Quantum chains with $GL_q(2)$ symmetry

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Usually quantum chains with quantum group symmetry are associated with representations of quantized universal algebras $U_q(g)$. Here we propose a method for constructing quantum chains with $C_q(G)$ global symmetry, where $C_q(G)$ is the algebra of functions on the quantum group. In particular we will construct a quantum chain with $GL_q(2)$ symmetry which interpolates between two classical Ising chains. It is shown that the Hamiltonian of this chain satisfies the generalized braid group algebra. © *1996 American Institute of Physics.* [S0022-2488(95)02912-8]

I. INTRODUCTION

Almost all integrable models in two-dimensional statistical models, quantum field theories in $1+1$ dimensions, and quantum chains[1] owe their integrability to some quantum group symmetry. For example, in lattice models, if one assigns the local Boltzman weights of a vertex or an IRF model to be the elements of the R matrix corresponding to a quantum group, then the model will be integrable due to the existence of a one-parameter family of commuting transfer matrices. In a sense one can say that local quantum group symmetry ensures integrability. Although global quantum group symmetry does not mean integrability, construction of models with such symmetries may be interesting and important as a first step toward understanding the mechanism of integrability.

Recently new types of two- and three-state quantum chains were constructed and shown to possess $U_q(\mathrm{sl}(2))$ symmetry.[2–4] The strategy followed in Ref. 4 was to define the Hamiltonian as

$$H=\sum_{j=1}^{L} id\otimes\cdots id\otimes H_j\otimes id\ldots.\otimes id, \tag{1}$$

where H_j acts on sites j and $j+1$ as

$$H_j=(\pi_j\otimes\pi_{j+1})[Q_j(\Delta(C))]. \tag{2}$$

Here j denotes the site of the lattice, C is the quadratic Casimir of $U_q(\mathrm{sl}(2))$, Δ is the coproduct, π_j is a typical type b representation[5] of $U_q(\mathrm{sl}(2))$ assigned to site j, and finally Q_j is a polynomial function of degree $d\leqslant m$ where the integer m is characterized by the value of $q(q^m=1)$. This Hamiltonian is by construction $U_q(\mathrm{sl}(2))$ invariant. The invariance is due to the centrality of the Casimir. For the particular form of the Hamiltonian of the two-state and three-state quantum chains see Ref. 4.

As is well known any quantum group is characterized by two algebras,[6,7] the first being the deformation of the universal enveloping algebra which is denoted by $U_q(g)$ and the second one which is the deformation of the algebra of functions on the group which is denoted by $C_q(G)$. So far everything which has been done concerning the construction of physical models with quantum group symmetry have been based on representation theory of $U_q(g)$. However, in the quantum case the second algebra, $C_q(G)$, has also a representation theory which is completely different from that of $U_q(g)$.[8,9]

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The novelty of the representations of $C_q(G)$ is best understood when one considers the classical $(q\to 1)$ limit of $C_q(G)$. In this limit, representations of $U_q(g)$ approach those of the classical Lie algebra g while those of $C_q(G)$ collapse to trivial one-dimensional representations, since $C_q(G)$ will become a commutative algebra. Therefore there is no parallelism between the representation theories in the deformed and the undeformed case. Naively one expects that paying attention to physical models which are $C_q(G)$ invariant may open up a new road in the study of integrable models. At the present stage this is only a hope and real justification for it will exist if one can somehow gauge a global symmetry of this kind in a particular physical model.

In this letter we construct a quantum chain which has a global $C_q(\mathrm{GL}(2))$ symmetry, hereafter called $\mathrm{GL}_q(2)$ symmetry for simplicity.

II. THE QUANTUM GROUP $GL_q(2)$ AND IT'S CYCLIC REPRESENTATIONS

The quantum group $\mathrm{GL}_q(2)$ is defined by the generators 1, a, b, c, and d, collected in the form of a quantum matrix[7]

$$T=\begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

and relations

$$\begin{gathered} ab=qba, \quad ac=qca, \quad bd=qdb, \\ cd=qdc, \quad bc=cb, \quad ad-da=(q-q^{-1})bc. \end{gathered} \tag{3}$$

The coproduct which is used in tensor multiplication of representations is defined by

$$\Delta\begin{pmatrix} a & b \\ c & d \end{pmatrix}=\begin{pmatrix} a & b \\ c & d \end{pmatrix}\otimes\begin{pmatrix} a & b \\ c & d \end{pmatrix}. \tag{4}$$

The quantum determinant $D_q=ad-qbc$ is central and grouplike; that is,

$$\Delta D_q=D_q\otimes D_q. \tag{5}$$

If q is a root of unity ($q^p=1$), in addition to the determinant, all the elements a^p, b^p, c^p, and d^p are central. In this case the algebra has a p-dimensional cyclic representation which is constructed as follows:[8] One first defines a state $|0\rangle$ which is a common eigenvector of b and c with eigenvalues μ and ν, respectively:

$$b|0\rangle=\mu|0\rangle, \quad c|0\rangle=\nu|0\rangle,$$

and then builds up the representation space V as the linear span of vectors $\{|n\rangle\equiv d^n|0\rangle,\ 0\leqslant n\leqslant p-1\}$. It is then easy to show that V is invariant under the action of $\mathrm{GL}_q(2)$:

$$\begin{gathered} d|n\rangle=|n+1\rangle, \quad d|p-1\rangle=\eta|0\rangle, \quad b|n\rangle=\mu q^n|n\rangle, \quad c|n\rangle=\nu q^n|n\rangle, \\ a|n\rangle=(\xi+q^{2n-1}\mu\nu)|n-1\rangle, \quad a|0\rangle=\frac{1}{\eta}(\xi+\mu\nu q^{-1})|p-1\rangle. \end{gathered} \tag{6}$$

Here η is the central value of d^p and ξ is the value of the q-determinant D_q.

It can be easily checked that the parameters η, ξ, μ, and ν are all independent and hence each representation is characterized by the values of these parameters and is denoted by $\pi(\eta,\xi,\mu,\nu)$.

III. QUANTUM CHAINS WITH $GL_q(2)$ SYMMETRY

We construct the quantum chains with $GL_q(2)$ symmetry as follows: To each site $1 \leqslant j \leqslant L$, we assign a representation $\pi_j = \pi(\eta_j, \xi_j, \mu_j, \nu_j)$, the Hilbert space is the tensor product $\otimes_{j=1}^{L} V_j$, where V_j is the p-dimensional representation space of π_j.

At first glance it seems that the analogue of the construction of Ref. 4 in the case of $C_q(\mathrm{GL}(2))$ is to replace the Casimir C in Eq. (2) by the quantum determinant D_q. However, this procedure leads to a trivial Hamiltonian due to the grouplike property of D_q [Eq. (5)], which makes $\pi_j \otimes \pi_{j+1}(Q_j(\Delta(D)))$ proportional to the identity. However, there is one interesting possibility and it is to define H_j as

$$H_j = \pi_j \otimes \pi_{j+1}(Q_j(\Delta(a^p), \Delta(b^p), \Delta(c^p), \Delta(d^p))). \tag{7}$$

Here the crucial point is that although in an irreducible representation a^p, b^p, c^p, and d^p are proportional to the identity, in a tensor product of representations they are not so due to the mixing of the generators in their coproducts [Eq. (4)]. The Hamiltonian constructed in this way is $GL_q(2)$ invariant by construction.

A. Two-state quantum chains

Now we restrict ourselves to the case $p=2$ $(q=-1)$. From Eq. (6) we obtain the two-dimensional cyclic representation of $GL_q(2)$, which in the explicit matrix notation takes the form

$$\begin{aligned} \pi(a) &= \begin{pmatrix} 0 & \gamma/\eta \\ \gamma & 0 \end{pmatrix}, \quad \pi(b) = \begin{pmatrix} \mu & 0 \\ 0 & -\mu \end{pmatrix}, \\ \pi(c) &= \begin{pmatrix} \nu & 0 \\ 0 & -\nu \end{pmatrix}, \quad \pi(d) = \begin{pmatrix} 0 & 1 \\ \eta & 0 \end{pmatrix}, \end{aligned} \tag{8}$$

where $\gamma = \xi - \mu\nu$. This represents a continuous four-parameter family of two-dimensional representations for $GL_q(2)$ (for $q=-1$). If t stands for a, b, c, or d, then a straightforward calculation shows that

$$(\pi_j \otimes \pi_{j+1})\Delta t^2 = l_t 1 \otimes 1 + n_t \sigma_x \otimes \sigma_x + p_t \sigma_y \otimes \sigma_y - i q_t \sigma_x \otimes \sigma_y - i r_t \sigma_y \otimes \sigma_x, \tag{9}$$

where

$$\begin{aligned} n_t &= \tfrac{1}{4}(1 - \eta_j - \eta_{j+1} + \eta_j \eta_{j+1}) m_t, \quad p_t = -\tfrac{1}{4}(1 + \eta_j + \eta_{j+1} + \eta_j \eta_{j+1}) m_t, \\ q_t &= \tfrac{1}{4}(-1 + \eta_j - \eta_{j+1} + \eta_j \eta_{j+1}) m_t, \quad r_t = \tfrac{1}{4}(-1 - \eta_j + \eta_{j+1} + \eta_j \eta_{j+1}) m_t, \end{aligned} \tag{10}$$

and

$$\begin{aligned} m_a &= \frac{2\gamma_j \gamma_{j+1} \mu_j \nu_{j+1}}{\eta_j \eta_{j+1}}, \quad m_b = -2\,\frac{\mu_j \mu_{j+1} \gamma_j}{\eta_j}, \\ m_c &= -2\,\frac{\nu_j \nu_{j+1} \gamma_{j+1}}{\eta_{j+1}}, \quad m_d = 2\mu_{j+1}\nu_j. \end{aligned} \tag{11}$$

The explicit expressions of l_ts are not necessary in this stage. As the simplest choice for the polynomial [in Eq. (7)] we set

$$Q_0 = \alpha_a a^2 + \alpha_b b^2 + \alpha_c c^2 + \alpha_d d^2, \tag{12}$$

where α_ts are arbitrary constants. Combination of Eqs. (9) and (12) leads to the following Hamiltonian:

$$H_j = A\sigma_x^j\sigma_x^{j+1} + B\sigma_y^j\sigma_y^{j+1} + -iC\sigma_x^j\sigma_y^{j+1} - iD\sigma_y^j\sigma_x^{j+1}, \tag{13}$$

where

$$\begin{aligned} A &= \beta_j(1-\eta_j-\eta_{j+1}+\eta_j\eta_{j+1}), \\ B &= -\beta_j(1+\eta_j+\eta_{j+1}+\eta_j\eta_{j+1}), \\ C &= \beta_j(-1+\eta_j-\eta_{j+1}+\eta_j\eta_{j+1}), \\ D &= \beta_j(-1-\eta_j+\eta_{j+1}+\eta_j\eta_{j+1}), \end{aligned} \tag{14}$$

and $\beta_j = \alpha_a m_a + \alpha_b m_b + \alpha_c m_c + \alpha_d m_d$. If the factor β_j is site independent, then modulo a constant overall factor the Hamiltonian becomes

$$\begin{aligned} H_0 = \sum_j \{&(1-\eta_j-\eta_{j+1}+\eta_j\eta_{j+1})\sigma_x^j\sigma_x^{j+1} - (1+\eta_j+\eta_{j+1}+\eta_j\eta_{j+1})\sigma_y^j\sigma_y^{j+1} - i(-1+\eta_j \\ &-\eta_{j+1}+\eta_j r_{j+1})\sigma_x^j\sigma_y^{j+1} - i(-1-\eta_j+\eta_{j+1}+\eta_j\eta_{j+1})\sigma_y^j\sigma_x^{j+1}\}. \end{aligned} \tag{15}$$

Now the condition of Hermiticity of the Hamiltonian restricts the parameters η_j and η_{j+1} to the following form:

$$\begin{aligned} \eta_j &= \alpha + i\sqrt{1-\alpha^2}, \\ \eta_{j+1} &= \eta_j^*, \end{aligned} \tag{16}$$

where α is a real parameter. Under this condition the Hamiltonian takes the following simple form:

$$H_0 = \sum_j \{(1-\alpha)\sigma_x^j\sigma_x^{j+1} - (1+\alpha)\sigma_y^j\sigma_y^{j+1} + \sqrt{1-\alpha^2}(\sigma_x^j\sigma_y^{j+1} - \sigma_y^j\sigma_x^{j+1})\}. \tag{17}$$

This is the desired Hamiltonian with $GL_q(2)$ symmetry.

Imposing the condition of site independence on β_j in Eq. (14), the m_ts are restricted to be site independent, as α_ts are arbitrary constants. Solving these conditions and using Eq. (16) results in the following relation between the parameters of the different representations of the sites:

$$\begin{aligned} &\gamma_j = \gamma_{j+2}, \quad \nu_j = \nu_{j+2}, \quad \mu_j = \mu_{j+2}, \\ &\frac{\gamma_j}{\eta_j} = \frac{\gamma_{j+1}}{\eta_{j+1}}, \quad \frac{\mu_j}{\nu_j} = \frac{\mu_{j+1}}{\nu_{j+1}}. \end{aligned} \tag{18}$$

So the whole representations of the sites specify only by four complex parameters ν_1, μ_1, ν_2, γ_1, and one real parameter α.

There are several observations on the above Hamiltonian [Eq. (17)]:

(1) Instead of the original continuous parameter q, the Hamiltonian depends on the continuous parameter α, which comes from the representation.
(2) In the two limits $\alpha=1$ and $\alpha=-1$, this Hamiltonian degenerates into an exactly solvable chain, that is $\Sigma_{j=1}^{L}\sigma_{\hat{n}}^j\sigma_{\hat{n}}^{j+1}$. So our $GL_q(2)$ invariant Hamiltonian interpolates between two **xx** and **yy** classical Ising chains, when α is changed continuously from -1 to 1.

(3) It is crucial to note that the Hamiltonian (17) is not equivalent to an $\hat{n}\hat{n}$ chain where $\hat{n}$ is a new unit vector in the $x-y$ plane. That is, the transformations $\sigma_x \to a\sigma_x + b\sigma_y$ and $\sigma_y \to c\sigma_x + d\sigma_y$ cannot diagonalize the Hamiltonian.

(4) If one defines $U_i = 2 + H_i$, then there exists the following interesting relations between U_i's:

$$U_i^2 = 4U_i,$$
$$(U_iU_{i\pm1}U_i - U_{i\pm1}U_iU_{i\pm1})(U_i - U_{i\pm1}) = 64(1-\alpha^2). \tag{19}$$

The above equation is the generalized braid group algebra.[2]

(5) The simplest situation in which H_0 can be solved exactly is the case of a two-site lattice. In this case there are four states with eigenvalues 2, 2, -2, and -2. It can be shown that the degenerate orthonormal states ($|2\rangle_\pm$ and $|-2\rangle_\pm$) are two-dimensional representations of $\Delta(t)$s.

B. Higher-state quantum chains

Choosing $p=3$, one may expect to obtain a three-state $GL_q(2)$ invariant quantum chain. However, for $q^3=1$ it is seen by computation that

$$\Delta a^3 = a^3\otimes a^3 + b^3\otimes c^3, \quad \Delta b^3 = a^3\otimes b^3 + b^3\otimes d^3,$$
$$\Delta c^3 = c^3\otimes b^3 + d^3\otimes d^3, \quad \Delta d^3 = c^3\otimes a^3 + d^3\otimes c^3,$$

which means that the Hamiltonian (7) is proportional to the identity. This phenomena may occur for all odd integers p.

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Quasi-exactly solvable systems and orthogonal polynomials

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This paper shows that there is a correspondence between quasi-exactly solvable models in quantum mechanics and sets of orthogonal polynomials $\{P_n\}$. The quantum-mechanical wave function is the generating function for the $P_n(E)$, which are polynomials in the energy E. The condition of quasi-exact solvability is reflected in the vanishing of the norm of all polynomials whose index n exceeds a critical value J. The zeros of the critical polynomial $P_J(E)$ are the quasi-exact energy eigenvalues of the system. © *1996 American Institute of Physics.* [S0022-2488(96)03201-X]

In quantum mechanics there exist potentials for which it is possible to find a finite portion of the energy spectrum and associated eigenfunctions exactly and in closed form. These systems are said to be quasi-exactly solvable.[1–5] In such systems the potential depends on a parameter J; for positive integer values of J one can find J eigenvalues and eigenfunctions exactly. The usual approach to the analysis of quasi-exactly solvable systems is an algebraic one in which the Hamiltonian is expressed as a nonlinear combination of generators of a Lie algebra, not belonging to the center of the corresponding enveloping algebra.[4] This technique is a modification of the dynamical symmetry approach to exactly solvable quantum-mechanical systems, in which one can find by algebraic means the *entire* spectrum in closed form.[6]

In this paper we propose an alternative approach to quasi-exact solvability. We show that the solution ψ to the Schrödinger equation for a quasi-exactly solvable model,

$$H\psi = E\psi, \tag{1}$$

is the generating function for a set of polynomials $\{P_n(E)\}$ in the energy variable E. These polynomials satisfy a three-term recursion relation and therefore form an orthogonal set with respect to some weight function $w(E)$. For positive integer values of the parameter J, corresponding to quasi-exact solvability, we find that the norm of $P_n(E)$ *vanishes* for $n \geqslant J$. Moreover, all polynomials $P_n(E)$ beyond a critical polynomial $P_J(E)$, factor into a product of two polynomials, one of which is $P_J(E)$:

$$P_{n+J}(E) = P_J(E)Q_n(E) \quad (n \geqslant 0). \tag{2}$$

The zeros of the critical polynomial $P_J(E)$ are precisely the quasi-exact energy eigenvalues of the quantum-mechanical model.

We illustrate these features of quasi-exactly solvable models with the following infinite class of Hamiltonians first discussed by A. Turbiner:[1]

$$H = -\frac{d^2}{dx^2} + \frac{(4s-1)(4s-3)}{4x^2} - (4s+4J-2)x^2 + x^6. \tag{3}$$

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Here, s is an arbitrary parameter. When s lies between $\frac{1}{4}$ and $\frac{3}{4}$, there is an attractive centrifugal term; for s outside this range the centrifugal term is repulsive. When $s=\frac{1}{4}$ or $s=\frac{3}{4}$, the centrifugal core term disappears leaving a nonsingular sextic oscillator Hamiltonian

$$H=-\frac{d^2}{dx^2}-(4s+4J-2)x^2+x^6. \tag{4}$$

When the parameter J in Eq. (3) is a nonnegative integer, the corresponding Schrödinger equation has J exact, closed-form solutions for any value of s.

We seek a solution $\psi(x)$ to the Schrödinger equation for H in Eq. (3) of the form

$$\psi(x)=\exp\left(-\frac{1}{4}x^4\right)x^{2s-1/2}\sum_{n=0}^{\infty}\left(-\frac{1}{4}\right)^n\frac{P_n(E)}{n!\Gamma(n+2s)}x^{2n}. \tag{5}$$

Observe that when $s=\frac{1}{4}$ this solution becomes an even-parity wave function of the oscillator Hamiltonian (4); when $s=\frac{3}{4}$, $\psi(x)$ becomes an odd-parity wave function of H in (4).

Demanding that $\psi(x)$ in Eq. (5) obey the Schrödinger equation (1) leads to the following recursion relation for the expansion coefficients $P_n(E)$:

$$P_n(E)=EP_{n-1}(E)+16(n-1)(n-J-1)(n+2s-2)P_{n-2}(E)\quad(n\geqslant 2), \tag{6}$$

subject to the initial conditions

$$P_0(E)=1\quad\text{and}\quad P_1(E)=E. \tag{7}$$

From these initial conditions the recursion relation (6) generates a set of monic[7] polynomials, the next four of which are

$$\begin{aligned}
P_2(E)&=E^2+(32-32J)s,\\
P_3(E)&=E^3+[(160-96J)s-32J+64]E,\\
P_4(E)&=E^4+[(448-192J)s-128J+352]E^2+(3072J^2-12288J+9216)s(s+1),\\
P_5(E)&=E^5+[(960-320J)s-320J+1120]E^3+[(15360J^2-81920J+91136)s^2\\
&\quad+(25600J^2-141312J+164864)s+6144J^2-36864J+49152]E.
\end{aligned} \tag{8}$$

These polynomials have a number of noteworthy properties. First, for all values of the parameters s and J they form an orthogonal set. This follows from the fact that they are generated by a second-order (three-term) recursion relation.[8] The appearance of a three-term recursion relation is a consequence of the form of the potential in Eq. (3). For example, the corresponding recursion relation for an x^4 anharmonic oscillator potential, whose Hamiltonian is not quasi-exactly solvable, is a higher-order recurrence relation. The harmonic oscillator system leads to a two-term recursion relation; this system is exactly solvable rather than quasi-exactly solvable.

Second, from the expansion (5) we can see that the wave function $\psi(x,E)$ is the generating function for the polynomials $P_n(E)$.

The third and most significant property of the polynomials $P_n(E)$ is that, when the parameter J takes positive integer values, the polynomials exhibit the factorization property in Eq. (2). This factorization occurs because the third term in the recursion relation (6) vanishes when $n=J+1$, so that all subsequent polynomials have the common factor $P_J(E)$. This factorization property holds for all values of the parameter s. Furthermore, this factorization leads to the result that the zeros

of the critical polynomial $P_J(E)$ are just the quasi-exact energy eigenvalues. This is true because the expansion in (5) truncates when E is a zero of $P_J(E)$; when this series truncates the wave function $\psi(x)$ is automatically normalizable.

To illustrate this factorization we list in factored form the first six polynomials $P_n(E)$ for the case $J=3$:

$$P_0(E)=1, \quad P_1(E)=E, \quad P_2(E)=E^2-64s,$$

$$P_3(E)=E^3-(128s+32)E, \quad P_4(E)=[E^3-(128s+32)E]E, \tag{9}$$

$$P_5(E)=[E^3-(128s+32)E](E^2+128s+192).$$

Observe that $P_3(E)$ is a common factor of $P_n(E)$ for $n\geqslant 3$. The zeros of $P_3(E)$ are

$$E=0, \quad E=\pm\sqrt{128s+32}, \tag{10}$$

which are the three exact energy eigenvalues for the quasi-exactly solvable Hamiltonian (3) when $J=3$. The corresponding exact eigenfunctions are obtained by evaluating $\psi(x)$ in Eq. (5) at these values of E:

$$\psi_0(x)= \exp\left(-\frac{1}{4}x^4\right)\frac{x^{2s-1/2}}{\Gamma(2s)}\left(1-\frac{x^4}{2s+1}\right),$$

$$\psi_+(x)= \exp\left(-\frac{1}{4}x^4\right)\frac{x^{2s-1/2}}{\Gamma(2s)}\left(1-\frac{\sqrt{128s+32}}{8s}x^2+\frac{x^4}{2s}\right), \tag{11}$$

$$\psi_-(x)= \exp\left(-\frac{1}{4}x^4\right)\frac{x^{2s-1/2}}{\Gamma(2s)}\left(1+\frac{\sqrt{128s+32}}{8s}x^2+\frac{x^4}{2s}\right).$$

Note that the energy levels may be ordered by the number of nodes of the corresponding wave function.

A fourth property of the polynomials $P_n(E)$ concerns their norms. The norm (squared) γ_n of $P_n(E)$ is defined as an integral:

$$\gamma_n=\int dE\, w(E)[P_n(E)]^2. \tag{12}$$

It is possible to determine the norms of an orthogonal set of polynomials directly from the recursion relation; it is not necessary to know explicitly the weight function $w(E)$ with respect to which the polynomials are orthogonal.[9] The procedure is simply to multiply the recursion relation (6) by $w(E)E^{n-2}$ and to integrate with respect to E. Using the fact that $P_n(E)$ is orthogonal to E^k, $k<n$, we obtain a simple, two-term recursion relation for γ_n:

$$\gamma_n=16n(J-n)(2s+n-1)\,\gamma_{n-1}. \tag{13}$$

The solution to this equation with $\gamma_0=1$ is

$$\gamma_n=\frac{16^n n!\,\Gamma(J)\Gamma(2s+n)}{\Gamma(J-n)\Gamma(2s)}. \tag{14}$$

This equation reveals that the space of orthogonal polynomials arising from a quasi-exactly solvable model is associated with a nonpositive definite norm. In particular, we can see from Eq.

(14) that γ_n vanishes for $n \geq J$ if J is a positive integer. The appearance of a vanishing norm coincides with the factorization mentioned above and is an alternative characterization of quasi-exact solvability.

It is interesting that while the polynomials $P_{n+J}(E)$ for $n \geq 0$ have vanishing norm when J is a positive integer, the quotient polynomials $Q_n(E)$ in Eq. (2) form a new orthogonal set of polynomials for each value of J.

Having determined the norms γ_n of the polynomials $P_n(E)$ it is natural to evaluate the integral of the square of the generating function (wave function) with respect to the weight function $w(E)$:

$$G(x) = \int dE w(E)[\psi(x,E)]^2, \tag{15}$$

where $\psi(x,E)$ is given in Eq. (5). Using the orthogonality of the polynomials $P_n(E)$, we can express $G(x)$ as a confluent hypergeometric function:

$$G(x) = \frac{\Gamma(J)}{\Gamma(2s)} \exp\left(-\frac{1}{2}x^4\right) \sum_{n=0}^{\infty} \frac{x^{4n+4s-1}}{n!\Gamma(n+2s)\Gamma(J-n)}. \tag{16}$$

When J is a positive integer, this sum truncates and we find that $G(x)$ can be expressed as a linear combination of the squares of the J quasi-exact eigenfunctions of the Hamiltonian H in Eq. (3). For example, when $J=3$, we have

$$\begin{aligned} G(x) &= \frac{1}{\Gamma(2s)} \exp\left(-\frac{1}{2}x^4\right) x^{4s-1}\left[1 + \frac{x^4}{s} + \frac{x^8}{2s(2s+1)}\right] \\ &= \Gamma(2s)\left(\frac{2s+1}{4s+1}[\psi_0(x)]^2 + \frac{s}{4s+1}[\psi_+(x)]^2 + \frac{s}{4s+1}[\psi_-(x)]^2\right), \end{aligned} \tag{17}$$

where $\psi_0(x)$ and $\psi_\pm(x)$ are taken from Eq. (11). We emphasize that this result is highly non-trivial. Expressing $G(x)$ as a linear combination of the squares of the eigenfunctions requires that one solve an overdetermined system of $2J-1$ equations for J expansion coefficients.

Let us now investigate the properties of the weight function $w(E)$. From the polynomials $P_n(E)$ we can calculate the moments of $w(E)$. Let a_n represent the $2n$th moment of $w(E)$:

$$a_n = \int dE w(E) E^{2n}. \tag{18}$$

(Because the polynomials have parity symmetry we know that the odd moments vanish.) We are free to normalize $w(E)$ so that its zeroth moment is unity:

$$a_0 = 1. \tag{19}$$

The remaining moments can then be determined algebraically:

$$\begin{aligned} a_1 &= 32(J-1)s, \\ a_2 &= 32^2(J-1)s(3Js-5s+J-2), \\ a_3 &= 32^3(J-1)s(15J^2s^2-60Js^2+61s^2+15J^2s-67Js+74s+4J^2-19J+22), \\ a_4 &= 32^4(J-1)s(105J^3s^3-735J^2s^3+1743Js^3-1385s^3+210J^3s^2-1596J^2s^2+4038Js^2 \end{aligned} \tag{20}$$

$$-3372s^2+147J^3s-1179J^2s+3114Js-2688s+34J^3-282J^2+765J-674),$$

$$\begin{aligned}a_5=32^5(J-1)s(&945J^4s^4-10080J^3s^4+40950J^2s^4-74400Js^4+50521s^4+3150J^4s^3\\&-35910J^3s^3+153990J^2s^3-292154Js^3+205228s^3+4095J^4s^2-48960J^3s^2+218337J^2s^2\\&-427524Js^2+307860s^2+2370J^4s-29306J^3s+134373J^2s-269085Js+197206s+496J^4\\&-6272J^3+29292J^2-59531J+44134).\end{aligned}$$

These moments have some interesting mathematical properties. For example, all the moments a_n, $n\geqslant 1$, have a factor of $(J-1)s$. Furthermore, in the residual factor the coefficient of $(Js)^{n-1}$ is $(2n-1)!!$ and the coefficient of s^{n-1} is the nth Euler number E_n.[10]

The outstanding property of the moments a_n concerns their rapid rate of growth. This rate of growth can be determined using the fact that there is a simple relationship between the moments a_n and the coefficients b_{n-1} of $P_{n-2}(E)$ in the recursion relation (6). Specifically, the Taylor series

$$f(z)=\sum_{n=0}^{\infty} a_n z^n, \tag{21}$$

whose coefficients are the moments in Eq. (18), is equivalent to a continued fraction

$$f(z)=1/(1-b_1z/(1-b_2z/(1-b_3z/(1-\ldots)))), \tag{22}$$

whose coefficients are b_n.[11] Since b_n is a cubic polynomial in n we deduce that the moments a_n grow like $(3n)!$.[11]

It is unusual to find orthogonal polynomials whose weight functions have moments that grow so rapidly. The classical orthogonal polynomials, such as the Hermite polynomials, typically have moments that grow like $n!$. This is also true of discrete versions of the classical orthogonal polynomials, such as the Hahn polynomials.[12] The Euler and Bernoulli polynomials are distinctive[13] in that their moments grow like $(2n)!$. However, the polynomials $P_n(E)$ associated with quasi-exact solvability are of an entirely new type due to the rapid rate of growth of their moments. Carleman's condition states that when the moments grow faster than $(2n)!$, the moment problem is not guaranteed to have a unique solution.[15] Almost certainly, the weight function $w(E)$ is not unique! This nonuniqueness corresponds to a kind of gauge invariance that underlies these quasi-exactly solvable systems. Indeed one may conjecture that the nonuniqueness of the weight function is related to the Lie algebraic symmetry of quasi-exact solvability.

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A rigorous treatment of conformal blocks in a model of bosonic conformal field theory

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A free massless field coupled to a background charge Q is considered. The conformal blocks of the theory are adequately described by the N-point vertex $V_{N;0}$ which is, up to a multiplicative constant, completely determined by the Knizhnik–Zamolodchikov equations and a set of Ward identities on the sphere. The N-point g-loop vertex $V_{N;g}$ for compact Riemann surfaces Σ_g of genus $g\neq 0$ is constructed by a sewing procedure. The main new result is a rigorous proof of the fact that $V_{N;0}$ is trace class for nonoverlapping disks. This allows one to show that the set of all N-point vertices (for all N) is a modular functor. © *1996 American Institute of Physics.* [S0022-2488(96)01301-3]

I. INTRODUCTION

In two-dimensional conformal invariant quantum field theory, the minimal models of Belavin, Polyakov, and Zamolodchikov[1] belong to the simplest ones. They are built upon a finite set of irreducible highest weight modules $L(h,c)$ of the Virasoro algebra with central charge $c=1-6(p'-p)^2/pp'$ parametrized by two positive and relatively prime integers p and p'. It has been realized in Ref. 2 that these models can be constructed using a free field in a background charge. More precisely, the spaces $L(h,c)$ are isomorphic to the BRST-cohomologies of certain complexes of free field Hilbert spaces. This connection allowed the computation of conformal blocks of minimal models on Riemann surfaces.[3,4]

In this paper, we study free field theories for their own sake. We present a rigorous construction of the N-point vertex $V_{N;g}$ on compact Riemann surfaces of arbitrary genus g. Out of it, it is easy to construct the conformal blocks (i.e., the holomorphic correlation functions) which contain all the information of the theory. One simply has to saturate the vertex with the states

$$\prod t_i'(0)^{-\beta_i(\beta_i-Q)/2}|0\rangle_{\beta_i}.$$

Our guideline throughout the paper is Segal's axiomatic framework[5] (Sec. VII). Starting with the N-point vertex on the sphere, we construct the N-point g-loop vertex by a sewing procedure. Our main new result is Theorem 13 which proves the validity of the whole construction. We also show that the result we get does not depend on our particular way of sewing. If this were the case, we would have a contradiction with Segal's fourth axiom. Finally, we establish the validity of the other axioms in Sec. X. An important remark is that the axiom (iii) is not true in the presence of a background charge, which implies a lack of physical positivity. In order for our construction to be really complete, we would still have to check that we can obtain all Riemann surfaces (up to equivalence) by only sewing disks together on the sphere. Whether this is true or not is not known to the author, but is an interesting open question.

Although this paper is organized in a self-consistent way, the interested reader can find more background and computational details in Ref. 6.

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II. FREE BOSONIC THEORY

For the sake of clarity and to fix the notation, we briefly review some properties of a free massless field. The coupling to a background charge Q will only play a role when we later introduce correlators.

We define the Heisenberg algebra $(a_n)_{n\in\mathbb{Z}}$ through the commutation relations

$$[a_n, a_m] = n\,\delta_{n+m,0}. \tag{1}$$

It is useful to know that for fixed $n>0$, the operators $a_n/\sqrt{n}$ and $a_{-n}/\sqrt{n}$ satisfy the canonical commutation relations

$$\left[\frac{a_n}{\sqrt{n}}, \frac{a_{-n}}{\sqrt{n}}\right] = 1.$$

a_0 is called the zero mode of the algebra. The algebra (1) has infinite dimensional representations π_μ characterized by a real number μ, a highest weight vector $|0\rangle_\mu$, and the relations

$$a_0|0\rangle_\mu = \mu|0\rangle_\mu, \quad a_n|0\rangle_\mu = 0, \quad n>0.$$

We further define e_n as the multiindex with 1 at position n and 0 otherwise. A basis of π_μ is given by

$$|\phi_\beta\rangle_\mu = \frac{a_{-1}^{\beta_1}\cdots a_{-k}^{\beta_k}}{\sqrt{\beta!}\sqrt{I^\beta}}\,|0\rangle_\mu,$$

where $\beta=(\beta_1,...,\beta_k)$ is a finite multiindex, $\beta!=\Pi\beta_i!$, $I^\beta = \Pi i^{\beta_i}$. Moreover we set $\|\beta\|=\Sigma i\beta_i$. We now have the relations

$$a_n|\phi_\beta\rangle_\mu = \sqrt{n\beta_n}\,|\phi_{\beta-e_n}\rangle_\mu, \quad n>0,$$

$$a_{-n}|\phi_\beta\rangle_\mu = \sqrt{n(\beta_n+1)}\,|\phi_{\beta+e_n}\rangle_\mu, \quad n>0,$$

where we set $|\phi_\beta\rangle_\mu=0$ if β has one or more negative components. The space π_μ of all finite linear combinations of basis vectors possesses a scalar product which is uniquely determined by the requirements $a_n^* = a_{-n}$ for all $n\in\mathbb{Z}$ and that $|0\rangle_\mu$ has norm one. We denote the completion of π_μ with respect to this scalar product by $\overline{\pi_\mu}$. The vectors $|\phi_\beta\rangle_\mu$ form an orthonormal basis of $\overline{\pi_\mu}$. We next introduce the operator

$$L_0 = \frac{1}{2}\,a_0(a_0-Q) + \sum_{n=1}^{\infty} a_{-n}a_n,$$

where the real number Q is called the background charge of the theory. L_0 is a well defined symmetric operator on π_μ and is bounded below.

Definition 1: For $R>0$ we define H_R^μ as the completion of π_μ with respect to the scalar product

$$(\varphi,\psi)_R = (R^{-L_0}\varphi, R^{-L_0}\psi).$$

It is easy to see that

$$\pi_\mu \subseteq H_R^\mu \subseteq H_{R'}^\mu, \subseteq H_1^\mu = \overline{\pi_\mu} \subseteq H_{R''}$$

for $0<R\leqslant R'\leqslant 1\leqslant R''$. An orthonormal basis of H_R^μ is given by the vectors $R^{L_0}|\phi_\alpha\rangle_\mu$. The fundamental fields of the theory are

$$J(z)=\sum_{n\in\mathbb{Z}} a_{-n}z^{n-1}=a_0 z^{-1}+\sum_{n\neq 0}\sqrt{|n|}\,\frac{a_{-n}}{\sqrt{|n|}}\,z^{n-1}$$

and

$$V_\beta(z)=T_\beta z^{\beta a_0}\exp\left(\beta\sum_{n=1}^{\infty}\frac{a_{-n}}{n}\,z^n\right)\exp\left(-\beta\sum_{n=1}^{\infty}\frac{a_n}{n}\,z^{-n}\right),\quad \beta\in\mathbb{R},$$

where $T_\beta:\pi_\mu\to\pi_{\mu+\beta}$ is the linear map sending $|\phi_\alpha\rangle_\mu$ to $|\phi_\alpha\rangle_{\mu+\beta}$ for all finite multi-indices α.

Definition 2: We define $TC_\mu^{\mu+\beta}$ as the space of all operators A with the following properties:

(a) $A(z):H_R^\mu\to H_{R'}^{\mu+\beta}$ *is an analytic (possibly many-valued) trace class operator for* $0<R<|z|<R'$.

(b) *The operator $J(z_1)A(z_2):H_R^\mu\to H_{R'}^{\mu+\beta}$ has a (possibly many-valued) trace class analytic continuation to the whole domain $R<|z_1|,|z_2|<R'$ with a possible pole at $z_1=z_2$.*

(c) *The analytic continuation is radial ordering for $|z_1|\neq|z_2|$.*

It is not too hard to show that $J\in TC_\mu^\mu$. Using generalized Laguerre polynomials,[6] it is possible to show the following result:

Proposition 3: $V_\beta\in TC_\mu^{\mu+\beta}$

To give the reader an idea of the techniques involved, we sketch the proof of property (a). The square of the Hilbert–Schmidt norm of $V_\beta(z):H_R^\mu\to H_{R'}^{\mu+\beta}$ is given by

$$\sum_{\|\alpha\|<\infty}\|R'^{-L_0}V_\beta(z)R^{L_0}|\phi_\alpha\rangle\|^2=c\sum_{\|\alpha\|<\infty}\left(\frac{R}{R'}\right)^{2\|\alpha\|}\exp\left(\sum_{k=1}^{\infty}\frac{|\beta|^2}{k}\left(\frac{|z|}{R'}\right)^{2k}\right)\times\prod_{k=1}^{\infty}L_{\alpha_k}\left(-\frac{|1-(|z|/R')^{2k}|^2}{(k/|\beta|^2)(|z|/R')^{2k}}\right),$$

where we have introduced the Laguerre polynomials

$$L_n(x)=\sum_{m=0}^{n}\binom{n}{m}\frac{(-x)^{n-m}}{(n-m)!}\tag{2}$$

The constant c comes from the purely zero mode contributions, and is therefore unimportant here. The expression we have in the sum is finite if and only if $|z|<R'$. Using the generating function

$$\sum_{n=0}^{\infty}t^n L_n(-x)=\frac{1}{1-t}\exp\left(\frac{tx}{1-t}\right),\quad |t|<1\tag{3}$$

we can compute the sum and find

$$\sum_{\|\alpha\|<\infty}\|R'^{-L_0}V_\beta(z)R^{L_0}|\phi_\alpha\rangle\|^2=c\,\exp\left(\sum_{k=1}^{\infty}\frac{|\beta|^2}{k}\left(\frac{|z|}{R'}\right)^{2k}\right)\prod_{k=1}^{\infty}\frac{1}{1-(R/R')^{2k}}\times\exp\left(\frac{(|\beta|^2/k)(R/|z|)^{2k}|1-(|z|/R')^{2k}|^2}{1-(R/R')^{2k}}\right).$$

It is not too hard to see that this sum is finite if and only if $R<|z|<R'$. Therefore, $V_\beta(z):H_R^\mu \to H_{R'}^{\mu+\beta}$ is a Hilbert–Schmidt operator for $R<|z|<R'$. A part of this result was found independently by Ref. 7 (albeit without the use of Laguerre polynomials). By a deformation argument similar to the one used in Theorem 16, we can prove that V_β is actually a trace class operator.

Considering radially ordered products of J's with V_β, we get new operators which have radial ordering as analytic continuation. We want to make this idea rigorous with the following:

Definition 4: We define the linear map $j:\pi_\beta \to TC_\mu^{\mu+\beta}$ recursively by the relations

$$j|0\rangle_\beta = V_\beta,$$

$$(j(a_n\psi))(z) = \frac{1}{2\pi i} \oint_z d\zeta (\zeta - z)^n J(\zeta)(j\psi)(z), \quad \forall \psi \in \pi_\beta, \quad \forall n \in \mathbb{Z},$$

where the arguments z and ζ are implicitly radially ordered.

As an operator $H_R \to H_{R'}$, $(j(a_n\psi))(z)$ can be practically computed as

$$(j(a_n\psi))(z) = \frac{1}{2\pi i} \oint_{|\zeta|=r'} d\zeta (\zeta - z)^n J(\zeta)(j\psi)(z) - \frac{1}{2\pi i} \oint_{|\zeta|=r} d\zeta (\zeta - z)^n (j\psi)(z) J(\zeta),$$

where $R<r<|z|<r'<R'$. All the operators $j\phi$ with $\phi \neq |0\rangle_\beta$ are called descendant fields.

Proposition 5:

(*a*) *j is well defined;*

(*b*) $(ja_{-n_1}\cdots a_{-n_k}|0\rangle_\beta)(z) = \dfrac{:\partial^{n_1-1}J\cdots\partial^{n_k-1}JV_\beta:(z)}{(n_1-1)!\cdots(n_k-1)!}$.

The dots ":" in (b) denote Wick ordering (it brings T_β and all the a_n with negative n to the left). What (a) says is that j respects the commutation relations $[a_n,a_m]=n\delta_{n+m;0}$ of the Heisenberg algebra, and that $j\psi$ is really in $TC_\mu^{\mu+\beta}$ for all $\psi \in \pi_\beta$, which can be easily proved by induction. An immediate consequence is that our operator algebra contains all fields of the form

$$:P(J,\partial J,\partial^2 J,\ldots)V_\beta:,$$

where P is an arbitrary polynomial. That it contains no other operators is the content of Theorem 6.

Theorem 6: *For all $\varphi \in \pi_{\beta_1}$, $\psi \in \pi_{\beta_2}$ the product $(j\varphi)(z_1)(j\psi)(z_2)$ is analytic (but possibly many-valued) in z_1, z_2 if $R'>|z_1|>|z_2|>R$ and has a (possibly many-valued) analytic trace class continuation to $R'>|z_1|,|z_2|>R$, $z_1 \neq z_2$. This analytic continuation can be expanded in the form*

$$(j\varphi)(z_1)(j\psi)(z_2) = (z_1-z_2)^{\beta_1\beta_2} \sum_{n \geqslant -N} (z_1-z_2)^n \psi_n(z_2),$$

where N is finite and $\psi_n \in TC_\mu^{\mu+\beta_1+\beta_2}$ are (finite sums of) descendant fields. The sum converges in the trace norm and therefore also in the operator norm if

$$|z_1-z_2| < \min(R'-|z_2|, |z_2|-R).$$

What this theorem means is that if we allow the values β of V_β to sit in a lattice L, we have a closed operator algebra in the following sense: the product of any two fields in the algebra can be expanded in a power series whose Laurent coefficients are again fields in the algebra. The operator algebra consists of all vertex operators V_β and their descendants. The properties we require of the lattice L are the following:

(a) $L \subset \mathbb{R}$;

(b) $\beta_1,\beta_2 \in L \Rightarrow \beta_1+\beta_2 \in L$;

(c) $\beta \in L \Rightarrow -\beta \in L$;

(d) $Q \in L$;
(e) L is a countable set.

III. DUAL SPACES

In order to define the N-point vertex $V_{N;0}$ in Sec. IV, and to extend the theory to Riemann surfaces, it is necessary to introduce the concept of dual module. The space π_β is graded by the eigenspaces of L_0:

$$\pi_\beta = \oplus_{n=0}^{\infty} \pi_{\beta,n},$$

where the subspace $\pi_{\beta,n}$ with L_0 eigenvalue $\frac{1}{2}\beta(\beta-Q)+n$ has dimension $p(n)$, the number of partitions of n. As a space, the dual module π_β^* is just the sum of the duals of the homogeneous components

$$\pi_\beta^* = \oplus_{n=0}^{\infty} \pi_{\beta,n}^*.$$

In addition, π_β^* is both a left and a right Heisenberg module. To see this, we have to define a left and a right action of the generators of the Heisenberg algebra on a general covector $\omega \in \pi_\beta^*$. By definition

$$(\omega a_n)(\varphi) = \omega(a_n \varphi)$$

and

$$(a_n \omega)(\varphi) = \omega((Q\delta_{n;0} - a_{-n})\varphi),$$

where $\varphi \in \pi_\beta$ and where $(\ \ )(\ \ )$ denotes duality. It is easy to check the relations

$$[a_n, a_m] = [Q\delta_{m;0} - a_{-m}, Q\delta_{n;0} - a_{-n}]$$

establishing the left module structure of π_β^*. Let us define

$$L_l = \frac{1}{2} \sum_{m \in Z} :a_m a_{l-m}: - \frac{1}{2} Q(l+1) a_l \tag{4}$$

which satisfy the Virasoro commutation relations

$$[L_n, L_m] = (n-m)L_{n+m} + \frac{c}{12} n(n^2-1)\delta_{n+m;0}$$

with $c = 1 - 3Q^2$. Now π_β^* also carries a left and right Virasoro structure. Indeed, using the definition of L_n, we find

$$(\omega L_n)(\varphi) = \omega(L_n \varphi)$$

and

$$(L_n \omega)(\varphi) = \omega(L_{-n}\varphi).$$

The vector ${}_\beta\langle 0| \in \pi_{\beta,0}^*$ with ${}_\beta\langle 0|0\rangle_\beta = 1$ is the highest weight vector of π_β^* with L_0 (left or right) eigenvalue $\frac{1}{2}\beta(\beta-Q)$. Since we will later work with the spaces $\oplus_{\beta \in L} \pi_\beta$, it is natural to define

$${}_\alpha\langle 0|0\rangle_\beta = \delta_{\alpha;\beta}. \tag{5}$$

Note that vectors in π_β^* have left a_0 eigenvalue $Q-\beta$. As a consequence, the spaces π_β^* and $\pi_{Q-\beta}$ are isomorphic as left Heisenberg modules, the isomorphism being

$$a_{n_1}\cdots a_{n_k\beta}\langle 0| \mapsto a_{n_1}\cdots a_{n_k}|0\rangle_{Q-\beta}. \tag{6}$$

IV. THE N-POINT VERTEX $V_{N;0}$

The purpose of this section is to introduce the N-point vertex $V_{N;0}$ for a free bosonic theory coupled to a background charge Q. It depends on N coordinate systems $t_1(z)=z+z_1,\ldots,t_N(z)=z+z_N$ on the Riemann sphere. In a later section, we will generalize it to arbitrary projective coordinates $t_1,\ldots,t_N$.

In any field theory, it is important to know the vacuum expectation value of a product of fields. In our case, this means the value of

$${}_Q\langle 0|(j|\psi_1\rangle)(z_1)\cdots(j|\psi_N\rangle)(z_N)|0\rangle_0 \tag{7}$$

for $|\psi_i\rangle \in \pi_{\beta_i}$ and $|z_1|>\cdots>|z_N|$. We interpret the out vacuum ${}_Q\langle 0|$ as having a charge Q. In other words, we couple the system to a charge Q sitting in the point ∞. We know from Sec. II that Eq. (7) has an analytic (possibly many-valued) continuation to noncoinciding points. Moreover, by the equality (5), the vacuum expectation value vanishes unless $\Sigma_i\beta_i=Q$. We define $V_{N;0}(t_1,\ldots,t_N)$ by

$$V_{N;0}(t_1,\ldots,t_N)|\psi_1\rangle\cdots|\psi_N\rangle={}_Q\langle 0|(j|\psi_1\rangle)(z_1)\cdots(j|\psi_N\rangle)(z_N)|0\rangle_0.$$

It is a multilinear form acting on $\pi_{\beta_1}\otimes\cdots\otimes\pi_{\beta_N}$. The next proposition states that $V_{N;0}$ is completely determined by its value on $|0\rangle_{\beta_1}\cdots|0\rangle_{\beta_N}$. Before we can state the proposition, we define $\mathscr{M}$ as the space of meromorphic functions which are regular at ∞ and have poles only at the points $t_1(0)=z_1,\ldots,t_N(0)=z_N$ with $|z_1|>\cdots>|z_N|$. In other words $\mathscr{M}$ consists of all finite linear combinations of functions of the type $(z-z_i)^m$, $m\leqslant 0$ an integer. For $f\in\mathscr{M}$ we define

$$a_{z_i}(f)=\frac{1}{2\pi i}\oint_{z_i} d\zeta\, f(\zeta)J(\zeta-z_i),$$

where the contour encircles the point z_i, but no other point z_j, $j\neq i$. Since f has at most a pole singularity at $z=z_i$, $a_{z_i}(f)$ leaves π_{β_i} invariant. By the definition of j, we can also write

$$(ja_{z_i}(f)\varphi)(z_i)=\frac{1}{2\pi i}\oint_{z_i} d\zeta\, f(\zeta)J(\zeta)(j\varphi)(z_i) \tag{8}$$

because Eq. (8) is true for all f of the form $f(z)=(z-z_i)^m$. Now comes a fundamental proposition:

Proposition 7: Let $f\in\mathscr{M}$, $|\varphi_i\rangle \in \pi_{\beta_i}$, $\Sigma\beta_i=Q$, $|z_1|>\cdots>|z_N|$. *Then*

$$\sum_{i=1}^{N} {}_Q\langle 0|(j|\varphi_1\rangle)(z_1)\cdots(j(a_{z_i}(f)|\varphi_i\rangle)(z_i))\cdots(j|\varphi_N\rangle)(z_N)|0\rangle_0$$
$$=Qf(\infty){}_Q\langle 0|(j|\varphi_1\rangle)(z_1)\cdots(j|\varphi_N\rangle)(z_N)|0\rangle_0, \tag{9}$$

where $f(\infty)=\lim_{z\to\infty} f(z)$.

These equalities are called Ward identities and reflect the $U(1)$ Kac–Moody symmetry generated by J. The proof of the proposition is a straightforward argument of contour deformation.

With Eq. (9), we can successively build down the degrees of the $|\varphi_i\rangle$ until we get a product of vacua (here, the degree of $a_{-n_1}\cdots a_{-n_k}|0\rangle_\beta$ is defined as $\Sigma_i n_i$). With the help of this proposition, it is possible to prove Proposition 8.

Proposition 8: We have

$$V_{N;0}=\delta_{\Sigma\beta_i;Q}\ {}_{\beta_1}\langle 0|\cdots{}_{\beta_N}\langle 0|\exp\left(\sum_{\substack{i,j=1\\ i<j}}^{N}\sum_{m,n=0}^{\infty} a_n^{(i)}a_m^{(j)}\,\frac{\partial_{z_i}^n}{n!}\,\frac{\partial_{z_j}^m}{m!}\log(z_i-z_j)\right).$$

Here, the upper index $^{(i)}$ means that the action is on the ith factor of the tensor product $\otimes\ \pi_{\beta_j}$.

V. THE KNIZHNIK–ZAMOLODCHIKOV EQUATIONS

In this paragraph, we want to extend the N-point vertex $V_{N;0}$ to general projective coordinates using the Knizhnik–Zamolodchikov equations. Let us start by defining the energy-momentum tensor

$$T(z)=\tfrac{1}{2}{:}(\partial\phi)^2{:}(z)-\tfrac{1}{2}Q\partial^2\phi(z)$$

with the expansion

$$T(z)=\sum_{n\in\mathbb{Z}} L_n z^{n-2}, \tag{10}$$

where the modes L_n are given by Eq. (4). Using the explicit formula we have for j (Proposition 5b) as well as the Leibniz rule for differentiating a product, we can check Proposition 9.

Proposition 9: We have the following operator equation (both sides are operators: $H_R^\alpha\to H_{R'}^{\alpha+\beta}$, $R<|z|<R'$):

$$(jL_{-1}\psi)(z)=\partial_z(j\psi)(z),\quad \psi\in\pi_\beta.$$

This proposition immediately implies that

$$\partial_{z_i}V_{N;0}(t_1,\ldots,t_N)=V_{N;0}(t_1,\ldots,t_N)L_{-1}^{(i)}. \tag{11}$$

Actually, Eq. (11) together with the Ward identities (9) uniquely characterize $V_{N;0}$ up to a multiplicative constant. The Ward identities fix its dependence on the states it acts on, while Eq. (11) fixes its dependence on t_i. From now on, we would like to admit more general projective transformations t_i. Proposition 9 tells us what happens to $V_{N;0}$ under translations. With the idea in mind that the energy-momentum tensor is the infinitesimal generator of conformal transformations, we would like to describe how $V_{N;0}$ changes under an infinitesimal projective transformation. The collection $t_1,\ldots,t_N$ of projective coordinate systems is called admissible if $t_i(0)\neq t_j(0)$ whenever $i\neq j$. Consider a connected, simply connected open neighbourhood U of one such collection $t_1^0,\ldots,t_N^0$ which contains only admissible collections of coordinates. Let ML_N be the space of multilinear forms

$$V:\pi_{\beta_1}\otimes\cdots\otimes\pi_{\beta_N}\to\mathbb{C}$$

which depend holomorphically on N coordinate systems $t_1,\ldots,t_N$ in U (for arbitrary but fixed β_i satisfying $\Sigma\beta_i=Q$). Let us now look at a coordinate change in U:

$$\tilde{t}_i(z)=t_i(z)+\epsilon v(z)\,\frac{d}{dz}\,t_i(z),$$

where $v(z)d/dz$ is some holomorphic vector field on the Riemann sphere, i.e., of the form

$$v(z)\,\frac{d}{dz}=\sum_{n=-1}^{1} v_n z^{n+1}\,\frac{d}{dz}$$

and ϵ is a real parameter. We define an action of v on π_{β_i} by

$$\pi(v)|\,\eta\rangle=-\sum_{n=-1}^{1} v_n L_n|\,\eta\rangle.$$

Only finitely many terms in the expansion

$$\frac{1}{2}\sum_{k\in\mathbb{Z}} :a_k a_{n-k}:$$

of L_n contribute for a given $|\,\eta\rangle \in \pi_{\beta_i}$, and the action is well defined. With the Lie bracket

$$\left[-z^{n+1}\,\frac{d}{dz},-z^{m+1}\,\frac{d}{dz}\right]=-(n-m)z^{n+m+1}\,\frac{d}{dz}$$

for vector fields, this becomes a Lie algebra action in correspondence with the Virasoro algebra commutation relations

$$[L_n,L_m]=(n-m)L_{n+m}$$

for $n,m\in\{-1,0,1\}$. We further define

$$\partial_v^{(i)}V(t_1,\ldots,t_N)=\frac{d}{d\epsilon}\,V(t_1,\ldots,\tilde{t}_i,\ldots,t_N)|_{\epsilon=0}$$

and

$$\nabla_v^{(i)}V=\partial_v^{(i)}V+V\pi(v)^{(i)}$$

for $V\in ML_N$. Both $\partial_v^{(i)}$ and $\nabla_v^{(i)}$ are linear maps: $ML_N\to ML_N$. Let $\mathscr{M}_N$ be the space of holomorphic functions

$$f:U\times\hat{\mathbb{C}}\to\hat{\mathbb{C}}$$

satisfying $f^{-1}(\infty)\subset\cup_{i=1}^{N}\{(t_1,\ldots,t_N,z)|z=t_i(0)\}$. We emphasize that f should have only pole singularities [in no other hyperplanes than $z=t_i(0)$]. This space carries a Lie algebra structure under the bracket

$$[f,g]=\sum_{i=1}^{N}\,\frac{1}{2\pi i}\,\oint_{z_i} g\,df=0,$$

where df denotes the differential of f with respect to z. The expression is zero because the 1-form gdf has no poles outside $z=z_i(=t_i(0))$. We now define an action of $f\in\mathscr{M}_N$ on the space ML_N by

$$(f\cdot V)(t_1,\ldots,t_N)=V(t_1,\ldots,t_N)\left(\sum_{i=1}^{N} a_{t_i}^{(i)}(f\,)-Qf(t_1,\ldots,t_N,\infty)\right),\tag{12}$$

where the upper index $^{(i)}$ *again means that the action is on the ith factor* π_{β_i} *and where* $a_t(f)$ is implicitly defined by the equation

$$j_t a_t(f)\varphi = \frac{1}{2\pi i} \oint_{t(0)} f(z)J(z)j_t\varphi \, dz. \tag{13}$$

For $t(z)=z+z_i$, we have $a_t(f) = a_{z_i}(f)$ by Eq. (8). By analyzing infinitesimal coordinate changes, we see that Eq. (13) is a good definition for $a_t(f)$ which means that $a_t(f)$ maps π_β to itself. Using the operator product

$$J(\zeta)J(z) = \frac{1}{(\zeta-z)^2} + \text{regular terms}$$

we can show that Eq. (12) defines a Lie algebra action of $\mathscr{M}_N$ on ML_N. We would now like to define the N-point vertex $V_{N;0} \in ML_N$ as a solution to the Knizhnik–Zamolodchikov equations

$$\nabla_v^{(i)} V = 0 \tag{14}$$

for all vector fields v and to the Ward identities

$$(f \cdot V) = 0 \tag{15}$$

for all $f \in \mathscr{M}_N$. That Eq. (14) is compatible is a consequence of Proposition 10.

Proposition 10: The connection ∇ *is flat, i.e.,*

$$[\nabla_u^{(i)}, \nabla_v^{(j)}] = \delta^{ij}\nabla_{[u,v]}^{(i)}.$$

Proof: For $i \neq j$ this is true because $\nabla_v^{(i)}$ and $\nabla_u^{(j)}$ act on different factors. If $i=j$, the relation is an immediate consequence of

$$[\partial_u, \partial_v] = \partial_{[u,v]}$$

and the fact that we have a Lie algebra action of vector fields. ■

We know from the previous section that the Ward identities

$$f \cdot V(t_1,\ldots,t_N) = 0, \quad \forall f \in \mathscr{M}_N$$

for the fixed collection of coordinate systems $t_i^0(z) = z + z_i$ determine the multilinear form V (for these particular t_i^0) uniquely up to a scalar multiple. The Knizhnik–Zamolodchikov equation (14) being first-order compatible differential equations allow us to extend this V uniquely to other coordinates t_i along each path starting at t_i^0 in our space of coordinate systems. The solution we get will be holomorphic in admissible $(t_1,\ldots,t_N) \in U$. Moreover, it is sufficient to impose $\nabla_v V = 0$ for $v(\zeta) = 1, \zeta, \zeta^2$. Let us call the solution we get the N-point vertex and denote it by $V_{N;0}$ (0 is the genus of the surface, which is 0 for the Riemann sphere). For all $f \in \mathscr{M}_N$ we have

$$\begin{aligned}
&(f \cdot V_{N;0})(t_1,\ldots,t_N)|\eta_1\rangle\cdots|\eta_N\rangle \\
&\quad = {}_Q\langle 0|\sum_{i=1}^N j_{t_1}|\eta_1\rangle\cdots j_{t_i}a_{t_i}^{(i)}(f)|\eta_i\rangle\cdots j_{t_N}|\eta_N\rangle|0\rangle_0 - Qf(t_1,\ldots,t_N,\infty)V_{N;0}|\eta_1\rangle\cdots|\eta_N\rangle \\
&\quad = \sum_{i=1}^N {}_Q\langle 0|\sum_{i=1}^N j_{t_1}|\eta_1\rangle\cdots \frac{1}{2\pi i}\oint_{t_i(0)} f(z)J(z)j_{t_i}|\eta_i\rangle dz\cdots j_{t_N}|\eta_N\rangle|0\rangle_0 \\
&\qquad - Qf(t_1,\ldots,t_N,\infty)V_{N;0}|\eta_1\rangle\cdots|\eta_N\rangle
\end{aligned}$$

$$
\begin{aligned}
&= {}_Q\langle 0|\ \frac{1}{2\pi i}\ \oint_{|z|\gg 1} f(z)J(z)dz\ j_{t_1}|\,\eta_1\rangle\cdots j_{t_N}|\,\eta_N\rangle|0\rangle_0 \\
&- {}_Q\langle 0|j_{t_1}|\,\eta_1\rangle\cdots j_{t_N}|\,\eta_N\rangle\ \frac{1}{2\pi i}\ \oint_0 f(z)J(z)dz|0\rangle_0 - Qf(t_1,\ldots,t_N,\infty)V_{N;0}|\,\eta_1\rangle\cdots|\,\eta_N\rangle \\
&= 0
\end{aligned}
$$

so $V_{N;0}$ automatically satisfies Eqs. (15) in all coordinate systems. Let us summarize what we have found in the following:

Proposition 11: The Ward identities (15) for a particular collection of admissible coordinate systems, together with the Knizhnik–Zamolodchikov equations (14) for all admissible $t_1,\ldots,t_N$ and $v(\zeta)=1,\zeta,\zeta^2$, determine $V \in ML_N$ uniquely up to a scalar multiple. We call this V the N-point vertex and denote it by $V_{N;0}$. It is analytic (but possibly many-valued) in $t_1,\ldots,t_N$. Moreover, it satisfies the Ward identities (15) for all admissible $t_1,\ldots,t_N$.

The next proposition gives an explicit form for $V_{N;0}$:

Proposition 12: Up to a multiplicative constant, $V_{N;0}$ is given by

$$
V_{N;0} = \delta_{\Sigma_{i=1}^N \beta_i;Q^{\beta_1}}\langle 0|\cdots_{\beta_N}\langle 0|\exp\left(-\sum_{\substack{i,j=1\\ i<j}}^{N}\ \sum_{n,m=0}^{\infty}\ \alpha_n^{(i)}D_{nm}(s_i t_j)\alpha_m^{(j)}\right), \tag{16}
$$

where t_i are projective coordinates, i.e., have the form

$$
t_i(z)=\frac{Az+B}{Cz+D},\quad AD-BC=1.
$$

$s_i t_j$ denotes composition of the maps s_i and t_j, and

$$
\alpha_n=\begin{cases} a_0, & n=0 \\ \dfrac{a_n}{\sqrt{|n|}}, & n\neq 0, \end{cases}
$$

$$
s_i(z)=\frac{1}{t_i^{-1}(z)},
$$

$$
D_{nm}(\gamma)=\frac{\sqrt{m}}{\sqrt{n}}\ \frac{\partial^m}{m!}\ \gamma(z)^n\Big|_{z=0},\quad n,\ m\neq 0,
$$

$$
D_{00}(\gamma)=\tfrac{1}{2}\log(\gamma'(z))\big|_{z=0},
$$

$$
D_{n0}(\gamma)=\frac{1}{\sqrt{n}}\ \gamma(z)^n\Big|_{z=0},\quad n\neq 0,
$$

$$
D_{0m}(\gamma)=\frac{1}{2}\ \sqrt{m}\ \frac{\partial^m}{m!}\log\ \gamma'(z)\Big|_{z=0},\quad m\neq 0.
$$

The proof splits into two parts. First, we must show that this expression agrees, up to a multiplicative constant, with the one we have found in the special case where $t_i(z)=z+z_i$. This is easy to check. The more lengthy but nevertheless straightforward part consists in checking the KZ equations.

VI. THE SCHOTTKY REPRESENTATION OF A RIEMANN SURFACE

In this section we describe how we can, starting from a punctured sphere, obtain compact Riemann surfaces. This will ultimately help us to extend the N-point vertex $V_{N;0}$ from the Riemann sphere to more general Riemann surfaces. Let S_μ $(\mu=1,...,g)$ be a set of g projective transformations, i.e.,

$$S_\mu(z)=\frac{a_\mu z+b_\mu}{c_\mu z+d_\mu}, \quad a_\mu d_\mu-b_\mu c_\mu=1 \tag{17}$$

having some characteristic circles (see below) all exterior to one another. The Schottky group $\mathscr{G}_g$ is the subgroup of PSL $(2,\mathbb{C})$ generated by the S_μ's. Therefore, an element $T\in\mathscr{G}_g$, except for the identity, can be written in the form

$$T=S_{\mu_1}^{n_1}\cdots S_{\mu_r}^{n_r}, \quad r=1,2,\ldots, \quad n_i\in\mathbb{Z}\backslash\{0\}, \quad \mu_i\neq\mu_{i+1}.$$

A more convenient way to specify the generators S_μ than Eq. (17) is by their multipliers k_μ and fixed points ξ_μ and η_μ defined by

$$\frac{S_\mu(z)-\eta_\mu}{S_\mu(z)-\xi_\mu}=k_\mu\frac{z-\eta_\mu}{z-\xi_\mu}, \quad 0<|k_\mu|<1.$$

Since for any $z\in\hat{\mathbb{C}}\{\xi_\mu,\eta_\mu\}$ we have

$$\lim_{n\to\infty} S_\mu(z)^n=\eta_\mu, \quad \lim_{n\to\infty} S_\mu(z)^{-n}=\xi_\mu$$

we call η_μ the attractive fixed point and ξ_μ the repulsive fixed point. The g generators S_μ and their inverse identify in the extended complex plane $2g$ circles $\mathscr{C}_\mu$ and $\mathscr{C}'_\mu$ for $\mu=1,...,g$, called isometric circles and defined, respectively, by

$$\left|\frac{dS_\mu}{dz}\right|^{-1}=|c_\mu z+d_\mu|^2=1, \quad \left|\frac{dS_\mu^{-1}}{dz}\right|^{-1}=|c_\mu z-a_\mu|^2=1.$$

It is easy to verify that the projective transformation S_μ maps $\mathscr{C}_\mu$ onto $\mathscr{C}'_\mu$ and that of course the inverse S_μ^{-1} maps $\mathscr{C}'_\mu$ onto $\mathscr{C}_\mu$. Moreover, the exterior of $\mathscr{C}_\mu$ will be mapped by S_μ into the interior of $\mathscr{C}'_\mu$ whereas the interior of $\mathscr{C}_\mu$ will be mapped into the exterior of $\mathscr{C}'_\mu$. In particular, this implies that the attractive fixed point η_μ is inside the circle $\mathscr{C}'_\mu$ while the repulsive fixed point ξ_μ is inside the circle $\mathscr{C}_\mu$. If we require these isometric circles to be all exterior to each other, we can deduce that the fundamental region of the Schottky group $\mathscr{G}_g$ is precisely the part of the extended complex plane which is exterior to all the circles. If we identify these circles in couple, g handles are formed and we obtain a Riemann surface Σ_g of genus g. More precisely, we have

$$\Sigma_g=\frac{\hat{\mathbb{C}}-\Lambda(\mathscr{G}_g)}{\mathscr{G}_g},$$

where $\Lambda(\mathscr{G}_g)$ is the limit set of the Schottky group, i.e., the set of accumulation points of its orbits.[8] Going around a cycle a_μ of the canonical homology basis of the Riemann surface corre-

sponds, in the Schottky representation, to going around $\mathscr{C}_\mu$ clockwise or $\mathscr{C}'_\mu$ anticlockwise while moving on a path that brings from a point z to the point $S_\mu(z) \in \mathscr{C}'_\mu$ corresponds to going around a b_μ cycle. Instead of choosing isometric circles, we could, for example, take a smaller circle $\tilde{\mathscr{C}}_\mu$ instead of $\mathscr{C}_\mu$, which is then mapped into a circle $\tilde{\mathscr{C}}'_\mu$ larger than $\mathscr{C}'_\mu$. All the properties of $\mathscr{C}_\mu$ and $\mathscr{C}'_\mu$ (apart from being isometric) remain true for $\tilde{\mathscr{C}}_\mu$ and $\tilde{\mathscr{C}}'_\mu$. In particular, we can require these new circles to be all exterior to each other, and forget about the old ones. Conversely, every compact Riemann surface Σ_g with a given homology basis can be obtained with a group of Schottky type (Ref. 9, retrosection theorem p. 222 of Ref. 10). A group of Schottky type, unlike a Schottky group, identifies pairs of analytic closed curves instead of pairs of circles, but it is still a group of projective transformations. The closed curves just mentioned correspond to the given homology basis. Unfortunately, not every group of Schottky type is a Schottky group as is shown in Ref. 11. Therefore, it is probably not true that we obtain all Riemann surfaces by sewing together pairs of circles (it may even not be true that we obtain a representative for each point in the moduli space of compact Riemann surfaces). Since we only consider Riemann spheres with N disjoint projective disks $t_1(D),\ldots,t_N(D)$ (D being the closed unit disk) and not spheres with general embedded disks, the whole discussion will be restricted to the Riemann surfaces Σ_g obtained by identifying pairs of circles $t_i(S^1)$.

VII. AXIOMATIC APPROACH

In Ref. 5, Segal formulated a set of properties or axioms which he thinks are characteristic of a conformal field theory. We now want to list these axioms in a slightly different setting, taking into account many-valuedness and the fact that we possibly do not get all compact Riemann surfaces using Schottky groups.

For Segal,[5] the basic object of a conformal field theory is a representation of the category $\mathscr{C}$ which we now want to describe. The starting point for defining $\mathscr{C}$ is a Riemann sphere with pairwise disjoint embedded disks (also called legs) $t_1(D),\ldots,t_{N+M}(D)$ where $t_1,\ldots,t_{N+M}$ are projective transformations. We can change the orientation of the disks $t_{N+1}(D),\ldots,t_{N+M}(D)$ by complex conjugation. We then get a Riemann sphere with legs $t_1(D),\ldots,t_N(D)$, $\bar{t}_{N+1}(D),\ldots,t_{N+M}(D)$ which we interpret as a morphism from N in-disks C_N to M out-disks C_M. A new morphism, i.e., a new Riemann surface, can be obtained by cutting out g pairs of in- and out-disks and sewing their boundary circles together. This is done using a Schottky group. More precisely, the sewing together of the circles $t_i(S^{-1})$ and $\bar{t}_j(S^1)$ is via the Schottky generator $t_i s_j$. We thus get g generators, and obtain a surface of genus g which carries a canonical homology basis, where the a cycles correspond to the pairs of circles that have been sewn together, and a path from a point on one circle to the corresponding point on its image circle corresponds to a b cycle. We will show later that there is a unique way to choose the homology class of the b cycle. The objects of $\mathscr{C}$ are therefore Cartesian products C_N of N unit disks D in the complex plane, and a morphism $C_N \to C_M$ is a compact (not necessarily connected) Riemann surface Σ with N in-legs and M out-legs. Each connected component of Σ is a Riemann surface X without boundary with a certain number of embedded disks $t_i(D)$ or $\bar{t}_j(D)$ and a fixed canonical homology basis (a,b). These t_i are local projective coordinates on X. Moreover, we associate to each unordered pair of distinct coordinates on X an integer $l_{ij} \in \mathbb{Z}$. Likewise, if the genus of X is not zero, we associate integers l_i^Q, l_μ^Q to each t_i (or $\bar{t}_i$) and each $a_\mu, l_{i\mu}$ to every pair t_i, a_μ, and $l_{\mu\nu} = l_{\nu\mu} \in \{0,1\}$ to every pair a_μ, a_ν (where this time μ and ν can be equal). In the case of the sphere, these integers fix a branch for each logarithm appearing in $V_{N;0}$. More precisely, the integers are defined so that

$$\pi l_{ij} \leqslant \mathrm{Im}(D_{00}(s_i t_j)) < \pi(l_{ij}+1)$$

making $V_{N;0}$ single-valued. In the same way, $V_{N;g}$ will be single-valued if the integers

$l_{i\mu}, l_{ij}, l_{\mu\nu}, l_i^Q, l_\mu^Q$ are specified along with a canonical homology basis [see the discussion after Eq. (28)]. Two morphisms Σ and Σ' which carry the same set of integers are identified whenever there exists a biholomorphic map

$$f:\Sigma \to \Sigma'$$

with $f\circ(t,\bar{t})=(t',\bar{t'})$ and $f(a_\mu)=a'_\mu, f(b_\mu)=b'_\mu$ for all $\mu\in\{1,...,g\}$. The last two equalities are to be understood in a homological sense.

Under composition of morphisms, the genus is additive, and as we will see later, the integers associated to the new surface, as well as the new homology basis are uniquely determined by the integers and homology basis we had before the sewing. The simplest example is provided by the semigroup of morphisms $C_0 \to C_0$. It is just the space of isomorphism classes of Riemann surfaces with a fixed homology basis and a fixed set of integers, the operation being disjoint union.

Let us consider the composition Σ of two morphisms corresponding to connected Riemann surfaces both coming from a Riemann sphere under the action of a Schottky group. Σ itself can be obtained from a Schottky group acting on a Riemann sphere because we can first sew both spheres together and then act with the larger Schottky group. Our space of morphisms consists of all finite unions of Riemann surfaces that we get from a sphere and a Schottky group, and what we have just shown is that a composition of morphisms is again a morphism. We are now in a position to define a conformal field theory. It consists of a complex Hilbert space $\mathscr{H}$ (the space of states) and of a continuous functor V from $\mathscr{C}$ to a category of Hilbert spaces. V is required to possess the following properties:

(i) $V(C_N)=\mathscr{H}^{\otimes N}$.

(ii) For each morphism $\Sigma:C_N\to C_M$, the operator $V:\mathscr{H}^{\otimes N}\to\mathscr{H}^{\otimes M}$ is trace class.

(iii) V is a *-functor, i.e., $V(\Sigma)^*=V(\bar{\Sigma})$ for each $(\Sigma,a,b):C_N\to C_M$ where $(\bar{\Sigma},a,-b):C_M\to C_N$ is the Riemann surface complex conjugate to Σ carrying the same set of integers as Σ but with the opposite sign.

(iv) V has the collapsing property that if a morphism $\Sigma:C_{N+R}\to C_{M+R}$ is made into a morphism $\hat{\Sigma}:C_N\to C_M$ by attaching the first R outgoing circles to the first R ingoing circles, then $V(\hat{\Sigma})=\mathrm{Tr}\, V(\Sigma)$ where the trace is taken over $\mathscr{H}^{\otimes R}$.

(v) Let $\tilde{\Sigma}:C^{N-1}\to C^{M+1}$ be the morphism obtained from $\Sigma:C^N\to C^M$ by reversing one leg (while keeping the homology basis and the integers fixed). If we interpret $V(\Sigma)$ as an operator from $\mathscr{H}^{N-1}$ to $\mathscr{H}^*\otimes\mathscr{H}^{\otimes M}$, then $V(\tilde{\Sigma})=(\varphi\otimes Id)\circ V(\Sigma)$ where $\varphi:\mathscr{H}^*\to\mathscr{H}$ is a (fixed) linear isomorphism.

A word of explanation is in order for the fourth property. By the remarks before the axioms, it is enough to know which b cycles and integers to select in the case where we sew together g pairs of circles on the sphere. What property (iv) says is that $V(\hat{\Sigma})$ is independent of the particular sewing used to obtain it.

The functor V is sometimes called modular because it only depends on the Riemann surface Σ through a homology basis, a set of integers, and the local projective coordinates t_i around the embedded disks. In the literature, modularity generally means more than this. One usually considers holomorphic and antiholomorphic sectors together and requires independence of the homology basis.

VIII. EXTENSION TO RIEMANN SURFACES

In this section, we would like to extend the N-point vertex $V_{N;0}$ from a sphere with N legs to other compact Riemann surfaces with legs by a sewing procedure. The extension will be such that the set of all N-point vertices so obtained (for all N) is a modular functor in the sense of the axioms above.

We would first like to associate $V_{N;0}$ to a Riemann sphere with N legs. The legs are $t_i(D)$, $i=1,\ldots,N$. Let us see how to get the N-point g-loop vertex $V_{N;g}$ starting with $V_{N+2g;0}$. For

notational simplicity, we label the first N legs of $V_{N+2g;0}$ with an index i running from 1 to N and divide the remaining $2g$ legs into ''odd'' legs labeled by $2\mu-1$ and ''even'' legs labeled by 2μ, $\mu=1,...,g$. This choice is particularly convenient because we will later sew together leg $2\mu-1$ with leg 2μ, $\mu=1,...,g$, thus generating g handles. The first operation we have to make is reverse the even legs. This means identifying $\mathscr{H}^*$ with $\mathscr{H}$ with the linear isomorphism (6), i.e.,

$$_{\beta_\mu+Q}\langle 0|a_{n_1}\cdots a_{n_k} \mapsto (Q\delta_{n_k;0}-a_{-n_k})\cdots(Q\delta_{n_1;0}-a_{-n_1})|0\rangle_{-\beta_\mu}$$

since

$$_{\beta_\mu+Q}\langle 0|a_{n_1}\cdots a_{n_k}=(Q\delta_{n_k;0}-a_{-n_k})\cdots(Q\delta_{n_1;0}-a_{-n_1})_{\beta_\mu+Q}\langle 0|.$$

Due to the special form of $V_{N;0}$, this corresponds to the prescription

$$_{\beta_\mu+Q}\langle 0|\mapsto|0\rangle_{-\beta_\mu}, \quad \alpha_n^{(\mu)}\mapsto\alpha_n^{+(\mu)}=-\alpha_{-n}^{(\mu)}+Q\delta_{n,0}. \tag{18}$$

This operation is motivated by the fact that by sewing together two spheres with $N+1$ and $M+1$ legs along a boundary circle, one gets a sphere with $M+N$ legs, i.e.,

$$V_{N+1;0}(1,2,\ldots,N,E)V_{M+1;0}(F^+,N+1,\ldots,N+M)=V_{N+M;0}(1,\ldots,N+M), \tag{19}$$

where F^+ means that the leg F has been reversed according to Eq. (18). Here, the Hilbert spaces of the two legs E and F have been identified. By conservation of charge, we must have

$$\beta_E=-\sum_{i=1}^{N}\beta_i+Q=-\beta_F+Q, \quad \beta_F=-\sum_{i=N+1}^{N+M}\beta_i+Q$$

so that the left-hand side of Eq. (19) can be written as

$$\begin{aligned}
&{}_{\beta_1}\langle 0|,\ldots,{}_{\beta_{N+M}}\langle 0|\,\delta_{\Sigma_{i=1}^{N+M}\beta_i;Q}\,\exp\left(-\sum_{\substack{i,j=1\\ i<j}}^{N}\sum_{n,m=0}^{\infty}\alpha_n^{(i)}D_{nm}(s_it_j)\alpha_m^{(j)}\right)\\
&\times\exp\left(-\sum_{\substack{i,j=N+1\\ i<j}}^{N+M}\sum_{n,m=0}^{\infty}\alpha_n^{(i)}D_{nm}(s_it_j)\alpha_m^{(j)}\right)\\
&\times{}_{\beta_E}\langle 0|\exp\left(-\sum_{i=1}^{N}\sum_{n,m=0}^{\infty}\alpha_n^{(i)}D_{nm}(s_it_E)\alpha_m^{(E)}\right)\\
&\times\exp\left(-\sum_{j=N+1}^{N+M}\sum_{n,m=0}^{\infty}\alpha_n^{+(E)}D_{nm}(s_Ft_j)\alpha_m^{(j)}\right)|0\rangle_{\beta_E}.
\end{aligned} \tag{20}$$

We compute the last two lines as follows: we interchange the two exponentials using the formula

$$e^Ae^B=e^{[A,B]}e^Be^A$$

and write $\alpha_0^{(E)}=\Sigma_{j=N+1}^{N+M}\beta_j$, $\alpha_0^{+(E)}=\Sigma_{i=1}^{N}\beta_i$. That way, we get

$$\exp\left(-\sum_{i=1}^{N}\sum_{j=N+1}^{N+M}\sum_{n,m=0}^{\infty}\sum_{l=1}^{\infty}\alpha_n^{(i)}D_{nl}(s_it_E)D_{lm}(s_Ft_j)\alpha_m^{(j)}\right)$$

$$\exp\left(-\sum_{i=1}^{N}\sum_{n=0}^{\infty}\alpha_n^{(i)}D_{n0}(s_it_E)\sum_{j=N+1}^{N+M}\beta_j\right)\exp\left(-\sum_{i=1}^{N}\beta_i\sum_{j=N+1}^{N+M}\sum_{m=0}^{\infty}D_{0m}(s_Ft_j)\alpha_m^{(j)}\right)$$
$$=\exp\left(-\sum_{i=1}^{N}\sum_{j=N+1}^{N+M}\sum_{n,m=0}^{\infty}\alpha_n^{(i)}D_{nm}(s_it_Es_Ft_j)\alpha_m^{(j)}\right),$$

where we have used the property

$$D_{nm}(\gamma_1\gamma_2)=\sum_{l=1}^{\infty}D_{nl}(\gamma_1)D_{lm}(\gamma_2)+D_{n0}(\gamma_1)\delta_{m,0}+D_{0m}(\gamma_2)\delta_{n,0}. \tag{21}$$

Together with the first two lines of Eq. (20) we get

$${}_{\beta_1}\langle 0|\cdots{}_{\beta_{N+M}}\langle 0|\,\delta_{\Sigma_{i=1}^{N+M}\beta_i;Q}\,\exp\left(-\sum_{\substack{i,j=1\\ i<j}}^{N+M}\sum_{n,m=0}^{\infty}\alpha_n^{(i)}D_{nm}(\tilde{s}_i\tilde{t}_j)\alpha_m^{(j)}\right)$$

with the new coordinates

$$\tilde{s}_i=\begin{cases}s_i, & i=N+1,\ldots,N+M\\ s_it_E\Gamma t_F^{-1}, & i=1,\ldots,N\end{cases},$$
$$\tilde{t}_i=\begin{cases}t_i, & i=N+1,\ldots,N+M\\ t_F\Gamma t_E^{-1}t_i, & i=1,\ldots,N\end{cases}, \tag{22}$$

where $\Gamma(z)=1/z$. We now understand the precise meaning of Eq. (19). The transformation $t_E\Gamma t_F^{-1}$ maps the "unit circle" $t_F(S^1)$ into the unit circle $t_E(S^1)$. The transformation Γ makes sure that the exterior of the circle $t_F(S^1)$ is mapped into the interior of $t_E(S^1)$. In view of the key role played by the identity (21), we check it for $n,m\neq 0$. By the explicit form of D_{nm}, we have to prove that

$$\frac{1}{m!}\frac{\sqrt{m}}{\sqrt{n}}\,\partial_z^m(\gamma_1\gamma_2(z))^n=\lim_{w\to 0}\sum_{l=1}^{\infty}\frac{1}{l!}\frac{\sqrt{l}}{\sqrt{n}}\,\partial_w^l(\gamma_1(w))^n\,\frac{1}{m!}\frac{\sqrt{m}}{\sqrt{l}}\,\partial_z^m(\gamma_2(z))^l$$

for $|z|\to 0$. It is enough to show the equality

$$(\gamma_1\gamma_2(z))^n=\sum_{l=1}^{\infty}\frac{1}{l!}\,\partial_w^l(\gamma_1(w))^n\Big|_{w=0}(\gamma_2(z))^l+(\gamma_1(0))^n.$$

The right-hand side is nothing but the Taylor expansion of the left-hand side. Let us return to the case of genus $g\geqslant 1$. According to Segal's last axiom, we have to take the partial trace

$$V_{N;g}=\prod_{\mu=1}^{g}\mathrm{Tr}_{(2\mu-1,2\mu)}V_{N+2g;0}^{+}$$

to get the g-loop vertex. The trace is to be understood as a sum over both zero and nonzero modes. More precisely, we now interpret the N-point vertex $V_{N;0}$ as acting on the N-fold tensor product $\mathscr{H}^{\otimes N}$ where the Hilbert space $\mathscr{H}$ is a direct sum of $\overline{\pi_\beta}$'s:

$$\mathscr{H}=\oplus_{\beta\in L}\overline{\pi_\beta}.$$

Here, L is the lattice of allowed zero modes. We rewrite the N-point vertex as

$$V_{N;0}=\sum_{\beta_1,\ldots,\beta_N\in L}\delta_{\Sigma_{i=1}^N\beta_i;Q}\,{}_{\beta_1}\langle 0|\cdots{}_{\beta_N}\langle 0|\exp\left(-\sum_{\substack{i,j=1\\ i<j}}^{N}\sum_{n,m=0}^{\infty}\alpha_n^{(i)}D_{nm}(s_it_j)\alpha_m^{(j)}\right). \tag{23}$$

Reversing the even legs, we get the expression

$$\begin{aligned}V^+_{N+2g;0}=&\sum_{\beta_1,\ldots,\beta_N\in L}\sum_{r_1,\ldots,r_g\in L}\delta_{\Sigma_{i=1}^N\beta_i+(g-1)Q;0}\,{}_{\beta_1}\langle 0|\cdots{}_{\beta_N}\langle 0|\\ &\times\exp\left(-\frac{1}{2}\sum_{\substack{i,j=1\\ i\neq j}}^{N}\sum_{n,m=0}^{\infty}\alpha_n^{(i)}D_{nm}(s_it_j)\alpha_m^{(j)}\right)\prod_{\substack{\mu=1\\ \text{odd}}}^{g}{}_{-r_\mu}\langle 0|\\ &\times\exp\left(-\sum_{i=1}^{N}\sum_{\mu=1}^{g}\sum_{n,m=0}^{\infty}\alpha_n^{(i)}(D_{nm}(s_it_{2\mu-1})\alpha_m^{(2\mu-1)}+D_{nm}(s_it_{2\mu})\alpha_m^{+(2\mu)})\right)\\ &\times\exp\left(-\frac{1}{2}\sum_{\substack{\mu,\nu=1\\ \mu\neq\nu}}^{g}\sum_{n,m=0}^{\infty}\alpha_n^{(2\mu-1)}D_{nm}(s_{2\mu-1}t_{2\nu-1})\alpha_m^{(2\nu-1)}\right.\\ &\left.+\alpha_n^{+(2\mu)}D_{nm}(s_{2\mu}t_{2\nu})\alpha_m^{+(2\nu)}\right)\\ &\times\exp\left(-\sum_{\mu,\nu=1}^{g}\sum_{n,m=0}^{\infty}\alpha_n^{+(2\mu)}D_{nm}(s_{2\mu}t_{2\nu-1})\alpha_m^{(2\nu-1)}\right)\prod_{\substack{\mu=1\\ \text{even}}}^{g}|0\rangle_{-r_\mu},\end{aligned} \tag{24}$$

where we have set $\beta_{2\mu}=r_\mu+Q$, $\beta_{2\mu-1}=-r_\mu$. Care is required here because the β_i still appearing in the formula correspond to the unsewn legs and are not fixed by the identities just given. Some exponents in our expression have a $\frac{1}{2}$ factor in front because we have used the property

$$D_{nm}(s_It_J)=D_{mn}(s_Jt_I).$$

The main result of this paper is Theorem 13.

Theorem 13: *$V_{N;0}:\mathscr{H}^{\otimes N}\to\mathbb{C}$ is trace class as soon as the closed disks $t_i(D)$ are all pairwise disjoint. If any two open disks $t_i(\mathring{D}),t_j(\mathring{D})$ overlap, the operator $V_{N;0}$ gets unbounded (i.e., cannot be extended to all $\mathscr{H}^{\otimes N}$ by the closed graph theorem).*

We will prove Theorem 13 in Sec. IX. Since $V^+_{N=2g;0}$ is the composition of $V_{N+2g;0}$ (which we here interpret as an operator $\mathscr{H}^{\otimes N+g}\to\mathscr{H}^{*\otimes g}$) and Eq. (18), and since Eq. (18): $\mathscr{H}^*\to\mathscr{H}$ is an isometry, the same statements with $V^+_{N+2g;0}$ instead of $V_{N+2g;0}$ are also true. This allows us to choose a basis to compute

$$V_{N:g}=\prod_{\mu=1}^{g}\mathrm{Tr}_{(2\mu-1,2\mu)}V^+_{N+2g;0}\,.$$

We first compute the trace over the nonzero modes using the coherent states method. In one dimension, the Hamiltonian of the harmonic oscillator is $H=a^*a$ with $a^*=1/\sqrt{2}(x-d/dx)$, $a=1/\sqrt{2}(x+d/dx)$ the creation and annihilation operators, respectively. A coherent state $|\alpha\rangle$ is an eigenstate of a with eigenvalue α. Explicitly

$$|\alpha\rangle=e^{\alpha a^*}|0\rangle,$$

where $|0\rangle = \pi^{-1/4} e^{-x^2/2}$ is the ground state of H. Recall that if $T: L^2(\mathbb{R}) \to L^2(\mathbb{R})$ is a trace class operator, its trace is equal to

$$\mathrm{Tr}\ T = \frac{1}{\pi} \int d^2\alpha\ e^{-|\alpha|^2} \langle \alpha | T | \alpha \rangle,$$

where the integral is over all $\alpha \in \mathbb{C}$. $V_{N;g}$ is therefore given by

$$V_{N:g} = \int \prod_{\mu=1}^{g} \prod_{n=1}^{\infty} \left(\frac{d^2\alpha_n^\mu}{\pi} \right) \exp\left[-\sum_{\mu=1}^{g} \sum_{n=1}^{\infty} |\alpha_n^\mu|^2 \right] \langle \alpha | V^+_{N+2g;0} | \alpha \rangle = \sum_{r_1,\dots,r_g \in L} \tilde{V}_{N:g}$$

which is a Gaussian functional integral. We first compute $\tilde{V}_{N:g}$. The trace calculation amounts to the substitutions

$$\alpha_n^{(2\mu-1)} \to \alpha_n^\mu, \quad \alpha_n^{+(2\mu)} \to -\bar{\alpha}_n^\mu \quad (n>0);$$

$$\alpha_0^{(2\mu-1)} \to -r_\mu, \quad \alpha_0^{+(2\mu)} \to r_\mu + Q.$$

In order to write our formulas in a more compact way, we adopt the following vectorlike notation:

$$(X_1 X_2) \begin{pmatrix} Y_1 \\ Y_2 \end{pmatrix} = \sum_{\mu=1}^{g} \sum_{n=1}^{\infty} \left((X_1)_n^\mu (Y_1)_n^\mu + (X_2)_n^\mu (Y_2)_n^\mu \right)$$

and get a result of the form

$$\tilde{V}_{N:g} = \sum_{\beta_1,\dots,\beta_N \in L} {}_{\beta_1}\langle 0| \cdots {}_{\beta_N}\langle 0|\, \delta_{\Sigma_{i=1}^N \beta_i + (g-1)Q;0}\ \exp(A) \int \prod_{\mu=1}^{g} \prod_{n=1}^{\infty} \left(\frac{d^2\alpha_n^\mu}{\pi} \right) \times \exp\left((B_1 B_2) \begin{pmatrix} \alpha \\ \bar{\alpha} \end{pmatrix} - \frac{1}{2} (\bar{\alpha}\alpha)(1-H) \begin{pmatrix} \alpha \\ \bar{\alpha} \end{pmatrix} \right), \tag{25}$$

where A denotes all the terms which do not depend on α_n^μ, $n \neq 0$. The 1 in the matrix $(1-H)$ comes from the Gaussian measure with respect to which we integrate. The integration over α_n^μ yields

$$\tilde{V}_{N;g} = \det(1-H)^{-(1/2)} {}_{\beta_1}\langle 0| \cdots {}_{\beta_N}\langle 0|\, \delta_{\Sigma_{i=1}^N \beta_i + (g-1)Q;0}\ \exp\left(A + \frac{1}{2} (B_1 B_2)(1-H)^{-1} \begin{pmatrix} B_2 \\ B_1 \end{pmatrix} \right). \tag{26}$$

If we use the explicit expressions for A, B_1, and B_2, it becomes clear that the exponent in the last expression can be separated into three pieces that are respectively quadratic, linear and independent of the zero modes r_μ. In other words, we can rewrite $\tilde{V}_{N;g}$ as

$$\tilde{V}_{N:g} = \sum_{\beta_1,\dots,\beta_N \in L} {}_{\beta_1}\langle 0| \cdots {}_{\beta_N}\langle 0|\, \delta_{\Sigma_{i=1}^N \beta_i + (g-1)Q;0}\ \det(1-H)^{-(1/2)} \times \exp\left(\frac{1}{2} \sum_{\mu,\nu=1}^{g} r_\mu C^{(1)}_{\mu\nu} r_\nu + \sum_{\mu=1}^{g} r_\mu C^{(2)}_\mu + C^{(3)} \right). \tag{27}$$

It is a lengthy, but straightforward task to compute the coefficients $C^{(1)}_{\mu\nu}, C^{(2)}_\mu, C^{(3)}$ and the determinant. The more difficult part consists in identifying the results with some geometric objects associated to the Riemann surface. A detailed account of the computation can be found in Ref. 12. In Ref. 6, the same computation was carried out more rigorously. The result is

$$\tilde{V}_{N;g} = {}_{\beta_1}\langle 0|\cdots{}_{\beta_N}\langle 0|\,\delta_{\Sigma_{i=1}^N \beta_i + (g-1)Q;0}\mathcal{N}\exp\left(\frac{\pi i}{2}\sum_{\mu,\nu=1}^{g} r_\mu (2\tau_{\mu\nu}+l_{\mu\nu})r_\nu\right)$$
$$\times\exp\left(-\sum_{\mu=1}^{g} r_\mu\left(\sum_{i=1}^{N}\sum_{m=0}^{\infty}\frac{a_m^{(i)}}{m!}\,\partial_z^m\left(\int_{z_0}^{t_i(z)}\omega_\mu\right)\Big|_{z=0} + 2\pi i Q\left(\Delta_\mu^{z_0}+\frac{1}{2}\right)\right)\right)$$
$$\times\exp\left(-\frac{1}{2}\sum_{\substack{i,j=1\\ i\neq j}}^{N}\sum_{n,m=0}^{\infty}\alpha_n^{(i)} D_{nm}(s_i t_j)\,\alpha_m^{(j)}\right)$$
$$\times\exp\left(\frac{1}{2}\sum_{i,j=1}^{N}\sum_{n,m=0}^{\infty} a_n^{(i)}\,\frac{\partial_z^n}{n!}\,\frac{\partial_y^m}{m!}\log\frac{E(t_i(z),t_j(y))}{t_i(z)-t_j(y)}\Big|_{y,z=0} a_m^{(j)}\right)$$
$$\times\exp\left(-\frac{1}{2}\,Q\sum_{i=1}^{N}\sum_{m=0}^{\infty} a_m^{(i)}\,\frac{\partial_z^m}{m!}\{\log t_i'(z) + 2\log\sigma(t_i(z))\}\Big|_{z=0}\right). \tag{28}$$

The coefficient $\mathcal{N}=\det(1-H)^{-(1/2)}$ is related to the inverse of the determinant of the scalar Laplacian on the Riemann surface Σ_g calculated in the subspace of the nonzero modes, and its dependence on the period matrix $\tau_{\mu\nu}$ is only through $\det(\mathrm{Im}\,\tau)$,[13] which is independent of the b cycles. The abelian differentials ω_μ only depend on the Riemann surface Σ_g through the a cycles. The prime form E remains invariant if its arguments are moved along a cycles, and is therefore also independent of our particular choice of b, but depends on the local coordinates t_i. The $g/2$ differential σ with no zeros or poles depends on Σ_g only through the coordinates t_i.[14] If we require $0\leqslant \mathrm{Im}(\log k_\mu) < 2\pi$ for all multipliers k_μ, we find that the vector of Riemann constants $\Delta_\mu^{z_0}$ is fixed modulo $\frac{1}{2}$. The z_0 dependence of $\tilde{V}_{N;g}$ drops out due to the Kronecker delta. The way Sciuto *et al.* obtained the period matrix $\tau_{\mu\nu}$ is ambiguous because the computation involved logarithms.[12] As a consequence, each matrix element is only clearly defined modulo $\frac{1}{2}$. If we fix a branch for each logarithm in the definition of $V_{N;0}$, i.e., if we fix each l_{ij}, this corresponds to a unique choice of b cycles. More precisely, if $V_{N;0}$ is unambiguously defined, the same is automatically true for $V_{N;g}$. The ambiguities of $V_{N;g}$ can be labeled by the set of integers $\tilde{l}_\mu^Q, \tilde{l}_{i\mu}, \tilde{l}_i^Q, \tilde{l}_{ij}$ corresponding to an unambiguous choice of the value of

$$\Delta_\mu^{z_0}, \int_{z_0}^{t_i(0)}\omega_\mu,\ \log t_i'(0) + 2\log\sigma(t_i(0))$$

and

$$D_{00}(s_i t_j) - \log\frac{E(t_i(0),t_j(0))}{t_i(0)-t_j(0)},$$

respectively, and by the choice of $l_{\mu\nu}$ and b cycles. All these integers as well as the b cycles can of course be expressed in terms of the l_{ij} on the sphere. Conversely, one can show that any choice of b cycles and of integers can be attained by a suitable choice of constants l_{ij} on the sphere. If we specify the lattice L of allowed zero modes, we can compute the sum over $r_1,\ldots,r_g \in L$, which leads to a theta function. What we have found is Proposition 14.

Proposition 14: $V_{N;g}$ is independent of the particular sewing used to obtain it. Therefore, the given construction of the g-loop vertex is consistent with axiom (iv). Indeed, the expression we get for $V_{N;g}$ depends on the Riemann surface Σ_g only through the coordinates t_i as well as a homology basis (a,b) and a set of integers.

IX. THE NONZERO MODE PROBLEM

In this section, we prove the analogous of Theorem 13 in the case of fixed zero modes. This provides a first step (the most important one) towards a proof of Segal's axioms. We start with a technical proposition

Proposition 15: Let a^* and a satisfy the commutation relation $[a,a^*]=1$. We have the following equalities:

$$\text{(a)}\quad e^{\mu a} r^{a^* a} = r^{a^* a} e^{\mu r a},$$
$$\text{(b)}\quad e^{\lambda a^*} r^{a^* a} = r^{a^* a} e^{(\lambda/r) a^*},$$
$$\text{(c)}\quad e^{\mu \sum_{n=1}^{\infty} \gamma^n a_n} r^{L_0} = r^{L_0} e^{\mu \sum_{n=1}^{\infty} \gamma^n r^n a_n},$$
$$\text{(d)}\quad e^{\lambda \sum_{n=1}^{\infty} \gamma^n a_{-n}} r^{L_0} = r^{L_0} e^{\lambda \sum_{n=1}^{\infty} \gamma^n r^{-n} a_{-n}}.$$

Proof: The core of the proposition is (a). (b), (c) and (d) are easy consequences thereof. We first observe that

$$\frac{d}{d\kappa}\, e^{-\kappa a^* a}\, a\; e^{\kappa a^* a} = e^{-\kappa a^* a}[a, a^* a] e^{\kappa a^* a} = e^{-\kappa a^* a}\, a\; e^{\kappa a^* a}.$$

Since $e^{-\kappa a^* a}\, a\; e^{\kappa a^* a}\big|_{\kappa=0} = a$, the solution of this differential equation is

$$e^{-\kappa a^* a}\, a\; e^{\kappa a^* a} = e^{\kappa} a.$$

Taking the nth power of this equation we get

$$e^{-\kappa a^* a} a^n\; e^{\kappa a^* a} = (e^{\kappa} a)^n.$$

Summing over all n with suitable coefficients leads to

$$e^{-\kappa a^* a}\; e^{\mu a}\; e^{\kappa a^* a} = e^{e^{\kappa} a \mu}.$$

If we set $e^{\kappa} = r$ we get (a). We prove (b) in exactly the same way, the only difference being the commutator $[a^*, a^* a] = -a^*$. (c) and (d) are infinite products of (a) and (b), respectively. ■

We now come to the main result. Let us consider $V_{N;0}$ as an operator from $\otimes\, \pi_{\beta_i}$ to $\mathbb{C}$ for fixed zero modes $\beta_1,\ldots,\beta_N$. We have Theorem 16.

Theorem 16: *Let D_r denote the closed disk of radius r centered around the origin. Then $V_{N;0}$ can be extended to $H^{\beta_1}_{r_1} \otimes \cdots \otimes H^{\beta_N}_{r_N}$ if the numbers r_i satisfy the following geometric condition:*

$$t_i(D_{r_i}) \cap t_j(D_{r_j}) = \varnothing, \quad i \neq j$$

Moreover, the extended map

$$V_{N;0} : H^{\beta_1}_{r_1} \otimes \cdots \otimes H^{\beta_N}_{r_N} \to \mathbb{C}$$

is trace class (meaning that $(V^*_{N;0} V_{N;0})^{1/2}$ is trace class).

Proof: We proceed in three steps. We first show that we can neglect all the contributions coming from the zero modes. Then, we show that the non zero mode core of $V_{N;0}$ is Hilbert–Schmidt and therefore bounded on $H_{r_i} \otimes \cdots \otimes H_{r_N}$. Finally, we use a deformation argument to show that $V_{N;0}$ is trace class.

We can forget the purely zero mode contributions in $V_{N;0}$ because they yield an overall constant factor. We next show that we can neglect the contributions coming from the coupling of the zero modes to the oscillators. More precisely, we claim that the map

$$\exp\left(-\sum_{n=1}^{\infty}\alpha_n^{(i)}D_{n0}(s_it_j)\alpha_0^{(j)}\right):H_r^{(i)}\to H_{\tilde r}^{(i)}$$

is Hilbert–Schmidt, and therefore bounded, as soon as $\tilde r>r$. Using multiindex notation, we can write

$$\exp\left(\sum_{n=1}^{\infty}\frac{a_n}{\sqrt{n}}\,\omega_n^+\right)|\phi_\alpha\rangle=\sum_{\gamma\leqslant\alpha}\frac{{\omega^+}^{\alpha-\gamma}}{(\alpha-\gamma)!}\frac{\sqrt{\alpha!}}{\sqrt{\gamma!}}\,|\phi_\gamma\rangle, \tag{29}$$

where $\alpha!=\Pi\alpha_i$, ${\omega^+}^{\alpha}=\Pi{\omega_i^+}^{\alpha_i}$, and where $\gamma\leqslant\alpha$ means $\gamma_j\leqslant\alpha_j$ for all j. To simplify the notation, we drop the superscript $^{(i)}$ and set $\alpha_0^{(j)}=-\beta$. We apply the exponential to a normed basis element of H_r and use Proposition 15(c) to get

$$\begin{aligned}\exp\left(\beta\sum_{n=1}^{\infty}\alpha_nD_{n0}(s_it_j)\right)r^{L_0}|\phi_\alpha\rangle&=r^{L_0}\exp\left(\beta\sum_{n=1}^{\infty}\frac{\alpha_n}{\sqrt{n}}(s_it_j(0))^nr^n\right)|\phi_\alpha\rangle\\&\overset{(29)}{=}r^{L_0}\sum_{\gamma\leqslant\alpha}\frac{{\omega^+}^{\alpha-\gamma}}{(\alpha-\gamma)!}\frac{\sqrt{\alpha!}}{\sqrt{\gamma!}}\,|\phi_\gamma\rangle,\end{aligned}$$

where $\omega_n^+=\beta(s_it_j(0))^nr^n/\sqrt{n}$. With $\|\gamma\|=\Sigma j\gamma_j$, the square of the Hilbert–Schmidt norm of the map is (we forget the zero mode factor coming from L_0)

$$\begin{aligned}\sum_{\alpha}\sum_{\gamma\leqslant\alpha}\left(\frac{r}{\tilde r}\right)^{2\|\gamma\|}\frac{|\omega^+|^{2(\alpha-\gamma)}}{(\alpha-\gamma)!^2}\frac{\alpha!}{\gamma!}&\overset{(2)}{=}\sum_{\alpha}\left(\frac{r}{\tilde r}\right)^{2\|\alpha\|}\prod_n L_{\alpha_n}\left(-|\omega_n^+|^2\left(\frac{\tilde r}{r}\right)^{2n}\right)\\&\overset{(3)}{=}\prod_n\frac{1}{1-(r/\tilde r)^{2n}}\exp\left(\frac{|\omega_n^+|^2}{1-(r/\tilde r)^{2n}}\right).\end{aligned}$$

This is convergent if $\Sigma_n|\omega_n^+|^2$ converges, which is the case if $r<|t_i^{-1}(t_j(0))|$. This last inequality is a consequence of the geometric condition. Similarly, the map

$$\exp\left(-\sum_{n=1}^{\infty}\alpha_0^{(i)}D_{0n}(s_it_j)\alpha_n^{(j)}\right):H_r^{(j)}\to H_{\tilde r}^{(j)}$$

is Hilbert–Schmidt if $\tilde r>r$. We are now left with the oscillatory part of $V_{N;0}$ which we denote by $\tilde V_{N;0}$.

An orthonormal basis of $H_{r_1}^{\beta_1}\otimes\cdots\otimes H_{r_N}^{\beta_N}$ is given by the vectors

$$r_1^{L_0^{(1)}}\cdots r_N^{L_0^{(N)}}|\phi_{\gamma^1}\rangle\cdots|\phi_{\gamma^N}\rangle,$$

where each γ^j ranges over all possible finite multi-indices. Using proposition 15(c), we get (forgetting the zero modes of $L_0^{(i)}$)

$$\tilde{V}_{N;0} r_1^{L_0^{(1)}} \cdots r_N^{L_0^{(N)}} |\phi_{\gamma^1}\rangle \cdots |\phi_{\gamma^N}\rangle$$
$$= \langle 0| \cdots \langle 0| \exp\left(- \sum_{\substack{i,j=1 \\ i<j}}^{N} \sum_{n,m=1}^{\infty} \alpha_n^{(i)} D_{nm}(s_i t_j) r_i^n r_j^m \alpha_m^{(j)} \right) |\phi_{\gamma^1}\rangle \cdots |\phi_{\gamma^N}\rangle. \qquad (30)$$

We now introduce a useful representation of the algebra a, a^* of the harmonic oscillator. This algebra can be realized on the space of polynomials in ψ as follows:

$$a f(\psi) = \frac{\partial}{\partial \psi} f(\psi), \quad a^* f(\psi) = \psi f(\psi).$$

Obviously, we have $[a, a^*] = 1$. The vacuum is represented by the function $f(\psi) = 1$ and more generally $|k\rangle = (a^*)^k / \sqrt{k!} |0\rangle$ is represented by the function $\psi^k / \sqrt{k!}$. The scalar product is represented by

$$\langle f, g \rangle = \overline{f}\left(\frac{\overline{\partial}}{\partial \psi} \right) g(\psi)|_{\psi=0}$$

because it is antilinear in the first and linear in the second factor and because

$$\langle k|l\rangle = \frac{1}{\sqrt{k!}} \left(\frac{\partial}{\partial \psi} \right)^k \frac{\psi^l}{\sqrt{l!}} \bigg|_{\psi=0} = \delta_{k,l}.$$

For expression (30), we introduce a variable ψ_n^i for each oscillator $\alpha_{-n}^{(i)}$, so we have the scalar product of

$$f(\psi^1, \ldots, \psi^N) = \frac{(\psi^1)^{\gamma^1}}{\sqrt{\gamma^1!}} \cdots \frac{(\psi^N)^{\gamma^N}}{\sqrt{\gamma^N!}}$$

with

$$g(\psi^1, \ldots, \psi^N) = \exp\left(- \sum_{\substack{i,j=1 \\ i<j}}^{N} \sum_{n,m=1}^{\infty} \psi_n^i D_{nm}(s_i t_j) r_i^n r_j^m \psi_m^j \right)$$

which is nothing else than

$$\frac{1}{\sqrt{\gamma^1!}} \left(\frac{\partial}{\partial \psi^1} \right)^{\gamma^1} \cdots \frac{1}{\sqrt{\gamma^N!}} \left(\frac{\partial}{\partial \psi^N} \right)^{\gamma^N} \exp\left(- \sum_{\substack{i,j=1 \\ i<j}}^{N} \sum_{n,m=1}^{\infty} D_{nm}(s_i t_j) r_i^n r_j^m \psi_n^i \psi_m^j \right) \bigg|_{\psi=0}.$$

The square of the Hilbert–Schmidt norm is given by

$$\sum_{\gamma^1, \ldots, \gamma^N} \frac{1}{\gamma^1! \cdots \gamma^N!} \left| \left(\frac{\partial}{\partial \psi^1} \right)^{\gamma^1} \cdots \left(\frac{\partial}{\partial \psi^N} \right)^{\gamma^N} \exp\left(- \sum_{\substack{i,j=1 \\ i<j}}^{N} \sum_{n,m=1}^{\infty} D_{nm}(s_i t_j) r_i^n r_j^m \psi_n^i \psi_m^j \right) \bigg|_{\psi=0} \right|^2.$$

It is finite if

$$\sum_{\gamma^1,\ldots,\gamma^N} \frac{1}{\gamma^1!\cdots\gamma^N!} \left| \left(\frac{\partial}{\partial\psi^1}\right)^{\gamma^1} \cdots \left(\frac{\partial}{\partial\psi^N}\right)^{\gamma^N} \exp\left(-\sum_{\substack{i,j=1\\ i<j}}^{N} \sum_{n,m=1}^{\infty} D_{nm}(s_i t_j) r_i^n r_j^m \psi_n^i \psi_m^j \right) \right|_{\psi=0}$$

is. We can rewrite the sum as

$$\begin{aligned} &\prod_{\substack{i,j=1\\ i<j}}^{N} \prod_{n,m=1}^{\infty} \sum_{\beta,\gamma=0}^{\infty} \frac{1}{\beta!\,\gamma!} \left| \left(\frac{\partial}{\partial\psi}\right)^{\beta} \left(\frac{\partial}{\partial\kappa}\right)^{\gamma} \exp(-D_{nm}(s_i t_j) r_i^n r_j^m \psi\kappa) \right|_{\psi=\kappa=0} \\ &= \prod_{\substack{i,j=1\\ i<j}}^{N} \prod_{n,m=1}^{\infty} \sum_{\beta,\gamma=0}^{\infty} \frac{1}{\beta!\,\gamma!} \left(\frac{\partial}{\partial\psi}\right)^{\beta} \left(\frac{\partial}{\partial\kappa}\right)^{\gamma} \exp(|D_{nm}(s_i t_j)| r_i^n r_j^m \psi\kappa) \Big|_{\psi=\kappa=0} \\ &= \exp\left(\sum_{\substack{i,j=1\\ i<j}}^{N} \sum_{n,m=1}^{\infty} |D_{nm}(s_i t_j)| r_i^n r_j^m \right). \end{aligned}$$

It remains to show the finiteness of the sums

$$\sum_{n,m=1}^{\infty} \left| \frac{1}{m!}\, \partial^m (s_i(t_j(z)))^n \Big|_{z=0} r_i^n r_j^m \right| \tag{31}$$

for all i,j with $i<j$ (we absorbed a factor $\sqrt{m}$ by making r_j slightly bigger). For a function $\gamma(z)$ which is analytic in a neighborhood of zero, we can write

$$\frac{1}{m!}\, \partial^m \gamma(z) \Big|_{z=0} = \frac{1}{2\pi i} \oint_0 \frac{\gamma(\zeta)}{\zeta^{m+1}}\, d\zeta,$$

where we integrate over a circle of radius R around zero with R smaller than the radius of convergence of the series

$$\sum_m \frac{1}{m!}\, \partial^m \gamma(z) \Big|_{z=0} \zeta^m.$$

Doing this for the function $\gamma(z)=(s_i t_j(z))^n$ we get the estimate

$$\left| \frac{1}{m!}\, \partial^m (s_i(t_j(z)))^n \Big|_{z=0} \right| \leqslant \frac{1}{R^m} \sup_{|\zeta|=R} |(s_i(t_j(\zeta)))^n|$$

so that our double sum (31) gets smaller than

$$\sum_{n,m=1}^{\infty} \left(\sup_{|\zeta|=R} |(s_i(t_j(\zeta)))| \right)^n r_i^n \left(\frac{r_j}{R}\right)^m.$$

We must choose R smaller than the absolute value of the pole of $s_i t_j$, which means that the circle $t_j(D_R)$ must not contain $t_i(0)$. In particular we may take R to be slightly bigger than r_j but still satisfying the geometric condition $t_i(D_{r_i}) \cap t_j(D_R) = \varnothing$. Such an R ensures the convergence of the m-sum above. As to the n-sum, it converges because $r_i < \inf_{|\zeta|=R} |t_i^{-1}(t_j(\zeta))|$. Therefore,

$$V_{N;0} : H_{r_1} \otimes \cdots \otimes H_{r_N} \to \mathbb{C}$$

is bounded. Let $\tilde{r}_i > r_i (i=1,\ldots,N)$ be such that the $t_i(D_{\tilde{r}_i})$ are still pairwise disjoint. We can decompose the map $V_{N;0}: \otimes H_{r_i} \to \mathbb{C}$ according to

$$\otimes H_{r_i} \overset{Id}{\to} \otimes_i H_{\tilde{r}_i} \overset{V_{N;0}}{\longrightarrow} \mathbb{C},$$

where Id is the embedding of $\otimes H_{r_i}$ in $\otimes H_{\tilde{r}_i}$. Since Id is trace class and since the second map is bounded, the composition is trace class. ■

The next proposition shows that the result we got is the best possible.

Proposition 17: Let $\mathring{D}_r$ denote the open disk with radius r around the origin. Then the map

$$V_{N;0}: H^{\beta_1}_{r_1} \otimes \cdots \otimes H^{\beta_N}_{r_N} \to \mathbb{C}$$

gets unbounded as soon as there exists i,j, $i \neq j$ with

$$t_i(\mathring{D}_{r_i}) \cap t_j(\mathring{D}_{r_j}) \neq \varnothing.$$

In other words $V_{N;0}$ cannot be extended to all $H^{\beta_1}_{r_1} \otimes \cdots \otimes H^{\beta_N}_{r_N}$ if the disks $t_i(\mathring{D}_{r_i})$ are not disjoint.

Proof: The effect of increasing one r_i is simply multiplication of the basis vectors

$$r_1^{L_0^{(1)}} \cdots r_N^{L_0^{(N)}} |\phi_{\gamma^1}\rangle \cdots |\phi_{\gamma^N}\rangle$$

with a constant whose norm is greater than one. Since we want to show that $V_{N;0}$ applied to these basis vectors are complex numbers whose norm is unbounded in $\gamma^1,\ldots,\gamma^N$, we can suppose without loss of generality that $t_1(\mathring{D}_{r_1})$ and $t_2(\mathring{D}_{r_2})$ are the only disks that overlap. Moreover, we can suppose that $r_i = 1$ for all $i=1,\ldots,N$ because the change from 1 to r_i is nothing else than the coordinate change $t_i(z) \mapsto \tilde{t}_i(z) = t_i(r_i z)$ [since $D_{nm}(s_j t_i) r_i^n = D_{nm}(s_j \tilde{t}_i)$ and $D_{nm}(s_i t_j) r_i^n = D_{nm}(\tilde{s}_i t_j)$]. It is enough to treat the case of small overlap, by which we mean that

$$\gamma(z) := s_1 t_2(z)$$

has the property

$$|\gamma(0)| < 1.$$

We are now ready to compute

$$\begin{aligned}
&V_{N;0} |\phi_{e_n}\rangle_{\beta_1} |\phi_{e_m}\rangle_{\beta_2} |0\rangle_{\beta_3} \cdots |0\rangle_{\beta_N} \\
&\quad = \text{const}\ {}_{\beta_2}\langle 0|_{\beta_1}\langle 0| \exp(-\alpha_n^{(1)} D_{nm}(s_1 t_2) \alpha_m^{(2)}) \exp\left(-\sum_{j\neq 1} \alpha_n^{(1)} D_{n0}(s_1 t_j) \beta_j \right) \\
&\qquad \times \exp\left(-\sum_{j\neq 2} \alpha_m^{(2)} D_{m0}(s_2 t_j) \beta_j \right) |\phi_{e_n}\rangle_{\beta_1} |\phi_{e_m}\rangle_{\beta_2} \\
&\quad = \text{const} \left(-D_{nm}(s_1 t_2) + \sum_{j\neq 1} \sum_{k\neq 2} D_{n0}(s_1 t_j) D_{m0}(s_2 t_k) \beta_j \beta_k \right) \\
&\quad = \text{const} \left(-D_{nm}(\gamma) + \left(\sum_{j\neq 1} D_{n0}(s_1 t_j) \beta_j \right) \left(\sum_{k\neq 2} D_{m0}(s_2 t_k) \beta_k \right) \right),
\end{aligned}$$

where const is a nonvanishing constant independent of n and m coming from the purely zero mode contributions. We want to show that this expression is unbounded in n and m. First of all, since $|s_i t_j(0)|<1$, $\forall i\neq j$, we see that

$$D_{n0}(s_i t_j) \to 0, \quad n \to \infty$$

so it is enough to show that $D_{nm}(\gamma)$ is unbounded in n and m. Suppose it were bounded, i.e.,

$$|D_{nm}(\gamma)|\leqslant c, \quad \forall n,m$$

for some constant c. Then for all $q,\tilde{q}<1$ and all $\varphi \in \mathbb{R}$, we would have convergence of the double sum

$$\sum_{n,m=0}^{\infty} \frac{1}{m!}\, \partial^m (\gamma(z))^n \Big|_{z=0} \tilde{q}^n (q\ e^{i\varphi})^m.$$

The m-sum yields

$$\sum_{n=0}^{\infty} \gamma(q\ e^{i\varphi})^n \tilde{q}^n.$$

For a suitable choice of q and φ, we have

$$|\gamma(q\ e^{i\varphi})|>1$$

by the overlap assumption, so the n-sum cannot converge for all $\tilde{q}<1$, a contradiction. ■

X. VERIFICATION OF THE AXIOMS

We now prove the axioms. We start with the proposition:

Proposition 18: V is a ∗ functor (i.e., the third axiom is true) if and only if $Q=0$.

Proof: We first check the proposition for the sphere (for notational simplicity, we restrict ourselves to the case $\mathscr{H}^{\otimes N} \to \mathbb{C}$). It is easy to see that

$$\bar{D}_{nm}(s_i t_j) = D_{nm}(\overline{s_i t_j})$$

so that

$$\begin{aligned}
(V_{N;0})^* &= \sum_{\beta_1,\ldots,\beta_N \in L} \left(\delta_{\sum_{i=1}^N \beta_i;Q}\, {}_{\beta_1}\langle 0|\cdots{}_{\beta_N}\langle 0| \exp\left(-\sum_{\substack{i,j=1\\ i<j}}^{N} \sum_{n,m=0}^{\infty} \alpha_n^{(i)} D_{nm}(s_i t_j) \alpha_m^{(j)} \right) \right)^* \\
&= \sum_{\beta_1,\ldots,\beta_N \in L} \delta_{\sum_{i=1}^N \beta_i;Q} \exp\left(-\sum_{\substack{i,j=1\\ i<j}}^{N} \sum_{n,m=0}^{\infty} \alpha_n^{(i)*} \bar{D}_{nm}(s_i t_j) \alpha_m^{(j)*} \right) |0\rangle_{\beta_N} \cdots |0\rangle_{\beta_1} \\
&= \sum_{\beta_1,\ldots,\beta_N \in L} \delta_{\sum_{i=1}^N \beta_i;Q} \exp\left(-\sum_{\substack{i,j=1\\ i<j}}^{N} \sum_{n,m=0}^{\infty} (-\alpha_{-n}^{(i)}) D_{nm}(\overline{s_i t_j}) (-\alpha_{-m}^{(j)}) \right) |0\rangle_{\beta_N} \cdots |0\rangle_{\beta_1} \\
&= \sum_{\beta_1,\ldots,\beta_N \in L} \delta_{\sum_{i=1}^N \beta_i;Q} \exp\left(-\sum_{\substack{i,j=1\\ i<j}}^{N} \sum_{n,m=0}^{\infty} (-(\alpha_{-n}^{(i)} - Q\delta_{n;0})) D_{nm}(\overline{s_i t_j}) (-(\alpha_{-m}^{(j)}\right.
\end{aligned}$$

$$
\left. -Q\delta_{m;0})) \right) |0\rangle_{\beta_N+Q} \cdots |0\rangle_{\beta_1+Q}
$$

$$
= \sum_{\beta_1,\ldots,\beta_N \in L} \delta_{\Sigma_{i=1}^N \beta_i;(N+1)Q} \exp\left(- \sum_{\substack{i,j=1 \\ i<j}}^{N} \sum_{n,m=0}^{\infty} \alpha_n^{(i)+} D_{nm}(\overline{s_i t_j}) \alpha_m^{(j)+} \right)
$$

$$
\times |0\rangle_{\beta_N} \cdots |0\rangle_{\beta_1}
$$

which is the N-point vertex for the complex conjugate sphere with differently oriented boundary if and only if $Q=0$ (the sum of the ''in-charges'' must be equal to the sum of the ''outcharges'' $+Q$). Under the change $D_{00} \mapsto \bar{D}_{00}$, all the integers l_{ij} change sign. Because the g-loop vertex is an appropriate trace of the zero-loop vertex, the results still hold for arbitrary genus. We finally note that taking the adjoint of Eq. (28) leads to the transformation

$$
i\pi(r_\mu(2\tau_{\mu\nu}+l_{\mu\nu})r_\nu) \mapsto i\pi(r_\mu(-2\bar{\tau}_{\mu\nu}-l_{\mu\nu})r_\nu),
$$

where $-\overline{\tau_{\mu\nu}}$ corresponds to the period matrix of the complex conjugate surface with cycles $(a, -b)$ because

$$
\int_{-b_\nu} \bar{\omega}_\mu = \overline{\int_{-b_\nu} \omega_\mu} = -2\pi i \bar{\tau}_{\mu\nu}.
$$

■

It can be shown that the axiom (iii) implies Osterwalder–Schrader positivity for symmetric surfaces (the only ones where ''time reversal'' has a meaning), so a scalar massless field coupled to a background charge $Q \neq 0$ is not a good field theory in that sense. However, it is useful in the context of minimal models.[2] We next prove Theorem 13, and then extend it to Riemann surfaces.

Proof: What we actually need is the special case $r_i=1$ for all i. The second part of the theorem follows from Proposition 17. It remains to show the first part. We note that any operator

$$
A: \mathscr{H}^{\otimes N} \to \mathbb{C}
$$

$$
A: \eta \mapsto (\psi, \eta), \quad \psi \in \mathscr{H}^{\otimes N}
$$

is trace class. Indeed,

$$
A^* A \eta = (\psi, \eta)\psi
$$

is a projection (times a constant). Its square root is also a projection, and projections on finite dimensional subspaces are trace class. Therefore, all we have to prove is that

$$
\sum_{\beta_1,\ldots,\beta_N \in L} \delta_{\Sigma_{i=1}^N \beta_i;Q\beta_1} \langle 0| \cdots {}_{\beta_N}\langle 0| \exp\left(-\frac{1}{2} \sum_{\substack{i,j=1 \\ i\neq j}}^{N} \sum_{n,m=0}^{\infty} \alpha_n^{(i)} D_{nm}(s_i t_j) \alpha_m^{(j)} \right)
$$

$$
\times \sum_{\gamma_1,\ldots,\gamma_N \in L} \exp\left(-\frac{1}{2} \sum_{\substack{i,j=1 \\ i\neq j}}^{N} \sum_{n,m=0}^{\infty} \alpha_{-n}^{(i)} \bar{D}_{nm}(s_i t_j) \alpha_{-m}^{(j)} \right) |0\rangle_{\gamma_N} \cdots |0\rangle_{\gamma_1} \tag{32}
$$

is finite. Without the β- and γ-sums, we know by theorem 16 that the expression is $\delta_{\beta_1,\gamma_1} \cdots \delta_{\beta_N,\gamma_N}$ times something finite, namely the square of the Hilbert–Schmidt norm of the map $V_{N;0}$ for the fixed zero modes $\beta_1,\ldots,\beta_N$.

Let us consider the case $Q=0$ first. By the proposition we have just proven, the second line of Eq. (32) represents the complex conjugate Riemann sphere with ''out-legs''

$$\bar{t}_i(D), \quad i=1,\ldots,N.$$

It is the mirror image of the sphere with ''in-legs''

$$t_i(D), \quad i=1,\ldots,N,$$

where the mirror symmetry is given by reflection about the x axis. The expression we have is therefore what we get by sewing together a sphere with its mirror image along the boundaries of the embedded disks. We can do the sewing in two steps: first, we only identify the legs number N. This gives us a Riemann sphere with $2N-2$ legs. Therefore, the summand of Eq. (32) is the trace over the nonzero modes of

$$\begin{aligned}
&{}_{\beta_1}\langle 0|\cdots{}_{\beta_{N-1}}\langle 0|\exp\Bigg(-\frac{1}{2}\sum_{\mu,\nu=1}^{N-1}\sum_{n,m=0}^{\infty}\alpha_n^{(2\mu-1)}D_{nm}(\tilde{s}_{2\mu-1}\tilde{t}_{2\nu-1})\alpha_m^{(2\nu-1)}\\
&\quad+\alpha_n^{+(2\mu)}D_{nm}(\tilde{s}_{2\mu}\tilde{t}_{2\nu})\alpha_m^{+(2\nu)}\Bigg)\\
&\quad\times\exp\Bigg(-\sum_{\mu,\nu=1}^{N-1}\sum_{n,m=0}^{\infty}\alpha_n^{+(2\mu)}D_{nm}(\tilde{s}_{2\mu}\tilde{t}_{2\nu-1})\alpha_m^{(2\nu-1)}\Bigg)|0\rangle_{\beta_{N-1}}\cdots|0\rangle_{\beta_1}
\end{aligned}\tag{33}$$

[see Eq. (24)], the new sum being over $\beta_1,\ldots,\beta_{N-1}\in L$. Here, $\alpha_n^{(2\mu-1)}$ acts on a vacuum to the left while $\alpha_n^{(2\mu)}$ acts on a vacuum to the right. By Eq. (22), the new coordinates are

$$\tilde{t}_{2\mu-1}=t_\mu, \quad \tilde{s}_{2\mu-1}=s_\mu,$$

$$\tilde{t}_{2\mu}=\bar{t}_N\Gamma t_N^{-1}t_\mu, \quad \tilde{s}_{2\mu}=s_\mu t_N\Gamma\bar{t}_N^{-1}.$$

The trace is to be understood as an identification of even and odd legs. Its calculation is a special case of what we have already done, namely the case where all the legs are sewn. We can read off the result (28), which means that Eq. (32) can be written as

$$\sum_{\beta_1,\ldots,\beta_{N-1}\in L}\det(1-H)^{-(1/2)}\exp\Bigg(\frac{1}{2}\sum_{\mu,\nu=1}^{N-1}\beta_\mu C_{\mu\nu}^{(1)}\beta_\nu+\sum_{\mu=1}^{N-1}\beta_\mu C_\mu^{(2)}+C^{(3)}\Bigg).$$

Since $C_{\mu\nu}^{(1)}=2\pi i\tau_{\mu\nu}$ modulo πi, and since period matrices have positive definite imaginary part,[15] the β-sum is finite. Let us now turn to the more complicated case $Q\neq 0$. The second exponential of Eq. (32) still represents the complex conjugate surface if we add an exponential which takes into account that $\alpha_0^+=Q-\alpha_0$. Instead of Eq. (33), we then find

$$\begin{aligned}
&{}_{\beta_1}\langle 0|\cdots{}_{\beta_{N-1}}\langle 0|\exp\Bigg(-\frac{1}{2}\sum_{\substack{\mu,\nu=1\\ \mu\neq\nu}}^{N-1}\sum_{n,m=0}^{\infty}(\alpha_n^{(2\mu-1)}D_{nm}(\tilde{s}_{2\mu-1}\tilde{t}_{2\nu-1})\alpha_m^{(2\nu-1)}\\
&\quad+\alpha_n^{+(2\mu)}D_{nm}(\tilde{s}_{2\mu}\tilde{t}_{2\nu})\alpha_m^{+(2\nu)})\Bigg)\exp\Bigg(-Q\sum_{m\geqslant 0}\Bigg(\sum_{\mu=1}^{N-1}D_{0m}(s_Nt_\mu)\alpha_m^{(2\mu-1)}+D_{0m}(\overline{s_Nt_\mu})(Q\\
&\quad-\alpha_m^{+(2\mu)})\Bigg)\Bigg)\exp\Bigg(-\sum_{\mu,\nu=1}^{N-1}\sum_{n,m=0}^{\infty}\alpha_n^{+(2\mu)}D_{nm}(\tilde{s}_{2\mu}\tilde{t}_{2\nu-1})\alpha_m^{(2\nu-1)}\Bigg)|0\rangle_{\beta_{N-1}}\cdots|0\rangle_{\beta_1}.
\end{aligned}$$

We can forget the exponential with the factor Q^2, because it has no influence on the convergence of the β sums. The two new exponentials with a factor Q have the effect of translating the factors B_1 and B_2 in the trace calculation by an amount independent of the zero modes, and of increasing the factor A by an amount linear in the zero modes. The contribution of Eq. (26) to $C^{(1)}_{\mu\nu}$ is therefore unchanged, and the sum over $\beta_1,...,\beta_{N-1}$ still converges. ■

Now axiom (ii) is true for the Riemann surfaces we have constructed because $V_{N;g}$ is a partial trace of the trace class operator $V_{N+2g;0}$, and partial traces are trace class. Finally, we have constructed $V_{N;g}$ so that axiom (iv) holds. More precisely, we have found that $V_{N;g}$ depends only on a canonical homology basis (a,b) and on local projective coordinates t_i associated to the Riemann surface, and is thus independent of the particular sewing used to obtain it. Identifying boundary circles on Σ_g is the same as initially identifying more pairs of circles on the sphere. Therefore, property (iv) holds and we have proved that V is a modular functor from a category of Riemann surfaces to a category of trace class operators over a Hilbert space.

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Integrable systems of group SO(1,2) and Green's functions

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Integrable quantum systems related with two-dimensional two- and one-sheeted hyperboloid are considered. The explicit expressions of the Green's functions of the free particles on the those homogenous spaces are given. © *1996 American Institute of Physics.* [S0022-2488(95)03012-1]

I. INTRODUCTION

There exists a number of exact results about the complete systems of quantum commuting observables (quantum integrals of motion) wave functions, spectra, and so on. The review[1] presents, from a general point of view, the results obtained in these subject. The dynamics of some of these systems is closely related to free motion in the symmetric space (SS). It is known that (SS) can be realized as a set of cossets K/G of connected Lie group G on its compact subgroup K. For example, the two-sheeted hyperboloid SO(2)/SO(1,2): $[x,x]=x_0^2-x_1^2-x_2^2$, $x_0>0$, constitutes the (SS) space $K=\mathrm{SO}(2)$ keeping the point $x=(1,0,0)$ fixed. The distance r between the fixed point $x=(1,0,0)$ and an arbitrary point $x=(x_0,x_1,x_2)$ on this (SS) defined by formula $\cosh Kr=[x,\ x]=x_0>1$ is real. However, in the case of one-sheeted hyperboloid $[x,\ x]=x_0^2-x_1^2-x_2^2=-1$, stationary subgroup of fixed point $x=(0,0,1)$ is a noncompact group SO(1,1) and the distance $r=\cosh Kr=|[x,x]|=|x_2|>0$ is piecewise defined, real when $\cosh Kr>1$ and imaginary when $\cosh Kr<1$.

This is the reason why the quantum systems related to (SS) K/G have only continuous spectra of scattering states, and the quantum systems related to homogeneous spaces H/G with noncompact stationary subgroup have continuous and discrete spectra.

This report carries on the research reviewed in Ref. 2. The key point of the relation between the theory of homogeneous spaces and quantum systems is the existence of a simple transformation of Laplace–Beltrami operators on homogeneous spaces to some Hamiltonious quantum systems.

We consider different coordinate systems on hyperboloids which reduce to three different quantum systems.

The paper is organized as follows: an introduction and three sections and two appendices. Sections I and II are devoted to quantum systems related to two- and one-sheeted hyperboloids correspondingly. The review of the results concerning the two-sheeted hyperboloid is introduced for complement and also for comparison with the case of the one-sheeted hyperboloid. In Sec. III the explicit expressions of the Green's function of the free particle on two- and one-sheeted hyperboloids are calculated. The Appendices are devoted to the basic facts of the representation theory of the group SO(1,2).

II. THE QUANTUM SYSTEMS RELATED TO TWO-SHEETED HYPERBOLOID

Consider the problem, inside the cone in the three-dimensional space, on three different coordinate systems.

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A. Spherical polar coordinates

The spherical polar coordinates are given by

$$x_0 = r \cosh \alpha,$$
$$x_1 = r \sin \alpha \sin \varphi, \tag{2.1}$$
$$x_2 = r \sin \alpha \cos \varphi,$$

where $\alpha \in [0,\infty)$ and $\varphi \in [0, 2\pi]$.

By (2.1) we have

$$(g_{ab}) = \text{diag}\,(1, -r^2, -r^2 \sinh^2 \alpha), \tag{2.2}$$

$$\sqrt{g} = (\det\,(g_{ab}))^{1/2} = r^2 \sinh \alpha. \tag{2.3}$$

The component of the Laplace–Beltrami operator

$$\Delta_{\mathrm{LB}} = \frac{-1}{\sqrt{g}}\, \partial_a g^{ab} \sqrt{g} \partial_b, \quad a,b = 1,2,3,\ldots, \tag{2.4}$$

on the hyperboloid $[x, x] = 1$ is in the following form:

$$\Delta_{\alpha,\varphi} = \frac{1}{\sinh \alpha} \frac{\partial}{\partial \alpha} \left(\sinh \alpha \frac{\partial}{\partial \alpha} \right) + \frac{1}{\sinh^2 \alpha} \frac{\partial^2}{\partial \varphi^2}. \tag{2.5}$$

The radial part of the Laplace equation,

$$\Delta_{\alpha,\varphi} \Phi(\alpha,\varphi) = \sigma(\sigma+1)\Phi(\alpha,\varphi), \tag{2.6}$$

where

$$\Phi(\alpha,\varphi) = \vartheta(\alpha) e^{in\varphi}, \tag{2.7}$$

has the form

$$\left[\frac{\partial^2}{\partial \alpha^2} + \frac{\cosh \alpha}{\sinh \alpha} \frac{\partial}{\partial \alpha} - \frac{n}{\sinh^2 \alpha} \right] \vartheta(\alpha) = \sigma(\sigma+1)\, \vartheta(\alpha) \tag{2.8}$$

using

$$dx = \sqrt{g} d\alpha\, d\varphi = \sinh \alpha d\alpha\, d\varphi, \tag{2.9}$$

and making the transformation

$$\vartheta(\alpha) = (\sinh \alpha)^{-1/2} \Psi(\alpha) \tag{2.10}$$

Eq. (2.8) becomes

$$\frac{\partial^2 \Psi(\alpha)}{\partial \alpha^2} + \left[-\frac{1}{4} - \sigma(\sigma+1) - \frac{n^2 - (1/4)}{\sinh^2 \alpha} \right] \Psi(\alpha) = 0. \tag{2.11}$$

Equivalently, defining

$$E=-\tfrac{1}{2}-\sigma(\sigma+1),\quad \sigma=-\tfrac{1}{2}+i\sqrt{E},\quad E>0, \tag{2.12}$$

$$V(\alpha)=\frac{n^2-(1/4)}{\sinh^2\alpha}, \tag{2.13}$$

Eq. (2.8) becomes the Schrödinger equation

$$\frac{\partial^2\Psi(\alpha)}{\partial\alpha^2}+[E-V(\alpha)]\Psi(\alpha)=0. \tag{2.14}$$

By considering the sign of the potential function (2.13) it is seen that only scattering takes place and that E takes positive values only. In Eq. (2.8) if the transformation

$$\vartheta(\alpha)=\left(\cosh\frac{\alpha}{2}\right)^{-n}\left(\sinh\frac{\alpha}{2}\right)^{n}W(\alpha) \tag{2.15}$$

is applied, the following equation is reached:

$$\left[\frac{d^2}{d\alpha^2}+\frac{2n+\cosh\alpha}{\sinh\alpha}\frac{d}{d\alpha}\right]W(\alpha)=\sigma(\sigma+1)W(\alpha). \tag{2.16}$$

In this equation, applying change of the variable

$$z=-\sinh^2\alpha/2, \tag{2.17}$$

the hyper-geometric equation

$$z(z-1)\frac{d^2W(z)}{dz^2}+[(n+1)-2z]\frac{dW(z)}{dz}-[-\sigma(\sigma+1)]W(z)=0 \tag{2.18}$$

is obtained. One solution of Eq. (2.18) is

$$W_1=F\left(\frac{1}{2}+i\sqrt{E},\ \frac{1}{2}-i\sqrt{E},\ n+1;-\sinh^2\frac{\alpha}{2}\right). \tag{2.19}$$

By (2.10) and (2.15) the regular solution of the Schrödinger equation at $\alpha=0$ is given by

$$\Psi(\alpha,\rho)=\frac{\Gamma(\frac{1}{2}+n+i\rho)}{\Gamma(\frac{1}{2}+i\rho)\Gamma(n+1)}\left(\sinh\frac{\alpha}{2}\right)^{1/2+n}\left(\cosh\frac{\alpha}{2}\right)^{1/2-n}$$
$$\times F\left(\frac{1}{2}+i\rho,\ \frac{1}{2}-i\rho,n+1;-\sinh^2\frac{\alpha}{2}\right), \tag{2.20}$$

where $\sqrt{E}=\rho$. On the other hand, using the relation (Ref. 3, p. 1043),

$$F(a,b,c;z)=\frac{\Gamma(c)\Gamma(b-a)}{\Gamma(b)\Gamma(c-a)}(-z)^{-a}F\left(a,a-c+1,b-a+1;\frac{1}{z}\right)$$
$$+\frac{\Gamma(c)\Gamma(a-b)}{\Gamma(a)\Gamma(c-a)}(-z)^{-b}F\left(b,b-c+1,b-a+1;\frac{1}{z}\right), \tag{2.21}$$

we find the asymptotic expression of (2.20) as

$$\Psi(\alpha,\rho)\underset{\alpha\to\infty}{\cong}A(\rho,n)e^{-i\rho\alpha}+\overline{A(\rho,n)}e^{i\rho\alpha}, \tag{2.22}$$

where

$$A(\rho,n)=\frac{\Gamma(n+1)\Gamma(-2i\rho)}{\Gamma(\frac{1}{2}-i\rho)\Gamma(\frac{1}{2}-i\rho+n)}. \tag{2.23}$$

From (2.22) it follows that the normalizing factor is chosen to satisfy the condition

$$\int_{-\infty}^{\infty}\Psi(\alpha,\rho)\overline{\Psi(\alpha,\rho')}d\alpha=\frac{1}{\rho\ \tanh\ \pi\rho}\ \delta(\rho-\rho'). \tag{2.24}$$

The S-matrix is found to be given by

$$S=\frac{A}{\bar{A}}=\frac{\Gamma(-2i\rho)\Gamma(\frac{1}{2}+i\rho)\Gamma(\frac{1}{2}+i\rho+n)}{\Gamma(2i\rho)\Gamma(\frac{1}{2}-i\rho)\Gamma(\frac{1}{2}-i\rho+n)}. \tag{2.25}$$

B. Hyperbolic coordinates

The hyperbolic coordinates are given as

$$\begin{gathered}x_0=r\ \cosh\ \gamma\ \cosh\ \beta,\\ x_1=r\ \cosh\ \gamma\ \sinh\ \beta,\\ x_2=r\ \sinh\ \gamma,\\ \gamma\in(-\infty,\infty),\quad \beta\in(-\infty,\infty).\end{gathered} \tag{2.26}$$

By (2.26), we have

$$(g_{ab})=\ \mathrm{diag}\ (1,-r^2,-r^2\ \cosh^{\,2}\ \gamma), \tag{2.27}$$

$$\sqrt{g}=(\det\ (g_{ab}))^{1/2}=r^2\ \cosh\ \gamma. \tag{2.28}$$

The component of the Laplace–Beltrami operator (2.4) on the hyperboloid $[x,\ x]=1$ is

$$\Delta_{\gamma,\beta}=\frac{1}{\cosh\ \gamma}\frac{\partial}{\partial\gamma}\left(\cosh\ \gamma\ \frac{\partial}{\partial\gamma}\right)+\frac{1}{\cosh^{\,2}\ \gamma}\frac{\partial^2}{\partial\beta^2}. \tag{2.29}$$

On the other hand, the equation

$$\Delta_{\gamma,\beta}\Phi(\gamma,\beta)=\sigma(\sigma+1)\Phi(\gamma,\beta) \tag{2.30}$$

is given by

$$\left(\frac{\partial^2}{\partial\gamma^2}+\frac{\sinh\ \gamma}{\cosh\ \gamma}\frac{\partial}{\partial\gamma}-\frac{\nu^2}{\cosh^{\,2}\ \gamma}\right)\vartheta(\gamma)=\sigma(\sigma+1)\,\vartheta(\gamma), \tag{2.31}$$

where

$$\Phi(\gamma,\beta)=\vartheta(\gamma)e^{i\nu\beta}. \tag{2.32}$$

Utilizing

$$dx=\sqrt{g}\ d\gamma d\beta=\ \cosh\ \gamma\ d\gamma d\beta \tag{2.33}$$

and making the transformation

$$\vartheta(\gamma)=(\cosh\ \gamma)^{-1/2}\psi(\gamma), \tag{2.34}$$

Eq. (2.31) reduces to

$$\frac{d^2\psi(\gamma)}{d\gamma^2}+\left[-\frac{1}{4}-\sigma(\sigma+1)-\frac{\nu^2+(1/4)}{\cosh^{\,2}\gamma}\right]\psi(\gamma)=0 \tag{2.35}$$

or, to the Schrödingers equation (2.14) with

$$E=-\tfrac{1}{4}-\sigma(\sigma+1),\quad \sigma=-\tfrac{1}{2}-i\sqrt{E}, \tag{2.36}$$

$$V(\gamma)=\frac{\nu^2+(1/4)}{\cosh^{\,2}\gamma}. \tag{2.37}$$

Applying the transformation

$$\vartheta(\gamma)=(\cosh\ \gamma)^{\sigma}w(\gamma) \tag{2.38}$$

in Eq. (2.31), we obtain

$$\frac{d^2w(\gamma)}{d\gamma^2}+(2\sigma+1)\ \tanh\ \gamma\ \frac{dw(\gamma)}{d\gamma}-\frac{\gamma^2+\sigma^2}{\cosh^{\,2}\gamma}\,w(\gamma)=0. \tag{2.39}$$

In Eq. (2.39), applying the change of variable

$$z=\ \tanh^{\,2}\gamma \tag{2.40}$$

we arrive at the hyper-geometric equation

$$z(1-z)\ \frac{d^2w(z)}{dz^2}+\left[\frac{1}{2}-(1-\sigma)z\right]\frac{dw(z)}{dz}-\frac{1}{4}\,(\nu^2+\sigma^2)w(z)=0. \tag{2.41}$$

A solution to this equation is

$$W_1=F\left(\frac{1}{4}-\frac{i\sqrt{E}}{2}-\frac{i\nu}{2},\ \frac{1}{4}-\frac{i\sqrt{E}}{2}+\frac{i\nu}{2};\ \frac{1}{2};\ \tanh^{\,2}\gamma\right). \tag{2.42}$$

The regular solution of the Schrödinger equation at $\alpha=0$ with $\sqrt{E}=\rho$ satisfying the condition

$$\int_{-\infty}^{\infty}\psi(\gamma,\rho)\overline{\psi(\gamma,\rho')}d\gamma=\frac{1}{\rho\ \tanh\ \rho\pi}\ \delta(\rho-\rho') \tag{2.43}$$

is found to be

$$\psi(\gamma,\rho)=\left(\frac{\cosh\ \pi\rho}{4\pi^3}\right)^{1/2}\Gamma\left(\frac{1}{4}+\frac{i\rho}{2}+\frac{i\nu}{2}\right)\Gamma\left(\frac{1}{4}+\frac{i\rho}{2}+\frac{i\nu}{2}\right)(\cosh\ \gamma)^{i\rho}$$
$$\times F\left(\frac{1}{4}-\frac{i\rho}{2}-\frac{i\nu}{2},\frac{1}{4}-\frac{i\rho}{2}+\frac{i\nu}{2};\frac{1}{2};\tanh^2\gamma\right). \tag{2.44}$$

On the other hand, considering

$$F(a,b,c;z)=\frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}(z)^{-a}F\left(a,a-c+1,a+b-c+1;1-\frac{1}{z}\right)+\frac{\Gamma(c)\Gamma(a+b-c)}{\Gamma(a)\Gamma(b)}$$
$$\times(1-z)^{c-a-b}(z)^{a-c}F\left(c-a,1-a,c-a-b+1;1-\frac{1}{z}\right),$$
$$|\arg z|<\pi,\quad |\arg(1-z)|<\pi,\quad c-a-b\neq m,\quad m=0,\pm1,\pm2,\ldots, \tag{2.45}$$

the asymptotic expression for (2.44) is

$$\psi(\gamma,\rho)=A(\rho,\nu)e^{-i\rho\gamma}+\overline{A(\rho,\nu)}e^{i\rho\gamma}, \tag{2.46}$$

where

$$A(\rho,\nu)=\frac{\Gamma(\frac{1}{2})\Gamma(-i\rho)}{\Gamma\left(\frac{1}{4}-\frac{i\rho}{2}-\frac{i\nu}{2}\right)\Gamma\left(\frac{1}{4}-\frac{i\rho}{2}+\frac{i\nu}{2}\right)}2^{i\rho}. \tag{2.47}$$

The S-matrix is

$$S=\frac{A}{\bar{A}}=\frac{\Gamma(i\rho)\Gamma\left(\frac{1}{4}-\frac{i\rho}{2}-\frac{i\nu}{2}\right)\Gamma\left(\frac{1}{4}-\frac{i\rho}{2}+\frac{i\nu}{2}\right)}{\Gamma(-i\rho)\Gamma\left(\frac{1}{4}+\frac{i\rho}{2}+\frac{i\nu}{2}\right)\Gamma\left(\frac{1}{4}+\frac{i\rho}{2}-\frac{i\nu}{2}\right)}. \tag{2.48}$$

C. Parabolic coordinates

The parabolic coordinates are given by

$$x_0=r[\cosh\ \tfrac{1}{2}t+\tfrac{1}{2}e^{(1/2)t}q^2],\quad x_1=r[\sinh\ \tfrac{1}{2}t+\tfrac{1}{2}e^{(1/2)t}q^2],$$
$$x_2=re^{(1/2)t}q,\quad t\in(-\infty,\infty),\ \ q\in(-\infty,\infty). \tag{2.49}$$

From (2.49), we have

$$(g_{ab})=\ \text{diag}\ (1,-\tfrac{1}{4}r^2,-r^2e^t), \tag{2.50}$$

$$\sqrt{g}=(\det\ (g_{ab}))^{1/2}=\tfrac{1}{2}r^2e^{(1/2)t}. \tag{2.51}$$

The component of the Laplace–Beltrami operator on parabola $[x,\ x]=1$ is given as

$$\Delta_{t,q}=4\frac{\partial^2}{\partial t^2}+2\frac{\partial}{\partial t}+\frac{1}{e^t}\frac{\partial^2}{\partial q^2}. \tag{2.52}$$

On the other hand, the equation

$$\Delta_{t,q}\Phi(t,q)=\sigma(\sigma+1)\Phi(t,q), \tag{2.53}$$

where

$$\Phi(t,q)=\vartheta(t)e^{i\nu q} \tag{2.54}$$

is equivalent to

$$\left[4\,\frac{\partial^2}{\partial t^2}+2\,\frac{\partial}{\partial t}-\frac{\nu^2}{e^t}\right]\vartheta(t)=\sigma(\sigma+1)\,\vartheta(t). \tag{2.55}$$

Making use of

$$dx=\sqrt{g}dtdq=\tfrac{1}{2}e^{(1/2)t}\,dtdq \tag{2.56}$$

and applying the transformation

$$\vartheta(t)=e^{-(1/4)t}\psi(t), \tag{2.57}$$

Eq. (2.55) becomes

$$\frac{d^2\psi(t)}{dt^2}+\left[-\frac{1}{16}-\frac{1}{4}\,\sigma(\sigma+1)-\frac{(1/4)\,\nu^2}{e^t}\right]\psi(t)=0, \tag{2.58}$$

which reduces to the Schrödinger equation where

$$E=-\tfrac{1}{16}-\tfrac{1}{4}\sigma(\sigma+1), \tag{2.59}$$

$$V(t)=\frac{(1/4)\,\nu^2}{e^t}. \tag{2.60}$$

Applying the change of variables

$$z=e^{-(1/2)t} \tag{2.61}$$

in Eq. (2.58), we arrive at the equation

$$z^2\,\frac{d^2\psi(z)}{dz^2}+z\,\frac{d\psi(z)}{dz}-[\,\nu^2z^2+(i\rho)^2]\psi(z)=0. \tag{2.62}$$

Equation (2.62) is reduced to

$$z^2\,\frac{d^2\psi(z)}{dz^2}+z\,\frac{d\psi(z)}{dz}-[z^2+(i\rho)^2]\psi(z)=0, \tag{2.63}$$

the modified Bessel equation. Inserting $z'=vz$ the solution satisfying the condition

$$\int_{-\infty}^{\infty}\psi(t,\rho)\overline{\psi(t,\rho')}dt=\frac{1}{\rho\,\tanh\,\pi\rho}\,\delta(\rho-\rho') \tag{2.64}$$

is found to be

$$\psi(t,\rho)=\left(\frac{2\ \cosh\ \pi\rho}{\pi}\right)^{1/2}K_{i\rho}(\nu e^{-(1/2)t}). \tag{2.65}$$

On the other hand, considering the asymptotic expression of $K_\mu(z)$ at $z\to\infty$, we have $\psi\to 0$ for $t\to-\infty$. The expression for ψ as $t\to\infty$ can be found by regarding

$$K_\mu=\frac{\pi}{2\ \sinh\ \pi\mu}\left[I_{-\mu}(z)-I_\mu(z)\right] \tag{2.66}$$

and

$$I_\mu(z)=\frac{(z/2)^\mu e^{-z}}{\Gamma(\mu+1)}F_1(\mu+\tfrac{1}{2};2\mu+1;2z), \tag{2.67}$$

we have

$$\psi(t,\rho)\underset{t\to\infty}{\cong}A(\rho,\nu)e^{-(1/2)i\rho t}+\overline{A(\rho,\nu)}e^{(1/2)i\rho t}. \tag{2.68}$$

Here

$$A(\rho,\nu)=\left(\frac{2\ \cosh\ \pi\rho}{\pi}\right)^{1/2}\frac{-\pi(\nu/2)^{i\rho}}{2i\ \sinh\ \pi\rho\Gamma(1+i\rho)} \tag{2.69}$$

and the S-matrix is given by

$$S=\frac{A}{\bar{A}}=\left(\frac{\nu}{2}\right)^{2i\rho}\frac{\Gamma(1-i\rho)}{\Gamma(1+i\rho)}. \tag{2.70}$$

The quantum system related to the two-sheeted hyperboloid was also considered in Refs. 4 and 5.

III. THE QUANTUM SYSTEMS RELATED TO ONE-SHEETED HYPERBOLOID

Consider the problem outside the cone ($[x,\ x]<0$) in three-dimensional space on three different coordinate systems.

A. Spherical polar coordinates

The spherical polar coordinates are given by

$$x_0=r\ \sinh\ \alpha,\quad x_1=r\ \cosh\ \alpha\ \sin\ \varphi,$$

$$x_2=r\ \cosh\ \alpha\ \cos\ \varphi,\quad r>0,\quad \alpha\in(-\infty,\infty),\quad \varphi\in[0,2\pi]. \tag{3.1}$$

By (3.1) we have

$$(g_{ab})=\ \text{diag}\ (-1,r^2,-r^2\ \cosh^{\,2}\ \alpha), \tag{3.2}$$

$$\sqrt{g}=(\det(g_{ab}))^{1/2}=r^2\ \cosh\ \alpha. \tag{3.3}$$

The component of the Laplace–Beltrami operator on the hyperboloid $[x,\ x]=-1$, is

$$\Delta_{\alpha,\varphi}=\frac{\partial^2}{\partial\alpha^2}+\tanh\ \alpha\ \frac{\partial}{\partial\alpha}-\frac{1}{\cosh^{\,2}\ \alpha}\ \frac{\partial^2}{\partial\varphi^2}. \tag{3.4}$$

On the other hand, the equation

$$\Delta_{\alpha,\varphi}\Phi(\alpha,\varphi)=\sigma(\sigma+1)\Phi(\alpha,\varphi), \tag{3.5}$$

where

$$\Phi(\alpha,\varphi)=\vartheta(\alpha)e^{in\varphi}, \tag{3.6}$$

becomes

$$\left[\frac{\partial^2}{\partial\alpha^2}+\tanh\,\alpha\,\frac{\partial}{\partial\alpha}+\frac{n^2}{\cosh^2\alpha}\right]\vartheta(\alpha)=\sigma(\sigma+1)\,\vartheta(\alpha). \tag{3.7}$$

Using

$$dx=\cosh\,\alpha\;d\alpha\;d\varphi \tag{3.8}$$

and applying the transformation

$$\vartheta(\alpha)=(\cosh\,\alpha)^{-1/2}\psi(\alpha), \tag{3.9}$$

Eq. (3.7) takes the form

$$\frac{\partial^2\psi(\alpha)}{\partial\alpha^2}+\left[-\frac{1}{4}-\sigma(\sigma+1)+\frac{n^2-(1/4)}{\cosh^2\alpha}\right]\psi(\alpha)=0, \tag{3.10}$$

or inserting

$$E=-\tfrac{1}{4}-\sigma(\sigma+1),\quad \sigma=-\tfrac{1}{2}+i\sqrt{E}, \tag{3.11}$$

$$V(\alpha)=-\frac{n^2-(1/4)}{\cosh^2\alpha}, \tag{3.12}$$

reduces the equation to the Schrödinger equation. As can be seen from (3.12), E takes positive and negative values. Let us seek solutions for positive values of E first. Making the transformation

$$\vartheta(\alpha)=(\cosh\,\alpha)^{\sigma}w(\alpha) \tag{3.13}$$

in Eq. (3.7), we arrive at the equation

$$\frac{d^2w(\alpha)}{d\alpha^2}+(2\sigma+1)\,\tanh\,\alpha\,\frac{dw(\alpha)}{d\alpha}+\frac{n^2-\sigma^2}{\cosh^2\alpha}\,w(\alpha)=0. \tag{3.14}$$

Changing to variable $z=\tanh^2\alpha$ in Eq. (3.14), we obtain the equation

$$z(z-1)\,\frac{d^2w(z)}{dz^2}+\left[\frac{1}{2}-(1-\sigma)z\right]\frac{dw(z)}{dz}-\frac{1}{4}\,(\sigma^2-n^2)]w(z)=0. \tag{3.15}$$

The solutions of this equation are given by

$$w_1=F\left(\frac{1}{4}-\frac{i\sqrt{E}}{2}-\frac{n}{2},\,\frac{1}{4}-\frac{i\sqrt{E}}{2}+\frac{n}{2};\,\frac{1}{2};z\right), \tag{3.16}$$

$$w_2 = z^{(1/2)} F\left(\frac{3}{4} - \frac{i\sqrt{E}}{2} - \frac{n}{2}, \frac{3}{4} - \frac{i\sqrt{E}}{2} + \frac{n}{2}; \frac{3}{2}; z\right). \tag{3.17}$$

The function $\Phi(x)$ on the hyperboloid $[x, x] = -1$ with respect to reflection $Rx = -x$ has even and odd components. We consider only the even components.

The regular solution of the Schrödinger equation at $\alpha = 0$ with $\sqrt{E} = \rho$, satisfying the condition

$$\int_{-\infty}^{\infty} \Psi(\alpha, \rho)\overline{\Psi(\alpha, \rho')} d\alpha = \frac{1}{\rho \tanh \pi\rho}\, \delta(\rho - \rho'),$$

are found to be

$$\psi_1(\alpha, \rho) = \frac{1}{\sqrt{2}} \frac{\Gamma\left(\frac{1}{4} + \frac{i\rho}{2} + \frac{n}{2}\right)}{\Gamma\left(\frac{3}{4} - \frac{i\rho}{2} + \frac{n}{2}\right)} (\cosh \alpha)^{i\rho} F\left(\frac{1}{4} - \frac{i\rho}{2} - \frac{n}{2}, \frac{1}{4} - \frac{i\rho}{2} + \frac{n}{2}, \frac{1}{2}; \tanh^2 \alpha\right) \tag{3.18}$$

for $n = 2k$, $k = 1,2,3,...$,

$$\psi_2(\alpha, \rho) = -\frac{1}{2} \frac{\Gamma\left(\frac{3}{4} + \frac{i\rho}{2} + \frac{n}{2}\right)}{\Gamma\left(\frac{1}{4} + \frac{i\rho}{2} + \frac{n}{2}\right)} (\tanh \alpha)(\cosh \alpha)^{i\rho} F\left(\frac{3}{4} - \frac{i\rho}{2} - \frac{n}{2}, \frac{3}{4} - \frac{i\rho}{2} + \frac{n}{2}, \frac{3}{2}; \tanh^2 \alpha\right) \tag{3.19}$$

for $n = 2k + 1$, $k = 1,2,3,...$.

Using the relation (2.21), we find the asymptotic solution of (3.18),

$$\psi_1(\alpha, \rho) = A(\rho, n) e^{-i\rho\alpha} + \overline{A(\rho, n)} e^{i\rho\alpha}, \tag{3.20}$$

where

$$A(\rho, n) = \frac{\Gamma\left(\frac{1}{2}\right)\Gamma(-i\rho)}{\Gamma\left(\frac{1}{4} - \frac{i\rho}{2} - \frac{n}{2}\right)\Gamma\left(\frac{1}{4} - \frac{i\rho}{2} + \frac{n}{2}\right)} 2^{i\rho}. \tag{3.21}$$

Similarly, the asymptotic expression for (3.19) is

$$\psi_2(\alpha, \rho) = A'(\rho, n) e^{-i\rho\alpha} + \overline{A'(\rho, n)} e^{i\rho\alpha}, \tag{3.22}$$

where

$$A'(\rho, n) = \frac{\Gamma\left(\frac{3}{2}\right)\Gamma(-i\rho)}{\Gamma\left(\frac{3}{4} - \frac{i\rho}{2} - \frac{n}{2}\right)\Gamma\left(\frac{3}{4} - \frac{i\rho}{2} + \frac{n}{2}\right)} 2^{i\rho}. \tag{3.23}$$

The S-matrices for (3.20) and (3.22) are

$$S=\frac{\Gamma(-i\rho)\Gamma\left(\frac{1}{4}+\frac{i\rho}{2}-\frac{n}{2}\right)\Gamma\left(\frac{1}{4}+\frac{i\rho}{2}+\frac{n}{2}\right)}{\Gamma(i\rho)\Gamma\left(\frac{1}{4}-\frac{i\rho}{2}-\frac{n}{2}\right)\Gamma\left(\frac{1}{4}-\frac{i\rho}{2}+\frac{n}{2}\right)},\quad n=2k, \tag{3.24}$$

and

$$S=\frac{\Gamma(-i\rho)\Gamma\left(\frac{3}{4}+\frac{i\rho}{2}-\frac{n}{2}\right)\Gamma\left(\frac{3}{4}+\frac{i\rho}{2}+\frac{n}{2}\right)}{\Gamma(i\rho)\Gamma\left(\frac{3}{4}-\frac{i\rho}{2}-\frac{n}{2}\right)\Gamma\left(\frac{3}{4}-\frac{i\rho}{2}+\frac{n}{2}\right)},\quad n=2k+1. \tag{3.25}$$

The square integrable solutions for the negatives values of E are obtained from (3.18) and (3.19). By substituting

$$\sigma=-\tfrac{1}{2}-i\sqrt{E}=-1-\ell, \tag{3.26}$$

we have

$$\psi_1(\alpha,\ell)=c_1(\cosh\,\alpha)^{-|n|+1/2+2k}F(-k,|n|-k;\tfrac{1}{2};\,\tanh^2\,\alpha) \tag{3.27}$$

for $|n|-\ell=2k+1$, $k=0,1,2,...$, and

$$\psi_2(\alpha,\ell)=-c_2(\tanh\,\alpha)(\cosh\,\alpha)^{-|n|+3/2+2k}F(-k,|n|-k;\tfrac{3}{2};\,\tanh^2\,\alpha) \tag{3.28}$$

for $|n|-\ell=2k+2$, $k=0,1,2,...$

Here the normalization factors c_1 and c_2,

$$|c_1|^2=\frac{2}{2\ell+1}\,\frac{\Gamma(\frac{1}{2}+k)\Gamma(-|n|+k+\frac{1}{2})\Gamma(|n|-k)}{\pi\Gamma(1+k)\Gamma(-|n|+2k+\frac{1}{2})\Gamma(|n|-2k-\frac{1}{2})} \tag{3.29}$$

and

$$|c_2|^2=\frac{8}{2\ell+1}\,\frac{\Gamma(\frac{3}{2}+k)\Gamma(-|n|+k+\frac{3}{2})\Gamma(|n|-k)}{\pi\Gamma(1+k)\Gamma(-|n|+2k+\frac{3}{2})\Gamma(|n|-2k+\frac{3}{2})}, \tag{3.30}$$

are chosen to satisfy the condition

$$\int\,|\Psi_i|^2\,d\alpha=\frac{1}{\ell+(1/2)},\quad i=1,2. \tag{3.31}$$

The calculating of the normalization factors c_1 and c_2 are given in Appendix B.

B. Hyperbolic coordinates

The hyperbolic coordinates for $|x_2|>1$ are given as

$$\begin{aligned} x_0&=r\,\sinh\,\gamma\,\cosh\,\beta,\\ x_1&=r\,\sinh\,\gamma\,\sinh\,\beta, \end{aligned} \tag{3.32}$$

$$x_2 = r\epsilon \cosh\ \gamma,$$

$$\gamma \in (-\infty,\infty), \quad \beta \in (-\infty,\infty), \quad \epsilon = \pm 1.$$

By (3.32), we have

$$(g_{ab}) = \text{ diag } (-1, r^2, -r^2 \sinh^2\ \gamma), \tag{3.33}$$

$$\sqrt{g} = (\det\ (g_{ab}))^{1/2} = r^2 \sinh\ \gamma. \tag{3.34}$$

The component of the Laplace–Beltrami operator on the hyperboloid $[x,\ x] = -1$ is

$$\Delta_{\gamma,\beta} = \frac{\partial^2}{\partial \gamma^2} + \coth\ \gamma \frac{\partial}{\partial \gamma} + \frac{1}{\sinh^2\ \gamma} \frac{\partial^2}{\partial \beta^2}. \tag{3.35}$$

The equation

$$\Delta_{\gamma,\beta} \Phi(\gamma,\beta) = \sigma(\sigma+1)\Phi(\gamma,\beta) \tag{3.36}$$

is given by

$$\left(\frac{\partial^2}{\partial \gamma^2} + \coth\ \gamma \frac{\partial}{\partial \gamma} + \frac{\nu^2}{\sinh^2\ \gamma} \right) \vartheta(\gamma) = \sigma(\sigma+1)\,\vartheta(\gamma), \tag{3.37}$$

where

$$\Phi(\gamma,\beta) = \vartheta(\gamma) e^{i\nu\beta}. \tag{3.38}$$

Utilizing

$$dx = \sinh\ \gamma d\gamma\ d\beta \tag{3.39}$$

and making the transformation

$$\vartheta(\gamma) = (\sinh\ \gamma)^{-1/2} \psi(\gamma), \tag{3.40}$$

Eq. (3.37) reduces to

$$\frac{d^2\psi(\gamma)}{d\gamma^2} + \left[-\frac{1}{4} - \sigma(\sigma+1) + \frac{\nu^2 + (1/4)}{\sinh^2\ \gamma} \right] \psi(\gamma) = 0, \tag{3.41}$$

or to the Schrödinger's equation (2.14) with

$$E = -\tfrac{1}{4} - \sigma(\sigma+1), \quad \sigma = -\tfrac{1}{2} + i\sqrt{E}, \quad \sqrt{E} = \rho, \tag{3.42}$$

$$V(\gamma) = -\frac{\nu^2 + (1/4)}{\sinh^2\ \gamma}. \tag{3.43}$$

Applying the transformation

$$\vartheta(\gamma) = \left(\cosh \frac{\gamma}{2} \right)^{-i\nu} \left(\sinh \frac{\gamma}{2} \right)^{-i\nu} w(\gamma) \tag{3.44}$$

in Eq. (3.37), we obtain

$$\left[\frac{d^2}{d\gamma^2}+\frac{2i\nu+\cosh\ \gamma}{\sinh\ \gamma}\frac{d}{d\gamma}\right]w(\gamma)=\sigma(\sigma+1)w(\gamma). \tag{3.45}$$

In Eq. (3.45), applying the change of variable

$$z=-\sinh^2\frac{\gamma}{2}, \tag{3.46}$$

we arrive at the hyper-geometric equation

$$z(1-z)\frac{d^2w(z)}{dz^2}+[(i\nu+1)-2z]\frac{dw(z)}{dz}-[-\sigma(\sigma+1)]w(z)=0. \tag{3.47}$$

The regular solutions of the Schrödinger equation at $\gamma=0$ are found to be

$$\psi_{\pm}(\gamma,\sigma)=\left(\cosh\frac{\gamma}{2}\right)^{1/2}\left(\sinh\frac{\gamma}{2}\right)^{1/2}P_{\sigma}^{\pm i\nu}(\cosh\ \gamma), \tag{3.48}$$

where

$$P_{\sigma}^{\pm i\nu}(\cosh\ \gamma)=\frac{1}{\Gamma(1\mp i\nu)}\left(\cosh\frac{\gamma}{2}\right)^{\pm i\nu}\left(\sinh\frac{\gamma}{2}\right)^{\mp i\nu}F\left(\sigma+1,-\sigma,1\mp i\gamma,-\sinh^2\frac{\gamma}{2}\right). \tag{3.49}$$

Satisfying the condition Eq. (2.43) the solutions of the equation (3.41) have the form[2]

$$\Psi(\gamma,\sigma)=\left(\cosh\frac{\gamma}{2}\right)^{1/2}\left(\sinh\frac{\gamma}{2}\right)^{1/2}[q(\nu,\sigma)P_{\sigma}^{-i\nu}(\cosh\ \gamma)+q(-\nu,\sigma)P_{\sigma}^{i\nu}(\cosh\ \gamma)], \tag{3.50}$$

where

$$q(\nu,\sigma)=q_{\nu}=\frac{1}{\pi\sqrt{2}}\frac{\pi}{i\ \sinh\frac{-\nu}{2}\pi}\sqrt{\Gamma(\sigma+1)\Gamma(-\sigma)\Gamma(\sigma+1+i\nu)\Gamma(-\sigma+i\nu)}$$

$$\times\sqrt{\cos\frac{\sigma}{2}\pi\ \sin\frac{\sigma}{2}\pi\ \cos\left(\frac{\sigma}{2}+\frac{i\nu}{2}\right)\pi\ \sin\left(\frac{\sigma}{2}-\frac{i\nu}{2}\right)\pi}, \tag{3.51}$$

we find the asymptotic expression of (3.50) with $\sigma=-\frac{1}{2}+i\rho$, $\rho=\sqrt{E}$ as

$$\underset{\gamma\to\infty}{\Psi(\gamma,\rho)}\cong(q_{\nu}A_{\nu}+q_{-\nu}A_{-\nu})e^{-i\rho\gamma}+(q_{\nu}B_{\nu}+q_{-\nu}B_{-\nu})e^{i\rho\gamma}, \tag{3.52}$$

where

$$A_{\nu}=\frac{\Gamma(-2i\rho)}{\Gamma(\frac{1}{2}-i\rho)\Gamma(\frac{1}{2}-i\rho+i\nu)}2^{2i\rho}, \tag{3.53}$$

$$B_{\nu}=\frac{\Gamma(2i\rho)}{\Gamma(\frac{1}{2}+i\rho)\Gamma(\frac{1}{2}+i\rho+i\nu)}2^{-2i\rho}. \tag{3.54}$$

Using the conditions

$$|q_\nu|^2|A_\nu|^2+|q_{-\nu}|^2|A_{-\nu}|^2+q_\nu A_\nu\overline{q_{-\nu}A_{-\nu}}+q_{-\nu}A_{-\nu}\overline{q_\nu A_\nu}+|q_\nu|^2|B_\nu|^2+|q_{-\nu}|^2|B_{-\nu}|^2$$
$$+q_\nu B_\nu\overline{q_{-\nu}B_{-\nu}}+q_{-\nu}B_{-\nu}\overline{q_\nu B_\nu}=\frac{\pi}{2\rho\ \tanh\ \pi\rho} \tag{3.55}$$

it can be verified that the condition (2.43) for $\Psi(\gamma,\sigma)$ is satisfied.

The S-matrix is found to be given by

$$S=\frac{q_\nu A_\nu+q_{-\nu}A_{-\nu}}{q_\nu B_\nu+q_{-\nu}B_{-\nu}}. \tag{3.56}$$

The square integrable solution of Eq. (3.41) is found from (3.49) by setting $\sigma=l=0,1,2$:

$$\Psi(\gamma,l)=q(l,\nu)\left(\cosh\frac{\gamma}{2}\right)^{1/2}\left(\sinh\frac{\gamma}{2}\right)^{1/2}\left[P_l^{i\nu}(t)-\frac{\Gamma(1+l+i\nu)}{\Gamma(1+l-i\nu)}\,P_e^{-i\nu}(t)\right], \tag{3.57}$$

where

$$q(l,\gamma)=2\sqrt{\pi}\sqrt{\cot g\,\frac{i\pi\nu}{2}}\,\sqrt{\Gamma(1+\sigma-i\nu)\Gamma(-\sigma-i\nu)},$$
$$t=\cosh\ \gamma. \tag{3.58}$$

Using the relation between Legendre functions[3]

$$Q_\gamma^\mu(z)\sin\ \mu\pi=\frac{\pi}{2}\,e^{i\mu\pi}\left[P_\nu^\mu(z)-\frac{\Gamma(\nu+\mu+1)}{\Gamma(\nu-\mu+1)}\,P_\nu^{-\mu}(z)\right] \tag{3.59}$$

we have

$$\Psi(\gamma,l)=\frac{2}{\pi}\sin\ i\nu\pi e^{-i\pi\nu}q(l,\nu)\left(\cosh\frac{\gamma}{2}\right)^{1/2}\left(\sinh\frac{\gamma}{2}\right)^{1/2}Q_l^{i\nu}(\cosh\ \gamma), \tag{3.60}$$

where

$$Q_l^{i\nu}(\cosh\ \gamma)=2^l(\cosh\ \gamma+1)^{-l-1+i\nu/2}(\cosh\ \gamma-1)^{-i\nu/2}\,\frac{\Gamma(1+l)\Gamma(1+l+i\nu)}{\Gamma(2+2l)}$$
$$\times F\left(1+l-i\nu,1+l,2+2l;\,\frac{2}{1+\cosh\ \gamma}\right). \tag{3.61}$$

The condition

$$\int_{-\infty}^{\infty}\Psi(\gamma,l)\overline{\Psi(\gamma,l')}d\gamma=\frac{1}{l+(1/2)}\,\delta ll' \tag{3.62}$$

follows from the condition

$$\int_{-\infty}^{\infty}\Psi(\gamma,\sigma)\overline{\Psi(\gamma,\sigma')}d\gamma=\frac{1}{2(\sigma+\frac{1}{2})\tanh(\sigma+\frac{1}{2})\pi}\,\delta(\sigma-\sigma') \tag{3.63}$$

by the analytic continuation.

C. Parabolic coordinates

The parabolic coordinates are given as

$$\begin{gathered} x_0 = r[\sinh \tfrac{1}{2}t - \tfrac{1}{2}e^{(1/2)t}q^2], \\ x_1 = r[\cosh \tfrac{1}{2}t + \tfrac{1}{2}e^{(1/2)t}q^2], \\ x_2 = re^{(1/2)t}q, \\ t \in (-\infty,\infty), \quad q \in (-\infty,\infty). \end{gathered} \tag{3.64}$$

By (3.64), we have

$$(g_{ab}) = \text{ diag } (-1, \tfrac{1}{4}r^2, -r^2e^t). \tag{3.65}$$

The component of the operator (2.14) on the hyperboloid $[x,\ x] = -1$ is

$$\Delta_{t,q} = 4\,\frac{\partial^2}{\partial t^2} + 2\,\frac{\partial}{\partial t} - \frac{1}{e^t}\,\frac{\partial^2}{\partial q^2}\,. \tag{3.66}$$

The equation

$$\Delta_{t,q}\Phi(t,q) = \sigma(\sigma+1)\Phi(t,q), \tag{3.67}$$

where

$$\Phi(t,q) = \vartheta(t)e^{i\nu q} \tag{3.68}$$

becomes

$$\left[4\,\frac{\partial^2}{\partial t^2} + 2\,\frac{\partial}{\partial t} + \frac{\nu^2}{e^t}\right]\vartheta(t) = \sigma(\sigma+1)\,\vartheta(t). \tag{3.69}$$

Using (2.56) and making the transformation (2.57), Eq. (3.37) becomes

$$\frac{d^2\Psi(t)}{dt^2} + \left[-\frac{1}{16} - \frac{1}{4}\,\sigma(\sigma+1) + \frac{(1/4)\,\nu^2}{e^t}\right]\Psi(t) = 0 \tag{3.70}$$

or reduces to the Schrödinger equation with

$$E = -\tfrac{1}{16} - \tfrac{1}{4}\sigma(\sigma+1), \tag{3.71}$$

$$V(t) = -\frac{(1/4)\,\nu^2}{e^t}. \tag{3.72}$$

Changing variables to (2.61) in Eq. (3.70) with $\sigma = -\frac{1}{2} + i\rho$ we obtain

$$z^2\,\frac{d^2\Psi(z)}{dz^2} + z\,\frac{d\Psi(z)}{dz} + [\nu^2z^2 + \rho^2]\Psi(z) = 0. \tag{3.73}$$

The solution which tends to zero for $t \to \infty$ and satisfies the condition (2.64),

$$\Psi(t,\rho)=\left(\frac{2\ \cosh\ \rho\pi}{\pi}\right)^{1/2}K_{i\rho}(i\nu e^{-(1/2)t}) \tag{3.74}$$

The square integrable solution of Eq. (3.73) with $\sigma(\sigma+1)=l(l+1)$ is

$$\Psi_l(t)=J_{l+1/2}(\nu e^{-(1/2)t}). \tag{3.75}$$

The orthonormality condition of Bessel functions has the form

$$\int_0^\infty J_{l+1/2}(z)J_{l'+1/2}(z)\ \frac{dz}{z}=\frac{l}{l+\frac{1}{2}}\ \delta ll'. \tag{3.76}$$

IV. THE EXPLICIT EXPRESSIONS ON THE GREEN'S FUNCTION OF THE FREE PARTICLE ON TWO- AND ONE-SHEETED HYPERBOLOIDS

A. Calculate Green's function of the free particle on hyperboloid $[x,\ x]=1$

First we consider the decomposition of the unitary representation

$$T(g)F(x)=F(xg),\quad g\in \mathrm{SO}(1,2), \tag{4.1}$$

in the space

$$\langle F_1,F_2\rangle=\int F_1(x)\overline{F_2(x)}dx \tag{4.2}$$

of function on hyperboloid. The irreducible representation $T_\sigma(g)$, $g\in$SO(1,2), can be realized in the space of the homogenous functions on cone

$$[y,\ y]=y_0^2-y_1^2-y_2^2=0,\quad y_0>0$$

(see Appendix A). Consider the functions $[x,\ y]^\sigma$, which for fixed x homogenous functions on cone

$$[x,\ dy]^\sigma=a^\sigma[x,\ y]^\sigma. \tag{4.3}$$

Since $[xg^{-1},\ y]=[x,\ yg]$, we have

$$[xg^{-1},\ s]^\sigma=(sg)_0^\sigma[x,\overline{sg}]^\sigma, \tag{4.4}$$

where $y=e^\alpha s$, $s=(1,\sin\varphi,\cos\varphi)$. The Fourier components $\tilde{F}(s;\rho)$ of the function $F(x)$ we define by formula

$$\tilde{F}(s,\rho)=\int F(x)[x,s]^{-1/2+i\rho}\ dx. \tag{4.5}$$

For the function $F_g(x)=F(xg)$ we have

$$\tilde{F}_g(s,\rho)=\int F_g(x)[x,s]^{-1/2+i\rho}\ dx=\int F(x)[xg^{-1},s]^{-1/2+i\rho}\ dx=(sg)_0^{-1/2+i\rho}F(\overline{sg},\rho). \tag{4.6}$$

Here we used Eq. (4.4) and the invariance of the volume element $dx=dxg$. Hence representation in the space of functions $F(s,\rho)$ is irreducible.

The expansion of the function $F(x)$ in an elementary harmonics reads[2]

$$F(x)=\frac{1}{\pi^2}\int \tilde{F}(s,\rho)[x,s]^{-1/2+i\rho}\rho\ \tanh\ \pi\rho\ d\rho\ ds. \tag{4.7}$$

The function $[x,\ s]^{\sigma}$ is an eigenfunction of the Laplace–Beltrami operator,

$$\Delta_{\mathrm{L,B}}[x,s]^{\sigma}=\sigma(\sigma+1)[x,s]^{\sigma}. \tag{4.8}$$

Therefore the Green's function of the quantum system with Hamiltonian

$$H=-\frac{1}{2mR^2}\Delta_{\mathrm{LB}} \tag{4.9}$$

reads

$$G(x_1,x_2;E)=\frac{1}{\pi^2}\int\int_S \frac{[x_1,s]^{-1/2+i\rho}[x_2,s]^{-1/2-i\rho}}{\frac{1}{2mR^2}\left(\rho^2+\frac{1}{4}\right)-E}\rho\ \tanh\ \pi\rho\ d\rho\ ds. \tag{4.10}$$

Using the addition theorem (see Appendix A),

$$\int\ [x_1,\ s]^{-1/2+i\rho}[x_2,\ s]^{-1/2-i\rho}\ ds=2\pi\int\ [\dot{x}g_{x_1}g_{x_2}^{-1},s]^{-1/2+i\rho}\ d\varphi, \tag{4.11}$$

and integral representation of first kind Legendre function,

$$P_{\sigma}(\cosh\ \alpha)=\frac{1}{2\pi}\int\ [x,\ s]^{\sigma}ds=\frac{1}{2\pi}\int\ (\cosh\ \alpha-\sinh\ \alpha\ \cos\ \varphi)^{\sigma}d\varphi, \tag{4.12}$$

and the relation between first kind and second kind Legendre functions (Ref. 3, p. 819),

$$\int_0^{\infty}\frac{x\ \tanh\ \pi x}{a^2+x^2}P_{-(1/2)+ix}(\cosh\ y)dx=Q_{a-(1/2)}(\cosh\ y), \tag{4.13}$$

we obtain

$$G(x_1,x_2;E)=8mR^2Q_{i\sqrt{2mR^2E-(1/4)}-(1/2)}([x_1,\ x_2]). \tag{4.14}$$

The same results were obtained by the path integral method in Refs. 6 and 7.

By a Fourier transformation we obtain the time-dependent propagator:

$$K(x_1,x_2;T)=\frac{1}{2\pi R^2}\int_0^{\infty}\exp\left[\frac{-iT(\rho^2+\frac{1}{4})}{2mR^2}\right]P_{-(1/2)+i\rho}([x_1,\ x_2])\rho\ \tanh\ \pi\rho\ d\rho. \tag{4.15}$$

The eigenfunction representation in terms of the Legendre function of the propagator is ''equivalent to the integral over classical parts.''[4,7]

Indeed, using the integral representation for the Legendre function[8]

$$\tanh(\pi\rho)P_{-(1/2)+i\rho}(\cosh\ \alpha)=\frac{\sqrt{2}}{\pi}\int_{\alpha}^{\infty}\frac{\sin\ \rho t\ dt}{(\cosh\ t-\cosh\ \alpha)^{1/2}} \tag{4.16}$$

and the formula;

$$\int_0^\infty \rho \sin(\rho t)\exp(-a\rho^2)d\rho = \sqrt{\frac{\pi}{a}}\,(t/4a)\exp(-t^2/4a) \tag{4.17}$$

we obtain

$$K(x_1,x_2;T)=\sqrt{2}\ \mathrm{Re}^{-i\pi/8mR^2}\left(\frac{m}{2\pi T}\right)^{3/2}\int_\alpha^\infty \frac{t\exp(-mRt^2/2T)dt}{(\cosh t-\cosh\alpha)^{1/2}}, \tag{4.18}$$

where $\cosh\alpha=[x_1, x_2]$.

B. The Green's function on one-sheeted hyperbolic $[x, x]=-1$

There exists the reflection operator R defined by

$$RF(x)=F(-x) \tag{4.19}$$

which commutes with the representation operator

$$T(g)F(x)=F(xg). \tag{4.20}$$

Therefore symmetric and antisymmetric parts $F^{\pm}(x)=\frac{1}{2}[F(x)\pm F(-x)]$ of the functions $F(x)$ define invariant subspaces. Notice that the one-sheeted hyperboloid $[x, x]=-1$ with identified of the opposite points x and $-x$ is called the imaginary Labochevsky space. From the results concerning the decomposition of the representation (4.20) into the irreducible components[2] follows that the Green's function in the imaginary Lobachevsky space is defined by

$$G(x_1,x_2;E)=\frac{1}{\pi}\int_0^\infty\int_S \frac{[x_1, s]^{-1/2+i\rho}[x_2, s]^{-1/2-i\rho}}{\frac{1}{2mR^2}(\rho^2+\frac{1}{4})-E}\rho\tanh\pi\rho\, d\rho\, ds$$

$$+\frac{1}{\pi}\sum_{l=0}^\infty \frac{(l+\frac{1}{2})\int|[x_1,s]|^{-1-l}|[x_2,s]|^l\, ds}{-\frac{1}{2mR^2}l(l+1)-E}. \tag{4.21}$$

By the addition theorem (see Appendix A) we get

$$G(x_1,x_2;E)=2\pi R^2\int_0^\infty \frac{P_{-(1/2)+i\rho}(|x_1,x_2|)\rho\tanh\pi\rho\, d\rho}{\rho^2-(2mR^2E+\frac{1}{4})}+2mR^2\sum_{l=0}^\infty \frac{(l+\frac{1}{2})P_l(|x_1,x_2|)}{-l(l+1)-2mR^2}. \tag{4.22}$$

In order to calculate the infinite series in (4.22) we use the Sommerfeld–Watson integral transformation

$$\sum_{l=0}^\infty \frac{(l+\frac{1}{2})}{-l(l+1)-E}P_l(t)=i\int_C d\sigma\,\frac{(\sigma+\frac{1}{2})\cos\pi\sigma}{\sin\pi\sigma[-\sigma(\sigma+1)-E]}P_\sigma(t)$$

$$=\int_{-\infty}^\infty \frac{d\rho\rho\tanh\pi\rho}{\rho^2+\frac{1}{4}+(-E)}P_{-(1/2)+i\rho}(t), \tag{4.23}$$

where contour C encounters the zeros of the function $\sin\pi l, l=0,1,2,\ldots$.

For $t>1$ then apply to last integral the formula (4.13), but for $t<1$ we define it by analytic continuation. Thus we obtain final expression for Green's function

$$G(x_1,x_2;E)=2mR^2[Q_{i\sqrt{(E/2mR^2)-(1/4)}-(1/2)}(|x_1x_2|)+Q_{i\sqrt{(-E/2mR^2)-(1/4)}-(1/2)}(|x_1x_2|)]. \tag{4.24}$$

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APPENDIX A: THE ORTHOGONALITY, COMPLETENESS CONDITIONS AND ADDITION THEOREM FOR PLANE VALUES $[x,\ s]^{\sigma}$

The irreducible representations of group SO(1,2) are constructed[9] in the space of infinitely differentiable homogenous functions $F(y)$ on the cone $[y,y]=0$; $y_0>0$,

$$F(ay)=a^{\sigma}F(y),\quad a>0. \tag{A1}$$

The representation

$$T_{\sigma}(g)F(y)=F(yg),\quad g\in \mathrm{SO}(1,2), \tag{A2}$$

can be realized in the space of infinitely differentiable functions on intersections of cone; for example, on the circle

$$T_{\sigma}(g)f(s)=(sg)_0^{\sigma}f(\overline{sg}), \tag{A3}$$

$$s=y|_{y_0=1}=(1,\ \sin\varphi,\ \cos\varphi),\quad y=y_0s=e^{\alpha}s. \tag{A4}$$

From $y'=yg$ we have

$$(sg)_0=e^{\alpha'-\alpha},\quad \overline{sg}=sg/(sg)_0=(1,\ \sin\varphi',\ \cos\varphi'). \tag{A5}$$

The unitary representation $T_{\sigma}(g)$, $g\in\mathrm{SO}(1,2)$ with respect to scalar product

$$\langle f_1,f_2\rangle=\int \overline{f_1(\varphi)}f_2(\varphi)d\varphi=\int \overline{f_1(s)}f_2(s)ds \tag{A6}$$

is defined by $\sigma=-(1/2)+i\rho$ (principle series). The unitary representation $T_{\sigma}(g)$ with respect to the scalar product

$$\langle f_1,f_2\rangle=\frac{1}{\Gamma(-r-\frac{1}{2})}\int [s,s']^{-1-\sigma}\overline{f_1(s)}f_2(s)ds\ ds' \tag{A7}$$

is defined by $-1<\sigma<0$ (complementary series) and by $\sigma=-1-l$, $l=0,1,2$ (discrete series). The matrix elements of the representation $T^{\sigma}_{0,n}(g)$ are defined by the formula

$$t^{\sigma}_{0,n}(g)=\langle 1,T_{\sigma}(g)e^{in\varphi}\rangle=\frac{1}{2\pi}\int (sg)_0^{\sigma}e^{in\varphi'}\ d\varphi'. \tag{A8}$$

Using the decomposition of the element $g\in\mathrm{SO}(1,2)$ related with the hyperboloid $[x,\ x]=1$

$$x=xg_x,\quad xK=x,\quad g=Kg_x,$$

we also have

$$t^{\sigma}_{0,n}(g_x)=\langle T_{-1-\sigma}(g_x^{-1}),e^{in\varphi}\rangle=\frac{1}{2\pi}\int (sg_x^{-1})_0^{-1-\bar{\sigma}}e^{in\varphi}\,d\varphi. \tag{A9}$$

Since

$$(sg_x^{-1})_0=[\mathring{x},\ sg_x^{-1}]=[\mathring{x}g_x,\ s]=[x,\ s],\quad \mathring{x}=(1,0,0)$$

we get

$$t^{\sigma}_{0,n}(g_x)=\frac{1}{2\pi}\int [x,s]^{-1-\bar{\sigma}}e^{in\varphi}\,d\varphi. \tag{A10}$$

Laplace–Beltrami operator Δ_{LB} on hyperboloid $[x,\ x]=1,\ x_0>0$, is a Casimir operator of the quasi-regular representation $T_g(g)F(x)=F(xg)$.

So, the matrix elements $t^{\sigma}_{0,n}(g_x)$ satisfy the equation

$$\Delta_{\mathrm{LB}}t^{\sigma}_{0,n}(g_x)=\sigma(\sigma+1)t^{\sigma}_{0,n}(g_x), \tag{A11}$$

and we have

$$\Delta_{\mathrm{LB}}[x,\ s]^{\sigma}=\sigma(\sigma+1)[x,\ s]^{\sigma}. \tag{A12}$$

The addition theorem for function $[x,s]^{-1+i\rho}$ follows from the relations

$$\sum_n t^{\sigma}_{0,n}(g_{x_1})\overline{t^{\sigma}_{0,n}(g_{x_2})}=\sum_n t^{\sigma}_{0,n}(g_{x_1})t^{\sigma}_{0,n}(g_{x_2}^{-1})=t^{\sigma}_{0,0}(g_{x_1}g_{x_2}^{-1}). \tag{A13}$$

Using the integral representation (A10) we have

$$\int [x_1,\ s]^{-(1/2)+i\rho}[x_2,\ s]^{-(1/2)-i\rho}\,ds=\frac{1}{2\pi}\int [\dot{x}g_{x_1}g_{x_2}^{-1},s]^{-(1/2)+i\rho}\,ds. \tag{A14}$$

The orthogonality condition for the matrix elements $t^{\sigma}_{0,n}(g_x)$ reads

$$\int t_{0,n}^{-(1/2)+i\rho}(g_x)\overline{t_{0,n}^{-(1/2)+i\rho'}}(g_x)dx=(2\pi)^2|c(\rho)|^2\delta(\rho-\rho')\,\delta_{nn'}, \tag{A15}$$

where $c(\rho)$, the so-called Harish–Chandra function, is defined asymptotically:[10]

$$t^{\sigma}_{0,n}(a(\alpha))\underset{\alpha\to\infty}{\cong}\int_0^{2\pi}(\cosh\,\alpha+\sinh\,\alpha\,\cos\,\varphi)^{\sigma}\,d\varphi=(\cosh\,\alpha)^{\sigma}c(\sigma), \tag{A16}$$

where

$$c(\sigma)=2^{\sigma}\frac{\Gamma(1+2\sigma)}{|\Gamma(1+\sigma)|^2}. \tag{A17}$$

Here we use Eq. (A8) and the fact that

$$\cos\,\varphi'\underset{\alpha\to\infty}{=}\frac{\sinh\,\alpha+\cosh\,\alpha\,\cos\,\varphi}{\cosh\,\alpha+\sinh\,\alpha\,\cos\,\varphi}\to 1. \tag{A18}$$

From Eq. (A15) we get to the orthogonality condition for functions $[x\ s]^{-(1/2)+i\rho}$:

$$\int [x,s]^{-(1/2)+i\rho}[x,s']^{-(1/2)-i\rho'}\,dx=\pi^2\,\frac{1}{\rho\,\tanh\,\pi\rho}\,\delta(\rho-\rho')\,\delta(s-s'). \tag{A19}$$

The completeness condition

$$\frac{1}{\pi^2}\int [x_1,\,s]^{-(1/2)+i\rho}[x_2,\,s]^{-(1/2)-i\rho}\rho\,\tanh\,\pi\rho\,d\rho\,ds=\frac{1}{\pi}\,\delta(x_1-x_2) \tag{A20}$$

follows from the fact that quantum systems related to the hyperboloid $[x,\,x]=1$, $x_0>0$, contain only scattering states (see Ref. 2).

In order to present the addition theorem for the eigenfunctions $|[x,\,s]|^{\sigma}$ of the Laplace–Beltrami operator on the one-sheeted hyperboloid $[x,\,x]=-1$ because the stationary subgroup of fixed point $x=(0,0,1)$ is noncompact $\mathrm{SO}(1,1)\equiv H$, we must consider the matrix elements of unitary representation $T_\sigma(g)$ in the basis associated with noncompact subgroup H. Realizing the representation (A2) in the space of function $f(p)=F(y)|_{x_2=\pm 1}$, where $p=(\cosh\beta,\ \sinh\beta,\epsilon)$, $\epsilon=\pm 1$, we get[2]

$$t^{\sigma,\epsilon}_{0,\nu}(g_x)=\frac{1}{2\pi}\int_S|[x,s]|^{-1-\sigma}[x,\,s]^{\sigma}\,\mathrm{sign}^{\epsilon}[x,s]\left\{\frac{[p^+,s]}{[p^-,s]}\right\}^{i\nu/2}ds, \tag{A21}$$

where $\epsilon=0,1$; $p^{\pm}=(1,\pm 1,0)$. Then from

$$\int_S t^{(\sigma,0)}_{0,0}(g_{x_1})t^{(\sigma,0)}_{0,\nu}(g^{-1}_{x_2})\,d\nu=t^{(\sigma,0)}_{0,0}(g_{x_1}g^{-1}_{x_2}) \tag{A22}$$

we obtain

$$\int_S|[x_1,s]|^{\sigma}|[x_2,s]|^{-1-\sigma}\,ds=\int_S|[xg_{x_1}g^{-1}_{x_2},s]|^{\sigma}|[x,s]|^{-1-\sigma}\,ds. \tag{A23}$$

Using the decomposition of the elements

$$g=h\tilde{g}h,\quad g\in\mathrm{SO}(1,2), \tag{A24}$$

where $\tilde{g}=a(\alpha)$ or $\tilde{g}=K(\theta)$ (see Ref. 2) associated with the hyperboloid $[x,\,x]=-1$. We have

$$t^{(\sigma,0)}_{0,0}(g)=t^{(\sigma,0)}_{0,0}(\tilde{g})=P_\sigma(t) \tag{A25}$$

for $|t|>1$, $t=\epsilon\cosh\alpha$, $\epsilon=\pm 1$, for $|t|<1$, $t=\cos\theta$.

APPENDIX B: CALCULATION OF THE NORMALIZATION FACTOR

To calculate the normalization factor in (3.27) we perform the change of variable $x=\tanh^2\alpha$ and use the formula [Ref. 11, 2.8 (17)]

$$F(-k,b;c;x)=\frac{\Gamma(c)}{\Gamma(c+k)}\,x^{1-c}(1-x)^{k+c-b}\,\frac{d^k}{dx^k}\,[x^{k+c-1}(1-x)^{b-c}]. \tag{B1}$$

Then we get

$$J=\frac{|c_1|^2\sqrt{x}}{\Gamma(\frac{1}{2}+k)}\int_0^1(1-x)^{-1}F\left(-k,n-k;\,\frac{1}{2};x\right)\frac{d^k}{dx^k}\,[x^{k-1/2}(1-x)^{n-k-1/2}]dx. \tag{B2}$$

After k-fold multiple integration by parts and using the formula [Ref. 11, 28 (25)]

$$\frac{d^k}{dx^k}\left[(1-x)^{-1}F(-k,b;c;x)\right]=\frac{\Gamma(k+1)\Gamma(c-b+k)\Gamma(c)}{\Gamma(c-b)\Gamma(c+k)}\,(1-x)^{-k-1}, \tag{B3}$$

from $J=1/[\ell+(1/2)]$ we obtain

$$|c_1|^2=\frac{2}{2\ell+1}\,\frac{\Gamma(\frac{1}{2}+k)\Gamma(-n+k+\frac{1}{2})\Gamma(n-k)}{\pi\Gamma(k+1)\Gamma(-n+2k+\frac{1}{2})\Gamma(n-2k-\frac{1}{2})}. \tag{B4}$$

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Two-dimensional supersymmetric harmonic oscillator carrying a representation of the GL(2|1) graded Lie algebra

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We study a supersymmetric two-dimensional harmonic oscillator which carries a representation of the general graded Lie algebra GL(2|1), formulate it on the superspace, and discuss its physical spectrum. © *1996 American Institute of Physics.* [S0022-2488(96)00201-X]

I. INTRODUCTION

Supersymmetry is an interesting symmetry which transforms bosons into fermions and vice versa.[1] Quantum mechanical (or classical) theories which are supersymmetric provide realizations of graded Lie algebras (GLA).[2] The most familiar GLA is the graded Poincaré algebra which leads to relativistic, supersymmetric quantum field theories, which include supergravity.

Examples of simple and extended global supersymmetries based on the grading of space-time symmetries are abundant in simple quantum mechanical systems—the one-dimensional supersymmetric harmonic oscillator being the simplest example of such systems.[3,4] However, there exist many other GLAs which involve grading internal symmetry algebras. The most familiar of such GLAs are the OS$p(2m|n)$ and SL$(m|n)$.[5] While realizations of such algebras arise naturally in integrable models, there does not yet exist a quantum or classical mechanical realization of the most general graded Lie algebra, namely, GL$(m|n)$. In this paper, we construct a supersymmetric two-dimensional harmonic oscillator which provides a realization of GL(2|1) as its symmetry algebra. In Sec. II, we discuss the GL(2|1) algebra with raising and lowering operators. In Sec. III we present our model of a supersymmetric harmonic oscillator and discuss all the symmetries associated with this system. We show that the symmetry algebra coincides with GL(2|1). In Sec. IV, we discuss the spectrum of states associated with this Hamiltonian and present a superspace description of this theory. Finally, we discuss our conclusions in Sec. V.

II. GRADED LIE ALGEBRA GL(2|1)

Graded Lie algebras[2] include both bosonic and fermionic generators satisfying commutation and anticommutation relations, respectively, and have the following general structure:

$$[B_m,B_n]_- = f_{mn}^k B_k, \quad [B_m,F_\alpha]_- = h_{m\alpha}^\beta F_\beta, \quad [F_\alpha,F_\beta]_+ = g_{\alpha\beta}^m B_m, \tag{1}$$

with the brackets $[...,...]_{\mp}$ denoting commutators and anticommutators, respectively, $k,m,n = 1,2,\ldots,N$, and $\alpha,\beta = 1,2,\ldots,M$. The even or bosonic generators B_m form the underlying Lie algebra, while the odd or fermionic generators F_α provide a grading of this algebra consistent with the generalized Jacobi identities.

In this section we shall study the graded Lie algebra GL(2|1) whose underlying bosonic algebra is GL(2)⊕GL(1). Here we shall use the boson/fermion representation obtained with the help of canonical realizations, i.e., realizations in terms of pairs of boson/fermion creation and annihilation operators satisfying canonical (anti)commutation relations. Consider the set of bosonic and fermionic operators

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$$\{a_k^\dagger, a_k; k=1,2\} \quad \text{and} \ \{a_3^\dagger, a_3\} \tag{2}$$

satisfying the canonical (anti)commutation relations

$$[a_k, a_m^\dagger]_- = \delta_{km}, \quad [a_3, a_3^\dagger]_+ = 1, \tag{3}$$

with all other (anti)commutators vanishing. The four bilinear operators $B \sim a_k^\dagger a_m$ define the generators of the underlying GL(2) algebra, which together with $B \sim a_3^\dagger a_3$ constitute the five bosonic generators of the GL(2|1) algebra. The four fermionic generators of this algebra are defined by the bilinear operators $F \sim a_3^\dagger a_k$ and $F \sim a_k^\dagger a_3$. All together these nine operators generate the Z_2 graded GL(2|1) algebra. It is a simple task to verify that they satisfy the algebra (1). For instance, if we denote these nine operators as

(a) bosonic generators:

$$\begin{gathered} B_1 = a_1^\dagger a_1, \quad B_2 = a_1^\dagger a_2, \quad B_3 = a_2^\dagger a_1, \\ B_4 = a_2^\dagger a_2, \quad B_5 = a_3^\dagger a_3, \end{gathered} \tag{4}$$

(b) fermionic generators:

$$\begin{gathered} F_1 = a_1^\dagger a_3, \quad F_2 = a_2^\dagger a_3, \\ F_3 = a_3^\dagger a_1, \quad F_4 = a_3^\dagger a_2, \end{gathered} \tag{5}$$

it is then a simple task to find the nonvanishing structure constants in Eq. (1).

For future convenience, we introduce a new basis of the fermionic generators as

$$\begin{gathered} Q_R = \frac{1}{\sqrt{2}}(a_1^\dagger a_3 - i a_2^\dagger a_3), \quad \bar{Q}_R = \frac{1}{\sqrt{2}}(a_3^\dagger a_1 + i a_3^\dagger a_2), \\ Q_L = \frac{i}{\sqrt{2}}(a_3^\dagger a_1 - i a_3^\dagger a_2), \quad \bar{Q}_L = \frac{-i}{\sqrt{2}}(a_1^\dagger a_3 + i a_2^\dagger a_3). \end{gathered} \tag{6}$$

The anticommutation relations among these charges are easily computed. We also redefine the five bosonic operators as

$$\begin{gathered} h_b = a_1^\dagger a_1 + a_2^\dagger a_2, \quad h_f = a_3^\dagger a_3, \\ \Delta_1 = a_1^\dagger a_1 - a_2^\dagger a_2, \quad i\Delta_2 = a_2^\dagger a_1 - a_1^\dagger a_2, \quad \Delta_3 = a_1^\dagger a_2 + a_2^\dagger a_1, \end{gathered} \tag{7}$$

and introduce the operator $H = h_b + h_f$. The algebra of the fermionic charges (6) becomes

$$\begin{gathered} [Q_R, \bar{Q}_R]_+ = \tfrac{1}{2}(H + \Delta_2 + h_f), \quad [Q_L, \bar{Q}_L]_+ = \tfrac{1}{2}(H - \Delta_2 + h_f), \\ [Q_R, Q_L]_+ = \tfrac{1}{2}(\Delta_3 + i\Delta_1), \quad [\bar{Q}_R, \bar{Q}_L]_+ = \tfrac{1}{2}(\Delta_3 - i\Delta_1). \end{gathered} \tag{8}$$

Similarly, the algebra of the new bosonic charges (7) can be computed straightforwardly, to give

$$\begin{gathered} [\Delta_k, \Delta_m]_- = 2i\epsilon_{kmn}\Delta_n, \quad [h_b, \Delta_m]_- = 0, \\ [h_f, \Delta_m]_- = 0, \quad [h_b, h_f]_- = 0, \end{gathered} \tag{9}$$

while the remaining nonvanishing boson–fermion commutation relations are

$$[h_f,Q_R]_-=-[h_b,Q_R]_-=-Q_R,\quad [h_f,\bar{Q}_R]_-=-[h_b,\bar{Q}_R]_-=+\bar{Q}_R,$$
$$[h_f,Q_L]_-=-[h_b,Q_L]_-=+Q_L,\quad [h_f,\bar{Q}_L]_-=-[h_b,\bar{Q}_L]_-=-\bar{Q}_L; \tag{10}$$

$$[\Delta_1,Q_R]_-=+i\bar{Q}_L,\quad [\Delta_1,\bar{Q}_R]_-=+iQ_L,$$
$$[\Delta_1,Q_L]_-=-i\bar{Q}_R,\quad [\Delta_1,\bar{Q}_L]_-=-iQ_R; \tag{11}$$

$$[\Delta_2,Q_R]_-=+Q_R,\quad [\Delta_2,\bar{Q}_R]_-=-\bar{Q}_R,$$
$$[\Delta_2,Q_L]_-=+Q_L,\quad [\Delta_2,\bar{Q}_L]_-=-\bar{Q}_L; \tag{12}$$

$$[\Delta_3,Q_R]_-=+\bar{Q}_L,\quad [\Delta_3,\bar{Q}_R]_-=-Q_L,$$
$$[\Delta_3,Q_L]_-=-\bar{Q}_R,\quad [\Delta_3,\bar{Q}_L]_-=+Q_R. \tag{13}$$

Using these relations we can verify that all generators satisfy the generalized Jacobi identities. Observe from Eqs. (9) and (10) that all nine generators of the GL(2|1) graded Lie algebra described above commute with H which stays in the center of the algebra.

III. TWO-DIMENSIONAL SUPERSYMMETRIC HARMONIC OSCILLATOR

In this section we introduce our model, a two-dimensional supersymmetric harmonic oscillator which, as mentioned in the Introduction, carries a representation of the graded GL(2|1) algebra described in Sec. II. This model is described by the following Lagrangian:

$$L=\frac{1}{2}\,(\dot{q}^T\dot{q}-q^Tq)+\frac{i}{2}\,\psi^T\left(\frac{d}{dt}-i\sigma_2\right)\psi, \tag{14}$$

where

$$q=\begin{pmatrix} q_1 \\ q_2 \end{pmatrix} \tag{15}$$

and

$$\psi=\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \tag{16}$$

are the oscillator's bosonic and fermionic coordinates, which are assumed to be real. We have chosen the mass and the frequency to be unity, for simplicity. Here σ_k stands for the Pauli matrices and q^T and ψ^T stand for matrix transposition, as usual. Note that up to total derivatives, we can also write the Lagrangian (14) as

$$L=-\frac{1}{2}\,q^T\left(\frac{d}{dt}-i\sigma_2\right)\left(\frac{d}{dt}+i\sigma_2\right)q+\frac{i}{2}\,\psi^T\left(\frac{d}{dt}-i\sigma_2\right)\psi. \tag{17}$$

It is important to mention that compared to the *usual* two-dimensional supersymmetric harmonic oscillator, the model under investigation here is constructed with half the number of fermionic

degrees of freedom, i.e., it has two second-order bosonic variables (or four first-order) and two first-order fermionic variables. In the two-dimensional matrix space of Eqs. (15) and (16), let us denote a complete basis of real, (2×2) matrices by

$$\tau_a=(\sigma_0,\sigma_1,i\sigma_2,\sigma_3);\quad a=0,1,2,3, \tag{18}$$

where σ_0 is the (2×2) identity matrix. It is straightforward to show that the action of the theory described by Eq. (14) is invariant under the four supersymmetry transformations

$$\delta q=\epsilon_a\tau_a\psi,\quad \delta\psi=i\left(\frac{d}{dt}+i\sigma_2\right)\epsilon_a\tau_a^T q, \tag{19}$$

with ϵ_a being four infinitesimal, constant Grassmann parameters that characterize the transformations. In the Hamiltonian language,[6] which is more appropriate for our purposes, the Hamiltonian operator is given by

$$H=\tfrac{1}{2}(p^Tp+q^Tq)-\tfrac{1}{2}\psi^T\sigma_2\psi \tag{20}$$

and enjoys the following set of global invariances:

(A) Supersymmetry

$$\delta q=\frac{1}{\sqrt{2}}\,\epsilon_a\tau_a\psi,\quad \delta\psi=\frac{i}{\sqrt{2}}\,\epsilon_a(\tau_a^Tp+i\sigma_2\tau_a^Tq),\quad \delta p=\frac{i}{\sqrt{2}}\,\epsilon_a\tau_a\sigma_2\psi. \tag{21}$$

The Noether supercharges generating these transformations are given by

$$Q_a=\frac{1}{\sqrt{2}}\,(p^T\tau_a\psi-iq^T\tau_a\sigma_2\psi). \tag{22}$$

Indeed, note that given the generalized Dirac brackets [see Eq. (A5)]

$$\{q_k,p_m\}=\delta_{km},\quad \{\psi_\alpha,\psi_\beta\}=-i\delta_{\alpha\beta}, \tag{23}$$

we obtain the supersymmetry transformations (21) above as

$$\delta A=\{A,\epsilon_aQ_a\}, \tag{24}$$

where A stands for q_k, p_k, and ψ_α. The invariance of the Hamiltonian implies that $\{H,Q_a\}=0$ which in turn shows that the Q_a's are constants of motion. Besides the four supersymmetries above, this Hamiltonian is also invariant under the following global symmetries.

(B) Rotation on the four-dimensional (bosonic) phase-space
(i) The transformations

$$\delta q=-i\alpha\sigma_2q,\quad \delta p=-i\beta\sigma_2p, \tag{25}$$

with α,β bosonic, constant infinitesimal parameters are clearly symmetries of H. However, in order to preserve the canonical commutation relations (23) we must have $\alpha=\beta$. These transformations are generated by the angular momentum operator

$$J_1=\frac{i}{2}\,(q^T\sigma_2p-p^T\sigma_2q). \tag{26}$$

Note that these transformations do not mix coordinate and momentum variables.

(ii) The transformations

$$\delta q=\lambda_a\tau_a p, \quad \delta p=-\lambda_a\tau_a q, \tag{27}$$

with λ_a constant, bosonic, infinitesimal parameters are also a set of symmetries of the Hamiltonian which preserve the Dirac brackets relations, as long as the index $a\neq 2$ [see Eq. (18)]. The charges generating these transformations are

$$L_0=\tfrac{1}{2}(p^Tp+q^Tq), \quad L_1=\tfrac{1}{2}(p^T\sigma_1 p+q^T\sigma_1 q), \quad L_3=\tfrac{1}{2}(p^T\sigma_3 p+q^T\sigma_3 q). \tag{28}$$

(C) Rotation on the two-dimensional fermionic phase-space

The generalized rotation in the fermionic phase-space

$$\delta\psi=\boldsymbol{\alpha}\cdot\boldsymbol{\sigma}\psi \tag{29}$$

with $\boldsymbol{\alpha}=(\alpha_1,\alpha_2,\alpha_3)$ being a set of constant bosonic parameters, is another group of symmetries in the action. Again, preservation of the canonical commutation relations (23) imposes $\alpha_1=\alpha_3=0$ as conditions over the possible values that these parameters can take. These transformations are generated by the following charge:

$$J_2=\tfrac{1}{2}\psi^T\sigma_2\psi \tag{30}$$

representing the fermionic contribution to the total angular momentum.

Now, in order to make contact with the graded algebra GL(2|1) defined in the preceeding section, let us redefine these charges as

$$\begin{gathered} h_b=L_0=\tfrac{1}{2}(p^Tp+q^Tq), \quad h_f=-J_2=-\tfrac{1}{2}\psi^T\sigma_2\psi, \\ \Delta_1=L_1=\tfrac{1}{2}(p^T\sigma_1 p+q^T\sigma_1 q), \quad \Delta_2=J_1=(i/2)(q^T\sigma_2 p-p^T\sigma_2 q), \\ \Delta_3=L_3=\tfrac{1}{2}(p^T\sigma_3 p+q^T\sigma_3 q). \end{gathered} \tag{31}$$

The canonical Dirac bracket algebra of these charges read

$$\{\Delta_k,\Delta_m\}=2\epsilon_{kmn}\Delta_n, \quad \{h_b,\Delta_k\}=0, \quad \{h_f,\Delta_k\}=0, \tag{32}$$

and can be seen to agree with the bosonic sector of the GL(2|1) algebra, Eq. (9), when the classical Dirac bracket algebra is quantized through the usual replacement $\{\ldots,\ldots\}\to -i[\ldots,\ldots]_{\mp}$.

Next we redefine the supersymmetry generators (22) as

$$\begin{gathered} Q_R=\frac{1}{2}(Q_0+iQ_2)=\frac{1}{\sqrt{2}}(p^T+iq^T)T_+\psi, \\ \bar{Q}_R=\frac{1}{2}(Q_0-iQ_2)=\frac{1}{\sqrt{2}}(p^T-iq^T)T_-\psi, \end{gathered} \tag{33}$$

$$Q_L=\frac{1}{2}(Q_1+iQ_3)=\frac{1}{\sqrt{2}}(p^T-iq^T)\sigma_1 T_+\psi,$$

$$\bar{Q}_L=\frac{1}{2}(Q_1-iQ_3)=\frac{1}{\sqrt{2}}(p^T+iq^T)\sigma_1 T_-\psi,$$

where $T_\pm=\frac{1}{2}(1\mp\sigma_2)$ is the "helicity" projection operator. Using the generalized Dirac brackets, Eq. (23), we can verify that the nine symmetry generating operators in Eqs. (31) and (33) possess an algebra whose quantum version is isomorphic to that presented in Sec. II. Moreover, if we introduce, as usual, the representation of the phase-space variables q_k and p_k in terms of creation and annihilation operators as

$$a_k=\frac{1}{\sqrt{2}}(q_k+ip_k),\quad a_k^\dagger=\frac{1}{\sqrt{2}}(q_k-ip_k), \tag{34}$$

and define

$$a_3=\frac{i}{\sqrt{2}}(\psi_1+i\psi_2),\quad a_3^\dagger=\frac{-i}{\sqrt{2}}(\psi_1-i\psi_2), \tag{35}$$

which, by virtue of Eq. (23) do satisfy Eq. (3), then we can write the generators of symmetry in Eqs. (31) and (33) in the same form as the graded Lie algebra generators (6) and (7), defined in Sec. II. It becomes a matter of simple calculation to verify that these nine charges (five bosonic and four fermionic) exactly satisfy the graded Lie algebra GL(2|1) found in Sec. II.

IV. SPECTRUM AND SUPERSPACE FORMULATION

Let us examine in this section the action of the GL(2|1) operators, defined in the previous sections, on the states of the Hilbert space of the quantum mechanical model. The spectrum of the normal ordered theory is given by $\{\mathscr{E}_n,|n\rangle\}$, where the eigenvalues and eigenvectors are

$$\mathscr{E}_n=n_++n_-+n_f,\quad |n\rangle=|n_+,n_-,n_f\rangle, \tag{36}$$

with $n_\pm=0,1,2,\ldots$ and $n_f=0,1$. Conventionally, the states with $n_f=0(1)$ are called bosonic (fermionic). Here $n_\pm$ and n_f are the eigenvalues of the bosonic and fermionic number operators, $N_\pm=a_\pm^\dagger a_\pm$ and $N_f=a_3^\dagger a_3$, and

$$a_\pm=\frac{1}{\sqrt{2}}(a_1\pm ia_2). \tag{37}$$

By inspection we see that the ground state is a nondegenerate bosonic state with zero energy. The first excited level is threefold degenerate, possessing one fermionic and two bosonic states. The second excited energy level is fivefold degenerate, with two fermionic and three bosonic states, and so on. The states of the first few levels are displayed below:

$$
\begin{aligned}
|0\rangle &= |0,0,0\rangle, \\
|1\rangle &= \{|1,0,0\rangle, |0,0,1\rangle, |0,1,0\rangle\}, \\
|2\rangle &= \{|2,0,0\rangle, |1,0,1\rangle, |1,1,0\rangle, |0,1,1\rangle, |0,2,0\rangle\}, \\
&\vdots .
\end{aligned}
\tag{38}
$$

In terms of the raising and lowering (chiral) operators (37), the GL(2|1) generators (6) and (7) read

$$
\begin{aligned}
&Q_R = a_+^\dagger a_3, \quad \bar{Q}_R = a_+ a_3^\dagger, \quad Q_L = i a_- a_3^\dagger, \\
&\bar{Q}_L = -i a_-^\dagger a_3, \quad \Delta_1 = a_+^\dagger a_- + a_-^\dagger a_+, \quad \Delta_2 = a_+^\dagger a_+ - a_-^\dagger a_-, \\
&i\Delta_3 = a_-^\dagger a_+ - a_+^\dagger a_-, \quad h_b = a_+^\dagger a_+ + a_-^\dagger a_-, \quad h_f = a_3^\dagger a_3 .
\end{aligned}
\tag{39}
$$

On the degenerate levels the supersymmetry generators take bosonic states into fermionic ones and vice versa as

$$
\begin{aligned}
Q_R|n_+,n_-,n_f\rangle &= \sqrt{n_+ + 1}\,\delta_{n_f,1}|n_+ + 1, n_-, n_f - 1\rangle, \\
\bar{Q}_R|n_+,n_-,n_f\rangle &= \sqrt{n_+}\,\delta_{n_f,0}|n_+ - 1, n_-, n_f + 1\rangle, \\
Q_L|n_+,n_-,n_f\rangle &= i\sqrt{n_-}\,\delta_{n_f 0}|n_+, n_- - 1, n_f + 1\rangle, \\
\bar{Q}_L|n_+,n_-,n_f\rangle &= -i\sqrt{n_- + 1}\,\delta_{n_f,1}|n_+, n_- + 1, n_f - 1\rangle.
\end{aligned}
\tag{40}
$$

Quite clearly the supersymmetry charge $Q_R(\bar{Q}_R)$ creates (destroys) a right-handed boson and destroys (creates) a fermion. Similarly the $Q_L(Q_L)$ destroys (creates) a left-handed boson while creating (destroying) a fermion. Note that Q_R and Q_R (Q_L and Q_L) have no effect on the $n_-(n_+)$ eigenvalues, showing the existence of a chiral supersymmetry which, ultimately, is due to the fact that we have twice as many bosonic variables as the fermionic ones. The supersymmetry charges can be used to generate the states in a given level once the highest state is given. Then, starting from the state $|0,n,0\rangle$, one can generate all the states belonging to the $\mathscr{E}_n$ subspace by consecutive applications of Q_L and Q_R until the state $|n,0,0\rangle$ is reached:

$$
|n,0,0\rangle \overset{Q_R}{\leftarrow} |n-1,0,1\rangle \overset{Q_L}{\leftarrow} |n-1,1,0\rangle \ldots |0,n-1,1\rangle \overset{Q_L}{\leftarrow} |0,n,0\rangle. \tag{41}
$$

Similarly, starting with the state $|n,0,0\rangle$ and using consecutively the charges $\bar{Q}_R$ and $\bar{Q}_L$ one generates the whole subspace $\mathscr{E}_n$ again.

$$
|n,0,0\rangle \xrightarrow{\bar{Q}_R} |n-1,0,1\rangle \xrightarrow{\bar{Q}_L} |n-1,1,0\rangle \ldots |0,n-1,1\rangle \xrightarrow{\bar{Q}_L} |0,n,0\rangle. \tag{42}
$$

This action of the supersymmetry charges is easily seen on the set of states shown in Eq. (38).

On the other hand, the action of the bosonic operators only connect states with the same fermion number. The operators h_f, h_b, and Δ_2 are diagonal in the chiral basis (36):

$$h_b|n_+,n_-,n_f\rangle=(n_++n_-)|n_+,n_-,n_f\rangle,$$
$$\Delta_2|n_+,n_-,n_f\rangle=(n_+-n_-)|n_+,n_-,n_f\rangle, \tag{43}$$
$$h_f|n_+,n_-,n_f\rangle=n_f|n_+,n_-,n_f\rangle.$$

These operators have the usual interpretation as bosonic and fermionic Hamiltonians (h_b and h_f), and chirality operator (Δ_2). Finally, the nondiagonal bosonic operators Δ_1 and Δ_3 play the role of chirality changing operators:

$$\tfrac{1}{2}(\Delta_1+i\Delta_3)|n_+,n_-,n_f\rangle=\sqrt{(n_-+1)n_+}|n_+-1,n_-+1,n_f\rangle,$$
$$\tfrac{1}{2}(\Delta_1-i\Delta_3)|n_+,n_-,n_f\rangle=\sqrt{(n_++1)n_-}|n_++1,n_--1,n_f\rangle. \tag{44}$$

Concluding, relations (40), (43), and (44) represent the action of all the GL(2|1) generators on the Hilbert space of the 2D SUSY harmonic oscillator.

We finish this section with a discussion of the superspace formulation of this problem. To this end we rewrite the supersymmetry transformations (19) in terms of the transformations generated by the chiral supersymmetry charges (33), which seem to be more appropriate for this model. The transformations generated by Q_R, $\bar{Q}_R$, Q_L, and $\bar{Q}_L$ are, respectively,

$$\delta_R q=\epsilon_R T_+\psi, \quad \delta_R\psi=\epsilon_R T_-\mathscr{D}_+ q, \tag{45}$$

$$\bar{\delta}_R q=\bar{\epsilon}_R T_-\psi, \quad \bar{\delta}_R\psi=\bar{\epsilon}_R T_+\mathscr{D}_- q, \tag{46}$$

$$\delta_L q=\epsilon_L T_+\sigma_1\psi, \quad \delta_L\psi=\epsilon_L T_+\sigma_1\mathscr{D}_- q, \tag{47}$$

$$\bar{\delta}_L q=\bar{\epsilon}_L T_-\sigma_1\psi, \quad \bar{\delta}_R\psi=\bar{\epsilon}_L T_-\sigma_1\mathscr{D}_+ q. \tag{48}$$

Here we have introduced the notation $\mathscr{D}_\pm=i(\partial_t\pm i)$. To obtain these four supersymmetries in a superfield language, we introduce two Grassman variables for each chiral sector as θ_R, $\bar{\theta}_R$, θ_L, and $\bar{\theta}_L$, and define two chiral superfields ϕ_R and ϕ_L. The transformation in the right chiral sector can be obtained from the following superfield and (differential operator) supercharge:

$$\phi_R=q+\theta_R T_+\psi+\bar{\theta}_R T_-\psi, \quad Q_R=T_+\frac{\partial}{\partial\theta_R}-\bar{\theta}_R T_-\mathscr{D}_+, \quad \bar{Q}_R=T_-\frac{\partial}{\partial\bar{\theta}_R}-\theta_R T_+\mathscr{D}_-, \tag{49}$$

while those in the left chiral sector come from

$$\phi_L=q+\theta_L T_+\sigma_1\psi+\bar{\theta}_L T_-\sigma_1\psi, \quad Q_L=T_+\frac{\partial}{\partial\theta_L}-\bar{\theta}_L T_-\mathscr{D}_-, \quad \bar{Q}_L=T_-\frac{\partial}{\partial\bar{\theta}_L}-\theta_L T_+\mathscr{D}_+. \tag{50}$$

These transformations can be organized in a matrixlike structure with the following form:

$$\delta\Phi=\epsilon^T\mathbf{Q}\Phi, \quad \bar{\delta}\Phi=\bar{\epsilon}^T\bar{\mathbf{Q}}\Phi, \tag{51}$$

where

$$\mathbf{Q}=\begin{pmatrix} Q_R & 0 \\ 0 & Q_L \end{pmatrix}, \tag{52}$$

$$\overline{\mathbf{Q}}=\begin{pmatrix} \bar{Q}_R & 0 \\ 0 & \bar{Q}_L \end{pmatrix} \tag{53}$$

are block-diagonal (4×4) matrices and

$$\Phi=\begin{pmatrix} \phi_R \\ \phi_L \end{pmatrix}, \tag{54}$$

$$\epsilon=\begin{pmatrix} \epsilon_R \\ \epsilon_L \end{pmatrix} \tag{55}$$

are (4×1) column matrices. We notice here that a matrix structure is essential for the superspace formulation since the GLA, in this case, grades an internal symmetry algebra [e.g., Eq. (8) involves not just the Hamiltonian, but the internal symmetry generators as well which would have a matrix representation]. The matrix structure of Q would depend on the internal space upon which it acts (unlike the usual space-time supersymmetry charges) and the form given here is appropriate only for the doublet space of q and ψ. Next we introduce the four covariant derivatives as

$$D_R=T_-\frac{\partial}{\partial\theta_R}+\bar{\theta}_R T_+\mathscr{D}_+, \quad \bar{D}_R=T_+\frac{\partial}{\partial\bar{\theta}_R}-\theta_R T_-\mathscr{D}_-, \tag{56}$$

$$D_L=T_-\frac{\partial}{\partial\theta_L}+\bar{\theta}_L T_+\mathscr{D}_-, \quad \bar{D}_L=T_+\frac{\partial}{\partial\bar{\theta}_L}-\theta_L T_-\mathscr{D}_+, \tag{57}$$

and define

$$\mathbf{D}=\begin{pmatrix} D_R & 0 \\ 0 & D_L \end{pmatrix}, \tag{58}$$

$$\overline{\mathbf{D}}=\begin{pmatrix} \bar{D}_R & 0 \\ 0 & \bar{D}_L \end{pmatrix}. \tag{59}$$

These covariant derivatives can be easily seen to anticommute with all supersymmetry charges $\mathbf{Q}$ and $\overline{\mathbf{Q}}$. In terms of these covariant derivatives, the Lagrangian of this theory can be written as

$$\begin{aligned} L&=\frac{1}{2}\sum_{A=R,L}\int d\theta_A\, d\bar{\theta}_A[(\overline{\mathbf{D}}\Phi)^T\cdot(\mathbf{D}\Phi)-\Phi^T\cdot\overline{\mathbf{D}}\mathbf{D}\Phi] \\ &=\frac{1}{2}\sum_{A=R,L}\int d\theta_A\, d\bar{\theta}_A[(\bar{D}_A\phi_A)^T\cdot(D_A\phi_A)-\phi_A^T\cdot\bar{D}_A D_A\phi_A]. \end{aligned} \tag{60}$$

V. CONCLUSION

In this work we have studied a supersymmetric harmonic oscillator possessing twice as many bosonic variables than fermionic ones. The model enjoys a chiral supersymmetry when the fermionic variables are interchanged with either one of the chiral bosonic sectors. Besides the supersymmetries, we have worked out all the global symmetries of the model and verified that the generators provide a representation of the general graded Lie algebra GL(2|1). We have worked out the physical spectrum of this model and constructed the superspace formulation. It is interest-

ing to see that in the superspace language the separation of the chiral sectors are clearly displayed, and the charges and the covariant derivatives carry a matrix structure essentially because the algebra represents the grading of an internal symmetry group.

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APPENDIX: GENERALIZED DIRAC BRACKETS VIA FADDEEV-JACKIW APPROACH

First-order Lagrangians are constrained systems and must be quantized with Dirac brackets instead of Poisson brackets.[7,8] The Dirac brackets of an arbitrary first-order system can be calculated with ease using the technique put forward by Faddeev and Jackiw a few years ago.[9] Consider an arbitray system with a finite number of degrees of freedom Z_A, whose Grassman parity is ϵ_A and is described by

$$L=\dot{Z}_A K_A(Z_A)-V(Z_A). \tag{A1}$$

The equations of motion read

$$\dot{Z}_B M_{BA}=-\frac{\partial V}{\partial Z_A}, \tag{A2}$$

where

$$M_{AB}=\frac{\partial K^B}{\partial Z_A}-(-1)^{\epsilon_A\epsilon_B}\frac{\partial K^A}{\partial Z_B} \tag{A3}$$

is the generalized sympletic matrix.[10] If the sympletic matrix is nonsingular, the equation of motion (A2) can be solved for the velocities as

$$\dot{Z}_A=(-1)^{\epsilon_A}M^{-1}_{AB}\frac{\partial V}{\partial Z_B} \tag{A4}$$

and be written in Hamiltonian form with the introduction of some generalized or Dirac bracket as

$$\{Z_A,Z_B\}=(-1)^{\epsilon_A}M^{-1}_{AB}. \tag{A5}$$

The equations of motion then take the following form:

$$\dot{Z}_A=\{Z_A,V(Z)\}. \tag{A6}$$

Using Eq. (A5) one can verify that the Dirac brackets for the fermionic variables of the supersymmetric two-dimensional oscillator are those given in Eq. (23).[11]

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Vertex normal ordering as a consequence of nonsymmetric bilinear forms in Clifford algebras

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We consider Clifford algebras with nonsymmetric bilinear forms. They parametrize the chosen ideal in the isomorphism class of the standard symmetric ones. Since the content of physical theories depends on the injection $\oplus^{n}\bigwedge^{n}\mathscr{V}\to CL(\mathscr{V},Q)$, one has to transform to the standard construction. The injection is described by the antisymmetric part of the bilinear form. This process results in the appropriate vertex normal ordering terms, which are now obtained from the theory itself and not added *ad hoc* via a regularization argument. © *1996 American Institute of Physics.* [S0022-2488(96)01601-1]

I. INTRODUCTION

Nonlinear spinor equations play an important role in high-energy, nuclear or solid state physics. Examples are the Heisenberg, Nambu, and Jona–Lasinio-like models[1,2] of elementary particle and nuclear physics. Nonlinear sigma models bear an analogous structure.[3] In solid state physics the Hubbard model[4] is applied to various phenomena from super conductivity up to spin chains and so on.

The general structure of such models is of the form

$$\left(\sum i\gamma^{\mu}\partial_{\mu}-m\right)_{II'}\Psi_{I'}=gV_{II'I''I'''}\Psi_{I'}\Psi_{I''}\Psi_{I'''}. \tag{1}$$

Here $\Sigma i\gamma^{\mu}\partial_{\mu}$ is the Dirac operator, with Euclidean or Lorentzian signature. The mass could be zero. With the multi index $I=\{K,\Lambda\}$ we represent the spinor and its adjoined by Λ and the other algebraic and spatio temporal indices by K.

If the adjoined spinor is fixed, the quadratic form of the Clifford algebra is completely determined. Usually canonical quantization is applied. The quantization procedure chooses in fact the ideal which generates the Clifford algebraic structure, i.e., the commutator

$$\{\Psi_I,\Psi_{I'}\}_{+}=\langle\Psi_I|\Psi_{I'}\rangle=\delta_{II'}. \tag{2}$$

There are several problems with these equations listed below.

(i) The equations are non-renormalizable.
(ii) In order to define a unique quantization procedure, one is troubled by the ordering problem.
(iii) The transition to normal ordered amplitudes yields additional Singularities. (In Fock space this is the Wick–Dyson normal ordering. The algebraic argument given below is also valid in the general case, defined in Ref. 5 but then only the two-point correlations are retracted.)

In solid state physics there seems to be no principal problem with (i), because there may be a physically motivated cutoff at the Brillouin zone. In the case of particle physics, several *ad hoc* regularizations become necessary. An approach to these topics will be given elsewhere[6] and we assume the theory to be regularized.

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The second point is usually solved using causality arguments. They imply a natural ordering in the polynomials of the fields at hand. Therefore time-ordered products are used in the covariant formulation, see for example, Ref. 7. In the Hamilton formalism, the (anti)symmetric ordering could be used.

Including a somehow given Vacuum state $|0\rangle_{Ph}$, which gives the representation of the field operators $\Pi_{Ph}(\Psi_I)$, all quantities are formally (formally, because one has to show uniqueness and existence of the defined objects too, which is a nontrivial problem) defined, see part III also. One should be able to calculate this vacuum state in a nonlinear theory, by solving the dynamical problem at hand in a sort of self consistent problem.

Now the third point causes trouble, because transition from one ordering to another yields infinities. In Fock space this transformation equals a Wick–Dyson normal ordering of the vertex.[8] The Fock space is only appropriate in free theories or in perturbation theory, which proves not useful in our case. A nonperturbative treatment is given in Ref. 5. This process results in the desired amplitudes and so-called contractions, which for bilinear and higher-order terms yields singularities at least on the light cone.

Even if the propagator function is finite on the light cone, the resulting terms would destroy the accuracy of the theory by additional corrections.

These contractions are related to the finite ground state energies, which become infinite by field quantization. With the convention that the vacuum has no nonzero quantum numbers, the vertex regularization is related to finite normal ordered amplitudes.[9] The field equations read now

$$\left(\sum i\gamma^{\mu}\partial_{\mu}-m\right)_{II'}\Psi_{I'}=gV_{II'I''I'''}:\Psi_{I'}\Psi_{I''}\Psi_{I'''}: . \tag{3}$$

With the physical propagator

$$P_{II'}:={}_{Ph}\langle 0|\mathscr{T}(\Psi_I\Psi_{I'})|0\rangle_{Ph} \tag{4}$$

the vertex term changes to

$$:\Psi_{I'}\Psi_{I''}\Psi_{I'''}:=\Psi_{I'}\Psi_{I''}\Psi_{I'''}+P_{I'I''}\Psi_{I'''}-P_{I'I'''}\Psi_{I''}+P_{I''I'''}\Psi_{I'} . \tag{5}$$

However, this procedure is nothing but a shift of the problem from one equation into another, because the time-ordered equation becomes singular. The first proposed theory is then ill defined, if we require the normal-ordered equation to be finite and vice versa. Changing the ordering thus yields singularities.

In this paper we want to show how an embedding of the theory in a Clifford algebra structure can overcome this problem by generating a normal ordering, which does not produce any additional singular contributions. So above item (iii) is resolved. We consider nonsymmetric bilinear forms and the associated Clifford algebras. The transformation from such algebras to the symmetric ones is an isomorphism, but the linear space of antisymmetric p-vectors is moved. As physical information is coded therein it is therefore altered.

Progress in the relation of states and operators was made in Ref. 10. The relation of Clifford algebras and quantum mechanics was studied in Ref. 11. The algebraic differences of matrix and conventional column spinors are analyzed in Ref. 12. Nonsymmetric Clifford algebras where introduced in a more mathematical way in Ref. 13.

In Sec. II, a brief introduction to the construction of Clifford algebras with arbitrary bilinear-forms is given. In Sec. III an application is given to quantum field theory. The Appendix gives a low-dimensional example of the desired algebraic structure.

II. CLIFFORD ALGEBRAS WITH NONSYMMETRIC BILINEAR FORMS

In this section we will present Clifford algebras with nonsymmetric bilinear forms, and various multivector constructions. Choosing the appropriate one, the nonsymmetric part of the form is removed.

Clifford algebras entered particle physics with Pauli and Dirac,[14] who used it to linearize the Laplacian and the D'Alambertian.

Let $\mathscr{V}$ be a vector space over R or C and Q a quadratic form on $\mathscr{V}$. The Clifford map is an injection from $\mathscr{V}$ into $CL(\mathscr{V},Q)$ with the property that every square of a vector element of the Clifford algebra is a scalar:

$$\begin{gathered}\gamma: V \to CL(\mathscr{V},Q), \quad e_i \mapsto \gamma_i = \gamma(e_i) \\ x^2 = xx = x \cdot x = Q(x) \in (R,C).\end{gathered} \tag{6}$$

With linearization we have on a generating set of $\mathscr{V}$

$$\begin{gathered}(e_i+e_j)(e_i+e_j) = e_i^2 + e_j^2 + e_i e_j + e_j e_i, \\ e_i e_j + e_j e_i = Q(e_i+e_j) - Q(e_i) - Q(e_j) \\ =: 2G(e_i,e_j) \in (R,C).\end{gathered} \tag{7}$$

The bilinear form G is symmetric. The whole algebra is now generated from reduced products of one-vectors. Let N be the set of ordered partitions of n pieces, $|\alpha|$ the cardinality of such a subset, and include the empty set. If we define $1_A = e_0$, then an algebra element read

$$\begin{gathered}A = \sum_{\alpha \in N} a_\alpha e_\alpha = \sum_{r=0}^{n} \sum_{|\alpha|=r} a_r e_r = A_0 + A_1 + \cdots + A_n, \\ e_\alpha := e_{i_1} \wedge e_{i_2} \wedge \cdots \wedge e_{i_r}, \quad i_1 < i_2 \cdots < i_r, \quad \alpha \in N, \quad |\alpha| = r.\end{gathered} \tag{8}$$

The A_r are homogeneous of degree r and the wedge product means antisymmetric multiplication as in the Grassmann case. Indeed as a linear space these two constructions are identical. Thereby the Clifford algebra has the direct sum decompositions

$$\begin{gathered}CL(V,Q) = CL_+ \oplus CL_- \quad \text{as algebra, and} \\ CL(V,Q) = \oplus^n \wedge^n \mathscr{V} \quad \text{as linear space.}\end{gathered} \tag{9}$$

However, the Clifford product intermingles the grades. Let $\langle\ \rangle_r$ be the projector to the homogeneous part of grade r. Then one has

$$A_r B_s = \langle AB \rangle_{|r-s|} + \langle AB \rangle_{|r-s+2|} + \cdots + \langle AB \rangle_{r+s}, \tag{10}$$

where in the Grassmann case $A_r B_s = \langle AB \rangle_{r+s}$ results.

Physicists consider the anticommuting elements of grade r as, e.g., scalars, spinors (vectors), spin tensors (tensors), and so on. That is, the physical content of the theory is coded explicitly in this structure.

Now let us see in which way it is possible to introduce nonsymmetric bilinear forms. It is obvious that we have to leave the above construction in favor of a more general one. This can be done by introducing algebra derivatives as proposed by Chevalley and Riesz[15,16] or analogous to Oziewicz.[13]

First of all, we introduce two more algebraic constructions for further use. An involution (a property sometimes called conjugation) J of period two and the also involutive Reversion$\tilde{}$ by the rules

$$J\begin{cases} K^2 & := \quad id_A \\ J(XY) & := \quad j(X)J(Y), \\ J(R,C) & := \quad (R,\overline{C}), \end{cases}$$
$$\tilde{}\begin{cases} \tilde{\tilde{}} & := \quad id_A, \\ \langle\tilde{}\rangle_{0+1} & := \quad id_{A_0+A_1}, \\ (XY)\tilde{} & := \quad \tilde{Y}\,\tilde{X}. \end{cases} \tag{11}$$

Now we may introduce the desired formulas ($a \in \mathscr{V}; B \in A$)

$$a\rfloor B := \tfrac{1}{2}(aB - J(B)a), \quad a\dot{\wedge} B := \tfrac{1}{2}(aB + J(B)a); \tag{12}$$

herewith we may decompose the Clifford product to

$$aB = a\rfloor B + a\dot{\wedge} B. \tag{13}$$

The contraction $\rfloor$ is a graded derivative of degree 1, as can be seen as follows (graded Leibnitz rule):

$$\begin{aligned} a\rfloor(bc) &:= \tfrac{1}{2}(abc - J(bc)a) \\ &= \tfrac{1}{2}(abc - J(b)ac + J(b)ac - J(b)J(c)a) \\ &= (a\rfloor b)c + J(b)(a\rfloor c). \end{aligned} \tag{14}$$

With $bc = 1$ we have $a\rfloor 1 = 2a\rfloor 1$, so $a\rfloor(R,C) = 0$, from which we could prove by induction the homogeneity of $a\rfloor B_r$. Obviously the contraction is linear, that is,

$$(\alpha X + \beta Y)\rfloor A = \alpha X\rfloor A + \beta Y\rfloor A. \tag{15}$$

These properties together state that $\rfloor$ is an algebra derivation. One can easy prove the useful formulas[17]

$$(u\wedge v)\rfloor X = u\rfloor(v\rfloor(X))$$

$$a\rfloor(x_{i_1}\wedge\cdots\wedge x_{i_n}) = \sum_{i=1}^{n}(-)^{i-1}(a\rfloor x_i)(x_1\wedge\cdots\wedge_{i-1}\wedge x_{i+1}\wedge\cdots\wedge x_n)$$
$$\det(x_i\rfloor x_j) = (x_n\wedge\cdots\wedge x_1)\rfloor(x_1\wedge\cdots\wedge x_n)$$
$$= x_n\rfloor(x_{n-1}\rfloor\cdots(x_1\rfloor(x_1\wedge\cdots\wedge x_n))\cdots). \tag{16}$$

Now the asymmetry of this result is obvious, and we may define an arbitrary nondegenerate bilinear form B exactly as the contraction. In a not-necessarily orthonormalized system of generating elements e_i of $\mathscr{V}$ we have

$$B = G + F = [B_{ij}] = [e_i\rfloor e_j], \tag{17}$$

$$G^T=G, \quad F^T=-F.$$

The injection, introduced by Chevalley, $\bigwedge \mathscr{V} \to CL(\mathscr{V},Q)$, is of course known by physicists in the disguise of the Kähler–Atiyah isomorphism. (See Ref. 17 for an account on that, and for a review on the historical development.)

We have identified the Clifford algebra as a subalgebra of $End(\oplus_n \bigwedge^n \mathscr{V})$, the endomorphism algebra of the Grassmann algebra. A very explicit example will be given in the appendix, in a manner closely related to the work of Lounesto.

Clearly, if we had chosen J to be the common use involution on $\mathscr{V}$, that is, $J(\mathscr{V})=-\mathscr{V}$, we would reobtain the original formulas, with a symmetric bilinearform

$$G_{ij}=\tfrac{1}{2}(e_ie_j-J(e_j)e_i)=\tfrac{1}{2}(e_ie_j+e_je_i). \tag{18}$$

Thus, if there exists a distinct involution of period two, we have the desired extension.

Now we have from (13),

$$e_{i_1}\wedge e_{i_2}=e_{i_1}e_{i_2}-e_{i_1}\rfloor e_{i_2}=e_{i_1}e_{i_2}-B_{i_1i_2}, \tag{19}$$

which is not antisymmetric with respect to the reversion as one can see as follows:

$$\begin{aligned}(e_{i_1}\wedge e_{i_2})^{\tilde{}} &=(e_{i_1}e_{i_2}-B_{i_1i_2})^{\tilde{}}\\ &=e_{i_2}e_{i_1}-B_{i_2i_1}+(B_{i_2i_1}-B_{i_1i_2})\\ &=e_{i_2}\wedge e_{i_1}+(B^T_{i_1i_2}-B_{i_1i_2})\\ &=e_{i_2}\wedge e_{i_1}+2F_{i_1i_2}\neq e_{i_2}\wedge e_{i_1}.\end{aligned} \tag{20}$$

Here T means matrix transposition. To avoid such a situation, and for establishing the reversion as the (Hermitian) transpose of the matrix representation, we are forced to choose the bi- and multivectors in a definite way. With $i_1<i_2<\cdots$, we set

$$\begin{aligned}e_{i_1}\dot{\wedge}e_{i_2}:&=\tfrac{1}{2}(e_{i_1}\wedge e_{i_2}-e_{i_2}\wedge e_{i_1})\\ &=\tfrac{1}{2}(e_{i_1}e_{i_2}-B_{i_1i_2}-e_{i_2}e_{i_1}+B_{i_2i_1})\\ &=\tfrac{1}{2}(e_{i_1}e_{i_2}-e_{i_2e_{i_1}})-\tfrac{1}{2}(B_{i_1i_2}+B_{i_2i_1})\\ &=e_{i_1}\wedge e_{i_2}-F_{i_1i_2}\end{aligned} \tag{21}$$

where B is now split into symmetric and antisymmetric parts $B=G_S+F_A$, with respect to the usual matrix transpose. We obtain the following rules, utilizing now the *standard* involution.

$$\begin{aligned}G_{i_1i_2}&=\tfrac{1}{2}(e_{i_1}e_{i_2}+e_{i_1}e_{i_2})\\ e_{i_1}\dot{\wedge}e_{i_2}&=\tfrac{1}{2}(e_{i_1}e_{i_2}-(e_{i_1}e_{i_2})^{\tilde{}})\\ &=\tfrac{1}{2}(e_{i_1}e_{i_2}-e_{i_2}e_{i_1})\\ &=\tfrac{1}{2}(e_{i_1}\rfloor e_{i_2}+e_{i_1}\wedge e_{i_2}-e_{i_2}\rfloor e_{i_1}-e_{i_2}\wedge e_{i_1})\\ &=e_{i_1}\wedge e_{i_2}+F_{i_1i_2},\end{aligned} \tag{22}$$

and therefore now

$$(e_{i_1}\dot{\wedge}e_{i_2})\tilde{} = e_{i_2}\dot{\wedge}e_{i_1} = -e_{i_1}\dot{\wedge}e_{i_2},$$
$$J(e_{i_1}\dot{\wedge}e_{i_2}) = e_{i_1}\dot{\wedge}e_{i_2}. \tag{23}$$

A third-order term will be given as

$$e_{i_1}\dot{\wedge}e_{i_2}\dot{\wedge}e_{i_3} = \tfrac{1}{2}(e_{i_1}e_{i_2}\dot{\wedge}e_{i_3} + e_{i_2}\dot{\wedge}e_{i_3}e_{i_1})$$
$$= e_{i_1}\wedge e_{i_2}\wedge e_{i_3} + F_{i_1i_2}e_{i_3} + F_{i_2i_3}e_{i_1} - F_{i_1i_3}e_{i_2}. \tag{24}$$

If we would like to have the transposition to act trivial on the matrix representation of the vector elements, we have to introduce a dual set of generating elements, as discussed in the Appendix.

We are now able to construct a new generating system of the Clifford algebra, which is antisymmetric with respect to the reversion, by using the corresponding wedge product $\dot{\wedge}$.

$$\{e_0; e_{i_1}; e_{i_1}\dot{\wedge}e_{i_2}; e_{i_1}\dot{\wedge}e_{i_2}\dot{\wedge}e_{i_3}; \dots\}, \quad \forall i_n; \quad i_1 < i_2 < \cdots . \tag{25}$$

We finish this section by recalling the main consequences of the analysis done, with respect to the application in Sec. III.

If there is a nonsymmetric part in the contraction, then the usual multivectors are not the desired algebraic elements. The nondiagonal part of the contraction leads to a refined treatment of the algebraic properties. The antisymmetric parts are incorporated in the multivectorial structure, where as the symmetric part should be handled with dual sets of generating elements. The matrix transposition is equivalent to the reversion only in this special situation, or if $G_{i_1i_2} = \delta_{i_1i_2}$ to the Cartesian case.

By looking at these constructions, we are forced to introduce a new kind of multivector. As a Clifford algebra, the two constructions prove to be isomorphic, at least in the nondegenerate case. However, the linear spaces $\oplus^n \wedge^n \mathscr{V}$ and $\oplus^n \mathrm{span}\{e_{i_1\dots i_n}\}$ are quite differently represented. This quite general result will be applied as an example to the nonlinear spinor theory, but is not confined to that case at all.

III. APPLICATION TO THE NONLINEAR SPINOR FIELD MODEL

In this section the vertex normal ordering is given as a consequence of the algebraic formalism. The connection between $\mathscr{T}$ and $\mathscr{N}$ ordered amplitudes is one-to-one, if the construction itself exists. No *ad hoc* regularization argument is needed.

Now we want to have a look at the vertex term of the nonlinear spinor field theory. This should correctly be done in the functional space formulation, which exhibits the structure more clearly.[5] For brevity and simplicity, we will give our arguments directly on the level of the field operators.

We should note that the above construction was made with a finite Set N, where as in field theory we use the continuum indices $(\vec{r},t)$ also. Therefore we should construct infinite Clifford algebras and prove their existence. Such things are far from being easy.[18] Of course we are still considering a singular theory before introduction of a here-not-specified regularization. So we proceed with formal algebraic arguments, valid only if the symbols used are defined. Otherwise one has to use increasing nets of finite lattices and to study convergence properties.

The quantization of fermionic fields is in effect the introduction of a Clifford algebra, or CAR algebra as in this context usually named:[6,19]

$$\{\Psi_K^\dagger, \Psi_{K'}\}_+ = \delta_{KK'}\,. \tag{26}$$

With our indexing $\Psi_I = \Psi_{K\Lambda} = \{\Psi_{K1}^\dagger; \Psi_{K2}\}$ we have

$$\{\Psi_I, \Psi_{I'}\} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}_{\Lambda\Lambda'} \delta_{KK'}\,. \tag{27}$$

This is, of course, a special basis; we may call it a Witt basis.[19] If the Hermitean conjugation is the usual one, then the connection to Fock space is very close.[20] Therefore we will expect to have an (in this formulation) invisible antisymmetric part. So it is essential to have non-Fock states. This relation can be rewritten in the form

$$\Psi_I \rfloor \Psi_{I'} + \Psi_{I'} \rfloor \Psi_I = 2G_{II'} = \delta_{II'}\,, \tag{28}$$

which now can be extended to an arbitrary bilinear form B. We obtain in this way the antisymmetric part, exhibiting a new term $2F_{II'}$

$$\begin{aligned}[\Psi_I, \Psi_{I'}] &= 2F_{II'} + 2\Psi_I \barwedge \Psi_{I'} \\ &= 2\Psi_I \dot{\barwedge} \Psi_{I'}\,.\end{aligned} \tag{29}$$

From the Clifford algebraic point of view, this corresponds to the scalar and bivector part, if we use the usual wedge product.

This entity is in fact related with the propagator of the theory:

$$\begin{aligned}P_{II'} &= {}_{Ph}\langle 0|\mathscr{T}(\Psi_I \Psi_{I'})|0\rangle_{Ph} \\ &= \tfrac{1}{2}{}_{Ph}\langle 0|\,\theta(t_I - t_{I'})\Psi_I\Psi_{I'} - \theta(t_{I'} - t_I)\Psi_{I'}\Psi_I|0\rangle_{Ph}\,.\end{aligned} \tag{30}$$

For equal times we have

$$\begin{aligned}P^t_{II'} &= \tfrac{1}{2}{}_{Ph}\langle 0|\Psi_I\Psi_{I'} - \Psi_{I'}\Psi_I|0\rangle_{Ph,t=t'} \\ &= {}_{Ph}\langle 0|F_{II'} + \Psi_I \barwedge \Psi_{I'}|0\rangle_{Ph,t=t'}\,.\end{aligned} \tag{31}$$

Now the $F_{II'}$ are ''scalars'', that is, in field theory a distribution-valued function, and act *not* as operators. We have the trace as the analogous algebra property only in the appropriate basis, which of course leads to

$${}_{Ph}\langle 0|\Psi_I \barwedge \Psi_{I'}|0\rangle_{Ph} = 0 \tag{32}$$

and thus to

$$P^t_{II'} = F_{II'}\,. \tag{33}$$

Looking in this way at the vertex term, we have antisymmetric products, and are free to choose the appropriate one, which absorbs the additional terms, resulting in the normal-ordering procedure. Of course, this should be done in such a way that the transposition and reversion behave in the right way, but here we will not bother about that. (See the remarks in the Appendix.)

By comparing the ''dot'' procedure defining[5]

$$:\Psi_{I'}\Psi_{I''}\Psi_{I'''}: \quad := \Psi_{I'}\Psi_{I''}\Psi_{I'''} - P_{I'I''}\Psi_{I'''} + P_{I'I'''}\Psi_{I''} - P_{I''I'''}\Psi_{I'} \tag{34}$$

with the derived equation

$$e_{i_1}\wedge e_{i_2}\wedge e_{i_3}=e_{i_1}\dot{\wedge}e_{i_2}\dot{\wedge}e_{i_3}-F_{i_1i_2}e_{i_3}+F_{i_1i_3}e_{i_2}-F_{i_2i_3}e_{i_1}, \tag{35}$$

it is shown, that if we choose $P_{II'}$ as the antisymmetric part of the contraction, then we are forced to introduce the normal-ordering terms in the field equation from the beginning. This is, because we want the usual conjugation and the multivectorial construction to hold in the algebraic and matrix case, as the usual normal-ordered field equation.

For the time-ordered field equation this yields

$$\left(\sum\ i\gamma^\mu\partial_\mu-m\right)_{II'}\Psi_{I'}=gV_{II'I''I'''}\Psi_{I'}\wedge\Psi_{I''}\wedge\Psi_{I'''}, \tag{36}$$

or

$$\left(\sum\ i\gamma^\mu\partial_\mu-m\right)_{II'}\Psi_{I'}+gV_{II'I''I'''}\{P_{I'I2''}\Psi_{I'''}-P_{I'I'''}\Psi_{I''}+P_{I''I'''}\Psi_{I'}\}$$
$$=gV_{II'I''I'''}\Psi_{I'}\dot{\wedge}\Psi_{I''}\dot{\wedge}\Psi_{I'''}. \tag{37}$$

Omitting now the interaction term [RHS of (37)] we are left with a still singular equation, but now the singularity is only the dynamical one. As proposed in the introduction, the dynamical singularities may also be treated in an algebraic manner, which will be shown elsewhere.

The Clifford algebraic point of view should of course be taken from the very beginning.

IV. CONCLUSION

With help of some results obtained by studying Clifford algebras with nonsymmetric bilinear forms, we are able to understand the process of normal ordering in a new and deeper way. We noticed the dependence of the multivectorial structure on the antisymmetric part of the contraction. Without this sort of tool, it seems hardly possible to recognize the algebraic difference between $\mathscr{T}$- and $\mathscr{N}$-ordered transition matrix elements. In fact, they belong to quite different multivector constructions.

In ordinary treatments the vertex normal ordering is done *ad hoc*, simply motivated by obtaining an afterwards finite theory. However, this is nothing but a shift of the singularities in the $\mathscr{T}$-ordered equation. The ''dot'' procedure connects singular and regular theories, which is obviously not an equivalence relation. The theory is altered by hand.

The algebraic method distinguishes the different products in a correct way, and is sensitive to the redefinition of the multivectorial structure. So a unique and one-to-one correspondence between $\mathscr{T}$- and $\mathscr{N}$-ordered equations is established, in the case where the objects do exist.

In the computation of composites one has to expect the appearance of nonsymmetric parts of the bilinear forms. This stems from the antisymmetric constructions of the composite, in which case the effective bilinearform should have such a part.

The next step is the observation that the usually obtained divergencies are related to the dynamical ones. Therefore it is obvious that they are irrelevant to the not yet well-defined theory, because they evaporate when the theory is regularized. *A posteriori* the ''dot'' procedure is thus justified as a heuristic method. However, the important thing is that we have, even in this case, to choose another time-ordered equation by introducing wedges between the vertex Ψ's. The construction itself gives the hint that we should start from the very beginning with Clifford methods. Thereby Clifford analysis, or monogenetic function theory, should provide us a finite theory, from first principles.

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APPENDIX A: PAULI ALGEBRA WITH NONSYMMETRIC BILINEAR FORM

In the Appendix an example is given, in the spirit of Lounesto.[17] Because all used quantities can only be constructed explicitly in very low-dimensional cases, we use the Pauli algebra. It is well known and the smallest Clifford algebra over the reals which exhibits a three-vector quantity.

The bilinear form is decomposed into symmetric and antisymmetric parts, using matrix transposition. We have the linear independent not normalized, not orthogonal set $\{e_1,e_2,e_3\}$ spanning $\mathscr{V}$. The algebra is generated by

$$\{Y_i\}=\{e_0;e_1,e_2,e_3;e_1\wedge e_2,e_2\wedge e_3,e_3\wedge e_1;e_1\wedge e_2\wedge e_3\}. \tag{A1}$$

In this basis the bilinear form is $(i,j \in 1,2,3)$

$$B=[B_{ij}]=[e_i\rfloor e_j]=[g_{ij}]+[f_{ij}],\quad [g_{ij}]^T=[g_{ij}],\quad [f_{ij}]^T=-[f_{ij}]. \tag{A2}$$

Next we search for a matrix representation. This can be done[17] by Clifford multiplying from the right an algebra element with all elements of the algebraic basis and expanding the result in homogeneous parts. Those are written as columns of the matrices. Matrix multiplication corresponds to the Clifford product. Of course we have

$$[1]=[\delta_{ij}], \tag{A3}$$

and we calculate as an example $[e_1]$

$$\begin{gathered}
e_1 1=e_1\\
e_1e_1=g_{11}\\
e_1e_2=e_1\rfloor e_2+e_1\wedge e_2=g_{12}+f_{12}+e_1\wedge e_2\\
e_1e_3=g_{13}+f_{13}+e_1\wedge e_3\\
e_1(e_1\wedge e_2)=e_1(e_1e_2-e_1\rfloor e_2)=g_{11}e_2-(g_{12}+f_{12})e_1\\
e_1(e_2\wedge e_3)=(g_{12}+f_{12})e_3-(g_{13}+f_{13})e_2+e_1\wedge e_2\wedge e_3\\
e_1(e_3\wedge e_1)=-g_{11}e_3+(g_{13}+f_{13})e_1\\
e_1(e_1\wedge e_2\wedge e_3)=g_{11}e_2\wedge e_3+(g_{12}+f_{12})e_3\wedge e_1+(g_{13}+f_{13})e_1\wedge e_2.
\end{gathered} \tag{A4}$$

The same can be done for the other elements, which yields

$$[e_1]=\begin{bmatrix}
0 & g_{11} & g_{12}+f_{12} & g_{13}+f_{13} & 0 & 0 & 0 & 0\\
1 & 0 & 0 & 0 & -g_{12}-f_{12} & 0 & g_{13}+f_{13} & 0\\
0 & 0 & 0 & 0 & g_{11} & -g_{13}-f_{13} & 0 & 0\\
0 & 0 & 0 & 0 & 0 & g_{12}+f_{12} & -g_{11} & 0\\
0 & 0 & 1 & 0 & 0 & 0 & 0 & g_{13}+f_{13}\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & g_{11}\\
0 & 0 & 0 & -1 & 0 & 0 & 0 & g_{12}+f_{12}\\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0
\end{bmatrix},$$

$$[e_2]=\begin{bmatrix}
0 & g_{21}+f_{21} & g_{22} & g_{23}+f_{23} & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & -f_{22} & 0 & g_{23}+f_{23} & 0\\
1 & 0 & 0 & 0 & g_{21}-f_{12} & -f_{23} & 0 & 0\\
0 & 0 & 0 & 0 & 0 & g_{22} & -g_{12}+f_{12} & 0\\
0 & -1 & 0 & 0 & 0 & 0 & 0 & g_{23}+f_{23}\\
0 & 0 & 0 & 1 & 0 & 0 & 0 & g_{12}-f_{12}\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & g_{22}\\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0
\end{bmatrix},$$

$$[e_3]=\begin{bmatrix}
0 & g_{13}-f_{13} & g_{23}-f_{23} & g_{33} & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & -g_{23}+f_{23} & 0 & g_{33} & 0\\
0 & 0 & 0 & 0 & g_{13}-f_{13} & -g_{33} & 0 & 0\\
1 & 0 & 0 & 0 & 0 & g_{23}-f_{23} & -g_{13}+f_{13} & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & g_{33}\\
0 & 0 & -1 & 0 & 0 & 0 & 0 & g_{13}-f_{13}\\
0 & 1 & 0 & 0 & 0 & 0 & 0 & g_{23}-f_{23}\\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0
\end{bmatrix}.$$

This 8×8-dimensional representation of the Pauli algebra is not reducible to a real 4×4 or complex 2×2 one. The matrix transposition is not the reversion, because the $[e_i]$ are not symmetric matrices. Also the trace is not a map in the image of (R,C) in the algebra, because there are elements with nonvanishing trace beside $[\delta_{ij}]$, which means that the trace is not a projection onto the homogeneous part of degree zero. So the matrix trace is not a linear form *in* the algebra. The trace is clearly a linear form on the matrix representation, but into the field (R,C) itself.

The element $e_1\dot{\wedge}e_2\dot{\wedge}e_3$ reads

$$[e_1\dot{\wedge}e_2\dot{\wedge}e_3]=[e_1\wedge e_2\wedge e_3-f_{12}e_3+f_{13}e_2-f_{23}e_1], \tag{A5}$$

which yields a matrix not easy to display. The entries are linear, quadratic, and cubic functions of the f_{ij} and g_{ij} parameters.

The same procedure can be done with the reordered basis, belonging to the dotted wedge product

$$\{e_1,e_2,e_3;e_1\dot{\wedge}e_2\dot{\wedge}e_3;e_0;e_1\dot{\wedge}e_2,e_2\dot{\wedge}e_3,e_3\dot{\wedge}e_1\}, \tag{A6}$$

ordered in odd and even elements. The vector elements read

$$[e_1]=\begin{bmatrix} 0 & 0 & 0 & 0 & 1 & -g_{12} & 0 & g_{31} \\ 0 & 0 & 0 & 0 & 0 & g_{11} & -g_{13} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & g_{12} & -g_{11} \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ g_{11} & g_{12} & g_{13} & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & g_{13} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & g_{11} & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & g_{12} & 0 & 0 & 0 & 0 \end{bmatrix},$$

$$[e_2]=\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -g_{22} & 0 & g_{23} \\ 0 & 0 & 0 & 0 & 1 & g_{12} & -g_{23} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & g_{22} & -g_{12} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ g_{12} & g_{22} & g_{23} & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & g_{23} & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & g_{12} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & g_{22} & 0 & 0 & 0 & 0 \end{bmatrix},$$

$$[e_3]=\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -g_{23} & 0 & g_{33} \\ 0 & 0 & 0 & 0 & 0 & g_{13} & -g_{33} & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & g_{23} & -g_{13} \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ g_{13} & g_{23} & g_{33} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & g_{33} & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & g_{13} & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & -g_{23} & 0 & 0 & 0 & 0 \end{bmatrix},$$

which yields a much more convenient and symmetric form. If the bilinear form is Euclidean, then this representation becomes symmetric with respect to the trace. In this case transposition and reversion are identical. The antisymmetric part has been absorbed fully in the multivectorial construction.

A fully satisfactory representation could be obtained by using a dual set of generating algebra elements, to the above ones. Therefore let the Volume element be

$$E:=e_1\dot{\wedge}e_2\dot{\wedge}e_3=-E^{\tilde{}},$$

$$E^{-1}=\frac{E^{\tilde{}}}{E^{\tilde{}}E},$$

$$E^{\tilde{}}E=\det G=|G|\neq 0. \tag{A7}$$

Then we may construct

$$e^i:=(-)^{i+1}e_1\dot{\wedge}\ldots e_{i-1}\dot{\wedge}e_{i+1}\dot{\wedge}\ldots e_nE^{-1} \tag{A8}$$

which is a generalization to nonsymmetric bilinear forms of the detailed results in Ref. 21.

Now the representation with the algebra basis $\{X^i\}$ yields via $[e_j X^i]$ symmetric matrices, even if the symmetric part of B is nontrivial.

This form is the most distinguished and symmetric one. Transposition and conjugation are the usual operations, but for arbitrary B the representation is still of dimension 8×8.

In this light, we have to change the ''quantization'' process, to use these dual elements. Therefore we should write

$$\Psi^I \Psi_{I'} + \Psi_{I'} \Psi^I = \delta^I_{I'} = 2G^I_{I'} . \tag{A9}$$

One can apply only in trivial cases (Euclidean G and vanishing F) ''canonical'' quantization without such a dual set and the above dotted wedge product.

In the general case the dual set depends on the possibly varying volume element of the algebra, and makes the definition of ''creation'' and ''annihilation'' operators position dependent. We may hope to get a better understanding of quantization on curved space in this way.

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Fermionic matter coupled to higher derivative Chern–Simons theories. II

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The diagrammatic and the Feynman rules for the higher derivative Chern–Simons theories in (2+1) dimensions coupled to fermionic matter are constructed. This is done by starting from the path-integral quantization. Once the diagrammatic and the Feynman rules are given, the regularization and renormalization problem of this higher derivative model is analysed in the framework of the perturbation theory. The unitarity problem related with the possible appearance of ghost states with negative norm is also discussed. Finally, the BRST formalism for the model is constructed and some interesting differences with respect to the formalism applied to usual Chern–Simons models are presented. © *1996 American Institute of Physics.* [S0022-2488(95)02512-9]

I. INTRODUCTION

In a recent paper,[1] we have constructed the classical and quantum formalism for the constrained Hamiltonian system with singular higher-order Lagrangian describing the Chern–Simons (CS) theories in (2+1) dimensions coupled to matter. To construct the classical generalized Hamiltonian formalism we have worked as close as possible to the Dirac algorithm. Then the canonical Dirac quantization has been performed. The path-integral quantization has also been done by extending the Faddeev–Senjanovic method,[2] to the higher-derivative case under consideration.

The classical and quantum CS theories in (2+1) dimensions have been investigated from a long time ago and with increasing interest in the last years.[3–9] Many interesting problems are present in the (2+1) dimensional physics.

Moreover, the dynamical systems described in terms of higher derivatives constitute an interesting problem of current research in quantum field theory.[10]

One of the reasons to consider these kinds of theories and in particular those containing higher derivative terms in the action, is because of their possible application to high-Tc superconductivity.

Another motivation exists from the point of view of the field theory itself. Maybe these theories have not been treated intensively not due to a lack of physical interest, but due to the underdeveloped knowledge on how to treat higher-derivative field theories. As it is well-known, they have a bad reputation because ghost states with negative norm can be causing unitarity violation.[11]

On the other hand, these theories have some kind of attraction, when terms of higher derivatives are added to the Lagrangian; the convergence of the corresponding Feynman diagrams can be improved.[12,13]

A natural higher derivative field theory is, for instance, the conformal supergravity in (2+1) dimensions which is also described by a CS term.[14] The constraints on curvatures make this feature evident and it is possible to see that the second-order canonical formalism is non-trivial

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when it is implemented.[15] Moreover, the conformal gravity in three dimensions is finite and exactly soluble.[16]

The dynamical unitary, and possible renormalizable topologically massive three-dimensional gravity, was also investigated.[17]

The motivation of the present paper is to continue the work developed in Ref. 1, by studying the diagrammatic and the Feynman rules for that higher derivative CS model. The BRST formalism for the model is also considered.

The paper is organized as follows. In section II, we briefly recall the main results obtained in Ref. 1, for the Abelian case. In section III, we find the diagrammatic of the model. This is obtained by defining the propagator for a suitable bosonic object. The unitarity of the model is also discussed. Finally, in section VI, the BRST formalim is found.

II. DEFINITIONS AND PRELIMINARIES

In Ref. 1, our starting point was the following singular Lagrangian density:

$$\mathscr{L}=\mathscr{L}_{top}+\mathscr{L}_{h}+\mathscr{L}_{f}+\mathscr{L}_{int}, \tag{2.1}$$

describing the matter coupled to Abelian CS theories in (2+1) dimensions. In equation (2.1), $\mathscr{L}_{top}$ is the electromagnetic Lagrangian density with a topological mass term, i.e. a CS term, and it is given by

$$\mathscr{L}_{top}=-\tfrac{1}{4}F_{\mu\nu}F^{\mu\nu}+\frac{\kappa}{4\pi}\varepsilon^{\mu\nu\rho}\partial_{\mu}A_{\nu}A_{\rho}. \tag{2.2a}$$

The part containing higher derivatives is

$$\mathscr{L}_{h}=-\frac{c^{2}}{4\pi}\partial_{\rho}F_{\mu\nu}\partial^{\rho}F^{\mu\nu}, \tag{2.2b}$$

and the fermionic and interacting pieces are, respectively, given by

$$\mathscr{L}_{f}=i\left(\frac{a+1}{2}\right)\bar{\psi}\gamma^{\mu}\partial_{\mu}\psi+i\left(\frac{a-1}{2}\right)\partial_{\mu}\bar{\psi}\gamma^{\mu}\psi-m\bar{\psi}\psi, \tag{2.2c}$$

$$\mathscr{L}_{int}=e\bar{\psi}\gamma^{\mu}\psi A_{\mu}. \tag{2.2d}$$

The constant κ is the topological mass of the gauge field and its dimension is $(length)^{-1}$, the dimensional constant c has dimension $(length)^{1}$. We will use the convention $\varepsilon^{012}=\varepsilon^{12}=1$, the Minkowskian metric $g_{\mu\nu}$ is $g_{\mu\nu}=diag(1,-1,-1)$ and the Dirac γ-matrices are $\gamma^{0}=\sigma^{3}$, $\gamma^{1}=i\sigma^{1}$ and $\gamma^{2}=i\sigma^{2}$ (σ' are the Pauli matrices).

After the Ostrogradski transformation[18] is performed, the momenta P^{μ}, Q^{μ}, $\overline{\Pi}^{(\alpha)}$ and $\Pi^{(\alpha)}$ canonically conjugate to the independent field variables A_{μ}, $B_{\mu}=\dot{A}_{\mu}$, ψ_{α} and $\bar{\psi}_{\alpha}$ remain defined and they are given by

$$P^{0}=-\frac{c}{\pi}\partial_{0}\partial_{i}F^{0i}, \tag{2.3a}$$

$$P^{i}=F^{i0}+\frac{\kappa}{4\pi}\varepsilon^{ij}A_{j}+\frac{c}{\pi}(\nabla^{2}F^{0i}+\partial_{0}\partial_{j}F^{ji})-\partial_{0}Q^{i}, \tag{2.3b}$$

$$Q^{0}=0, \tag{2.3c}$$

$$Q^i = -\frac{c}{\pi}\partial_0 F^{0i}, \tag{2.3d}$$

$$\Pi_{(\alpha)}(x) = i\left(\frac{a-1}{2}\right)\gamma_0\psi_{(\alpha)}, \tag{2.3e}$$

$$\overline{\Pi}_{(\alpha)}(x) = -i\left(\frac{a+1}{2}\right)\bar{\psi}_{(\alpha)}\gamma_0, \tag{2.3f}$$

where the italic indices take the values $i,\ j\ =\ 1,2$.

The Poisson brackets for pairs of canonical conjugate variables are the usuals. The equations (2.3) show that the primary constraints are

$$\Phi_1(x) = Q^0(x) \approx 0, \tag{2.4a}$$

$$\Omega_{(\alpha)}(x) = \Pi_{(\alpha)}(x) - i\left(\frac{a-1}{2}\right)\gamma_0\psi_{(\alpha)} \approx 0, \tag{2.4b}$$

$$\overline{\Omega}_{(\alpha)}(x) = \overline{\Pi}_{(\alpha)}(x) + i\left(\frac{a+1}{2}\right)\bar{\psi}_{(\alpha)}\gamma_0 \approx 0. \tag{2.4c}$$

So, the classical canonical Hamiltonian is given by

$$\mathscr{H}_{can} = B_\mu P^\mu + \dot{B}_\mu Q^\mu + \dot{\bar{\psi}}_{(\alpha)}\Pi^{(\alpha)} + \overline{\Pi}^{(\alpha)}\dot{\psi}_{(\alpha)} - \mathscr{L}. \tag{2.5}$$

The extended Hamiltonian $H_E = \int d^2x.\mathscr{H}_E$ generator of time evolution, remains defined in terms of the following Hamiltonian density:

$$\mathscr{H}_E = \mathscr{H}_{can} + \delta\Phi_1 + \overline{\lambda}_{(\alpha)}\Omega^{(\alpha)} + \overline{\Omega}^{(\alpha)}\lambda_{(\alpha)}, \tag{2.6}$$

where δ is a bosonic Lagrange multiplier and $\overline{\lambda}$ and λ are the fermionic Lagrange multipliers.

Now, going on with the Dirac algorithm,[19] the secondary constraints can be easily found. Once the set of constraints are known, we must find all the first class ones associated with the gauge symmetries of the system, and write the Dirac brackets. Finally, the Hamiltonian system for this model is given by the total Hamiltonian,

$$H_T = \int d^2x(\mathscr{H}_{can} + \beta^a\Phi_a), \tag{2.7}$$

where β^a $(a = 1,2,3)$ are three arbitrary parameters and Φ_a are the first class constraints given by

$$\Phi_1(x) = Q^0(x) \approx 0, \tag{2.8a}$$

$$\Phi_2(x) = -P^0(x) + \partial_i Q^i(x) \approx 0, \tag{2.8b}$$

$$\Phi_3(x) = -ie(\bar{\psi}_{(\alpha)}(x)\Pi^{(\alpha)}(x) + \overline{\Pi}^{(\alpha)}(x)\psi_{(\alpha)}(x)) - \frac{\kappa}{4\pi}\partial_i A_j(x)\varepsilon^{ij} - \partial_i P^i(x) \approx 0. \tag{2.8c}$$

The equal time commutators (or anticommutators) we have found in the canonical quantum formalism are

$$[A_\mu(x),P^\nu(y)]_D=-\frac{i}{\hbar}\delta^\nu_\mu\delta(x-y), \tag{2.9a}$$

$$[B_\mu(x),Q^\nu(y)]_D=-\frac{i}{\hbar}\delta^\nu_\mu\delta(x-y), \tag{2.9b}$$

$$\{\psi_{(\alpha)}(x),\bar{\psi}_{(\beta)}(y)\}_D=\frac{i}{\hbar}(\gamma_0)_{(\alpha)(\beta)}\delta(x-y). \tag{2.9c}$$

In the next section we are going to use these results to study the diagrammatic of the model.

III. DIAGRAMMATIC AND FEYNMAN RULES

The partition function for higher derivative theories in the Hamiltonian formalism we have proposed in Ref. 1 is

$$\begin{aligned}Z=\int\ &\mathscr{D}A_\mu\mathscr{D}P^\mu\mathscr{D}B_\nu\mathscr{D}Q^\nu\mathscr{D}\bar{\psi}_{(\alpha)}\mathscr{D}\Pi^{(\alpha)}\mathscr{D}\psi_{(\beta)}\mathscr{D}\overline{\Pi}^{(\beta)}\delta(\Phi_1)\,\delta(\Phi_2)\,\delta(\Phi_3)\\ &\times\delta(f_1)\,\delta(f_2)\,\delta(f_3)\det[\Phi_1,\Phi_2,\Phi_3,f_1,f_2,f_3]_D\,\delta(\Omega_{(\alpha)})\,\delta(\Omega_{(\beta)})\det[\Omega_{(\alpha)},\Omega_{(\beta)}]\\ &\times\exp\,i\left[\int d^3x(B_\mu P^\mu+\dot{B}_\nu Q^\nu+\bar{\psi}\dot{\Pi}+\overline{\Pi}\dot{\psi})-H_E\right],\end{aligned} \tag{3.1}$$

where the functional integration is performed over all phase space volume corresponding to the independent dynamical variables A_μ, B_ν, P^μ and Q^ν.

The quantities f_1, f_2 and f_3 are gauge fixing conditions. A convenient set of such conditions compatible with the equations of motion and verifiying $\det[f_a,\Phi_b]_D\neq 0$ for all first-class constraints Φ_a, are

$$f_1=\partial_i A^i\approx 0, \tag{3.2a}$$

$$f_2=B_0\approx 0, \tag{3.2b}$$

$$f_3=\frac{\kappa}{2\pi}\nabla^2A_0+e\varepsilon_{ik}\partial^k(\bar{\psi}\gamma^i\psi)+\Box\left(1-\frac{c^2}{\pi}\Box\right)\partial_kA_i\varepsilon^{ik}\approx 0. \tag{3.2c}$$

When in equation (3.1), the determinants are explicitly computed and the path integral over the fields B_0, P^μ, Q^μ, $\overline{\Pi}^{(\alpha)}$ and $\Pi^{(\alpha)}$ have been made, the partition function results:

$$Z=\int\mathscr{D}A_\mu\mathscr{D}B_i\mathscr{D}\bar{\psi}_{(\alpha)}\mathscr{D}\psi_{(\beta)}\delta(f_1)\,\delta(f_3)\exp\,i\left[\int d^3x\mathscr{L}_{eff}\right]. \tag{3.3}$$

The Lagrangian density $\mathscr{L}_{eff}$ defined in (3.3) is given by

$$\begin{aligned}\mathscr{L}_{eff}=&-\tfrac{1}{4}F_{ij}F^{ij}-\frac{c^2}{4\pi}G_{ij}G^{ij}-\tfrac{1}{2}(B_i-\partial_iA_0)(B_i-\partial_iA_0)-\frac{c^2}{2\pi}\dot{B}_i\dot{B}^i-\frac{c^2}{4\pi}\partial_iF_{jk}\partial^iF^{jk}+\frac{c^2}{2\pi}B_j\nabla^2B^j\\ &-\frac{c^2}{\pi}\nabla^2B_j\partial^jA_0-\frac{c^2}{2\pi}(\nabla^2A_0)^2-\frac{\kappa}{4\pi}\partial_iA_0A_j\varepsilon^{ij}+\frac{\kappa}{4\pi}(\partial_iA_j)A_0\varepsilon^{ij}+\frac{\kappa}{4\pi}B_iA_j\varepsilon^{ij}\\ &+i\left(\frac{a+1}{2}\right)\bar{\psi}\gamma^\mu\partial_\mu\psi+i\left(\frac{a-1}{2}\right)(\partial_\mu\bar{\psi})\,\gamma^\mu\psi-m\bar{\psi}\psi+e\bar{\psi}\gamma_\mu\psi A^\mu,\end{aligned} \tag{3.4}$$

where $G_{ij} = \partial_i B_j - \partial_j B_i$ and $\nabla^2 = \partial_i \partial^i$.

From equation (3.3) we can see that the quantum problem remains defined in terms of a path integral in which there are four independent fields. Consequently, it is possible to apply diagrammatic techniques defining proper Feynman rules for propagators and vertices corresponding to the fields A_μ, B_i, $\psi_{(\alpha)}$ and $\bar{\psi}_{(\alpha)}$.

Alternatively, the path integral equation (3.3) can be written:

$$Z = \int \mathscr{D}A_\mu \mathscr{D}B_i \mathscr{D}\bar{\psi}_{(\alpha)} \mathscr{D}\psi_{(\beta)} \mathscr{D}\Lambda_1 \mathscr{D}\Lambda_3 \exp\, i\left[\int d^3x \mathscr{L}^*\right], \tag{3.5}$$

where

$$\mathscr{L}^* = \mathscr{L}_{eff} - \Lambda_1 f_1 - \Lambda_3 f_3, \tag{3.6}$$

for the Lagrange multipliers Λ_1 and Λ_3.

As it was carried out in a different context,[20] we can define a bosonic vector quantity X_Σ, having the same dimension as the vector field A_μ, whose components are given by

$$X_\Sigma = \left(A_\mu, cB_i, c\Lambda_1, \frac{1}{c}\Lambda_3\right), \tag{3.7}$$

where the compound index Σ takes the seven values $0,1,\ldots,6$.

Therefore, when the action is written in terms of the vector quantity (3.7) we can easily recognise the propagators defined by the quadratic part of the Lagrangian (3.6) and the remaining part of it can be represented by vertices. Consequently, the equation (3.6) can be seen as the Lagrangian density which defines the effective action for a system describing the boson vector field X_Σ coupled to a matter Dirac spinor field. The effective action $\mathscr{S}^*$ can be written:

$$\mathscr{S}^* = \mathscr{S}^*(X_\Sigma) + \mathscr{S}^*(\psi) + \mathscr{S}^*_{\text{int}}(X_\Sigma, \psi), \tag{3.8}$$

where, taking into account equation (3.4), it is

$$\mathscr{S}^*(\psi) = \int d^3x \mathscr{L}_f, \tag{3.9a}$$

$$\mathscr{S}^*(X_\Sigma, \psi) = \int d^3x [e\bar{\psi}(\Gamma_\Sigma X^\Sigma)\psi], \tag{3.9b}$$

$$\mathscr{S}^*(X_\Sigma) = \int d^3x [\tfrac{1}{2} X_\Sigma (D^{-1})^{\Sigma\Lambda} X_\Lambda]. \tag{3.9c}$$

The seven matrices $\Gamma_\Sigma = (\Gamma_{A_0}, \Gamma_{A_i}, \Gamma_{B_i}, \Gamma_{\Lambda_1}, \Gamma_{\Lambda_3})$, defined in equation (3.9b) are

$$\Gamma_{A_0} = \gamma_0, \quad \Gamma_{A_i} = \gamma_i, \quad \Gamma_{B_i} = 0, \quad \Gamma_{\Lambda_1} = 0, \quad \Gamma_{\Lambda_3} = c\gamma^i \varepsilon_{ik} \partial^k. \tag{3.10}$$

The 7×7 matrix $(D^{-1})^{\Sigma\Lambda}$ defined in equation (3.9c) is the inverse of the propagator of the bosonic object X_Σ given in (3.7). The matrix $(D^{-1})^{\Sigma\Lambda}$ is Hermitian and non-degenerate and it can be invertible and so the propagator $D_{\Sigma\Lambda}$ can be evaluated. The computation of the matrix elements $D_{\Sigma\Lambda}$ of the propagator in the general case is difficult and very complicated expressions are obtained. We can conclude that it could be useful to define a mixed propagator of the bosonic object X_Σ in order to study the simple case $\kappa = 0$, but not the general case.

To obtain a suitable expression for the bosonic propagator in the general $\kappa \neq 0$ case, we are going to give an alternative approach.

Remarking the arbitrariness of the gauge fixing conditions (3.2), instead of (3.2c), we can take a different gauge fixing condition $f_3=\partial_i B^i \approx 0$. This new gauge fixing condition is also compatible with the equation of motion and independent of f_1 in the Hamiltonian formalism where the partition function (3.1) is proposed.

The condition (3.2c) is obtained from the spatial component of the Lagrangian field equation of A_μ. The presence of the gauge fixing condition (3.2c) in the partition function equation (3.1), allows to come again on the original field A_μ. Now, to come back to the original field A_μ when the new gauge fixing condition $f_3=\partial_i B^i \approx 0$ is used, we must add to the action a term of the form $\int d^3x \Lambda^\mu (B_\mu - \dot{A}_\mu)$ with arbitrary multipliers Λ^μ and perform the integration on all their possible values. Consequently, the partition function (3.1) is written:

$$
\begin{aligned}
Z=\int \mathscr{D}A_\mu \mathscr{D}P^\mu \mathscr{D}B_\nu \mathscr{D}Q^\nu \mathscr{D}\bar{\psi}_{(\alpha)} \mathscr{D}\Pi^{(\alpha)} \mathscr{D}\psi_{(\beta)} \mathscr{D}\overline{\Pi}^{(\beta)} \delta(\Phi_1)\,\delta(\Phi_2)\,\delta(\Phi_3)\,\delta(f_1) \\
\times \delta(f_2)\,\delta(f_3) \det[\Phi_1,\Phi_2,\Phi_3,f_1,f_2,f_3]_D \delta(\Omega_{(\alpha)})\,\delta(\Omega_{(\beta)})\,\delta(B_\mu - \dot{A}_\mu) \\
\times \det[\Omega_{(\alpha)},\Omega_{(\beta)}] \exp\, i\left[\int d^3x (B_\mu P^\mu + \dot{B}_\nu Q^\nu + \dot{\bar{\psi}}\Pi + \overline{\Pi}\dot{\psi}) - H_E\right].
\end{aligned}
\tag{3.11}
$$

Therefore, in equation (3.11) also the path-integral over the field B_μ can be performed, and instead of the expression (3.3), the partition function reads as

$$
Z=\int \mathscr{D}A_\mu \mathscr{D}\bar{\psi}_{(\alpha)} \mathscr{D}\psi_{(\beta)} \delta(f_1)\,\delta(f_3) \exp\, i\left[\int d^3x \mathscr{L}_{eff}\right],
\tag{3.12}
$$

where $\mathscr{L}_{eff}$ given in (3.4) must be written in terms of A_μ.

As usual, we must transfer the integration measure defined on the surface $f_1=\partial_i A^i=0$, to the surface $f_1'=\partial_\mu A^\mu=0$, which defines the Lorentz gauge. The same argument can be used on the surface f_3. Moreover, once the path integral over the field B_μ is performed in the equation (3.11), the surface f_3 becomes the time derivative of the surface f_1.

Also in higher derivative models, it is convenient to work in a generalized gauge defined by

$$
\partial_\mu A^\mu(x)=\alpha_1(x),
\tag{3.13a}
$$

$$
\partial_\mu \dot{A}^\mu(x)=\dot{\alpha}_1(x)=\alpha_2(x),
\tag{3.13b}
$$

where $\alpha_1(x)$ and $\alpha_2(x)$ are arbitrary matrices.

Finally, as the partition function (3.12) does not depend neither on α_1 nor on α_2, by integrating over both quantities with a Gaussian weight: $\exp(i\lambda_1 tr\int d^3x \alpha_1^2(x) + ic^2\lambda_2 tr\int d^3x \alpha_2^2(x))$, the following extended Lagrangian density remains defined:

$$
\mathscr{L}^*=\mathscr{L}_{eff}-\frac{\lambda_1}{2}(\partial_\mu A^\mu)^2-\frac{\lambda_2}{2}(\partial_\mu \dot{A}^\mu)^2.
\tag{3.14}
$$

Looking at the Lagrangian density (3.14), we can see that in this context the inverse of the A_μ propagator is given by the 3×3 matrix $(D^{-1})^{\mu\nu}$, defined again by the quadratic piece in A_μ. In the momentum space, this matrix has the following elements:

$$
[D^{-1}]^{00}=(1-c^2\mathbf{k}^2)\mathbf{k}^2-\lambda k_0^2,
$$

$$[D^{-1}]^{01}=[D^{-1}]^{10*}=(\lambda-1+c^2\mathbf{k}^2)k_0k_1-i\frac{\kappa}{2\pi}k_2,$$

$$[D^{-1}]^{02}=[D^{-1}]^{20*}=(\lambda-1+c^2\mathbf{k}^2)k_0k_2+i\frac{\kappa}{2\pi}k_1,$$

$$[D^{-1}]^{11}=-(1-c^2\varepsilon)(\varepsilon-k_1^2)-\lambda k_1^2, \tag{3.15}$$

$$[D^{-1}]^{12}=[D^{-1}]^{21*}=(1-c^2\varepsilon-\lambda)k_2k_1-i\frac{\kappa}{2\pi}k_0,$$

$$[D^{-1}]^{22}=-(1-c^2\varepsilon)(\varepsilon-k_2^2)-\lambda k_2^2.$$

In the above equations we have renamed the parameter c in such a way that it is not necessary to write the constant π explicitly, and we called $\mathbf{k}^2=k_1^2+k_2^2$, $\varepsilon=\mathbf{k}^2-k_0^2$ and $\lambda=\lambda_1+\lambda_2c^2k_0^2$.

Now, the propagator $D_{\mu\nu}$ can be evaluated and the following matrix elements are obtained:

$$D_{00}=\frac{(1-c^2\varepsilon)\varepsilon}{\Delta}[\lambda\mathbf{k}^2-(1-c^2\varepsilon)k_0^2]-\frac{(\kappa/2\pi)^2k_0^2}{\Delta},$$

$$D_{01}=D_{10}^*=-\frac{k_0k_1}{\Delta}\left[(1-c^2\mathbf{k}^2-\lambda)(1-c^2\varepsilon)\varepsilon+\left(\frac{\kappa}{2\pi}\right)^2\right]-i\frac{\kappa k_2}{2\pi\Delta}[-\lambda\varepsilon+c^2k_0^4],$$

$$D_{02}=D_{20}^*=-\frac{k_0k_2}{\Delta}\left[(1-c^2\mathbf{k}^2-\lambda)(1-c^2\varepsilon)\varepsilon+\left(\frac{\kappa}{2\pi}\right)^2\right]+i\frac{\kappa k_1}{2\pi\Delta}[-\lambda\varepsilon+c^2k_0^4],$$

$$\begin{aligned}D_{11}=&-\frac{k_1^2}{\Delta}\left[(1-c^2\mathbf{k}^2)(1-c^2\varepsilon-\lambda)\varepsilon+c^2k_0^4(1-c^2\mathbf{k}^2-\lambda)+\left(\frac{\kappa}{2\pi}\right)^2\right]\\&+\frac{1}{\Delta}(1-c^2\mathbf{k}^2)c^2\mathbf{k}^2k_0^4+\frac{\lambda}{\Delta}[(c^2\mathbf{k}^2-1)\varepsilon^2-c^2k_0^6],\end{aligned}$$

$$D_{12}=D_{21}^*=-\frac{k_1k_2}{\Delta}\left[(1-c^2\mathbf{k}^2)(1-c^2\varepsilon-\lambda)\varepsilon+c^2k_0^4(1-c^2\mathbf{k}^2-\lambda)+\left(\frac{\kappa}{2\pi}\right)^2\right]-i\lambda\frac{\kappa k_0\varepsilon}{2\pi\Delta},$$

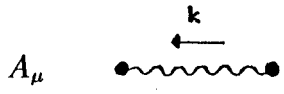
$$\begin{aligned}D_{22}=&-\frac{k_2^2}{\Delta}\left[(1-c^2\mathbf{k}^2)(1-c^2\varepsilon-\lambda)\varepsilon+c^2k_0^4(1-c^2\mathbf{k}^2-\lambda)+\left(\frac{\kappa}{2\pi}\right)^2\right]\\&+\frac{1}{\Delta}(1-c^2\mathbf{k}^2)c^2\mathbf{k}^2k_0^4+\frac{\lambda}{\Delta}[(c^2\mathbf{k}^2-1)\varepsilon^2-c^2k_0^6].\end{aligned} \tag{3.16}$$

In equations (3.16) $\Delta=\det[D^{-1}(k)]$ and it is given by

$$\Delta=\lambda\left[(1-c^2\mathbf{k}^2)(1-c^2\varepsilon)\varepsilon+\left(\frac{\kappa}{2\pi}\right)^2\right]\varepsilon^2+\lambda c^2k_0^6(1-c^2\varepsilon)\varepsilon-c^2\mathbf{k}^2k_0^4$$
$$\times\left[(1-c^2\mathbf{k}^2)(1-c^2\varepsilon)\varepsilon+\left(\frac{\kappa}{2\pi}\right)^2\right]. \tag{3.17}$$

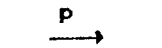
Subsequently, the Feynman rules propagators and vertices can be written.

(i) Propagators: We associate with the propagator $D_{\mu\nu}$ of the bosonic field A_μ, a wavy line connecting two generic points:



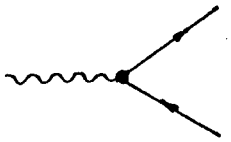
$$\equiv D_{\mu\nu}(k)\,,$$

and with a simple line the usual propagator of the fermionic field ψ



$$\equiv \frac{-i}{\gamma.p+m}=\frac{i(\gamma.p-m)}{p^2+m^2}$$

(ii) Vertices: Then, the three legs vertex of the model is:

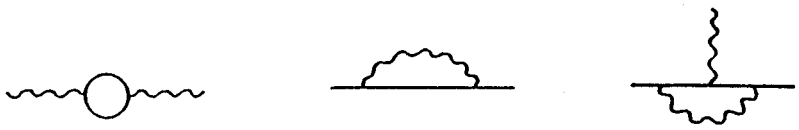


$$\equiv -ie\gamma_\mu\,.$$

Moreover, as it is usual we have to take into account a minus sign for every closed fermion loop and other minus signs for diagrams related to the exchange of two fermion lines, internal or external. A combinatorial factor correcting for double counting in case that identical particles occur, also must be taken into account.

IV. PERTURBATIVE METHOD IN HIGHER DERIVATIVE QED. ONE-LOOP STRUCTURE

Now, we proceed to examine the perturbative treatment of this gauge theory which describes the interaction of the bosonic field A_μ with the Dirac spinor field. Using the above rules, a power-counting analysis shows that the superficial degrees of divergence G are essentially those of the usual QED, so we are led to the following one loop diagrams:



which correct the fundamental parameters and fields of the theory.

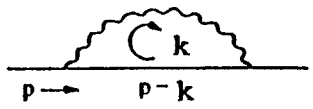
If we call $\Pi_{\mu\nu}(k)$, the correction to the boson line or vacuum polarization diagram, it can be written as

$\Pi_{\mu\nu}(k) =$ 

$$= -e^2 \int \frac{d^3p}{(2\pi)^3} \frac{1}{(p^2+m^2)[(p+k)^2+m^2]} \times Tr[\gamma_\mu(\gamma.p+\gamma.k-m)\gamma_\nu(\gamma.p-m)]. \tag{4.1}$$

So, the correction to the boson line is similar to the non higher model, therefore the ultraviolet behavior of the integral (4.1) is the same as in the usual QED, i.e for large momentum p, the Feynman integral (4.1) behaves as $\sim\int dp$ and so this diagram is linearly divergent. This must be expected, because this model is a higher derivative only with respect to the boson field, and the propagator of that field does not appear in the vacuum polarization diagram. Consequently, the evaluation of the integral (4.1) is carried out by introducing a Feynman parameter and the new loop momentum $p' = p + kx$. We note that in the case in which the complete CS Lagrangian (2.2a) (with $\kappa \neq 0$) is considered, the dimensional regularization cannot be used safely due to the presence of the volume form $\varepsilon^{\mu\nu\rho}$. In that case, another gauge invariant regularization method, for instance a Pauli–Villars one,[13] must be used. The renormalization procedure is implemented as in the usual QED.

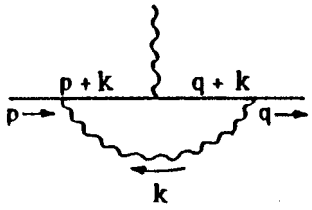
Now, we consider the second diagram given above. Let $\Sigma(p)$ be the correction to the fermion line (suppressing spinor indices). This diagram is given by the following integral expression:

$\Sigma(p) =$ 

$$= -ie^2 \int \frac{d^3k}{(2\pi)^3} \frac{\gamma_\mu(\gamma.p-\gamma.k-m)\gamma_\nu}{(p-k)^2+m^2} \times D_{\mu\nu}(k). \tag{4.2}$$

From equations (3.16), it can be seen that, for large momentum, the propagator $D_{\mu\nu}$ behaves like k^{-4}. Therefore the new propagator has an ultraviolet behavior in such a manner that the Feynman integral (4.2) gives a convergent result (for large k the integral behaves as $\sim\int dk/k^3$).

The last one-loop diagram we consider is the vertex correction, which we call $V_\xi(p,q)$, and is written as

$V_\xi(p,q) =$ 

$$= -ie^3 \int \frac{d^3k}{(2\pi)^3} \gamma_\mu \frac{(\gamma.p+\gamma.k-m)}{(p+k)^2+m^2} \gamma_\xi \times \frac{(\gamma.q+\gamma.k-m)}{(q+k)^2+m^2} \gamma_\nu \times D_{\mu\nu}(k). \tag{4.3}$$

Once more, by introducing the expressions (3.16) for the boson propagator $D_{\mu\nu}$, we can see that the diagram is also convergent, because for large momentum the integral behaves as $\sim \int dk/k^4$.

We conclude that in one-loop diagrams in which the propagator $D_{\mu\nu}$ of the field A_μ takes place, the ultraviolet behavior is improved and the divergence of these diagrams are eliminated. The remaining diagrammatic with a fermionic loop does not change and the degree of divergence is that of the usual QED. Therefore, the use of higher derivative terms in the Lagrangian allows us to improve the behavior of the correspondent propagators at large momentum, rendering the theory less divergent.

V. UNITARITY

At this stage, another important problem to take into account is the unitarity problem. It is well known,[11] that in higher derivative theories, the unitarity can be violated when ghost states with negative norm are present. To say something about the unitarity, we must analyze more carefully the bosonic propagator we have defined.

First we note that the Hermitian matrix $D_{\mu\nu}(k)$ defined in (3.16) can be diagonalized and so its eigenvalues are determined. As it is possible to see, the corresponding secular equation depends only on k^2 and k_0 and therefore we can study the problem for a given value of the three-vector k_μ. Let $k_\mu=(k_0,k_1=0,k_2)$ be the value for the three-vector momentum.

From equation (3.17) we see that Δ can be written as a six-order polynomial in the parameter ε. As the model is described by a second-order Lagrangian, there are two physical roots which are the two single poles appearing in the propagator. The remaining roots of the polynomial Δ are non-physical ones.

For appropriated values of the parameter c^2 and the topological mass κ, it is possible to obtain a factorized expression for the polynomial Δ. Considering the dimensional parameter c^2 in the physical regimes verifying the condition $c^2\mathbf{k}^2-1>0$ (i.e., $k_0^2>0$) and for values of the topological mass κ verifying $c^2\kappa^2/(c^2\mathbf{k}^2-1)\ll 1$, the polynomial Δ can be written as

$$\Delta=(\varepsilon-\alpha_1)(\varepsilon-\alpha_2)f(\lambda,\mathbf{k},\varepsilon), \tag{5.1}$$

where α_1 and α_2 are the two real roots of the polynomial $c^2\varepsilon^2-\varepsilon+[\kappa^2/4\pi^2(c^2\mathbf{k}^2-1)]=0$. These roots, which are independent of the gauge parameters, in the above approximation for the topological mass makes

$$\alpha_1\cong\frac{1}{c^2}-\frac{\kappa^2}{4\pi^2(c^2\mathbf{k}^2-1)},\qquad \alpha_2\cong\frac{\kappa^2}{4\pi^2(c^2\mathbf{k}^2-1)}. \tag{5.2}$$

Moreover, $f(\lambda,\mathbf{k},\varepsilon=\alpha_{1,2})$ is a finite and different from zero function.

As we can see, in the limit $\kappa=0$, the two poles are displaced to the values $\varepsilon_1=1/c^2$ and $\varepsilon_2=0$, respectively.

In the limit $c^2\to 0$ the only remaining pole is located at $\varepsilon=-\kappa^2/4\pi^2$, as it must be expected. The propagator (3.16) covariantly written takes the form

$$D_{\mu\nu}(k)=\frac{1}{(\varepsilon+\kappa^2/4\pi^2)}\left[g_{\mu\nu}+\left(1-\frac{1}{\lambda_1}-\frac{\kappa^2/4\pi^2}{\lambda_1\varepsilon}\right)\frac{k_\mu k_\nu}{\varepsilon}-i\frac{\kappa}{2\pi}\varepsilon_{\mu\nu\rho}\frac{k^\rho}{\varepsilon}\right]. \tag{5.3}$$

Now, the propagator (3.16) can be written as

$$D_{\mu\nu}=\frac{1}{\Delta}\times K^R_{\mu\nu}. \tag{5.4}$$

The 3×3 matrix $K^R_{\mu\nu}$ is called matrix residue. It can be diagonalized and it has three different non-zero eigenvalues $\xi_{(\alpha)}$ $((\alpha)=1,2,3)$, which can be given, for example, as power series of ε with proper coefficients depending on $\mathbf{k}^2$.

Consequently, we can define a set of real currents $J^{(\alpha)}_\mu(k)$, one for every non-zero eigenvalue, which are mutually orthogonal and eigenstates of the matrix $K^R_{\mu\nu}(k)$,[21] i.e.

$$J^{(\alpha)}_\mu(k)J^{(\beta)}_\mu(k)=0, \quad \text{if}(\alpha)\neq(\beta), \tag{5.5a}$$

$$K^R_{\mu\nu}(k)J^{(\alpha)}_\nu(k)=e^{(\alpha)}(k)J^{(\alpha)}_\mu(k). \tag{5.5b}$$

For instance, the real bosonic currents for emission of a particle corresponding to incoming particles of the S-matrix, when all the eigenvalues of the matrix K^R are positive, must be normalized in such a way that

$$J^{(\alpha)}_\mu(k)K^R_{\mu\nu}(k)J^{(\alpha)}_\nu(k)=+1. \tag{5.6}$$

The source currents thus defined are properly normalized for emission of a particle (or an antiparticle). When absorption of a particle (or an antiparticle) is considered, in the matrix K^R appearing in equation (5.5b), k must be replaced by $-k$.

On the other hand, once the matrix residue $K^R_{\mu\nu}$ is diagonalized, the above equations (5.5) imply that the currents are of the form

$$J^{(\alpha)}=(0,1/\sqrt{\xi_{(\alpha)}},0),$$

and obviously results in

$$\sum_{(\alpha)} J^{(\alpha)}J^{(\alpha)}=[K^R]^{-1}. \tag{5.7}$$

The equation (5.7) holds when the eigenvalues of the matrix K^R at the pole are positive, that is to say when the unitarity is preserved and the normalization (5.6) holds. In the case of negative eigenvalues, to recover the unitarity, the normalization in (5.6) must be done with a minus one. As it is well known, when the matrix residue K^R has a negative eigenvalue at the pole, it corresponds to states with negative norm, and they are physically unacceptable. The corresponding particles are called ghosts. This is the prescription to retrieve the unitarity of the theory and it is usually called indefinite metric prescription.

Let us consider the secular equation corresponding to the matrix K^R, which is written as

$$\xi^3-\xi^2 Tr[D_{\mu\nu}]+\xi\Delta Tr[(D^{-1})^{\mu\nu}]-\Delta^2=0. \tag{5.8}$$

From equation (5.8) it is possible to analyze the residue of the eigenvalues at every pole. The residue is given by the coefficient of ξ^2, i.e, $Tr[D_{\mu\nu}]$. At the poles $\alpha_{1,2}$ the residues, respectively, are written as

$$Tr[D_{\mu\nu}(\varepsilon=\alpha_1)]=-\frac{k_0^2}{(c^2\mathbf{k}^2-1)}\Bigg[c^4k_0^4\mathbf{k}^2(c^2\mathbf{k}^2-1)-\frac{\kappa^2}{4\pi^2}c^4k_0^4 +\lambda\left(\mathbf{k}^2(c^2\mathbf{k}^2-2)(c^2\mathbf{k}^2-1)+\frac{\kappa^2}{2\pi^2}c^2k_0^2\right)\Bigg], \tag{5.9a}$$

$$Tr[D_{\mu\nu}(\varepsilon=\alpha_2)]=-\frac{k_0^2}{(c^2\mathbf{k}^2-1)}\Bigg[c^2k_0^4(c^2\mathbf{k}^2-1)^2+\frac{\kappa^2}{4\pi^2}c^4k_0^4 +\lambda\left(c^2\mathbf{k}^4(c^2\mathbf{k}^2-1)-\frac{\kappa^2}{2\pi^2}(c^2\mathbf{k}^2+1)\right)\Bigg]. \tag{5.9b}$$

By looking at the equations (5.9), we can assert that the sign of the residues depend on λ. For instance, the signs can be determined in the physical region $c^2\mathbf{k}^2>2$ and in the Feynman gauge $\lambda_1=\lambda_2=1$. In this case, in both equations (5.9) results in $Tr[D_{\mu\nu}]<0$, and therefore the normalization in (5.6) must be given with the minus one.

Finally, as it is easy to note, when the limit $c^2=0$ is taken in the model, the set of constraints are modified. The fermionic constraints do not change, but the bosonic constraints (2.4a) disappear in this case, leaving $P^0=0$ as the unique primary bosonic constraint. The consistency condition on the constraints gives only one secondary constraint. Subsequently, it is possible to find the two first class constraints characteristic to the usual electrodynamic with the CS term. The two correspondent gauge fixing conditions are given by $f_1=\partial_i A^i\approx 0$ and $f_2=A_0\approx 0$. The partition function analogous to (3.1), after integrated in the variable A_0 by using the function $\delta(f_2)$, is reduced to

$$Z=\int \mathscr{D}A_i\mathscr{D}\bar{\psi}\mathscr{D}\psi\delta(f_2)\ \exp\, i[S_{eff}], \tag{5.10}$$

where S_{eff} is now the effective action for the electrodynamic with the topological CS term.

VI. THE BRST FORMALISM

The BRST formalism for the constrained Hamiltonian system under consideration is contructed by using most of the tools of Refs. 22–27. As it was shown, the Hamiltonian system is defined by the three first class constraints Φ_a given in (2.8), the Dirac brackets (2.9) and the Hamiltonian given in equation (2.7). The Hamiltonian density appearing in (2.7) can be written as follows:

$$\mathscr{H}=\mathscr{H}_0+\lambda^a\Phi_a, \tag{6.1}$$

where we call $\mathscr{H}_0$ the quantity given by

$$\mathscr{H}_0=\mathscr{H}_{can}+B_0\Phi_2. \tag{6.2}$$

Therefore, the following equations hold:

$$[\Phi_a,\Phi_b]_D=C^c{}_{ab}\Phi_c=0, \tag{6.3a}$$

$$[H_0,\Phi_a]_D=V_a^b\Phi_b, \tag{6.3b}$$

where $H_0=\int d^2x\mathscr{H}_0$. From now on we will write the Dirac brackets without the sub-script "D".

We note that in a usual CS theory,[24] all the coefficients V_a^b vanish for a suitable choice of the Hamiltonian density $\mathscr{H}_0$. In the present case, because of the presence of the higher derivative terms, there is no possible choice of $\mathscr{H}_0$ that could allow us the elimination of all the V_a^b

components. When we work with the Hamiltonian $\mathscr{H}_0$ given in (4.2) it results in $V_2^3 = -1$, and the other components of V_a^b are all vanishing. This is the choice that allows the elimination of the greatest number of V_a^b components.

At this stage it is convenient to treat the Lagrange multipliers λ^a defined in (6.1), on the same footing as the remainders dynamical variables, and to associate with them an equal number of canonical momenta, such that

$$[\lambda^a, \mathscr{P}_b] = \delta^a{}_b . \tag{6.4}$$

With the purpose of not changing the dynamical structure of the theory, classically the momenta are constrained to vanish. The constraints $\mathscr{P}_a$ generate the gauge transformation $\lambda^a \rightarrow \lambda^a + u^a$ of the multipliers, making evident their arbitrariness.

Consequently, from now on our dynamical variables will be

$$\boldsymbol{A}_\Sigma = (A_\mu, B_\mu, \bar{\psi}, \psi, \lambda_a). \tag{6.5}$$

The corresponding canonical conjugate momenta are written as

$$\boldsymbol{P}^\Sigma = (P^\mu, Q^\mu, \Pi, \overline{\Pi}, \mathscr{P}^a), \tag{6.6}$$

and the new set of constraints are given by

$$G_A = (\Phi_a, \mathscr{P}_b), \quad a,b = 1,2,3 \quad \text{and} \quad A = 1, \ldots, 6. \tag{6.7}$$

Therefore, the equations (6.3) take the form

$$[G_A, G_B] = 0, \tag{6.8a}$$

$$[H_0, G_A] = V_A^B G_B, \quad \text{with} \quad V_2^3 = -1. \tag{6.8b}$$

Now, by introducing the fermionic ghost fields (Majorana spinors) η_A and their canonical conjugate variables π^A, the BRST invariant gauge fixed Hamiltonian can be written as

$$H_\chi = H_0 + \pi_B V_A^B \eta^A + [\chi, Q], \tag{6.9}$$

where $\chi = \pi_B \omega^B$, being ω^B the gauge fixing conditions given by the set of quantities,

$$\omega^B = (\lambda^a, f^b). \tag{6.10}$$

Furthermore, as we deal with an Abelian model, the BRST generator Q is given by the well known expression:

$$Q = \eta_A G^A. \tag{6.11}$$

As the constraints (6.7) can be divided in two subsets, we assume that the ghosts and the antighosts are introduced in such a way that

$$\eta_A = (\eta_a, \pi_a), \tag{6.12a}$$

$$\pi^A = (\bar{\pi}^a, \bar{\eta}^a). \tag{6.12b}$$

Therefore, the following canonical brackets hold:

$$[\eta_a, \bar{\pi}^b]_+ = \delta_a^b, \tag{6.13a}$$

$$[\pi_a, \bar{\eta}^b]_+ = \delta_a^b, \tag{6.13b}$$

that is, we are working in the mixed representation in which both the ghosts and the antighosts are diagonal.

When an integration in the last term of equation (6.9) is performed, the following Hamiltonian density can be written:

$$\mathscr{H}_\chi = \mathscr{H}_0 + \lambda^a \Phi_a + f^a \mathscr{P}_a + \bar{\pi}^a \pi_a - \bar{\pi}^3 \eta_2 + \bar{\eta}^a [f_a, \Phi^b] \eta_b . \tag{6.14}$$

Thus, the BRST Lagrangian density $\mathscr{L}^{BRST}$ is given by

$$\mathscr{L}^{BRST} = B_\mu P^\mu + \dot{B}_\nu Q^\nu + \dot{\bar{\psi}}\Pi + \overline{\Pi}\dot{\psi} + \dot{\lambda}^a \mathscr{P}_a + \bar{\eta}^a \pi_a + \bar{\pi}^a \dot{\eta}_a - \mathscr{H}_\chi . \tag{6.15}$$

As in the present case, when the constrained system has first and second class constraints, the partition function in the BRST formalism is written by means of the following path integral[27]:

$$Z = \int \mathscr{D}A_\Sigma \mathscr{D}P^\Sigma \mathscr{D}\bar{\eta}_a \mathscr{D}\eta_a \mathscr{D}\bar{\pi}^a \mathscr{D}\pi^a \delta(\Omega^{(\alpha)}) \delta(\overline{\Omega}_{(\alpha)}) \times \exp\, i\left[\int d^3x \mathscr{L}^{BRST} \right]. \tag{6.16}$$

Looking at the equation (6.15), we can see that the variables P_μ do not explicitly appear in $\mathscr{L}^{BRST}$, and so the path integral over this variable must be included in the normalizing factor. Similarly, this occurs with the field components B_0 and Q_0, since the Hamiltonian $\mathscr{H}_0$ in (6.2) was chosen precisely to eliminate as dynamical variables B_0, and so its canonical momentum Q^0.

The path integral over the variables $\bar{\pi}^a$, π^a and Q^i are Gaussian and they are easily performed. The path integral over the momenta $\overline{\Pi}^{(\alpha)}$ and $\Pi^{(\alpha)}$ are also elementary by using the two Dirac's delta functions appearing in (6.16). Therefore, the partition function (6.16) takes the form

$$Z = \int \mathscr{D}A_\mu \mathscr{D}B_i \mathscr{D}\bar{\psi} \mathscr{D}\psi \mathscr{D}\lambda \mathscr{D}\mathscr{P} \mathscr{D}\bar{\eta}^a \mathscr{D}\eta^a \times \exp\, i\left[\int d^3x \mathscr{L}^* \right], \tag{6.17}$$

where the Lagrangian density we call $\mathscr{L}^*$ is written as

$$\mathscr{L}^* = \mathscr{L}_{eff} - \lambda^a \Phi_a + (\dot{\lambda}^a - f^a)\mathscr{P}_a - \bar{\eta}^a [f_a, \Phi^b] \eta_b - [\dot{\bar{\eta}}^a \eta_a + \tfrac{1}{4}\bar{\eta}^2 \eta_2 - \tfrac{1}{2}(\dot{\bar{\eta}}^3 \eta_2 + \bar{\eta}^2 \dot{\eta}_3)], \tag{6.18}$$

and we have called $\mathscr{L}_{eff}$ the Lagrangian density defined in (3.4).

With the aim to recover the expression (3.1) for the partition function in the Faddeev–Senjanovic form, the next task is to go on a relativistic gauge or non-canonical gauge (see Refs. 24 and 26). To do this we make the following replacement:

$$f_a \to \frac{1}{\tau} f'_a , \quad \mathscr{P} \to \tau \mathscr{P}_a , \quad \bar{\eta}^a \to \tau \bar{\eta}'^a ,$$

where the two last substitutions represent a change in the corresponding path integral variables. Later on, the parameter τ will go to zero by virtue of the Fradkin–Vilkovisky theorem, which has stated that the transition amplitude does not depend on this parameter. Once this is done, the partition function results:

$$Z=\int \mathscr{D}A_\mu \mathscr{D}B_i \mathscr{D}\bar{\psi}\mathscr{D}\psi \mathscr{D}\lambda^a \mathscr{D}\mathscr{P}'_a \mathscr{D}\bar{\eta}'^a \mathscr{D}\eta^a$$

$$\times \exp\, i\left[\int d^3x(\mathscr{L}_{eff}-\lambda^a\Phi_a - f'^a\mathscr{P}'_a - \bar{\eta}'^a[f'_a,\Phi^b]\eta_b)\right]. \tag{6.19}$$

After the integration over the path integral variables λ^a , $\mathscr{P}'_a$, $\bar{\eta}'^a$and η_a are performed, the final form for the partition function we can obtain is

$$Z=\int \mathscr{D}A_\mu \mathscr{D}B_i \mathscr{D}\bar{\psi}\mathscr{D}\psi\,\delta(\Phi_a)\,\delta(f'^a)\det[f'^a_{,}\,\Phi^b]\exp\, i\left[\int d^3x\mathscr{L}_{eff}\right]. \tag{6.20}$$

This last expression for the partition function can be confronted with that written in section III. Our starting expression used above in the framework of the canonical formalism to construct the diagrammatic, was proposed following the Faddeev–Senjanovic procedure. So we can conclude that both different methods give the same basic results and therefore, they can be considered as alternatives.

VII. CONCLUSIONS

To go on with the work beginning in Ref. 1, in the present paper we found the diagrammatic and the Feynman rules for a higher-derivative model coupled to matter. This was done by defining a suitable propagator of the bosonic field. The fermionic propagator for the matter field is the usual one. The model has an unique three legs vertex; and all the diagrams are obtained by connecting vertices and sources by means of the propagators thus defined. Using the perturbative theory, the one loop structure of the model was analyzed. The results obtained for the one loop diagrams in which the boson field propagator takes place allows us to guarantee that the ultraviolet behavior is improved and the divergence of these diagrams are eliminated. Therefore, we conclude that the presence of higher-derivative terms in the Lagrangian density gives rise to a new bosonic propagator, which yield that the theory is less divergent.

We have also proved, unlike what occurs in the usual quantum electrodynamics, that in this higher-derivative model there are two single poles; one of them is going to infinity in the limit $c\to 0$; and so the electrodynamic singularity is recovered.

Moreover, the prescription to eliminate the ghost states with negative norm, in such a way that the unitarity can be preserved, was also given.

Finally, by using well known tools and methods, the BRST formalism was constructed. When this formalism is applied to theories containing higher-derivative terms in the Lagrangian, there are some differences contained in the equation (6.3) upon which we have remarked. As it was shown the partition function of the model, in the BRST formalism written in the relativistic non-canonical gauge, is consistent with those obtained by means of a suitable extension of the Faddeev–Senjanovic procedure.

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Asymptotic algebra for charged particles and radiation

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A C^*-algebra of asymptotic fields which properly describes the infrared structure in quantum electrodynamics is proposed. The algebra is generated by the null asymptotic of electromagnetic field and the time asymptotic of charged matter fields which incorporate the corresponding Coulomb fields. As a consequence Gauss' law is satisfied in the algebraic setting. Within this algebra the observables can be identified by the principle of gauge invariance. A class of representations of the asymptotic algebra is constructed which resembles the Kulish–Faddeev treatment of electrically charged asymptotic fields. © *1996 American Institute of Physics.* [S0022-2488(96)01701-X]

I. INTRODUCTION

It is frequently stated that the excellent experimental confirmation of quantum electrodynamics is not matched by sufficient understanding of its theoretical foundations yet. Indeed, the need for better understanding of the theory seems to be confirmed by steady fundamental research. One could even point out that experimental verification has to be considered as provisory, as long as the theory has no completely firm status. This refers not only to the existing experimental evidence. New experimental arrangements may be needed to test the results of further theoretical investigations.

This may especially be the case in relation to the problems connected with the long-range character of the electromagnetic interaction, Gauss' law, and the proper description of charged states. These problems manifest themselves in the infrared divergencies of perturbational QED,[1] the structure of uncountably many superselection sectors,[2,3] the infraparticle problem,[4,5] and the spontaneous breaking of the Lorentz group in charged representations of local observables.[5,6] All these questions have been investigated in various theoretical setups, with varying emphasis on mathematical rigor on the one hand, and concrete calculations on the other. An important step in the development of understanding of the long-range structure was the realization that it is the timelike, resp. lightlike, asymptotic structure that is relevant here.[2,7–9] The work of Kulish and Faddeev deserves special mentioning, as it generalized Dollard's idea[10] of asymptotic dynamics to the Gupta–Bleuler formulation of quantum electrodynamics. A more careful analysis of asymptotical charged states within this formalism was given by Morchio and Strocchi.[11] In rigorous mathematical terms, within the algebraic framework in quantum field theory, the asymptotic electromagnetic field has been obtained as an LSZ-type limit by Buchholz.[3] For reviews see the book by Jauch and Rohrlich,[1] the lecture notes by Morchio and Strocchi,[12] and the book by Haag.[13]

In spite of the progress brought by these works, our understanding of what an electron is is still not very concrete. So far there only exist abstract, though rigorous, characterizations of electrically charged particles.[14,15] Even more importantly, the concrete algebraic structure of the asymptotic quantum fields is still unclear. Thus investigations of properties such as the spontaneous breaking of the Lorentz group in charged sectors or the nonexistence of sharp masses (infraparticles) are frequently based on *ad hoc* assumptions. Most general results are therefore of the ''no-go'' type (see, e.g., Ref. 5).

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It is the aim of the present work to propose a concrete formulation of the algebraic structure of asymptotic fields (and observables) of electrons interacting with radiation. This algebra resembles various elements of standard knowledge on the infrared problem. However, we would like to point out three novel aspects of our formulation.

(i) A clear and consistent algebraic framework is obtained. The asymptotic algebra is a C^*-algebra, thereby placing the problem on firm mathematical grounds.

(ii) We do not have to consider the fully interacting quantum field theory. In particular, the canonical quantization (which is taken for granted in the treatment of Kulish and Faddeev) is avoided. In fact, this heuristic procedure for obtaining the algebraic structure may fail in the field of long-range problems, as we shall discuss. Instead we base our construction on the asymptotic structure of classical electrodynamics (Maxwell and Dirac) which has been established in Ref. 16. These results lead naturally via the correspondence principle to our quantum algebra.

(iii) The algebra incorporates the Coulomb fields of the asymptotic (outgoing) particles. In this respect it resembles the theory of the quantized Coulomb field of Staruszkiewicz.[17] However, the latter is an idealized theory of certain isolated degrees of freedom, and it seems to have no natural embedding into a larger scheme.

The plan of the paper is as follows. In Sec. II we describe briefly the asymptotic structure of the classical theory. Part of the material is shifted to the Appendix. In Sec. III this structure is then quantized according to the correspondence principle. Heuristical physical considerations are presented which lead to formal algebraic relations for the fields. These relations are made mathematically precise in Sec. IV, and lead to our asymptotic C^*-algebra. A class of representations of the algebra is constructed in Sec. V. The question of physical relevance of these representations is left for future work. Section VI brings some final remarks, and comments on future perspectives of this work.

II. CLASSICAL ASYMPTOTIC STRUCTURE

In this section we give a short account of the asymptotic structure of a classical field theory with electromagnetic interaction, discussed at length in Ref. 16. For the definiteness we considered the Dirac field interacting with radiation. Complete rigorous results were obtained along the lines summarized here for the both external field problems, but the extension to the full theory is possible, as argued in Ref. 16, under plausible conjectures. (The relation of our asymptotic variables to those used by Flato *et al.*[18] in their recent solution of the Cauchy problem and proof of asymptotic completeness of the Maxwell–Dirac system is an open problem.) The aim of this summary is also, for the convenience of the reader, to rewrite in the tensor form the properties and formulas for the asymptotics of the electromagnetic field which were discussed in the two-component spinor language in Ref. 16. Equivalence to the original formulation is proved in the Appendix.

The idea of the approach deviates from the standard formulation of the scattering problem as the limit of constant time configurations with time tending to infinity. Rather, the advantage is taken of the different propagation velocities of matter and radiation, to consider their asymptotics in different space–time regions. For the electromagnetic field the known methods of the null infinity asymptotics[19,20] are applied, formulated in terms of homogeneous functions (without Penrose's space–time compactification) and further developed in some specific aspects. For the matter field a method is developed which leads to the determination of an asymptotic field inside the forward lightcone—this is sufficient, as eventually every massive particle enters the cone. Plausible arguments then indicate that asymptotics thus defined contain the full information on the system and the total Poincaré quantities (energy-momentum and four-dimensional angular momentum) of the theory may be expressed in terms of them.

The electromagnetic field of the system admits a class of gauges of the potential with the null asymptotic of the form [Eq. (2.45) in Ref. 16]

$$\lim_{R\to\infty} RA_a(x+Rl)=V_a(x\cdot l,l). \tag{2.1}$$

Here x is any space–time point in Minkowski space M and l is a future-pointing null vector. The function $V_a(s,l)$ (s is a real variable) is homogeneous of degree -1,

$$V_a(\mu s,\mu l)=\mu^{-1}V_a(s,l), \tag{2.2}$$

($\mu>0$), and satisfies

$$l\cdot V(s,l)=Q, \tag{2.3}$$

where Q is the charge of the field. Its s-derivative $\dot{V}_a(s,l):=(\partial/\partial s)V_a(s,l)$ falls off according to

$$|\dot{V}_a(s,l)|<\frac{\text{const}}{(1+|s|)^{1+\epsilon}} \tag{2.4}$$

for some $\epsilon>0$, so $V_a(s,l)$ has limits for $s\to\pm\infty$, which we denote $V_a(\pm\infty,l)$. [Null vectors l are scaled in (2.4) to $l^0=1$ in arbitrarily chosen, fixed Minkowski frame; change of frame results only in change of bounding constant.] Gauge freedom consists of the transformation $V_a(s,l)\to V_a(s,l)+\alpha(s,l)l_a$.

Further properties of the limit values $V_a(\pm\infty,l)$ involve differentiation on cone variables. A simple and explicitly Lorentz-covariant way to express the differentiations in directions tangent to the cone is to use the operator $l_a\partial_b-l_b\partial_a(\partial_a:=\partial/\partial l^a)$. One applies the operator to any differentiable extension to some neighborhood of the cone of a function defined on the cone itself, and restricts the result again to the cone. The result is independent of the extension used.

The limit values $V_a(\pm\infty,l)$ are constrained by the following gauge-invariant condition:

$$l_{[a}\partial_b V_{c]}(\pm\infty,l)=0 \tag{2.5}$$

[this is the tensor form of the conditions (3.32) with (2.54)–(2.57) in Ref. 16; see also the Appendix]. The physical content of the condition, which is satisfied in standard scattering situations, is that it allows the identification of the total angular momentum of the system, as discussed in Ref. 16. The properties (2.2), (2.3), and (2.5) allow another simple representation of $V_a(\pm\infty,l)$. It follows from (2.2) and (2.3) that $(l_b\partial_a-l_a\partial_b)V^b(\pm\infty,l)+V_a(\pm\infty,l)\propto l_a$. We denote

$$(l_b\partial_a-l_a\partial_b)V^b(+\infty,l)+V_a(+\infty,l)=2q(l)l_a, \tag{2.6}$$

$$(l_b\partial_a-l_a\partial_b)V^b(-\infty,l)+V_a(-\infty,l)=2\kappa(l)l_a. \tag{2.7}$$

Here $q(l)$ and $\kappa(l)$ are homogeneous functions of degree -2. If, for the sake of differentiation, the extensions of $V_a(\pm\infty,l)$ are chosen so as to satisfy (2.3) also in a neighborhood of the cone, then

$$q(l)=-\tfrac{1}{2}\partial_b V^b(+\infty,l),\quad \kappa(l)==-\tfrac{1}{2}\partial_b V^b(-\infty,l). \tag{2.8}$$

The charge of the field is recovered from the functions $q(l)$ and $\kappa(l)$ by the formulas

$$Q=\frac{1}{2\pi}\int q(l)d^2l=\frac{1}{2\pi}\int \kappa(l)d^2l. \tag{2.9}$$

By d^2l we denote that measure on the set of null directions which gives a Lorentz invariant result when applied to a homogeneous function of l of degree -2 (see Ref. 16 and references given there). The measure itself is homogeneous of degree 2, and for l's scaled to $l^0=1$ in any fixed

Minkowski frame it is the rotationally invariant measure on the unit sphere of vectors **l**. For future reference we note that if $\alpha(l)$ is differentiable and homogeneous of degree -2, then (see Appendix)

$$\int (l_a\partial_b - l_b\partial_a)\alpha(l)d^2l = 0. \tag{2.10}$$

Now conversely, one can show that if $q(l)$ and $\kappa(l)$ are homogeneous functions of degree -2 satisfying (2.9), then the vector functions $V_a(\pm\infty,l)$ constrained by (2.2), (2.3), and (2.5) are determined by (2.6) and (2.7) uniquely up to a gauge [Ref. 16, after Eq. (2.61)].

Physical interpretation of $\kappa(l)$ is of importance: this function determines the flux of the electromagnetic field in spacelike infinity. Explicitly, if x is any point and y a spacelike vector, then

$$\lim_{R\to\infty} R^2F_{ab}(x+Ry) = K_a(y)y_b - K_b(y)y_a, \tag{2.11}$$

where

$$K_a(y) = \frac{1}{2\pi y^2}\,\nabla_a \int \kappa(l)\,\mathrm{sgn}\, y\cdot l\, d^2l. \tag{2.12}$$

If the potential is decomposed in the standard way into the advanced and the free outgoing part $A_a = A^{\mathrm{adv}}{}_a + A^{\mathrm{out}}{}_a$, then $A^{\mathrm{adv}}{}_a$ and $A^{\mathrm{out}}{}_a$ have again asymptotics of the type (2.1) with $V_a(+\infty,l)$ and $V^{\mathrm{out}}{}_a(s,l) := V_a(s,l) - V_a(+\infty,l)$ replacing $V_a(s,l)$ on the right-hand side (rhs) of (2.1), respectively. This brings the physical interpretation of $q(l)$: this function determines the asymptotic Coulomb field of the outgoing currents.

The free outgoing field is completely determined by its asymptotic according to the formula

$$A^{\mathrm{out}}{}_a(x) = -\frac{1}{2\pi}\int \dot{V}^{\mathrm{out}}{}_a(x\cdot l,l)d^2l. \tag{2.13}$$

The flux of the field $F^{\mathrm{out}}{}_{ab}(x)$ at the spacelike infinity is again given by the formulas (2.11) and (2.12) in which $\kappa(l)$ is replaced by $\sigma(l) := \kappa(l) - q(l) = -(1/2)\partial^b V^{\mathrm{out}}{}_b(-\infty,l)$, which is therefore interpreted as the infrared characteristic of the free field. The vector function $V^{\mathrm{out}}{}_a(-\infty,l)$ is again determined up to a gauge by $\sigma(l)$, but in this case a more explicit representation is possible. One shows that Eq. (2.5) [satisfied by $V^{\mathrm{out}}{}_a(-\infty,l)$] and the condition $l\cdot V^{\mathrm{out}}(-\infty,l)=0$ together imply the existence of a real function $\Phi(l)$ homogeneous of degree 0 such that (see the Appendix)

$$l_{[a}V^{\mathrm{out}}{}_{b]}(-\infty,l) = l_{[a}\partial_{b]}\Phi(l). \tag{2.14}$$

Here $\Phi(l)$ is determined by this condition up to an additive constant. We make the choice of this constant characterize classes of gauges of $V^{\mathrm{out}}{}_a(-\infty,l)$ as follows. First, fix $\Phi(l)$ with some choice of the constant. Then, choose an antisymmetric real tensor function $G_{ab}(l) = -G_{ba}(l)$, homogeneous of degree 0, such that

$$l_{[a}G_{bc]}(l) = 0, \quad G_{ab}(l)l^b = \Phi(l)l_a. \tag{2.15}$$

This tensor is then of the form $G_{ab}(l) = l_a g_b(l) - l_b g_a(l)$, where $g_a(l)$ is homogeneous of degree -1, satisfies

$$l\cdot g(l) = \Phi(l), \tag{2.16}$$

and is determined by $G_{ab}(l)$ up to $g_a(l)\to g_a(l) + \alpha(l)l_a$. Finally, put

$$V^{\text{out}}{}_a(-\infty,l)=(l_b\partial_a-l_a\partial_b)g^b(l)+g_a(l). \tag{2.17}$$

One shows that

(i) (2.17) satisfies (2.14);
(ii) every gauge of $V^{\text{out}}{}_a(-\infty,l)$ may be represented in this way and the correspondence with the tensors $G_{ab}(l)$ is 1:1;
(iii) gauges corresponding to the choices of G_{ab}'s with a fixed constant in $\Phi(l)$ form equivalence classes with respect to the following equivalence relation: $V_1^{\text{out}}{}_a(-\infty,l)\sim V_2^{\text{out}}{}_a(-\infty,l)$ iff $\int\alpha(l)d^2l=0$, where $V_1^{\text{out}}{}_a(-\infty,l)-V_2^{\text{out}}{}_a(-\infty,l)=\alpha(l)l_a$. We shall see in Sec. III that the interpretation imposed by the above procedure on the additive constant in $\Phi(l)$ is a very natural one from the point of view of the symplectic form for electromagnetic field.

The asymptotic of the Dirac field $\psi(x)$ inside the forward lightcone is determined by considering the behavior of $\psi(\lambda v)$ for large λ, where the four-velocity v lies on the hyperboloid $H:=\{v\in M|v^2=1,\ v^0>0\}$. Physically, the most important condition for the validity of our discussion is such a choice of gauge of the electromagnetic potential, that $|v\cdot A(\lambda v)|<\text{const}\,\lambda^{-1-\epsilon}$, ($\epsilon>0$). That this is possible in our context is shown in Ref. 16 where further details are also given. One shows then that if we put

$$\psi(\lambda v)=-i\lambda^{-3/2}e^{-i(m\lambda+\pi/4)\gamma\cdot v}f_\lambda(v)$$

(γ^a are the Dirac matrices), then $\lim_{\lambda\to\infty}f_\lambda(v)=f(v)$. For the external field problem it is shown that this limit is reached strongly in the Hilbert space $\mathscr{K}$ of four-component functions on the hyperboloid H with the scalar product

$$(f,g)=\int\overline{f(v)}\gamma\cdot v g(v)d\mu(v), \tag{2.18}$$

where bar denotes the usual Dirac conjugation and $d\mu(v)=d^3v/v^0$ is the invariant measure on the hyperboloid. Moreover, free outgoing field may be determined by

$$\psi^{\text{out}}(x)=\left(\frac{m}{2\pi}\right)^{3/2}\int e^{-imx\cdot v\gamma\cdot v}\gamma\cdot v f(v)d\mu(v). \tag{2.19}$$

$\psi^{\text{out}}(x)$ has the same asymptotic as $\psi(x)$. It is argued that the structure is essentially the same in the full theory. In that case the characteristic $q(l)$ of the Coulomb field of the outgoing currents is expressed in terms of their asymptotic

$$q(l)=e\int\overline{f(v)}\gamma\cdot v f(v)\,\frac{d\mu(v)}{2(v\cdot l)^2} \tag{2.20}$$

(e is the charge of the electron).

We note for future use that explicitly Lorentz-covariant differentiation on H may be discussed with the use of operators defined in exactly the same way as it has been done in the case of the lightcone in the paragraph preceding (2.5). In the case of hyperboloid the operator contracted with v^b contains the whole information

$$\delta_a f(v):=(\partial_a-v_a v\cdot\partial)f(v). \tag{2.21}$$

Finally, total Poincaré quantities are expressed in terms of the outgoing fields. One finds that these quantities are the sums of the respective quantities for the free fields ${F^{\text{out}}}_{ab}(x)$ and $\psi^{\text{out}}(x)$ [determined by (2.13) and (2.19), respectively], with, however, one additional term in the case of angular momentum

$$\Delta M_{ab} = -\frac{1}{2\pi}\int q(l)(l_a\partial_b - l_b\partial_a)\Phi(l)d^2l. \tag{2.22}$$

This term is seen to mix the outgoing matter characteristic $q(l)$ with the infrared characteristic $\Phi(l)$. (It originates from the mixed adv–out terms of the asymptotics in null directions of the electromagnetic energy-momentum tensor.) This mixing of the long-range degrees of freedom corresponds to this remnant of interaction which is responsible for the validity of the Gauss' law. Its appearance shows that a Poisson bracket structure separating the two fields asymptotically remains in contradiction not only with the Gauss' law, but also with the Poincaré structure of the theory.

III. QUANTIZATION

We assume now that the asymptotic structure of the quantum theory may be described by quantum variables analogous to $V_a(s,l)$ and $f(v)$. By that we mean that these analogs generate an algebra, the states of which may be interpreted as scattering states in quantum electrodynamics. In the present section we give heuristic arguments which lead us to the formulation of quantization conditions for these variables. In Sec. IV, then, the appropriate algebra is constructed.

The usual quantization of the free electromagnetic field is achieved by the use of the symplectic form

$$\{F_1, F_2\} = \frac{1}{4\pi}\int_\Sigma ({F_1}^{ab}A_{2b} - {F_2}^{ab}A_{1b})d\sigma_a, \tag{3.1}$$

the integration extending over a Cauchy surface Σ. It has been observed by other authors before[18,19] that the integration surface may be shifted so as to become the future null infinity hypersurface (in the language of the compactified Minkowski space), as the fields are determined by their data on this surface. This corresponds in our language (no compactification) to the integration of "radiated" symplectic form. This is calculated in exactly the same way in which the radiated energy-momentum and angular momentum were determined in Ref. 16, Eqs. (3.6)–(3.14). The explicitly Lorentz-invariant result, denoted by $\{V_1, V_2\}$, is

$$\{V_1, V_2\} = \frac{1}{4\pi}\int (\dot{V}_1\cdot V_2 - \dot{V}_2\cdot V_1)(s,l)ds\ d^2l, \tag{3.2}$$

where V_i are asymptotics (2.1). However, we observe that also in the presence of sources the electromagnetic field is locally free in the null asymptotic region, so one can try to use the same symplectic form for the asymptotics of the interacting theory. The form (3.2) is now extended without formal change to asymptotics of all fields admitted by the framework of Sec. II. [The reason for taking (3.2) rather than directly the "radiated" analog of (3.1) for general fields as a basis for generalization is that for charged fields with nonvanishing infrared part the latter form yields no Lorentz invariant result. If the calculation is performed in a frame with the time-axis along the positive unit timelike vector t, then the result differs from (3.2) by

$$\frac{Q_2}{4\pi}\int t^a {V_1^{\text{out}}}_a(-\infty,l)\,\frac{d^2l}{t\cdot l} - \frac{Q_1}{4\pi}\int t^a {V_2^{\text{out}}}_a(-\infty,l)\,\frac{d^2l}{t\cdot l},$$

where Q_i are the charges (2.3).]

If V's are split into the free and the Coulomb part $V_a(s,l)=V^{\text{out}}{}_a(s,l)+V_a(+\infty,l)$, then

$$\{V_1,V_2\}=\{V_1^{\text{out}},V_2^{\text{out}}\}+\frac{1}{4\pi}\int (V_1(+\infty,l)\cdot V_2^{\text{out}}(-\infty,l)-V_2(+\infty,l)\cdot V_1^{\text{out}}(-\infty,l))d^2l.$$

Substituting in the second term (2.17), integrating by parts with the use of (2.10), and finally using (2.6) and (2.16) one obtains

$$\{V_1,V_2\}=\frac{1}{4\pi}\int (\dot{V}_1^{\text{out}}\cdot V_2^{\text{out}}-\dot{V}_2^{\text{out}}\cdot V_1^{\text{out}})(s,l)ds\ d^2l+\frac{1}{2\pi}\int (q_1\Phi_2-q_2\Phi_1)(l)d^2l. \quad (3.3)$$

The first term on the rhs is gauge invariant, while the second depends on gauge only through the choice of the additive constant in $\Phi(l)$, that is, on the choice of one of the equivalence classes of $V^{\text{out}}{}_a(-\infty,l)$ discussed after Eq. (2.17). The above compact form of the second term supplies justification for our interpretation of the constant in $\Phi(l)$.

Let now $V^{\text{op}}{}_a(s,l)$ be a quantum field and $V_a(s,l)$ a classical test field. The heuristic quantization rule is

$$[\{V_1,V^{\text{op}}\},\{V_2,V^{\text{op}}\}]=i\{V_1,V_2\},$$

where the real multiplicative constant on the rhs is fixed by the condition that the quantization reduces to the standard one for free infrared–regular test fields. In the Weyl exponentiated form this becomes $W(V_1)W(V_2)=e^{-(i\beta^2/2)\{V_1,V_2\}}W(V_1+V_2)$, where we put $W(V)=e^{-i\beta\{V,V^{\text{op}}\}}$, with β a real constant to be determined shortly. The Weyl operators are assumed to depend only on those variables, which enter nontrivially into the symplectic form (3.3), that is, they are insensitive to the gauge of $V^{\text{out}}{}_a(s,l)$ for finite s and to the gauge of $V_a(+\infty,l)$, and they depend on the gauge of $V^{\text{out}}{}_a(-\infty,l)$ only through the choice of constant in $\Phi(l)$. Therefore we shall write sometimes $W(V)=W(\xi,\Phi,q)$, where $\xi_{ab}(s,l):=l_aV^{\text{out}}{}_b(s,l)-l_bV^{\text{out}}{}_a(s,l)$. [Remember that $\Phi(l)$ is determined by $\xi_{ab}(-\infty,l)$ up to an additive constant.] The form (3.3) determines the physical interpretation of the Weyl operator for $q=0$, $\xi=0$, $\Phi=c=$const: $W(0,c,0)=e^{i\beta cQ^{\text{op}}}$, where Q^{op} is the operator of the charge of the field. From Weyl relations we have then

$$e^{i\beta cQ^{\text{op}}}W(V)=W(V)e^{i\beta c(Q^{\text{op}}+\beta Q)},$$

where Q is the charge of the electromagnetic test field V. For the interpretation of the classical and the quantum charge to agree we set $\beta=1$. Then the Weyl operator $W(V)$ carries a quantum charge equal to the classical charge of the test field V. More generally, it may be interpreted to carry the asymptotic field characterized by $V_a(s,l)$. The Weyl algebra

$$W(V_1)W(V_2)=e^{-(i/2)\{V_1,V_2\}}W(V_1+V_2) \quad (3.4)$$

may be considered as a theory of the asymptotic electromagnetic field. The quantization of charge demands that the space of test fields be restricted to the Abelian additive group of those Vs which carry the multiple of the elementary charge $Q=(1/2\pi)\int q(l)d^2l=ne$. The subgroup of zero-charge test fields forms a vector space. (For the discussion of an ''adiabatic limit'' of such a theory, in which only the long-range characteristics of the field survive, we refer the reader to Ref. 21.) However, the theory thus formulated is physically incomplete—it admits Coulomb fields, but there are no particles present to carry these fields. We turn now to the description of these particles.

Let us forget for the moment that there is some ''Gauss coupling'' between the asymptotic electromagnetic and Dirac fields which has to modify the Poisson bracket structure (as compared with the structure of two independent fields). Then the quantum field $f^{\text{op}}(v)$ which is to corre-

spond to the classical $f(v)$ is quantized in the standard Dirac way. We denote the quantum field smeared with the test field $f(v)$ by $B(f)$ and replace $f^{\mathrm{op}}(v)$ by $B(v)$, so that symbolically $B(f) = \int \overline{f(v)}\gamma\cdot v B(v) d\mu(v)$, where f is in $\mathscr{K}$, the Hilbert space introduced before (2.18). The standard quantization law in our notation reads

$$[B(f),\, B(g)]_+ = 0, \quad [B(f),\, B(g)^*]_+ = (f,g).$$

It will be convenient for our purposes to have fermionic operators depending on fs linearly. We introduce notation

$$B^0(f) = B(f^c) = \int B^0(v)\gamma\cdot v f(v) d\mu(v), \tag{3.5}$$

$$\bar{B}(f) = B(f)^* = \int \bar{B}(v)\gamma\cdot v f(v) d\mu(v), \tag{3.6}$$

where f^c is the charge conjugation of f defined by

$$f^c = C\bar{f}^T, \tag{3.7}$$

with C a unitary, antisymmetric matrix inducing the transformation $C^{-1}\gamma^a C = -\gamma^{aT}$. The involution law is then

$$B^0(f)^* = \bar{B}(f^c), \tag{3.8}$$

and anticommutation relations

$$[B^0(f),\, B^0(g)]_+ = 0, \quad [B^0(f),\, \bar{B}(g)]_+ = (f^c, g), \tag{3.9}$$

or, symbolically,

$$[B^0(v)_\alpha,\, B^0(v)_\beta]_+ = 0, \quad [B^0(v)_\alpha, \bar{B}(u)_\beta]_+ = \delta(v,u)(C^{-1}\gamma\cdot v)_{\alpha\beta}, \tag{3.10}$$

where $\delta(v,u)$ is the Dirac "δ-function" in the two velocities with respect to the measure $d\mu(v)$.

Physical interpretation of $B(f)$ and $B^0(f)$ justified by the Fock representation is that these operators annihilate an electron and/or create a positron. This means that they locally create charge $-e$ (if e is the charge of electron). More specifically, the operators $B(v)$ and $B^0(v)$ [resp. $\bar{B}(v)$] (forget for the moment mathematical subtleties) create the charge $-e$ (resp. e) moving with a constant four-velocity v. However, if the Gauss' law is again brought into play, creation of a charged particle must have electromagnetic consequences. Therefore, we want to extend the effect of Bs in such a way that they create (or annihilate) also the Coulomb field accompanying the charge. Basing the intuitions on pictures from perturbation calculations and on the algebraic discussion of superselection sectors of local observables, we want to admit the possibility that charged particles are in addition accompanied by "clouds" of radiation. Let the potential of the total field (Coulomb+radiation) accompanying charge e moving with velocity v be characterized by the asymptotic $V_a(v) = V_a(v;s,l)$. Then for each v this asymptotic is in the class discussed in Sec. II, and, moreover, its Coulomb part is, up to a gauge, the asymptotic of the potential $A_a(x) = ev_a/v\cdot x$, that is $V_a(v;+\infty,l) = ev_a/v\cdot l + \text{gauge}$. Now we seek operators $B^0_{-V_1}(v)$ and $\bar{B}_{V_2}(v)$ analogous to $B^0(v)$ and $\bar{B}(v)$ respectively, which, however, beside creating or annihilating material particles should also carry accompanying electromagnetic fields with asymptotics $-V_1(v)$ and $V_2(v)$, respectively, where V_1 and V_2 are in the class introduced above. Thus formulated, the problem almost uniquely determines its solution—the objects which do the electromagnetic part of the task are already there, the Weyl operators $W(-V_1(v))$, and $W(V_2(v))$ carry

exactly those charged fields. For the purpose of obtaining commutation relations we imagine the operators $B^0_{-V_1}(v)$ [resp. $\bar{B}_{V_2}(v)$] to be formed as products of $B^0(v)$ [resp. $\bar{B}(v)$] and $W(-V_1(v))$ [resp. $W(V_2(v))$] (mutually commuting). On the other hand, having attached charged fields to the matter particles in this way, we do not need any longer, as independent objects, the Weyl operators $W(V)$ for test fields with nonvanishing Coulomb part. From now on the asymptotic V in $W(V)$ is always a free-field asymptotic $[V_a(+\infty,l)=0]$.

The (naive) commutation relations resulting from the above discussion are

$$B^0_{-V_1}(v)W(V)=e^{(i/2)\{V_1(v),V\}}B^0_{-V_1+V}(v),$$

$$\bar{B}_{V_2}(v)W(V)=e^{-(i/2)\{V_2(v),V\}}\bar{B}_{V_2+V}(v),$$

$$e^{(i/2)\{V_1(v),V_2(u)\}}B^0_{-V_1}(v)_\alpha B^0_{-V_2}(u)_\beta+e^{(i/2)\{V_2(u),V_1(v)\}}B^0_{-V_2}(u)_\beta B^0_{-V_1}(v)_\alpha=0,$$

$$\begin{aligned}e^{-(i/2)\{V_1(v),V_2(u)\}}B^0_{-V_1}(v)_\alpha\bar{B}_{V_2}(u)_\beta+e^{-(i/2)\{V_2(u),V_1(v)\}}\bar{B}_{V_2}(u)_\beta B^0_{-V_1}(v)_\alpha\\ =\delta(v,u)(C^{-1}\gamma\cdot v)_{\alpha\beta}W(V_2(v)-V_1(v)),\end{aligned}$$

supplemented with the Weyl relations. Note that the asymptotic in the Weyl operator in the last line is a free-field asymptotic, as $V_2(v;+\infty,l)-V_1(v;+\infty,l)=0$.

For a precise formulation of the above quantization conditions it will not suffice, in contrast to the case of the Dirac field algebra, to have objects smeared with one-particle test functions as generating elements. Smeared products of $B^0_{-V_1}(v)$, $\bar{B}_{V_2}(v)$ and $W(V_2(v)-V_1(v))$ have to be defined, and the phase factors appearing in the above relations must become multipliers in the space of test fields. This construction is given in Sec. IV.

Before we go over to this task we want to draw attention to a known fact concerning physical interpretation of Weyl operators, which, however, in our context is of decisive importance and must not be overlooked. We illustrate our point first on the simplest possible example, the Weyl algebra of a single pair of canonical variables in quantum mechanics, $[x,p]=i\mathbf{1}$. The Weyl formulation reads in that case

$$W(x_1,p_1)W(x_2,p_2)=e^{-(i/2)\{x_1,p_1;x_2,p_2\}}W(x_1+x_2,p_1+p_2),$$

where x_i and p_i are classical ''test''-position and momentum variables, the symplectic form is $\{x_1,p_1;x_2,p_2\}=x_1p_2-x_2p_1$, and the Weyl operator is interpreted as $W(x_1,p_1)=e^{-i\{x_1,p_1;x,p\}}$. We want to point out a certain duality in the interpretation of $W(x_1,p_1)$. Let us set for simplicity $p_1=0$. Then, on the one hand, if treated as a function of observables, the Weyl operator $W(x_1,0)=e^{-ix_1p}$ ''measures'' the probability distribution of a state with respect to the momentum. On the other hand we have $W(x_1,0)^*xW(x_1,0)=x+x_1$. Hence, if treated as a unitary transformation operator, $W(x_1,0)$ ''carries'' the translation x_1; that is, when applied to a vector in Hilbert space it increases its position characteristic by the ''test''-position x_1. The characteristic which is ''carried'' by a Weyl operator in this sense is thus the one given by the test-quantity, while the ''measured'' one is dual to it, in the sense of the symplectic form. Going back to our objects we see that $B^0_{-V_1}(v)$, $\bar{B}_{V_2}(v)$ and $W(V)$ carry the respective fields in the above sense, in the case of $W(V)$ a free field. However, from the symplectic form (3.3) one reads off that the asymptotic of a free-field potential has as its dual the asymptotic of the total field, which is therefore what is ''measured'' by $W(V)$.

IV. THE ALGEBRA

Consider the set of C^∞ functions $V_a(s,l)$ [differentiations with respect to l in the sense discussed before Eq. (2.5), outside some neighborhood of the vertex of the cone] satisfying conditions (2.2)–(2.5). In this set introduce the following equivalence relation: $V_2(s,l)\sim V_1(s,l)$ iff $V_2(s,l)=V_1(s,l)+\alpha(s,l)l$ and $\int(\alpha(-\infty,l)-\alpha(+\infty,l))\,d^2l=0$ [this is the equivalence relation for the infrared characteristics of the free field component of V_a, introduced in (iii) after (2.17)]. The set of equivalence classes with respect to this relation will be denoted by L_Q. Another way of characterizing elements of L_Q is by the triples (ξ,Φ,q) introduced in the paragraph preceding Eq. (3.4). In order not to burden the notation, the elements of L_Q will be denoted by $V_a(s,l)$, but always the equivalence classes are understood. The set $\hat{L}:=\cup_{n\in\mathbf{Z}}L_{ne}$ has in a natural way the structure of an Abelian additive group. With the map $\{.,.\}:\hat{L}\times\hat{L}\to\mathbf{R}$ defined by (3.2), it becomes a symplectic group, on which $\{.,.\}$ is nondegenerate. The subgroup $L_0\subset\hat{L}$ has the structure of a vector space. Its subspace consisting of elements satisfying in addition $V_a(+\infty,l)\propto l_a$ (no Coulomb field) will be denoted by L. This symplectic space is again nondegenerate. Without loss of generality it may be assumed that for all Vs in L there is $V_a(+\infty,l)=0$. Elements of L will be the test functions of Weyl operators.

Consider, next, the class of all functions $V_a(v)$ on the hyperboloid H with values in L_e, such that

(i) $V^a(v;+\infty,l)=V_e{}^a(v,l)+\text{gauge}$, where $V_e{}^a(v,l):=ev^a/v\cdot l$, or, equivalently, $q(v,l)=q_e(v,l):=(e/2)(v\cdot l)^{-2}$;

(ii) for each $V(v)$ there is a function $F_V(v)$ such that

$$\{V(v),V(u)\}=F_V(v)-F_V(u) \tag{4.1}$$

for every v and u;

(iii) representants $V_a(v;s,l)$ may be chosen in C^∞ in v [differentiations in the sense of (2.21)] and for each $k=0,1,...$ there are constants $C_k\in\mathbf{R}$ and $m_k\in\mathbf{N}\cup\{0\}$ such that

$$|\delta_{a_1}\cdots\delta_{a_k}\dot{V}_b(v;s,l)|<C_k(v^0)^{m_k}(|s|+1)^{-1-\epsilon}$$

(in a fixed Minkowski frame, with scaling of ls fixed by $l^0=1$; the change of frame induces only a change of C_k).

Let $\mathscr{S}at_e$ be a subclass of this family of functions, such that

(iv) if $V_1(v)\in\mathscr{S}at_e$ and $V_0\in L$, then $V_2(v)=V_1(v)+V_0\in\mathscr{S}at_e$; this condition is fulfilled if $\mathscr{S}at_e$ consists of all functions satisfying (i)–(iii).

Denote, moreover, $\mathscr{S}at_{-e}:=-\mathscr{S}at_e$ and $\mathscr{R}ad:=\mathscr{S}at_e+\mathscr{S}at_{-e}$. The elements of $\mathscr{S}at_e$ and $\mathscr{S}at_{-e}$ will be the fields accompanying particles. Free fields from the class $\mathscr{R}ad$ will serve to define smeared Weyl operators.

Physical meaning of the first condition has been explained before. The next two conditions are of technical nature. The second one will guarantee the boundedness of the fermionic operators. The third implies that for $V_1,V_2\in\mathscr{S}at_e\cup\mathscr{S}at_{-e}\cup\mathscr{R}ad$ the symplectic form $\{V_1(v),V_2(u)\}$, and phase factors containing it linearly in exponent, are C^∞ functions in both variables, bounded polynomially in each of them. These properties make them multipliers in the space of Schwartz functions on $H^{\times n}$. Finally, the fourth condition says that a free field may be added to the cloud of the particle.

After these preliminaries our algebra may be constructed. We introduce formal symbols $W(V)$ for $V\in L$, W_V for $V\in\mathscr{R}ad$, B_V^0 for $V\in\mathscr{S}at_{-e}$, and B_V for $V\in\mathscr{S}at_e$. The symbol to which a given V is attached determines the class to which it belongs, so there is no need for special notation of Vs for each case separately. Let D be any finite sequence of these four symbols and χ a Schwartz function having one four-velocity argument for each of the symbols W_V, B_V^0, and B_V, and one index taking the values $\alpha=1,...,4$, for each of the symbols B_V^0 and B_V. If the sequence D

contains n symbols W_V, B^0_V and $\bar{B}_V$, and m symbols B^0_V and $\bar{B}_V$, then $\chi \in \mathscr{S}(H^n, \mathbf{C}^{4^m})$. We introduce a new symbol $[D](\chi)$, linear by assumption in χ. For a symbol consisting of only one of the operators W_V, B^0_V, or B_V, the symbolic notation is introduced

$$W_V(\chi) = \int W_V(v)\chi(v)d\mu(v), \tag{4.2}$$

$$B^0_V(f\ ) = \int B^0_V(v)\gamma\cdot v f(v)d\mu(v), \tag{4.3}$$

$$\bar{B}_V(f\ ) = \int \bar{B}_V(v)\gamma\cdot v f(v)d\mu(v), \tag{4.4}$$

[cf. (3.5) and (3.6)] and extended by linearity to general symbols $[D](\chi)$. The set of all formal finite sums of these symbols forms a vector space. We divide this space by its subspace generated by the following identifications [$G_V(v)$ is any of the symbols $W_V(v)$, $B^0_V(v)$, or $B_V(v)$]:

$$e^{(i/2)\{V_1,V_2\}}W(V_1)W(V_2) = W(V_1+V_2), \tag{4.5}$$

$$e^{(i/2)\{V_1,V_2(v)\}}W(V_1)G_{V_2}(v) = G_{V_1+V_2}(v), \tag{4.6}$$

$$e^{(i/2)\{V_2(v),V_1\}}G_{V_2}(v)W(V_1) = G_{V_1+V_2}(v), \tag{4.7}$$

$$e^{(i/2)\{V_1(v),V_2(u)\}}W_{V_1}(v)G_{V_2}(u) - e^{(i/2)\{V_2(u),V_1(v)\}}G_{V_2}(u)W_{V_1}(v) = 0, \tag{4.8}$$

$$e^{(i/2)\{V_1(v),V_2(u)\}}B^\sharp_{V_1}(v)_\alpha B^\sharp_{V_2}(u)_\beta + e^{(i/2)\{V_2(u),V_1(v)\}}B^\sharp_{V_2}(u)_\beta B^\sharp_{V_1}(v)_\alpha = 0, \tag{4.9}$$

$$\begin{aligned} &e^{(i/2)\{V_1(v),V_2(u)\}}B^0_{V_1}(v)_\alpha \bar{B}_{V_2}(u)_\beta + e^{(i/2)\{V_2(u),V_1(v)\}}\bar{B}_{V_2}(u)_\beta B^0_{V_1}(v)_\alpha \\ &\quad = \delta(v,u)(C^{-1}\gamma\cdot v)_{\alpha\beta}W_{V_1+V_2}(v); \end{aligned} \tag{4.10}$$

if $V(v) = V_0 = \text{const}(v)$ on the support of $\chi(...,v,...)$ in v, the variable connected with $W_V(v)$, then

$$[\cdots W_V \cdots](\chi) = [\cdots W(V_0)\cdots]\left(\int \chi(...,v,...)d\mu(v)\right). \tag{4.11}$$

In Eq. (4.9) $\sharp = 0$ or the bar sign, the same at both Bs. The phase factors appearing in (4.5)–(4.10) are to be understood to multiply test functions χ in the symbols $[D](\chi)$. The last relation says that constant smeared Weyl operators are identical with the standard ones.

The elements of the factor space thus obtained will be again denoted by $\Sigma_{i=1}^N [D_i](\chi_i)$ without a risk of confusion. This vector space becomes a *-algebra $\mathscr{B}$ with the multiplication and involution laws defined by

$$[D_1](\chi_1)[D_2](\chi_2) = [D_1D_2](\chi_1\otimes\chi_2), \tag{4.12}$$

$$[D](\chi)^* = [D^*](\chi^c), \tag{4.13}$$

and the unit $\mathbf{1} = W(0)$. D_1D_2 is the sequence of symbols formed of the two sequences D_1 and D_2, D_2 following D_1. χ^c results from χ by the application of the sequence of three operations: complex conjugation, reflection of the order of the variables and indices, and the matrix multipli-

cation by $C\gamma^{0T}=-\gamma^0 C$ applied to each of the indices [cf. (3.7)]. The sequence D^* results from D by reflection of its order and subsequent replacements: $W(V)\to W(-V)$, $W_V\to W_{-V}$, $B^0_V\to B_{-V}$, $B_V\to B^0_{-V}$.

In the last step we consider now the problem of introducing a C^*-norm on the *-algebra $\mathscr{B}$. Let $\mathscr{R}$ be the class of all C^*-seminorms p on $\mathscr{B}$ such that

(i) $p([D](\chi))$ is continuous in χ in the topology of $\mathscr{S}$ for each D;

(ii)

$$p(W_V(\chi))\leqslant\|\chi\|_{L^1(H,d\mu)}. \tag{4.14}$$

A comment on each of the conditions is in place. The second one is a necessary condition for the admitted representations of the smeared Weyl operators $W_V(\chi)$ to be indeed given by integrals of unitary operators with the test function χ. To see the meaning of the first condition let us compare our present context with that of the standard algebra of the Dirac field. In the latter case one has in the algebra the elements $[B^{\sharp_1}\cdots B^{\sharp_n}](f^1\otimes\cdots\otimes f^n):=B^{\sharp_1}(f^1)\cdots B^{\sharp_n}(f^n)$, ($\sharp_i=0$ or the bar sign), where $f^i\in\mathscr{S}(H,\mathbf{C}^4)\subset\mathscr{K}$. These elements are norm continuous in each of the functions f^i in the $\mathscr{S}$-topology, so by the nuclear theorem for Schwartz functions one obtains in the algebra the unique linear extension $[B^{\sharp_1}\cdots B^{\sharp_n}](\chi)$ to the whole of $\mathscr{S}(H^n,\mathbf{C}^{4^n})$, norm continuous in χ in the topology of $\mathscr{S}$. Their analogs in our algebra are symbols $[D](\chi)$. However, we had to define them from the beginning for the whole space $\mathscr{S}$ to be able to formulate the algebraic conditions. Condition (i) will guarantee that also here they will be continuous extensions of products of the basic objects.

Proposition 4.1: The class $\mathscr{R}$ contains the maximal element $p_{\max}$. A C^*-seminorm p on $\mathscr{B}$ is in $\mathscr{R}$ iff $p\leqslant p_{\max}$.

The second statement is obviously true, if the first is proved. The proof is preceded by two lemmas.

Lemma 4.2: For any C^*-seminorm $p\neq 0$ on $\mathscr{B}$ there is $p(W(V))=1$ for all $V\in L$, and $p(B^0_{V_1}(f))=p(\bar{B}_{V_2}(f))=\|f\|_{\mathscr{K}}$ for all $V_1\in\mathscr{S}at_{-e}$, $V_2\in\mathscr{S}at_e$, and $f\in\mathscr{S}$.

Proof: The first statement is the consequence of the Weyl relations. The proof of the second one is a slightly more involved version of the analogous proof for the C^*-norm on the Dirac field algebra. Let $\{V(v),V(u)\}=F(v)-F(u)$. Then (4.9) for $V_1=V_2=V$ takes the form

$$e^{iF(v)}B^0_V(v)_\alpha B^0_V(u)_\beta+e^{iF(u)}B^0_V(u)_\beta B^0_V(v)_\alpha=0.$$

For $\chi=f\otimes g$ this yields $B^0_V(e^{iF}f)B^0_V(g)+B^0_V(e^{iF}g)B^0_V(f)=0$, and for $g=f$, in particular, $B^0_V(e^{iF}f)B^0_V(f)=0$. In the same way one obtains from (4.10)

$$B^0_V(f)\bar{B}_{-V}(g)+\bar{B}_{-V}(e^{-iF}g)B^0_V(e^{iF}f)=(f^c,g). \tag{4.15}$$

The last two equations imply

$$B^0_V(f)B^0_V(g)^*B^0_V(f)=(g,f)B^0_V(f). \tag{4.16}$$

Multiplying this equation on the left by $B^0_V(f)^*$ and setting $g=f$ one obtains easily $p(B^0_V(f))=\|f\|_{\mathscr{K}}$ or 0. Assume that there is V and $g\neq 0$ such that $p(B^0_V(g))=0$. Then from (4.16) there is $|(g,f)|p(B^0_V(f))=0$ for all f, hence $p(B^0_V(f))=0$ for all such f that $(g,f)\neq 0$. Each f may be represented as $f=f_1+f_2$ with $(g,f_i)\neq 0$, so $p(B^0_V(f))=0$ for all f, which contradicts (4.15) and ends the proof of the lemma. □

Let $\chi\in\mathscr{S}(H^n,\mathbf{C}^{4^m})$, $m\leqslant n$. There always exists a representation $\chi=\Sigma_{i=1}^{\infty}f_i^1\otimes\cdots\otimes f_i^n$, where for a given k all f_i^k are either in $\mathscr{S}(H,\mathbf{C})$ or in $\mathscr{S}(H,\mathbf{C}^4)$ and the sum converges in the topology of

$\mathscr{S}$ (e.g., the N-representation[22]). There are various orders of spaces $\mathscr{S}(H,\mathbf{C})$ and $\mathscr{S}(H,\mathbf{C}^4)$ in this representation possible. Denote a fixed order by $\flat$ and the above representation with this order by $\chi=\Sigma_{i=1}^{\infty} f_i^1\otimes_\flat\cdots\otimes_\flat f_i^n$. Let

$$d_\flat(\chi):=\inf_{\chi=\Sigma_{i=1}^{\infty} f_i^1\otimes_\flat\cdots\otimes_\flat f_i^n}\sum_{i=1}^{\infty}\|f_i^1\|_\bullet\cdots\|f_i^n\|_\bullet, \tag{4.17}$$

where $\|f\|_\bullet=\|f\|_{L^1(H,d\mu)}$ if $f\in\mathscr{S}(H,\mathbf{C})$ and $\|f\|_\bullet=\|f\|_{\mathscr{K}}$ if $f\in\mathscr{S}(H,\mathbf{C}^4)$.

Lemma 4.3: $d_\flat$ are norms on $\mathscr{S}(H^n,\mathbf{C}^{4^m})$, continuous in the topology of $\mathscr{S}$.

Proof: We show first that $d_\flat$ is bounded by one of the seminorms defining the topology of $\mathscr{S}$. We assume for simplicity that $\chi\in\mathscr{S}(H^2,\mathbf{C}^4)$ and we are interested in the norm $d_\flat$ for the order of spaces $(\mathscr{S}(H,\mathbf{C}),\mathscr{S}(H,\mathbf{C}^4))$. The general case differs only by more involved notation. Choose a Minkowski frame and denote $\chi'_\alpha(v,u)=v^0(u^0)^{-1/2}\Sigma_{\beta=1}^4 S^{-1}(u)_{\alpha\beta}\chi_\beta(v,u)$, where the matrix $S^{-1}(u)=(2(u^0+1))^{-1/2}(1+\gamma^0\gamma\cdot u)$ induces the transformation $f\gamma\cdot ug=(S^{-1}(u)f)^\dagger(S^{-1}(u)g)$ (the dagger denoting the matrix Hermitian conjugation). Consider χ' as a function of variables $\vec{v}$ and $\vec{u}$ and expand it in the N-representation: $\chi'_\alpha(v,u)=\Sigma_{i=1}^{\infty} f_i(\vec{v})g_{i\alpha}(\vec{u})$, where fs and gs are multiples of products of the Hermite functions. The sum converges in $\mathscr{S}$ and $\Sigma_{i=1}^{\infty}\|f_i\|_{L^1(\mathbf{R}^3,d^3v)}(\Sigma_{\alpha=1}^4\|g_{i\alpha}\|_{L^2(\mathbf{R}^3,d^3v)})$ is bounded by one of the fundamental seminorms of χ', which in turn may be bounded by one of the seminorms of χ. Now it suffices to observe that $\Sigma_{i=1}^{\infty}(v^0)^{-1}f_i(\vec{v})(u^0)^{1/2}(S(u)g_i(\vec{u}))_\alpha$ converges to χ in $\mathscr{S}$ and $\Sigma_{i=1}^{\infty}\|(v^0)^{-1}f_i(\vec{v})\|_{L^1(H,d\mu)}\|(u^0)^{1/2}(S(u)g_i(\vec{u}))\|_{\mathscr{K}}<\text{const}\,\Sigma_{i=1}^{\infty}\|f_i\|_{L^1(\mathbf{R}^3,d^3v)}(\Sigma_{\alpha=1}^4\|g_{i\alpha}\|_{L^2(\mathbf{R}^3,d^3v)})$ to get $d_\flat(\chi)<\rho(\chi)$, where ρ is one of the fundamental seminorms. The properties of a seminorm are easily checked for $d_\flat$. That $d_\flat(\chi)=0$ implies $\chi=0$ is again illustrated in our special case. Let $\chi=\Sigma_{i=1}^{\infty} f_i\otimes g_i$, $f_i\in\mathscr{S}(H,\mathbf{C})$, $g_i\in\mathscr{S}(H,\mathbf{C}^4)$, and also choose any $h_1\in\mathscr{S}(H,\mathbf{C})$ and $h_2\in\mathscr{S}(H,\mathbf{C}^4)$. Then

$$\left|\int h_1(v)\overline{h_2(u)}\gamma\cdot u\chi(v,u)d\mu(v)d\mu(u)\right|\leqslant\sup_v|h_1(v)|\sum_{i=1}^{\infty}\|f_i\|_{L^1}\|g_i\|_{\mathscr{K}}.$$

Hence, if $d_\flat(\chi)=0$, then the lhs vanishes for all h_1 and h_2 and $\chi=0$. □

Proof of Proposition 4.1: Let $\flat(D)$ be the order of spaces $\mathscr{S}(H,\mathbf{C})$ and $\mathscr{S}(H,\mathbf{C}^4)$ corresponding to the order of symbols W_V and $B_V^\sharp$, respectively, in the sequence D. Then by the assumption (4.14) and Lemma 4.2 one has for any $p\in\mathscr{R}$

$$p([D](f^1\otimes_{\flat(D)}\cdots\otimes_{\flat(D)}f^n))\leqslant\|f^1\|_\bullet\cdots\|f^n\|_\bullet.$$

If $\chi=\Sigma_{i=1}^{\infty} f_i^1\otimes_{\flat(D)}\cdots\otimes_{\flat(D)}f_i^n$, then by the assumed continuity $p([D](\chi))\leqslant\Sigma_{i=1}^{\infty}\|f_i^1\|_\bullet\cdots\|f_i^n\|_\bullet$. Hence for any element of $\mathscr{B}$ one has

$$p\left(\sum_{k=1}^{N}[D_k](\chi_k)\right)\leqslant\sum_{k=1}^{N}d_{\flat(D_k)}(\chi).$$

We define the seminorm $p_{\max}$ on $\mathscr{B}$ by

$$p_{\max}(A)=\sup_{p\in\mathscr{R}}p(A).$$

There is $p_{\max}([D](\chi))\leqslant d_{\flat(D)}(\chi)$, so $p_{\max}\in\mathscr{R}$. □

The answer to the question whether $p_{\max}$ is a norm on $\mathscr{B}$ is not known yet. If it is not, one divides $\mathscr{B}$ through the ideal $\mathscr{T}$ of those elements for which $p_{\max}$ vanishes. The seminorm $p_{\max}$ induces then a C^*-norm $\|.\|$ on $\mathscr{B}/\mathscr{T}$ in the standard way. The completion of $\mathscr{B}/\mathscr{T}$ in this norm is

a C^*-algebra $(\mathscr{F},\|.\|)$. We propose to regard this algebra as the base of a theory of asymptotic fields. With regard to the interpretation of electromagnetic ingredients of the algebra, one should have in mind the remarks made at the end of Sec. III.

It is easy to see that representations of the algebra $(\mathscr{F},\|\cdot\|)$ are in natural 1:1 correspondence with those representations π of $\mathscr{B}$ for which $p(.)=\|\pi(.)\|\in\mathscr{R}$.

In the asymptotic algebra of fields there is no place more for the local gauge transformations. The only gauge-dependent quantity in the electromagnetic test fields is the additive constant in $\Phi(l)$. This freedom is closely connected with the global gauge transformation of the charge carrying fields, which is implemented in the algebra itself. Let $W(V)=W(0,c)$, $c=$const, (i.e., $V=$pure gauge, $\Phi=c$), and set $\gamma_c(A)=\underline{W}(0,c)AW(0,\underline{c})^*$. Then $\gamma_c(A)=A$ for $A=W(V)$ or $W_V(\chi)$, and $\gamma_c(B_V^0(f))=e^{-ice}B_V^0(f)$, $\gamma_c(B_V(f))=e^{+ice}B_V(f)$. Algebra $\mathscr{B}$ is the linear span of its subspaces $\mathscr{B}_k$, $k\in\mathbf{Z}$, where $\gamma_c=e^{icke}$ id on $\mathscr{B}_k$. The subspace $\mathscr{B}_0$ is a *-subalgebra of $\mathscr{B}$. If $\mathscr{I}\neq 0$, then it is easily seen that $\mathscr{I}$ is the linear span of $\mathscr{I}_k:=\mathscr{B}_k\cap\mathscr{I}$. The decomposition is therefore inherited by $\mathscr{F}$, and $\mathscr{F}_0$ is a C^*-algebra, which may be interpreted as the algebra of observables $\mathscr{A}\equiv\mathscr{F}_0$.

The algebraic relations of $\mathscr{B}$ have been obtained by treating $B_V^\sharp(v)$ heuristically as products of $B^\sharp(v)$ and Weyl operators for charged fields $W(V(v))$. In Sec. V we shall see that this heuristic idea may be also used to obtain a class of representations of $\mathscr{B}$ (and $\mathscr{F}$).

V. A CLASS OF REPRESENTATIONS

Let $W_0(V)$ be a representation in a Hilbert space $\mathscr{H}_1$ of the Weyl algebra over the test function space $\hat{L}$ with the symplectic form (3.2). We assume that for any $V(.)\in\mathscr{S}at_e$ it satisfies the following conditions:

(i) for every $\varphi\in\mathscr{H}_1$ the vectors $W_0(V(v))\varphi$, $v\in H$, span a separable subspace;

(ii) for every φ, $\psi\in\mathscr{H}_1$, the function $(\varphi,W_0(V(v))\psi)$ is measurable in v.

(The class of representations satisfying the conditions is nonempty—this may be shown by an explicit construction making use of the usual Fock representation and one of representations discussed in Ref. 21.) It follows that $(\varphi,W_0(V_1(v_1))...W_0(V_n(v_n))\psi)$ is also measurable. For $V_i\in\mathscr{S}at_e\cup\mathscr{S}at_{-e}\cup\mathscr{R}ad$, $i=1,\ldots,n$, $\chi\in L^1(H^n,d\mu^n)$, we denote

$$[W_{0V_1}\cdots W_{0V_n}](\chi)=\int W_0(V_1(v_1))\cdots W_0(V_n(v_n))\chi(v_1,\ldots,v_n)d\mu(v_1)\cdots d\mu(v_n),$$

the integral in the weak sense. The Weyl algebra relations imply

$$[W_{0V_1}W_{0V_2}](\chi)=[W_{0V_2}W_{0V_1}](\chi'), \tag{5.1}$$

where $\chi'(u,v)=e^{-i\{V_1(v),V_2(u)\}}\chi(v,u)$. If, in particular, $\{V_1(v),V_2(u)\}=F_{12}(v)-F_{12}(u)$, then

$$W_{0V_1}(\chi_1)W_{0V_2}(\chi_2)=W_{0V_2}(e^{iF_{12}}\chi_2)W_{0V_1}(e^{-iF_{12}}\chi_1). \tag{5.2}$$

Let further $B(f)$ [and $B^\sharp(f)$] be a concrete realization (representation) of the Dirac field algebra in a Hilbert space $\mathscr{H}_2$. We would like to define $B_V^0(v)$ as a product of $W_0(V(v))$ and $B^0(v)$, that is, to give sense to the expression

$$B_V^0(f)=\int W_0(V(v))\otimes B^0(v)\gamma\cdot v f(v)d\mu(v)$$

for $f\in\mathscr{S}(H,\mathbf{C}^4)$. [When constructing the representation we shall use the simplified notation $B_V^0(f)$ instead of the more appropriate $\pi(B_V^0(f))$, etc., which may be restored at the end of construction.] Let $\{e_i\}$ be an orthonormal basis of the Hilbert space $\mathscr{K}$. If we "expand" $B^0(v)$ in this basis, we are led to the following formulation. Consider a family of bounded operators on $\mathscr{K}_1\otimes\mathscr{K}_2$

$$B_V^0(f)_n := \sum_{i=1}^{n} W_{0V}(\overline{e_i}\Gamma f)\otimes B^0(e_i),$$

where $(\Gamma f)(v)=\gamma\cdot v f(v)$.

Proposition 5.1. The sequence of operators $B_V^0(f)_n$ converges *-strongly to a bounded operator $B_V^0(f)$, with $\|B_V^0(f)\|\leqslant\|f\|_{\mathscr{K}}$.

Proof: Let $\{V(v),V(u)\}=F(v)-F(u)$. From the Dirac field anticommutation relations and (5.2) we obtain

$$(B_V^0(f)_n-B_V^0(f)_m)^*(B_V^0(f)_n-B_V^0(f)_m)+(B_V^0(e^{-iF}f)_n-B_V^0(e^{-iF}f)_m)$$

$$(B_V^0(e^{-iF}f)_n-B_V^0(e^{-iF}f)_m)^*=\left(\sum_{i=m+1}^{n} w_i^* w_i\right)\otimes\mathbf{1},$$

where $w_i = W_{0V}(\overline{e_i}\Gamma f)$. For any vector $\psi\in\mathscr{H}_1\otimes\mathscr{H}_2$, there is then

$$\|(B_V^0(f)_n-B_V^0(f)_m)\psi\|^2+\|(B_V^0(e^{-iF}f)_n^*-B_V^0(e^{-iF}f)_m^*)\psi\|^2=p_\psi\left(\sum_{i=m+1}^{n} w_i^* w_i\right), \quad (5.3)$$

where $p_\psi(A):=(\psi,A\otimes\mathbf{1}\psi)$ agrees for positive A with one of the seminorms defining the σ-weak topology on the space of bounded operators on $\mathscr{H}_1$. We shall show below that

$$\sum_{i=1}^{\infty} w_i^* w_i=\|f\|^2\mathbf{1}, \quad (5.4)$$

and that the series converges σ-strongly. Hence $B_V^0(f)_n$ and $B_V^0(e^{-iF}f)_n^*$ converge strongly to bounded operators for all f, which implies the *-strong convergence of $B_V^0(f)_n$ for all f. Putting $m=0$ in (5.3) and taking the limit in n we obtain the bound of the norm. To prove (5.4) observe first that for any x, $y\in\mathscr{H}_1$ we have $(y,w_i x)=\int(y,W_0(V(v))x)\overline{e_i(v)}\gamma\cdot v f(v)d\mu(v)$ $=(e_i,(y,W_0(V(.))x)f)_{\mathscr{K}}$, so that

$$\sum_{i=1}^{\infty}|(y,w_i x)|^2=\|(y,W_0(V(.))x)f\|_{\mathscr{K}}^2.$$

For fixed x let $\{\varphi_j\}$ be an orthonormal basis of the subspace of $\mathscr{H}_1$ spanned by $W_0(V(v))x$, $v\in H$. Then

$$\sum_{i=1}^{\infty}(x,w_i^* w_i x)=\sum_{i,j=1}^{\infty}|(\varphi_j,w_i x)|^2=\sum_{j=1}^{\infty}\int|(\varphi_j,W_0(V(v))x)|^2\overline{f(v)}\gamma\cdot v f(v)d\mu(v)=\|f\|_{\mathscr{K}}^2\|x\|^2,$$

the last equality by the Lebesgue theorem. As $\Sigma_{i=1}^{n} w_i^* w_i$ is an increasing sequence of positive operators, the above calculation shows that (5.4) holds in the σ-strong sense (e.g., Ref. 23, Lemma 2.4.19). □

The building blocks of the representation acting on $\mathscr{K}_1\otimes\mathscr{K}_2$ are now defined by

$$W(V)=W_0(V)\otimes\mathbf{1}, \quad V\in L, \quad (5.5)$$

$$W_V(\chi)=W_{0V}(\chi)\otimes\mathbf{1}, \quad V\in\mathscr{R}ad, \quad \chi\in\mathscr{S}(H,\mathbf{C}), \quad (5.6)$$

$$B_V^\sharp(f)=\sum_{i=1}^{\infty} W_{0V}(\overline{e_i}\Gamma f)\otimes B^\sharp(e_i),\quad V\in\mathscr{S}at_e\cup\mathscr{S}at_{-e},\quad f\in\mathscr{S}(H,\mathbf{C}^4). \tag{5.7}$$

The definition of $B_V^\sharp$ is independent of the choice of the basis $\{e_i\}$, as it is easily shown that

$$(x_1\otimes y_1,B_V^\sharp(f)x_2\otimes y_2)=(y_1,B^\sharp((x_1,W_0(V(.))x_2)f)y_2). \tag{5.8}$$

If D is any sequence of the symbols $W(V)$, W_V, and $B_V^\sharp$, and $(f^1,\ldots,f^n)$ form a sequence of type $\flat(D)$, then we define $[D](f^1\otimes\cdots\otimes f^n)$ as the product of the "building blocks." In view of Prop. 5.1 and of the obvious bound $\|W_V(\chi)\|\leqslant\|\chi\|_{L^1}$, this element is norm continuous in each of f's in the topology of $\mathscr{S}$. By the nuclear theorem it extends then to the function $[D](\chi)$ norm continuous in χ in the $\mathscr{S}$-topology. The conditions (4.12) and (4.13) are satisfied, and the operator norm fulfills the defining conditions of the class $\mathscr{R}$. To complete the proof that we have thus obtained a representation of the algebra $\mathscr{F}$ it remains to show that the relations (4.5)–(4.11) are satisfied.

The conditions (4.5) and (4.11) are obviously satisfied. It is sufficient to check the other relations for elements $[D](\chi)$ with Ds being sequences of two symbols. The relations (4.6) and (4.7) are then quite obvious as well. Equation (4.8) for $G_V=W_V$ follows from (5.1). For $G_V=B_V^\sharp$ it is easy to show that

$$(x_1\otimes y_1,[W_{V_1}B_{V_2}^\sharp](\chi)x_2\otimes y_2)=\left(y_1,B^\sharp\left(\int(x_1,W_0(V_1(v))W_0(V_2(.))x_2)\chi(v,.)d\mu(v)\right)y_2\right),$$

and similarly in the opposite order of symbols, which implies (4.8).

To prove (4.9) and (4.10) we have to make a digression on the extension of products $B^{\sharp_1}(f)B^{\sharp_2}(g)$ in the algebra of the Dirac field. We have mentioned such an extension to the space of Schwartz functions, but now we need a wider family.

Let $\mathscr{K}\otimes\mathscr{K}$ be the tensor product Hilbert space. This space consists of measurable functions $\chi_{\alpha\beta}(v,u)$, for which

$$\sum_{\substack{\alpha,\alpha'\\ \beta,\beta'}}\int\chi^*_{\alpha\beta}(v,u)(\gamma^0\gamma\cdot u)_{\alpha\alpha'}(\gamma^0\gamma\cdot u)_{\beta\beta'}\chi_{\alpha'\beta'}(v,u)d\mu(v)d\mu(u)<\infty.$$

Let, further, $\mathscr{K}\otimes_1\mathscr{K}$ be the subspace of $\mathscr{K}\otimes\mathscr{K}$ consisting of those $\chi\in\mathscr{K}\otimes\mathscr{K}$ for which

$$\|\chi\|_1:=\inf_{\chi=\Sigma_{i=1}^{\infty}f_i\otimes g_i}\sum_{k=1}^{\infty}\|f_k\|\|g_k\|<\infty.$$

$\|.\|_1$ is a norm on $\mathscr{K}\otimes_1\mathscr{K}$, $\|\chi\|<\|\chi\|_1$ for $\chi\in\mathscr{K}\otimes_1\mathscr{K}$, and $(\mathscr{K}\otimes_1\mathscr{K},\|.\|_1)$ is a Banach space. These statements follow most simply from the following two observations.

(i) $(\mathscr{K}\otimes\mathscr{K},\|.\|)$ is isomorphic with the space of Hilbert–Schmidt operators on $\mathscr{K}$ by the map $\chi\to\mathscr{O}_\chi$, where for $\chi=\Sigma_{i=1}^{\infty}f_i\otimes g_i$ the operator $\mathscr{O}_\chi$ is defined by

$$\mathscr{O}_\chi h=\sum_{i=1}^{\infty}(h^c,f_i)g_i. \tag{5.9}$$

(ii) Under the same map $(\mathscr{K}\otimes_1\mathscr{K},\|.\|_1)$ is isomorphic with the Banach space of trace class operators on $\mathscr{K}$.[24] Thus, if $\chi_n\to\chi$ in $\mathscr{K}\otimes_1\mathscr{K}$, then $\chi_n\to\chi$ in $\mathscr{K}\otimes\mathscr{K}$.

Extension of the product of fundamental elements in the Dirac field algebra is now easily achieved. For $\chi=\Sigma_{i=1}^n f_i\otimes g_i$, $f_i, g_i\in\mathscr{K}$, we set $[B^{\sharp_1}B^{\sharp_2}](\chi)=\Sigma_{i=1}^n B^{\sharp_1}(f_i)B^{\sharp_2}(g_i)$. This defines a linear map of the algebraic product $\mathscr{K}\otimes_{\text{alg}}\mathscr{K}$ (densely contained in $\mathscr{K}\otimes_1\mathscr{K}$) into the

algebra, with the norm bound $\|[B^{\sharp_1}B^{\sharp_2}](\chi)\| \leqslant \|\chi\|_1$. Hence the map extends to the whole $\mathscr{K}\otimes_1\mathscr{K}$, with the conservation of the bound. For $\chi\in\mathscr{S}$ this reduces to the extension mentioned previously.

The anticommutation relations may be now extended from $\mathscr{K}\otimes_{\mathrm{alg}}\mathscr{K}$ to the whole $\mathscr{K}\otimes_1\mathscr{K}$, which gives

$$[B^{\sharp}B^{\sharp}](\chi+\chi^T)=0, \tag{5.10}$$

$$[B^0\bar{B}](\chi)+[\bar{B}B^0](\chi^T)=\mathrm{Tr}\,\mathscr{O}_\chi\mathbf{1}, \tag{5.11}$$

where ${\chi^T}_{\alpha\beta}(v,u)=\chi_{\beta\alpha}(u,v)$, and $\mathrm{Tr}\,\mathscr{O}_\chi$ is the trace of the operator (5.9), $\mathrm{Tr}\,\mathscr{O}_\chi=\Sigma_{i=1}^{\infty}(f_i^c,g_i)$ for $\chi=\Sigma_{i=1}^{\infty}f_i\otimes g_i$.

After these preparations we take up the proof of the relations (4.9) and (4.10). For $x_1,x_2\in\mathscr{H}_1$ let φ_j be an orthonormal basis of the linear span of vectors $W_0(V_1(v))^*x_1$ and $W_0(V_1(v))x_2$, $v\in H$. Let, further, ψ_λ be an orthonormal basis (not necessarily countable) of $\mathscr{H}_2$, and $f,g\in\mathscr{S}(H,\mathbf{C}^4)$. Expanding $B^{\sharp_2}_{V_2}(g)x_2\otimes y_2$ in the basis $\varphi_j\otimes\psi_\lambda$ and using (5.8) one finds

$$\begin{aligned}&(x_1\otimes y_1,B^{\sharp_1}_{V_1}(f\,)B^{\sharp_2}_{V_2}(g)x_2\otimes y_2)\\&\quad=\sum_{i=1}^{\infty}(y_1,[B^{\sharp_1}B^{\sharp_2}]((x_1,W_0(V_1(.))\varphi_i)f\otimes(\varphi_i,W_0(V_2(.))x_2)g)y_2).\end{aligned}$$

We have

$$\begin{aligned}&\sum_{i=1}^{\infty}\|(x_1,W_0(V_1(.))\varphi_i)f\|_{\mathscr{K}}\|(\varphi_i,W_0(V_2(.))x_2)g\|_{\mathscr{K}}\\&\quad\leqslant\left(\sum_{i=1}^{\infty}\|(W_0(V_1(.))^*x_1,\varphi_i)f\|^2_{\mathscr{K}}\right)^{1/2}\left(\sum_{i=1}^{\infty}\|(\varphi_i,W_0(V_2(.))x_2)g\|^2_{\mathscr{K}}\right)^{1/2}\\&\quad=\|x_1\|\|x_2\|\|f\|_{\mathscr{K}}\|g\|_{\mathscr{K}},\end{aligned}$$

the last equality by the Lebesgue theorem. Hence, the series

$$\sum_{i=1}^{\infty}(x_1,W_0(V_1(.))\varphi_i)f\otimes(\varphi_i,W_0(V_2(.))x_2)g \tag{5.12}$$

converges both in $\mathscr{K}\otimes_1\mathscr{K}$ and $\mathscr{K}\otimes\mathscr{K}$, to the same element. The limit in $\mathscr{K}\otimes\mathscr{K}$ is easily found as the point limit of functions, which yields $(x_1,W_0(V_1(v))W_0(V_2(u))x_2)f(v)g(u)$. Thus we have proved that if $\chi\in\mathscr{K}\otimes_{\mathrm{alg}}\mathscr{K}$, then

$$\begin{aligned}&(x_1,W_0(V_1(.))W_0(V_2(.))x_2)\chi\in\mathscr{K}\otimes_1\mathscr{K},\\&\|(x_1,W_0(V_1(.))W_0(V_2(.))x_2)\chi\|_1\leqslant\|x_1\|\|x_2\|\|\chi\|_1,\end{aligned} \tag{5.13}$$

and for $\chi\in\mathscr{S}(H,\mathbf{C}^4)\otimes_{\mathrm{alg}}\mathscr{S}(H,\mathbf{C}^4)\subset\mathscr{K}\otimes_{\mathrm{alg}}\mathscr{K}$

$$(x_1\otimes y_1,[B^{\sharp_1}_{V_1}B^{\sharp_2}_{V_2}](\chi)x_2\otimes y_2)=(y_1,[B^{\sharp_1}B^{\sharp_2}]((x_1,W_0(V_1(.))W_0(V_2(.))x_2)\chi)y_2). \tag{5.14}$$

By continuity (5.13) remains true for $\chi\in\mathscr{K}\otimes_1\mathscr{K}$, and (5.14) for $\chi\in\mathscr{S}(H^2,\mathbf{C}^{4^2})\subset\mathscr{K}\otimes_1\mathscr{K}$. Denote $\chi'_{\alpha\beta}(v,u)=e^{(i/2)\{V_1(v),V_2(u)\}}\chi_{\alpha\beta}(v,u)$ and $\chi''_{\alpha\beta}(v,u)=e^{(i/2)\{V_2(u),V_1(v)\}}\chi^T_{\alpha\beta}(v,u)$. Using the Weyl relations for W_0 one obtains from (5.14)

$$(x_1\otimes y_1,([B^{\sharp_1}_{V_1}B^{\sharp_2}_{V_2}](\chi')+[B^{\sharp_2}_{V_2}B^{\sharp_1}_{V_1}](\chi''))x_2\otimes y_2)=(y_1,([B^{\sharp_1}B^{\sharp_2}](\Psi)+[B^{\sharp_2}B^{\sharp_1}](\Psi^T))y_2),$$

where $\Psi_{\alpha\beta}(v,u)=(x_1,W_0(V_1(v)+V_2(u))x_2)\chi_{\alpha\beta}(v,u)$. The relation (4.9) follows now from (5.10). The proof of (4.10) will be complete by (5.11) and the definition (5.6) if we show that

$$\mathrm{Tr}\,\mathscr{O}_\Psi=\int (x_1,W_0(V_1(v)+V_2(v))x_2)\sum_{\alpha,\beta}(C^{-1}\gamma\cdot v)_{\alpha\beta}\chi_{\alpha\beta}(v,v)d\mu(v).$$

The rhs may be written as

$$\int (x_1,W_0(V_1(v))W_0(V_2(v))x_2)\sum_{\alpha,\beta}(C^{-1}\gamma\cdot v)_{\alpha\beta}\chi'_{\alpha\beta}(v,v)d\mu(v).$$

This formula defines a distribution on $\chi'\in\mathscr{S}$, so it is sufficient to take $\chi'=f\otimes g$, $f,g\in\mathscr{S}(H,\mathbf{C}^4)$. Then Ψ is given by (5.12) and

$$\begin{aligned}\mathrm{Tr}\,\mathscr{O}_\Psi&=\sum_{i=1}^{\infty}\overline{((x_1,W_0(V_1(.))\varphi_i)f^c}\,,(\varphi_i,W_0(V_2(.))x_2)g)\\&=\sum_{i=1}^{\infty}\int (x_1,W_0(V_1(.))\varphi_i)(\varphi_i,W_0(V_2(.))x_2)\overline{f^c(v)}\,\gamma\cdot v g(v)d\mu(v),\end{aligned}$$

which yields the desired relation by the Lebesgue theorem. This ends the proof of the conditions of our algebra.

VI. DISCUSSION AND OUTLOOK

We have shown how heuristic quantization of the asymptotic structure of classical field electrodynamics leads to the construction of an asymptotic algebra of fields, whose states may be expected to describe the structure of collision states in quantum electrodynamics, including the charged states. This algebra is a C^*-algebra, so there is no need for the indefinite metric formalism. The charged fields are accompanied by Coulomb fields, which solves the problem of Gauss' law in charged states. The construction depends on the choice of a class of ''satellite'' fields. This choice was left open to some extent. It corresponds to selecting various ''clouds'' of free radiation field accompanying the particle in addition to the Coulomb field. Three classes of satellite fields satisfying the defining conditions (i)–(iv) in Sec. IV are worth mentioning:

(a) the class of all fields satisfying the conditions (i)–(iv);
(b) the subclass consisting of fields of the form $V_a(v;s,l)=V_{ea}(v,l)+V_{0a}(s,l)$, where $V_{ea}(v,l)$, defined in (i), corresponds to the Coulomb field, and $V_{0a}\in L$;
(c) the subclass of fields for which $V_a(v;-\infty,l)$ does not depend on v.

The first choice is the most general one within the limits of our construction. The second possibility is the simplest one. In that case the smeared Weyl elements reduce to the (simple) Weyl elements, as the space $\mathscr{R}ad$ is then naturally isomorphic with L. We mention as an aside that an explicit faithful representation of the corresponding algebra can be constructed. The choice (c) has a clear physical interpretation: the long-range tail of the cloud accompanying the particle is chosen to compensate the velocity dependence of the tail of the Coulomb field. The total satellite field has then a velocity independent flux at spatial infinity.

The last possibility seems to be the one closest to the picture emerging from the analysis of superselection sectors structure in the algebraic framework of local observables. However, we leave the problem of specifying the physically justified choice of satellite fields open at present.

The solution of this problem may depend on the answer to the important question of whether our algebra may be obtained by some limiting procedure from the field algebra of the full theory. This seems a difficult problem, but the classical theory gives hints, how such a limiting process could look like. The quantum version of the null infinity limit of the electromagnetic field may be thought of as an LSZ-type limit in lightlike directions, which brings in mind the construction of Buchholz.[3] For the matter field one would have to choose a gauge in a class supplying a quantum analog of the class mentioned in Sec. II. An LSZ-type limit on the hyperboloid $x^2=\lambda^2$, $x^0>0$, with $\lambda\to\infty$ may then be expected to exist.

Important as the latter problem may be, the asymptotic algebra also deserves further investigations on its own. The following physically interesting problems may be posed within this framework.

(i) How can the local observables be characterized and what is their relation to the nonlocal ones? That the latter observables are present may be read off from the properties of the symplectic form.
(ii) The Poincaré group acts naturally on the algebra as a group of automorphisms. Do there exist irreducible Poincaré-covariant representations of the algebra? If so, which superselection structure of the algebra of local observables is implied? (We recall that in charged superselection sectors the Lorentz group has to be spontaneously broken.)
(iii) What is the measure class of the spectrum of energy-momentum in translation-covariant, positive energy representations (infraparticle problem)?

Finally, let us mention for completeness that the construction given in this paper may be reflected in time, yielding the asymptotic ''in''-algebra. If these two algebras fit into the interacting theory, the scattering problem may be considered. One may hope, for instance, that the perturbation calculus in a suitable gauge, starting from the quasi-free theory supplied by our algebra, should be infrared-regular.

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APPENDIX: EQUIVALENCE OF SPINOR AND TENSOR FORMULAS

We prove here the equivalence of tensor and spinor versions of those formulas which appear in Sec. II, but were given only in the spinor form in Ref. 16.

For $l_a=o_A\bar{o}_{A'}$ in the notation of Ref. 16, $\partial_A=\partial/\partial o^A$ and $\partial_a=\partial/\partial l^a$, one has $\partial_A\alpha(l)=\bar{o}^{A'}\partial_{AA'}\alpha(l)$, hence

$$(l_a\partial_b-l_b\partial_a)\alpha(l)=-(\epsilon_{A'B'}o_{(A}\partial_{B)}+\epsilon_{AB}\bar{o}_{(A'}\partial_{B')})\alpha(l), \tag{A1}$$

and the integral identity (2.10) is then equivalent to (A8) of Ref. 16.

The electromagnetic field tensor and spinor are connected by $F_{ab}=\epsilon_{A'B'}\varphi_{AB}+\epsilon_{AB}\bar{\varphi}_{A'B'}$, hence the field $\varrho_{AA'}(x)=\varphi_{AB}(x)x^B_{A'}$ [(2.28) in Ref. 16] is equivalently expressed as $\varrho_a(x)=x^b\,{}^-F_{ba}(x)$, where ${}^-F_{ba}$ is the anti-selfdual part of F_{ba}. Its null asymptotic $\lim_{R\to\infty}R\varrho_a(x+Rl)=N_a(x\cdot l,l)$ is given by $N_a(s,l)=\partial_{A'}\zeta_A(s,l)$, where $\zeta_A(s,l)=o_{A'}V^{A'}_A$, $V_a(s,l)$ defined in (2.1) [see Ref. 16, Eq. (2.44)]. We have

$$\partial_{A'}\zeta_A=-V_a+o_{B'}\partial_{A'}V^{B'}_A=-V_a-\tfrac{1}{2}\epsilon_{B'A'}o^{C'}\partial_{C'}V^{B'}_A+o_{(B'}\partial_{A')}V^{B'}_A\,.$$

In view of homogeneity (2.2) and using (A1) this may be written as

$$N_a(s,l)=\tfrac{1}{2}(s\dot{V}_a(s,l)-V_a(s,l))+{}^{+}(l_a\partial_b-l_b\partial_a)V^b(s,l),$$

where ${}^{+}(l_a\partial_b-l_b\partial_a)$ is the selfdual part of $l_a\partial_b-l_b\partial_a$. It was shown in Ref. 16 (and may be also shown without use of spinors) that from (2.2) and (2.3) now follows that the limit values $N_a(\pm\infty,l)$ are proportional to l_a, that is,

$$-\tfrac{1}{2}V_a(+\infty,l)+{}^{+}(l_a\partial_b-l_b\partial_a)V^b(+\infty,l)=-l_aq(l),$$

$$-\tfrac{1}{2}V_a(-\infty,l)+{}^{+}(l_a\partial_b-l_b\partial_a)V^b(-\infty,l)=-l_a\kappa(l),$$

which corresponds with the equations (2.54) and (2.56) of Ref. 16 (there we used $\sigma=\kappa-q$ instead of κ). The conditions of reality of q and κ [(3.32) in Ref. 16], and the above equations in that case are now equivalent to (2.5), and (2.6) and (2.7), respectively.

It was shown in Ref. 16 [Eq. (2.64)] that

$$o^{A'}V^{\text{out}}{}_{A'A}(-\infty,l)=\partial_A\Phi(l) \tag{A2}$$

for some $\Phi(l)$ homogeneous of degree 0. In view of (A1) this is equivalent to (2.14). The gauge of $V^{\text{out}}{}_a(-\infty,l)$ (2.17) is written with the use of (A1) as

$$V^{\text{out}}{}_a(-\infty,l)=\partial_A(o^Bg_{BA'}(l))+\partial_{A'}(o^{B'}g_{B'A}(l)).$$

As $o^Bg_{BA'}(l)$ are in 1:1 correspondence with G_{ab}, the gauge has the form $V^{\text{out}}{}_a(-\infty,l)=\partial_Ah_{A'}(o,\bar{o})+\partial_{A'}h_A(o,\bar{o})$, where $h_{A'}(\alpha o,\overline{\alpha o})=\bar{\alpha}^{-1}h_{A'}(o,\bar{o})$, $h_{A'}(o,\bar{o})o^{A'}=\Phi(l)$, and in the statements (i)–(iii) following (2.17) the tensor G_{ab} may be replaced by $h_{A'}(o,\bar{o})$ satisfying these conditions. This representation satisfies (A2), so (i) is proved. We get a special gauge choosing

$$h_{A'}(o,\bar{o})=\frac{t_{A'A}o^A}{t\cdot l}\,\Phi(l),$$

where t is any unit, positive timelike vector. Any other gauge differs by $\beta(l)l_a$, $\beta(l)$ homogeneous of degree -2. Let $\alpha(l)=\beta(l)-c(t\cdot l)^{-2}$, with such a constant c that $\int\alpha(l)d^2l=0$. There exists then a homogeneous of degree 0 function $A(l)$, such that $\partial_A\partial_{A'}A(l)=\frac{1}{2}o_Ao_{A'}\alpha(l)$. $A(l)$ is determined up to an additive constant. The new gauge is then determined by

$$h'_{A'}(o,\bar{o})=\frac{t_{A'A}o^A}{t\cdot l}\,(\Phi(l)+c)+\partial_{A'}A(l).$$

With this formula the statements (ii) and (iii) following (2.17) are seen to be true.

Finally, the angular momentum term ΔM_{ab} (2.22) is the tensor version of the angular momentum spinor term $\Delta\mu_{AB}=1/2\pi\int qo_{(A}\partial_{B)}\Phi d^2l$, easily obtained from $\Delta M_{ab}=\epsilon_{A'B'}\Delta\mu_{AB}+\epsilon_{AB}\overline{\Delta\mu}_{A'B'}$ by the use of (A1).

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General properties between the canonical correlation and the independent-oscillator model on a partial *-algebra

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We consider a quantum particle in thermal equilibrium with any quantum system in a finite volume under some conditions. For the Heisenberg operator of the momentum operator of the quantum particle, we show that, on a partial *-algebra, the Heisenberg operator satisfies a quantum Langevin equation, which is similar to the work of Ford *et al.* [G. W. Ford, J. T. Lewis, and R. F. O'Connell, Phys. Rev. A **37**, 4419 (1988)]. Through the Langevin equation, we show general and mathematical properties between the canonical correlation and the independent-oscillator model.
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I. INTRODUCTION

The independent-oscillator (IO) model is the model of the quantum particle surrounded by a large number of independent heat bath particles, each attached to the quantum particle by a spring. The Hamiltonian of the system is given by

$$H_{\mathrm{IO}} \overset{\mathrm{def}}{=} \frac{p^2}{2m} + V(x) + \sum_{j=1}^{\infty} \left[\frac{p_j^2}{2m_j} + \frac{1}{2} m_j \omega_j^2 (q_j - x)^2 \right]. \tag{1}$$

Here x and p are the coordinate and momentum operators of the quantum particle of mass m, while q_j and p_j are those of the jth heat bath particle of mass m_j. Of course, we have the usual commutation relations:

$$[x,\ p] = i\hbar, \quad [q_j,\ p_{j'}] = i\hbar\,\delta_{jj'}. \tag{2}$$

Here, $V(x)$ is the potential energy of the external force on the quantum particle. This model appeared in the literature.[1–5] Especially, Ford, Lewis, and O'Connell found the IO model to be convenient since other heat bath models can generally be related to the IO model in Ref. 4. They showed in Sec. IV of Ref. 4 that from the IO model H_{IO} we can derive the generalized quantum Langevin equation:

$$\frac{d}{dt} p(t) + \int_{-\infty}^{t} ds\ \mu(t-s) \frac{p(s)}{m} + V'(x) = F(t), \tag{3}$$

which is the momentum operator version of (2.1) in Ref. 4, where the prime denotes the derivative with respect to x. Here, $\mu(t)$ is the memory function given by

$$\mu(t) = \sum_{j=1}^{\infty} m_j \omega_j^2 \cos(\omega_j t)\, \theta(t), \tag{4}$$

where $\theta(t)$ is the Heaviside step function, and $F(t)$ is an operator-valued random force with mean zero, and a mean force characterized by a memory function $\mu(t)$. The symmetrized correlation function of $F(t)$ is given by

$$\frac{1}{2}\langle F(t)F(s)+F(s)F(t)\rangle_B=\frac{1}{2}\sum_{j=1}^{\infty}\hbar m_j\omega_j^3\coth(\hbar\omega_j/2kT)\cos[\omega_j(t-s)], \tag{5}$$

and the nonequal-time commutator of $F(t)$ is

$$[F(t),\,F(s)]=-i\sum_{j=1}^{\infty}\hbar m_j\omega_j^3\sin[\omega_j(t-s)]. \tag{6}$$

Here, for operator O, $\langle O\rangle_B$ means that $\langle O\rangle_B \overset{\text{def}}{=} \mathrm{tr}(Oe^{-H_B/kT})/\mathrm{tr}(e^{-H_B/kT})$, where

$$H_B \overset{\text{def}}{=} \sum_j\left[\frac{1}{2m_j}p_j^2+\frac{1}{2}m_j\omega_j^2q_j^2\right],$$

k is the Boltzmann constant, and T is absolute temperature. The Fourier–Laplace transform of the memory function is given as

$$[\mu](z)\overset{\text{def}}{=}\int_0^{\infty}dt\;e^{itz}\mu(t)=\frac{i}{2}\sum_{j=1}^{\infty}m_j\omega_j^2\left[\frac{1}{z-\omega_j}+\frac{1}{z+\omega_j}\right] \tag{7}$$

for every $\mathrm{Im}\,z>0$.

Furthermore, Li, Ford, and O'Connell investigated the symmetrized correlation of the coordinate operator and the quantum random force of the generalized quantum Langevin equation in Ref. 5.

Ford, Lewis, and O'Connell showed that properties (5) and (6) are characterization of the operator-valued random force $F(t)$ by the memory function $\mu(t)$ (see (2.2), (2.3), (4.13), and (4.14) in Ref. 4). And besides, in Sec. 3 in Ref. 1 Ford and Kac remarked that, in the generalized quantum Langevin equation, the correlation and commutator for the operator-valued random force must have the forms (5) and (6). Then, in this paper, we prove general properties including (5) and (6) between canonical correlation and the IO model on a partial *-algebra.[6–8] The partial *-algebra which we treat in this paper is given by a completion of a set of quantum operators. The completion is done by the Bogoliubov scalar product which gives the canonical correlation. In order to deal directly with bosonic operators which are unbounded, we choose the partial *-algebra, not C^*-algebra, for unbounded operators.

We consider a quantum particle in thermal equilibrium with any quantum system in a finite volume under conditions (**A.1**)–(**A.4**) below. From now on, we set the Planck constant $\hbar=1$. Let $H_{q,p,s}$ be an arbitrary total Hamiltonian which governs our system of the quantum particle with the quantum system such that $e^{-\beta H_{q,p,s}}$ is a trace class operator (where $\beta\equiv 1/kT$ denotes the inverse temperature). $H_{q,p,s}$ has the form of $H_{q,p,s}=p^2/2m+V(x)+H_{q,s}+H_{int}$, where $H_{q,s}$ denotes the Hamiltonian of a quantum system surrounding the quantum particle with (x,p), and H_{int} is the interaction Hamiltonian between the quantum particle and the quantum system. Here, of course, the form of $H_{q,s}+H_{\mathrm{int}}$ is unknown now. The canonical correlation function $R_p(t_1,t_2)$ for the momentum operator p is defined by

$$R_p(t_1,t_2)\overset{\text{def}}{=}\frac{1}{\beta\mathrm{tr}(e^{-\beta H_{q,p,s}})}\int_0^{\beta}d\lambda\;\mathrm{tr}(e^{-(\beta-\lambda)H_{q,p,s}}e^{iH_{q,p,s}t_1}pe^{-iH_{q,p,s}t_1}e^{-\lambda H_{q,p,s}}e^{iH_{q,p,s}t_2}pe^{-iH_{q,p,s}t_2}).$$

In Secs. II and III, for any p and $H_{q,p,s}$ satisfying (**A.1**)–(**A.4**), we prove that, on a partial *-algebra $\mathbf{X}_c(H_{q,p,s})$ which is called the Liouville space, the Heisenberg operator $p(t)\overset{\text{def}}{=}e^{iH_{q,p,s}t}pe^{-iH_{q,p,s}t}$ satisfies a quantum Langevin equation with a quantum fluctuation $I(t)$,

which has the similar form to (3) [see (17) in the main theorem]. Here we note that we cannot apply theories in Ref. 9 nor Ref. 10 to the momentum operator because of a condition (see Remark 3.2). We show that the memory function $\mu(t)$ for the IO model characterizes a fluctuation–dissipation relation in our Langevin equation and the canonical correlation function $R_p(t_1,t_2)$ [see (19) and (20) in the main theorem], which means that $H_{\rm int}$ is characterized by $[\mu](z)$. Furthermore the symmetrized autocorrelation and nonequal-time commutator of $I(t)$ have the similar representation to (5) and (6), which are implied by our fluctuation–dissipation relation [see (21) and (22) in the main theorem]. They are general results for p and $H_{q,p,s}$ in mathematics, so they give additional mathematical evidence that the IO model represents the system of the quantum particle with the most general quantum system, which was indicated by Ford, Lewis, and O'Connell in Ref. 4. It is a symmetry with respect to the canonical correlation that derives the close relations between the canonical correlation and the distribution of the memory function of the IO model (see Lemma 3.8 in this paper).

As mentioned above, some properties of the IO model was studied in Refs. 1–5. Especially Ford and Kac say on p.808 in Ref. 1: ''*since we have derived the quantum Langevin equation only for very special oscillator models (i.e. the IO model), one might wonder to what extent we have demonstrated the universality of the equation. The answer, of course, is that we have not. Rather, the logic is reversed: if there is a universal description, then it must be of the form we have obtained.*'' Ford, Lewis, and O'Connell showed in Ref. 4 that a number of other heat-bath models within the framework of the general macroscopic description of the quantum Langevin equation are reduced to the IO model by physically adequate reasons. In this paper, for the momentum operator of our system we shall derive a quantum Langevin equation by the general theory by Mori,[11,12] and show general properties between canonical correlation and the IO model. The author thinks that this argument is valid over not only the momentum operator of our system but also observables which are realized as self-adjoint operators in some class, which gives a physical and mathematical proof for Ford and Kac's remark above.

In Sec. IV B, we give some examples of the Hamiltonian $H_{q,p,s}$ and the momentum operator p satisfying assumptions (**A.1**)–(**A.4**).

II. THE STATEMENT OF THE MAIN THEOREM

In this section, in order to introduce canonical correlation functions defined by the Bogoliubov scalar product, the Liouville space, and explain our main theorem, we set up a general framework.

We consider a quantum particle in thermal equilibrium with any quantum system in the finite volume. So, we give a state space for our system by a separable infinite-dimensional Hilbert space, which is denoted simply by $\mathscr{F}_{q,p,s}$. And we denote the inner product of $\mathscr{F}_{q,p,s}$ by $(\ ,\ )_{q,p,s}$.

Let x and p be the coordinate and momentum operators of the quantum particle of mass m and $V(x)$ be the potential energy of the external force on the quantum particle.

For our system, there exists a Hamiltonian $H_{q,p,s}$ whose form is given by $H_{q,p,s}=p^2/2m+V(x)+H_{q,s}+H_{\rm int}$, where $H_{q,s}$ denotes the Hamiltonian of the quantum system surrounding the quantum particle with (x,p), and $H_{\rm int}$ is the interaction Hamiltonian between the quantum particle and the quantum system. Here, of course, the form of $H_{q,s}+H_{\rm int}$ is unknown now. So $H_{q,p,s}$ may be nonquadratic, but must be realized as a self-adjoint operator acting in the Hilbert space $\mathscr{F}_{q,p,s}$. Since we are now considering the thermal equilibrium quantum system, $H_{q,p,s}$ is a self-adjoint operator acting in $\mathscr{F}_{q,p,s}$ and we have the following assumption.

(**A.1**) $e^{-\tau H_{q,p,s}}$ is a trace class operator on $\mathscr{F}_{q,p,s}$ for every $\tau\in(0,\beta]$, where $\beta\equiv 1/kT$ is the inverse temperature. This condition implies that the spectra of $H_{q,p,s}$ are purely discrete and the eigenvectors $\{\varphi_n | n\in\mathbf{N}^*\}$ of $H_{q,p,s}$ form a complete orthonormal system of $\mathscr{F}_{q,p,s}$, where $\mathbf{N}^* \underset{\rm def}{=} \{0,1,\cdots\}$. We count the eigenvalues λ_n $(n\in\mathbf{N}^*)$ of $H_{q,p,s}$ in such a way that $H_{q,p,s}\varphi_n=\lambda_n\varphi_n$ and $0<\lambda_0\leqslant\lambda_1\leqslant\cdots\leqslant\lambda_n\leqslant\lambda_{n+1}\leqslant\cdots\nearrow\infty$.

For the Hamiltonian $H_{q,p,s}$, we can construct a Liouville space $\mathbf{X}_c(H_{q,p,s})$, which is a set of adequate quantum operators acting in $\mathscr{F}_{q,p,s}$.[9,13] We denote the linear hull of $\{\varphi_n | n \in \mathbf{N}^*\}$ by $\mathbf{D}_{q,p,s}$, i.e., $\mathbf{D}_{q,p,s} \stackrel{\text{def}}{=} \mathbf{L.h.}[\{\varphi_n | n \in \mathbf{N}^*\}]$. From here on, we denote the linear hull of a set S by $\mathbf{L.h.}[S]$. Obviously $\mathbf{D}_{q,p,s}$ is dense in $\mathscr{F}_{q,p,s}$. Further, we denote by $\mathbf{B}(\mathbf{D}_{q,p,s}, \mathscr{F}_{q,p,s})$ the space of bounded linear operators from $\mathbf{D}_{q,p,s}$ to $\mathscr{F}_{q,p,s}$. Every element A in $\mathbf{B}(\mathbf{D}_{q,p,s}, \mathscr{F}_{q,p,s})$ has a unique extension to an element in $\mathbf{B}(\mathscr{F}_{q,p,s})$, the space of bounded linear operators on $\mathscr{F}_{q,p,s}$. We denote the extension of A by A^-, and $A^* \restriction \mathbf{D}_{q,p,s}$ by A^+, which means that the domain of operator A^* is restricted to $\mathbf{D}_{q,p,s}$.

We first define a class $\mathbf{T}(H_{q,p,s})$ of quantum operators, which is a set of quantum operators A satisfying the following conditions: (**T.1**) the domain of each operator is equal to $\mathbf{D}_{q,p,s}$, and the domain of the adjoint operator of each operator includes $\mathbf{D}_{q,p,s}$ [i.e., $\mathrm{D}(A) = \mathbf{D}_{q,p,s}$ and $\mathrm{D}(A^*) \supset \mathbf{D}_{q,p,s}$, where $\mathrm{D}(B)$ denotes the domain of each operator B]; (**T.2**) for all τ in $(0,\beta]$ operators $e^{-\tau H_{q,p,s}} A$ and $A e^{-\tau H_{q,p,s}}$ are in $\mathbf{B}(\mathbf{D}_{q,p,s}, \mathscr{F}_{q,p,s})$, furthermore, $(e^{-\tau H_{q,p,s}} A)^-$ and $(A e^{-\tau H_{q,p,s}})^-$ are Hilbert–Schmidt operators on $\mathscr{F}_{q,p,s}$. We must now turn our attention to the unboundedness of operators because it is known that limits on the precision of the measurement of observables for bounded operators (e.g., fermion) and unbounded operators (e.g., boson) are different.[14–16] For unbounded operators, the problem of their domains is delicate, so we provide condition (**T.1**). Condition (**T.2**) addresses convergency with respect to the Bogoliubov scalar product.[9,13,17] We note here that $\mathbf{T}(H_{q,p,s})$ is a linear space. We can then introduce the Bogoliubov (Kubo–Mori) scalar product $\langle\ ;\ \rangle$ as

$$\langle A;B\rangle \stackrel{\text{def}}{=} \frac{1}{\beta Z(\beta)} \int_0^\beta d\lambda\ \mathrm{tr}((e^{-(\beta-\lambda)H_{q,p,s}} A^*)^- (e^{-\lambda H_{q,p,s}} B)^-), \quad A,B \in \mathbf{T}(H_{q,p,s}),$$

where $Z(\beta) \stackrel{\text{def}}{=} \mathrm{tr}(e^{-\beta H_{q,p,s}})$. It can be easily proven that $\langle\ ;\ \rangle$ is an inner product of $\mathbf{T}(H_{q,p,s})$ (see Ref. 13). The inner product introduces a norm: $\|A\|_{H_{q,p,s}} \stackrel{\text{def}}{=} \langle A;A\rangle^{1/2}$. We can therefore obtain the Liouville space $\mathbf{X}_c(H_{q,p,s})$ defined by a Hilbert space which is the completion of $\mathbf{T}(H_{q,p,s})$ with respect to the norm $\|\ \|_{H_{q,p,s}}$. It is interesting to note that $\mathbf{X}_c(H_{q,p,s})$ is a partial *-algebra with a unit (see Proposition 3.14 in Ref. 13). The definition of partial *-algebras is given in Refs. 6–8. We also note here that an element in $\mathbf{X}_c(H_{q,p,s})$ is not always an operator acting in $\mathscr{F}_{q,p,s}$. It is noteworthy that Naudts *et al.* attempted to argue in general about linear response theory on the Hilbert space which is constructed by a completion of a von Neumann algebra with KMS-state.[18] Roughly speaking, the von Neumann algebra with the KMS-state can be regarded as a set of quantum operators which can be taken as a statistical average with the KMS-condition, however the operators are bounded. So, for our purpose we do use the partial *-algebra instead of the von Neumann algebra because the operators we treat are unbounded. And we deal with Mori's theory on $\mathbf{X}_c(H_{q,p,s})$, which is just the partial *-algebra constructed by the completion concerning the Bogoliubov scalar product.

In order to introduce the Heisenberg operator $p(t)$ of the momentum operator, we define here the Liouville operator $\mathscr{L}_{q,p,s}$ determined by the Hamiltonian $H_{q,p,s}$.

We can define, for adequate operators A, the Liouville operator $\mathscr{L}_{q,p,s}$ by $\mathscr{L}_{q,p,s} A \stackrel{\text{def}}{=} [H_{q,p,s}, A] = H_{q,p,s} A - A H_{q,p,s}$ (see Lemma 3.8 in Ref. 13). The domain $\mathrm{D}(\mathscr{L}_{q,p,s})$ of the Liouville operator $\mathscr{L}_{q,p,s}$ then contains a dense subspace $\mathscr{D}_{q,p,s}$ of all elements $A \in \mathbf{T}(H_{q,p,s})$ satisfying that $H_{q,p,s} A$ and $A H_{q,p,s} \restriction \mathbf{D}_{q,p,s}$ are in $\mathbf{T}(H_{q,p,s})$; furthermore, Ax, $A^+ x$, $H_{q,p,s} Ax$, $H_{q,p,s} A^+ x$, $A H_{q,p,s} x$, and $A^+ H_{q,p,s} x$ are in $\mathbf{D}_{q,p,s}$ for all x in $\mathbf{D}_{q,p,s}$. Actually, the subspace $\mathscr{D}_{q,p,s}$ is a core for $\mathscr{L}_{q,p,s}$ [see (66) in Sec. IV B, Lemmas 3.7 and 3.8 in Ref. 13].

For every $A \in \mathbf{X}_c(H_{q,p,s})$, we denote the Heisenberg operator of A by $A(t)$ in the Liouville space $\mathbf{X}_c(H_{q,p,s})$, i.e.,

$$A(t) \stackrel{\text{def}}{=} e^{i\mathscr{L}_{q,p,s}t}A.$$

And we define the canonical autocorrelation function of A by

$$R_A(t) \stackrel{\text{def}}{=} R_A(0,t) \equiv \langle A(0);A(t)\rangle.$$

Remark 2.1: The time evolution $A(t)$ coincides with the Heisenberg picture $e^{iH_{q,p,s}t}Ae^{-iH_{q,p,s}t}$ for every quantum operator A in $\mathscr{D}_{q,p,s}$ and $t \in \mathbf{R}$ (see Proposition 3.13 in Ref. 13).

So, we denote the canonical autocorrelation function of the momentum operator p by $R_p(t)$. We define here a function $[R_p](z)$ ($z \in \mathbf{C}$ with $\operatorname{Im} z > 0$) by the Fourier–Laplace transform as

$$[R_p](z) \stackrel{\text{def}}{=} \int_0^\infty dt\ e^{itz}R_p(t).$$

Here, we have the properties concerning poles of $[R_p](z)$:

The spectra of $\mathscr{L}_{q,p,s}$ is given by the closure of the set of all $\lambda_m - \lambda_n$'s:

$$\sigma(\mathscr{L}_{q,p,s}) = \overline{\{\lambda_m - \lambda_n | m,n \in \mathbf{N}^*\}}^{\text{ closure}}, \tag{8}$$

which is proved in Lemma 3.1 in the following section.

There exist non-negative constants $A_{m,n}$ ($m,n \in \mathbf{N}^*$) such that

$$R_p(t) = \sum_{m,n \in \mathbf{N}^*} A_{m,n}e^{it(\lambda_m - \lambda_n)}, \tag{9}$$

whose proof is given by Lemma 3.2 in the following section.

We denote the set of all positive poles of $[R_p](z)$ by $\mathbf{P}_+^R$, and the set of all negative poles of $[R_p](z)$ by $\mathbf{P}_-^R$. Then, by (9) and the following assumption, each poles of $[R_p](z)$ agree with differences of two λ_n's.

(**A.2**) For $\mathbf{P}_+^R = \{\varepsilon_k | k = 0,1,\cdots\}$, $\inf_{k \in \mathbf{N}^*}(\varepsilon_{k+1} - \varepsilon_k) > 0$. Moreover, for $\mathbf{P}_-^R = \{\eta_k | k = 0,1,\cdots\}$, $\inf_{k \in \mathbf{N}^*}(\eta_k - \eta_{k+1}) > 0$.

We set the last two conditions: Because we consider a system governed by the Hamiltonian $H_{q,p,s} \equiv p^2/2m + V(x) + H_{q,s} + H_{\text{int}}$ with (**A.1**), the condition that $p \in \mathbf{T}(H_{q,p,s})$ is natural assumption.

(**A.3**) $p \in \mathbf{T}(H_{q,s,p})$. Furthermore,

$$\sum_{k=0}^{\infty} \left(\lim_{z \to \varepsilon_k} \frac{1}{i}(z - \varepsilon_k)[R_p](z) \right) \varepsilon_k^2 < \infty,$$

and

$$\sum_{k=0}^{\infty} \left(\lim_{z \to \eta_k} \frac{1}{i}(z - \eta_k)[R_p](z) \right) (-\eta_k)^2 < \infty.$$

(**A.4**) $\lim_{z \to 0; z \in \mathbf{C}^+} z[R_p](z) = 0$, where $\mathbf{C}^+ \stackrel{\text{def}}{=} \{z \in \mathbf{C} | \operatorname{Im} z > 0\}$.

Here we introduce the symmetrized autocorrelation function $S_p(t)$ by using well-known relation in Theorem 3 in Ref. 19. For $R_A(t)$ $(A \in \mathbf{X}_c(H_{q,p,s}))$, since $R_A(t)$ is continuous and positive-definite, there exists a unique measure Δ_A^{can} such that

$$R_A(t) = \int_{-\infty}^{\infty} e^{it\omega} \Delta_A^{\mathrm{can}}(d\omega)$$

according to Bochner's theorem. Then, we define the symmetrized autocorrelation function $S_A(t)$ for $A \in \mathbf{X}_c(H_{q,p,s})$ by

$$S_A(t) \underset{=}{\mathrm{def}} \int_{-\infty}^{\infty} e^{it\omega} \beta E_\beta(\omega) \Delta_A^{\mathrm{can}}(d\omega), \tag{10}$$

where $E_\beta(\omega)$ is the average energy of the harmonic oscillator with the frequency ω at temperature $T = 1/k\beta$,

$$E_\beta(\omega) = \frac{\hbar\omega}{2} \coth \frac{\beta\hbar\omega}{2}. \tag{11}$$

(We note here that we set $\hbar = 1$ in this paper.)

For $A \in \mathbf{X}_c(H_{q,p,s})$, we define the response function $P_A(t)$ by

$$P_A(t) \underset{=}{\mathrm{def}} -\beta \frac{d}{dt} \langle A; A(t) \rangle. \tag{12}$$

We have another Liouville space $\mathbf{X}_\beta(H_{q,p,s})$ by completion of $\mathbf{T}(H_{q,p,s})$ by the following inner product:[20] For $A, B \in \mathbf{T}(H_{q,p,s})$, we set

$$\langle A|B \rangle \underset{=}{\mathrm{def}} Z(\beta)^{-1} \mathrm{tr}(\{(Ae^{-\beta H_{q,p,s}/2})^-\} * \{(Be^{-\beta H_{q,p,s}/2})^-\}). \tag{13}$$

Then, we can define the Liouville operator $\mathscr{L}^{q,p,s}$ with certain dense domain in $\mathbf{X}_\beta(H_{q,p,s})$ (see Secs. II and III in Ref. 20) in the same way as $\mathscr{L}_{q,p,s}$. So we can get the Heisenberg operator $e^{i\mathscr{L}^{q,p,s}t} A$ for $A \in \mathbf{X}_\beta(H_{q,p,s})$, which denotes

$$A[t] \underset{=}{\mathrm{def}} e^{i\mathscr{L}^{q,p,s}t} A \in \mathbf{X}_\beta(H_{q,p,s}) \tag{14}$$

in order to distinguish it from $A(t) \in \mathbf{X}_c(H_{q,p,s})$.

We denote $Z(\beta)^{-1}$ tr $(Oe^{-\beta H q,p,s})$ by $\langle O \rangle$. Then, of course, the well-known relation (see Theorem 3 in Ref. 19) means the following proposition in our Liouville's spaces: If A is a symmetric operator acting in $\mathscr{F}_{q,p,s}$ with $A \in \mathbf{X}_c(H_{q,p,s})$ and $A \in \mathbf{X}_\beta(H_{q,p,s})$, then

$$S_A(t) = \tfrac{1}{2} \langle AA[t] + A[t]A \rangle. \tag{15}$$

We will prove this relation in Proposition 3.3 in the following section.

Furthermore, concerning the response function, of course a well-known fact in our version holds: If A is a symmetric operator acting in $\mathscr{F}_{q,p,s}$ with $A \in \mathbf{X}_c(H_{q,p,s})$ and $A \in \mathbf{X}_\beta(H_{q,p,s})$, then

$$P_A(t) = -i \langle [A, A[t]] \rangle, \tag{16}$$

where, of course, $[A, A[t]] = AA[t] - A[t]A$.We will also prove this relation in Proposition 3.4 in the following section.Now, we can state our main theorem.

Theorem: *Suppose that the total Hamiltonian $H_{q,p,s}$ of the system of the quantum particle with the quantum system, and the momentum operator p of the quantum particle, satisfy assumptions* (**A.1**), (**A.2**), (**A.3**), *and* (**A.4**). *Then the function* $[R_p](z)$ can be extended to a meromorphic function on the complex plane, *and the set* $\{\omega_j\}_{j=1}^{\infty}$ *of all positive zero points of* $[R_p]$ *is counted in such a way that*

$$\omega_j \in (\varepsilon_{j-1}, \varepsilon_j), \text{ with } \varepsilon_j > 0, \ j \in \mathbf{N}.$$

Give the mass m_j *of the particle of the quantum system by*

$$m_j = \frac{2mR_p(0)}{\omega_j^2 i[R_p]'(\omega_j)}, \text{ where } [R_p]'(z) \equiv d[R_p](z)/dz.$$

Let $\mu(t)$ *be the memory function of* H_{IO} *with frequency* ω_j *and mass* m_j *above, i.e.,*

$$\mu(t) = \sum_{j=1}^{\infty} m_j \omega_j^2 \cos(\omega_j t)\,\theta(t).$$

Then, there exist a memory function $\kappa_\tau(t)$ *and quantum fluctuation* $I(t)$ *such that the Heisenberg operator* $p(t) \equiv e^{i\mathscr{L}_{q,p,s}t}p$ *of the momentum operator satisfies the following quantum Langevin equation* :

$$\frac{d}{dt}p(t) + \lim_{\tau \uparrow t} \int_{-\infty}^{t} ds\ \kappa_\tau(t-s)\frac{p(s)}{m} = I(t) \tag{17}$$

on the Liouville space $\mathbf{X}_c(H_{q,p,s})$ *with*

$$\lim_{\tau \to \infty} \kappa_\tau(t) = \mu(t), \quad t > 0, \tag{18}$$

a fluctuation-dissipation relation :

$$\frac{R_p(0)}{m}\mu(t) = \langle I(0); I(t) \rangle, \quad t > 0, \tag{19}$$

with

$$\langle p; I(t) \rangle = 0, \quad t \in \mathbf{R},$$

and

$$[R_p](z) = R_p(0)\frac{1}{-iz + [\mu](z)/m}, \quad z \in \mathbf{C} \backslash \{\omega_j\}_{j=1}^{\infty}. \tag{20}$$

Furthermore, the fluctuation-dissipation relation (19) *implies that the symmetrized autocorrelation function* $S_I(t)$ *of* $I(t)$ *is*

$$S_I(t) = \frac{1}{2kT}\sum_{j=1}^{\infty} m_j \omega_j^3 \coth\left(\frac{\omega_j}{2kT}\right)\cos(\omega_j t), \tag{21}$$

and response function $P_I(t)$ *is*

$$P_I(t)=\frac{R_p(0)}{mkT}\sum_{j=1}^{\infty} m_j\omega_j^3 \sin(\omega_j t). \tag{22}$$

(*We note here we set* $\hbar=1$ *now.*)

Remark 2.2: $I(t)$ may be decomposed into a summation of $V'(x)$ and a certain quantum force $F(t)$. However, information in the theorem is not enough to decompose $I(t)$ in such a way. As a matter of fact, the fluctuation $I(t)$ is Mori's fluctuation on the Liouville space $\mathbf{X}_c(H_{q,p,s})$, and then $\mu(t)$ agrees with Mori's memory function multiplied by the mass m for $t\geqslant 0$ [see (42) and Lemma 3.10(c) in the following section].

III. PROOFS OF THE RESULTS

A. Preliminaries

We first prove some properties concerning the poles of $[R_p]\,(z)$.

The proof of (8) is given by the following lemma:

Lemma 3.1: The spectra of $\mathscr{L}_{q,p,s}$ is the closure of the set of all $\lambda_m-\lambda_n$'s:

$$\sigma(\mathscr{L}_{q,p,s})=\overline{\{\lambda_m-\lambda_n|m,n\in\mathbf{N}^*\}}^{\text{ closure}}.$$

Proof: Simple calculation implies that linear operators $\Phi_{m,n}\colon \mathbf{D}_{q,p,s}\to\mathbf{D}_{q,p,s}$, $m,n\in\mathbf{N}^*$ defined by

$$\begin{aligned} &\mathrm{D}(\Phi_{m,n})\overset{\text{def}}{=}\mathbf{D}_{q,p,s},\\ &\Phi_{m,n}x\overset{\text{def}}{=}\beta^{1/2}Z(\beta)^{1/2}W_{m,n}^{1/2}(\varphi_n,x)_{q,p,s}\varphi_m, \qquad x\in\mathbf{D}_{q,p,s};m,n\in\mathbf{N}^*, \end{aligned} \tag{23}$$

are eigenvectors of $\mathscr{L}_{q,p,s}$ (see Proposition 3.9 in Ref. 9), where

$$W_{m,n}\overset{\text{def}}{=}\begin{cases} \dfrac{\lambda_n-\lambda_m}{e^{-\beta\lambda_m}-e^{-\beta\lambda_n}} \text{ if } \lambda_m\neq\lambda_n,\\ \beta^{-1}e^{\beta\lambda_m} \text{ if } \lambda_m=\lambda_n. \end{cases}$$

The set of all $\Phi_{m,n}$'s is also a complete orthonormal system of $\mathbf{X}_c(H_{q,p,s})$ such that

$$\mathscr{L}_{q,p,s}\Phi_{m,n}=(\lambda_m-\lambda_n)\Phi_{m,n}, \quad m,n\in\mathbf{N}^*, \quad \Phi_{m,n}^{+}=\Phi_{n,m}, m,n\in\mathbf{N}^* \tag{24}$$

(see Proposition 3.9 in Ref. 9). It must be noted that

$$W_{m,n}>0, \quad m,n\in\mathbf{N}^*, \quad W_{m,n}=W_{n,m}, \quad m,n\in\mathbf{N}^*. \tag{25}$$

The complete orthonormal system, $\{\Phi_{m,n},|m,n\in\mathbf{N}^*\}$, gives a proof that the set of all spectra of the Liouville operator $\mathscr{L}_{q,p,s}$ are equal to the closure of the set of $\lambda_m-\lambda_n$ $(m,n\in\mathbf{N}^*)$. Q.E.D.

The proof of (9) is given as follows:

Lemma 3.2: There exist non-negative constants $A_{m,n}$ $(m,n\in\mathbf{N}^*)$ such that

$$R_p(t)=\sum_{m,n\in\mathbf{N}^*} A_{m,n}e^{it(\lambda_m-\lambda_n)}.$$

Proof: By the proof of Lemma 3.1, we obtain

$$R_p(t)=\langle p;e^{i\mathscr{L}_{q,p,s}t}p\rangle=\sum_{m,n\in\mathbf{N}^*}|\langle\Phi_{m,n};p\rangle|^2e^{it(\lambda_m-\lambda_n)}. \tag{26}$$

So taking

$$A_{m,n}=|\langle\Phi_{m,n};p\rangle|^2, \tag{27}$$

we get our lemma. Q.E.D.

The proofs of (15) and (16) are given in the following Propositions 3.3 and 3.4.

Proposition 3.3: If A is a symmetric operator acting in $\mathscr{F}_{q,p,s}$ with $A\in\mathbf{X}_c(H_{q,p,s})$ and $A\in\mathbf{X}_\beta(H_{q,p,s})$, then

$$S_A(t)=\tfrac{1}{2}\langle AA[t]+A[t]A\rangle=\tfrac{1}{2}\{\langle A|A[t]\rangle+\langle A[t]|A\rangle\}.$$

Proof: According to Sec. III in Ref. 20, we define operators $\Psi_{m,n}:\mathbf{D}_{q,p,s}\to\mathbf{D}_{q,p,s}$ by

$$\begin{gathered}\mathrm{D}(\Psi_{m,n})\underset{=}{\text{def}}\mathbf{D}_{q,p,s},\\ \Psi_{m,n}x\underset{=}{\text{def}}Z(\beta)^{1/2}e^{\beta\lambda_n/2}(\varphi_n,x)_{q,p,s}\varphi_m,\qquad x\in\mathbf{D}_{q,p,s};m,n\in\mathbf{N}^*,\end{gathered} \tag{28}$$

which are eigenvectors of $\mathscr{L}^{q,p,s}$ (see Proposition 3.9 in Ref. 20). They make also a complete orthonormal system of $\mathbf{X}_\beta(H_{q,p,s})$ such that

$$\mathscr{L}^{q,p,s}\Psi_{m,n}=(\lambda_m-\lambda_n)\Psi_{m,n},m,n\in\mathbf{N}^*,\quad \Psi^+_{m,n}=e^{\beta(\lambda_n-\lambda_m)/2}\Psi_{n,m},m,n\in\mathbf{N}^* \tag{29}$$

(see Proposition 3.9 in Ref. 20). Using expansions of A and $A[t]$ by $\Psi_{m,n}$'s, we have $\langle A|A[t]\rangle=\langle AA[t]\rangle$ and $\langle A[t]|A\rangle=\langle A[t]A\rangle$, where we used the assumption that A is symmetric.

Since $\frac{1}{2}\{\langle A|A[t]\rangle+\langle A[t]|A\rangle\}$ is continuous and positive-definite, there exists a unique measure Δ_A^{sym} such that

$$\frac{1}{2}\{\langle A|A[t]\rangle+\langle A[t]|A\rangle\}=\int_{-\infty}^{\infty}e^{it\omega}\Delta_A^{\mathrm{sym}}(d\omega)$$

according to Bochner's theorem.

By using expansions

$$A(t)=\sum_{m,n}\langle\Phi_{m,n};A\rangle e^{it(\lambda_m-\lambda_n)}\Phi_{m,n}\quad\text{in}\quad\mathbf{X}_c(H_{q,p,s}),$$

$$A[t]=\sum_{m,n}\langle\Psi_{m,n}|A\rangle e^{it(\lambda_m-\lambda_n)}\Psi_{m,n}\quad\text{in}\quad\mathbf{X}_\beta(H_{q,p,s}),$$

we have

$$\Delta_A^{\mathrm{can}}(d\omega)=\sum_{m,n}|\langle\Phi_{m,n};A\rangle|^2\delta_{(\lambda_m-\lambda_n)}(d\omega), \tag{30}$$

$$\Delta_A^{\mathrm{sym}}(d\omega)=\sum_{m,n}|\langle\Psi_{m,n}|A\rangle|^2\frac{1}{2}(\delta_{(\lambda_m-\lambda_n)}(d\omega)+\delta_{(\lambda_n-\lambda_m)}(d\omega))$$

$$=\sum_{m,n}\frac{|\langle\Psi_{m,n}|A\rangle|^2+|\langle\Psi_{n,m}|A\rangle|^2}{2}\delta_{(\lambda_m-\lambda_n)}(d\omega). \tag{31}$$

We note here

$$\langle\Phi_{m,n};A\rangle=\beta^{-1/2}Z(\beta)^{-1/2}W_{m,n}^{-1/2}(\varphi_m,A\varphi_n)_{q,p,s} \tag{32}$$

by (27) in Ref. 9, and

$$\langle\Psi_{m,n}|A\rangle=Z(\beta)^{-1/2}e^{-\beta\lambda_n/2}(\varphi_m,A\varphi_n)_{q,p,s}$$

by (46) in Ref. 20. So, we have

$$\left(\frac{|\langle\Psi_{m,n}|A\rangle|^2+|\langle\Psi_{n,m}|A\rangle|^2}{2}\right)(|\langle\Phi_{m,n};A\rangle|^2)^{-1}$$

$$=\frac{\beta W_{m,n}}{2}(e^{-\beta\lambda_m}+e^{-\beta\lambda_n})$$

$$=\frac{\beta(\lambda_m-\lambda_n)}{2}\,\frac{e^{\beta(\lambda_m-\lambda_n)}+1}{e^{\beta(\lambda_m-\lambda_n)}-1}$$

$$=\frac{\beta(\lambda_m-\lambda_n)}{2}\coth\left(\frac{\beta(\lambda_m-\lambda_n)}{2}\right).$$

Therefore, we obtain

$$\Delta_A^{\mathrm{sym}}(d\omega)=\beta\frac{\omega}{2}\coth\left(\frac{\beta\omega}{2}\right)\Delta_A^{\mathrm{can}}(d\omega). \tag{33}$$

Remember we set $\hbar=1$, and (33) implies our proposition. Q.E.D.

Proposition 3.4: If A is a symmetric operator acting in $\mathscr{F}_{q,p,s}$ with $A\in\mathbf{X}_c(H_{q,p,s})$ and $A\in\mathbf{X}_\beta(H_{q,p,s})$, then

$$P_A(t)=-i\langle[A,A[t]]\rangle=-i\{\langle A|A[t]\rangle-\langle A[t]|A\rangle\}.$$

Proof: This proposition is proved in the same way as Proposition 3.3. Q.E.D.

By (26), it is clear that, for any ε_k and η_k $(k\in\mathbf{N}^*)$ there exist $m^+(k),n^+(k)\in\mathbf{N}^*$; and $m^-(k),n^-(k)\in\mathbf{N}^*$ such that

$$\varepsilon_k=-(\lambda_{m^+(k)}-\lambda_{n^+(k)}), \tag{34}$$

$$\eta_k=-(\lambda_{m^-(k)}-\lambda_{n^-(k)}), \tag{35}$$

and for the zero, 0, there exist $m^0(k),n^0(k)\in\mathbf{N}^*$ such that

$$0=-(\lambda_{m^0(k)}-\lambda_{n^0(k)}). \tag{36}$$

For every $z\in\mathbf{C}$ with $z\neq0$ and $z\notin\mathbf{P}_\pm^R$, there exists a point $c\in\{0\}\cup\mathbf{P}_+^R\cup\mathbf{P}_-^R$ such that $|z-c|\leqslant|z-c'|$ for all $c'\in\{0\}\cup\mathbf{P}_+^R\cup\mathbf{P}_-^R$ by the assumption (**A.2**). So, we have

$$\left|\int_0^\infty dt\ e^{-itc'}e^{itz}\right|\leqslant\frac{1}{|z-c|}$$

if Im $z>0$. Thus, by applying Lebesgue's dominated convergence theorem to (26), we note that for Im $z>0$

$$[R_p](z)=i\sum_{k=0}^{\infty}\left(\sum_{\substack{m^+(k),n^+(k);\\ \lambda_{m^+(k)}-\lambda_{n^+(k)}=-\varepsilon_k}} A_{m^+(k),n^+(k)}\right)\frac{1}{z-\varepsilon_k}$$
$$+i\sum_{k=0}^{\infty}\left(\sum_{\substack{m^-(k),n^-(k);\\ -\lambda_{n^-(k)}=-\eta_k\lambda_{m^-(k)}}} A_{m^-(k),n^-(k)}\frac{1}{z-\eta_k}\right.$$
$$+i\sum_{k=0}^{\infty}\left(\sum_{\substack{m^0(k),n^0(k);\\ \lambda_{m^0(k)-\lambda_{n^0(k)}=0}} A_{m^0(k),n^0(k)}\right)\frac{1}{z}. \tag{37}$$

And, for $z\notin\{0\}\cup\mathbf{P}_+^R\cup\mathbf{P}_-^R$,

$$\left|\frac{d}{dz}\left(\frac{1}{z-c'}\right)\right|\leqslant\frac{1}{|z-c|^2}.$$

Thus, by applying Weierstrass' M-test to (37), it is evident that $[R_p](z)$ can be extended into a meromorphic function on the complex plain with singularities only at points in $\{0\}\cup\mathbf{P}_+^R\cup\mathbf{P}_-^R$ by (**A.3**) and (37).

For instance, for any $z\in\mathbf{C}$ with $|z-\varepsilon_k|<\min(\varepsilon_k-\varepsilon_{k-1},\varepsilon_{k+1}-\varepsilon_k)/2$, inequalities $|z-\varepsilon_k|\leqslant|z-\varepsilon_{k'}|$ and $|z-\varepsilon_k|\leqslant|z-\eta_{k'}|$ $(k'\in\mathbf{N}^*)$ hold. So, we get $|(z-\varepsilon_k)[R_p](z)|\leqslant\|p\|_{H_{q,p,s}}^2$ for the z above. Then, the following lemma is derived from (27) and (37) by Weierstrass' M-test.

Lemma 3.5: For each $k\in\mathbf{N}^*$,

$$\lim_{z\to\varepsilon_k}\frac{1}{i}(z-\varepsilon_k)[R_p](z)=\sum_{\substack{m^+(k),n^+(k);\\ \lambda_{m^+(k)}-\lambda_{n^+(k)}=-\varepsilon_k}} A_{m^+(k),n^+(k)},$$

$$\lim_{z\to\eta_k}\frac{1}{i}(z-\eta_k)[R_p](z)=\sum_{\substack{m^-(k),n^-(k);\\ \lambda_{m^-(k)}-\lambda_{n^-(k)}=-\eta_k}} A_{m^-(k),n^-(k)},$$

$$\lim_{z\to 0}\frac{1}{i}z[R_p](z)=\sum_{\substack{m^0(k),n^0(k);\\ \lambda_{m^0(k)-\lambda_{n^0(k)}=0}} A_{m^0(k),n^0(k)}.$$

Lemma 3.6: $p\in\mathrm{D}(\mathscr{L}_{a,b})$.

Proof: Assumption (**A.3**) and Lemma 3.5 imply our lemma. Q.E.D.

By using (34), (35), (36), and (37), we can decompose $R_p(t)$ into $R_p(t)=R_0+R_1(t)+R_2(t)$, where

$$R_0\overset{\text{def}}{=}-i\lim_{z\to 0;z\in\mathbf{C}^+}z[R_p](z)=\sum_{k=0}^{\infty}\left(\sum_{\substack{m^0(k),n^0(k);\\ \lambda_{m^0(k)-\lambda_{n^0(k)}=0}} A_{m^0(k),n^0(k)}\right),$$

$$R_1(t) \overset{\text{def}}{=} \sum_{k=0}^{\infty} \left(\sum_{\substack{m^+(k),n^+(k);\\ \lambda_{m^+(k)}-\lambda_{n^+(k)}=-\varepsilon_k}} A_{m^+(k),n^+(k)} \right) e^{-it\varepsilon_k}$$

$$= \sum_{k=0}^{\infty} \left(\sum_{\substack{m^+(k),n^+(k);\\ \lambda_{m^+(k)}-\lambda_{n^+(k)}=-\varepsilon_k}} |\langle \Phi_{m^+(k),n^+(k)}; p\rangle|^2 e^{it(\lambda_{m^+(k)}-\lambda_{n^+(k)})} \right), \tag{38}$$

$$R_2(t) \overset{\text{def}}{=} \sum_{k=0}^{\infty} \left(\sum_{\substack{m^-(k),n^-(k);\\ \lambda_{m-(k)}-\lambda_{n-(k)}=-\eta_k}} A_{m^-(k),n^-(k)} \right) e^{-it\eta_k}$$

$$= \sum_{k=0}^{\infty} \left(\sum_{\substack{m^-(k),n^-(k);\\ \lambda_{m-(k)}-\lambda_{n-(k)}=-\eta_k}} |\langle \Phi_{m^-(k),n^-(k)}; p\rangle|^2 e^{it(\lambda_{m^-(k)}-\lambda_{n^-(k)})} \right). \tag{39}$$

So, by (**A.4**), we have

$$R_p(t) = R_1(t) + R_2(t). \tag{40}$$

Then we define Mori's frequency ω_0 by

$$\omega_0 \overset{\text{def}}{=} -\langle p; \mathscr{L}_{q,p,s} p\rangle \langle p; p\rangle^{-1}. \tag{41}$$

(We changed the original definition of this frequency[11,12] into the above definition, see Sec. IV A.)

Next, we define Mori's fluctuation $I(t)$ for p by

$$I(t) \overset{\text{def}}{=} ie^{i\mathscr{L}_1 t}(1-\Pi_0)\mathscr{L}_{q,p,s} p, \quad t \in \mathbf{R}, \tag{42}$$

where Π_0 is an orthogonal projection operator onto the closed subspace $\mathbf{X}_c^-(H_{q,p,s})$ generated by p, i.e., $\Pi_0 \mathbf{X}_c(H_{q,p,s}) = \mathbf{X}_c^-(H_{q,p,s}) \overset{\text{def}}{=} \overline{\{\alpha p \in \mathbf{X}_c(H_{q,p,s}) | \alpha \in \mathbf{C}\}}^{\|\ \|_{H_{q,p,s}}}$.[9,13] We denote here the closure of a linear subspace S of $\mathbf{X}_c(H_{q,p,s})$ by $\bar{S}$. And $\mathscr{L}_1$ is a self-adjoint operator acting in the Hilbert space $(1-\Pi_0)\mathbf{X}_c(H_{q,p,s})$, which is defined by $\mathscr{L}_1 A \overset{\text{def}}{=} (1-\Pi_0)\mathscr{L}_{q,p,s} A$ for $A \in \mathrm{D}(\mathscr{L}_1) \overset{\text{def}}{=} \mathrm{D}(\mathscr{L}_{q,p,s}) \cap (1-\Pi_0)\mathbf{X}_c(H_{q,p,s})$.[10]

We now define symmetric operator $\mathscr{V}$ acting in $\mathbf{X}_c(H_{q,p,s})$ by $D(\mathscr{V}) \overset{\text{def}}{=} D(\mathscr{L}_{q,p,s})$; and $\mathscr{V} \overset{\text{def}}{=} -(\Pi_0 \mathscr{L}_{q,p,s} + \mathscr{L}_{q,p,s}\Pi_0) + \Pi_0 \mathscr{L}_{q,p,s}\Pi_0$. We note here that $\Pi_0 C \in D(\mathscr{L}_{q,p,s})$ for every $C \in \mathbf{X}_c(H_{q,p,s})$ since $p \in D(\mathscr{L}_{q,p,s})$. It is evident that $(1-\Pi_0)\mathscr{L}_{q,p,s}(1-\Pi_0) = \mathscr{L}_{q,p,s} + \mathscr{V}$ on $D(\mathscr{L}_{q,p,s})$. Let $C_n \in D(\mathscr{L}_{q,p,s})$ $(n \in \mathbf{N})$ with conditions $\sup_{n\in\mathbf{N}} \|C_n\|_{H_{q,p,s}} < \infty$, and $\sup_{n\in\mathbf{N}} \|\mathscr{L}_{q,p,s} C_n\|_{H_{q,p,s}} < \infty$. Then, there exist subsequences $\{C_\kappa\}_\kappa \subset \{C_n\}_n$ and vectors $B_1, B_2 \in \mathbf{X}_c(H_{q,p,s})$ such that $\mathrm{w}-\lim_{\kappa\to\infty} C_\kappa = B_1$ and $\mathrm{w}-\lim_{\kappa\to\infty} \mathscr{L}_{q,p,s} C_\kappa = B_2$. It follows that $\mathrm{s}-\lim_{\kappa\to\infty} \Pi_0 C_\kappa = \Pi_0 B_1$ and $\mathrm{s}-\lim_{\kappa\to\infty} \Pi_0 \mathscr{L}_{q,p,s} C_\kappa = \Pi_0 B_2$ since Π_0 is a finite rank operator, so a compact operator. And besides, we have

$$\mathscr{L}_{q,p,s}\Pi_0 C_\kappa = \frac{\langle p; C_\kappa\rangle}{\langle p, p\rangle} \mathscr{L}_{q,p,s} p \to \frac{\langle p; B_1\rangle}{\langle p; p\rangle} \mathscr{L}_{q,p,s} p$$

as $\kappa\to\infty$. Therefore, we have

$$\mathscr{V}C_\kappa\to-\Pi_0B_2+\frac{\langle p;B_1\rangle}{\langle p;p\rangle}(-\mathscr{L}_{q,p,s}p+\Pi_0\mathscr{L}_{q,p,s}p)$$

as $\kappa\to\infty$. Thus, $\mathscr{V}$ is relatively compact with respect to $\mathscr{L}_{q,p,s}$, so that $\mathscr{L}_{q,p,s}+\mathscr{N}$ is self-adjoint, and $\sigma_{ess}(\mathscr{L}_{q,p,s})=\sigma_{ess}(\mathscr{L}_{q,p,s}+\mathscr{V})$, where $\sigma_{ess}(A)$ denotes the set of all essential spectra of closed operator A. Hence following lemma follows from Lemma 3.1:

Lemma 3.7: The spectrum of projected Liouville operator $\mathscr{L}_1$ has isolated points and their accumulating points only, and

$$\sigma_{ess}(\mathscr{L}_1)\subset\overline{\{\lambda_m-\lambda_n|m,n\in\mathbf{N}^*\}}^{\text{closure}}.$$

Remark 3.1: Under the condition of $\mathscr{L}_{q,p,s}\Pi_0\supset\Pi_0\mathscr{L}_{q,p,s}$, the same statement as Lemma 3.7 was proved in Theorem 4.7 in Ref. 9. However, the method in the proof of Lemma 3.7 tells us that the condition above is superfluous and so strong that the discussion of Mori's theory (see Erratum for Ref. 9). So, arguments in Secs. IV and V in Ref. 9 do not need the condition of $\mathscr{L}_{q,p,s}\Pi_0\supset\Pi_0\mathscr{L}_{q,p,s}$.

Quite generally, the Heisenberg operator $p(t)\overset{\text{def}}{=}e^{i\mathscr{L}_{q,p,s}t}p$ satisfies Mori's memory kernel equation (or Langevin equation)[9,11,12] if $p\in\mathrm{D}(\mathscr{L}_{q,p,s})$:

$$\frac{d}{dt}p(t)=-i\omega_0p(t)-\int_0^t ds\ \phi(t-s)p(s)+I(t),\quad t\in\mathbf{R}\tag{43}$$

on $\mathbf{X}_c(H_{q,p,s})$ (see Sec. IV A in this paper). Mori's memory kernel equation (43) shows the existence of Mori's memory function $\phi(t)$ satisfying the fluctuation-dissipation relation. Namely, Mori's memory function $\phi(t)$ is related to the canonical autocorrelation function of Mori's fluctuation $I(t)$ by the following fluctuation-dissipation relation:

$$\langle p;p\rangle\phi(t)=\langle I(0);I(t)\rangle,\quad t\in\mathbf{R},\tag{44}$$

with orthogonality between p and $I(t)$ $(t\in\mathbf{R})$, i.e.,

$$\langle p;I(t)\rangle=0,\quad t\in\mathbf{R}.\tag{45}$$

We note that (43) and (45) imply that

$$\frac{d}{dt}R_p(t)=-i\omega_0R_p(t)-\int_0^t ds\ \phi(t-s)R_p(s),\quad t\in\mathbf{R}.\tag{46}$$

We define here a function $[\phi](z)$ $(z\in\mathbf{C}$ with $\mathrm{Im}\,z>0)$ by

$$[\phi](z)\overset{\text{def}}{=}\int_0^\infty dt\ e^{itz}\phi(t).$$

For proving our main theorem, we prepare some lemmas.

The following Lemma 3.8 shows important symmetric properties which the Bogoliubov scalar product has:

Lemma 3.8:

(a) For each $m,n\in\mathbf{N}^*$, $|\langle\Phi_{m,n};p\rangle|^2=|\langle\Phi_{n,m};p\rangle|^2$ holds. Namely, $A_{m,n}=A_{n,m}$.

(b) For every $t\in\mathbf{R}$, $R_1(-t)=R_2(t)$, so $R_p(t)=R_1(t)+R_1(-t)$ and $R_1(0)=R_2(0)=R_p(0)/2$.

(c) For every $t\in\mathbf{R}$, $-\dot{R}_1(-t)=\dot{R}_2(t)$, where $\dot{R}_j(t)\overset{\text{def}}{=}dR_j(t)/dt$ $(j=1,2)$. So, $\dot{R}_p(t)=\dot{R}_1(t)-\dot{R}_1(-t)$ and $\dot{R}_p(0)=0$.

(d) For each $k\in\mathbf{N}^*$, $\varepsilon_k=-\eta_k$.

Proof: By (23) and (25), we have

$$\begin{aligned}\beta^{-1/2}Z(\beta)^{-1/2}W_{m,n}^{-1/2}\langle\Phi_{m,n};p\rangle&=(\varphi_m,p\varphi_n)_{q,p,s}\\&=(p\varphi_m,\varphi_n)_{q,p,s}\\&=\overline{(\varphi_n,p\varphi_m)_{q,p,s}}\\&=\beta^{-1/2}Z(\beta)^{-1/2}W_{m,n}^{-1/2}\overline{\langle\Phi_{n,m};p\rangle},\end{aligned}$$

which implies

$$\langle\Phi_{m,n};p\rangle=\overline{\langle\Phi_{n,m};p\rangle},\quad m,n\in\mathbf{N}^*. \tag{47}$$

Therefore, we obtain part (a).

Let $\mathcal{N}(\mathcal{L}_{q,p,s}-\alpha)$ be the space of the all eigenvectors of $\mathcal{L}_{q,p,s}$ with the eigenvalue α. By part (a), if $\langle\Phi_{m^+(k),n^+(k)};p\rangle\neq 0$, then $\langle\Phi_{n^+(k),m^+(k)};p\rangle\neq 0$, and $\varepsilon_k=\lambda_{n^+(k)}-\lambda_{m^+(k)}>0$. So, by the expansion (26) of $R_p(t)$, the point $-\varepsilon_k$ must be a negative pole of $[R_p](z)$, i.e., $-\varepsilon_k\in\mathbf{P}_-^R$. Thus, for any $k\in\mathbf{N}^*$ there exists $\tilde{k}\in\mathbf{N}^*$ such that $-\varepsilon_k=\eta_{\tilde{k}}$, i.e.,

$$-(\lambda_{m^+(k)}-\lambda_{n^+(k)})=\varepsilon_k=-\eta_{\tilde{k}}=\lambda_{m^-(\tilde{k})}-\lambda_{n^-(\tilde{k})}. \tag{48}$$

Conversely, for any $k'\in\mathbf{N}^*$ there exists $\overline{k'}\in\mathbf{N}^*$ such that $-\eta_{k'}=\varepsilon_{\overline{k'}}$, i.e.,

$$-(\lambda_{m^-(k')}-\lambda_{n^-(k')})=\eta_{k'}=-\varepsilon_{\bar{k}'}=\lambda_{m^+(\bar{k}')}-\lambda_{n^+(\bar{k}')}. \tag{49}$$

By assumption (**A.2**), there is a one-to-one correspondence ι between $\mathbf{N}^*$ and $\mathbf{N}^*$, which induces a one-to-one correspondence ϑ between $\mathbf{P}_+^R$ and $\mathbf{P}_-^R$, i.e.,

$$\iota:\mathbf{N}^*\ni k\mapsto\iota(k)\overset{\text{def}}{=}\tilde{k}\in\mathbf{N}^*,\quad \iota^{-1}:\mathbf{N}^*\ni k'\mapsto\iota^{-1}(k')\overset{\text{def}}{=}\bar{k}'\in\mathbf{N}^*,$$

$$\vartheta:\mathbf{P}_+^R\ni\varepsilon_k\mapsto\vartheta(\varepsilon_k)\overset{\text{def}}{=}\eta_{\tilde{k}}=-\varepsilon_k\in\mathbf{P}_-^R,$$

$$\vartheta^{-1}:\mathbf{P}_-^R\ni\eta_{k'}\mapsto\vartheta^{-1}(\eta_{k'})\overset{\text{def}}{=}\varepsilon_{\bar{k}'}=-\eta_{k'}\in\mathbf{P}_+^R.$$

Moreover, by (48), $\Phi_{n^+(k),m^+(k)}$ is an eigenvector of $\mathcal{L}_{q,p,s}$ with the eigenvalue $\lambda_{m^-(\tilde{k})}-\lambda_{n^-(\tilde{k})}=-\eta_{\tilde{k}}$, i.e.,

$$\Phi_{n^+(k),m^+(k)}\in\mathcal{N}(\mathcal{L}_{q,p,s}+\eta_{\iota(k)}). \tag{50}$$

Similarly, by (49) we get

$$\Phi_{n^-(k'),m^-(k')}\in\mathcal{N}(\mathcal{L}_{q,p,s}+\varepsilon_{\iota^{-1}(k')}). \tag{51}$$

We define a map $\Xi:\cup_{\alpha\in\sigma(\mathcal{L}_{q,p,s})}\mathcal{N}(\mathcal{L}_{q,p,s}-\alpha)\to\cup_{\alpha\in\sigma(\mathcal{L}_{q,p,s})}\mathcal{N}(\mathcal{L}_{q,p,s}-\alpha)$ by $\Xi\Phi_{m,n}\overset{\text{def}}{=}\Phi_{n,m}$. By (50) and (51), we have

$$\Xi\Phi_{m^+(k),n^+(k)}\in\mathcal{N}(\mathscr{L}_{q,p,s}+\eta_{\iota(k)}),$$

$$\Xi\Phi_{m^-(\iota(k)),n^-(\iota(k))}\in\mathcal{N}(\mathscr{L}_{q,p,s}+\varepsilon_{\iota^{-1}(\iota(k))})=\mathcal{N}(\mathscr{L}_{q,p,s}+\varepsilon_k).$$

Hence it follows that

$$\Xi\mathcal{N}(\mathscr{L}_{q,p,s}+\varepsilon_k)=\mathcal{N}(\mathscr{L}_{q,p,s}+\eta_{\tilde{k}}),\quad k\in\mathbf{N}^*. \tag{52}$$

In the same way, we get

$$\Xi\mathcal{N}(\mathscr{L}_{q,p,s}+\eta_{k'})=\mathcal{N}(\mathscr{L}_{q,p,s}+\varepsilon_{\bar{k}'}),\quad k'\in\mathbf{N}^*. \tag{53}$$

We have

$$\sum_{\substack{m^-(\tilde{k}),n^-(\tilde{k});\\ \lambda_{m^-(\tilde{k})}-\lambda_{n^-(\tilde{k})}=-\eta_{\tilde{k}}}}|\langle\Phi_{n^+(k),m^+(k)};p\rangle|^2=\sum_{\substack{m^-(\tilde{k}),n^-(\tilde{k});\\ \lambda_{m^-(\tilde{k})}-\lambda_{n^-(\tilde{k})}=-\eta_{\tilde{k}}}}|\langle\Phi_{m^-(\tilde{k}),n^-(\tilde{k})};p\rangle|^2 \tag{54}$$

since ι and ϑ are one-to-one correspondences, equalities (52) and (53) hold, and the pair $(m^-(\tilde{k}),n^-(\tilde{k}))$ in the summation of

$$\sum_{\substack{m^-(\tilde{k}),n^-(\tilde{k});\\ \lambda_{m-(\tilde{k})}-\lambda_{n-(\tilde{k})}=-\eta_{\tilde{k}}}}|\langle\Phi_{n^+(k),m^+(k)};p\rangle|^2$$

runs over all indices of eigenvectors of $\mathscr{L}_{q,p,s}$ with eigenvalue $-\eta_{\tilde{k}}$. So, by using part (a), (48), the one-to-one correspondences, and (54), we have

$$\begin{aligned}
R_1(-t)&=\sum_{k=0}^{\infty}\left(\sum_{\substack{m^+(k),n^+(k);\\ \lambda_{m^+(k)}-\lambda_{n^+(k)}=-\varepsilon_k}}|\langle\Phi_{m^+(k),n^+(k)};p\rangle|^2\exp[-it(\lambda_{m^+(k)}-\lambda_{n^+(k)})]\right)\\
&=\sum_{k=0}^{\infty}\left(\sum_{\substack{m^+(k),n^+(k);\\ \lambda_{m^+(k)}-\lambda_{n^+(k)}=-\varepsilon_k}}|\langle\Phi_{n^+(k),m^+(k)};p\rangle|^2\exp[it\varepsilon_k]\right)\\
&=\sum_{\tilde{k}=0}^{\infty}\left(\sum_{\substack{m^-(\tilde{k}),n^-(\tilde{k});\\ \lambda_{m^-(\tilde{k})}-\lambda_{n^-(\tilde{k})}=-\eta_{\tilde{k}}}}|\langle\Phi_{n^+(k),m^+(k)};p\rangle|^2\right)\exp[-it\eta_{\tilde{k}}]\\
&=\sum_{\tilde{k}=0}^{\infty}\left(\sum_{\substack{m^-(\tilde{k}),n^-(\tilde{k});\\ \lambda_{m^-(\tilde{k})}-\lambda_{n^-(\tilde{k})}=-\eta_{\tilde{k}}}}|\langle\Phi_{m^-(\tilde{k}),n^-(\tilde{k});p}\rangle|^2\right)\exp[-it\eta_{\tilde{k}}]\\
&=\sum_{k=0}^{\infty}\left(\sum_{\substack{m^-(k),n^-(k);\\ \lambda_{m^-(k)}-\lambda_{n^-(k)}=-\eta_k}}|\langle\Phi_{m^-(k),n^-(k)};p\rangle|^2\right)\exp[-it\eta_k]\\
&=\sum_{k=0}^{\infty}\left(\sum_{\substack{m^-(k),n^-(k);\\ \lambda_{m^-(k)}-\lambda_{n^-(k)}=-\eta_k}}|\langle\Phi_{m^-(k),n^-(k)};p\rangle|^2\exp[it(\lambda_{m^-(k)}-\lambda_{n^-(k)})]\right)=R_2(t),
\end{aligned}$$

thus, we have $R_1(-t)=R_2(t)$. Since we know the decomposition of $R_p(t)=R_1(t)+R_2(t)$ in (40) and $R_1(-t)=R_2(t)$, we get $R_p(0)=R_1(0)+R_2(0)=2R_1(0)=2R_2(0)$. So, we obtain part (b). Part (c) depends on part (b).

Part (d) follows from (48), (49) and $\varepsilon_k<\varepsilon_{k+1}$, $\eta_{k+1}<\eta_k$ in (**A.2**). Q.E.D.

Remark 3.2: The fact, $\lim_{z\to 0}[R_p](z)=0$ in the following Lemma 3.9(a) means that we cannot deal with the momentum operator p in our case in the same way as Ref. 9. Furthermore, we cannot apply the theory KMO-Langevin equation[10] to our case.

Lemma 3.9:

(a) $\omega_0=0$ holds, and $\lim_{z\to 0}[R_p](z)=0$.

(b) $[R_p]\,(z)$ can be extended to a meromorphic function on the complex plane.

(c) $[\phi](z)$ can be also extended to a meromorphic function on the complex plane. And the set of all positive zero points of $[R_p]\,(z)$ is equal to the set of all positive poles of $[\phi](z)$. Furthermore, if γ is a pole of $[\phi](z)$, then γ is a pole of the first order of $[\phi](z)$, and besides, there exists $k\in\mathbf{N}^*$ such that $\gamma\in(\varepsilon_k,\,\varepsilon_{k+1})$ or $\gamma\in(-\varepsilon_{k+1},-\varepsilon_k)$, and $-\gamma$ is an eigenvalue of the projected Liouville operator $\mathscr{L}_1$.

Proof: First, we prove part (a). By Lemma 3.8(c), we have $\omega_0\equiv-\langle p;\mathscr{L}_{q,p,s}p\rangle\langle p;p\rangle^{-1}=i\dot{R}_p(0)/R_p(0)=0$, where the dot denotes the derivative with respect to t.

We note here assumption (**A.2**) implies that $\inf\{\varepsilon_k|\langle\Phi_{m^+(k),n^+(k)};p\rangle\neq 0\}=\varepsilon_0>0$. Then, by (38), (39), and (40), we have by Lemma 3.8

$$[R_p](z)=i\sum_{k=0}^{\infty}\left(\sum_{\substack{m^+(k),n^+(k);\\ \lambda_{m^+(k)}-\lambda_{n^+(k)}=-\varepsilon_k}}A_{m^+(k),n^+(k)}\right)\left(\frac{1}{z-\varepsilon_k}+\frac{1}{z+\varepsilon_k}\right),\tag{55}$$

and for any $z\in\mathbf{C}$ with $|z|<\varepsilon_0/2$ and $|z|\leqslant\inf_{k\in\mathbf{N}}(\varepsilon_{k+1}-\varepsilon_k)/2$, we get $\varepsilon_0/2\leqslant|z\pm\varepsilon_0|\leqslant|z\pm\varepsilon_k|$ $(k\in\mathbf{N}^*)$, so we have

$$\sum_{k=0}^{\infty}\left(\sum_{\substack{m^+(k),n^+(k);\\ \lambda_{m^+(k)}-\lambda_{n^+(k)}=-\varepsilon_k}}A_{m^+(k),n^+(k)}\right)\left|\frac{1}{z\pm\varepsilon_k}\right|\leqslant\frac{2}{\varepsilon_0}\sum_{k=0}^{\infty}\sum_{\substack{m^+(k),n^+(k);\\ \lambda_{m^+(k)}-\lambda_{n^+(k)}=-\varepsilon_k}}A_{m^+(k),n^+(k)}.$$

By using the above inequality and Weierstrass' M-test, we obtain

$$\lim_{z\to 0}[R_p](z)=i\sum_{k=0}^{\infty}\left(\sum_{\substack{m^+(k),n^+(k);\\ \lambda_{m^+(k)}-\lambda_{n^+(k)}=-\varepsilon_k}}A_{m^+(k),n^+(k)}\right)\left(-\frac{1}{\varepsilon_k}+\frac{1}{\varepsilon_k}\right)=0,$$

which is a proof of part (a).

Part (b) follows from (55).

The Fourier–Laplace transform of (46) implies that

$$[R_p](z)=\frac{R_p(0)}{i\omega_0-iz+[\phi](z)}.\tag{56}$$

So, by part (a) and (56), we have

$$[\phi](z)=iz+\frac{R_p(0)}{[R_p](z)}.\tag{57}$$

We note that $[\phi](z)$ is meromorphic on the complex plane by (57). Let $-\gamma'$ be a pole of $[\phi](z)$. Then $-\gamma'$ is a zero point of $[R_p]\,(z)$ by (57), so there exists $p\in\mathbf{N}^*$ such that $-\gamma'\in(\varepsilon_k,\varepsilon_{k+1})$ by solving the following equation:

$$0=\frac{1}{i}[R_p](z)=\sum_{k=0}^{\infty}\left(\sum_{\substack{m^+(k),n^+(k);\\ \lambda_{m^+(k)}-\lambda_{n^+(k)}=-\varepsilon_k}} A_{m^+(k),n^+(k)}\right)\left(\frac{\mathrm{Re}\ z-\varepsilon_k}{(\mathrm{Re}\ z-\varepsilon_k)^2+(\mathrm{Im}\ z)^2}\right.$$
$$\left.+\frac{\mathrm{Re}\ z+\varepsilon_k}{(\mathrm{Re}\ z+\varepsilon_k)^2+(\mathrm{Im}\ z)^2}\right)-i(\mathrm{Im}\ z)\sum_{k=0}^{\infty}\left(\sum_{\substack{m^+(k),n^+(k);\\ \lambda_{m^+(k)}-\lambda_{n^+(k)}=-\varepsilon_k}} A_{m^+(k),n^+(k)}\right)$$
$$\times\left(\frac{1}{(\mathrm{Re}\ z-\varepsilon_k)^2+(\mathrm{Im}\ z)^2}+\frac{1}{(\mathrm{Re}\ z+\varepsilon_k)^2+(\mathrm{Im}\ z)^2}\right)$$

by (55), and

$$\lim_{z\to-\gamma'}\frac{1}{i}(z+\gamma')[\phi](z)=\lim_{z\to-\gamma'}\left((z+\gamma')z-iR_p(0)\frac{z+\gamma'}{[R_p](z)-[R_p](-\gamma')}\right)$$
$$=-i\frac{R_p(0)}{\dfrac{d}{dz}[R_p](z)\rceil_{z=-\gamma'}}$$

by (57) because $[R_p](-\gamma')=0$. And besides, by (55), we get

$$\frac{d[R_p](z)}{dz}=-i\sum_{k=0}^{\infty}\left(\sum_{\substack{m^+(k),n^+(k);\\ \lambda_{m^+(k)}-\lambda_{n^+(k)}=-\varepsilon_k}} A_{m^+(k),n^+(k)}\right)\left(\frac{1}{(z-\varepsilon_k)^2}+\frac{1}{(z+\varepsilon_k)^2}\right),$$

which implies

$$i\frac{d[R_p](z)}{dz}\rceil_{z=-\gamma'}=\sum_{k=0}^{\infty}\left(\sum_{\substack{m^+(k),n^+(k);\\ \lambda_{m^+(k)}-\lambda_{n^+(k)}=-\varepsilon_k}} A_{m^+(k),n^+(k)}\right)\left(\frac{1}{(\gamma'+\varepsilon_k)^2}+\frac{1}{(\gamma'-\varepsilon_k)^2}\right)>0.$$

Thus, $-\gamma'$ is a pole of the first order of $[\phi](z)$.

Let $\mathscr{P}^1(d\xi)$ be the spectral measure of $\mathscr{L}_1$:

$$\mathscr{L}_1=\int_{\mathbf{R}}\xi\ d\mathscr{P}^1_\xi.$$

Let $\tilde{p}\overset{\mathrm{def}}{=}(1-\Pi_0)\mathscr{L}_{q,p,s}p$. The equality

$$\left\langle\tilde{p};\frac{1}{-z-\mathscr{L}_1}\tilde{p}\right\rangle=i\langle p;p\rangle[\phi](z)$$

follows from (42), (44) and a simple calculation. And, by well-known fact, we have for every $\delta>0$

$$\mathscr{P}^1((\gamma'-\delta,\gamma'))=\mathrm{s}-\lim_{\delta_2\downarrow0}\mathrm{s}-\lim_{\delta_1\downarrow0}\frac{1}{2\pi i}\int_{\gamma'-\delta+\delta_2}^{\gamma'-\delta_2}\left(\frac{1}{x-i\delta_1-\mathscr{L}_1}-\frac{1}{x+i\delta_1-\mathscr{L}_1}\right)dx.$$

Remember that all poles of $[\phi](z)$ are isolated since $[\phi](z)$ is meromorphic, and the spectra of $\mathscr{L}_1$ consist of isolated points and their accumulating points by Lemma 3.7. Since $-\gamma'$ is a pole of the first order of $[\phi](z)$, the principal part of the Laurent expansion of $[\phi](z)$ at $z=-\gamma'$ has the form of const$\times 1/(z+\gamma')$. So, we have for sufficiently small $\delta>0$

$$\langle \tilde{p};\mathscr{P}^1((\gamma'-\delta,\gamma'))\tilde{p}\rangle = i\langle p;p\rangle \lim_{\delta_2\downarrow 0}\lim_{\delta_1\downarrow 0}\frac{1}{2\pi i}\int_{\gamma'-\delta+\delta_2}^{\gamma'-\delta_2}([\phi](i\delta_1-x)-[\phi](-i\delta_1-x))dx$$

$$=0.$$

Hence it follows that $\mathscr{P}^1((\gamma'-\delta,\gamma'))\tilde{p}=0$. In the same way, we have $\mathscr{P}^1((\gamma',\gamma'+\delta))\tilde{p}=0$. Thus, if $-\gamma'$ is a pole of $[\phi](z)$, then $\gamma'\in\sigma_p(\mathscr{L}_1)$, where $\sigma_p(\mathscr{L}_1)$ is the all point spectra of $\mathscr{L}_1$. Otherwise, suppose here that $-\gamma'$ is a pole of $[\phi_-](z)$ satisfying $\mathscr{P}^1(\{\gamma'\})=0$. By the arguments above, there exists $\delta>0$ such that $\mathscr{P}^1((\gamma'-\delta,\gamma'+\delta)\backslash\{\gamma'\})\tilde{p}=0$. Thus, we get

$$\mathscr{P}^1((\gamma'-\delta,\gamma'+\delta))\tilde{p}=(\mathscr{P}^1(\{\gamma'\})+\mathscr{P}^1((\gamma'-\delta,\gamma'+\delta)\backslash\{\gamma'\}))\tilde{p}=0,$$

which is a contradiction because $-\gamma'$ is a pole of $[\phi](z)$. Therefore, we obtain part (c). Q.E.D.

Lemma 3.10:

(a) $[R_p](-z)=-[R_p](z)$, so if γ is a zero point of $[R_p](z)$, then γ is also a zero point of $[R_p](-z)$.

(b) $[R_p]'(-z)=[R_p]'(z)$.

(c) Let $\{\omega_j\}_{j=1}^{\infty}$ be the set of all positive zero points of $[R_p](z)$. Then,

$$\phi(t)=2R_p(0)\sum_{j=1}^{\infty}\frac{1}{i[R_p]'(\omega_j)}\cos(t\omega_j).$$

So,

$$[\phi](z)=R_p(0)\sum_{j=1}^{\infty}\frac{1}{[R_p]'(\omega_j)}\left(\frac{1}{z-\omega_j}+\frac{1}{z+\omega_j}\right).$$

Proof: By (55), we have

$$[R_p](-z)=-[R_p](z),$$

which is part (a).

Part (b) follows from part (a).

By Lemma 3.9(c), there are eigenvectors $\widetilde{\Phi}_{m,n}$ $(m,n=1,2,\cdots)$ of $\mathscr{L}_1$ such that $\mathscr{L}_1\widetilde{\Phi}_{m,n}=\mu_{m,n}\widetilde{\Phi}_{m,n}$ $(\mu_{m,n}\in\sigma_p(\mathscr{L}_1))$, and $\phi(t)=\langle p;p\rangle^{-1}\Sigma_{m,n=1}^{\infty}|\langle\widetilde{\Phi}_{m,n};(1-\Pi_0)\times\mathscr{L}_{q,p,s}p\rangle|^2\exp[it\mu_{m,n}]$.

Here, let $\{\gamma_j\}_{j=1}^{\infty}$ be the set of all distinct poles of $[\phi](z)$ (i.e., $\gamma_j\neq\gamma_{j'}$ if $j\neq j'$) with $\langle\widetilde{\Phi}_{m,n};(1-\Pi_0)\mathscr{L}_{q,p,s}p\rangle\neq 0$, where, for any $j\in\mathbf{N}$, there exist $m(j),n(j)\in\mathbf{N}$ such that $-\gamma_j=\mu_{m(j),n(j)}$. So,

$$[\phi](z)=\frac{i}{\langle p;p\rangle}\sum_{m,n=1}^{\infty}|\langle\widetilde{\Phi}_{m,n};(1-\Pi_0)\mathscr{L}_{q,p,s}p\rangle|^2\frac{1}{z+\mu_{m,n}}$$

$$=\frac{i}{\langle p;p\rangle}\sum_{j;\ \langle\widetilde{\Phi}_{m(j),n(j)};(1-\Pi_0)\mathscr{L}_{q,p,s}p\rangle\neq 0}$$

$$\times\left(\sum_{\substack{m(j),n(j);\\ -\gamma_j=\mu_{m(j),n(j)}}} |\langle\widetilde{\Phi}_{m(j),n(j)};(1-\Pi_0)\mathscr{L}_{q,p,s}p\rangle|^2\right)\frac{1}{z-\gamma_j}. \tag{58}$$

Thus, we obtain by (57) and (58)

$$\begin{aligned}\sum_{\substack{m(j),n(j);\\ \mu_{m(j),n(j)}=-\gamma_j}} |\langle\widetilde{\Phi}_{m(j),n(j)};(1-\Pi_0)\mathscr{L}_{q,p,s}p\rangle|^2 &= \lim_{z\to\gamma_j}\frac{1}{i}(z-\gamma_j)[\phi](z)\langle p;p\rangle \\ &= \frac{1}{i}(R_p(0))^2\lim_{z\to\gamma_j}\frac{z-\gamma_j}{[R_p](z)-[R_p](\gamma_j)} \\ &= (R_p(0))^2\frac{1}{i[R_p]'(\gamma_j)}>0. \end{aligned}\tag{59}$$

Here, we used the fact that $[R_p](\gamma_j)=0$ by Lemma 3.9(c). By (58), we have

$$\phi(t)=\frac{1}{R_p(0)}\sum_{j=1}^{\infty}\left(\sum_{\substack{m(j),n(j);\\ \mu_{m(j),n(j)}=-\gamma_j}} |\langle\widetilde{\Phi}_{m(j),n(j)};(1-\Pi_0)\mathscr{L}_{q,p,s}p\rangle|^2\right)e^{-it\gamma_j}.$$

Therefore, by (59), we obtain

$$\phi(t)=R_p(0)\sum_{j=1}^{\infty}\frac{1}{i[R_p]'(\gamma_j)}e^{-it\gamma_j}. \tag{60}$$

By part (b), we have

$$\frac{1}{[R_p]'(\omega_j)}=\frac{1}{[R_p]'(-\omega_j)}. \tag{61}$$

And besides, by Lemma 3.9(c) and part (a), the set of all poles of $[\phi](z)$ is given by $\{\pm\omega_j\}_{j=1}^{\infty}$. Therefore, we obtain part (c) from (60) and (61). Q.E.D.

B. Proof of the main theorem

We define $\kappa_\tau(t)$ by

$$\kappa_\tau(t)\underset{=}{\text{def}} m\phi(t)\chi_{[0,\tau]}(t), \tag{62}$$

where $\chi_{[0,\tau]}(t)$ denotes the characteristic function of $[0,\tau]$.

The quantum Langevin equation (17) follows from (43), Lemma 3.9(a) and Lemma 3.10(c).

For $t>0$, it is evident that $lim_{\tau\uparrow\infty}\kappa_\tau(t)=m\phi(t)$, which implies (18).

The fluctuation-dissipation relation follows from (44) and (45).

The Fourier–Laplace transform of (46) implies (20).

Concerning the proof of (21), first we get

$$S_I(t)=\int_{-\infty}^{\infty}e^{it\omega}\beta E_\beta(\omega)\Delta_I^{\text{can}}(d\omega)$$

by the definition of symmetrized autocorrelation function (10), and

$$\Delta_I^{\mathrm{can}}(d\omega)=\sum_{j=1}^{\infty} m_j\omega_j^2\left(\frac{\delta_{\omega_j}(d\omega)+\delta_{-\omega_j}(d\omega)}{2}\right)$$

by (19). Thus, since $E_\beta(\omega)=E_\beta(-\omega)$, we have

$$S_I(t)=\frac{1}{2}\sum_{j=1}^{\infty} m_j\omega_j^2\beta(E_\beta(\omega_j)e^{it\omega_j}+E_\beta(-\omega_j)e^{-it\omega_j})=\sum_{j=1}^{\infty} m_j\omega_j^2\beta E_\beta(\omega_j)\cos(\omega_j t),$$

which implies (21).

The last equality (22) depends on (19).

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APPENDIX

1. Mori's memory kernel equation

In this Appendix, we recall briefly Mori's memory kernel equation.[11,12] Let $\mathbf{X}$ be a Hilbert space with an inner product $(,)_{\mathbf{X}}$, $\mathscr{L}$ a self-adjoint operator in $\mathbf{X}$ with domain $\mathrm{D}(\mathscr{L})$, and A a non-zero element in $\mathrm{D}(\mathscr{L})$, where the inner product $(,)_{\mathbf{X}}$ is linear in the right vector.

We consider a stationary curve $\{A(t)|t\in\mathbf{R}\}$ defined by $A(t)\overset{\mathrm{def}}{=}e^{it\mathscr{L}}A, t\in\mathbf{R}$, and the autocorrelation function R_A of A given by $R_A(t)\overset{\mathrm{def}}{=}(A(0),A(t))_{\mathbf{X}}$.

Let $\mathbf{X}_0$ be the closed subspace generated by A, and Π_0 and $\mathbf{X}_1$ the orthogonal projection operator on $\mathbf{X}_0$ and the complementary subspace of $\mathbf{X}_0$ in $\mathbf{X}$, respectively. Then we define a linear operator $\mathscr{L}_1$ on the Hilbert space $\mathbf{X}_1$ by

$$\mathrm{D}(\mathscr{L}_1)\overset{\mathrm{def}}{=}(1-\Pi_0)\mathbf{X}\cap\mathrm{D}(\mathscr{L})$$

$$\mathscr{L}_1 x\overset{\mathrm{def}}{=}(1-\Pi_0)\mathscr{L}x,\quad x\in\mathrm{D}(\mathscr{L}_1)\ .$$

From this, we note that $\mathscr{L}_1$ is a self-adjoint operator acting in the Hilbert space $\mathbf{X}_1$.[10,11] And we define Mori's frequency ω_A, fluctuation $I_A(t), t\in\mathbf{R}$ and memory function ϕ_A by

$$\omega_A\overset{\mathrm{def}}{=}-(A(0),\mathscr{L}A(0))_{\mathbf{X}}(A(0),A(0))_{\mathbf{X}}^{-1}.\quad I_A(t)\overset{\mathrm{def}}{=}ie^{it\mathscr{L}_1}(1-\Pi_0)\mathscr{L}A,\quad t\in\mathbf{R},$$

$$\phi_A(t)\overset{\mathrm{def}}{=}(I_A(0),I_A(t))_{\mathbf{X}}(A(0),A(0))_{\mathbf{X}}^{-1},\quad t\in\mathbf{R}. \tag{A1}$$

We note here that we change the original definition of Mori's frequency into (A1) to discuss our argument. Then we have the following theorem.

Theorem A.1 (Refs. 10–12):

(a) *For all* $t\in\mathbf{R}$,

$$\frac{d}{dt}R_A(t) = -i\omega_A R_A(t) - \int_0^t ds\ \phi_A(t-s)R_A(s).$$

(b) *For all* $z \in \mathbf{C}^+ \underset{=}{\text{def}} \{z \in \mathbf{C} | \text{Im } z > 0\}$,

$$\int_0^\infty dt\ \ e^{itz}R_A(t) = R_A(0)\frac{1}{i\omega_A - iz + \int_0^\infty dt\ e^{itz}\phi_A(t)}.$$

(c) *For all* $t \in \mathbf{R}$,

$$\frac{d}{dt}A(t) = -i\omega_A A(t) - \int_0^t ds\ \phi_A(t-s)A(s) + I_A(t). \tag{A2}$$

Equation (A2) is *Mori's memory kernel equation*, or *Mori's Langevin equation*.

2. An example of the Hamiltonian and the momentum operator satisfying the assumptions

Let

$$\overline{\mathscr{D}_{q,p,s}} \underset{=}{\text{def}} \{A \in \mathbf{T}(H_{q,p,s}) | H_{q,p,s}A, AH_{q,p,s} \lceil \mathbf{D}_{q,p,s} \in \mathbf{T}(H_{q,p,s})\}.$$

Then, for every $A \in \overline{\mathscr{D}_{q,p,s}}$, by (32)

$$\begin{aligned}
\sum_{m,n=0}^{\infty} (\lambda_m - \lambda_n)^2 |\langle \Phi_{m,n}; A\rangle|^2 &\leqslant 2\sum_{m,n=0}^{\infty} (\lambda_m^2 + \lambda_n^2)|\langle \Phi_{m,n}; A\rangle|^2 \\
&= 2\sum_{m,n=0}^{\infty} (\lambda_m^2 + \lambda_n^2)\frac{|(\varphi_m, A\varphi_n)_{q,p,s}|^2}{\beta Z(\beta) W_{m,n}} \\
&= 2\sum_{m,n=0}^{\infty} \frac{1}{\beta Z(\beta) W_{m,n}}(|(\varphi_m, H_{q,p,s}A\varphi_n)_{q,p,s}|^2 \\
&\quad + |(\varphi_m, AH_{q,p,s}\varphi_n)_{q,p,s}|^2) \\
&= 2(\|H_{q,p,s}A\|^2_{H_{q,p,s}} + \|AH_{q,p,s}\|^2_{H_{q,p,s}}) < \infty.
\end{aligned} \tag{A3}$$

Therefore, we have

$$\mathscr{D}_{q,p,s} \subset \overline{\mathscr{D}_{q,p,s}} \subset \mathrm{D}(\mathscr{L}_{q,p,s}). \tag{A4}$$

Next, we prepare basic tools from Ref. 21. Let $\mathscr{F}_b^\infty$ be the symmetric Fock space, which is the Hilbert space complete of the symmetric tensor algebra over $L^2(\mathbf{R})$:

$$\mathscr{F}_b^\infty \underset{=}{\text{def}} \oplus_{n=0}^\infty \mathscr{F}_n,$$

where $\mathscr{F}_n$ is the space of n noninteracting bosons:

$$\mathscr{F}_0 \stackrel{\text{def}}{=} \mathbf{C},$$

$$\mathscr{F}_n \stackrel{\text{def}}{=} \underbrace{L^2(\mathbf{R})\otimes_s L^2(\mathbf{R})\otimes_s \cdots \otimes_s L^2(\mathbf{R})}_{n\text{factors}}, \quad n=1,2,\ldots .$$

We use the standard annihilation and creation operators $b(k)$ and $b^+(k)$, defined by

$$(b(k)\psi)_{n-1}(k_1,\ldots,k_{n-1}) \stackrel{\text{def}}{=} n^{1/2}\psi_n(k,k_1,\ldots,k_{n-1})$$

on the dense subset of vectors $\psi \equiv \{\psi_0,\psi_1,\ldots\} \in \mathscr{F}_b^\infty$ with $\psi_n=0$ for large n. And

$$(b^+(k)\psi)_{n+1}(k_1,\ldots,k_{n+1}) \stackrel{\text{def}}{=} (n+1)^{-1/2}\sum_{j=1}^{n+1} \delta(k-k_j)\psi_n(k_1,\ldots,\widehat{k_j},\ldots,k_{n+1}).$$

Here $\widehat{k_j}$ means that k_j is omitted.

For finite volume $V>0$, we define a set of lattice points $\mathbf{\Gamma}_V$ by

$$\mathbf{\Gamma}_V \stackrel{\text{def}}{=} \left\{ k \mid k=\frac{2\pi n}{V}, n=0,\pm 1,\pm 2,\ldots \right\}. \tag{A5}$$

We can define the Fock space $\mathscr{F}_b^V$ for volume V as

$$\mathscr{F}_b{}^V \stackrel{\text{def}}{=} \mathbf{C}\oplus l^2(\mathbf{\Gamma}_V)\oplus(l^2(\mathbf{\Gamma}_V)\otimes_s l^2(\mathbf{\Gamma}_\mathbf{V}))\oplus(l^2(\mathbf{\Gamma}_\mathbf{V})\otimes_s l^2(\mathbf{\Gamma}_\mathbf{V})\otimes_s l^2(\mathbf{\Gamma}_\mathbf{V}))\ldots . \tag{A6}$$

Then we can identify $\mathscr{F}_b^V$ with the subspace of $\mathscr{F}_b^\infty$ consisting of piecewise constant functions which are constant on each cube of volume $(2\pi/V)^j$ centered about a lattice point $(k_1,\ldots,k_j)\in \mathbf{\Gamma}_\mathbf{V}\times\mathbf{\Gamma}_\mathbf{V}\ldots\times\mathbf{\Gamma}_\mathbf{V}$.

The periodic annihilation and creation operators $b_V(k)$ and $b_V^+(k)$ are defined by

$$b_V(k) \stackrel{\text{def}}{=} \left(\frac{V}{2\pi}\right)^{1/2}\int_{-\pi/V}^{\pi/V} b(k+l)dl, \tag{A7}$$

$$b_V^+(k) \stackrel{\text{def}}{=} \left(\frac{V}{2\pi}\right)^{1/2}\int_{-\pi/V}^{\pi/V} b^+(k+l)dl, \tag{A8}$$

and can be extended from $\mathscr{F}_b^V$ to $\mathscr{F}_b^\infty$. We regard $\mathscr{F}_b^V$ as $\mathscr{F}_{q,p,s}$.

We define annihilation and creation operators of a quantum harmonic oscillator by

$$a \stackrel{\text{def}}{=} b_V(0), \quad a^+ \stackrel{\text{def}}{=} b_V^+(0),$$

furthermore annihilation and creation operators of bosons by

$$b_k \stackrel{\text{def}}{=} b_V(k), \quad b_k^+ \stackrel{\text{def}}{=} b_V^+(k), \quad k\in\mathbf{\Gamma}_V\backslash\{0\}.$$

And let $\mathscr{F}_{q,p,s}\equiv\mathscr{F}_b^V$.

Let w_0 be a positive number, and $\{w_k\}_{k\in\mathbf{\Gamma}_V\setminus\{0\}}$ a sequence of positive numbers with $\Sigma_{k\in\mathbf{\Gamma}_V\setminus\{0\}}w_k^{-2}<\infty$. We give a free Hamiltonian H_0 by

$$H_0 \overset{\text{def}}{=} w_0 a^+ a + \sum_{k\in\mathbf{\Gamma}_V\setminus\{0\}} w_k b_k^+ b_k .$$

Let H_I be a self-adjoint operator satisfying

$$\left.\begin{aligned} H_I &\geqslant 0, \\ H_{q,p,s} = H_0 + H_I &\text{ is essentially self}-\text{adjoint} \\ &\text{on a core } C^\infty(H_0)\cap \mathrm{D}(H_I), \\ \mathrm{D}(p) &\supset \mathrm{D}(H_I), \\ [H_I, p] &= 0. \end{aligned}\right\} \tag{A9}$$

For instance, for $n\in\mathbf{N}$, let

$$:\phi^{2n}: \equiv \lambda\int_{-\infty}^{\infty} :\phi_V(x)^{2n}: g(x)\,dx \lceil C^\infty\left(w_0 a^+ a + \sum_{k\in\mathbf{\Gamma}_V\setminus\{0\}} w_k b_k^+ b_k\right),$$

where $\lambda>0$, g is a positive function in Schwartz's class, and

$$\phi_V(x) \overset{\text{def}}{=} \frac{1}{(2V)^{1/2}} \sum_{k\in\mathbf{\Gamma}_V\setminus\{0\}} e^{-ikx}(b_k^+ + b_{-k}) w_k^{-1/2}.$$

It is well known that for $\mathscr{F}_b^V$ there exist a measure space $\mathbf{Q}$ and the Gaussian measure $d\mu_0$ such that $\mathscr{F}_b^V$ is unitary equivalent to $L^2(\mathbf{Q},d\mu_0)$. From now on, we identify $\mathscr{F}_b^V$, so $\mathscr{F}_{q,p,s}$ with $L^2(\mathbf{Q},d\mu_0)$. Let P_1 and P_2 be positive polynomials of x and $x_1,x_2,\ldots,x_n$, respectively, satisfying $P_1(p)P_2(:\phi^2:,:\phi^4:,\ldots,:\phi^2:)\in L^2(\mathbf{Q},d\mu_0)$. Then, by Theorem X.59 in Ref. 22, $H_0+P_1(p)P_2(:\phi^2:,:\phi^4:,\ldots,:\phi^2:)$ is essentially self-adjoint on $C^\infty(H_0)\cap\mathrm{D}(H_1)$ and positive. This $P_1(p)P_2(:\phi^2:,:\phi^4:,\ldots,:\phi^{2n}:)$ is an example of H_I with (71).

More concrete example is given as follows: Let

$$H_{0,I} \overset{\text{def}}{=} \lambda\int_{-\infty}^{\infty} :\phi_V(x)^4: g(x)\,dx \lceil C^\infty\left(w_0 a^+ a + \sum_{k\in\mathbf{\Gamma}_V\setminus\{0\}} w_k b_k^+ b_k\right),$$

where $\lambda>0$, g is a positive function in Schwartz's class. Since $H_{0,I}$ is extended to self-adjoint operator by claim in p.176 of Ref. 23 and Theorem VIII.33 in Ref. 24. And, we can represent p using projection valued measure E_ξ as

$$p = \int_{-\infty}^{\infty} \xi\, dE_\xi .$$

We define p_K $(K>0)$ by

$$p_K \equiv \int_{-K}^{K} \xi\, dE_\xi .$$

Let $H_{b,I}$ be a bounded symmetric operator acting in

$$\mathbf{L.h}\left[\left\{\frac{1}{\sqrt{n_{k_1}!}\cdots\sqrt{n_{k_N}!}}(b_{k_1}^{+})^{n_{k_1}}\cdots(b_{k_N}^{+})^{n_{k_N}}\Omega_0 | n_{k_1},\ldots,n_{k_N}\in\mathbf{N}^*;k_1,\ldots,k_N\in\mathbf{\Gamma}_V;N\in\mathbf{N}^*\right\}\right].$$

Here Ω_0 denotes the Fock vacuum. Then, it is clear that $H_{0,I}+p_K H_{b,I}$ is an example of H_I with (A9). Here we note that $[p_K, H_{b,I}]=0$.

For H_I with (A9), we obtain the following proposition:

Proposition B.1.

(a) $e^{-tH_{q,p,s}}$ is trace class for every $t>0$.

(b) $p\in \mathrm{D}(\mathscr{L}_{q,p,s})$.

Remark B.1: By this proposition, we know that $H_{q,p,s}$ and p argued in this subsection satisfy our assumptions (**A.1**) and (**A.3**).

Proof of Proposition B.1: First part (a) follows from Golden–Thompson inequality Corollary on p.320 in Ref. 25.

We note that

$$[H_0,q]=-iw_0p,\quad [H_0,p]=iw_0q, \tag{A10}$$

and there exist positive constants $c_n(q)$ and $c_n(p)$ $(n=1,2...)$ such that

$$\|q^n x\|\leqslant c_n(q)\|(H_0+I)^n x\|,\quad \|p^n x\|\leqslant c_n(p)\|(H_0+I)^n x\|, \tag{A11}$$

for $x\in C^\infty(H_0)$.

Here we note that by Proposition 1 in Ref. 26

$$\|H_0x\|+\|H_Ix\|\leqslant \mathrm{const}_1(\|H_{q,p,s}x\|+\|x\|) \tag{A12}$$

for all $x\in \mathrm{D}(H_0+H_I)$.

By using inequalities (A11), (A12), and the facts that $D(p)\supset C^\infty(H_0)\cap \mathrm{D}(H_I)$; $C^\infty(H_0)\cap \mathrm{D}(H_I)$ is a core for $H_{q,p,s}$; and p is closed, we have $D(p)=\mathrm{D}(p^*)\supset \mathrm{D}(H_{q,p,s})$, which implies that p satisfies (**T.1**), and $\mathrm{D}(pH_{q,p,s})\supset \mathbf{D}_{q,p,s}$. In the same way, we get $\mathrm{D}(q)\supset \mathbf{D}_{q,p,s}$. Since $H_{q,p,s}p=pH_{q,p,s}+iw_0q$, we have $\mathrm{D}(H_{q,p,s}p)=\mathrm{D}(pH_{q,p,s}+iw_0q)=\mathrm{D}(pH_{q,p,s})\cap \mathrm{D}(q)\supset \mathbf{D}_{q,p,s}$. Therefore, we can show that $pH_{q,p,s}$ and $H_{q,p,s}p$ satisfy (**T.1**).

Here we put for $t>0$,

$$A \overset{\mathrm{def}}{=} tH_0,$$

$$B \overset{\mathrm{def}}{=} tH_I,$$

$$C \overset{\mathrm{def}}{=} \|e^{-A/2}e^{-B}e^{-A/2}\|\leqslant e^{-t\inf\sigma(H_I)}\|e^{-A}\|.$$

Remember (A11) and (A12). In the same way as the proof of Theorem X.57 (Segal's lemma) in Ref. 25, since $(e^{-2^{-(n+1)}A}e^{-2^{-n}B}e^{-2^{-(n+1)}A})^{2^n}$ converges to $e^{-(A+B)}$ as $n\to\infty$, and $\|e^{-2^{-(n+1)}A}e^{-2^{-n}B}e^{-2^{-(n+1)}A}\|\leqslant C^{2^{-n}}$, we have for $x\in \mathrm{D}(p)$

$$\|e^{-(A+B)}px\|=\lim_{n\to\infty}\|(e^{-2^{-(n+1)}A}e^{-2^{-n}B}e^{-2^{-(n+1)}A})^{2^n}px\|$$

$$\leqslant c_1(p)\lim_{n\to\infty}C^{1-2^{-n}}\|e^{-A}\left(\frac{A}{t}+I\right)\|\|e^{(1-2^{-(n+1)})A}\|\|x\|$$

$$\leqslant c_1(p)e^{-t\inf\sigma(H_I)}\lim_{n\to\infty}C^{-2^{-n}}\|e^{-A}\left(\frac{A}{t}+I\right)\|\|e^{(-2^{-(n+1)})A}\|\|x\|$$

$$=c_1(p)e^{-t\inf\sigma(H_I)}\lim_{n\to\infty}C^{-2^{-n}}e^{(-2^{-(n+1)})t\inf\sigma(H_I)}\|e^{-A}\left(\frac{A}{t}+I\right)\|\|x\|$$

$$=c_1(p)e^{-t\inf\sigma(H_I)}\|e^{-A}\left(\frac{A}{t}+I\right)\|\|x\|.$$

Therefore, $e^{-tH_{q,p,s}}p$ is bounded, and similarly, $e^{-tH_{q,p,s}}q$ is also bounded. So, it follows that $e^{-tH_{q,p,s}}p$ and $e^{-tH_{q,p,s}}q$ are trace class from part (a) and boundedness of $e^{-tH_{q,p,s}}p$ and $e^{-tH_{q,p,s}}q$. Taking adjoint of them, we know $pe^{-tH_{q,p,s}}$ and $qe^{-tH_{q,p,s}}$ are also trace class. So, $pH_{q,p,s}e^{-tH_{q,p,s}}=pe^{-tH_{q,p,s}/2}H_{q,p,s}e^{-tH_{q,p,s}/2}$ is trace class. Furthermore, since $pH_{q,p,s}=H_{q,p,s}p-iw_0q$,

$$\begin{aligned}e^{-tH_{q,p,s}}pH_{q,p,s}&=e^{-tH_{q,p,s}}H_{q,p,s}p-iw_0e^{-tH_{q,p,s}}q\\&=e^{-tH_{q,p,s}/2}H_{q,p,s}e^{-tH_{q,p,s}/2}p-iw_0e^{-tH_{q,p,s}}q\end{aligned}$$

is trace class. In the same way, $e^{-tH_{q,p,s}}H_{q,p,s}p=e^{-tH_{q,p,s}/2}H_{q,p,s}e^{-tH_{q,p,s}/2}p$ is trace class, and since $H_{q,p,s}p=pH_{q,p,s}+iw_0q$,

$$H_{q,p,s}pe^{-tH_{q,p,s}}=pH_{q,p,s}e^{-tH_{q,p,s}}+iw_0qe^{-tH_{q,p,s}}=pe^{-tH_{q,p,s}/2}H_{q,p,s}e^{-tH_{q,p,s}/2}+iw_0qe^{-tH_{q,p,s}}$$

is also trace class. Thus, $p, pH_{q,p,s}$, and $H_{q,p,s}p$ satisfy (**T.2**).

Therefore, we obtain that $p\in\overline{\mathscr{D}_{q,p,s}}$. So, by (66), $p\in\mathrm{D}(\mathscr{S}_{q,p,s})$. Q.E.D.

When condition (**A.2**) and (**A.4**) do not hold, we consider the following smeared momentum operator. We can expand p as

$$p=\sum_{m,n}\langle\Phi_{m,n};p\rangle\Phi_{m,n}$$

in $\mathbf{X}_c(H_{q,p,s})$.

Definition B.1: By an observation, select ε_p and η_p with (**A.2**). Then, for p, we define the *smeared momentum operator* p^{sm} by

$$\begin{aligned}p^{sm}&\equiv p^{sm}(\varepsilon_p,\eta_p;p\in\mathbf{N}^*)\\&\overset{\mathrm{def}}{=}\sum_{k=0}^{\infty}\left(\sum_{\substack{m^+(k),n^+(k);\\ \lambda_{m^+(k)}-\lambda_{n^+(k)}=-\varepsilon_k}}\langle\Phi_{m^+(k),n^+(k)};p\rangle_{H_{q,p,s}}\right)\Phi_{m^+(k),n^+(k)}\\&\quad+\sum_{k=0}^{\infty}\left(\sum_{\substack{m^-(k),n^-(k);\\ \lambda_{m^-(k)}-\lambda_{n^-(k)}=-\eta_k}}\langle\Phi_{m^-(k),n^-(k)};p\rangle_{H_{q,p,s}}\right)\Phi_{m^-(k),n^-(k)}.\end{aligned}$$

It is evident that p^{sm} satisfies (**A.4**) automatically.

The Hamiltonian $H_{q,p,s}$ and smeared momentum operator p^{sm} which are argued in this subsection satisfy our assumptions (**A.1**)-(**A.4**), and more complicated model than the IO model is included.

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Solution to three-magnon problem for $S=1/2$ periodic quantum spin chains with elliptic exchange

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The method of solving the three-particle quantum elliptic Calogero–Moser problem is applied to the description of three-magnon wave functions for the $S=1/2$ quantum Heisenberg chains with the exchange interaction given by the Weierstrass ϱ function. The Bethe-like algebraic equations for the three-magnon case are presented in the explicit form. © *1996 American Institute of Physics.* [S0022-2488(96)02101-X]

I. INTRODUCTION

Despite the remarkable progress in studying integrable models of field theory and statistical mechanics, the universal method of constructing their solutions in the quantum case is not found. The well-known techniques of the coordinate Bethe ansatz and its algebraic version based on the Yang–Baxter equation are still not applicable to 1-D problems proposed a long time ago within the framework of the classical Lax representation and proved also to be quantum integrable.[2,3] They can be interpreted as the systems of particles on a torus $T_{\omega_1,\omega_2}=\mathbf{C}/\mathbf{Z}\omega_1+\mathbf{Z}\omega_2, \mathcal{I}m(\omega_1\omega_2^{-1})\neq 0$, with the quantum Hamiltonian

$$H_p^{(M)}=-\frac{1}{2}\sum_{j=1}^{M}\left(\frac{\partial}{\partial x_j}\right)^2+n(n-1)\sum_{j<l}^{M}\wp(x_j-x_l), \tag{1}$$

where $\wp(x)$ is the elliptic Weierstrass function with periods ω_1 and ω_2,

$$\begin{aligned}\wp(x)&=x^{-2}+\sum_{m\in\mathbf{Z}^2,m_1^2+m_2^2\neq 0}[(x+m_1\omega_1+m_2\omega_2)^{-2}-(m_1\omega_1+m_2\omega_2)^{-2}]\\&=\left(\frac{\pi}{\omega_2}\right)^2\left(-\frac{1}{3}+\sum_{m\in\mathbf{Z}}\left[\sin\left(\pi\,\frac{x-m\omega_1}{\omega_2}\right)\right]^{-2}-2\sum_{m\in\mathbf{Z}_+}\left[\sin\frac{m\omega_1}{\omega_2}\,\pi\right]^{-2}\right).\end{aligned} \tag{2}$$

Moreover, the superintegrability of these systems at $n\in\mathbf{Z}_+$ was conjectured,[4,5] i.e., at least as $\omega_1\to\infty$ the ring of well-defined operators commuting with $H_p^{(M)}$ is larger than it is required for classical integrability in the Liouville sense. Although a number of results have been obtained in various degenerate cases of $\omega_1,\omega_2\to 0,\infty$,[2,4–8] any explicit eigenvectors of $H_p^{(M)}$ at arbitrary ω_1, ω_2 and $M>2$ have not been found.

Recently, several approaches have been proposed for explaining the phenomenon of the integrability of elliptic many-body systems and describing the spectrum of the commutative family of differential operators which includes (1). One is based on the relationship of integrable many-body problems to the theory of semisimple and affine Lie groups[9] and the use of the quantum Hamiltonian reduction described first in Ref. 10. It results in the interpretation of the eigenfunctions of the trigonometric analog of (1) as traces of the operators which intertwine some representations of gl_M.[11] The generalization of the treatment to affine Lie groups leads to the parabolic differential

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equation which is viewed as a reduction of the KZB equations.[12] In the case of $M=2$, it has been proved in Ref. 12 that the asymptotics of the integral representations of its solutions at critical level gives the eigenfunctions of (1) at $n\in\mathbf{Z}_+$. It has been found also that there is the natural extension of the systems (1) to the relativistic Hamiltonians[13] with the symmetry related to the gauged WZW theory and quantum groups.[14]

The important results for the spectrum and eigenfunctions of (1) at $M\leqslant 3$, $n\in\mathbf{R}_+$, have been obtained within the framework of the general scheme of the separation of variables.[15]

The promising way of embedding the systems (1) into the Yang–Baxter structures is related to the construction of the representations of quadratic Sklyanin algebra with Belavin's elliptic R matrix by means of difference operators[16] and further reduction to differential ones. Being most general at the present time, this approach is still not realized completely in writing down the explicit expressions for the solutions of the eigenvalue problem for the operator (1).

In this paper, we address mainly to the lattice analogs of $H_p^{(M)}$ which are the Hamiltonians of interacting $S=1/2$ quantum spins,

$$H_s=-\frac{1}{2}\sum_{j\neq l}^{N}\wp(j-l)\left(\frac{\vec{\sigma}_j\vec{\sigma}_l-1}{2}\right). \tag{3}$$

Here $\{\sigma_j\}$ are the usual Pauli matrices labelled by the indices of lattice sites and $\wp(x)$ is defined on the torus $T_{N,\omega}$, i.e., the real period of $\wp$ coincides with the total number of spins N. The real part of ω has to vanish if H_s is self-adjoint. The corresponding lattice Schrödinger equation reads

$$\begin{aligned}L(n_1\cdots n_M)&=\sum_{\beta=1}^{M}\sum_{s\neq n_1\cdots n_M}^{N}\wp(n_\beta-s)\psi^{(M)}(n_1\cdots n_{\beta-1},s,n_{\beta+1}\cdots n_M)\\&=-\left[\sum_{\alpha\neq\beta}^{M}\wp(n_\alpha-n_\beta)+E_M-ME_0\right]\psi^{(M)}(n_1\cdots n_M),\end{aligned} \tag{4}$$

where $E_0=\Sigma_{j=1}^{N-1}\wp(j)$ and $n_1\cdots n_M$ denote the positions of spins turned over the state in which all spins are aligned identically. The M-magnon wave function $\psi^{(M)}$ must be symmetric in all its arguments.

The limits of $\mathcal{I}m\,\omega\to 0,\infty$ have been investigated by Bethe[17] and Haldane.[18] In these limits, the underlying symmetry of the model has been established by explicit construction of transfer matrices which satisfy Yang–Baxter relations.[19,20] The eigenvectors of H_s for infinite spin chains at arbitrary values of $\mathcal{I}m\,\omega$ have been completely described recently.[21]

However, in the general case of finite N and $\omega\neq 0,\infty$, which is of more interest for thermodynamics, the explicit solutions have been indicated only for the simplest two-magnon sector.[22] One of possible ways of extension of these results to $M>2$ is in finding the lattice analogs of the powerful algebraic approaches to continuous elliptic many-particle problems proposed in Refs. 9–12. However, they do not provide useful expressions for the eigenfunctions of (1) and (3) at present stage of the development. Hence the search for more simple methods is worth a trial.

In the present paper we would like to show that the eigenfunctions of the particle and spin Hamiltonians (1) and (3) can be found explicitly also for $M=3$ by using its analytic properties without any appeals to the concept of superintegrability.

It is worthwhile to outline the situation at $M=2$, $n=2$ for convenience and introduction of some basic notation. As for the two-particle interaction, the problem reduces to the well-known Lamè equation,

$$\left[-\frac{1}{2}\left(\frac{d}{dx}\right)^2+\wp(x)\right]\varphi=E\varphi. \tag{5}$$

The solutions to (4) were given by Hermite[23] more than a century ago,

$$\varphi(x)=\exp(ikx)\,\frac{\sigma(x+\gamma)}{\sigma(x)}, \tag{6}$$

where k and E are easily expressed through an arbitrary phase γ,

$$ik=-\zeta(\gamma), \quad E=-\tfrac{1}{2}\wp(\gamma).$$

Here $\zeta(x)$ and $\sigma(x)$ are the Weierstrass functions related to $\wp(x)$ as follows:

$$\frac{d\zeta(x)}{dx}=-\wp(x), \ \lim_{x\to 0}[\zeta(x)-x^{-1}]=0; \quad \frac{d\,\ln\,\sigma(x)}{dx}=\zeta(x), \ \lim_{x\to 0}\,\sigma(x)x^{-1}=1. \tag{7}$$

Unlike $\wp$, zeta and sigma are not periodic. Nevertheless both these functions can be treated on the torus T_{ω_1,ω_2} due to their quasiperiodicity,

$$\zeta(x+\omega_j)=\zeta(x)+\eta_j, \quad \sigma(x+\omega_j)=\sigma(x)\exp\left[\pi i+\eta_j\left(x+\frac{\omega_j}{2}\right)\right], \quad j=1,2, \tag{8}$$

where $\eta_1=2\zeta(\omega_1/2)$ and $\eta_2=2\zeta(\omega_2/2)$ obey the Legendre relation

$$\eta_1\omega_2-\eta_2\omega_1=2\pi i. \tag{9}$$

As it follows from (2.7), the only simple pole of $\zeta(x)$ and zero of $\sigma(x)$ on T_{ω_1,ω_2} are located at $x=0$. The Hermite result (6) is one of the consequences of the addition theorem for $\wp(x)$ and $\zeta(x)$:

$$\wp(x)+\wp(y)+\wp(x+y)=[\zeta(x)+\zeta(y)-\zeta(x+y)]^2, \quad x,y\in\mathbf{C}. \tag{10}$$

The two-magnon wave functions, as it was pointed in Ref. 22, also have the Hermite form (6), but the connection between γ and other parameters is not so simple. It will be shown in two subsequent sections that the analogy of particle and spin dynamics still takes place in the more complicated $M=3$ problem.

II. THE SOLUTION TO THREE-PARTICLE PROBLEM AT $n=2$

Let us consider a three-particle equation of Lamè type,

$$H_p^{(3)}\varphi=\left\{-\frac{1}{2}\sum_{\alpha=1}^{3}\left(\frac{\partial}{\partial x_\alpha}\right)^2+2[\wp(x_1-x_2)+\wp(x_2-x_3)+\wp(x_3-x_1)]\right\}\varphi=E\varphi. \tag{11}$$

As $H_p^{(3)}$ commutes with each of the operators $S_j^{(\alpha)}$ shifting jth argument of φ to the period ω_α of the Weierstrass function, it is natural to search for the solutions of (7) in accordance with the Floquet–Bloch theory, i.e., as quasiperiodic functions in each argument $\{x_j\}$:

$$\varphi(x_1+l_1\omega_\alpha,x_2+l_2\omega_\alpha,x_3+l_3\omega_\alpha)=\exp\left(i\sum_{j=1}^{3}q_j^{(\alpha)}l_j\right)\varphi(x_1,x_2,x_3), \quad l_1,l_2,l_3\in\mathbf{Z}. \tag{12}$$

The only singularity of $\wp(x)$ on the torus T_{ω_1,ω_2} is the second-order pole at $x=0$. Then it follows from (11) that $\varphi(x_1,x_2,x_3)$ is meromorphic on $(T_{\omega_1,\omega_2})^3$ with simple poles at $x_1=x_2$, $x_2=x_3$, $x_3=x_1$, i.e., it can be represented in the form

$$\varphi(x_1,x_2,x_3)=\frac{\Phi(x_1,x_2,x_3)}{\sigma(x_1-x_2)\sigma(x_2-x_3)\sigma(x_3-x_1)}, \tag{13}$$

where $\Phi(x_1,x_2,x_3)$ is analytic on $(T_{\omega_1,\omega_2})^3$. One can show that this condition, being combined with (12), determines the structure of Φ up to eight arbitrary parameters. In particular, the constants $q_\alpha^{(j)}$ in (12) cannot be chosen independently but are related by

$$\Omega=\sum_{j=1}^{3}\left[\omega_1 q_j^{(2)}-\omega_2 q_j^{(1)}\right]\in 2\pi(\mathbf{Z}\omega_1+\mathbf{Z}\omega_2).$$

So it is always possible to choose $\{q_j^{(\alpha)}\}$ such as Ω vanishes.

Note that the solutions to (11) of the type (12) contain only four arbitrary parameters (the common normalization factor and three particle quasimomenta). Hence finding these solutions is equivalent to some purely algebraic problem, i.e., extracting some four-dimensional manifold from $\{\Phi\}$. To formulate it in a constructive way, one needs an appropriate parametrization of $\{\Phi\}$. It can be chosen as

$$\Phi(x_1,x_2,x_3)=A\,\exp\left[i\sum_{\alpha=1}^{3}k_\alpha x_\alpha\right]\sigma(x_1-x_2+\gamma_{12})\sigma(x_2-x_3+\gamma_{23})\sigma(x_3-x_1+\gamma_{31})$$
$$\times[B+\zeta(x_1-x_2+\gamma_{12})+\zeta(x_2-x_3+\gamma_{23})+\zeta(x_3-x_1+\gamma_{31})]. \tag{14}$$

Since the poles of $\zeta(x)$ coincide with zeroes of $\sigma(x)$, the functions of the type (14) are analytic on $(T_{\omega_1,\omega_2})^3$ as required. The parameters $q_j^{(\alpha)}$ in (12) are easily expressed through $\{k\}$ and $\{\gamma\}$ with the use of (8),

$$q_j^{(\alpha)}=k_j\omega_\alpha-i\eta_\alpha(\gamma_{jl}+\gamma_{jm}), \tag{15}$$

where the auxiliary phases $\gamma_{21},\gamma_{32},\gamma_{13}$ are introduced by the relation

$$\gamma_{jm}=-\gamma_{mj} \tag{16}$$

and (jlm) is an arbitrary combination of the numbers from 1 to 3.

Upon substituting (13) and (14) into (11) one arrives at the equation

$$L(x_1,x_2,x_3)=A\,\exp\left[i\sum_{\alpha=1}^{3}k_\alpha x_\alpha\right]\frac{\sigma(y_{12})\sigma(y_{23})\sigma(y_{31})}{\sigma(z_{12})\sigma(z_{23})\sigma(z_{31})}\{[B+\zeta(y_{12})+\zeta(y_{23})+\zeta(y_{31})][-\epsilon$$
$$+i\zeta(z_{12})(k_1-k_2)+i\zeta(z_{23})(k_2-k_3)+i\zeta(z_{31})(k_3-k_1)+3(\zeta(z_{12})\zeta(z_{23})$$
$$+\zeta(z_{12})\zeta(z_{31})+\zeta(z_{23})\zeta(z_{31}))-(\zeta(y_{12})-\zeta(y_{31}))(ik_1-\zeta(z_{12})+\zeta(z_{31}))-(\zeta(y_{23})$$
$$-\zeta(y_{12}))(ik_2-\zeta(z_{23})+\zeta(z_{12}))-(\zeta(y_{31})-\zeta(y_{23}))(ik_3-\zeta(z_{31})+\zeta(z_{23}))-\zeta^2(y_{12})$$
$$-\zeta^2(y_{23})-\zeta^2(y_{31})+\zeta(y_{12})\zeta(y_{23})+\zeta(y_{12})\zeta(y_{31})+\zeta(y_{23})\zeta(y_{31})+\wp(y_{12})+\wp(y_{23})$$
$$+\wp(y_{31})]+[ik_1-\zeta(z_{12})+\zeta(z_{31})+\zeta(y_{12})-\zeta(y_{31})][\wp(y_{12})-\wp(y_{31})]+[ik_2$$
$$-\zeta(z_{23})+\zeta(z_{12})+\zeta(y_{23})-\zeta(y_{12})][\wp(y_{23})-\wp(y_{12})]+[ik_3-\zeta(z_{31})+\zeta(z_{23})$$
$$+\zeta(y_{31})-\zeta(y_{23})][\wp(y_{31})-\wp(y_{23})]+\wp'(y_{12})+\wp'(y_{23})+\wp'(y_{31})\}=0, \tag{17}$$

where

$$\epsilon = E - \tfrac{1}{2}(k_1^2 + k_2^2 + k_3^2), \quad z_{\alpha\beta} = x_\alpha - x_\beta, \quad y_{\alpha\beta} = x_\alpha - x_\beta + \gamma_{\alpha\beta}.$$

Note that $L(x_1, x_2, x_3)$, like $\varphi(x_1, x_2, x_3)$, is quasiperiodic in each argument. Let us choose one of them (say, x_1) and fix two others. When treated as a function of x_1, L obeys the relations

$$L(x_1 + \omega_j, x_2, x_3) = \exp(i q_1^{(j)}) L(x_1, x_2, x_3), \quad j = 1,2, \tag{18}$$

with $q_1^{(j)}$ given by (15). At $\gamma_{12} - \gamma_{31} \notin \mathbf{Z}\omega_1 + \mathbf{Z}\omega_2$ one has

$$q_1^{(1)}\omega_2 - q_1^{(2)}\omega_1 \notin 2\pi(\mathbf{Z}\omega_1 + \mathbf{Z}\omega_2). \tag{19}$$

The singularities of L on T_{ω_1,ω_2} at fixed x_2, x_3 are second-order poles at $x_1 = x_2$ and $x_1 = x_3$. Near these points one can write the Laurent decompositions of L as

$$\exp\left(-i\sum_{\alpha=1}^{3} k_\alpha x_\alpha\right) L(x_1, x_2, x_3) = \lambda_{-2}^{(j)}(z)(x_1 - x_j)^{-2} + \lambda_{-1}^{(j)}(z)(x_1 - x_j)^{-1} + \lambda_0^{(j)}(z, x_1 - x_j),$$

$$j = 2,3,$$

where $z = x_2 - x_3$ and $\lambda_0^{(j)}$ are regular when $x_1 \to x_j$. If one proves that all $\lambda_{-2}^{(j)}(z), \lambda_{-1}^{(j)}(z)$ vanish, then L as a function of x_1 will be analytic on T_{ω_1,ω_2}. However, according to the Liouville theorem, the only analytic function on this torus under the conditions (18) and (19) is zero. Hence (17) is equivalent to four simpler equations:

$$\lambda_{-2}^{(2)}(z) = 0, \quad \lambda_{-2}^{(3)}(z) = 0, \tag{20}$$

$$\lambda_{-1}^{(2)}(z) = 0, \quad \lambda_{-1}^{(3)}(z) = 0. \tag{21}$$

Let us first consider the equations (20). After calculation of the explicit form of leading singularities in (17) they can be written as

$$[B + \zeta(\gamma_{12}) + \zeta(z + \gamma_{23}) - \zeta(z - \gamma_{31})][i(k_1 - k_2) + 2\zeta(\gamma_{12}) + \zeta(z - \gamma_{31}) - \zeta(z + \gamma_{23})]$$
$$+ \wp(z - \gamma_{31}) + \wp(z + \gamma_{23}) - 2\wp(\gamma_{12}) = 0, \tag{22}$$

$$[B + \zeta(\gamma_{31}) + \zeta(z + \gamma_{23}) - \zeta(z - \gamma_{12})][i(k_3 - k_1) + 2\zeta(\gamma_{31}) + \zeta(z - \gamma_{12}) - \zeta(z + \gamma_{23})]$$
$$+ \wp(z - \gamma_{12}) + \wp(z + \gamma_{23}) - 2\wp(\gamma_{31}) = 0. \tag{23}$$

The left-hand sides of (22) and (23) are double periodic (i.e., elliptic) functions of z with the first-order poles at $z = -\gamma_{23}, \gamma_{31}$ for (22) and $z = -\gamma_{23}, \gamma_{12}$ for (23). If the pole residues and constant terms in the Laurent decompositions of these functions equal to zero, then, according to the Liouville theorem, they must vanish identically. These conditions can be expressed in the form of four purely algebraic equations for the parameters $B, \{k\}, \{\gamma\}$,

$$B - i(k_1 - k_2) - \zeta(\gamma_{12}) + 2\zeta(\gamma_{31} + \gamma_{23}) = 0, \tag{24}$$

$$B - i(k_3 - k_1) - \zeta(\gamma_{31}) + 2\zeta(\gamma_{12} + \gamma_{23}) = 0, \tag{25}$$

$$[B + \zeta(\gamma_{12}) + \zeta(\gamma_{31} + \gamma_{23})][i(k_1 - k_2) + 2\zeta(\gamma_{12}) - \zeta(\gamma_{31} + \gamma_{23})]$$
$$- 2\wp(\gamma_{12}) - \wp(\gamma_{31} + \gamma_{23}) = 0, \tag{26}$$

$$[B+\zeta(\gamma_{31})+\zeta(\gamma_{12}+\gamma_{23})][i(k_3-k_1)+2\zeta(\gamma_{31})-\zeta(\gamma_{12}+\gamma_{23})]$$
$$-2\wp(\gamma_{31})-\wp(\gamma_{12}+\gamma_{23})=0. \tag{27}$$

Upon eliminating k_1-k_2 and k_3-k_1 by (24) and (25), Eqs. (26) and (27) can be written as

$$[B+\zeta(\gamma_{12})+\zeta(\gamma_{31}+\gamma_{23})]^2=2\wp(\gamma_{12})+\wp(\gamma_{31}+\gamma_{23}), \tag{28}$$

$$[B+\zeta(\gamma_{31})+\zeta(\gamma_{12}+\gamma_{23})]^2=2\wp(\gamma_{31})+\wp(\gamma_{12}+\gamma_{23}). \tag{29}$$

Since the difference of (28) and (29) is linear in B, this parameter can also be expressed easily through the phases $\{\gamma\}$,

$$B=-[\zeta(\gamma_{12})+\zeta(\gamma_{23})+\zeta(\gamma_{31})]+3[\wp(\gamma_{12})-\wp(\gamma_{23})][\wp(\gamma_{23})-\wp(\gamma_{31})][\wp(\gamma_{31})-\wp(\gamma_{12})]$$
$$\times\{\wp'(\gamma_{12})[\wp(\gamma_{23})-\wp(\gamma_{31})]+\wp'(\gamma_{23})[\wp(\gamma_{31})-\wp(\gamma_{12})]+\wp'(\gamma_{31})[\wp(\gamma_{12})-\wp(\gamma_{23})]\}^{-1}. \tag{30}$$

After the substitution of (30) into one of Eqs. (28) and (29), one obtains the nonlinear constraint for $\gamma_{12},\gamma_{23},\gamma_{31}$. At first sight it seems to be enormously cumbersome but can be essentially simplified with the use of addition theorems for zeta functions,

$$\zeta(x)+\zeta(y)+\zeta(z)-\zeta(x+y+z)=2[\wp(x)-\wp(y)][\wp(y)-\wp(z)][\wp(z)-\wp(x)]\{\wp'(x)[\wp(y)$$
$$-\wp(z)]+\wp'(y)[\wp(z)-\wp(x)]+\wp'(z)[\wp(x)-\wp(y)]\}^{-1},$$
$$\wp(x)-\wp(y)=[\zeta(x)-\zeta(y)-\zeta(x+z)+\zeta(y+z)][\zeta(x)+\zeta(y)+\zeta(z)-\zeta(x+y+z)], \tag{31}$$

which are valid for all $x,y,z\in\mathbf{C}$. The result of simple but tedious calculations is

$$[\zeta(\gamma_{12})+\zeta(\gamma_{23})+\zeta(\gamma_{31})-\zeta(\gamma_{12}+\gamma_{23}+\gamma_{31})]\{9\zeta(\gamma_{12}+\gamma_{23}+\gamma_{31})$$
$$-4[\zeta(\gamma_{12}+\gamma_{23})+\zeta(\gamma_{23}+\gamma_{31})+\zeta(\gamma_{12}+\gamma_{31})]-[\zeta(\gamma_{12})+\zeta(\gamma_{23})+\zeta(\gamma_{31})]\}=0. \tag{32}$$

All zeroes of the first factor in (32) coincide with the poles of the second one as it follows from the relation

$$\zeta(x)+\zeta(y)+\zeta(z)-\zeta(x+y+z)=\frac{\sigma(x+y)\sigma(y+z)\sigma(z+x)}{\sigma(x)\sigma(y)\sigma(z)\sigma(x+y+z)}. \tag{33}$$

Hence this factor must be omitted and one finally obtains the constraint for $\{\gamma\}$ in the form

$$\zeta(\gamma_{12})+\zeta(\gamma_{23})+\zeta(\gamma_{31})+4[\zeta(\gamma_{12}+\gamma_{23})+\zeta(\gamma_{23}+\gamma_{31})+\zeta(\gamma_{31}+\gamma_{12})]-9\zeta(\gamma_{12}+\gamma_{23}+\gamma_{31})=0. \tag{34}$$

The left-hand side of (34) as a function of one of the phases (say, γ_{12}) at fixed values of two others is double periodic and has four simple poles on $\mathbf{C}/\mathbf{Z}\omega_1+\mathbf{Z}\omega_2$. So there are four roots of Eq. (34) and γ_{12} can be treated as a four-valued function of γ_{23} and γ_{31} on $(\mathbf{C}/\mathbf{Z}\omega_1+\mathbf{Z}\omega_2)^2$. The analysis of degenerate cases $\omega_1,\omega_2\to\infty$ shows that the uniformization problem for the constraint (34) is relatively complicated and its solution seems to be very nontrivial.

With the use of (24)–(27), (30), and (34) one can express the parameter B and the differences $\{k_\alpha-k_\beta\}$ through the phases $\{\gamma\}$. The result reads

$$B=\tfrac{1}{2}[\zeta(\gamma_{12})+\zeta(\gamma_{23})+\zeta(\gamma_{31})-3\zeta(\gamma_{12}+\gamma_{23}+\gamma_{31})], \tag{35}$$

$$i(k_\alpha - k_\beta) = \tfrac{1}{2}[\zeta(\gamma_{\beta\delta}) - \zeta(\gamma_{\alpha\delta}) - \zeta(\gamma_{\alpha\beta}) + 4\zeta(\gamma_{\beta\delta} - \gamma_{\alpha\delta}) - 3\zeta(\gamma_{\alpha\beta} + \gamma_{\beta\delta} - \gamma_{\alpha\delta})], \quad (36)$$

where $(\alpha\beta\delta)$ is an arbitrary permutation of (123).

The next step in constructing the solutions to (11) consists in solving Eqs. (21). The explicit form of them is as follows:

$$\begin{aligned}\lambda_{-1}^{(2)}(z) = {} & [B + \zeta(\gamma_{12}) + \zeta(z+\gamma_{23}) - \zeta(z-\gamma_{31})]\{-\epsilon + 3\wp(z) + \wp(z+\gamma_{23}) - \zeta^2(\gamma_{12}) - \wp(\gamma_{12}) \\ & + \zeta(\gamma_{12})[\zeta(z+\gamma_{23}) - \zeta(z-\gamma_{31})] - [\zeta(z+\gamma_{23}) - \zeta(z-\gamma_{31})]^2 - 3[\zeta(z) - \zeta(z-\gamma_{31})] \\ & \times [\zeta(z) - \zeta(z+\gamma_{23})] + i(k_1 - k_3)[\zeta(z) - \zeta(\gamma_{12}) - \zeta(z-\gamma_{31})] + i(k_2 - k_3)[\zeta(z) \\ & + \zeta(\gamma_{12}) - \zeta(z+\gamma_{23})]\} - \wp'(\gamma_{12}) + \wp'(z+\gamma_{23}) + [\wp(z-\gamma_{31}) - \wp(z+\gamma_{23})][i(k_3 - k_2) \\ & + \zeta(\gamma_{12}) - \zeta(z-\gamma_{31}) - 2\zeta(z+\gamma_{23}) + 3\zeta(z)] = 0, \end{aligned} \quad (37)$$

$$\begin{aligned}\lambda_{-1}^{(3)}(z) = {} & [B + \zeta(\gamma_{31}) + \zeta(z+\gamma_{23}) - \zeta(z-\gamma_{12})]\{-\epsilon + 3\wp(z) + \wp(z+\gamma_{23}) - \zeta^2(\gamma_{31}) - \wp(\gamma_{31}) \\ & + \zeta(\gamma_{31})[\zeta(z+\gamma_{23}) - \zeta(z-\gamma_{12})] - [\zeta(z+\gamma_{23}) - \zeta(z-\gamma_{12})]^2 - 3[\zeta(z) - \zeta(z-\gamma_{12})] \\ & \times [\zeta(z) - \zeta(z+\gamma_{23})] + i(k_2 - k_1)[\zeta(z) - \zeta(\gamma_{31}) - \zeta(z-\gamma_{12})] + i(k_2 - k_3)[\zeta(z) \\ & + \zeta(\gamma_{31}) - \zeta(z+\gamma_{23})]\} - \wp'(\gamma_{31}) + \wp'(z+\gamma_{23}) + [\wp(z-\gamma_{12}) - \wp(z+\gamma_{23})][i(k_3 - k_2) \\ & + \zeta(\gamma_{31}) - \zeta(z-\gamma_{12}) - 2\zeta(z+\gamma_{23}) + 3\zeta(z)] = 0. \end{aligned} \quad (38)$$

It is easy to see that both $\lambda_{-1}^{(2)}(z)$ and $\lambda_{-1}^{(3)}(z)$ are elliptic functions of z with poles at $z = 0, -\gamma_{23}, \gamma_{31}$ for (37) and at $z = 0, -\gamma_{23}, \gamma_{12}$ for (38). At arbitrary values of $B, \{k\}, \{\gamma\}$ the pole at $z = 0$ is simple and two others are of second order. With the use of (35) and (36) one can show, however, that $\lambda_{-1}^{(2)}$ and $\lambda_{-1}^{(3)}$ are analytic at $z = 0$ and the remaining poles are simple. Hence, according to the Liouville theorem, $\lambda_{-1}^{(2)}$ and $\lambda_{-1}^{(3)}$ must vanish if their residues at $z = \gamma_{23}$ and values at $z = 0$ are equal to zero. In other words, (37) and (38) are reduced to four algebraic equations,

$$\begin{aligned} & \epsilon + i(k_1 - k_3)[-\zeta(\gamma_{31}) + \zeta(\gamma_{12})] + i(k_2 - k_3)[\zeta(\gamma_{31} + \gamma_{23}) - \zeta(\gamma_{12}) - \zeta(\gamma_{31})] + 2\wp(\gamma_{31} + \gamma_{23}) \\ & \quad - 3\wp(\gamma_{31}) + \wp(\gamma_{12}) + \zeta^2(\gamma_{12}) + \zeta^2(\gamma_{31} + \gamma_{23}) + 3\zeta^2(\gamma_{31}) - \zeta(\gamma_{31} + \gamma_{23})[\zeta(\gamma_{12}) + 3\zeta(\gamma_{31})] \\ & \quad + [B + \zeta(\gamma_{12}) + \zeta(\gamma_{31} + \gamma_{23})][-i(k_1 - k_3) + 3\zeta(\gamma_{31}) - \zeta(\gamma_{12}) - \zeta(\gamma_{31} + \gamma_{23})] = 0, \end{aligned} \quad (39)$$

$$\begin{aligned} & [B + \zeta(\gamma_{12}) + \zeta(\gamma_{23}) + \zeta(\gamma_{31})][-\epsilon - 3\wp(\gamma_{31}) - 2\wp(\gamma_{23}) - \wp(\gamma_{12}) - \zeta^2(\gamma_{12}) - (\zeta(\gamma_{23}) + \zeta(\gamma_{31}))^2 \\ & \quad + \zeta(\gamma_{12})(\zeta(\gamma_{23}) + \zeta(\gamma_{31})) + 3\zeta(\gamma_{23})\zeta(\gamma_{31}) + i(k_1 - k_3)(\zeta(\gamma_{31}) - \zeta(\gamma_{12})) + i(k_2 - k_3) \\ & \quad \times (\zeta(\gamma_{12}) - \zeta(\gamma_{23}))] + [\wp(\gamma_{31}) - \wp(\gamma_{23})][i(k_1 - k_3) + \zeta(\gamma_{12}) + \zeta(\gamma_{23}) - 2\zeta(\gamma_{31})] \\ & \quad - 3\wp'(\gamma_{31}) - 2\wp'(\gamma_{23}) - \wp'(\gamma_{12}) = 0, \end{aligned} \quad (40)$$

$$\begin{aligned} & \epsilon + i(k_2 - k_1)[-\zeta(\gamma_{12}) + \zeta(\gamma_{31})] + i(k_2 - k_3)[\zeta(\gamma_{12} + \gamma_{23}) - \zeta(\gamma_{12}) - \zeta(\gamma_{31})] + 2\wp(\gamma_{12} + \gamma_{23}) \\ & \quad - 3\wp(\gamma_{12}) + \wp(\gamma_{31}) + \zeta^2(\gamma_{31}) + \zeta^2(\gamma_{12} + \gamma_{23}) + 3\zeta^2(\gamma_{12}) - \zeta(\gamma_{12} + \gamma_{23})[\zeta(\gamma_{31}) + 3\zeta(\gamma_{12})] \\ & \quad + [B + \zeta(\gamma_{31}) + \zeta(\gamma_{12} + \gamma_{23})][-i(k_2 - k_1) + 3\zeta(\gamma_{12}) - \zeta(\gamma_{31}) - \zeta(\gamma_{12} + \gamma_{23})] = 0, \end{aligned} \quad (41)$$

$$[B+\zeta(\gamma_{12})+\zeta(\gamma_{23})+\zeta(\gamma_{31})][-\epsilon-3\wp(\gamma_{12})-2\wp(\gamma_{23})-\wp(\gamma_{31})-\zeta^2(\gamma_{31})]-(\zeta(\gamma_{23})+\zeta(\gamma_{12}))^2$$
$$+\zeta(\gamma_{31})(\zeta(\gamma_{12})+\zeta(\gamma_{23}))+3\zeta(\gamma_{23})\zeta(\gamma_{12})+i(k_2-k_1)(\zeta(\gamma_{12})-\zeta(\gamma_{31}))+i(k_2-k_3)(\zeta(\gamma_{31})$$
$$-\zeta(\gamma_{23}))]+[\wp(\gamma_{12})-\wp(\gamma_{23})][i(k_2-k_1)+\zeta(\gamma_{31})+\zeta(\gamma_{23})-2\zeta(\gamma_{12})]-3\wp'(\gamma_{12})$$
$$-2\wp'(\gamma_{23})-\wp'(\gamma_{31})=0. \tag{42}$$

The essential simplification of (40) and (42) can be made if the formula

$$\wp'(x)+2\wp'(y)+3\wp'(z)=2[\wp(z)-\wp(y)][\zeta(x)+\zeta(y)-\zeta(x+y)]+[\zeta(x+y+z)-\zeta(x)$$
$$-\zeta(y)-\zeta(z)]\{6[\wp(x)+\wp(y)+\wp(z)]+2[\zeta(x)+\zeta(y)-\zeta(x+y)]$$
$$\times[\zeta(x+y)+\zeta(x+z)+\zeta(y+z)-2\zeta(x)-2\zeta(y)-2\zeta(z)]\}$$

is taken into account. Finally, with the use of (31), (35), and (36) it is possible after long calculations to show that all Eqs. (39)–(42) are mutually equivalent. Any extra constraints on the parameters $\{\gamma\}$ are absent and (39)–(42) determine the three-particle energy,

$$E=\tfrac{1}{2}(k_1^2+k_2^2+k_3^2)-\tfrac{1}{2}[\zeta^2(\gamma_{12})+\zeta^2(\gamma_{23})+\zeta^2(\gamma_{31})]+\tfrac{3}{2}\zeta(\gamma_{12}+\gamma_{23}+\gamma_{31})[\zeta(\gamma_{12})+\zeta(\gamma_{23})$$
$$+\zeta(\gamma_{31})]-2[\zeta(\gamma_{12})\zeta(\gamma_{23}+\gamma_{31})+\zeta(\gamma_{23})\zeta(\gamma_{12}+\gamma_{31})+\zeta(\gamma_{31})\zeta(\gamma_{12}+\gamma_{23})]+2[\wp(\gamma_{12})$$
$$+\wp(\gamma_{23})+\wp(\gamma_{31})]-\tfrac{9}{4}[\zeta(\gamma_{12}+\gamma_{23}+\gamma_{31})-\zeta(\gamma_{12})-\zeta(\gamma_{23})-\zeta(\gamma_{31})]^2.$$

[This result, together with the formulas (35) and (36), has been announced in Ref. 24.] Further simplification of E can be reached by extracting the energy of the center-of-mass motion with a total momentum $K=k_1+k_2+k_3$ and using expressions for relative quasimomenta $\{k_\alpha-k_\beta\}$ (36) in combination with addition theorems (10) and (31) for the Weierstrass functions,

$$E=\frac{K^2}{6}+\frac{1}{12}\{27\wp(\gamma_{12}+\gamma_{23}+\gamma_{31})-8[\wp(\gamma_{12}+\gamma_{23})+\wp(\gamma_{23}+\gamma_{31})+\wp(\gamma_{12}+\gamma_{31})]-[\wp(\gamma_{12})$$
$$+\wp(\gamma_{23})+\wp(\gamma_{31})]\}. \tag{43}$$

Formulas (13), (14), (35), (36), and (43) give a complete solution to the problem of finding the quasiperiodic functions $\varphi(x_1,x_2,x_3)$ obeying (11). Note also that with the use of (33) one can write φ's only in terms of sigma functions,

$$\varphi(x_1,x_2,x_3)=\frac{A\ \exp(i\Sigma_{\alpha=1}^3 k_\alpha x_\alpha)}{\sigma(x_1-x_2)\sigma(x_2-x_3)\sigma(x_3-x_1)}$$
$$\times\left\{\frac{\sigma(x_1-x_2+\gamma_{12})\sigma(x_2-x_3+\gamma_{23})\sigma(x_3-x_1+\gamma_{31})}{2\sigma(\gamma_{12})\sigma(\gamma_{23})\sigma(\gamma_{31})}\right.$$
$$\left.+\frac{\sigma(x_1-x_2+\gamma_{12}-\Delta)\sigma(x_2-x_3+\gamma_{23}-\Delta)\sigma(x_3-x_1+\gamma_{31}-\Delta)}{\sigma(\gamma_{12}-\Delta)\sigma(\gamma_{23}-\Delta)\sigma(\gamma_{31}-\Delta)}\right\}, \tag{44}$$

where $\Delta=\gamma_{12}+\gamma_{23}+\gamma_{31}$ and the connections (36) between ks and γs are implied. The resemblance of (44) to the classical Hermite form (6) of the solution to the Lamè equation is evident.

III. THREE-MAGNON PROBLEM

First, let us note that the lattice equation (4) always has solutions of the type

$$\psi_d^{(M)}(n_1\cdots n_M)=\sum_{\beta=1}^{M}\psi^{(M-1)}(n_1\cdots n_{\beta-1}n_{\beta+1}\cdots n_M),\quad E_M=E_{M-1}, \tag{45}$$

where $\psi^{(M-1)}(n_1\cdots n_{M-1})$ obeys the equation of the type (4) with M replaced by $M-1$. The wave functions (45) describe the M-magnon states which are generated from $(M-1)$-magnon ones by the action of the component of total spin operator reducing the absolute value of S_z. The remained M-magnon states corresponding to the lowest possible eigenvalue of the total spin are described by ψs which cannot be presented in the form (45). Now let us construct three-magnon states of this type in terms of the ansatz which is similar to the symmetrized three-particle wave function (13) and (14):

$$\psi^{(3)}(n_1,n_2,n_3)=\sum_{P\in\pi_3}\frac{\exp(i\Sigma_{\alpha=1}^{3}k_\alpha n_{P\alpha})}{\sigma(n_{P1}-n_{P2})\sigma(n_{P2}-n_{P3})\sigma(n_{P3}-n_{P1})}\left[B+\frac{\partial}{\partial\gamma_{12}}+\frac{\partial}{\partial\gamma_{23}}\right.$$
$$\left.+\frac{\partial}{\partial\gamma_{31}}\right]\sigma(n_{P1}-n_{P2}+\gamma_{12})\sigma(n_{P2}-n_{P3}+\gamma_{23})\sigma(n_{P3}-n_{P1}+\gamma_{31}). \tag{46}$$

Here π_3 is the group of all permutations of the numbers from 1 to 3. The Weierstrass functions are defined on the torus $T_{N,\omega}$. Unlike the particle case, ks and γs have to be restricted by the periodicity of ψ in each argument,

$$Nk_\alpha-i\eta_1(\gamma_{\alpha\beta}+\gamma_{\alpha\delta})=2\pi l_\alpha,\quad l_\alpha\in\mathbf{Z}, \tag{47}$$

where the auxiliary phases are defined by (16).

To calculate the left-hand side of (4) at $M=3$ with the use of (46), one should represent in a closed form the sum over lattice sites of the following type,

$$W(k,\{\gamma\},\{l\})=\sum_{s=1;s\neq l_1,l_2}^{N-1}\exp(iks)\wp(s)\,\frac{\sigma(s-l_1+\gamma_1)\sigma(s-l_2+\gamma_2)}{\sigma(s-l_1)\sigma(s-l_2)},\quad l_1,l_2\in\mathbf{Z}, \tag{48}$$

where k, γ_1, and γ_2 are chosen so as to ensure the periodicity of the summands in (48) with respect to s,

$$kN-i\eta_1(\gamma_1+\gamma_2)=0(\mathrm{mod}\,2\pi).$$

It can be done by using the technique based on the Liouville theorem and described earlier in Refs. 12 and 13. The result reads

$$W(k,\{\gamma\},\{l\})=\left[\prod_{\alpha=1}^{2}\frac{\sigma(l_\alpha-\gamma_\alpha)}{\sigma(l_\alpha)}\right]\left\{\epsilon(k,\gamma_1,\gamma_2)+f(k,\gamma_1,\gamma_2)\sum_{\alpha=1}^{2}[\zeta(l_\alpha)-\zeta(l_\alpha-\gamma_\alpha)]\right.$$
$$-[\zeta(l_1)-\zeta(l_1-\gamma_1)][\zeta(l_2)-\zeta(l_2-\gamma_2)]+\frac{1}{2}\sum_{\alpha=1}^{2}[\wp(l_\alpha-\gamma_\alpha)-\wp(l_\alpha)$$
$$\left.-(\zeta(l_\alpha)-\zeta(l_\alpha-\gamma_\alpha))^2]\right\}+2\sum_{\alpha=1}^{2}\exp(ikl_\alpha)\left[\prod_{\beta\neq\alpha}^{2}\frac{\sigma(l_\alpha-l_\beta+\gamma_\beta)}{\sigma(l_\alpha-l_\beta)}\right]\sigma(\gamma_\alpha)$$
$$\times\left\{\wp(l_\alpha)\left[f(k,\gamma_1,\gamma_2)-\zeta(\gamma_\alpha)-\sum_{\beta\neq\alpha}(\zeta(l_\alpha-l_\beta+\gamma_\beta)-\zeta(l_\alpha-l_\beta))\right]-\wp'(l_\alpha)\right\},$$

where

$$f(k,\gamma_1,\gamma_2)=\zeta_1\left(-\frac{k\omega}{2\pi}+\frac{i}{\pi}\,\zeta\left(\frac{\omega}{2}\right)(\gamma_1+\gamma_2)\right)+(\pi i)^{-1}\left[ik\zeta_1\left(\frac{\omega}{2}\right)+2\zeta_1\left(\frac{1}{2}\right)\zeta\left(\frac{\omega}{2}\right)(\gamma_1+\gamma_2)\right],$$

$$\epsilon(k,\gamma_1,\gamma_2)=\frac{1}{2}\left[\wp_1\left(-\frac{k\omega}{2\pi}+\frac{i}{\pi}\,\zeta\left(\frac{\omega}{2}\right)(\gamma_1+\gamma_2)\right)-f^2(k,\gamma_1,\gamma_2)\right],$$

and the notation $\wp_1(x),\zeta_1(x)$ is used for the Weierstrass functions defined on the torus $T_{1,\omega}$.

Now the lhs of (4) at $M=3$ can be divided into two parts,

$$L(n_1,n_2,n_3)=L_1(n_1,n_2,n_3)+L_2(n_1,n_2,n_3),$$

where

$$L_1(n_1,n_2,n_3)=\sum_{P\in\pi_3}\sum_{\alpha=1}^{3}\chi_\alpha(n_{P1},n_{P2},n_{P3}),$$

$$L_2(n_1,n_2,n_3)=\sum_{P\in\pi_3}\sum_{\alpha=1}^{3}[\mu_\alpha^{(1)}(n_{P1},n_{P2},n_{P3})+\mu_\alpha^{(2)}(n_{P1},n_{P2},n_{P3})], \tag{49}$$

and

$$\begin{aligned}\chi_1(l_1,l_2,l_3)=\exp\left(i\sum_{\alpha=1}^{3}k_\alpha l_\alpha\right)&\frac{\sigma(l_1-l_2+\gamma_{12})\sigma(l_2-l_3+\gamma_{23})\sigma(l_3-l_1+\gamma_{31})}{\sigma(l_1-l_2)\sigma(l_2-l_3)\sigma(l_3-l_1)}\{[B+\zeta(l_2-l_3\\&+\gamma_{23})+\zeta(l_1-l_2+\gamma_{12})+\zeta(l_3-l_1+\gamma_{31})][\epsilon(k_1,\gamma_{12},\gamma_{13})+(f(k_1,\gamma_{12},\gamma_{13})\\&-\zeta(\gamma_{12}))(\zeta(l_1-l_2+\gamma_{12})-\zeta(l_1-l_2))+(f(k_1,\gamma_{12},\gamma_{13})-\zeta(\gamma_{13}))(\zeta(l_1-l_3+\gamma_{13})\\&-\zeta(l_1-l_3))-(\zeta(l_1-l_2+\gamma_{12})-\zeta(l_1-l_2))(\zeta(l_1-l_3+\gamma_{13})-\zeta(l_1-l_3))-\wp(l_1\\&-l_2)-\wp(l_1-l_3)-\tfrac{1}{2}(\zeta^2(\gamma_{12})+\zeta^2(\gamma_{13})-\wp(\gamma_{12})-\wp(\gamma_{13}))]+[\zeta(l_1-l_2+\gamma_{12})\\&-\zeta(l_1-l_2)][\wp(\gamma_{12})-\wp(l_1-l_3+\gamma_{13})]+[\zeta(l_1-l_3+\gamma_{13})-\zeta(l_1-l_3)][\wp(l_1-l_2\\&+\gamma_{12})-\wp(\gamma_{13})]-\wp(l_1-l_2+\gamma_{12})[f(k_1,\gamma_{12},\gamma_{13})-\zeta(\gamma_{12})]+\wp(l_1-l_3+\gamma_{13})\\&\times[f(k_1,\gamma_{12},\gamma_{13})-\zeta(\gamma_{13})]-\wp(\gamma_{12})\zeta(\gamma_{12})+\wp(\gamma_{13})\zeta(\gamma_{13})+\tfrac{1}{2}[\wp'(\gamma_{13})\\&-\wp'(\gamma_{12})]\},\end{aligned} \tag{50}$$

$$\begin{aligned}\mu_1^{(1)}(l_1,l_2,l_3)=\exp[i(l_2(k_1+k_2)+k_3l_3)]&\frac{\sigma(l_2-l_3+\gamma_{23})\sigma(l_2-l_3+\gamma_{13})}{\sigma^2(l_2-l_3)}\sigma(\gamma_{12})\{[B+\zeta(l_2-l_3\\&+\gamma_{23})-\zeta(l_2-l_3+\gamma_{13})+\zeta(\gamma_{12})][\wp(l_1-l_2)(f(k_1,\gamma_{12},\gamma_{13})-\zeta(\gamma_{12})-\zeta(l_2-l_3\\&+\gamma_{13})+\zeta(l_2-l_3))+\wp'(l_1-l_2)]+\wp(l_1-l_2)[\wp(\gamma_{12})-\wp(l_2-l_3+\gamma_{13})]\},\end{aligned} \tag{51}$$

$$\mu_2^{(1)}(l_1,l_2,l_3)=\exp[i(l_3(k_1+k_3)+k_2l_2)]\,\frac{\sigma(l_2-l_3+\gamma_{23})\sigma(l_2-l_3-\gamma_{12})}{\sigma^2(l_2-l_3)}\,\sigma(\gamma_{13})\{[B+\zeta(l_2-l_3+\gamma_{23})-\zeta(l_2-l_3-\gamma_{12})-\zeta(\gamma_{13})][\wp(l_3-l_1)(f(k_1,\gamma_{12},\gamma_{13})-\zeta(\gamma_{13})+\zeta(l_2-l_3-\gamma_{12})-\zeta(l_2-l_3))+\wp'(l_1-l_3)]+\wp(l_3-l_1)[-\wp(\gamma_{13})+\wp(l_2-l_3-\gamma_{12})]\}. \tag{52}$$

The quantities $\chi_2,\mu_2^{(1)},\mu_2^{(2)}$ and $\chi_3,\mu_3^{(1)},\mu_3^{(2)}$ are obtained from (50)–(52) by cyclic permutations (123)→(231), (123)→(312) of the indices in $\{k_\alpha\},\{l_\alpha\},\{\gamma_{\alpha\beta}\}$. Note that $L_2(n_1,n_2,n_3)$ can be transformed as follows. If, for example, Q is the transposition $(1\leftrightarrow 2)$, then

$$\sum_{P\in\pi_3}\mu_2^{(2)}(n_{P1},n_{P2},n_{P3})=\sum_{PQ\in\pi_3}\mu_2^{(2)}(n_{PQ1},n_{PQ2},n_{PQ3})=\sum_{P\in\pi_3}\mu_2^{(2)}(n_{P2},n_{P1},n_{P3}).$$

Hence the terms in (49) can be combined as

$$\sum_{P\in\pi_3}\{[\mu_1^{(1)}(n_{P1},n_{P2},n_{P3})+\mu_2^{(2)}(n_{P2},n_{P1},n_{P3})]+[\mu_1^{(2)}(n_{P1},n_{P2},n_{P3})+\mu_3^{(1)}(n_{P3},n_{P2},n_{P1})]+[\mu_2^{(1)}(n_{P1},n_{P2},n_{P3})+\mu_3^{(2)}(n_{P1},n_{P3},n_{P2})]\}. \tag{53}$$

Now one can see with the use of the explicit expressions (51) and (52) that the terms in all the three braces of (53) vanish under the conditions which are very similar to the conditions (22) and (23) for vanishing of the second-order poles in the left-hand side of the three-particle equation (17):

$$[B+\zeta(\gamma_{12})+\zeta(z+\gamma_{23})-\zeta(z-\gamma_{31})][-f(k_1,\gamma_{12},\gamma_{13})+f(k_2,\gamma_{23},\gamma_{21})+2\zeta(\gamma_{12})+\zeta(z-\gamma_{13})-\zeta(z+\gamma_{23})]-2\wp(\gamma_{12})+\wp(z-\gamma_{31})+\wp(z+\gamma_{23})=0, \tag{54}$$

$$[B+\zeta(\gamma_{31})+\zeta(z+\gamma_{23})-\zeta(z-\gamma_{12})][-f(k_3,\gamma_{32},\gamma_{31})+f(k_1,\gamma_{12},\gamma_{13})+2\zeta(\gamma_{31})+\zeta(z-\gamma_{12})-\zeta(z+\gamma_{23})]-2\wp(\gamma_{31})+\wp(z-\gamma_{12})+\wp(z+\gamma_{23})=0, \tag{55}$$

$$z=n_{P2}-n_{P3}.$$

Really, the equations (22), (23) and (54), (55) exactly coincide after changing $k_\alpha\to if(k_\alpha,\gamma_{\alpha\beta},\gamma_{\alpha\delta})$. Hence one can use all the techniques of Sec. II for determining the relations between the parameters of the three-magnon wave function (46).

Since $L_2(n_1,n_2,n_3)$ vanishes if the conditions (54) and (55) are fulfilled, the final step of construction consists in the investigation of the structure of $L_1(n_1,n_2,n_3)$. It can be done along the lines of Sec. II with some minimal changes. One finds that $\psi(n_1,n_2,n_3)$ obeys (4) if B is expressed through the γs as in (35), ks and γs are connected by (36) after changing $ik_\alpha\to -f(k_\alpha,\gamma_{\alpha\beta},\gamma_{\alpha\delta})$, and the three-magnon energy is given by

$$E_3=\varepsilon(k_1,\gamma_{12},\gamma_{13})+\varepsilon(k_2,\gamma_{21},\gamma_{23})+\varepsilon(k_3,\gamma_{31},\gamma_{32})+\tfrac{1}{6}[f(k_1,\gamma_{12},\gamma_{13})+f(k_2,\gamma_{21},\gamma_{23})+f(k_3,\gamma_{31},\gamma_{32})]^2-\tfrac{1}{12}\{27\wp(\gamma_{12}+\gamma_{23}+\gamma_{31})-8[\wp(\gamma_{12}+\gamma_{23})+\wp(\gamma_{23}+\gamma_{31})+\wp(\gamma_{31}+\gamma_{12})]-\wp(\gamma_{12})-\wp(\gamma_{23})-\wp(\gamma_{31})\},$$

where

$$\varepsilon(k,\gamma_1,\gamma_2)=\frac{2}{\omega}\left[\zeta_1\left(\frac{\omega}{2}\right)-N\zeta\left(\frac{\omega}{2}\right)\right]-\frac{1}{2}\wp_1\left(-\frac{k\omega}{2\pi}+\frac{i}{\pi}\zeta\left(\frac{\omega}{2}\right)(\gamma_1+\gamma_2)\right).$$

The relations of the type (36) can be simplified by using the periodicity conditions (47) and Legendre relation (9). The result reads

$$\zeta_1\left(\frac{\gamma_{\alpha\beta}+\gamma_{\alpha\delta}-l_\alpha\omega}{N}\right)-\zeta_1\left(\frac{\gamma_{\beta\alpha}+\gamma_{\beta\delta}-l_\beta\omega}{N}\right)+2\zeta_1\left(\frac{\omega}{2}\right)\frac{l_\alpha-l_\beta}{N}+\frac{2}{N\omega}\left[N\zeta\left(\frac{\omega}{2}\right)-\zeta_1\left(\frac{\omega}{2}\right)\right](2\gamma_{\alpha\beta}$$

$$+\gamma_{\alpha\delta}-\gamma_{\beta\delta})+\frac{1}{2}[\zeta(\gamma_{\alpha\beta})+\zeta(\gamma_{\alpha\delta})-\zeta(\gamma_{\beta\delta})+4\zeta(\gamma_{\alpha\delta}-\gamma_{\beta\delta})+3\zeta(\gamma_{\alpha\beta}+\gamma_{\beta\delta}-\gamma_{\alpha\delta})]=0,$$

where $(\alpha\beta\gamma)$ is an arbitrary combination of (123) and $l_1,l_2,l_3\in\mathbf{Z}$. The corresponding three-magnon wave functions are determined by the solutions of these three transcendental constraints. As $\omega\to 0$, (56) transform to the Bethe-ansatz equations[17] for the periodic XXX Heisenberg chain with nearest-neighbor spin interaction. As it follows directly from the definition, the wave functions of the form (45) for three magnons are expressed through two-magnon ones found earlier in Ref. 22.

IV. SUMMARY AND DISCUSSION

The results presented above can be treated as a first step to the solution of the most general integrable 1-D translationally invariant Heisenberg chain with elliptic exchange which might provide rigorous proof of the validity of the use of asymptotic Bethe ansatz for thermodynamic description of infinite particle and spin systems with the short-range interaction $(\sinh \alpha r)^{-2}$. It is natural to expect that almost all previous results of Bethe, Sutherland, and Haldane in the integrable 1-D quantum chains will be unified by this hypothetical solution. The study of analytic properties may serve, as it was demonstrated above, as a guide to its construction.

It would be highly desirable to explain the reasons of the appearance of the Bethe-like transcendental equations (56) by clarifying the algebraic structures which give rise to the integrability of these spin chains. Some progress has been made recently in constructing the family of the operators which commute with the Hamiltonian (3).[25] The way of their extracting from some generalized transfer matrix has not yet been found. It is worth noting also that the analogy of spin and particle dynamics is extended further to give the correspondence between multimagnon wave functions and their many-particle double quasiperiodic counterparts. The details of the proof will be given elsewhere.

However, some problems are open even for the three-magnon case. In particular, it will be of interest to show that the solutions to (56) give a complete set of $\frac{1}{6}N(N-1)(N-5)$ three-magnon eigenvectors of the Hamiltonian (3) with total spin $S=S_z=N/2-3$. In the two-magnon case the answer to the similar question is positive.[26] The selection of the ground state in $M=3$ sector for antiferromagnetic type of coupling still demands nontrivial algebraic ideas and needs further detailed investigation.

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On the quantum deformations of Hamiltonian systems

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In this paper we analyze the relationship between operatorial quantization and deformation quantization for Hamiltonian systems on R^{2n}. We define heuristically generalized symbols for the operators, which make this connection. We construct explicitly deformations which are not equivalent to the Moyal one and show that an infinitesimal, classical canonical transformation does not change the equivalence class of the deformation. The results are applied to the quantum integrability of some two dimensional Hamiltonian systems. © *1996 American Institute of Physics.* [S0022-2488(96)01001-6]

I. INTRODUCTION

The relationship between classical and quantum mechanics is not completely understood. Given a classical Hamiltonian system defined on the $2n$ dimensional phase space R^{2n}, with coordinates (q_i, p_i), $i=1,\ldots,n$, the quantization map is a linear map which sends a real function $f \in C^\infty(R^{2n})$ on the phase space to an Hermitian operator $\hat{f}$ on the Hilbert space of square integrable functions of variables $q_i, L^2(R^n)$. The usual rule of quantization is to associate Hermitian operators $(\hat{q}_i, \hat{p}_j)$ to the basic functions (q_i, p_j) such that,

$$\hat{q}_i \Psi(q) = q_i \Psi(q),$$
$$\hat{p}_j \Psi(q) = -i\hbar \frac{\partial}{\partial q_j} \Psi(q), \tag{1}$$

and the constant function 1 is mapped to the identity operator. The Lie bracket of these operators is related with the Poisson bracket of the corresponding functions on the phase space by

$$[\hat{q}_i, \hat{p}_j] = i\hbar \{q_i, p_j\}\hat{} = i\hbar \delta_{ij}. \tag{2}$$

As it is well known, this rule does not completely determine the quantization map. Consider for example a polynomial $q^n p^m$. We can associate several operators to it, corresponding to different ordering rules. The first attempt to select an ordering rule is due to Dirac.[1] According to the Dirac rule, one tries to associate Hermitian operators to real functions in phase space in such a way that the relation between Lie brackets and Poisson brackets (2) is maintained for all functions,

$$[\hat{f}, \hat{g}] = i\hbar \{f, g\}\hat{}; \quad f, g \in C^\infty(R^n). \tag{3}$$

It is also known that this rule is inconsistent (see Ref. 2, Chap. 5, Sec. 4 for a proof). Dirac itself noticed this could happen, and proposed to relax the rule by requiring that it were valid only to first order in $\hbar$.

There is a wide variety of ordering rules. All of them satisfy the last requirement, and can be expressed through the formal integral,[3]

$$\hat{f} = \int d^n s d^n t \mathcal{F}\left(\frac{i}{\hbar} s \cdot t\right) \bar{f}(s,t) \exp\left(\frac{i}{\hbar} (s \cdot \hat{p} + t \cdot \hat{q})\right), \tag{4}$$

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where

$$\bar{f}(s,t)=\frac{1}{(2\pi\hbar)^{2n}}\int d^nq\,d^np\,\exp\left(-\frac{i}{\hbar}(s\cdot p+t\cdot q)\right)f(q,p) \tag{5}$$

is the Fourier transform of the classical observable, and $\mathscr{F}$ is an arbitrary function. Some of them associate Hermitian operators to real functions, as for example the Weyl rule, which corresponds to take $\mathscr{F}=1$.[4]

The ordering rule is not the only origin of arbitrariness in the process of quantization. One could consider quantizing a function $g(q,p,\hbar)$ whose limit when $\hbar\to 0$ is $f(q,p)$. Since the inverse process to quantization involves taking a limit $\hbar\to 0$, the operator associated to $g(q,p,\hbar)$ is a physically admissible quantization of the classical observable $f(q,p)$.

Finally, let us consider the effect of making a classical canonical transformation, $(q,p)\mapsto(Q(q,p),P(q,p))$. Let f be a classical observable, and let $\hat{f}$ and $\hat{F}$ be the corresponding quantum observables according to the Weyl rule, in the old and new canonical coordinates respectively. The map $\hat{f}\mapsto\hat{F}$ is not a unitary transformation (or more generally, an isometry[5]) for a general canonical transformation, since (3) is inconsistent. So both quantization maps are different, and as before, both are physically admissible. Each quantum theory has its own quantum canonical transformations (i.e. unitary or isometric transformations) but generally the map $\hat{f}\mapsto\hat{F}$ may not correspond to any of them. This is also true for the map given by different ordering rules.

So there is a big degree of arbitrariness when facing the problem of selecting a quantum theory once the classical theory is given. The only thing we know for sure is that the classical theory must be the limit when $\hbar\to 0$, and this limit is a sort of collapsing limit, which does not admit a unique inverse process. In order to make a selection, we must add other criteria, as for example, maintaining the symmetries present in the classical theory.

There are other methods of approaching the problem of quantization. For instance, a powerful one is the deformation theory.[6] The quantization process is understood as a deformation of the Poisson bracket of functions on phase space in terms of the parameter $\hbar$. The deformation is just an inverse process of the "contraction" $\hbar\to 0$. A deformation of the Poisson algebra was written by Moyal,[7] and it is indeed a sort of fundamental deformation on a flat Poisson manifold. The Moyal bracket is related with the Weyl quantization rule through a kind of symbols (Weyl symbols) associated to pseudodifferential operators. Other deformations are related with operators by means of other kinds of symbols. The purpose of this paper is to clarify the relationship between both methods of quantization, the deformation and operatorial approaches.

In Section II we explore the connection between symbols and ordering rules. In Section III we review some facts about deformations of Poisson algebras, construct explicitly deformations nonequivalent to the Moyal one and analyze the effect of a classical canonical transformation when going to the quantum theory. In Section IV we make some applications to the quantum integrability of two dimensional Hamiltonian systems. Finally, in Section V we state our conclusions.

II. SYMBOLS AND ORDERING RULES

A symbol of a pseudodifferential operator is a function associated to it in such a way that the operator can be obtained if the symbol is known. The product of symbols is defined as the symbol of the composite operator. The subject of pseudodifferential operators and their symbols is a well studied subject, and we only make here a rapid survey. Exact statements and proofs concerning τ-symbols can be found for example in Ref. 8.

Let us consider a differential operator A of order m which acts on $u\in C^\infty(R^n)$ through

$$Au(q)=\sum_{|\alpha|\leq m}a_\alpha(q)P^\alpha u(q), \tag{6}$$

where $\alpha=(\alpha^1,...,\alpha^n)$ is a multiindex with $\alpha^j=0,\ldots,m$ and $|\alpha|=\alpha_1+...+\alpha_n$. In what follows a greek character will denote a multiindex, and a Latin one a simple index. $a_\alpha(q)\in C^\infty(R^n)$, $P=(P_1,\ldots,P_n)$, $P_j=-i\hbar(\partial/\partial q^j)$ and $P^\alpha=P_1^{\alpha_1}\ldots P_n^{\alpha_n}$.

Let $u(q)\in S(R^n)$, the Schwartz space, and consider the Fourier transform

$$\bar{u}(p)=\frac{1}{(2\pi\hbar)^n}\int d^nq\ \exp\left(-\frac{i}{\hbar}\,q\cdot p\right)u(q),$$
$$u(q)=\int d^np\ \exp\left(\frac{i}{\hbar}\,q\cdot p\right)\bar{u}(p). \tag{7}$$

Let us apply the operator A on the second expression of (7),

$$Au(q)=\frac{1}{(2\pi\hbar)^n}\int d^npd^nq'\ \exp\left(\frac{i}{\hbar}\,p\cdot(q-q')\right)\sigma_A(q,p)u(q'), \tag{8}$$

where we have introduced the standard symbol of A as the function

$$\sigma_A(q,p)=\sum_{|\alpha|\leqslant m}a_\alpha(q)p^\alpha=\exp\left(-\frac{i}{\hbar}\,q\cdot p\right)A\ \exp\left(\frac{1}{\hbar}\,q\cdot p\right). \tag{9}$$

Equation (8) is valid even for more general functions $u(q)$ by conveniently regularizing the integral, so one can consider (8) as the definition of the operator A through his standard symbol.

One can consider more general operators,

$$Bu(q)=\frac{1}{(2\pi\hbar)^n}\int d^npd^nq'\ \exp\left(\frac{i}{\hbar}\,p\cdot(q-q')\right)b(q,q',p)u(q'), \tag{10}$$

where the function $b(q,q',p)$ is the amplitude of the operator belonging to a suitably restricted class of functions. It is a remarkable fact that an operator like (10) can be uniquely written as

$$Bu(q)=\frac{1}{(2\pi\hbar)^n}\int d^npd^nq'\ \exp\left(\frac{i}{\hbar}\,p\cdot(q-q')\right).\sigma_A^\tau((1-\tau)q+\tau q',p)u(q') \tag{11}$$

for any $\tau\in R$. The function $\sigma_A^\tau(x,p)$ is the τ-symbol of the operator A. The standard symbol (or left symbol) corresponds to take $\tau=0$. For $\tau=1$ it is called the right symbol, and for $\tau=1/2$ it is called the Weyl symbol. A differential operator is a special case of (10), so one can define its τ-symbol for any τ, and not only the standard symbol. Let τ_1 and τ_2 be two arbitrary real numbers. One can obtain the τ_2-symbol of a differential operator in terms of the τ_1-symbol through the formula,

$$\sigma^{\tau_2}(x,p)=\sum_\alpha\ (\tau_1-\tau_2)^{|\alpha|}\partial_p^\alpha P^\alpha\sigma^{\tau_1}(x,p). \tag{12}$$

An interesting point about symbols is that they have a composition rule. Let A' and A'' be differential operators with symbols σ'^τ and σ''^τ respectively, then the symbol of the composition $A'\circ A''$ has the form

$$\sigma^\tau(x,p)=\sum_{\beta,\gamma}\ \frac{(-1)^{|\beta|}\tau^{|\beta|}(1-\tau)^{|\gamma|}}{\beta!\,\gamma!}\,(\partial_p^\gamma P^\beta\sigma'^\tau(x,p))(\partial_p^\beta P^\gamma\sigma''^\tau(x,p)). \tag{13}$$

The composition formula defines an associative, noncommutative product on the space of symbols, different for each τ which we denote by $\sigma'^{\tau} *_{\tau} \sigma''^{\tau}$.

The Weyl symbol has the property

$$\sigma_A^{1/2}(x,p) = \overline{\sigma_{A^\dagger}^{1/2}(x,p)}, \tag{14}$$

where the bar means complex conjugation and $A^\dagger$ is the adjoint operator. So $A = A^\dagger$ is equivalent to the real valuedness of the Weyl symbol.

We want now to compute the standard symbol of the operator associated to a function on the phase space by one of the ordering rules (4).[3] We assume that the function $\mathscr{F}((i/\hbar)s\cdot t)$, which determines the ordering rule, is always different from zero, has $\mathscr{F}(0)=1$ and can be expanded as

$$\mathscr{F}\left(\frac{i}{\hbar}\, s\cdot t\right) = \sum_m \mathscr{F}_m \left(\frac{i}{\hbar}\, s\cdot t\right)^m. \tag{15}$$

Using that

$$\exp\left(\frac{i}{\hbar}\,(t\cdot\hat{q} + s\cdot\hat{p})\right) = \exp\frac{is\cdot t}{2\hbar}\exp\frac{it\cdot\hat{q}}{\hbar}\exp\frac{is\cdot\hat{p}}{\hbar}, \tag{16}$$

the operator $\hat{f}$ in (4) can be written as

$$\hat{f} = \int d^n s\, d^n t\, \mathscr{F}\left(\frac{i}{\hbar}\, s\cdot t\right) \bar{f}(s,t) \exp\frac{is\cdot t}{2\hbar}\exp\frac{it\cdot\hat{q}}{\hbar}\exp\frac{is\cdot\hat{p}}{\hbar}. \tag{17}$$

So, according to (9), the standard symbol of this operator is

$$\sigma_{\hat{f}}^0 = \int d^n s\, d^n t\, \mathscr{F}\left(\frac{i}{\hbar}\, s\cdot t\right) \bar{f}(s,t) \exp\frac{is\cdot t}{2\hbar}\exp\frac{it\cdot q}{\hbar}\exp\frac{is\cdot p}{\hbar} \tag{18}$$

and substituting the Taylor expansion for $\mathscr{F}$(15) and for the exponential, it is easy to see that the standard symbol $\sigma_{\hat{f}}^0(q,p)$ of $\hat{f}$ is

$$\sigma_{\hat{f}}^0(q,p) = \sum_m (-i\hbar)^m F_m \left(\sum_{i=1}^n \partial p_i \partial q_i\right)^m f(q,p), \tag{19}$$

where

$$F_m = \sum_{k=0}^m \mathscr{F}_k \frac{1}{(m-k)!}\left(\frac{1}{2}\right)^{m-k}, \tag{20}$$

that is,

$$e^{x/2}\mathscr{F}(x) = \sum_m F_m x^m. \tag{21}$$

For a monomial $f = q^l p^r$,

$$\sigma_{\hat{f}}^0(q,p) = \sum_m (-i\hbar)^m F_m \frac{1}{(l-m)!\,l!\,(r-m)!\,r!}\, q^{l-m} p^{r-m}. \tag{22}$$

Let us see some examples. If $\mathscr{F} = \exp(-is\cdot t/2\hbar)$, then

$$\sigma^0_{\hat f}(q,p)=f(q,p), \tag{23}$$

so quantizing with this ordering rule is equivalent to consider the functions on the phase space as standard symbols of the quantum operators. More generally, if $\mathscr{T}=\exp((is\cdot t)/2\hbar(\tau-1/2))$, the τ-symbol of the quantum operator is the function itself.

For a general ordering rule, the same interpretation is possible. The classical observable is considered as a new kind of symbol of the quantum operator. One can express this new symbol in the same way as (11). Let us express the action of operator $\hat f$ through the standard symbol (19),

$$\begin{aligned}\hat f u(q)&=\frac{1}{(2\pi\hbar)^n}\int d^n p\,d^n q'\,\exp\left(\frac{i}{\hbar}\,p\cdot(q-q')\right)\sigma^0_{\hat f}(q,p)u(q')\\&=\frac{1}{(2\pi\hbar)^n}\int d^n p\,d^n q'\,\exp\left(\frac{i}{\hbar}\,p\cdot(q-q')\right)\cdot\sum_m\,(-i\hbar)^m F_m\left(\sum_{i=1}^n\,\partial_{p_i}\partial_{q_i}\right)^m f(q,p)u(q').\end{aligned} \tag{24}$$

Integrating by parts ∂_{p_i},

$$\begin{aligned}\hat f u(q)&=\sum_m\,F_m\,\frac{1}{(2\pi\hbar)^n}\int d^n p\,d^n q'\,\exp\left(\frac{i}{\hbar}\,p\cdot(q-q')\right)\cdot\partial^m_\rho f(q+\rho(q'-q),p)|_{\rho=0}u(q')\\&=\sum_m\,F_m\,\frac{1}{(2\pi\hbar)^n}\,\frac{1}{2\pi\hbar}\int d^n p\,d^n q'\,d\rho\,d\zeta\,\exp\left(\frac{i}{\hbar}\,p\cdot(q-q')\right)\\&\quad\times\exp\left(-\frac{i\zeta\rho}{\hbar}\right)\cdot\left(\frac{i\zeta}{\hbar}\right)^m f(q+\rho(q'-q),p)u(q'),\end{aligned} \tag{25}$$

and finally,

$$\begin{aligned}\hat f u(q)&=\frac{1}{(2\pi\hbar)^n}\int d^n p\,d^n q'\,\exp\left(\frac{i}{\hbar}\,p\cdot(q-q')\right)\cdot\,\frac{1}{2\pi\hbar}\int d\rho\,d\zeta\\&\quad\times\exp\left(-\frac{i\zeta}{\hbar}\left(\rho-\frac{1}{2}\right)\right)\mathscr{T}\left(\frac{i\zeta}{\hbar}\right)f(q+\rho(q'-q),p)u(q').\end{aligned} \tag{26}$$

It is easy to see that for $\mathscr{T}(is\cdot t/\hbar)=\exp((is\cdot t)/2\hbar(\tau-1/2))$, one gets τ-symbol. Equation (26) can also be interpreted in the following way. For each ρ, the function $f(q+\rho(q'-q),p)$ gives, under the integral, a different operator, and we are taking a linear superposition of all of them, whose coefficients are a distribution which is the Fourier transform of the function $F(i\zeta/\hbar)=\exp(i\zeta/2\hbar)\mathscr{T}(i\zeta/\hbar)$. We will call these symbols $\mathscr{T}$-symbols, and will denote them by $\sigma^{\mathscr{T}}$.

Let $\mathscr{T}_1,\mathscr{T}_2$ be two arbitrary functions. By using the standard symbol, one can obtain the $\mathscr{T}_2$-symbol of an operator in terms of the $\mathscr{T}_1$-symbol,

$$\sigma^{\mathscr{T}^2}(q,p)=\sum_m\,(-i\hbar)^m F^{12}_m\left(\sum_{i=1}^n\,\partial_{p_i}\partial_{q_i}\right)^m\sigma^{\mathscr{T}^1}(q,p), \tag{27}$$

where

$$F^{12}_m=\sum_{r=0}^m\,F^1_{m-r}\tilde F^2_r,\quad \frac{1}{F^2(x)}=\sum_m\,\tilde F^2_m x^m,\quad \frac{F^1(x)}{F^2(x)}=\frac{\mathscr{T}^1(x)}{\mathscr{T}^2(x)}=\sum_m\,F^{12}_m x^m. \tag{28}$$

The composition formula for $\mathscr{T}$-symbols can be computed from the composition formula (13) for $\tau=0$ and substituting the standard symbols in terms of the $\mathscr{T}$-symbols, (19). The result is that the $\mathscr{T}$-symbol of the composition of operators $A'\circ A''$ in terms of the symbols $\sigma'^{\mathscr{T}}$ and $\sigma''^{\mathscr{T}}$ of A' and A'', is

$$\sigma^{\mathscr{T}}=\sigma'^{\mathscr{T}}*_{\mathscr{T}}\sigma''^{\mathscr{T}}=\sum_{\delta+\epsilon=\mu+\nu}(-i\hbar)^{|\delta+\epsilon|}C_{\delta,\epsilon,\mu,\nu}(\partial_p^{\delta}\partial_q^{\mu}\sigma'^{\mathscr{T}})(\partial_p^{\epsilon}\partial_q^{\nu}\sigma''^{\mathscr{T}}), \tag{29}$$

where

$$C_{\delta,\epsilon,\mu,\nu}=\sum_{\beta=0}^{\min(\delta,\mu)}\sum_{\gamma=0}^{\min(\epsilon,\nu)}\sum_{\alpha=0}^{\min(\delta-\beta,\nu-\gamma)}\tilde{F}_{|\delta+\epsilon-\beta-\gamma-\alpha|}F_{|\beta|}F_{|\gamma|}\cdot\frac{(\delta+\epsilon\beta-\gamma-\alpha)!}{\beta!\,\gamma!(\mu-\beta)!(\epsilon-\gamma)!\,\alpha!(\delta-\beta-\alpha)!(\nu-\gamma-\alpha)!}. \tag{30}$$

It is also easy to see that if $F_m=0$ for odd m, then Hermitian operators have real $\mathscr{T}$-symbols.

III. DEFORMATIONS OF POISSON ALGEBRAS

We consider a symplectic manifold M with local symplectic coordinates (q_i,p_i), $i=1,\ldots,n$, and symplectic two form, ω. On the associative, commutative algebra $N=C^{\infty}(M)$ there is a Poisson algebra structure given by

$$\{f,g\}=\omega(X_f,X_g), \tag{31}$$

where $f,g\in N$ and X_f,X_g are the Hamiltonian vector fields associated to f,g defined by

$$df(\cdot)=\omega(X_f,\cdot). \tag{32}$$

Let $E(N,\lambda)$ be the space of formal series in λ with coefficients in N. A formal deformation of the associative commutative algebra of pointwise multiplication $C^{\infty}(M)$ is a bilinear map $*:E(N,\lambda)\times E(N,\lambda)\to E(N,\lambda)$ given by a formal series

$$u*v=\sum_{r=0}^{\infty}\lambda^r C_r(u,v)\quad u,v\in E(N,\lambda) \tag{33}$$

with $C_r(u,v)$ bidifferential operators, $C_0(u,v)=uv$, and such that it satisfies the associativity condition

$$(u*v)*w=u*(v*w)\quad u,v,w\in E(N,\lambda). \tag{34}$$

In general, formal deformations are not commutative. Let M be R^{2n}; the product of $\mathscr{T}$-symbols (29) is a formal deformation of the associative algebra $C^{\infty}(R^{2n})$, with deformation parameter $i\hbar$. The bidifferential operators $C_r(u,v)$ have constant coefficients and the associativity is guaranteed by the associativity of the composition of operators. These deformations satisfy the additional condition

$$C_1(u,v)-C_1(v,u)=\{u,v\}. \tag{35}$$

For τ-symbols, notice that (13) can be expressed as

$$u(q,p)*_r v(q,p)=\sum_m \frac{(i\hbar)^m}{m!}\left((\tau-1)\sum_{i=1}^{n}\partial'_{p_i}\partial''_{q_i}+\tau\sum_{i=1}^{n}\partial''_{p_i}\partial'_{q_i}\right)^m (u(q,p),v(q,p)), \tag{36}$$

where the notation means

$$\partial'_p\partial''_q(u(q,p),v(q,p))=\partial_p u(q,p)\partial_q v(q,p), \tag{37}$$

so formally one can write

$$u(q,p)*_\tau v(q,p)=\exp(i\hbar)\left((\tau-1)\sum_{i=1}^{n}\partial'_{p_i}\partial''_{q_i}+\tau\sum_{i=1}^{n}\partial''_{p_i}\partial'_{q_i}\right)^m\cdot(u(q,p),v(q,p)). \tag{38}$$

For $\tau=1/2$, the argument in the exponential is (one half of) the Poisson bracket. It has been shown in Ref. 6 that the exponential is the only function of the Poisson bracket which gives an associative formal deformation.

The bracket $\{u,v\}^{(\mathcal{F})}=(i\hbar)^{-1}(u*_{\mathcal{F}}v-v*_{\mathcal{F}}u)$ satisfies the Jacobi Identity,

$$S\{\{u,v\}^{(\mathcal{F})},w\}^{(\mathcal{F})}=0, \tag{39}$$

where S means circular symmetrization with respect to the entries, u,v,w. For the formal deformation associated to any ordering rule, the zero order term in $\hbar$ of this bracket is the Poisson bracket, so we have a formal deformation of the Poisson bracket. For $\tau=1/2$, the corresponding deformation is the Moyal bracket[7]

$$\{u,v\}^{(M)}=2\sinh\left(\frac{\nu}{2}\left(\sum_{i=1}^{n}\partial''_{p_i}\partial'_{q_i}-\sum_{i=1}^{n}\partial'_{p_i}\partial''_{q_i}\right)\right)(u,v) \tag{40}$$

with $\nu=(i\hbar)^2$.

Consider an associative formal deformation, for example de Weyl deformation, $u*_W v$. Let T be a map $T:E(N,\lambda)\to E(N,\lambda)$, such that it can be expressed by the formal series

$$T=Id+\sum_{s=1}^{\infty}\lambda^s T_s, \tag{41}$$

where T_s are differential operators on N. One can construct the formal deformation given by

$$u*_T v=T(T^{-1}u*_W T^{-1}v), \tag{42}$$

where T^{-1} has an obvious meaning. It is associative by construction. One can define the T-symbol of an operator $\hat{f}$ as

$$\sigma^T_{\hat{f}}=T\sigma^W_{\hat{f}} \tag{43}$$

and the product of T-symbols is the deformation written above (42). If the series T in $\lambda=i\hbar$ is such that $T_r=0$ for odd r, then the T-symbol of an Hermitian operator is real. We must point out that in order for this definition of T-symbols to be meaningful, the formal series (43) must be convergent, so some restrictions on T or on the class of functions which are T-symbols, should be imposed. We are not going to elucidate this point in this paper.

In general, two associative formal deformations are called equivalent if there is a series T connecting them by means of Eq. (42). It is easy to see that this is an equivalence relation.

All deformations (29) are equivalent by means of the formal series (27). The quantization maps (that is, the interpretation of functions on the phase space as symbols of operators) given by

two equivalent deformations are not the same, since they associate different operators to the same classical observable. But there exists a "classical" observable $g(q,p,\hbar)$ related to the classical observable $f(q,p)$ by $g=Tf$ (in particular, $g\to f$ when $\hbar\to 0$) and such that the operator associated to g with one quantization map is the same as the operator associated to f with the other quantization map. In this sense, one can say that the quantum theories are essentially equivalent.

The commutator of T-symbols is also a formal deformation of the Poisson bracket. Following Ref. 6, two formal deformations

$$\begin{aligned}\{u,v\}^{(A)}&=\{u,v\}+\sum_{r=1}^{\infty}\lambda^r C_r^{(A)}(u,v),\\ \{u,v\}^{(B)}&=\{u,v\}+\sum_{r=1}^{\infty}\lambda^r C_r^{(B)}(u,v),\end{aligned}\tag{44}$$

are c-equivalent if there is a formal series (41) such that the relation

$$T\{u,v\}^{(A)}=\{Tu,Tv\}^{(B)}\tag{45}$$

is formally satisfied. Two equivalent associative formal deformations can give the same deformation of the Poisson bracket, and in this case the map sending the operators obtained with one quantization map to the operators obtained with the other quantization map preserves commutators, so it is a unitary transformation, irrelevant in the quantum theory. In this way, we can focus on the easier issue of equivalence of deformations of the Poisson bracket.

We are going to construct inequivalent deformations. Given a formal series like (44), it is a formal deformation if the Jacobi identity (39) is satisfied. At each order, the Jacobi identity is

$$S\sum_{r+s=t} C_s(C_r(u,v),w)=0 \quad r,s\geqslant 0,\tag{46}$$

which can be written as

$$\partial C_t(u,v,w)=SC_t(\{u,v\},w)+S\{C_t(u,v),w\}=-S\sum_{r+s=t} C_s(C_r(u,v),w) \quad r,s\geqslant 1.\tag{47}$$

The ∂ symbol in the left hand side of Eq. (47) is the differential operator of the Chevalley cohomology, acting on p-cochains which are alternate p-differential maps of N^p to N. If the Jacobi identity is satisfied up to order $t-1$, then the right hand side of Eq. (47) (notice that it only depends on C_r, $r<t$) is a 3-cocycle, and in order for the Jacobi identity to be satisfied up to order t, it must be a cobord. For $t=0$ the identity is trivially satisfied and for $t=1$

$$\partial C_1(u,v,w)=0,\tag{48}$$

which means that C_1 is a 2-cocycle in the Chevalley cohomology.

Let us write Eq. (45) at order t,

$$\sum_{r+s=t} T_s C_r^{(A)}(u,v)-\sum_{r+s+s'=t} C_r^{(B)}(T_s u,T_{s'}v)=0, \quad r,s,s'\geqslant 0,\tag{49}$$

which can be rewritten as

$$C_t^{(A)}(u,v)-C_t^{(B)}(u,v)+G_t(u,v)=\partial T_t(u,v),\tag{50}$$

where G_t collects all terms depending on $C_r^{(A)}$, $C_r^{(B)}$ and T_r for $r<t$. For our purposes, it will be enough to say that $G_t=0$ if $T_r=0$ for $r<t$. Two deformations are equivalent at order 1 if the difference of the two cocycles $C_1^{(A)}-C_1^{(B)}$ is a cobord ∂T_1. If the cocycle C_1 is itself a cobord, the deformation is equivalent to the zero deformation at order 1, and we say that the deformation is trivial to this order. For the Moyal deformation $C_1^{(M)}$ is a nontrivial 2-cocycle. Indeed, the dimension of the second order cohomology space is one for a flat Poisson manifold, so we have that at order one there is only one nontrivial possibility.

Consider a deformation $\{u,v\}^{(A)}$ as in Eq. (45). Let us construct another deformation, by modifying $C_2^{(A)}$ with a term proportional to $C_1^{(A)}$:

$$C_1^{(B)}=C_1^{(A)}, \quad C_2^{(B)}=C_2^{(A)}+\mu C_1^{(A)}. \tag{51}$$

It can be shown inductively that there is a general solution for $C_r^{(B)}$ satisfying the Jacobi identity, of the form

$$C_r^{(B)}=\sum_{s=0}^{r} \mu_s \binom{r-s}{s} C_{r-s}^{(A)}, \tag{52}$$

in terms of the binomial coefficients $\binom{r-s}{s}$. Notice that at each order the expansion in μ is finite. If we modify the term of order $t+1$ instead of the order two, then the form of the successive $C_r^{(B)}$ is

$$C_r^{(B)}=\sum_{s=0}^{[r/t]} \mu_s \binom{r-ts}{s} C_{r-ts}^{(A)}, \tag{53}$$

where $[r/t]$ is the integer part of r/t. If the cocycle $C_1^{(A)}$ is nontrivial, the deformations obtained in this way are not equivalent, neither to the original deformation, nor equivalent between them. The Moyal bracket has this feature, so this mechanism produces deformations which are not equivalent to the Moyal bracket.

Now we are going to consider the effect of making a canonical transformation. The Moyal bracket can be expressed in a covariant way by writing the differential operators $C_r^{(M)}$ as

$$C_r^{(M)}(u,v)=\frac{1}{2^{2r}(2r+1)!}\, P^{2r+1}(u,v), \tag{54}$$

$$P^r(u,v)=\Lambda^{i_1 j_1}\cdots\Lambda^{i_r j_r}\nabla_{i_1\cdots i_r}u\,\nabla_{j_1\cdots j_r}v, \tag{55}$$

where Λ^{ij} is the 2-tensor which is the inverse matrix of the symplectic form, and ∇ is the covariant derivative associated to a flat symplectic connection, that is, such that $\nabla\Lambda=0$. The bracket satisfies the Jacobi identity if both conditions are satisfied (See Ref. 6). In $M=\mathrm{R}^{2n}$, one can choose coordinates (q,p) in such way that the coefficients of the connection are zero, and we recover the Moyal bracket as in (40). If we change the flat connection, the Moyal bracket will be different, but in some symplectic coordinates (Q,P), it is expressed again in the usual form. Therefore, to quantize in different global symplectic coordinates corresponds to take the Moyal bracket with different flat connections. We can ask if the Moyal deformations obtained with different flat connections are equivalent (notice that the map T which realizes the equivalence can change even the basic commutators). We do not have a rigorous answer to that question, but we are going to show that making an infinitesimal canonical transformation we stay in the same equivalence class.

Let us make the canonical transformation $(q,p)\to(Q(q,p),P(q,p))$. A function of the phase space $\mathscr{F}$ has local representations $f(q,p)$, and $F(Q,P)$ in the old and new symplectic coordinates respectively, satisfying

$$f(q,p)=F(Q(q,p),P(q,p)). \tag{56}$$

If the transformation is infinitesimal with parameter ϵ, then

$$f(q,p)=F(Q(q,p),P(q,p))\approx F(q,p)+\epsilon\{F(q,p),\eta(q,p)\} \tag{57}$$

or

$$F(q,p)\approx f(q,p)-\epsilon\{f(q,p),\eta(q,p)\}, \tag{58}$$

where the function η is the generator of the infinitesimal canonical transformation. We denote by superindices A and B the Moyal deformations corresponding to the symplectic coordinates (q,p) and (Q,P) respectively. Let $H(Q,P)$ be the local representation of $\{\mathscr{F},\mathscr{G}\}^{(B)}$. Using (57)

$$H(Q(q,p),P(q,p))\approx H(q,p)+\epsilon\{H(q,p),\eta(q,p)\} \tag{59}$$

and

$$\begin{aligned} H(q,p)&=\{F(q,p),G(q,p)\}^{(A)}\\ &\approx\{f(q,p),g(q,p)\}^{(A)}-\epsilon\{\{f(q,p),\eta(q,p)\},g(q,p)\}^{(A)}\\ &\quad+\epsilon[\{f(q,p),\{\eta(q,p),g(q,p)\}\}^{(A)}]. \end{aligned} \tag{60}$$

So in the local representation (q,p),

$$\{\mathscr{F},\mathscr{G}\}^{(B)}-\{\mathscr{F},\mathscr{G}\}^{(A)}=\epsilon\{\{f,g\}^{(A)},\eta\}-\epsilon[\{\{f,\eta\},g\}^{(A)}-\{f,\{g,\eta\}\}^{(A)}]. \tag{61}$$

Let us look at this equation order by order in $\nu=(i\hbar)^2$,

$$\begin{aligned} C_1^{(B)}-C_1^{(A)}&\approx\epsilon[\{C_1^{(A)}(f,g),\eta\}-C_1^{(A)}(\{f,\eta\},g)-C_1^{(A)}(f,\{g,\eta\})]\\ &=\epsilon[\partial(C_1^{(A)}(.,\eta))(f,g)-\partial C_1^{(A)}(f,g,\eta)], \end{aligned} \tag{62}$$

and since $\partial C_1^{(A)}=0$, then $T_1=\epsilon C_1^{(A)}(.,\eta)$. At order r, using that the bracket A satisfies the Jacobi identity, one can see that

$$(C_r^{(B)}-C_r^{(A)}+G_t)(f,g)\approx\epsilon[\partial(C_r^{(A)}(.,\eta))(f,g)], \tag{63}$$

so $T_r=\epsilon C_r^{(A)}(.,\eta)$.

In this way we have shown that for global symplectic coordinates differing by an infinitesimal transformation, the Moyal brackets belong to the same equivalence class of deformations. It seems that all deformations used in physics to quantize a Hamiltonian system fall in the same equivalence class, and perhaps other deformations, as the ones we constructed below, inequivalent to the Moyal bracket, do not admit a representation by Hermitian operators on a Hilbert space, in the same way that the trivial deformation, the Poisson bracket, does not admit one.

IV. APPLICATIONS TO QUANTUM INTEGRABILITY OF TWO DIMENSIONAL HAMILTONIAN SYSTEMS

A Hamiltonian system with 2 degrees of freedom is classically integrable if there is a function $I(q,p)$ independent of the Hamiltonian such that the Poisson bracket $\{H,I\}=0$. A quantization map sends H and I to the operators $\hat{H}$ and $\hat{I}$, but in general, these operators do not commute. One can ask if there exists an ordering rule which makes the corresponding operators commute, or more generally, if there exists a particular quantization map for which the operators commute. We have found, when dealing with the examples that the first possibility is not satisfied in most of the

cases, so we ask for more general quantization maps. This seems possible because one can find a classical canonical transformation where H and I are the new momenta, and the Weyl quantization map brings them to operators which commute trivially. Of course, such canonical transformation could be very difficult to find, or might not be globally well defined, so this procedure seems to be impractical in order to analyze the problem of quantum integrability.

But we saw in Section III that infinitesimal classical canonical transformations are reflected in the commutator of symbols as a change to a equivalent deformation. Assuming that this is true for finite canonical transformations we can look for deformations, equivalent to the Moyal bracket, such that H and I have a vanishing bracket. The corresponding quantization map consists in interpreting the functions on the phase space as T-symbols of the quantum operators. The Weyl symbols of the quantum operators are related with the T-symbols by

$$\sigma^W_{\hat{F}} = T^{-1}\sigma^T_{\hat{F}} = T^{-1}F = VF. \tag{64}$$

In Ref. 9 the problem of quantum integrability of some two dimensional systems is analyzed in terms of the Moyal bracket. They found that one has to add, in most of the cases, quantum correction terms (of order $O(\hbar)$) to I, and sometimes to H, in order to write the Weyl symbol of the commuting quantum operators which make the system quantum integrable. So all we have to check is if these expansions in $\hbar$ for the Weyl symbols can be written in the form (64) for a series of differential operators $T^{-1}=V$.

We are going to analyze some examples of integrable systems which present quantum corrections. The quantum integrability of all the examples we use has been proved by Hietarinta.[9] We show here explicitly that the quantum corrections come from a series V satisfying (64) and consequently, that the quantum corrections can be eliminated by an appropriate choice of the quantization map, in terms of T-symbols.

Example 1: The following Hamiltonian is classically integrable

$$H_1 = \frac{1}{2}(p_x^2+p_y^2) + \frac{16}{3}y^3 + yx^2 + \frac{a}{2}(x^2+16y^2) + \mu x^{-2} + \nu x^{-6}, \tag{65}$$

with the invariant given by

$$\begin{aligned} I_1 = {} & p_x^4 + p_x^2(2ax^2 + 4x^2y + 4\mu x^{-2} + 4\nu x^{-6}) - \frac{4}{3}p_x p_y x^3 - \frac{4}{3}ax^4y - \frac{4}{3}x^4y^2 \\ & + \frac{8}{3}\mu y + 8\nu y x^{-4} - \frac{2}{9}x^6 + a^2x^4 + 4(a\nu+\mu^2)x^{-4} + 8\mu\nu x^{-8} + 4\nu^2 x^{-12}. \end{aligned} \tag{66}$$

In order to the Moyal bracket $\{H_1, I_1\}^{(M)}$ vanish, the invariant must be corrected with

$$\Delta I_1 = -\hbar^2(6\mu x^{-4} + 42\nu x^{-8}), \tag{67}$$

so the Weyl symbol of the quantum operator is $I_1 + \Delta I_1$. We want to know if there is a quantization map in which the classical observable, without quantum corrections, is the symbol of the quantum operators. It can be proven that there is no ordering rule satisfying this condition. Nevertheless, for this particular example, a trick that consists in adding a term αH_1^2 to I_1 and considering a unusual ordering rule works. This is done in Ref. 9, but we obtained a different numerical result. The value of α is -4, and the ordering rule must be such that

$$\mathscr{F}'(0) = 0; \quad \mathscr{F}''(0) = 65/128. \tag{68}$$

Both results become the same if in the computation of Ref. 9 the effect of changing the ordering rule in the new terms H_1^2 is taken into account. Nevertheless, this method does not work for other Hamiltonians, and we are lead to consider more general quantization maps.

The series

$$V_1 = Id + (i\hbar)^2\left(\frac{1}{8}\,\partial_{p_x}^2\partial_x^2 - \left(\frac{a}{16}+\frac{y}{8}\right)\partial_{p_x}^2\partial_x^2\partial_y\right), \tag{69}$$

when applied to H_1 and I_1 reproduces the quantum corrections, so the T-symbols of the quantum operators are H_1 and I_1. Since that the series V_1 is truncated at order $\hbar^2$, it is easy to get the inverse series T_1,

$$\begin{aligned} V_1 &= Id + (i\hbar)^2 A_1, \\ T_1 &= Id + \sum_{r=1} (-1)^r (i\hbar)^{2r} A_1^r. \end{aligned} \tag{70}$$

From here, we can see that if the Weyl symbol $\sigma_{\hat{F}}^W$ of an operator is a polynomial function of p_x, then the series $T_1\sigma_{\hat{F}}^W$ is truncated at some order in $(i\hbar)^2$. This is a sufficient, although not necessary, condition for the T-symbol of the operator $\hat{F}$ be well defined.

Example 2: This is another example of classically integrable system:

$$H_2 = \tfrac{1}{2}\,(p_x^2+p_y^2) + x^4 + 6x^2y^2 + 8y^4 + \kappa(x^2+4y^2) + \mu x^{-2} + \nu x^{-6} + \lambda y^{-2}, \tag{71}$$

$$\begin{aligned} I_2 = {} & p_x^4 + 4p_x^2(x^4 + 6x^2y^2 + \kappa x^2 + \mu x^{-2} + \nu x^{-6}) - 16p_xp_yx^3y + 4p_y^2x^4 + 8\lambda y^{-2}x^4 + 4\mu^2x^{-4} \\ & + 8\mu\nu x^{-8} + 8\mu x^2 + 16\mu y^2 + 4\mu^2x^{-12} + 8\nu\kappa x^{-4} + 8\nu x^{-2} + 48\nu 2x^{-4}y^2 + 4\kappa^2x^4 + 8\kappa x^6 \\ & + 16\kappa x^4y^2 + 4x^8 + 16x^6y^2 + 16x^4y^4, \end{aligned} \tag{72}$$

and the quantum corrections are

$$\Delta I_2 = -\hbar^2(6\mu x^{-4} + 42\nu x^{-8} + 12x^2). \tag{73}$$

The series V_2 is,

$$V_2 = Id + (i\hbar)^2\left(\frac{1}{8}\,\partial_x^2\partial_{p_x}^2 + \frac{a}{48}\,\partial_x^3\partial_y\partial_{p_x}\partial_{p_y} + \frac{y}{8}\,\partial_x^3\partial_{p_x}\partial_{p_y}\right). \tag{74}$$

In this example, the condition for the finiteness of the series is that the Weyl symbol of the operator must be a polynomial function of p_x and p_y.

In the following examples, the Hamiltonian also needs quantum corrections in order to be quantum integrable. In those cases, it is obvious that no ordering rule will restore the integrability.

Example 3: For the Holt Hamiltonian,[10]

$$H_3 = \tfrac{1}{2}\,(p_x^2+p_y^2) + \tfrac{3}{4}\,x^{4/3} + y^2x^{-2/3} + \delta x^{-2/3}, \tag{75}$$

which is classically integrable, the integral is

$$I_3 = p_y^3 + \tfrac{3}{2}\,p_yp_x^2 + p_y(-\tfrac{9}{2}\,x^{4/3} + 3x^{-2/3}y^2 + 3\delta x^{-2/3}) + 9x^{1/3}yp_x. \tag{76}$$

The quantum corrections are

$$\Delta H_3 = -\frac{5}{72}\hbar^2 x^{-2}, \quad \Delta I_3 = -\frac{5}{72}\hbar^2 p_y x^{-2}. \tag{77}$$

The operator reproducing the quantum corrections is

$$V_3 = Id + (i\hbar)^2 \frac{5}{144} x^{-4/3}\partial_y^2. \tag{78}$$

The series is truncated if the Weyl symbol is a polynomial function of y.

Example 4: The Hamiltonian,[11]

$$H_4 = \tfrac{1}{2}(p_x^2 + p_y^2) + (xy)^{-2/3}, \tag{79}$$

is classically integrable,[11]

$$I_4 = p_y p_x (x p_y - y p_x) + 2(xy)^{-2/3}(x p_x - y p_y). \tag{80}$$

The quantum corrections are

$$\Delta H_4 = -\frac{5}{72}\hbar^2 (x^{-2} + y^{-2}), \quad \Delta I_4 = -\frac{5}{72}\hbar^2 (x p_x y^{-2} - y p_y x^{-2}). \tag{81}$$

The operator reproducing the quantum corrections is

$$V_4 = Id + (i\hbar)^2 \frac{5}{72}\left(\frac{9(xy)^{8/3}}{10y^4}\partial_x^2 + \frac{9(xy)^{8/3}}{10x^4}\partial_y^2\right) + (i\hbar)^2 \frac{5}{72}\left(\frac{1}{xy}\partial_{p_x}\partial_{p_y} + \frac{6y}{5x^2}\partial_{p_x}^2\partial_y + \frac{6x}{5y^2}\partial_{p_y}^2\partial_x\right). \tag{82}$$

In this example, it is more difficult to analyze the convergence of the series because the non-polynomial terms in the coefficients of V_4. But let us make a canonical point transformation,

$$x = X^{-3/2}, \quad p_x = -\frac{2}{3}P_X X^{5/2}, \quad x = X^{-3/2}, \quad p_x = -\frac{2}{3}P_X X^{5/2}. \tag{83}$$

The Hamiltonian and the integral have polynomial form,

$$\begin{aligned} H_5 &= \frac{2}{9}(P_X^2 X^5 + P_Y^2 Y^5) + XY, \\ I_5 &= \frac{4}{3}(P_Y X Y^2 + P_X Y X^2) + \frac{8}{27}(P_X^2 P_Y X^5 Y + P_Y^2 P_X Y^5 X). \end{aligned} \tag{84}$$

The Hamiltonian is now ordering dependent, but the quantum corrections are also polynomial,

$$\Delta H_5 = \hbar^2 \frac{5}{18}(X^3 + Y^3), \quad \Delta I_5 = \hbar^2 \frac{10}{27}(P_Y X^3 Y + P_X Y^3 X), \tag{85}$$

and the series V_5 is now very easy to compute,

$$V_5 = Id - (i\hbar)^2 \frac{1}{32}(\partial_X^2 \partial_{P_X}^2 + \partial_Y^2 \partial_{P_Y}^2). \tag{86}$$

The series giving the T-symbol in terms of the Weyl symbol is truncated if the Weyl symbol is polynomial in P_X and P_Y.

V. CONCLUSIONS

In this paper we have analyzed the relationship between the quantum deformations of the Poisson algebra of classical observables and the operatorial quantization. We have described this relationship in terms of generalized symbols of operators, not only for different ordering rules but for more general quantization maps. We have found that the effect of an infinitesimal classical canonical transformation in the quantum theory is just a change to an equivalent deformation. This result suggests that all quantization maps currently used fall into the same equivalence class of deformations. We have explicitly written deformations inequivalent to the Moyal bracket. It is an open question if these deformations have a representation in terms of operators on a Hilbert space.

We have applied these results to the study of two dimensional integrable systems. For the examples considered, we have eliminated the quantum corrections which arise when one requires the preservation of the symmetry in the quantum theory. This procedure could be generalized to other systems presenting more complicated symmetries.

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Left–right asymmetry and minimal coupling

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In this paper we deal with an alternative approach to the description of massless particles of arbitrary spin. Within this scheme chiral components of a spinor field are regarded as fundamental quantities and treated as independent field variables. The free field Lagrangian is built up from the requirement of chiral invariance. This formulation is parallel to the neutrino theory and allows for a formulation that generalizes, to particles of arbitrary spin, the two-component neutrino theory. We achieve a spinor formulation of electrodynamics. In the case of the photon, the nonzero helicity components satisfy Weyl's equations and are associated to observables (electromagnetic fields) whereas the zero helicity components are related to nonobservables (electromagnetic potentials). Within the spinor formulation of electrodynamics the minimal coupling substitution follows as a consequence of the linearity of the interaction and the preference of nature for chiral components, that is, of the left–right asymmetry of nature. © *1996 American Institute of Physics.* [S0022-2488(96)01310-4]

I. INTRODUCTION

Nowadays there is plenty of evidence that nature is asymmetric with respect to chirality (left and right handedness).[1] Within the realm of the fundamental interactions this asymmetry has been realized since the *V-A* theory[2] of weak interactions and has been verified empirically in 1957 in a parity violating process occurring as a result of weak processes.[3] In this paper we will show that, within an alternative scheme for treating massless particles, electrodynamics is also a left–right asymmetric theory. In this way we extend even further the notion that fundamental interactions violate left–right symmetry.

Within the usual formulation of electrodynamics (the tensorial method) the seemingly asymmetrical magnetism[1] cannot be entirely understood in view of the fact that the electromagnetic fields are fundamentally symmetrical (the Lagrangians, in terms of these fields, do not exhibit any left–right asymmetry). Within the spinor method, the one that will be employed in this paper, one has an equivalent formulation of electrodynamics allowing us to understand that magnetism and electrodynamics is, in fact, a basic departure from the left–right asymmetry of nature.

The spinorial formulation proposed here allows us to formulate theories involving massless spin 1 particles in close analogy with massless spin $\frac{1}{2}$ particles. The requirement of chiral invariance, at the free field level, leads to Maxwell's equation in vacuum. The requirement of chiral asymmetry for the linear interaction of the spinor field with matter leads to Maxwell's equation in the presence of matter. Previous spinorial formulations of electrodynamics can be found in Refs. 4 and 5.

In order to generalize the left–right asymmetry to other interactions, as will be done in this paper, let us recall that for massless spin $\frac{1}{2}$ particles one can define chiral components ψ_L and ψ_R of a basic field ψ as follows:

$$\psi_R = \tfrac{1}{2}(I+\gamma^5)\psi, \quad \psi_L = \tfrac{1}{2}(I-\gamma^5)\psi.$$

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Furthermore, under space reflection (P) these components transform as

$$\psi_R \overset{P}{\rightarrow} \psi_R'(x') = \xi \gamma_0 \psi_L(-\mathbf{x},t), \quad \psi_L \overset{P}{\rightarrow} \psi_L'(x') = \xi \gamma_0 \psi_L(-\mathbf{x},t).$$

The intriguing aspect of the weak interactions is that, at low energies, the right and left components interact in a different way with ordinary matter. As a matter of fact, there is no evidence at all that the right-hand component interacts with ordinary matter. Weak interactions are definitely asymmetric with regard to left and right. This follows from the fact that right and left components interact with different strength to matter.

At the Lagrangian level this preference of nature for chiral components can be formulated in a simple way by stating that the Lagrangian is not invariant under the transformation

$$\psi_R \rightarrow \psi_L .$$

Due to the transformation properties of $\psi_R(\psi_L)$ under space reflections, the noninvariance of the Lagrangian under the left–right transformation implies breakdown of space reflection.

The first question that we deal with in this paper is the possibility of extending, to massless particles of arbitrary spin, the usual neutrino theory. We shall see that the spinor method provides an approach that permits us such a generalization. Within the spinor method it is possible to generalize the notion of chiral invariance for particles of arbitrary spin as well as to define chiral components analogous to the ones associated to massless particles of spin $\frac{1}{2}$. Within the spinor method one assigns to a particle of spin s a symmetric spinor ψ of rank $2s$. The definition of chiral components, for a particle of arbitrary spin, is the tensor product of the usual ones.

We propose that these chiral components should be treated as independent variables and that they satisfy extended Dirac equations analogous to the ones satisfied by the left and right neutrino field components. These equations, as will be shown later, follow from the requirement that the free field Lagrangian be chiral invariant.

The generalized chiral components provide a very simple criterion on whether a theory involving masslessness is left–right symmetric or not. The theory is left–right symmetric if the Lagrangian is invariant under the subscript interchange $L \rightarrow R$ (or $R \rightarrow L$). Otherwise the theory is $L-R$ asymmetric. The theory is left–right asymmetric if the coupling of the chiral components to the matter fields occurs with different strengths.

As a byproduct of the formulation of zero-mass particles in terms of chiral components, we will show that it is possible to generalize the two-component neutrino theory to particles of arbitrary spin. The generalized two-component fields satisfy generalized Weyl's equations.

It seems to be worthwhile to analyze whether, besides the neutrinos, there is other evidence in nature of an asymmetric coupling of chiral components of zero-mass particles to ordinary matter. The next, nontrivial, zero-mass particles that couple to ordinary particles are the photons. We find that the coupling of photons reflects some kind of asymmetry between the coupling of chiral components to ordinary matter. We will show that, as in other theories, in electrodynamics chiral asymmetry and parity nonconservation are intimately connected. We shall see that, in electrodynamics, the only consequence of violation of these symmetries is a dynamical one, namely, the minimal substitution way of coupling the electromagnetic fields to matter.

In Sec. II we present a novel approach to the study of massless particles of arbitrary spin. In close analogy with the spin $\frac{1}{2}$ particles we generalize, to arbitrary spin s particles, the usual spin $\frac{1}{2}$ chiral components. One can also generalize the two-component neutrino theory to massless particles of arbitrary spin. This extension is possible in the context of the Bargmann–Wigner (BW) theory. The totally right (left) components have generalized helicity components s $(-s)$ and obey the generalized Weyl's equation.

In order to illustrate how the spinor method works we present in Sec. III the BW theory for spin 1 massive particles. The interesting point here is that clearly BW theory leads to a complete

description of massive particles by associating to these particles a symmetric rank 2 tensor field instead of associating particles to a rank 1 tensor (the usual procedure). The subsidiary condition $\partial^\mu B_\mu = 0$, for instance, follows naturally from the decomposition of the basic BW field into the spinor space and the BW equation.

In Sec. IV we present an alternative approach to spin 1 massless particles. We show how Maxwell's equation in vacuum emerges from the requirement of chiral invariance and the treatment of the chiral components as independent variables.

In Sec. V we formulate electrodynamics in terms of the chiral components ψ_{RR}, ψ_{RL}, ψ_{LR}, and ψ_{LL}. Here we show explicitly that one can formulate QED as long as matter couples only to some components of the chiral fields. That is, QED is manifestly left–right asymmetric.

In Sec. VI we touch on the question of the quantization of the BW fields. This is achieved by imposing an appropriate commutation relation among the BW components.

We end this paper with a section dedicated to conclusions.

II. ALTERNATIVE METHOD FOR THE DESCRIPTION OF MASSLESS PARTICLES

A. Bargmann–Wigner method—Massive particles

It has long been recognized that spinor quantities can be regarded as fundamental in any particle description within the field theoretical approach. In this chapter we will describe the spinor method, proposed by Bargmann and Wigner,[6] for studying massive particles and an alternative method, based on treating the chiral components of a spinor field as independent variables, for the description of massless particles.

Before setting the framework it is important to recall that the description of processes involving particles, within the field theoretic approach, requires the assignment to every particle a set of basic fields. In order to have Lorentz covariance explicitly the fields should have a well defined Lorentz transformation property. It just happens that, as in the case of spin 1 particles, the fields contain more degrees of freedom than the particles they are describing. These extra degrees of freedom of the field are eliminated by imposing complementary conditions on the fields. The case of massive (mass m) spin 1 particles is a very good example of this situation. In this case one associates to these particles (three polarization states) a four-component vector field B_μ. In order to eliminate the extra degree of freedom one imposes the covariant restriction

$$\partial_\mu B^\mu = 0. \tag{2.1}$$

The free field equation is

$$\partial_\mu G^{\mu\nu} = 0, \tag{2.2}$$

where

$$G_{\mu\nu} = \partial_\nu B_\mu - \partial_\mu B_\nu . \tag{2.3}$$

It was pointed out by Bargmann and Wigner[6] that the assignment particle→field is not unique. In fact, within the Bargmann–Wigner method one assigns to a massive particle of mass m and spin s a spinor field of rank $2s$:

$$\psi_{a_1 a_2 \cdots a_{2s}}(x), \quad a_k = 1,2,3,4. \tag{2.4}$$

Since the rank $2s$ spinor field contains, for particles of spin larger than $\frac{1}{2}$, much more degrees of freedom than the particle description requires, one has to impose further restrictions on the field ψ. One requires, as proposed by Bargmann–Wigner, that ψ be symmetric in its spin indices and imposes further that ψ satisfies a set of $2s$ Dirac-like equations; that is,

$$i\partial\!\!\!/_{a_k a_k'}\psi_{a_1\cdots a_k'\cdots a_{2s}}(x)=m\psi_{a_1\cdots a_k\cdots a_{2s}}(x),$$
$$k=1\ldots 2s. \tag{2.5}$$

The set of equations (2.5) can be written under the equivalent form, or permutation of it,

$$i\partial\!\!\!/\otimes I\otimes\cdots\otimes I\psi=m\psi. \tag{2.6}$$

It is then evident, from (2.6), that the Bargmann–Wigner approach is just an extension of Dirac's theory to particles of arbitrary spin.

As a final remark on the whole framework, not only valid for the Bargmann–Wigner method but also for the generalized four-component and two-component theory that will be presented next, we would like to emphasize the need for an explicit representation for $2s$ rank spinors. The method that will be used is to express the $2s$ rank spinor fields as linear combinations of symmetric 4×4 matrices (within the four-spinor framework), or symmetric 2×2 matrices (for the two-spinor framework). The coefficients in these expansions are new fields. The properties of the new fields allow us to establish the connection of our approach to the usual electrodynamics.

In the four-spinor case the symmetric matrices are, by using the notation of Bjorken and Drell,[7]

$$(\sigma_{\mu\nu}C)\quad\text{and}\quad(\gamma_\mu C), \tag{2.7}$$

whereas in the two-spinor case the symmetric matrices are

$$(\sigma^k C_1),\quad k=1,2,3, \tag{2.8}$$

where C is charge conjugation matrix and C_1 is the 2×2 charge conjugation matrix (see Appendix B).

As an example, let us write the decomposition of the rank 2 spinor field $\psi_{a_1a_2}$ associated to a mass m and spin 1 particle in terms of the symmetric matrices $(\gamma^\mu C)$ and $(\sigma^{\mu\nu}C)$. $\psi_{a_1a_2}$ admits the following decomposition:

$$\psi_{a_1a_2}(x)=\sqrt{m}\left\{B_\mu(x)(\gamma^\mu C)_{a_1a_2}-\frac{1}{2m}G_{\mu\nu}(x)(\sigma^{\mu\nu}C)_{a_1a_2}\right\}, \tag{2.9}$$

where the field $B_\mu(x)$ is a vector field (which, as will be shown later, is the usual spin 1 field), and $G_{\mu\nu}(x)$ is a field not yet determined and that, in principle, should involve derivatives of the $B_\mu(x)$ field. This is actually what happens. As will be shown in the next section, from (2.6) and (2.9) it follows that $G_{\mu\nu}$ in (2.9) can be written as

$$G_{\mu\nu}(x)=\partial_\nu B_\mu(x)-\partial_\mu B_\nu(x). \tag{2.10}$$

B. Massless particles—Chiral components

For the description of spin $\frac{1}{2}$ massless particles (neutrinos) one defines, as usual, the right and left components of a four-component spinor $\tilde{\psi}$ as

$$\tilde{\psi}_R=\tfrac{1}{2}(I+\gamma^5)\tilde{\psi}, \tag{2.11a}$$

$$\tilde{\psi}_L=\tfrac{1}{2}(I-\gamma^5)\tilde{\psi}. \tag{2.11b}$$

The free field Lagrangian, in terms of the right and left components, is

$$L=\bar{\tilde{\psi}}_R i\ \partial\!\!\!/\psi_L+\bar{\tilde{\psi}}_L i\ \partial\!\!\!/\psi_R\equiv\bar{\psi} i\ \partial\!\!\!/\psi. \tag{2.12}$$

By treating the left and right components independently one gets as equations of motion the following equations:

$$i\partial\!\!\!/\psi_R=0, \tag{2.13a}$$

$$i\partial\!\!\!/\psi_L=0. \tag{2.13b}$$

For the description of massless particles of arbitrary spin we assume, in analogy with the BW theory for massive particles, that a particle of spin s is associated to a symmetric spinor field of rank $2s$:

$$\tilde{\psi}_{a_1\cdots a_k\cdots a_{2s}}(x),\quad a_k=1,2,3,4. \tag{2.14}$$

For the rank $2s$ spinor field (2.14) one can define a set of chiral components as follows:

$$\tilde{\psi}_{R\cdots R}(x)\equiv\tilde{\psi}_{R_{a_1}\cdots R_{a_{2s}}}(x)=\tfrac{1}{2}(I+\gamma^5)_{a_1a_1'}\tfrac{1}{2}(I+\gamma^5)_{a_2a_2'}\cdots\tfrac{1}{2}(I+\gamma^5)_{a_{2s}a_{2s}'}\tilde{\psi}_{a_1'\cdots a_{2s}'}(x),$$

$$\tilde{\psi}_{R\cdots RL}(x)\equiv\tilde{\psi}_{R_{a_1}\cdots R_{a_{2s-1}}L_{a_{2s}}}(x)=\tfrac{1}{2}(I+\gamma^5)_{a_1a_1'}\cdots\tfrac{1}{2}(I+\gamma^5)_{a_{2s-1}a_{2s-1}'}\cdot\tfrac{1}{2}(I-\gamma^5)_{a_{2s}a_{2s}'}\tilde{\psi}_{a_1'\cdots a_{2s}'}(x),$$

$$\vdots$$

$$\tilde{\psi}_{L\cdots L}(x)\equiv\tilde{\psi}_{L_{a_1}\cdots L_{a_{2s}}}(x)=\tfrac{1}{2}(I-\gamma^5)_{a_1a_1'}\cdots\tfrac{1}{2}(I-\gamma^5)_{a_{2s}a_{2s}'}\tilde{\psi}_{a_1'\cdots a_{2s}'}(x). \tag{2.15}$$

We propose that these components satisfy an equation analogous to (2.13); that is,

$$i\partial\!\!\!/_{a_1a_1'}\tilde{\psi}_{R_{a_1'}R_{a_2}\cdots R_{a_{2s}}}(x)=0,$$

$$i\partial\!\!\!/_{a_1a_1'}\tilde{\psi}_{R_{a_1'}R_{a_2}\cdots L_{a_{2s}}}(x)=0,$$

$$\vdots$$

$$i\partial\!\!\!/_{a_1a_1'}\tilde{\psi}_{L_{a_1'}L_{a_2}\cdots L_{a_{2s}}}(x)=0. \tag{2.16}$$

We shall see in Sec. IV A that these equations follows from chiral invariance of the free Lagrangian.

C. Massless particles—Generalized two-component theory[8]

It is well known that massless particles of spin $\frac{1}{2}$ can be described by a two-component theory. We will show that this is also true for massless particles of arbitrary spin. That is, we will show that one can describe massless particles of arbitrary spin by means of a generalized two-component theory. Furthermore, we will show that these components satisfy equations analogous to Weyl's equations for particles of spin $\frac{1}{2}$.

In order to extend the two-component neutrino theory we just recall that one can write a four-component spinor as

$$\tilde{\psi}(x)=\begin{bmatrix}\xi(x)\\ \dot{\chi}(x)\end{bmatrix}=\psi_R+\psi_L\,, \tag{2.17}$$

where $\xi(x)$ and $\dot{\eta}(x)$ are two-component spinors, and ψ_R, ψ_L are defined in (2.11).

The set of equations (2.13) for ψ_R and ψ_L is equivalent to the following Weyl's equations for the two-component spinors ξ and $\dot{\eta}$:

$$(-i\sigma_0\partial_0 - i\boldsymbol{\sigma}\cdot\boldsymbol{\nabla})\,\xi(x)=0, \quad (-i\sigma_0\partial_0 + i\boldsymbol{\sigma}\cdot\boldsymbol{\nabla})\,\dot{\eta}(x)=0. \tag{2.18}$$

The two-component spinors ξ and $\dot{\chi}$ are eigenstates of the helicity operator $\frac{1}{2}\boldsymbol{\sigma}\cdot\mathbf{n}(\mathbf{n}=\mathbf{p}/|\mathbf{p}|)$ with eigenvalues $\pm\frac{1}{2}$.

The formulation of massless particles, in terms of generalized two-component spinors, can now be implemented by recalling that if $\tilde{\psi}$ transforms, under a Poincaré transformation, as a tensor product of $2s$ bispinors,

$$\tilde{\psi}\sim\begin{bmatrix}\xi_I\\ \dot{\chi}_I\end{bmatrix}\otimes\cdots\otimes\begin{bmatrix}\xi_{IIS}\\ \dot{\chi}_{IIS}\end{bmatrix}, \tag{2.19}$$

then, in chiral representation, the one that we will use from now on in the massless case, $\tilde{\psi}_{R\cdots R}, \tilde{\psi}_{R\cdots RL}, \tilde{\psi}_{L\cdots L}$, will transform like

$$\begin{aligned}
\tilde{\psi}_{R\cdots R}&\sim\begin{bmatrix}\xi_I\\ 0\end{bmatrix}\otimes\cdots\otimes\begin{bmatrix}\xi_{IIS}\\ 0\end{bmatrix}=\begin{bmatrix}\xi_I\cdots\xi_{IIS}\\ 0\\ \vdots\\ 0\end{bmatrix},\\
\tilde{\psi}_{R\cdots RL}&\sim\begin{bmatrix}\xi_I\\ 0\end{bmatrix}\otimes\cdots\otimes\begin{bmatrix}\xi_{IIS_{-1}}\\ 0\end{bmatrix}\otimes\begin{bmatrix}0\\ \dot{\chi}_{IIS}\end{bmatrix}=\begin{bmatrix}0\\ \xi_I\cdots\xi_{IIS_{-1}}\dot{\chi}_{IIS}\\ 0\\ \vdots\\ 0\end{bmatrix},\\
&\vdots\\
\tilde{\psi}_{L\cdots L}&\sim\begin{bmatrix}0\\ \dot{\chi}_I\end{bmatrix}\otimes\cdots\otimes\begin{bmatrix}0\\ \dot{\chi}_{IIS}\end{bmatrix}=\begin{bmatrix}0\\ \vdots\\ 0\\ \dot{\chi}_I\cdots\dot{\chi}_{IIS}\end{bmatrix}.
\end{aligned} \tag{2.20}$$

From (2.20), one can write, by using (2.15),

$$\begin{aligned}
\tilde{\psi}_{R\cdots R}&\sim\begin{bmatrix}\varphi^{(1)}\\ 0\\ \vdots\\ 0\end{bmatrix},\\
\tilde{\psi}_{R\cdots RL}&\sim\begin{bmatrix}0\\ \varphi^{(2)}\\ 0\\ \vdots\\ 0\end{bmatrix},\\
&\vdots
\end{aligned} \tag{2.21}$$

$$\tilde{\psi}_{L\cdots L}\sim\begin{bmatrix}0\\ \vdots\\ 0\\ \varphi^{(2s)}\end{bmatrix},$$

where $\varphi^{(1)},\varphi^{(2)},...,\varphi^{(2s)}$, are, respectively, the only nonzero components of $\tilde{\psi}_{R\cdots R},\tilde{\psi}_{R\cdots RL},\ldots,\tilde{\psi}_{L\cdots L}$ and are two-component spinors of rank $2s$:

$$\begin{aligned}\varphi^{(1)}&=\varphi_{b_1b_2\cdots b_{2s}},\\ \varphi^{(2)}&=\varphi'_{b_1b_2\cdots b_{2s}},\\ &\vdots\\ \varphi^{(2s)}&=\varphi^{(2s-1)}_{b_1b_2\cdots b_{2s}},\\ b_1,b_2,\ldots,b_{2s}&=1,2.\end{aligned}\tag{2.22}$$

Using Eqs. (2.16) we can see that $\varphi^{(1)}$ and $\varphi^{(2s)}$ satisfy generalized Weyl's equations:

$$(-i\sigma^0\partial_0-i\boldsymbol{\sigma}\cdot\boldsymbol{\nabla})\otimes\mathbf{1}\otimes\cdots\otimes\mathbf{1}\varphi^{(1)}(x)=0,\tag{2.23a}$$

$$(-i\sigma^0\partial_0+i\boldsymbol{\sigma}\cdot\boldsymbol{\nabla})\otimes\mathbf{1}\otimes\cdots\otimes\mathbf{1}\varphi^{(2s)}(x)=0,\tag{2.23b}$$

where $\varphi^{(1)}$ and $\varphi^{(2s)}$ are symmetric two-component spinors of rank $2s$. Equation (2.23b) can be derived from (2.23a) by space reflection, so one can consider just one of the equations (2.23).

The other components $\varphi^{(2)},...,\varphi(2s-1)$ satisfy equations analogous to Weyl's.

Since the spin operator, in chiral representation, is given by

$$\boldsymbol{\Sigma}=\tfrac{1}{2}(\boldsymbol{\Sigma}\otimes\mathbf{1}\otimes\mathbf{1}\cdots\otimes\mathbf{1}+\cdots+\mathbf{1}\otimes\mathbf{1}\otimes\mathbf{1}\cdots\otimes\boldsymbol{\Sigma}),\tag{2.24}$$

then the generalized helicity operator W is

$$W=\mathbf{n}\cdot\boldsymbol{\Sigma}.\tag{2.25}$$

The eigenvalues of $W(\omega)$ lie in the range $-s\leqslant\omega\leqslant s$. In particular, we have

$$W\psi_{R\cdots R}=s\psi_{R\cdots R},\quad W\psi_{L\cdots L}=-s\psi_{L\cdots L}.\tag{2.26}$$

Our proposal for treating massless particles is then parallel to the neutrino theory. For the free field theory one requires chiral invariance. For massless particles it is sensible to define chiral components and treat them as independent variables. For free fields, by using four-spinors, these equations are (2.16), whereas, by using two-spinors, the basic equations are (2.23). We shall see that this leads to Maxwell's equation in vacuum in the case of spin 1 particles.

III. BW THEORY FOR MASSIVE SPIN 1 PARTICLES

A. Free fields

This chapter shows how one describes massive spin 1 particles with the spinor method proposed by Bargmann and Wigner.

Within the BW method a spin 1 massive particle of mass m is described, in the noninteracting case, by a rank 2 symmetric spinor $\psi_{a_1a_2}(x)$ obeying a system of two Dirac-type equations:

$$(i\partial\!\!\!/\otimes I)\psi = m\psi, \quad (I\otimes i\partial\!\!\!/)\psi = m\psi. \tag{3.1}$$

Equations (3.1) may be derived from the following Lagrangian:[6]

$$\mathscr{L}_0 = \bar{\psi}\left\{\frac{i}{2}[\gamma^\mu\otimes I + I\otimes\gamma^\mu]\partial_\mu - mI\otimes I\right\}\psi. \tag{3.2}$$

If we treat the field $\psi_{a_1a_2}$ as the independent variable, one gets, in particular,

$$\{i\partial\!\!\!/ - m\}_{a_1a_s'}\psi_{a_1'a_2}(x) = 0. \tag{3.3}$$

We replace $\psi_{a_1'a_2}$ in (3.3) by its decomposition (2.9) and obtain

$$\begin{aligned} i\gamma^\alpha_{a_1a_1'}\partial_\alpha\left\{B_\mu(x)(\gamma^\mu C)_{a_1'a_2} - \frac{1}{2m}G_{\mu\nu}(x)(\sigma^{\mu\nu}C)_{a_1'a_2}\right\} \\ = m\left\{B_\mu(x)(\gamma^\mu C)_{a_1a_2} - \frac{1}{2m}G_{\mu\nu}(x)(\sigma^{\mu\nu}C)_{a_1a_2}\right\}. \end{aligned} \tag{3.4}$$

In order to see that (3.4) leads to the usual equations one has to make some simple operations involving γ matrices. For instance, if one multiplies (3.4) by $(C^{-1})_{a_2a_1}$ and sums over a_1a_2, one gets

$$i\partial_\alpha B_\mu \operatorname{Tr}(\gamma^\alpha\gamma^\mu) = 0,$$

from which it follows that

$$\partial_\mu B^\mu = 0. \tag{3.5}$$

It is interesting to see that the subsidiary condition $\partial_\mu B^\mu = 0$ follows directly from the BW equation. If, on the other hand, one multiplies (3.4) by $(C^{-1}\gamma^\beta)_{a_2a_1}$, one gets

$$-\frac{1}{2m}\partial_\alpha G_{\mu\nu}\operatorname{Tr}(\gamma^\alpha\sigma^{\mu\nu}\gamma^\beta) = mB_\mu\operatorname{Tr}(\gamma^\mu\gamma^\beta),$$

from which one gets

$$-\partial^\mu G_{\mu\beta} + m^2 B_\beta = 0. \tag{3.6}$$

Finally, if we multiply (3.4) by $(C^{-1}\gamma^\beta\gamma^\lambda)_{a_2a_1}$, one gets

$$i\partial_\alpha B_\mu \operatorname{Tr}(\gamma^\alpha\gamma^\mu\gamma^\beta\gamma^\lambda) = -\frac{1}{2m}G_{\mu\nu}\operatorname{Tr}(\sigma^{\mu\nu}\gamma^\beta\gamma^\lambda),$$

from which it follows that

$$\partial_\mu B^\mu g^{\beta\lambda} + \partial^\lambda B^\beta - \partial^\beta B^\lambda = G^{\beta\lambda}. \tag{3.7}$$

By using (3.5) in (3.7) one gets

$$G^{\beta\lambda} = \partial^\lambda B^\beta - \partial^\beta B^\lambda; \tag{3.8}$$

that is, in the decomposition (2.9) of the field ψ, the only acceptable tensor is $\partial^\nu B^\mu - \partial^\mu B^\nu$.

We have then seen that BW equations lead to the following restrictions upon the fields B^{μ} and $G^{\mu\nu}$:

$$\partial^{\mu}B_{\mu}=0, \quad G_{\mu\nu}=\partial_{\nu}B_{\mu}-\partial_{\mu}B_{\nu}, \quad -\partial^{\mu}G_{\mu\nu}+m^{2}B_{\nu}=0. \tag{3.9}$$

In order to see the equivalence between the BW method and the usual approach, in which we assign to a vector field B_{μ} a spin 1 particle, let us now write $\mathscr{L}_0$ in terms of B_{μ}.

By using decomposition (2.9) one gets

$$\mathscr{L}_0=4m^{2}B^{\mu}B_{\mu}-2G^{\mu\nu}G_{\mu\nu} \tag{3.10}$$

or, using (3.8),

$$\mathscr{L}_0=4m^{2}B^{\mu}B_{\mu}+4\partial^{\mu}B^{\nu}(\partial_{\nu}B_{\mu}-\partial_{\mu}B_{\nu}). \tag{3.11}$$

If we consider B_{μ} as the independent field, then one gets from (3.11) the usual Euler–Lagrange for the B_{μ} field; that is,

$$m^{2}B_{\nu}-\partial^{\mu}G_{\mu\nu}=0, \tag{3.12}$$

where

$$G_{\mu\nu}=\partial_{\nu}B_{\mu}-\partial_{\mu}B_{\nu}.$$

Equation (3.12) is the same as Eq. (3.6).

B. Interacting fields

Let us consider the interaction of massive spin 1 particles with massive spin $\frac{1}{2}$ particles, described, as usual, by a rank 1 spinor field η.

If we restrict ourselves to Lagrangians that are linear in the ψ fields (which leads, ultimately, to renormalizable models), then the forms that are compatible with Lorentz invariance are

$$\mathscr{L}_{\text{int}}=g_1\bar{\psi}_{a_1a_2}\eta^{c}_{a_1}\eta^{c}_{a_2}+g_2\bar{\psi}_{a_1a_2}\eta^{c}_{a_1}\eta^{c}_{a_2}+\text{h.c.}=g_1\eta^{c}\bar{\psi}\eta+g_2\eta\bar{\psi}\eta+\text{h.c.}, \tag{3.13}$$

where g_1 and g_2 are constants with dimension $[L]^{1/2}=1/[M]^{1/2}$.

In the following we shall take $g_2=0$. As we shall see later in the zero-mass limit nature seems to prefer this type of coupling.

We shall study the following total Lagrangian for a spin 1 massive field interacting with a spin $\frac{1}{2}$ massive field:

$$\mathscr{L}=\bar{\psi}\{\tfrac{1}{2}(\gamma^{\mu}\otimes I+I\otimes\gamma^{\mu})\partial_{\mu}-mI\otimes I\}\psi+g_1\eta^{c}\bar{\psi}\eta+\bar{\eta}(i\partial\!\!\!/-m_f)\eta. \tag{3.14}$$

Treating now $\bar{\psi}_{a_1a_2}$, $\psi_{a_1a_2}$, η as independent fields, we obtain using (3.9) and Lagrange equations

$$\partial_{\mu}G^{\rho\mu}=-m^{2}B^{\rho}+g_1\frac{\sqrt{m}}{4}\bar{\eta}\gamma^{\rho}\eta. \tag{3.15}$$

Model (3.15) leads to equations analogous to Maxwell's. In fact, in analogy with the massless case, we name

$$G^{0k}=E^{k}, \quad G^{jk}=\epsilon^{ljk}H^{l}. \tag{3.16}$$

We obtain from (3.15) the following set of equations:

$$\nabla\cdot\mathbf{E}+m^2B^0=g_1\frac{\sqrt{m}}{4}\,\bar{\eta}\gamma^0\eta,$$

$$\partial^0\mathbf{E}-\nabla\wedge\mathbf{H}-m^2\mathbf{B}=-g_1\frac{\sqrt{m}}{4}\,\bar{\eta}\gamma^0\eta,$$

$$\nabla\cdot\mathbf{H}=0,\quad \partial^0\mathbf{H}+\nabla\wedge\mathbf{E}=0. \tag{3.17}$$

Equations (3.17) are analogous to Maxwell's. That is, we get a set of coupled equations of first order in terms of the observables **E** and **H**.

C. Hamiltonian

We take the form (3.14) of $\mathscr{L}$ as a starting point. The two fields η and ψ are independent. We construct conjugate momenta from $\mathscr{L}$ by the standard prescription, so we obtain

$$\pi_{a_1a_2}=\frac{\partial\mathscr{L}}{\partial(\partial^0\psi)_{a_1a_2}}=\bar{\psi}_{a_1'a_2'}\frac{i}{2}\{\gamma^0_{a_1'a_1}\delta_{a_2'a_2}+\delta_{a_1'a_1}\gamma^0_{a_2'a_2}\},$$
$$\pi_{a_1}=\frac{\partial\mathscr{L}}{\partial(\partial^0\eta)_{a_1}}=\bar{\eta}_{a_2}i\gamma^0_{a_2a_1}. \tag{3.18}$$

The Hamiltonian is defined by

$$\mathbf{H}=\pi_{a_1a_2}\partial^0\psi_{a_1a_2}+\pi_{a_1}\partial^0\eta_{a_1}-\mathscr{L}. \tag{3.19}$$

Replacing $\psi_{a_1a_2}(\bar{\psi}_{a_1a_2})$ by its decomposition (2.9), one gets

$$\mathbf{H}=4\{G^{0\mu}\partial_0B_\mu+\partial_0B_\mu G^{0\mu}\}-4\{m^2B^\mu B_\mu-\tfrac{1}{2}G^{\mu\nu}G_{\mu\nu}\}$$
$$+g_1\sqrt{m}\left\{B_\mu\bar{\eta}\gamma^\mu\eta-\frac{1}{2m}\,G_{\mu\nu}\bar{\eta}\sigma^{\mu\nu}\eta\right\}-\bar{\eta}(i\gamma^k\partial_k-m_f)\eta, \tag{3.20}$$

where

$$k,j=1,2,3,$$

$$\mu,\nu=0,1,2,3.$$

Now, following Bjorken–Drell[7] we adopt the notation

$$E^j=E^j_l+E^j_t=-\partial_jB^0-\partial_0B^j$$

and we assume that the fields **E** and **H** are real, so we obtain

$$\mathbf{H}=4(\mathbf{H}^2+\mathbf{E}_t^2)-4\mathbf{E}_l^2-4m^2B^\mu B_\mu+g_1\sqrt{m}\left\{B^0\bar{\eta}\gamma^0\eta+B_j\bar{\eta}\gamma^j\eta-\frac{1}{2m}\,G_{\mu\nu}\bar{\eta}\sigma^{\mu\nu}\eta\right\}$$
$$-\bar{\eta}(i\gamma^k\partial_k-m_f)\eta. \tag{3.21}$$

IV. ALTERNATIVE APPROACH TO SPIN 1 MASSLESS PARTICLES

A. Spin 1 massless particles

In this section we will see how one can apply the two-component and the four-component spinorial formalism in the description of spin 1 massless particles. In this case one works with a rank 2 spinor field ψ_{ab}. Our starting point could be the zero-mass limit of (3.2). The Lagrangian that one gets in this limit is

$$\mathscr{L}_0=\bar{\psi}\left\{\frac{i\partial\!\!\!/}{2}\otimes\mathbf{1}+\mathbf{1}\otimes\frac{i\partial\!\!\!/}{2}\right\}\psi. \tag{4.1}$$

Lagrangian (4.1) is not, however, the appropriate Lagrangian for spin 1 massless particles. The reason why the extension of the Bargmann–Wigner theory, in this case, is not straightforward is chiral symmetry. $\mathscr{L}_0$ defined in (4.1) is not invariant under the generalized chiral transformation

$$\psi\rightarrow\psi'=e^{i\alpha\gamma_5}\otimes e^{i\alpha\gamma_5}\psi. \tag{4.2}$$

Only the equivalent Lagrangians

$$\mathscr{L}=\bar{\psi}(i\partial\!\!\!/\otimes 1)\psi \quad [\mathscr{L}'=\bar{\psi}(1\otimes i\partial\!\!\!/)\psi] \tag{4.3}$$

are invariant under the chiral transformations

$$\psi\rightarrow\psi'=(e^{i\alpha\gamma_5}\otimes 1)\psi \quad [\psi'=(1\otimes e^{i\alpha\gamma_5})\psi]. \tag{4.4}$$

Expressions (4.3) suggest that the Lagrangian for massless spin 1 particles is not uniquely defined. This would be the case if the field ψ is asymmetric. However, for a symmetric ψ field both expressions in (4.3) are equivalent. The problem is that we are not able to impose, at the Lagrangian level, the symmetry properties of the ψ field.

The need to work with asymmetric ψ fields lead us eventually to difficulties in dealing with discrete symmetries. This is due to the fact that depending on the Lagrangian we take we might get a different transformation law for the fields ψ. These transformation laws are equivalent only in the case of symmetric ψ fields. This is just to call attention to the fact that some care is needed when dealing with discrete symmetries.

For the Lagrangian $\mathscr{L}$ ($\mathscr{L}'$) one can introduce, in close analogy with the spin $\frac{1}{2}$ case, the chiral components

$$\begin{aligned}
\psi_{RR}&=\frac{(1+\gamma_5)}{2}\otimes\frac{(1+\gamma_5)}{2}\,\psi, \quad \psi_{RL}=\frac{(1+\gamma_5)}{2}\otimes\frac{(1-\gamma_5)}{2}\,\psi,\\
\psi_{LR}&=\frac{(1-\gamma_5)}{2}\otimes\frac{(1+\gamma_5)}{2}\,\psi, \quad \psi_{LL}=\frac{(1-\gamma_5)}{2}\otimes\frac{(1-\gamma_5)}{2}\,\psi,
\end{aligned} \tag{4.5}$$

where, by definition,

$$\psi=\psi_{RL}+\psi_{RR}+\psi_{LR}+\psi_{LL}. \tag{4.6}$$

These chiral components are eigenstates of the chirality operator $\gamma_5\otimes 1(1\otimes\gamma_5)$ with eigenvalues $+1$ or (-1). That is, they are polarized either to the right or to the left.

For massless particles the most general decomposition of the ψ field is now

$$\psi_{a_1a_2}=C_1A_\mu(\gamma^\mu C)_{a_1a_2}-C_2F_{\mu\nu}(\sigma^{\mu\nu}C)_{a_1a_2}, \tag{4.7}$$

where C_1 and C_2 in (4.7) are arbitrary constants that, in the massless case, cannot be related to each other as in the massive case [expression (2.9)], since C_1 and C_2 are dimensional constants having different dimensions.

The chiral components defined in (4.5) assume, after inserting (4.7) in (4.5), the following form:

$$\begin{aligned}
(\psi_{RR}(x))_{a_1a_2} &= -C_2[\tfrac{1}{2}(1+\gamma_5)\sigma^{\mu\nu}C]_{a_1a_2}F_{\mu\nu},\\
(\psi_{RL}(x))_{a_1a_2} &= C_1[\tfrac{1}{2}(1+\gamma_5)\gamma^{\mu}C]_{a_1a_2}A_{\mu},\\
(\psi_{LR}(x))_{a_1a_2} &= C_1[\tfrac{1}{2}(1-\gamma_5)\gamma^{\mu}C]_{a_1a_2}A_{\mu},\\
(\psi_{LL}(x))_{a_1a_2} &= -C_2[\tfrac{1}{2}(1-\gamma_5)\sigma^{\mu\nu}C]_{a_1a_2}F_{\mu\nu}.
\end{aligned} \tag{4.8}$$

That is, ψ_{RL},ψ_{RR} are related to potentials whereas ψ_{RR},ψ_{LL} are related to observables (electromagnetic fields).

Our proposal for treating massless spin 1 particles is, in close analogy with spin $\frac{1}{2}$ particles, to treat all chiral components $(\psi_{RL},\psi_{LR},\psi_{LL},\psi_{RR})$ as independent field variables. These chiral components describe, in principle, different species of spin 1 massless particles. In this way we consider all chiral components as dynamical variables. This approach leads to a formulation of QED in which potentials and observable fields are treated on equal footing. It is simple to check that the substitution of (4.6) into (4.3) leads to the following Lagrangian density:

$$\tilde{\mathscr{L}}_0=\bar{\tilde{\psi}}_{RL}(i\partial\!\!\!/\otimes I)\tilde{\psi}_{RR}+\bar{\tilde{\psi}}_{LR}(i\partial\!\!\!/\otimes I)\tilde{\psi}_{LL}+\bar{\tilde{\psi}}_{RR}(i\partial\!\!\!/\otimes I)\tilde{\psi}_{RL}+\bar{\tilde{\psi}}_{LL}(i\partial\!\!\!/\otimes I)\tilde{\psi}_{LR}. \tag{4.9}$$

By treating all chiral components as independent field variables one gets the following equations of motion:

$$\begin{aligned}
&(i\partial\!\!\!/\otimes I)\tilde{\psi}_{RR}=0, \quad (i\partial\!\!\!/\otimes I)\tilde{\psi}_{RL}=0,\\
&(i\partial\!\!\!/\otimes I)\tilde{\psi}_{LR}=0, \quad (i\partial\!\!\!/\otimes I)\tilde{\psi}_{LL}=0.
\end{aligned} \tag{4.10}$$

We will be interested in analyzing whether the interaction of photons with matter exhibits any preference of nature with regard to chiral components and, if this occurs, if there is violation of parity. The free field Lagrangian is invariant under space reflection ($\mathbf{x}\to-\mathbf{x}$) if the chiral fields transform as

$$\begin{aligned}
\psi_{LP} &\overset{P}{\to} \psi'_{LR}(x')=\xi(\gamma_0\otimes 1)\psi_{RR}(+\mathbf{x},t),\\
\psi_{LL} &\overset{P}{\to} \psi'_{LL}(x')=\xi(\gamma_0\otimes 1)\psi_{RL}(+\mathbf{x},t),\\
\psi_{RR} &\overset{P}{\to} \psi'_{RR}(x')=\xi(\gamma_0\otimes 1)\psi_{LR}(+\mathbf{x},t),\\
\psi_{RL} &\overset{P}{\to} \psi'_{RL}(x')=\xi(\gamma_0\otimes 1)\psi_{LL}(+\mathbf{x},t).
\end{aligned} \tag{4.11}$$

From (4.11) and (4.8) one would conclude that the mirror fields of the potentials are the observable fields (**E** and **H**) and vice-versa. This example illustrates, as pointed out before, the difficulty which we might run into when dealing with discrete symmetries within the spinors method.

There are two alternatives in dealing with discrete symmetries that can easily be checked taking the explicit example of space reflection. In the first case one can use the explicitly symmetric representation (4.7) in any of the alternative forms in (4.3) and analyze the symmetry properties of the Lagrangian in terms of the fields A_μ and $F_{\mu\nu}$. The Lagrangian is the standard one of electromagnetism as we shall see later.

The other alternative is to impose, from the very beginning, that ψ is symmetric. Under these circumstances Lagrangians (4.3) and (4.1) are equivalent. These equivalent Lagrangians would now be invariant under space reflections if the chiral fields transform as

$$\psi'_{RR}(x')=\xi(\gamma^0\otimes\gamma^0)\psi_{LL}(x), \quad \psi'_{RL}(x')=\xi(\gamma^0\otimes\gamma^0)\psi_{LR}(x),$$

$$\psi'_{LR}(x')=\xi(\gamma^0\otimes\gamma^0)\psi_{RL}(x), \quad \psi'_{LL}(x')=\xi(\gamma^0\otimes\gamma^0)\psi_{RR}(x).$$

It can be checked explicitly that these transformations lead to the proper transformation properties of the A_μ and $F_{\mu\nu}$ fields.

The generalized helicity operator W is now

$$\tfrac{1}{2}(\boldsymbol{\Sigma}\cdot\mathbf{n}\otimes I+I\otimes\boldsymbol{\Sigma}\cdot\mathbf{n})\equiv W, \quad \mathbf{n}=\frac{\mathbf{p}}{|\mathbf{p}|}. \tag{4.12}$$

It is straightforward to show that $\psi_{RR},\psi_{RL},\psi_{LR},\psi_{LL}$ are eigenstates of W with eigenvalues $+1,0,-1$; that is,

$$\begin{aligned}&\tfrac{1}{2}(\boldsymbol{\Sigma}\cdot\mathbf{n}\otimes I+I\otimes\boldsymbol{\Sigma}\cdot\mathbf{n})\tilde{\psi}_{RR}=\psi_{RR}, \quad \tfrac{1}{2}(\boldsymbol{\Sigma}\cdot\mathbf{n}\otimes I+I\otimes\boldsymbol{\Sigma}\cdot\mathbf{n})\tilde{\psi}_{RL}=0,\\ &\tfrac{1}{2}(\boldsymbol{\Sigma}\cdot\mathbf{n}\otimes I+I\otimes\boldsymbol{\Sigma}\cdot\mathbf{n})\tilde{\psi}_{LR}=0, \quad \tfrac{1}{2}(\boldsymbol{\Sigma}\cdot\mathbf{n}\otimes I+I\otimes\boldsymbol{\Sigma}\cdot\mathbf{n})\tilde{\psi}_{LL}=-\psi_{LL}.\end{aligned} \tag{4.13}$$

B. Free electrodynamics

Let us check, finally, that the Lagrangian density (4.9) provides an alternative formulation of free electrodynamics. By substituting (4.8) into Eqs. (4.10) and furthermore multiplying (4.10) by (C) and taking the trace, we get

$$\partial^\mu A_\mu=0; \tag{4.14}$$

that is, we get a Lorentz condition. Furthermore, multiplying (4.10) by $(C^{-1}\gamma^\beta)$ we get the equation of motion for the $F^{\mu\nu}$ field,

$$\partial^\mu F_{\mu\nu}=0. \tag{4.15}$$

We shall see, by employing the two-spinor approach, that $F_{\mu\nu}$ can be written, in terms of an antisymmetric field tension $\mathscr{F}_{\mu\nu}$, as

$$F_{\mu\nu}=\mathscr{F}_{\mu\nu}+i\tilde{\mathscr{F}}_{\mu\nu}, \tag{4.16}$$

where

$$\tilde{\mathscr{F}}^{\mu\nu}=\tfrac{1}{2}\epsilon^{\mu\nu\alpha\beta}\mathscr{F}_{\alpha\beta}. \tag{4.17}$$

The equation of motion for $\mathscr{F}_{\mu\nu}$ and $\tilde{\mathscr{F}}_{\mu\nu}$ is, from (4.15),

$$\partial_\mu \mathscr{F}^{\mu\nu}=0, \quad \partial_\mu \tilde{\mathscr{F}}^{\mu\nu}=0. \tag{4.18}$$

It should be pointed out at this point that since in the massless case ψ_{RL} and ψ_{RR} components are treated as independent variables there is no connection between $\mathscr{F}^{\mu\nu}$ and the derivatives of the field A_μ. That is, in this case A_μ and $F_{\mu\nu}$ are independent field variables. We shall see, however, that within the generalized two-component theory of massless spin 1 particles this connection emerges from Maxwell's equations for the observable fields. We shall see that, also in this case, one can write

$$\mathscr{F}^{\mu\nu}=\partial^\mu A^\nu-\partial^\nu A^\mu \tag{4.19}$$

and, as a result, from (4.19) and (4.14), it follows that the A^μ field satisfies, by using (4.18),

$$\Box A^\mu=0. \tag{4.20}$$

C. Two-component formulation of free electrodynamics

We shall now consider the formulation of free electrodynamics within the generalized two-component theory presented in Sec. I. In the case of spin 1 particles the field ψ transforms as

$$\psi\sim\begin{bmatrix}\xi^I\\ \dot{\chi}^I\end{bmatrix}\otimes\begin{bmatrix}\xi^{II}\\ \dot{\chi}^{II}\end{bmatrix} \tag{4.21}$$

so that the fields $\psi_{RL},\psi_{LR},\psi_{RR},\psi_{LL}$ defined in (4.5) transform like

$$\begin{aligned}
&\tilde{\psi}_{RR}\sim\begin{bmatrix}\xi^I\\ 0\end{bmatrix}\otimes\begin{bmatrix}\xi^{II}\\ 0\end{bmatrix}, \quad \tilde{\psi}_{RL}\sim\begin{bmatrix}\xi^I\\ 0\end{bmatrix}\otimes\begin{bmatrix}0\\ \dot{\chi}^{II}\end{bmatrix},\\
&\tilde{\psi}_{LR}\sim\begin{bmatrix}0\\ \dot{\chi}^I\end{bmatrix}\otimes\begin{bmatrix}\xi^{II}\\ 0\end{bmatrix}, \quad \tilde{\psi}_{LL}\sim\begin{bmatrix}0\\ \dot{\chi}^I\end{bmatrix}\otimes\begin{bmatrix}0\\ \dot{\chi}^{II}\end{bmatrix}.
\end{aligned} \tag{4.22}$$

The generalized Weyl's equations satisfied by the nonzero components of ψ_{RR} and ψ_{LL} are

$$\begin{aligned}
&(-i\sigma^0\partial_0-i\boldsymbol{\sigma}\cdot\boldsymbol{\nabla})_{aa'}\xi^I_{a'}\xi^{II}_b=0,\\
&(-i\sigma^0\partial_0+i\boldsymbol{\sigma}\cdot\boldsymbol{\nabla})_{aa'}\dot{\chi}^I_{a'}\dot{\chi}^{II}_b=0,
\end{aligned} \tag{4.23}$$

where symmetrization in the spin indices is assumed in Eq. (4.23).

Equations (4.23) can be written, in terms of $\varphi^{(1)}$ and $\varphi^{(4)}$ defined in (2.21), as

$$(-i\sigma^0\partial_0-i\boldsymbol{\sigma}\cdot\boldsymbol{\nabla})\varphi^{(1)}(\mathbf{x},t)=0, \tag{4.24a}$$

$$(-i\sigma_0\partial_0+i\boldsymbol{\sigma}\cdot\boldsymbol{\nabla})\varphi^{(4)}(\mathbf{x},t)=0. \tag{4.24b}$$

We are now ready to get the field equations of electrodynamics. As in the generalized four-component approach, one tries to write $\varphi^{(1)}$ and $\varphi^{(4)}$ as a linear combination of 2×2 symmetric matrices. In this case, the candidate matrices are the matrices (2.8), $\boldsymbol{\sigma}C_1$, where C_1 is the 2×2 charge conjugation matrix. One can then write

$$\varphi^{(1)}(x)=\mathbf{f}(x)(\boldsymbol{\sigma}\cdot C_1), \tag{4.25}$$

where $\mathbf{f}$ is a vector that satisfies, after substituting (4.25) into (4.24), the following equations:

$$\nabla \cdot \mathbf{f} = 0, \tag{4.26}$$

$$i\partial^0 \mathbf{f} = \nabla \times \mathbf{f}. \tag{4.27}$$

We have shown in Sec. IV A that $\varphi^{(1)}$ and $\varphi^{(4)}$ (or, equivalently, ψ_{RR} and ψ_{LL}) should be built from an antisymmetric tensor $F_{\mu\nu}$. More specifically, it follows from (4.8) and (4.25) that the ith component f_i can be written as

$$f_i = \tfrac{1}{2}\,\epsilon_{0i\alpha\beta}F^{\alpha\beta} = \tfrac{1}{2}\,\epsilon_{i\alpha\beta}F^{\alpha\beta}, \tag{4.28}$$

with $i,\alpha,\beta = 1,2,3$.

As pointed out in Ref. 5 $F_{\mu\nu}$ in (4.28) should be self-dual. In this way if one assumes that $\mathscr{F}_{\mu\nu}$ is an antisymmetrical tensor, then one can construct from this tensor a self-dual one by writing

$$F^{\mu\nu} = \mathscr{F}^{\mu\nu} + i\tilde{\mathscr{F}}^{\mu\nu}, \tag{4.29}$$

where

$$\tilde{\mathscr{F}}^{\mu\nu} = \tfrac{1}{2}\epsilon^{\mu\nu\alpha\beta}\mathscr{F}_{\alpha\beta}. \tag{4.30}$$

If one defines further,

$$E^i \equiv \mathscr{F}_0 i, \quad H^i = \tilde{\mathscr{F}}_0 i. \tag{4.31}$$

It follows that Eqs. (4.26) and (4.27) for $\mathbf{f}$ imply Maxwell's equations for the $\mathbf{E}$ and $\mathbf{H}$ fields defined in (4.31). That is,

$$\begin{gathered} \nabla \cdot \mathbf{E} = 0, \quad \nabla \cdot \mathbf{H} = 0, \\ \nabla \times \mathbf{E} - \partial_0 \mathbf{E} = 0, \quad \nabla \times \mathbf{H} - \partial_0 \mathbf{H} = 0. \end{gathered} \tag{4.32}$$

Finally, it follows from Maxwell's equation (4.32) and from (4.31) that $\mathscr{F}_{\mu\nu}$ can be written as

$$\mathscr{F}_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu. \tag{4.33}$$

It is worth commenting, at this point, on the connection between $\mathscr{F}_{\mu\nu}$ and the derivatives of the field A_μ in the case of massless particles. In the massive case the connection analogous to (4.33) follows from the restriction imposed by BW equations. In the massless case the possibility of writing $\mathscr{F}_{\mu\nu}$ under the form (4.33) follows from Maxwell's equations that allows us to write the observable fields in terms of derivatives of the four-potentials. We will show, in the interaction case, how expression (4.33) can be derived by adding chiral violating terms to the Lagrangian.

The conclusion is that, within the spinor method proposed here, Maxwell's equation in vacuum emerges from the requirement of chiral invariance of the free field Lagrangian. Maxwell's equations for the fields $\mathbf{E}$ and $\mathbf{H}$ emerge from the equations analogous to Weyl's equation in the two-component neutrino theory.

V. INTERACTING FIELDS—QED

A. Linear interactions

Let us now consider the interaction of massless spin 1 fields. We will mainly be concerned with the interaction of these particles with ordinary matter. That is, we will be concerned with the most general interaction Lagrangian describing massless spin 1 particles interacting with spin $\frac{1}{2}$ massive (m_f) particles.

The most general Lagrangian involving the interaction of the chiral fields (4.5) with ordinary matter (here represented by the Fermi on field η) is

$$\mathscr{L}=\bar{\psi}_{RL}(i\partial\!\!\!/\otimes 1)\psi_{RR}+\bar{\psi}_{LR}(i\partial\!\!\!/\otimes 1)\psi_{LL}+\bar{\psi}_{RR}(i\partial\!\!\!/\otimes 1)\psi_{RL}+\bar{\psi}_{LL}(i\partial\!\!\!/\otimes 1)$$
$$\times\psi_{LR}+\bar{\eta}(i\partial\!\!\!/-m)\eta+\mathscr{L}_{\text{int}}(\psi_{RR},\ \psi_{RL},\ \psi_{LR},\ \psi_{LL},\ \eta). \tag{5.1}$$

By imposing that the Lagrangian is linear in the ψ fields, then the most general form that is bilinear in the matter field η that we can construct with the four independent fields ψ_{RR}, ψ_{RL}, ψ_{LR}, and ψ_{LL} is

$$\mathscr{L}_{\text{int}}=A\bar{\psi}_{R_{a_1}R_{a_2}}\eta_{a_1}\eta_{a_2}+B\bar{\psi}_{L_{a_1}L_{a_2}}\eta_{a_1}\eta_{a_2}+D\bar{\psi}_{R_{a_1}L_{a_2}}\eta_{a_1}\eta_{a_2}+E\bar{\psi}_{L_{a_1}R_{a_2}}\eta_{a_1}\eta_{a_2}+F\bar{\psi}_{R_{a_1}R_{a_2}}\eta^c_{a_1}\eta_{a_2}$$
$$+J\bar{\psi}_{L_{a_1}L_{a_2}}\eta^c_{a_1}\eta_{a_2}+K\bar{\psi}_{R_{a_1}L_{a_2}}\eta^c_{a_1}\eta_{a_2}+L\bar{\psi}_{L_{a_1}R_{a_2}}\eta^c_{a_1}\eta_{a_2}+\text{h.c.}, \tag{5.2}$$

where A, B, D, E, F, J, K, and L are arbitrary constants.

The reason for so many terms is that we shall assume, to start with, that ordinary matter couples with different strengths to the chiral components of the field ψ. As a matter of fact, we shall see that, in this case, only the zero helicity components couple to ordinary matter.

It is trivial to check that if nature is asymmetric with regard to left and right (that is, if it prefers chiral components), then the theory violates parity [in the sense that the Lagrangian is not invariant under transformations (4.11)]. The physical consequences, however, depend on how this symmetry is broken. We will show that within the field theoretical context the breakdown of parity, and consequently of left–right symmetry, does not lead always to processes occurring with different probabilities in the actual system or in its mirror image. That is, for theories in which not all the fields are observables, the parity symmetry breakdown might not be accompanied by observable effects. Electrodynamics follow into this category of field theories. In order to illustrate this relevant aspect let us consider two parity nonconserving Lagrangians:

$$\mathscr{L}_1^{\text{int}}=D(\psi_{LR})\eta_c\eta, \tag{5.3}$$

$$\mathscr{L}_2^{\text{int}}=K(\psi_{RL}+\psi_{LR})\eta_c\eta, \tag{5.4}$$

where K and D are coupling constants.

The first Lagrangian leads to left–right asymmetry leading to observable effects as far as parity breaking is concerned. In fact, Lagrangian (5.3) describes essentially the interaction of a vector field A_μ coupled to a vector and axial vector current $[\bar{\eta}(1-\gamma_5)\gamma_\mu\eta]$. As will be shown in the next section, the Lagrangian (5.4) is an equivalent formulation of QED.

If one wants to ensure that there are no observable effects in the breakdown of parity of Lagrangian (5.2), one has to require that

$$\begin{aligned} A&=B, \quad D=E,\\ F&=J, \quad K=L. \end{aligned} \tag{5.5}$$

Under restrictions (5.5), the most general interaction Lagrangian is then

$$\mathscr{L}_{\text{int}}=A(\bar{\psi}_{RR}\eta\eta+\bar{\psi}_{LL}\eta\eta)+D(\bar{\psi}_{RL}\eta\eta+\bar{\psi}_{LR}\eta\eta)+F(\bar{\psi}_{RR}\eta^c\eta+\bar{\psi}_{LL}\eta^c\eta)$$
$$+K(\bar{\psi}_{RL}\eta^c\eta+\bar{\psi}_{LR}\eta^c\eta). \tag{5.6}$$

We now consider the particular interaction Lagrangian obtained by taking $A=D=K=0$:

$$\mathscr{L}_{\text{int}} = F(\bar{\tilde{\psi}}_{RR}\eta^c\eta + \bar{\tilde{\psi}}_{LL}\eta^c\eta). \tag{5.7}$$

The complete Lagrangian is then

$$\begin{aligned}\mathscr{L} = {} & \bar{\tilde{\psi}}_{RL}(i\partial\!\!\!/\otimes I)\tilde{\psi}_{RR} + \bar{\tilde{\psi}}_{LR}(i\partial\!\!\!/\otimes I)\tilde{\psi}_{LL} + \bar{\tilde{\psi}}_{RR}(i\partial\!\!\!/\otimes I)\tilde{\psi}_{RL} \\ & + \bar{\tilde{\psi}}_{LL}(i\partial\!\!\!/\otimes I)\tilde{\psi}_{LR} + F(\bar{\tilde{\psi}}_{RR}\eta^c\eta + \bar{\tilde{\psi}}_{LL}\eta^c\eta) + \bar{\eta}(i\partial\!\!\!/ - m_f)\eta.\end{aligned} \tag{5.8}$$

Writing Lagrange equations explicitly, one has

$$i\partial\!\!\!/\otimes I\bar{\tilde{\psi}}_{LR} + F\eta^c\eta = 0, \tag{5.9a}$$

$$i\partial\!\!\!/\otimes I\bar{\tilde{\psi}}_{RL} + F\eta^c\eta = 0, \tag{5.9b}$$

$$i\partial\!\!\!/\otimes I\bar{\tilde{\psi}}_{RR} = 0, \tag{5.9c}$$

$$i\partial\!\!\!/\otimes I\bar{\tilde{\psi}}_{LL} = 0. \tag{5.9d}$$

Equations (5.9) and (4.8) imply, in particular, the following relations:

$$2iC_1\partial_\mu A^\mu = F\bar{\eta}\eta, \tag{5.10}$$

$$\partial^\mu F_{\mu\nu} = 0. \tag{5.11}$$

The conclusion is that Lagrangian (5.8) describes the interaction of massless spin 1 particles with matter but this theory is not electrodynamics.

B. Electrodynamics and chiral asymmetry

Let us consider now the interaction of massless particles with ordinary matter described by the interaction Lagrangian:

$$\mathscr{L}_{\text{int}} = K\{\bar{\tilde{\psi}}_{RL}\eta^c\eta + \bar{\tilde{\psi}}_{LR}\eta^c\eta\}. \tag{5.12}$$

By adding the free field Lagrangians we end up with the following total Lagrangian:

$$\begin{aligned}\mathscr{L} = {} & \bar{\tilde{\psi}}_{RL}(i\partial\!\!\!/\otimes I)\tilde{\psi}_{RR} + \bar{\tilde{\psi}}_{LR}(i\partial\!\!\!/\otimes I)\tilde{\psi}_{LL} + \bar{\tilde{\psi}}_{RR}(i\partial\!\!\!/\otimes I)\tilde{\psi}_{RL} + \bar{\tilde{\psi}}_{LL}(i\partial\!\!\!/\otimes I)\tilde{\psi}_{LR} \\ & + K\{\bar{\tilde{\psi}}_{RL}\eta^c\eta + \bar{\tilde{\psi}}_{LR}\eta^c\eta\} + \bar{\eta}(i\partial\!\!\!/ - m_f)\eta + \alpha\bar{\tilde{\psi}}_{RR}\psi_{LL} + \alpha\bar{\tilde{\psi}}_{LL}\psi_{RR}.\end{aligned} \tag{5.13}$$

One of the basic features of this approach is that although only some chiral components couple with the usual matter, all chiral components should be considered as dynamical variables. That is, one should write five Lagrange equations, one for each of the independent fields (ψ_{RR}, ψ_{RL}, ψ_{LR}, ψ_{LL}, and η).

With $\mathscr{L}$ given by (5.13), they lead to

$$i\partial\!\!\!/\otimes I\tilde{\psi}_{RL} + \alpha\tilde{\psi}_{LL} = 0, \tag{5.14a}$$

$$i\partial\!\!\!/\otimes I\tilde{\psi}_{RR} + K\eta^c\eta = 0, \tag{5.14b}$$

$$i\partial\!\!\!/\otimes I\tilde{\psi}_{LL} + K\eta^c\eta = 0, \tag{5.14c}$$

$$i\partial\!\!\!/\otimes I\tilde{\psi}_{LR} + \alpha\tilde{\psi}_{RR} = 0, \tag{5.14d}$$

$$K\eta^c\{\bar{\tilde{\psi}}_{RL}+\bar{\tilde{\psi}}_{LR}\}-m_f\bar{\eta}-i\partial_\mu(\bar{\eta})\gamma^\mu=0. \tag{5.14e}$$

From equation (5.14e) it follows that

$$K\eta^c_{a_1}\{\bar{\tilde{\psi}}_{RL}+\bar{\tilde{\psi}}_{LR}\}_{a_1a_2}-m_f\bar{\eta}_{a_2}-i\partial_\mu\bar{\eta}_{a_1}\gamma^\mu_{a_1a_2}=0. \tag{5.15}$$

Or, replacing $\bar{\tilde{\psi}}_{RL}$ and $\bar{\tilde{\psi}}_{LR}$ by expression (4.8),

$$-KC_1\bar{\eta}_{a_1}A_\mu(\gamma^\mu)_{a_1a_2}-m_f\bar{\eta}_{a_2}-i\partial_\mu\bar{\eta}_{a_1}\gamma^\mu_{a_1a_2}=0. \tag{5.16}$$

Taking the Hermitian conjugate of (5.16) one gets

$$(i\partial\!\!\!/-m_f)_{a_1a_2}\eta_{a_2}=KC_1(\gamma^\mu)_{a_1a_2}A_\mu\eta_{a_2}. \tag{5.17}$$

Now adding (5.14b) and (5.14c) and replacing $\tilde{\psi}_{RR}$ and $\tilde{\psi}_{LL}$ by expressions (4.8) we get

$$\partial_\mu F^{\beta\mu}=-\frac{K}{4C_2}\,\bar{\eta}\gamma^\beta\eta. \tag{5.18}$$

Similarly, adding (5.14a) and (5.14d) and replacing $\tilde{\psi}_{LR}$ and $\tilde{\psi}_{RL}$ by expressions (4.8) we get the following constraint:

$$\partial^\mu A_\mu=0; \tag{5.19}$$

that is, one gets the Lorentz condition and

$$\mathscr{F}^{sr}=\frac{C_1}{2\alpha C_2}(\partial^sA^r-\partial^rA^s). \tag{5.20}$$

This implies the usual relationship if one takes

$$\frac{C_1}{2\alpha C_2}=1. \tag{5.21}$$

The conclusion is that, by adding chiral asymmetric terms in the Lagrangian, one can get the usual relation (4.33).

We have seen in Sec. IV that the most general form for $F_{\mu\nu}$ is

$$F_{\mu\nu}=\mathscr{F}_{\mu\nu}+i\tilde{\mathscr{F}}_{\mu\nu}. \tag{5.22}$$

Replacing $F_{\mu\nu}$ given by (5.22) in Eq. (5.18) we get an alternative form for Eq. (5.18). This alternative form is

$$\begin{cases}\partial_\mu\mathscr{F}^{\beta\mu}=-\dfrac{K}{4C_2}\,\bar{\eta}\gamma^\beta\eta,\\ \partial_\mu\tilde{\mathscr{F}}^{\beta\mu}=0.\end{cases} \tag{5.23}$$

These are Maxwell's equations in Lorentz gauge if one writes $\mathscr{F}_{\mu\nu}$ under the form (4.33) and imposes the restriction

$$-\frac{K}{4C_2}=e. \tag{5.24}$$

In order to see this equivalence in terms of the observables **E** and **H** one writes

$$f^{ok}=E^k,$$
$$f^{jk}=e^{ljk}H^l, \quad k,j,l=1,2,3. \tag{5.25}$$

Equations (5.23) give rise to the following equations;

$$\nabla\cdot\mathbf{E}=e\bar{\eta}\gamma^0\eta, \quad \partial^0\mathbf{E}-\nabla\wedge\mathbf{H}=-e\bar{\eta}\boldsymbol{\gamma}\eta,$$
$$\nabla\cdot\mathbf{H}=0, \quad \partial^0\mathbf{H}+\nabla\wedge\mathbf{E}=0. \tag{5.26}$$

Equations (5.26) are Maxwell's equation in the presence of matter.

As a final remark we would like to show the equivalence between the spinor method and the usual tensor method. In order to show this all one has to do is to substitute in Lagrangian (5.13) the expression for the chiral components (4.8). In terms of the fields $F_{\mu\nu}$ and A_μ the Lagrangian density can be written as

$$\mathscr{L}[F^{\mu\nu},\ A^\mu]=-8\alpha C_2^2\{F^{*\mu\nu}(\partial_\nu A_\mu-\partial_\mu A_\nu)-A_\mu^*(\partial_\nu F^{\mu\nu}-\partial_\nu F^{\mu\nu})\}+2K\alpha C_2\bar{\eta}\gamma^\mu\eta A_\mu^*$$
$$+\bar{\eta}(i\partial\!\!\!/-m_f)\eta-8\alpha C_2^2F_{\mu\nu}^*F^{\mu\nu}, \tag{5.27}$$

where we have used condition (5.21).

By treating $F_{\mu\nu}^*$, A_μ^*, and η as independent field variables one gets the following equations:

$$\partial_\nu F^{\mu\nu}=-\frac{K}{4C_2}\,\bar{\eta}\gamma^\mu\eta, \tag{5.28}$$

$$(i\partial\!\!\!/-m_f)\eta=-2K\alpha C_2\gamma^\mu\eta A_\mu, \tag{5.29}$$

$$\mathscr{F}_{\mu\nu}=\partial^\mu A_\nu-\partial^\nu A^\mu. \tag{5.30}$$

Finally, one gets the usual Lagrangian of electrodynamics in terms of A_μ if one uses (5.30) and makes a proper choice of the constant α.

VI. QUANTIZATION

In this section we will consider the quantization of massive fields within the BW theory. We also propose an extension to the zero-mass case. We show that there is no basic distinction between this method and the usual approach. The relevant point is that it is possible to quantize the spinor fields by imposing appropriate commutation relations for these fields.

We quantize the BW fields by imposing the following commutation relations for BW's massive fields:

$$[\psi_{a_1a_2\cdots a_{2s}}(x),\ \psi^+_{a_1'a_2'\cdots a_{2s}'}(y)]_s=(-i)^{2s-1}\kappa\sum_{\mathscr{P}}\ i(i\partial\!\!\!/_x+m)_{a_1a_1'}\cdots i(i\partial\!\!\!/_x+m)_{a_{2s}a_{2s}'}\Delta(x-y),$$
$$a_1,\ldots,a_1',\ldots=1,2,3,4. \tag{6.1}$$

$\Delta(x-y)$ is the Jordan Pauli function, κ is a constant to be determined, $\mathscr{P}$ denotes all possible permutations among the spinor indices, and we use, in (6.1), the following notation:

$$[\phi,\psi]_s=\phi\psi+(-1)^{2s-1}\phi\psi, \tag{6.2}$$

where s is the spin of the fields in (6.2).

In the case of massless particles, and as pointed out in Sec. II, the fundamental objects are two-component spinors of rank $2s$ $\varphi^{(1)}\cdots\varphi^{(2s)}$. For the massless case the quantization is carried out by imposing the following commutation relations for the two-component Weyl spinors φ:

$$[\varphi_{b_1\cdots b_{2s}}(x),\ \varphi^{+}_{b'_1\cdots b'_{2s}}(y)]_x=(-i)^{2s-1}\kappa\sum_{\mathscr{P}} i(i\sigma^0\partial_0-i\boldsymbol{\sigma}\cdot\boldsymbol{\nabla})_{b_1b'_1}\cdots i(i\sigma^0\partial_0-i\boldsymbol{\sigma}\cdot\boldsymbol{\nabla})_{b_{2s}b'_{2s}} \times D(x-y), \tag{6.3}$$

where $D(x-y)$ is the Jordan Pauli function for massless particles, κ is a constant to be determined, $\mathscr{P}$ denotes all possible permutations among the spinor indices, and where we use convention (6.2).

One can now use, for spin 1 massive particles, the decomposition (2.9) and write the usual plane wave expansion for the field B_μ. In the case of the photon this decomposition for the A_μ field is

$$A^\mu(x)=\frac{1}{(2\pi)^3}\int\frac{d^3\mathbf{p}}{\sqrt{2p^0}}\sum_{\lambda=1}^{2}\epsilon^\mu(p,\lambda)[A(p,\lambda)e^{-ipx}+A^+(p,\lambda)e^{ipx}], \tag{6.4}$$

where $p=(p^0,\mathbf{p})$.

If one uses the decomposition (4.25) with $\mathbf{f}$ given by (4.28), then the commutation relations (6.3) imply the following commutation relations for the creation (A^+) and annihilation (A) operators:

$$[A(p,\lambda),A^+(p',\lambda')]=\delta^3(p-\mathbf{p}')\delta_{\lambda\lambda'}. \tag{6.5}$$

By analyzing the behavior of observables such as the energy, as we did in Sec. III C, and momentum we would realize that these fields describe particles.

We shall not further analyze the question of the quantization of the spinor fields. We just wanted to point out that one can provide a quantization method for spinor fields as well Feynman rules for the interaction of these fields. Most of the questions on computing cross sections for specific processes and the analysis of renormalization can be carried out in a simpler manner within the usual approach (tensor method).

VII. CONCLUSIONS

In this paper we have presented the description of electrodynamics in terms of spinors. The spinor method provides a description of massless particles in terms of chiral components when they are treated as independent field variables.

We have shown that, within the spinorial approach proposed here, photons can be described in close analogy with neutrinos. The requirement of chiral invariance, at the free field level, leads to Maxwell's equation in vacuum. The requirement of chiral asymmetry for the linear interaction of the spinor field with matter fields leads, for a proper choice of chiral components, to Maxwell's equations in the presence of matter.

One of the advantages of this approach is that it allows one to formulate electrodynamics in terms of potentials or, by using two-component spinors, in terms of the observable fields (Maxwell equation) E and H.

The question is whether electrodynamics is a left–right asymmetric theory. If matter does not distinguish between chiral components, then it should couple with the field ψ. That is not, however, the case. On the other hand, if ordinary matter couples only with $\psi_{RR}\psi_{LL}$ we would have electrodynamics formulated entirely in terms of observables. That is not the alternative that nature chooses either.

The usual QED is compatible with a theory in which only $\psi_{LR}+\psi_{RL}$ couples with ordinary matter. From this point of view QED is another example of an asymmetric interaction between chiral components. The conclusion is that the Lagrangian describing electrodynamics, in this four-component (chiral components) framework, is

$$\mathscr{L}_{\mathrm{QED}}=\bar{\psi}_{RL}(i\partial\!\!\!/\otimes 1)\psi_{RR}+\bar{\psi}_{LR}(i\partial\!\!\!/\otimes 1)\psi_{LL}+\bar{\psi}_{RR}(i\partial\!\!\!/\otimes 1)\psi_{RL}+\bar{\psi}_{LL}(i\partial\!\!\!/\otimes I)\psi_{LR}+\bar{\eta}(i\partial\!\!\!/-m)\eta+F(\bar{\psi}_{RL}+\bar{\psi}_{LR})\eta_c\eta.$$

Within this spinor framework it is easy to see that electrodynamics is a parity nonconserving theory. Although electrodynamics is asymmetric with regard to left and right and usually chiral asymmetry is connected to parity nonconservation, it is obvious that in this case the consequence of symmetry does not lead to processes occurring differently in the actual systems or in its mirror image. There are no observable consequences for the breakdown of parity.

There is a dynamical consequence for the particular way in which nature chooses to break chiral symmetry. Violation of chiral symmetry in this case reflects the preference of matter in interacting through the electromagnetic potentials rather than interacting through the electromagnetic fields. The linear nature of the interaction and the breakdown of the symmetry implies the minimal coupling substitution.

Our conclusion is that the linearity of the theory and left–right asymmetry implies the minimal substitution way of coupling the electromagnetic fields to matter.

The extension of this method to spin 2 field is under preparation.[9,10]

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APPENDIX A: RANK 2*s* FOUR SPINORS

Remembering that a rank one spinor transforms, under Poincaré transformation, as

$$\eta(x)\to\eta'(x')=D(l)\eta(x),$$

a $2s$ rank spinor $\psi(x)$ transforms as

$$\psi(x)\to\psi'(x')=\underbrace{D(l)\otimes\cdots\otimes D(l)}_{2s\ \text{factors}}\psi(x).$$

Analogously, the $2s$ rank spinor $\bar{\psi}(x)$ defined by

$$\bar{\psi}(x)=\psi^{+}(x)\underbrace{\gamma^0\otimes\cdots\otimes\gamma^0}_{2s\ \text{factors}}$$

transforms like

$$\bar{\psi}(x)\to\bar{\psi}'(x')=\bar{\psi}(x)\underbrace{D^{-1}(l)\otimes\cdots\otimes D^{-1}(l)}_{2s\ \text{factors}},$$

where we have used the property that

$$\gamma^0 D^+(l)\gamma^0 = D^{-1}(l).$$

APPENDIX B: NOTATION AND γ MATRICES

(1) The metric used is $g_{\mu\nu}=(1,-1,-1,-1)$.
(2) Dirac's matrices commutation rules are those of Bjorken and Drell.[7]
(3) In chiral representation

$$\gamma^5=\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix},\quad \mathbf{\Sigma}=\begin{bmatrix}\boldsymbol{\sigma} & 0\\ 0 & \boldsymbol{\sigma}\end{bmatrix},\quad \gamma^{\mu}_{\alpha\dot{\beta}}=\begin{bmatrix}0 & -(\sigma_\mu)_{\alpha\dot{\beta}}\\ -(\sigma^\mu)^{\alpha\dot{\beta}} & 0\end{bmatrix}.$$

(4) Charge conjugation matrix

$$(C)_{\alpha\dot{\beta}}=\begin{bmatrix}-i\sigma^2_{\alpha\dot{\beta}}=C_1 & 0\\ 0 & i\sigma^2_{\alpha\dot{\beta}}=C_1\end{bmatrix}.$$

(5) Pauli matrices are defined by

$$\sigma^0=\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix},\quad \sigma^1=\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix},\quad \sigma^2=\begin{bmatrix}0 & -i\\ i & 0\end{bmatrix},\quad \sigma^0=\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}.$$

By convention $\sigma^\mu=(\sigma^0=1,\ \boldsymbol{\sigma})$ designates $(\sigma^\mu)_{\alpha\dot{\beta}}$.

We have used also the property that

$$(\sigma^0)_{\alpha\dot{\beta}}=(\sigma_0)_{\alpha\dot{\beta}},\quad (\sigma^k)_{\alpha\dot{\beta}}=-(\sigma_k)_{\alpha\dot{\beta}}.$$

C_1 denotes the charge conjugation matrix in (2,2) space and obeys ${}^tC_1=-C_1$, $C_1^+=C_1^{-1}$.

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Involutions on the algebra of physical observables from reality conditions

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Some aspects of the algebraic quantization program proposed by Ashtekar are revisited in this article. It is proven that, for systems with first-class constraints, the involution introduced on the algebra of quantum operators via reality conditions can never be projected unambiguously to the algebra of physical observables, i.e., of quantum observables modulo constraints. It is nevertheless shown that, under sufficiently general assumptions, one can still induce an involution on the algebra of physical observables from reality conditions, though the involution obtained depends on the choice of particular representatives for the equivalence classes of quantum observables. © *1996 American Institute of Physics.* [S0022-2488(96)03801-8]

I. INTRODUCTION

Recently, Ashtekar *et al.*[1–3] have elaborated a program for the nonperturbative quantization of dynamical systems with first-class constraints. This program is specially designed to deal with the problem of quantizing general relativity, and has already been carried out successfully in a number of lower dimensional gravitational models, including minisuperspaces[4–6] and $2+1$ gravity.[1,3,7] The program proposed by Ashtekar is an extension, based on the algebraic approach to quantum mechanics,[8] of Dirac's canonical quantization method.[9] One of the main novelties with respect to Dirac's procedure is the introduction of a prescription to find the inner product in the space of quantum states. This allows one to adhere to the standard probabilistic interpretation of quantum mechanics when the quantization can be achieved.

Ashtekar's program consists of a series of steps that, after completion, should provide us with a consistent quantum theory. It can be applied, in principle, to any classical system whose phase space Γ is a real symplectic manifold.[1]

One must first choose a subspace S of the vector space of smooth complex functions on Γ. This subspace must contain the unit function and be closed both under complex conjugation and Poisson brackets.[2] In addition, S has to be complete, in the sense that any sufficiently regular complex function on phase space should be expressable as a sum of products of elements in S (or as a limit of this type of sums).[2]

Each element X in S is to be regarded as an elementary classical variable which is unambiguously associated with an abstract operator $\hat{X}$. One then constructs the free associative algebra $\mathcal{F}$ generated by these elementary quantum operators. On this algebra, one imposes the commutation relations that follow from the classical Poisson brackets, namely, if $X, Y \in S$, one must demand that (at least up to terms proportional to $\hbar^2$)

$$[\hat{X},\hat{Y}]-i\hbar\widehat{\{X,Y\}}=\hat{0}. \tag{1.1}$$

If there exist algebraic relations of the form

$$f_i(X_1,\ldots,X_n)=0 \quad (i=1,\ldots,m) \tag{1.2}$$

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between the elements in S (e.g., when the dimension of S is greater than that of Γ), such relations have also to be imposed on the corresponding quantum operators, with a suitable choice of factor ordering, if needed.[2] The imposition of these commutation and algebraic relations simply amounts to taking the quotient of the free algebra $\mathscr{F}$ by the ideal $\mathscr{T}_{\mathscr{F}}$ generated by the left-hand sides of Eq. (1.1) and the quantum counterpart of Eq. (1.2). The algebra of operators obtained in this way will be called $\mathscr{A}$.

At this point one should promote the complex conjugation relations in S to an involution on $\mathscr{A}$. We recall that an involution $\star$ on the algebra $\mathscr{A}$ is a map $\star: \mathscr{A}\rightarrow\mathscr{A}$ that satisfies

$$(\hat{X}^{\star})^{\star}=\hat{X}, \tag{1.3}$$

$$(\hat{X}+\lambda\hat{Y})^{\star}=\hat{X}^{\star}+\overline{\lambda}\hat{Y}^{\star}, \quad (\hat{X}\hat{Y})^{\star}=\hat{Y}^{\star}\hat{X}^{\star}, \tag{1.4}$$

for all $\hat{X},\hat{Y}\in\mathscr{A}$ and complex numbers λ. Here, $\overline{\lambda}$ is the complex conjugate to λ. To introduce the desired involution on $\mathscr{A}$, one can proceed in the following manner. For every $X,Y\in S$ such that Y is the complex conjugate to X, define $\hat{X}^{\star}=\hat{Y}$, and use properties (1.4) to extend this definition to all the operators in the free algebra $\mathscr{F}$. It is straightforward to check that one then gets an involution on $\mathscr{A}$ provided that the ideal $\mathscr{T}_{\mathscr{F}}$ of operators which vanish modulo commutation and algebraic relations is invariant under the $\star$-operation, i.e., that $\mathscr{T}_{\mathscr{F}}$ is a $\star$-ideal of $\mathscr{F}$. We will assume hereafter that this is in fact the case, and denote the resulting $\star$-algebra by $\mathscr{A}^{(\star)}$. The $\star$-relations in $\mathscr{A}^{(\star)}$ are usually called reality conditions,[1] for they capture the complex conjugation relations between elementary classical variables.

The next step in the quantization consists in finding a faithful representation for the abstract algebra $\mathscr{A}$ by linear operators acting on a complex vector space V. If the classical system possesses first-class constraints $\{C_i\}$, these constraints must now be explicitly represented by operators $\{\hat{C}_i\}$. In general, a choice of factor ordering, and of regularization in infinite dimensional systems,[2,3] are needed at this point in order to get a consistent algebra of quantum constraints,[9] that is, to guarantee that

$$[\hat{C}_i,\ \hat{C}_j]=\hat{f}_{ij}{}^{k}\hat{C}_k, \tag{1.5}$$

where $\hat{f}_{ij}{}^{k}\in\mathscr{A}$ and we use the convention that pairs of contracted indices are summed over.

The kernel $V_p\subset V$ of the constraints $\{\hat{C}_i\}$ supplies the vector subspace of quantum states. One must then determine the subalgebra $\mathscr{A}_p\subset\mathscr{A}$ of operators which leave V_p invariant. These operators commute weakly with the quantum constraints,

$$\hat{A}\in\mathscr{A}_p\Leftrightarrow[\hat{A},\ \hat{C}_i]=\hat{h}_i{}^{j}\hat{C}_j \quad (\hat{h}_i{}^{j}\in\mathscr{A}). \tag{1.6}$$

Let us define now

$$\mathscr{T}_C\equiv\{\hat{X}^i\hat{C}_i;\hat{X}^i\in\mathscr{A}\}. \tag{1.7}$$

Using Eqs. (1.5) and (1.6) one can show that $\mathscr{T}_C\subset\mathscr{A}_p$ and that, $\forall\hat{I}\in\mathscr{T}_C$ and $\forall\hat{A}\in\mathscr{A}_p$, both $\hat{A}\hat{I}$ and $\hat{I}\hat{A}$ belong to $\mathscr{T}_C$, so that $\mathscr{T}_C$ is an ideal of $\mathscr{A}_p$. On the other hand, if $\hat{A}\in\mathscr{A}_p$, all the operators of the form $\hat{B}=\hat{A}+\hat{I}$, with $\hat{I}\in\mathscr{T}_C$, have exactly the same action on quantum states, for V_p is annihilated by the quantum constraints. In order to obtain the algebra $\mathscr{A}'_p$ of operators with a well-defined action on V_p, one should therefore take the quotient of $\mathscr{A}_p$ by the ideal $\mathscr{T}_C$:[2]

$$\mathscr{A}'_p\equiv\mathscr{A}_p/\mathscr{T}_C. \tag{1.8}$$

The operators in $\mathscr{A}'_p$ are the quantum physical observables of the system.[10]

The quantization program presented so far leaves a certain freedom in the following steps: (a) the selection of the subspace S of elementary classical variables, (b) the construction of the linear

representation for the algebra $\mathscr{A}$ of quantum operators, and (c) the choice of factor ordering in the quantum constraints $\{\hat{C}_i\}$. The final result of the quantization process will depend on these inputs.[2] In particular, Ashtekar and Tate[2] assumed at this stage that, with a judicious choice of such inputs and at least for a large variety of physical systems, the involution defined on $\mathscr{A}^{(\star)}$ would induce an involution on $\mathscr{A}'_p$.

It is worth remarking in this sense that the $\star$-relations will project unambiguously to the algebra of physical observables only if two conditions are fulfilled. On the one hand, $\mathscr{A}_p \subset \mathscr{A}$ must be invariant under the $\star$-operation: $\forall \hat{A} \in \mathscr{A}_p$, $\hat{A}^\star \in \mathscr{A}_p$. On the other hand, it is necessary that $\mathscr{I}_C \subset \mathscr{A}_p$ be a $\star$-ideal of $\mathscr{A}_p$: $\forall \hat{I} \in \mathscr{I}_C$, $\hat{I}^\star \in \mathscr{I}_C$. When this is the case, the $\star$-operation provides a uniquely defined map between equivalence classes in $\mathscr{A}'_p$ which satisfies the properties (1.3) and (1.4) of an involution. The involution induced on $\mathscr{A}'_p$ will be denoted again by $\star$, and the resulting $\star$-algebra of physical observables by $\mathscr{A}'^{(\star)}_p$.

The idea suggested by Ashtekar[1–3] is to employ the involution on $\mathscr{A}'^{(\star)}_p$ to select the inner product $\langle , \rangle$ on V_p and, therefore, the Hilbert space $\mathscr{H}$ of physical states (normalizable quantum states). More specifically, he proposed to determine the inner product on V_p by demanding that the $\star$-relations between physical observables are realized as adjoint relations on the Hilbert space $\mathscr{H}$, i.e.,

$$\langle \Psi, \hat{A}' \Phi \rangle = \langle \hat{B}' \Psi, \Phi \rangle \quad \forall \Phi, \Psi \in \mathscr{H}, \quad \forall \hat{A}', \hat{B}' = (\hat{A}')^\star \in \mathscr{A}'^{(\star)}_p. \tag{1.9}$$

Rendall showed[11] that this condition is such a severe restriction on the inner product that, if an admissible inner product exists, it is unique (up to a positive global factor) under very general assumptions.

This completes the quantization program put forward by Ashtekar. If this program can be carried out for a given classical system, one would arrive at a mathematically consistent quantum theory in which real physical observables would be represented by self-adjoint operators acting on a Hilbert space of physical states.

The purpose of this work is to demonstrate however that there exists an impediment to achieving one of the steps of the above quantization method. We will prove in Sec. II that the $\star$-relations in $\mathscr{A}^{(\star)}$ never project unambiguously to the algebra of physical observables. This problem can be nonetheless overcome by slightly modifying Ashtekar's program, as we will show in Sec. III. The price to be paid is to allow a new freedom in the quantization process. A particular procedure to introduce an involution on $\mathscr{A}'_p$ from reality conditions should then be adopted. The subtleties that arise in defining such an involution are illustrated in Sec. IV by considering some simple physical systems. We finally discuss the physical implications of our results and conclude in Sec. V.

II. AMBIGUITIES IN THE REALITY CONDITIONS ON PHYSICAL OBSERVABLES

We want to prove that reality conditions (i.e., the $\star$-relations between quantum operators) never project unambiguously to the algebra of physical observables when there exist first-class constraints on the system. We will assume that the faithful, linear representation constructed for the algebra $\mathscr{A}$ of quantum operators is irreducible. Otherwise, one should decompose it in irreducible components, and apply the proof to follow to each component separately.

We have seen that, in order to obtain a uniquely defined involution on physical observables from reality conditions, it is necessary that both $\mathscr{A}_p$ and $\mathscr{I}_C$ be invariant under the $\star$-operation. In particular, we should have

$$\forall \hat{I} \in \mathscr{I}_C, \quad \hat{I}^0 \equiv \hat{I}^\star \in \mathscr{I}_C. \tag{2.1}$$

Select now in $\mathscr{T}_C$ one of the quantum constraints, e.g., $\hat{C}_1$, and consider also all the operators of the form $\hat{I}_1=\hat{Z}\hat{C}_1\in\mathscr{T}_C$, with $\hat{Z}\in\mathscr{A}$. Employing condition (2.1), and recalling definition (1.7), we obtain

$$\hat{C}_1^\star=\hat{Y}_1^j\hat{C}_j\,, \tag{2.2}$$

$$(\hat{I}_1)^\star=\hat{C}_1^\star\hat{Z}^\star=\hat{Y}_1^j\hat{C}_j\hat{Z}^\star\equiv\hat{I}_1^0=\hat{X}_1^k\hat{C}_k\,, \tag{2.3}$$

for some $\hat{Y}_1^j,\hat{X}_1^k\in\mathscr{A}$.

On the other hand, the image $\hat{Z}^\star$ of all the operators $\hat{Z}\in\mathscr{A}$ is again the whole algebra $\mathscr{A}$, because the $\star$-operation is an involution. Relation (2.3) therefore implies that, $\forall\,\hat{Z}\in\mathscr{A}$, there exist $\hat{X}_1^k\in\mathscr{A}$ such that

$$\hat{Y}_1^j\hat{C}_j\hat{Z}=\hat{X}_1^k\hat{C}_k\,. \tag{2.4}$$

This identity between operators must hold on any element of V, the vector space on which $\mathscr{A}$ has been represented. Choosing then $\Phi\in V_p\subset V$ with Φ different from zero, it follows from Eq. (2.4) that, $\forall\,\hat{Z}\in\mathscr{A}$,

$$\hat{Y}_1^j\hat{C}_j(\hat{Z}\Phi)=\hat{X}_1^k\hat{C}_k\Phi=0, \tag{2.5}$$

for the physical state Φ is annihilated by all quantum constraints. Besides, since the representation constructed is irreducible and $\Phi\neq0$, the range of $\hat{Z}\Phi(\forall\,\hat{Z}\in\mathscr{A})$ must be the whole vector space V. So, the above equation states that V is the kernel of the operator $\hat{Y}_1^j\hat{C}_j$. Being the representation for $\mathscr{A}$ faithful, we then must have

$$\hat{Y}_1^j\hat{C}_j=\hat{0}. \tag{2.6}$$

But this is clearly inconsistent with the fact that the $\star$-operation is an involution, because, using Eqs. (2.2) and (2.6), we get that $\hat{C}_1=(\hat{C}_1^\star)^\star=\hat{0}$. In this way, we conclude that, when there exist first-class constraints, $\mathscr{T}_C$ can never be invariant under the $\star$-operation and, therefore, reality conditions do not project unambiguously to the algebra of physical observables.

Moreover, it is generally the case that the $\star$-image of $\mathscr{T}_C$ is not even contained in $\mathscr{A}_p$, so that $\mathscr{A}_p$ is not a $\star$-subalgebra of $\mathscr{A}$. This can be proved, for instance, under the assumptions that (a) Eq. (2.2) holds for a certain quantum constraint $\hat{C}_1$ and (b) there exists at least one operator $\hat{W}\in\mathscr{A}$ whose commutator with $\hat{C}_1$ does not belong to $\mathscr{A}_p$. One can then check that, while $\hat{W}^\star\hat{Y}_1{}^j\hat{C}_j$ belongs to $\mathscr{T}_C$, its $\star$-conjugate, given by $\hat{C}_1\hat{W}$, is not included in $\mathscr{A}_p$. Hence, even though one could find a representative $\hat{A}$ for a given physical observable $\hat{A}'$ such that $\hat{A}^\star\in\mathscr{A}_p$, the $\star$-conjugates of all other operators in the equivalence class $\hat{A}'$ (i.e., the operators $\hat{A}+\hat{I}$, with $\hat{I}\in\mathscr{T}_C$) will in general not belong to the algebra $\mathscr{A}_p$.

For the sake of an example, let us consider a classical system whose phase space admits a set of global coordinates of the form $s\equiv\{t,H,x,p\}$, with $t,H,x,p\in\mathbb{R}$, and H and p the momenta canonically conjugate to t and x, respectively. Suppose, in addition, that there exists only one first-class constraint on the system, given by $H=0$. This extremely simple example describes, for instance, a Kantowski–Sachs model with positive cosmological constant.[5]

As elementary classical variables, we can choose the complex vector space spanned by s and the unity. The $\star$-operation on the corresponding algebra $\mathscr{A}$ of quantum operators is defined by

$$\hat{t}^\star=\hat{t},\quad \hat{H}^\star=\hat{H}, \tag{2.7}$$

$$\hat{x}^\star=\hat{x},\quad \hat{p}^\star=\hat{p},\quad \hat{1}^\star=\hat{1}, \tag{2.8}$$

and the properties (1.4) of an involution. The only quantum constraint is $\hat{H}=0$. On the other hand, it is not difficult to prove that the equivalence classes of the operators $\hat{1}$, $\hat{x}$, and $\hat{p}$ form a complete set of physical observables. We point out, nevertheless, that the algebra $\mathscr{A}_p$ is not generated by $\{\hat{1},\hat{x},\hat{p},\hat{H}\}$, but contains also operators like $\hat{t}\hat{H}$ and $(\hat{t})^2\hat{H}$ which are elements in $\mathscr{T}_C$. From Eq. (2.8) it follows that each equivalence class of observables possesses at least a representative whose $\star$-conjugate belongs to $\mathscr{A}_p$. In general, however, the $\star$-image of different representatives do not coincide modulo the constraint $H=0$, because the $\star$-operation does not leave the ideal $\mathscr{T}_C$ invariant. Namely, from Eqs. (2.7), (2.8) and the commutator $[\hat{t},\hat{H}]=i\hbar\hat{1}$, we get

$$(\hat{t}\hat{H})^\star=\hat{t}\hat{H}-i\hbar\hat{1}, \quad ((\hat{t})^2\hat{H})^\star=(\hat{t})^2\hat{H}-2i\hbar\hat{t}, \tag{2.9}$$

so that the $\star$-conjugate to $\hat{t}\hat{H}$ belongs to $\mathscr{A}_p$, but not to $\mathscr{T}_C$, whereas the $\star$-conjugate to $(\hat{t})^2\hat{H}$ is not even in $\mathscr{A}_p$.

III. INVOLUTIONS ON PHYSICAL OBSERVABLES

We have seen that the $\star$-relations in $\mathscr{A}^{(\star)}$ do not project unambiguously to $\mathscr{A}'_p$, because the $\star$-operation never maps all the representatives of a class of physical observables into another equivalence class. In order to define the $\star$-conjugate to a physical observable, one is therefore forced to choose first a particular representative for it. We now want to discuss under which circumstances it is possible to introduce an involution on $\mathscr{A}'_p$ by this procedure.

To construct an involution $\star$ on $\mathscr{A}'_p$, it actually suffices to define the $\star$-operation on an (over-) complete set of physical observables, and demand that this operation verifies conditions (1.4). Suppose then that $\{\hat{U}'_a\}$ is a complete set in $\mathscr{A}'_p$, that is, that $\mathscr{A}'_p$ can be obtained from the free associative algebra $\mathscr{B}'$ generated by $\{\hat{U}'_a\}$ by imposing the commutation relations between the observables $\hat{U}'_a$, as well as any algebraic relation that could exist between them. Assume also that one can find representatives $\{\hat{U}_a\}$ of the observables $\{\hat{U}'_a\}$ such that their $\star$-conjugates $\{\hat{U}^\star_a\}$ belong to $\mathscr{A}_p$. One might then hope that the $\star$-operation on $\mathscr{A}'_p$ could be defined by

$$(\hat{U}'_a)^\star=(\hat{U}^\star_a)', \tag{3.1}$$

where $(\hat{U}^\star_a)'$ denotes the equivalence class of $\hat{U}^\star_a$. However, we will prove that the assumptions introduced above do not guarantee that Eq. (3.1) leads to a well-defined involution on the algebra of physical observables.

The proof makes use of the fact that, being $\{\hat{U}'_a\}$ complete in $\mathscr{A}'_p$, any operator in the algebra $\mathscr{A}_p$ should be expressable, modulo an element in the ideal $\mathscr{T}_C$ (1.7), as (possibly a limit of) a sum of products of the representatives $\{\hat{U}_a\}$. In particular, since every $\hat{U}^\star_a\in\mathscr{A}_p$, one gets

$$\hat{U}^\star_a=\sum_n \lambda_a^{b_1\cdots b_n}\hat{U}_{b_1}\cdots\hat{U}_{b_n}+\hat{X}^i_a\hat{C}_i, \tag{3.2}$$

with $\hat{X}^i_a\in\mathscr{A}$ and the $\lambda_a^{b_1\cdots b_n}$'s some complex numbers. Hence, from Eq. (3.1),

$$(\hat{U}'_a)^\star=\sum_n \lambda_a^{b_1\cdots b_n}\hat{U}'_{b_1}\cdots\hat{U}'_{b_n}. \tag{3.3}$$

This $\star$-operation will be an involution on $\mathscr{A}'_p$ only if $((\hat{U}'_a)^\star)^\star=\hat{U}'_a$ for all $\hat{U}'_a$. This, together with Eqs. (1.4), (3.1), and (3.3), implies

$$\hat{U}'_a=\sum_n \overline{\lambda_a^{b_1\cdots b_n}}(\hat{U}^\star_{b_n})'\cdots(\hat{U}^\star_{b_1})'. \tag{3.4}$$

On the other hand, we have from Eq. (3.2)

$$\hat{U}_a = \sum_n \overline{\lambda_a^{b_1 \cdots b_n}} \hat{U}^\star_{b_n} \cdots \hat{U}^\star_{b_1} + \hat{C}_i^\star \hat{X}_a^{i\star}, \tag{3.5}$$

since the $\star$-operation is an involution on $\mathscr{A}^{(\star)}$. Consistency of Eq. (3.4) with (3.5) requires then

$$\hat{C}_i^\star \hat{X}_a^{i\star} = \hat{Y}^i_a \hat{C}_i\,, \tag{3.6}$$

for some operators $\hat{Y}^i_a \in \mathscr{A}$. This condition will not be satisfied by generic operators $\hat{X}^i_a \hat{C}_i \in \mathscr{I}_C$, because the ideal $\mathscr{I}_C$ is not invariant under the $\star$-operation when there exist first-class constraints on the system. Therefore, the $\star$-relations (3.3) will not supply in general an involution on $\mathscr{A}'_p$. To obtain that involution, it is necessary that both conditions (3.2) and (3.6) are satisfied by the representatives of our complete set of physical observables.

We will study now the case in which these requirements hold for our particular choice of representatives. Our previous discussion shows that the $\star$-operation defined by Eqs. (3.3) and (1.4) is then an involution on $\mathscr{B}'$, the free associative algebra generated by $\{\hat{U}'_a\}$. Recalling that the algebra $\mathscr{A}'_p$ of physical observables can be obtained from $\mathscr{B}'$ by imposing on its generators the commutation relations and any existing algebraic relations, we conclude that the $\star$-operation introduced on $\mathscr{B}'$ straightforwardly supplies an involution on $\mathscr{A}'_p$ provided that such an operation is compatible with the relations imposed on the generators $\{\hat{U}'_a\}$. In other words, the ideal of $\mathscr{B}'$ generated by those relations should be invariant under the $\star$-operation. When this requisite is fulfilled, one gets an involution on $\mathscr{A}'_p$ which captures the reality conditions on quantum operators.

Notice that the involution at which one arrives depends, nevertheless, on two choices: the complete set of physical observables and the representatives for them. In general, distinct choices may lead to different involutions on the algebra of physical observables. We will comment on this point further in Sec. V.

A situation which is often encountered in physical applications[4,5] is that one can find a complete set in $\mathscr{A}'_p$ admitting representatives $\{\hat{U}_a\}$ such that the complex vector space spanned by them is closed under reality conditions, i.e.,

$$\hat{U}^\star_a = \lambda^b_a \hat{U}_b\,. \tag{3.7}$$

In this case, assumption (3.2) holds with $\hat{X}^i_a \hat{C}_i = \hat{0}$, so that Eq. (3.6) is trivially satisfied. It is then at least possible to obtain an involution on the free algebra $\mathscr{B}'$ by replacing the operators $\hat{U}_a$ in Eq. (3.7) with their corresponding equivalence classes of physical observables.

IV. EXAMPLES

Let us illustrate our discussion by dealing with some examples. Consider, for instance, the physical system that was analyzed at the end of Sec. II. A complete set of physical observables for this system is $\mathscr{O}' \equiv \{\hat{1}', \hat{x}', \hat{p}'\}$, where $\hat{1}'$, $\hat{x}'$, and $\hat{p}'$ are the equivalence classes of the operators $\hat{1}$, $\hat{x}$, and $\hat{p}$, respectively. We can select these operators as the representatives of $\mathscr{O}'$. The associated reality conditions, which are given by Eq. (2.8), have the form (3.7). So, hypotheses (3.2) and (3.6) apply. We can therefore try to induce an involution on $\mathscr{A}'_p$ by the procedure explained in Sec. III. Since there exist no algebraic relations in $\mathscr{O}'$, the only consistency requirement that must be satisfied in order to get the desired involution is that reality conditions (2.8) are compatible with the commutators of the physical observables in $\mathscr{O}'$. There is just one commutator different from zero: $[\hat{x}', \hat{p}'] = i\hbar \hat{1}'$. On the other hand, we obtain from Eqs. (2.8) and (3.1)

$$(\hat{x}')^\star = \hat{x}', \tag{4.1}$$

$$(\hat{p}')^\star=\hat{p}', \quad (\hat{1}')^\star=\hat{1}'. \tag{4.2}$$

Taking then the $\star$-conjugate to $[\hat{x}', \hat{p}']$, we get

$$([\hat{x}', \hat{p}'])^\star=[(\hat{p}')^\star, (\hat{x}')^\star]=[\hat{p}', \hat{x}']=-i\hbar\hat{1}', \tag{4.3}$$

which is precisely $(i\hbar\hat{1}')^\star$. All other commutators between $(\hat{1}')^\star$, $(\hat{x}')^\star$, and $(\hat{p}')^\star$ vanish identically. Hence, the $\star$-operation constructed is compatible with the structure of $\mathscr{A}'_p$, and provides an involution on this algebra.

Let us consider now other choices of representatives of $\mathscr{O}'$. Adopt, e.g., the choice $\{\hat{1}, \hat{x}+\hat{t}(\hat{H})^2, \hat{p}\}$. It follows from Eqs. (2.7) and (2.8) that

$$(\hat{x}+\hat{t}(\hat{H})^2)^\star=\hat{x}+\hat{t}(\hat{H})^2-2i\hbar\hat{H}, \quad \hat{p}^\star=\hat{p}, \quad \hat{1}^\star=\hat{1}. \tag{4.4}$$

These reality conditions are of the type (3.2), with $\hat{X}^i_a\hat{C}_i=-2i\hbar\hat{H}$ for $\hat{U}_a=\hat{x}+\hat{t}(\hat{H})^2$, vanishing otherwise. In particular, assumption (3.6) is verified. Therefore, one can introduce a $\star$-operation on $\mathscr{A}'_p$ by applying Eq. (3.1) to the present case. In this way, one recovers the $\star$-relations (4.1) and (4.2), and thus the same involution on the algebra of physical observables that was obtained above.

Choose now the operators $\hat{1}$, $\hat{x}+\hat{t}\hat{H}$, and $\hat{p}$ as representatives of $\mathscr{O}'$. The reality conditions are then given by

$$(\hat{x}+\hat{t}\hat{H})^\star=\hat{x}+\hat{t}\hat{H}-i\hbar\hat{1}, \quad \hat{p}^\star=\hat{p}, \quad \hat{1}^\star=\hat{1}. \tag{4.5}$$

These reality conditions are of the form (3.7), and induce on $\mathscr{A}'_p$ the $\star$-operation defined through Eq. (4.2) and

$$(\hat{x}')^\star=\hat{x}'-i\hbar\hat{1}'. \tag{4.6}$$

Since Eqs. (4.2) and (4.6) imply again relation (4.3), and $(\hat{1}')^\star$ commutes with $(\hat{x}')^\star$ and $(\hat{p}')^\star$, the introduced $\star$-operation is compatible with the commutators of the physical observables, and is therefore an involution on $\mathscr{A}'_p$. However, this involution differs from that obtained in Eqs. (4.1) and (4.2). This proves that the involution induced on $\mathscr{A}'_p$ from reality conditions depends on the particular selection of representatives made for the complete set of physical observables under consideration.

Note, nonetheless, that the two involutions induced on $\mathscr{A}'_p$ in the example discussed above are equivalent in the sense that the two resulting $\star$-algebras $\mathscr{A}'^{(\star)}_p$ are isomorphic, as one can easily check by identifying the physical observable $\hat{x}'$ in Eq. (4.1) with $\hat{x}'-i(\hbar/2)\hat{1}'$ in (4.6). For infinite dimensional systems, however, one should expect that the involutions constructed by choosing different complete sets in $\mathscr{A}'_p$ and appropriate representatives for them would lead in general to inequivalent $\star$-algebras of physical observables.

Suppose, on the other hand, that we can represent the $\star$-relations on $\mathscr{A}'_p$ as adjoint relations on a Hilbert space of physical states, as suggested by Ashtekar. From the involution provided by Eqs. (4.1) and (4.2), we would then arrive at a quantum theory in which the observable $\hat{x}'$ would be self-adjoint. The involution defined through Eqs. (4.2) and (4.6) would lead instead to a quantum theory in which $\hat{x}'$ would not be represented by a self-adjoint operator, so that it should not correspond to a real physical observable of the system. In order to resolve this ambiguity one can insist, for instance, on that the real classical variable x should be represented by the quantum observable $\hat{x}'$. One would thus expect that the spectrum of $\hat{x}'$ should be real to guarantee that this observable has always real expectation values. Hence, $\hat{x}'$ should be self-adjoint. By itself, this condition supports the use of involution (4.1), (4.2) in the quantization, rather than other possible $\star$-relations on $\mathscr{A}'_p$ which, like relation (4.6), are inconsistent with the identification of $\hat{x}'$ as the quantum physical observable corresponding to x.

To close this section, we will present an example in which the involution induced on $\mathscr{B}'$ via reality conditions is not compatible with the structure of the algebra of physical observables. Let us consider a physical system with a first-class constraint of the form $H=0$, where $H\in\mathbb{R}$ is the momentum canonically conjugate to a certain variable $t\in\mathbb{R}$. We will assume that the reduced phase space of the system is the cotangent bundle over the unit circle S^1. As elementary variables, we can choose the complex vector space spanned by $\{1, t, H, c_\theta\equiv\cos\theta, s_\theta\equiv\sin\theta, p_\theta\}$. Here, $\theta\in S^1$, and $p_\theta\in\mathbb{R}$ is the momentum conjugate to θ. The reality conditions on the corresponding algebra $\mathscr{A}^{(\star)}$ of quantum operators are given by Eq. (2.7) and

$$\hat{c}_\theta^\star=\hat{c}_\theta,\quad \hat{s}_\theta^\star=\hat{s}_\theta,\quad \hat{p}_\theta^\star=\hat{p}_\theta,\quad \hat{1}^\star=\hat{1}. \tag{4.7}$$

Besides, since $\cos^2\theta+\sin^2\theta=1$, we will impose the algebraic relation

$$(\hat{c}_\theta)^2+(\hat{s}_\theta)^2=\hat{1}. \tag{4.8}$$

A complete set of physical observables is $\mathscr{O}'\equiv\{\hat{1}',\hat{c}'_\theta,\hat{s}'_\theta,\hat{p}'_\theta\}$, the prime denoting equivalence classes. The only nonvanishing commutators in $\mathscr{O}'$ are

$$[\hat{c}'_\theta,\hat{p}'_\theta]=-i\hbar\hat{s}'_\theta,\quad [\hat{s}'_\theta,\hat{p}'_\theta]=i\hbar\hat{c}'_\theta. \tag{4.9}$$

In addition, relation (4.8) implies that the physical observables in $\mathscr{O}'$ must satisfy

$$(\hat{c}'_\theta)^2+(\hat{s}'_\theta)^2=\hat{1}'. \tag{4.10}$$

If one chooses $\hat{1}$, $\hat{c}_\theta$, $\hat{s}_\theta$, and $\hat{p}_\theta$ as the representatives of $\mathscr{O}'$, the procedure explained in Sec. III allows one to obtain a $\star$-operation on $\mathscr{B}'$ (the free associative algebra generated by $\mathscr{O}'$) which is compatible with the commutators (4.9) and the algebraic relation (4.10), and hence provides an involution on $\mathscr{A}'_p$. Let us select instead the representatives $\mathscr{O}\equiv\{\hat{1},(\hat{c}_\theta+\hat{t}\hat{H}),\hat{s}_\theta,\hat{p}_\theta\}$. From Eqs. (2.7) and (4.7) (and the commutator of $\hat{t}$ and $\hat{H}$), we get

$$\hat{1}^\star=\hat{1},\quad (\hat{c}_\theta+\hat{t}\hat{H})^\star=(\hat{c}_\theta+\hat{t}\hat{H})-i\hbar\hat{1},\quad \hat{s}_\theta^\star=\hat{s}_\theta,\quad \hat{p}_\theta^\star=\hat{p}_\theta. \tag{4.11}$$

These reality conditions are of the type (3.7). Thus, we can apply the results of Sec. III to arrive at an involution on $\mathscr{B}'$ which is defined through the $\star$-relations (4.11), but imposed on equivalence classes in $\mathscr{O}'$. However, such a $\star$-operation is incompatible with the algebraic relation (4.10), because

$$((\hat{c}'_\theta)^2+(\hat{s}'_\theta)^2-\hat{1})^\star=(\hat{c}'_\theta-i\hbar\hat{1}')^2+(\hat{s}'_\theta)^2-\hat{1}'\neq 0. \tag{4.12}$$

So, the involution introduced on $\mathscr{B}'$ does not supply a well-defined involution on the algebra $\mathscr{A}'_p$ of physical observables. This example shows that the freedom in choosing representatives of the complete set of physical observables is in general restricted by the consistency of the algebraic structures with the $\star$-operation constructed on $\mathscr{A}'_p$.

V. CONCLUSIONS AND FURTHER COMMENTS

We have shown that, in systems with first-class constraints, the involution defined on the algebra $\mathscr{A}^{(\star)}$ of quantum operators does not ever project unambiguously to the algebra $\mathscr{A}'_p$ of physical observables. The reason for this is that the $\star$-conjugates of all the representatives of any class of observables never belong to the same equivalence class in $\mathscr{A}_p$, and, in general, not even to $\mathscr{A}_p$.

We have also proved that, under sufficiently general circumstances, it is nevertheless possible to obtain a well-defined involution on $\mathscr{A}'_p$ via reality conditions by making a particular choice of

representatives for the equivalence classes of physical observables. The procedure to arrive at this involution is the following. One must first find a complete set of physical observables $\{\hat{U}'_a\}$ in $\mathscr{A}'_p$, and select representatives $\{\hat{U}_a\}$ of them such that their $\star$-conjugates $\{\hat{U}^\star_a\}$ satisfy requirements (3.2) and (3.6), namely, such that every $\hat{U}^\star_a$ belongs to the free associative algebra generated by $\{\hat{U}_a\}$ up to an operator which, as well as its $\star$-conjugate, vanish modulo quantum constraints. One can then introduce an involution $\star$ in the free associative algebra $\mathscr{B}'$ by defining $(\hat{U}'_a)^\star$ as the equivalence class of the observable $\hat{U}^\star_a$ [see Eqs. (3.2),(3.3)]. This involution on $\mathscr{B}'$ straightforwardly supplies an involution on $\mathscr{A}'_p$, provided that the constructed $\star$-operation is compatible with the commutation and algebraic relations which exist between the physical observables in the complete set $\{\hat{U}'_a\}$.

The involution obtained in this way on $\mathscr{A}'_p$ depends on the selection of a complete set of physical observables and of specific representatives for them. While these choices are severely restricted by the consistency conditions explained above, there is in general some freedom left, so that, by adopting different choices, one might in principle arrive at nonequivalent involutions on the algebra of physical observables.

This extra freedom in the quantization method suggested by Ashtekar, rather than being a supplementary complication, might actually become an additional help when attempting to complete the quantization. This is due to the fact that, given an involution $\star$ on the algebra $\mathscr{A}'_p$ and a certain representation for $\mathscr{A}'_p$ on a vector space V_p of quantum states, there is *a priori* no guarantee that there exists an inner product on V_p with respect to which the $\star$-relations on physical observables are realized as Hermitian adjoint relations in the resulting Hilbert space. Thus if such an inner product does not exist for a particular involution on $\mathscr{A}'_p$, one can always try to induce a different involution on this algebra via reality conditions, and see whether it is possible to then find an inner product with the desired properties.

We notice, on the other hand, that the introduction of an involution on $\mathscr{A}'_p$ amounts essentially to determine the $\star$-conjugate to a complete set of physical observables. When one expects that a set of this kind, or at least some of its elements, correspond classically to real observables of the system, it is reasonable to assume that they should be represented by self-adjoint operators. The involution defined on $\mathscr{A}'_p$ should therefore ensure that these operators coincide with their $\star$-conjugates. These requirements clearly restrict the physically admissible involutions on $\mathscr{A}'_p$. Moreover, in the case that this type of physical arguments would apply to a complete set in $\mathscr{A}'_p$, one would fully specify the involution on this algebra. In this way, one can use physical intuition as a guideline to resolve (either partially or totally) the ambiguity encountered when inducing an involution on the algebra of physical observables from reality conditions.

Finally, an alternative strategy to remove such an ambiguity could consist in adopting a specific procedure to induce the involution $\star$ on $\mathscr{A}'_p$. A procedure of this type might be, e.g., the following:[12] Let us denote by $\mathscr{A}_s \subset \mathscr{A}_p$ the subalgebra formed by all the strong quantum observables of the theory (that is, the operators which commute exactly with all the quantum constraints $\{\hat{C}_i\}$), and define $\mathscr{I}_s \equiv \mathscr{I}_C \cap \mathscr{A}_s$. It is immediate to check that $\mathscr{I}_s$ is an ideal of $\mathscr{A}_s$. Suppose then that, in the system under consideration, the involution $\star$ defined on $\mathscr{A}^{(\star)}$ and the representation constructed for the algebra $\mathscr{A}$ and for the constraints $\{C_i\}$ are such that: (a) The complex vector space spanned by the quantum constraints $\{\hat{C}_i\}$ is closed under reality conditions, i.e., $\hat{C}^\star_i = \lambda^j_i \hat{C}_j$, where the λ^j_i's are complex numbers. (b) The algebra $\mathscr{A}'_s \equiv \mathscr{A}_s / \mathscr{I}_s$ is isomorphic to $\mathscr{A}'_p$. (c) The ideal $\mathscr{I}_s$ is invariant under the $\star$-operation. Notice that hypothesis (c) is in principle compatible with the fact that $\mathscr{I}_C$ is not a $\star$-ideal of $\mathscr{A}_p$. Requirement (b), on the other hand, guarantees that each physical observable in $\mathscr{A}'_p$ possesses (at least) one representative which is a strong observable.

Using condition (a), it is possible to prove that the $\star$-operation leaves $\mathscr{A}_s$ invariant. Assumption (c) ensures then that the $\star$-relations project unambiguously to $\mathscr{A}'_s$. One hence obtains a well-defined involution on $\mathscr{A}'_s$ which, given condition (b), supplies a unique involution on $\mathscr{A}'_p$ through the existing isomorphism between these two algebras. So, provided that hypotheses (a)–

(c) are satisfied, the above strategy allows one to induce an unambiguous involution on $\mathscr{A}'_p$ from reality conditions.

In fact, this strategy is partially motivated by the refined version of Ashtekar's program which has been recently proposed.[13] In this new version of the program, it is supposed that all first-class constraints can be represented by self-adjoint operators on an auxiliary Hilbert space on which one has constructed a $\star$-representation of $\mathscr{A}^{(\star)}$. Hypothesis (a) must hence hold. Besides, rather than considering the whole algebra $\mathscr{A}_p$, one restricts one's attention to a certain $\star$-subalgebra of strong observables $\mathscr{B}^{(\star)}_{\rm phys} \subset \mathscr{A}_s$.[13] After completion of the quantization, one obtains a physical Hilbert space $\mathscr{H}_{\rm phys}$ which carries a $\star$-representation of $\mathscr{B}^{(\star)}_{\rm phys}$. Let us point out that this representation will not be faithful in general, for there may exist a subalgebra $\mathscr{I}_{\mathscr{B}} \subset \mathscr{B}^{(\star)}_{\rm phys}$ that annihilates the whole space of physical states. It seems reasonable to assume that $\mathscr{I}_{\mathscr{B}} = \mathscr{I}_C \cap \mathscr{B}^{(\star)}_{\rm phys}$, i.e., that the operators in $\mathscr{B}^{(\star)}_{\rm phys}$ with zero action on physical states are those which vanish modulo constraints.[14] On the other hand, it is possible to show[14] that Ashtekar's refined program can be consistently implemented only if $\mathscr{I}_{\mathscr{B}}$ is a $\star$-ideal of $\mathscr{B}^{(\star)}_{\rm phys}$, requirement which is the analog of hypothesis (c) above.

According to our discussion, $\mathscr{H}_{\rm phys}$ should finally provide a faithful representation of $\mathscr{B}'_{\rm phys} \equiv \mathscr{B}^{(\star)}_{\rm phys}/\mathscr{I}_{\mathscr{B}}$. In order that all relevant physical information can be extracted from the quantum theory obtained, it is then necessary that $\mathscr{B}'_{\rm phys}$ be isomorphic to $\mathscr{A}'_p$ (or at least to a sufficiently large subalgebra of it). This last condition parallels hypothesis (b). In this sense, the strategy presented here to induce an involution on $\mathscr{A}'_p$ actually is implicitly incorporated in Ashtekar's refined program, with the only generalization that one can consider a $\star$-subalgebra of strong observables $\mathscr{B}^{(\star)}_{\rm phys}$ as the substitute for $\mathscr{A}_s$.

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Group quantization on configuration space

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New features of a previously introduced group approach to quantization are presented. We show that the construction of the symmetry group associated with the system to be quantized (the ''quantizing group'') does not require, in general, the explicit construction of the phase space of the system, i.e., does not require the actual knowledge of the general solution of the classical equations of motion; in many relevant cases an implicit construction of the group can be given, directly, on configuration space. To show an application, we construct the symmetry group for the conformally invariant massless scalar and electromagnetic fields and the scalar and Dirac fields evolving in a symmetric curved space-time or interacting with symmetric classical electromagnetic fields. Further generalizations of the present procedure are also discussed and in particular the conditions under which non-Abelian groups (mainly affine groups and more general gauge groups) can be included. © *1996 American Institute of Physics.* [S0022-2488(96)02401-7]

I. INTRODUCTION

The conventional perturbative methods of quantization do not work properly with several relevant field theories. In addition, even in the case of theories for which a perturbative approach is possible, some information cannot be obtained by perturbative techniques because of its global nature. Therefore, it is necessary to look for other nonperturbative methods to extract this information from these quantum theories. A quantization method which might be especially suitable to perform this task is the group approach to quantization (GAQ) formalism.

The GAQ formalism was introduced several years ago (see, e.g., Refs. 1 and 2, and references therein) as an improved version of the geometric quantization and the Kirillov coadjoint orbit methods of quantization.[3,4] One of the major aims in the construction of the algorithm was to achieve the quantum solutions of a given physical system without explicitly solving the corresponding classical equation of motion, thus allowing for a quantum system for which a classical limit is not properly defined or the classical equations do not have a well-defined general solution. However, the required understanding of the basic symmetry group[5] is so accurate that, in many cases, the effort to finding it could be nearly equivalent to solving the problem. In this sense, GAQ is perhaps more useful as a tool for associating exactly solved (quantum systems) with already

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classified Lie groups than as a method to quantize physical systems originally defined by a Lagrangian.

This paper is intended to be a first step in the opposite direction, i.e., towards the construction of quantizing groups, closely related to actual Lagrangians (or, equivalently, equations of motions), and dependent on fields given in configuration space, that is to say, formal groups of sections of a given fiber bundle on space–time directly attached to the physical system. We shall call this *configuration-space image* of the formalism. As the basic result, prior to this goal, it will be shown that the construction of the quantizing group does not, in principle, require the previous step of going to the phase space of the system; i.e., the explicit solution of the classical equations of motion is not required.

The configuration-space image of the formalism will also provide us a clearer view of the exact nature of the quantizing group and will clarify the relationship of this formalism with the Lagrangian and canonical formalisms.

We shall also show some of the advantages of expressing the formalism in the configuration-space image by constructing the quantizing group for several nontrivial fields in a natural and straightforward way: the conformally invariant massless scalar and electromagnetic fields, and the scalar field in symmetric curved space–time or interacting with arbitrary symmetric classical electromagnetic fields (Sec. III).

This image of the formalism, as well as the examples presented here, can also serve as a guide for further generalizations. We shall discuss some of these, arguing that a direct generalization for non-Abelian affine groups, or more general Kac–Moody groups and gauge groups[6,7] (see also Refs. 8 and 9), requires the equations of motion to be of first order. We shall show by means of two examples that this is not the case for other types of non-Abelian groups (Sec. IV).

In this article we shall not discuss the subtleties of the proper quantization procedure. The interested reader may explore these in some of the quoted references.

II. THE HARMONIC OSCILLATOR AND THE KLEIN–GORDON FIELD

In this section we shall use two simples examples, the harmonic oscillator and the Klein–Gordon field, to present the basic features of the GAQ formalism when the quantizing group can be written in terms of fields in configuration space.

The group law proposed in Ref. 1 for the one-dimensional harmonic oscillator [the extended one-dimensional Galilei group, the quantizing group for the nonrelativistic free particle can be obtained as the limiting case $\omega\to 0$] was

$$A''=A+A'\cos\omega B+\left(\frac{V'}{\omega}\right)\sin\omega B,$$

$$V''=V+V'\cos\omega B-\omega A'\sin\omega B,\quad B''=B+B', \tag{2.1}$$

$$\zeta''=\zeta\zeta'\exp\frac{i}{2}\left[V\left(A'\cos\omega B+\frac{V'}{\omega}\sin\omega B\right)-A(V'\cos\omega B-\omega A'\sin\omega B)\right].$$

Nevertheless, apart from the fact that the algebra of this group is isomorphic to the algebra of the basic observables of the harmonic oscillator little has been explained concerning the manner in which this group is actually associated with the harmonic oscillator (HO). Let us consider, however, the harmonic oscillator (HO) from the Lagrangian viewpoint. The action is

$$S_{\mathrm{HO}}=\frac{1}{2}m\int dt[\dot{q}^2-\omega^2q^2]. \tag{2.2}$$

The equations of motion are

$$\left[\frac{d^2}{dt^2}+\omega^2\right]q=0 \tag{2.3}$$

with the general solution

$$q(t)=q_0\ \cos\ \omega t+\frac{\dot{q}_0}{\omega}\ \sin\ \omega t,\quad \Rightarrow\dot{q}(t)=\dot{q}_0\ \cos\ \omega t-\omega q_0\ \sin\ \omega t. \tag{2.4}$$

Hence, by means of the identification $A\equiv q_0$, $V\equiv\dot{q}_0$, $t\equiv B$; and associating a time evolution to the coordinates of the phase space in the natural manner, the group law in Eq. (2.1) can be written in the form

$$\begin{gathered}A''=A+A'(B),\quad V''=V+V'(B),\quad B''=B+B',\\ \zeta''=\zeta\zeta'\ \exp\frac{i}{2}\,m[VA'(B)-AV'(B)].\end{gathered} \tag{2.5}$$

Now, taking into account that $\dot{q}\equiv\dot{A}=V$, this group law can straightforwardly be written on configuration space:

$$\begin{gathered}B''=B+B',\quad q''(t)=q(t)+q'(t+B),\\ \zeta''=\zeta'\zeta\ \exp\frac{i}{2}\,m[\dot{q}(t)q'(t+B)-q(t)\dot{q}'(t+B)]_{t=t_0}.\end{gathered} \tag{2.6}$$

Instead of discussing here what we can learn from the simple manipulations above and the results obtained, it is preferable to consider first the case of a field such as the Klein–Gordon field. The action and equations of motion are

$$S_{\mathrm{KG}}=\frac{1}{2}\int d^4x[\partial^\mu\phi\partial_\mu\phi-m^2\phi^2], \tag{2.7}$$

$$\Rightarrow[\Box+m^2]\phi=0. \tag{2.8}$$

The analogy with the harmonic oscillator can serve as a guide to propose a quantizing group for the fields directly on configuration space (to simplify the discussion we shall not consider here Lorentz transformations, but only the symmetries associated with space–time translations). Let us consider the following composition law:

$$a''=a+a',\quad a\ \in\ R^4,\quad \phi''(x)=\phi(x)+\phi'(x+a), \tag{2.9}$$

$$\zeta''=\zeta'\zeta\ \exp\frac{i}{2}\,\xi_{\mathrm{KG}}(g',g)\equiv\zeta'\zeta\ \exp\frac{i}{2}\int_\Sigma d\sigma_\mu(x).\mathscr{T}^\mu_{\mathrm{KG}}(g,g')(x),$$

where

$$\mathscr{T}^\mu_{\mathrm{KG}}(g,g')(x)=\partial^\mu\phi(x)\phi'(x+a)-\phi(x)\partial^\mu\phi'(x+a) \tag{2.10}$$

and Σ is any spacelike hypersurface.

Now, let us expand the fields ϕ that solve the equation of motion (2.8) in Fourier modes by means of

$$\phi(x)=\int \frac{d^3k}{2k^0}\,(\Phi(k)e^{-ikx}+\Phi^+(k)e^{ikx}). \tag{2.11}$$

It is not difficult to see that for the Fourier modes $\Phi(k)$ we get the composition law postulated in Ref. 10. This implies that the composition law above is actually a group law. Nonetheless, it is easy to see that we need not use the general solution (2.11) to show that Eqs. (2.9) and (2.10) define a group law. In fact, the requirement that the fields in Eq. (2.10) be solutions of the equation of motion is enough to show that

(a) the quantity $\xi(g',g)$ fulfills the cocycle property:

$$\xi(g'',g')+\xi(g''*g',g)=\xi(g'',g'*g)+\xi(g',g) \tag{2.12}$$

and that

(b) the current $\mathscr{T}^\mu$ is conserved:

$$\partial_\mu \mathscr{T}^\mu=0. \tag{2.13}$$

In fact, in all the cases studied in this paper there is a double implication (a) $\Leftrightarrow$ (b): Finding a divergenceless current composed of the fields solution of the equations of motion has consistently proved sufficient for the quantity ξ, constructed on it, to fulfill the cocycle property. We do not know whether this is the general case.

We can, therefore, state the following features of the formalism expressed in configuration space:

(1) The basic group (the group to be centrally extended) is a group irrespective of whether or not the fields involved fulfill the equations of motion.

(2) The central extension involves the integral of a divergenceless current $\mathscr{T}^\mu$ over an hypersurface Σ. This current has null divergence only over the fields that obey the equations of motion.

Therefore, the centrally extended group, the quantizing group, *involves only the fields that are solutions of the equations of motion*. It is constructed upon the *phase space* of the system. [For the (covariant) description of the phase space of a system as the set of all solutions of the classical equations of motion see, e.g., Ref. 11, and references therein.]

In this phase space, different coordinates can be chosen. The choice of the Fourier modes $\Phi(k)$ leads us to the composition law in Ref. 10. Another choice is the familiar one of fields and timelike derivatives of the fields in the hypersurface Σ. We can write the group law in these coordinates by using the following propagation property:

$$\phi(y)=\int_\Sigma d\sigma_\mu(x)[\,\partial^\mu\Delta(y-x)\,\phi(x)-\Delta(y-x)\,\partial^\mu\phi(x)\,], \tag{2.14}$$

where the propagator Δ obeys the equation of motion:[12]

$$[\Box+m^2]\Delta=0. \tag{2.15}$$

(3) The classical equations of motion, *but not their general solution*, are required to show that the quantizing group is, in fact, a group.

(4) The equations of motion are not uniquely determined by the group; Eq. (2.13) implies Eq. (2.8) for *some* m but not for a particular m. Therefore Eq. (2.13) *almost* implies Eq. (2.8) but there is not a complete implication. The groups in configuration space for the harmonic oscillator and the free particle are the same, whereas the equations of motion are not. It is in terms of phase-space coordinates that the difference between these systems explicitly appears in the group.

III. APPLICATIONS

In this section we shall construct the quantizing group for several physically interesting systems to present an application of the formalism presented above: the conformally invariant massless scalar and electromagnetic fields, the scalar and Dirac field in a symmetric curved space–time, and these same fields interacting with symmetric electromagnetic fields.

[Unlike in the previous section, where the semidirect action of the space-time symmetries was given in a rather unnatural way—a way adapted to the Schrödinger representation—in the sequel we shall write the quantizing groups in the natural way; the other expression can be obtained by a simple change of coordinates.]

A. Conformally invariant fields

The conformal group, for which the composition law has not, up to now, been given in a closed form, is made up of compositions of the following actions on the space–time:

(a) space time translations: $(ux)^{\alpha}=x^{\alpha}+a^{\alpha}$;

(b) Lorentz transformations: $(ux)^{\alpha}=\Lambda^{\alpha}_{\mu}x^{\mu}$;

(c) dilatations: $(ux)^{\alpha}=e^{\lambda}x^{\alpha}$;

(d) special conformal tranformations: $(ux)^{\alpha}=\dfrac{x^{\alpha}+c^{\alpha}x^{2}}{1+2cx+c^{2}x^{2}}$.

1. The massless scalar field

The group law (in four dimensions, in which case the conformal dimension of a scalar field is $l=-1$) is

$$\begin{aligned} u''&=u'*\dot{u}, \quad \text{conformal (sub)group,}\\ \phi''(x)&=\phi'(x)+\Omega^{-1}(u'^{-1},x)\,\phi(u'^{-1}(x)), \end{aligned} \tag{3.1}$$

$$\zeta''=\zeta'\zeta\,\exp\frac{i}{2}\,\xi_{MS}(g',g)=\zeta\zeta'\,\exp\frac{i}{2}\int_{\Sigma}d\sigma_{\mu}(x).\mathscr{T}^{\mu}_{MS}, \tag{3.2}$$

where

$$\mathscr{T}^{\mu}_{MS}=\phi'(x)\partial^{\mu}[\Omega^{-1}(u'^{-1},x)\,\phi(u'^{-1}(x))]-\partial^{\mu}\phi'(x)[\Omega^{-1}(u'^{-1},x)\,\phi(u'^{-1}(x))] \tag{3.3}$$

and the function Ω is given by

$$\Omega(u,x)=\begin{cases} 1+2cx+c^{2}x^{2} & \text{for special conformal transformation}\\ e^{-\lambda} & \text{for dilatations}\\ 1 & \text{for the Poincaré subgroup}\end{cases}.$$

The function Ω for a general conformal transformation can be obtained by using its property

$$\Omega(u,x)\Omega(u',ux)=\Omega(u'u,x) \tag{3.4}$$

which is required for Eq. (3.1) to define a group.

It is not difficult to show that if $\phi(x)$ and $\phi'(x)$ are solution of the equations of motion

$$\partial^{\mu}\partial_{\mu}\phi(x)=0 \tag{3.5}$$

so is $\phi''(x)$. It is also straightforward to show, by using Eqs. (3.4) and (3.5), that the current $\mathcal{T}^{\mu}$ is divergenceless and fulfills the cocycle property (2.12).

2. The electromagnetic field

The group law is given by

$$\begin{aligned} &u''=u'*u, \quad \text{conformal (sub)group,} \\ &A''_{\mu}(x)=A'_{\mu}(x)+\frac{\partial u'^{-1\alpha}}{\partial x^{\mu}}A_{\alpha}(u'^{-1}x)\equiv A'_{\mu}(x)+(S(u'^{-1})A)_{\mu}(x), \end{aligned} \tag{3.6}$$

where S is the representation of the conformal group that acts on the electromagnetic vector field. This action is the natural one and means that the potential vector has null conformal weight. This action induces the following one on the tensor field $F_{\mu\nu}$:

$$F''_{\mu\nu}(x)=F'_{\mu\nu}(x)+\frac{\partial u'^{-1\alpha}}{\partial x^{\mu}}\frac{\partial u'^{-1\beta}}{\partial x^{\nu}}F_{\alpha\beta}(u'^{-1}x), \tag{3.7}$$

$$\equiv F'_{\mu\nu}(x)+(S(u'^{-1})F)_{\mu\nu}(x). \tag{3.8}$$

It is easy to show that this action leaves invariant Maxwell's action:

$$S_M=\int d^4x\ F_{\mu\nu}F^{\mu\nu} \tag{3.9}$$

and, therefore, leaves Maxwell's equations invariant.

The central extension is given by

$$\zeta''=\zeta'\zeta\ \exp\frac{i}{2}\,\xi_M(g',g)=\zeta'\zeta\ \exp\frac{i}{2}\int_{\Sigma}d\sigma_{\mu}(x).\mathcal{T}^{\mu}_M(g',g)(x) \tag{3.10}$$

with divergenceless current

$$\mathcal{T}^{\mu}_M(g',g)(x)=F'^{\mu\nu}(x)(S(u'^{-1})A)_{\nu}(x)-A'_{\nu}(x)(S(u'^{-1})F)^{\mu\nu}(x). \tag{3.11}$$

If we restrict ourselves to the symmetry group of space–time translations, the group is written

$$\begin{aligned} &a''=a+a', \quad A''_{\mu}(x)=A'_{\mu}(x)+A_{\mu}(x-a'), \\ &\zeta''=\zeta\zeta'\ \exp\frac{i}{2}\int_{\Sigma}d\sigma_{\mu}(x).\mathcal{T}^{\mu}_M(g',g)(x), \end{aligned} \tag{3.12}$$

with a current

$$\mathcal{T}^{\mu}_M(g',g)(x)=F'^{\mu\nu}(x)A_{\nu}(x-a')-A'_{\nu}(x)F^{\mu\nu}(x-a'). \tag{3.13}$$

In this last example, we again see the issue discussed above: The current $\mathcal{T}^{\mu}_M$ is divergenceless and fulfills the cocycle property if Maxwell equations are obeyed, but a Proca-like equation $\partial_{\mu}F^{\mu\nu}+m^2A^{\nu}=0$, with a non-null mass m, is also allowed. This is, however, no longer the case when the full conformal group is considered.

B. Matter fields in a symmetric curved space–time

In this section we shall present the quantizing group for matter fields, the Klein–Gordon and Dirac fields, evolving in a symmetric, but on the other hand arbitrary, curved space–time with metric $g_{\mu\nu}$.

Let us assume that a set of transformations v is a group of isometries of the metric (see, e.g., Refs. 13 and 14). Then we have

$$g_{\mu\nu}(vx)\,\frac{\partial(vx)^{\mu}}{\partial x^{\alpha}}\,\frac{\partial(vx)^{\nu}}{\partial x^{\beta}}=g_{\alpha\beta}(x) \tag{3.14}$$

and, in the same way,

$$g^{\mu\nu}(vx)=g^{\alpha\beta}(x)\,\frac{\partial(vx)^{\mu}}{\partial x^{\alpha}}\,\frac{\partial(vx)^{\nu}}{\partial x^{\beta}}. \tag{3.15}$$

1. The scalar field

The equations of motion for a scalar field evolving in this background metric are (see, e.g., Refs. 15 and 16):

$$[\Box(x)+\alpha R(x)+m^2]\phi(x)=0 \tag{3.16}$$

with

$$\Box(x)\phi(x)\equiv\frac{1}{\sqrt{g(x)}}\,\partial_{\mu}(\sqrt{g(x)}g^{\mu\nu}(x)\partial_{\nu})\phi(x). \tag{3.17}$$

The group law that would describe the quantum dynamics of this system is given by

$$v''=v'*v,\quad \phi''(x)=\phi'(x)+\phi(v'^{-1}(x)), \tag{3.18}$$

$$\zeta''=\zeta\zeta'\,\exp\frac{i}{2}\int_{\Sigma}d\sigma_{\mu}(x)\mathscr{T}^{\mu}_{SCS} \tag{3.19}$$

with

$$\mathscr{T}^{\mu}_{SCS}=\sqrt{g(x)}g^{\mu\nu}(x)[\phi'(x)\partial_{\nu}[\phi(v'^{-1}(x))]-\partial_{\nu}\phi'(x)\phi(v'^{-1}(x))]. \tag{3.20}$$

[Notice that Eq. (3.14) implies $\Box(x)=\Box(vx)$ and $R(vx)=R(x)$ (see also Ref. 14).]

2. The Dirac field

Let Ψ be a Dirac field with equations of motion (see, e.g., Refs. 13 and 15):

$$[i\hat{\gamma}^{\mu}(\partial_{\mu}+\tfrac{1}{2}i\Gamma^{a}{}_{\mu}{}^{b}\Sigma_{ab})-m]\Psi=0, \tag{3.21}$$

where

$$g_{\mu\nu}=\eta_{ab}e^{a}_{\mu}e^{b}_{\nu}, \tag{3.22}$$

$$\hat{\gamma}^{\mu}=\gamma^{a}e_{a}{}^{\mu},\quad \Sigma_{ab}=\tfrac{1}{4}i[\gamma_a,\gamma_b], \tag{3.23}$$

$$\Gamma^{c}_{ab}=e^{c}{}_{\nu}e^{\mu}_{a}(\partial_{\mu}e_{b}{}^{\nu}+e_{b}{}^{\lambda}\Gamma^{\nu}_{\mu\lambda}). \tag{3.24}$$

The transformations v, being isometries, imply that there exists a set of local Lorentz transformations $\Lambda(v,x)$ such that

$$e^a{}_\mu(vx)\,\frac{\partial(vx)^\mu}{\partial x^\lambda}=\Lambda(v,x)^a{}_c e^c{}_\lambda(x). \tag{3.25}$$

On these grounds it can be shown that the following set of transformations is a (super)group:

$$\begin{gathered} v''=v'*v, \\ \Psi''(x)=\Psi'(x)+\rho(\Lambda(v'^{-1},x))\Psi(v'^{-1}(x)), \end{gathered} \tag{3.26}$$

$$\begin{gathered} \overline{\Psi}''(x)=\overline{\Psi}'(x)+\overline{\Psi}(v'^{-1}(x))\rho(\Lambda(v'^{-1},x))^{-1}, \\ \zeta''=\zeta'\zeta\,\exp\frac{i}{2}\,\xi_{DCS}(g',g)=\zeta'\zeta\,\exp\frac{i}{2}\int_\Sigma d\sigma_\mu(x)\mathscr{T}^\mu_{DCS}(g',g)(x), \end{gathered} \tag{3.27}$$

where

$$\begin{aligned} \mathscr{T}^\mu_{DCS}(g',g)(x)=i[&\overline{\Psi}'(x)\hat{\gamma}^\mu(x)\rho(\Lambda(v'^{-1},x))\Psi(v'^{-1}x) \\ &-\overline{\Psi}(v'^{-1}x)\rho(\Lambda(v'^{-1},x))^{-1}\hat{\gamma}^\mu(x)\Psi'(x)] \end{aligned} \tag{3.28}$$

and ρ is the usual spin representation of the Poincaré group which verifies

$$\rho(\Lambda)^{-1}\gamma^a\rho(\Lambda)=\Lambda^a{}_b\gamma^b. \tag{3.29}$$

C. Matter fields coupled to symmetric electromagnetic fields

In this section, we shall present the quantizing group for matter fields, the Klein–Gordon and Dirac fields, coupled to a symmetric, but on the other hand arbitrary, electromagnetic field.

The space–time in this section will be flat, with a Minkowskian metric $\eta_{\mu\nu}$. The set of transformation v will be any subgroup of the Poincaré group leaving the electromagnetic field invariant: $A_\mu(vx)=A_\mu(x)$.

1. The Klein–Gordon field

Let the scalar field ϕ obeys the equations of motion

$$(D_\mu D^\mu+m^2)\phi=0 \tag{3.30}$$

with $D_\mu\equiv\partial_\mu-iA_\mu$.

Then the following composition law defines a group:

$$v''=v'*v, \tag{3.31}$$

$$\phi''(x)=\phi'(x)+\phi(v'^{-1}(x)), \tag{3.32}$$

$$\zeta''=\zeta'\zeta\,\exp\frac{i}{2}\,\xi_{SAF}(g',g)=\zeta'\zeta\,\exp\frac{i}{2}\int_\Sigma d\sigma_\mu(x)\mathscr{T}^\mu_{SAF}(g',g)(x) \tag{3.33}$$

with

$$\mathscr{T}^\mu_{SAF}(g',g)(x)=D^\mu\phi(v'^{-1})\phi^{*\prime}(x)-\phi(v'^{-1})(D^\mu\phi)^{*\prime}(x)$$

$$+(D^{\mu}\phi(v'^{-1}))^{*}\phi'(x)-\phi(v'^{-1})^{*}(D^{\mu}\phi)'(x). \tag{3.34}$$

2. The Dirac field

Let Ψ be a Dirac field with equations of motion:

$$(i\gamma^{\mu}D_{\mu}-m)\Psi=0. \tag{3.35}$$

Then the following set of transformations is a group:

$$v''=v'*v,$$

$$\Psi''(x)=\Psi'(x)+\rho(\Lambda(v'^{-1}))\Psi(v'^{-1}(x)), \tag{3.36}$$

$$\overline{\Psi}''(x)=\overline{\Psi}'(x)+\overline{\Psi}(v'^{-1}(x))\rho(\Lambda(v'^{-1}))^{-1},$$

$$\zeta''=\zeta'\zeta\ \exp\frac{i}{2}\,\xi_{DAF}(g',g)=\zeta'\zeta\ \exp\frac{i}{2}\int_{\Sigma}d\sigma_{\mu}(x).\mathscr{T}^{\mu}_{DAF}(g',g)(x) \tag{3.37}$$

with

$$\mathscr{T}^{\mu}_{DAF}(g',g)(x)=i[\overline{\Psi}'(x)\gamma^{\mu}\rho(\Lambda(v'^{-1}))\Psi(v'^{-1}x)-\overline{\Psi}(v'^{-1}x)\rho(\Lambda(v'^{-1}))^{-1}\gamma^{\mu}\Psi'(x)]. \tag{3.38}$$

Comments: We should point out here that the requirement of being symmetric for the classical ''source'' fields considered above, such as the space-time metric or the electromagnetic field in Secs. III B and III C, respectively, is not a strict requirement: many relevant systems, such as the one of fields evolving in a Schwarzchild black hole background,[15,17] are not excluded by this constraint.

IV. GENERALIZATIONS. THE VIRASORO GROUP AND THE SCHWARZIAN DERIVATIVE

Let us consider from another perspective the manner in which we arrived at the group law for the harmonic oscillator in Sec. II, Eq. (2.1). (Similar considerations can be made on the group laws for the other fields mentioned above.) We started with an Abelian gauge group (the group of functions on R with values in a group G and pointwise group composition) (composed in a semidirect way with the temporal translations which are the zero modes of the group of diffeomorphisms of the real line). From this group, we extracted the subgroup of the functions that obey certain differential equations (the equations of motion). The subgroup obtained this way can be extended, the principal ingredient for the extension being a divergenceless current.

This point of view leads us immediately to a possible generalization: instead of an Abelian gauge group let us consider more general, non-Abelian gauge groups. However, we should ask what differential equations (equations of motion) are to be applied to the basic group. In other words, the question is: what differential equation is there such that if $g(t)$ and $h(t)$ are solutions of this equation, $g(t)*h(t)$ is also for a general non-Abelian affine group? (This is a kind of symmetry that goes beyond those usually considered in the literature.) For the Abelian group, the solution was obvious: any linear differential equation is such that if $h(t),g(t)$ are solutions so is $h(t)+g(t)$. From this simple property, we have constructed the quantizing group for the harmonic oscillator, the nonrelativistic free particle, the Klein–Gordon and Maxwell fields, etc. We might ask though what differential equation fulfills this property for, say, a current SU(2) group.

There are strong indications that no equation of order greater than one with this property exists for any non-Abelian gauge group. In fact, let us consider the Lie algebra of these gauge groups. For any Abelian gauge group, the basic Lie algebra is

$$\{\varphi_a(x),\varphi_b(y)\}=0. \tag{4.1}$$

From this algebra, we have to extract the subalgebra made up of the tangent fields that obey the (linearized) equations of motion and further extend it. In the Abelian case, this can be done with the result

$$\{\varphi_a(x),\varphi_b(y)\}=\Delta_{ab}(x-y), \tag{4.2}$$

where Δ_{ab} is the propagator similar to that of Eqs. (2.14) and (2.15). [If $\Delta(x-y)$ is the propagator for the Klein–Gordon field, the propagator for the Dirac field is $\Delta_D(x-y)=(i\gamma^\mu\partial_\mu+m)\Delta(x-y)$ and for the electromagnetic (or Proca) field is $\Delta_{M_{\mu\nu}}(x-y)=-\eta_{\mu\nu}\Delta(x-y)$. For the harmonic oscillator it is $\Delta_{\mathrm{HO}}(B)=(1/\omega)\sin\omega B$ and for the nonrelativistic free particle $\Delta_{FP}(B)=B$.] This central extension is consistent with the (linearized) equations of motion for the tangent fields.

For non-Abelian fields, we should start from the basic Lie algebra:

$$\{T^a(x),T^b(y)\}=f_c^{ab}T^c(x)\,\delta(x-y). \tag{4.3}$$

The Lie bracket of two elements of the Lie algebra

$$X=\int dx\ f_a(x)T^a(x),\quad Y=\int dx\ g_a(x)T^a(x) \tag{4.4}$$

is given by

$$[X,Y]=\int dx\ f_a(x)g_b(x)f_c^{ab}T^c(x). \tag{4.5}$$

Therefore the Lie algebra (4.3) can equivalently be written in terms of the coefficient functions f as follows:

$$[f,g]_c(x)=f_a(x)g_b(x)f_c^{ab}. \tag{4.6}$$

For any equation of motion that we impose now on the group elements, the induced linearized equations of motion for the elements of the Lie algebra will, of course, be linear. But, for non-null structure constants f_c^{ab}, Eq. (4.6) implies that no subalgebra can be defined by linear equations of an order greater than one.

This result is a sort of *no-go* theorem which implies that the construction above for Abelian groups (fields), with equations of motion of a second order, cannot be *directly* extended to non-Abelian groups (fields). This extension would require the equations of motion to be of a typically Hamiltonian form. Only in the case of Abelian centrally extended gauge groups (fields), the splitting of coordinate momentum can be made without breaking the group structure.

Now, we shall show that this obstruction is not present in other kinds of non-Abelian groups. Let us consider, as an example, the Schwarzian derivative $S(f)$:

$$S(f)=\partial_t\left\{\frac{\partial_t^2 f}{\partial_t f}\right\}-\frac{1}{2}\left(\frac{\partial_t^2 f}{\partial_t f}\right)^2=\frac{\partial_t^3 f}{\partial_t f}-\frac{3}{2}\left(\frac{\partial_t^2 f}{\partial_t f}\right)^2. \tag{4.7}$$

This operator fulfills the so-called Cayley property:

$$S(fog)=S(f)og(\dot g)^2+S(g), \tag{4.8}$$

where o stands for composition of functions. Therefore we shall find that

$$S(f)=0,\quad S(g)=0\Rightarrow S(fog)=0. \tag{4.9}$$

Therefore, for the Virasoro group, the group of diffeomorphisms of the real line, the vanishing of the Schwarzian derivative is a differential equation with the property we were seeking. (We will say that the Schwarzian derivative is *closed* under the Virasoro group.) Since the group of diffeomorphisms *does not have* a pointwise composition law, it does not fulfill the hypothesis of the no-go theorem above, and we shall show that it does not fulfill its thesis either.

The algebra of the group of diffeomorphisms on R is the Lie algebra of all vector fields $v(t)\partial_t$ with the Lie bracket:

$$\{u,v\}(t)=-(\dot{u}(t)v(t)-u(t)\dot{v}(t)). \tag{4.10}$$

If the functions of the group satisfy $S(f)=0$, by taking variation and taking into account that the identity function is $f(t)=t$, we arrive at the following (of course, linear) equation for the functions in the Lie algebra of the group

$$\partial_t^3 v(t)=0. \tag{4.11}$$

It is straightforward to show by applying the linear operator ∂_t^3 to both sides of Eq. (4.10) that the set of functions which satisfy Eq. (4.11) close into a subalgebra.

The general solution of Eq. (4.11) is a general linear combination of $1,t,t^2$ which generates the general solution of the equation $S(f)=0$:

$$f(t)=\frac{at+b}{ct+d} \quad \text{with} \quad ad-bc=1. \tag{4.12}$$

Therefore the subgroup of the Virasoro group generated by functions obeying $S(f)=0$ is the SL(2,R) group.

A. The Virasoro gauge group and the induced 2D gravity in the light-cone gauge

A construction similar to the one presented above for the Virasoro group can also be made for the *Virasoro gauge group*. [This group should not be confused with the affine Virasoro group, which is a realization of the Virasoro group (generators), the Sugawara construction, in terms of currents from an affine (Kac–Moody) algebra (see Ref. 8).] This is the set of functions

$$\begin{gathered} f: R \rightarrow \text{Virasoro}, \\ \sigma \rightarrow f(\sigma) \end{gathered} \tag{4.13}$$

with the composition law $(f*g)(\sigma)(\tau)=(f(\sigma)og(\sigma))(\tau)$. The elements of this group are, therefore, parametrized by two coordinates, σ and τ, and can be considered to be functions of two variables, $f(\sigma,\tau)$.

The vanishing of the Schwarzian derivative

$$\{f(\sigma,\tau),\tau\}=0 \tag{4.14}$$

is, of course, a *closed* equation for this group, thus defining a subgroup, the SL(2,R) affine group in this case.

The identifications $\sigma\equiv x^+=t+x$, $\tau\equiv x^-=t-x$ transform Eq. (4.14) into the equation of motion, $\{f,x^-\}=0$, of the induced 2D gravity in the light-cone gauge.[11] Moreover, in this gauge, the symplectic form is the canonical one of the SL(2,R) affine (sub)group. All this would indicate that the quantum theory of this system should be described in terms of irreducible, unitary representations of the SL(2,R) affine group. However, it is well known that there are no unitary, standard highest-weight representations with a nonzero central charge. In fact, a more rigorous analysis of this theory based on a local form of the action shows that its true reduced phase space

is quite different from that proposed above and cannot be obtained as a constrained version of the former.[11] Therefore, the role played by the SL(2,*R*) affine symmetry is in any case different from the one expected from the analysis of the nonlocal theory in the light-cone gauge.

V. DISCUSSION

We have presented the basic features of the GAQ formalism when the quantizing group can be written in terms of fields given on configuration space. It was not our intention to be exhaustive. On the contrary: many question have been raised which will have to be addressed in future publications.

The quantizing groups for several physically relevant systems have been given, albeit most of them in an implicit form. However, one might question the utility of writing down the quantizing group in this implicit form. The key point in considering the quantizing group is that it collects all the information about both the classical and the quantum theories. Of course, we can achieve the most with it when we know the general solution of the equations of motion, i.e., the phase space of the theory (and, in fact, there are many important examples in which this is the case), but we believe that, even when the general solution is not known, there can still be a large amount of information of the quantum theory that we can possibly extract from the quantizing group.

An interesting case occurs when we know only *some* of the classical solutions of the theory. With the GAQ formalism, we would be able to quantize these solutions, provided that we were able to find pairs of solutions that are coordinate-momentum conjugates of each other. (In the GAQ formalism, the cocycle may be viewed as a sort of ''symplectic product'' which measures the extent to which two classical solutions are coordinate-momentum conjugates of each other.) This sort of *minisuperspace* approach would provide us with a preliminary draft of the quantum theory and deserves independent study.

In addition, the phase space of any classical theory is, in some sense, always roughly known: it is characterized by the fields and time derivative of the fields in a Cauchy hypersurface and evolve in time in accordance with the classical equations of motion. Putting aside topological or, in general, global issues of the phase space, the GAQ formalism equipped with this rough description of the phase space must necessarily work better than the familiar canonical quantization does.

Furthermore, the configuration-space image of the GAQ formalism appears as a well-suited formalism to deal with gauge theories. Indeed, gauge symmetries, far from being a mere useful tool to solve a previously given theory, determine the theory, and this philosophy is the same that inspires the GAQ formalism. However, we have proven in Sec. IV a sort of no-go theorem which delimits the type of equations of motion in a (nonlinear) system defined by a non-Abelian basic current group; these equations must be kept in a Hamiltonian-like, first-order form, since the restriction to the pure coordinate space satisfying second-order equations would destroy the group structure. This situation resembles that of WZW models[18] where the Kac–Moody symmetry comes out in a natural way when written in a set of coordinates (light-cone coordinates) where the Lagrangian is not regular, making this way the difference between the modified and ordinary Hamilton principle.

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Fermion pair production from an electric field varying in two dimensions

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The Hamiltonian describing fermion pair production from an arbitrarily time-varying electric field in two dimensions is studied using a group-theoretic approach. We show that this Hamiltonian can be encompassed by two, commuting SU(2) algebras, and that the two-dimensional problem can therefore be reduced to two one-dimensional problems. We compare the group structure for the two-dimensional problem with that previously derived for the one-dimensional problem, and verify that the Schwinger result is obtained under the appropriate conditions. © *1996 American Institute of Physics.* [S0022-2488(96)01201-4]

I. INTRODUCTION

Fermion pair production takes place in a large number of physical situations; a comprehensive review of its applications in atomic, nuclear, elementary particle physics, astrophysics, and cosmology is given in Ref. 1. Consequently, the problem of pair production from classical external electric fields has been the subject of considerable theoretical interest.[2–17] The rate of fermion pair production from a uniform, static electric field was originally calculated by Schwinger[2] to be

$$\omega = \frac{\alpha E^2}{\pi^2} \sum_{n=1}^{\infty} \frac{1}{n^2} \exp\left(- \frac{n \pi m^2}{|eE|} \right), \tag{1}$$

where m is the mass of the produced fermions. To date, an analytic formalism that successfully addresses the general problem of fields which vary arbitrarily in both time and space has not been developed. However, numerous approaches have been suggested which address particular special cases. We previously discussed an approach for predicting the rate of pair production from a spatially homogeneous but arbitrarily time-varying field, provided the field is constrained to point in a fixed direction.[17] We now investigate an extension to this formalism that allows for a field varying in two dimensions.

We begin by writing the interaction Hamiltonian for fermions in an electric field. We adopt the gauge

$$A_0 = 0, \quad A_i = - \int_{-\infty}^{t} E_i(t) dt. \tag{2}$$

The interaction Hamiltonian is then given by

$$H_I = - e A_i \int d^3x \; \bar{\psi}_{\rm in}(x) \gamma_i \psi_{\rm in}(x), \tag{3}$$

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where γ_i is the ith 4×4 Dirac γ-matrix, and summation over like indices is assumed. The incoming Dirac field ψ_{in} is that of free fermions,

$$\psi_{\text{in}}=\int \frac{d^3\mathbf{k}}{(2\pi)^{3/2}}\sqrt{\frac{m}{k_0}}\sum_{\beta}\left[b_\beta(k)u_\beta(k)e^{-ik\cdot x}+d^\dagger_\beta(\tilde{k})v_\beta(\tilde{k})e^{ik\cdot x}\right], \tag{4}$$

where b and $d^\dagger$ are the usual fermion creation and antifermion annihilation operators, and u and v are the two-component fermion and antifermion spinors. We use the symbol k to denote the four-vector $(k_0,\mathbf{k})$ and $\tilde{k}$ to denote $(k_0,-\mathbf{k})$; k represents the initial momentum of the fermions, and is a time-independent quantity. The mass of the created fermions is given by m, and their charge by e.

We chose the one-dimensional configuration as a starting point because, if the field varies in only one direction, the Hamiltonian contains only one Dirac γ-matrix, and an SU(2) algebra is sufficient to encompass the Hamiltonian. In the two-dimensional case, the Hamiltonian contains two Dirac γ-matrices. The appropriate algebra is then an SO(4) algebra, which is isomorphic to two commuting SU(2) algebras, as we illustrate below.

II. PAIR EMISSION FROM A TWO-DIMENSIONAL ELECTRIC FIELD

For an electric field that varies in the plane defined by the directions $i=1,2$, the interaction picture Hamiltonian is

$$H=\int d^3\mathbf{k}\left\{\left(2k_0-2e\frac{A_ik_i}{k_0}\right)J_0(k)-\frac{e\mu_iA_i}{k_0}\left[J^{(i)}_+(k)+J^{(i)}_-(k)\right]\right\}, \tag{5}$$

where summation of i over indices 1 and 2 is implied. μ_i in this expression is defined as $\mu_i=\sqrt{k_0^2-k_i^2}$. We have defined the operators in analogy to the one-dimensional case:[17]

$$\begin{aligned} J^{(i)}_+&=\frac{m}{\mu_i}\sum_{\alpha\beta}b^\dagger_\alpha(k)d^\dagger_\beta(\tilde{k})\bar{u}_\alpha(k)\gamma_iv_\beta(\tilde{k}),\quad i=1,2,\\ J^{(i)}_-&=[J^{(i)}_+]^\dagger,\quad i=1,2,\\ J_0&=\frac{1}{2}\sum_\alpha\left[b^\dagger_\alpha(k)b_\alpha(k)-d_\alpha(\tilde{k})d^\dagger_\alpha(\tilde{k})\right]. \end{aligned} \tag{6}$$

With an additional operator,

$$Q=\sum_{\alpha\beta}\left[b^\dagger_\alpha b_\beta\bar{u}_\alpha\gamma_3\gamma_5u_\beta+d_\alpha d^\dagger_\beta\bar{v}_\alpha\gamma_3\gamma_5v_\beta\right], \tag{7}$$

these operators form an SO(4) algebra.

From linear combinations of these operators, we can form two commuting SU(2) algebras, which we denote by $I_{+,-,0}$ and $T_{+,-,0}$, as follows:

$$\begin{aligned} I_+&=aJ^{(1)}_++a^*J^{(2)}_+,\\ I_-&=[I_+]^\dagger,\\ I_0&=\frac{1}{2}J_0+\frac{m}{4\mu}Q, \end{aligned} \tag{8}$$

$$T_+ = a^* J_+^{(1)} + a J_+^{(2)},$$
$$T_- = [T_+]^\dagger, \tag{9}$$

and

$$T_0 = \frac{1}{2} J_0 - \frac{m}{4\mu} Q,$$

where

$$a = \sqrt{\frac{\mu_1 \mu_2}{8(\mu_1 \mu_2 - k_1 k_2)}} + i \sqrt{\frac{\mu_1 \mu_2}{8(\mu_1 \mu_2 + k_1 k_2)}}, \tag{10}$$

and we have defined $\mu = \sqrt{k_0^2 - k_1^2 - k_2^2}$. Each of these SU(2) algebras is in the $j = \frac{1}{2}$ representation.

The group-theoretic approach has been previously discussed by Perelemov,[18] but the algebras we have derived are distinct from the algebras he considered. The SU(2) algebras utilized in Ref. 18 are constructed from the Dirac γ-matrices, whereas the SU(2) commutation relations of the operators in Eqs. (8) and (9) follow from the completeness and orthogonality of the Dirac spinors $u(p)$ and $v(p)$.

The Hamiltonian in Eq. (5) can be rewritten as a linear combination of elements of these two SU(2) algebras, and diagonalized via a Bogoliubov[19] transformation. The Bogoliubov transformation takes the usual form

$$\tilde{b}_\alpha(k) = \mathscr{U}_{\alpha\beta}(k) b_\beta(k) + \mathscr{V}_{\alpha\beta}(k) d_\beta^\dagger(\tilde{k}), \tag{11}$$

$$\tilde{d}_\alpha(\tilde{k}) = \mathscr{X}_{\alpha\beta}(k) d_\beta(\tilde{k}) + \mathscr{Y}_{\alpha\beta}(k) b_\beta^\dagger(k), \tag{12}$$

where the coefficients are time-dependent, 2×2 matrices. Requiring that the transformation preserve the canonical commutation relations constrains the coefficients to satisfy the relations

$$\mathscr{U}\mathscr{U}^\dagger + \mathscr{V}\mathscr{V}^\dagger = 1, \quad \mathscr{X}\mathscr{X}^\dagger + \mathscr{Y}\mathscr{Y}^\dagger = 1,$$
$$\mathscr{U}\mathscr{V}^T + \mathscr{V}\mathscr{X}^T = 0.$$

We further require that the Bogoliubov transformation yield the diagonal Hamiltonian,

$$H = \int d^3\mathbf{k}\ \epsilon(k) \sum_{\alpha\beta} [\tilde{b}_\alpha^\dagger(k) \tilde{b}_\alpha(k) - \tilde{d}_\alpha(\tilde{k}) \tilde{d}_\alpha^\dagger(\tilde{k})], \tag{13}$$

where ϵ is the total energy

$$\epsilon = \sqrt{m^2 + (\mathbf{k} - e\mathbf{A})^2}.$$

This requirement constrains the coefficients to be

$$\mathscr{U} = \cos\ \theta I \tag{14}$$

and

$$\mathscr{Z} = \mathscr{U}^{-1}\mathscr{V} = \frac{-mA_i \tan\ \theta}{\sqrt{k_0^2 \mathbf{A}^2 - (\mathbf{A}\cdot\mathbf{k})^2}} [\bar{u}_\alpha \gamma_i v_\beta], \tag{15}$$

and summation over i is implied. θ is defined by the relations

$$\cos\ \theta = \sqrt{\frac{\epsilon+\rho}{2\epsilon}}, \quad \sin\ \theta = -\sqrt{\frac{\epsilon-\rho}{2\epsilon}}, \tag{16}$$

and ρ is defined by

$$\rho = k_0 - \frac{e\mathbf{A}\cdot\mathbf{k}}{k_0}. \tag{17}$$

Alternatively, one can write the Bogoliubov transformation as a linear operator,

$$R = R_1 R_2, \tag{18}$$

such that

$$\tilde{b} = R(t) b R^{\dagger}(t). \tag{19}$$

R_1 and R_2 can each be written in terms of only one of the two commuting SU(2) algebras:

$$\begin{aligned} R_1 &= \exp[\,\eta I_+]\exp[\log(1+|\,\eta|^2) I_0]\exp[-\eta^* I_-], \\ R_2 &= \exp[\,\eta^* T_+]\exp[\log(1+|\,\eta|^2) T_0]\exp[-\eta T_-], \end{aligned} \tag{20}$$

where

$$\eta = \frac{-1}{(a^2 - a^{*2})}\left[\frac{\tan\ \theta(a\mu_1 A_1 - a^*\mu_2 A_2)}{\sqrt{k_0^2\mathbf{A}^2 - (\mathbf{A}\cdot\mathbf{k})^2}}\right] \tag{21}$$

gives the desired diagonal Hamiltonian.

Writing the Bogoliubov transformation as a linear operator is useful when calculating the rate of pair production from an electric field. The physical vacuum after the field has been turned off ($t>T$), $|Z(T)\rangle$, is related to the vacuum before the field was turned on ($t<-T$), $|0_i\rangle$, by

$$|Z(T)\rangle = R(T)|0_i\rangle. \tag{22}$$

Similarly, the physical creation operators for fermions and antifermions at times $t>T$ are $\tilde{b}^{\dagger}(k)$ and $\tilde{d}^{\dagger}(k)$, respectively.[17] The probability amplitude of producing no pairs, S_0, is therefore given by

$$S_0 = \lim_{t\to\infty}\langle Z|U_I|0_i\rangle = \langle 0_i|\tilde{U}|0_i\rangle, \tag{23}$$

where $\tilde{U} = R^{\dagger}U_I$. One can solve for $\tilde{U}$ directly, through

$$i\,\frac{d\tilde{U}}{dt} = \tilde{H}\tilde{U},$$

where

$$\tilde{H} = R^{\dagger}HR - iR^{\dagger}R. \tag{24}$$

The probability amplitude for producing no pairs is related to the rate of pair production ω by

$$|S_0|^2 = e^{-\int \omega \, d^4x}. \tag{25}$$

The operator R_1 has the matrix representation

$$R_1 = \begin{pmatrix} \cos\dfrac{\alpha_1}{2} & \sin\dfrac{\alpha_1}{2}\, e^{-i\gamma_1} \\ -\sin\dfrac{\alpha_1}{2}\, e^{-i\gamma_1} & \cos\dfrac{\alpha_1}{2} \end{pmatrix}, \tag{26}$$

where $\eta = \tan(\alpha/2)e^{-i\gamma}$. R_2 is defined analogously. One observes that, to satisfy Eq. (20), $\alpha_1 = \alpha_2$ and $\gamma_1 = -\gamma_2$; the subscripts on α and γ are therefore dropped. The matrix representation allows one to easily calculate the Hamiltonian $\tilde{H}$. By substituting Eqs. (8) and (9) into the Hamiltonian of Eq. (5), one can show that this Hamiltonian can be written $H = H_1 + H_2$, where

$$H_1 = \int d^3k \left\{ \left(2k_0 - \frac{2eA_i k_i}{k_0} \right) I_0 + 2ie\mu \left[\left(\frac{aA_1}{\mu_2} - \frac{a^*A_2}{\mu_1} \right) I_+ - \left(\frac{a^*A_1}{\mu_2} - \frac{aA_2}{\mu_1} \right) I_- \right] \right\} \tag{27}$$

and

$$H_2 = \int d^3k \left\{ \left(2k_0 - \frac{2eA_i k_i}{k_0} \right) T_0 + 2ie\mu \left[\left(\frac{-a^*A_1}{\mu_2} + \frac{aA_2}{\mu_1} \right) T_+ + \left(\frac{aA_1}{\mu_2} - \frac{a^*A_2}{\mu_1} \right) T_- \right] \right\}. \tag{28}$$

It follows that $\tilde{H}$ can be written $\tilde{H} = \tilde{H}_1 + \tilde{H}_2$, where

$$\tilde{H}_1 = R_1^\dagger H_1 R_1 - i R_1^\dagger \dot{R}_1 \tag{29}$$

and

$$\tilde{H}_2 = R_2^\dagger H_2 R_2 - i R_2^\dagger \dot{R}_2. \tag{30}$$

The explicit expressions for $\tilde{H}_1$ and $\tilde{H}_2$ are then

$$\tilde{H}_1 = \int d^3k \left\{ \left[2\epsilon(k) + 2\left(\dot{\gamma} \sin^2\frac{\alpha}{2} \right) \right] I_0 - \frac{1}{2} \left[(i\dot{\alpha} + \dot{\gamma} \sin\alpha) e^{-i\gamma} I_+ + (-i\dot{\alpha} + \dot{\gamma} \sin\alpha) e^{i\gamma} I_- \right] \right\}, \tag{31}$$

$$\tilde{H}_2 = \int d^3k \left\{ \left[2\epsilon(k) - 2\left(\dot{\gamma} \sin^2\frac{\alpha}{2} \right) \right] T_0 - \frac{1}{2} \left[(i\dot{\alpha} - \dot{\gamma} \sin\alpha) e^{i\gamma} T_+ + (-i\dot{\alpha} - \dot{\gamma} \sin\alpha) e^{-i\gamma} T_- \right] \right\}. \tag{32}$$

If we now write $\tilde{U}$ as a product, $\tilde{U} = \tilde{U}_1 \tilde{U}_2$, where $\tilde{U}_1$ and $\tilde{U}_2$ are each written in the most general form of an element of the respective SU(2) groups:

$$\tilde{U}_1 = \exp\left[-i \int d^3\mathbf{k} \; \phi_1 I_0 \right] \exp\left[\int d^3\mathbf{k} \; \tau_1 I_+ \right] \exp\left[\int d^3\mathbf{k} \; \log(1 + |\tau_1|^2) I_0 \right] \exp\left[-\int d^3\mathbf{k} \; \tau_1^* I_- \right] \tag{33}$$

and

$$\tilde{U}_2 = \exp\left[-i \int d^3\mathbf{k} \; \phi_2 T_0 \right] \exp\left[\int d^3\mathbf{k} \; \tau_2 T_+ \right] \exp\left[\int d^3\mathbf{k} \; \log(1 + |\tau_2|^2) T_0 \right] \exp\left[-\int d^3\mathbf{k} \; \tau_2^* T_- \right], \tag{34}$$

then the differential equation for $\tilde{U}$,

$$i\,\frac{d\tilde{U}}{dt}=\tilde{H}\tilde{U},$$

separates into two independent equations for $\tilde{U}_1$ and $\tilde{U}_2$. We show this as follows:

$$i\,\frac{d\tilde{U}}{dt}=i\,\frac{d\tilde{U}_1}{dt}\,\tilde{U}_2+i\tilde{U}_1\,\frac{d\tilde{U}_2}{dt}=(\tilde{H}_1+\tilde{H}_2)\tilde{U}_1\tilde{U}_2. \tag{35}$$

This is the sum of the two equations:

$$\left[i\,\frac{d\tilde{U}_1}{dt}=\tilde{H}_1\tilde{U}_1\right]\tilde{U}_2 \tag{36}$$

and

$$\tilde{U}_1\left[i\,\frac{d\tilde{U}_2}{dt}=\tilde{H}_2\tilde{U}_2\right]. \tag{37}$$

These are independent differential equations for $\tilde{U}_1$ and $\tilde{U}_2$, each equation containing elements of only one SU(2) algebra. When we insert our ansatz for $\tilde{U}_1$ and $\tilde{U}_2$ into the above differential equations, we obtain differential equations for the coefficients τ_1, τ_2, ϕ_1, and ϕ_2. One can proceed to solve these differential equations in precisely the same manner as in the one-dimensional case.[17]

Let

$$z=\tau\,\exp(-i\phi+i\gamma). \tag{38}$$

The resulting differential equation for z_1 is

$$i\dot{z}_1=-\tfrac{1}{2}(\dot{\gamma}\,\sin\,\alpha+i\dot{\alpha})+2[\epsilon(k)-\dot{\gamma}\,\cos\,\alpha]z_1+\tfrac{1}{2}(\dot{\gamma}\,\sin\,\alpha-i\dot{\alpha})z_1^2. \tag{39}$$

The corresponding differential equation for z_2 is

$$i\dot{z}_2=-\tfrac{1}{2}(-\dot{\gamma}\,\sin\,\alpha+i\dot{\alpha})+2[\epsilon(k)+\dot{\gamma}\,\cos\,\alpha]z_2+\tfrac{1}{2}(-\dot{\gamma}\,\sin\,\alpha-i\dot{\alpha})z_2^2. \tag{40}$$

One can write $\dot{\alpha}$ and $\dot{\gamma}$ explicitly, in terms of the electric field and vector potential. The expression for $\dot{\alpha}$ is

$$\dot{\alpha}=\left(\frac{e}{\epsilon^2}\right)\frac{[(\mathbf{k}-e\mathbf{A})\times\mathbf{E}]\cdot(\mathbf{k}\times\mathbf{A})+m^2(\mathbf{E}\cdot\mathbf{A})}{\sqrt{k_0^2\mathbf{A}^2-(\mathbf{A}\cdot\mathbf{k})^2}}, \tag{41}$$

with $\dot{\alpha}=0$ at $t=-\infty$. The expression for $\dot{\gamma}$ is

$$\dot{\gamma}=-\frac{\mu k_0|\mathbf{A}\times\mathbf{E}|}{k_0^2\mathbf{A}^2-(\mathbf{A}\cdot\mathbf{k})^2}. \tag{42}$$

Note that only $\dot{\gamma}$ appears explicitly in the equations; when calculating $|\tau|$ (see Eq. (43) below), the initial condition on γ is irrelevant. When $\mathbf{A}$ and $\mathbf{E}$ are parallel ($\dot{\gamma}=0$), Eqs. (39) and (40) reduce to the corresponding equation calculated for the one-dimensional case.[17] When $\dot{\gamma}\neq 0$, the two-dimensional nature of the equations is manifested.

Finally, one can calculate the rate of pair production ω via S_0. The above definitions give

$$S_0=\langle 0_i|\tilde{U}|0_i\rangle=\exp\left[i\int d^3\mathbf{k}\left(\frac{\phi_1+\phi_2}{2}\right)\right]\exp\left[-\int d^3\mathbf{k}\,\log\sqrt{(1+|\tau_1|^2)(1+|\tau_2|^2)}\right]. \quad (43)$$

Then

$$|S_0|^2=|\langle 0_i|\tilde{U}|0_i\rangle|^2=\exp\left\{-\int d^3\mathbf{k}\,\log[(1+|z_1|^2)(1+|z_2|^2)]\right\}. \quad (44)$$

Once the differential equations have been solved for z_1 and z_2 (in general, this must be done numerically), the rate of pair production is easily obtained.

To verify this approach, consider the very simple example of a uniform, static electric field which is oriented at an angle θ to the x-axis. Then $|\mathbf{E}\times\mathbf{A}|=0$, and $\dot{\gamma}=0$. In this case, $\dot{\alpha}$ reduces to

$$\dot{\alpha}=\frac{ek_\perp E_0}{\epsilon^2}, \quad (45)$$

where

$$k_\perp=\sqrt{k_0^2-k_\parallel^2}=\sqrt{k_0^2-\frac{(\mathbf{k}\cdot\mathbf{E})^2}{\mathbf{k}^2}}. \quad (46)$$

With these values, the expressions for $i\dot{z}_1$ and $i\dot{z}_2$ are identical, and each is equal to the expression which applied in the one-dimensional case.[17] With $z_1=z_2$, Eq. (44) reduces to

$$|S_0|^2=|\langle 0_i|\tilde{U}|0_i\rangle|^2=\exp\left[-2\int d^3\mathbf{k}\,\log(1+|z_1|^2)\right], \quad (47)$$

which again is identical to the one-dimensional result.[17] In this case, the rate of pair production has been shown to be equal to that calculated by Schwinger, given in Eq. (1).

III. CONCLUSIONS

We have shown that the Hamiltonian describing fermion pair production from an arbitrarily time-varying electric field in two dimensions is encompassed by an SO(4) algebra. We have also explicitly constructed the two commuting SU(2) algebras in the direct product SU(2)×SU(2), which is isomorphic to this SO(4) algebra. The one-dimensional problem is described by an SU(2) algebra in the $j=1$ representation, while the two-dimensional problem is described by two SU(2) algebras in the $j=\frac{1}{2}$ representation. However, when the one-dimensional problem and the two-dimensional problem are each considered in the lowest-dimensional representation, one sees that the off-diagonal elements are real in the one-dimensional case and complex in the two-dimensional case. The extra degree of freedom present in the two-dimensional case is manifested in this way. Indeed, it can easily be shown that the factor γ in Eq. (38) is the Berry's phase.

This group-theoretic approach may simplify the calculation of the rate of fermion pair production from the field, since the two-dimensional problem can in this way be reduced to two one-dimensional problems. We verify our approach by showing that the Schwinger formula for pair production can be obtained for the special case of a uniform, static electric field.

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Hidden local gauge invariance in the one-dimensional Heisenberg *XXZ* model with the general boundary terms

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Hidden local gauge invariance in the one-dimensional Heisenberg *XXZ* model with the general boundary terms is studied in the framework of the quantum inverse scattering method. The Bethe ansatz equations are established for the model with the special boundary terms. Our results show that the Hamiltonian and its eigenvectors are explicitly gauge dependent whereas the energy eigenvalues and the Bethe ansatz equations are gauge invariant. © *1996 American Institute of Physics.* [S0022-2488(95)01512-6]

I. INTRODUCTION

One of the recent developments of the theory of completely integrable quantum systems is Sklyanin's work[1] on the reflection equations (RE),[2] who showed that there is a variant of the usual formalism of the quantum inverse scattering method (QISM)[3–5] which may be used to describe systems on a finite interval with independent boundary conditions on each end. Central to his approach is the introduction of a new algebraic structure-RE called the quantum Sklyanin algebras. The latter plays the same role in the theory of a completely integrable quantum systems with boundary terms as the quantum Yang–Baxter algebras (QYBA) do in the usual formalism of QISM. Now much attention has been paid to the solutions of RE which present the boundary K matrices compatible with the integrability.[6–9] Recently, the general boundary K matrices have been constructed by de Vega and González Ruiz[6] for the six-vertex model.

On the other hand, de Vega and Lopes[10] studied an interesting feature of completely integrable quantum systems with periodic boundary conditions, i.e., what they referred to as hidden local gauge invariance (see also, Refs. 5, 11–13). They showed that the combination of the quantum integrability, i.e., the existence of the R matrix, with a global gauge transformation group leads to an Abelian local gauge invariance in the Heisenberg *XXZ* model. As a consequence, one may construct a more general family of completely integrable quantum systems. Further, they also showed that in this model the exact energy spectrum turns out to be gauge invariant whereas the eigenvectors are explicit gauge dependent. Thus, it seems interesting to explore hidden local gauge invariance in completely integrable lattice spin systems with boundary terms.

The aim of this article is to give a detailed study of hidden local gauge invariance in the one-dimensional (1-D) Heisenberg *XXZ* model with the general boundary terms. We show that the Hamiltonian and its eigenvectors are explicitly gauge dependent whereas the energy eigenvalues and the Bethe ansatz equations are gauge invariant.

The outline of this article is the following. In Sec. II, we define the basic notations for later use. In Sec. III, we discuss hidden local gauge invariance in the 1-D Heisenberg *XXZ* model with the general boundary terms. In Sec. IV, we present a derivation of the Bethe ansatz equations for

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the gauge-transformed system with the special boundary terms. Lastly, Sec. V is devoted to the conclusions.

II. BASIC NOTATIONS

To describe completely integrable quantum systems on a finite interval with independent boundary conditions on each end, Sklyanin[1] has introduced two algebras $\mathscr{T}_+$ and $\mathscr{T}_-$ associated with a given R matrix, defined by the generators $(\mathscr{T}_+)_{\alpha\beta}$ and $(\mathscr{T}_-)_{\alpha\beta}$ ($\alpha,\beta=1,2,...,\dim W_0, W_0$ is the auxiliary space), and by the relations (called Sklyanin relations)

$$R_{12}(u_1-u_2)\overset{1}{\mathscr{T}}_-(u_1)R_{12}(u_1+u_2)\overset{2}{\mathscr{T}}_-(u_2)=\overset{2}{\mathscr{T}}_-(u_2)R_{12}(u_1+u_2)\overset{1}{\mathscr{T}}_-(u_1)R_{12}(u_1-u_2) \tag{1}$$

and

$$R_{12}(-u_1+u_2)\overset{1}{\mathscr{T}}{}^{t_1}_+(u_1)R_{12}(-u_1-u_2-2\eta)\overset{2}{\mathscr{T}}{}^{t_2}_+(u_2)$$

$$=\overset{2}{\mathscr{T}}{}^{t_2}_+(u_2)R_{12}(-u_1-u_2-2\eta)\overset{1}{\mathscr{T}}{}^{t_1}_+(u_1)R_{12}(u_1-u_2), \tag{2}$$

respectively. Here $\overset{1}{X}\equiv X\otimes id_{V_2}$, $\overset{2}{X}\equiv id_{V_1}\otimes X$ for any matrix $X\in\mathrm{End}(V)(V=W_0)$. It follows that the transfer matrices $\tau(u)$ defined by

$$\tau(u)=\mathrm{tr}\,\mathscr{T}_+(u)\mathscr{T}_-(u) \tag{3}$$

commute with each other for different values of the spectral parameter u. Therefore, one may consider $\tau(u)$ (3) as a generating function of the integrals of motion for quantum systems defined by specifying some concrete representations of the algebras $\mathscr{T}_\pm$ on the quantum spaces $W_\pm$. A class of important realizations of the algebras $\mathscr{T}_\pm$ are provided by the 1-D lattice spin models with boundary terms. In these cases, the explicit realizations of the algebras $\mathscr{T}_\pm$ may be chosen in the form

$$\mathscr{T}_-(u)=T(u)K_-(u)T^{-1}(-u) \tag{4}$$

and

$$\mathscr{T}_+(u)=K_+(u), \tag{5}$$

respectively. Here $K_\pm(u)$ are representations of $\mathscr{T}_\pm$ in C^1, i.e., C-number matrices, while $T(u)\equiv L_N(u)\cdots L_1(u)$ is the representation of the associative algebra T on the quantum space $\mathscr{H}\equiv W_N\otimes W_{N-1}\cdots\otimes W_1$. The algebra T is defined by the generators $T_{\alpha\beta}(u)$ ($\alpha,\beta=1,2,...,\dim W_0$), considered as the elements of the square matrix $T(u)$, and by the relations (QYBA)

$$R(u_1-u_2)\overset{1}{T}(u_1)\overset{2}{T}(u_2)=\overset{2}{T}(u_2)\overset{1}{T}(u_1)R(u_1-u_2). \tag{6}$$

Here and hereafter, we assume that the L matrix $L_n(u)$ coincides with the R matrix $R(u)$ in the space $W_n\otimes W_0$

$$L_n(u)=R_{n0}(u). \tag{7}$$

Further, $R(u)$ and $K_-(u)$ satisfy $R_{mn}(0)=P_{mn}$ and $K_-(0)=1$, respectively, and P_{mn} is the permutation operator in $W_m\otimes W_n$, satisfying $P(x\otimes y)=y\otimes x$, for $x,y\in W$. It follows that there exists a relation between the transfer matrix $\tau(u)$ and the Hamiltonian for the lattice spin open chain:

$$\tau'(0)=2H\ \mathrm{tr}\ K_+(0)+\mathrm{tr}\ K'_+(0), \tag{8}$$

where

$$H=\sum_{j=1}^{N-1} H_{j,j+1}+\frac{1}{2}\ \mathrm{tr}\ P_{10}K'_-(0)P_{10}^{-1}+\frac{\mathrm{tr}\ K_+(0)L'_{N0}(0)P_{N0}}{\mathrm{tr}\ K_+(0)}, \tag{9}$$

with

$$H_{j,j+1}=L'_{j,j+1}(0)P_{j,j+1}^{-1}. \tag{10}$$

Here the prime denotes the derivative with respect to the spectral parameter u.

III. HIDDEN LOCAL GAUGE INVARIANCE

Let us now study hidden local gauge invariance in the 1-D Heisenberg *XXZ* open chain with the general boundary terms. Notice that for a given R matrix $R(u)$, if there exist $N\times N$ ($N=\dim W_0$) matrices g and h satisfying

$$[g\otimes g,\ R]=0, \tag{11}$$

$$[h\otimes h,\ R]=0, \tag{12}$$

then the Sklyanin relations (1) and (2) are invariant under the gauge transformation

$$L_j^{(g)}(u)=g(k_j)L_j(u)h^{-1}(l_j). \tag{13}$$

Further, the transformed transfer matrix $\tau^{(g)}(u)$ defined by

$$\tau^{(g)}(u)=\mathrm{tr}\ K_+(u)T^{(g)}(u)K_-(u)(T^{(g)}(-u))^{-1}, \tag{14}$$

with

$$T^{(g)}(u)=L_N^{(g)}(u)\cdots L_1^{(g)}(u) \tag{15}$$

and the transformed Hamiltonian $H^{(g)}$ still satisfy Eq. (8). That is,

$$\tau^{(g)\prime}(0)=\sum_{j=1}^{N-1} H_{j,j+1}^{(g)}+\frac{1}{2}\ \mathrm{tr}\ P_{10}^{(g)}K'_-(0)(P_{10}^{(g)})^{-1}+\frac{\mathrm{tr}\ K_+(0)(L_{N0}^{(g)}(0))'(P_{N0}^{(g)})^{-1}}{\mathrm{tr}\ K_+(0)}, \tag{16}$$

where

$$H_{j,j+1}^{(g)}=P_{j+1,0}^{(g)}L_{j,0}^{\prime(g)}(0)(P_{j,0}^{(g)})^{-1}(P_{j+1,0}^{(g)})^{-1}, \tag{17}$$

with

$$P_{j,0}^{(g)}=g(k_j)P_{j,0}h^{-1}(l_j). \tag{18}$$

For the 1-D Heisenberg *XXZ* open chain, the L matrix is

$$L_j(u)=\begin{pmatrix} \frac{\sinh(u+\eta)+\sinh u}{2}+\frac{\sinh(u+\eta)-\sinh u}{2}\sigma_j^z & \sinh\ \eta\sigma_j^- \\ \sinh\ \eta\sigma_j^+ & \frac{\sinh(u+\eta)+\sinh u}{2}-\frac{\sinh(u+\eta)-\sinh u}{2}\sigma_j^z \end{pmatrix}, \tag{19}$$

with the corresponding R matrix

$$R(u)=\begin{pmatrix} \sinh(u+\eta) & 0 & 0 & 0 \\ 0 & \sinh u & \sinh\ \eta & 0 \\ 0 & \sinh\ \eta & \sinh u & 0 \\ 0 & 0 & 0 & \sinh(u+\eta) \end{pmatrix}. \tag{20}$$

According to de Vega and González,[6] the boundary K matrices $K_\pm$ may be taken as

$$K_-(u)=K_-(u,k_-,\lambda_-,u_-,\xi_-)=\begin{pmatrix} k_-\ \sinh(u+\xi_-) & u_-\ \sinh 2u \\ \lambda_-\ \sinh 2u & -k_-\ \sinh(u-\xi_-) \end{pmatrix}, \quad k_-=\frac{1}{\sinh\ \xi_-} \tag{21}$$

and

$$K_+(u)=K_+(u,k_+,\lambda_+,u_+,\xi_+)=\begin{pmatrix} k_+\ \sinh(u+\eta+\xi_+) & u_+\ \sinh 2(u+\eta) \\ \lambda_+\ \sinh 2(u+\eta) & -k_+\ \sinh(u-\xi_++\eta) \end{pmatrix}, \tag{22}$$

respectively. From Eqs. (11), (12), and (20), we get

$$g(k_j)=h(k_j)=\begin{pmatrix} e^{ik_j} & 0 \\ 0 & e^{-ik_j} \end{pmatrix}, \quad k_j\in R. \tag{23}$$

From Eqs. (14)–(18), we immediately obtain the transformed Hamiltonian for the 1-D Heisenberg *XXZ* model with the general boundary terms

$$\begin{aligned} H^{(9)}=&\sum_{j=1}^{N-1}\left[\cosh\ \eta\sigma_j^z\sigma_{j+1}^z+2e^{2i(k_j-l_{j+1})}\sigma_j^-\sigma_{j+1}^++2e^{-2i(k_j-l_{j+1})}\sigma_j^+\sigma_{j+1}^-\right] \\ &+\sinh\ \eta\Bigg[\coth\ \xi-\sigma_1^z+\coth\ \xi_+\sigma_N^z+2\lambda_-e^{2il_1}\sigma_1^-+\frac{2\lambda_+}{k_+\ \sinh\ \xi_+}e^{2ik_N}\sigma_N^- \\ &+2u_-e^{-2il_1}\sigma_1^++2\frac{u_+}{k_+\ \sinh\ \xi_+}e^{-2ik_N}\sigma_N^+\Bigg]. \end{aligned} \tag{24}$$

In particular, setting $\lambda_\pm=0$, $u_\pm=0$, and $k_+=1$, one gets

$$\begin{aligned} H^{(g)}=&\sum_{j=1}^{N-1}\left[\cosh\ \eta\sigma_j^z\sigma_{j+1}^z+2e^{2i(k_j-l_{j+1})}\sigma_j^-\sigma_{j+1}^++2e^{-2i(k_j-l_{j+1})}\sigma_j^+\sigma_{j+1}^-\right] \\ &+\sinh\ \eta(\sigma_1^z\coth\ \xi_-+\sigma_N^z\coth\ \xi_+). \end{aligned} \tag{25}$$

This is the transformed Hamiltonian of the model first solved in Ref. 14 by the coordinate Bethe ansatz approach.

IV. BETHE ANSATZ EQUATIONS

The diagonalization of the transfer matrix for the model Hamiltonian (24) is not an easy problem,[6] so we restrict ourselves to study the model Hamiltonian (25). This can be done by using the algebraic Bethe ansatz approach modified by Sklyanin.[1]

Repeating the same reasoning as in Ref. 1, we can diagonalize the transfer matrix for the Hamiltonian (25)

$$\tau^{(g)}(u)|v_1\cdots v_m\rangle = V^{(g)}(u)|v_1\cdots v_m\rangle, \tag{26}$$

where the eigenvalue $V^{(g)}(u)$ is given by

$$\begin{aligned} V^{(g)}(u) = \frac{(-1)^N}{\sinh(2u+\eta)\sinh\ \eta_-\,\delta\{T^{(g)}(-u-(1/2)\,\eta)\}}\Bigg[& \sinh(2u+2\,\eta)\sinh(u+\xi_+) \\ & \times\sinh(u+\xi_-)\sinh^{2N}(u+\eta)\prod_{m=1}^{M}\ \frac{\sinh(u-v_m-(1/2)\,\eta)\sinh(u+v_m-(1/2)\,\eta)}{\sinh(u-v_m+(1/2)\,\eta)\sinh(u+v_m+(1/2)\,\eta)} \\ & +\sinh 2u\ \sinh(u-\xi_++\eta)\sinh(u-\xi_-+\eta)\sinh^{2N} \\ & \times u\prod_{m=1}^{M}\ \frac{\sinh(u-v_m+(3/2)\,\eta)\sinh(u+v_m+(3/2)\,\eta)}{\sinh(u-v_m+(1/2)\,\eta)\sinh(u+v_m+(1/2)\,\eta)}\Bigg], \end{aligned} \tag{27}$$

with $\delta\{T^{(g)}(-u-\frac{1}{2}\eta)\}$ the quantum determinant of the matrix $T^{(g)}(-u-\frac{1}{2}\eta)$

$$\delta\{T^{(g)}(-u-\tfrac{1}{2}\eta)\} = \sinh^N(u+\eta)\sinh^N(u-\eta). \tag{28}$$

This result holds, provided that the parameters $\{v_1, v_2, \ldots, v_m\}$ satisfy the Bethe ansatz equations

$$\begin{aligned} \prod_{\substack{k=1\\k\neq m}}^{M}\ \frac{\sinh(v_m-v_k+\eta)\sinh(v_m+v_k+\eta)}{\sinh(v_m-v_k-\eta)\sinh(v_m+v_k-\eta)} & \\ = \frac{\sinh(v_m+\xi_+-(1/2)\,\eta)\sinh(v_m+\xi_--(1/2)\,\eta)\sinh^{2N}(v_m+(1/2)\,\eta)}{\sinh(v_m-\xi_++(1/2)\,\eta)\sinh(v_m-\xi_-+(1/2)\,\eta)\sinh^{2N}(v_m-(1/2)\,\eta)}, & \\ (m=1,2,\ldots,M). & \end{aligned} \tag{29}$$

Since the transformed transfer matrices $\tau^{(g)}(u)$ for different values of the spectral parameter u commute, the eigenvectors are u-independent and then the eigenvalues of the Hamiltonian (25) can be determined from Eq. (8). Explicitly, we have

$$\begin{aligned} E^{(g)} = & -\frac{\coth\ \eta}{\sinh\ \xi_-}+\coth 2\eta+\frac{1}{2}\,(1+\coth\ \xi_-)-\frac{1}{2}\tanh\ \eta+N\ \coth\ \eta \\ & +\sinh\ \eta\sum_{m=1}^{M}\ \frac{1}{\sinh(v_m+(1/2)\,\eta)\sinh(v_m-(1/2)\,\eta)}. \end{aligned} \tag{30}$$

From this we see that the eigenvalues of the gauge-transformed transfer matrix $\tau^{(g)}(u)$ and hence those of the Hamiltonian as well as the Bethe ansatz equations are gauge invariant whereas the Hamiltonian and its eigenvectors are explicitly gauge dependent. These results are different from those for the 1-D Heisenberg *XXZ* model with the periodic boundary conditions.[7] Evidently, this difference results from the fact that the transfer matrix for the open chain involves both $T(u)$ and

$T^{-1}(-u)$, while the corresponding transfer matrix in the case of the periodic boundary conditions involves only $T(u)$. This implies that the eigenvalues of the transfer matrix for the open chain on the pseudovacuum are gauge invariant, while the eigenvalues of the transfer matrix for the periodic chain are not. Thus, our conclusion must be a consequence of the fact that the gauge factors appearing in the eigenvalues of the transfer matrix as well as in the Bethe ansatz equations only originate from the eigenvalues of the transfer matrix on the pseudovacuum.

V. CONCLUSION

In this article we have studied hidden local gauge invariance in the 1-D Heisenberg *XXZ* model with the general boundary terms in the framework of QISM. The Bethe ansatz equations are established for the model with the special boundary terms. From this we have concluded that the Hamiltonian and its eigenvectors are explicitly gauge dependent whereas the energy eigenvalues and the Bethe ansatz equations are gauge invariant.

In conclusion we would like to point out that the model Hamiltonian (25) may be mapped into a 1-D lattice model of fermions by the Jordan–Wigner transformation.[15–17] Since the model (25) has the quantum symmetry $U_q(su_2)$ for a special choice of boundary terms,[18–20] we may expect that the 1-D lattice model of fermions (the 1-D small-polaron model) for a special choice of the boundary terms also has the quantum symmetry $U_q(su_2)$. This requires us to construct a new realization of the generators of the quantum algebra $U_q(su_2)$ in terms of the lattice fermion operators. Thus, further work is required for an understanding of the unclear algebraic structure of lattice models of fermions with boundary terms.

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New solution of the wave equation with a uniformly moving point source

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A new solution of the inhomogeneous d'Alembert equation with the point uniformly moving charge is found. The comparison of the new solution with the Kirchhoff formula solution is performed. © *1996 American Institute of Physics.* [S0022-2488(96)00101-0]

I. INTRODUCTION

The problem of determination of a field created by the unaccelerated point charge is the eldest problem of classical electrodynamics (see Ref. 1, and references therein). We discuss this problem from the point of view of the Goursat problem (GP) in which the boundary conditions are given over the characteristics $\xi=ct-z$ and $\eta=ct+z$.[2,3] In such a formulation of the problem the fundamental solutions (FS) of the wave equation (WE) (the so-called Riemann functions) are classified as belonging to the two-dimensional Minkowski space M^2.[4] In particular, in the timelike space $M^2_{(+)}$, where $\xi\eta=c^2t^2-z^2\geqslant 0$ the Riemann function has a form:[5]

$$G_R^{(+)}=J_0(\sqrt{\xi\eta(-\Delta_\perp)})|i\rangle, \tag{1}$$

where J_0 is the Bessel function of the first kind and zero order, $\Delta_\perp=(\partial^2/\partial x_1^2)+(\partial^2/\partial x_2^2)$ is the two-dimensional Laplace operator, and $|i\rangle$ is the boundary condition on the characteristics $\xi=0$ and $\eta=0$. Using this boundary value in the form of the two-dimensional delta function we obtain the Riemann function $G_R^{(+)}$:[4,5]

$$G_R^{(+)}=\frac{\delta(\sqrt{\xi\eta}-x_\perp)}{2\pi x_\perp}=\frac{\delta(|t|-r/c)}{2\pi cr}=\frac{1}{\pi c^2}\,\delta(t^2-r^2/c^2), \tag{2}$$

where $x_\perp=\sqrt{x_1^2+x_2^2}$.

In spacelike $M^2_{(-)}$ where $-\xi\eta=z^2-c^2t^2\geqslant 0$ the Riemann function $G_R^{(-)}$ is[5]

$$G_R^{(-)}=J_0(\sqrt{(-\xi\eta)\Delta_\perp})|i\rangle, \tag{3}$$

where $|i\rangle$ is a nonlocalized and smooth delta function (here we have used the Feinberg terminology). It is constructed from the Macdonald function K_0:

$$|i\rangle=\frac{1}{2\pi}\int_0^\infty K_0(kx_\perp)k\,dk=\frac{1}{2\pi x_\perp^2}. \tag{4}$$

After the substitution of Eq. (4) into Eq. (3) we can find the FS of WE:[5]

$$G_R^{(-)}=\frac{1}{2\pi}\,\frac{1}{(-\xi\eta+x_\perp^2)}=\frac{1}{2\pi}\,\frac{1}{(r^2-c^2t^2)}>0. \tag{5}$$

The GP solutions with the Riemann function $G_R^{(+)}$ for WE with the source ρ:

$$\Box^2\phi(x_1,x_2,z,t)=-4\pi\rho(x_1,x_2,z,t)$$

and zero boundary conditions on the characteristics have the following form:

$$\phi(x_1,x_2,z,t)=\int_0^{ct-z}d\xi'\int_0^{ct+z}d\eta'\int(d\mathbf{x}'_\perp)\,\frac{\delta(\sqrt{(ct-z-\xi')(ct+z-\eta')}-|\mathbf{x}_\perp-\mathbf{x}'_\perp|)}{2|\mathbf{x}_\perp-\mathbf{x}'_\perp|}$$
$$\times Q(x'_1,x'_2,\xi',\eta') \tag{6}$$

in $M^2_{(+)}$ space and, respectively,

$$\phi(x_1,x_2,z,t)=-\frac{1}{2\pi}\int_0^{z-ct}d\xi'\int_0^{ct+z}d\eta'\int d(\mathbf{x}'_\perp)$$
$$\times\frac{Q(x'_1,x'_2,\xi',\eta')}{(z-ct-\xi')(z+ct-\eta')+|\mathbf{x}_\perp-\mathbf{x}'_\perp|^2} \tag{7}$$

in $M^2_{(-)}$ space, where $Q(x_1,x_2,\xi,\eta)=\rho[x_1,x_2(\eta-\xi)/2,(\eta+\xi)/2c]$.

The existence and uniqueness of the GP solutions in the general case should be a subject of the special consideration and will not be discussed here.

The aim of this paper is to obtain the solutions of the WE on the background of expressions (6) and (7) for the unaccelerated source and their comparison with the Kirchhoff formula results, in which only the retarded potential has been used. Special attention will be paid to the performance of the Lorentz condition.

II. THE FIELD OF A CHARGE MOVING WITH THE SUBLUMINAL VELOCITY

Let the charge density ρ and the current density J_z of the point charge (source) which moves with a constant velocity $v<c$ have the form

$$\rho(x_1,x_2,z,t)=e\,\delta(x_1,x_2)\,\delta(z-vt),\quad J_z=\rho v \tag{8}$$

or, in the characteristic variables,

$$\rho(x_1,x_2,z,t)=Q(x_1,x_1,\xi,\eta)=\frac{2ec}{c+v}\,\delta(\xi-\alpha\eta)\,\delta(x_1,x_2), \tag{9}$$

where the parameter α is

$$\alpha=\frac{c-v}{c+v}. \tag{10}$$

In the following we shall apply either formula (6) or (7) depending on the sign α.

For the charge at rest one has that $\alpha=1$, and the line $\xi=\eta$ belongs to the $M^2_{(+)}$ space. In this case formula (6) gives the potential of the immovable charge[5]

$$\phi=e\Theta(\sqrt{\xi\eta}-x_\perp)/r,\quad x_\perp=\sqrt{x_1^2+x_2^2}, \tag{11}$$

where $\Theta(\tau)$ is the Heaviside step function. The condition $\sqrt{\xi\eta}>x_\perp$ is equivalent to the condition $c|t|>r$. The potential (11) is not the solution of the Maxwell equations for the charge at rest because it does not comply with the Lorentz condition $(1/c)(\partial\phi/\partial t)=0$, but it satisfies the more weak condition $\Box^2[(1/c)(\partial\phi/\partial t)]=0$.

The possibility of the existence of electrodynamics with the weak Lorentz condition was considered by many authors.[6–8] To satisfy the Lorentz condition we determine the vector potential **A**, obeying the homogeneous WE:

$$\mathbf{A}=\nabla\chi, \quad \text{div } \mathbf{A}=\Delta\chi=-\frac{1}{c}\frac{\partial\phi}{\partial t}=-e\epsilon(t)\delta(\sqrt{\xi\eta}-x_\perp)/x_\perp, \tag{12}$$

where $\epsilon(t)$ is the sign function. The scalar function χ of the gauge transformation satisfies not only the homogeneous wave equation but also the inhomogeneous nonrelativistic Poisson equation (12).

Using the FS of the Poisson equation $-1/4\pi|\mathbf{r}-\mathbf{r}'|$ we obtain the partial solution of Eq. (12) in the form

$$\chi=e\epsilon(t)\left[\frac{c|t|}{r}\,\Theta(x_\perp-\sqrt{\xi\eta})+\Theta(\sqrt{\xi\eta}-x_\perp)\right] \tag{13}$$

with the time derivative $(1/c)(\partial\chi/\partial t)=e\Theta(x_\perp-\sqrt{\xi\eta})/r$. Next we calculate the field strength created by the potentials **A** and ϕ:

$$\mathbf{E}=-\frac{1}{c}\frac{\partial\mathbf{A}}{\partial t}-\nabla\phi=-\nabla\left(\frac{1}{c}\frac{\partial\chi}{\partial t}+\phi\right)=-e\nabla\left(\frac{\Theta(x_\perp-\sqrt{\xi\eta})}{r}+\frac{\Theta(\sqrt{\xi\eta}-x_\perp)}{r}\right)=\frac{e\mathbf{r}}{r^3}. \tag{14}$$

Thus, the new Coulomb solution (11) differs from the usual Coulomb potential by the gauge.

Next we consider the subluminal source that has the velocity $v\to c-0$ (it is the ultrarelativistic case). In this case the parameter $\alpha\to+0$ and formula (6) gives the potential

$$\phi=e\Theta(\sqrt{\xi\eta}-x_\perp)/|\xi|, \quad A_z=\frac{v}{c}\,\phi=\phi. \tag{15}$$

The potential (15) has the singularity on the characteristics $\xi=0$. For the point source with the density $\rho=e\delta(x_1,x_2)\delta(z-ct)$ it should be multiplied by $\Theta(\xi)$ [this means that the variables $\xi=ct-z$, $\eta=ct+z$ in Eq. (15) belong to $M^2_{(+)}$—the future space], or by $-\Theta(-\xi)$ (the variables ξ,η belong to $M^2_{(+)}$—the past space). The solution (15) does not satisfy the Lorentz condition either because

$$\frac{1}{c}\frac{\partial\phi}{\partial t}+\frac{\partial A_z}{\partial z}=\frac{e\delta(\sqrt{\xi\eta}-x_\perp)\Theta(\xi)}{x_\perp}\neq 0. \tag{16}$$

To satisfy the Lorentz condition in the Lorentz gauge we introduce the transverse vector **A** by the relations

$$A_i=\frac{\partial\chi}{\partial x_i}, \quad \partial_i A_i=\Delta_\perp\chi=-\frac{2\partial\phi}{\partial\eta}=-\frac{e\delta(\sqrt{\xi\eta}-x_\perp)}{x_\perp}\,\Theta(\xi), \tag{17}$$

where $i=1,2$ and the scalar function χ obeys not only the homogeneous WE but also the two-dimensional Poisson equation with the fundamental solution

$$\frac{1}{2\pi}\log\sqrt{(x_1-x_1')^2+(x_2-x_2')^2}. \tag{18}$$

The partial solution of Eq. (17):

$$\chi=-e[\log x_\perp\Theta(x_\perp-\sqrt{\xi\eta})+\log\sqrt{\xi\eta}\Theta(\sqrt{\xi\eta}-x_\perp)]\Theta(\xi) \tag{19}$$

creates the potentials

$$A_i=\frac{\partial\chi}{\partial x_i}=-e(x_i/x_\perp^2)\Theta(x_\perp-\sqrt{\xi\eta})\Theta(\xi) \tag{20}$$

that enables us to find the strengths **E** and **H**. It will be convenient to introduce the cylindrical coordinates with the basic unit vectors $\mathbf{x}^0$, $\boldsymbol{\psi}^0$, $\mathbf{z}^0$, by the relations

$$\mathbf{x}^0=\left(\frac{x_1}{x_\perp},\frac{x_2}{x_\perp},0\right),\quad \boldsymbol{\psi}^0=\left(-\frac{x_2}{x_\perp},\frac{x_1}{x_\perp},0\right),\quad \mathbf{z}^0=(0,0,1). \tag{21}$$

Thus the electric field strength **E** is

$$\mathbf{E}=\mathbf{x}^0E_x+\mathbf{z}^0E_z, \tag{22}$$

where

$$E_x=e\left(\frac{\delta(\sqrt{\xi\eta}-x_\perp)}{x_\perp}\frac{z}{x_\perp}\Theta(\xi)+\frac{\delta(\xi)}{x_\perp}\right)=e\left(\frac{\delta(t-r/c)}{cr}\frac{z}{x_\perp}\Theta(\xi)+\frac{\delta(\xi)}{x_\perp}\right), \tag{23}$$

$$E_z=-e\left(\frac{\delta(\sqrt{\xi\eta}-x_\perp)}{x_\perp}\right)\Theta(\xi)=-e\,\frac{\delta(t-r/c)}{cr}\Theta(\xi), \tag{24}$$

and the magnetic field strength is

$$\mathbf{H}=\mathrm{rot}\,\mathbf{A}=e\boldsymbol{\psi}^0\left(\frac{\delta(t-r/c)}{cr}\frac{ct}{x_\perp}\Theta(\xi)+\frac{\delta(ct-z)}{x_\perp}\right). \tag{25}$$

As follows from formulas (23) and (25), the field strengths can be rewritten in the form

$$\mathbf{E}=\mathbf{E}^{(0)}+\mathbf{E}^{(1)},\quad \mathbf{H}=\mathbf{H}^{(0)}+\mathbf{H}^{(1)}, \tag{26}$$

where

$$\mathbf{E}^{(1)}=e\,\frac{\delta(\sqrt{\xi\eta}-x_\perp)}{x_\perp}\Theta(\xi)\left(\mathbf{x}^0\frac{z}{x_\perp}-\mathbf{z}^0\right)=e\,\frac{\delta(t-r/c)}{cr}\Theta(\xi)(\mathbf{x}^0\cot\theta-\mathbf{z}^0), \tag{27}$$

$$\mathbf{H}^{(1)}=e\,\frac{\delta(\sqrt{\xi\eta}-x_\perp)}{x_\perp}\Theta(\xi)\boldsymbol{\psi}^0\frac{ct}{x_\perp}=e\,\frac{\delta(t-r/c)}{cr}\frac{\boldsymbol{\psi}^0}{\sin\theta}\Theta(\xi), \tag{28}$$

and

$$\mathbf{E}^{(0)}=e\,\frac{\delta(ct-z)}{x_\perp}\mathbf{x}^0=e\,\frac{\delta(ct-r\cos\theta)}{r\sin\theta}\mathbf{x}^0, \tag{29}$$

$$\mathbf{H}^{(0)}=e\,\frac{\delta(ct-r\cos\theta)}{r\sin\theta}\boldsymbol{\psi}^0, \tag{30}$$

where θ is the polar angle between the directions of the vectors $\mathbf{z}^0$ and $\mathbf{r}^0=\mathbf{r}/r=\mathbf{x}^0\sin\theta+\mathbf{z}^0\cos\theta$.

It is easy to verify that

$$|\mathbf{E}^{(1)}|=|\mathbf{H}^{(1)}|, \quad \mathbf{E}^{(1)}=\mathbf{H}^{(1)}\times\mathbf{r}^0, \quad \mathbf{H}^{(1)}=\mathbf{r}^0\times\mathbf{E}^{(1)}, \tag{31}$$

where $\mathbf{E}^{(1)}$ and $\mathbf{H}^{(1)}$ are called the radiation fields. The strengths $\mathbf{E}^{(0)}$ and $\mathbf{H}^{(0)}$ which fall off with the fixed r as $1/r^2$ must be called quasistationary. The electric field strength $\mathbf{E}^{(0)}$ plays an important role in the validity of Gauss' theorem

$$\int \text{div } \mathbf{E}(d\mathbf{r})= \oint \mathbf{E}^{(0)}\mathbf{r}^0 r^2 \, d\Omega = 2\pi e \int_0^\pi \delta(ct/r-\cos\,\theta)\sin\,\theta \, d\theta = 4\pi e. \tag{32}$$

The Poynting vector $\mathbf{S}$ which determines the energy flux at large distances from the point charge is connected with the radiation fields $\mathbf{E}^{(1)}$ and $\mathbf{H}^{(1)}$ only:

$$\mathbf{S}=\frac{c}{4\pi}\,\mathbf{E}^{(1)}\times\mathbf{H}^{(1)}=\frac{c}{4\pi}\,\mathbf{E}^{(1)^2}\mathbf{r}^0. \tag{33}$$

To end with the radiation one needs to consider the energy balance and the force balance following the Maxwell equations. The energy balance in the integral form for the solution of Eqs. (23)–(25) is represented by the formula

$$\int (d\mathbf{r})\,\frac{\partial}{\partial t}\left(\frac{E^2+H^2}{8\pi}\right)=-\int (d\mathbf{r})(\mathbf{JE})-\frac{c}{4\pi}\oint d\boldsymbol{\sigma}, \quad \mathbf{E}\times\mathbf{H}. \tag{34}$$

The term on the left-hand side of Eq. (34) represents, by itself, the change of the total electromagnetic field energy, besides in the wave zone ($r\to\infty$ or $t\to\infty$) it tends to zero. The latter means that the energy losses per time unit are equal to the energy emitted by the ultrarelativistic source

$$\int (d\mathbf{r})J_zE_z=-\frac{c}{4\pi}\oint d\boldsymbol{\sigma}, \quad \mathbf{E}\times\mathbf{H}. \tag{35}$$

The substitution of expressions (23)–(25) into Eq. (35) shows that the energy losses

$$\int (d\mathbf{r})J_zE_z=-e^2c\int_0^\infty k\,dk\to -ce^2k^2 \tag{36}$$

and the energy flux per the time unit which is integrated over the sphere of radius r:

$$\frac{c}{4\pi}\oint d\boldsymbol{\sigma}, \quad \mathbf{E}\times\mathbf{H}=\frac{e^2}{c}\,[\delta(t-r/c)]^2\to e^2\omega^2/c \tag{37}$$

are infinite. Being interpreted in terms of the cutting parameters ω and k they become finite. From Eqs. (35)–(37) we obtain the relation connecting the cutting parameters. It is valid only for the electromagnetic waves in vacuum:

$$k=\frac{\omega}{c}=\frac{2\pi}{\lambda}. \tag{38}$$

Let us calculate the volume density of the Lorentz force in the fields (23)–(25):

$$\mathbf{f}=\rho\mathbf{E}+\frac{1}{c}\,(\mathbf{J}\times\mathbf{H})=\rho\mathbf{E}^{(1)}+\frac{1}{c}\,(\mathbf{J}\times\mathbf{H}^{(1)})=\mathbf{z}^0\rho E_z=\mathbf{r}^0\rho E_z\,. \tag{39}$$

We recall that

$$\rho = e\,\delta(x_1,x_2)\,\delta(z-ct), \quad E_z = -e\,\frac{\delta(t-r/c)}{cr}\,\Theta(ct-z), \quad \mathbf{J}=(0,0,c\rho).$$

In Eq. (39) we take into account the relation

$$\rho\mathbf{E}^{(0)} + \frac{1}{c}\,(\mathbf{J}\times\mathbf{H}^{(0)}) = 0. \tag{40}$$

Except this, the multiplication by the above delta functions leads to the relations $z=r=ct$ and $\mathbf{z}^{(0)}=\mathbf{r}^{(0)}$.

Thus the Lorentz force $\mathbf{f}$ is indeed the spatial component of the four-dimensional vector f_μ:

$$f_\mu = (\mathbf{f}, i\rho E_z), \quad f_\mu^2 = f^2 - f_0^2 = 0. \tag{41}$$

This vector has a zero four-dimensional length, that is, the energy momentum tensor $T_{\mu v}$ of the field created by the ultrarelativistic source possesses the correct properties under the Lorentz transformation.

One can calculate the number of the photons N of the frequency ω emitted on the path $d=ct$:

$$N = (e^2\omega^2/c)(d/c)(1/h\omega) = 2\pi(e^2/hc)(d/\lambda). \tag{42}$$

In conclusion to this section we want to note that the solution (15) is absent in the classical electrodynamics. It appears only in the Goursat problem.[8]

III. THE FIELD OF SUPERLUMINAL SOURCE

For the point source that moves with the velocity $v>c$ the parameter $\alpha<0$ [see Eq. (10)] and the characteristic variables of the source belong to the space $M^2_{(-)}$. Using formula (7) we obtain[5]

$$\phi = -(e/R)\log(vt-z-R)/(vt-z+R), \quad A_z = (v/c)\,\phi, \tag{43}$$

where

$$R = \sqrt{(vt-z)^2 - (v^2/c^2-1)x_\perp^2}. \tag{44}$$

Solution (43) depends on z and t in the combination $\zeta = vt-z$ so that the Lorentz condition performs automatically. In solution (43) the wave operator is

$$\Box^2 = -(v^2/c^2-1)\,\frac{\partial^2}{\partial\zeta^2} + \Delta_\perp\,. \tag{45}$$

As $v\to c+0$ $(R=|vt-z|)$ solution (43) does not exist because the wave operator is independent of z and t. This dependence remains in the source density. By the Kirchhoff formula the potential of the superluminal source is equal to

$$\phi = \frac{2e}{R}. \tag{46}$$

This is the Heaviside–Sommerfeld solution.[9] The potential (43) as well as the potential (46) cannot be created by the source with the density $e\,\delta(x_1,x_2)\,\delta(z-vt)$. This fact will take place even if they are multiplied by steps $\theta(\zeta - \sqrt{v^2/c^2-1}\,x_\perp)\,\theta(\zeta)$. Let us emphasize that

$$\lim_{vt-z\to 0,\ x_\perp\to 0} R(x_\perp, vt-z) \neq \lim_{x_\perp\to 0,\ vt-z\to 0} R(x_\perp, vt-z). \tag{47}$$

The latter fact induced Sommerfeld to refuse the point source model. The analysis of solutions (43) and (46) shows that the inhomogeneous WE at the source velocity $v \geqslant c+0$ has no solution.

IV. CONCLUSION

Formula (42) allows us to make the following conclusion: the charged particle that moves uniformly along the straight line in vacuum emits electromagnetic waves only in the ultrarelativistic case $(v \to c-0)$. This contradicts the assertion that the free uniformly moving particle in vacuum can radiate electromagnetic waves at $v > c$.[9]

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Transitive symplectic manifolds in 1+2 dimensions

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A complete list of all transitive symplectic manifolds of the Poincaré and Galilei group in 1+2 dimensions is given. © *1996 American Institute of Physics.* [S0022-2488(96)00601-6]

I. INTRODUCTION

Recently the author gave a complete analysis of the projective unitary irreducible representations of the Poincaré and Galilei groups in 1+2 dimensions.[1,2] In the context of constant interest in physics in 1+2 dimensions, the author believes it useful to provide the same analysis in the framework of Hamiltonian mechanics. Namely, to provide a complete list of all the transitive symplectic actions for the Poincaré and Galilei groups in 1+2 dimensions. The method used is, essentially, the orbit method of Kostant, Souriau, and Kirillov.[3–6] However, if we want the complete list of these symplectic actions (not only up to a covering like in the usual formulation of the orbit method) one needs a generalization of this method appearing in Ref. 7.

Section II presents the method following Ref. 7 In Secs. III and IV the method for the Poincaré and the Galilei groups, respectively are applied. The first case is rather standard and offers no surprises. The second case is on the contrary a very good ''laboratory'' for practically all the symplectic techniques described in full generality in Sec. II.

After some preliminaries, in Sec. IV C the transitive symplectic manifolds of the (proper orthochronous) Galilei group in a rather abstract way directly following the method outlined in Sec. II is described. In Secs. V A–V D to give more explicit realizations of some of these manifolds using the coadjoint orbits of the Galilei group and of his central extensions.

Note that some of these coadjoint orbits have appeared in Ref. 8.

II. TRANSITIVE SYMPLECTIC ACTIONS OF LIE GROUPS

A. Basic definitions

Let (M_i,Ω_i) $i=1,2$ be symplectic manifolds. A diffeomorphism $\phi: M_1 \to M_2$ is called *symplectic* if

$$\phi^* \Omega_2 = \Omega_1 . \tag{2.1}$$

Let (M,Ω) be a symplectic manifold and G a Lie group (not necessarily connected) acting on $M: G \ni g \mapsto \phi_g \in Diff(M)$.

This action is called *symplectic* and (M,Ω) is called a *G-symplectic manifold* if:

$$(\phi_g)^* \Omega = \Omega, \quad \forall g \in G. \tag{2.2}$$

If (M_i,Ω_i) $i=1,2$ are two G-symplectic manifolds, they are called *G-symplectomorphic* if there exists a symplectic map $\phi: M_1 \to M_2$ which is also G-equivariant.

Physically, a G-symplectic manifold can be considered as the phase space of a given Hamiltonian system for which G is the covariance group. Two such Hamiltonian system are identical from the physical point of view if the corresponding G-symplectic manifolds are

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G-symplectomorphic. One can also argue that elementary systems are described by transitive G-symplectic manifolds. The orbit method describes transitive G-symplectic manifolds up to G-symplectomorphisms.

B. The basic theorem

Denote by $\mathrm{Lie}(G)\equiv T_e(G)$ the Lie algebra of G, by $G \ni g\mapsto Ad_g \in \mathrm{End}(\mathrm{Lie}(G))$ the adjoint action and by $G \ni g\mapsto Ad_g^{\#} \in \wedge(\mathrm{Lie}(G)^*)$ the (dual) action of G (see Ref. 6, p. 172). In particular, the restriction of $Ad_g^{\#}$ to $(\mathrm{Lie}(G))^*$ is the usual coadjoint action of G. Call $Ad_g^{\#}$ *the induced action*. A 2-*cocycle* for $\mathrm{Lie}(G)$ is a bilinear antisymmetric map: $\sigma:\mathrm{Lie}(G)\times\mathrm{Lie}(G)\to\mathbb{R}$ verifying the cocycle identity:[6]

$$\sigma([X_1,X_2],X_3)+\textit{cyclic permutations}=0 \quad \forall\, X_i \in \mathrm{Lie}(G)\ (i=1,2,3). \tag{2.3}$$

Denote by $Z^2(\mathrm{Lie}(G),\mathbb{R})$ the linear space of all 2-cocycles. If $\sigma \in Z^2(\mathrm{Lie}(G),\mathbb{R})$ we define:

$$h_\sigma\equiv\{X\in\mathrm{Lie}(G)\,|\,\sigma(X,Y)=0,\forall Y\in\mathrm{Lie}(G)\} \tag{2.4}$$

and one finds out that $h_\sigma\subset\mathrm{Lie}(G)$ is a Lie subalgebra. Denote by $H_\sigma\subset G$ the connected Lie subgroup immersed in G and associated to the Lie subalgebra h_σ.

The natural action of G on $Z^2(\mathrm{Lie}(G),\mathbb{R})$, namely the induced action is given by:

$$(Ad_g^{\#}\sigma\,)(X_1,X_2)\equiv\ \sigma(Ad_{g^{-1}}(X_1),Ad_{g^{-1}}(X_2)). \tag{2.5}$$

Denote by $G_\sigma\subset G$ the stability subgroup of σ with respect to this action. H_σ is a normal subgroup of G_σ. An $Ad^{\#}$-orbit $\mathcal{O}$ in $Z^2(\mathrm{Lie}(G),\mathbb{R})$, is called *regular* if for some $\sigma \in \mathcal{O}$ (then for all $\sigma \in \mathcal{O}$), the subgroup H_σ is closed.

If K is a Lie group and $N\subset K$ is a normal subgroup denote by K/N the factor Lie group. Two subgroups $Q,Q'\subset K/N$ are called *conjugated* if there exists $k_0 \in K$ such that

$$Q'=\{k_0kk_0^{-1}N\,|\,kN\in Q\}. \tag{2.6}$$

Now formulate the main theorem[7]:

Theorem 1: Take one representative σ from every regular orbit in $Z^2(\mathrm{Lie}(G),\mathbb{R})$. Let $\mathcal{H}_\sigma$ be the set of discrete subgroups of G_σ/H_σ and $\mathcal{C}_\sigma$ the set of conjugacy classes in $\mathcal{H}_\sigma$. Let $\bar{H} \in \mathcal{H}_\sigma$ be a representative of a given conjugacy class $[\bar{H}] \in \mathcal{C}_\sigma$ and

$$H\equiv\{h\in G_\sigma\,|\,hH_\sigma\in\bar{H}\}. \tag{2.7}$$

Then $H\subset G$ is a closed subgroup and G/H is a G-symplectic manifold with the symplectic form Ω^σ uniquely determined by

$$\sigma=(\pi^*\Omega^\sigma)_e. \tag{2.8}$$

(Here $\pi:G\to G/H$ is the canonical submersion.)

Every G-symplectic manifold of G is G-symplectomorphic to a manifold of the form $(G/H,\Omega^\sigma)$ described above. Moreover, to different couples $(\sigma,[\bar{H}])=(\sigma',[\bar{H}'])$ correspond G-symplectic manifolds which are not G-symplectomorphic.

This theorem is quite general and affords a complete classification in a very constructive way. Loosely speaking, the regular orbits classify the G-symplectic manifolds, up to a covering; the various coverings are classified by the classes of discrete subgroups in G_σ/H_σ. It is an improvement of a similar result from Ref. 6 (see p. 178) where it is shown that every G-symplectic manifold is covered by a *maximal* G-symplectic manifold, i.e., a manifold constructed as in the statement of the theorem for $H=H_\sigma$.

In applications, one determines for every regular orbit the maximal symplectic manifold. Then the various symplectic manifolds covered by this maximal manifold will be determined by factorizing $(G/H_\sigma,\Omega^\sigma)$ to the (symplectic) action of some suitable chosen discrete subgroup of G.

C. A particular case

A 2-*coboundary* is an element of $Z^2(\mathrm{Lie}(G),\mathbb{R})$ of the form

$$\sigma(X_1,X_2)=-\langle \eta,[X_1,X_2]\rangle, \quad \forall X_1,X_2\in \mathrm{Lie}(G). \tag{2.9}$$

Here $\langle,\rangle$ is the duality form between $\mathrm{Lie}(G)$ and $(\mathrm{Lie}(G)^*$ and $\eta\in(\mathrm{Lie}(G)^*$ is arbitrary. The linear space of all 2-coboundaries is denoted by $B^2(\mathrm{Lie}(G),\mathbb{R})$. We will also need the *second cohomology group* with real coefficients:

$$H^2(\mathrm{Lie}(G),\mathbb{R})\equiv Z^2(\mathrm{Lie}(G),\mathbb{R})/B^2(\mathrm{Lie}(G),\mathbb{R}).$$

Finally, a 1-*cocycle* for $\mathrm{Lie}(G)$ is any element $\eta\in(\mathrm{Lie}(G))^*$ verifying

$$\langle \eta,[X_1,X_2]\rangle>=0, \quad \forall X_1,X_2\in \mathrm{Lie}(G). \tag{2.10}$$

Denote by $Z^1(\mathrm{Lie}(G),\mathbb{R})$ the linear space of all 1-cocycles and by $H^1(\mathrm{Lie}(G),\mathbb{R})=Z^1(\mathrm{Lie}(G),\mathbb{R})$ the *first cohomology group* with real coefficients.

Now consider the coadjoint action of G in $(\mathrm{Lie}(G))^*$ defined similarly to Eq. (2.5):

$$(Ad_g^*\eta)(X)\equiv \eta(Ad_{g^{-1}}(X)), \tag{2.11}$$

and let $\mathcal{O}\subset(\mathrm{Lie}(G))^*$ be an orbit with respect to this action (i.e., a coadjoint orbit). For every $X\in\mathrm{Lie}(G)$, let $X_\mathcal{O}$ be the associated vector field on $\mathcal{O}$:

$$X_\mathcal{O}\equiv \frac{d}{ds}Ad^*_{\exp(-sX)}\big|_{s=0}. \tag{2.12}$$

Then we have Corollary 1.

Corollary 1: Let $\mathcal{O}\subset(\mathrm{Lie}(G))^*$ *be a coadjoint orbit. Then* $\mathcal{O}$ *becomes a symplectic manifold with respect to the Kostant–Souriau–Kirillov* (KSK) *symplectic form* Ω^{KSK} *which is uniquely determined by*

$$\Omega^{\mathrm{KSK}}_\eta(X_\mathcal{O},Y_\mathcal{O})=-\langle \eta,[X,Y]\rangle \tag{2.13}$$

$(\forall \eta\in\mathcal{O},\forall X,Y\in\mathrm{Lie}(G))$.

Two different coadjoint orbits are not G-symplectomorphic.

Suppose that $H^i(\mathrm{Lie}(G),\mathbb{R})=0$ $(i=1,2)$. If the stability subgroup G_η ($\eta\in\mathcal{O}$ arbitrary) is connected, then every transitive G-symplectic manifold is G-symplectomorphic with a coadjoint orbit. If G_η is not connected, then the coadjoint orbits are the minimal symplectic manifolds and the various symplectic manifolds covering $\mathcal{O}$ are classified by the conjugacy classes in $G_\eta/(G_\eta)^0$.

(See Theorem 25.2 of Refs. 6 and 7).

In applications one can use the factorization method outlined at the end of Sec. II B. If $H^i(\mathrm{Lie}(G),\mathbb{R})\neq 0$ for $i=1$ or $i=2$ then the list of all transitive G-symplectic manifolds is not exhausted by the construction outlined above and based on coadjoint orbits.

D. Extended coadjoint orbits

This section closes with another interesting construction. As seen in Sec. II C, if $H^i(\mathrm{Lie}(G),\mathbb{R}) = 0$ $(i = 1,2)$ then one can conveniently describe transitive G-symplectic manifolds as coadjoint orbits of G (or their factorization). One may wonder if something analogous works in the general case. The answer is positive and the construction works as follows.[4,5]

Let c be a 2-cocycle for the Lie group G, i.e., a map $c: G\times G\to\mathbb{R}$ verifying

$$c(g_1,g_2) + c(g_1g_2,g_3) = c(g_2,g_3) + c(g_1,g_2g_3) \quad (\forall\ g_1,g_2,g_3 \in G), \tag{2.14}$$

$$c(e,g)=c(g,e) = 0 \quad (\forall\ g \in G). \tag{2.15}$$

We construct the *central extension* G^c of G which is set-theoretically $G^c=G\times\mathbb{R}$ with the composition law

$$(g;\zeta)\cdot(g';\zeta')=(gg';\zeta +\zeta' +c(g,g')). \tag{2.16}$$

Then if c is smooth, G^c is also a Lie group. One identifies $\mathrm{Lie}(G^c) \simeq \mathrm{Lie}(G) + \mathbb{R}$ and $(\mathrm{Lie}(G^c))^* \simeq (\mathrm{Lie}(G))^* + \mathbb{R}$ in a natural way.

Then one can show that the coadjoint action of G^c has the form

$$Ad^*_{g;\zeta}(\eta;\rho)=(Ad^*_g(\eta)+\rho\alpha_{g^{-1}};\rho). \tag{2.17}$$

Here $\alpha_g \in (\mathrm{Lie}(G))^*$ is given by

$$\langle\alpha_g,X\rangle=\frac{d}{ds}[c(g,e^{sX})-c(e^{sAd_g(X)},g)]|_{s=0}. \tag{2.18}$$

One notices that the orbits of the action (2.17) are of the form $(\mathcal{O};\rho)$ where $\mathcal{O}$ are orbits in $(\mathrm{Lie}(G))^*$ relative to a modified coadjoint action. In particular, we consider the case $\rho=1$ and obtain the modified coadjoint action:

$$Ad^c_g(\eta)\equiv Ad^*_g(\eta)+\alpha_{g^{-1}}. \tag{2.19}$$

Because Ad^*_g is modified only by an η-independent translation, it is clear that Ad^c_g will remain a symplectic transformation with respect to Ω^{KSK}. It follows that in this way we obtain modified coadjoint orbits as transitive G-symplectic manifolds.

One can prove that two constructions of this type, based on the 2-cocycles c_1 and c_2, respectively, give the same result (up to a G-symplectomorphism) *if* c_1 and c_2 are cohomologous, i.e.,

$$c_1(g,g')-c_2(g,g')=d(g)-d(gg')+d(g') \tag{2.20}$$

for some smooth $d: G\to\mathbb{R}$.

In conclusion one can obtain new G-symplectic manifolds (beside the usual coadjoint orbits), by classifying all 2-cocycles of G, up to the equivalence relation (2.20), selecting a representative from every cohomology class and working with the central extension G^c.

There is no guarantee that one will obtain all the transitive G-symplectic manifolds in this way although this happens, for instance, for the Galilei group in 1+3 dimensions. In fact the Galilei group in 1+2 dimensions provide an example for which one does not obtain all the transitive G-symplectic manifolds in this way. However, the list can be completed by some simple tricks performed on the coadjoint orbits.

Finally, note that if a transitive symplectic manifold can be realized as an (extended) coadjoint orbit then one can obtain a momentum map in an obvious way.

III. TRANSITIVE SYMPLECTIC ACTIONS FOR THE POINCARÉ GROUP IN 1+2 DIMENSIONS

Denote by M the 1+2-dimensional Minkowski space i.e., $\mathbb{R}^3$ with coordinates (x^0,x^1,x^2) and with the Minkowski bilinear form

$$\{x,y\}\equiv x^0y^0-x^1y^1-x^2y^2. \tag{3.1}$$

One also needs the Minkowski norm: $\|x\|^2 \equiv \{x,x\}$.

The Lorentz group is

$$\mathscr{L}\equiv\{\Lambda\in \mathrm{End}(M)\,|\,\{Lx,Ly\}=\{x,y\},\forall x,y\in M\}$$

considered as a group with respect to operator multiplication.

The proper orthochronous Lorentz group is $\mathscr{L}_+^\uparrow\subset\mathscr{L}$:

$$\mathscr{L}_+^\uparrow\equiv\{\Lambda\in\mathscr{L}\,|\det(L)=1,L_{00}>0\}.$$

The proper orthochronous Poincaré group is a semidirect product: set theoretically $\mathscr{P}_+^\uparrow$ is formed from couples (L,a) with $L\in\mathscr{L}_+^\uparrow$ and $a\in M$ and the composition law is

$$(L,a)\cdot(L',a')=(LL',a+La'). \tag{3.2}$$

It is well known that: $H^i(\mathrm{Lie}(\mathscr{P}_+^\uparrow),\mathbb{R})=0$ $(i=1,2)$ (see, e.g. Ref. 6) so we can apply the corollary from Sec. II 2C.

One can identify $(\mathrm{Lie}(\mathscr{P}_+^\uparrow))^*\simeq\wedge^2M+M$ (see Ref. 6). One can naturally extend to this space the Minkowski bilinear form $\{,\}$ and the Minkowski norm $\|\cdot\|$. Next, one easily computes the coadjoint action of $\mathscr{P}_+^\uparrow$ in this representation:

$$Ad^*_{L,a}(\Gamma,P)=(L\Gamma+a\wedge LP,LP). \tag{3.3}$$

Here $\Gamma\to L\Gamma$ is the action of the Lorentz group on $\wedge^2M$ (it is defined in an elementary way on decomposable elements and afterwards is extended by linearity).

One can easily compute the coadjoint orbits of $\mathscr{P}_+^\uparrow$. If e_0,e_1,e_2 is the canonical base in M, then they are:

(a) $M^\epsilon_{m,s}\equiv\{(\Gamma,P)\,|\,\|P\|^2=m^2,\mathrm{sign}(P_0)=\epsilon,\Gamma\wedge P=\epsilon ms e_0\wedge e_1\wedge e_2\}$ $(m\in\mathbb{R}_+,s\in\mathbb{R},\epsilon=\pm)$;

(b) $M^\epsilon_s\equiv\{(\Gamma,P)\,|\,\|P\|^2=0,\mathrm{sign}(P_0)=\epsilon,\Gamma\wedge P=\epsilon s\, e_0\wedge e_1\wedge e_2\}$ $(s\in\mathbb{R},\epsilon=\pm)$;

(c) $M_{m,s}\equiv\{(\Gamma,P)\,|\,\|P\|^2=-m^2,\Gamma\wedge P=ms\, e_0\wedge e_1\wedge e_2\}$ $(m\in\mathbb{R}_+,s\in\mathbb{R})$;

(d1) $M^\epsilon_m\equiv\{(\Gamma,0)\,|\,\|*\Gamma\|^2=m^2,\mathrm{sign}((*\Gamma)_{00})=\epsilon\}$ $(m\in\mathbb{R}_+,\epsilon=\pm)$;

(d2) $M^\epsilon\equiv\{(\Gamma,0)\,|\,\|*\Gamma\|^2=0,\ \mathrm{sign}((*\Gamma)_{00})=\epsilon\}$ $(\epsilon=\pm)$;

(d3) $M_m\equiv\{(\Gamma,0)\,|\,\|*\Gamma\|^2=-m^2\}$ $(m\in\mathbb{R}_+)$.

(Here $*$ is the Hodge operator.)

Computing the stability subgroups for a given reference point from every orbit we obtain only connected Lie subgroups. Applying the corollary from Sec. II C it follows that (a)–(d) is the complete list of the transitive $\mathscr{P}_+^\uparrow$-symplectic manifolds.

A different realization of $M^\epsilon_{m,s}$ also appeared in Ref. 9. It is interesting to establish the connection between these two realizations. The idea is to identify

$$\wedge^2M\ni\Gamma\leftrightarrow J=*\Gamma\in M. \tag{3.4}$$

Then the action (3.3) becomes

$$Ad^*_{L,a}(J,P)=(LJ+a\times LP,LP), \tag{3.5}$$

where, for any $a,b \in M$ we define $a\times b \in M$ according to

$$(a\times b)^{\rho}\equiv\varepsilon^{\rho\mu\nu}a_{\mu}b_{\nu}. \tag{3.6}$$

The manifolds (a)–(d) above are mapped into $(J,P) \in M\times M$:
(a) $M^{\epsilon}_{m,s}\equiv\{(J,P)|\|P\|^2=m^2,\text{sign}(P_0)=\epsilon,\{J,P\}=\epsilon ms\}$ $(m\in\mathbb{R}_+,s\in\mathbb{R},\epsilon=\pm)$;
(b) $M^{\epsilon}_{s}\equiv\{(J,P)\mid\|P\|^2=0,\text{sign}(P_0)=\epsilon,\{J,P\}=\epsilon s\}$ $(s\in\mathbb{R},\epsilon=\pm)$;
(c) $M_{m,s}\equiv\{(J,P)|\|P\|^2=m^2,\{J,P\}=ms\}$ $(m\in\mathbb{R}_+,s\in\mathbb{R})$;
(d1) $M^{\epsilon}_{m}\equiv\{(J,0)|\|J\|^2=m^2,\text{sign}(J_0)=\epsilon\}$ $(m\in\mathbb{R}_+,\epsilon=\pm)$;
(d2) $M^{\epsilon}\equiv\{(J,0)|\|J\|^2=0,\text{sign}(J_0)=\epsilon\}$ $(\epsilon=\pm)$;
(d3) $M_m\equiv\{(J,0)|\|J\|^2=-m^2\}$ $(m\in\mathbb{R}_+)$.

Remark 1: One can investigate now the notion of localizability for the systems described above following the lines of Ref. 10. *It is not hard to establish that only the system corresponding to* $M^{\epsilon}_{m,s}$ *can be localizable, namely on the Euclidean space* $\mathbb{R}^2$.

Remark 2: If we compare the actions above with the list of projective unitary irreducible representations of the same group[1] *it is apparent that there are representations which do not have a classical analog.*

IV. THE TRANSITIVE SYMPLECTIC ACTIONS FOR THE GALILEI GROUP IN 1+2 DIMENSIONS

A. Notations

We define directly the proper orthochronous Galilei group in $1+2$ dimensions $\mathcal{G}^{\uparrow}_{+}$ as the group of 4×4 real matrices of the form

$$(R,\mathbf{v},\tau,\mathbf{a})\equiv\begin{pmatrix} R & \mathbf{v} & \mathbf{a}\\ 0 & 1 & \tau\\ 0 & 0 & 1\end{pmatrix}, \tag{4.1}$$

where $\tau\in\mathbb{R}$, $R\in SO(2)$ is a 2×2 real orthogonal matrix and the vectors $\mathbf{v},\mathbf{a}\in\mathbb{R}^2$ are considered as column matrices.

As for any matrix group, we identify the Lie algebra $\text{Lie}(\mathcal{G}^{\uparrow}_{+})$ with the linear space of 4×4 real matrices of the form

$$(\alpha,\mathbf{u},t,\mathbf{x})\equiv\begin{pmatrix} \alpha A & \mathbf{u} & \mathbf{x}\\ 0 & 0 & t\\ 0 & 0 & 0\end{pmatrix}. \tag{4.2}$$

Here $\mathbf{u},\mathbf{x}\in\mathbb{R}^2,t,\ \alpha\in\mathbb{R}$, and

$$A\equiv\begin{pmatrix} 0 & 1\\ -1 & 0\end{pmatrix}.$$

One obtains the Lie bracket as

$$[(\alpha_1,\mathbf{u}_1,t_1,\mathbf{x}_1),(\alpha_2,\mathbf{u}_2,t_2,\mathbf{x}_2)]=(0,A(\alpha_1\mathbf{u}_2-\alpha_2\mathbf{u}_1),0,A(\alpha_1\mathbf{x}_2-\alpha_2\mathbf{x}_1)+t_2\mathbf{u}_1-t_1\mathbf{u}_2). \tag{4.3}$$

We have established[2] that $H^2(\text{Lie}(\mathcal{G}^{\uparrow}_{+}),\mathbb{R})\neq0$ (in fact it is a three-dimensional real space) so we will have to apply directly the theorem from Sec. II B.

First we choose a convenient representation for an arbitrary element from the 2-cocycle space $Z^2(\mathrm{Lie}(\mathscr{G}_+^\uparrow),\mathbb{R})$. From Ref. 2 it follows that a generic element is of the form $[m,F,S,\mathbf{G},\mathbf{P}]$ $(m,F,S\in\mathbb{R},\mathbf{G},\mathbf{P}\in\mathbb{R}^2)$ given by the following formula:

$$[m,F,S,\mathbf{G},\mathbf{P}]=m\xi_0+F\xi_1+S\xi_2+[\mathbf{G},\mathbf{P}], \tag{4.4}$$

where ξ_0,ξ_1,ξ_2 are nontrivial cocycles (i.e., they are not coboundaries) and they have the following expressions:

$$\xi_0((\alpha_1,\mathbf{u}_1,t_1,\mathbf{x}_1),(\alpha_2,\mathbf{u}_2,t_2,\mathbf{x}_2))=\mathbf{x}_1\cdot\mathbf{u}_2-\mathbf{x}_1\cdot\mathbf{u}_2, \tag{4.5}$$

$$\xi_1((\alpha_1,\mathbf{u}_1,t_1,\mathbf{x}_1),(\alpha_2,\mathbf{u}_2,t_2,\mathbf{x}_2))=\langle\mathbf{u}_1,\mathbf{u}_2\rangle, \tag{4.6}$$

$$\xi_2((\alpha_1,\mathbf{u}_1,t_1,\mathbf{x}_1),(\alpha_2,\mathbf{u}_2,t_2,\mathbf{x}_2))=\alpha_1t_2-\alpha_2t_1 \tag{4.7}$$

and $[\mathbf{G},\mathbf{P}]$ is a coboundary of the form

$$[\mathbf{G},\mathbf{P}]((\alpha_1,\mathbf{u}_1,t_1,\mathbf{x}_1),(\alpha_2,\mathbf{u}_2,t_2,\mathbf{x}_2))=\langle\mathbf{P},\alpha_1\mathbf{x}_2-\alpha_2\mathbf{x}_1\rangle+\mathbf{P}\cdot(t_2\mathbf{u}_1-t_1\mathbf{u}_2)-\langle\mathbf{G},\alpha_1\mathbf{u}_2-\alpha_2\mathbf{u}_1\rangle. \tag{4.8}$$

We have denoted the usual scalar product in $\mathbb{R}^2$ by $\mathbf{x}\cdot\mathbf{y}$ and $\langle,\rangle$ is the symplectic form on $\mathbb{R}^2$:

$$\langle\mathbf{x},\mathbf{y}\rangle\equiv\mathbf{x}\cdot A\mathbf{y}. \tag{4.9}$$

B. Orbits of $\mathscr{G}_+^\uparrow$ in $Z^2(\mathrm{Lie}(\mathscr{G}_+^\uparrow),\mathbb{R})$

First, we compute from Eqs. (4.1) and (4.2) the adjoint action:

$$\begin{aligned}Ad_{R,\mathbf{v},\tau,\mathbf{a}}(\alpha,\mathbf{u},t,\mathbf{x})&=(R,\mathbf{v},\tau,\mathbf{a})(\alpha,\mathbf{u},t,\mathbf{x})(R,\mathbf{v},\tau,\mathbf{a})^{-1}\\&=(\alpha,R\mathbf{u}-\alpha A\mathbf{v},t,R\mathbf{x}+t\mathbf{v}+\alpha A(\tau\mathbf{v}-\mathbf{a})-\tau R\mathbf{u}).\end{aligned} \tag{4.10}$$

Then, applying Eq. (2.5) we get the desired induced action:

$$Ad^{\#}_{R,\mathbf{v},\tau,\mathbf{a}}[m,F,S,\mathbf{G},\mathbf{P}]=[m,F,S,R(\mathbf{G}+m\mathbf{a})-\tau R(\mathbf{P}+m\mathbf{v})-FA\mathbf{v},R\mathbf{P}+m\mathbf{v}]. \tag{4.11}$$

It is clear that the structure of the orbits with respect to this induced action will depend on F. In particular we have two cases $F=0$ and $F\neq0$.

(I) $\underline{F=0}$

In this case the orbits are

(a) $\mathscr{O}^1_{m,S}\equiv\{[m,0,S,\mathbf{G},\mathbf{P}]\,|\,\mathbf{G},\mathbf{P}\in\mathbb{R}^2\}\quad m\in\mathbb{R}^*,\quad S\in\mathbb{R}$,

(b) $\mathscr{O}^2_{S,k,\lambda}\equiv\{[0,0,S,\mathbf{G},\mathbf{P}]\,|\,\mathbf{P}^2=k^2,\mathbf{G}\wedge\mathbf{P}=\lambda k\mathbf{e}_1\wedge\mathbf{e}_2\}\quad k\in\mathbb{R}_+,\quad S,\lambda\in\mathbb{R}$,

(c) $\mathscr{O}^3_{S,k}\equiv\{[0,0,S,\mathbf{G},\mathbf{0}]\,|\,\mathbf{G}^2=k^2\}\quad k\in\mathbb{R}_+\cup\{0\},\quad S\in\mathbb{R}$

(II) $\underline{F\in\mathbb{R}^*}$

The orbits are

(a) $\mathscr{O}^4_{m,F,S}\equiv\{[m,F,S,\mathbf{G},\mathbf{P}]\,|\,\mathbf{G},\mathbf{P}\in\mathbb{R}^2\}\quad m\in\mathbb{R}^*,\quad S\in\mathbb{R}$,

(b) $\mathscr{O}^5_{F,S,k}\equiv\{[0,F,S,\mathbf{G},\mathbf{P}]\,|\,\mathbf{G}\in\mathbb{R}^2,\mathbf{P}^2=k^2\}\quad k\in\mathbb{R}_+\cup\{0\},\quad S\in\mathbb{R}$.

Above we have denoted with $\mathbf{e}_1$ and $\mathbf{e}_2$ the natural basis in $\mathbb{R}^2$.

C. Computation of the transitive symplectic actions

As indicated in the statement of Theorem 1, one needs to provide a list of subgroups $H \subset \mathcal{G}_+^\uparrow$ such that $\mathcal{G}_+^\uparrow/H$ is a symplectic manifold with the symplectic form given by Eq. (2.8). Of course, this is a very implicit way to exhibit the symplectic transitive actions of $\mathcal{G}_+^\uparrow$.

As suggested in Sec. IV B, one divides the study in two cases corresponding to $F=0$ and $F\neq 0$, respectively. One has to take some reference point σ on every orbit $\mathcal{O}^i$ $(i=1,...,5)$ and thereafter to compute G_σ and H_σ and the discrete subgroups of G_σ/H_σ. The computations are elementary and we provide only the final results. We point out that in all the cases the action of G_σ on G_σ/H_σ is trivial, so $\mathcal{C}_\sigma = \mathcal{H}_\sigma$ (in the notations of the theorem from Sec. II B).

(I) $\underline{F=0}$

(a) $\underline{\sigma=[m,0,S,\mathbf{0},\mathbf{0}]}$, $m\in\mathbb{R}^*$, $\quad S\in\mathbb{R}$.

One finds two subcases:

(a1) $\underline{S=0}$

$$H_\sigma=\{(R,\mathbf{0},\tau,\mathbf{0})|R\in SO(2),\tau\in)\mathbb{R}\};$$

(a2) $\underline{S\neq 0}$

$$H_\sigma=\{(\ \mathbf{1},\mathbf{0},0,\mathbf{0})\}.$$

In both cases we have

$$G_\sigma=\{(R,\mathbf{0},\tau,\mathbf{0})|R\in SO(2),\tau\in\mathbb{R}\}.$$

So, in the case (a1), G_σ/H_σ is trivial and in the case (a2) $G_\sigma/H_\sigma\simeq G_\sigma\simeq SO(2)\times\mathbb{R}$.

(b) $\underline{\sigma=[0,0,S,\lambda\ \mathbf{e}_1,k\mathbf{e}_2]}$, $k\in\mathbb{R}_+$, $S,\lambda\in\mathbb{R}$.

One finds

$$H_\sigma=\{(\mathbf{1},\mathbf{v},0,\mathbf{a})|v_2=0,\quad a_1=0\},$$

$$G_\sigma=\{(\mathbf{1},\mathbf{v},0,\mathbf{a})|\mathbf{v},\quad \mathbf{a}\in\mathbb{R}^2\},$$

$$G_\sigma/H_\sigma\simeq\{(\mathbf{1},\mathbf{v},0,\mathbf{a})|v_1=0,\quad a_2=0\}\simeq\mathbb{R}\times\mathbb{R}.$$

(c) $\underline{\sigma=[0,0,S,k\ \mathbf{e}_2,\mathbf{0}]}$, $k\in\mathbb{R}_+\cup\{0\}$, $S\in\mathbb{R}$.

Again we have two subcases:

(c1) $\underline{k\in\mathbb{R}_+}$:

$$H_\sigma=\left\{(\mathbf{1},\mathbf{v},\tau,\mathbf{a})\middle| v_1=-\frac{S}{k}\tau,\tau,v_2\in\mathbb{R},\ \mathbf{a}\in\mathbb{R}^2\right\},$$

$$G_\sigma=\{(\mathbf{1},\mathbf{v},\tau,\mathbf{a})|\tau\in\mathbb{R},\ \mathbf{v},\mathbf{a}\in\mathbb{R}^2\},$$

$$G_\sigma/H_\sigma\simeq\{(\mathbf{1},\mathbf{v},0,\mathbf{0})|v_2=0\}\simeq\mathbb{R}.$$

(c2) $\underline{k=0}$

If $S\neq 0$, we have

$$H_\sigma=\{(\mathbf{1},\mathbf{v},0,\mathbf{a})|\mathbf{v},\mathbf{a}\in\mathbb{R}^2\},$$

$$G_\sigma=\mathcal{G}_+^\uparrow,$$

$$G_\sigma/H_\sigma\simeq\{(R,\mathbf{0},\tau,\mathbf{0})|R\in SO(2),\tau\in\mathbb{R}\}\simeq SO(2)\times\mathbb{R}.$$

If $S=0$, we have $G_\sigma=H_\sigma=\mathscr{P}_+^\uparrow$ so this case is trivial.

(II) $F\in\mathbb{R}^*$

(a) $\sigma=[m,F,S,\mathbf{0},\mathbf{0}]$, $m\in\mathbb{R}^*$, $S\in\mathbb{R}$.

We obtain the same subgroups G_σ and H_σ as in the case $F=0$.

(b) $\sigma=[0,F,S,\mathbf{0},k\mathbf{e}_2]$, $k\in\mathbb{R}_+\cup\{0\}$, $S\in\mathbb{R}$.

We have two subcases:

(b1) $k\in\mathbb{R}_+$.

$$H_\sigma=\left\{\left(\mathbf{1},v\mathbf{e}_1,\frac{Fv}{k},\left(\frac{SFv}{k^2}+\frac{Fv^2}{2k}\right)\mathbf{e}_1+a\mathbf{e}_2\right)\middle| v,a\in\mathbb{R}\right\},$$

$$G_\sigma=\left\{\left(\mathbf{1},v\mathbf{e}_1,\frac{Fv}{k},\mathbf{a}\right)\middle| v\in\mathbb{R},\mathbf{a}\in\mathbb{R}^2\right\},$$

$$G_\sigma/H_\sigma=\{(\mathbf{1},\mathbf{0},0,b\mathbf{e}_1)|b\in\mathbb{R}\}\simeq\mathbb{R}.$$

(b2) $k=0$.

There are two possibilities:

(b2.1) $S\neq0$.

$$H_\sigma=\{(\mathbf{1},\mathbf{0},0,\mathbf{a})|\mathbf{a}\in\mathbb{R}^2\}.$$

(b2.2) $S=0$.

$$H_\sigma=\{(R,\mathbf{0},\tau,\mathbf{a})|R\in SO(2),\tau\in\mathbb{R},\mathbf{a}\in\mathbb{R}^2\}.$$

Regardless of the value of S we have

$$G_\sigma=\{(R,\mathbf{0},\tau,\mathbf{a})|R\in SO(2),\tau\in\mathbb{R},\mathbf{a}\in\mathbb{R}^2\}.$$

So we have for the first possibility

$$G_\sigma/H_\sigma=\{(R,\mathbf{0},\tau,\mathbf{0})|R\in SO(2),\quad\tau\in\mathbb{R}\}\simeq SO(2)\times\mathbb{R}$$

and for the second possibility the factor group is trivial.

Regarding the discrete subgroups of G_σ/H_σ we have only three nontrivial possibilities: $\mathbb{R}$, $\mathbb{R}\times\mathbb{R}$, and $SO(2)\times\mathbb{R}$ as is apparent from the list above. It is well known that the discrete subgroups are in these cases $H_\gamma\equiv\gamma\mathbf{Z}$, $H_{\gamma_1,\gamma_2}\equiv\gamma_1\mathbf{Z}\times\gamma_2\mathbf{Z}$ and $H_{r,\gamma}\equiv Z_r\times\gamma\mathbf{Z}$, respectively. Here $\gamma,\gamma_1,\gamma_2\in\mathbb{R}_+\cup\{0\}$ and $Z_r\in SO(2)$ is the cyclic group of order $r\in\mathbb{N}^*$: $Z_r\equiv\{R(2\pi k/r)|k=0,\ldots,r-1\}$ (as usual $R(\phi)=e^{\phi A}$ is the rotation of angle ϕ).

Combining the results obtained above, we can formulate the main result:

Proposition 1: Every transitive $\mathscr{P}_+^\uparrow$-symplectic manifold is $\mathscr{P}_+^\uparrow$-symplectomorphic to one of the form $(\mathscr{P}_+^\uparrow/H,\Omega^\sigma)$ where H and σ can be

$$(1)\qquad H^1=\{(R,\mathbf{0},\tau,\mathbf{0})|R\in SO(2),\quad\tau\in\mathbb{R}\},$$

$$\sigma^1=[m,F,0,\mathbf{0},\mathbf{0}]\quad m\in\mathbb{R}^*,\quad F\in\mathbb{R};$$

$$(2)\qquad H^2=\{(R(2\pi k/r),\mathbf{0},n\gamma,\mathbf{0})|k=0,\ldots,r-1,n\in\mathbf{Z}\},$$

$$\sigma^2=[m,F,S,\mathbf{0},\mathbf{0}]\quad m,S\in\mathbb{R}^*,\quad F\in\mathbb{R},\quad r\in\mathbb{N}^*,\quad\gamma\in\mathbb{R}_+\cup\{0\};$$

$$(3)\qquad H^3=\{(\ \mathbf{1},v\mathbf{e}_1+\gamma_1 n\mathbf{e}_2,0,\gamma_2 m\mathbf{e}_1+a\mathbf{e}_2)\,|\,v,a\in\mathbb{R},m,n\in\mathbf{Z}\},$$

$$\sigma^3=[0,0,S,\lambda\mathbf{e}_1,k\mathbf{e}_2]\quad k\in\mathbb{R}_+,\ \lambda,S\in\mathbb{R},\ \gamma_1,\gamma_2\in\mathbb{R}_+\cup\{0\};$$

$$(4)\qquad H^4=\left\{\left(\mathbf{1},v\mathbf{e}_1,\frac{Fv}{k},\left(\frac{SFv}{k^2}+\frac{Fv^2}{2k^2}+\gamma n\right)\mathbf{e}_1+a\mathbf{e}_2\right)\middle|\,v,a\in\mathbb{R},n\in\mathbf{Z}\right\}$$

$$\sigma^4=[0,F,S,\mathbf{0},k\mathbf{e}_2]\quad k\in\mathbb{R}_+,\quad S\in\mathbb{R},\quad F\in\mathbb{R}^*,\quad \gamma\in\mathbb{R}_+\cup\{0\};$$

$$(5)\qquad H^5=\left\{\left(\ \mathbf{1},\left(n\gamma-\frac{S\tau}{k}\right)\mathbf{e}_1+v\mathbf{e}_2,\tau,\mathbf{a}\right)\middle|\,\tau,v\in\mathbb{R},\ \mathbf{a}\in\mathbb{R}^2,n\in\mathbf{Z}\right\},$$

$$\sigma^5=[0,0,S,k\mathbf{e}_2,\mathbf{0}],\quad k\in\mathbb{R}_+,\quad S\in\mathbb{R},\quad \gamma\in\mathbb{R}_+\cup\{0\};$$

$$(6)\qquad H^6=\{(R(2\pi\ k/r),\ \mathbf{v},n\gamma,\mathbf{a})\,|\,k=0,\ldots,r-1,\mathbf{v},\mathbf{a}\in\mathbb{R}^2,n\in\mathbf{Z}\},$$

$$\sigma^6=[0,0,S,\mathbf{0},\mathbf{0}]\quad S\in\mathbb{R}^*,r\in\mathbb{N}^*,\gamma\in\mathbb{R}_+\cup\{0\};$$

$$(7)\qquad H^7=\{(R(2\pi\ k/r),\mathbf{0},n\gamma,\mathbf{a})\,|\,k=0,\ldots,r-1,\mathbf{a}\in\mathbb{R}^2,n\in\ \mathbf{Z},$$

$$\sigma^7=[0,F,S,\mathbf{0},\mathbf{0}]\quad F,S\in\mathbb{R}^*,\quad r\in\mathbb{N}^*,\quad \gamma\in\mathbb{R}_+\cup\{0\};$$

$$(8)\qquad H^8=\{(R,\ \mathbf{0},\tau,\mathbf{a})\,|\,R\in SO(2),\tau\in\mathbb{R},\mathbf{a}\in\mathbb{R}^2\},$$

$$\sigma^8=[0,F,0,\mathbf{0},\mathbf{0}]\quad F\in\mathbb{R}^*.$$

For distinct couples $(H,\Omega)\neq(H',\Omega')$ the corresponding manifolds are not $\mathscr{P}_+^\uparrow$-symplectomorphic.

V. SOME EXPLICIT REALIZATIONS

In principle, the analysis of the transitive symplectic manifolds for $\mathscr{P}_+^\uparrow$ was completed above. However, it is interesting to give various realizations of these manifolds. In this way one could conjecture perhaps a reasonable physical interpretation. One will obtain some of these representations systematically using the extended action from 2D; this will be done in Secs. V A and V B. Sections V C and V D contain some unsystematic guesses for some other cases not covered by the previous analysis.

A. Central extensions of $\mathscr{G}_+^\uparrow$

As outlined in Sec. II D we first need $H^2(\mathscr{G}_+^\uparrow,\mathbb{R})$. One computes this group taking advantage of the knowledge of $H^2(\tilde{\mathscr{G}}_+^\uparrow,\mathbb{R})$ which was determined in Ref. 2. For the definitions of $\tilde{\mathscr{G}}_+^\uparrow$ and of the covering map $\delta:\tilde{\mathscr{G}}_+^\uparrow\to\mathscr{G}_+^\uparrow$ see also Ref. 2.

Let $c\in Z^2(\mathscr{G}_+^\uparrow,\mathbb{R})$ be arbitrary. One defines $\tilde{c}:\tilde{\mathscr{G}}_+^\uparrow\times\tilde{\mathscr{G}}_+^\uparrow\to\mathbb{R}$ by

$$\tilde{c}(\tilde{g},\tilde{g}')\equiv c(\delta(\tilde{g}),\delta(\tilde{g}')).$$

Then it is elementary to show that $\tilde{c}\in Z^2(\tilde{\mathscr{G}}_+^\uparrow,\mathbb{R})$. Applying the result obtained in Ref. 2 it follows that $\tilde{c}$ is cohomologous to $m\tilde{c}_0+F\tilde{c}_1+S\tilde{c}_2$ where:

$$\tilde{c}_0(\tilde{g},\tilde{g}')\equiv\tfrac{1}{2}[\mathbf{a}\cdot R(x)\mathbf{v}'-\mathbf{v}\cdot R(x)\mathbf{a}'+\tau'\mathbf{v}\cdot R(x)\mathbf{v}'], \tag{5.1}$$

$$\tilde{c}_1(\tilde{g},\tilde{g}')\equiv\tfrac{1}{2}\langle\mathbf{v},R(x)\mathbf{v}'\rangle, \tag{5.2}$$

$$\tilde{c}_2(\tilde{g},\tilde{g}')\equiv\tau x'. \tag{5.3}$$

Here $\tilde{g}=(x,\mathbf{v},\tau,\mathbf{a}),\tilde{g}'=(x',\mathbf{v}',\tau',\mathbf{a}')$. Explicitly one has

$$c(\delta(\tilde{g}),\delta(\tilde{g}'))=m\tilde{c}_0(\tilde{g},\tilde{g}')+F\tilde{c}_1(\tilde{g},\tilde{g}')+S\tilde{c}_2(\tilde{g},\tilde{g}')+\tilde{d}(\tilde{g})-\tilde{d}(\tilde{g}\tilde{g}')+\tilde{d}(\tilde{g}') \tag{5.4}$$

with $\tilde{d}:\tilde{\mathscr{G}}_+^\uparrow\to\mathbb{R}$ a smooth function. By redefining $\tilde{d}\to\tilde{d}'$ where

$$\tilde{d}'(x,\mathbf{v},\tau,\mathbf{a})=\tilde{d}(x,\mathbf{v},\tau,\mathbf{a})-\frac{x}{2\pi}\tilde{d}(2\pi,\mathbf{0},0,\mathbf{0})$$

one still has Eq. (5.4) but the new $\tilde{d}$ also verifies

$$\tilde{d}(0,\mathbf{0},0,\mathbf{0})=\tilde{d}(2\pi,\mathbf{0},0,\mathbf{0})=0.$$

If we make $x\to x+2\pi$ in Eq. (5.4) one gets more, namely that the function $\tilde{d}$ is periodic in x with period 2π. Finally, if one makes $x'\to x'+2\pi$ in Eq. (5.4) one gets $S=0$. Then it follows from Eq. (4.15) that

$$c(g,g')=mc_0(g,g')+Fc_1(g,g')+d(g)-d(gg')+d(g'),$$

where

$$c_0(g,g')\equiv\tfrac{1}{2}(\mathbf{a}\cdot R\mathbf{v}'-\mathbf{v}\cdot R\mathbf{a}'+\tau'\mathbf{v}\cdot R\mathbf{v}'), \tag{5.5}$$

$$c_1(g,g')\equiv\tfrac{1}{2}\langle\mathbf{v},R\mathbf{v}'\rangle \tag{5.6}$$

with $g=(R,\mathbf{v},\tau,\mathbf{a})$, $g'=(R',\mathbf{v}',\tau',\mathbf{a}')$ and d is uniquely determined by $d\circ\delta=\tilde{d}$.

Proposition 2: $H^2(\mathscr{G}_+^\uparrow,\mathbb{R})$ is a two-dimensional real space. Explicitly, every 2-cocycle of $\mathscr{G}_+^\uparrow$ is cohomologous to one of the form mc_0+Fc_1.

Remark 3: In Ref. 8 only the central extensions of $\mathscr{G}_+^\uparrow$ are considered. So in computing the corresponding coadjoint orbits one finds out only the case $S=0$ from our analysis.

According to Sec. II D one must consider the central extension $(\mathscr{G}_+^\uparrow)^c$ where $c=mc_0+Fc_1$.

It is to be expected that one will obtain only the symplectic manifolds corresponding to $S=0$ from the list included in the statement of Proposition 1.

B. Coadjoint orbits of $(\mathscr{G}_+^\uparrow)^c$

First compute the function α_g according to Eq. (2.18). An elementary computation gives

$$\alpha_{R,\mathbf{v},\tau,\mathbf{a}}(\alpha,\mathbf{u},t,\mathbf{x})=m(R^{-1}\mathbf{a}\cdot\mathbf{u}-R^{-1}\mathbf{v}\cdot\mathbf{x}-\alpha\langle\mathbf{a},\mathbf{v}\rangle-\tfrac{1}{2}t\mathbf{v}^2)+F(\tfrac{1}{2}\alpha\mathbf{v}^2+\langle R^{-1}\mathbf{v},\mathbf{u}\rangle). \quad (5.7)$$

To compute the extended action (2.17) one identifies $(\mathrm{Lie}(\mathscr{G}_+^\uparrow))^*\simeq\mathbb{R}+\mathbb{R}^2+\mathbb{R}+\mathbb{R}^2$ using the duality form

$$\langle(\beta,\mathbf{G},E,\mathbf{P}),(\alpha,\mathbf{u},t,\mathbf{x})\rangle=-\beta\alpha-\mathbf{G}\cdot\mathbf{u}-Et+\mathbf{P}\cdot\mathbf{x}. \quad (5.8)$$

Then Eq. (2.19) gives for the modified coadjoint action:

$$\begin{aligned}Ad^c_{R,\mathbf{v},\tau,\mathbf{a}}(\beta,\mathbf{G},E,\mathbf{P})=(&\beta+\langle R\mathbf{G}+m\mathbf{a},\mathbf{v}\rangle-\langle R\mathbf{P},\mathbf{a}\rangle-\tfrac{1}{2}F\mathbf{v}^2,\\ &R\mathbf{G}+m\mathbf{a}-\tau(R\mathbf{P}+m\mathbf{v})-FA\mathbf{v},\\ &E+R\mathbf{P}\cdot\mathbf{v}+\tfrac{1}{2}m\mathbf{v}^2,R\mathbf{P}+m\mathbf{v}).\end{aligned} \quad (5.9)$$

It is elementary to compute the orbits of this action. They are

(a) $\mathscr{O}^{*1}_{m,s,F,\mathscr{E}}\equiv\{(\beta,\mathbf{G},E,\mathbf{P})|\|\mathbf{P}\wedge\mathbf{G}-(FE-m\beta)\mathbf{e}_1\wedge\mathbf{e}_2\|=ms,E-\mathbf{P}^2/2m=\mathscr{E}\}$, $m\in\mathbb{R}^*$, $s\in\mathbb{R}_+\cup\{0\},F,\mathscr{E}\in\mathbb{R}$.

(b) $\mathscr{O}^{*2}_{k,\lambda,F}\equiv\{(\beta,\mathbf{G},E,\mathbf{P})|\mathbf{P}\wedge\mathbf{G}=(FE-\lambda k)\mathbf{e}_1\wedge\mathbf{e}_2,\mathbf{P}^2=k^2\}$, $k\in\mathbb{R}_+$, $\lambda,F\in\mathbb{R}$.

(c) $\mathscr{O}^{*3}_{E,s,F}\equiv\{(\beta,\mathbf{G},E,\mathbf{0})|2F\beta+\mathbf{G}^2=s\}$, $s,E,F\in\mathbb{R}$.

Now it is easy to match these coadjoint orbits with symplectic manifolds appearing in the statement of Proposition 1 and corresponding to $S=0$. One will get maximal manifolds as it is easy to anticipate. Namely one has

(1) $\mathscr{O}^{*1}_{m,s,F,\mathscr{E}}$ is for any $s,\mathscr{E}$ the maximal manifold of case (1);

(2) $\mathscr{O}^{*2}_{k,\lambda,F}$ is the maximal manifold of cases (3) and (4), respectively (both for $S=0$);

(3) $\mathscr{O}^{*3}_{E,s,F}$ is for any E, s the maximal manifold of cases (5) (for $S=0$) and (8), respectively.

The fact that one can obtain some of the maximal symplectic manifolds of $\mathscr{G}_+^\uparrow$ using the action Ad^c has an accidental nature as already mentioned at the end of paragraph of Sec. II D. However it is quite possible that results of a general nature can be established.

C. Maximal symplectic manifolds for $S\neq 0$

To obtain case (1) one gives another realization of case (2), namely $M=\mathbb{R}^2\times\mathbb{R}^2$ with coordinates $(\mathbf{q},\mathbf{p})$, the symplectic form

$$\Omega=\sum_{i=1}^{2}dq_i\wedge dp_i+\frac{2F}{m^2}dp_1\wedge dp_2 \quad (5.10)$$

and the action of $\mathscr{G}_+^\uparrow$:

$$\phi_{R,\mathbf{v},\tau,\mathbf{a}}(\mathbf{q},\mathbf{p})=\left(R\mathbf{q}+\mathbf{a}-\frac{\tau}{m}(R\mathbf{p}+m\mathbf{v}),R\mathbf{p}+m\mathbf{v}\right). \quad (5.11)$$

One can see in Ref. 7 the corresponding 1+3-dimensional case. Taking a suggestion from this case one builds case (1) as follows. $M=\mathbb{R}^2\times\mathbb{R}^2\times S^1\times\mathbb{R}$ with coordinates $(\mathbf{q},\mathbf{p},\nu,l)$, the symplectic form

$$\Omega=\sum_{i=1}^{2} dq_i\wedge dp_i+\frac{2F}{m^2}dp_1\wedge dp_2+\frac{S}{m}d\varphi\wedge dl \tag{5.12}$$

where $\nu=(\cos(\varphi),\sin(\varphi))$, and the action

$$\phi_{R,\mathbf{v},\tau,\mathbf{a}}(\mathbf{q},\mathbf{p},\nu,l)=\left(R\mathbf{q}+\mathbf{a}-\frac{\tau}{m}(R\mathbf{p}+m\mathbf{v}),R\mathbf{p}+m\mathbf{v},R\nu,l+m\tau\right). \tag{5.13}$$

In the cases (3)–(5) for $S\neq 0$, the trick is to modify a little the extended action (5.9), namely

$$Ad^{c,S}_{R,\mathbf{v},\tau,\mathbf{a}}(\beta,\mathbf{G},E,\mathbf{P})=(\beta+\langle R\mathbf{G},\mathbf{v}\rangle-\langle R\mathbf{P},\mathbf{a}\rangle-\tfrac{1}{2}F\mathbf{v}^2-S\tau,R\mathbf{G}-\tau R\mathbf{P}-FA\mathbf{v},E+R\mathbf{P}\cdot\mathbf{v},R\mathbf{P}) \tag{5.14}$$

and to keep the KSK-symplectic form unchanged.

Case (6) can be realized by $M=\mathbb{R}\times S^1$ with coordinates (T,ν), the symplectic form

$$\Omega=S\ d\varphi\wedge dT \tag{5.15}$$

and the action

$$\phi_{R,\mathbf{v},\tau,\mathbf{a}}(T,\nu)=(T+\tau,R\nu). \tag{5.16}$$

Here $\nu=(\cos(\varphi),\sin(\varphi))$ as above.

Finally case (7) is given by $M=\mathbb{R}\times\mathbb{R}^2\times S^1$ with coordinates $(T,\mathbf{V},\nu)$, the symplectic form

$$\Omega=F\ dV_1\wedge dV_2+S\ d\varphi\wedge dT+k(-\sin(\varphi)dV_1+\cos(\varphi)dV_2)\wedge dT \tag{5.17}$$

and the action

$$\phi_{R,\mathbf{v},\tau,\mathbf{a}}(T,\mathbf{V},\nu)=(T+\tau,R\mathbf{V}+\mathbf{v},R\nu). \tag{5.18}$$

Of course in Eqs. (5.15) and (5.17) $\nu=(\cos(\varphi),\sin(\varphi))$ as in case (1).

D. Factorized symplectic manifolds

In all cases except (1) and (8) one has, beside the maximal manifolds exhibited above, some families of factorized manifolds. The results in these remaining cases are indicated briefly.

(2) If $\gamma=0$ and $r=2,3,\ldots$ then modify Eq. (5.13) as follows:

$$\phi_{R,\mathbf{v},\tau,\mathbf{a}}(\mathbf{q},\mathbf{p},\nu,l)=\left(R\mathbf{q}+\mathbf{a}-\frac{\tau}{m}(R\mathbf{p}+m\mathbf{v}),R\mathbf{p}+m\mathbf{v},R^r\nu,l+m\tau\right). \tag{5.19}$$

To obtain the cases with $\gamma\in\mathbb{R}_+$ one factorizes the previous cases by the following action of $\mathbf{Z}$:

$$n\cdot(\mathbf{q},\mathbf{p},\nu,l)=(\mathbf{q},\mathbf{p},\nu,l+n\gamma m). \tag{5.20}$$

(3) One factorizes the maximal manifolds to an action of $\mathbf{Z}\times\mathbf{Z}$, namely,

$$(n,m)\cdot(\beta,\mathbf{G},E,\mathbf{P})=(\beta+mk\gamma_2,\mathbf{G},E+nk\gamma_1,\mathbf{P}). \tag{5.21}$$

(4)–(5) The maximal manifold is factorized to the following action of $\mathbf{Z}$:

$$n\cdot(\beta,\mathbf{G},E,\mathbf{P})=(\beta+nk\gamma,\mathbf{G},E,\mathbf{P}). \tag{5.22}$$

(6) If $\gamma=0$ and $r=2, 3,...$ proceed as case (2) above, namely modify Eq. (5.16) to

$$\phi_{R,\mathbf{v},\tau,\mathbf{a}}(T,\nu)=(T+\tau,R^r\nu). \tag{5.23}$$

The case $\gamma \in \mathbb{R}_+$ is obtained factorizing the previous cases to the following action of $\mathbf{Z}$:

$$n\cdot(T,\nu)=(T+n\gamma,\nu). \tag{5.24}$$

(7) Similarly with (6): the action on the variable $\mathbf{V}$ is not changed.

Remark 4: The notion of localizability can be investigated as in Ref. 10. It is manifest from the first part of Sec. V F that cases (1) and (2) (i.e., nonzero mass systems) are localizable on $\mathbb{R}^2$. One also finds that the cases (5)–(7) are localizable on S^1.

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Dielectric screening in a plasma: Some rigorous results

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In this article, we give some rigorous results about the properties of the solution of Poisson's equation describing dielectric screening by electrons trapped and/or untrapped in the Coulomb field of the test charge. © *1996 American Institute of Physics.* [S0022-2488(96)02501-6]

I. INTRODUCTION

Introduction of a test charge q (say, at $\mathbf{r}=\mathbf{0}$) polarizes the plasma and produces a shielding cloud around the charge. If the plasma were cold and there were no thermal agitation, the shielding would be perfect and the potential of the test charge would drop to zero outside the cloud. The test charge would be electrically invisible there! If the plasma were not cold, however, there would be a few particles at the edge of the cloud which would have enough thermal energy to escape from the cloud so that the shielding will not be complete.

The effective potential field $\phi(\mathbf{r})$ around the test charge q is calculated by taking into account the dielectric screening produced by other charged particles. Poisson's equation gives

$$\nabla^2\phi=-4\pi(n_i-n_e)-4\pi q\,\delta(\mathbf{r}), \tag{1}$$

where n is the number density of the particles and the subscripts i and e denote the ions and the electrons, respectively. The ions are assumed not to participate in the shielding process and to form only a uniform neutralizing background, so

$$n_i=n_0. \tag{2}$$

The full (trapped plus untrapped) electrons subjected to the Coulomb field of the test charge are assumed to be distributed in space according to the Boltzmann distribution

$$n_e(\mathbf{r})=n_0 e^{(e\phi)/kT_e}, \tag{3}$$

T being the temperature.

If the plasma is weakly coupled, the coupling parameter Γ satisfies

$$\Gamma=\frac{\text{mean Coulomb interaction energy}}{\text{thermal energy}}\sim\left|\frac{e\phi}{KT_e}\right|\ll 1. \tag{4}$$

Equation (4), in conjunction with Eqs. (2) and (3), leads to a linearization of Eq. (1):

$$\nabla^2\phi_{\text{lin}}=\lambda_D^{-2}\phi_{\text{lin}}-4\pi q\,\delta(\mathbf{r}) \tag{5}$$

with the well-known solution[1]

$$\phi_{\text{lin}}=\frac{q}{r}\,e^{-(r)/\lambda_D}, \tag{6}$$

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where λ_D is the Debye length

$$\lambda_D = \sqrt{\frac{KT_e}{4\pi n_0 e^2}}.$$

On the other hand, the electrons untrapped by the Coulomb field of the test charge are distributed according to the Maxwell–Boltzmann distribution

$$f_e^{(u)}(\mathbf{r},\mathbf{v}) = \begin{cases} n_0\left(\frac{m_e}{2\pi KT_e}\right)^{3/2} \exp\left[-\left(\frac{m_e\nu^2}{2} - e\phi\right)\frac{1}{KT_e}\right], & \frac{m_e\nu^2}{2} > |e\phi| \\ 0, & \frac{m_e\nu^2}{2} < |e\phi| \end{cases}. \tag{7}$$

The number density of the untrapped electrons is then given by

$$n_e^{(u)}(\mathbf{r}) = \int_0^\infty f_e^{(u)}(\mathbf{r},\mathbf{v}) 4\pi\nu^2 \, d\nu = n_0\left\{ e^{(e\phi)/KT_e}\left[1 - erf\left(\sqrt{\frac{e\phi}{KT_e}}\right)\right] + \frac{2}{\sqrt{\pi}}\sqrt{\frac{e\phi}{KT_e}}\right\}. \tag{8}$$

The number of the trapped electrons, from Eqs. (3) and (8), is thus given by

$$n_e^{(t)}(\mathbf{r}) = n_e(\mathbf{r}) - n_e^{(u)}(\mathbf{r}) = n_0\left[e^{(e\phi)/KT_e} erf\left(\sqrt{\frac{e\phi}{KT_e}}\right) - \frac{2}{\sqrt{\pi}}\sqrt{\frac{e\phi}{KT_e}}\right]. \tag{9}$$

In this paper, we propose to give some rigorous results about the properties of the solution of Eq. (1) in conjunction with Eq. (3), (8), or (9).

II. SCREENING BY THE FULL ELECTRONS

Let us nondimensionalize according to

$$\hat{\phi} = \frac{e\phi}{KT_e}, \quad \hat{r} = \frac{r}{\lambda_D}, \tag{10}$$

and drop the hats. Equation (1), on using Eqs. (2) and (3), then becomes

$$(r\phi)'' = r(e^\phi - 1) - rq\,\delta(\mathbf{r}), \tag{11}$$

where primes denote differentiation with respect to r.

Lampert and Crandall[2] rigorously proved that the solution of Eq. (11) is monotonically decreasing. The occurrence of dielectric screening would indicate that this result can be sharpened further, as given below.

Theorem 1: Let ϕ be a solution of

$$(r\phi)'' = r(e^\phi - 1) - rq\,\delta(\mathbf{r}). \tag{11}$$

Then ϕ decreases more rapidly than the shieldless decay law $1/r$, $\forall r$.

Proof: The proof is adapted from that given by Lampert and Crandall.[2]

Let $\phi > 0$, $\forall r$. Upon integrating Eq. (11) once over $0 < r_1 \leqslant r \leqslant r_2 < \infty$, we obtain

$$(r\phi)_2' - (r\phi)_1' = \int_{r_1}^{r_2} r(e^\phi - 1)\,dr. \tag{12}$$

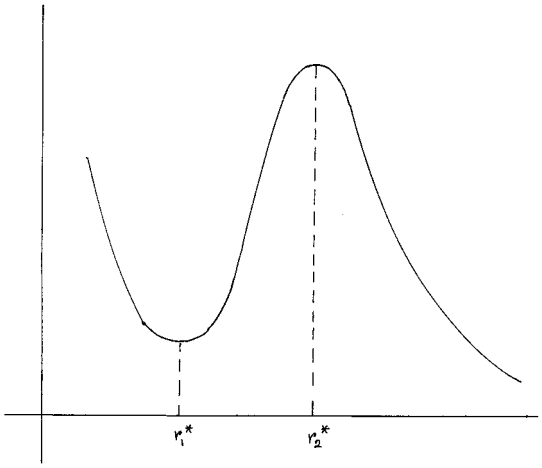

FIG. 1. $r\phi$ vs r.

If we now suppose that $(r\phi)$ does not decrease monotonically with r, then $(r\phi)$ must have a minimum for $r = r_1^* < \infty$. However, since

$$e^{\phi} - 1 \approx \phi, \quad \phi \ll 1 \tag{13}$$

ϕ must eventually decrease more rapidly than $1/r$; so it is clear that $(r\phi)$ must have a maximum for $r = r_2^*$ with $r_1^* < r_2^* < \infty$ (see Fig. 1).

Taking $r_1 = r_1^*$ and $r_2 = r_2^*$, Eq. (12) gives

$$0 = \int_{r_1^*}^{r_2^*} r(e^{\phi} - 1)\, dr$$

which is, of course, impossible since $\phi > 0$, $\forall r$.

Now, according to Eq. (13), the dielectric screening by the full electrons resembles, in the far field ($r \gg 1$), a linearized screening. (Physically this is appreciable because, according to Eqs. (8) and (9), the untrapped electrons outnumber the trapped electrons, for $r \gg 1$.) However, the numerical work of Lampert and Crandall[2] as well as that of Mak[3] indicated that the linearization condition (4) is unnecessarily stringent and that the exact solution of Eq. (11) remains close to the linearized solution (6) well after the linearization condition (4) is violated. Actually, the exact solution is bounded from below by the linearized solution (6), as shown below.

Lemma 1: The function

$$f(\phi) = e^{\phi} - 1 - \phi, \quad \phi > 0 \tag{14}$$

is positive and monotonically increasing (see Fig. 2).

Theorem 2: Let ϕ be a solution of

$$(r\phi)'' = r(e^{\phi} - 1) - rq\,\delta(\mathbf{r}). \tag{11}$$

Then, ϕ is bounded from below, $\forall r$, by the linearized solution

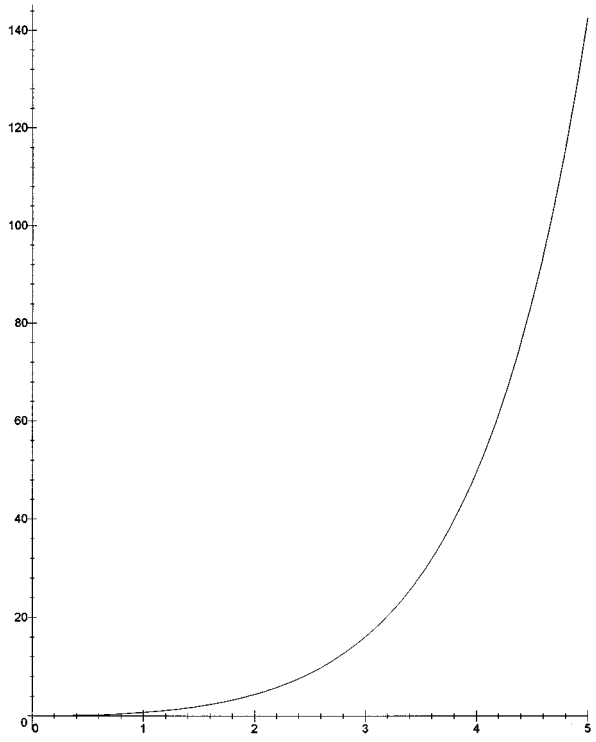

FIG. 2. $f(\phi)$ vs ϕ.

$$\phi_{\text{lin}}=\frac{q}{r}\,e^{-\mathbf{r}}. \tag{6}$$

Proof: The exact solution of Eq. (11) can be written formally as

$$(r\phi)=\int_r^\infty (r'-r)r'[\phi(r')+\{e^{\phi(r')}-1-\phi(r')\}-q\,\delta(\mathbf{r}')]dr \tag{15}$$

from which

$$(r\phi)=q\;e^{-r}+\int_r^\infty (r'-r)r'[e^{\phi(r')}-1-\phi(r')]dr'. \tag{16}$$

Using Lemma 1, Eq. (16) then implies that

$$(r\phi)\geqslant q\;e^{-r},\quad \forall r.$$

Q.E.D.

According to Theorem 2, the exact screening of the test change is weaker than linearized screening for the full electrons.

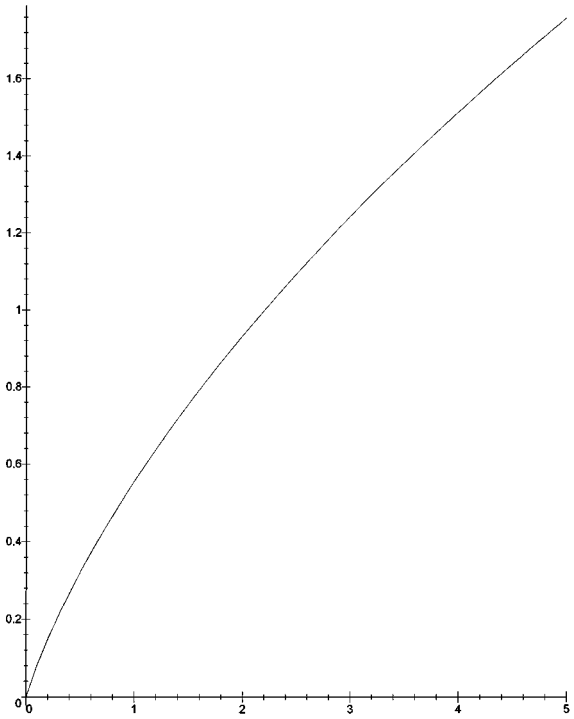

FIG. 3. $F(\phi)$ vs ϕ.

III. SCREENING BY UNTRAPPED ELECTRONS

On nondimensionalizing according to Eq. (10), and using Eqs. (2) and (8), Eq. (1) gives for the untrapped-electron screening

$$(r\phi)''=r\left[e^{\phi}\{1-erf(\sqrt{\phi})\}+\frac{2}{\sqrt{\pi}}\sqrt{\phi}-1\right]-rq\delta(\mathbf{r}). \tag{17}$$

The occurrence of dielectric screening again implies that the solution of Eq. (17) decreases more rapidly than the shieldless decay law $1/r$, $\forall r$, as deduced below.

Lemma 2: The function

$$F(\phi)=e^{\phi}[1-erf(\sqrt{\phi})]+\frac{2}{\sqrt{\pi}}\sqrt{\phi}-1 \tag{18}$$

is positive and monotonically increasing (see Fig. 3).

Theorem 3: Let ϕ be a solution of

$$(r\phi)''=r\left[e^{\phi}\{1-erf(\sqrt{\phi})\}+\frac{2}{\sqrt{\pi}}\sqrt{\phi}-1\right]-rq\delta(\mathbf{r}). \tag{19}$$

Then, ϕ decreases more rapidly than $1/r$, $\forall r$.

Proof: The proof is similar to that for Theorem 1.

Let $\phi>0$, $\forall r$. Upon integrating Eq. (17) once over $0<r_1\leqslant r\leqslant r_2<\infty$, we obtain

$$(r\phi)_2'-(r\phi)_1'=\int_{r_1}^{r_2}\left[e^{\phi}\{1-erf(\sqrt{\phi})\}+\frac{2}{\sqrt{\pi}}\sqrt{\phi}-1\right]dr. \tag{20}$$

If we now suppose that $(r\phi)$ does not decrease monotonically with r, then $(r\phi)$ must have a minimum for $r=r_1^*<\infty$. However, since

$$e^{\phi}[1-erf(\sqrt{\phi})]+\frac{2}{\sqrt{\pi}}\sqrt{\phi}-1\approx\phi,\quad \phi\ll 1$$

we have from Eq. (17) that

$$\phi_{\text{lin}}\sim\frac{q}{r}e^{-r},\quad r\gg 1 \tag{21}$$

showing that ϕ eventually decreases more rapidly than $1/r$. Therefore, $(r\phi)$ must have a maximum for $r=r_2^*$ with $r_1^*<r_2^*<\infty$.

Taking $r_1=r_1^*$ and $r_2=r_2^*$ Eq. (19) then gives

$$0=\int_{r_1^*}^{r_2^*}r\left[e^{\phi}\{1-erf(\sqrt{\phi})\}+\frac{2}{\sqrt{\pi}}\sqrt{\phi}-1\right]dr$$

which, from Lemma 2, is impossible.

Therefore, $(r\phi)$ must decrease monotonically, $\forall r$.

Now, in view of Eq. (20), the dielectric screening by untrapped electrons resembles, in the far field ($r\gg 1$), a linearized screening. However, the exact screening of the test charge by the untrapped electrons turns out to be stronger than linearized screening, as deduced below.

Lemma 3: The function

$$G(\phi)=e^{\phi}[1-erf(\sqrt{\phi})]+\frac{2}{\sqrt{\pi}}\sqrt{\phi}-1-\phi \tag{22}$$

is negative and monotonically decreasing (see Fig. 4).

Theorem 4: Let ϕ be a solution of

$$(r\phi)''=r\left[e^{\phi}\{1-erf(\sqrt{\phi})\}+\frac{2}{\sqrt{\pi}}\sqrt{\phi}-1\right]-rq\delta(\mathbf{r}). \tag{19}$$

Then, ϕ is bounded from above, $\forall r$, by the linearized solution

$$\phi_{\text{lin}}=\frac{q}{r}e^{-r}. \tag{6}$$

Proof: The exact solution of Eq. (17) can be written formally as

$$(r\phi)=\int_r^{\infty}(r'-r)r'\left[\phi(r')+\left\{e^{\phi(r')}[1-erf(\sqrt{\phi(r')})]+\frac{2}{\sqrt{\pi}}\sqrt{\phi(r')}-1-\phi(r')\right\}-q\delta(\mathbf{r}')\right]dr' \tag{23}$$

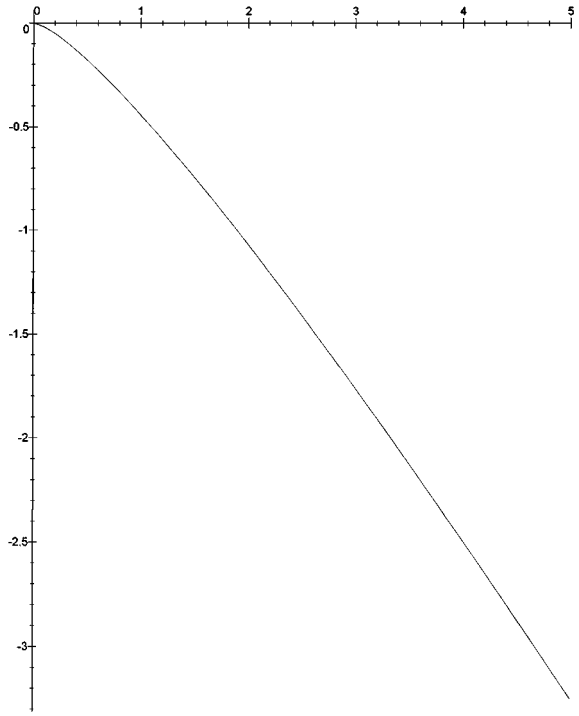

FIG. 4. $G(\phi)$ vs ϕ.

from which

$$(r\phi)=q\ e^{-r}+\int_r^{\infty}(r'-r)r'\left\{e^{\phi(r')}[1-erf(\sqrt{\phi(r')})]+\frac{2}{\sqrt{\pi}}\sqrt{\phi(r')}-1-\phi(r')\right\}dr'. \tag{24}$$

Using Lemma 3, Eq. (24) then implies that

$$(r\phi)\leqslant q\ e^{-r},\ \ \forall r.$$

$Q.E.D.$

According to Theorem 4, the exact screening of the test change is stronger than linearized screening for the untrapped electrons.

IV. SCREENING BY TRAPPED ELECTRONS

Nondimensionalizing according to Eq. (10), and using Eqs. (2) and (9), Eq. (1) gives for the trapped-electron screening,

$$(r\phi)''=r\left[e^{\phi}erf(\sqrt{\phi})-\frac{2}{\sqrt{\pi}}\sqrt{\phi}\right]-rq\,\delta(\mathbf{r}). \tag{25}$$

The solution of Eq. (2) decreases again more rapidly than the shieldless decay law $1/r$, $\forall r$, as deduced below.

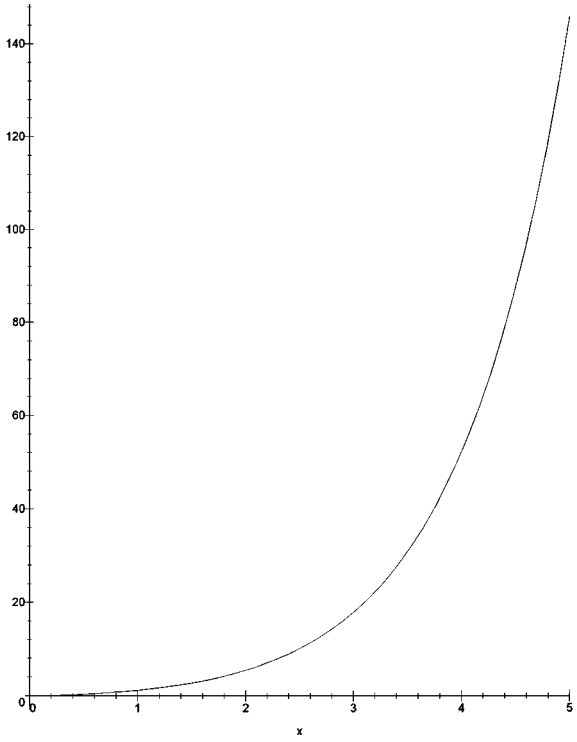

FIG. 5. $H(\phi)$ vs ϕ.

Lemma 4: The function

$$H(\phi)=e^{\phi}erf(\sqrt{\phi})-\frac{2}{\sqrt{\pi}}\sqrt{\phi} \tag{26}$$

is positive and monotonically increasing (see Fig. 5).

Theorem 5: Let ϕ be a solution of

$$(r\phi)''=r\left[e^{\phi}erf(\sqrt{\phi})-\frac{2}{\sqrt{\pi}}\sqrt{\phi}\right]-rq\delta(\mathbf{r}). \tag{25}$$

Then, ϕ decreases more rapidly than $1/r$, $\forall r$.

Proof: The proof is entirely similar to that of Theorem 3 and uses Lemma 4. Q.E.D.

Now, since

$$e^{\phi}erf(\sqrt{\phi})-\frac{2}{\sqrt{\pi}}\sqrt{\phi}\approx\frac{2}{\sqrt{\pi}}\phi^{3/2},\quad \phi\ll 1 \tag{27}$$

observe that the dielectric screening by trapped electrons does not resemble, in the far field, a linearized screening. However, on using Eq. (27), Eq. (25) becomes

$$(r\phi)''\approx\frac{2}{\sqrt{\pi}}r\phi^{3/2}-rq\delta(\mathbf{r}) \tag{28}$$

so that the classical trapped-electron dielectric screening process approaches, in the far field ($r \gg 1$), the semiclassical Thomas–Fermi screening (Ashcroft and Mermin[4]) regime!

V. DISCUSSION

In this paper, we have given some rigorous results about the properties of the solution of Poisson's equation describing dielectric screening by electrons trapped and/or untrapped in the Coulomb field of the test charge. For the full (untrapped) electrons, the exact screening of the test charge is shown to be weaker (stronger) than linearized screening; this is due to the fact that the linearized screening overestimates (underestimates) the screening of the test charge for the full (untrapped) electrons.

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Global cocycle dynamics for infinite mean field quantum systems interacting with the boson gas

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In the framework of operator algebraic quantum statistical mechanics, the global nonequilibrium dynamics for a general class of interactions of infinite mean field quantum lattice systems with the boson field is investigated. The associated interaction operators consist of arbitrary powers of the collective density operators of the mean field system and are linear with respect to the bosonic field operators. Instead of the usual perturbation expansions, here the interacting dynamics are studied by means of cocycle techniques. The cocycle methods are more appropriate to the considered class of interactions, and lead to explicit closed expressions for the dynamical automorphism groups. The cocycle equations connect the classical, collective dynamical behavior of the mean field system with the one-boson dynamics. In physical applications such systems are due to collectively ordered finite-level atoms or the Josephson junction in the thermodynamic limit weakly interacting with the electromagnetic field. © *1996 American Institute of Physics.* [S0022-2488-(96)00801-4]

I. INTRODUCTION

There is a great variety of papers where (starting from a microscopic quantum description) many aspects of the usual phenomenological descriptions of the Josephson effect and Josephson oscillator are obtained in the thermodynamic limit. The limit is performed as the particle number N becomes infinite with fixed particle density. The commonly accepted interpretation of the Josephson effect is in terms of a nondissipative process between two weakly linked superconductors, where the weakness of the interaction is expressed by the factor N^{-1} for each superconductor.

The same weak link also is taken for the Josephson oscillator; here, in addition, the two superconductors are coupled to the quantized electromagnetic field.[1]

In quantum optics such a weak coupling has been used for the Dicke model in the thermodynamic limit $N\to\infty$ (here N means the number of two-level atoms; the coupling strength also is rescaled by N^{-1}).[2–4]

In many theoretical treatments of the BCS model and the Josephson effect the thermodynamic limit has been performed within the formalism of infinite mean field quantum lattice systems. However, the Josephson oscillator model in Ref. 1, as well as the infinite atom Dicke model in Refs. 2 and 5, are not calculated within the mean field setup.

For the coupling of the photon field to some kind of (postulated) finite-dimensional classical material system in Refs. 2 and 5, Davies used cocycle techniques to obtain an explicit closed form for the unitary time evolution group in some specific Hilbert space representation. The results of Refs. 2 and 5 are used in Ref. 1.

Here we generalize the above ''limiting'' weak couplings and investigate the nonequilibrium dynamics for a general class of interactions of infinite mean field quantum lattice systems with the boson field. Inspired by the methods of Davies, we develop cocycle techniques for the description of the interacting systems. The cocycle equations connect the classical, collective dynamical behavior of the mean field system with the one-boson dynamics. Each solution of the cocycle equations leads to a different interaction. And thus, the whole of all solutions gives our treated class of interactions, which correspond to coupling operators of the form

$$P=\sum_{k=1}^{l}\left[D_k\otimes a_b^*(\phi_k)+D_k^*\otimes a_b(\phi_k)\right]. \tag{1.1}$$

Here the mean field part of P consists of arbitrary powers D_k of the collective density operators, i.e., the D_k are arbitrary classical observables of the mean field system. And the $a_b^{\#}(\phi_k)$ denote the bosonic annihilation, resp., creation operators smeared with the one-boson ''test functions'' ϕ_k. The ϕ_k express the coupling constants between the mean field system (e.g., an atomic system, or some superconductors) and the modes of the boson system (e.g., the electromagnetic field). In suitable subrepresentations the interacting cocycle dynamics are approximated by local (finite volume) expressions in the thermodynamic limit (see Theorem 4.10 below). Indeed, the above-mentioned weak couplings for the Josephson oscillator and the Dicke model lead in the thermodynamic limit to a special form of (1.1) for the interaction operators.

In contrast to the Hilbert space ansatz in Refs. 1, 2, and 5, here we use the general operator algebraic approach. We use the concept of global dynamical descriptions, where the dynamics in the Schrödinger picture is given by a group of affine bijections on some suitable convex subset (folium)—the physical states—of the state space of the associated C^*-algebra so that the expectation values are time continuous (cf. Definition 1.2 below). This dynamical concept is more general than those of C^*- and W^*-dynamical systems. Below it is presented in detail. Even for the free time evolutions of the infinite mean field, as well as of the boson system, it is necessary to work with the global dynamical concept, if one wants to cover a great variety of states, which show some continuity concerning their time evolutions.

Recently, great progress has been made concerning the rigorous formulation of the general, i.e. nonequilibrium dynamics of infinite quantum lattice systems with mean field interactions.[6–9] Due to the extremely long range of the interaction, the mean field limiting dynamics is not given as an automorphism group on the original quasilocal C^*-algebra,[10] but with the general global dynamical concept on the folium generated by the perturbation invariant states. The collective (classical) observables are the continuous functions on a classical phase space, the dynamics of which is given by a classical phase flow, which is generated by a Hamiltonian function Q and which is the restriction of the above limiting mean field dynamics.

The (quasi-)free boson dynamics is defined in terms of Bogoliubov transformations on (an enlargement of) the associated bosonic Weyl algebra (CCR algebra). It is well known that here one does not have a C^*-dynamical system. A global dynamical description with time continuity of the expectation values is not obtained for all states, but on the folium of states, which are chosen to be continuous with respect to some topology τ on the one-boson test function space.

Because here we cover such a great variety of states (i.e., very large folia, resp. representations) for both systems, the infinite mean field systems and the boson gas, the free dynamics are not given as W^*-dynamical systems. But the perturbation expansions (Ref. 11, Sec. 5.4.1) (with the interaction operator as perturbation) need the W^*-time continuity for the free evolution group. Hence, it is not possible to introduce interactions by using the perturbation theory. The unboundedness of the considered interaction operators (1.1) would be a second problem for the convergence of the perturbational expansion series. The difficulties of introducing the above class of mean field–boson interactions we overcome by the cocycle techniques. The advantage of the cocycle methods is that one directly obtains an explicit closed form (and not only an expansion series, as in the perturbational case) for the coupled time evolution automorphisms. More exactly, with the cocycle techniques we first construct the class of dynamical groups of interacting automorphisms, and then, in a second step, we determine the associated interactions.

Using the cocycle dynamics of the present investigation in Ref. 12 for very general initial states of the total system, we consider the infinite time limit ($t\to\infty$) of the boson field. In the resulting bosonic time-asymptotic states one partially rediscovers the collective ordering of the infinite mean field quantum lattice system, which also reflects the influence of the interaction (1.1) to the bose gas (cf. also Refs. 13 and 14).

In Ref. 4 for the special case of the infinite Dicke model in a specific (covariant) GNS representation, the opposite way has also been carried through. There, by means of Trotter's product formula and perturbation techniques the explicit expressions for the unitary time evolutions are derived. The emitted radiation, i.e. the time-asymptotic photon states, turns out to be quantum optically coherent,[15] which follows from the influence of the collective atomic behavior.[3,16]

An application of the present investigation and the one of the time-asymptotic boson states[12] to the general weakly coupled Dicke model is found in Ref. 17, and an application to the Josephson microwave radiation in Ref. 18.

The preparatory section (II) is devoted to the considered class of infinite mean field models. In Sec. III we develop the global dynamical description of the free boson field. In the main part of the paper (Sec. IV) the global interacting cocycle dynamics is investigated.

We start our exposition with the global dynamical concept we are confrontated in the subsequent sections, at the free systems, the mean field lattice, resp. the boson gas, and at the interacting system.

A. The algebraic dynamical concept

Let $\mathscr{A}$ be an arbitrary C^*-algebra with state space $\mathscr{S}(\mathscr{A})$ describing a physical system. Denote by $\mathscr{M}^u \equiv \mathscr{M}^u(\mathscr{A})$ the universal enveloping W^*-algebra of $\mathscr{A}$ associated with the universal representation Π^u, and its center by $\mathscr{Z}^u$.[19,20] We do not distinguish between a state on $\mathscr{A}$ and its unique normal extension to $\mathscr{M}^u$.

The notion of a folium was introduced by Haag *et al.*[21] (cf. also Ref. 22). A folium $\mathscr{F}$ of $\mathscr{A}$ is a norm-closed, convex subset of $\mathscr{S}(\mathscr{A})$, which is invariant under "perturbations," in the sense that $\omega \in \mathscr{F}$ implies $\omega_B \in \mathscr{F}$ for all $B \in \mathscr{A}$ with $\langle \omega;\ B^*B\rangle \neq 0$, where ω_B is the state on $\mathscr{A}$ given by $\langle \omega_B; \cdot \rangle = \langle \omega; B^* \cdot B\rangle / \langle \omega; B^*B\rangle$.

Folia arise naturally as the set of Π-normal states of any representation Π of $\mathscr{A}$. More exactly, we have the following well-known results (see, e.g., Refs. 21 and 20).

Proposition 1.1: There is a one-to-one correspondence between the folia of $\mathscr{A}$, the quasiequivalence classes of representations, and the orthogonal projectors in the center $\mathscr{Z}^u$, which preserves the partial orderings, respectively. That is, if for $j \in \{1,2\}$ $\mathscr{F}_j$, Π_j, and $c_j \in \mathscr{Z}^u$ are in correspondence, then

$$\mathscr{F}_1 \subseteq \mathscr{F}_2 \subseteq \mathscr{S}(\mathscr{A}) \Leftrightarrow \Pi_1 \leqslant \Pi_2 \leqslant \Pi^u \Leftrightarrow c_1 \leqslant c_2 \leqslant \mathbb{1}^u.$$

Moreover, if $\mathscr{F}$, $\Pi_{\mathscr{F}}$, and $c_{\mathscr{F}}$ are in correspondence one has $\mathscr{M}_{\mathscr{F}} := \Pi_{\mathscr{F}}(\mathscr{A})'' = c_{\mathscr{F}}\mathscr{M}^u$, $\mathscr{Z}_{\mathscr{F}} := \mathscr{M}_{\mathscr{F}} \cap \mathscr{M}'_{\mathscr{F}} = c_{\mathscr{F}}\mathscr{Z}^u$, $\mathscr{F}$ are just the $\Pi_{\mathscr{F}}$-normal states, that is, $\mathscr{M}_{\mathscr{F}} = LH(\mathscr{F})^*$. $\Pi_{\mathscr{F}}$ extends to a normal representation $\tilde{\Pi}_{\mathscr{F}}$ of $\mathscr{M}^u$ with $\tilde{\Pi}_{\mathscr{F}}(\mathscr{M}^u) = \mathscr{M}_{\mathscr{F}}$, $\tilde{\Pi}_{\mathscr{F}}(\mathscr{Z}^u) = \mathscr{Z}_{\mathscr{F}}$.

A folium $\mathscr{F}$ expresses classical, macroscopic aspects of the physical system, which one also may refind in the center $\mathscr{Z}_{\mathscr{F}}$ of the associated W^*-algebra $\mathscr{M}_{\mathscr{F}}$. Thus, dealing with a subfolium of $\mathscr{F}$ instead of $\mathscr{F}$ itself, means a restriction of the considered collective, macroscopic aspects of the physical system. Disjoint folia give macroscopically totally different aspects and define two superselection sectors, which is also demonstrated by the orthogonality of the associated central projectors.

In the Schrödinger picture Roos[24] introduced the following dynamical description on the folium $\mathscr{F}$ of $\mathscr{A}$.

Definition 1.2: Let $\nu \equiv \{\nu_t | t \in \mathbb{R}\}$ be a one-parameter group of affine maps $\nu_t : \mathscr{F} \to \mathscr{F}$, that is, ν_0 is the identity and $\nu_s \circ \nu_t = \nu_{s+t}$, $\forall s,t \in \mathbb{R}$, which obeys the continuity conditions

$$\lim_{t \to 0} \langle \nu_t(\omega); A\rangle = \langle \omega; A\rangle, \quad \forall \omega \in \mathscr{F}, \quad \forall A \in \mathscr{A}. \tag{1.2}$$

Then the triple $(\mathscr{A}, \mathscr{F}, \nu)$ is denoted a dynamical description of our physical system.

Obviously, the group property yields each ν_t to be an affine bijection on $\mathscr{F}$. By duality, for each $t\in\mathbb{R}$ there exists a unique Jordan automorphism τ_t on $\mathscr{M}_{\mathscr{F}}$ (Ref. 25, Theorem 3.2.8), such that

$$\langle \nu_t(\omega);A\rangle=\langle \omega;\tau_t(A)\rangle,\quad \forall\,\omega\in\mathscr{F},\quad \forall A\in\mathscr{M}_{\mathscr{F}}. \tag{1.3}$$

Since in applications the dynamics is motivated by Hamiltonians, in the sequel we always assume τ_t to be an automorphism (cf., e.g., Ref. 26 and Subsection 2.3, where ν_t is approximated by finite Hamiltonian dynamics). The group $\tau\equiv\{\tau_t|t\in\mathbb{R}\}$ describes the dynamics in the Heisenberg picture on the W^*-algebra $\mathscr{M}_{\mathscr{F}}$, which is denoted by $(\mathscr{M}_{\mathscr{F}},\tau)$.

Roos's dynamical concept is a generalization of Kadison's classical definition of a dynamical system;[23] the difference is that here the weak* continuity of $\omega\in\mathscr{F}\mapsto\nu_t(\omega)$ on $\mathscr{A}$, t fixed, is dropped. This weak* continuity property is equivalent to $\tau_t(\mathscr{A})\subseteq\mathscr{A}$, and its failure plays a crucial role for the mechanisms of symmetry breaking.[10]

Because of the restricted continuity in time (1.2), in general $(\mathscr{M}_{\mathscr{F}},\tau)$ does not define a W^*-dynamical system (e.g. Ref. 11, Definition 2.7.1). However, $(\mathscr{M}_{\mathscr{F}},\tau)$ is a W^*-dynamical system, if (1.2) is also valid for each $A\in\mathscr{M}_{\mathscr{F}}$, that is, $t\mapsto\nu_t(\omega)$ is $\sigma(\mathscr{M}_{\mathscr{F}*},\mathscr{M}_{\mathscr{F}})$ continuous for every $\omega\in\mathscr{F}$, which by Ref. 25, Corollary 3.1.8 is equivalent to the norm continuity of $t\mapsto\nu_t(\omega)$. Then, by duality, $t\mapsto\tau_t(A)$ is $\sigma(\mathscr{M}_{\mathscr{F}},\mathscr{M}_{\mathscr{F}*})$ continuous for all $A\in\mathscr{M}_{\mathscr{F}}$.

The C^*-dynamical system $(\mathscr{A},\tau)$ is obtained (e.g., Ref. 11, Definition 2.7.1), if the folium $\mathscr{F}$ is the whole state space $\mathscr{S}(\mathscr{A})$: By duality arguments, each τ_t leaves $\mathscr{A}$ invariant and the $\sigma(\mathscr{A}^*,\mathscr{A})$ continuity of $t\mapsto\nu_t(\omega)$, $\forall\omega\in\mathscr{S}(\mathscr{A})$ from (1.2) is equivalent to the $\sigma(\mathscr{A},\mathscr{A}^*)$ continuity of $t\mapsto\tau_t(A)$, $\forall A\in\mathscr{A}$, which by Ref. 25, Corollary 3.1.8 leads to $\lim_{t\to0}\|\tau_t(A)-A\|=0$ for each $A\in\mathscr{A}$.

Definition 1.3: If $\mathscr{F}'\subseteq\mathscr{F}$ is a ν-invariant subfolium, that is $\nu_t(\mathscr{F}')\subseteq\mathscr{F}'$, $\forall t\in\mathbb{R}$, then $(\mathscr{A},\mathscr{F}',\nu)$ is called a dynamical subdescription of $(\mathscr{A},\mathscr{F},\nu)$.

If one has the continuity condition, $\lim_{t\to0}\|\nu_t(\omega)-\omega\|=0$, $\forall\omega\in\mathscr{F}'$, which is stronger than (1.2), then the dynamical (sub-)description $(\mathscr{A},\mathscr{F}',\nu)$ is called covariant.

$(\mathscr{A},\mathscr{F}',\nu)$ to be a dynamical subdescription is equivalent to $\tau_t(c_{\mathscr{F}'})=c_{\mathscr{F}'}$, $\forall t\in\mathbb{R}$ for the central projector $c_{\mathscr{F}'}\in\mathscr{Z}_{\mathscr{F}}$ associated with the subfolium $\mathscr{F}'$, $\mathscr{M}_{\mathscr{F}'}=c_{\mathscr{F}'}\mathscr{M}_{\mathscr{F}}$, of the above proposition. The associated dynamics in the Heisenberg picture $(\mathscr{M}_{\mathscr{F}'},\tau)$ is obtained by restricting τ from $\mathscr{M}_{\mathscr{F}}$ to $\mathscr{M}_{\mathscr{F}'}=c_{\mathscr{F}'}\mathscr{M}_{\mathscr{F}}$ with the central projection $c_{\mathscr{F}'}$.

Consequently, if one wants to consider a very great variety of collective, macroscopic observables of the physical system (in the center $\mathscr{Z}_{\mathscr{F}}$), which may evolve in time, it is necessary to work with a dynamical description $(\mathscr{A},\mathscr{F},\nu)$ with some folium $\mathscr{F}$, which is chosen as large as possible.

The covariance of $(\mathscr{A},\mathscr{F}',\nu)$ is equivalent for $(\mathscr{M}_{\mathscr{F}'},\tau)$ to constitute a W^*-dynamical system. In a standard representation of $\mathscr{M}_{\mathscr{F}'}$ on the standard Hilbert space $\mathscr{H}^{\rm std}_{\mathscr{F}'}$[27] then one gets a strongly continuous unitary group $e^{it\mathrm{H}}$, $t\in\mathbb{R}$, on $\mathscr{H}^{\rm std}_{\mathscr{F}'}$, which implements the Heisenberg dynamics τ: $\tau_t(M)=e^{it\mathrm{H}}Me^{-it\mathrm{H}}$, $\forall M\in\mathscr{M}_{\mathscr{F}'}$, $\forall t\in\mathbb{R}$. However, in general, $e^{it\mathrm{H}}\notin\mathscr{M}_{\mathscr{F}'}$, that is, the renormalized Hamiltonian H is not affiliated with $\mathscr{M}_{\mathscr{F}'}$. These results are proven with the general modular formalism.[28,20,29,30]

Selecting in our dynamical description $(\mathscr{A},\mathscr{F},\nu)$ those $\omega\in\mathscr{F}$, which fulfill the norm continuity $\lim_{t\to0}\|\nu_t(\omega)-\omega\|=0$, leads to a subfolium $\mathscr{F}_{\rm cov}\subseteq\mathscr{F}$ invariant with respect to the Schrödinger dynamics ν. Hence $(\mathscr{A},\mathscr{F}_{\rm cov},\nu)$ gives the largest covariant dynamical subdescription of $(\mathscr{A},\mathscr{F},\nu)$, an idea that goes back to Ref. 31 (cf. also Refs. 8 and 32).

If $\omega\in\mathscr{F}$ is a ν-invariant state, then, $\nu_t(\mathscr{F}_\omega)=\mathscr{F}_\omega$, $\forall t\in\mathbb{R}$, where $\mathscr{F}_\omega$ is the subfolium of $\mathscr{F}$ generated by ω (the smallest folium containing ω), and $(\mathscr{A},\mathscr{F}_\omega,\nu)$ is a dynamical subdescription. Because of the uniqueness of the GNS representation $(\Pi_\omega,\mathscr{H}_\omega,\Omega_\omega)$ of ω up to unitary equivalence, there exist unitary operators U_t^ω on $\mathscr{H}_\omega$ with $\tau_t(M)=U_t^\omega MU_t^\omega$, $\forall M\in\mathscr{M}_{\mathscr{F}_\omega}\equiv\mathscr{M}_\omega$, and $U_t^\omega\Omega_\omega=\Omega_\omega$ for each $t\in\mathbb{R}$. By (1.2) one easily checks the strong continuity of $t\mapsto U_t^\omega$. Consequently, $\mathscr{F}_\omega\subseteq\mathscr{F}_{\rm cov}$, and thus $\mathscr{F}_\omega$ defines a covariant subdescription.

II. INFINITE MEAN FIELD QUANTUM LATTICE SYSTEMS

In this section, we give a short self-contained description of the theory of infinite mean field systems and their dynamics for the extent necessary for the present purposes. For more information and additional references, we refer the reader to the original works.[35,6,7,32,8] Our notation resembles the one in Ref. 8.

For the numbering of the spatial lattice we use the natural numbers $\mathbb{N}$. The set of finite subsets Λ of $\mathbb{N}$, $\mathcal{L}:=\{\Lambda\subset\mathbb{N}||\Lambda|<\infty\}$, where $|\Lambda|$ denotes the cardinality of Λ, is directed by inclusion. Quantities indexed by $\Lambda\in\mathcal{L}$ are usually called local. The limit of a net of local elements $(a_\Lambda)_{\Lambda\in\mathcal{L}}$ we denote by $\lim_{\Lambda\in\mathcal{L}} a_\Lambda$.

At each lattice point $n\in\mathbb{N}$ we have the same finite subsystem described by the $m\times m$ matrices $\mathbb{M}_m$ as algebra of observables. The observables for the finite lattice region $\Lambda\in\mathcal{L}$ are given by $\mathcal{A}(\Lambda):=\otimes_{n\in\Lambda}\mathbb{M}_m$, and for the total infinite system by the C^*-inductive limit $\mathcal{A}:=\otimes_{n\in\mathbb{N}}\mathbb{M}_m$.[33,34] The C^*-algebra $\mathcal{A}$ is simple, and thus any nontrivial representation of $\mathcal{A}$ is faithful. The local algebras $\mathcal{A}(\Lambda)$, $\Lambda\in\mathcal{L}$ are embedded into $\mathcal{A}$ by adjoining the unit $\mathbb{1}_m$ of $\mathbb{M}_m$ at the lattice points $n\notin\Lambda$.

A. Kinematical structure

Denote by $\mathcal{F}_a^p$ the folium of $\mathcal{A}$ generated by the permutation invariant states $\mathcal{S}^p(\mathcal{A})$ [smallest folium containing $\mathcal{S}^p(\mathcal{A})$], and let Π_a^p be the associated representation with corresponding von Neumann algebra $\mathcal{M}_a^p:=\Pi_a^p(\mathcal{A})''$ by Proposition 1.1. Then, for every $a\in\mathbb{M}_m$ the limit

$$m(a)=s-\lim_{\Lambda\in\mathcal{L}}\Pi_a^p(m_\Lambda(a))\in\mathcal{Z}_a^p,$$

of the local density operators,

$$m_\Lambda(a):=\frac{1}{|\Lambda|}\sum_{n\in\Lambda}\mathbb{1}_m\otimes\cdots\otimes\mathbb{1}_m\otimes\underbrace{a}_{n\text{th place}}\otimes\mathbb{1}_m\otimes\mathbb{1}_m\otimes\cdots\in\mathcal{A}(\Lambda),\quad\Lambda\in\mathcal{L},\tag{2.1}$$

exists in the strong operator topology and is an element of the center $\mathcal{Z}_a^p$ of $\mathcal{M}_a^p$. Let us denote by $\mathcal{N}_{\mathrm{cl}}$ the C^*-subalgebra of the center $\mathcal{Z}_a^p$, which is generated by the set $\{m(a)|a\in\mathbb{M}_m\}$, respectively, by $\{m(a)|a\in\mathcal{G}\}$, where

$$\mathcal{G}:=\{a\in\mathbb{M}_m|a=a^*,\ \mathrm{tr}[a]=0\},$$

the Lie algebra corresponding to the Lie group $SU(m)$.

$\mathcal{N}_{\mathrm{cl}}$ is a commutative C^*-algebra, which we want to identify with the C^*-algebra $C(P)$ of continuous functions on the state space $P\equiv\mathcal{S}(\mathbb{M}_m)$ of $\mathbb{M}_m$. We also regard P as a compact, convex subset of the vector space dual $\mathcal{G}^*$ of the Lie algebra $\mathcal{G}$, which is a real vector space of dimension m^2-1. The duality relation $\langle x;a\rangle$ for $x\in\mathcal{G}^*$ and $a\in\mathcal{G}\subset\mathbb{M}_m$ is a restriction of the duality relation on $\mathbb{M}_m$.

$a\in\mathcal{G}\mapsto\exp\{im(a)\}\in\mathcal{Z}_a^p$ is a unitary representation of the additive group $\mathcal{G}$. Thus, by the SNAG theorem there exists a unique projection-valued measure $\mathcal{P}$ from the Borel subsets of $\mathcal{G}^*$ into the set of orthogonal projections of the center $\mathcal{Z}_a^p$ such that $m(a)=\int_{\mathcal{G}^*}\langle x;a\rangle d\mathcal{P}(x)$ for each $a\in\mathcal{G}$, respectively, for each $a\in\mathbb{M}_m$. It follows that P is just the support of $\mathcal{P}$. Now the spectral calculus defines the desired isomorphism,

$$\hat{\mathcal{P}}:C(P)\to\mathcal{N}_{\mathrm{cl}},\quad\xi\mapsto\int_P\xi(x)d\mathcal{P}(x).$$

$\mathcal{N}_{\mathrm{cl}} \cong C(P)$ is interpreted as the C^*-algebra of classical observables for the infinite mean field system. Let us define the enlargement $\mathcal{A}_e := \mathcal{A} \otimes C(P)$ of the original C^*-algebra $\mathcal{A}$ with the associated classical $C(P)$. $\mathcal{A}_e$ is isomorphic to the C^*-algebra $C(P, \mathcal{A})$ of continuous $\mathcal{A}$-valued functions on P.

The representation Π_a^p of $\mathcal{A}$ extends to a representation of $\mathcal{A}_e$ by defining $\Pi_a^p(X \otimes \xi) = \Pi_a^p(X)\hat{\mathcal{P}}(\xi) \in \mathcal{M}_a^p$ for $X \in \mathcal{A}$ and $\xi \in C(P)$. That is, $\Pi_a^p(\mathcal{A}_e)$ is just the C^*-subalgebra of $\mathcal{M}_a^p$, which is generated by $\Pi_a^p(\mathcal{A})$ and $\mathcal{N}_{\mathrm{cl}}$. Since the folium $\mathcal{F}_a^p$ of $\mathcal{A}$ agrees with the normal states on $\mathcal{M}_a^p$, it follows that $\mathcal{F}_a^p$ is just the folium of $\mathcal{A}_e$ associated with the representation Π_a^p of $\mathcal{A}_e$ (cf. Proposition 1.1).

B. The classical phase space

The state space of $C(P)$ is the convex set $M_+^1(P)$ of (positive) probability measures on P. Thus, the restriction $\omega|_{\mathcal{N}_{\mathrm{cl}}}$ of $\omega \in \mathcal{S}^p(\mathcal{A})$ from $\mathcal{M}_a^p$ to $\mathcal{N}_{\mathrm{cl}}$ gives the probability measure $\omega|_{\mathcal{N}_{\mathrm{cl}}} \circ \hat{\mathcal{P}}^{-1} =: \mu_\omega$ on P, which implies the affine bijection $\omega \mapsto \mu_\omega$ from $\mathcal{S}^p(\mathcal{A})$ onto $M_+^1(P)$. The point measure at $x \in P$ gives the product state $\omega_x = \otimes_{n \in \mathbb{N}} x$ on $\mathcal{A}$. Consequently, the permutation invariant states $\mathcal{S}^p(\mathcal{A})$ of $\mathcal{A}$ form a Bauer simplex with the extreme boundary $\partial_e \mathcal{S}^p(\mathcal{A}) = \{\omega_x | x \in P\}$. The probability measure $\mu_\omega \in M_+^1(P)$ gives the central decomposition of $\omega \in \mathcal{S}^p(\mathcal{A})$, $\omega = \int_P \omega_x \, d\mu_\omega(x)$.[36,8]

P is the classical phase space of the considered mean field system. The tangent space at each point $x \in P$ of the manifold P is just the dual $\mathcal{G}^*$, and the cotangent space is $\mathcal{G}^{**}$, which is canonically identified with $\mathcal{G}$. With the Lie product on $\mathcal{G}$ (i times the commutator $[\cdot, \cdot]$) the Poisson bracket $\{\xi, \eta\}$ of two differentiable, real-valued functions ξ, η on the manifold P is introduced by

$$\{\xi, \eta\}(x) := i\langle x; [d\xi_x, d\eta_x] \rangle, \quad \forall x \in P, \tag{2.2}$$

which uses the differentials $d\xi_x \in \mathcal{G}$ and $d\eta_x \in \mathcal{G}$ at $x \in P$. However, (2.2) is not quite a Poisson bracket in the sense of the theory of classical Hamiltonian mechanics (e.g., Ref. 37), since the underlying symplectic form is degenerate (for more details see Refs. 7, 32, and 38).

C. The limiting dynamics

With a fixed orthonormal base $\{a^1, \ldots, a^{m^2-1}\}$ of $\mathcal{G}$ (with respect to the Hilbert–Schmidt scalar product), $\mathcal{G}^*$ is parametrized, and thus $\mathcal{G}^* \cong \mathbb{R}^{m^2-1}$.

The dynamics is given with an arbitrary real-valued polynomial Q on $\mathbb{R}^{m^2-1} \cong \mathcal{G}^*$ in terms of the local Hamiltonians,

$$A_\Lambda := |\Lambda| Q(m_\Lambda(a^1), \ldots, m_\Lambda(a^{m^2-1})), \quad \forall \Lambda \in \mathcal{L}, \tag{2.3}$$

which define the local time evolutions,

$$\alpha_t^{Q,\Lambda}(\cdot) = \exp\{itA_\Lambda\} \cdot \exp\{-itA_\Lambda\}, \quad t \in \mathbb{R}, \quad \Lambda \in \mathcal{L}. \tag{2.4}$$

New developments[9] generalize to arbitrary $\mathcal{C}^\infty$-functions Q.

1. The Schrödinger picture

For each $t \in \mathbb{R}$ there exists an affine bijection ν_t^Q on the folium $\mathcal{F}_a^p$ such that

$$\langle \nu_t^Q(\omega); X \rangle = \lim_{\Lambda \in \mathcal{L}} \langle \omega; \Pi_a^p(\alpha_t^{Q,\Lambda}(X)) \rangle, \quad \forall X \in \mathcal{A}, \quad \forall \omega \in \mathcal{F}_a^p.$$

The group $\nu^Q \equiv \{\nu_t^Q | t \in \mathbb{R}\}$ induces the dynamical descriptions $(\mathcal{A}, \mathcal{F}_a^p, \nu^Q)$ and $(\mathcal{A}_e, \mathcal{F}_a^p, \nu^Q)$ in the sense of Definition 1.2.

2. The Heisenberg picture

By the duality (1.3) we get the dynamics $(\mathscr{M}_a^p, \alpha^Q)$ in the Heisenberg picture. The group $\alpha^Q \equiv \{\alpha_t^Q | t \in \mathbb{R}\}$ of automorphisms on $\mathscr{M}_a^p$ leaves the represented algebra $\Pi_a^p(\mathscr{A})$ invariant, if and only if Q is linear. But α^Q leaves the C^*-algebra $\Pi_a^p(\mathscr{A}_e) \subset \mathscr{M}_a^p$ invariant, and lifts to the C^*-dynamical system $(\mathscr{A}_e, \alpha^Q)$ (since the representation Π_a^p of $\mathscr{A}_e$ is faithful). We also regard $(\mathscr{A}_e, \alpha^Q)$ as the dynamics in the Heisenberg picture.

D. The classical (sub-)dynamics

1. The classical Hamiltonian phase flow

With the Poisson bracket (2.2) and the polynomial Q as a Hamiltonian function it is introduced the Hamiltonian vector field $\lambda_Q : P \mapsto \mathscr{G}^*$ in the standard way, $\langle \lambda_Q(x); a \rangle := \{Q,a\}(x), \forall a \in \mathscr{G}$ for $x \in P$ (here $a \in \mathscr{G} = \mathscr{G}^{**}$ is considered as a mapping on P). The associated classical Hamiltonian phase flow $\varphi^Q \equiv \{\varphi_t^Q | t \in \mathbb{R}\}$ on the classical phase space P then is obtained from the differential equation $(d/dt)\varphi_t^Q(x) = \lambda_Q(\varphi_t^Q(x)), \forall x \in P$.

2. The Schrödinger picture

The group ν^Q leaves $\partial_e \mathscr{S}^p(\mathscr{A})$ and $\mathscr{S}^p(\mathscr{A})$ invariant. More exactly, it is $\nu_t^Q(\omega_x) = \omega_{\varphi_t^Q(x)}, \forall x \in P$ with the above phase flow φ^Q. The time evolution $\nu_t^Q(\omega)$ for $\omega \in \mathscr{S}^p(\mathscr{A})$ then is given by $\mu_\omega \circ \varphi_{-t}^Q =: (\varphi_t^Q)^{**}(\mu_\omega)$ with the associated measure $\mu_\omega \in M_+^1(P)$. This implies $(\mathscr{N}_{\mathrm{cl}}, \mathscr{S}^p(\mathscr{A}), \nu^Q) \cong (C(P), M_+^1(P), (\varphi^Q)^{**})$ to be the dynamical description of the classical part of the mean field system in the Schrödinger picture.

Thus we have $\|\nu_t^Q(\omega_x) - \omega_x\| = \|\omega_{\varphi_t^Q(x)} - \omega_x\| = 2$ for small t for some $x \in P$, whenever Q is not constant (since $\|\omega_x - \omega_y\| = 2$ for $x \neq y$), which demonstrates that the dynamical description $(\mathscr{A}, \mathscr{F}_a^p, \nu^Q)$ is not covariant (cf. Definition 1.3).

3. The Heisenberg picture

Let us turn to the classical dynamics in the Heisenberg picture. It is $\alpha_t^Q(\mathscr{N}_{\mathrm{cl}}) = \mathscr{N}_{\mathrm{cl}} \forall t \in \mathbb{R}$, and via the isomorphism $\hat{\mathscr{P}}$ the restriction is given by $\alpha_t^Q|_{\mathscr{N}_{\mathrm{cl}}} = \hat{\mathscr{P}} \circ (\varphi_t^Q)^* \circ \hat{\mathscr{P}}^{-1}$, where $(\varphi_t^Q)^*(\xi) := \xi \circ \varphi_t^Q$ for $\xi \in C(P)$. Thus the C^*-dynamical system $(\mathscr{N}_{\mathrm{cl}}, \alpha^Q)$ is isomorphic to $(C(P), (\varphi^Q)^*)$, the well-known classical dynamics of the observables.

III. THE BOSON FIELD

The one-boson test function space (E, σ) is a real vector space E equipped with the symplectic form σ [i.e., $\sigma : E \times E \to \mathbb{R}$ is bilinear with $\sigma(f,g) = -\sigma(g,f), \forall f,g \in E$], which may be degenerate.

A. The C^*-Weyl algebra of the boson field

The C^*-algebra for the boson system is set up as the Weyl algebra $\mathscr{W}(E,\sigma)$ over (E,σ), which is constructed from unitary elements $W(f), f \in E$—the Weyl operators—satisfying for all $f,g \in E$,

$$W(f)W(g) = \exp\left\{-\frac{i}{2}\sigma(f,g)\right\} W(f+g), \quad W(f)^* = W(-f), \tag{3.1}$$

and by means of the minimal regular norm.[39,11,40,13] $\mathscr{W}(E,\sigma)$ is simple, if and only if σ is nondegenerate [i.e., $\sigma(f,g) = 0, \forall g \in E$ implies $f = 0$]. For the subspace $D \subseteq E$ the C^*-subalgebra of $\mathscr{W}(E,\sigma)$ generated by $\{W(f) | f \in D\}$ just agrees with the Weyl algebra $\mathscr{W}(D,\sigma)$. It holds $\mathscr{W}(D,\sigma) = \mathscr{W}(E,\sigma)$, if and only if $D = E$.

A linear mapping $b:E\to E$ is denoted a symplectic transformation on (E,σ), if b is bijective and satisfies $\sigma(bf,bg)=\sigma(f,g),\forall f,g\in E$. For each symplectic b on (E,σ) there exists a unique automorphism β_b on $\mathscr{W}(E,\sigma)$ with $\beta_b(W(f))=W(bf),\forall f\in E$, which is called the associated Bogoliubov transformation.

A representation Π of $\mathscr{W}(E,\sigma)$ is called regular, if for each $f\in E$ the unitary group $t\in\mathbb{R}\mapsto\Pi(W(tf))$ is strongly continuous. Their generators $\Phi_\Pi(f),f\in E$, are the so-called field operators, $\Pi(W(tf))=\exp\{it\Phi_\Pi(f)\},\forall t\in\mathbb{R}$. Obviously, $f\in E\mapsto\Phi_\Pi(f)$ is linear, and on suitable dense domains they fulfill the canonical commutation relations $\Phi_\Pi(f)\Phi_\Pi(g)-\Phi_\Pi(g)\Phi_\Pi(f)=i\sigma(f,g)\mathbb{1}_\Pi,\forall f,g\in E$.

The characteristic function of the state ω on $\mathscr{W}(E,\sigma)$ is defined to be the mapping $C_\omega:E\to\mathbb{C}$, $f\mapsto\langle\omega;W(f)\rangle=C_\omega(f)$. Let us characterize the state space of $\mathscr{W}(E,\sigma)$ by the characteristic functions. $\mathsf{C}(E,\sigma)$ is the convex set of functions $C:E\to\mathbb{C}$ with $C(0)=1$ and for which the map $(f,g)\mapsto\exp\{(i/2)\sigma(f,g)\}C(g-f)$ constitutes a positive-definite kernel $E\times E\to\mathbb{C}$.[41] From Eqs. (2.17) and (3.2) in Ref. 39 (cf. also Ref. 15) it follows the affinity and bijectivity of the map

$$\mathscr{S}(\mathscr{W}(E,\sigma))\to\mathsf{C}(E,\sigma),\quad \omega\mapsto C_\omega. \tag{3.2}$$

B. The folium of τ-continuous states

Definition 3.1: Denote by $\mathscr{T}(E,\sigma)$ the set of all topologies τ on E such that for each $f\in E$ the maps $g\in E\mapsto f+g\in E$ and $g\in E\mapsto\sigma(f,g)\in\mathbb{R}$ are continuous with respect to the τ topology.

Proposition 3.2: For each $\tau\in\mathscr{T}(E,\sigma)$ the set of τ-continuous states,

$$\mathscr{F}_b^\tau(E,\sigma):=\{\omega\in\mathscr{S}(\mathscr{W}(E,\sigma))|C_\omega\ \text{ is }\ \tau\ \text{ continuous}\},$$

is a folium on $\mathscr{W}(E,\sigma)$.

Proof: Let $\omega\in\mathscr{F}_b^\tau(E,\sigma)$. Obviously $\mathscr{F}_b^\tau(E,\sigma)$ is convex. Using an $\epsilon/3$ argument one easily checks that $\mathscr{F}_b^\tau(E,\sigma)$ is norm closed. For $\omega\in\mathscr{F}_b^\tau(E,\sigma)$ the map (use the Weyl relations)

$$f\in E\mapsto\langle\omega;W(g)W(f)W(h)\rangle=\exp\left\{-\frac{i}{2}(\sigma(g,f)+\sigma(g+f,h))\right\}\langle\omega;W(g+f+h)\rangle$$

is τ continuous, from which by an $\epsilon/3$ argument the continuity of $f\in E\mapsto\langle\omega;B^*W(f)B\rangle$ for each $B\in\mathscr{W}(E,\sigma)$ follows. ■

The natural ordering on $\mathscr{T}(E,\sigma)$ obviously carries over to the associated folia:

$$\tau_1\leqslant\tau_2\leqslant d\ \Rightarrow\ \mathscr{F}_b^{\tau_1}(E,\sigma)\subseteq\mathscr{F}_b^{\tau_2}(E,\sigma)\subseteq\mathscr{F}_b^{d}(E,\sigma)=\mathscr{S}(\mathscr{W}(E,\sigma)),$$

where $d\in\mathscr{T}(E,\sigma)$ means the discrete topology.

Proposition 3.3: Let $\tau\in\mathscr{T}(E,\sigma)$, then $f\in E\mapsto\Pi_b^\tau(W(f))=:W_b^\tau(f)$ is continuous with respect to the topology τ on E and the strong operator topology on $\mathscr{M}_b^\tau:=\Pi_b^\tau(\mathscr{W}(E,\sigma))''$, where Π_b^τ is the representation associated with $\mathscr{F}_b^\tau(E,\sigma)$.

Proof: Let $\omega\in\mathscr{F}_b^\tau(E,\sigma)$. For $f,g,h\in E$ by the Weyl relations one gets

$$\begin{aligned}&\|(\Pi_\omega(W(f))-\Pi_\omega(W(g)))\Pi_\omega(W(h))\Omega_\omega\|^2\\&\quad=\langle\omega;W(-h)(W(-f)-W(-g))(W(f)-W(g))W(h)\rangle\\&\quad=2-2\ \mathrm{Re}(\exp\{(i/2)\sigma(f,g)+i\sigma(h,g-f)\}\langle\omega;W(g-f)\rangle),\end{aligned}$$

from which by an $\epsilon/3$ argument it follows the continuity of $f\in E\mapsto\Pi_\omega(W(f))$. Now observe that $\Pi_b^\tau=\oplus_{\omega\in\mathscr{F}_b^\tau}\Pi_\omega$, and the assertion is proved. ■

We mention, because of Proposition 3.3 the representation Π_b^τ is regular, if $t\in\mathbb{R}\mapsto tf\in E$ is τ continuous for each $f\in E$. Thus, in the case of a vector space topology $\tau\in\mathcal{T}(E,\sigma)$ the field operators $\Phi_b^\tau(f),f\in E$, associated with Π_b^τ exist.

C. The (quasi-)free boson dynamics

The subsequent definition of a quasi-free dynamics generalizes an idea in Ref. 24.

The single particle dynamics is given by a group $v\equiv\{v_t|t\in\mathbb{R}\}$ of symplectic transformations v_t on a larger symplectic space $(\mathcal{E},\sigma)\supseteq(E,\sigma)$ (i.e., v_0 is the identity, and $v_s\circ v_t=v_{s+t},\forall s,t\in\mathbb{R}$). Unfortunately, in many physical cases E is a proper subspace of $\mathcal{E}$, which is not v invariant [i.e., $v_t(E)$ is not a subset of E for some $t\neq0$].

The group of v on $\mathcal{E}$ is assumed to be connected with E by a topology τ fulfilling

- $\tau\in\mathcal{T}(\mathcal{E},\sigma)$ is a locally convex topology on $\mathcal{E}$;
- $f\in\mathcal{E}\mapsto v_tf\in\mathcal{E}$ is τ-τ continuous for each $t\in\mathbb{R}$;
- $t\in\mathbb{R}\mapsto v_tf\in\mathcal{E}$ is τ continuous for each $f\in\mathcal{E}$;
- $\mathcal{E}$ is τ-complete, and E is τ dense in $\mathcal{E}$.

1. The Schrödinger picture

By construction for every $\omega\in\mathcal{F}_b^\tau(E,\sigma)$, the characteristic function $C_\omega\in\mathsf{C}(E,\sigma)$ τ continuously extends to $C_\omega\in\mathsf{C}(\mathcal{E},\sigma)$. Moreover, for each $\omega\in\mathcal{F}_b^\tau(E,\sigma)$ the mapping $f\in E\mapsto C_\omega(v_tf)$ is τ continuous and an element of $\mathsf{C}(E,\sigma)$, and thus by the relation (3.2) and Proposition 3.2 defines a unique state $\nu_t^v(\omega)\in\mathcal{F}_b^\tau(E,\sigma)$. One easily checks that the mapping ν_t^v is affine and bijective on the folium $\mathcal{F}_b^\tau(E,\sigma)$. The continuity of $t\mapsto v_t$ and the group property of v imply $\nu^v\equiv\{\nu_t^v|t\in\mathbb{R}\}$ to be a group that satisfies the continuity conditions (1.2). Summarizing, we have shown the following.

Proposition 3.4: $(\mathcal{W}(E,\sigma),\mathcal{F}_b^\tau(E,\sigma),\nu^v)$ *is a dynamical description in the sense of Definition 1.2, where* $C_{\nu_t^v(\omega)}=C_\omega\circ v_t,\forall t\in\mathbb{R}$ *for each* $\omega\in\mathcal{F}_b^\tau(E,\sigma)$.

Let us give some physically relevant examples.

Example 3.5: For thermodynamical reasons the Weyl algebra $\mathcal{W}(E,\sigma)$ *should have a quasilocal structure.*[11] *Thus one usually takes* $E=\mathcal{D}(\mathbb{R}^p)$ *the space of all infinitely differentiable functions with compact support in* $\mathbb{R}^p$ *and* σ *to be the imaginary part of the scalar product* $\langle f|g\rangle=\int_{\mathbb{R}^p}\bar{f}g\,d^px$. *On* $\mathcal{W}(E,\sigma)$ *the thermodynamic limits for local Gibbs states are performed. The local Gibbs states are defined on the local algebras* $\mathcal{W}(\mathcal{D}(\Gamma),\sigma)$, *where the* Γ *are open, bounded regions of* $\mathbb{R}^p$ *(e.g., for the Bose–Einstein condensation, cf. Refs. 42, 43, 11, and 24).*

The one-particle dynamics of the bosons is $v_t=\exp\{-it\Delta\}$ *on* $\mathsf{L}^2(\mathbb{R}^p)$. *It is obtained by the thermodynamic limit of the local time translations* $\exp\{-it\Delta_\Gamma\}$, *where the local Laplacians* $-\Delta_\Gamma$ *obey some boundary conditions for the local regions* Γ. *It is well known that for* $0\neq f\in\mathcal{D}(\mathbb{R}^p)$ *the evolved* $v_t(f)$ *no longer has compact support, i.e.,* $v_t(f)\notin\mathcal{D}(\mathbb{R}^p)$ *for* $t\neq0$.

There are several possibilities for choosing a larger symplectic space $(\mathcal{E},\sigma)$ *and a suitable topology* τ *fulfilling the above assumptions. For example, let* $\mathcal{E}$ *be the set of functions with rapid decrease on* $\mathbb{R}^p$, *equipped with the natural Fréchet topology* τ_{Fr}, *which leads to the folium* $\mathcal{F}_b^{Fr}$ *of* τ_{Fr}*-continuous states on* $\mathcal{W}(E,\sigma)$. *Or,* $\mathcal{E}=\mathsf{L}^2(\mathbb{R}^p)$ *with the scalar product topology* τ_s, *which gives the folium* $\mathcal{F}_b^s$ *of* τ_s*-continuous states on* $\mathcal{W}(E,\sigma)$. *Since* $\tau_s<\tau_{Fr}$, $\mathcal{F}_b^s$ *is a proper subfolium of* $\mathcal{F}_b^{Fr}$. *And the dynamical description* $(\mathcal{W}(E,\sigma),\mathcal{F}_b^s,\nu^v)$ *is a dynamical subdescription of* $(\mathcal{W}(E,\sigma),\mathcal{F}_b^{Fr},\nu^v)$. *The limiting Gibbs states, however, are elements of* $\mathcal{F}_b^{Fr}$ *but not of* $\mathcal{F}_b^s$. *In Sec. IV C further examples are given.*

For photons one has a similar situation,[44] *where the one-photon Hamiltonians are the square roots of the Laplacians.*

2. The Heisenberg picture

As an immediate consequence of (3.2) and the Propositions 3.2, 3.3, and 3.4 we have that the restrictions of the states in $\mathcal{F}_b^\tau(\mathcal{E},\sigma)$ from the enlarged Weyl algebra $\mathcal{W}(\mathcal{E},\sigma)$ to the subalgebra

$\mathscr{W}(E,\sigma)$ just give the folium $\mathscr{F}_b^\tau(E,\sigma)$, which in the sequel is denoted by $\mathscr{F}_b^\tau$. Moreover, the representation Π_b^τ of $\mathscr{W}(E,\sigma)$ is the restriction of the representation Π_b^τ of $\mathscr{W}(\mathscr{E},\sigma)$, and $\mathscr{M}_b^\tau=\Pi_b^\tau(\mathscr{W}(\mathscr{E},\sigma))''=\Pi_b^\tau(\mathscr{W}(E,\sigma))''$.

By the duality (1.3) we get from $(\mathscr{W}(E,\sigma),\mathscr{F}_b^\tau,\nu^v)$ the dynamics $(\mathscr{M}_b^\tau,\beta^v)$ in the Heisenberg picture. The group β^v is just the Π_b^τ-normal extension to $\mathscr{M}_b^\tau$ of the group of Bogoliubov transformations $\beta^v\equiv\{\beta_t^v|t\in\mathbb{R}\}$ (denoted by the same symbol) on the enlarged Weyl algebra $\mathscr{W}(\mathscr{E},\sigma)$, $\beta_t^v(W(f))=W(v_t f),\forall f\in\mathscr{E}$ for every $t\in\mathbb{R}$. From $\|W(f)-W(g)\|=2$ for $f\neq g$ it immediately follows that $(\mathscr{W}(\mathscr{E},\sigma),\beta^v)$ is not a C^*-dynamical system (whenever v is nontrivial). We also regard $(\mathscr{W}(\mathscr{E},\sigma),\beta^v)$ as the dynamics in the Heisenberg picture for our boson field.

IV. COCYCLE DYNAMICS FOR THE INTERACTING SYSTEM

Here let us fix an arbitrary polynomial Q for the dynamics of the mean field system and an arbitrary one-boson dynamics $v\equiv\{v_t|t\in\mathbb{R}\}$ on the larger symplectic space $(\mathscr{E},\sigma)\supseteq(E,\sigma)$ with the associated topology τ from Sec. III C.

The free dynamics in the Schrödinger picture is the dynamical description $(\mathscr{C},\mathscr{F},\nu)$ on the C^*-algebra $\mathscr{C}:=\mathscr{A}\otimes\mathscr{W}(E,\sigma)$ of the composite mean field–boson system. Here $\mathscr{F}:=\mathscr{F}_a^p\otimes\mathscr{F}_b^\tau$ is the folium of $\Pi_a^p\otimes\Pi_b^\tau$-normal states on $\mathscr{C}$, and $\nu_t:=\nu_t^Q\otimes\nu_t^v,\forall t\in\mathbb{R}$.

Let $\gamma_t:=\alpha_t^Q\otimes\beta_t^v,\forall t\in\mathbb{R}$. The free dynamics in the Heisenberg picture is $(\mathscr{M},\gamma)$, where $\mathscr{M}:=\mathscr{M}_a^p\overline{\otimes}\mathscr{M}_b^\tau=\Pi_a^p\otimes\Pi_b^\tau(\mathscr{C})''=\Pi_a^p\otimes\Pi_b^\tau(\mathscr{C}_e)''$, which is obtained from $(\mathscr{C},\mathscr{F},\nu)$ by the duality relation (1.3).

Another formulation of the dynamics in the Heisenberg picture is given in terms of the extended C^*-algebras. For the mean field we have the C^*-dynamical system $(\mathscr{A}_e,\alpha^Q)$, and for the bosons we have the time-noncontinuous group of Bogoliubov transformations $(\mathscr{W}(\mathscr{E},\sigma),\beta^v)$. The tensor product gives the Heisenberg dynamics $(\mathscr{C}_e,\gamma)$ with the extended composite C^*-algebra,

$$\mathscr{C}_e:=\mathscr{A}_e\otimes\mathscr{W}(\mathscr{E},\sigma)=\mathscr{A}\otimes C(P)\otimes\mathscr{W}(\mathscr{E},\sigma)\cong C(P,\mathscr{A}\otimes\mathscr{W}(\mathscr{E},\sigma))\cong\mathscr{A}\otimes C(P,\mathscr{W}(\mathscr{E},\sigma))$$

[which is unique since $\mathscr{A}$ and $C(P)$ are nuclear], where $C(P,\mathscr{V})$ ($\mathscr{V}$ is Banach space) denotes the Banach space of all continuous $\mathscr{V}$-valued functions with the uniform norm $\|X\|_\infty=\sup_{x\in P}\|X(x)\|$ [as usual $C(P)\equiv C(P,\mathbb{C})$].

With the help of cocycle techniques we first construct a class of interacting dynamics in the Heisenberg picture as time-noncontinuous groups of automorphisms on $\mathscr{C}_e$. Each solution of the cocycle equations gives a different interaction. And thus, the whole of all solutions gives our treated class of interactions.

Then we extend by W^*-continuity to $\mathscr{M}$, i.e., in the representation $\Pi_a^p\otimes\Pi_b^\tau$ of $\mathscr{C}_e$. Here we need the generalized spectral integral, which is presented in the Appendix. And in a third step we formulate the above class of interactions in the Schrödinger picture as dynamical descriptions (see Definition 1.2) on the folium $\mathscr{F}$ of $\mathscr{C}$, resp., of $\mathscr{C}_e$.

We investigate the cocycle dynamics in suitable covariant subrepresentations, which leads to an enlarged system of cocycle equations for the unitary implementation of the cocycle automorphism group. We finally turn to some concretizations and realize the cocycle dynamics as a thermodynamic limit in suitable subrepresentations.

Let us mention that similar to the previous sections it would also be possible to start with the Schrödinger dynamical description of the interacting systems, and then to turn over to the Heisenberg picture.

A. The algebraic cocycle dynamics

1. The Heisenberg dynamics on the extended C^*-algebra

Using the above isomorphies for $\mathscr{C}_e$ we have the following.

Theorem 4.1: *Let $\psi:\mathbb{R}\times P\to\mathscr{E}$, $(t,x)\mapsto\psi(t,x)$ be a function so that $x\in P\mapsto\sigma(\psi(t,x),f)$ is continuous for all $t\in\mathbb{R}$ and each $f\in\mathscr{E}$. Then, for each $t\in\mathbb{R}$,*

$$\gamma_t^{\psi}(Z)(x) := [1_{\mathscr{A}} \otimes W(\psi(t,x))][\gamma_t(Z)(x)][1_{\mathscr{A}} \otimes W(-\psi(t,x))], \quad \forall x \in P, \quad Z \in \mathscr{C}_e,$$

defines the automorphism γ_t^{ψ} *on* $\mathscr{C}_e$. $\psi \equiv 0$ *gives the free time evolutions* $\gamma_t^0 = \gamma_t$, $\forall t \in \mathbb{R}$.

Moreover, if $\psi(t,x)$ *satisfies the cocycle equations*

$$\psi(s+t,x) = \psi(s,x) + v_s \psi(t, \varphi_s^Q x), \quad \forall x \in P, \quad \forall s,t \in \mathbb{R}, \tag{4.1}$$

then $\gamma^{\psi} \equiv \{\gamma_t^{\psi} | t \in \mathbb{R}\}$ *is a group, i.e.,* $\gamma_s^{\psi} \circ \gamma_t^{\psi} = \gamma_{s+t}^{\psi}$, $\forall s,t \in \mathbb{R}$, *and* γ_0^{ψ} *is the identity.*

Proof: We define the implementing map for $Z \in \mathscr{C}_e \cong C(P, \mathscr{A} \otimes \mathscr{W}(\mathscr{E},\sigma))$ and $t \in \mathbb{R}$,

$$\chi_t(Z): P \to \mathscr{A} \otimes \mathscr{W}(\mathscr{E},\sigma), \quad x \mapsto [1_{\mathscr{A}} \otimes W(\psi(t,x))] Z(x) [1_{\mathscr{A}} \otimes W(-\psi(t,x))].$$

By the unitarity of the Weyl operators one gets $\|\chi_t(Z)\|_{\infty} = \|Z\|_{\infty}$. We prove the continuity of the function $\chi_t(Z)$. First, let $Z = X \otimes W(f)$ with $X \in \mathscr{A}_e \cong C(P, \mathscr{A})$ and $f \in \mathscr{E}$. The Weyl relations yield $\chi_t(Z)(x) = \exp\{-i\sigma(\psi(t,x), f)\} X(x) \otimes W(f)$, $\forall x \in P$, which is continuous in $x \in P$. Now we approximate an arbitrary $Z \in \mathscr{C}_e$ by linear combinations of elements $X \otimes W(f)$, and the continuity follows with an $\epsilon/3$ argument.

$\chi_t : \mathscr{C}_e \to \mathscr{C}_e$, $Z \mapsto \chi_t(Z)$ obviously is an automorphism on $\mathscr{C}_e$, whose inverse is given by $\chi_t^{-1}(Z)(x) = [1_{\mathscr{A}} \otimes W(-\psi(t,x))] Z(x) [1_{\mathscr{A}} \otimes W(\psi(t,x))], \forall Z \in \mathscr{C}_e$, $\forall t \in \mathbb{R}, \forall x \in P$. Consequently, $\gamma_t^{\psi} = \chi_t \circ \gamma_t$ is an automorphism too.

Let (4.1) be valid. From Sec. II it immediately follows that $\alpha_t^Q \otimes id_{\mathscr{W}(\mathscr{E},\sigma)}$ maps $1_{\mathscr{A}} \otimes Y \in 1_{\mathscr{A}} \otimes C(P, \mathscr{W}(\mathscr{E},\sigma)) \subset \mathscr{C}_e$ onto the continuous function $1_{\mathscr{A}} \otimes Y(\varphi_t^Q(\cdot)) \in \mathscr{C}_e$. Now, for $Z = A \otimes Y$, where $A \in \mathscr{A}$ and $Y \in C(P, \mathscr{W}(\mathscr{E},\sigma))$, one checks that for all $s,t \in \mathbb{R}$ and each $x \in P$,

$$\gamma_s \circ \chi_t(Z)(x) = [1_{\mathscr{A}} \otimes W(v_s \psi(t, \varphi_s^Q(x)))][\gamma_s(Z)(x)][1_{\mathscr{A}} \otimes W(-v_s \psi(t, \varphi_s^Q(x)))],$$

which then extends to all $Z \in \mathscr{C}_e$. Using this and the Weyl relations, the group property of γ^{ψ} is immediate. Since (4.1) yields $\psi(0,x) = 0$, $\forall x \in P$, we have that γ_0^{ψ} is the identity on $\mathscr{C}_e$. ■

Obviously, for each solution ψ of the cocycle equations (4.1) we have a different group γ^{ψ} of automorphisms on $\mathscr{C}_e$. The cocycle equations define an initial value problem.

Theorem 4.2: *For any* $\phi \in C(P,\mathscr{E})$ *it holds: The cocycle equations (4.1) with the initial value* $(\partial\psi/\partial t)(0,x) = \phi(x), \forall x \in P$ *are uniquely solvable, with the solution* $\psi : \mathbb{R} \times P \to \mathscr{E}$,

$$\psi(t,x) = \int_{r=0}^{t} v_r \phi(\varphi_r^Q x) dr, \quad x \in P, \quad t \in \mathbb{R}. \tag{4.2}$$

The integrals and the derivatives are understood with respect to the τ *topology, where their existences are ensured by the completeness of* $\mathscr{E}$.

Proof: That (4.2) fulfills the cocycle equations (4.1) is easily checked. The cocycle equations imply $\psi(0,x) = 0, \forall x \in P$. $t \to 0$ in $[\psi(s+t,x) - \psi(s,x)]/t = v_s \psi(t, \varphi_s^Q x)/t$ gives the partial differential equation $(\partial\psi/\partial s)(s,x) = v_s \phi(\varphi_s^Q x)$, which is uniquely solvable with the initial value $\psi(0,x) = 0$. ■

The above theorem characterizes the solutions $\psi \equiv \psi^{\phi}$ of the cocycle equations by their initial values $\phi \in C(P,\mathscr{E})$. In the sequel we will call the initial value ϕ a *coupling function* for our mean field–boson system. Every coupling function $\phi \in C(P,\mathscr{E})$ gives rise to an interaction between the mean field system and the boson field, and the interacting dynamics is given by the group γ^{ψ} on $\mathscr{C}_e$. And thus, the interactions treated in the present work may be indexed by $C(P,\mathscr{E})$. In Proposition 4.5 it becomes transparent how the coupling operator corresponding to the coupling function ϕ looks.

2. The Heisenberg dynamics on the composite W*-algebra

Here the time-noncontinuous Heisenberg dynamics $(\mathscr{C}_e,\gamma^\psi)$ from Theorem 4.1 for an arbitrary solution ψ of the cocycle equations is considered in the representation $\Pi_a^p \otimes \Pi_b^\tau$ of $\mathscr{C}_e=\mathscr{A}_e\otimes\mathscr{W}(\mathscr{E},\sigma)$, i.e., on the W^*-tensor product, $\mathscr{M}=\mathscr{M}_a^p\overline{\otimes}\mathscr{M}_b^\tau$.

However, we need some preparatories. With the projection-valued measure $\mathscr{P}$ of Sec. II A and the general spectral integral of the Appendix we define

$$V(\zeta;\eta):=\int_P \exp\{i\zeta(x)\}[\mathbb{1}_a^p\otimes W_b^\tau(\eta(x))]d(\mathscr{P}(x)\otimes\mathbb{1}_b^\tau)\in\mathscr{Z}_a^p\overline{\otimes}\mathscr{M}_b^\tau, \tag{4.3}$$

for every $\zeta\in C(P,\mathbb{R})$ and $\eta\in C(P,\mathscr{E})$. For the existence of the integrals observe the continuity of $x\in P\mapsto W_b^\tau(\eta(x))$ in the strong operator topology by Proposition 3.3.

Lemma 4.3: Let $\zeta_1,\zeta_2,\zeta\in C(P,\mathbb{R})$ and $\eta_1,\eta_2,\eta\in C(P,\mathscr{E})$. Then

(a) $V(\zeta;\eta)$ is unitary with $V(\zeta;\eta)^*=V(-\zeta;-\eta)$.

(b) $V(\zeta_1;\eta_1)V(\zeta_2;\eta_2)=V(\zeta_{1,2};\eta_1+\eta_2)$, where

$$\zeta_{1,2}(x):=\zeta_1(x)+\zeta_2(x)-\tfrac{1}{2}(\eta_1(x),\eta_2(x)),\quad \forall x\in P.$$

(c)$\alpha_s^Q\otimes\beta_t^v(V(\zeta;\eta))=V(\zeta\circ\varphi_s^Q;v_t(\eta\circ\varphi_s^Q)),\forall s,t\in\mathbb{R}$, where

$$v_t(\eta\circ\varphi_s^Q):P\to\mathscr{E},\quad x\mapsto v_t\eta(\varphi_s^Q x).$$

Proof: The proof is easily checked by the weak definition of $V(\zeta;\eta)$ in Theorem A.1 of the Appendix and by observing $\alpha_t^Q(\int_P\xi\,d\mathscr{P})=\int_P\xi\circ\varphi_t^Q\,d\mathscr{P}$ for $\xi\in C(P)$ (see Sec. II D). ■

Theorem 4.4: *Let $\psi:\mathbb{R}\times P\to\mathscr{E},(t,x)\mapsto\psi(t,x)=:\psi_t(x)$ be a continuous function. Then, for each $t\in\mathbb{R}$ the automorphism γ_t^ψ on $\mathscr{C}_e$ in the representation $\Pi_a^p\otimes\Pi_b^\tau$ W^*-continuously extends to an automorphism on $\mathscr{M}$ denoted by the same symbol, which with arbitrary $\zeta\in C(P,\mathbb{R})$ (one may choose $\zeta=0$) is given by*

$$\gamma_t^\psi(Z)=V(\zeta;\psi_t)\,\gamma_t(Z)V(\zeta;\psi_t)^*,\quad \forall Z\in\mathscr{M}.$$

Proof: For each $t\in\mathbb{R}$ $\tilde{\gamma}_t^\psi(\cdot):=V(0;\psi_t)\,\gamma_t(\cdot)V(0;\psi_t)^*$ is an automorphism on $\mathscr{M}$. With Lemma 4.3 and $V(0;g)=\mathbb{1}_a^p\otimes W_b^\tau(g)$ (where $g\in\mathscr{E}$ is considered as a constant function on P) one establishes for each $X\in\mathscr{M}_a^p$ and $f\in\mathscr{E}$,

$$\begin{aligned}V(\zeta;\psi_t)\,\gamma_t(X\otimes W_b^\tau(f\ ))V(\zeta;\psi_t)^*&=V(\zeta;\psi_t)[\alpha_t^Q(X)\otimes\mathbb{1}_b^\tau][\mathbb{1}_a^p\otimes W_b^\tau(v_tf\ )]V(\zeta;\psi_t)^*\\&=[\alpha_t^Q(X)\otimes\mathbb{1}_b^\tau][V(\zeta;\psi_t)V(0;v_tf\ )V(-\zeta;-\psi_t)]\\&=[\alpha_t^Q(X)\otimes\mathbb{1}_b^\tau]V(-\sigma(\psi_t(\cdot),v_tf\ );v_tf\ )\\&=[\alpha_t^Q(X)\otimes\mathbb{1}_b^\tau][V(0;\psi_t)V(0;v_tf\ )V(0;-\psi_t)]\\&=\tilde{\gamma}_t^\psi(X\otimes W_b^\tau(f\ )).\end{aligned}$$

We now prove the agreement of $\tilde{\gamma}_t^\psi\circ(\Pi_a^p\otimes\Pi_b^\tau)$ with $(\Pi_a^p\otimes\Pi_b^\tau)\circ\gamma_t^\psi$,

$$\begin{aligned}\tilde{\gamma}_t^\psi(X\otimes W_b^\tau(f\ ))&=[\alpha_t^Q(X)\otimes\mathbb{1}_b^\tau]V(-\sigma(\psi_t(\cdot),v_tf\ );v_tf\ )\\&=[\alpha_t^Q(X)\otimes\mathbb{1}_b^\tau]\left(\int_P\exp\{-i\sigma(\psi_t(x),v_tf\ )\}d\mathscr{P}(x)\right)\otimes W_b^\tau(v_tf\ )\\&=\left[\int_P\exp\{-i\sigma(\psi_t(x),v_tf\ )\}d\mathscr{P}(x)\otimes\mathbb{1}_b^\tau\right][\gamma_t(X\otimes W_b^\tau(f\ ))].\end{aligned}$$

On the other side $\gamma_t^{\psi}(X\otimes W(f))(x)=\exp\{-i\sigma(\psi_t(x),v_tf)\}\,\gamma_t(X\otimes W(f))(x)$. ■

As a corollary of the above proof we have the explicit evaluation on elements of the form $X\otimes W_b^{\tau}(f)$, where $X\in\mathscr{M}_a^p$ and $f\in\mathscr{E}$:

$$\gamma_t^{\psi}(X\otimes W_b^{\tau}(f))=\Bigg[\underbrace{\left(\int_P \exp\{-i\sigma(\psi(t,x),v_tf)\}d\mathscr{P}(x)\right)}_{\in\mathscr{Z}_a^p=\mathscr{M}_a^p\cap\mathscr{M}_a^{p\prime}}\alpha_t^Q(X)\Bigg]\otimes W_b^{\tau}(v_tf).$$

3. Coupling functions and interaction operators

Let us first consider an arbitrary C^*- or W^*-dynamical system $(\mathscr{B},\tau)$, which we perturb with $P=P^*\in\mathscr{B}$. If δ is the generator of τ, $\delta=(d/dt)\tau_t|_{t=0}$, then $\delta+i[P,\cdot]$ is the generator of the perturbed dynamical one-parameter group τ^P on $\mathscr{B}$. τ^P may be calculated by the Dyson expansion (Ref. 11, Proposition 5.4.1),

$$\tau_t^P(B)=\sum_{n=0}^{\infty} i^n\int_{t_1=0}^{t}dt_1\cdots\int_{t_n=0}^{t_{n-1}}dt_n[\tau_{t_n}(P),[\cdots[\tau_{t_1}(P),\tau_t(B)]\cdots]],\quad B\in\mathscr{B}. \tag{4.4}$$

From the unperturbed (free) dynamics τ and the perturbed (interacting) dynamics τ^P, the perturbation P is obtained back by $i[P,B]=(d/dt)\tau_t^P(\tau_{-t}(B))|_{t=0},\forall B=\mathscr{B}$.

As in the above case of a bounded perturbation of a C^*- or W^*-dynamical system we now determine the perturbation (interaction) operator P^{ϕ} associated with our interacting dynamics γ^{ψ} by comparing with the free dynamics γ, where $\psi=\psi^{\phi}$ is the solution (4.2) of the cocycle equations (4.1) associated with the coupling function $\phi\in C(P,\mathscr{E})$. Formally we have $i[P^{\phi},Z]=(d/dt)\gamma_t^{\psi}(\gamma_{-t}(Z))|_{t=0}$ for $Z\in\mathscr{M}$. Since $\gamma_t^{\psi}(\gamma_{-t}(Z))=V(0;\psi_t)ZV(0;\psi_t)^*,\forall Z\in\mathscr{M}$, we conclude that P^{ϕ} is affiliated to $\mathscr{M}$ and given (up to an additive term in the center of $\mathscr{M}$) by

$$P^{\phi}=\frac{d}{dt}\,V(0;\psi_t)|_{t=0}. \tag{4.5}$$

Proposition 4.5: The formal calculation of the derivation in (4.5) gives

$$P^{\phi}=\int_P[\mathbb{1}_a^p\otimes\Phi_b^{\tau}(\phi(x))]d(\mathscr{P}(x)\otimes\mathbb{1}_b^{\tau}),$$

which justifies our above notion of a coupling function for $\phi\in C(P,\mathscr{E})$, and where $\Phi_b^{\tau}(f)$, $f\in\mathscr{E}$, are the field operators associated with the representation Π_b^{τ} of $\mathscr{W}(\mathscr{E},\sigma)$.

Sketch of Proof: Suppose $h:\mathbb{R}\to\mathscr{E}$ to be continuously differentiable. With the Weyl relations we obtain, in a regular representation of $\mathscr{W}(\mathscr{E},\sigma)$,

$$\begin{aligned}\frac{d}{dt}\,W(h(t))&=\lim_{\epsilon\to0}\frac{1}{\epsilon}\,(W(h(t+\epsilon))-W(h(t)))\\&=\lim_{\epsilon\to0}\frac{\exp\{(i/2)\sigma(h(t+\epsilon),h(t))\}-1}{\epsilon}\,W(h(t+\epsilon)-h(t))W(h(t))\\&\quad+\lim_{\epsilon\to0}\frac{\exp\{i\Phi(h(t+\epsilon)-h(t))\}-\mathbb{1}}{\epsilon}\,W(h(t))\\&=i(\tfrac{1}{2}\,\sigma(h'(t),h(t))+\Phi(h'(t)))W(h(t)),\end{aligned}$$

where we have used the formal calculation

$$\frac{\exp\{i\Phi(h(t+\epsilon)-h(t))\}-\mathbb{1}}{\epsilon}=i\Phi\left(\frac{h(t+\epsilon)-h(t)}{\epsilon}\right)\sum_{n=1}^{\infty}\frac{i^{n-1}}{n!}\,\Phi(h(t+\epsilon)-h(t))^{n-1}$$

$$\xrightarrow{\epsilon\to 0} i\Phi(h'(t)).$$

Now, with $\psi(0,x)=0$ and $(\partial\psi/\partial t)(0,x)=\phi(x)$, the differentiation in (4.5) is easily performed. ■

4. The cocycle dynamics in the Schrödinger picture

The unitary $V(\zeta;\eta)\in\mathscr{M}$ from Eq. (4.3) uniquely defines an affine bijection $\kappa(\zeta;\eta)$ on the folium $\mathscr{F}$, satisfying

$$\langle\kappa(\zeta;\eta)(\omega);Z\rangle:=\langle\omega;V(\zeta;\eta)ZV(\zeta;\eta)^*\rangle,\quad\forall\,\omega\in\mathscr{F},\quad\forall\,Z\in\mathscr{M}.$$

Thus, for each $t\in\mathbb{R}$ the affine bijection ν_t^{ψ} on the folium $\mathscr{F}$ of normal states on $\mathscr{M}$, which is obtained from γ_t^{ψ} by the duality relation (1.3), is given by

$$\nu_t^{\psi}=\kappa(\zeta,\psi_t)\circ\nu_t,\quad\forall\,\zeta\in C(P,\mathbb{R}).$$

As an immediate consequence of the weak definition of the spectral integral in Theorem A.1 we get the following.

Theorem 4.6: *Let $\psi:\mathbb{R}\times P\to\mathscr{E},(t,x)\mapsto\psi(t,x)=:\psi_t(x)$ be a continuous function. Then $t\in\mathbb{R}\mapsto V(0,\psi_t)$ is continuous in the strong operator topology.*

Thus, if ψ satisfies the cocycle equations (4.1), then $(\mathscr{C},\mathscr{F},\nu^{\psi})$ and $(\mathscr{C}_e,\mathscr{F},\nu^{\psi})$ are dynamical descriptions in the sense of Definition 1.2.

B. Unitary cocycle dynamics

1. The cocycle dynamics in subrepresentations

Let $\mathscr{F}_a\subseteq\mathscr{F}_a^p$ and $\mathscr{F}_b\subseteq\mathscr{F}_b^{\tau}$ be subfolia, invariant with respect to the free dynamics ν^Q and ν^v, respectively. Then $(\mathscr{A},\mathscr{F}_a,\nu^Q)$ and $(\mathscr{W}(E,\sigma),\mathscr{F}_b,\nu^v)$ are dynamical subdescriptions. Denote by $c_a\in\mathscr{Z}_a^p$ and $c_b\in\mathscr{Z}_b^{\tau}$ the associated central projections, and by $\Pi_a\leqslant\Pi_a^p$, resp $\Pi_b\leqslant\Pi_b^{\tau}$, the corresponding subrepresentations. Moreover, let $\mathscr{M}_a:=\Pi_a(\mathscr{A})''=c_a\mathscr{M}_a^p$ and $\mathscr{M}_b:=\Pi_b(\mathscr{W}(E,\sigma))''=c_b\mathscr{M}_b^{\tau}$ (cf. Proposition 1.1). The normal states on $\mathscr{M}_{a,b}:=\mathscr{M}_a\overline{\otimes}\mathscr{M}_b=(c_a\otimes c_b)\mathscr{M}$ are given by $\mathscr{F}_{a,b}=\mathscr{F}_a\otimes\mathscr{F}_b\subseteq\mathscr{F}$.

The central projection $c_a\otimes c_b\in\mathscr{Z}_a^p\overline{\otimes}\mathscr{Z}_b^{\tau}\subset\mathscr{M}$ is invariant with respect to the Heisenberg dynamics γ^{ψ} on $\mathscr{M}$. Consequently, $\mathscr{F}_{a,b}$ is ν^{ψ} invariant, and the associated cocycle dynamics in both, the Schrödinger and the Heisenberg picture, are obtained by restricting ν^{ψ}, resp. γ^{ψ}, to $\mathscr{F}_{a,b}$, resp. $\mathscr{M}_{a,b}$, in the manner described in the Introduction.

Let $\mathscr{P}_a:=c_a\mathscr{P}$ be the restriction of the projection-valued measure $\mathscr{P}$, which now has values in the set of orthogonal projections of the center $\mathscr{Z}_a$ of $\mathscr{M}_a$. From the theory of the infinite mean field systems, it is well known that the support $P_a\subseteq P$ of $\mathscr{P}_a$ is invariant with respect to the flow φ^Q. Denote by $\mathbb{1}_a\cong c_a$ the unit in $\mathscr{M}_a$ and $\mathbb{1}_b\cong c_b$ the one in $\mathscr{M}_b$. $W_b(f):=c_bW_b^{\tau}(f)\in\mathscr{M}_b$, $f\in\mathscr{E}$, are the represented Weyl operators with respect to $\Pi_b\leqslant\Pi_b^{\tau}$. Then the restriction of the unitaries (4.3) from $\mathscr{M}$ to $\mathscr{M}_{a,b}$ is

$$V_{a,b}(\zeta;\eta):=(c_a\otimes c_b)V(\zeta;\eta)=\int_{P_a}\exp\{i\zeta(x)\}[\mathbb{1}_a\otimes W_b(\eta(x))]\,d(\mathscr{P}_a(x)\otimes\mathbb{1}_b)\in\mathscr{Z}_a\overline{\otimes}\mathscr{M}_b.$$

And thus it suffices that the functions ζ and η are defined on P_a.

2. Unitary implementations of the cocycle dynamics

From now on let us suppose that the dynamical (sub-)descriptions $(\mathscr{A},\mathscr{F}_a,\nu^Q)$ and $(\mathscr{W}(E,\sigma),\mathscr{F}_b,\nu^v)$ are covariant, which is equivalent that $(\mathscr{M}_a,\alpha^Q)$ and $(\mathscr{M}_b,\beta^v)$ both are W^*-dynamical systems. By Theorem 4.6, $t\mapsto V(0;\psi_t)$ is strongly continuous. Thus, it follows that the dynamical (sub-)description $(\mathscr{C},\mathscr{F}_{a,b},\nu^\psi)$ is covariant, or equivalently, that the Heisenberg (sub-)dynamics $(\mathscr{M}_{a,b},\gamma^\psi)$ defines a W^*-dynamical system.

Let us assume standard representations of $\mathscr{M}_a$ and $\mathscr{M}_b$ on the Hilbert spaces $\mathscr{H}_a^{\mathrm{std}}$ and $\mathscr{H}_b^{\mathrm{std}}$, respectively, such that the W^*-groups α^Q and β^v are unitarily implementable with the Hamiltonians A_a, resp. B_b,

$$\alpha_t^Q(X)=e^{itA_a}Xe^{-itA_a},\quad \forall X\in\mathscr{M}_a,\quad \beta_t^v(Y)=e^{itB_b}Ye^{-itB_b},\quad \forall Y\in\mathscr{M}_b. \tag{4.6}$$

We now search for a strongly continuous unitary group, which implements $(\mathscr{M}_{a,b},\gamma^\psi)$.

Theorem 4.7: *Let $\zeta:\mathbb{R}\times P\to\mathbb{R}$, $(t,x)\mapsto\zeta(t,x)=:\zeta_t(x)$ and $\psi:\mathbb{R}\times P\to\mathscr{E}$, $(t,x)\mapsto\psi(t,x)=:\psi_t(x)$ be continuous functions. For each $t\in\mathbb{R}$ it follows that γ_t^ψ is implemented by the unitary*

$$U_t^{\psi,\zeta}:=V_{a,b}(\zeta_t;\psi_t)[e^{itA_a}\otimes e^{itB_b}], \tag{4.7}$$

that is, $\gamma_t^\psi(Z)=U_t^{\psi,\zeta}Z(U_t^{\psi,\zeta})^*$, $\forall Z\in\mathscr{M}_{a,b}$.

Moreover, the family $U^{\psi,\zeta}\equiv\{U_t^{\psi,\zeta}\mid t\in\mathbb{R}\}$ defines a strongly continuous group on $\mathscr{H}_a^{\mathrm{std}}\otimes\mathscr{H}_b^{\mathrm{std}}$, if ψ and ζ satisfy the cocycle equations,

$$\psi(s+t,x)=\psi(s,x)+v_s\psi(t,\varphi_s^Q x), \tag{4.8}$$

$$\zeta(s+t,x)=\zeta(s,x)+\zeta(t,\varphi_x^Q x)-\tfrac{1}{2}\,\sigma(\psi(s,x),v_s\psi(t,\varphi_s^Q x)), \tag{4.9}$$

for all $s,t\in\mathbb{R}$ and each $x\in P_a$.

Proof: $\gamma_t^\psi(\cdot)=U_t^{\psi,\zeta}\cdot(U_t^{\psi,\zeta})^*$ is obvious. With Lemma 4.3 and (4.6) we get

$$\begin{aligned}U_s^{\psi,\zeta}U_t^{\psi,\zeta}&=V_{a,b}(\zeta_s;\psi_s)[e^{isA_a}\otimes e^{isB_b}]V_{a,b}(\zeta_t;\psi_t)[e^{itA_a}\otimes e^{itB_b}]\\&=V_{a,b}(\zeta_s;\psi_s)V_{a,b}(\zeta_t\circ\varphi_s^Q;v_s(\psi_t\circ\varphi_s^Q))[e^{i(s+t)A_a}\otimes e^{i(s+t)B_b}]\\&=V_{a,b}(\zeta_{s,t};\psi_s+v_s(\psi_t\circ\varphi_s^Q))[e^{i(s+t)A_a}\otimes e^{i(s+t)B_b}],\end{aligned}$$

with $\zeta_{s,t}:=\zeta(s,x)+\zeta(t,\varphi_s^Q x)-(1/2)\sigma(\psi(s,x),\,v_s\psi(t,\varphi_s^Q x))$. This agrees with $U_{s+t}^{\psi,\zeta}$, if the cocycle equations (4.8) and (4.9) are fulfilled. ∎

The cocycle equations (4.8) are the restriction of (4.1) to the φ^Q-invariant subset P_a of the classical phase space P. Analogously to Theorem 4.2, the unique solution $\psi:\mathbb{R}\times P_a\to\mathscr{E}$ of (4.8) with initial value $(\partial\psi/\partial t)(0,x)=\phi(x)$, $\forall x\in P_a$, where $\phi\in C(P_a,\mathscr{E})$ is an arbitrary coupling function, is given by Eq. (4.2), but for $x\in P_a\subseteq P$. Using a solution ψ for (4.8) we may solve the equations (4.9), that determine the correct phase of the group $U^{\psi,\zeta}$. Similar to Theorem 4.2, one proves the following.

Theorem 4.8: *Let $\psi(t,x)=\int_{r=0}^t v_r\phi(\varphi_r^Q x)dr,\forall x\in P_a$ be the unique solution of (4.8) with the initial value $\phi\in C(P_a,\mathscr{E})$ by Theorem 4.2. Then, for arbitrary $\lambda\in C(P_a,\mathbb{R})$ it holds: The cocycle equations (4.9) with the initial value $(\partial\zeta/\partial t)(0,x)=\lambda(x),\forall x\in P_a$ are uniquely solvable, and the solution $\zeta:\mathbb{R}\times P_a\to\mathbb{R}$ is given by*

$$\zeta(t,x)=\int_{r=0}^t\lambda(\varphi_r^Q x)dr-\frac{1}{2}\int_{p=0}^t\int_{r=0}^p\sigma(v_r\phi(\varphi_r^Q x),v_p\phi(\varphi_p^Q x))dr\,dp.$$

3. The generator of the unitary cocycle dynamics

Here, let us assume the solutions ψ and ζ of the cocycle equations given with the initial values $\phi \in C(P_a, \mathscr{E})$ and $\lambda \in C(P_a, \mathbb{R})$ by Theorem 4.8.

Similar to Proposition 4.5, one formally calculates the Hamiltonian H^ϕ associated with the unitary group $U^{\psi,\zeta}$ of Theorem 4.7,

$$H^\phi := -i \frac{d}{dt} U_t^{\psi,\zeta}\Big|_{t=0} = A_a \otimes \mathbb{1}_b + \mathbb{1}_a \otimes B_b + \int_{P_a} [\mathbb{1}_a \otimes \Phi_b(\phi(x))] d(\mathscr{P}_a(x) \otimes \mathbb{1}_b) + \left(\int_{P_a} \lambda \, d\mathscr{P}_a \right) \otimes \mathbb{1}_b , \tag{4.10}$$

where the $\Phi_b(f)$, $f \in \mathscr{E}$, denote the field operators associated with the representation Π_b of $\mathscr{W}(\mathscr{E},\sigma)$. The central part $\int_{P_a} \lambda \, d\mathscr{P}_a \in \mathscr{Z}_a$ in H^ϕ is irrelevant for the Heisenberg dynamics $(\mathscr{M}_{a,b}, \gamma^\psi)$. Thus, in the sequel let us assume $\lambda \equiv 0$. The interacting part of H^ϕ agrees with $(c_a \otimes c_b) P^\phi$, where P^ϕ is from Proposition 4.5.

C. The cocycle dynamics as a thermodynamic limit

If E and thus $\mathscr{E}$ are complex vector spaces (the multiplication with the complex i is τ continuous), and σ is the imaginary part of a τ-continuous positive sesquilinear form $\langle \cdot | \cdot \rangle$ on $\mathscr{E}$, then one may introduce the annihilation and creation operators, $a_b(f) := (1/\sqrt{2})(\Phi_b(f) + i\Phi_b(if))$ and $a_b^*(f)$ as the adjoint, for the regular representation Π_b of $\mathscr{W}(\mathscr{E},\sigma)$. Throughout the present section we consider the coupling function

$$\phi(x) = \sqrt{2} \sum_{k=1}^{l} \xi_k(x) \phi_k , \quad x \in P, \tag{4.11}$$

for some $l \in \mathbb{N}_0$, where $\xi_k \in C(P)$ and $\phi_k \in \mathscr{E}$. With this ϕ we obtain the familiar form [cf. Eq. (1.1)] of the interaction operator from Proposition 4.5,

$$P^\phi = \sum_{k=1}^{l} \left[\left(\int_P \xi_k \, d\mathscr{P} \right) \otimes a_b^*(\phi_k) + \left(\int_P \overline{\xi_k} \, d\mathscr{P} \right) \otimes a_b(\phi_k) \right]. \tag{4.12}$$

The local time evolutions $\alpha^{Q,\Lambda}$, $\Lambda \in \mathscr{L}$, of the mean field system from Eq. (2.4) converge in the representation Π_a^p of $\mathscr{A}$ in some sense to the limiting Heisenberg dynamics α^Q. Also, the mean field parts $\int_P \xi_k \, d\mathscr{P} \in \mathscr{Z}_a^p$ of the above interaction P^ϕ may be approximated by uniformly bounded (with respect to $\Lambda \in \mathscr{L}$) local polynomials Ξ_k^Λ of the local density operators $m_\Lambda(b)$ from Eq. (2.1).

Thus, it should be possible that the interacting dynamics γ^ψ is approximated by the local time evolution groups $\gamma^{\psi,\Lambda}$, $\Lambda \in \mathscr{L}$, which are given by the perturbation of $\alpha^{Q,\Lambda} \otimes \beta^v$ with the local interaction

$$P^{\phi,\Lambda} = \sum_{k=1}^{l} [\Xi_k^\Lambda \otimes a_b^*(\phi_k) + (\Xi_k^\Lambda)^* \otimes a_b(\phi_k)].$$

For such an approximation procedure we want to use perturbation techniques. Because the field operators (respectively, the annihilation and creation operators) are unbounded, for general bosonic representations $\Pi_b \leqslant \Pi_b^\tau$ it is not possible to control the growth of the expansion series (4.4) uniformly for $\Lambda \in \mathscr{L}$.

However, for the field, annihilation, and creation operators there exist estimates on the finite particle vectors in Fock space. This suggests that the necessary growth control of the expansion series can be done for Fock-like representations Π_b of $\mathscr{W}(E,\sigma)$. A Fock-like representation Π_b, for example, is obtained as the GNS representation of a suitable (ν^v-invariant) gauge-invariant

quasi-free factor state on $\mathscr{W}(E,\sigma)$, where the GNS–Hilbert space is the tensor product of two Fock spaces.[40,11,45] Let us outline in more detail a typical situation, where here the temperature states (without condensation) of the boson system are considered. The associated estimates for the perturbation expansions are derived in Ref. 47.

E usually is chosen to be a complex pre-Hilbert space with (right-linear) scalar product $\langle\cdot|\cdot\rangle$ (σ is the imaginary part of $\langle\cdot|\cdot\rangle$). The single particle Hamiltonian S (self-adjoint operator on the completion E of E with respect to $\langle\cdot|\cdot\rangle$) is positive, not having zero as its eigenvalue. We assume $E\subseteq D(S^{-1/2})=:\mathscr{E}$ to be a core for $S^{-1/2}$. The τ topology is chosen to arise from the inner product $\langle f|g\rangle_\tau:=\langle f|g\rangle+\langle S^{-1/2}f|S^{-1/2}g\rangle$, which defines the graph norm of $S^{-1/2}$. The one-boson dynamics is $v_t:=e^{itS}|_{\mathscr{E}}$, $t\in\mathbb{R}$. That $v=\{v_t|t\in\mathbb{R}\}$ is a strongly continuous unitary group on the Hilbert space $\mathscr{E}=(D(S^{-1/2}),\langle\cdot|\cdot\rangle_\tau)$ is immediate.

Remark 4.9: If E is any subset of the domain $D(S^{-1/2})$, which is invariant with respect to the one-boson dynamics v, then by Ref. 46, Theorem 4 E is a core for $S^{-1/2}$.

In the special case, where $E=\mathscr{D}(\mathbb{R}^p)$ is from Example 3.5, and $S=-\Delta$, resp. $S=\sqrt{-\Delta}$, then E is a core for $S^{-1/2}$ (cf. Refs. 44, 24, and 42).

Let $T_\beta:=e^{-\beta S}(\mathbb{1}-e^{-\beta S})^{-1}$ for $\beta>0$, and $T_\infty:=0$ for $\beta=\infty$. Then by

$$\langle\omega_b^\beta;W(f\ )\rangle=\exp\{-\tfrac{1}{4}\|f\|^2-\tfrac{1}{2}\|T_\beta^{1/2}f\|^2\},\quad f\in E,$$

the characteristic function of the temperature state ω_b^β for the inverse temperature $\beta\in]0,\infty]$ is given (for $\beta=\infty$ the Fock vacuum state is obtained). Since for each $\beta\in]0,\infty[$ the graph norm for $T_\beta^{1/2}$ is equivalent to the above $\|\cdot\|_\tau$, and $D(T_\beta^{1/2})=D(S^{-1/2})$, it follows that ω_b^β is an element of the folium $\mathscr{F}_b^\tau$ of τ-continuous states on $\mathscr{W}(E,\sigma)$.

Since ω_b^β is invariant with respect to the dynamical description $(\mathscr{W}(E,\sigma),\mathscr{F}_b^\tau,\nu^v)$, its GNS representation $(\Pi_b^\beta,\mathscr{H}_b^\beta,\Omega_b^\beta)$ defines a covariant dynamical subdescription (cf. the Introduction). The above Hamiltonian $B_b\equiv B_b^\beta$ is chosen so that $B_b^\beta\Omega_b^\beta=0$.

With (2.3) we define in the representation $\Pi_a^p\otimes\Pi_b^\beta$ the local interacting Hamiltonians,

$$H^{\phi,\Lambda}:=A_\Lambda\otimes\mathbb{1}_b^\beta+\mathbb{1}_a^p\otimes B_b^\beta+P^{\phi,\Lambda},$$

which are essentially self-adjoint.[47] Then the local perturbed time evolutions are

$$\gamma_t^{\psi;\Lambda}(\cdot):=\exp\{itH^{\phi,\Lambda}\}\cdot\exp\{-itH^{\phi,\Lambda}\},\quad \Lambda\in\mathscr{L}.$$

Since ω_b^β is a gauge-invariant quasi-free factor state on $\mathscr{W}(E,\sigma)$, we are in the above mentioned situation, and the expansion (4.4) can be controlled uniformly in $\Lambda\in\mathscr{L}$,[47] which gives the following result proven in Ref. 13 ($\odot$ means the algebraic tensor product).

Theorem 4.10: *$\gamma_t^\psi(Z)=s-\lim_{\Lambda\in\mathscr{L}}\gamma_t^{\psi,\Lambda}(Z)$, for $Z\in\Pi_a^p(\mathscr{A})\odot\Pi_b^\beta(\mathscr{W}(\mathscr{E},\sigma))$.*

The result is also interesting insofar that the perturbation techniques are valid here for the free dynamics γ on $\mathscr{M}_a^p\overline{\otimes}\mathscr{M}_b^\beta$, which is not a W^*-dynamical system.

With the above perturbation techniques using the Fock-like temperature representation Π_b^β in addition to the above result it is also possible to make rigorous the differentiation in the formal sketch of proof of Proposition 4.5; we refer to Refs. 47 and 13.

Theorem 4.11: *Let $\Pi_a\leqslant\Pi_a^p$ be a covariant subrepresentation for α^Q as in Sec. IV D. Then*

$$H^\phi=A_a\otimes\mathbb{1}_b^\beta+\mathbb{1}_a\otimes B_b^\beta+(c_a\otimes c_b^\beta)P^\phi,$$

where P^ϕ is from (4.12), is essentially self-adjoint, and is indeed the generator of the unitary group $U^{\psi,\zeta}$ on $\mathscr{H}_a^{std}\otimes\mathscr{H}_b^\beta$ [cf. Eq. (4.10)].

APPENDIX: SPECTRAL INTEGRALS

For integrating general operator-valued functions with respect to a projection-valued measure, there are very strong conditions[48] (cf. also Ref. 49, Chap. 6). Here, however, we have some special cases of such integrals, for which the conditions for existence are weaker.

Let $\mathscr{H}$ and $\mathscr{K}$ be (complex) Hilbert spaces, $\mathscr{B}(\mathscr{K})$ the bounded operators of $\mathscr{K}$, and $\mathscr{P}$ a projection-valued measure from the Borel subsets $B(\mathbb{R}^p)$ of $\mathbb{R}^p$ ($p\in\mathbb{N}$) into the orthogonal projections of $\mathscr{H}$. Then, the map $\Delta\in B(\mathbb{R}^p)\mapsto\mathscr{P}(\Delta)\otimes 1_{\mathscr{K}}$ is a projection-valued measure on $\mathscr{H}\otimes\mathscr{K}$. For operator-valued functions $X:\mathbb{R}^p\to\mathscr{B}(\mathscr{K})$ we now develop the theory of the spectral integrals,

$$\int_{\mathbb{R}^p}(1_{\mathscr{H}}\otimes X(x))d(\mathscr{P}(x)\otimes 1_{\mathscr{K}}). \tag{A1}$$

We do not give the long proofs here and refer the reader to Ref. 13, Sec. A.4, where the connection with the direct integral is also pointed out.

Theorem A.1: *Let $X:\mathbb{R}^p\to\mathscr{B}(\mathscr{K})$ be weakly measurable with $\sup\{\|X(x)\|\,|x\in\mathbb{R}^p\}<\infty$. Then by*

$$\left\langle \phi_1\otimes\psi_1\middle|\int_{\mathbb{R}^p}(1_{\mathscr{H}}\otimes X(x))d(\mathscr{P}(x)\otimes 1_{\mathscr{K}})\phi_2\otimes\psi_2\right\rangle := \int_{\mathbb{R}^p}\langle\psi_1|X(x)\psi_2\rangle d\langle\phi_1|\mathscr{P}(x)\phi_2\rangle,$$

$$\forall\,\phi_1,\phi_2\in\mathscr{H},\quad \forall\,\psi_1,\psi_2\in\mathscr{K},$$

and by linear and continuous extension on $\mathscr{H}\otimes\mathscr{K}$ the bounded operator (A1) is well defined. Moreover,

(a) $\|\int_{\mathbb{R}^p}(1_{\mathscr{H}}\otimes X(x))d(\mathscr{P}(x)\otimes 1_{\mathscr{K}})\|\leq\sup\{\|X(x)\|\;\;|x\in\mathbb{R}^p\}$.

(b) $(\int_{\mathbb{R}^p}(1_{\mathscr{H}}\otimes X(x))d(\mathscr{P}(x)\otimes 1_{\mathscr{K}}))^*=\int_{\mathbb{R}^p}(1_{\mathscr{H}}\otimes(X(x))^*)d(\mathscr{P}(x)\otimes 1_{\mathscr{K}})$.

(c) *If $\mathscr{H}$ and $\mathscr{K}$ are separable, then we have the product property*

$$\int_{\mathbb{R}^p}(1_{\mathscr{H}}\otimes X(x)Y(x))d(\mathscr{P}(x)\otimes 1_{\mathscr{K}})=\int_{\mathbb{R}^p}(1_{\mathscr{H}}\otimes X(x))d(\mathscr{P}(x)\otimes 1_{\mathscr{K}})\int_{\mathbb{R}^p}(1_{\mathscr{H}}\otimes Y(x))d(\mathscr{P}(x)\otimes 1_{\mathscr{K}}).$$

(d) *If $\mathscr{K}$ is separable, then the measurability of $x\in\mathbb{R}^p\mapsto\|X(x)\|$ follows, and for all $\xi\in\mathscr{H}\otimes\mathscr{K}$ it is*

$$\left\|\int_{\mathbb{R}^p}(1_{\mathscr{H}}\otimes X(x))d(\mathscr{P}(x)\otimes 1_{\mathscr{K}})\xi\right\|^2\leq\int_{\mathbb{R}^p}\|X(x)\|^2 d\langle\xi|(\mathscr{P}(x)\otimes 1_{\mathscr{K}})\xi\rangle.$$

With some stronger conditions for $X:\mathbb{R}^p\to\mathscr{B}(\mathscr{K})$ and $Y:\mathbb{R}^p\to\mathscr{B}(\mathscr{K})$, we may drop in (c) the separability condition for $\mathscr{H}$ and $\mathscr{K}$. Let $P\in B(\mathbb{R}^p)$. We call $X:P\to\mathscr{B}(\mathscr{K})$ with $\sup\{\|X(x)\|\;\;|x\in P\}<\infty$ a $\mathscr{T}$ function, if X is approximable for $\mathscr{P}$—almost all $x\in P$ in the strong operator topology by a sequence of elementary functions $X_n:P\to\mathscr{B}(\mathscr{K})$ for which $\|X_n(x)\|\leq c$, $\forall x\in P$, $\forall n\in\mathbb{N}$ for some $c>0$ (cf. Ref. 50, Appendix to IV.5, p. 115). [An elementary function is of the form $\Sigma_{k=1}^m\chi_{\Delta_k}Q_k$, where χ_Δ is the characteristic function of $\Delta\in B(P)$ and $Q_k\in\mathscr{B}(\mathscr{K})$.] If $X:P\to\mathscr{B}(\mathscr{K})$ and $Y:P\to\mathscr{B}(\mathscr{K})$ are $\mathscr{T}$ functions, so are $XY:P\to\mathscr{B}(\mathscr{K})$, $x\mapsto X(x)Y(x)$, and $X^*:P\to\mathscr{B}(\mathscr{K})$, $x\mapsto X(x)^*$. Especially, each with respect to the strong operator topology piecewise continuous function $X:P\to\mathscr{B}(\mathscr{K})$ with $\sup\{\|X(x)\|\;\;|x\in P\}<\infty$ is of class $\mathscr{T}$. Each $\mathscr{T}$ function is weakly measurable, and hence the operator $\int_P(1_{\mathscr{H}}\otimes X(x))d(\mathscr{P}(x)\otimes 1_{\mathscr{K}})$ exists.

Proposition A.2: Let $X:P\to\mathscr{B}(\mathscr{K})$ be a $\mathscr{T}$ function with some associated sequence $(X_n)_{n\in\mathbb{N}}$ of elementary functions. Then it follows in the strong operator topology,

$$\int_P(1_{\mathscr{H}}\otimes X(x))d(\mathscr{P}(x)\otimes 1_{\mathscr{K}})=s-\lim_{n\to\infty}\int_P(1_{\mathscr{H}}\otimes X_n(x))d(\mathscr{P}(x)\otimes 1_{\mathscr{K}}).$$

Corollary A.3: If $X:P\to\mathcal{B}(\mathcal{K})$ and $Y:P\to\mathcal{B}(\mathcal{K})$ are $\mathcal{T}$ functions, then the product property is valid in any case concerning the separability or nonseparability of $\mathcal{H}$ and $\mathcal{K}$.

Moreover, in each case, where the product property of Theorem A.1(c) is valid, one has for all $\phi\in\mathcal{H}$ and $\psi\in\mathcal{K}$,

$$\left\| \int_P (1_{\mathcal{H}}\otimes X(x))d(\mathcal{P}(x)\otimes 1_{\mathcal{K}})\phi\otimes\psi \right\|^2 = \int_P \|X(x)\psi\|^2 d\langle\phi|\mathcal{P}(x)\phi\rangle.$$

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On stochastic diffusion equations and stochastic Burgers' equations

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In this paper we construct a strong solution for the stochastic Hamilton Jacobi equation by using stochastic classical mechanics before the caustics. We thereby obtain the viscosity solution for a certain class of inviscid stochastic Burgers' equations. This viscosity solution is not continuous beyond the caustics of the corresponding Hamilton Jacobi equation. The Hopf–Cole transformation is used to identify the stochastic heat equation and the viscous stochastic Burgers' equation. The exact solutions for the above two equations are given in terms of the stochastic Hamilton Jacobi function under a no-caustic condition. We construct the heat kernel for the stochastic heat equation for zero potentials in hyperbolic space and for harmonic oscillator potentials in Euclidean space thereby obtaining the stochastic Mehler formula. © *1996 American Institute of Physics.* [S0022-2488(96)00401-8]

I. INTRODUCTION

Inspired by Maslov's quasiclassical asymptotics of quantum mechanics,[1] Truman,[2] Elworthy and Truman[3–5] developed the path-space Hamilton Jacobi theory (elementary formula method or semiclassical analysis) in order to treat the deterministic heat equation (and Schrödinger equation) to get quasiclassical expansions for their solutions. It was proved that before the caustic time the Hamilton Jacobi equation has a $C^{1,2}$ solution which gives the exact solution of the diffusion equation (and Schrödinger equation) geared to small time asymptotics. From Varadhan's or Wentzell–Freidlin's large deviation theories (Varadhan,[6] Freidlin and Wentzell[7]), we only know that the Hamilton Jacobi function gives the leading term. The new method resulted in the discovery of a new ''Brownian Riemannian'' bridge process on manifolds and an elegant new version of the Feynman–Kac formula in curved space geared to simplifying small-time and small-$\hbar$ asymptotics. The same methods have been applied to traveling waves for nonlinear reaction diffusion equations in Elworthy, Truman, and Zhao.[8] A generalization of this Brownian Riemannian bridge process has been obtained in Watling.[9] Quite recently we developed the corresponding stochastic Hamilton Jacobi theory in Truman and Zhao.[10] Using these results, certain stochastic partial differential equations have been solved explicitly and heat kernels and small time asymptotics have been obtained. The stochastic Hamilton Jacobi theory is the main tool used to obtain the results in the present paper.

In this paper we first construct a strong solution for the stochastic Hamilton Jacobi equation and examine the stochastic heat equation with Stratonovich white noise in time. As long as the map defined by the stochastic Hamiltonian system is a diffeomorphism on the configuration space the stochastic Hamilton Jacobi equation has a strong solution. Here we simplify the Feynman–Kac integral for the solution of the stochastic heat equation and get a rigorous semiclassical representation by changing measures using the stochastic Hamilton Jacobi theory. As applications, we take the limits $\mu\to 0$ to get WKB expansions for the solutions. We continue by considering the heat kernel on a complete Riemannian manifold with a pole and using the harmonic oscillator potential we obtain the stochastic Mehler formula.

By the well known Hopf–Cole transformation, the stochastic heat equation is equivalent to the viscous stochastic Burgers' equation which is the KPZ model for the dynamics of the interface introduced by Kardar, Parisi, and Zhang.[11] (See Sec. V for more details.) In the limit $\mu\to 0$ the

equation is the inviscid stochastic Burgers' equation which is the gradient of the stochastic Hamilton Jacobi equation. Using the logarithmic transformation and the stochastic Hamilton Jacobi theory, we get a rigorous formula relating the solutions for the viscous stochastic Burgers' equation and inviscid stochastic Burgers' equation before the caustic time of the corresponding stochastic classical mechanics. We identify the inviscid limit and semiclassical limit under the no-caustics condition. Beyond the caustics we show the solution of the inviscid Burgers' equation is discontinuous. For certain types of equations we prove the existence and uniqueness of the viscosity solution and generalize Wentzell–Freidlin's large deviation theory from deterministic heat equations to stochastic ones as an easy consequence of our theory. Some examples of random shock waves beyond the caustics are given. Needless to say, the occurrence of caustics for the heat equation leads to the appearance of shock waves for the corresponding inviscid Burgers' equation. Indeed a classification of the caustics could lead to a classification of shock waves (Arnold[12]).

In this paper we restrict the Stratonovich white noise term to be white noise in time. We are currently investigating whether our treatment can be generalized to include white noise in space and the (much more difficult) white noise in space–time. The method can clearly be extended to include random initial data but we do not do so here because of restrictions on the length of the paper.

II. THE STOCHASTIC HAMILTON JACOBI EQUATIONS AND STOCHASTIC DIFFUSION EQUATIONS

(1) Let M be an n-dimensional Riemannian manifold. For $c\in C^{1,2}([0,+\infty)\times M,R)$, $S_0\in C^2(M,R)$ and $k\in C^{1,2}([0,+\infty)\times M,R^m)$ and an m-dimensional Brownian motion w_s on probability space $(\Omega,\mathcal{F}_t,P)$, define $\Phi_s:M\times\Omega\to M$ by the following stochastic mechanical system for each $x\in M$:

$$\begin{cases} d\dot{\Phi}_s(x)=-\nabla c(s,\Phi_s(x))ds-\nabla\langle k(s,\Phi_s(x)),dw_s\rangle \\ \dot{\Phi}_0(x)=\nabla S_0(x), \quad \Phi_0(x)=x \end{cases}. \tag{2.1}$$

Here $\langle\cdot,\cdot\rangle$ denotes the inner product in R^m. For a mechanical system without noise set $k\equiv 0$. This shows that c is a potential energy function.

First we prove a diffeomorphism result:

Proposition 2.1: If M is compact or if M is complete, ∇c, $\nabla^2 c$, ∇k, $\nabla^2 k$, ∇S_0, $\nabla^2 S_0$ and the curvature tensor R of the manifold M are all bounded, then there exists $T(\omega)>0$ a.s. such that $\Phi_s(\omega):M\to M$ is a diffeomorphism for $0\leqslant s\leqslant T(\omega)$ for a.e. $\omega\in\Omega$.

Proof: Integrating Eq. (2.1) we obtain

$$\dot{\Phi}_s(x)=\nabla S_0(x)-\int_0^s \nabla c(\sigma,\Phi_\sigma(x))d\sigma-\int_0^s \nabla\langle k(\sigma,\Phi_\sigma(x)),dw_\sigma\rangle.$$

It follows that $\dot{\Phi}_s(x)$ is bounded P-a.s. for $s\in[0,T^*]$ for any fixed $T^*>0$. To investigate the gradients of Φ_s, for $v\in T_xM$ and $q:(-1,1)\to M$ with $q(0)=x$ and $\dot{q}(0)=v$, we have

$$d\,\frac{\partial}{\partial s}\,\frac{\partial}{\partial s'}\,\Phi_s(q(s'))=\frac{D}{\partial s'}\,d\,\frac{\partial}{\partial s}\,\Phi_s(q(s'))+R\left\{\frac{\partial}{\partial s}\,\Phi_s(q(s')),\,\frac{\partial}{\partial s'}\,\Phi_s(q(s'))\right\}\dot{\Phi}_s(q(s'))ds.$$

Taking $s'=0$ and from Eq. (2.1) again we have

$$d\,\frac{\partial}{\partial s}\,T_x\Phi_s(v)=R(\dot{\Phi}_s(x),T_x\Phi_s(v))\dot{\Phi}_s(x)ds-\nabla^2 c_s(\Phi_s(x))T_x\Phi_s(v)ds$$

$$-\nabla^2\langle k_s(\Phi_s(x)),dw_s\rangle T_x\Phi_s(v)$$

with $T_x\Phi_0(v)=I$ and $T_x\dot{\Phi}_0(v)=\nabla^2 S_0(x)$. Note that the above equation for $T_x\Phi_s(v)$ is a perturbed linear one with some perturbation, $R(\dot{\Phi}_s(x),T_x\Phi_s(v))\dot{\Phi}_s(x)$ which is bounded P-a.s. because $\dot{\Phi}_s$ is bounded P-a.s. Therefore, the solution $T_x\Phi_s(v)$ is bounded P-a.s. for $s\in[0,T^*]$ for any fixed $T^*>0$. Integration of the above equation gives a semimartingale

$$T_x\Phi_t(v)=I+\nabla^2 S_0(x)t+\int_0^t\int_0^\sigma R(\dot{\Phi}_s(x),T_x\Phi_s(v))\dot{\Phi}_s(x)ds\ d\sigma$$
$$-\int_0^t\int_0^\sigma \nabla^2 c_s(\Phi_s(x))T_x\Phi_s(v)ds\ d\sigma-\int_0^t\int_0^\sigma \nabla^2\langle k_s(\Phi_s(x)),dw_s\rangle T_x\Phi_s(v)d\sigma.$$

It is clear now that there exists $T(\omega)>0$ (let $T<T^*$ if necessary) such that for $0\leqslant t\leqslant T(\omega)$, the matrix norm $\|\nabla^2 S_0(x)t+\int_0^t\int_0^\sigma R(\dot{\Phi}_s(x),T_x\Phi_s(v))\dot{\Phi}_s(x)ds\ d\sigma-\int_0^t\int_0^\sigma\nabla^2 c_s(\Phi_s(x))T_x\Phi_s(v)ds\ d\sigma-\int_0^t\int_0^\sigma\nabla^2\langle k_s(\Phi_s(x)),dw_s\rangle T_x\Phi_s(v)d\sigma\|<1$ for a.e. $\omega\in\Omega$. By a similar argument to the one in Elworthy and Truman[4] we know for $0\leqslant t\leqslant T(\omega)$, $T_x\Phi_t(v)(\omega)$ is nonsingular. The diffeomorphism follows from the global inverse function theorem. (See, Ref. 4 for example.) ■

For $t\geqslant 0$, $y\in M$ define $\tilde{S}:[0,+\infty)\times M\to R$ by the following nonanticipating Itô stochastic integral:

$$\tilde{S}_t(y,\omega)=\frac{1}{2}\int_0^t|\dot{\Phi}_s(y)|^2ds+S_0(y)-\int_0^t c(s,\Phi_s(y))ds-\int_0^t\langle k(s,\Phi_s(y)),dw_s\rangle. \tag{2.2}$$

We assume a no-caustic condition: there exists $T(\omega)>0$ a.s. such that for $0\leqslant s\leqslant T(\omega)$, $\Phi_s(\omega):M\to M$ is a diffeomorphism for a.e. $\omega\in\Omega$. This is always true provided the conditions in Proposition 2.1 are satisfied. With this assumption we define $S_t(\omega):M\to R^1$ for a.e. $\omega\in\Omega$ and $0\leqslant t\leqslant T(\omega)$ by

$$S_t(x)=\tilde{S}_t(\Phi_t^{-1}(x)). \tag{2.3}$$

We proved the following theorem in Truman and Zhao:[10]

Theorem 2.1 (Truman and Zhao[10]): (i) *Let* Φ *be defined by* Eq. (2.1) *and satisfy the no-caustic condition for* $0\leqslant t\leqslant T(\omega)$ *and* $S_t(x)$ *be defined by* Eq. (2.3) *for* a.e. $\omega\in\Omega$. *Then for any* $0\leqslant t\leqslant T(\omega)$, $x\in M$ *for* a.e. $\omega\in\Omega$:

$$\dot{\Phi}_t(x)=\nabla S_t(\Phi_t(x)). \tag{2.4}$$

(ii) *For any* $0\leqslant t\leqslant T(\omega)$, $x\in M$ *for* a.e. $\omega\in\Omega$, *S satisfies the following stochastic Hamilton Jacobi equation*:

$$dS_t(x)+[\tfrac{1}{2}\|\nabla S_t(x)\|^2+c(t,x)]dt+\langle k(t,x),dw_t\rangle=0. \tag{2.5}$$

Note that $S(t,x)$ is continuous with respect to t and C^2 with respect to x for $0\leqslant t\leqslant T(\omega)$. We call $S(t,x)$ a strong solution of the stochastic Hamilton Jacobi equation (2.5). Another useful identity is the following continuity equation:

Theorem 2.2: *Define* $\phi_t(\omega):M\to R$ *by* $\phi(t,x)=|\det T_x\Phi_t^{-1}|$ (*using the Riemannian metric of* M) *for any* $0\leqslant t\leqslant T(\omega)$ *for* a.e. $\omega\in\Omega$. *Then* ϕ *satisfies the continuity equation*

$$\frac{\partial\phi}{\partial t}(t,x)+\operatorname{div}(\phi(t,x)\nabla S(t,x))=0. \tag{2.6}$$

Proof: Take any C^∞ function $f:M\to R$ with compact support. Integrating by parts,

$$\int_M \operatorname{div}(\phi(t,-)\nabla S(t,-))(x)f(x)dx = -\int_M \phi(t,x)\langle \nabla S(t,x), \nabla f(x)\rangle dx$$

$$= -\int_M \langle \nabla S(t,\Phi_t(x)), \nabla f(\Phi_t(x))\rangle dx$$

$$= -\int_M df(\dot{\Phi}_t(x))dx = -\frac{d}{dt}\int_M f(\Phi_t(x))dx$$

$$= -\frac{d}{dt}\int_M f(x)\phi(t,x)dx$$

$$= -\int_M f(x)\frac{\partial}{\partial t}\phi(t,x)dx$$

using Eq. (2.4). As f is an arbitrary $C^\infty(M,R)$ function then the continuity equation follows. ■

(2) Consider the following stochastic diffusion equation:

$$\begin{cases} du_t^\mu(x) = \left[\frac{1}{2}\mu^2\Delta u_t^\mu(x) + \frac{1}{\mu^2}c(t,x)u_t^\mu(x)\right]dt + \frac{1}{\mu^2}u_t^\mu(x)\langle k(t,x), \partial w_t\rangle \\ u_0^\mu(x) = T_0(x)\exp\left\{-\frac{S_0(x)}{\mu^2}\right\} \end{cases}, \tag{2.7}$$

where $x \in M$, an n-dimensional Riemannian manifold and Δ its Laplace–Beltrami operator, $c \in C^{1,2}(R^1 \times M, R^1)$, $k \in C^{1,2}(R^1 \times M, R^m)$ and w_t an m-dimensional Brownian motion, ∂ being the Stratonovich derivative. Given $T_0 : M \to R^1$ a bounded measurable function and $S_0 : M \to R^1$ a C^2 function, let $u_t^\mu(x)$ denote the solution of Eq. (2.7). We do not treat the existence theory of the solution for the stochastic diffusion equation here. For this we refer the readers to Flandoli.[13] In the following we always suppose the solution to Eq. (2.7) exists and is regular. Clearly the solution is positive if $T_0 > 0$ and in this case for given mild conditions on c and k there is a unique positive solution to Eq. (2.7).

For such $c \in C^{1,2}([0,+\infty)\times M, R)$ and $k \in C^{1,2}([0,+\infty)\times M, R)$ and $S_0 \in C^2(M,R)$, let $S_t(x)$ be defined by Eq. (2.3) for $0 \leqslant t \leqslant T(\omega)$ for a.e. $\omega \in \Omega$ if the map $\Phi_t : M \to M$ satisfies the no-caustic condition for $0 \leqslant t \leqslant T(\omega)$ in configuration space M for a.e. $\omega \in \Omega$.

Here we use some of the results of Eells and Elworthy (Elworthy[14]). Let $\Pi : O(M) \to M$ be the orthonormal frame bundle of M. The Levi-Civita connection of M determines a map $\chi : O(M) \times R^n \to TO(M)$ into the tangent space to $O(M)$, which trivializes the horizontal tangent bundle of M. Let $\tilde{A}_t : O(M) \to TO(M)$ be its horizontal lift: so $T\Pi(\tilde{A}_t(\mathscr{U})) = A_t(\Pi(\mathscr{U}))$, $0 \leqslant t \leqslant \tau$, $\mathscr{U} \in O(M)$, where $T\Pi : TO(M) \to TM$ is the derivative map of Π.

For $x_0 \in M$ take $\mathscr{U}_0 \in \Pi^{-1}(x_0)$ and consider the Stratonovich stochastic equation for $\mathscr{U} : [0,\xi_A) \times \hat{\Omega} \to O(M)$ with $\mathscr{U}(0,\hat{\omega}) = \mathscr{U}_0$, $0 \leqslant s \leqslant t$:

$$d\mathscr{U}_s^{t,\mu} = \mu\chi(\mathscr{U}_s^{t,\mu}) \cdot dB_s + \tilde{A}_s^t(\mathscr{U}_s^{t,\mu})ds, \tag{2.8}$$

where B_s is an n-dimensional Brownian motion defined on the probability space $(\hat{\Omega}, \hat{\mathscr{F}}, \hat{P})$. Define $\hat{\mathscr{F}}_s = \sigma\{B_{s_1} : 0 \leqslant s_1 \leqslant s\}$. The solution $\mathscr{U}_s^{t,\mu}$ with explosion time $0 < \xi_A \leqslant +\infty$ for all $\hat{\omega} \in \hat{\Omega}$ is $\hat{\mathscr{F}}_s$ measurable. Finally we define $X_s^{t,\mu}$ on M by $X_s^{t,\mu} = \Pi(\mathscr{U}_s^{t,\mu})$. Let $\{B_s^{t,\mu} : 0 \leqslant s \leqslant t\}$ be the solution of Eq. (2.8) with $A \equiv 0$. Note that $B_s^{t,\mu}$, $X_s^{t,\mu} \in \hat{\mathscr{F}}_s$.

Given the initial condition $u_0^\mu(x)$ for Eq. (2.7), then by the Feynman–Kac formula we have

$$u_t^\mu(x)=\hat{E}T_0(B_t^{t,\mu})\exp\left\{-\frac{1}{\mu^2}S_0(B_t^{t,\mu})+\frac{1}{\mu^2}\int_0^t c(t-s,B_s^{t,\mu})ds+\frac{1}{\mu^2}\int_0^t\langle k(t-s,B_s^{t,\mu}),dw_{t-s}\rangle\right\}. \tag{2.9}$$

Given a drift A_s^t, we have a solution X_s^t to Eq. (2.8). If X_s^t is nonexplosive and the stochastic integral $\int_0^t\langle k(t-s,X_s^{t,\mu}(x)),dw_{t-s}\rangle$ is well defined in the Itô sense, then we can use the Maruyama–Girsanov–Cameron–Martin formula to give

$$u_t^\mu(x)=\hat{E}T_0(X_t^{t,\mu}(x))\exp\left\{-\frac{1}{\mu^2}S_0(X_t^{t,\mu}(x))+\frac{1}{\mu^2}\int_0^t c(t-s,X_s^{t,\mu}(x))ds+\frac{1}{\mu^2}\int_0^t\langle k(t-s,X_s^{t,\mu}(x)),dw_{t-s}\rangle\right\}\mathscr{M}_t^\mu, \tag{2.10}$$

where

$$\mathscr{M}_t^\mu=\exp\left\{-\frac{1}{\mu}\int_0^t\langle A_s^t(X_s^{t,\mu}(x)),\mathscr{C}_s^{t,\mu}dB_s\rangle-\frac{1}{2\mu^2}\int_0^t\|A_s^t(X_s^{t,\mu}(x))\|^2ds\right\}. \tag{2.11}$$

On the other hand if we choose $A_s^t=\nabla Y_s^t$ for some suitable $Y_s^t:0\leqslant s\leqslant t$, then Itô's formula yields

$$Y_t(X_t^{t,\mu}(x))-Y_0(x)=\int_0^t\{\langle\nabla Y_s(X_s^{t,\mu}(x)),\mu\mathscr{C}_s^{t,\mu}\,dB_s\rangle+[\tfrac{1}{2}\mu^2\Delta Y_s(X_s^{t,\mu}(x))+\langle\nabla Y_s(X_s^{t,\mu}(x)),A_s(X_s^{t,\mu}(x))\rangle]ds+dY_s(X_s^{t,\mu}(x))\}. \tag{2.12}$$

Substituting $\int_0^t\langle\nabla Y_s(X_s^{t,\mu}(x)),\mathscr{C}_s^{t,\mu}\,dB_s\rangle$ in Eq. (2.11) by solving for $\int_0^t\langle\nabla Y_s(X_s^{t,\mu}(x)),\mathscr{C}_s^{t,\mu}\,dB_s\rangle$ in Eq. (2.12) we get

$$\mathscr{M}_t^\mu=\exp\left\{\frac{1}{\mu^2}(Y_0(x)-Y_t(X_t^{t,\mu}(x)))+\frac{1}{2}\int_0^t\Delta Y_s(X_s^{t,\mu}(x))ds+\frac{1}{\mu^2}\int_0^t\left(dY_s(X_s^{t,\mu}(x))+\frac{1}{2}\|A_s^t(X_s^{t,\mu}(x))\|^2ds\right)\right\}. \tag{2.13}$$

(3) Denote $w_s^*=w_{t-s}$ and $\mathscr{F}_s^*$ to be the enlargement of the filtration $\{\mathscr{F}_s^0\}$, where

$$\mathscr{F}_s^0=\sigma\{w_r^*:r\leqslant s\}. \tag{2.14}$$

Then $w_{t-s}=w_s^*$ is $\mathscr{F}_s^*$ measurable and $\mathscr{F}_{s_1}^*\subset\mathscr{F}_{s_2}^*$ if $s_1\leqslant s_2$. See Rogers and Williams[15] for the filtration $\mathscr{F}_s^*$.

If we take $Y_s=-S_{t-s}$ and if ∇S_{t-s} is $\mathscr{F}_s^*$ measurable for $0\leqslant s\leqslant t$ for fixed t, then we have a $\mathscr{F}_s^*$ measurable solution $X_s^{t,\mu}(x)$ to Eq. (2.8). Then we have the following theorem:

Theorem 2.3: *Assume* $c\in C^{1,2}([0,+\infty)\times M,R^1)$, $k\in C^{1,2}([0,+\infty)\times M,R^m)$ *and* $S_0\in C^2(M,R)$ *and* $T_0:M\to R^1$ *bounded and measurable,* w_t *is an* m*-dimensional Brownian motion on probability space* $(\Omega,\mathscr{F},P)$*. Let the map defined by Eq. (2.1) satisfy the no-caustic condition for* $0\leqslant t\leqslant T(\omega)$ *for a.e.* $\omega\in\Omega$ *and let* $S_t(x)$ *be the Hamilton Jacobi function defined by Eqs. (2.2) and (2.3) and* $X_s^{t,\mu}(x)$ *be the Markov process defined by Eq. (2.8) with* $Y_s=-S_{t-s}$*. If* $X_s^{t,\mu}(x)$ *is* $\mathscr{F}_s^*$ *measurable for fixed* t *and nonexplosive, then for* $0\leqslant t\leqslant T(\omega)$ *for a.e.* $\omega\in\Omega$,

$$u_t^\mu(x)=\exp\left\{-\frac{S_t(x)}{\mu^2}\right\}\hat{E}T_0(X_t^{t,\mu}(x))\exp\left\{-\frac{1}{2}\int_0^t \Delta S_{t-s}(X_s^{t,\mu}(x))ds\right\}. \tag{2.15}$$

Proof: Taking $Y_s=-S_{t-s}$, as long as $X_s^{t,\mu}(x)$ is $\mathscr{F}_s^*$ measurable and nonexplosive for $0\leqslant s\leqslant t$ for any fixed t, from Eqs. (2.10) and (2.13) we have

$$\begin{aligned}u_t^\mu(x)=\hat{E}T_0(X_t^{t,\mu}(x))\exp\Bigg\{&-\frac{1}{\mu^2}S_0(X_t^{t,\mu}(x))+\frac{1}{\mu^2}\int_0^t c(t-s,X_s^{t,\mu}(x))ds\\&+\frac{1}{\mu^2}\int_0^t\langle k(t-s,X_s^{t,\mu}(x)),dw_{t-s}\rangle\Bigg\}\\&\times\exp\Bigg\{\frac{1}{\mu^2}\{-S_t(x)+S_0(X_t^{t,\mu}(x))\}-\frac{1}{2}\int_0^t\Delta S_{t-s}(X_s^{t,\mu}(x))ds\\&+\frac{1}{\mu^2}\int_0^t\Bigg(-dS_{t-s}(X_s^{t,\mu}(x))+\frac{1}{2}\|\nabla S_{t-s}(X_s^{t,\mu}(x))\|^2ds\Bigg)\Bigg\}.\end{aligned}$$

From the stochastic Hamilton–Jacobi equation, i.e.,

$$-dS_{t-s}(X_s^{t,\mu}(x))+\{\tfrac{1}{2}\|\nabla S_{t-s}(X_s^{t,\mu}(x))\|^2+c(t-s,X_s^{t,\mu}(x))\}ds+\langle k(t-s,X_s^{t,\mu}(x)),dw_{t-s}\rangle=0,$$

formula (2.15) follows. ■

Remark 2.1: For $\mu=1$, we get Theorem 2.1 in Truman and Zhao.[10]

From Theorem 2.2 we have

$$-\Delta S(t,x)=\frac{\partial}{\partial t}\log\,\phi(t,x)+\langle\nabla\,\log\,\phi(t,x),\nabla S(t,x)\rangle. \tag{2.16}$$

In particular we obtain

$$-\Delta S(t-s,z_s^t(x))=-\frac{\partial}{\partial s}\log\,\phi(t-s,z_s^t(x)), \tag{2.17}$$

where $z_s^t(x)=\Phi_{t-s}(\Phi_t^{-1}(x))$. By Eq. (2.4) we have

$$\frac{\partial}{\partial s}z_s^t(x)=-\nabla S_{t-s}(z_s^t(x)). \tag{2.18}$$

For each $\omega\in\Omega$, if ∇S_{t-s} is bounded then as $\mu\to 0$, $X_s^{t,\mu}(x)\to z_s^t(x)$ in $\hat{P}$ probability. Therefore, applying Lebesgue's dominated convergence theorem to Eq. (2.15) we have

$$\lim_{\mu\to 0}\exp\left\{\frac{S_t(x)}{\mu^2}\right\}u_t^\mu(x)=T_0(z_t^t(x))\exp\left\{-\frac{1}{2}\int_0^t\Delta S_{t-s}(z_s^t(x))ds\right\}$$

for each $\omega\in\Omega$. The following theorem follows from Eq. (2.17).

Theorem 2.4: *Assume all the conditions in Theorem* 2.3 *and, for a.e.* $\omega\in\Omega$, ∇S *is bounded and* ΔS *is bounded from below for* $0\leqslant t\leqslant T(\omega), x\in M$, *and* T_0 *is continuous. Then for a.e.* $\omega\in\Omega$, $0\leqslant t\leqslant T(\omega)$:

$$\lim_{\mu\to 0}\exp\left\{\frac{S_t(x)}{\mu^2}\right\}u_t^\mu(x)=T_0(\Phi_t^{-1}(x))\sqrt{\phi_t(x)}. \tag{2.19}$$

Here $\phi_t(x)=|\det T_x\Phi_t^{-1}|$

For $0\leqslant t\leqslant T(\omega)$, let

$$\psi(t,x)=T_0(\Phi_t^{-1}(x))\sqrt{\phi_t(x)}. \tag{2.20}$$

Then if T_0 is positive and C^1 we have the continuity equation for $\psi_t(x)$. It turns out that

$$\frac{\partial}{\partial t}\log\,\psi_t(x)=-\frac{1}{2}\,\Delta S_t(x)-\langle\nabla\,\log\,\psi_t(x),\nabla S_t(x)\rangle. \tag{2.21}$$

Now take $Y(s,a)=-S(t-s,a)+\mu^2\log\,\psi_{t-s}(a)$ and let $X_s^{t,\mu}(x)$ be the solution of Eq. (2.8) for Y. Note X_s is nonexplosive if ∇S and $\nabla\log\psi$ are bounded P-a.s. By Eq. (2.13) we calculate the martingale $\mathscr{M}_t^\mu$:

$$\begin{aligned}\mathscr{M}_t^\mu=&\exp\Bigg\{\frac{1}{\mu^2}\,[-S_t(x)+\mu^2\,\log\,\psi_t(x)+S_0(X_t^{t,\mu}(x))-\mu^2\,\log\,\psi_0(X_t^{t,\mu}(x))]\\&-\frac{1}{2}\int_0^t\Delta S_{t-s}(X_s^{t,\mu}(x))ds+\frac{1}{2}\int_0^t\mu^2\Delta\,\log\,\psi_{t-s}(X_s^{t,\mu}(x))ds+\frac{1}{\mu^2}\int_0^t\Bigg[-dS_{t-s}(X_s^{t,\mu}(x))\\&+\Bigg(\mu^2\frac{\partial}{\partial s}\log\,\psi_{t-s}(X_s^{t,\mu}(x))+\frac{1}{2}\,\|-\nabla S_{t-s}(X_s^{t,\mu}(x))+\mu^2\nabla\,\log\,\psi_{t-s}(X_s^{t,\mu}(x))\|^2\Bigg)ds\Bigg]\Bigg\}\\=&\exp\Bigg\{-\frac{S_t(x)}{\mu^2}\Bigg\}\psi_t(x)\exp\Bigg\{\frac{1}{\mu^2}\,S_0(X_t^{t,\mu}(x))-\log\,\psi_0(X_t^{t,\mu}(x))-\frac{1}{2}\int_0^t\Delta S_{t-s}(X_s^{t,\mu}(x))ds\\&+\frac{1}{2}\,\mu^2\int_0^t\psi_{t-s}^{-1}(X_s^{t,\mu}(x))\Delta\psi_{t-s}(X_s^{t,\mu}(x))ds-\frac{1}{2}\int_0^t\mu^2\|\nabla\,\log\,\psi_{t-s}(X_s^{t,\mu}(x))\|^2ds\\&+\frac{1}{\mu^2}\int_0^t\Bigg\{-dS_{t-s}(X_s^{t,\mu}(x))+\frac{1}{2}\,\|\nabla S_{t-s}(X_s^{t,\mu}(x))\|^2ds\Bigg\}+\int_0^t\Bigg[\frac{\partial}{\partial s}\log\,\psi_{t-s}(X_s^{t,\mu}(x))\\&-\langle\nabla S_{t-s}(X_s^{t,\mu}(x)),\nabla\,\log\{\psi_{t-s}(X_s^{t,\mu}(x))\rangle\Bigg]ds+\frac{1}{2}\int_0^t\mu^2\|\nabla\,\log\,\psi_{t-s}(X_s^{t,\mu}(x))\|^2ds\Bigg\}.\end{aligned}$$

Therefore by Eqs. (2.21) and (2.10) and the stochastic Hamilton–Jacobi equation we have the following formula as long as $\int_0^t\langle k(t-s,X_s^{t,\mu}(x)),dw_{t-s}\rangle$ is well defined.

Theorem 2.5: *Assume that c and k and* S_0 *are* C^3 *with all the conditions of Theorem* 2.3 *and also that* ∇S *and* $\nabla\log\psi_t$ *are bounded and* ψ_{t-s} *is* $\mathscr{T}_s^*$ *measurable for any* $0\leqslant s\leqslant t$ *and fixed* t. *Then for any* $\mu\neq 0$, $0\leqslant t\leqslant T(\omega)$ *for a.e.* $\omega\in\Omega$,

$$u_t^\mu(x)=\exp\Bigg\{-\frac{1}{\mu^2}\,S_t(x)\Bigg\}\psi_t(x)\hat{E}\,\exp\Bigg\{\frac{1}{2}\,\mu^2\int_0^t\psi_{t-s}^{-1}(X_s^{t,\mu}(x))\Delta\psi_{t-s}(X_s^{t,\mu}(x))ds\Bigg\}, \tag{2.22}$$

where $X_s^{t,\mu}(x)$ *is defined by Eq.* (2.8) *with* $Y_s=-S_{t-s}+\mu^2\log\psi_{t-s}$.

Remark 2.2: For $k\equiv 0$, we get Formula B of Elworthy and Truman.[5]

As $\mu\to 0$, $X_s^{t,\mu}(x)$ converges to $z_s^t(x)$ in $\hat{P}$ probability for each $\omega\in\Omega$. As long as $\psi^{-1}\Delta\psi$ is bounded we can apply Lebesgue's dominated convergence theorem and the Taylor expansion theorem to give the following post-WKB expansion:

Theorem 2.6: *Assume all the conditions of Theorem* 2.5 *and* $\psi^{-1}\Delta\psi$ *is bounded for all* $0\leqslant t\leqslant T(\omega)$ *for a.e.* $\omega\in\Omega$ *and* $x\in M$. *Then for sufficiently small* $\mu\neq 0$, $0\leqslant t\leqslant T(\omega)$ *for a.e.* $\omega\in\Omega$:

$$u_t^{\mu}(x)=\exp\left\{-\frac{1}{\mu^2}S_t(x)\right\}\psi_t(x)\left\{1+\frac{1}{2}\mu^2\int_0^t\psi_{t-s}^{-1}(z_s^t(x))\Delta\psi_{t-s}(z_s^t(x))ds+\circ(\mu^2)\right\}. \tag{2.23}$$

Remark 2.3: As long as the stochastic integral $\int_0^t\langle k(t-s,X_s^{t,\mu}),dw_{t-s}\rangle$ is well defined in Itô's sense, Theorems 2.3–2.6 are still true. In most of the situations, this condition is satisfied.

III. THE HEAT KERNEL

(1) Let M be an n-dimensional Riemannian manifold, with global normal coordinates and a Riemannian metric $r(\cdot,\cdot)$. Consider the following stochastic heat equation:

$$du_t(x)=[\tfrac{1}{2}\Delta u_t(x)+c(t,x)u_t(x)]dt+u_t(x)(\langle\gamma(t),\partial w_t\rangle+\langle x,\eta\partial w_t\rangle), \tag{3.1}$$

where $x\in M$, Δ is a Laplace Beltrami operator, w_t is an m-dimensional Brownian motion, $\eta:R^m\to R^n$ is a linear map, $\gamma\in C^1([0,\infty),R^m)$ is bounded. Let $p_t^{\lambda}(x,y)$ be the solution of Eq. (3.1) with the initial condition

$$p_0^{\lambda}(x,y)=\frac{1}{(2\pi\lambda)^{n/2}}\exp\left\{-\frac{r^2(x,y)}{2\lambda}\right\}. \tag{3.2}$$

Then the heat kernel $p_t(x,y)$ of Eq. (3.1) is given by

$$p_t(x,y)=\lim_{\lambda\to 0}p_t^{\lambda}(x,y). \tag{3.3}$$

Suppose $y\in M$ is a pole for M so that $\exp_y:T_yM\to M$ is a C^{∞} diffeomorphism. Denote $x=\exp_y(v)$. Therefore we have a global system of normal coordinates from y in which the geodesics from y are represented as straight lines from the origin. Let $\theta_y(v)$ be the Jacobian determinant of $\exp_y$ at v (Ruses' invariant): $\theta_y(v)=|\det_M T_v\exp_y|$, where $\det_M$ indicates that the inner product of T_yM and $T\exp_y(v)M$ are used to define the determinant. We shall often write θ for θ_y.

From now on let the stochastic process $X_s^{t,\lambda}$ be defined in our normal coordinates by Eq. (2.8) where we take $\mu=1$ with

$$A_s^{t,\lambda}(x)=\eta w_{t-s}-\frac{v+\int_0^{t-s}\eta w_\sigma\,d\sigma}{\lambda+t-s}-\frac{1}{2}\nabla\log\theta\left(v+\int_0^{t-s}\eta w_\sigma\,d\sigma\right). \tag{3.4}$$

Let $\xi_s^{t,\lambda}=v_s^{t,\lambda}+\int_0^{t-s}\eta w_\sigma\,d\sigma$. Then from Eq. (2.8) $\xi_s^{t,\lambda}$ satisfies an equation which does not include the stochastic process w except for the initial condition $\xi_0^{t,\lambda}=v_0+\int_0^t\eta w_\sigma\,d\sigma$. Thus we can write $\xi_s^{t,\lambda}=F_s^{t,\lambda}(v_0+\int_0^t\eta w_\sigma\,d\sigma)$ for some functional $F_s^{t,\lambda}$ which is independent of w. Recall $v_s^{t,\lambda}=\xi_s^{t,\lambda}-\int_0^{t-s}\eta w_\sigma\,d\sigma=F_s^{t,\lambda}(v_0+\int_0^t\eta w_\sigma\,d\sigma)-\int_0^t\eta w_\sigma\,d\sigma+\int_{t-s}^t\eta w_\sigma\,d\sigma$. Thus the stochastic integral $\int_0^t\langle X_s^{t,\lambda},\eta\,dw_{t-s}\rangle$ is well defined in Itô's sense.

Lemma 3.1: As $\lambda\to 0$, $\{X_s^{t,\lambda}:0\leqslant s\leqslant t\}$ converges in law $(\hat{P})$ to the process $\{X_s^t(x):0\leqslant s\leqslant t\}$ which is sample continuous, agrees with $X_s^{t,0}$ for $0\leqslant s<t$ and $X_t^t(x)=y$.

Proof: As for $0\leqslant s<t$, as $\lambda\to 0$, $A_s^{t,\lambda}\to Z_s^t$ where

$$Z_s^t=\eta w_{t-s}-\frac{v_s+\int_0^{t-s}\eta w_\sigma\,d\sigma}{t-s}-\frac{1}{2}\nabla\log\theta\left(v_s+\int_0^{t-s}\eta w_\sigma\,d\sigma\right),\quad 0\leqslant s<t. \tag{3.5}$$

It follows from Sec. 4 Chap. VIII and Theorem 8C of Chap. VII of Elworthy[14] [that as $\lambda\to 0$ so $X_s^{t,\lambda}$ converges in $\hat{P}$ probability for $0\leqslant s<t$, to a standard Brownian motion $X_s^{t,0}$ with a drift Z_s^t. Note that Z_s^t as well as $A_s^{t,\lambda}$ depends on the Brownian motion w_s on the probability space

$(\Omega,\mathcal{F},P)$. However this does not affect our argument. To see what happens at time t define $r_s: M \to R$ by $r_s(v) = r(v + \int_0^{t-s} \eta w_\sigma \, d\sigma, y)$. Then $r_s(-)$ is C^2 on $M - \{y\}$ while, if $n \geqslant 2$, and $x \neq y$, with $\hat{P}$ probability one $X_s^{t,\lambda}$ avoids y for $0 \leqslant s < t$ as does $X_s^{t,0}(x)$ for $0 \leqslant s < t$. Therefore by Itô's formula, for $0 \leqslant s < t$,

$$r_s(v_s^t) = r_0(x) + \int_0^s dr_\sigma(\mathscr{U}_\sigma \, dB_\sigma) + \int_0^s dr_\sigma \, Z_\sigma^t(v_\sigma^t) d\sigma + \frac{1}{2} \int_0^s \Delta r_\sigma(v_\sigma^t) d\sigma + \int_0^s \frac{\partial r_\sigma}{\partial \sigma}(v_\sigma^t) d\sigma. \tag{3.6}$$

We see from Elworthy[14] that

$$\Delta r = \frac{n-1}{r} + \frac{\partial}{\partial r} \log \theta. \tag{3.7}$$

Then it follows that

$$\frac{1}{2} \Delta r_\sigma(v_\sigma) = \frac{1}{2} \frac{n-1}{r(v_\sigma^t + \int_0^{t-\sigma} \eta w_\sigma \, d\sigma)} + \frac{1}{2} \frac{\partial}{\partial r} \log \theta \left(v_\sigma^t + \int_0^{t-\sigma} \eta w_\sigma \, d\sigma \right). \tag{3.8}$$

In our coordinates

$$\nabla r_\sigma(v) = \frac{v + \int_0^{t-\sigma} \eta w_\sigma \, d\sigma}{|v + \int_0^{t-\sigma} \eta w_\sigma \, d\sigma|}.$$

Therefore,

$$dr_\sigma \, Z_\sigma^t(v_\sigma) = dr_\sigma \, \eta w_{t-\sigma} - \frac{r(v_\sigma^t + \int_0^{t-\sigma} \eta w_\sigma \, d\sigma)}{t-\sigma} - \frac{1}{2} \frac{\partial}{\partial r} \log \theta \left(v_\sigma^t + \int_0^{t-\sigma} \eta w_\sigma \, d\sigma \right). \tag{3.9}$$

Therefore if we let $r_s = r(v_s^t(x) + \int_0^{t-s} \eta w_\sigma \, d\sigma)$ and $\tilde{B}_s = \int_0^s dr_\sigma(\mathscr{U}_\sigma \, dB_\sigma)$, and note the cancellation of the terms $dr_\sigma \, \eta w_{t-\sigma}$ and $\partial r_\sigma / \partial \sigma(v_\sigma^t)$, then

$$r_s = r_0(x) + \tilde{B}_s + \frac{1}{2}(n-1) \int_0^s \frac{d\sigma}{r_\sigma} - \int_0^s \frac{r_\sigma}{t-\sigma} \, d\sigma. \tag{3.10}$$

It turns out from Ikeda and Watanabe[16] that with $\hat{P}$ probability one, r_s converges to 0 as $s \to t$. That is to say $X_s^t(x) \to y$ as $s \to t$. ■

We call $\{X_s^t(x): 0 \leqslant s \leqslant t\}$ a stochastic Brownian Riemannian bridge from x to y in time t on M.

(2) Now if $f: M \to R$ is smooth with $f(x) = F[r(x)]$ for some smooth $F: (0, +\infty) \to R$, then by Elworthy,[17]

$$\Delta f(x) = \frac{\partial^2 F}{\partial r^2} + \left(\frac{n-1}{r(x)} + \frac{\partial}{\partial r} (\log \theta(x)) \right) \frac{\partial F}{\partial r}. \tag{3.11}$$

In particular

$$-\Delta r^2 = -2 - 2(n-1) - 2r \frac{\partial}{\partial r} \log \theta = -2n - 2r \frac{\partial}{\partial r} \log \theta. \tag{3.12}$$

Moreover

$$-\tfrac{1}{2}\,\Delta\,\log\,\theta=\theta^{1/2}\Delta\,\theta^{-(1/2)}-|\nabla\,\log\,\theta^{1/2}|^2. \tag{3.13}$$

We give the heat kernel representation theorem in terms of the stochastic Brownian Riemannian bridge as follows:

Theorem 3.1: *Suppose y is a pole on the n-dimensional Riemannian manifold M. If $\theta^{1/2}\Delta\theta^{-1/2}$ and $c\in C^{1,2}(R\times M,R)$ are bounded above and $\gamma\in C^1(R,R^m)$ is bounded, then the heat kernel of Eq. (3.1) on the Riemannian manifold M is given by*

$$\begin{aligned}p_t(x,y)=&\frac{1}{(2\pi t)^{n/2}}\,\theta^{-(1/2)}\left(\exp(\exp^{-1}(x)+\int_0^t\eta w_s\,ds)\right)\exp\left\{\int_0^t\langle\gamma(s),dw_s\rangle+\frac{1}{2}\int_0^t|\eta w_s|^2ds\right.\\&\left.+\langle x,\eta w_t\rangle-\frac{r^2\{\exp(\exp^{-1}(x)+\int_0^t\eta w_s\,ds),y\}}{2t}\right\}\\&\cdot\hat{E}\,\exp\left\{\frac{1}{2}\int_0^t(\theta^{1/2}\Delta\theta^{-(1/2)})\left(\exp\left(v_s^t+\int_0^{t-s}\eta w_\sigma\,d\sigma\right)\right)ds+\int_0^t c(t-s,X_s^t)ds\right\},\end{aligned} \tag{3.14}$$

where $X_s^t=\exp(v_s^t)$ is the stochastic Brownian Riemannian bridge from x to y at time t on M.

Proof: Define $S_t^\lambda(x)$ by

$$S_t^\lambda(x)=-\int_0^t\langle\gamma(\sigma),dw_\sigma\rangle-\frac{1}{2}\int_0^t|\eta w_\sigma|^2d\sigma-\langle x,\eta w_t\rangle+\frac{r^2(\exp(v+\int_0^t\eta w_\sigma\,d\sigma),y)}{2(\lambda+t)}. \tag{3.15}$$

Take $Y_s^{t,\lambda}(x)=-S_{t-s}^\lambda(x)-\frac{1}{2}\log\theta(v+\int_0^{t-s}\eta w_\sigma\,d\sigma)$. Then $A_s^{t,\lambda}$ is defined by Eq. (3.4) and the stochastic process $X_s^{t,\lambda}\in\mathcal{F}_s^*$. Thus we can use Eq. (2.13) to calculate $\mathcal{M}_t^\lambda$ as follows:

$$\begin{aligned}\mathcal{M}_t^\lambda=\exp&\left\{-S_t^\lambda(x)-\frac{1}{2}\log\,\theta\left(v+\int_0^t\eta w_s\,ds\right)+\frac{r^2(X_t^{t,\lambda},y)}{2\lambda}+\frac{1}{2}\log\,\theta(X_t^{t,\lambda})\right.\\&+\frac{1}{2}\int_0^t\left[-\frac{\Delta r^2(v_s^{t,\lambda}+\int_0^{t-s}\eta w_\sigma\,d\sigma)}{2(\lambda+t-s)}-\frac{1}{2}\Delta\,\log\,\theta\left(v_s^{t,\lambda}+\int_0^{t-s}\eta w_\sigma\,d\sigma\right)\right]ds\\&+\int_0^t\left[-dS_{t-s}(X_s^{t,\lambda})+\left(\nabla\,\log\,\theta^{-(1/2)}\left(v_s^{t,\lambda}+\int_0^{t-s}\eta w_\sigma\,d\sigma\right)(-\eta w_{t-s})\right.\right.\\&+\frac{1}{2}\left\|\eta w_{t-s}-\frac{r(v_s^{t,\lambda}+\int_0^{t-s}\eta w_\sigma\,d\sigma)\nabla r(v_s^{t,\lambda}+\int_0^{t-s}\eta w_\sigma\,d\sigma)}{\lambda+t-s}\right\|^2\\&+\frac{1}{2}\left\|\nabla\,\log\,\theta^{-(1/2)}\left(v_s^{t,\lambda}+\int_0^{t-s}\eta w_\sigma\,d\sigma\right)\right\|^2+\nabla\,\log\,\theta^{-(1/2)}\left(v_s^{t,\lambda}+\int_0^{t-s}\eta w_\sigma\,d\sigma\right)\eta w_{t-s}\\&+\frac{1}{2}\frac{r(v_s^{t,\lambda}+\int_0^{t-s}\eta w_\sigma\,d\sigma)\nabla r(v_s^{t,\lambda}+\int_0^{t-s}\eta w_\sigma\,d\sigma)}{\lambda+t-s}\\&\left.\left.\cdot\nabla\,\log\,\theta\left(v_s^{t,\lambda}+\int_0^{t-s}\eta w_\sigma\,d\sigma\right)\right)ds\right]\right\}.\end{aligned}$$

The first cancellation comes out from $\nabla\log\theta^{-(1/2)}(v_s^{t,\lambda}+\int_0^{t-s}\eta w_\sigma\,d\sigma)(-\eta w_{t-s})+\nabla\log\theta^{-(1/2)}(v_s^{t,\lambda}+\int_0^{t-s}\eta w_\sigma\,d\sigma)\,\eta w_{t-s}\equiv 0$. Then by Eqs. (3.12) and (3.13) we have

$$\mathscr{M}_t = \exp\{-S_t^\lambda(x)\}\theta^{-(1/2)}\left(v+\int_0^t \eta w_s\, ds\right)\cdot\exp\left\{\frac{r^2(X_t^{t,\lambda},y)}{2\lambda}+\frac{1}{2}\log\,\theta(X_t^{t,\lambda})\right.$$
$$+\frac{1}{2}\int_0^t\left[-\frac{n}{\lambda+t-s}-\frac{r(v_s^{t,\lambda}+\int_0^{t-s}\eta w_\sigma\, d\sigma)}{\lambda+t-s}\cdot\frac{\partial}{\partial r}\log\,\theta\left(v_s^{t,\lambda}+\int_0^{t-s}\eta w_\sigma\, d\sigma\right)\right.$$
$$+\theta^{1/2}\left(v_s^{t,\lambda}+\int_0^{t-s}\eta w_\sigma\, d\sigma\right)\Delta\,\theta^{-(1/2)}\left(v_s^{t,\lambda}+\int_0^{t-s}\eta w_\sigma\, d\sigma\right)$$
$$-\left|\nabla\,\log\,\theta^{1/2}\left(v_s^{t,\lambda}+\int_0^{t-s}\eta w_\sigma\, d\sigma\right)\right|^2\Bigg]ds+\int_0^t\Bigg[-dS_{t-s}(X_s^{t,\lambda})$$
$$+\left(\frac{1}{2}\|\nabla S_{t-s}(X_s^{t,\lambda})\|^2+\frac{1}{2}\left\|\nabla\,\log\,\theta^{-(1/2)}\left(v_s^{t,\lambda}+\int_0^{t-s}\eta w_\sigma\, d\sigma\right)\right\|^2\right.$$
$$\left.\left.+\frac{1}{2}\frac{r(v_s^{t,\lambda}+\int_0^{t-s}\eta w_\sigma\, d\sigma)}{\lambda+t-s}\cdot\frac{\partial}{\partial r}\log\,\theta\left(v_s^{t,\lambda}+\int_0^{t-s}\eta w_\sigma\, d\sigma\right)\right)ds\Bigg]\right\}.$$

Thus after the cancellations we have

$$\mathscr{M}_t = \exp\{-S_t^\lambda(x)\}\theta^{-(1/2)}\left(v+\int_0^t \eta w_s\, ds\right)\left(\frac{\lambda}{\lambda+t}\right)^{n/2}\exp\left\{\frac{r^2(X_t^{t,\lambda},y)}{2\lambda}+\frac{1}{2}\log\,\theta(X_t^{t,\lambda})\right.$$
$$+\frac{1}{2}\int_0^t\theta^{1/2}\left(v_s^{t,\lambda}+\int_0^{t-s}\eta w_\sigma\, d\sigma\right)\Delta\,\theta^{-(1/2)}\left(v_s^{t,\lambda}+\int_0^{t-s}\eta w_\sigma\, d\sigma\right)ds$$
$$\left.+\int_0^t\left[-dS_{t-s}(X_s^{t,\lambda})+\frac{1}{2}\|\nabla S_{t-s}(X_s^{t,\lambda})\|^2 ds\right]\right\}. \tag{3.16}$$

Now by the definition of $p_t^\lambda(x,y)$ and Eq. (2.10),

$$p_t^\lambda(x,y)=\frac{1}{(2\pi\lambda)^{n/2}}\hat{E}\,\exp\left\{-\frac{r^2(X_t^{t,\lambda},y)}{2\lambda}+\int_0^t c(t-s,X_s^{t,\lambda})ds\right.$$
$$\left.+\int_0^t\langle\gamma(t-s),dw_{t-s}\rangle+\int_0^t\langle X_s^{t,\lambda},\eta\, dw_{t-s}\rangle\right\}\cdot\mathscr{M}_t. \tag{3.17}$$

From Eq. (3.16) and the fact that S^λ satisfies the stochastic Hamilton Jacobi equation (Truman and Zhao[10]):

$$-dS_{t-s}(X_s^{t,\lambda})+\tfrac{1}{2}\|\nabla S_{t-s}(X_s^{t,\lambda})\|^2 ds+\langle\gamma(t-s),dw_{t-s}\rangle+\langle X_s^{t,\lambda},\eta\, dw_{t-s}\rangle\equiv 0, \tag{3.18}$$

it turns out that

$$p_t^{\lambda}(x,y)=\frac{1}{(2\pi(t+\lambda))^{n/2}}\,\theta^{-(1/2)}\left(v+\int_0^t \eta w_s\,ds\right)\exp\left\{\int_0^t\langle\gamma(t-s),dw_{t-s}\rangle+\frac{1}{2}\int_0^t|\eta w_s|^2ds\right.$$
$$\left.+\langle x,\eta w_t\rangle-\frac{r^2(\exp(v+\int_0^t\eta w_s\,ds),y)}{2(\lambda+t)}\right\}$$
$$\cdot\hat{E}\,\exp\left\{\frac{1}{2}\int_0^t\theta^{1/2}\left(v_s^{t,\lambda}+\int_0^{t-s}\eta w_\sigma\,d\sigma\right)\Delta\theta^{-(1/2)}\left(v_s^{t,\lambda}+\int_0^{t-s}\eta w_\sigma\,d\sigma\right)ds\right.$$
$$\left.+\int_0^t c(t-s,X_s^{t,\lambda})ds+\frac{1}{2}\log\,\theta(X_t^{t,\lambda})\right\}. \tag{3.19}$$

The theorem follows by taking the limit $\lambda\to 0$ in Eq. (3.19) and applying Lebesgue's dominated convergence theorem and Lemma 3.1. ■

With the representation theorem in our hands, using the iterated logarithm law of Brownian motion, the small time asymptotics is a straightforward corollary of Theorem 3.1.

Corollary 3.1: Assume all the conditions of Theorem 3.1. Then for x,y in any compact subset of M as $t\to 0$, the heat kernel $p_t(x,y)$ of Eq. (3.1) satisfies

$$p_t(x,y)=\frac{1}{(2\pi t)^{n/2}}\exp\left\{-\frac{r^2(x,y)}{2t}\right\}\left\{1+\circ\left(\left(t\,\log\frac{1}{t}\right)^{1/2}\right)\right\}\quad P-\text{a.s.} \tag{3.20}$$

If $M=R^n$, then $\theta\equiv 1$, the following theorem in Truman and Zhao[10] follows from Theorem 3.1.

Theorem 3.2 (Truman and Zhao[10]): *Consider Eq. (3.1) for the case $M=R^n$. Assume $c\in C^{1,2}([0,\infty)\times R^n,R^1)$ and $\gamma\in C^1([0,\infty),R^m)$ with c bounded above and γ bounded. Then the heat kernel is given by*

$$p_t(x,y)=\frac{1}{(2\pi t)^{n/2}}\exp\left\{\int_0^t\langle\gamma(\sigma),dw_\sigma\rangle+\frac{1}{2}\int_0^t|\eta w_\sigma|^2d\sigma+\langle x,\eta w_t\rangle-\frac{r^2(x+\int_0^t\eta w_\sigma\,d\sigma,y)}{2t}\right\}$$
$$\cdot\hat{E}\,\exp\left\{\int_0^t c(t-s,X_s^t)ds\right\}. \tag{3.21}$$

Here $\{X_s^t:0\leqslant s\leqslant t\}$ is the stochastic semiclassical bridge in R^n from x to y in time t.

If $\eta\equiv 0$, $\gamma\equiv 0$, Eq. (3.1) is a deterministic equation on M. The Elworthy and Truman[5] Theorem follows from Theorem 3.1.

Theorem 3.3 (Elworthy and Truman[5]): *Suppose y is a pole on the Riemannian manifold M. If $\theta^{1/2}\Delta\theta^{-(1/2)}$ and c are bounded, then the heat kernel of Eq. (3.1) for $\eta\equiv 0$, $\gamma\equiv 0$ on the Riemannian manifold M is given by*

$$p_t(x,y)=\frac{1}{(2\pi t)^{n/2}}\,\theta^{-(1/2)}(x)\exp\left\{-\frac{r^2(x,y)}{2t}\right\}$$
$$\times\hat{E}\,\exp\left\{\frac{1}{2}\int_0^t\theta^{1/2}(X_s^t)\Delta\theta^{-(1/2)}(X_s^t)ds+\int_0^t c(t-s,X_s^t)ds\right\}, \tag{3.22}$$

where X_s^t is the Brownian Riemannian bridge from x to y at time t on M.

(3) For hyperbolic n-space H^n with constant sectional curvatures $-(1/R^2)$ we have

$$\theta_y(x)=\left(\frac{R}{r}\sinh\frac{r}{R}\right)^{n-1}$$

for $r(x)=r(x,y)$. From Elworthy[14] we see that

$$\frac{1}{2}\,\theta^{1/2}\Delta\,\theta^{-(1/2)}=-\frac{(n-1)^2}{8R^2}+\frac{(n-1)(n-3)}{8}\left\{r^{-2}-\left(R^2\,\sinh^2\left(\frac{r}{R}\right)\right)^{-1}\right\}.$$

Therefore the heat kernel of Eq. (3.1) on H^n is given by

$$\begin{aligned}p_t(x,y)=&\frac{1}{(2\pi t)^{n/2}}\\&\times\left[\frac{r\{\exp(\exp^{-1}(x)+\int_0^t\eta w_s\,ds),y\}}{R}\,\frac{1}{\sinh[r\{\exp(\exp^{-1}(x)+\int_0^t\eta w_s\,ds),y\}/R]}\right]^{(n-1)/2}\\&\cdot\exp\left\{\int_0^t\langle\gamma(s),dw_s\rangle+\frac{1}{2}\int_0^t|\eta w_s|^2ds+\langle x,\eta w_t\rangle-\frac{r^2\{\exp(\exp^{-1}(x)+\int_0^t\eta w_s\,ds),y\}}{2t}\right.\\&\left.-\frac{(n-1)^2}{8R^2}\,t\right\}\cdot\hat{E}\,\exp\left\{\frac{(n-1)(n-3)}{8}\int_0^t\left[r^{-2}\left(\exp\left\{\exp^{-1}(X_s^t(x))\right.\right.\right.\\&\left.\left.\left.+\int_0^{t-s}\eta w_\sigma\,d\sigma\right\},y\right)-\left(R^2\,\sinh^2\left(\frac{r(\exp\{\exp^{-1}(X_s^t(x))+\int_0^{t-s}\eta w_\sigma\,d\sigma\},y)}{R}\right)\right)^{-1}\right]ds\right\}.\end{aligned}\tag{3.23}$$

Here $X_s^t(x)$ is the stochastic Brownian Riemannian bridge on H^n. In particular for hyperbolic 3-space H^3, we have

$$\begin{aligned}p_t(x,y)=&\frac{1}{(2\pi t)^{3/2}}\\&\times\frac{r\{\exp(\exp^{-1}(x)+\int_0^t\eta w_s\,ds),y\}}{R}\,\frac{1}{\sinh[r\{\exp(\exp^{-1}(x)+\int_0^t\eta w_s\,ds),y\}/R]}\\&\times\exp\left\{\int_0^t\langle\gamma(s),dw_s\rangle+\frac{1}{2}\int_0^t|\eta w_s|^2ds+\langle x,\eta w_t\rangle-\frac{r^2\{\exp(\exp^{-1}(x)+\int_0^t\eta w_s\,ds),y\}}{2t}\right.\\&\left.-\frac{1}{2R^2}\,t\right\}.\end{aligned}\tag{3.24}$$

IV. THE STOCHASTIC MEHLER FORMULA

(1) Consider the following stochastic harmonic oscillator in R^1

$$\begin{cases}d\dot{\Phi}_s=-\alpha^2\Phi_s\,ds-\eta\,dw_s\\ \Phi_0(x)=x,\quad \Phi_0(x)=\dfrac{x}{\lambda}\end{cases},\tag{4.1}$$

where $\alpha,\lambda>0,\eta\geqslant 0$ are constants, which is Eq. (2.1) in the case $c(s,x)=\frac{1}{2}\alpha^2x^2$, $k(s,x)=\eta x$, and $S_0(x)=x^2/2\lambda$ and $M=R^1$. See McKean,[18] Markus and Weerasinghe,[19] and Albeverio *et al.*[20] for some important properties of the stochastic harmonic oscillator. Solving Eq. (4.1) we have

$$\Phi_s(x)=x\,\cos\,\alpha s+\frac{x}{\lambda\alpha}\,\sin\,\alpha s-\frac{\eta}{\alpha}\int_0^s\sin\,\alpha(s-\sigma)dw_\sigma.\tag{4.2}$$

The map $\Phi_s: R^1 \to R^1$ satisfies the no caustic condition for $s < (1/\alpha)\mathrm{ctg}^{-1}(-(1/\alpha\lambda))$ and the inverse function is given by

$$\Phi_t^{-1}(x) = \frac{\lambda(\alpha x + \eta \int_0^t \sin\ \alpha(t-\sigma) dw_\sigma)}{\alpha\lambda\ \cos\ \alpha t + \sin\ \alpha t} \quad \text{for } 0 < t < \frac{1}{\alpha}\ \mathrm{ctg}^{-1}\left(-\frac{1}{\alpha\lambda}\right). \tag{4.3}$$

By the definition of $\tilde{S}_t(x)$, Eq. (2.2), and careful calculations we have

$$\begin{aligned}\tilde{S}_{t,\lambda}(y) = &\left[\frac{\sin 2\alpha t}{4\alpha\lambda^2} + \frac{\cos 2\alpha t}{2\lambda} - \frac{1}{4}\ \alpha\ \sin 2\alpha t\right] y^2 \\ &- \frac{\eta}{\alpha\lambda}\ (\alpha\lambda\ \cos\ \alpha t + \sin\ \alpha t) \int_0^t \cos\ \alpha(t-\sigma) dw_\sigma\ y \\ &+ \frac{1}{2}\ \eta^2 \int_0^t \left\{ \left(\int_0^s \cos\ \alpha(s-\sigma) dw_\sigma \right)^2 - \left(\int_0^s \sin\ \alpha(s-\sigma) dw_\sigma \right)^2 \right\} ds \\ &+ \frac{\eta^2}{\alpha} \int_0^t \int_0^s \sin\ \alpha(s-\sigma) dw_\sigma\ dw_s .\end{aligned}$$

It turns out from the definition of S_t, Eq. (2.3),

$$\begin{aligned}S_{t,\lambda}(x) = \tilde{S}_{t,\lambda}[\Phi_t^{-1}(x)] = &\left[\frac{\sin 2\alpha t}{4\alpha\lambda^2} + \frac{\cos 2\alpha t}{2\lambda} - \frac{1}{4}\ \alpha\ \sin 2\alpha t\right] \frac{\lambda^2(\alpha x + \eta \int_0^t \sin\ \alpha(t-\sigma) dw_\sigma)^2}{(\alpha\lambda\ \cos\ \alpha t + \sin\ \alpha t)^2} \\ &- \frac{\eta}{\alpha} \int_0^t \cos\ \alpha(t-\sigma) dw_\sigma \left(\alpha x + \eta \int_0^t \sin\ \alpha(t-\sigma) dw_\sigma \right) + \frac{1}{2}\ \eta^2 \int_0^t \left\{ \left(\int_0^s \cos\ \alpha(s \right.\right. \\ &\left.\left. - \sigma) dw_\sigma \right)^2 - \left(\int_0^s \sin\ \alpha(s-\sigma) dw_\sigma \right)^2 \right\} ds + \frac{\eta^2}{\alpha} \int_0^t \int_0^s \sin\ \alpha(s-\sigma) dw_\sigma\ dw_s \end{aligned} \tag{4.4}$$

for $0 < t < (1/\alpha)\mathrm{ctg}^{-1}[-(1/\alpha\lambda)]$. It is a very complicated formula. However we can simplify it by taking the limit $\lambda \to 0$ to get an illuminating formula for S:

$$\begin{aligned}S_t(x) = \lim_{\lambda \to 0} S_{t,\lambda}(x) = &\frac{\cos\ \alpha t}{2\alpha\ \sin\ \alpha t} \left(\alpha x + \eta \int_0^t \sin\ \alpha(t-\sigma) dw_\sigma \right)^2 - \frac{\eta}{\alpha} \int_0^t \cos\ \alpha(t-\sigma) dw_\sigma \\ &\times \left(\alpha x + \eta \int_0^t \sin\ \alpha(t-\sigma) dw_\sigma \right) + \frac{1}{2}\ \eta^2 \int_0^t \left\{ \left(\int_0^s \cos\ \alpha(s-\sigma) dw_\sigma \right)^2 \right. \\ &\left. - \left(\int_0^s \sin\ \alpha(s-\sigma) dw_\sigma \right)^2 \right\} ds + \frac{\eta^2}{\alpha} \int_0^t \int_0^s \sin\ \alpha(s-\sigma) dw_\sigma\ dw_s \end{aligned} \tag{4.5}$$

for $t < \pi/\alpha$. Note $T_{\alpha,\lambda} = (1/\alpha)\mathrm{ctg}^{-1}[-(1/\alpha\lambda)]$ is the caustic time of our stochastic oscillator (4.1). $T_\alpha = \pi/\alpha$ is the $\lambda \to 0$ limit of the caustic time $T_{\alpha,\lambda}$.

At the moment let us consider the Stratonovich stochastic heat equation with the harmonic oscillator potential

$$du_t = [\tfrac{1}{2}\Delta u_t + \tfrac{1}{2}\alpha^2 x^2 u_t] dt + \eta x u_t \partial w_t . \tag{4.6}$$

Here $x \in R^1$. Let $p_t^\lambda(x)$ be the solution of Eq. (4.6) with the initial condition $p_0^\lambda(x) = (1/\sqrt{2\pi\lambda})\exp\{-(x^2/2\lambda)\}$ and $p_t(x) = \lim_{\lambda\to 0} p_t^\lambda(x)$. We shall apply Theorem 2.5. Note first $\psi_{t,\lambda}(x) = \sqrt{\alpha/2\pi}(\alpha\lambda\cos\alpha t + \sin\alpha t)$ by Eqs. (2.20) and (4.3) so that $\nabla\psi_{t-s,\lambda} \equiv 0$ for $0 \leqslant s \leqslant t < T_{\alpha,\lambda}$. Moreover for $0 \leqslant s \leqslant t < T_{\alpha,\lambda}$,

$$\nabla S_{t-s,\lambda}(x) = \left[\frac{\sin 2\alpha(t-s)}{4\alpha\lambda^2} + \frac{\cos 2\alpha(t-s)}{2\lambda} - \frac{1}{4}\,\alpha\,\sin 2\alpha(t-s)\right] \cdot \frac{2\alpha\lambda^2(\alpha x + \eta\int_0^{t-s}\sin\alpha(t-s-\sigma)dw_\sigma)}{(\alpha\lambda\cos\alpha(t-s) + \sin\alpha(t-s))^2} - \eta\int_0^{t-s}\cos\alpha(t-s-\sigma)dw_\sigma .$$

Let $\xi_s^{t,\lambda} = X_s^{t,\lambda} + \eta/\alpha\int_0^{t-s}\sin\alpha(t-s-\sigma)dw_\sigma$. Then from Eq. (2.8) $\xi_s^{t,\lambda}$ satisfies an equation which does not include the stochastic process w except for the initial condition $\xi_0^{t,\lambda} = x + \eta/\alpha\int_0^t \sin\alpha(t-\sigma)dw_\sigma$. Thus we can write $\xi_s^{t,\lambda} = F_s^{t,\lambda}(x + \eta/\alpha\int_0^t \sin\alpha(t-\sigma)dw_\sigma)$. Recall $X_s^{t,\lambda} = \xi_s^{t,\lambda} - \eta/\alpha\int_0^{t-s}\sin\alpha(t-s-\sigma)dw_\sigma = F_s^{t,\lambda}(x + \eta/\alpha\int_0^t \sin\alpha(t-\sigma)dw_\sigma) - \eta/\alpha\int_0^t \times\sin\alpha(t-s-\sigma)dw_\sigma + \eta/\alpha\int_{t-s}^t \sin\alpha(t-s-\sigma)dw_\sigma$. Thus $\eta\int_0^t X_s^{t,\lambda}\,dw_{t-s}$ is well defined in Itô's sense for fixed $t < T_{\alpha,\lambda}$. Then applying Eq. (2.22) of Theorem 2.5 and Remark 2.3 we have

$$p_t^\lambda(x) = \sqrt{\frac{\alpha}{2\pi(\alpha\lambda\cos\alpha t + \sin\alpha t)}}\,\exp\{-S_{t,\lambda}(x)\}. \tag{4.7}$$

It turns out by taking the limits $\lambda \to 0$ in Eq. (4.7) that

Theorem 4.1: For $0 < t < \pi/\alpha$,

$$\begin{aligned} p_t(x) = \sqrt{\frac{\alpha}{2\pi\sin\alpha t}}\,\exp\Bigg\{ & -\frac{\cos\alpha t}{2\alpha\sin\alpha t}\left(\alpha x + \eta\int_0^t \sin\alpha(t-\sigma)dw_\sigma\right)^2 \\ & + \frac{\eta}{\alpha}\int_0^t \cos\alpha(t-\sigma)dw_\sigma\left(\alpha x + \eta\int_0^t \sin\alpha(t-\sigma)dw_\sigma\right) \\ & - \frac{1}{2}\,\eta^2\int_0^t\left\{\left(\int_0^s \cos\alpha(s-\sigma)dw_\sigma\right)^2 - \left(\int_0^s \sin\alpha(s-\sigma)dw_\sigma\right)^2\right\}ds \\ & - \frac{\eta^2}{\alpha}\int_0^t\int_0^s \sin\alpha(s-\sigma)dw_\sigma\,dw_s\Bigg\}. \end{aligned} \tag{4.8}$$

And as $t \to \pi/\alpha$, $p_t(x) \to +\infty$ P-a.s. for any $x \neq -\eta/\alpha\int_0^t \sin\alpha(t-\sigma)dw_\sigma$.

Proof: Formula (4.8) follows taking the limits $\lambda \to 0$ in Eq. (4.7). The rest of the theorem is easy to see if we notice that the last three terms in the $\exp\{-\}$ in Eq. (4.8) remain bounded when we take the limit $t \to \pi/\alpha$.

Remark 4.1: For $\eta = 0$, then for $0 < t < \pi/\alpha$:

$$p_t(x) = \sqrt{\frac{\alpha}{2\pi\sin\alpha t}}\,\exp\left\{-\frac{\alpha\cos\alpha t}{2\sin\alpha t}\,x^2\right\} \tag{4.9}$$

which was given in Elworthy, Truman, and Zhao.[8]

(2) Similarly we consider

$$\begin{cases} d\dot{\Phi}_s^1 = \alpha^2\Phi_s^1\,ds - \eta\,dw_s \\ \Phi_0^1(x) = x, \quad \dot{\Phi}_0^1(x) = \dfrac{x}{\lambda}, \end{cases} \tag{4.10}$$

where $\alpha>0$, which is Eq. (2.1) in the case $c(s,x)=-\frac{1}{2}\alpha^2x^2$, $k(s,x)=\eta x$ *and* $S_0(x)=x^2/2\lambda$. *Similarly with* (1) *we have*

$$\Phi_s^1(x)=x\cosh\alpha s+\frac{x}{\lambda\alpha}\sinh\alpha s-\frac{\eta}{\alpha}\int_0^s\sinh\alpha(s-\sigma)dw_\sigma. \tag{4.11}$$

The map $\Phi_s^1:R^1\to R^1$ satisfies the no-caustic condition for $0\leqslant s<+\infty$ and the inverse function is given by

$$\Phi_t^{1^{-1}}(x)=\frac{\lambda(\alpha x+\eta\int_0^t\sinh\alpha(t-\sigma)dw_\sigma)}{\alpha\lambda\cosh\alpha t+\sinh\alpha t}. \tag{4.12}$$

Similar calculations give

$$\begin{aligned}S_t^1(x)=&\frac{\cosh\alpha t}{2\alpha\sinh\alpha t}\left(\alpha x+\eta\int_0^t\sinh\alpha(t-\sigma)dw_\sigma\right)^2\\&-\frac{\eta}{\alpha}\int_0^t\cosh\alpha(t-\sigma)dw_\sigma\left(\alpha x+\eta\int_0^t\sinh\alpha(t-\sigma)dw_\sigma\right)\\&+\frac{1}{2}\eta^2\int_0^t\left\{\left(\int_0^s\cosh\alpha(s-\sigma)dw_\sigma\right)^2+\left(\int_0^s\sinh\alpha(s-\sigma)dw_\sigma\right)^2\right\}ds\\&+\frac{\eta^2}{\alpha}\int_0^t\int_0^s\sinh\alpha(s-\sigma)dw_\sigma\,dw_s.\end{aligned} \tag{4.13}$$

A quick way to get these formulas is to write Eq. (4.10) as $d\Phi_s^1=-(\alpha i)^2\Phi_s^1\,ds-\eta\,dw_s$. Then $\Phi_s^1(x,\alpha)=\Phi_s(x,\alpha i)$ and $S_t^1(x,\alpha)=S_t(x,\alpha i)$. Note $\cos(\alpha is)=\cosh\alpha s$ and $(1/i)\sin(\alpha is)=\sinh\alpha s$.

Consider the Stratonovich stochastic heat equation with harmonic oscillator potential

$$du_t=[\tfrac{1}{2}\Delta u_t-\tfrac{1}{2}\alpha^2x^2u_t]dt+\eta xu_t\partial w_t. \tag{4.14}$$

Here $x\in R^1$. As before we can prove $\eta\int_0^tX_s^{t,\lambda}dw_{t-s}$ is well defined in Itô's sense for any fixed $t\geqslant0$. Let $q_t^\lambda(x)$ be the solution of Eq. (4.14) with the initial condition $q_0^\lambda(x)=(1/\sqrt{2\pi\lambda})\times\exp\{-(x^2/2\lambda)\}$ and $q_t(x)=\lim_{\lambda\to0}q_t^\lambda(x)$. It turns out from Eqs. (4.12) and (2.22) in Theorem 2.5 and Remark 2.3 that

$$q_t^\lambda(x)=\sqrt{\frac{\alpha}{2\pi(\alpha\lambda\cosh\alpha t+\sinh\alpha t)}}\exp\{-S_{t,\lambda}^1(x)\}. \tag{4.15}$$

Here it is enough to know $S_{t,\lambda}^1(x)\to S_t^1(x)$ as $\lambda\to0$ since we have written $S_t^1(x)$ in Eq. (4.13). One can write $S_{t,\lambda}^1(x)$ explicitly without any difficulty. Taking the limit $\lambda\to0$ we have

Theorem 4.2: For any $t>0$,

$$\begin{aligned}q_t(x)=&\sqrt{\frac{\alpha}{2\pi\sinh\alpha t}}\exp\left\{-\frac{\cosh\alpha t}{2\alpha\sinh\alpha t}\left(\alpha x+\eta\int_0^t\sinh\alpha(t-\sigma)dw_\sigma\right)^2\right.\\&\left.+\frac{\eta}{\alpha}\int_0^t\cosh\alpha(t-\sigma)dw_\sigma\left(\alpha x+\eta\int_0^t\sinh\alpha(t-\sigma)dw_\sigma\right)\right.\end{aligned}$$

$$-\frac{1}{2}\,\eta^2\int_0^t\left\{\left(\int_0^s \cosh\,\alpha(s-\sigma)dw_\sigma\right)^2+\left(\int_0^s \sinh\,\alpha(s-\sigma)dw_\sigma\right)^2\right\}ds$$
$$-\frac{\eta^2}{\alpha}\int_0^t\int_0^s \sinh\,\alpha(s-\sigma)dw_\sigma\,dw_s\Bigg\}. \tag{4.16}$$

Corollary 4.1: For $\eta\equiv 0$ we get

$$q_t(x)=\sqrt{\frac{\alpha}{2\pi\,\sinh\,\alpha t}}\exp\left\{-\frac{\alpha\,\cosh\,\alpha t}{2\,\sinh\,\alpha t}\,x^2\right\}. \tag{4.17}$$

Remark 4.2: Formula (4.17) is the classical Mehler formula (cf. Berline, Getzler, and Vergne[21]). Therefore we call Eq. (4.16) the stochastic Mehler formula. Note for any $t>0$, $q_t(x)$ is well defined.

Remark 4.3: For $\alpha=0$, Eqs. (4.8) and (4.16) are no longer true. However we have the formulas given in Sec. III and Truman and Zhao[10] instead.

(3) Now we consider the more interesting case: the Itô stochastic heat equation with the harmonic oscillator potential

$$du_t(x)=[\tfrac{1}{2}\Delta u_t(x)+\tfrac{1}{2}\alpha^2x^2u_t]dt+\eta x u_t\,dw_t. \tag{4.18}$$

For a given initial condition $u_0(x)$ from the Feynman–Kac formula we have

$$u_t(x)=\hat{E}u_0(B_t^x)\exp\left\{\frac{1}{2}\,(\alpha^2-\eta^2)\int_0^t(B_s^x)^2ds+\eta\int_0^t B_s^x\,dw_s\right\}.$$

Here $B_s^x=x+B_s$, B_s is a one-dimensional Brownian motion in the probability space $(\hat{\Omega},\hat{\mathcal{F}},\hat{P})$ with $B_0=0$ P-a.s. Therefore $u_t(x)$ satisfies the following Stratonovich stochastic heat equation:

$$du_t(x)=[\tfrac{1}{2}\Delta u_t(x)+\tfrac{1}{2}(\alpha^2-\eta^2)x^2u_t]dt+\eta x u_t\partial w_t. \tag{4.19}$$

Let $p_t^\lambda(x)(I)$ denote the solution of Eq. (4.18) with the initial condition $p_0^\lambda(x)(I)=(1/\sqrt{2\pi\lambda})\exp\{-(x^2/2\lambda)\}$ and $p_t(x)(I)=\lim_{\lambda\to 0}p_t^\lambda(x)(I)$. From the results on the Stratonovich equation we easily formulate the following theorem:

Theorem 4.3: (i) For $|\eta|<|\alpha|$, let $\alpha_1=\sqrt{\alpha^2-\eta^2}$, then for $0<t<\pi/\alpha_1$,

$$p_t(x)(I)=\sqrt{\frac{\alpha_1}{2\pi\,\sin\,\alpha_1 t}}\exp\left\{-\frac{\cos\,\alpha_1 t}{2\alpha_1\,\sin\,\alpha_1 t}\left(\alpha_1 x+\eta\int_0^t \sin\,\alpha_1(t-\sigma)dw_\sigma\right)^2\right.$$
$$+\frac{\eta}{\alpha_1}\int_0^t \cos\,\alpha_1(t-\sigma)dw_\sigma\left(\alpha_1 x+\eta\int_0^t \sin\,\alpha_1(t-\sigma)dw_\sigma\right)$$
$$-\frac{1}{2}\,\eta^2\int_0^t\left\{\left(\int_0^s \cos\,\alpha_1(s-\sigma)dw_\sigma\right)^2-\left(\int_0^s \sin\,\alpha_1(s-\sigma)dw_\sigma\right)^2\right\}ds$$
$$\left.-\frac{\eta^2}{\alpha_1}\int_0^t\int_0^s \sin\,\alpha_1(s-\sigma)dw_\sigma\,dw_s\right\}. \tag{4.20}$$

And as $t\to\pi/\alpha_1$, $p_t(x)(I)\to+\infty$ P-a.s. for any $x\neq-(\eta/\alpha_1)\int_0^t\sin\,\alpha_1(t-\sigma)dw_\sigma$.

(ii) For $|\eta|=|\alpha|$ we have

$$p_t(x)(I)=\frac{1}{\sqrt{2\pi t}}\exp\left\{-\frac{(x+\int_0^t \eta w_\sigma\, d\sigma)^2}{2t}+\eta x w_t+\frac{1}{2}\int_0^t \eta^2 w_\sigma^2\, d\sigma\right\}. \tag{4.21}$$

(iii) For $|\eta|>|\alpha|$, let $\alpha_2=\sqrt{\eta^2-\alpha^2}$, we have for any $t>0$,

$$\begin{aligned}p_t(x)(I)=&\sqrt{\frac{\alpha_2}{2\pi\sinh\alpha_2 t}}\exp\left\{-\frac{\cosh\alpha_2 t}{2\alpha_2\sinh\alpha_2 t}\left(\alpha_2 x+\eta\int_0^t \sinh\alpha_2(t-\sigma)dw_\sigma\right)^2\right.\\&+\frac{\eta}{\alpha_2}\int_0^t\cosh\alpha_2(t-\sigma)dw_\sigma\left(\alpha_2 x+\eta\int_0^t\sinh\alpha_2(t-\sigma)dw_\sigma\right)\\&-\frac{1}{2}\eta^2\int_0^t\left\{\left(\int_0^s\cosh\alpha_2(s-\sigma)dw_\sigma\right)^2+\left(\int_0^s\sinh\alpha_2(s-\sigma)dw_\sigma\right)^2\right\}ds\\&\left.-\frac{\eta^2}{\alpha_2}\int_0^t\int_0^s\sinh\alpha_2(s-\sigma)dw_\sigma\,dw_s\right\}.\end{aligned} \tag{4.22}$$

V. STOCHASTIC BURGERS' EQUATIONS

(1) As the simplest model for the differential equation of fluid flow, Burgers[22,23] introduced the equation (called viscous Burgers' equation nowadays)

$$\frac{\partial}{\partial t}v^\mu(t,x)+v^\mu(t,x)\frac{\partial}{\partial x}v^\mu(t,x)=\frac{1}{2}\mu^2\frac{\partial^2}{\partial x^2}v^\mu(t,x). \tag{5.1}$$

The well known logarithm transformation

$$v^\mu(t,x)=-\mu^2\nabla\log u^\mu(t,x) \tag{5.2}$$

given by Hopf in his pioneering work (Hopf[24]) on Burgers' equation transforms the nonlinear Burgers' equation into a linear heat equation

$$\frac{\partial u^\mu(t,x)}{\partial t}=\frac{1}{2}\mu^2\frac{\partial^2 u^\mu(t,x)}{\partial x^2} \tag{5.3}$$

with the initial condition $u^\mu(0,x)=\exp\{[\int_0^x v^\mu(0,x)dx/\mu^2]\}$. Very recently stochastic Burgers' equations have been studied by Kardar, Parisi, and Zhang,[11] Bertini, Cancrini, and Jona-Lasinio,[25] Bertini and Cancrini,[26] Albeverio, Molchanov, and Surgailis,[27] Da Prato, Debusche, and Temam,[28] Holden *et al.*,[29,30] Oksendal,[31] and Newman,[32] to name but a few. The KPZ model has been given and a representation theorem for the solution of the viscous stochastic Burgers' equation has been obtained by initial condition and a diffusion process via a stochastic heat equation for which the solution can be represented by a Feynman–Kac formula. In this section of this paper we consider the following viscous stochastic Burgers' equation

$$dv^{\mu}(t,x)+v^{\mu}(t,x)\,\frac{\partial}{\partial x}\,v^{\mu}(t,x)dt=\frac{1}{2}\,\mu^{2}\,\frac{\partial^{2}v^{\mu}(t,x)}{\partial x^{2}}\,dt+e_{1}(t,x)dt+e_{2}(t,x)dw_{t}, \tag{5.4}$$

with the initial condition $v^{\mu}(0,x)=\nabla S_{0}(x)$ for a certain C^{2} function S_{0}. Here w_{t} is a one-dimensional Brownian motion. For simplicity we suppose initially the configuration space is R^{1}. Assume $e_{1},e_{2}\in C^{1,1}([0,+\infty)\times R^{1},R^{1})$. Let us also make the transformation (5.2). Suppose there exist functions $c(t,x)$ and $k(t,x)$ such that $e_{1}(t,x)=-(\partial/\partial x)c(t,x)$ and $e_{2}(t,x)=-(\partial/\partial x)k(t,x)$. Direct computation using Itô's formula gives the stochastic heat equation of the Stratonovich type

$$du^{\mu}(t,x)=\left[\frac{1}{2}\,\mu^{2}\Delta u^{\mu}(t,x)+\frac{c(t,x)}{\mu^{2}}\,u^{\mu}(t,x)\right]dt+\frac{k(t,x)}{\mu^{2}}\,u^{\mu}(t,x)\partial w_{t} \tag{5.5}$$

with the initial condition $u^{\mu}(t,x)=\exp\{-S_{0}(x)/\mu^{2}\}$.

(2) Consider the related inviscid stochastic Burgers' equation

$$dv(t,x)+v(t,x)\,\frac{\partial}{\partial x}\,v(t,x)dt=e_{1}(t,x)dt+e_{2}(t,x)dw_{t} \tag{5.6}$$

with the initial condition $v(0,x)=\nabla S_{0}(x)$. Note it can be obtained by letting $\mu=0$ in Eq. (5.4). More importantly we note the solution $v(t,x)$ of Eq. (5.6) is the gradient of the solution $S(t,x)$ of the stochastic Hamilton Jacobi equation

$$dS(t,x)+[\tfrac{1}{2}\,|\nabla S(t,x)|^{2}+c(t,x)]dt+k(t,x)dw_{t}=0 \tag{5.7}$$

with the initial condition $S(0,x)=S_{0}(x)$, which was studied in Sec. II.

As before let Φ be defined by Eq. (2.1). In our case

$$\begin{cases} d\dot{\Phi}_{s}(x)=e_{1}(s,\Phi_{s}(x))ds+e_{2}(s,\Phi_{s}(x))dw_{s} \\ \dot{\Phi}_{0}(x)=v(0,x), \quad \Phi_{0}(x)=x \end{cases}. \tag{5.8}$$

Suppose for $0\leqslant s\leqslant T(\omega)$, $\Phi_{s}:R^{1}\to R^{1}$ satisfies the no-caustic condition for a.e. $\omega\in\Omega$. From Sec. II we know that for a.e. $\omega\in\Omega$ and $0\leqslant t\leqslant T(\omega)$, $v(t,x)=\nabla S(t,x)$ is well defined and continuous with respect to t and C^{1} with respect to x. Later we will prove that $v(t,x)$ is not continuous at the caustic points of the stochastic classical mechanics.

Let us come back to study the viscous stochastic Burgers' equation under the no-caustic condition. We always suppose the existence and uniqueness of the regular solution for the viscous equation as from the existence and uniqueness of the regular solutions of the stochastic heat equations studied by Flandoli.[13] In the following we give the explicit formulas between the solution of the viscous stochastic Burgers' equation and the solution of the inviscid one under the no-caustic condition. Let $X_{s}^{t,\mu}(x)$ be the solution of Eq. (2.8) with $Y(s,-)=-S(t-s,-)$. That is,

$$dX_{s}^{t,\mu}(x)=\mu\ dB_{s}-v_{t-s}(X_{s}^{t,\mu}(x))ds, \quad X_{0}^{t,\mu}(x)=x. \tag{5.9}$$

Here B_{s} is a one-dimensional Brownian motion on the probability space $(\hat{\Omega},\hat{\mathscr{F}},\hat{P})$ from the origin.

Theorem 5.1: *Assume all the conditions of Theorem* 2.3 *and the map defined by* Eq. (5.8) *satisfies the no-caustic condition for* $0\leqslant t\leqslant T(\omega)$ *for* a.e. $\omega\in\Omega$ *and* $S(t,x)$ *is defined by* Eq. (2.3). *Then for* a.e. $\omega\in\Omega$ *and any* $0\leqslant t\leqslant T(\omega)$, *the solution* $v(t,x)$ *of the inviscid stochastic Burgers' equation* (5.6) *exists and is given by* $v(t,x)=\nabla S(t,x)$.

Let $X_{s}^{t,\mu}(x)$ *be defined by* Eq. (5.9). *If* $X_{s}^{t,\mu}(x)$ *is nonexplosive and* $\mathscr{F}_{s}^{*}$ *measurable then for any* $\mu\neq 0$, *the solution* $v^{\mu}(t,x)$ *(if it exists and is unique) of the viscous stochastic Burger's equation* (5.4) *is given by*

$$v^{\mu}(t,x)=v(t,x)-\mu^2\nabla\ \log\ \hat{E}\exp\left\{-\frac{1}{2}\int_0^t\frac{\partial}{\partial x}v(t-s,X_s^{t,\mu}(x))ds\right\},\tag{5.10}$$

for a.e. $\omega\in\Omega$ *and any* $0\leqslant t\leqslant T(\omega)$.

Proof: Claim $v(t,x)=\nabla S(t,x)$ was already shown. The solution $u^{\mu}(t,x)$ of Eq. (5.5) is given by Eq. (2.15) where $T_0=1$. Therefore, $u_t^{\mu}(t,x)>0$ for a.e. $\omega\in\Omega$ and $0\leqslant t\leqslant T(\omega)$. Take the logarithm to Eq. (2.15) and differentiate it with respect to x. We get Eq. (5.11) from $v^{\mu}(t,x)=-\mu^2\nabla\log u^{\mu}(t,x)$. ■

Recall $\psi(t,x)=(|\det T_x\Phi_t^{-1}|)^{1/2}>0$ for a.e. $\omega\in\Omega$ and $0\leqslant t\leqslant T(\omega)$. Instead of Eq. (5.10) now we let $X_s^{t,\mu}(x)$ be defined by

$$\begin{cases}dX_s^{t,\mu}(x)=\mu\ dB_s-v_{t-s}(X_s^{t,\mu}(x))ds+\mu^2\nabla\ \log\ \psi(t-s,X_s^{t,\mu}(x))ds\\ X_0^{t,\mu}(x)=x\end{cases}.\tag{5.11}$$

If $X_s^{t,\mu}(x)$ is $\mathcal{F}_s^*$ measurable and nonexplosive we have the solution $u^{\mu}(t,x)$ given by Eq. (2.22) and $u^{\mu}(t,x)>0$ for a.e. $\omega\in\Omega$ and $0\leqslant t\leqslant T(\omega)$. Take logarithms of Eq. (2.22) and differentiate it with respect to x. By Eq. (5.2) we have the following theorem:

Theorem 5.2: *Assume all the conditions of Theorem* 2.5. *Then for any* $\mu\neq 0$, a.e. $\omega\in\Omega$ *and* $0\leqslant t\leqslant T(\omega)$ *the solution* $v^{\mu}(t,x)$ *(if it exists and is unique) of the viscous stochastic Burgers' equation* (5.4) *is given by*

$$v^{\mu}(t,x)=v(t,x)-\mu^2\nabla\log\psi(t,x)-\mu^2\nabla\log$$
$$\hat{E}\exp\left\{\frac{1}{2}\mu^2\int_0^t\psi^{-1}(t-s,X_s^{t,\mu}(x))\Delta\psi(t-s,X_s^{t,\mu}(x))ds\right\},\tag{5.12}$$

if $X_s^{t,\mu}(x)$ is $\mathcal{F}_s^*$ measurable and nonexplosive, where $X_s^{t,\mu}(x)$ is defined by Eq. (5.11).

Remark 5.1: Theorems 5.1 and 5.2 are true for any $\mu\neq 0$. Therefore Eqs. (5.10) and (5.12) are exact solutions rather than asymptotic solutions of the viscous stochastic Burgers' equation. It seems that this solution cannot be easily obtained by the Maslov canonical operator method (Mishchenko, Shatalov, and Sternin[33]).

Remark 5.2: It is trivial to get from Theorem 5.2 that for a.e. $\omega\in\Omega$ and $0\leqslant t\leqslant T(\omega)$, $v^{\mu}(t,x)\to v(t,x)$ as $\mu\to 0$ as long as $\nabla\log\psi$ and $\psi^{-1}\Delta\psi$ are bounded. That means the inviscid limit is the semiclassical limit under the no-caustic condition.

(3) In the following we will prove that $v(t,x)$, the solution of the inviscid equation (5.6), is not continuous at the caustic points of the stochastic classical mechanics. Examples given later demonstrate shock waves in the presence of the caustics.

By Eq. (2.4) we have for a.e. $\omega\in\Omega$ and $0\leqslant t\leqslant T(\omega)$:

$$\dot{\Phi}_t(x)=v(t,\Phi_t(x)).\tag{5.13}$$

Note this is the same as the characteristic equation in a lot of the literature for the deterministic inviscid Burgers' equations [of course when $e_2(t,x)=0$, Eq. (5.6) is deterministic] (see Smoller [34]).

Let $\tau(a)$ be first time such that there exist $x_1\neq x_2, x_1, x_2\in R^1$ such that $\Phi_\tau(x_1)=\Phi_\tau(x_2)=a$ and $\dot{\Phi}_\tau(x_1)\neq\dot{\Phi}_\tau(x_2)$, i.e., τ is a caustic time at point a.

Theorem 5.3: The function $v(t,x)$ is discontinuous at (τ,a).

Proof: For any $t<\tau$ from Eq. (5.13), we have $\dot{\Phi}_t(x_1)=v(t,\Phi_t(x_1))$ and $\dot{\Phi}_t(x_2)=v(t,\Phi_t(x_2))$. If $v(t,x)$ is continuous at (τ,a) we can take the limit $t\to\tau$ to $v(t,\Phi_t(x_1))$ and $v(t,\Phi_t(x_2))$. Thus $\lim_{t\to\tau}v(t,\Phi_t(x_1))=v(\tau,a)=\lim_{t\to\tau}v(t,\Phi_t(x_2))$. It turns out that $\dot{\Phi}_\tau(x_1)=\dot{\Phi}_\tau(x_2)$. This is in contradiction to our hypothesis on (τ,a). The theorem follows. ■

Remark 5.3: If $e_2 \equiv 0$, one can prove that the assumption that there exist $x_1 \neq x_2, x_1, x_2 \in R^1$ such that $\Phi_\tau(x_1) = \Phi_\tau(x_2)$ implies $\dot{\Phi}_\tau(x_1) \neq \dot{\Phi}_\tau(x_2)$ from the uniqueness of the backward deterministic ordinary differential equation. Therefore $\tau(a)$ is the first time such that there exist $x_1 \neq x_2, x_1, x_2 \in R^1$ such that $\Phi_\tau(x_1) = \Phi_\tau(x_2) = a$.

Remark 5.4: Apparently this theorem is true for any manifold M as our configuration space.

If c and k are smooth and bounded, then the stochastic heat equation (5.5) has a classical solution therefore the viscous stochastic Burgers' equation (5.4) has a classical solution $v^\mu(t,x)$. Therefore we have the following important remark:

Remark 5.5: Beyond the caustics, Eqs. (5.10) and (5.12) can hardly be true as in general v^μ is smooth and v is discontinuous at the caustics by Theorem 5.3. This leads us to pose an open problem:

Problem: What change of measure should be used to deduce the detailed asymptotics of the solution beyond the caustics?

The answer to this problem is not clear even in Elworthy and Truman's deterministic Hamilton Jacobi theory (deterministic here means that the Hamilton Jacobi equation is deterministic).

(4) In order to understand some of the simplest inviscid stochastic Burgers' equations beyond caustics we first give a very simple lemma which transforms a certain class of the stochastic equations to random equations which are easily handled. For this let g be the solution of the nonlinear random equation

$$g_t(t,x) + g(t,x)g_x(t,x) = f\left(t, x - \int_0^t \eta w_\sigma \, d\sigma, g_x, g_{xx}, \ldots\right), \tag{5.14}$$

where $g_x(t,x) = (\partial/\partial x)g(t,x)$, etc. The equation can be treated as a deterministic equation as $\int_0^t \eta w_\sigma \, d\sigma$ is a continuous stationary process. All the conclusions on deterministic equations are still true for Eq. (5.14). The following lemma can be proved directly by calculations:

Lemma 5.1: The function

$$v(t,x) = g\left(t, x + \int_0^t \eta w_\sigma \, d\sigma\right) - \eta w_t \tag{5.15}$$

satisfies the following stochastic equation:

$$dv(t,x) + v(t,x)\frac{\partial}{\partial x} v(t,x)dt = f(t,x,v_x,v_{xx},\ldots)dt - \eta \, dw_t, \quad v(0,x) = g(0,x). \tag{5.16}$$

Conversely if $v(t,x)$ is a solution of Eq. (5.16), then $g(t,x) = v(t, x - \int_0^t \eta w_\sigma \, d\sigma) + \eta w_t$ is a solution of Eq. (5.14).

Lemma 5.1 is true for some special cases such as the viscous stochastic Burgers' equation, the inviscid stochastic Burgers' equation which are studied in this paper and the stochastic KdV equation (Dankel[35]).

(5) Consider the inviscid stochastic Burgers' equation

$$dv(t,x) + v(t,x)\frac{\partial}{\partial x} v(t,x)dt = -\eta \, dw_t \tag{5.17}$$

with $v(0,x) = 1$ for $x < 0$ and $v(0,x) = 0$ for $x > 0$. Let g be the solution of the Burgers' equation $(\partial/\partial t)g(t,x) + g(t,x)(\partial/\partial x)g(t,x) = 0$ with the same initial condition. It is well known that g is a discontinuous solution and $g(t,x) = 1$ for $x < \frac{1}{2}t$ and $g(t,x) = 0$ for $x > \frac{1}{2}t$ (see, e.g., Smoller[34]). It is a deterministic shock wave. From Lemma 5.1 we have $v(t,x) = 1 - \eta w_t$ for $x < \frac{1}{2}t - \int_0^t \eta w_\sigma \, d\sigma$ and $v(t,x) = -\eta w_t$ for $x > \frac{1}{2}t - \int_0^t \eta w_\sigma \, d\sigma$. This is the simplest example of stochastic shock

waves. The wave front is a random curve $x=\frac{1}{2}t-\int_0^t \eta w_\sigma\, d\sigma$, the structure of the wave is that: the trough $-\eta w_t$ and the crest $1-\eta w_t$, both behave randomly as a Brownian motion. Note $\tau=0$ is the caustic of the classical mechanics.

(6) We shall demonstrate another shock wave from the harmonic oscillator. Consider the deterministic equation first:

$$\frac{\partial}{\partial t}\, g(t,x)+g(t,x)\,\frac{\partial}{\partial x}\, g(t,x)=-x, \quad g(0,x)=x. \tag{5.18}$$

From formula (4.4) where we take $\lambda=1$, $\alpha=1$, $\eta=0$ we have

$$g(t,x)=\nabla S_\lambda(t,x)=\frac{\cos t-\sin t}{\cos t+\sin t}\, x. \tag{5.19}$$

For $t<\frac{3}{4}\pi, g(t,x)$ is smooth and as $t\uparrow\frac{3}{4}\pi, g(t,x)\to+\infty$ for $x<0$ and $g(t,x)\to-\infty$ for $x>0$. Note $\frac{3}{4}\,\pi$ is the caustic time of the classical mechanics and Theorem 5.3. If we consider the stochastic Burgers' equation

$$dv(t,x)+v(t,x)\,\frac{\partial}{\partial x}\, v(t,x)dt=-x\, dt-\eta\, dw_t, \quad v(0,x)=x, \tag{5.20}$$

then from Eq. (4.4) where we take $\lambda=1,\alpha=1$,

$$v(t,x)=\frac{\cos t-\sin t}{\cos t+\sin t}\left(x+\eta\int_0^t \sin(t-\sigma)dw_\sigma\right)-\eta\int_0^t \cos(t-\sigma)dw_\sigma. \tag{5.21}$$

Therefore for $t<\frac{3}{4}\pi, v(t,x)$ is well defined and continuous and as $t\uparrow\frac{3}{4}\pi, v(t,x)\to+\infty$ P-a.s. for $x<-\eta\int_0^{(3/4)\pi}\sin(\frac{3}{4}\pi-\sigma)dw_\sigma$ and $v(t,x)\to-\infty$ $P-$a.s. for $x>-\eta\int_0^{(3/4)\pi}\sin(\frac{3}{4}\pi-\sigma)dw_\sigma$.

(7) We have not proved the existence of the piecewise continuous solution for the inviscid stochastic Burgers' equation. Nevertheless, we believe

Conjecture: Given some bounds on e_1 and e_2 the stochastic Burgers' equation (5.6) has a unique viscosity solution.

It may not be true if e_1 and e_2 are not bounded. See Sec. V (6) for a counterexample. For some more special equations we can prove:

Theorem 5.4: If $V(t,x)=\int_0^{x-\int_0^t \eta w_\sigma\, d\sigma} e_1(t,y)dy$ is bounded below and strictly convex in space variable x, then the stochastic Burgers' equation

$$dv(t,x)+v(t,x)\,\frac{\partial}{\partial x}\, v(t,x)=e_1(t,x)dt-\eta dw_t \tag{5.22}$$

with a bounded initial condition has a unique viscosity solution.

Proof: From Davies and Truman[36] we know $G(t,x)=\min\{\frac{1}{2}\int_0^t|\dot z(s)|^2ds+\int_0^t V(s,z(s))ds+\int_0^{z_t}v(0,y)dy: z_0=x, z_s$ is absolutely continuous for $0\leqslant s\leqslant t\}$ has a unique global solution and from Fleming[37,38] we know $G(t,x)$ satisfies the following Hamilton Jacobi equation:

$$\frac{\partial}{\partial t}\, G(t,x)+\frac{1}{2}\,|\nabla G(t,x)|^2+c^*(t,x)=0 \tag{5.23}$$

with $G(0,x)=\int_0^x v(0,x)dx$ and $c^*=-V$. Although $V(t,x)$ is random here it does not affect the argument. By Rademacher's theorem a Lipschitz continuous function is differentiable almost everywhere, therefore almost everywhere $g(t,x)=\nabla G(t,x)$ satisfies

$$\frac{\partial}{\partial t} g(t,x)+g(t,x)\ \frac{\partial}{\partial x} g(t,x)=e_1\left(t,x-\int_0^t \eta w_\sigma\ d\sigma\right). \tag{5.24}$$

Let $v(t,x)=g(t,x+\int_0^t \eta w_\sigma\ d\sigma)-\eta w_t$. By Lemma 5.1, for almost everywhere $v(t,x)$ is the solution of Eq. (5.22). By the uniqueness of Eqs. (5.23) and (5.24) we have the uniqueness of Eq. (5.22). The theorem follows. ■

Here we have not striven for the maximum generality. For alternative formulations see Fleming.[37,38]

Theorem 5.5: Consider the solution $u^\mu(t,x)$ of the following stochastic heat equation on R^1:

$$\begin{cases} du_t^\mu(x)=\left[\frac{1}{2}\ \mu^2\Delta u_t^\mu(x)+\frac{1}{\mu^2}\ c(t,x)u_t^\mu(x)\right]dt+\frac{1}{\mu^2}\ \eta x u_t^\mu(x)\partial w_t \\ u_0^\mu(x)=T_0(x)\exp\left\{-\frac{S_0(x)}{\mu^2}\right\} \end{cases}. \tag{5.25}$$

Assume $-c(t,x-\int_0^t \eta w_\sigma\ d\sigma)$ is bounded below and strictly convex in space variable x. Then the following stochastic Hamilton Jacobi equation:

$$dS(t,x)+[\tfrac{1}{2}|\nabla S(t,x)|^2+c(t,x)]dt+\eta x\ dw_t=0, \tag{5.26}$$

with the initial condition $S(0,x)=S_0(x)$ has a unique Lipschitz continuous solution. If T_0 is bounded and positive, then

$$\lim_{\mu\to 0}\ \mu^2\ \log\ u^\mu(t,x)=-S(t,x), \tag{5.27}$$

uniformly in any compact subset of $[0,+\infty)\times R^1, P$-a.s.

Proof: The existence and uniqueness of the Lipschitz continuous solution to Eq. (5.26) follows from Theorem 5.4. Let

$$dJ^\mu(t,x)+[\tfrac{1}{2}|\nabla J^\mu(t,x)|^2+c(t,x)]dt+\eta x\ dw_t=\tfrac{1}{2}\mu^2\Delta J^\mu(t,x)dt \tag{5.28}$$

with $J^\mu(0,x)=S_0(x)$. Let G^μ and G satisfy

$$\frac{\partial}{\partial t} G^\mu(t,x)+\frac{1}{2}\ |\nabla G^\mu(t,x)|^2+c\left(t,x-\eta\int_0^t w_\sigma\ d\sigma\right)=\frac{1}{2}\ \mu^2\Delta G^\mu(t,x) \tag{5.29}$$

and

$$\frac{\partial}{\partial t} G(t,x)+\frac{1}{2}\ |\nabla G(t,x)|^2+c\left(t,x-\eta\int_0^t w_\sigma\ d\sigma\right)=0 \tag{5.30}$$

with $G^\mu(0,x)=G(0,x)=S_0(x)$. Then direct calculations give that J is unique and $J^\mu(t,x)=G^\mu(t,x+\eta\int_0^t w_\sigma\ d\sigma)-\eta x w_t-\frac{1}{2}\eta^2\int_0^t w_\sigma^2\ d\sigma$, $S(t,x)=G(t,x+\eta\int_0^t w_\sigma\ d\sigma)-\eta x w_t\ -\frac{1}{2}\eta^2\int_0^t w_\sigma^2\ d\sigma$. From the results of Hopf[24] and Fleming[37] we know as $\mu\to 0$, $G^\mu(t,x)\to G(t,x)$ uniformly in any compact subset of $[0,+\infty)\times R^1$ P-a.s. The randomness does not affect the result. Therefore $\mu\to 0$, $J^\mu(t,x)\to S(t,x)$ uniformly in any compact subset of $[0,+\infty)\times R^1$ P-a.s. Let the stochastic process $X_s^{t,\mu}(x)$ be defined by

$$dX_s^{t,\mu}(x)=\mu\ dB_s-\nabla J^\mu(t-s,X_s^{t,\mu}(x))ds,\quad X_0^{t,\mu}(x)=x. \tag{5.31}$$

As in Sec. III we know $\int_0^t X_s^{t,\mu}(x)dw_{t-s}$ is well defined in Itô's sense. Then using formulas (2.10), (2.13), and (5.28) we have

$$u^\mu(t,x)=\exp\left\{-\frac{J^\mu(t,x)}{\mu^2}\right\}\hat{E}T_0(X_t^{t,\mu}(x)), \quad P\text{-a.s.} \tag{5.32}$$

Therefore $\mu^2 \log u^\mu(t,x)=-J^\mu(t,x)+\mu^2 \log \hat{E}T_0(X_t^{t,\mu}(x))$ P-a.s. Thus Eq. (5.27) follows. ■

Remark 5.6: We believe that Eq. (5.32) is of independent interest.

Remark 5.7: We also believe Eq. (5.27) is true in general

Conjecture: As long as the stochastic Hamilton Jacobi equation (2.5) has a Lipschitz solution $S(t,x)$, the solution of stochastic heat equation (2.7) satisfies

$$\lim_{\mu\to 0} \mu^2 \log u^\mu(t,x)=-S(t,x),$$

uniformly in any compact subset of $[0,+\infty)\times M, P$-a.s.

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The squared eigenfunctions of the massive Thirring model in laboratory coordinates

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We demonstrate a simple procedure for finding the squared eigenfunctions of an integrable system and illustrate the method by deriving the squared eigenfunctions of the massive Thirring model. We give the formula for the inner products between the direct squared eigenfunction problem and its adjoint. We also demonstrate closure and express the variations of the potentials in terms of variations of the scattering data. © *1996 American Institute of Physics.* [S0022-2488(96)02201-9]

I. INTRODUCTION

Besides being a simple integrable model in field theory, the massive Thirring model[1] also plays a certain role in nonlinear optics in a problem of wave propagation in a periodically modulated nonlinear fiber.[2]

Naturally, in such situations, one at times needs to understand how perturbations can affect such a system. For this, one needs to know the squared eigenfunctions for the appropriate eigenvalue problem and their closure. In this paper, we solve that problem.

There are two standard methods for finding squared eigenfunctions. One method, the first one discovered,[3] involves obtaining the equations for perturbations solving the adjoint problem and then determining the inner products between the original eigenfunctions and the adjoint eigenfunctions. The main part of this technique consists of finding the equation for the squared eigenfunctions, which can require much trial and error, and thus the success of the method significantly depends on the researcher's ingenuity. On the other hand, there is a procedure based on the Riemann–Hilbert method that will always work.[4] However, in the interesting case when one is interested in the perturbation on the background of a soliton (or a N-soliton solution), this method becomes technically very complex.

We have found a simple regular procedure that allows one to eliminate the trial and error from the former method. We do not start by seeking an equation for the squared eigenfunctions, but instead assume a particular general structure for the Wronskian relation between certain eigenstates related to the original eigenvalue problem. Then one proceeds to determine the coefficients in the general Wronskian relation. The method is simple to use and is straightforward to apply. There seem to be no serious restrictions on the structure of the original eigenvalue problem. In particular, it would work even in the case where eigenvalues can occur in an arbitrary polynomial form inside the eigenvalue problem. We note, however, that at the moment our method does not allow one to find the equation for the squared eigenfunctions; we discuss this point later in Secs. III and VI.

In Sec. II, we review the direct and inverse scattering problems for the massive Thirring model. In Sec. III, we solve the above for variations of the scattering data in terms of variations of the potentials. We then discuss the problem of inverting this relation in order to obtain the variations of the potentials in terms of variations of the scattering data. Then, in Sec. IV, we solve

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this problem by the method outlined in the preceding paragraph. We start from a general Wronkian relation and use the original and adjoint eigenvalue problems to fully determine all coefficients in it. This results in obtaining the specific Wronskian relation required for the massive Thirring model. Now it becomes trivial to obtain the inner products and a bit less trivial to verify closure, which we do in Sec. V. Also in that section, we give the variations of the potentials in terms of variations of the scattering data. In Sec. VI we make some concluding remarks. In the Appendix the method based on the Riemann–Hilbert formulation is briefly considered.

II. THE DIRECT AND INVERSE SCATTERING PROBLEMS

We consider the equations of the massive Thirring model (MTM) in the laboratory coordinates:

$$i(u_x+u_t)+v+u|v|^2=0, \quad i(-v_x+v_t)+u+v|u|^2=0. \tag{1}$$

Here x and t are the space and time coordinates, respectively. The initial conditions for the fields u and v are

$$u(x,t=0)=u_0(x), \quad v(x,t=0)=v_0(x) \tag{2}$$

on the whole x-axis $\mathbf{R}$, and $|u_0(x)|$ and $|v_0(x)|$ are assumed to be integrable on $\mathbf{R}$ and sufficiently smooth (e.g., from the Schwartz class). Equations (1) are the compatibility condition for the following linear system:[1]

$$\left(\frac{\partial}{\partial x}-L\right)\psi=0, \tag{3a}$$

$$\left(\frac{\partial}{\partial t}-A\right)\psi=0, \tag{3b}$$

where ψ is a two-vector and L and A are 2×2 matrices. Here we will only need the expression for L:

$$L=\frac{i}{4}(|u|^2-|v|^2)\sigma_3-\frac{i\lambda}{2}\begin{pmatrix}0 & v^*\\ v & 0\end{pmatrix}+\frac{i}{2\lambda}\begin{pmatrix}0 & u^*\\ u & 0\end{pmatrix}+\frac{i}{4}\left(\lambda^2-\frac{1}{\lambda^2}\right)\sigma_3, \tag{4}$$

where we have used the notations for the Pauli matrices:

$$\sigma_1=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \quad \sigma_2=\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}, \quad \sigma_3=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}.$$

An asterisk in (4) and everywhere below stands for complex conjugation. Notice that the notations in (4) are slightly different from those in Ref. 1, where the representation (3) was first found.

The problem that we solve in this paper is the following: what quadratic combinations of the eigenfunctions (we will term them ''squared eigenfunctions'' for brevity) of (3a) does one need in order to be able to expand over them the variations $\delta u, \delta u^*, \delta v, \delta v^*$ of the potentials u and v of the operator L. Before passing to the solution of the problem stated we will give a brief summary of the results on the direct and inverse scattering problems for the operator L, obtained in Ref. 1.

Let us introduce two pairs of the Jost solutions of (3a):

$$\chi(\lambda)\to\begin{pmatrix}0\\1\end{pmatrix}\exp(-ikx),\quad x\to-\infty$$

$$\bar{\chi}(\lambda)\to\begin{pmatrix}1\\0\end{pmatrix}\exp(ikx),\quad x\to-\infty \tag{5a}$$

$$\phi(\lambda)\to\begin{pmatrix}1\\0\end{pmatrix}\exp(ikx),\quad x\to+\infty$$

$$\bar{\phi}(\lambda)\to\begin{pmatrix}0\\-1\end{pmatrix}\exp(-ikx),\quad x\to+\infty \tag{5b}$$

where $k\equiv k(\lambda)=\frac{1}{4}(\lambda^2-\lambda^{-2})$. The operator L satisfies the relation

$$\sigma_2 L^*(\lambda^*)\sigma_2=L(\lambda). \tag{6}$$

So if $\psi(x,\lambda)$ is a solution of (3a), then

$$\bar{\psi}(x,\lambda)=i\sigma_2\psi^*(x,\lambda^*) \tag{7}$$

is another solution. In particular, the solutions $\bar{\chi}$ and $\bar{\phi}$ are related by involution (7) to χ and ϕ, respectively. Also,

$$\tilde{\psi}(x,\lambda)=\pm\sigma_3\psi(x,-\lambda) \tag{8}$$

is yet another solution of (3a). If ψ is any of the Jost solutions, then it is invariant under transformation (8), with the sign in the rhs of (8) being chosen in accordance with asymptotics (5). The Wronskian

$$W(f,g)=\det\begin{pmatrix}f_1 & g_1\\ f_2 & g_2\end{pmatrix}$$

of any two solutions f and g of (3a) with the same λ is independent of x. This yields that $\bar{\psi}(\lambda)$ and $\psi(\lambda)$ are linearly independent (i.e., their Wronskian is nonzero), where the ψ denotes any of the Jost solutions.

Now let us introduce the scattering matrix for $\mathrm{Im}\,\lambda^2=0$:

$$\phi=a(\lambda)\bar{\chi}+b(\lambda)\chi,\quad \bar{\phi}=-\bar{a}(\lambda)\chi+\bar{b}(\lambda)\bar{\chi}. \tag{9a}$$

From (7) it follows that

$$\bar{a}(\lambda)=a^*(\lambda^*),\quad \bar{b}(\lambda)=b^*(\lambda^*). \tag{10}$$

In a standard way one shows that $\chi(\lambda)e^{ikx}$ and $\phi(\lambda)e^{-ikx}$ are analytic where $\mathrm{Im}\,\lambda^2\geqslant 0$, and $\bar{\chi}(\lambda)e^{-ikx}$ and $\bar{\phi}(\lambda)e^{ikx}$ are analytic where $\mathrm{Im}\,\lambda^2\leqslant 0$. From (9a) one finds

$$a=W(\phi,\chi),\quad b=W(\bar{\chi},\phi), \tag{11}$$

whence $a(\lambda)$ is analytic for $\mathrm{Im}\,\lambda^2>0$, and accordingly $\bar{a}(\lambda)$ is analytic for $\mathrm{Im}\,\lambda^2<0$; $b(\lambda)$ and $\bar{b}(\lambda)$ are, in general, defined only for $\mathrm{Im}\,\lambda^2=0$. From (11), (8), and (5) it follows that

$$a(-\lambda)=a(\lambda),\quad b(-\lambda)=-b(\lambda), \tag{12}$$

and also that, for $\mathrm{Im}\,\lambda^2=0$,

$$a\bar{a}+b\bar{b}=1. \tag{13}$$

From (9a) and (13) one determines the inverse of (9a):

$$\chi=-a\bar{\phi}+\bar{b}\phi, \quad \bar{\chi}=\bar{a}\phi+b\bar{\phi}. \tag{9b}$$

At the points of the discrete spectrum $\lambda_n(\mathrm{Im}\,\lambda_n^2>0)$ and $\lambda_n^*\equiv\lambda_{\bar{n}}$ such that $a(\lambda_n)=\bar{a}(\lambda_{\bar{n}})=0$, one has

$$\begin{aligned} &\chi_n=\bar{b}_n\phi_n, \quad \bar{\chi}_{\bar{n}}=b_{\bar{n}}\bar{\phi}_{\bar{n}}, \\ &\phi_n=b_n\chi_n, \quad \bar{\phi}_{\bar{n}}=\bar{b}_{\bar{n}}\bar{\chi}_{\bar{n}}, \end{aligned} \tag{9c}$$

where $\phi_n=\phi(x,\lambda_n)$, etc. Note that these points appear in pairs: if λ_n is an eigenvalue, then so is $-\lambda_n$, since $a(\lambda)$ is an even function. The asymptotic values of $a(\lambda)$ can be obtained from (3a) and (11):

$$\left.\begin{array}{ll} \underline{\lambda\to\infty} & a(\lambda)\to\exp(-i\hat{Q}) \\ \underline{\lambda\to 0} & a(\lambda)\to\exp(i\hat{Q}) \end{array}\right\} \mathrm{Im}(\lambda^2)\geqslant 0, \tag{14}$$

where $\hat{Q}=\frac{1}{4}\int_{-\infty}^{\infty}(|u|^2+|v|^2)dx$. The asymptotics of the Jost solutions for large and small λ are the following (for $\mathrm{Im}\,\lambda_n^2\geqslant 0$):

$$\begin{aligned} \underline{\lambda\to\infty} \quad \chi&\to\begin{pmatrix} v^*\lambda^{-1} \\ 1 \end{pmatrix}(1+\mathcal{O}(\lambda^{-1}))\exp(-ikx-iQ^-(x)), \\ \phi&\to\begin{pmatrix} 1 \\ -v\lambda^{-1} \end{pmatrix}(1+\mathcal{O}(\lambda^{-1}))\exp(ikx-iQ^+(x)), \end{aligned} \tag{15a}$$

$$\begin{aligned} \underline{\lambda\to 0} \quad \chi&\to\begin{pmatrix} \lambda u^* \\ 1 \end{pmatrix}(1+\mathcal{O}(\lambda))\exp(-ikx+iQ^-(x)), \\ \phi&\to\begin{pmatrix} 1 \\ -\lambda u \end{pmatrix}(1+\mathcal{O}(\lambda))\exp(ikx+iQ^+(x)), \end{aligned} \tag{15b}$$

where

$$Q^{\pm}(x)=\pm\frac{1}{4}\int_x^{\pm\infty}(|u|^2+|v|^2)dx'.$$

To complete the review of the discrete and inverse scattering problems for the operator L, we present the singular integral equation which allows one to reconstruct the Jost solutions from known scattering data $S=\{\rho(\lambda)=b/a|\lambda^2$ is real; λ_n, $c_n=b_n/\dot{a}_n|n=-N,\ldots,N,\ n\neq 0\}$:

$$Y(x,\lambda)=\sum_{n=-N,n\neq 0}^{N}\frac{c_n\chi_n e^{-ik_nx}}{\lambda-\lambda_n}+\begin{pmatrix}1\\0\end{pmatrix}e^{iQ^-(x)}+\frac{1}{2\pi i}\int_\Gamma\frac{\rho(\lambda')\chi(x,\lambda')e^{-ik'x}}{\lambda'-\lambda}\,d\lambda', \tag{16a}$$

where

$$Y(x,\lambda)=\begin{cases}(\phi/a)e^{-ikx}, & \mathrm{Im}\,\lambda^2>0, \\ \bar{\chi}e^{-ikx}, & \mathrm{Im}\,\lambda^2<0. \end{cases} \tag{16b}$$

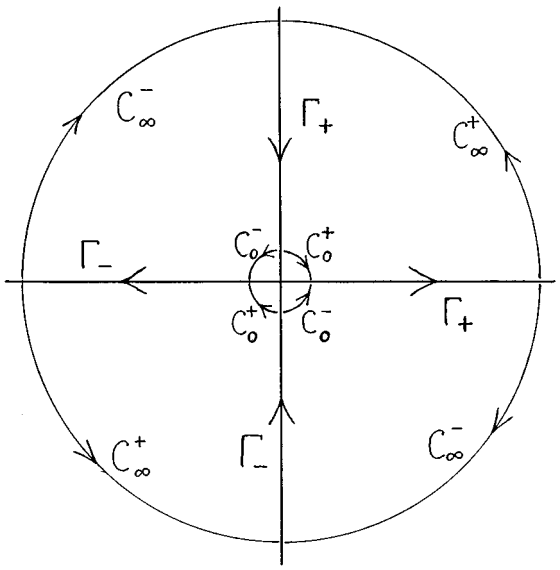

FIG. 1. Contours $C_0^{\pm}$, $C_\infty^{\pm}$, and $\Gamma^{\pm}$ in the complex λ-plane. Contour Γ is the union of Γ^+ and Γ^-.

Above we have used the following notations: $\dot{a}_n = (da/d\lambda)|_{\lambda=\lambda_n}$, $k_n=k(\lambda_n)$, $k'=k(\lambda')$, $\lambda_{-n}=-\lambda_n$, and the contour Γ is shown in Fig. 1.

Now let us pass to the solution of the problem stated in the beginning. We have four variations of the potentials: δu, δu^*, δv, and δv^*. In order to map them one-to-one into variations of the scattering data, we need four independent components of the latter. If we ignore for now the discrete spectrum, then we seem to have only two functions: $\rho(\lambda)$ and $\overline{\rho}(\lambda)=\rho^*(\lambda^*)$ on Γ. However, in reality we have exactly four of these. Indeed, the natural spectral parameter for (3a) is not the λ but rather $k(\lambda)$. On Γ, $k(\lambda)$ is fourfold degenerate since, for each value of k, there are four different possible values of λ, namely, λ itself, $-\lambda$, and $\pm i\lambda^{-1}$. As λ moves along each of the four rays of which the contour Γ is composed, k ranges from $-\infty$ to ∞. From (12) one deduces the relation $\rho(-\lambda)=-\rho(\lambda)$ [and consequently, $\overline{\rho}(-\lambda)=-\overline{\rho}(\lambda)$]. Thus, although the scattering data at $-\lambda$ is always related to the scattering data at λ, there is no such a relation connecting the scattering data at $\pm i\lambda^{-1}$ with that at λ. Therefore, the four independent functions in the set of scattering data are $\rho(\lambda)$ and $\overline{\rho}(\lambda)$ on contour Γ_+ (see Fig. 1).

III. VARIATIONS OF POTENTIALS AND SCATTERING DATA

Before going on to the solution of the problem, we note the following. As it was pointed out in the Introduction, there exist two equivalent ways of finding variations of the potentials via the components of the Jost solutions. The first way (see, for example, Ref. 4) employs the Riemann–Hilbert formulation of the corresponding scattering problem. This method would readily give us the answer if no discrete spectrum was present, but it becomes technically very cumbersome when one seeks to obtain the contribution to the variations of the potentials from the variation of the discrete spectrum. Therefore, here we have chosen to use the other method, which is based on calculating the variations of the scattering data via the variations of the potentials, and then inverting this relation. This latter method was used, for example, in Refs. 3, 5–8. In the Appendix we give, for the sake of completeness of presentation, a brief exposition of the former method.

Thus, we first find the variation of $\rho(\lambda)$ corresponding to variations of the potentials u and v. Then in a standard way (see, for example, Ref. 9) we find from (3a), (11), (5), and (9):

$$\delta\rho=\frac{i}{4a^2}\,\langle Z(\phi(x,\lambda))|\,\delta p(x)\rangle,\quad \delta\bar{\rho}=\frac{i}{4\bar{a}^2}\,\langle \bar{Z}(\phi(x,\lambda))|\,\delta p(x)\rangle, \tag{17}$$

where

$$\begin{gathered}\langle f|g\rangle\equiv\int_{-\infty}^{\infty}dx f(x)g(x),\quad \delta p=(\delta u,\delta u^*,\delta v,\delta v^*)^T,\\ Z=(Z_1,Z_2,Z_3,Z_4),\quad \bar{Z}(\phi)\equiv Z(\bar{\phi}),\\ Z_1(\phi)=2\left(-\frac{1}{\lambda}\,\phi_1{}^2+u^*\phi_1\phi_2\right),\quad Z_2(\phi)=2\left(\frac{1}{\lambda}\,\phi_2{}^2+u\,\phi_1\phi_2\right),\\ Z_3(\phi)=2(\lambda\,\phi_1{}^2-v^*\phi_1\phi_2),\quad Z_4(\phi)=2(-\lambda\,\phi_2{}^2-v\,\phi_1\phi_2),\end{gathered} \tag{18}$$

and ϕ_i in the above is the ith ($i=1,2$) component of ϕ, the Jost solutions defined in (5b). We omit arguments of functions wherever those are obvious or unimportant. In what follows it will be convenient for us to use the following notations:

$$V_i(fg)=f_ig_i,\quad i=1,2;\quad V_3(fg)=f_1g_2+f_2g_1, \tag{19}$$

and $V_i(f)=V_i(ff)$, $i=1,2,3$.

Let us now show how (17) should be inverted to find $\delta p(x)$. To simplify the subsequent calculations, let us suppose for the moment that L has no discrete spectrum. Then $\delta\rho$ and $\delta\bar{\rho}$ are its only scattering data. In order to invert these, we would require a set of adjoint functions, $Z^A(x,\lambda)$, orthogonal to the set Z in (18). Suppose for the moment that we have such a set where

$$\frac{i}{4}\int_\Gamma (Z^A(x',\lambda),\bar{Z}^A(x',\lambda))\begin{pmatrix} Z(x,\lambda)/a^2(\lambda)\\ \bar{Z}(x,\lambda)/\bar{a}^2(\lambda)\end{pmatrix}d\lambda=\delta(x'-x)\cdot I_4, \tag{20}$$

where I_n is the $n\times n$ unit matrix. Let us use the notation $\hat{Z}$ for the matrix $\left(\begin{smallmatrix} Z/a^2\\ \bar{Z}/\bar{a}^2\end{smallmatrix}\right)$ and $\hat{Z}^A$ for the matrix $(Z^A,\bar{Z}^A)$. Using (20), we could then obtain from (17)

$$\delta p(x)=\int_\Gamma d\lambda\,\hat{Z}^A(x,\lambda)\begin{pmatrix}\delta\rho(\lambda)\\ \delta\bar{\rho}(\lambda)\end{pmatrix}. \tag{21}$$

One way to find the form of $\hat{Z}^A$ would be to start with the expression dual to (20). Namely, if one multiplies (21) by $\hat{Z}$, integrates over x, and then takes into account (17), then one would obtain

$$\frac{i}{4}\,\langle\hat{Z}(x,\lambda)|\hat{Z}^A(x,\lambda')\rangle=\delta(\lambda-\lambda')\cdot I_2. \tag{22}$$

Once one has such a set of orthogonality relations as in (22), then one could identify $\hat{Z}_A$ from the integrands. This is how we shall proceed.

In earlier works,[3,5–8] the explicit form of $\hat{Z}^A$ was found in the following way. First, find the integro-differential equation for Z of the form

$$\Lambda Z=0; \tag{23a}$$

with the integro-differential operator Λ being of the form

$$\Lambda=\Lambda_0+\lambda\quad\text{or}\quad\Lambda=\Lambda_0+\lambda^2,\quad\text{etc.}, \tag{23b}$$

where Λ_0 is a λ-independent part. For the cases in Refs. 3,5–8, it was always found that this could be done even when the original L-operator contained both positive and negative powers of λ (see Ref. 8). Once (23) had been found, it was then straightforward to determine Z^A as a solution of the adjoint equation (hence the superscript 'A') and the inner product between Z and Z^A. The apparent drawback of this procedure was that the form of Λ had always been found by trial and error, which sometimes was a nontrivial matter.[5–8] In the case of the MTM in laboratory coordinates, we have been unable to easily find such an analogue of representation (23). The most apparent difficulty in doing this is that upon taking a derivative of Z_i, $i=1,...,4$, one then has derivatives of the potentials u,u^*,v,v^* as multiplying factors, which is a complicating feature. Nevertheless, we have found that it is still possible to find the explicit form of Z^A and determine its inner product with Z by means of another technique. Below we will describe this technique in detail since we believe that it will be useful in other related problems.

IV. METHOD OF FINDING Z^A FROM THE WRONSKIAN RELATIONS

First, from (3a), for the vector $\vec{V}=(V_1,V_2,V_3)^T$ one straightforwardly obtains

$$\left[I_3 \frac{\partial}{\partial x} - 2i(w+k) \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & r \\ 0 & 0 & q \\ 2q & 2r & 0 \end{pmatrix} \right] \vec{V}=0, \tag{24a}$$

where $k\equiv k(\lambda)$, $w=\frac{1}{4}(|u|^2-|v|^2)$, $r=(i/2)(\lambda v^*-u^*/\lambda)$, and $q=(i/2)(\lambda v-u/\lambda)$. Defining the solution $\vec{V}^A$ of the adjoint problem as the vector satisfying

$$\left[-I_3 \frac{\partial}{\partial x} - 2i(w+k) \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 2q \\ 0 & 0 & 2r \\ r & q & 0 \end{pmatrix} \right] \vec{V}^A=0, \tag{24b}$$

one finds that $\vec{V}^A=(V_2,V_1,-V_3/2)$. Thus the solution of the adjoint problem is related to that of the original one by a similarity transformation.

Now we make the observation that, in all the previous cases, one was able to obtain from the corresponding integro-differential equation, (23), a Wronskian relation from the analogue of Eq. (24) in the following form:

$$\frac{\partial}{\partial x}\left[\alpha(\lambda,\lambda')V_1^A V_1+\beta(\lambda,\lambda')V_2^A V_2+\gamma(\lambda,\lambda')V_3^A V_3\right]=h(\lambda,\lambda')(Z_1^A Z_1+Z_2^A Z_2+Z_3^A Z_3+Z_4^A Z_4). \tag{25}$$

In (25), the Vs and Zs are functions of x and λ, the adjoint states V^As and Z^As are functions of x and λ', and the coefficients α, β, γ, and h are independent of x. So, if this is the form which always results, is it possible to start with (25), then use all the above relations and uniquely determine α, β, γ, h, and Z^A? Indeed, such is the case.

We start with (24) and the definition of $\vec{V}^A$. Then (25) becomes of the form (summation over repeated indices is implied)

$$h(\lambda,\lambda')Z_i^A Z_i=V_j' M_{js} V_s, \tag{26a}$$

with

$$M=\begin{pmatrix} 0 & -2i\beta(k-k') & q'\gamma-q\beta \\ 2i\alpha(k-k') & 0 & r'\gamma-r\alpha \\ q\gamma-q'\alpha & r\gamma-r'\beta & 0 \end{pmatrix}, \tag{26b}$$

where $V_j \equiv V_j(\lambda)$, $V_j' \equiv V_j(\lambda')$, etc. From (18) one has

$$Z_i = m_{is} V_s \tag{27a}$$

with

$$m=\begin{pmatrix} -2\lambda^{-1} & 0 & u^* \\ 0 & 2\lambda^{-1} & u \\ 2\lambda & 0 & -v^* \\ 0 & -2\lambda & -v \end{pmatrix}. \tag{27b}$$

Substituting (27a) into the lhs of (26a), one sees that the resulting equation is linear in V_s. Then, after formally differentiating it with respect to V_s, one obtains

$$h(\lambda,\lambda')Z_i^A m_{is} = V_j' M_{js}. \tag{28}$$

One cannot invert it to find Z^A because m is not a square matrix. However, if Z^A exists, then it is seen from (28) that it must be of the form

$$Z_i^A = m_{ij}^A V_j', \tag{29}$$

for some yet unknown 4×3 matrix m^A. The key to determining m^A lies in the fact that the entries of m^A may depend on λ', but not on λ. Upon substituting (29) into (28) and formally differentiating with respect to V_j', one obtains

$$h m_{ij}^A m_{is} = M_{js}. \tag{30}$$

Let us introduce the following notations [see (26b) and (27b)]:

$$M=\begin{pmatrix} A & B \\ C & 0 \end{pmatrix}, \quad m=(D,E), \quad m^A=(F,G),$$

where A, B, and C are 2×2, 2×1, and 1×2 matrices, respectively. The (22)-entry of M is the number zero, D and F are 4×2 matrices, and E and G are 4×1 matrices. Notice that A and D are independent of the potentials. With these notations, (30) rewrites as follows:

$$\begin{aligned} hF^T\cdot D = A, \quad hF^T\cdot E = B, \\ hG^T\cdot D = C, \quad G^T\cdot E = 0. \end{aligned} \tag{31}$$

Consider the first matrix equation in (31). Using (26b) and (27b) and the explicit form of q,r, one obtains

$$-\frac{1}{\lambda}F_{11}+\lambda F_{31}=0, \tag{32a}$$

$$h\left(-\frac{1}{\lambda}F_{12}+\lambda F_{32}\right)=i(k-k')\beta, \tag{32b}$$

$$h\left(-\frac{1}{\lambda}F_{21}+\lambda F_{41}\right)=i(k-k')\alpha, \tag{32c}$$

$$-\frac{1}{\lambda}F_{22}+\lambda F_{42}=0. \tag{32d}$$

Let $F_{ij}=F_{ij}^0+F_{ij}^p$, where F_{ij}^0, F_{ij}^p are the potential-independent and potential-dependent parts, respectively. Then one easily finds that

$$F_{1j}^p=\lambda^2 F_{3j}^p, \quad F_{2j}^p=\lambda^2 F_{4j}^p, \quad j=1,2. \tag{33}$$

Since the matrix m^A is independent of λ, then from (33) it follows that the potential-dependent part of F must be zero.

Using the second equation in (31), one obtains

$$h(u^*F_{11}+uF_{21}-v^*F_{31}-vF_{41})=\frac{i}{2}\left[v(\gamma\lambda'-\beta\lambda)+u\left(\frac{\beta}{\lambda}-\frac{\gamma}{\lambda'}\right)\right], \tag{34a}$$

$$h(u^*F_{12}+uF_{22}-v^*F_{32}-vF_{42})=\frac{i}{2}\left[v^*(\gamma\lambda'-\alpha\lambda)+u^*\left(\frac{\alpha}{\lambda}-\frac{\gamma}{\lambda'}\right)\right]. \tag{34b}$$

Since F has been found to be potential independent, one immediately sees that

$$F_{11}=F_{31}=F_{22}=F_{42}=0, \tag{35a}$$

$$hF_{21}=\frac{i}{2}\left(\frac{\beta}{\lambda}-\frac{\gamma}{\lambda'}\right), \tag{35b}$$

$$hF_{41}=\frac{i}{2}(\beta\lambda-\gamma\lambda'), \tag{35c}$$

$$hF_{12}=\frac{i}{2}\left(\frac{\alpha}{\lambda}-\frac{\gamma}{\lambda'}\right), \tag{35d}$$

$$hF_{41}=\frac{i}{2}(\alpha\lambda-\gamma\lambda'). \tag{35e}$$

Substituting (35b) and (35c) into (32c) and (35d) and (35e) into (32b), one obtains two linear equations for α, β, and γ, from which one straightforwardly deduces

$$\alpha=\beta, \quad \gamma=\alpha\cdot\frac{\lambda^2+\lambda'^2}{2\lambda\lambda'}. \tag{36}$$

Without loss of generality, one can set $\alpha=1$.

Let $G=(g_1,g_2,g_3,g_4)^T$. Then from the third equation in (31) and Eq. (36) it follows

$$h\left(-\frac{1}{\lambda}g_1+\lambda g_3\right)=\frac{i}{4}\left[\lambda v\,\frac{\lambda^2-\lambda'^2}{2\lambda\lambda'}+\frac{u}{\lambda}\,\frac{\lambda^2-\lambda'^2}{2\lambda\lambda'}\right], \tag{37a}$$

$$h\left(\frac{1}{\lambda}g_2-\lambda g_4\right)=\frac{i}{4}\left[\lambda v^*\,\frac{\lambda^2-\lambda'^2}{2\lambda\lambda'}+\frac{u^*}{\lambda}\,\frac{\lambda^2-\lambda'^2}{2\lambda\lambda'}\right]. \tag{37b}$$

Since the entries of G are to be independent of λ, then it must be

$$g_1=-\frac{u}{2}f(\lambda'),\quad g_2=\frac{u^*}{2}f(\lambda'),$$

$$g_3=\frac{v}{2}f(\lambda'),\quad g_4=-\frac{v^*}{2}f(\lambda'), \tag{38}$$

$$h=\frac{i(\lambda^2-\lambda'^2)}{4\lambda\lambda' f(\lambda')},$$

where $f(\lambda')$ is an arbitrary function. Then the fourth equation in (31) is satisfied identically. As one can see from (35) and (38), the function $f(\lambda')$ simply multiplies the matrix m^A by an arbitrary function of λ'. In order to have a simple form for Z^A, we take $f(\lambda')=1$. Finally, using (35), (36), and (38), one obtains the desired Wronskian relation:

$$\frac{\partial}{\partial x}\left[V_1^A V_1+V_2^A V_2+\frac{\lambda^2+\lambda'^2}{2\lambda\lambda'}V_3^A V_3\right]=\frac{i(\lambda'^2-\lambda^2)}{8\lambda\lambda'}\cdot(Z_1Z_2'+Z_2(-Z_1')+Z_3Z_4'+Z_4(-Z_3')), \tag{39}$$

where $Z_j\equiv Z_j(\lambda)$, $Z_j'\equiv Z_j(\lambda')$, $j=1,...,4$. With this we can define the inner product that we need. We note that a formula, which proves to be equivalent to (39), was given (without derivation) in Ref. 1.

V. COMPLETENESS OF THE SQUARED EIGENFUNCTIONS

From (39), it follows that we may take

$$Z^A=\frac{i}{2\pi}(Z_2,-Z_1,Z_4,-Z_3)^T,\quad \bar{Z}^A=-\frac{i}{2\pi}(\bar{Z}_2,-\bar{Z}_1,\bar{Z}_4,-\bar{Z}_3)^T,$$

and we choose to evaluate the Z- and Z^A-states using the Jost solutions ϕ and χ, respectively. Then, from (5) and (39), we obtain, for $\mathrm{Im}\,\lambda^2=0$,

$$\frac{i}{4}\langle\hat{Z}|\hat{Z}'^A\rangle=2\lambda\lambda'\delta(\lambda^2-\lambda'^2)\cdot I_2. \tag{40}$$

Similarly, the inner products involving the discrete spectrum are

$$\langle\hat{Z}_n|\hat{Z}_m^A\rangle=0, \tag{41a}$$

$$\langle\hat{D}_n|\hat{D}_m^A\rangle=\begin{pmatrix}\frac{2}{\pi}\lambda_n\dot{a}_n\ddot{a}_n(\delta_{n,m}+\delta_{n,-m}) & 0\\ 0 & \frac{2}{\pi}\lambda_{\bar{n}}\dot{\bar{a}}_{\bar{n}}\ddot{\bar{a}}_{\bar{n}}(\delta_{\bar{n},\bar{m}}+\delta_{\bar{n},-\bar{m}})\end{pmatrix}, \tag{41b}$$

$$\langle\hat{D}_n|\hat{Z}_m^A\rangle=\langle\hat{Z}_n|\hat{D}_m^A\rangle=\begin{pmatrix}\frac{2}{\pi}\lambda_n\dot{a}_n^2(\delta_{n,m}+\delta_{n,-m}) & 0\\ 0 & \frac{2}{\pi}\lambda_{\bar{n}}\dot{\bar{a}}_{\bar{n}}^2(\delta_{\bar{n},\bar{m}}+\delta_{\bar{n},-\bar{m}})\end{pmatrix}, \tag{41c}$$

for $m,n=-N,\ldots,N$; $m,n\neq 0$. In (41), we have used the following shorthand notations:

$$\hat{Z}_n=(Z^T(x,\lambda_n),\bar{Z}^T(x,\lambda_{\bar{n}}))^T,\quad \hat{D}_n=\left(\frac{\partial}{\partial\lambda}Z^T(x,\lambda)\Big|_{\lambda_n},\frac{\partial}{\partial\lambda}\bar{Z}^T(x,\lambda)\Big|_{\lambda_{\bar{n}}}\right)^T,$$

$$\hat{Z}_n^A=(Z^A(x,\lambda_n),\bar{Z}^A(x,\lambda_{\bar{n}})),\quad \hat{D}_n^A=\left(\frac{\partial}{\partial\lambda}Z^A(x,\lambda)\Big|_{\lambda_n},\frac{\partial}{\partial\lambda}\bar{Z}^A(x,\lambda)\Big|_{\lambda_{\bar{n}}}\right).$$

Let us now derive a generalization of (20) to the case when the L-operator (3a) has a discrete spectrum. Taking into account (40), consider the following principal value integral:

$$\frac{i}{8}\not\int_\Gamma\frac{d\lambda}{\lambda}\,\hat{Z}^A(\chi(x))\cdot\hat{Z}(\phi(y))$$

$$=\begin{cases}-\dfrac{i}{8}\left[\left(\displaystyle\int_{C_0^+}+\int_{C_\infty^+}\right)\dfrac{d\lambda}{\lambda a^2}\,Z^A(\chi(x))Z(\phi(y))+\left(\displaystyle\int_{C_0^-}+\int_{C_\infty^-}\right)\dfrac{d\lambda}{\lambda\bar{a}^2}\,\bar{Z}^A(\chi(x))\bar{Z}(\phi(y))\right]\\ \quad-\dfrac{\pi}{4}\,(\text{D.Sp.}),\quad \text{for } y\geqslant x;\\ -\dfrac{i}{8}\left[\left(\displaystyle\int_{C_0^+}+\int_{C_\infty^+}\right)\dfrac{d\lambda}{\lambda a^2}\,(2Z^A(\chi\phi(x))Z(\chi\phi(y))-Z^A(\phi(x))Z(\chi(y)))+\left(\displaystyle\int_{C_0^-}+\int_{C_\infty^-}\right)\right.\\ \quad\left.\times\dfrac{d\lambda}{\lambda\bar{a}^2}\,(2\bar{Z}^A(\chi\phi(x))\bar{Z}(\chi\phi(y))-\bar{Z}^A(\phi(x))\bar{Z}(\chi(y)))\right]-\dfrac{\pi}{4}\,(\text{D.Sp.}),\quad \text{for } y\leqslant x;\end{cases}\tag{42a}$$

where, for instance, $Z(\chi\phi(y))$ is evaluated for the functions $\chi(y,\lambda)$ and $\phi(y,\lambda)$ as in (19); $Z_n(\phi(y))=Z(\phi(y,\lambda_n))$, etc. Now in (42a), each case contains the term (D.Sp.), which is the contribution to (42a) of the discrete spectrum. This term is given by

$$(\text{D.Sp.})=\sum_{n=-N,n\neq 0}^{N}\left\{-\left(\frac{\dot{a}_n+\lambda_n\ddot{a}_n}{\dot{a}_n^3\lambda_n^2}\right)Z_n^A(\chi(x))Z_n(\phi(y))+\frac{1}{\dot{a}_n^2\lambda_n}\,[D_n^A(\chi(x))Z_n(\phi(y))\right.$$
$$\left.+Z_n^A(\chi(x))D_n(\phi(y))]\right\}-\{\text{same quantities with the bar}\}.\tag{42b}$$

The contours $C_0^\pm$, $C_\infty^\pm$ are shown in Fig. 1. In deriving (42), we have used the analyticity of the Jost functions in their corresponding domains, and also we made use of relations (9) to obtain the representation of the lhs in the regions $y\geqslant x$ and $y\leqslant x$ (see Ref. 5). Now, one can use the asymptotics (14) and (15) to evaluate the continuous spectrum part in the rhs of (42a) and then ''pull back'' onto the contour Γ, after deleting those terms which give vanishing contributions at infinity. In this way, upon also using the identities

$$\not\int_\Gamma\frac{d\lambda}{\lambda^3}\,e^{ik(\lambda)x}=\not\int_\Gamma\lambda\,d\lambda\,e^{ik(\lambda)x}=8\pi\delta(x),$$

we arrive at the formula which is the main result of this paper:

$$\frac{i}{8}\oint_\Gamma \frac{d\lambda}{\lambda}\,\hat{Z}^A\cdot\hat{Z}+\frac{\pi}{4}\sum_{n=-N,n\neq 0}^{N}\left\{-\hat{Z}_n^A\cdot\begin{pmatrix}(\dot a_n+\lambda_n\ddot a_n)Z_n/(\dot a_n^3\lambda_n^2)\\ -(\dot{\bar a}_{\bar n}+\lambda_{\bar n}\ddot{\bar a}_{\bar n})\bar Z_{\bar n}/(\dot{\bar a}_{\bar n}^3\lambda_{\bar n}^2)\end{pmatrix}+\hat{D}_n^A\cdot\begin{pmatrix}Z_n/(\dot a_n^2\lambda_n)\\ -\bar Z_{\bar n}/(\dot{\bar a}_{\bar n}^2\lambda_{\bar n})\end{pmatrix}+\hat{Z}_n^A\right.$$
$$\left.\cdot\begin{pmatrix}D_n/(\dot a_n^2\lambda_n)\\ -\bar D_{\bar n}/(\dot{\bar a}_{\bar n}^2\lambda_{\bar n})\end{pmatrix}\right\}=\delta(x-y)\cdot I_4. \tag{43}$$

In (43) each Z^A and D^A are to be evaluated for $\chi(x,\lambda)$ and each Z and D are to be evaluated for $\phi(y,\lambda)$. Notice that, making use of symmetry (8) and (12), one may restrict the summation in (42b) and (43), and formulae (45) and (46) below to be over $n=1,\ldots,N$ (one should then take the overall coefficient in front of the sum sign to be a factor of 2 larger), and at the same time, replace $\oint_\Gamma$ by $2\int_{\Gamma^+}$.

Now we can produce formulas for the expansions of both the potential $p(x)=(u,u^*,v,v^*)^T$ and $\delta p(x)$ over the complete set $\{Z^A\}$. In the standard way (see Ref. 10) one obtains

$$\delta\lambda_n=\frac{i}{4b_n\dot a_n}\langle Z_n(\phi)|\,\delta p\rangle, \tag{44a}$$

$$\delta c_n=\frac{i}{4\dot a_n^2}\left[-\left(\frac{\ddot a_n}{\dot a_n}\right)\langle Z_n(\phi)|\,\delta p\rangle+\langle D_n(\phi)|\,\delta p\rangle\right]; \tag{44b}$$

the quantity c_n was defined before formula (16). Note that in the derivation of (44), one must take into account the fact that $b_n,\dot a_n$ depend on the potential $p(x)$ both implicitly, as functionals, and explicitly, through their dependence on λ_n. Equations (17), (44), and (43) now lead to the following expansion formula for δp:

$$\delta p=\frac{1}{2}\oint_\Gamma\frac{d\lambda}{\lambda}\,\hat{Z}^A(\chi)\begin{pmatrix}\delta\rho\\ \delta\bar\rho\end{pmatrix}-i\pi\sum_{n=-N,n\neq 0}^{N}\left[\hat{Z}_n^A\begin{pmatrix}\delta(c_n/\lambda_n)\\ -\delta(\bar c_{\bar n}/\lambda_{\bar n})\end{pmatrix}+\hat{D}_n^A\begin{pmatrix}(c_n/\lambda_n)\delta\lambda_n\\ -(\bar c_{\bar n}/\lambda_{\bar n})\delta\lambda_{\bar n}\end{pmatrix}\right]. \tag{45}$$

From the third row in (24a) one easily finds the inner products between the Z-states and the potential $p(x)$. Whence one obtains

$$\begin{pmatrix}\sigma_3 & 0\\ 0 & \sigma_3\end{pmatrix}p(x)=\frac{1}{2}\oint_\Gamma\frac{d\lambda}{\lambda}\,\hat{Z}^A(\chi)\begin{pmatrix}\rho\\ -\bar\rho\end{pmatrix}-i\pi\sum_{n=-N,n\neq 0}^{N}\hat{Z}_n^A(\chi)\begin{pmatrix}c_n/\lambda_n\\ \bar c_{\bar n}/\lambda_{\bar n}\end{pmatrix}. \tag{46}$$

Note that the D_n^A states are absent in (46).

For possible applications, we present below the exact expressions of the one-soliton potentials $u_s(x)$ and $v_s(x)$, the corresponding scattering data, and the Jost solutions $\chi(x,\lambda)$ and $\chi(x,\lambda_1)$, from which the Z- and Z^A- states may be computed as needed:

$$u_s(x,t)=\sin Q\ \operatorname{sech}(\Theta-iQ/2)e^{i\beta},\quad v_s(x,t)=-\sin Q\ \operatorname{sech}(\Theta+iQ/2)e^{i\beta}; \tag{47}$$

$$0\leqslant Q\leqslant\pi,\quad \Theta=x\sin Q,\quad \beta=-t\cos Q,$$

$$\lambda_1=\exp(iQ/2),\quad c_1=\sin Q\cdot e^{i\beta}, \tag{48}$$

$$a(\lambda)=\frac{\lambda^2-\lambda_1^2}{\lambda^2-\lambda_1^{*2}}\,e^{-iQ},\quad b(\lambda)=0\quad\text{for Im }\lambda^2=0;$$

$$\chi(x,\lambda_1)=\frac{1}{2}\begin{pmatrix}i\ \operatorname{sech}(\Theta+iQ/2)\cdot\exp(-i\beta+iA(x)+(\Theta-iQ)/2)\\ \operatorname{sech}(\Theta-iQ/2)\cdot\exp(-iA(x)-(\Theta-iQ)/2)\end{pmatrix}, \tag{49}$$

where

$$A(x)=\arctan\left(\tan\left(\frac{Q}{2}\right)\tanh\,\Theta\right)+\frac{Q}{2},$$

$$\chi(x,\lambda)=\begin{pmatrix}0\\1\end{pmatrix}e^{-iA(x)-ik(\lambda)x}-\frac{\exp(-ik(\lambda)x)\cdot\sin\,Q}{\lambda^2-\lambda_1^{*2}}\cdot\begin{pmatrix}\lambda\ \operatorname{sech}(\Theta+iQ/2)\cdot\exp(-i\beta-iQ+iA(x))\\ i\ \operatorname{sech}(\Theta-iQ/2)\cdot\exp(\Theta-iA(x)-iQ/2)\end{pmatrix}. \tag{50}$$

Formulas (49) and (50) were obtained from (16) and (48).

VI. CONCLUDING REMARKS

The main difference between the result of the present work and those of the earlier ones[4–9] on this subject is a new method for finding squared eigenfunctions. Previously, one has been able to find both the exact form of the ''squared eigenfunctions'' and the operator Λ_0 [see (23)], whose eigenfunctions were the ''squared eigenfunctions.'' The knowledge of that operator allowed one to construct a hierarchy of integrable evolutional equations and Hamiltonian structures, related to a given L-operator, and the corresponding infinite series of conservation laws. Let us note, however, that the infinite series of the conservation laws for equations (1) was obtained in Ref. 1 by standard ''elementary'' means, and thus the whole hierarchy of integrable evolutional equations of which the massive Thirring model in laboratory coordinates is a member, is in principle known. We have proposed a regular procedure by which the structure of the inner product, and thus the explicit form of Z^A, can be determined. This procedure gave us the result for equations (1), and we believe that it will be useful in other related problems.

Note added in proof: It has recently been pointed out to us by V. S. Gerdjikov that one could also use the method outlined in Refs. 11 and 12 to find the recursion operator (i.e., the operator whose eigenfunctions are the ''squared eigenfunctions'') for the operator (3a). With the notations

$$X_{uv}f\equiv-\begin{pmatrix}u\\-u^*\end{pmatrix}\int_x^\infty dy(v^*,v)f,$$

defining operators X_{uv}, etc., acting on a two-component vector f, and also with

$$T=\begin{pmatrix}1+\frac{i}{2}X_{uu} & -\frac{i}{2}X_{uv}\\ -\frac{i}{2}X_{vu} & -1+\frac{i}{2}X_{vv}\end{pmatrix},\quad T^{-1}=\begin{pmatrix}1-\frac{i}{2}X_{uu} & -\frac{i}{2}X_{uv}\\ -\frac{i}{2}X_{vu} & -1-\frac{i}{2}X_{vv}\end{pmatrix},$$

$$\tilde{\Lambda}=\begin{pmatrix}1 & 0\\ 0 & 2(i-X_{vv})\end{pmatrix}\cdot\begin{pmatrix}0 & 1\\ -\frac{1}{2}(i-X_{uu}) & \sigma_3\partial_x+2iw-\frac{1}{2}(X_{vu}+X_{uv})\end{pmatrix},$$

$$\tilde{\Lambda}^{-1}=\begin{pmatrix}-2(i+X_{uu}) & 0\\ 0 & 1\end{pmatrix}\cdot\begin{pmatrix}\sigma_3\partial_x+2iw-\frac{1}{2}(X_{vu}+X_{uv}) & \frac{1}{2}(i+X_{vv})\\ 1 & 0\end{pmatrix},$$

$$\hat{\sigma}_2=\operatorname{diag}(\sigma_2,\sigma_2),$$

one can define two operators,

$$\Lambda=\hat{\sigma}_2 T\tilde{\Lambda}T^{-1}\hat{\sigma}_2, \quad \Lambda^{-1}=\hat{\sigma}_2 T\tilde{\Lambda}^{-1}T^{-1}\hat{\sigma}_2,$$

such that

$$(\Lambda-\lambda^2)Z=0, \quad (\Lambda^{-1}-\lambda^{-2})Z=0,$$

where Z was defined in (18), and $w=(|u|^2-|v|^2)/4$. Given this, one could find the adjoint vector Z^A and then proceed as outlined after Eq. (23) in the text. However, this method of finding the recursion operator is known (V. S. Gerdjikov, private communication) not to work (at least in a straightforward way) for, e.g., a quartic bundle,[12] while for the method described in Sec. IV of the present paper there seems to be no restriction on the maximum power of λ in the Lax operator. The question of whether this is indeed the case and, in particular, whether or not our method would work for the quartic bundle, needs further investigation.

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APPENDIX: RIEMANN–HILBERT FORMULATION

Here we demonstrate how the form of the ''squared eigenfunctions'' can be found from the Riemann–Hilbert (RH) formulation of the inverse scattering problem for operator (4). Below we will assume that the coefficients $a(\lambda)$, $\bar{a}(\lambda)$ are nonzero in their respective domains of analyticity.

The second equations in (9a) and (9b) can be rewritten in the form

$$\Psi^+=\Psi^- G, \quad \lambda\in\Gamma, \tag{A1a}$$

where the 2×2 matrices $\Psi^{\pm}$, G are

$$\Psi^+=\left(\frac{\phi}{a}\,e^{-ikx},\chi e^{ikx}\right), \quad \Psi^-=\left(\bar{\chi}e^{-ikx},-\frac{\bar{\phi}}{\bar{a}}\,e^{ikx}\right), \quad G=\begin{pmatrix}1+\rho\bar{\rho} & \bar{\rho}e^{2ikx}\\ \rho e^{-2ikx} & 1\end{pmatrix}. \tag{A1b}$$

In deriving (A1), Eq. (13) was used. $\Psi^{\pm}$ are analytic where $\mathrm{Im}\,\lambda^2\gtrless0$, respectively. If the potentials in (4) vary, then $\Psi^{\pm}$, G will vary according to the equation

$$\delta\Psi^+(\Psi^+)^{-1}=\delta\Psi^-(\Psi^-)^{-1}+\Psi^-\delta G(\Psi^+)^{-1}, \quad \lambda\in\Gamma, \tag{A2}$$

where we have used $G=\Psi^+(\Psi^-)^{-1}$. Matrices $(\Psi^{\pm})^{-1}$ are nonsingular [see (11)], thus $\delta\Psi^{\pm}(\Psi^{\pm})^{-1}$ are analytic in the corresponding domains of the λ-plane. Then (A2) constitutes a simple RH problem, whose solution is

$$\delta\Psi(x,\lambda)=\delta\Psi^0(x)\Psi(x,\lambda)+\frac{1}{2i\pi}\int\!\!\!\!\!\!\diagup_{\Gamma}\frac{\Phi(x,\xi)d\xi}{\xi-\lambda}\,\Psi(x,\lambda), \tag{A3}$$

where $\Psi(x,\lambda)$ is the solution of (A1). In (A3),

$$\Phi=\Psi^-\delta G(\Psi^+)^{-1}, \tag{A4a}$$

or, in the component form,

$$\Phi_{11}=-\Phi_{22}=\delta\rho\chi_1\chi_2-\delta\bar{\rho}\bar{\chi}_1\bar{\chi}_2,\quad \Phi_{12}=-\delta\rho\chi_1^2+\delta\bar{\rho}\bar{\chi}_1^2,\quad \Phi_{21}=\delta\rho\chi_2^2-\delta\bar{\rho}\bar{\chi}_2^2. \tag{A4b}$$

Matrix $\delta\Psi^0(x)$ in (A3) should be determined from the asymptotics at $\lambda\to 0$ and $\lambda\to\infty$. Taking into account symmetry (8) and (12), it is convenient to rewrite (A3) as follows:

$$\delta\Psi(x,\lambda)=\delta\Psi^0(x)\Psi(x,\lambda)+\frac{1}{i\pi}\int_{\Gamma^+}\frac{d\xi}{\xi^2-\lambda^2}\left[\xi\begin{pmatrix}\Phi_{11} & 0\\ 0 & -\Phi_{11}\end{pmatrix}+\lambda\begin{pmatrix}0 & \Phi_{12}\\ \Phi_{21} & 0\end{pmatrix}\right]\Psi(x,\lambda). \tag{A5}$$

The desired variations $\delta u,\delta u^*,\delta v,\delta v^*$ are found from the asymptotics of (A5) for $\lambda\to 0$ and $\lambda\to\infty$. From (14) and (15) one finds

$$\underline{\lambda\to 0}\quad \Psi^+\to\begin{pmatrix}e^{-iQ^-} & \lambda u^* e^{iQ^-}\\ -\lambda u e^{-iQ^-} & e^{iQ^-}\end{pmatrix}, \tag{A6a}$$

$$\underline{\lambda\to\infty}\quad \Psi^+\to\begin{pmatrix}e^{iQ^-} & \lambda^{-1}v^* e^{-iQ^-}\\ -\lambda^{-1}v e^{iQ^-} & e^{-iQ^-}\end{pmatrix}, \tag{A6b}$$

where $Q^-\equiv Q^-(x)$. Substituting (A6a) into (A5), one finds

$$\delta\Psi^0_{12}(x)=\delta\Psi^0_{21}(x)=0; \tag{A7a}$$

$$I_2\left(i\,\delta Q^-+\frac{1}{i\pi}\int_{\Gamma^+}\frac{\Phi_{11}d\xi}{\xi}\right)+\sigma_3\ \mathrm{diag}(\delta\Psi^0_{11}(x),\delta\Psi^0_{22}(x))=0; \tag{A7b}$$

$$\delta u=-\frac{1}{i\pi}\int_{\Gamma^+}\frac{\Phi_{21}d\xi}{\xi^2}+2i\,\delta Q^- u; \tag{A7c}$$

$$\delta u^*=\frac{1}{i\pi}\int_{\Gamma^+}\frac{\Phi_{12}d\xi}{\xi^2}-2i\,\delta Q^- u^*. \tag{A7d}$$

Substituting (A6b) into (A5) and using (A7), one obtains

$$\delta\Psi^0_{11}(x)=-\delta\Psi^0_{22}(x)=i\,\delta Q^-=-\frac{1}{2i\pi}\int_{\Gamma^+}\frac{\Phi_{11}d\xi}{\xi},$$

and then

$$\begin{aligned}
\delta u&=-\frac{1}{i\pi}\int_{\Gamma^+}\left(\frac{\Phi_{21}}{\xi^2}+u\,\frac{\Phi_{11}}{\xi}\right)d\xi;\\
\delta u^*&=\frac{1}{i\pi}\int_{\Gamma^+}\left(\frac{\Phi_{12}}{\xi^2}+u^*\,\frac{\Phi_{11}}{\xi}\right)d\xi;\\
\delta v&=\frac{1}{i\pi}\int_{\Gamma^+}\left(\Phi_{21}+v\,\frac{\Phi_{11}}{\xi}\right)d\xi;\\
\delta v^*&=-\frac{1}{i\pi}\int_{\Gamma^+}\left(\Phi_{12}+v^*\,\frac{\Phi_{11}}{\xi}\right)d\xi.
\end{aligned} \tag{A8}$$

Equations (A8) are equivalent to formula (45) without the contribution from the discrete spectrum. As it is known, the discrete spectrum is introduced into the RH problem through the solution of a certain system of algebraic equations. Working with the variation of this system, occurring due to the variation of the discrete scattering data, is much more cumbersome than simply picking up the contribution from the poles in the corresponding integrals [formula (42)], therefore we did not pursue the former way here.

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Exact interaction of solitary waves for certain nonintegrable equations

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Physically interesting exact solutions are constructed for a large class of nonlinear nonintegrable evolution equations. These solutions describe the interaction of traveling waves. They exhibit rich phenomenology including breaking of solitary waves. Generalized conditional symmetries and bilinearity are used to derive these exact results. © *1996 American Institute of Physics.* [S0022-2488(96)03601-5]

I. INTRODUCTION

We have recently introduced a new method for finding physically important exact solutions of certain nonintegrable equations.[1] Our method uses the fact that there exist nonintegrable equations which share an ''integrable sector'' with integrable equations. We recall that there exist two well-known types of integrable equations: Equations like Burgers which can be linearized by an explicit change of variables,[2] and equations like Korteweg–de Vries (KdV) which can be linearized by the inverse spectral method.[3] We have found nonintegrable equations associated with both Burgers and KdV. For example, the Newell–Whitehead equation[4]

$$3u_t = u_{xx} + u - 2u^3 \tag{1.1}$$

shares the two-shock solution $\partial_x \log(K_1 e^{(1/\sqrt{2})x+(1/2)t} + K_2 e^{-(1/\sqrt{2})x+(1/2)t} + K_3)$, K_1, K_2, and K_3 are arbitrary constants with the Burgers equation

$$u_t = u_{xx} + 2uu_x. \tag{1.2}$$

Similarly, the equation

$$u_t = 2\gamma u u_{xx} + (1-\gamma)u_x^2 + (2+4\gamma)u^2 u_x + \alpha u_x + (1+\gamma)(u^4 - \alpha u^2 + \beta), \quad \alpha,\beta,\gamma \text{ const} \tag{1.3}$$

shares the two-soliton solution $\partial_x \log[K_1 e^{k_1[x+(k_1^2+3k_2^2)t]} + K_2 e^{-k_1[x+(k_1^2+3k_2^2)t]} + K_3 e^{k_2[x+(3k_1^2+k_2^2)t]} + K_4 e^{-k_2[x+(3k_1^2+k_2^2)t]}]$, $k_1 = [(\alpha + \sqrt{\alpha^2-4\beta})/2]^{1/2}$, $k_2 = [(\alpha - \sqrt{\alpha^2-4\beta})/2]^{1/2}$, K_1, K_2, and K_3 are arbitrary constants and $k_1^2 K_1 K_2 = k_2^2 K_3 K_4$, with the potential KdV equation

$$u_t = u_{xxx} + 6u_x^2. \tag{1.4}$$

We note that multisoliton and multishock solutions have similar mathematical characterization. Actually multisolitons can be obtained from multishocks by differentiation with respect to x. Throughout this article we use this approach to obtain soliton-type solutions from shock-type solutions.

Our method is based on the introduction of a new type of symmetry, which we have called generalized conditional symmetry (GCS). A smooth function of u, u_x, u_{xx},..., denoted by $\sigma(u)$,

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is a GCS of the evolution equation $u_t=K(u)$, where K is a smooth function of u, u_x, u_{xx},..., iff $[\sigma,K]=0$ when $\sigma=0$, where $[\sigma,K]\doteq\sigma'[K]-K'[\sigma]$ and the prime denotes Fréchet differentiation, i.e.,

$$\sigma'(u)=\frac{\partial\sigma}{\partial u}+\frac{\partial\sigma}{\partial u_x}\,\partial_x+\frac{\partial\sigma}{\partial u_{xx}}\,\partial_x^2+\cdots\ .$$

GCS's are generalizations of conditional symmetries,[5] in the same way that generalized symmetries[6] are generalizations of symmetries. It turns out that GCS's have the following important properties:

(a) The equations $\sigma=0$ and $u_t=K$ are compatible, thus in general they share a common manifold of solutions. Many physical important solutions, such as multishock and multisoliton solutions, can be characterized precisely as such manifolds. (b) If σ is a GCS of $u_t=K(u)$, then σ is also a GCS of $u_t=K(u)+G(u,\sigma)$, where G is an *arbitrary* function of u, u_x, u_{xx},... and of σ, σ_x, σ_{xx},..., which only satisfies the condition $G(u,0)=0$.

The method used in Ref. 1 is based on the following steps: (a) Find the GCS σ which characterizes the multishock or the multisoliton solutions of a given integrable equation $u_t=K(u)$. (b) Construct the family of equations $u_t=K(u)+G(u,\sigma)$. Since this family also admits σ as a GCS, it shares the same multishock or multisoliton solution with the original equation. For example, the two-shock solution of the Burgers equation is uniquely characterized as the common solution of Eq. (1.2) and of $\sigma=0$, where

$$\sigma=u_{xx}+3uu_x+u^3+\alpha(u_x+u^2)+\beta u. \tag{1.5}$$

Taking $G=-2\sigma/3$ with $\alpha=0$, $\beta=-1/2$, the equation $u_t=K+G$ becomes Eq. (1.1), which therefore also possesses the same two-shock solution. Similarly, the two-soliton solution of the potential KdV equation is associated with

$$\sigma=2uu_{xx}-u_x^2+4u^2u_x+u^4-\alpha u^2+\beta. \tag{1.6}$$

Taking $G=-\sigma_x/(2u)+(1+c)\sigma$, it follows that Eq. (1.3) also possesses the same two-soliton solution.

In this article we further extend the above results:

(a) In Ref. 1 we found the GCS characterizing the N-shock solution of Burgers, and the GCS's for one-, two- and three-soliton solutions of KdV. In Sec. II we show that the GCS characterizing the N-soliton solution of the KdV hierarchy

$$u_t=\sum_{m=0}^{M}\alpha_m(\partial_x^2+4u+2u_x\partial_x^{-1})^m u_x,\quad M\in\mathbb{Z},\quad \alpha_m \text{ const} \tag{1.7}$$

is given by

$$\sigma=\sum_{n=0}^{N}c_n(\partial_x+u\partial_x^{-1})^n u. \tag{1.8}$$

(b) In Sec. III we construct two new GCS's for the hierarchy of equations

$$u_t=\partial_x\left[\sum_{m=0}^{M}\alpha_m(\partial_x+u)^{2m}u\right],\quad M\in\mathbb{Z},\quad \alpha_m \text{ const.} \tag{1.9}$$

We call this hierarchy the "even" Burgers hierarchy, since Eq. (1.9) with $(\partial_x+u)^{2m}$ replaced by $(\partial_x+u)^m$ is the usual Burgers hierarchy.

These GCS's are given by

$$\sigma_1=\sum_{n=0}^{N-1}(-1)^n s_n \sum_{i=1}^{2N-2n-1}(-1)^{i-1}[(\partial_x+u)^{i-1}u][(\partial_x+u)^{2N-2n-i-1}u]+(-1)^N s_N \tag{1.10}$$

and

$$\sigma_2=\sum_{n=0}^{N-1}(-1)^n s_n \sum_{i=0}^{2N-2n}(-1)^{i}[(\partial_x+u)^{i-1}u][(\partial_x+u)^{2N-2n-i-1}u]+(-1)^N s_N, \tag{1.11}$$

where s_n are elementary symmetric polynomials for the set of numbers $(k_1^2,k_2^2,\ldots,k_N^2)$. For example, σ_1 with $N=2$ is

$$\sigma_1^{(2)}=2uu_{xx}-u_x^2+4u^2u_x+u^4-(k_1^2+k_2^2)u^2+k_1^2k_2^2,$$

and σ_2 with $N=2$ is

$$\sigma_2^{(2)}=2u_{xxx}+6uu_{xx}+7u_x^2+8u^2u_x+u^4-(k_1^2+k_2^2)(2u_x+u^2)+k_1^2k_2^2.$$

The equation $\sigma_1=0$ together with Eq. (1.9) specifies the solution

$$u=\partial_x\log\left[\sum_{i=1}^{N}(K_{2i-1}e^{n_i}+K_{2i}e^{-n_i})\right],\quad n_i\doteq k_i\left[x+\left(\sum_{m=0}^{M}\alpha_n k_i^{2m}\right)t\right], \tag{1.12}$$

where the constants k_i and K_i satisfy the constraint

$$\sum_{i=1}^{N}k_i^2\left[\prod_{j\neq i}(k_i^2-k_j^2)\right]K_{2i-1}K_{2i}=0. \tag{1.13}$$

Similarly the equation $\sigma_2=0$ together with Eq. (1.9) characterizes the solution

$$u=\partial_x\log\left[\sum_{i=1}^{N}(K_{2i-1}e^{n_i}+K_{2i}e^{-n_i})+K_{2N+1}\right],\quad n_i\doteq k_i\left[x+\left(\sum_{m=0}^{M}\alpha_n k_i^{2m}\right)t\right], \tag{1.14}$$

where the constants k_i and K_i satisfy the constraint

$$K_{2N+1}^2=4\left(\prod_{i=1}^{N}k_i^{-2}\right)\left\{\sum_{i=1}^{N}k_i^2\left[\prod_{j\neq i}(k_i^2-k_j^2)\right]K_{2i-1}K_{2i}\right\}. \tag{1.15}$$

The equations $u_t=K(u)+G(u,\sigma_1)$ and $u_t=K(u)+G(u,\sigma_2)$, where $K(u)$ is the right-hand side of Eq. (1.9) also possess these solutions. For example, the second order evolution equation

$$u_t=uu_{xx}-u_x^2+u^2u_x, \tag{1.16}$$

which corresponds to $K=u_{xxx}+3uu_{xx}+3u_x^2+3u^2u_x+(k_1^2+k_2^2)u_x$, $\sigma_1=\sigma_1^{(2)}$, $G=-\sigma_{1x}/(2u)$, admits the solution

$$\begin{gathered}u=\partial_x\log(K_1e^{n_1}+K_2e^{-n_1}+K_3e^{n_2}+K_4e^{-n_2}),\\ n_1\doteq k_1[x+(k_1^2+2k_2^2)t],\quad n_2\doteq k_2[x+(2k_1^2+k_2^2)t],\end{gathered} \tag{1.17}$$

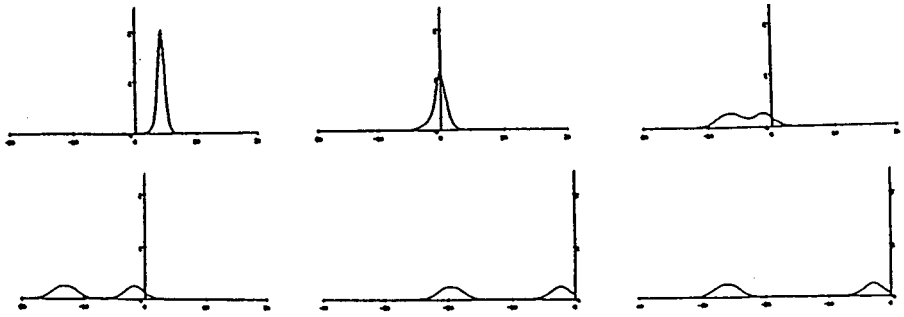

FIG. 1. Breaking of solitary waves.

where the constants k_i and K_i satisfy the constraint

$$k_1^2 K_1 K_2 = k_2^2 K_3 K_4. \tag{1.18}$$

This solution describes the interaction of two solitary waves with arbitrary wave speeds. Similarly the first order evolution equation

$$u_t = u_x^2 + 2u^2 u_x + u^4 - \alpha u^2 + \beta, \quad \alpha, \beta \text{ const}, \tag{1.19}$$

which corresponds to $K = -2u_{xxx} - 6uu_{xx} - 6u_x^2 - 6u^2 u_x + 2\alpha u_x$, $\sigma_2 = \sigma_2^{(2)}$ with $k_1 = [(\alpha + \sqrt{\alpha^2 - 4\beta})/2]^{1/2}$, $k_2 = [(\alpha - \sqrt{\alpha^2 - 4\beta})/2]^{1/2}$, $G = \sigma_2$, admits the solution

$$\begin{gathered} u = \partial_x \log(K_1 e^{n_1} + K_2 e^{-n_1} + K_3 e^{n_2} + K_4 e^{-n_2} + K_5), \\ n_1 \doteq k_1(x + 2k_2^2 t), \quad n_2 \doteq k_2(x + 2k_1^2 t), \quad K_5^2 \doteq 4\left(\frac{1}{k_1^2} - \frac{1}{k_2^2}\right)(k_1^2 K_1 K_2 - k_2^2 K_3 K_4), \end{gathered} \tag{1.20}$$

where K_1, K_2, K_3, and K_4 are arbitrary constants. If all the K_i's are different from zero this solution describes the interaction of two solitary waves with fixed wave speeds; however, if say $K_1 = 0$ this solution describes the interaction between one and two solitary waves, see Fig. 1. This figure corresponds to the real value of k_1 and k_2. For the imaginary value we obtain breather-type solutions. One such solution is plotted in Fig. 2.

It is remarkable that the potential KdV (1.4) can be obtained from Eq. (1.9) with $M = 1$, $\alpha_0 = 3(k_1^2 + k_2^2)$, $\alpha_1 = -2$, i.e., from

$$u_t = -2u_{xxx} - 6uu_{xx} - 6u_x^2 - 6u^2 u_x + 3(k_1^2 + k_2^2)u_x, \tag{1.21}$$

using $\sigma = \sigma_1^{(2)}$. This means that the two-soliton solution of the potential KdV can be traced back to the three-shock solution of Eq. (1.21).

(c) It is natural to ask if the equations considered in (b) have any other special property in addition to possessing certain exact solutions. We have found that these equations are in general equivalent to multilinear (i.e., bilinear, trilinear, etc.) equations. In Secs. IV and V we investigate a particular class of such equations, namely the bilinear ones. We note that these equations *cannot* in general be written in a concise form using Hirota's bilinear operators D_x and D_t. We consider the equation

$$u_t = \sum_{i,j \geq 0} \alpha_{ij}[(\partial_x + u)^{i-1} u][(\partial_x + u)^{j-1} u], \tag{1.22}$$

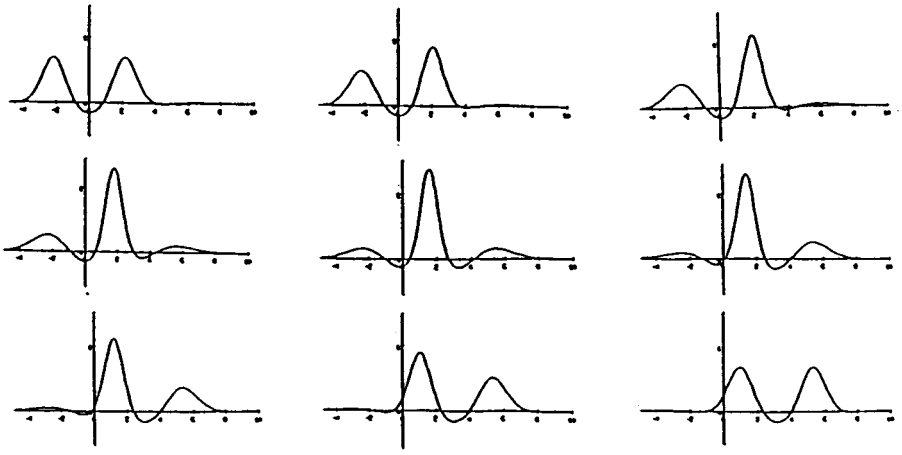

FIG. 2. Breather-type solitary waves.

where we define $(\partial_x+u)^{-1}u=1$. This equation, under the Cole–Hopf transformation $u=f_x/f$, becomes the bilinear equation

$$ff_{xt}-f_xf_t=\sum_{i,j\geqslant 0}\alpha_{ij}(\partial_x^i f)(\partial_x^j f). \tag{1.23}$$

In Sec. IV we find certain exact solutions of Eq. (1.22). These solutions are associated with bilinear GCS's. We find it more convenient to find these solutions directly without using the associated GCS's. These solutions are similar to Eqs. (1.11) and (1.12) and (1.13) and (1.14). For example, we find that Eq. (1.3), in addition to possess the two-soliton solution, also admits the solitary wave solution

$$u=\partial_x\ \log[K_1e^{k_1[x+(k_1^2+(3+2\gamma)k_2^2)t]}+K_2e^{-k_1[x+(k_1^2+(3+2\gamma)k_2^2)t]}+K_3], \tag{1.24}$$

where K_1 and K_2 are arbitrary constants and

$$K_3^2=4\left(1-\frac{1-\gamma}{1+\gamma}\frac{k_1^2}{k_2^2}\right)K_1K_2. \tag{1.25}$$

In Sec. V we find exact solutions of Eq. (1.22) which are associated with multilinear GCS's. For example, we find that the third order evolution equation

$$u_t=a_1u_{xxx}+4a_3uu_{xx}+3(2a_1-a_3)u_x^2+6a_3u^2u_x+a_3u^4+bu^2+c, \tag{1.26}$$

admits two types of exact solutions:

$$u=\partial_x\ \log[K_1e^{k_1x+l_1t}+K_2e^{-(k_1x+l_1t)}+K_3e^{k_2x+l_2t}+K_4e^{-(k_2x+l_2t)}], \tag{1.27}$$

where K_1, K_2, and K_3 are arbitrary constants,

$$k_1=\sqrt{\frac{-b+\sqrt{b^2-4a_3c}}{2a_3}},\quad k_2=\sqrt{\frac{-b-\sqrt{b^2-4a_3c}}{2a_3}},$$
$$l_1=k_1[a_1k_1^2+(3a_1-2a_3)k_2^2],\quad l_2=k_2[(3a_1-2a_3)k_1^2+a_1k_2^2],\quad k_1^2K_1K_2=k_2^2K_2K_3, \tag{1.28}$$

and

$$u=\partial_x \log[K_1e^{k_1x+l_1t}+K_2e^{-(k_1x+l_1t)}+K_3e^{k_2x+l_2t}+K_4e^{-(k_2x+l_2t)}+K_5e^{k_3x+l_3t}+K_6e^{-(k_3x+l_3t)}], \tag{1.29}$$

where K_1, K_2, and K_5 are arbitrary constants,

$$k_1=\sqrt{\frac{-b+\sqrt{b^2-4a_3c}}{2a_3}},\quad k_2=\sqrt{\frac{-b-\sqrt{b^2-4a_3c}}{2a_3}},\quad k_3=-\tfrac{1}{2}(k_1+k_2),$$

$$l_1=a_1(k_1^3+3k_1^2k_3+3k_1k_3^2-3k_3^3)-2a_3k_1^2k_2,$$

$$l_2=a_1(k_2^3+3k_2^2k_3+3k_2k_3^2-3k_3^3)-2a_3k_1k_2^2,\quad l_3=k_3(4a_1k_3^2-2a_3k_1k_2), \tag{1.30}$$

$$K_3=\frac{(k_1-k_3)[3a_1(k_1-k_3)-4a_3k_1]^2[3a_1(k_1-k_2)^2+16a_3k_1k_2]}{a_3(k_1-k_3)^3[3a_1(k_2-k_3)-4a_3k_2]^2}\frac{K_1K_2^2}{K_5^2},$$

$$K_4=\frac{a_3(k_1-k_3)(k_2-k_3)}{3a_1(k_1-k_2)^2+16a_3k_1k_2}\frac{K_5^2}{K_2},$$

$$K_6=\frac{[3a_1(k_1-k_3)-4a_3k_1][3a_1(k_1-k_2)^2+16a_3k_1k_2]}{a_3(k_2-k_3)^2[3a_1(k_2-k_3)-4a_3k_2]}\frac{K_1K_2}{K_5}.$$

Both of these solutions describe the interaction of two solitary waves.

We also find that the generalized CDGSK-KdV equation

$$\begin{aligned}u_t=&a_1(u_{xxxxx}+30u_xu_{xxx}+60u_x^3)+a_2(uu_{xxxx}-3u_xu_{xxx}+2u^2u_{xxx}+2u_{xx}^2+10uu_xu_{xx}\\&+2u^3u_{xx}-9u_x^3+6u^2u_x^2+u^4u_x)+b_1(u_{xxx}+6u_x^2)+b_2(uu_{xx}-u_x^2+u^2u_x)\end{aligned} \tag{1.31}$$

admits the exact solution

$$\begin{aligned}u=\partial_x \log[&K_1e^{k_1x+l_1t}+K_2e^{-(k_1x+l_1t)}+K_3e^{k_2x+l_2t}+K_4e^{-(k_2x+l_2t)}\\&+K_5e^{k_3x+l_3t}+K_6e^{-(k_3x+l_3t)}+K_7e^{k_4x+l_4t}+K_8e^{-(k_4x+l_4t)}],\end{aligned} \tag{1.32}$$

where k_1, k_2, K_1, K_3, K_5, and K_7 are arbitrary constants,

$$\begin{gathered}k_1+k_2+k_3+k_4=0,\quad k_1^2+k_2^2+k_3^2+k_4^2=-\frac{2b_2}{a_2},\quad l_i=\sum_{j\neq i}\frac{P(k_i,-k_j)}{k_i+k_j},\\K_2=\frac{A_{23}A_{24}A_{34}}{AK_1},\quad K_4=\frac{A_{13}A_{14}A_{34}}{AK_3},\quad K_6=\frac{A_{12}A_{14}A_{24}}{AK_5},\quad K_8=\frac{A_{12}A_{13}A_{23}}{AK_7}\end{gathered} \tag{1.33}$$

and

$$\begin{gathered}P(x,y)=\tfrac{1}{2}(x-y)^2[a_1(x-y)^4+a_2xy(x^2-xy+y^2)+b_1(x-y)^2+b_2xy],\\A_{ij}=(k_i-k_j)(l_i-l_j)-2P(k_i,k_j),\quad A=\pm\left(-\frac{A_{12}A_{13}A_{14}A_{23}A_{24}A_{34}}{K_1K_3K_5K_7}\right)^{1/2}.\end{gathered} \tag{1.34}$$

This solution describes the exact interaction of three solitary waves. We note that Eq. (1.31) can be written in a concise bilinear form. Indeed, using $u=f_x/f$, Eq. (1.31) becomes

$$D_xD_tf\cdot f=a_1D_x^6f\cdot f+a_2(D_x^4f_x\cdot f_x+D_x^2f_{xx}\cdot f_{xx})+b_1D_x^4f\cdot f+b_2D_x^2f_x\cdot f_x. \tag{1.35}$$

We hope that the rich phenomenology of the interaction of solitary waves described in this article will motivate the search for appropriate physical circumstances that such nonlinear interactions occur.

II. GENERALIZED CONDITIONAL SYMMETRIES OF THE KdV HIERARCHY

It was found in Ref. 1, using the Bäcklund transformation, that the GCS characterizing the three-soliton solution of the KdV hierarchy is given by

$$\begin{gathered}\sigma=(p_{xx}+ab+bc+ca)^2-4(p_x+2abc)v^2,\\ p\doteq v_x+v^2,\quad a\doteq p-k_1^2-k_2^2+k_3^2,\quad b\doteq p-k_2^2-k_3^2+k_1^2,\quad c\doteq p-k_3^2-k_1^2+k_2^2.\end{gathered} \tag{2.1}$$

The three-soliton solution of the potential KdV hierarchy is

$$\begin{gathered}v=\partial_x\log[e^{-(\eta_1+\eta_2+\eta_3)}+A_{12}A_{13}A_{23}e^{\eta_1+\eta_2+\eta_3}+A_{12}e^{\eta_1+\eta_2-\eta_3}+e^{-(\eta_1+\eta_2-\eta_3)}+A_{13}e^{\eta_1-\eta_2+\eta_3}\\ +e^{-(\eta_1-\eta_2+\eta_3)}+A_{23}e^{-\eta_1+\eta_2+\eta_3}+e^{-(-\eta_1+\eta_2+\eta_3)}],\\ \eta_i=k_i\left[x+\left(\sum_{m=0}^{M}\alpha_m(2k_i)^{2m}\right)t\right]+\eta_i^0,\quad A_{ij}=\left(\frac{k_i-k_j}{k_i+k_j}\right)^2\quad(i,j=1,2,3).\end{gathered} \tag{2.2}$$

Letting $u=2v_x$ it follows that u satisfies the KdV hierarchy (1.7). We note that under differentiation, the equation $\sigma=0$ implies

$$[p_{xxx}+2(a+b+c)p_x]v-(p_{xx}+ab+bc+ca)v_x=4p_xv^3, \tag{2.3}$$

i.e.,

$$\begin{gathered}vv_{xxxx}-v_xv_{xxx}+2v^2v_{xxx}+10vv_xv_{xx}+2v^3v_{xx}-5v_x^3+6v^2v_x^2\\ +v^4v_x-2A(vv_{xx}-v_x^2+v^2v_x)+Bv_x=0,\\ A\doteq k_1^2+k_2^2+k_3^2,\quad B\doteq k_1^4+k_2^4+k_3^4-2k_1^2k_2^2-2k_1^2k_3^2-2k_2^2k_3^2.\end{gathered} \tag{2.4}$$

We can now use Eq. (2.4) to construct nonintegrable equations which possess the three-soliton solution (2.2). For example, the fifth order evolution equation

$$\begin{gathered}v_t=v_{xxxxx}+(20-C)v_xv_{xxx}+10v_{xx}^2+5(8-C)v_x^3+C[vv_{xxxx}+2v^2v_{xxx}+10vv_xv_{xx}+2v^3v_{xx}\\ +6v^2v_x^2+v^4v_x-2A(vv_{xx}-v_x^2+v^2v_x)+Bv_x],\quad A,B,C\text{ const}\end{gathered}$$

admits Eq. (2.2) with arbitrary k_1 and

$$k_2=[\tfrac{1}{2}(A-k_1^2+\sqrt{B-2k_1^2A-3k_1^4})]^{1/2},\quad k_3=[\tfrac{1}{2}(A-k_1^2-\sqrt{B-2k_1^2A-3k_1^4})]^{1/2},$$

$$\eta_i=k_i(x+16k_i^4t)+\eta_i^0.$$

Although in principle we can use the Bäcklund transformation to derive the GCS characterizing the N-soliton solution this procedure is quite complicated. In this article we derive these GCS's in the form of Eq. (1.8), using Bargmann's method:[7] We consider the Schrödinger spectral equation

$$\phi_{xx}+(u+k^2)\phi=0. \tag{2.5}$$

Letting $\phi=e^{ikx}F$, $\mu=2ik$, we find $F_{xx}+\mu F_x+uF=0$. Assuming that $F=\mu^N+\Sigma_{n=1}^{N}a_n\mu^{N-n}$, it follows that

$$a_{1x}+u=0, \quad a_{n-1,x}+a_{nxx}+a_nu=0 \quad (n=1,2,\ldots,N-1), \quad a_{Nxx}+a_Nu=0.$$

Thus

$$a_n=(-1)^n(\partial_x+\partial_x^{-1}u)^{n-1}\partial_x^{-1}u \quad (n=1,2,\ldots,N-1) \quad (\partial_x+u\partial_x^{-1})^Nu=0.$$

For example, for $N=2$, we find

$$u=-a_x, \quad b=-a_x+\tfrac{1}{2}a^2+c_1$$

and

$$aa_{xx}-\tfrac{1}{2}a_x^2-a^2a_x+\tfrac{1}{8}a^4+\tfrac{1}{2}c_1a^2+c_2=0.$$

The left-hand side of this equation is the GCS (1.6) ($a\to-2u$) which characterizes the two-soliton. For $N=3$, we find

$$u=-a_x, \quad b=-a_x+\tfrac{1}{2}a^2+c_1, \quad c=a_{xx}-aa_x-\partial_x^{-1}a_x^2+\tfrac{1}{6}a^3+c_1a+c_2$$

and

$$a_{xxx}-aa_{xx}-\tfrac{5}{2}a_x^2+\tfrac{1}{2}a^2a_x+a\partial_x^{-1}a_x^2-\tfrac{1}{24}a^4+c_1(a_x-\tfrac{1}{2}a^2)-c_2a+c_3=0,$$

which implies Eq. (2.5) ($a\to-2v$).

It is a general conjecture that equations admitting three-soliton solutions with arbitrary wave numbers are integrable.[8] However, using our approach, it follows that this cannot be true. For example, the three-soliton (2.2) satisfies the ODE:

$$\left\{\prod_{i,j,m=\pm1}[\partial_x+(-1)^ik_1+(-1)^jk_2+(-1)^mk_3]\right\}f=0,$$

i.e.,

$$\partial_x^8f+a_1\partial_x^7f+\cdots+a_8f=0$$

for certain constants a_i. Since

$$\partial_x^nf=p_n(v)f, \quad p_0\doteq1, \quad p_1\doteq v, \quad p_{n+1}\doteq p_{nx}+vp_n,$$

we find

$$p_8+a_1p_7+\cdots+a_8p_0=0,$$

which implies that the functions $p_0(v)$, $p_1(v),\ldots,p_8(v)$ are functional dependent, thus their Wronskian determinant

$$\sigma = W(p_0(v), p_1(v), \ldots, p_8(v)) = 0.$$

Therefore, all the equations in the form of $v_t = v_{xxx} + 6v_x^2 + G(v, \sigma)$, where G satisfies $G(v,0) = 0$, admit the three-soliton solution (2.2) with arbitrary wave numbers k_i. Since $G(v, \sigma)$ is essentially arbitrary, it is doubtful that all these equations are integrable.

III. GENERALIZED CONDITIONAL SYMMETRIES AS REDUCTIONS OF LINEAR ONES

It was shown in Ref. 1 that the Burgers hierarchy

$$u_t = \partial_x \left[\sum_{i=0}^{M} \alpha_m (\partial_x + u)^m u \right] \tag{3.1}$$

admits the GCS:

$$\sigma = \sum_{n=0}^{N+1} c_n (\partial_x + u)^{n-1} u. \tag{3.2}$$

Associated with this σ is the N-shock solution

$$u = \partial_x \log \left(\sum_{i=1}^{N+1} K_i e^{k_i x + l_i t} \right), \quad l_i = \sum_{m=0}^{M} \alpha_m k_i^{m+1}, \tag{3.3}$$

where $k_1, \ldots, k_{N+1}$ are the $N+1$ roots of the equation $\Sigma_{n=0}^{N+1} c_n k^n = 0$. This fact becomes more clear under the Cole–Hopf transformation

$$u = (\log f)_x. \tag{3.4}$$

Under this transformation, Eq. (3.1) becomes a linear evolution equation:

$$f_t = \sum_{m=0}^{M} \alpha_m \partial_x^{m+1} f; \tag{3.5}$$

σ becomes linear in f:

$$\sigma = \sum_{n=0}^{N+1} c_n \partial_x^n f; \tag{3.6}$$

and $\sigma = 0$ implies that

$$f = \sum_{i=1}^{N+1} K_i e^{k_i x + l_i t}. \tag{3.7}$$

Therefore the GCS's associated with the multishock solution can be explicitly linearized.

Now we derive some other type of GCS's. These new GCS's cannot be linearized. However, they satisfy bilinear equations and furthermore can be obtained from the previous GCS's through the process of reductions. We say that a GCS σ_1 is a reduction of another GCS σ_2 iff $\sigma_2 = G(u, \sigma_1)$ for some function G satisfying $G(u,0) = 0$. This means that $\sigma_1 = 0$ implies $\sigma_2 = 0$. As a simple example, we consider the ODE:

$$f_{xxxx} - \alpha f_{xx} + \beta f = 0, \tag{3.8}$$

whose general solution is

$$f=K_1e^{k_1x}+K_2e^{-k_1x}+K_3e^{k_2x}+K_4e^{-k_2x}, \tag{3.9}$$

where k_1 and k_2 are given by

$$\alpha=k_1^2+k_2^2, \quad \beta=k_1^2k_2^2, \tag{3.10}$$

and K_i $(i=1,2,3,4)$ are arbitrary and independent to x. A simple reduction can be obtained by multiplying Eq. (3.8) by f_x and then integrating it. This yields

$$2f_xf_{xxx}-f_{xx}^2-\alpha f_x^2+\beta f^2=0. \tag{3.11}$$

Substituting Eq. (3.9) into Eq. (3.11), we find the constraint condition

$$k_1^2K_1K_2=k_2^2K_3K_4.$$

Equations (3.9) and (3.11) are compatible with the linear evolution equation

$$f_t=\sum_{m=0}^{M}\alpha_m\partial_x^{2m+1}f. \tag{3.12}$$

Thus the even Burgers hierarchy (1.9) admits the GCS:

$$\sigma=2uu_{xx}-u_x^2+4u^2u_x+u^4-\alpha u^2+\beta. \tag{3.13}$$

We call this GCS σ bilinear since the equation $\sigma=0$ is equivalent to the bilinear equation (3.11).

The solution associated to this GCS is the two-soliton

$$u=\partial_x\log[K_1e^{k_1x+l_1t}+K_2e^{-(k_1x+l_1t)}+K_3e^{k_2x+l_2t}+K_4e^{-(k_2x+l_2t)}], \tag{3.14a}$$

$$l_i=\sum_{m=0}^{M}\alpha_mk_i^{m+1} \quad (i=1,2), \quad k_1^2K_1K_2=k_2^2K_3K_4. \tag{3.14b}$$

As a second example of a reduction, we consider the ODE:

$$f_{xxxxx}-\alpha f_{xxx}+\beta f_x=0, \tag{3.15}$$

whose general solution is

$$f=K_1e^{k_1x}+K_2e^{-k_1x}+K_3e^{k_2x}+K_4e^{-k_2x}+K_5, \tag{3.16}$$

where k_1 and k_2 are given by Eqs. (3.10) and K_i $(i=1,2,3,4,5)$ are arbitrary and independent to x. Multiplying this equation by f and integrating it, we find

$$2ff_{xxxx}-2f_xf_{xxx}+f_{xx}^2-\alpha(2ff_{xx}-f_x^2)+\beta f^2=0. \tag{3.17}$$

The constraint condition is

$$K_5^2=4\left(\frac{1}{k_1^2}-\frac{1}{k_2^2}\right)(k_1^2K_1K_2-k_2^2K_3K_4).$$

Thus the even Burgers hierarchy admits the bilinear GCS:

$$\sigma=2u_{xxx}+6uu_{xx}+7u_x^2+8u^2u_x+u^4-2\alpha u_x-\alpha u^2+\beta. \tag{3.18}$$

The solution associated to this GCS is

$$u=\partial_x \log[K_1e^{k_1x+l_1t}+K_2e^{-(k_1x+l_1t)}+K_3e^{k_2x+l_2t}+K_4e^{-(k_2x+l_2t)}+K_5], \tag{3.19a}$$

$$l_i=\sum_{m=0}^{M}\alpha_m k_i^{m+1} \quad (i=1,2), \quad K_5^2=4\left(\frac{1}{k_1^2}-\frac{1}{k_2^2}\right)(k_1^2K_1K_2-k_2^2K_3K_4). \tag{3.19b}$$

The following theorem generalizes these results.

Theorem 3.1: (a) The evolution equation

$$u_t=\partial_x\left[\sum \alpha_m(\partial_x+u)^{2m}u\right]+G\Bigg(u,\sum_{n=0}^{N-1}(-1)^n s_n \sum_{i=1}^{2N-2n-1}(-1)^{i-1}[(\partial_x+u)^{i-1}u] \times[(\partial_x+u)^{2N-2n-i-1}u]+(-1)^N s_N\Bigg) \tag{3.20}$$

admits the exact solution

$$u=(\log f)_x, \quad f=\sum_{i=1}^{N}(K_{2i-1}e^{n_i}+K_{2i}e^{-n_i}),$$
$$n_i=k_i\left[x+\left(\sum \alpha_m k_i^{2m}\right)t\right], \quad \sum_{i=1}^{N}k_i^2\left[\prod_{j\neq i}(k_i^2-k_j^2)\right]K_{2i-1}K_{2i}=0. \tag{3.21}$$

(b) The evolution equation

$$u_t=\partial_x\left[\sum \alpha_m(\partial_x+u)^{2m}u\right]+G\Bigg(u,\sum_{n=0}^{N-1}(-1)^n s_n \sum_{i=0}^{2N-2n}(-1)^{i}[(\partial_x+u)^{i-1}u] \times[(\partial_x+u)^{2N-2n-i-1}u]+(-1)^N s_N \tag{3.22}$$

admits the exact solution

$$u=(\log f)_x, \quad f=\sum_{i=1}^{N}(K_{2i-1}e^{n_i}+K_{2i}e^{-n_i})+K_{2N+1},$$
$$n_i=k_i\left[x+\left(\sum \alpha_m k_i^{2m}\right)t\right], \quad K_{2N+1}^2=4\left(\prod_{i=1}^{N}k_i^{-2}\right)\left\{\sum_{i=1}^{N}k_i^2\left[\prod_{j\neq i}(k_i^2-k_j^2)\right]K_{2i-1}K_{2i}\right\}, \tag{3.23}$$

where $G(u,\sigma)$ is a function of u and σ and their derivatives satisfying $G(u,0)=0$, and s_n are elementary symmetric polynomials for the set of numbers $(k_1^2,k_2^2,\ldots,k_N^2)$,

$$s_0=1, \quad s_1=\sum_{i=1}^{N} k_i^2, \quad s_2=\sum_{i<j} k_i^2 k_j^2, \ \ldots, \quad s_N=\prod_{i=1}^{N} k_i^2. \tag{3.24}$$

Proof: We only prove part (a); part (b) can be proved similarly. We need to prove

$$\sum_{n=0}^{N-1} (-1)^n s_n \sum_{i=1}^{2N-2n-1} (-1)^{i-1} (\partial_x^i f)(\partial_x^{2N-2n-i} f) + (-1)^N s_N f^2 = 0. \tag{3.25}$$

Substituting Eq. (3.21b) into this equation, we find that the sum of the coefficients of e^{-2n_p} is

$$K_{2p-1}^2 \left[\sum_{n=0}^{N-1} (-1)^n s_n \sum_{i=1}^{2N-2n-1} (-1)^{i-1} k_p^{2N-2n} + (-1)^N s_N \right] = K_{2p-1}^2 \left[\sum_{n=0}^{N} (-1)^n s_n k_p^{2N-2n} \right] = 0$$

and the sum of the coefficients of $e^{-n_p-n_q}$ is

$$\begin{aligned} &2K_{2p-1}K_{2q-1}\left[\sum_{n=0}^{N-1} (-1)^n s_n \sum_{i=1}^{2N-2n-1} (-1)^{i-1} k_p^i k_q^{2N-2n-i} + (-1)^N s_N \right] \\ &= 2K_{2p-1}K_{2q-1}\left[\frac{k_q}{k_p-k_q} \sum_{n=0}^{N} (-1)^N s_n k_p^{2N-2n} + \frac{k_p}{k_q-k_p} \sum_{n=0}^{N} (-1)^N s_n k_q^{2N-2n} \right] = 0. \end{aligned}$$

Similarly, we find that the sums of the coefficients of e^{2n_p}, $e^{\pm n_p \pm n_q}$ are all zeros. The only terms left come from the multiplication of e^{n_p} and e^{-n_p} for $p=1,2,\ldots,N$, which are

$$\begin{aligned} &2K_{2p-1}K_{2p}\left[\sum_{n=0}^{N-1} (-i)^n s_n \sum_{i=1}^{2N-2n-1} (-1)^{i-1} k_p^i (-k_p)^{2N-2n-i} + (-1)^N s_N \right] \\ &= 2K_{2p-1}K_{2p}\left[-\sum_{n=0}^{N-1} (-1)^n s_n (2N-2n-1) k_p^{2N-2n} + (-1)^N s_N \right] \\ &= -4K_{2p-1}K_{2p}k_p^2\left[\sum_{n=0}^{N-1} (-1)^n s_n (N-n) k_i^{2N-2n-2} \right] \\ &= -4K_{2p-1}K_{2p}k_p^2\left[\sum_{n=0}^{N-1} (-1)^n s_n^{(p)} k_p^{2N-2n-2} \right] = -4K_{2p-1}K_{2p}k_p^2 \prod_{q\neq p} (k_p^2-k_q^2), \end{aligned}$$

where we denote by $s_n^{(p)}$ the elementary symmetric polynomials for $(k_1^2,\ldots,k_{p-1}^2,k_{p+1}^2,\ldots,k_N^2)$, and have used the relation $s_n=s_n^{(p)}+k_p^2 s_{n-1}^{(p)}$. Thus Eq. (3.21d) implies Eq. (3.25).

Remark: More general reductions can be obtained by integrating $(\Sigma \alpha_n \partial_x^{2n+1} f)(\Sigma \beta_n \partial_x^{2n} f)=0$.

Example 3.1: The third order equation

$$u_t = a_1 u_{xxx} + a_2 u u_{xx} + (6a_1 - a_2 + a_3) u_x^2 + (a_2 + 2a_3) u^2 u_x + a_3 u^4 + b u^2 + c \tag{3.26}$$

admits the exact solutions (3.14a) and (3.14c) with

$$k_1 = \sqrt{\frac{-b+\sqrt{b^2-4a_3c}}{2a_3}}, \tag{3.27a}$$

$$k_2=\sqrt{\frac{-b-\sqrt{b^2-4a_3c}}{2a_3}}, \tag{3.27b}$$

$$l_1=k_1[a_1k_1^2+(3a_1-a_2+2a_3)k_2^2], \tag{3.27c}$$

$$l_2=k_2[(3a_1-a_2+2a_3)k_1^2+a_1k_2^2]. \tag{3.27d}$$

Proof: The right-hand side of Eq. (3.26) can be written as

$$(-2a_1+a_2-2a_3)(u_{xxx}+3uu_{xx}+3u_x^2+3u^2u_x)+a(3a_1-a_2+2a_3)u_x$$
$$+\left[\frac{1}{2u}(3a_1-a_2+2a_3)\partial_x+a_3\right]\sigma+(b+\alpha a_3)u^2+c-\beta a_3,$$

where σ is given by Eq. (3.13). Letting $\alpha=-b/a_3$ and $\beta=c/a_3$, which imply Eqs. (3.27a) and (3.27b), we find that Eq. (3.26) admits two-soliton solutions [Eqs. (3.13a) and (3.13c)] with

$$l_i=k_i[(-2a_1+a_2-2a_3)k_i^2+\alpha(3a_1-a_2+2a_3)] \quad (i=1,2).$$

Example 3.2: The third order equation

$$u_t=a_1u_{xxx}+a_2uu_{xx}+(6a_1-a_2)u_x^2+a_2u^2u_x \tag{3.28}$$

admits the exact solutions (3.14a) and (3.14c) with arbitrary wave numbers and $l_1=k_1[a_1k_1^2+(3a_1-a_2)k_2^2]$, $l_2=k_2[(3a_1-a_2)k_1^2+a_1k_2^2]$.

Example 3.3: The third order equation

$$u_t=a_1u_{xxx}+3a_1uu_{xx}+(3a_1+a_3)u_x^2+(3a_1+2a_3)u^2u_x+a_3u^4+bu^2+c \tag{3.29}$$

admits the exact solutions (3.19a) and (3.19c) with

$$k_1=\sqrt{\frac{-b+\sqrt{b^2-4a_3c}}{2a_3}}, \quad k_2=\sqrt{\frac{-b-\sqrt{b^2-4a_3c}}{2a_3}},$$

$$l_1=k_1(a_1k_1^2+2a_3k_2^2), \quad l_2=k_2(2a_3k_1^2+a_1k_2^2). \tag{3.30}$$

IV. EXACT SOLUTIONS OF BILINEAR EVOLUTION EQUATIONS ASSOCIATED WITH BILINEAR GENERALIZED CONDITIONAL SYMMETRIES

Although in principle we can construct all the equations which admit exact solutions associated with bilinear GCS's from the Burgers-type equations, the resulting equations are quite complicated. Therefore, we look directly for simple equations admitting exact solutions. In particular we consider the bilinear equation (1.23). In this section, we search for exact solutions for this equation directly. Without loss of generality, we assume that $\alpha_{ij}=\alpha_{ji}$. We define

$$P(x,y)=\sum \alpha_{ij}x^iy^j, \tag{4.1}$$

then Eq. (1.23) can be written as

$$(\partial_x-\partial_{x'})(\partial_t-\partial_{t'})f(x,t)f(x',t')\big|_{x'=x,t'=t}=2P(\partial_x,\partial_{x'})f(x,t)f(x',t')\big|_{x'=x,t'=t}. \tag{4.2}$$

We look for solutions which are sums of exponentials

$$f(x,t)=\sum K_p e^{n_p}, \quad n_p=k_p x+l_p t. \tag{4.3}$$

Substituting in Eq. (1.23), we find that

$$\sum_{p<q}(k_p-k_q)(l_p-l_q)K_pK_q e^{n_p+n_q}=\sum_{p,q} P(k_p,k_q)K_pK_q e^{n_p+n_q},$$

i.e.,

$$\sum_{p<q}[(k_p-k_q)(l_p-l_q)-2P(k_p,k_q)]K_pK_q e^{n_p+n_q}-\sum_p P(k_p,k_p)K_p^2 e^{2n_p}=0. \tag{4.4}$$

Therefore, we have the following results:

Theorem 4.1: The bilinear evolution equation (1.22) with even P, admits the following exact solutions:

(a)

$$u=(\log f)_x, \quad f=\sum_{i=1}^{n}[K_{2i-1}e^{k_i x+l_i t}+K_{2i}e^{-(k_i x+l_i t)}], \tag{4.5}$$

where

$$P(k_i,k_i)=0, \quad l_i=\frac{P(k_i,k_j)}{k_i-k_j}+\frac{P(k_i,-k_j)}{k_i+k_j} \quad (\forall j\neq i), \quad \sum_{i=1}^{n}[2k_i l_i-P(k_i,-k_i)]K_{2i-1}K_{2i}=0, \tag{4.6}$$

provided that

$$\frac{P(k_i,k_j)}{k_i-k_j}+\frac{P(k_i,-k_j)}{k_i+k_j}=\frac{P(k_i,k_m)}{k_i-k_m}+\frac{P(k_i,-k_m)}{k_i+k_m} \quad (\forall i\neq j\neq m); \tag{4.7}$$

(b)

$$u=(\log f)_x, \quad f=\sum_{i=1}^{n}[K_{2i-1}e^{k_i x+l_i t}+K_{2i}e^{-(k_i x+l_i t)}]+K_{2n+1}, \tag{4.8}$$

where

$$P(k_i,k_i)=0, \quad l_i=\frac{2}{k_i}P(k_i,0), \quad P(0,0)K_{2n+1}^2=2\sum_{i=1}^{n}[4P(k_i,0)-P(k_i,-k_i)]K_{2i-1}K_{2i}, \tag{4.9}$$

provided that

$$\frac{2}{k_i}P(k_i,0)=\frac{P(k_i,k_j)}{k_i-k_j}+\frac{P(k_i,-k_j)}{k_i+k_j} \quad (\forall i\neq j). \tag{4.10}$$

Applying this theorem to the third order equation (3.26), we find that this equation admits not only two-soliton solutions (3.27), but also the following traveling wave solution:

$$u=(\log f)_x, \quad f=K_1e^{kx+lt}+K_2e^{-(kx+lt)}+K_3,$$
$$k=\sqrt{\frac{-b\pm\sqrt{b^2-4a_3c}}{2a_3}}, \quad l=k[(a_1-2a_3)k^2-2b], \tag{4.11}$$
$$K_3^2=4\left[1+\frac{1}{c}(-3a_1+a_2-a_3)k^4\right]K_1K_2.$$

Applying this theorem to the bilinear equation (1.23) with $i+j\leqslant 6$, we obtain the following results.

Example 4.1: The equation

$$u_t=a_1(\partial_x+u)^5u+a_2u(\partial_x+u)^4u+a_3[(\partial_x+u)u][(\partial_x+u)^3u]+a_4[(\partial_x+u)^2u]^2$$
$$+b_1(\partial_x+u)^3u+b_2u(\partial_x+u)^2u+b_3[(\partial_x+u)u]^2+cu^2+d \tag{4.12}$$

admits the two-soliton solution (3.14a) where

$$(a_1+a_2+a_3+a_4)k_i^6+(b_1+b_2+b_3)k_i^4+ck_i^2+d=0 \quad (i=1,2),$$
$$l_1=k_1[-(a_2+a_3+a_4)k_1^4-a_4k_1^2k_2^2+(a_3+a_4)k_2^4-(b_2+b_3)k_1^2+b_3k_2^2-c],$$
$$l_2=k_2[-(a_2+a_3+a_4)k_2^4-a_4k_1^2k_2^2+(a_3+a_4)k_1^4-(b_2+b_3)k_2^2+b_3k_1^2-c], \tag{4.13}$$
$$k_1^2[a_3k_1^2+(a_3+a_4)k_2^2+b_3]K_1K_2=k_2^2[(a_3+a_4)k_1^2+a_3k_2^2+b_3]K_3K_4,$$

and the traveling wave solution (4.11) where

$$(a_1+a_2+a_3+a_4)k^6+(b_1+b_2+b_3)k^4+ck^2+d=0,$$
$$l=-k[(a_1+2a_2+2a_3+2a_4)k^4+(b_1+2b_2+2b_3)k^2+2c], \tag{4.14}$$
$$K_3^2=-\frac{4k^2}{d}[(a_1+a_2+2a_3+a_4)k^4+(b_1+b_2+2b_3)k^2+c]K_1K_2.$$

Example 4.2: The equation

$$u_t=a_1(\partial_x+u)^5u-(a_1+a_3+a_4)u(\partial_x+u)^4u+a_3[(\partial_x+u)u][(\partial_x+u)^3u]$$
$$+a_4[(\partial_x+u)^2u]^2+b_1(\partial_x+u)^3u-(b_1+b_3)u(\partial_x+u)^2u+b_3[(\partial_x+u)u]^2, \tag{4.15}$$

whose bilinear form is

$$D_xD_tf\cdot f=a_1D_x^6f\cdot f-(5a_1+a_3+a_4)D_x^4f_x\cdot f_x-(5a_1+3a_3+4a_4)$$
$$\times D_x^2f_{xx}\cdot f_{xx}+b_1D_x^4f\cdot f-(3b_1+b_3)D_x^2f_x\cdot f_x+c_1D_x^2f\cdot f, \tag{4.16}$$

admits the two-soliton solution (3.14a) with arbitrary wave numbers and

$$l_1=k_1[a_1k_1^4-a_4k_1^2k_2^2+(a_3+a_4)k_2^4+b_1k_1^2+b_3k_2^2],$$
$$l_2=k_2[a_1k_2^4-a_4k_1^2k_2^2+(a_3+a_4)k_1^4+b_1k_2^2+b_3k_1^2], \tag{4.17}$$
$$k_1^2[a_3k_1^2+(a_3+a_4)k_2^2+b_3]K_1K_2=k_2^2[(a_3+a_4)k_1^2+a_3k_2^2+b_3]K_3K_4.$$

Example 4.3: The equation

$$u_t=a_1(\partial_x+u)^5u+a_2u(\partial_x+u)^4u+a_4\{-2[(\partial_x+u)u][(\partial_x+u)^3u]+[(\partial_x+u)^2u]^2\}$$
$$+b_1(\partial_x+u)^3u+b_2u(\partial_x+u)^2u+b_3[(\partial_x+u)u]^2+cu^2+d \tag{4.18}$$

with

$$a_1+a_2\neq a_4,\quad (a_1+a_2)b_3+(b_1+b_2)a_4=0, \tag{4.19}$$

admits the exact solution

$$u=(\log f)_x, \tag{4.20a}$$
$$f=K_1e^{k_1x+l_1t}+K_2e^{-(k_1x+l_1t)}+K_3e^{k_2x+l_2t}+K_4e^{-(k_2x+l_2t)}+K_5e^{k_3x+l_3t}+K_6e^{-(k_3x+l_3t)}, \tag{4.20b}$$
$$(a_1+a_2-a_4)k_i^6+(b_1+b_2+b_3)k_i^4+ck_i^2+d=0\quad (i=1,2,3), \tag{4.20c}$$
$$l_1=k_1[(-a_2+a_4)k_1^4+a_4k_2^2k_3^2-(b_2+b_3)k_1^2-c], \tag{4.20d}$$
$$l_2=k_2[(-a_2+a_4)k_2^4+a_4k_3^2k_1^2-(b_2+b_3)k_2^2-c], \tag{4.20e}$$
$$l_3=k_3[(-a_2+a_4)k_3^4+a_4k_1^2k_2^2-(b_2+b_3)k_3^2-c], \tag{4.20f}$$
$$\frac{k_1^2}{k_2^2-k_3^2}K_1K_2+\frac{k_2^2}{k_3^2-k_1^2}K_3K_4+\frac{k_3^2}{k_1^2-k_2^2}K_5K_6=0. \tag{4.20g}$$

Example 4.4: The equation

$$u_t=uu_{xxxx}-2u_xu_{xxx}+3u^2u_{xxx}+u_{xx}^2+8uu_xu_{xx}+4u^3u_{xx}$$
$$-6u_x^3+6u^2u_x^2+2u^4u_x+b(uu_{xx}-u_x^2+u^2u_x), \tag{4.21}$$

whose bilinear form is

$$D_xD_tf\cdot f=D_x^4f_x\cdot f_x+2D_x^2f_{xx}\cdot f_{xx}+bD_x^2f_x\cdot f_x, \tag{4.22}$$

admit the exact solutions (4.20b) and (4.20g) with arbitrary k_1 and k_2 and

$$k_1^2+k_2^2+k_3^2=-b,\quad l_1=k_1k_2^2k_3^2,\quad l_2=k_1^2k_2k_3^2,\quad l_3=k_1^2k_2^2k_3.$$

Example 4.5: The equation

$$u_t=a_1\partial_x(\partial_x+u)^4u+a_4\{-2[(\partial_x+u)u][(\partial_x+u)^3u]+[(\partial_x+u)^2u]^2\}$$
$$+b_1\partial_x(\partial_x+u)^2u+b_3[(\partial_x+u)u]^2+cu^2+d\quad (a_4\neq0) \tag{4.23}$$

admits the exact solution

$$
\begin{gathered}
u=(\log f)_x,\\
f=K_1e^{k_1x+l_1t}+K_2e^{-(k_1x+l_1t)}+K_3e^{k_2x+l_2t}+K_4e^{-(k_2x+l_2t)}+K_5e^{k_3x+l_3t}+K_6e^{-(k_3x+l_3t)}+K_7,\\
a_4k_i^6-b_3k_i^4-ck_i^2-d=0 \quad (i=1,2,3),\\
l_1=k_1[(a_1+a_4)k_1^4+a_4k_2^2k_3^2+(b_1-b_3)k_1^2-c],\\
l_2=k_2[(a_1+a_4)k_2^4+a_4k_3^2k_1^2+(b_1-b_3)k_2^2-c],\\
l_3=k_3[(a_1+a_4)k_3^4+a_4k_1^2k_2^2+(b_1-b_3)k_3^2-c],\\
K_7^2=-\frac{4(k_1^2-k_2^2)(k_2^2-k_3^2)(k_3^2-k_1^2)}{k_1^2k_2^2k_3^2}\left(\frac{k_1^2}{k_2^2-k_3^2}K_1K_2+\frac{k_2^2}{k_3^2-k_1^2}K_3K_4+\frac{k_3^2}{k_1^2-k_2^2}K_5K_6\right).
\end{gathered}
\tag{4.24}
$$

Since the exact solutions we derived in this article are in the form of sums of exponentials, they describe in general the interaction of traveling waves. Here we use the solution (1.20) of Eq. (1.19) to show that these solutions may describe breaking traveling waves. We assume that $k_1>k_2>0$. In the moving coordinate $\eta=x+at$, we get

$$
f=K_1e^{k_1\eta+(l_1-k_1a)t}+K_2e^{-k_1\eta+(-l_1+k_1a)t}+K_3e^{k_2\eta+(l_2-k_2a)t}+K_4e^{-k_2\eta+(-l_2+k_2a)t}+K_5.
$$

For $l_1-k_1a=l_2-k_2a$, i.e., $a=-2k_1k_2$, we get

$$
f\sim e^{2k_1k_2(k_1+k_2)t}(K_1e^{k_1\eta}+K_3e^{k_2\eta}),\quad u\sim\partial_x\log(K_1e^{k_1\eta}+K_3e^{k_2\eta}),\quad t\to+\infty,
$$

and

$$
f\sim e^{2k_1k_2(k_1+k_2)t}(K_2e^{-k_1\eta}+K_4e^{-k_2\eta}),\quad u\sim\partial_x\log(K_2e^{-k_1\eta}+K_4e^{-k_2\eta}),\quad t\to-\infty.
$$

For $l_1-k_1a=-l_2+k_2a$, i.e., $a=2k_1k_2$, we get

$$
f\sim e^{2k_1k_2(-k_1+k_2)t}(K_2e^{-k_1\eta}+K_3e^{k_2\eta}),\quad u\sim\partial_x\log(K_2e^{-k_1\eta}+K_3e^{k_2\eta}),\quad t\to+\infty,
$$

and

$$
f\sim e^{2k_1k_2(k_1-k_2)t}(K_1e^{k_1\eta}+K_4e^{-k_2\eta}),\quad u\sim\partial_x\log(K_1e^{k_1\eta}+K_4e^{-k_2\eta}),\quad t\to-\infty.
$$

For $l_1-k_1a=0$, i.e., $a=2k_2^2$, we get

$$
\begin{array}{lll}
f\sim K_3e^{k_2\eta+2k_2(k_1^2-k_2^2)t}, & u\sim k_2 & (K_3\neq0),\\
f\sim K_1e^{k_1\eta}+K_2e^{-k_1\eta}+K_5, & u\sim\partial_x\log(K_1e^{k_1\eta}+K_2e^{-k_1\eta}+K_5) & (K_3=0),
\end{array}
\quad t\to+\infty,
$$

and

$$
\begin{array}{lll}
f\sim K_4e^{-k_2\eta-2k_2(k_1^2-k_2^2)t}, & u\sim -k_2, & (K_4\neq0),\\
f\sim K_1e^{k_1\eta}+K_2e^{-k_1\eta}+K_5, & u\sim\partial_x\log(K_1e^{k_1\eta}+K_2e^{-k_1\eta}+K_5), & (K_4=0),
\end{array}
\quad t\to-\infty.
$$

Therefore, if all K_i $(i=1,2,3,4)$ are nonzero, this solution describes the interaction of two solitary waves and if one of these K_i is zero, then it describes the interaction of one and two solitary waves. The following general result is valid for exact solutions containing six exponentials.

Lemma 4.1: The exact solution (1.29), where $k_1>k_2>k_3>0$, $K_i\neq0$ $(i=1,2,3,4,5,6)$, describes the interaction of three solitary waves if $a_{12}<a_{13}<a_{23}$ with one of the following:

$$b_{12}<b_{13}<b_{23}, \quad b_{23}<b_{12}<b_{13}, \quad b_{13}<b_{23}<b_{12},$$

or if $a_{23}<a_{13}<a_{12}$ with one of the following:

$$b_{12}<b_{23}<b_{13}, \quad b_{13}<b_{12}<b_{23}, \quad b_{23}<b_{13}<b_{12}.$$

The constants a_{ij} and b_{ij} are defined by

$$a_{ij}=\frac{l_i-l_j}{k_i-k_j}, \quad b_{ij}=\frac{l_i+l_j}{k_i+k_j}.$$

If the above conditions are violated, it describes the interaction of two solitary waves. If some of the K_i's equal zero, this solution in general describes breaking of solitary waves. Applying this result to the solutions (1.29) and (1.30), we find that it describes the interaction of two solitary waves.

V. EXACT SOLUTIONS OF BILINEAR EVOLUTION EQUATIONS ASSOCIATED WITH MULTILINEAR GENERALIZED CONDITIONAL SYMMETRIES

There exist exact solutions, for example the three-soliton solution (2.2), which are associated with multilinear as oppose to bilinear GCS's. Since these GCS's are quite complicated, we construct equations admitting this kind of solutions directly. In this section, we consider again Eq. (1.23). But now we are interested in the cases that, for f in the form of the sum of exponentials, the product of two exponentials is identical to the product of some other two exponentials in Eq. (1.23). For f with even terms, we have the following cases:

$$\text{(a)} \ \ n_1+n_2+n_3+n_4=0, \quad \text{(b)} \ \ n_1+n_2+2n_3=0, \quad \text{(c)} \ \ n_1+3n_2=0,$$

and for f with odd terms, we still have these cases as well as two additional ones:

$$\text{(d)} \ \ n_1+n_2+n_3=0, \quad \text{(e)} \ \ n_1+2n_2=0.$$

As an example, we consider the solution of Eq. (1.23) with even $P(x,y)$ in the form of

$$f=K_1e^{n_1}+K_2e^{-n_1}+K_3e^{n_2}+K_4e^{-n_2}+K_5e^{n_3}+K_6e^{-n_3},$$

with the condition $n_1+n_2+2n_3=0$. We substitute this f into Eq. (1.23) to find the conditions for f. The coefficients of e^{2n_1} and e^{2n_2} yield

$$P(k_1,k_1)=P(k_2,k_2)=0.$$

The coefficients of $e^{n_i-n_j}$ $(i\neq j)$ yield

$$l_1+l_2=\frac{2P(k_1,-k_2)}{k_1+k_2}, \quad l_1+l_3=\frac{2P(k_1,-k_3)}{k_1+k_3}, \quad l_2+l_3=\frac{2P(k_2,-k_3)}{k_2+k_3}.$$

The coefficients of $e^{n_1+n_2}=e^{-2n_3}$ and $e^{-n_1-n_2}=e^{2n_3}$ yield

$$A_{12}K_1K_3=P(k_3,k_3)K_6^2, \quad A_{12}K_2K_4=P(k_3,k_3)K_5^2,$$

where we denote

$$A_{ij}=(k_i-k_j)(l_i-l_j)-2P(k_i,k_j).$$

The coefficients of $e^{n_1+n_3}=e^{-n_2-n_3}$ and $e^{n_2+n_3}=e^{-n_1-n_2}$ yield

$$A_{13}K_1K_5+A_{23}K_4K_6=0, \quad A_{13}K_2K_6+A_{23}K_3K_5=0.$$

The constant terms yield

$$[2k_1l_1-P(k_1,-k_1)]K_1K_2+[2k_2l_2-P(k_2,-k_2)]K_3K_4+[2k_3l_3-P(k_3,-k_3)]K_5K_6=0.$$

From all these requirements, we get the following result.

Theorem 5.1: Suppose $P(x,y)$ is even and k_1 and k_2 are two roots of $P(x,x)$, $k_3=-(k_1+k_2)/2$, and

$$\begin{aligned} &P(k_1,k_3)=P(k_2,-k_3),\\ &[2k_3l_3-P(k_3,-k_3)]A_{12}A_{13}A_{23}=P(k_3,k_3)\{[2k_1l_1-P(k_1,-k_1)]A_{23}^2\\ &\qquad\qquad +[2k_2l_2-P(k_2,-k_2)]A_{13}^2\}, \end{aligned} \tag{5.1}$$

where

$$\begin{aligned} &A_{ij}=(k_1-k_j)(l_i-l_j)-2P(k_i,k_j) \quad (i\neq j),\\ &l_1=\frac{P(k_1,-k_2)}{k_1+k_2}+\frac{2P(k_1,-k_3)}{k_1+k_3}, \quad l_2=\frac{P(k_1,-k_2)}{k_1+k_2}+\frac{2P(k_2,-k_3)}{k_2+k_3}, \quad l_3=-\frac{P(k_1,-k_2)}{k_1+k_2}. \end{aligned} \tag{5.2}$$

Then Eq. (1.22) admits the exact solution

$$\begin{aligned} &u=(\log f)_x,\\ &f=K_1e^{k_1x+l_1t}+K_2e^{-(k_1x+l_1t)}+K_3e^{k_2x+l_2t}+K_4e^{-(k_2x+l_2t)}+K_5e^{k_3x+l_3t}+K_6e^{-(k_3x+l_3t)}, \end{aligned} \tag{5.3}$$

where K_1, K_2, and K_5 are arbitrary and

$$K_3=\frac{A_{12}A_{13}^2}{A_{23}^2P(k_3,k_3)}\frac{K_1K_2^2}{K_5^2}, \quad K_4=\frac{P(k_3,k_3)}{A_{12}}\frac{K_5^2}{K_2}, \quad K_6=-\frac{A_{12}A_{13}}{A_{23}P(k_3,k_3)}\frac{K_1K_2}{K_5}. \tag{5.4}$$

Applying this result to Eq. (3.26), we find $a_2=4a_3$ and the exact solutions (1.29) and (1.30) of Eq. (1.26).

We have also found the requirements for Eq. (1.23) to admit solutions with six terms satisfying $n_1+3n_2=0$, and seven terms satisfying $n_1+n_2+2n_3=0$ or $n_1+n_2+n_3=0$. In the following we give one example for each case.

Example 5.1: Equation (4.12) admits the exact solution (5.3) with arbitrary K_3, K_4, and K_5, and

$$\begin{aligned} &K_1=\frac{k_2^2-k_3^2}{3(k_1^2-k_3^2)}\frac{K_4^2}{K_3}, \quad K_2=\frac{k_2^2-k_3^2}{3(k_1^2-k_3^2)}\frac{K_3^2}{K_4}, \quad K_6=\frac{64k_2^6}{k_3^2(k_1^2-k_3^2)^2}\frac{K_3K_4}{K_5},\\ &l_1=-\tfrac{1}{9}k_1[a_1k_1^4+2(5a_1+5a_2+11a_3+12a_4)k_1^2k_3^2-27(a_3+2a_4)k_3^4], \quad l_2=-\tfrac{1}{3}l_1.\\ &l_3=-\tfrac{1}{9}k_3[(a_1+a_2+4a_3+6a_4)k_1^4+2(5a_1-9a_2-18a_4)k_1^2k_3^2+9(a_2+a_3)k_3^4], \end{aligned} \tag{5.5}$$

for fixed wave numbers k_1, k_2, and k_3 with $k_2=-k_1/3$, provided that

$$b_1=-\tfrac{10}{9}a_1k_1^2-(a_1+a_2+a_3)k_3^2, \quad b_2=-\tfrac{10}{9}a_2k_1^2-2a_4k_3^2,$$

$$b_3=-\tfrac{1}{9}(11a_3+12a_4)k_1^2+(a_3+3a_4)k_3^2,$$

$$c=\tfrac{1}{9}(a_1+2a_3+3a_4)k_1^4+\tfrac{2}{9}(5a_1+5a_2+a_3-3a_4)k_1^2k_3^2-(a_3+2a_4)k_3^4, \tag{5.6}$$

$$d=-\tfrac{1}{9}(a_1+a_2+2a_3)k_1^4k_3^2+(a_3+2a_4)k_1^2k_3^4.$$

Example 5.2: The equation

$$\begin{aligned}u_t=&a_1\partial_x(\partial_x+u)^4u+a_3[(\partial_x+u)u][(\partial_x+u)^3u]+a_4[(\partial_x+u)^2u]^2+[(\tfrac{5}{3}a_1+a_3+\tfrac{4}{3}a_4)k_1k_2\\&-5a_1k_3^2](\partial_x+u)^3u+[-(\tfrac{5}{3}a_1+2a_3+\tfrac{10}{3}a_4)k_1k_2+5a_1k_3^2]u(\partial_x+u)^2u+[(3a_3+4a_4)k_1k_2\\&-(\tfrac{11}{2}a_3+6a_4)k_3^2][(\partial_x+u)u]^2+[a_3(k_1^2k_2^2+\tfrac{3}{2}k_1^2k_3^2+\tfrac{3}{2}k_2^2k_3^2)+a_4(k_1^2k_2^2+2k_1^2k_3^2+2k_2^2k_3^2)]u^2\\&-(\tfrac{3}{2}a_3+4a_4)k_1^2k_2^2k_3^2\end{aligned} \tag{5.7}$$

admits the exact solution

$$u=(\log f)_x,$$

$$f=K_1e^{k_1x+l_1t}+K_2e^{-(k_1x+l_1t)}+K_3e^{k_2x+l_2t}+K_4e^{-(k_2x+l_2t)}+K_5e^{k_3x+l_3t}+K_6e^{-(k_3x+l_3t)}+K_7, \tag{5.8}$$

where K_1, K_2, and K_5 are arbitrary and

$$l_1=-\tfrac{1}{12}a_1k_1^3(3k_1^2+10k_1k_2+15k_2^2)+\tfrac{1}{3}(3a_3+4a_4)k_1k_2(k_1^3-3k_2k_3^2),$$

$$\begin{gathered}l_2=-\tfrac{1}{12}a_1k_2^3(3k_2^2+10k_1k_2+15k_1^2)+\tfrac{1}{3}(3a_3+4a_4)k_1k_2(k_2^3-3k_1k_3^2),\quad l_3=-\tfrac{1}{2}(l_1+l_2),\\K_3=\frac{16k_1^6(k_1-k_3)}{k_2^2k_3^2(k_2-k_3)^3}\frac{K_1K_2^2}{K_5^2},\quad K_4=\frac{k_3^2(k_1-k_3)(k_2-k_3)}{16k_1^2k_2^2}\frac{K_5^2}{K_2},\\K_6=\frac{16k_1^4}{k_3^2(k_2-k_3)^2}\frac{K_1K_2}{K_5},\quad K_7=\pm\frac{2(k_1-k_2)^2(k_2-k_3)}{k_2^2k_3}\sqrt{K_1K_2}.\end{gathered} \tag{5.9}$$

Example 5.3: The equation

$$\begin{aligned}u_t=&a_1\partial_x(\partial_x+u)^4u+a_3[(\partial_x+u)u][(\partial_x+u)^3u]+a_4[(\partial_x+u)^2u]^2\\&+b_1(\partial_x+u)^3u+b_2u(\partial_x+u)^2u+b_3[(\partial_x+u)u]^2+cu^2+d\end{aligned} \tag{5.10}$$

with $b_3=6(a_3+a_4)(3b_1+b_2)/(10a_1+3a_3+2a_4)$, admits the exact solution (5.8), where k_1, k_2, and k_3 are the three roots of the cubic polynomial $(a_3+a_4)x^3+(b_1+b_2+b_3)x^2+cx+d$, K_1, K_3, and K_5 are arbitrary and

$$\begin{aligned}l_1&=k_1[a(k_1^4-5k_1^2k_2k_3-5k_2^2k_3^2)+b_1(k_1^2-k_2k_3)],\\l_2&=k_2[a(k_2^4-5k_2^2k_3k_1-5k_3^2k_1^2)+b_1(k_2^2-k_3k_1)],\\l_3&=k_3[a(k_3^4-5k_3^2k_1k_2-5k_1^2k_2^2)+b_1(k_3^2-k_1k_2)],\end{aligned} \tag{5.11}$$

$$K_7=2\left[\frac{(k_1-k_2)(k_1-k_3)(k_2-k_3)}{k_1k_2k_3}\right]^{2/3}(K_1K_3K_5)^{1/3},\quad K_2=\frac{1}{4}\left[\frac{k_2k_3}{(k_1-k_2)(k_1-k_3)}\right]^2\frac{K_7^2}{K_1},$$

$$K_4=\frac{1}{4}\left[\frac{k_1k_3}{(k_1-k_2)(k_2-k_3)}\right]^2\frac{K_7^2}{K_3},\quad K_6=\frac{1}{4}\left[\frac{k_1k_2}{(k_1-k_3)(k_2-k_3)}\right]^2\frac{K_7^2}{K_5}.$$

Solutions of Eq. (1.22) with eight terms may describe the interaction of three solitary waves provided $n_1+n_2+n_3+n_4=0$:

Theorem 5.2: Suppose $P(x,y)$ is even and k_i $(i=1,2,3,4)$ are four roots of $P(x,x)$ and

$$\begin{gathered}k_1+k_2+k_3+k_4=0,\\ P(k_1,-k_2)=P(k_3,-k_4),\quad P(k_1,-k_3)=P(k_2,-k_4),\quad P(k_1,-k_4)=P(k_2,-k_3),\\ [2k_1l_1-P(k_1,-k_1)]A_{23}A_{24}A_{34}+[2k_2l_2-P(k_2,-k_2)]A_{13}A_{14}A_{34}\\ +[2k_3l_3-P(k_3,-k_3)]A_{12}A_{14}A_{24}+[2k_4l_4-P(k_4,-k_4)]A_{12}A_{13}A_{23}=0,\end{gathered}\tag{5.12}$$

where

$$l_i=\sum_{j\neq i}\frac{P(k_i,-k_j)}{k_i+k_j},\quad A_{ij}=(k_i-k_j)(l_i-l_j)-2P(k_i,k_j).\tag{5.13}$$

Then Eq. (1.22) admits the exact solution

$$\begin{gathered}u=(\log f)_x,\\ f=K_1e^{k_1x+l_1t}+K_2e^{-(k_1x+l_1t)}+K_3e^{k_2x+l_2t}+K_4e^{-(k_2x+l_2t)}+K_5e^{k_3x+l_3t}+K_6e^{-(k_3x+l_3t)}\\ +K_7e^{k_4x+l_4t}+K_8e^{-(k_4x+l_4t)},\end{gathered}\tag{5.14}$$

where K_1, K_3, K_5, and K_7 are arbitrary and

$$\begin{gathered}K_2=\frac{A_{23}A_{24}A_{34}}{AK_1},\quad K_4=\frac{A_{13}A_{14}A_{34}}{AK_3},\quad K_6=\frac{A_{12}A_{14}A_{24}}{AK_5},\quad K_8=\frac{A_{12}A_{13}A_{23}}{AK_7},\\ A=\pm\left(-\frac{A_{12}A_{13}A_{14}A_{23}A_{24}A_{34}}{K_1K_3K_5K_7}\right)^{1/2}.\end{gathered}\tag{5.15}$$

This solution describes the interaction of three solitary waves. Applying this result to Eq. (4.12), we find Eq. (1.31) and its exact solutions (1.32)–(1.34). We can also consider the cases that n_1, n_2, n_3, and n_4 satisfy two linear relations, which can be either $n_3=3n_1$, $n_4=2n_1+n_2$, or $n_3=3n_1$, $n_4=4n_1+n_2$, or $n_3=2n_1+n_2$, $n_4=3n_1+2n_2$. The details for these results can be found in Ref. 9.

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Geometry of spaces with the Jacobi metric

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The generalized Maupertuis principle is formulated for systems with the natural Lagrangian and an indefinite form of the kinetic energy. The generalization is applied to the theory of gravity and cosmology. For such systems, the metric determined by the kinetic energy form has a Lorentz signature. The theorem is proved concerning the behavior of trajectories in a neighborhood of the boundary of the region admissible for motion. This region is not a smooth manifold but turns out to be a differential space of constant differential dimension. This fact allows us to use geometric methods analogous to those elaborated for smooth manifolds. It is shown that singularities of the Jacobi metric are not dangerous for the motion; its trajectories are smooth in the sense of the theory of differential spaces. © *1996 American Institute of Physics.* [S0022-2488(95)00412-1]

I. INTRODUCTION

In the present work we study mechanical systems with Lagrange functions L which do not depend on time and are of second order in velocities, i.e., $L = \frac{1}{2}g_{\alpha\beta}\dot{q}^{\alpha}\dot{q}^{\beta} - V(q)$, where $V: M \to \mathbf{R}$ is a potential function. According to the classical Maupertuis principle, trajectories of the system, with the total energy $E = \frac{1}{2}g_{\alpha\beta}\dot{q}^{\alpha}\dot{q}^{\beta} + V(q)$, are geodesics of the Jacobi metric $\hat{g}_{\alpha\beta} = (E - V)g_{\alpha\beta}$. From the energy integral it follows that, for such systems, the motion occurs in the region for which $E - V \geqslant 0$. If $\sup_M(V) < E$, then the description of motion reduces to the study of the Riemann geometry. As far as applications to cosmology and the theory of gravity are concerned, the kinetic energy form is indefinite and the metric has the Lorentz signature. In the present work we generalize the Maupertuis principle to this case and prove the corresponding generalized Jacobi theorem. It turns out that the problem of motion is reduced to the behaviour of geodesics in certain domains of the configuration space. Spaces with the Jacobi metric are spaces with boundaries at which the metric is degenerate (we use the term ''boundary'' although in some cases below it is rather a boundary set than a boundary in a standard sense). In the case of positively definite kinetic energy form they are Riemann spaces (sections II and IV), whereas in our case they are pseudo-Riemannian spaces (sections III and V).

First non-trivial results concerning the behaviour of trajectories of classical systems with degenerate Jacobi metrics were obtained by Seifert.[1] However, intensive investigation of the domains admissible for motion $\{x \in M: V(x) \leqslant E\}$ began with Refs. 2 and 3. These works focused on the existence of closed trajectories with endpoints at the boundary $\{x \in M: E = V\}$. Kozlov's papers[3] contain a review of the obtained results. Our motivations are different. We aim at finding an invariant description of chaos in gauge theories. Our main tool is the study of separation of nearby geodesics in terms of the normal component of the separation vector satisfying the geodesic deviation equation. The present paper is a generalization of the series of previous results.[4]

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The fact that the Jacobi metric degenerates at the boundary of the domain admissible for motion creates some difficulties. We show, however, that these difficulties are not dangerous since the set of the natural parameter values for which the trajectory remains at the boundary is a zero-measure subset in the set of all boundary points. This allows us to use the geodesic deviation equation (objections of Burd and Tavakol[5] notwithstanding) in spite of the fact that it is singular at the boundary.

In general, spaces with the Jacobi metric can be regarded as simple generalizations of differentiable manifolds known as differential spaces of constant differential dimension (section VI). Differential spaces were first introduced by Sikorski[6] and applied to the geometry of space–time by Gruszczak *et al.*[7] Classical analysis and differential geometry can be naturally done on such spaces. This allows us to investigate, in the precise manner, the behaviour of trajectories in a neighbourhood of the boundary of the domain admissible for motion. Such a domain can carry a Lorentz metric. This fact is important since spaces with Lorentz metrics are needed to describe systems with the indefinite kinetic energy form. It should be stressed that such mechanical systems are as important as usual classical mechanical systems. We show that for systems with both positive definite and indefinite kinetic energy forms hyperregular Lagrange functions can be defined which implies that for these systems the Lagrange and Hamiltonian formulations of mechanics are equivalent (section VII). This fact puts the Maupertuis principle on the firm base.

There exist alternative approaches to the main problem of the present work. Motion can be investigated either with the help of Euler–Lagrange equations with the metric taken from the kinetic energy form (well defined on the entire space), or with the help of the geodesic equations. In the latter case, since the Jacobi metric on the boundary is degenerate, and the geodesic equation breaks down at the boundary, one should develop the theory of motion in terms of structure tensors with lower indices as it is done in the theory of sub-Riemannian manifolds (which have found their applications to the steering theory). However, one has to remember that to apply this theory to our case, one should generalize it in two directions: to the case of the Lorentz metric and to the case of manifold with boundary (again, the theory of differential spaces could be used).

The Maupertuis principle in our approach can be regarded as a method of geometrization of a broader class of dynamical problems. It can be applied to the Hamiltonian systems with the natural Lagrange function. For instance, in the classical case (if the kinetic energy form is positive definite), this method can be used to the study of dynamics of collisionless n-body gravitating system.[8] In the non-classical case (the kinetic energy form is indefinite), the generalized Maupertuis principle can be used to the investigation of dynamical systems in general relativity and cosmology. In the so-called ADM formulation of general relativity, the dynamics of space–time is equivalent to the study of non-classical dynamical systems with a suitable potential function which is determined by the geometry of spacelike sections and the matter content in the non-vacuum case.[9] Another important field of applications of the generalized Maupertuis principle is given by the dynamics of homogeneous anisotropic cosmological models. In this case, the potential function is determined by the Lie algebras of the corresponding isometry groups acting on spacelike sections of space–time.[10]

It is worthwhile noticing that it would be meaningless to apply our method to a certain class of problems as, for instance, to the problem of motion of a test particle in the external gravitational field in general relativity. Such test particles already move along geodesics in a given space–time, and their dynamics is already geometrized. In this case, the geodesic motion is determined by the Hamilton function which coincides with the kinetic energy form.

II. CLASSICAL MECHANICS OF SIMPLE MECHANICAL SYSTEMS

In the present section we define classical mechanics of simple mechanical systems, introduce standard concepts, mainly to establish terminology, and prove the Jacobi theorem for the case of

simple mechanical systems with an indefinite kinetic energy form. This will allow us to generalize the Maupertuis principle to the case of mechanical systems within the framework of general relativity and cosmology.

Definition 1: Classical mechanics of simple mechanical systems is the triple $(\mathscr{M},K,V)$, *where* $\mathscr{M}$ *is a smooth manifold (a configuration space),* K *is the kinetic energy form defined by the Riemann metric on* $\mathscr{M}$, *i.e.,* $K(v)=\frac{1}{2}g(v,v)$ *for every* $v \in T_x\mathscr{M}$, $x \in \mathscr{M}$, *and* V *is the potential energy of the system.*,[8,11]

These systems are called *classical* since their kinetic energy form is positively definite; they are called *simple* since they have a natural Lagrangian.

For a given total energy E of the system the *admissible configuration space* is given by

$$\hat{\mathscr{M}}_E=\{x\in\mathscr{M}: V(x)\leqslant E\}.$$

To the total energy E there corresponds the Jacobi metric g_E of the simple classical mechanical system $(\mathscr{M},K,V)$ given by

$$g_E(x):=2(E-V(x))g(x).$$

This is a Riemann metric on a configuration space M_E parametrized by E. It is non-degenerate on $M_E=\{x \in \mathscr{M}: V(x)<E\}$, and degenerate on the boundary $\partial M_E=\{x \in \mathscr{M}: V(x)=E\}$.

As is well known, one obtains the trajectories of a simple mechanical system by extremalizing the action

$$I[C]=\int_a^b L(C(t))dt,$$

where $L(x,v)=\frac{1}{2}g_x(v,v)-V(x)$. The Maupertuis principle, in its original formulation, consisted in considering only those trajectories which satisfy the condition

$$\tfrac{1}{2}g(\dot{C}(t),\dot{C}(t))=E-V(C(t)),$$

where a dot means differentiation with respect to t.

Historically, the Maupertuis principle preceded a simpler Hamilton principle. The precise formulation of the Maupertuis principle we owe to Jacobi (see Ref. 2). After taking into account the above Maupertuis condition, the first variation of the action assumes the form

$$\delta I[C]=\delta\int_a^b g(\dot{C},\dot{C})dt=\delta\int_a^b\{2[E-V(C(t))]g(\dot{C},\dot{C})\}^{1/2}dt=0.$$

Consequently, physical trajectories of the system with the total energy E are geodesics of the Jacobi metric $2(E-V)g$. This heuristic argumentation can be repeated for the case with the indefinite kinetic energy form. To this end, it is enough to replace the expression $2(E-V(C(t)))$ by $2|E-V(C(t))|$.

Theorem 1 (Jacobi): *Physical trajectories of a simple classical system* $(\mathscr{M},K,V)$ *[or equivalently* (M,g,V)*] with the total energy* E *are geodesics on the Riemann manifold* (M_E,g_E).

Since the proof of this theorem is well known we shall present only those of its aspects which will allow us to generalize the above theorem to the case with the indefinite kinetic energy form (in section III).

The proof of the Jacobi theorem consists in considering the Lagrange-Euler equations in a local map, i.e.,

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}^i(t)}=\frac{\partial L}{\partial x^i(t)}, \tag{1}$$

where

$$L=\tfrac{1}{2}g(\dot{C}(t),\dot{C}(t))-V(C(t))=\tfrac{1}{2}g_{ij}(x(t))\dot{x}^i(t)\dot{x}^j(t))-V(x(t)). \tag{2}$$

After inserting (2) into (1) we obtain

$$\ddot{x}^p(t)+\Gamma^p_{rs}(x(t))\dot{x}^r\dot{x}^s=-g^{pi}\partial_i V(x(t))=-(\mathrm{grad}V)^p(x(t)) \tag{3}$$

or, equivalently, the Euler-Lagrange equation

$$\nabla_{\dot{C}(t)}\dot{C}(t)=-\mathrm{grad}V(C(t)).$$

Equation (3) with the convention

$$e^{2f}=2|E-V|$$

assumes the form

$$\ddot{x}^i(t)+\hat{\Gamma}^i_{jk}(x(t))\dot{x}^j(t)\dot{x}^k(t)=\frac{d}{dt}\ln|E-V(x(t))|\dot{x}^i(t), \tag{4}$$

where $\hat{\Gamma}^i_{jk}$ are Christofell symbols with respect to the Jacobi metric $\hat{g}_E$. We have taken into account the equality $2df(\dot{C})=2\dot{x}^i(t)(\partial_i f)x(t)$ (for detailed calculations see, Refs. 8, 11).

Now, we introduce the reparametrization $s=s(t)$ to obtain

$$\left(\frac{ds}{dt}\right)^2 x^i(s)''+\frac{d^2s}{dt^2}x^i(s)'+\left(\frac{ds}{dt}\right)^2\hat{\Gamma}^i_{jk}x^j(s)'x^k(s)'=\left\{\left[\frac{d}{dt}\ln|E-V(x(t))|\right]\frac{ds}{dt}\right\}x^i(s)', \tag{5}$$

where prime denotes differentiation with respect to s. After eliminating the terms with first derivatives of x^i from equation (5), we obtain

$$\frac{ds}{dt}=\kappa|E-V(x(t))|,$$

where κ is a real number. We choose $\kappa=2$ to guarantee

(1) that s should be a monotonic function of the Newtonian time t,

(2) that the tangent vector to the geodesic should be normed to $+1$, or to -1, or that it should be a null vector, i.e.,

$$g_E(x',x')=\mathrm{sgn}(E-V). \tag{6}$$

Therefore, if we take the natural parameter s for the Jacobi metric, i.e.,

$$\frac{ds}{dt}=2|E-V|, \tag{7}$$

the trajectory equation assumes the form of the geodesic equation

$$x^i(s)'' + \hat{\Gamma}^i_{jk}(x(t))x^j(s)'x^k(s)' = 0, \tag{8}$$

which ends the proof. □

III. NON-CLASSICAL MECHANICS OF SIMPLE MECHANICAL SYSTEMS

Definition 2: Non-classical mechanics of simple mechanical systems is the triple $(\mathcal{M},K,V)$ *(or* (M,g,V)*) where* $\mathcal{M}$ *is a smooth manifold (configuration space), K is the indefinite kinetic energy form,* $K(v)=\frac{1}{2}g(v,v)$*, and V is the potential energy of the system.*

These systems are called non-classical since their kinetic energy form is indefinite. We assume that the signature of g is $(+,+,\ldots,+,-)$.

In the configuration space of simple non-classical mechanical systems we define the following subsets

(a) D_T: the subset of the configuration space $\mathbf{R}^N$ on which $E-V<0$,

(b) D_S: the subset of $\mathbf{R}^N$ on which $E-V>0$,

(c) ∂D: the subset of $\mathbf{R}^N$ on which $V=E$.

In the theory of gravity (cosmology included), especially interesting is the class of simple mechanical systems with $E=0$, we shall call them *zero constraint mechanical systems* (ZC-systems).

Definition 3: In the tangent space to the configuration space $\mathbf{R}^N$ *of simple non-classical mechanical systems, we define the following classes of vectors*

(a) $v \in T_q\mathbf{R}^N$ *is timelike if* $g_{\alpha\beta}(q)v^\alpha v^\beta<0, q \in M$,

(b) $v \in T_q\mathbf{R}^N$ *is spacelike if* $g_{\alpha\beta}(q)v^\alpha v^\beta>0, q \in M$,

(c) $v \in T_q\mathbf{R}^N$ *is null if* $g_{\alpha\beta}(q)v^\alpha v^\beta=0, q \in M$.

The Hamiltonian constraint $(H=E=0)$ implies the following properties of the tangent vector to any trajectory

(a′) any tangent vector in the domain D_T is timelike,

(b′) any tangent vector in the domain D_S is spacelike,

(c′) the tangent vector to any trajectory through a point $q_0 \in \partial D$ is a null vector, i.e., it is situated on the surface given by $g_{\alpha\beta}(q_0)\xi^\alpha\xi^\beta=0$.

The above regularities allow us to generalize the Jacobi theorem to the case of non-classical simple mechanical systems.

Theorem 2: *Physical trajectories of a non-classical simple mechanical system with the total energy E are geodesics on a pseudo-Riemannian manifold without a boundary on which the Jacobi metric is degenerate.*

Proof follows from that for the classical case together with definitions 2 and 3, and their consequences. □

IV. APPLICATION OF THE MAUPERTUIS PRINCIPLE TO SIMPLE CLASSICAL MECHANICAL SYSTEMS

We shall distinguish two cases

(1) $E>\max_M V$,

(2) $E\leqslant\max_M V$.

Of course, we assume that the potential function has no critical points on $\{V=E\}$. In case (1), $\hat{M}_E$ coincides with the entire configuration space. For instance, the problem of the existence of periodic solutions to the equations of motion reduces to the problem of finding closed geodesics on a smooth Riemann manifold. In general, we can use known theorems about the behaviour of geodesics on Riemann manifolds to solve various problems, but this case is seldom physically interesting.[3]

Example 1: Let us consider a torus T^2 with a Riemann metric. Among all closed curves with m rotations in the parallel surface and n rotations in the orthogonal surface, there exists the curve

of the minimal length. It is a closed geodesic. T^2 is a position space of a double plane pendulum. It follows that, for any integers m and n, there exists a periodic motion of the double pendulum in which one arm performs m rotations and the other arm performs n rotations.

In case (2), the boundary ∂M_E is non-empty, and the Jacobi metric has a singularity on ∂M_E; lengths of all curves in ∂M_E are equal to zero. In this case, the geometry of the admissible configuration space is different from that of the ordinary Riemann compact manifolds. (For a review of the problem of geodesics on spaces with the Jacobi metrics degenerating at the boundary, see Refs. 3, 12.)

The theory of closed geodesics was intensively investigated beginning from the classical Poincaré works. These works were a part of the program of the qualitative study of mechanical systems. The problem of the periodic trajectories was reduced by Poincaré to the existence of closed geodesics. Later on it was investigated by many authors.

With the additional assumptions that the configuration space M_E is compact and has the non-empty boundary ∂M_E, which is an $(N-1)$-dimensional smooth manifold, Kozlov was able to prove the following propositions[3]:

(1) Let us consider the motion $q(t)$ of a simple classical mechanical system with the initial condition at $t=0$: $q(0)=q_0$, $\dot{q}(0)=v_0$. $q(-t)$ is a solution of the same equations with the initial condition $q(0)=q_0$, $\dot{q}(0)=-v_0$, and $q(\pm t)=q(\mp t)$. The proof follows directly from properties of Lagrange equations and from the theorem on the uniqueness of solutions for the Lagrange systems with a positive definite kinetic energy form (as far as we know, for systems with an indefinite kinetic energy form the uniquness was never proved). The fact that $q(t)=q(-t)$ is a simple consequence of the above, i.e., if the trajectory $q(t)$ reaches the boundary at $t=0$ then the motion, after colliding with the boundary, will continue in the opposite direction along the same trajectory.

(2) There are no solutions of the motion equations the trajectories of which cross the boundary at more than two different points. The proof is elementary, and it follows from the fact that if a trajectory crossed the boundary at three points, A, B, C say, then a point m moving from A would reach B, and then—in agreement with (1)—it would continue in the opposite direction along the same trajectory. After a certain period of time it would again reach A, etc.

(3) If trajectories of motion have two common points with the boundary, they can have no other common points with the boundary, and the solution is periodic.

(4) In the close neighbourhood of the boundary, trajectories of motion are orthogonal to the boundary. To illustrate this proposition let us consider a simple classical mechanical system with the Lagrange function

$$\mathscr{L}=\tfrac{1}{2}K\delta_{ij}\dot{q}^i\dot{q}^j-V(q),$$

where $K=\text{const}$. Since the metric $g_{ij}=K\delta_{ij}$ is constant, the Christoffel symbols vanish and the Euler–Lagrange equations are

$$\ddot{\mathbf{q}}=-\nabla V.$$

Let us consider the trajectory of the system with the initial condition $\mathbf{q}_0 \in \partial D$, where $\dot{\mathbf{q}}(0)=0$ (at the boundary $t=0$). This trajectory can be presented in the form

$$\mathbf{x}(t)=\mathbf{x}_0+\dot{\mathbf{x}}(0)t+\tfrac{1}{2}\ddot{\mathbf{x}}(0)t^2+\cdots=\mathbf{x}_0-\tfrac{1}{2}\nabla V(\mathbf{x}_0)t^2+\cdots,$$

that is, for small $t<\varepsilon$ (near the boundary), the trajectory is determined by the gradient vector (which is orthogonal to the equipotential surface). This means that the particle moves orthogonally to the boundary, for $|t|<\varepsilon$.

To see how the Maupertuis principle works in simple classical mechanical systems let us consider a harmonic oscillator.[8]

Example 2: In the case of a harmonic oscillator the Lagrange function is

$$\mathscr{L}=\frac{m\dot{x}^2}{2}+\frac{m\omega^2x^2}{2}$$

which implies that the metric (of the kinetic energy form) g is equal to m.

The Jacobi metric is

$$\hat{g}=2\left(E-\frac{m\omega^2x^2}{2}\right)m,$$

the domain admissible for motion

$$D_E=\left\{x\in\mathbf{R},-\frac{1}{\omega}\left(\frac{2E}{m}\right)^{1/2}\leqslant x\leqslant\frac{1}{\omega}\left(\frac{2E}{m}\right)^{1/2}\right\}$$

and its boundary

$$\partial D_E=\left\{-\frac{1}{\omega}\left(\frac{2E}{m}\right)^{1/2},\frac{1}{\omega}\left(\frac{2E}{m}\right)^{1/2}\right\},$$

the only non-vanishing Christofell symbol

$$\hat{\Gamma}^1_{11}=-\frac{m\omega^2x}{2E-m\omega^2x^2}\left(\frac{dx}{ds}\right)^2=0.$$

The normalization condition of the tangent vector $\|u\|^2=1$ reduces to

$$m(2E-m\omega^2x^2)\left(\frac{dx}{ds}\right)^2=1.$$

This equation defines the natural parameter s along the geodesic. After differentiating the above equation with respect to s one obtains the geodesic equation. Therefore, the geodesic equation informs us that the norm of the tangent vector is preserved if one changes the parameter s. The solution of the above equation is

$$x(t)=\frac{1}{\omega}\left(\frac{2E}{m}\right)^{1/2}\sin\,\omega(t-t_0),$$

$$x(s)\arcsin\left(\omega\sqrt{\frac{m}{2E}}x\right)+\omega\sqrt{\frac{m}{2E}}x\left(1-\frac{\omega^2m}{2E}x^2\right)^{1/2}=\frac{\omega}{E}(s-s_0),$$

and

$$s(t)=E\left[(t-t_0)+\frac{\sin 2\omega(t-t_0)}{m}\right]+s_0.$$

Of course, $s(t)$ is a strictly monotonic function of the Newtonian time t.

V. APPLICATIONS OF THE MAUPERTUIS PRINCIPLE TO SIMPLE NON-CLASSICAL MECHANICAL SYSTEMS

The problem of the dynamics of non-classical simple mechanical systems in the Maupertuis approach is, in principle, an open question. Kozlov's theorems should be generalized to the two following cases: (1) to Lagrange systems with the natural Lagrangian and indefinite form of the kinetic energy; (2) to non-classical systems with and without a boundary which is not a smooth manifold.

The following theorem is a counterpart for the pseudoriemannian case of Kozlov's property 4 (see section IV):

Theorem 3: *A trajectory of a system with the natural Lagrangian and an indefinite form of the kinetic energy, when passing through the boundary of the region admissible for motion, changes the sector of the cone which is determined by the kinetic energy form.*

Proof follows from the construction of the Maupertuis principle and from properties of the tangent vector to the trajectory (properties (a′) – (c′) in section 3). □

Let us consider the following example. Let the energy function be

$$\mathscr{E}=\tfrac{1}{2}k\,\eta_{\mu\nu}\dot{x}^{\mu}\dot{x}^{\nu}+V(x),$$

where

$$\eta_{\mu\nu}=\mathrm{diag}\|-1,1,1,\ldots\|,k=\mathrm{const.}$$

We assume that the boundary ∂D of the region D admissible for the motion is a smooth manifold. For $x\in\partial D$ one has $\eta_{\mu\nu}\dot{x}^{\mu}\dot{x}^{\nu}=0$. In the case of a non-classical system, $\dot{x}^{\mu}(0)\neq 0$ at the boundary! We investigate the motion in a small neighbourhood of the boundary. The trajectory starts in this neighbourhood at $t=0$. For small times, $|t|<\varepsilon$ the linear approximation is valid

$$\mathbf{x}(t)=\mathbf{x}_0+\dot{\mathbf{x}}_0t+\cdots,$$

i.e., for $|t|<\varepsilon$, the motion is determined by the vector $\dot{\mathbf{x}}_0$ which is situated on the cone.

Example 3: As a special case of the above system, let us consider a Hamiltonian system describing the dynamics of the Friedman cosmological model with the scalar field.[13] The Hamiltonian of this system is

$$\mathscr{H}=\mathscr{H}(p_1,p_2,q^1,q^2)=\tfrac{1}{2}\eta^{\mu\nu}p_{\mu}p_{\nu}+V(q^1,q^2),$$

where

$$\eta^{\mu\nu}=\mathrm{diag}(-1,1),$$

$$V(q^1,q^2)=\tfrac{1}{2}[-(q^1)^2+(q^2)^2+m^2(q^1)^2(q^2)^2].$$

The Hamiltonian constraint is $\mathscr{H}=0$ which is typical for gravitational systems. Therefore, the motion takes place in the region given by

$$-(\dot{q}^1)^2+(\dot{q}^2)^2=-(q^1)^2+(q^2)^2+m^2(q^1)^2(q^2)^2=-2V(q^1,q^2).$$

In this case, the kinetic energy form is indefinite and divides the configuration space into subdomains.

Kozlov[3] claims that some theorems concerning the behaviour of trajectories, in the general case of the reversible Hamiltonian systems, are valid independently of generalizations (1) and (2). For instance, one has

Theorem 4 (Kozlov): *Let* $x:(-\varepsilon,\varepsilon)\to B$ *be a motion of a system with a natural Lagrangian and* $x(0)\in\partial D$. *Then* $x(t)=x(-t)$ *for every* $-\varepsilon<t<\varepsilon$.

It seems that this theorem cannot be applied to the case with an indefinite kinetic energy form. If a point hits ∂D, it moves along the same trajectory in the oppposite direction. In the work by Hofer and Toland,[14] the existence of libration motions has been proved provided that D_T is compact and convex, and there are no critical points of the potential function on the boundary ∂D. The proof uses topological theorems about fixed points of smooth mappings.

Hoffer and Toland[14] consider also the existence of periodic motions of non-classical systems with the Lagrangian $(S\dot{x},\dot{x})/2-V(x)$, where $(\cdot,\cdot)$ is the scalar product in $\mathbf{R}^N$, and S is a symmetric, non-degenerate, linear operator with one negative eigenvalue. Let $\Sigma=\{y\in\mathbf{R}^n:(Sy,y)<0\}$ be a cone in $\mathbf{R}^n$. If $x(\cdot)$ is a motion with the vanishing total energy starting in the region $C=\{x:V(x)>0\}$ then $\dot{x}\in\Sigma$. Since Σ consists of two connected components, the transition from one component to another component can occur only at the boundary C.

Some theorems, which are true for simple classical mechanical systems (as, for example, Kozlov's theorem), have no counterparts for simple non-classical mechanical systems. This is illustrated by the following example.

Example 4: A simple non-classical mechanical system in a neighbourhood of the boundary ∂D_E. Let us consider a system with the natural Lagrangian $\mathscr{L}=\frac{1}{2}\eta_{\alpha\beta}\dot{q}^\alpha\dot{q}^\beta-V(q)$, where $\eta_{\alpha\beta}=\mathrm{diag}\|1,\ldots,-1\|$ is a metric with the Lorentz signature. We synchronize time so that $t=0$ corresponds to the moment at which the particle is at ∂D_E and $V(x_0^1,\ldots,x_0^n)=0$. The tangent vector to the cone $\eta_{\mu\nu}(x_0^1,\ldots,x_0^n)\xi^\mu\xi^\nu=0$, $\xi^\mu\equiv\partial x^\mu/\partial t,$, is

$$x^\mu(t)=x_0^\mu+t\dot{x}_0^\mu+\frac{t^2}{2}\ddot{x}_0^\mu+O(t^2). \tag{9}$$

For a 2-dimensional case, the above equation has the form

$$\begin{aligned} x(t)&=x_0+t\dot{x}_0+\frac{t^2}{2}\frac{\partial V}{\partial x}(x_0,y_0)+O(t^2),\\ y(t)&=y_0\pm t\dot{x}_0+\frac{t^2}{2}\frac{\partial V}{\partial y}(x_0,y_0)+O(t^2), \end{aligned} \tag{10}$$

where (x,y) are Cartesian coordinates of the trajectory, $\dot{x}_0=\pm\dot{y}_0$, and $V(x_0,y_0)=0$ on the boundary ∂D_E.

Expansion (9), when applied to classical systems, leaves only terms with even exponents α in t^α. To see this, it is enough to notice that, for a 1-dimensional system, the trajectory $q(t)$, for small t, is given by

$$q(t)=q_0-\frac{t^2}{2}\frac{\partial V}{\partial q}(q_0)+O(t^2). \tag{11}$$

Indeed, since the velocity of the particle at the boundary ∂D_E vanishes, expansion (9) leaves the terms with even exponents of t, for instance:

$$\dddot{q}(t)=\frac{d}{dt}(\ddot{q}(t))=\frac{-\partial^2 V}{\partial q^2}\dot{q}=0,\qquad \dddot{q}(t)=\frac{\partial^2 V}{\partial q^2}\ddot{q}\neq 0$$

at the boundary ∂D_E.

This is not true as far as non-classical mechanical systems are concerned and, consequently, Kozlov's generalization is not correct. This can be seen already in the linear approximation (see (10)). However, the assertion remains true that if $q(t)$ is a solution of the Euler-Lagrange equation

with the initial condition $q(0)=q_0,\dot{q}(0)=v_0$, then $q(-t)$ is also a solution with the initial condition $q(0)=q_0,\dot{q}(0)=-v_0$. It is enough to notice that if $t\to -t$, $\dot{x}_0\to -\dot{x}_0$, $\dot{y}_0\to -\dot{y}_0$, and $x(0)=x_0$, $y(0)=y_0$, one obtains the trajectory $(x(t),y(t))$. For classical mechanical systems, from (11) one has $q(\pm t)=q(\mp t)$.

To study our system in a neighbourhood of ∂D_E let us consider the squared length of the tangent vector $\dot{\mathbf{x}}$ to the trajectory

$$\|\dot{\mathbf{x}}\|^2 \equiv \eta_{\mu\nu}\frac{dx^\mu}{d\tau}\frac{dx^\nu}{d\tau} = -2V(x). \tag{12}$$

By using (9) in the linear approximation of the potential and the trajectory we obtain: for a 2-dimensional system

$$\begin{aligned}\|\dot{\mathbf{x}}\|^2 &= -2(x_0+t\dot{x}_0, y_0\pm t\dot{x}_0)\\ &= -2V(x_0,y_0)-2t\left[\frac{\partial V}{\partial x}(x_0,y_0)\dot{x}_0\pm\frac{\partial V}{\partial y}(x_0,y_0)\dot{x}_0\right]\\ &= -2V(x_0,y_0)-2t\left[\frac{\partial V}{\partial x}(x_0,y_0)\dot{x}_0\pm\frac{\partial V}{\partial y}(x_0,y_0)\dot{x}_0\right],\end{aligned} \tag{13}$$

and for a multidimensional system

$$\|\dot{\mathbf{x}}\|^2 = -2(x_0^1+t\dot{x}_0^1, x_0^2+t\dot{x}_0^2, \ldots, x_0^n+t\dot{x}_0^n) = -2t\sum_{\mu=1}^{n}\frac{\partial V}{\partial x^\mu}(x_0^1,\ldots,x_0^n)\dot{x}_0^\mu. \tag{14}$$

From (14) it can be seen that, for small t, the function f of the squared velocity is an odd function of t, and it changes the sign when passing through ∂D_E, i.e.,

$$\|\dot{\mathbf{x}}\|^2 = \begin{cases} f>0 & \text{if} \quad t<0\\ f=0 & \text{if} \quad t=0.\\ f<0 & \text{if} \quad t>0\end{cases}$$

To describe the behaviour of trajectories further away from the boundary ∂D_E one should take into account at least second order terms in expansion (9) and (10). Taking into account second order terms in (9) and (10), in the second order approximation of the function $\|\dot{\mathbf{x}}\|^2$ (see (14)), for the 1-dimensional and multidimensional cases, we obtain, respectively,

$$\begin{aligned}\|\dot{\mathbf{x}}\|^2 &= -2V\left(x_0+t\dot{x}_0-\frac{t^2}{2}\frac{\partial V}{\partial x}(x_0,\,y_0), y_0\pm t\dot{x}_0+\frac{t^2}{2}\frac{\partial V}{\partial y}(x_0,\,y_0)\right)\\ &= -2V(x_0,y_0)-2t\left[\frac{\partial V}{\partial x}(x_0,\,y_0)\dot{x}_0\pm\frac{\partial V}{\partial y}(x_0,y_0)\dot{x}_0\right]-t^2\left[\left(\frac{\partial V}{\partial x}\right)^2(x_0,\,y_0)+\left(\frac{\partial V}{\partial y}\right)^2(x_0,y_0)\right.\\ &\quad\left.+\frac{\partial^2 V}{\partial x^2}(x_0,\,y_0)\dot{x}_0^2+\frac{\partial^2 V}{\partial y^2}(x_0,y_0)\dot{x}_0^2\mp\frac{\partial^2 V}{\partial x\partial y}(x_0,y_0)\dot{x}_0^2\right]+\mathcal{O}(t^2),\end{aligned}$$

$$\|\dot{\mathbf{x}}\|^2=-2t\sum_{\mu=1}^{n}\frac{\partial V}{\partial x^\mu}(x_0^1,\ldots,x_0^n)\dot{x}_0^i-t^2\left[\sum_{\mu=1}^{n-1}(-1)\left(\frac{\partial V}{\partial x^\mu}\right)^2+\left(\frac{\partial V}{\partial x^n}\right)^2+\frac{\partial^2 V}{\partial x^{i2}}(\dot{x}_0^i)^2+\frac{\partial^2 V}{\partial x^i\partial x^j}\dot{x}_0^i\dot{x}_0^j\right]. \tag{15}$$

From (15) one can deduce that, after a certain time t_{cr}, the trajectory will return to the boundary. For the n-dimensional case one has

$$t_{cr}=\left.\frac{\sum_{\mu=1}^{n}\frac{\partial V}{\partial x^\mu}(x_0^1,\ldots,x_0^n)\dot{x}_0^\mu}{\sum_{\mu=1}^{n-1}\left(\frac{\partial V}{\partial x^\mu}\right)^2-\left(\frac{\partial V}{\partial x^n}\right)^2+\frac{\partial^2 V}{\partial x^{i2}}(\dot{x}_0^i)^2+\frac{\partial^2 V}{\partial x^i\partial x^j}\dot{x}_0^i\dot{x}_0^j}\right|_{(x_0^1,\ldots,x_0^n)\in C}, \tag{16}$$

where C is given by $\Sigma_{\mu=1}^{n-1}(x^\mu)^2-(x^n)^2=0$.

If t_{cr} exists and is finite, one can similarly compute the next cycle after which the system will be again at the boundary ∂D_E. Systems are known for which there are infinitely many such cycles.

VI. SPACES WITH THE JACOBI METRIC AS DIFFERENTIAL SPACES

The existence of a singular boundary in the Maupertuis image of dynamics creates serious problems with using standard analysis on smooth manifolds. In the present section, we show that the problem can be dealt with in the framework of the theory of the so-called differential spaces. The differential space concept generalizes the concept of smooth manifold to such an extent that every subset of $\mathbf{R}^n$ is a differential space (d-space, for short).[6] We shall need only especially nice (and easy workable) subclass of d-spaces, namely the d-spaces of constant differential dimension. These d-spaces are similar to smooth manifolds: local calculations are the same as on manifolds; in particular, tensors can be dealt with locally and globally as on manifolds; the majority of objects (e.g., external forms) behave in the natural way.

As is well known, a smooth manifold can be defined as a pair $(M,\mathscr{C})$ where $\mathscr{C}=C^\infty(M)$ is a family of smooth real functions on a set M satisfying the following axioms: (i) $\mathscr{C}$ is closed with respect to localization, (ii) $\mathscr{C}$ is closed with respect to composition with the set $C^\infty(\mathbf{R})^n$ of all smooth functions on $\mathbf{R}^n$, i.e., for any $n\in\mathbf{N}$, and $\omega\in C^\infty(\mathbf{R})^n$, $f_1,\ldots,f_n\in\mathscr{C}$ implies that $\omega\circ(f_1,\ldots,l_n)\in\mathscr{C}$, (iii) M is locally diffeomorphic to $\mathbf{R}^n$. One considers the weakest topology on M in which the functions of $\mathscr{C}$ are continuous. Axiom (i) requires the following concept. A function defined on $U\subset M$ is said to be a *local* $\mathscr{C}$-function if for every $p\in U$ there is a neighbourhood V of p (in the topology on U induced from that on M) and a function $g\in\mathscr{C}$ such that $f|V=g|V$. The set of all local $\mathscr{C}$-functions is denoted by $\mathscr{C}_U$. One has $\mathscr{C}|U\subset\mathscr{C}_U$, and consequently $\mathscr{C}\subset\mathscr{C}_M$. If $\mathscr{C}=\mathscr{C}_M$, the family $\mathscr{C}$ is said to be *closed with respect to localization.* If we drop axiom (iii) we obtain the definition of a differential space. $\mathscr{C}$ is called a differential structure and M its *support.*

Most of calculation tools for d-spaces is developed in terms of tangent vectors. A tangent vector to a d-space $(M,\mathscr{C})$ at $p\in M$ is a linear mapping $v:\mathscr{C}\to\mathbf{R}$ satisfying the Leibniz rule. The set of all tangent vectors at $p\in M$ is the *tangent space* $T_p(M,\mathscr{C})$ to a d-space $(M,\mathscr{C})$ at $p\in M$.

A d-space $(M,\mathscr{C})$ is said to be of *constant differential dimension n* if, for every $p\in M$, there exist an open neighbourhood W in the topology of M and a smooth manifold $\tilde{M}$ of the minimal dimension n such that $C^\infty(M)_W=C_W$, $W\subset\tilde{M}$, where $C=(C^\infty(\mathbf{R}_n))_M$ is the differential structure on M.

First we shall prove (1) that the region admissible for motion of any classical or non-classical system is a d-space of constant differential dimension; (2) that singularities of trajectories of

classical or non-classical systems are not malicious in the sense that the set of point-instances at which a particle is at the boundary consists of isolated points (it contains no interval).

(1) follows from the following:

Lemma 1: If $M\subset\mathbf{R}^n$ *satisfies the condition* $\overline{\mathrm{Int}M}=M$, *then* $\dim T_pM=n$ *for any* $p\in M$.

Proof. Let $p\in \mathrm{Int}M$. Since $\mathrm{Int}M$ is open in $\mathbf{R}^n$, $\dim T_pM=n$. Now, let $p\in M\backslash \mathrm{Int}M$, i.e., p is an accumulation point of M. Let $\tilde{M}$ be a smooth manifold of the minimal dimension k such that there exists an open neighbourhood W of p and $W\subset\tilde{M}$, $C^\infty(\tilde{M})_W=C_W$. Since p is an accumulation point of M, $W\cap\mathrm{Int}M$ is a non-empty open subset of $\mathbf{R}^n$. It follows that $\tilde{M}$ contains an open subset of $\mathbf{R}^n$, $\dim\tilde{M}=k\geqslant n$. We know, however, that $k\leqslant n$, since $\tilde{M}\subset\mathbf{R}^n$. □

Since $\overline{\mathrm{Int}\Omega}=\Omega$, statement (1) follows.

To prove (2) let us notice that in the classical case trajectories do not go ''physically'' through the boundary ∂D. Let $c:[-\varepsilon,\varepsilon]\to\mathbf{R}^n$ be a curve passing through ∂D. For non-classical systems, the geodesic equation $\hat{\nabla}_{C'(s)}C'(s)=0$ can be written on the entire $\mathbf{R}^n$. The only problem is what happens at the boundary. Let us define the set of parameters for which the trajectory remains at the boundary (where the metric is degenerate) by $c^{\#}=\{s:c(s)\in\partial D\}$. Two cases should be considered: (a) $c^{\#}$ consists of isolated points, (b) $c^{\#}$ contains an interval of parameters.

In case (a), the trajectory is uniquely defined by the geodesic equation on the set $D_T\cup D_S$ and can be uniquely prolonged to ∂D. Since $[-\varepsilon,\varepsilon]\backslash c^{\#}$ is dense in $[-\varepsilon,\varepsilon]$, this follows from continuity (moreover c is a smooth geodesic in the sense of the d-space theory).

Case (b) implies that the tangent vector to the geodesic has a component which is tangent to ∂D along a certain interval. In the case of classical systems it is impossible since the velocity $\|u\|$ at the boundary is zero. In the non-classical case, trajectories go through the boundary transversally changing the sector of the cone. (Let us notice that if a trajectory remained in ∂D, for a certain time interval, the motion would not be determined.)

The singularity problem for non-classical systems is not dangerous since trajectories can be suitably prolonged through the boundary (and made smooth in the sense of d-space theory), and the motion can occur in the entire $\mathbf{R}^n$. For classical systems singularities, if they exist, are physical, and the motion can take place only in a region of $\mathbf{R}^n$ limited by the surface of the zero velocity.

VII. EQUIVALENCE OF LAGRANGE AND HAMILTON FORMULATION OF MECHANICS

In the present section, we shall show, by using methods of differential spaces, that for both classical and non-classical simple mechanical systems the Lagrange formulation of mechanics is equivalent to the Hamilton formulation of mechanics. This fact gives a solid base to the Maupertuis principle as it was presented in the preceding sections. Let us begin with simple classical mechanical systems.

Let M be a differential space of class $\mathscr{D}_0$, and $L:TM\to\mathbf{R}$ a smooth Lagrange function. We define a fibre derivative $\mathscr{L}:TM\to T^*M$, where T^*M is the space of covectors, by

$$\langle\mathscr{L}(u),v\rangle=\left.\frac{d}{dt}\right|_{t=0}(t\mapsto L(u+tv))$$

for $u,v\in TM$ such that $\pi(u)=\pi(v)$, where $\pi:TM\to M$ is the canonical projection of the tangent bundle. In the literature, fibre derivative is known as Legendre transformation (see, for instance, Ref. 15). In the case of simple classical mechanical systems, Lagrange function L is said to be hyperregular if $\mathscr{L}$ is a global diffeomorphism. It is evident that in such a case the Lagrange formulation of mechanics is equivalent to that of Hamilton. A mechanical system $(\mathscr{M},K,V)$ with the Lagrange function $L=K-V\circ\pi$ is an example of a mechanical system with the hyperregular Lagrange function. We shall show even more, namely that a simple classical mechanical system

with a Jacobi metric on its configuration space with boundary is a mechanical system the Lagrange function of which is hyperregular (provided that tangent and cotangent spaces are suitably chosen).

Let, as before, $\bar{M}_E=\{x \in M: V(x)\leqslant E\}$ be the admissible configuration space with the Jacobi metric g_E such that $g_E|\partial M_E=0$. Let us consider the Lagrange function of g_E, $L_E: T\bar{M}_E\to\mathbf{R}$, given by $L_E(v)=\frac{1}{2}g_E(v,v)$. Physically, it describes the motion of a free particle on the space with boundary carrying the Jacobi metric.

Now, we introduce (after Spallek[16]) the concept of locally integrable vector field. A vector field $X \in \mathscr{X}(\bar{M}_E)$ is said to be locally integrable if, for any point $p \in \bar{M}_E$, there locally exists an integral curve of X. For smooth manifolds every smooth vector field is locally integrable. However, for spaces with singularities this need not be the case. Spallek[16] has demonstrated that, in the case of a differential space of constant dimension having the form $M_E \cup \partial M_E$, locally integrable vector fields are tangent to the boundary ∂M_E.

Following Spallek's suggestion[17] that to every problem on spaces with singularities one should choose a suitable concept of tangent space (and that of differentiation), we shall consider the submodule $\tilde{\mathscr{X}}^i(\bar{M}_E)\subset\mathscr{X}^i(\bar{M}_E)$ of locally integrable vector fields on $\bar{M}_E$ which vanish at the boundary $\partial\bar{M}_E$. Let us notice that the fields $\tilde{\mathscr{X}}^i(M_E)$ have a physical meaning. With this choice we are able to prove the following theorem

Theorem 5: *Legendre transformation* $\mathscr{L}: T^i\bar{M}_E\to T^{*i}\bar{M}_E$, *where* $T^i\bar{M}_E=\{v \in T\bar{M}_E: \exists X \in \tilde{\mathscr{X}}^i(\bar{M}_E), X(\pi(v))=v\}$ *and* $T^{*i}\bar{M}_E=\mathscr{L}(T^i\bar{M}_E)$ *is a cotangent space with the natural differential structure induced by* $\mathscr{L}$, *is a global diffeomorphism.*

Proof: It can be easily seen that $T^i_p\bar{M}_E=\{0\}$ for any $p \in \partial M_E$. Of course, $\mathscr{L}$ is a global diffeomorphism over M_E which implies that it is an isomorphism on fibres. Over boundary points the zero fibre is transformed into the zero fibre (the zero vector into the zero vector) which ends the proof. □

The equivalence of the Lagrange and Hamilton formulations of mechanics following from the hyperregularity of the Lagrange function is a strong conclusion which removes all objections against the Maupertuis principle.[18]

In particular, it is clear that the existence of the boundary ∂M_E does not violate the precise formulation of the Maupertuis principle. To see what exactly happens on the boundary let us consider a more general situation of a configuration space M with singularities (which can be organized into a kind of boundary) such that there exist a differentiable manifold $\tilde{M}$ and a surjection $\tilde{\pi}:\tilde{M}\to M$ with the property that, for regular (non-singular) points of M, $\tilde{\pi}$ is a covering. Any Lagrange function $L: TM\to\mathbf{R}$ determines a Lagrange function $\tilde{L}=L\circ\tilde{\pi}$ on the tangent bundle $T\tilde{M}$. Projections of the tangent vector fields to $\tilde{M}$ which are compatible with the mapping $\tilde{\pi}$ (i.e., such that for any $p,q \in \tilde{M}, \tilde{\pi}(p)=\tilde{\pi}(q)$ implies $\tilde{\pi}_*(X(p))=\tilde{\pi}_*(X(q)), X \in \mathscr{X}(\bar{M})$) are vector fields locally integrable on M. The Lagrange formalism on M is fully determined by the Lagrange formalism on $\tilde{M}$ (with the Lagrangian $\tilde{L}$). This implies that the singularities in the configuration space M are fully analyzable. As a simple example one could consider the configuration space $M\backslash\partial M_E$ of a harmonic oscillator, where $M\backslash\partial M_E$ is an interval (without the endpoints) which could be covered by a circle $\tilde{M}$ with the natural projection $\tilde{\pi}:\tilde{M}\to M$.

Now, let us consider a non-classical simple mechanical system (M,K,V). Let $g_E=2|E-V|$ be the Jacobi metric with g being the Lorentz metric $K(v)=\frac{1}{2}g(v,v)$. The Jacobi metric g_E is degenerate on the set $\Xi=\{x: V(x)=E\}$, $\Xi\subset M$, which is a boundary set.

Larsen[19] has investigated the behaviour of geodesics on spaces with degenerate semi-Riemannian metrics. His theorem 4.1 concerns geodesics of a conformally singular metric (with a smooth conformal factor). He shows that there exists a geodesic passing through the boundary set Ξ with the zero velocity in a locally unique way, i.e., if γ_1 and γ_2 are geodesics such that $\mathrm{dom}\gamma_1=\mathrm{dom}\gamma_2 \neq \varnothing$, then there exists an interval $[-t,t]$ such that $\gamma_1[-t,t]=\gamma_2[-t,t]$. By applying methods of differential spaces to the case with a non-continuous conformal factor in the

metric and by adapting Larsen's theorem to our case, one can easily see the existence and the local uniqueness of a piecewise smooth geodesic passing through the boundary set Ξ. (Details of all constructions sketched in the present section will be published in a forthcoming paper.)

Now, we shall describe the local behaviour of geodesics (of the metric g_E) in a neighbourhood of the boundary set Ξ for points $p \in M$ at which $(dV)(p) \neq 0$. There exist a neighbourhood U of p such that $\Xi \cap U$ is a hypersurface in U, and a map x (with a suitably shrinked domain D_x) such that $\Xi \cap D_x$ is a subset of the surface of the coordinate system axes, with respect to which D_x is symmetric. Therefore, we have reduced the considered case to a smooth manifold symmetric with respect to the boundary set Ξ on which the Jacobi metric vanishes.

Let $\mathbf{Z}_2$ be an Abelian group acting as a reflexion group on this manifold with respect to Ξ. A quotient half-space $\mathbf{R}^n/\mathbf{Z}_2$ is a manifold with boundary (symmetric points are identified). On $\mathbf{R}^n/\mathbf{Z}_2$ the Jacobi metric $g_E^+ = 2(E-V)g$ is defined. A similar theorem as for simple classical mechanical systems can be proved.

Theorem 6: *The Lagrange function* $L:\tilde{T}(\mathbf{R}^n/\mathbf{Z}_2) \to \mathbf{R}$ *given by* $L(v) = \frac{1}{2} g_E^+(v,v)$ *is hyperregular.*

Therefore, the Maupertuis principle finds its strict formulation also for simple non-classical mechanical systems. Analogous theorem to the above one can also be proved for the Jacobi metric $\bar{g}_E = -2(E-V)g$. In such a case, the condition $\gamma(-t) = \gamma(t)$, found by Kozlov,[3] is valid. It is also evident that a geodesic passing through the boundary set Ξ changes the sector of the null-cone.

We should notice that the mechanics on the quotient space $\mathbf{R}^n/\mathbf{Z}_2$ is a π-invariant projection of the mechanics on $\mathbf{R}^n$, where $\pi:\mathbf{R}^n \to \mathbf{R}^n/\mathbf{Z}_2$ is the canonical projection. In a forthcoming paper we shall investigate relationships between mechanics on a (quotient) space with singularities and mechanics on the covering space.

VIII. CONCLUDING REMARKS

In the present work we focused on two problems: (1) a generalization of the Maupertuis principle to the case with the natural Lagrangian and an indefinite kinetic energy form (non-classical simple mechanical systems); (2) demonstration that the region admissible for the motion of a system with the Jacobi metric is a differential space of constant differential dimension. Owing to the last property the analysis usually carried out on smooth manifolds can be done on more general spaces including some sorts of singularities. In the framework of such spaces, the behaviour of trajectories in a close neighbourhood of singular boundaries becomes a workable problem. Differentiable space methods allowed us also to show that for both classical and non-classical simple mechanical systems the Lagrange and Hamilton formulations of mechanics are equivalent.

The theory of non-classical simple mechanical systems is still *in statu nascendi*, and the situation in this field is analogous to that which once compelled mathematicians to investigate spaces with Lorentz metrics. We hope that first steps in the correct direction have been made in the present work.

Simple non-classical mechanical systems (ZC-systems) have natural applications in cosmology and the gravity theory.[4] In such systems the indefinite character of the kinetic energy form (in the Hamiltonian formulation) is a relic of the Lorentz structure of space–time. Non-classical systems can also be applied to the investigation of deterministic chaos or, more precisely, to the investigation of separation of nearby trajectories, basing on the equation of the geodesic deviation. This is important as far as the invariant definition of deterministic chaos in gauge theories is concerned.[4,5]

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Induced matter theory and embeddings in Riemann flat space–times

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A class of five-dimensional space-times that contain four-dimensional hypersurfaces whose intrinsic metrics are of cosmological interest is investigated. First, the five-dimensional space–time is assumed to be Riemann flat—the problem of determining the intrinsic metrics of the four-dimensional hypersurfaces then becomes a problem of embedding in flat space–time. Second, the Riemann flat solutions are used as a starting point to find solutions to Einstein's vacuum field equations in five dimensions that are not Riemann flat. In particular, a new general class of five-dimensional vacuum solutions is found. © *1996 American Institute of Physics.* [S0022-2488(96)04201-8]

I. INTRODUCTION

Recently, several authors have been interested in Einstein's theory of general relativity in five dimensions[1–7] (higher-dimensional theories have also been considered[8,9]). In these studies the higher-dimensional field equations were taken to be the vacuum Einstein field equations, and the primary goal in several[1–3,6,7] of these studies was to determine whether the four-dimensional properties of matter could be interpreted as being purely geometrical in origin[10]—the embedding of the four-dimensional space–time in the vacuum five-dimensional space-time was interpreted as producing an effective four-dimensional stress–energy tensor.

Curiously, Mc Manus[7] recently observed that a class of five-dimensional vacuum (i.e., Ricci flat) solutions of Ponce de Leon[6] were, in fact, completely (Riemann) flat, that is to say that the five-dimensional Riemann tensor associated with these metrics was identically zero. Thus, one is immediately prompted to ask the following question: are any of the other known five-dimensional Ricci flat solutions also Riemann flat? Of course, it is not very instructive to just simply systematically calculate the Riemann tensor for the known five-dimensional vacuum solutions to determine if the Riemann tensor vanishes. It would be far more beneficial if we could find some general results. Consequently, we now pose the following question: what is the class of Lorentzian four-metrics that can be embedded in five-dimensional Minkowski space-time? In theory, the general solution to this problem is known.[11] For example, consider the following class of Riemann flat five-metrics:

$$ds^2=g_{\alpha\beta}(x^\gamma,y)dx^\alpha\, dx^\beta+\phi^2(x^\gamma,y)dy^2. \tag{1}$$

where the intrinsic metric, $g_{\alpha\beta}(x^\gamma,y)\big|_{y=\text{const}}$, of the four-dimensional hypersurfaces $y=$constant is Lorentzian in signature. The fact that the full five-dimensional metric is flat imposes necessary and sufficient conditions on the Riemann tensor, $R_{\alpha\beta\gamma\delta}$, of the intrinsic metric and on the extrinsic curvature, $K_{\alpha\beta}$, of the hypersurface $y=$const, namely that

$$R_{\alpha\beta\gamma\delta}=K_{\alpha\gamma}K_{\beta\delta}-K_{\alpha\delta}K_{\beta\gamma}, \tag{2}$$

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$$K_{\alpha\beta;\gamma}=K_{\alpha\gamma;\beta}, \tag{3}$$

where here ";" denotes covariant differentiation with respect to the intrinsic metric $g_{\alpha\beta}$. (In general,[11] the four-metric ${}^4ds^2=g_{\alpha\beta}(x^\gamma)dx^\alpha\,dx^\beta$ can be embedded in a five-dimensional Riemann flat space–time if and only if there exists a symmetric tensor $\Omega_{\alpha\beta}$ that satisfies ${}^4R_{\alpha\beta\gamma\delta}=2\Omega_{\alpha[\gamma}\Omega_{\delta]\beta}$ and $\Omega_{\alpha[\beta;\gamma]}=0$.) Furthermore, the extrinsic curvature of the surface $y=$const is given by

$$K_{\alpha\beta}=\frac{1}{2\phi}\frac{\partial}{\partial y}(g_{\alpha\beta}), \tag{4}$$

for the above metric. Unfortunately, the above equations are too complex for an explicit coordinate representation for the metric functions $g_{\alpha\beta}$ and ϕ to be found, in general.

In this paper, we consider the following class of metrics:

$$ds^2=-e^{2F(t,r,y)}\,dt^2+e^{2G(t,r,y)}(dr^2+r^2\,d\Omega^2)+e^{2K(t,r,y)}\,dy^2, \tag{5}$$

where $d\Omega^2\equiv d\theta^2+\sin^2(\theta)d\phi^2$. Various forms of the metric (5) have been extensively investigated in the literature[1,2,6,7]—the vacuum Einstein field equations, $R_{ij}=0$, have been solved for certain subclasses of the metric (5). Although several metrics of the form (5) have been noted to be Riemann flat,[7,13] most notably the Ponce de Leon solutions,[6] the general form of the Riemann flat solutions has not been found.

Therefore, we wish to determine all metrics of the form (5) that are Riemann flat. In other words, we want to find all solutions of the equations $R_{ijkl}=0$ where the metric is given by (5). In principle, the problem is trivial since locally all solutions are Minkowski space-time; however, one has to implement various nontrivial diffeomorphisms to get the solution into this form. However, we shall only permit diffeomorphisms of the form $x^\alpha\to\bar{x}^\alpha(x^\beta)$ and $y\to\bar{y}(y)$. Thus, by restricting the permissible diffeomorphisms we ensure that the four-dimensional intrinsic metrics $ds^2=g_{\alpha\beta}(x^\gamma,y)|_{y=\text{const}}\,dx^\alpha\,dx^\beta$ are not necessarily Riemann flat, even though the five-dimensional metrics are Riemann flat. In technical language, we confine our analysis to four-dimensional metrics of embedding class $p=1$ (see Refs. 8 and 12 for further discussions on the embedding problem).

If we calculate the extrinsic curvature, $K_{\alpha\beta}$, for the metric (5) using (4), then we find that it has the form

$$K_{\alpha\beta}=Av_\alpha v_\beta+Bg_{\alpha\beta}, \tag{6}$$

where $g_{\alpha\beta}v^\alpha v^\beta=-1$. Equation (2) can then be employed to show that the stress–energy tensor associated with the intrinsic metric $g_{\alpha\beta}$ has the form of a perfect fluid, namely $T_{\alpha\beta}=(\mu+P)v_\alpha v_\beta+Pg_{\alpha\beta}$. Now, standard results of embedding theory[12,14,15] tell us about the allowable perfect fluid solutions. In the case $\mu+P\neq0$, the solution belongs to either the class of generalized interior Schwarzschild solutions if the expansion of the fluid velocity, v_α, is zero, or the class of generalized Friedmann cosmological models if the fluid expansion is nonzero. In the case that $\mu+P=0$, the solutions are de Sitter space–times (that is, space–times of constant curvature). All of these spherically symmetric solutions are conformally flat.

The purpose of our paper is twofold; not only do we wish to find the explicit form for all the Riemann flat solutions of the form (5), but we also wish to find new Ricci flat solutions. In particular, we wish to employ our knowledge of the Riemann flat solutions as an aid to construct new Ricci flat solutions.

The paper is organized as follows: In Sec. II, we analyze the Riemann flat equations for the metric (5), and both classify and find all the five-dimensional solutions explicitly. In Sec. III, we discuss the solutions found in Sec. II, paying particular attention to their interpretation in the

context of induced matter theory. Finally, in Sec. IV, we use the Riemann flat solutions as an aid to construct some Ricci flat solutions of the metric (5) that are not Riemann flat.

II. FIELD EQUATIONS

We shall now proceed to solve the equations $R_{ijkl}=0$ for the metric (5). However, we will restrict the allowable diffeomorphisms to diffeomorphisms of the form $x^{\alpha}\rightarrow\bar{x}^{\alpha}(x^{\beta})$, $y\rightarrow\bar{y}(y)$. We start our analysis by noting that the pivotal equations are $R^{\theta}{}_{tr\theta}=0$ and $R^{\theta}{}_{ry\theta}=0$, which yield

$$G_{rt}=G_tF_r\,. \tag{7}$$

$$G_{ry}=G_yK_r\,, \tag{8}$$

respectively. (The complete set of the components of the Riemann tensor are listed in the Appendix.) Thus, we immediately observe that we can divide the solutions into four classes: (1) $G=G(r)$; (2) $G=G(r,y)$ with $G_y\neq0$ and $\exp(K)=G_y/\alpha$; (3) $G=G(r,t)$ with $G_t\neq0$ and $\exp(F)=G_t/\beta$; and (4) $G=G(t,r,y)$ with $G_tG_y\neq0$, and $\exp(K)=G_y/\alpha$ and $\exp(F)=G_t/\beta$, where both α and β are nonzero functions of t and y only.

A. $G=G(r)$

The equation $R^{\theta}{}_{rr\theta}=0$ yields the differential equation

$$rG_{rr}+G_r=0, \tag{9}$$

which can easily be solved to get

$$G=c_1\,\ln(r)+c_2\,, \tag{10}$$

where c_1 and c_2 are arbitrary constants. The field equation $R^{\phi}{}_{\theta\theta\phi}=0$ now reduces to

$$c_1(c_2+2)=0. \tag{11}$$

We can take $c_1=c_2=0$ without loss of generality. (The solutions $c_1=0$ and $c_2=-2$ are related by the transformation $r\rightarrow1/r$.) Equations $R^{\theta}{}_{tt\theta}=0$ and $R^{\theta}{}_{yy\theta}=0$ imply that the functions F and K are both independent of the variable r. Thus, the metric may be written as

$$ds^2=-A^2(t,y)dt^2+dr^2+r^2\,d\Omega^2+B^2(t,y)dy^2, \tag{12}$$

where the metric functions A and B must satisfy the following equation:

$$\frac{\partial}{\partial y}\left(\frac{1}{B}\frac{\partial A}{\partial y}\right)=\frac{\partial}{\partial t}\left(\frac{1}{A}\frac{\partial B}{\partial t}\right). \tag{13}$$

Equation (13) follows directly from the equation $R^{t}{}_{yty}=0$. (The remaining equations $R^{i}{}_{jkl}=0$ are trivially satisfied.)

B. $G_t=0$, $G_y\neq0$

For this class of solutions, we have that the metric function K satisfies

$$e^K=G_y/\alpha(t,y), \tag{14}$$

where $\alpha\neq0$. The equation $R^{r}{}_{tyr}=0$ implies that $\alpha=(y)$. The equation $R^{\theta}{}_{rr\theta}=0$ then yields the following differential equation for G:

$$G_{rr}+\frac{1}{r}\,G_r+\alpha^2 e^{2G}=0, \tag{15}$$

which can easily be solved to obtain the solution

$$G=\frac{1}{2}\ln\left[\frac{a^2 b}{\alpha^2}\,\frac{r^{a-2}}{(1+br^c)^2}\right], \tag{16}$$

where a and b are arbitrary functions of y only. Furthermore, the equation $R^{\phi}{}_{\theta\theta\phi}=0$ reduces to

$$G_r^2+\frac{2}{r}\,G_r+\alpha^2 e^{2G}=0. \tag{17}$$

Inserting the solution (16) for G into (17) implies that $a^2=4$ (we can take $a=2$ without loss of generality). Thus, the solution for G is

$$G=\frac{1}{2}\ln\left[\frac{4b(y)}{\alpha^2(y)}\,\frac{1}{(1+b(y)r^2)^2}\right]. \tag{18}$$

Note that we can write the solution for G in the above form, since the equation $R^{\theta}{}_{rr\theta}=0$ implies that $G_r\neq 0$ if $G_t=0$ and $G_y\neq 0$.

For simplicity, we introduce the function A defined by

$$A=e^F. \tag{19}$$

The equations $R^{t}{}_{rtr}=0$ and $R^{\theta}{}_{tt\theta}=0$ now reduce to

$$\frac{1}{\alpha^2}\,G_y(A_{rr}-G_rA_r)+A_y e^{2G}=0. \tag{20}$$

$$\frac{1}{\alpha^2}\,G_y\left(G_r+\frac{1}{r}\right)A_r+A_y e^{2G}=0. \tag{21}$$

respectively. Subtracting (21) from (20) yields

$$A_{rr}-2A_rG_r-\frac{1}{r}\,A_r=0, \tag{22}$$

which can be integrated to obtain

$$A_r=re^{2G}l(t,y), \tag{23}$$

where $l(t,y)$ is an arbitrary function. Furthermore, Eq. (21) implies that

$$A_y=-\frac{l}{\alpha^2}\,G_y(1+rG_r). \tag{24}$$

With the aid of Eq. (18), Eq. (23) can now be integrated to yield

$$A=-\frac{2l}{\alpha^2}\,\frac{1}{1+br^2}+m(t,y). \tag{25}$$

where $m(t,y)$ is an arbitrary function. In addition, the equation $R^{t}{}_{rty}=0$ reduces to

$$G_r A_{ry} - G_y^2 A_r - A_y G_{ry} = 0, \tag{26}$$

which can be integrated to obtain

$$\frac{A_y}{G_y} = A + n(t,y), \tag{27}$$

where $n(t,y)$ is an arbitrary function. If we divide Eq. (24) by G_y and compare the result to (27), then we find that A must be of the form

$$A = -\frac{l}{\alpha^2}\frac{1-br^2}{1+br^2} - n. \tag{28}$$

If we combine Eqs. (25) and (28), then we obtain that the function A may be written as

$$A = \frac{p(t,y) + b(y)q(t,y)r^2}{1+b(y)r^2}. \tag{29}$$

where $p = n - l/\alpha^2$ and $q = n + l/\alpha^2$. In addition, the above solution must also satisfy Eq. (24). Inserting the above solution into Eq. (24), we find that Eq. (24) becomes a power series in r. Thus, equating the various coefficients of r to zero, we find the following equations:

$$(p-q)\left(\frac{b_y}{b} - 2\frac{\alpha_y}{\alpha}\right) = 4p_y, \tag{30}$$

$$(p-q)b_y = 2(q_y + p_y), \tag{31}$$

$$(p-q)\left(\frac{b_y}{b} + 2\frac{\alpha_y}{\alpha}\right) = 4q_y. \tag{32}$$

Equation (31) is redundant since it can be obtained by adding Eqs. (30) and (32) together. Subtracting Eq. (32) from Eq. (30), we find that

$$2(p_y - q_y) + (p-q)\frac{\alpha_y}{\alpha} = 0, \tag{33}$$

which can be integrated to yield the solutions

$$p = u(t)\left[\frac{2}{\alpha} + \int \frac{dy}{\alpha}\frac{b_y}{b}\right] + v(t), \tag{34}$$

$$q = u(t)\left[-\frac{2}{\alpha} + \int \frac{dy}{\alpha}\frac{b_y}{b}\right] + v(t), \tag{35}$$

where u and v are arbitrary functions. The remaining equations $R^i{}_{jkl} = 0$ are trivially satisfied.

Thus, if we make the coordinate transformation $Y = \frac{1}{2}\ln b(y)$ and introduce the function $a = -\ln \alpha$, then the metric can be written as

$$ds^2 = -A^2\, dt^2 + \frac{4e^{2(a+Y)}}{(1+e^{2Y}r^2)^2}(dr^2 + r^2\, d\Omega^2) + \frac{e^{2a}}{(1+e^{2Y}r^2)^2}[(a_Y+1) + (a_Y-1)e^{2Y}r^2]^2\, dY^2, \tag{36}$$

where $a=a(Y)$ is an arbitrary function and A can be set to

$$A=\begin{cases} 1 \quad [\text{if } u(t)=0], \\ v(t)+2e^{2a}\dfrac{1-e^{2Y}r^2}{1+e^{2Y}r^2}+2\displaystyle\int e^a\,dY \quad [\text{if } u(t)\neq 0], \end{cases} \tag{37}$$

where $v(t)$ is an arbitrary function.

C. $G_y=0$, $G_t\neq 0$

This class is very similar to the previous class. Thus, we forgo writing down the steps of the calculation since they are, in essence, the same as those employed in the derivation of the class (2) solutions. We merely quote the results: there exist coordinates such that the class (3) solutions may be written as

$$ds^2=-\frac{e^{2a}}{(1-e^{2T}r^2)^2}\left[(a_T+1)-(a_T-1)e^{2T}r^2\right]^2\,dT^2+\frac{4e^{2(a+T)}}{(1-e^{2T}r^2)^2}\,(dr^2+r^2\,d\Omega^2)+B^2\,dy^2, \tag{38}$$

where $a=a(T)$ is an arbitrary function and B can be set equal to

$$B=\begin{cases} 1 \quad (\text{if } B_r=0), \\ v(y)+2e^{2a}\dfrac{1+e^{2T}r^2}{1-e^{2T}r^2}+2\displaystyle\int e^a\,dT \quad (\text{if } B_r\neq 0), \end{cases} \tag{39}$$

where $v(y)$ is an arbitrary function.

D. $G_tG_y\neq 0$

In this case, the functions F and K satisfy the relationships

$$e^K=G_y/\alpha(t,y), \tag{40}$$

$$e^F=G_t/\beta(t,y). \tag{41}$$

Now, the equations $R^{\theta}{}_{rr\theta}=0$ and $R^{\phi}{}_{\theta\theta\phi}=0$ yield

$$G_{rr}+\frac{1}{r}\,G_r+ae^{2G}=0, \tag{42}$$

$$G_r^2+\frac{2}{r}\,G_r+ae^{2G}=0, \tag{43}$$

respectively, where

$$a\equiv\alpha^2-\beta^2. \tag{44}$$

The above equations can be solved to obtain the solution

$$G=\frac{1}{2}\ln\left[\frac{4b^2}{(a+b^2r^2)^2}\right], \tag{45}$$

where $b=b(t,y)$ is an arbitrary function. Furthermore, the equation $R^t{}_{rty}=0$ reduces to

$$G_{yt}=G_tG_y+\frac{\alpha_y}{\alpha}\,G_t+\frac{\beta_t}{\beta}\,G_y\,. \tag{46}$$

Using the solution (45), we can expand the above equation in a power series in r. We find that the following two equations must be satisfied:

$$b_{ty}=(\partial_t \ln \beta)b_y+(\partial_y \ln \alpha)b_t\,, \tag{47}$$

$$\partial_t\left(\frac{\alpha_y}{\beta}\right)+\frac{1}{\beta}\left[\alpha(\partial_t \ln b)(\partial_y \ln b)-\alpha_y\partial_t \ln b-\alpha_t\partial_y \ln b\right]$$

$$=\partial_y\left(\frac{\beta_t}{\alpha}\right)+\frac{1}{\alpha}\left[\beta(\partial_t \ln b)(\partial_y \ln b)-\beta_y\partial_t \ln b-\beta_t\partial_y \ln b\right]. \tag{48}$$

(Actually, there is a third equation, but it is automatically satisfied on account of the first two equations.)

The remaining equations $R^i{}_{jkl}=0$ can all be shown to be trivially satisfied. First, using Eq. (46) we find that the equation $R^t{}_{rtr}=0$ can be written as

$$\frac{\partial}{\partial r}\left[2G_{rr}-G_r^2+ae^{2G}\right]=0, \tag{49}$$

which is trivially satisfied due to (45). Similarly, the equation $R^r{}_{yyr}=0$ reduces to

$$\frac{\partial}{\partial y}\left[2G_{rr}-G_r^2+ae^{2G}\right]=0. \tag{50}$$

Both the equations $R^t{}_{rty}=0$ and $R^y{}_{try}=0$ reduce to

$$\frac{\partial}{\partial r}\left[G_{yt}-G_tG_y-\frac{\alpha_y}{\alpha}\,G_t-\frac{\beta_t}{\beta}\,G_y\right]=0 \tag{51}$$

which is trivially satisfied because of Eq. (46). Furthermore, using Eq. (46), the equations $R^\theta{}_{tt\theta}=0$ and $R^y{}_{\theta\theta y}=0$ can be shown to reduce to

$$rG_{rtr}=G_{rt}(1+2rG_r), \tag{52}$$

$$rG_{ryr}=G_{ry}(1+2rG_r), \tag{53}$$

respectively, which again are trivially satisfied on account of Eq. (45). Finally, after a long calculation employing Eqs. (42)–(48), the equation $R^t{}_{yty}=0$ can be shown to be trivially satisfied.

In summary, the metric is given by

$$ds^2=-\left(\frac{G_t}{\beta(t,y)}\right)^2 dt^2+e^{2G}(dr^2+r^2\,d\Omega^2)+\left(\frac{G_y}{\alpha(t,y)}\right)^2 dy^2, \tag{54}$$

where

$$e^{2G}\equiv\frac{4b(t,y)^2}{(\alpha^2-\beta^2+b(t,y)^2r^2)^2}, \tag{55}$$

and α, β and b satisfy (47)–(48).

III. DISCUSSION

We should, of course, determine where the known Riemann flat solutions of the form (5) fit into the above classification scheme. As was noted by Mc Manus,[7] the following three Ponce de Leon metrics[6] are all Riemann flat:

$$ds^2=-y^2\ dt^2+t^{2/\gamma}y^{2/(1-\gamma)}[dr^2+r^2\ d\Omega^2]+\left(\frac{\gamma}{\gamma-1}\right)^2 t^2\ dy^2, \tag{56}$$

$$ds^2=-y^2\ dt^2+y^2e^{2t}[dr^2+r^2\ d\Omega^2]+dy^2, \tag{57}$$

$$ds^2=-dt^2+t^2e^{2y}[dr^2+r^2\ d\Omega^2]+t^2\ dy^2, \tag{58}$$

where $\gamma(\neq 0,1)$ is an arbitrary constant. Clearly, all the above metrics belong to class (4), since $G=G(t,y)$ with $G_tG_y\neq 0$. In particular, the above solutions belong to the special case $a=0$ [that is, $\alpha=\beta$—see Eqs. (40)–(42)]. However, the solution (43) appears to depend on r; this dependency can be removed by the coordinate transformation $r\rightarrow\bar{r}=2/r$. Also note that in this special case Eq. (46) is automatically satisfied. Class (4) solutions with $\alpha\neq\beta$ are known to exist. For instance, the metric

$$ds^2=-dt^2+\frac{1}{4}\ t^2(e^y-\kappa e^{-y})^2\ \frac{dr^2+r^2\ d\Omega^2}{[1+(\kappa/4)r^2]^2}+t^2\ dy^2, \tag{59}$$

given in Ref. 7, is Riemann flat for all values of the constant κ.

In addition, we recall that metrics of the form (5) were originally investigated in the context of induced matter theory.[2] In induced matter theory, the field equations are usually taken to be the the vacuum Einstein field equations in $4+n$-dimensional space–time.[1–3] However, for our analysis we wish to examine the consequences of taking the field equations to be the five-dimensional Riemann flat equations. (Of course, we are immediately neglecting a whole variety of well-known solutions of Einstein's field equations, most notably the Schwarzschild solution that can, at best, be embedded in six-dimensional Minkowski space-time.) Matter is introduced into the theory by considering the embedding of the physical four-dimensional space–time in the full five-dimensional space–time. Basically, the physically relevant metric is taken to be the intrinsic metric on the four-dimensional slices $y=$const.

The class (1) and (3) solutions, namely (12) and (37)–(38), induce Riemann flat four-metrics on the slices $y=$const, and are thus physically uninteresting within the context of induced matter theory. The class (2) solutions induce conformally flat four-metrics. The class (2) solutions with $A=1$ [see Eqs. (36)–(37)] represent static Friedman–Robertson–Walker metrics, such that the three-space $t=$const has positive constant curvature. The class (2) solutions with $A\neq 1$ can be interpreted as perfect fluid models with constant density,

$$\mu=\frac{3}{e^{2a}}, \tag{60}$$

and non-constant pressure,

$$P=-\frac{1}{e^{2a}}-\frac{4}{e^{2a}}\left[2+e^{-2a}V(t)\ \frac{1+e^{2y}r^2}{1-e^{2y}r^2}\right]^{-1}, \tag{61}$$

where $V(t)\equiv v(t)+2\int^t \exp[a(y)]dy$. The intrinsic metric of these class (2) solutions (on the hypersurface $Y=$const),

$$ds^2=-\left\{v(t)+2e^{2a}\,\frac{1-e^{2Y}r^2}{1+e^{2Y}r^2}+2\int e^a\,dY\right\}^2 dt^2+\frac{4e^{2(a+Y)}}{(1+e^{2Y}r^2)^2}\,(dr^2+r^2\,d\Omega^2). \tag{62}$$

belongs to the class of generalized interior Schwarzschild solutions.[12,14] The diffeomorphism (with $Y=\text{const}$),

$$R=\frac{2e^{2a}e^Y}{1+e^{2Y}r^2}, \tag{63}$$

reduces the above metric to the standard form,

$$ds^2=-\{v(t)+\sqrt{1-C^2R^2}\}^2\,dt^2+\frac{dR^2}{1-C^2R^2}+R^2\,d\Omega^2, \tag{64}$$

where $C(=\exp[-a(Y)]_{Y=\text{const}})$ is an arbitrary constant. We note that a specific embedding for the interior Schwarzschild solution, $v(t)=\text{const}$, into a six-dimensional Riemann flat solution is known (see Ref. 16). However, to our knowledge, the metric (36) with $A\neq 1$ [see (37)] is the first time that an explicit embedding for the interior Schwarzschild solution into five-dimensional Riemann flat space–time has appeared in the literature.

The class (4) solutions also induce conformally flat four-metrics, and can be interpreted as perfect fluid models whose associated density and pressure are

$$\mu=3\alpha^2, \tag{65}$$

$$P=-3\alpha^2+2\alpha\alpha_t\{\partial_t\,\ln[b^{-1}(\alpha^2-\beta^2+b^2r^2)]\}^{-1}. \tag{66}$$

These solutions belong to the class of generalized Friedmann solutions.[14]

It is clear from (2) that there exist algebraic relationships between $K_{\alpha\beta}$ ($\Omega_{\alpha\beta}$), $R_{\alpha\beta}$ (and hence $T_{\alpha\beta}$), and the Weyl tensor $C_{\alpha\beta\gamma\delta}$. *All the Riemann flat solutions* [classes (1)–(4)] *induce four-metrics that are conformally flat*. Indeed, all the perfect fluid solutions of embedding class one must necessarily be either of Petrov type O (conformally flat) or of Petrov type D.[12] Curiously, results about the embedding of conformally flat four-dimensional metrics into Riemannian flat five-dimensional Lorentzian space-time do not seem to appear in the literature. Results about the embedding of conformally flat four-dimensional metrics into Riemannian flat five-dimensional Euclidean space–times (positive definite metrics) are known (see Refs. 17 and 18). For completeness, we now state the following theorem without proof: If a four-dimensional conformally flat Lorentzian metric is of embedding class one, then its Riemann tensor is given by $R_{\alpha\beta\gamma\delta}=2\Omega_{\alpha[\gamma}\Omega_{\delta]\beta}$, where $\Omega_{\alpha[\beta;\gamma]}=0$, and furthermore Ω must be of the form

$$\Omega_{\alpha\beta}=An_\alpha n_\beta+Bg_{\alpha\beta}, \tag{67}$$

where n_α is a unit space-like or time-like vector (that is, $n_\alpha n^\alpha=\pm 1$).

IV. RICCI FLAT SOLUTIONS

All the solutions discussed in Secs. II and III are Riemann flat and thus are also automatically Ricci flat. To date, the majority of the known Ricci flat solutions where the metric has the form (5) have been found by examining the special ansatz that the metric functions are separable in the variables t, r, and y. In this section, our aim is to find a class of Ricci flat solutions that contain a subclass of the Riemann flat solutions. Thus, we use the Riemann flat solutions of the previous sections as a springboard to construct new Ricci flat solutions.

We base our first ansatz on the form of the class (2) solutions [we chose the class (2) solutions because (i) they are not as complicated as the class (4) solutions; and (ii) the class (1) and (3) solutions have an uninteresting interpretation in terms of induced matter theory]. Hence, we consider metrics of the following form:

$$e^F=\frac{A(t,y)+B(t,y)r^2}{\alpha(y)+b^2(y)r^2}, \tag{68}$$

$$e^G=\frac{2b(y)+C(y)r^2}{\alpha(y)+b^2(y)r^2}, \tag{69}$$

$$e^K=\frac{D(y)+E(y)r^2}{\alpha(y)+b^2(y)r^2}. \tag{70}$$

Thus, the field equations $R_{ij}=0$ will all reduce to power series in r. The coefficients of each of the power series will, in general, be partial differential equations in t and y only and they must be identically zero. After a lengthy calculation (see Ref. 19 for full details), we find the following equation:

$$C_y=C\,\frac{b_y}{b}. \tag{71}$$

Thus, we find that either (i) $C=0$ or (ii) $C=\pm b\neq 0$. In case (i), the solutions can eventually be shown to reduce to the Riemann flat class (2) solutions. In case (ii), the metric can be shown to be equivalent to

$$ds^2=-y^{-1}\,dt^2+y(dr^2+r^2\,d\Omega^2)+dy^2. \tag{72}$$

The above metric was discussed in Ref. 7 and belongs to the class of generalized Kasner metrics.[9,20,21]

In the process of determining the Riemann flat solutions and the above solutions, we observed that if the metric functions F, G, and K appearing in (5) had a particular form, then some of the Ricci flat field equations could be easily integrated. Thus, based upon our observations, we are led to our second ansatz; we shall now consider metrics of the following form:

$$ds^2=-e^{F(t,r,y)}\,dt^2+e^{2G(r)}[dr^2+r^2\,d\Omega^2]+e^{2K(r,y)}\,dy^2. \tag{73}$$

This ansatz includes both the class (1) Riemann flat solutions and the Davidson–Owen–Gross–Perry solutions.[4,5]

The field equation $R_{\theta\theta}=0$ for metric (73) implies that $(G_r+1/r)F_{tr}=0$. Thus, either (i) $G_r=-1/r$ or (ii) $F_{tr}=0$.

In case (i) we can set $G=0$ without loss of generality by an appropriate diffeomorphism. The field equations $R_{rr}=0$ and $R_{\theta\theta}=0$ can then be employed to show that $F_r=0=K_r$. The remaining field equations can then be used to show that the metric reduces to the class (1) Riemann flat solutions, (12)–(13), with $B=1$.

In case (ii) we find that $F=A(t,y)+B(r,y)$. The equation $R_{\theta\theta}=0$ then yields the additional result $(B+K)_{ry}=0$, and thus $K=-B(r,y)+C(r)$. Furthermore, the equation $R_{rr}=0$ yields $B_{ry}(2B_r-C_r)=0$, which implies that $K=K(r)$ and $F=A(t,y)+B(r)$. Finally, the equation $R_{ry}=0$ implies that $A_y(B_r-K_r)=0$. Thus, either (a) $A_y=0$ or (b) $B_r=K_r$. In case (a), we can take $A=1$ without loss of generality, and the metric then reduces to the Davidson–Owen–Gross–Perry class of soliton solutions,[4,5] namely,

$$ds^2=-\left(\frac{ar-1}{ar+1}\right)^{2\epsilon k}dt^2+\left(\frac{a^2r^2-1}{a^2r^2}\right)^2\left(\frac{ar+1}{ar-1}\right)^{2\epsilon(k-1)}[dr^2+r^2\,d\Omega^2]+\left(\frac{ar+1}{ar-1}\right)^{2\epsilon}dy^2, \tag{74}$$

where ϵ and k are subject to the constraint $\epsilon^2(k^2-k+1)=1$.

In case (b), the general form of the metric may be written as

$$ds^2=-A^2(t,y)e^{2K(r)}\,dt^2+e^{2G(r)}[dr^2+r^2\,d\Omega^2]+e^{2K(r)}\,dy^2. \tag{75}$$

The field equation $R_{tt}=0$ can be employed to show that

$$A_{yy}=\kappa A \tag{76}$$

and

$$e^{2K}[K_{rr}+2K_r^2+K_rG_r+(2/r)K_r]+\kappa e^{2G}=0, \tag{77}$$

where κ is a constant (κ can always be chosen to be equal to either 0 or ±1). Finally, the equations $R_{rr}=0$ and $R_{\theta\theta}=0$ yield

$$K_{rr}+K_r^2-K_rG_r+G_{rr}+\frac{1}{r}G_r=0, \tag{78}$$

$$2K_rG_r+\frac{2}{r}K_r-G_{rr}+\frac{3}{r}G_r+G_r^2=0, \tag{79}$$

respectively. We note that the above system of equations (77)–(79) only has rank 2—Eq. (79) is a first integral of (77) and (78).

If $\kappa=0$, then the above system of equations, (77)–(79), can be solved completely to yield the solution

$$ds^2=-\left(\frac{ar+1}{ar-1}\right)^{2/\sqrt{3}}[\alpha(t)y+\beta(t)]^2\,dt^2+\left(\frac{a^2r^2-1}{a^2r^2}\right)^2\left(\frac{ar-1}{ar+1}\right)^{4/\sqrt{3}}[dr^2+r^2\,d\Omega^2]$$
$$+\left(\frac{ar+1}{ar-1}\right)^{2/\sqrt{3}}dy^2, \tag{80}$$

where a is an arbitrary constant, and α and β are arbitrary functions of t. If $\alpha=0$ then the above metric is a particular solution belonging to the Davidson–Owen–Gross–Perry class of solutions[4,5] [that is, metric (74) with $\epsilon=1/\sqrt{3}$ and $k=-1$]. If $\alpha\neq0$, then we can always set $\alpha=1$: this particular solution was originally found by Ponce de Leon and Wesson[22]—the solution is also very similar in form to the time-dependent soliton solution found by Wesson, Liu, and Lim.[3]

If $\kappa\neq0$, then the equations (77)–(79) are not so simple to solve. For convenience, we introduce the new variable,

$$\rho=\ln r. \tag{81}$$

Equations (77)–(79) can then be reduced to the following system of differential equations:

$$G_{\rho\rho}=-G_\rho^2-2K_\rho G_\rho-2K_\rho-2G_\rho, \tag{82}$$

$$K_{\rho\rho}=-K_\rho^2+3K_\rho G_\rho+G_\rho^2+2G_\rho+3K_\rho, \tag{83}$$

with the first integral

$$4K_\rho G_\rho + G_\rho^2 + K_\rho^2 + 2G_\rho + 4K_\rho + \kappa e^{2(G-K+\rho)} = 0. \tag{84}$$

Equations (82) and (83) form a two-dimensional autonomous system of differential equations. A specific solution can be found by demanding that $K = G + \rho$; Eqs. (82) and (84) then imply that $\kappa = -1$ and that

$$G = \left(-1 \pm \frac{1}{\sqrt{3}} \right) \rho, \tag{85}$$

$$K = \pm \frac{1}{\sqrt{3}}\, \rho. \tag{86}$$

Thus, if we make the transformation $R = r^{\pm 1/\sqrt{3}}$, then the metric, in this special case, may be written as

$$ds^2 = -\cos^2(y + \alpha(t)) R^2\, dt^2 + 3\, dR^2 + R^2\, d\Omega^2 + R^2 dy^2. \tag{87}$$

A. Remarks

Of course, Eqs. (82)–(83) can easily be analyzed as a two-dimensional dynamical systems.[19] It can be shown that the system has four fixed points at finite values and six fixed points at infinity (full details are given in Ref. 19). Analysis of the finite fixed points shows that there are two saddles, an attracting focus and a repelling focus. Both the attracting focus and the repelling focus are described by the metric (87) [for which $\kappa = -1$] and are valid for R tends to infinity and R tends to zero, respectively. The corresponding class of solutions are consequently asymptotically flat in general, in the sense that all components of the Riemann tensor asymptotically vanish (as $r \to \infty$ for the attractor and as $r \to 0$ for the repellor). The corresponding four-dimensional models have the property that asymptotically the stress-energy tensor may be interpreted as an anisotropic fluid, with $p_\parallel = 0$ and $\mu = 2p_\perp$, where $p_\parallel$ and $p_\perp$ are the fluid pressures parallel and perpendicular to the fluid four-velocity, respectively. (At the two saddles the corresponding exact solutions have $\kappa = 0$ and the associated four-dimensional solutions that are also flat.)

Analysis of the singular points at infinity shows that there are two sinks, two sources, and two saddles (appearing in pairs). The asymptotic form of the solution corresponding to the sources at infinity is given by

$$G(r) \approx (\ln r)^{1 - 2/\sqrt{3}}, \quad K(r) \approx (\ln r)^{1/\sqrt{3}} \tag{88}$$

[note that $K \to \infty$, $G \to 0$, and that $\det(g_{ij}) \to \infty$ as $r \to \infty$], while for the sinks,

$$G(r) \approx (\ln r)^{1 + 2/\sqrt{3}}, \quad K(r) \approx (\ln r)^{-1/\sqrt{3}}. \tag{89}$$

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APPENDIX: THE RIEMANN TENSOR

The nonzero components of the Riemann tensor, up to the usual symmetries, for the metric (5) are

$$R^t{}_{rtr} = F_{rr} + F_r^2 - F_r G_r - e^{2(G-F)} \{ G_{tt} + G_t^2 - F_t G_t \} + e^{2(G-K)} F_y G_y, \tag{A1}$$

$$R^{t}{}_{rty}=F_{ry}+F_rF_y-F_rG_y-F_yK_r\,, \tag{A2}$$

$$R^{r}{}_{tyr}=G_{ty}+G_tG_y-F_yG_t-K_tG_y \quad (=R^{\theta}{}_{ty\theta}=R^{\phi}{}_{ty\phi}), \tag{A3}$$

$$R^{\theta}{}_{tt\theta}=G_{tt}+G_t^2-F_tG_t-F_r(G_r+1/r)e^{2(F-G)}-e^{2(F-K)}F_yG_y \quad (=R^{\phi}{}_{tt\phi}), \tag{A4}$$

$$R^{\theta}{}_{tr\theta}=G_{rt}-G_tF_r \quad (=R^{\phi}{}_{tr\phi}), \tag{A5}$$

$$R^{t}{}_{yty}=F_{yy}+F_y^2-F_yK_y+e^{2(K-G)}F_rK_r-e^{2(K-F)}\{K_{tt}+K_t^2-F_tK_t\}, \tag{A6}$$

$$R^{y}{}_{try}=K_{rt}+K_rK_t-K_tF_r-G_tK_r\,, \tag{A7}$$

$$R^{\theta}{}_{rr\theta}=G_{rr}+\frac{1}{r}\,G_r-e^{2(G-F)}G_t^2+e^{2(G-K)}G_y^2 \quad (=R^{\phi}{}_{rr\phi}), \tag{A8}$$

$$R^{\theta}{}_{ry\theta}=G_{ry}-K_rG_y \quad (=R^{\phi}{}_{ry\phi}), \tag{A9}$$

$$R^{r}{}_{yyr}=G_{yy}+G_y^2-G_yK_y+e^{2(K-G)}\{K_{rr}+K_r^2-G_rK_r\}-e^{2(K-F)}G_tK_t\,, \tag{A10}$$

$$R^{\phi}{}_{\theta\theta\phi}=r^2\left\{G_r^2+\frac{2}{r}\,G_r-e^{2(G-F)}G_t^2+e^{2(G-K)}G_y^2\right\}, \tag{A11}$$

$$R^{\theta}{}_{yy\theta}=G_{yy}+G_y^2-G_yK_y-e^{2(K-F)}G_tK_t+e^{2(K-G)}K_r(G_r+1/r) \quad (=R^{\phi}{}_{yy\phi})\,. \tag{A12}$$

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A new algebraic approach for calculating the heat kernel in quantum gravity

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It is shown that the heat kernel operator for the Laplace operator on any covariantly constant curved background, i.e., in symmetric spaces, may be presented in the form of an averaging over the Lie group of isometries with some nontrivial measure. Using this representation, the heat kernel diagonal, i.e., the heat kernel in coinciding points is obtained. Related topics concerning the structure of symmetric spaces and the calculation of the effective action are discussed. © *1996 American Institute of Physics.* [S0022-2488(96)00501-7]

I. INTRODUCTION

The heat kernel, a very powerful tool for investigating the effective action in quantum field theory and quantum gravity, has been the subject of much investigation in recent years in physical as well as in mathematical literature (Refs. 1–22). The subject of the present investigation is the low-energy limit of the one-loop contribution of a set of quantized fields ϕ on a d-dimensional Riemannian manifold M of metric $g_{\mu\nu}$ with Euclidean signature to the effective action, which can best be presented using the ζ-function regularization in the form[1]

$$\Gamma_{(1)}=-\frac{1}{2}\,\zeta'(0), \tag{1.1}$$

where

$$\zeta(p)=\mu^{2p}\ \mathrm{Tr}\ F^{-p}=\frac{\mu^{2p}}{\Gamma(p)}\int_0^\infty dt\ t^{p-1}\ \mathrm{Tr}\ U(t), \tag{1.2}$$

$$F=-\Box+Q+m^2, \tag{1.3}$$

$$U(t)=\exp(-tF), \tag{1.4}$$

with $\Box=g^{\mu\nu}\nabla_\mu\nabla_\nu$, Tr meaning the functional trace, μ being a renormparameter introduced to preserve dimensions, $Q(x)$ an arbitrary matrix-valued function (potential term), m a mass parameter, and ∇_μ a covariant derivative. The covariant derivative includes, in general, not only the Levi-Civita connection, but also the appropriate spin one as well as the vector gauge connection, and is determined by the commutator $[\nabla_\mu,\nabla_\nu]\phi=.\mathscr{R}_{\mu\nu}\phi$. The Riemann curvature tensor, the curvature of background connection, and the potential term completely describe the background metric and connection, at least locally. In the following we will call these quantities the *background curvatures* or simply curvatures and denote them symbolic by $\mathfrak{R}=\{R_{\mu\nu\alpha\beta},\mathscr{R}_{\mu\nu},Q\}$.

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Exact evaluation of the heat kernel $U(t)$ is obviously impossible. Therefore, one should make use of various approximations. First of all, let us note the very important so-called Schwinger–De Witt asymptotic expansion of the heat kernel at $t\to 0$,[1–5]

$$\mathrm{Tr}\ U(t)\sim(4\pi t)^{-d/2}\ \exp(-tm^2)\sum_{k=0}^{\infty}\ \frac{(-t)^k}{k!}\,B_k\,, \tag{1.5}$$

$$B_k=\int_M dx\ g^{1/2}\ \mathrm{tr}\ b_k\,. \tag{1.6}$$

This expansion is purely local and does not depend, in fact, on the global structure of the manifold. In manifolds with boundary additional terms in B_k as well as new terms of order $t^{-d/2+k/2}$ in the form of surface integrals over the boundary ∂M appear. For details see Refs. 12 and 13, where all coefficients for arbitrary boundary conditions up to terms of order $t^{-d/2+5/2}$ are calculated. Its coefficients b_k [we call them Hadamard–Minakshisundaram–De Witt–Seeley (HMDS) coefficients] are local invariants built from the curvature, the potential term, and their covariant derivatives.[1,5,6,14] They play a very important role, both in physics and mathematics, and are closely connected with various sections of mathematical physics.[14,22] Therefore, the calculation of HMDS coefficients is in itself of great importance. Various methods were used for calculating these coefficients, beginning from the direct De Witt's method[1] to modern mathematical methods, which make use of pseudodifferential operators, functorial properties of the heat kernel, etc.[5–13] Very good reviews of the calculation of the HMDS coefficients are given in recent papers.[14]

Nowadays, in the general case only the first four coefficients are explicitly calculated. The first three coefficients were calculated in Ref. 9. An effective covariant technique for calculating HMDS coefficients is elaborated in Refs. 10 and 4, where also the first four coefficients are computed. In the case of scalar operators the fourth coefficient is also calculated in Ref. 11. Analytic approach was developed in Ref. 7, where a closed form for the intrinsic symbol of the resolvent parametrix was obtained. The leading terms in all the volume coefficients B_k quadratic in the background curvatures were calculated completely independently in Refs. 15 and 16.

Although the Schwinger–De Witt expansion is good for small t (viz. $t\mathfrak{R}\ll 1$), and thereby in the case of massive quantized fields in weak background fields when $\mathfrak{R}\ll m^2$, it is absolutely inadequate for large t in strongly curved manifolds and strong background fields ($\mathfrak{R}\gg m^2$). For investigating these cases one needs some other methods.

A possibility to exceed the limits of the Schwinger–De Witt expansion is to employ the direct partial summation.[2] Namely, one can compare all the terms in HMDS coefficients B_k (1.6), pick up the main (the largest in some approximation) terms, and sum up the corresponding partial sum. There is always a lack of uniqueness concerned with the global structure of the manifold, when doing so. But, hopefully, fixing the topology, e.g. the trivial one, one can obtain a unique, well-defined, expression that would reproduce the Schwinger–De Witt expansion, being expanded in curvature. The main advantage of such an approach is that although the result will be *not exact*, it will be *covariant* and *general*.

Actually, the effective action is a covariant functional of the metric and depends on the geometry of the manifold as a whole, i.e., it depends on both local characteristics of the geometry, like invariants of the curvature tensor, and its global topological structure. However, *we will not investigate in this paper the influence of the topology*, but concentrate our attention, as a rule, on the *local effects*. That means that we restrict ourselves to those physical problems where the contribution of the global effects may be neglected, in comparison with local ones. Then the possible approximations for evaluating the effective action can be based on the assumptions about the local behavior of the background fields, dealing with the real physical gauge invariant variations of the local geometry, i.e. with the curvature invariants, but not with the behavior of the

metric and the connection that is not invariant. Comparing the value of the curvature with that of its covariant derivatives one comes to two possible approximations: (i) the short-wave (or high-energy) approximation characterized by $\mathbf{\nabla\nabla}\mathfrak{R}\gg\mathfrak{R}\mathfrak{R}$, and (ii) the long-wave (or low-energy) one $\mathbf{\nabla\nabla}\mathfrak{R}\ll\mathfrak{R}\mathfrak{R}$.

The idea of partial summation was realized in short-wave approximation for investigating the nonlocal aspects of the effective action (in other words, the high-energy limit of that) in Refs. 15 and 4, where all the terms in the HMDS coefficients B_k with higher derivatives (quadratic in the curvature and potential term) are calculated, and the corresponding asymptotic expansion is summed up. Another approach to study the high-energy limit of the effective action, so-called covariant perturbation theory, is developed in Ref. 17.

II. LOW-ENERGY APPROXIMATION AND ITS CONSEQUENCES

The low-energy effective action, in other words, the effective potential, presents a very natural tool for investigating the vacuum of the theory, its stability, and the phase structure.[23] Here only partial success is achieved and various approaches to the problem are only outlined (see, e.g., the excellent review of Camporesi in Ref. 22 with an ample bibliography and our recent papers[20,21]).

The long-wave (or low-energy) approximation is determined, as it was already stressed above, by strong slowly varying background fields. This means that the derivatives of all invariants are much smaller than the products of the invariants themselves. The zeroth order of this approximation corresponds to covariantly constant background curvatures,

$$\mathbf{\nabla}_\mu R_{\alpha\beta\gamma\delta}=0, \quad \mathbf{\nabla}_\mu \mathscr{R}_{\alpha\beta}=0, \quad \mathbf{\nabla}_\mu Q=0. \tag{2.1}$$

In this case the HMDS coefficients are simply polynomials in curvature invariants and potential term of dimension $\mathfrak{R}^k$ up to terms with one or more covariant derivatives of the background curvatures $O(\mathbf{\nabla}\mathfrak{R})$,

$$b_k=\sum_{n=0}^{k}\binom{k}{n}Q^{k-n}a_n+O(\mathbf{\nabla}\mathfrak{R}), \tag{2.2}$$

$$a_k=b_k|_{Q=\mathbf{\nabla}R=0}=\sum R^k. \tag{2.3}$$

Note that the commutators $[Q,\mathscr{R}_{\mu\nu}]$ are of order $O(\mathbf{\nabla\nabla}\mathfrak{R})$, and therefore are neglected here.

Then, after summing the Schwinger–De Witt expansion (1.5), we obtain for the heat kernel, the ζ function and the effective action,

$$\mathrm{Tr}\ U(t)=\int_M dx\ g^{1/2}(4\pi t)^{-d/2}\ \mathrm{tr}\{\exp(-t(m^2+Q))(\Omega(t)+O(\mathbf{\nabla}\mathfrak{R}))\}, \tag{2.4}$$

$$\zeta(p)=\int_M dx\ g^{1/2}(4\pi)^{-d/2}\ \frac{\mu^{2p}}{\Gamma(p)}\int_0^\infty dt\ t^{p-d/2-1}\ \mathrm{tr}\{\exp(-t(m^2+Q))(\Omega(t)+O(\mathbf{\nabla}\mathfrak{R}))\}, \tag{2.5}$$

$$\Gamma_{(1)}=\int_M dx\ g^{1/2}\{V(\mathfrak{R})+O(\mathbf{\nabla}\mathfrak{R})\}, \tag{2.6}$$

with

$$V(\mathfrak{R})=\frac{1}{2}\,(4\pi)^{-d/2}\,\frac{1}{\Gamma(d/2+1)}\int_0^\infty dt\left(\log(\mu^2 t)+\psi\left(\frac{d}{2}+1\right)\right)$$
$$\times\left(\frac{\partial}{\partial t}\right)^{d/2+1}\operatorname{tr}\{\exp(-t(m^2+Q))\Omega(t)\},\tag{2.7}$$

for even d and

$$V(\mathfrak{R})=\frac{1}{2}\,(4\pi)^{-d/2}\,\frac{1}{\Gamma(d/2+1)}\int_0^\infty dt\;t^{-1/2}\left(\frac{\partial}{\partial t}\right)^{(d+1)/2}\operatorname{tr}\{\exp(-t(m^2+Q))\Omega(t)\},\tag{2.8}$$

for odd d, where

$$\Omega(t)\sim\sum_{k=0}^{\infty}\frac{(-t)^k}{k!}\,a_k,\tag{2.9}$$

is a function of local invariants of the curvatures (but not of the potential).

It is natural to call the functions $\Omega(t)$ and $V(\mathfrak{R})$ that do not contain the *covariant* derivatives at all and so determine the zeroth order of the heat kernel and that of the effective action, the *generating function* for covariantly constant terms in HMDS coefficients and the *effective potential* in quantum gravity, respectively.

Let us note that such a definition of the effective potential is not conventional. It differs from the definition that is often found in the literature.[24] What is meant usually under the notion of the effective potential is a function of the potential term only Q, because it does not contain derivatives of the background fields (in contrast to Riemann curvature $R_{\alpha\beta\gamma\delta}$ that contains second derivatives of the metric and the curvature $\mathscr{R}_{\mu\nu}$ with first derivatives of the connection). So, e.g., in Ref. 24, the potential term Q is summed up exactly, but an expansion is made not only in covariant derivatives but also in powers of curvatures $R_{\mu\nu\alpha\beta}$ and $\mathscr{R}_{\mu\nu}$, i.e. the curvatures are treated perturbatively. Thereby the validity of this approximation for the effective action is limited to small curvatures $\mathscr{R}_{\mu\nu},R_{\mu\nu\alpha\beta}\ll Q$. Such an expansion is called ''expansion of the effective action in covariant derivatives.'' Without the potential term ($Q=0$) the effective potential in such a scheme is trivial. Hence we stress here once again that the effective potential in our definition contains, in fact, *much more information* than the usual effective potential does when using the ''expansion in covariant derivatives.'' As a matter of fact, what we mean is the *low-energy limit of the effective action* formulated in a covariant way.

Note that the conditions (2.1) are local. They determine the geometry of the *locally* symmetric spaces. However, the manifold is a *globally* symmetric one only in the case when it satisfies additionally some global topological restrictions (e.g., it is sufficient if it is simply connected and complete) and the condition (2.1) is valid everywhere, i.e. at any point of the manifold.[25,26]

In most *physical* problems, the situation is radically different. The correct setting of the problem seems to be as follows. The low-energy effective action depends, in general, also essentially on the global topological properties of the space-time manifold, i.e. on the existence of closed geodesics, boundaries, or singularities that might act similarly to boundaries. But, as it was noted above, we do not investigate in this paper the influence of the topology. Therefore, consider a complete noncompact asymptotically flat manifold without a boundary that is homeomorphic to $\mathbb{R}^d$. Let a finite not small, in general, domain of the manifold exists that is strongly curved and quasihomogeneous, i.e. the invariants of the curvature in this region vary very slowly. Then, the geometry of this region is *locally* very similar to that of a symmetric space. However, one should have in mind that there are *always* regions in the manifold where this condition is not fulfilled. This is, first of all, the asymptotic Euclidean region that has small curvature and, therefore, the opposite short-wave approximation is valid.

The general situation in the correct setting of the problem is the following. From infinity with small curvature and possibly radiation, where[17] $\mathfrak{R}\mathfrak{R}\ll\nabla\nabla\mathfrak{R}$, we pass on to the quasihomogeneous region where the local properties of the manifold are close to those of symmetric spaces. The size of this region can tend to zero. Then the curvature is nowhere large and the short-wave approximation is valid anywhere. If one tries to extend the limits of such a region to infinity, then one has also to analyze the topological properties. The space can be compact or noncompact, depending on the sign of the curvature. But first we will come across a coordinate horizon-like singularity, although no one true physical singularity really exists.

This construction can be intuitively imagined as follows. Take the flat Euclidean space $\mathbb{R}^d$, cut out from it a region M with some boundary ∂M, and stick to it smoothly along the boundary, instead of the piece cut out, a piece of a curved symmetric space with the same boundary ∂M. Such a construction will be homeomorphic to the initial space and at the same time will contain a finite highly curved homogeneous region. Let us stress that this surgery can be always done *smoothly*, so that in the region where the curved and the flat regions are joined no discontinuity in the curvature appears that could cause the reflected waves to produce Casimir-like effects. By the way, the exact effective action for a symmetric space differs from the effective action for built construction by a purely topological contribution. This fact seems to be useful when analyzing the effects of topology.

Thus, the problem is to calculate the low-energy effective action (2.7) and (2.8), i.e. the heat kernel for covariantly constant background. Although this quantity, generally speaking, depends essentially on the topology and other global aspects of the manifold, one can disengage oneself from these effects fixing the trivial topology. Since the asymptotic Schwinger–De Witt expansion does not depend on the topology, one can hold that we thereby sum up all the terms without covariant derivatives in it.

We stress here once again that our analysis is purely local. Of course, there are always special global effects (Casimir-like effects, influence of boundaries, closed geodesics, etc.), that do not show up in the local expansion of the heat kernel. The aim of this paper is to study only such situations where the contribution of these effects is small in comparison with the local part, i.e. the effective action is *approximately* given by the integration of the local formula.

In other words, the problem is the following. One has to obtain a local covariant function of the invariants of the curvature $\Omega(t)$ (2.9) that would describe adequately the low-energy limit of the trace of the heat kernel and that would, being expanded in curvatures, reproduce all terms without covariant derivatives in the asymptotic expansion of the heat kernel, i.e. the HMDS coefficients a_k (2.3). If one finds such an expression, then one can simply determine the ζ function (2.5) and, therefore, the low-energy limit of the effective action (2.7) and (2.8).

III. SYMMETRIC SPACES

In this paper we will get the most out of the properties of symmetric spaces. Let us list below some known ideas, facts, and formulas about symmetric spaces presented in the form that is most convenient for calculating the heat kernel and the effective action.

First of all, we give some definitions (see Refs. 25 and 26 and Sec. III D). A Riemannian locally symmetric space that is simply connected and complete is globally symmetric space (or, simply, symmetric space).[26] A symmetric space is said to be of *compact*, *non-compact*, or *Euclidean type* if *all* sectional curvatures $K(u,v)=R_{abcd}u^a v^b u^c v^d$ are positive, negative, or zero. A direct product of symmetric spaces of compact and noncompact types is called *semisimple* symmetric space. It is well known[25,26] that a generic complete simply connected Riemannian symmetric space is a direct product of a flat space and a semisimple symmetric space (also see Sec. III D). Although in the Sec. IV we will need actually only symmetric spaces of compact type the whole exposition of the Sec. III is valid for a more general case of semisimple symmetric spaces.

So, what are the direct consequences of the condition of covariant constancy of the curvature (2.1)?

A. Geometrical framework

First of all, to carry out the calculations in the curved space in a covariant way we need some auxiliary two-point geometric objects, namely the geodetic interval (or world function) $\sigma(x,x')$, defined as one-half the square of the length of the geodesic connecting the points x and x', the tangent vectors $\sigma_\mu(x,x')=\nabla_\mu\sigma(x,x')$ and $\sigma_{\mu'}(x,x')=\nabla_{\mu'}\sigma(x,x')$ to this geodesic at the points x and x', respectively, and a frame $e^\mu_a(x,x')$, which is covariantly constant (parallel) along the geodesic between points x and x', i.e. $\sigma^\mu\nabla_\mu e^\nu_a=0$. We denote the frame components of the tangent vector by $\sigma^a(x,x')=g^{ab}e^{\mu'}_a(x')\nabla_{\mu'}\sigma(x,x')$.

Any tensor $T^{a\cdots}_{b\cdots}$, can then be presented in the form of covariant Taylor series,

$$T^{a\cdots}_{b\cdots}=\sum_{n\geqslant 0}\frac{(-1)^n}{n!}\,\sigma^{\mu'_1}\cdots\sigma^{\mu'_n}[\nabla_{(\mu_1}\cdots\nabla_{\mu_n)}T^{\alpha\cdots}_{\beta\cdots}](x')e^a_{\alpha'}\cdots e^{\beta'}_b\,. \tag{3.1}$$

Therefrom, it is clear that the frame components of a *covariantly* constant tensor are *simply* constant.

In the case of covariantly constant curvature one can express the mixed second derivatives of the geodetic interval, i.e. the matrix

$$\sigma^a{}_b(x,x')=e^a_{\mu'}(x')e^\alpha_b(x)\nabla^{\mu'}\nabla_\alpha\sigma(x,x'), \tag{3.2}$$

explicitly in terms of the curvature at a fixed point x'. Introducing a matrix $K=\{K^a{}_b(x,x')\}$,

$$K^a{}_b=R^a{}_{cbd}\sigma^c\sigma^d, \tag{3.3}$$

one can sum up the Taylor series, obtaining a closed form,[4]

$$\sigma^a{}_b=-\left(\frac{\sqrt{K}}{\sin\sqrt{K}}\right)^a_b. \tag{3.4}$$

This expression, as well as any other similar expressions below, should be always understood as a *power series* in the curvature.

B. Curvature

Let us consider the Riemann tensor in more detail (we follow here Secs. 3.7–3.10 of the first paper in Ref. 25). The components of the curvature tensor of *any* Riemannian manifold can be always presented in the form

$$R_{abcd}=\beta_{ik}E^i{}_{ab}E^k{}_{cd}, \tag{3.5}$$

where E^i_{ab} $(i=1,\ldots,p;p\leqslant d(d-1)/2)$, is some set of antisymmetric matrices (2-forms) and β_{ik} is some symmetric nondegenerate matrix.

Then define the traceless matrices $D_i=\{D^a{}_{ib}\}$,

$$D^a{}_{ib}=-\beta_{ik}E^k{}_{cb}g^{ca}=-D^a{}_{bi}, \tag{3.6}$$

so that

$$R^a{}_{bcd}=-D^a{}_{ib}E^i{}_{cd},\quad R^a{}_b{}^c{}_d=\beta^{ik}D^a{}_{ib}D^c{}_{kd}, \tag{3.7}$$

$$R^a_b=-\beta^{ik}D^a{}_{ic}D^c{}_{kb},\quad R=-\beta^{ik}D^a{}_{ic}D^c{}_{ka}=-\beta^{ik}\,\mathrm{tr}(D_iD_k), \tag{3.8}$$

where $\beta^{ik}=(\beta_{ik})^{-1}$. Because of the curvature identities, we have identically

$$D^a{}_{j[b}E^j{}_{cd]}=0. \tag{3.9}$$

The matrices D_i are known to be the generators of the *holonomy algebra*, i.e. the Lie algebra of the restricted holonomy group, $\mathscr{H}$ (the first paper in Ref. 25, p. 97) of dimension $\dim\mathscr{H}=p$,

$$[D_i,D_k]=F^j{}_{ik}D_j, \quad \text{or} \quad D^a{}_{ic}D^c{}_{kb}-D^a{}_{kc}D^c{}_{ib}=F^j{}_{ik}D^a{}_{jb}. \tag{3.10}$$

The structure constants $F^j{}_{ik}$ of the holonomy algebra are completely determined by these commutation relations and satisfy the Jacobi identities

$$F^i{}_{j[k}F^j{}_{mn]}=0, \quad \text{or} \quad [F_i,F_k]=F^j{}_{ik}F_j, \tag{3.11}$$

where $F_i=\{F^k{}_{il}\}$ are the generators of the holonomy algebra in adjoint representation. Note that the restricted holonomy group H is always compact, as it is a subgroup of the orthogonal group (in the Euclidean case), and connected.

Now let us rewrite the condition of integrability of the relations (2.1) given simply by the commutator of covariant derivatives,

$$[\boldsymbol{\nabla}_\mu,\boldsymbol{\nabla}_\nu]R_{\alpha\beta\gamma\delta}=-2\{R_{\mu\nu\lambda[\alpha}R^\lambda{}_{\beta]\gamma\delta}+R_{\mu\nu\lambda[\gamma}R^\lambda{}_{\delta]\alpha\beta}\}=0, \tag{3.12}$$

in terms of introduced quantities. It is not difficult to show that it looks like

$$E^i{}_{ac}D^c{}_{bk}-E^i{}_{bc}D^c{}_{ak}=E^j{}_{ab}F^i{}_{jk}. \tag{3.13}$$

This equation takes place *only in symmetric spaces* and is the most important one. It is this equation that makes a Riemannian manifold the symmetric space.

From Eqs. (3.10) and (3.13) we now have

$$\beta_{ik}F^k{}_{jm}+\beta_{mk}F^k{}_{ji}=0, \quad \text{or} \quad F_i^T=-\beta F_i\beta^{-1}, \tag{3.14}$$

which means that the adjoint and coadjoint representations of the restricted holonomy group are equivalent.

Equation (3.13) leads also to some identities for the curvature tensor

$$D^a{}_{i[b}R_{c]ade}+D^a{}_{i[d}R_{e]abc}=0, \tag{3.15}$$

$$R^a{}_cD^c{}_{ib}=D^a{}_{ic}R^c{}_b, \tag{3.16}$$

which means, in particular, that the Ricci tensor matrix commutes with all matrices D_i and is, therefore, an invariant matrix of the holonomy algebra.

Actually, Eq. (3.13) brings into existence a much wider algebra $\mathscr{G}$ of dimension $\dim\mathscr{G}=D=p+d$, in other words, it closes this algebra. Really, let us introduce new quantities $C^A{}_{BC}=-C^A{}_{CB}$ $(A=1,\ldots,D)$,

$$C^i{}_{ab}=E^i{}_{ab}, \quad C^a{}_{ib}=D^a{}_{ib}, \quad C^i{}_{kl}=F^i{}_{kl}, \quad C^a{}_{bc}=C^i{}_{ka}=C^a{}_{ik}=0, \tag{3.17}$$

forming the matrices $C_A=\{C^B{}_{AC}\}=(C_a,C_i)$,

$$C_a=\begin{pmatrix}0 & D^b{}_{ai}\\ E^j{}_{ac} & 0\end{pmatrix}, \quad C_i=\begin{pmatrix}D^b{}_{ia} & 0\\ 0 & F^j{}_{ik}\end{pmatrix}, \tag{3.18}$$

and symmetric nondegenerate matrix,

$$\gamma_{AB}=\begin{pmatrix} g_{ab} & 0 \\ 0 & \beta_{ik} \end{pmatrix}. \tag{3.19}$$

Then one can show, first, that as a consequence of the identities (3.9)–(3.13) the quantities $C^A{}_{CB}$ satisfy the Jacobi identities

$$C^E{}_{D[A}C^D{}_{BC]}=0, \quad \text{or} \quad [C_A,C_B]=C^C{}_{AB}C_C, \tag{3.20}$$

and are, therefore, the structure constants of some Lie algebra $\mathscr{G}$, the matrices C_A being then the generators of this algebra in adjoint representation. More precisely, the commutation relations have the form

$$[C_a,C_b]=E^i{}_{ab}C_i, \quad [C_a,C_i]=D^b{}_{ai}C_b, \quad [C_i,C_k]=F^j{}_{ik}C_j. \tag{3.21}$$

And, second, using the definition of D matrices and Eq. (3.14), one can show that the structure constants also satisfy the identity

$$\gamma_{AB}C^B{}_{CD}+\gamma_{DB}C^B{}_{CA}=0, \quad \text{or} \quad C_A^T=-\gamma C_A\gamma^{-1}, \tag{3.22}$$

meaning the equivalence of the adjoint and coadjoint representations of the algebra $\mathscr{G}$.

In other words, the Jacobi identities (3.22) are equivalent to the identities (3.12) that the curvature must satisfy in the symmetric space. This means that the set of structure constants $C^A{}_{BC}$, satisfying the Jacobi identities, determines the curvature tensor of symmetric space $R^a{}_{bcd}$. *Vice versa*, the structure of the algebra $\mathscr{G}$ is completely determined by the curvature tensor of symmetric space at a fixed point x'.

Now, consider the curvature of background connection $\mathscr{R}_{ab}$. One can show analogously to (3.12) that because of the integrability conditions of Eq. (2.1),

$$[\boldsymbol{\nabla}_\mu,\boldsymbol{\nabla}_\nu]\mathscr{R}_{\alpha\beta}=[\mathscr{R}_{\mu\nu},\mathscr{R}_{\alpha\beta}]-2R_{\mu\nu\lambda[\alpha}\mathscr{R}^\lambda{}_{\beta]}=0, \tag{3.23}$$

the curvature of background connection $\mathscr{R}_{ab}$ in *semisimple* symmetric spaces must have the form

$$\mathscr{R}_{ab}=\mathscr{R}_iE^i{}_{ab}, \tag{3.24}$$

where $E^i{}_{ab}$ are the same 2-forms and $\mathscr{R}_i$ are some matrices forming a representation of the holonomy algebra,

$$[\mathscr{R}_i,\mathscr{R}_k]=F^j{}_{ik}\mathscr{R}_j. \tag{3.25}$$

In a generic symmetric space with a flat subspace there are additional Abelian contributions to the curvature $\mathscr{R}_{ab}$ (3.24) corresponding to the flat directions.

Finally, from (2.1) it follows that the potential term should commute with the curvature $\mathscr{R}_{\mu\nu}$,

$$[\boldsymbol{\nabla}_\mu,\boldsymbol{\nabla}_\nu]Q=[\mathscr{R}_{\mu\nu},Q]=0, \tag{3.26}$$

and, therefore, with all the matrices $\mathscr{R}_i$,

$$[\mathscr{R}_i,Q]=0. \tag{3.27}$$

C. Isometries

On the covariantly constant background (2.1), i.e. in symmetric spaces, one can easily solve the Killing equations,

$$\mathscr{L}_\xi g_{\mu\nu}=2\boldsymbol{\nabla}_{(\mu}\xi_{\nu)}=0, \tag{3.28}$$

where $\mathscr{L}_\xi$ means the Lie derivative. Indeed, by differentiating the equation

$$\mathscr{L}_\xi \Gamma^\lambda_{\mu\nu} = \nabla_{(\mu}\nabla_{\nu)}\xi^\lambda + R^\lambda{}_{(\mu|\alpha|\nu)}\xi^\alpha = 0, \tag{3.29}$$

having in mind $\nabla R = 0$, and symmetrizing the derivatives we get

$$\nabla_{(\mu_1}\cdots\nabla_{\mu_{2n})}\xi^\lambda = (-1)^n R^\lambda{}_{(\mu_1|\alpha_1|\mu_2} R^{\alpha_1}{}_{\mu_3|\alpha_2|\mu_4}\cdots R^{\alpha_{n-1}}{}_{\mu_{2n-1}|\alpha_n|\mu_{2n})}\xi^{\alpha_n}, \tag{3.30}$$

$$\nabla_{(\mu_1}\cdots\nabla_{\mu_{2n+1})}\xi^\lambda = (-1)^n R^\lambda{}_{(\mu_1|\alpha_1|\mu_2} R^{\alpha_1}{}_{\mu_3|\alpha_2|\mu_4}\cdots R^{\alpha_{n-1}}{}_{\mu_{2n-1}|\alpha_n|\mu_{2n}}\nabla_{\mu_{2n+1})}\xi^{\alpha_n}. \tag{3.31}$$

Thereby we have found all the coefficients of the covariant Taylor series (3.1) for the Killing vectors of symmetric spaces. Moreover, one can now sum it up obtaining a closed form,

$$\xi^\mu(x) = e^\mu{}_a\left\{ (\cos\sqrt{K})^a{}_b\xi^b(x') - \left(\frac{\sin\sqrt{K}}{\sqrt{K}}\right)^a_b \sigma^c \xi^b{}_{;c}(x')\right\}, \tag{3.32}$$

where $\xi^b{}_{;c} = \xi^\mu{}_{;\nu} e^b_\mu e^\nu_c$.

Therefore, all Killing vectors at any point x are determined in terms of initial values of the vectors themselves $\xi^b(x')$ and their first derivatives $\xi^b{}_{;c}(x')$ at a fixed point x'. The set of all Killing vectors $\hat{\mathscr{G}} = \{\xi_{\hat{A}}\}, (\hat{A} = 1,\ldots,\hat{D})$, dim $\hat{\mathscr{G}} = \hat{\mathscr{D}}$, can be split in two essentially different sets: $\mathscr{M} = \{P_a\}$, dim $\mathscr{M} = d$, with P_a defined by

$$P^\mu{}_a(x) = e^\mu{}_b(\cos\sqrt{K})^b{}_c P^c{}_a(x'), \tag{3.33}$$

and $\hat{\mathscr{H}} = \{L_{\hat{i}}\}, (\hat{i} = 1,\ldots,\hat{p})$, i.e. dim $\hat{\mathscr{H}} = \hat{p} = \hat{D} - d$, where

$$L^\mu{}_{\hat{i}}(x) = -e^\mu{}_b\left(\frac{\sin\sqrt{K}}{\sqrt{K}}\right)^b_a \sigma^c L^a{}_{\hat{i};c}(x'), \tag{3.34}$$

according to the values of their initial parameters,

$$P^\mu{}_a|_{x=x'} \neq 0, \quad L^\mu{}_{\hat{i}}|_{x=x'} = 0. \tag{3.35}$$

Note that for a general symmetric space $\hat{p} \neq p$, and hence, $\hat{D} \neq D$!

The Killing vector fields $\xi_{\hat{A}} = \xi^\mu_{\hat{A}}\nabla_\mu$ (or $P_a = P^\mu{}_a\nabla_\mu$ and $L_{\hat{i}} = L^\mu{}_{\hat{i}}\nabla_\mu$) (acting on scalar fields) form the Lie *algebra of isometries*, $\hat{\mathscr{G}}$,

$$[\xi_{\hat{A}}, \xi_{\hat{B}}] = \hat{C}^{\hat{C}}{}_{\hat{A}\hat{B}}\xi_{\hat{C}}, \tag{3.35a}$$

or, more explicitly,

$$[P_a, P_b] = \hat{E}^{\hat{i}}{}_{ab}L_{\hat{i}}, \quad [P_{\hat{i}}, L_i] = \hat{D}^b{}_{a\hat{i}}P_b,$$

$$[L_{\hat{i}}, L_{\hat{k}}] = \hat{F}^{\hat{j}}{}_{\hat{i}\hat{k}}L_{\hat{j}}, \tag{3.35b}$$

where $\{\hat{C}^{\hat{C}}{}_{\hat{A}\hat{B}}\} = \{\hat{E}^{\hat{i}}{}_{ab}, \hat{D}^b{}_{a\hat{i}}, \hat{F}^{\hat{j}}{}_{\hat{i}\hat{k}}\}$ are the structure constants of the algebra of isometries. One sees now that the generators $L_{\hat{i}}$ vanishing at the point x' form a subalgebra (3.35b) of the algebra of isometries $\hat{\mathscr{G}}$ (3.35a) called the *isotropy* algebra, $\hat{\mathscr{H}}$.

In fact, all odd symmetrized derivatives of $P^\mu{}_a$ and all even symmetrized derivatives of $L^\mu{}_i$ as well as $L^\mu{}_{\hat{i}}$ themselves vanish at the point x',

$$\nabla_\nu P^\mu{}_a|_{x=x'} = \nabla_{(\mu_1}\cdots\nabla_{\mu_{2n+1})}P^\mu{}_a|_{x=x'} = 0, \tag{3.36}$$

$$L^{\mu}{}_{\hat{i}}|_{x=x'} = \nabla_{(\mu_1}\cdots\nabla_{\mu_{2n})}L^{\mu}{}_{\hat{i}}|_{x=x'} = 0. \tag{3.37}$$

All the parameters $P^b{}_a(x')$ are independent and, therefore, there are exactly d such parameters. The maximal number of the parameters $L^b{}_{\hat{i};c}$ is $d(d-1)/2$, since they are antisymmetric; in other words $\dim \hat{\mathscr{H}} \leqslant d(d-1)/2$. However, they are not independent. This can be seen immediately if one recalls that the equation

$$\mathscr{L}_{L_{\hat{i}}} R_{\alpha\beta\gamma\delta} = 2\{L^\sigma{}_{\hat{i};[\gamma}R_{\delta]\sigma\beta\alpha} + L^\sigma{}_{\hat{i};[\alpha}R_{\beta]\sigma\delta\gamma}\} = 0, \tag{3.38}$$

holds in symmetric spaces. This equation is, actually, the integrability condition for Killing equations (3.26). It imposes strict constraints on the possible initial parameters $L^b{}_{\hat{i};c}(x')$. One can show that for the *semisimple* symmetric spaces the number of independent parameters $L^b{}_{\hat{i};c}(x')$ is equal to p, i.e. the dimension of the isotropy algebra $\hat{\mathscr{H}}$ (3.35b) is equal to the dimension of the holonomy algebra $\mathscr{H}$ (3.10),.

$$\hat{p} \equiv \dim\, \hat{\mathscr{H}} = \dim\, \mathscr{H} \equiv p.$$

Therefore, the dimension of the algebra of isometries $\hat{\mathscr{G}}$, i.e. the total number of the Killing vectors, in semisimple symmetric spaces, is equal to the dimension of the algebra $\mathscr{G}$ (3.20) defined in previous Sec. III B,

$$\hat{D} \equiv \dim\, \hat{\mathscr{G}} = \dim\, \mathscr{G} \equiv D.$$

This means that there is no difference between the ordinary latin indices and the indices with overcarets. Hence, one can omit the overcarets everywhere. In a symmetric space of general type having a flat subspace there are additional trivial Killing vectors corresponding to flat directions. Therefore, in general,

$$\dim\, \mathscr{H} \leqslant \dim\, \hat{\mathscr{H}} \leqslant d(d-1)/2, \quad \dim\, \mathscr{G} \leqslant \dim\, \hat{\mathscr{G}} \leqslant d(d+1)/2.$$

The spaces with a maximal number of independent isometries, i.e. with $p = d(d-1)/2$ and $D = d + p = d(d+1)/2$, are the spaces of constant curvature, and only those.

Thus, taking into account (3.15), it is evident that one can put

$$P^a{}_b(x') = \delta^a_b, \quad L^a{}_{i;b}(x') = -D^a{}_{ib}. \tag{3.39}$$

Therefore, the generators of isometries in semisimple symmetric spaces take the form

$$P_a = P^\mu{}_a \nabla_\mu = -(\sqrt{K}\,\cot\sqrt{K})^b{}_a \mathscr{D}_b, \tag{3.40}$$

$$L_i = L^\mu{}_i \nabla_\mu = -D^b{}_{ia}\sigma^a \mathscr{D}_b, \tag{3.41}$$

where

$$\mathscr{D}_a = (\sigma^a{}_b)^{-1} e^\mu{}_b \nabla_\mu = \frac{\partial}{\partial \sigma^a}. \tag{3.42}$$

Moreover, one can show[25,26] that for semisimple symmetric spaces the isotropy algebra $\hat{\mathscr{H}}$ (3.35b) is *isomorphic* to the holonomy algebra $\mathscr{H}$ (3.10) and the algebra of isometries $\hat{\mathscr{G}}$ (3.35a) is isomorphic to the algebra $\mathscr{G}$ (3.20) determined by the curvature tensor. Therefore, the commutation relations (3.35a) and (3.35b) can be rewritten in the form

$$[\xi_A,\xi_B]=C^C{}_{AB}\xi_C \tag{3.43}$$

and

$$[P_a,P_b]=E^i{}_{ab}L_i,\quad [P_a,L_i]=D^b{}_{ai}P_b,\quad [L_i,L_k]=F^j{}_{ik}L_j, \tag{3.44}$$

with the same structure constants as in (3.20) and (3.21) defined by (3.5), (3.6), (3.10), and (3.17). Hence, we conclude that the curvature tensor of the *semisimple* symmetric space completely determines the structure of the isotropy algebra and the algebra of isometries. For a generic symmetric space the curvature determines the algebra of isometries up to an Abelian ideal. Let us stress once again that in the case of semisimple symmetric spaces there is no need to distinguish in notation between the isotropy algebra $\hat{\mathscr{H}}$ and the holonomy algebra $\mathscr{H}$ and, therefore, between $\hat{\mathscr{G}}$ and $\mathscr{G}$ as well.

D. General structure

As we already noted above, the simply connected symmetric space M is isomorphic to the quotient space of the group of isometries by the isotropy subgroup $M=\hat{G}/\hat{H}$.[25] It is, in general, reducible, and has the following general structure:[25]

$$M=M_0\times M_s, \tag{3.45a}$$

$$M_s=M_+\times M_-, \tag{3.45b}$$

where M_0, M_s, M_+, and M_- are the Euclidean, semisimple, compact, and noncompact components. The corresponding algebra of isometries is a direct sum of ideals,

$$\hat{\mathscr{G}}=\mathscr{G}_0\oplus\mathscr{G}_s,\quad \mathscr{G}_s=\mathscr{G}_+\oplus\mathscr{G}_-, \tag{3.46}$$

where $\mathscr{G}_0$ is an Abelian ideal, $\mathscr{G}_s$ is the semisimple ideal, and $\mathscr{G}_+$ and $\mathscr{G}_-$ are the semisimple compact and noncompact ones.

There is a remarkable duality relation $*$ between compact and noncompact objects. For any semisimple algebra of isometries $\mathscr{G}=\mathscr{M}+\mathscr{H}=\{P_a,L_k\}$, one defines the dual one according to $\mathscr{G}^*=i\mathscr{M}+\mathscr{H}=\{iP_a,L_k\}$, the structure constants of the dual algebra being

$$\{C^{*A}{}_{BC}\}=\{E^i{}_{ab},D^c{}_{dk},F^j{}_{lm}\}^*=\{-E^i{}_{ab},D^c{}_{dk},F^j{}_{lm}\}. \tag{3.47}$$

So, the asterisk $*$ only changes the sign of $E^i{}_{ab}$, but does not act on all other structure constants. This means also that the matrix γ (3.19) for dual algebra should have the form

$$\gamma^*{}_{AB}=\begin{pmatrix} g_{ab} & 0\\ 0 & \beta_{ik}\end{pmatrix}^*=\begin{pmatrix} g_{ab} & 0\\ 0 & -\beta_{ik}\end{pmatrix}, \tag{3.48}$$

and, therefore, the curvature of the dual manifold has the opposite sign,

$$R^*{}_{abcd}=-R_{abcd}. \tag{3.49}$$

IV. HEAT KERNEL

It should be noted once more that our analysis in this paper is purely *local* (see the discussion in Sec. II.) We are looking for a *universal local* function of the curvature, $\Omega(t)$, (2.9) that describes adequately the low-energy limit of the heat kernel diagonal (up to ''global'' nonanalytical effects that are not studied in this paper!). Our minimal requirement is that this function should

reproduce *all* the terms without covariant derivatives of the curvature in the local Schwinger–De Witt asymptotic expansion of the heat kernel, i.e. it should give *all* the HMDS coefficients a_k (2.3) for *any* symmetric space.

It is well known that the HMDS coefficients have a *universal* explicit structure,[5] i.e. a_k are scalar polynomials of the curvature of the order k with *universal* numerical coefficients that do not depend on the particular form of the symmetric space, on the dimension, etc. It is obvious that any flat subspaces do not contribute in a_k. Moreover, since HMDS coefficients a_k are analytic in the curvature, it is evident that to find this universal structure it is sufficient to consider only symmetric spaces of the *compact* type with positive curvature. Using the factorization property of the heat kernel[5] and the duality between compact and noncompact symmetric spaces, we can obtain then the results for the general case by analytical continuation.

That is why below in this paper we consider only the case of symmetric spaces of the *compact* type when the matrices β_{ik} and γ_{AB} are *positive* definite. Besides, we restrict ourselves, for simplicity, to the scalar operators, i.e. $\mathscr{R}_{\alpha\beta}=0$. The general case will be investigated in a future work.

A. Heat kernel operator

It is not difficult to show that the metric of the symmetric space can be presented in the form

$$g^{\mu\nu}=\gamma^{AB}\xi_A^\mu\xi_B^\nu=g^{ab}P^\mu{}_a P^\nu{}_b+\beta^{ik}L^\mu{}_i L^\nu{}_k\,. \tag{4.1}$$

Indeed, by making use of Eqs. (3.7) and recalling the definition of the matrix K (3.3), it is easy to obtain (4.1) using the explicit expressions (3.33) and (3.34).

Now, having the metric (4.1), we can build the Laplacian for the scalar ($\mathscr{R}_{\alpha\beta}=0$) case,

$$\Box=g^{\mu\nu}\nabla_\mu\nabla_\nu=\gamma^{AB}\xi_A\xi_B\,, \tag{4.2}$$

where $\xi_A=\xi_A^\mu\nabla_\mu$ and the Killing equation (3.5) has been used.

It is not difficult to show that the Laplacian belongs to the center of the enveloping algebra, i.e. it commutes with all the generators of the algebra,

$$[\Box,\xi_A]=0\,. \tag{4.3}$$

Let us now try to represent the heat kernel in terms of a group average, i.e. let us find a formula like

$$\exp(t\Box)=\int dk\ \gamma^{1/2}\Phi(t|k)\exp(k^A\xi_A)\,. \tag{4.4}$$

We formulate first the answer in form of a theorem and prove it below.

Theorem 1: For any compact D-dimensional Lie group generated by ξ_A,

$$[\xi_A,\xi_B]=C^C{}_{AB}\xi_C\,, \tag{4.5}$$

the operator identity takes place,

$$\exp(t\Box)=(4\pi t)^{-D/2}\int dk\ \gamma^{1/2}\ \det\left(\frac{\sinh(k^AC_A/2)}{k^AC_A/2}\right)^{1/2}$$
$$\times\exp\left\{-\frac{1}{4t}\,k^A\gamma_{AB}k^B+\frac{1}{6}\,R_G t\right\}\exp(k^A\xi_A)\,, \tag{4.6}$$

where $\Box=\gamma^{AB}\xi_A\xi_B$, $\gamma^{AB}=(\gamma_{AB})^{-1}$, $\gamma=\det\gamma_{AB}$, γ_{AB} is a symmetric nondegenerate positive definite matrix connecting the generators in adjoint $C_A=(C^B{}_{AC})$ and coadjoint C_A^T representations,

$$C_A^T=-\gamma C_A\gamma^{-1}, \tag{4.7}$$

R_G is the scalar curvature of the group manifold,

$$R_G=-\tfrac{1}{4}\,\gamma^{AB}C^C{}_{AD}C^D{}_{BC}, \tag{4.8}$$

and the integration is to be taken over the whole Euclidean space $\mathbb{R}^D$.

The proof: Let us consider the integral

$$\Psi(t)=\int dk\ \gamma^{1/2}\Phi(k,t)\exp(k^A\xi_A), \tag{4.9}$$

where

$$\Phi(t|k)=(4\pi t)^{-D/2}\ \det\left(\frac{\sinh(k^AC_A/2)}{k^AC_A/2}\right)^{1/2}\ \exp\left\{-\frac{1}{4t}\,k^A\gamma_{AB}k^B+\frac{1}{6}\,R_Gt\right\}. \tag{4.10}$$

To prove the theorem we have to show that $\Psi(t)=\exp(t\Box)$, in other words, that it satisfies the operator equation

$$\partial_t\Psi=\Box\Psi, \tag{4.11}$$

with the initial condition

$$\Psi(t)|_{t=0}=1. \tag{4.12}$$

First, one can show that

$$\xi_B\ \exp(k^A\xi_A)=X_B\ \exp(k^A\xi_A), \tag{4.13}$$

where

$$X_A=X^M{}_A(k)\ \frac{\partial}{\partial k^M} \tag{4.14}$$

are the left-invariant vector fields on the group that have in canonical coordinates the explicit form

$$X^M{}_A(k)=\left(\frac{k^AC_A}{\exp(k^AC_A)-1}\right)^M{}_A. \tag{4.15}$$

Therefore, from the definition of the Laplacian we have

$$\Box\ \exp(k^A\xi_A)=X_2\ \exp(k^A\xi_A), \tag{4.16}$$

$$X_2=\gamma^{AB}X_AX_B. \tag{4.17}$$

Then, introducing the metric on the group manifold,

$$G_{MN}=\gamma_{AB}X^{-1A}{}_MX^{-1B}{}_N, \tag{4.18}$$

and its determinant,

$$G=\det G_{MN}=\gamma \det X^{-2}=\gamma \det\left(\frac{\sinh(k^A C_A/2)}{k^A C_A/2}\right)^2, \tag{4.19}$$

one can obtain the transposition relation

$$(G^{1/2}X_2G^{-1/2})^T=X_2. \tag{4.20}$$

Now, making use of (4.9), (4.16), and (4.20) and integrating by parts, we obtain

$$\Box\Psi(t)=\int dk\ \gamma^{1/2}\ \exp(k^A\xi_A)(G^{1/2}X_2G^{-1/2}\Phi). \tag{4.21}$$

On the other hand, one has, from (4.9),

$$\partial_t\Psi(t)=\int dk\ \gamma^{1/2}\ \partial_t\Phi\ \exp(k^A\xi_A). \tag{4.22}$$

Thus, to prove (4.11) we have to show that

$$\partial_t\Phi=G^{1/2}X_2G^{-1/2}\Phi. \tag{4.23}$$

Substituting the explicit expression for Φ,

$$\Phi(t|k)=\gamma^{-1/4}G^{1/4}(k)(4\pi t)^{-D/2}\ \exp\left\{-\frac{1}{4t}\,k^A\gamma_{AB}k^B+\frac{1}{6}\,R_G t\right\}, \tag{4.24}$$

and using the relations

$$X_2G^{-1/4}=\tfrac{1}{6}\,R_GG^{-1/4} \tag{4.25}$$

and

$$k^A\frac{\partial}{\partial k^A}\,G^{-1/4}=\frac{1}{2}\,(D-\mathrm{tr}\,X)G^{-1/4}, \tag{4.26}$$

where

$$\mathrm{tr}\,X=X^A_A=\mathrm{tr}(k^AC_A\,\coth(k^AC_A)), \tag{4.27}$$

which hold on the group manifold, we convince ourselves that Eq. (4.23) is correct. Thereby it is shown that $\Psi(t)$ really satisfies Eq. (4.11).

Further, from (4.10) it follows immediately that

$$\Phi(t|k)|_{t=0}=\gamma^{-1/2}\delta(k), \tag{4.28}$$

and, therefore, the initial condition (4.12). Thus, we found $\Psi(t)=\exp(t\Box)$ that proves the theorem.

B. Heat kernel diagonal

So, we have found a very nontrivial representation (4.6) that holds on any compact Lie group. How can we proceed now with this useful theorem?

First, we can express the scalar curvature of the group manifold in terms of the scalar curvature of the symmetric space R and that of the isotropy subgroup R_H,

$$R_G=-\,\tfrac{1}{4}\,\gamma^{AB}C^C{}_{AD}C^D{}_{BC}=\tfrac{3}{4}\,R+R_H, \tag{4.29}$$

where

$$R_H = -\tfrac{1}{4}\,\beta^{ik}F^m{}_{il}F^l{}_{km}\,. \tag{4.30}$$

The representation (4.6) is valid for any generators ξ_A satisfying the commutation relations (4.5), and so it is also valid for the infinitesimal isometries (3.40) and (3.41) of the symmetric space. In this case $\Box$ is the usual Laplacian and $\exp(t\Box)$ is the heat kernel operator.

For further use it is convenient to rewrite the integral (4.6) splitting the integration variables $k^A=(q^a,\omega^i)$ in the form

$$\exp(t\Box) = (4\pi t)^{-D/2}\int dq\ d\omega\ \eta^{1/2}\beta^{1/2}\ \det\left(\frac{\sinh((q^aC_a+\omega^iC_i)/2)}{(q^aC_a+\omega^iC_i)/2}\right)^{1/2}$$
$$\times\exp\left\{-\frac{1}{4t}\,(q^ag_{ab}q^b+\omega^i\beta_{ik}\omega^k)+\left(\frac{1}{8}\,R+\frac{1}{6}\,R_H\right)t\right\}\exp(q^aP_a+\omega^iL_i), \tag{4.31}$$

where $\beta=\det\beta_{ik}$, $\eta=\det g_{ab}$. To get the heat kernel explicitly in coordinate representation we have to act with the heat kernel operator $\exp(t\Box)$ on the delta function on M,

$$\exp(t\Box)(x,x') = \exp(t\Box)\,\delta(x,x') = \int dq\ d\omega\ \eta^{1/2}\beta^{1/2}\Phi(t|q,\omega)\exp(q^aP_a+\omega^iL_i)\,\delta(x,x')\,. \tag{4.32}$$

To learn how the operator $\exp(k^A\xi_A)$ acts on a scalar function $f(x)$, let us introduce a new function,

$$\phi(s,k,x) = \exp(sk^A\xi_A)f(x). \tag{4.33}$$

This function satisfies the first-order differential equation,

$$\partial_s\phi = k^A\xi_A\phi = k^A\xi^\mu{}_A(x)\,\partial_\mu\phi, \tag{4.34}$$

with the initial condition of the form

$$\phi|_{s=0} = f(x). \tag{4.35}$$

It is not difficult to prove that

$$\phi(s,k,x) = f(x_0(s,k,x)), \tag{4.36}$$

where $x_0(s,k,x)$ satisfies the equation of characteristics,

$$\frac{dx_0^\mu}{ds} = k^A\xi_A^\mu(x_0), \tag{4.37}$$

with the initial condition

$$x_0^\mu|_{s=0} = x^\mu. \tag{4.38}$$

Therefore, we have

$$\exp(k^A\xi_A)\,\delta(x,x') = \delta(x_0(1,k,x),x'). \tag{4.39}$$

Consider now the operator integrals of the form we need,

$$I(x,x')=\int dq\ d\omega\ \eta^{1/2}\beta^{1/2}Z(q,\omega)\exp(q^aP_a+\omega^iL_i)\,\delta(x,x'),\tag{4.40}$$

where $Z(q,\omega)$ is some analytic function. Using Eq. (4.39), we have

$$\exp(q^aP_a+\omega^iL_i)\,\delta(x,x')=\delta(x_0(1,q,\omega,x,x'),x')=\eta^{-1/2}J(\omega,x,x')\,\delta(q-\bar{q}),\tag{4.41}$$

where $\bar{q}=\bar{q}(\omega,x,x')$ is to be determined from the equation

$$x_0(1,\bar{q},\omega,x,x')=x'\tag{4.42}$$

and $J(\omega,x,x')$ is the Jacobian computed at $x_0=x'$,

$$J(\omega,x,x')=g'^{-1/2}\eta^{1/2}\ \det\left|\frac{\partial x_0^\mu}{\partial q^a}\right|^{-1}_{q=\bar{q},s=1}.\tag{4.43}$$

So, we can now simply integrate over q in (4.40) to get

$$I(x,x')=\int d\omega\ \beta^{1/2}Z(\bar{q}(\omega,x,x'),\omega)J(\omega,x,x').\tag{4.44}$$

If we are interested in the coincidence limit then one has to put finally $x=x'$,

$$I(x,x)=\int d\omega\ \beta^{1/2}Z(\bar{q}(\omega,x,x),\omega)J(\omega,x,x).\tag{4.45}$$

Consider now the equation of characteristics at greater length. Making a change of variables,

$$x^\mu\to\sigma_0^a=\sigma^a(x_0,x')=e^a_{\mu'}(x')\sigma^{\mu'}(x_0,x'),\tag{4.46}$$

we arrive to the equation of a more explicit form,

$$\frac{d\sigma_0^a}{ds}=-(\sqrt{K(\sigma_0)}\cot\sqrt{K(\sigma_0)})^a{}_bq^b-\omega^iD^a{}_{ib}\sigma_0^b.\tag{4.47}$$

Let $\sigma_0^a=\sigma_0^a(s,q,\omega,\sigma^b)$ be the solution of the equation (4.47). Then $\bar{q}$ is to be determined from an equation like (4.42),

$$\sigma_0^a(1,\bar{q},\omega,\sigma^b)=0\tag{4.48}$$

and

$$J(\omega,x,x')=\det\left|-\frac{\partial\sigma_0^a}{\partial q^b}\right|^{-1}_{q=\bar{q},s=1},\tag{4.49}$$

where it has been taken into account $\det(e_a^{\mu'})=g'^{-1/2}\eta^{1/2}$.

Therefore, we have to find the solution to the equation (4.47) near the zero, i.e. assuming σ_0^a to be small. Moreover, we consider mostly the case when the points x and x' are close to each other which means that σ^a is small as well. The equation (4.47) near the point $\sigma_0^a=0$ looks like

$$\frac{d\sigma_0^a}{ds}=-q^a,\tag{4.50}$$

meaning that the momentums q^a are of the same small order.

More precisely, we assume

$$\sigma_0^a \sim \sigma^b \sim q^c \sim \epsilon \ll 1, \tag{4.51}$$

and look for a solution of Eq. (4.47) in the form of a power series in ϵ, i.e. in the form of a Taylor series in σ^a and q^a.

In this way one simply obtains up to quadratic terms

$$\sigma_0^a(s,q,\omega,x,x') = (\exp(-s\omega^i D_i))^a{}_b \sigma^b + \left(\frac{\exp(-s\omega^i D_i)-1}{\omega^i D_i}\right)^a{}_b q^b + O(\epsilon^2). \tag{4.52}$$

With the same accuracy the solution of Eq. (4.48) is

$$\bar{q}^a = \left(\frac{\omega^i D_i \exp(-s\omega^i D_i)}{1-\exp(-s\omega^i D_i)}\right)^a{}_b \sigma^b + O(\sigma^{a2}). \tag{4.53}$$

Further, one finds from (4.52),

$$\det\left|-\frac{\partial \sigma_0^a}{\partial q^b}\right|_{q=\bar{q},s=1} = \det\left(\frac{\sinh(\omega^i D_i/2)}{\omega^i D_i/2}\right) + O(\sigma^a), \tag{4.54}$$

and so, from (4.49),

$$J(\omega,x,x') = \det\left(\frac{\sinh(\omega^i D_i/2)}{\omega^i D_i/2}\right)^{-1} + O(\sigma^a). \tag{4.55}$$

Substituting (4.53) and (4.55) in (4.44) and expanding $Z(\bar{q},\omega)$, we can calculate the integral (4.40) for near points x and x' in the form of an expansion in $\sigma^a(x,x')$.

Therefore, we have found, in particular, a useful exact result for coincidence limit (4.45).

Lemma 2: For an analytical function $Z(q,\omega)$ there holds

$$\begin{aligned} I(x,x) &= \int dq\ d\omega\ \eta^{1/2}\beta^{1/2} Z(q,\omega)\exp(q^a P_a + \omega^i L_i)\,\delta(x,x')|_{x=x'} \\ &= \int d\omega\ \beta^{1/2} Z(0,\omega)\det\left(\frac{\sinh(\omega^i D_i/2)}{\omega^i D_i/2}\right)^{-1}, \end{aligned} \tag{4.56}$$

with the operators P_a and L_i given by (3.40) and (3.41).

Using the obtained results (4.53), (4.55), and (4.56) and substituting the explicit form of our integral (4.31), we get the heat kernel in coordinate representation,

$$\begin{aligned} \exp(t\Box)(x,x') = (4\pi t)^{-D/2}\int d\omega\ \beta_H^{1/2}\ \det\left(\frac{\sinh(\omega^i C_i/2)}{\omega^i C_i/2}\right)^{1/2} \det\left(\frac{\sinh(\omega^i D_i/2)}{\omega^i D_i/2}\right)^{-1} \\ \times\exp\left\{-\frac{1}{4t}\,(\omega^i\beta_{ik}\omega^k + \sigma^a g_{ac}B^c{}_b(\omega)\sigma^b) + \left(\frac{1}{8}R + \frac{1}{6}R_H\right)t\right\} + O(\sigma^a), \end{aligned} \tag{4.57}$$

where $B(\omega) = \{B^a{}_b(\omega)\}$ is a matrix of the form

$$B(\omega)=\left(\frac{\sinh(\omega^i D_i/2)}{\omega^i D_i/2}\right)^{-2}. \tag{4.58}$$

Now, from (3.18) it is not difficult to find that

$$\det\left(\frac{\sinh(\omega^i C_i/2)}{\omega^i C_i/2}\right)=\det\left(\frac{\sinh(\omega^i D_i/2)}{\omega^i D_i/2}\right)\det\left(\frac{\sinh(\omega^i F_i/2)}{\omega^i F_i/2}\right). \tag{4.59}$$

Therefore, the final result, after taking into account (4.59), looks like

$$\exp(t\Box)(x,x')=(4\pi t)^{-D/2}\int d\omega\ \beta^{1/2}\ \det\left(\frac{\sinh(\omega^i F_i/2)}{\omega^i F_i/2}\right)^{1/2}\det\left(\frac{\sinh(\omega^i D_i/2)}{\omega^i D_i/2}\right)^{-1/2}$$
$$\times\exp\left\{-\frac{1}{4t}\,(\omega^i\beta_{ik}\omega^k+\sigma^a g_{ac}B^c_b(\omega)\sigma^b)+\left(\frac{1}{8}\,R+\frac{1}{6}\,R_H\right)t\right\}+O(\sigma^a). \tag{4.60}$$

The coincidence limit of this heat kernel is then simply derived by putting $x=x'$, i.e. $\sigma^a=0$,

$$\exp(t\Box)(x,x)=(4\pi t)^{-D/2}\int d\omega\ \beta^{1/2}\ \det\left(\frac{\sinh(\omega^i F_i/2)}{\omega^i F_i/2}\right)^{1/2}\det\left(\frac{\sinh(\omega^i D_i/2)}{\omega^i D_i/2}\right)^{-1/2}$$
$$\times\exp\left\{-\frac{1}{4t}\,\omega^i\beta_{ik}\omega^k+\left(\frac{1}{8}\,R+\frac{1}{6}\,R_H\right)t\right\}. \tag{4.61}$$

Note that this formula is exact (up to possible nonanalytic topological contributions, see the discussion in Sec. II). This gives a nontrivial example of how the heat kernel can be constructed using only the algebraic properties of the isometries of the symmetric space.

One can derive an alternative nontrivial *formal* representation of this result. Substituting the equation,

$$(4\pi t)^{-p/2}\beta^{1/2}\ \exp\left(-\frac{1}{4t}\,\omega^i\beta_{ik}\omega^k\right)=(2\pi)^{-p}\int dp\ \exp(ip_k\omega^k-tp_k\beta^{kn}p_n) \tag{4.62}$$

into the integral (4.61), and integrating over ω we obtain

$$\exp(t\Box)(x,x)=(4\pi t)^{-d/2}\ \exp\left\{t\left(\frac{1}{8}\,R+\frac{1}{6}\,R_H\right)\right\}\int dp\ \exp(-tp_n\beta^{nk}p_k)$$
$$\times\det\left(\frac{\sinh(-i\ \partial^k F_k/2)}{-i\ \partial^k F_k/2}\right)^{1/2}\det\left(\frac{\sinh(-i\ \partial^k D_k/2)}{-i\ \partial^k D_k/2}\right)^{-1/2}\delta(p), \tag{4.63}$$

where $\partial^k=\partial/\partial p_k$. Therefrom, integrating by parts and changing the integration variables $p_k\to it^{-1/2}p_k$ we get finally an expression without any integration,

$$\exp(t\Box)(x,x)=(4\pi t)^{-d/2}\ \exp\left(t\left(\frac{1}{8}\,R+\frac{1}{6}\,R_H\right)\right)\det\left(\frac{\sinh(\sqrt{t}\partial^k F_k/2)}{\sqrt{t}\partial^k F_k/2}\right)^{1/2}$$
$$\times\det\left(\frac{\sinh(\sqrt{t}\partial^k D_k/2)}{\sqrt{t}\partial^k D_k/2}\right)^{-1/2}\exp(p_n\beta^{nk}p_k)\Big|_{p=0}. \tag{4.64}$$

This formal solution should be understood as a power series in the derivatives ∂^i that is well defined and determines the heat kernel asymptotic expansion at $t\to 0$.

C. Heat kernel asymptotics

Using the obtained result one can get easily the explicit form of the generating function for HMDS coefficients (2.9),

$$\Omega(t|x,x)=(4\pi t)^{-p/2}\int d\omega\ \beta^{1/2}\ \det\left(\frac{\sinh(\omega^i F_i/2)}{\omega^i F_i/2}\right)^{1/2}\ \det\left(\frac{\sinh(\omega^i D_i/2)}{\omega^i D_i/2}\right)^{-1/2}$$
$$\times\exp\left\{-\frac{1}{4t}\,\omega^i\beta_{ik}\omega^k+\left(\frac{1}{8}\,R+\frac{1}{6}\,R_H\right)t\right\}. \tag{4.65}$$

This formula can be used now to generate *all* HMDS coefficients a_k for *any* symmetric space, i.e. for *any space with covariantly constant curvature*, simply by expanding it in a power series in t.

Changing the integration variables $\omega\to\sqrt{t}\omega$ and introducing a Gaussian averaging over ω,

$$\langle f(\omega)\rangle=(4\pi)^{-p/2}\int d\omega\ \beta^{1/2}\ \exp\left(-\frac{1}{4}\,\omega^i\beta_{ik}\omega^k\right)f(\omega), \tag{4.66}$$

we get

$$\Omega(t|x,x)=\exp\left\{\left(\frac{1}{8}\,R+\frac{1}{6}\,R_H\right)t\right\}\left\langle\det\left(\frac{\sinh(\sqrt{t}\omega^i F_i/2)}{\sqrt{t}\omega^i F_i/2}\right)^{1/2}\det\left(\frac{\sinh(\sqrt{t}\omega^i D_i/2)}{\sqrt{t}\omega^i D_i/2}\right)^{-1/2}\right\rangle. \tag{4.67}$$

Using the standard Gaussian averages,

$$\langle 1\rangle=1,\quad \langle\omega^i\rangle=0,\quad \langle\omega^i\omega^k\rangle=\tfrac{1}{2}\,\beta^{ik},$$
$$\langle\omega^i_1\cdots\omega^{i_{2n+1}}\rangle=0,$$
$$\langle\omega^{i_1}\cdots\omega^{i_{2n}}\rangle=\frac{(2n)!}{2^{2n}n!}\,\beta^{(i_1i_2}\cdots\beta^{i_{2n-1}i_{2n})}, \tag{4.68}$$

one can obtain now all HMDS coefficients in terms of various foldings of the quantities $D^a{}_{ib}$ and $F^j{}_{ik}$ with the help of matrix β^{ik}. All these quantities are curvature invariants and can be expressed directly in terms of a Riemann tensor. Thereby one finds *all covariantly constant terms in all HMDS coefficients* in a manifestly covariant way. We are going to obtain the explicit formulas in a further work.

V. CONCLUDING REMARKS

In the present paper we continued the study of the heat kernel that we conducted in our papers (Refs. 4, 10, 15, and 21). Here we have discussed some ideas connected with the point that was left aside in previous papers, namely, the problem of calculating the low-energy limit of the effective action in quantum gravity. We have analyzed in detail the status of the low-energy limit in quantum gravity and stressed the central role playing by the Lie group of isometries that naturally appears when generalizing consistently the low-energy limit to curved space.

We have proposed a promising, to our mind, approach for calculating the low-energy heat kernel and realized, thereby, the idea of partial summation of the terms without covariant derivatives in local asymptotic expansion for computing the effective action that was suggested in Refs. 2 and 4.

Of course, there are many unsolved problems left. First of all, one has to obtain *explicitly* the covariantly constant terms in HMDS coefficients. This would be the opposite case to the high-derivative approximation[15,16] and can be of certain interest in mathematical physics. Then, we still do not know how to calculate the low-energy heat kernel in the general case of covariantly constant curvatures, i.e. when all background curvatures ($\mathfrak{R}=\{R_{\mu\nu\alpha\beta},\mathscr{R}_{\mu\nu},Q\}$) are present. Besides, it is not perfectly clear how to do the analytical continuation of Euclidean low-energy effective action to the space of Lorentzian signature for obtaining physical results.

Let us make a final remark concerning the relation of our work to that of previous authors, who seems to treat almost the same problem (see the review paper of Camporesi in Ref. 22 and references therein and Ref. 27). What we have been trying to do in the present paper is rather different from what the other authors did. These are the *global* topological problems and effects that are of *prime* interest in those papers. The authors of those papers make use of the techniques of geometric analysis on homogenous spaces, with an emphasis on the *exact* results. That is why only very special concrete examples of symmetric spaces (group manifolds, spheres, rank-one symmetric spaces, split-rank symmetric spaces, etc.), which allow us to obtain closed formulas were considered. The results obtained in this way are presented in terms of the root vectors and their multiplicities. The complexity of the method depends critically on the rank of symmetric space. As far as we know the explicit results for the heat kernel are obtained for rank-one and for some rank-two symmetric spaces.

We are interested, in contrary, first of all in *local* effects of strongly curved *approximately homogeneous* manifolds. Therefore, our approach is thought of only as a *framework for a perturbation theory* in nonhomogeneity. In typical physical problems we need a rather *general approximation scheme* instead of exact exceptional results. The point is that we need the effective action as a functional of a *generic* metric that could be varied to obtain the physical currents.

There is, of course, the difficult question, of whether the global effects might be neglected in comparison with local ones. This question is *open*. We can only say that if it is the case, i.e. *if the local effects are dominant*, then the heat kernel is given by explicit covariant formulas obtained in Sec. IV.

VI. NOTE ADDED

After this paper was completed we became aware of the similar results on the heat kernel in symmetric spaces by Fegan (Ref. 27). Though they were obtained in a completely different rather geometrical setting incorporating the nontrivial global topology, one would, due to intrinsic locality of the heat kernel expansion, expect that the two expressions, i.e. ours and that of Ref. 27, should coincide under an appropriate representation of the special functions obtained in Ref. 27.

Another comment concerns the meaning of the effective potential. If the symmetry in question is that of Euclidean space (that is not the case, in general!) our expansion should reduce to the quasilocal expansion of Brown and Duff,[28] which was extended to curved spaces by Hu and O'Connor.[29] Therefore, one might consider our work as an extension of the quasilocal expansion to a symmetric space and quasihomogeneous setting.

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Massive NGT and spherically symmetric systems

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The arguments leading to the introduction of the massive Nonsymmetric Gravitational action are reviewed [J. W. Moffat, J. Math. Phys. **36**, 3722 (1995), Phys. Lett. B **355**, 447 (1995)], leading to an action that gives asymptotically well-behaved perturbations on General Relativity (GR) backgrounds. Through the analysis of spherically symmetric perturbations about GR (Schwarzschild) and Nonsymmetric Gravitational Theory (NGT) (Wyman-type) static backgrounds, it is shown that spherically symmetric systems are not guaranteed to be static, and hence Birkhoff's theorem is not valid in NGT. This implies that in general one must consider time dependent exteriors when looking at spherically symmetric systems in NGT. For the surviving monopole mode considered here there is no energy flux as it is short ranged by construction. Further work on the spherically symmetric case will be motivated through a discussion of the possibility that there remain additional modes that do not show up in weak field situations, but nonetheless exist in the full theory and may again result in bad global asymptotics. A presentation of the action and field equations in a general frame is given in the course of the paper, providing an alternative approach to dealing with the algebraic complications inherent in NGT, as well as offering a more general framework for discussing the physics of the antisymmetric sector. © *1996 American Institute of Physics.* [S0022-2488(96)01501-5]

I. INTRODUCTION

In General Relativity (GR), just as in Maxwell's electrodynamics, one finds that given a spherically symmetric system, there are no dynamical degrees of freedom in the theory. This is Birkhoff's theorem, and it implies that a time dependent source will not excite modes in the gravitational system, so that outside this source the system must be physically equivalent to the Schwarzschild solution (the nontrivial static spherically symmetric spacetime). It has been further established[1,2] that the solution is stable when perturbed, so that small deviations from spherical symmetry do not alter the large scale features of the spacetime, and systems that are only approximately spherically symmetric are therefore still very well modeled by the Schwarzschild solution. This establishes that the phenomenology of the Schwarzschild solution is physically relevant.

To see that Birkhoff's theorem is not a generic feature of physical theories one need look no further than a scalar field. However the example that is important for this work is the (massive) Kalb–Ramond action[3] which (as will be demonstrated in Section III) has a single mode that is time dependent in general. As will be shown in Section II, the massive Nonsymmetric Gravitational Theory[4,5] (mNGT as opposed to the older versions of the theory, referred to as NGT, or massless NGT) becomes identically a massive Kalb–Ramond field with an additional curvature coupling term when considered as a perturbation about a Ricci-flat GR background, so the result that NGT has a monopole mode is not surprising. The mode considered here is short ranged, so that far enough away from the source one finds that the solution will be dominated by Schwarzschild behavior, and there is no energy flux. However, after demonstrating that spherically symmetric fields in the skew sector are not static in general, it will be shown in Section VI that the symmetric sector will also no longer be static, through examination of a similar perturbation about the mNGT background discussed in Section V. This means that no static solutions can be consid-

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ered rigorously as an exterior solution unless the solution is globally static (i.e. the interior is static as well).

The results in this paper are obtained through an examination of linearized perturbations, although the conclusions must hold in general as Birkhoff's theorem would imply that these fields must be static as well. What cannot be examined in this fashion is whether in the full nonlinear theory more modes become excited. In particular, one will see in the case of a perturbation about a GR background (in Section II) that there are three propagating modes, even though the absence of gauge invariant kinetic terms in the full theory would suggest that all six modes in the antisymmetric metric could be independent degrees of freedom (as yet, the number of degrees of freedom in mNGT has not been rigorously established). Although this issue is not addressed directly in this work, the ability to recast the theory in a general basis given in Section IV sets the stage for a complete analysis of the spherically symmetric system in NGT. Given that there is an additional mode in the general spherically symmetric system, how the fields may or may not approach an asymptotically flat spacetime should then be addressed, and also whether evolution singularities of the type discussed in Ref. 6 are encountered.

II. MASSIVE NGT

The original version of NGT[7] grew out of a re-interpretation of the Einstein-Straus[8,9] unified field theory as a purely gravitational system. The antisymmetric part of the metric and connection operationally produce different modes of parallel transport and index contraction,[7,10,11] where the algebra is consistent with an enlargement of the tangent vector space to its hyperbolic complex extension.[12–14] It is important to note that the action cannot support the additional Bianchi identities and gauge invariance related to the extension of the tangent bundle, simply because the base manifold is locally diffeomorphic to $\mathbb{R}^4$, and the variational principle is based on an integration over this real manifold. Any change of gauge that mixes real and hyperbolic complex covectors will cause the volume element to pick up a hyperbolic complex piece, and the action will no longer be real.

The hyperbolic complex structure is unnecessary for an operational discussion of the theory (although it may be relevant for a more fundamental discussion of its physical interpretation), and in this paper all quantities will be considered real, allowing antisymmetric contributions to the metric and connection coefficients. The dynamics of the theory will be determined from the first order action ($G=c=1$):

$$S=\int d^4x\{-\mathbf{g}^{\mu\nu}R^{\mathrm{NS}}_{\mu\nu}[\Gamma]-\mathbf{g}^{\mu\nu}\partial_{[\mu}W_{\nu]}+\mathbf{l}^{\mu}\Gamma_{\mu}+\tfrac{1}{2}\alpha\mathbf{g}^{(\mu\nu)}W_{\mu}W_{\nu}+\tfrac{1}{4}m^2\mathbf{g}^{[\mu\nu]}g_{[\mu\nu]}\}+S_M\,, \quad (1)$$

where

$$\frac{\delta S_M}{\delta g^{\mu\nu}}=\mathbf{T}_{\mu\nu}\,, \quad (2)$$

is the matter stress energy tensor derived from the variation of the matter action S_M, that acts as a source in the gravitational field equations. The Ricci-like tensor for NGT appearing in (1) is written as:

$$R^{\mathrm{NS}}_{\mu\nu}=\partial_{\alpha}\Gamma^{\alpha}_{\mu\nu}-\tfrac{1}{2}(\partial_{\nu}\Gamma^{\alpha}_{\mu\alpha}+\partial_{\mu}\Gamma^{\alpha}_{\alpha\nu})+\Gamma^{\alpha}_{\mu\nu}\Gamma^{\beta}_{(\alpha\beta)}-\Gamma^{\alpha}_{\beta\nu}\Gamma^{\beta}_{\mu\alpha}\,, \quad (3)$$

and a mass term for $g_{[]}$ has been included along with a term quadratic in W as new features of the action. As will become clear shortly, α may be fixed uniquely by requiring good asymptotic behavior of perturbations about GR backgrounds. The new parameter in the massive action (m) is an inverse length scale that must be constrained by experiment, and l is a Lagrange multiplier employed to enforce the vanishing of the trace of the antisymmetric part of the connection coefficients: $\Gamma_{\mu}=\Gamma^{\alpha}_{[\mu\alpha]}$.

The field equations related to the metric compatibility conditions are derived through the variations:

$$\frac{\delta S}{\delta \mathbf{l}^{\mu}} = \Gamma_{\mu} = 0, \tag{4a}$$

$$\frac{\delta S}{\delta W_{\mu}} = \partial_{\nu}\mathbf{g}^{[\nu\mu]} + \alpha \mathbf{g}^{(\mu\nu)} W_{\nu} = 0, \tag{4b}$$

$$\begin{aligned}\frac{\delta S}{\delta \Gamma^{\gamma}_{\sigma\omega}} = {} & \partial_{\gamma}\mathbf{g}^{\sigma\omega} - \mathbf{g}^{\sigma\omega}\Gamma^{\alpha}_{(\gamma\alpha)} + \mathbf{g}^{\alpha\omega}\Gamma^{\sigma}_{\alpha\gamma} + \mathbf{g}^{\sigma\alpha}\Gamma^{\omega}_{\gamma\alpha} - \tfrac{1}{2}\delta^{\omega}_{\gamma}(\partial_{\alpha}\mathbf{g}^{\sigma\alpha} + \mathbf{g}^{\alpha\beta}\Gamma^{\sigma}_{\alpha\beta} - \mathbf{l}^{\sigma}) \\ & - \tfrac{1}{2}\delta^{\sigma}_{\gamma}(\partial_{\alpha}\mathbf{g}^{\alpha\omega} + \mathbf{g}^{\alpha\beta}\Gamma^{\omega}_{\alpha\beta} + \mathbf{l}^{\omega}).\end{aligned} \tag{4c}$$

Contracting on either index of (4c) and solving for the (anti-)symmetric parts of the divergence of the densitized inverse metric results in the determination of the Lagrange multiplier using (4b): $\mathbf{l}^{\sigma} = (\alpha/3)\,\mathbf{g}^{(\sigma\omega)}W_{\omega}$. This also allows one to simplify the Kronecker-δ terms, and determine the compatibility conditions in undensitized form as:

$$\partial_{\gamma} g_{\mu\nu} - g_{\mu\alpha}\Gamma^{\alpha}_{\nu\gamma} - g_{\alpha\nu}\Gamma^{\alpha}_{\gamma\mu} = \tfrac{2}{3}\alpha(g_{\mu[\gamma}g_{\alpha]\nu} + \tfrac{1}{2}g_{\mu\nu}g_{[\gamma\alpha]})g^{(\alpha\beta)}W_{\beta}, \tag{5}$$

where the inverse of the metric has been defined by $g_{\mu\alpha}g^{\alpha\nu} = \delta^{\nu}_{\mu}$, which has been used in order to rewrite the compatibility conditions in terms of the components of the metric $g_{\mu\nu}$.

The remaining field equations derived from the variation of the action with respect to $g^{\mu\nu}$ may be written as:

$$\mathscr{R}_{\mu\nu} := R^{\mathrm{NS}}_{\mu\nu} + \partial_{[\mu}W_{\nu]} - \tfrac{1}{2}\alpha W_{\mu}W_{\nu} - \tfrac{1}{4}m^{2}(g_{[\mu\nu]} - g_{\alpha\mu}g_{\nu\beta}g^{[\alpha\beta]} + \tfrac{1}{2}g_{\nu\mu}g^{[\alpha\beta]}g_{[\alpha\beta]}) = T_{\mu\nu} - \tfrac{1}{2}g_{\nu\mu}T, \tag{6}$$

where $T = g^{\mu\nu}T_{\mu\nu}$, and the tensor $\mathscr{R}$ has been introduced in order to simplify the discussion of the field equations. One may translate the conventions used here to those in Ref. 4 by taking $W \to -\frac{2}{3}W, T_{\mu\nu} \to -8\pi T_{\mu\nu}$, $\alpha \to -\frac{9}{4}\sigma$, and adjusting the definitions of the inverse metric: $g^{\mu\nu} \to g^{\nu\mu}$. To see the equivalence of the action, one further needs to rewrite Γ in terms of the unconstrained W connection, and drop the contribution from the Lagrange multiplier l.

The action for massless NGT is given by (1) with $m = \alpha = 0$. As will be demonstrated, the new terms have been introduced in order to make all skew modes short ranged when considering perturbations about GR backgrounds. One performs this expansion about a symmetric, Ricci-flat background, where one assumes that all background curvatures fall off at worst as $1/r$ as $r \to \infty$. This allows one to talk sensibly of energy-momentum and decompose fields via a spin projection, so that higher order poles and negative energy (ghost) modes may be identified, as well as avoiding the full nonsymmetric structure of a more general background that would make the analysis far more complicated. One considers a perturbation of all quantities about a symmetric GR background as in[15]:

$$g_{\mu\nu} \to g_{(\mu\nu)} + h_{\mu\nu}, \quad \Gamma^{\alpha}_{\mu\nu} \to \left\{ \begin{matrix} \alpha \\ \mu\nu \end{matrix} \right\} + \gamma^{\alpha}_{\mu\nu}, \tag{7}$$

where W, l and T are considered to be first order in the perturbation (as the background is assumed to be Ricci-flat, there one has $T_{\mu\nu} = 0$). As usual, indices will be ''raised'' and ''lowered'' by the symmetric background metric, and the covariant derivative ∇ is associated with the back-

ground Christoffel symbols { } determined from the background metric in the usual manner. Corrections to the background curvatures, field equations and Lagrangian at each order in the perturbation will be indicated by a superscript as: ${}^0R, {}^1R \cdots$.

The first order correction to the compatibility equation (5) can be solved explicitly for γ to yield:

$$\gamma^{\alpha}_{\mu\nu} = \tfrac{1}{2} g^{\alpha\beta}(\nabla_\nu h_{\beta\mu} + \nabla_\mu h_{\nu\beta} - \nabla_\beta h_{\mu\nu}) + \tfrac{2}{3}\alpha \delta^{\alpha}_{[\mu} W_{\nu]}, \tag{8}$$

and $\gamma_\mu = \gamma^{\alpha}_{[\mu\alpha]}$ is seen to vanish by the linearization of the skew divergence equation:

$$-\nabla_\nu h^{[\mu\nu]} = \alpha W^\mu. \tag{9}$$

In massless NGT,[10] one had (8), (9) with $\alpha = 0$, and hence there was no relation between the metric degrees of freedom and those of W. The skew part of the linearization of equation (6) with $m = 0$ as well as $\alpha = 0$ became:

$${}^1\mathscr{R}_{[\mu\nu]} = {}^1R^{\mathrm{NS}}_{[\mu\nu]} + \partial_{[\mu} W_{\nu]} = \nabla_\alpha \gamma^{\alpha}_{[\mu\nu]} + \partial_{[\mu} W_{\nu]} = T_{[\mu\nu]}. \tag{10}$$

The symmetric contribution, are the equations for a metric perturbation in GR,[16] and will be ignored in the remainder of this section. Using (9) with $\alpha = 0$, the assumption that the background is Ricci-flat (${}^0R_{\mu\nu} = 0$), and the commutation relation (for an arbitrary tensor B):

$$\nabla_{[\alpha}\nabla_{\beta]} B_{\mu\nu} = -\tfrac{1}{2}(B_{\omega\nu}\,{}^0R^{\omega}{}_{\mu\alpha\beta} + B_{\mu\omega}\,{}^0R^{\omega}{}_{\nu\alpha\beta}), \tag{11}$$

(10) simplifies to:

$$\nabla^\alpha \nabla_\alpha h_{[\mu\nu]} - 2\partial_{[\mu} W_{\nu]} - 4\,{}^0R^{\alpha}{}_{\mu}{}^{\beta}{}_{\nu} h_{[\alpha\beta]} = \nabla^\alpha F_{\mu\nu\alpha} - 2\partial_{[\mu} W_{\nu]} - 8\,{}^0R^{\alpha}{}_{\mu}{}^{\beta}{}_{\nu} h_{[\alpha\beta]} = -2T_{[\mu\nu]}. \tag{12}$$

The second form is given in terms of the curl of the skew metric ($F_{\gamma\mu\nu} = \partial_\gamma h_{\mu\nu} + \partial_\nu h_{\gamma\mu} + \partial_\mu h_{\nu\gamma}$), in order to more easily demonstrate the result found previously by Damour, Deser, and McCarthy[17,18] (using the fact that $\nabla^\gamma \nabla^\nu F_{\mu\nu\gamma} = 0$ about a Ricci-flat background), that these antisymmetric perturbations will in general have bad asymptotic behavior. Although written as if the skew metric were a gauge field, the presence of the curvature coupling term implies that the associated gauge invariance is not present,[19] and one is not allowed to make any choice of gauge in order to simplify this sector. One proceeds by taking the divergence of (12) and choosing the gauge $\nabla^\alpha W_\alpha = 0$ (the theory had a $U(1)$ invariance as W only appeared in the action in a curl) to find:

$$\nabla^\alpha \nabla_\alpha W_\mu - 8\nabla^\nu [\,{}^0R^{\alpha}{}_{\mu}{}^{\beta}{}_{\nu} h_{[\alpha\beta]}] = -2\nabla^\nu T_{[\mu\nu]}. \tag{13}$$

Notice that the background curvature acts as a source here, so that even if one postulates that the matter source is conserved, this curvature coupling (and in general other nonlinear terms) will still exist as a source, causing W to propagate and have asymptotic behavior consistent with a massless field ($\sim 1/r$ along the forward light cone). Using this asymptotic behavior to determine h from (12) results in a source with $\sim 1/r$ behavior, causing the field h not to fall off as $r \to \infty$ along the forward light cone. This analysis is correct since one has assumed that the background curvature falls off fast enough, and hence the potential term in (13) can be treated as a source, without changing the asymptotic behavior of the fields. It must be stressed that one is assuming that the background *and* the radiative fields fall off at least as fast as $\sim 1/r$, and what has actually been derived here is a contradiction of this, since h is driven to a constant and can no longer be considered as a perturbative mode.

Any analysis of this sort also supposes that a solution of the linearized field equations does in fact correspond to an exact solution of the full nonlinear field equations. This is the case in GR[16,20]

at least for source free equations, but no such result exists yet for any of the models considered here. It is possible to take the stance that NGT is not linearization-stable, so that this sort of analysis necessarily produces spurious results that do not correspond to global solutions, but then one is denying the ability to do any sort of perturbative analysis without the existence of an exact solution to back it up. Due to the scarcity of solutions, and the apparent existence of weak-field perturbative situations, this would seem an unreasonable position to adopt.

This result is not confined to curved backgrounds, and in fact the analysis about Minkowski space will serve to explicitly demonstrate the higher order pole leading to bad fall-off. Since this curvature coupling, and any nonlinear effects in general, will act as a nonconserved source term in the skew sector, the linearization that correctly represents the full nonlinear field equations in the asymptotic region will have a nonconserved source term. This is no more than the observation that once again, the full NGT action does not possess any form of additional gauge invariance in the skew sector. A gauge field coupled to a source (or matter) in a manner that violates gauge invariance may have drastically different behavior than the empty space and apparently gauge invariant field equations, if indeed the action is consistent at all. Any analysis that attempts to determine the propagator or asymptotic behavior of the field must take the form of the source (or coupling to other fields) into account.

A trivial example of this is given by considering the Maxwell action. Coupling the usual gauge invariant kinetic terms to a nonconserved source gives an inconsistent set of field equations, and adding some sort of gauge fixing term will give a consistent set of equations, but the scalar ghost mode will be excited and depending on the gauge there may be higher order poles in the solution. The linearized field equations considered outside the source resemble those of the gauge invariant theory in a particular gauge, but treating them as such will not give asymptotic behavior that follows from coupling to the nonconserved source. The situation in NGT is more akin to enforcing the gauge condition in the action through the use of an auxiliary field as: $b\partial_\mu A^\mu$.[21,22] Source conservation and absence of ghosts relies on whether or not the scalar Lagrange multiplier field b has a source or not in the wave equation that determines it, and is thus a global question. Given that the source for A is not conserved, then b propagates and there are higher order poles in the solution for A, leading to fields that do not fall off as $r\to\infty$ along the forward light cone.

Considering the field equations for massless NGT linearized from (12) about Minkowski space:

$$\Box h_{[\mu\nu]}-2\partial_{[\mu}W_{\nu]}=-2T_{[\mu\nu]}, \tag{14a}$$

$$\partial_\nu h^{[\mu\nu]}=0, \tag{14b}$$

($\partial^\nu T_{[\nu\mu]}\neq 0$), one may take a divergence (to find a wave equation for W) or a curl (to remove W) of the first of these, resulting in the unique consistent solution:

$$h_{[\mu\nu]}=-2\Box^{-1}[T_{[\mu\nu]}+2\Box^{-1}\partial^\alpha\partial_{[\mu}T_{[\alpha\nu]]}],$$

$$W_\mu=-2\Box^{-1}\partial^\nu T_{[\mu\nu]}. \tag{15}$$

The presence of the higher order pole (and consequent bad fall-off) is now obvious from the presence of the $\Box^{-2}$ term in the Green's function solution, and is no more than the result of vanNieuwenhuizen[23] who showed that the only healthy quadratic actions built of antisymmetric tensor fields are the so-called Kalb–Ramond[3] (massless or massive) actions. One also notes that there are 5 modes here: 3 in h, since 3 are determined algebraically by the second equation in (14), and 2 in W due to the previously mentioned $U(1)$ gauge invariance.[24] If it is assumed that the (matter) source is conserved, the higher order poles are removed at linear order, but show up in the second order correction to the fields, again causing a breakdown of the perturbative analysis.

This analysis correctly represents the asymptotic behavior of the fields (W,h), and is equivalent to equation (18) of Ref. 25, where the higher order pole resides in the projection operator: $P(1^+)$. One also sees the true propagating nature of W, and this is borne out by the analysis in Refs. 26 and 27 where there are five degrees of freedom evolving from each Cauchy surface, the extra two of which are associated with the field W. That a Lagrange multiplier is propagating merely signifies that it is a determined multiplier, with its evolution derived from the field equations[15] and not freely fixable as was done in Refs. 28 and 29 and in the next to last section of Ref. 24 where *ad hoc* constraints were imposed on the linearized theory in order to obtain the dynamics of a Kalb–Ramond theory. That these constraints cannot exist is clear from the lack of gauge invariance in the full NGT action.

The result of vanNieuwenhuizen does however motivate a potential solution to this problem, since the massive Kalb–Ramond theory does not require a conserved current and yet has no ghost modes, higher order poles or tachyons. The additional terms in the action for mNGT (1) are introduced in order to allow the linearized field equations of NGT to take on this form in the antisymmetric sector. These two terms play slightly different roles: the W^2 term causes W to be determined in terms of metric functions directly (α is fixed in order to find the correct form of the kinetic energy terms), and the mass term for $g_{[]}$ makes the skew sector short-ranged, and ensures that the linearized field equations remain consistent when expanding about a flat background.

Thus mNGT should have a linearization about Minkowski space of the form:

$$\partial^\alpha F_{\mu\nu\alpha}+m^2 h_{[\mu\nu]}=J_{[\mu\nu]}. \tag{16}$$

The solution to (16) can be found by taking a divergence and substituting back in to find:

$$h_{[\mu\nu]}=\Box^{-1}\left[J_{[\mu\nu]}+\frac{2}{m^2}\partial^\alpha\partial_{[\mu}J_{[\alpha\nu]]}\right],$$

$$\partial^\nu h_{[\mu\nu]}=\frac{1}{m^2}\partial^\nu J_{[\mu\nu]}. \tag{17}$$

The higher order poles have disappeared, and it can be shown that the linearized Hamiltonian is weakly positive definite and that ghost modes are removed through the algebraic conditions that couple them locally to the source in (17). About a more general background one can allow a curvature coupling term, since it will not affect the behavior of the fields asymptotically once the background is assumed to fall off appropriately. Choosing the theory that results in this behavior in the linearized theory will fix α uniquely.

Returning now to the field equations of mNGT expanded about a GR background following from (6), one finds:

$${}^1\mathscr{R}_{\mu\nu}={}^1R_{\mu\nu}+\frac{1}{\alpha}\nabla_{[\mu}\nabla^\alpha h_{[\alpha\nu]]}-\frac{1}{2}m^2 h_{[\mu\nu]}=T_{\mu\nu}-\frac{1}{2}g_{\nu\mu}T, \tag{18}$$

where the first order correction to the ''Ricci'' tensor is given by:

$${}^1R_{\mu\nu}=\nabla_\alpha\gamma^\alpha_{\mu\nu}-\nabla_{(\nu}\gamma^\alpha_{\alpha\mu)}. \tag{19}$$

Again ignoring the symmetric GR perturbations, the antisymmetric part of (18) is:

$$\nabla_\alpha\gamma^\alpha_{[\mu\nu]}+\frac{1}{\alpha}\nabla_{[\mu}\nabla^\alpha h_{[\alpha\mu]]}-\tfrac{1}{2}m^2 h_{[\mu\nu]}=-\tfrac{1}{2}(\nabla^\alpha F_{\mu\nu\alpha}+m^2 h_{[\mu\nu]})-2\nabla^\alpha\nabla_{[\mu}h_{[\alpha\nu]]}$$
$$+\frac{1}{\alpha}\left[1+\frac{2}{3}\alpha\right]\nabla_{[\mu}\nabla^\alpha h_{[\alpha\nu]]}=T_{[\mu\nu]}. \tag{20}$$

Requiring that this reduce to the massive Kalb–Ramond field equations (16) determines the (previously arbitrary) coupling: $\alpha=3/4$. The last two terms can be reduced to a curvature term to give:

$$\nabla^{\alpha}F_{\mu\nu\alpha}+m^2h_{[\mu\nu]}-4^0R^{\alpha}{}_{[\mu}{}^{\beta}{}_{\nu]}h_{[\alpha\beta]}=-2T_{[\mu\nu]}, \tag{21}$$

so the skew sector perturbations are well-behaved when perturbing about any asymptotically flat GR background.

Expanding the action (1) to second order (ignoring surface terms) gives:

$${}^2\mathscr{L}=-{}^2R-\tfrac{1}{2}h^1R+h^{\mu\nu 1}R_{\mu\nu}+h^{\mu\nu}\partial_{[\mu}W_{\nu]}+\tfrac{1}{2}\alpha W^{\mu}W_{\mu}+l^{\mu}\Gamma_{\mu}-\tfrac{1}{4}m^2h^{[\mu\nu]}h_{[\mu\nu]} \tag{22}$$

and once compatibility is imposed, followed by the removal of W, this becomes:

$${}^2\mathscr{L}=\frac{1}{12}F^{\mu\nu\gamma}F_{\mu\nu\gamma}-\frac{1}{4}m^2h^{[\mu\nu]}h_{[\mu\nu]}-\nabla^{\gamma}h^{[\mu\nu]}\nabla_{\nu}h_{[\gamma\mu]}-\left(\frac{1}{2\alpha}+\frac{1}{3}\right)\nabla_{\nu}h^{[\mu\nu]}\nabla^{\gamma}h_{[\mu\gamma]}. \tag{23}$$

Choosing $\alpha=3/4$ results in kinetic terms identical to those of Kalb–Ramond theory on a GR background, giving the skew sector action:

$${}^2\mathscr{L}=\tfrac{1}{12}F^{\mu\nu\gamma}F_{\mu\nu\gamma}-\tfrac{1}{4}m^2h^{[\mu\nu]}h_{[\mu\nu]}-h^{[\mu\nu]}h^{[\alpha\beta]0}R_{\alpha\mu\beta\nu}, \tag{24}$$

which reproduces the linearized field equations (21). Thus the massive NGT action will be (1) with $\alpha=3/4$,[4] giving the action (24) for perturbations about a GR background and guaranteeing good asymptotic behavior for these fields.

Although it has been established that the perturbation equations about a GR background are a consistent system resulting in good fall-off for the skew sector, it is not clear whether an asymptotic perturbation actually corresponds to a global solution (linearization stability). The (seemingly contrived) asymptotic limit of gauge invariant kinetic terms cannot be reflected in the full action, since there is no room for the additional gauge invariance in theories constructed from antisymmetric fields in this manner. This means that in general that one expects more (perhaps all 6) degrees of freedom in the skew sector evolving as degrees of freedom in a Cauchy analysis, whereas in any spacetime that has an asymptotically flat region only three will survive. This situation could be similar to that found in Ref. 6, where vector fields were seen to increase their degrees of freedom when gravitational effects are taken into account. In order to obtain an asymptotically flat spacetime (with the reduced degrees of freedom of the vector fields) from physically reasonable initial data, the evolution equations were seen to have to encounter singularities. This is generally considered to be a sign of instability, and certainly not a desirable feature in any theory. Perturbations about NGT backgrounds should also be considered, since the physically interesting NGT solutions are most likely those that are not ''close'' to a GR solution.[30] It is hoped that a more complete analysis of the general spherically symmetric system should be able to say something about this issue, since it will certainly tell one how many degrees of freedom survive and how they couple to external fields, and hopefully something about how the system may or may not approach an asymptotically flat spacetime.

It is also true that the form of the action (1) is far from unique. In particular, one could replace the W^2 term with some combination of W^2 and $(1/\sqrt{-g})\,g_{(\mu\nu)}\partial_{\alpha}[\mathbf{g}^{[\mu\alpha]}]\partial_{\gamma}[\mathbf{g}^{[\nu\gamma]}]$, giving the same perturbation equations (21), and resulting in an arbitrary coupling constant in the action. Further, since there is nothing preventing one from adding $\Gamma_{[]}$ terms (they are tensors) or even infinite strings of terms of the form: $g_{(\alpha\beta)}g^{(\beta\gamma)}\cdots$ or $g_{[\alpha\beta]}g^{[\beta\gamma]}\cdots$ (which conveniently disappear in the asymptotic expansion), there is clearly an infinite number of actions that do this. These examples seem extremely unnatural and will not be considered further here, although the results of this paper would not change significantly for these more general actions.

III. SPHERICALLY SYMMETRIC PERTURBATION OF THE SCHWARZSCHILD SOLUTION IN A COORDINATE BASIS

The absence of a Birkhoff theorem may be derived from the perturbation equations (21) developed in Section II. In general the spherically symmetric fields in the skew sector will not be static, although the symmetric sector will remain static in the perturbation about the GR solution considered here. The background metric is Schwarzschild with (coordinate basis) metric written as: $g=\mathrm{diag}[A(r),-1/A(r),-r^2,-r^2\sin^2(\theta)]$, where $A(r)=1-2M_s/r$ and M_s is the Schwarzschild mass parameter. The perturbation considered will be one that is spherically symmetric but not necessarily static. A Killing vector analysis yields the general form of the spherically symmetric perturbation:

$$|h_{\mu\nu}|=\begin{bmatrix} h_{00}(t,r) & h_{(01)}(t,r)+h_{[01]}(t,r) & 0 & 0 \\ h_{(01)}(t,r)-h_{[01]}(t,r) & h_{11}(t,r) & 0 & 0 \\ 0 & 0 & h_{22}(t,r) & h_{[23]}(t,r)\sin(\theta) \\ 0 & 0 & -h_{[23]}(t,r)\sin(\theta) & h_{22}(t,r)\sin^2(\theta) \end{bmatrix}. \tag{25}$$

Making a change of coordinates of the background geometry is equivalent to making a change of gauge on the perturbation: $\delta h=\pounds_\varepsilon[g]$, where ε is the spherically symmetric vector gauge parameter generating diffeomorphisms between spherically symmetric spacetimes. This allows one to simplify the form of the perturbation by a suitable choice of gauge. Choosing the gauge parameter as:

$$\varepsilon^0=-\int\left(\frac{h_{(01)}}{A(r)}-\frac{\partial_t[h_{22}]}{2rA(r)^2}\right)dr, \tag{26a}$$

$$\varepsilon^1=\frac{h_{22}}{2r}, \tag{26b}$$

removes the $\theta-\theta$, $\phi-\phi$, and symmetric $t-r$ perturbations altogether, and a remaining gauge transformation $\varepsilon^0=\epsilon(t)$ allows one to remove an arbitrary function from the $t-t$ component of the form: $\delta h_{00}=2A(r)\epsilon(t)$.

The field equations will be written without the source terms for simplicity although it is straightforward to include them and relate the constants of integration to properties of the source. First reviewing how the symmetric (in this case identically GR) perturbations become static, it is simplest to begin with the field equation: ${}^1\mathscr{R}_{(01)}=0$, which implies:

$$\partial_t[h_{11}(t,r)]=0, \tag{27}$$

immediately showing that h_{11} must be static. By considering ${}^1\mathscr{R}_{22}=0$, it is determined to be:

$$h_{11}(t,r)=-\frac{2\delta M_s}{rA^2}, \tag{28}$$

where the integration constant has been combined with M_s and interpreted as a perturbation of the Schwarzschild mass parameter: δM_s. Then one considers: $g^{00}\,{}^1\mathscr{R}_{00}-g^{11}\,{}^1\mathscr{R}_{11}=0$, leading to:

$$h_{00}(t,r)=B(t)A-\frac{2\delta M_s}{r}, \tag{29}$$

also giving a contribution arising from the perturbed mass parameter, as well as an arbitrary function of time as an integration constant, removable by the remaining choice of gauge noted above with: $\epsilon(t)=-B(t)/2$. Thus one has that the symmetric perturbations are static and interpretable as being due to a small change in the total energy of the system: δM_s.

In the skew sector, the $t-r$ field equation gives:

$$^1\mathscr{R}_{[01]}=\tfrac{1}{2}(2A''-m^2)h_{[01]}=0, \tag{30}$$

from which one must conclude that $h_{[01]}$ vanishes outside the source. (Primes will denote the derivative of a function of one variable where convenient.) In massless Kalb–Ramond theory, this is the surviving spherically symmetric ghost mode which in that case is pure gauge. When a mass term is added, although these modes are now no longer pure gauge, they do not propagate since they are locally coupled to the source. It is these modes that one eventually must worry about, since in the full theory they may play a nontrivial dynamical role. In the $\theta-\phi$ sector:

$$^1\mathscr{R}_{[23]}=-\frac{1}{2}\left\{\frac{1}{A}\partial_t^2[h_{[23]}]-A\partial_r^2[h_{[23]}]-\left(A'-\frac{2A}{r}\right)\partial_r[h_{[23]}]+\left(\frac{4}{r^2}(1-A)+m^2\right)h_{[23]}\right\}\sin(\theta)=0. \tag{31}$$

In order to derive the asymptotic form of this perturbation, it is convenient to define $h_{[23]}=rf(t,r)$, leading to:

$$\frac{1}{A}\partial_t^2[f]-A\partial_r^2[f]-A'\partial_r[f]+\left(\frac{3A'}{r}+\frac{2A}{r^2}+m^2\right)f=0. \tag{32}$$

Introducing the coordinate:

$$r^*=\int\frac{dr}{A(r)}=r+2M_s\ln\left(\frac{r}{2M_s}-1\right), \tag{33}$$

one obtains (after multiplying by A) the partial differential equation for f in normal form:

$$\partial_t^2[f]-\partial_{r^*}^2[f]+A\left(m^2+\frac{2A}{r^2}+\frac{3A'}{r}\right)f=0, \tag{34}$$

where r is considered as a function of r^* as are $A(r)$ and $\partial_r A(r)$, and the perturbation $f=f(t,r^*)$. In this form it is obvious that (34) is a hyperbolic wave equation, and that the field f is therefore nonlocally related to the source.

Using the fact that $1/r-1/r^*\sim o(1/(r^*)^2)$ as $r^*\to\infty$, one keeps only the constant mass term asymptotically, as all other potential terms will be dominated by it. This leaves the massive scalar wave equation to determine the asymptotic form of the perturbation:

$$\partial_t^2[f]-\partial_{r^*}^2[f]+m^2f\sim 0. \tag{35}$$

The static solution of this is easily seen to have the asymptotic form:

$$h_{[23]}(r)\sim F_0\frac{r}{m}e^{-mr^*}\sim F_0\frac{r}{m}e^{-mr}\left(\frac{r}{2M_s}\right)^{-2mM_s}, \tag{36}$$

where a factor of m has been introduced in order to make the constant F_0 dimensionless. The general time dependent case may be handled by noting that the retarded and advanced Green's functions for the massive scalar wave equation[31] ($x^2=t^2-\vec{x}^2$):

$$D^{\text{ret, adv}}(x)=D^{\text{ret, adv}}(t,r)=\frac{1}{2\pi}\theta(\pm x^0)\left[\delta(x^2)-\frac{m\theta(x^2)}{2\sqrt{x^2}}J_1(m\sqrt{x^2})\right], \tag{37}$$

depends only on (t,r), and $r^*D^{\text{ret, adv}}(t,r^*)$ will solve (35). The asymptotic behavior of $h_{[23]}$ is then determined from:

$$h_{[23]}\sim rr^*D^{\text{ret, adv}}(t,r^*). \tag{38}$$

Note that the behavior on the light cone is determined from just the massless Green's function $\delta(x^2)$,[32] and so it would appear that $h_{[23]}$ will behave as r as $r\to\infty$ along the forward light cone. This is misleading, as it can be demonstrated explicitly[33] that for C^∞ initial data with compact spatial support, a massive Klein-Gordon field is bounded everywhere by: $\phi\leqslant d(1+|t|)^{-3/2}$, for some constant d, and therefore cannot radiate energy. This can also be understood by noting that because the field is massive, the effects propagating on the light cone must be fields of infinite energy, and given some physically reasonable source distribution, these infinite energy modes will not be excited.

The existence of time dependent solutions thus proves that Birkhoff theorem is not valid in mNGT, although the short-ranged nature of the skew sector implies that monopole radiation will not exist. The symmetric sector has remained static in this system, but as will be shown in Section VI, through a perturbation about an approximated mNGT solution, this will not be the case in general. The perturbation equations about a mNGT background have not been given in covariant form, primarily due to the complication involved (although it is possible in principle using a generalization of the inversion of the compatibility equation given in Ref. 34). Instead the system may be developed in each case separately, and the analysis simplified by considering the field equations in a vierbein frame given in the next Section.

IV. NONSYMMETRIC THEORIES IN A GENERAL FRAME

The structure of the compatibility relations and field equations in nonsymmetric theories can be formulated in terms of components in a general moving frame (in the sense of global section of the general linear frame bundle $GL\mathbf{M}$ of all linear frames over $\mathbf{M}$). The formalism given here is essentially a more systematic development of the approach in Ref. 35, and differs slightly from that of Hlavaty[36] in that the (in general nonsymmetric in a coordinate basis) connection coefficients have been split up into a connection that is torsion free, and another that is purely antisymmetric, instead of defining two types of covariant derivative, one associated with the NGT Christoffel symbols, and another that is in general nonsymmetric and not in general torsion-free. The construction here has the advantage of only defining one covariant derivative, and the fact that it is torsion-free implies that the antisymmetric components in a general (noncoordinate) frame are related in the standard way to the structure constants. In a coordinate basis this is the usual split between the symmetric and antisymmetric components, however it is easily generalized to any basis by considering the antisymmetric components as a separate antisymmetric tensor, and the symmetric components as a torsion-free but generally noncompatible connection.

This provides a simple way to split the GR and NGT contribution in weak field situations, as well as generating computationally simpler systems to solve when inverting the compatibility relations. Note that although the formalism is developed for a general basis, the specialization to a vierbein basis (the reduction of $GL\mathbf{M}$ to $L\mathbf{M}$, the Lorentz frame bundle consisting of all Lorentz frames above $\mathbf{M}$) which will be utilized in the rest of this paper, is accomplished through the choice of the fiber metric as $g_{()}\to\eta$ above all points of the manifold. This is possible in NGT for the same reason that it is possible in GR: mathematically formulating a physical theory in a diffeomorphism invariant manner will always allow the introduction of these general linear frames. The reduction to Lorentz frames is also possible as one is assuming that the symmetric part of the metric that one is attempting to diagonalize is nondegenerate, allowing the reduction of

the frame bundle. This construction will be of importance when considering the canonical analysis of NGT, as one would like to work in a surface compatible (generally noncoordinate) basis in order to avoid specialization to a particular choice of time parameter fixed by the foliation of the manifold, and is easily applied to other systems with a nonsymmetric metric and connection.[29]

A. Metric, compatibility and curvature

The compatibility conditions in a coordinate basis (5) will be written for convenience as:

$$\partial_\gamma[g_{\mu\nu}]-g_{\mu\alpha}\Gamma^\alpha_{\nu\gamma}-g_{\alpha\nu}\Gamma^\alpha_{\gamma\mu}=-\Delta^0_{\gamma\mu\nu}, \tag{39}$$

where Δ^0 depends only on the metric or quantities directly derivable from it (and possibly other quantities, but for the purposes of this construction it does not depend on the connection coefficients). Parallel transport (and the related covariant derivative) will then be defined using just the symmetric part of the coordinate basis connection, and its action on the (coordinate) basis vectors is:

$$\nabla_{e_\alpha}[e]_\beta=\Gamma^\gamma_{(\alpha\beta)}e_\gamma,\nabla_{e_\alpha}[\theta]^\gamma=-\Gamma^\gamma_{(\alpha\beta)}\theta^\beta, \tag{40}$$

and the connection is split into a symmetric connection and an antisymmetric tensor:

$$\Gamma^\gamma_{\mu\nu}\rightarrow\Gamma^\gamma_{(\mu\nu)}+\Lambda^\gamma_{[\mu\nu]}. \tag{41}$$

Thus Γ will refer from this point onwards to the torsion-free (symmetric in a coordinate basis) part of the connection, and Λ to the remaining tensor contribution. In this way, Γ is a torsion-free (but noncompatible) covariant derivative since:

$$T^\gamma_{\mu\nu}=\theta^\gamma[\nabla_{e_\mu}e_\nu-\nabla_{e_\nu}e_\mu-[e_\mu,e_\nu]]=2\Gamma^\gamma_{[\mu\nu]}=0. \tag{42}$$

The compatibility equation (39) then becomes:

$$\nabla_{e_\gamma}[g]_{\mu\nu}=e_\gamma[g_{\mu\nu}]-g_{\mu\alpha}\Gamma^\alpha_{\gamma\nu}-g_{\alpha\nu}\Gamma^\alpha_{\gamma\mu}=g_{\mu\alpha}\Lambda^\alpha_{\nu\gamma}+g_{\alpha\nu}\Lambda^\alpha_{\gamma\mu}-\Delta^0_{\gamma\mu\nu}, \tag{43}$$

where the basis vectors are just directional derivatives along the coordinates: $e_\gamma[\,]=\partial_\gamma[\,]$.

With this definition of the covariant derivative and related connection coefficients, the geometric curvature is found as usual from:

$$R^\alpha_{\beta\mu\nu}=\theta^\alpha[(\nabla_{e_\mu}\nabla_{e_\nu}-\nabla_{e_\nu}\nabla_{e_\mu}-\nabla_{[e_\mu,e_\nu]})e_\beta]=e_\mu[\Gamma^\alpha_{\nu\beta}]-e_\nu[\Gamma^\alpha_{\mu\beta}]+\Gamma^\gamma_{\nu\beta}\Gamma^\alpha_{\mu\gamma}-\Gamma^\gamma_{\mu\beta}\Gamma^\alpha_{\nu\gamma}, \tag{44}$$

and defining the two independent contractions:

$$R^1_{\mu\nu}=R^\alpha_{\mu\alpha\nu}=e_\alpha[\Gamma^\alpha_{\nu\mu}]-e_\nu[\Gamma^\alpha_{\alpha\mu}]+\Gamma^\gamma_{\nu\mu}\Gamma^\alpha_{\alpha\gamma}-\Gamma^\gamma_{\alpha\mu}\Gamma^\alpha_{\nu\gamma}, \tag{45a}$$

$$R^2_{\mu\nu}=R^\alpha_{\alpha\mu\nu}=e_\mu[\Gamma^\alpha_{\nu\alpha}]-e_\nu[\Gamma^\alpha_{\mu\alpha}]. \tag{45b}$$

The Ricci tensor will be defined as:

$$R_{\mu\nu}=R^1_{\mu\nu}-\tfrac{1}{2}R^2_{\mu\nu}=e_\alpha[\Gamma^\alpha_{\nu\mu}]-\tfrac{1}{2}(e_\nu[\Gamma^\alpha_{\alpha\mu}]+e_\mu[\Gamma^\alpha_{\nu\alpha}])+\Gamma^\gamma_{\nu\mu}\Gamma^\alpha_{\alpha\gamma}-\Gamma^\gamma_{\alpha\mu}\Gamma^\alpha_{\nu\gamma}. \tag{46}$$

This particular combination is symmetric, and obviously reduces to the GR Ricci tensor when the NGT antisymmetric terms vanish. Decomposition of (3) into $R_{\mu\nu}$ and another that depends on Λ as: $R^{\rm NS}_{\mu\nu}=R_{\mu\nu}+R^\Lambda_{\mu\nu}$ where $(\Lambda_\mu=\Lambda^\alpha_{\mu\alpha})$ gives:

$$R^{\Lambda}_{\mu\nu}=\nabla_{e_\alpha}[\Lambda]^{\alpha}_{\mu\nu}+\nabla_{e_{[\mu}}[\Lambda]_{\nu]}+\Lambda^{\alpha}_{\mu\beta}\Lambda^{\beta}_{\nu\alpha}. \tag{47}$$

A more general basis is introduced at each point on the manifold through $e_A=E^{\mu}_{A}e_{\mu}$, where E is locally an element of $Gl(4,\mathbb{R})$, and these bases are smoothly joined up to form sections of the tangent bundle $T(\mathbf{M})$.[37,38] The general basis vectors are then given in terms of a coordinate basis through the vierbein-like quantities, which can be used to translate tensors from one choice of basis to the other:

$$e_A=E^{\mu}_{A}e_{\mu}, \quad E^{\mu}_{A}E^{\nu}_{B}g_{\mu\nu}=g_{AB}, \text{ etc.} \tag{48}$$

(In the usual orthonormal basis, one transforms the symmetric part of the metric to the Minkowski space metric, and the E's provide the isomorphism between coordinate basis tensors and locally Lorentzian tensors.) The dual basis of $T^*(\mathbf{M})$ is introduced through the usual relation: $\theta^A[e_B]=\delta^A_B$, and the inverse of the vierbeins is defined through: $E^{\mu}_{A}E^{A}_{\nu}=\delta^{\mu}_{\nu}$. In this paper capital letters from the beginning of the alphabet: $A,B,C,\cdots$ will refer to components of the object decomposed in the general basis.

Parallel transport of the basis vectors now defines the generalized connection coefficients:

$$\nabla_{e_A}[e]_B=\Gamma^{C}_{AB}e_C, \nabla_{e_A}[\theta]^C=-\Gamma^{C}_{AB}\theta^B. \tag{49}$$

The definition of the basis in (48) implies that it is no longer a coordinate basis in general, and hence the directional derivatives no longer necessarily commute, giving rise to the structure constants:

$$[e_A,e_B]=C_{AB}{}^{C}e_C, \tag{50a}$$

given by:

$$C_{AB}{}^{C}=E^{C}_{\nu}(E^{\mu}_{A}\partial_{\mu}[E^{\nu}_{B}]-E^{\mu}_{B}\partial_{\mu}[E^{\nu}_{A}]), \tag{50b}$$

calculated by noting that $e_A[\,]=E^{\mu}_{A}\partial_{\mu}[\,]$. This also implies that a torsion-free connection will no longer be symmetric, and vanishing torsion now gives:

$$T^{A}_{BC}=\theta^A[\nabla_{e_B}e_C-\nabla_{e_C}e_B-[e_B,e_C]]=2\Gamma^{A}_{[BC]}-C_{BC}{}^{A}=0, \tag{51}$$

allowing one to determine the antisymmetric part as usual from the structure constants. This is the motivation for splitting up the connection in this way. Given some alternate split where Γ is not torsion free, one would have to distinguish between the effects of the general basis on the skew part of the connection coefficients, and that of the NGT effects (themselves tensors).

The compatibility condition (39) can now be written as:

$$\nabla_{e_C}[g]_{AB}=g_{AD}\Lambda^{D}_{BC}+g_{DB}\Lambda^{D}_{CA}-\Delta^{0}_{CAB}, \tag{52}$$

where since Δ^0 and Λ are tensors, they are just redefined by multiplication by the appropriate combination of vierbeins. The symmetric part of this can now be solved for the symmetric part of Γ in terms of the antisymmetric part, the structure constants, and Λ, to give:

$$\Gamma_{C(AB)}=\tfrac{1}{2}\Delta_{C(AB)}-\Gamma_{A[BC]}+\Gamma_{B[CA]}-A^{D}_{A}\Lambda_{DBC}+A^{D}_{B}\Lambda_{DCA}, \tag{53}$$

where the quantities:

$$\Gamma_{ABC}=g_{(AD)}\Gamma^{D}_{BC}, \quad \Lambda_{ABC}=g_{(AD)}\Lambda^{D}_{BC}, \quad A^{A}_{B}=S^{(AC)}g_{[CB]}, \tag{54}$$

have been defined for convenience, and S is the inverse of the symmetric part of the metric defined by: $S^{(AB)}g_{(BC)}=\delta^A_C$. Also appearing is the symmetric part of:

$$\Delta_{CAB}=e_B[g_{CA}]+e_A[g_{BC}]-e_C[g_{AB}]+\Delta^0_{BCA}+\Delta^0_{ABC}-\Delta^0_{CAB}. \tag{55}$$

The antisymmetric part of the compatibility conditions can now be recast [using (53)] as 24 algebraic equations for Λ:

$$\Lambda_{CAB}-A^D_AA^E_B\Lambda_{ECD}-A^D_AA^E_C\Lambda_{EBD}+A^D_BA^E_A\Lambda_{ECD}+A^D_BA^E_C\Lambda_{EAD}=\Omega_{C[AB]}, \tag{56}$$

where:

$$\begin{aligned}\Omega_{C[AB]}=&\tfrac{1}{2}(\Delta_{C[AB]}+A^D_B\Delta_{D(CA)}-A^D_A\Delta_{D(BC)})+A^D_A(\Gamma_{B[CD]}+\Gamma_{C[BD]})\\&-A^D_B(\Gamma_{A[CD]}+\Gamma_{C[AD]})-A^D_C\Gamma_{D[AB]}.\end{aligned} \tag{57}$$

The method for solving the compatibility conditions is to first determine the auxiliary quantities appearing in this relation: $(A,\Gamma_{[\,]},\Delta,\Omega)$ in terms of the vierbeins and metric quantities, then solve for Λ through (56), determine $\Gamma_{(\,)}$ from (53), and then use S with $\Gamma_{[\,]}$ and $\Gamma_{(\,)}$ to form Γ^A_{BC} and Λ^A_{BC}. This may not seem like much of a simplification, but when specialized to a Lorentz frame, many of these quantities simplify considerably (as is the case in the Wyman sector in Section V).

The curvature tensor (44) becomes:

$$\begin{aligned}R^A_{BCD}=&\theta^A[(\nabla_{e_C}\nabla_{e_D}-\nabla_{e_D}\nabla_{e_C}-\nabla_{[e_C,e_D]})e_B]\\=&e_C[\Gamma^A_{DB}]-e_D[\Gamma^A_{CB}]+\Gamma^E_{DB}\Gamma^A_{CE}-\Gamma^E_{CB}\Gamma^A_{DE}-C_{CD}{}^E\Gamma^A_{EB},\end{aligned} \tag{58}$$

and the contractions:

$$R^1_{AB}=R^C_{ACB}=e_C[\Gamma^C_{BA}]-e_B[\Gamma^C_{CA}]+\Gamma^D_{BA}\Gamma^C_{CD}-\Gamma^D_{CA}\Gamma^C_{BD}-C_{CB}{}^D\Gamma^C_{DA}, \tag{59a}$$

$$R^2_{AB}=R^C_{CAB}=e_A[\Gamma^C_{BC}]-e_B[\Gamma^C_{AC}]-C_{AB}{}^D\Gamma^C_{DC}, \tag{59b}$$

combine to give the Ricci tensor:

$$\begin{aligned}R_{AB}=&R^1_{AB}-\tfrac{1}{2}R^2_{AB}=e_C[\Gamma^C_{BA}]-e_B[\Gamma^C_{CA}]-\tfrac{1}{2}e_A[\Gamma^C_{BC}]+\tfrac{1}{2}e_B[\Gamma^C_{AC}]\\&+\Gamma^D_{BA}\Gamma^C_{CD}-\Gamma^D_{CA}\Gamma^C_{BD}-C_{CB}{}^D\Gamma^C_{DA}+\tfrac{1}{2}C_{AB}{}^D\Gamma^C_{DC}\\=&e_C[\Gamma^C_{BA}]-e_B[\Gamma^C_{CA}]-\tfrac{1}{2}e_A[\Gamma^C_{BC}]+\tfrac{1}{2}e_B[\Gamma^C_{AC}]+\Gamma^D_{BA}\Gamma^C_{CD}-\Gamma^D_{CB}\Gamma^C_{DA}+\Gamma^D_{[AB]}\Gamma^C_{DC}.\end{aligned} \tag{60}$$

In the split $R^{\rm NS}_{AB}=R_{AB}+R^\Lambda_{AB}$:

$$R^\Lambda_{AB}=\nabla_{e_C}[\Lambda]^C_{AB}+\nabla_{e_{[A}}[\Lambda]_{B]}+\Lambda^C_{AD}\Lambda^D_{BC} \tag{61}$$

as expected.

Since by construction Γ is a torsion free connection, and (58) is the standard curvature tensor constructed from it, one obtains the usual Bianchi identities[38] on the curvature tensor. One should note though that the connection is not compatible, and so the rotation coefficients are not antisymmetric. The relevant Ricci tensors are also not constructed in the same manner as in GR, so the implications of these identities are somewhat different. The first Bianchi identity gives the usual cyclic identity on the last three indices of (58), and leads to the result:

$$R^1_{[AB]} = \tfrac{1}{2} R^2_{AB} \tag{62}$$

when one contracts on any lowered index. (This can also be proven directly using the Jacobi identity.) This tells us that the NGT Ricci tensor is symmetric ($R_{[AB]}=0$) in general, not just in a coordinate basis.

A detailed study of the contractions of the second Bianchi identity (the cyclic covariant derivative):

$$\nabla_{e_C}[R]^A_{BDE} + \nabla_{e_D}[R]^A_{BEC} + \nabla_{e_E}[R]^A_{BCD} = 0, \tag{63}$$

should result in a derivation of the equations of motion for matter fields[39,40] from the field equations.

B. The NGT action and field equations in a general basis

The translation of the field equations (4b), (5), (6) is accomplished through an almost straightforward substitution:

$$\Lambda_A = 0, \tag{64a}$$

$$\nabla_{e_B}[\mathbf{g}]^{[AB]} = \alpha \mathbf{g}^{(AB)} W_B, \tag{64b}$$

$$\mathscr{R}_{AB} := R^{NS}_{AB} + \nabla_{e_{[A}}[W]_{B]} - \tfrac{1}{2}\alpha W_A W_B - \tfrac{1}{4} m^2 M_{AB} = 0, \tag{64c}$$

where the density is $\sqrt{-g} = \sqrt{-\det(g_{AB})}$, the mass tensor:

$$M_{AB} = g_{[AB]} - g_{CA} g_{BD} g^{[CD]} + \tfrac{1}{2} g_{BA} g^{[CD]} g_{[CD]} \tag{65}$$

has been defined, and the tensor appearing in the compatibility equations is:

$$\Delta^0_{CAB} = -\tfrac{2}{3}\alpha (g_{A[C} g_{D]B} + \tfrac{1}{2} g_{AB} g_{[CD]}) g^{(DE)} W_E. \tag{66}$$

One must be careful to treat totally antisymmetric derivatives properly (the structure constants now come into the curl of a vector), and translate the metric density properly.

In order to define the action, one should note that the inverse of the metric is now: $g_{AB} g^{BC} = g^{CB} g_{BA} = \delta^C_A$, and the direct translation of the density results in: $\sqrt{-g} \to \sqrt{-E g E^t} = E\sqrt{-g}$ where $g = \det(g_{AB})$ and $E = \det(E^A_\mu)$. Then (1) is rewritten:

$$S = \int d^4x E \{ -\mathbf{g}^{AB} R^{\mathrm{NS}}_{AB} - \mathbf{g}^{AB} \nabla_{e_{[A}}[W]_{B]} + \mathbf{l}^A \Lambda_A + \tfrac{1}{2}\alpha \mathbf{g}^{(AB)} W_A W_B + \tfrac{1}{4} m^2 \mathbf{g}^{[AB]} g_{[AB]} \}. \tag{67}$$

(Note that in a Lorentz basis, the inverse of the metric is not η.)

Deriving the equations of motion from this action should be approached with care. As it stands there are too many fields (the metric and the vierbeins share degrees of freedom) and one typically must choose either a coordinate basis (as in Section II), a Lorentz basis (so that all symmetric metric degrees of freedom are contained in the vierbeins), or a well-defined combination of the two. One must also realize that (67) as it stands assumes that the connection Γ is torsion-free *a priori*, so that when varying the vierbein, $\Gamma_{[\,]}$ must be varied as well. As an alternative, one may impose the torsion-free condition through additional Lagrange multiplier terms: $L^{BC}_A T^A_{BC}$ in the action, varying the full connection coefficients and vierbeins separately.

V. APPROXIMATION OF THE WYMAN SECTOR SOLUTION IN A VIERBEIN BASIS

In general, the spherically symmetric Killing vector analysis for a (0,2) tensor gives both $t-r$ and $\theta-\phi$ skew components. However it is possible to show from the general spherically symmetric field equations that it is consistent to put either (or both) of these skew components to zero separately, since in either case one loses the corresponding field equation, and the system of equations remains consistent. Whether it is physically reasonable to do this or not depends on the details of the matter coupling in the theory, and how it alters the global behavior of the skew sector. Here will be considered the field equations for what will be referred to as the Wyman sector[41] (keeping just the $\theta-\phi$ sector), although the asymptotics of the $t-r$ sector will be discussed briefly at the end of this section, where it will be argued that there are no static solutions with asymptotic behavior that is dominated by Schwarzschild (or equivalently, Newtonian) effects. This will allow an analysis of the perturbation equations for the spherically symmetric modes, in order to see the effects of the antisymmetric background.

In a coordinate basis, the Wyman metric looks like:

$$|g_{\mu\nu}| = \text{diag}[\gamma(r), -\alpha(r), -r^2, -r^2 \sin^2(\theta)], \quad g_{[23]} = f(r)\sin(\theta). \tag{68}$$

(An appropriate coordinate system has been chosen in order to remove the symmetric $t-r$ metric component, and fix the $\theta-\theta$ component.) Introducing the usual choice of vierbein (using the functions defined by: $F=f(r)/r^2, E_0=1/\sqrt{\gamma(r)}, E_1=1/\sqrt{\alpha(r)}$):

$$E_A^{\mu} = \text{diag}\left[E_0^{\ 0}=E_0, E_1^{\ 1}=E_1, E_2^{\ 2}=\frac{1}{r}, E_3^{\ 3}=\frac{1}{r\ \sin(\theta)} \right], \tag{69}$$

the metric becomes:

$$|g_{(AB)}| = \eta_{AB}, \quad g_{[23]} = F, \tag{70}$$

and the density $\sqrt{-g}=\sqrt{1+F^2}$.

At this point one can invert the compatibility conditions and compute the field equations using the method of Section IV, given in some detail in Appendix A. No attempt will be made here to solve the field equations exactly, although numerical evidence for the existence of an exact solution with asymptotic behavior that matches that given here has been found,[42] ensuring that the approximations given come from a global solution. Instead, an approximation will be given that describes the asymptotic behavior of the exact solution. The idea will be to consider the skew sector as a small correction (of order some small dimensionless parameter κ, to be explicitly defined later) to the Schwarzschild solution far enough away from the source. This should be reasonable since one expects from the results of the perturbation in Section III that the skew sector will behave asymptotically as a decaying exponential, while the symmetric sector should behave as $\sim 1/r$, so that far enough away from the gravitational source the skew sector should be completely dominated by GR effects.

To lowest order in κ (the skew sector) the work is already done, as the field equation for the skew function will be essentially the same as the static perturbation about a Schwarzschild background already considered in Section III. In the vierbein basis, this is derived as before from $\mathscr{R}_{[23]}$ (A8), and gives:

$$A\partial_r^2[F] + \left(A' + \frac{2A}{r} \right) \partial_r[F] - \frac{2}{r}\left(A' + \frac{A}{r} \right) F - m^2 F = 0, \tag{71}$$

and it is trivial to see that when using: $F=f/r$, this reduces to the static limit of (32), giving the asymptotic form for F:

$$F \sim F_0 \frac{e^{-mr^*}}{mr}. \tag{72}$$

One now must consider how the presence of the skew sector affects the symmetric sector, particularly whether it really is a higher order effect. The asymptotic form of these corrections due to F may be calculated by considering order κ^2 corrections to the vierbeins (order κ terms will not depend on F, and so will be solely δM_s corrections), calculated from the symmetric field equations with F from (72) acting as a source. Writing the corrections to the vierbeins as: $E_{0,1} \to E_{0,1} + E^{(2)}_{0,1}$, and the corrections to the field equations as $\mathscr{R}^{(2)}$, one calculates:

$$\mathscr{R}^{(2)}_{00} + \mathscr{R}^{(2)}_{11} = -\frac{2A}{r}\partial_r\left[\sqrt{A}E^{(2)}_0 + \frac{E^{(2)}_1}{\sqrt{A}}\right] - AFF'' - \frac{3}{2}A(F')^2 - \frac{2A}{r}FF' = 0, \tag{73}$$

which, after translating it into a differential equation in r^* and keeping only the asymptotically dominant terms, results in:

$$\partial_{r^*}\left[\sqrt{A}E^{(2)}_0 + \frac{E^{(2)}_1}{\sqrt{A}}\right] \sim -\frac{5}{4}(F_0)^2\frac{e^{-2mr^*}}{r^*}. \tag{74}$$

This integrates to give (the constant of integration is ignored as one could eliminate it through an appropriate choice of gauge as in Section III):

$$\sqrt{A}E^{(2)}_0 + \frac{E^{(2)}_1}{\sqrt{A}} \sim \frac{5}{4}(F_0)^2\frac{e^{-2mr^*}}{2mr^*}. \tag{75}$$

Considering next $\mathscr{R}^{(2)}_{33}$ and using (73) leads to the asymptotic equation:

$$\partial_{r^*}[r\sqrt{A}E^{(2)}_1] \sim -\tfrac{5}{4}(F_0)^2 e^{-2mr^*}. \tag{76}$$

The solution of this combined with the results of (75) gives (once again the constant of integration is ignored, this time as it would be interpretable as a perturbation of the mass parameter and not due to the effects of the skew sector):

$$E^{(2)}_1 \sim \frac{5}{4}(F_0)^2\frac{e^{-2mr^*}}{2mr^*}, \quad E^{(2)}_0 \sim o\left(\frac{e^{-2mr^*}}{(r^*)^2}\right), \tag{77}$$

where the dominant correction to the symmetric sector is $E^{(2)}_1$, and $E^{(2)}_0$ is down by $o(1/r^*)$. It is not hard to see that these corrections are indeed of an order higher than the effects in the skew sector. Clearly one may define a small parameter $\kappa = F_0 \exp(-mr^*_0)$, where r^*_0 is chosen such that $F(r^*_0) \ll 1$, to define the small size of the skew sector when $r^* > r^*_0$. The corrections to the symmetric sector are seen to be of order κ^2, and will therefore be neglected in the approximation of the background required in Section VI.

One may attempt to do the same sort of analysis keeping the $g_{[01]}$ component, however the linearized field equation implies immediately that the field must vanish (it is identical to (30)). Considering higher orders in the field in an attempt to generate a solution other than this trivial result, the third order correction gives [writing $W(r) = \sqrt{-X(r)}$, where the sign has been chosen so that the asymptotic behavior determined below results in a real $W(r)$]

$$\mathscr{R}_{[01]} = \frac{\sqrt{-X}}{6}\left[A\partial_r^2[X] + \left(A' + \frac{2A}{r}\right)\partial_r[X] + \left(\frac{12A}{r^2} + \frac{4A'}{r} + \frac{3}{2}m^2\right)X - \frac{12A'}{r} - 3m^2\right] = 0. \tag{78}$$

Writing $X=Y/r$ and transforming to the r^* coordinate as before gives in canonical form:

$$\partial_{r^*}^2[Y]+A\left(\frac{12A}{r^2}+\frac{3A'}{r}+\frac{3}{2}m^2\right)Y-A(12A'+3m^2r)=0, \tag{79}$$

and keeping the dominant terms:

$$\partial_{r^*}^2[Y]+\tfrac{3}{2}m^2Y-3m^2r^*=0, \tag{80}$$

easily giving the asymptotic form of the solution:

$$W^2(r^*)=2+\frac{a}{r^*}\cos(\sqrt{\tfrac{3}{2}}mr^*)+\frac{b}{r^*}\sin(\sqrt{\tfrac{3}{2}}mr^*), \tag{81}$$

(where (a,b) are arbitrary constants). The dominant part of this solution implies that W is not in fact a small correction to the Schwarzschild metric asymptotically, and must therefore be discarded. This is not surprising as one is trying to match a function that is small asymptotically (by hypothesis) to one that is constant keeping higher orders in W will clearly not change this result, implying that nontrivial static solutions that include this sector will fail to be dominantly Schwarzschild for large r. This of course does not exclude solutions with symmetric metric components whose asymptotic behavior does not match that of the Schwarzschild solution, nor can one exclude the possibility that W is nonvanishing only inside some finite radius.

VI. SPHERICALLY SYMMETRIC PERTURBATION ABOUT A WYMAN BACKGROUND

In an attempt to consider the perturbation equations for NGT about a general non-symmetric background, one finds that the compatibility conditions prevent one from formulating the inversion in a useful form. This means that a fairly straightforward covariant formulation (like that given in Section II) is not feasible, and instead one must treat each situation separately, in this case a spherically symmetric perturbation about the approximated mNGT Wyman solution given in the previous section. Here it is demonstrated that despite the remaining gauge freedom in the symmetric sector, both symmetric functions will in general pick up time dependence from the skew sector. Although this cross coupling is demonstrated explicitly in a perturbative scenario, it will certainly persist in a more general sense. The results here will show that the perturbations in the symmetric sector pick up time dependence that is algebraically determined by the skew function F, without themselves becoming independent degrees of freedom. The canonical analysis of the general spherically symmetric system will address rigorously how many degrees of freedom exist in each sector. If there are more in the nonperturbative theory, one can examine the dynamical approach to an asymptotically flat spacetime looking for possible singular behavior similar to that found in Ref. 6.

The perturbation of the Wyman metric (70) in a coordinate basis will look identical to (25) (using the gauge choice to simplify it as before). The background vierbeins will be the same as those in the Wyman solution (69), where now the perturbations of the vierbeins and skew metric functions are related to perturbations in the coordinate basis by:

$$\delta W=\frac{h_{[01]}(t,r)}{\sqrt{\alpha(r)\gamma(r)}},\quad \delta F=\frac{\delta h_{[23]}(t,r)}{r^2},\quad \delta E_0=-\frac{1}{2}\frac{h_{00}(t,r)}{\gamma(r)^{3/2}},\quad \delta E_1=-\frac{1}{2}\frac{h_{11}(t,r)}{\alpha(r)^{3/2}}. \tag{82}$$

In the vierbein basis the metric perturbation has nonvanishing components:

$$h_{[01]}=\delta W,\quad h_{[23]}=\delta F. \tag{83}$$

The approximation of the background Wyman solution given in Section V greatly simplifies the algebra necessary to develop the perturbation given in Appendix B. Approximating the symmetric sector by the Schwarzschild solution and the antisymmetric sector by (72), first order in this static antisymmetric background is kept, as is the first order in the perturbations. As one shall see, this will be a reasonable approximation since it will be possible to keep the perturbations small compared to the background by an appropriate choice of integration constants (similarly to δM_s in the Schwarzschild case).

The field equation: ${}^1\mathscr{R}_{[01]}=0$, yields precisely the same field equation as in the Schwarzschild case (30), allowing one to immediately set $\delta W=0$. The symmetric part: ${}^1\mathscr{R}_{(01)}=0$, can be written as a total time derivative:

$$ {}^1\mathscr{R}_{(01)}=\partial_t\left[\frac{2}{r\sqrt{A}}\delta E_1+\frac{3}{2}F'\delta F+\left(\frac{1}{r}-\frac{A'}{2A}\right)F\delta F+F\partial_r[\delta F]\right]=0. \tag{84}$$

This last field equation is then integrated, introducing an arbitrary static function $\delta E(r)$:

$$ \frac{2}{r\sqrt{A}}(\delta E_1-\delta E)=-\frac{3}{2}F'\delta F-\left(\frac{1}{r}-\frac{A'}{2A}\right)F\delta F-F\partial_r[\delta F]. \tag{85}$$

Now computing $(\mathrm{Tr}[\mathscr{R}_{AB}]:=\mathscr{R}_{00}+\mathscr{R}_{11}+2\mathscr{R}_{22})$:

$$ \begin{aligned}\mathrm{Tr}[{}^1\mathscr{R}_{AB}]=&\frac{4}{r^2}\partial_r[r\sqrt{A}\delta E_1]-\frac{F}{A}\partial_t^2[\delta F]+3AF\partial_r^2[\delta F]+\left(\frac{8A}{r}F+2A'F+5AF'\right)\partial_r[\delta F]\\&+\left(3AF''+\frac{8A}{r}F'+2A'F'-m^2F\right)\delta F=0,\end{aligned} \tag{86}$$

and inserting (85) gives:

$$ \begin{aligned}\mathrm{Tr}[{}^1\mathscr{R}_{AB}]=&\frac{4}{r^2}\partial_r[r\sqrt{A}\delta E]-\frac{F}{A}\partial_t^2[\delta F]+AF\partial_r^2[\delta F]+\left(A'+\frac{2A}{r}\right)F\partial_r[\delta F]\\&-\left(\frac{2A'}{r}+\frac{2A}{r^2}+m^2\right)F\delta F=0.\end{aligned} \tag{87}$$

Also,

$$ \begin{aligned}{}^1\mathscr{R}_{00}+{}^1\mathscr{R}_{11}=&\frac{2A}{r}\partial_r\left[\sqrt{A}\delta E_0+\frac{\delta E_1}{\sqrt{A}}\right]+\frac{F}{A}\partial_t^2[\delta F]+AF\partial_r^2[\delta F]+A\left(\frac{2F}{r}+3F'\right)\partial_r[\delta F]\\&+A\left(\frac{2F'}{r}+F''\right)\delta F=0,\end{aligned} \tag{88}$$

gives the equality of spatial derivatives of $\sqrt{A}\,\delta E_0$ and $\delta E_1/\sqrt{A}$ up to order F. This will be useful when considering:

$$
\begin{aligned}
{}^1\mathscr{R}_{[23]} &= \left(\frac{F}{r}-\frac{F'}{2}\right)A\partial_r\left[\frac{\delta E_1}{\sqrt{A}}-\sqrt{A}\,\delta E_0\right]-\left[AF''+\left(A'+\frac{2A}{r}\right)F'-\frac{2}{r}\left(A'+\frac{A}{r}\right)F\right]\frac{\delta E_1}{\sqrt{A}} \\
&\quad+\frac{1}{2}\left(\frac{1}{A}\partial_t^2[\,\delta F]-A\partial_r^2[\,\delta F]-\left(A'+\frac{2A}{r}\right)\partial_r[\,\delta F]+\left(\frac{2A'}{r}+\frac{2A}{r^2}+m^2\right)\delta F\right) \\
&= \left(\frac{F}{r}-\frac{F'}{2}\right)A\partial_r\left[\frac{\delta E_1}{\sqrt{A}}-\sqrt{A}\,\delta E_0\right]-m^2F\frac{\delta E_1}{\sqrt{A}} \\
&\quad+\frac{1}{2}\left(\frac{1}{A}\partial_t^2[\,\delta F]-A\partial_r^2[\,\delta F]-\left(A'+\frac{2A}{r}\right)\partial_r[\,\delta F]+\left(\frac{2A'}{r}+\frac{2A}{r^2}+m^2\right)\delta F\right)=0,
\end{aligned}
\tag{89}
$$

where use has been made of (71). One derives a simple field equation by inserting (89) in (87) and dropping the resulting terms that are of second order in the background skew field F:

$$
\partial_r[\,r\sqrt{A}\,\delta E]=0\rightarrow\delta E=\frac{\delta M_s}{r\sqrt{A}}, \tag{90}
$$

where the constant of integration has been identified with the GR-like perturbation of the Schwarzschild mass parameter.

Now (88) can be used to replace δE_0 with δE_1 at this order, and (85) to replace δE_1 with δE to find:

$$
\begin{aligned}
{}^1\mathscr{R}_{[23]} &= \frac{1}{2}\left\{\frac{1}{A}\partial_t^2[\,\delta F]-A\partial_r^2[\,\delta F]-\left(A'+\frac{2A}{r}\right)\partial_r[\,\delta F]+\left(\frac{2A'}{r}+\frac{2A}{r^2}+m^2\right)\delta F\right\} \\
&\quad-A\left(F'-\frac{2F}{r}\right)\partial_r\left[\frac{\delta E}{\sqrt{A}}\right]-m^2F\frac{\delta E}{\sqrt{A}}=0,
\end{aligned}
\tag{91}
$$

and using (90) in this yields the wave equation for δF:

$$
\begin{aligned}
&\frac{1}{A}\partial_t^2[\,\delta F]-A\partial_r^2[\,\delta F]-\left(A'+\frac{2A}{r}\right)\partial_r[\,\delta F]+\left(m^2+\frac{2A}{r^2}+\frac{2A'}{r}\right)\delta F \\
&\quad=\frac{\delta M_s}{rA}\left[m^2F+4\left(\frac{F}{r}-\frac{F'}{2}\right)\left(\frac{A}{r}+A'\right)\right].
\end{aligned}
\tag{92}
$$

Note that this is a static source and so will not in itself induce any wave solutions, but as before the effects of a matter source will show up asymptotically. The static part of the solution may be derived using the methods in Section III:

$$
\delta F=-2F_0\frac{\delta M_s}{r}e^{-2mr^*}\ln\left(\frac{r^*}{2M_s}\right), \tag{93}
$$

and is consistent with the static solution (72) derived about a Schwarzschild background with mass parameter $M_s+\delta M_s$. Time dependent solutions are identical to those found from (71), and will

induce time dependence in the symmetric sector through (85). Since δE_1 is related to δF locally, it is not an independent degree of freedom, and since the skew field is short-ranged, it will not radiate energy at infinity.

Using (92) and (71), one reduces (88) to an algebraic relation for δE_0:

$$\frac{2A}{r}\partial_r\left[\sqrt{A}\,\delta E_0+\frac{\delta E}{\sqrt{A}}\right]+AF\partial_r^2[\delta F]+\left(\frac{3A'}{2}F+\frac{2A}{r}F+\frac{A}{2}F'\right)\partial_r[\delta F]$$
$$+\left[\left(A'+\frac{A}{2r}\right)F'-\left(\frac{(A')^2}{2A}+\frac{7A'}{2r}+\frac{3A}{r^2}+\frac{3}{4}m^2\right)F\right]\delta F=0. \tag{94}$$

The solution for δE_0 can be written as:

$$\sqrt{A}\,\delta E_0=\sqrt{A}\,\delta\tilde{E}-\frac{\delta E}{\sqrt{A}}+B(t), \tag{95}$$

where $B(t)$ is an arbitrary function of time (removable in the usual way using the remaining gauge transformation), the second term corresponds to the static Schwarzschild perturbation from Section III, and $\delta\tilde{E}$ solves the remainder of (94). Note that although not independent degrees of freedom, neither δE_0 nor δE_1 is static. This is in fact what one would expect when considering the effect of a spherically symmetric matter field to which Birkhoff's theorem does not apply, on the GR background. The presence of the nonstatic field will induce time dependence in the gravitational fields, without exciting any independent modes. This is expected to continue to be the case in NGT: the general spherically symmetric system should only have degrees of freedom in the skew sector.

VII. CONCLUSIONS

The asymptotic behavior of the antisymmetric sector for the case of a static Wyman-type metric has been determined, and the corrections to the symmetric sector shown to be negligible provided one considers regions of spacetime far enough away from the gravitational source. It has also been determined that if one keeps the antisymmetric $t-r$ component, then one cannot have asymptotic behavior that is dominated by the Schwarzschild metric, and so it must be discarded. This analysis was facilitated by the introduction of a vierbein basis, although the formalism has been given for a general basis for completeness.

By considering a spherically symmetric perturbation of the Schwarzschild metric, it has been shown that NGT does not have a rigorous Birkhoff theorem as the antisymmetric sector will not remain static in general. (This has also been noted previously in a Unified Field Theory based on Lyra geometries.[43]) Perturbing an approximate Wyman background in a vierbein basis has shown that the symmetric sector is also not static in general, although no additional modes become excited. This is important phenomenologically since one cannot consider the static solutions (Schwarzschild and Wyman) as the only spherically symmetric exterior solutions to the field equations, and one must therefore match an interior solution to a nonstatic exterior in general.

Perturbations of GR backgrounds have been shown to have good asymptotic behavior in general, since the ghost modes do not become excited and the remaining degrees of freedom are short ranged by construction. However this is not good enough since one expects that the physically interesting solutions to mNGT will not be the purely GR solutions, and one would therefore like to examine the behavior of perturbations on generic, asymptotically-flat, mNGT backgrounds. A covariant perturbative scheme, although possible in principle, would seem to be too complex to

be of any practical value. Instead one may treat each case separately and consider the behavior of (perhaps several) modes about a particular background, as was done here for the spherically symmetric perturbation about a Wyman background.

However this also may not be adequate to fully understand the dynamics of the skew sector in mNGT. The lack of additional gauge invariance in the skew sector may mean that there are more modes in the rigorous theory that will be seen in any sort of weak field, perturbative analysis. To determine whether or not this is the case will require a canonical analysis of the full theory. Partial information may be obtained by considering the full set of fields in a spherically symmetric system, and looking for global information about the behavior of the skew modes given a general coupling to external sources. This is not likely to be a tractable problem in a coordinate basis, and even in a Lorentz frame the field equations are not expected to be particularly enlightening, due to their complication alone. However the canonical analysis of this system will show which fields propagate in the general case, and allow one to get at the dynamics of the approach to an asymptotically well behaved spacetime.

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APPENDIX A: WYMAN SECTOR FIELD EQUATIONS

Here the details of the calculation of the Wyman field equations are given, following the steps outlined in Section IV. Beginning with $A^A_B = \eta^{AC} g_{[CB]}$ from (54), one finds the remaining components:

$$A^2_3 = -A^3_2 = F. \tag{A1}$$

The inverse of the symmetric part of the metric is the Minkowski metric: η, whereas the full inverse metric is:

$$|g^{AB}| = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -\dfrac{1}{1+F^2} & -\dfrac{F}{1+F^2} \\ 0 & 0 & \dfrac{F}{1+F^2} & -\dfrac{1}{1+F^2} \end{bmatrix}, \tag{A2}$$

and is necessary in order to compute the mass tensor (65). The structure constants, and hence the skew components of the connection Γ, are then easily found to be:

$$\Gamma^0_{[10]}=\frac{1}{2}C_{10}{}^0=\frac{1}{2}E_1\partial_r[\ln(E_0)],$$

$$\Gamma^2_{[12]}=\Gamma^3_{[13]}=\frac{1}{2}C_{12}{}^2=\frac{1}{2}C_{13}{}^3=-\frac{1}{2r}E_1, \tag{A3}$$

$$\Gamma^3_{[23]}=\frac{1}{2}C_{23}{}^3=-\frac{1}{2r}\cot(\theta).$$

Then Δ from (55) may be determined:

$$-\Delta_{1[23]}=\Delta_{3[12]}=\Delta_{2[31]}=E_1\partial_r[F], \tag{A4}$$

and Ω from (57):

$$\Omega_{1[23]}=E_1\left(\frac{F}{r}-\frac{1}{2}\partial_r[F]\right),\quad \Omega_{3[12]}=\Omega_{2[31]}=\tfrac{1}{2}E_1\partial_r[F]. \tag{A5}$$

Now (56) is solved for Λ and (53) to calculate the connection components (Γ):

$$\Lambda^3_{12}=\Lambda^2_{31}=-\frac{1}{2}\frac{E_1F'}{1+F^2},$$

$$\Lambda^1_{23}=-\frac{E_1F}{r}+\frac{1}{2}E_1F'-\frac{1}{2}E_1F\partial_r[\ln(1+F^2)], \tag{A6}$$

and:

$$\Gamma^0_{01}=\Gamma^1_{00}=-E_1\partial_r[\ln(E_0)],\quad \Gamma^1_{22}=\Gamma^1_{33}=-\frac{E_1}{r}-\frac{1}{2}E_1\partial_r[\ln(1+F^2)],$$

$$\Gamma^2_{21}=\Gamma^3_{31}=\frac{E_1}{r}+\frac{1}{4}E_1\partial_r[\ln(1+F^2)],\quad \Gamma^2_{12}=\Gamma^3_{13}=\frac{1}{4}E_1\partial_r[\ln(1+F^2)],$$

$$\Gamma^3_{32}=-\Gamma^2_{33}=\frac{1}{r}\cot(\theta). \tag{A7}$$

The field equations that remain are:

$$\mathscr{R}_{00}=E_1\partial_r[\Gamma^1_{00}]+\Gamma^1_{00}(\Gamma^0_{01}+2\Gamma^2_{21})+\frac{m^2}{4}\frac{F^2}{1+F^2}=0,$$

$$\mathscr{R}_{11}=-E_1\partial_r[\Gamma^0_{01}]-2E_1\partial_r[\Gamma^2_{21}]-(\Gamma^0_{01})^2-2(\Gamma^2_{21})^2-2(\Lambda^3_{12})^2-\frac{m^2}{4}\frac{F^2}{1+F^2}=0,$$

$$\mathscr{R}_{22}=\mathscr{R}_{33}=E_1\partial_r[\Gamma^1_{22}]+\frac{1}{r^2}+\Gamma^1_{22}(\Gamma^0_{01}+4\Gamma^2_{[21]})-2\Lambda^3_{12}\Lambda^1_{23}+\frac{m^2}{4}\frac{F^2}{1+F^2}=0,$$

$$\mathscr{R}_{[23]}=E_1\partial_r[\Lambda^1_{23}]+(\Gamma^0_{01}-4\Gamma^2_{[12]})\Lambda^1_{23}+2\Gamma^1_{22}\Lambda^3_{12}-\frac{m^2}{4}\left(F+\frac{F}{1+F^2}\right)=0. \tag{A8}$$

It can be shown that in the absence of any skew sector altogether, the Schwarzschild field equations are obtained, and in the absence of the mass term one has the Wyman Field equations.[41]

APPENDIX B: PERTURBATION EQUATIONS

The background field will be that given in Appendix A, approximated by considering only first order contributions from the skew sector. The spherically symmetric perturbations about this background are given here in detail, keeping only first order in the background F, and setting $\alpha = 3/4$ throughout. One may begin by calculating first order corrections to metric quantities, first the density:

$$\delta\sqrt{-g} = \sqrt{-g} F\, \delta F, \tag{B1}$$

and the inverse of the full metric is:

$$|\delta g^{AB}| = \begin{bmatrix} 0 & \delta W & 0 & 0 \\ -\delta W & 0 & 0 & 0 \\ 0 & 0 & 2F\,\delta F & -\delta F \\ 0 & 0 & \delta F & 2F\,\delta F \end{bmatrix}. \tag{B2}$$

The tensor δA has remaining components:

$$\delta A^0_{\ 1} = \delta A^1_{\ 0} = \delta W, \quad \delta A^2_{\ 3} = -\delta A^3_{\ 2} = -\delta F, \tag{B3}$$

and the perturbation of the antisymmetric connection coefficients, derived from (50b):

$$\delta\Gamma^0_{[10]} = \frac{1}{2}\delta C^{\ 0}_{10} = \frac{1}{2}\left(\delta E_1 \partial_r[\ln(E_0)] + \frac{E_1}{E_0}\partial_r[\delta E_0] - \frac{E_1}{E_0}\partial_r[\ln(E_0)]\delta E_0 \right),$$

$$\delta\Gamma^1_{[01]} = \frac{1}{2}\delta C^{\ 1}_{01} = \frac{1}{2}\frac{E_0}{E_1}\partial_t[\delta E_1], \tag{B4}$$

$$\delta\Gamma^2_{[12]} = \delta\Gamma^3_{[13]} = \frac{1}{2}\delta C^{\ 2}_{12} = \frac{1}{2}\delta C^{\ 3}_{13} = -\frac{1}{2}\frac{\delta E_1}{r}.$$

The last equation of (64) is now solved to determine δW in terms of metric functions to find:

$$\delta W_0 = \frac{4}{3}E_1\left(\partial_r[\delta W] + \frac{2\,\delta W}{r} \right), \quad \delta W_1 = \frac{4}{3}E_0\partial_t[\delta W], \quad \delta W_2 = \delta W_3 = 0. \tag{B5}$$

It is then fairly straightforward to calculate the remaining $\delta\Delta^0$:

$$\begin{gathered} \delta\Delta^0_{0[01]} = -\tfrac{1}{4}\delta W_1, \quad \delta\Delta^0_{1[01]} = -\tfrac{1}{4}\delta W_0, \\ \delta\Delta^0_{2[a2]} = \delta\Delta^0_{3[a3]} = -\tfrac{1}{4}\delta W_a, \quad \delta\Delta^0_{2(3a)} = -\delta\Delta^0_{3(2a)} = \tfrac{1}{4}F\,\delta W_a, \end{gathered} \tag{B6}$$

where $a \in \{0,1\}$ here and in the following. The remaining Δ's are:

$$\delta\Delta_{2(a3)}=-\delta\Delta_{3(a2)}=-\tfrac{1}{2}F\,\delta W_a,\quad \delta\Delta_{0[10]}=2E_0\partial_t[\delta W]-\tfrac{1}{2}\delta W_1,$$
$$\delta\Delta_{1[10]}=2E_1\partial_r[\delta W]-\tfrac{1}{2}\delta W_0,\quad \delta\Delta_{2[2a]}=\delta\Delta_{3[3a]}=-\tfrac{1}{2}\delta W_a,$$
$$\delta\Delta_{0[23]}=-E_0\partial_t[\delta F],\quad \delta\Delta_{1[23]}=-E_1\partial_r[\delta F]-\delta E_1\partial_r[F],$$
$$\delta\Delta_{3[02]}=-\delta\Delta_{2[03]}=E_0\partial_t[\delta F],\quad \delta\Delta_{3[12]}=-\delta\Delta_{2[13]}=E_1\partial_r[\delta F]+\delta E_1\partial_r[F]. \tag{B7}$$

Then $\delta\Omega$ can be calculated:

$$\delta\Omega_{0[10]}=E_0\partial_t[\delta W]-\tfrac{1}{4}\delta W_1,\quad \delta\Omega_{1[10]}=E_1\partial_r[\delta W]-\tfrac{1}{4}\delta W_0,$$
$$\delta\Omega_{2[02]}=\delta\Omega_{3[03]}=\frac{1}{4}\delta W_0-\frac{E_1\delta W}{r},\quad \delta\Omega_{2[12]}=\delta\Omega_{3[13]}=\frac{1}{4}\delta W_1,$$
$$\delta\Omega_{0[23]}=-\frac{1}{2}E_0\partial_t[\delta F],\quad \delta\Omega_{1[23]}=-\frac{1}{2}E_1\partial_r[\delta F]+\frac{F\delta E_1}{r}+\frac{E_1\delta F}{r}-\frac{1}{2}\delta E_1\partial_r[F], \tag{B8}$$
$$\delta\Omega_{3[02]}=-\delta\Omega_{2[03]}=\tfrac{1}{2}E_0\partial_t[\delta F],\quad \delta\Omega_{3[12]}=-\delta\Omega_{2[13]}=\tfrac{1}{2}E_1\partial_r[\delta F]+\tfrac{1}{2}\delta E_1\partial_r[F].$$

One is now in a position to invert the compatibility conditions (56) to solve for the perturbations to the connection coefficients. First the corrections to Λ:

$$\delta\Lambda^0_{01}=-\frac{2}{3}E_0\partial_t[\delta W],\quad \delta\Lambda^1_{01}=-\frac{2}{3}E_1\left(\frac{\delta W}{r}-\partial_r[\delta W]\right),$$
$$\delta\Lambda^2_{20}=\delta\Lambda^3_{30}=-\frac{1}{3}E_1\left(\frac{\delta W}{r}-\partial_r[\delta W]\right),\quad \delta\Lambda^2_{21}=\delta\Lambda^3_{31}=\frac{1}{3}E_0\partial_t[\delta W],$$
$$\delta\Lambda^0_{23}=-\frac{1}{2}E_0\partial_t[\delta F],\quad \delta\Lambda^1_{23}=-\frac{E_1\delta F}{r}-\frac{\delta E_1 F}{r}+\frac{1}{2}\frac{\delta E_1 F'}{r}+\frac{1}{2}\frac{E_1\partial_r[\delta F]}{r}, \tag{B9}$$
$$\delta\Lambda^2_{03}=\delta\Lambda^3_{20}=\tfrac{1}{2}E_0\partial_t[\delta F],\quad \delta\Lambda^2_{13}=\delta\Lambda^3_{21}=\tfrac{1}{2}E_1\partial_r[\delta F]+\tfrac{1}{2}F'\delta E_1,$$

and then to Γ:

$$\delta\Gamma^0_{01}=\delta\Gamma^1_{00}=-\frac{E_1}{E_0}\partial_r[\delta E_0]-\delta E_1\partial_r[\ln(E_0)]+\frac{E_1}{E_0}\delta E_0\partial_r[\ln(E_0)],$$
$$\delta\Gamma^0_{11}=\delta\Gamma^1_{10}=-\frac{E_0}{E_1}\partial_t[\delta E_1],\quad \delta\Gamma^2_{03}=\delta\Gamma^2_{30}=-\delta\Gamma^3_{02}=-\delta\Gamma^3_{20}=\frac{1}{2}E_1F'\delta W,$$
$$\delta\Gamma^0_{22}=\delta\Gamma^0_{33}=2\,\delta\Gamma^2_{02}=2\,\delta\Gamma^2_{20}=2\,\delta\Gamma^3_{03}=2\,\delta\Gamma^3_{30}=E_0F\partial_t[\delta F],$$
$$\delta\Gamma^1_{22}=\delta\Gamma^1_{33}=-\frac{\delta E_1}{r}-E_1F\partial_r[\delta F]-E_1F'\delta F,\quad \delta\Gamma^2_{12}=\delta\Gamma^3_{13}=\tfrac{1}{2}E_1F\partial_r[\delta F]+\frac{1}{2}E_1F'\delta F,$$
$$\delta\Gamma^2_{21}=\delta\Gamma^3_{31}=\frac{\delta E_1}{r}+\frac{1}{2}E_1F\partial_r[\delta F]+\frac{1}{2}E_1F'\delta F. \tag{B10}$$

The remaining field equations will be: ${}^1\mathscr{R}_{00}, {}^1\mathscr{R}_{(01)}, {}^1\mathscr{R}_{[01]}, {}^1\mathscr{R}_{11}, {}^1\mathscr{R}_{22} = {}^1\mathscr{R}_{33}$ and ${}^1\mathscr{R}_{[23]}$. The relevant combinations will be quoted in Section VI.

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Angular momentum and Killing potentials

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When the Penrose–Goldberg (PG) superpotential is used to compute the angular momentum of an axial symmetry, the Killing potential $Q^{\mu\nu}_{(\varphi)}$ for that symmetry is needed. Killing potentials used in the PG superpotential must satisfy Penrose's equation. It is proved for the Schwarzschild and Kerr solutions that the Penrose equation does not admit a $Q^{\mu\nu}_{(\varphi)}$ at finite r and therefore the PG superpotential can only be used to compute angular momentum asymptotically. © *1996 American Institute of Physics.* [S0022-2488(95)03312-9]

I. INTRODUCTION

In this work computing angular momentum with the use of Killing potentials is studied for the Schwarzschild and Kerr solutions. Killing potentials are bivectors $Q^{\mu\nu}$ whose divergence yields a Killing vector. Both solutions have explicit rotational Killing symmetries, spherical for Schwarzschild and axial for Kerr, and we have obtained an axial Killing potential $Q^{\mu\nu}_{(\varphi)}$ for both solutions. We expected to use that $Q^{\mu\nu}_{(\varphi)}$ in the Penrose–Goldberg (PG) superpotential[1] to compute angular momentum in the same way that $Q^{\mu\nu}_{(\mathrm{t})}$ has been previously used to compute mass[2] and found, to our surprise, that this was not possible.

Killing potentials used in the PG superpotential must satisfy Penrose's equation[3]

$$\mathbf{P}^{\alpha\mu\nu}:=\boldsymbol{\nabla}^{(\alpha}Q^{\mu\nu)}-\boldsymbol{\nabla}^{(\alpha}Q^{\nu)\mu}+g^{\alpha[\mu}Q^{\nu]\beta}{}_{;\beta}=0 \tag{1}$$

such that $\boldsymbol{\nabla}_\beta Q^{\alpha\beta}$ is a Killing vector. Penrose showed that ten independent $Q^{\mu\nu}$ exist in Minkowski space, but there can be no solutions in a general space–time which has no Killing symmetries. For Penrose's quasi-local mass integral we exhibit, in the following section, a Killing potential for the Kerr spacetime which satisfies (1) and yields a quasi-local Kerr mass. Unfortunately, one cannot use the PG superpotential to compute quasi-local angular momentum and so this work has a **negative** result. It is proved for the Schwarzschild and Kerr solutions that the Penrose equation does not admit a $Q^{\mu\nu}_{(\varphi)}$ at finite r and thus the PG superpotential **cannot** be used to compute angular momentum at finite r.

A Newman–Penrose null tetrad for the Kerr solution is given in Appendix A together with the details of an anti-self-dual bivector basis. Bivector components of the Penrose equation are presented in Appendix B. The conformal Penrose equation is given in Appendix C. Sign conventions used here are $2A_{\nu;[\alpha\beta]}=A_\mu R^\mu{}_{\nu\alpha\beta}$, and $R_{\mu\nu}=R^\alpha{}_{\mu\nu\alpha}$.

II. KILLING POTENTIALS

For Killing vector k^α there is an antisymmetric Killing potential $Q^{\alpha\beta}$ such that

$$k^\alpha=\tfrac{1}{3}\boldsymbol{\nabla}_\beta Q^{\alpha\beta}.$$

It is the Killing potential which is the core of the PG superpotential for computing conserved Noether quantities such as mass and angular momentum. The PG superpotential is

$$U^{\alpha\beta}=\sqrt{-g}\,\tfrac{1}{2}G^{\alpha\beta}{}_{\mu\nu}Q^{\mu\nu}, \tag{2}$$

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where $G^{\alpha\beta}{}_{\mu\nu}$ is the negative right and left dual of the Riemann tensor. In order for

$$\nabla_\beta U^{\alpha\beta}=\sqrt{-g}G^{\alpha\nu}k_\nu,$$

it is necessary that the Killing potential $Q^{\mu\nu}$ satisfy the Penrose equation.

The Kerr solution has two Killing vectors, stationary $k^\alpha_{(t)}$ and axial $k^\alpha_{(\varphi)}$, and the metric, in Boyer–Lindquist coordinates, is given by

$$g^{\text{Kerr}}_{\alpha\beta}\,dx^\alpha dx^\beta=\Psi\ dt^2-(\Sigma/\Delta)dr^2+(1-\Psi)2a\ \sin^2\theta\ dtd\varphi-\Sigma d\theta^2 - \sin^2\theta[\Sigma+(2-\Psi)a^2\ \sin^2\theta]d\varphi^2, \tag{3}$$

where $R=r-ia\cos\theta$, $\Sigma=R\bar{R}$, $\Delta=r^2+a^2-2mr$, and $\Psi=1-2mr/\Sigma$. The Killing potential for $k^\alpha_{(t)}$ is

$$Q^{\alpha\beta}_{(t)}=-\tfrac{1}{2}(RM^{\alpha\beta}+\bar{R}\bar{M}^{\alpha\beta}). \tag{4}$$

Here $M^{\alpha\beta}$ is an anti-self-dual bivector, $M^{*\alpha\beta}=-iM^{\alpha\beta}$, given in terms of Newman–Penrose null vectors in Appendix A. One-third the divergence of Eq. (4) yields the stationary Killing vector

$$k^\alpha_{(t)}=n^\alpha+(\Delta/2\Sigma)l^\alpha+(ia\sin\theta/\sqrt{2}\Sigma)(\bar{R}m^\alpha-R\bar{m}^\alpha). \tag{5}$$

Direct substitution of $Q^{\alpha\beta}_{(t)}$ in Eq. (1) verifies that $Q_{(t)}$ satisfies the Penrose equation. One can now use the stationary Killing potential with the PG superpotential to compute the mass^2 of the Kerr source:

$$M(S^2)=-\frac{1}{16\pi}\oint_{S^2}\sqrt{-g}C^{\alpha\beta}_{\mu\nu}Q^{\mu\nu}_{(t)}dS_{\alpha\beta} \tag{6}$$

where S^2 is a closed $t=$const, $r=$const two-surface. The result is m for any r beyond the outer event horizon.

An axial Killing potential for the Kerr solution is given by

$$Q^{\alpha\beta}_{(\varphi)}=Q_1M^{\alpha\beta}+Q_2V^{\alpha\beta}+\text{c.c.},$$
$$Q_1=\frac{ar\sin^2\theta}{2\Sigma}(r^2+3a^2\cos^2\theta),\quad Q_2=\frac{ir\sin\theta}{\sqrt{2}R}(r^2+3a^2\cos^2\theta), \tag{7}$$

and one-third the divergence of $Q^{\alpha\beta}_{(\varphi)}$ yields the axial Killing vector

$$k^\alpha_{(\varphi)}=-a\sin^2\theta\left[n^\alpha+\left(\frac{\Delta}{2\Sigma}\right)l^\alpha\right]-\left[\frac{i(r^2+a^2)\sin\theta}{\sqrt{2}\Sigma}\right](\bar{R}m^\alpha-R\bar{m}^\alpha). \tag{8}$$

When the Kerr rotation parameter is set to zero, one obtains the Schwarzschild results

$$Q^{\alpha\beta}_{(\varphi)}=\frac{ir^2\sin\theta}{\sqrt{2}}V^{\alpha\beta}+\text{c.c.}, \tag{9}$$

$$k^\alpha_{(\varphi)}=-\frac{ir\sin\theta}{\sqrt{2}}m^\alpha+\text{c.c.} \tag{10}$$

Neither the $Q_{(\varphi)}$ for Kerr nor the $Q_{(\varphi)}$ for Schwarzschild satisfy the Penrose equation.

III. NO AXIAL PENROSE SOLUTION

We will show for the Schwarzschild solution and the Kerr solution that the Penrose equation does not allow an axial Killing potential at finite r. Penrose's equation,[3] $\nabla_{A'}{}^{(A}W^{BC)}=0$ for symmetric spinor W^{BC} (equivalent to the antisymmetric Killing potential $Q^{\mu\nu}$), was used in linearized theory where Penrose[4] showed existence of ten independent Killing potentials, one for each Minkowski Killing vector. In Goldberg's generalization[1] to a fully curved metric there is no discussion of the existence of solutions of the Penrose equation at finite r. We know that a solution exists for $Q_{(t)}$. It is given in Eq. (4) for the Kerr solution with anti-self-dual components

$$Q_0=0, \quad Q_1=-\tfrac{1}{2}R, \quad Q_2=0, \tag{11}$$

where

$$Q^{\mu\nu}=Q_0U^{\mu\nu}+Q_1M^{\mu\nu}+Q_2V^{\mu\nu}+\text{c.c.}$$

We also know that Penrose obtained asymptotic results for angular momentum J. For axial symmetry $k_{(\varphi)}$ at the conformal boundary he found $J=0$ for Schwarzschild's solution and $J=ma$ for Kerr's, so it is reasonable to expect a $Q_{(\varphi)}$ for use in the PG superpotential at finite r.

The argument presented below assumes that $Q_{(\varphi)}$ exists, goes through a long set of equations which are the components of the bivector form of Penrose's equation given in Appendix B, and ends with no possible $Q_{(\varphi)}$. To integrate the equations it is assumed that Q_0, Q_1, and Q_2 are independent of t and φ, i.e., it is assumed that $\mathscr{L}_\xi Q^{\mu\nu}_{(\varphi)}=0$ where ξ^α is a Killing vector that commutes with the Kerr $k^\alpha_{(t)}$ and $k^\alpha_{(\varphi)}$. If this assumption is false, then $\mathscr{L}_\xi Q^{\mu\nu}_{(\varphi)}=X^{\mu\nu}$. Penrose's equation (1) with $\nabla_\beta Q^{\nu\beta}=3k^\nu$ can be written as

$$\nabla_\beta Q^{\mu\nu}=\nabla^{[\mu}Q^{\nu]}{}_\beta+3k^{[\mu}\delta^{\nu]}{}_\beta. \tag{12}$$

Since the Lie and covariant derivatives commute, the nonzero bivector $X^{\mu\nu}$ must satisfy

$$\boldsymbol{\nabla}_\beta X^{\mu\nu}=\boldsymbol{\nabla}^{[\mu}X^{\nu]}{}_\beta. \tag{13}$$

The Kerr and Schwarzschild solutions do not admit a nonzero $X^{\mu\nu}$ at finite r.

We investigate the existence of $Q_{(\varphi)}$ for the Schwarzschild solution since the equations are simpler with the Kerr rotation parameter set to zero but the argument can be extended in a straightforward manner to the Kerr solution. The null tetrad and spin coefficients given in Appendix A are used. Penrose's equation (B4) has n^α component

$$L_0=0=\partial_r Q_0, \tag{14}$$

with solution $Q_0=h(\theta)$; h an arbitrary function. The $\bar{m}^\alpha$ component is

$$M_0=0=\frac{1}{\sqrt{2}r}\,(\partial_\theta Q_0-\cot\,\theta Q_0), \tag{15}$$

with solution $Q_0=f(r)\sin\theta$, f arbitrary. The two separate solutions require

$$Q_0=c_0\,\sin\,\theta,\ c_0\ \text{const.} \tag{16}$$

Equation (B2) has l^α component

$$N_2=0=r(r-2m)\partial_r Q_2-2mQ_2, \tag{17}$$

with solution $Q_2=(1-2m/r)h(\theta)$. The m^α component is

$$B_2=0=\frac{1}{\sqrt{2}r}\,(\partial_\theta Q_2-\cot\,\theta Q_2), \tag{18}$$

with solution $Q_2=f(r)\,\sin\,\theta$. The two solutions for Q_2 require

$$Q_2=c_2(1-2m/r)\sin\,\theta,\ c_2\ \text{const.} \tag{19}$$

The n^α component of (B2) is

$$L_2-2B_1=0,\quad \partial_r Q_2-\frac{2}{r}\,Q_2-\frac{\sqrt{2}}{r}\,\partial_\theta Q_1=0. \tag{20}$$

Using Q_2 from (19) we find

$$Q_1=c_2\sqrt{2}(1-3m/r)\cos\,\theta+f(r). \tag{21}$$

We now have functional forms for Q_0, Q_1, and Q_2. The Q components are further restricted by using the $\bar{m}^\alpha$ component of (B2):

$$\begin{gathered} M_2-2N_1=0,\\ \frac{1}{\sqrt{2}r}\,(\partial_\theta Q_2+\cot\,\theta Q_2)+\left(1-\frac{2m}{r}\right)\left(\partial_r Q_1-\frac{1}{r}\,Q_1\right)=0. \end{gathered} \tag{22}$$

Using Q_2 from (19) and Q_1 from (21) we obtain the equation

$$\frac{c_2 6\sqrt{2}m}{r^2}\cos\,\theta+\partial_r f-\frac{1}{r}\,f=0. \tag{23}$$

No solution is possible unless one chooses $c_2=0$. Then $Q_1=c_1 r$. The Q components are now

$$Q_0=c_0\,\sin\,\theta,\quad Q_1=c_1 r,\quad Q_2=0. \tag{24}$$

The l^α component of (B4) is

$$\begin{gathered} N_0-2M_1=0,\\ \frac{1}{2}\left(1-\frac{2m}{r}\right)\partial_r Q_0+\frac{m}{r^2}\,Q_0-\frac{1}{r}\left(1-\frac{2m}{r}\right)Q_0+\frac{\sqrt{2}}{r}\,\partial_\theta Q_1=0. \end{gathered} \tag{25}$$

Substituting (24) requires $c_0=0$. Comparing (24) and (11) one can now see that the only solution possible is the one for $Q_{(t)}$ given above.

We have proved that, for the Schwarzschild and Kerr solutions, only the timelike Killing vector $k_{(t)}$ can have a Killing potential that satisfies the Penrose equation at finite r.

IV. NULL INFINITY

We proceed to solve the Penrose equation at the boundary of Schwarzschild space–time. The Schwarzschild solution is given in outgoing null coordinates as

$$g_{\mu\nu}\,dx^\mu dx^\nu=(1-2m/r)du^2+2\,dudr-r^2(d\theta^2+\sin^2\theta\,d\varphi^2). \tag{26}$$

We use the null tetrad

$$l_\alpha\, dx^\alpha = du, \quad n_\alpha\, dx^\alpha = \tfrac{1}{2}(1-2m/r)du + dr, \quad m_\alpha\, dx^\alpha = -(r/\sqrt{2})(d\theta + i\,\sin\,\theta\, d\varphi),$$

and spin coefficients given in Eq. (A2) with Kerr rotation parameter $a=0$. The general equations for a conformal map are given in Appendix C. We choose $\Omega = 1/r = z$. On $\mathscr{I}^+$, where $z=0$, the metric is

$$\hat{g}_{\mu\nu}\, dx^\mu dx^\nu = -2\, du dz - (d\theta^2 + \sin^2\theta\, d\varphi^2). \tag{27}$$

Here the conformal Bondi frame is

$$\hat{l}_\alpha\, dx^\alpha = du, \quad \hat{n}_\alpha\, dx^\alpha = -dz, \quad \hat{m}_\alpha\, dx^\alpha = -(1/\sqrt{2})(d\theta + i\,\sin\,\theta\, d\varphi),$$

with nonzero spin coefficients

$$\hat{\beta} = \frac{\cot\,\theta}{2\sqrt{2}} = -\hat{\alpha}.$$

The Penrose equation comprises eight complex equations (B2)–(B4) for $\hat{Q}_0$, $\hat{Q}_1$, and $\hat{Q}_2$. Three establish finite values for the Qs on the boundary:

$$\partial_z \hat{Q}_0 = 0, \quad \partial_z \hat{Q}_1 + \tfrac{1}{2}(\hat{\delta} - 2\hat{\alpha})\hat{Q}_0 = 0, \quad \partial_z \hat{Q}_2 + 2(\hat{\delta})\hat{Q}_1 = 0,$$

where $\hat{D} = -\partial_z$, $\hat{\Delta} = \partial_u$, and on $\mathscr{I}^+$ $(\hat{\delta} + 2s\hat{\alpha})\eta = -\eth\eta$ for η a spin weight s scalar (we use the original definition[5] of edth with spin weight opposite to the helicity of outgoing radiation). In the following a zero superscript denotes independence of z, and $(\hat{Q}_0^0, \hat{Q}_1^0, \hat{Q}_2^0)$ have spin weights $(1,0,-1)$. The remaining five equations on $\mathscr{I}^+$ are

$$\partial_u \hat{Q}_2^0 = 0, \tag{28a}$$

$$\bar{\eth}\hat{Q}_2^0 = 0, \tag{28b}$$

$$\bar{\eth}\hat{Q}_2^0 + 2\,\partial_u \hat{Q}_1^0 = 0, \tag{28c}$$

$$\eth\hat{Q}_0^0 = 0, \tag{28d}$$

$$2\eth\hat{Q}_1^0 + \partial_u \hat{Q}_0^0 = 0. \tag{28e}$$

The solutions are

$$\hat{Q}_2^0 = k^m{}_{-1}Y_{1m}, \quad \hat{Q}_1^0 = -\tfrac{1}{2}u\;\eth\hat{Q}_2^0 + f(\theta,\varphi), \quad \hat{Q}_0^0 = \tfrac{1}{2}\,u^2\eth^2\hat{Q}_2^0 - 2u\eth f + c^m{}_1Y_{1m}, \tag{29}$$

where k^m and c^m are complex constants. Here we can go beyond Goldberg[1] and integrate (28e) since the Schwarzschild null surfaces are shear-free. The asymptotic Killing vectors are

$$\hat{k}_u = \hat{Q}^0{}_1 + \text{c.c.}, \quad \Omega\hat{k}_\theta = \text{c.c.}(\hat{Q}^0{}_2), \quad \Omega\hat{k}_\varphi = \hat{Q}^0{}_2. \tag{30}$$

The supertranslations of the BMS group have a full function's worth of freedom in $\hat{Q}^0{}_1$ but at the Schwarzschild boundary $f(\theta,\varphi)$ is restricted to four parameters for ordinary translations and $\eth f = 0$.

The solution of the Penrose equation for $Q_{(t)}$ is contained above. The nonzero anti-self-dual component of Eq. (4) is $Q_1 = -r/2$ or $\hat{Q}_1 = -\frac{1}{2}$. This solution coincides with the values $k^m = 0$, $c^m = 0$, and $f(\theta,\varphi) = -\frac{1}{2}$.

Now lets take the asymptotic solutions found above in (29) and (30) and use them to construct a Killing potential $Q_{(\varphi)}$. Thus our candidate has the form

$$Q^{\mu\nu}_{(\varphi)}=(r^2Q^0_2)V^{\mu\nu}+\text{c.c.} \tag{31}$$

For the Schwarzschild solution we compute the divergence:

$$\frac{1}{3}\,\nabla_\nu Q^{\mu\nu}_{(\varphi)}=-[rQ^0{}_2]m^\mu+\left[\frac{r}{\sqrt{2}}\,(\partial_\theta+\cot\,\theta)Q^0{}_2\right]l^\mu+\text{c.c.} \tag{32}$$

Equating with

$$k^\mu_{(\varphi)}=-\frac{ir\,\sin\,\theta}{\sqrt{2}}\,m^\mu+\text{c.c.}$$

yields

$$Q^0{}_2=\frac{i\,\sin\,\theta}{\sqrt{2}}.$$

The l^μ term in (32) vanishes when the complex conjugate is added. We have constructed the Killing potential which was already given above as Eq. (9). The anti-self-dual components are

$$Q_0=0,\quad Q_1=0,\quad Q_2=(i/\sqrt{2})r^2\,\sin\,\theta. \tag{33}$$

Of the twelve terms entering the Penrose equation (defined in Appendix B), four are nonzero for the components of Eq. (33):

$$L_2=i\sqrt{2}r\,\sin\,\theta,\quad N_2=(i/\sqrt{2})(3m-r)\,\sin\,\theta,$$

$$M_2=ir\,\cos\,\theta,\quad B_1=(i/\sqrt{2})r\,\sin\,\theta.$$

Although Q_2 has the r^2 dependence that one expects for an asymptotic solution and the angular dependence dictated by $k_{(\varphi)}$, the components of Eq. (B2), particularly $N_2=0$, show directly that this Killing potential fails to satisfy the Penrose equation.

V. CONCLUSION

To find a Killing potential one can write the divergence equation relating k^α and $Q^{\alpha\beta}$ as a three-form relation, one-third the exterior derivative of dual Q equal to the dual of $k_\alpha\,dx^\alpha$,

$$\tfrac{1}{3}d{*}Q={*}(k_\alpha\,dx^\alpha),$$

and then integrate (if possible). We have seen that not just any Killing potential can be used in the PG superpotential but only one which satisfies Penrose's equation. Although a $Q^{\alpha\beta}_{(\varphi)}$ whose divergence yielded the axial Killing vector was presented for the Kerr solution, it could not be used to compute quasi-local angular momentum although asymptotically it yields ma. It has been shown that a $Q^{\alpha\beta}_{(\varphi)}$ **cannot** be found for either the Kerr or Schwarzschild solutions which will satisfy the Penrose equation in curved space and so the PG superpotential cannot be used to compute quasi-local angular momentum.

Some interesting questions remain. What are the complete integrability conditions for the Penrose equation? What is the physical reason that no quasi-local Killing potential for rotational symmetry can satisfy the Penrose equation?

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APPENDIX A: NULL TETRAD AND BIVECTORS

A Newman–Penrose tetrad $(l^\alpha, n^\alpha, m^\alpha, \bar{m}^\alpha)$ for the Kerr metric (3) with l^α and n^α as principal null vectors is chosen as

$$\begin{aligned} l^\alpha \partial_\alpha &= \frac{1}{\Delta}\left[(r^2+a^2)\partial_t + \Delta\partial_r + a\partial_\varphi\right], \\ n^\alpha \partial_\alpha &= \frac{1}{2\Sigma}\left[(r^2+a^2)\partial_t - \Delta\partial_r + a\partial_\varphi\right], \\ m^\alpha \partial_\alpha &= \frac{1}{\sqrt{2}\bar{R}}\left[ia\,\sin\,\theta\partial_t + \partial_\theta + \frac{i}{\sin\,\theta}\,\partial_\varphi\right], \end{aligned} \tag{A1}$$

where $R = r - ia\cos\theta$, $\Sigma = R\bar{R}$, and $\Delta = r^2 + a^2 - 2mr$. The nonzero spin coefficients and Weyl tensor component are

$$\begin{aligned} &\rho = -\frac{1}{R}, \quad \mu = -\frac{\Delta}{(2\Sigma R)}, \quad \tau = -\frac{ia\,\sin\,\theta}{\sqrt{2}\Sigma}, \quad \pi = \frac{ia\,\sin\,\theta}{\sqrt{2}R^2}, \\ &\gamma = \mu + \frac{r-m}{2\Sigma}, \quad \beta = \frac{\cot\,\theta}{2\sqrt{2}\bar{R}}, \quad \alpha = \pi - \bar{\beta}, \quad \psi_2 = -\frac{m}{R^3}. \end{aligned} \tag{A2}$$

A basis of anti-self-dual bivectors is given by

$$U^{\mu\nu} = 2\bar{m}^{[\mu}n^{\nu]}, \quad M^{\mu\nu} = 2l^{[\mu}n^{\nu]} - 2m^{[\mu}\bar{m}^{\nu]}, \quad V^{\mu\nu} = 2l^{[\mu}m^{\nu]}. \tag{A3}$$

Their inner products are $U^{\mu\nu}V_{\mu\nu} = \bar{U}^{\mu\nu}\bar{V}_{\mu\nu} = 2$, $M^{\mu\nu}M_{\mu\nu} = \bar{M}^{\mu\nu}\bar{M}_{\mu\nu} = -4$, and all others zero. As a basis, they satisfy the completeness relation

$$\tfrac{1}{2}(g^{\alpha\beta\mu\nu} + i\,\eta^{\alpha\beta\mu\nu}) = U^{\alpha\beta}V^{\mu\nu} + V^{\alpha\beta}U^{\mu\nu} - \tfrac{1}{2}M^{\alpha\beta}M^{\mu\nu}, \tag{A4}$$

where $g^{\alpha\beta\mu\nu} = g^{\alpha\mu}g^{\beta\nu} - g^{\alpha\nu}g^{\beta\mu}$, and $\frac{1}{2}\eta^{\alpha\beta\mu\nu}$ is the dual tensor. It is useful to list their covariant derivatives:

$$\begin{aligned} &\nabla_\beta U^{\mu\nu} = -2U^{\mu\nu}a_\beta + M^{\mu\nu}b_\beta, \quad a_\beta = \epsilon n_\beta + \gamma l_\beta - \alpha m_\beta - \beta\bar{m}_\beta, \\ &\nabla_\beta M^{\mu\nu} = -2U^{\mu\nu}c_\beta + 2V^{\mu\nu}b_\beta, \quad b_\beta = \pi n_\beta + \nu l_\beta - \lambda m_\beta - \mu\bar{m}_\beta, \\ &\nabla_\beta V^{\mu\nu} = 2V^{\mu\nu}a_\beta - M^{\mu\nu}c_\beta, \quad c_\beta = \kappa n_\beta + \tau l_\beta - \rho m_\beta - \sigma\bar{m}_\beta. \end{aligned} \tag{A5}$$

APPENDIX B: THE PENROSE EQUATION

Equation (1), which a Killing potential must satisfy in order to be valid for use in the PG superpotential, can be written in terms of anti self-dual bivectors with the definition

$$Q^{\mu\nu} = Q_0 U^{\mu\nu} + Q_1 M^{\mu\nu} + Q_2 V^{\mu\nu} + \text{c.c.} \tag{B1}$$

Substituting the bivector expansion into (1) provides equations for the components Q_0, Q_1, Q_2, which can be most simply written with the use of twelve terms:

$$L_0=(D-2\epsilon)Q_0-2\kappa Q_1, \quad L_1=DQ_1-\kappa Q_2+\pi Q_0, \quad L_2=(D+2\epsilon)Q_2+2\pi Q_1,$$

$$N_0=(\Delta-2\gamma)Q_0-2\tau Q_1, \quad N_1=\Delta Q_1-\tau Q_2+\nu Q_0, \quad N_2=(\Delta+2\gamma)Q_2+2\nu Q_1,$$

$$M_0=(\delta-2\beta)Q_0-2\sigma Q_1, \quad M_1=\delta Q_1-\sigma Q_2+\mu Q_0, \quad M_2=(\delta+2\beta)Q_2+2\mu Q_1,$$

$$B_0=(\bar{\delta}-2\alpha)Q_0-2\rho Q_1, \quad B_1=\bar{\delta}Q_1-\rho Q_2+\lambda Q_0, \quad B_2=(\bar{\delta}+2\alpha)Q_2+2\lambda Q_1.$$

Here $D=l^\alpha\nabla_\alpha$, $\Delta=n^\alpha\nabla_\alpha$, and $\delta=m^\alpha\nabla_\alpha$. The Penrose equation has the following $U_{\mu\nu}$, $M_{\mu\nu}$, and $V_{\mu\nu}$ components, respectively:

$$l^\alpha(3N_2)+n^\alpha(L_2-2B_1)-m^\alpha(3B_2)-\bar{m}^\alpha(M_2-2N_1)=0, \tag{B2}$$

$$l^\alpha(M_2-2N_1)+n^\alpha(B_0-2L_1)+m^\alpha(2B_1-L_2)+\bar{m}^\alpha(2M_1-N_0)=0, \tag{B3}$$

$$l^\alpha(N_0-2M_1)+n^\alpha(3L_0)-m^\alpha(B_0-2L_1)-\bar{m}^\alpha(3M_0)=0. \tag{B4}$$

If $Q^{\mu\nu}$ is to be a Killing potential for k^μ, then its divergence must satisfy

$$3k^\mu=l^\mu(N_1+M_2)-n^\mu(B_0+L_1)-m^\mu(B_1+L_2)+\bar{m}^\mu(N_0+M_1)+\text{c.c.} \tag{B5}$$

APPENDIX C: THE CONFORMAL PENROSE EQUATION

For asymptotically simple space–times with future null infinity $\mathscr{I}^+$ we follow Penrose and Rindler[6] case (iv) to conformally map from the physical metric $g_{\alpha\beta}$ to the unphysical metric $\hat{g}_{\alpha\beta}$:

$$\hat{g}_{\alpha\beta}=\Omega^2 g_{\alpha\beta} \tag{C1}$$

with the spinor basis mapping as $\hat{o}_A=o_A$, $\hat{\imath}_A=\Omega\imath_A$. Here $\Omega=0$ defines the future null boundary with $\nabla_\alpha\Omega$ a null vector tangent to the generators of $\mathscr{I}^+$. It follows from the map of the spinor basis that the tetrad derivatives transform as

$$\hat{D}=\Omega^{-2}D, \quad \hat{\delta}=\Omega^{-1}\delta, \quad \hat{\Delta}=\Delta. \tag{C2}$$

The spin coefficients conformally map as

$$\hat{\kappa}=\Omega^{-3}\kappa, \quad \hat{\rho}=\Omega^{-2}\rho-\Omega^{-3}D\Omega,$$

$$\hat{\sigma}=\Omega^{-2}\sigma, \quad \hat{\tau}=\Omega^{-1}\tau-\Omega^{-2}\delta\Omega,$$

$$\hat{\epsilon}=\Omega^{-2}\epsilon, \quad \hat{\alpha}=\Omega^{-1}\alpha-\Omega^{-2}\bar{\delta}\Omega,$$

$$\hat{\beta}=\Omega^{-1}\beta, \quad \hat{\gamma}=\gamma-\Omega^{-1}\Delta\Omega,$$

$$\hat{\nu}=\Omega\nu, \quad \hat{\mu}=\mu+\Omega^{-1}\Delta\Omega,$$

$$\hat{\lambda}=\lambda, \quad \hat{\pi}=\Omega^{-1}\pi+\Omega^{-2}\bar{\delta}\Omega.$$

Since the Killing potential obeys the conformal transformation $\hat{Q}^{\alpha\beta}=\Omega^{-1}Q^{\alpha\beta}$, it's anti-self-dual bivector components map as

$$\hat{Q}_0 = Q_0, \quad \hat{Q}_1 = \Omega Q_1, \quad \hat{Q}_2 = \Omega^2 Q_2. \tag{C3}$$

The twelve terms in Appendix B which comprise the components of the Penrose equation map as

$$\hat{L}_0 = \Omega^{-2} L_0, \quad \hat{L}_1 = \Omega^{-1} L_1 + Q_0(\Omega^{-2}\bar{\delta}\Omega) + Q_1(\Omega^{-2} D\Omega),$$

$$\hat{L}_2 = L_2 + 2Q_1(\Omega^{-1}\bar{\delta}\Omega) + 2Q_2(\Omega^{-1} D\Omega), \quad \hat{N}_0 = N_0 + 2Q_0(\Omega^{-1}\Delta\Omega) + 2Q_1(\Omega^{-1}\delta\Omega),$$

$$\hat{N}_1 = \Omega N_1 + Q_1(\Delta\Omega) + Q_2(\delta\Omega), \quad \hat{N}_2 = \Omega^2 N_2,$$

$$\hat{M}_0 = \Omega^{-1} N_0, \quad \hat{M}_1 = M_1 + Q_0(\Omega^{-1}\Delta\Omega) + Q_1(\Omega^{-1}\delta\Omega),$$

$$\hat{M}_2 = \Omega M_2 + 2Q_1(\Delta\Omega) + 2Q_2(\delta\Omega), \quad \hat{B}_0 = \Omega^{-1} B_0 + 2Q_0(\Omega^{-2}\bar{\delta}\Omega) + 2Q_1(\Omega^{-2} D\Omega),$$

$$\hat{B}_1 = B_1 + Q_1(\Omega^{-1}\bar{\delta}\Omega) + Q_2(\Omega^{-1} D\Omega), \quad \hat{B}_2 = \Omega B_2.$$

Finally, by direct substitution of the twelve terms above into Eqs. (B2)–(B4) we find the anti-self-dual components of the Penrose equation conformally transform as

$$(\hat{\mathrm{B}}2) = (\mathrm{B}2), \quad (\hat{\mathrm{B}}3) = \Omega^{-1}(\mathrm{B}3), \quad (\hat{\mathrm{B}}4) = \Omega^{-2}(\mathrm{B}4). \tag{C4}$$

This result is confirmed by the conformal maps

$$\hat{\mathbf{P}}^{\alpha\mu\nu} = \Omega^{-3}\mathbf{P}^{\alpha\mu\nu} \tag{C5}$$

and

$$\hat{U}_{\mu\nu} = \Omega^3 U_{\mu\nu}, \quad \hat{M}_{\mu\nu} = \Omega^2 M_{\mu\nu}, \quad \hat{V}_{\mu\nu} = \Omega V_{\mu\nu}. \tag{C6}$$

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Exact solutions for the Tikekar superdense star

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We analyze a relativistic model for superdense stars proposed by Tikekar [R. Tikekar, J. Math. Phys. **31**, 2454 (1990)]. In this model the hypersurfaces generated by $\{t=\text{const}\}$ have the geometry of the 3-spheroid which gives the solutions a clear geometrical characterization. The solution of the Einstein field equations is reduced to integrating a second order ordinary differential equation. New classes of solutions are presented by restricting the choice of the spheroidal parameter K so that polynomial solutions are admitted for the first solution and then we find that there exists another solution which is a product of polynomials and algebraic functions. A remarkable feature of the class of solutions generated is that they are expressible completely in terms of polynomials and algebraic functions. Some physical aspects of the solutions are briefly considered. We regain the Tikekar solution as a special case when $K=-7$. As another example we explicitly present the form of the solution when $K=-2$. © *1996 American Institute of Physics.* [S0022-2488(96)02301-8]

I. INTRODUCTION

Models of relativistic stars are important for the description of astrophysical processes. We may model relativistic stars by finding static spherically symmetric solutions to the Einstein field equations. In addition a number of conditions are normally placed on the energy density, the pressure, and the gravitational potentials to ensure that the model is physically reasonable. However, we should point out that it is rare to find a model that rigorously satisfies all these conditions. For a comprehensive list of exact solutions to the Einstein field equations, many of which may be used to describe the gravitational behavior of stars, see Kramer *et al.*[1] Knutsen[2,3] provides a comprehensive treatment, in particular stellar models, of the conditions to be satisfied for a realistic matter distribution. Even though the static and spherically symmetric conditions are highly simplified they allow the construction of models of physically reasonable superdense stars such as neutron stars.[4]

In an attempt to reduce the complexity of the field equations one normally places some restriction on the metric functions. Vaidya and Tikekar[5] made the observation that one could utilize the geometry of the spacelike hypersurfaces generated by $\{t=\text{const}\}$ to find exact solutions in some cases. This property is very useful in the case of space-times which are static and spherically symmetric, and the hypersurfaces $\{t=\text{const}\}$ are that of the 3-spheroid. The spheroidal condition provides a clear geometrical characterization of the space–times concerned. This is a desirable feature as it is difficult to characterize geometrically many of the solutions in the literature which have been obtained using other techniques. One of the metric functions may be immediately determined from geometrical arguments and the energy density is specified. We are then in a position to determine the remaining gravitational and thermodynamical variables from Einstein's equations. The model that is generated may be applied to superdense stars. Tikekar[6] has performed an analysis of the physical properties of these solutions and found them to be physically viable. The Tikekar model is applicable in the last stages of stellar evolution and satisfies the

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physical requirements placed on fluid configurations at ultrahigh densities and pressures. The values of the maximum mass of the superdense star obtained are close to those of Rhodes and Ruffini.[7] Knutsen[3] has demonstrated that solutions with a spheroidal geometry are stable with respect to infinitesimal radial pulsations.

Our intention in this paper is to obtain new solutions to the field equations for the Tikekar[6] model. The ideal is to obtain models with physically acceptable gravitational behavior in the interior of the star when the 3-spaces $\{t=\text{const}\}$ are spheroidal. In Sec. II we present the field equations for static spherically symmetric gravitational fields. We review the superdense model of Tikekar and generate the second order field equation that has to be integrated. The first solution, in terms of polynomials, is presented in Sec. III. In Sec. IV we generate the second solution in terms of polynomials and algebraic functions by generalizing a solution previously found. Some particular solutions, from the new classes of solutions presented, are explicitly derived in Sec. V. In Sec. VI we briefly consider certain aspects of physically reasonable stellar models. Finally in Sec. VII we review the results obtained and discuss possibilities for further research.

II. THE TIKEKAR MODEL

In standard coordinates, $(x^i)=(t,r,\theta,\phi)$, the line element for static spherically symmetric space–times may be written as[1]

$$ds^2=-e^{2\nu(r)}\,dt^2+e^{2\lambda(r)}\,dr^2+r^2(d\theta^2+\sin^2\,\theta\,d\phi^2), \tag{1}$$

where the quantities $\nu(r)$ and $\lambda(r)$ are gravitational potentials. For a perfect fluid energy-momentum tensor and the static spherically symmetric line element (1) we obtain the following Einstein field equations:

$$\frac{1}{r^2}\,[r(1-e^{-2\lambda})]'=\rho, \tag{2}$$

$$-\frac{1}{r^2}\,(1-e^{-2\lambda})+\frac{2\nu'}{r}\,e^{-2\lambda}=p, \tag{3}$$

$$e^{-2\lambda}\left[\nu''+\nu'^2+\frac{\nu'}{r}-\nu'\lambda'-\frac{\lambda'}{r}\right]=p, \tag{4}$$

where ρ is the energy density and p is the isotropic pressure. In the above equations, primes denote differentiation with respect to r. We rewrite the above systems (2)–(4) so that it is easier to compare with the results of Tikekar.[6] Note that our notation and signature differ from those of Tikekar. However, we generate the same field equations and our results are consistent. For the hypersurface $\{t=\text{const}\}$ to be a 3-spheroid we require that

$$e^{2\lambda}=\frac{1-Kr^2/R^2}{1-r^2/R^2}.$$

The geometry of the 3-spheroid is governed by the parameters R and K. The metric function $e^{2\lambda}$ is regular and well behaved for $r<R$ for which the parameter values $K<1$. We neglect the cases $K=0,1$: for $K=0$ we obtain the Schwarzschild interior solution and, when $K=1$, the hypersurfaces $\{t=\text{const}\}$ are flat. With the above form of $e^{2\lambda}$ the field equations (2)–(4) become

$$\rho=\frac{1-K}{R^2}\,\frac{3-Kr^2/R^2}{(1-Kr^2/R^2)^2}, \tag{5}$$

$$p=\left(\frac{2\nu'}{r}+\frac{1}{r^2}\right)\frac{1-r^2/R^2}{1-Kr^2/R^2}-\frac{1}{r^2}, \tag{6}$$

$$p=\left(\nu''+\nu'^2+\frac{\nu'}{r}\right)\frac{1-r^2/R^2}{1-Kr^2/R^2}-\left(\nu'+\frac{1}{r}\right)\frac{(1-K)(r/R^2)}{(1-Kr^2/R^2)^2}. \tag{7}$$

The equation

$$(1-r^2/R^2)(1-Kr^2/R^2)\left(\nu''+\nu'^2-\frac{\nu'}{r}\right)-(1-K)(r/R^2)\left(\nu'+\frac{1}{r}\right)$$
$$+(1-K)(1/R^2)(1-Kr^2/R^2)=0 \tag{8}$$

follows directly from Eqs. (6) and (7) and is the condition for pressure isotropy.

It is clear from inspection of the systems (5)–(7) that, if a functional form for the metric function ν is known, then we have a solution to the field equations. The differential equation (8) determines the behavior of ν. We can transform Eq. (8) to simpler form if we let

$$\psi=e^{\nu}, \quad x^2=1-r^2/R^2.$$

Then Eq. (8) takes the equivalent form

$$(1-K+Kx^2)\frac{d^2\psi}{dx^2}-Kx\frac{d\psi}{dx}+K(K-1)\psi=0. \tag{9}$$

For the parameter value $K=-7$ Tikekar[6] obtained the particular solution

$$\psi=A\psi_1+B\psi_2=A(1-\tfrac{7}{2}x^2+\tfrac{49}{24}x^4)+Bx(1-\tfrac{7}{8}x^2)^{3/2}, \tag{10}$$

where A and B are arbitrary constants. We present new classes of solutions to the differential equation (9) in subsequent sections.

III. THE FIRST SOLUTION

The special solution (10) contains the quartic term $(1-\frac{7}{2}x^2+\frac{49}{24}x^4)$. This suggests that Eq. (9) may admit solutions ψ_1 in the form of a series which would terminate for some values of K. Therefore we seek solutions to Eq. (9) of the form

$$\psi_1=\sum_{i=0}^{\infty}a_i x^i,$$

where a_i are constants. We find that this series terminates and we obtain two classes of polynomial solutions, the first in even powers of x and the second in odd powers of x, for particular values of the parameter K as would be expected from the form of Eq. (9). The appropriate values of K are

$$\text{even powers in } x: \quad K=2-(2n-1)^2,$$

$$\text{odd powers in } x: \quad K=2-4n^2.$$

Note that we require $n>1$, for even powers of x, and $n>0$, for odd powers of x, so that $K<1$ to ensure regularity of the metric functions.

For even powers we obtain the difference equation

$$a_{i+1}=-\frac{[(2n-1)^2-2]}{n(n-1)}\frac{(n-i)(n+i-1)}{(i+1)(2i+1)}a_i$$

which may be solved for the coefficients a_i. Then we can show that the polynomial in even powers of x is of the form

$$\psi_1=\sum_{i=0}^{n}a_ix^{2i}=\sum_{i=0}^{n}\frac{(n+i-2)!}{(n-i)!(2i)!}(-\lambda)^ix^{2i}, \tag{11}$$

where the constants λ and K are given by

$$\lambda=4-\frac{1}{n(n-1)},\quad K=2-(2n-1)^2.$$

The difference equation for odd powers is given by

$$a_{i+1}=-\frac{8(2n^2-1)}{4n^2-1}\frac{(n-i)(n+i)}{(2i+2)(2i+3)}a_i.$$

Consequently the polynomial in odd powers of x has the form

$$\psi_1=\sum_{i=0}^{n}a_ix^{2i+1}=\sum_{i=0}^{n}\frac{(n+i-1)!}{(n-i)!(2i+1)!}(-\mu)^ix^{2i+1}, \tag{12}$$

where we define

$$\mu=4-\frac{4}{4n^2-1},\quad K=2-4n^2.$$

The polynomial solutions (11) and (12) comprise the first solution ψ_1 of Eq. (9) for the appropriate values of K. It is clear that Eq. (11) contains the quartic term $(1-\frac{7}{2}x^2+\frac{49}{24}x^4)$ in Tikekar's solution (10). The second solution to Eq. (9) cannot be expressed solely in terms of polynomial functions as demonstrated in Sec. IV.

IV. THE SECOND SOLUTION

The Tikekar[6] solution (10) contains $x(1-\frac{7}{8}x^2)^{3/2}$ as the second solution. This algebraic function is a special case of

$$\psi_2=(1-K+Kx^2)^{3/2}u(x),$$

where $u(x)=x$ and $K=-7$. We notice that other values of K generate particular solutions to Eq. (9) and $u(x)$ is a polynomial. This suggests that the above form for ψ_2 is a generic solution to the differential equation (9). For ψ_2 to be a solution of Eq. (9) the function $u(x)$ has to satisfy the following equation:

$$(1-K+Kx^2)\frac{d^2u}{dx^2}+5Kx\frac{du}{dx}+K(K+2)u=0. \tag{13}$$

As for the first solution we can find polynomials that satisfy Eq. (13) for certain values of K. The procedure is very similar to that given in Sec. III. However, it is important to note that there is a reversal of role for the parameter K in the characterization of the even and odd polynomials:

$$\text{odd powers in } x: \quad K=2-(2n-1)^2,$$

$$\text{even powers in } x: \quad K=2-4n^2.$$

In other words, u will contain odd (even) powers of x when ψ_1 has even (odd) powers of x. The oddness and evenness of the two solutions is not unexpected from the form of Eq. (9). That both are finite expressions (in the sense of Poincaré) is perhaps somewhat unexpected.

The difference equation for $K=2-(2n-1)^2$ is

$$a_{i+1}=-\frac{[(2n-1)^2-2]}{2n(n-1)}\frac{(n+i+1)(n-i-2)}{(2i+2)(2i+3)}a_i$$

which we have solved in general. Then the polynomial in odd powers of x is given by

$$u=\sum_{i=0}^{n-2}a_i x^{2i+1}=\sum_{i=0}^{n-2}\frac{(n+i)!}{(n-i-2)!(2i+1)!}(-\lambda)^i x^{2i+1},$$

where the constants λ and K satisfy

$$\lambda=4-\frac{1}{n(n-1)}, \quad K=2-(2n-1)^2.$$

The difference equation for $K=2-4n^2$ is given by

$$a_{i+1}=-\frac{8(2n^2-1)}{4n^2-1}\frac{n^2-(i+1)^2}{(2i+1)(2i+2)}a_i$$

which may be solved for the constants a_i. The polynomial in even powers of x has the form

$$u=\sum_{i=0}^{n-1}a_i x^{2i}=\sum_{i=0}^{n-1}\frac{(n+i-1)!}{(n-i)!(2i)!}(-\mu)^i x^{2i},$$

where we have

$$\mu=4-\frac{4}{4n^2-1}, \quad K=2-4n^2.$$

With these expressions for u we have that the second solution, with u containing odd powers of x, is given by

$$\psi_2=(1-K+Kx^2)^{3/2}\sum_{i=0}^{n-2}\frac{(n+i)!}{(n-i-2)!(2i+1)!}(-\lambda)^i x^{2i+1}. \tag{14}$$

The second solution, with u containing even powers of x, is

$$\psi_2=(1-K+Kx^2)^{3/2}\sum_{i=0}^{n-1}\frac{(n+i)!}{(n-i-1)!(2i)!}(-\mu)^i x^{2i}. \tag{15}$$

Solutions (14) and (15) generate the second solutions of Eq. (9) which are clearly linearly independent from the first solutions (11) and (12), respectively.

Thus we have generated general solutions to the differential equation (9) by restricting the values of K so that polynomials and products of polynomials with algebraic functions are possible as solutions. The solutions for the various cases are given by Eqs. (11), (12), (14), and (15). Collecting these results we have the first category of solutions:

$$\psi=A\sum_{i=0}^{n}\frac{(n+i-2)!}{(n-i)!(2i)!}(-\lambda)^i x^{2i}+B(1-K+Kx^2)^{3/2}\sum_{i=0}^{n-2}\frac{(n+i)!}{(n-i-2)!(2i+1)!}(-\lambda)^i x^{2i+1} \tag{16}$$

for $K=2-(2n-1)^2$. The second category of solutions is given by

$$\psi=A\sum_{i=0}^{n}\frac{(n+i-1)!}{(n-i)!(2i+1)!}(-\mu)^i x^{2i+1}+B(1-K+Kx^2)^{3/2}\sum_{i=0}^{n-1}\frac{(n+i)!}{(n-i-1)!(2i)!}(-\mu)^i x^{2i}, \tag{17}$$

where $K=2-4n^2$. In Eqs. (16) and (17) the constants λ and μ depend on n:

$$\lambda=4-\frac{1}{n(n-1)},\quad \mu=4-\frac{4}{4n^2-1}.$$

We have generalized the solution of Tikekar[6] and obtained new classes of solution applicable to superdense stars. It is remarkable that the solutions (16) and (17) are expressed completely as combinations of polynomials and algebraic functions. This is directly related to the restriction placed on the spheroidal parameter K. It is rare to find solutions, especially such large classes as Eqs. (16) and (17), to the field equations in terms of elementary functions. Because of their simplicity our solutions will have the advantage of simplifying the analysis of the physical properties of the superdense star.

V. SOME PARTICULAR CASES

We may generate many solutions found previously from our general class of solutions (16) and (17). With $K=-7$ $(n=2)$, $\lambda=7/2$. Then it is easy to verify that Eq. (16) becomes

$$\psi=A(1-\tfrac{7}{2}x^2+\tfrac{49}{24}x^4)+Bx(1-\tfrac{7}{8}x^2)^{3/2}.$$

Thus we have regained the Tikekar[6] solution from our results. Other solutions found in the literature are also contained in our general class of functions. However, there exist solutions found previously that cannot be regained from our results. For example, the Durgapal and Bannerji solution[8] for which

$$e^{2\lambda}=\frac{2(1+Cr^2)}{2-Cr^2},$$

where C is a positive constant does not fall into our class of solutions. A study of the various possibilities that arise and their relationship to particular existing solutions would be a formidable task. Also we may obtain other explicit functional forms for ψ which could be useful in applications for superdense stars. As a simple example suppose that $K=-2(n=1)$ so that $\mu=8/3$. Then it follows that

$$\psi=A(x-\tfrac{4}{9}x^3)+B(3-2x^2)^{3/2}$$

from Eq. (17).

VI. SOME PHYSICAL ASPECTS

As we have pointed out previously the condition of 3-spheroidal hypersurfaces permits a clear geometrical interpretation which is not the case in many other exact solutions. The spheroidal assumption in the $\{t=\text{const}\}$ hypersurfaces is physically reasonable as it represents a deviation from spherical symmetry. This situation is likely to occur in the central core regions of superdense stars because of highly nonlinear gravitational effects. It should be emphasized that we have little information about the nature of the behavior of matter in the central regions of superdense stars. Clearly we should attempt to construct a model under assumptions that allow for fairly general behavior. In this regard solutions generated by computers are not helpful as we cannot specify *a priori* a equation of state with great certainty for the core regions. The spheroidal assumption has produced models which are consistent with densities of the order 2×10^{14} gm cm^{-3} as demonstrated by Tikekar.[6] These values are consistent with the results of Rhodes and Ruffini[7] and indicate that the spheroidal assumption produces physically viable static models for relativistic stars.

If $0<K<1$ then ρ remains positive in the region $r^2<3R^2/K$ which restricts the size of the configuration. When $K<0$ there is no restriction on ρ. Thus $\rho>0$ in the interior of the star. It is clear from Eq. (5) that $\rho'<0$ so that the density decreases from the center. We require that the pressure must vanish at the boundary $r=a$ which implies that

$$\left(\frac{4}{R^2}\frac{1}{\psi}\frac{d\psi}{dx}\right]_a-\frac{1}{a^2}\right)\frac{1-a^2/R^2}{1-Ka^2/R^2}+\frac{1}{a^2}=0,$$

where ψ is given by Eq. (16) or (17). Essentially this places a restriction on the constants A and B. The gradient of the pressure is

$$p'=-(\rho+p)\frac{pr^3+2m(r)}{2r[r-2m(r)]},\quad m(r)=\frac{1}{2}\frac{(1-K)r/R^2}{1-Kr^2/R^2}.$$

This implies that the pressure gradient is negative if $p>0$ (the energy density $\rho>0$) and consequently the pressure will be decreasing outwards. The interior metric (1) should continuously match with the exterior Schwarschild line element

$$ds^2=-\left(1-\frac{2m}{r}\right)dt^2+\left(1-\frac{2m}{r}\right)^{-1}dr^2+r^2(d\theta^2+\sin^2\theta\,d\phi^2)$$

at $r=a$. This requirement implies that

$$1-\frac{2m}{a}=e^{2\nu(a)}=A\psi_1(a)+B\psi_2(a),$$

$$\left(1-\frac{2m}{a}\right)^{-1}=e^{2\lambda(a)}=\frac{1-Ka^2/R^2}{1-a^2/R^2}.$$

The quantities considered above can be explicitly investigated for various models. In particular Tikekar[6] and Vaidya and Tikekar[5] have comprehensively studied the cases $K=-7$ and $K=-2$, respectively; they demonstrated that the physical requirements for a regular, stable star are satisfied.

VII. DISCUSSION

The Tikekar[6] model has the advantage of being well behaved and satisfies the physical requirements for a superdense star. Unlike many other solutions it has a clear geometrical interpre-

tation: the 3-spaces $\{t=\text{const}\}$ have the geometry of the spheroid. We have integrated the field equation (9) to obtain new solutions by restricting the spheroidal parameter K to take on values so that polynomial solutions exist. The accuracy of the results has been verified with the assistance of the algebraic computing package MATHEMATICA.[9] The distinguishing feature of solutions (16) and (17) is that they are written completely in terms of polynomial functions and algebraic functions. This is a desirable feature and is particularly helpful when considering the physical properties of stars such as the mass, red shift, etc. We regained the physically reasonable Tikekar[6] model of a superdense star from our general class of solutions for $K=-7$ and presented a particular solution for $K=-2$. We briefly discussed some of the physical properties of the new solutions presented. This is important for applications and should be pursued in greater detail in the future. The models generated in our analysis are likely to be physically reasonable as they contain the Tikekar superdense model.

The solutions obtained have arisen essentially because we have imposed spheroidal symmetry. The use of other symmetries may generate new solutions. For example, Herrera *et al.*,[10] Herrera and Ponce de Leon,[11–13] and Maartens and Maharaj[14] have generated conformally invariant static fluid spheres by assuming a conformal symmetry on space–time. We have obtained solutions to the differential equation (9) by restricting the values of K. There exist other solutions to Eq. (9) for different values of K. To demonstrate this let

$$\psi=y(x), \quad x=-2\sqrt{1-1/K}x+\sqrt{1-1/K}.$$

Then the isotropy of pressure condition (9) becomes

$$x(1-x)\frac{d^2y}{dx^2}-\left(x-\frac{1}{2}\right)\frac{dy}{dx}+(1-K)y=0$$

which is the hypergeometric equation.[15] This has solutions in terms of special functions, namely the hypergeometric function. Whether the greater generality of the solution in terms of hypergeometric functions outweighs the tractability of the solutions presented here is a matter for conjecture.

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The initial singularity in solutions of the Einstein–Vlasov system of Bianchi type I

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The dynamics of solutions of the Einstein–Vlasov system with Bianchi I symmetry is discussed in the case of massive or massless particles. It is shown that in the case of massive particles the solutions are asymptotic to isotropic dust solutions at late times. The initial singularity is more difficult to analyze. It is shown that the asymptotic behavior there must be one of a small set of possibilities, but it is not clear whether all of these possibilities are realized. One solution is exhibited in the case of massless particles, which behaves quite differently near the singularity from any Bianchi I solution with perfect fluid as a matter model. In particular, the matter is not dynamically negligible near the singularity for this solution. © *1996 American Institute of Physics.* [S0022-2488(96)03901-4]

I. INTRODUCTION

The simplest of all anisotropic cosmological models are those of Bianchi type I. They are the space–times that admit a three-dimensional Abelian symmetry group whose orbits are space-like. (For general information on Bianchi models see Ref. 1.) Just how simple their dynamics is depends significantly on the nature of the matter content of the space–time. For a perfect fluid with a linear equation of state, it has been known for a long time how to analyze the dynamics.[2,3] For a noninteracting mixture of two fluids with linear equations of state, the time evolution is also well understood and is asymptotic near the singularity and at large times to that of a single fluid.[4] The case of a fluid with a nonlinear equation of state is discussed in an Appendix to the present paper. The dynamics does not differ much from the picture in the linear case. When a magnetic field is added to the fluid, things are already more complicated. In fact, as was shown by Collins,[5] a Bianchi type I model with fluid and magnetic field resembles a model of the more complicated Bianchi type II with fluid alone. It is also interesting to note that models of type VI_0 with perfect fluid and a magnetic field have a dynamical behavior resembling the notoriously complicated ''Mixmaster'' behavior of Bianchi type IX models.[6] Thus, changing the matter model can have effects on the complexity of the dynamics comparable with those encountered when passing to more general symmetry types.

A matter model for which the details of the global dynamics of Bianchi type I space–times has not previously been studied mathematically is the collisionless gas, described by the Vlasov equation. The only general facts that are known are that, with an appropriate choice of time orientation, (i) the space–time is future geodesically complete (when maximally extended toward the future); and (ii) there is a crushing singularity in the past where, except in the vacuum case, the curvature invariant $R_{\alpha\beta}R^{\alpha\beta}$ tends to infinity.

These fundamental facts were proved in Ref. 7, where it was shown that they hold for any Bianchi type other than IX and for a general class of matter models. The aim of this paper is to refine (i) and (ii) in the case of Bianchi type I symmetry and matter described by the Vlasov equation so as to get more detailed information about the asymptotics of the expanding phase and the nature of the initial singularity. An aspect of the situation that makes this more difficult than in the case of many other matter models is that for general initial data it is not possible to derive an explicit closed system of ordinary differential equations that describes the dynamics. This is because certain integrals that occur cannot be evaluated. In one special case, where massless

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particles are considered and the initial phase space density has the form of the characteristic function of a ball, these integrals have been computed by Lukash and Starobinski.[8] However, the explicit expressions they obtain are sufficiently complicated that they do not seem to make a rigorous analysis of the global dynamics any easier. On the other hand, they would probably be useful for numerical calculations, since they would allow costly numerical evaluation of integrals to be avoided.

The dynamics at late times of the models with massive particles can be described precisely. All solutions become isotropic and can be approximated by dust solutions in this limit (Theorem 5.4). On the other hand, the results of this paper do not give a complete picture of the dynamics near the initial singularity of the space–times being studied. They merely reduce the possible types of asymptotic behavior to a small number of alternatives. Improving on this is likely to require new techniques. These results leave open the possibility that Bianchi I space–times with a matter content described by kinetic theory may show complicated oscillatory behavior, and thus may be very different from those with other types of matter content studied up to now. The mechanism that allows for this complexity is simply the presence of anisotropy in the pressure that may respond to changes in the geometry. It may be that the only reason that the dynamics is so simple in the case of a perfect fluid is that this mechanism is excluded by a special symmetry assumption (the isotropy of the pressure). The one conclusion that emerges and that applies to all solutions considered here is that the ratio of the mean pressure to the energy density tends to one-third as the singularity is approached. This means that in a certain weak sense the dynamics for particles of unit mass m is approximated near the singularity by that for massless particles. For this reason both cases are often considered together in the following, although the main emphasis is on the case $m=1$.

The results will now be summarized. There are, broadly speaking, two possible types of asymptotic behavior of solutions of the Einstein–Vlasov system with Bianchi I symmetry near the singularity. They will be referred to as convergent and oscillatory. Let λ_i denote the eigenvalues of the second fundamental form of the homogeneous hypersurfaces. Then the mean curvature of the homogeneous hypersurfaces is given by $\mathrm{tr}\, k=\lambda_1+\lambda_2+\lambda_3$. Define the generalized Kasner exponents by $p_i=\lambda_i/\mathrm{tr}\, k$. In the convergent type, the p_i tend to limits as the singularity is approached. There are three different cases, depending on these limiting values. The first case is that where the limiting values are $(\frac{1}{3},\frac{1}{3},\frac{1}{3})$. The well-known homogeneous and isotropic solutions of the Einstein–Vlasov system[9] are of this type. The second is that the limiting values are $(0,\frac{1}{2},\frac{1}{2})$ or some permutation thereof. The existence of solutions of this kind in the case of massless particles is shown in Sec. VI. These limiting values of the generalized Kasner exponents are not realized by any Bianchi type I space–time when the matter model is a perfect fluid (see the Appendix). The third is that the limiting values satisfy the Kasner relation $p_1^2+p_2^2+p_3^2=1$. Any solution for which one of the eigenvalues becomes negative at some time has this asymptotic behavior, and so there are plenty of examples. This is proved in Theorem 5.1. Note that the special case of this result when two of the p_i are equal is closely related to the homogeneous special case of a result of Rein[10] for plane symmetric space–times. In the oscillatory type the p_i undergo infinitely many oscillations, in a sense that will now be specified. There are two cases to be considered, according to whether two of the eigenvalues are always equal or not. Consider first the case where two eigenvalues are equal and suppose, without loss of generality, that $\lambda_2=\lambda_3$. Associate to any solution a string of symbols (which may be finite or infinite, depending on the solution) as follows. Moving backward from some fixed time, add an x to the string each time that $\lambda_1-\lambda_2$ changes from being $\leqslant 0$ to being >0 and add a y each time it changes from being $\geqslant 0$ to being <0. That this makes sense follows from the fact, proved in Sec. II, that the set of times where $\lambda_1=\lambda_2$ can have no limit point unless this equality holds at all times. Thus, a finite time interval can only contribute a finite number of symbols. The solution is said to undergo infinitely many oscillations if the resulting string of symbols is infinite. Similarly, if there is some time where all eigenvalues are distinct, then a string

of symbols is associated to the solution by adding x, y, or z each time λ_1, λ_2, or λ_3, respectively, becomes strictly larger than the other two eigenvalues.

Unfortunately it could not be shown whether any oscillatory solutions exist. If they did, then the behavior of Bianchi I models with kinetic theory as matter model would be much more complicated than in the case of a perfect fluid. If it could be shown that they existed, the question would remain whether the sequences of symbols they produce have some regularity or whether they are chaotic. In the absence of analytical techniques capable of deciding this question, it would be desirable to carry out a numerical investigation. This could provide evidence as to the existence (or otherwise) and nature of oscillatory behavior. It might also suggest new approaches to proving theorems about the global dynamics.

To each type of solution discussed above corresponds a characteristic behavior of the pressures. The solutions considered in the following all have diagonal energy-momentum tensors, and so three pressures P_i are defined by three diagonal components. The remaining diagonal component is the energy density ρ. The quantities $R_i = P_i/\rho$ must have a sum that converges to unity at the singularity. When the limiting values of the p_i are $(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ or $(0,\frac{1}{2},\frac{1}{2})$, then the limiting values of the R_i are $(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ or $(0,\frac{1}{2},\frac{1}{2})$, respectively. When the sum of the squares of the limiting values of the p_i is equal to unity, then the R_i tend to $(0,\frac{1}{2},\frac{1}{2})$ or a permutation thereof, unless one p_i has the limiting value zero. In the latter case the R_i tend to (1,0,0) or a permutation thereof.

The paper is organized as follows. In Sec. II some basic facts about the solutions are collected. Section III is concerned with a simplified system, which in some cases models the asymptotic behavior of the solutions of the original system. Some estimates for the pressures are derived in Sec. IV. Section V contains the main results. Section VI contains proofs of the existence or nonexistence of solutions with certain kinds of asymptotic behavior.

II. BASIC FACTS

The Einstein–Vlasov system is the system of equations that describes the kinetic theory of self-gravitating particles in general relativity. A thorough introduction to general relativistic kinetic theory and to the collisionless case, in particular, can be found in Ref. 11. For particles all of the same mass $m \geqslant 0$, the system can be written in the following form in the case of Bianchi type I symmetry:

$$-k_{ij}k^{ij} + (\mathrm{tr}\ k)^2 = 16\pi\rho, \tag{2.1}$$

$$T_{0i} = 0, \tag{2.2}$$

$$\partial_t g_{ij} = -2k_{ij}, \tag{2.3}$$

$$\partial_t k_{ij} = \mathrm{tr}\ k k_{ij} - 2k_{il}k^l_j - 8\pi T_{ij} - 4\pi\rho g_{ij} + 4\pi\ \mathrm{tr}\ T g_{ij}, \tag{2.4}$$

$$\frac{\partial f}{\partial t} + 2k^i_j v^j \frac{\partial f}{\partial v^i} = 0, \tag{2.5}$$

$$\rho = \int f(t,v^k)(m^2 + g_{rs}v^r v^s)^{1/2}(\det g)^{1/2}\, dv^1\, dv^2\, dv^3, \tag{2.6}$$

$$T_{ij} = \int f(t,v^k) v_i v_j (m^2 + g_{rs}v^r v^s)^{-1/2}(\det g)^{1/2}\, dv^1\, dv^2\, dv^3. \tag{2.7}$$

Equations (2.1)–(2.4) are the Einstein equations written in 3+1 form, (2.5) is the Vlasov equation, and (2.6) and (2.7) are the definition of the energy-momentum tensor in terms of the matter fields needed to complete the system. In these equations g_{ij} is the induced metric of the homogeneous

hypersurfaces, k_{ij} is the second fundamental form, f is the phase space density of particles, ρ is the energy density, T_{0i} and T_{ij} are components of the energy-momentum tensor, and tr k is the mean curvature $g^{ij}k_{ij}$. With the exception of f all these quantities depend only on the time coordinate t. This time coordinate is Gaussian, i.e., it is constant on each homogeneous hypersurface and defines a parametrization by proper time when restricted to any geodesic normal to these hypersurfaces. The space–time metric is of the form

$$ds^2 = -dt^2 + g_{ij}(t)dx^i\,dx^j. \tag{2.8}$$

In the following it is always assumed, when talking about solutions of (2.1)–(2.7), that the function $f(t,v)$ is non-negative and has compact support for each fixed t. It is assumed that f is C^1 except in Sec. III, where f may be a distribution. The case of primary interest here is the case $m=1$. Since, however, solutions of (2.1)–(2.7) with $m=1$ resemble solutions with $m=0$ close to the singularity, it is useful to also allow the case $m=0$ from the beginning. Note that the real distinction here is between massless particles on the one hand and, on the other hand, massive particles, which all have the same mass. In the latter case it is convenient to choose the mass of a particle as a unit of mass so that the numerical value of the mass of a particle in the system of units used is unity.

For a given Bianchi I geometry, the Vlasov equation can be solved explicitly. (This is not possible for the other Bianchi types. The reason is explained in Ref. 12.) The result is that if f is expressed in terms of the covariant components v_i then it is independent of time. This means that if t_0 is some fixed time and $f_0(v_i)=f(t_0,v_i)$, then (2.6) can be rewritten as

$$\rho = \int f_0(v_i)(m^2+g^{rs}v_rv_s)^{1/2}(\det g)^{-1/2}\,dv_1\,dv_2\,dv_3, \tag{2.9}$$

and (2.7) can be rewritten in a similar way. The explicit solution allows certain special subclasses of solutions of (2.1)–(2.7) to be identified. The first of these will be referred to as reflection-symmetric, and is defined by the conditions that

$$f_0(v_1,v_2,v_3)=f_0(-v_1,-v_2,v_3)=f_0(v_1,-v_2,-v_3), \tag{2.10}$$

and that the initial values of g_{ij} and k_{ij} are diagonal. Equation (2.10) implies that T_{ij} is diagonal. It then follows from (2.3) and (2.4) that g_{ij} and k_{ij} are always diagonal. The second case, which will be referred to as LRS (locally rotationally symmetric) is obtained by supplementing (2.10) by the conditions that

$$f_0(v_1,v_2,v_3)=F((v_1)^2+(v_2)^2,v_3), \tag{2.11}$$

for some function F and that $g_{11}=g_{22}$, $k_{11}=k_{22}$ initially. Equation (2.11) implies that $T_{11}=T_{22}$ and it follows from (2.3) and (2.4) that $g_{11}=g_{22}$ and $k_{11}=k_{22}$ everywhere. A solution will also be called LRS if it satisfies the definition obtained from that just given by a permutation of the indices 1,2,3. A solution will be called isotropic if

$$f_0(v_1,v_2,v_3)=F((v_1)^2+(v_2)^2+(v_3)^2), \tag{2.12}$$

and if g_{ij} and k_{ij} are proportional to δ_{ij} on the initial hypersurface, and hence everywhere. If a solution satisfies the conditions on g_{ij} and k_{ij} in the definition of reflection-symmetric, LRS or isotropic for all t in some interval, but no assumption is made on f then the solution will be said to have reflection-symmetric, LRS or isotropic geometry, respectively, on that interval. It follows from (2.4) that T_{ij} has a corresponding symmetry property.

In this paper only reflection-symmetric solutions of (2.1)–(2.7) are considered. The alternative notation $a^2=g_{11}/g_{11}(t_0)$, $b^2=g_{22}/g_{22}(t_0)$, $c^2=g_{33}/g_{33}(t_0)$ is used when it is convenient. Yet another form of (2.6) can then be obtained by doing a change of variables in (2.9),

$$\rho=\int f_0(aw_1,bw_2,cw_3)(m^2+\delta^{rs}w_rw_s)^{1/2}\,dw_1\,dw_2\,dw_3. \tag{2.13}$$

The geometric interpretation of the w_i is that they are the components of the momentum in an orthonormal frame. Similarly,

$$T^i_i=\int f_0(aw_1,bw_2,cw_3)w_i^2(m^2+\delta^{rs}w_rw_s)^{-1/2}\,dw_1\,dw_2\,dw_3. \tag{2.14}$$

In order to study the dynamics of the solutions of the system (2.1)–(2.7) in detail, it is useful to introduce certain dimensionless variables that remain finite at the singularity. It follows from (2.1) that $\operatorname{tr} k$ never vanishes, except in the case of flat space–time, which is excluded from consideration in the following. By replacing t by $-t$ if necessary, it can be arranged that $\operatorname{tr} k<0$ everywhere. It will be assumed that this has been done. Define

$$\hat{k}_{ij}=k_{ij}/\operatorname{tr} k, \tag{2.15}$$

$$\hat{\rho}=\rho/(\operatorname{tr} k)^2, \tag{2.16}$$

$$\hat{T}_{ij}=T_{ij}/(\operatorname{tr} k)^2, \tag{2.17}$$

$$\tau(t)=-\int_{t_0}^{t}\operatorname{tr} k(t')dt'. \tag{2.18}$$

In terms of these variables equations (2.1) and (2.4) become

$$-\hat{k}^i_j\hat{k}^j_i+1=16\pi\hat{\rho}, \tag{2.19}$$

$$\partial_\tau\hat{k}^i_j=-12\pi\hat{\rho}(\hat{k}^i_j-\tfrac{1}{3}\delta^i_j)+8\pi\hat{T}^i_j+4\pi(\hat{k}^i_j-\delta^i_j)\operatorname{tr}\hat{T}. \tag{2.20}$$

The following lemma provides some information about the range of τ.

Lemma 2.1: Let a solution of (2.1)–(2.7) with $m=0$ or $m=1$ be given, which is the maximal globally hyperbolic development of initial data on the hypersurface $t=t_0$. Then $\operatorname{tr} k(t)$ is a monotonic function defined on an interval (t_1,∞). By translating t, it can be assumed that $t_1=0$. Then $\lim_{t\to 0}\operatorname{tr} k=-\infty$ and $\lim_{t\to\infty}\operatorname{tr} k=0$. Moreover, $-3/t\leqslant\operatorname{tr} k(t)\leqslant -1/t$.

Proof: That $\operatorname{tr} k(t)$ is monotonic and defined on an interval of the form (t_1,∞) with $\lim_{t\to t_1}\operatorname{tr} k=-\infty$ was shown for the case $m=1$ in Ref. 13. Essentially the same argument applies for $m=0$. In the latter case the coefficients of the characteristic system are only Lipschitz instead of C^1, but this causes no problems. Now it follows from (2.4) that $\frac{1}{3}(\operatorname{tr} k)^2\leqslant\partial_t(\operatorname{tr} k)\leqslant(\operatorname{tr} k)^2$. Comparing the solution with the ordinary differential equations corresponding to these inequalities then gives the desired estimates (cf. Ref. 7).

This result implies that the integral defining τ diverges as $t\to 0$ and as $t\to\infty$. Hence, the solution of (2.19)–(2.20) exists globally in τ.

The solution of (2.19)–(2.20), of course, contains only a small part of the information of that contained in the solution of (2.1)–(2.7). The former is only a projection of the latter. Nevertheless, it will be seen that a lot of information about the solution of the full equations can be obtained by studying this projection. Consider now the set K of triples of real numbers $\hat{k}^1_1,\hat{k}^2_2,\hat{k}^3_3$ that satisfy $\Sigma_i(\hat{k}^i_i)^2\leqslant 1$ and $\Sigma_i\hat{k}^i_i=1$. This is a compact subset of $\mathbf{R}^3$. In fact, it is a disk in a plane. A solution

of (2.19)–(2.20) defines a point of K at each time τ. It is on the boundary of K in the plane if f is identically zero and in the interior otherwise. This point depending on τ, considered as a mapping from $\mathbf{R}$ to K, will be referred to as the projection of the given solution. The projection of a vacuum solution, which lies on the boundary of K, is constant. The vacuum solutions are, of course, the well-known Kasner solutions and the boundary of K may be referred to as the "Kasner circle." Let C denote the point $(\frac{1}{3},\frac{1}{3},\frac{1}{3})$. If a solution has isotropic geometry on a time interval, then its projection lies at the point C during this time. Conversely, if its projection lies at C on a given time interval, then it can be made to have isotropic geometry by a time-independent rescaling of the spatial coordinates. Let L_1, L_2, and L_3 be the subsets of K defined by $\hat{k}_2^2=\hat{k}_3^3$, $\hat{k}_1^1=\hat{k}_3^3$, and $\hat{k}_1^1=\hat{k}_2^2$, respectively. A solution has LRS geometry on a time interval (up to a constant rescaling of the spatial coordinates as above), if and only if its projection lies on one of the lines L_1, L_2, or L_3 during this time. Let L_i^+ denote the open half of L_i which ends at the point with coordinates $(-\frac{1}{3},\frac{2}{3},\frac{2}{3})$ or a permutation thereof, and let L_i^- denote the opposite half-line, which ends at the point with coordinates (1,0,0) or a permutation thereof. Let V_i^+ and V_i^- denote these end points. Let A_1 be the open region bounded by L_2^+,L_3^+ and the boundary of K, and let A_2 and A_3 be defined by cyclically permuting (1,2,3) in this definition. Let B_i be the subset of K where $\hat{k}_i^i \leqslant 0$.

The components of the metric satisfy the evolution equations

$$\frac{dg_{ii}}{d\tau}=2\hat{k}_i^i g_{ii}, \quad \frac{d}{d\tau}\left(\frac{g_{ii}}{g_{jj}}\right)=2(\hat{k}_i^i-\hat{k}_j^i)\left(\frac{g_{ii}}{g_{jj}}\right), \tag{2.21}$$

which imply that g_{ii} or their ratios increase or decrease exponentially if certain sign conditions are satisfied by the $\hat{k}_i^i$. There are, of course, corresponding statements for the scale factors a, b, and c. Given an initial datum f_0 for f the quantities ρ and T_i^i are determined uniquely by the g_{ii} by means of Eqs. (2.13) and (2.14). The quantities $\hat{\rho}$ and $\hat{T}_i^i$ are given in terms of ρ and T_i^i and tr k by the definitions (2.16) and (2.17), while the off-diagonal components $\hat{T}_j^i$ are zero by assumption. Thus, (2.19), (2.20), and (2.21), together with the equation

$$\partial_\tau(\text{tr } k)=-(\text{tr } k)(1-12\pi\hat{\rho}+4\pi \text{ tr } \hat{T}), \tag{2.22}$$

derive from (2.4), form a closed system of ordinary differential equations, which, for fixed f_0, formally determine the quantities $\hat{k}_i^i$, g_{ii}, and tr k as functions of τ in terms of initial data. If the coefficients of this system were locally Lipschitz, it would follow from the standard uniqueness theorem for ordinary differential equations that they determine them uniquely. It will now be shown that, in fact, for $m=1$ this dependence is analytic. To do this it is convenient to use the expressions for ρ and T_i^i of the type (2.9). Analyticity is a consequence of the following lemma.

Lemma 2.2: Let W be a mapping of $U\times\mathbf{R}^3$ to $\mathbf{R}$, where U is an open subset of $\mathbf{R}^3$. Suppose that W extends to a C^1 mapping $\tilde{W}$ of $\tilde{U}\times\mathbf{R}^3$ to $\mathbf{C}$, where $\tilde{U}$ is an open neighborhood of U in $\mathbf{C}^3$, and that $\tilde{W}(\cdot,y)$ satisfies the Cauchy–Riemann equations for each fixed $y\in R^3$. Finally, suppose that each $z\in W$ has an open neighborhood V such that the supports of the functions $W(z,\cdot)$ are contained in a common compact subset K of $\mathbf{R}^3$. Then the function $F(x)=\int_{\mathbf{R}^3}W(x,y)dy$ is analytic.

Proof: It suffices to show that the function $\tilde{F}(z)=\int_{\mathbf{R}^3}\tilde{W}(z,y)dy$ is complex analytic, and this is true if $\tilde{F}$ is C^1 and satisfies the Cauchy–Riemann equations.[14] The assumptions on the smoothness and support of $\tilde{W}$ justify differentiation under the integral, and so the Cauchy–Riemann equations for $\tilde{F}$ follow from the Cauchy–Riemann equations for $\tilde{W}$.

A consequence of the analyticity of the coefficients in the system of ordinary differential equations is that the solutions are analytic. It follows that if a solution with $m=1$ has LRS or isotropic geometry on some nonempty open time interval, then it must have LRS or isotropic geometry, respectively, for all values of τ. The same conclusion holds if there is a sequence of times having a limit point where the geometry is LRS or isotropic, respectively.

III. THE ASYMPTOTIC SYSTEM

In this section a certain system of ordinary differential equations is introduced and the qualitative behavior of its solutions analyzed. This system is used later to study the asymptotic behavior of solutions of the system (2.1)–(2.7). This system can be obtained formally from (2.1)–(2.7) by replacing the C^1 function $f(t,v_1,v_2,v_3)$ by a measure of the form $f(t,v_1)\delta(v_2-\bar{v}_2(t))\delta(v_3-\bar{v}_3(t))$, where δ is a Dirac measure, and taking $m=0$. Solutions of this system can be interpreted as certain distributional solutions of the Einstein–Vlasov system for massless particles. These are intermediate between smooth solutions and the even more singular solutions, which are in one to one correspondence with dust solutions. (For the correspondence between dust and distributional solutions of the Vlasov equation see Ref. 15.) The mathematical results that will now be derived are independent of this interpretation.

The system of ODEs to be considered is the special case of the equations (2.19) and (2.20) obtained by setting $\hat{T}_1^1=\hat{T}_2^2=0$ and $\hat{T}_3^3=\hat{\rho}$. Note that, in contrast to the general case of (2.19) and (2.20), these specialized equations suffice to determine all unknowns occurring in them from initial data. The explicit form of (2.20) in this case is

$$\partial_\tau \hat{k}_1^1=-8\pi\hat{\rho}\hat{k}_1^1, \tag{3.1}$$

$$\partial_\tau \hat{k}_2^2=-8\pi\hat{\rho}\hat{k}_2^2, \tag{3.2}$$

$$\partial_\tau \hat{k}_3^3=-8\pi\hat{\rho}(\hat{k}_3^3-1). \tag{3.3}$$

If initial data are chosen at some time that satisfy the condition $\Sigma_i(\hat{k}_i^i)=1$, then the solution also satisfies it. Only solutions with this property are considered here. It follows from (3.1) and (3.2) that $\partial_\tau(\hat{k}_2^2/\hat{k}_1^1)=0$ whenever $\hat{k}_1^1\neq 0$. Let r be the constant value of $\hat{k}_2^2/\hat{k}_1^1$. Then

$$\hat{k}_2^2=r\hat{k}_1^1, \tag{3.4}$$

$$\hat{k}_3^3=1-(1+r)\hat{k}_1^1. \tag{3.5}$$

Substituting (2.19), (3.4), and (3.5) into (3.1) gives

$$\partial_\tau \hat{k}_1^1=(\hat{k}_1^1)^2[(1+r+r^2)\hat{k}_1^1-(1+r)]. \tag{3.6}$$

Proposition 3.1: Let $(\hat{k}_1^1,\hat{k}_2^2,\hat{k}_3^3)$ be a solution of (3.1)–(3.3) satisfying $\Sigma_i(\hat{k}_i^i)=1$ and $\Sigma_i(\hat{k}_i^i)^2<1$. Define $r=\hat{k}_2^2/\hat{k}_1^1$ whenever $\hat{k}_1^1\neq 0$. Then

(i) if $\hat{k}_1^1$ is zero initially it is always zero;
(ii) if $\hat{k}_1^1$ is initially (and hence always) nonzero, then r is constant;
(iii) when $\hat{k}_1^1\neq 0$ it is a monotonic function with $\lim_{\tau\to-\infty}\hat{k}_1^1=(1+r)/(1+r+r^2)$ and $\lim_{\tau\to\infty}\hat{k}_1^1=0$; and
(iv) in that case $\lim_{\tau\to-\infty}(\hat{k}_3^3-\hat{k}_2^2)=-r(r+2)/(1+r+r^2)$.

Proof: Statement (i) follows from (3.1). Statement (ii) has been demonstrated above. Statement (iii) follows from (3.6). The last conclusion is then an immediate consequence of the definitions.

Of course analogous statements hold if $\hat{k}_1^1$ and $\hat{k}_2^2$ are interchanged, since these two quantities occur symmetrically in the hypotheses.

IV. PRESSURE ESTIMATES

The results of this section are all variations on the theme that if the space–time is expanding in a certain direction, then the pressure in that direction tends to decrease. It is assumed throughout

that the geometry is reflection-symmetric. A solution of (2.1)–(2.7) with $m=0$ satisfies $\text{tr}\, T/\rho=1$. This condition never holds when $m=1$, but the next lemma shows that it does hold asymptotically.

Lemma 4.1: Suppose that some solution of (2.1)–(2.7) with $m=1$ is defined on an interval $(-\infty,\tau_1)$, with f not identically zero. Then $\lim_{\tau\to-\infty} \text{tr}\, T/\rho=1$.

Proof: It was shown in Ref. 7 that $\lim_{\tau\to-\infty}\rho=\infty$. Thus, the result will follow if it can be shown that $\rho\to\infty$ implies $\text{tr}\, T/\rho\to 1$. To do this, choose some radius $L>0$ and write $\rho=\rho_1+\rho_2$ and $\text{tr}\, T=(\text{tr}\, T)_1+(\text{tr}\, T)_2$, where the first summand is the integral over the region $|w|<L$ of the integrand in (2.13) or (2.14), respectively, and the second is the integral over the complementary region. Using the fact that $(1+x^2)^{1/2}-x^2/(1+x^2)^{1/2}=(1+x^2)^{-1/2}$, it can be seen that $\rho_2-(\text{tr}\, T)_2\leqslant(1+L^2)^{-1}\rho_2$. Hence

$$(\text{tr}\, T)_2\geqslant\frac{L^2}{1+L^2}\,\rho_2 \tag{4.1}$$

and

$$\text{tr}\, T\geqslant\text{tr}\, T_2\geqslant\frac{L^2}{1+L^2}\left(\rho-\left(\frac{4\pi}{3}\right)L^3(1+L^2)^{1/2}\|f_0\|_\infty\right). \tag{4.2}$$

By choosing L sufficiently large, the quantity $L^2/(1+L^2)$ can be made as close to unity as desired. For fixed L, the quantity in brackets on the right-hand side of (4.2) approaches ρ as ρ becomes large. This suffices to give the conclusion of the lemma.

For a given initial datum f_0, the equation (2.14) defines the pressures T_i^i as functions of a, b, and c. The following results concern the qualitative behavior of these functions.

Lemma 4.2: If f_0 is not identically zero and $a\leqslant C'\min\{1,b,c\}$ for some constant $C'>0$, there exists a constant $C>0$ such that $T_1^1\geqslant Ca^{-2}b^{-1}c^{-1}$ and $T_2^2/T_1^1\leqslant C(a/b)^{4/3}$. In the case $m=0$ the conclusion holds under the weaker hypothesis that $a\leqslant C'\min\{b,c\}$.

Proof: Let p be a point of $\mathbf{R}^3$ where $f_0\neq 0$, whose first coordinate w_1 is nonzero. Let δ be a positive number such that f is bounded below by some positive constant η on the closed cube W of side 2δ centered at p and such that w_1 does not vanish anywhere on this cube. Consider now the image W' of the cube W under the mapping $(w_1,w_2,w_3)\mapsto(a^{-1}w_1,b^{-1}w_2,c^{-1}w_3)$. On W the functions w_2/w_1 and w_3/w_1 are bounded. Under the assumptions of the lemma they are bounded by the same constant on W'. It follows that $|w_1|/(1+|w|^2)^{1/2}$ is bounded below on any such cube by a positive constant that is independent of a, b, and c, which satisfy the hypotheses of the lemma. The integral defining T_1^1 can be bounded from below by the integral of the same quantity over W. It follows that

$$T_1^1\geqslant C\eta a^{-2}b^{-1}c^{-1}, \tag{4.3}$$

and this proves the first part of the lemma. To get a lower bound for T_1^1/T_2^2, the domain of integration in the definition of these two quantities will be divided into the regions $|w_2|>R|w_1|$ and $|w_2|<R|w_1|$, where R is a positive number that will be specified later. Corresponding to this decomposition of the domain of integration, there are decompositions $T_1^1=T_{11}^1+T_{12}^1$ and $T_2^2=T_{21}^2+T_{22}^2$. The volume of the region where $|w_2|>R|w_1|$ and $f(aw_1,bw_2,cw_3)\neq 0$ can be bounded by an expression of the form $CR^{-1}c^{-1}b^{-2}$, and so $T_{21}^2\leqslant CR^{-1}c^{-1}b^{-3}$. On the other hand, $T_{22}^2\leqslant R^2T_{12}^1$. Thus,

$$T_2^2\leqslant CR^{-1}c^{-1}b^{-3}+R^2T_1^1\leqslant(CR^{-1}(a/b)^2+R^2)T_1^1, \tag{4.4}$$

where in the last step (4.3) has been used. Choosing $R=(a/b)^{2/3}$ gives $T_2^2\leqslant C(a/b)^{4/3}T_1^1$, and this proves the result for T_2^2/T_1^1.

Lemma 4.3: Suppose that some solution of (2.1)–(2.7) is defined on the interval $(-\infty,\tau_1)$, with f not identically zero. If $\hat{k}_1^1-\hat{k}_2^2\geqslant A$ and $\hat{k}_1^1-\hat{k}_3^3\geqslant A$ on this interval for some $A>0$, then $T_i^i/T_1^1\leqslant Ce^{4A\tau/3}$ for $i=2,3$.

Proof: It suffices to note that under the assumptions of this lemma there will be a time interval $(-\infty,\tau_2)$ where the hypotheses of Lemma 4.2 hold, so that (4.4) can be applied.

The time derivatives of the quantities $\hat{T}_i^i$ cannot, in general, be expressed in terms of the dimensionless quantities (2.9)–(2.11), so as to get a closed system of ordinary differential equations. However, they can be estimated in terms of these quantities. Note first that

$$\frac{d\hat{T}_i^i}{d\tau}=-(\text{tr } k)^{-3}\frac{dT_i^i}{dt}+2\hat{T}_i^i[1-12\pi\hat{\rho}+4\pi \text{ tr } \hat{T}]. \tag{4.5}$$

Next, a change of variables in (2.7) gives, in the diagonal case,

$$T_i^i=g^{ii}\int f_0(v_1,v_2,v_3)(v_i)^2(m^2+g^{rs}v_rv_s)^{-1/2}(\det g)^{-1/2}\,dv_1\,dv_2\,dv_3. \tag{4.6}$$

Hence,

$$\begin{aligned}\frac{dT_1^1}{dt}=&(3k_1^1+k_2^2+k_3^3)T_1^1+g^{11}\int f_0(v_1,v_2,v_3)(v_1)^2F(v_1,v_2,v_3)\\&\times(m^2+g^{rs}v_rv_s)^{-3/2}(\det g)^{-1/2}\,dv_1\,dv_2\,dv_3,\end{aligned} \tag{4.7}$$

where

$$F(v_1,v_2,v_3)=(-g^{11}k_1^1(v_1)^2-g^{22}k_2^2(v_2)^2-g^{33}k_3^3(v_3)^2). \tag{4.8}$$

Note now that

$$|F(v_1,v_2,v_3)|\leqslant(|k_1^1|+|k_2^2|+|k_3^3|)(m^2+g^{rs}v_rv_s), \tag{4.9}$$

and so the integral in (4.7) can be bounded in modulus by $3\,\text{tr}\,kT_1^1$. Putting this information into (4.5) gives the desired bound.

Lemma 4.4: Consider a maximally extended solution of (2.1)–(2.7) with $m=1$ and f not identically zero. If $g_{ii}\to\infty$ as $\tau\to\infty$, then $\lim_{\tau\to\infty}T_i^i/\rho=0$. If, on the other hand, g_{11} is bounded above and all g_{ii} are bounded below by a positive constant on an interval of the form $[\tau_1,\infty)$, then T_1^1/ρ is bounded below by a positive constant on that interval.

Proof: It follows from (2.13) and (2.14) that $T_1^1\leqslant Ca^{-2}\rho$, and this proves the first statement. To get the other conclusion, choose a cube C_1 as in the proof of Lemma 4.2. Then $T_1^1\geqslant Ca^{-1}b^{-1}c^{-1}$ while $\rho\leqslant Ca^{-1}b^{-1}c^{-1}$. Hence, $T_1^1/\rho\geqslant C>0$.

V. THE MAIN RESULTS

Lemma 5.1 (compactness lemma): Let a sequence of reflection-symmetric global solutions of Eqs. (2.1)–(2.7) be given. Then there exists a subsequence such that $\hat{k}_j^i$ and $\hat{\rho}$ converge uniformly on compact sets of $\mathbf{R}$. Here $\hat{T}_i^i$ also converges uniformly on compact subsets (after possibly passing to a subsequence once more), and the limiting quantities satisfy (2.19) and (2.20).

Proof: The quantities $\hat{k}_j^i$ are contained in the compact set K and so are, in particular, uniformly bounded. By (2.19), $\hat{\rho}$ is uniformly bounded. It follows that $\hat{T}_j^i$ is uniformly bounded. Equation (2.20) now shows that $\partial_\tau\hat{k}_j^i$ is uniformly bounded. By Ascoli's theorem there exists a subsequence such that $\hat{k}_j^i$ converges uniformly on the interval $[-1,1]$. Applying the theorem again shows that this subsequence has a subsequence such that $\hat{k}_j^i$ converges uniformly on $[-2,2]$. Continuing in

this way, we obtain a collection of subsequences indexed by a positive integer n with the properties that for the nth subsequence $\hat{k}_j^i$ converges uniformly on $[-n,n]$, and each sequence is a subsequence of the previous one. The diagonal sequence has the property that $\hat{k}_j^i$ converges on each compact subset of the real line. By the Hamiltonian constraint $\hat{\rho}$ also converges uniformly on compact sets along this subsequence. In the diagonal case the derivatives $\partial_\tau \hat{T}_i^i$ are bounded, as was shown in Sec. IV and applying Ascoli's theorem as before gives the remaining conclusions.

Theorem 5.1: Let a global solution of Eqs. (2.1)–(2.7) be given for which f is not identically zero. If at some time τ_1, the projection of the solution lies in the set B_i for some i, then (i) the projection lies in B_i for all $\tau \leqslant \tau_1$; (ii) if there exists some $\tau_2 > \tau_1$ such that the projection of the solution lies in the complement of B_i, then it lies in the complement of all B_j for $\tau > \tau_2$; and (iii) as $\tau \to -\infty$ the projection converges to a point of the boundary of the region K that is not one of the points V_i^-.

Proof: Suppose without loss of generality that $i=1$. It follows from (2.20) that

$$\partial_\tau \hat{k}_1^1 = -4\pi(\hat{\rho} - \text{tr}\ \hat{T})(3\hat{k}_1^1 - 1) - 8\pi\ \text{tr}\ \hat{T}\hat{k}_1^1 + 8\pi\hat{T}_1^1. \tag{5.1}$$

If at some time $\hat{k}_1^1 \leqslant 0$, then the first and second terms on the right-hand side of (5.1) are nonnegative while the third term is positive. Hence $\partial_\tau \hat{k}_1^1 > 0$. This implies the first conclusion of the theorem. Moreover, it means that if the projection once leaves B_1 it can never reenter it. A similar statement, of course, applies to any other B_j, and this gives (ii). To prove (iii) note first that $\partial_\tau \hat{k}_1^1$ is bounded below by a positive constant as long as $\hat{\rho}$ is. This shows that $\liminf_{\tau \to -\infty} \hat{\rho} = 0$. Equation (5.1) also implies that the integral of $\hat{\rho}$ on the interval $(-\infty, \tau_1]$ must be finite so that for each i the integral of the right-hand side of (2.20) is absolutely convergent. Hence, each $\hat{k}_i^i$ tends to a limit as $\tau \to -\infty$. By what has already been said it can only be a point of the boundary of K. The monotonicity of $\hat{k}_1^1$ shows that this limit cannot be one of the points V_i^-.

Theorem 5.2: Let a global solution of Eqs. (2.1)–(2.7) be given for which f is not identically zero. If at some time τ_1 the projection of the solution lies in the set A_i for some i, then as τ decreases either (i) the projection converges to a point of the boundary of K as $\tau \to -\infty$; or (ii) it reaches L_j^+ for some j or C at a finite time before τ_1; or (iii) it stays in A_i for all $\tau < \tau_1$ and it has a point of one of the lines L_j^+ or the point C as an accumulation point.

Proof: Suppose without loss of generality that $i=1$. When the projection lies in A_1 the inequalities $k_1^1 > k_2^2$, $k_1^1 > k_3^3$, and $\hat{k}_1^1 > \frac{1}{3}$ hold. Suppose that on the time interval $(-\infty, \tau_1)$ the inequalities $\hat{k}_1^1 - \hat{k}_2^2 \geqslant A$ and $\hat{k}_1^1 - \hat{k}_3^3 \geqslant A$ are satisfied for some $A > 0$. Then, by Lemma 4.3, it follows that on this time interval T_1^1/T_2^2 and T_1^1/T_3^3 can be bounded below by a decreasing function, which tends to ∞ as $\tau \to -\infty$. Moreover, by Lemma 4.1, $\text{tr}\ T/\rho \to 1$ as $\tau \to -\infty$. Now, define a sequence of solutions of (2.1)–(2.7) by $u_n(\tau) = u(\tau - n)$, $\tau \in (-\infty, \tau_1)$, where u denotes any of the functions that make up the solution and n is a positive integer. By Lemma 5.1 there exists a subsequence such that $\hat{k}_j^i$ and $\hat{\rho}$ converge uniformly on compact subsets. By the statements made above, $\text{tr}\ \hat{T}$ must tend to the same limit as $\hat{\rho}$ along this sequence. Also, $\hat{T}_1^1$ tends to this same limit and $\hat{T}_2^2$ and $\hat{T}_3^3$ tend to zero. Applying Lemma 5.1 again shows that the limits of these sequences satisfy (2.19) and (2.20). Because of the values of the limits they, in fact, satisfy the asymptotic system (3.1)–(3.3). The solution of the asymptotic system obtained inherits the properties that $\hat{k}_1^1 \geqslant \hat{k}_2^2$ and $\hat{k}_1^1 \geqslant \hat{k}_3^3$. The only solutions of the asymptotic system that satisfy these inequalities on an interval of the form $(-\infty, \tau_1)$ are the vacuum solutions. If for some choice of subsequence this vacuum solution is not that corresponding to the point V_1^-, then the projection of the original solution must converge to that point, by Theorem 5.1. Otherwise every subsequence of the sequence of translated solutions has a subsequence that converges to the same solution of the asymptotic system. Hence, the whole sequence converges to this solution and the projection of the original solution converges to V_1^-. In both cases the solution of the original system converges to a point of the boundary of K.

It remains to consider the case where the above estimate is not satisfied for any $A>0$. If the solution does not reach L_j^+ for some j or C in finite time, then it stays in A_i for all $\tau<\tau_1$. Then it must have as an accumulation point either a point on L_j^+ for some j, C, or V_j^+ for some j. In the first two cases this gives case (iii) of the conclusion of the theorem. In the third case the solution enters B_j, and so by Theorem 5.1, case (i) of the conclusion holds.

In case (iii) of this theorem we can also consider a limit of translates of the solutions whose existence is guaranteed by Lemma 5.1. If the ratios a/b and a/c tended to zero as $\tau\to-\infty$ for the original solution, then by Lemma 4.2 the ratios T_1^1/T_2^2 and T_1^1/T_3^3 would tend to infinity and the solution would belong to case (i). Thus, in case (iii) it can be assumed without loss of generality (after possibly interchanging the indices 2 and 3) that b/a is bounded as $\tau\to-\infty$. Hence $\int_{-\infty}^{\tau_1}(\hat{k}_1^1-\hat{k}_2^2)$ is finite. Since $\partial_\tau(\hat{k}_1^1-\hat{k}_2^2)$ is bounded, it follows that $\hat{k}_1^1-\hat{k}_2^2\to0$ as $\tau\to-\infty$. Hence, the solution obtained as a limit of translates has LRS geometry. It also satisfies $\rho=\mathrm{tr}\,T$. Information about the asymptotics of LRS solutions can thus be used to obtain information about the asymptotics of the solutions, which fit into case (iii) of Theorem 5.2 but do not fit into case (i).

Theorem 5.3: Let a solution of Eqs. (2.19)–(2.20) be given that satisfies the LRS condition $k_2^2=k_3^3$. If at some time τ_1 the projection satisfies $\hat{k}_1^1<\frac{1}{3}$, then either (i) the projection of the solution tends to the point $(-\frac{1}{3},\frac{2}{3},\frac{2}{3})$ as $\tau\to-\infty$; (ii) it tends to the point $(0,\frac{1}{2},\frac{1}{2})$ as $\tau\to-\infty$; (iii) it reaches the point $(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ at a finite time before τ_1; or (iv) it tends to the point $(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ as $\tau\to-\infty$.

Proof: Suppose first that $\hat{k}_1^1\leqslant\frac{1}{3}-A$ for some $A>0$. Then by Lemma 4.2 the ratio of $T_2^2=T_3^3$ to T_1^1 increases without limit. Passing to a limit of translates in the familiar way gives a solution of the equation $\partial_\tau\hat{k}_1^1=-8\pi\hat{k}_1^1\hat{\rho}$ for which $\hat{k}_1^1$ satisfies the same inequality as before. There are only two such solutions, namely that for which $\hat{\rho}=0$ and that for which $\hat{k}_1^1=0$. In the first of these cases the original solution must enter the region B_1, and hence by Theorem 5.1 belong to case (i) of the conclusion of the present theorem. The only way of avoiding this is if, no matter which subsequence is chosen, the limiting value of $\hat{k}_1^1$ is zero. Hence, the projection of the original solution must converge to the point $(0,\frac{1}{2},\frac{1}{2})$. Thus, the solution belongs to case (ii) of the conclusion. Now consider the case where there is no $A>0$ with the given property. If, despite this, the ratio of T_2^2 to T_1^1 tends to infinity, we can argue as before to show that the solution belongs to case (i) or (ii). If, on the other hand, this ratio remains bounded, then the ratio a/b must remain bounded, and hence if $\hat{k}_1^1$ remains smaller than $\frac{1}{3}$ forever then $\int_{-\infty}^{\tau_1}(\frac{1}{3}-\hat{k}_1^1)$ is finite. It then follows as in the discussion following the proof of Theorem 5.2 that $\hat{k}_1^1\to\frac{1}{3}$. Thus the solution either belongs to case (iii) or case (iv).

Theorem 5.4: Let a solution of the equations (2.1)–(2.7) with $m=1$ and f not identically zero be given. Then $\hat{k}_i^i\to\frac{1}{3}$ and $T_i^i/\rho\to0$ for each i as $\tau\to\infty$.

Proof: In Ref. 13, it was shown that the scale factors a, b, and c are bounded below by a positive constant on any interval of the form $[\tau_1,\infty)$. Using (5.1), this statement can be strengthened. Suppose that $\hat{k}_1^1$ were negative on an interval of the form $[\tau_1,\infty)$. Then it would follow, as in the proof of Theorem 5.1, that the integral of $\hat{\rho}$ on this interval was finite. But $\hat{\rho}$ is increasing on this interval, a contradiction. It follows that each $\hat{k}_i^i$ must become zero after a finite time, and once this happens it must immediately become positive and stay positive. Thus, for τ_1 sufficiently large, a, b, and c are increasing. Consider now the behavior of the quantity $\min\{a,b,c\}$. Suppose first that it tends to infinity as $\tau\to\infty$. Then, by Lemma 4.4 the ratios T_i^i/ρ tend to zero as $\tau\to\infty$. Construct a limit of translates as in the proof of Theorem 5.2, except that this time the translations should be done in the opposite direction. Then the limiting solution satisfies $\partial_\tau\hat{k}_i^i=-12\pi\hat{\rho}(\hat{k}_i^i-\frac{1}{3})$. This is the equation that is satisfied by a Bianchi I solution of the Einstein equations coupled to dust. It is well known and also easy to see directly that in the case of dust each $\hat{k}_i^i$ converges to $\frac{1}{3}$ as $\tau\to\infty$. Because a convergent subsequence can be extracted from any subsequence of the sequence of translates by integers, it follows that $\hat{k}_i^i\to\frac{1}{3}$ for the original solution of the Einstein–Vlasov system as well. Next, consider the case where a is bounded on an interval of the form $[\tau_1,\infty)$ while $\min\{b,c\}\to\infty$ as $\tau\to\infty$. Then, by Lemma 4.4 the ratios T_2^2/ρ and T_3^3/ρ converge to zero as $\tau\to\infty$ while T_1^1/ρ remains bounded away from zero. Equation (5.1) implies that $\partial_\tau\hat{k}_1^1$ is

bounded below by a positive constant if $\hat{k}_1^1 < \frac{1}{3}$ and T_2^2/T_1^1 and T_3^3/T_1^1 are less than $1-A$ for some constant $A>0$. However, this contradicts the boundedness of a. Since the volume tends to infinity as $\tau\to\infty$, at least one of a, b, or c must tend to infinity. It follows that to complete the proof we may assume without loss of generality that a and b are bounded while c tends to infinity. By Lemma 4.4, $T_3^3/\rho\to 0$, while T_1^1/ρ and T_2^2/ρ are bounded below by a positive constant. Now the integral $\int_{\tau_1}^{\infty}\hat{k}_i^i(\tau)d\tau$ is finite for $i=1,2$ and $\partial_\tau\hat{k}_i^i$ is bounded. Hence, $\hat{k}_1^1$ and $\hat{k}_2^2$ tend to zero as $\tau\to\infty$ and $\hat{k}_3^3\to 1$. But the given behavior of the pressures shows that for $\hat{k}_3^3\geqslant\frac{1}{3}$ and sufficiently large times $\partial_\tau k_3^3$ is negative, a contradiction. This completes the proof.

VI. A COMPACTIFICATION

This section is devoted to a finer examination of LRS solutions of the Einstein–Vlasov system with massless particles. For LRS solutions with $k_2^2=k_3^3$, let $k=\hat{k}_1^1$, $q=b/a$, $Q=T_1^1/\rho$. Then $\hat{k}_2^2=\frac{1}{2}(1-k)$ and $\hat{\rho}=(1/16\pi)(\frac{1}{2}+k-\frac{3}{2}k^2)$. The essential equations describing the dynamics are

$$\partial_\tau k=\tfrac{1}{4}(1+3k)(1-k)(Q-k), \tag{6.1}$$

$$\partial_\tau q=\tfrac{1}{2}(1-3k)q. \tag{6.2}$$

The quantity Q can be expressed entirely in terms of q and the initial data as follows:

$$Q=q^2\left[\frac{\int f_0(v_i)v_1^2(q^2v_1^2+v_2^2+v_3^2)^{-1/2}\,dv_1\,dv_2\,dv_3}{\int f_0(v_i)(q^2v_1^2+v_2^2+v_3^2)^{1/2}\,dv_1\,dv_2\,dv_3}\right]. \tag{6.3}$$

Substituting (6.3) into (6.1) makes the equations (6.1) and (6.2) into an autonomous system of ordinary differential equations for k and q. Lemma 4.2 shows that $Q(q)=O(q^{4/3})$ as $q\to 0$. This means that the system (6.1)–(6.2) can be extended in a C^1 manner to the boundary $q=0$. Moreover, Q does not contribute to the linearization of the extended system at the critical point $q=0$, $k=0$. The eigenvectors of the linearization are directed along the k and q axes, with eigenvalues $-\frac{1}{4}$ and $\frac{1}{2}$, respectively. It follows (see, e.g., Ref. 16) that the dynamical system has an unstable manifold that is a curve tangent to the k axis at the point (0,0). This shows that for any initial value f_0 it is possible to find LRS solutions of the Einstein–Vlasov system, where the distribution function has the initial value f_0 and where the quantities $\hat{k}_i^i$ converge to $(0,\frac{1}{2},\frac{1}{2})$ as $\tau\to-\infty$. Note that the stable manifold is just the k axis, and so does not give rise to any smooth solutions of the Einstein–Vlasov system. The information about the linearization also determines the nature of the phase portrait near the singular point, and shows that there are solutions for which $\hat{k}_1^1$ approaches zero, but turns back before reaching it. A typical feature of Bianchi models is that the matter becomes dynamically negligible near the singularity. No attempt will be made here to make this notion precise, but one aspect of it is that the projection of the solution should tend to a point of the boundary of K as $\tau\to-\infty$. The solution whose existence has just been shown is an exception to the rule. For anisotropic Bianchi I models with a perfect fluid, no exceptional solutions of this kind exist. However, they do occur for other Bianchi types.[17]

The critical points of the system (6.1)–(6.2) in the region where $0<q$ and $-\frac{1}{3}<k<1$ are the points of the form $(\frac{1}{3},q_0)$, where q_0 has the property that $Q(q_0)=\frac{1}{3}$. Differentiating (6.3) and estimating the result in an elementary way leads to the inequality $qQ'\geqslant Q(1-Q)$. This shows that the function Q is strictly increasing for $q>0$. Taking account of the limiting values of Q, it follows that there is precisely one value q_0 for which $Q(q_0)=\frac{1}{3}$. Moreover, at this point $qQ'\geqslant\frac{2}{9}$. The eigenvalues of the linearization at the corresponding critical point are $-\frac{1}{6}\pm\frac{1}{2}\sqrt{\frac{1}{9}-q_0Q'(q_0)}$. They both have negative real parts and the critical point is a sink. In particular, no solution emerges from this critical point. Thus, it is seen that if the projection of any LRS solution for massless particles approaches the point C as $\tau\to-\infty$, then the projection must stay at C for all time, i.e., the

solution must have isotropic geometry. This should be compared with the results of Newman[18] on isotropic singularities in solutions of the Einstein equations coupled to a radiation fluid.

APPENDIX: FLUIDS WITH NONLINEAR EQUATION OF STATE

Consider a perfect fluid with equation of state $p=f(\rho)$ that satisfies the following general assumptions: (i) f is a continuous function from $[0,\infty)$ to itself with $f(0)=0$, which is C^1 for $\rho>0$; (ii) $0\leqslant f'(\rho)\leqslant 1$ for all $\rho>0$; and (iii) there exists a constant $C<1$ such that $p\leqslant C\rho$ for $\rho<1$.

Assumptions (i) and (ii) are standard. The third assumption is, when (i) and (ii) are satisfied, equivalent to the assumption made in Ref. 7 that the equation of state is not asymptotically stiff at low densities. In the case of a linear equation of state $f(\rho)=k\rho$, the assumptions (i)–(iii) are satisfied if and only if $0\leqslant k<1$. In a Bianchi I space–time, it follows from the momentum constraint (2.2) that the four-velocity of the fluid is orthogonal to the hypersurfaces of homogeneity. Hence, the energy density ρ measured by an observer whose word line is orthogonal to the hypersurfaces of homogeneity, is the same as that measured by a comoving observer. Equations (2.19) and (2.20) are valid, as in the case of the Einstein–Vlasov system. For a fluid, it can be assumed without loss of generality that the solution is reflection symmetric, because given any initial data, it suffices to do a linear transformation of the coordinates that simultaneously diagonalizes the metric and second fundamental form in order to transform the given data to data for a reflection-symmetric space–time.

In the case of a fluid $T^i_j=p\,\delta^i_j$ and hence $\hat{T}^i_j=\hat{p}\,\delta^i_j$, where $\hat{p}=p/(\mathrm{tr}\,k)^2$. If the equation of state is linear, then $\hat{p}$ can be expressed as a function of $\hat{\rho}$ alone, and (2.19) and (2.20) then reduce to a system of ordinary differential equations that suffice to determine $\hat{k}^i_j$ from initial data. For a nonlinear equation of state, this is no longer the case. The equations (2.19) and (2.20) no longer form a closed system and must instead be considered as the projection of a bigger system, as in the case of the Vlasov equation. This is one reason why the linear case has been studied preferentially in the literature. Nevertheless, it turns out that the projection can be analyzed very effectively in the general case.

The first question that needs to be addressed is that of global existence in τ, i.e., the equivalent of Lemma 2.1 for a fluid. This follows from the results of Ref. 7. The assumption (iii) has been used at this stage. A direct calculation shows that the quantity $(\hat{k}^1_1-\hat{k}^2_2)/(\hat{k}^1_1-\hat{k}^3_3)$ is independent of τ whenever $\hat{k}^1_1-\hat{k}^3_3$ is nonzero. Moreover, if $\hat{k}^1_1-\hat{k}^3_3$ is zero at some time, it remains zero. Hence, the projection of each solution is constrained to move on a straight line in K passing through the center C. This is already a much stronger statement than could be proved in the case of the Vlasov equation. To find out how the projection moves on this straight line, the time derivative of the dimensionless version of the density will be calculated. For a fluid it is given by

$$\partial_\tau\hat{\rho}=(\hat{\rho}-\hat{p})(1-24\pi\hat{\rho}). \tag{A1}$$

Noting that the Hamiltonian constraint implies that $24\pi\hat{\rho}\leqslant 1$ with equality only at the point C, it can now be seen that the projection moves monotonically from the boundary of K at $\tau=-\infty$ to the center C of K at $\tau=\infty$. This qualitative behavior is independent of the equation of state, satisfying (i)–(iii). The only difference is in the speed with which the projection moves along the radial line at different times. Equation (A1) also makes clear that this picture changes completely if the equations of state considered here are replaced by the limiting case of a stiff fluid, $p=\rho$.

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Majorana parafermions

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A Majorana analog to the parafermion algebra is constructed and shown to be isomorphic to so(n). Ansatz realizations of this algebra are constructed and used to establish the properties of particular representations. The construction of specific so(n) representations is discussed for odd and even n, and for even n the procedure is illustrated explicitly in the case of so(4). By contracting the Majorana parafermion algebra, the para-Grassman algebra and its representation theory are obtained.
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I. INTRODUCTION

Systems of parabosons and parafermions were introduced in Ref. 1, and have been considered extensively[2,3] as generalizations of ordinary bosons and fermions. Recently, representations of these systems in terms of deformed bosonic operators,[4–8] examination of their connections with the Calogero–Vasiliev oscillator,[9,10] and attempts to quantum deform them[11–14] have all led to a renewal of interest.

In this paper we construct a Majorana analog to the parafermion, interpret it as a Lie algebra, and investigate the properties of its representations.

After a brief review in Sec. II of parafermions and their ansatz representations, we move directly in Sec. III to the construction of real Majorana parafermions (MPFs) out of the standard complex parafermions and the establishment of the algebra which these new operators satisfy. In Sec. IV we establish that the algebra of n MPFs is isomorphic to so($n+1$), which is a generalization of the well-known result that n parafermions generate so($2n+1$). In Sec. V we introduce a minor modification to the standard fermionic realization of the Green ansatz, and use this in a straightforward way to obtain ansatz realizations of the MPFs. Using these we develop a procedure for establishing complete sets of the algebraic relations for MPFs representations of any order of statistics. We illustrate this procedure for $p=2$. In Sec. VI we look at the construction of so($2n+1$) and so($2n$) representations using MPFs. For so($2n+1$) this only involves a restatement of the unique vacuum conditions for a parafermion system in terms of MPFs, and we find that MPFs, when acting on a Fock space, are grouped into related pairs, so that the overall symmetry between MPFs is lost. For so($2n$) we are in a new situation. We show how to project a MPF realization of so($2n+1$) onto so($2n$), and how, after implementing this projection, to reduce the number of MPFs involved to its natural minimum. The purpose of this procedure is to obtain so($2n$) in a form in which its constituent MPFs are clearly related to its raising and lowering operators. This is illustrated explicitly for so(4), for which we also construct all representations in MPF terms.

Finally, in Sec. VII we show that by means of a simple contraction, the para-Grassman algebra[15] can be obtained from the MPF algebra. Consequently the properties of the para-Grassman representations for any order of statistics follow from the contraction of the corresponding MPF representations.

II. DIRAC PARAFERMIONS

A system of n oscillators a_i and their conjugates $a_i^\dagger$ which satisfy the trilinear commutation relations

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$$[[a_i^\dagger,\ a_j],\ a_k^\dagger]=2\,\delta_{ik}a_j, \tag{1}$$

$$[[a_i,\ a_j],\ a_k]=0, \tag{2}$$

together with their conjugates, for $i,j,k=1,2,\ldots,n$ is referred to in previous work as a system of n parafermions. In this paper we shall refer to these oscillators as Dirac parafermions (DPFs). It is well known that all of the irreducible representations of the DPFs on a Fock space with a unique vacuum state $|0\rangle$ satisfying $a_i|0\rangle=0$ are labeled by a single positive integer p, the order of statistics, such that $a_i a_i^\dagger|0\rangle = p|0\rangle$ for all i, and that all of these representations are included among the Green ansatz representations.[2] Recently the following realization of this ansatz in terms of Dirac and Majorana fermions has been studied by[16]

$$a_i=\sum_{\alpha=1}^{p} f_{i\alpha}s_\alpha, \quad a_i^\dagger=\sum_{\alpha=1}^{p} f_{i\alpha}^\dagger s_\alpha. \tag{3}$$

Here $f_{i\alpha}$ and s_α are, respectively, Dirac and Majorana fermions. These have commutation relations

$$\{f_{i\alpha},f_{j\beta}\}=0, \quad \{f_{i\alpha},f_{j\beta}^\dagger\}=\delta_{ij}\delta_{\alpha\beta}, \quad \{s_\alpha,s_\beta\}=2\,\delta_{\alpha\beta}, \quad \{f_{i\alpha},s_\beta\}=0, \tag{4}$$

as well as $s_\alpha^\dagger = s_\alpha$.

III. CONSTRUCTION OF MAJORANA PARAFERMIONS

In this section we construct a parafermionic analog to the Majorana fermion, and establish the algebraic properties of such operators. Essentially the same operators were defined in Ref. 17, although there they were introduced only as a part of the analysis of the DPF algebra, and not considered in their own right. We define Majorana parafermions (MPFs) in terms of DPFs by analogy with the well-known definition of Majorana fermions in terms of Dirac fermions, so that, for example

$$c_1=a_1+a_1^\dagger, \quad c_2=i(a_1-a_1^\dagger). \tag{5}$$

Here c_1 and c_2 are MPFs. It is clear from these definitions that $c_1^\dagger = c_1$ and $c_2^\dagger = c_2$. To establish the MPF algebra we must also define

$$\begin{aligned} c_3&=a_2+a_2^\dagger, \quad c_4=i(a_2-a_2^\dagger),\\ c_5&=a_3+a_3^\dagger, \quad c_6=i(a_3-a_3^\dagger). \end{aligned} \tag{6}$$

Now consider

$$[[a_1^\dagger,\ a_1],\ a_1^\dagger]=2a_1^\dagger \quad \text{and} \quad [[a_1^\dagger,\ a_1],\ a_1]=-2a_1. \tag{7}$$

Writing this in MPF form we obtain

$$[[c_1+ic_2,c_1-ic_2],\ c_1\pm ic_2]=\pm 8c_1+8ic_2, \tag{8}$$

which reduces to

$$[[c_1,\ c_2],\ c_2]=4c_1, \quad [[c_1,\ c_2],\ c_1]=-4c_2. \tag{9}$$

The form of each of these equations is the same. By using Eqs. (1), (2), and (6) it is straightforward to check that the form of the two particle trilinear is the same for any pair of MPFs. Further, by replacing MPFs with their DPF equivalents, and using Eqs. (1) and (2) it is easy to show that all three particle MPF trilinear are trivial.

For example, to show that $[[c_1, c_2], c_3]=0$, add $[[a_1^\dagger, a_1], a_2] = 0$ and $[[a_1^\dagger, a_1], a_2^\dagger] = 0$. Collecting our results into a single expression, we have

$$[[c_i, c_j], c_k]=4\delta_{jk}c_i-4\delta_{ik}c_j. \tag{10}$$

Taking this to be the definition of the MPF algebra, the requirement that it be invariant under Hermitian conjugation gives us the freedom $c_i^\dagger = \eta_i c_i$, where $\eta_i=\pm 1$. Augmenting our definition by $\eta_i=+1$ for all i we restrict ourselves to the compact real form of the algebra. The odd looking factors of 4 on the right-hand side of Eq. (10) arise because we have constructed MPFs out of DPFs in exact analogy to the construction of Majorana fermions out of Dirac fermions, and these could easily be scaled away. However, for our purposes the scale factor in Eq. (10) is convenient, since it avoids the introduction of noninteger factors into the algebras (20), (21), and (22) associated with MPFs of specific orders of parastatistics. This construction is completely reversible, so the algebra of $2n$ MPFs is isomorphic to the algebra of n DPFs. It is well known[17] that this algebra is so$(2n+1)$. Although the MPFs were derived in such a way that we obtained two from each DPF, there is no memory of this in the MPF algebra which gives all c_is the same properties. Because of this there is no obstacle to consideration of systems containing an odd number of MPFs. Unlike systems containing an even number of MPFs, these are essentially different from the well-known DPF systems, and lead to new results.

IV. THE LIE ALGEBRAIC INTERPRETATION OF MPFs

As stated above, it is known that n DPFs generate so$(2n+1)$, and consequently that the same must be true of $2n$ MPFs. We now establish the more general result, which includes systems containing an odd number of MPFs.

Using n MPFs, labeled $c_1, c_2, \ldots c_n$ we can define operators $L_{\alpha\beta}$ with $\alpha, \beta=1,2,\ldots,n$ as follows:

$$L_{\alpha\beta}=\frac{[c_\alpha, c_\beta]}{4}. \tag{11}$$

Clearly $L_{\alpha\beta}=-L_{\beta\alpha}$. It follows directly from the MPF algebra (10) that these satisfy

$$[L_{\alpha\beta}, L_{\gamma\nu}]=\delta_{\beta\gamma}L_{\alpha\nu}+\delta_{\alpha\nu}L_{\beta\gamma}-\delta_{\beta\nu}L_{\alpha\gamma}-\delta_{\alpha\gamma}L_{\beta\nu} \tag{12}$$

and

$$[c_\alpha, L_{\gamma\nu}]=\delta_{\gamma\alpha}c_\nu-\delta_{\nu\alpha}c_\gamma. \tag{13}$$

We now define

$$L_{0\alpha}=\frac{ic_\alpha}{2}. \tag{14}$$

Then Eqs. (11) and (13) can be written as

$$[L_{0\alpha}, L_{0\beta}]=-L_{\alpha\beta}, \quad [L_{0\alpha}, L_{\gamma\nu}]=\delta_{\nu\alpha}L_{0\gamma}+\delta_{\gamma\alpha}L_{0\nu}, \tag{15}$$

both of which have the same form as Eq. (12). These relationships extend the range of the indices on the $L_{\alpha,\beta}$ in Eq. (12) to $\alpha, \beta=0,1,2,\ldots,n$, but this is just the algebra so$(n+1)$, and by our

construction we see that it is isomorphic to an algebra of n MPFs. Thus we have established the general result, that $n-1$ MPFs generate so(n). For even n this corresponds to the familiar result that n DPFs generate so($2n+1$), but for odd n our result is new, and provides those so(n) algebras which DPFs alone cannot generate in a canonical way.

Note that to establish the order of statistics of a given representation, we can construct the MPF equivalent of the su(2) Casimir operator out if any pair. This gives

$$c_i^2+c_j^2-\frac{[c_i,\,c_j]^2}{4}=p(p+2). \tag{16}$$

V. ANSATZ REPRESENTATIONS OF MPFs

We now construct a MPF analog of the Green ansatz. To do this in the most convenient way we first of all note that the realization of the Green ansatz given by Eqs. (3) and (4) remains valid if we modify Eq. (4) so that the Dirac fermions commute with the Majorana fermions, that is, Eq. (4) becomes

$$\{f_{i\alpha},f_{j\beta}\}=0,\quad \{f_{i\alpha},f_{j\beta}^{\dagger}\}=\delta_{ij}\delta_{\alpha\beta},\quad \{s_\alpha,s_\beta\}=\delta_{\alpha\beta},\quad [f_{i\alpha},\,s_\beta]=0, \tag{17}$$

where $s_\alpha^{\dagger}=s_\alpha$ for all α. This may appear somewhat unnatural, though it is less so if we view the Dirac and Majorana elements as fermions of different colors. The point of making this change is that doing so greatly simplifies manipulation of the MPF ansatz realizations, which, using Eq. (5), we can write down directly as

$$c_i=\sum_{\alpha=1}^{p} k_{i\alpha}s_\alpha. \tag{18}$$

Here $\{k_{i\alpha}\}$ and $\{s_\alpha\}$ are commuting sets of Majorana fermions, that is,

$$\{k_{i\alpha},k_{j\beta}\}=\delta_{ij}\delta_{\alpha\beta},\quad \{s_\alpha,s_\beta\}=\delta_{\alpha\beta},\quad [k_{i\alpha},\,s_\beta]=0. \tag{19}$$

We note that because the $p=1$ ansatz is the fundamental representation, it is known from representation theory that all representations of so(n) appear (at least once) in the reduction of this ansatz for some p. For $p=1$ all we have are the ordinary Majorana fermions, the properties of which are well known. For $p=2$ the algebra is

$$c_i^3=4c_i,\quad c_ic_jc_k+c_kc_jc_i=4\delta_{jk}c_i+4\delta_{ij}c_k. \tag{20}$$

In general to obtain the algebras associated with $p>1$ we must first establish the single MPF algebra. The most direct way to do this is to notice that each ansatz term $k_{i\alpha}s_\alpha$ (no sum on α) has eigenvalues ±1. From this we can see that an MPF of order p satisfies the following characteristic equation:

$$(c+p)(c+p-2)(c+p-4),\ldots,(c-p+4)(c-p+2)(c-p)=0.$$

This can be more conveniently written as follows:

$$\begin{aligned}&\text{For even } p\text{:}\quad (c^2-p^2)(c^2-(p-2)^2),\ldots,(c^2-2^2)c=0,\\ &\text{for odd } p\text{:}\quad (c^2-p^2)(c^2-(p-2)^2),\ldots,(c^2-3^2)(c^2-1)=0.\end{aligned} \tag{21}$$

For example,

$$p=2,\quad c^3=4c,\quad p=3,\quad c^4=10c^2-9, \tag{22}$$

$$p=4, \quad c^5=20c^3-64c.$$

To obtain the algebraic relations between different MPFs their characteristic equations need to be inserted into commutators. As an example we obtain the $p=2$ algebra as given in Eq. (20). First of all use the characteristic equation $c^3=4c$ to obtain

$$[[c_1,\ c_2],\ c_2^3]=4[[c_1,\ c_2],\ c_2]. \tag{23}$$

When the left-hand side of this is evaluated using Eq. (10), and the result is solved simultaneously with Eq. (10), those relations from Eq. (20) which involve only two MPEs are obtained. To obtain the three MPF relations as well we put the two MPF relations into a commutator involving a new MPF. In this case (i.e., for $p=2$) we need only use $c_1c_2c_1=0$ to obtain the expression

$$[[c_1,\ c_3],\ c_1c_2c_1]=0. \tag{24}$$

Expanding this, we find that $c_1c_2c_3+c_3c_2c_1=0$ which completes our derivation of the relations (20). For $p>2$ we can establish the algebra using essentially the same method as we have illustrated here. However, because in general the p specific relations are of order $p+1$, to get a complete set of these it is necessary to use an iterative procedure in which the characteristic equation, itself of order $p+1$, is commuted up to p times with terms of the form $[c_i,c_j]$, each commutation inserting a new MPF into the algebra.

VI. MPFs AND REPRESENTATIONS OF so(n) ALGEBRAS

In this section we look at representations of so(n) algebras on Fock spaces which have a unique vacuum state. In the case of odd n this involves a restatement of the familiar DPF results in MPF language, and we include these only for completeness. For the more complicated even n case, we show how to construct so($2n$) representations out of $2n-1$ MPFs by making use of a projection from so($2n+1$). This is illustrated for so(4).

A. so($2n+1$) representations in terms of MPFs

In terms of DPFs, a particular so($2n+1$) representation having a unique vacuum state $|0\rangle$ is defined by the following conditions:

$$a_j|0\rangle=0, \quad a_ja_j^\dagger|0\rangle=p|0\rangle \quad \text{for all } j. \tag{25}$$

Here p is a positive definite integer, the order of the parastatistics. From Eq. (5) we can express the DPFs in these expressions as follows:

$$a_j=\frac{c_{j+}-ic_{j-}}{2}, \quad a_j^\dagger=\frac{c_{j+}+c_{j-}}{2}. \tag{26}$$

Here c_{j+} and c_{j-} are independent MPFs, the $j\pm$ notation being used only for convenience. In terms of MPFs the representation defining conditions (25) become

$$c_{j+}|0\rangle=ic_{j-}|0\rangle, \quad (c_{j+}^2+c_{j-}^2)|0\rangle=2p|0\rangle. \tag{27}$$

These conditions clearly involve a pairing of MPFs based on their properties with respect to the Fock space. So although within the algebra there is complete symmetry between the MPFs, this is broken by their action on the Fock space. The fact that even after this symmetry is broken we are able to group $2n$ MPFs into n symmetric pairs (i.e., each of the n pairs having the same algebraic properties) is the origin of the DPF algebra.

B. Representation of so(4) constructed using three MPFs

Consider first so(5), with its elements expressed in DPF notation. The root diagram of this algebra contains the points $\pm e_1$, $\pm e_2$, $\pm e_1+e_2$, $\pm e_1-e_2$, where e_1 and e_2 are othogonal unit vectors. The correspondence between the DPF algebra elements and the root vectors is

$$a_1^\dagger \leftrightarrow e_1, \quad a_1 \leftrightarrow -e_1, \quad a_2^\dagger \leftrightarrow e_2, \quad a_2 \leftrightarrow -e_2,$$

$$[a_1^\dagger, a_2^\dagger] \leftrightarrow e_1+e_2, \quad [a_1^\dagger, a_2] \leftrightarrow e_1-e_2, \quad [a_1, a_2^\dagger] \leftrightarrow -e_1+e_2, \quad [a_1, a_2] \leftrightarrow -e_1-e_2.$$

The four vectors of length $\sqrt{2}$ are the roots of the so(4) subalgebra. To construct so(4) representations in terms of MPFs we restrict our attention to these. We define

$$J_{1z}=\frac{[a_1^\dagger, a_1]+[a_2^\dagger, a_2]}{4}, \quad J_{1+}=\frac{[a_2^\dagger, a_1^\dagger]}{2}, \quad J_{1-}=\frac{[a_1, a_2]}{2} \tag{28}$$

and

$$J_{2z}=\frac{[a_1^\dagger, a_1]-[a_2^\dagger, a_2]}{4}, \quad J_{2+}=\frac{[a_2, a_1^\dagger]}{2}, \quad J_{2-}=\frac{[a_1, a_2^\dagger]}{2}. \tag{29}$$

These operators form two commuting su(2) algebras, displaying the su(2)$\oplus$su(2) structure of so(4). To express these operators in terms of MPFs we use

$$a_1^\dagger=\frac{c_1+ic_2}{2}, \quad a_1=\frac{c_1-ic_2}{2}, \tag{30}$$

$$a_2^\dagger=\frac{c_3+ic_4}{2}, \quad a_2=\frac{c_3-ic_4}{2}. \tag{31}$$

We find

$$\begin{aligned}
J_{1z}&=\frac{i[c_2, c_1]+i[c_4, c_3]}{8},\\
J_{1\pm}&=\frac{\mp[c_1, c_3]\pm[c_2, c_4]-i[c_2, c_3]-i[c_1, c_4]}{8},\\
J_{2z}&=\frac{i[c_2, c_1]-i[c_4, c_3]}{8},\\
J_{2\pm}&=\frac{\mp[c_1, c_3]\mp[c_2, c_4]-i[c_2, c_3]+i[c_1, c_4]}{8}.
\end{aligned} \tag{32}$$

Here we have constructed a representation of so(4) using four MPFs. However our theorem tells us that so(4) is isomorphic to the algebra of only three MPFs. This isomorphism can be made explicit if we first use Eq. (11) to rewrite our MPF realization of so(4) in terms of $L_{\alpha\beta}$ operators:

$$J_{1z}=\frac{i(L_{21}+L_{43})}{2}, \quad J_{1\pm}=\frac{(\mp L_{13}\pm L_{24}-iL_{23}-iL_{14})}{2}, \tag{33}$$

$$J_{2z}=\frac{i(L_{21}-L_{43})}{2},\quad J_{2\pm}=\frac{(\mp L_{13}\mp L_{24}-iL_{23}+iL_{14})}{2}.$$

Now, since the index 0 does not appear in any of these expressions, we can, without altering the algebra in any way, replace the index 4 in each by the index 0. If we do this, and then use Eqs. (11) and (14) to transform our results back into MPF notation we obtain

$$\begin{aligned} J_{1z}&=i\,\frac{[c_2,\,c_1]}{8}-\frac{c_3}{4},\quad J_{1\pm}=\frac{\mp[c_1,\,c_3]-i[c_2,\,c_3]}{8}-\frac{c_1\pm ic_2}{4},\\ J_{2z}&=i\,\frac{[c_2,\,c_1]}{8}+\frac{c_3}{4},\quad J_{2\pm}=\frac{\mp[c_1,\,c_3]-i[c_2,\,c_3]}{8}+\frac{c_1\pm ic_2}{4}. \end{aligned} \tag{34}$$

These expressions involve only three MPFs, so we have obtained the so(4) algebra explicitly in terms of three MPFs, as we set out to do. It is particularly interesting to observe the following expressions for J_{ix}, J_{iy}, J_{iz} $(i=1,2)$ in which the symmetry between the three MPFs is made manifest:

$$J_{1x}=-i\,\frac{[c_2,\,c_3]}{8}-\frac{c_1}{4},\quad J_{1y}=-i\,\frac{[c_3,\,c_1]}{8}-\frac{c_2}{4},\quad J_{1z}=-i\,\frac{[c_1,\,c_2]}{8}-\frac{c_3}{4}; \tag{35}$$

$$J_{2x}=-i\,\frac{[c_2,\,c_3]}{8}+\frac{c_1}{4},J_{2y}=-i\,\frac{[c_3,\,c_1]}{8}+\frac{c_2}{4},\quad J_{2z}=-i\,\frac{[c_1,\,c_2]}{8}+\frac{c_3}{4}. \tag{36}$$

Due to the su(2)⊕su(2) structure of so(4) we can construct specific so(4) representations by choosing a ground state $|0\rangle$ such that

$$J_{1-}|0\rangle=J_{2-}|0\rangle=0,\quad J_{1z}|0\rangle=-j_1|0\rangle,\quad J_{2z}|0\rangle=-j_2|0\rangle. \tag{37}$$

Here j_1 and j_2 are the spins of the two su(2) subalgebra representations. In conventional su(2) notation, this ground state would be written as $|j_1,-j_1,j_2,j_2\rangle$. In terms of MPFs the conditions (37) become

$$(c_1-ic_2)|0\rangle=0, \tag{38}$$

$$i[c_1,\,c_2]|0\rangle=(c_1^2+c_2^2)|0\rangle=4(j_1+j_2)|0\rangle, \tag{39a}$$

$$c_3|0\rangle=2(j_1-j_2)|0\rangle. \tag{39b}$$

Note that Eqs. (38) and (39a) are essentially the same as Eq. (27). As in the so$(2n+1)$ case the overall symmetry among the MPFs is lost in the transition to Fock space representations.

Relations (35) and (36) can be inverted to yield the MPF matrix representations associated with specific so(4) representations. The relationship is

$$c_i=2(J_{2i}-J_{1i}). \tag{40}$$

If the J_{1i} and J_{2i} operators have spins n and m, respectively, so that we are looking at the (n,m) representation of so(4), then by Eq. (16) the MPFs have $p=2(n+m)$. As an example, if $\{\sigma_\alpha\}$ are the Pauli matrices, then the $(\frac{1}{2},\frac{1}{2})$ representation has $j_{1\alpha}=\sigma_\alpha/2\otimes 1$ and $j_{2\alpha}=1\otimes\sigma_\alpha/2$, so that $p=2$, and by Eq. (40) $c_\alpha=1\otimes\sigma_\alpha-\sigma_\alpha\otimes 1$.

Realizations of higher so$(2n)$ algebras in terms of MPFs can be constructed in a similar way by projecting down from the well-known parafermionic realizations of so$(2n+1)$.

VII. MPFs AND THE PARA-GRASSMAN ALGEBRA

If we define (real) elements ϵ_i by $c_i = l\epsilon_i$ for all i, where l is a contraction parameter, and take the limit $l \to 0$ we obtain the algebra

$$[[\epsilon_i,\ \epsilon_j],\ \epsilon_k] = 0. \tag{41}$$

This is just the para-Grassman algebra,[15] considered extensively in connection with the representation theory of DPFs. Our results and ansatz representations for specific MPF algebras can likewise be contracted, leading to results in para-Grassman representation theory. For example contraction of Eq. (20) yields

$$\epsilon_i\epsilon_j\epsilon_k + \epsilon_k\epsilon_j\epsilon_i = 0 \tag{42}$$

and Eq. (21) contracted leads to the very simple relation $\epsilon_i^{p+1} = 0$ for all i.

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The projective unitary irreducible representations of the Galilei group in 1+2 dimensions

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We give an elementary analysis of the multiplicator group of the Galilei group in 1+2 dimensions $\mathscr{G}_+^\uparrow$. For a nontrivial multiplicator we give a list of all the corresponding projective unitary irreducible representations of $\mathscr{G}_+^\uparrow$. © *1996 American Institute of Physics.* [S0022-2488(96)00701-5]

I. INTRODUCTION

Recently a complete list of all projective unitary irreducible representations of the Poincaré group in $1+2$ dimensions was determined.[1] This paper intended to provide a similar analysis for the Galilei group (more precisely for the proper orthochronous Galilei group).

The main technical obstacle seems to be the rather complicated structure of the multiplier group (see Ref. 2, Appendix A). In Sec. II the reader is provided with the basic facts concerning the determination of the projective irreducible representations of a certain group by the Mackey method. (Follow as closely as possible Ref. 3). Section III gives an elementary analysis of the second cohomology group of the universal covering group $\widetilde{\mathscr{G}}_+^\uparrow$ of the Galilei group $\mathscr{G}_+^\uparrow$ in $1+2$ dimensions.

Section IV constructs for every nontrivial multiplier a certain extension of $\widetilde{\mathscr{G}}_+^\uparrow$ which exhibits a semidirect product group structure. One is able to apply the Mackey induced representations method to determine the desired representations. In this paper only nontrivial multipliers are considered. The case of true representation (i.e., trivial multipliers) is elementary to analyze and raises no problems.[1]

II. PROJECTIVE UNITARY IRREDUCIBLE REPRESENTATIONS

Following Ref. 3, the classification of all projective unitary irreducible representations of a certain group G is done following the steps below:

(1) One identifies the universal covering group $\tilde{G}$ of G. Let one denote by $\pi:\tilde{G}\to G$ the canonical projection. If $\alpha:G\to \mathrm{Aut}(\mathscr{P}(\mathscr{H}))$ is a morphism of G into the group of automorphisms of the lattice of the orthogonal projectors in the Hilbert space $\mathscr{H}$ (i.e., a *symmetry*) then

$$\tilde{\alpha}\equiv\alpha\circ\pi \tag{2.1}$$

is a morphism of $\tilde{G}$ into the group of automorphisms of the same lattice $\mathscr{P}(\mathscr{H})$ verifying the condition

$$\tilde{\alpha}_{g_0}=id \tag{2.2}$$

for any $g_0\in Ker(\pi)$.

Conversely, any morphism of $\tilde{G}$ in $\mathrm{Aut}(\mathscr{P}(\mathscr{H}))$ verifying Eq. (2.2) determines a morphism of G via formula (2.1). It will be clear immediately that it is more convenient to study morphisms of

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$\tilde{G}$ instead of morphisms of G. According to Wigner theorem, the morphism $\tilde{\alpha}$ is induced by projective unitary irreducible representation V of $\tilde{G}$ in the Hilbert space $\mathscr{H}$.

One easily discovers, applying the Schur lemma, that the condition (2.2) is equivalent to the condition

$$V_{g_0} = \lambda \times id \tag{2.3}$$

for any $g_0 \in Ker(\pi)$. Here λ is a complex number of modulus 1. So in the following one will determine the projective unitary irreducible representation of the group $\tilde{G}$ verifying Eq. (2.3).

(2) One determines the cohomology group $H^2(\tilde{G},\mathbb{R})$ using infinitesimal arguments. This is possible because for connected and simply connected Lie groups one has $H^2(\tilde{G},\mathbb{R}) \simeq H^2(\mathrm{Lie}(\tilde{G}),\mathbb{R})$.

(3) One determines from $H^2(\tilde{G},\mathbb{R})$ the multiplier group, i.e., $H^2(\tilde{G},\mathbf{T})$ where $\mathbf{T}$ is the multiplicative group of complex numbers of modulus 1. The corresponding 2-cocycles are also called multipliers. One selects a multiplier from every cohomology class and tries to classify the unitary irreducible representations of $\tilde{G}$ and afterwards selects those verifying the condition (2.3).

For this last step one tries to first exhibit a semidirect product group. To fix the notations we remind the reader the content of the Mackey theorem. Let $H \times_t A$ be a semidirect product of the locally compact groups H and A which verify the second axiom of countability. Suppose that A is Abelian. Here: $t: H \to \mathrm{Aut}(A)$ is a group homomorphism. To classify all the unitary irreducible representations of $H \times_t A$ one goes through the following steps.[3]

(a) One considers the dual $\hat{A}$ of A and the action of H on it given by

$$(h \cdot \omega)(a) \equiv \omega(t_{h^{-1}}(a)). \tag{2.4}$$

(b) One computes all the H-orbits in $\hat{A}$. We suppose there exists a Borel cross section $\Sigma \subset \hat{A}$ intersecting once every H-orbit.

(c) For $\forall \omega \in \Sigma$ one computes the *little group*:

$$H_\omega \equiv \{h \in H | h \cdot \omega = \omega\}. \tag{2.5}$$

(d) We suppose that we know the complete list of the unitary irreducible representations of $H_\omega, \forall \omega \in \Sigma$.

(e) Let $\mathscr{O} \subset \hat{A}$ be a H-orbit in $\hat{A}, \omega_0 \equiv \mathscr{O} \cap \Sigma$ and π a unitary irreducible representation of H_{ω_0} acting in the (complex) Hilbert space $\mathscr{K}$. As it is well known[3] one can associate to every π a $(H,\mathscr{O},\mathscr{K})$-cocyle ϕ^π, i.e., a Borel map $\phi^\pi: H \times \mathscr{O} \to \mathscr{U}(\mathscr{K})$ [here $\mathscr{U}(\mathscr{K})$ is the group of unitary operators in $\mathscr{K}$] such that a.e. in $H \times \mathscr{O}$:

$$\phi^\pi(h_1, h_2 \cdot \omega)\phi^\pi(h_2, \omega) = \phi^\pi(h_1 h_2, \omega) \tag{2.6}$$

and $\forall h \in H_{\omega_0}$:

$$\pi(h) = \phi^\pi(h, \omega_0). \tag{2.7}$$

A convenient way to construct ϕ^π is as follows. Let $c: \mathscr{O} \to H$ be a Borel section, i.e., a Borel map such that $\forall \omega \in \mathscr{O}$,

$$c(\omega) \cdot \omega_0 = \omega. \tag{2.8}$$

Then we can take

$$\phi^\pi(h, \omega) = \pi(c(h \cdot \omega)^{-1} h c(\omega)). \tag{2.9}$$

(f) For every H-orbit $\mathcal{O}$ and every unitary irreducible representation π of H_{ω_0} in $\mathcal{K}$ we consider the Hilbert space $\mathcal{H}\equiv L^2(\mathcal{O},d\alpha,\mathcal{K})$ (where α is an H-quasi-invariant measure on $\mathcal{O}$) and define: $\mathcal{W}_{h,a}^{(\mathcal{O},\pi)}:\mathcal{H}\to\mathcal{H}$ as follows:

$$(\mathcal{W}_{h,a}^{(\mathcal{O},\pi)}f)(\omega)=\omega(a)(r_h(h^{-1}\cdot\omega))^{1/2}\phi^{\pi}(h,h^{-1}\cdot\omega)f(h^{-1}\cdot\omega) \tag{2.10}$$

(where $r_h(\cdot)$ is a version of the Radon–Nicodym derivative $d\alpha^{h^{-1}}/d\alpha$).

Then $\mathcal{W}$ is a unitary irreducible representation of $H\times_t A$.

The Mackey theorem asserts that if the orbit structure is smooth (see Ref. 3) then every unitary irreducible representation of $H\times_t A$ is unitary equivalent to a representation of the form $\mathcal{W}^{(\mathcal{O},\pi)}$ and moreover to distinct couples $(\mathcal{O},\pi)\neq(\mathcal{O}',\pi')$ corresponding representations $\mathcal{W}^{(\mathcal{O},\pi)}$ and $\mathcal{W}^{(\mathcal{O},\pi)}$ which are not unitary equivalent.

III. THE GALILEI GROUP IN 1+2 DIMENSIONS

A. Notations

By definition the orthochronous Galilei group in $1+2$ dimensions $\mathcal{G}^{\uparrow}$ is set-theoretically $O(2)\times\mathbb{R}^2\times\mathbb{R}\times\mathbb{R}^2$ with the composition law

$$(R_1,\mathbf{v}_1,\eta_1,\mathbf{a}_1)\cdot(R_2,\mathbf{v}_2,\eta_2,\mathbf{a}_2)=(R_1R_2,\mathbf{v}_1+R_1\mathbf{v}_2,\eta_1+\eta_2,\mathbf{a}_1+R_1\mathbf{a}_2+\eta_2\mathbf{v}_1). \tag{3.1}$$

Organize $\mathbb{R}^2$ as column vectors, $O(2)$ as the 2×2 real orthogonal matrices, and consistently use matrix notations. This group acts naturally on $\mathbb{R}\times\mathbb{R}^2$:

$$(R,\mathbf{v},\eta,\mathbf{a})\cdot(T,\mathbf{X})=(T+\eta,R\mathbf{X}+T\mathbf{v}+\mathbf{a}). \tag{3.2}$$

One can also consider the proper orthochronous Galilei group $\mathcal{G}^{\uparrow}_{+}$ defined as

$$\mathcal{G}^{\uparrow}_{+}\equiv\{(R,\mathbf{v},\eta,\mathbf{a})\,|\det(R)=1\} \tag{3.3}$$

and the universal covering group $\widetilde{\mathcal{G}}^{\uparrow}_{+}$ of $\mathcal{G}^{\uparrow}_{+}$. We can take $\widetilde{\mathcal{G}}^{\uparrow}_{+}=\mathbb{R}\times\mathbb{R}^2\times\mathbb{R}\times\mathbb{R}^2$ with the composition law

$$(x_1,\mathbf{v}_1,\eta_1,\mathbf{a}_1)\cdot(x_2,\mathbf{v}_2,\eta_2,\mathbf{a}_2)=(x_1+x_2,\mathbf{v}_1+R(x_1)\mathbf{v}_2,\eta_1+\eta_2,\mathbf{a}_1+R(x_1)\mathbf{a}_2+\eta_2\mathbf{v}_1), \tag{3.4}$$

where

$$R(x)\equiv\begin{pmatrix}\cos(x) & \sin(x)\\ -\sin(x) & \cos(x)\end{pmatrix}. \tag{3.5}$$

The covering homomorphism δ: $\widetilde{\mathcal{G}}^{\uparrow}_{+}\to\mathcal{G}^{\uparrow}_{+}$ is

$$\delta(x,\mathbf{v},\eta,\mathbf{a})=(R(x),\mathbf{v},\eta,\mathbf{a}). \tag{3.6}$$

Finally we describe the Lie algebra of $\widetilde{\mathcal{G}}^{\uparrow}_{+}$, $\mathrm{Lie}(\widetilde{\mathcal{G}}^{\uparrow}_{+})\simeq\mathrm{Lie}(\mathcal{G}^{\uparrow}_{+})$ using the fact that $\mathcal{G}^{\uparrow}_{+}$ can be organized as a matrix group. Indeed one has the group isomorphism:

$$\mathcal{G}^{\uparrow}_{+}\ni(R,\mathbf{v},\eta,\mathbf{a})\leftrightarrow\begin{pmatrix}R & \mathbf{v} & \mathbf{a}\\ 0 & 1 & \eta\\ 0 & 0 & 1\end{pmatrix}\in M_{\mathbb{R}}(4,4). \tag{3.7}$$

Then $\mathrm{Lie}(\mathcal{G}^{\uparrow}_{+})$ can be identified with the linear space of 4×4 real matrices of the form

$$(\alpha,\mathbf{u},t,\mathbf{x})\equiv\begin{pmatrix}\alpha A & \mathbf{u} & \mathbf{x}\\ 0 & 0 & t\\ 0 & 0 & 0\end{pmatrix}. \tag{3.8}$$

Here $\mathbf{u},\mathbf{x}\in\mathbb{R}^2, t,\alpha\in\mathbb{R}$ and $A\equiv\left(\begin{smallmatrix}0 & 1\\ -1 & 0\end{smallmatrix}\right)$. One obtains the Lie bracket as

$$[(\alpha_1,\mathbf{u}_1,t_1,\mathbf{x}_1),(\alpha_2,\mathbf{u}_2,t_2,\mathbf{x}_2)]=(0,A(\alpha_1\mathbf{u}_2-\alpha_2\mathbf{u}_1),0,A(\alpha_1\mathbf{x}_2-\alpha_2\mathbf{x}_1)+t_2\mathbf{u}_1-t_1\mathbf{u}_2). \tag{3.9}$$

B. Computation of $H^2(\mathrm{Lie}(\widetilde{\mathscr{G}}^{\uparrow}_{+}),\mathbb{R})$

As was outlined in the preceding section, to classify all multipliers of a Lie group G one starts by first computing the second cohomology group of $\mathrm{Lie}(G)$ with real coefficients.[3] As was said in the Introduction, an elementary derivation of this group is provided (see also Ref. 4). If $\xi\in Z^2(\mathrm{Lie}(\tilde{\mathscr{G}}^{\uparrow}_{+}),\mathbb{R})$ the cocycle equation is written as:

$$\xi([(\alpha_1,\mathbf{u}_1,t_1,\mathbf{x}_1),(\alpha_2,\mathbf{u}_2,t_2,\mathbf{x}_2)],(\alpha_3,\mathbf{u}_3,t_3,\mathbf{x}_3))+\text{perm.}=0. \tag{3.10}$$

Here $\xi:\mathrm{Lie}(\widetilde{\mathscr{G}}^{\uparrow}_{+})\times\mathrm{Lie}(\widetilde{\mathscr{G}}^{\uparrow}_{+})\to\mathbb{R}$ is, by definition, bilinear and antisymmetric. Using Eq. (3.9), one can explicitate (3.10):

$$\xi((0,A(\alpha_1\mathbf{u}_2-\alpha_2\mathbf{u}_1),0,A(\alpha_1\mathbf{x}_2-\alpha_2\mathbf{x}_1)+t_2\mathbf{u}_1-t_1\mathbf{u}_2),(\alpha_3,\mathbf{u}_3,t_3,\mathbf{x}_3))+\text{perm.}=0. \tag{3.11}$$

One can consider some distinct cases of this equation:
(i) $t_i=0$, $\mathbf{x}_i=\mathbf{0}$ $(i=1,2,3)$
One obtains

$$\xi((0,A(\alpha_1\mathbf{u}_2-\alpha_2\mathbf{u}_1),0,\mathbf{0}),(\alpha_3,\mathbf{u}_3,t_3,\mathbf{x}_3))+\text{perm.}=0. \tag{3.12}$$

From bilinearity one has

$$\xi((0,\mathbf{u},0,\mathbf{0}),(0,\mathbf{u}',0,\mathbf{0}))=\mathbf{u}^tC\mathbf{u}', \tag{3.13}$$

where C is a 2×2 real matrix. From antisymmetry one finds $C^t=-C$ so necessarily $C=\frac{1}{2}FA(F\in\mathbb{R})$. So one has

$$\xi((0,\mathbf{u},0,\mathbf{0}),(0,\mathbf{u}',0,\mathbf{0}))=\tfrac{1}{2}F\langle\mathbf{u},\mathbf{u}'\rangle, \tag{3.14}$$

where $\langle\cdot,\cdot\rangle$is the sesquilinear form on $\mathbb{R}^2$ given by

$$\langle\mathbf{u},\mathbf{v}\rangle\equiv\mathbf{u}^tA\mathbf{v}. \tag{3.15}$$

It is easy to see that Eq. (3.12) becomes an identity.
(ii) $\alpha_i=0$, $\mathbf{u}_i=\mathbf{0}$ $(i=1,2,3)$
Equation (3.11) becomes an identity.
(iii) $t_1=0$, $\mathbf{x}_1=\mathbf{0}$, $\alpha_i=0$, $\mathbf{u}_i=\mathbf{0}$ $(i=2,3)$
One easily obtains from Eq. (3.11),

$$\xi((0,\mathbf{0},t,\mathbf{x}),(0,\mathbf{0},t',\mathbf{x}'))=0. \tag{3.16}$$

(iv) $t_i=0$, $\mathbf{x}_i=\mathbf{0}$ $(i=1,2)$, $\alpha_3=0$, $\mathbf{u}_3=\mathbf{0}$
Equation (3.11) becomes

$$\xi((0,\mathrm{A}(\alpha 1\mathbf{u}2-\alpha 2\mathbf{u}1),0,\mathbf{0}),(0,\mathbf{0},t3,\mathbf{x}3))+\xi((0,\mathbf{0},0,\alpha 2A\mathbf{x}3+t3\mathbf{u}2),(\alpha 1,\mathbf{u}1,0,\mathbf{0}))$$

$$+\xi((0,\mathbf{0},0,-\alpha_1 A\mathbf{x}_3-t_3\mathbf{u}_1),(\alpha_2,\mathbf{u_2},0,\mathbf{0}))=0. \tag{3.17}$$

From bilinearity one has

$$\xi((0,\mathbf{u},0,\mathbf{0}),(0,\mathbf{0},0,\mathbf{x})=\mathbf{x}^t D\mathbf{u}, \tag{3.18}$$

where D is a 2×2 real matrix.

If one takes in Eq. (3.17) $\alpha_2=0$, $t_3=0$ and inserts expression (3.18) one gets

$$[D,A]=0\Leftrightarrow D=-\tau\times id+cA \quad (\tau,c\in\mathbb{R}) \tag{3.19}$$

so, Eq. (3.18) takes the form

$$\xi((0,\cdot\,\mathbf{u},0,\mathbf{0}),(0,\mathbf{0},0,\mathbf{x})=-\tau\mathbf{x}\cdot\mathbf{u}+c\langle\mathbf{x},\mathbf{u}\rangle. \tag{3.20}$$

If one inserts Eq. (3.20) into Eq. (3.17) one gets $c=0$ and

$$\xi((0,A\mathbf{u},0,\mathbf{0}),(0,\mathbf{0},1,\mathbf{0}))+\xi((0,\mathbf{0},0,\mathbf{u}),(1,\mathbf{0},0,\mathbf{0}))=0. \tag{3.21}$$

Because of linearity one has

$$\xi((0,\mathbf{0},1,\mathbf{0}),(0,\mathbf{u},0,\mathbf{0}))=\mathbf{P}\cdot\mathbf{u} \quad (\mathbf{P}\in\mathbb{R}^2) \tag{3.22}$$

and the preceding relation gives

$$\xi((0,\mathbf{0},0,\mathbf{x}),(1,\mathbf{0},0,\mathbf{0}))=\langle\mathbf{P},\mathbf{x}\rangle. \tag{3.23}$$

Finally Eq. (3.20) reduces to

$$\xi((0,\mathbf{u},0,\mathbf{0}),(0,\mathbf{0},0,\mathbf{x})=\tau\mathbf{x}\cdot\mathbf{u}. \tag{3.24}$$

Denote

$$S\equiv\xi((1,\mathbf{0},0,\mathbf{0}),(0,\mathbf{0},1,\mathbf{0})) \tag{3.25}$$

and use linearity to obtain.

$$\xi((1,\mathbf{0},0,\mathbf{0}),(0,\mathbf{u},0,\mathbf{0})=\langle\mathbf{G},\mathbf{u}\rangle \quad (\mathbf{G}\in\mathbb{R}^2). \tag{3.26}$$

Finally reconstruct the cocyle ξ from Eqs. (3.14)–(3.26):

$$\xi(\alpha_1,\mathbf{u}_1,t_1,\mathbf{x}_1),(\alpha_2,\mathbf{u}_2,t_2,\mathbf{x}_2)=\langle\mathbf{G},\alpha_1\mathbf{u}_2-\alpha_2\mathbf{u}_1\rangle+\tfrac{1}{2}F\langle\mathbf{u}_1,\mathbf{u}_2\rangle+S(\alpha_1 t_2-\alpha_2 t_1)$$
$$-\langle\mathbf{P},\alpha_1\mathbf{x}_2-\alpha_2\mathbf{x}_1\rangle+\mathbf{P}\cdot(t_2\mathbf{u}_1-t_1\mathbf{u}_2)+\tau(\mathbf{x}_1\cdot\mathbf{u}_2-\mathbf{x}_2\cdot\mathbf{u}_1). \tag{3.27}$$

If one takes the generic element of $C^1(\text{Lie}(\widetilde{\mathscr{G}}^{\uparrow}_{+}),\mathbb{R})\simeq(\text{Lie}(\widetilde{\mathscr{G}}^{\uparrow}_{+})^*$ to be $(\beta,\mathbf{G},E,\mathbf{P})$ defined by

$$\langle(\beta,\mathbf{G},E,\mathbf{P}),(\alpha,\mathbf{u},t,\mathbf{x})\rangle\equiv-\beta\alpha-\mathbf{G}\cdot\mathbf{u}-Et+\mathbf{P}\cdot\mathbf{x} \tag{3.28}$$

then it is elementary to see that Eq. (3.27) rewrites as

$$\xi=\tau\xi_0+F\xi_1+S\xi_2+\partial(0,\mathbf{G},0,\mathbf{P}), \tag{3.29}$$

where $\xi_0,\xi_1,\xi_2\in Z^2(\text{Lie}(\widetilde{\mathscr{G}}^{\uparrow}_{+}),\mathbb{R})$ are

$$\xi_0((\alpha_1,\mathbf{u}_1,t_1,\mathbf{x}_1),(\alpha_2,\mathbf{u}_2,t_2,\mathbf{x}_2))\equiv\mathbf{x}_1\cdot\mathbf{u}_2-\mathbf{x}_1\cdot\mathbf{u}_2, \tag{3.30}$$

$$\xi_1((\alpha_1,\mathbf{u}_1,t_1,\mathbf{x}_1),(\alpha_2,\mathbf{u}_2,t_2,\mathbf{x}_2))\equiv\tfrac{1}{2}\langle\mathbf{u}_1,\mathbf{u}_2\rangle, \tag{3.31}$$

$$\xi_2((\alpha_1,\mathbf{u}_1,t_1,\mathbf{x}_1),(\alpha_2,\mathbf{u}_2,t_2,\mathbf{x}_2))\equiv\alpha_1t_2-\alpha_2t_1 \tag{3.32}$$

and ∂ is the coboundary operator defined as

$$(\partial\beta)(X,X')=-\beta([X,X']),\quad \forall X,X'\in\mathrm{Lie}(\widetilde{\mathscr{G}}^{\uparrow}_{+}),\quad \forall\beta\in(\mathrm{Lie}\,(\widetilde{\mathscr{G}}^{\uparrow}_{+}))^{*}. \tag{3.33}$$

So every cocycle $\xi\in Z^2(\mathrm{Lie}(\widetilde{\mathscr{G}}^{\uparrow}_{+}),\mathbb{R})$ is cohomologous with a cocyle of the form $\tau\xi_0+F\xi_1+S\xi_2$.

It is easy to establish now that this cocycle is not a coboundary. One can summarize the preceding discussion as the following:

Proposition 1: $H^2(\mathrm{Lie}(\widetilde{\mathscr{G}}^{\uparrow}_{+}),\mathbb{R})$ *is a three-dimensional real space. In every cohomology class there exists exactly one cocyle of the type* $\tau\xi_0+F\xi_1+S\xi_2$.

C. Computation of $H^2(\widetilde{\mathscr{G}}^{\uparrow}_{+},\mathbb{R})$

As in Ref. 3 one uses the fact that for G a connected and simply connected Lie group, $H^2(G,\mathbb{R})$ is isomorphic to $H^2(\mathrm{Lie}(G),\mathbb{R})$. So, to determine $H^2(G,\mathbb{R})$ one should determine for ξ_0,ξ_1,ξ_2 some corresponding group cocyles. One easily determines (see Ref. 2)

$$\omega_0(g,g')=1/2[\mathbf{a}\cdot R(x)\mathbf{v}'-\mathbf{v}\cdot R(x)\mathbf{a}'+\eta'\mathbf{v}\cdot R(x)\mathbf{v}'], \tag{3.34}$$

$$\omega_1(g,g')=1/2\langle\mathbf{v},R(x)\mathbf{v}'\rangle, \tag{3.35}$$

$$\omega_2=\eta x', \tag{3.36}$$

where $g=(x,\mathbf{v},\eta,\mathbf{a})$, $g'=(x',\mathbf{v}',\eta',\mathbf{a}')$.

The correspondence between the Lie group and Lie algebra cocycles is checked using Lemma 7.36 from Ref. 3, Chap. VII. The content of this lemma is the following. Let G be connected and simply connected Lie group and $c\in Z^2(G,\mathbb{R})$. Define the Lie algebra 2-cochain ξ_c by

$$\xi_c(X,X')\equiv\frac{\partial^2}{\partial s\,\partial s'}[c(\exp(sX),\exp(s'X'))-(X\leftrightarrow X')]_{s=s'=0}. \tag{3.37}$$

Then $\xi_c\in Z^2(\mathrm{Lie}(G),\mathbb{R})$ and the correspondence $c\to\xi_c$ factorizes to an isomorphism between $H^2(G,\mathbb{R})$ and $H^2(\mathrm{Lie}(G),\mathbb{R})$.

So one has the following:

Corollary 1: $H^2(\widetilde{\mathscr{G}}^{\uparrow}_{+},\mathbb{R})$ *is a three-dimensional real linear space. In every cohomology class there exists exactly one cocycle of the type* $\tau\omega_0+F\omega_1+S\omega_2$.

Finally, applying Thm. 7.37 of Ref. 3 one has the following:

Theorem 1: *Every multiplier of* $\widetilde{\mathscr{G}}^{\uparrow}_{+}$ *is equivalent to a multiplier of the form*

$$m_{\tau,F,S}(g,g')\equiv\exp\left\{\frac{i\tau}{2}[\mathbf{a}\cdot R(x)\mathbf{v}'-\mathbf{v}\cdot R(x)\mathbf{a}'+\eta'\mathbf{v}\cdot R(x)\mathbf{v}']\right\}\exp\left\{\frac{iF}{2}\langle\mathbf{v},R(x)\mathbf{v}'\rangle+iS\,\eta x'\right\}. \tag{3.38}$$

Moreover $m_{\tau,F,S}\sim m_{\tau',F',S'}$ *iff* $\tau=\tau'$, $F=F'$, $S=S'$.

Remark 1: In 1+3 dimensions it is well known that only a multiplier of type $m_{\tau,0,0}$ *survives. So,* $m_{0,F,S}$ *is characteristic to 1+2 dimensions. According to the general theory of the projective*

unitary representations, one has to consider the most general multiplier $m_{\tau,F,S}$. In Ref. 1 only the multiplier $m_{\tau,0,0}$ was considered, so the statement of Theorem 2 in this reference is rather carelessly formulated.

Remark 2: One will find it convenient to denote $m_\tau \equiv m_{\tau,0,0}$, $m_F \equiv m_{0,F,0}$, $m_S \equiv m_{0,0,S}$.

Also note that $m_{\tau,F,S} = m_\tau m_F m_S$.

IV. THE PROJECTIVE UNITARY IRREDUCIBLE REPRESENTATIONS OF THE GALILEI GROUP IN 1+2 DIMENSIONS

A. The method

As anticipated, classify here the unitary irreducible $m_{\tau,F,S}$-representations of $\widetilde{\mathscr{G}}^{\uparrow}_{+}$. We try to mimic the method from Ref. 3 which consists of two steps:

(a) One first applies a simple result, namely a generalization of Theorem 7.16 from Ref. 3.

Proposition 2: Let $m_0,\ldots,m_p$ be multipliers for the group G and let $U(g\mapsto U_g)$ be an $m_0,\ldots,m_p$ representation of G in a (separable) Hilbert $\mathscr{H}$ space over the complex numbers. Let $G_{m_0,\ldots,m_p} \equiv G\times \underbrace{\mathbf{T}\times\cdots\times\mathbf{T}}_{(p+1)-times}$ with the composition law:

$$(g;\zeta_0,\ldots,\zeta_p)\cdot(g';\zeta_0',\ldots,\zeta_p') = (gg';\zeta_0\zeta_0' m_0(g,g'),\ldots,\zeta_p\zeta_p' m_p(g,g')). \tag{4.1}$$

Then $G_{m_0,\ldots,m_p}$ is a group, and

$$(g;\zeta_0,\ldots,\zeta_p)\mapsto V_{g;\zeta_0,\ldots,\zeta_p} \equiv \zeta_0^{-1},\ldots,\zeta_p^{-1} U_g \tag{4.2}$$

is a representation of $G_{m_0,\ldots,m_p}$ in $\mathscr{H}$ such that

$$V_{e;\zeta_0,\ldots,\zeta_p} = \zeta_0^{-1},\ldots,\zeta_p^{-1}\times id. \tag{4.3}$$

Conversely, if V is a representation of $G_{m_0,\ldots,m_p}$ in $\mathscr{H}$ such that Eq. (4.3) is verified, then if one writes

$$U_g \equiv V_{g;\ \underbrace{1,\ldots,1}_{(p+1)-times}}. \tag{4.4}$$

$g\mapsto U_g$ is an $m_0,\ldots,m_p$-representation of G in $\mathscr{H}$ and the connection (4.2) between U and V is true.

The proof is elementary and Theorem 7.16 of Ref. 3 is the particular case $p=0$.

It is clear that one can apply Proposition 2 with $G=\widetilde{\mathscr{G}}^{\uparrow}_{+}$, $p=2$, and $m_0=m_\tau$, $m_1=m_F$, $m_2=m_S$. Denote the corresponding group $G_{m_0 m_1 m_2}$ by $\widetilde{\mathscr{G}}^{\uparrow}_{+}{}^{\tau,F,S}$.

(b) Remember that in Ref. 3, where, in the four-dimensional case, one has to study only $\widetilde{\mathscr{G}}^{\uparrow}_{+}{}^{\tau,0,0}$ (see Chap. IX, Sec. 8), a semidirect product group structure is exhibited, so one can apply the induction procedure. The same procedure works for $\widetilde{\mathscr{G}}^{\uparrow}_{+}{}^{\tau,F,S}$. Indeed one has a group isomorphism $\widetilde{\mathscr{G}}^{\uparrow}_{+}{}^{\tau,F,S} \simeq H^F \times_{t^{\tau,S}} A$.

Define the group $H \equiv \mathbb{R}\times\mathbb{R}^2$ with the composition law:

$$(x,\mathbf{v})\cdot(x',\mathbf{v}') = (x+x',\mathbf{v}+R(x)\mathbf{v}') \tag{4.5}$$

then $H^F \equiv H \times \mathbf{T}$ with the composition law

$$(h_1;\zeta_1)\cdot(h_2;\zeta_2)=(h_1h_2;\zeta_1\zeta_1' m_F(h,h')). \tag{4.6}$$

The notation $m_F(h,h')$ makes sense because on the right-hand side of Eq. (3.35) only the variables x and $\mathbf{v}$ appear.

$A \equiv \mathbb{R}\times\mathbb{R}^2\times\mathbf{T}\times\mathbf{T}$ with the composition law

$$(\eta,\mathbf{a};\zeta_0,\zeta_2)\cdot(\eta',\mathbf{a}';\zeta_0',\zeta_2')=(\eta+\eta',\mathbf{a}+\mathbf{a}';\zeta_0\zeta_0',\zeta_2\zeta_2'). \tag{4.7}$$

$t^{\tau,S}: H^F \to \mathrm{Aut}(A)$ is given by

$$t^{\tau,S}_{h;\zeta_1}(a;\zeta_0,\zeta_2)=\left(t_h(a);\zeta_0\ \exp\left\{-\frac{i\tau}{2}[2\mathbf{v}\cdot R(x)\mathbf{a}+\eta\mathbf{v}^2]\right\},\zeta_2 e^{-iS\eta x}\right). \tag{4.8}$$

Here $a \equiv (\eta,\mathbf{a})$ and

$$t_h(\eta,\mathbf{a})=(\eta,R(x)\mathbf{a}+\eta\mathbf{v}). \tag{4.9}$$

The semidirect product structure follows from the homomorphism property of $t^{\tau,S}$. Then the isomorphism is

$$H^F \times_{t^{\tau,S}} A \ni \{(x,\mathbf{v};\zeta_1),(\eta,\mathbf{a};\zeta_0,\zeta_2)\} \leftrightarrow \left(x,\mathbf{v},\eta,\mathbf{a};\zeta_0\ \exp\left(\frac{i\tau}{2}\mathbf{a}\cdot\mathbf{v}\right),\zeta_1,\zeta_2 e^{iS\eta x}\right) \in \widetilde{\mathscr{G}}^{\uparrow\ \tau,F,S}_{+}. \tag{4.10}$$

We note that A is Abelian, so we will be able to apply the Mackey induction procedure.

Remark 3: One may wonder why Proposition 2 was not applied with $p=0$ *and* $m_0=m_\tau m_F m_S$. *The reason is that it did not succeed to find a convenient semidirect product structure for* G_{m_0} *in this case.*

Taking into account Eq. (4.10) the representations of $\widetilde{\mathscr{G}}^{\uparrow\ \tau,F,S}_{+}$ follow from representations of $H^F \times_{t^{\tau,S}} A$ according to

$$W_{(x,\mathbf{v},\eta,\mathbf{a};\zeta_0,\zeta_1,\zeta_2)}=\mathscr{W}_{(x,\mathbf{v},\eta,\mathbf{a};\zeta_0\ \exp\{-(i\tau/2)\,\mathbf{a}\cdot\mathbf{v}\},\zeta_1,\zeta_2 e^{-iS\eta x})}. \tag{4.11}$$

According to Proposition 2 one is looking for unitary irreducible representations of $\widetilde{\mathscr{G}}^{\uparrow\ \tau,F,S}_{+}$ verifying

$$W_{e;\zeta_0,\zeta_1,\zeta_2}=\zeta_0^{-1}\zeta_1^{-1}\zeta_2^{-1}\times id. \tag{4.12}$$

Follow the method of induced representations as presented in Sec. II.

B. Computation of the orbits

It is clear that every character of $A^{\tau,S}$ has the form

$$\chi_{p_0,\mathbf{p};n_0,n_2}(\eta,\mathbf{a};\zeta_0,\zeta_2)=\zeta_0^{n_0}\zeta_2^{n_2}\ \exp\{i(\eta p_0+\mathbf{a}\cdot\mathbf{p})\}, \tag{4.13}$$

where $p_0 \in \mathbb{R}, \mathbf{p} \in \mathbb{R}^2$, and $n_0, n_2 \in \mathbf{Z}$. So, $\widehat{A^{\tau,S}} \equiv \mathbb{R}\times\mathbb{R}^2\times\mathbf{Z}\times\mathbf{Z}$ with the generic element denoted by $[p_0,\mathbf{p};n_0,n_2]$. One easily computes the dual action of $t^{\tau,S}_{h;\zeta_1}$, namely,

$$(x,\mathbf{v};\zeta_1)\cdot[p_0,\mathbf{p};n_0,n_2]=[p_0-\mathbf{v}\cdot R(x)\mathbf{p}-1/2n_0\tau\mathbf{v}^2+Sn_2x,R(x)\mathbf{p}+n_0\tau\mathbf{v};n_0,n_2]. \tag{4.14}$$

The classification of the orbits of this action is elementary. We distinguish three cases which must be studied separately:

(a) $\tau \neq 0, \quad S=0.$

The orbits are

$$Z^1_{n_2,p_0} \equiv \{[p_0,\mathbf{0};0,n_2]\}; \quad p_0 \in \mathbb{R}, \quad n_2 \in \mathbf{Z},$$

$$Z^2_{n_2,r} \equiv \{[p_0,\mathbf{p};0,n_2] | \mathbf{p}^2 = r^2, \quad p_0 \in \mathbb{R}\}; \quad r \in \mathbb{R}_+, \quad n_2 \in \mathbf{Z},$$

$$Z^3_{n_0,n_2,\rho} \equiv \{[p_0,\mathbf{p};n_0,n_2] | \mathbf{p}^2 + 2n_0\tau p_0 = \rho\}; \quad \rho \in \mathbb{R}, \quad n_0 \in \mathbf{Z}^*, \quad n_2 \in \mathbf{Z}.$$

(b) $\tau = 0, \ S \neq 0.$

$$Z^4_{n_0,p_0} \equiv \{[p_0,\mathbf{0};n_0,0]\}; \quad p_0 \in \mathbb{R}, \quad n_0 \in \mathbf{Z},$$

$$Z^5_{n_0,n_2} \equiv \{[p_0,\mathbf{0};n_0,n_2] | p_0 \in \mathbb{R}\}, \quad n_0 \in \mathbf{Z}, \quad n_2 \in \mathbf{Z}^*,$$

$$Z^6_{n_0,n_2,r} \equiv \{[p_0,\mathbf{p};n_0,n_2] | \mathbf{p}^2 = r^2, p_0 \in \mathbb{R}\}; \quad r \in \mathbb{R}_+, \ n_0,n_2 \in \mathbf{Z}.$$

(c) $\tau \neq 0, \ S \neq 0.$

$$Z^7_{p_0} \equiv \{[p_0,\mathbf{0};0,0]\}; \quad p_0 \in \mathbb{R},$$

$$Z^8_{n_2} \equiv \{[p_0,\mathbf{0};0,n_2] | p_0 \in \mathbb{R}\}, \quad n_2 \in \mathbf{Z}^*,$$

$$Z^9_{n_0,\rho} \equiv \{[p_0,\mathbf{p};n_0,0] | \mathbf{p}^2 + 2n_0\tau p_0 = \rho\}; \quad \rho \in \mathbb{R}, \quad n_0 \in \mathbf{Z}^*,$$

$$Z^{10}_{n_0,n_2} \equiv \{[p_0,\mathbf{p};n_0,n_2] | \mathbf{p} \in \mathbb{R}^2, p_0 \in \mathbb{R}\}; \quad n_0,n_2 \in \mathbf{Z}^*.$$

(d) $\tau = 0, \ S = 0.$

$$Z^{11}_{p_0,n_0,n_2} \equiv \{[p_0,\mathbf{0};n_0,n_2]|\}; \quad p_0 \in \mathbb{R}, \quad n_0,n_2 \in \mathbf{Z},$$

$$Z^{12}_{r,n_0,n_2} \equiv \{[p_0,\mathbf{p};n_0,n_2] | p_0 \in \mathbb{R}, \mathbf{p}^2 = r^2\}; \quad r \in \mathbb{R}_+, \quad n_0,n_2 \in \mathbf{Z}.$$

(Note that Z^{11} is a point.) It is not hard to see that condition (4.12) cannot be fulfilled by the induced representations corresponding to the orbits: Z^1, Z^2, Z^4, Z^7, Z^8, and Z^9. So, analyze only the cases $Z^3, Z^5, Z^6, Z^{10}, Z^{11}$, and Z^{12}. One by one of these six cases are analyzed.

C. The representations

The unitary irreducible representations of the little groups are computed, then the corresponding cocycles as in Sec. II and finally the projective representations of $\mathscr{G}^{\uparrow}_{+}$ we are looking for, are exhibited.

(a) $\tau \neq 0, \ S = 0.$

In this case, $Z = Z^3_{n_0,n_2,\rho}$. A reference point is $[\rho/2n_0\tau, \mathbf{0}; n_0, n_2]$ and we have

$$H^F_{[\rho/2n_0\tau,\mathbf{0};n_0,n_2]} = \{(x,\mathbf{0};\zeta_1) | x \in \mathbb{R}, \zeta_1 \in \mathbf{T}\} \simeq \mathbb{R} \times \mathbf{T}. \tag{4.15}$$

The unitary irreducible representations of this Abelian subgroup are of the form $\pi^{(s,n_1)}$ ($s \in \mathbb{R}, n_1 \in \mathbf{Z}$); they are one-dimensional and are acting in $\mathbf{C}$ as follows:

$$\pi^{(s,n_1)}(x,\mathbf{0};\zeta_1)=e^{isx}\ \zeta_1^{n_1}. \tag{4.16}$$

In this case one can find explicitly a corresponding cocycle ϕ^{π}, namely,

$$\phi^{(s,n_1)}((x,\mathbf{v};\zeta_1),[p_0,\mathbf{p};n_0,n_2])=e^{isx}\ \zeta_1^{n_1}\ \exp\left\{\frac{in_1F}{2n_0\tau}\langle\mathbf{v},R(x)\mathbf{p}\rangle\right\}. \tag{4.17}$$

As in Ref. 3 identify $Z^3\simeq\mathbb{R}^2$ according to: $[(\rho-\mathbf{p}^2)/2n_0\tau,\mathbf{p};n_0,n_2]\leftrightarrow\mathbf{p}$ and consider the strictly invariant Lebesgue measure $d\mathbf{p}$ on $\mathbb{R}^2$.

Applying Eq. (4.11), the corresponding induced representation is acting in $\mathscr{H}=L^2(\mathbb{R}^2,d\mathbf{p})$ according to

$$(W_{(x,\mathbf{v},\eta,\mathbf{a};\zeta_0,\zeta_1,\zeta_2)}f)(\mathbf{p})=\zeta_0^{n_0}\zeta_1^{n_1}\zeta_2^{n_2}\ \exp\left\{i\left[-\frac{n_0\tau}{2}\ \eta\mathbf{a}\cdot\mathbf{v}+\eta\ \frac{\rho-\mathbf{p}^2}{2n_0\tau}+\mathbf{a}\cdot\mathbf{p}+sx\right]\right\}$$
$$\times\exp\left\{i\left[\frac{n_1F}{2n_0\tau}\langle\mathbf{v},\mathbf{p}\rangle\right]\right\}f(R(x)^{-1}(\mathbf{p}-n_0\tau\mathbf{v}). \tag{4.18}$$

The condition (4.12) imposes $n_0=n_1=n_2=-1$. The factor $\exp(-(i\eta\rho/2\tau))$ can be dropped because one is looking for projective representations. One gets the projective representations $V^{\tau,s}(\tau\in\mathbb{R}^*,s\in\mathbb{R})$ acting in $L^2(\mathbb{R}^2,d\mathbf{p})$ as follows:

$$(V^{\tau,s}_{x,\mathbf{v},\eta,\mathbf{a}}f)(\mathbf{p})=\exp\left\{i\left(sx+\mathbf{a}\cdot\mathbf{p}+\frac{\eta\mathbf{p}^2}{2\tau}+\frac{\tau}{2}\mathbf{a}\cdot\mathbf{v}+\frac{F}{2\tau}\langle\mathbf{v},\mathbf{p}\rangle\right)\right\}f(R(x)^{-1}(\mathbf{p}+\tau\mathbf{v})). \tag{4.19}$$

(b) $\tau=0$, $S\neq0$.

(b1) $Z=Z^5_{n_0,n_2}$.

A reference point is $[0,\mathbf{0};n_0,n_2]$ and one has

$$H^F_{[0,\mathbf{0};n_0,n_2]}=\{(0,\mathbf{v};\zeta_1)|\mathbf{v}\in\mathbb{R}^2,\zeta_1\in\mathbf{T}\}, \tag{4.20}$$

i.e., a central extension of the Abelian group $\mathbb{R}^2$. Let π be a unitary irreducible representation of this group. Because of Eq. (4.12) one must have

$$\pi_{(0,\mathbf{0};\zeta_1)}=\zeta_1^{-1}\times id. \tag{4.21}$$

This easily implies that one has

$$\pi_{(0,\mathbf{v};1)}\pi_{(0,\mathbf{v}';1)}=\exp\left\{-\frac{iF}{2}\langle\mathbf{v},\mathbf{v}'\rangle\right\}\pi_{(0,\mathbf{v}+\mathbf{v}';1)}, \tag{4.22}$$

i.e., $\mathbf{v}\mapsto\pi_{(0,\mathbf{v};1)}$ is a unitary irreducible representation of the canonical commutation relations in Weyl form. According to Stone–von Neumann theorem there exists (up to unitary equivalence) exactly one such representation, denoted π^{CCR} and acting in the Hibert space $\mathscr{H}$ (for an explicit expression see, e.g., Ref. 5, Chap. 3.1). So, the representations of $H^F_{[0,\mathbf{0};n_0,n_2]}$ one is looking for are of the form

$$\pi_{(0,\mathbf{v};\zeta_1)}=\zeta_1^{-1}\pi^{\mathrm{CCR}}_{\mathbf{v}}. \tag{4.23}$$

A corresponding cocycle is clearly

$$\phi^{\mathrm{CCR}}((x,\mathbf{v};\zeta_1),[p_0,\mathbf{0};n_0,n_2])=\zeta_1^{-1}\pi^{\mathrm{CCR}}_{\mathbf{v}}. \tag{4.24}$$

If one identifies naturally $Z^5 \simeq \mathbb{R}$ with the strictly invariant measure dp_0, then the corresponding induced representation is acting in $\mathscr{H}=L^2(\mathbb{R},\mathscr{K},dp_0)$ as follows:

$$(W_{(x,\mathbf{v},\eta,\mathbf{a};\zeta_0,\zeta_1,\zeta_2)}f)(p_0)=\zeta_0^{n_0}(\zeta_2\ e^{-iS\eta x})^{n_2}\ e^{i\eta p_0}\zeta_1^{-1}(\pi_{\mathbf{v}}^{\mathrm{CCR}}f)(p_0-Sn_2x). \tag{4.25}$$

Again Eq. (4.12) imposes $n_0=n_2=-1$ and one is left with the projective representations V^{CCR} acting in $\mathscr{H}=L^2(\mathbb{R},\mathscr{K},dp_0)$ according to

$$(V^{\mathrm{CCR}}_{x,\mathbf{v},\eta,\mathbf{a}}f)(p_0)=e^{i\eta(p_0+Sx)}(\pi_{\mathbf{v}}^{\mathrm{CCR}}f)(p_0+Sx). \tag{4.26}$$

(b2) $Z=Z^6_{n_0,n_2,\rho}$.

A reference point is $[0,r\mathbf{e_1};n_0,n_2]$ and one easily obtains

$$H^F_{[0,r\mathbf{e}_1;n_0,n_2]}=\left\{\left(2\pi n,\frac{2\pi nSn_2}{r}\ \mathbf{e_1}+\alpha\mathbf{e_2};\zeta_1\right)\middle|\ n\in\mathbf{Z},\alpha\in\mathbb{R},\zeta\in\mathbf{T}\right\}. \tag{4.27}$$

If one denotes

$$(n,\alpha;\zeta_1)\equiv\left(2\pi n,\frac{2\pi nSn_2}{r}\ \mathbf{e_1}+\alpha\mathbf{e_2};\zeta_1\right) \tag{4.28}$$

then the composition law is

$$(n,\alpha;\zeta_1)\cdot(n',\alpha';\zeta_1')=(n+n',\alpha+\alpha';\zeta_1\zeta_1'\ \exp\{ik(\alpha n'-\alpha' n)\}), \tag{4.29}$$

i.e., the little group is in this case a central extension of the Abelian group $\mathbf{Z}\times\mathbb{R}$. Here $k=2\pi FSn_2/r$. Let $(n,\alpha;\zeta_1)\mapsto\pi_{(n,\alpha;\zeta_1)}$ be a unitary irreducible representation fulfilling

$$\pi_{(0,0;\zeta_1)}=\zeta_1^{-1}\times id. \tag{4.30}$$

(The argument leading to this relation is similar to the argument leading to Eq. (4.21).)

One has for $\pi_{n,\alpha}\equiv\pi_{n,\alpha;1}$:

$$\pi_{n,\alpha}\pi_{n',\alpha'}=\exp\{ik(\alpha n'-\alpha' n)\}\pi_{n+n',\alpha+\alpha'}. \tag{4.31}$$

(b21) First analyze the case $k\neq 0\Leftrightarrow F\neq 0$.

The resemblance of this relation to the Weyl system (4.22) suggests an association to Eq. (4.31), a sort of imprimitivity system.[3] Denote: $\pi_{1,0}\equiv V$ and $\pi_\alpha=\pi_{0,\alpha}$. It is clear that Eq. (4.31) is equivalent to

$$\pi_{n,0}=V^n;\quad V\pi_\alpha V^{-1}=e^{2ik\alpha}\pi_\alpha;\quad \pi_\alpha\pi_{\alpha'}=\pi_{\alpha+\alpha'}. \tag{4.32}$$

So, it is sufficient to find an irreducible couple (V,π_α) fulfilling the last two relations of Eq. (4.32). According to a well-known theorem in harmonic analysis [Stone, Naimark, Ambrose, and Godement (SNAG)theorem][6,7] π_α is of the form

$$\pi_\alpha=\int_{\mathbb{R}}e^{i\lambda\alpha}\ dP(\lambda), \tag{4.33}$$

where $\Delta\mapsto P_\Delta$ is a projection valued measure in the Hilbert space $\mathscr{K}$. The second relation (4.32) is equivalent to

$$VP_\Delta V^{-1}=P_{\Delta-2k}. \tag{4.34}$$

Applying the same idea as in Ref. 3 Lemma 6.10, we can prove that P is homogeneous, i.e., $\mathscr{K}=L^2(\mathbb{R},\mathbf{C}^n,\beta)$ where β is a measure on $\mathbb{R}$ quasi-invariant with respect to the transformation $\lambda\mapsto\lambda+2k$ and

$$(P_\Delta f)(\lambda)=\chi_\Delta(\lambda)f(\lambda). \tag{4.35}$$

Moreover, like in Ref. 3, Theorem 6.12, one can show that V has the "diagonal" expression

$$(Vf)(\lambda)=r_V(\lambda+2k)^{1/2}v(\lambda)f(\lambda+2k) \tag{4.36}$$

(here r_V is a Radon–Nicodym derivative).

It is easy to see that for $n>1$ the system (V,P_Δ) is not irreducible. So, $n=1$. Moreover one can show that $\mathrm{supp}(\beta)$ must be discrete with period $2k$, i.e., $\mathrm{supp}(\beta)=\{\lambda+2km|m\in\mathbf{Z}\},\lambda\in\mathbb{R}$.

It is clear that one can take $\beta=\Sigma_{m\in\mathbf{Z}}\delta_{\lambda+2km}$. In this case one can also take $\mathscr{K}=l^2$ (i.e., sequences $\{f_m\}_{m\in\mathbf{Z}}$ such that $\Sigma_{m\in\mathbf{Z}}|f_m|^2<\infty$) and $P=\beta$. It follows that one has

$$(\pi_\alpha f)_m=e^{i(\lambda+2km)\alpha}f_m;\quad (Vf)_m=v_m f_{m+1}(\forall m\in\mathbf{Z}). \tag{4.37}$$

(Here $v_m\in\mathbf{T}$.)

The system (V,π_α) is irreducible. So, the unitary irreducible representations of the little group $H^F_{[0,r\mathbf{e_1};n_0,n_2]}$ verifying Eq. (3.25) are of the form $\pi^\lambda(\lambda\in\mathbb{R})$ acting in l^2 according to

$$(\pi^\lambda_{n,\alpha;\zeta_1}f)_m=\zeta_1^{-1}e^{i[\lambda+k(2m+n)]\alpha}f_{m+n}. \tag{4.38}$$

Consider the unitary transformation

$$(Uf)_m=f_{m+n}. \tag{4.39}$$

Then, one easily obtains that

$$U\pi^\lambda U^{-1}=\pi^{\lambda+n},\quad \forall n\in\mathbf{Z}, \tag{4.40}$$

i.e., $\pi^\lambda\sim\pi^{\lambda+n}\forall n\in\mathbf{Z}$.

Conversely, suppose that $\pi^{\lambda_1}\sim\pi^{\lambda_2}$. Then the spectra of the infinitesimal generators $(1/i)\ (d/d\alpha)\ \pi^{\lambda_i}_{0,\alpha}|_{\alpha=0}\ i=1,2$ must coincide. But these spectra are $\{\lambda_i+kn|n\in\mathbf{Z}\}$, so one necessarily gets $\lambda_1-\lambda_2\in k\mathbf{Z}$.

It follows that the parameter λ takes values in $\mathbb{R}(\mathrm{mod}\,k)$.

Denote by ϕ^λ a cocycle corresponding to π^λ. (The author has not been able to find a simple expression for this cocycle.) Then, if one identifies $Z^6\simeq\mathbb{R}\times S^1$ with the strictly invariant measure $dp_0\otimes d\Omega$, in the end one gets the projective representation $V^{r,\lambda}$ acting in $L^2(\mathbb{R}\times S^1,l^2,dp_0\otimes d\Omega)$ according to

$$\begin{aligned}(V^{r,\lambda}_{x,\mathbf{v},\eta,\mathbf{a}}f)(p_0,\mathbf{p})=&\exp\{i[\eta(p_0+Sx)+\mathbf{a}\cdot\mathbf{p}]\}\phi^\lambda((x,\mathbf{v};1),[p_0+\mathbf{v}\cdot\mathbf{p}+Sx,R(x)^{-1}\mathbf{p}])\\&\times f(p_0+\mathbf{v}\cdot\mathbf{p}+Sx,R(x)^{-1}\mathbf{p}).\end{aligned} \tag{4.41}$$

(b22) Analyze the case $k=0\Leftrightarrow F=0$.

In this case Eq. (4.31) states that π is a unitary irreducible representation of the Abelian group $\mathbf{Z}\times\mathbb{R}$. So $\pi\sim\pi^{(s,t)}$ with $s\in\mathbb{R}(\mathrm{mod}\,1),t\in\mathbb{R}$ where $\pi^{(s,t)}$ are one-dimensional and have the expression

$$\pi^{(s,t)}_{n,\alpha}=e^{2\pi ins}\ e^{it\alpha}. \tag{4.42}$$

A corresponding cocycle is

$$\phi^{(s,t)}((x,\mathbf{v}),[p_0,\mathbf{p}])=\exp\left\{i\left(sx-t\,\frac{\langle\mathbf{v},R(x)\mathbf{p}\rangle}{r}\right)\right\}. \tag{4.43}$$

The corresponding induced representation is $V^{r,s,t}$ acting in $L^2(\mathbb{R}\times S^1,dp_0\otimes d\Omega)$ according to

$$(V^{r,s,t}_{x,\mathbf{v},\eta,\mathbf{a}}f)(p_0,\mathbf{p})=\exp\left\{i\left[\eta(p_0+Sx)+\mathbf{a}\cdot\mathbf{p}+sx+S\frac{\langle\mathbf{p},\mathbf{v}\rangle}{r}\right]\right\}\ f(p_0+\mathbf{v}\cdot\mathbf{p}+Sx,R(x)^{-1}\mathbf{p}). \tag{4.44}$$

(c) $\tau\neq 0$, $S\neq 0$.

Only the orbit $Z^{10}_{n_0,n_2}$ is involved. A reference point is $[0,\mathbf{0};n_0,n_2]$ and we have

$$H^F_{[0,\mathbf{0};n_0,n_2]}=\{(0,\mathbf{0};\zeta_1)\,|\,\zeta_1\in\mathbf{T}\}\simeq\mathbf{T} \tag{4.45}$$

with the unitary irreducible representations of the form π^{n_1} acting in $\mathbf{C}$ according to

$$\pi^{n_1}_{(0,\mathbf{0};\zeta_1)}=\zeta_1^{n_1}. \tag{4.46}$$

A corresponding cocycle can be found:

$$\phi^{n_1}((x,\mathbf{v};\zeta_1),[p_0,\mathbf{p};n_0,n_2])=\zeta_1^{n_1}\exp\left\{\frac{iFn_1}{2n_0\tau}\langle\mathbf{v},R(x)\mathbf{p}\rangle\right\}. \tag{4.47}$$

Identify $Z^{10}\simeq\mathbb{R}\times\mathbb{R}^2$ with the strictly invariant measure $dp_0\otimes d\mathbf{p}$. The induced representations obey Eq. (4.12) *iff* $n_0=n_1=n_2=-1$ and we get projective representations V^τ acting in $L^2(\mathbb{R}\times\mathbb{R}^2,dp_0\ d\mathbf{p})$ according to

$$\begin{aligned}(V^\tau_{x,\mathbf{v},\eta,\mathbf{a}}f)(p_0,\mathbf{p})=&\exp\left\{i\left[\eta(p_0+Sx)+\frac{\tau}{2}\mathbf{a}\cdot\mathbf{v}+\mathbf{a}\cdot\mathbf{p}+\frac{F}{2\tau}\langle\mathbf{v},\mathbf{p}\rangle\right]\right\}\\&\times f(p_0+Sx+\mathbf{v}\cdot\mathbf{p}+\tfrac{1}{2}\tau\mathbf{v}^2,R(x)^{-1}(\mathbf{p}+\tau\mathbf{v})).\end{aligned} \tag{4.48}$$

(d) $\tau=0$, $S=0$.

In this case only the nontrivial orbit Z^{12} counts. A reference point is $[0,r\mathbf{e}_1;n_0,n_2]$ and we have

$$H^F_{[0,r\mathbf{e}_1;n_0,n_2]}=\{(2\pi n,\alpha\mathbf{e}_2;\zeta 1)\,|\,n\in\mathbf{Z},\alpha\in\mathbb{R},\zeta\in\mathbf{T}\}\simeq\mathbf{Z}\times\mathbb{R}\times\mathbf{T}. \tag{4.49}$$

The unitary irreducible representations are $\pi^{(s,t,n_1)}(s\in\mathbb{R}(\mathrm{mod}\,1),t\in\mathbb{R},n_1\in\mathbf{Z})$ acting in $\mathbf{C}$ according to

$$\pi^{(s,t,n_1)}((2\pi n,\alpha\mathbf{e}_2;\zeta 1)=e^{2\pi ins}\ e^{it\alpha}\zeta_1^{n_1}. \tag{4.50}$$

Let $\phi^{(s,t,n_1)}$ be an associated cocycle. Then the induced representation corresponds to the choice $n_0=n_1=n_2=-1$ and acts in $L^2(\mathbb{R}\times S^1,dp_0\otimes d\Omega)$ according to

$$(V'^{,r,s,t}_{x,\mathbf{v},\eta,\mathbf{a}}f)(p_0,\mathbf{p})=e^{i(\eta p_0+\mathbf{a}\cdot\mathbf{p})}\phi^{(s,t,-1)}((x,\mathbf{v};1),[p_0+\mathbf{v}\cdot\mathbf{p}])f(p_0+\mathbf{v}\cdot\mathbf{p},R(x)^{-1}\mathbf{p}). \tag{4.51}$$

Theorem 2: *Every projective unitary irreducible representation of* $\widetilde{\mathscr{G}}^{\uparrow}_{+}$ *with a nontrivial multiplier is unitary equivalent to a representation of the type* $V^{\tau,s},V^{\mathrm{CCR}},V^{r,\lambda},V^{r,s,t},V^{\tau}$, *or* $V^{\prime,r,s,t}$ *described by Eqs. (4.19), (4.26), (4.41), (4.44), (4.48), and (4.51), respectively. Two different*

representations from this list are not unitary equivalent. Only the representations (4.19) and (4.51) verify the condition (2.3) so only these representations correspond to Galilean invariant systems.

Remark 4: Consider the representations (4.19) and (4.51) from the point of view of localizability.[3] *The representation (4.19) is localizable. Indeed, by restricting the covering group of the Euclidean group SE(2) we obtain*

$$(V^{\tau,s}_{x,\mathbf{a}}f)(\mathbf{p})=e^{i(sx+\mathbf{a}\cdot\mathbf{p})}f(R(x)^{-1}\mathbf{p}). \tag{4.52}$$

Performing a Fourier transform one gets

$$(V^{\tau,s}_{x,\mathbf{a}}f)(\mathbf{X})=e^{isx}\ f(R(x)^{-1}(\mathbf{X}-\mathbf{a})). \tag{4.53}$$

If $P_\Delta=\chi_\Delta$ *then* $(V^{\tau,s},P)$ *is a system of imprimitivity based on* $\mathbb{R}^2$ *relative to the action*

$$(x,\mathbf{a})\cdot\mathbf{X}=R(x)\mathbf{X}+\mathbf{a} \tag{4.54}$$

so one has localizability.

The representations (4.51) are not localizable on $\mathbb{R}^2$ *(the argument is similar to the one in Ref. 3 and is based on the existence of the constraint* $\mathbf{p}^2=r^2$*).*

Remark 5: The representations (4.19) obtained in case (a) are the analogues of the representations obtained in 1+3 dimensions (see, Ref. 3, Chap. IX, Subsection 8). The infinitesimal generators of this representation are

$$(Hf)(\mathbf{p})=\frac{\mathbf{p}^2}{2\tau}\ f, \tag{4.55}$$

$$(\mathbf{P}f)(\mathbf{p})=\mathbf{p}f, \tag{4.56}$$

$$(Jf)(\mathbf{p})=i\left(p_1\frac{\partial f}{\partial p_2}-p_2\frac{\partial f}{\partial p_1}\right)+sf, \tag{4.57}$$

$$(\mathbf{K}f)(\mathbf{p})=-i\tau\frac{\partial f}{\partial\mathbf{p}}+\frac{F}{2\tau}A\mathbf{p}f. \tag{4.58}$$

So τ *and s must be interpreted as the mass and the spin of the system, respectively. The interpretation of F is not clear. Because F appears from a central extension of a translation group (see Eq. (4.22)), it is tempting to associate F with some kind of magnetic force. For another interpretation of the parameter F (based on the nonrelativistic limit) see Ref. 8.*

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A $\mathbb{Z}_3$-graded generalization of supermatrices

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We introduce $\mathbb{Z}_3$-graded objects which are the generalization of the more familiar $\mathbb{Z}_2$-graded objects that are used in supersymmetric theories and in many models of non-commutative geometry. First, we introduce the **$\mathbb{Z}_3$-graded Grassmann algebra**, and we use this object to construct the **$\mathbb{Z}_3$-matrices**, which are the generalizations of the **supermatrices**. Then, we generalize the concepts of **supertrace** and **superdeterminant**. © *1996 American Institute of Physics.* [S0022-2488(96)00901-9]

I. INTRODUCTION

$\mathbb{Z}_2$-graded algebras, which are the basic objects of supersymmetry, are well known since the works of Berezin, Kac, Leites, Wess and Zumino,[1–5] who introduced the concepts of supermatrices, supertrace and superdeterminant. These concepts will be generalized here.

Recently, there have been many attempts to generalize $\mathbb{Z}_2$-graded constructions to the $\mathbb{Z}_3$-graded case.[6–10] Many such attempts, though, were aimed at the description of exotic statistics. We think that our construction could describe some properties of the *quarks*, in particular the *ternary* aspects of their associations.

II. THE $\mathbb{Z}_3$-GRADED GRASSMANN ALGEBRA

The ordinary Grassmann algebra is generated by anticommuting entities:

$$\eta_i \eta_j = -\eta_j \eta_i .$$

This can be viewed in the following way. $\mathbb{Z}_2$ is the group of the permutations of two elements. It can be represented by the real numbers (-1) and 1:

$$\underset{+1}{\begin{pmatrix} A & B \\ A & B \end{pmatrix}} \quad \underset{-1}{\begin{pmatrix} A & B \\ B & A \end{pmatrix}}.$$

When an element of the permutation group is applied to the product of two generators, it is followed by the multiplication by the number representing this permutation.

Similar operations can be performed with $\mathbb{Z}_3$, which is faithfully represented by the complex numbers 1, j and j^2, where j is a cubic root of 1, $e^{2i\pi/3}$:

$$\underset{1}{\begin{pmatrix} A & B & C \\ A & B & C \end{pmatrix}} \quad \underset{j}{\begin{pmatrix} A & B & C \\ B & C & A \end{pmatrix}} \quad \underset{j^2}{\begin{pmatrix} A & B & C \\ C & A & B \end{pmatrix}}.$$

When one applies an element of the cyclic permutation group to the product of *three* generators, it is multiplied by the complex number representing this permutation:

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$$\theta_i\theta_k\theta_l = j\,\theta_k\theta_l\theta_i\,.$$

The generators defined in this way have the following properties: their cubes vanish, as also does a product of any four generators:[8]

$$\theta_i^3 = 0, \quad \theta_i\theta_k\theta_l\theta_m = 0.$$

Therefore the dimension of the algebra generated by N independent elements is

$$\underset{\theta' s}{N} + \underset{\theta\theta' s}{N^2} + \underset{\theta\theta\theta' s}{\frac{N^3-N}{3}}.$$

To restore the symmetry between grades 1 (the θ's) and 2 (the $\theta\theta$'s), we can add N grade 2 generators $\bar{\theta}_i$ that behave like the products of two θ's, that is

$$\bar{\theta}_i\bar{\theta}_k\bar{\theta}_l = j^2\bar{\theta}_k\bar{\theta}_l\bar{\theta}_i\,, \quad \theta_i\bar{\theta}_k = j\,\bar{\theta}_k\theta_i\,.$$

In the case of the ordinary Grassmann algebra, the products of an odd number of generators are automatically anticommutative, whereas the products of an even number of generators commute with all other elements. In the $\mathbb{Z}_3$-graded case, this is no longer true. For example,

$$\theta_i\theta_k\bar{\theta}_l = j\,\theta_i\bar{\theta}_l\theta_k = j^2\bar{\theta}_l\theta_i\theta_k\,;$$

but in the same time, $\theta_k\bar{\theta}_l$ and $\bar{\theta}_l\theta_i$, as grade 0 elements, should commute with all other elements, leading to the relations $\theta_i(\theta_k\bar{\theta}_l) = (\theta_k\bar{\theta}_l)\theta_i$ and $\theta_i\theta_k\bar{\theta}_l = j^2(\bar{\theta}_l\theta_i)\theta_k = j^2\theta_k(\bar{\theta}_l\theta_i)$, which are clearly contradictory.

This leads us to impose the following relations on all elements of a definite grade (the grade of the product of two elements being the sum of their grades, modulo 3). Let us denote by $a, b, \ldots$, the elements of grade 0, by $A, B, \ldots$, the elements of grade 1, by $\bar{A}, \bar{B}, \ldots$, the elements of grade 2 and by $\mathscr{X}$ an element of arbitrary grade. Then the rules

$$a.\mathscr{X} = .\mathscr{X}a, \quad A\bar{A} = j\bar{A}A,$$

define entirely the $\mathbb{Z}_3$-graded Grassmann algebra. We obtain the ternary rules $\theta_i\theta_k\theta_l = j\,\theta_k\theta_l\theta_i$ and $\bar{\theta}_i\bar{\theta}_k\bar{\theta}_l = j^2\bar{\theta}_k\bar{\theta}_l\bar{\theta}_i$ directly from the second rule by replacing A and $\bar{A}$ with products of one or two generators θ or $\bar{\theta}$.

With the unit element $\mathbb{I}$, the algebra contains the following elements:

Grade 0: $\mathbb{I}, \theta\bar{\theta}, \theta\theta\theta, \bar{\theta}\bar{\theta}\bar{\theta},$

Grade 1: $\theta, \bar{\theta}\bar{\theta},$

Grade 2: $\bar{\theta}, \theta\theta,$

and its dimension is

$$D=1+2N+3N^2+2\frac{N^3-N}{3}=\frac{3+4N+9N^2+2N^3}{3}.$$

One can note that the grade 0 elements recall formally the only observable combinations of *quark fields* in chromodynamics based on the $SU(3)$ symmetry, that is, the mesons which are the combinations $q\bar{q}$ of one quark and one antiquark, and the hadrons which are the combinations qqq or $\bar{q}\bar{q}\bar{q}$ of three quarks or three antiquarks.

From now on, we shall denote the grade of an object X by ∂X.

III. $\mathbb{Z}_3$-MATRICES

We define the $\mathbb{Z}_3$-matrices in analogy with the supermatrices, which form a $\mathbb{Z}_2$-graded matrix algebra and whose entries are elements of a Grassmann algebra.

First, we define a $\mathbb{Z}_3$-graded complex matrix algebra by dividing the algebra $\mathscr{A}$ of 3×3 block matrices into three parts: $\mathscr{A}=\mathscr{A}_0\oplus\mathscr{A}_1\oplus\mathscr{A}_2$. A matrix is an element of $\mathscr{A}_0$ (resp., $\mathscr{A}_1$, $\mathscr{A}_2$) and is of grade 0 (resp., 1, 2) if it has the form shown below:

$$\begin{pmatrix} A & 0 & 0\\ 0 & B & 0\\ 0 & 0 & C\end{pmatrix}, \text{ resp. } \begin{pmatrix} 0 & A & 0\\ 0 & 0 & B\\ C & 0 & 0\end{pmatrix}, \begin{pmatrix} 0 & 0 & A\\ B & 0 & 0\\ 0 & C & 0\end{pmatrix}.$$

This gives a $\mathbb{Z}_3$-graded structure to the algebra of matrices, in the sense that the grade of the product of two matrices is the sum of the grades of these matrices modulo 3.

We can then tensorize this graded algebra with our $\mathbb{Z}_3$-graded Grassmann algebra, the grade of a $\mathbb{Z}_3$-matrix being the sum *modulo 3* of the grade of the matrix and of the grade of the Grassmann element. So a $\mathbb{Z}_3$-matrix is of grade 0 (resp., 1, 2) if its blocks contain only Grassmann elements with the respective grades:

$$\underset{\text{grade 0}}{\begin{pmatrix} 0 & 2 & 1\\ 1 & 0 & 2\\ 2 & 1 & 0\end{pmatrix}}, \underset{\text{grade 1}}{\begin{pmatrix} 1 & 0 & 2\\ 2 & 1 & 0\\ 0 & 2 & 1\end{pmatrix}}, \underset{\text{grade 2}}{\begin{pmatrix} 2 & 1 & 0\\ 0 & 2 & 1\\ 1 & 0 & 2\end{pmatrix}}.$$

It is easy to verify that the grade of the product of two $\mathbb{Z}_3$-matrices is the sum of their grades modulo 3.

The algebra of $\mathbb{Z}_3$-matrices contains a neutral element, $\mathscr{T}$, the $\mathbb{Z}_3$-matrix whose only non-vanishing elements are the unit of the Grassmann algebra occupying the main diagonal. The existence of this element enables us to define the invertibility of a $\mathbb{Z}_3$-matrix.

Theorem 1 (a): *A block of a $\mathbb{Z}_3$-matrix is invertible if and only if the block matrix formed with the coefficients of $\mathbb{I}$ in the development of the elements of the block over the grade 0 elements of the Grassmann algebra* ($\mathbb{I}$, $\theta\theta$, $\theta\theta\theta$, $\bar{\theta}\bar{\theta}\bar{\theta}$) *is invertible.*

(b) *A $\mathbb{Z}_3$-matrix is invertible if and only if its grade 0 blocks are invertible. The inverse of a grade 1 (resp., 2, 0) $\mathbb{Z}_3$-matrix is a grade 2 (resp., 1, 0) $\mathbb{Z}_3$-matrix.*

(c) *The product of two invertible $\mathbb{Z}_3$-matrices is an invertible $\mathbb{Z}_3$-matrix.*

Proof:

(a)–Let us decompose a $\mathbb{Z}_3$-matrix M into its complex component matrices along the elements of the Grassmann algebra: $M=M_\phi\mathbb{I}+M_\mu\theta_\mu+\bar{M}_\mu\bar{\theta}_\mu+M_{\mu\nu}\theta_\mu\theta_\nu+\bar{M}_{\mu\nu}\theta_\mu\bar{\theta}_\nu+\tilde{M}_{\mu\nu}\theta_\mu\bar{\theta}_\nu + M_{\mu\nu\eta}\theta_\mu\theta_\nu\theta_\eta+\bar{M}_{\mu\nu\eta}\theta_\mu\theta_\nu\bar{\theta}_\eta$. We also consider another $\mathbb{Z}_3$-matrix N that we decompose in the same way. Then it is easy to see that the component of MN along $\mathbb{I}$ is $M_\phi N_\phi$ (no product of two generators different from $\mathbb{I}$ can give something proportional to $\mathbb{I}$), so that for M to be invertible, its component M_ϕ must be invertible. Conversely, if M_ϕ is invertible, let us put

$N_\phi=(M_\phi)^{-1}$. Then the product MN differs from $\mathscr{I}$ only in terms of degree 2 and higher. However, we can choose $N_\mu=-(M_\phi)^{-1}M_\mu(M_\phi)^{-1}$ and $\bar{N}_\mu=-(M_\phi)^{-1}\bar{M}_\mu(M_\phi)^{-1}$. This way, MN differs from $\mathscr{I}$ only in terms of degree 3 and higher. Choosing the higher-level components of N in the same way, it is easy to expel these terms to higher degrees, until we have actually constructed the inverse of M, because of the finite number of terms in the development and of their cubic nilpotence.

(b) For this part of the theorem, we can use the proof of part (a) by noting that the component M_ϕ of a matrix M has non-zero coefficients only in positions corresponding to grade 0 blocks. $\mathscr{I}$ being of grade 0, it is obvious that the sum of the grades of a $\mathbb{Z}_3$-matrix and of its inverse should be 0 modulo 3.

(c) The component along $\mathbb{I}$ of the product of two invertible matrices is the product of their components along $\mathbb{I}$, which are invertible matrices by virtue of (b) and (a). These components being ordinary matrices, their product is an invertible matrix. We use (b) once more to conclude.■

The left (resp., right) product of a supermatrix by an element λ of the ordinary Grassmann algebra is defined as its left (resp., right) multiplication by the supermatrix

$$\begin{pmatrix} \lambda & \\ & (-1)^{\partial\lambda}\lambda \end{pmatrix}.$$

Generalizing this idea, we define the left (resp., right) product of a $\mathbb{Z}_3$-matrix by an element λ of the Grassmann algebra as its left (resp., right) multiplication by the following diagonal $\mathbb{Z}_3$-matrix:

$$\begin{pmatrix} \lambda & & \\ & j^{2\partial\lambda}\lambda & \\ & & j^{\partial\lambda}\lambda \end{pmatrix}.$$

Note that in general, $\lambda M \neq M\lambda$, but we have $\lambda(MN)=(\lambda M)N$, $(M\lambda)N=M(\lambda N)$, $M(N\lambda)=(MN)\lambda$ and $\lambda(M\mu)=(\lambda M)\mu$ which give our algebra the structure of a bimodule with respect to the Grassmann algebra.

Definition 2: Let us define a $\mathbb{Z}_3$-matrix M with the following block structure:

$$M=\begin{pmatrix} A & B & C \\ D & E & F \\ G & H & I \end{pmatrix}.$$

Its $\mathbb{Z}_3$-trace *is defined by:* $\mathrm{tr}_{\mathbb{Z}_3}(M)=\mathrm{tr}(A)+j^{2(1-\partial M)}\mathrm{tr}(E)+j^{(1-\partial M)}\mathrm{tr}(I)$; that is:

- If M is of grade 0, then $\mathrm{tr}_{\mathbb{Z}_3}(M)=\mathrm{tr}(A)+j^2.\mathrm{tr}(E)+j.\mathrm{tr}(I)$.
- If M is of grade 1, then $\mathrm{tr}_{\mathbb{Z}_3}(M)=\mathrm{tr}(A)+\mathrm{tr}(E)+\mathrm{tr}(I)$.
- If M is of grade 2, then $\mathrm{tr}_{\mathbb{Z}_3}(M)=\mathrm{tr}(A)+j\mathrm{tr}(E)+j^2\mathrm{tr}(I)$.

The supertrace of a supermatrix

$$M=\begin{pmatrix} A & B \\ C & D \end{pmatrix}$$

was defined by $\mathrm{str}\ M=\mathrm{tr}(A)+(-1)^{1-\partial M}\mathrm{tr}(D)$.

The following theorem can be easily proved:

Theorem 3: *(a) If M and N are of the same grade,*

$$\mathrm{tr}_{\mathbb{Z}_3}(M+N)=\mathrm{tr}_{\mathbb{Z}_3}(M)+\mathrm{tr}_{\mathbb{Z}_3}(N).$$

(b) $\mathrm{tr}_{\mathbb{Z}_3}(\lambda M)=\lambda\mathrm{tr}_{\mathbb{Z}_3}(M)$ *and* $\mathrm{tr}_{\mathbb{Z}_3}(M\lambda)=\mathrm{tr}_{\mathbb{Z}_3}(M)\lambda$.

(*c*) • *If M and N are of grade 0 then* $\mathrm{tr}_{\mathbb{Z}_3}(MN)=\mathrm{tr}_{\mathbb{Z}_3}(NM)$.

• *If M is of grade 1 and N of grade 2, then* $\mathrm{tr}_{\mathbb{Z}_3}(MN)=j\mathrm{tr}_{\mathbb{Z}_3}(NM)$.

Corollary 4: • *If M,N and P are of grade 1 then* $\mathrm{tr}_{\mathbb{Z}_3}(MNP)=j\ \mathrm{tr}_{\mathbb{Z}_3}(NPM)$.

• *If M,N and P are of grade 2 then* $\mathrm{tr}_{\mathbb{Z}_3}(MNP)=j^2\mathrm{tr}_{\mathbb{Z}_3}(NPM)$.

The proofs are straightforward, and the only nontrivial observation concerns the fact that $\mathrm{tr}(MN)=\mathrm{tr}(NM)$ is not always true if the M and N's coefficients are not numbers.

Finally, we can define the generalization of the superdeterminant this way.

Definition 5, $\mathbb{Z}_3$*-determinant: If M is a* grade 0 *invertible* $\mathbb{Z}_3$*-matrix, then its* $\mathbb{Z}_3$-determinant *is*

$$\begin{aligned}\det_{\mathbb{Z}_3}(M)=&\det(A-CI^{-1}G-(B-CI^{-1}H)(E-FI^{-1}H)^{-1}(D-FI^{-1}G))\\&\times(\det(E-FI^{-1}H))^{j^2}(\det I)^j.\end{aligned}$$

Theorem 6: *If M and N are two invertible grade 0* $\mathbb{Z}_3$*-matrices,*

$$\det_{\mathbb{Z}_3}(MN)=(\det_{\mathbb{Z}_3}M)(\det_{\mathbb{Z}_3}N).$$

Proof: Any grade 0 invertible $\mathbb{Z}_3$-matrix can be decomposed into the product of three $\mathbb{Z}_3$-matrices: $M=M_1M_0M_2$ with

$$M_1=\begin{pmatrix}1 & (B-CI^{-1}H)(E-FI^{-1}H)^{-1} & CI^{-1}\\ 0 & 1 & FI^{-1}\\ 0 & 0 & 1\end{pmatrix},$$

$$M_0=\begin{pmatrix}A-CI^{-1}G-(B-CI^{-1}H)(E-FI^{-1}H)^{-1}(D-FI^{-1}G) & 0 & 0\\ 0 & E-FI^{-1}H & 0\\ 0 & 0 & I\end{pmatrix},$$

$$M_2=\begin{pmatrix}1 & 0 & 0\\ (D-FI^{-1}G)(E-FI^{-1}H)^{-1} & 1 & 0\\ I^{-1}G & I^{-1}H & 1\end{pmatrix}. \tag{1}$$

It is very easy to show that the theorem is true for any M if N is block-diagonal or inferior-block-triangular with the identity in the diagonal blocks. It is also easy to generalize to an arbitrary N in the case where M is block-diagonal or superior-block-triangular with the identity in the diagonal blocks. Therefore, we have

$$\begin{aligned}\det_{\mathbb{Z}_3}(MN)&=\det_{\mathbb{Z}_3}(M_1)\det_{\mathbb{Z}_3}(M_0)\det_{\mathbb{Z}_3}(M_2N_1)\det_{\mathbb{Z}_3}(N_0)\det_{\mathbb{Z}_3}(N_2)\\&=\det_{\mathbb{Z}_3}(M)\det_{\mathbb{Z}_3}(M_2N_1)\det_{\mathbb{Z}_3}(N),\end{aligned}$$

and the theorem remains to be proved only for M of the form

$$\begin{pmatrix} 1 & 0 & 0 \\ A & 1 & 0 \\ B & C & 1 \end{pmatrix}$$

and N of the form

$$\begin{pmatrix} 1 & D & E \\ 0 & 1 & F \\ 0 & 0 & 1 \end{pmatrix}.$$

One can note that

$$\begin{pmatrix} 1 & 0 & B \\ 0 & 1 & C \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & C' \\ 0 & 0 & 1 \end{pmatrix}=\begin{pmatrix} 1 & 0 & B \\ 0 & 1 & C+C' \\ 0 & 0 & 1 \end{pmatrix},$$

$$\begin{pmatrix} 1 & A & B \\ 0 & 1 & C \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} 1 & A' & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}=\begin{pmatrix} 1 & A+A' & B \\ 0 & 1 & C \\ 0 & 0 & 1 \end{pmatrix},$$

and

$$\begin{pmatrix} 1 & A & B \\ 0 & 1 & C \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 & B' \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}=\begin{pmatrix} 1 & A & B+B' \\ 0 & 1 & C \\ 0 & 0 & 1 \end{pmatrix},$$

so that we can construct the matrix N_1, element by element, starting from the matrix that contains only its diagonal blocks, using left multiplication by a series of matrices that contain only one non-zero element out of the diagonal blocks.

We show the theorem for M of the form of M_2 and N containing only one element out of the diagonal blocks, using the fact that if $\partial X \neq 0$, then $(1+X)^{\alpha}=1+\alpha X+[\alpha(\alpha-1)/2]X^2$. If $N_1=N_1^0N_1^1$ we can decompose $M_2N_1^0$ in the form 1. Then,

$$\begin{aligned}\det_{\mathbb{Z}_3}(M_2N_1)&=\det_{\mathbb{Z}_3}((M_2N_1^0)_1(M_2N_1^0)_0(M_2N_1^0)_2.N_1^1)\\&=\det_{\mathbb{Z}_3}((M_2N_1^0)_0)\det_{\mathbb{Z}_3}((M_2N_1^0)_2.N_1^1)=\det_{\mathbb{Z}_3}((M_2N_1^0)_0),\end{aligned}$$

if N_1^1 contains only one element out of its diagonal blocks. But $\det_{\mathbb{Z}_3}((M_2N_1^0)_0)=\det_{\mathbb{Z}_3}(M_2N_1^0)$. We can perform the same operation, until only the product of M_2 and the matrix formed with the diagonal blocks of N_1 (which are the identity) remains. Thus $\det_{\mathbb{Z}_3}(M_2N_1)=1$. ■

Theorem 7: *If M is a grade 0 invertible $\mathbb{Z}_3$-matrix, its $\mathbb{Z}_3$-determinant can also be expressed in the following five alternative ways:*

$$\begin{aligned}\det_{\mathbb{Z}_3}(M)&=\det(A-CI^{-1}G)\\&\quad\times(\det(E-FI^{-1}H-(D-FI^{-1}G)(A-CI^{-1}G)^{-1}(B-CI^{-1}H)))^{j^2}(\det I)^j,\end{aligned}$$

$$\det_{\mathbb{Z}_3}(M) = (\det A).(\det(E - DA^{-1}B - (F - DA^{-1}C)(I - GA^{-1}C)^{-1}(H - GA^{-1}B)))^{j^2}(\det(I - GA^{-1}C))^{j},$$

$$\det_{\mathbb{Z}_3}(M) = (\det A)(\det(E - DA^{-1}B))^{j^2}(\det(I - GA^{-1}C - (H - GA^{-1}B)(E - DA^{-1}B)^{-1}(F - DA^{-1}C)))^{j},$$

$$\det_{\mathbb{Z}_3}(M) = (\det(A - BE^{-1}D - (C - BE^{-1}F)(I - HE^{-1}F)^{-1}(G - HE^{-1}D)))(\det E)^{j^2}(\det(I - HE^{-1}F))^{j},$$

$$\det_{\mathbb{Z}_3}(M) = (\det(A - BE^{-1}D)(\det E))^{j^2}(\det(I - HE^{-1}F - (G - HE^{-1}D)(A - BE^{-1}D)^{-1}(C - BE^{-1}F)))^{j}.$$

Proof: We use the following decompositions of M:

$$\begin{pmatrix} A - CI^{-1}G & 0 & C \\ D - FI^{-1}G & E - FI^{-1}H - (D - FI^{-1}G)(A - CI^{-1}G)^{-1}(B - CI^{-1}H) & F \\ 0 & 0 & I \end{pmatrix} \begin{pmatrix} 1 & (A - CI^{-1}G)^{-1}(B - CI^{-1}H) & 0 \\ 0 & 1 & 0 \\ I^{-1}G & I^{-1}H & 1 \end{pmatrix},$$

$$\begin{pmatrix} 1 & 0 & 0 \\ DA^{-1} & 1 & (F - DA^{-1}C)(I - GA^{-1}C)^{-1} \\ GA^{-1} & 0 & 1 \end{pmatrix} \begin{pmatrix} A & B & C \\ 0 & E - DA^{-1}B - (F - DA^{-1}C)(I - GA^{-1}C)^{-1}(H - GA^{-1}B) & 0 \\ 0 & H - GA^{-1}B & I - GA^{-1}C \end{pmatrix},$$

$$\begin{pmatrix} 1 & 0 & 0 \\ DA^{-1} & 1 & 0 \\ GA^{-1} & (H - GA^{-1}B)(E - DA^{-1}B)^{-1} & 1 \end{pmatrix} \begin{pmatrix} A & B & C \\ 0 & E - DA^{-1}B & F - DA^{-1}C \\ 0 & 0 & I - GA^{-1}C - (H - GA^{-1}B)(E - DA^{-1}B)^{-1}(F - DA^{-1}C) \end{pmatrix},$$

$$\begin{pmatrix} 1 & BE^{-1} & (C-BE^{-1}F)(I-HE^{-1}F)^{-1} \\ 0 & 1 & 0 \\ 0 & HE^{-1} & 1 \end{pmatrix} \begin{pmatrix} A-BE^{-1}D-(C-BE^{-1}F)(I-HE^{-1}F)^{-1}(G-HE^{-1}D) & 0 & 0 \\ D & E & F \\ 0 & 0 & I-HE^{-1}F \end{pmatrix},$$

$$\begin{pmatrix} A-BE^{-1}D & B & 0 \\ 0 & E & 0 \\ G-HE^{-1}D & H & I-HE^{-1}F-(G-HE^{-1}D)(A-BE^{-1}D)^{-1}(C-BE^{-1}F) \end{pmatrix} \begin{pmatrix} 1 & 0 & (A-BE^{-1}D)^{-1}(C-BE^{-1}F) \\ E^{-1}D & 1 & E^{-1}F \\ 0 & 0 & 1 \end{pmatrix},$$

and make use of the Theorem 6. ■

In the case of the superdeterminant, the following two expressions are equivalent:

$$\mathrm{sdet}\begin{pmatrix} A & B \\ C & D \end{pmatrix} = \det(A-BD^{-1}C).(\det D)^{-1} = \det A.(\det(D-CA^{-1}B))^{-1}.$$

This restores the symmetry between the two diagonal elements on the one hand, and between the two off diagonal elements on the other hand. Here we have six expressions, restoring the S_3 symmetry between the three grade 0, grade 1 and grade 2 elements of the $\mathbb{Z}_3$-matrix which is broken in any expression separately chosen.

Theorem 8: *If M is a grade 0 invertible 3×3 $\mathbb{Z}_3$-matrix, then*

$$\det_{\mathbb{Z}_3}(\exp M) = \exp(\mathrm{tr}_{\mathbb{Z}_3} M).$$

Proof: Let M be the matrix:

$$M = \begin{pmatrix} a & \bar{A} & A \\ B & b & \bar{B} \\ \bar{C} & C & c \end{pmatrix},$$

where a,b,c are three grade 0 invertible elements of the Grassmann algebra (they must be invertible in order for M to be invertible; see Theorem 1), A,B,C are three grade 1 elements of the Grassmann algebra, and $\bar{A},\bar{B},\bar{C}$ are three grade 2 elements of the Grassmann algebra. Assuming that a,b,c are distinct, straightforward calculus give the following expression for the exponential of the matrix M:

$$\exp M=\begin{pmatrix} e^a+f(a,b)\bar{A}B+f(a,c)A\bar{C} & h(a,b)\bar{A}+l(a,b,c)AC & h(a,c)A+l(a,b,c)\bar{A}\bar{B} \\ \quad +g(a,b,c)(\bar{A}\bar{B}\bar{C}+j.CBA) & e^b+j^2f(b,c)C\bar{B}+j.f(b,a)\bar{A}B & h(b,c)\bar{B}+l(a,b,c)BA \\ h(a,b)B+l(a,b,c)\bar{B}\bar{C} & \quad +j.g(b,c,a)(\bar{A}\bar{B}\bar{C}+j.CBA) & e^c+j^2.f(c,a)A\bar{C}+f(c,b)C\bar{B} \\ h(a,c)\bar{C}+l(a,b,c)CB & h(b,c)C+l(a,b,c)\bar{C}\bar{A} & \quad +j^2.g(c,a,b)(\bar{A}\bar{B}\bar{C}+j.CBA) \end{pmatrix},$$

where

$$f(x,y)=\frac{(x-y-1)e^x+e^y}{(x-y)^2},$$

$$g(x,y,z)=\left[\frac{1}{(x-y)(x-z)}-\frac{1}{(x-y)(x-z)^2}-\frac{1}{(x-z)(x-y)^2}\right]e^x+\frac{e^y}{(y-z)(y-x)^2}+\frac{e^z}{(z-y)(z-x)^2},$$

$$h(x,y)=\frac{e^x-e^y}{x-y},$$

$$l(x,y,z)=\frac{e^x}{(x-y)(x-z)}+\frac{e^y}{(y-z)(y-x)}+\frac{e^z}{(z-x)(z-y)}.$$

From this we compute

$$\begin{aligned}\det{}_{\mathbb{Z}_3}(\exp M)=e^{a+j^2b+jc}[&\mathbb{I}+(e^{-a}f(a,b)+e^{-b}f(b,a)-e^{-(a+b)}(h(a,b))^2)\bar{A}B+(e^{-a}f(a,c)+e^{-c}f(c,a)-e^{-(a+c)}(h(a,c))^2)A\bar{C}+j(e^{-c}f(c,b)\\&+e^{-b}f(b,c)-e^{-(b+c)}(h(b,c))^2)C\bar{B}+[e^{-a}g(a,b,c)+e^{-b}g(b,c,a)+e^{-c}g(c,a,b)+e^{-(a+b+c)}h(a,b)h(b,c)h(c,a)\\&-(e^{-(a+b)}h(a,b)+e^{-(a+c)}h(a,c)+e^{-(b+c)}h(b,c))l(a,b,c)](\bar{A}\bar{B}\bar{C}+j.CBA)],\end{aligned}$$

and it is then easy to verify that all terms inside the brackets vanish, except for $\mathbb{I}$. The cases where $a=b$, $b=c$ or $c=a$ are just limits of the previous case. ■

These constructions will be used in a forthcoming paper concerning the construction of a gauge theory based on a $\mathbb{Z}_3$-graded non-commutative geometry model similar to the one used by Coquereaux *et al.*,[11] using instead Kerner's differential whose cube is zero, whereas its square is not.[8]

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A q-superdimension formula for irreps of type I quantum superalgebras

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We derive a closed formula for the q-superdimensions of a wide class of irreps, including all unitary irreps, of the type I quantum superalgebras. © *1996 American Institute of Physics.* [S0022-2488(95)03512-7]

I. INTRODUCTION

It is well known that quantum algebras[1] play an extensive role in the study of integrable systems derived through the quantum inverse scattering method. Not only do these algebras appear as underlying symmetries of these systems, but it is their quasitriangular structure which in essence allows the algebraic Bethe ansatz to be applied to diagonalize the Hamiltonians of these models. Likewise, the $\mathbb{Z}_2$-graded analogues of quantum algebras, known as quantum superalgebras,[2–4] play a similar role in integrable systems with supersymmetry. Recently, these models have attracted considerable attention since within this class of models are a number which describe correlated electron systems. These include the supersymmetric $t-j$ model,[5] the supersymmetric extended Hubbard model,[6] and the Hubbard model with correlated hopping and electron pair hopping.[7]

In the investigation of such models it is desirable to have a well-developed representation theory of the underlying symmetry algebras. The representation theory of quantum superalgebras is more complicated than that of quantum algebras. Here we will restrict our attention to the type I quantum superalgebras consisting of $U_q(\mathrm{gl}(m|n))$ and $U_q(\mathrm{osp}(2|2n))$ where several developments have been made. A description of finite-dimensional irreducible representations (irreps) is understood in terms of the induced module construction[8] generalizing that of Kac,[9] whereby the irreps fall into two distinct classes, typical and atypical. This construction also provides a means to naturally induce bilinear forms. Symmetry relations satisfied by Clebsch-Gordan coefficients defined with respect to these forms have been obtained in Ref. 10 and these results have been used to determine the eigenvalues of families of Casimir invariants in any irrep (see also Ref. 11).

The most important aspect of the type I quantum superalgebras is that they are the only ones which admit finite-dimensional unitary irreps. These are the representations which are necessary to use in describing physical models where unitarity is a requirement. For example, the correlated electron models[5–7] mentioned above are all based on unitary irreps. A classification of the unitary irreps is known[12,13] which was achieved through the use of the induced bilinear forms.

In this article, we will be concerned with developing another aspect of the representation theory of the type I quantum superalgebras; viz. the determination of the q-superdimensions of irreps which we will achieve using the results of Ref. 10. Previously, a general formula for q-superdimensions has been lacking (with the exception of the typical irreps which all have zero q-superdimension) since all the classical techniques used for non-graded algebras (e.g., see Ref. 14) fail to extend to the superalgebra case. Our results apply to a large number of irreps, including all unitary irreps (which include all covariant and contravariant tensor irreps) as we will show, and consequently will have applications to systems with physical significance. The surprising aspect of our formula is that it shows that the q-superdimension is nonzero only when the irrep has maximal atypicality. Using the results of Refs. 12 and 13 enables us to classify all the unitary irreps which have this property.

The q-superdimension formula we derive is new even in the classical ($q\to 1$) limit and agrees

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with some particular studies using other methods such as super Young diagrams.[15] The formula is presented as a natural generalization of the Weyl dimension formula for irreps of Lie algebras. These results have an important role in the computation of link invariants as discussed in Ref. 16.

II. PRELIMINARIES

Let g denote a basic classical Lie superalgebra of rank $l+1$ with the usual generators $\{e_i,f_i,h_i\}_{i=0}^{l}$. Let $\{\alpha_i\}_{i=0}^{l}$ be the distinguished set of simple roots of g in the sense of Kac[9] and let $(,)$ be a fixed invariant bilinear form on H^*, the dual of the Cartan subalgebra H of g. We also let $\Phi^+=\Phi_0^+\cup\Phi_1^+$ denote the full set of roots with Φ_0^+ (resp. Φ_1^+) the subset of even (resp. odd) roots. Throughout, we adopt the convention that α_0 denotes the unique odd simple root. Associated with g one can define the quantum superalgebra $U_q(g)$ (q is assumed not a root of unity) which has the structure of a $\mathbb{Z}_2$-graded quasi-triangular Hopf algebra.[3] We will not give the full defining relations of $U_q(g)$ here and refer to Ref. 4 for details. We note, however, that $U_q(g)$ has a co-product structure given by

$$\Delta(q^{\pm(1/2)h_i})=q^{\pm(1/2)h_i}\otimes q^{\pm(1/2)h_i},\quad \Delta(x)=x\otimes q^{-(1/2)h_i}+q^{(1/2)h_i}\otimes x,\quad x=e_i,f_i,$$

which is extended to an algebra homomorphism to all of $U_q(g)$ in the usual way. It is important to point out that the multiplication rule for the tensor product is defined for homogeneous elements $a,b,c,d\in U_q(g)$ by

$$(a\otimes b)(c\otimes d)=(-1)^{[b][c]}(ac\otimes bd) \tag{1}$$

and extended linearly to all of $U_q(g)\otimes U_q(g)$. Here $[a]\in\mathbb{Z}_2$ denotes the degree of the homogeneous element $a\in U_q(g)$, which is defined for the elementary generators by

$$[h_i]=0,\quad [e_i]=[f_i]\equiv[i]=\delta_{i0},\quad \forall 0\leqslant i\leqslant l,$$

and extended to all homogeneous elements of $U_q(g)$ through

$$[ab]=[a]+[b](\mathrm{mod}\ 2),\quad \forall a,b\in U_q(g).$$

The twist map $T:U_q(g)\otimes U_q(g)\to U_q(g)\otimes U_q(g)$ is defined by

$$T(a\otimes b)=(-1)^{[a][b]}b\otimes a \tag{2}$$

for all homogeneous $a,b\in U_q(g)$: we set $\overline{\Delta}=T.\Delta$. Then there exists a canonical element $R\in U_q(g)\otimes U_q(g)$ called the universal R-matrix which is even and invertible and satisfies the following relations:[3]

$$R\Delta(a)=\overline{\Delta}(a)R,\quad \forall a\in U_q(g), \tag{3}$$

$$(\Delta\otimes I)R=R_{13}R_{23},\quad (I\otimes\Delta)R=R_{13}R_{12}, \tag{4}$$

where we have adopted the conventional notation. From Eqs. (3) and (4) it follows that the universal R-matrix satisfies the graded Yang–Baxter equation

$$R_{12}R_{13}R_{23}=R_{23}R_{13}R_{12}. \tag{5}$$

We emphasize that multiplication of the tensor products is to obey Eq. (1).

Let $\rho\in H^*$ denote the graded half-sum of positive roots of g and let h_ρ denote the unique element of H defined by $\alpha_i(h_\rho)=(\rho,\alpha_i)$, $\forall\alpha_i\in H^*$. We recall from Ref. 17 the following result.

Theorem 1: Let π be a fixed, but arbitrary, finite-dimensional representation of $U_q(g)$ with representation space V and set

$$\Delta_\pi = (\pi \otimes I)\Delta.$$

If $w \in U_q(g) \otimes \text{End } V$ satisfies

$$\Delta_\pi(a)w = w\Delta_\pi(a), \quad \forall a \in U_q(g), \tag{6}$$

then

$$s\tau_q(w) = (\text{str} \otimes I)(\pi(q^{2h_\rho}) \otimes I)w$$

belongs to the center Z of $U_q(g)$, where str denotes the supertrace. □

Theorem 1 enables a family of Casimir invariants to be constructed for $U_q(g)$ utilizing the universal R-matrix. Defining $R^T = TR$, it is clear from (3) that

$$R^T R\Delta(a) = \Delta(a)R^T R, \quad \forall a \in U_q(g).$$

Setting

$$A = (q - q^{-1})^{-1}(\pi \otimes I)(I \otimes I - R^T R), \tag{7}$$

then $A^l, l \in \mathbb{Z}^+$, satisfies (6). We thus obtain the family of Casimir invariants

$$C_l = s\tau_q(A^l).$$

The preceding discussion applies for any quantum superalgebra, not only those of type I. Let π_μ denote a $U_q(g)$ irrep with highest weight $\mu \in D^+$ where $D^+ \subset H^*$ is the set of dominant weights. For type I quantum superalgebras, $\mu \in D^+$ if and only if[8,9]

$$\langle \mu, \alpha_i \rangle = \frac{2(\mu, \alpha_i)}{(\alpha_i, \alpha_i)} \in \mathbb{Z}^+, \quad 1 \leqslant i \leqslant l,$$

while (μ, α_0) can take arbitrary complex values. When acting in π_μ the invariants C_l act as scalar multiples of the identity operator (Schur's lemma), which we denote by $\chi_\mu(C_l)$. In Ref. 10 a general formula for these eigenvalues is presented. We say that π_μ admits an *infinitesimal character* χ_μ which determines an algebra homomorphism

$$\chi_\mu : Z \to \mathbb{C}, \quad z \to \chi_\mu(z).$$

Recall that for type I quantum superalgebras we say that $\mu \in H^*$ is *typical* if[8,9]

$$(\mu + \rho, \alpha) \neq 0, \quad \forall \alpha \in \Phi_1^+,$$

and *atypical* otherwise. It is known[9] that for typical $\mu \in D^+$, the irrep π_μ is uniquely characterized by the infinitesimal character χ_μ. This is not the case for atypical irreps.

Finally, in view of Theorem 1, it is natural to define the q-superdimension of an irrep π_μ by

$$sd_q[\mu] = \text{str } \pi_\mu(q^{2h_\rho}),$$

which reduces to the usual superdimension when $q \to 1$. Below we will present a method of determining this quantity for a large class of irreps.

III. A q-SUPERDIMENSION FORMULA

Throughout, we let $V(\mu)$ denote the $U_q(g)$ module which affords the representation π_μ. Let $U_q(g_0)\subset U_q(g)$ be the (nongraded) quantum algebra generated by $\{e_i,f_i,h_i\}_{i=1}^l$. Each $U_q(g)$ module $V(\mu)$ reduces completely into $U_q(g_0)$ modules; i.e.,

$$V(\mu)=\bigoplus_\nu m_\nu V_0(\nu), \tag{8}$$

where m_ν denotes the multiplicity of $V_0(\nu)$. Each of the weights ν has a degree $[\nu]\in\mathbb{Z}_2$. We adopt the convention that $[\mu]=0$. Let $\Pi_+(\mu)$ denote the $U_q(g_0)$ highest weights occurring in the decomposition (8). For later use we define the following.

Definition 1. We say that $\mu\in D^+$ is *quasi-typical* if

$$\chi_\nu\neq\chi_\mu, \quad \forall\,\nu\neq\mu, \quad \nu\in\Pi_+(\mu);$$

i.e., χ_μ occurs once in the set $\{\chi_\nu|\nu\in\Pi_+(\mu)\}$.

Note that the class of quasi-typical weights includes the typical weights in D^+.

Let $\delta\in H^*$ be orthogonal to all even elements of H^* and satisfy $(\delta,\alpha_0)=1$. Clearly $(\delta,\alpha)=1$, $\forall\alpha\in\Phi_1^+$. Choosing $\beta\in\mathbb{C}$, $|\beta|\ll 1$, such that $\beta\delta,\nu+\beta\delta$ are all typical, then (8) implies the $U_q(g)$ tensor product decomposition[10]

$$V(\mu)\otimes V(\beta\delta)=\bigoplus_\nu m_\nu V(\nu+\beta\delta). \tag{9}$$

Let $P[\nu+\beta\delta]$ denote orthogonal projections onto the isotypic components $\overline{V(\nu+\beta\delta)}\equiv m_\nu V(\nu+\beta\delta)$. Since the weights $\nu+\beta\delta$ are all typical, we have, as noted previously,

$$\chi_{\nu+\beta\delta}\neq\chi_{\mu+\beta\delta}, \quad \forall\,\nu\neq\mu, \quad \nu\in\Pi_+(\mu).$$

This implies that there exists $z\in Z$ such that the central projection

$$P[\mu+\beta\delta]=\prod_{\nu\neq\mu}\left(\frac{\Delta(z)-\chi_{\nu+\beta\delta}(z)}{\chi_{\mu+\beta\delta}(z)-\chi_{\nu+\beta\delta}(z)}\right) \tag{10}$$

is well defined. Using Theorem 1 we may construct the Casimir invariant

$$\gamma_\beta=s\tau_q(P[\mu+\beta\delta]).$$

From Ref. 10 we have the following result.

Proposition 1: For any $\overline{V(\nu)}\subset V(\mu)\otimes V(\Lambda)$ such that ν and Λ are both typical and dominant, then

$$\chi_\Lambda(s\tau_q(P[\nu]))=(-1)^{[\nu]}m_\nu\prod_{\alpha\in\Phi_0^+}\frac{[(\nu+\rho,\alpha)]_q}{[(\Lambda+\rho,\alpha)]_q}\prod_{\alpha\in\Phi_1^+}\frac{[(\Lambda+\rho,\alpha)]_q}{[(\nu+\rho,\alpha)]_q},$$

where

$$[x]_q=\frac{q^x-q^{-x}}{q-q^{-1}}.$$

□

Applying Proposition 1 to the invariant γ_β we find

$$\chi_{\beta\delta}(\gamma_\beta)=\prod_{\alpha\in\Phi_0^+}\frac{[(\mu+\beta\delta+\rho,\alpha)]_q}{[(\beta\delta+\rho,\alpha)]_q}\prod_{\alpha\in\Phi_1^+}\frac{[(\beta\delta+\rho,\alpha)]_q}{[(\mu+\beta\delta+\rho,\alpha)]_q}. \tag{11}$$

Taking the limit $\beta\to 0$, Eq. (9) becomes

$$V(\mu)\otimes K(0)=\oplus_\nu m_\nu K(\nu),$$

where $K(\nu)$ denotes the Kac module[8,9] of highest weight ν. Note that $K(\nu)=V(\nu)$ if ν is typical. In the case of atypical ν, $K(\nu)$ is not irreducible but still admits the infinitesimal character χ_ν. Provided μ is quasi-typical, the central projection

$$P[\mu]=\lim_{\beta\to 0} P[\mu+\beta]$$

is well defined. Observe that $P[\mu]$ acts as the identity operator on $V(\mu)\otimes V(0)$ so

$$\chi_0(\gamma_\beta)|_{\beta=0}=sd_q[\mu].$$

On the other hand, $\chi_0(\gamma_\beta)|_{\beta=0}$ is given by (11) in the limit $\beta\to 0$ since $K(0)$ admits the infinitesimal character χ_0. Define

$$\Phi_1^+(\mu)=\{\alpha\in\Phi_1^+|(\mu+\rho,\alpha)\neq 0\}$$

and call $a_\mu=|\Phi_1^+|-|\Phi_1^+(\mu)|$ the *atypicality index* of μ. We remark that the maximal possible atypicality index is given by a_0 corresponding to the trivial one dimensional irrep. We then have the following.

Proposition 2: Suppose μ is quasi-typical. Then

$$sd_q[\mu]=\delta_{a_0 a_\mu}\prod_{\alpha\in\Phi_0^+}\frac{[(\mu+\rho,\alpha)]_q}{[(\rho,\alpha)]_q}\frac{\Pi_{\alpha\in\Phi_1^+(0)}[(\rho,\alpha)]_q}{\Pi_{\alpha\in\Phi_1^+(\mu)}[(\mu+\rho,\alpha)]_q}.$$

Proof: We may write (11) in the form

$$\chi_{\beta\delta}(\gamma_\beta)=[\beta]_q^{a_0-a_\mu}\prod_{\alpha\in\Phi_0^+}\frac{[(\mu+\beta\delta+\rho,\alpha)]_q}{[(\beta\delta+\rho,\alpha)]_q}\frac{\Pi_{\alpha\in\Phi_1^+(0)}[(\beta\delta+\rho,\alpha)]_q}{\Pi_{\alpha\in\Phi_1^+(\mu)}[(\mu+\beta\delta+\rho,\alpha)]_q}.$$

Taking the limit $\beta\to 0$, it is clear that we have a nonzero result if and only if $a_\mu=a_0$ since a_0 is the maximal atypicality index as indicated above. The proposition then follows. □

The above shows that the q-superdimension of a quasi-typical irrep π_μ vanishes identically unless $\mu\in D^+$ has maximal atypicality index.

IV. UNITARY IRREPS

Next we will show that Proposition 2 applies to all unitary irreps. The two types of unitary irreps have been classified in Refs. 12 and 13 and we refer to those articles for details. We have the following result from Ref. 18.

Proposition 3: Let C_L denote the universal second-order Casimir invariant of g. Let $V(\mu)$ be a unitary module with g_0 decomposition (8).

(i) If π_μ is a type I unitary irrep, then

$$\chi_\mu(C_L)-\chi_\nu(C_L)=(\mu-\nu,\mu+\nu+2\rho)\geqslant 0$$

with equality if and only if $\nu=\mu$.

(ii) If π_μ is a type II unitary irrep, then

$$\chi_\mu(C_L)-\chi_\nu(C_L)=(\mu-\nu,\mu+\nu+2\rho)\leqslant 0$$

with equality if and only if $\nu=\mu$. □

Proposition 3 shows that μ is quasi-typical for all unitary irreps of the Lie superalgebra g. This must also be true upon deformation into an irrep of $U_q(g)$, which is also unitary, so we can apply Proposition 2 to give the following.

Proposition 4: The q-superdimension of a finite dimensional unitary irrep π_μ is given by

$$sd_q[\mu]=\delta_{a_0 a_\mu}\prod_{\alpha\in\Phi_0^+}\frac{[(\mu+\rho,\alpha)]_q}{[(\rho,\alpha)]_q}\frac{\Pi_{\alpha\in\Phi_1^+(0)}[(\rho,\alpha)]_q}{\Pi_{\alpha\in\Phi_1^+(\mu)}[(\mu+\rho,\alpha)]_q}.$$

□

Using the classification scheme of Ref. 12, we can characterize all of the unitary irreps of $U_q(\mathrm{gl}(m|n))$ with maximal atypicality index $a_0=\min(m,n)$.

Proposition 5: For $U_q(\mathrm{gl}(m|n))$ choose $\{\varepsilon_i\}_{i=1}^{m+n}$ as a basis for H^* satisfying $(\varepsilon_i,\varepsilon_j)=(-1)^{[i]}\delta_{ij}$ where $[i]=0$ for $i=1,2,\ldots,m$ and $[i]=1$ for $i=m+1,\ldots,m+n$. In this basis, any weight $\mu\in H^*$ is expressed as $\mu=\Sigma_i\mu_i\varepsilon_i\equiv(\mu_1,\ldots,\mu_m|\mu_{m+1},\ldots,\mu_{m+n})$.

(i) Suppose $m\geqslant n$. The irrep π_μ is type I unitary with $a_\mu=n$ if and only if

$$\mu=(\mu_1,\ldots,\mu_{m-n},\dot{0}_n|\dot{0}_n), \tag{12}$$

and is type II unitary with $a_\mu=n$ if and only if

$$\mu=(\dot{0}_k,\mu_{k+1},\ldots,\mu_m|\mu_{m+1},\ldots,\mu_{m+n}),\quad k\geqslant n, \tag{13}$$

where

$$\mu_{m+j}=i_j+j-m-1,\quad j=1,\ldots,n, \tag{14}$$

and

$$\begin{aligned} i_1&=k,\\ i_j&=n+1-j,\ldots,i_{j-1}-1,\quad j=2,\ldots,n. \end{aligned} \tag{15}$$

(ii) Suppose $m\leqslant n$. The irrep π_μ is type I unitary with $a_\mu=m$ if and only if

$$\mu=(\mu_1,\ldots,\mu_m|\mu_{m+1},\ldots,\mu_{m+k-1},\dot{0}_{n-k+1}),\quad k\leqslant n-m+1,$$

where

$$\mu_i=i+j_i-m-1,\quad i=1,\ldots,m,$$

and

$$\begin{aligned} j_m&=k,\\ j_i&=j_{i+1}+1,\ldots,n+1-i,\quad i=1,\ldots,m-1. \end{aligned}$$

The irrep π_μ is type II unitary with $a_\mu=m$ if and only if

$$\mu=(\dot{0}_m|\dot{0}_m,\mu_{2m+1},\ldots,\mu_{m+n}).$$

Proof: First we will consider the case when $m\geqslant n$ and π_Λ is type I unitary. From Ref. 12 we have that μ must satisfy

$$(\mu+\rho,\varepsilon_m-\varepsilon_{m+k})=(\mu,\varepsilon_k-\varepsilon_{m+n})=0 \tag{16}$$

for some odd index $m+1\leqslant m+k\leqslant m+n$ in order to be type I unitary. For μ to have maximal atypicality requires that for each $1\leqslant j\leqslant n$, there exists $1\leqslant i_j\leqslant m$ such that

$$(\mu+\rho,\varepsilon_{i_j}-\varepsilon_{m+j})=0. \tag{17}$$

Note that the index i_j is uniquely determined since

$$(\mu+\rho,\varepsilon_i-\varepsilon_{m+j})>(\mu+\rho,\varepsilon_l-\varepsilon_{m+j}),\quad 1\leqslant i<l\leqslant m.$$

Now

$$(\mu+\rho,\varepsilon_{i_j}-\varepsilon_{m+j})=(\mu+\rho,\varepsilon_m-\varepsilon_{m+k})+(\mu+\rho,\varepsilon_{i_j}-\varepsilon_m)+(\mu+\rho,\varepsilon_{m+k}-\varepsilon_{m+j})$$

so that

$$(\mu+\rho,\varepsilon_{i_j}-\varepsilon_m)=-(\mu+\rho,\varepsilon_{m+k}-\varepsilon_{m+j}).$$

Lexicality of μ requires that $k\leqslant j$, $\forall 1\leqslant j\leqslant n$, implying that $k=1$. In view of (16) we can choose w.l.o.g.

$$\mu_m=\mu_{m+1}=\cdots=\mu_{m+n}=0.$$

Now from (17) we have

$$\mu_i=i_j+j-m-1$$

and again the lexicality of μ demands that

$$\mu_i\geqslant\mu_l\geqslant 0,\quad \forall 1\leqslant i<l<m$$

because of the choice $\mu_m=0$. There is only one solution to this system of equations which is given by

$$i_j=m+1-j,$$

and this in turn gives $\mu_{m+1-j}=0$, $j=1,\ldots,n$. All other μ_i, $i\leqslant m-n$, are arbitrary so we obtain (12).

Next we will consider the case when π_μ is type II unitary. From Ref. 12 we have that μ must satisfy

$$(\mu+\rho,\varepsilon_k-\varepsilon_{m+1})=(\mu,\varepsilon_1-\varepsilon_k)=0, \tag{18}$$

for some even index $1\leqslant k\leqslant m$. From Eq. (18) we can choose w.l.o.g.

$$\mu_1=\mu_2=\cdots=\mu_k=0. \tag{19}$$

Now for μ to have maximal atypicality requires that for each $1\leqslant j\leqslant n$ there is an even index $1\leqslant i_j\leqslant m$ such that

$$(\mu+\rho,\varepsilon_{i_j}-\varepsilon_{m+j})=0. \tag{20}$$

Equation (20) also implies that

$$(\mu+\rho,\varepsilon_{i_j}-\varepsilon_{i_l})=-(\mu+\rho,\varepsilon_{m+l}-\varepsilon_{m+j})$$

from which we deduce $i_j<i_l$ whenever $l<j$. Clearly $i_1=k$ so we conclude that $k\geqslant n$. For consistency, the remaining values of i_j must be restricted to the range of values given by (15). Equation (20) may be written as

$$\mu_{i_j}+\mu_{m+j}=i_j+j-m-1.$$

However, we see from (19) that $\mu_{i_j}=0\ \forall 1\leqslant j\leqslant n$, which then gives us (14). The remaining μ_i, $k+1\leqslant i\leqslant m$, may take arbitrary values. The case for $m\leqslant n$ may be treated similarly and this completes the proof.

Note: An interesting example is the case of $U_q(\mathrm{gl}(m|m))$. The above shows that apart from the exception of the trivial irrep with $\mu=(\dot{0}_m|\dot{0}_m)$, all unitary irreps have zero q-superdimension.

For the case of $U_q(\mathrm{osp}(2|2n))$, all irreps have atypicality index of either 0 or 1. Thus the unitary irreps with maximal atypicality are simply the atypical unitary irreps. From Ref. 13 we have the following classification.

Proposition 6: For $U_q(\mathrm{osp}(2|2n))$, choose $\{\varepsilon_i\}_{i=0}^n$ as a basis for H^* satisfying $(\varepsilon_i,\varepsilon_j)=(-1)^{\delta_{i0}}\delta_{ij}$. The irrep π_μ is type I unitary with $a_\mu=1$ if and only if

$$(\mu,\varepsilon_0-\varepsilon_1)=0.$$

The irrep π_μ is type II unitary with $a_\mu=1$ if and only if there exists an index $j\in\{1,\ldots,n\}$ such that

$$(\mu+\rho,\varepsilon_0+\varepsilon_j)=(\mu,\varepsilon_1-\varepsilon_j)=0;$$

or $\mu=0$.

V. CONCLUSION

We have derived a formula for the q-superdimensions of a class of irreps, referred to as quasi-typical, for the type I quantum superalgebras. The quasi-typical irreps are a natural generalization of typical irreps and include the important class of all unitary irreps. In future work we aim to characterize and investigate the properties of the quasi-typical irreps.

Our q-superdimension formula is new even in the classical ($q\to 1$) limit. It has long been known that all the typical irreps have zero q-superdimension.[9,17] Our formula gives the surprising result that the quasi-typical irreps with maximal atypicality index have nonzero q-superdimension, while all other quasi-typical irreps have q-superdimension equal to zero. For the unitary irreps, we have given a classification of those with maximal atypicality index in terms of the highest weight labels. An example of an application of these results is in the computation of link invariants as discussed in Ref. 16.

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Calabi–Yau compactifications and the global structure of the standard group

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The ''standard group'' of elementary particle theory is *locally* isomorphic to SU(3) $\times$SU(2)$\times$U(1). The *global* structure is completely fixed in unified theories, often in a subtle way; and such theories can be physically unacceptable if they predict the ''wrong'' global structure for the standard group. A particularly striking example of this is provided by Calabi–Yau compactifications of string theory with the *linear* (rather than the more conventional spinor) connection interpreted as an E_8 connection. Remarkably, these more unconventional compactifications break E_8 to a group which is locally isomorphic to the standard group (instead of E_6); but they are physically unacceptable, and we argue that the basic reason for this is their failure to produce the correct global structure. © *1996 American Institute of Physics.* [S0022-2488(96)03701-9]

I. INTRODUCTION

One of the most remarkable results of work on Kaluza–Klein theories[1] was the discovery that higher-dimensional theories can yield chiral fermions only if K, the internal manifold, admits a nontrivial vacuum gauge potential. The geometry of K itself supplies, through parallel transport, candidates for this vacuum gauge potential; if these are used for this purpose, one says[2] that the ''spin connection is embedded in the gauge group.''

However, a closer analysis of this procedure reveals a basic ambiguity. Every Riemannian spin manifold[3] carries at least *two* distinct principal bundles defined by its geometry: a bundle of oriented orthonormal frames, SO(K) (with structural group SO(n),$n=\dim K$), and at least one bundle of spinor frames spin(K) (with structural group spin(n)). The familiar Levi–Civitá connection on K may be regarded as a one-form ω_L on SO(K), but it also defines a ''Dirac connection'' ω_D on spin(K). (This, in turn, defines the spinor covariant derivative.) The question now is this: when, as in string theory, we use the geometry of K to define a vacuum gauge potential, how are we to decide whether to use ω_L or ω_D?

The distinction between ω_L and ω_D can most usefully be expressed as follows. Suppose that K is a Calabi–Yau manifold. Then, as is well-known, its *linear* holonomy group is a subgroup of SO(6) which happens to be isomorphic to SU(3). Notice that the *linear* holonomy group (i.e., the holonomy group defined by the Levi–Civitá connection ω_L) is necessarily a subgroup of SO(6). On the other hand, the Dirac connection ω_D, like every connection, also has a holonomy group; but *this* group is necessarily a subgroup of spin(6), *not* SO(6). In fact, it can be shown that under certain reasonable technical conditions, the holonomy group of ω_D is also abstractly isomorphic to SU(3). Nevertheless, ω_L and ω_D are distinct objects, and this distinction is expressed through the fact that one holonomy group is a subgroup of SO(6), while the other is a subgroup of spin(6).

The usual procedure[2] in string theory is to embed SU(3) in the exceptional group E_8 through SU(3)$\cdot E_6$. (Here and henceforth, the dot denotes a direct product modulo some finite subgroup—in this case, the cyclic group of order three, $\mathbb{Z}_3$.) It can be shown that this is equivalent to an embedding through spin(6)$\cdot$spin(10) (which is a subgroup of spin(16)/$\mathbb{Z}_2$, a maximal connected subgroup of E_8). Thus we see that the standard procedure in string theory is to use the Dirac connection ω_D to define the vacuum E_8 gauge potential on K. But why should we do this—why not use the (more fundamental) Levi–Civitá connection ω_L? In this article, we shall

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investigate the consequences of doing so: i.e., we embed SU(3) in E_8 through SO(6) instead of spin(6). The results are rather striking. Instead of E_6, we find that E_8 is broken directly to a group which is locally isomorphic to $SU(3)\times SU(2)\times U(1)$. However, the global structure (including discrete symmetries) is unsatisfactory, and so these unconventional compactifications must be rejected. (We stress that this result has no bearing on the conventional Calabi–Yau compactifications which do indeed break E_8 to E_6; we merely wish to clarify the importance of making the correct choice between ω_D and ω_L.)

II. REMARKS ON THE GLOBAL STRUCTURE OF THE STANDARD GROUP

The gauge group of the standard model is usually given as $SU(3)\times SU(2)\times U(1)$. However, it is often argued[4,5] that the correct form (the "true group") is $[SU(3)\times SU(2)]\cdot U(1)$, where the dot indicates that a finite subgroup has been factored out. This finite subgroup is $\mathbb{Z}_3\times\mathbb{Z}_2(=\mathbb{Z}_6)$. The argument is essentially as follows. If G is a Lie group and F is a finite normal subgroup, then every representation of G/F is likewise a representation of G; but the converse is not true. Thus in passing from $SU(3)\times SU(2)\times U(1)$ to $[SU(3)\times SU(2)]\cdot U(1)$, some representations are "lost." However, it so happens that these representations invariably correspond to particles which apparently do not exist. For example, all charged quarks are assigned to representations of $SU(3)\cdot U(1)^q$ (where $U(1)^q$ is the electromagnetic subgroup of $SU(2)\cdot U(1)$); the representations of $SU(3)\times U(1)^q$ that fail to "factor through" are never used.[5]

The reader may be inclined to dismiss this as hair splitting—after all, the fact is that all representations of $SU(3)\cdot U(1)^q$ are representations of $SU(3)\times U(1)^q$—but the question is of genuine interest if discrete symmetries are included. Let us write $SU(3)\times U(1)$ as $SU(3)\times SO(2)$. Then $SU(3)\cdot SO(2)$ is obtained by factoring out the $\mathbb{Z}_3$ generated by the pair (u,v), where u and v are fixed central elements of order three in SU(3) and SO(2), respectively. This $\mathbb{Z}_3$ is of course normal in $SU(3)\times SO(2)$. But now consider the *disconnected* group $SU(3)\times O(2)$. The reader can readily verify that $\mathbb{Z}_3$ is *not* a normal subgroup of this group—notice that, unlike SO(2), O(2) is not Abelian. Hence $\mathbb{Z}_3$ cannot be factored out, and $SU(3)\times O(2)$ has no representations which restrict to representations of $SU(3)\cdot SO(2)$. In this case, we can definitely assert that $SU(3)\times O(2)$ must be rejected on physical grounds, despite the fact that its *local* structure is identical to that of $SU(3)\times U(1)$ and $SU(3)\cdot U(1)$. In short, global properties can have unacceptable consequences even if the local structure is correct.

III. CALABI–YAU COMPACTIFICATIONS BASED ON LINEAR HOLONOMY

In this section we investigate unconventional Calabi–Yau compactifications with SU(3) embedded in E_8 through SO(6), instead of the usual spin(6) subgroup.

As we shall see, the final gauge group is necessarily disconnected. We can turn this to good account by gauging the CP operator, as advocated in Ref. 6. In string theories, CP always has a natural geometric interpretation in terms of antiholomorphic isometries of K. Let β be such an isometry, with $\beta^2=1$, and let α be the parity isometry of M_4: then CP is related[2] to $\alpha\beta$. As M_4 is flat, the bundle $SO^+(M_4\times K)$ consisting of time and space oriented orthonormal frames over $M_4\times K$ is reducible to an SU(3) bundle P. But while the natural lift[7] of $\alpha\beta$, denoted $\tilde{\alpha}\tilde{\beta}$, is an automorphism of $SO^+(M_4\times K)$ (because α and β are orientation-reversing on M_4 and K separately, so that $\alpha\beta$ is orientation-preserving), it does not restrict to an automorphism of P. Therefore we adjoin to P all those frames in $SO^+(M_4\times K)$ obtained by reversing directions according to the action of the matrix

$$\sigma=\mathrm{diag}(1,-1,-1,-1,1,1,1,-1,-1,-1).$$

Then σ is an element of $\mathrm{SO}^+(1,9)$; it generates a cyclic subgroup of order 2. (The first four entries act on frames over M_4; the last six act on frames over K.) The resulting bundle P^* over $M_4\times K$ is an $\mathrm{SU}(3)\rtimes\mathbb{Z}_2$ bundle, where the product is semidirect and $\mathbb{Z}_2$ acts on SU(3) by complex conjugation. (Note that SU(3) is embedded in $\mathrm{SO}^+(1,9)$ through

$$A+iB\to\mathrm{diag}\left(I_4,\begin{pmatrix}A & -B\\ B & A\end{pmatrix}\right)\in\mathrm{SO}^+(1,9),$$

so that conjugation by σ does indeed map $A+iB$ to $A-iB$.) Clearly $\tilde{\alpha}\tilde{\beta}$ does restrict to an automorphism of P^*. Our objective is to extend the latter to an E_8 bundle, and so we must embed $\mathrm{SU}(3)\rtimes\mathbb{Z}_2$ in E_8.

As explained above, we wish to embed SU(3) in E_8 through SO(6) (just as SU(3) is embedded in $\mathrm{SO}^+(1,9)$ through SO(6)). There is a very natural way to do this, as follows. E_8 contains $\mathrm{SU}(2)\cdot E_7$ as a maximal connected subgroup, and E_7 likewise contains $\mathrm{SU}(3)\cdot\mathrm{SU}(6)$. Thus E_8 contains $[\mathrm{SU}(2)\times\mathrm{SU}(3)]\cdot\mathrm{SU}(6)$, the dot as usual meaning that the respective centers (both isomorphic to $\mathbb{Z}_2\times\mathbb{Z}_3=\mathbb{Z}_6$) are identified in E_8, so that the product is not direct in the usual sense. As SU(6) contains SO(6) in an obvious way, we have our embedding of SO(6) in E_8. In fact, we can even embed O(6) in E_8 in much the same way. To see this, let (a,b,c) denote any element of $[\mathrm{SU}(2)\times\mathrm{SU}(3)]\cdot\mathrm{SU}(6)$. (Because of the identifications mentioned earlier, all triples of the form (x^3I_2,x^2I_3,xI_6), where x is any sixth root of unity, are identified in this group.) Now let S be the element of this group given by (recall the definition of σ)

$$S=\left(z^3\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix},\quad z^2\begin{pmatrix}-1 & 0 & 0\\ 0 & -1 & 0\\ 0 & 0 & -1\end{pmatrix},\quad z\cdot\mathrm{diag}(1,1,1,-1,-1,-1)\right),$$

where z is a primitive 12th root of unity. Then $S^2=1$, and, if SO(6) is the real subgroup of SU(6), it is clear that

$$\mathrm{O}(6)=\mathrm{SO}(6)\cup S\cdot\mathrm{SO}(6)$$

is indeed isomorphic to O(6). Thus we have O(6) as a subgroup of $[\mathrm{SU}(2)\times\mathrm{SU}(3)]\cdot\mathrm{SU}(6)$, and hence as a subgroup of E_8. This in turn yields the desired embedding of $\mathrm{SU}(3)\rtimes\mathbb{Z}_2$ in E_8.

The $\mathrm{SU}(3)\rtimes\mathbb{Z}_2$ bundle P^* may now be extended to an E_8 bundle,[8] denoted E, and the Levi–Civitá connection on P^* induces a connection ω on E. In this way, we equate the gauge connection to the linear connection, and at the same time associate an element of E_8 with the action of $\alpha\beta$ on $M_4\times K$ (i.e., we "gauge" the CP operator.[6] See below for the precise construction of the E_8 element associated with $\alpha\beta$.)

The final gauge symmetry group of this theory is the group of all those automorphisms of E which cover the cyclic group of order two generated by $\alpha\beta$, and which preserve ω. That is, we need to study the group of all maps $F:E\to E$ which commute with the action of E_8 on E, which satisfy $F^*\omega=\omega$, and which induce either $\alpha\beta$ or the identity map on the base manifold. This group is naturally isomorphic to a subgroup of E_8, as follows. First, the subgroup V_ω which covers the identity (i.e., the group of *vertical* automorphisms preserving ω) is isomorphic[9] to the centralizer of the holonomy group in E_8. This centralizer, which we also denote by V_ω, depends on the embedding of SU(3) in E_8: when the embedding is through spin(6), it is isomorphic to E_6, but not when the embedding is through SO(6). Second, the automorphisms covering $\alpha\beta$ correspond to the E_8 elements of the form $S\cdot V_\omega$, where S was defined above. Hence the full symmetry group is

$$V_\omega\cup S\cdot V_\omega,$$

which has the structure $V_\omega \rtimes \mathbb{Z}_2$. (Note that as conjugation by S is an automorphism of SU(3), it is also an automorphism of the centralizer of SU(3) in any group containing S and SU(3).) With the spin(6) embedding, this means that E_8 is broken to a subgroup of the form $E_6 \rtimes \mathbb{Z}_2$, as one expects if CP is gauged. To find the corresponding subgroup in the SO(6) case, we need to compute the centralizer of SU(3) with that embedding.

As SU(6) is embedded in E_8 through $[\mathrm{SU}(2)\times\mathrm{SU}(3)]\cdot\mathrm{SU}(6)$, it is clear that the centralizer of SO(6) must contain SU(2)×SU(3). In fact, the *full* centralizer is the disconnected group[10]

$$[\mathrm{SU}(2)\times\mathrm{SU}(3)]\rtimes\mathbb{Z}_2,$$

where the product is semidirect, and where $\mathbb{Z}_2$ is generated by an element R_0 contained in E_8 (but not in $[\mathrm{SU}(2)\times\mathrm{SU}(3)]\cdot\mathrm{SU}(6)$), such that $R_0^2=1$ and conjugation by R_0 induces complex conjugation on SU(2), SU(3), and SU(6). In fact we shall find it more convenient to describe $[\mathrm{SU}(2)\times\mathrm{SU}(3)]\rtimes\mathbb{Z}_2$ in the following slightly different way. Let Q be the element of $[\mathrm{SU}(2)\times\mathrm{SU}(3)]\cdot\mathrm{SU}(6)$ defined by

$$Q=\left(z^3\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}, I_3, I_6\right),$$

where z is as in the definition of S. Defining

$$R=QR_0,$$

we see that $R^2=1$, and so we may regard R as the generator of $\mathbb{Z}_2$ in $[\mathrm{SU}(2)\times\mathrm{SU}(3)]\rtimes\mathbb{Z}_2$. Note that R commutes with SO(6), and that

$$SR=SQR_0=QSR_0=QR_0\bar{S}=R\bar{S},$$

where

$$\bar{S}=\left(\bar{z}^3\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}, \quad \bar{z}^2\begin{pmatrix}-1 & 0 & 0\\ 0 & -1 & 0\\ 0 & 0 & -1\end{pmatrix}, \quad \bar{z}\cdot\mathrm{diag}(1,1,1,-1,-1,-1)\right).$$

But the latter is just the product of $(\bar{z}^6 I_2, \bar{z}^3 I_3, \bar{z}^2 I_6)$ with S; and since $\bar{z}^2$ is a sixth root of unity, we find that $\bar{S}=S$. Thus in fact $SR=RS$. In short, the centralizer of SO(6) in E_8 is $[\mathrm{SU}(2)\times\mathrm{SU}(3)]\rtimes\mathbb{Z}_2$, where the generator of $\mathbb{Z}_2$ can be chosen to commute with S.

If the holonomy group of K were isomorphic to SO(6), then, we would obtain a gauge group with identity component SU(2)×SU(3), which is of course too small to be useful. But within SO(6), SU(3) commutes with all matrices of the form

$$\begin{bmatrix} I_3\cos\theta & -I_3\sin\theta\\ I_3\sin\theta & I_3\cos\theta\end{bmatrix},$$

and so the gauge group acquires *an additional factor*, isomorphic to U(1), if the holonomy group is SU(3). Note that this U(1) contains the $\mathbb{Z}_2$ in the center of SU(6) (generated by $-I_6$) but *not* the $\mathbb{Z}_3$, since that latter is not generated by a real matrix. Thus U(1) intersects the SU(2) factor in $[\mathrm{SU}(2)\times\mathrm{SU}(3)]\rtimes\mathbb{Z}_2$ nontrivially, but not the SU(3) factor. In our earlier agreed notation, the identity component of the final gauge group is

$$[\mathrm{U}(1)\cdot\mathrm{SU}(2)]\times\mathrm{SU}(3).$$

Thus indeed the linear connection ω_L breaks E_8 differently:instead of the E_6 produced by the Dirac connection, we obtain a group which is locally indistinguishable from the standard group. This result is all the more striking when we recall that, even with the aid of the ''Hosotani mechanism,'' the conventional approach[2] cannot produce a final gauge group of rank lower than five.

These alternative string theories must, however, be rejected. One can show this in various ways; but the most fundamental defect of these theories is that they do not produce an acceptable global structure for the gauge group.

The group $[\mathrm{U}(1)\cdot\mathrm{SU}(2)]\times\mathrm{SU}(3)$ is not globally isomorphic to the ''true group'' of Ref. 4; the latter is obtained by identifying the center of SU(3) with the $\mathbb{Z}_3$ subgroup of U(1). That is, our gauge group is a covering group of the true group. But this in itself is not a fatal objection: it becomes so only when we consider the structure of the full, disconnected gauge group. Setting $G_0=[\mathrm{U}(1)\cdot\mathrm{SU}(2)]\times\mathrm{SU}(3)$, we have found that the full gauge group, including CP, is the E_8 subgroup

$$G=G_0\cup S\cdot G_0\cup R\cdot G_0\cup RS\cdot G_0.$$

Here, S and R satisfy $S^2=R^2=1$, $RS=SR$; conjugation by S acts as conjugation by

$$\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$$

on SU(2), as complex conjugation on U(1) (because

$$\begin{pmatrix} I_3 & 0 \\ 0 & -I_3 \end{pmatrix}\begin{pmatrix} I_3\cos\theta & -I_3\sin\theta \\ I_3\sin\theta & I_3\cos\theta \end{pmatrix}\begin{pmatrix} I_3 & 0 \\ 0 & -I_3 \end{pmatrix}=\begin{pmatrix} I_3\cos\theta & I_3\sin\theta \\ -I_3\sin\theta & I_3\cos\theta \end{pmatrix},$$

which is complex conjugation for U(1) as a subgroup of SO(6)), and trivially on SU(3). Conjugation by R acts as complex conjugation followed by

$$\mathrm{Ad}\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$$

on SU(2), trivially on U(1), and as complex conjugation on SU(3). Conjugation by RS therefore acts simply as complex conjugation on all three factors, and so it is RS that corresponds to the conventional CP operator. Thus finally E_8 is broken to a subgroup isomorphic to a semidirect product of $[\mathrm{U}(1)\cdot\mathrm{SU}(2)]\times\mathrm{SU}(3)$ with $\mathbb{Z}_2\times\mathbb{Z}_2$.

Now the subgroup which must be factored out if the identity component is to coincide with the true group[4] (i.e., $[\mathrm{SU}(3)\times\mathrm{SU}(2)\times\mathrm{U}(1)]/\mathbb{Z}_6$), is the diagonal subgroup of the central subgroup $\mathbb{Z}_3\times\mathbb{Z}_3\subset\mathrm{U}(1)\times\mathrm{SU}(3)$. But it is clear that, since $\mathrm{Ad}(R)$ and $\mathrm{Ad}(S)$ act differently on the two $\mathbb{Z}_3$ factors, the diagonal subgroup is *not* normal in any group containing either R or S. It *is* normal in $G_0=[\mathrm{U}(1)\cdot\mathrm{SU}(2)]\times\mathrm{SU}(3)$, and also in $G_0\cup RS\cdot G_0$, but not in the full group with four connected components. Consequently the latter does not possess representations that can accommodate the known elementary particles, and the theory must therefore be rejected.

IV. CONCLUSION

We argue that there are two ways of interpreting, in string theory, the construction of a nontrivial vacuum gauge potential. The usual procedure is based on spinor parallel transport. In this article we have investigated the alternative, using linear (vector) parallel transport. Despite being initially attractive, these unconventional compactifications must be rejected; and this conclusion probably cannot be evaded, since it is obtained by very general (topological) arguments.

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$ISO_q(3)$ and $ISO_q(2,1)$

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We prove the embedding of $ISO_q(3) \hookrightarrow ISU^{\mathrm{ex}}_{\sqrt{q}}(2)$ and $ISO_q(2,1) \hookrightarrow ISL^{\mathrm{ex}}_q(2,R)$ as $*$-algebras and give a Hilbert space representation of $ISU^{\mathrm{ex}}_{\sqrt{q}}(2)$. © *1996 American Institute of Physics.* [S0022-2488(96)00301-9]

I. INTRODUCTION

The inhomogenized extensions of a large list of standard quantized Lie groups[1] have been given in Refs. 2–7. They form quantized versions of the classical inhomogeneous groups. For a real deformation parameter q the representation theory of the homogeneous parts (e.g., corepresentations of the function algebra) is basically the same as for the classical groups, whereas for q root of unity it is completely different. However, the representation theory of the noncommutative function algebra differs for any $q \neq 1$ from the classical situation. Its relevance stems from the question of whether a deformation exists on the C^*-algebra level.[8]

In Sec. II we recall the properties of inhomogeneous quantum groups. In Sec. III we examine the algebraic embedding of the $ISO_q(3)$ into $ISU^{\mathrm{ex}}_{\sqrt{q}}(2)$ and $ISO_q(2,1)$ into $ISL^{\mathrm{ex}}_q(2,R)$. Here the "extended inhomogeneous" quantum algebra IG^{ex} designates inhomogeneous quantum algebras containing two sets of coordinate functions.

In Sec. IV we examine the representation theory of the $ISU^{\mathrm{ex}}_{\sqrt{q}}(2)$.

II. THE HOPF ALGEBRA STRUCTURE OF INHOMOGENEOUS QUANTUM GROUPS

Quantum groups may be considered to be deformations of the function algebra over the corresponding Lie groups. The deformation is given by a parameter $q \in \mathbb{C}$ which has to be further restricted in order to get special cases of deformations. Quantum groups exhibit a Hopf algebra structure. The noncommutative algebra structure is controlled by an $\hat{R}$ matrix fulfilling the quantum Yang–Baxter equation $\hat{R}_{12}\hat{R}_{23}\hat{R}_{12} = \hat{R}_{23}\hat{R}_{12}\hat{R}_{23}$. In this paper we refer to $\hat{R}$ matrices in their standard form given in Ref. 1. They are defined by their projector decomposition making use of the antisymmetrizer $\hat{A}^{ij}_{q\,kl}$, the symmetrizer $\hat{S}^{ij}_{q\,kl}$, and the trace projector $\hat{T}^{ij}_{q\,kl} \propto C^{ij}C_{kl}$ with the metric C_{ij}, existing for the q-orthogonal groups only:

$$\hat{R}^{ij}_{q\,kl} = \begin{cases} q\hat{S}^{ij}_{q\,kl} - q^{-1}\hat{A}^{ij}_{q\,kl}, & [\text{for } SL_q(N)] \\ q\hat{S}^{ij}_{q\,kl} - q^{-1}\hat{A}^{ij}_{q\,kl} + q^{1-N}\hat{T}^{ij}_{q\,kl}, & [\text{for } SO_q(N)]\ . \end{cases} \tag{1}$$

The algebra relations for the generators M^i_j of the unital $\mathbb{C}$ algebra $\mathscr{A}$ are

$$\hat{R}^{ij}_{q\,j'i'} M^{j'}{}_{j''} M^{i'}{}_{i''} = M^i{}_{i'} M^j{}_{j'} \hat{R}^{i'j'}_{q\,j''i''} \tag{2}$$

and

$$\begin{cases} \det M = \dfrac{(-1)^{N-1}}{[N]!}\, \epsilon^{k_1,\ldots,k_N} M^{l_1}{}_{k_1} \ldots M^{l_N}{}_{k_N} \epsilon_{l_1,\ldots,l_N} = \mathbf{1}\ , & [SL_q(N)]\ , \\ C_{ij} M^i{}_{i'} M^j{}_{j'} = C_{i'j'}\mathbf{1}\ , & [SO_q(N)]\ . \end{cases} \tag{3}$$

For the unimodularity condition we use the q-antisymmetric tensors ϵ_q defined in Refs. 2 and 3.

In order to obtain inhomogeneous quantum groups the set of generators has to be enlarged not only by the coordinate functions x_i but by an invertible scaling operator $\bar{w}$ as well. Its existence is required by consistency of the comultiplication. The additional algebra relations of the extended Hopf algebra $\mathscr{A}^I$ are

$$\begin{aligned} &\text{(i)}\quad x^i M^j{}_k = \gamma \hat{R}^{ij}_{q\,lm} M^l{}_k x^m, && \text{(iv)}\quad w M^i{}_j = M^i{}_j w, \\ &\text{(ii)}\quad \bar{w} w = \mathbf{1}, && \text{(v)}\quad \bar{w} x^i = \frac{q}{\gamma}\, x^i \bar{w}, \\ &\text{(iii)}\quad \bar{w} M^i{}_j = M^i{}_j \bar{w}, && \text{(vi)}\quad w x^i = \frac{\gamma}{q}\, x^i w, \end{aligned} \tag{4}$$

with

$$\gamma = \begin{cases} q^{-1/N}, & [\text{for } SL_q(N)], \\ 1, & [\text{for } SO_q(N)]. \end{cases} \tag{5}$$

The comultiplication $\Phi: \mathscr{A}^I \to \mathscr{A}^I \otimes \mathscr{A}^I$, counit $e: \mathscr{A}^I \to \mathbb{C}$ and the antipode $\kappa: \mathscr{A}^I \to \mathscr{A}^I$ are very easily given in matrix notation. With

$$M^I = \begin{pmatrix} wM & \mathbf{x} \\ 0 & 1 \end{pmatrix} \tag{6}$$

we get

$$\Phi(M^I) = M^I \dot{\otimes} M^I \tag{7}$$

and

$$e(M^I) = \begin{pmatrix} E & \mathbf{0} \\ 0 & 1 \end{pmatrix} \tag{8}$$

with the unity matrix E. The antipode is given as

$$\kappa(M^I) = \begin{pmatrix} \kappa(M)\bar{w} & -\kappa(M)\bar{w}\mathbf{x} \\ 0 & \mathbf{1} \end{pmatrix}. \tag{9}$$

A. Complex conjugation

The $*$-operations on $\mathscr{A}$ are defined quite differently in the cases $q \in \mathbb{R}^+$ and $|q| = 1$.

1. $q \in \mathbb{R}^+$

With the unitarity condition $(M^i_j)^* = \kappa(M^j_i)$, the quantum group $SL_q(N)$ becomes an $SU_q(N)$ quantum group. The same $*$-structure holds for the orthogonal quantum groups $SO_q(N)$.

2. $|q| = 1$

For such q the R_q matrix has the property $R_q^* = R_q^{-1}$. With the reality condition $(M^i_j)^* = M^i_j$ one finds the real representation of the quantum group $SL_q(N)$ called $SL_q(N,R)$ and the orthogonal quantum groups in this case have a metric which is indefinite, i.e., for N even we get $SO_q(n,n)$ and for N odd $SO_q(n,n+1)$, with $N = 2n$ or $N = 2n+1$, respectively.

The complex conjugation for the inhomogeneous extensions of these function algebras have to be treated separately as well.

(a) In the case $q \in \mathbf{R}^+$ we have to enlarge the generating set of the $*$-Hopf algebra $\mathscr{A}^l$ by the conjugate coordinate functions $\bar{x}_i$. The additional algebra relations are

$$\begin{aligned} &\text{(i)} \quad M^l{}_s \bar{x}_j = \frac{1}{\gamma} \hat{R}_q^{al}{}_{ij} \bar{x}_a M^i{}_s, \quad &&\text{(iii)} \quad \bar{w}\bar{x}_i = \frac{q}{\gamma} \bar{x}_i \bar{w}, \\ &\text{(ii)} \quad w\bar{x}_i = \frac{\gamma}{q} \bar{x}_i w, &&\text{(iv)} \quad x^i \bar{x}_j = \frac{1}{q} \bar{x}_a x^b \hat{R}_q^{ai}{}_{bj}. \end{aligned} \tag{10}$$

The comultiplication of $\bar{x}_i$ follows from being an $*$-homomorphism and the antipode from the fact that $\kappa \circ * \circ \kappa \circ * = id$.

(b) When $|q| = 1$ the coordinate functions may be chosen to be real ($x_i^* = x_i$), since applying the $*$ to Eq. (4i) and taking into account that $R_q^{ij*}{}_{kl} = R_q^{-1ij}{}_{kl}$, we get

$$M^j{}_k x^i = \gamma^{-1} R_q^{-1ji}{}_{lm} x^m M^l{}_k \tag{11}$$

or

$$\gamma \hat{R}_q^{rs}{}_{ji} M^j{}_k x^i = \delta^r_m \delta^s_l x^m M^l{}_k. \tag{12}$$

III. ALGEBRAIC EMBEDDING

The $\hat{R}$-matrix of $SU_{\sqrt{q}}(2)$ is decomposed using the q-antisymmetric ϵ-tensor:

$$\hat{R}^{\mu\nu}_{\sqrt{q}\rho\sigma} = \sqrt{q}\, \delta^\mu_\rho \delta^\sigma_\nu + \epsilon^{\mu\nu} \epsilon_{\rho\sigma} \tag{13}$$

with

$$\epsilon_{\mu\nu} := \begin{pmatrix} 0 & q^{-1/4} \\ -q^{1/4} & 0 \end{pmatrix}_{\mu\nu} = -e^{\mu\nu}.$$

For the homogeneous parts the embedding $SO_q(3) \hookrightarrow SU_{\sqrt{q}}$ is well known.[9] With the q-deformed Clebsch–Gordan coefficients $c^i_{\mu\nu}$ of the product decomposition of the $SU_{\sqrt{q}}(2)$:[10]

$$c^1_{\mu\nu} := \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}_{\mu\nu}, \quad c^2_{\mu\nu} := \frac{1}{\sqrt{1+q}} \begin{pmatrix} 0 & \sqrt{q} \\ 1 & 0 \end{pmatrix}_{\mu\nu}, \quad c^3_{\mu\nu} := \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}_{\mu\nu} \tag{14}$$

and $c^i_{\mu\nu} = c^{\mu\nu}_i$ the matrix elements M^i_j of $SO_q(3)$ are given in terms of $SU_{\sqrt{q}}(2)$ elements m^μ_ν by

$$M^i{}_j := c^i_{\mu\nu} m^\mu{}_\rho m^\nu{}_\sigma c^{\rho\sigma}_j. \tag{15}$$

This is verified by checking the $\hat{R}$-matrix of the $SO_q(3)$ group to be

$$\frac{1}{q}\, \eta^i{}_{i'} \eta^j{}_{j'} c^{i'}_{\mu\rho} c^{j'}_{\sigma\lambda} \hat{r}^{\mu\nu}{}_{\mu'\nu'} \hat{r}^{\rho\sigma}{}_{\nu\tau} \hat{r}^{\tau\lambda}{}_{\tau'\lambda'} \hat{r}^{\nu'\tau'}{}_{\rho'\sigma'} c^{\mu'\rho'}_{k'} c^{\sigma'\lambda'}_{l'} \bar{\eta}^{k'}{}_k \eta^{l'}{}_l, \tag{16}$$

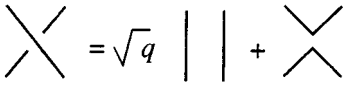
where $\hat{r}$ denotes the $\hat{R}$-matrix of the $SU_{\sqrt{q}}(2)$ group and $\eta = \mathrm{diag}(1,i,1)$, i being the imaginary unit. It just produces a base change to more convenient coordinates. Note as well the decomposition of the symmetric projector $\hat{S}^{\mu\nu}_{\sqrt{q}\rho\sigma} = c^{\mu\nu}_i c^i_{\rho\sigma}$.

In order to clear out nasty indices we want to make use of a graphical notation, which has been given in Ref. 11. With

$c^i_{\mu\nu} :=$ 

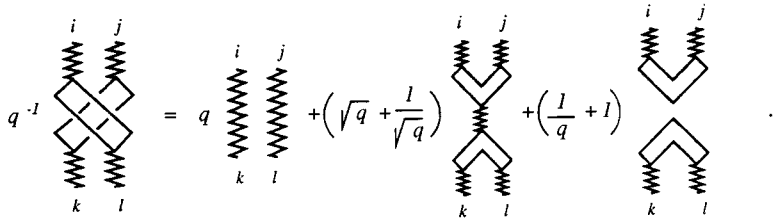
(17)

and the equality



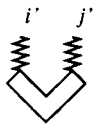
(18)

we can disentangle the matrix



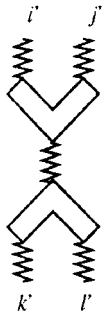
(19)

This is the $\hat{R}$-matrix of $SO_q(3)$ since obviously

$C^{ij} = \eta^i{}_{i'}\eta^j{}_{j'}$ 

(20)

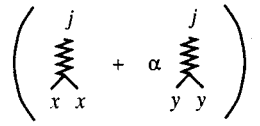
and

$\hat{A}^{ij}_{q\,kl} = \eta^i{}_{i'}\eta^j{}_{j'}$  $\bar{\eta}^{k'}{}_k\bar{\eta}^{l'}{}_l$.

(21)

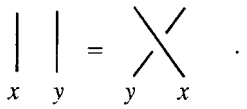
Of course the same construction holds for the $SO_q(2,1)$ group. Then η has to be chosen as an identity matrix

Since we know the q-antisymmetrizer we are able to find the $SO_q(3)$ covariant quantum plane in terms of spinor variables. To obtain sufficiently many degrees of freedom we have to take at least two copies of q-spinors x and y having the same commutation relations with m. This provides an extended inhomogeneous algebra called $ISU^{\mathrm{ex}}_{\sqrt{q}}(2)$. We want to mention that the extended algebra does not have a correct coalgebra structure. This is not important for the algebraic embedding. The three-dimensional quantum space has the form

$z^i = \eta^i{}_j$ 

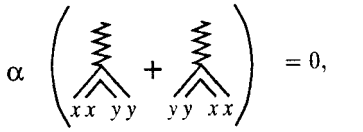
(22)

We fix the x,y-relations such that the element $\epsilon_{\nu\mu}x^\nu y^\mu$ commutes with the coordinate functions and get



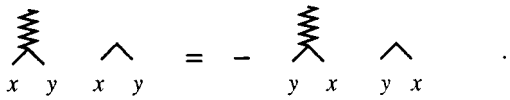
(23)

We still have to prove that $\hat{A}^{ij}_{q\,kl}z^i z^j$ vanishes. This follows from the equation



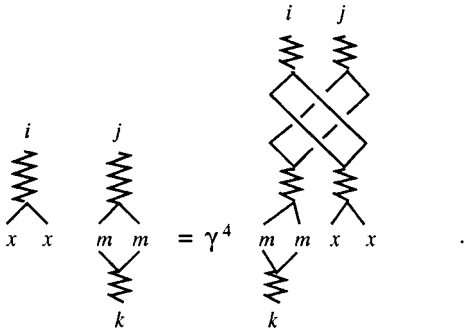
(24)

or



(25)

Next we observe that



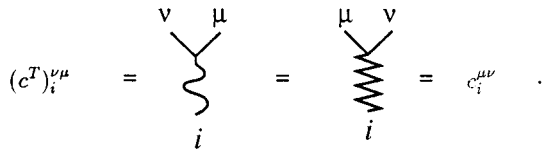
(26)

Now we have to take a look to the $*$-operation. The behavior is for q complex quite different from q real, since $(c^i_{\mu\nu})^* = c^i_{\nu\mu}$ in the first and $(c^i_{\mu\nu})^* = c^i_{\mu\nu}$ in the second case. From this we see

immediately that the algebraic embedding in the case of $ISO_q(2,1)$ respects the $*$-operation, whereas for the $ISO_q(3)$ quantum group we have to examine the $*$-structure more closely. At first for the homogeneous part we have

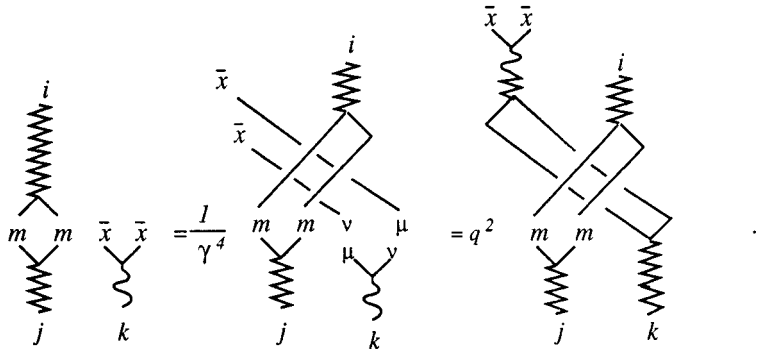
$$\kappa(c^i_{\mu\nu}m^\mu_\rho m^\nu_\sigma c^{\rho\sigma}_j)=c^i_{\mu\nu}(m^\sigma_\nu)^*(m^\rho_\mu)^*c^{\rho\sigma}_j=(c^j_{\rho\sigma}m^\rho_\mu m^\sigma_\nu c^{\mu\nu}_i)^*. \tag{27}$$

To use the graphical technique for the translations we have to introduce the ''transposed c-matrix'' c^T:



(28)

Of course $(z^i)^*=:\bar{z}_i=(c^T_i)^{\mu\nu}\bar{x}_\mu\bar{x}_\nu$. Calculating now the mixed commutation relations one has



(29)

To reproduce the correct $z-\bar{z}$ relations which use diagrams similar to that of Eq. (29) we have to redefine z as $z\to z^i=x^\mu x^\nu c^i_{\mu\nu}\bar{\omega}^n$. Now the calculation is similar to the one above and we find $n=2/3$. This relation finishes the proof of the algebraic embedding.

A. Remarks

(a) The antipode of the coordinates z just differs by a minus sign, when expressed in terms of $\kappa(x)$.

(b) The coproduct of the coordinates z cannot be embedded for obvious reasons.

IV. HILBERT SPACE REPRESENTATION FOR $ISO_q(3)$

The problem to find a representation for $ISO_q(3)$ and $ISO_q(2,1)$ is now reduced to that of representing $ISU^{\mathrm{ex}}_{\sqrt{q}}(2)$ and $ISL^{\mathrm{ex}}_q(2,\mathbb{R})$.

Here we restrict ourselves to the representation of $ISO_q(3)$. [We want to mention that $SL_q(2,\mathbb{R})$ does not exist on the C^*-algebra level anyhow.[12]] As well we confine the value of q to (0,1). However, the case $q>1$ is isomorphic. The relations of $SU_{\sqrt{q}}(2)$ are ($\mu=\sqrt{q}$):

$$\begin{gathered}\alpha\gamma=\mu\gamma\alpha,\quad \alpha\gamma^*=\mu\gamma^*\alpha,\quad \gamma\gamma^*=\gamma^*\gamma,\\ \alpha^*\alpha+\gamma^*\gamma=1,\quad \alpha\alpha^*+\mu^2\gamma^*\gamma=1.\end{gathered} \tag{30}$$

The second coordinate has the following commutation relations (remember that in our convention the quantum plane coordinates are $x^{(\tau)}$, $\tau=1,2$.):

$$x^{(2)}\alpha=\mu^{-1}\alpha x^{(2)},\quad x^{(2)}\gamma=\mu\gamma x^{(2)},$$
$$x^{(2)}\alpha^*=\mu\alpha^* x^{(2)},\quad x^{(2)}\gamma^*=\mu^{-1}\gamma^* x^{(2)}. \tag{31}$$

Applying the antipode to Eq. (31) gives

$$\alpha^*\kappa(x^{(2)})=\mu^{-1}\kappa(x^{(2)})\alpha^*,\quad \gamma\kappa(x^{(2)})=\mu\kappa(x^{(2)})\gamma,$$
$$\alpha\kappa(x^{(2)})=\mu\kappa(x^{(2)})\alpha,\quad \gamma^*\kappa(x^{(2)})=\mu^{-1}\kappa(x^{(2)})\gamma^*. \tag{32}$$

Those relations hold for any $SU_{\sqrt{q}}(2)$-covariant plane.

We have other relations for the functions on the quantum planes $x^{(\tau)}$ and $y^{(\tau)}$, $\tau=1,2$:

$$x^{(2)}y^{(2)}=\mu y^{(2)}x^{(2)},\quad \kappa(x^{(2)})\kappa(y^{(2)})=\mu^{-1}\kappa(y^{(2)})\kappa(x^{(2)}),$$
$$x^{(\tau)}\kappa(x^{(\delta)})=\mu^{-2}\kappa(x^{(\delta)})x^{(\tau)},\quad x^{(\tau)}\kappa(y^{(\delta)})=\mu^{-1}\kappa(y^{(\delta)})x^{(\tau)},$$
$$\kappa(x^{(2)})\overline{\kappa(y^{(2)})}=\mu^2\overline{\kappa(y_2)}\kappa(x_2), \tag{33}$$
$$\overline{a_\nu}\kappa(b^{(\tau)})=\kappa(b^{(\tau)})\overline{a_\nu},\quad a,b\in\{x,y\},$$
$$y^{(\tau)}\kappa(x^{(\delta)})=\mu^{-1}\kappa(x^{(\delta)})y^{\tau}+(\mu^{-2}-1)\kappa(y^{(\delta)})x^{(\tau)},$$

where $\delta,\tau\in\{1,2\}$.

These and the conjugated relations together with the obvious relations for ω contain the whole algebraic information of $ISU_{\sqrt{q}}(2)$ since

$$a^{(1)}=(\mu\gamma)^{(-1)}[\omega\kappa(a^{(2)})+\alpha a^{(2)}],\quad a,b\in\{x,y\}. \tag{34}$$

Remember that γ is an invertible element.

The algebra may still be simplified by a nonlinear transformation in the functions of coordinates. With $Q^4=\mu^2=q$ and $v^3=\omega$ we define

$$\rho_1=\overline{v^2}\gamma^{-1}x^{(2)},\quad \Theta_1=q^{-1}v\gamma^{-1}\kappa(x^{(2)}),$$
$$\rho_2=\overline{v^2}\gamma^{-1}y^{(2)},\quad \Theta_2=q^{-1}v\gamma^{-1}\kappa(y^{(2)}). \tag{35}$$

All algebraic relations with coordinate functions are given by

$$\rho_i\alpha=Q\alpha\rho_i,\quad \Theta_i\alpha=Q\alpha\Theta_i,\quad \Theta_i\Theta_i^*=\Theta_i^*\Theta_i,$$
$$\rho_i\alpha^*=Q^{-1}\alpha^*\rho_i,\quad \Theta_i\alpha^*=Q^{-1}\alpha^*\Theta_i,\quad \rho_i\rho_i^*=Q^2\rho_i^*\rho_i,$$
$$\rho_i\gamma=Q\gamma\rho_i,\quad \Theta_i\gamma=Q^{-1}\gamma\Theta_i,\quad \rho_i\Theta_i=Q^{-3}\Theta_i\rho_i, \tag{36}$$
$$\rho_i\gamma^*=Q^{-1}\gamma^*\rho_i,\quad \Theta_i\gamma^*=Q\gamma^*\Theta_i,\quad \rho_i^*\Theta_i=Q^{-1}\Theta_i\rho_i^*,$$

with $i=1,2$:

$$\begin{gathered}\Theta_1\Theta_2=Q^2\Theta_2\Theta_1, \quad \rho_1\rho_2^*=Q^2\rho_2^*\rho_1,\\ \rho_1\rho_2=Q^2\rho_2\rho_1, \quad \Theta_1\rho_2^*=Q\rho_2^*\Theta_1,\\ \rho_1\Theta_2=Q^{-1}\Theta_2\rho_1, \quad \Theta_2\rho_1^*=Q\rho_1^*\Theta_2,\\ \Theta_1\rho_2=(Q^2-Q^{-2})\Theta_2\rho_1+Q\rho_2\Theta_1, \quad \Theta_1\Theta_2^*=\Theta_2^*\Theta_1.\end{gathered} \tag{37}$$

It is easy to find a maximal real subalgebra $\mathscr{D}$ of commuting elements. In order to connect the representation of $ISO_q(3)$ to that of $SU_{\sqrt{q}}(2)$ we choose

$$\mathscr{D}:=\{\alpha\alpha^*,\gamma\gamma^*,\rho_1\rho_1^*,\Theta_1\Theta_1^*,\Theta_2\Theta_2^*,v\}. \tag{38}$$

These operators are used to label the eigenvectors of the Hilbert space. They are normalized so that the representation is given by

$$\begin{gathered}\pi(\alpha)|n,m,k,r,s,v\rangle=\sqrt{1-Q^{4n}}|n-1,m,k,r,s,v\rangle,\\ \pi(\alpha^*)|n,m,k,r,s,v\rangle=\sqrt{1-Q^{4(n+1)}}|n+1,m,k,r,s,v\rangle,\\ \pi(\gamma)|n,m,k,r,s,v\rangle=Q^{2n}|n,m-1,k,r,s,v\rangle,\\ \pi(\gamma^*)|n,m,k,r,s,v\rangle=Q^{2n+2}|n,m+1,k,r,s,v\rangle,\\ \pi(v)|n,m,k,r,s,v\rangle=|n,m,k-1,r,s,v\rangle,\\ \pi(v^*)|n,m,k,r,s,v\rangle=|n,m,k+1,r,s,v\rangle,\\ \pi(\rho_1)|n,m,k,r,s,v\rangle=Q^{-(n+m+k)+r+2s-v}|n,m,k,r-1,s,v\rangle,\\ \pi(\rho_1^*)|n,m,k,r,s,v\rangle=Q^{-(n+m+k)+r+1+2s-v}|n,m,k,r+1,s,v\rangle,\\ \pi(\rho_2)|n,m,k,r,s,v\rangle=Q^{-(n+m+k)+2r+3s-v}|n,m,k,r-1,s,v-1\rangle,\\ \pi(\rho_2^*)|n,m,k,r,s,v\rangle=Q^{-(n+m+k)+2r+1+3s-v}|n,m,k,r+1,s,v+1\rangle,\\ \pi(\Theta_1)|n,m,k,r,s,v\rangle=Q^{-(n-m+k+r+v)}|n,m,k,r,s-1,v\rangle,\\ \pi(\Theta_1^*)|n,m,k,r,s,v\rangle=Q^{-(n-m+k+r+v)}|n,m,k,r,s+1,v\rangle,\\ \pi(\Theta_2)|n,m,k,r,s,v\rangle=Q^{-(n-m+k+r-s+v)}|n,m,k,r,s-1,v-1\rangle,\\ \pi(\Theta_2^*)|n,m,k,r,s,v\rangle=Q^{-(n-m+k+r-s+v)}|n,m,k,r,s+1,v+1\rangle.\end{gathered} \tag{39}$$

V. CONCLUSIONS

We have given the algebraic embedding of two q-Euclidean groups in three dimensions. We have given an irreducible Hilbert space representation for the function algebra of $ISO_q(3)$. With a reasoning along the lines of Ref. 8 it should be possible to prove that $ISO_q(3)$ exists on a C^*-algebra level.

ACKNOWLEDGMENTS

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Spinor structures and nonlinear connections in vector bundles, generalized Lagrange and Finsler spaces

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It is our purpose here to show that the spinor theory admits generalization for curved spaces with local anisotropy (for example, for Finsler, Lagrange, and generalized Lagrange spaces). © *1996 American Institute of Physics.* [S0022-2488(95)02210-7]

I. INTRODUCTION

The space–times with local anisotropy have generated growing interest in theoretical and mathematical physics.[1–8] In different models of locally anisotropic space–times one considers nonlinear and linear connections and metric structures in vector bundles (isotopic anisotropy) and tangent bundles (space–time anisotropy) on locally isotropic space–times [(pseudo)-Riemannian, Einstein–Cartan, or more general types of curved spaces with torsion and nonmetricity]. It seems likely that locally anisotropic space–times (la-spaces) make up a more convenient geometrical background for developing, in a self-consistent manner, classical and quantum statistical and field theories in dispersive media with radiational or turbulent and random processes. In this connection, the formulation of spinor theory on la-spaces presents substantial interest. Questions on spinors and la-space geometry were considered, for example, in the frame of Finsler bundles on space–time[5] and of the spinor gauge field theory,[9] but up to the present, we do not have a *rigorous* mathematical definition of spinors on la-spaces.

The aim of this paper is to present a geometric study of the Clifford and spinor structures in vector and tangent bundles provided with nonlinear and linear connections and metric structures and to formulate the spinor theory for spaces with the most general anisotropy of metric called *generalized Lagrange spaces*[1,2,10] GL-spaces.

The geometry of vector bundles, endowed with mutually adapted nonlinear connection, distinguished connection and metric structures and the geometry of GL-spaces are briefly reviewed in Sect. II. Distinguished Clifford algebras are introduced in Sec. III. Then, in Sec. IV, we define Clifford bundles and spinor structures on vector bundles and GL-spaces. Almost complex spinor structures on GL-spaces are studied in Sec. V. A brief introduction into algebraic and geometric theory of distinguished spinors in vector bundles and GL-spaces is given in Sec. VI. Finally, the results presented in the paper are discussed in Sec. VII.

II. NONLINEAR CONNECTIONS IN VECTOR BUNDLES AND GENERALIZED LAGRANGE SPACES

In this section we present for our further considerations the necessary definitions and basic results on vector bundles and spaces with local anisotropy.[1,2,11,12]

Let us introduce differentiable bundle spaces: the principal bundle, denoted as $\mathscr{P}=(P,\pi,\mathrm{Gr},M)$ where P and M are differentiable manifolds, map $\pi:P\to M$ is a differentiable surjection, and Gr is the structural group, the vector bundle, v-bundle, denoted as $\xi=(E,p,M)=(E,p,\mathrm{Gr},M,F)$ where differentiable manifolds E and M are called, respectively, the total ($E=\mathrm{tot}\,\xi$) and base ($M=\mathrm{bas}\,\xi$) spaces of v-bundle ξ, map $p:E\to M$ is a differentiable surjection, typical fiber F is a real vector space of dimension m, $\dim F=m$, and as the structural group Gr of bundle ξ we consider the group of linear transforms of F, i.e., $\mathrm{Gr}=GL(m,\mathbb{R})$.

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For a base space M of dimension n, bundle ξ has E a space of dimension $n+m$. Local coordinates on ξ are denoted as $u=(u^\alpha)=(x^i,y^a)$, $(i=1,2,\ldots,n)$, $(a=1,2,\ldots,m)$, where $x=(x^i)$ are considered as local coordinates on M and y^a as coordinates on fiber F_x. Coordinate transforms on v-bundle ξ are defined as

$$u^\alpha=(x^i,y^a)\rightarrow u^{\alpha'}=(x^{i'},y^{a'}), \tag{1}$$

where $x^{k'}=x^{k'}(x^k)$, $\operatorname{rank}(\partial x^{k'}/\partial x^k)=n$,

$$y^{a'}=M_a^{a'}(x)y^a, \|M_a^{a'}(x)\|\in \text{ Gr},$$

matrices $M_a^{a'}$ have the property that for a superposition of coordinate transforms $(x^i,y^a)\rightarrow(x^{i'},y^{a'})\rightarrow(x^{i'},y^{a'})$,

$$M_a^{a''}(x')M_a^{a'}(x)=M_a^{a''}(x), M_a^{a'}(x)=\delta_a^{a'}.$$

The concept of nonlinear connection, i.e., N-connection, was introduced in the frame of Finsler geometry; the definition of N-connection as a global geometric structure was first given in Ref. 13 (see related topics in Refs. 14 and 15). In Refs. 1, 2, 9, and 10 N-connection structures are studied in detail.

Definition 1: A nonlinear connection in a vector bundle ξ is a distribution $\{E_u\rightarrow H_uE, T_uE=H_uE\otimes V_uE\}$ on E defining a global decomposition, as a Whitney sum, into horizontal, HE, and vertical, VE, subbundles of the tangent bundle TE:

$$TE=HE\otimes VE. \tag{2}$$

To a N-connection one associates a covariant derivation

$$\nabla_X A=X^i\left\{\frac{\partial A^a}{\partial x^i}+N_i^a(x,\,A)\right\}s_a \tag{3}$$

on M, where s_a are local linear independent sections of (E,p,M), $A=A^a s_a$ is a tensor field in E, and $X=X^i s_i$ is a vector field on M decomposed on local basis s_i.

Differentiable functions N_i^a from (3) written as functions on x^i and y^a, $N_i^a(x,\,y)$ are called coefficients of the N-connection and satisfy these transformation laws under coordinate transforms (1) and (2):

$$N_{i'}^{a'}\frac{\partial x^{i'}}{\partial x^i}=M_a^{a'}N_i^a-\frac{\partial M_a^{a'}(x)}{\partial x^i}y^a.$$

Remark 1: Linear connections are particular cases of N-connections, when $N_i^a(x,\,y)$ are parametized as $N_i^a(x,\,y)=K^a{}_{bi}(x)X^i y^b$; functions $K^a{}_{bi}(x)$ defined on M are called as Christoffel coefficients.

In vector bundle ξ we can introduce a local frame basis adapted to the given N-connection,

$$X_\alpha=\frac{\delta}{\delta u^\alpha}=\left(X_i=\frac{\delta}{\delta x^i}=\partial_i-N_i^a(x,\,y)\,\frac{\partial}{\partial y^a}, X_a=\frac{\delta}{\delta y^a}=\frac{\partial}{\partial y^a}\right). \tag{4}$$

The dual to (4) basis is defined as

$$X^\alpha=du^\alpha=(dX^i=\delta x^i=dx^i,\; X^a=\delta y^a=dy^a+N_i^a(x,\,y)dx^i). \tag{4a}$$

By using adapted bases (4) and (4a) one introduces algebra $DT(E)$ of tensorial distinguished fields (d-fields, d-tensors, d-objects) on ξ, $\mathscr{T}=\mathscr{T}^{pr}_{qs}$ which is equivalent to the tensorial algebra of the v-bundle $\pi_d: HE\otimes VE\to E$, hereafter briefly denoted as ξ_d. An element $t\in\mathscr{T}^{\rm pr}_{\rm qs}$, d-tensor field of type $\binom{pr}{qs}$ can be written in local form as

$$t=t^{i_1\cdots i_p\ a_1\cdots a_r}_{j_1\cdots j_q\ b_1\cdots b_s}(x,\ y)\ \frac{\delta}{\delta x^{i_1}}\otimes\cdots\otimes\frac{\delta}{\delta x^{i_p}}\otimes dx^{j_1}\otimes\cdots\otimes dx^{j_q}\otimes\frac{\partial}{\partial y^{a_1}}\otimes\cdots\otimes\frac{\partial}{\partial y^{a_r}}\otimes\delta y^{b_1}\otimes\cdots\otimes\delta y^{b_s}.$$

In addition to d-tensors we can introduce d-objects with various group and coordinate transforms adapted to global splitting (2). For example, we define linear d-connections in this form.

Definition 2: A linear d-connection on E is a linear connection D on E conserving under parallelism the global decomposition (2) into horizontal and vertical sub-bundles of the tangent bundle TE.

By using decompositions of N-adapted frames (4) we define components of connection D, $\tilde{\Gamma}^{\alpha}{}_{\beta\gamma}$, as covariant $\tilde{D}$-derivations of X_β:

$$\tilde{D}_\gamma X_\beta:=\tilde{D}_{X_\gamma}X_\beta=\tilde{\Gamma}^{\alpha}{}_{\beta\gamma}X_\alpha.$$

Torsion $\tilde{T}^{\alpha}{}_{\beta\gamma}$ and curvature $\tilde{R}_{\beta}{}^{\alpha}{}_{\gamma\delta}$ of connection $\tilde{\Gamma}^{\alpha}{}_{\beta\gamma}$ can be introduced in standard manner:[1,2,10]

$$\tilde{T}(X_\gamma,X_\beta)=\tilde{T}^{\alpha}{}_{\beta\gamma}X_\alpha,$$

where

$$\tilde{T}^{\alpha}{}_{\beta\gamma}=\tilde{\Gamma}^{\alpha}{}_{\beta\gamma}-\tilde{\Gamma}^{\alpha}{}_{\gamma\beta}+\omega^{\alpha}{}_{\beta\gamma}, \tag{5}$$

and, respectively, $\tilde{R}(X_\delta,X_\gamma,X_\beta)=\tilde{R}_{\beta}{}^{\alpha}{}_{\gamma\delta}X_\alpha$, where

$$\tilde{R}_{\beta}{}^{\alpha}{}_{\gamma\delta}=X_\delta\tilde{\Gamma}^{\alpha}{}_{\beta\gamma}-X_\gamma\tilde{\Gamma}^{\alpha}{}_{\beta\cdot\delta}+\tilde{\Gamma}^{\varphi}{}_{\beta\gamma}\tilde{\Gamma}^{\alpha}{}_{\varphi\delta}-\tilde{\Gamma}^{\varphi}{}_{\beta\delta}\tilde{\Gamma}^{\alpha}{}_{\varphi\gamma}+\tilde{\Gamma}^{\alpha}{}_{\beta\varphi}\omega^{\varphi}{}_{\gamma\delta}. \tag{6}$$

In formulas (5) and (6) we have used nonholonomy coefficients $w^{\alpha}{}_{\beta\gamma}$ of adapted frames, defined as

$$[X_\alpha,X_\beta]=X_\alpha X_\beta-X_\beta X_\alpha=w^{\gamma}{}_{\alpha\beta}X_\gamma. \tag{7}$$

Let us consider v-bundle $\xi=(E,\ p,\ M)$ with paracompact base M.

Definition 3: The metric structure G on total space E of vector bundle ξ is defined as a second-order covariant, tensor field nondegenerate, and of constant signature.

In the adapted frame metric G on E is expressed as

$$G=G_{\alpha\beta}(u)\,\delta u^\alpha\otimes\delta u^\beta=g_{ij}(x,\ y)dx^i\otimes dx^j+q_{ab}(x,\ y)\,\delta y^a\otimes\delta y^b. \tag{8}$$

Definition 4: Distinguished connection structure D on E is compatible with metric structure G on E if

$$\tilde{D}_\alpha G_{\gamma\delta}=0. \tag{9}$$

In Lagrange and Finsler geometry the basic geometric constructions are realized on the tangent bundle (TM,τ,M) In this case, an N-connection, with local coefficients $N^i_j(x^k,y^l)$ is associated to a global Whitney sum decomposition:

$$TTM=HTM\oplus VTM. \tag{10}$$

Let consider a d-metric $g_{ij}(x, y)$ on M (fundamental tensor on M) as a second-order covariant and nondegenerate tensorial d-field on M.

Definition 5 (see Refs. 1, 2, and 10): A pair $M^n=(M, g_{ij}(x, y))$ is called a generalized Lagrange space (GL-space).

Remark 2: Lagrange spaces L^n are a particular case of GL-spaces: when the d-metric on M can be expressed as

$$g_{ij}(x,y)=\frac{\partial^2 \mathscr{L}}{\partial y^i\ \partial y^j},$$

where $\mathscr{L}:TM\to\mathbb{R}$ ($\mathbb{R}$ is the real number field) is a differentiable function, called a Lagrangian on M.

Remark 3: We obtain a Finsler space (M,L), also as a particular case, if $\mathscr{L}=L^2$, where L is a Finsler metric on M.

For our purposes it is convenient to use Miron's[1,2] almost Hermitian model $H^{2n}(M,G,J)$ of a GL-space, denoted H^{2n}-space, a correspondingly defined lift of $M^n=(M, g_{ij}(x, y))$ to TM, which is almost compatible with complex structure $J^\alpha{}_\beta=\begin{pmatrix} 0 & \delta^i_j \\ -\delta^i_j & 0 \end{pmatrix}$ on TM, with $J\cdot J=-I$. In the construction of H^{2n}-spaces it is a very important fact that the N-connection on TM uniquely determines the metric structure G on TM, the H^{2n}-metric,

$$G(u)=g_{ij}(x,y)dx^i\otimes dx^j+g_{ij}(x,y)\,\delta y^i\otimes \delta y^j \tag{11}$$

[with components of d-metric $g_{ij}(x, y)$ defined from relations $g_{ij}-N^k{}_i g_{kj}=0$] being compatible with the $\tilde{D}$-connection, i.e.,

$$\tilde{D}_\alpha G_{\beta\gamma}=0, \tag{12}$$

and with the almost complex structure, i.e.,

$$J_\alpha{}^\beta J_\gamma{}^\delta G_{\beta\delta}=G_{\alpha\gamma} \quad \text{and} \quad D_\alpha J^\gamma{}_\beta=0.$$

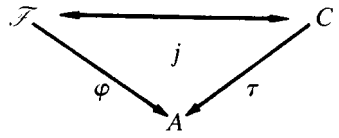
The spinor formalism proposed in this paper will be formulated for v-bundles provided with an N-connection structure compatible with the corresponding d-connection and metric structures (8) and satisfying metricity conditions (9). We point out that for GL-spaces, H^{2n}-metric (11) satisfying metricity conditions (12) is uniquely determined by the N-connection; we shall construct Clifford bundles and define spinor structures generated by this nonlinear connection structure.

III. DISTINGUISHED CLIFFORD ALGEBRAS

The typical fiber of v-bundle ξ_d, $\pi_d:HE\oplus VE\to E$ is a d-vector space $\mathscr{F}=h\mathscr{F}\oplus v\mathscr{F}$, split into vertical $v\mathscr{F}$ and horizontal $h\mathscr{F}$ subspaces, with metric $G(g, q)$ induced by v-bundle metric (8) [or by H^{2n}-metric (11) in the case when $E=TM$]. Clifford algebras (see, for example, Refs. 16–18) formulated for d-vector spaces will be called Clifford d-algebras. In this section we shall consider the main properties of Clifford d-algebras. The proof of theorems will be based on the technique developed in Ref. 16 correspondingly adapted to the distinguished character of spaces in consideration.

Let k be a number field (for our purposes $k=\mathbb{R}$ or $k=\mathbb{C}$, $\mathbb{R}$ and $\mathbb{C}$ are, respectively, real and complex number fields) and define $\mathscr{F}$ as a d-vector space on k provided with nondegenerate symmetric quadratic form (metric) G. Let C be an algebra on k (not necessarily commutative) and $j:\mathscr{F}\to C$ a homomorphism of underlying vector spaces such that $j(u)^2=G(u)\cdot 1$ (1 is the unity in algebra C and d-vector $u\in\mathscr{F}$). We are interested in definition of the pair (C, j) satisfying the next

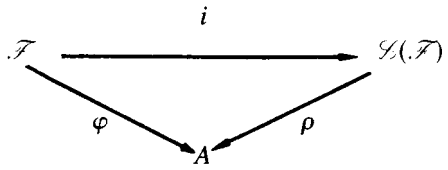
universality conditions. For every k-algebra A and arbitrary homomorphism $\varphi: \mathcal{F} \to A$ of the underlying d-vector spaces, such that $(\varphi(u))^2 \to G(u) \cdot 1$, there is a unique homomorphism of algebras $\psi: C \to A$ transforming the diagram



into a commutative one. The algebra solving this problem will be denoted as $C(\mathcal{F},G)$ [equivalently as $C(G)$ or $C(\mathcal{F})$] and called as Clifford d-algebra associated with pair $(\mathcal{F}, G)$.

Theorem 1: The above-presented diagram has a unique solution (C, j) up to isomorphism.

Proof: (We adapt for d-algebras that of Ref. 16, p. 127.) For a universal problem the uniqueness is obvious if we prove the existence of solution $C(G)$. To do this we use tensor algebra $\mathcal{S}(\mathcal{F}) = \oplus \mathcal{S}^{pr}_{qs}(\mathcal{F}) = \oplus_{i=0}^{\infty} T^i(\mathcal{F})$, where $T^0(\mathcal{F}) = k$ and $T^i(\mathcal{F}) = \mathcal{F} \otimes \cdots \otimes \mathcal{F}$ for $i > 0$. Let $I(G)$ be the bilateral ideal generated by elements of form $\epsilon(u) = u \otimes u - G(u) \cdot 1$ where $u \in \mathcal{F}$ and 1 is the unity element of algebra $\mathcal{S}(\mathcal{F})$. Every element from $I(G)$ can be written as $\Sigma_i \lambda_i \epsilon(u_i) \mu_i$, where λ_i, $\mu_i \in \mathcal{S}(\mathcal{F})$ and $u_i \in \mathcal{F}$. Let $C(G) = \mathcal{S}(\mathcal{F})/I(G)$ and define $j: \mathcal{F} \to C(G)$ as the composition of monomorphism $i: \mathcal{F} \to \mathcal{S}^1(\mathcal{F}) \subset \mathcal{S}(\mathcal{F})$ and projection $p: \mathcal{S}(\mathcal{F}) \to C(G)$. In this case pair $(C(G), j)$ is the solution of our problem. From the general properties of tensor algebras the homomorphism $\varphi: \mathcal{F} \to A$ can be extended to $\mathcal{S}(\mathcal{F})$, i.e., the diagram



is commutative, where ρ is a monorphism of algebras. Because $(\varphi(u))^2 = G(u) \cdot 1$, then ρ vanishes on ideal $I(G)$ and in this case the necessary homomorphism τ is defined. As a consequence of uniqueness of ρ, the homomorphism τ is unique.

Tensor d-algebra $\mathcal{S}(\mathcal{F})$ can be considered as a $\mathbb{Z}/2$ graded algebra. Really, let us introduce $\mathcal{S}^{(0)}(\mathcal{F}) = \Sigma_{i=1}^{\infty} T^{2i}(\mathcal{F})$ and $\mathcal{S}^{(1)}(\mathcal{F}) = \Sigma_{i=1}^{\infty} T^{2i+1}(\mathcal{F})$. Setting $I^{(\alpha)}(G) = I(G) \cap \mathcal{S}^{(\alpha)}(\mathcal{F})$ [$(\alpha) = (1),(2)$], we have $I(G) = I^{(0)}(G) \oplus I^{(1)}(G)$. Define $C^{(\alpha)}(G)$ as $p(\mathcal{S}^{(\alpha)}(\mathcal{F}))$, where $p: \mathcal{S}(\mathcal{F}) \to C(G)$ is the canonical projection. Then $C(G) = C^{(0)}(G) \oplus C^{(1)}(G)$ and in consequence we obtain that the Clifford d-algebra is $\mathbb{Z}/2$ graded.

It is obvious that Clifford d-algebra functorially depends on pair $(\mathcal{F}, G)$. If $f: \mathcal{F} \to \mathcal{F}'$ is a homomorphism of k-vector spaces, such that $G'(f(u)) = G(u)$, where G and G' are, respectively, metrics on $\mathcal{F}$ and $\mathcal{F}'$, then f induces an homomorphism of d-algebras

$$C(f): C(G) \to C(G')$$

with identities $C(\varphi \cdot f) = C(\varphi) C(f)$ and $C(\mathrm{Id}_{\mathcal{F}}) = \mathrm{Id}_{C(\mathcal{F})}$.

If $\mathcal{A}^{\alpha}$ and $\mathcal{B}^{\beta}$ are $\mathbb{Z}/2$-graded d-algebras, then their graded tensorial product $\mathcal{A}^{\alpha} \otimes \mathcal{B}^{\beta}$ is defined as a d-algebra for k-vector d-space $\mathcal{A}^{\alpha} \otimes \mathcal{B}^{\beta}$ with the graded product induced as $(a \otimes b)(c \otimes d) = (-1)^{\alpha\beta} ac \otimes bd$, where $b \in \mathcal{B}^{\beta}$ and $c \in \mathcal{A}^{\alpha}$ $(\alpha, \beta = 0,1)$.

Now we reformulate for d-algebras the Chevalley theorem.[19]

Theorem 2: The Clifford d-algebra $C(h\mathcal{F} \oplus v\mathcal{F}, g + q)$ is naturally isomorphic to $C(g) \hat{\otimes} C(q)$.

Proof: Let $n: h\mathcal{F} \to C(g)$ and $n': v\mathcal{F} \to C(q)$ be canonical maps and map $m: h\mathcal{F} \oplus v\mathcal{F} \to C(g) \hat{\otimes} C(q)$ is defined as $m(x, y) = n(x) \otimes 1 + 1 \otimes n'(y)$, $x \in h\mathcal{F}$, $y \in v\mathcal{F}$. We

have $(m(x,\,y))^2=[(n(x))^2+(n'(y))^2]\cdot 1=[g(x)+q(y)]$. Taking into account the universality property of Clifford d-algebras we conclude that m induces the homomorphism

$$\zeta: C(h\mathscr{F}\oplus v\mathscr{F}, g\oplus q)\to C(h\mathscr{F}, g)\hat{\otimes} C(v\mathscr{F}, q).$$

We also can define a homomorphism

$$\upsilon: C(h\mathscr{F},\, g)\hat{\otimes} C(v\mathscr{F},\, q)\to C(h\mathscr{F}\oplus v\mathscr{F},\, g\oplus q)$$

by using formula $\upsilon(x\otimes y)=\delta(x)\,\delta'(y)$, where homomorphisms δ and δ' are, respectively, induced by imbeddings of $h\mathscr{F}$ and $v\mathscr{F}$ into $h\mathscr{F}\oplus v\mathscr{F}$:

$$\delta: C(h\mathscr{F},\, g)\to C(h\mathscr{F}\oplus v\mathscr{F}, g\oplus q),$$

$$\delta': C(v\mathscr{F},\, q)\to C(h\mathscr{F}\oplus v\mathscr{F}, g\oplus q).$$

Because $x\in C^{(\alpha)}(g)$ and $y\in C^{(\alpha)}(q)$, $\delta(x)\,\delta'(y)=(-1)^{\alpha'}\delta'(y)\,\delta(x)$.

Superpositions of homomorphisms ζ and υ lead to identities

$$\begin{aligned}\upsilon\zeta&=\mathrm{Id}_{C(h\mathscr{F},\, g)\hat{\otimes} C(v\mathscr{F},\, q)},\\ \zeta\upsilon&=\mathrm{Id}_{C(h\mathscr{F},\, g)\hat{\otimes} C(v\mathscr{F},\, q)}.\end{aligned}\tag{13}$$

Really, d-algebra $C(h\mathscr{F}\oplus v\mathscr{F}, g+q)$ is generated by elements of type $m(x,\,y)$. Calculating

$$\upsilon\zeta(m(x,\,y))=\upsilon(n(x)\otimes 1+1\otimes n'(y))=\delta(n(x))\,\delta(n'(y))=m(x,\,0)+m(0,\,y)=m(x,\,y),$$

we prove the first identity in (13).

On the other hand, d-algebra $C(h\mathscr{F}, g)\hat{\otimes} C(v\mathscr{F}, q)$ is generated by elements of type $n(x)\otimes 1$ and $1\otimes n'(y)$. Because $(\zeta\upsilon)(n(x)\otimes 1)=\psi(\delta(n(x))=n(x)\otimes 1$ and $(\zeta\upsilon)(1\otimes n'(y))=\psi(\delta'(n(y))=1\otimes n'(y)$, we prove the second identity in (13).

Following from the above-mentioned properties of homomorphisms ζ and υ we can assert that the natural isomorphism is explicitly constructed. □

In consequence of theorem 2 we conclude that all operations with Clifford d-algebras can be reduced to calculations for $C(h\mathscr{F}, g)$ and $C(v\mathscr{F}, q)$ which are usual Clifford algebras of dimension 2^n and, respectively, 2^m.[16,20]

Of special interest is the case when $k=\mathbb{R}$ and $\mathscr{F}$ is isomorphic to vector space $\mathbb{R}^{p+q,a+b}$ provided with quadratic form $-x_1^2-\cdots-x_p^2+\cdots+x_{p+q}^2-y_1^2-\cdots-y_a^2+\cdots+y_{a+b}^2$. In this case, the Clifford algebra, denoted as $(C^{p,q},\, C^{a,b})$, is generated by symbols $e_1^{(x)}$, $e_2^{(x)},\ldots,e_{p+q}^{(x)}$, $e_1^{(y)}$, $e_2^{(y)},\ldots,e_{a+b}^{(y)}$ satisfying properties $(e_i)^2=-1$ $(1\leqslant i\leqslant p)$, $(e_j)^2=-1$ $(1\leqslant j\leqslant a)$, $(e_k)^2=1$ $(p+1\leqslant k\leqslant p+q)$, $(e_j)^2=1$ $(n+1\leqslant s\leqslant a+b)$, $e_ie_j=-e_je_i$, $i\neq j$. Explicit calculations of $C^{p,q}$ and $C^{a,b}$ are possible by using isomorphisms[16,18]

$$C^{p+n,q+n}\approx C^{p,q}\otimes M_2(\mathbb{R})\otimes\cdots\otimes M_2(\mathbb{R})\simeq C^{p,q}\otimes M_{2^n}(\mathbb{R})\cong M_{2^n}(C^{p,q}),$$

where $M_s(A)$ denotes the ring of quadratic matrices of order s with coefficients in ring A. Here we write the simplest isomorphisms $C^{1,0}\simeq\mathbb{C}$, $C^{0,1}\simeq\mathbb{R}\oplus\mathbb{R}$ and $C^{2,0}=\mathbb{H}$, where by $\mathbb{H}$ is denoted the body of quaternions. We summarize this calculus as (as in Ref. 20)

$$C^{0,0}=\mathbb{R},\quad C^{1,0}=\mathbb{C},\quad C^{0,1}=\mathbb{R}\oplus\mathbb{R},$$

$$C^{2,0}=\mathbb{H},\quad C^{0,2}=M_2(\mathbb{R}),\quad C^{3,0}=\mathbb{H}\oplus\mathbb{H},\quad C^{0,3}=M_2(\mathbb{R}),$$

$$C^{4,0}=M_2(\mathbb{H}),\quad C^{0,4}=M_2(\mathbb{H}),\quad C^{5,0}=M_4(\mathbb{C}),\quad C^{0,5}=M_2(\mathbb{H})\oplus M_2(\mathbb{H}),$$

$$C^{6,0}=M_8(\mathbb{R}),\quad C^{0,6}=M_4(\mathbb{H}),\quad C^{7,0}=M_8(\mathbb{R})\oplus M_8(\mathbb{R}),\quad C^{0,7}=M_8(\mathbb{C}),$$

$$C^{8,0}=M_{16}(\mathbb{R}),\quad C^{0,8}=M_{16}(\mathbb{R}).$$

One of the most important properties of real algebras $C^{0,p}(C^{0,a})$ and $C^{p,0}(C^{a,0})$ is the eightfold periodicity of $p(a)$.

Now, we emphasize that H^{2n}-spaces admit locally a structure of Clifford algebra on complex vector spaces. Really, by using almost Hermitian structure $J_\alpha{}^\beta$ and considering complex space $\mathbb{C}^n$ with nondegenerate quadratic form $\Sigma_{a=1}^{a}|z_a|^2$, $z_a\in\mathbb{C}^2$ induced locally by metric (8) (rewritten in complex coordinates $z_a=x_a+iy_a$) we define Clifford algebra $\check{C}^n=\underbrace{\check{C}^1\otimes\cdots\otimes\check{C}^L}_{n}$, where $\check{C}^1=\mathbb{C}\otimes_{\mathbb{R}}\mathbb{C}=\mathbb{C}\oplus\mathbb{C}$ or, in consequence, $\check{C}^n\simeq C^{n,0}\otimes_{\mathbb{R}}\mathbb{C}\simeq C^{0,n}\otimes_{\mathbb{R}}\mathbb{C}$. Explicit calculations lead to isomorphisms $\check{C}^2=C^{0,2}\otimes_{\mathbb{R}}\mathbb{C}\simeq M_2(\mathbb{R})\otimes_{\mathbb{R}}\mathbb{C}\simeq M_2(\mathbb{C})$, $\check{C}^{n+2}\simeq M_2(\check{C}^n)$, $C^{2p}\approx M_{2^p}(\mathbb{C})$ and $\check{C}^{2p+1}\approx M_{2^p}(\mathbb{C})\oplus M_{2^p}(\mathbb{C})$, which show that complex Clifford algebras, defined locally for H^{2n}-spaces, have periodicity 2 on p.

Considerations presented in the proof of theorem 2 show that map $j:\mathscr{F}\to C(\mathscr{F})$ is monomorphic, so we can identify space $\mathscr{F}$ with its image in $C(\mathscr{F},G)$. On the other hand, endomorphism $u\to -u$ of space $\mathscr{F}$ induces an involution on $C(\mathscr{F},G)$, denoted as $u\to\bar{u}$, if $u\in C^{(0)}(\mathscr{F},G)$ ($u\in C^{(1)}(\mathscr{F},G)$); then $u=\bar{u}$ (respectively, $\bar{u}=-u$).

Definition 6: The set of elements $u\in C(G)^*$, where $C(G)^*$ denotes the multiplicative group of invertible elements of $C(\mathscr{F},G)$ satisfying $\bar{u}\mathscr{F}u^{-1}\in\mathscr{F}$, is called the *twisted Clifford d-group*, denoted as $\tilde{\Gamma}(\mathscr{F})$.

Let $\tilde{\rho}:\tilde{\Gamma}(\mathscr{F})\to GL(\mathscr{F})$ be the homomorphism given by $u\to\rho\tilde{u}$, where $\tilde{\rho}_u(w)=\bar{u}wu^{-1}$. We can verify that $\ker\tilde{\rho}=\mathbb{R}^*$ is a subgroup in $\tilde{\Gamma}(\mathscr{F})$.

Canonical map $j:\mathscr{F}\to C(\mathscr{F})$ can be interpreted as the linear map $\mathscr{F}\to C(\mathscr{F})^0$ satisfying the universal property of Clifford d-algebras. This leads to a homomorphism of algebras, $C(\mathscr{F})\to C(\mathscr{F})^t$, considered by an anti-involution of $C(\mathscr{F})$ and denoted as $u\to{}^tu$. More exactly, if $\lambda\in u_1\cdots u_n\in\mathscr{F}$, then ${}^tu=u_n\cdots u_1$ and ${}^t\bar{u}=\overline{{}^tu}=(-1)^nu_n\cdots u_1$.

Definition 7: The spinor norm of arbitrary $u\in C(\mathscr{F})$ is defined as $S(u)={}^t\bar{u}\cdot u\in C(\mathscr{F})$.

It is obvious that if $u,u',u''\in\tilde{\Gamma}(\mathscr{F})$, then $S(u,u')=S(u)S(u')$ and $S(uu'u'')=S(u)S(u')S(u'')$. For $u,u'\in\mathscr{F}$ $S(u)=-G(u)$ and $S(u,u')=S(u)S(u')=S(u'u)$.

Let us introduce the orthogonal group $\mathrm{O}(G)\subset GL(G)$ defined by metric G on $\mathscr{F}$ and denote sets $\mathrm{SO}(G)=\{u\in\mathrm{O}(G),\ \det|u|=1\}$, $Pin(G)=\{u\in\tilde{\Gamma}(\mathscr{F}),\ \mathrm{S}(u)=1\}$ and $Spin(G)=Pin(G)\cap C^0(\mathscr{F})$. For $\mathscr{F}\cong\mathbb{R}^{n+m}$ we write $Spin(n+m)$. By straightforward calculations (see similar considerations in Ref. 16) we can verify the exactness of these sequences:

$$1\to\mathbb{Z}/2\to Pin(G)\to\mathrm{O}(G)\to 1,$$

$$1\to\mathbb{Z}/2\to Spin(G)\to\mathrm{SO}(G)\to 0,$$

$$1\to\mathbb{Z}/2\to Spin(n+m)\to\mathrm{SO}(n+m)\to 1.$$

We conclude this section by emphasizing that the spinor norm was defined with respect to a quadratic form induced by a metric in the v-bundle ξ_d (or by an H^{2n}-metric in the case of GL-spaces). This approach differs from that presented in Refs. 5 and 9.

IV. CLIFFORD BUNDLES AND SPINOR STRUCTURES ON VECTOR BUNDLES AND GL-SPACES

There are two possibilities for generalizing our spinor constructions defined for d-vector spaces to the case of vector bundle spaces with the structure of N-connection. The first is to use

the extension to the category of vector bundles. The second is to define the Clifford fibration associated with compatible linear d-connection and metric G on a vector bundle (or with an H^{2n}-metric on GL-space). Let us consider both variants.

A. Clifford *d*-module structures in vector bundles

Because functor $\mathscr{F}\to C(\mathscr{F})$ is smooth we can extend it to the category of vector bundles of type $\xi_d=\{\pi_d: HE\oplus VE\to E\}$. Recall that by $\mathscr{F}$ we denote the typical fiber of such bundles. For ξ_d we obtain a bundle of algebras, denoted as $C(\xi_d)$, such that $C(\xi_d)_u=C(\mathscr{F}_u)$. Multiplication in every fiber defines a continuous map $C(\xi_d)\times C(\xi_d)\to C(\xi_d)$. If ξ_d is a vector bundle on number field k, the structure of the $C(\xi_d)$-module, the d-module, on ξ_d is given by the continuous map $C(\xi_d)x_E\xi_d\to\xi_d$ with every fiber $\mathscr{F}_u$ provided with the structure of the $C(\mathscr{F}_u)$-module, correlated with its k-module structure. Because $\mathscr{F}\subset C(\mathscr{F})$, we have a fiber to fiber map $\mathscr{F}x_E\xi_d\to\xi_d$, inducing on every fiber the map $\mathscr{F}_u x_E\xi_{d(u)}\to\xi_{d(u)}$ ($\mathbb{R}$-linear on the first factor and k-linear on the second one). Inversely, every such bilinear map defines on ξ_d the structure of the $C(\xi_d)$-module by virtue of universal properties of Clifford d-algebras. Equivalently, the above-mentioned bilinear map defines a morphism of v-bundles $m:\xi_d\to\mathrm{HOM}(\xi_d,\xi_d)$ [$\mathrm{HOM}(\xi_d,\xi_d)$ denotes the bundle of homomorphisms] when $(m(u))^2=G(u)$ on every point.

Vector bundles ξ_d provided with $C(\xi_d)$-structure are objects of the category with morphisms being morphisms of v-bundles, which induce on every point $u\in\xi$ morphisms of $C(\xi_d)$-modules. This is a Banach category contained in the category of finite-dimensional d-vector spaces on field k. We shall not use category formalism in this work, but point to its advantages in further formulation of new directions of K-theory (see, for example, an introduction in Ref. 16) concerned with generalized Lagrange spaces.

Let us denote by $H^s(\xi,GL_{n+m}(\mathbb{R}))$ the s-dimensional cohomology group of the algebraic sheaf of germs of continuous maps of v-bundle ξ with group $GL_{n+m}(\mathbb{R})$ the group of automorphisms of $\mathbb{R}^{n+m}$ (for the language of algebraic topology see, for example, Refs. 16 and 21). We shall also use the group $SL_{n+m}(\mathbb{R})=\{A\subset GL_{n+m}(\mathbb{R}),\ \det A=1\}$. Here we point out that cohomologies $H^s(M,\mathrm{Gr})$ characterize the class of a principal bundle $\pi:P\to M$ on M with structural group Gr. Taking into account that we deal with bundles distinguished by an N-connection we introduce into consideration cohomologies $H^s(\xi,GL_{n+m}(\mathbb{R}))$ as distinguished classes (d-classes) of bundles ξ provided with a global N-connection structure.

For a real vector bundle ξ_d on compact base ξ we can define the orientation on ξ_d as an element $\alpha_d\in H^1(\xi,GL_{n+m}(\mathbb{R}))$ whose image on map

$$H^1(\xi,SL_{n+m}(\mathbb{R}))\to H^1(\xi,GL_{n+m}(\mathbb{R}))$$

is the d-class of bundle ξ.

Definition 8: The spinor structure on ξ_d is defined as the element $\beta_d\in H^1(\xi,Spin(n+m))$ whose image in the composition

$$H^1(\xi,Spin(n+m))\to H^1(\xi,\mathrm{SO}(n+m))\to H^1(\xi,GL_{n+m}(\mathbb{R}))$$

is the d-class of ξ.

The above definition of spinor structures can be reformulated in terms of principal bundles. Let ξ_d be a real vector bundle of rank $n+m$ on a compact base ξ. If there is a principal bundle P_d with structural group $\mathrm{SO}(n+m)$ [or $Spin(n+m)$], this bundle ξ_d can be provided with orientation (or spinor) structure. The bundle P_d is associated with element $\alpha_d\in H^1(\xi,\mathrm{SO}(n+m))$ [or $\beta_d\in H^1(\xi,Spin(n+m))$].

We remark that a real bundle is oriented if and only if its first Stiefel–Whitney d-class vanishes,

$$w_1(\xi_d)\in H^1(\xi,\mathbb{Z}/2)=0,$$

where $H^1(\xi/\mathbb{Z}/2)$ is the first group of Chech cohomology with coefficients in $\mathbb{Z}/2$. Considering the second Stiefel–Whitney class $w_2(\xi_d) \in H^2(\xi,\mathbb{Z}/2)$ it is well known that vector bundle ξ_d admits the spinor structure if and only if $w_2(\xi_d)=0$. Finally, in this subsection, we emphasize that taking into account that base space ξ is also a v-bundle, $p:E\to M$, we have to make explicit calculations in order to express cohomologies $H^s(\xi,GL_{n+m})$ and $H^s(\xi,\mathrm{SO}(n+m))$ through cohomologies $H^s(M,GL_n)$, $H^s(M,\mathrm{SO}(n))$, which depends on global topological structures of spaces M and ξ. For general bundle and base spaces this requires a cumbersome cohomological calculus.

B. Clifford fibration

Another way of defining the spinor structure is to use Clifford fibrations. Consider the principal bundle with the structural group Gr being a subgroup of orthogonal group $\mathrm{O}(G)$, where G is a quadratic nondegenerate form [see (8)] defined on the base (also being a bundle space) space ξ [we deal with H^{2n}-metric (11) in the case when the base space is a H^{2n}-space] and denote it as $P(\xi, \mathrm{Gr})$ [$P(H^{2n}, \mathrm{Gr})$]. The fibration associated to principal fibration $P(\xi, \mathrm{Gr})$ [or $P(H^{2n}, \mathrm{Gr})$] with a typical fiber having Clifford algebra $C(G)$ is, by definition, the Clifford fibration $PC(\xi, \mathrm{Gr})$ [or $PC(H^{2n}, \mathrm{Gr})$]. We can always define a metric on the Clifford fibration if every fiber is isometric to $PC(\xi, G)$ (this result is proved for arbitrary quadratic forms G on pseudo-Riemannian bases[17]). If, additionally, $\mathrm{Gr}\subset\mathrm{SO}(G)$ a global section can be defined on $PC(G)$.

Let $\mathscr{P}(\xi, \mathrm{Gr})$ [or $\mathscr{P}(H^{2n}, \mathrm{Gr})$] be the set of principal bundles with differentiable base ξ (or H^{2n}-space) and structural group Gr. If $g:\mathrm{Gr}\to\mathrm{Gr}'$ is an homomorphism of Lie groups and $P(\xi, \mathrm{Gr})\subset\mathscr{P}(\xi, \mathrm{Gr})$ [or $P(H^{2n}, \mathrm{Gr})\subset\mathscr{P}(H^{2n}, \mathrm{Gr})$] (for simplicity in this section we shall denote mentioned bundles and sets of bundles as P, P' and, respectively, $\mathscr{P}$, $\mathscr{P}'$], we can always construct a principal bundle with the property that there is an homomorphism $f:P'\to P$ of principal bundles which can be projected to the identity map of ξ (or H^{2n}) and corresponds to isomorphism $g:\mathrm{Gr}\to\mathrm{Gr}'$. If the inverse statement also holds the bundle P' is called as the extention of P associated to $\mathbf{g}$ and f is called the extension homomorphism denoted as $\tilde{\mathbf{g}}$.

Now we can define distinguished spinor structures on bundle spaces (compare with definition 8).

Definition 9: Let $P\in\mathscr{P}(\xi,O(G))$ [or $P\in\mathscr{P}(H^{2n}), O(G)$] be a principal bundle. A distinguished spinor structure of P, equivalently a ds-structure on ξ (or on H^{2n}) is an extension $\tilde{P}$ of P associated to homomorphism $h:PinG\to\mathrm{O}(G)$ where $\mathrm{O}(G)$ is the group of orthogonal rotations, generated by metric G, in bundle ξ (or in H^{2n}-space).

So, if $\tilde{P}$ is a spinor structure of the space ξ (or H^{2n}), then $\tilde{P}\in\mathscr{P}(\xi,PinG)$ [or $\tilde{P}\in\mathscr{P}(H^{2n}, PinG)$].

The definition of spinor structures on varieties was given in Ref. 22. In Refs. 23 and 24 it is proved that a necessary and sufficient condition for a space time to be orientable is to admit a global field of orthonormal frames. We mention that spinor structures can be also defined on varieties modeled on Banach spaces.[25] As we have shown in this subsection, similar constructions are possible for the cases when space time has the structure of a v-bundle with an N-connection (or an H^{2n}-space).

Definition 10: A special distinguished spinor structure, ds-structure, of principal bundle $P=P(\xi,\mathrm{SO}(G))$ [or $P=P(H^{2n},\mathrm{SO}(G))$] is a principal bundle $\tilde{P}=\tilde{P}(\xi,SpinG)$ [or $\tilde{P}=\tilde{P}(H^{2n},SpinG)$] for which a homomorphism of principal bundles $\tilde{p}:\tilde{P}\to P$, projected on the identity map of ξ (or of H^{2n}) and corresponding to representation

$$R:SpinG\to\mathrm{SO}(G),$$

is defined.

In the case when the base space variety is oriented, there is a natural bijection between tangent spinor structures and special spinor structures with a common base. For special ds-structures we

can define, as for any spinor structure, the concepts of spin tensors, spinor connections, and spinor covariant derivations (see Sec. VI in this paper) a detailed version will be presented in Ref. 26).

V. ALMOST COMPLEX SPINOR STRUCTURES ON GENERALIZED LAGRANGE SPACES

Almost complex structures are an important characteristic of H^{2n}-spaces. As we have mentioned in Sec. IV, we can rewrite H^{2n}-metric (11) in complex form:

$$G=H_{ab}(z,\xi)dz^a\otimes dz^b, \tag{14}$$

where

$$z^a=x^a+iy^a,\quad \bar{z}^a=x^a-iy^a,\quad H_{ab}(z,\bar{z})=g_{ab}(x,y)\big|^{x=x(z,\bar{z})}_{y=y(z,\bar{z})},$$

and define almost complex spinor structures. For given metric (14) on H^{2n}-space there is always a principal bundle P^U with unitary structural group $\mathrm{U}(n)$ which allows us to transform H^{2n}-space into v-bundle $\xi^U\approx P^U x_{U(n)}\mathbb{R}^{2n}$. This statement will be proved after we introduce complex spinor structures on oriented real vector bundles.[16]

Let us consider momentarily $k=\mathbb{C}$ and introduce into consideration [instead of the group $Spin(n)$] the group $Spin^c(n)=Spin(n)x_{\mathbb{Z}/2}$, $\mathrm{U}(1)$ being the factor group of the product $Spin(n)xU(1)$ with the respect to equivalence

$$(y,\ a)\sim(-y,\ -a),\quad y\in Spin(m).$$

This way we define the short exact sequence

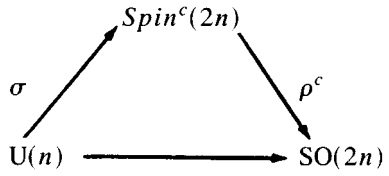
$$1\to \mathrm{U}(1)\to Spin^c(n)\overset{S^c}{\to}\mathrm{SO}(n)\to 1,$$

where $\rho^c(y,a)=\rho^c(y)$. If λ is a oriented, real, and rank n, γ-bundle $\pi:E_\lambda\to M^n$, with base M^n, the complex spinor structure, spin structure, on λ is given by the principal bundle P with structural group $Spin^c(m)$ and isomorphism $\lambda\approx Px_{Spin^c(n)}\mathbb{R}^n$. For such bundles the categorial equivalence can be defined as

$$\epsilon^c:\mathscr{E}^T_{\mathbb{C}}(M^n)\to\mathscr{E}^\lambda_{\mathbb{C}}(M^n), \tag{15}$$

where $\epsilon^c(E^c)=P\Delta_{Spin^c(n)}E^c$ is the category of trivial complex bundles on M^n, $\mathscr{E}^\lambda_{\mathbb{C}}(M^n)$ is the category of complex v-bundles on M^n with action of Clifford bundle $C(\lambda)$, $P\Delta_{Spin^c(n)}$ and E^c is the factor space of the bundle product Px_ME^c with respect to the equivalence $(p,\ e)\sim(p\hat{g}^{-1},\ \hat{g}e)$, $p\in P$, $e\in E^c$, where $\hat{g}\in Spin^c(n)$ acts on E by via the imbedding $Spin(n)\subset C^{o,n}$ and the natural action $\mathrm{U}(1)\subset\mathbb{C}$ on complex v-bundle ξ^c, $E^c=\mathrm{tot}\,\xi^c$, for bundle $\pi^c:E^c\to M^n$.

Now we return to the bundle ξ. A real v-bundle (not being a spinor bundle) admits a complex spinor structure if and only if there exists a homomorphism $\sigma:\mathrm{U}(n)\to Spin^c(2n)$ making the diagram



commutative. The explicit construction of σ for arbitrary γ-bundles is given in Refs. 16 and 20. For H^{2n}-spaces it is obvious that a diagram similar to (16) can be defined for the tangent bundle TM^n, which directly points to the possibility of defining the ${}^cSpin$-structure on H^{2n}-spaces.

Let λ be a complex, rank n, spinor bundle with

$$\tau: Spin^c(n) x_{\mathbb{Z}/2} \mathrm{U}(1) \to \mathrm{U}(1) \tag{17}$$

the homomorphism defined by formula $\tau(\lambda,\delta)=\delta^2$. For P_S being the principal bundle with fiber $Spin^c(n)$ we introduce the complex linear bundle $L(\lambda^c) = P_S x_{Spin^c(n)} \mathbb{C}$ defined as the factor space of $P_S x \mathbb{C}$ on equivalence relation $(pt,z)\sim(p,l(t)^{-1}z)$, where $t \in Spin^c(n)$. This linear bundle is associated to complex spinor structure on λ^c.

If λ^c and $\lambda^{c'}$ are complex spinor bundles, the Whitney sum $\lambda^c \oplus \lambda^{c'}$ is naturally provided with the structure of the complex spinor bundle. This follows from the holomorphism

$$\omega^c: Spin^c(n) \times Spin^c(n') \to Spin^c(n+n'), \tag{18}$$

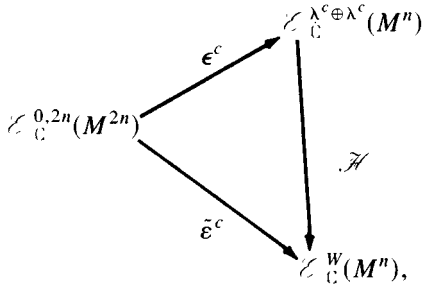
given by formula $[(\beta, z),(\beta', z')] \to [\omega(\beta, \beta'), zz']$, where ω is the homomorphism making the following diagram commutative;

$$\begin{array}{ccc} Spin(n)\times Spin(n') & \longrightarrow & Spin(n+n') \\ \downarrow & & \downarrow \\ \mathrm{O}(n)\times \mathrm{O}(n') & \longrightarrow & \mathrm{O}(n+n') \end{array}$$

Here, $z,z' \in \mathrm{U}(1)$. It is obvious that $L(\lambda^c \oplus \lambda^{c'})$ is isomorphic to $L(\lambda^c) \otimes L(\lambda^{c'})$.

We conclude this section by formulating our main result on complex spinor structures for H^{2n}-spaces:

Theorem: Let λ^c be a complex spinor bundle of rank n and H^{2n}-space considered as a real vector bundle $\lambda^c \oplus \lambda^c$ provided with almost complex structure $J^\alpha{}_\beta$; multiplication on i is given by $\begin{pmatrix} 0 & -\delta^i_j \\ \delta^i_j & 0 \end{pmatrix}$. Then, the diagram below is commutative up to isomorphism

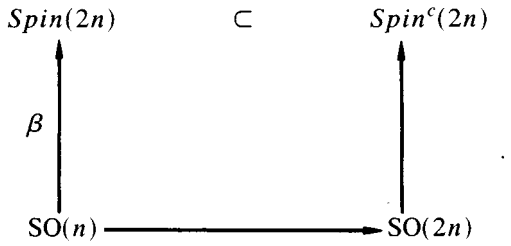


where ϵ^c and $\tilde{\epsilon}^c$ are defined as in (15), $\mathscr{H}$ is functor $E^c \to E^c \otimes L(\lambda^c)$ and $\mathscr{E}_{\mathbb{C}}^{0,2n}(M^n)$ is defined by functor $\mathscr{E}_{\mathbb{C}}(M^n) \to \mathscr{E}_{\mathbb{C}}^{0,2n}(M^n)$ given as correspondence $E^c \to \Lambda(\mathbb{C}^n) \otimes E^c$ (which is a categorial equivalence), $\Lambda(\mathbb{C}^n)$ is the exterior algebra on $\mathbb{C}^n$. W is the real bundle $\lambda^c \oplus \lambda^c$ provided with complex structure.

Proof: We use composition of homomorphisms

$$\mu: Spin^c(2n) \overset{\pi}{\to} \mathrm{SO}(n) \overset{r}{\to} \mathrm{U}(n) \overset{\sigma}{\to} Spin^c(2n) = Spin(2n) x_{\mathbb{Z}/2} \mathrm{U}(1),$$

commutative diagram



and introduce composition of homomorphisms

$$\mu: Spin^c(n) \overset{\Delta}{\to} Spin^c(n) \times Spin^c(n) \overset{\omega^c}{\to} Spin^c(n),$$

where Δ is the diagonal homomorphism and ω^c is defined as in (18). Using homomorphisms (17) and (18) we obtain formula $\mu(t) = \mu(t) r(t)$.

Now we consider bundle $Px_{Spin^c(n)} Spin^c(2n)$ as the principal $Spin^c(2n)$-bundle, associated to $M \oplus M$ being the factor space of the product $PxSpin^c(2n)$ on the equivalence relation $(p, t, h) \sim (p, \mu(t)^{-1} h)$. In this case the categorial equivalence (15) can be rewritten as

$$\epsilon^c(E^c) = Px_{Spin^c(n)} Spin^c(2n) \Delta_{Spin^c(2n)} E^c$$

and seen as factor space of $PxSpin^c(2n) x_M E^c$ on equivalence relation $(pt, h, e) \sim (p, \mu(p)^{-1} h, e)$ and $(p, h_1, h_2, e) \sim (p, h_1, h_2^{-1} e)$ (projections of elements p and e coincides on base M). Every element of $\epsilon^c(E^c)$ can be represented as $P\Delta_{Spin^c(n)} E^c$, i.e., as factor space of $Px_M E^c$ on equivalence relation $(pt, e) \sim (p, \mu(t)^{-1} e)$, where $t \in Spin^c(n)$.

On the other hand, the principal $Spin^c(2n)$-bundle associated to complex structure on $M \oplus M$ is $Px_{Spin^c(n)} Spin^c(2n)$ and in consequence $\epsilon^c(E^c)$ can be represented as $P\Delta_{Spin^c(n)} E^c$, i.e., as a factor space $P\Delta E^c$ on equivalence relation $(pt, e) \sim (p, \mu^c(t)^{-1}, e)$, when $t \in Spin^c(n)$.

The complex line bundle $L(\lambda^c)$ can be interpreted as the factor space of $Px_{Spin^c(n)} \mathbb{C}$ on equivalence relation $(pt, \delta) \sim (p, r(t)^{-1} \delta)$.

Putting $(p, e) \otimes (p, \delta)(p, \delta e)$ we introduce morphism

$$\epsilon^c(E) \times L(\lambda^c) \to \epsilon^c(\lambda^c)$$

with properties $(pt, e) \otimes (pt, \delta) \to (pt, \delta e) = (p, \mu^c(t)^{-1} \delta e)$, $(p, \mu^c(t)^{-1} e) \otimes (p, l(t)^{-1} e) \to (p, \mu^c(t) r(t)^{-1} \delta e)$ pointing to the fact that we have defined the isomorphism correctly and that it is an isomorphism on every fiber. □

VI. SPINORS IN VECTOR BUNDLES WITH NONLINEAR CONNECTIONS

In this section we present a brief introduction to the theory of d-spinors in v-bundles and H^{2n}-spaces. To generate Clifford d-algebra we start with Clifford–Dirac equations written in the form[18]

$$\sigma_\alpha(u) \sigma_\beta(u) + \sigma_\beta(u) \sigma_\alpha(u) = -G_{\alpha\beta}(u) I, \tag{19}$$

where distinguished complex matrices $\sigma_\alpha(u)$ are parametrized as

$$\sigma_\alpha(u) = \begin{pmatrix} \sigma_i(u) & 0 \\ 0 & \sigma_a(u) \end{pmatrix},$$

$\sigma_i(u)$, $\sigma_a(u)$ being matrices of dimension $N_h \times N_h$ ($N_v \times N_v$) $N_h = 2^{n/2}$ ($N_v = 2^{m/2}$ for even values of $n(m)$ and $N_h = 2^{(n+1)/2}$ ($N_v = 2^{(m+1)/2}$) for odd values of $n(m)$.

To relate the succeeding constructions with Clifford d-algebra (see Sec. III) it is convenient to use frame decomposition of metric (8) [or (11)]:

$$G_{\alpha\beta}=l^{\hat{\alpha}}_{\alpha}(u)l^{\hat{\beta}}_{\beta}(u)g_{\hat{\alpha}\hat{\beta}},$$

where the frame components are distinguished as

$$l^{\hat{\alpha}}_{\alpha}(u)=\begin{pmatrix} l^{\hat{i}}_{j}(u) & 0 \\ 0 & l^{\hat{a}}_{a}(u) \end{pmatrix}, \quad g_{\hat{\alpha}\hat{\beta}}=\begin{pmatrix} g_{\hat{i}\hat{j}} & 0 \\ 0 & g_{\hat{a}\hat{b}} \end{pmatrix},$$

where $g_{\hat{i}\hat{j}}$ and $g_{\hat{a}\hat{b}}$ are diagonal matrices with $g_{\hat{i}\hat{j}}=g_{\hat{a}\hat{b}}=\pm 1$. In general, we can treat indices $\hat{\alpha},\hat{\beta},\hat{i},j,\hat{a},\hat{b},\ldots$ as abstract tensorial indices.[18]

Introducing matrices $\sigma_{\hat{\alpha}}=l^{\alpha}_{\hat{\alpha}}\sigma_{\alpha}$ (matrix $l^{\alpha}_{\hat{\alpha}}$ is inverse to $l^{\hat{\alpha}}_{\alpha}$) we rewrite Eqs. (17) as algebraic equations for components of constant matrices σ^{n}_{α}:

$$\sigma_{\hat{\alpha}}\sigma_{\hat{\beta}}+\sigma_{\hat{\beta}}\sigma_{\hat{\alpha}}=-G_{\hat{\alpha}\hat{\beta}}I. \tag{20}$$

We consider that matrices $\sigma_{\hat{\alpha}}$ act on corresponding d-vector space $\mathscr{F}=h\mathscr{F}\oplus v\mathscr{F}$. To specify elements we can introduce abstract spinor indices [locally adapted to bases (4) and (5)]:

$$\sigma_{\hat{\alpha}}=\left\{(\sigma_{\hat{\alpha}})_{\rho}{}^{\gamma}=\begin{pmatrix} (\sigma_{\hat{i}})_{j}{}^{k} & 0 \\ 0 & (\sigma_{\hat{a}})_{b}{}^{c} \end{pmatrix}\right\},$$

where ρ, γ,... refer to spin space $S=S_{(h)}\oplus S_{(v)}$; j, k and b, c refer, respectively, to spin spaces $S_{(h)}$ and $S_{(v)}$ [$S_{(h)}$ and $S_{(v)}$ are associated to h- and, respectively, γ-decomposition of bundle ξ_d (of H^{2n}-space)]. Suggesting that algebra generated by σ_2 is irreducible, it is necessary that $\dim S_{(h)}=N_{(h)}$ and, respectively, $\dim S_{(v)}=N_{(v)}$, where

$$N_{(h)}=\begin{cases} 2^{n/2}, & n=2k, \\ 2^{(n-1)/2}, & n=2k+1, \end{cases} \quad \text{and} \quad N_{(v)}=\begin{cases} 2^{m/2}, & m=2k, \\ 2^{(m-1)/2}, & m=2k+1 \end{cases}$$

[the minimal dimension of matrices satisfying Eqs. (18) is $N\times N$, where $N=N_{(h)}+N_{(v)}$].

The Clifford d-algebra is generated by sums of $n+1$ elements of the form

$$A_1 I+B^{\hat{i}}\sigma_{\hat{i}}+C^{\hat{i}\hat{j}}\sigma_{\hat{i}\hat{j}}+D^{\hat{i}\hat{j}\hat{k}}\sigma_{\hat{i}\hat{j}\hat{k}}+\cdots \tag{21}$$

and sums of $m+1$ elements of the form

$$A_2 I+B^{\hat{a}}\sigma_{\hat{a}}+C^{\hat{a}\hat{b}}\sigma_{\hat{a}\hat{b}}+D^{\hat{a}\hat{b}\hat{c}}\sigma_{\hat{a}\hat{b}\hat{c}}+\cdots$$

with antisymmetric coefficients $C^{\hat{i}\hat{j}}=C^{[\hat{i}\hat{j}]}$, $C^{\hat{a}\hat{b}}=C^{[\hat{a}\hat{b}]}$, $D^{\hat{i}\hat{j}\hat{k}}=D^{[\hat{i}\hat{j}\hat{k}]}$, $D^{\hat{a}\hat{b}\hat{c}}=D^{[\hat{a}\hat{b}\hat{c}]}$,... and matrices $\sigma_{\hat{i}\hat{j}}=\sigma_{[\hat{i}}\sigma_{\hat{j}]}$, $\sigma_{\hat{a}\hat{b}}=\sigma_{[\hat{a}}\sigma_{\hat{b}]}$, $\sigma_{\hat{i}\hat{j}\hat{k}}=\sigma_{[\hat{i}}\sigma_{\hat{j}}\sigma_{\hat{k}]}$,... . Really, we have 2^{n+1} coefficients $(A_1,C^{\hat{i}\hat{j}},D^{\hat{i}\hat{j}\hat{k}},\ldots)$ and 2^{m+1} coefficients $(A_2,C^{\hat{a}\hat{b}},D^{\hat{a}\hat{b}\hat{c}},\ldots)$ of Clifford d-algebra on $\mathscr{F}$.

Let us define finite (because of a finite number of elements $\sigma_{[\hat{i},\hat{j},\ldots,\hat{k}]}$ and $\sigma_{[\hat{a}\hat{b}\cdots\hat{c}]}$) sums:

$${}^{(\pm)}E^{ij}_{km}=\delta^{i}_{k}\delta^{j}_{m}+\frac{2}{1!}(\sigma_{\hat{i}})_{k}{}^{i}(\sigma^{\hat{i}})_{m}{}^{j}+\frac{2^2}{2!}(\sigma_{\hat{i}\hat{j}})_{k}{}^{i}(\sigma^{\hat{i}\hat{j}})_{m}{}^{j}+\frac{2^3}{3!}(\sigma_{\hat{i}\hat{j}\hat{k}})_{k}{}^{i}(\sigma^{\hat{i}\hat{j}\hat{k}})_{m}{}^{j}+\cdots, \tag{22}$$

$${}^{(\pm)}E^{ab}_{cd}=\delta^{a}_{c}\delta^{b}_{d}+\frac{2}{1!}(\sigma_{\hat{a}})_{c}{}^{a}(\sigma^{\hat{a}})_{d}{}^{b}+\frac{2^2}{2!}(\sigma_{\hat{a}\hat{b}})_{c}{}^{a}(\sigma^{\hat{a}\hat{b}})_{d}{}^{b}+\frac{2^3}{3!}(\sigma_{\hat{a}\hat{b}\hat{c}})_{c}{}^{a}(\sigma^{\hat{a}\hat{b}\hat{c}})_{d}{}^{b}+\ldots. \tag{23}$$

TABLE I. Symmetry properties of ϵ-objects (O, S, and A denote correspondingly vanishing, symmetry, and antisymmetry of ϵ-objects).

n(mod 8) [m(mod 8)]	${}^{(+)}\epsilon_{lm}$, ${}^{(+)}\epsilon^{lm}$ (${}^{(+)}\epsilon_{ab}$, ${}^{(+)}\epsilon^{ab}$)	${}^{(-)}\epsilon_{lm}$, ${}^{(-)}\epsilon^{lm}$ (${}^{(-)}\epsilon_{ab}$, ${}^{(-)}\epsilon^{ab}$)
0	S	S
1	O	S
2	A	S
3	A	O
4	A	A
5	O	A
6	S	A
7	S	O

E-objects (22) can be factorized as

$$
\begin{aligned}
&{}^{(\pm)}E^{ij}_{km}=N_{(h)}\,{}^{(\pm)}\epsilon_{km}\,{}^{(\pm)}\epsilon^{ij}, \quad \text{for } n=2k,\\
&{}^{(+)}E^{ij}_{km}=2N_{(h)}\epsilon_{km}\epsilon^{ij}, {}^{(-)}E^{ij}_{km}=0, \quad \text{for } n=3(\text{mod } 4),\\
&{}^{(+)}E^{ij}_{km}=0, \quad {}^{(-)}E^{ij}_{km}=2N_{(h)}\epsilon_{km}\epsilon^{ij}, \quad \text{for } n=1(\text{mod } 4)
\end{aligned}
\tag{24}
$$

[in a similar manner we can factorize E-objects (23), correspondingly, for values $m=2k$, $m=3(\text{mod } 4)$ and $m=1(\text{mod } 4)$].

From definition (21), factorization (24), and antisymmetry of $\sigma_{\hat{i}\hat{j}\hat{k}\ldots}$ and $\sigma_{\hat{a}\hat{b}\hat{c}\ldots}$ one follows the symmetry properties of ϵ-objects summarized in Table I (coordinated with canonical isomorphisms of Clifford algebras $C^{p,0}$ and $C^{0,p}$; see Sec. III in this work and similar considerations for isotropic spaces in Ref. 18. We omit proofs which in most cases are mechanical but rather tedious. By straightforward calculations the presented formulas show direct relationships between relations for Clifford d-algebra (21)–(25) and symmetric properties of spinor metrics and σ-objects on the corresponding periodicity of dimensions n and m (see Tables I and II).

For even values of $n(m)$ we can continue reduction of ${}^{\pm}E$- and ${}^{\pm}\epsilon$-objects. We define new ϵ-objects

$$
\begin{aligned}
&\epsilon^{lm}=\tfrac{1}{2}({}^{(+)}\epsilon^{lm}+{}^{(-)}\epsilon^{lm}), \quad \epsilon_{lm}=\tfrac{1}{2}({}^{(+)}\epsilon_{lm}+{}^{(-)}\epsilon_{lm}),\\
&\tilde{\epsilon}^{lm}=\tfrac{1}{2}({}^{(+)}\epsilon^{lm}-{}^{(-)}\epsilon^{lm}), \quad \epsilon_{lm}=\tfrac{1}{2}({}^{(+)}\epsilon_{lm}-{}^{(-)}\epsilon_{lm})
\end{aligned}
$$

TABLE II. ϵ-isomorphisms.

n	Spinor metrics		Juggling of indices	Canonical isomorphisms
0 (mod 4)	$\epsilon^{MN}=-\epsilon^{NM}$, $\epsilon_{MN}=-\epsilon_{NM}$,	$\epsilon^{M'N'}=-\epsilon^{N'M'}$ $\epsilon_{M'N'}=-\epsilon_{N'M'}$	$\zeta_{A'}=\epsilon_{A'B'}\zeta^{B'}$, $\zeta^{A}=\epsilon^{AB}\zeta_{B}$	$S_{(h)}\cong\tilde{S}'_{(h)}$ $\tilde{S}_{(h)}\cong S'_{(h)}$
2 (mod 4)	$\epsilon^{RS'}$, $\epsilon^{R'S}$,	$\epsilon_{RS'}$ $\epsilon_{R'S}$	$\zeta_{A'}=\epsilon_{A'B}\zeta^{B}$, $\zeta^{A'}=\epsilon^{A'B}\zeta_{B}$	$S_{(h)}\cong\tilde{S}'_{(h)}$ $S'_{(h)}\cong\tilde{S}_{(h)}$
$2k+1$ $k=0,1,2,\ldots$	ϵ^{lm},	ϵ_{lm}	$\zeta_{l}=\epsilon_{lm}\zeta^{m}$, $\zeta^{m}=\epsilon^{mn}\zeta_{n}$	$S_{(h)}\cong\tilde{S}_{(h)}$

(by similar formulas we introduce objects ϵ^{ab}, ϵ_{ab}, $\tilde{\epsilon}^{ab}$, $\tilde{\epsilon}_{ab}$ on fibers of bundle ξ_d). For simplicity, hereafter, in this section, we shall restrict our considerations only to horizontal spinor subspaces $S_{(h)}$. Introducing splitting of indices $l=L\oplus L'$, $m=M\oplus M'$, $a=A\oplus A',\ldots$, we parametrize the spinor metrics in this form:

$$\epsilon^{lm}=\begin{pmatrix}\epsilon^{LM} & 0\\ 0 & 0\end{pmatrix},\quad \tilde{\epsilon}^{lm}=\begin{pmatrix}0 & 0\\ 0 & \tilde{\epsilon}^{L'M'}\end{pmatrix},\quad \text{for } n=0(\text{mod } 4),$$

$$\epsilon^{lm}=\begin{pmatrix}0 & 0\\ \epsilon^{L'M} & 0\end{pmatrix},\quad \tilde{\epsilon}^{lm}=\begin{pmatrix}0 & \epsilon^{LM'}\\ 0 & 0\end{pmatrix},\quad \text{for } n=2(\text{mod } 4)$$

(the same formulas holds for ϵ-objects with covariant spinor indices).

From Table I we conclude that ϵ^{MN}, ϵ_{MN}, $\tilde{\epsilon}^{M'N'}$, $\tilde{\epsilon}_{M'N'}$ are symmetric (antisymmetric) for $n=0(\text{mod } 8)$ $(n=4(\text{mod } 8))$, $\tilde{\epsilon}^{AB'}=\epsilon^{B'A}$, $\tilde{\epsilon}_{AB'}=\pm\epsilon_{B'A}$ for $n=6(\text{mod } 8)$ and $\tilde{\epsilon}^{AB'}=-\epsilon^{B'A}$, $\tilde{\epsilon}_{AB'}=-\epsilon_{B'A}$ for $n=2(\text{mod } 8)$.

Let us denote horizontal spinors as $\zeta^N\in\mathbb{S}_{(h)}$, $\zeta^{N'}\in\mathbb{S}'_{(h)}$, $\zeta_N\in\tilde{\mathbb{S}}_{(h)}$ ($\tilde{\mathbb{S}}_{(h)}$ is dual to $\mathbb{S}_{(h)}$), $\zeta_{N'}\in\mathbb{S}'_{(h)}$ ($\tilde{\mathbb{S}}'_{(h)}$ is dual to $\mathbb{S}'_{(h)}$), $\zeta^l\in S_{(h)}$, and $\zeta_l\in\tilde{S}_{(h)}$ ($\tilde{S}_{(h)}$ is dual to $S_{(h)}$). By using ϵ-objects we can raise and lower indices in both cases of irreduced and reduced spinor spaces [for $n=2(\text{mod } 4)$ we can exclude, for example, primed indices, or inversely]. These properties and canonical isomorphisms between corresponding spaces are summarized in Table II.

The last subject to be considered in this section is the mutual transformation of d-tensors and d-spinors on ξ_d (or on H^{2n}). Really σ-objects from (19) or (20) allow us to obtain, for example, for $n=2(\text{mod } 4)$, from d-tensor $B^{\alpha}{}_{\beta}$ a spinor d-tensor (d-spinor): $B^{MM'}{}_{NN'}=(\sigma_\alpha)^{MM'}(\sigma'^3)_{NN'}B^{\alpha}{}_{\beta}$. On the other hand, a spinor d-tensor φ^{lm}, for example, for $n=2k+1$, can be transformed into d-vector $\varphi_\alpha=(\sigma_\alpha)_{lm}\varphi^{lm}$. So, by using σ-objects $[(\sigma_\alpha)_i{}^m,(\sigma_\alpha)_{RS},(\sigma_\alpha)^{AB},\ldots]$ we can transform σ-tensors into d-spinors and inversely d-spinors into d-tensors. We note that d-spinor–d-tensor mutual transformations are compatible to Whitney sums (2) [or (10)] for bundle ξ_d (or H^{2n}-space); i.e., "horizontal" ("vertical") d-tensorial indices must be transformed into "horizontal" ("vertical") spinor indices and inversely.

We end this section by emphasizing that the next step in the formulation of locally anisotropic spinor theory should be the development of the spinor differential geometry for $1a$-spaces.[26–28]

VII. OUTLOOK AND CONCLUSIONS

We have investigated the problem of definition of spinors on spaces with local anisotropy. Our approach is based on the formalism of Clifford d-algebras. We have introduced spinor structures on la-spaces as Clifford d-module structures on v-bundles. We have also proposed the second definition, as distinguished spinor structures, by using Clifford fibrations. It has been shown that H^{2n}-spaces admit as a proper characteristic the almost complex spinor structure. We have argued that one of the most important properties of spinors in both v-bundles with compatible nonlinear connection and metric and in H^{2n}-spaces is the periodicity 8 on the dimension of the base and on the dimension of the typical fiber spaces.

It should be noted that in this paper the distinguished Clifford and spinor structures have been introduced in an algebraic topological manner, and that in our considerations the compatibility of the d-connection and the metric, adapted to a given N-connection, plays a crucial role. Only Miron's approach to modeling on tangent bundles of spaces and media with local anisotropy admits a rigorous geometric definition of spinors. For models of Finsler and Lagrange spaces with noncompatible connection and metric structure, the definition of spinors is more sophisticated, if spinors are introduced locally with respect to the given metric quadratic form, the spinor constructions will not be invariant on parallel transport. We shall introduce corresponding discordance

laws and values and define nonstandard spinor structures by using a nonmetrical d-tensor (see similar constructions for locally isotropic curved spaces, in general with torsion and nonmetricity, in Ref. 29).

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Differential Hopf algebra structures on the universal enveloping algebra of a Lie algebra

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We discuss a method to construct a De Rham complex (differential algebra) of Poincaré–Birkhoff–Witt type on the universal enveloping algebra of a Lie algebra $\mathfrak{g}$. We determine the cases in which this gives rise to a differential Hopf algebra that naturally extends the Hopf algebra structure of $U(\mathfrak{g})$. The construction of such differential structures is interpreted in terms of color Lie superalgebras. © *1996 American Institute of Physics.* [S0022-2488(95)02112-5]

I. INTRODUCTION

Recently noncommutative differential geometry has attracted considerable interest, both mathematically and as a framework for certain models in theoretical physics. In particular, there is much activity in differential geometry on quantum groups. A noncommutative differential calculus on quantum groups has been developed by Woronowicz[1] following general ideas of Connes.[2] This general theory has been reformulated by Wess and Zumino[3] in a less abstract way. Their approach may be more suitable for specific applications in physics. A large number of papers have been written since and a few other methods to construct a noncommutative differential geometry on a quantum group or to define a differential geometric structure (a De Rham complex) on a given noncommutative algebra have been proposed and discussed by several authors (e.g., Refs. 4–6).

In this paper we present a differential calculus on the enveloping algebra of a given Lie algebra. This differential structure turns out to be a differential Hopf algebra, which can be interpreted in a very interesting way in terms of color Lie superalgebras. The commutative case has been studied previously (see, e.g., Ref. 7). Notice that our approach is different from the standard methods to construct noncommutative differential structures on Hopf algebras and quantum groups, in the sense that our starting point is not the algebra of functions on the (quantum) group but its dual the (quantized) universal enveloping algebra.

In the classical limit a quantized universal enveloping algebra defines a co-Poisson–Hopf algebra structure on the universal enveloping algebra (see Ref. 8). Further research is in progress concerning the compatibility between the differential calculus and the Poisson cobracket in order to define a differential Hopf algebra structure on the quantized universal enveloping algebra. We will report on this in the near future.

II. A DE RHAM COMPLEX ON $U(\mathfrak{g})$

Let A be an associative algebra over the field of complex numbers. A differential algebra on A (or a De Rham complex on A, see Ref. 4) is an $\mathbb{N}$-graded associative algebra Ω equipped with a linear operator d that has the following properties: (1) d is homogeneous of degree 1, i.e. $d(\Omega^p)\subset\Omega^{p+1}$ for all $p\in\mathbb{N}$. (2) d is a differential, i.e. $d^2=d\circ d=0$. (3) d is a graded derivation (of degree 1), i.e.

$$d(ab)=d(a)b+(-1)^p a d(b), \quad a\in\Omega^p, \ \ b\in\Omega. \tag{1}$$

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Furthermore, the algebra Ω has to be generated by $\Omega^0 \cup d(\Omega^0)$, where Ω^0 is isomorphic to A. For A we take the universal enveloping algebra of a Lie algebra and discuss the construction of De Rham complexes on such an algebra.

Let $\mathfrak{g}$ be a finite-dimensional Lie algebra over $\mathbb{C}$ with basis $\{x^1,x^2,\ldots,x^n\}$ and corresponding structure constants C_k^{ij}, which are defined by the property $[x^i,x^j]=C_k^{ij}x^k$. Throughout this paper we will make use of the Einstein summation convention. The universal enveloping algebra of $\mathfrak{g}$, which we denote by $U(\mathfrak{g})$, can be viewed as the quotient algebra of the free associative algebra on the alphabet $\{x^1,x^2,\ldots,x^n\}$ modulo the ideal generated by the relations

$$x^i x^j - x^j x^i = C_k^{ij} x^k. \tag{2}$$

From the Poincaré–Birkhoff–Witt Theorem we know that the monomials $x^{i_1}x^{i_2}\cdots x^{i_p}$ with $p \geqslant 0$ and $i_1 \leqslant i_2 \leqslant \cdots \leqslant i_p$ form a basis of $U(\mathfrak{g})$. The main idea behind the construction of Ω on $U(\mathfrak{g})$ is that we demand Ω to be of the PBW type; by this we mean that the monomials

$$dx^{j_1}\, dx^{j_2}\cdots dx^{j_q}x^{i_1}x^{i_2}\cdots x^{i_p}, \quad \text{with } j_1<j_2<\cdots<j_q, \quad i_1\leqslant i_2\leqslant\cdots\leqslant i_p, \quad p,q\geqslant 0, \tag{3}$$

are a basis of the associative algebra Ω. From here on we will write y^j to denote the element $dx^j=d(x^j)$ in Ω^1.

In order to construct Ω we have to impose certain commutation relations between the elements x^i and y^j. On account of the homogeneity and the PBW property, we impose relations of the form

$$x^i y^j = y^k(\Theta_{lk}^{ij}x^l + A_k^{ij}), \tag{4}$$

where both Θ_{lk}^{ij} and A_k^{ij} are arbitrary complex numbers. Since we want to obtain an ideal that is invariant under the action of the differential, we adjoin the following commutation relations for the elements y^i and y^j:

$$y^i y^j = -\Theta_{lk}^{ij} y^k y^l. \tag{5}$$

This is simply the consequence of applying d to the relations (4). Let Ω be the quotient algebra of the free associative algebra on the alphabet $\{x^1,x^2,..,x^n,y^1,y^2,..,y^n\}$ modulo the ideal J that is generated by the relations (2), (4), and (5). The $\mathbb{N}$ grading of Ω is induced by giving the elements x^i degree 0 and the elements y^j degree 1. The differential d is defined by $d(x^i)=y^i$, $d(y^i)=0$ and the derivation property (1).

The coefficients Θ_{lk}^{ij} and A_k^{ij} should satisfy a number of conditions in order that Ω has the above mentioned properties of a De Rham complex on $U(\mathfrak{g})$. The first condition arises from $d(J)\subset J$, i.e. the d invariance of the ideal J. By applying d to (2) we obtain

$$y^i x^j + x^i y^j - y^j x^i - x^j y^i = C_k^{ij} y^k,$$

which, on account of the relations (4), can be written as

$$y^i x^j + y^k(\Theta_{lk}^{ij}x^l + A_k^{ij}) - y^j x^i - y^k(\Theta_{lk}^{ji}x^l + A_k^{ji}) = C_k^{ij} y^k.$$

The PBW property of Ω implies that

$$A_k^{ij} - A_k^{ji} = C_k^{ij} \quad \text{and} \quad y^i x^j - y^j x^i + (\Theta_{lk}^{ij} - \Theta_{lk}^{ji}) y^k x^l = 0.$$

We can write this in the following compact form:

$$(I-P)A = C \quad \text{and} \quad I - P + \Theta P - P\Theta P = (I-P)(I+\Theta P) = 0. \tag{6}$$

In these equations we consider A and C as $n^2\times n$ and Θ, I, and P as $n^2\times n^2$ matrices over $\mathbb{C}$, the product is just the ordinary matrix multiplication. The permutation matrix P is defined by $P^{ij}_{kl}=\delta^i_l\delta^j_k$ where δ denotes the Kronecker delta. Since the relations (5) have been found by applying d to the relations (4), and since $d^2=0$, there are no further conditions arising from the d invariance.

The PBW property yields a number of compatibility conditions that are closely related to the well-known Diamond Lemma (see, e.g., Ref. 9). The ordering is a lexicographic total degree ordering with $y^i<y^j<x^k<x^l$ for all $i<j$ and $k<l$. According to this the monomials of the form (3) are precisely the irreducible monomials. The compatibility conditions arise from rewriting terms of the form $x^ix^jx^k$, $x^ix^jy^k$, $x^iy^jy^k$, and $y^iy^jy^k$. Evidently, rewriting the terms $x^ix^jx^k$ does not lead to any conditions since it simply boils down to the proof of the Poincaré–Birkhoff–Witt Theorem. We can rewrite $x^ix^jy^k$ as

$$x^ix^jy^k=x^i(y^l(\Theta^{jk}_{pl}x^p+A^{jk}_l))=y^m(\Theta^{il}_{nm}x^n+A^{il}_m)(\Theta^{jk}_{pl}x^p+A^{jk}_l),$$

but also as

$$\begin{aligned}x^ix^jy^k&=(x^jx^i+C^{ij}_lx^l)y^k\\&=x^jy^m(\Theta^{ik}_{nm}x^n+A^{ik}_m)+C^{ij}_ly^p(\Theta^{lk}_{mp}x^m+A^{lk}_p)\\&=y^p(\Theta^{jm}_{lp}x^l+A^{jm}_p)(\Theta^{ik}_{nm}x^n+A^{ik}_m)+C^{ij}_ly^p(\Theta^{lk}_{mp}x^m+A^{lk}_p).\end{aligned}$$

Due to the PWB property of Ω, the linear part of the expressions should coincide, yielding

$$A^{jk}_lA^{il}_m=A^{ik}_pA^{jp}_m+C^{ij}_lA^{lk}_m.$$

We introduce matrices A^i by $(A^i)^j_k=A^{ij}_k$. Thus, the equation above can be written as

$$A^jA^i-A^iA^j=C^{ij}_lA^l. \tag{7}$$

The rest of the expressions give rise to the equation

$$y^my^n(A^{jk}_l\Theta^{il}_{nm}+\Theta^{jk}_{nl}A^{il}_m-A^{ik}_p\Theta^{jp}_{nm}-\Theta^{ik}_{np}A^{jp}_m-C^{ij}_l\Theta^{lk}_{nm})+y^mx^ny^p(\Theta^{jk}_{pl}\Theta^{il}_{nm}-\Theta^{ik}_{pl}\Theta^{jl}_{nm})=0.$$

By making use of the following equality:

$$x^nx^p=\tfrac{1}{2}\,(x^nx^p+x^nx^p)=\tfrac{1}{2}\,(x^nx^p+x^px^n+C^{np}_lx^l),$$

the PBW basis gives rise to two consistency conditions. The highest-order part yields

$$\Theta^{jk}_{pl}\Theta^{il}_{nm}-\Theta^{ik}_{pl}\Theta^{jl}_{nm}+\Theta^{jk}_{nl}\Theta^{il}_{pm}-\Theta^{ik}_{nl}\Theta^{jl}_{pm}=0,$$

which can shortly be written as

$$[\Theta^i_n,\Theta^j_p]=[\Theta^j_n,\Theta^i_p], \tag{8}$$

where the matrices Θ^i_j are defined by $(\Theta^i_j)^k_l=\Theta^{ik}_{jl}$. Similarly, the second-order part coefficients give the condition

$$2([A^j,\Theta^i_n]+[\Theta^j_n,A^i]-C^{ij}_l\Theta^l_n)+(\Theta^j_p\Theta^i_q-\Theta^i_p\Theta^j_q)C^{pq}_n=0. \tag{9}$$

We apply the same method to handle terms like $x^iy^jy^k$. We obtain

$$x^iy^jy^k=y^m(\Theta^{ij}_{lm}x^l+A^{ij}_m)y^k$$

$$= \Theta^{ij}_{lm} y^m y^p (\Theta^{lk}_{qp} x^q + A^{lk}_p) + A^{ij}_m y^m y^k$$
$$= \Theta^{ij}_{lm} \Theta^{lk}_{qp} y^m y^p x^q + (\Theta^{ij}_{lm} A^{lk}_p - A^{ij}_l \Theta^{lk}_{pm}) y^m y^p,$$

and on the other hand we can write

$$x^i y^j y^k = (\Theta^{jk}_{lm} A^{im}_p \Theta^{pl}_{ts} - \Theta^{jk}_{lm} \Theta^{im}_{ps} A^{pl}_t) y^s y^t - \Theta^{jk}_{lm} \Theta^{im}_{qp} \Theta^{ql}_{ts} y^p y^s x^t.$$

We remark that the relations (5) can be rewritten in the form

$$(I+S)^{ij}_{kl} y^k y^l = 0,$$

where S is a matrix with the property $S^2 = I$. On account of the PBW property of Ω, we obtain the conditions

$$(\Theta^{ij}_{lp} \Theta^{lk}_{ts} + S^{jk}_{ml} \Theta^{im}_{qp} \Theta^{ql}_{ts}) y^p y^s x^t = 0 \quad \text{and} \quad (I+S)^{jk}_{ml} (\Theta^{im}_{sp} A^{sl}_q - A^{im}_s \Theta^{sl}_{qp}) y^p y^q = 0.$$

Due to the fact that $1/2(I+S)$ is a projection, the preceding equations are equivalent to

$$(I+S)^{jk}_{ml} \Theta^{im}_{qp} \Theta^{ql}_{ts} (I-S)^{ps}_{uv} = 0, \quad (I+S)^{jk}_{ml} (\Theta^{im}_{sp} A^{sl}_q - A^{im}_s \Theta^{sl}_{qp}) (I-S)^{pq}_{uv} = 0. \tag{10}$$

The first condition can be written in the following elegant form:

$$(I+S)_{12} \Theta_{31} \Theta_{32} (I-S)_{12} = 0. \tag{11}$$

The subscripts denote the positions used to embed the $n^2 \times n^2$ matrices into the $n^3 \times n^3$ matrices, e.g., $(\Theta_{12})^{ijk}_{pqr} = \Theta^{ij}_{pq} \delta^k_r$. The consistency condition arising from rewriting the terms $y^i y^j y^k$ is

$$((I+S)_{12} \Theta_{31} \Theta_{32})^{ijk}_{pqr} y^p y^q y^r = 0.$$

This is evidently satisfied if (11) holds, so this gives no further conditions for the coefficients.

The conclusion is that the set of conditions (6), (7), (8), (9), and (10) is sufficient to define a De Rham complex Ω on $U(\mathfrak{g})$ with the PBW property. In the next section we investigate the possibility to define a differential Hopf algebra on $U(\mathfrak{g})$.

III. A DIFFERENTIAL HOPF ALGEBRA ON $U(\mathfrak{g})$

It is well known that the universal enveloping of a Lie algebra $\mathfrak{g}$ has a natural Hopf algebra structure (see, e.g., Ref. 10), its comultiplication $\Delta: U(\mathfrak{g}) \to U(\mathfrak{g}) \otimes U(\mathfrak{g})$ is defined by $\Delta(x) = 1 \otimes x + x \otimes 1$, its counit $\epsilon: U(\mathfrak{g}) \to \mathbb{C}$ by $\epsilon(x) = 0$ for all x in $\mathfrak{g}$. They both are algebra morphisms. The antipode $S: U(\mathfrak{g}) \to U(\mathfrak{g})$ is the unique antialgebra morphism satisfying $S(x) = -x$. In the preceding section we discussed the construction of a differential algebra on $U(\mathfrak{g})$, which essentially is an algebra extension of $U(\mathfrak{g})$ equipped with a differential operator d. In this section we discuss the possibility of extending Δ, ϵ, and S from $U(\mathfrak{g})$ to Ω in such a way that Ω becomes a differential Hopf algebra.

Let us first recall the notion of a differential bialgebra, for a complete description we refer to Ref. 4. A differential bialgebra is a differential algebra Ω equipped with a comultiplication Δ and a counit ϵ that are differential algebra morphisms. Note that a differential algebra morphism $\varphi: \Omega \to \Omega'$ simply is an algebra morphism of degree zero that commutes with the differentials, i.e. $\varphi \circ d = d' \circ \varphi$.

In order to write down explicitly the conditions for Δ and ϵ we need to explain the differential algebra structures of $\Omega \otimes \Omega$ and $\mathbb{C}$. The $\mathbb{N}$ grading of $\Omega \otimes \Omega$ is defined by

$$(\Omega \otimes \Omega)^p = \bigoplus_{0 \le q \le p} \Omega^q \otimes \Omega^{p-q}, \tag{12}$$

and its multiplication $\mu_{\otimes}:\Omega\otimes\Omega\otimes\Omega\otimes\Omega\to\Omega\otimes\Omega$ by

$$\mu_{\otimes}=(\mu\otimes\mu)\circ\sigma_{23}, \tag{13}$$

where μ denotes the multiplication of Ω. The linear map σ_{23} denotes the graded flip $\sigma:\Omega\otimes\Omega\to\Omega\otimes\Omega$, which is defined by

$$\sigma(a\otimes b)=(-1)^{pq}b\otimes a, \quad a\in\Omega^p, \ b\in\Omega^q, \tag{14}$$

applied to the second and third component of the tensor product. The differential $d_{\otimes}$ of $\Omega\otimes\Omega$ is given by $d_{\otimes}=d\otimes id+\tau\otimes d$, where $\tau:\Omega\to\Omega$ is the linear map of degree zero satisfying $\tau(a)=(-1)^p a$ for all $a\in\Omega^p$. Written out explicitly, this gives

$$d_{\otimes}(a\otimes b)=d(a)\otimes b+(-1)^p a\otimes d(b), \quad a\in\Omega^p, \ b\in\Omega. \tag{15}$$

Henceforth, the condition that Δ should be a differential algebra morphism means that Δ is an algebra morphism with the property

$$d_{\otimes}\circ\Delta=(d\otimes id+\tau\otimes d)\circ\Delta=\Delta\circ d. \tag{16}$$

Note that this is the analog of the derivation property (1) that can be written as $d\circ\mu=\mu\circ d_{\otimes}$. We consider $\mathbb{C}$ to be a differential algebra with $\mathbb{C}^0=\mathbb{C}$ and $\mathbb{C}^p=0$ for all $p>0$. Hence, ϵ is a differential algebra morphism if and only if it is an algebra morphism satisfying $\epsilon\circ d=0$.

Since Ω is generated by $\Omega^0\cup d(\Omega^0)$, it suffices to define the actions of Δ and ϵ on $\{x^1,x^2,\ldots,x^n,y^1,y^2,\ldots,y^n\}$. Naturally the actions on elements x^i coincide with the previously described actions on $U(\mathfrak{g})$. The above mentioned conditions for Δ and ϵ uniquely determine the actions on the elements y^j:

$$\Delta(y^i)=\Delta\circ d(x^i)=d_{\otimes}\circ\Delta(x^i)=d_{\otimes}(x^i\otimes 1+1\otimes x^i)=y^i\otimes 1+1\otimes y^i, \tag{17}$$

$$\epsilon(y^i)=\epsilon\circ d(x^i)=0. \tag{18}$$

Here we have used that $d(1)=0$, which is a direct consequence of the derivation property of d.

In order for ϵ and Δ to be well defined, the ideal J needs to be a (two-sided) coideal, i.e. $\epsilon(J)=0$ and $\Delta(J)\subset\Omega\otimes J+J\otimes\Omega$. The first condition is clearly satisfied. To verify the second we apply Δ to the relations (2), (4), and (5). Naturally the relations (2) do not give rise to any conditions for the coefficients Θ^{ij}_{lk} and A^{ij}_k. The relations (4) yield

$$\begin{aligned}\Delta(x^iy^j-\Theta^{ij}_{lk}y^k(x^l+A^{ij}_k))&=\Delta(x^i)\Delta(y^j)-\Theta^{ij}_{lk}\Delta(y^k)(\Delta(x^l)+A^{ij}_k 1\otimes 1)\\&=1\otimes x^iy^j+x^i\otimes y^j+y^j\otimes x^i+x^iy^j\otimes 1\\&\quad-\Theta^{ij}_{lk}(1\otimes y^kx^l+x^l\otimes y^k+y^k\otimes x^l+y^kx^l\otimes 1+A^{ij}_k(1\otimes y^k+y^k\otimes 1))\\&=x^i\otimes y^j+y^j\otimes x^i-\Theta^{ij}_{lk}(y^k\otimes x^l+x^l\otimes y^k)\mathrm{mod}(\Omega\otimes J+J\otimes\Omega).\end{aligned}$$

Again, on account of the PBW property of Ω, we obtain

$$x^i\otimes y^j=\Theta^{ij}_{lk}x^l\otimes y^k \quad\text{and}\quad y^j\otimes x^i=\Theta^{ij}_{lk}y^k\otimes x^l, \tag{19}$$

which evidently implies $\Theta=I$. Similarly, we find

$$\Delta(y^iy^j+\Theta^{ij}_{lk}y^ky^l)=y^i\otimes y^j-y^j\otimes y^i+\Theta^{ij}_{lk}(y^k\otimes y^l-y^l\otimes y^k)\mathrm{mod}(J\otimes\Omega+\Omega\otimes J),$$

which boils down to the condition $(I-\Theta)(I-P)=0$. Therefore, the conclusion is that Ω can only be a differential bialgebra on $U(\mathfrak{g})$ if $\Theta=I$. In that case the conditions (6), (7), (8), and (9) reduce to

$$(I-P)A=C \quad \text{and} \quad [A^j,A^i]=C_l^{ij}A^l, \tag{20}$$

due to the fact that $P^2=I$ and $S^2=I$. The commutation relations (4) and (5) take the following form:

$$x^iy^j=y^jx^i+A_k^{ij}y^k \quad \text{and} \quad y^iy^j=-y^jy^i. \tag{21}$$

We remark that we did not check the coassociativity of Δ, i.e. $(\Delta\otimes id)\circ\Delta=(id\otimes\Delta)\circ\Delta$. This is a direct consequence of the coassociativity of Δ on $U(\mathfrak{g})=\Omega^0$ since

$$\begin{aligned}(\Delta\otimes id)\circ\Delta\circ d(\Omega^0)&=(\Delta\otimes id)\circ d_\otimes\circ\Delta(\Omega^0)\\&=(d_\otimes\otimes id+\tau\otimes\tau\otimes d)\circ(\Delta\otimes id)\circ\Delta(\Omega^0)\\&=(d\otimes id\otimes id+\tau\otimes d_\otimes)\circ(id\otimes\Delta)\circ\Delta(\Omega^0)\\&=(id\otimes\Delta)\circ d_\otimes\circ\Delta(\Omega^0)=(id\otimes\Delta)\circ\Delta\circ d(\Omega^0).\end{aligned}$$

By a similar reasoning one can show that the counit property of ϵ on Ω is induced by the same property of ϵ on $U(\mathfrak{g})$.

The next step is to consider a differential Hopf algebra structure on Ω. We recall that Ω is a differential Hopf algebra (see Ref. 4) if it is a differential bialgebra that possesses an antipode S. An antipode S is an element of $End(\Omega)$ satisfying $S\star id=id\star S=\eta\circ\epsilon$, where $\star$ denotes the convolution product on $End(\Omega)$ (see Ref. 10) defined by

$$f\star g=\mu\circ(f\otimes g)\circ\Delta, \quad f,g\in End(\Omega). \tag{22}$$

By $\eta:\mathbb{C}\to\Omega$ we denote the unit element of Ω, i.e. $\eta(1)=1$. Since $\eta\circ\epsilon$ is the unit element in $End(\Omega)$ with respect to the convolution product, one can describe the antipode as the unique inverse of the identity. An important property of the antipode is that it is an antialgebra morphism; this means that $S\circ\mu\circ\sigma=(S\otimes S)\circ\mu$ and $S\circ\eta=\eta$ [or equivalently $S(1)=1$].

We try to extend the antipode of $U(\mathfrak{g})=\Omega^0$ to Ω. In order to do that we make the following observation. Suppose that f and g are homogeneous endomorphisms on Ω of degree zero that commute with the differential operator d. Then the properties $d_\otimes\circ\Delta=\Delta\circ d$ and $\mu\circ d_\otimes=d\circ\mu$ imply that

$$\begin{aligned}d\circ(f\star g)&=d\circ\mu\circ(f\otimes g)\circ\Delta\\&=\mu\circ d_\otimes\circ(f\otimes g)\circ\Delta\\&=\mu\circ(d\otimes id+\tau\otimes d)\circ(f\otimes g)\circ\Delta\\&=\mu\circ(f\otimes g)\circ(d\otimes id+\tau\otimes d)\circ\Delta\\&=\mu\circ(f\otimes g)\circ d_\otimes\circ\Delta\\&=\mu\circ(f\otimes g)\circ\Delta\circ d=(f\star g)\circ d.\end{aligned}$$

Hence, the convolution product $f\star g$ also commutes with d. By inductive use of this argument we can conclude that d commutes with $f^n=f\star f\star\cdots\star f$ for all positive values of n if f is a homoge-

neous endomorphism of degree zero satisfying $d\circ f=f\circ d$. For f we can choose the identity. This makes it plausible that d commutes with $id^{-1}=S$. So, we extend the antipode by demanding $d\circ S=S\circ d$. In particular, this yields

$$S(y^i)=S\circ d(x^i)=d\circ S(x^i)=-d(x^i)=-y^i. \tag{23}$$

For S to be a well-defined antialgebra morphism on Ω, it must leave the ideal J invariant $[S(J)\subset J]$. To verify this condition, it suffices to apply S to the relations (21). We will only write out the first; the second can be handled similarly,

$$\begin{aligned} S(x^iy^j-y^jx^i-A^{ij}_k y^k)&=S(y^j)S(x^i)-S(x^i)S(y^j)-A^{ij}_k S(y^k)\\ &=y^jx^i-x^iy^j+A^{ij}_k y^k\\ &=-(x^iy^j-y^jx^i-A^{ij}_k y^k)\in J. \end{aligned}$$

In order to check that S is indeed an antipode, we can confine ourselves to verifying the defining property of S for a set of generators of Ω. Since S is the extension of the antipode of $U(\mathfrak{g})$, we only need to compute

$$(S\star id)(y^i)=\mu\circ(S\otimes id)(1\otimes y^i+y^i\otimes 1)=1\cdot y^i-y^i\cdot 1=0=\eta\circ\epsilon(y^i).$$

So, at the end of this section we come to the following conclusion. In order to obtain a differential Hopf algebra Ω on $U(\mathfrak{g})$, it is necessary that the matrix Θ in (4) and (5) equals the identity matrix I. In that case necessary and sufficient conditions for the coefficients A^{ij}_k are given by (20), and the corresponding Hopf algebraic extension is described by (17), (18), and (23).

IV. A LIE ALGEBRAIC INTERPRETATION

The comultiplication of the universal enveloping algebra of a Lie algebra is cocommutative. We can easily verify that the cocommutativity of Δ on Ω^0 gives rise to graded cocommutativity for the extension of Δ to Ω:

$$\sigma\circ\Delta\circ d(\Omega^0)=\sigma\circ d_{\otimes}\circ\Delta(\Omega^0)=d_{\otimes}\circ\sigma\circ\Delta(\Omega^0)=d_{\otimes}\circ\Delta(\Omega^0)=\Delta\circ d(\Omega^0),$$

or, more explicitly,

$$\sigma\circ\Delta(y^i)=\sigma(1\otimes y^i+y^i\otimes 1)=y^i\otimes 1+1\otimes y^i=\Delta(y^i).$$

We call the property $\sigma\circ\Delta=\Delta$ graded cocommutativity because σ denotes the graded flip.

It is well known (see, e.g., Ref. 11) that a cocommutative Hopf algebra H, which has a compatible filtering, is isomorphic to the Hopf algebra corresponding to the universal enveloping algebra of the Lie algebra of primitive elements of H. Note that the set of primitive elements of H is defined by

$$P(H)=\{x\in H\,|\,\Delta(x)=1\otimes x+x\otimes 1\}, \tag{24}$$

which has the structure of a Lie algebra with the commutator $[x,y]=xy-yx$. By a compatible filtering we mean an increasing family of subspaces $(F_p)_{p\in N}$ of H satisfying

$$\mu(F_p\otimes F_q)\subset F_{p+q}\ \Delta(F_p)\subset\sum_{0\leqslant q\leqslant p}F_q\otimes F_{p-q}\ \bigcup_{p\in N}F_p=H. \tag{25}$$

With respect to the graded cocommutative Hopf algebra Ω, we remark that $F_p=\oplus_{0\leqslant q\leqslant p}\Omega^q$ defines a compatible filtering. Due to the graded cocommutativity, $P(\Omega)$ does not have the struc-

ture of an ordinary Lie algebra. Instead of the usual commutator we define a "color" commutator on Ω by $[x,y]=xy-(-1)^{pq}yx$ for $x\in\Omega^p$ and $y\in\Omega^q$. The set $P(\Omega)$ is closed under this bracket since

$$\begin{aligned}\Delta([x,y]) &= \Delta(xy-(-1)^{pq}yx)\\ &= \Delta(x)\Delta(y)-(-1)^{pq}\Delta(y)\Delta(x)\\ &= (1\otimes x+x\otimes 1)(1\otimes y+y\otimes 1)-(-1)^{pq}(1\otimes y+y\otimes 1)(1\otimes x+x\otimes 1)\\ &= 1\otimes xy+x\otimes y+(-1)^{pq}y\otimes x+xy\otimes 1-(-1)^{pq}(1\otimes yx+y\otimes x+(-1)^{pq}x\otimes y+yx\otimes 1)\\ &= 1\otimes(xy-(-1)^{pq}yx)+(xy-(-1)^{pq}yx)\otimes 1\\ &= 1\otimes[x,y]+[x,y]\otimes 1,\end{aligned}$$

for all $x\in P(\Omega)^p$ and $y\in P(\Omega)^q$. Note that the $\mathbb{N}$ grading of Ω induces an $\mathbb{N}$ grading on $P(\Omega)$, since Δ is homogeneous of degree zero. By this argument we have derived that $P(\Omega)$ is a color Lie superalgebra. For the definition of a color Lie superalgebra we refer to Ref. 12. The corresponding 2-cocyle α is given by

$$\alpha:\mathbb{N}\times\mathbb{N}\to\mathbb{C}^*,\quad \alpha(p,q)=(-1)^{pq}. \tag{26}$$

Since $\alpha(q,q)=(-1)^{q^2}=(-1)^q$, the elements of $P(\Omega)^q$ are even (odd) if and only if q is even (odd). As in the case of ordinary Lie algebras, one can define the universal enveloping algebra of a color Lie superalgebra and a corresponding Hopf algebraic structure on it. Analogous to the above mentioned result of Ref. 11, the Hopf algebra Ω is isomorphic to the Hopf algebra $U(P(\Omega))$.

The question is what $P(\Omega)$ explicitly looks like. The set of primitive elements of Ω certainly contains the linear span of $\{x^1,x^2,..,x^n,y^1,y^2,..,y^n\}$ [see (17)], which we will denote by L. We consider L as the $\mathbb{N}$-graded vector space $L=\oplus_{p\in N}L^p$ with

$$L^0=\langle x^i\rangle_{1\leqslant i\leqslant n},\quad L^1=\langle y^i\rangle_{1\leqslant i\leqslant n}\quad L^p=0\quad (p\geqslant 2).$$

According to the relations (2) and (21), we have

$$[x^i,x^j]=C^{ij}_k x^k,\quad [x^i,y^j]=A^{ij}_k y^k,\quad \text{and}\quad [y^i,y^j]=0, \tag{27}$$

so L is a color Lie supersubalgebra in $P(\Omega)$. Since the elements of L^0 are even and the elements of L^1 are odd, a basis of $U(L)$ can be given by (see, e.g., Ref. 12)

$$y^{j_1}y^{j_2}\cdots y^{j_q}x^{i_1}x^{i_2}\cdots x^{i_p}\quad \text{with}\ j_1<j_2<\cdots<j_q,\quad i_1\leqslant i_2\leqslant\cdots\leqslant i_p,\quad \text{and}\quad p,q\geqslant 0.$$

A comparison of this basis with the described basis of Ω [see (3)], proves that the Hopf algebra Ω is isomorphic to the Hopf algebra $U(L)$. Hence, $P(\Omega)=L$.

The preceding reasoning enables us to interpret the construction of a differential Hopf algebra on the universal enveloping of a Lie algebra $\mathfrak{g}$ in terms of a color Lie superalgebraic extension of $\mathfrak{g}$. The problem to be solved can be reformulated as follows. Given is a Lie algebra $\mathfrak{g}$ with basis $\{x^1,x^2,\ldots,x^n\}$. Let L be the $\mathbb{N}$-graded vector space given by $L^0=\mathfrak{g}$, $L^1=\langle y^i\rangle_{1\leqslant i\leqslant n}$ and $L^p=0$ for all $p\geqslant 2$. Define a bilinear operation $[\ ,\ ]$ on L of degree zero extending the commutator of $\mathfrak{g}$ in such a way that $[x^i,y^j]=A^{ij}_k y^k$. This bracket expresses the commutation relations (21). The conditions (20) for the coefficients A^{ij}_k are equivalent to demanding that L equipped with this commutator becomes a color Lie superalgebra with 2-cocycle α given by (26), satisfying the additional property that the linear map d defined by $d(x^i)=y^i$ and $d(y^i)=0$ is a graded derivation of degree

1 on L. The corresponding differential Hopf algebra on $U(\mathfrak{g})$ is then given by the Hopf algebra $U(L)$ equipped with the unique extension of the derivation d from L to $U(L)$.

V. CONCLUDING REMARKS

We have presented a framework to construct a De Rham complex on the universal enveloping algebra of a Lie algebra $\mathfrak{g}$. The fundamental property of the differential algebra is that it possesses a so-called PBW basis. We have proven that the differential algebra can be given a Hopf algebra structure extending the natural Hopf algebra $U(\mathfrak{g})$. In our presentation we assumed $\mathfrak{g}$ to be finite dimensional. This is definitely not a necessary condition; one can easily see that this framework can also be applied in the infinite-dimensional case. For more details on this and some explicit examples we refer to Ref. 13. Naturally, a De Rham complex on $U(\mathfrak{g})$ brings to surface the notion of cohomology. It would be very interesting to investigate this De Rham cohomology.

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Path integrals for spinning particles, stationary phase and the Duistermaat–Heckmann theorem

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We examine the problem of the evaluation of both the propagator and of the partition function of a spinning particle in an external field at the classical as well as the quantum level, in connection with the asserted exactness of the stationary phase approximation. At the classical level we argue that exactness of this approximation stems from the fact that the dynamics (on the two-sphere S^2) of a spinning particle in a magnetic field is the reduction from $\mathbf{R}^4$ to S^2 of a linear dynamical system on $\mathbf{R}^4$. At the quantum level, however, and within the path integral approach, the restriction, inherent to the use of the stationary phase approximation, to regular paths clashes with the fact that no regulators are present in the action that enters the path integral. This is shown to lead to a prefactor for the path integral that is strictly divergent, except in the classical limit. A critical comparison is made with the various approaches that have been presented in the literature. The validity of a formula given in literature for the spin propagator is extended to the case of motion in an arbitrary magnetic field. © *1996 American Institute of Physics.* [S0022-2488(96)04501-5]

I. INTRODUCTION

Since the early days of path integration, how to do a path integral for spinning particles was recognized[1] as one of the major difficulties of the formalism. Schulman[2] (but also see Ref. 3) made a first attempt toward a formulation of a path integral for spinning particles, one which was, however, rather a related path integral, namely that for a spinning top.

Much progress has been made since with the systematic use, initiated by Klauder,[4,5] of the resolution of the identity associated with spin-coherent states[6,7] in the discretized-time (or time-sliced) approach to the path integral. Path integral quantization using coherent states will be discussed extensively in the sequel. Other versions of the path integral not making an explicit use of coherent states have been discussed instead in Refs. 8 and 9 (also see Ref. 10), as well as in Ref. 11 specifically for the calculation of the spin tunneling in the semiclassical limit.

Already at the classical level, a spin (classically a vector **S** of fixed magnitude s) presents some peculiarities as a dynamical system. While the Hamiltonian description is essentially straightforward if one assumes the Poisson brackets:

$$\{S_i, S_j\} = \epsilon_{ijk} S_k, \tag{1}$$

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among the components of the spin vector, it has been pointed out by Balachandran *et al.*[12] that no global Lagrangian description can be given as long as one sticks to the natural configuration space of the spin, which is the compact two-sphere S^2. The same authors have shown that a global Lagrangian can be associated with a classical spin by lifting the description of the system from S^2 to the group manifold of SU(2), which is the three-sphere S^3, as follows. Considering the usual spin-$\frac{1}{2}$ representation of SU(2), one can define a vector $\mathbf{S}$ in S^2 via the Hopf map, i.e.

$$\tilde{S}=\mathbf{S}\cdot\boldsymbol{\sigma}=sg\sigma_3 g^{-1}, \tag{2}$$

with $\boldsymbol{\sigma}=(\sigma_1,\sigma_2,\sigma_3)$ the Pauli matrices. Then it can be shown[12] that the (global) Lagrangian on TSU(2):

$$L=is\ \mathrm{Tr}(\sigma_3 g^{-1}\dot{g})-\frac{\mu}{2}\ \mathrm{Tr}(\tilde{S}\tilde{B}), \tag{3}$$

where μ is the Bohr magneton and $\tilde{B}=\mathbf{B}\cdot\boldsymbol{\sigma}$, yields the correct equations of motion for a classical spin in an external magnetic field $\mathbf{B}$. The same equations can be derived, of course, at the Hamiltonian level using the Poisson brackets (1) and the Hamiltonian:

$$H=\mu\mathbf{S}\cdot\mathbf{B}. \tag{4}$$

As it is clear from the fact that the spin is recovered via the Hopf projection (2), this approach introduces an extra, nondynamical U(1) gauge degree of freedom. Indeed, under $g\rightarrow g\ \exp[i\gamma\sigma_3/2]$, (2) is invariant while L changes by a total time derivative (i.e., it is "weakly invariant"[12]):

$$L\rightarrow L-s\dot{\gamma}. \tag{5}$$

This is also evident if we parametrize SU(2) with the Euler angles as

$$g=e^{-i\phi\sigma_3/2}e^{-i\theta\sigma_2/2}e^{-i\gamma\sigma_3/2} \tag{6}$$

($0\leqslant\theta\leqslant\pi, 0\leqslant\phi\leqslant 2\pi, 0\leqslant\gamma\leqslant 4\pi$), which yields the (local) Lagrangian:

$$L=s(\dot{\phi}\ \cos\ \theta+\dot{\gamma})+\mu\mathbf{S}\cdot\mathbf{B}. \tag{7}$$

Although it can be shown[13] that this extra gauge degree of freedom has interesting consequences for the path integral quantization of (3), and namely that it leads in a straightforward way to spin quantization (i.e., $2s/\hbar=$integer), we would like to stress here the fact that (3) (or (7) for that matter) being linear in the time derivatives, a spinning particle is described as a constrained dynamical system. Canonical quantization requires then the use of Dirac's theory[14] of constraints, and it has been shown by Balachandran *et al.*[12] that this does indeed yield the correct quantum mechanical description of the spin, including spin quantization. As pointed out, e.g., in Ref. 9, it turns out that the (semiclassical) Bohr–Sommerfeld quantization is exact for a spin Hamiltonian. This is a strong indication that the stationary phase approximation to the path integral for, say, the propagator should be exact as well. Exactness of the stationary phase approximation implies, of course, that we discuss the applicability to the present problem of the Duistermaat–Heckman theorem, which provides a rigorous framework.

Concerning the path integral approach and the legitimacy of evaluating the path integral within the stationary phase approximation, which is the main problem addressed in the present paper, a Lagrangian of the form (7) poses another problem, and namely that, the classical equations of motion being first order in time, the saddle point problem becomes *overdetermined*, as the

solutions of the saddle point equations have to obey two boundary conditions, and not a single one. Different ways to overcome this problem have been proposed in the literature, and notably by Klauder,[4,5] Keski-Vakkuri *et al.*,[15] and Suzuki.[16]

This paper is devoted mainly to the discussion of two questions, namely that of the legitimacy of some approximations that are currently made in the coherent state formulation of the path integral for spins and that of the still unsettled problem, which has also been widely discussed in the literature, that the stationary phase approximation to the path integral yields the exact result for both the propagator and/or the partition function of a quantum spin. While the stationary phase approximation is almost trivially exact for quadratic Hamiltonians, here the apparently surprising fact is that it turns out to be exact also for the Hamiltonian (4) and/or the Lagrangian (7) that are far from being quadratic.

The paper is organized as follows. In the Appendix we briefly review the Duistermaat–Heckman theorem and the stationary phase approximation. In Sec. II we apply the latter to the calculation of the partition function of a classical spin and show that the deep reason of the validity of such an approximation is that a classical spin, when viewed as a dynamical system, can be shown to result from the reduction of a linear dynamical system from $\mathbf{R}^4$ to S^2. In Sec. III, we begin by discussing briefly the use of spin-coherent state path integral approach to the calculation of the propagator and/or of the partition function of a quantum spin. We show there that the approximation currently used in literature restricting the paths in the functional integral to be continuous leads to incorrect and diverging prefactors. Then we review briefly the approaches of Klauder and Suzuki to the same problem. We clarify the origin of some apparently mysterious terms that are added to the action in Klauder's approach. Then we analyze why the stationary phase approximation yields the exact result in Suzuki's approach, by arguing that his main result stems simply from the exactness of the Ehrenfest theorem in the present context. In Sec. IV we discuss in more detail the coherent state approach by using the holomorphic representation for the latter, applying the complex stationary phase approximation to the discrete version of the spin path integral. Section V is devoted to a general discussion and to some conclusions.

II. THE CLASSICAL SPIN

Let us start our considerations from a *classical* (nonrelativistic) spin in a time-independent magnetic field $\mathbf{B}=(B_1,B_2,B_3)$.

Since the only degree of freedom for a spin is its direction, we describe it by means of a three-dimensional vector $(S_1,S_2,S_3)\in\mathbf{R}^3$ of a fixed norm: $S_1^2+S_2^2+S_3^2=s^2$, where the three classical variables $S_j (j=1,2,3)$ satisfy the Poisson brackets (1). Thus, the phase space for a classical spin is the two-dimensional manifold $S^2(s)$, equipped with the symplectic two-form

$$\Omega=\frac{1}{2s^2}\,\epsilon_{ijk}S_i\,dS_j\wedge dS_k\,. \tag{8}$$

The Hamiltonian that describes a classical spin in a magnetic field is given by (4). For simplicity we will set $\mu\equiv 1$ in the following so that

$$H=\mathbf{B}\cdot\mathbf{S}. \tag{9}$$

The Hamiltonian vector field Δ associated to (9), which is determined by the symplectic form Ω, is given by

$$\Delta=\epsilon_{ijk}B_jS_k\,\frac{\partial}{\partial S_i}, \tag{10}$$

so that the classical equations of motion, $i_\Delta\Omega=dH$, read as

$$\dot{S}_i = \epsilon_{ijk} B_j S_k \,. \tag{11}$$

Without any loss of generality, we will set $\mathbf{B}=(0,0,B)$ $(B>0)$ from now on. In this case, the Hamiltonian (9) and the equations of motion (11) assume a very simple form if we use spherical coordinates $S_1 = s \sin\theta\cos\phi$, $S_2 = s \sin\theta\sin\phi$, $S_3 = s\cos\theta$. They become, respectively,

$$H = sB \cos\theta \tag{12}$$

and

$$\cos\theta\dot{\theta} = 0, \quad \sin\theta(\dot{\phi} - B) = 0. \tag{13}$$

The latter can be easily integrated, and one sees that the classical orbits are circles parallel to the equator, the spin processing about the magnetic field with a period $\tau = 2\pi/B$.

In spherical coordinates, it is also very easy to compute the *exact* partition function for the Hamiltonian (9):

$$\mathcal{Z}_{\mathrm{cl}}(\beta) = \int_{S^2(s)} \Omega e^{-\beta H}. \tag{14}$$

Indeed, one gets

$$\mathcal{Z}_{\mathrm{cl}}(\beta) = s \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta \, d\theta \, e^{-\beta sB\cos\theta} = \frac{2\pi}{\beta B} \left(e^{\beta sB} - e^{-\beta sB}\right). \tag{15}$$

From (15), one recognizes that the classical partition function can be written as the weighted sum of two terms, each given by the evaluation of $e^{-\beta H}$ at the two critical points $\theta=\pi$ and $\theta=0$ of the Hamiltonian, for which $\Delta_{\mathbf{S}=(0,0,\pm s)} = 0$. In addition, it is not hard to check that the weights $(\pm 2\pi/\beta B)$ are exactly the ones coming from the calculation of the contributions to the integral (15) of the Gaussian fluctuations around the stationary points of H.

Everybody is familiar with such a result whenever dealing with (multidimensional) harmonic oscillators, or, in general, with a quadratic Hamiltonian on the linear manifold $\mathbf{R}^{2n}$. Even if the Hamiltonian (9) is not of this kind, the stationary phase approximation is exact as well. A spin in a magnetic field is, in fact, the simplest (nontrivial) application of the Duistermaat–Heckman theorem,[17,18] which establishes under which conditions a phase-space integral, such as (14), can be evaluated exactly in the stationary phase approximation. We refer to the Appendix for a review of the Duistermaat–Heckman theorem and for the proof of its applicability to the system of a spin in a magnetic field. Here we recall only that this result holds essentially for the two following geometrical reasons: (1) the Hamiltonian (12) is invariant under an $U(1)$ action, given by rotations about the third axis (i.e., the axis of the constant magnetic field); (2) the associated Hamiltonian vector field, given by

$$\Delta = B\left(-S_2 \frac{\partial}{\partial S_1} + S_1 \frac{\partial}{\partial S_2}\right), \tag{16}$$

is proportional to the generator of this $U(1)$ action. This is clear in spherical coordinates, where $\Delta = B(\partial/\partial\phi)$. However, while (16) defines it globally on $S^2(s)$, the spherical coordinate representation becomes singular at $\theta = 0, \pi$.

The Duistermaat–Heckman theorem gives some abstract mathematical conditions for the stationary phase approximation to be exact. In the following we will show that for a spin in a magnetic field there is, however, a deeper reason why this holds: the dynamical system that describes a spin in the magnetic field is the reduction of a bigger system, which is described by a

quadratic Hamiltonian on the linear manifold $\mathbf{R}^4$.[19] Such a situation has already been considered in the literature (see Ref. 20 and references therein), even if not much in the context of the stationary phase approximation, but mainly in the context of integrable systems, for which there exists the conjecture[20] that every integrable system is the reduction of a bigger *linear* dynamical system. To show what happens in the case of a spin, let us consider the linear manifold $\mathbf{R}^4=\{(x_1,x_2,x_3,x_4)\}=\mathbf{C}^2=\{(z_1,z_2):z_1=x_1+ix_2,z_2=x_3+ix_4\}$, equipped with the symplectic two-form $\Omega=(1/2s)(dx_1\wedge dx_2+dx_3\wedge dx_4)=(1/2s)(1/2i)(dz_1^*\wedge dz_1+dz_2^*\wedge dz_2)$.

There is a natural action of SU(2) on $\mathbf{R}^4=\mathbf{C}^2$, which is simply given by left multiplication:

$$\begin{bmatrix}\alpha & -\beta^*\\ \beta & \alpha^*\end{bmatrix}\begin{bmatrix}z_1\\ z_2\end{bmatrix}=\begin{bmatrix}\alpha z_1-\beta^* z_2\\ \beta z_1+\alpha^* z_2\end{bmatrix},$$

where $\left[\begin{smallmatrix}\alpha & -\beta^*\\ \beta & \alpha^*\end{smallmatrix}\right]$, with $|\alpha|^2+|\beta|^2=1$, is an element of SU(2) in the fundamental representation. This action is symplectic and Hamiltonian,[21] and its Lie algebra is spanned by the vector fields:

$$\begin{gathered}\bar{\chi}_1=x_4\partial_1-x_3\partial_2+x_2\partial_3-x_1\partial_4,\quad \bar{\chi}_2=-x_3\partial_1-x_4\partial_2+x_1\partial_3+x_2\partial_4,\\ \bar{\chi}_3=x_2\partial_1-x_1\partial_2-x_4\partial_3+x_3\partial_4.\end{gathered}\tag{17}$$

Hence, it is easy to prove that the linear vector field $\bar{\Delta}=\Sigma_{j=1}^3 B_j\bar{\chi}_j$ is a Hamiltonian vector field with a quadratic Hamiltonian, namely

$$\bar{H}=\sum_{j=1}^{3} B_j f_j,\tag{18}$$

where

$$\begin{gathered}f_1=\frac{1}{2s}(x_1x_3+x_2x_4)=\frac{1}{2s}\,\mathrm{Re}\,z_1^*z_2,\quad f_2=\frac{1}{2s}(x_1x_4-x_2x_3)=\frac{1}{2s}\,\mathrm{Im}\,z_1^*z_2,\\ f_3=\frac{1}{4s}(x_1^2+x_2^2-x_3^2-x_4^2)=\frac{1}{4s}(|z_1|^2-|z_2|^2).\end{gathered}\tag{19}$$

Here we can identify $\mathbf{R}^4$ with $T^*\mathbf{R}^2$ with canonical coordinates x_1, x_3 and momenta $p_1=x_2/2s$ and $p_2=x_4/2s$.

The SU(2) action we are considering leaves the three-dimensional spheres $S^3(R)=\{(x_1,x_2,x_3,x_4):x_1^2+x_2^2+x_3^2+x_4^2=R^2\}=\{(z_1,z_2):|z_1|^2+|z_2|^2=R^2\}$ invariant, so that we can restrict the dynamics from the full $\mathbf{R}^4$ to the submanifolds $S^3(R)$ on which the classical orbits lie. In the following we choose $R=2s$ and work on $S^3(2s)$.

The functions (19) and hence the Hamiltonian (18) have an additional symmetry, being invariant under the action of U(1), given by

$$(z_1,z_2)\mapsto(e^{i\theta}z_1,e^{i\theta}z_2),\quad \theta\in[0,2\pi[.$$

This allows us to project the Hamiltonian (18) from $S^3(2s)$ down to the two-dimensional manifold $S^3(2s)/\mathrm{U}(1)$, which is homeomorphic to the two-dimensional sphere. Indeed, the three functions $(x_1,x_2,x_3,x_4)\mapsto S_j\equiv f_j(x_1,x_2,x_3,x_4)$ $(j=1,2,3)$ given in (19) are the components of the projection map from the three-sphere $S^3(2s)$ to the two-sphere $S^2(s)$ of the Hopf bundle, $\mathrm{U}(1)\to S^3\to S^2$.[22]

On $S^2(s)$ the Hamiltonian (18) becomes simply $H=\Sigma_{j=1}^3 B_jS_j$ and therefore coincides with the Hamiltonian (9) for a spin in a magnetic field. This shows that the latter is the reduction of a quadratic Hamiltonian defined on a linear manifold. To prove this rigorously, we should show also

that the restriction to $S^3(2s)$ of the symplectic two-form $\overline{\Omega}$ is the pull-back of the symplectic two-form Ω we defined on $S^2(s)$. The proof of this statement is straightforward, so we will omit details here.

The situation we have examined here has some resemblance with the problem discussed, for example, in Ref. 23, namely with the possibility of finding solutions of the wave and Laplace equations on the Euclidean plane R^2, the two-sphere S^2, and the Lobachevski plane L^2 by a descent process, starting, respectively, from R^3, S^3, L^3. We would like to remark here, however, that the dynamical system we have chosen to consider on R^4 is not equivalent to a *single* spin in a magnetic field. Indeed, the Hamiltonian (18) on R^4 simultaneously describes all values of the spin, the latter getting fixed to the single value s only when we restrict the dynamics to the submanifold $S^3(R)$ with $R=2s$.

III. COHERENT STATE PATH INTEGRALS FOR SPIN

Let us consider now the quantum mechanics of a spinning particle, described by the Hamiltonian

$$\hat{H}=\mathbf{B}\cdot\hat{\mathbf{S}}, \tag{20}$$

where the spin operators $\hat{S}_j (j=1,2,3)$ satisfy the usual commutation relations ($\hbar=1$):

$$[\hat{S}_i,\hat{S}_j]=i\epsilon_{ijk}\hat{S}_k. \tag{21}$$

We have already mentioned in the Introduction that the semiclassical Bohr–Sommerfeld quantization turns out to be exact for this problem, and this seems to suggest that the stationary phase approximation to the path integral for the propagator and/or the partition function could be exact as well. In addition, for such a simple problem, one can evaluate the partition function exactly. Its expression,

$$\mathcal{Z}(\beta)=\mathrm{Tr}\{e^{-\beta\hat{H}}\}=\frac{e^{\beta Bs}}{1-e^{-\beta B}}+\frac{e^{-\beta Bs}}{1-e^{\beta B}}, \tag{22}$$

can be thought of as the sum of two terms, each corresponding to one of the two poles of the sphere ($S_3=\pm s$), similarly to what happens in the classical case.

In this section we will briefly review the existing literature on the evaluation of the partition function for a quantum spin in a magnetic field, and, in particular, on the validity of the stationary phase approximation applied to this problem.

Let us begin by considering a set $|l\rangle$ of generalized coherent states[4,7] labeled by one or more continuous variables that we denote collectively as l. The $|l\rangle$'s will be assumed to be normalized. They are, however, overcomplete, because although there is a resolution of the identity associated with them,

$$1=\int dl|l\rangle\langle l|, \tag{23}$$

with "dl" a suitable measure, in general, they fail to be an orthonormal set: $\langle l|l'\rangle\neq 0$.

Here we are interested in the group SU(2), which is generated by the spin-operator algebra (21). Coherent states[7] for a spin s ($2s$ being an integer) can be constructed as

$$|\theta,\phi\rangle=e^{-i\phi\hat{S}_3}e^{-i\theta\hat{S}_2}|0\rangle, \tag{24}$$

where $|0\rangle$ denotes the highest-weight state of the spin-s representation of SU(2) ($\hat{S}_3|0\rangle\equiv s|0\rangle$) and θ,ϕ are the two angular coordinates parametrizing S^2: $0\leqslant\theta\leqslant\pi$; $0\leqslant\phi\leqslant 2\pi$. It is well known[6,7] that

$$\langle \theta', \phi' | \theta, \phi \rangle = \left[\cos \frac{\theta'}{2} \cos \frac{\theta}{2} e^{i(\phi' - \phi)/2} + \sin \frac{\theta'}{2} \sin \frac{\theta}{2} e^{-i(\phi' - \phi)/2} \right]^{2s}, \tag{25}$$

and that the resolution of the identity associated with spin-coherent states is

$$1 = \frac{2s+1}{4\pi} \int_0^{2\pi} \int_0^{\pi} |\theta, \phi\rangle \langle \theta, \phi| \sin \theta \, d\theta \, d\phi. \tag{26}$$

Going back to the general case, let $\hat{H}$ be the Hamiltonian of a quantum system. The matrix element of the propagator,

$$K(l_F, l_I, T) = \langle l_F | e^{-i\hat{H}T} | l_I \rangle, \tag{27}$$

can be represented as the following path integral:

$$K(l_F, l_I, T) = \lim_{\epsilon \to 0} \int \prod_{k=1}^{N} (dl_k) \prod_{k=0}^{N} \langle l_{k+1} | e^{-i\epsilon \hat{H}} | l_k \rangle, \tag{28}$$

where $\epsilon = T/N$ and $|l_0\rangle \equiv |l_I\rangle, |l_{N+1}\rangle \equiv |l_F\rangle$. Equation (28) can be rewritten as

$$K(l_F, l_I; T) = \lim_{\epsilon \to 0} \int \prod_{k=1}^{N} (dl_k) \prod_{k=0}^{N} e^{iA(l_{k+1}, l_k)}, \tag{29}$$

where

$$A(l_{k+1}, l_k) = -i \ln \langle l_{k+1} | l_k \rangle - \epsilon H(l_{k+1}, l_k) \tag{30}$$

and

$$H(l_{k+1}, l_k) = \frac{\langle l_{k+1} | \hat{H} | l_k \rangle}{\langle l_{k+1} | l_k \rangle}. \tag{31}$$

It is usually assumed that, for ϵ small, $|l_{k+1}\rangle$ is so close to $|l_k\rangle$ that one is allowed to expand the former around the latter to leading order in ϵ. This leads to

$$H(l_{k+1}, l_k) \sim H(l_k) = \langle l_k | \hat{H} | l_k \rangle \tag{32}$$

and to

$$\ln \langle l_{k+1} | l_k \rangle \sim \langle \delta l_k | l_k \rangle, \tag{33}$$

where $|\delta l_k\rangle = |l_{k+1}\rangle - |l_k\rangle$. Hence, the continuum version of the path integral reads as

$$\int \mathscr{D}l \, \exp\left[i \int_0^T dt [i \langle l | \dot{l} \rangle - H(l)] \right], \tag{34}$$

where $|\dot{l}\rangle = d|l\rangle/dt$. This procedure is justified when the Hamiltonian contains an explicit kinetic term that can act as a regulator, concentrating the functional measure on continuous paths. This is the case of the Wiener integral, where[24,25] the measure is concentrated on paths $q(t)$ satisfying the Lipschitz condition: $|q(t+\epsilon) - q(t)| = O(\epsilon^{1/2})$. The same holds true for the Feynman path integrals for massive particles in not too singular potentials.[1]

In the case of spin, the Hamiltonian (20) contains no regulators and the straightforward application of (32) and (33) is questionable. We will see, indeed, that it may lead to serious problems. Let us be more specific. Taking again the magnetic field along the positive z axis we have, in terms of spin-coherent states (24):

$$\langle l|\hat{H}|l\rangle \to \langle \theta,\phi|\hat{H}|\theta,\phi\rangle = sB\ \cos\ \theta \tag{35}$$

and

$$i\langle l|\dot{l}\rangle \to i\langle \theta,\phi|\frac{d}{dt}|\theta,\phi\rangle = s\ \cos\ \theta\dot{\phi}. \tag{36}$$

So we obtain the path integral:

$$\langle \theta_F,\phi_F|e^{-iB\hat{S}_3 T}|\theta_I,\phi_I\rangle = \int \mathscr{D}\Omega\ \exp\left[i\int_0^T [s\ \cos\ \theta\dot{\phi} - sB\ \cos\ \theta]dt\right], \tag{37}$$

where $\mathscr{D}\Omega = \sin\theta\mathscr{D}\theta\,\mathscr{D}\phi$. From (37) we can obtain the canonical partition function $\mathscr{Z}(\beta)$ by setting $T=-i\beta, |\theta_F,\phi_F\rangle = |\theta_I,\phi_I\rangle$ and by tracing over the angles. Following the standard procedure and Ref. 8, we evaluated $\mathscr{Z}(\beta)$ by time slicing the path integral and using the resolution of the identity (26) at each intermediate (Euclidean) time. In order to include paths turning around the North Pole any number of times, we had to extend, at every time slice, the domain of integration of the variable ϕ from $[0,2\pi]$ to $[-\infty,+\infty]$. In fact without following such a procedure one would have gotten, as in Ref. 8, a completely wrong partition function. Denoting with $\mathscr{Z}_N(\beta)$ the result for N time slices, we found for it, without any further approximation, the expression[13]

$$\mathscr{Z}_N(\beta) = \left(1+\frac{1}{2s}\right)^N \mathscr{Z}(\beta), \tag{38}$$

where $\mathscr{Z}(\beta)$ on the right-hand side is the exact partition function (22).

As one can easily notice by simple inspection, in the limit $N\to\infty$, $\mathscr{Z}_N$ coincides with the exact partition function up to a diverging prefactor. Such divergency disappears only in the classical limit, namely $\hbar\to 0$, $s\to\infty$, with $\hbar s = \text{const}$. On the other hand, the only approximations we used are those given by Eqs. (32) and mainly (33), which again are exact in the classical limit. In the sequel of this paper we shall come back to this point.

We discuss now briefly two different approaches[5,16] that lead to the conclusion that in the case of a spinning particle in a magnetic field the stationary phase approximation to the path integral for the propagator does indeed yield the exact result. This holds again up to a normalization factor not taken into account in Refs. 15 and 16, since the calculation is done in the continuum.

Klauder[5] has proposed a modified form for the action that appears in the path integral (34), redefining the latter as

$$K(l_F,l_I;T) = \lim_{\epsilon\to 0}\int \mathscr{D}l\ \exp\left[i\int_0^T dt\left[i\langle l|\dot{l}\rangle + \frac{1}{2}\,i\epsilon\langle\dot{l}|(1-|l\rangle\langle l|)|\dot{l}\rangle - H(l)\right]\right]. \tag{39}$$

The prescription here is that the limit for $\epsilon\to 0$ should be taken after having evaluated the path integral in the stationary phase approximation. For the case of a spin in a magnetic field, (39) becomes

$$K(\theta_F,\phi_F,\theta_I,\phi_I;T) = \lim_{\epsilon\to 0}\int \mathscr{D}\Omega\ \exp\left[i\int_0^T\left[s\ \cos\ \theta\dot{\phi} + \frac{1}{4}\,is\epsilon(\dot{\theta}^2+\sin^2\ \theta\dot{\phi}^2) - sB\ \cos\ \theta\right]dt\right], \tag{40}$$

and the action in (40) becomes essentially that of a particle of charge s and mass $m=1/2s\epsilon$ moving on the two-sphere S^2, coupled both with a magnetic monopole of unit strength located at the center of the sphere and with a constant electric-type field directed along the z axis. In this context, Dirac's quantization condition[26] becomes identical with the spin quantization condition, i.e., $2s=$integer.

The classical equations of motion that can be derived from the action in (40) are now second order in time for $\epsilon\neq 0$, and hence are not plagued by the already mentioned problem of overdetermination. Klauder has proved that they can be solved explicitly and that the resulting stationary phase approximation to the path integral (or, better, what he calls the ''dominant stationary phase approximation,'' namely approximating the path integral with $e^{iS_{\rm cl}}$, without any prefactor originating from the integration of Gaussian fluctuations) is indeed exact. Actually, only the free-spin case $B=0$ has been considered in Ref. 5, but the extension to $B\neq 0$ is straightforward.[13] It should be noted, incidentally, that the term that Klauder has added to the action is in the form of a kinetic energy term, thus providing the required regulator justifying the assumption of continuously varying paths.

The origin of the additional kinetic-type term, that looks somewhat mysterious in Klauder's original paper,[4] can be clarified as follows. If we push the expansion of the logarithm in (33) one step further beyond first order, we obtain, with $|\delta l\rangle\sim\epsilon|\dot{l}\rangle+\epsilon^2/2|\ddot{l}\rangle$:

$$\ln\langle l_{k+1}|l_k\rangle\sim\epsilon\langle\dot{l}_k|l_k\rangle+\frac{\epsilon^2}{2}\langle\ddot{l}_k|l_k\rangle-\frac{\epsilon^2}{2}(\langle\dot{l}_k|l_k\rangle)^2, \tag{41}$$

leading, in the continuum limit, to

$$\lim_{\epsilon\to 0}\exp\left[i\int_{t_i}^{t_f}dt\left[i\langle l|\dot{l}\rangle+\frac{1}{2}i\epsilon(-\langle\ddot{l}|l\rangle+\langle\dot{l}|l\rangle\langle l|\dot{l}\rangle)\right]\right], \tag{42}$$

where we have used $\langle l|\dot{l}\rangle=-\langle\dot{l}|l\rangle$. A final integration by parts of the term containing the second derivative yields precisely Klauder's additional term.

Suzuki[16] has adopted quite a different approach. Introducing two additional resolutions of the identity, the propagator

$$K(l_F,l_I,T)=\int_{l(0)=l_I}^{l(T)=l_F}\mathscr{D}l\ e^{iA_{FI}(l)}, \tag{43}$$

where

$$A_{FI}(l)=\int_0^T dt[i\langle l|\dot{l}\rangle-H(l)], \tag{44}$$

is rewritten in Ref. 16 in the form

$$K(l_F,l_I,T)=\int\int dl_f\,dl_i\langle l_F|l_f\rangle\langle l_f|e^{-i\hat{H}T}|l_i\rangle\langle l_i|l_I\rangle=\int\int dl_f\,dl_i\langle l_F|l_f\rangle\langle l_i|l_I\rangle\int_{l(0)=l_i}^{l(T)=l_f}\mathscr{D}l\ e^{iA_{fi}(l)}. \tag{45}$$

In general, the parameter(s) l labeling a coherent state can be defined in terms of the expectation values of a suitable set of operators: position and momentum for the free particle and the harmonic oscillator, spin components in the case of spins. Taking then the latter as Cauchy data for the canonical equations of motion, one can determine how they evolve classically in time, thus

determining a ''classical'' coherent state $|l(t)\rangle$ as the coherent state labeled by $l(t)$, the evoluted at time t of any given initial parameter set l. Then, Suzuki has argued that the stationary phase approximation to the last integral leads to

$$\int_{l(0)=l_i}^{l(T)=l_f} \mathscr{D}l\ e^{iA_{fi}(l)} \sim \delta(l_f - l_i(T)) e^{iA_{fi}}, \tag{46}$$

where $l_i(T)$ is the evoluted at time T of l_i, and that the final result of the application of the stationary phase approximation is the semiclassical propagator,

$$K_{\mathrm{sc}}(l_F, l_I, T) = \int dl_i \langle l_F | l_i(T) \rangle \langle l_i | l_I \rangle e^{iA_{fi}}, \tag{47}$$

where A_{fi} is the classical action evaluated along the classical path leading from $l(0)=l_i$ to $l(T)$. Once again, the semiclassical propagator (47) yields the exact result for the propagator of a spinning particle.

We would like to show here that the possible exactness of Eq. (47) has very little to do with the path integral formalism itself, and that it follows rather from a single assumption, one that amounts basically to assuming that the Ehrenfest theorem be applicable in the present case. Let $\hat{l}$ be the set of operators whose expectation values label a given coherent state. To each coherent state $|l\rangle$ we can associate two different time-dependent states: the ''classically'' time evoluted state $|l(t)\rangle$ defined above, and therefore such that

$$\langle l(t) | \hat{l} | l(t) \rangle = l_{\mathrm{cl}}(t), \tag{48}$$

$l_{\mathrm{cl}}(t)$ being the classical trajectory; and the quantum time evoluted state $|l,t\rangle$ obtained through the application of the full quantum evolution operator:

$$|l,t\rangle = e^{-i\hat{H}t} |l\rangle. \tag{49}$$

We require now the expectation values on the quantum evoluted state to evolve in time according to the classical equations of motion:

$$\langle l,t | \hat{l} | l,t \rangle = l_{\mathrm{cl}}(t). \tag{50}$$

In other words, we are assuming, as anticipated, the validity of the Ehrenfest theorem. A sufficient condition for this to happen is that the Heisenberg equations of motion be linear equations. This is certainly true for quadratic Hamiltonians with conventional canonical coordinates and momenta and the standard Poisson brackets among them. For spins, the Hamiltonian (4) is not of the quadratic type, but the Poisson brackets (1) lead, nonetheless, to linear equations of the motion, and hence to the validity of the Ehrenfest theorem. If we now assume that the set of operators $\hat{l}$ act irreducibly on the Hilbert space of states (which is true, e.g., for harmonic oscillators and for spin systems), the two states $|l,t\rangle$ and $|l(t)\rangle$ will differ, at most, by a phase, i.e.:

$$|l,t\rangle = e^{i\chi(t)} |l(t)\rangle. \tag{51}$$

Differentiating with respect to time, we obtain

$$\langle l(t) | \frac{d}{dt} | l(t) \rangle = -i\dot{\chi} + + \langle l,t | \frac{d}{dt} | l,t \rangle, \tag{52}$$

and hence

$$\langle l|\dot{l}\rangle_{\rm cl} = -i\dot{\chi} - i\langle l,t|\hat{H}|l,t\rangle. \tag{53}$$

If, as it is presently the case, the Hamiltonian does not contain time derivatives, we obtain, furthermore,

$$\dot{\chi} = i\langle l|\dot{l}\rangle_{\rm cl} - \langle l(t)|\hat{H}|l(t)\rangle = i\langle l|\dot{l}\rangle_{\rm cl} - H(l(t)), \tag{54}$$

and eventually, integrating the last equation and up to an irrelevant constant phase,

$$\chi(t) = \int_0^t [i\langle l|\dot{l}\rangle_{\rm cl} - H(l)]dt'. \tag{55}$$

The rhs of (55) is exactly the classical action, hence $\chi(t) = A_{\rm cl}(t)$. Then Suzuki's result follows at once from

$$K(l_F, l_I, T) = \langle l_F|e^{-i\hat{H}T}|l_T\rangle = \int dl_i \langle l_F|e^{-i\hat{H}T}|l_i\rangle\langle l_i|l_I\rangle = \int dl_i \langle l_F|l_i(T)\rangle\langle l_i|l_I\rangle e^{i\chi(T)}$$

$$= \int dl_i \langle l_F|l_i(T)\rangle\langle l_i|l_I\rangle e^{iA_{\hbar}}, \tag{56}$$

which is the desired result.

Let us analyze (56) in the specific case of a spinning particle. As already pointed out, the Hamiltonian (4) leads to linear Heisenberg equations of motion and hence to the validity of formula (56). It seems to us that this is the ultimate reason for the apparently surprising fact that stationary phase approximation to path integrals and/or semiclassical quantization leads to the exact result for the quantum propagator of a spinning particle. We would like to stress here that this is also true for the motion in a magnetic field with an arbitrary dependence on time. Formula (56) reduces therefore the quantum problem of the calculation of the spin propagator in an arbitrary magnetic field to the solution of the classical equation of motion.

The expression for the propagator can, of course, be worked out explicitly only when the classical equation of motion can be solved analytically. With a constant magnetic field along the z axis, formula (47) reads as

$$K(\theta_F, \phi_F, \theta_I, \phi_I; T) = \frac{2s+1}{4\pi} \int d\Omega_i \langle \theta_F, \phi_F|\theta_i(T), \phi_i(T)\rangle\langle \theta_i, \phi_i\theta_I, \phi_I\rangle e^{iA_{\rm cl}}. \tag{57}$$

Since the solutions of the classical equations of motion are $\theta_i(T) = \theta_i$; $\phi_i(T) = \phi_i + BT$, while $A_{\rm cl} = 0$, the above expression becomes

$$K(\theta_F, \phi_F, \theta_I, \phi_I; T) = \frac{2s+1}{4\pi} \int d\Omega_i \langle \theta_F, \phi_F|\theta_i, \phi_i + BT\rangle\langle \theta_i, \phi_i|\theta_I, \phi_I\rangle. \tag{58}$$

The integral in (58) can be done easily by noting that $\langle \theta_F, \phi_F|\theta_i, \phi_i + BT\rangle = \langle \theta_F, \phi_F - BT|\theta_i, \phi_i\rangle$ and using the resolution of the identity. We obtain, eventually,

$$K(\theta_F, \phi_F, \theta_I; \phi_I; T) = \langle \theta_F, \phi_F - BT|\theta_I, \phi_I\rangle, \tag{59}$$

which indeed gives the exact propagator, upon using formula (25) for the overlap of two coherent states.

IV. THE COMPLEX SADDLE POINT

We devote this section to another approach to the path integral for spin. It has been used, for example, in Refs. 15 and 27, where, however, only continuous and hence formal expressions for the action and the path integral have been studied.

Here we will study the path integral *discrete* version for the propagator (34). The method is based on a different choice of the spin-coherent states. Instead of (24), we consider the following states, labeled by a complex parameter μ:

$$|\mu\rangle = \frac{e^{\mu \hat{S}^-}}{(1+|\mu|^2)^s}\,|0\rangle, \tag{60}$$

where we have set $\hat{S}^{\pm}=\hat{S}_1 \pm i\hat{S}_2$. To be more precise, μ parametrizes the homogeneous space SU(2)/U(1)$=S^2$ by means of the stereographic projection of S^2 onto $\mathbf{R}^2$. With respect to the spherical coordinates θ and ϕ used previously, one has $\mu=\tan(\theta/2)e^{i\phi}$, and it is also not difficult to check that the state (60) coincides up to a phase with the state $|\theta,\phi\rangle$ defined in (24).

To write down an explicit expression for the path integral in terms of the coherent states (60), we need the matrix elements

$$\langle \lambda|\mu\rangle = \frac{(1+\lambda^*\mu)^{2s}}{(1+|\mu|^2)^s(1+|\lambda|^2)^s}, \quad \langle \lambda|\hat{S}_3|\mu\rangle = \langle \lambda|\mu\rangle s\,\frac{1-\lambda^*\mu}{1+\lambda^*\mu},$$
$$\langle \mu|\dot{\mu}\rangle = \frac{s}{1+|\mu|^2}\,(\dot{\mu}\mu^* - \dot{\mu}^*\mu), \tag{61}$$

and the explicit formula for the resolution of the identity:

$$\frac{2s+1}{\pi}\int \frac{d^2\mu}{(1+|\mu|^2)^2}\,|\mu\rangle\langle\mu| = 1, \tag{62}$$

where $d^2\mu = d(\mathrm{Re}\,\mu)d(\mathrm{Im}\,\mu)$. After some algebra, one finds that the path integral representation of the propagator is given by

$$K(\mu_F^*,\mu_I;T) = \int_{\substack{\mu(0)=\mu_I \\ (\mu(T))^*=\mu_F^*}} \frac{d^2\mu}{(1+|\mu|^2)^2}\,e^A, \tag{63}$$

where the action for a spin in a magnetic field is

$$A = is\int_0^T dt\left(i\,\frac{\dot{\mu}\mu^* - \mu\dot{\mu}^*}{1+|\mu|^2} - B\,\frac{1-|\mu|^2}{1+|\mu|^2}\right). \tag{64}$$

Again, the saddle point equations that are derived by extremizing (64):

$$\dot{\mu} = iB\mu, \quad \dot{\mu}^* = -iB\mu^*, \tag{65}$$

are first order, so that they do not admit a solution for boundary conditions of the form

$$\mu(0)=\mu_I, \quad (\mu(T))^* = \mu_F^*, \tag{66}$$

with arbitrary μ_I and μ_F.

This problem does, however, admit of solutions[15,28] if we enlarge our variable space from $\mathbf{C}$ to $\mathbf{C}^2$, and look for saddle point solutions for which $\mu(t)$ and $\mu^*(t)$ are *not* complex conjugate one of the other. In other words, we have to consider μ and μ^* as independent complex variables, and look for solutions of (65) satisfying the boundary conditions

$$\mu(0)=\mu_I, \quad \mu^*(T)=\mu_F^*. \tag{67}$$

These so-called complex saddle point solutions are easily found to be

$$\mu(t)=e^{iBt}\mu_I, \quad \mu^*(t)=e^{iB(T-t)}\mu_F^*, \tag{68}$$

and, to complete the stationary phase approximation, one has further to evaluate the contributions of the Gaussian fluctuations around the solutions (68).

This has been done by the authors of Refs. 15 and 27, who have concluded that one can obtain the exact propagator in this way. They have, however, worked with the continuous expression (64), and therefore they have performed only formal calculations. Funahashi *et al.*[29] have considered the discrete version of the integral, but they have applied a stationary phase approximation to the calculation of the partition function only. This problem, as pointed out by the same authors, is simpler than the calculation of the propagator, since the overdetermination problem can be overcome without enlarging the variable space from $\mathbf{C}$ to $\mathbf{C}^2$.

Our aim in this section is to examine whether the stationary phase approximation to the path integral (63) is exact, by performing the calculation in the *discrete* version of the path integral. The latter is given by (29), where now the generic index l stands for the complex parameter μ. By using (61) and rearranging the terms, one eventually gets

$$K(\mu_F^*,\mu_I,T)=\mathcal{N}\int\prod_{j=1}^{N-1}\frac{d^2\mu_j}{(1+\mu_j^*\mu_j)^2}\,e^A, \tag{69}$$

with

$$\mathcal{N}=\left(\frac{2s+1}{\pi}\right)^{N-1}\frac{1}{(1+|\mu_F|^2)^s(1+|\mu_I|^2)^s}, \tag{70}$$

whereas the discretized action A is given by

$$A=\sum_{j=1}^{N}\left[A_{j,j-1}+H_{j,j-1}\right]+2s\,\ln(1+\mu_F^*\mu_N), \tag{71}$$

$$A_{j,j-1}\equiv 2s\,\ln\frac{1+\mu_j^*\mu_{j-1}}{1+\mu_j^*\mu_j} \tag{72}$$

$$H_{j,j-1}=-iBs\epsilon\,\frac{1-\mu_j^*\mu_{j-1}}{1+\mu_j^*\mu_{j-1}}. \tag{73}$$

The expression for $A_{j,j-1}$ given in (72) comes from the exponentiation of the overlaps $\langle\mu_j|\mu_{j-1}\rangle$ $(j=1,\ldots,N)$. Let us remark that we have *not* expanded the overlaps to first order in the difference $|\mu_j\rangle-|\mu_{j-1}\rangle$, as is usually done to recover the continuum version [see (33)]. As already pointed out, such an expansion would be correct only in the presence of a regulating term in the action. Thus, we will work only with (72) and we will proceed now to evaluate the stationary phase approximation to the multidimensional integral (69), according to the formula

$$K(\mu_F^*,\mu_I,T)_{\rm sc}=\mathcal{N}\prod_{j=1}^{N-1}\left(\frac{1}{(1+\mu_j^*\mu_j)^2}\right)_{\rm cl} e^{A_{\rm cl}}\frac{\pi^{N-1}}{(\det M_N)^{1/2}}, \tag{74}$$

where M_N is the $2(N-1)\times 2(N-1)$ matrix of quadratic fluctuations around the classical solutions of the discretized action (71):

$$A=A_{\rm cl}+(\delta\mu_1^*,\delta\mu_1,\ldots,\delta\mu_{N-1}^*,\delta\mu_{N-1})M_N\begin{pmatrix}\delta\mu_1\\ \delta\mu_1^*\\ \vdots\\ \delta\mu_{N-1}\\ \delta\mu_{N-1}^*\end{pmatrix}. \tag{75}$$

The subscript ''cl'' means that the function (the action in this case) has to be evaluated on the classical solution, which satisfies the saddle point equations:

$$\begin{aligned}\frac{\mu_{j+1}^*-\mu_j^*}{1+\mu_j^*\mu_j}&=-i\epsilon B\,\frac{\mu_{j+1}^*}{1+\mu_{j+1}^*\mu_j},\\ \frac{\mu_j-\mu_{j-1}}{1+\mu_j^*\mu_j}&=+i\epsilon B\,\frac{\mu_{j-1}}{1+\mu_j^*\mu_{j-1}}.\end{aligned} \tag{76}$$

In (76), as well as in (71), we have explicitly written $|\mu_j|^2$ as $\mu_j\mu_j^*$ to stress the fact that in the search of the saddle point solutions we have to treat μ_j and μ_j^* as independent complex variables. Indeed, exactly as in the continuum, the equations (76) are incompatible with the boundary conditions

$$\mu_0=\mu_I,\quad \mu_N^*=\mu_F^*, \tag{77}$$

unless μ_j and μ_j^* are treated as independent variables.

We know that the classical solution has to fulfill the property $\mu_{j+1}|_{\rm cl}=\mu_j|_{\rm cl}+O(\epsilon)$, so that we can approximate the denominators on the right-hand side of (76), to get

$$\begin{aligned}\frac{\mu_{j+1}^*-\mu_j^*}{1+\mu_j^*\mu_j}&=-i\epsilon B\,\frac{\mu_j^*}{1+\mu_j^*\mu_j}+O(\epsilon^2),\\ \frac{\mu_j-\mu_{j-1}}{1+\mu_j^*\mu_j}&=+i\epsilon B\,\frac{\mu_{j-1}}{1+\mu_j^*\mu_j}+O(\epsilon^2).\end{aligned} \tag{78}$$

To order ϵ, we find for the solutions satisfying the boundary conditions (77) and for the classical action, the expressions

$$\mu_j=(1+i\epsilon B)^j\mu_I,\quad \mu_j^*=(1+i\epsilon B)^{N-j}\mu_F^*, \tag{79}$$

$$A_{\rm cl}=-isBT. \tag{80}$$

To complete the calculation of the right-hand side of (74), we have to compute the determinant of the Gaussian fluctuation matrix M_N. As for the solutions of the classical equations (76), we evaluate the matrix elements to the order $O(\epsilon)$. Neglecting therefore all the terms of at least order $O(\epsilon^2)$, we find that the only nonzero matrix elements are

$$a_j \equiv \left.\frac{\partial^2 A}{\partial \mu_j^* \, \partial \mu_j}\right|_{\rm cl} = \left.\frac{\partial^2 A}{\partial \mu_j \, \partial \mu_j^*}\right|_{\rm cl} = \left.\frac{-2s}{(1+\mu_j^* \mu_j)^2}\right|_{\rm cl} = \frac{-2s}{(1+(1+i\epsilon B)^N \mu_F^* \mu_I)^2}, \tag{81}$$

$$b_j \equiv \left.\frac{\partial^2 A}{\partial \mu_j \, \partial \mu_{j+1}^*}\right|_{\rm cl} = \left.\frac{\partial^2 A}{\partial \mu_{j+1}^* \, \partial \mu_j}\right|_{\rm cl} = \left[\frac{2s}{1+\mu_{j+1}^* \mu_j}\right]_{\rm cl} \left[\frac{1}{1+\mu_j^* \mu_j} + i\epsilon B \, \frac{1}{(1+\mu_{j+1}^* \mu_j)^2}\right]_{\rm cl}$$

$$= \frac{2s(1+i\epsilon B)}{(1+(1+i\epsilon B)^N \mu_I \mu_F^*)^2}. \tag{82}$$

Defining

$$A_i = \begin{pmatrix} a_i & 0 \\ 0 & a_i \end{pmatrix}, \quad B_i = \begin{pmatrix} 0 & 0 \\ 0 & b_i \end{pmatrix}, \quad C_i = \begin{pmatrix} b_i & 0 \\ 0 & 0 \end{pmatrix}, \tag{83}$$

the matrix M_N is given by

$$M_N = \begin{pmatrix} A_1 & B_1 & & & & \\ C_1 & A_2 & B_2 & & & \\ & & \ddots & & & \\ & & & C_{N-3} & A_{N-2} & B_{N-2} \\ & & & & C_{N-1} & A_{N-1} \end{pmatrix}. \tag{84}$$

Thus, we have

$$\det M_N = a_1^2 \cdots a_{N-1}^2 = \left[\frac{-2s}{(1+(1+i\epsilon B)^N \mu_I \mu_F^*)^2}\right]^{2(N-1)}, \tag{85}$$

which can be finally inserted, together with (80), in (74), yielding

$$K(\mu_F^*, \mu_I, T)_{\rm sc} = \left(1+\frac{1}{2s}\right)^{N-1} \frac{e^{-isBT}(1+\mu_I \mu_F^* (1+iBT/N)^N)^{2s}}{(1+|\mu_F|^2)^s (1+|\mu_I|^2)^s}. \tag{86}$$

This is again the expected result up to the divergent normalization factor $(1+1/2s)^{N-1}$. Indeed, since $\lim_{N\to\infty}(1+iBT/N)^N = e^{iBT}$, but for the prefactor, we obtain

$$K(\mu_F^*, \mu_I, T)_{\rm sc} = \frac{e^{-isBT}(1+\mu_I \mu_F^* e^{iBT})^{2s}}{(1+|\mu_F|^2)^s (1+|\mu_I|^2)^s}, \tag{87}$$

which coincides with the exact propagator.

V. CONCLUSIONS

In this paper we have examined the problem of spin in a magnetic field. We have seen that the stationary phase approximation applied to the calculation of the classical partition function yields the correct result. In quantum mechanics the situation is more complicated. We have reexamined the different approaches that have been used in literature to prove the exactness of stationary phase approximation in the calculation of the quantum propagator and partition function. All these methods, in particular those proposed by Klauder[5] and Keski-Vakkuri *et al.*,[15] make use of the continuum expression of the path integral, and hence reproduce the correct result only formally.

To test the validity of the stationary phase approximation for a spin system, we decided to work with the very definition of the path integral, namely with its discrete version. We have

written the discrete path integral for the partition function and the propagator in terms of spin coherent states and then considered two different kinds of approximations. In Sec. III we have expanded the overlaps $\langle l_k|_{lk-1}\rangle$ to first order in $\epsilon=T/N$ and then performed an exact integration. On the contrary, in Sec. IV we have made no expansion for the overlaps and applied instead the complex saddle point method to evaluate the stationary phase approximation of the path integral. In both cases, we have found that the exact result is reproduced correctly only up to an infinite normalization factor, $\lim_{N\to\infty}(1+1/2s)^N$, which goes to 1 in the classical limit $s\to\infty$, provided the latter is performed first. Notice that this fact is not a drawback just of the Hamiltonian for a spinning particle. Indeed, one can repeat easily the calculation for $H\equiv 0$ and get the same infinite constant.

A very similar conclusion has also been reached by Enz and Schilling.[11] They have examined the semiclassical theory for the tunneling of a magnetic ion in a crystal field and an applied magnetic field. In particular, they have calculated the quantum ground state energy E_0, which classically is doubly degenerate, as well as the tunnel splitting energy ΔE_0 as a function of the spin s. By performing the calculations by means of spin-coherent states, they have found that the path integral does not yield the correct semiclassical results for these physical quantities.

All this seems to suggest that, for those Hamiltonians that do not contain a regulating term (such as a kinetic part), any approximation that restricts the class of quantum paths in phase space, by imposing some regularity conditions on them, yields a wrong result. In our case this shows up in the appearance of an infinite prefactor.

We would like to conclude by commenting on the paper by Funahashi *et al.*,[29] who have been able to reproduce the exact partition function (with the correct prefactor) by performing the stationary phase approximation in the discrete path integral, written again in terms of spin-coherent states. They have obtained this result by also taking into account the Gaussian fluctuations coming from the factor $1/(1+|\mu|^2)^2=\sin\theta/4$ appearing in the integration measure. We do not want to explain this technique, which is described in detail in Ref. 29. Here we notice only that the inclusion of fluctuations coming from the measure induces a shift in the multiplicative factor appearing in front of the action from $2s$ to $2s+1$. Effectively, we can say that such a method amounts to choosing $2s+1$ as a parameter for the semiclassical expansion. If so, we should not evaluate the path integral following (74), but according to

$$K(\mu_F^*,\mu_I,T)_{\rm sc}=\mathcal{N}\prod_{j=1}^{N-1}\left(\frac{e^{-\tilde{A}/(N-1)}}{(1+\mu_j^*\mu_j)^2}\right)_{\rm cl}\frac{\pi^{N-1}e^{(2s+1)\tilde{A}_{\rm cl}}}{(\det\tilde{M}_N)^{1/2}}, \tag{88}$$

where $\tilde{A}=A/2s$ and $\tilde{M}_N$ is the matrix of Gaussian fluctuations of $(2s+1)\tilde{A}$ around the classical solution, so that

$$\det\tilde{M}_N=a_1^2\cdots a_{N-1}^2=\left[\frac{-2(s+1)}{(1+(1+i\epsilon B)^N\mu_I\mu_F^*)^2}\right]^{2(N-1)}. \tag{89}$$

It is exactly the factor $2s+1$ in (89) that cancels the same factor in $\mathcal{N}$, yielding the correct propagator.

This is quite a remarkable result. In our opinion, however, the derivation presented in Ref. 29 needs some clarification. To us, it seems to be inconsistent to include Gaussian fluctuations of the measure factor in the calculation of the stationary phase approximation without considering also its contributions to the saddle point equations. In Ref. 29 this method works only because the first derivatives of the measure factor *do* vanish at the classical solution, which in this case correspond to $\mu=0$ or $\mu=\infty$ ($\theta=0$, π in angular coordinates). But this would not be the case in slightly more complicated situations, for example for the calculation of the propagator or when considering complex saddle point solutions.

APPENDIX: THE DUISTERMAAT–HECKMAN THEOREM

Let us consider an oscillatory integral of the kind

$$I(t)\equiv\left(\frac{t}{2\pi}\right)^n\int_M \sigma e^{itf}, \tag{A1}$$

over a $(2n)$-dimensional manifold M with volume form σ. If M is a Riemannian manifold, under rather mild hypotheses, namely that the function f be a Morse function, i.e., that the Hessian matrix of f be nonsingular at all critical points of f [$\det \mathrm{Hess}_P(f)\neq 0$ if $\nabla f(P)=0$], it is possible to show[30] that for large values of the parameter t, one has

$$I(t)=\sum_P c_P e^{itf(P)}+O(t^{-1}), \tag{A2}$$

where the sum ranges over all critical points of f and the coefficients are given in terms of the determinant of the Gaussian fluctuations of f around the critical points:

$$c_P=\exp\left[i\,\frac{\pi}{4}\,\mathrm{sgn}\ \mathrm{Hess}_P(f)\right][\det \mathrm{Hess}_P(f)]^{-1/2}. \tag{A3}$$

Here the signature $\mathrm{sgn}\,A$ of a symmetric real-valued nonsingular matrix A is defined as the number of its positive eigenvalues minus the number of its negative eigenvalues.

Everybody is familiar with the elementary result that the remainder term $O(t^{-1})$ vanishes identically if M is the linear manifold $\mathbf{R}^{2n}$ with volume form $\sigma=dx_1\cdots dx_{2n}$, and the function f is a quadratic form: $f=\frac{1}{2}Q\vec{x}\cdot\vec{x}-\vec{\xi}\cdot\vec{x}$, Q being any symmetric real-valued $(2n)$-dimensional nonsingular matrix. In this case, the only critical point of f is $\vec{x}_0=Q^{-1}\vec{\xi}$ and $\mathrm{Hess}_{\vec{x}_0}(f)=Q$, so that (A2) with $O(t^{-1})\equiv 0$ gives simply the formula for a Gaussian integral.

The theorem of Duistermaat–Heckman[17] and its generalization due to Berline and Vergne[18] establish under which conditions an integral of the kind (A1) can be exactly evaluated in the stationary phase approximation, i.e., when $O(t^{-1})\equiv 0$.

Let M be a compact $(2n)$-dimensional manifold with symplectic two-form Ω and suppose M is acted upon by a compact Lie group G, whose action is symplectic and Hamiltonian.[30] Let us denote with χ_η the fundamental vector field on M generated by the action of the element η in the Lie algebra G of G and with f_η the associated Hamiltonian function ($i_{\chi_\eta}\Omega = df_\eta$, where i denotes the contraction). Then, if χ_η is nondegenerate, i.e., if it is zero only at the fixed points of G, the following results hold:[30]

(1) f_η is a Morse function;

(2)

$$\left(\frac{t}{2\pi}\right)^n\int_M \frac{\Omega^n}{n!}\,e^{itf_\eta}=\sum_P c_P e^{itf_\eta(P)}, \tag{A4}$$

where the the sum ranges over the critical points of f, i.e., over the points P, such that $\chi_\eta(P)=0$ and the coefficients c_P are given by

$$c_P=\frac{i^n}{\lambda_1\lambda_2\cdots\lambda_n}, \tag{A5}$$

the λ_j's being the coefficients appearing in the matrix L_P of the derivatives at P of the components of the vector field χ_η, $[L_P]^{ij}=(\partial\chi_\eta^i/\partial x_j)_P$, which in a suitable *positively oriented* basis can always be written as

$$L_P=\begin{bmatrix} 0 & \lambda_1 & & & & & \\ -\lambda_1 & 0 & & & & & \\ & & 0 & \lambda_2 & & & \\ & & -\lambda_2 & 0 & & & \\ & & & & \cdots & 0 & \lambda_n \\ & & & & & -\lambda_n & 0 \end{bmatrix}.$$

If M is equipped with a Riemannian metric, formula (A5) is seen to coincide with (A3).

From a physical point of view, (A4) can be applied to classical statistical mechanics for the computation of the partition function:

$$\mathcal{Z}=\int_M \frac{\Omega^n}{n!}\, e^{-\beta \mathrm{H}}. \tag{A6}$$

In this case the vector field χ_η is given by the Hamiltonian vector field Δ_{H}, where now H plays the role of the function f_η. The assumptions of the Duistermaat–Heckman theorem require Δ_{H} to be nondegenerate and to be the fundamental vector field associated with an element η of the Lie algebra G of a compact Lie group G, acting symplectically on the manifold M. If these two conditions holds, we can apply formula (A4) to conclude that (we have set $\beta=-it$):

$$\mathcal{Z}(\beta)=\left(\frac{2\pi}{i\beta}\right)^n \sum_P c_P e^{-\beta H(P)}, \tag{A7}$$

where (i) the sum ranges over the stationary points of the Hamiltonian, $\Delta_{\mathrm{H}}(P)=0$; (ii) the coefficients c_P are given by (A5) in terms of the λ_j's, the latter being the coefficients of the matrix $[L_P]_{ij}=(\partial \Delta_H^i/\partial x_j)_P$, written in a suitable positive oriented basis.

Let us go back now to the problem of a spin in a magnetic field. We want to show that the Duistermaat–Heckman theorem can be applied to this problem, so that the *exact* partition function can be calculated by means of formula (A7). The Hamiltonian vector field associated to the Hamiltonian (9) is

$$\Delta=B\left(-S_2\,\frac{\partial}{\partial S_1}+S_1\,\frac{\partial}{\partial S_2}\right), \tag{A8}$$

and it is easy to recognize that it is proportional to the generator $\chi_\eta=\partial/\partial\phi$ of the rotations about the third axis (i.e., the axis along the constant magnetic field). Thus, the Lie group that acts symplectically on the phase space manifold $S^2(s)$ is simply given by $U(1)$ in this case.

To apply (A7) we have, first of all, to find the critical points of the Hamiltonian, which are given by the North and the South Poles of the sphere:

$$P_\pm \equiv (0,0,\pm s), \tag{A9}$$

and then to compute the coefficients $c_{P_\pm}$ according to (A5). In the tangent space of P_+ and P_-, we choose to work with the positively oriented basis $(\partial/\partial S_1, \partial/\partial S_2)$ and $(\partial/\partial S_2, \partial/\partial S_1)$, respectively. With respect to these bases,

$$L_{P_\pm}(\Delta)=\mp B\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \tag{A10}$$

so that

$$c_{P_{\pm}} = \mp \frac{i}{B}. \tag{A11}$$

We can finally compute the partition function in the stationary phase approximation as

$$\mathcal{Z} = \frac{2\pi}{\beta B} (e^{\beta B s} - e^{-\beta B s}), \tag{A12}$$

which, in agreement with the Duistermaat–Heckman theorem, coincides with the exact partition function (15) for a spin in a magnetic field.

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Semilocal Chern–Simons defects

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We find both radially symmetric and more general solutions in a Chern–Simons–Higgs model with a Higgs doublet. They are of the kind of the so-called semilocal defects, and show richer properties than those previously known in another type of Higgs models. © *1996 American Institute of Physics.* [S0022-2488(96)00602-2]

I. INTRODUCTION

Planar solitons arising in models enjoying both global and gauge, i.e. local symmetries, have been recently discovered by Vachaspati and Achúcarro.[1] They are called semilocal topological defects and fit in the general theme of cosmological strings,[2] although not always the magnetic flux is concentrated. The appearance took place in the extended Higgs model, the bosonic sector of the Standard Model at Weinberg angle $\Theta_W=\pi/2$, where the SU(2)-weak isospin symmetry becomes global, in the search for stable strings in variations of the Electroweak Theory.[3]

The problem of studying the stability of semilocal topological defects was addressed thereafter by Hindmarsh,[4] who showed by numerical computations that they are indeed stable. He also made the important observation that semilocal topological defects are hybrids of CP^1 lumps and Higgs vortices; the solution depends on a continuous parameter varying between zero and infinity, such that at the extreme values it is either a Higgs vortex or a CP^1 lump.

The apparent paradox of finding stability without meeting the necessary topological conditions, at least at first sight, attracted a lot of attention to the problem. In an interesting paper,[5] Gibbons *et al.* observed that the crux of the matter is the Hopf fibration, and they were also able to recognize the moduli space of solutions by means of an analysis à là Jaffe–Taubes.[6] Their results were used in Ref. 7 by Leese and Samols to elucidate the low-energy scattering of these semilocal topological defects as geodesic motion in their moduli space.

In this paper we address the issue of the existence of semilocal topological defects in a similar model. We consider an extended Chern–Simons–Higgs theory: the generalization of the model thoroughly discussed by Jackiw *et al.* in Ref. 8 to a doublet of Higgs fields. The charged scalar fields are assembled in the fundamental representation of SU(2), which is a global symmetry of the Lagrangian; meanwhile they are minimally coupled to a U(1) gauge field for which the kinetic energy is of the Chern–Simons form. The richest structure of the set of Chern–Simons–Higgs planar solitons as compared to the solitons of the Abelian Higgs model tells us that a detailed analysis of the model is worthwhile. We thus find, besides the expected semilocal topological defects associated to the topological vortices of the CSH model, a new kind related to the so-called nontopological solitons with or without vorticity. We present both radially symmetric solutions solving an interesting mechanical problem by applying the methods of Sprück and Yang[9] and describe more general situations using the ideas of Wang.[10] This latter approach, combined with index theorems à là Weinberg,[11] afford us a good knowledge of the moduli space with specially interesting results in the nontopological sectors.

From a phenomenological point of view, the model could provide a Ginzburg–Landau theory of the kind proposed by Kivelson *et al.*[12] for the Fractional Quantum Hall Effect. A pathology in the filling factor series with fraction $n=\frac{5}{2}$ has been discovered by Eisestein *et al.*[13] Hall conductivity $\rho_{xy}=\frac{5}{2}(h/e^2)$ is anomalous, in the sense that even denominators are very rare. Moreover, the

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same team of experimentalists has determined that the incompressible state is not completely spin polarized.[14] The electron wave function is a spinor and the procedure of Ref. 12, leading from the microscopic theory to a phenomenological model in a parallel development, where the electrons are not polarized, requires a spinorial order parameter and free energy obtainable from our Lagrangian by looking at static configurations. Finally, we expect links between our vortices and Laughlin states similar to those occurring in the usual case of completely polarized electrons and odd denominator fractions (see Ref. 12).

The organization of the paper is as follows: In Sec. II, we present the model, analyze the topology of the configuration space, and propose the self-duality equations. We perform the study of radial solutions in Sec. III. Solutions with arbitrary centers as well as their moduli space are discussed in Sec. IV. To conclude, we elaborate in Sec. V on the stability of the semilocal topological defects and speculate on how to study the low-energy scattering.

II. THE MODEL

Our model is described by the action

$$S=\int d^3x\left\{\frac{\kappa}{4}\,\epsilon^{\alpha\beta\gamma}A_\alpha F_{\beta\gamma}+\frac{1}{2}\,D_\mu\Phi^\dagger D^\mu\Phi-U(\Phi)\right\}, \tag{1}$$

where the tridimensional Minkowski space–time metric is $\eta_{\mu\nu}=\mathrm{diag}(1,-1,-1)$, $\Phi=\binom{\phi_1}{\phi_2}$ is a doublet of complex scalar fields, $D_\mu\Phi=\partial_\mu\Phi-iA_\mu\Phi$, and $\mathrm{U}(\Phi)=(\lambda/8)\Phi^\dagger\Phi(\Phi^\dagger\Phi-1)$.[2] This system shows gauge invariance against the hybrid global-local $SU(2)\times U(1)$ transformations,

$$\Phi\rightarrow\Phi'=e^{(i/2)\omega_a\sigma_a}e^{i\chi(x)}\Phi, \tag{2}$$

$$A_\mu\rightarrow A'_\mu=A_\mu+\partial_\mu\chi, \tag{3}$$

where $\{\sigma_a\}$ $a=1,2,3$ are the Pauli matrices and the ω_a coefficients do not depend on the coordinates. This type of mixed Symmetry is called semilocal.[1] The action functional (1) is akin to the action for the bosonic sector of electroweak theory at Weinberg angle $\Theta_{\mathrm{W}}=\pi/2$; here the Maxwell terms for the neutral fields are replaced by the Chern–Simons term for the A_μ field, the counterpart of the massive Z field of the weak interactions. The SU(2) global symmetry would correspond thus to weak isospin symmetry, whereas the U(1) gauge group would be connected to the hypercharge.

The choice of the scalar potential $U(\Phi)$, however, is guided by the expectation of self-duality in the conventional Chern–Simons–Higgs model.[15] The theory exhibits two phases, respectively, built around the two degenerate vacua: the symmetric $\Phi=0$ and the asymmetric $\{\Phi^\dagger\Phi=1\}$. In the symmetric phase, the symmetry remains totally unbroken and four scalar bosons of mass $m_s=\sqrt{\lambda}/2$ arise, while the vector field does not propagate. In the asymmetric phase, the Higgs–Kibble mechanism takes place to produce one scalar particle of mass $m_H=\sqrt{\lambda}$ and one vector meson of mass $\mu_A=1/\kappa$. There are also two Goldstone bosons, the broken SU(2) symmetry is global, and we are left with a global U(1) symmetry that is the diagonal subgroup of $\mathrm{U}(1)\times\mathrm{U}(1)$ corresponding to the electromagnetic charge.

Classically, the dynamics follows from the field equations yield by varying (1):

$$\frac{\kappa}{2}\,\epsilon^{\mu\alpha\beta}F_{\alpha\beta}=J^\mu, \tag{4}$$

$$D_\mu\,D^\mu\Phi=2\,\frac{\partial U}{\partial\Phi^\dagger}, \tag{5}$$

where $J^\mu=-(i/2)[\Phi^\dagger\ D^\mu\Phi-\Phi\ D^\mu\Phi^\dagger]$ is a conserved current. Among them is specially interesting the modified Gauss law,

$$\kappa F_{12}=J^0=-A_0\Phi^\dagger\Phi-\frac{i}{2}\,[\Phi^\dagger\ \partial_0\Phi-\Phi\ \partial_0\Phi^\dagger], \tag{6}$$

or, in integral terms,

$$Q=\int d^2x\ J^0=\kappa\int d^2x\ F_{12}=\kappa\Phi_{\mathrm{M}}; \tag{7}$$

this equality forces the particle-like excitations of the model to be anionic.[16]

Our interest in this paper is limited to the study of the topological and nontopological defects emerging from (1), and so we will work in the space $\mathscr{C}$ of finite energy stationary configurations. For stationary configurations satisfying the modified Gauss law (6), the energy is minus the action by unit of time: $E=\int d^2x\ T_{00}=-S/T$. Plugging (6) in (1),

$$E=\int d^2x\left\{\frac{1}{4}\,\frac{\kappa}{\Phi^\dagger\Phi}\,F_{ij}F_{ij}+\frac{1}{2}\,D_k\Phi^\dagger D_k\Phi+U(\Phi)\right\}, \tag{8}$$

and we obtain a semilocal Higgs generalized model where a dielectric function $G(\Phi)=\kappa/\Phi^\dagger\Phi$ is incorporated.[17] Finite energy implies

$$F_{12}|_{\partial R^2}=0,\quad D_k\Phi|_{\partial R^2}=0,\quad \Phi|_{\partial R^2}\in V, \tag{9}$$

$V=\{\Phi=0$ or $\Phi^\dagger\Phi=1\}\cong\{0\}\cup S^3$ being the vacuum orbit of the scalar field. Due to $\Pi_0(V)=Z_2$, we can define a topological charge,

$$Q_0^T:\mathscr{C}\to Z_2,\quad Q_0^T=\Phi^\dagger\Phi|_{\partial R^2}, \tag{10}$$

but the surprising fact is that, although $\Pi_1(V)=\{0\}$, the Hopf fibration $S^3(CP^1,U(1))$ allows us to introduce a vortical topological charge, S^3 being locally isomorphic to $CP^1\times U(1)$.[1] The reason is that for the covariant derivative to vanish in the infinity of the plane when $Q_0^T=1$, it is necessary that $\Phi(\infty,\theta)=g(\infty)\Phi_0$, where g is a map from $\partial R^2\cong S^1$ to the U(1) fiber of S^3 passing by Φ_0. In addition, $A_\mu|_{\partial R^2}=-ig^{-1}\partial_\mu g$, so that $(1/2\pi)\oint_{\partial R^2}A_\mu\ dx^\mu$ gives the winding number of g. Thus

$$Q_1^T:\mathscr{C}\to Z,\quad Q_1^T=\frac{1}{2\pi}\ \oint_{\partial R^2}A_\mu\ dx^\mu=\frac{\Phi_{\mathrm{M}}}{2\pi} \tag{11}$$

is a topological charge. As a consequence, $\mathscr{C}$ breaks in topological sectors as follows

$$\mathscr{C}=\cup_{l\in Z}\mathscr{C}_0^l\cup_{n\in Z}\mathscr{C}_1^n,\quad Q_0^T[\mathscr{C}_a^b]=a,\quad Q_1^T[\mathscr{C}_a^b]=b. \tag{12}$$

Now, the problem is to find solutions of the field equations in $\mathscr{C}$ space. We can proceed by realizing that (8) admits the splitting

$$\begin{aligned}E=&\int d^2x\left\{\frac{\kappa^2}{2\Phi^\dagger\Phi}\left[F_{12}\mp\frac{\sqrt{\lambda}}{2\kappa}\,\Phi^\dagger\Phi(1-\Phi^\dagger\Phi)\right]^2+\frac{1}{2}|D_1\Phi\pm iD_2\Phi|^2\right\}\\&\pm\frac{1}{2}\int d^2x\ F_{12}\pm\frac{1}{2}\,(\kappa\sqrt{\lambda}-1)\int d^2x(1-\Phi^\dagger\Phi)F_{12}.\end{aligned} \tag{13}$$

In the Bogomolny limit $\sqrt{\lambda} = 1/\kappa$ (i.e., $\mu_A = m_H = m$), we have a lower bound for the energy, $E \geqslant \frac{1}{2}\left|\int d^2x\ F_{12}\right|$, and the bound is reached if and only if the Bogomolny equations,

$$F_{12} = \pm \frac{m^2}{2}\, \Phi^\dagger \Phi (1 - \Phi^\dagger \Phi), \tag{14}$$

$$D_1 \Phi \pm i\ D_2 \Phi = 0, \tag{15}$$

are satisfied. Configurations fulfilling (14), (15) are minima of the energy functional, and thus also represent solutions of the second-order Euler–Lagrange equations.

III. RADIALLY SYMMETRIC SOLUTIONS

We will now be concerned with the search for radially symmetric solutions of (14), (15). By applying a global SU(2) and a local trivial U(1) transformations, any configuration of such a kind can be set in the general form

$$\Phi = \begin{bmatrix} g(r) e^{in\theta} \\ \eta(r) \end{bmatrix}, \quad A_k = \epsilon_{kj}\, \frac{a(r) - n}{r^2}\, x_j, \tag{16}$$

where $g(r) \in R$ and $\eta(r) \in \mathbf{C}$. Substitution of the ansatz (16) in (14), (15) gives

$$\frac{1}{r}\frac{da}{dr} = \frac{m^2}{2}\, (g^2 + |\eta|^2)(g^2 + |\eta|^2 - 1), \tag{17}$$

$$\frac{dg}{dr} = \frac{ag}{r}, \tag{18}$$

$$\frac{d\eta}{dr} = \frac{a - n}{r}\, \eta. \tag{19}$$

Given that (16) is tantamount to $A_r = 0$, $A_\theta = n - a(r)$ for configurations in the $\mathscr{C}_l^n$ sector, regularity at the origin imposes the conditions

$$n g(0) = 0, \quad \eta(0) = \eta_0 e^{i\gamma}, \quad a(0) = n, \tag{20}$$

and finite energy requires

$$g(\infty) = l, \quad \eta(\infty) = 0, \quad a(\infty) = (l - 1)\alpha, \tag{21}$$

where *a priori* η_0, α are arbitrary real numbers that determine, together with n and l, the behavior of the solutions, both at the origin and infinity. From (18), (19), $\eta(r) = K g(r)/r^n$, $K \in \mathbf{C}$, and by defining $v(r) = \frac{1}{2} \ln g(r) + \ln(1 + |K|^2/r^{2n})$ the system (16)–(19) reduces to

$$\frac{d^2 v}{dr^2} + \frac{1}{r}\frac{dv}{dr} = m^2 e^v (e^v - 1) + \frac{4n^2 |K|^2 r^{2n-2}}{(r^{2n} + |K|^2)^2}, \tag{22}$$

$$\Phi = \frac{1}{\sqrt{r^{2n} + |K|^2}} \begin{pmatrix} r^n e^{in\theta} \\ K \end{pmatrix} e^{v(r)/2}, \quad a(r) = \frac{1}{r}\frac{dv}{dr} + \frac{n|K|^2}{r^{2n} + |K|^2}. \tag{23}$$

Equation (22) adopts a particularly appealing form by making the change $t = \ln r$ (from a geometric point of view, an isometric transformation from the plane to an infinite cone) that leads to

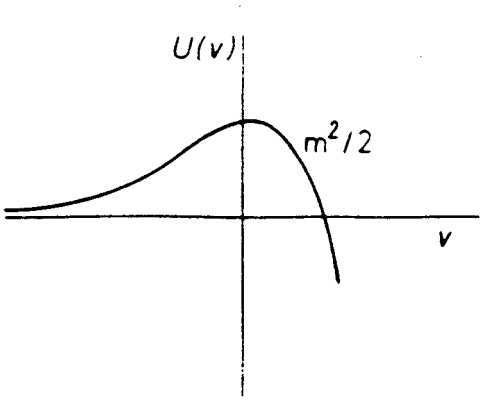

FIG. 1. A plot of U as a function of v. It could be understood as the "potential" felt by the particle at $t=0$.

$$\ddot{v}=m^2e^{2t}T(v)+F(t), \tag{24}$$

where $T(v)=e^v(e^v-1)$, $F(t)=4n^2|K|e^{2nt}/(e^{2nt}+|K|^2)^2$. Thus, we are facing a mechanical problem: one particle whose coordinate is v, submitted to a position and time depending force. The velocity of the particle is related to the vector field a by means of

$$\dot{v}=2a-\frac{2n|K|^2}{e^{2nt}+|K|^2}, \tag{25}$$

and the boundary conditions (20), (21) fix the asymptotic behavior of the movement for $t=\pm\infty$. Accordingly, we will consider each sector separately:

I. $\mathscr{C}_1^0$ sector: Here $F(t)=0$ and $\ddot{v}=-e^{2t}(dU/dv)$, $U=m^2e^v(1-e^v/2)$. From (20) and (21) we get

$$v(-\infty)=v_0, \quad \dot{v}(-\infty)=0, \tag{26}$$

$$v(+\infty)=0, \quad \dot{v}(+\infty)=0. \tag{27}$$

A glance at Fig. 1 leads us to the conclusion that $v(t)=0$ is the only possible solution compatible with (26) and (27), leading therefore to finite energy lumps: The only solution is thus the trivial one, the asymmetric vacuum.

II. $\mathscr{C}_0^n$ sector (nontopological vortices): The asymptotic conditions of the movement are

$$v(-\infty)=v_0, \quad \dot{v}(-\infty)=0, \tag{28}$$

$$v(+\infty)=-\infty, \quad \dot{v}(+\infty)=-2\alpha, \tag{29}$$

and therefore the function $v=v(t)$ has the behavior shown in Fig. 2. Bearing in mind (24), (28), and (29), it follows that v_0 is necessarily smaller than zero. Moreover, it can be shown that, if $v_0\ll 0$, v does not reach positive values, and, since $T(v)<0$ if $v<0$, the e^{2t} factor pushes the particle toward $v=-\infty$ when $t\to\infty$. To see how this can happen, let us forget about the $e^{2t}T(v)$ term in (24) at a first stage of the movement. Then the equation proves to be integrable, and from it we deduce that the particle reaches $\hat{v}<-\ln 2$ in the instant $\hat{t}\approx(2\ln K-v_0+\hat{v})/2n$ with speed $\dot{v}\approx 2n$. But the actual acceleration in (24) is more negative, and so we conclude that either the

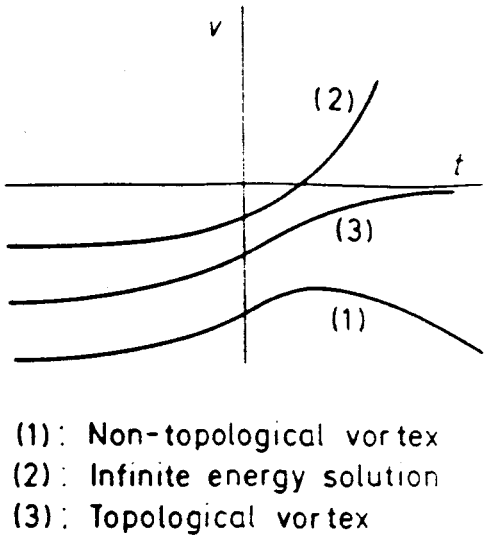

FIG. 2. Trajectories of the particles leading to (1) nontopological vortices, (2) infinite energy solutions, and (3) topological vortices.

particle does not reach $\hat{v}$ or arrives at this point for $t>\hat{t}$. Now, since $\hat{t}$ is great, for $t>\hat{t}$, $F(t)$ can be taken as $F(t) \approx 4n^2\kappa^2 e^{v_0}$, and while the particle continues moving between $\hat{v}$ and $-\ln 2$, we have

$$\ddot{v}<m^2e^{2t}T(\hat{v})+4n^2\kappa^2e^{v_0}. \tag{30}$$

If (30) were an equality, one would have that for $t=\hat{t}+\frac{1}{2}\ln[4n/m^2T(\hat{v})]$ there would be a turning point and we could always choose $\hat{v}$ so that this point would be at the left of $-\ln 2$. Since in (30) we have an upper bound for $\ddot{v}$, the turning point is in fact reached even before.

Hence, the existence of nontopological vortices is guaranteed, and from Fig. 2 and (17)–(21) it is easy to give a qualitative description of the fields: $a(r)$ and $|\eta(r)|$ decrease monotonically with r, while $g(r)$ and $|\Phi(r)|$ present a maximum; $F_{12}(r)$ presents one maximum value that splits in two if the turning point of the particle occurs for $v>-\ln 2$ (see Figs. 3, 4, and 5). The magnetic flux is $\Phi_M=2\pi(n+\alpha)$, and therefore the charge is $Q=2\pi\kappa(n+\alpha)$.

It is interesting to consider in (22), (23) the extreme situations $K=0$, $|K|\to\infty$. In the first case, $\phi_2(r,\theta)=0$, and we come back to the CSH conventional model.[8] Hence, for $K=0$ we obtain all the CSH nontopological vortices as a special limit of our solutions. To understand the other limit we note that in (23) $\Phi=\hat{\Phi}e^{v/2}$, where $\hat{\Phi}$ is exactly a CP^1 lump of topological charge n; meanwhile the $e^{v/2}$ factor is determined by (22) and the boundary conditions. Then, for general $|K|$ we can interpret our nontopological vortices as CP^1 lumps modulated by certain radial functions, the solutions of the mechanical problem (22), (28), and (29). The interesting point is that, for $|K|\to\infty$, (20)–(23) lead us to the mechanical problem

$$\ddot{v}=m^2e^{2t}e^{v}(e^{v}-1), \tag{31}$$

$$v(-\infty)=v_0, \quad \dot{v}(-\infty)=0, \tag{32}$$

$$v(+\infty)=-\infty, \quad v(-\infty)=-2\alpha-2n=-2\alpha', \tag{33}$$

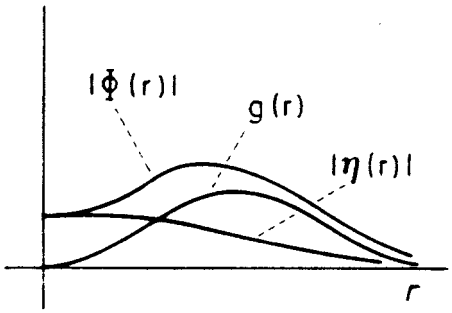

FIG. 3. Behavior of the scalar field for nontopological vortices.

corresponding exactly to the equations of a CSH nontopological soliton.[9] These limits seem to suggest that, for finite $|K|$, the nontopological vortices of the extended model interpolates between the nontopological vortices and the nontopological solitons of the standard CSH model times a CP^1 lump. The α parameter in (29) varies accordingly as a function of $|K|$: $\alpha<\alpha(|K|)$ and $2<\alpha(K)<2+2n$.[9]

III. $\mathscr{C}_1^n$ sector (topological vortices): In this sector the movement is subject to the conditions

$$v(-\infty)=v_0, \quad \dot{v}(-\infty)=0, \tag{34}$$

$$v(+\infty)=0, \quad \dot{v}(+\infty)=0, \tag{35}$$

and the $v=v(t)$ function has the appearance shown in Fig. 2. We have seen that the model contains nontopological vortices satisfying $v(+\infty)=-\infty$. Moreover, in the semilocal Abelian Higgs model there are solutions having $v(+\infty)=+\infty$,[4] and, since for $v<0$ the acceleration in (24) is less negative than the one corresponding to that model, (24) also has solutions with such behavior. The separatrix between these two types of movements satisfies (34) and (35) and corresponds to a topological vortex. In a similar way to the nontopological vortices, it is easy to understand the shape of the fields at a qualitative level (see Figs. 6–8). The magnetic flux is now $\Phi_M=2\pi n$ and the charge amounts $Q=2\pi\kappa n$. The $K\to 0$ limit of a topological vortex is a CSH

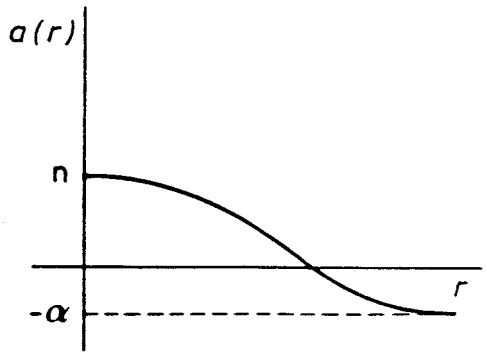

FIG. 4. The vector field of a nontopological vortex.

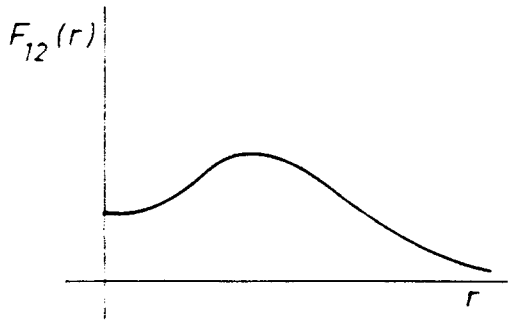

FIG. 5. Distribution of the magnetic field of nontopological vortices.

topological vortex. When $|K|\to\infty$, from (31), (34), and (35) we obtain $v(t)=0$ and arrive at a CP^1 lump of charge n, whereas for arbitrary $|K|$ we have a CP^1 lump modulated by the $e^{v/2}$ factor determined in (24), (34), and (35).

IV. $\mathscr{C}_0^0$ sector (nontopological solitons). In this case $F(t)=0$ and the mechanical problem is (31) with boundary conditions (28), (29), and a solution corresponding to a CSH nontopological soliton. Taking $n=0$ in (23), we can build the fields, which are essentially the same as for a CSH soliton, whose detailed description can be found in Refs. 8 and 9.

IV. MORE GENERAL SOLUTIONS

After having studied the radially symmetric solutions, we now will focus on the description of the space of general solutions in $\mathscr{C}$. In the topological sectors, the method put forward in Ref. 6 allows a very precise characterization based on the location on the plane of the zeros of Φ. In the nontopological ones however, the appearance of an asymptotic zero located at the infinity produces some novelties that we will show by means of an index theorem.

Following Ref. 5, we will first consider the general topological vortices in $\mathscr{C}_1^n$. In order to do so, we introduce the usual complex notation $z=x_1+ix_2$, $\partial_z=\frac{1}{2}(\partial_1-i\partial_2)$, $A=\frac{1}{2}(A_1-iA_2)$, and write (14), (15) as

$$(\partial_z-i\bar{A})\,\phi_1=0, \tag{36}$$

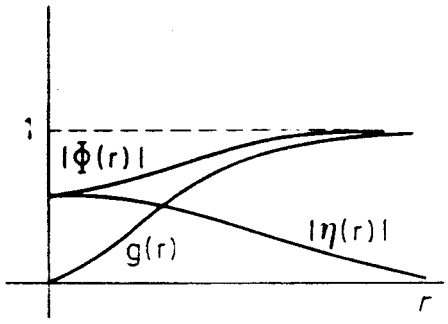

FIG. 6. The scalar field for topological vortices.

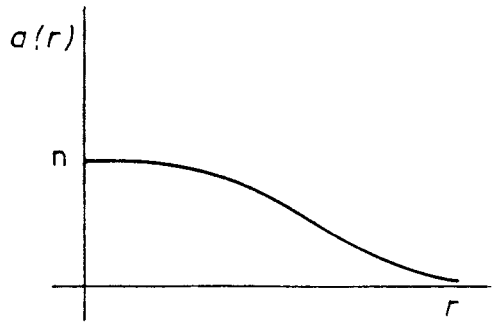

FIG. 7. The vector field of a topological vortex.

$$\partial_{\bar{z}} \ln w = 0, \tag{37}$$

$$\partial_{\bar{z}} A - \partial_z \bar{A} = -\frac{i}{4} m^2 |\phi_1|^2 (1+|w|^2)[1-|\phi_1|^2(1+|w|^2)], \tag{38}$$

where $\phi_2(z) = w(z)\phi_1(z)$. Expression (36) and boundary conditions (20), (21) imply that ϕ_1 has n zeros, say $z_1, z_2, \ldots, z_n$. Furthermore, it is possible to choose a gauge in which $\phi_1(z) = e^{1/2[u(z)+i\theta(z)]}$, where $\theta = 2\Sigma_{i=1}^{n} \arg(z-z_i)$ and $u(z)$ is a real function satisfying

$$\Delta u + m^2[1-e^u(1+|w|^2)][e^u(1+|w|^2)] = 4\pi \sum_{k=1}^{n} \delta(z-z_k), \tag{39}$$

and $\lim_{|z|\to\infty} u(z) = 0$. Equation (37) plus the boundary condition $\lim_{|z|\to\infty} w(z) = 0$ has general solution $w(z) = Q_n(z)/P_n(z)$, where $P_n(z) = \Pi_{k=1}^{n}(z-z_k)$ and $Q_n(z) = \Sigma_{k=0}^{n-1} q_n z^k$, the q_k coefficients being arbitrary. By using this in (39) and introducing $v = u + \ln(1+|w|^2)$, we conclude that the problem is tantamount to studying the equation

$$\Delta v + m^2 e^v (1-e^v) = \Delta \ln(|P_n|^2 + |Q_n|^2), \tag{40}$$

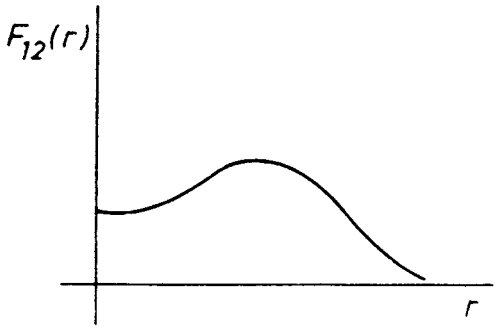

FIG. 8. Distribution of the magnetic field of topological vortices.

whose solution gives us the vortex fields as

$$\Phi=\frac{1}{\sqrt{|P_n|^2+|Q_n|^2}}\begin{pmatrix}P_n\\ Q_n\end{pmatrix}e^{v/2},\quad A=\frac{i}{2}\,\partial_z(u-i\,\theta). \tag{41}$$

For $Q_n=0$, (40) has one only solution,[10] and so the moduli space in $\mathscr{C}_1^n$ $\mathscr{M}_1^n$, has dimension $2n$ and is parametrized by the points $\{z_n\}$, where ϕ_1 vanishes. For general Q_n, proof of existence and uniqueness of solutions of (40) comes from a slight modification of the Sovolev analysis developed by Wang by writing (40) as the variational equation for a strictly convex functional of v. This leads to the conclusion that, since Q_n depends on $2n$ parameters, dim $\mathscr{M}_1^n=4n$. Instead of plunging into too technical a work, here we will exploit an index calculation that, besides giving us information about the others sectors, provides the announced result for $\mathscr{M}_1^n$.

The departure point[8,11] is to take a solution (A_k,Φ) of (14) and (15) and deform it into another $(A_k+\delta A_k,\Phi+\delta\Phi)$, at the same time imposing the Coulomb gauge condition $\partial_k\ \delta A_k=0$. This is equivalent to the requirement $\mathscr{D}(\frac{\delta\Phi}{\delta A_k})=0$, where $\mathscr{D}=iP_k\partial_k+Q$ and

$$P_1=\begin{pmatrix}-i&0&0\\0&-i&0\\0&0&-\sigma_2\end{pmatrix},\quad P_2=\begin{pmatrix}-\sigma_2&0&0\\0&-\sigma_2&0\\0&0&-i\end{pmatrix}, \tag{42}$$

$$Q=\begin{pmatrix}A_2+i\sigma_2A_1&0&\varphi_2+i\sigma_2\varphi_1\\0&A_2+i\sigma_2A_1&\psi_2+i\sigma_2\psi_1\\K\varphi&K\psi&0\end{pmatrix}, \tag{43}$$

$$\xi=\varphi\quad\text{or}\quad\psi,K\xi=\begin{pmatrix}\xi_1\mathscr{U}&\xi_2\mathscr{U}\\0&0\end{pmatrix},\quad \mathscr{U}=m(1-2\Phi^\dagger\Phi), \tag{44}$$

where we have changed the notation and put $\Phi=\binom{\varphi}{\psi}$. Thus, the dimension of the moduli space on $\mathscr{C}_a^n$, $\mathscr{M}_a^n$, essentially corresponds to the dimension of the kernel of $\mathscr{D}$, except for four global gauge modes of $\mathrm{SU}(2)_g\times\mathrm{U}(1)_\mathrm{I}$ not excluded by the Coulomb gauge in the nontopological sectors, and hence

$$\dim\mathscr{M}_1^n=\dim\ker\mathscr{D},\quad \dim\mathscr{M}_0^n=\dim\ker\mathscr{D}-4. \tag{45}$$

Now, the following operator

$$T=\begin{pmatrix}i\bar{\varphi}&i\bar{\psi}&2\partial_z\\ i\bar{\varphi}&i\bar{\psi}+1&2\partial_z\\1&0&0\\0&-i\varphi&0\\0&-i\varphi&0\\0&0&-i\varphi\\0&0&-i\varphi\end{pmatrix}, \tag{46}$$

where

$$i\xi=\begin{pmatrix}\xi_2&-\xi_1\\ \xi_1&\xi_2\end{pmatrix},\quad 2\partial_z=\begin{pmatrix}\partial_1&\partial_2\\-\partial_2&\partial_1\end{pmatrix} \tag{47}$$

satisfies Ker $T=\{0\}$, Ker $T\mathscr{D}^\dagger=\{0\}$ (except for the existence of a nongeneric zero mode of the Schrödinger operator $-\nabla^2-|\Phi|^2U$), as it is easy to verify, and so Ker $\mathscr{D}^\dagger=\{0\}$, and we have

$$\text{ind } \mathscr{D}=\dim \ker \mathscr{D}. \tag{48}$$

To compute ind $\mathscr{D}$ we shall use the heat-kernel method. We define

$$h(t)=\text{Tr } e^{-t\mathscr{D}^\dagger\mathscr{D}}-\text{Tr } e^{-t\mathscr{D}\mathscr{D}^\dagger}, \tag{49}$$

and, because of the supersymmetric pairing between the $\mathscr{D}\mathscr{D}^\dagger$ and $D^\dagger\mathscr{D}$ eigenstates corresponding to nonvanishing spectral values, we obtain

$$\text{ind } \mathscr{D}=h(0)+\Delta, \tag{50}$$

where the correction Δ must be considered in the nontopological sectors because the boundary conditions in them produce differences between the spectral densities of both operators. On the topological sectors, boundary conditions allow R^2 to be compactified to a sphere,[18] and hence $\Delta=0$. To compute $h(0)$, we build the second-order operators,

$$\mathscr{D}^\dagger\mathscr{D}=-\nabla^2+i[P_kQ^\dagger+QP_k^\dagger]\partial_k+iP_k(\partial_kQ^\dagger)+QQ^\dagger, \tag{51}$$

$$\mathscr{D}\mathscr{D}^\dagger=-\nabla^2+i[P_k^\dagger Q+Q^\dagger P_k]\partial_k+iP_k^\dagger(\partial_kQ)+Q^\dagger Q, \tag{52}$$

and realizing that $\{P_k^\dagger,P_j\}=\{P_k,P_j^\dagger\}=2\delta_{kj}$, we obtain

$$h(0)=\lim_{t\to 0}h(t)=-\frac{i}{4\pi}\int d^2x\ \text{tr}[P_k^\dagger(\partial_kQ)-P_k(\partial_kQ^\dagger)]=4\Phi_{\text{M}}. \tag{53}$$

It remains to compute Δ. For this, we observe that if Ψ_λ is an eigenstate of $\mathscr{D}^\dagger\mathscr{D}$ with eigenvalue λ^2, $\tilde{\Psi}_\lambda=(1/\lambda)\mathscr{D}\Psi_\lambda$ is also eigenstate of $\mathscr{D}\mathscr{D}^\dagger$ with the same eigenvalue, and, as a consequence,

$$\Delta=\lim_{t\to 0}\int d\lambda\int d^2x[(\tilde{\Psi}_\lambda(x),\tilde{\Psi}_\lambda(x))-(\Psi_\lambda(x),\Psi_\lambda(x))]e^{-t\lambda^2}, \tag{54}$$

and, via partial integration,

$$\Delta=\lim_{t\to 0}\int d\lambda\int_0^{2\pi}r\ d\theta(\Psi_\lambda,-iP_r^\dagger\ \mathscr{D}\Psi_\lambda)\ \frac{e^{-t\lambda^2}}{\lambda^2}\bigg|_{r=\infty}, \tag{55}$$

where $P_r=x_kP_k/r$, $P_\theta=\epsilon_{ik}x_iP_k/r^2$, and in polar coordinates $\mathscr{D}=iP_r\partial_r+iP_\theta\partial_\theta+Q$. Introducing $\mathscr{D}=iP_r[\partial_r+T_r]$,

$$\Delta=\lim_{t\to 0}\int d\lambda\int_0^{2\pi}r\ d\theta(\Psi_\lambda,[\partial_r+T_\infty]\Psi_\lambda)\ \frac{e^{-t\lambda^2}}{\lambda^2}\bigg|_{r=\infty}, \tag{56}$$

where $\mathscr{D}^\dagger\mathscr{D}_\infty=\lim_{r\to\infty}\mathscr{D}^\dagger\mathscr{D}=-\partial_r^2-(1/r)\partial_r+T_\infty^2-(1/r)(\partial_r+T_\infty)$ and

$$T_\infty = \begin{pmatrix} L & 0 & 0 \\ 0 & L & 0 \\ 0 & 0 & \dfrac{i}{r}\,\sigma_2\partial_\theta \end{pmatrix}, \quad L = \frac{1}{r}\,[-i\sigma_2\partial_\theta + n - a(\infty)]. \tag{57}$$

By using the complete orthonormal system $\{\Psi_{k\mu}(r,\theta) = e^{ikr}/\sqrt{2\pi r} f_\mu(\theta)\}$ in (56), one can show that

$$\Delta = \tfrac{1}{2}\,\eta_{T_\infty}(0) = 2 - 4\ \ Fracc[n - a(\infty)], \tag{58}$$

where $\eta_{T_\infty}(0)$ is the spectral asymmetry of the T_∞ operator and by $Fracc[\alpha]$ we denote the fractionary part of α; this, together with (45), (50), (53), (20), and (21), leads to

$$\dim \mathscr{M}_1^n = 4\Phi_{\mathrm{M}} = 4n, \quad \dim \mathscr{M}_0^n = 4\ \mathrm{Int}[\Phi_{\mathrm{M}}] - 2, \tag{59}$$

a result that in all the sectors has $2[\Phi_{\mathrm{M}}]$ parameters more than in the CSH case,[8] owing to the new degrees of freedom associated with the ϕ_2 field.

V. FURTHER COMMENTS

We now briefly consider the issue of the stability of the defects found in the model. For the topological ones, stability is sure because Bogomolny equations are associated in the topological sectors to a lower bound of the energy. The same is not true for nontopological defects, and thus it is necessary to study the spectrum of the Hessian operator, whose form restricted to the ϕ_2 deformations of a radially symmetric configuration (the ϕ_1 deformations are exactly the same as in the CSH model and lead to stability) is the following:

$$\mathscr{H} = -\frac{1}{r}\frac{d}{dr}\left(r\,\frac{d}{dr}\right) + \frac{(a-n+l)^2}{r^2} + \frac{1}{r}\frac{da}{dr}, \tag{60}$$

when operating on deformations of the form $\delta\phi_2(r,\theta) = \xi(r)e^{il\theta}$. Accordingly, the $l=0$ case is the most unfavorable, and it will suffice to concentrate on it. We do not dispose of an exact expression for the fields, but we can approximate the problem by taking

$$a(r) = \begin{cases} n - \Lambda r, & \text{if } r < \gamma/\Lambda, \\ n - \gamma, & \text{if } r > \gamma/\Lambda, \end{cases} \tag{61}$$

where $\gamma = n$ for a topological vortex and takes an arbitrary value for a nontopological defect, and Λ is a parameter that specifies the defect size. Thus, near the defect core,

$$\mathscr{H} = \mathscr{H}_{\mathrm{COUL}} + \Lambda^2, \quad \mathscr{H}_{\mathrm{COUL}} = -\frac{1}{r}\frac{d}{dr}\left(r\,\frac{d}{dr}\right) - \frac{\Lambda}{r}, \tag{62}$$

and it is known that $\mathscr{H}_{\mathrm{COUL}}$ has one only bound state with eigenvalue $-\Lambda^2$. So $\mathscr{H}$ does not have negative eigenvalues, and this can be taken as strong evidence of stability for all the defects that we have studied.

In this paper we have addressed the static semilocal CSH defects. It would be interesting to pursue the investigation by considering the low-energy scattering of these defects, as has been done in the semilocal Abelian Higgs Model.[7] The main difference is that, since our defects have an anyonic nature, the low energy Lagrangian will include a "$\epsilon_{ij}q^i q^j$" term that will prevent defects from following geodesics in the moduli space, although presumably the 90° scattering will be also present in our model.

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Coherent states over Grassmann manifolds and the WKB exactness in path integral

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U(N) coherent states over Grassmann manifold, $G_{N,n}\simeq \mathrm{U}(N)/(\mathrm{U}(n)\times \mathrm{U}(N-n))$, are formulated to be able to argue the WKB exactness in the path integral representation of a character formula. The phenomena is the so-called localization of Duistermaat–Heckman. The exponent in the path integral formula is proportional to an integer k labeling the U(N) representation. Thus, when $k\to\infty$ a usual semiclassical approximation, by regarding $k\sim 1/\hbar$, can be performed to yield a desired conclusion. The mechanism of the localization is uncovered by the help of the (generalized) Schwinger boson technique. The discussion on the Feynman kernel is also presented. © *1996 American Institute of Physics.* [S0022-2488(96)03102-0]

I. INTRODUCTION

In any physical situation it is often difficult to find an exact response, therefore, some approximation method must be employed. Apart from the well-known perturbation theories, the Wentzel–Kramers–Brillouin (WKB) approximation, known as the $\hbar$ expansion, seems most suitable to the path integral formalism; since the exponent in the path integral is usually given by a quantity divided by Planck's constant $\hbar$. These approximation methods can be straightforwardly performed without specifying a path measure rigorously, which apparently has been a main reason that the path integral plays a major role in modern physics. On the other hand, due to this handiness there always accompanies some skepticism, such as the problem of operator ordering,[1] since only c numbers appear, or a vague relationship of the change of variables to the canonical operator formalism.[2] What we have learned through various efforts is that the path integral can produce reliable as well as consistent results under the *time slicing method*. A simple example can be seen as follows: take a bosonic oscillator, defined by a Hamiltonian $H\equiv \omega a^\dagger a$ with $[a,a^\dagger]=\mathbf{I}$, $[\mathbf{I},a]=[\mathbf{I},a^\dagger]=0$, and calculate the quantity $\mathrm{Tr}\, e^{-iHT}$. First, write the exponential operator such that

$$\mathrm{Tr}\, e^{-iHT}=\lim_{M\to\infty}\mathrm{Tr}(\mathbf{I}-i\,\Delta t\,H)^M;\quad \Delta t\equiv\frac{T}{M}, \tag{1.1}$$

which is the starting point of the time slicing method. With the aid of canonical coherent states,[3] (1.1) becomes

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$$\mathrm{Tr}\, e^{-i\omega a^\dagger a T} = \lim_{M\to\infty} \int_{\mathrm{PBC}} \prod_{j=1}^{M} \frac{dz(j)d\bar{z}(j)}{\pi} \exp\Bigg[-\sum_{k=1}^{M} \{\bar{z}(k)(z(k)-z(k-1)) + i\omega\, \Delta t\, \bar{z}(k)z(k-1)\}\Bigg], \tag{1.2}$$

where "PBC" denotes $z(0)=z(M)$ and $dz\, d\bar{z} \equiv d\,\mathrm{Re}(z)\, d\,\mathrm{Im}(z)$. By taking a formal limit, $M\to\infty$, the continuum representation is obtained:

$$\mathrm{Tr}\, e^{-i\omega a^\dagger a T} \to \int_{\mathrm{PBC}0\leqslant t\leqslant T} \prod dz\, d\bar{z} \exp\left\{ -\int_0^T dt(\dot{\bar{z}}z + i\omega \bar{z}z)\right\}, \tag{1.3}$$

where "PBC" reads as $z(T)=z(0)$ in this case. In spite of the formal limit, we still could impart a meaning to the functional measure by means of the functional determinant:

$$(1.3) \equiv \det\left(\frac{d}{dt} + i\omega\right)^{-1} = \frac{1}{2i\, \sin(\omega T/2)}, \tag{1.4}$$

with the aid of the ζ-function regularization. The result does not, however, match to the correct one, obtained from (1.2),

$$\frac{1}{2i\, \sin(\omega T/2)} \neq \frac{1}{1-e^{-i\omega T}} = \frac{e^{i\omega T/2}}{2i\, \sin(\omega T/2)}. \tag{1.5}$$

Therefore, we must pay the price whenever we have adopted the continuum path integral representation, which would apparently be suitable for a geometrical treatment.

In some situation an approximation scheme happens to lead to an exact answer: the harmonic oscillator is WKB exact, because of the integration being Gaussian. (The cross section of the Coulomb interaction is another well-known example,[4] which furthermore reveals that the Born approximation yields the exact result.) In recent years, however, a new possibility of finding the WKB exactness has been opened up.[5–10] Works have been stimulated by the Duistermaat–Heckman (DH) theorem.[11–13] A key word to understand these new classes of the WKB exactness would be "*localization*",[14–16] commonly understood in terms of equivariant cohomology.[17]

Inspired by these facts, we have convinced ourselves of the WKB exactness in the path integral formulas obtained through the generalized coherent states[18] in cases of $\mathbf{C}P^1$ and $\mathbf{C}P^N$,[9,10] as well as their noncompact counter parts in the foregoing papers. Even if another representation is adopted[19] for the $\mathbf{C}P^1$ case to give the Nielsen–Rohrlich form,[20] the same localization has been clarified.[21] As a natural generalization in this paper, we try to examine the Grassmann manifold, $G_{N,n} \simeq \mathrm{U}(N)/(\mathrm{U}(n)\times\mathrm{U}(N-n))$. In order to carry out the program we need to build up coherent states of $\mathrm{U}(N)$ over $G_{N,n}$.

The plan of the paper is as follows. An interpretation of the DH theorem, stated in terms of finite-dimensional integrations, is presented in Sec. II, since the WKB exactness is sometimes regarded as a generalization to the infinite-dimensional case. In order to achieve the path integral expression, there needs to construct coherent states over Grassmann manifolds. We develop two ways: one is the algebraic method according to the Perelomov's prescription[18] and the other is due to the canonical coherent state[3] combined with the Schwinger boson technique.[22] These are the contents of Sec. III A and III B, respectively. The path integral representation of the character formula is then given in Sec. IV A and the WKB approximation is performed in Sec. IV B. The mechanism of the WKB exactness is clarified in Sec. IV C by making use of the Schwinger boson.

The final section is devoted to related topics and remarks. In Appendix A, proofs for the theorems in the Sec. III A, are given. Finally, in Appendix B a discussion on the WKB exactness in terms of the Feynman kernel is provided.

II. THE DH FORMULA ON GRASSMANN MANIFOLDS

In this section, we demonstrate the validity of the DH formula on $G_{N,n}$ as a preparation for later discussions.

A. Classical mechanics on $G_{N,n}$

Let $\mathbf{C}^n$ be the n-dimensional complex vector space. We denote the space of $m\times n$ matrices over $\mathbf{C}$ by $M(m,n;\mathbf{C})$ and abbreviate $M(n,n;\mathbf{C})$ by $M(n;\mathbf{C})$. Regard $G_{N,n}\simeq \mathrm{U}(N)/(\mathrm{U}(n)\times \mathrm{U}(N-n))$ as a phase space, assuming $N\geqslant 2n$ for brevity's sake, and write

$$G_{N,n}=\{P\in M(N;\mathbf{C})\,|\,P^2=P, P^\dagger=P \quad \text{and tr } P=n\}. \tag{2.1}$$

P can be parametrized in terms of $\xi\in M(N-n,n;\mathbf{C})$, such that

$$P=\begin{pmatrix} \dfrac{1}{1_n+\xi^\dagger\xi} & \dfrac{1}{1_n+\xi^\dagger\xi}\,\xi^\dagger \\ \xi\,\dfrac{1}{1_n+\xi^\dagger\xi} & \xi\,\dfrac{1}{1_n+\xi^\dagger\xi}\,\xi^\dagger \end{pmatrix}=U(\xi)P_{1,\ldots,n}U^\dagger(\xi), \tag{2.2}$$

where

$$P_{1,\ldots,n}\equiv\begin{pmatrix} 1_n & 0 \\ 0 & 0 \end{pmatrix} \tag{2.3}$$

and

$$U(\xi)\equiv\begin{pmatrix} \dfrac{1}{\sqrt{1_n+\xi^\dagger\xi}} & -\dfrac{1}{\sqrt{1_n+\xi^\dagger\xi}}\,\xi^\dagger \\ \xi\,\dfrac{1}{\sqrt{1_n+\xi^\dagger\xi}} & \dfrac{1}{\sqrt{1_{N-n}+\xi\xi^\dagger}} \end{pmatrix}. \tag{2.4}$$

The parametrization (2.2) cannot cover the whole phase space: indeed there exist other parametrizations such as

$$(P_{\mu_1,\ldots,\mu_n})_{\rho\lambda}=\sum_{a=1}^{n}\delta_{\rho,\mu_a}\delta_{\lambda,\mu_a},\quad 1\leqslant\mu_a\leqslant N, \tag{2.5}$$

which tells us that there need $\binom{N}{n}$ kinds of local parametrization. (Throughout the paper we use a convention for indices: $1\leqslant\mu,\nu\leqslant N$; $1\leqslant a,b\leqslant n$; $n+1\leqslant i,j\leqslant N$.) In order to obtain an appropriate parametrization in the neighborhood of $P_{\mu_1,\ldots,\mu_n}$, we can utilize a unitary transformation $U(\mu_1,\ldots,\mu_n|1,\ldots,n)$ satisfying

$$U(\mu_1,\ldots,\mu_n|1,\ldots,n)P_{1,\ldots,n}U^\dagger(\mu_1,\ldots,\mu_n|1,\ldots,n)=P_{\mu_1,\ldots,\mu_n}. \tag{2.6}$$

The symplectic structure on $G_{N,n}$ is defined through the symplectic 2-form,

$$\omega=i\ \mathrm{tr}(P\ dP\wedge dP), \tag{2.7}$$

whose explicit form, under (2.2), reads as

$$\omega = i\ \mathrm{tr}\{(1_n+\xi^\dagger\xi)^{-1}\ d\xi^\dagger \wedge (1_{N-n}+\xi\xi^\dagger)^{-1}\ d\xi\}, \tag{2.8}$$

yielding to the $U(N)$ invariant measure on $G_{N,n}$,

$$\det[(1_{N-n}+\xi\xi^\dagger)^{-1}\otimes\{(1_n+\xi^\dagger\xi)^{-1}\}^{\mathscr{T}}](d\xi\ d\bar{\xi})^{n(N-n)} = \frac{1}{\{\det(1_n+\xi^\dagger\xi)\}^N}\ (d\xi\ d\bar{\xi})^{n(N-n)}, \tag{2.9}$$

where the superscript $\mathscr{T}$ denotes the transpose of matrix and an abbreviation,

$$(dz\ d\bar{z})^{mn} \equiv \prod_{\substack{1\leqslant i\leqslant m\\ 1\leqslant a\leqslant n}} d\ \mathrm{Re}(z_{ia})d\ \mathrm{Im}(z_{ia}), \tag{2.10}$$

has been employed. Our convention of the tensor product is

$$A\otimes B = \begin{pmatrix} a_{11}B & a_{12}B & \cdots \\ a_{21}B & a_{22}B & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}, \quad \text{for } A=(a_{ij}), \quad B=(b_{ij}).$$

Dynamical variables are defined through a linear mapping,

$$X\in H(N) \mapsto F_X = \mathrm{tr}(PX) \in \mathbf{R}, \tag{2.11}$$

where $H(N)$ is the space of Hermitian matrices:

$$H(m) = \{X | X\in M(m;\mathbf{C}), X^\dagger = X\}. \tag{2.12}$$

The Poisson bracket is given, with the aid of (2.7), by

$$\{F_X, F_Y\}_{\mathrm{P.B.}} = \omega^{-1}(V_X, V_Y) = F_{-i[X,Y]}, \tag{2.13}$$

with $[X,Y]=XY-YX$, where V_X is a vector field on $G_{N,n}$ associated with F_X:

$$V_X = \sum_{i,a}\left(\frac{\partial F_X}{\partial \xi_{ia}}\frac{\partial}{\partial \xi_{ia}} + \frac{\partial F_X}{\partial \bar{\xi}_{ia}}\frac{\partial}{\partial \bar{\xi}_{ia}}\right).$$

Note that the Poisson bracket (2.13) generates the $u(N)$ algebra.

An explicit form of the Hamiltonian function for a Hermitian matrix X,

$$X = \begin{pmatrix} A & B \\ B^\dagger & D \end{pmatrix}, \quad A\in H(n), \quad B\in M(n,N-n;\mathbf{C}), \quad D\in H(N-n), \tag{2.14}$$

is read as

$$F_X = \mathrm{tr}\{(1_n+\xi^\dagger\xi)^{-1}\Phi_X\}, \quad \Phi_X = A + B\xi + \xi^\dagger B^\dagger + \xi^\dagger\ D\xi. \tag{2.15}$$

Introduce a 1-form θ_κ,

$$d\theta_\kappa = \omega, \quad \theta_\kappa = i\ \mathrm{tr}[\{\kappa\xi^\dagger\ d\xi - (1-\kappa)d\xi^\dagger\ \xi\}(1_n+\xi^\dagger\xi)^{-1}]; \quad \kappa\in\mathbf{R}. \tag{2.16}$$

Here κ is an arbitrary parameter that does not affect kinematics at all and is usually fixed by putting $\kappa=\frac{1}{2}$. The action functional for this Hamiltonian system is thus found as

$$S=\int_{t_1}^{t_2}(\theta_\kappa-F_X\,dt)=\int_{t_1}^{t_2}dt\ \mathrm{tr}[(1_n+\xi^\dagger\xi)^{-1}\{i(\kappa\xi^\dagger\dot{\xi}-(1-\kappa)\dot{\xi}^\dagger\xi)-(A+B\xi+\xi^\dagger B^\dagger+\xi^\dagger D\xi)\}], \tag{2.17}$$

giving us equations of motion,

$$\begin{aligned}\dot{\xi}&=i(\xi A-D\xi-B^\dagger+\xi B\xi),\\ \dot{\xi}^\dagger&=-i(A\xi^\dagger-\xi^\dagger D+\xi^\dagger B^\dagger\xi^\dagger-B).\end{aligned} \tag{2.18}$$

The solution can be found by putting

$$\exp(-iXt)=\begin{pmatrix}\alpha(t) & \beta(t)\\ \gamma(t) & \delta(t)\end{pmatrix}, \tag{2.19}$$

with X being given by (2.14), such that

$$\xi(t)=\{\gamma(t)+\delta(t)\xi(0)\}\{\alpha(t)+\beta(t)\xi(0)\}^{-1}. \tag{2.20}$$

The solution (2.20) takes the simplest form in the case of a block-diagonal Hamiltonian given by $B=0$:

$$\xi(t)=U(t)\xi(0)V^\dagger(t), \tag{2.21}$$

where matrices $V(t)\in\mathrm{U}(n)$ and $U(t)\in\mathrm{U}(N-n)$ are given as

$$V(t)=\exp(-iAt),\quad U(t)=\exp(-i\,Dt). \tag{2.22}$$

In terms of $\xi(t)$ (2.20), the time dependence of P (2.2) is read as

$$P(t)=\begin{pmatrix}\dfrac{1}{1_n+\xi^\dagger(t)\xi(t)} & \dfrac{1}{1_n+\xi^\dagger(t)\xi(t)}\,\xi^\dagger(t)\\ \xi(t)\,\dfrac{1}{1_n+\xi^\dagger(t)\xi(t)} & \xi(t)\,\dfrac{1}{1_n+\xi^\dagger(t)\xi(t)}\,\xi^\dagger(t)\end{pmatrix}, \tag{2.23}$$

so that

$$P(t)=e^{-iXt}P(0)e^{iXt}. \tag{2.24}$$

Therefore we can recognize that the equations (2.18) describe an action of $\mathrm{U}(N)$ on $G_{N,n}$ (in a local coordinate system). In this way classical mechanics on $G_{N,n}$ can have geometric interpretation.

As a final remark, note that only $\xi(t)=0$ $(0\leqslant t\leqslant T)$ is allowed under the periodic boundary condition $\xi(T)=\xi(0)$ for arbitrary T and X. In the subsequent section the same situation is found when performing the WKB approximation.

B. The DH formula

We now discuss the Duistermaat–Heckamn localization formula for the classical system defined above. Start with a classical partition function,

$$\mathcal{Z}_{\rm cl}(\beta)=\int d\mu(\xi)\exp(-\beta F_H),\quad \beta>0, \tag{2.25}$$

where

$$d\mu(\xi)\equiv\frac{1}{\{\det(1_n+\xi^\dagger\xi)\}^N}\left(\frac{d\xi\,d\bar{\xi}}{\pi}\right)^{n(N-n)}, \tag{2.26}$$

which satisfies

$$\int d\mu(\xi)=\mathcal{N}(n,N-n), \tag{2.27}$$

with

$$\mathcal{N}(n,p)\equiv\frac{0!1!\cdots(n-1)!}{p!(p+1)!\cdots(p+n-1)!}\quad (p=0,1,2,\ldots). \tag{2.28}$$

[The verification of (2.27) is found in the next section. Putting $k\to 0$ in (3.48) we have (2.27).] Here $F_{\rm H}$ is a Hamiltonian, in terms of a real diagonal matrix,

$$H=\mathrm{diag}(h_1,\ldots,h_n,h_{n+1},\ldots,h_N),\quad 0<h_1<\cdots<h_N, \tag{2.29}$$

such that

$$F_{\rm H}=\mathrm{tr}\{(1_n+\xi^\dagger\xi)^{-1}(H_u+\xi^\dagger H_d\xi)\},$$

$$H_u=\mathrm{diag}(h_1,\ldots,h_n),\quad H_d=\mathrm{diag}(h_{n+1},\ldots,h_N). \tag{2.30}$$

The first task is to find critical points of the Hamiltonian by solving

$$\frac{\partial F_{\rm H}}{\partial\xi_{ia}}=0,\quad \frac{\partial F_{\rm H}}{\partial\bar{\xi}_{ia}}=0, \tag{2.31}$$

which coincide with the right-hand sides of the equations of motion (2.18). In view of (2.25) these critical points are nothing but the *saddle points* of the integral. For the present case, the saddle point conditions (2.31) become

$$H_u\xi^\dagger-\xi^\dagger H_d=0,\quad \xi H_u-H_d\xi=0. \tag{2.32}$$

Note that if $\xi\neq 0$ these conditions cannot be met, owing to the assumption, $h_1<\cdots<h_N$. Therefore there remains only one case, $\xi=0$, *under this parametrization* of $G_{N,n}$, in other words, there exists a unique fixed point under the action of $\mathrm{U}(n)\times\mathrm{U}(N-n)$ [torus, $\mathrm{U}(1)^N$, in this case] (2.21). Now calculate the second derivative of $F_{\rm H}$ at $\xi=0$; the Hessian of the Hamiltonian,

$$\left.\frac{\partial^2 F_{\rm H}}{\partial\xi_{ia}\,\partial\bar{\xi}_{jb}}\right|_{\xi=0}=(H_u)_{ab}\delta_{ji}-\delta_{ab}(H_d)_{ji}. \tag{2.33}$$

Hence, the contribution from this critical point to (2.25) is found to be

$$\int \left(\frac{d\xi\, d\bar{\xi}}{\pi}\right)^{n(N-n)} \exp\{-\beta \text{ tr } H_u - \beta \text{ tr}(H_d \xi\xi^\dagger - H_u \xi^\dagger \xi)\} = \frac{\exp(-\beta \Sigma_{a=1}^n h_a)}{\beta^{n(N-n)} \Pi_{a=1}^n \Pi_{i=n+1}^N (h_i - h_a)}. \tag{2.34}$$

As was stressed above, there need $\binom{N}{n}$ local parametrizations to cover the whole phase space, contributions from other critical points must be taken into account. To this end, recall the unitary transformation given in (2.6). A change of the local parametrization,

$$P = U(\xi) P_{1,\ldots,n} U^\dagger(\xi) \mapsto P_U = U(\mu_1,\ldots,\mu_n|1,\ldots,n) P U^\dagger(\mu_1,\ldots,\mu_n|1,\ldots,n), \tag{2.35}$$

is equivalent to that of the Hermitian matrix in the Hamiltonian function,

$$F_{\mathrm{H}}(P) = \text{tr}(PH) \mapsto F_{\mathrm{H}}(P_U) = F_{H'}(P) = \text{tr}(PH'), \tag{2.36}$$

with

$$H' = U^\dagger(\mu_1,\ldots,\mu_n|1,\ldots,n) H U(\mu_1,\ldots,\mu_n|1,\ldots,n). \tag{2.37}$$

Once recognizing this, we can easily carry out the task; since the new Hamiltonian after the transformation is again diagonal without degeneracy so that a critical point is always located at $\xi = 0$ in each local parametrization. Summing up those contributions, therefore we obtain, as a result of the saddle point approximation,

$$\mathcal{Z}_{\mathrm{cl}}(\beta) \simeq \sum_{\mu_1 < \cdots < \mu_n} \frac{\exp(-\beta \Sigma_{a=1}^n h_{\mu_a})}{\beta^{n(N-n)} \Pi_{a=1}^n \Pi_{\nu \in \bar{\mu}} (h_\nu - h_{\mu_a})}, \tag{2.38}$$

where

$$\bar{\mu} \equiv \{1,\ldots,N\} \backslash \{\mu_1,\ldots,\mu_n\}. \tag{2.39}$$

The DH theorem tells us that the sum on the right-hand side gives an exact result. To see that this is true, consider, instead of (2.25), the following expression:

$$\int_{H(n)} d\lambda \int_{M(N,n;C)} \left(\frac{dz\, d\bar{z}}{\pi}\right)^{Nn} \exp[-\beta \text{ tr}(Z^\dagger H Z) + i \text{ tr}\{\lambda(Z^\dagger Z - 1)\}], \tag{2.40}$$

where the integration domain of λ is $H(n)$ and new variables,

$$Z = \begin{pmatrix} Z_u \\ Z_d \end{pmatrix}, \quad Z \in M(N,n;\mathbf{C}),$$

$$Z_u = \begin{pmatrix} z_{1,1} & \cdots & z_{1,n} \\ \vdots & & \vdots \\ z_{n,1} & \cdots & z_{n,n} \end{pmatrix}, \quad Z_d = \begin{pmatrix} z_{n+1,1} & \cdots & z_{n+1,n} \\ \vdots & & \vdots \\ z_{N,1} & \cdots & z_{N,n} \end{pmatrix}, \tag{2.41}$$

have been introduced. An explicit form of λ is given as

$$\lambda = \begin{pmatrix} \lambda_1 & \lambda_{1,2} & \cdots & \lambda_{1,n} \\ \overline{\lambda_{1,2}} & \lambda_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \lambda_{n-1,n} \\ \overline{\lambda_{1,n}} & \cdots & \overline{\lambda_{n-1,n}} & \lambda_n \end{pmatrix}, \tag{2.42}$$

$$\lambda_a \in \mathbf{R} \quad (a=1,\ldots,n),$$

$$\lambda_{a,b}=\frac{x_{a,b}-iy_{a,b}}{2}, \quad x_{a,b},y_{a,b}\in\mathbf{R}, \quad (1\leqslant a\leqslant b\leqslant n), \tag{2.43}$$

so that the measure is

$$d\lambda=\prod_{a=1}^{n}\frac{d\lambda_a}{2\pi}\prod_{a<b}\frac{dx_{a,b}\,dy_{a,b}}{(2\pi)^2}. \tag{2.44}$$

The λ integration leads us to delta functions which can be handled by means of the following change of variables:

$$Z=\begin{pmatrix}1_n\\ \xi\end{pmatrix}\frac{1}{\sqrt{1_n+\xi^\dagger\xi}}\,\zeta; \quad \xi\in M(N-n,n;\mathbf{C}), \quad \zeta\in M(n;\mathbf{C}), \tag{2.45}$$

which brings

$$Z^\dagger Z=\zeta^\dagger\zeta, \tag{2.46}$$

$$\left(\frac{dz\,d\bar{z}}{\pi}\right)^{Nn}=\left(\frac{d\xi\,d\bar{\xi}}{\pi}\right)^{n(N-n)}\frac{1}{\{\det(1_n+\xi^\dagger\xi)\}^N}\left(\frac{d\zeta\,d\bar{\zeta}}{\pi}\right)^{n^2}\{\det(\zeta^\dagger\zeta)\}^{N-n}. \tag{2.47}$$

Then the integration with respect to ζ in (2.40) is easily performed yielding to (2.25). From this observation we can grasp the role of λ, which is to reduce the number of degrees of freedom from Nn to $Nn-n^2=n(N-n)$. Therefore λ is called a multiplier and whose coefficient is referred to as constraint:[23]

$$\psi_{ab}\equiv(Z^\dagger Z)_{ab}-\delta_{ab}\approx 0. \tag{2.48}$$

On the contrary, if $z_{\mu,a}$'s integrations that is *Gaussian* are first performed, we obtain

$$\int_{H(n)}d\lambda\,\frac{\exp(-i\ \mathrm{tr}\ \lambda)}{\det(\beta H\otimes 1_n-i1_N\otimes\lambda^{\mathcal{T}})}. \tag{2.49}$$

With the help of the decomposition,[24]

$$\lambda=\Omega\lambda_0\Omega^\dagger, \quad \lambda_0=\mathrm{diag}(l_1,\ldots,l_n), \quad \Omega\in\mathrm{SU}(n), \tag{2.50}$$

the Ω integration gives

$$(2.40)=\int_{-\infty}^{+\infty}\frac{1}{n!}\prod_{a=1}^{n}\frac{dl_a}{2\pi}\prod_{a<b}(l_a-l_b)^2\,\frac{\exp(-i\Sigma_{a=1}^{n}l_a)}{\Pi_{a=1}^{n}\Pi_{\mu=1}^{N}(\beta h_\mu-il_a)}, \tag{2.51}$$

which, by considering poles and zeros, leads to

$$(2.40)=\sum_{\mu_1<\cdots<\mu_n}\frac{\exp(-\beta\Sigma_{a=1}^{n}h_{\mu_a})}{\beta^{n(N-n)}\Pi_{a=1}^{n}\Pi_{\nu\in\bar{\mu}}(h_\nu-h_{\mu_a})}, \tag{2.52}$$

where again $\bar{\mu}$ is given by (2.39). This is exactly the same expression as (2.38). Thus, *the saddle point approximation (2.38) itself contains the full information of the partition function* $\mathcal{Z}_{\mathrm{cl}}$.

We consider in what follows a quantum version of the DH theorem, that is, the WKB exactness in a path integral. Our interpretation to the DH formula put here will be very helpful in the analysis.

III. COHERENT STATES OF U(N) OVER $G_{N,n}$

In order to obtain the path integral representation, we construct coherent states of U(N) in this section. We consider first the algebraic method proposed by Perelomov, then a generalization of the Schwinger boson technique.

A. Algebraic construction

The $u(N)$ algebra in terms of generators $E_{\mu\nu}$ is

$$[E_{\mu\nu},E_{\rho\sigma}]=\delta_{\nu\rho}E_{\mu\sigma}-\delta_{\mu\sigma}E_{\rho\nu},\quad (1\leqslant\mu,\nu,\rho,\sigma\leqslant N). \tag{3.1}$$

First, build up the coherent state in the fundamental representation. The generators are expressed as

$$(E_{\mu\nu})_{\rho\sigma}=\delta_{\mu\rho}\delta_{\nu\sigma}. \tag{3.2}$$

Introduce an orthonormal set of basis vectors in $\mathbf{C}^N$,

$$(\mathbf{e}_\mu)_\nu=\delta_{\mu\nu},\quad \mathbf{e}_\mu^\dagger\mathbf{e}_\nu=\delta_{\mu\nu}; \tag{3.3}$$

to define a fiducial vector, by picking up first n $\mathbf{e}_a$ $(a=1,\ldots,n)$ vectors out of N vectors, such that

$$\mathscr{E}_{N,n}=\frac{1}{\sqrt{n!}}\sum_{\sigma\in\mathscr{S}_n}\operatorname{sgn}(\sigma)\mathbf{e}_{\sigma(1)}\otimes\cdots\otimes\mathbf{e}_{\sigma(n)}\in\mathbf{C}^{N^n}, \tag{3.4}$$

where $\mathscr{S}_n$ denotes the symmetric group of order n. Consider the map

$$\rho_1:GL(N;\mathbf{C})\mapsto GL(N^n;\mathbf{C}),\quad \rho_1(x)\equiv\otimes^n x(=x\otimes\overset{n}{\cdots}\otimes x), \tag{3.5}$$

then it is obvious that

$$d\rho_1\left(\sum_{a=1}^{n}E_{aa}-\sum_{i=n+1}^{N}E_{ii}\right)\mathscr{E}_{N,n}=n\mathscr{E}_{N,n}, \tag{3.6}$$

$$d\rho_1(E_{\mu i})\mathscr{E}_{N,n}=0, \tag{3.7}$$

where

$$d\rho_1(E)\equiv\frac{d}{dt}\bigg|_{t=0}\rho_1(\exp tE)=\sum_{p=1}^{n}\otimes^{p-1}1_N\otimes E\otimes^{n-p}1_N, \tag{3.8}$$

for $E\in u(N)$. As for this fiducial vector $\mathscr{E}_{N,n}$, the following fact should be noted.

Lemma III.1: On the fiducial vector $\mathscr{E}_{N,n}$, there holds

$$\rho_1(B)\mathscr{E}_{N,n}=\det a\cdot\mathscr{E}_{N,n}, \tag{3.9}$$

where

$$B \in GL(N;\mathbf{C}), \quad B=\begin{pmatrix} a & b \\ 0 & c \end{pmatrix}, \tag{3.10}$$

with

$$a \in GL(n;\mathbf{C}), \quad b \in M(n,N-n;\mathbf{C}), \quad c \in GL(N-n;\mathbf{C}). \tag{3.11}$$

The proof of this lemma is obvious so that we can omit it. (However, some comments would be useful: what this lemma signifies is that $\det a(\mathscr{E}_{N,n})$ is an eigenvalue (eigenvector) of $\rho_1(B)$. If we put $n=N$ in (3.9), the relation is nothing but the definition of the determinant.)

Now consider an element of SU(N) generated by an orthogonal complement of the Lie algebra of U(n)×U($N-n$),

$$S=\exp\begin{pmatrix} 0 & -\alpha^\dagger \\ \alpha & 0 \end{pmatrix}; \quad \alpha \in M(N-n,n;\mathbf{C}), \tag{3.12}$$

which can be rewritten as

$$S=\begin{pmatrix} \dfrac{1}{\sqrt{1_n+\xi^\dagger\xi}} & -\dfrac{1}{\sqrt{1_n+\xi^\dagger\xi}}\,\xi^\dagger \\ \xi\,\dfrac{1}{\sqrt{1_n+\xi^\dagger\xi}} & \dfrac{1}{\sqrt{1_{N-n}+\xi\xi^\dagger}} \end{pmatrix}; \quad \xi \in M(N-n,n;\mathbf{C}), \tag{3.13}$$

with

$$\xi=\alpha\,\frac{1}{\sqrt{\alpha^\dagger\alpha}}\tan\sqrt{\alpha^\dagger\alpha}. \tag{3.14}$$

Noting the Gauss' decomposition $S=LMU$, with

$$L=\begin{pmatrix} 1_n & 0 \\ \xi & 1_{N-n} \end{pmatrix}, \quad M=\begin{pmatrix} \dfrac{1}{\sqrt{1_n+\xi^\dagger\xi}} & 0 \\ 0 & \sqrt{1_{N-n}+\xi\xi^\dagger} \end{pmatrix}, \quad U=\begin{pmatrix} 1_n & -\xi^\dagger \\ 0 & 1_{N-n} \end{pmatrix}, \tag{3.15}$$

we can obtain a desired (normalized) coherent state:

$$|\xi;1\rangle \equiv \rho_1(LMU)\mathscr{E}_{N,n}=\frac{1}{\{\det(1_n+\xi^\dagger\xi)\}^{1/2}}\,\rho_1(L)\mathscr{E}_{N,n}, \tag{3.16}$$

where we have used Lemma III.1. While the unnormalized one is given by

$$|\xi;1\rangle \equiv \rho_1(L)\mathscr{E}_{N,n}, \quad (\xi;1|\xi;1)=\det(1_n+\xi^\dagger\xi), \tag{3.17}$$

whose second relation can be verified as follows: by noting that $L\mathbf{e}_a=\mathbf{e}_a+\Sigma_{i=n+1}^{N}\xi_{ia}\mathbf{e}_i$; $(1\leqslant a\leqslant n)$, we find

$$|\xi;1\rangle=\frac{1}{\sqrt{n!}}\sum_{\sigma\in\mathscr{S}_n}\operatorname{sgn}(\sigma)(\mathbf{e}_{\sigma(1)}+\xi_{i_1\sigma(1)}\mathbf{e}_{i_1})\otimes\cdots\otimes(\mathbf{e}_{\sigma(n)}+\xi_{i_n\sigma(n)}\mathbf{e}_{i_n}). \tag{3.18}$$

(Here and for a while repeated indices imply summation for brevity's sake.) Further, noting

$$(\mathbf{e}_\sigma^\dagger + \boldsymbol{\xi}_{i\sigma}\mathbf{e}_i^\dagger)(\mathbf{e}_\tau + \eta_{j\tau}\mathbf{e}_j) = \delta_{\sigma\tau} + (\xi^\dagger\eta)_{\sigma\tau}, \tag{3.19}$$

then we find

$$(\xi;1|\,\eta;1) = \det(1_n + \xi^\dagger\eta), \tag{3.20}$$

so that

$$\langle\xi;1|\,\eta;1\rangle = \det\{(1_n + \xi^\dagger\xi)^{-1/2}(1_n + \xi^\dagger\eta)(1_n + \eta^\dagger\eta)^{-1/2}\}. \tag{3.21}$$

Next, discuss matrix elements of generators: in view of (3.8) the task is to calculate

$$(\xi;1|d\rho_1(E_{\mu\nu})|\,\eta;1) = \sum_{p=1}^{n} (\xi;1|\otimes^{p-1}1_N\otimes E_{\mu\nu}\otimes^{n-p}1_N|\,\eta;1), \tag{3.22}$$

which can be found, after somewhat lengthy calculations, as

$$(\xi;1|d\rho_1(E_{ab})|\,\eta;1) = \det(1_n + \xi^\dagger\eta)\left(\frac{1}{1_n + \xi^\dagger\eta}\right)_{ba}, \tag{3.23}$$

$$(\xi;1|d\rho_1(E_{ai})|\,\eta;1) = \det(1_n + \xi^\dagger\eta)\left(\eta\,\frac{1}{1_n + \xi^\dagger\eta}\right)_{ia}, \tag{3.24}$$

$$(\xi;1|d\rho_1(E_{ia})|\,\eta;1) = \det(1_n + \xi^\dagger\eta)\left(\frac{1}{1_n + \xi^\dagger\eta}\,\xi^\dagger\right)_{ai}, \tag{3.25}$$

$$(\xi;1|d\rho_1(E_{ij})|\,\eta;1) = \det(1_n + \xi^\dagger\eta)\left(\eta\,\frac{1}{1_n + \xi^\dagger\eta}\,\xi^\dagger\right)_{ji}. \tag{3.26}$$

Armed with these, we obtain the matrix element of an arbitrary Hermitian matrix,

$$H = \sum_{\mu,\nu} h_{\mu\nu}E_{\mu\nu} = \sum_{a,b} h_{ab}E_{ab} + \sum_{a,i} h_{ai}E_{ai} + \sum_{j,b} h_{jb}E_{jb} + \sum_{i,j} h_{ij}E_{ij} \equiv \begin{pmatrix} H_{uu} & H_{ud} \\ H_{du} & H_{dd} \end{pmatrix}, \tag{3.27}$$

such that

$$(\xi;1|d\rho_1(H)|\,\eta;1) = (\xi;1|\,\eta;1)\mathrm{tr}\left\{\frac{1}{1_n + \xi^\dagger\eta}\,(H_{uu} + H_{ud}\eta + \xi^\dagger H_{du} + \xi^\dagger H_{dd}\eta)\right\}, \tag{3.28}$$

which is further rewritten to

$$(\xi;1|d\rho_1(H)|\,\eta;1) = (\xi;1|\,\eta;1)\mathrm{tr}\{P(\xi,\eta)H\}, \tag{3.29}$$

or, equivalently,

$$\langle\xi;1|d\rho_1(H)|\,\eta;1\rangle = \langle\xi;1|\,\eta;1\rangle\mathrm{tr}\{P(\xi,\eta)H\}, \tag{3.30}$$

where we have introduced a projection $P(\xi,\eta)$,

$$P(\xi,\eta) = \begin{pmatrix} 1_n \\ \eta \end{pmatrix}(1_n + \xi^\dagger\eta)^{-1}(1_n \quad \xi^\dagger), \tag{3.31}$$

giving

$$\mathrm{tr}\{P(\xi,\eta)H\}=\mathrm{tr}\left\{\frac{1}{1_n+\xi^\dagger\eta}\,(H_{uu}+H_{ud}\eta+\xi^\dagger H_{du}+\xi^\dagger H_{dd}\eta)\right\}. \tag{3.32}$$

[It should be noted that although the definition of $P(\xi,\eta)$ looks singular in the domain $\{(\xi,\eta)|\det(1_n+\xi^\dagger\eta)=0\}$, there is no harm; since the quantity $\mathrm{tr}\{P(\xi,\eta)H\}$ is always accompanied with $\langle\xi;1|\eta;1\rangle$, including $\det(1_n+\xi^\dagger\eta)$ in the numerator.]

Now we generalize the above result to a higher-dimensional representation. Consider a tensor product of the coherent state,

$$|\xi;1\rangle\mapsto|\xi;k\rangle\equiv\otimes^k|\xi;1\rangle,\quad k=0,1,2,\ldots, \tag{3.33}$$

as well as that of the representation,

$$\rho_k(x)\equiv\otimes^k(\rho_1(x)),\quad x\in GL(N,\mathbf{C}), \tag{3.34}$$

to put

$$|\xi;k\rangle=\rho_k(LMU)\mathscr{E}^{\,k}_{N,n},\quad \mathscr{E}^{\,k}_{N,n}\equiv\otimes^k\mathscr{E}_{N,n}. \tag{3.35}$$

We designate this representation as the kth representation. The following relations are obvious:

$$d\rho_k\left(\sum_{a=1}^{n}E_{aa}-\sum_{i=n+1}^{N}E_{ii}\right)\mathscr{E}^{\,k}_{N,n}=kn\,\mathscr{E}^{\,k}_{N,n}, \tag{3.36}$$

$$d\rho_k(E_{\mu i})\mathscr{E}^{k}_{N,n}=0. \tag{3.37}$$

And it is straightforward to find (i) the inner product between coherent states,

$$\langle\xi;k|\eta;k\rangle=[\det\{(1_n+\xi^\dagger\xi)^{-1/2}(1_n+\xi^\dagger\eta)(1_n+\eta^\dagger\eta)^{-1/2}\}]^k; \tag{3.38}$$

(ii) and matrix elements of generators,

$$\langle\xi;k|d\rho_k(E_{\mu\nu})|\eta;k\rangle=k\ \mathrm{tr}\{P(\xi,\eta)E_{\mu\nu}\}\langle\xi;k|\eta;k\rangle, \tag{3.39}$$

hence

$$\langle\xi;k|d\rho_k(H)|\eta;k\rangle=k\ \mathrm{tr}\{P(\xi,\eta)H\}\langle\xi;k|\eta;k\rangle. \tag{3.40}$$

In view of these relations, there follow that (i) the inner product has a form $\{\langle\xi;1|\eta;1\rangle\}^k$ and (ii) the matrix element of a Hamiltonian is proportional to the parameter k. This fact tells us that the exponent of the path integral is proportional to k. Therefore we can perform the $1/k$ expansion when k goes to large like the usual WKB expansion with respect to $\hbar$.

If we declare that the state $|\xi;k\rangle$ is a coherent state, we must check that the resolution of unity does hold:

$$\mathbf{1}_k=\int d\mu(\xi;k)|\xi;k\rangle\langle\xi;k|, \tag{3.41}$$

with

$$d\mu(\xi;k)\equiv\frac{\mathscr{N}(n,k)}{\mathscr{N}(n,N-n+k)}\,\frac{1}{\{\det(1_n+\xi^\dagger\xi)\}^N}\left(\frac{d\xi\ d\bar{\xi}}{\pi}\right)^{n(N-n)}, \tag{3.42}$$

where $\mathcal{N}(n,k)$ has been given by (2.28) and $\mathbf{1}_k$ is the identity operator on the representation space. To this end the following formulas are indispensable.

Theorem III.2: *Let dg be the normalized Haar measure on* $\mathrm{U}(n)$. *Then for* $^\forall p \in \mathbf{Z}_+$ *with* $\mathbf{Z}_+ = \{0\} \cup \mathbf{N}$ *and* $^\forall X \in M(n;\mathbf{C})$, *there holds an integration formula,*

$$\int_{\mathrm{U}(n)} \frac{dg}{(\det g)^p} \exp\{\mathrm{tr}(gX)\} = \mathcal{N}(n,p)|X|^p, \tag{3.43}$$

$$\mathcal{N}(n,p) \equiv \frac{0!1!\cdots(n-1)!}{p!(p+1)!\cdots(p+n-1)!}. \tag{3.44}$$

Theorem III.3: *For* $^\forall X \in M(n;\mathbf{C})$ *and* $^\forall p \in \mathbf{Z}_+$, *there holds a differential formula,*

$$|\partial_X||X|^p = p(p+1)\cdots(p+n-1)|X|^{p-1}, \tag{3.45}$$

where $|X| = \det X$ *and* $|\partial_X|$ *is defined by*

$$|\partial_X| \equiv \det\left(\frac{\partial}{\partial x_{ij}}\right), \quad \text{for } X = (x_{ij}), \tag{3.46}$$

which is valid even if p is negative integer, provided that $X + X^\dagger$ *is positive definite and* $|X| \neq 0$. Proofs of these formulas are straightforward, but need a bit lengthy calculations; therefore we relegate them to Appendix A. (Although the proof of Theorem III.3, known as Cayley's formula, could be found somewhere, for example, by using Capelli's identity,[25] we supply our own proof.)

Practically our target is to show, instead of (3.41),

$$(\alpha;k|\beta;k) = \int d\mu(\xi;k)(\alpha;k|\xi;k\rangle\langle\xi;k|\beta;k); \quad \alpha,\beta \in M(N-n,n;\mathbf{C}), \tag{3.47}$$

that is,

$$\begin{aligned}\{\det(1_n + \alpha^\dagger\beta)\}^k &= \int d\mu(\xi;k)\, \frac{\{\det(1_n + \alpha^\dagger\xi)\}^k\{\det(1_n + \xi^\dagger\beta)\}^k}{\{\det(1_n + \xi^\dagger\xi)\}^k} \\ &= \frac{\mathcal{N}(n,k)}{\mathcal{N}(n,N-n+k)} \int \left(\frac{d\xi\, d\bar{\xi}}{\pi}\right)^{n(N-n)} \frac{1}{\{\det(1_n + \xi^\dagger\xi)\}^N} \\ &\quad \times \frac{\{\det(1_n + \alpha^\dagger\xi)\}^k\{\det(1_n + \xi^\dagger\beta)\}^k}{\{\det(1_n + \xi^\dagger\xi)\}^k}.\end{aligned} \tag{3.48}$$

Establishing (3.48) is equal to establishing (3.41); since these relations hold for any $|\alpha;k)$ and $|\beta;k)$. To this end, two other relations are needed.

Corollary III.4: For $^\forall k \in \mathbf{Z}_+$, *there holds a formula for Gaussian-type integration over* $M(m+n,n;\mathbf{C})$:

$$\int \left(\frac{dz\, d\bar{z}}{\pi}\right)^{n(m+n)} |Z^\dagger Z|^k \exp\{-\mathrm{tr}(Z^\dagger Z)\} = \frac{\mathcal{N}(n,m)}{\mathcal{N}(n,m+k)}. \tag{3.49}$$

Proof: By making use of an identity,

$$|Z^\dagger Z|^k \exp\{-\mathrm{tr}(Z^\dagger Z)\} = (-1)^{nk}|\partial_X|^k|_{X=1_n} \exp\{-\mathrm{tr}(XZ^\dagger Z)\}, \tag{3.50}$$

the left-hand side of (3.49) is rewritten as

$$(-1)^{nk}|\partial_X|^k|_{X=1_n}\int\left(\frac{dz\ d\bar{z}}{\pi}\right)^{n(m+n)}\exp\{-\mathrm{tr}(XZ^\dagger Z)\}=(-1)^{nk}|\partial_X|^k|_{X=1_n}|X|^{-(m+n)}, \tag{3.51}$$

which becomes, by a repeated use of the formula III.3, to

$$(3.51)=\frac{(m+n)!}{m!}\times\frac{(m+n+1)!}{(m+1)!}\times\cdots\times\frac{(m+n+k-1)!}{(m+k-1)!}=\frac{\mathscr{N}(n,m)}{\mathscr{N}(n,m+k)}. \tag{3.52}$$

Corollary III.5: For $^\forall p,q\in\mathbf{Z}_+$ *and* $^\forall A,B\in M(m+n,n;\mathbf{C})$, *there holds*

$$\int_{\mathrm{U}(n)}\frac{dg}{(\det g)^p}\int\left(\frac{dz\ d\bar{z}}{\pi}\right)^{n(m+n)}|Z^\dagger Z|^q\exp\{-\mathrm{tr}(Z^\dagger Z-Z^\dagger A-gB^\dagger Z)\}$$
$$=\frac{\mathscr{N}(n,p)\mathscr{N}(n,m+p)}{\mathscr{N}(n,m+p+q)}|B^\dagger A|^p. \tag{3.53}$$

Proof: Integrate with respect to $Z,Z^\dagger$ and follow a similar procedure as above to find

$$(3.53)=(-1)^{nq}|\partial_X|^q|_{X=1_n}\int_{\mathrm{U}(n)}\frac{dg}{(\det g)^p}\exp\{\mathrm{tr}(gB^\dagger AX^{-1})\}|X|^{-(m+n)}. \tag{3.54}$$

The formula III.2 enables us to perform the g integration, giving

$$(3.54)=(-1)^{nq}|\partial_X|^q|_{X=1_n}|X|^{-(m+n+p)}\mathscr{N}(n,p)|B^\dagger A|^p, \tag{3.55}$$

which turns out, again, by the repeated use of the formula III.3, to be the right-hand side of (3.53).

Now we can proceed to our target: first rewrite the left-hand side of (3.48) by use of the formula III.2 as

$$\{\det(1_n+\alpha^\dagger\beta)\}^k=\frac{1}{\mathscr{N}(n,k)}\int_{\mathrm{U}(n)}\frac{dg}{(\det g)^k}\exp[\mathrm{tr}\{g(1_n+\alpha^\dagger\beta)\}], \tag{3.56}$$

whose integrand can be expressed by the Gaussian integration with respect to $Z\in M(N,n;\mathbf{C})$,

$$\exp[\mathrm{tr}\{g(1_n+\alpha^\dagger\beta)\}]=\int\left(\frac{dz\ d\bar{z}}{\pi}\right)^{Nn}\exp\left[-\mathrm{tr}\left\{Z^\dagger Z-Z^\dagger\begin{pmatrix}1_n\\ \beta\end{pmatrix}-(1_n,\alpha^\dagger)Zg\right\}\right]. \tag{3.57}$$

A change of variables, $Z\to(\xi,\zeta)$, as was from (2.45) to (2.46), gives

$$(3.57)=\int\left(\frac{d\xi\ d\bar{\xi}}{\pi}\right)^{n(N-n)}\frac{1}{\{\det(1_n+\xi^\dagger\xi)\}^N}\int\left(\frac{d\zeta\ d\bar{\zeta}}{\pi}\right)^{n^2}(\det\zeta^\dagger\zeta)^{N-n}\exp[-\mathrm{tr}\{\zeta^\dagger\zeta-\zeta^\dagger(1_n$$
$$+\xi^\dagger\xi)^{-1/2}(1_n+\xi^\dagger\beta)-g(1_n+\alpha^\dagger\xi)(1_n+\xi^\dagger\xi)^{-1/2}\zeta\}]. \tag{3.58}$$

Substituting (3.58) into (3.56), then integrating with respect to ζ and g with the aid of the formula III.5, we find

$$\text{rhs of }(3.56)=\frac{\mathscr{N}(n,k)}{\mathscr{N}(n,N-n+k)}\int\left(\frac{d\xi\ d\bar{\xi}}{\pi}\right)^{n(N-n)}\frac{1}{\{\det(1_n+\xi^\dagger\xi)\}^N}$$
$$\times\frac{\{\det(1_n+\alpha^\dagger\xi)\}^k\{\det(1_n+\xi^\dagger\beta)\}^k}{\{\det(1_n+\xi^\dagger\xi)\}^k}, \tag{3.59}$$

which is nothing but the right-hand side of (3.48).

We now consider another version of the coherent state with the aid of the Schwinger boson technique.

B. Coherent state via Schwinger boson

As was stressed in Sec. II B, the essence of the classical DH theorem can easily be grasped by increasing degrees of freedom while balancing them with the aid of the multiplier λ: we call such a viewpoint as that of the constrained system. If we could find a similar way in quantum cases, then establishment of the localization would be obvious. Fortunately, we know such a candidate that might realize our expectation: the method of a Schwinger boson. There, in order to obtain a group representation, generators of a group are expressed by creation and annihilation operators. The representation space is thus the Fock space, whose dimension is too large for a group. Therefore there needs to be some constraint to reduce the whole space. In a simple case such as $\mathbf{C}P^N$,[9,10] it is realized by fixing the total particle number. In this way, the scenario would be hopeful.

Consider operators,

$$a=\begin{pmatrix} a_u \\ a_d \end{pmatrix}, \quad a_u=\begin{pmatrix} a_{1,1} & \cdots & a_{1,n} \\ \vdots & & \vdots \\ a_{n,1} & \cdots & a_{n,n} \end{pmatrix}, \quad a_d=\begin{pmatrix} a_{n+1,1} & \cdots & a_{n+1,n} \\ \vdots & & \vdots \\ a_{N,1} & \cdots & a_{N,n} \end{pmatrix}, \tag{3.60}$$

which obey $(1\leqslant \mu,\nu\leqslant N;\ 1\leqslant a,b\leqslant n)$

$$[a_{\mu,a},a^\dagger_{\nu,b}]=\delta_{\mu\nu}\delta_{ab}, \quad [a_{\mu,a},a_{\nu,b}]=[a^\dagger_{\mu,a},a^\dagger_{\nu,b}]=0. \tag{3.61}$$

In terms of these operators, $u(N)$ generators are realized:

$$\hat{E}_{\mu\nu}=\mathrm{tr}(a^\dagger E_{\mu\nu}a); \tag{3.62}$$

$$[\hat{E}_{\mu\nu},\hat{E}_{\rho\sigma}]=(\delta_{\nu\rho}\hat{E}_{\mu\sigma}-\delta_{\sigma\mu}\hat{E}_{\rho\nu}). \tag{3.63}$$

The Fock space $\mathscr{F}$ is designated as

$$\mathscr{F}=\mathrm{Span}\{|(n_{\mu,a})\rangle=\prod_{\mu,a}\ \frac{1}{\sqrt{n_{\mu,a}!}}\,a^{\dagger\,n_{\mu,a}}_{\mu,a}|0\rangle, \quad a_{\mu,a}|0\rangle=0, \quad n_{\mu,a}\in\mathbf{Z}_+\}. \tag{3.64}$$

Introduce a usual canonical coherent state:[3]

$$|Z\rangle\equiv\exp\{\mathrm{tr}(a^\dagger Z-Z^\dagger a)\}|0\rangle=\exp\{-\tfrac{1}{2}\,\mathrm{tr}(Z^\dagger Z)\}\exp\{\mathrm{tr}(a^\dagger Z)\}|0\rangle, \tag{3.65}$$

$$\mathbf{1}=\int\left(\frac{dz\ d\bar{z}}{\pi}\right)^{Nn}|Z\rangle\langle Z|, \tag{3.66}$$

$$\langle Z|Z'\rangle=\exp\{-\tfrac{1}{2}\,\mathrm{tr}(Z^\dagger Z+Z'^\dagger Z')+\mathrm{tr}(Z^\dagger Z')\}, \tag{3.67}$$

where **1** denotes the identity operator on $\mathscr{F}$ and Z has been given by (2.41).

Consider a Hermitian projection operator,

$$P_k\equiv\int\left(\frac{dz\ d\bar{z}}{\pi}\right)^{Nn}\int_{\mathrm{U}(n)}\frac{dg}{(\det g)^k}\,|Zg\rangle\langle Z|. \tag{3.68}$$

A simple inspection leads to

$$P_k P_{k'} = P_k \delta_{k,k'}, \quad P_k^\dagger = P_k. \tag{3.69}$$

In what follows we see that this projection operator indeed reduces $\mathscr{F}$ to the space of the kth representation in the previous section, but before proceeding it is instructive to discuss how to find the form of P_k as (3.68). By noting

$$\exp\{i\ \mathrm{tr}(\lambda a^\dagger a)\}|Z\rangle = |Z_g\rangle, \quad g = e^{i\lambda} \in U(n), \tag{3.70}$$

so that

$$\frac{1}{(\det g)^k}|Z_g\rangle = \exp[\,i\ \mathrm{tr}\{\lambda(a^\dagger a - k)\}]|Z\rangle, \tag{3.71}$$

which immediately reminds us of the multiplier part of (2.40) by replacing $a(a^\dagger)$ with $Z(Z^\dagger)$. [However, note that the difference of the integration domain of λ; in (2.40) it is infinite but in (3.68) it is bounded. Details on this issue are found in Sec. V.]

The trace of P_k can be calculated as

$$\begin{aligned}
\mathrm{Tr}\ P_k &= \int \left(\frac{dz\ d\bar{z}}{\pi}\right)^{Nn} \int_{U(n)} \frac{dg}{(\det g)^k} \langle Z|Zg\rangle \\
&= \mathscr{N}(n,k) \int \left(\frac{dz\ d\bar{z}}{\pi}\right)^{Nn} |Z^\dagger Z|^k \exp\{-\mathrm{tr}(Z^\dagger Z)\} \\
&= \frac{\mathscr{N}(n,k)\mathscr{N}(n,N-n)}{\mathscr{N}(n,N-n+k)},
\end{aligned} \tag{3.72}$$

where we have used (3.67), then the formula III.4. [We have employed the notation $\mathrm{Tr}(\cdots)$ for the trace over the Fock space while $\mathrm{Tr}_k(\cdots)$ emerging below for that over the kth representation space. Those should be distinguished from $\mathrm{tr}(\cdots)$ used for matrix-valued quantities.] (3.72) implies the dimension of the kth representation, that is, the number of independent vectors in $\mathscr{F}$ obeying n^2 physical state conditions:

$$(a^\dagger a)_{a,b}|\mathrm{phys}\rangle = k\,\delta_{a,b}|\mathrm{phys}\rangle. \tag{3.73}$$

In particular, for the case of $k=1$, the relation (3.72) implies an arbitrariness of choosing a fiducial vector (3.4). It is symmetric with respect to n and $N-n$, which clearly reflects the nature of the base manifold $G_{N,n}$, namely $G_{N,n} \cong G_{N,N-n}$, and is easily checked by an explicit calculation:

$$\frac{\mathscr{N}(n,k)\mathscr{N}(n,N-n)}{\mathscr{N}(n,N-n+k)} = \frac{\mathscr{N}(N-n,k)\mathscr{N}(N-n,n)}{\mathscr{N}(N-n,n+k)}. \tag{3.74}$$

Now we show that

$$P_k = \int d\mu(\xi;k)|\xi;k\rangle\langle\xi;k|, \tag{3.75}$$

where $|\xi;k\rangle$ is the coherent state of $U(N)$ over $G_{N,n}$ derived previously, but now given by

$$|\xi;k\rangle \equiv \frac{1}{\{\det(1_n + \xi^\dagger\xi)\}^{k/2}} \exp\{\mathrm{tr}(a_d^\dagger \xi a_u)\}\sqrt{\mathscr{N}(n,k)}(\det a_u^\dagger)^k|0\rangle. \tag{3.76}$$

Thus, we can regard (3.75) as the resolution of unity (3.41).

In order to reach the resolution of unity (3.75) and the coherent state (3.76), first rewrite (3.68) to

$$P_k=\int\left(\frac{dz\ d\bar{z}}{\pi}\right)^{Nn}\int_{U(n)}\frac{dg_1\ dg_2}{\{\det(g_1g_2)\}^k}\,|Zg_1\rangle\langle Zg_2^\dagger|, \tag{3.77}$$

which can be recognized directly by putting $Zg_2^\dagger\mapsto Z$ and $g_1g_2\mapsto g$ and finally performing the trivial integration with respect to g_2. Then note that from (3.67),

$$\begin{aligned}|Zg\rangle&=\exp\{-\tfrac{1}{2}\,\mathrm{tr}(Z^\dagger Z)\}\exp\{\mathrm{tr}(a^\dagger Zg)\}|0\rangle\\&=\exp\{-\tfrac{1}{2}\,\mathrm{tr}(Z^\dagger Z)\}\exp[\,\mathrm{tr}\{(a_u^\dagger Z_u+a_d^\dagger Z_d)g\}\,]|0\rangle\\&=\exp\{-\tfrac{1}{2}\,\mathrm{tr}(\zeta^\dagger\zeta)\}\exp\{\mathrm{tr}(a_d^\dagger\xi a_u)\}\exp\{\mathrm{tr}(a_u^\dagger\Lambda^{-1/2}\zeta g)\}|0\rangle,\end{aligned} \tag{3.78}$$

with $\Lambda=1_n+\xi^\dagger\xi$, where we have utilized the change of variables (2.45) and the Campbell–Baker–Hausdorff formula to the final expression. [As was discussed in the previous section, employing (2.45) is nothing but choosing some fiducial vector.] Therefore (3.78) with the formula III.2 leads to

$$\int_{U(n)}\frac{dg_1}{(\det g_1)^k}\,|Zg_1\rangle=\mathcal{N}(n,k)\exp\left\{-\frac{1}{2}\,\mathrm{tr}(\zeta^\dagger\zeta)\right\}\exp\{\mathrm{tr}(a_d^\dagger\xi a_u)\}\{\det(a_u^\dagger\Lambda^{-1/2}\zeta)\}^k|0\rangle. \tag{3.79}$$

Also note the relation, obtained from the formula III.4,

$$\int\left(\frac{d\zeta\ d\bar{\zeta}}{\pi}\right)^{n^2}|\zeta^\dagger\zeta|^{N-n+k}\exp\{-\mathrm{tr}(\zeta^\dagger\zeta)\}=\frac{1}{\mathcal{N}(n,N-n+k)}. \tag{3.80}$$

Substituting (3.79) (and whose conjugate) into (3.77) then utilizing (3.80), we finally arrive at

$$\begin{aligned}P_k=\frac{\mathcal{N}(n,k)^2}{\mathcal{N}(n,N-n+k)}\int\left(\frac{d\xi\ d\bar{\xi}}{\pi}\right)^{n(N-n)}&\frac{1}{\{\det(1_n+\xi^\dagger\xi)\}^{N+k}}\times\exp\{\mathrm{tr}(a_d^\dagger\xi a_u)\}\\&\times(\det a_u^\dagger)^k|0\rangle\langle 0|(\det a_u)^k\exp\{\mathrm{tr}(a_u^\dagger\xi^\dagger a_d)\}.\end{aligned} \tag{3.81}$$

Therefore we have established (3.75) and (3.76). By comparing (3.76) with (3.16) and (3.33), the state $\sqrt{\mathcal{N}(n,k)}(\det a_u^\dagger)^k|0\rangle$ can be identified as $\vec{\mathscr{E}}^k_{N,n}$. Therefore the projection operator onto the subspace can now be regarded as the resolution of unity in the space of the kth representation.

IV. PATH INTEGRAL AND WKB

In this section we first build up a path integral representation of a character formula by means of the coherent states developed previously. We then perform the WKB approximation. The mechanism of exactness is clarified with the aid of the generalized Schwinger boson technique.

A. Path integral representation

Take a Hamiltonian in the kth representation,

$$\hat{H}=d\rho_k(H),\quad H=\mathrm{diag}(h_1,\ldots,h_N),\ \ h_\mu\in\mathbf{R},\ \ h_1<\cdots<h_N. \tag{4.1}$$

Consider the trace of the time evolution operator, which we call the *character formula* of the kth representation:

$$\mathcal{Z}_k(T)\equiv \mathrm{Tr}_k\ \rho_k(e^{-iHT})=\lim_{M\to\infty}\int d\mu(\xi;k)\langle\xi;k|\{d\rho_k(1_N-i\ \Delta t\ H)\}^M|\xi;k\rangle, \tag{4.2}$$

where $\Delta t=T/M$. Insert the resolution of unity (3.41) to obtain

$$\mathcal{Z}_k(T)=\lim_{M\to\infty}\int_{\mathrm{PBC}}\prod_{j=1}^{M} d\mu(\xi(j);k)\langle\xi(j);k|d\rho_k(1_N-i\ \Delta t\ H)|\xi(j-1);k\rangle, \tag{4.3}$$

where as before "PBC" means $\xi(0)=\xi(M)$. From (3.40) we have

$$\begin{aligned}\langle\xi(j);k|d\rho_k(1_N-i\ \Delta t\ H)|\xi(j-1);k\rangle&=\langle\xi(j);k|\xi(j-1);k\rangle[1-ik\ \Delta t\ \mathrm{tr}\{P(\xi(j),\xi(j-1))H\}]\\&=\langle\xi(j);k|\xi(j-1);k\rangle\exp[-ik\ \Delta t\ \mathrm{tr}\{P(\xi(j),\xi(j-1))H\}]\\&\quad\times\{1+O((\Delta t)^2)\}.\end{aligned} \tag{4.4}$$

Employing the expression (3.38) to $\langle\xi(j);k|\xi(j-1);k\rangle$, we obtain

$$\begin{aligned}\mathcal{Z}_k(T)=\lim_{M\to\infty}\int_{\mathrm{PBC}}\prod_{j=1}^{M} d\mu(\xi(j);k)\exp\Bigg[-k\sum_{i=1}^{M}\mathrm{tr}\{\log(1_n+\xi^\dagger(i)\xi(i))-\log(1_n+\xi^\dagger(i)\\\times\xi(i-1))\}\Bigg]\exp\Bigg[-ik\ \Delta t\sum_{j=1}^{M}\mathrm{tr}\{P(\xi(j),\xi(j-1))H\}\Bigg],\end{aligned} \tag{4.5}$$

where we have discarded terms of $O((\Delta t)^2)$, whose fact also brings us to

$$\begin{aligned}\mathcal{Z}_k(T)=(\det\ V(T))^k\lim_{M\to\infty}\int_{\mathrm{PBC}}\prod_{j=1}^{M} d\mu(\xi(j);k)\exp\Bigg[-k\sum_{i=1}^{M}\mathrm{tr}\{\log(1_n+\xi^\dagger(i)\xi(i))\\-\log(1_n+\xi^\dagger(i)U(\Delta t)\xi(i-1)V^\dagger(\Delta t))\}\Bigg],\end{aligned} \tag{4.6}$$

where $U(t)$ and $V(t)$ have been defined by (2.22),

$$U(t)=e^{-iH_dt}\in U(N-n),\quad V(t)=e^{-iH_ut}\in U(n), \tag{4.7}$$

$$H_u=\mathrm{diag}(h_1,\ldots,h_n),\quad H_d=\mathrm{diag}(h_{n+1},\ldots,h_N). \tag{4.8}$$

By noting that

$$\begin{aligned}&\exp[-k\ \mathrm{tr}\{\log(1_n+\xi^\dagger(i)\xi(i))-\log(1_n+\xi^\dagger(i)U(\Delta t)\xi(i-1)V^\dagger(\Delta t))\}]\\&=\left\{\frac{\det(1_n+\xi^\dagger(i)U(\Delta t)\xi(i-1)V^\dagger(\Delta t))}{\det(1_n+\xi^\dagger(i)\xi(i))}\right\}^k,\end{aligned} \tag{4.9}$$

(4.6) becomes

$$\mathcal{Z}_k(T)=(\det\ V(T))^k\lim_{M\to\infty}\int_{\mathrm{PBC}}\prod_{i=1}^{M} d\mu(\xi(i);k)\times\prod_{j=1}^{M}\langle\xi(j)V(\Delta t);k|U(\Delta t)\xi(j-1);k\rangle, \tag{4.10}$$

where use has been made of (3.38). The relation (3.48) enables us to perform the multiple integration, giving

$$\mathcal{Z}_k(T)=(\det\, V(T))^k\int d\mu(\xi;k)\left\{\frac{\det(1_n+\xi^\dagger U(T)\xi V^\dagger(T))}{\det(1_n+\xi^\dagger\xi)}\right\}^k. \tag{4.11}$$

(See a further discussion in Appendix B.)

B. The WKB approximation

Now examine the WKB approximation of the path integral expression (4.6). Equations of motion are

$$\xi(j)\{1_n+\xi^\dagger(j)\xi(j)\}^{-1}=U(\Delta t)\xi(j-1)V^\dagger(\Delta t)\{1_n+\xi^\dagger(j)U(\Delta t)\xi(j-1)V^\dagger(\Delta t)\}^{-1}, \tag{4.12}$$

$$\{1_n+\xi^\dagger(j)\xi(j)\}^{-1}\xi^\dagger(j)=\{1_n+V^\dagger(\Delta t)\xi^\dagger(j+1)U(\Delta t)\xi(j)\}^{-1}V^\dagger(\Delta t)\xi^\dagger(j+1)U(\Delta t). \tag{4.13}$$

Recall here that solutions should meet the periodic boundary condition $\xi(0)=\xi(M)$. Clearly, only $\xi(j)=0$ for all $1\leqslant j\leqslant M$ can fulfill the condition. Therefore, by putting $\xi=z/\sqrt{k}$ and noting

$$\frac{\mathcal{N}(n,k)}{\mathcal{N}(n,N-n+k)}\overset{k\to\infty}{\sim}k^{n(N-n)}, \tag{4.14}$$

the dominant contribution from this classical solution is read as

$$\tilde{\mathcal{Z}}_k(T)\overset{k\to\infty}{\sim}\lim_{M\to\infty}\int_{\mathrm{PBC}}\prod_{j=1}^{M}\left(\frac{dz(j)d\bar{z}(j)}{\pi}\right)^{n(N-n)}\times\exp\left[-\sum_{j=1}^{M}\mathrm{tr}\, z^\dagger(j)\{z(j)-U(\Delta t)z(j-1)V^\dagger(\Delta t)\}\right], \tag{4.15}$$

where

$$\tilde{\mathcal{Z}}_k(T)\equiv\frac{\mathcal{Z}_k(T)}{(\det\, V(T))^k}. \tag{4.16}$$

To perform the integration further, it is convenient to utilize the Fourier transformation respecting "PBC:"

$$z(j)=\sum_{r=0}^{M-1}\frac{1}{\sqrt{M}}e^{-2\pi ijr/M}\tilde{z}(r),\quad \tilde{z}(r)\in M(N-n,n;\mathbf{C}), \tag{4.17}$$

which enables us to write

$$\sum_{j=1}^{M}z^\dagger(j)\{z(j)-U(\Delta t)z(j-1)V^\dagger(\Delta t)\}=\sum_{r=0}^{M-1}\tilde{z}^\dagger(r)\{\tilde{z}(r)-U(\Delta t)\tilde{z}(r)V^\dagger(\Delta t)e^{2\pi ir/M}\}. \tag{4.18}$$

Since the Jacobian is trivial, the integration with respect to $\tilde{z},\tilde{z}^\dagger$ can readily be performed to give

$$\tilde{\mathcal{Z}}_k(T)=\lim_{M\to\infty}\frac{1}{\Pi_{r=0}^{M-1}\det\{1_{N-n}\otimes 1_n-e^{2\pi ir/M}U(\Delta t)\otimes\bar{V}(\Delta t)\}},\tag{4.19}$$

where $\bar{V}$ is the complex conjugate of V. Utilizing the identity

$$\prod_{r=0}^{M-1}(1_m-e^{2\pi ir/M}X)=1_m-X^M,\tag{4.20}$$

holding for any $X\in M(m;\mathbf{C})$, we finally obtain

$$\tilde{\mathcal{Z}}_k(T)=\frac{1}{\det\{1_{N-n}\otimes 1_n-U(T)\otimes\bar{V}(T)\}}=\frac{1}{\Pi_{i=n+1}^{N}\Pi_{a=1}^{n}\{1-e^{-i(h_i-h_a)T}\}}.\tag{4.21}$$

Similar to the classical case, the number of classical solutions is $\binom{N}{n}$. Taking all the contributions into account [while paying attention to the relation (4.16)], we arrive at

$$\mathcal{Z}_k(T)\overset{k\to\infty}{\sim}\sum_{\mu_1<\cdots<\mu_n}\frac{\exp(-ik\Sigma_{a=1}^{n}h_{\mu_a}T)}{\Pi_{a=1}^{n}\Pi_{\nu\in\bar{\mu}}\{1-e^{-i(h_\nu-h_{\mu_a})T}\}},\tag{4.22}$$

with $\bar{\mu}$ being given by (2.39).

By noticing that the right-hand side of (4.22) can be rewritten, by means of the Laplace expansion of determinant, such that

$$\text{rhs of (4.22)}=\frac{|\epsilon^{N-1+k},\ldots,\epsilon^{N-n+k},\epsilon^{N-n-1},\ldots,\epsilon^{1},1|}{|\epsilon^{N-1},\ldots,\epsilon^{1},1|}\tag{4.23}$$

where

$$|\epsilon^{m_1},\ldots,\epsilon^{m_N}|\equiv\begin{vmatrix}\epsilon_1^{m_1}&\cdots&\epsilon_1^{m_N}\\ \vdots&\vdots&\vdots\\ \epsilon_N^{m_1}&\cdots&\epsilon_N^{m_N}\end{vmatrix},\quad \epsilon_\mu\equiv e^{-ih_\mu T},\tag{4.24}$$

the conclusion that the WKB approximation is exact in this case can be derived; since (4.23) is nothing but the Weyl character formula[26] of $U(N)$. [It is easy to find a similar expression for the classical counterpart (2.38).] The mechanism of this exactness then must be examined.

C. The mechanism of exactness

In view of (4.6), or even after $M-1$ integrations as in (4.11), the remaining integration looks still hard to perform. However, the method of the (generalized) Schwinger boson betters the situation.

As in (3.62), any element $E_{\mu\nu}\in u(N)$ has an operator counterpart on $\mathcal{F}$. Since any $N\times N$ Hermitian matrix is expandable in terms of these basis matrices, a quantum Hamiltonian is expressed as a self-adjoint operator on $\mathcal{F}$:

$$\hat{X}\equiv\mathrm{tr}(a^\dagger Xa),\quad X\in H(N).\tag{4.25}$$

Adopting the diagonal matrix H in (4.1) for X to define $\hat{H}$, we start with the character formula

$$\mathcal{Z}_k(T)=\mathrm{Tr}_k\,\exp(-i\hat{H}T),\tag{4.26}$$

in this new formulation. Recall now the fact that the operator P_k (3.68) is not only the resolution of unity in the kth representation space, but also the projection operator onto the subspace of the Fock space. Therefore we can rewrite (4.26) to

$$\mathcal{Z}_k(T)=\mathrm{Tr}\{\exp(-i\hat{H}T)P_k\}=\int_{U(n)}\frac{dg}{(\det g)^k}\int\left(\frac{dz\ d\bar{z}}{\pi}\right)^{Nn}\langle Z|e^{-i\hat{H}T}|Zg_\epsilon\rangle, \tag{4.27}$$

where we have introduced a regularization parameter ϵ,

$$g\mapsto g_\epsilon=e^{-\epsilon}g, \tag{4.28}$$

which is set to zero after all and legitimatizes the exchange of order of integrations. Apart from the g integration, the right-hand side of (4.27) can be brought into a path integral form by dividing the time duration into M segments and inserting the resolution of unity (3.66) successively:

$$\int\left(\frac{dz\ d\bar{z}}{\pi}\right)^{Nn}\langle Z|e^{-i\hat{H}T}|Zg_\epsilon\rangle=\lim_{M\to\infty}\int_{\mathrm{TBC}}\prod_{i=1}^{M}\left(\frac{dz(i)d\bar{z}(i)}{\pi}\right)^{Nn}\prod_{j=1}^{M}\langle Z(j)|(\mathbf{1}-i\hat{H}\ \Delta t)|Z(j-1)\rangle, \tag{4.29}$$

where "TBC" means a twisted boundary condition $Z(0)=Z(M)g_\epsilon$. Since the Hamiltonian is bilinear with respect to $a^\dagger$ and a, it is a simple task to arrive at

$$(4.29)=\lim_{M\to\infty}\int_{\mathrm{TBC}}\prod_{i=1}^{M}\left(\frac{dz(i)d\bar{z}(i)}{\pi}\right)^{Nn}\exp\left[-\sum_{j=1}^{M}\ \mathrm{tr}\ Z^\dagger(j)\{Z(j)-(1_N-iH\ \Delta t)Z(j-1)\}\right]. \tag{4.30}$$

In order to carry out the Gaussian integrals, follow a similar procedure from (4.17) to (4.21) except employing the Fourier transformation met with "TBC,"

$$z(j)=\sum_{r=0}^{M-1}\ \frac{1}{\sqrt{M}}\,e^{-2\pi ijr/M}\tilde{z}(r)(g_\epsilon)^{j/M}, \tag{4.31}$$

giving

$$(4.27)=\int_{U(n)}\frac{dg}{(\det g)^k}\frac{1}{\det(1_N\otimes 1_n-e^{-iHT}\otimes g_\epsilon^{\mathscr{T}})}. \tag{4.32}$$

The g integration can be performed such that one can use the decomposition[27,24]

$$g=\Omega g_0\Omega^\dagger,\quad g_0=\mathrm{diag}(e^{i\theta_1},\ldots,e^{i\theta_n}),\quad \Omega\in SU(n), \tag{4.33}$$

then integrate Ω to give

$$(4.32)=\int_0^{2\pi}\left(\frac{d\theta}{2\pi}\right)^n\frac{1}{n!}\prod_{a<b}|e^{i\theta_a}-e^{i\theta_b}|^2\,\frac{\exp(-ik\Sigma_{a=1}^n\theta_a)}{\Pi_{\mu=1}^N\Pi_{a=1}^n(1-e^{-ih_\mu T+i\theta_a-\epsilon})}. \tag{4.34}$$

By putting $w_a=e^{-i\theta_a}$ the integration over the maximal torus is converted into a multiple contour integrations:

$$(4.34)=\frac{1}{n!}\oint\left(\frac{dw}{2\pi i}\right)^n\prod_{a\neq b}(w_a-w_b)\,\frac{\Pi_{a=1}^n w_a^{N-n+k}}{\Pi_{\mu=1}^N\Pi_{a=1}^n(w_a-e^{-ih_\mu T-\epsilon})}. \tag{4.35}$$

Taking into account all the contributions from poles, we finally obtain

$$\mathcal{Z}_k(T)=\sum_{\mu_1<\cdots<\mu_n}\frac{\exp(-ik\Sigma_{a=1}^{n}h_{\mu_a}T)}{\Pi_{a=1}^{n}\Pi_{\nu\in\bar{\mu}}\{1-e^{-i(h_\nu-h_{\mu_a})T}\}}, \tag{4.36}$$

where again we have used the notation (2.39). (4.36) exactly matches with (4.22). Hence, the WKB approximation is exact in the path integral for the character formula (4.2), which is now interpreted as that of U(N) represented over $G_{N,n}$.

The reason is now quite obvious, since the path integral representation, in view of (4.30), is essentially Gaussian with an additional g integration, regarded as imposing the physical state condition. Evidently there is no room for the emergence of k^{-1}. As is stated in Ref. 14, we may conclude that the path integral expression we have discussed is kinematically nonlinear but dynamically free. [The situation would correspond to a free field over nontrivial phase space, which should compare to the harmonic oscillator (free field!) over a flat phase space.]

V. DISCUSSION

We have clarified the exactness of the WKB approximation for the U(N) character formula expressed as a path integral over $G_{N,n}$. We have employed a time slicing method as well as coherent states to build up a path integral representation. We have made two different approaches: Perelomov's generalized coherent state and a method of (generalized) Schwinger boson. The latter provides a view of constrained system and can clarify the reason for exactness in both cases, classical (2.38) as well as (4.22): the targets, the classical partition function (2.25), and the character formula (4.2), are essentially Gaussian.

Note, however, the difference between the classical and the quantum cases: critical points are controlled by eigenvalues of the Hermitian matrix, (2.32) or (2.38) in the former case but by those of the unitary matrix, (4.12), (4.13) or (4.22) in the latter case. The origin of the difference lies in the form of constraints: although in the classical case (2.40) constraints (2.48) can be interpreted as the result of inserting the delta function naively to the trivial partition function, in other words, the integration domain of the multiplier λ is *unbounded*, it is *compact* in the quantum case, as can be seen from (3.68).

The compactness of the integration domain is indispensable in the quantum case. To see the situation clearly let us examine the $\mathbf{C}P^1$ example:

$$H=\mathbf{z}^\dagger h\mathbf{z},\quad h=\begin{pmatrix}a & b\\ \bar{b} & d\end{pmatrix}\in H(2),\quad \mathbf{z}=\begin{pmatrix}z_1\\ z_2\end{pmatrix}\in\mathbf{C}^2, \tag{5.1}$$

with a constraint

$$\psi\equiv\mathbf{z}^\dagger\mathbf{z}-p\approx 0,\quad p\in\mathbf{R}_+. \tag{5.2}$$

The fundamental Poisson brackets are

$$\{z_\mu,\bar{z}_\nu\}=-i\delta_{\mu\nu},\quad \{z_\mu,z_\nu\}=\{\bar{z}_\mu,\bar{z}_\nu\}=0,\quad (\mu,\nu=1,2). \tag{5.3}$$

In order to reduce the (flat) manifold to $\mathbf{C}P^1$, there needs an additional constraint to fix the phase of a complex number, say z_1. To this end, a change of variables,

$$\mathbf{z}=\begin{pmatrix}1\\ \xi\end{pmatrix}\frac{1}{\sqrt{1+|\xi|^2}}\,\zeta, \tag{5.4}$$

is utilized. The constraint (5.2) is read as $\psi=|\zeta|^2-p$, and the desired one is found as

$$\chi=\frac{1}{2i}\log\left(\frac{\zeta}{\bar{\zeta}}\right)-\phi_0, \quad 0\leqslant\phi_0<2\pi. \tag{5.5}$$

They satisfy

$$\{\psi,\chi\}=1, \tag{5.6}$$

so that the Dirac brackets can be constructed to give

$$\{\xi,\bar{\xi}\}_{\mathrm{D}}=-\frac{i}{p}(1+|\xi|^2)^2. \tag{5.7}$$

In this way classical mechanics on the reduced phase space can be obtained without any problems.

A prescription to quantum theory would be found by means of a path integral developed by Faddeev–Senjanovic (FS):[28]

$$\begin{aligned}\mathscr{Z}_p^{(\mathrm{FS})}\equiv\lim_{M\to\infty}\int\prod_{\mathrm{PBC}i=1}^{M}\frac{(dz(i)d\bar{z}(i))^2}{\pi}\,\delta(\psi(i))\delta(\chi(i))\\ \times\exp\left[i\sum_{j=1}^{M}\{i\mathbf{z}^{\dagger}(j)\Delta\mathbf{z}(j)-\Delta t\ \mathbf{z}^{\dagger}(j)h\mathbf{z}(j-1)\}\right],\end{aligned} \tag{5.8}$$

where

$$\Delta\mathbf{z}(j)\equiv\mathbf{z}(j)-\mathbf{z}(j-1). \tag{5.9}$$

Although the way of finding (5.8) is rather heuristic, the result seems convincing, provided that constrained systems are given in the configuration space, such as the sphere.[29] Therefore we employ this as a starting point of quantum theory.

With the aid of the change of variables (5.4), (5.8) becomes

$$\begin{aligned}\mathscr{Z}_p^{(\mathrm{FS})}=\lim_{M\to\infty}\int\prod_{\mathrm{PBC}i=1}^{M}\frac{d\xi(i)d\bar{\xi}(i)}{\pi(1+|\xi(i)|^2)^2}\,d\zeta(i)d\bar{\zeta}(i)|\zeta(i)|^2\delta(\psi(i))\delta(\chi(i))\\ \times\exp\left[i\sum_{j=1}^{M}\left\{i|\zeta(j)|^2-i\bar{\zeta}(j)\zeta(j-1)\,\frac{1+\bar{\xi}(j)\xi(j-1)}{(1+\bar{\xi}(j)\xi(j))^{1/2}(1+\bar{\xi}(j-1)\xi(j-1))^{1/2}}\right.\right.\\ -\Delta t\bar{\zeta}(j)\zeta(j-1)\\ \left.\left.\times\frac{a+b\xi(j-1)+\bar{\xi}(j)\bar{b}+\bar{\xi}(j)d\xi(j-1)}{(1+\bar{\xi}(j)\xi(j))^{1/2}(1+\bar{\xi}(j-1)\xi(j-1))^{1/2}}\right\}\right].\end{aligned} \tag{5.10}$$

A trivial integration with respect to ζ leads to

$$\mathscr{Z}_p^{(\mathrm{FS})} = \lim_{M\to\infty} \int_{\mathrm{PBC}} \prod_{i=1}^{M} \frac{p\, d\xi(i) d\bar{\xi}(i)}{\pi(1+|\xi(i)|^2)^2} \times \exp\left[-p \sum_{j=1}^{M} \left\{ 1 - \frac{1+\bar{\xi}(j)\xi(j-1)}{(1+\bar{\xi}(j)\xi(j))^{1/2}(1+\bar{\xi}(j-1)\xi(j-1))^{1/2}} + i\,\Delta t\, \frac{a+b\xi(j-1)+\bar{\xi}(j)\bar{b}+\bar{\xi}(j)d\xi(j-1)}{(1+\bar{\xi}(j)\xi(j))^{1/2}(1+\bar{\xi}(j-1)\xi(j-1))^{1/2}} \right\} \right], \tag{5.11}$$

which should be compared with the correct one, the $\mathbf{C}P^1$ version of (4.5),

$$\mathscr{Z}_k(T) = \lim_{M\to\infty} \int_{\mathrm{PBC}} \prod_{i=1}^{M} \frac{(k+1) d\xi(i) d\bar{\xi}(i)}{\pi(1+|\xi(i)|^2)^2} \exp\left[-k \sum_{j=1}^{M} \left\{ \log(1+|\xi(j)|^2) - \log(1+\bar{\xi}(j)\xi(j-1)) + i\,\Delta t\, \frac{a+b\xi(j-1)+\bar{\xi}(j)\bar{b}+\bar{\xi}(j)d\xi(j-1)}{1+\bar{\xi}(j)\xi(j-1)} \right\} \right]. \tag{5.12}$$

In view of these, even if an arbitrary parameter p in (5.11) would be set to $k \in \mathbf{Z}_+$, a failure of the FS prescription for the present model is now obvious. Nevertheless, a formal continuum limit of (5.11) seems reasonably geometric and respects the feature of the classical system. First, rely on a naive expansion,

$$\xi(j-1) \sim \xi(j) - \Delta t \dot{\xi}(j), \tag{5.13}$$

which brings (5.11) to

$$(5.11) \to \int_{\mathrm{PBC}} \prod_{0\le t\le T} \frac{p\, d\xi(t) d\bar{\xi}(t)}{\pi(1+|\xi(t)|^2)^2} \exp\left[ip \int_0^T dt \left\{ \frac{i}{2} \frac{\bar{\xi}\dot{\xi} - \dot{\bar{\xi}}\xi}{1+|\xi|^2} - \frac{1}{1+|\xi|^2} (a + b\xi + \bar{b}\dot{\bar{\xi}} + \bar{\xi} d\xi) \right\} \right], \tag{5.14}$$

whose exponent consists of (classical) $\mathbf{C}P^1$ action. [Of course, we can also arrive at (5.14), starting from (5.12) with a replacement, $k+1 \to p$, in the measure, then taking the same limit.]

We should, therefore, discard or modify the expression (5.8) in order to find a correct quantum theory. In order to convince the importance of the compactness of the multiplier, we modify the expression as

$$\mathscr{Z}_p^{(\text{FS-I})} \equiv \lim_{M\to\infty} \int_{\mathrm{PBC}} \prod_{i=1}^{M} \left(\frac{dz(i) d\bar{z}(i)}{\pi} \right)^2 \int_{-\infty}^{\infty} \frac{\Delta t}{2\pi} d\lambda(i) \times \exp\left[i \sum_{j=1}^{M} \{ i\mathbf{z}^\dagger(j)\Delta\mathbf{z}(j) - \Delta t\, \mathbf{z}^\dagger(j) h \mathbf{z}(j-1) + \Delta t\, \lambda(j)(\mathbf{z}^\dagger(j)\mathbf{z}(j-1) - p) \} \right]. \tag{5.15}$$

Here the χ constraints have been discarded while the ψ constraints now read as $\mathbf{z}^\dagger(j)\mathbf{z}(j-1) - p \approx 0$ and have been Fourier transformed in (5.8). Note that λ plays the role of the multiplier and still travels in an *infinite range*. If we notice that a change of variables,

$$\mathbf{z}(j) = \mathbf{z}'(j) \exp\left\{ i\, \Delta t \sum_{k=1}^{j} \lambda(k) \right\}, \tag{5.16}$$

$$\lambda(j)=\sum_{r=0}^{M-1}\frac{1}{\sqrt{M}}\,e^{-2\pi ijr/M}\tilde{\lambda}(r), \tag{5.17}$$

wipes out almost all $\tilde{\lambda}(r)$, leaving only $\tilde{\lambda}(0)$ [the constant mode of $\lambda(j)$] in the integrand we further modify (5.8), by throwing away infinities from $\tilde{\lambda}(r)$'s, to

$$\mathscr{Z}_p^{(\mathrm{FS\text{-}II})}\equiv\lim_{M\to\infty}\int_{\mathrm{TBC}}\prod_{i=1}^{M}\left(\frac{dz(i)d\bar{z}(i)}{\pi}\right)^2\int_{-\infty}^{\infty}\frac{d\lambda}{2\pi}\,e^{-ip\lambda}$$
$$\times\exp\left[i\sum_{j=1}^{M}\{i\mathbf{z}^{\dagger}(j)\Delta\mathbf{z}(j)-\Delta t\;\mathbf{z}^{\dagger}(j)h\mathbf{z}(j-1)\}\right], \tag{5.18}$$

where, as before, "TBC" denotes $\mathbf{z}(0)=\mathbf{z}(M)e^{i\lambda}$ and all primes have been removed. The Gaussian integrations with respect to $\mathbf{z}$'s can be performed by introducing a regularization parameter $\epsilon>0$, to give

$$\mathscr{Z}_p^{(\mathrm{FS\text{-}II})}=\lim_{\epsilon\to\infty}\int_{-\infty}^{+\infty}\frac{d\lambda}{2\pi}\,e^{-ip\lambda}\,\frac{1}{(1-e^{-ih_1T+i\lambda-\epsilon})(1-e^{-ih_2T+i\lambda-\epsilon})}, \tag{5.19}$$

where h_i's are eigenvalues of h in (5.1). In view of (5.19), p must be some positive integer, otherwise the result is zero, which leads us, furthermore, to the conclusion that the integration domain of λ in (5.19) *must be replaced by a compact one* $0\leqslant\lambda\leqslant 2\pi$. (Since otherwise we obtain infinitely many copies of the same integration.) Therefore we should have

$$\mathscr{Z}_p^{(\mathrm{correct})}=\lim_{\epsilon\to\infty}\int_{0}^{2\pi}\frac{d\lambda}{2\pi}\,e^{-ip\lambda}\,\frac{1}{(1-e^{-ih_1T+i\lambda-\epsilon})(1-e^{-ih_2T+i\lambda-\epsilon})}, \tag{5.20}$$

that is

$$\mathscr{Z}_p^{(\mathrm{correct})}=\lim_{M\to\infty}\int_{\mathrm{TBC}}\prod_{i=1}^{M}\left(\frac{dz(i)d\bar{z}(i)}{\pi}\right)^2\int_{0}^{2\pi}\frac{d\lambda}{2\pi}\,e^{-ip\lambda}$$
$$\times\exp\left[i\sum_{j=1}^{M}\{i\mathbf{z}^{\dagger}(j)\Delta\mathbf{z}(j)-\Delta t\;\mathbf{z}^{\dagger}(j)h\mathbf{z}(j-1)\}\right]. \tag{5.21}$$

In this way the importance of the compactness in the domain of multipliers is understood, which clarifies an indispensable use of projection operator P_k (3.68) given in Sec. III B.

APPENDIX A: PROOF OF THE THEOREMS

In this appendix, we prove our main theorems in Sec. III A

1. Theorem III.2

The statement is

$$\int_{U(n)}\frac{dg}{(\det g)^p}\exp\{\mathrm{tr}(gX)\}=\mathscr{N}(n,p)|X|^p, \tag{A1}$$

where

$$\mathcal{N}(n,p)=\frac{0!1!\cdots(n-1)!}{p!(p+1)!\cdots(p+n-1)!}, \tag{A2}$$

with the assumptions being given in the text.

We use the following facts without proof.

(I) Invariant measure on $\mathrm{U}(n)$:

$$dg\propto\frac{1}{(\det g)^n}\prod_{1\leqslant i,j\leqslant n}dg_{ij}, \tag{A3}$$

where dg_{ij}'s denote n^2 independent differentials. Each g_{ij} is complex and the number of independent components is n^2 in terms of real variables.

(II) Local decomposition of $\mathrm{U}(n)$:

$$g\in\mathrm{U}(n)\Rightarrow g=\begin{pmatrix}a & 0\\ 0 & B\end{pmatrix}\exp\begin{pmatrix}0 & -\alpha^\dagger\\ \alpha & 0\end{pmatrix}, \tag{A4}$$

where $a\in\mathrm{U}(1)$, $B\in\mathrm{U(n-1)}$, and $\alpha\in\mathbf{C}^{n-1}$ is the parameter for $\mathbf{C}P^{n-1}$. Rewrite (A4) to

$$\begin{pmatrix}a & 0\\ 0 & B\end{pmatrix}\begin{pmatrix}\dfrac{1}{\sqrt{1+|\xi|^2}} & -\dfrac{1}{\sqrt{1+|\xi|^2}}\,\xi^\dagger\\ \xi\,\dfrac{1}{\sqrt{1+|\xi|^2}} & \dfrac{1}{\sqrt{1_{n-1}+\xi\xi^\dagger}}\end{pmatrix},\quad \xi=\frac{\alpha}{|\alpha|}\tan|\alpha|, \tag{A5}$$

so that

$$dg\propto d\mu_{n-1}(\xi)\,\frac{da}{a}\,\frac{\Pi dB_{ij}}{(\det B)^{n-1}}. \tag{A6}$$

Note that the $\mathrm{U}(n)$ measure is decomposed into $\mathbf{C}P^{n-1}$, $\mathrm{U}(1)$, and $\mathrm{U}(n-1)$ in order of mention. Therefore a repeated use of this procedure results in

$$dg\propto\prod_{j=1}^{n-1}d\mu_j(\xi^{(j)})\prod_{i=1}^{n}\frac{da_i}{a_i}, \tag{A7}$$

which signifies that the invariant measure of $\mathrm{U}(n)$ is given by the product of $\mathbf{C}P^j$'s measure $(1\leqslant j\leqslant n-1)$ and the tori of $\mathrm{U}(n)$, corresponding to the local decomposition of $\mathrm{U}(n)$:

$$\frac{\mathrm{U}(n)}{\mathrm{U}(1)\times\mathrm{U}(n-1)}\times\frac{\mathrm{U}(n-1)}{\mathrm{U}(1)\times\mathrm{U}(n-2)}\times\cdots\times\frac{\mathrm{U}(2)}{\mathrm{U}(1)\times\mathrm{U}(1)}\times\mathrm{U}(1)^n\cong\mathbf{C}P^{n-1}\times\mathbf{C}P^{n-2}\times\cdots\mathbf{C}P^1\times\mathrm{U}(1)^n. \tag{A8}$$

(III) Integration formula on $\mathbf{C}P^N$:

$$\frac{(k+N)!}{k!}\int\frac{(d\xi\,d\bar{\xi})^N}{\pi^N(1+|\xi|^2)^{N+1+k}}\,(1+a^\dagger\xi)^k(1+\xi^\dagger b)^k=(1+a^\dagger b)^k, \tag{A9}$$

holds for $^\forall a,b\in\mathbf{C}^N$ and $^\forall k\in\mathbf{Z}_+$.

Since both sides of (A1) are regular functions of x_{ij}, the case, $|X|=0$, can be regarded as a limit of $|X|\neq 0$ so that without loss of generality we can assume

$$X=\begin{pmatrix}\alpha & \beta\\ \gamma & \delta\end{pmatrix},\quad \alpha\in\mathbf{C},\beta^T,\gamma\in\mathbf{C}^{n-1},\delta\in M(n-1;\mathbf{C}),\tag{A10}$$

with $\alpha\det\delta\neq 0$.

The proof is done by induction:

(i) For $n=1$, (A1) is verified by a direct calculation:

$$\oint\frac{da}{2\pi i a^{k+1}}\sum_{k=0}^{\infty}\frac{1}{k!}(aX)^k=\frac{X^k}{k!}.\tag{A11}$$

(ii) Assume (A1) holds for $n\leqslant m$. Then adopt (A5) for $g\in U(m+1)$ to find

$$\operatorname{tr} g\begin{pmatrix}\alpha & \beta\\ \gamma & \delta\end{pmatrix}=a\frac{\alpha-\xi^\dagger\gamma}{\sqrt{1+|\xi|^2}}+\operatorname{tr}\left\{B\left(\frac{\xi\beta}{\sqrt{1+|\xi|^2}}+\frac{1}{\sqrt{1_m+\xi\xi^\dagger}}\,\delta\right)\right\}.\tag{A12}$$

According to the assumption of induction, when $n=m+1$, the integration with respect to a and B on the left-hand side of (A1) gives

$$\frac{\mathcal{N}(m,p)}{p!}\int\frac{m!(d\xi\,d\bar{\xi})^m}{\pi^m(1+|\xi|^2)^{m+1}}\left\{\frac{\alpha-\xi^\dagger\gamma}{\sqrt{1+|\xi|^2}}\right\}^p\left\{\det\left(\frac{\xi\beta}{\sqrt{1+|\xi|^2}}+\frac{1}{\sqrt{1_m+\xi\xi^\dagger}}\,\delta\right)\right\}^p.\tag{A13}$$

By means of a relation,

$$\det\left(\frac{\xi\beta}{\sqrt{1+|\xi|^2}}+\frac{1}{\sqrt{1_m+\xi\xi^\dagger}}\,\delta\right)=\frac{1+\beta\delta^{-1}\xi}{\sqrt{1+|\xi|^2}}\det\,\delta,\tag{A14}$$

(A13) is rewritten as

$$\frac{m!\mathcal{N}(m,p)}{p!}(\alpha\,\det\,\delta)^p\int\frac{(d\xi\,d\bar{\xi})^m}{\pi^m(1+|\xi|^2)^{m+1+p}}(1-\xi^\dagger\gamma\alpha^{-1})^p(1+\beta\,\delta^{-1}\xi)^p,\tag{A15}$$

which finally turns out, with the aid of (A9), to be

$$(\text{A15})=\frac{m!}{(p+m)!}\mathcal{N}(m,p)(\alpha\,\det\,\delta)^p(1-\beta\,\delta^{-1}\gamma\,\alpha^{-1})^p=\frac{m!}{(p+m)!}\mathcal{N}(m,p)\left\{\det\begin{pmatrix}\alpha & \beta\\ \gamma & \delta\end{pmatrix}\right\}^p.\tag{A16}$$

Hence, (A1) holds for $n=m+1$ as well as for $n\leqslant m$.
This completes the proof.

2. Theorem III.3

Next, consider the second theorem:

$$|\partial_X||X|^p=p(p+1)\cdots(p+n-1)|X|^{p-1},$$

$$p=0,\pm 1,\pm 2,\ldots\ .\tag{A17}$$

A. Proof for $p \geqslant 0$

In this case, the formula (A1) is utilized to rewrite the left-hand side of (A17) as

$$|\partial_X||X|^p = \frac{1}{\mathcal{N}(n,1)\mathcal{N}(n,p)} \int_{U(n)} \frac{dg_1\, dg_2}{\det g_1 (\det g_2)^p} \exp\{\mathrm{tr}(g_1 \partial_X)\} \exp\{\mathrm{tr}(g_2 X)\}. \tag{A18}$$

Regard $\partial_{ij} = \partial/\partial x_{ij}$ and x_{ij} as operators upon functions of x_{ij}. Then the both sides of (A18) are now considered to operate on 1. Apply the Campbell–Baker–Hausdorff formula to the exponential factors on the right-hand side to give

$$\begin{aligned} \text{rhs of (A18)} = \frac{1}{\mathcal{N}(n,1)\mathcal{N}(n,p)} \int_{U(n)} \frac{dg_1\, dg_2}{\det g_1 (\det g_2)^p} \exp\{\mathrm{tr}(g_1 g_2)\} \\ \times \exp\{\mathrm{tr}(g_2 X)\} \exp\{\mathrm{tr}(g_1 \partial_X)\}, \end{aligned} \tag{A19}$$

so that the last exponential factor can be dropped. Finally, g_1 integration leads to

$$\begin{aligned} |\partial_X||X|^P = \frac{1}{\mathcal{N}(n,p)} \int_{U(n)} \frac{dg}{(\det g)^{p-1}} \exp\{\mathrm{tr}(gX)\} = \frac{\mathcal{N}(n,p-1)}{\mathcal{N}(n,p)} |X|^{p-1} \\ = p(p+1)\cdots(p+n-1)|X|^{p-1}, \end{aligned} \tag{A20}$$

which complete the proof for $p \in \mathbf{Z}_+$. Note that there is no restriction to $X \in M(n;\mathbf{C})$ in this case.

B. Proof for $p<0$

Start with the following relation:

$$|\partial_X||X|^{-p} = |\partial_X| \int \left(\frac{dz\, d\bar{z}}{\pi}\right)^{np} \exp\{-\mathrm{tr}(XZZ^\dagger)\} = (-1)^n \int \left(\frac{dz\, d\bar{z}}{\pi}\right)^{np} |ZZ^\dagger| \exp\{-\mathrm{tr}(XZZ^\dagger)\}, \tag{A21}$$

for

$$X = A + iB, \quad A^\dagger = A, \quad B^\dagger = B, \quad A > 0, \tag{A22}$$

where we have put $p \to -p$ so that p is positive here and hereafter.

First, consider the case $p \leqslant n-1$ in which the relation,

$$\det ZZ^\dagger = \det(Z \quad 0) \begin{pmatrix} Z^\dagger \\ 0 \end{pmatrix} = 0, \tag{A23}$$

tells us that the right-hand side of (A21) trivially vanishes. Hence, it is enough to examine the case $p \geqslant n$. Before proceeding, we recall a well-known fact: under the condition (A22) A and B are simultaneously diagonalized by means of an appropriate invertible matrix K, such that

$$K^\dagger A K = 1_n, \quad K^\dagger B K = B_D = \mathrm{diag}(\beta_1, \ldots, \beta_n). \tag{A24}$$

Accordingly, a change of variables, $Z \mapsto Z' = K^{-1}Z$, gives

$$(\text{A21}) = \frac{(-1)^n}{|A|^{p+1}} \int \left(\frac{dz\, d\bar{z}}{\pi}\right)^{np} |ZZ^\dagger| \exp[-\mathrm{tr}\{(1_n + iB_D)ZZ^\dagger\}]. \tag{A25}$$

Then rewrite the matrix $1_n + iB_D$ as

$$1_n + iB_D = \begin{pmatrix} 1+i\beta_1 & & 0 \\ & \ddots & \\ 0 & & 1+i\beta_n \end{pmatrix} = F\Phi, \tag{A26}$$

$$F \equiv \begin{pmatrix} f_1 & & 0 \\ & \ddots & \\ 0 & & f_n \end{pmatrix}, \quad \Phi \equiv \begin{pmatrix} e^{i\phi_1} & & 0 \\ & \ddots & \\ 0 & & e^{i\phi_n} \end{pmatrix}, \tag{A27}$$

$$0 < f_i, \quad -\frac{\pi}{2} < \phi_i < \frac{\pi}{2} \quad (i = 1,\ldots,n). \tag{A28}$$

Further, a change of variables $Z \mapsto Z' = \sqrt{F}Z$ leads to

$$(\text{A25}) = \frac{(-1)^n}{|A|^{p+1}|F|^{p+1}} \int \left(\frac{dz\ d\bar{z}}{\pi}\right)^{np} |ZZ^\dagger| \exp\{-\mathrm{tr}(\Phi Z Z^\dagger)\}, \tag{A29}$$

which is rewritten, by use of the formula (A1), as

$$(\text{A29}) = \frac{(-1)^n n!}{|A|^{p+1}|F|^{p+1}} \lim_{\epsilon \to 0} \int_{U(n)} \frac{dg}{\det g} \int \left(\frac{dz\ d\bar{z}}{\pi}\right)^{np} \exp[-\mathrm{tr}\{(\Phi - ge^{-\epsilon})ZZ^\dagger\}]. \tag{A30}$$

Now the Gaussian integration with respect to Z is performed, giving

$$(\text{A30}) = \frac{(-1)^n n!}{|A|^{p+1}|F|^{p+1}} \lim_{\epsilon \to 0} \int_{U(n)} \frac{dg}{\det g} \frac{1}{\det(\Phi - ge^{-\epsilon})^p}, \tag{A31}$$

which becomes, after a change of variable $g \mapsto \Phi^{-1}g$,

$$\begin{aligned}(\text{A31}) &= \frac{(-1)^n n!}{|A|^{p+1}|F|^{p+1}|\Phi|^{p+1}} \lim_{\epsilon \to 0} \int_{U(n)} \frac{dg}{\det g} \frac{1}{\det(1_n - ge^{-\epsilon})^p} \\ &= \frac{(-1)^n n!}{|X|^{p+1}} \lim_{\epsilon \to 0} \int_{U(n)} \frac{dg}{\det g} \frac{1}{\det(1_n - ge^{-\epsilon})^p}. \end{aligned} \tag{A32}$$

In view of (A32) and (A17) (with $p \to -p$), our remaining task is therefore to prove

$$\lim_{\epsilon \to 0} \int_{U(n)} \frac{dg}{\det g} \frac{1}{\det(1_n - ge^{-\epsilon})^p} = \binom{p}{n}. \tag{A33}$$

In order to accomplish the g integration, recall the decomposition,[27,24]

$$g = \Omega g_0 \Omega^\dagger, \quad g_0 = \mathrm{diag}(e^{i\theta_1},\ldots,e^{i\theta_n}), \quad \Omega \in SU(n), \tag{A34}$$

then integrate Ω to obtain

$$\lim_{\epsilon \to 0} \int_{U(n)} \frac{dg}{\det g} \frac{1}{\det(1_n - ge^{-\epsilon})^p} = \lim_{\epsilon \to 0} \int_0^{2\pi} \left(\frac{d\theta}{2\pi}\right)^n \frac{1}{n!} \prod_{a<b} |e^{i\theta_a} - e^{i\theta_b}|^2 \prod_{a=1}^n \frac{e^{-i\theta_a}}{(1 - e^{-\epsilon + i\theta_a})^p}$$

$$= \lim_{\epsilon \to 0} \int_0^{2\pi} \left(\frac{d\theta}{2\pi} \right)^n \frac{1}{n!} \sum_{\sigma,\tau \in \mathcal{S}_n} \operatorname{sgn}(\sigma\tau) \prod_{a=1}^{n} \sum_{l_a=0}^{\infty} \binom{p+l_a-1}{l_a}$$
$$\times \exp[i\{l_a - 1 + \sigma(a) - \tau(a)\}\theta_a - l_a\epsilon]. \tag{A35}$$

Finally, carry out the θ integrations and put $\epsilon \to 0$ to find

$$(\text{A35}) = \begin{vmatrix} p & \binom{p+1}{2} & \binom{p+2}{3} & \cdots & \binom{p+n-1}{n} \\ 1 & p & \binom{p+1}{2} & \ddots & \vdots \\ 0 & 1 & p & \ddots & \binom{p+2}{3} \\ \vdots & \ddots & \ddots & \ddots & \binom{p+1}{2} \\ 0 & \cdots & 0 & 1 & p \end{vmatrix}. \tag{A36}$$

We denote this determinant as $\mathcal{D}(n,p)$, $n=0,1,2,...$, defining $\mathcal{D}(0,p)=1$. Now our goal is to show

$$\mathcal{D}(n,p) = \binom{p}{n}. \tag{A37}$$

Prove this again by induction: first note the recursion relation, obtained by expanding $\mathcal{D}(n,p)$ with respect to its first row,

$$\mathcal{D}(n,p) = \sum_{r=1}^{n} (-1)^{1+r} \binom{p+r-1}{r} \mathcal{D}(n-r,p). \tag{A38}$$

Assume (A37) for $0 \leqslant m \leqslant n-1$, then rewrite (A38) as

$$\mathcal{D}(n,p) = \sum_{r=1}^{n} (-1)^{1+r} \binom{p+r-1}{r} \binom{p}{n-r} = \frac{p}{n} \sum_{r=1}^{n} (-1)^{1+r} \binom{n}{r} \binom{p+r-1}{p+r-n}. \tag{A39}$$

Utilize the generating function, giving us

$$\binom{p+r-1}{p+r-n} = \frac{1}{p!} \left(\frac{d}{dx} \right)^p \Bigg|_{x=0} \sum_{l=0}^{\infty} \binom{l+n-1}{l} x^{l+n-r}, \tag{A40}$$

to find

$$\binom{p}{n} - \mathcal{D}(n,p) = \frac{p}{n} \sum_{r=0}^{n} (-1)^r \binom{n}{r} \binom{p+r-1}{p+r-n} = \frac{p}{n} \frac{1}{p!} \left(\frac{d}{dx} \right)^p \Bigg|_{x=0} \sum_{r=0}^{n} (-1)^r \binom{n}{r}$$
$$\times \sum_{l=0}^{\infty} \binom{l+n-1}{l} x^{l+n-r}$$
$$= \frac{p}{n} \frac{1}{p!} \left(\frac{d}{dx} \right)^p \Bigg|_{x=0} \sum_{r=0}^{n} \binom{n}{r} (-1)^r x^{n-r} \left(\frac{1}{1-x} \right)^n = (-1)^n \frac{p}{n} \frac{1}{p!} \left(\frac{d}{dx} \right)^p \Bigg|_{x=0} 1 = 0. \tag{A41}$$

Thus (A37) also holds for $m=n$. This completes the proof.

APPENDIX B: FEYNMAN KERNEL AND THE WKB APPROXIMATION

In order to make a comparison to the DH theorem, our concentration has been on the character formula in the text. However, from a quantum mechanical point of view, the Feynman kernel is more primitive so that in this appendix a brief sketch is presented, giving a path integral representation that enables us to discuss the WKB approximation.

1. The Feynman kernel by the generalized coherent states

Take a Hermitian matrix,

$$H\equiv\begin{pmatrix} A & B \\ B^\dagger & D \end{pmatrix}\in H(N), \tag{B1}$$

with the same convention given in (2.14); then consider the Feynman kernel,

$$K_k(\xi_F,\xi_I;T)\equiv\langle\xi_F;k|\rho_k(e^{-iHT})|\xi_I;k\rangle. \tag{B2}$$

Follow a similar procedure from (4.2) to (4.6) to obtain

$$\begin{aligned} K_k(\xi_F,\xi_I;T)=&\frac{1}{[\det\{(1_n+\xi_F^\dagger\xi_F)(1_n+\xi_I^\dagger\xi_I)\}]^{k/2}}\lim_{M\to\infty}\int\prod_{i=1}^{M-1}d\mu(\xi(i);k)\\ &\times\exp\left[-k\sum_{j=1}^{M-1}\operatorname{tr}\log(1_n+\xi^\dagger(j)\xi(j))+k\sum_{j=1}^{M}\operatorname{tr}\log(1_n+\xi^\dagger(j)\xi(j-1))\right]\\ &\times\exp\left[-ik\,\Delta t\sum_{j=1}^{M}\operatorname{tr}\{P(\xi(j),\xi(j-1))H\}\right], \end{aligned} \tag{B3}$$

where $\xi(0)=\xi_I$, $\xi(M)=\xi_F$. Introduce a one-parameter subgroup of U(N),

$$g(t)=\exp(-iHt)=\begin{pmatrix} \alpha(t) & \beta(t) \\ \gamma(t) & \delta(t) \end{pmatrix},\quad t\in\mathbf{R}, \tag{B4}$$

and write

$$\mathbf{L}(i,j)\equiv\alpha(i-j)+\xi^\dagger(i)\gamma(i-j)+\beta(i-j)\xi(j)+\xi^\dagger(i)\delta(i-j)\xi(j), \tag{B5}$$

with the abbreviation $\alpha(j\Delta t)=\alpha(j)$, etc.; then discard $O((\Delta t)^2)$ terms to obtain

$$\begin{aligned} K_k(\xi_F,\xi_I;T)=&\frac{1}{[\det\{(1_n+\xi_F^\dagger\xi_F)(1_n+\xi_I^\dagger\xi_I)\}]^{k/2}}\lim_{M\to\infty}\int\prod_{i=1}^{M-1}d\mu(\xi(i);k)\\ &\times\exp\left[k\sum_{j=1}^{M}\operatorname{tr}\log\mathbf{L}(j,j-1)-k\sum_{j=1}^{M-1}\operatorname{tr}\log\mathbf{L}(j,j)\right], \end{aligned} \tag{B6}$$

whose jth integration part is

$$\int\frac{d\mu(\xi(j);k)}{\{\det(1_n+\xi^\dagger(j)\xi(j))\}^k}[\det\{\mathbf{L}(j+1,j)\mathbf{L}(j,j-1)\}]^k. \tag{B7}$$

To carry out this integration, write

$$\det\{\mathbf{L}(j+1,j)\mathbf{L}(j,j-1)\}=\det\{\alpha(1)+\xi^{\dagger}(j+1)\gamma(1)\}\det\{1_n+\{\xi^{\dagger}(j+1)*g(1)\}\xi(j)\}$$
$$\times\det\{1_n+\xi^{\dagger}(j)\{g(1)*\xi(j-1)\}\}\det\{\alpha(1)+\beta(1)\xi(j-1)\}, \tag{B8}$$

where

$$g(j)*\xi=\{\gamma(j)+\delta(j)\xi\}\{\alpha(j)+\beta(j)\xi\}^{-1},$$
$$\xi^{\dagger}*g(j)\equiv\{\alpha(j)+\xi^{\dagger}\gamma(j)\}^{-1}\{\beta(j)+\xi^{\dagger}\delta(j)\}. \tag{B9}$$

Utilizing the formula (3.48), we find

$$(\mathrm{B7})=\det\{\alpha(1)+\xi^{\dagger}(j+1)\gamma(1)\}^{k}[\det\{1_n+\{\xi^{\dagger}(j+1)*g(1)\}\{g(1)*\xi(j-1)\}\}]^{k}$$
$$\times\det\{\alpha(1)+\beta(1)\xi(j-1)\}^{k}, \tag{B10}$$

which is nothing but

$$(\mathrm{B7})=\{\det\mathbf{L}(j+1,j-1)\}^{k}, \tag{B11}$$

since $g(t)$ is an element of the one-parameter subgroup (B4). Hence, after $M-1$ times of this manipulation we obtain

$$K_k(\xi_F,\xi_I;T)=\left[\frac{\det\{\alpha(T)+\xi_F^{\dagger}\gamma(T)+\beta(T)\xi_I+\xi_F^{\dagger}\delta(T)\xi_I\}}{\det\{(1_n+\xi_F^{\dagger}\xi_F)(1_n+\xi_I^{\dagger}\xi_I)\}^{1/2}}\right]^{k}. \tag{B12}$$

2. The Feynman kernel by the Schwinger boson

First introduce an integral representation of the inner product between coherent states:

$$\langle\xi;k|\eta;k\rangle=\frac{\mathcal{N}(n,N-n+k)}{\mathcal{N}(n,k)}\int\left(\frac{d\zeta\,d\bar{\zeta}}{\pi}\right)^{n^2}\{\det(\zeta^{\dagger}\zeta)\}^{N-n}\int_{U(n)}\frac{dg}{(\det g)^{k}}\langle Z(\xi,\zeta)|Z(\eta,\zeta)g\rangle, \tag{B13}$$

where

$$|Z(\xi,\zeta)\rangle\equiv\exp\{\mathrm{tr}(a^{\dagger}Z(\xi,\zeta)-Z^{\dagger}(\xi,\zeta)a)\}|0\rangle \tag{B14}$$

is the canonical coherent state, with $Z(\xi,\zeta)$ being defined by

$$\xi\in M(N-n,n;\mathbf{C}),\quad \zeta\in M(n;\mathbf{C})\mapsto Z(\xi,\zeta)\equiv\begin{pmatrix}1_n\\ \xi\end{pmatrix}\frac{1}{\sqrt{1_n+\xi^{\dagger}\xi}}\,\zeta\in M(N,n;\mathbf{C}). \tag{B15}$$

[The relation (B13) can be verified by use of the formulas III.2 and III.3.) Then the Feynman kernel (B2) is expressed as

$$K_k(\xi_F,\xi_I;T)=\frac{\mathcal{N}(n,N-n+k)}{\mathcal{N}(n,k)}\int\left(\frac{d\zeta\,d\bar{\zeta}}{\pi}\right)^{n^2}\{\det(\zeta^{\dagger}\zeta)\}^{N-n}\int_{U(n)}\frac{dg}{(\det g)^{k}}\langle Z(\xi_F,\zeta)|$$
$$\times\exp(-i\hat{H}T)|Z(\xi_I,\zeta)g\rangle, \tag{B16}$$

where $\hat{H}$ has been given by (4.25) for H in (B1). Write

$$\langle Z(\xi_F,\zeta)|\exp(-i\hat{H}T)|Z(\zeta_I,\zeta)g\rangle=\exp\{-\mathrm{tr}(\zeta^\dagger\zeta)\}\lim_{M\to\infty}\int\prod_{i=1}^{M-1}\left(\frac{dz(i)d\bar{z}(i)}{\pi}\right)^{Nn}$$
$$\times\exp\left[-\mathrm{tr}\left\{\sum_{j=1}^{M-1}Z^\dagger(j)Z(j)\right.\right.$$
$$\left.\left.-\sum_{j=1}^{M}Z^\dagger(j)g(1)Z(j-1)\right\}\right], \tag{B17}$$

where $Z(0)=Z(\xi_I,\zeta)g$, $Z^\dagger(M)=Z^\dagger(\xi_F,\zeta)$, which becomes

$$(\mathrm{B17})=\exp[-\mathrm{tr}\{\zeta^\dagger\zeta-g\zeta^\dagger\mathbf{K}(\xi_F,\xi_I;T)\zeta\}], \tag{B18}$$

where

$$\mathbf{K}(\xi_F,\xi_I;T)\equiv(1_n+\xi_F^\dagger\xi_F)^{-1/2}\mathbf{L}(M,0)(1_n+\xi_I^\dagger\xi_I)^{-1/2}$$
$$=(1_n+\xi_F^\dagger\xi_F)^{-1/2}\{\alpha(T)+\xi_F^\dagger\gamma(T)+\beta(T)\xi_I+\xi_F^\dagger\delta(T)\xi_I\}(1_n+\xi_I^\dagger\xi_I)^{-1/2}. \tag{B19}$$

Substituting (B18) into (B16) and carrying out g and ζ integrations, we find

$$K_k(\xi_F,\xi_I;T)=\{\det\mathbf{K}(\xi_F,\xi_I;T)\}^k=\left[\frac{\det\{\alpha(T)+\xi_F^\dagger\gamma(T)+\beta(T)\xi_I+\xi_F^\dagger\delta(T)\xi_I\}}{\det\{(1_n+\xi_F^\dagger\xi_F)(1_n+\xi_I^\dagger\xi_I)\}^{1/2}}\right]^k, \tag{B20}$$

which, of course, matches the previous result (B12). However, this representation can again provide an interpretation of the WKB exactness.

3. The WKB approximation

From the path integral expression (B6), the action is read as

$$S=\sum_{j=1}^{M}\mathrm{tr}\log\mathbf{L}(j,j-1)-\sum_{j=1}^{M-1}\mathrm{tr}\log\mathbf{L}(j,j). \tag{B21}$$

and therefore equations of motion read as

$$\{\gamma(1)+\delta(1)\xi(j-1)\}\mathbf{L}^{-1}(j,j-1)=\xi(j)\mathbf{L}^{-1}(j,j), \tag{B22}$$

$$\mathbf{L}^{-1}(j+1,j)\{\beta(1)+\xi^\dagger(j+1)\delta(1)\}=\mathbf{L}^{-1}(j,j)\xi^\dagger(j), \tag{B23}$$

for $1\leqslant j\leqslant M-1$. These can be solved locally by

$$\xi(j)=\{\gamma(1)+\delta(1)\xi(j-1)\}\{\alpha(1)+\beta(1)\xi(j-1)\}^{-1}, \tag{B24}$$

$$\xi^\dagger(j)=\{\alpha(1)+\xi^\dagger(j+1)\gamma(1)\}^{-1}\{\beta(1)+\xi^\dagger(j+1)\delta(1)\}, \tag{B25}$$

so that the classical solution, under the boundary condition $\xi(0)=\xi_I$, $\xi(M)=\xi_F$, is found such that

$$\xi_c(j)=\{\gamma(j)+\delta(j)\xi_I\}\{\alpha(j)+\beta(j)\xi_I\}^{-1}, \tag{B26}$$

$$\xi_c^\dagger(j)=\{\alpha(M-j)+\xi_F^\dagger\gamma(M-j)\}^{-1}\{\beta(M-j)+\xi_F^\dagger\delta(M-j)\}. \tag{B27}$$

Note that $\xi_c(j)$ and $\xi_c^\dagger(j)$ are not Hermitian conjugated to each other. This is not so surprising, although it is often emphasized. A similar situation can be met even in a simple Gaussian integration:

$$\int \frac{dz\ d\bar{z}}{\pi} \exp(-\bar{z}z+\bar{a}z+\bar{z}b), \tag{B28}$$

for $a,b\in\mathbf{C}$. Complete the square to find

$$\bar{z}z-\bar{a}z-\bar{z}b=(\bar{z}-\bar{a})(z-b)-\bar{a}b. \tag{B29}$$

Then the shift, $z,\bar{z}\to z+b,\bar{z}+a$, leading to

$$\int \frac{dz\ d\bar{z}}{\pi} \exp(-\bar{z}z+\bar{a}b)=e^{\bar{a}b}, \tag{B30}$$

is asymmetric, but there is no problem. The point is that they should be regarded as independent, which also clarifies that there is no overspecification problem often stressed by authors working in a continuum version of the path integral, since there seems to be two boundary conditions in the first-order differential equation. (The confusion emerges from regarding variables as complex conjugates to each other.)

Turn back to the main subject and evaluate the action (B21) and its Hessian at classical solutions (B26) and (B27). To this end note the following relation:

$$\mathbf{L}(j,j)_c\{\alpha(j)+\beta(j)\xi_I\}=\mathbf{L}(j,j-1)_c\{\alpha(j-1)+\beta(j-1)\xi_I\}, \tag{B31}$$

where the subscript c designates quantities of the classical solutions. Then

$$\begin{aligned} S_c &\equiv \sum_{j=1}^{M} \operatorname{tr}\log \mathbf{L}(j,j-1)_c - \sum_{j=1}^{M-1} \operatorname{tr}\log \mathbf{L}(j,j)_c \\ &= \operatorname{tr}\log[\mathbf{L}(M,M-1)_c\{\alpha(M-1)+\beta(M-1)\xi_I\}]=\operatorname{tr}\log \mathbf{L}(M,0), \end{aligned} \tag{B32}$$

with $\mathbf{L}(M,0)\in M(n;\mathbf{C})$ being given by (B5): explicitly, $\mathbf{L}(M,0) = \alpha(T) + \xi_F^\dagger\gamma(T) + \beta(T)\xi_I + \xi_F^\dagger\delta(T)\xi_I$. Introduce another one-parameter subgroup,

$$\tilde{g}(t)\equiv\begin{pmatrix} \delta^\dagger(t) & -\beta^\dagger(t) \\ -\gamma^\dagger(t) & \alpha^\dagger(t) \end{pmatrix}, \tag{B33}$$

to define

$$\tilde{\mathbf{L}}(i,j)\equiv\delta^\dagger(i-j)-\xi(j)\gamma^\dagger(i-j)-\beta^\dagger(i-j)\xi^\dagger(i)+\xi(j)\alpha^\dagger(i-j)\xi^\dagger(i). \tag{B34}$$

The Hessian of the action is then found as

$$\frac{\partial^2 S}{\partial\xi_{ia}(l)\partial\bar{\xi}_{jb}(m)}=-\delta_{l,m}\tilde{\mathbf{L}}^{-1}(m,m)_{ji}\mathbf{L}^{-1}(m,m)_{ab}+\delta_{l,m-1}\tilde{\mathbf{L}}^{-1}(m,m-1)_{ji}\mathbf{L}^{-1}(m,m-1)_{ab}. \tag{B35}$$

Shifting the variables such that

$$\xi(j)=\xi_c(j)+z(j),\quad \xi^\dagger(j)=\xi_c^\dagger(j)+z^\dagger(j), \tag{B36}$$

and truncate the Taylor series up to the bilinear terms of z and $z^\dagger$ to obtain

$$S \sim S_c - \sum_{j=1}^{M-1} \mathrm{tr}\{z^\dagger(j)\tilde{\mathbf{L}}^{-1}(j,j)_c z(j)\mathbf{L}^{-1}(j,j)_c\} + \sum_{j=2}^{M-1} \mathrm{tr}\{z^\dagger(j)\tilde{L}^{-1}(j,j-1)_c z(j-1) \times \mathbf{L}^{-1}(j,j-1)_c\}. \tag{B37}$$

The measure is also approximated as

$$d\mu(\xi(j);k)|_c \overset{k\to\infty}{\sim} \frac{k^{n(N-n)}}{\{\det \mathbf{L}(j,j)_c\}^N} \left(\frac{dz(j)d\bar{z}(j)}{\pi}\right)^{n(N-n)} \{1+O(k^{-1})\}, \tag{B38}$$

where use has been made of the definition of the measure (3.42) with (4.14). Therefore, in view of (B37) and (B38) the Gaussian integration of $\bar{z}(j), z(j)$ gives

$$\det\{\tilde{\mathbf{L}}^{-1}(j,j)_c \otimes (\mathbf{L}^{-1}(j,j)_c)^{\mathscr{T}}\}^{-1} = \{\det \mathbf{L}(j,j)_c\}^N, \tag{B39}$$

which, together with $(\pi/k)^{n(N-n)}$, cancels the prefactor in (B38), yielding the leading contribution to the WKB approximation:

$$\begin{aligned} K_k(\xi_F,\xi_I;T) &\overset{k\to\infty}{\sim} \frac{1}{[\det\{(1_n+\xi_F^\dagger\xi_F)(1_n+\xi_I^\dagger\xi_I)\}]^{k/2}} \exp\{k \ \mathrm{tr} \log \mathbf{L}(M,0)\} \\ &= \left[\frac{\det\{\alpha(T)+\xi_F^\dagger\gamma(T)+\beta(T)\xi_I+\xi_F^\dagger\delta(T)\xi_I\}}{\det\{(1_n+\xi_F^\dagger\xi_F)(1_n+\xi_I^\dagger\xi_I)\}^{1/2}}\right]^k. \end{aligned} \tag{B40}$$

The result is equal to the Feynman kernel (B12), (B20). Thus, *the WKB approximation is again exact for the Feynman kernel*. The fact can also be clarified in view of (B16) as well as (B17), since the integrand is Gaussian.

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Berry's phase on SU(n)/S(U(1)×U($n-1$)) manifolds

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It is shown that the Berry phase/matrix for Hamiltonians parametrized by the points of $M \equiv \mathrm{SU}(n)/\mathrm{S}(\mathrm{U}(1)\times\mathrm{U}(n-1))$ and having no accidental degeneracy is expressible in terms of Riemannian connection on M and representations of $\mathrm{S}(\mathrm{U}(1)\times\mathrm{U}(n-1))$. © *1996 American Institute of Physics.* [S0022-2488(95)01812-3]

I. INTRODUCTION

Berry's phase has appeared to be the most exciting recent discovery in the field of elementary quantum mechanics. It has found a wide range of applications as, for example, the Born–Oppenheimer treatment of molecular systems,[2] the quantum Hall effect,[3] gauge anomalies,[4] or light propagation in optical fibers.[5]

Much attention has also been paid to the mathematical structure of Berry's phase. It was quickly realized that Berry's phase, as well as its generalization to the case of degenerate levels[6]—the Berry matrix, is related to the geometry of some fiber bundles.[7–10] In particular, in Ref. 10 a general approach was proposed that is applicable in the case of Hamiltonians generated by the action of a unitary representation of some Lie group G. Within the approach proposed there the relation between Berry's phase/matrix and the geometry of homogeneous space G/H becomes transparent, and some general structural questions are easily addressed. For example, the general criteria can be given under which the Berry phase is determined by the Riemannian connection on G/H and the representation of H.

The present paper is devoted to the proof of the statement that for $G=\mathrm{SU}(n)$ and $H=\mathrm{S}(\mathrm{U}(1)\times\mathrm{U}(n-1))$ the Berry phase/matrix for any Hamiltonian with no degeneracy (to be defined below) is determined in this way. In Sec. II we outline the method developed in Ref. 10 and recall some basic facts concerning the geometry of homogeneous spaces. Then in Sec. III, we prove our basic statement. Our main tool in Gelfand–Tseytlin explicit construction of representations of U(n) groups.

II. GEOMETRY OF BERRY'S PHASE AND HOMOGENEOUS SPACES

We recall briefly the group-theoretical approach to Berry's phase developed in Ref. 10. Let $\{\Pi_n\}$ be any spectral decomposition of unity,

$$\Pi_n\Pi_m=\delta_{nm}\Pi_m, \quad \Pi_n^+=\Pi_n, \quad \sum_n \Pi_n=1. \tag{1}$$

Assume further that $G\ni g\mapsto U(g)$ is a unitary representation of compact semisimple Lie group G acting in the Hilbert space of states. Consider family of projectors defined by

$$\Pi_n(g)=U(g)\Pi_n U^+(g). \tag{2}$$

Let $H\subset G$ be subgroup of G consisting of all elements $g\in G$ such that $U(g)\Pi_n U^+(g)=\Pi_n$ for any n. Then the family $\{\Pi_n(g)\}$ is parametrized by the points $\zeta\in G/H$. Finally, let $\{E_n(\zeta)\}$ be a set of real-valued functions on G/H such that $E_n(\zeta)\neq E_m(\zeta)$, $n\neq m$; we define the family of Hamiltonians,

$$\mathscr{H}(\zeta)\equiv\sum_n E_n(\zeta)\Pi_n(\zeta). \tag{3}$$

Our task is to calculate the Berry phases/matrices for this family. The following answer to this problem is given in Ref. 10. Let (V,A) be the Lie algebra of G while (V)—that of H. The relevant commutation rules read as follows:

$$[V_i,V_j]=ic_{ij}^k V_k, \quad [V_i,A_\alpha]=ic_{i\alpha}^\beta A_\beta, \quad [A_\alpha,A_\beta]=ic_{\alpha\beta}^k V_k+ic_{\alpha\beta}^\gamma A_\gamma. \tag{4}$$

We always assume that basis (V,A) provides an orthogonal decomposition of Lie algebra with respect to the Cartan product,

$$\mathrm{Tr}(\mathrm{Ad}\ V_i\cdot \mathrm{Ad}\ A_\alpha)=0, \tag{5}$$

and we put

$$\mathrm{Tr}(\mathrm{Ad}\ V_i\cdot \mathrm{Ad}\ V_j)=\eta_{ij}, \quad \mathrm{Tr}(\mathrm{Ad}\ A_\alpha\cdot \mathrm{Ad}\ A_\beta)=\eta_{\alpha\beta}. \tag{6}$$

The Cartan forms are defined as follows:

$$U^+(\zeta)dU(\zeta)=i\,\eta_\mu^i\ d\zeta^\mu\cdot V_i+i\omega_\mu^\alpha\ d\zeta^\mu A_\alpha. \tag{7}$$

Finally, we denote

$$V_i^{(n)}\equiv\Pi_n V_i\Pi_n, \quad A_\alpha^{(n)}\equiv\Pi_n A_\alpha\Pi_n. \tag{8}$$

The main result of Ref. 10 is as follows. Given any closed curve $\gamma\subset G/H$, the corresponding Berry's matrix for the nth level is given by the parallel transport along γ defined by the connection

$$\frac{D}{dt}=\frac{\partial}{\partial t}+i\ \frac{d\zeta^\mu}{dt}\ (\omega_\mu^\alpha A_\alpha^{(n)}+\eta_\mu^k V_k^{(n)}). \tag{9}$$

This formula gives the group-theoretical description of Berry's aholonomy for the family of Hamiltonians defined by Eq. (3). One can now use the geometrical techniques to obtain more detailed information concerning Berry's phase/matrix.

Let us remind some basic facts concerning the geometry of homogeneous spaces. Putting

$$\omega^\alpha\equiv\omega_\mu^\alpha\ d\zeta^\mu, \quad \eta^i\equiv\eta_\mu^i\ d\zeta^\mu, \tag{10}$$

and taking the external derivative of both sides of Eq. (7), we arrive at the so-called Cartan–Maurer equations,

$$d\omega^\gamma=\tfrac{1}{2}c_{\alpha\beta}^\gamma\omega^\alpha\wedge\omega^\beta+c_{k\alpha}^\gamma\eta^k\wedge\omega^\alpha, \tag{10a}$$

$$d\eta^i=\tfrac{1}{2}c_{\alpha\beta}^i\omega^\alpha\wedge\omega^\beta+\tfrac{1}{2}c_{lk}^i\eta^l\wedge\eta^k. \tag{10b}$$

Note that $\omega_\mu^\alpha(\zeta)$ can be viewed as orthonormal repers; in particular,

$$g_{\mu\nu}(\zeta)\equiv\eta_{\alpha\beta}\omega_\mu^\alpha(\zeta)\omega_\nu^\beta(\zeta) \tag{11}$$

is an invariant metric on G/H. Let us define

$$\Omega_\beta^\alpha\equiv-\eta^i c_{i\beta}^\alpha, \tag{12a}$$

$$T_{\beta\gamma}^\alpha\equiv c_{\beta\gamma}^\alpha, \tag{12b}$$

$$R_{\beta\gamma\rho}^\alpha\equiv-c_{i\beta}^\alpha c_{\gamma\rho}^i. \tag{12c}$$

Equations (10) can be now written in the form

$$d\omega^{\alpha}+\Omega^{\alpha}_{\beta}\wedge\omega^{\beta}=\tfrac{1}{2}T^{\alpha}_{\beta\gamma}\omega^{\beta}\wedge\omega^{\gamma}, \tag{13a}$$

$$d\Omega^{\alpha}_{\beta}+\Omega^{\alpha}_{\rho}\wedge\Omega^{\rho}_{\beta}=\tfrac{1}{2}R^{\alpha}_{\beta\gamma\rho}\omega^{\gamma}\wedge\omega^{\beta}. \tag{13b}$$

Therefore, $T^{\alpha}_{\beta\gamma}$ and $R^{\alpha}_{\beta\gamma\rho}$ are torsion and curvature, respectively. In particular, if G/H is a symmetric space, $c^{\alpha}_{\beta\gamma}=0$, the torsion vanishes. Then Ω^{α}_{β} is the Riemannian connection on G/H. If G/H is homogeneous only, Ω^{α}_{β} differs from the Riemannian connection by a torsion term; in both cases the metric tensor (11) is covariantly constant. In the *nonsymmetric* case the Riemannian connection reads as

$$\Omega^{\alpha}_{R\beta}=-\eta^{i}c^{\alpha}_{i\beta}-\tfrac{1}{2}c^{\alpha}_{\gamma\beta}\omega^{\gamma}. \tag{14}$$

Indeed, $\Omega_{R\alpha\beta}$ is antisymmetric; moreover, it follows from Eq. (12a) that the corresponding torsion vanishes. The direct proof of Eq. (14) can be also obtained by calculating Christoffel symbols from the metric (11) and using the formula

$$\Omega^{\alpha}_{R\beta}=\omega^{\alpha}_{\nu}\Gamma^{\nu}_{\mu}\omega^{\mu}_{\beta}+\omega^{\alpha}_{\nu}\,d\omega^{\nu}_{\beta}. \tag{15}$$

In the above formula the first index of ω^{α}_{β} is raised (lowered) with the help of $\eta^{\alpha\beta}(\eta_{\alpha\beta})$ while the second one by $g^{\mu\nu}(\zeta)(g_{\mu\nu}(\zeta))$.

If G/H is symmetric space, the Riemannian connection can be viewed as a connection in a bundle associated with the principal bundle $P(G/H,H)$.

Let us pose the following question: *for which Hamiltonians (3) the Berry matrices for all levels n are expressible in terms of Riemannian connection on G/H and the representations of H*. It follows from Eq. (9) that one should then have

$$A^{(n)}_{\alpha}=0, \tag{16}$$

and, moreover, G/H should be symmetric space. All generators V_i have a block-diagonal form,

$$V_i=\sum_n V^{(n)}_i. \tag{17}$$

We assume that there is no accidental degeneracy, i.e., H is a maximal symmetry group of all Hamiltonians of the family under consideration. Then all eigenspaces carry irreducible representations of H. Our problem becomes now a purely group-theoretical one. Given group G and subgroup $H\subset G$ such that G/H is a symmetric space, find all irreducible representations of G such that Eq. (16) holds for all irreducible subspace (n) of subduced representation $G\downarrow H$.

It is not easy to solve this question in whole generality. Instead, in the next section we present some general example of such a situation.

III. BERRY'S AHOLONOMY FOR SU(n)/S(U(1)×U($n-1$)) SYSTEMS

Here we solve the problem posed in the last section for $G=\mathrm{SU}(n)$ and $H=\mathrm{S}(\mathrm{U}(1)\times\mathrm{U}(n-1))$.

The generators of SU(n) can be introduced as follows.[11] First, we define generators of GL($n,\mathbb{R}$),

$$(A_{ij})_{kl}=\delta_{il}\delta_{jk}, \tag{18}$$

verifying

$$[A_{ij},A_{kl}]=\delta_{jk}A_{il}-\delta_{il}A_{kj}. \tag{19}$$

Then we put

$$M_{kl}\equiv A_{kl}+A_{lk}, \quad \tilde{M}_{kl}\equiv i(A_{kl}-A_{lk}), \quad 1\leqslant k<l\leqslant n, \tag{20a}$$

$$M_{ll}\equiv A_{ll}-A_{l+1l+1}, \quad 1\leqslant l\leqslant n-2, \tag{20b}$$

$$M_{n-1n-1}\equiv \mathrm{diag}(1,\ldots,1,1-n). \tag{20c}$$

Then $H=\mathrm{S}(\mathrm{U}(1)\times\mathrm{U}(n-1))$ subgroup is generated by M_{kl}, $\tilde{M}_{kl}$, $1\leqslant k<l\leqslant n-1$ and M_{ll}, $l=1,\ldots,n-1$; the remaining ones (generating the cosets) are M_{kn}, $\tilde{M}_{kn}$, $k=1,\ldots,n-1$.

We are looking for the irreducible representations of SU(n) for which Eq. (16) holds. To this end we adopt the following strategy.[12] First, we note that any irreducible representation of SU(n) is obtained by subducing some irreducible representations of U(n). Indeed, it is sufficient to add to the set of generators (20) an additional one,

$$M_{nn}=I. \tag{21}$$

Then the operators M_{kl}, $\tilde{M}_{kl}$, $1\leqslant k<l\leqslant n-1$, M_{ll}, $l=1,\ldots,n-1$ span the Lie algebra of U(n) while M_{kl}, $\tilde{M}_{kl}$, $1\leqslant k<l\leqslant n-1$, M_{ll}, $1\leqslant l\leqslant n-2$ and

$$M\equiv\frac{1}{n}\,(M_{n-1n-1}+(n-1)M_{nn}), \tag{22}$$

span the Lie algebra of U($n-1$); the coset space is generated by $2n-1$ operators $M_{kn},\tilde{M}_{kn},M_{nn}$. In any irreducible representation M_{nn} is proportional to unit operator and poses no problems.

We have only to check for which representations of U(n) Eq. (16) holds for any irreducible representation of U($n-1$) and any operator M_{kn}, $\tilde{M}_{kn}$, $k=1,\ldots,n-1$. First, we note that

$$[M_{kl},M_{in}]=-i(\delta_{il}\tilde{M}_{kn}+\delta_{ik}\tilde{M}_{ln}), \tag{23a}$$

$$[\tilde{M}_{kl},\tilde{M}_{in}]=i(\delta_{il}\tilde{M}_{kn}-\delta_{ik}\tilde{M}_{ln}), \tag{23b}$$

$$[\tilde{M}_{kl},M_{in}]=i(\delta_{il}M_{kn}-\delta_{ik}M_{ln}). \tag{23c}$$

We see that the generators $\tilde{M}_{kl}$, $1\leqslant k<l\leqslant n-1$ span SO($n-1$) algebra and M_{in}, $\tilde{M}_{in}$, $i=1,\ldots,n-1$ form the vector representations of this algebra. Therefore, for any $l=1,\ldots,n-1$ there exist $g_l,\tilde{g}_l\in\mathrm{SO}(n-1)\subset\mathrm{S}(\mathrm{U}(1)\times\mathrm{U}(n-1))$, such that

$$M_{ln}=U(g_l)M_{n-1n}U^{+}(g_l), \quad \tilde{M}_{ln}=U(\tilde{g}_l)\tilde{M}_{n-1n}U^{+}(\tilde{g}_l). \tag{24}$$

But $U(g_l),U(\tilde{g}_l)$ leave invariant the irreducible subspaces of $\mathrm{S}(\mathrm{U}(1)\times\mathrm{U}(n-1))$. Therefore it is sufficient to check the validity of Eq. (16) for M_{n-1n} and $\tilde{M}_{n-1n}$ only. To this end we use the Gelfand–Tseytlin method.[11] Consider the chain of subalgebras,

$$u(n)\supset u(n-1)\supset\cdots\supset u(1). \tag{25}$$

It is well known that any irreducible representation of $u(k)$, when subduced to $u(n-1)$, contains a given irreducible representation of $u(k-1)$, at most, once; moreover, irreducible representations of $u(1)$ are one dimensional. Therefore we can enumerate the basis vector of a given representation of $u(n)$ by indicating to which representation of $u(k),k=1,\ldots,n-1$, it belongs. This is the essence of the Gelfand–Tseytlin scheme.

Now, M_{n-1n} and $\tilde{M}_{n-1n}$ commute with all $u(k),k=1,\ldots,n-2$. Therefore, in a Gelfand–Tseytlin basis, their nonvanishing matrix elements are either diagonal or correspond to the vectors

belonging to different irreducible representation of $u(n-1)$. So, we have to check Eq. (16) for diagonal elements M_{n-1n} and $\tilde{M}_{n-1n}$, or, equivalently, of A_{n-1n} and A_{nn-1}. However, it follows from general Gelfand–Tseytlin formulas[11] that the diagonal matrix element of $A_{n-1,n}$ and $A_{n,n-1}$ vanish for all irreducible representations of U(n).

We conclude that for any n and any irreducible representation of SU(n), the Hamiltonians generated by SU(n), parametrized by the points of coset space SU(n)/S(U(1)×U($n-1$)) and exhibiting no accidental degeneracy give rise to Berry's phases/matrices expressible in terms of Riemannian connection on SU(n)/S(U(1)×U($n-1$)) and the representations of S(U(1)×U($n-1$)).

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Quantization of the multifold Kepler system

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For over a century, the Kepler problem and the harmonic oscillator have been known as the only central force dynamical systems, all of whose bounded motions are periodic. Two of the authors (T. I. and N. K.) have found an infinite number of dynamical systems possessing such a periodicity property, which have been called multi-fold Kepler systems or ν-fold Kepler systems, with ν a positive rational number. If ν is allowed to take the real positive numbers, say $\nu=\alpha$, then for the α-fold Kepler system, all the bounded motions become periodic or not, according to whether the parameter α is a rational number or not. A purpose of this paper is to quantize the α-fold Kepler system and thereby to figure out a quantum analog of the closed orbit property of the α-fold Kepler system. It will turn out that the quantized α-fold Kepler system admits accidental degeneracy in energy levels or not, according to whether α is a rational number or not. © *1996 American Institute of Physics.* [S0022-2488(96)00902-1]

I. INTRODUCTION

For many years, the Taub–NUT metric on $\mathbf{R}^4-\{0\}$ has been investigated from various points of view. For instance, the motion of well-separated two monopoles can be described approximately by the geodesic motion associated with the Taub–NUT (Taub–Newman–Unti–Tambrino) metric.[1–5] It is also known, from a symmetry point of view, that the geodesic motion of this metric admits a Kepler-type symmetry when the geodesic flow system is reduced to a three-degrees-of-freedom system.[5–8]

In previous papers,[9–11] Iwai and Katayama have generalized the Taub–NUT metric so that the associated reduced system may admit a Kepler-type symmetry. In a continuation of those papers,[12] they have made further generalization of the Taub–NUT metric, which is described as follows: Let (x_j) be the Cartesian coordinates in $\dot{\mathbf{R}}^4:=\mathbf{R}^4-\{0\}$. The generalized Taub–NUT metric is expressed as

$$ds_G^2=4rf(r)\sum_{j=1}^{4}dx_j^2+4\left(\frac{g(r)}{r^2}-f(r)\right)(-x_2\,dx_1+x_1\,dx_2-x_4\,dx_3+x_3\,dx_4)^2, \tag{1.1}$$

with $f(r)$ and $g(r)$ given, respectively, by

$$f(r)=r^{1/\alpha-2}(a_0+a_1r^{1/\alpha}) \quad \text{and} \quad g(r)=\frac{r^{1/\alpha}(a_0+a_1r^{1/\alpha})}{1+a_2r^{1/\alpha}+a_3r^{2/\alpha}}, \tag{1.2}$$

where r is the squared radius,

$$r=\sum_{j=1}^{4}x_j^2,$$

and the parameter α is a positive real number and a_j's real constants.

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The reduced system from the geodesic flow system associated with this metric has a remarkable periodicity property. Consider the cotangent bundle $T^*\dot{\mathbf{R}}^4$ of $\dot{\mathbf{R}}^4$ with the standard symplectic form $d\theta=\Sigma_{j=1}^4 dy_j\wedge dx_j$, (x_j,y_j) being the Cartesian coordinates in $\dot{\mathbf{R}}^4\times\mathbf{R}^4\simeq T^*\dot{\mathbf{R}}^4$. Then the geodesic flow system is described as a Hamiltonian system on the phase space $(T^*\dot{\mathbf{R}}^4,d\theta)$ along with a certain Hamiltonian function H containing $f(r)$ and $g(r)$. Owing to a $U(1)$ symmetry, the Hamiltonian system $(T^*\dot{\mathbf{R}}^4,d\theta,H)$ can be reduced to a Hamiltonian system $(T^*\dot{\mathbf{R}}^3,\omega_\mu,H_\mu)$, where $T^*\dot{\mathbf{R}}^3\simeq\dot{\mathbf{R}}^3\times\mathbf{R}^3$ denotes the cotangent bundle of $\dot{\mathbf{R}}^3:=\mathbf{R}^3-\{0\}$, ω_μ is the reduced symplectic form composed of the canonical one plus the two-form describing Dirac's monopole field of strength $-\mu$, $\mu\in\mathbf{R}$, and H_μ is a reduced Hamiltonian, which also depends on $f(r)$ and $g(r)$. See Refs. 12, 13, or 14 for the reduction procedure, for example. For $f(r)$ and $g(r)$ given by (1.2), the reduced Hamiltonian system $(T^*\dot{\mathbf{R}}^3,\omega_\mu,H_\mu)$ has a remarkable periodicity property; according as the parameter α in H_μ is a rational number or not, all the bounded motions become periodic or not. In this paper, this Hamiltonian system will be referred to as the "α-fold Kepler system," whichever number the α takes, rational or irrational.

The aim of this paper is to develop a quantum theory for the α-fold Kepler system. Like in the classical case, a significant feature will be found out for the quantized α-fold Kepler system: According to whether the α is rational or not, accidental degeneracies in the energy levels arise or not.

The contents of this paper are outlined as follows: Section II contains a setting up of the classical α-fold Kepler system, which is defined to be a Hamiltonian system reduced from the geodesic flow system for the generalized Taub–NUT metric ds_G^2 through the reduction by a $U(1)$ action. It is remarked that the α-fold Kepler system covers a class of dynamical systems of interest.

In Sec. III, the geodesic flow system for ds_G^2 is quantized, through the Schrödinger procedure, since the classical Hamiltonian can be expressed in the Cartesian coordinates, and since no problem of noncommutativity of operators arises. It is to be noted that the Hamiltonian operator obtained, $\hat{H}$, is not equal to $-\frac{1}{2}$ times the Laplace–Beltrami operator for ds_G^2. This definition of $\hat{H}$ seems to contradict the ordinary principle that the Hamiltonian operator to be associated with the metric is the Laplace–Beltrami operator. For example, in Refs. 5–7, the Laplace–Beltrami operator associated with the Taub–NUT metric was used as a Hamiltonian operator. This discrepancy will be cleared out in Sec. VI. Note also that the Hilbert space in which $\hat{H}$ is to be defined densely is taken to be $L^2(\mathbf{R}^4;4rf(r)dx)$, the space of square-integrable functions on $\mathbf{R}^4$ with respect to the volume form $4rf(r)dx_1\cdots dx_4$. To avoid excessive singularity, we assume that $f(r)>0$ for $r>0$ in the following. The eigenvalue problem of $\hat{H}$ is solved for bound states. It is shown further that the energy eigenvalues for $\hat{H}$ become equal to those obtained already in Refs. 5–7, when ds_G^2 is restricted to the Taub–NUT metric.

In Sec. IV, the quantized α-fold Kepler system is defined to be the reduced system of the quantized geodesic flow system defined in Sec. III. A key to the reduction procedure is the fact that the configuration space $\dot{\mathbf{R}}^4$ is made into a principal U(1) bundle $\pi:\dot{\mathbf{R}}^4\to\dot{\mathbf{R}}^3$. Then the geometric setting for the reduction is to form the complex line bundle L_m, $m\in\mathbf{Z}$, associated with the principal bundle $\pi:\dot{\mathbf{R}}^4\to\dot{\mathbf{R}}^3$. The restriction of $L^2(\mathbf{R}^4;4rf(r)dx)$ to the ρ_m-equivariant functions[15,16] gives rise to the Hilbert space of square integrable cross sections in L_m, denoted by Γ_m. According to this reduction procedure, the quantized α-fold Kepler system is to be defined in Γ_m, with the Hamiltonian operator $\hat{H}_m$ reduced from the $\hat{H}$, which contains the covariant derivation operator with respect to the linear connection on L_m. The eigenvalue problem of $\hat{H}_m$ is studied accordingly. On account of the reduction procedure, the eigenvalues of $\hat{H}_m$ come from those of $\hat{H}$.

In Sec. V, degeneracy in energy levels for $\hat{H}_m$ is discussed. Owing to the spherical symmetry, the quantized α-fold Kepler system admits an SU(2) symmetry, which causes degeneracy in the energy levels of $\hat{H}_m$. In addition, it will be shown that additional "accidental" degeneracy occurs

or not, according to whether α is a rational number or not. This can be thought of as a quantum analog to the periodicity property of the classical α-fold Kepler system.

Section VI contains the comparison of the operator $\hat{H}$ with the Laplace–Beltrami operator Δ for the generalized Taub–NUT metric ds_G^2. A necessary and sufficient condition for $\hat{H}=-(1/2)\Delta$ will be given.

II. A REVIEW OF THE MULTIFOLD KEPLER SYSTEM

In this section, we make a brief review of the multifold Kepler system. To define the multifold Kepler system on $T^*\dot{\mathbf{R}}^3$ with $\dot{\mathbf{R}}^3=\mathbf{R}^3-\{0\}$, we start with a U(1) reduction of the phase space $(T^*\dot{\mathbf{R}}^4, d\theta)$, where $\dot{\mathbf{R}}^4=\mathbf{R}^4-\{0\}$, and $d\theta$ is the standard symplectic two-form that is expressed as $d\theta=\Sigma_{i=1}^4\, dy_i\wedge dx_i$ in the Cartesian coordinates $(x,y)\in\dot{\mathbf{R}}^4\times\mathbf{R}^4\simeq T^*\dot{\mathbf{R}}^4$. The symplectic SO(2) $\simeq$U(1) action, denoted by S_t, is defined to be

$$S_t:(x,y)\mapsto(T(t)x,T(t)y), \tag{2.1}$$

with

$$T(t)=\begin{pmatrix} R(t) & 0 \\ 0 & R(t)\end{pmatrix},\quad R(t)=\begin{pmatrix} \cos t/2 & -\sin t/2 \\ \sin t/2 & \cos t/2\end{pmatrix}. \tag{2.2}$$

The moment map J associated with S_t takes the form

$$J(x,y)=\tfrac{1}{2}(-x_2y_1+x_1y_2-x_4y_3+x_3y_4). \tag{2.3}$$

According to the Weinstein–Marsden reduction method,[17] the reduced phase space is defined to be the quotient space $J^{-1}(\mu)/\mathrm{U}(1)$ for a fixed $\mu\in\mathbf{R}$, which turns out to be realized as the cotangent bundle $T^*\dot{\mathbf{R}}^3$ of $\dot{\mathbf{R}}^3$ as follows:[13,14] We define a map of $\dot{\mathbf{R}}^4\times\mathbf{R}^4$ to $\dot{\mathbf{R}}^3\times\mathbf{R}^3$ by

$$\Pi(x,y):=\left(P(x)x,\frac{1}{2r}\,P(x)y\right), \tag{2.4a}$$

where

$$P(x)=\begin{pmatrix} x_3 & x_4 & x_1 & x_2 \\ -x_4 & x_3 & x_2 & -x_1 \\ x_1 & x_2 & -x_3 & -x_4\end{pmatrix},\quad r:=\sum_{j=1}^4 x_j^2. \tag{2.4b}$$

The mapping (2.4a) is also known as the Kustaanheimo–Stiefel transformation.[18] Then the restriction of Π to $J^{-1}(\mu)\subset T^*\dot{\mathbf{R}}^4$, denoted by π_μ, gives rise to the projection

$$\pi_\mu:J^{-1}(\mu)\to T^*\dot{\mathbf{R}}^3\simeq J^{-1}(\mu)/\mathrm{U}(1), \tag{2.5}$$

which proves our assertion. We denote the Cartesian coordinates in the reduced phase space $\dot{\mathbf{R}}^3\times\mathbf{R}^3$ by (q,p); $\Pi(x,y)=(q,p)$ with $(x,y)\in J^{-1}(\mu)$. We reduce the symplectic form $d\theta$ in turn. On letting $\iota_\mu:J^{-1}(\mu)\to T^*\dot{\mathbf{R}}^4$ be the inclusion map, the reduced symplectic form ω_μ on the reduced phase space is determined through $\pi_\mu^*\omega_\mu=\iota_\mu^*\, d\theta$, which turns out to take the form

$$\omega_\mu=\sum_{k=1}^3 dp_k\wedge dq_k-\frac{\mu}{r^3}\,(q_1\, dq_2\wedge dq_3+\text{cyclic}). \tag{2.6}$$

The second term of the right-hand side of (2.6) corresponds to the magnetic flux of Dirac's monopole field $\mathbf{B}=-\mu\mathbf{q}/r^3$.

Let H be a Hamiltonian function on $T^*\dot{\mathbf{R}}^4$. If it is $U(1)$ invariant, it can be reduced, through $H\circ\iota_\mu = H_\mu\circ\pi_\mu$, to a Hamiltonian function H_μ on $T^*\dot{\mathbf{R}}^3$. In what follows, we are to reduce the Hamiltonian system describing the geodesic flows for the generalized Taub–NUT metrics ds_G^2 given by (1.1) and (1.2). The Hamiltonian function H associated with ds_G^2 is given by

$$H=\frac{1}{2}\cdot\frac{1}{4rf(r)}\left[\sum_{j=1}^{4}y_j^2+\left(\frac{rf(r)}{g(r)}-\frac{1}{r}\right)(-x_2y_1+x_1y_2-x_4y_3+x_3y_4)^2\right]. \tag{2.7}$$

Throughout this paper, to get rid of excessive singularities of H, we assume that $a_0\geqslant 0$ and $a_1>$, so that $f(r)>0$ for $r>0$. Note again that the α is a positive number, and a_j's real constants. Since the H is invariant under the U(1) action (2.1), it proves to be reduced to the Hamiltonian function

$$H_\mu=\frac{1}{2f(r)}\sum_{k=1}^{3}p_k^2+\frac{\mu^2}{2g(r)}\quad\left(r^2=\sum_{k=1}^{3}q_k^2\right). \tag{2.8}$$

Note that the reduction procedure works for arbitrary functions $f(r)$ and $g(r)$. In a summary, we have the following.[12]

Proposition 2.1: The Hamiltonian system $(T^*\dot{\mathbf{R}}^4,d\theta,H)$ *describing the geodesic flows for the generalized Taub–NUT metric* ds_G^2 *is reduced by the* U(1) *action to the Hamiltonian system* $(T^*\dot{\mathbf{R}}^3,\omega_\mu,H_\mu)$, $\mu\in\mathbf{R}$, *which is called the* α*-fold Kepler system.*

The α-fold Kepler system has a significant property in their bounded trajectories.[12]

Theorem 2.2: *For the* α*-fold Kepler system* $(T^*\dot{\mathbf{R}}^3,\omega_\mu,H_\mu)$, *all the bounded trajectories are closed if and only if the parameter* α *in the Hamiltonian function (2.8) with (1.2) is a rational number.*

In closing this section, we make a few remarks. When the parameters in $f(r)$ and $g(r)$ are set to be

$$a_0=4c,\quad a_1=1,\quad a_2=\frac{1}{2c},\quad a_3=\frac{1}{16c^2},\quad\text{and}\quad\alpha=1, \tag{2.9}$$

the metric ds_G^2 becomes the Taub–NUT metric, where c is a constant. Further, if we set the parameters to be

$$a_0=a_3=0,\quad a_1=1,\quad a_2=-\frac{2\kappa}{\mu^2}\ (\kappa>0,\text{const}),\quad\text{and}\quad\alpha=1, \tag{2.10}$$

the reduced Hamiltonian (2.8) becomes that for the MIC (McIntosch–Cisneros)–Kepler problem. For the MIC–Kepler problem, see a series of papers.[13,15,19,20] Further, in the case of

$$a_0=a_3=0,\quad a_1=\frac{1}{4},\quad a_2=-\frac{\kappa}{2\mu^2},\quad\text{and}\quad\alpha=2, \tag{2.11}$$

the reduced system becomes the two-fold Kepler system studied in Ref. 11, which is the Hamiltonian system reduced from the four-dimensional Kepler problem on $(T^*\dot{\mathbf{R}}^4,d\theta)$.

III. THE QUANTUM SYSTEM ASSOCIATED WITH THE GEODESIC FLOW SYSTEM FOR ds_G^2

A. Quantization of the geodesic flow system

We wish to quantize the geodesic flow system $(T^*\dot{\mathbf{R}}^4,d\theta,H)$, with H given by (2.7). Since H is expressed in the Cartesian coordinates, and since no problem of noncommutativity of operators

occurs, we choose to adopt the Schrödinger procedure in order to associate a Hamiltonian operator with H. According to that procedure, y_j are replaced by $-i\partial/\partial x_j$, so that Eq. (2.7) gives rise to

$$\hat{H}=-\frac{1}{2}\cdot\frac{1}{4rf(r)}\left[\sum_{j=1}^{4}\frac{\partial^2}{\partial {x_j}^2}+\left(\frac{rf(r)}{g(r)}-\frac{1}{r}\right)\left(-x_2\frac{\partial}{\partial x_1}+x_1\frac{\partial}{\partial x_2}-x_4\frac{\partial}{\partial x_3}+x_3\frac{\partial}{\partial x_4}\right)^2\right]. \tag{3.1}$$

As a Hamiltonian operator, we could have chosen $-\frac{1}{2}$ times the Laplace–Beltrami operator associated with ds_G^2, following the usual principle. However, we dared to adopt the operator (3.1). We postpone the comparison of these two quantization procedures to Sec. VI. Instead of the comparison, here we claim that our procedure is based upon the consideration of energy manifolds of the classical system. Let us define a function K_λ to be

$$K_\lambda=4rf(r)(H-\lambda), \tag{3.2}$$

where λ is a constant. Then, the energy manifolds $H^{-1}(E)$ and $K_\lambda^{-1}(0)$ with $E=\lambda$ are identical in $T^*\dot{\mathbf{R}}^4$. Further, the Hamiltonian flows generated by H and by K_E coincide up to "time" parameters. In fact, a straightforward calculation shows that $X_{K_\lambda}=4rf(r)X_H$ on the energy manifold mentioned above. We are to quantize H on the hope that quantum analogy of (3.2) holds. That is, we assume that if Hamiltonian operators $\hat{H}$ and $\hat{K}_\lambda$ are defined suitably, they will possibly satisfy

$$\hat{K}_\lambda=4rf(r)(\hat{H}-\lambda). \tag{3.3}$$

This equation implies that eigenfunctions for $\hat{K}_E=0$ become those for $\hat{H}=E$, and vice versa. The quantization of K_λ is easy to make, since K_λ takes the simple form

$$K_\lambda=\frac{1}{2}\left[\sum_{j=1}^{4}y_j^2+\left(\frac{rf(r)}{g(r)}-\frac{1}{r}\right)(-x_2y_1+x_1y_2-x_4y_3+x_3y_4)^2\right]-4\lambda rf(r), \tag{3.4}$$

to which the Schrödinger procedure is easy to apply. Hence, the Hamiltonian operator $\hat{H}$ is expressed as in (3.1) on account of (3.3).

We have to describe what Hilbert space is suitable for $\hat{H}$. We wish to define a Hilbert space so that $\hat{H}$ may be at least a symmetric operator in it. To this end, we consider the space of square integrable functions on $\mathbf{R}^4$ with respect to the volume element $4rf(r)dx=4rf(r)dx_1\cdots dx_4$, which is denoted by $L^2(\mathbf{R}^4;4rf(r)dx)$. Incidentally, it is well known that $C_0^\infty(\mathbf{R}^4)$, the space of smooth functions on $\mathbf{R}^4$ with compact support, is dense in $L^2(\mathbf{R}^4)$, the usual L^2 space. Moreover, the space $C_0^\infty(\mathbf{R}^4)$ remains to be dense in $L^2(\mathbf{R}^4;4rf(r)dx)$, as is easily shown. Now, for any ϕ, $\psi\in C_0^\infty(\mathbf{R}^4)$, integration by parts shows that

$$\int_{\mathbf{R}^4}\overline{(\hat{H}\phi)(x)}\psi(x)4rf(r)dx=\int_{\mathbf{R}^4}\overline{\phi(x)}(\hat{H}\psi)(x)4rf(r)dx. \tag{3.5}$$

Thus, the Hamiltonian operator $\hat{H}$ is a symmetric operator in $L^2(\mathbf{R}^4;4rf(r)dx)$. Summarizing the above, we come to the following definition.

Definition 3.1: The quantized system associated with the geodesic flow system for the generalized Taub–NUT metric ds_G^2 is defined as the pair $(L^2(\mathbf{R}^4;4rf(r)dx),\hat{H})$, where $\hat{H}$ is given by (3.1).

Before going to the eigenvalue problem of $\hat{H}$, we have to make a remark on $\hat{H}$. As was remarked in Sec. II, if the parameters are set as in (2.9), the generalized Taub–NUT metric ds_G^2 becomes the usual Taub–NUT metric. Correspondingly, the Hamiltonian operator $\hat{H}$ becomes

identical with $-\frac{1}{2}$ times the Laplace–Beltrami operator for the Taub–NUT metric, which was studied in Refs. 5–7. However, as will be shown in Sec. VI, the $\hat{H}$ is not equal to $-\frac{1}{2}$ times the Laplace–Beltrami operator for ds_G^2 in general.

B. The eigenvalue problem of $\hat{H}$

We are to solve the eigenvalue problem of $\hat{H}$ for the bound states. To this end, it is convenient to introduce curvilinear coordinates in $\dot{\mathbf{R}}^4$ as follows:

$$\begin{aligned} x_1 &= \sqrt{r}\,\cos\frac{\theta}{2}\cos\frac{\psi+\phi}{2}, \quad x_2 = \sqrt{r}\,\cos\frac{\theta}{2}\sin\frac{\psi+\phi}{2}, \\ x_3 &= \sqrt{r}\,\sin\frac{\theta}{2}\cos\frac{\psi-\phi}{2}, \quad x_4 = \sqrt{r}\,\sin\frac{\theta}{2}\sin\frac{\psi-\phi}{2}, \end{aligned} \tag{3.6}$$

where $r>0$, $0\leqslant\theta\leqslant\pi$, and $0\leqslant\psi-\phi$, $\psi+\phi\leqslant 4\pi$. In terms of (r,θ,ϕ,ψ), the operator $\hat{H}$ is written as

$$\hat{H} = -\frac{1}{2f(r)}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{1}{4r^2}\Delta_3+\left(\frac{f(r)}{g(r)}-\frac{1}{r^2}\right)\left(\frac{\partial}{\partial\psi}\right)^2\right], \tag{3.7}$$

where Δ_3 is the Laplace–Beltrami operator on the three-dimensional unit sphere S^3 with the canonical metric;

$$\Delta_3 = 4\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\left(\frac{\partial^2}{\partial\phi^2}-2\cos\theta\frac{\partial^2}{\partial\phi\,\partial\psi}+\frac{\partial^2}{\partial\psi^2}\right)\right]. \tag{3.8}$$

Let us take an ansatz $R(r)Q(\theta,\phi,\psi)$ as an eigenfunction of $\hat{H}$, after the method of a separation of variables. We may assume that the angular part $Q(\theta,\phi,\psi)$ is an eigenfunction of the Δ_3, which is expanded into a series of Wigner's $\mathscr{D}$ functions $\{\mathscr{D}^J_{ML}(\psi,\theta,\phi)\}$, a complete orthogonal basis of $L^2(S^3)$. In this paper, we follow Edmonds' definition;[21]

$$\mathscr{D}^J_{ML}(\psi,\theta,\phi) = \exp(iM\psi)\exp(iL\phi)d^J_{ML}(\theta), \tag{3.9a}$$

with

$$d^J_{ML}(\theta) = \left[\frac{(J+M)!(J-M)!}{(J+L)!(J-L)!}\right]^{1/2}\left(\cos\frac{\theta}{2}\right)^{M+L}\left(\sin\frac{\theta}{2}\right)^{M-L}P^{(M-L,M+L)}_{J-M}(\cos\theta), \tag{3.9b}$$

where $P^{(M-L,M+L)}_{J-M}$'s denote the Jacobi polynomials.[21] The suffices J, L, and M of $\mathscr{D}^J_{ML}$ are subject to

$$J\text{:non-negative half-integer}, \quad L,M = J,J-1,\cdots-J+1,-J. \tag{3.10}$$

Since every $\mathscr{D}$ function is an eigenfunction for Δ_3,

$$\Delta_3\mathscr{D}^J_{ML} = -4J(J+1)\mathscr{D}^J_{ML}, \tag{3.11}$$

our ansatz can take a more specified form, $R(r)\mathscr{D}^J_{ML}(\psi,\theta,\phi)$. We note here that $\mathscr{D}^J_{ML}$ is simultaneously an eigenfunction of $-i\partial/\partial\psi$;

$$\frac{\partial}{\partial\psi}\mathscr{D}^J_{ML} = iM\mathscr{D}^J_{ML}. \tag{3.12}$$

Then, further calculation shows that the radial part $R(r)$ must satisfy

$$\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)-\frac{J(J+1)}{r^2}+\frac{1}{r^2}\,(c_0 r^{1/\alpha}+c_1 r^{2/\alpha})\right]R(r)=0, \tag{3.13a}$$

with

$$c_0=2Ea_0-M^2a_2, \quad c_1=2Ea_1-M^2a_3, \tag{3.13b}$$

where J, M, and L are subject to (3.10). The energy eigenvalues and the eigenfunctions are hence obtained by solving (3.13) under the boundary condition

$$\int_0^\infty |R(r)|^2 2r^2 f(r)dr<+\infty, \tag{3.14}$$

since $R(r)Q(\theta,\phi,\psi)\in L^2(\mathbf{R}^4,4rf(r)dx)$. The calculation of eigenfunctions and eigenvalues is given in the Appendix.

From the Appendix, we see that the eigenvalues depend on a number n defined, for a non-negative integer N, by

$$n=N+\tfrac{1}{2}+\alpha(J+\tfrac{1}{2}). \tag{3.15}$$

We express Eqs. (A14a) and (A14b) as

$$E^+_{J,N;M}=\frac{1}{2a_0^2}\left(a_0a_2M^2-2a_1\left(\frac{n}{\alpha}\right)^2+2\frac{n}{\alpha}\sqrt{\left(\frac{n}{\alpha}\right)^2a_1^2+a_0(a_0a_3-a_1a_2)M^2}\right), \tag{3.16a}$$

for $a_0\neq 0$, and as

$$E^0_{J,N;M}=\frac{a_3M^2}{2a_1}-\frac{\alpha^2a_2^2M^4}{8a_1n^2}, \tag{3.16b}$$

for $a_0=0$, respectively. Further, we set

$$\epsilon=\alpha\sqrt{a_3M^2-2a_1E^\sigma_{J,N;M}} \quad (\sigma=+,0). \tag{3.17}$$

Then from (A12), we find that Eq. (3.13) is satisfied by the function

$$R^\sigma_{J,N;M}(r)=\exp(-\epsilon r^{1/\alpha})r^JF(-N,\alpha(2J+1)+1,2\epsilon r^{1/\alpha}), \tag{3.18}$$

where F denotes the confluent hypergeometric function.

We are now in a position to give solutions to the eigenvalue problem (3.13) with (3.14).

Theorem 3.2: *The eigenvalues of $\hat{H}$ for the bound states are given by (3.16a) or (3.16b), according to whether the constants a_j, $j=0,\ldots,3$, are subject to the condition*

$$(P)\quad a_0>0, \quad a_1\geqslant 0, \quad \text{and } (a_0a_3-a_1a_2)M^2\neq 0, \tag{3.19}$$

or

$$(Z)\quad a_0=0, \quad a_1>0 \quad \text{and } M\neq 0.$$

The suffixes J and M are subject to (3.10), and N to $N=0,1,2,\ldots$. If the constants a_j, $j=0,1,2,3$, are not subject to the conditions listed in (3.19), no bound states for $\hat{H}$ exist under the assumption that $f(r)>0$ for $r>0$.

It is to be noted that the conditions $(a_0a_3-a_1a_2)M^2\neq 0$ and $M\neq 0$ in (3.19) are necessary for $\epsilon>0$.

Theorem 3.3: *The* $2J+1$ *linearly independent eigenfunctions,*

$$\Psi^{\sigma}_{L,J,N;M}(r,\theta,\phi,\psi)=R^{\sigma}_{J,N;M}(r)\mathscr{D}^{J}_{ML}(\psi,\theta,\phi) \quad (L=J,J-1,\ldots,-J), \tag{3.20}$$

are associated with the eigenvalue $E^{\sigma}_{J,N;M}$ *of* $\hat{H}$*, where the suffixes J and M are subject to (3.10), and N to* $N=0,1,2,\ldots$ *. The* σ *is chosen to be* $\sigma=+$ *in the case of* (P)*, and* $\sigma=0$ *in the case of* (Z)*.*

In particular, in the case of the Taub–NUT metric, the constants a_j, $j=0,\ldots,3$, are chosen as in (2.9), so that the eigenvalues (3.16a) become

$$E^{+}_{J,N;M}=\frac{1}{(4c)^2}\,(M^2-n^2+n\sqrt{n^2-M^2}) \quad (n=N+J+1), \tag{3.21}$$

which are equal to those already known.[5–7] The same energy eigenvalues are obtained by other methods, say, by the path integral method, *et al.*,[22–25] in relation to the Kaluza–Klein monopole system in five dimensions.[26,27] We have to note here that $\alpha=1$ for the Taub–NUT metric. What the condition of $\alpha=1$ means will be investigated in the last section. Moreover, if the constants a_j take the values given in (2.10), the eigenvalues (3.16b) become $E^{0}_{J,N;M}=-\kappa^2/2(N+J+1)^2=-2\kappa^2/(n'+2)^2$ with $n'=2N+2J$ a non-negative integer, which are already known as energy eigenvalues for the quantized MIC–Kepler problem.[15]

In closing this section, we have to make a remark on the differential equation (3.13a). This equation can be regarded as the radial Schrödinger equation for the potential

$$V(r)=-\tfrac{1}{2}c_0r^{1/\alpha-2}-\tfrac{1}{2}c_1r^{2/\alpha-2}, \tag{3.22}$$

along with the zero energy, where $c_0>0$ and $c_1<0$ are constants. From this point of view, Khare *et al.*[28–30] investigated Eq. (3.13a).

IV. THE QUANTIZED α-FOLD KEPLER SYSTEM

A. The quantization of the α-fold Kepler system

In this section, we reduce the quantum system $(L^2(\mathbf{R}^4;4rf(r)dx),\hat{H})$ in order to define the quantized α-fold Kepler system on the analogy to the reduction procedure for defining the classical α-fold Kepler system. The geometric setting of the reduction procedure has been established in Iwai and Uwano,[15] which is reviewed as follows.

A point to make is to observe that the configuration space $\dot{\mathbf{R}}^4$ is made into a principal U(1) bundle; $\pi:\dot{\mathbf{R}}^4\to\dot{\mathbf{R}}^3$. The $\mathrm{U}(1)\simeq\mathrm{SO}(2)$ action on $\dot{\mathbf{R}}^4$ is defined by

$$x\mapsto T(t)x \quad (x\in\dot{\mathbf{R}}^4), \tag{4.1}$$

where $T(t)$ is given by (2.2). The projection π is realized as

$$\pi(x)=P(x)x \quad (x\in\dot{\mathbf{R}}^4), \tag{4.2}$$

where $P(x)$ is the matrix defined by (2.4b).

Let ρ_m, $m\in\mathbf{Z}$, denote a unitary irreducible representation of $\mathrm{U}(1)\simeq\mathrm{SO}(2)$ on $\mathbf{C}$;

$$\rho_m(T(t)):\zeta\mapsto\exp(imt/2)\zeta \quad (\zeta\in\mathbf{C}). \tag{4.3}$$

Then, the U(1) action on the product space $\dot{\mathbf{R}}^4\times\mathbf{C}$,

$$(x,\zeta)\mapsto(T(t)x,\exp(imt/2)\zeta) \quad (x\in\dot{\mathbf{R}}^4,\zeta\in\mathbf{C}), \tag{4.4}$$

gives rise to the quotient manifold denoted by $\dot{\mathbf{R}}^4\times_m\mathbf{C}$, which is made into a complex line bundle $L_m=(\dot{\mathbf{R}}^4\times_m\mathbf{C},\pi_m,\dot{\mathbf{R}}^3)$. Here, the π_m is the projection, $\pi_m:\dot{\mathbf{R}}^4\times_m\mathbf{C}\to\dot{\mathbf{R}}^3$. The L_m is called the complex line bundle associated with the U(1) bundle $\pi:\dot{\mathbf{R}}^4\to\dot{\mathbf{R}}^3$.[15,16] Denoting by pr the natural projection of $\dot{\mathbf{R}}^4\times\mathbf{C}$ to $\dot{\mathbf{R}}^4\times_m\mathbf{C}$, one has the commutative diagram
rw

$$\begin{array}{ccc} \dot{\mathbf{R}}^4\times C & \xrightarrow{\quad pr\quad} & \dot{\mathbf{R}}^4\times_m C \\ {\scriptstyle p_1}\downarrow & & {\scriptstyle \pi_m}\downarrow \\ \dot{\mathbf{R}}^4 & \xrightarrow{\quad \pi\quad} & \dot{\mathbf{R}}^3 \end{array}, \tag{4.5}$$

where p_1 is the projection onto the first factor.

A complex-valued function F on $\dot{\mathbf{R}}^4$ is called ρ_m equivariant, if it satisfies

$$F(T(t)x)=\exp(imt/2)F(x). \tag{4.6}$$

It is well known that ρ_m-equivariant functions on $\dot{\mathbf{R}}^4$ are in one-to-one correspondence with cross sections in L_m.[15,16] We denote by q_m the correspondence; to a ρ_m-equivariant function F, there corresponds a cross section γ in L_m,

$$(q_mF)(q)=\gamma(q)\quad(q\in\dot{\mathbf{R}}^3). \tag{4.7}$$

On the basis of (4.7), we are to reduce the Hilbert space $L^2(\mathbf{R}^4;4rf(r)dx)$ to a Hilbert space of cross sections in L_m. Let γ's be cross sections in L_m such that $q_m^{-1}\gamma$'s are in $L^2(\mathbf{R}^4;4rf(r)dx)$. Then, the inner product in $L^2(\mathbf{R}^4;4rf(r)dx)$ gives rise to the inner product in the space of cross sections in L_m;

$$\langle\gamma_1,\gamma_2\rangle_m=\frac{1}{4\pi}\int_{\mathbf{R}^4}\overline{(q_m^{-1}\gamma_1)(x)}(q_m^{-1}\gamma_2)(x)4rf(r)dx. \tag{4.8}$$

We note here that, since $q_m^{-1}\gamma$'s are ρ_m equivariant, the integrand in (4.8) is invariant under the U(1) action, so that the integration on the right-hand side of (4.8) is reduced to that on $\mathbf{R}^3$. We denote by Γ_m the Hilbert space of square integrable cross sections in L_m with respect to $\langle\ ,\ \rangle_m$. Thus, $L^2(\mathbf{R}^4;4rf(r)dx)$ is reduced to Γ_m by restricting $L^2(\mathbf{R}^4;4rf(r)dx)$ to the space of ρ_m-equivariant functions.

We here remark that Dirac's monopole field is already encompassed in this setting.[15,16] This is because the complex line bundle L_m is endowed with the linear connection associated with the natural connection defined in the U(1) bundle $\dot{\mathbf{R}}^4$ and because Dirac's monopole field is the curvature 2-form of this linear connection.

We turn to the reduction of the Hamiltonian operator $\hat{H}$ given by (3.1). For this purpose, we define a one-parameter group of unitary transformations U_t to be

$$(U_tF)(x)=F(T(-t)x)\quad(F\in L^2(\dot{\mathbf{R}}^4;4rf(r)dx)). \tag{4.9}$$

Then, it is an easy matter to verify that the Hamiltonian operator $\hat{H}$ is invariant under U_t; $U_t\hat{H}U_t^{-1}=\hat{H}$. To reduce $\hat{H}$, we have only to restrict the domain of $\hat{H}$ to the space of ρ_m-equivariant functions. For $\hat{H}$ and ρ_m-equivariant functions F, we can define a reduced operator $\hat{H}_m$ through

$$\hat{H}_m(q_mF)=q_m(\hat{H}F), \tag{4.10}$$

since $\hat{H}F$ is ρ_m equivariant because of $U_t\hat{H}U_t^{-1}=\hat{H}$ and of $U_tF=\exp(-imt/2)F$. To put $\hat{H}_m$ in an explicit form, we express $\hat{H}$ in terms of the momentum operator $\hat{J}$ and the horizontal lifts $(\partial/\partial q_k)^*$ of the vector fields $\partial/\partial q_k$ on $\dot{\mathbf{R}}^3$,

$$\hat{H}=-\frac{1}{2f(r)}\sum_{k=1}^{3}\left[\left(\frac{\partial}{\partial q_k}\right)^*\right]^2+\frac{1}{2g(r)}(\hat{J})^2, \tag{4.11}$$

where $(\partial/\partial q_k)^*$ and $\hat{J}$ are given,[15] respectively, by

$$\begin{pmatrix}(\partial/\partial q_1)^*\\(\partial/\partial q_2)^*\\(\partial/\partial q_3)^*\end{pmatrix}=\frac{1}{2r}P(x)\begin{pmatrix}\partial/\partial x_1\\\partial/\partial x_2\\\partial/\partial x_3\\\partial/\partial x_4\end{pmatrix}, \tag{4.12a}$$

and

$$\hat{J}=\frac{1}{2i}\left(-x_2\frac{\partial}{\partial x_1}+x_1\frac{\partial}{\partial x_2}-x_4\frac{\partial}{\partial x_3}+x_3\frac{\partial}{\partial x_4}\right). \tag{4.12b}$$

Operating ρ_m-equivariant functions with (4.11) provides

$$\hat{H}_m=-\frac{1}{2f(r)}\sum_{k=1}^{3}\nabla_k^2+\frac{(m/2)^2}{2g(r)}, \tag{4.13}$$

where $\boldsymbol{\nabla}_k$ is the covariant derivation with respect to $\partial/\partial q_k$.[15] Comparison of (2.8) with (4.13) shows that the $\hat{H}_m$ is the quantization of H_μ by replacing p_k and μ with $-i\boldsymbol{\nabla}_k$ and $-m/2$, respectively. Thus, we obtain the following theorem.

Theorem 4.1: *The quantized system* $(L^2(\mathbf{R}^4;4rf(r)dx),\hat{H})$ *for the geodesic flow system associated with the generalized Taub–NUT metric* ds_G^2 *is reduced to the quantum system* $(\Gamma_m,\hat{H}_m)$, *where* Γ_m *is the Hilbert space of square integrable cross sections in* L_m, *and* $\hat{H}_m$ *is the Hamiltonian operator given by (4.13). We refer to the quantum system* $(\Gamma_m,\hat{H}_m)$ *as the quantized* α*-fold Kepler system*.

B. The eigenvalue problem

We proceed to the eigenvalue problem of $\hat{H}_m$. In view of the definition of the quantized α-fold Kepler system, the eigenvalues and the eigencross sections for $(\Gamma_m,\hat{H}_m)$ are expected to be obtained from those for $(L^2(\mathbf{R}^4,4rf(r)dx),\hat{H})$ through the U(1) reduction method.

From the definition (4.10) of $\hat{H}_m$, the eigenvalues of $\hat{H}_m$ must be eigenvalues of $\hat{H}$. Hence the eigencross sections of $\hat{H}_m$ come from eigenfunctions of $\hat{H}$, so that our task amounts to picking up ρ_m-equivariant eigenfunctions of $\hat{H}$. Let us be reminded that the eigenfunctions of $\hat{H}$ are expressed as linear combinations of functions of the form $R(r)Q$, where Q's are spherical harmonics on the unit sphere S^3. Since the ρ_m equivariance of eigenfunctions is concerned with only the spherical harmonics part, we can restrict ourselves to spherical harmonics on S^3 in picking up ρ_m-equivariant eigenfunctions. Moreover, since spherical harmonics on S^3 are the restriction of solid harmonics on $\mathbf{R}^4$, we have only to give a method of picking up ρ_m-equivariant solid harmonics. Incidentally, a generating function of solid harmonics of degree $2J$ is given by

$$G(z,\bar{z};\tau)=(\tau z_1+z_2)^p(\bar{z}_1-\tau\bar{z}_2)^q,\quad p+q=2J,\quad \tau\in\mathbf{R}, \tag{4.14}$$

where p and q are non-negative integers, and

$$z_1=x_1+ix_2,\quad z_2=x_3+ix_4. \tag{4.15}$$

Moreover, the U(1) action on $\mathbf{C}^2 \cong \mathbf{R}^4$ given by (4.1) is expressed as

$$(z_1, z_2) \mapsto (e^{it/2} z_1, e^{it/2} z_2). \tag{4.16}$$

Then, the generating function (4.14) transforms according to

$$G(e^{it/2} z, e^{-it/2} \bar{z}; \tau) = e^{it(p-q)/2} G(z, \bar{z}; \tau), \tag{4.17}$$

so that the ρ_m-equivariant solid harmonics are singled out by the condition that $p-q=m$. Thus, we have found the method of picking up ρ_m-equivariant eigenfunctions in the manner independent of the choice of local coordinates in S^3.

To carry out the above procedure in terms of local coordinates (θ, ϕ, ψ) in S^3, we first notice that the U(1) action is expressed as

$$\psi \mapsto \psi + t, \quad \text{the others fixed.} \tag{4.18}$$

Then the $\mathscr{D}$ functions, spherical harmonics on S^3, transform according to

$$\mathscr{D}^J_{ML}(\psi + t, \theta, \phi) = \exp(iMt) \mathscr{D}^J_{ML}(\psi, \theta, \phi). \tag{4.19}$$

Thus we have the following.

Lemma 4.2: The eigenfunction $\Psi^{\sigma}_{L,J,N;M}$ for $\hat{H}$ associated with the eigenvalue $E^{\sigma}_{J,N;M}$ is ρ_m equivariant if and only if $M=m/2$.

It is to be noted here that the generating function $G(z, \bar{z}; \tau)$ with $p=J+M$, $q=J-M$, and $|z_1|^2 + |z_2|^2 = 1$ is expanded into

$$G(z, \bar{z}; \tau) = \sum_{|L| \leqslant J} \tau^{J+L} \left[\frac{(J+M)!(J-M)!}{(J+L)!(J-L)!} \right]^{1/2} \mathscr{D}^J_{ML}(\psi, \theta, \phi), \tag{4.20}$$

where we have used (3.6) together with (4.15). We are now in a position to describe eigenspaces for the quantized α-fold Kepler system $(\Gamma_m, \hat{H}_m)$.

Theorem 4.3: *The eigenvalues of the quantized α-fold Kepler system $(\Gamma_m, \hat{H}_m)$ are given by $E^{\sigma}_{J,N;m/2}$, and the associated eigenspace is isomorphic with the eigenspace of $(L^2(\mathbf{R}^4, 4rf(r)dx), \hat{H})$ assigned by $E^{\sigma}_{J,N;m/2}$.*

We notice here that $q_m(\Psi^{\sigma}_{L,J,N;m/2}(r, \theta, \phi, \psi))$'s provide locally-defined eigencross sections through $\psi = -\phi$ or $\psi = \phi$.

V. DEGENERACIES IN THE ENERGY LEVELS

Now that we have solved the eigenvalue problem for the quantized α-fold Kepler system, we are to study degeneracies in the energy levels for this system. Degeneracies are broken up into two. One is concerned with the rotational symmetry of the quantized α-fold Kepler system, and the other depends on whether α is a rational number or not.

A. Normal degeneracies

Theorems 3.3 and 4.3 are put together to show that the eigenspace of $\hat{H}_m$ associated with the energy level $E^{\sigma}_{J,N;m/2}$ is of dimension $2J+1$, at least. Namely, the energy level $E^{\sigma}_{J,N;m/2}$ is degenerate at least $(2J+1)$-fold. In this section, we show that this degeneracy is caused by the spherical symmetry of the quantized α-fold Kepler system, so that it will be suitably called normal degeneracy after Wigner.[31]

To start with, let us identify $\mathbf{R}^4$ with $\mathbf{C}^2$ through the map given in (4.15). Further, we denote by $g_{\mathbf{R}}$ the 4×4 real matrix associated with $g \in \mathrm{SU}(2)$. Then, the SU(2) action on $\mathbf{R}^4$ gives rise to a unitary operator W_g on $L^2(\mathbf{R}^4; 4rf(r)dx)$ through

$$(W_g F)(x) = F(g_{\mathbf{R}}^{-1} x) \quad (g \in \mathrm{SU}(2), F \in L^2(\mathbf{R}^4; 4rf(r)dx)). \tag{5.1}$$

We can verify that the W_g is indeed a unitary operator by using the fact that $g_{\mathbf{R}}$ leaves the volume form $4rf(r)dx$ invariant. Further calculation shows that the Hamiltonian operator $\hat{H}$ is invariant under W_g;

$$W_g \hat{H} W_g^{-1} = \hat{H}. \tag{5.2}$$

Thus, the SU(2) proves to be a symmetry group of $(L^2(\mathbf{R}^4; 4rf(r)dx), \hat{H})$.

The action of W_g on the eigenfunctions can be described in a usual manner from the representation theory. To show this, we choose to identify S^3 with SU(2) through

$$(z_1, z_2) \mapsto \begin{pmatrix} z_1 & z_2 \\ -\overline{z_2} & \overline{z_1} \end{pmatrix}, \quad \text{with } \sum_{l=1}^{2} |z_l|^2 = 1. \tag{5.3}$$

Then the representation theory shows that

$$\mathscr{D}^J_{ML}(g_{\mathbf{R}}^{-1} x/|x|) = \sum_{M'=-J}^{J} \mathscr{D}^J_{MM'}(x/|x|) \overline{\mathscr{D}^J_{M'L}(g)} \quad (g \in SU(2)), \tag{5.4}$$

where $x = (x_1, \ldots, x_4)^T$, a column vector, $|x|^2 = \Sigma_{j=1}^4 x_j^2$, and $\mathscr{D}$ functions are viewed as defined on $\mathrm{SU}(2) \simeq S^3 \subset \mathbf{R}^4$. Equations (5.4) and (3.20) are put together to show that the energy eigenspace admits the SU(2) action.

We proceed to show that the SU(2) symmetry treated above will provide the SU(2) symmetry of the quantized α-fold Kepler system. Since the U(1) action U_t given by (4.9) and the SU(2) action W_g given by (5.1) commute, we can restrict W_g to the subspace of ρ_m-equivariant functions in $L^2(\mathbf{R}^4; 4rf(r)dx)$ to define the SU(2) action $W_g^{(m)}$ on the Hilbert space Γ_m;

$$W_g^{(m)} \circ q_m = q_m \circ W_g. \tag{5.5}$$

Put together with Theorem 4.3, this implies the following.

Theorem 5.1: *The quantized α-fold Kepler system $(\Gamma_m, \hat{H}_m)$ admits SU(2) as a symmetry group, which acts unitarily on each eigenspace through $W_g^{(m)}$.*

Remark: The operator $W_g^{(m)}$ can be expressed in a simple form. Let us define a map $\chi_g : \dot{\mathbf{R}}^4 \times \mathbf{C} \to \dot{\mathbf{R}}^4 \times \mathbf{C}$ by $(x, \zeta) \mapsto (g_{\mathbf{R}} x, \zeta)$, and a map $\chi_g^{(m)} : L_m \to L_m$ through

$$\chi_g^{(m)} \circ \pi_m = \pi_m \circ \chi_g \quad (g \in SU(2)). \tag{5.6}$$

Then, from the commutative diagram (4.5) and the definition (5.5), it follows that

$$(W_g^{(m)} \gamma)(\pi(x)) = \chi_g^{(m)}(\gamma(\pi(g_{\mathbf{R}}^{-1} x))) \quad (x \in \dot{\mathbf{R}}^4). \tag{5.7}$$

Further calculation shows that

$$(W_{-g}^{(m)} \gamma)(q) = (-1)^m (W_g^{(m)} \gamma)(q) \quad (q \in \dot{\mathbf{R}}^3). \tag{5.8}$$

Hence, if m is even, the SU(2) symmetry stated above reduces to the SO(3) symmetry, since $\mathrm{SU}(2)/\mathbf{Z}_2 \simeq SO(3)$, $\mathbf{Z}_2 = \{I, -I\}$, with I the identity of SU(2).

B. Accidental degeneracies

We wish to show that another degeneracy takes place in the energy levels of $\hat{H}_m$, which is not attributed to the SU(2) symmetry, but to the α dependence of the energy levels. The following lemma is easy to prove.

Lemma 5.2: Let σ and m be fixed in the energy eigenvalues $E^{\sigma}_{J,N;m/2}$ of $\hat{H}_m$. Then two of the eigenvalues, $E^{\sigma}_{J_1,N_1;m/2}$ and $E^{\sigma}_{J_2,N_2;m/2}$, become identical if and only if

$$(N_1+\tfrac{1}{2})+\alpha(J_1+\tfrac{1}{2})=(N_2+\tfrac{1}{2})+\alpha(J_2+\tfrac{1}{2}). \tag{5.9}$$

We now rewrite (5.9) in the form

$$(N_1-N_2)=-\alpha(J_1-J_2), \tag{5.10}$$

which shows that there are no pairs of different half-integers, (J_1,N_1) and (J_2,N_2), satisfying (5.10) if α is an irrational number. Conversely, if α is a rational number, one can find out those integers satisfying (5.10); for example, on putting $\alpha=q/p$ with q and p mutually prime integers, we find that (5.10) is valid, at least, for the pair of integers, (J_1,N_1) and $(J_2,N_2)=(J_1+p,N_1-q)$. Lemma 5.2 then implies that the energy levels $E^{\sigma}_{J_1,N_1;m/2}$ and $E^{\sigma}_{J_2,N_2;m/2}$ coincide for those pairs. Clearly, this degeneracy has nothing to do with the $SU(2)$ symmetry of the quantized α-fold Kepler system. We may call this degeneracy an ''accidental'' one after Wigner.[31] Thus, we come to the following conclusion.

Theorem 5.3: *In the energy levels of the quantized α-fold Kepler system, accidental degeneracies take place, if and only if α is a rational number.*

In the rest of this section, we wish to observe how the energy level splitting for the quantized α-fold Kepler system occurs when α varies from a rational number. Let us take the parameters contained in $\hat{H}_m$ to be

$$a_0=4c,\quad a_1=1,\quad a_2=\frac{1}{2c},\quad a_3=\frac{1}{16c^2}\quad (c>0),\quad \text{and } m=2. \tag{5.11}$$

If $\alpha=1$ in addition to (5.11) (without the condition of $m=2$), the generalized Taub–NUT metric ds^2_G becomes the Euclidean Taub–NUT metric. Taking $c=1$, we evaluate numerically the energy levels, $E^{+}_{J,N;1}$, of $\hat{H}_2$ in the case of $\alpha=1$ and of $\alpha=1+\pi/5000$. In both cases, the energy levels, $E^{+}_{J,N;1}$, to be evaluated are subject to

$$500\leqslant N+J\leqslant 510,\quad J\geqslant 1,\quad N\geqslant 0\quad (J,N:\text{integers}). \tag{5.12}$$

Figures 1(a) and 1(b) show the energy levels for $\alpha=1$ and for $\alpha=1+\pi/5000$, respectively. These figures show that distinct energy levels split as α varies from $\alpha=1$ to $\alpha=1+\pi/5000$. Indeed, the bands painted out in black in Fig. 1(b) consist of more than 5000 distinct energy levels. It is worth noting that, in Fig. 1(a), each of the energy levels are degenerate approximately 2.5×10^5-fold. In contrast with this, each of the energy levels in Fig. 1(b) admits $2J+1$-fold normal degeneracy, which is less than 1100-fold. We have to remark that the numerical evaluation, of course, cannot describe the energy-level behavior completely, because we cannot deal with any irrational numbers on computers! In our example, however, the numerical evaluation seems to work quite well.

VI. REMARKS ON THE HAMILTONIAN OPERATOR $\hat{H}$

As we stated in Sec. III, the Hamiltonian operator $\hat{H}$ is not equal to $-\frac{1}{2}$ times the Laplace–Beltrami operator, which are usually supposed to be the Hamiltonian operator associated with the energy function of the geodesic flows. Let g_{jk} be the components of the generalized Taub–NUT metric ds^2_G, and $(g^{jk})=(g_{jk})^{-1}$;

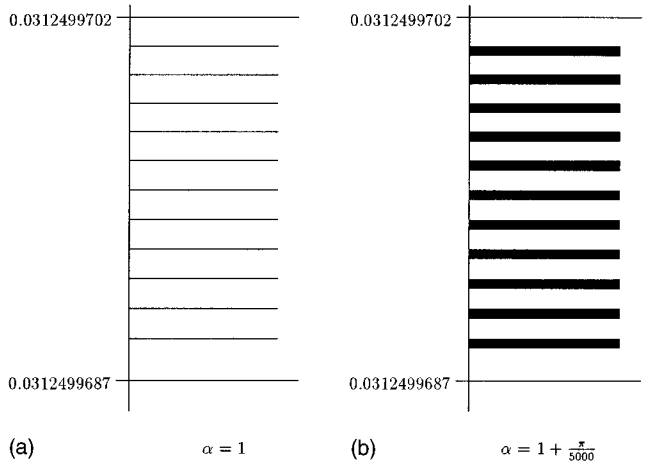

FIG. 1. The energy levels of $\hat{H}_2$.

$$ds_G^2 = \sum_{j,k=1}^{4} g_{jk}\, du^j\, du^k = f(r)(dr^2 + r^2(d\theta^2 + \sin^2\theta\, d\phi^2)) + g(r)(d\psi + \cos\theta\, d\phi)^2, \quad (6.1)$$

where $(u^j) = (r, \theta, \phi, \psi)$, and $f(r)$ and $g(r)$ are given by (1.2). Let $\tilde{\nabla}_j$ be the Levi–Civita connection formed from g_{jk}. Then $-\frac{1}{2}$ times the Laplace–Beltrami operator is expressed as

$$-\frac{1}{2}\Delta = -\frac{1}{2}\sum_{j,k} g^{jk}\, \tilde{\nabla}_j \tilde{\nabla}_k = \hat{H} - \frac{(f(r)g(r))'}{4f(r)^2 g(r)}\frac{\partial}{\partial r}, \quad (6.2)$$

where $\hat{H}$ is the Hamiltonian operator given by (3.7), and the prime $'$ denotes the derivative with respect to r. From (6.2) it then follows that $\hat{H} = -\frac{1}{2}\Delta$ if and only if $(f(r)g(r))' = 0$. Investigating this equation, we obtain the following.

Proposition 6.1: The Hamiltonian operator $\hat{H}$ and $-\frac{1}{2}$ times the Laplace–Beltrami operator coincide, if and only if

$$\alpha = 1, \quad a_2 = 2a_1/a_0, \quad a_3 = (a_1/a_0)^2 \quad (a_0 \neq 0),$$

or (6.3)

$$\alpha = 2, \quad a_1 \neq 0, \quad a_2 = a_3 = 0 \quad (a_0 = 0).$$

According to whether the condition $\alpha = 1,...,$ holds or the condition $\alpha = 2,...,$ does, the generalized Taub–NUT metric ds_G^2 becomes a constant multiple of the Taub–NUT metric or of the standard flat metric. Therefore, for the Taub–NUT metric, our Hamiltonian operator is equal to $-\frac{1}{2}$ times the Laplace–Beltrami operator, so that the energy levels (3.16a) become equal to those obtained from $-\frac{1}{2}$ times the Laplace–Beltrami operator for the Taub–NUT metric. This fact was already remarked in (3.21) without any comments.

In conclusion, we remark also that for $\alpha = 1$ the generalized Taub–NUT metric ds_G^2 is Einstein if and only if $a_2 = 2a_1/a_0$, $a_3 = (a_1/a_0)^2$ $(a_0 \neq 0)$.[9] In view of this, we would like to say that if the Riemannian manifold is Einstein, the generally accepted principle that $-\frac{1}{2}$ times the Laplace–Beltrami operator is the Hamiltonian operator associated with the geodesic flow system holds true. However, if the Riemannian manifold is not Einstein, the other principle of quantization would be worth applying.

APPENDIX: CALCULATION OF EIGENFUNCTIONS AND EIGENVALUES

We are to give solutions to (3.13). In view of the classical method for finding the functional form of $f(r)$ and $g(r)$,[12] we make a change of the variable r by setting

$$r^{1/\alpha}=\rho. \tag{A1}$$

Then the unknown function $y(\rho)=R(r)$ turns out to satisfy the differential equation

$$y''(\rho)+\frac{1+\alpha}{\rho}\,y'(\rho)+\alpha^2\left(c_1+\frac{c_0}{\rho}-\frac{J(J+1)}{\rho^2}\right)y(\rho)=0. \tag{A2}$$

Introducing a function $v(\rho)$ by

$$y(\rho)=\rho^{-(1/2)(1+\alpha)}v(\rho), \tag{A3}$$

we find that $v(\rho)$ satisfies

$$v''(\rho)+\left(\alpha^2c_1+\alpha^2\,\frac{c_0}{\rho}+\frac{1}{\rho^2}\left(\frac{1}{4}\,(1-\alpha^2)-\alpha^2J(J+1)\right)\right)v(\rho)=0. \tag{A4}$$

As ρ tends to infinity, Eq. (A4) has an asymptotic solution $e^{-\alpha\sqrt{-c_1}\rho}$, subject to the condition that $y(\rho)\to 0$. Here we have assumed that $c_1=2a_1E-M^2a_3<0$, which is a quantum analog of one of the classical conditions, $2a_1E-a_3\mu^2<0$, for bounded trajectories of the multifold Kepler system to occur.[12] Note also that the boundary condition (3.14) is now expressed as

$$\int_0^\infty |y(\rho)|^2(a_0+a_1\rho)\rho^\alpha\,d\rho<+\infty. \tag{A5}$$

On setting

$$v(\rho)=e^{-\alpha\sqrt{-c_1}\rho}z(\rho), \tag{A6}$$

it follows from (A4) that $z(\rho)$ is subject to

$$z''(\rho)-2\alpha\sqrt{-c_1}z'(\rho)+\left(\alpha^2\,\frac{c_0}{\rho}+\frac{1}{\rho^2}\left(\frac{1}{4}\,(1-\alpha^2)-\alpha^2J(J+1)\right)\right)z(\rho)=0. \tag{A7}$$

This equation has a solution of the form

$$z(\rho)=\rho^s w(\rho),\quad w(\rho)=\sum_{m=0}^{\infty}b_m\rho^m,\quad b_0\neq 0. \tag{A8}$$

Equations (A7) and (A8) are put together to provide

$$s=\tfrac{1}{2}+\alpha(J+\tfrac{1}{2}), \tag{A9}$$

and

$$w''(\rho)+\left(\frac{1}{\rho}\,(1+\alpha(2J+1))-2\alpha\sqrt{-c_1}\right)w'(\rho)+\frac{1}{\rho}\,(\alpha^2c_0-(\alpha+\alpha^2(2J+1))\sqrt{-c_1})w(\rho)=0. \tag{A10}$$

This equation can be expressed as the confluent hypergeometric equation, and therefore its solution is expressed in terms of confluent hypergeometric functions;

$$w(\rho)=F\left(\frac{1}{2}+\alpha\left(J+\frac{1}{2}\right)-\frac{\alpha c_0}{2\sqrt{-c_1}},1+\alpha(2J+1),2\alpha\sqrt{-c_1}\rho\right). \tag{A11}$$

Thus the radial equation has a solution of the form

$$R(r)=\exp(-\alpha\sqrt{-c_1}r^{1/\alpha})r^J F\left(\frac{1}{2}+\alpha\left(J+\frac{1}{2}\right)-\frac{\alpha c_0}{2\sqrt{-c_1}},1+\alpha(2J+1),2\alpha\sqrt{-c_1}r^{1/\alpha}\right). \tag{A12}$$

The boundary condition (A5) requires that F should be a polynomial in ρ, so that there is a non-negative integer N, satisfying

$$N+\frac{1}{2}+\alpha\left(J+\frac{1}{2}\right)=\frac{\alpha c_0}{2\sqrt{-c_1}}, \tag{A13}$$

and thereby the energy levels are obtained as follows: For $a_0\neq 0$,

$$E=\frac{1}{2a_0^2}\left(a_0a_2M^2-2a_1\left(\frac{n}{\alpha}\right)^2\pm 2\frac{n}{\alpha}\sqrt{\left(\frac{n}{\alpha}\right)^2 a_1^2+a_0(a_0a_3-a_1a_2)M^2}\right), \tag{A14a}$$

and for $a_0=0$,

$$E=\frac{a_3M^2}{2a_1}-\frac{\alpha^2a_2^2M^4}{8a_1n^2}, \tag{A14b}$$

where n is defined to be

$$n=\left(N+\frac{1}{2}\right)+\alpha\left(J+\frac{1}{2}\right)\quad (N\text{:non-negative integer}). \tag{A15}$$

We have to take "+" in (A14a). This is because if "−" were chosen, the energy levels would not have a minimum, which is not acceptable.

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The canonical connection in quantum mechanics

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In this paper we investigate the form of induced gauge fields that arises in two types of quantum systems. In the first we consider quantum mechanics on coset spaces G/H, and argue that G invariance is central to the emergence of the H connection as induced gauge fields in the different quantum sectors. We then demonstrate why the same connection, now giving rise to the non-Abelian generalization of Berry's phase, can also be found in systems that have slow variables taking values in such a coset space. © *1996 American Institute of Physics.* [S0022-2488(96)02602-0]

I. INTRODUCTION

There are various instances in quantum mechanics when a gauge field appears in a system whose initial formulation did not contain such fields. The most familiar example of this is the emergence of Berry's connection[1] in systems with degeneracies, which leads to a holonomy in energy eigenspaces, i.e., a non-Abelian generalization of Berry's phase. Another example is to be found in the different quantum sectors that arise when quantizing on a coset space.[2] For both of these cases, the gauge field that emerges is often found to be of a specific type. Indeed, when the effective configuration space is a coset space G/H, the resulting connection can usually be identified with the so-called *H connection*, which is a (possibly topological) solution of the Yang–Mills equation on this space. The prime aim of this paper is to clarify why and when this connection arises in these systems.

More precisely, in the context of Berry's phase, the origin of the connection is in some sense obvious from the outset, that is, it comes from the ambiguity in choosing a set of basis vectors in the instantaneous energy eigenspaces. However, what is not obvious and hence remarkable is that in a wide variety of systems of physical interest, Berry's connection often (though not always) takes the form of the H connection.[3–5] Such systems arise when considering the coupled dynamics of slow and fast variables. In this case we wish to know the form of the connection, also occurring in the Hamiltonian of the effective slow system, in advance. By giving a precise identification of when it is the H connection the need to calculate energy eigenstates can be avoided.

In contrast, in the context of inequivalent quantizations on coset spaces, the origin of the connection is not quite obvious, and the question is why the specific H connection can appear at all when quantized. In the account presented in Ref. 2, which relies (basically) on Mackey's approach,[6] the system of a ''free particle'' on G/H is considered, where the Hamiltonian is fixed by requiring that there is no operator ordering ambiguity. This is clearly an important criterion, and

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leads to a system minimally coupled to the H connection. However, this is not a criterion geometrically motivated, and more importantly, in any attempt at extending these results to field theories such a reliance on a factor ordering argument is unnatural and, indeed, unworkable. What we will show in this paper is that an invariance argument can be developed that highlights the need for such a connection.

The emergence of gauge fields is also recognized recently by a number of other groups[7–9] using different approaches to quantization. For instance, in Ref. 7, spheres S^n embedded in $\mathbb{R}^{n+1}$ are taken as the configuration space and gauge fields are seen to emerge at the quantum level. It will be shown, however, in this paper that these induced gauge fields are none other than the H connection. This will perhaps support the view that the emergence of gauge fields is not just an artifact of a particular quantization approach but a ''norm'' when quantizing on coset spaces.

The plan of this paper is as follows. In Sec. II we will demonstrate how the H connection emerges in the quantum description of a point particle moving freely on a coset space. In Sec. III we prove that the connection that arises in the quantization scheme of Ref. 7 is just the H connection. In Sec. IV the conditions under which Berry's connection reduces to the H connection will be presented. Section V is devoted to our conclusions and discussions.

II. QUANTIZING ON A COSET

We begin by arguing that the H connection—observed by Landsman and Linden[2] in investigating the dynamical aspect of the quantum theory on a coset space G/H—is indeed the natural connection in the quantum system.

Let us first, though, fix our notation (which follows those in Ref. 10). We take G to be a compact Lie group with Lie algebra $\mathfrak{g}$, and H a compact subgroup of G with Lie algebra $\mathfrak{h}$. The Lie algebra $\mathfrak{g}$ has an orthogonal decomposition,

$$\mathfrak{g}=\mathfrak{h}\oplus\mathfrak{r}, \tag{2.1}$$

where $\mathfrak{r}=\mathfrak{h}^{\perp}$ is the orthogonal complement of $\mathfrak{h}$ in $\mathfrak{g}$. This is, in fact, a reductive decomposition, i.e.,

$$[\mathfrak{h},\mathfrak{r}]\subset\mathfrak{r}. \tag{2.2}$$

We shall denote bases of the spaces by

$$\begin{aligned}\mathfrak{g}&=\mathrm{span}\{T_m\},\quad m=1,\ldots,\dim\ G,\\ \mathfrak{h}&=\mathrm{span}\{T_i\},\quad i=1,\ldots,\dim\ H,\\ \mathfrak{r}&=\mathrm{span}\{T_a\},\quad a=1,\ldots,\dim(G/H).\end{aligned} \tag{2.3}$$

Let us recall that in Mackey's account of quantizing on G/H,[6] a set of fundamental relations, called a *system of imprimitivity*, is introduced whose irreducible representations give the quantum theories (a full discussion of this can be found in Ref. 10). The upshot of this is that the Hilbert space $\mathscr{H}(G/H)$ on the coset space consists of L^2 functions on G/H belonging to the linear space $\mathscr{H}_\chi$ of some irreducible unitary representation χ of the subgroup H: $\mathscr{H}(G/H)\simeq L^2(G/H,\mathscr{H}_\chi)$. Locally, we may take a basis set $\{|q,\chi,\mu\rangle\}$ of the Hilbert space $\mathscr{H}(G/H)$ by

$$|q,\chi,\mu\rangle:=|q\rangle\otimes|\chi,\mu\rangle, \tag{2.4}$$

where $|q\rangle$ are the eigenstates in the coordinate representation on G/H and $|\chi,\mu\rangle$ the orthonormal basis vectors in $\mathscr{H}_\chi$. Thus, the states in the basis set (2.4) satisfy the orthonormality condition

$$\langle q,\chi,\mu|q',\chi,\nu\rangle=\delta_{\mu\nu}\delta(q-q'), \tag{2.5}$$

with $\delta(q-q')$ being the delta function on the coset space G/H.

In order to have a singularity-free description we need to introduce a set of patches to cover the coset space G/H. Let $\{U_\alpha\}$ be the local patches introduced, and $\sigma_\alpha: U_\alpha \mapsto G$ be a continuous section on the patch U_α. On overlaps $U_\alpha \cap U_\beta$ the sections are related by a gauge transformation, namely, for $q \in U_\alpha \cap U_\beta$,

$$\sigma_\beta(q) = \sigma_\alpha(q) h_{\alpha\beta}(q), \tag{2.6}$$

where $h_{\alpha\beta} \in H$. Accordingly, we consider a sectional basis $\{|q,\chi,\mu\rangle^\alpha\}$, which is a basis set given independently on the patch U_α. Using standard partition of unity arguments, we can define an inner product on these and see that all is well defined. The wave functions are then defined to be

$$\psi^\alpha_\mu(q) = {}^\alpha\langle q,\chi,\mu|\psi\rangle. \tag{2.7}$$

An important ingredient in Mackey's quantization[6] is that associated with the G action $q \to g^{-1}q$ for $g \in G$, which relates any two points on the coset space, there is a corresponding action on the wave functions furnished by the *induced representation*,

$$(U(g)\psi)^\alpha_\mu(q) = \sum_\nu \pi^\chi_{\mu\nu}((\sigma_\alpha(q))^{-1} g \sigma_\beta(g^{-1}q))\psi^\beta_\nu(g^{-1}q). \tag{2.8}$$

Here the matrix elements of the unitary operator $\pi^\chi(h)$, implementing the irreducible representation χ, are

$$\pi^\chi_{\mu\nu}(h) := \langle\chi,\mu|\pi^\chi(h)|\chi,\nu\rangle, \tag{2.9}$$

and a choice of section has been made on each of the patch, $q \in U_\alpha$ and $g^{-1}q \in U_\beta$. On the sectional basis, this action (2.8) reads as

$$U(g)|q,\chi,\mu\rangle^\alpha = \sum_\nu |gq,\chi,\nu\rangle^\beta \pi^\chi_{\nu\mu}((\sigma_\beta(gq))^{-1} g \sigma_\alpha(q)), \tag{2.10}$$

where we put $g \to g^{-1}$ for later convenience. In effect, the induced representation (2.10) consists of a rotation in the space $\mathscr{H}_\chi$ and a translation in the coset space G/H, both determined by g and q. Using the naturally defined measure on the coset space G/H, one can readily show that (2.10) indeed provides a unitary representation of G.[10]

Now we shall consider the quantum mechanics of a point particle moving freely on the coset space G/H. Here the term "free" is meant to indicate that the system under consideration is *homogeneous* over G/H, and that the dynamics of the particle is that of a free particle when observed locally. Note that in order to get the Schrödinger equation for the wave functions (2.7) describing the point particle of this system, we need to use the G action to ensure the homogeneity (as it is the only means available on G/H for this purpose). But since the G action on the wave functions (2.8) is section dependent, we need a covariant derivative (with respect to q) such that the section dependence disappears in the physical dynamics.

To be explicit, let us consider the state

$$|\chi,\bar{\mu}\rangle := \sum_\nu |e,\chi,\nu\rangle^\beta \pi_{\nu\mu}((\sigma_\beta(e))^{-1}), \tag{2.11}$$

where e is the identity point in the coset G/H. Then (2.10) allows us to write the basis states at q as

$$|q,\chi,\mu\rangle^\alpha = U(\sigma_\alpha(q))|\chi,\bar{\mu}\rangle, \tag{2.12}$$

which shows that the G action allows for obtaining all the basis states over G/H by the unitary G action from the reference state (2.11). It is then easy to see from (2.10) that, under the change of section (2.6), the basis states undergo the rotation

$$|q,\chi,\mu\rangle^{\alpha}\rightarrow|q,\chi,\mu\rangle^{\beta}=U(\sigma_{\alpha}h_{\alpha\beta})|\chi,\bar{\mu}\rangle=\sum_{\nu}|q,\chi,\nu\rangle^{\alpha}\pi^{\chi}_{\nu\mu}(h_{\alpha\beta}). \tag{2.13}$$

Thus, the connection used in the covariant derivative must compensate the derivative factor in the Schrödinger equation arising from the rotation in (2.13). Actually, in the theory of vector bundles associated with the principal bundle $G(G/H,H)$, the term "connection" already implies this property. This, however, is not enough to single out the connection relevant to our system on G/H.

The crucial point in specifying the connection is the homogeneity over the coset G/H mentioned above. We note that for the system to be homogeneous the connection must also be homogeneous physically, that is, it must be invariant under the G action up to a gauge transformation of the group H (i.e., up to a change of section). In other words, the curvature of the connection is constant over G/H. Now the theory of invariant connections (see Theorem 11.1 on p. 103 of Ref. 11) asserts that such a connection is always given by the H connection $A^{H}:=\sigma_{\alpha}^{-1}(q)d\sigma_{\alpha}(q)|_{\mathfrak{h}}$, which is the (pullback of the) canonical 1-form projected down to the subspace $\mathfrak{h}\subset\mathfrak{g}$. In the present context, the invariant connection that arises in the covariant derivative acting on the wave functions (2.7) is the H connection in the representation χ:

$$\sum_{i}A^{H}_{i}(q)(T_{i})_{\mu\nu}=\langle\chi,\bar{\mu}|U^{-1}(\sigma_{\alpha}(q))dU(\sigma_{\alpha}(q))|_{\mathfrak{h}}|\chi,\bar{\nu}\rangle. \tag{2.14}$$

One can readily confirm that its curvature is indeed constant over G/H and that it does transform as a connection under the change of section (2.6).

In short, we see that the covariant derivative used for the Schrödinger equation must contain the H connection in the form (2.14), if we are to consider the homogeneous free particle system over G/H requiring the independence of the choice of section. This G invariance is, we feel, more fundamental than the factor ordering criterion adopted in Ref. 2. However, for completeness, we now need to see what form of Hamiltonian comes out of our analysis.

To begin with, let us note that our vector-valued wave functions $\psi^{\alpha}_{\mu}(q)$, provided by the irreducible representation χ of H, may be expanded in terms of the "harmonics" $U^{\Lambda}_{\xi}(\sigma_{\alpha}^{-1}(q))$ over the coset space G/H,[12]

$$\psi^{\alpha}_{\mu}(q)=\sum_{\Lambda}\sum_{\rho,\xi}c^{\Lambda}_{\rho\xi}U^{\Lambda}_{\xi}(\sigma_{\alpha}^{-1}(q))_{\mu\rho}. \tag{2.15}$$

In this expansion, ξ is the index of multiplicity of the representation χ appearing in the irreducible representation Λ of G upon restriction to H, and the range of ρ equals the dimension of the representation Λ.

We recall that the Frobenius reciprocity theorem tells us that in the above summation only those Λ of G occur that contain the representation χ of H when restricted to the subgroup. (For brevity we henceforth omit α, which labels the patch to which the point q belongs.) But the message important to us here is that we can now work with the section variable $\sigma^{-1}(q)$ instead of the coordinates q on the coset space. We shall, for the sake of simplicity, consider the principal bundle $G(G/H,H)$ first. Because our vector bundle in question is the associated bundle via the irreducible representation of H, the covariant derivative in the vector bundle will follow immediately from that of the principal bundle.

Consider now the vector fields X_{m} defined by the relation

$$X_{m}\sigma^{-1}(q)=\sigma^{-1}(q)T_{m}. \tag{2.16}$$

These vector fields are just the generalizations of the usual Killing vector fields regarded as first-order differential operators. (In the context of Berry's phase these are modified symmetry generators for effective Hamiltonians.[5]) The fact that such vector fields do exist can be seen explicitly by examining the infinitesimal version of $g\sigma(q)=\sigma(gq)h(g,q)$, which leads to a first-order differential operators for X_m satisfying the commutation relations of the Lie algebra $\mathfrak{g}$.

We shall then consider the following covariant derivative:

$$\boldsymbol{\nabla}_m := -\mathscr{D}^{\,n}_{\,m}(\sigma^{-1})X_n\,, \tag{2.17}$$

where $\mathscr{D}^{\,n}_{\,m}(\sigma)$ is the "adjoint matrix" (the matrix of the adjoint representation of G in the basis T_m), defined by

$$\sigma^{-1}(q)T_m\sigma(q)=\mathscr{D}^{\,n}_{\,m}(\sigma)T_n\,, \tag{2.18}$$

Using this, we may invert (2.16) to get

$$\mathscr{D}^{\,m}_{\,n}(\sigma^{-1})X_m\sigma^{-1}=T_n\sigma^{-1}. \tag{2.19}$$

Hence, we find that our covariant derivative (2.17) satisfies

$$\boldsymbol{\nabla}_m\sigma^{-1}=-T_m\sigma^{-1}, \tag{2.20}$$

that is, it behaves just as $-T_m$ on σ^{-1}.

The $\mathfrak{r}$ component of $\boldsymbol{\nabla}_m$ is the covariant derivative with respect to the H connection. To see this, following the standard line of argument,[13] one decomposes the canonical 1-form as $\sigma^{-1}\,d\sigma=-d(\sigma^{-1})\sigma=A^H+e$, where $A^H=A^i_\alpha T_i\,dq^\alpha$ is the H connection and $e=\sigma^{-1}\,d\sigma|_{\mathfrak{r}}=e^a_\alpha T_a\,dq^\alpha$ is the vielbein, with $T_i\in\mathfrak{h}$ and $T_r\in\mathfrak{r}$ in the orthogonal decomposition $\mathfrak{g}=\mathfrak{h}\oplus\mathfrak{r}$. Using the inverse of the vielbein, $e^\alpha{}_a e_\alpha{}^b=\delta^b_a$, one may cast the canonical 1-form into the vielbein frame. This yields

$$(\partial_a+e_a{}^\alpha A^i_\alpha T_i)\sigma^{-1}=-T_a\sigma^{-1}=\boldsymbol{\nabla}_a\sigma^{-1}, \tag{2.21}$$

where (2.20) is used in the last equality, therefore proving our claim.

When we go over to the vector bundle from the principal bundle, we have to act with the covariant derivative on the expansion (2.15); hence, we are to use the particular representation χ for the generators T_i of $\mathfrak{h}$. It is then clear that the covariant derivative acts in an extremely simple manner on the wave functions. In fact, the property (2.20) shows that the covariant derivative in the representation χ is indeed the representation of the element T_m on such wave functions. Hence, if we adopt for the Hamiltonian the quadratic Casimir $X_mX^m=\boldsymbol{\nabla}_m\boldsymbol{\nabla}^m$ of the group G—which is G invariant by construction—we find that the Hamiltonian is given by the square of the covariant derivative $\boldsymbol{\nabla}_a\boldsymbol{\nabla}^a$ modulo a constant that is the value of the quadratic Casimir of the subgroup H evaluated on the irreducible representation χ. Thus, the free, homogeneous Hamiltonian given by the quadratic Casimir leads precisely to the Hamiltonian for the particle minimally coupled to the H connection, that is, the Hamiltonian argued by Landsman and Linden.[2]

III. QUANTIZING ON AN *n* SPHERE

In the approach to quantizating on spheres S^n proposed by Ohnuki and Kitakado[7] there appeared (possibly topological) gauge fields on the spheres as a result of inequivalent quantizations. These (infinitely) many inequivalent quantizations are labeled by the irreducible representations of the group SO(n)—an important feature shared with Mackey's approach,[6] where one

regards S^n as $\mathrm{SO}(n+1)/\mathrm{SO}(n)$. Thus, it would be natural to expect that the gauge fields observed in Ref. 7 may coincide with the H connection found by Landsman and Linden[2] in Mackey's approach. We shall show below that this is indeed the case.

But let us first recall the quantization and the gauge fields discussed in Ref. 7. There, quantization is prescribed by embedding the sphere S^n in $\mathbb{R}^{n+1}$ and then postulating a "fundamental algebra" as a set of quantum relations, generalizing the conventional canonical commutation relations. The fundamental algebra is the Lie algebra of $E(n+1)$, the Euclidean group in $n+1$ dimensions given by the semidirect product of $\mathrm{SO}(n+1)$ and $\mathbb{R}^{n+1}$, and finding the Hilbert space $\mathscr{H}(S^n)$ amounts to finding the representations of the group, taking into account the constraint that restricts to the sphere. Wigner's technique then allows for constructing explicitly the representations of $E(n+1)$ from the irreducible representations of the subgroup $\mathrm{SO}(n)$, which is the isometry group of $\mathrm{SO}(n+1)$ acting on S^n. According to this, the representations (of the Lie algebra) of $E(n+1)$ may be found by looking at the infinitesimal generators of the Wigner rotation. In Mackey's language the Wigner rotation corresponds to the matrix element

$$Q_{\mu\nu}(g,q) := \pi^{\chi}_{\mu\nu}((\sigma(q))^{-1} g \sigma(g^{-1}q)), \tag{3.1}$$

representing the rotations in the components of the vector-valued wave function in the induced representation (2.8). (Here we assume for simplicity that q and $g^{-1}q$ are in the same patch, where a single section σ is available.) In the present case $g \in \mathrm{SO}(n+1)$ and q stands for a vector on the sphere S^n embedded in $\mathbb{R}^{n+1}$, and we take the radius of the sphere to be unity, $\Sigma_{\alpha=1}^{n+1}(q^\alpha)^2=1$. In this embedding we adopt the convention that any function on S^n is smoothly extended to $\mathbb{R}^{n+1}$ by continuing the value of the function constantly along the direction of the radius. This implies that any function $f(q)$ defined this way obeys the condition, $q^\alpha \partial_\alpha f(q)=0$, where $\partial_\alpha = \partial/\partial q^\alpha$.

We label the basis of the Lie algebra $\mathrm{so}(n+1)$ by antisymmetric operators $T_{\alpha\beta}$ with α and β running over $1,\ldots,n+1$. The $\mathrm{so}(n)$ subalgebra is identified with the generators T_{ab}, where a and b can take values $1,\ldots,n$. The reductive decomposition $\mathrm{so}(n+1)=\mathrm{so}(n)\oplus\mathfrak{r}$ is then given by $\mathrm{so}(n+1)=\mathrm{span}\{T_{ab}\}\oplus\mathrm{span}\{T_a\}$, where $T_a = T_{a,n+1}$. The commutation relations are then

$$\begin{aligned}
[T_{ab},T_{cd}] &= \delta_{ad}T_{bc} + \delta_{bc}T_{ad} - \delta_{ac}T_{bd} - \delta_{ba}T_{ac}, \\
[T_{ab},T_c] &= \delta_{bc}T_a - \delta_{ac}T_b, \\
[T_a,T_b] &= -T_{ab}.
\end{aligned} \tag{3.2}$$

To make the presentation easier we now omit the label π^χ for the representation used.

Corresponding to the infinitesimal transformation $g = e^{1/2\epsilon_{\alpha\beta}T_{\alpha\beta}} = 1 + \frac{1}{2}\epsilon_{\alpha\beta}T_{\alpha\beta}$ with $\epsilon_{\alpha\beta}$ being real antisymmetric parameters, we have the Wigner rotation

$$Q(g,q) = 1 + \tfrac{1}{2}\epsilon_{\alpha\beta} f_{\alpha\beta}(q), \tag{3.3}$$

where $f_{\alpha\beta}(q)$ are the generators of the rotation. Then, the combination[7]

$$A_\alpha(q) := f_{\alpha\beta}(q) q^\beta, \tag{3.4}$$

is seen to appear in the Hamiltonian in the form covariantly coupled to a particle, and hence is regarded as an induced gauge field. We now show that this gauge field (3.4) is, in fact, the H connection.

To this end, observe first that from (3.1) the generators in (3.3) are given by

$$f_{\alpha\beta}(q) = \sigma^{-1}(q) T_{\alpha\beta} \sigma(q) - \sigma^{-1}(q)\partial_\mu \sigma(q) \left.\frac{\partial q^\mu(\epsilon)}{\partial \epsilon_{\alpha\beta}}\right|_{\epsilon=0}, \tag{3.5}$$

where $q^\mu(\epsilon) := (gq)^\mu = q^\mu + \frac{1}{2}\epsilon_{\alpha\beta}(T^{\rm def}_{\alpha\beta})_{\mu\nu}q^\nu$, and $(T^{\rm def}_{\alpha\beta})_{\mu\nu} = \delta_{\alpha\mu}\delta_{\alpha\nu} - \delta_{\alpha\nu}\delta_{\beta\mu}$ is the defining representation of so$(n+1)$. From this we get

$$\left.\frac{\partial q^\mu(\epsilon)}{\partial \epsilon_{\alpha\beta}}\right|_{\epsilon=0} = \delta^{\alpha\mu}q^\beta - \delta^{\beta\mu}q^\alpha. \tag{3.6}$$

It is then easy to see that under the change of section $\sigma(q)\to\sigma(q)h(q)$ for some $h(q)\in SO(n)$ the gauge field (3.4) transforms as a connection,

$$A_\alpha(q)\to h^{-1}(q)A_\alpha(q)h(q) - h^{-1}(q)\partial_\alpha h(q). \tag{3.7}$$

This is also evident from the expression

$$A_\alpha(q) = \sigma^{-1}(q)T_{\alpha\beta}q^\beta\sigma(q) - \sigma^{-1}(q)\partial_\alpha\sigma(q), \tag{3.8}$$

obtained from the definition (3.4).

Consider now the section

$$\sigma(q) = e^{\theta^a(q)T_a}, \tag{3.9}$$

which provides a local mapping from S^n to $G = \mathrm{SO}(n+1)$. The inverse mapping is given by

$$q^a := \theta^a\,\frac{\sin|\theta|}{|\theta|}, \quad a=1,\ldots,n, \quad q^{n+1} := \cos|\theta|, \tag{3.10}$$

where $\theta^t = (\theta^1,\ldots,\theta^n)$ and $|\theta| = \sqrt{\theta^t\theta} = \sqrt{\Sigma_a(\theta^a)^2}$. With the section (3.9) one finds that the relevant parts of the adjoint matrix (2.18),

$$\begin{aligned}\sigma^{-1}(q)T_{ab}\sigma(q) &= \mathscr{D}^{\ cd}_{ab}T_{cd} + \mathscr{D}^{\ c}_{ab}T_c,\\ \sigma^{-1}(q)T_a\sigma(q) &= \mathscr{D}^{\ bc}_{a}T_{bc} + \mathscr{D}^{\ b}_{a}T_b,\end{aligned} \tag{3.11}$$

take the form[5]

$$\mathscr{D}^{\ bc}_{a} = \tfrac{1}{2}(q^b\delta^c_a - q^c\delta^b_a) \tag{3.12}$$

and

$$\mathscr{D}^{\ cd}_{ab} = \frac{1}{2}\,(\delta^c_a\delta^d_b - \delta^c_b\delta^d_a) + \frac{q_b(q^c\delta^d_a - q^d\delta^c_a) + q_a(q^d\delta^c_b - q^c\delta^d_b)}{2(1+q^{n+1})}. \tag{3.13}$$

To show that (3.8) is the H connection, we note that the $\mathfrak{h}$ part in the first term on the right-hand side of (3.8) vanishes,

$$\sigma^{-1}(q)T_{\alpha\beta}q^\beta\sigma(q)|_{\mathfrak{h}} = 0. \tag{3.14}$$

For $\alpha = n+1$, this is obvious since the middle piece $T_{\alpha\beta}q^\beta$ that is conjugated under $\sigma(q)$ is precisely proportional to the argument in the exponential of $\sigma(q)$; see (3.9) and (3.10). For $\alpha = a \neq n+1$, using (3.12), (3.13) and the antisymmetry of T_{cd}, we have

$$\sigma^{-1}(q)T_{\alpha\beta}q^\beta\sigma(q)|_{\mathfrak{h}} = (q^b\mathscr{D}^{\ cd}_{ab} + q^{n+1}\mathscr{D}^{\ cd}_{a})T_{cd} = 0, \tag{3.15}$$

which establishes (3.14).

Now since the gauge field (3.8) must lie anyway in the space $\mathfrak{h}=\mathrm{so}(n)$ by construction [because it is formed out of the generators of the SO(n) Wigner rotation], we see that the $\mathfrak{r}$ part of the two terms in the right-hand side of (3.8) must precisely cancel each other. Combined with (3.14), this implies that

$$A_\alpha(q)=-\sigma^{-1}(q)\partial_\alpha\sigma(q)|_{\mathfrak{h}}, \tag{3.16}$$

that is, Ohnuki–Kitakato's gauge field (3.4) is, in fact, the H connection (up to the irrelevant sign). In terms of the section (3.9) the H connection reads as

$$\sigma^{-1}(q)d\sigma(q)|_{\mathfrak{h}}=\frac{1}{1+q^{n+1}}\sum_{a,b}^{n} q_a\, dq_b\, T_{ab}, \tag{3.17}$$

which, of course, agrees with the expression found in Ref. 7.

In passing, we mention that in a recent paper[15] it is pointed out that the gauge field (3.4) can be mapped into the ''generalized BPST instanton'' solution found earlier[16]—a solution of the Yang–Mills equation on S^n, which is topologically nontrivial for n even and trivial for n odd. The above result implies that this solution is essentially identical to the H connection, although the meaning of self-duality can change under the mapping. (The confirmation by a direct computation is also given in Ref. 14.)

IV. BERRY'S CONNECTION AS THE *H* CONNECTION

Berry's phase arises in systems where the Hamiltonian has degenerate eigenstates labeled by a collection of parameters, which are identified with the slow degrees of freedom. Adiabatically decoupling the fast variables from these slow ones results in an effective theory with a gauge structure in the slowly varying system.[1] The form of the gauge field that emerges is governed by the geometry of the slow system. In applications the degeneracies reflect a symmetry of the system; hence the slow system is usually identified with a coset space G/H. Such an identification emerges from a Hamiltonian of the form

$$H(q)=U(q)H_0U^{-1}(q), \tag{4.1}$$

where $q\in G/H$ are the slow variables, $U(g)$ is a unitary irreducible representation of G, and H_0 is typically an element of the enveloping algebra of the subgroup H, commuting with the restriction of the representation U to H. It is readily confirmed[3–5] that if we let $U(q)$ be in the form $U(\sigma(q))$, then (2.12) furnishes the eigenstates of the Hamiltonian with $|\chi,\bar{\mu}\rangle$ being the eigenstates of H_0 labeled by some irreducible representation χ of H. Thus, our representation χ is obtained from the given representation of G by restriction to H, followed by a further restriction to an invariant subspace. Using the states (2.12) (again dropping the label α for the patch to which q belongs) Berry's connection reads as

$$\begin{aligned}\sum_m A_m^{\mathrm{Berry}}(q)(T_m)_{\mu\nu}&=\langle q,\chi,\mu|d|q,\chi,\nu\rangle\\ &=\langle\chi,\bar{\mu}|U^{-1}(\sigma(q))dU(\sigma(q))|\chi,\bar{\nu}\rangle\\ &=\sum_i A_i^H(q)(T_i)_{\mu\nu}+\sum_a e_a(q)\\ &\quad\times\langle\chi,\bar{\mu}|U(T_a)|\chi,\bar{\nu}\rangle.\end{aligned} \tag{4.2}$$

The identification of this connection with the H connection clearly depends on whether the final term is zero or not. In applications this term is often set equal to zero by hand.[4,5] That this term is not always zero, though, is best seen through an explicit example.

Consider the situation where the slow variables parametrize a three sphere S^3, now viewed as the coset space SO(4)/SO(3). This would arise, for example, from (4.1) by taking H_0 to be the quadratic Casimir for SO(3). In the Lie algebra of SO(4) we take the reductive decomposition

$$\mathfrak{g}=\mathfrak{h}\oplus\mathfrak{r}=\mathrm{span}\{T_i\}\oplus\mathrm{span}\{T_d\},\quad i,a=1,2,3, \tag{4.3}$$

with the T_i's forming an su(2) algebra, $[T_i,T_j]=\epsilon_{ijk}T_k$, and the remaining commutators being

$$[T_i,T_a]=\epsilon_{iab}T_b \tag{4.4}$$

and

$$[T_a,T_b]=\epsilon_{abi}T_i\,. \tag{4.5}$$

The non-H-connection part of Berry's connection is, in this example, $\Sigma_a e_a\langle jm|T_a|jm'\rangle$, where we have reverted to the familiar notation for the representation of angular momentum. We now show that the matrix element $\langle jm|T_a|jm'\rangle$ need not be zero in general.

For this, we note first that the commutator (4.4) implies that the basis vectors in $\mathfrak{r}$ transform as a vector (spin 1) operator. To emphasize this fact we will, henceforth, denote these operators by ${T_a}^{(1)}$. The Wigner–Eckart theorem then tells us that the m, m', and a dependence of this matrix element resides in the Clebsch–Gordan coefficients $\langle jm'1a|jm\rangle$:

$$\langle jm|{T_a}^{(1)}|jm'\rangle=\langle jm'1a|jm\rangle\langle j\|T^{(1)}\|j\rangle, \tag{4.6}$$

where $\langle j\|T^{(1)}\|j\rangle$ is the reduced matrix element, which is independent of m, m', and a. In terms of the basis $T_\pm:=i(T_1\pm iT_2)$, $T_0:=iT_3$, the Clebsch–Gordan coefficients are given by

$$\langle jm'1a|jm\rangle=\frac{\delta_{m'+a,m}}{\sqrt{j(j+1)}}\begin{cases}\mp\sqrt{(j\pm m)(j\mp m+1)/2}, & \text{if } a=\pm;\\ m, & \text{if } a=0.\end{cases} \tag{4.7}$$

Upon identifying the same a and i, we find that these coefficients are related to the representation matrix elements $\langle jm'|T_i|jm\rangle$ of the $su(2)$ generators T_i, $i=+,-,0$. This allows us to rewrite (4.6) as

$$\langle jm|T_a^{(1)}|jm'\rangle=a_j\langle jm'|T_i|jm\rangle, \tag{4.8}$$

where the prefactor a_j is

$$a_j=-\frac{\langle j\|T^{(1)}\|j\rangle}{\sqrt{j(j+1)}}. \tag{4.9}$$

We recall that the action of any vector operator on the state $|jm'\rangle$ is determined by two reduced matrix elements. For $T^{(1)}$ these are a_j and the reduced matrix element $\langle j-1\|T^{(1)}\|j\rangle$. However, the action of $T^{(1)}$ is also fixed by the fact that it comes from a representation of SO(4). Exploiting these two facts allows us to determine the allowed values for a_j.

The irreducible unitary representations of SO(4) are labeled by two numbers (k_0,c), where $k_0=0,\ \frac{1}{2},\ 1,\ \frac{3}{2},\ldots$, and $c=\pm(k_1+1)$ with $k_1=k_0,k_0+1,k_0+2,\ldots$. (For a clear account of this see Ref. 17.) The representation space is then decomposed into the direct sum

$$\mathscr{R}(k_0,c)=\bigoplus_{j=k_0}^{k_1}\mathscr{R}^j, \tag{4.10}$$

of the irreducible representations $\mathscr{R}^j$ of SO(3) spanned by the angular momentum states, $|jm\rangle$, $m=-j,\ldots,j$. In such a representation one finds that a_j is given by

$$a_j=\frac{k_0c}{j(j+1)}. \tag{4.11}$$

From this we deduce that if $k_0\neq 0$, then Berry's connection does not correspond to the H connection.

This example can be extended to more general coset spaces in much the same way by using the generalized Wigner–Eckart theorem (see, for example, Ref. 18). The conclusion reached is that, in general, Berry's connection is not the H connection. The question we now want to address is what additional structures are needed in order to ensure that they do coincide. To motivate our analysis of this problem it is again useful to return to the three sphere example discussed above.

From (4.11) we see that the relevant reduced matrix element vanishes only when $k_0=0$. In this case (and only in this case) the representations $(k_0=0,c)$ and $(k_0=0,-c)$ of SO(4) are unitarily equivalent (there is no parity doubling[17]). The representation space becomes the direct sum,

$$\mathscr{R}(0,n)=\bigoplus_{j=0}^{n-1}\mathscr{R}^j, \quad \text{where } n=1,2,\ldots . \tag{4.12}$$

The action of T_i on $\mathscr{R}^j$ is the standard one, changing the value of m by ± 1. From (4.4) one can also show that the action of $T_a^{(1)}$ on $\mathscr{R}^j$ changes the value of j by ± 1. Thus, the state $|jm\rangle=|n-1,n-1\rangle$ is both a highest weight vector for the irreducible representation on $\mathscr{R}^{n-1}$ of SO(3), and for the irreducible representation on $\mathscr{R}(0,n)$ of SO(4). This cannot hold for any of the other $(k_0\neq 0)$ representations of SO(4) since the parity doubling found in those representations would then imply that such a vector was a highest weight for two inequivalent representations.

We shall use this example as a motivation for the following restriction on the allowed states $|\chi,\overline{\mu}\rangle$ that occur in (4.2). Recall first that by definition the reference basis states satisfy

$$U(h)|\chi,\bar{\mu}\rangle=\sum_{\nu}|\chi,\bar{\nu}\rangle\pi^{\chi}_{\nu\mu}(h), \quad \text{for } h\in H. \tag{4.13}$$

Let Λ be the highest weight labeling the representation of the group G in question. We shall consider the *highest subspace* $\mathscr{H}_\Lambda$, which is the subspace of the representation space $\mathscr{H}$ of G realizing (4.13) and also contains the vector $|\Lambda\rangle$ corresponding to the highest weight. We then claim that, for a wide class of systems, by choosing the subspace as a highest subspace we will manage to obtain merely the $\mathfrak{h}$ part of Berry's connection. To prove this it is convenient to develop an alternative description of the highest subspace $\mathscr{H}_\Lambda$.

For this, let us restrict ourselves to cosets G/H, where the subgroup H is given by the centralizer S_K of some element $K\in\mathfrak{g}$. This corresponds to the Hamiltonian (4.1) whose parameter space is the coadjoint orbit of the group G passing through K discussed in Refs. 3 and 5. If K is a regular semisimple element[19] of $\mathfrak{g}$, then H in this case is just the Cartan subgroup T regarded as the maximal torus containing K, but if not then H is greater than T. Let Σ be the root system of G relative to T, and let Σ_K be the root system of H relative to T. By considering the complexification $\mathfrak{g}_c$ of $\mathfrak{g}$ we have the Cartan decomposition,

$$\mathfrak{g}_c=\mathfrak{t}_c\oplus\sum_{\alpha\in\Sigma}\mathfrak{g}_\alpha, \tag{4.14}$$

where $\mathfrak{t}_c$ is the complexification of the Cartan subalgebra $\mathfrak{t}$, and $\mathfrak{g}_\alpha$ is the root space corresponding to the root α. Similarly, we have

$$\mathfrak{h}_c = \mathfrak{t}_c \oplus \sum_{\alpha \in \Sigma_K} \mathfrak{h}_\alpha . \tag{4.15}$$

Next, let W be a Weyl chamber of $\mathfrak{t}$ relative to G, and W_K be a Weyl chamber of $\mathfrak{t}$ relative to H. We can define the positive roots Σ^+ (Σ_K^+) of Σ (Σ_K) with respect to W (W_K). It is then guaranteed[20] that there exists a "K admissible Weyl chamber," satisfying (i) $\Sigma^+ \cap \Sigma_K = \Sigma_K^+$ and (ii) if $\alpha \in \Sigma^+ - \Sigma_K^+$, $\beta \in \Sigma_K$ and $\alpha + \beta \in \Sigma$, then $\alpha + \beta \in \Sigma - \Sigma_K^+$.

Armed with this, we then show that the highest subspace $\mathscr{H}_\Lambda$ can alternatively be characterized by

$$\mathscr{H}_\Lambda = \{ |\phi\rangle \in \mathscr{H} \mid \ U(T_\alpha)|\phi\rangle = 0, \quad \forall \alpha \in \Sigma^+ - \Sigma_K^+ \}. \tag{4.16}$$

Note first that the states defined by (4.16) are invariant under the action of H in $\mathscr{H}$. Indeed, for those generators of $\mathfrak{h}$ belonging to the Cartan subalgebra $\mathfrak{t}$ this is obvious since for $T_i \in t$, $[T_i, T_\alpha] = \alpha(T_i) T_\alpha$. If T_β is a generator of $\mathfrak{h}$ not in $\mathfrak{t}$ then, using the reductivity of the decomposition $\mathfrak{g} = \mathfrak{h} \oplus \mathfrak{r}$, we get, for $\alpha \in \Sigma^+ - \Sigma_K^+$,

$$U(T_\alpha)U(T_\beta)|\phi\rangle = U(T_\beta)U(T_\alpha)|\phi\rangle + U([T_\alpha, T_\beta])|\phi\rangle = C_{\alpha\beta}^{\alpha+\beta} U(T_{\alpha+\beta})|\phi\rangle, \tag{4.17}$$

which vanishes since $\alpha + \beta \in \Sigma^+ - \Sigma_K^+$.

Second, the unitary action in (4.16) is also irreducible. To see this, suppose that it is reducible. Then there exists some $|\Omega\rangle \neq |\Lambda\rangle$ for which

$$U(T_\beta)|\Omega\rangle = 0, \quad \text{for } \beta \in \Sigma_K^+ , \tag{4.18}$$

i.e., $U(T_\beta)$ is a step operator in $\mathfrak{h}$ annihilating this state. It then follows that both the operators $U(T_\alpha)$ and $U(T_\beta)$, where $\alpha \in \Sigma^+ - \Sigma_K^+$ and $\beta \in \Sigma_K^+$, annihilate $|\Omega\rangle$. Hence, this state is annihilated by any $U(T_\alpha)$ for $\alpha \in \Sigma^+$, which implies that $|\Omega\rangle$ is a highest weight. But since we cannot have two highest weights, we see that $\mathscr{H}_\Lambda$ defined by (4.16) is irreducible and hence must be the highest subspace satisfying (4.13).

Having established (4.16), we now find, for such highest subspace states,

$$\sum_{\alpha \in \Sigma - \Sigma_K} e_\alpha(q) \langle \chi, \bar{\mu} | U(T_\alpha) | \chi, \bar{\nu} \rangle = 0, \tag{4.19}$$

on account of $T_{-\alpha} = T_\alpha{}^\dagger$. Clearly, then, we can conclude that if a highest subspace is used in the construction of Berry's connection, then there will be no $\mathfrak{r}$ part, and hence it will be the H connection—the claim we wished to prove.

V. CONCLUSIONS AND DISCUSSIONS

In this paper we have argued that the induced connection that appears on a coset space in Mackey's quantization scheme admits a natural interpretation, that is, it arises from the homogeneity criterion required for the Hamiltonian. This led to an alternative account from Ref. 2 of why the Hamiltonian on G/H involves the induced H connection. Being geometrical, our criterion will be useful, even in other quantization approaches and, possibly, in attempts at extending the quantization scheme to field theories. Indeed, we have shown that the gauge field induced in a slightly different approach[7] is again the H connection—a fact suggesting a universal feature of the quantum theory on such topologically nontrivial spaces. In connection with this, it is worth mentioning

that even in the ''confining approach''[21] to quantization, which is totally different from Mackey's approach, one can still observe an induced gauge field, which is also appears to be of the type of the H connection.[8,9]

The appearance of the H connection in the other context—Berry's phase—was then analyzed in the setting where the parameter space is given by a coset space G/H. We have seen that Berry's connection becomes the H connection if the energy eigenspace we are looking at possesses the highest weight state of the unitary representation of the group G that characterizes the system. Notice also that such highest subspaces can be used to define the so-called vectorial coherent states[22] for the group G. Indeed, by choosing the states $|\chi,\overline{\mu}\rangle$ as the ones belonging to a highest subspace, the states of (2.12) become the vectorial coherent states. The physical implications of this condition for the energy eigenspaces need to be investigated, but we have at least seen an interesting fact that in such cases the effective theory describing the slow variables bears an unexpected resemblance with the quantum theory on coset spaces.

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Poisson brackets of Wilson loops and derivations of free algebras

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We describe a finite analog of the Poisson algebra of Wilson loops in Yang–Mills theory. It is shown that this algebra arises in an apparently completely different context: as a Lie algebra of vector fields on a noncommutative space. This suggests that noncommutative geometry plays a fundamental role in the manifestly gauge invariant formulation of Yang–Mills theory. We also construct the deformation of the algebra of loops induced by quantization, in the large-N_c limit. © *1996 American Institute of Physics.* [S0022-2488(96)03001-5]

I. ALGEBRAS OF WILSON LOOPS

A central problem of particle physics is to find a formulation of Yang–Mills theory in terms of gauge invariant variables. There is a large amount of literature on this subject, starting with pioneering work of Mandelstam.[1] Such a reformulation of Yang–Mills theory must involve as yet unknown geometrical principles, as the principle of gauge invariance would be empty. We should discover these geometrical structures by starting with the conventional formalism of gauge theory and rewriting it in terms of gauge invariant variables. A loose analogy can be made with the process by which symplectic geometry was discovered to be the foundation of classical mechanics.

In this article we will show that the fundamental Poisson brackets of Yang–Mills theory have an interpretation as an algebra of vector fields in a noncommutative space, a sort of noncommutative generalization of the Virasoro algebra. The precise mathematical formulation is possible only for a finite (regularized) version of the theory, but the ideas extend in a formal way to the continuum theory.

A natural choice of gauge invariant variable in Yang–Mills theory is the Wilson loop variable. It is just the trace of the parallel transport operator around a loop. We can describe the symplectic structure of classical Yang–Mills theory in terms of Poisson brackets of these variables. However, in the usual canonical formalism, where initial data is given on a spacelike surface, this leads to either a trivial answer or to an impossibly complicated one. If the loop lies entirely on a spacelike surface, the Poisson brackets will vanish since the components of the gauge field on a spacelike surface commute: they are like the q variables of classical mechanics. If the loop has a finite extension into the timelike direction on the other hand, the Poisson brackets cannot be obtained without solving the equations of motion: this is like asking for $\{q(t),q(t')\}$ at unequal times in classical mechanics. One way around this impasse is to introduce loop variables involving the electric field (which is the canonical conjugate of the Yang–Mills potential) but this does not have the elegance and simplicity of a formalism involving Wilson loop variables alone.

We showed in some recent papers[2] that the Wilson loops in classical Yang–Mills theory which lie on a null surface satisfy simple Poisson brackets. (There is also a large amount of literature on the null cone formalism for gauge theories. See, e.g., Ref. 3.) In a formalism in which initial data is given on null surfaces there is thus a natural way of encoding the canonical structure of

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Yang–Mills theory in terms of gauge invariant variables. In this article we will show that an analog of this Loop algebra arises as derivations of the free algebra on a finite number of variables. This allows us to construct a Lie group of which the finite loop algebra is the Lie algebra. Moreover, we will construct a symplectic realization analogous to the realization on the Yang–Mills phase space. We will also obtain a quantum deformation of this algebra and obtain the contraction corresponding to the large-N_c limit. It is conjectured that this large-N_c limit algebra also has a symplectic realization, but we are as yet unable to construct it. This would be of great interest in Yang–Mills theory, as it would help us discover the phase space of gauge invariant observables of that theory.

We will reserve the phrase ''loop algebra'' to describe the algebras formed by Wilson loops in gauge theories. This should not be confused with another meaning of this term often found in the literature: the Lie algebra of the so-called loop group, the group of functions from a circle to a Lie group.

Let us now describe the situation a little more explicitly.[2] We will consider pure Yang–Mills theory on flat Minkowski space, with initial data given on a null cone. The field will then be determined at all points in the future of the cone by the Yang–Mills equations. (See Ref. 2 for details.) It will be particularly convenient to choose as initial surface the null cone at past timelike infinity (called $\mathscr{I}^-$ in Ref. 4) so that all points not on the cone are in its future. (This will also restore spatial translation invariance.) This can be accomplished by using a conformally equivalent metric

$$\hat{d}s^2 = dU(dU+2dR) - \sin^2 R q_{ij}(z)dz^i\, dz^j \tag{1}$$

instead of the flat metric on Minkowski space. (Here, q_{ij} is the standard metric on S^2.) Yang–Mills equations are conformally invariant in four dimensions, so this conformal change of the metric will not change the theory. $\partial/\partial U$ is a timelike vector and $\partial/\partial R$ is a null vector. We will regard $\partial/\partial U$ as defining the time direction. Also, Minkowski space corresponds to the region

$$-\pi < U < \pi \quad -\pi < U+2R < \pi. \tag{2}$$

The null cone at past timelike infinity $\mathscr{I}^-$ will be the surface $U=-\pi$.

Since the Yang–Mills equations are of first order in the time variable U, initial data consist of prescribing the value of the gauge potential on $\mathscr{I}^-$. We can set $A_R=0$, by a choice of gauge. Also, A_U is just a Lagrange multiplier (its time derivative does not appear in the Lagrangian) so that the dynamical variables are the transverse components A_i. The main simplification of the null formalism is that these variables are in a sense canonically conjugate to each other with equal time Poisson brackets

$$\{A^a_{ib}(z,R),A^c_{jd}(z',R')\} = \tfrac{1}{2}\delta^a_d\delta^c_b q_{ij}(z)\,\delta(z-z')\,\mathrm{sgn}(R-R'). \tag{3}$$

Here $a,b=1,2,\ldots,N_c$. We will consider the gauge group to be U(N_c) so that the matrices A_i are Hermitian. These Poisson brackets follow from the Yang–Mills action by a straight forward application of the canonical formalism.

We thus define the inverse of the symplectic form on the phase space of Yang–Mills theory:

$$\omega^{ab}_{ijcd}(z,R,z',R') = \delta^a_d\delta^b_c\omega_{ij}(z,R,z',R'), \tag{4}$$

where

$$\omega_{ij}(z,R,z',R') = \tfrac{1}{2}q_{ij}(z)\,\delta(z-z')\,\mathrm{sgn}(R-R'). \tag{5}$$

Now let $\xi: S^1 \to \mathscr{I}^-$ be a closed curve on the light cone. Given a Yang–Mills field A, we can define a complex valued function $W[\xi]$ on the space of closed curves, the trace of the parallel transport operator (holonomy) in the basic N_c dimensional representation. In the case of $U(N_c)$, this loop variable is complex valued, but it satisfies the condition

$$W[\bar{\xi}] = W^*[\xi], \tag{6}$$

where $\bar{\xi}$ is the curve ξ with the opposite orientation.

This $W[\xi]$ is the "Wilson loop" associated to this Yang–Mills configuration. For each ξ, $W[\xi]$ is a function on the Yang–Mills phase space so that it is possible to compute the Poisson bracket of a pair of loop variables. We will get

$$\{W[\xi], W[\tilde{\xi}]\} = \int ds\ dt\ \dot{\xi}^i(s)\dot{\tilde{\xi}}^j(t)\omega_{ij}(\xi(s), \tilde{\xi}(t)) W[\xi \circ_{st} \tilde{\xi}].$$

Due to the delta function in the symplectic form, only points s,t where $\xi^i(s) = \tilde{\xi}^i(t)$ will contribute to the integral; i.e., the projections of the curves to the sphere must intersect at parameter value s for the first curve and t for the second. There will be a null line segment joining the points $\xi(s)$ and $\tilde{\xi}(t)$ for this intersection. In this case, $\xi \circ_{st} \tilde{\xi}$ is the product curve, defined as follows: describe the curve ξ starting and ending at s; jump to the point $\tilde{\xi}(t)$ along the null line segment; describe the curve $\tilde{\xi}$ starting and ending at $\tilde{\xi}(t)$; jump back to $\xi(s)$ along the null segment. Thus the product is also a closed curve. The pieces of the curve along null lines will not contribute to $W[\xi \circ_{st} \tilde{\xi}]$ since we have chosen a gauge where the null component of the gauge field vanishes. Also, there will be generically only a finite number of intersection points, so that the integral on the right-hand side can be actually evaluated to yield a finite sum. We will not need the explicit expression, which is given in Ref. 2. This last property depends on the dimension of space–time being four; in higher than four dimensions generically there are no intersections while in lower dimensions there is a continuum of such intersections.

The Poisson brackets above could have been motivated based purely on the geometry of loops on the null cone. Causality requires that loops on a null cone which have no intersections when projected to the spacelike surface must commute. This explains the delta function in $\omega(z,R,z',R')$. The factor sgn $(R-R')$ is also natural, as it simply keeps track of which event is to the future along the null direction, and makes the bracket antisymmetric.

Indeed, geometrically, these are the most natural definitions possible for ω as well as the product of the loops. Note that the bracket is invariant under the change of parametrization of the loop. In fact the right-hand side will only depend on q_{ij} only through the angle of intersection of the tangent vectors $\dot{\xi}(s), \dot{\tilde{\xi}}(t)$; thus the algebra is invariant under conformal transformation of the metric on the two sphere. But every metric on the two sphere is conformal to the standard one, so we see that the algebra is in fact independent of the choice of metric also.

Once the Poisson brackets are postulated, the Jacobi identity can be proved directly. The Yang–Mills phase space then arises as the solutions of some algebraic constraints satisfied by the loop variables, due to Mandelstam. We proposed that these constraints be viewed as describing the coadjoint orbits of the above Lie algebra. In this way, Yang–Mills theories with different unitary groups as gauge groups, would arise as different realizations of the same universal Lie algebra. For more details we refer the reader to Ref. 2.

We would like to understand the above Lie algebra of loops better. In particular we would like to have a finite analog which can be studied by more rigorous methods; also it would be good to have a different situation in which this loop algebra arises so that we can have a point of view to Yang–Mills theory not based on the gauge group. Another natural object to study is the group associated to the above Loop algebra. Finally it is very important to understand the quantum deformations of this algebra and its large-N_c limit. In this paper we will in fact arrive at a finite

analog of the loop algebras and their groups, starting from considerations quite different from Yang–Mills theories; i.e., the derivations and automorphisms of free algebras. We will also construct a quantum deformation and its large-N_c limit.

Another situation where Poisson brackets of Wilson loops appears is in Chern–Simons theory. There, also, the spatial components of the gauge field are canonically conjugate to each other; the Wilson loops on a spacelike 2-surface satisfy the above algebra except that

$$\omega_{i,j}(z,z') = \epsilon_{ij}(z)\,\delta^2(z-z'), \tag{7}$$

where $\epsilon_{ij}(z)dz^i \wedge dz^j$ is the volume form on the spacelike surface. The product of loops relative to a pair of coincident points is defined as before as one loop followed by the other. Thus our considerations should also be of interest in the context of topological field theories.

II. THE FREE ALGEBRA AND ITS AUTOMORPHISMS

Let $\mathscr{T}_M$ be the real free algebra on M variables.[5] It is a graded vector space, the part of order m (for $m=0,1,2,...$) being just the set of all tensors of type $(0,m)$ on an M-dimensional real vector space. Note that no symmetry of any kind is required on these tensors. The multiplication rule on the algebra is defined by the direct (or tensor) product. $\mathscr{T}_M$ is a noncommutative but associative algebra with identity.

More explicitly, introduce variables ξ^i for $i=1,\ldots,M$ satisfying no relations whatever. A typical element of $\mathscr{T}_M$ is a polynomial in these variables,

$$T(\xi) = \sum_{m=0}^{\infty} T_{i_1 i_2,\ldots,i_m}\xi^{i_1}\xi^{i_2},\ldots,\xi^{i_m}. \tag{8}$$

$T_{i_1 i_2,\ldots,i_m}$ are the components with respect to some basis in R^M of a tensor T of type $(0,m)$. Since $T(\xi)$ is assumed to be a polynomial, only a finite number of terms on the right-hand side of the above series are nonzero: only a finite number of the tensors $T_{i_1,\ldots,i_m}$ are nonzero.

In this language, multiplication is defined as follows:

$$(ST)(\xi) = \sum_{m,n=0} S_{i_1,\ldots,i_m} T_{j_1,\ldots,j_n}\xi^{i_1},\ldots,\xi^{i_m}\xi^{j_1},\ldots,\xi^{j_n}. \tag{9}$$

There is no problem with convergence of the series since only a finite number of terms are nonzero. In fact this comment applies to almost all the formally infinite series below. (The exception is where we speak of inverting a transformation of the variables.)

If these variables ξ had commuted with each other, the algebra would just have been the commutative algebra of functions (polynomials) on R^M. The tensors would all have been symmetric and multiplication would have been the symmetrized tensor product. This algebra has as automorphisms the group of diffeomorphisms of R^M. (Actually a diffeomorphism will in general map a polynomial to an infinite series, so we will really need $\mathscr{T}_M$ to extend to an appropriate topological vector space to make this possible.) Infinitesimally, this would correspond to the Lie algebra of vector fields, whose components are polynomials, which form the derivations of the commutative algebra.

Thus we can regard $\mathscr{T}_M$ as the set of ''functions'' on a noncommutative space in the spirit of noncommutative geometry.[6] This is perhaps the most noncommutative case in the sense that the coordinates satisfy no relations at all. Now let us determine the Lie algebra of derivations $\mathscr{V}_M$ which will be the noncommutative analog of the algebra of vector fields. A derivation v is determined by its effect on the generators:

$$v(\xi)^i=\sum_{m=1} v^i_{i_1,\ldots,i_m}\xi^{i_1},\ldots,\xi^{i_m}, \tag{10}$$

where it is assumed that only a finite number of terms in the sum are nonzero. The effect of v on an arbitrary element of $\mathscr{T}_M$ is given by the Leibnitz rule:

$$v(T)(\xi)=\sum_{m,n=1}^{\infty}\sum_{k=1}^{m} T_{i_1,\ldots,i_m}v^{i_k}_{j_1,\ldots,j_n}\xi^{i_1},\ldots,\xi^{i_{k-1}}\xi^{j_1},\ldots,\xi^{j_n}\xi^{i_{k+1}},\ldots,\xi^{i_m}. \tag{11}$$

A basis (analogous to the Weyl basis for $gl(M)$) for $\mathscr{V}_M$ is given by the elements $E_i^{i_1,\ldots,i_m}$ defined by

$$E_i^{i_1,\ldots,i_m}(\xi)^j=\delta_i^j\xi^{i_1},\ldots,\xi^{i_m}. \tag{12}$$

In the commutative case they correspond to the vector fields $\xi^{i_1},\ldots,\xi^{i_m}(\partial/\partial\xi^i)$. They satisfy the commutation relations

$$[E_i^{i_1,\ldots,i_m},E_j^{j_1,\ldots,j_n}]=\sum_{l=1}^{n}\delta_i^{j_l}E_j^{j_1,\ldots,j_{l-1}i_1,\ldots,i_m j_{l+1},\ldots,j_n}-\sum_{k=1}^{m}\delta_j^{i_k}E_i^{i_k,\ldots,i_{k-1}j_1,\ldots,j_n i_{k+1},\ldots,i_m}.$$

In the special case $M=1$, all the noncommutativity dissappears, and $\mathscr{V}_1$ is just the algebra of polynomial vector fields on the real line. Since all the indices must take the value 1, there is just one generator with m superscripts. Suppose we call it L_{m-1} for $m=0,1,\ldots$. Then the above commutation relation becomes

$$[L_m,L_n]=(n-m)L_{m+n}\quad\text{for } m=-1,0,1,2,\ldots\ . \tag{13}$$

This is just the subalgebra of the Virasoro algebra on which the central term vanishes. Thus our algebras are, in a sense, generalizations of this familiar algebra.

Now let g_{ij} be a symmetric positive tensor on R^M and define $\mathscr{V}_M^-$ to be the subalgebra of tensors that preserve the element $g(\xi)=|\xi|^2=g_{ij}\xi^i\xi^j$. In the commutative case these are all the vector fields tangential to the spheres centered at the origin; these preserve the distance function $|\xi|^2$. The simplest among these are the rotations. In the case of a free algebra, we can see easily that the algebra $\mathscr{V}_M^-$ consists of the set of all elements of the form

$$v^i_{i_1,\ldots,i_m}=g^{ii_0}w_{i_0i_1,\ldots,i_m}, \tag{14}$$

where $w_{i_0i_1,\ldots,i_m}$ is a *cyclically antisymmetric tensor*. Of course such tensors exist only when m is odd. There is a basis for $\mathscr{V}_M^-$,

$$G^{i_0,\ldots,i_m}=\sum_{k=0}^{m}(-1)^k g^{i_kj}E_j^{i_{k+1},\ldots,i_0i_m,\ldots,i_{k-1}} \tag{15}$$

in which the Lie brackets become

$$[G^{i_0,\ldots,i_m},G^{j_0,\ldots,j_n}]=\sum_{k,l=0}^{k=m,l=n}(-1)^{k+l+1}g^{i_kj_l}G^{i_{k+1},\ldots,i_mi_1,\ldots,i_{k-1}j_{l+1},\ldots,j_nj_1,\ldots,j_{l-1}}. \tag{16}$$

In an exactly analogous fashion, let ω be an antisymmetric nondegenerate tensor. (Clearly this exists only if M is even, which will be assumed in the following.) This defines an element

$$\omega(\xi)=\omega_{ij}\xi^i\xi^j. \tag{17}$$

This is a symplectic analog of the distance function. This would have vanished identically in the commutative case.

The subalgebra $\mathscr{V}_M^+$ which preserves $\omega(\xi)$ is just the set of elements such that

$$v^i_{i_1,\ldots,i_m}=\omega^{ii_0}w_{i_0i_1,\ldots,i_m}, \tag{18}$$

where $w_{i_0i_1,\ldots,i_m}$ is a *cyclically symmetric* tensor. There is a basis for $\mathscr{V}_M^+$,

$$F^{i_1,\ldots,i_m}=\sum_{k=1}^{m}\omega^{i_kj}E^{i_{k+1},\ldots,i_1i_m,\ldots,i_{k-1}}_j \tag{19}$$

in which the Lie brackets become

$$[F^{i_1,\ldots,i_m},F^{j_1,\ldots,j_n}]=\sum_{k,l=1}^{k=m,l=n}\omega^{i_kj_l}F^{i_{k+1},\ldots,i_mi_1,\ldots,i_{k-1}j_{l+1},\ldots,j_nj_1,\ldots,j_{l-1}}. \tag{20}$$

Now we will show that this algebra is just a finite version of the loop algebra we found for Wilson loops. Let us think of the index $I=i_1,\ldots,i_m$ on the F^I variable as a map $I:Z_m\to\{1,\ldots,M\}$. Due to cyclic symmetry, this can be viewed as a ''loop'' from the cyclic permutation group Z_m (which is a discrete model for the circle) to a space which contains just a finite number M of points. The product of two loops at point k,l is defined as the loop I starting at i_{k+1} and ending at i_{k-1} followed by the loop J starting at j_{l+1} and ending at j_{l-1}:

$$I\circ_{kl}J=i_{k+1},\ldots,i_mi_1,\ldots,i_{k-1}j_{l+1},\ldots,j_nj_1,\ldots,j_{l-1}. \tag{21}$$

This is just the discrete analog of the product we introduced earlier. The commutation relations of the Lie algebra $\mathscr{V}_M^+$ are then

$$[F^I,\ F^J]=\sum_{kl}\omega^{i_kj_l}F^{I\circ_{kl}J}. \tag{22}$$

The Wilson loop algebra can be understood as the limiting case where the finite set Z_m is replaced by S^1 and the set $\{1,2,\ldots,M\}$ is replaced by the light cone $S^2\times R^+$. Thus by studying the algebra $\mathscr{V}_M^+$ we are studying a finite model for the algebra of Wilson loops. The algebras $\mathscr{V}_M$, $\mathscr{V}_M^-$, $\mathscr{V}_M^+$ are all graded Lie algebras. The point is that the Lie bracket of a tensor with m indices and one of with n indices has $m+n-2$ indices. Thus if we assign a grade of $m-1$ to the space of tensors with m indices, we have a graded Lie algebra. The range of the grading is $-1,0,1,2$; the space of grade -1, if nonempty, is a subalgebra with vanishing brackets.

Although we have introduced $\mathscr{V}_M^+$ as a complex Lie algebra, its unitary form, obtained by imposing

$$v_I^*=v_{\bar{I}} \tag{23}$$

on the coefficients of an element $v=\Sigma v_IF^I$, will be of particular interest. To save on notation we will also call this real Lie algebra $\mathscr{V}_M^+$. Here,

$$\bar{I}=i_mi_{m-1},\ldots,i_1 \tag{24}$$

is the loop with the opposite orientation. The conjugation $v_I\to v_I^*$ is an antilinear involution of the complex algebra, therefore it makes sense to talk about its unitary form.

The algebra $\mathscr{V}_M^-$ is the finite analog of the commutation relations of the Wilson loop in supersymmetric Yang–Mills theory. In the case of supersymmetric QCD in two dimensions, e.g., the bosonic components of the gauge field can be removed by gauge fixing, and the analog of the Wilson loop variables involve only the fermionic fields in the adjoint representation. Thus it is of equal interest to study $\mathscr{V}_M^-$; we can develop the two cases in parallel; but mostly we will speak of $\mathscr{V}_M^+$.

III. AUTOMORPHISM GROUPS $G_M^{\pm}$

It is now possible to understand the Lie groups of which $\mathscr{V}_M^{\pm}$ are Lie algebras. Thus, we will solve in a finite context the problem of exponentiating the Lie algebra of Wilson loops.

First of all, let us consider a group of which $\mathscr{V}_M$ is the Lie algebra. Consider the vector space of tensors of type $(1,m)$ for $m=0,1,...$. In terms of the variables ξ^i, a typical element would be

$$\phi^i(\xi)=\sum_{m=1}^{\infty}\phi^i_{i_1,\ldots,i_m}\xi^{i_1},\ldots,\xi^{i_m}. \tag{25}$$

Define the composition law of such functions of ξ in the obvious way:

$$(\tilde{\phi}\circ\phi)^i(\xi)=\sum_{m=0}^{\infty}\tilde{\phi}^i_{i_1,\ldots,i_m}\phi(\xi)^{i_1},\ldots,\phi(\xi)^{i_m}. \tag{26}$$

This operation is clearly associative and has identity.

If we now restrict to the subset of functions ϕ such that the first tensor in the series above, is invertible,

$$G_M=\{\phi|\det\ \phi^i_j\neq 0\} \tag{27}$$

we have a group under the above composition law. To see this, we note that given any such ϕ, a unique inverse ψ can be constructed solving the equation

$$\psi^i(\phi)(\xi)=\xi^i \tag{28}$$

recursively:

$$\psi^i_j\phi^j_k=\delta^i_k,$$

$$\psi^i_j\phi^j_{j_1j_2}+\psi^i_{i_1i_2}\phi^{i_1}_{j_1}\phi^{i_2}_{j_2}=0,$$

etc. The term of order m will determine $\psi^i_{i_1,\ldots,i_m}$ in terms of lower order components of ψ thus establishing the existence and uniqueness of an inverse. In general, ψ will have an infinite number of nonzero terms even when ϕ is a polynomial. [We must enlarge our space of allowed transformations to include infinite series, in order to be able to define an inverse. We do not address the issue of convergence of these series, although it should be possible to define an appropriate topology on the space of such series with respect to which G_M is a Lie group. The Lie algebra of G_M will in fact be the completion of our polynomial derivations $\mathscr{V}_M$ in such a topology.] This is an algebraic analog of the inverse function theorem: ϕ^i_j is the analog of the derivative at the origin of the function $\phi^i(\xi)$, so that if it is invertible, we should expect ϕ to be invertible at least locally.

Thus G_M is a group under the above composition law; by infinitesimalizing the composition law we see that this group has as Lie algebra $\mathscr{V}_M$. We see that G_M is a noncommutative analog of the diffeomorphism group of R^M.

Now it is clear that groups of which the Lie algebras are $\mathscr{V}_M^{\pm}$ may be defined as below:

$$G_M^- = \{\phi | \det\ \phi_j^i \neq 0; g_{ij}\phi^i(\xi)\phi^j(\xi) = g_{ij}\xi^i\xi^j\},$$

$$G_M^+ = \{\phi | \det\ \phi_j^i \neq 0; \omega_{ij}\phi^i(\xi)\phi^j(\xi) = \omega_{ij}\xi^i\xi^j\}$$

which are just the conditions for the distance functions to be invariant.

IV. SYMPLECTIC REALIZATIONS

It would obviously be interesting to look at representations of the above loop algebras. This should be interesting, e.g., in the quantum Yang–Mills theory. However, it is quite possible that the relevant algebras are different in the quantum theory: quantization could deform the algebra itself. Therefore we first study the classical analog of a representation, a realization of the Lie algebra $\mathscr{V}_M^+$ in terms of Poisson brackets of some functions on symplectic space.

Let η_b^{ia} be a set of complex variables satisfying the Hermiticity condition

$$\eta_b^{ia*} = \eta_a^{ib}. \tag{29}$$

Here, $i = 1,\ldots,M$ and $a,b = 1,\ldots,N_c$ for some positive integer N_c. We will consider only the case of even M. (The indices a and b will be called color indices, since we will soon see an analogy to Yang–Mills theory.) Now impose the Poisson brackets

$$\{\eta_b^{ia}, \eta_d^{jc}\} = \omega^{ij}\delta_d^a\delta_b^c. \tag{30}$$

Thus we are just considering the real vector space $R^{MN_c^2}$ with a symplectic form that is invariant under the adjoint action of $U(N_c)$. Now consider the space of polynomials invariant under the adjoint action of $U(N_c)$. A basis for this space is labeled by a discrete loop $I: Z_m \to \{1,2,\ldots,M\}$:

$$f^I(\eta) = \mathrm{Tr}\ \eta^{i_1}\eta^{i_2},\ldots,\eta^{i_m}. \tag{31}$$

The cyclic symmetry of the trace assures us that f^I is independent of the starting point of the loop I. Moreover,

$$f^{I*} = f^{\bar{I}}. \tag{32}$$

This implies that the coefficients a_I of an element $a = \Sigma a_I f^I$ are complex numbers satisfying $a_I^* = a_{\bar{I}}$.

Now it is a simple matter to verify that the Poisson brackets of these functions provide a realization of the Lie algebra $\mathscr{V}_M^+$:

$$\{f^I, f^J\} = \sum_{kl}\ \omega^{i_k, j_l} f^{I\circ_{k,l}J}. \tag{33}$$

The analogy of this realization with the Poisson brackets of the Wilson loops is obvious.

At the level of the group, we also have an action of the group on invariant polynomials of the variables η^j by a sort of "pull-back":

$$\phi^*(h)(\eta) = h(\psi(\eta)), \tag{34}$$

where ψ is the inverse of ϕ and

$$[\psi(\eta)]^i = \sum_{m=1}\ \psi^i_{i_1,\ldots,i_m}\eta^{i_1},\ldots,\eta^{i_m} \tag{35}$$

matrix multiplication being implied on the right-hand side. If we restrict to the subgroup G_M^+ the matrix valued function $\omega_{ij}\eta^i\eta^j$ is invariant under this action. This ''symplectic distance'' function has an obvious meaning in this realization: it is the generator of infinitesimal gauge transformations. If u is a constant anti-Hermitian matrix,

$$\{\mathrm{Tr}\ u\omega_{ij}\eta^i\eta^j, \eta^k\} = [u, \eta^k] \tag{36}$$

so that the traces $f^{i_1,\ldots,i_m}$ are invariant under this action.

Clearly if the number of ''colors'' N_c is one, the realization described above has a large kernel. The variables η^i then satisfy the relation

$$\eta^i\eta^j - \eta^j\eta^i = 0 \tag{37}$$

since they commute. The functions f^I then satisfy the ''Mandelstam identity''

$$f^{I\circ_{kl}J} - f^I f^J = 0 \tag{38}$$

relative to any way of multiplying the two loops I and J at points k and l. More generally, there will be an identity that says that the antisymmetric part in N_c+1 indices is zero; these are the finite analogs of the Mandelstam identities. For simplicity, let us state the $N_c=2$ case:

$$f^{I_1\circ I_2\circ I_3} + f^{I_1\circ I_3\circ I_2} - f^{I_1\circ I_2} f^{I_3} - f^{I_1\circ I_3} f^{I_2} - f^{I_2\circ I_3} f^{I_1} + f^{I_1} f^{I_2} f^{I_3} = 0. \tag{39}$$

Here, I_1 actually denotes the set $i_1, i_2, \ldots, i_{k_1}$, I_2 denotes $j_1, \ldots, j_{k_2}$ and I_3 refers to $l_1, \ldots, l_{k_3}$. The circles are the products we introduced which corresponds to combining the corresponding sequences. Similarly, one can see that writing the all possible antisymmetric combinations and taking the trace, we get a relation satisfied by N_c+1 generators of the representation. This gives us combinations of generators with all possible permutations multiplied with the appropriate sign of the permutation. If we take the cycle decomposition of a permutation π of N_c+1 numbers, and denote each cycle as π_k, we can write the result as

$$\sum_{\pi} (-1)^{\pi} f^{I_{\pi_1}} f^{I_{\pi_2}}, \ldots, f^{I_{\pi_s}} = 0, \tag{40}$$

where we used a short hand $f^{I_{\pi_k}}$ to denote $f^{I_{l_{r_{k-1}}}\circ,\ldots,\circ I_{l_{r_k}}}$. Here the length of the cycle π_k is given by $r_k - r_{k-1}$ and circles again correspond to products.

These are precisely the analogs of the identities satisfied by the Wilson loop for finite N_c (see Ref. 2). They simply describe the fact that f^I is the trace of an $N_c \times N_c$ matrix. As $N_c \to \infty$ these identities should disappear which must be a reason for the simplicity of the large-N_c limit.

We remark that if we introduce Grassmann variables ψ_b^{ia} which anticommute,

$$\psi_b^{ia}\psi_d^{jc} + \psi_d^{jc}\psi_b^{ia} = 0 \tag{41}$$

and satisfy the super-Poisson bracket

$$\{\psi_b^{ia}, \psi_d^{jc}\} = g^{ij}\delta_d^a\delta_b^c \tag{42}$$

we also have a supersymplectic realization of $\mathscr{V}_M^-$:

$$G^I \mapsto \mathrm{Tr}\ \psi^{i_1}, \ldots, \psi^{i_m}. \tag{43}$$

Clearly these G^I are cyclically antisymmetric and a short computation will show that their super-Poisson brackets form a realization of $\mathscr{V}_M^-$. By replacing the above Grassmann algebra by a Clifford algebra:

$$\psi_b^{ia} * \psi_d^{jc} + \psi_d^{jc} * \psi_b^{ia} = \hbar g^{ij} \delta_d^a \delta_b^c \tag{44}$$

we also have a quantum deformation for $\mathscr{V}_M^-$, analogous to the one in the Sec. V.

V. FREE ORTHOGONAL ALGEBRA

Let us consider the SO(N_c) Yang–Mills theory, and obtain a similar formalism of loops. If we think of SO(N_c) as the real part of U(N_c), then Wilson loops satisfy

$$W[\xi] = W[\bar{\xi}], \quad W^*[\xi] = W[\xi]. \tag{45}$$

The loop algebra should also reflect this symmetry, therefore for SO(N_c) Yang–Mills theory, we obtain the result

$$\{W[\xi_1], W[\xi_2]\} = \int ds\ dt (\dot{\xi}_1^i(s)\dot{\xi}_2^j(t)\omega_{ij}(\xi_1(s), \xi_2(t)) W[\xi_1 \circ_{st} \xi_2] + \dot{\xi}_1^i(s)\dot{\bar{\xi}}_2^j(t)\omega_{ij}(\xi_1(s), \bar{\xi}_2(t)) W[\xi_1 \circ_{st} \bar{\xi}_2]).$$

One can see that the algebra is invariant under $\xi \leftrightarrow \bar{\xi}$.[2]

We will see that the real subalgebra of the unitary algebra is in fact the above algebra of Wilson loops. The real form can be obtained by imposing the conditions

$$v_I = v_{\bar{I}}, \quad v_I^* = v_I \tag{46}$$

for the coefficients of an element $v = \Sigma v_I F^I$. One can check that a basis for them is given by

$$H^I = F^I + F^{\bar{I}}. \tag{47}$$

We can now calculate the commutator of these basis elements;

$$[H^I, H^J] = \sum_{k,l} \omega^{i_k j_l} (F^{I \circ_{kl} J} + F^{I \circ_{kl} \bar{J}} + F^{\bar{I} \circ_{kl} J} + F^{\bar{I} \circ_{kl} \bar{J}}), \tag{48}$$

using the previous result on the commutators of F^I's. Due to the cyclic symmetry we can show that $F^{I \circ_{kl} J} = F^{\bar{I} \circ_{kl} \bar{J}}$. Thus the above expression can be reorganized as

$$[H^I, H^J] = \sum_{kl} \omega^{i_k j_l} (H^{I \circ_{kl} J} + H^{I \circ_{kl} \bar{J}}). \tag{49}$$

This also shows explicitly that the above set of elements constitute a subalgebra. We will also briefly describe a symplectic realization of the above algebra. Let us consider the real symmetric matrices η_b^{ia}, where $i = 1,2,\ldots,M$ and $a,b = 1,2,\ldots,N_c$, with the Poisson bracket

$$\{\eta_b^{ia}, \eta_d^{jc}\} = \omega^{ij}(\delta_d^a \delta_b^c + \delta^{ac} \delta_{bd}). \tag{50}$$

If we define the SO(N_c) invariant polynomials,

$$h^I = \mathrm{Tr}\ \eta^{i_1} \eta^{i_2}, \ldots, \eta^{i_n} \tag{51}$$

they provide a symplectic realization of the above algebra. We have the condition $h^I = h^{\bar{I}}$ and the Mandelstam constraints as the kernel of this realization.

It is also possible to discuss the deformation of this symplectic realization but we will only consider the more physically relevant case of unitary algebras. The derivation given below can be extended to the orthogonal case.

VI. QUANTUM DEFORMATION

It is interesting to see what happens to the above realization upon quantization. One approach to quantization is the deformation of the commutative product of the functions of η_b^{ia} by the so-called Moyal product:

$$f*g(\eta)=[e^{-i(\hbar/2)\omega^{ij}(\partial/\partial\eta_b^{ia})(\partial/\partial\eta_a'^{jb})}f(\eta)g(\eta')]_{\eta=\eta'}. \tag{52}$$

(This particular definition of the product corresponds to Weyl ordering.[7]) If we apply this multiplication rule to the $U(N_c)$-invariant polynomials f^I, we will get a noncommutative associative algebra. The commutator of this multiplication defines a Lie algebra, which is a quantum deformation of our loop algebra $\mathscr{Y}_M^+$. To first order in $\hbar$ this commutator is just the Poisson bracket, so that in this limit we recover the previous algebra as a contraction of the quantum algebra. But the general answer is quite formidable, at each order r in $\hbar$, there will be terms involving up to r products of loops.

On the other hand, it is to be expected that some simplifications will occur in the limit as $N_c\to\infty$. The point is that the leading contribution will come from terms where there are the largest number of possible independent traces, so that we must keep the terms with the largest number of loops. All the other terms are subleading order. Nevertheless, it turns out that there is such a term of leading order in $1/N_c^2$ at each order in $\hbar$; the limit $N_c\to\infty$ is quite different from the limit $\hbar\to 0$. But this is also a ''classical'' limit in that the commutators of color invariant observables is of order $1/N_c^2$, so that they become simultaneously measurable in the limit $N_c\to\infty$. It is of utmost importance to understand the large-N_c limit of gauge theories; our discussion identifies the canonical structure (Poisson brackets of loop variables) of color singlet observables in the large-N_c limit.

Let us now calculate the deformed brackets more explicitly. First of all note that

$$\frac{\partial f^I}{\partial\eta_b^{ka}}=0 \tag{53}$$

unless k is equal to one of the elements of the loop $\{i_1,i_2,\ldots,i_m\}$. In the case $k=i_\mu$ for some $\mu=1,2,\ldots,m$,

$$\frac{\partial f^I}{\partial\eta_b^{i_\mu a}}=[\eta^{i_{\mu+1}}\eta^{i_{\mu+2}},\ldots,\eta^{i_m}\eta^{i_1},\ldots,\eta^{i_{\mu-1}}]_a^b. \tag{54}$$

Thus differentiation with respect to η^{i_μ} cuts the loop at the point with parameter value μ.

More generally,

$$\frac{\partial^r f^I}{\partial\eta_{b_1}^{k_1a_1},\ldots,\partial\eta_{b_r}^{k_ra_r}}=0 \tag{55}$$

unless the set $\{k_1,k_2,\ldots,k_r\}$ is a subset of the set $\{i_1,i_2,\ldots,i_m\}$. Suppose $\{\mu_1,\mu_2,\ldots,\mu_r\}\subset\{1,2,\ldots,m\}$ and moreover that $\mu_1<\mu_2,\ldots,<\mu_r$. Then we can see that

$$\frac{\partial^r f^I}{\partial \eta^{i_{\mu_1} a_1}_{b_1},\ldots,\partial \eta^{i_{\mu_r} a_r}_{b_r}} = [\,\eta^{i_{\mu_1+1}}\eta^{i_{\mu_1+2}},\ldots,\eta^{i_{\mu_2-1}}]^{b_1}_{a_1}$$
$$\times [\,\eta^{i_{\mu_2+1}}\eta^{i_{\mu_2+2}},\ldots,\eta^{i_{\mu_3-1}}]^{b_2}_{a_2}\cdots[\,\eta^{i_{\mu_r+1}}\eta^{i_{\mu_r+2}},\ldots,\eta^{i_{\mu_1-1}}]^{b_r}_{a_r}$$

which corresponds to cutting the loop at points $\mu_1,\mu_2,...,\mu_r$. It is clearly convenient to introduce the matrix, for $\mu_1<\mu_2\in\{1,2,...,m\}$:

$$P^b_a(I(\mu_1,\mu_2)) = [\,\eta^{i_{\mu_1+1}}\eta^{i_{\mu_1+2}},\ldots,\eta^{i_{\mu_2-1}}]^b_a, \tag{56}$$

which represents the parallel transport operator for the piece of the loop I from μ_1 to μ_2. Then, for $\mu_1<\mu_2,...,<\mu_r$,

$$\frac{\partial^r f^I}{\partial \eta^{i_{\mu_1} a_1}_{b_1},\ldots,\partial \eta^{i_{\mu_r} a_r}_{b_r}} = P^{b_1}_{a_1}(I(\mu_1,\mu_2))P^{b_2}_{a_2}(I(\mu_2,\mu_3)),\ldots,P^{b_r}_{a_r}(I(\mu_r,\mu_1)).$$

Now let us consider the general term in the definition of the deformed product of color invariant functions of the η:

$$f^I * f^J = f^I f^J + \sum_{r=1}^{\infty} \frac{1}{r!}\left(-\frac{i\hbar}{2}\right)^r \omega^{i_{\mu_1} j_{\nu_1}},\ldots,\omega^{i_{\mu_r} j_{\nu_r}} \frac{\partial^r f^I}{\partial \eta^{i_{\mu_1} a_1}_{b_1},\ldots,\partial \eta^{i_{\mu_r} a_r}_{b_r}} \frac{\partial^r f^J}{\partial \eta^{j_{\nu_1} b_1}_{a_1},\ldots,\partial \eta^{j_{\nu_r} b_r}_{a_r}}.$$

We can, using the symmetry of the derivatives, and relabeling of indices, always bring the indices in the first derivative factor to the order $\mu_1<\mu_2,...,<\mu_r$. However, once this is done, there is no reason that the indices $\nu_1,\nu_2,...,\nu_r$ are in any particular order. This is because the contraction of the color indices links μ_k to ν_k. Thus, the general term in the series will involve quite complicated ways of contracting the color indices.

In the large-N_c limit, however, the leading term will have the largest number of traces. This will happen when the ν indices are in *decreasing* order: $\{\nu_1>\nu_2,...,>\nu_r\}$. (Of course, the ordering we use is a cyclic ordering; i.e., $\mu_1>\mu_2,...,\mu_r$ means also $\mu_2>\mu_3,...,\mu_r>\mu_1$, etc.) This is the term that involves a product of r Wilson loops, so that

$$f^I * f^J = f^I f^J + \sum_{r=1}^{\infty} \sum_{\substack{\mu_1<\mu_2,\ldots,<\mu_r \\ \nu_1>\nu_2,\ldots,>\nu_r}} \times\left(-\frac{i\hbar}{2}\right)^r \omega^{i_{\mu_1} j_{\nu_1}},\ldots,\omega^{i_{\mu_r} j_{\nu_r}} f^{I(\mu_1,\mu_2)J(\nu_2,\nu_1)} f^{I(\mu_2,\mu_3)J(\nu_3,\nu_2)}\cdots f^{I(\mu_r,\mu_1)J(\nu_1,\nu_r)} + \cdots .$$

Here $I(\mu_1,\mu_2)J(\nu_2,\nu_1)$, e.g., is the loop $i_{\mu_1+1}i_{\mu_1+2},\ldots,i_{\mu_2-1}j_{\nu_2+1},\ldots,j_{\nu_1-1}$.

Now, as the large-N_c limit is taken, we usually have to multiply physical quantities by some N_c-dependent factor, in order that the limit be well-defined. The proper normalization of f^I, e.g., is not obvious. We propose that f^I be normalized such that its vacuum expectation value remains finite in the limit. Now the vacuum expectation value depends on the choice of the Hamiltonian, which we have not made yet. The simplest case would be a quadratic function, $H=g_{ij}\,\mathrm{Tr}\,\eta^i\eta^j$. (This corresponds to having a free theory; if the coupling constants in the interacting case are scaled properly by powers of N_c as well, the counting rules in powers of N_c will not be affected.) The vacuum expectation value of a product of two η's is then $\langle \eta^{ia}_b \eta^{jc}_d\rangle = \epsilon^{ij}\delta^a_d\delta^c_b$. (Here ϵ^{ij} is a tensor built from g_{ij} and ω_{ij} whose explicit form is not necessary.) The vacuum expectation value of the product of an odd number of η's will vanish; for an even number of η's it is given by the

Wick formula. A short calculation will show that, for even m, the expectation value of f^I is of order $N_c^{m/2+1}$. This is independent of the particular form of the Hamiltonian.

Thus we define the normalized functions

$$\tilde{f}^I = \frac{1}{N_c^{m/2+1}} f^I. \tag{57}$$

Now one can check that

$$\tilde{f}^I * \tilde{f}^J = \tilde{f}^I \tilde{f}^J + \frac{1}{N_c^2} \sum_{r=1}^{\infty} \sum_{\substack{\mu_1 < \mu_2, \ldots, < \mu_r \\ \nu_1 > \nu_2, \ldots, > \nu_r}} \left(-\frac{i\hbar}{2} \right)^r \omega^{i\mu_1 j\nu_1}, \ldots, \omega^{i\mu_r j\nu_r} \tilde{f}^{I(\mu_1,\mu_2)J(\nu_2,\nu_1)}$$

$$\times \tilde{f}^{I(\mu_2,\mu_3)J(\nu_3,\nu_2)} \cdots \tilde{f}^{I(\mu_r,\mu_1)J(\nu_1,\nu_r)} + O\left(\frac{1}{N_c^3} \right).$$

Thus the pointwise product is again the leading contribution in the large-N_c limit.

The commutator of the $\tilde{f}^I$'s is of order $1/N_c^2$. This is consistent with the idea that the large-N_c limit is a classical theory, with $1/N_c^2$ measuring the size of the quantum corrections: analogous to the $\hbar$ of the conventional classical limit. Indeed, the Poisson algebra of the large-N_c limit of (regularized) Yang–Mills theory is

$$\{\tilde{f}^I, \tilde{f}^J\}_* = 2i \sum_{r=1,\text{odd}}^{\infty} \sum_{\substack{\mu_1 < \mu_2, \ldots, < \mu_r \\ \nu_1 > \nu_2, \ldots, > \nu_r}} \left(-\frac{i\hbar}{2} \right)^r \omega^{i\mu_1 j\nu_1}, \ldots, \omega^{i\mu_r j\nu_r} \tilde{f}^{I(\mu_1,\mu_2)J(\nu_2,\nu_1)}$$

$$\times \tilde{f}^{I(\mu_2,\mu_3)J(\nu_3,\nu_2)} \cdots \tilde{f}^{I(\mu_r,\mu_1)J(\nu_1,\nu_r)}.$$

The Poisson manifold defined by these relations is the phase space of the large-N_c limit of Yang–Mills theory. It is quite different from the phase space of the conventional classical limit. (This is in fact quite typical of such large-N_c limits.) We believe that the above Poisson algebra plays a fundamental role in the physics of strongly interacting particles.

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Zero modes of rotationally symmetric generalized vortices and vortex scattering

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Zero modes of rotationally symmetric vortices in a hierarchy of generalized Abelian Higgs models are studied. Under the finite energy and the smoothness condition, it is shown, that in all models, n self-dual vortices superimposed at the origin have $2n$ modes. The relevance of these modes for vortex scattering is discussed: first, in the context of the slow-motion approximation; second, a corresponding Cauchy problem for an all head-on collision of n vortices is formulated. It is shown that the solution of this Cauchy problem has a π/n symmetry. © *1996 American Institute of Physics.* [S0022-2488(96)03301-6]

I. INTRODUCTION

Since their discovery,[1] vortices in the Abelian Higgs model have attracted much attention. This is mainly due to the fact that the static solutions of this model describe flux tubes in superconductors. As objects in two-dimensional space, they also provide simple examples of topologically nontrivial structures. Recently, the Abelian Higgs model was generalized, and rotationally symmetric vortices were found in these models.[2] The *generalized* Abelian Higgs models form a hierarchy of two-dimensional $U(1)$ models labeled by an integer parameter p. The significance of p is that the pth member of this hierarchy has been derived by subjecting the pth member of the hierarchy of the $4p$-dimensional scale-invariant SO($4p$) Yang–Mills models to dimensional descent.[3] The $p=1$ members of both these hierarchies are the usual Abelian Higgs model and the Yang–Mills model in 2 and 4 dimensions, respectively.

A mathematically rigorous proof for the existence and uniqueness of the rotationally symmetric self-dual vortices of the hierarchy of generalized Abelian Higgs models was subsequently given in Ref. 4. These rotationally symmetric solutions describe vortices superimposed at the origin, and provide us with objects qualitatively similar to, but quantitatively different from the vortices in the Abelian Higgs model. In the case of the Abelian Higgs model, actually, a $2n$-parameter family of vortices exists.[5] In this article, we show that, at least near the rotationally symmetric vortices, there is also a $2n$-parameter family of generalized vortices.

In the Abelian Higgs model, the knowledge gained from the study of the zero modes has been used to investigate the scattering of vortices. Vortex scattering has been studied in the context of the slow-motion approximation,[6] and with the help of the theory of partial differential equations.[7] Among the most interesting processes studied is 90° scattering of two vortices in a head-on collision (or its generalization: π/n scattering in all head-on collisions of n vortices). We will show that some of the results, in particular the π/n symmetry of the scattering process, generalize to generalized vortices.

The paper is organized as follows. In Sec. II, we highlight those aspects of the generalized

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Abelian Higgs models, and of their rotationally symmetric vortices, important to our discussion of the zero modes. In Sec. III, following steps taken by Weinberg in the case of the Abelian Higgs model,[8] we derive the fluctuation equations for rotationally symmetric generalized vortices. We show that these equations have a $2n$-parameter family of smooth finite-energy solutions. In Sec. IV, the scattering of n generalized vortices shortly before and after they form a rotationally symmetric vortex is discussed, first, briefly, in the context of the slow-motion approximation. A corresponding Cauchy problem is then formulated. It is shown that its solution has a π/n symmetry.

II. THE MODELS AND THEIR RADIALLY SYMMETRIC SOLUTIONS

The models we study are the generalized Abelian Higgs models in $(2+1)$-dimensional space–time, given by the Lagrangian densities

$$\begin{aligned}\mathscr{L}^{(p)}=&(\eta^2-|\phi|^2)^{2(p-2)}([(\eta^2-|\phi|^2)F_{\mu\nu}+\iota(p-1)D_{[\mu}\phi^*D_{\nu]}\phi]^2\\&+4p(2p-1)(\eta^2-|\phi|^2)^2|D_\mu\phi|^2+2(2p-1)^2(\eta^2-|\phi|^2)^4)\end{aligned}\tag{1}$$

for any integer $p>1$. For $p=1$, Eq. (1) reduces to the usual Abelian Higgs model. ϕ is the complex Higgs field, $D_\mu\phi=\partial_\mu\phi+\iota A_\mu\phi$, $\mu=0,1,2$, is the covariant derivative, and the gauge fields $F_{\mu\nu}$ are defined in terms of the real gauge potentials A_μ as $F_{\mu\nu}=\partial_\mu A_\nu-\partial_\nu A_\mu=\partial_{[\mu}A_{\nu]}$ $\mu,\nu=0,1,2$. The square brackets mean antisymmetrization in the indices. For any tensor $T_{\mu\nu,\ldots}$, $(T_{\mu\nu,\ldots})^2$ means $T_{\mu\nu,\ldots}T^{\mu\nu,\cdots}$. The indices are raised and lowered with the metric tensor $g=\mathrm{diag}$ $(-1,+1,+1)$. Our task is to find, and study, smooth finite-energy solutions of the corresponding Euler–Lagrange equations.

As in the case of the Abelian Higgs model, the Euler–Lagrange equations of the generalized Abelian Higgs models are solved by certain first-order equations. For the Abelian Higgs model, these equations were found by Bogomol'nyi.[9] For the Lagrangian (1), the first-order equations arise as follows: In the case $A_0=0$, and for time-independent Higgs field and gauge potentials, the Lagragian can be written in the form $\mathscr{L}^{(p)}=I^2+J^2+\epsilon_{ij}\partial^i\Omega^j$, where I^2 and J^2 are the positive definite terms

$$I^2=(\eta^2-|\phi|^2)^{2(p-2)}(((\eta^2-|\phi|^2)F_{ij}+\iota(p-1)D_{[i}\phi^*D_{j]}\phi)-(2p-1)\epsilon_{ij}(\eta^2-|\phi|^2)^2)^2,\tag{2}$$

$$J^2=2p(2p-1)(\eta^2-|\phi|^2)^{2(p-1)}|D_i\phi-\iota\epsilon_{ij}D^j\phi|^2,\tag{3}$$

and where

$$\Omega^j=4(2p-1)\eta^{2(2p-1)}A^j+\sum_{s=1}^{2p-1}\frac{4\iota}{s}(2p-1)^2\eta^{2(2p-1-s)}\binom{2p-2}{s-1}(-|\phi|^2)^{s-1}\phi^*D^j\phi.\tag{4}$$

The special structure of the Lagrangian $\mathscr{L}^{(p)}$ is no accident, but arises naturally through dimensional reduction of the generalized Yang–Mills model on $R^2\times S^{4p-2}$.[2] The divergence $\epsilon_{ij}\partial^i\Omega^j$ is the dimensionally reduced form of the Chern–Pontryagin density. $I=0$ and $J=0$ stem from the self-duality equations of the generalized Yang–Mills theory.[3] Setting I and J equal to zero means minimizing the energy in a given tological sector, and yields the desired first-order equations. We have simplified the task of finding time-independent solutions with $A_0=0$, to solving the following equations:

$$(\eta^2-|\phi|^2)F_{ij}+\iota(p-1)D_{[i}\phi^*D_{j]}\phi=(2p-1)\epsilon_{ij}(\eta^2-|\phi|^2)^2,\tag{5}$$

$$D_i\phi=\iota\epsilon_{ij}D^j\phi.\tag{6}$$

For the rotationally symmetric ansatz,

$$\phi = \eta g(r) \exp(-\imath n \theta), \tag{7}$$

$$A_i = \epsilon_{ij} x^j \frac{a(r)-n}{r^2}, \tag{8}$$

with integer vortex number n, Eqs. (5) and (6) reduce to

$$(1-g^2)\frac{da}{dr} = \frac{2}{r}(p-1)a^2 g^2 - \eta^2(2p-1)r(1-g^2)^2, \tag{9}$$

$$\frac{dg}{dr} = \frac{ag}{r}. \tag{10}$$

In Ref. 3, for all n, existence and uniqueness of a solution to these equations with the desired asymptotic behavior was shown. For small r, a goes to n, and g goes like $C_n r^n$, where the C_n are constants which have to be determined numerically. For large r, g goes to 1, and $a/(1-g^2)$ goes like $\sqrt{(2p-1)/(2p)}\,\eta r$. In Sec. III, we will study the zero modes of these rotationally symmetric solutions.

III. THE FLUCTUATION EQUATIONS AND THE ZERO MODES

We write the fluctuations about the rotationally symmetric solutions in the following form:

$$\delta\phi = \eta g(r) h(r,\theta) \exp(-\imath n \theta), \tag{11}$$

$$\delta A_1 = \frac{1}{r}(-b(r,\theta)\sin\theta + c(r,\theta)\cos\theta), \tag{12}$$

$$\delta A_2 = \frac{1}{r}(b(r,\theta)\cos\theta + c(r,\theta)\sin\theta). \tag{13}$$

Here, b and c are real functions, and $h = h^1 + \imath h^2$ is a complex function. To count the number of modes, we will later fix the gauge by setting h^2 equal to zero. To discuss the smoothness of the modes, we will have to use the gauge freedom and find suitable functions h^2.

Equations (5) and (6), linearized in the functions h, b, and c, then yield the fluctuation equations. Equation (6) leads to expressions for the functions b and c in terms of the function h:

$$b = -r\frac{\partial h^1}{\partial r} - \frac{\partial h^2}{\partial \theta}, \tag{14}$$

$$c = \frac{\partial h^1}{\partial \theta} - r\frac{\partial h^2}{\partial r}. \tag{15}$$

Using these expressions, we obtain from Eq. (5) the following equation for h:

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial h^1}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 h^1}{\partial \theta^2} - \frac{4(p-1)ag^2}{r(1-g^2)}\frac{\partial h^1}{\partial r} - g^2\left(2(2p-1)\eta^2 + \frac{4(p-1)a^2}{r^2(1-g^2)^2}\right)h^1 = 0. \tag{16}$$

Note that h^2 does not occur in Eq. (16). Therefore, the finite-energy solutions of Eq. (16), which lead to smooth fields in a suitable gauge, yield the zero modes. There are no other modes, since we can impose the gauge condition, $h^2=0$.

We attempt to solve Eq. (16) in terms of a Fourier series for h^1,

$$h^1(r,\theta)=\sum_{k=0}^{\infty}(h_k^{(1)}(r)\cos k\theta+h_k^{(2)}(r)\sin k\theta). \tag{17}$$

The Fourier coefficient functions $h_k^{(i)}$ have to satisfy the equation

$$\frac{d^2h_k^{(i)}}{dr^2}+\left(\frac{1}{r}-\frac{4(p-1)ag^2}{r(1-g^2)}\right)\frac{dh_k^{(i)}}{dr}-\left(\frac{k^2}{r^2}+2(2p-1)\eta^2g^2+\frac{4(p-1)a^2g^2}{r^2(1-g^2)^2}\right)h_k^{(i)}=0. \tag{18}$$

We want to find all solutions such that, in a suitable gauge, the rotationally symmetric background fields plus the fluctuations are C^∞ functions on R^2 with finite energy.

For small r, Eq. (18) reduces to $r^2y''+ry'=k^2y$, where $y=h_k^{(i)}$. The general solution to this equation is $y=c_1r^k+c_2r^{-k}$ for $k>0$, and $y=c_1+c_2\ln r$ for $k=0$. The uniqueness of radially symmetric vortices rules out nontrivial fluctuations for $k=0$. (We assume here that the uniqueness result, rigorously proven in Ref. 4 for $p=2$, is in fact true for all p.) For large r,

$$y''-(p-1)\sqrt{\frac{8(2p-1)}{p}}\,\eta y'-\frac{2(2p-1)^2}{p}\,\eta^2y=0 \tag{19}$$

holds, with the general solution

$$y=c_3\exp\left(\sqrt{\frac{2}{p}}\,(2p-1)^{3/2}\eta r\right)+c_4\exp\left(-\sqrt{\frac{2(2p-1)}{p}}\,\eta r\right). \tag{20}$$

Because of the finite-energy condition, we have to set $c_3=0$. c_4 is an arbitrary coefficient. One can now show that all exponentially decreasing solutions at infinity lead to solutions at the origin with $c_2\neq0$. Assume the contrary: Then for $c_4>0$ there must be a maximum with positive y. However, Eq. (18) shows that, when the first derivative vanishes, the second derivative is positive. This is a contradiction. (An analogous argument holds when c_4 is negative and y has to attain a minimum.) Hence, acceptable nontrivial behavior at infinity leads to an r^{-k} term at the origin. For $k>n$ this implies that the energy is infinite.

We are left with the $2n$ modes $h_k^{(i)}$ (with all the other $h_l^{(j)}$, for $j\neq i$ or $l\neq k$, equal to zero) for $0<k\leqslant n$ and $i=1,2$. Supplemented with suitable functions h^2, these modes lead to the following smooth finite-energy solutions: For the first set of n functions, the fluctuations are of the form

$$\delta\phi=\eta g(r)h_k^{(1)}(r)\exp(-\iota(n-k)\theta), \tag{21}$$

$$\delta A_1=-\left(\frac{dh_k^{(1)}}{dr}+\frac{k}{r}\,h_k^{(1)}\right)\sin((k-1)\theta), \tag{22}$$

$$\delta A_2=-\left(\frac{dh_k^{(1)}}{dr}+\frac{k}{r}\,h_k^{(1)}\right)\cos((k-1)\theta). \tag{23}$$

For the second set of n functions, the fluctuations are of the form

$$\delta\phi=-\iota\eta g(r)h_k^{(2)}(r)\exp(-\iota(n-k)\theta), \tag{24}$$

$$\delta A_1 = \left(\frac{dh_k^{(2)}}{dr} + \frac{k}{r} h_k^{(2)} \right) \cos((k-1)\theta), \tag{25}$$

$$\delta A_2 = -\left(\frac{dh_k^{(2)}}{dr} + \frac{k}{r} h_k^{(2)} \right) \sin((k-1)\theta). \tag{26}$$

IV. SYMMETRIES AND VORTEX SCATTERING

In the Abelian Higgs model, the zero modes can be used to study vortex scattering in the context of the slow-motion approximation.[10] The idea of this approximation is that for low velocities, at each point in time the fields A_1, A_2, and ϕ are given by one of the static solutions; i.e., as an ansatz for these functions one can choose the family of static solutions after making the parameters time dependent. A_0 is then determined from its equation of motion, which is of zero order in t. Finally, with this ansatz the action is minimized.

For our purpose, this idea can be implemented as follows. Near the rotationally symmetric vortices, we expand the fields

$$\phi^i = \hat{\phi}^i + s^i(t)\,\delta\phi^i, \quad A^i = \hat{A}^i + s^{2+i}(t)\,\delta A^i. \tag{27}$$

Here, $\hat{\phi} = \hat{\phi}^1 + \iota\hat{\phi}^2$ and $\hat{A}^i$ are the static solutions (7) and (8). $\delta\phi^i$ and δA^i are the fluctuations (21), (22), and (23) or (24), (25), and (26). The equation, which has to be solved for A_0, is the first (for $\nu=0$) of the following three equations:

$$\begin{aligned} &\partial_\mu((\eta^2-|\phi|^2)^{2p-3}((\eta^2-|\phi|^2)F^{\mu\nu}+\iota(p-1)D^{[\mu}\phi^*D^{\nu]}\phi))+(p-1)(\eta^2-|\phi|^2)^{2p-4} \\ &\quad\times(((\eta^2-|\phi|^2)F^{\mu\nu}+\iota(p-1)D^{[\mu}\phi^*D^{\nu]}\phi)(\phi^*D_\mu\phi+\phi D_\mu\phi^*))-\iota p(2p-1) \\ &\quad\times(\eta^2-|\phi|^2)^{2p-2}(\phi D^\nu\phi^*-\phi^*D^\nu\phi)=0. \end{aligned} \tag{28}$$

[The other two equations (for $\nu=1,2$) are the second-order equations of motion for A_1 and A_2, which we will need later.]

The dynamics, as described by the functions $s^\alpha(t)$, is now given by the Lagrange function

$$\begin{aligned} L^{(p)} = \int_{R^2} &(\eta^2-|\phi|^2)^{2(p-2)}(2((\eta^2-|\phi|^2)F_{0i}+\iota(p-1)D_{[0}\phi^*D_{i]}\phi)^2 \\ &+4p(2p-1)(\eta^2-|\phi|^2)^2|D_0\phi|^2)d^2x. \end{aligned} \tag{29}$$

The functions s^α are found by solving the Euler–Lagrange equations of this Lagrange function. Obviously, the slow-motion approximation still leaves us with very complicated equations to solve. With our ansatz (27), however, we only attempt to study the neighborhood of rotationally symmetric vortices; i.e., we can neglect higher order terms in the functions s^α. Even though we are allowed to linearize in s^α, we were not able to solve Eq. (28) for $\nu=0$.

In the Abelian Higgs model, the Gauss equation corresponds to Eq. (28) for $\nu=0$. Following the same steps we have just discussed for our models, in the Abelian Higgs model one finds that $A_0=0$, and that the s^α are functions linear in time, in the neighborhood of the rotationally symmetric vortices. For the modes with real smooth $\delta\phi$ this implies π/n scattering, if only times shortly before and shortly after the vortices coincide are considered. We see that the slow-motion approximation yields more results in the Abelian Higgs model. Another difference between the models discussed here and the Abelian Higgs model is that in the Abelian Higgs model the validity of the slow-motion approximation has been rigorously proven.[11]

Instead of pursuing the slow-motion approximation any further, we will now formulate a corresponding Cauchy problem and use the symmetries to study the full Euler–Lagrange equations of the Lagrangian (1). We work with the vector $\psi^T=(A_0,\partial_t A_0,A_1,\partial_t A_1,A_2,\partial_t A_2,\phi,\partial_t\phi)$, and impose the following initial conditions:

$$\psi(0,\mathbf{x})^T=(\hat{A}_0,0,\hat{A}_1,\delta A_1,\hat{A}_2,\delta A_2,\hat{\phi},\delta\phi). \tag{30}$$

Here $\hat{\phi}$ and $\hat{A}_i$ are the static solutions (7) and (8). $\delta\phi$ and δA_i are the fluctuations (21), (22), and (23) for $k=n$. We concentrate on this type of fluctuation for simplicity, and because they lead to the interesting π/n symmetry in the n vortex scattering process. $\hat{A}_0$ is the solution of Eq. (28) for $\nu=0$ at time $t=0$.

The equations of motion for ϕ and A_μ we consider are the following second-order equations. The second-order equation for A_0 is $\partial_{tt}A^0+\partial_i\partial_t A^i=0$. (This equation follows from the Lorentz condition $\partial_\mu A^\mu=0$.) The second-order equations for A_1 and A_2 are given by Eq. (28) for $\nu=1,2$. The second-order equation for ϕ is its Euler–Lagrange equation,

$$\begin{aligned}
&\iota\partial_\mu((\eta^2-|\phi|^2)^{2p-4}[(\eta^2-|\phi|^2)F^{\nu\mu}+\iota(p-1)D^{[\nu}\phi^*D^{\mu]}\phi](p-1)D_\nu\phi^*+p(2p-1)\\
&\quad\times(\eta^2-|\phi|^2)^2D^\mu\phi^*)+\tfrac{1}{2}(p-2)(\eta^2-|\phi|^2)^{2p-3}([(\eta^2-|\phi|^2)F_{\mu\nu}+\iota(p-1)D_{[\mu}\phi^*D_{\nu]}\phi]^2\\
&\quad+4p(2p-1)(\eta^2-|\phi|^2)^2|D_\mu\phi|^2+2(2p-1)^2(\eta^2-|\phi|^2)^4)\phi^*-\tfrac{1}{2}(\eta^2-|\phi|^2)^{2(p-2)}\\
&\quad\times(((\eta^2-|\phi|^2)F^{\mu\nu}+\iota(p-1)D^{[\mu}\phi^*D^{\nu]}\phi)(F_{\mu\nu}\phi^*-(p-1)A_{[\mu}D_{\nu]}\phi^*)-2p(2p-1)\\
&\quad\times(\eta^2-|\phi|^2)|D_\mu\phi|^2\phi^*+\iota p(2p-1)(\eta^2-|\phi|^2)^2A^\mu D_\mu\phi^*-2(2p-1)^2(\eta^2-|\phi|^2)^3\phi^*)=0.
\end{aligned} \tag{31}$$

The Lorentz condition and Eq. (28) for $\nu=0$ are considered as constraints, which, by our choice of initial data, are satisfied at $t=0$. In the Abelian Higgs model, it has been proven that the analogous Cauchy problem has a unique solution, and that the constraints are propagated.[7] In the following, we will assume that in the present case a unique solution also exists, although a rigorous proof is still missing. (Because of the complexity of the equations, to rigorously prove existence of a unique solution seems a very difficult task.)

For a given solution $\psi(t,\mathbf{x})$, we define the functions $\psi_i(t,\mathbf{x})=M_i\psi(t,\mathbf{x}_{(i)})$ for $i=1,2$, where $\mathbf{x}_{(1)}=S\mathbf{x}$ with

$$S=\begin{pmatrix}\cos\dfrac{2\pi}{n} & -\sin\dfrac{2\pi}{n}\\[2ex] \sin\dfrac{2\pi}{n} & \cos\dfrac{2\pi}{n}\end{pmatrix}, \tag{32}$$

and where $\mathbf{x}_{(2)}^T=(x_1,-x_2)^T$. The matrices M_i are defined as

$$M_1=\begin{pmatrix}I & 0 & 0 & 0\\ 0 & A & B & 0\\ 0 & -B & A & 0\\ 0 & 0 & 0 & I\end{pmatrix},\quad I=\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix},\quad A=\cos\frac{2\pi}{n}I,\quad B=\sin\frac{2\pi}{n}I \tag{33}$$

and

$$M_2=\begin{pmatrix} -I & 0 & 0 & 0 \\ 0 & -I & 0 & 0 \\ 0 & 0 & I & 0 \\ 0 & 0 & 0 & C \end{pmatrix}, \quad CV=V^*. \tag{34}$$

We can now show that, if $\psi(t,\mathbf{x})$ is a solution of the Cauchy problem, so are $\psi_1(t,\mathbf{x})$ and $\psi_2(t,\mathbf{x})$. (To find the symmetries of the initial data $A_0(0,\mathbf{x})$, we have assumed that Eq. (28) for $\nu=0$ has a unique smooth solution with asymptotic decay sufficient to satisfy the finite-energy condition.) The uniqueness of the solution of the Cauchy problem now implies that, actually, ψ, ψ_1, and ψ_2 are all the same function. This, in turn, implies that functions like $|\phi|^2$, F_{ij}^2, or the energy density $\mathscr{E}$ are invariant under a $2\pi/n$ rotation, and under a reflection with respect to the x_1 axis. This leads to the following conclusion: If by using functions like $|\phi|^2$, F_{ij}^2, or $\mathscr{E}$, there is a way of defining the positions $(x_1^a(t),x_2^a(t))$, $a=1,\ldots,n$, of exactly n separate vortices, these n positions must lie on n radial lines separated by an angle $2\pi/n$ with equal distance from the origin. (As in Ref. 7, we can use the minima of $|\Phi|^2$ to define these positions, near the rotationally symmetric vortices.) Furthermore, one of these radial lines must be the positive x_1 axis, or make an angle π/n with the positive x_1 axis. Any vortex that does not satisfy these conditions immediately leads to $2n-1$ other vortices, because of the symmetries of our solution. For continuous solutions, these positions will change continuously such that at $t=0$ the n positions coincide, and after the collision the vortices move again on the radial lines just described. Therefore, they can either go back on the radial lines they came in on, or go back on radial lines shifted by an angle π/n. We will study a further symmetry to show that the second case is realized.

The last transformation we study is $\mathbf{x}\to M\mathbf{x}$, where M is the orthogonal matrix

$$M=\begin{pmatrix} \cos\dfrac{\pi}{n} & -\sin\dfrac{\pi}{n} \\ \sin\dfrac{\pi}{n} & \cos\dfrac{\pi}{n} \end{pmatrix}. \tag{35}$$

Under this transformation the initial data change as follows:

$$\psi(0,M\mathbf{x})=M_3\psi(0,\mathbf{x}),$$

with

$$M_3=\begin{pmatrix} -\sigma & 0 & 0 & 0 \\ 0 & C & -D & 0 \\ 0 & D & C & 0 \\ 0 & 0 & 0 & -\sigma \end{pmatrix}, \quad \sigma=\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad C=\cos\frac{\pi}{n}\,\sigma, \quad D=\sin\frac{\pi}{n}\,\sigma. \tag{36}$$

[We have again assumed the uniqueness of the smooth finite-energy solution, $A_0(0,\mathbf{x})$, of Eq. (28) for $\nu=0$.] From the uniqueness of the solution of the Cauchy problem, $\psi(-t,M\mathbf{x})=M_3\psi(t,\mathbf{x})$ follows, and we see that the functions $|\phi|^2$, F_{ij}^2, and $\mathscr{E}$ are invariant under the transformation $(t,\mathbf{x})\to(-t,M\mathbf{x})$. This establishes π/n scattering for n vortices.

V. CONCLUSIONS

The study of vortices in a hierarchy of generalized Abelian Higgs models, and the comparison with the Abelian Higgs model was continued. In previous studies we had seen that the rotationally symmetric generalized vortices are qualitatively similar to, but quantitatively different from the

vortices. Here similar structures were found in the neighborhood of the rotationally symmetric vortices. We found that the zero modes of the generalized vortices have the same angular dependence as, but radial behavior different from that of the zero modes of the vortices in the Abelian Higgs model.

The slow-motion approximation turned out to be of limited value. (Since the time-independent solutions are not known explicitly even in the Abelian Higgs model, the slow-motion approximation is not very successful in this model either.) On the reasonable assumption that a certain Cauchy problem has a unique solution, we were, however, able to study the symmetries of certain solutions. Each solution describes a process where n vortices approach and form one structure, namely a rotationally symmetric vortex. From this structure n vortices emerge. The pattern the vortices create for time t is the same as that for time $-t$, after a π/n rotation.

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Time-dependent plane-wave spectrum representations for radiation from volume source distributions

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A new time-domain spectral theory for radiation from a time-dependent source distribution, is presented. The full spectral representation is based on a Radon transform of the source distribution in the four-dimensional space-time domain and consists of time-dependent plane waves that propagate in all space directions and with all (spectral) propagation speeds v_κ. This operation, termed the *slant stack transform*, involves projection of the time-dependent source distribution along planes normal to the spectral propagation direction and stacking them with a progressive delay corresponding to the spectral propagation speed v_κ along this direction. Outside the source domain, this three-fold representation may be contracted into a two-fold representation consisting of time-dependent plane waves that satisfy the spectral constraint $v_\kappa = c$ with c being the medium velocity. In the two-fold representation, however, the complete spectral representation involves both propagating time-dependent plane waves and evanescent time-dependent plane waves. We explore the separate role of these spectral constituents in establishing the causal field, and determine the space-time regions where the field is described only by the propagating spectrum. The spectral theory is presented here for scalar wave fields, but it may readily be extended to vector electromagnetic fields. [S0022-2488(96)01801-4]

I. INTRODUCTION

With the increase in the bandwidth of radiation and detection hardware there is a growing interest, for various applications, in the radiation, propagation and diffraction of ultra-wideband, short-pulse fields. Of particular interest is the problem of synthesizing source distributions for well collimated short pulse fields, sometimes referred to as pulsed beams.[1–6] Because of the broad frequency band of these fields, the conventional use of frequency domain techniques is often less efficient and physically less transparent than direct treatment in the space-time domain where the fields are well localized. The general goal of the present research is thus toward developing a time-domain theory for spectral analysis and synthesis of physically realizable pulsed fields and sources. This includes representation theorems and processing tools as well as ''time-domain thinking.'' Emphasis in this paper is placed on clarifying the physical role of various portions of the plane wave spectra in generating the causal field in different space-time regions.

The time-dependent plane-wave realization of general short pulse fields have been considered in Refs. 7–9. It has been shown in Ref. 7 how the time-dependent plane-wave spectrum can be matched to a prescribed pulsed radiation pattern in the far zone, thereby determining the field at all times and in particular the initial distribution at $t=0$. This representation, however, has addressed only the initial field distributions after the source had shut-off (i.e., a source-free field), but not the time-dependent source problem which models physical antennas. As such, it has been restricted to wave fields without evanescent spectrum, and in particular to electromagnetic ''bullets'' whose radiation pattern vanishes identically outside a certain ''radiation cone.'' Strictly speaking, such fields cannot be synthesized by finite support sources. Refs. 8–9, on the other hand, have addressed only planar source (aperture) realizations.

In the present paper we explore the time-dependent plane-wave spectral representation due to

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a general source distribution of finite support. As will be shown (Sec. VI), in certain space-time regions the field may be described only by the propagating spectrum, but such a representation is not valid everywhere. A full description, in particular in the near zone, must include the time-dependent evanescent field. We shall therefore explore the physical role of the various spectral constituents in establishing the causal field. Some of the observations, concerning the space-time regions where the evanescent spectrum does not contribute have been derived in Ref. 10 from asymptotic considerations in the frequency domain. Here, however, all the results are obtained directly from the time-domain spectral contributions.

Transient plane-wave representations have been used in the past mainly for the analysis of scattering and diffraction of point-source excited pulsed fields. Several techniques have been introduced for the evaluation of the resulting spectral integrals.[11–16]. Recent studies were concerned with time-dependent spectral synthesis of collimated pulsed beam fields (space-time wave-packets), and with the scattering of such fields.[17,18] The present paper, on the other hand, presents a general formulation for source distributions.

We consider the time-dependent plane wave representation for the field radiated by a pulsed source distribution in a uniform medium with wave speed c. The field u satisfies the time-dependent wave equation

$$\left(\nabla^2-\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)u(\mathbf{r},t)=-q(\mathbf{r},t) \tag{1.1}$$

in a three-dimensional domain $\mathbf{r}=(x,y,z)$. It is assumed that the source distribution $q(\mathbf{r},t)$ is confined in a volume V bounded within a sphere of radius R_0 centered at the origins and that its time history is a continuous pulse of duration T, namely

$$q(\mathbf{r},t)\neq 0 \quad \text{only} \quad \text{if} \quad \mathbf{r}\in V \quad \text{and} \quad 0<t<T. \tag{1.2}$$

The solution of (1.1) is given by the well known retarded potential integral

$$u(\mathbf{r},t)=\int_V d^3r'\, q[\mathbf{r}',t-|\mathbf{r}-\mathbf{r}'|/c]/4\pi|\mathbf{r}-\mathbf{r}'|. \tag{1.3}$$

Here, however, we shall explore alternative time-dependent plane wave representations for the field.

The time-dependent spectral theory will be derived here only for scalar fields. An extension to radiation of vector electromagnetic fields, expressed in the terminology of antenna theory is under preparation.

The presentation starts, methodically, with the well known spectral representations of time-harmonic fields (Sec. II). In Sec. III we construct the full time-domain spectral representation which is valid everywhere, including the source domain. It involves plane waves that propagate in all directions and with all wave-speeds v_κ, $0<v_\kappa<\infty$. This spectral representation is obtained via a Radon transform of the source distribution in the four-dimensional $(\mathbf{r},t)$ domain. Physically, this operation involves projection of the distribution along planes normal to the propagation direction and stacking them with a progressive delay that corresponds to the spectral wave-speed v_κ, and it is therefore termed the *slant stack transform*. Note that ''plane-wave'' constituents for which $v_\kappa \neq c$ are not solutions of the wave equation.

For observation points *outside* the source region the complete three-fold representation above may be contracted into a representation involving only spectral constituents constraint by the dispersion relation $v_\kappa=c$, i.e., lying on the *light cone* (Sec. IV). This representation, however, involves both propagating (homogeneous) and evanescent time-dependent plane-wave spectra. The time-dependent evanescent spectrum is described most effectively by the analytic signal

representation, obtained by extending the field solutions into the complex time domain. However, we also present explicit expressions for the evaluation of the time-dependent evanescent field directly from the real time-dependent data.

Next we explore the physical meaning of the time-dependent evanescent plane waves by considering first the special case of a pulsed point-source (Sec. V), and then extending the results to distributed sources (Sec. VI). It is shown that the contribution of the evanescent spectrum vanishes identically after a certain time t_E that may be determined a priori, so that for $t>t_E$ the field is described only by a spectrum of propagating time-dependent plane waves. In certain regions in space t_E occurs prior to the causal arrival time t_0, leaving the causal field at $t>t_0$ described only by the propagating spectrum. Prior to t_0, however, the propagating spectrum generates non-vanishing non-causal contributions that are canceled only by the contributions of the evanescent spectrum.

Motivated by these results we consider in Sec. VII some general properties of the field solutions that are generated by a spectrum of *propagating* (homogeneous) time-dependent plane waves. Specifically we explore the fields described by a conical spectral range with angle Θ, centered about the propagation direction to the observer. The analysis covers a wide range of parameters, from a very narrow spectral range (small Θ) up to $\Theta=\pi$ where the plane waves emerge from the source in all directions (a Wittaker-type expansion). Again we determine the space-time window wherein such spectral representation provides a faithful description of the field.

II. TIME-HARMONIC REPRESENTATIONS

A. Full spectral representation

We start with a brief review of alternative plane wave representations for time-harmonic solutions. We use an over caret to denote time-harmonic constituents with suppressed time-dependence $\exp(-i\omega t)$. We introduce the 3D spatial spectrum of the time-harmonic source distribution $\hat{q}(\mathbf{r},\omega)$

$$\hat{\tilde{q}}(\mathbf{K},\omega)=\int d^3r\,\hat{q}(\mathbf{r},\omega)e^{-i\mathbf{K}\cdot\mathbf{r}} \tag{2.1}$$

and its inverse

$$\hat{q}(\mathbf{r},\omega)=\frac{1}{(2\pi)^3}\int d^3K\,\hat{\tilde{q}}(\mathbf{K},\omega)e^{i\mathbf{K}\cdot\mathbf{r}}, \tag{2.2}$$

where $\mathbf{K}=(K_x,K_y,K_z)$. Applying the transform in (2.1) to the time-harmonic wave equation we obtain the well-known result for the time-harmonic field

$$\hat{u}(\mathbf{r},\omega)=\frac{1}{(2\pi)^3}\int d^3K\frac{\hat{\tilde{q}}(\mathbf{K},\omega)}{K^2-k^2}e^{i\mathbf{K}\cdot\mathbf{r}}, \tag{2.3}$$

where $K=|\mathbf{K}|$ and $k=\omega/c$.

B. Contracted (2D) spectral representation: Weyl representation

Expression (2.3) is valid both inside and outside the source region. For observation points outside the source region V, the 3D integral can be contracted to a 2D plane-wave integral. Without loss of generality we shall contract the spectrum about the z-axis and therefore denote $\mathbf{r}=(\mathbf{x},z)$ with $\mathbf{x}=(x_1,x_2)$ being the transverse coordinates. For $|z|>R_0$ we may evaluate the K_z integral in (2.3) via Cauchy's theorem, obtaining

$$\hat{u}(\mathbf{r},\omega)=\frac{1}{(2\pi)^2}\int d^2k_x e^{i\mathbf{k}_x\cdot\mathbf{x}\pm ik_z z}\frac{1}{-2ik_z}\hat{\tilde{q}}(\mathbf{K},\omega)\Big|_{\mathbf{K}=(\mathbf{k}_x,\pm k_z)}, \tag{2.4}$$

where upper and lower signs are for $z>R_0$ and $z<-R_0$, respectively. To distinguish between the full (3D) and the contracted (2D) representations we have replaced the spectral coordinates (K_{x_1},K_{x_2}) by $\mathbf{k}_x=(k_{x_1},k_{x_2})$. The longitudinal wavenumber is determined by $\mathbf{k}_x$ via

$$k_z=\begin{cases}\sqrt{k^2-|\mathbf{k}_x|^2}, & |\mathbf{k}_x|<k\\ i\sqrt{|\mathbf{k}_x|^2-k^2}, & |\mathbf{k}_x|>k.\end{cases} \tag{2.5}$$

Unlike (2.3), Eq. (2.4) expresses the field as a superposition of plane-wave solutions of the wave equation. It consists, however, of both propagating and evanescent spectra: The propagating part of the spectrum ($|\mathbf{k}_x|<k$) depends on the value of $\hat{\tilde{q}}(\mathbf{K})$ on the Ewald sphere $|\mathbf{K}|=k$, while the evanescent part ($|\mathbf{k}_x|>k$) depends on the analytic continuation of $\hat{\tilde{q}}(\mathbf{K})$ to $\mathbf{K}=(\mathbf{k}_x,\pm i\sqrt{|\mathbf{k}_x|^2-k^2})$ for $z\gtrless R_0$, respectively.

The integral representation in (2.4) is valid only if $|z|>R_0$. If $|z|<R_0$, the contracted representation is more complicated and involves both forward and backward propagating waves. We shall not address this case here. If, however, $|z|<R_0$ but $\mathbf{r}$ is located outside the sphere R_0, then this difficulty can be circumvented by rotating the coordinates to a different contraction axis, say z' for which $|z'|>R_0$.

III. FULL SPECTRAL REPRESENTATION: 4D RADON TRANSFORM IN SPACE–TIME

The time-dependent field will be recovered here via an inverse Fourier transform to the time domain. To simplify the analytic manipulations we shall use analytic signal representation. Among other advantages, this formulation also enables a treatment of the propagating and the evanescent spectra in the same analytical framework.

An analytic signal $\overset{+}{f}(t)$ corresponding to the real signal $f(t)$ with frequency spectrum $\hat{f}(\omega)$ is defined by the analytic inverse Fourier transform

$$\overset{+}{f}(t)=\frac{1}{\pi}\int_0^\infty d\omega e^{-i\omega t}\hat{f}(\omega),\qquad \mathrm{Im}\ t\leqslant 0. \tag{3.1}$$

This integral definition implies that $\overset{+}{f}(t)$ is an analytic function in the lower half of the complex t-plane. The physical signal $f(t)$ for real t is obtained via

$$f(t)=\mathrm{Re}\ \overset{+}{f}(t),\qquad t\ \text{real}. \tag{3.2}$$

An alternative definition of $\overset{+}{f}(t)$ directly from the real data $f(t)$ is given in (A7). Other properties are summarized in Appendix A.

A key feature in the time-dependent spectral representation is the use of frequency-normalized spectral variables

$$\boldsymbol{\kappa}=\mathbf{K}/k=(\kappa_x,\kappa_y,\kappa_z). \tag{3.3}$$

Clearly $\boldsymbol{\kappa}$ has a pure *frequency independent* geometrical interpretation in terms of the plane-wave angle. We shall also denote conveniently $\hat{\tilde{q}}(\mathbf{K},\omega)|_{\mathbf{K}=k\boldsymbol{\kappa}}$ as $\hat{\tilde{q}}(\boldsymbol{\kappa},\omega)$.

The space–time spectrum $\overset{+}{\tilde{q}}(\boldsymbol{\kappa},t)$ is defined now by

$$\overset{+}{\tilde{q}}(\boldsymbol{\kappa},\tau)=\frac{1}{\pi}\int_0^\infty d\omega e^{-i\omega\tau}\overset{+}{\tilde{q}}(\boldsymbol{\kappa},\omega), \tag{3.4}$$

where τ is the spectral time variable. Rewriting (2.1)–(2.2) in terms of $\boldsymbol{\kappa}$, and applying (3.1) we have

$$\overset{+}{\tilde{q}}(\boldsymbol{\kappa},\tau)=\frac{1}{\pi}\int_0^\infty d\omega\int_V d^3r\hat{q}(\mathbf{r},\omega)e^{-i\omega(\tau+\boldsymbol{\kappa}\cdot\mathbf{r}/c)}, \tag{3.5}$$

$$\overset{+}{q}(\boldsymbol{\kappa},t)=\frac{1}{\pi}\int_0^\infty d\omega\frac{k^3}{(2\pi)^3}\int d^3\kappa\hat{\tilde{q}}(\boldsymbol{\kappa},k)e^{-i\omega(t-\boldsymbol{\kappa}\cdot\mathbf{r}/c)}. \tag{3.6}$$

Switching the order of integrations and performing the ω integrations first (justified for Im $t,\tau<0$ and in the limit of real t,τ) we obtain the analytic time-domain transform pair

$$\overset{+}{\tilde{q}}(\boldsymbol{\kappa},\tau)=\int_V d^3r\overset{+}{q}(\mathbf{r},\tau+\ \kappa\cdot\mathbf{r}/c), \tag{3.7}$$

$$\overset{+}{q}(\mathbf{r},t)=\frac{-i\partial_t^3}{(2\pi c)^3}\int d^3\kappa\overset{+}{\tilde{q}}(\boldsymbol{\kappa},t-\boldsymbol{\kappa}\cdot\mathbf{r}/c) \tag{3.8}$$

where $\overset{+}{q}(\mathbf{r},t)$ is the analytic signal corresponding to the real source function $q(\mathbf{r},t)$ and $\partial_t\equiv\partial/\partial t$.

The *real signal* equivalent of this analytic transform pair is obtained by taking its real part (see (3.2)). Noting that the $(-i)$ is replaced by $\mathscr{H}$ (see (A2)) we obtain

$$\tilde{q}(\boldsymbol{\kappa},\tau)=\int_V d^3rq(\mathbf{r},\tau+\boldsymbol{\kappa}\cdot\mathbf{r}/c), \tag{3.9}$$

$$q(\mathbf{r},t)=\mathscr{H}\partial_t^3\frac{1}{(2\pi c)^3}\int d^3\kappa\tilde{q}(\boldsymbol{\kappa},t-\boldsymbol{\kappa}\cdot\mathbf{r}/c). \tag{3.10}$$

Note that the integration, the differentiation and the Hilbert transform operations in (3.10) can commute.

The transformation-pair in (3.9)–(3.10) (or, equivalently, (3.7)–(3.8)) is termed the *slant stack transform*. To gain further insight we note that the operation in (3.9) can be cast in a two step cascade

$$\tilde{q}(\boldsymbol{\kappa},\tau)=\int d\sigma\mathscr{P}_{\hat{\kappa}}[q](\sigma,\tau+\kappa\sigma/c) \tag{3.11}$$

$$\mathscr{P}_{\hat{\kappa}}[q](\sigma,\tau)=\int d^2rq(\mathbf{r},\tau)|_{\mathbf{r}\cdot\hat{\kappa}=\sigma}. \tag{3.12}$$

Equation (3.12) is the projection of the time-dependent distribution $q(\mathbf{r},t)$ onto the direction $\hat{\boldsymbol{\kappa}}\equiv\boldsymbol{\kappa}/\kappa$ where $\kappa\equiv|\boldsymbol{\kappa}|$. It is obtained by integrating q along the plane $\mathbf{r}\cdot\hat{\boldsymbol{\kappa}}=\sigma$ normal to $\hat{\boldsymbol{\kappa}}$, with

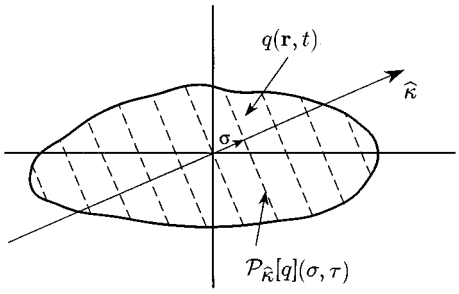


FIG. 1. Schematization of the time-dependent plane-wave transform.

σ being position along the $\hat{\boldsymbol{\kappa}}$ axis. In (3.11) these projections are stacked along this axis with a progressive delay corresponding to the spectral propagation speed (see Fig. 1)

$$v_\kappa = c/\kappa. \tag{3.13}$$

Note that spectral points on the 4D cone $|\boldsymbol{\kappa}|=1$ correspond to plane-wave data with propagation speed c. In the frequency domain, they correspond to points on the Ewald sphere $|\mathbf{K}|=\omega/c$. Points lying off this cone describe faster or slower spectral components.

Equations (3.9)–(3.10) are identified as a Radon transform pair in the four dimensional $(\mathbf{r},t)\leftrightarrow(\boldsymbol{\kappa},\tau)$ domains. In fact, defining the 4D vector $\mathbf{x}=(\mathbf{r},ct)$ we find from (B1) that

$$\tilde{q}(\boldsymbol{\kappa},\tau)=c^{-1}\sqrt{1+\kappa^2}\,\check{q}(p,\hat{\mathbf{p}}) \tag{3.14}$$

with $\check{q}(p,\hat{\mathbf{p}})$ being the conventional definition of the Radon transform and

$$p=c\tau/\sqrt{1+\kappa^2}, \qquad \hat{\mathbf{p}}=(-\boldsymbol{\kappa},1)/\sqrt{1+\kappa^2}. \tag{3.15}$$

Equation (3.10) can be identified as the 4D inverse Radon transform (B18).

The analytic time-dependent field is obtained now by rewriting (2.3) in terms of $\boldsymbol{\kappa}$ and transforming the result to the time domain. Following the same procedure as in (3.4)–(3.8) we obtain

$$\overset{+}{u}(\mathbf{r},t)=\frac{i\partial_t}{(2\pi)^3 c}\int d^3\kappa\,\frac{\overset{+}{\tilde{q}}(\boldsymbol{\kappa},t-\boldsymbol{\kappa}\cdot\mathbf{r}/c)}{\kappa^2-1}, \tag{3.16}$$

hence the real field is found from the real spectral function $\tilde{q}(\boldsymbol{\kappa},\tau)$ via

$$u(\mathbf{r},t)=-\mathscr{H}\partial_t\frac{1}{(2\pi)^3 c}\int d^3\kappa\,\frac{\tilde{q}(\boldsymbol{\kappa},t-\kappa\cdot\mathbf{r}/c)}{\kappa^2-1}, \tag{3.17}$$

where the real spectral function $\tilde{q}$ is defined in (3.9). Equations (3.16)–(3.17) describe the field as a superposition of time-dependent ''plane waves'' that propagate in all directions with the spectral propagation speed v_κ of (3.13).

In the far radiation zone the time-dependent spectral integral (3.17) reduces asymptotically to a point contribution from the spectral component $\tilde{q}$ that propagates at the speed of light $v_\kappa=c$ in the observation direction $\hat{\mathbf{r}}$. Thus the field has the asymptotic form

$$u(\mathbf{r},t)\sim\frac{g(\hat{\mathbf{r}},t-r/c)}{4\pi r},\quad r\to\infty, \tag{3.18}$$

where $r=|\mathbf{r}|$, $\hat{\mathbf{r}}=\mathbf{r}/r$ and the time-dependent radiation pattern

$$g(\hat{\mathbf{r}},t-r/c)=\tilde{q}(\boldsymbol{\kappa},\tau)\Big|_{\boldsymbol{\kappa}=\hat{\mathbf{r}},\tau=t-r/c}. \tag{3.19}$$

IV. CONTRACTED (WEYL-TYPE) REPRESENTATION: TIME-DEPENDENT PROPAGATING AND EVANESCENT SPECTRA

Expression (3.17) describes the field as a 3D spectral superposition of time-dependent plane waves that propagate in all directions, and with all propagation speeds $0<v_\kappa<\infty$ (see (3.13)). For observation points outside the source region one may obtained a contracted representation involving only time-dependent plane waves with wave-speed c. This representation, however, includes evanescent time-dependent plane waves.

For the contracted spectrum representation we replace the spectral wavenumber $\mathbf{k}_x$ of (2.4) by the frequency-normalized spectral coordinates (cf. (3.3))

$$\boldsymbol{\xi}=\mathbf{k}_x/k=(\xi_1,\xi_2), \tag{4.1}$$

and

$$\zeta=\begin{cases}\sqrt{1-|\boldsymbol{\xi}|^2}, & |\boldsymbol{\xi}|<1\\ i\sqrt{|\boldsymbol{\xi}|^2-1}, & |\boldsymbol{\xi}|>1.\end{cases} \tag{4.2}$$

The use of analytic signals enables us to treat the contributions of the propagating ($|\boldsymbol{\xi}|<1$) and the evanescent ($|\boldsymbol{\xi}|>1$) spectra in a single framework (see (4.13)–(4.14)). However, to clarify the mathematical details we shall first consider these contributions separately.

A. Time-dependent propagating spectrum

We rewrite the time-harmonic integral for the propagating spectrum in (2.4) as

$$\hat{u}_P(\mathbf{r},\omega)=\frac{ik}{2(2\pi)^2}\int_{|\boldsymbol{\xi}|<1}d^2\xi\frac{1}{\zeta}\hat{\tilde{q}}(\mathbf{K}^{\pm},\omega)e^{ik(\boldsymbol{\xi}\cdot\mathbf{x}\pm\zeta z)}, \tag{4.3}$$

where upper and lower signs are for $z>R_0$ and $z<R_0$, respectively, $\mathbf{K}^{\pm}=k(\boldsymbol{\xi},\pm\zeta)$, and from (2.1)

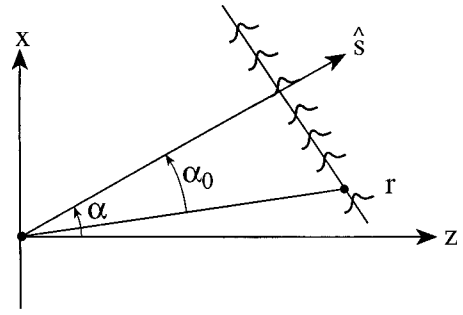
$$\hat{\tilde{q}}(\mathbf{K}^{\pm},\omega)=\int_V d^3r'\hat{q}(\mathbf{r}',\omega)e^{-ik(\boldsymbol{\xi}\cdot\mathbf{x}'\pm\zeta z')}. \tag{4.4}$$

Henceforth we shall assume that $z>R_0$ and shall omit the $\pm$ sign.

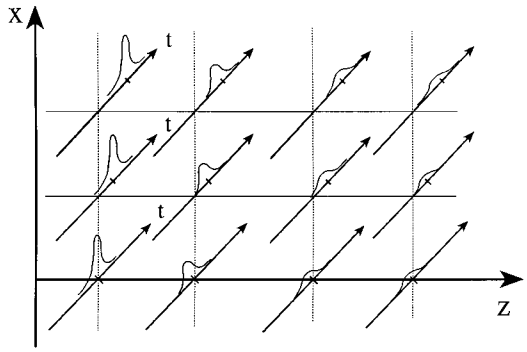
The time-dependent field is obtained by applying (3.1) to (4.3). Substituting (4.4), switching the order of integrations and performing the ω-integration first as in (3.5) and (3.7) yields

$$\overset{+}{u}_p(\mathbf{r},t)=\frac{-\partial_t}{(2\pi)^2 2c}\int_{|\boldsymbol{\xi}|<1}d^2\xi\frac{1}{\zeta}\hat{\tilde{q}}(\boldsymbol{\kappa},t-\boldsymbol{\kappa}\cdot\mathbf{r}/c)\Big|_{\boldsymbol{\kappa}=(\boldsymbol{\xi},\zeta)}, \tag{4.5}$$

where $\overset{+}{\tilde{q}}$ is the analytic time-dependent spectral function as calculated from the time-dependent source via (3.7).



(a)



(b)

FIG. 2. Time-dependent plane wave integral. (a) Propagating spectrum: Schematization of a single pulsed plane wave at a fixed observation time. $\hat{\mathbf{s}}$ is the plane-wave direction, $\mathbf{r}$ is a typical observation point, and α_0 is introduced in connection with (5.10). (b) Evanescent spectrum: Schematization of an evanescent pulsed plane wave at several observation points along three axes parallel to the z-axis. The diagonal axes denote the time axis at each observation point. The evanescent plane wave propagates in the x-direction and that the pulses decay and broaden as z grows.

The *real* field u_P is obtained from the real part of $\overset{+}{u}_P$. Thus, it can be calculated directly from the *real* spectral function $\tilde{q}$ by using $\tilde{q}$ instead of $\overset{+}{\tilde{q}}$ in (4.5). Note also that $\tilde{q}$ is found directly from the *real* data $q(\mathbf{r},t)$ via (3.10).

Expression (4.5) constitutes an angular spectrum of time-dependent plane waves as schematized in Fig. 2(a). The integrand defines time-dependent plane waves propagating with speed c along the unit vector directions

$$\hat{\mathbf{s}}=(\xi_1,\xi_2,\zeta)=(\sin\,\alpha\,\cos\,\beta,\sin\,\alpha\,\sin\,\beta,\cos\,\alpha), \tag{4.6}$$

where (α,β) are the polar and azimuthal angles with respect to the z-axis. Using these angle coordinates, the real propagating spectrum integral simplifies into

$$u_P(\mathbf{r},t)=\frac{-\partial_t}{(2\pi)^2 2c}\int_{-\pi}^{\pi} d\beta \int_0^{\pi/2} d\alpha\,\sin\,\alpha\tilde{q}(\hat{\mathbf{s}},t-\hat{\mathbf{s}}\cdot\mathbf{r}/c). \tag{4.7}$$

B. Time-dependent evanescent spectrum

The time-harmonic evanescent spectrum is given by (4.3) but with the integration limit now replaced by $|\boldsymbol{\xi}|>1$. Here, however, $\zeta=i|\zeta|$ hence as follows from (4.5), $\hat{\tilde{q}}(\mathbf{K}^{\pm},\omega)$ now grows exponentially as $\omega\to\infty$. To transform this representation to the time domain we rewrite the evanescent spectrum part of (2.4) in a regularized form

$$\hat{u}_E(\mathbf{r},\omega)=\frac{ik}{2(2\pi)^2}\int_{|\boldsymbol{\xi}|>1} d^2\xi\,\frac{1}{\zeta}\hat{\tilde{q}}_0(\mathbf{K}^{+},\omega)e^{ik[\boldsymbol{\xi}\cdot\mathbf{x}+\zeta(z-R_0)]} \tag{4.8}$$

with

$$\hat{\tilde{q}}_0(\mathbf{K}^{+},\omega)=\int_V d^3r'\,\hat{q}(\mathbf{r}',\omega)e^{-ik[\boldsymbol{\xi}\cdot\mathbf{x}'+\zeta(z'-R_0)]}, \tag{4.9}$$

where R_0 is the support of the source and, as before, it is assumed that $z>R_0$. Noting also that $z'<R_0$ for $\mathbf{r}'\in V$ it follows that the exponents in (4.8) and (4.9) decay for $\zeta=i|\zeta|$ as $\omega\to\infty$.

The time-dependent field is obtained now by applying (3.1) to (4.8)–(4.9) and performing the ω integration first. We obtain

$$\overset{+}{u}_E(\mathbf{r},t)=\frac{-\partial_t}{(2\pi)^2 2c}\int_{|\boldsymbol{\xi}|>1} d^2\xi\,\frac{1}{\zeta}\,\overset{+}{\tilde{q}}_0[(\boldsymbol{\xi},\zeta),t-\boldsymbol{\xi}\cdot\mathbf{x}/c-\zeta(z-R_0)/c] \tag{4.10}$$

with

$$\overset{+}{\tilde{q}}_0[(\boldsymbol{\xi},\zeta),\tau]=\int_V d^3r'\,\overset{+}{q}[\mathbf{r}',\tau+\boldsymbol{\xi}\cdot\mathbf{x}'/c+\zeta(z'-R_0)/c], \tag{4.11}$$

where $\overset{+}{\tilde{q}}_0$ is the analytic time-dependent spectrum of $q(\mathbf{r},t)$ (compare (3.7)). Here, however, it is calculated for an imaginary spectral variable $\zeta=i|\zeta|$, and it is also space-shifted by R_0. Note that since $z>R_0$ and $z'<R_0$, the time-arguments in the integrands of (4.10)–(4.11) have negative imaginary parts as required by the analytic signal theory.

Expression (4.10) is identified as a superposition of *time-dependent evanescent plane waves*. This interpretation follows from the fact that analytic signals generally decay as their time-argument goes deeper into the lower half of the complex plane (see (3.1)). Since $\zeta=i|\zeta|$ here, the integrand $\overset{+}{\tilde{q}}$ in (4.10) decays as z increases, as schematized in Fig. 2(b). The *real* spectral delay in the argument of $\overset{+}{\tilde{q}}$ is given by $\boldsymbol{\xi}\cdot\mathbf{x}/c$, hence the time-dependent evanescent waves "propagate" transversely in the $\boldsymbol{\xi}$ direction with propagation speed $v_E=c/|\boldsymbol{\xi}|<c$ (Fig. 2(b)).

The *real* field u_E is obtained from (4.10) via $\mathrm{Re}\,\overset{+}{u}_E$. Unlike (4.5), however, in (4.10) one cannot replace $\overset{+}{\tilde{q}}_0$ by the real spectral function $\tilde{q}$ since here the time-argument in the integrand is complex even for real t.

It is therefore required in (4.11) to calculate the extension of the source signal $q(\mathbf{r},t)$ to the analytic function $\overset{+}{q}(\mathbf{r},t)$ for complex t. In certain cases, $\overset{+}{q}$ can be found analytically. Otherwise, it should be calculated numerically. One route is by the analytic Fourier inversion (3.4) of $\hat{\tilde{q}}(\kappa,\omega)$ to complex t with $\mathrm{Im}\ t\leqslant 0$. This route, however, is rather intricate since, given $q(\mathbf{r},t)$, it requires the calculation $\hat{q}(\mathbf{r},\omega)$ for all $\mathbf{r}$, then of $\hat{\tilde{q}}(\boldsymbol{\kappa},\omega)$ and finally of $\overset{+}{q}(\mathbf{r},t)$ via (3.4).

Alternatively, the extension of the real data $q(\mathbf{r},t)$ to complex t can be calculated *directly in the time domain* by convolving the real signal with the analytic $\overset{+}{\delta}$ function as in (A7). Via this route, the analytic kernel $\overset{+}{\tilde{q}}_0[(\xi,\zeta),\tau]$ in (4.11) can be calculated via the *real data* integration

$$\overset{+}{\tilde{q}}[(\boldsymbol{\xi},\zeta),\tau]=\int_V d^3r' \int_{-\infty}^{\infty} dt' q(\mathbf{r}',t')\frac{1}{\pi i}\frac{1}{\tau+\boldsymbol{\xi}\cdot\mathbf{x}'/c+\zeta(z'-R_0)/c-t'}, \quad \text{Im } \tau<0. \tag{4.12}$$

To recover the radiated field via (4.10), this kernel should be calculated for $\zeta=i\sqrt{|\boldsymbol{\xi}|^2-1}$ and for complex τ: $\tau=t-\boldsymbol{\xi}\cdot\mathbf{x}/c-i|\zeta|(z-R_0)/c$ where t is the real observation time.

C. A unified representation

The analysis in (4.8)–(4.9) implies that the evanescent time-dependent plane-wave representation is valid only if the source is located entirely behind the reference plane. Choosing a reference plane $z=z_0 > R_0$ yields a representation that includes both the propagating and the evanescent spectra. With respect to this plane we have

$$\overset{+}{u}(\mathbf{r},t)=\frac{-\partial_t}{(2\pi)^2 2c}\int_{-\infty}^{\infty} d^2\xi \ \frac{1}{\zeta}\ \overset{+}{\tilde{q}}_0[(\boldsymbol{\xi},\zeta),t-\boldsymbol{\xi}\cdot\mathbf{x}/c-\zeta(z-z_0)/c], \quad z>z_0, \tag{4.13}$$

with (compare (4.5) and (4.10))

$$\overset{+}{\tilde{q}}_0[(\boldsymbol{\xi},\zeta),\tau]=\int_V d^3r' \overset{+}{q}[\mathbf{r}',\tau+\boldsymbol{\xi}\cdot\mathbf{x}'/c+\zeta(z'-z_0)/c]. \tag{4.14}$$

The unified representation in (4.13) now includes *both the propagating and the evanescent time-dependent spectra*. The real field is obtained by taking the real part of (4.13). The details are similar to those discussed in connection with (4.7) and (4.10).

V. SPECIAL CASE: POINT SOURCE

To clarify the causal properties of the time-dependent plane wave representation we shall consider first the simplified problem of the time-dependent Green's function $G(\mathbf{r},t)$, due to a pulsed point-source

$$q(\mathbf{r},t)=f(t)\,\delta(\mathbf{r}), \tag{5.1}$$

where it is assumed that the source history $f(t)$ vanishes for $t<0$.

We shall obtain closed-form expressions for the time-dependent propagating and evanescent spectra that clarify their respective role in establishing the causal radiated field. These properties will be used in Sec. VI to establish the causal properties of the time-dependent plane-wave representations under more general conditions.

A. The spectral integrals

From (3.7), the plane-wave spectrum of the source is

$$\tilde{q}(\boldsymbol{\kappa},\tau)=f(\tau), \tag{5.2}$$

hence from (4.13), the (Weyl-type) spectral expansion for the time-dependent analytic Green's function is

$$\overset{+}{G}(\mathbf{r},t)=\frac{1}{(2\pi)^2}\frac{-1}{2c}\int_{-\infty}^{\infty}d^2\xi\frac{1}{\zeta}\overset{+}{f}{}'[t-(\boldsymbol{\xi}\cdot\mathbf{x}+\zeta z)/c], \tag{5.3}$$

where the prime denotes a derivative with respect to the argument. Expression (5.3) is a unified expression that includes both the propagating and the evanescent time-dependent spectra.

As before, we explore separately the field contributions G_P and G_E from the propagating and evanescent spectral ranges, respectively. The propagating spectrum consists of pulsed plane waves propagating in the unit vector directions $\hat{\mathbf{s}}$ in (4.6). Using the plane-wave unit vector direction $\hat{\mathbf{s}}$ and the spherical angles (α,β) of (4.6), the integral for the propagating spectrum becomes (see (4.7))

$$\overset{+}{G}_P(\mathbf{r},t)=\frac{-1}{(2\pi)^2 2c}\int_{-\pi}^{\pi}d\beta\int_0^{\pi/2}d\alpha\ \sin\alpha\overset{+}{f}{}'[t-\hat{\mathbf{s}}\cdot\mathbf{r}/c], \tag{5.4}$$

and the *real* field G_P is given by the same expression with $\overset{+}{f}\to f$. Since $\hat{\mathbf{s}}\cdot\mathbf{r}\leqslant r$ for all $\hat{\mathbf{s}}$, all the pulsed plane waves in (5.4), except for the one that propagates along the direction from the source to $\mathbf{r}$, arrive to $\mathbf{r}$ *prior* to the causal arrival time $t_0=r/c$. This yields a non-causal contribution that is canceled out by the contribution of the pulsed evanescent spectrum. As we shall see below, in certain space-regions the integrated non-causal contribution vanishes prior to the causal arrival time t_0, so that it may be time-separated from the physical signal at $t>t_0$.

The contribution of the evanescent spectrum is given by

$$\overset{+}{G}_E(\mathbf{r},t)=\frac{-1}{(2\pi)^2 2c}\int_{|\boldsymbol{\xi}|>1}d^2\xi\frac{1}{\zeta}\overset{+}{f}{}'[t-(\boldsymbol{\xi}\cdot\mathbf{x}+\zeta z)/c], \tag{5.5}$$

where here $\zeta=i|\zeta|$. This expression may be described as an integration in the complex α plane but we shall not pursue this formal extension here. The interpretation of (5.5) has been discussed in connection with (4.10). The implications of the observations noted there will be discussed later on.

Expression (5.5) requires the calculation of the dual analytic function $\overset{+}{f}$ for complex t. As mentioned in connection with (4.12), unless f is known analytically, this extension should be done numerically either by Fourier inversion of $\hat{f}(\omega)$ to complex t via (3.1) or directly in the time domain as in (A7). Substituting (A7) in (5.5) we obtain an expression that involves processing only of the *real* data f

$$G_E(\mathbf{r},t)=\frac{1}{(2\pi)^3 c}\int_{|\boldsymbol{\xi}|>1}d^2\xi\frac{1}{|\zeta|}\int_{-\infty}^{\infty}dt' f'(t')\mathrm{Re}\,\frac{1}{t-t'-\boldsymbol{\xi}\cdot\mathbf{x}/c-i|\zeta|z/c} \tag{5.6}$$

$$=\frac{1}{(2\pi)^3 c}\int_{|\boldsymbol{\xi}|>1}d^2\xi\frac{1}{|\zeta|}\int_{-\infty}^{\infty}dt' f(t')\mathrm{Re}\,\frac{-1}{(t-t'-\boldsymbol{\xi}\cdot\mathbf{x}/c-i|\zeta|z/c)^2}, \tag{5.7}$$

where in (5.7) the time-derivative has been commuted, yielding an expression in terms of f rather than f'.

B. Evaluation of the propagating spectrum integral and the role of the evanescent spectrum

To gain insight we consider first an observation point on the z-axis $\mathbf{r}=(0,0,z)$. Here $\hat{\mathbf{s}}\cdot\mathbf{r}=z\cos\alpha$ and the integral in (5.4) is β-independent, giving

$$G_P(\mathbf{r},t)=\frac{-1}{4\pi c}\int_0^{\pi/2} d\alpha\ \sin\ \alpha f'[t-(z/r)\cos\ \alpha].$$

Changing the integration variable to $\tau=(z/c)\cos\ \alpha$ we obtain

$$G_P(\mathbf{r},t)=\frac{1}{4\pi z}\int_{z/c}^{0} d\tau\ f'(t-\tau)=f(t-z/c)/4\pi z-f(t)/4\pi z. \tag{5.8}$$

The first term in (5.8) is the actual field G on the z-axis, hence the remainder should be canceled by the evanescent spectrum, i.e.,

$$G_E(\mathbf{r},t)=f(t)/4\pi z. \tag{5.9}$$

Expression (5.9) will be re-derived in (5.21) by direct evaluation of integral (5.5) for G_E.

Next, we consider general observation points off the z-axis. Let $\mathbf{r}=(r,\theta,\phi)$ where θ and ϕ are the conventional spherical angles and, without loss of generality, let $\phi=0$. To evaluate the spectral integral G_P it is convenient to use the spectral spherical angles (α_0,β_0) that are centered about the observation direction $\hat{\mathbf{r}}$: α_0 and β_0 are the plane wave polar and azimuthal angles with respect to the $\hat{\mathbf{r}}$-axis, with $\beta_0=0$ on the $\phi=0$ plane. One readily finds that the plane wave direction $\hat{\mathbf{s}}$ in (4.6) is described by

$$\begin{aligned}(\xi_1,\xi_2,\zeta)=(&\cos\ \theta\ \sin\ \alpha_0\ \cos\ \beta_0+\sin\ \theta\ \cos\ \alpha_0,\ \ \sin\ \alpha_0\ \sin\ \beta_0,\ \ \cos\ \theta\ \cos\ \alpha_0\\ &-\sin\ \theta\ \sin\ \alpha_0\ \cos\ \beta_0).\end{aligned} \tag{5.10}$$

The condition $\zeta\geqslant 0$ that defines the propagating plane wave spectrum in (5.4) can therefore be expressed as $0\leqslant\alpha_0\leqslant\bar{\alpha}_0(\beta_0)$ where

$$\bar{\alpha}_0(\beta_0)=\tan^{-1}(\cot\ \theta/\cos\ \beta_0). \tag{5.11}$$

Using $\mathbf{r}\cdot\hat{\mathbf{s}}=r\ \cos\ \alpha_0$ we obtain from (5.4)

$$G_P=\frac{1}{(2\pi)^2}\frac{-1}{2c}\int_0^{2\pi} d\beta_0\int_0^{\bar{\alpha}_0(\beta_0)} d\alpha_0\ \sin\ \alpha_0\ f'[t-(r/c)\cos\ \alpha_0]. \tag{5.12}$$

Changing integration variable to $\tau=(r/c)\cos\ \alpha_0$ we obtain, as in (5.8)

$$\begin{aligned}G_P&=\frac{1}{4\pi r}\frac{1}{2\pi}\int_0^{2\pi} d\beta_0\{f[t-r/c]-f[t-(r/c)\cos\ \bar{\alpha}_0(\beta_0)]\}\\ &=\frac{f[t-r/c]}{4\pi r}-\frac{1}{4\pi r}\int_0^{2\pi}\frac{d\beta_0}{2\pi} f[t-(r/c)\cos\ \bar{\alpha}_0(\beta_0)],\end{aligned} \tag{5.13}$$

hence the evanescent spectrum contribution

$$G_E=\frac{1}{4\pi r}\int_0^{2\pi}\frac{d\beta_0}{2\pi} f[t-(r/c)\cos\ \bar{\alpha}_0(\beta_0)]. \tag{5.14}$$

Noting that the maximum and minimum values of $\bar{\alpha}_0(\beta_0)$ are $\bar{\alpha}_0(0)=\pi/2-\theta$ and $\bar{\alpha}_0(\pi)=\pi/2+\theta$, respectively, one finds that the latest and earliest spectral delays in the integrand (5.14) are $\pm x_1/c$, respectively (recall that we assumed that $x_2=0$). It therefore follows that $G_E\neq 0$ only for $-x_1/c<t<T+x_1/c$. Generalizing this result for any $\mathbf{r}$ we have

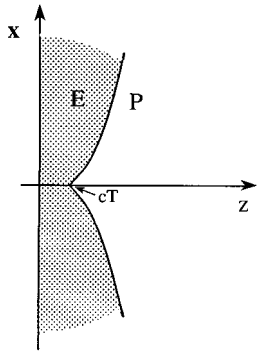


FIG. 3. Space-time regions for the propagating and the evanescent spectral contributions. In region E, the causal field (at times $t>r/c$) is described by both the propagating and the evanescent spectra. In region P, the field may be described only by the propagating spectrum for all causal times.

$$G_E\neq 0 \text{ only for } -\rho/c<t<T+\rho/c\equiv t_E, \tag{5.15}$$

where $\rho=\sqrt{x_1^2+x_2^2}$. Thus $G=G_P$ for all $t>t_E$. Recalling that the physical arrival time is $t_0\equiv r/c$, it follows that in the space region where $t_E<t_0$, i.e.,

$$r>\rho+cT \tag{5.16}$$

(region P in Fig. 3), the field is described only by G_P for all t in the causal window $t>t_0$ (in fact, even for $t_E<t<t_0$). In region E where $r<\rho+cT$, the contribution of G_E does not vanish prior to t_0 hence the total field in the causal window $t>t_0$ consists of both G_P and G_E.

C. Impulsive source: $f(t)=\delta(t)$

To further clarify the discussion above we consider the special case $f(t)=\delta(t)$ in which the spectral integrals may be evaluated in closed form. The analytic excitation here is $\overset{+}{f}(t)=\overset{+}{\delta}(t)$ where $\overset{+}{\delta}(t)=(\pi i t)^{-1}$ is the analytic delta function (see (A5)). Substituting in (5.5) and using the evanescent spectrum coordinates $\boldsymbol{\xi}=(\xi_1,\xi_2)=\xi(\cos\beta,\sin\beta)$ with $\xi>1$, we obtain

$$\overset{+}{G}_E=\frac{1}{(2\pi)^3 c}\frac{\partial}{\partial t}\int_1^\infty d\xi\int_{-\pi}^{\pi} d\beta\,\frac{\xi}{\sqrt{\xi^2-1}}\,\frac{1}{t-(\xi x_1\cos\beta+iz\sqrt{\xi^2-1})/c}, \tag{5.17}$$

where it is assumed, without loss of generality, that $x_2=0$. Evaluating the β integral yields

$$\overset{+}{G}_E=\frac{1}{(2\pi)^3 c}\frac{\partial}{\partial t}\int_1^\infty d\xi\,\frac{\xi}{\sqrt{\xi^2-1}}\,\frac{2\pi c}{[(ct)^2+z^2-\xi^2 r^2-2ictz\sqrt{\xi^2-1}]^{1/2}},$$

where $r=\sqrt{x_1^2+z^2}$. This result may be generalized for $x_2\neq 0$ by replacing $x_1\to\rho$. Changing integration variable to $\eta=\sqrt{\xi^2-1}$ we obtain

$$\overset{+}{G}_E=\frac{1}{(2\pi)^2}\frac{\partial}{\partial t}\int_0^\infty d\eta\,\frac{1}{\sqrt{\Phi}}$$

where $\Phi=(ct)^2-\rho^2-2ictz\eta-\eta^2 r^2$, and then

$$\overset{+}{G}_E=\frac{1}{(2\pi)^2}\frac{i}{r}\frac{\partial}{\partial t}\ln\left(ct-\frac{ir^2\eta}{z}+\frac{r}{z}\sqrt{\Phi}\right)\Bigg|_0^\infty=\frac{c}{(2\pi)^2}\frac{i}{r}\frac{ctr/z-i\eta r+\sqrt{\Phi}}{[ct-ir^2\eta/z+(r/z)\sqrt{\Phi}]\sqrt{\Phi}}\Bigg|_0^\infty.$$

Since the limit at infinity vanishes we finally obtain

$$\overset{+}{G}_E=\frac{1}{(2\pi)^2 iz}\frac{t+(z/r)\sqrt{t^2-(\rho/c)^2}}{t+(r/z)\sqrt{t^2-(\rho/c)^2}}\frac{1}{\sqrt{t^2-(\rho/c)^2}}. \tag{5.18}$$

In all the expressions above, the square roots are defined with branch cuts in the upper half of the complex t plane, giving analytic function in the lower half of the t-plane. In particular in the final expression (5.18) we use for real t,

$$\sqrt{t^2-(\rho/c)^2}=\begin{cases}\sqrt{t^2-(\rho/c)^2} & t>\rho/c,\\ -i\sqrt{(\rho/c)^2-t^2} & -\rho/c<t<\rho/c,\\ -\sqrt{t^2-(\rho/c)^2} & t<-\rho/c,\end{cases}$$

where all the square roots on the right hand side are defined to be positive real. Taking the real part of (5.18), using (V.3.), we obtain for the *real* evanescent field

$$G_E=\frac{1}{(2\pi)^2}\frac{z/c^2}{(r/c)^2-t^2}\frac{1}{\sqrt{(\rho/c)^2-t^2}} \tag{5.19}$$

for $-\rho/c<t<\rho/c$, and zero elsewhere.

Expression (5.19) (or (5.18)) is our main result. For $t\to\rho/c$ such that $|t-\rho/c|\ll 2\rho/c$ we obtain from (5.18) and (5.19)

$$\overset{+}{G}_E\simeq\frac{1}{(2\pi)^2 i}\frac{1}{z\sqrt{2\rho/c}}\frac{1}{\sqrt{t-\rho/c}},\quad\text{hence}\quad G_E\simeq\frac{1}{(2\pi)^2}\frac{1}{z\sqrt{2\rho/c}}\frac{H(\rho/c-t)}{\sqrt{\rho/c-t}} \tag{5.20}$$

where H is the Heaviside function. As one observes, the peak for $t\to\rho/c$ increases as $\rho\to 0$. Indeed, using $\rho=0$ in (5.18) we obtain *on* the axis

$$\overset{+}{G}_E=\frac{1}{4\pi z}\frac{1}{\pi i t}=\frac{1}{4\pi z}\overset{+}{\delta}(t),\quad\text{hence}\quad G_E=\frac{1}{4\pi z}\delta(t). \tag{5.21}$$

Expression (5.21) is in agreement with (5.9), while (5.19) explains the conclusion in (5.15) and the discussion thereafter (see Fig. 3).

Expression (5.19) is similar to Eq. (C.7a) in Ref. 15 up to a factor of 2, which is due to the fact that in Ref. 15, the contribution of the evanescent spectrum has been calculated indirectly using the ''causality trick,'' i.e., by adding the noncausal Green's function to the causal Green's function, and calculating the combined response.

Plots of G_E and of G_P at a constant distance $r=1$ from the source but for several observation directions θ are shown in Fig. 4. Their sum synthesizes the Green's function $G=f(t-r/c)/4\pi r$. The input in this figure is a smoothed δ pulse

$$f(t)=\mathrm{Re}\ \overset{+}{\delta}(t-i\tfrac{1}{2}T)=\frac{1}{\pi}\frac{\frac{1}{2}T}{t^2+(\frac{1}{2}T)^2} \tag{5.22}$$

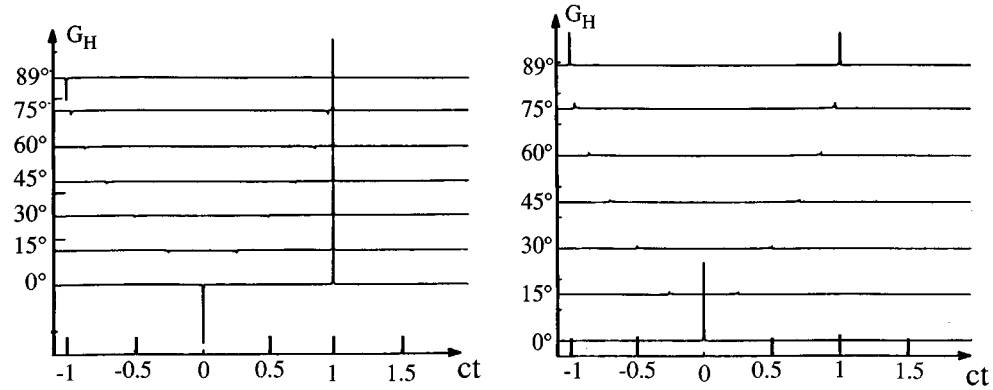


FIG. 4. Plots of G_E and of G_P at a constant distance $r=1$ from the source and for several observation directions θ.

with $T=2\,10^{-3}$ is the half-amplitude pulse length. The spectral contributions G_p and G_E for this excitation pulse are obtained *in closed form* by substituting $t\rightarrow t-i\,\frac{1}{2}\,T$ in the analytic impulse response (5.18) and then taking the real part.

D. Conical spectrum of propagating time-dependent plane-waves

In the previous section we explored, separately, the fields generated by the time-dependent propagating and evanescent spectra. Here we consider the fields generated by a spectrum of propagating time-dependent plane waves. Specifically, we shall consider a conical spectral range of angle Θ centered about the observation direction $\hat{\mathbf{r}}$. From (5.4) it is defined by

$$G_P^{\Theta}=\frac{-1}{(2\pi)^2 2c}\int_{-\pi}^{\pi}d\beta_0\int_0^{\Theta}d\alpha_0\,\sin\,\alpha_0\,f'[t-(r/c)\cos\,\alpha_0], \tag{5.23}$$

where (α_0,β_0) are the plane wave angles with respect to $\hat{\mathbf{r}}$ (see (5.10)). Following the analysis in (5.8) we find that

$$G_P^{\Theta}=\frac{f(t-r/c)}{4\pi r}-\frac{f(t-(r/c)\cos\,\Theta)}{4\pi r}. \tag{5.24}$$

The second term represents the effect of spectral truncation. It vanishes for (cf. (5.15))

$$t>t_{\Theta}\,,\quad t_{\Theta}\equiv T+(r/c)\cos\,\Theta. \tag{5.25}$$

Following the same reasoning as in (5.16) we find that if

$$r(1-\cos\,\Theta)>cT \tag{5.26}$$

then G can be described by G_P^{Θ} for all $t>t_0\equiv r/c$. Condition (5.26) defines the narrowest angular spectrum range needed in order to described correctly the signal G for causal times $t>t_0$. For $r\gg cT$ we find that

$$\Theta>\cos^{-1}(1-cT/r)\simeq\sqrt{2cT/r}. \tag{5.27}$$

Replacing T by ω^{-1}, this condition becomes $\Theta\sim\sqrt{1/kr}$ which is the asymptotic expressison (for $kr\gg 1$) for the contributing spectral range in a conventional stationary point evaluation of the time-harmonic plane-wave integral.

The wave function G_P^{Θ} is a superposition of propagating time-dependent plane waves and therefore is also a source-free solution of the wave equation. Indeed one finds from (5.24) that for $r\to 0$

$$G_P^{\Theta}\simeq \frac{f'(t)[1-\cos\,\Theta]}{4\pi c}=\text{bounded}. \tag{5.28}$$

An important special case of (5.23) is the Wittaker's expansion wherein the propagating plane-wave spectrum comprises all 4π directions (i.e., $\Theta=\pi$). From (5.24) we obtain

$$G_P^{\pi}=\frac{f(t-r/c)}{4\pi r}-\frac{f(t+r/c)}{4\pi r}. \tag{5.29}$$

Thus G_P^{π} is the Schwinger function, consisting of a sum of the causal and the non-causal (adjoint) Green's functions

$$G_P^{\pi}=G-G^{\dagger}\equiv\mathscr{G}. \tag{5.30}$$

Clearly G_P^{π} is a source-free solution of the wave-equation and is regular at $r\simeq 0$ (see also (5.28)).

VI. ON THE ROLE OF THE EVANESCENT SPECTRUM IN THE CAUSAL FIELD

Having established the causal properties of the propagating and evanescent spectra of the point-source configuration, we return now to the distributed source configuration $q(\mathbf{r},t)$. We shall determine the space-time region wherein the total field u is described *only* by the propagating spectrum u_P in (4.5)–(4.7).

For a single point-source at the origin we have shown in (5.15) that u_E vanishes for all $t>t_E=T+\rho/c$ where $\rho=\sqrt{x_1^2+x_2^2}$ is the transverse distance of $\mathbf{r}$ from the point source. Thus for the distributed source, u_E vanishes for all $t>t_E$ where t_E is determined by the point $\mathbf{r}'$ in the source domain with the greatest transverse distance from $\mathbf{r}$, i.e., $t_E=T+\max|\mathbf{x}-\mathbf{x}'|$. Recalling that the source is bounded within a sphere of radius R_0, it follows that

$$u_E=0 \quad \text{for} \quad t>t_E\equiv T+(\rho+R_0)/c. \tag{6.1}$$

Since the causal signal arrives to $\mathbf{r}$ at $t_0=(r-R_0)/c$, we find that the region in space wherein $t_E<t_0$ is given by

$$r-\rho>2R_0+cT \tag{6.2}$$

(region P in Fig. 3). In this region the field u can be described only by u_P for all causal times $t>t_0$ (in fact for all $t>t_E$). In region E where $r-\rho<2R_0+cT$ the contribution of u_E does not vanish within the causal time window $t>t_0$, hence the field representation there consists of both u_P and u_E. It should be emphasized that in any case, u_P generates non-causal contributions that are canceled by u_E, such that the total field is causal. If the observer is in region P, these non-causal contributions vanish prior to the causal arrival time t_0.

VII. ON FIELDS DESCRIBED BY A SPECTRUM OF PROPAGATING PLANE WAVES

A. Conical spectrum of propagating time-dependent plane waves

As mentioned in the introduction, in certain cases it might be preferable to consider only a portion of the propagating spectrum. In this section we consider the field u_P^{Θ} generated by a conical spectral range with angle Θ, centered about the observation direction $\hat{\mathbf{r}}$. Without loss of generality we may assume here that $\mathbf{r}$ is on the z-axis, hence from (4.7) we have

$$u_P^{\Theta}(\mathbf{r},t)=\frac{-\partial_t}{(2\pi)^2 2c}\int_{-\pi}^{\pi}d\beta\int_0^{\Theta}d\alpha\ \sin\alpha\ \tilde{q}[\hat{\mathbf{s}},t-\hat{\mathbf{s}}\cdot\mathbf{r}/c]. \tag{7.1}$$

Here $\tilde{q}(\hat{\mathbf{s}},t)$ may be any function of the plane-wave direction $\hat{\mathbf{s}}(\alpha,\beta)$ and of time t. Clearly u_P^{Θ} is a source-free solution of the time-dependent wave equation. However, to be specific we shall take $\tilde{q}$ to be the time-dependent plane-wave spectrum of $q(\mathbf{r},t)$ as obtained by the slant-stack transform (3.9) (restricted to the light cone whereon $|\boldsymbol{\kappa}|=1$). We shall then explore under what conditions u_P^{Θ} represent the actual field u radiated by $q(\mathbf{r},t)$. It will also be assumed here that

$$\Theta>\sin^{-1}(R_0/z), \tag{7.2}$$

where $\sin^{-1}(R_0/z)$ is the polar angle formed by the tangent from $\mathbf{r}$ to the ball R_0 supporting the source domain V. This implies that *all* the observation directions from all $\mathbf{r}'\in V$ to $\mathbf{r}$ are included in the spectral range in (7.1).

To explore the properties of u_P^{Θ}, we shall express (7.1) as a Green's function integral

$$u_P^{\Theta}(\mathbf{r},t)=\int_V d^3r'\int dt'\,q(\mathbf{r}',t')G_P^{\Theta}(\mathbf{r},t,\mathbf{r}',t'), \tag{7.3}$$

where (see (5.4) and (5.23))

$$G_P^{\Theta}(\mathbf{r},t,\mathbf{r}',t')=\frac{-1}{(2\pi)^2 2c}\int_{-\pi}^{\pi}d\beta\int_0^{\Theta}d\alpha\ \sin\alpha\ \ \delta'[t-t'-\hat{\mathbf{s}}\cdot(\mathbf{r}-\mathbf{r}')/c] \tag{7.4}$$

is *the truncated spectrum part of the time-dependent Green's function.*

The expression for $G_P^{\Theta}(\mathbf{r},t,\mathbf{r}',t')$ can be simplified by using the spherical spectral angles (α_0,β_0) that are centered about the observation direction from $\mathbf{r}'$ to $\mathbf{r}$ as in (5.10), with $\beta_0=0$ on the plane that includes the z axis. In this coordinate system, the plane-wave direction $=(\xi_1,\xi_2,\zeta)$ in the conventional (x_1,x_2,z) coordinate system is described by (5.10) where θ is now the observation angle from $\mathbf{r}'$ to $\mathbf{r}$, i.e.,

$$\theta(\mathbf{r}')=\tan^{-1}[\rho'/(z-z')],\quad \rho'=\sqrt{x'^2_1+x'^2_2}. \tag{7.5}$$

For a given β_0, the spectrum is truncated at an angle $\bar{\alpha}_0(\beta_0,\mathbf{r}')$, which is the spectral angle α_0 at $\mathbf{r}'$ where the spectral direction $\hat{\mathbf{s}}$ coincides with the spectral truncation cone $\alpha=\Theta$. From (5.10) it is found by solving the equation

$$\zeta=-\sin\ \theta(\mathbf{r}')\sin\ \alpha_0\ \cos\ \beta_0+\cos\ \theta(\mathbf{r}')\cos\ \alpha_0=\cos\ \Theta, \tag{7.6}$$

where $\theta(\mathbf{r}')$ is defined in (7.5). In view of (7.2), this equation has a solution $\bar{\alpha}_0>0$.

Following an analysis similar to (5.11)–(5.13) we find that

$$G_P^{\Theta}(\mathbf{r},t,\mathbf{r}',t')=\frac{-1}{(2\pi)^2 2c}\int_{-\pi}^{\pi}d\beta_0\int_0^{\bar{\alpha}_0(\beta_0,\mathbf{r}')}d\alpha_0\ \sin\alpha_0\ \ \delta'[t-t'-c^{-1}|\mathbf{r}-\mathbf{r}'|\ \cos\ \alpha_0] \tag{7.7}$$

and finally

$$G_P^{\Theta}=\frac{\delta[t-t'-|\mathbf{r}-\mathbf{r}'|/c]}{4\pi|\mathbf{r}-\mathbf{r}'|}-\frac{1}{4\pi|\mathbf{r}-\mathbf{r}'|}\int_{-\pi}^{\pi}\frac{d\beta_0}{2\pi}\delta[t-t'-c^{-1}|\mathbf{r}-\mathbf{r}'|\ \cos\ \bar{\alpha}_0(\beta_0,\mathbf{r}')], \tag{7.8}$$

where $\bar{\alpha}_0(\beta_0,\mathbf{r}')$ is defined in (7.6).

The first term in (7.8) is readily recognized as the time-dependent Green's function. Thus the spectral truncation effect is included in the second term which consists of a spectrum of pulsed plane waves arriving at $\mathbf{r}$ *prior* to the causal arrival time $|\mathbf{r}-\mathbf{r}'|/c$. The *latest* arrival is obtained for the smallest $\bar{\alpha}_0(\beta_0,\mathbf{r}')$ i.e., when $\beta_0=0$. From (7.6) we obtain, as expected

$$\bar{\alpha}_0|_{min}=\Theta-\theta(\mathbf{r}'). \tag{7.9}$$

Thus the spectral truncation term in (7.8) vanishes for $t-t' > c^{-1}|\mathbf{r}-\mathbf{r}'|\cos(\Theta-\theta(\mathbf{r}'))$.

Returning to (7.3) we may determine now the space-time region where the effect of the spectral truncation vanishes so that the homogeneous wave solution uP^{Θ} of (7.1) represents the source excited field u. We therefore look for $\mathbf{r}' \in V$ that maximizes $\tau\equiv c^{-1}|\mathbf{r}-\mathbf{r}'|\cos(\Theta-\theta(\mathbf{r}'))$. Recalling that $\mathbf{r}$ is on the z-axis and that $\tan\theta(\mathbf{r}')=\rho'/(z-z')$ we obtain $c\tau=(z-z')\cos\Theta+\rho'\sin\Theta=z\cos\Theta-r'\cos(\Theta+\theta')$ where in the second expression (r',θ') denote the polar coordinates of $\mathbf{r}'$. The maximum occurs at $(r',\theta')=(R_0,\pi-\Theta)$, where $c\tau=z\cos\Theta+R_0$. It therefore follows that *the effect of the spectral truncation on the total solution vanishes for*

$$t>t_{\Theta}\equiv T+(z\cos\Theta+R_0)/c. \tag{7.10}$$

Next, the region wherein the effect of the spectral truncation vanishes before the causal arrival at $t_0=(z-R_0)/c$ is found from $t_{\Theta}<t_0$, giving

$$z>(cT+2R_0)/(1-\cos\Theta). \tag{7.11}$$

This condition determines the space region wherein the truncated spectral integral u_P^{Θ} of (7.1) describes the causal part of the actual radiated field u. We finally note that if the observation point is not situated on the z axis then z in (7.10)–(7.11) should be replaced by r.

Special case: The far zone spectral cone. The narrowest spectral cone of propagating time-dependent plane waves needed in order to synthesize the total causal field at a given remote observation point is found from the large z approximation of (7.11), giving

$$\Theta\simeq\sqrt{2(cT+2R_0)/z}\to 0. \tag{7.12}$$

Special case: $\Theta=\pi/2$. In this case, (7.11) is a special case of the result in (6.2), as one may readily be verified by setting $\rho=0$ in (6.2).

B. Wittaker's expansion: $\Theta=\pi$

Here we consider the field generated by a spectrum of propagating time-dependent plane-waves propagating in all directions. From (7.1), it is given by

$$u_P^{\pi}(\mathbf{r},t)=\frac{-\partial_t}{(2\pi)^2 2c}\int_{-\pi}^{\pi}d\beta\int_0^{\pi}d\alpha\,\sin\alpha\;\tilde{q}[\hat{\mathbf{s}},t-\hat{\mathbf{s}}\cdot\mathbf{r}/c], \tag{7.13}$$

where, as mentioned after (7.1), $\tilde{q}$ may be any proper function of $(\hat{\mathbf{s}},t)$, but is taken here to be the time-dependent plane-wave spectrum of $q(\mathbf{r},t)$ as obtained by the *slant stack transform* (3.9). Clearly, u_P^{π} is a source-free solution hence it does not describe the actual field u radiated by $q(\mathbf{r},t)$. To determine the relation between the two we note from (7.3) that u_P^{π} can also be expressed as

$$u_P^{\pi}(\mathbf{r},t)=\int_V d^3r'\int dt'\,q(\mathbf{r}',t')\mathscr{G}(\mathbf{r},t,\mathbf{r}',t'), \tag{7.14}$$

where $\mathcal{G} \equiv G_P^{\pi}$ is the Schwinger function as given by (5.29)–(5.30) with $f \to \delta$. Its spectral representation is given by (7.4) with $\Theta \to \pi$.

It follows from (7.14) that u_P^{π} describes the actual radiated field u for all $t > T$.[10] Furthermore, the space-region wherein $u_P^{\pi} = u$ describes the total causal field (for $t > t_0 = (r - R_0)/c$) is found by setting $\Theta = \pi$ in (7.11), giving

$$r > cT/2 + R_0 . \tag{7.15}$$

In view of (7.14), this condition is identified as a requirement that the contributions of the noncausal Green's function (which vanish for $t > T - (r - R_0)/c$) will vanish prior to the causal arrival time of the actual field at $t_0 = (r - R_0)/c$.

VIII. CONCLUSIONS

We presented a new time-domain spectral theory for radiation from a time-dependent source distribution. In a companion paper (Ref. 19) we consider alternative representation strategies using pulsed multipoles, and determine their relation to the present time-dependent plane-wave representations. The theory has been derived here only for scalar fields: An extension to vector electromagnetic fields, expressed in the terminology of antenna theory is under preparation.

The main results and expressions are summarized below:

(1) The spectral theory is based on the *time-dependent plane-wave spectrum* of the source $\tilde{q}(\boldsymbol{\kappa}, \tau)$, calculated via the *slant stack transform* (3.9) of the time-dependent source distribution $q(\mathbf{r}, t)$. This operation involves (i) projection of $q(\mathbf{r}, t)$ along planes normal to the spectral propagation direction (see (3.11)) and (ii) stacking the projections with a progressive delay corresponding to the spectral propagation speed v_κ along this direction (see (3.12)). The plane-wave direction and its speed v_κ are determined by $\boldsymbol{\kappa}$ (see (3.13)). $\boldsymbol{\kappa} = (\kappa_1, \kappa_2, \kappa_3)$ is a frequency-normalized wavenumber as defined in (3.3).

The *slant-stack transform* $\tilde{q}(\boldsymbol{\kappa}, \tau)$ is related to a Radon transform of $q(\mathbf{r}, t)$ in the four-dimensional space-time domain. The relation to the conventional definition of the Radon transform $\check{q}$ (see Appendix B) is given in (3.14)–(3.15).

(2) The full (three-fold) spectral representation in (3.17) consists of a spectrum of "time dependent plane waves" $\tilde{q}(\boldsymbol{\kappa}, \tau)$ that propagate in all space directions and with all (spectral) propagation speeds v_κ. Note that only those "plane waves" whose propagation speed v_κ equals c (i.e., those on the light cone $|\boldsymbol{\kappa}| = 1$) are solutions of the wave equation.

(3) The time-dependent radiation pattern $g(\hat{\mathbf{r}}, t)$ is described by the value of $\tilde{q}(\boldsymbol{\kappa}, \tau)$ on the "light-cone" $|\boldsymbol{\kappa}| = 1$ (see (3.18)).

(4) Outside the source domain, the field can be described by a contracted (two-fold) representation consisting of time-dependent plane waves $\tilde{q}(\boldsymbol{\kappa}, \tau)|_{|\kappa| = 1}$ that satisfy the spectral constraint $v_\kappa = c$. Here, however, the complete spectral representation involves both *propagating* and *evanescent* time-dependent plane waves. Their separate contributions, u_P and u_E are given by (4.5)–(4.7) and by the real part of (4.10), respectively. The integrand in (4.10) requires an analytic extension of the real data to complex times as performed in (4.12).

The analytic signal representation also enables the unified formulation (4.13) that incorporates both the propagating and the evanescent time-dependent spectra in a single integral.

In the contracted spectral integrals above, ξ is a frequency normalized transverse wavenumber as defined in (4.1).

(5) To clarify the physical meaning of the time-dependent evanescent spectrum we have explored first the special case of a pulsed point-source (Sec. V), and then extended the results to distributed sources (Sec. VI).

In the point-source case, the analytic time-dependent Green's function $\overset{+}{G}$ is given by the Weyl-type integral (5.3). The separate contributions of the time-dependent propagating and evanescent spectra, G_P and G_E, are given, respectively by (5.4) and (5.5). The latter involves an extension of the real source function to complex times (see (5.6)–(5.7)). It has been established that the G_E vanishes identically after a time t_E in (5.15). Furthermore, in certain regions in space this contribution vanishes *before* the causal time t_0 (i.e., $t_E<t_0$), hence the causal field there may be described only by the time-dependent propagating spectrum (see (5.16)).

Finally, the time-dependent propagating and the evanescent spectra has been evaluated explicitly for the special case of an *impulsive point-source* (see (5.19)). The results agree with the general observations mentioned above.

(6) The point-source results were extended to the case of a general source distribution. We have determined in (6.1) the time t_E after which the contribution of the time-dependent evanescent spectrum vanishes, and in (6.2) the region in space wherein the causal part of the field may be described only by the propagating spectrum.

(7) Finally, we explored the properties of the fields $u_P^{\Theta}(\mathbf{r},t)$ obtained by truncating the spectrum of the time-dependent propagating plane waves in a conical range of angle Θ. The special case $\Theta=\pi$ is the time-domain Wittaker's expansion. These fields are non-causal, source-free solutions of the wave equation. In (7.3) and (7.8), they have been described as a sum of the actual radiating field and a spectral truncation term. The latter vanishes identically after the time t_{Θ} in (7.10). Consequently we determined the space-time regions wherein the truncated representation gives the correct solution to the actual field ((7.10)–(7.11)). Finally, the special case of the time-domain Wittaker's expansion has been considered as examples for the general spectral conditions.

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APPENDIX A: ANALYTIC SIGNALS

Analytic signals are defined by the positive frequency inverse Fourier transform in (3.1) (see (A7) for an alternative definition). This integral definition implies that $\overset{+}{f}(t)$ is an analytic function in the lower half of the complex t-plane. Its *real* t limit is related to the *real* signal $f(t)$ via

$$\overset{+}{f}(t)=f(t)+i\mathscr{H}f(t), \qquad t \text{ real}, \tag{A1}$$

where $\mathscr{H}$ denotes the Hilbert transform

$$\mathscr{H}f(t)\equiv\frac{-\mathscr{P}}{\pi t}\otimes f(t)=\frac{-1}{\pi}\int_{-\infty}^{\infty}dt'\mathscr{P}\frac{f(t')}{t'-t}, \tag{A2}$$

$\mathscr{P}$ denotes a principal value and $\otimes$ is a convolution operator. From (A2), the real signal $f(t)$ for real t is recovered via $f(t)=\mathrm{Re}\ \overset{+}{f}(t)$.

The analytic signals possess the following convolution property: If $\hat{h}(\omega)=\hat{f}(\omega)\hat{g}(\omega)$ then

$$\overset{+}{h}(t)=\frac{1}{2}\overset{+}{f}\otimes\overset{+}{g}\equiv\frac{1}{2}\int_{-\infty}^{\infty}dt'\overset{+}{f}(t-t')\overset{+}{g}(t'), \tag{A3}$$

where Im $t\leqslant 0$ and the t'-integration can be carried along any contour with $0\geqslant \mathrm{Im}\, t'\geqslant \mathrm{Im}\, t$. If one of the signals, say g, is known only in its real form for real t then

$$\overset{+}{h}(t)=\overset{+}{f}\otimes g\equiv\int_{-\infty}^{\infty}dt'\,\overset{+}{f}(t-t')g(t'), \tag{A4}$$

where here Im $t\leqslant 0$ but the integration is carried along the real t' axis.

A special case of these relations is provided by the analytic δ function defined by

$$\overset{+}{\delta}(t)=\begin{cases}1/\pi it, & \mathrm{Im}\, t<0,\\ \delta(t)+\mathscr{P}/\pi\mathrm{it}, & \mathrm{Im}\, t=0,\end{cases} \tag{A5}$$

where the second expression is the distributional limit of the first one for real t. Via Cauchy theorem one readily verifies the identity

$$\overset{+}{f}(t)=\frac{1}{2}\overset{+}{f}\otimes\overset{+}{\delta}=\frac{1}{2\pi i}\int_{-\infty}^{\infty}dt'\,\frac{\overset{+}{f}(t')}{t-t'}. \tag{A6}$$

Finally, from (A4) and (A6) the analytic function $\overset{+}{f}(t)$ for Im $t\leqslant 0$ can be calculated from the real function $f(t)$ for real t via

$$\overset{+}{f}(t)=f\otimes\overset{+}{\delta}=\frac{1}{\pi i}\int_{-\infty}^{\infty}dt'\,\frac{f(t')}{t-t'}, \tag{A7}$$

where the integration is carried out along the real t' axis.

APPENDIX B: ANALYTIC SIGNAL REPRESENTATION OF THE RADON TRANSFORM

The time-dependent spectral theory in this paper can be structured as a Radon transform in 4D space-time domain. Since a unified time-domain theory involves analytic signals in order to accommodate the evanescent spectrum (see Sections IV B and IV C), we summarize below an analytic signal representation of the Radon transform theory.[21]

1. Definition in the configuration space

Let $f(\mathbf{x})$, with $\mathbf{x}\in R^n$, be a real function in $\mathscr{S}_2$. Its Radon transform is defined by[20]

$$\check{f}(p,\hat{\mathbf{p}})=\int d^n x\; f(\mathbf{x})\,\delta(p-\hat{\mathbf{p}}\cdot\mathbf{x})=\int d^{n-1}x\; f(\mathbf{x})\Big|_{\hat{\mathbf{p}}\cdot\mathbf{x}=p}, \tag{B1}$$

where $p\in R$ while $\hat{\mathbf{p}}\in R^n$ is a unit vector $|\hat{\mathbf{p}}|=1$. The analytic Radon transform is defined by

$$\overset{+}{\check{f}}(p,\hat{\mathbf{p}})=\int d^n x\; f(\mathbf{x})\,\overset{+}{\delta}(p-\hat{\mathbf{p}}\cdot\mathbf{x}),\qquad \mathrm{Im}\, p\leqslant 0\ , \tag{B2}$$

where we used $\overset{+}{\delta}(p)=1/\pi ip$ (see (A5)). Henceforth we use the over plus symbol to define analytic functions of p in the l.h.p. Note that unlike the definition of the real Radon transform, the integral in (B2) cannot be reduced into an $(n-1)$ dimensional integral over the plane $\hat{\mathbf{p}}\cdot\mathbf{x}=p$ since here p is complex. For real p, however, we obtain via the distributional limit in (A5)

$$\overset{+}{\check{f}}(p,\hat{\mathbf{p}})=\check{f}(p,\hat{\mathbf{p}})+i\mathscr{H}_p\check{f}(p,\hat{\mathbf{p}}),\qquad \mathrm{Im}\, p=0, \tag{B3}$$

where $\mathscr{H}_p$ is the Hilbert transform operator (see (A2))

$$\mathscr{H}_p \check{f}(p,\hat{\mathbf{p}}) = \frac{-1}{\pi}\int_{-\infty}^{\infty} dp' \mathscr{P}\frac{\check{f}(p',\hat{\mathbf{p}})}{p'-p}. \tag{B4}$$

The definition of the analytic Radon transform implies the symmetry property

$$[\overset{+}{\check{f}}(p,\hat{\mathbf{p}})]^* = \overset{+}{\check{f}}(-p^*,-\hat{\mathbf{p}}), \qquad \text{Im } p \leqslant 0. \tag{B5}$$

(Note that $-p^*$ is symmetric to p with respect to the imaginary axis in the l.h.p.) For real p we obtain the expected result

$$\check{f}(p,\hat{\mathbf{p}}) = \check{f}(-p,-\hat{\mathbf{p}}) \tag{B6}$$

and also: $\mathscr{H}_p \check{f}(p,\hat{\mathbf{p}}) = -\mathscr{H}_p \check{f}(-p,-\hat{\mathbf{p}})$.

2. Relation to the Fourier transform: The analytic Fourier slice theorem

The Fourier spectrum of f is defined by

$$\tilde{f}(\mathbf{X}) = \int d^n x\ f(\mathbf{x}) e^{i\mathbf{X}\cdot\mathbf{x}}, \quad \mathbf{X}\in R^n. \tag{B7}$$

To sow the relation of $\tilde{f}$ and $\overset{+}{\check{f}}$ we replace the $\overset{+}{\delta}$ function in (B2) by its integral definition, valid for Im $p \leqslant 0$, obtaining

$$\overset{+}{\check{f}}(p,\hat{\mathbf{p}}) = \int d^n x\ f(\mathbf{x}) \frac{1}{\pi}\int_0^{\infty} dX\ e^{-iX(p-\hat{\mathbf{p}}\cdot\mathbf{x})}, \qquad \text{Im } p \leqslant 0. \tag{B8}$$

Switching the orders of integrations (legitimate for Im $p \leqslant 0$) we note that the x-integral yields $\tilde{f}(\mathbf{X}=X\hat{\mathbf{p}})$. Thus $\overset{+}{\check{f}}(p,\hat{\mathbf{p}})$ and $\tilde{f}(\mathbf{X}) \equiv \tilde{f}(X,\hat{\mathbf{p}})$ are related via the 1D analytic Fourier transform

$$\overset{+}{\check{f}}(p,\hat{\mathbf{p}}) = \frac{1}{\pi}\int_0^{\infty} dX\ \tilde{f}(X,\hat{\mathbf{p}}) e^{-iXp}, \qquad \text{Im } p \leqslant 0 \tag{B9}$$

and consequently

$$\tilde{f}(X,\hat{\mathbf{p}}) = \frac{1}{2}\int_{-\infty}^{\infty} dp\ \overset{+}{\check{f}}(p,\hat{\mathbf{p}}) e^{ipX}. \tag{B10}$$

The integration in (B10) may be performed along any path in the lower half of the complex p-plane but is taken, conveniently, along the real axis. Note also that since $\overset{+}{\check{f}}$ is analytic in the l.h.p., then $\tilde{f}(X,\hat{\mathbf{p}}) = 0$ for $X<0$.

The distributional limit counterpart of (B9)–(B10) for real p is found now by noting from (B3) that for real p, $\check{f} = \frac{1}{2}(\overset{+}{\check{f}} + \overset{+}{\check{f}}{}^*)$, and from (B9) that $\overset{+}{\check{f}}{}^*(p,\hat{\mathbf{p}}) \leftrightarrow \tilde{f}^*(X,-\hat{\mathbf{p}})$, so that

$$\check{f}(p,\hat{\mathbf{p}}) = \frac{1}{2\pi}\int_0^{\infty} dX\{\tilde{f}(X,\hat{\mathbf{p}}) e^{-iXp} + \tilde{f}(X,-\hat{\mathbf{p}}) e^{iXp}\}. \tag{B11}$$

To simplify this expression we extend the definition of X to negative values via $\mathbf{X}=X\hat{\mathbf{p}}=(-X)\times(-\hat{\mathbf{p}})$. Consequently $\tilde{f}(X,-\hat{\mathbf{p}})=\tilde{f}(-X,\hat{\mathbf{p}})$ and we finally obtain

$$\check{f}(p,\hat{\mathbf{p}})=\frac{1}{2\pi}\int_{-\infty}^{\infty}dX\ \tilde{f}(X,\hat{\mathbf{p}})e^{-iXp}, \tag{B12}$$

and

$$\tilde{f}(X,\hat{\mathbf{p}})=\int_{-\infty}^{\infty}dp\ \check{f}(p,\hat{\mathbf{p}})e^{ipX}. \tag{B13}$$

The transform pair in (B12)–(B13) is called the ''Fourier slice theorem'' since it relates a slice in the X-domain to the projections of f transverse to the direction $\hat{\mathbf{p}}$. Equations (B9)–(B10) are the analytic counterparts of this theorem.

3. Analytic inversion

We start with the inverse of (B7)

$$f(\mathbf{x})=\frac{1}{(2\pi)^n}\int d^nX\ \tilde{f}(\mathbf{X})e^{-i\mathbf{X}\cdot\mathbf{x}} \tag{B14}$$

$$=\mathrm{Re}\frac{2}{(2\pi)^n}\int_{\Omega/2}d^{n-1}\hat{\mathbf{p}}\int_0^{\infty}dXX^{n-1}\tilde{f}(X,\hat{\mathbf{p}})e^{-iX\hat{\mathbf{p}}\cdot\mathbf{x}} \tag{B15}$$

where in (B15) we used $\mathbf{X}=X\hat{\mathbf{p}}$ as before, and also $\tilde{f}(X,\hat{\mathbf{p}})=\tilde{f}^*(X,-\hat{\mathbf{p}})$ (since f is real). Consequently the $\hat{\mathbf{p}}$-integration is performed over the ''half sphere'' domain $\Omega/2$ consisting of all directions $\hat{\mathbf{p}}$ but excluding the reverse directions $-\hat{\mathbf{p}}$. The X integral may be evaluated via the Fourier slice theorem (B9), using also $X\leftrightarrow i\partial_p$, giving

$$f(\mathbf{x})=\mathrm{Re}\ \frac{i^{n-1}}{(2\pi)^{n-1}}\int_{\Omega/2}d^{n-1}\hat{\mathbf{p}}(\partial_p^{n-1}\overset{+}{\check{f}}(p,\hat{\mathbf{p}}))\ \Big|_{p=\hat{\mathbf{p}}\cdot\mathbf{x}}. \tag{B16}$$

This expression can be rewritten in terms of real functions. Taking the real part and using (B3) for $\overset{+}{\check{f}}$ with real p, we obtain the inversion formulas[20]

$$f(\mathbf{x})=\frac{(-)^{(n-1)/2}}{(2\pi)^{n-1}}\int_{\Omega/2}d^{n-1}\hat{\mathbf{p}}(\partial_p^{n-1}\check{f}(p,\hat{\mathbf{p}}))\ \Big|_{p=\hat{\mathbf{p}}\cdot\mathbf{x}},\qquad n\quad\text{odd} \tag{B17}$$

$$f(\mathbf{x})=\frac{(-)^{n/2}}{(2\pi)^{n-1}}\int_{\Omega/2}d^{n-1}\hat{\mathbf{p}}(\partial_p^{n-1}\mathscr{H}_p\check{f}(p,\hat{\mathbf{p}}))\ \Big|_{p=\hat{\mathbf{p}}\cdot\mathbf{x}},\qquad n\quad\text{even}. \tag{B18}$$

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Time-dependent multipoles and their application for radiation from volume source distributions

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The radiation from a pulsed source distribution is expressed directly in the time-domain using a sum of time-dependent spherical (multipole) wave functions. Two alternative expressions for the time-dependent multipole moments (the excitation pulses) are derived. It is shown how they are related to the time-dependent plane-wave spectrum of the source (obtained via a Radon transform of the source distribution in the four space-time coordinates). Furthermore, the time-dependent multipole moments, and thereby the total time-dependent field outside the source region, are completely determined by the time-dependent radiation pattern. The series convergence is addressed by showing that the high order multipole moments tend to the quasistatic extension of the static multipole moments. This also puts an upper limit on the spatial resolution that can be achieved by a source distribution with specified size and pulse length. © *1996 American Institute of Physics.* [S0022-2488(96)01901-0]

I. INTRODUCTION

With the increased bandwidth of radiation and detection systems there is a growing interest in the analysis of radiation propagation and scattering of short-pulse fields. Because of the wide band of these fields, solution techniques directly in the time-domain, where the fields are localized, are preferable over the more conventional approach of transforming the frequency-domain solutions into the time domain. A recent review of short pulse systems, applications, and of analysis techniques may be found in Ref. 1.

One of most significant characteristics of time-dependent fields is *causality*. Solution techniques that are structured around causality are therefore preferable. One example of an a priori causal representation is the time-dependent Green's function integral i.e., the retarded potential superposition integral (see e.g., Ref. 2). An alternative representation is the time-dependent plane-wave spectral integral.[3] However, because of their global nature, the individual pulsed plane waves are non-causal, i.e., each one may contribute at the observer prior to the physical (causal) arrival time of the field. These non-causal contributions cancel each other in the complete spectral superposition, thereby generating the correct causal field. Thus, if the causal arrival time is known a priori, for example via ray tracing, then these non-causal spectral constituents can be rejected a priori for causal observation windows, yielding a simplified spectral representation. This idea has been explored in Ref. 3 where the separate role of selected spectral constituents in establishing the causal radiated field has been determined directly in the time domain (see also Refs. 4 and 5).

In this paper we consider a different set of basic function, namely the time-dependent multipoles. A major advantage of this set for radiation problems is that these basis functions are spherically outgoing and therefore a priori causal. These functions are the time-domain counterparts of the time-harmonic multipoles which were used extensively in direct and inverse scattering and in spectral theory (see e.g., Refs. 6, 7, 8–10, and 11, respectively), as well as in establishing fundamental limits in antenna theory.[12–14]

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Time-dependent multipole expansions have already been suggested before.[15,16] In Sec. III C we rederive this expansion directly from its frequency domain counterpart. In Sec. III B we introduce an alternative new expansion, which is more closely related to the time-dependent plane-wave spectrum representation of Ref. 3.

The time-dependent multipole expansion will be developed for the prototype problem of pulsed radiation in a uniform 3-dimensional medium $\mathbf{r}=(x,y,z)$, where the field $u(\mathbf{r},t)$ satisfies the wave equation

$$\left(\nabla^2-\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)u(\mathbf{r},t)=-q(\mathbf{r},t). \tag{1.1}$$

It is assumed that the source distribution $q(\mathbf{r},t)$ occupies a volume V bounded by a sphere of radius R_0 about the origin, and that $q(\mathbf{r},t)\neq 0$ only for $0<t<T$.

The time-dependent multipole wave-functions can be extended analytically so that they describe radiation from multipoles located in a complex coordinate space.[17] The resulting fields are highly collimated pulsed beams (space-time wavepackets) that propagate along ray trajectories.[18] Such basis functions are useful for efficient expansion of pulsed highly collimated source distributions.[17]

II. TIME-HARMONIC FIELDS: SPHERICAL WAVE EXPANSION

With a suppressed time-dependence $e^{-i\omega t}$, the spherical wave functions of order (l,m) with $l=0,1,\ldots$ and $m=0,\pm 1,\ldots \pm l$ are defined by

$$\hat{\varphi}_{l,m}(\mathbf{r})=(4\pi)j_l(kr)Y_{l,m}(\hat{\mathbf{r}}), \tag{2.1}$$

$$\hat{\psi}_{l,m}(\mathbf{r})=(4\pi)^{-1}ikh_l^{(1)}(kr)Y_{l,m}(\hat{\mathbf{r}}). \tag{2.2}$$

Here $\mathbf{r}=(r,\theta,\phi)$ is the space coordinate, $\hat{\mathbf{r}}=(\theta,\phi)$ is a unit vector in the direction of $\hat{\mathbf{r}}$, j_l and $h_l^{(1)}$ are the spherical Bessel functions of order l and $Y_{l,m}$ are the spherical harmonics (we use the standard definition of Ref. 6; see Appendix A). Here and henceforth a caret over a wave constituents denotes the time harmonic amplitude, while a caret over a vector denotes a unit vector.

The 3D Green's function

$$\hat{G}(\mathbf{r},\mathbf{r}')=e^{ik|\mathbf{r}-\mathbf{r}'|}/4\pi|\mathbf{r}-\mathbf{r}'| \tag{2.3}$$

can be expressed now as

$$\hat{G}(\mathbf{r},\mathbf{r}')=\sum_{l,m} ikj_l(kr_<)h_l^{(1)}(kr_>)Y_{l,m}(\hat{\mathbf{r}})Y_{l,m}^*(\hat{\mathbf{r}}'), \tag{2.4}$$

where $r_<$ and $r_>$ denote, respectively, the lesser and greater between r and r' and the asterisks denotes a complex conjugate. Denoting by $\hat{q}(\mathbf{r})$ the time-harmonic counterpart of the source distribution in (1.1), the radiated field can be expressed as

$$\hat{u}(\mathbf{r})=\int_V d^3r'\hat{G}(\mathbf{r},\mathbf{r}')\hat{q}(\mathbf{r}'). \tag{2.5}$$

Outside the sphere R_0 that encloses V, $\hat{u}(\mathbf{r})$ can therefore be expressed as a series of spherical (or multipole) waves

$$\hat{u}(\mathbf{r})=\sum_{l,m}\hat{q}_{l,m}\hat{\psi}_{l,m}(\mathbf{r}), \quad r>R_0, \tag{2.6}$$

where the ''multipole moments'' are found from

$$\hat{q}_{l,m}=\int_V d^3r'\,\hat{\varphi}^*_{l,m}(\mathbf{r}')\hat{q}(\mathbf{r}'). \tag{2.7}$$

An alternative expression for the multipole moments is obtained if we use the plane-wave expansion of $\hat{\varphi}_{l,m}(\mathbf{r}')$

$$\hat{\varphi}_{l,m}(\mathbf{r})=\int_{4\pi} d^2\hat{r}'(-i)^l Y_{l,m}(\hat{\mathbf{r}}')e^{ik\hat{\mathbf{r}}'\cdot\mathbf{r}} \tag{2.8}$$

or its inverse representation, i.e., the multiple expansion of a plane-wave

$$e^{ik\hat{\mathbf{r}}'\cdot\mathbf{r}}=\sum_{l,m} i^l\hat{\varphi}_{l,m}(\mathbf{r})Y^*_{l,m}(\hat{\mathbf{r}}'), \tag{2.9}$$

where in (2.8) $d^2\hat{r}'=\sin\theta' d\theta' d\phi'$ and the integration comprises all 4π spherical directions. Substituting (2.8) into (2.7) and inverting order of integrations we obtain

$$\hat{q}_{l,m}=\int_{4\pi} d^2\hat{r}'\,i^l Y^*_{l,m}(\hat{\mathbf{r}}')\hat{\tilde{q}}(\mathbf{K})|_{\mathbf{K}=k\hat{\mathbf{r}}'}, \tag{2.10}$$

where

$$\hat{\tilde{q}}(\mathbf{K})=\int_V d^3r'\,\hat{q}(\mathbf{r}')e^{-i\mathbf{K}\cdot\mathbf{r}'} \tag{2.11}$$

is the 3D Fourier transform of $\hat{q}(\mathbf{r})$. From (2.10), the multipole moments are the coefficients in the spherical harmonic expansion of the spatial spectrum $\hat{\tilde{q}}(\mathbf{K})$ on the Ewald sphere $|\mathbf{K}|=k$.

In the far zone the radiated field has the form

$$\hat{u}(\mathbf{r})|_{r\to\infty}=\frac{e^{ikr}}{4\pi r}\hat{g}(\hat{\mathbf{r}}) \tag{2.12}$$

where the ''radiation pattern'' in the direction $\hat{\mathbf{r}}$ is given by

$$\hat{g}(\hat{\mathbf{r}})=\hat{\tilde{q}}(k\hat{\mathbf{r}}) \tag{2.13}$$

$$=\sum_{l,m}\hat{q}_{l,m}(-i)^l Y_{l,m}(\hat{\mathbf{r}}). \tag{2.14}$$

Equation (2.13) is obtained directly from (2.5) and (2.11) by using $\hat{G}(\mathbf{r},\mathbf{r}')\sim(e^{ikr}/4\pi r)e^{-ik\hat{\mathbf{r}}\cdot\mathbf{r}'}$. It states that the far field pattern is determined by the value of $\hat{\tilde{q}}(\mathbf{K})$ on the Ewald sphere $|\mathbf{K}|=k$. In view of (2.10), expression (2.14) is simply a spherical harmonic expansion of (2.13). Alternatively (2.14) follows from (2.6) using $h_l^{(1)}\times(kr)\sim(-i)^l(e^{ikr}/ikr)$ as $r\to\infty$.

III. TIME-DEPENDENT MULTIPOLE EXPANSION

The time-dependent field will be recovered via an inverse Fourier transform to the time-domain. We shall use analytic signal representation that simplifies the manipulations, but we shall also express the final results explicitly in terms of real signals.

An analytic signal $\overset{+}{f}(t)$ corresponding to the real signal $f(t)$ with frequency spectrum $\hat{f}(\omega)$ is defined by the positive frequency inverse Fourier transform

$$\overset{+}{f}(t)=\frac{1}{\pi}\int_0^\infty d\omega e^{-i\omega t}\hat{f}(\omega), \qquad \text{Im } t \leqslant 0. \tag{3.1}$$

This integral definition implies that $\overset{+}{f}(t)$ is an analytic function in the lower half of the complex t-plane. Its *real* t limit is related to the *real* signal $f(t)$ via

$$\overset{+}{f}(t)=f(t)+i\mathscr{H}f(t), \qquad t \text{ real}, \tag{3.2}$$

where $\mathscr{H}$ is the Hilbert transform

$$\mathscr{H}f(t)\equiv\frac{-1}{\pi}\int_{-\infty}^{\infty}dt'\mathscr{P}\frac{f(t')}{t'-t} \tag{3.3}$$

and $\mathscr{P}$ denotes a principal value. The physical signal $f(t)$ (for real t) is therefore recovered via $f(t)=\text{Re}\overset{+}{f}(t)$.

A. Time-dependent multipole wave functions

The *analytic* time-dependent multipole wave functions of order (l,m) with $l=0,1,\ldots$ and $m=0,\pm 1,\ldots \pm l$ are defined via

$$\overset{+}{\psi}_{l,m}(\mathbf{r},t)=\frac{1}{\pi}\int_0^\infty d\omega e^{-i\omega t}i^l\hat{\psi}_{l,m}(\mathbf{r})\hat{f}(\omega) \tag{3.4}$$

where $\hat{\psi}_{l,m}$ are defined in (2.2) and $\hat{f}(\omega)$ is a rather general pulse spectrum. Substituting [Ref. 19, Eq. (10.1.8–9)]

$$h_l^{(1)}(z)=\frac{e^{iz}}{iz}(-i)^l\sum_{n=0}^{l}\frac{(l+n)!}{n!(l-n)!}(-2iz)^{-n}, \tag{3.5}$$

and inverting the order of integration and summation we get

$$\overset{+}{\psi}_{l,m}(\mathbf{r},t)=(4\pi r)^{-1}Y_{l,m}(\hat{\mathbf{r}})\mathscr{L}_l\overset{+}{f}(\tau), \qquad \tau=t-r/c, \tag{3.6}$$

where

$$\mathscr{L}_l=\sum_{n=0}^{l}\frac{(l+n)!}{n!(l-n)!}\left(\frac{c}{2r}\right)^n\partial_\tau^{-n} \tag{3.7}$$

and $\partial_\tau^{-n}\equiv(\partial/\partial t)^{-n}$ denotes an nth order integration. The procedure above is justified analytically for $\text{Im } t<0$ and in the limit of real t. It is also assumed the $f(t)$ is l times integrable.

The *real* multipole wave functions are given now by

$$\psi_{l,m}^{(j)}(\mathbf{r},t)=(4\pi r)^{-1}S_{l,m}^{(j)}(\hat{\mathbf{r}})\mathscr{L}_l f(\tau), \tag{3.8}$$

where $S_{l,m}^{(j)}$ are the real spherical harmonics in (A6) with $l=0,1,\ldots,$ $m=0,1,\ldots l$ and $j=1,2$. The relation between the analytic set $\overset{+}{\psi}_{l,m}$ with $-l\leqslant m\leqslant l$ and the real set $\psi_{l,m}^{(j)}$ with $0\leqslant m\leqslant l$, is found by substituting in (3.6) $Y_{l,m}=S_{l,m}^{(1)}+iS_{l,m}^{(2)}$ for $m\geqslant 0$ and using the symmetry relation (A5) for $m<0$. Using also the real t relation (see (3.2)) $\overset{+}{f}=f+i\mathscr{H}f$ we obtain

$$\overset{+}{\psi}_{l,m}=\psi_{l,m}^{(1)}-\mathscr{H}\psi_{l,m}^{(2)}+i[\mathscr{H}\psi_{l,m}^{(1)}+\psi_{l,m}^{(2)}], \tag{3.9a}$$

$$(-1)^m\overset{+}{\psi}_{l,-m}=\psi_{l,m}^{(1)}+\mathscr{H}\psi_{l,m}^{(2)}+i[\mathscr{H}\psi_{l,m}^{(1)}-\psi_{l,m}^{(2)}], \tag{3.9b}$$

where $m\geqslant 0$ here and $\mathscr{H}\psi_{l,m}^{(j)}(\mathbf{r},t)$ are given by (3.8) with $f(\tau)\to\mathscr{H}f(\tau)$.

B. Multipole wave expansion based on time-dependent plane-wave representation

Applying (3.1) to (2.6), using (3.4) and (3.6) we find that the analytic time-dependent field at $r>R_0$ can be expressed as a sum of multipole wave functions

$$\overset{+}{u}(\mathbf{r},t)=\sum_{l=0}^{\infty}\sum_{m=-l}^{l}(4\pi r)^{-1}Y_{l,m}(\hat{\mathbf{r}})\mathscr{L}_l\overset{+}{q}_{l,m}(\tau), \tag{3.10}$$

where the operation $\mathscr{L}_l$ is defined in (3.7) and the time-dependent multipole moments are related to the time-harmonic ones in (2.6) via

$$\overset{+}{q}_{l,m}(\tau)=\frac{1}{\pi}\int_0^{\infty}d\omega(-i)^l\hat{q}_{l,m}e^{-i\omega\tau}. \tag{3.11}$$

Using (2.10)–(2.11), we find a time-domain expression for the multipole moments

$$\overset{+}{q}_{l,m}(\tau)=\int_{4\pi}d^2\hat{r}'Y_{l,m}^*(\hat{\mathbf{r}}')\overset{+}{\tilde{q}}(\hat{\mathbf{r}}',\tau), \tag{3.12}$$

where

$$\overset{+}{\tilde{q}}(\hat{\mathbf{r}}',\tau)=\frac{1}{\pi}\int_0^{\infty}d\omega e^{-i\omega\tau}\tilde{q}(k\hat{\mathbf{r}}')=\frac{1}{\pi}\int_0^{\infty}d\omega\int_V d^3r\hat{q}(\mathbf{r})e^{-i\omega(\tau+\hat{\mathbf{r}}'\cdot\mathbf{r}/c)}.$$

Inverting the order of integrations (legitimate for $\mathrm{Im}\,\tau<0$ and in the limit of real τ) and evaluating the ω integration yields

$$\overset{+}{\tilde{q}}(\hat{\mathbf{r}}',\tau)=\int_V d^3r\overset{+}{q}(\mathbf{r},\tau+\hat{\mathbf{r}}'\cdot\mathbf{r}/c). \tag{3.13}$$

In (3.13) $\overset{+}{q}(\mathbf{r},t)$ is the analytic extension of the source distribution $q(\mathbf{r},t)$. The function $\overset{+}{\tilde{q}}(\hat{\mathbf{r}}',\tau)$ is termed the analytic *time-dependent plane-wave spectrum* of $q(\mathbf{r},t)$,[3] describing the source-excited time-dependent plane wave in the direction $\hat{\mathbf{r}}'$. The operation in (3.13) is termed a "slant-stack transform"[3] since, as implied by (3.13), it is obtained by projecting the source distribution $q(\mathbf{r},t)$ along planes normal to the propagation direction $\hat{\mathbf{r}}'$ and stacking these projections with a progressive delay corresponding to a time-dependent plane wave that propagates in that direction (see Ref. 3; Eqs. (3.11)–(3.12) and Fig. 1). Thus, this operation extracts from $q(\mathbf{r},t)$ the time-dependent plane-wave information in the direction of $\hat{\mathbf{r}}'$. Mathematically, (3.13) is a Radon transform of $q(\mathbf{r},t)$ in the four-dimensional $(\mathbf{r},t)$ coordinate space.

On taking the real part of (3.10) we obtain the final result for the *real field*

$$u(\mathbf{r},t)=\sum_{l=0}^{\infty}\sum_{m=0}^{l}\sum_{j=1}^{2}(4\pi r)^{-1}\alpha_m S_{l,m}^{(j)}(\hat{\mathbf{r}})\mathscr{L}_l q_{l,m}^{(j)}(\tau), \tag{3.14}$$

where $S_{l,m}^{(j)}$ are the real spherical harmonics, $\alpha_m=1$ or 2 for $m=0$ or $m\geqslant 1$, respectively, and

$$q_{l,m}^{(j)}(\tau)=\int_{4\pi} d^2\hat{r}'\, S_{l,m}^{(j)}(\hat{\mathbf{r}}')\tilde{q}(\hat{\mathbf{r}}',\tau) \tag{3.15}$$

with

$$\tilde{q}(\hat{\mathbf{r}}',\tau)=\int_V d^3 r\, q(\mathbf{r},\tau+\hat{\mathbf{r}}'\cdot\mathbf{r}/c). \tag{3.16}$$

Equations (3.14)–(3.16) are the real analog of (3.10)–(3.13), and their interpretation is basically the same. The real field is expressed in (3.14) as a sum of time-dependent multipole wave functions with time-dependent moments $q_{l,m}^{(j)}(\tau)$. From (3.15), these moments are projections of the *real* time-dependent plane-wave spectrum $\tilde{q}(\hat{\mathbf{r}}',\tau)$ of (3.16) onto the *real spherical harmonics* $S_{l,m}^{(j)}$. In (3.18)–(3.20) this operation will be identified as a projection of the time-dependent radiation pattern. Finally, the series convergence will be considered in (3.30)–(3.32).

In the far zone, the field has the form

$$u(\mathbf{r},t)\big|_{r\to\infty}\sim\frac{g(\hat{\mathbf{r}},\tau)}{4\pi r},\ \tau=t-r/c. \tag{3.17}$$

In the multipole expansion (3.14), the time-dependent radiation pattern is obtained from the lowest order $(n=0)$ term in the operator $\mathscr{L}_l$ in (3.7) which yields $\mathscr{L}_l\to 1$. Thus, from (3.14)

$$g(\hat{\mathbf{r}},\tau)=\sum_{l=0}^{\infty}\sum_{m=0}^{l}\sum_{j=1}^{2}\alpha_m S_{l,m}^{(j)}(\hat{\mathbf{r}})q_{l,m}^{(j)}(\tau). \tag{3.18}$$

Equation (3.18) is a spherical harmonics expansion of $g(\hat{\mathbf{r}},\tau)$. Thus, for a given radiation pattern $g(\hat{\mathbf{r}},\tau)$ the multipole moment functions $q_{l,m}^{(j)}(\tau)$ are given by

$$q_{l,m}^{(j)}(\tau)=\int_{4\pi} d^2\hat{r}\, S_{l,m}^{(j)}(\hat{\mathbf{r}})g(\hat{\mathbf{r}},\tau). \tag{3.19}$$

Comparing (3.15) and (3.19) it also follows that the time-dependent radiation pattern g is directly related to the time-dependent plane-wave spectrum

$$g(\hat{\mathbf{r}},\tau)=\tilde{q}(\hat{\mathbf{r}},\tau)=\int_V d^3r'\,q(\mathbf{r}',\tau+\hat{\mathbf{r}}\cdot\mathbf{r}'/c). \tag{3.20}$$

This expression is also derived in Ref. 3; Eq. (3.18)–(3.19) using time-dependent plane wave analysis. Thus, the time-dependent multipole moments $q_{l,m}^{(j)}(\tau)$, and from (3.14) also the total field at $r>R_0$, are completely determined by the time-dependent radiation pattern $g(\hat{\mathbf{r}},\tau)$.

C. A multipole expansion based on weighted volume contribution

Here we use (Ref. 19; 9.1.20)

$$j_l(z)=\frac{(z/2)^l}{2l!}\int_{-1}^{1} d\eta(1-\eta^2)e^{iz\eta} \tag{3.21}$$

so that from (2.7)

$$k^{-l}\hat{q}_{l,m}=\frac{4\pi}{l!2^{l+1}}\int_V d^3r'\,\hat{q}(\mathbf{r}')Y_{l,m}^*(\hat{\mathbf{r}}')(r')^l\int_{-1}^{1} d\eta(1-\eta^2)^l e^{ikr'\eta}. \tag{3.22}$$

In this expression, the function $(r')^l\int_{-1}^{1}d\eta(1-\eta^2)^l e^{ikr'\eta}$ can be regarded as a weighting factor (or, in antenna terminology, an array factor) for sources located on the r' sphere.

Applying the analytic inverse Fourier transform (3.1) yields the time-dependent multipole expansion of (3.10) wherein the time-dependent multipole moments are related to the frequency domain ones as in (3.11). In this section, however, we shall obtain the time-domain expression for the multipole moments by substituting (3.22) into (3.11) and inverting the order of integration, giving

$$\overset{+}{q}_{l,m}(\tau)=\int_V d^3r'\,Y_{l,m}^*(\hat{\mathbf{r}}')(r')^l\overset{+}{\bar{q}}_l(\mathbf{r}',\tau), \tag{3.23}$$

where

$$\overset{+}{\bar{q}}_l(\mathbf{r}',\tau)=\frac{1}{\pi}\int_0^{\infty} d\omega e^{-i\omega\tau}(-ik)^l\hat{q}(\mathbf{r}')\frac{4\pi}{l!2^{l+1}}\int_{-1}^{1} d\eta(1-\eta^2)^l e^{ikr'\eta}.$$

Inverting the order of integrations (see remark after (3.7)) we obtain

$$\overset{+}{\bar{q}}_l(\mathbf{r}',\tau)=\frac{4\pi}{l!2^{l+1}}\left(\frac{d}{cd\tau}\right)^l\int_{-1}^{1} d\eta(1-\eta^2)^l\overset{+}{q}(\mathbf{r}',\tau+\eta r'/c). \tag{3.24}$$

Taking the real part of (3.10) with (3.23)–(3.24) we find that the real time-dependent field is given by the multipole expansion in (3.14) with

$$q_{l,m}^{(j)}(\tau)=\int_V d^3r'\,S_{l,m}^{(j)}(\hat{\mathbf{r}}')(r')^l\bar{q}_l(\mathbf{r}',\tau) \tag{3.25}$$

with

$$\bar{q}_l(\mathbf{r}',\tau)=\frac{4\pi}{l!2^{l+1}}\left(\frac{d}{cd\tau}\right)^l\int_{-1}^{1} d\eta(1-\eta^2)^l q(\mathbf{r}',\tau+\eta r'/c). \tag{3.26}$$

Note that the operation $\mathscr{L}_l(d/d\tau)^l$ in (3.14) with (3.25) and (3.26) involves only positive power derivatives of $q(\mathbf{r}',\tau)$, having the form $(d/d\tau)^{l-n}$ with $n=0,\ldots,l$.

The multipole expansion in (3.14) with (3.25)–(3.26) has been derived previously using time-domain manipulations. Here it has been derived from the well known time-harmonic multipole expansion (2.6)–(2.7). In Sec. III B we have derived a different representation which explicitly shows that the time-dependent multipole moments are the coefficients in a spherical expansion of the time-dependent plane-wave spectrum (or of the time-dependent radiation pattern).

Note that the operation in (3.26) (or (3.24)) is, for a given $\mathbf{r}'$, a weighted average of the signal in the time-window $(\tau\pm r'/c)$, accounting for the fact that this source point is located on a sphere of radius r'. The η integration therefore yields the effective "array factor" for each source point $\mathbf{r}'$.

If the source signal is approximately constant within the time-window $(\tau\pm r'/c)$, then

$$\bar{q}_l(\mathbf{r}',\tau)\simeq\frac{4\pi}{(2l+1)!!}\left(\frac{d}{cd\tau}\right)^l q(\mathbf{r}',\tau), \tag{3.27}$$

where $(2l+1)!!=1\cdot3\cdot5...(2l+1)$. Let T be a measure of the source rate of change (in particular T can be the pulse-length). Noting that the effective width of the $(1-\eta^2)^l$ kernel in (3.26) is $[\int_{-1}^{1}d\eta\,\eta^2(1-\eta^2)^l]^{1/2}=[2(2l)!!/(2l+3)!!]^{1/2}$, where $(2l)!!=2\cdot4\cdot6...(2l)$, we find that the approximation in (3.27) is valid if

$$2r'/cT\ll\sqrt{(2l+3)!!/(2l)!!}\sim(2\pi^{-1/4})(l/e)^{3/4}, \tag{3.28}$$

where the large l approximation is obtained using Stirling's formula. Thus the approximation in (3.27) is valid for small r' or for large l.

For large l such that

$$2R_0/cT\ll\sqrt{(2l+3)!!/(2l)!!}\sim(2\pi^{-1/4})(l/e)^{3/4}, \tag{3.29}$$

where R_0 is the source support (see (1.1)), (3.27) can be applied for *all* points in the source region, and the time-dependent multipole moments become

$$q_{l,m}^{(j)}(\tau)\simeq\frac{4\pi}{(2l+1)!!}\left(\frac{d}{cd\tau}\right)^l\int_V d^3r'S_{l,m}^{(j)}(\hat{\mathbf{r}}')(r')^l q(\mathbf{r}',\tau). \tag{3.30}$$

The multipole expansion (3.14) with the multipole moments of (3.30) is recognized as the quasi-static extension of the static multipole expansion (Ref. 6; Sec. 4.1).

Noting that for large l the main contribution in (3.30) comes from $r\simeq R_0$, one obtains

$$q_{l,m}^{(j)}(\tau)\simeq\frac{4\pi R_0^{l+3}}{(2l+1)!!(l+3)}\left(\frac{d}{cd\tau}\right)^l Q_{l,m}^{(j)}(\tau)\simeq\frac{4\pi R_0^{l+3}(e/2)^{l+3/2}}{l^{l+2}}\left(\frac{d}{cd\tau}\right)^l Q_{l,m}^{(j)}(\tau), \tag{3.31}$$

where

$$Q_{l,m}^{(j)}(\tau)=\int_{4\pi}d^2\hat{r}S_{l,m}^{(j)}(\hat{\mathbf{r}})q(R_0\hat{\mathbf{r}},\tau) \tag{3.32}$$

is the spherical harmonics expansion of the source distribution situated on the external ball R_0. In (3.31) we also used the Stirling approximation for $(2l+1)!!$. Using in (3.31) $\partial_\tau\sim O(T^{-1})$, it follows that the multipole moments $q_{l,m}^{(j)}$ decay rapidly like $l^{-2}(R_0/cTl)^l$ for $l>R_0/cT$. In view

of (3.18), this defines a fundamental limit on the space-time resolution of the time-dependent radiation pattern that can be achieved by a given pulsed source distribution. This subject will be explored elsewhere.

IV. CONCLUSIONS

In this paper we described the radiation from a pulsed source distribution by a time-dependent multipole expansion. The spherical (multipole) wave functions have been introduced in Sec. III A using two formulations: An analytic signal formulation in (3.6) and later on a real signal formulation (3.8). The latter is expressed in terms of a real source function $f(t)$ and utilizes the real spherical harmonics $S_{l,m}^{(j)}$, whereas the former requires the analytic extension of the source data $\overset{+}{f}(t)$ and the complex spherical harmonics $Y_{l,m}$. Clearly the real signal formulation is the practical one, but for analytical convenience we also considered the analytic signal one (identified by an over plus). In the expressions above, the source function $f(t)$ is an arbitrary signal: In the multipole expansions of Secs. III B and C, it is replaced by the corresponding time-dependent multipole moment of the source distribution.

The time-dependent multipole expansion of the field is given in (3.14) wherein $q_{l,m}^{(j)}(t)$ are the corresponding time-dependent multipole moments (see also (3.10) for the analytic signal formulation; henceforth, however, we shall mention only the final, real signal expressions). We derived two alternative formulations for the calculation of the time-dependent multipole moments directly from the time-dependent source distribution $q(\mathbf{r},t)$. The one in Sec. III B (Eqs. (3.15)–(3.16)) is closely related to the time-dependent plane-wave spectrum of the source considered in Ref. 3. In this formulation the source $q(\mathbf{r},t)$ is first projected on planar wavefronts via the slant-stack transform (3.16), thereby providing the time-dependent plane-wave spectrum of the source, and subsequently projected onto the real spherical harmonics (see (3.15)). In the formulation of Sec. III C (Eqs. (3.25)–(3.26)), on the other hand, the time-dependent source function is first projected on spherical wavefronts centered in the origin (see (3.26)). This formulation has been derived before.[15]

Finally, we addressed the series convergence by showing that the high order multipole moments tend to the quasistatic extension of the static multipole moments (see (3.29)–(3.30)). This also puts an upper limit on the spatial resolution that can be achieved by a source distribution with specified size and pulse length (see (3.31)–(3.32)).

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APPENDIX: THE REAL SPHERICAL HARMONICS $S_{l,m}^{(j)}$

We use the standard definition of the spherical harmonics[6]

$$Y_{l,m}(\hat{\mathbf{r}}) = y_{l,m} P_l^m(\cos\theta) e^{im\phi}, \tag{A1a}$$

$$y_{l,m} = \sqrt{(2l+1)(l-m)!/(l+m)!}/\sqrt{4\pi}, \tag{A1b}$$

where $l=0,1,\ldots$, $m=0,\pm 1,\ldots \pm l$ and $\hat{\mathbf{r}}$ is a unit vector, defined by the spherical angles (θ,ϕ). Here

$$P_l^m(x) = \frac{(-1)^m}{2^l l!}(1-x^2)^{m/2}\left(\frac{d}{dx}\right)^{l+m}(x^2-1)^l \tag{A2}$$

are the associated Legendre functions which may be rewritten in the computationally convenient form (Ref. 19; Eq. 22.5.60 and 22.5.20)

$$P_l^m(x)=\frac{(-1)^m(l+m)!}{2^m l!}(1-x^2)^{m/2}P_{l-m}^{(m,m)}(x), \tag{A2a}$$

where $P_m^{(\alpha,\beta)}$ are the Jacobi polynomials.

The spherical harmonics satisfy the orthogonality, completeness and symmetry conditions

$$\int_{4\pi} d^2\hat{r}\,Y_{l,m}^*(\hat{\mathbf{r}})Y_{l',m'}(\hat{\mathbf{r}})=\delta_{l,l'}\delta_{m,m'}, \tag{A3}$$

$$\sum_{l,m} Y_{l,m}(\hat{\mathbf{r}})Y_{l,m}^*(\hat{\mathbf{r}}')=\delta(\hat{\mathbf{r}}-\hat{\mathbf{r}}'), \tag{A4}$$

$$Y_{l,-m}(\hat{\mathbf{r}})=(-1)^m Y_{l,m}^*(\hat{\mathbf{r}}), \tag{A5}$$

where the asterisks denote a complex conjugate. In (A3) the $d^2\hat{r}=\sin\theta\,d\theta\,d\phi$ integration comprises all 4π spherical directions and in (A5), $\delta(\hat{\mathbf{r}}-\hat{\mathbf{r}}')=(1/\sin\theta)\delta(\phi-\phi')\delta(\theta-\theta')$.

For the real time-domain fields it is convenient to use the *real* spherical harmonics $S_{l,m}^{(j)}$, where $l=0,1,\ldots\ m=0,1,\ldots l$ and $j=1,2$,

$$S_{l,m}^{(1)}=\mathrm{Re}\ Y_{l,m},\ S_{l,m}^{(2)}=\mathrm{Im}\ Y_{l,m}. \tag{A6}$$

Clearly they are given by (A1) with $e^{im\phi}$ replaced by $\cos m\phi$ and $\sin m\phi$, respectively. One may readily show that they satisfy the orthogonality and completeness conditions

$$\int_{4\pi} d^2\hat{r}\,S_{l,m}^{(j)}(\hat{\mathbf{r}})S_{l',m'}^{(j')}(\hat{\mathbf{r}})=\delta_{l,l'}\delta_{m,m'}\delta_{j,j'}\frac{1}{\alpha_m}, \tag{A7}$$

$$\sum_{l=1}^{\infty}\sum_{m=0}^{l}\sum_{j=1,2}\alpha_m S_{l,m}^{(j)}(\hat{\mathbf{r}})S_{l,m}^{(j)}(\hat{\mathbf{r}}')=\delta(\hat{\mathbf{r}}-\hat{\mathbf{r}}'), \tag{A8}$$

where $\alpha_m=1$ or 2 for $m=0$ or $m\geqslant 1$, respectively.

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Topological Yang–Mills theory with scalar and vector fields in two and three dimensions

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We study the topological Yang–Mills theory of scalar and vector fields in two and three dimensions in the superconnection framework. We modify the horizontality condition in such a way that we can take care of the topological symmetry of the $\delta A_\mu = \beta_\mu$ type, as well as the usual gauge symmetry of the $\delta A_\mu = D_\mu c$ type. We then obtain a complete set of BRST and anti-BRST transformation rules of the component fields in a systematic way. © *1996 American Institute of Physics.* [S0022-2488(96)03501-9]

I. INTRODUCTION

The classical action of Witten's four-dimensional topological Yang–Mills theory[1]

$$\mathscr{S}_4 = \int d^4x \ \mathrm{Tr}[\,\epsilon^{\mu\nu\rho\sigma} F_{\mu\nu} F_{\rho\sigma}] \tag{1}$$

is invariant under the transformation

$$\delta_\beta A_\mu = \beta_\mu , \tag{2}$$

as well as under the usual gauge transformation

$$\delta_\alpha A_\mu = D_\mu c . \tag{3}$$

The transformation (2) is the characteristic symmetry of the action (1). Using Eq. (2) as well as Eq. (3) in the BRST quantization formalism, Baulieu and Singer and Perry and Teo reproduced Witten's quantum action which generates the Donaldson invariants.[2–4]

On the other hand, Baulieu and Grossman[5] found that in three dimensions the classical action

$$\mathscr{S}_3 = \int d^3x \ \mathrm{Tr}[\,\epsilon^{\mu\nu\lambda} F_{\mu\nu} D_\lambda \varphi], \tag{4}$$

where $D_\lambda \varphi = \partial_\lambda \varphi + [A_\lambda , \varphi]$, is invariant under the following transformations:

$$\delta A_\mu = D_\mu c + \beta_\mu , \quad \delta\varphi = [\varphi,\ c] + \gamma. \tag{5}$$

Then they studied the BRST symmetry of Eq. (4), and related its quantum action with the scattering of slowly moving magnetic monopoles. Chapline and Grossman[6] found that the classical action in two dimensions,

$$\mathscr{S}_2 = \int d^2x \ \mathrm{Tr}[\,\epsilon^{\mu\nu} D_\mu \varphi D_\nu \varphi], \tag{6}$$

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is also invariant under the transformations (5). They studied the BRST symmetry of Eq. (6), and its quantum action in connection with the theory of vortices and knots.

In this paper we study the BRST and anti-BRST symmetries of Eq. (5) in the superconnection framework. In Sec. II we briefly explain the ''superconnection'' formalism (introduced by Refs. 7–9) and the ''horizontality condition'' (introduced by Ref. 10), which are essential tools in the present work. In this paper, the superconnection will contain only zero and one forms, thus this term has more restrictive meaning than the general one that appeared in Refs. 7 and 8, and in this sense it is similar to the one that appeared in Ref. 9. However, we would like to note that the authors of Ref. 8 also considered a similar case including the Higgs field for the spontaneous symmetry breaking mechanism. From here on, we shall freely use this terminology (and remove the double quotes) as it was used in the quoted references, and we shall not have to provide any further interpretation for the geometrical meaning of the horizontality condition in terms of the geometry of principal bundles. In Sec. III we combine the scalar field φ and the vector field A_μ in a superconnection. We modify the horizontality condition such that it takes care of the symmetry (5) which contains the topological symmetry as well as the usual gauge symmetry. Then using this modified horizontality condition, we obtain the BRST and anti-BRST transformation rules of the component fields in the superconnection framework. In Sec. IV, which constitutes discussions and conclusion, we interpret the three- and two-dimensional topological actions (4) and (6) in analogy with the correspondence between the four-dimensional topological action (1) and the Chern–Simons action.

II. SUPERCONNECTION AND HORIZONTALITY CONDITION

In order to study the theory with scalar and vector gauge fields, it is much easier to work in the superconnection framework, since the theory contains both even and odd form fields. The superalgebra multiplication law is given as follows: for general supermatrices $\mathscr{X}$ and $\mathscr{X}'$, which have arbitrary degree forms X and X' as their supermatrix elements,[8,9]

$$\mathscr{X}\cdot\mathscr{X}' = (a\otimes X)(a'\otimes X') = (-1)^{|X||a'|}(aa')\otimes(XX'), \tag{7}$$

where

$$\mathscr{X} = (a\otimes X) = \begin{pmatrix} A & C \\ D & B \end{pmatrix}, \quad \mathscr{X}' = (a'\otimes X') = \begin{pmatrix} P & R \\ S & Q \end{pmatrix}. \tag{8}$$

In Eq. (7), $|X|$ and $|a|$ are form grade and supermatrix grade, respectively. $|X|$ is one for odd form, zero for even form. $|a|$ is zero for even (diagonal) supermatrix and one for odd (off-diagonal) supermatrix. Equation (7) can be written more explicitly as

$$\mathscr{X}\cdot\mathscr{X}' = \begin{pmatrix} A & C \\ D & B \end{pmatrix}\begin{pmatrix} P & R \\ S & Q \end{pmatrix} = \begin{pmatrix} AP+(-1)^{|C|}CS & (-1)^{|A|}AR+CQ \\ DP+(-1)^{|B|}BS & (-1)^{|D|}DR+BQ \end{pmatrix}. \tag{9}$$

The exterior derivative which is consistent with the superalgebra multiplication law (7) is given by

$$\mathbf{d}.\mathscr{X} = \begin{pmatrix} d & 0 \\ 0 & d \end{pmatrix}\begin{pmatrix} P & R \\ S & Q \end{pmatrix} = \begin{pmatrix} dP & -dR \\ -dS & dQ \end{pmatrix} \tag{10}$$

for the general supermatrix $\mathscr{X}$ since $\mathbf{d}$ is an even supermatrix and $d\equiv dx^\mu(\partial/\partial x^\mu)$ is one form in the base manifold. This exterior derivative satisfies the following Leibniz rule:

$$\mathbf{d}(\mathscr{X}\cdot\mathscr{X}') = \mathbf{d}((a\otimes X)(a'\otimes X')) = (\mathbf{d}.\mathscr{X})\cdot\mathscr{X}' + (-1)^{|a|+|X|}\mathscr{X}\cdot(\mathbf{d}.\mathscr{X}') \tag{11}$$

for general supermatrices $\mathscr{X}'$ and $\mathscr{X}''$. Here one can introduce a ''matrix differentiation'' operation satisfying the same Leibniz rule, the so-called matrix derivative,[11] which is a graded commutator operation with a constant zero form matrix. However, we shall not consider this operation here, and it was considered in our previous article[4] on the pure topological Yang–Mills theory in four dimensions. In this sense, here we are following the approach of Ref. 8 more closely, although ours is more restrictive as we explained in the Introduction. The superconnection is defined as[8]

$$\mathscr{A}=\begin{pmatrix}\omega_0 & L_{01}\\ L_{10} & \omega_1\end{pmatrix}=\mathscr{A}_{\mathrm{ev}}+\mathscr{A}_{\mathrm{od}}=\begin{pmatrix}\omega_0 & 0\\ 0 & \omega_1\end{pmatrix}+\begin{pmatrix}0 & L_{01}\\ L_{10} & 0\end{pmatrix}, \tag{12}$$

where the even supermatrix elements ω_0, ω_1 are odd degree differential forms, and the odd elements L_{01}, L_{10} are even degree forms. Since the superconnection in Eq. (12) has odd and even degree forms for even and odd supermatrix elements, respectively, the exterior derivative **d** satisfies the following Leibniz rule from Eq. (11):

$$\mathbf{d}(\mathscr{A}\mathscr{X}')=(\mathbf{d}\mathscr{A})\mathscr{X}'-\mathscr{A}(\mathbf{d}\mathscr{X}') \tag{13}$$

for the superconnection $\mathscr{A}$ and the general supermatrix $\mathscr{X}'$. We note that Eq. (13) is the same Leibniz rule as that for the ordinary one-form gauge field A which is given by $d(AX)=(dA)X-A(dX)$, where X is an arbitrary differential form. From the superconnection in Eq. (12) we have the supercurvature $\mathscr{F}$ as

$$\mathscr{F}=\mathbf{d}\mathscr{A}+\mathscr{A}\mathscr{A} \tag{14}$$

$$=\begin{pmatrix}d\omega_0+\omega_0\omega_0+L_{01}L_{10} & -dL_{01}-\omega_0L_{01}+L_{01}\omega_1\\ -dL_{10}+L_{10}\omega_0-\omega_1L_{10} & d\omega_1+L_{10}L_{01}+\omega_1\omega_1\end{pmatrix}. \tag{15}$$

Now, we explain the horizontality condition by showing how it gives rise to the BRST transformation rules in the ordinary gauge theory. In the usual non-Abelian gauge theory we have a one-form connection A:

$$A=A_\mu\,dx^\mu, \tag{16}$$

where x^μ is the coordinate of the space-time base manifold. We adopt the differential form notation. The curvature is given by

$$F=dA+AA, \tag{17}$$

where $d=dx^\mu(\partial/\partial x^\mu)$ is the exterior derivative and $AA=A\wedge A$. We omit the wedge for the product of differential forms.

In order to obtain the BRST transformations in a simple way, Ne'eman and Thierry-Mieg introduced[10] new coordinates y^N and extended A to the following algebraic object $\tilde{A}$:

$$\tilde{A}=A+c=A_\mu\,dx^\mu+c_N\,dy^N, \tag{18}$$

where $c=c_N\,dy^N$ plays the role of a gauge field along the direction of the gauge group and turns out to be the ghost field of the BRST symmetry. The curvature in the fiber-bundle space is given by

$$\tilde{F}=\tilde{d}\tilde{A}+\tilde{A}\tilde{A}=(d+s)(A+c)+(A+c)(A+c), \tag{19}$$

where $\tilde{d}=d+s$ and $s=dy^N(\partial/\partial y^N)$ is the exterior derivative in the gauge group direction.

Then Ne'eman and Thierry-Mieg showed that the horizontality condition, which is the Maurer–Cartan equation,

$$\tilde{F}=F \tag{20}$$

gives rise to the BRST transformation rules which satisfy the nilpotency condition $s^2=\bar{s}^2=s\bar{s}+\bar{s}s=0$. That is, when we expand Eq. (20) in terms of form degree, we get the following well-known BRST transformation rules:

$$\begin{aligned}(dx)^1(dy)^1&: sA=-dc-Ac-cA,\\ (dy)^2&: sc=-cc.\end{aligned} \tag{21}$$

The horizontality condition was first studied by Ne'eman and Thierry-Mieg,[10] and it has played important roles in investigating the geometrical meaning of the BRST symmetry.[10,12–14]

III. TOPOLOGICAL BRST AND ANTI-BRST SYMMETRIES WITH SCALAR AND VECTOR FIELDS

In this section we apply the horizontality condition in the superconnection framework, in order to study the BRST symmetry of a system which contains both scalar and vector gauge fields. Then we modify the horizontality condition in such a way that we can take care of the symmetry (5), which contains the topological symmetry of the type (2), as well as the usual gauge symmetry of the type (3). At the beginning we consider only the BRST symmetry, and then both the BRST and anti-BRST symmetries.

In order to study a system which contains both scalar and vector fields, we combine one form gauge field A and zero form scalar gauge field φ in the superconnection as

$$\mathscr{A}=\begin{pmatrix} A & \varphi \\ \varphi & A \end{pmatrix}, \tag{22}$$

where $A=A_\mu\, dx^\mu$ is one-form and φ is zero-form. Here A and φ are Lie algebra valued, that is, $A=A_aT_a$ and $\varphi=\varphi_aT_a$, where T_a are gauge group generators, for example, SU(N) group generators. The ghost and auxiliary fields below are also Lie algebra valued in the same way. The superconnection in the fiber-bundle space is given by

$$\tilde{\mathscr{A}}=\begin{pmatrix} A+\alpha & \varphi \\ \varphi & A+\alpha \end{pmatrix}, \tag{23}$$

where

$$A+\alpha=A_\mu\, dx^\mu+\alpha_N\, dy^N, \quad \varphi=\varphi. \tag{24}$$

The supercurvature in the base manifold $\mathscr{F}$ and that in the fiber-bundle space $\tilde{\mathscr{F}}$ are given by

$$\mathscr{F}=\mathbf{d}\mathscr{A}+\mathscr{A}\mathscr{A}, \tag{25}$$

$$\tilde{\mathscr{F}}=(\mathbf{s}+\mathbf{d})\tilde{\mathscr{A}}+\tilde{\mathscr{A}}\tilde{\mathscr{A}}. \tag{26}$$

Then the horizontality condition is given by

$$\tilde{\mathscr{F}}=\mathscr{F}. \tag{27}$$

From Eq. (27) we get the BRST transformation rule of $\tilde{\mathscr{A}}$,

$$\mathbf{s}\tilde{\mathscr{A}} = -\mathbf{d}\tilde{\mathscr{A}} - \tilde{\mathscr{A}}\tilde{\mathscr{A}} + \mathscr{F}. \tag{28}$$

However, in order to make sure that **s** in Eq. (28) is really a BRST transformation, we should check that $\mathbf{ss}\tilde{\mathscr{A}} = 0$ is satisfied. From Eq. (28) we have

$$\mathbf{ss}\tilde{\mathscr{A}} = \mathbf{d}(\mathbf{s}\tilde{\mathscr{A}}) - (\mathbf{s}\tilde{\mathscr{A}})\tilde{\mathscr{A}} + \tilde{\mathscr{A}}(\mathbf{s}\tilde{\mathscr{A}}) + \mathbf{s}\mathscr{F} = \mathbf{d}\mathscr{F} + \tilde{\mathscr{A}}\mathscr{F} - \mathscr{F}\tilde{\mathscr{A}} + \mathbf{s}\mathscr{F}. \tag{29}$$

On the right-hand side of Eq. (29) there is no term with a ghost number greater than one in our case with $\mathscr{A}$ in Eq. (22) and $\tilde{\mathscr{A}}$ in Eq. (23). Therefore $\mathbf{ss}\tilde{\mathscr{A}} = 0$ is satisfied in the system composed of scalar and vector gauge fields with usual gauge symmetry. Expanding Eq. (28) in terms of form degree, we get the usual BRST transformation rules of both the gauge fields A, φ, and the ghost field α without topological symmetry:

$$\begin{aligned} (dx)^1(dy)^1 &: sA = -D\alpha, \\ (dy)^1 &: s\varphi = -[\alpha,\ \varphi], \\ (dy)^2 &: s\alpha = -\alpha\alpha, \end{aligned} \tag{30}$$

where $[\ ,\ ]$ is the graded commutator and $Df \equiv df + [A,\ f]$. By explicit application of s in Eq. (30) we can show that s is nilpotent, that is, $s^2 = 0$.

In order to take care of the topological symmetry of Eq. (5), we extend $\tilde{\mathscr{F}}$ in Eq. (26) to

$$\tilde{\mathscr{F}}_T \equiv \tilde{\mathscr{F}} + \tilde{\mathscr{F}}'. \tag{31}$$

In our case where $\tilde{\mathscr{A}}$ is given by Eq. (23), $\tilde{\mathscr{F}}'$ is assigned as

$$\tilde{\mathscr{F}}' = \begin{pmatrix} \beta + \phi & \gamma \\ \gamma & \beta + \phi \end{pmatrix}, \tag{32}$$

where

$$\beta + \phi = \beta_{\mu N}\, dx^{\mu} \wedge dy^N + \tfrac{1}{2}\phi_{MN}\, dy^M \wedge dy^N, \quad \gamma = \gamma_N\, dy^N. \tag{33}$$

Note that each component field of $\tilde{\mathscr{F}}'$ is assigned to have one more ghost number than the corresponding field of $\tilde{\mathscr{A}}$ in Eq. (23). Then we modify the horizontality condition (27) to

$$\tilde{\mathscr{F}}_T = \mathscr{F}. \tag{34}$$

From Eq. (34) we have the modified version of Eq. (28),

$$\mathbf{s}\tilde{\mathscr{A}} = -\mathbf{d}\tilde{\mathscr{A}} - \tilde{\mathscr{A}}\tilde{\mathscr{A}} + \mathscr{F} - \tilde{\mathscr{F}}'. \tag{35}$$

By applying **s** on the both sides of Eq. (35), and requiring the nilpotency for $\tilde{\mathscr{A}}$, $\mathbf{ss}\tilde{\mathscr{A}} = 0$, we get the BRST transformation rule of $\tilde{\mathscr{F}}'$,

$$\mathbf{s}\tilde{\mathscr{F}}' = -\mathbf{d}\tilde{\mathscr{F}}' - \tilde{\mathscr{A}}\tilde{\mathscr{F}}' + \tilde{\mathscr{F}}'\tilde{\mathscr{A}} + \mathbf{d}\mathscr{F} + \tilde{\mathscr{A}}\mathscr{F} - \mathscr{F}\tilde{\mathscr{A}} + \mathbf{s}\mathscr{F}. \tag{36}$$

In reality, the last four terms of the right-hand side of Eq. (36) do not contribute to $\mathbf{s}\tilde{\mathscr{F}}'$ in the system composed of scalar and vector gauge fields, since none of them has a ghost number greater than one, whereas all the components of $\mathbf{s}\tilde{\mathscr{F}}'$ have ghost numbers greater than one. Again, we should check $\mathbf{ss}\tilde{\mathscr{F}}' = 0$. From Eqs. (35) and (36) we have

$$\mathbf{ss}\tilde{\mathscr{F}}' = -\tilde{\mathscr{A}}(\mathbf{d}\mathscr{F}) - (\mathbf{d}\mathscr{F})\tilde{\mathscr{A}} - \tilde{\mathscr{A}}(\mathbf{s}\mathscr{F}) - (\mathbf{s}\mathscr{F})\tilde{\mathscr{A}} - \mathbf{ds}\mathscr{F}. \tag{37}$$

There is no term with a ghost number greater than two on the right-hand side of Eq. (37) in our case with $\mathscr{A}$ in Eq. (22), $\tilde{\mathscr{A}}$ in Eq. (23), and $\tilde{\mathscr{F}}'$ in Eq. (32), whereas all the components of $\mathbf{ss}\tilde{\mathscr{F}}'$ have ghost numbers greater than two. Therefore $\mathbf{ss}\tilde{\mathscr{F}}'=0$ is satisfied in our case. Then it is confirmed that Eqs. (35) and (36) give the BRST transformation rules of the topological Yang–Mills theory with scalar and vector gauge fields.

In order to obtain the BRST transformation rules of the component fields, we expand Eqs. (35) and (36) in terms of form degree. Through this expansion we obtain

[even part]

$$\begin{gathered}(dx)^1(dy)^1{:}\,sA=-D\alpha-\beta,\\ (dy)^2{:}\,s\alpha=-\alpha\alpha-\phi,\\ (dx)^1(dy)^2{:}\,s\beta=-D\phi-[\alpha,\ \beta],\\ (dy)^3{:}\,s\phi=-[\alpha,\ \phi];\end{gathered}\tag{38}$$

[odd part]

$$\begin{gathered}(dy)^1{:}\,s\varphi=-[\alpha,\ \varphi]+\gamma,\\ (dy)^2{:}\,s\gamma=-[\alpha,\ \gamma]-[\phi,\ \varphi],\end{gathered}\tag{39}$$

where $[\ ,\ ]$ is the graded commutator and $Df\equiv df+[A,\ f]$. Equations (38) and (39) constitute a complete set of the BRST transformation rules of the component fields.

Now, let us consider both BRST and anti-BRST symmetries by assigning

$$\tilde{\mathscr{A}}=\begin{pmatrix} A+\alpha+\bar{\alpha} & \varphi \\ \varphi & A+\alpha+\bar{\alpha}\end{pmatrix},\tag{40}$$

$$\tilde{\mathscr{F}}'=\begin{pmatrix} \beta+\bar{\beta}+\phi+\rho+\bar{\phi} & \gamma+\bar{\gamma} \\ \gamma+\bar{\gamma} & \beta+\bar{\beta}+\phi+\rho+\bar{\phi}\end{pmatrix},\tag{41}$$

where

$$\begin{gathered}A+\alpha+\bar{\alpha}=A_\mu\,dx^\mu+\alpha_N\,dy^N+\bar{\alpha}_{\bar{N}}\,d\bar{y}^{\bar{N}},\\ \varphi=\varphi,\\ \beta+\bar{\beta}+\phi+\rho+\bar{\phi}=\beta_{\mu N}\,dx^\mu\wedge dy^N+\bar{\beta}_{\mu\bar{N}}\,dx^\mu\wedge d\bar{y}^{\bar{N}}+\tfrac{1}{2}\phi_{MN}\,dy^M\wedge dy^N\\ +\rho_{M\bar{N}}\,dy^M\wedge d\bar{y}^{\bar{N}}+\tfrac{1}{2}\bar{\phi}_{\bar{M}\bar{N}}\,d\bar{y}^{\bar{M}}\wedge d\bar{y}^{\bar{N}},\\ \gamma+\bar{\gamma}=\gamma_N\,dy^N+\bar{\gamma}_{\bar{N}}\,d\bar{y}^{\bar{N}}.\end{gathered}\tag{42}$$

In the above ϕ, ρ, and $\bar{\phi}$ fields are ghost for ghost fields which are necessary to fix the residual gauge symmetries of β and $\bar{\beta}$. The forms in Eqs. (40) and (41) are defined on the tangent and cotangent manifolds of the fiber as well as on the space-time base manifold, that is, they are defined in the fiber-bundle space. The component fields with odd forms in dy and $d\bar{y}$ directions have wrong spin statistics and reduce the physical degrees of freedom. Here, α, $\bar{\alpha}$, β, and $\bar{\beta}$ are such fields.

In analogy with Eqs. (35) and (36), the BRST and anti-BRST transformation rules are given by

$$(\mathbf{s}+\overline{\mathbf{s}})\tilde{\mathscr{A}}=-\mathbf{d}\tilde{\mathscr{A}}-\tilde{\mathscr{A}}\tilde{\mathscr{A}}+\mathscr{F}-\tilde{\mathscr{F}}', \tag{43}$$

$$(\mathbf{s}+\overline{\mathbf{s}})\tilde{\mathscr{F}}'=-\mathbf{d}\tilde{\mathscr{F}}'-\tilde{\mathscr{A}}\tilde{\mathscr{F}}'+\tilde{\mathscr{F}}'\tilde{\mathscr{A}}+\mathbf{d}\mathscr{F}+\tilde{\mathscr{A}}\mathscr{F}-\mathscr{F}\tilde{\mathscr{A}}+(\mathbf{s}+\overline{\mathbf{s}})\mathscr{F}. \tag{44}$$

We obtain the following BRST and anti-BRST transformation rules of the component fields by expanding Eqs. (43) and (44) in terms of form degree:

[even part]

$$\begin{gathered}
(dx)^1(dy)^1{:}\,sA=-D\alpha-\beta,\\
(dx)^1(d\bar{y})^1{:}\,\bar{s}A=-D\bar{\alpha}-\bar{\beta},\\
(dy)^2{:}\,s\alpha=-\alpha\alpha-\phi,\\
(d\bar{y})^2{:}\,\bar{s}\bar{\alpha}=-\bar{\alpha}\bar{\alpha}-\bar{\phi},\\
(dy)^1(d\bar{y})^1{:}\,s\bar{\alpha}+\bar{s}\alpha=-[\alpha,\ \bar{\alpha}]-\rho,\\
(dx)^1(dy)^2{:}\,s\beta=-D\phi-[\alpha,\ \beta],\\
(dx)^1(d\bar{y})^2{:}\,\bar{s}\bar{\beta}=-D\bar{\phi}-[\bar{\alpha},\ \bar{\beta}],\\
(dx)^1(dy)^1(d\bar{y})^1{:}\,s\bar{\beta}+\bar{s}\beta=-[\alpha,\ \bar{\beta}]-[\bar{\alpha},\ \beta]-D\rho,\\
(dy)^3{:}\,s\phi=-[\alpha,\ \phi],\\
(d\bar{y})^3{:}\,\bar{s}\bar{\phi}=-[\bar{\alpha},\ \bar{\phi}],\\
(dy)^2(d\bar{y})^1{:}\,\bar{s}\phi+s\rho=-[\alpha,\ \rho]-[\bar{\alpha},\ \phi],\\
(dy)^1(d\bar{y})^2{:}\,s\bar{\phi}+\bar{s}\rho=-[\bar{\alpha},\ \rho]-[\alpha,\ \bar{\phi}];
\end{gathered} \tag{45}$$

[odd part]

$$\begin{gathered}
(dy)^1{:}\,s\varphi=-[\alpha,\ \varphi]+\gamma,\\
(d\bar{y})^1{:}\,\bar{s}\varphi=-[\bar{\alpha},\ \varphi]+\bar{\gamma},\\
(dy)^2{:}\,s\gamma=-[\alpha,\ \gamma]-[\phi,\ \varphi],\\
(d\bar{y})^2{:}\,\bar{s}\bar{\gamma}=-[\bar{\alpha},\ \bar{\gamma}]-[\bar{\phi},\ \varphi],\\
(dy)^1(d\bar{y})^1{:}\,s\bar{\gamma}+\bar{s}\gamma=-[\alpha,\ \bar{\gamma}]-[\bar{\alpha},\ \gamma]-[\rho,\ \varphi].
\end{gathered} \tag{46}$$

The equations of $(dy)^1(d\bar{y})^1$, $(dx)^1(dy)^1(d\bar{y})^1$, $(dy)^2(d\bar{y})^1$, and $(dy)^1(d\bar{y})^2$ in Eq. (45) and that of $(dy)^1(d\bar{y})^1$ in Eq. (46) do not completely specify the transformation rules of the component fields. Therefore we need to introduce the auxiliary fields t, m, n, $\bar{n}$, and u given below to solve these equations:

$$
\begin{aligned}
s\bar{\alpha} &\equiv t, \quad \bar{s}\alpha = -t - [\alpha, \bar{\alpha}] - \rho, \\
s\bar{\beta} &\equiv m, \quad \bar{s}\beta = -m - [\alpha, \bar{\beta}] - [\bar{\alpha}, \beta] - D\rho, \\
s\rho &\equiv n, \quad \bar{s}\phi = -n - [\alpha, \rho] - [\bar{\alpha}, \phi], \\
s\bar{\phi} &\equiv \bar{n}, \quad \bar{s}\rho = -\bar{n} - [\bar{\alpha}, \rho] - [\alpha, \bar{\phi}], \\
s\bar{\gamma} &\equiv u, \quad \bar{s}\gamma = -u - [\alpha, \bar{\gamma}] - [\bar{\alpha}, \gamma] - [\rho, \varphi].
\end{aligned} \tag{47}
$$

From Eq. (47) we get the following transformation rules of the auxiliary fields:

$$
\begin{aligned}
st &= sm = sn = s\bar{n} = su = 0, \\
\bar{s}t &= -[\bar{\alpha}, t] + \bar{n}, \\
\bar{s}m &= -[D\alpha, \bar{\phi}] - D\bar{n} - [\beta, \bar{\phi}] - [\bar{\beta}, t] - [\bar{\alpha}, m], \\
\bar{s}n &= -[\alpha\alpha, \bar{\phi}] - [\alpha, \bar{n}] - [\bar{\alpha}, n] - [\phi, \bar{\phi}] - [\rho, t], \\
\bar{s}\bar{n} &= -[\bar{\alpha}, \bar{n}] - [\bar{\phi}, t], \\
\bar{s}u &= -[\bar{\alpha}, u] - [\bar{\gamma}, t] - [\varphi, \bar{n}] - [\gamma, \bar{\phi}] + [[\alpha, \varphi], \bar{\phi}].
\end{aligned} \tag{48}
$$

Equations (45), (46), (47), and (48) constitute a complete set of the BRST and anti-BRST transformation rules of the component fields of the topological Yang–Mills theory with scalar and vector gauge fields.

IV. DISCUSSIONS AND CONCLUSION

It is well known that $\mathscr{S}_4$ in Eq. (1) can be expressed as

$$
\mathscr{S}_4 = \mathrm{Tr} \int_{M_4} FF = \mathrm{Tr} \int_{M_4} d(A\, dA + \tfrac{2}{3} AAA). \tag{49}
$$

From this property we get the Chern–Simons action in three dimensions:

$$
\mathscr{S}_3^{\mathrm{CS}} = \mathrm{Tr} \int_{M_3} (A\, dA + \tfrac{2}{3} AAA), \tag{50}
$$

which is invariant under the usual gauge transformation $sA = -D\alpha$. At the same time, the fact that $\mathscr{S}_4$ is a total derivative of something as in Eq. (49) explains why $\mathscr{S}_4$ is invariant under the topological symmetry $sA = -\beta$ which is equivalent to Eq. (2). This is true because $sd = -ds$, and β is set to be zero at the boundary.

$\mathscr{S}_3$ in Eq. (4) and $\mathscr{S}_2$ in Eq. (6) are also invariant under the topological symmetry (5). Then we expect that $\mathscr{S}_3$ and $\mathscr{S}_2$ can also be expressed as total derivatives of something. This is also true as we can see below:

$$
\mathscr{S}_3 = \mathrm{Tr} \int_{M_3} F\, D\varphi = \mathrm{Tr} \int_{M_3} d(\varphi F), \tag{51}
$$

$$\mathscr{S}_2 = \mathrm{Tr} \int_{M_2} D\varphi \; D\varphi = \mathrm{Tr} \int_{M_2} d(\varphi \; d\varphi). \tag{52}$$

Actually, we can say that for some action, having a topological symmetry and being able to be expressed as a total derivative of something are equivalent. From Eqs. (51) and (52) we have the following two- and one-dimensional Chern–Simons actions:[15]

$$\mathscr{S}_2^{\mathrm{CS}} = \mathrm{Tr} \int_{M_2} \varphi F, \tag{53}$$

$$\mathscr{S}_1^{\mathrm{CS}} = \mathrm{Tr} \int_{M_1} \varphi \; d\varphi, \tag{54}$$

which are invariant under the usual gauge transformation of $sA = -D\alpha$ and $s\varphi = -[\alpha, \varphi]$.

In this paper we studied the topological Yang–Mills theory of a system composed of scalar and vector gauge fields in two and three dimensions. Since the system contains both even and odd form gauge fields, we worked in the superconnection framework. Furthermore, in order to take care of the topological symmetry of the $\delta A_\mu = \beta_\mu$ type as well as the usual gauge symmetry of the $\delta A_\mu = D_\mu c$ type, we modified the horizontality condition. In this scheme it was possible to understand the BRST and anti-BRST symmetries geometrically. That is, by applying the modified horizontality condition in the superconnection framework, we could obtain a complete set of the BRST and anti-BRST transformation rules of the component fields in a systematic way.

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(2,0) superconformal anomaly

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The (2,0) supersymmetric Wess–Zumino–Polyakov action is constructed and the (2,0) superconformal anomaly is given. The anomalous Ward-identity in the right sector is derived and the known operator product expansion of the $N=2$ superstress energy tensor is recovered. © *1996 American Institute of Physics.* [S0022-2488(95)04509-6]

I. INTRODUCTION

The Beltrami differentials are the basic objects in the context of two-dimensional conformal structures, and play an important role in conformal field theory and perturbative string theory[1,2] where they couple to the energy momentum tensors.[3] Furthermore, Beltrami differentials which parametrize a conformal class of metrics[4] are considered as the proper tool for describing the Riemann surfaces and the Beltrami parametrization makes the so-called factorization[5] manifest at all levels.[1,4,6] The generalizations of these topics to super Riemann surfaces have been pursued by various authors, e.g. Refs. 7–10, and prove equally important for superstrings.[11–13]

Recently, the constructions of conformally covariant differential operators on compact Riemann surfaces in terms of projective connections[14] have been of considerable interest since their applications to conformal[15] and integrable[16] models. The study is based on the superdiffeomorphism anomaly which is not well defined on the compact Riemann surface and has to be modified by the inclusion of projective connection. On the other hand, the $N=1$ superconformal anomaly on a super Riemann surface has been determined[17] and its modification by the superprojective connections in order to be well defined on compact $N=1$ super Riemann surfaces was quite recently reached.[18] The generalization of these subjects to $N=2$ super Riemann surfaces requires familiarity with the $N=2$ superconformal anomaly. This is the purpose of this article in which we construct the (2,0) superconformal anomaly and the corresponding Wess–Zumino–Polyakov action. The anomalous Ward-identity is derived and the known operator product expression of the superstress energy tensor is recovered.

The article is organized as follows. In Sec. II, we present the (2,0) superconformal transformations of the derivatives, their duals, and the super Beltrami variables which are defined in the same way as in Refs. 8 and 9. The integrating factor equations, the BRST transformations, and the superconformal transformations of the ghost superfields are obtained. In Sec. III, we construct the (2,0) supersymmetric Wess–Zumino–Polyakov action and its variation gives the (2,0) superconformal anomaly. Section IV, contains the anomalous Ward-identity and the operator product expansion of the $N=2$ superconformal theory. Section V is devoted the conclusion.

II. (2,0) SUPERCONFORMAL TRANSFORMATIONS AND BELTRAMI SUPERFIELDS

The objective of this section is to discuss the super Beltrami differentials and superconformal models for the (2,0) supersymmetric case by following the development of Ref. 17(c). However, the (2,0) superspace is locally parametrized by $(z,\bar{z},\theta^+,\theta^-)$ with $\theta^+\equiv\theta^+_-$ and $\theta^-\equiv\theta^-_-$ where the lower index corresponds to the Lorentz indices and the upper to the U(1) charges. According to this choice the (2,0) super-derivatives are given by

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$$D_\theta^+ \equiv D_+^+ = \frac{\partial}{\partial \theta^-} + \theta^+ \partial_z \equiv \partial_\theta^+ + \theta^+ \partial_z ,$$
$$D_\theta^- \equiv D_+^- = \frac{\partial}{\partial \theta^+} + \theta^- \partial_z \equiv \partial_\theta^- + \theta^- \partial_z \tag{2.1}$$

which satisfy the relations

$$\{D_\theta^+ , D_\theta^-\} = 2\partial_z , \quad (D_\theta^+)^2 = 0 = (D_\theta^-)^2 . \tag{2.2}$$

$A(2,0)$ super Riemann surface is a supermanifold which is equipped with a superconformal structure meaning that it admits local coordinates $(Z, \bar{Z}, \Theta^+, \Theta^-)$ and any two sets of such coordinates.

$$(Z, \bar{Z}, \Theta^+, \Theta^-) \to (Z', \bar{Z}', \Theta^{+\prime}, \Theta^{-\prime})$$

are related by a superconformal transformation if it satisfies

$$Z' = Z'(Z, \Theta^+, \Theta^-), \quad \Theta'^{\pm} = \Theta'^{\pm}(Z, \Theta^+, \Theta^-), \quad \bar{Z}' = \bar{Z}'(\bar{Z}). \tag{2.3}$$

These are equivalent to the following (2,0) superconformal conditions:

$$D_\Theta^\pm Z' = \Theta'^{+}(D_\Theta^\pm \Theta'^{-}) + \Theta'^{-}(D_\Theta^\pm \Theta'^{+}), \tag{2.4}$$

$$D_\Theta^\pm = (D_\Theta^\pm \Theta'^{+}) D_\Theta{}^{-\prime} + (D_\Theta^\pm \Theta'^{-}) D_\theta{}^{+\prime}, \tag{2.5}$$

where the canonical basis of the supertangent space is

$$\partial_Z , \quad \partial_{\bar{Z}}, \quad D_\Theta^+ = \partial_\Theta^+ + \Theta^+ \partial_Z , \quad D_\Theta^- = \partial_\Theta^- + \Theta^- \partial_Z , \tag{2.6}$$

and the graded Lie brackets between these are

$$\{D_\Theta^+ , D_\Theta^-\} = 2\partial_Z , \quad (D_\Theta^+)^2 = 0 = (D_\Theta^-)^2 . \tag{2.7}$$

The conditions (2.4) must be supplemented by either[11]

$$D_\Theta^+ \Theta'^{-} = 0 = D_\Theta^- \Theta'^{+} \tag{2.8}$$

or

$$D_\Theta^+ \Theta'^{+} = 0 = D_\Theta^- \Theta'^{-} \tag{2.9}$$

which mean that $D_\Theta^\pm$ transform homogeneously under superconformal transformations. Note that the condition (2.9) can always be chosen for a surface with $N=2$, U(1) superconformal structure.[11] Therewith we have

$$D_\Theta{}^{+\prime} = e^W D_\Theta^+ , \quad D_\Theta{}^{-\prime} = e^{\bar{W}} D_\Theta^- , \tag{2.10}$$

with

$$e^W = (D_\Theta^+ \Theta'^{-})^{-1}, \tag{2.11}$$

and where $-$ is the U(1) charge conjugation. Furthermore, the constraint (2.4), which is rewritten with the choices (2.9) as

$$(D^+_\Theta Z') = \Theta'^+ (D^+_\Theta \Theta'^-), \tag{2.12.1}$$

$$(D^-_\Theta Z') = \Theta'^- (D^-_\Theta \Theta'^+) \tag{2.12.2}$$

leads to

$$e^{-W} e^{-\bar{W}} = \partial_Z Z' + \Theta'^+ (\partial_Z \Theta'^-) + \Theta'^- (\partial_Z \Theta'^+) = (D^-_\Theta \Theta'^+)(D^+_\Theta \Theta'^-) \tag{2.13}$$

and

$$(D^+_\Theta \Theta'^-)(D_\Theta{}^+ {}'\Theta^-) = 1 = (D^-_\Theta \Theta'^+)(D_\Theta{}^- {}'\Theta^+) \tag{2.14}$$

with the use of relations (2.7). These show that

$$e^{-W} = e^{i\alpha} [\partial_Z Z' + \Theta'^+ (\partial_Z \Theta'^-) + \Theta'^- (\partial_Z \Theta'^+)]^{1/2} \tag{2.15}$$

which is defined up to the U(1) phase $e^{i\alpha}$.[19] Furthermore, the transformations of ∂_Z and $\partial_{\bar{Z}}$ are given by

$$\partial_{Z'} = e^W e^{\bar{W}} [\partial_Z + (D^+_\Theta \bar{W}) D^-_\Theta + (D^-_\Theta W) D^+_\Theta],$$

$$\partial_{\bar{Z}'} = \left(\frac{\partial \bar{Z}}{\partial \bar{Z}'} \right) \partial_{\bar{Z}}. \tag{2.16}$$

On the other hand, the derivatives (2.6) are dual to the set of the one-forms

$$e^Z = dZ + \Theta^+ d\Theta^- + \Theta^- d\Theta^+,$$

$$e^{\Theta^+} = d\Theta^+, \quad e^{\Theta^-} = d\Theta^-, \quad e^{\bar{Z}} = d\bar{Z} \tag{2.17}$$

and the graded Lie brackets (2.7) are equivalent to

$$de^Z + e^{\Theta^+} e^{\Theta^-} + e^{\Theta^-} e^{\Theta^+} = 0,$$

$$de^{\Theta^+} = 0, \quad de^{\Theta^-} = 0, \quad de^{\bar{Z}} = 0. \tag{2.18}$$

In terms of these one-forms, the exterior derivative is given by

$$d = e^Z \partial_Z + e^{\Theta^+} D^-_\Theta + e^{\Theta^-} D^+_\Theta + e^{\bar{Z}} \partial_{\bar{Z}} \tag{2.19}$$

and the (2,0) superconformal transformations of $e^Z, e^{\Theta^\pm}$, and $e^{\bar{Z}}$ can be deduced from Eq. (2.19) with the use of Eqs. (2.10) and (2.16). These are given by

$$\begin{aligned}
&e^{Z'} = e^{-(W+\bar{W})} e^Z, && (1)\\
&e^{\Theta'^+} = e^{-\bar{W}} [e^{\Theta^+} - e^Z (D^+_\Theta \bar{W})], && (2)\\
&e^{\Theta'^-} = e^{-W} [e^{\Theta^-} - e^Z (D^-_\Theta W)], && (3)\\
&e^{\bar{Z}'} = \frac{\partial \bar{Z}'}{\partial \bar{Z}} e^{\bar{Z}}. && (4)
\end{aligned} \tag{2.20}$$

In analogy with $\underline{N}=0$ and $N=1$ superconformal cases, we assume that the (2,0) superconformal coordinates $(Z,\bar{Z},\Theta^+,\Theta^-)$ have been obtained from a reference system of superconformal coordinates $(z,\bar{z},\theta^+,\theta^-)$ by a smooth change of coordinates

$$(z,\bar{z},\theta^+,\theta^-)\to(Z(z,\bar{z},\theta^+,\theta^-),\bar{Z}(\bar{z}),\Theta^{\pm}(z,\bar{z},\theta^+,\theta^-)). \tag{2.21}$$

Now let us express the one-forms in terms of the reference coordinate basis as

$$\begin{aligned} e^Z &= e^z E_z^Z + e^{\bar{z}} E_{\bar{z}}^Z + e^{\theta^+} E_{\theta^+}^Z + e^{\theta^-} E_{\theta^-}^Z, \quad (1)\\ e^{\Theta^{\pm}} &= e^{\theta^+} E_{\theta^+}^{\Theta^{\pm}} + e^{\theta^-} E_{\theta^-}^{\Theta^{\pm}} + e^z E_z^{\Theta^{\pm}} + e^{\bar{z}} E_{\bar{z}}^{\Theta^{\pm}}, \quad (2)\\ e^{\bar{Z}} &= e^{\bar{z}} E_{\bar{z}}^{\bar{Z}} + e^z E_z^{\bar{Z}} + e^{\theta^+} E_{\theta^+}^{\bar{Z}} + e^{\theta^-} E_{\theta^-}^{\bar{Z}}. \quad (3) \end{aligned} \tag{2.22}$$

The identification of Eq. (2.17), with the help of the exterior derivative in the reference system of superconformal coordinates $(z,\bar{z},\theta^+,\theta^-)$, with Eq. (2.21) leads to

$$\begin{aligned} E_z^Z &= \partial_z Z + \Theta^+ \partial_z \Theta^- + \Theta^- \partial_z \Theta^+,\\ E_{\bar{z}}^Z &= \partial_{\bar{z}} Z + \Theta^+ \partial_{\bar{z}} \Theta^- + \Theta^- \partial_{\bar{z}} \Theta^+,\\ E_{\theta^+}^Z &= D_\theta^- Z - \Theta^+ D_\theta^- \Theta^- - \Theta^- D_\theta^- \Theta^+,\\ E_{\theta^-}^Z &= D_\theta^+ Z - \Theta^+ D_\theta^+ \Theta^- - \Theta^- D_\theta^+ \Theta^+, \end{aligned} \tag{2.23}$$

$$E_{\theta^\pm}^{\Theta^+} = D_\theta^{\mp} \Theta^+, \quad E_z^{\Theta^+} = \partial_z \Theta^+, \quad E_{\bar{z}}^{\Theta^+} = \partial_{\bar{z}} \Theta^+, \tag{2.24}$$

$$E_{\theta^+}^{\Theta^-} = D_\theta^{\pm} \Theta^-, \quad E_z^{\Theta^-} = \partial_z \Theta^-, \quad E_{\bar{z}}^{\Theta^-} = \partial_{\bar{z}} \Theta^-, \tag{2.25}$$

$$E_{\bar{z}}^{\bar{Z}} = \partial_{\bar{z}} \bar{Z}, \quad E_z^{\bar{Z}} = \partial_z \bar{Z}, \quad E_{\theta^\pm}^{\bar{Z}} = D_\theta^{\mp} \bar{Z}. \tag{2.26}$$

From Eq. (2.22) we can define the super Beltrami variables which are inert under the superconformal transformation (2.3). In fact, since the one-form e^Z transforms homogeneously under Eq. (2.3), the unaffected coefficients of e^Z can be obtained directly by factorizing E_z^Z in Eq. (2.22.1) which gives

$$e^Z = [e^z + e^{\bar{z}} H_{\bar{z}}^z + e^{\theta^+} H_{\theta^+}^z + e^{\theta^-} H_{\theta^-}^z]\Lambda \tag{2.27}$$

with

$$\Lambda \equiv E_z^Z \tag{2.28}$$

and

$$H_a^z = \frac{E_a^z}{E_z^Z}, \quad a = z,\bar{z},\theta^{\pm} \tag{2.29}$$

are the super Beltrami coefficients of e^Z. Furthermore, the super Beltrami variables of $e^{\bar{Z}}$ are defined in the same way as

$$e^{\bar{Z}} = [e^{\bar{z}} + e^z H_z^{\bar{z}} + e^{\theta^+} H_{\theta^+}^{\bar{z}} + e^{\theta^-} H_{\theta^-}^{\bar{z}}]\overline{\Lambda} \tag{2.30}$$

with

$$\overline{\Lambda}=E_{\bar{z}}^{\bar{Z}} \tag{2.31}$$

and

$$H_a^{\bar{z}}=\frac{E_a^{\bar{Z}}}{E_{\bar{z}}^{\bar{Z}}}, \quad a=z,\bar{z},\theta^{\pm}. \tag{2.32}$$

The (2,0) superconformal transformations (2.20.2–3) with the use of the expansions (2.22.2) and (2.27) lead to

$$\begin{aligned} &E_{\theta^+}^{\Theta'^+}=e^{-\bar{W}}[E_{\theta^+}^{\Theta^+}-H_{\theta^+}^{z}(D_\Theta^+\bar{W})\Lambda], \quad E_z^{\Theta'^+}=e^{-\bar{W}}[E_z^{\Theta^+}-(D_\theta^+\bar{W})\Lambda], \\ &E_{\bar{z}}^{\Theta'^+}=e^{-\bar{W}}[E_{\bar{z}}^{\Theta^+}-H_{\bar{z}}^{z}(D_\Theta^+\bar{W})\Lambda], \quad E_{\theta^-}^{\Theta'^+}=e^{-\bar{W}}[E_{\theta^-}^{\Theta^+}-H_{\theta^-}^{z}(D_\Theta^+\bar{W})\Lambda] \end{aligned} \tag{2.33.1}$$

and

$$\begin{aligned} &E_{\theta^+}^{\Theta'^-}=e^{-W}[E_{\theta^+}^{\Theta^-}-H_{\theta^+}^{z}(D_\Theta^-W)\Lambda], \quad E_{\theta^-}^{\Theta'^-}=e^{-W}[E_{\theta^-}^{\Theta^-}-H_{\theta^+}^{z}(D_\Theta^-W)\Lambda], \\ &E_z^{\Theta'^-}=e^{-W}[E_z^{\Theta^-}-(D_\Theta^-W)\Lambda], \quad E_{\bar{z}}^{\Theta'^-}=e^{-W}[E_{\bar{z}}^{\Theta^-}-H_{\bar{z}}^{z}(D_\Theta^-W)\Lambda]. \end{aligned} \tag{2.33.2}$$

These expressions show that the coefficients of $e^{\Theta^{\pm}}$ do not transform homogeneously and by some particular combinations of them one can construct the corresponding super Beltrami variables given in Refs. 8 and 9 namely.

$$H_a^{\theta^{\pm}}=\frac{1}{\sqrt{\Lambda}}[E_a^{\Theta^{\pm}}-H_a^{z}E_z^{\Theta^{\pm}}], \quad a=z,\bar{z},\theta^{\pm} \tag{2.34}$$

which are by construction inert variables. Therefore, the expansions of $e^{\Theta^{\pm}}$ in terms of these variables are given by

$$e^{\Theta^{\pm}}=[e^{z}+e^{\theta^+}H_{\theta^+}^{z}+e^{\theta^-}H_{\theta^-}^{z}+e^{\bar{z}}H_{\bar{z}}^{z}]\tau^{\pm}+[e^{\theta^+}H_{\theta^+}^{\theta^{\pm}}+e^{\bar{z}}H_{\bar{z}}^{\theta^{\pm}}+e^{\theta^-}H_{\theta^-}^{\theta^{\pm}}]\sqrt{\Lambda} \tag{2.35}$$

with

$$\tau^{\pm}=E_z^{\Theta^{\pm}}.$$

However, the parametrization contained in Eqs. (2.27), (2.30), and (2.34) can be expressed by using the decomposition given in Ref. 9 namely

$$(e^{Z},e^{\bar{Z}},e^{\Theta^+},e^{\Theta^-})=(e^{z},e^{\bar{z}},e^{\theta^+},e^{\theta^-})M\Lambda, \tag{2.36.1}$$

where the matrices M and Λ are given by

$$M=\begin{vmatrix} 1 & H_z^{\bar{z}} & 0 & 0 \\ H_{\bar{z}}^{z} & 1 & H_z^{\theta^+} & H_z^{\theta^-} \\ H_{\theta^+}^{z} & H_{\theta^+}^{\bar{z}} & H_{\theta^+}^{\theta^+} & H_{\theta^+}^{\theta^-} \\ H_{\theta^-}^{z} & H_{\theta^-}^{\bar{z}} & H_{\theta^-}^{\theta^+} & H_{\theta^-}^{\theta^-} \end{vmatrix}, \quad \Lambda=\begin{vmatrix} \Lambda & 0 & \tau^+ & \tau^- \\ 0 & \bar{\Lambda} & 0 & 0 \\ 0 & 0 & \sqrt{\Lambda} & 0 \\ 0 & 0 & 0 & \sqrt{\Lambda} \end{vmatrix}. \tag{2.36.2}$$

The coefficients Λ and $\tau^{\pm}$ transform under superconformal transformations as

$$\Lambda' = e^{-(W+\bar{W})}\Lambda, \quad \tau^{+\prime} = e^{-\bar{W}}[\tau^{+} - \Lambda(D_{\theta}^{+}\bar{W})], \quad \tau^{-\prime} = e^{-W}[\tau^{-} - \Lambda(D_{\theta}^{-}W)]. \tag{2.37}$$

We note that in Ref. 9 some gauge fixing choices are used in order to obtain the BRST transformations of the super Beltrami variables. However, these choices can be validated by considering a change of the reference coordinate system $(z,\bar{z},\theta^{+},\theta^{-})$ with

$$D^{+}z' = \theta'^{+}(D^{+}\theta'^{-}), \quad D^{-}z' = \theta'^{-}(D^{-}\theta'^{+}) \tag{2.38}$$

and

$$(D^{+}\theta'^{+}) = 0 = (D^{-}\theta'^{-}).$$

Therewith, the one basis forms transform as

$$e^{z'} = e^{-(\omega+\bar{\omega})}e^{z},$$

$$e^{\theta'^{+}} = e^{-\bar{\omega}}[e^{\theta^{+}} - e^{z}(D^{+}\bar{\omega})],$$

$$e^{\theta'^{-}} = e^{-\omega}[e^{\theta^{-}} - e^{z}(D^{-}\omega)],$$

$$e^{\bar{z}} = \left(\frac{\partial \bar{z}}{\partial \bar{z}'}\right)e^{\bar{z}'} \tag{2.39}$$

and the substitution of these expressions in Eq. (2.36.1) leads to the transformation of the coefficients $\Lambda,\bar{\Lambda},\tau^{\pm}$ and the super Beltrami variables H_{a}^{b} namely

$$\Lambda' \equiv \Lambda_{z'}^{z} = e^{(\omega+\bar{\omega})}Y\Lambda_{z}^{z}, \tag{2.40.1}$$

$$\tau^{\pm} \equiv \tau_{z'}^{\Theta^{\pm}} = e^{(\omega+\bar{\omega})}Y[\tau_{z}^{\Theta^{\pm}} + Y^{-1}(D^{+}\bar{\omega})H_{\theta^{+}}^{\theta^{\pm}}\sqrt{\Lambda} + Y^{-1}(D^{-}\omega)H_{\theta^{-}}^{\theta^{\pm}}\sqrt{\Lambda}], \tag{2.40.2}$$

$$\bar{\Lambda}' \equiv \bar{\Lambda}_{z'}^{\bar{z}} = \left(\frac{\partial \bar{z}}{\partial \bar{z}'}\right)\bar{\Lambda}_{z}^{\bar{z}} \tag{2.40.3}$$

and

$$H_{\bar{z}'}^{z'} = e^{-(\omega+\bar{\omega})}Y^{-1}\left(\frac{\partial \bar{z}}{\partial \bar{z}'}\right)H_{\bar{z}}^{z},$$

$$H_{\theta^{+}}^{z'} = e^{-\omega}Y^{-1}H_{\theta^{+}}^{z},$$

$$H_{\theta'^{-}}^{z'} = e^{-\bar{\omega}}Y^{-1}H_{\theta^{-}}^{z},$$

$$H_{\theta'^{+}}^{\theta'^{+}} = e^{-(\omega-\bar{\omega})/2}Y^{-1/2}[H_{\theta^{+}}^{\theta^{+}} - Y^{-1}H_{\theta^{+}}^{z}(H_{\theta^{+}}^{\theta^{+}}D^{+}\bar{\omega} + H_{\theta^{-}}^{\theta^{+}}D^{-}\omega)],$$

$$H_{\theta'^{-}}^{\theta'^{+}} = e^{(\omega-\bar{\omega})/2}Y^{-1/2}[H_{\theta^{-}}^{\theta^{+}} - Y^{-1}H_{\theta^{-}}^{z}(H_{\theta^{+}}^{\theta^{+}}D^{+}\bar{\omega} + H_{\theta^{-}}^{\theta^{+}}D^{-}\omega)],$$

$$H_{\bar{z}'}^{\theta'^{\pm}} = e^{-(\omega+\bar{\omega})/2}Y^{-1/2}\left(\frac{\partial \bar{z}}{\partial \bar{z}'}\right)[H_{\bar{z}}^{\theta^{\pm}} - Y^{-1}H_{\bar{z}}^{z}(H_{\theta^{+}}^{\theta^{\pm}}D^{+}\bar{\omega} + H_{\theta^{-}}^{\theta^{\pm}}D^{-}\omega)],$$

$$H^{\theta'^-}_{\theta'^+}=e^{-(\omega-\bar\omega)/2}Y^{-1/2}[H^{\theta^-}_{\theta^+}-Y^{-1}H^z_{\theta^+}(H^{\theta^+}_{\theta^+}D^+\bar\omega+H^{\theta^-}_{\theta^-}D^-\omega)],$$

$$H^{\theta^-\prime}_{\theta^-\prime}=e^{(\omega-\bar\omega)/2}Y^{-1/2}[H^{\theta^-}_{\theta^-}-Y^{-1}H^z_{\theta^-}(H^{\theta^-}_{\theta^+}D^+\bar\omega+H^{\theta^-}_{\theta^-}D^-\omega)],$$

$$H^{\bar z'}_{z'}=e^{(\omega+\bar\omega)}\left(\frac{\partial\bar z'}{\partial\bar z}\right)[H^{\bar z}_z+(D^+\bar\omega)H^{\bar z}_{\theta^+}+(D^-\omega)H^z_{\theta^-}],$$

$$H^{\bar z'}_{\theta'^+}=e^{\bar\omega}\left(\frac{\partial\bar z'}{\partial\bar z}\right)H^{\bar z}_{\theta^+},$$

$$H^{\bar z'}_{\theta'^-}=e^{\omega}\left(\frac{\partial\bar z'}{\partial\bar z}\right)H^{\bar z}_{\theta^-} \tag{2.41}$$

with

$$Y=1+(D^+\bar\omega)H^z_{\theta^+}+(D^-\omega)H^z_{\theta^-}. \tag{2.42}$$

Therefore, the choices $H^z_{\theta^\pm}=0$ taken in Refs. 8 and 9 are invariant under the change of the reference coordinate system and simplify all the other super Beltrami variable transformations. In fact, with these choices the transformations of $H^{\theta^\pm}_{\theta^\pm}$ and $H^{\theta^\mp}_{\theta^\pm}$ become homogeneous. Furthermore, we have seen that[9] the variables $H^{\bar z}_{\theta^\pm}$ and $H^z_{\bar z}$ are the fundamental super Beltrami variables. Indeed, from Eq. (2.17) and by the use of similar equations written in the reference coordinate system namely

$$de^z+e^{\theta^+}e^{\theta^-}+e^{\theta^-}e^{\theta^+}=0,\quad de^{\theta^+}=0=de^{\theta^-},\quad de^{\bar z}=0 \tag{2.43}$$

and the expansions (2.27), (2.30), (2.35) we find that the super Beltrami variables and the superconformal factors are related to each other by a set of equations. Among them we have

$$\begin{aligned}
&\partial_{\bar z}\Lambda-\partial_z(H^z_{\bar z}\Lambda)+2H^{\theta^-}_{\bar z}\tau^+\sqrt{\Lambda}+2H^{\theta^+}_{\bar z}\tau^-\sqrt{\Lambda}=0,\\
&D^+\Lambda+\partial_z(H^z_{\theta^-}\Lambda)+2H^{\theta^-}_{\theta^-}\tau^+\sqrt{\Lambda}+2H^{\theta^+}_{\theta^-}\tau^-\sqrt{\Lambda}=0,\\
&D^-\Lambda+\partial_z(H^z_{\theta^+}\Lambda)+2H^{\theta^-}_{\theta^+}\tau^+\sqrt{\Lambda}+2H^{\theta^+}_{\theta^+}\tau^-\sqrt{\Lambda}=0,
\end{aligned} \tag{2.44}$$

$$\begin{aligned}
&D^+(H^z_{\theta^+}\Lambda)+D^-(H^z_{\theta^-}\Lambda)-2\Lambda+2[H^z_{\theta^+}H^{\theta^-}_{\theta^-}+H^z_{\theta^-}H^{\theta^-}_{\theta^+}]\tau^+\sqrt{\Lambda}\\
&\quad+2[H^z_{\theta^-}H^{\theta^+}_{\theta^+}+H^z_{\theta^+}H^{\theta^+}_{\theta^-}]\tau^-\sqrt{\Lambda}+2[H^{\theta^+}_{\theta^+}H^{\theta^-}_{\theta^-}+H^{\theta^+}_{\theta^-}H^{\theta^-}_{\theta^+}]\Lambda=0,\\
&2\tau^+-D^+(H^z_{\theta^+}\tau^+)-D^-(H^z_{\theta^-}\tau^+)-D^+(H^{\theta^+}_{\theta^+}\sqrt{\Lambda})-D^-(H^{\theta^+}_{\theta^-}\sqrt{\Lambda})=0,\\
&2\tau^--D^+(H^z_{\theta^+}\tau^-)-D^-(H^z_{\theta^-}\tau^-)-D^+(H^{\theta^-}_{\theta^+}\sqrt{\Lambda})-D^-(H^{\theta^-}_{\theta^-}\sqrt{\Lambda})=0,
\end{aligned} \tag{2.45}$$

$$\begin{aligned}
&\partial_{\bar z}\overline{\Lambda}-\partial_{\bar z}(H^z_z\overline{\Lambda})=0,\\
&D^\pm\overline{\Lambda}-\partial_{\bar z}(H^{\bar z}_{\theta^\mp}\overline{\Lambda})=0.
\end{aligned} \tag{2.46}$$

From this set of equations we obtain the following results:

$$h=(H^{\theta^+}_{\theta^+}H^{\theta^-}_{\theta^-}+H^{\theta^+}_{\theta^-}H^{\theta^-}_{\theta^+})=1-\tfrac{1}{2}(D^+-H^z_{\theta^-}\partial_z)H^z_{\theta^+}-\tfrac{1}{2}(D^--H^z_{\theta^+}\partial_z)H^z_{\theta^-},$$

$$H^{\theta^-}_{\theta^+}=\frac{1}{2H^{\theta^+}_{\theta^+}}(D^--H^z_{\theta^+}\partial_z)H^z_{\theta^+},$$

$$H^{\theta^+}_{\theta^-}=\frac{1}{2H^{\theta^-}_{\theta^-}}(D^+-H^z_{\theta^-}\partial_z)H^z_{\theta^-},$$

$$H^{\theta^\pm}_{\bar z}=\frac{1}{2h}[H^{\theta^\pm}_{\theta^+}(\partial_{\bar z}-H^z_{\bar z}\partial_z)H^z_{\theta^-}-H^{\theta^\pm}_{\theta^-}(\partial_{\bar z}-H^z_{\bar z}\partial_z)H^z_{\theta^+}$$
$$+H^{\theta^\pm}_{\theta^+}(D^+-H^z_{\theta^-}\partial_z)H^z_{\bar z}-H^{\theta^\pm}_{\theta^-}(D^--H^z_{\theta^+}\partial_z)H^z_{\bar z}],$$
$$H^{\bar z}_{\bar z}=\tfrac{1}{2}(D^+-H^{\bar z}_{\theta^-}\partial_{\bar z})H^{\bar z}_{\theta^+}+\tfrac{1}{2}(D^-_\theta-H^{\bar z}_{\theta^+}\partial_{\bar z})H^{\bar z}_{\theta^-},$$

$$\tau^\pm=\frac{1}{2h}[(D^+-H^z_{\theta^-}\partial_z)(H^{\theta^\pm}_{\theta^+}\sqrt{\Lambda})+(D^--H^z_{\theta^+}\partial_z)(H^{\theta^\pm}_{\theta^-}\sqrt{\Lambda})] \tag{2.47}$$

which show that the super Beltrami variables $H^{\theta^-}_{\theta^+}, H^{\theta^+}_{\theta^-}, H^{\theta^\pm}_{\bar z}, H^{\bar z}_{\bar z}$ and the coefficients $\tau^\pm$ are expressed in terms of the basic super Beltrami variables $H^z_{\theta^\pm}$, $H^{\theta^-}_{\theta^-}$, $H^{\bar z}_{\theta^\pm}$, and $H^z_{\bar z}$ which remain undetermined. However, the particular choices

$$H^z_{\theta^\pm}=0 \tag{2.48}$$

lead to

$$\begin{aligned} &H^{\theta^\pm}_{\bar z}=\frac{1}{2H^{\theta^\mp}_{\theta^\mp}}[\pm D^\pm H^z_{\bar z}], \quad (1)\\ &\tau^\pm=\tfrac{1}{2}[D^\pm(H^{\theta^\pm}_{\theta^\pm}\sqrt{\Lambda})] \qquad (2)\end{aligned} \tag{2.49}$$

with

$$H^{\theta^+}_{\theta^+}H^{\theta^-}_{\theta^-}=1, \tag{2.50}$$

$$H^{\theta^-}_{\theta^+}=0=H^{\theta^+}_{\theta^-}. \tag{2.51}$$

These latter relations are equivalent to the fixing choice in Ref. 9 in order to decouple the BRST transformations of the super Beltrami variables.

On the other hand, the substitution of the previous results (2.47) in Eqs. (2.44) yields the following differential equations:

$$\partial_{\bar z}\Lambda-\left[H^z_{\bar z}+\frac{1}{2h}H^{\theta^-}_{\bar z}(H^z_{\theta^-}H^{\theta^+}_{\theta^+}+H^z_{\theta^+}H^{\theta^+}_{\theta^-})+\frac{1}{2h}H^{\theta^+}_{\bar z}(H^z_{\theta^-}H^{\theta^-}_{\theta^+}+H^z_{\theta^+}H^{\theta^-}_{\theta^-})\right]\partial_z\Lambda+\frac{1}{2h}$$
$$\times(H^{\theta^-}_{\bar z}H^{\theta^+}_{\theta^+}+H^{\theta^+}_{\bar z}H^{\theta^-}_{\theta^+})D^+\Lambda+\frac{1}{2h}(H^{\theta^-}_{\bar z}H^{\theta^+}_{\theta^-}+H^{\theta^+}_{\bar z}H^{\theta^-}_{\theta^-})D^-\Lambda$$

$$-\Big[\partial_z H_z^z-\frac{1}{h}H_z^{\theta^-}(D^+-H_{\theta^-}^z\partial_z)H_{\theta^+}^{\theta^+}-\frac{1}{h}H_z^{\theta^-}(D^--H_{\theta^+}^z\partial_z)H_{\theta^-}^{\theta^+}-\frac{1}{h}H_z^{\theta^+}$$
$$\times(D^+-H_{\theta^-}^z\partial_z)H_{\theta^+}^{\theta^-}-\frac{1}{h}H_z^{\theta^+}(D^--H_{\theta^+}^z\partial_z)H_{\theta^-}^{\theta^-}\Big]\Lambda=0, \tag{2.52}$$

$$D^{\mp}\Lambda+\frac{1}{h}H_{\theta^{\mp}}^{\theta^-}H_{\theta^{\mp}}^{\theta^+}D^{\mp}\Lambda+\frac{1}{2}\Big(H_{\theta^{\mp}}^z-\frac{2}{h}H_{\theta^{\pm}}^zH_{\theta^{\mp}}^{\theta^-}H_{\theta^{\mp}}^{\theta^+}\Big)\partial_z\Lambda+\Big[\partial_z H_{\theta^{\mp}}^z+\frac{1}{h}H_{\theta^{\mp}}^{\theta^-}$$
$$\times(D^+-H_{\theta^-}^z\partial_z)\,H_{\theta^+}^{\theta^+}+\frac{1}{h}H_{\theta^{\mp}}^{\theta^-}(D^--H_{\theta^+}^z\partial_z)H_{\theta^-}^{\theta^+}+\frac{1}{h}H_{\theta^{\mp}}^{\theta^+}$$
$$\times(D^+-H_{\theta^-}^z\partial_z)H_{\theta^+}^{\theta^-}+\frac{1}{h}H_{\theta^{\mp}}^{\theta^+}(D^--H_{\theta^+}^z\partial_z)H_{\theta^-}^{\theta^-}\Big]\Lambda=0 \tag{2.53}$$

which contain as for the $N=1$ supersymmetric case[17(c)] the bosonic theory equations and take a simple form for the choices (2.48).

The BRST transformations of the super Beltrami variables corresponding to (2,0) superdiffeomorphisms can be generated by the ghost vector superfield $\xi^M(M=z,\bar{z},\theta^+,\theta^-)$ such that

$$i_\xi e^M=\xi^M, \tag{2.54}$$

where i_ξ is the contraction operator along the ghost vector superfield ξ^M. Therewith, one can define suitable ghost superfields by using Eqs. (2.27), (2.30), and (2.35) in the following way:

$$i_\xi(e^Z)=[\xi^z+\xi^{\bar{z}}H_{\bar{z}}^z+\xi^{\theta^+}H_{\theta^+}^z+\xi^{\theta^-}H_{\theta^-}^z]\Lambda\equiv\Sigma^z\Lambda, \tag{2.55.1}$$

$$i_\xi(e^{\bar{Z}})=[\xi^{\bar{z}}+\xi^zH_z^{\bar{z}}+\xi^{\theta^+}H_{\theta^+}^{\bar{z}}+\xi^{\theta^-}H_{\theta^-}^{\bar{z}}]\overline{\Lambda}\equiv\Sigma^{\bar{z}}\overline{\Lambda} \tag{2.55.2}$$

and similarly

$$i_\xi(e^{\Theta^\pm})=\Sigma^{\Theta^\pm}\sqrt{\Lambda}+\Sigma^z\tau^\pm. \tag{2.55.3}$$

Thereby the BRST transformations of the coordinate system Z, $\bar{Z}$, and $\Theta^\pm$ can be deduced from Eq. (2.55) with the help of Eqs. (2.17). These are given by

$$s\Theta^\pm=\Sigma^{\theta^\pm}\sqrt{\Lambda}+\Sigma^z\tau^\pm,\quad sZ=\Sigma^z\Lambda-\Theta^+s\Theta^--\Theta^-s\Theta^+,\quad s\bar{Z}=\Sigma^{\bar{z}}\overline{\Lambda}. \tag{2.56}$$

The nilpotency property of the BRST operator on the coordinate system $Z,\bar{Z},\Theta^\pm$ leads to the BRST transformations of the ghost superfields Σ^z, $\Sigma^{\theta^\pm}$, and $\Sigma^{\bar{z}}$ in terms of the superconformal factors and the spinorial superfields $\tau^\pm$ namely

$$s\Sigma^z=\Sigma^z s\,\log\,\Lambda+2\Sigma^z\Big[\Sigma^{\theta^-}\frac{\tau^+}{\sqrt{\Lambda}}+\Sigma^{\theta^+}\frac{\tau^-}{\sqrt{\Lambda}}\Big]+2\Sigma^{\theta^+}\Sigma^{\theta^-},$$

$$s\Sigma^{\theta^\pm}=\Sigma^{\theta^\pm}s\,\log\,\Lambda-\frac{\tau^\pm}{\sqrt{\Lambda}}s\Sigma^z+\Sigma^z\frac{1}{\sqrt{\Lambda}}s\tau^\pm,\quad s\Sigma^{\bar{z}}=\Sigma^{\bar{z}}s\,\log\,\overline{\Lambda}. \tag{2.57}$$

Furthermore, the BRST_transformations of $\Lambda,\bar{\Lambda},\tau^{\pm}$ can be deduced by the evaluation of the differentials $dZ,d\Theta^{\pm},d\bar{Z}$ variations and the use of the relation $sd+ds=0$. These are given by

$$s\tau^{\pm}=-\partial_z[\Sigma^{\theta^{\pm}}\sqrt{\Lambda}+\Sigma^z\tau^{\pm}],$$

$$s\Lambda=-\partial_z[\Sigma^z\Lambda]-2[\Sigma^{\theta^-}\tau^+ +\Sigma^{\theta^+}\tau^-]\sqrt{\Lambda},\quad s\Lambda=-\partial_{\bar{z}}[\Sigma^{\bar{z}}\Lambda]. \tag{2.58}$$

The substitution of these expressions in Eq. (2.57) leads to

$$s\Sigma^z=-\Sigma^z\partial_z\Sigma^z+2\Sigma^{\theta^+}\Sigma^{\theta^-},$$

$$s\Sigma^{\theta^{\pm}}=-\Sigma^z\partial_z\Sigma^{\theta^{\pm}}-\tfrac{1}{2}\Sigma^{\theta^{\pm}}\partial_z\Sigma^z,$$

$$s\Sigma^z=-\Sigma^{\bar{z}}\partial_{\bar{z}}\Sigma^{\bar{z}}. \tag{2.59}$$

We remark that the introduction of the U(1) connection as a new degrees of freedom which closed the multiplet of the super Beltrami variables can be made in a straightforward way. In fact, this can be taken into account by considering the new covariant derivative

$$d\to d\pm A \tag{2.60}$$

on objects having + and −U(1) charges, respectively. This is equivalent to modifying Eqs. (2.23)–(2.26) by covariantizing the derivatives of the fermionic variables with respect to the U(1) connection. The latter can also be redefined in a particular form[8,9] in order to maintain the super Beltrami multiplet inert under Eq. (2.3) namely

$$\mathscr{A}_a=A_a-H_a^zA_z+H_a^{\theta^+}\frac{\tau^-}{\sqrt{\Lambda}}-H_a^{\theta^-}\frac{\tau^+}{\sqrt{\Lambda}}+2H_a^z\frac{\tau^+\tau^-}{\sqrt{\Lambda}} \tag{2.61}$$

with

$$\mathscr{A}_z=0.$$

In the same way as the procedure which gives Eq. (2.58), the BRST variations corresponding to superdiffeomorphisms of the super Beltrami variables are given by[8,9]

$$sH_z^z=(\partial_{\bar{z}}-H_z^z\partial_z)\Sigma^z-2(H_z^{\theta^-}\Sigma^{\theta^+}+H_z^{\theta^+}\Sigma^{\theta^-})+\Sigma^z\partial_zH_z^z, \tag{1}$$

$$sH_{\theta^{\pm}}^z=(D^{\mp}-H_{\theta^{\pm}}^z\partial_z)\Sigma^z-2(H_{\theta^{\pm}}^{\theta^-}\Sigma^{\theta^+}+H_{\theta^{\pm}}^{\theta^+}\Sigma^{\theta^-})+\Sigma^z\partial_zH_{\theta^{\pm}}^z, \tag{2}$$

$$sH_z^{\theta^{\pm}}=(\partial_{\bar{z}}-H_z^z\partial_z)\Sigma^{\theta^{\pm}}+\Sigma^z\partial_zH_z^{\theta^{\pm}}+\tfrac{1}{2}(\Sigma^{\theta^{\pm}}\partial_zH_z^z-H_z^{\theta^{\pm}}\partial_z\Sigma^z), \tag{3}$$

$$sH_{\theta^+}^{\theta^{\pm}}=(D^--H_{\theta^+}^z\partial_z)\Sigma^{\theta^{\pm}}+\Sigma^z\partial_zH_{\theta^+}^{\theta^{\pm}}+\tfrac{1}{2}(\Sigma^{\theta^{\pm}}\partial_zH_{\theta^+}^z-H_{\theta^+}^{\theta^{\pm}}\partial_z\Sigma^z), \tag{4}$$

$$sH_{\theta^-}^{\theta^{\pm}}=(D^+-H_{\theta^-}^z\partial_z)\Sigma^{\theta^{\pm}}+\Sigma^z\partial_zH_{\theta^-}^{\theta^{\pm}}+\tfrac{1}{2}(\Sigma^{\theta^{\pm}}\partial_zH_{\theta^-}^z-H_{\theta^-}^{\theta^{\pm}}\partial_z\Sigma^z), \tag{5}$$

$$sH_z^{\bar{z}}=(\partial_z-H_z^{\bar{z}}\partial_{\bar{z}})\Sigma^{\bar{z}}+\Sigma^{\bar{z}}\partial_{\bar{z}}H_z^{\bar{z}},\quad sH_{\theta^{\pm}}^{\bar{z}}=(D^{\mp}-H_{\theta^{\pm}}^{\bar{z}}\partial_{\bar{z}})\Sigma^{\bar{z}}+\Sigma^{\bar{z}}\partial_{\bar{z}}H_{\theta^{\pm}}^{\bar{z}}, \tag{2.62}$$

where we have to use the covariantization (2.60) if we take into account the U(1) symmetry. Finally, we would like to note that the expressions (2.57) are invariant under superconformal changes of the reference coordinate system. Therefore, with the use of the transformations (2.40) we deduce

$$\Sigma^{z'}=Y^{-1}e^{-(\omega+\bar{\omega})}\Sigma^{z},$$

$$\Sigma^{\theta'^{\pm}}=Y^{-1/2}e^{-(\omega+\bar{\omega})/2}[\Sigma^{\theta^{\pm}}-Y^{-1}\Sigma^{z}(D^{+}\bar{\omega})H_{\theta^{+}}^{\theta^{\pm}}-Y^{-1}\Sigma^{z}(D^{-}\omega)H_{\theta^{-}}^{\theta^{\pm}}],$$

$$\Sigma^{\bar{z}'}=\left(\frac{\partial\bar{z}'}{\partial\bar{z}}\right)\Sigma^{\bar{z}} \tag{2.63}$$

with these formulations of (2,0) superconformal structures parametrized in terms of Beltrami superfields we can study the extension to the (2,0) supersymmetric case of the Wess–Zumino–Polyakov action and the conformal anomaly.

III. (2,0) SUPERCONFORMAL ANOMALY

Before giving the (2,0) super Wess–Zumino–Polyakov action, we point out that, as in the $N=1$ superconformal case,[17(c)] we can define covariant derivatives with which the integrating factor equations (2.52) and (2.53) may be expressed. For this reason we introduce an intermediate coordinate system noted by $(\tilde{z},\tilde{\bar{z}},\widetilde{\theta^{+}},\widetilde{\theta^{-}})$ such that

$$(z,\bar{z},\theta^{+},\theta^{-})\rightarrow(\tilde{z},\tilde{\bar{z}},\widetilde{\theta^{+}},\widetilde{\theta^{-}})\equiv(Z,\bar{z},\Theta^{+},\Theta^{-})\rightarrow(Z,\bar{Z},\Theta^{+},\Theta^{-}). \tag{3.1}$$

The passage from the reference coordinate system to the intermediate one is described by the following matrices:

$$M_1\Lambda_1=\begin{bmatrix}1&0&0&0\\ H_z^z&1&H_z^{\theta^+}&H_z^{\theta^-}\\ H_{\theta^+}^z&0&H_{\theta^+}^{\theta^+}&H_{\theta^+}^{\theta^-}\\ H_{\theta^-}^z&0&H_{\theta^-}^{\theta^+}&H_{\theta^-}^{\theta^-}\end{bmatrix}\begin{bmatrix}\Lambda&0&\tau^+&\tau^-\\ 0&1&0&0\\ 0&0&\sqrt{\Lambda}&0\\ 0&0&0&\sqrt{\Lambda}\end{bmatrix} \tag{3.2}$$

with

$$s\ \det M_1\Lambda_1=[H_{\theta^+}^{\theta^+}H_{\theta^-}^{\theta^-}-H_{\theta^+}^{\theta^-}H_{\theta^-}^{\theta^+}]=f^{-1}. \tag{3.3}$$

Therewith we have

$$\begin{bmatrix}\tilde{\partial}\\ \tilde{\bar{\partial}}\\ \tilde{D}^{+}\\ \tilde{D}^{-}\end{bmatrix}=\Lambda_1^{-1}M_1^{-1}\begin{bmatrix}\partial\\ \bar{\partial}\\ D^{+}\\ D^{-}\end{bmatrix} \tag{3.4}$$

which leads explicitly to

$$\tilde{\partial}=\Lambda^{-1}\Bigg\{\partial+\frac{\tau^+}{f\sqrt{\Lambda}}[H_{\theta^+}^{\theta^-}(D^{+}-H_{\theta^-}^{z}\partial)-H_{\theta^-}^{\theta^-}(D^{-}-H_{\theta^+}^{z}\partial)]$$

$$+\frac{\tau^-}{f\sqrt{\Lambda}}[H_{\theta^-}^{\theta^+}(D^{-}-H_{\theta^+}^{z}\partial)-H_{\theta^+}^{\theta^+}(D^{+}-H_{\theta^-}^{z}\partial)]\Bigg\},$$

$$\tilde{\bar{\partial}}=(\bar{\partial}-H_z^z\partial)-\frac{1}{f}(H_z^{\theta^+}H_{\theta^-}^{\theta^-}-H_z^{\theta^-}H_{\theta^-}^{\theta^+})(D^{-}-H_{\theta^+}^{z}\partial)-\frac{1}{f}(H_z^{\theta^-}H_{\theta^+}^{\theta^+}-H_z^{\theta^+}H_{\theta^+}^{\theta^-})(D^{+}-H_{\theta^-}^{z}\partial),$$

$$\tilde{D}^+=\frac{1}{f\sqrt{\Lambda}}\,[H^{\theta^+}_{\theta^+}(D^+-H^z_{\theta^-}\partial)-H^{\theta^+}_{\theta^-}(D^--H^z_{\theta^+}\partial)],$$

$$\tilde{D}^-=\frac{1}{f\sqrt{\Lambda}}\,[H^{\theta^-}_{\theta^-}(D^--H^z_{\theta^+}\partial)-H^{\theta^-}_{\theta^+}(D^+-H^z_{\theta^-}\partial)]. \tag{3.5}$$

Consequently, the integrating factor Eqs. (2.52) become

$$\tilde{\bar{\partial}}\Lambda=\Lambda\Big\{\partial H^z_{\bar{z}}-\frac{1}{h}\,H^{\theta^-}_{\bar{z}}\,[(D^+-H^z_{\theta^-}\partial)H^{\theta^+}_{\theta^+}+(D^--H^z_{\theta^+}\partial)H^{\theta^+}_{\theta^-}]$$
$$-\frac{1}{h}\,H^{\theta^+}_{\bar{z}}\,[(D^+-H^z_{\theta^-}\partial)H^{\theta^-}_{\theta^+}+(D^--H^z_{\theta^+}\partial)H^{\theta^-}_{\theta^-}]\Big\}. \tag{3.6}$$

This differential equation simplifies for the choices (2.48) namely

$$\tilde{\bar{\partial}}\Lambda=\Lambda\{\partial H^z_{\bar{z}}-H^{\theta^-}_{\bar{z}}D^+H^{\theta^+}_{\theta^+}-H^{\theta^+}_{\bar{z}}D^-H^{\theta^-}_{\theta^-}\}. \tag{3.7}$$

As we have seen in the previous section the (2,0) superconformal structures are parametrized by the super Beltrami variables $H^z_{\bar{z}}$, $H^{\bar{z}}_{\theta^\pm}$, and $H^{\theta^+}_{\theta^+}$ (or $H^{\theta^-}_{\theta^-}$) which are independent. However, the extended Wess–Zumino–Polyakov action to the (2,0) supersymmetric case is given in the right sector by

$$\Gamma_{\mathrm{WZP}}=\frac{1}{2}\int d^3z^{--}H^z_{\bar{z}}[D^+,D^-]\ln\,\Lambda, \tag{3.8}$$

where $d^3z^{--}=d^2z\,d\theta^+\,d\theta^-$, and

$$\Lambda=\partial_z Z+\Theta^+\partial_z\Theta^-+\Theta^-\partial_z\Theta^+. \tag{3.9}$$

Furthermore, the choices (2.48), which will be henceforth taken, and the expressions (2.23) and (2.29) lead to

$$D^-Z-\Theta^+D^-\Theta^--\Theta^-D^-\Theta^+=0,\quad D^+Z-\Theta^+D^+\Theta^--\Theta^-D^+\Theta^+=0; \tag{3.10}$$

these equations can be combined in order to get

$$\Lambda=(D^+\Theta^+)(D^-\Theta^-)+(D^+\Theta^-)(D^-\Theta^+). \tag{3.11}$$

Moreover, the induced conditions (2.51) are equivalent to

$$(D^+\Theta^+)=0=(D^-\Theta^-) \tag{3.12}$$

which are nothing but Eq. (2.9). Therefore, the coefficient Λ is restricted with these convenient choices to

$$\Lambda=(D^+\Theta^-)(D^-\Theta^+). \tag{3.13}$$

The BRST variation of the action (3.8) is given by

$$s\Gamma_{\mathrm{WZP}}=\frac{1}{2}\int d^3z^{--}\{(\bar{\partial}-H^z_{\bar{z}}\partial)\Sigma^z-2(H^{\theta^-}_z\Sigma^{\theta^+}+H^{\theta^+}_z\Sigma^{\theta^-})+\Sigma^z\partial H^z_{\bar{z}}\}[D^+,D^-]\ln\Lambda$$

$$-\frac{1}{2}\int d^3z^{--}[D^+,D^-]H^z_{\bar{z}}\{\partial\Sigma^z+\Sigma^z\partial\ln\Lambda+\Sigma^{\theta^-}D^+H^{\theta^+}_{\theta^+}+\Sigma^{\theta^+}D^-H^{\theta^-}_{\theta^-}$$

$$+\tfrac{1}{2}\Sigma^{\theta^-}H^{\theta^+}_{\theta^+}D^+\ln\Lambda+\tfrac{1}{2}\Sigma^{\theta^+}H^{\theta^-}_{\theta^-}D^-\ln\Lambda\},\tag{3.14}$$

where we have used the expression (2.49.2). Moreover, the choices (2.48) and the resulting Eqs. (2.50) and (2.51) allow us to have

$$\begin{aligned}D^+\ln\Lambda&=-2H^{\theta^-}_{\theta^-}(D^+H^{\theta^+}_{\theta^+})=2H^{\theta^+}_{\theta^+}(D^+H^{\theta^-}_{\theta^-}),\\ D^-\ln\Lambda&=-2H^{\theta^+}_{\theta^+}(D^-H^{\theta^-}_{\theta^-})=2H^{\theta^-}_{\theta^-}(D^-H^{\theta^+}_{\theta^+}).\end{aligned}\tag{3.15}$$

These equations, with the use of Eq. (2.2), imply

$$\partial\ln\Lambda=H^{\theta^-}_{\theta^-}(D^+D^-H^{\theta^+}_{\theta^+})+H^{\theta^+}_{\theta^+}(D^-D^+H^{\theta^-}_{\theta^-})\tag{3.16}$$

and the variation (3.14) becomes

$$s\Gamma_{\mathrm{WZP}}=\frac{1}{2}\int d^3z^{--}\{\Sigma^z\partial[D^-,D^+]H^z_{\bar{z}}+\text{couplings in } H^z_{\bar{z}},H^{\theta^\pm}_{\theta^\pm},\Sigma^z\}=\mathscr{A}(\Sigma^z,H^z_{\bar{z}},H^{\theta^\pm}_{\theta^\pm}).\tag{3.17}$$

We note that we have used the relations

$$D^+\Sigma^z=2H^{\theta^-}_{\theta^-}\Sigma^{\theta^+},\quad D^-\Sigma^z=2H^{\theta^+}_{\theta^+}\Sigma^{\theta^-},\quad D^-\Sigma^{\theta^-}=0=D^+\Sigma^{\theta^-}\tag{3.18}$$

which follow from the BRST transformations of the super Beltrami variables $H^z_{\theta^\pm}$, $H^{\theta^-}_{\theta^+}$, and $H^{\theta^+}_{\theta^-}$ fixed to zero. The (2,0) superconformal anomaly is contained in the first term of Eq. (3.17) and the super Beltrami variables $H^{\theta^+}_{\theta^+}$ and $H^{\theta^-}_{\theta^-}$ which are constrained by the following condition

$$H^{\theta^+}_{\theta^+}H^{\theta^-}_{\theta^-}=1$$

contain only auxiliary fields. Therefore, if these variables are fixed as

$$H^{\theta^+}_{\theta^+}=1=H^{\theta^-}_{\theta^-}\tag{3.19}$$

in addition to Eq. (2.48) then

$$(D^+\Theta^-)^2=\Lambda=(D^-\Theta^+)^2\tag{3.20}$$

and Eqs. (3.15) become

$$D^\pm\ln\Lambda=0$$

which are equivalent to

$$\Lambda=(D^+\Theta^-)^2=(D^-\Theta^+)^2=1.\tag{3.21}$$

These choices are equivalent to the gauge choices of the Polyakov's chiral gauge action in the pseudo-Riemannian framework and its generalization to the $N=1$ supersymmetric case.[17(d),20]

Finally, in terms of field components the (2,0) superconformal anomaly (3.17) is given by

$$\mathscr{A}=\int d^2z^{--}\{\Sigma^z\partial^3\mu_z^z+2\Sigma^{\theta^-}\partial^2\mu_z^{\theta^+}+2\Sigma^{\theta^+}\partial^2\mu_z^{\theta^-}\}, \tag{3.22}$$

where we have used Eqs. (2.49.1) and (3.18) with the choice (3.19). Note in Eq. (3.17) and consequently Eq. (3.22) the absence of the U(1) gauge anomaly since the U(1) connection has been omitted from the beginning. At this stage, the anomalous (2,0) supersymmetric Ward-identities and the operator product expansions can be obtained. This is the subject of the next section.

IV. (2,0) SUPERSYMMETRIC WARD-IDENTITIES FOR $H^z_{\theta^\pm}=0$, $H^{\theta^\pm}_{\theta^\pm}=1$

The (2,0) supersymmetric Wess–Zumino–Polyakov action in the right sector Eq. (3.8) can be rewritten as follows:

$$\Gamma_{\mathrm{WZP}}=2\int d^3z^{--}\ \frac{1}{(D^+\Theta^-)(D^-\Theta^+)}\{(\partial\Theta^-)(\bar\partial-H_z^z\partial)\Theta^+-(\partial\Theta^+)(\bar\partial-H_z^z\partial)\Theta^-\}, \tag{4.1}$$

where we have used the following identities:

$$\begin{aligned}&D^+[\bar\partial Z+\Theta^+\bar\partial\Theta^-+\Theta^-\bar\partial\Theta^+]=2(\bar\partial\Theta^+)(D^+\Theta^-),\\ &D^-[\bar\partial Z+\Theta^+\bar\partial\Theta^-+\Theta^-\bar\partial\Theta^+]=2(\bar\partial\Theta^-)(D^-\Theta^+)\end{aligned} \tag{4.2}$$

which proceed from Eq. (3.10). Note that if we want to take into account the connection of the U(1) symmetry one has to covariantize the derivatives $\bar\partial\Theta^+$ and $\bar\partial\Theta^-$ namely

$$\bar\partial\Theta^\pm\to(\bar\partial\pm\mathscr{A}_{\bar z})\Theta^\pm. \tag{4.3}$$

Therefore, the expression (4.1) becomes

$$\Gamma_{\mathrm{WZP}}=2\int d^3z^{--}\ \frac{1}{(D^+\Theta^-)(D^-\Theta^+)}\{(\partial\Theta^-)(\bar\partial+\mathscr{A}_{\bar z}-H_z^z\partial)\Theta^+-(\partial\Theta^+)(\bar\partial-\mathscr{A}_{\bar z}-H_z^z\partial)\Theta^-\} \tag{4.4}$$

and its BRST variation allows to obtain in addition to Eq. (3.17) the contribution of the U(1) gauge anomaly.

The Ward-identity operator acting on the generating functional is given in the right sector by

$$B(\lambda\cdot\partial)=\int d^3z^{--}\delta_\lambda H_z^z\frac{\delta}{\delta H_z^z} \tag{4.5}$$

with $\delta_\lambda H_z^z$ the BRST variation (2.62.1) where the ghost superfields Σ^z, $\Sigma^{\theta^\pm}$ are replaced by the superparameters $\lambda^a(a=z,\theta^\pm)$. The anomalous Ward-identity which is given in the right sector by

$$B(\lambda\cdot\partial)Z_c[H_z^z]\alpha.\mathscr{A}(\lambda^z,H_z^z) \tag{4.6}$$

takes the explicit form

$$\int d^3z^{--}[(\bar{\partial}-H_z^z\partial)\lambda^z-2(H_z^{\theta^-}\lambda^{\theta^+}+H_z^{\theta^+}\lambda^{\theta^-})+\lambda^z\partial H_z^z]\frac{\delta Z_c[H_z^z]}{\delta H_z^z}=k\int d^3z^{--}\lambda^z\partial[D^-,D^+]H_z^z \tag{4.7}$$

which is equivalent to

$$\left[\bar{\partial}-H_z^z\partial+\frac{1}{2}(D^-H_z^z)D^+ +\frac{1}{2}(D^-H_z^z)D^- -\partial H_z^z\right]\frac{\delta Z_c[H_z^z]}{\delta H_z^z}=k\partial[D^-,D^+]H_z^z, \tag{4.8}$$

where k is an arbitrary constant. Furthermore, as for the bosonic and $N=1$ supersymmetric cases[17(d)] we define the following (2,0) superspace identity

$$-\Pi\,\delta^3_{--}(Z_1,Z_2)=\frac{\bar{\partial}^2}{\Box}[D^+,D^-]\ln[Z_{12},\bar{z}_{12}] \tag{4.9}$$

which contains the ordinary distributional relation, Z_{12} and $\bar{z}_{12}$ are defined by

$$Z_{12}=z_1-z_2-\theta_1^+\theta_2^- -\theta_1^-\theta_2^+, \quad \bar{z}_{12}=\bar{z}_1-\bar{z}_2 \tag{4.10}$$

and

$$\delta^3_{--}(Z_1,Z_2)=\delta^2(z_1-z_2)(\theta_1^+-\theta_2^+)(\theta_1^--\theta_2^-)$$

Therefore, multiplying Eq. (4.8) by $\bar{\partial}/\Box[D^+,D^-]\ln[Z_{12}\cdot\bar{z}_{12}]$ and after integrating we obtain

$$\frac{\pi}{2}\frac{\delta Z_c}{\delta H_z^z(Z_2)}=\int d^3z_1^{--}H_z^z\left\{\left|\frac{\theta_{12}^+\theta_{12}^-}{Z_{12}}\partial+\frac{\theta_{12}^+\theta_{12}^-}{Z_{12}^2}+\frac{\theta_{12}^+}{2Z_{12}}D^- -\frac{\theta_{12}^-}{2Z_{12}}D^+\right|\frac{\delta Z_c}{\delta H_z^z}+\frac{2k}{Z_{12}^2}\right\}. \tag{4.11}$$

Then a second derivation of this expression with respect to H_z^z leads to

$$\frac{\pi}{2}\frac{\delta^2 Z_c}{\delta H_z^z(Z_1)\delta H_z^z(Z_2)}\bigg|_{H_z^z=0}=\frac{2k}{Z_{12}^2}+\left|\frac{\theta_{12}^+\theta_{12}^-}{Z_{12}^2}+\frac{\theta_{12}^+\theta_{12}^-}{Z_{12}}\partial+\frac{\theta_{12}^+}{2Z_{12}}D^- -\frac{\theta_{12}^-}{2Z_{12}}D^+\right|\frac{\delta Z_c}{\delta H_z^z}\bigg|_{H_z^z=0}. \tag{4.12}$$

The variation of the generating functional Z_c with respect to the super Beltrami variable H_z^z gives rise[9] to the following (2,0) superstress energy tensor:

$$T_z(Z_1)=\frac{\delta Z_c}{\delta H_z^z(Z_1)} \tag{4.13}$$

and consequently, Eq. (4.12) is nothing but the operator product expansion of the (2,0) superstress energy tensor T_z (Refs. 21 and 19) namely

$$T_z(Z_1)T_z(Z_2)=\frac{c}{2Z_{12}^2}+\left|\frac{\theta_{12}^+\theta_{12}^-}{Z_{12}^2}+\frac{\theta_{12}^+\theta_{12}^-}{Z_{12}}\partial+\frac{\theta_{12}^+}{2Z_{12}}D^- -\frac{\theta_{12}^-}{2Z_{12}}D^+\right|T_z(Z_2)+\text{regular terms}, \tag{4.14}$$

where c is the central charge of the $N=2$ superconformal algebra. Finally, we note that if we consider the dependence of the generated functional with respect to $H_z^{\theta^\pm}$ instead of H_z^z and we reexpress the (2,0) superconformal anomaly in terms of $\Sigma^{\theta^\pm}$ and $H_z^{\theta^\pm}$ by the use of Eqs. (2.49.1) and (3.18) we obtain anomalous Ward-identities which contain variations of Z_c with respect to $H_z^{\theta^\pm}$. These latter lead in the same way to the operator product expansions of the following spinorial superstress energy tensor:[9]

$$T_{\theta^\pm} = \frac{\delta Z_c}{\delta H_z^{\theta^\pm}}$$

V. CONCLUSION

In this article we have derived the (2,0) superconformal transformations of the conformal factors, the super Beltrami variables and their corresponding ghost superfields. We have seen that the choices $H^z_{\theta^\pm} = 0$ fixed in Refs. 8 and 9 are invariant under the change of the reference coordinate and simplify all the other super Beltrami variable transformations as in the $N=1$ supersymmetric case. Therefore, the transformations of $H^{\theta^\pm}_{\theta^\pm}$ and $H^{\theta^\mp}_{\theta^\pm}$ become homogeneous. The BRST variations of the super Beltrami variables are obtained. We remark that these correspond to only superdiffeomorphism transformations. In order to recover the complete BRST transformations given in Refs. 8 and 9 in which the U(1) symmetry is apparent, we have to covariantize the derivatives acting on fermionic objects having + and −U(1) charges with respect to the U(1) connection. This latter is necessary in order to close the multiplet of the super Beltrami variables. Furthermore, the Wess–Zumino–Polyakov action is extended to the (2,0) supersymmetric case for the convenient choices $H^z_{\theta^\pm} = 0$. The BRST variation of this action leads to the (2,0) superconformal anomaly. For $H^{\theta^+}_{\theta^+} = 1 = H^{\theta^-}_{\theta^-}$ we recover the gauge choice of the Polyakov's chiral gauge action. Finally, we remark that the use of anomalous Ward-identity in the right sector of the (2,0) superspace allows to deduce the known operator product expansion of the $N=2$ superconformal theory.

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Imaging of velocity singularities with multiscale operators

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In this paper, by using the multiscale operator and based on the Beylkin's formula [J. Math. Phys. **26**, 99–108 (1985)], the inversion method of velocity singularities is presented, and by applying the multiscale operator to upward scattered data represented by the Kirchhoff approximation, the multiscale imaging formula is shown. For the band-limited inverse problem, based on the multiscale imaging formula in this paper, the behavior of the velocity singularities can be analyzed across the multiscale and the formula to reconstruct the velocity is obtained from the output of the multiscale operator interpreted in the terms of the Kirchhoff-approximate data. Particularly, at wide offset and even postcritical case, for the full-band input data, the same result with Beylkin's in the above reference about the velocity discontinuities is obtained. Our method in this paper can suppress the effects of the noise in the real world data and analyze the effect produced by band-limited input data. © *1996 American Institute of Physics.* [S0022-2488(96)02601-5]

I. INTRODUCTION

Beylkin presented a theory for asymptotic inversion of observation for the constant-density acoustic wave equation.[1] It allows for a completely general background sound speed in the inverse problem, as well as an assortment of possible source–receiver configurations broad enough to accommodate most of the cases of interest in seismic exploration and other applications. Thus, for the full-band inverse problem his method provides a unified inversion theory for all source–receiver configurations used in practice. However, in practice, the input data are band limited. To solve the band-limited inverse problems, Bleistein and his colleague have done a lot of investigations in Refs. 2 and 3 based on Beylkin's formula. The inversion operator $\beta(x)$ was introduced, and by using the velocity singularities, the authors have shown that $\beta(x)$ is a band-limited delta function on the interior surface, for the band-limited input data. From Refs. 2 and 3 we know that the small parameter constraint of the Born approximation in Ref. 1 can be at least partially eliminated by applying Bleistein's methods.

Despite the fundamental significance of Bleistein's results, further analysis is necessary. Because the inversion operator $\beta(x)$ is a generalization of the derivative operator $\partial\alpha(z)/\partial z$ in Ref. 4, $\beta(x)$ is highly sensitive to the noise in real world data. On other hand, the inversion operator $\beta(x)$, which is a band-limited delta function on the reflector, would be affected by the band-limited data. Hence, for the band-limited inverse problem, it is necessary to develop some new inverse methods which can suppress the noise and can analyze the effect.

Until recently, the Fourier transform was the main mathematical tool for singularity detection. The Fourier transform is global and provides a description of overall regularity of functions, but it is not well adapted for finding the location and the spatial distribution of singularities. However, based on the wavelet theory,[5] the multiscale operator in this paper is proposed. It is adapted for

finding the location and the spatial distribution of velocity singularities for the band-limited inverse problem. In this paper, a new inversion method for velocity singularities using multiscale operators is presented. For the band-limited inverse problem, the multiscale image formula for velocity singularities is given by applying the multiscale operator to upward scattered data represented by the Kirchhoff approximation. Based on the multiscale imaging formula, we can analyze the behavior of velocity singularities across multiscales. Particularly, at wide offset and even postcritical case, for the full-band imput data, we can obtain the same results as Beylkin's in Ref. 1 about the velocity discontinuities. Furthermore, our inversion method can suppress the effects of the noise in real world data and analyze the effect produced by band-limited input data.

This paper is motivated by Beylkin (Ref. 1) and Mallat (Ref. 5).

II. IMAGING OF VELOCITY SINGULARITIES WITH MULTISCALE OPERATOR

The Beylkin (Ref. 1) inversion formula in 3-D is

$$\alpha(x)=\int d\omega \int\int_{\Omega} d^2\xi B(x,\xi)\exp\{-i\omega\varphi(x,\xi)\}u_s(x_g,x_s,\omega), \tag{1}$$

where

$$B(x,\xi)=\frac{1}{8\pi^3}\frac{|h(x,\xi)|c^2(x)}{a(x,\xi)}, \tag{2}$$

$$h(x,\xi)=\det\begin{bmatrix} \nabla_x\varphi(x,\xi) \\ \dfrac{\partial}{\partial\xi_1}\nabla_x\varphi(x,\xi) \\ \dfrac{\partial}{\partial\xi_2}\nabla_x\varphi(x,\xi) \end{bmatrix}, \tag{3}$$

$$\varphi(x,\xi)=\tau(x,x_s(\xi))+\tau(x_g(\xi),x), \tag{4}$$

$$a(x,\xi)=A(x,x_s(\xi))A(x_g(\xi),x). \tag{5}$$

At this point A and τ are the 3-D amplitude and phase of the WKB Green's function, but with initial points being either the source point x_s or the receiver point x_g, both of which are parametrized by $\xi=(\xi_1,\xi_2)$ on the datum surface Ω, i.e.,

$$x_s=x_s(\xi_1,\xi_2), \quad x_g=x_g(\xi_1,\xi_2). \tag{6}$$

Here $\alpha(x)$ is the perturbation correction to the given reference velocity $c(x)$, with the total velocity $v(x)$ being given by

$$\frac{1}{v^2(x)}=\frac{1}{c^2(x)}[1+\alpha(x)]. \tag{7}$$

Here $u_s(x_g,x_s,\omega)$ denotes the observed data at x_g due to the source at x_s.

To consider the important question, that of limited bandwidth, we modify the formula (1) as

$$\alpha(x)=\int F(\omega)d\omega\int\int_{\Omega} d^2\xi B(x,\xi)\ \exp\{-i\omega\varphi(x,\xi)\}u_s(x_g,x_s,\omega). \tag{8}$$

The domain of integration in ω is limited by the symmetric filter $F(\omega)$.

We take as the symmetric filter $F(\omega)$ the following

$$F(\omega)=\begin{cases}1, & \omega\in(\omega_0,\omega_1) \text{ or } (-\omega_1,-\omega_0),\\ 0, & \text{otherwise},\end{cases} \tag{9}$$

where $\omega_1>\omega_0>0$.

In Ref. 1, only for the full-bandwidth case, Beylkin showed that the discontinuities of the function $\alpha(x)$ in (1) are located at the reflectors in the earth. In Refs. 2 and 3, Bleistein introduced a new inversion operator $\beta(x)$ and showed that $\beta(x)$ is a band-limited delta function for the band-limited case. What then is the effect of bandlimiting on the function $\alpha(x)$ in (8)? It is still unclear from Beylkin's results[1] and Bleistein's results.[2,3] In this paper, by choosing a multiscale function $\psi(x)$, we obtain the imaging formula of a velocity singularity, for the band-limited inversion problem (8). This imaging formula shows the effect of band limiting on $\alpha(x)$ very clearly.

We call a three-dimensional smoothing function, any function whose triple integral is nonzero. We define three functions which are, respectively, the partial derivatives along x_1, x_2, and x_3 of a three-dimensional smoothing function $\theta(x_1,x_2,x_3)$:

$$\psi^k(x)=\frac{\partial\theta(x)}{\partial x_k}, \tag{10}$$

where $k=1, 2, 3$, and $x=(x_1,x_2,x_3)$.

Let $\theta_s(x)=1/s^3\,\theta(x/s)$ and $\psi_s^k(x)=(1/s^3)\,\psi^k(x/s)$. The multiscale transforms are given by

$$W_s^k\alpha(x)=(\alpha*\psi_s^k)(x)=s\,\frac{\partial}{\partial x_k}\,(\alpha*\theta_s)(x), \tag{11}$$

in which "$*$" is the convolution operator and s is the multiscale.

Under the scale s, the three-dimensional multiscale operator W is given by

$$W_s\alpha(x)=\begin{bmatrix}W_s^1\alpha(x)\\ W_s^1\alpha(x)\\ W_s^1\alpha(x)\end{bmatrix}=s\begin{bmatrix}\dfrac{\partial}{\partial x_1}\,(\alpha*\theta_s)(x)\\ \dfrac{\partial}{\partial x_2}\,(\alpha*\theta_s)(x)\\ \dfrac{\partial}{\partial x_3}\,(\alpha*\theta_s)(x)\end{bmatrix}=s\nabla(\alpha*\theta_s)(x), \tag{12}$$

where "∇" is gradient operator.

In this paper, we choose $\theta(x)$ equal to a Gaussian, i.e.,

$$\theta(x)=\frac{1}{2\pi\sqrt{2\pi}}\exp\left(-\frac{x_1^2+x_2^2+x_3^2}{2}\right). \tag{13}$$

Now we assume that the upward-scattered response $u_s(x_g,x_s,\omega)$ in (8) arises from a single reflector S. Then, we use the Kirchhoff approximation which can be found in Ref. 3 to represent those data, for example. In the notation used here, the result is

$$u_s(x_g,x_r,\omega)\approx i\omega\int\int_S R(\bar{x},x_s)a(\bar{x},\xi)\hat{n}\cdot\nabla_{\bar{x}}\varphi(\bar{x},\xi)\exp\{i\omega\varphi(\bar{x},\xi)\}dS. \tag{14}$$

In this equation, $\varphi(\bar{x},\xi)$ and $a(\bar{x},\xi)$ are defined by (4) and (5), respectively: $R(\bar{x},x_s)$ is the geometrical optics reflection coefficient

$$R(\bar{x},x_s)=\frac{\left|\frac{\partial}{\partial n}\,\tau(\bar{x},x_s)\right|-\left\{1/c_+^2(\bar{x})-1/c^2(\bar{x})+\left[\frac{\partial}{\partial n}\,\tau(\bar{x},x_s)\right]^2\right\}^{1/2}}{\left|\frac{\partial}{\partial n}\,\tau(\bar{x},x_s)\right|+\left\{1/c_+^2(\bar{x})-1/c^2(\bar{x})+\left[\frac{\partial}{\partial n}\,\tau(\bar{x},x_s)\right]^2\right\}^{1/2}}. \tag{15}$$

The unit normal $\hat{n}$ points upward and $\partial/\partial n=\hat{n}\cdot\nabla_{\bar{x}}$; $c_+(x)$ is the propagation speed below the reflector. The surface S is described parametrically in terms of two parameters (σ_1,σ_2) by an equation of the form $\bar{x}=\bar{x}(\sigma)$, $\sigma=(\sigma_1,\sigma_2)$. In terms of these parameters, $dS=\sqrt{g}\,d\sigma_1\,d\sigma_2$. Equation (14) is to be substituted into (8). By using the stationary phase method, exactly as in (14), (15), and (18) in Ref. 3, for x near the reflector S we obtain

$$\alpha(x)\approx -R(\bar{x},x_s)\,\frac{a(\bar{x},x_s)}{a(x,x_s)}\,\frac{|h(x,\xi)|}{\sqrt{\det[\Phi_{\xi,\sigma}]}}\,\hat{n}$$
$$\cdot\,\nabla_{\bar{x}}\varphi(\bar{x},\xi)c^2(x)\sqrt{g}\,\frac{1}{2\pi}\int F(\omega)\,\frac{1}{i\omega}\exp\{i\omega\Phi(x,\bar{x},\xi)\}d\omega, \tag{16}$$

in which

$$\Phi(x,\bar{x},\xi)=\varphi(\bar{x},\xi)-\varphi(x,\xi), \tag{17}$$

$$g=\left|\frac{\partial\bar{x}}{\partial\sigma_1}\times\frac{\partial\bar{x}}{\partial\sigma_2}\right|^2=\left|\det\left[\frac{\partial\bar{x}}{\partial\sigma_k}\cdot\frac{\partial\bar{x}}{\partial\sigma_m}\right]\right|,\quad k,m=1,2, \tag{18}$$

$$[\Phi_{\xi,\sigma}]=\begin{bmatrix}\frac{\partial^2\Phi}{\partial\xi_k\partial\xi_m} & \frac{\partial^2\Phi}{\partial\xi_k\partial\sigma_m}\\ \frac{\partial^2\Phi}{\partial\xi_k\partial\sigma_m} & \frac{\partial^2\Phi}{\partial\sigma_k\partial\sigma_m}\end{bmatrix},\quad k,m=1,2. \tag{19}$$

By Ref. 3, we obtain the following equation:

$$\Phi(x,\bar{x},\xi)=0,\ \text{only for}\ x\ \text{on surface}\ S. \tag{20}$$

Now we apply the multiscale operator W in (13) to $\alpha(x)$ in (16), we obtain the following results, and the proof will be found in Sec. III.

Theorem 1: For the band-limited inverse problem (8), if x is near to surface S, then

$$|W_s\alpha(x)|\approx\frac{8s|R(\bar{x},x_s)|}{\pi c(\bar{x})}\cos^3\theta\,\exp\left(-\frac{b^2}{4a}\right)\left|\int_{\omega_0}^{\omega_1}\exp(-a\omega^2)d\omega+z(a,b,\omega_0,\omega_1)\right|. \tag{21}$$

In this equation, $a=2s^2\cos^2\theta/c^2(\bar{x})$, $b=\Phi(x,\bar{x},\xi)$, θ is the angle between the upward normal to the surface S and the incident and reflected rays on the surface S, and $z(a,b,\omega_0,\omega_1)$ satisfies the following inequality:

$$\left|\exp\left(-\frac{b^2}{4a}\right)z(a,b,\omega_0,\omega_1)\right|\leqslant\frac{1}{a}\left[\exp(-a\omega_1^2)+\exp(-a\omega_0^2)\right]\exp\left\{-\frac{(b^2-\tau_0^2)}{4a}\right\}, \tag{22}$$

in which $\tau_0\in(0,b)$ as $b>0$, or $\tau_0\in(b,0)$ as $b<0$, and $z(a,b,\omega_0,\omega_1)=0$ as $b=0$.

Based on (20)–(22), the following corollary holds.

Corollary 1: If x is on the surface S, then the value of $|W_s\alpha(x)|$ is maximal, and

$$\max|W_s\alpha(x)|\approx\frac{8s|R(\bar{x},x_s)|}{\pi c(\bar{x})}\cos^3\theta\int_{\omega_0}^{\omega_1}\exp(-a\omega^2)d\omega. \tag{23}$$

Especially at wide offset and even postcritical case, for the full-band input data, i.e., as $\omega_0\to 0^+$ and $\omega_1\to+\infty$, from inequality (22) we have

$$\exp\left(-\frac{b^2}{4a}\right)z(a,b,\omega_0,\omega_1)\to 0 \tag{24}$$

and

$$\int_{\omega_0}^{\omega_1}\exp(-a\omega^2)d\omega=\int_{-\infty}^{\infty}\exp(-a\omega^2)d\omega=\sqrt{\frac{\pi}{a}}=\frac{c(\bar{x})}{\sqrt{2}s\cos\theta}. \tag{25}$$

So, we have the second corollary.

Corollary 2: At wide offset and even postcritical case, from the full-band input data, then

$$|W_s\alpha(x)|\approx\frac{8|R(\bar{x},x_s)|}{\sqrt{2\pi}}\cos^2\theta\exp\left(-\frac{b^2}{4a}\right) \tag{26}$$

and for x on surface S

$$\max|W_s\alpha(x)|\approx\frac{8|R(\bar{x},x_s)|}{\sqrt{2\pi}}\cos^2\theta. \tag{27}$$

Remark (i): From (21), by detecting the maxima of $|W_s\alpha(x)|$, we obtain a reconstruction algorithm for the band-limited inverse problem. The approximation in (21) not only reconstructs the place, where the gradient of $\alpha(x)$ is large, for the band-limited inverse problem, but also shows the effect of the band-limited nature of the input data very clearly. Particularly, at wide offset and even postcritical case, for the full-band input data, the Corollary 2 shows that the effect of the band-limited nature disappears. In this sense the formula in (26) provides an algorithm for imaging the discontinuities of the function $\alpha(x)$.

Remark (ii): Based on Theorem 1, we can detect the velocity singularities to the band-limited inverse problem with the multiscale transform, and then we get the information on the differences between the velocity singularities and the noise singularities. On this information, we can easily suppress the effect of the noise from the imaging of the velocity singularities, by analyzing the behavior of the multiscale operator maxima across scales s. The detail discussion will be found in Sec. IV.

III. ASYMPTOTIC INVERSION

Bleistein in Ref. 3 showed that

$$\hat{n}\cdot\nabla_{\bar{x}}\varphi(\bar{x},\xi)=-\frac{2\cos\theta}{c(\bar{x})}, \tag{28}$$

$$|\nabla_{\bar{x}}\varphi(\bar{x},\xi)|=\frac{2\cos\theta}{c(\bar{x})}, \tag{29}$$

and x on surface S

$$\frac{|h(x,\xi)|}{\sqrt{|\det[\Phi_{\xi,\sigma}]}}\sqrt{g}=\frac{2\cos\theta}{c(x)}. \tag{30}$$

Let the reference velocity $c(x)$ in (7) be a continuous function and all the singularities of the total velocity $v(x)$ be contained in function $\alpha(x)$. In (16), define

$$I(x)=\frac{1}{\pi}\int F(\omega)\,\frac{1}{i\omega}\exp\{i\omega\Phi(x,\bar{x},\xi)\}d\omega. \tag{31}$$

Based on (28)–(31), from (16) we know that $\alpha(x)$ is equal to $I(x)$ multiplied by "a slowly varying function," i.e.,

$$\alpha(x)\approx 2R(\bar{x},x_s)\cos^2\theta I(x), \quad \text{for } x \text{ near enough to surface } S. \tag{32}$$

Applying the multiscale operator W in (13) to $\alpha(x)$ in (32), we obtain

$$W_s\alpha(x)\approx 2R(\bar{x},x_s)\cos^2\theta W_s I(x). \tag{33}$$

In (31), we expand the phase function $\Phi(x,\bar{x},\xi)$ into Taylor's series about the point $x=\bar{x}$. Saving the first two terms of the Taylor's series of $\Phi(x,\bar{x},\xi)$,

$$\Phi(x,\bar{x},\xi)\approx\Phi(x,\bar{x},\xi)|_{x=\bar{x}}+\nabla_x\Phi(x,\bar{x},\xi)|_{x=\bar{x}}\cdot(x-\bar{x})+\cdots, \tag{34}$$

and, using (20), we find that

$$\Phi(x,\bar{x},\xi)\approx\boldsymbol{\nabla}_x\Phi(x,\bar{x},\xi)|_{x=\bar{x}}\cdot(x-\bar{x})\approx-\nabla_x\varphi(x,\xi)|_{x=\bar{x}}\cdot(x-\bar{x}), \tag{35}$$

and

$$I(x)\approx\frac{1}{\pi}\int F(\omega)\,\frac{1}{i\omega}\exp\{-i\omega\boldsymbol{\nabla}_x\varphi(x,\xi)|_{x=\bar{x}}\cdot(x-\bar{x}\}d\omega. \tag{36}$$

Next, let us calculate the $W_sI(x)$. First, we calculate $W_s^kI(x)$. From (10), (11), and (13)

$$\begin{aligned}W_s^kI(x)&=s\,\frac{\partial}{\partial x_k}\,(I*\theta_x)(x)\\&=-\frac{s}{2\pi^2\sqrt{2\pi}}\,\nabla_{x_k}\varphi(x,\xi)\Big|_{x=\bar{x}}\\&\quad\times\int F(\omega)\,d\omega\int_{-\infty}^{\infty}\exp\Big\{i\omega\nabla_x\varphi(x,\xi)\Big|_{x=\bar{x}}\cdot\big[y-(x-\bar{x})\big]\Big\}\,\frac{1}{s^3}\\&\quad\times\exp\left\{-\frac{y_1^2+y_2^2+y_3^2}{2s^2}\right\}dy_1dy_2dy_3.\end{aligned} \tag{37}$$

By using the formula

$$\int_{-\infty}^{\infty} \exp(i\omega x - x^2/2)dx = (2\pi)^{1/2} \exp(-\omega^2/2), \tag{38}$$

from (37) we obtain

$$W_s^k I(x) = -\frac{s}{\pi} \nabla_{x_k} \varphi(x,\xi)|_{x=\bar{x}} \int F(\omega) \exp(-a\omega^2 + ib\omega)d\omega, \tag{39}$$

in which $a = 2s^2 \cos^2 \theta / c^2(\bar{x})$, and

$$b = -\nabla_x \varphi(x,\xi)|_{x=\bar{x}} \cdot (x-\bar{x}) \approx \Phi(x,\bar{x},\xi).$$

Define

$$z_1(b) = \int F(\omega) \exp(-a\omega^2) \cos(b\omega)d\omega, \tag{40}$$

$$z_2(b) = \int F(\omega) \exp(-a\omega^2) \sin(b\omega)d\omega. \tag{41}$$

From Eq. (9) we obtain

$$z_1(b) = 2\int_{\omega_0}^{\omega_1} \exp(-a\omega^2) \cos(b\omega)d\omega, \quad z_2(b) = 0.$$

Since

$$\frac{dz_1(b)}{db} = -\frac{b}{a} z_1(b) + \frac{1}{a}[\exp(-a\omega_1^2)\sin b\omega_1 - \exp(-a\omega_0^2) \sin b\omega_0], \tag{42}$$

one obtains

$$z_1(b) = 2\exp\left(-\frac{b^2}{4a}\right)\left\{\int_{\omega_0}^{\omega_1} \exp(-a\omega^2)d\omega + \int_0^b [\exp(-a\omega_1^2) \sin \tau\omega_1 - \exp(-a\omega_0^2)\sin \tau\omega_0] \frac{1}{2a} \exp\left(\frac{\tau^2}{4a}\right)d\tau\right\}. \tag{43}$$

Substituting (43) into (39) one obtains

$$W_s^k I(x) = -\frac{2s}{\pi} \nabla_{x_k} \varphi(x,\xi)|_{x=\bar{x}} \exp\left(-\frac{b^2}{4a}\right)\left[\int_{\omega_0}^{\omega_1} \exp(-a\omega^2)d\omega + z(a,b,\omega_0,\omega_1)\right], \tag{44}$$

where

$$z(a,b,\omega_0,\omega_1) = \int_0^b [\exp(-a\omega_1^2) \sin \tau\omega_1 - \exp(-a\omega_0^2) \sin \tau\omega_0]\exp\left(\frac{\tau^2}{4a}\right)d\tau. \tag{45}$$

It is easy to check that $z(a,b,\omega_0,\omega_1)$ satisfies the following inequality:

$$\left|\exp\left(-\frac{b^2}{4a}\right)z(a,b,\omega_0,\omega_1)\right| \leq \frac{1}{a}[\exp(-a\omega_1^2) + \exp(-a\omega_0^2)] \exp\left\{-\frac{b^2-\tau_0^2}{4a}\right\}, \tag{46}$$

where $\tau_0 \in (0,b)$ for $b>0$, $\tau_0 \in (b,0)$ for $b<0$, and $z(a,b,\omega_0,\omega_1)=0$ for $b=0$.

From (12), one obtains

$$|W_s I(x)| = \sqrt{|W_s^1 I(x)|^2 + |W_s^2 I(x)|^2 + |W_s^3 I(x)|^2}. \tag{47}$$

Substituting (44) into (47), we have

$$|W_s I(x)| = \frac{2s}{\pi} |\nabla_x \varphi(x,\xi)|_{x=\bar{x}}| \exp\left(-\frac{b^2}{4a}\right) \left| \int_{\omega_0}^{\omega_1} \exp(-a\omega^2) d\omega + z(a,b,\omega_0,\omega_1) \right|. \tag{48}$$

Furthermore, by (29), one obtains

$$|W_s I(x)| = \frac{4s \cos\theta}{\pi c(\bar{x})} \exp\left(-\frac{b^2}{4a}\right) \left| \int_{\omega_0}^{\omega_1} \exp(-a\omega^2) d\omega + z(a,b,\omega_0,\omega_1) \right|. \tag{49}$$

Substituting (49) into (33), we have

$$|W_s \alpha(x)| \approx \frac{8s|R(\bar{x},x_s)|}{\pi c(\bar{x})} \cos^3\theta \exp\left(-\frac{b^2}{4a}\right) \left| \int_{\omega_0}^{\omega_1} \exp(-a\omega^2) d\omega + z(a,b,\omega_0,\omega_1) \right|. \tag{50}$$

This equation shows that Eq. (21) in Theorem 1 is true.

IV. THE RECONSTRUCTION OF THE VELOCITY FUNCTION

By the above analyses, we can calculate the approximate value of $W_s \alpha(x)$ from the input data $u_s(x_g, x_s, \omega)$. Now, let us explain how to determine the velocity $c_+(x)$ below the surface S. Based on (23), in order to reconstruct $c_+(x)$, first we have to determine the value of θ. Similar to (9), let us define a multiscale filter $F_1(\omega)$ as follows:

$$F_1(\omega) = \begin{cases} \exp(-s_0^2\omega^2), & \omega \in (\omega_0,\omega_1) \text{ or } \omega \in (-\omega_1,-\omega_0), \\ 0, & \text{otherwise} \end{cases}, \tag{51}$$

where $\omega_1 > \omega_0 > 0$ and s_0 is a parameter to be chosen.

Using the filter $F_1(\omega)$ to replace $F(\omega)$ in (8), similar to (32) we obtain

$$a(x) \approx 2R(\bar{x},x_s) \cos^2\theta I_{s_0}(x), \tag{52}$$

for x near enough to surface S.

Here

$$I_{s_0}(x) = \frac{1}{\pi} \int \frac{1}{i\omega} \exp\{-s_0^2\omega^2 + i\omega\Phi(x,\bar{x},\xi)\} d\omega. \tag{53}$$

Define

$$\bar{W}_{s_0} \alpha(x) = 2R(\bar{x},x_s) \cos^2\theta \nabla_x I_{s_0}(x). \tag{54}$$

Similar to the proof of (50), for x near to S we obtain

$$|\bar{W}_{s_0} \alpha(x)| \approx \frac{8R(\bar{x},x_s)}{\pi c(\bar{x})} \cos^3\theta \exp\left(-\frac{b^2}{4s_0}\right) \left[\int_{\omega_0}^{\omega_1} \exp(-s_0^2\omega^2) d\omega + z(s_0,b,\omega_0,\omega_1) \right] \tag{55}$$

in which $b = \Phi(x,\bar{x},\xi)$ and $z(s_0,b,\omega_0,\omega_1)$ is given in (45), s_0^2 being in the place of a.

Note that in deriving (55) from (54) we have not used the linearization of phase Φ, but we have used the exact phase.

Thus, by (55),

$$\max|\bar{W}_{s_0}\alpha(x)| \approx \frac{8|R(\bar{x},x_s)|}{\pi c(\bar{x})} \cos^3\theta \int_{\omega_0}^{\omega_1} \exp(-s_0^2\omega^2)d\omega. \tag{56}$$

From (23), (56), and noting that $a=2s^2\cos^2\theta/c^2(\bar{x})$ in (23), we obtain

$$\frac{\max|W_s\alpha(x)|}{\max|\bar{W}_{s_0}\alpha(x)|} \approx \frac{s\int_{\omega_0}^{\omega_1}\exp\{-2s^2\omega^2\cos^2\theta/c^2(\bar{x})\}d\omega}{\int_{\omega_0}^{\omega_1}\exp\{-s_0^2\omega^2\}d\omega}. \tag{57}$$

Based on (57), from $\max|W_s\alpha(x)|$ and $\max|\bar{W}_{s_0}\alpha(x)|$ we can determine $\cos\theta$. In fact,

$$\frac{\cos^2\theta}{c^2(\bar{x})} \approx \frac{s_0^2}{2s^2} - \frac{1}{2s^2\omega_1^2}\ln\frac{\max|W_s\alpha(x)|}{s\max|\bar{W}_{s_0}\alpha(x)|}. \tag{58}$$

After $\cos\theta$ has been determined, we can use (23) or (56) to calculate $R(\bar{x},x_s)$. That is to say, from input data $u_s(x_g,x_s,\omega)$ we can calculate $|W_s\alpha(x)|$ and $|\bar{W}_{s_0}\alpha(x)|$, and then determine the values of $\cos\theta$ and $R(\bar{x},x_s)$.

Next, let us reconstruct the velocity c_+ below the surface S. Under the stationary conditions (see Ref. 3), one obtains

$$\frac{\partial\tau(\bar{x},x_s)}{\partial n} = \frac{\cos\theta}{c(\bar{x})}.$$

Hence, (15) can be rewritten as

$$R(\bar{x},x_s) = \frac{\dfrac{\cos\theta}{c(\bar{x})} - \left[\dfrac{1}{c_+^2(\bar{x})} - \dfrac{\sin^2\theta}{c^2(\bar{x})}\right]^{1/2}}{\dfrac{\cos\theta}{c(\bar{x})} + \left[\dfrac{1}{c_+^2(\bar{x})} - \dfrac{\sin^2\theta}{c^2(\bar{x})}\right]^{1/2}}. \tag{59}$$

From (59), $c_+(\bar{x})$ can easily be expressed as

$$c_+(\bar{x}) = \frac{c(\bar{x})}{\sqrt{1-4R\cos^2\theta/(1+R)^2}}. \tag{60}$$

V. CHARACTERIZATION OF VELOCITY SINGULARITY

To map more precisely the location of the reflector surface, it is useful to analyze the velocity singularity for the band-limited inverse problem. In mathematics, singularities are generally characterized by their Lipschitz exponents.

Definition 1: Let $0\leqslant\gamma\leqslant 1$. A function $f(x)$ is Lipschitz γ at x_0 if and only if there exists a constant k such that for all x in a neighborhood of x_0, we have

$$|f(x)-f(x_0)| \leqslant k|x-x_0|^r. \tag{61}$$

The function $f(x)$ is uniformly Lipschitz γ over an open interval (a,b) if and only if there exists a constant k such that (61) holds for any x, $x_0\in(a,b)$.

According to the Definition 1, if $f(x)$ is continuously differentiable at x_0, then it is Lipschitz $\gamma=1$. If $f(x)$ is discontinuous but bounded at x_0, for example, $f(x)$ is a step function at x_0, then its Lipschitz exponent $\gamma=0$.

In three dimensions, Lipschitz exponents are defined with a simple extension of Definition 1. Let $0\leqslant\gamma\leqslant1$ and $x\in R^3$. A function $f(x)$ is said to be Lipschitz γ at a given point $x_0\in R^3$, if and only if there exists $\delta>0$ as well as $k>0$ such that for any $x\in U(x_0,\delta)=\{x|x\in R^3,|x-x_0|<\delta\}$,

$$|f(x)-f(x_0)|\leqslant k\delta^{\gamma}. \tag{62}$$

If there exists a constant k such that (62) is satisfied for any points x_0 and x within an open set of R^3, the function $f(x)$ is uniformly Lipschitz γ over this open set.

From (12), the modulus of the multiscale operator at the scale s can be defined by

$$|W_s\alpha(x)|=\sqrt{|W_s^1\alpha(x)|^2+|W_s^2\alpha(x)|^2+|W_s^3\alpha(x)|^2}. \tag{63}$$

Based on (64), Jaffard's result in Ref. 6 can be extended as follows. Suppose that the wavelet $\psi^j(x)$, $j=1,2,3$, are continuously differentiable and $|\psi^j(x)|=0(1/(1+|x|^2))$, as $|x|\to\infty$. Then we have the following lemma.

Lemma 1: Let $0<\gamma<1$ and $f(x)\in L^2(R^3)$. A function $f(x)$ is uniformly Lipschitz γ over an open set A of R^3 if and only if there exists a constant $B>0$ such that for all $x\in A$, the modulus of the wavelet operator satisfies

$$|W_sf(x)|\leqslant Bs^{\gamma}. \tag{64}$$

The proof of this lemma is a simple extension of the proof of the Jaffard's result in Ref. 6.

Lemma 1 characterizes uniform Lipschitz exponents over an open set but not pointwise Lipschitz exponents. To study isolated singularities, however, according to Mallat's view in Ref. 5, Lemma 1 is sufficient. We shall say that a function has an isolated singularity as x_0 if there exists a neighborhood $U(x_0,\delta)$ of x_0, where the worst singularity is at x_0. In other words, the uniform Lipschitz regularity of the function over $U(x_0,\delta)$ is equal to the pointwise Lipschitz regularity at x_0.

Based on (22) in Theorem 1, (23) in Corollary 1, and (64) in Lemma 1, we obtain the following theorem.

Theorem 2: For the band-limited inverse problem (8), on the surface S in the Earth, the Lipschitz exponent γ of $\alpha(x)$ is not less than zero.

Particularly, at wide offset and even postcritical case, for the full band case by (26) and (27) in Corollary 2, and (64) in Lemma 1, we know that the Lipschitz exponent γ of $\alpha(x)$ is equal to zero on the surface S in the Earth. Hence, we have the following corollary.

Corollary 3: At wide offset and even postcritical case, for the full band case, the function $\alpha(x)$ is a step function and its discontinuity is on the surface S.

Theorem 2 and Corollary 3 show clearly the characterization of the velocity singularity, respectively, for band-limited and full-band input data. Using this information about the velocity singularity, we can easily suppress the effect of noise in real world data.

Because there always exists noise in the observed data, it is important to find a velocity inversion method which can suppress the noise.

First, let us consider the effects of noise in the data. Suppose that $u_s(x_g,x_s,\omega)$ in (8) is affected by $\hat{n}(\omega)$ and the observed data becomes $u_s(x_g,x_s,\omega)+\hat{n}(\omega)$; here $\hat{n}(\omega)$ is the Fourier transform of the noise $n(t)$. Then, the function $\alpha(x)$ in (8) correspondingly becomes $\bar{\alpha}(x)$, that is

$$\bar{\alpha}(x)=\alpha(x)+n_1(x). \tag{65}$$

In this equation,

$$n_1(x)=\int F(\omega)d\omega\int\int_{\Omega} d^2\xi B(x,\xi)\ \exp\{-i\omega\varphi(x,\xi)\}\hat{n}(\omega). \tag{66}$$

Equation (66) implies that the noise in the observed data should affect the function $\alpha(x)$ in (8). If $n(t)$ is real wide sense stationary white noise, by using the methods provided by Mallat in Ref. 5 we can calculate the Lipschitz exponent γ of $n_1(x)$ in (66). For a few special cases (for example, for the zero offset constant background case), we have known that the Lipschitz exponent γ of $n_1(x)$ in (66) is less than zero. That is to say, there exists a constant B_1 such that

$$|W_s n_1(x)|\leqslant B_1 s^{\gamma}. \tag{67}$$

In this equation, γ is less than zero.

Therefore, if we apply the wavelet operator W to (65), we obtain

$$W_s\bar{\alpha}=W_s\alpha(x)+W_s n_1(x). \tag{68}$$

Inequality (67) implies that $|W_s n_1(x)|$ should decrease when the scale s increases. On the other hand, by Theorem 2 and Lemma 1, the amplitude of $|W_s\alpha(x)|$ should decrease only when the scale s decreases. This means the $|W_s\alpha(x)|$ should increase or remain constant when the scale s increases. Hence, we can take advantage of the spatial coherence of the image of the velocity singular structure to suppress the effects of noise in observed data when the scale s increase.

VI. EXAMPLE AND DISCUSSION

Suppose surface S is a tilted plane and its equation is

$$x_1\sin\mu\cos\nu+x_2\sin\mu\sin\nu+x_3\cos\nu-h\cos\nu=0, \tag{69}$$

with speed $c(x)\equiv c_0$ above the plane, and speed $c_+(x)\equiv c_1$ below the plane. Let $\xi=(\xi_1,\xi_2,0)$ be a point on the Earth surface. Suppose a unit impulse is set off at the Earth surface. About this model, for the constant background (i.e., $c(x)\equiv c_0$) and zero-offset (i.e., $x_s\equiv x_g$, this implies $\cos\theta\equiv 1$), $\alpha(x)$ in (32) can be expressed as follows:

$$\alpha(x)=\frac{2R}{\pi}\int F(\omega)d(\omega)\ \frac{1}{i\omega}\exp\{2i\omega[(-x_1\cos\nu-x_2\sin\nu)\sin\mu+(h-x_3)\cos\nu]/c_0\}.$$

Here $R=(c_1-c_0)/(c_1+c_0)$.

One obtains

$$|W_s\alpha(x)|=\frac{8sR}{\pi c_0}\exp\left\{-\frac{b^2}{4a}\right\}\left|\int_{\omega_0}^{\omega_1}\exp(-a\omega^2)d\omega+z(a,b,\omega_0,\omega_1)\right|. \tag{70}$$

Here $a=2s^2/c_0$, $b=2[(-x_1\cos\nu-x_2\sin\nu)\sin\mu+(h-x_3)\cos\nu]/c_0$, and $z(a,b,\omega_0,\omega_1)$ satisfies (45) and (46).

By (70), we can easily show that

$$\max|W_s\alpha(x)|=\frac{8sR}{\pi c_0}\int_{\omega_1}^{\omega_0}\exp(-a\omega^2)d\omega,$$

if and only if $b=0$.

This implies that only for the point $x=(x_1,x_2,x_3)$ on the tilted plane S is the value of $|W_s\alpha(x)|$ maximum.

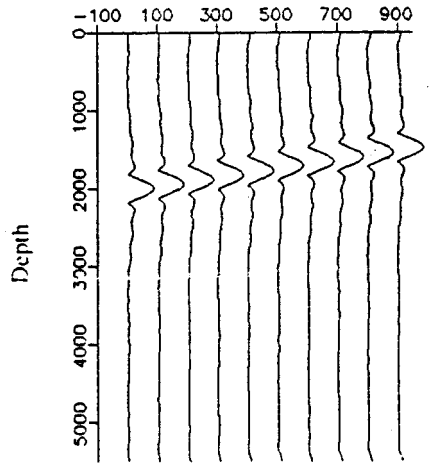

FIG. 1. A 6–50-Hz bandwidth representation of $|W_s\alpha(x)|$, scale $s=2^1$.

Here we simply describe the numerical procedure to calculate $W_s\alpha(x)$.

(1) By use of fast Fourier transform and the inverse Fourier transform, the calculations of $\alpha(x)$ can be carried out from the input data $u_s(\xi,t)$. The details can be found, for instance, in Ref. 7.
(2) By use of fast wavelet transform, which can be found in Ref. 5 or Ref. 8, we can calculate $W_s\alpha(x)$.
(3) Choose the maximum of $|W_s\alpha(x)|$ to detect the location of the reflector surface.

In (69), let $\mu=30°$, $\nu=0$, $h=2000$ m, $c_0=4500$ m/s, and $c_1=5500$ m/s. Figure 1 shows that the image of the reflector plane produced by max $|W_s\alpha(x)|$ corresponds to the plane S correctly. Furthermore, we add the real white noise to input data $u_s(\xi,t)$ and the peak amplitude of the noise is three-fifths of the peak amplitude of the signal. The image produced by $\partial\alpha/\partial n$ is shown in Fig. 2. The effects of the noise in Fig. 2 are apparent, and we cannot know the location of the planar

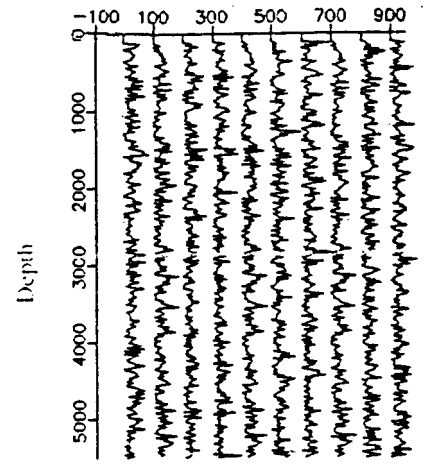

FIG. 2. Adding real white noise to input data, a 6–50-Hz bandwidth depth section determined by $\partial\alpha/\partial n$.

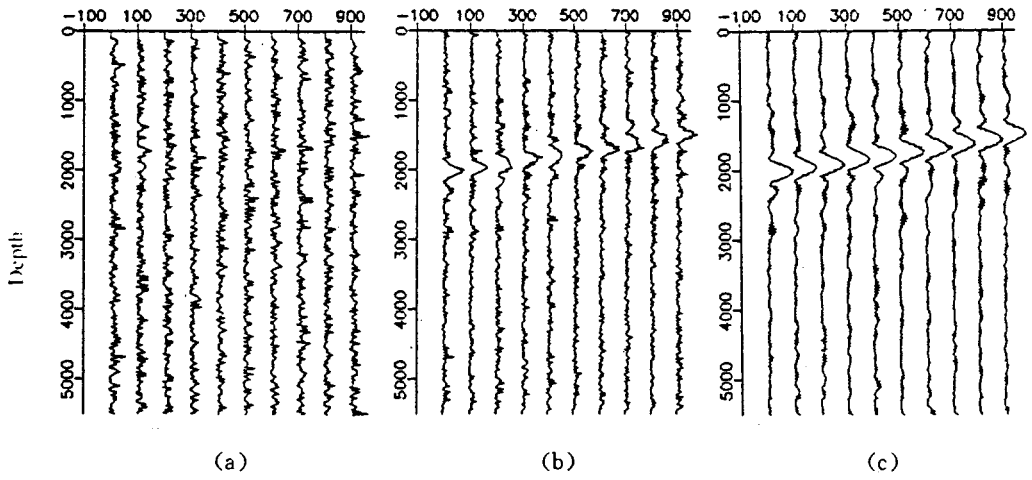

FIG. 3. (a)–(c) Adding real white noise to input data, 6–50-Hz bandwidth depth section determined by $|W_s\overline{\alpha}(x)|$ under scales s taking 2^0, 2^1, and 2^3, respectively.

reflector nor how many reflectors there are. However, in Fig. 3(a)–3(c), the images produced by $|W_s\alpha(x)|$ are far more desirable. As the scale s increases, the image of the reflector becomes progressively cleaner. However, the scale s should stay in a suitable range for seismic data because of spatial resolution being lost for increasing scale. Detailed analysis of how to choose the scale s can be found in Ref. 8. Here we give an example only to demonstrate the effectiveness of the results in this paper.

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Feynman–Kac kernels in Markovian representations of the Schrödinger interpolating dynamics

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Probabilistic solutions of the so-called Schrödinger boundary data problem provide for a unique Markovian interpolation between any two strictly positive probability densities designed to form the input–output statistics data for the process taking place in a finite-time interval. The key issue is to select the jointly continuous in all variables positive Feynman–Kac kernel, appropriate for the phenomenological (physical) situation. We extend the existing formulations of the problem to cases when the kernel is *not* a fundamental solution of a parabolic equation, and prove the existence of a continuous Markovian interpolation in this case. Next, we analyze the compatibility of this stochastic evolution with the original parabolic dynamics, which is assumed to be governed by the temporally adjoint pair of (parabolic) partial differential equations, and prove that the pertinent random motion is a diffusion process. In particular, in conjunction with Born's statistical interpretation postulate in quantum theory, we consider stochastic processes which are compatible with the Schrödinger picture quantum evolution. © *1996 American Institute of Physics.* [S0022-2488(96)00702-9]

I. MOTIVATION: SCHRÖDINGER'S INTERPOLATION PROBLEM THROUGH FEYNMAN–KAC KERNELS

The issue of *deriving* a microscopic dynamics from the (phenomenologically or numerically motivated, by approximating the frequency distributions) input–output statistics data was addressed, as the Schrödinger problem of a probabilistic interpolation, in a number of publications.[1–10] We shall consider Markovian propagation scenarios so remaining within the well-established framework, where for any two Borel sets $A,B\subset R$ on which the respective strictly positive boundary densities $\rho(x,0)$ and $\rho(x,T)$ are defined, the transition probability $m(A,B)$ from the set A to the set B in the time interval $T>0$ has a density given in a specific factorized form:

$$m(x,y)=f(x)k(x,0,y,T)g(y), \quad m(A,B)=\int_A dx\int_B dy m(x,y), \tag{1}$$

$$\int dy m(x,y)=\rho(x,0), \quad \int dx m(x,y)=\rho(y,T).$$

Here, $f(x),g(y)$ are the *a priori* unknown functions, which come out as solutions of the integral (Schrödinger) system of equations (1), provided that in addition to the density boundary data we have in hand any strictly positive, continuous in-space variables *function* $k(x,0,y,T)$. Our notation makes explicit the dependence (in general irrelevant) on the time interval endpoints. It anticipates an important restriction we shall impose, that $k(x,0,y,T)$ must be a strongly continuous dynamical semigroup kernel: it will secure the Markov property of the sought after stochastic process.

It is the major mathematical discovery[4] that, without the semigroup assumption *but* with the prescribed, nonzero boundary data $\rho(x,0)$, $\rho(y,T)$ *and* with the strictly positive continuous func-

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tion $k(y,0,x,T)$, the Schrödinger system (1) of integral equations admits a unique solution in terms of two nonzero, locally integrable functions $f(x),g(y)$ of the same sign (positive, everything is up to a multiplicative constant).

If $k(y,0,x,T)$ is a particular, confined to the time interval endpoints, form of a concrete semigroup kernel $k(y,s,x,t),0\leqslant s\leqslant t<T$, let it be a fundamental solution associated with (5) (whose existence *a priori* is *not* granted), then there exists[5,7,8,9,10] a function $p(y,s,x,t)$:

$$p(y,s,x,t)=k(y,s,x,t)\,\frac{\theta(x,t)}{\theta(y,s)}, \tag{2}$$

where

$$\theta(x,t)=\int dy k(x,t,y,T)g(y), \quad \theta_*(y,s)=\int dx k(x,0,y,s)f(x) \tag{3}$$

which implements a consistent propagation of the density $\rho(x,t)=\theta(x,t)\theta_*(x,t)$ between its boundary versions, according to

$$\rho(x,t)=\int p(y,s,x,t)\rho(y,s)dy, \quad 0\leqslant s<t\leqslant T. \tag{4}$$

For a given semigroup which is characterized by its generator (Hamiltonian), the kernel $k(y,s,x,t)$ and the emerging transition probability density $p(y,s,x,t)$ are unique in view of the uniqueness of solutions $f(x),g(y)$ of (1). For Markov processes, the knowledge of the transition probability density $p(y,s,x,t)$ for all intermediate times $0\leqslant s<t\leqslant T$ suffices for the derivation of all other relevant characteristics.

In the framework of the Schrödinger problem the choice of the integral kernel $k(\dot{y},0,x,T)$ is arbitrary, except for the strict positivity and continuity demand. As long as there is no ''natural'' physical motivation for its concrete functional form, the problem is abstract and of no direct physical relevance.

However, in the context of parabolic partial differential equations this ''natural'' choice is automatically settled if the Feynman–Kac formula can be utilized to represent solutions. Indeed, in this case an unambiguous strictly positive semigroup kernel, which is a continuous function of its arguments, can be introduced for a broad class of (admissible[11]) potentials. Time-dependent potentials are here included as well.[12,13] Moreover, in Ref. 8 we have discussed a possible phenomenological significance of the Feynman–Kac potentials, as contrasted to the usual identification of Smoluchowski drifts with force fields affecting particles (up to a coefficient) in the standard theory of stochastic diffusion processes.

In the existing probabilistic investigations,[5,6,8,9,14] based on the exploitation of the Schrödinger problem strategy, it was generally assumed that the kernel actually *is* a fundamental solution of the parabolic equation. It means that the kernel is a function with continuous derivatives: first order with respect to time, second order with respect to space variables. Then, the transition probability density defined by (2) is a fundamental solution of the Fokker–Planck (second Kolmogorov) equation in the pair x,t of variables, and as such is at the same time a solution of the backward (first Kolmogorov) equation in the pair y,s. This feature was exploited in Refs. 8 and 9.

There are a number of mathematical subtleties involved in the fundamental solution notion, since, in this case, the Feynman–Kac kernel must be a solution of the parabolic equation itself. In general, Feynman–Kac kernels may have granted the existence status, even as continuous functions,[11,13,15] but may not be differentiable, and need not be solutions of any conceivable partial differential equations.

To our knowledge, this complication in the study of Markovian representations of the Schrödinger interpolating dynamics (and the quantum Schrödinger picture dynamics in particular) has never been addressed in the literature. Moreover, it is far from being obvious that this Markovian interpolation actually *is* a diffusion process.

II. SCHRÖDINGER'S INTERPOLATION PROBLEM: GENERAL DERIVATION OF THE STOCHASTIC EVOLUTION

A. The Schrödinger system of integral equations

We shall complement our previous analysis[8,9] by discussing the issue in more detail. It turns out the crucial step lies in a *proper* choice of the strictly positive and continuous function $k(y,s,x,t), s<t$, which, if we want to construct a Markov process, has to satisfy the Chapman–Kolmogorov (semigroup composition) equation. To proceed generally, let us consider a pair of partial differential equations for real functions $u(x,t)$ and $v(x,t)$:

$$\partial_t u(x,t)=\Delta u(x,t)-c(x,t)u(x,t),$$

$$\partial_t v(x,t)=-\Delta v(x,t)+c(x,t)v(x,t), \tag{5}$$

where we have eliminated all unnecessary dimensional parameters.

Usually,[11,15] $c(x,t)$ is assumed to be a continuous and bounded-from-below function. We shall adopt weaker conditions. Namely, let us decompose $c(x,t)$ into a sum of positive and negative terms: $c(x,t)=c_+(x,t)-c_-(x,t)$, $c_\pm\geqslant 0$, where (a) $c_-(x,t)$ is bounded, while (b) $c_+(x,t)$ is bounded on compact sets of $R\times[0,\ T]$. It means that $c(x,t)$ is bounded from below and locally bounded from above. Clearly, $c(x,t)$ need not be a continuous function and then we encounter weak solutions of (5) which admit discontinuities.

With the first (forward) equation (5) we can immediately associate an integral kernel of the time-dependent semigroup (the exponential operator should be understood as the time-ordered expression):

$$k(y,s,x,t)=\left[\exp\left(-\int_s^t H(\tau)d\tau\right)\right](y,x), \tag{6}$$

where $H(\tau)=-\Delta+c(\tau)$. It is clear that for discontinuous $c(x,t)$, no fundamental solutions are admitted by (5).

By the Feynman–Kac formula,[12,13] we obtain

$$k(y,s,x,t)=\int \exp\left[-\int_s^t c(\omega(\tau),\tau)d\tau\right]d\mu_{(x,t)}^{(y,s)}(\omega), \tag{7}$$

where $d\mu_{(x,t)}^{(y,s)}(\omega)$ is the conditional Wiener measure over sample paths of the standard Brownian motion.

It is well known that k is strictly positive in case of $c(x,t)$, which is continuous and bounded from below; typical proofs are given under an additional assumption that c does not depend on time.[15] However, our assumptions about $c(x,t)$ were weaker, and to see that nonetheless k is strictly positive we shall follow the idea of Theorem 3.3.3 in Ref. 15. Namely, the conditional Wiener measure $d\mu_{(x,t)}^{(y,s)}$ can be written as follows

$$d\mu_{(x,t)}^{(y,s)}=[4\pi(t-s)]^{-1/2}\exp\left[-\frac{(x-y)^2}{4(t-s)}\right]d\nu_{(x,t)}^{(y,s)}, \tag{8}$$

where $d\nu_{(x,t)}^{(y,s)}$ is the normalized Wiener measure.[11] We can always choose a certain number $r>0$ to constrain the event (sample path) set

$$\Omega(r)=[\omega: X_s(\omega)=y, X_t(\omega)=x, \sup_{s\leqslant\tau\leqslant t}|X_\tau(\omega)|\leqslant r]. \tag{9}$$

It comprises these sample trajectories which are bounded by r on the time interval $[s,\ t]$. In the above, $X_t(\omega)$ is the value taken by the random variable $X(t)$ at time t, while a concrete ωth path is sampled. By properly tuning r, we can always achieve

$$\int_{\Omega(r)} d\nu_{(x,t)}^{(y,s)} \geqslant \frac{1}{2}, \tag{10}$$

which implies that

$$k(y,s,x,t)\geqslant \frac{1}{2}\,[4\pi(t-s)]^{-1/2}\exp\left[-\frac{(x-y)^2}{4(t-s)}\right]\exp[-(t-s)C]>0,$$
$$C=\sup_{s\leqslant\tau\leqslant t,\,\omega\in\Omega(r)} c_+(X_\tau(\omega),\tau), \tag{11}$$

where, by our assumptions, c_+ is bounded on compact sets. Consequently, the kernel k is *strictly positive*.

With the Schrödinger boundary data problem in mind, we must settle an issue of the *continuity* of the kernel. To this end, let us invoke a well-known procedure of rescaling of path integrals:[11,16] by passing from the ''unscaled'' sample paths $\omega(t)$-over which the conditional Wiener measure integrates, to the ''scaled'' paths of the Brownian bridge, the (y,x) conditioning can be taken away from the measure. Then, instead of sample paths ω connecting points y and x in the time interval $t-s>0$, we consider the appropriately ''scaled'' paths of the Brownian bridge α connecting the point 0 with 0 again, in the (scaled) time 1. It is possible, in view of the decomposition:[11,16]

$$\omega(\tau)=\left(\frac{t}{t-s}-\frac{\tau}{t-s}\right)y+\left(\frac{\tau}{t-s}-\frac{s}{t-s}\right)x+\sqrt{t-s}\,\alpha\left(\frac{\tau}{t-s}-\frac{s}{t-s}\right), \tag{12}$$

where α stands for the ''scaled'' Brownian bridge. Then, we can write

$$k(y,s,x,t)=[4\pi(t-s)]^{-1/2}\exp\left[-\frac{(x-y)^2}{4(t-s)}\right]\int d\mu(\alpha)$$
$$\times\exp\left[-\int_s^t c\left(\frac{t-\tau}{t-s}\,y+\frac{\tau-s}{t-s}\,x+\sqrt{t-s}\,\alpha\left(\frac{\tau-s}{t-s}\right),\tau\right)d\tau\right], \tag{13}$$

where $d\mu(\alpha)=d\nu_{(0,1)}^{(0,0)}(\omega)$ is the normalized Wiener measure integrating with respect to the ''scaled'' Brownian bridge paths, which begin and terminate at the origin 0 in-between ''scaled time'' instants: 0 corresponding to $\tau=s$ and 1 corresponding to $\tau=t$.

This representation of k, *if* combined with the assumption that $c(x,t)$ is a continuous function, allows us to conclude[11] that the kernel is continuous in all variables. However, our previous assumptions were weaker, and it is instructive to know that through suitable approximation techniques, Theorem B.7.1 in Ref. 13 proves that the kernel is jointly continuous in our case as well.

It is also clear that $k(y,s,x,t)$ satisfies the Chapman–Kolmogorov composition rule. So, the first equation (5) can be used to define the Feynman–Kac kernel, appropriate for the Schrödinger problem analysis in terms of a Markov stochastic process.

Let us consider an arbitrary (at the moment) pair of strictly positive, but not necessarily continuous, boundary densities $\rho_0(x)$ and $\rho_T(x)$. By Jamison's principal theorem[4] there exists a

unique pair of strictly positive, locally (i.e., on compact sets) integrable functions $f(x)$ and $g(x)$ solving the Schrödinger system (1), e.g., such that $\rho_0(x)=f(x)\int k(x,0,y,T)g(y)dy$ and $\rho_T(x)=g(x)\int k(y,0,x,T)f(y)dy$ with the kernel $k(y,s,x,t)$ given by (7).

Let us define

$$g(x,t)=\int k(x,t,y,T)g(y)dy, \quad f(x,t)=\int k(y,0,x,t)f(y)dy. \tag{14}$$

The above integrals exist at least for almost every x so that there appears the problem of the existence of a unique and continuous transition probability density $p(y,s,x,t)$ [Eq. (2)]. We shall assume that the function $g(y)$ is bounded at infinity. This means that there exists a constant $C>0$ and a compact set $K\subset R$ such that $g(y)\leqslant C$ for all $y\in R\backslash K$. Then, for all $t<T$ and any sequences $h_n\to 0$, $s_n\to 0$, as $n\to\infty$ we obtain (lim stands for $\lim_{n\to\infty}$)

$$\begin{aligned}\lim|g(x+h_n,t+s_n)-g(x,t)| &\leqslant \lim\left|\int_K [k(x+h_n,t+s_n,y,T)-k(x,t,y,T)]g(y)dy\right| \\ &\quad +\lim\left|\int_{R\backslash K}[k(x+h_n,t+s_n,y,T)-k(x,t,y,T)]g(y)dy\right| \\ &\leqslant \lim\sup_{y\in K}|k(x+h_n,t+s_n,y,T)-k(x,t,y,T)|\int_K g(y)dy \\ &\quad +C\lim\int_{R\backslash K}|k(x+h_n,t+s_n,y,T)-k(x,t,y,T)|dy. \end{aligned}\tag{15}$$

The first term tends to zero because k is jointly continuous and g is locally integrable. The second one tends to zero because of the Lebesgue bounded convergence theorem. Consequently, our assumption suffices to make $g(x,t)$ continuous on $R\times[0,T)$. Similarly, we can prove that $g(x,t)$ is bounded.

Now, we can set, according to (2), $p(y,s,x,t)=k(y,s,x,t)g(x,t)/g(y,s)$. Then, $p(y,s,x,t),0\leqslant s<t\leqslant T$, becomes a transition probability density of a Markov stochastic process with a factorized density $\rho(x,t)=f(x,t)g(x,t)$. Clearly, this stochastic process interpolates between the boundary data ρ_0 and ρ_T as time continuously varies from 0 to T. Notice that (15) implies the continuity of p in the time interval $[0,T)$.

Although $p(y,s,x,t)$ is continuous in all variables, we cannot be sure that the interpolating stochastic process has continuous trajectories, and no specific (e.g., Fokker–Planck) partial differential equation can be readily associated with this dynamics. Therefore, we must explicitly verify whether the associated process is stochastically continuous. If so, we should know whether it is continuous (i.e., admits continuous trajectories). Eventually, we should check the validity of conditions under which the investigated interpolation can be regarded as a diffusion process. The subsequent analysis will prove that this ultimate goal results only due to the gradual strengthening of conditions imposed on the parabolic system (5).

B. Stochastic continuity of the process

Apart from the generality of formulation of the Schrödinger interpolation problem, which appears to preclude an unambiguous identification (diffusion or not) of the constructed stochastic process, we can prove in the present case a fundamental property of a stochastic dynamics called a stochastic continuity of the process. In this connection, compare, e.g., Refs. 5, 17 and 18, where

this property is linked to the uniqueness of the corresponding Markov semigroup generator. The stochastic continuity property is a necessary condition for the process to admit continuous trajectories.

The stochastic process is stochastically continuous, if for the probability of the occurrence of sample paths ω, such that the random variable values $X_t(\omega)$ along the trajectory obey $|X_t(\omega)-X_s(\omega)|\geqslant\epsilon$, $s<t$, the following limiting behavior is recovered:

$$\lim_{t\downarrow s} P[\omega:|X_t(\omega)-X_s(\omega)|\geqslant\epsilon]=0 \tag{16}$$

for every positive ϵ. This demand can be written in a more handy way in terms of the transition probability density $p(y,s,x,t)$ and the density $\rho(x,t)$ of the process:

$$\lim_{t\downarrow s}\left[\int_{-\infty}^{+\infty} dy\rho(y,s)\int_{|x-y|\geqslant\epsilon} p(y,s,x,t)dx\right]=0. \tag{17}$$

So, for the transition density to be stochastically continuous, it suffices that

$$\lim_{\Delta s\downarrow 0}\int_{|x-y|\geqslant\epsilon} p(y,s,x,s+\Delta s)dx=0 \tag{18}$$

for almost every $y\in R$.

In view of our construction [Eq. (2)], we have

$$\lim_{\Delta s\downarrow 0}\int_{|x-y|\geqslant\epsilon} p(y,s,x,s+\Delta s)dx=\frac{1}{g(y,s)}\lim_{\Delta s\downarrow 0}\int_{|x-y|\geqslant\epsilon} dxk(y,s,x,s+\Delta s)\times\int_{-\infty}^{+\infty} k(x,s+\Delta s,z,T)g(z)dz. \tag{19}$$

By changing the order of integrations (allowed by positivity of the involved functions) we obtain

$$\lim_{\Delta s\downarrow 0}\int_{|x-y|\geqslant\epsilon} p(y,s,x,s+\Delta s)dx=\frac{1}{g(y,s)}\lim_{\Delta s\downarrow 0}\int_{-\infty}^{+\infty} dzg(z)\times\left[\int_{|x-y|\geqslant 0} dxk(y,s,x,s+\Delta s)k(x,s+\Delta s,z,T)\right]. \tag{20}$$

Because the potential is bounded from below, $c\geqslant -M$ for some $M>0$, we easily arrive at the estimates (use the ''scaled'' Brownian bridge argument)

$$k(y,s,x,s+\Delta s)\leqslant(4\pi\Delta s)^{-1/2}\exp\left[-\frac{(x-y)^2}{4\Delta s}\right]\exp(M\Delta s) \tag{21}$$

and

$$k(x,s+\Delta s,z,T)\leqslant[4\pi(T-s-\Delta s)]^{-1/2}\exp\left[-\frac{(z-x)^2}{4(T-s-\Delta s)}\right]\exp[M(T-s-\Delta s)]. \tag{22}$$

Then we obtain

$$0 \leqslant \lim_{\Delta s \downarrow 0} \int_{|x-y| \geqslant \epsilon} k(y,s,x,s+\Delta s) k(x,s+\Delta s,z,T) dx$$
$$\leqslant [4\pi(T-s)]^{-1/2} \exp[M(T-s)] \lim_{\Delta s \downarrow 0} (4\pi \Delta s)^{-1/2}$$
$$\times \int_{|x-y| \geqslant \epsilon} dx \, \exp\left[- \frac{(x-y)^2}{4\Delta s} \right] \exp\left[- \frac{(z-x)^2}{4(T-s-\Delta s)} \right] = 0. \tag{23}$$

So, by the classic Lebesgue bounded (dominated) convergence theorem, the required limiting property $\lim_{\Delta s \to 0} \int_{|x-y| \geqslant \epsilon} p(y,s,x,s+\Delta s) dx = 0$ follows and (16) holds true.

As mentioned before, the stochastic continuity of the Markov process is a necessary condition for the process to be continuous in a more pedestrian sense, i.e., to admit continuous sample paths. However, it is insufficient. Hence, additional requirements are necessary to allow for a standard diffusion process realization of solutions of the general Schrödinger problem [Eqs. (1)–(3)].

In the next section we shall prove that our process can be regarded as continuous, by requiring a certain correlation between the kernel $k(y,s,x,t)$ and a function $g(x,t)$ [Eq. (14)].

C. Continuity of the process

It is well known that a solution of a parabolic equation cannot tend to zero arbitrarily fast, when $|x| \to \infty$.[19] Roughly speaking, it cannot fall off faster than a fundamental solution (provided it exists). In fact, the solution is known to fall off as fast as the fundamental solution, when the initial boundary data coincide with the Dirac measure. If a support of the initial data is spread (i.e., not pointwise), then the solution falloff is slower than this of the fundamental one.

In our discussion, where $g(x,t)$ is a generalized solution and $k(y,s,x,t)$ is a Feynman–Kac kernel which does not need to be a fundamental solution, we expect a similar behavior. Mathematically, our demand will be expressed as follows. Let $t-s$ be small and K be a compact subset in R. Because $g(x,t)$ is supported on the whole R, in the decomposition

$$g(y,s) = \int_K k(y,s,x,t) g(x,t) dx + \int_{R \setminus K} k(y,s,x,t) g(x,t) dx, \tag{24}$$

the second term becomes relevant when $|y| \to \infty$. It amounts to [in the denominator there appears $g(y,s)$]

$$\lim_{|y| \to \infty} \frac{\int_{-\infty}^{+\infty} k(y,s,x,t) g(x,t) \chi_K(x) dx}{\int_{-\infty}^{+\infty} k(y,s,x,t) g(x,t) dx} = 0, \tag{25}$$

where χ_K is an indicator function of the set K, which equals one for $x \in K$ and zero otherwise.

By means of the transition probability density $p(y,s,x,t)$ let us introduce a transformation

$$(T_s^t f\ )(y) = \int_{-\infty}^{+\infty} p(y,s,x,t) f(x) dx. \tag{26}$$

of a function $f(x)$, continuous and vanishing at infinity (we shall use an abbreviation $f \in C_\infty(R)$ to express this fact). It is clear that $(T_s^t f\ )(x)$ is a continuous function. For a suitable compact set K we can always guarantee the property $|f(x)| < \epsilon$ for every $x \in R \setminus K$. Then, if we exploit the property $\int_{R \setminus K} p(y,s,x,t) dx \leqslant 1$ if $s < t$ and the definition of p in terms of k and g, we arrive at

$$|(T_s^t f)(y)| \leqslant \int_K p(y,s,x,t) |f(x,t)| dx + \int_{R \setminus K} p(y,s,x,t) |f(x,t)| dx$$

$$\leqslant\left[\int_K p(y,s,x,t)dx\right]\int_K|f(x,t)|dx+\sup_{x\in R\setminus K}|f(x,t)|\int_{R\setminus K}p(y,s,x,t)dx$$

$$\leqslant\left[\int_K|f(x,t)|dx\right]\frac{\int_K k(y,s,x,t)g(x,t)dx}{\int_{-\infty}^{+\infty}k(y,s,x,t)g(x,t)dx}+\epsilon. \tag{27}$$

It implies that for small $t-s$, $\lim_{|y|\to\infty}(T_s^t f\,)(y)=0$, and so T_s^t forms an inhomogeneous-in-time semigroup of positive contractions on $C_\infty(R)$. For arbitrary t and s the result follows by the obvious decomposition property $T_s^t = T_s^{s_1}T_{s_1}^{s_2}\cdots T_{s_n}^t$. In the well-established terminology, our $p(y,s,x,t)$ is a C_∞-Feller transition function and leads to a regular Markov process.[17] Moreover, by the stochastic continuity of $p(y,s,x,t), T_s^t$ is strongly continuous.

As yet, we do not know whether the process itself is continuous, i.e., has continuous sample paths. To this end, it suffices to check whether the so-called ''Dynkin condition,''[20]

$$\lim_{t\downarrow s}\frac{1}{t-s}\sup_{y\in K}\left[\int_{|x-y|>\epsilon}p(y,s,x,t)dx\right]=0, \tag{28}$$

is valid for every $\epsilon>0$ and every compact set K. We have [remember that $g(x,t)$ is strictly positive, continuous and bounded]

$$\sup_{y\in K}\int_{|x-y|>\epsilon}p(y,s,x,t)dx=\sup_{y\in K}\frac{1}{g(y,s)}\int_{|x-y|>\epsilon}k(y,s,x,t)g(x,t)dx$$

$$\leqslant\frac{\sup_x g(x,t)}{\inf_{y\in K}g(y,s)}\int_{|x-y|>\epsilon}k(y,s,x,t)dx\leqslant C\int_{|x-y|>\epsilon}k_0(x-y,t-s)dx, \tag{29}$$

where [compare, e.g., the previous estimate (22)]

$$C=\frac{\sup_x g(x,t)}{\inf_{y\in K}g(y,s)}\exp[M(t-s)] \tag{30}$$

and $k_0(x-y,t-s)$ is the heat kernel.

Finally, we arrive at

$$\lim_{t\downarrow s}\frac{1}{t-s}\sup_{y\in K}\left[\int_{|x-y|>\epsilon}p(y,s,x,t)dx\right]\leqslant C\lim_{t\downarrow s}\frac{1}{t-s}\int_{|z|>\epsilon}k_0(z,t-s)dz=0. \tag{31}$$

So, the stochastic process we are dealing with is continuous. Interestingly, ''a continuous in time parameter stochastic process, which possesses the (strong) Markov property and for which the sample paths $X(t)$ are almost always (i.e., with probability one) continuous functions of t, is called a diffusion process,'' see, e.g., Ch. 15 of Ref. 20.

D. The interpolating stochastic dynamics: Compatibility with the temporally adjoint parabolic evolutions

The formulas (14) determine what is called[12] the generalized solution of a parabolic equation: it admits functions which are not necessarily continuous and if continuous, then not necessarily differentiable. Previously, we have established the continuity of the generalized solution $g(x,t)$

under the rather mild assumption about the behavior of $g(x)$ at spatial infinity. In fact, the same assumption works for $f(x,t)$. However, nothing has been said about the differentiability of $f(x,t)$ and $g(x,t)$.

Consequently, our reasoning seems to be somewhat divorced from the original partial differential equations (5), for which we can take for granted that certain solutions $u(x,t)$ and $v(x,t)$ exist in the time interval $0\leqslant t\leqslant T$. For this, we must assume that $c(x,t)$ is a continuous function.

Let us consider the solutions of (5) that are bounded functions of their arguments. It is instructive to point out that we do not impose any restrictions on the growth of $c(x,t)$ when $|x|\to\infty$, and consequently we do not assume that solutions of parabolic equations (5) have bounded derivatives. Then,[12] the solution $u(x,t)$ of the forward parabolic equation (5) is known to admit the Feynman–Kac representation with the integral kernel (7) and (13), where

$$u(x,t)=\int k(y,s,x,t)u(y,s)dy \tag{32}$$

for $0\leqslant s<t\leqslant T$. At this point let us define

$$U(x,t)=v(x,T-t) \tag{33}$$

for all $t\in[0,\ T]$ and observe that, as a consequence of the time-adjoint equation (5) for which $v(x,t)$ is a solution, the newly introduced function $U(x,t)$ solves the forward equation (5):

$$\partial_t U(x,t)=\Delta U(x,t)-c(x,T-t)U(x,t) \tag{34}$$

with a slightly rearranged potential: $c(x,t)\to c(x,T-t)$. By the assumed boundedness of the solution $v(x,t)$ of (5), we arrive at the Feynman–Kac formula

$$U(x,t)=\int K(y,s,x,t)U(y,s)dy \tag{35}$$

with the corresponding kernel $K(y,s,x,t)$ of the (time ordering implicit) operator $\exp[-\int_s^t H(T-\tau)d\tau]$, where $H(T-\tau)=-\Delta+c(T-\tau)$. Let us emphasize that in the case of the time-independent potential, $c(x,t)=c(x)$ for all $0\leqslant t\leqslant T$, the kernel K coincides with k.

The previous Brownian bridge argument (12) and (13) retains its validity, and we have

$$K(y,s,x,t)=[4\pi(t-s)]^{-1/2}\exp\left[-\frac{(x-y)^2}{4(t-s)}\right]\int d\mu(\alpha)$$
$$\times\exp\left[-\int_s^t c\left(\frac{t-\tau}{t-s}\,y+\frac{\tau-s}{t-s}\,x+\sqrt{t-s}\,\alpha\left(\frac{\tau-s}{t-s}\right),T-\tau\right)d\tau\right], \tag{36}$$

which, after specializing to the case of $s=0$, $t=T$ and accounting for the invariance of the Brownian bridge measure with respect to the replacement of sample paths $\omega(\tau)$ by sample paths $\omega(T-\tau)$,[7,21] gives rise to

$$K(y,0,x,T)=(4\pi T)^{-1/2}\exp\left[-\frac{(x-y)^2}{4T}\right]\int d\mu(\alpha)$$
$$\times\exp\left[-\int_0^T c\left(\frac{\sigma}{T}\,y+\left(1-\frac{\sigma}{T}\right)x+\sqrt{T}\,\alpha\left(\frac{\sigma}{T}\right),\sigma\right)d\sigma\right], \tag{37}$$

where $\sigma=T-\tau$.

A comparison of (37) with (13) proves that we have derived an identity

$$K(y,0,x,T)=k(x,0,y,T) \tag{38}$$

whose immediate consequence is the formula

$$U(x,T)=v(x,0)=\int k(x,0,y,T)v(y,T)dy \tag{39}$$

for the backward propagation of $v(y,T)$ into $v(x,0)$.

We shall utilize (39) and (32), under an *additional* assumption that the previous, hitherto arbitrary, probability density data $\rho_0(x),\rho_T(x)$ actually are determined by the initial and terminal values of the solutions $u(x,t),v(x,t)$ of (5) according to

$$\rho_0(x)=u(x,0)v(x,0), \quad \rho_T(x)=u(x,T)v(x,T). \tag{40}$$

Our present aim is to show that with this assumption, we can identify the (still abstract) functions $f(x,t),g(x,t)$, (14), with $u(x,t)$ and $v(x,t)$, respectively. By (32) and (39) there holds

$$\begin{aligned}\rho_0(x)&=u(x,0)\int k(x,0,y,T)v(y,T)dy,\\ \rho_T(x)&=v(x,T)\int k(y,0,x,T)u(y,0)dy\end{aligned} \tag{41}$$

and, in view of the uniqueness of solution of the Schrödinger system, once the boundary densities and the continuous strictly positive kernel are specified, we realize that the propagation formulas (14) involve solutions of (5) through the respectively initial and terminal data:

$$f(x)=u(x,0), \quad g(x)=v(x,T). \tag{42}$$

Moreover, (5) and (14) imply that $f(x,t)=u(x,t)$ holds true identically for all $t\in[0,\,T]$.

What remains to be settled is whether the function $g(x,t)$ can be identified with the solution $v(x,t)$ of (5) for all $t\in[0,T]$.

This property is obvious, when the time-independent potential $c(x)$ is investigated instead of the more general $c(x,t)$. Also, the identification is with no doubt in the case when $k(y,s,x,t)$ is a fundamental solution of the parabolic equation in variables x,t. In this case, $k(y,s,x,t)$ is a unique solution of the system (5), and solves the adjoint equation in variables y,s.[22–24] Then, because $f(x),g(x)$ are locally integrable, an immediate consequence is[25] that $f(x,t)$ and $g(x,t)$ are positive solutions of (5). The identification of them with $u(x,t)$ and $v(x,t)$, respectively, follows from the uniqueness of positive solutions.[23]

Let us begin from a minor generalization of (22) and define

$$U_s(x,t)=v(x,T+s-t), \quad t\in[s,T]. \tag{43}$$

Clearly, a parabolic equation (34) is satisfied by $U_s(x,t)$, if instead of $c(x,T-t)$, the potential $c(x,T+s-t)$ is introduced. An immediate propagation formula follows:

$$U_s(x,t)=\int K_s(y,s,x,t)U_s(y,s)dy. \tag{44}$$

The integral kernel K_s differs from the previous K, (36), in the explicit time dependence of the potential $c(x,T-\tau)\to c(x,T+s-\tau)$. By putting $T=t$ in (44) we obtain

$$v(x,s)=\int K_s(y,s,x,T)v(y,T)dy, \tag{45}$$

and by the previous part of our demonstration we know that

$$g(x,s)=\int k(x,s,y,T)v(y,T)dy. \tag{46}$$

At this point, it is enough to prove that the identity [cf. (38)]

$$K_s(y,s,x,T)=k(x,s,y,T) \tag{47}$$

takes place for any s; $0\leqslant s\leqslant T$.

Let us exploit the Brownian bridge scaling (13) again, so that

$$k(x,s,y,T)=[4\pi(T-s)]^{-1/2}\exp\left[-\frac{(x-y)^2}{4(T-s)}\right]\int d\mu(\alpha)$$
$$\times\exp\left[-\int_s^T c\left(\frac{T-\tau}{T-s}x+\frac{\tau-s}{T-s}y+\sqrt{T-s}\,\alpha\left(\frac{\tau-s}{T-s}\right),\tau\right)d\tau\right], \tag{48}$$

and, analogously,

$$K_s(y,s,x,T)=[4\pi(T-s)]^{-1/2}\exp\left[-\frac{(x-y)^2}{4(T-s)}\right]\int d\mu(\alpha)$$
$$\times\exp\left[-\int_s^T c\left(\frac{T-\tau}{T-s}y+\frac{\tau-s}{T-s}x+\sqrt{T-s}\,\alpha\left(\frac{\tau-s}{T-s}\right),T+s-\tau\right)d\tau\right]. \tag{49}$$

By changing

$$\alpha\left(\frac{\tau-s}{T-s}\right)\Rightarrow\alpha\left(1-\frac{\tau-s}{T-s}\right)=\alpha\left(\frac{T-\tau}{T-s}\right) \tag{50}$$

and substituting $\sigma=T+s-\tau$, where τ only is the running variable, we finally recover

$$K_s(y,s,x,T)=[4\pi(T-s)]^{-1/2}\exp\left[-\frac{(x-y)^2}{T-s}\right]\int d\mu(\alpha)\exp\left[-\int_T^s c\left(\frac{\sigma-s}{T-s}y+\frac{T-\sigma}{T-s}x\right.\right.$$
$$\left.\left.+\sqrt{T-s}\,\alpha\left(\frac{\sigma-s}{T-s}\right),\sigma\right)(-d\sigma)\right]=k(x,s,y,T). \tag{51}$$

Hence,

$$g(x,s)=v(x,s) \tag{52}$$

is valid for all time instants $0\leqslant s\leqslant T$. This implies that $p(y,s,x,t)=k(y,s,x,t)v(x,t)/v(y,s)$ defines a consistent transition probability density of the continuous Markovian interpolation.

We have succeeded to prove the following.

(i) If a continuous, strictly positive Feynman–Kac kernel of the forward parabolic equation (5) is employed to solve the Schrödinger boundary data problem (1) for an *arbitrary* pair of nonzero probability densities $\rho_0(x)$ and $\rho_T(x)$, then we can construct a Markov stochastic process, which is continuous and provides for an interpolation between these boundary data in the time interval $[0, T]$.

(ii) Given the time-adjoint parabolic system (5) with bounded solutions $u(x,t),v(x,t)$ in the time interval $[0, T]$, if the boundary densities are defined according to (40), then the Schrödinger problem (1)–(3) provides us with a unique continuous Markov interpolation that is compatible with the time evolution of $\rho(x,t)=u(x,t)v(x,t)$, $t\in[0, T]$.

E. Whence diffusions?

Our strategy of deducing a probabilistic solution of the Schrödinger boundary data problem in terms of Markov stochastic processes running in a continuous time was accomplished in a number of steps, accompanied by the gradual strengthening of restrictions imposed on the Feynman–Kac potential, to yield a continuous process (cf. Sec. II C), and eventually to get it compatible with a given *a priori* parabolic evolution (Sec. II D). In a broad sense,[20] it can be named a diffusion.

However, this rather broad definition of the diffusion process is significantly narrowed in the physical literature: while demanding the continuity of the process, the additional restrictions are imposed to guarantee that the mean and variance of the infinitesimal displacements of the process have the standard meaning of the drift and diffusion coefficient, respectively.[25]

According to the general wisdom, diffusions arise in conjunction with the parabolic evolution equations, since then only the conditional averages are believed to make sense in the local description of the dynamics. It is not accidental that forward parabolic equations (5) are commonly called the generalized diffusion equations. Also, the fact that the Feynman–Kac formula involves the integration over sample paths of the Wiener process seems to suggest some diffusive features of the Schrödinger interpolation, even if we are unable to establish this fact in a canonical manner.

Clearly, the conditions valid for any $\epsilon>0$,

(a) there holds $\lim_{t\downarrow s}[1/(t-s)]\int_{|y-x|>\epsilon}p(y,s,x,t)dx=0$ [notice that (a) is a direct consequence of the stronger, Dynkin condition, (28)],
(b) there exists a drift function $b(x,s)=\lim_{t\downarrow s}[1/(t-s)]\int_{|y-s|\leqslant\epsilon}(y-x)p(x,s,y,t)dy$,
(c) there exists a diffusion function $a(x,s)=\lim_{t\downarrow s}[1/(t-s)]\int_{|y-x|\leqslant\epsilon}(y-x)^2p(x,s,y,t)dy$,

are conventionally interpreted to define a diffusion process.[25]

To our knowledge, no rigorous demonstration is available in the Schrödinger problem context, in the case when the involved semigroup kernel is *not* a fundamental solution of the parabolic equation.

Let us impose a restriction on a lower bound of a solution $v(x,t)$ of the backward equation (5). Namely, we assume that there exist constants $c_1>0$, $c_2>0$ such that $v(y,s)\geqslant c_1\exp(-c_2y^2)$ for all $s\in[0, t]$, $t<T$. This property was found to be respected by a large class of parabolic equations,[26] and it automatically ensures that the condition (25) of Sec. II C is satisfied. Indeed,

$$
\begin{aligned}
0&\leqslant \lim_{|y|\to\infty}\frac{1}{v(y,s)}\int_{-\infty}^{+\infty}k(y,s,x,t)v(x,t)\chi_K(x)dx\\
&\leqslant\frac{1}{c_1}[4\pi(t-s)]^{-1/2}\exp[M(t-s)][\sup_{x\in K}v(x,t)]\lim_{|y|\to\infty}\\
&\quad\times\exp(c_2y^2)\int_K\exp\left[-\frac{(x-y)^2}{4(t-s)}\,dx\right]=0,
\end{aligned}
\tag{53}
$$

if $t-s\geqslant\epsilon$ for sufficiently small $\epsilon>0$ (like, for example, $\epsilon=1/16c_2$).

It is our purpose to complete the previous analysis by demonstrating that, with the above assumption on $v(x,t)$, the continuous Markov process we have constructed actually *is* the diffusion process.

Our subsequent arguments will rely on the Dynkin treatise.[17] It is well known that the infinitesimal (local) characteristics of a continuous Markov process can be defined in terms of its so called characteristic operator. It is closely linked with the standard infinitesimal (Markov) generator of the process, and we shall take advantage of this link in below. Let us agree, following Dynkin, to call a continuous Markov process a diffusion, if its characteristic operator $\mathscr{U}$ is defined on twice-differentiable functions (we skip more detailed definition[17]). In this case $x\to x-x_0$ and $x\to(x-x_0)^2$ allow for the definition of a drift and diffusion function, respectively:

$$[\mathscr{U}(x-x_0)](x_0,s)=b(x_0,s),\quad [\mathscr{U}((x-x_0)^2)](x_0,s)=a(x_0,s). \tag{54}$$

By results of Secs. II C and II D we know that our transition probability density $p(y,s,x,t)=k(y,s,x,t)v(x,t)/v(y,s)$, inspired by the Schrödinger boundary data problem, gives rise to a continuous Markov process. To see whether it can be regarded as a diffusion, we must verify the above two defining properties (54).

At first, let us consider the infinitesimal operator A (Markov generator) of the corresponding strongly continuous semigroup $T_s^t: C_\infty(R)\to C_\infty(R)$, which we have introduced via the formula (26). We are interested in domain properties of A, in view of the fact that the characteristic operator $\mathscr{U}$ is a natural extension of $A, A\subset\mathscr{U}$.[17]

We denote $C_c^2(R)$ as the space of continuous functions with compact support which possess continuous derivatives up to second order. For $h\in C_c^2(R)$ we have

$$\lim_{\delta\downarrow 0}\frac{1}{\delta}\left[\int_{-\infty}^{+\infty}p(y,s,x,s+\delta)h(x)dx-h(y)\right]$$
$$=\frac{1}{v(y,s)}\lim_{\delta\downarrow 0}\frac{1}{\delta}\left[\int_{-\infty}^{+\infty}k(y,s,x,s+\delta)v(x,s+\delta)h(x)dx-v(y,s)h(y)\right]. \tag{55}$$

Because v is continuously differentiable with respect to time, we have

$$v(x,s+\delta)=v(x,s)+\delta\partial_s v(x,s') \tag{56}$$

where (cf. the standard Taylor expansion formula) $s'=s+\vartheta\delta$, $0\leqslant\vartheta\leqslant 1$. Hence

$$\lim_{\delta\downarrow 0}\frac{1}{\delta}\left[\int_{-\infty}^{+\infty}p(y,s,x,s+\delta)h(x)-h(y)\right]$$
$$=\frac{1}{v(y,s)}\lim_{\delta\downarrow 0}\frac{1}{\delta}\left[\int_{-\infty}^{+\infty}dxk(y,s,x,s+\delta)v(x,s)h(x)-v(y,s)h(x)\right]$$
$$+\frac{1}{v(y,s)}\lim_{\delta\downarrow 0}\left[\int_{-\infty}^{+\infty}k(y,s,x,s+\delta)\partial_s v(x,s')h(x)dx\right]. \tag{57}$$

We shall exploit the strongly continuous semigroup evolution associated with the parabolic system (5). Because of the domain property $C_c^\infty(R)\subset D(H)$, the smooth functions with compact support are acted upon by $H=\Delta-c(x,s)$ and H is closed as an operator on $C_\infty(R)$. But then also $C_c^2(R)\subset D(H)$ and so the first term in (57) takes the form

$$\frac{1}{v(y,s)}[\Delta(vh)(y,s)-c(y,s)v(y,s)h(y)] \tag{58}$$

while the second equals

$$\frac{1}{v(y,s)}[\partial_s v(y,s)]f(y)=\frac{1}{v(y,s)}[-\Delta v(y,s)+c(y,s)v(y,s)]f(y). \tag{59}$$

Thus, (55) is pointwise convergent:

$$\begin{aligned}
&\lim_{\delta\downarrow 0}\frac{1}{\delta}\left[\int_{-\infty}^{+\infty}p(y,s,x,s+\delta)h(x)dx-h(y)\right]\\
&\quad=\frac{1}{v(y,s)}[(\Delta v(y,s))h(y)+2\nabla v(y,s)\nabla h(y)+v(y,s)\Delta h(y)-c(y,s)v(y,s)h(y)\\
&\qquad-(\Delta v(y,s))h(y)+c(y,s)v(y,s)h(y)]\\
&\quad=\Delta h(y)+2\left(\frac{\nabla v}{v}\right)(y,s)\nabla h(y).
\end{aligned}\tag{60}$$

Now, we shall establish the boundedness of

$$\sup_{y\in R;0<\delta<\epsilon}\left[\frac{1}{\delta}\left|\int_{-\infty}^{+\infty}p(y,s,x,s+\delta)h(x)dx-h(y)\right|\right] \tag{61}$$

for some small ϵ.

Because $C_c^2(R)\subset D(H)$, so there holds

$$\frac{1}{\delta}\left[\int_{-\infty}^{+\infty}k(y,s,x,s+\delta)v(x,s)h(x)dx-v(y,s)h(y)\right]\to[\Delta-c(y,s)](vf)(y,s) \tag{62}$$

uniformly in y, as $\delta\to 0$. It implies that for any compact set K there is

$$\begin{aligned}
&\sup_{y\in K;0<\delta<\epsilon}\frac{1}{\delta}\left|\int_{-\infty}^{+\infty}p(y,s,x,s+\delta)h(x)-h(y)\right|\\
&\quad\leqslant[\sup_{y\in K}\frac{1}{v(y,s)}]\sup_{y\in K;0<\delta<\epsilon}\left[\frac{1}{\delta}\left|\int_{-\infty}^{+\infty}k(y,s,x,s+\delta)v(x,s)h(x)dx-v(y,s)h(y)\right|\right.\\
&\qquad\left.+\int_{-\infty}^{+\infty}k(y,s,x,s+\delta)\partial_s v(x,s')h(x)dx\right|<\infty.
\end{aligned}\tag{63}$$

We have thus the required boundedness for all $y\in K$, i.e., on compact sets.

For $y\in R\backslash K$ we shall make the following estimations. Because the support of h is compact, we can define $\operatorname{supp} h\subset[-n,\ n]$ for some natural number n. Let $K=[-3n,\ 3n]$. Then,

$$\begin{aligned}
&\sup_{y\in R\backslash K;0<\delta<\epsilon}\frac{1}{\delta}\left|\int_{-\infty}^{+\infty}p(y,s,x,s+\delta)h(x)dx-h(y)\right|\\
&\quad=\sup_{y\in R\backslash K;0<\delta<\epsilon}\frac{1}{\delta}\left|\int_{K}p(y,s,x,s+\delta)h(x)dx\right|\\
&\quad\leqslant[\sup_{x\in K}|h(x)|]\sup_{y\in R\backslash K;0<\delta<\epsilon}\frac{1}{\delta}\frac{1}{v(y,s)}\int_{K}k(y,s,x,s+\delta)v(x,s+\delta)dx
\end{aligned}$$

$$\leqslant[\sup_{x\in K}|h(x)|][\sup_{x\in K;s\leqslant s'\leqslant s+\epsilon} v(x,s')]\sup_{y\in R\setminus K;0<\delta<\epsilon}\frac{1}{\delta}\frac{1}{v(y,s)}\int k(y,s,x,s+\delta)dx. \tag{64}$$

In view of our assumption $v(y,s)\geqslant c_1\exp(-c_2y^2)$, there holds

$$\sup_{y\in R\setminus K;0<\delta<\epsilon}\frac{1}{\delta}\left|\int p(y,s,x,s+\delta)h(x)dx\right|$$

$$\leqslant C\cdot\sup_{|y|\geqslant 3n;0<\delta<\epsilon}\exp(c_2y^2)\delta^{-3/2}\int_{-n}^{+n}\exp\left[-\frac{(x-y)^2}{4\delta}\right]dx, \tag{65}$$

where

$$C=c_1(4\pi)^{-1/2}\exp(M\epsilon)[\sup_{x\in K}|h(x)|]\sup_{x\in K;s<s'<s+\epsilon}v(x,s'). \tag{66}$$

If we choose $\epsilon=1/16c_2$, then

$$\exp(c_2y^2)\int\exp\left[-\frac{(x-y)^2}{4\delta}\right]dx\leqslant 4\delta\exp\left(-\frac{n^2}{\delta}\right) \tag{67}$$

for every $|y|\geqslant 3n$, and so

$$\sup_{y\in R\setminus K;0<\delta<\epsilon}\frac{1}{\delta}\left|\int p(y,s,x,s+\delta)h(x)dx\right|\leqslant 4C\sup_{0<\delta<\epsilon}\delta^{-1/2}\exp\left(-\frac{n^2}{\delta}\right)<\infty. \tag{68}$$

Consequently, the desired boundedness (62) holds true for all $y\in R$, together with the previously established pointwise convergence (61).

Altogether, it means[17] that the weak generator of T_s^t is defined at least on $C_c^2(R)$. Moreover, while acting on $h\in C_c^2(R)$ it gives $\Delta h+(\nabla\ln v)\nabla h$. Because T_s^t is strongly continuous in $C_\infty(R)$, the Markov generator A coincides with the weak generator,[17] i.e., $A=\Delta+(\nabla\ln v)\nabla$ on $C_c^2(R)$.

Finally, let us choose $h_0\in C_c^2(R)$ such that $h_0(x)=1$ in some neighborhood of the point x_0. Then, $(x-x_0)h_0(x)$ and $(x-x_0)^2h_0(x)$ both belong to $C_c^2(R)$ and therefore

$$\begin{aligned}A[(x-x_0)h_0](x_0,s)&=\Delta[(x-x_0)h_0](x_0)+2(\nabla\ln v)(x_0,s)\nabla[(x-x_0)h_0](x_0)\\&=2(\nabla\ln v)(x_0,s)=2(\nabla\ln v)(x_0,s),\\A[(x-x_0)^2h_0](x_0,s)&=2.\end{aligned} \tag{69}$$

Because $A\subset\mathscr{U}$ and $\mathscr{U}$ is a local operator,[17] we have the following inclusion $C_c^2(R)\subset D(\mathscr{U})$ and (we can get rid of h_0)

$$\begin{aligned}[\mathscr{U}(x-x_0)](x_0,s)&=2(\nabla\ln v)(x_0,s),\\[\mathscr{U}(x-x_0)^2](x_0,s)&=2.\end{aligned} \tag{70}$$

It means that we indeed obtain a diffusion process with the drift $\nabla\ln v$ and a constant diffusion coefficient, according to the standards of Refs. 5, 21, and 28.

It is worth emphasizing that since $(x-x_0)h_0(x)$ and $(x-x_0)^2h_0(x)$ belong to $D(A)$, and since functions from $C_c^2(R)$ can be used to approximate, under an integral, an indicator function of the set $[x_0-\epsilon,x_0+\epsilon]$, $\epsilon>0$, we can directly evaluate

$$\lim_{t\downarrow s}\frac{1}{t-s}\int_{-\infty}^{+\infty}p(x_0,s,x,t)(x-x_0)h_0(x)dx$$

$$=\lim_{t\downarrow s}\frac{1}{t-s}\int_{|x-x_0|\leqslant\epsilon}p(x_0,s,x,t)(x-x_0)dx$$

$$=2(\nabla\ \ln v)(x_0,s), \tag{71}$$

and similarly

$$\lim_{t\downarrow s}\frac{1}{t-s}\int_{|x-x_0|\leqslant\epsilon}p(x_0,s,x,t)(x-x_0)^2\ dx=2. \tag{72}$$

Because the Dynkin condition (28) implies that

$$\lim_{t\downarrow s}\frac{1}{t-s}\int_{|x-x_0|>\epsilon}p(x_0,s,x,t)dx=0, \tag{73}$$

we arrive at the commonly accepted definition of the diffusion process, summarized in formulas (71)–(73), with the functional expression for the drift, (71), given in the familiar,[5,8,27] gradient form.

III. NONSTATIONARY SCHRÖDINGER DYNAMICS: FROM THE FEYNMAN–KAC KERNEL TO DIFFUSION PROCESS

In our previous paper,[9] the major conclusion was that in order to give a definitive probabilistic description of the quantum dynamics as a *unique* diffusion process solving Schrödinger's interpolation problem, a suitable Feynman–Kac semigroup must be singled out. Let us point out that the measure-preserving dynamics, permitted in the presence of conservative force fields, was investigated in Ref. 8 (see also Refs. 12 and 29).

The present analysis was performed quite generally and extends to the dynamics affected by time-dependent external potentials, with no clear-cut discrimination between the nonequilibrium statistical physics and essentially quantum evolutions. The formalism of Sec. II encompasses both groups of problems. Presently, we shall restrict our discussion to the free Schrödinger picture quantum dynamics. Following Ref. 9 we shall discuss the rescaled problem so as to eliminate all dimensional constants.

The free Schrödinger evolution $i\partial_t\psi=-\Delta\psi$ implies the following propagation of a specific Gaussian wave packet,

$$\psi(x,0)=(2\pi)^{-1/4}\exp\left(-\frac{x^2}{4}\right)\rightarrow\psi(x,t)=\left(\frac{2}{\pi}\right)^{1/4}(2+2it)^{-1/2}\exp\left[-\frac{x^2}{4(1+it)}\right], \tag{74}$$

so that

$$\rho_0(x)=|\psi(x,0)|^2=(2\pi)^{-1/2}\exp\left[-\frac{x^2}{2}\right]$$

$$\rightarrow\rho(x,t)=|\psi(x,t)|^2=[2\pi(1+t^2)]^{-1/2}\exp\left[-\frac{x^2}{2(1+t^2)}\right] \tag{75}$$

and the Fokker–Planck equation [easily derivable from the standard continuity equation $\partial_t\rho=-\nabla(v\rho)$, $v(x,t)=xt/(1+t^2)$] holds true:

$$\partial_t \rho = \Delta \rho - \nabla(b\rho), \quad b(x,t) = -\frac{1-t}{1+t^2}\, x. \tag{76}$$

The Madelung factorization $\psi = \exp(R+iS)$ implies [notice that $v = 2\nabla S$ and $b = 2\nabla(R+S)$] that the related real functions $\theta(x,t) = \exp[R(x,t)+S(x,t)]$ and $\theta_*(x,t) = \exp[R(x,t)-S(x,t)]$ read

$$\begin{aligned} \theta(x,t) &= [2\pi(1+t^2)]^{-1/4} \exp\left(-\frac{x^2}{4}\frac{1-t}{1+t^2} - \frac{1}{2}\arctan t \right), \\ \theta_*(x,t) &= [2\pi(1+t^2)]^{-1/4} \exp\left(-\frac{x^2}{4}\frac{1+t}{1+t^2} + \frac{1}{2}\arctan t \right). \end{aligned} \tag{77}$$

They solve a suitable version of the general parabolic equations (5), namely,

$$\partial_t \theta = -\Delta\theta + c\theta, \quad \partial_t \theta_* = \Delta\theta_* - c\theta_*, \tag{78}$$

with

$$c(x,t) = \frac{x^2}{2(1+t^2)^2} - \frac{1}{1+t^2} = 2\frac{\Delta\rho^{1/2}}{\rho^{1/2}}. \tag{79}$$

Anticipating further discussion, let us mention that the Feynman–Kac kernel, in this case, *is* a fundamental solution of the time-adjoint system (78). For clarity of exposition, let us recall that a *fundamental solution* of the forward parabolic equation (5) is a continuous function $k(y,s,x,t)$, defined for all $x,y, \in R$ and all $0 \leqslant s < t \leqslant T$, which has the following two properties:

(a) For any fixed $(y,s) \in R \times (0,T)$, the function $(x,t) \to k(y,s,x,t)$ is a regular (i.e., continuous and continuously differentiable the needed number of times) solution of the forward equation (5) in $R \times (s,T]$.

(b) For all continuous functions $\phi(x)$ with a compact support, there holds $\lim_{(t,x)\to(s,z)} \int_{-\infty}^{+\infty} k(y,s,x,t)\phi(y)dy = \phi(z)$.

First, we need to verify (this will be done self-explanatorily) that $c(x,t)$, (79), is Hölder continuous of exponent one on every compact subset of $R \times [0, T]$. It follows from direct estimates:

$$\begin{aligned} |c(x_2,t_2) - c(x_1,t_1)| &\leqslant \frac{1}{2}\left| \frac{x_2^2}{(1+t_2^2)^2} - \frac{x_1^2}{(1+t_1^2)^2} \right| + \left| \frac{1}{1+t_2^2} - \frac{1}{1+t_1^2} \right| \\ &\leqslant \frac{1}{2}\left| \frac{x_2}{1+t_2^2} - \frac{x_1}{1+t_1^2} \right| \left(\frac{|x_2|}{1+t_2^2} + \frac{|x_1|}{1+t_1^2} \right) + |t_2 - t_1| \frac{|t_1|+|t_2|}{(1+t_1^2)(1+t_2^2)}. \end{aligned} \tag{80}$$

However, in the case of $|x_1|, |x_2| \leqslant K$ and $|t_1|, |t_2| \leqslant T$ we have

$$|c(x_2,t_2) - c(x_1,t_1)| \leqslant K\left| \frac{x_2}{1+t_2^2} - \frac{x_1}{1+t_1^2} \right| + 2T|t_2 - t_1| \tag{81}$$

Furthermore,

$$\left| \frac{x_2}{1+t_2^2} - \frac{x_1}{1+t_1^2} \right| \leqslant \left| \frac{x_2 - x_1}{(1+t_2^2)(1+t_1^2)} \right| + \left| \frac{x_2 t_1^2 - x_1 t_2^2}{(1+t_2^2)(1+t_1^2)} \right| \leqslant |x_2 - x_1| + T^2|x_2 - x_1| + 2KT|t_2 - t_1| \tag{82}$$

implies (the new constant C majorizes all remaining ones)

$$|c(x_2,t_2)-c(x_1,t_1)|\leqslant C(|x_2-x_1|+|t_2-t_1|)\leqslant\sqrt{2}C[(x_2-x_1)^2+(t_2-t_1)^2]^{1/2}. \tag{83}$$

Let us also notice that we can introduce an auxiliary function $h(x,t)=\arctan t$ such that there holds

$$\Delta h-c(x,t)h-\partial_t h=-\frac{x^2h(x,t)}{2(1+t^2)^2}\leqslant 0. \tag{84}$$

We have thus satisfied the crucial assumptions I and II of Ref. 24. As a consequence, we have granted the existence of a fundamental solution $k(y,s,x,t)\geqslant 0$. Moreover, for every bounded and continuous function $\phi(x),|\phi(x)|\leqslant C$, where $C>0$ is arbitrary, the function

$$u(x,t)=\int_{-\infty}^{+\infty}k(y,0,x,t)\,\phi(y)\,dy \tag{85}$$

is a solution of the Cauchy problem, i.e., solves (79) under the initial condition $u(x,0)=\phi(x)$, so that $|u(x,t)|\leqslant C$. All that implies the uniqueness of the fundamental solution $k(y,s,x,t)$, and in view of $-c(x,t)\leqslant 1$ its strict positivity. The function $k(y,s,x,t)$ is also a solution of the adjoint equation with respect to variables y,s: $\partial_s k=-\Delta_y k+c(y,s)k$ in $R\times[0,T)$. It is obvious that the Chapman–Kolmogorov composition rule holds true, in view of the validity of the Feynman–Kac representation in the present case.

Basically, we must be satisfied with the Feynman–Kac representation of the fundamental solution, whose existence we have granted so far. In our case, the so-called parametrix method,[22] can be used to construct fundamental solutions. In fact, since $c(x,t)$ is locally Lipschitz, i.e., Hölder continuous of exponent one and quadratically bounded $|c(x,t)|\leqslant x^2+1$, the infinite series

$$k(y,s,x,t)=\sum_{n=0}^{+\infty}(-1)^n k_n(y,s,x,t), \tag{86}$$

where $k_0(y,s,x,t)=[4\pi(t-s)]^{-1/2}\exp[-(x-y)^2/4(t-s)]$ is the heat kernel and

$$k_n(y,s,x,t)=\int_s^t d\tau\int_{-\infty}^{+\infty}dz\,c(z,\tau)k_{n-1}(y,s,z,\tau)k_0(z,\tau,x,t) \tag{87}$$

are known to converge for all $x,y\in R$, $0\leqslant s<t\leqslant T$, and $t-s<T_0$ where $T_0<T$, and define the fundamental solution.[30]

By putting $p(y,s,x,t)=k(y,s,x,t)\,\theta(x,t)/\theta(y,s)$ we arrive at the fundamental solution of the second Kolmogorov (Fokker–Planck) equation

$$\partial_t p(y,s,x,t)=\Delta_x p(y,s,x,t)-\nabla_x[b(x,t)p(y,s,x,t)], \tag{88}$$

where $b=2\nabla\theta/\theta$ and $\rho=uv$, and, in particular, $\rho=\theta\theta_*=|\psi|^2$, are consistently propagated by p. It is the transition probability density of the Nelson diffusion associated with the solution (74) of the Schrödinger equation, and at the same time a solution of the first Kolmogorov (backward diffusion) equation

$$\partial_s p(y,s,x,t)=-\Delta_y p(y,s,x,t)-b(y,s)\nabla_y p(y,s,x,t). \tag{89}$$

Equations (88) and (89) prove that the pertinent process is a diffusion: it has the standard local (infinitesimal) characteristics of the diffusion process.[25]

Obviously, the above definition of p in terms of k induces the validity of the compatibility condition

$$c(x,t)=2\left[\partial_t \ln\ \theta(x,t)+\frac{1}{2}\left[\frac{b^2(x,t)}{2}+\nabla b(x,t)\right]\right] \tag{90}$$

connecting the drift of the diffusion process with the Feynman–Kac potential governing its local dynamics: cf. Refs. 8, 29, and 31 where the Ehrenfest theorem analogue was formulated for general (non-quantal included) Markovian diffusions.

Let us point out that our quantally motivated example was chosen not to show up a typical for quantum wave functions property of vanishing somewhere. In fact, because of restricting our considerations to strictly positive Feynman–Kac kernels and emphasizing the uniqueness of solutions, we have left aside an important group of topics pertaining to solution of the Schrödinger boundary data problem when

(i) the boundary densities have zeros, and
(ii) the interpolation itself is capable of producing zeros of the probability density, even if the boundary ones have none.

Only the case (i) can be (locally) addressed by means of strictly positive semigroup kernels; however, the uniqueness of solution is generally lost in space dimension higher than one.[2–4] General existence theorems are available[28,29] and indicate that one deals with diffusion-type processes in this case (see also, e.g., Refs. 5, 6, and 8). The case (ii) seems to never be considered in the literature (see however Ref. 32).

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A uniform diffusion limit for random wave propagation with turning point

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A random wave propagation problem with turning point is considered for a refractive, layered random medium. The variations of the medium structure are assumed to have two spatial scales; microscopic random fluctuations are superposed upon slowly varying macroscopic variations. An extension of a limit theorem for stochastic differential equations with multiple spatial scales is derived and proved to obtain a uniformly valid diffusion limit for random multiple scattering up to the turning point region. The scale dependence of the infinitesimal generator of the backward Kolmogorov equation provides an insight into the interplay of internal refraction and random scattering as one approaches the turning point. © *1996 American Institute of Physics.* [S0022-2488(96)01002-9]

I. INTRODUCTION

Waves are expected to undergo some scales of fluctuations when they propagate in a randomly inhomogeneous medium. If the random inhomogeneities are strong, multiple scattering and the interference of waves produce phenomena in which the waves are localized around the region where they are generated. They lose coherence and eventually they are totally converted to random fluctuations; the waves do not propagate at all. Localization phenomena can be found in one or two dimensional settings of layered media even when the random inhomogeneities are weak. Anderson[1] discovered these localization phenomena in connection with electronic waves in semiconductors in 1958. Then a substantial theory of Anderson localization has been developed in the eighties.[2,3] Recently, an analogous localization of light has also started getting attention from physicists.[4,5] Light in a certain class of strongly scattering dielectric microstructure exhibits localized modes. It took time, however, before localization of various types of classical waves became fully appreciated,[6] although localization for one-dimensional Schrödinger equation with random potential was well understood.[7] One reason[3] for this is that localization phenomena are observed usually over the long range of distances unless the random scattering is very strong and the dissipation is rather weak. In this paper, we study a wave propagation problem with turning point in a layered random medium in which we combine a geometric optics limit for the large scale structure of the medium with wave localization of multiply-scattered fields.

One typical type of randomly inhomogeneous medium, i.e. a one-dimensional refractive, randomly-layered medium, is considered here. When we have a point source off a medium, one can think of it as launching rays in all directions. We consider an oblique wave incident upon the medium from an adjoining homogeneous medium. Average wave field parameters are assumed to vary with propagation direction so that an obliquely incident wave, undergoing some random fluctuation, turns at some point in the medium, leading to stochastic turning point problem. To see the variations of the large-scale structure of the medium, the wave needs to have short wavelength compared to the length scales of the macrostructure but to acquire the statistical properties of the details of the random inhomogeneities, the wavelength needs to be long compared to the size of the random microstructure. This allows us to combine both a geometrical optics-like accommo-

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dation of the large-scale macroscopic variations and a Central Limit Theorem or diffusion limit theorem for the random microscopic details. The combined limits can reveal the very rich structures of stochastic wave propagation problems for suitably defined quantities. Our modeling hypothesis is this separation of scales with random layering of the medium. The interplay of total internal refraction and diffusion effects produced by random multiple scattering is to be analyzed based on this hypothesis.

Limit theorems for stochastic differential equations with a small parameter remain our mathematical tool. They say in brief that a large class of random processes defined by the following stochastic differential equations, not of Itô type,[9] converge weakly to a diffusion Markov process which solves a parabolic partial differential equation, the backward Kolmogorov equation, whose adjoint equation is the Fokker–Planck equation for the transition probability density:

$$\frac{dx}{d\tau}=\frac{1}{\epsilon}F(\tau,\tau/\epsilon^2,x,\omega),\quad 0\leqslant\tau\leqslant\tau_0\sim O(1),\quad \omega\in\Omega, \tag{1a}$$

$$x(0)=x_0, \tag{1b}$$

where the random field F has zero-mean and Ω denotes an underlying probability space. Such a type of theory was first called to attention by Stratonovich[10] in 1963 for problems of nonlinear vibrations in the presence of noise. Then mathematical theory was developed by Khasminskii[11] and extended by Papanicolaou and Kohler.[12] The theory has been applied effectively in the probabilistic approaches to a variety of problems[8,13–19] including wave propagation theory. In particular, it became a fundamental tool to derive transport equations for the statistics of multiply-scattered wave fields in the analysis of waves in random media. Our stochastic turning point problem, however, requires an extension of this theory to an asymptotically infinite interval. We present a limit theorem in general terms for stochastic equation of type (1) over an extended interval:

$$\frac{dx}{d\tau}=\frac{1}{\epsilon}F(\tau,\tau/\epsilon^2,x,\omega),\quad 0\leqslant\tau\leqslant\tau_0/\epsilon\sim O(\epsilon^{-1}),\quad \omega\in\Omega, \tag{2a}$$

$$x(0)=x_0. \tag{2b}$$

We quantify, in Sec. II, the scaling condition for multiscale structure of the medium. We introduce a stochastic turning point problem for a one-dimensional refractive, randomly layered medium. Using the propagator matrix of an effective system, we formulate a stochastic boundary value problem for the scattering variables. In terms of a new stretched variable, we recast it as a nonlinear stochastic initial value problem (the Riccati equation) for the reflection coefficient. In Sec. III, we derive a diffusion limit theorem for stochastic differential equations on an extended interval in general terms and subsequently apply this theorem to the turning point problem established in Sec. II. As a result, the stochastic quantities of interest are characterized as expectations of functions of the reflection coefficient. In Sec. IV, the subtle interplay of refraction and localization effect is explained in terms of the frequency and scale dependence of the backward Kolmogorov equation. The extended limit theorem is proved in Sec. V.

II. RANDOM WAVE PROPAGATION WITH TURNING POINT

We consider a monochromatic, time-harmonic, plane wave incidence upon a half space $z\leqslant 0$ from a homogeneous medium occupying the region $z>0$. The medium has a one-dimensional, randomly-layered fine structure; it is homogeneous in the transverse directions. The wave propagation model considered here is provided by a system of differential equations

$$\frac{d}{dz}\psi(z,\omega)=i\omega\mathscr{A}(z)\psi(z,\omega),\quad -\infty<z<\infty, \tag{3}$$

where matrix $\mathscr{A}(z)$ represents the material properties of the medium in the z direction. The physical waves represented by this system may be of a large number of different kinds (waves in a waveguide, acoustic waves, electromagnetic waves, etc).

Within the medium, matrix $\mathscr{A}(z)$ is assumed to vary with z in a manner that superposes a randomly-fluctuating component upon a slowly-varying mean value. We introduce a small positive parameter ϵ to quantify this two-scale dependence, i.e. a smooth deterministic macroscale and a random microscale, of the medium:

$$\mathscr{A}(z)=\mathscr{A}(z,z/\epsilon^2),\quad -\infty<z\leqslant 0, \tag{4}$$

where each component of matrix $\mathscr{A}(z,z/\epsilon^2)$ is unit correlation length random function of the second argument while the first argument accounts for deterministic nonstationary modulation; the actual correlation length of the processes is, therefore, ϵ^2. Let the frequency of the incident wave also be scaled by

$$\omega=\bar{\omega}/\epsilon, \tag{5}$$

where $\bar{\omega}$ is $O(1)$ (the overbar will subsequently be omitted throughout). Consequently the orders $O(1)$, $O(\epsilon)$ and $O(\epsilon^2)$ correspond to the large-scale structure of the medium, the wavelength of incident wave and the correlation length of the random features of the medium, respectively. This means that the wavelength is large enough to average over microscopic random effects and small enough to probe macroscopic variation. A limit is, therefore, possible which combines a diffusion limit for fine-scale random fluctuation with a geometric optics-like limit for large-scale deterministic variation. Also the high-frequency scale will permit the use of WKB analysis.

From now on, we consider a random system in the form

$$\frac{d}{dz}\psi(z,\omega)=\frac{i\omega}{\epsilon}\mathscr{A}(z,z/\epsilon^2)\psi(z,\omega),\quad -\infty<z\leqslant 0, \tag{6}$$

where matrix $\mathscr{A}(z,z/\epsilon^2)$ is decomposed into the sum of a deterministic part $\mathscr{A}_0(z)$ and a mean-zero random part $\mathscr{A}_1(z,z/\epsilon^2)$, each of which takes the form

$$\mathscr{A}_0(z)=\begin{bmatrix}0 & \alpha_0(z)\\ \beta_0(z) & 0\end{bmatrix},\quad \mathscr{A}_1(z,z/\epsilon^2)=\begin{bmatrix}0 & \alpha_1(z,z/\epsilon^2)\\ \beta_1(z,z/\epsilon^2) & 0\end{bmatrix}. \tag{7}$$

We assume that the averaged functions $\alpha_0(z)$ and $\beta_0(z)$ vary with z in such a way that the eigenvalues of $(i\omega/\epsilon)\mathscr{A}_0(z)$ vanish at some point, say $z=z_0$, and they are pure imaginary on $z_0<z<0$ and real valued on $z<z_0$; in the effective medium, waves propagate in the region $z_0<z<0$ and evanesce in the region $z<z_0$. The point z_0 will remain the dividing point for the stochastic problem in our scaling and it is called the turning point of our stochastic problem.

In order to obtain quantities exhibiting a limiting stochastic behavior as $\epsilon\downarrow 0$ in our turning point problem, one needs to remove the rapid deterministic variations of (6) so that there is only a mean-zero term on the right-hand side of (6). For this step of centering, we need a propagator matrix of the following system:

$$\frac{d}{dz}\psi(z,\omega)=\frac{i\omega}{\epsilon}\mathscr{A}_0(z)\psi(z,\omega),\quad -\infty<z\leqslant 0. \tag{8}$$

Let us introduce a WKB approximant for the propagator matrix of the effective system (8); we denote this approximant by $\Phi(z,\omega)$. Then a new dependent vector variable $\mathbf{u}(z,\omega)$ is introduced by

$$\psi(z,\omega)=\Phi(z,\omega)\mathbf{u}(z,\omega), \quad \mathbf{u}(z,\omega)\equiv[\mathbf{u}^+(z,\omega),\mathbf{u}^-(z,\omega)]^t. \tag{9}$$

For brevity, we omit the ω-dependence of field variables from now on. In a uniform medium, $\mathbf{u}^+(z)$ and $\mathbf{u}^-(z)$ are constant and the total wave field is exactly splitted into two physically identifiable components propagating in two opposite directions; $\mathbf{u}^+(z)$ represents a reflected or up-going wave amplitude while $\mathbf{u}^-(z)$ will correspond to an incident or down-going one. In a general inhomogeneous medium, however, the splitted wave fields provide only a mathematical decomposition. Random system (6) for wave fields now transforms into the following system for scattering variables $\mathbf{u}^+(z)$ and $\mathbf{u}^-(z)$:

$$\frac{d}{dz}\mathbf{u}(z)=\frac{i\omega}{\epsilon}\Phi^{-1}(z)\mathscr{A}_1(z,z/\epsilon^2)\Phi(z)\mathbf{u}(z)+\Phi^{-1}(z)\left(\frac{i\omega}{\epsilon}\mathscr{A}_0(z)\Phi(z)-\frac{d}{dz}\Phi(z)\right)\mathbf{u}(z), \tag{10}$$

where the second term on the right side of (10) would vanish if $\Phi(z)$ were an exact propagator matrix for the effective system (8).

To produce a two-point boundary value problem, we consider a unit incident wave in $z>0$ impinging upon the random medium, while for simplicity we assume total reflection at some point $\bar{z}<z_0$. For a physical point of view, the presence of a turning point at z_0 makes the nature of the termination at $\bar{z}$ irrelevant. Thus, using notation Γ_z for reflection coefficient at z, we impose the following boundary conditions:

$$\mathbf{u}^+(\bar{z})=\Gamma_{\bar{z}}\mathbf{u}^-(\bar{z}), \quad \mathbf{u}^-(0)=1, \tag{11}$$

where $|\Gamma_{\bar{z}}|=1$.

Let

$$\Phi(z)=\begin{bmatrix}\phi_{11}(z) & \phi_{12}(z)\\ \phi_{21}(z) & \phi_{22}(z)\end{bmatrix}. \tag{12}$$

If a propagator matrix $\Phi(z)$ can be chosen to have the second component on the right-hand side of the exact random system (10) negligible, then (10) becomes essentially centered. To obtain such a $\Phi(z)$ explicitly, we use results of Lynn and Keller[20] from which it follows that $\det\Phi(z)=2$ and the $\phi_{ij}(z)$'s are

$$\phi_{1j}(z)=\alpha_0^{1/2}(z)\zeta(z)\Theta_j(\lambda^{2/3}\phi), \quad j=1,2, \tag{13a}$$

$$\begin{aligned}\phi_{2j}(z)=&\lambda^{-1}\alpha_0^{-1/2}(z)(\alpha_0'(z)\zeta(z)/2\alpha_0(z)+\zeta'(z))\Theta_j(\lambda^{2/3}\phi)\\ &+\lambda^{-1/3}\alpha_0^{-1/2}(z)\zeta^{-1}(z)\Theta_j'(\lambda^{2/3}\phi),\end{aligned} \tag{13b}$$

where $\lambda=i\omega/\epsilon$ and the functions $\zeta(z)$ and $\phi(z)$ are defined to be

$$\zeta^4(z)=\phi(z)/\alpha_0(z)\beta_0(z), \quad \phi^{3/2}(z)=(3/2)\tau(z) \tag{14}$$

and the functions Θ_1 and Θ_2 are defined as follows in terms of the Airy functions:

$$\Theta_1(x)=\pi^{1/2}\lambda^{1/6}e^{-i(\omega/\epsilon)\tau_0}\{-iAi(x)+Bi(x)\}, \quad \Theta_2(x)=-2\pi^{1/2}\lambda^{1/6}e^{i(\omega/\epsilon)\tau_0}Ai(x). \tag{15}$$

Here we used the travel time defined by

$$\tau(z)=\int_{z_0}^{z}\sqrt{\alpha_0(s)\beta_0(s)}ds \tag{16}$$

and notation $\tau_0=\tau(0)$. It is worth noting that $\tau(z)$, $\phi(z)$ and $\zeta(z)$ are real positive functions on $z_0<z<0$ but are complex-valued functions on $z<z_0$.

If we use properties of the Airy functions,[21] the right-hand side of system (10) can be simplified and some underlying group structure of (10) can be revealed. First one can obtain the following conjugacy relations among the $\phi_{ij}(z)$'s:

$$\phi_{12}(z)=-\phi_{11}^{*}(z),\quad \phi_{22}(z)=\phi_{21}^{*}(z). \tag{17}$$

Due to these relations, one can show that both components of the coefficient matrix on the right-hand side of (10) have a common structure that generates propagator matrices belonging to a Lie group SU(1,1).[22] It means that the Lynn and Keller approximant preserves the group structure of the propagator matrices for the exact problem. With this observation and relations (17), one can prove that the time average energy flux for a time-harmonic wave, defined by $\underline{\mathbf{I}}=(1/2)Re(\boldsymbol{\psi}_1\boldsymbol{\psi}_2^{*})$,[23] is same as $(1/2)(|\mathbf{u}^{+}|^2-|\mathbf{u}^{-}|^2)$ and it is invariant. This leads to the fact that we have total reflection everywhere in the random slab $\bar{z}\leqslant z\leqslant 0$.

From now on, only the region $z_0\leqslant z\leqslant 0$ is considered. We stretch this region by defining a new argument

$$\eta=(\omega/\epsilon)^{2/3}\phi(z). \tag{18}$$

Then, using the relation $d\eta=(\omega/\epsilon)^{2/3}\zeta^{-2}(z)dz$, one can rewrite the exact system (10) in terms of the new variable. The asymptotic expansions of the Airy functions and their first derivatives provide the identification of the growth or decay behavior of components of the exact system as they reach the outer region after starting at the turning point z_0. Here we use the terminology ''transition region'' and ''outer region,'' respectively, for a region in distance of order $O(1)$ in the η-scale from the turning point and the rest of the transition region. It can be shown from the asymptotic behavior of the Airy functions that the second coefficient matrix of the exact system (10) is negligible uniformly (i.e. when one rescales back to z); the major contribution in the diffusion limit comes from the first coefficient matrix of (10) in both the transition region and the outer region. If we use the moduli and phases for the Airy functions and their first derivatives, i.e.

$$Ai(-\eta)+iBi(-\eta)=M(\eta)e^{i\{\Omega(\eta)+\pi/4\}}, \tag{19a}$$

$$Ai'(-\eta)+iBi'(-\eta)=N(\eta)e^{i\{\Psi(\eta)+3\pi/4\}}, \tag{19b}$$

then we can obtain the following centered system after neglecting the small terms:

$$\frac{d}{d\eta}\begin{bmatrix}\mathbf{u}^{+}\\ \mathbf{u}^{-}\end{bmatrix}=(i/2)(\omega/\epsilon)^{2/3}\pi\alpha_0\zeta^4M^2(\eta)\beta_1(\eta/\epsilon^{4/3})\begin{bmatrix}1 & -e^{2i\{(\omega/\epsilon)\tau_0+\Omega\}}\\ e^{-2i\{(\omega/\epsilon)\tau_0+\Omega\}} & -1\end{bmatrix}\begin{bmatrix}\mathbf{u}^{+}\\ \mathbf{u}^{-}\end{bmatrix}$$
$$+(i/2)\pi\alpha_0^{-1}N^2(\eta)\alpha_1(\eta/\epsilon^{4/3})\begin{bmatrix}1 & e^{2i\{(\omega/\epsilon)\tau_0+\Psi\}}\\ -e^{-2i\{(\omega/\epsilon)\tau_0+\Psi\}} & -1\end{bmatrix}\begin{bmatrix}\mathbf{u}^{+}\\ \mathbf{u}^{-}\end{bmatrix}, \tag{20a}$$

$$0\leqslant\eta\leqslant\eta_0\equiv(3\omega\tau_0/2\epsilon)^{2/3},\quad \mathbf{u}^{+}(0)=\Gamma_0\mathbf{u}^{-}(0),\quad \mathbf{u}^{-}(\eta_0)=1. \tag{20b}$$

We note from the asymptotic expansion of $M(\eta)$ and $N(\eta)$ that the first term on the right-hand side of system (20) is a dominant term in both the transition region and the outer region, while the second term will not contribute in the transition region but it will become as significant in the outer region as the first term.

The linear two point stochastic boundary value problem for the scattering variables $\mathbf{u}^+(\eta)$ and $\mathbf{u}^-(\eta)$ can be recast as a nonlinear stochastic initial value problem for the reflection coefficient. In this section, we already noted that the reflection coefficient is unimodular in the random slab of our interest. The problem reduces to a consideration of the phase of the unimodular reflection coefficient. Let

$$\frac{\mathbf{u}^+(\eta)}{\mathbf{u}^-(\eta)} = e^{-i\psi(\eta)}. \tag{21}$$

Then system (20) for the scattering variables $\mathbf{u}^+(\eta)$ and $\mathbf{u}^-(\eta)$ leads to the Riccati differential equation for the phase $\psi(\eta)$ of the reflection coefficient as follows:

$$\frac{d\psi}{d\eta} = \epsilon^{-2/3} F_1(\eta, \eta/\epsilon^{4/3}, \psi) + F_2(\eta, \eta/\epsilon^{4/3}, \psi), \quad 0 \leqslant \eta \leqslant \eta_0, \tag{22a}$$

$$\psi(0) = \psi_0, \tag{22b}$$

where ψ_0 is the phase of the reflection coefficient at the turning point and it is considered known for present discussion and the random fields F_1 and F_2 are given by

$$F_1(\eta, \eta/\epsilon^{4/3}, \psi) = \omega^{2/3}\pi\alpha_0\zeta^4 M^2(\eta)\beta_1(\eta/\epsilon^{4/3})\{1-\cos(\psi + 2(\omega\tau_0/\epsilon + \Omega(\eta)))\}, \tag{22c}$$

$$F_2(\eta, \eta/\epsilon^{4/3}, \psi) = \pi\alpha_0^{-1} N^2(\eta)\alpha_1(\eta/\epsilon^{4/3})\{1+\cos(\psi + 2(\omega\tau_0/\epsilon + \Psi(\eta)))\}. \tag{22d}$$

From the above stochastic initial value problem, a number of facts should be noted. The Riccati equation (22) is expressed in terms of the stretched variable η (transition region scale); $\epsilon^{2/3}\eta$ and $\eta/\epsilon^{4/3}$ correspond to z (or $\phi(z)$) and z/ϵ^2 in the z-scale, respectively. The deterministic functions α_0 and ζ depend on only a slow-variable $\epsilon^{2/3}\eta$ and thus they behave like constants in the η-scale. Both random fields F_1 and F_2 have the form of a mean-zero nonstationary random function, either α_1 or β_1, times deterministic functions. In short, stochastic initial value problem (22) has the form of model problem introduced in Sec. I. The interval $0 \leqslant \eta \leqslant \eta_0$ considered in our case, however, is not a bounded interval; it is order $O(\epsilon^{-2/3})$. Thus the mean-zero random field F_2 must be retained (not like the case of previously known theory). It will contribute in the diffusion limit since it is significant in the outer region. Hence it requires an extension of known limit theorems for stochastic differential equations with a small parameter to understand the diffusion effects caused by random multiple scattering. This work will be performed in the following sections. Usual differential equation existence and uniqueness theory tells us that the solutions of (22) are well-defined stochastic processes. Our goal is to characterize stochastic quantities of interest as expectations of functions of solutions of the stochastic differential equation, using an extended limit theorem that will be described in the next section.

III. AN EXTENDED DIFFUSION LIMIT THEOREM

In this section, we state in general terms a result about the extension of Khasminskii's limit theorem to an unbounded interval. Then we apply our results to the stochastic turning point problem formulated in Sec. II. As a result, we obtain a uniformly valid infinitesimal generator for the limiting diffusion Markov process.

We first establish notation and hypotheses before stating our theorem. Let $(\Omega, \mathcal{F}, P)$ be a probability space and let $\mathcal{F}_s^t$, $0 \leqslant s \leqslant t \leqslant \infty$, be a family of σ-algebra contained in $\mathcal{F}$ such that

$$\mathcal{F}_{s_1}^{t_1} \subset \mathcal{F}_{s_2}^{t_2}, \quad 0 \leqslant s_2 \leqslant s_1 \leqslant t_1 \leqslant t_2 \leqslant \infty. \tag{23}$$

We assume the strong mixing condition in the sense that

$$\sup_{s\geqslant 0}\sup_{A\in\mathscr{F}_{s+t}^{\infty},B\in\mathscr{F}_0^s}|P(A|B)-P(A)|=\rho(t)\downarrow 0,\quad \text{as } t\uparrow\infty. \tag{24}$$

The monotonically decreasing nonnegative function ρ is called the mixing rate which is assumed to satisfy the following rate condition:

$$\int_0^\infty \rho^{1/2}(s)ds<\infty. \tag{25}$$

For example, ergodic Markov processes on a compact state space are mixing processes with an exponential mixing rate. Note that decreasing monotonicity (24) and rate condition (25) imply that $\rho(1/\epsilon)/\epsilon$ is uniformly bounded in $\epsilon\in(0,1]$ and $\int_0^\infty\rho(s)ds<\infty$ and $\int_0^\infty s\rho(s)ds<\infty$. The conditional probabilities relative to $\mathscr{F}_0^s$, $0\leqslant s\leqslant\infty$, are assumed to have a regular version so that we are able to have the following representation almost everywhere:

$$E\{\cdot|\mathscr{F}_0^s\}=\int_\Omega\cdot P_s(d\omega|\omega')\quad a.e. \tag{26}$$

Let $F(\eta,\nu,x,\omega)$ be a function from $[0,\infty)\times[0,\infty)\times\mathscr{R}\times\Omega$ into $\mathscr{R}$, where $\mathscr{R}$ denotes the set of real numbers. The random field F is assumed to be jointly measurable with respect to its arguments and, for fixed η, ν and x, $F(\eta,\nu,x,\omega)$ is $\mathscr{F}_\nu^\nu$ measurable as a function of $\omega\in\Omega$.

We introduce the one-point compactification of $\mathscr{R}$, denoted by $\mathscr{R}_c$, and $\mathscr{C}^0$ denotes the space of continuous real valued functions on $\mathscr{R}_c$ with the supremum norm $\|\cdot\|$. Let $\mathscr{C}^k$ denote the space of real valued functions on $\mathscr{R}_c$ with bounded continuous derivatives up to order k with norm $\|\cdot\|_k$ the sum of the supremum norm of the function and its derivatives up to order k. Then the spaces $\mathscr{C}^k$ are separable Banach spaces and dense subspaces of $\mathscr{C}^0$ such that $\mathscr{C}^k\subset\mathscr{C}^{k-1}$ and $\|f\|_{k-1}\leqslant\|f\|_k$, $\forall f\in\mathscr{C}^k$.

With a positive parameter ϵ, we consider the following stochastic initial value problem on an $O(\epsilon^{-1})$ interval which is a generalized form of our model problem (22):

$$\frac{d}{d\tau}x^\epsilon(\tau,\sigma,x)=\frac{1}{\epsilon}F(\tau,\tau/\epsilon^2,x^\epsilon(\tau,\sigma,x),\omega),\quad 0\leqslant\sigma\leqslant\tau\leqslant\eta_0\sim O(\epsilon^{-1}), \tag{27a}$$

$$x^\epsilon(\sigma,\sigma,x)=x, \tag{27b}$$

where the solution $x^\epsilon(\tau,\sigma,x)$ is $\mathscr{F}_{\sigma/\epsilon^2}^{\tau/\epsilon^2}$ measurable as a function of ω for any fixed x.

To develop a limit theory for our problem of interest, it is convenient to introduce solution operators $U^\epsilon(\sigma,\tau)$, called random propagators, associated with (27); we define $U^\epsilon(\sigma,\tau)$ by

$$(U^\epsilon(\sigma,\tau)f)(x)=f(x^\epsilon(\tau,\sigma,x)), \tag{28}$$

for arbitrary $f\in\mathscr{C}^0$. These are contraction operators on $\mathscr{C}^0\to\mathscr{C}^0$. The function $U^\epsilon(\sigma,\tau)f$, $f\in\mathscr{C}^0$, is strongly $\mathscr{F}_{\sigma/\epsilon^2}^{\tau/\epsilon^2}$ measurable. It is also useful to define the following random differential operator $V(\tau)$:

$$(V(\tau)f)(x)=F(\tau,\tau/\epsilon^2,x)\partial_x f(x), \tag{29}$$

for arbitrary $f\in\mathscr{C}^k$, $k\geqslant 1$. Note that the ϵ dependence of $V(\tau)$ is not explicitly expressed here. For each $f\in\mathscr{C}^k$, $V(\tau)f$ is strongly $\mathscr{F}_{\tau/\epsilon^2}^{\tau/\epsilon^2}$ measurable.

Let the interval $0\leqslant\tau\leqslant\eta_0$ be covered by $O(1)$ intervals $I_n=[\sigma_{n-1},\sigma_n]$ such that

$$0=\sigma_0<\sigma_1<\cdots<\sigma_n<\cdots<\sigma_{m_0}=\eta_0, \quad m_0\sim O(\epsilon^{-1}). \tag{30}$$

We adopt, throughout, the convention that, for each fixed n, ϵ dependent constant $C_{n,\epsilon}$ introduced in the following theorem is not necessarily the same constant; constant multiples of $C_{n,\epsilon}$ will again be denoted by $C_{n,\epsilon}$.

Now we are ready to state our main result. The proof of the following theorem will be given in the next section.

Theorem: *Let $U^\epsilon(\sigma,\tau)$ and $V(\tau)$, $0\leqslant\sigma\leqslant\tau\leqslant\eta_0\equiv\tau_0/\epsilon\sim O(\epsilon^{-1})$, be the operators, respectively, defined by (28) and (29) corresponding to stochastic initial value problem (27). Suppose the strong mixing condition (24)–(25) and the hypotheses stated above are satisfied. Let us assume the following conditions (i)–(iv) hold:*

(i) For arbitrary $f\in\mathscr{C}^1$,

$$E\{V(\tau)f\}=0. \tag{31}$$

(ii) There are positive constants α_k and β_k independent of σ, τ and ϵ such that for arbitrary $f\in\mathscr{C}^k$, $k=1,2$,

$$\|U^\epsilon(\sigma,\tau)f\|_k\leqslant\beta_k\{1+(\tau-\sigma)/\epsilon+\cdots+((\tau-\sigma)/\epsilon)^{k-1}\}e^{\alpha_k[(\tau-\sigma)/\epsilon]}\|f\|_k \quad a.e. \tag{32}$$

(iii) For each interval I_n, there is a positive constant $C_{n,\epsilon}$ such that

$$\sup_{\tau\in I_n}\|V(\tau)f\|_{k-1}\leqslant C_{n,\epsilon}\|f\|_k \quad a.e., \quad \forall f\in\mathscr{C}^k, \quad 1\leqslant k\leqslant 4. \tag{33}$$

The above constants $C_{n,\epsilon}$, $n=1,2,\ldots,m_0$, are uniformly bounded in n by a constant independent of ϵ and satisfy, for some number $\gamma<1$, the following decay condition:

$$\sum_{n=1}^{m_0} C_{n,\epsilon}\sim O(\epsilon^{-\gamma}). \tag{34}$$

(iv) Let $(A^\epsilon(\sigma,\tau)f)(x)$ denote the solution $u^\epsilon(\sigma,\tau,x;f)$ of the backward Kolmogorov equation

$$\partial_\sigma u(\sigma,\tau,x)+\mathscr{L}^\epsilon_\sigma u(\sigma,\tau,x)=0, \quad \sigma<\tau, \quad u(\tau,\tau,x)=f(x), \tag{35}$$

with infinitesimal generator $\mathscr{L}^\epsilon_\sigma$ defined on $\mathscr{C}^2\to\mathscr{C}^0$ by

$$\mathscr{L}^\epsilon_\sigma f=\int_0^{1/\epsilon}E\{V(\sigma)V(\sigma+\epsilon^2 t)f\}dt, \tag{36}$$

and let the averaged backward propagators $A^\epsilon(\sigma,\tau)$ satisfy the following inequality for some positive constants a_k independent of $\epsilon>0$:

$$\sup_{0\leqslant\sigma\leqslant\tau\leqslant\eta_0}\|A^\epsilon(\sigma,\tau)f\|_k\leqslant a_k\|f\|_k, \quad \forall f\in\mathscr{C}^k, \quad 1\leqslant k\leqslant 4. \tag{37}$$

We assume that the strong limit in $\mathscr{C}^0$ of $A^\epsilon(\sigma,\tau)f$, as $\epsilon\to 0$, exists uniformly in σ and τ and the limit, denoted by $A(\sigma,\tau)f$, satisfies the rate of approach

$$\sup_{0\leqslant\tau\leqslant\eta_0}\|A^\epsilon(0,\tau)f-A(0,\tau)f\|_0\leqslant\epsilon^{1-\gamma}C_{\tau_0}\|f\|_2, \quad \forall f\in\mathscr{C}^2. \tag{38}$$

Then, for arbitrary $f\in\mathscr{C}^4$, we have the estimate

$$\sup_{0\leqslant\tau\leqslant\eta_0}\|E\{U^\epsilon(0,\tau)f\}-A(0,\tau)f\|_0\leqslant\epsilon^{1-\gamma}C(f;\tau_0), \tag{39}$$

where $C(f;\tau_0)$ is a positive constant depending on f and its derivatives up to order 4 and τ_0 (which comes from $\eta_0=\tau_0/\epsilon$) but independent of ϵ.

Remark: The known limit theorems so far have dealt with the random field of the form $\epsilon^{-1}F=\epsilon^{-1}F_1+F_2$ for some mean-zero random fields F_1 and F_2 on a finite scaled interval. In this case, the random field F_2 can be ignored in the diffusion limit. On the interval of infinite scale considered here, however, F_2 may grow and become comparable to $\epsilon^{-1}F_1$ as η increases while F_1 remains controlled. Then the random field F_2 cannot be ignored anymore in the diffusion limit. This is the case for the turning point problem established in the previous section. Unless such a problem is dealt with separately in two different regions, therefore, we need the above theorem for a uniformly valid diffusion limit on the whole interval.

IV. INTERPLAY OF REFRACTION AND RANDOM SCATTERING

Now we apply the theorem in Sec. III to our stochastic turning point problem in Sec. II with the appropriate strong mixing condition for the random functions $\alpha_1(\eta/\epsilon^{4/3})$ and $\beta_1(\eta/\epsilon^{4/3})$. The necessary hypotheses described in the theorem are satisfied. In particular, the constant $C_{n,\epsilon}$ can be taken as

$$C_{n,\epsilon}=c_1((n-1)\eta_1)^{-1/2}+c_2\epsilon^{2/3}(n\eta_1)^{1/2},\quad n=2,3,\ldots m_0, \tag{40}$$

where the corresponding σ_n in (30) is given by $n\eta_1$ for a fixed $O(1)$ interval η_1, and c_1 and c_2 are some positive constants ($C_{1,\epsilon}$ can be defined as a fixed positive number since η_1 is finite). Note also that the decay condition (34) corresponds to $\gamma=1/2$:

$$\sum_{n=1}^{m_0}C_{n,\epsilon}\sim O(\epsilon^{-1/3}). \tag{41}$$

We present here explicitly, with exact scales, the ϵ-dependent single-frequency infinitesimal generator of the corresponding diffusion Markov process for our turning point problem. This is an adjoint form of the infinitesimal generator of the Fokker-Planck equation for the transition probability density of the diffusion process:

$$\begin{aligned}\mathscr{L}_\eta^\epsilon f=&[\gamma_{22}^\epsilon\omega^{4/3}\pi^2\alpha_0^2\zeta^8M^4(\eta)\{1-\cos\Omega^\epsilon(\eta,\omega,\psi,\tau_0)\}^2+\epsilon^{2/3}\gamma_{21}^\epsilon\omega^{2/3}\pi^2\zeta^4M^2(\eta)N^2(\eta)\\&\times\{1-\cos\Omega^\epsilon(\eta,\omega,\psi,\tau_0)\}\{1+\cos\Psi^\epsilon(\eta,\omega,\psi,\tau_0)\}+\epsilon^{2/3}\gamma_{12}^\epsilon\omega^{2/3}\pi^2\zeta^4M^2(\eta)N^2(\eta)\\&\times\{1-\cos\Omega^\epsilon(\eta,\omega,\psi,\tau_0)\}\{1+\cos\Psi^\epsilon(\eta,\omega,\psi,\tau_0)\}+\epsilon^{4/3}\gamma_{11}^\epsilon\pi^2\alpha_0^{-2}N^4(\eta)\\&\times\{1+\cos\Psi^\epsilon(\eta,\omega,\psi,\tau_0)\}^2]\partial_{\psi\psi}^2f+[\gamma_{22}^\epsilon\omega^{4/3}\pi^2\alpha_0^2\zeta^8M^4(\eta)\{1-\cos\Omega^\epsilon(\eta,\omega,\psi,\tau_0)\}\\&\times\sin\Omega^\epsilon(\eta,\omega,\psi,\tau_0)-\epsilon^{2/3}\gamma_{21}^\epsilon\omega^{2/3}\pi^2\zeta^4M^2(\eta)N^2(\eta)\{1-\cos\Omega^\epsilon(\eta,\omega,\psi,\tau_0)\}\\&\times\sin\Psi^\epsilon(\eta,\omega,\psi,\tau_0)+\epsilon^{2/3}\gamma_{12}^\epsilon\omega^{2/3}\pi^2\zeta^4M^2(\eta)N^2(\eta)\sin\Omega^\epsilon(\eta,\omega,\psi,\tau_0)\\&\times\{1+\cos\Psi^\epsilon(\eta,\omega,\psi,\tau_0)\}-\epsilon^{4/3}\gamma_{11}^\epsilon\pi^2\alpha_0^{-2}N^4(\eta)\sin\Psi^\epsilon(\eta,\omega,\psi,\tau_0)\\&\times\{1+\cos\Psi^\epsilon(\eta,\omega,\psi,\tau_0)\}]\partial_\psi f,\end{aligned} \tag{42a}$$

where $\Omega^\epsilon(\eta,\omega,\psi,\tau_0)$ and $\Psi^\epsilon(\eta,\omega,\psi,\tau_0)$ are given by

$$\Omega^\epsilon(\eta,\omega,\psi,\tau_0)=\psi+2(\omega\tau_0/\epsilon+\Omega(\eta)),\quad \Psi^\epsilon(\eta,\omega,\psi,\tau_0)=\psi+2(\omega\tau_0/\epsilon+\Psi(\eta)) \tag{42b}$$

and γ_{ij}^ϵ's, $i,j=1,2$, correspond to the following quantities in the z-scale:

$$\gamma_{ij}^{\epsilon}(z)=\int_0^{1/\epsilon}\gamma_{ij}(z,z/\epsilon^2;t)dt,\quad \Gamma_t(z,z/\epsilon^2)\equiv(\gamma_{ij}(z,z/\epsilon^2;t)), \tag{42c}$$

$$\Gamma_t(z,z/\epsilon^2)\equiv\begin{bmatrix} E\{\alpha_1(z,z/\epsilon^2)\alpha_1(z,z/\epsilon^2)\} & E\{\alpha_1(z,z/\epsilon^2)\beta_1(z,z/\epsilon^2)\} \\ E\{\beta_1(z,z/\epsilon^2)\alpha_1(z,z/\epsilon^2)\} & E\{\beta_1(z,z/\epsilon^2)\beta_1(z,z/\epsilon^2)\}\end{bmatrix}.$$

The above generator is uniformly valid in the region above the turning point (transition as well as outer regions). Note that there is a competition among diffusion and drift coefficients due to the asymptotic behavior of $M(\eta)$ and $N(\eta)$; the terms involving γ_{22}^{ϵ}, γ_{21}^{ϵ}, γ_{12}^{ϵ} and γ_{11}^{ϵ} are of orders $O(1)$, $O(\epsilon^{2/3})$, $O(\epsilon^{2/3})$ and $O(\epsilon^{4/3})$, respectively, in the transition region whereas all of these are of comparable $O(\epsilon^{2/3})$ order in the outer region. In (42c), the limits are finite in view of the mixing rate condition (25). These quantities represent the noise intensity where z represents the nonstationary slow-scale $(\epsilon^{2/3}\eta)$ dependence while z/ϵ^2 represents the fast random-scale $(\eta/\epsilon^{4/3})$ dependence.

For the frequency range of interest, the scale dependence of diffusion and drift terms in each region displays the subtle interplay of refraction and multiple scattering. Significant multiple scattering by the random layering occurs in both regions with diffusive spreading of the phase angle of the reflection coefficient. Note that the order $O(\epsilon^{2/3})$ in the η-scale corresponds to the order $O(1)$ in the z-scale. In particular, the singular scale, i.e. $O(\epsilon^{-2/3})$ in the z-scale, of diffusion and drift terms in the transition region indicates that the refraction of the wave plays little role near the turning point. This implies physically that the randomization effect is enhanced as the rays become aligned with random layers. As the frequency increases in the valid range of our analysis, the multiple scattering is even more pronounced near the turning point than in the outer region; the diffusion term grows with the frequency of order $\epsilon^{-2/3}\omega^{4/3}$ in the z-scale near the turning point whereas it grows with the order of $\omega^{2/3}$ in the outer region. At higher frequencies, the randomization due to the increased multiple scattering is expected to be much stronger even in the outer region so that the wave field becomes relatively insensitive to the turning point. The simulation study of Ref. 18 in the geophysical context has shown this behavior well. The coherent energy suffers attenuation due to this randomization process and the multiple scattering with wave interference tends to localize the energy.

V. PROOF OF THE EXTENDED LIMIT THEOREM

To prove the limit theorem established in the previous section, we begin with finite propagator property and the variation of constants formulas for the random propagators $U^{\epsilon}(\sigma,\tau)$ and the averaged backward propagators $A^{\epsilon}(\sigma,\tau)$.

(i) finite propagator property:

$$U^{\epsilon}(\sigma,\eta)U^{\epsilon}(\eta,\tau)=U^{\epsilon}(\sigma,\tau),\quad U^{\epsilon}(\tau,\tau)=I. \tag{43a}$$

(ii) infinitesimal forward and backward propagator properties:

$$I+\epsilon^{-1}\int_{\sigma}^{\tau}U^{\epsilon}(\sigma,\eta)V(\eta)d\eta=U^{\epsilon}(\sigma,\tau)=I+\epsilon^{-1}\int_{\sigma}^{\tau}V(\eta)U^{\epsilon}(\eta,\tau)d\eta. \tag{43b}$$

The property (i) comes from the uniqueness of solutions of the differential equation. If one differentiates the identity $(U^{\epsilon}(\sigma,\tau)f)(x)=f(x^{\epsilon}(\tau,\sigma,x))$ with respect to τ, then one can obtain a differential equation whose integral form is the first identity of (43b). If one differentiates (43a) with respect to η and let $\eta\downarrow\sigma$, then one obtains an equivalent form of the second identity of (43b). Also the averaged backward propagators $A^{\epsilon}(\sigma,\tau)$ satisfy

$$A^\epsilon(\sigma,\eta)A^\epsilon(\eta,\tau)=A^\epsilon(\sigma,\tau),\quad A^\epsilon(\sigma,\sigma)=I, \tag{44a}$$

$$A^\epsilon(\sigma,\tau)=I+\int_\sigma^\tau \mathscr{L}^\epsilon_\eta A^\epsilon(\eta,\tau)d\eta. \tag{44b}$$

Then, using (43) and (44), one can obtain for arbitrary $f\in\mathscr{C}^4$

$$\begin{aligned}E\{U^\epsilon(0,\tau)f\}-A^\epsilon(\sigma,\tau)f=&\sum_{n=1}^m E\{U^\epsilon(0,\sigma_{n-1})\{E\{U^\epsilon(\sigma_{n-1},\sigma_n)g_n\}-A^\epsilon(\sigma_{n-1},\sigma_n)g_n\}\}\\&+\sum_{n=1}^m E\{U^\epsilon(0,\sigma_{n-1})\{U^\epsilon(\sigma_{n-1},\sigma_n)g_n-E\{U^\epsilon(\sigma_{n-1},\sigma_n)g_n\}\}\},\end{aligned} \tag{45}$$

where $g_n=A^\epsilon(\sigma_n,\tau)f$ is a deterministic function in $\mathscr{C}^4$ and $\|g_n\|_4\leqslant a_4\|f\|_4$. Since the propagators $U^\epsilon(0,\sigma_{n-1})$ are contraction operators on $\mathscr{C}^0\to\mathscr{C}^0$, the $\|\cdot\|_0$ norm of the above (45) satisfies the following inequality:

$$\|E\{U^\epsilon(0,\tau)f\}-A^\epsilon(0,\tau)f\|_0\leqslant\sum_{n=1}^m(\mathbf{I}_n^1(f)+\mathbf{I}_n^2(f)), \tag{46a}$$

$$\mathbf{I}_n^1(f)\equiv\|E\{U^\epsilon(\sigma_{n-1},\sigma_n)g_n\}-A^\epsilon(\sigma_{n-1},\sigma_n)g_n\|_0, \tag{46b}$$

$$\mathbf{I}_n^2(f)\equiv\|E\{U^\epsilon(0,\sigma_{n-1})U^\epsilon(\sigma_{n-1},\sigma_n)g_n\}-E\{U^\epsilon(0,\sigma_{n-1})E\{U^\epsilon(\sigma_{n-1},\sigma_n)g_n\}\}\|_0. \tag{46c}$$

From now on, we will show that

$$\mathbf{I}_n^1(f),\quad \mathbf{I}_n^2(f)\leqslant\epsilon C_{n,\epsilon}\|f\|_4,\quad \forall f\in\mathscr{C}^4. \tag{47}$$

Once (47) is proved, then the estimate (39) of the theorem follows immediately from (38) and the decay condition (34) for $C_{n,\epsilon}$. The estimate for $\mathbf{I}_n^1(f)$ roughly corresponds to a limit theorem on each $O(1)$ interval I_n in our context. Since it would follow basically the same idea of proof as in previously known limit theorems,[11,12] we omit here the lengthy proof[24] of the estimate for $\mathbf{I}_n^1(f)$. The main tool for the estimate of $\mathbf{I}_n^2(f)$ is the following p-norm version of mixing lemma.[25]

Lemma 1: Let $F(\omega',\omega)$ be a function on $\Omega\times\Omega$ such that for fixed ω, $F(\cdot,\omega)$ is $\mathscr{F}_0^s$ measurable and for fixed ω', $F(\omega',\cdot)$ is $\mathscr{F}_{s+t}^\infty$ measurable and $|F(\omega',\omega)|\leqslant\phi(\omega')\psi(\omega)$, $E\{\phi^q\}<\infty$ and $E\{\psi^p\}<\infty$ with $1/q+1/p=1$ and $p,q>1$. Let $\mathscr{F}_s^t$ and P satisfy the hypotheses in Sec. III and set

$$\bar{F}(\omega')\equiv E\{F(\omega',\cdot)\}=\int_\Omega F(\omega',\omega)P(d\omega).$$

Then

$$|E\{F\}-E\{\bar{F}\}|\leqslant 2\rho^{1/q}(t)E^{1/q}\{\phi^q\}E^{1/p}\{\psi^p\}. \tag{48}$$

If one uses the backward propagator property (43b) for $U^\epsilon(\sigma_{n-1},\sigma_n)$, then one can represent $\mathbf{I}_n^2(f)$ as follows:

$$\mathbf{I}_n^2(f)=\sup_{x\in\mathscr{R}_c}\mathbf{I}_n^2(f,x), \tag{49a}$$

$$\mathbf{I}_n^2(f,x) \equiv \sup_{x\in\mathscr{R}_c} \epsilon^{-1} \left| \int_{\sigma_{n-1}}^{\sigma_n} \{E\{U^\epsilon(0,\sigma_{n-1})V(s)U^\epsilon(s,\sigma_n)\} - E\{U^\epsilon(0,\sigma_{n-1})E\{V(s)U^\epsilon(s,\sigma_n)\}\}\} g_n(x)ds \right|. \tag{49b}$$

Note that between $U^\epsilon(0,\sigma_{n-1})$, which is $\mathscr{F}_0^{\sigma_{n-1}/\epsilon^2}$ measurable, and $V(s)U^\epsilon(s,\sigma_n)$, which is $\mathscr{F}_{s/\epsilon^2}^{\infty}$ measurable, a gap has been created. This allows us to apply Lemma 1 to the integral of (49b) if the corresponding random variables $\phi(\omega')$ and $\psi(\omega)$ can be found appropriately. From now on, we give the estimate of $\mathbf{I}_n^2(f)$ in the context of Lemma 1. The corresponding random field is given by

$$F_n(\omega',\omega) = F(s,s/\epsilon^2,x^\epsilon(\sigma_{n-1},0,x,\omega'),\omega)\partial_x g_n(x^\epsilon(\sigma_n,s,x^\epsilon(\sigma_{n-1},0,x,\omega'),\omega)) \times \partial_x x^\epsilon(\sigma_n,s,x^\epsilon(\sigma_{n-1},0,x,\omega'),\omega). \tag{50}$$

The random field averaged with respect to $d\omega$ is denoted by

$$\bar{F}_n(\omega') = E\{F_n(\omega',\cdot)\}. \tag{51}$$

We wish to control random variables $\psi_n(\omega)$ and $\phi_n(\omega')$ defined as

$$\phi_n(\omega') = \sup_{s\in I_n, x\in\mathscr{R}_c \omega\in\Omega} \sup |F(s,s/\epsilon^2,x,\omega)\partial_x g_n(x^\epsilon(\sigma_n,s,x,\omega))|, \tag{52a}$$

$$\psi_n(\omega) = \sup_{s\in I_n, x\in\mathscr{R}_c} |\partial_x x^\epsilon(\sigma_n,s,x,\omega)|. \tag{52b}$$

Anticipating Lemma 2, we now apply Lemma 1 (with $p=q=2$) to each integrand of (49). Then we get the inequality

$$\mathbf{I}_n^2(f,x) \leqslant \epsilon C_{n,\epsilon}\|f\|_4 \int_0^\infty \rho^{1/2}(u)du \tag{53}$$

for all $x \in \mathscr{R}_c$, where the notational convention for $C_{n,\epsilon}$ was used. Then the assumed mixing rate condition implies the desired estimate for $\mathbf{I}_n^2(f)$. To complete the estimate for $\mathbf{I}_n^2(f)$, therefore, we are left to prove the following lemma.

Lemma 2: Let $x^\epsilon(\tau,\sigma,x)$ be the solution of stochastic initial value problem (27). Then on each interval I_n we have

$$\sup_{\sigma,\tau\in I_n, \sigma\leqslant\tau} \sup_{x\in\mathscr{R}_c} E^{1/p}\{|\partial_x x^\epsilon(\tau,\sigma,x)|^p\} \leqslant 1 + C_{n,\epsilon} \tag{54}$$

and thus the p^{th} moment of $\partial_x x^\epsilon(\tau,\sigma,x)$ is bounded uniformly in n by a constant. The random variables ψ_n and ϕ_n defined by (52) satisfy

$$E^{1/p}\{\psi_n^p(\omega)\} \leqslant 1 + C_{n,\epsilon}, \quad E^{1/q}\{\phi_n^q(\omega')\} \leqslant C_{n,\epsilon}\|f\|_4. \tag{55}$$

Proof: The second inequality in (55) holds because of condition (33). The first inequality will follow from the dominated convergence theorem, once (54) is proved. From now on, therefore, we focus on the estimate of the pth moment of $\partial_x x^\epsilon(\tau,\sigma,x)$. In order to estimate the pth moment of $\partial_x x^\epsilon(\tau,\sigma,x)$ on $O(1)$ interval I_n, we use the following variational argument.

First we define the following (vector) notation for convenience:

$$x_1^\epsilon(\tau,\sigma,x)\equiv x^\epsilon(\tau,\sigma,x),\quad x_2^\epsilon(\tau,\sigma,x)\equiv\partial_x x^\epsilon(\tau,\sigma,x),\tag{56a}$$

$$F_1(\tau,\tau/\epsilon^2,x^\epsilon(\tau,\sigma,x))\equiv F(\tau,\tau/\epsilon^2,x^\epsilon(\tau,\sigma,x)),\tag{56b}$$

$$F_2(\tau,\tau/\epsilon^2,x^\epsilon(\tau,\sigma,x))\equiv\partial_x F(\tau,\tau/\epsilon^2,x^\epsilon(\tau,\sigma,x))\partial_x x^\epsilon(\tau,\sigma,x).\tag{56c}$$

Then, from the random differential equation (27), we obtain

$$x_2^\epsilon(\tau,\sigma,x)=1+\epsilon^{-1}\int_\sigma^\tau F_2(s,s/\epsilon^2,x^\epsilon(s,\sigma,x))ds.\tag{57}$$

Using the Gronwall inequality, one can get the following local estimate; if $\sigma,\tau\in I_n$ and $0\leqslant\tau-\sigma\leqslant\epsilon$, then

$$|x_2^\epsilon(\tau,\sigma,x)|\leqslant e^{C_{n,\epsilon}},\quad |\partial_x x_2^\epsilon(\tau,\sigma,x)|\leqslant C_{n,\epsilon}.\tag{58}$$

Note that, once one can show the inequality (54) for any even integer $2p$, the same result is true for any positive integer p by the Cauchy–Schwartz inequality. So we consider only the case of even integer power of $|x_2^\epsilon(\tau,\sigma,x)|$ to prove Lemma 2. Let us first divide the interval $[\sigma,\tau]\subset I_n$ into ϵ-length segments such that

$$\sigma=\tau_0<\tau_1<\tau_2<\cdots<\tau_k<\cdots<\tau_{r-1}<\tau_r=\tau,\quad \tau_k=\sigma+k\epsilon,$$

where ϵ can be chosen such that $r=(\tau-\sigma)/\epsilon$ is an integer without loss of generality. If one takes the $2p$-power of (57) and differentiates with respect to τ and integrates it from σ to τ, then one can get

$$\{x_2^\epsilon(\tau,\sigma,x)\}^{2p}-\{x_2^\epsilon(\sigma,\sigma,x)\}^{2p}=2p/\epsilon\int_\sigma^\tau\left[1+1/\epsilon\int_\sigma^s F_2(t,t/\epsilon^2,x^\epsilon(t,\sigma,x))dt\right]^{2p-1}\times F_2(s,s/\epsilon^2,x^\epsilon(s,\sigma,x))ds,\tag{59}$$

which, from (57), leads to

$$\{x_2^\epsilon(\tau,\sigma,x)\}^{2p}=1+2p/\epsilon\int_\sigma^\tau F_2(s,s/\epsilon^2,x^\epsilon(s,\sigma,x))\{x_2^\epsilon(s,\sigma,x)\}^{2p-1}ds.\tag{60}$$

We decompose the integral on the right side of (60) into the integrals on the ϵ-length segments:

$$\{x_2^\epsilon(\tau,\sigma,x)\}^{2p}=1+2p/\epsilon\sum_{k=0}^{r-1}J_k^\epsilon(x),\tag{61a}$$

$$J_k^\epsilon(x)\equiv\int_{\tau_k}^{\tau_{k+1}}F_2(s,s/\epsilon^2,x^\epsilon(s,\sigma,x))\{x_2^\epsilon(s,\sigma,x)\}^{2p-1}ds,\quad k=0,1,\ldots,r.\tag{61b}$$

For $k=0$, in particular, the following estimate from (33) and (58) holds:

$$|J_0^\epsilon(x)|\leqslant\epsilon C_{n,\epsilon}\quad a.e.,\tag{62}$$

where the uniform boundedness of $C_{n,\epsilon}$, $n=1,2,..,m_0$, and the notational convention for $C_{n,\epsilon}$ were used. Combining (61) and (62), one obtains the inequality

$$E\{|x_2^\epsilon(\tau,\sigma,x)|^{2p}\}\leqslant 1+C_{n,\epsilon}+2p/\epsilon\sum_{k=1}^{r-1}|E\{J_k^\epsilon(x)\}|. \tag{63}$$

This inequality will have the form to which the discrete version of the Gronwall inequality can be used if the following inequality holds:

$$|E\{J_k^\epsilon(x)\}|\leqslant \epsilon^2 C_{n,\epsilon}E\{\{x_2^\epsilon(\tau_{k-1},\sigma,x)\}^{2p}\},\quad k=1,2,\ldots,r-1. \tag{64}$$

Suppose this is true [(64) will be proved in Lemma 3]. Then we can get estimate (54) with even integer $2p$ in the following way. Using the notation

$$E_k(\sigma,x,2p)\equiv|E\{\{x_2^\epsilon(\tau_k,\sigma,x)\}^{2p}-1\}|,\quad k=0,1,\ldots,r, \tag{65}$$

for convenience, one can obtain from assumption (64) that (63) becomes

$$E_r(\sigma,x,2p)\leqslant C_{n,\epsilon}+\epsilon C_{n,\epsilon}\sum_{k=1}^{r-1}E_k(\sigma,x,2p), \tag{66}$$

where the fact that $r=O(\epsilon^{-1})$ and the notational convention for $C_{n,\epsilon}$ were used. With the notation $\Lambda_j(\sigma,x,2p)$ defined by

$$\Lambda_0(\sigma,x,2p)\equiv 0,\quad \Lambda_j(\sigma,x,2p)\equiv\sum_{k=1}^{j}E_k(\sigma,x,2p),\quad j=1,2,\ldots,r, \tag{67}$$

inequality (66) can be expressed as

$$\Lambda_r(\sigma,x,2p)\leqslant C_{n,\epsilon}+(1+\epsilon C_{n,\epsilon})\Lambda_{r-1}(\sigma,x,2p). \tag{68}$$

Now we apply the discrete version of the Gronwall inequality to (68). Then

$$\Lambda_r(\sigma,x,2p)\leqslant C_{n,\epsilon}\frac{(1+\epsilon C_{n,\epsilon})^r-1}{\epsilon C_{n,\epsilon}}\leqslant\frac{e^{r\epsilon C_{n,\epsilon}}-1}{\epsilon}. \tag{69}$$

By substituting this inequality (corresponding to $r-1$ instead of r) into (68), we have

$$E_r(\sigma,x,2p)=\Lambda_r(\sigma,x,2p)-\Lambda_{r-1}(\sigma,x,2p)\leqslant C_{n,\epsilon}+\epsilon C_{n,\epsilon}\frac{e^{(r-1)\epsilon C_{n,\epsilon}}-1}{\epsilon}\equiv C_{n,\epsilon}. \tag{70}$$

Therefore, the desired estimate (54) follows for even integer $2p$. To complete the proof of Lemma 2, we are left to show inequality (64). Let us explicitly restate this inequality as follows by substituting (61b) into (64).

Lemma 3: For $\sigma_{n-1}\leqslant\sigma\leqslant\cdots\leqslant\tau_k\leqslant\tau_{k+1}\leqslant\cdots\leqslant\tau\leqslant\sigma_n$, we have the estimate

$$\left|E\left\{\int_{\tau_k}^{\tau_{k+1}}F_2(s,s/\epsilon^2,x^\epsilon(s,\sigma,x))\{x_2^\epsilon(s,\sigma,x)\}^{2p-1}ds\right\}\right|\leqslant\epsilon^2C_{n,\epsilon}E\{\{x_2^\epsilon(\tau_{k-1},\sigma,x)\}^{2p}\}. \tag{71}$$

Proof: To derive the estimate (71), we first introduce some useful identities. These identities provide the creation of gaps to allow the mixing lemma (Lemma 1) to be used. By differentiation and integration, one can have

$$\{x_2^\epsilon(s,\sigma,x)\}^{2p-1}=\{x_2^\epsilon(\tau_{k-1},\sigma,x)\}^{2p-1}+(2p-1)/\epsilon\int_{\tau_{k-1}}^{s}F_2(\nu,\nu/\epsilon^2,x^\epsilon(\nu,\sigma,x))\times\{x_2^\epsilon(\nu,\sigma,x)\}^{2(p-1)}d\nu, \tag{72}$$

where $\tau_k\leqslant s\leqslant\tau_{k+1}$. We also have the following identity by the fundamental theorem of calculus and chain rule:

$$F_2(s,s/\epsilon^2,x^\epsilon(s,\sigma,x))=F_2(s,s/\epsilon^2,x^\epsilon(\tau_{k-1},\sigma,x))+1/\epsilon\int_{\tau_{k-1}}^{s}(\partial_{\underline{x}}F_2(s,s/\epsilon^2,x^\epsilon(\nu,\sigma,x)),\underline{F}(\nu,\nu/\epsilon^2,x^\epsilon(\nu,\sigma,x)))d\nu, \tag{73}$$

where $\underline{x}=[x_1,x_2]^t$, $\underline{F}=[F_1,F_2]^t$ and $(\ ,\ )$ denote the inner product. From the above two identities (72) and (73), the integral on the left side of inequality (71) becomes

$$\begin{aligned}J_k^\epsilon(x)=&\int_{\tau_k}^{\tau_{k+1}}F_2(s,s/\epsilon^2,x^\epsilon(\tau_{k-1},\sigma,x))\{x_2^\epsilon(\tau_{k-1},\sigma,x)\}^{2p-1}ds\\&+(2p-1)/\epsilon\int_{\tau_k}^{\tau_{k+1}}\int_{\tau_{k-1}}^{s}F_2(s,s/\epsilon^2,x^\epsilon(\tau_{k-1},\sigma,x))F_2(\nu,\nu/\epsilon^2,x^\epsilon(\nu,\sigma,x))\\&\times\{x_2^\epsilon(\nu,\sigma,x)\}^{2(p-1)}d\nu ds\\&+1/\epsilon\int_{\tau_k}^{\tau_{k+1}}\int_{\tau_{k-1}}^{s}(\partial_{\underline{x}}F_2(s,s/\epsilon^2,x^\epsilon(\nu,\sigma,x)),\underline{F}(\nu,\nu/\epsilon^2,x^\epsilon(\nu,\sigma,x)))\\&\times\{x_2^\epsilon(\tau_{k-1},\sigma,x)\}^{2p-1}d\nu ds\\&+(2p-1)/\epsilon^2\int_{\tau_k}^{\tau_{k+1}}\int_{\tau_{k-1}}^{s}\int_{\tau_{k-1}}^{s}(\partial_{\underline{x}}F_2(s,s/\epsilon^2,x^\epsilon(\nu,\sigma,x)),\underline{F}(\nu,\nu/\epsilon^2,x^\epsilon(\nu,\sigma,x)))\\&\times F_2(\mu,\mu/\epsilon^2,x^\epsilon(\mu,\sigma,x))\{x_2^\epsilon(\mu,\sigma,x)\}^{2(p-1)}d\mu d\nu ds.\end{aligned} \tag{74}$$

There are, therefore, four terms to be estimated for the proof of Lemma 3. For the estimation of these terms, we repeatedly use the following inequalities which can be derived without difficulty:

Lemma 4: For $\sigma_{n-1}\leqslant\sigma\leqslant\cdots\leqslant\tau_k\leqslant\tau_{k+1}\leqslant\cdots\leqslant\tau\leqslant\sigma_n$, we have the estimate

$$|x_2^\epsilon(\nu,\sigma,x)|\leqslant e^{C_{n,\epsilon}}|x_2^\epsilon(\tau_{k-1},\sigma,x)|,\quad \tau_{k-1}\leqslant\nu\leqslant\tau_k, \tag{75}$$

$$\int_{\tau_k}^{\tau_{k+1}}\int_{\tau_{k-1}}^{s}\rho((s-\nu)/\epsilon^2)d\nu ds\leqslant\epsilon^3\int_0^\infty\rho(t)dt. \tag{76}$$

We present here an estimation for only one term (for example, the second term) of (74) since the other terms can be estimated in a similar way:

$$
\begin{aligned}
&\left| E\left\{ (2p-1)/\epsilon \int_{\tau_k}^{\tau_{k+1}} \int_{\tau_{k-1}}^{s} F_2(s,s/\epsilon^2,x^\epsilon(\tau_{k-1},\sigma,x)) F_2(\nu,\nu/\epsilon^2,x^\epsilon(\nu,\sigma,x)) \right.\right. \\
&\quad \left.\left. \times \{x_2^\epsilon(\nu,\sigma,x)\}^{2(p-1)} d\nu ds \right\} \right| \\
&= \left| E\left\{ (2p-1)/\epsilon \int_{\tau_k}^{\tau_{k+1}} \int_{\tau_{k-1}}^{s} E\{\partial_x F(s,s/\epsilon^2,x^\epsilon(\tau_{k-1},\sigma,x)) | \mathscr{F}_0^{\nu/\epsilon^2}\} \partial_x F(\nu,\nu/\epsilon^2,x^\epsilon(\nu,\sigma,x)) \right.\right. \\
&\quad \left.\left. \times x_2^\epsilon(\tau_{k-1},\sigma,x) \{x_2^\epsilon(\nu,\sigma,x)\}^{2p-1} d\nu ds \right\} \right| \\
&\leq E\left\{ (2p-1)/\epsilon \int_{\tau_k}^{\tau_{k+1}} \int_{\tau_{k-1}}^{s} 2\rho((s-\nu)/\epsilon^2) d\nu ds C_{n,\epsilon}^2 e^{2(2p-1)C_{n,\epsilon}} |x_2^\epsilon(\tau_{k-1},\sigma,x)|^{2p} \right\} \\
&\leq \epsilon^2 C_{n,\epsilon} E\{|x_2^\epsilon(\tau_{k-1},\sigma,x)|^{2p}\},
\end{aligned}
$$

where a property of conditional expectation, Lemma 1, (75) and (76), sequentially, with the notational convention for $C_{n,\epsilon}$. Therefore, Lemma 3 is proved.

VI. FINAL REMARKS

The random wave propagation problem considered in this paper has the two divided regions, i.e. propagating region and evanescent region, determined by effective medium theory. Our extended limit theorem leads to a uniform description of diffusion Markov process for random multiple scattering occurring in the propagating region. The scale dependence of the coefficients of the backward Kolmogorov equation provides an insight into the orchestral interplay of refraction and multiple scattering as one approaches to the turning point of our wave propagation problem. The intermediate frequency scaling considered here, however, needs to be extended in order to understand the problem for the full range of frequencies.

The problem of interest in the evanescent region requires different scattering variables from those introduced in this paper since the error term in the Lynn and Keller approximant is not small at all in this region. Consequently we need a limit theorem for stochastic differential equations with a right-hand side that consists of a rapidly varying deterministic part plus a zero-mean random fluctuation part. There is already a result[26] for this type of problem (stochastic Boltzmann equations). The scaling there, however, is different from our case. If the limit process of a diffusion-type can be obtained for evanescent waves, which will appear later, it would adjoin at the turning point with the limiting diffusion process obtained in this paper and provide a global limit law for the same physical problem; we will need to use a transformation at the turning point to obtain a marching limiting process in the whole region of the medium.

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Stochastic mechanics of reciprocal diffusions

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The dynamics and kinematics of reciprocal diffusions were examined in a previous paper [J. Math. Phys. **34**, 1846 (1993)], where it was shown that reciprocal diffusions admit a chain of conservation laws, which close after the first two laws for two disjoint subclasses of reciprocal diffusions, the Markov and quantum diffusions. For the case of quantum diffusions, the conservation laws are equivalent to Schrödinger's equation. The Markov diffusions were employed by Schrödinger [Sitzungsber. Preuss. Akad. Wiss. Phys. Math Kl. 144 (1931); Ann. Inst. H. Poincaré **2**, 269 (1932)], Nelson [*Dynamical Theories of Brownian Motion* (Princeton University, Princeton, NJ, 1967); *Quantum Fluctuations* (Princeton University, Princeton, NJ, 1985)], and other researchers to develop stochastic formulations of quantum mechanics, called stochastic mechanics. We propose here an alternative version of stochastic mechanics based on quantum diffusions. A procedure is presented for constructing the quantum diffusion associated to a given wave function. It is shown that quantum diffusions satisfy the uncertainty principle, and have a locality property, whereby given two dynamically uncoupled but statistically correlated particles, the marginal statistics of each particle depend only on the local fields to which the particle is subjected. However, like Wigner's joint probability distribution for the position and momentum of a particle, the finite joint probability densities of quantum diffusions may take negative values. © *1996 American Institute of Physics.* [S0022-2488(96)03402-8]

I. INTRODUCTION

Since the early days of quantum mechanics, many researchers have attempted to formulate quantum mechanics in terms of diffusions processes. These efforts were originally motivated by the observation that as the real time t is converted to imaginary time it, the Schrödinger and Fokker–Planck equations, which describe, respectively, the time evolutions of the wave function in quantum mechanics and the density of a Markov diffusion, are transformed into each other. This is, for example, the correspondence that was exploited by Kac[1] to derive a stochastic interpretation of Feynman path integrals.[2] This analogy has been used in recent years to develop a stochastic formulation of quantum mechanics, called Euclidean quantum mechanics, which relies on Markov diffusions.[3,4] However, since this interpretation is based on the Wick rotation $t \rightarrow it$, the resulting stochastic models can be viewed as evocative analogies, but not as a picture of physical reality.

Other attempts at relating quantum mechanics and diffusion processes are more radical, in the sense that they go beyond analogies and seek to demonstrate that these two theories are, in fact, equivalent. This line of investigation was initiated by Schrödinger[5] in 1931, who focused his attention on Markov diffusions. Unfortunately, Schrödinger's work was somewhat premature, since descriptions of Markov diffusions in terms of stochastic differential equations were not yet

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available, and as a consequence his results were not immediately exploited, and were taken up only later by Zambrini[6] and Nagasawa.[7] Inspired by the early work of Fenyes,[8] a slightly different approach was proposed by Nelson[9,10] and other researchers[11] to formulate quantum mechanics in terms of Markov diffusions. The key aspect of this theory, which is usually called Markovian stochastic mechanics, is that it employs the calculus of stochastic differential equations to give a precise meaning to kinematic quantities such as velocity and acceleration. Given the wave function of a quantum process, one associates to it a Markov diffusion with an identical probability density, where the gradient of the wave function phase specifies the mean velocity obtained by averaging the forward and backward drifts of the diffusion. However, like Bohm's hidden variables interpretation of quantum mechanics,[12] both the Schrödinger and Nelson versions of stochastic mechanics are *nonlocal*, in the sense that a ''quantum potential'' needs to be introduced to relate the forward and backward Fokker–Planck equations of the Markov diffusions with the Schrödinger equation of the matching wave function. This potential has the feature that for two dynamically uncoupled and widely separated particles, changes in their joint probability density affect immediately the forces acting on each particle. This lack of locality gives rise to significant differences[10,13] between Markovian stochastic mechanics and standard quantum mechanics.

We propose here an alternative form of stochastic mechanics based on a subclass of reciprocal diffusions, called the quantum diffusions. Reciprocal processes were introduced by Bernstein in 1932,[14] who was influenced by Schrödinger's above mentioned attempt at a stochastic formulation of quantum mechanics. Reciprocal processes were subsequently studied by Jamison,[15] who showed that over a finite interval, they could be constructed from Markov processes by applying a change of measure to the joint probability distribution of the end-point values of the process. This procedure can be used to construct reciprocal diffusions directly from Markov diffusions. In Refs. 16 and 17, Krener showed that reciprocal diffusions satisfy locally a stochastic form of Newton's law, which in the Gaussian case,[18] can be used to express reciprocal diffusions as the solutions of second-order stochastic differential equations. In Ref. 19, a stochastic quantization procedure was introduced to associate a class of reciprocal diffusions to a dynamical system satisfied by its Hamiltonian. This construction was used to characterize the kinematics and dynamics of reciprocal diffusions. It was shown that reciprocal diffusions satisfy a chain of conservation laws, which is generally infinite, but closes after the first two laws for two disjoint subclasses, the Markov and quantum diffusions. The quantum diffusions derive their name from the equivalence existing between their conservation laws and Schrödinger's equation for the associated Hamiltonian.

The stochastic mechanics described here associates to the wave function of a quantum system a matching quantum diffusion. This construction selects, in the equivalence class of reciprocal diffusions associated to a Hamiltonian, the diffusion which models the corresponding quantum process. The quantum diffusions have the feature that the closure rule satisfied by their conservation laws is essentially equivalent to Heisenberg's uncertainty principle for the position and momentum variables. Unlike Markovian stochastic mechanics,[10,13] the stochastic mechanics of quantum diffusions is local, in the sense that given two dynamically uncoupled but statistically correlated particles, the marginal probability density of each particle does not depend on the parameters of the potentials acting on the other particle. However, one interesting feature of this new stochastic mechanics is that the end-point densities that must be applied to model certain quantum processes, such as the excited states of the harmonic oscillator, can take negative values. The appearance of such negative densities should not come as a true surprise if one considers that the finite joint densities for the positions at successive times obtained here form an extension of the Wigner joint position-momentum distribution,[20,21] which also has the feature of taking negative values. Note that the marginal density for the position at a single time is always positive, so that, as argued in Ref. 22, the negativity of densities is not a real drawback, as long as one considers that observable quantum events have always positive probabilities.

The paper is organized as follows. The stochastic quantization procedure used to associate a

class of reciprocal diffusions to a dynamical system specified by its Hamiltonian is described in Sec. II, where the dynamical properties of reciprocal diffusions are reviewed. In Sec. III, the subclass of quantum diffusions is introduced, and a method is presented for constructing the quantum diffusion matching the wave function of a quantum system. This construction is simplified for the case of Gaussian processes in Sec. IV, and then illustrated by considering the minimum uncertainty wavepacket for a free particle and the ground state of the harmonic oscillator. In Sec. V, we prove that quantum diffusions satisfy Heisenberg's position-momentum uncertainty relation. The locality property of quantum diffusions is demonstrated in Sec. VI. Finally, it is shown in Sec. VII that negative probabilities must be allowed if one seeks to model certain quantum processes, such as the excited states of the harmonic oscillator.

II. DYNAMICAL SYSTEMS AND RECIPROCAL DIFFUSIONS

As a starting point, we recall that a process $x(t)\in\mathbb{R}^n$ defined over $[0,T]$ is reciprocal if for arbitrary subintervals $[s,t]$ of $[0,T]$, the process interior to $[s,t]$ is independent of the process exterior to $[s,t]$, given $x(s)$ and $x(t)$. When $x(\cdot)$ admits finite joint probability densities, it was shown by Jamison[15] that $x(\cdot)$ is completely specified by (i) the joint probability density $p(x_0,0;x_T,T)$ of its values $x(0)$ and $x(T)$ at the ends of the interval $[0,T]$; and (ii) its reciprocal transition density $r(x,s;y,t;z,u)$, which is the conditional density of $x(t)=y$, given that $x(s)=x$ and $x(u)=z$, with $s<t<u$. In order to correspond to a reciprocal density, a function r must satisfy two conditions. First, it must be a probability density in y, i.e.

$$\int r(x,s;y,t;z,u)dy=1, \tag{2.1a}$$

and the identity

$$r(w,s;x,t;z,v)r(x,t;y,u;z,v)=r(w,s;y,u;z,v)r(w,s;x,t;y,u), \tag{2.1b}$$

must hold for all $0\leqslant s<t<u<v\leqslant T$. This last condition is the analog for reciprocal processes of the Chapman–Kolmogorov equation of Markov processes. From this characterization, one can immediately deduce that if a process is Markov, it is necessarily reciprocal, but the converse does not hold, in general. Also, two reciprocal processes with the same transition density *r(x,s;y,t;z,u)* are said to belong to the same reciprocal class, since they exhibit the same local stochastic behavior.

Let $\mathbb{R}^n$ be the standard n-dimensional Euclidean space with metric $\delta_{ij}=1$ for $i=j$, and $=0$ otherwise. Consider a dynamical system with Hamiltonian

$$H(x,p,t)=\tfrac{1}{2}(p^i-A^i(x,t))(p_i-A_i(x,t))+\phi(x,t), \tag{2.2}$$

where $\{\phi,A_i\}$ denotes a scalar and vector potential pair, and where we employ the standard tensor contraction convention with repeated upper and lower indices corresponding to a summation. Under certain smoothness conditions for the potentials $\{\phi,A_i\}$, a stochastic quantization procedure was proposed in Ref. 19, which associates a class of reciprocal diffusions to the system (2.2).

The first step of this quantization procedure consists in replacing the momentum p_j by $-\boldsymbol{\nabla}_j$ inside the Hamiltonian $H(x,p,t)$, where $\boldsymbol{\nabla}_j$ denotes the differentiation with respect to x^j. This correspondence rule is the stochastic analog of the quantization rule $p_j\leftrightarrow -i\boldsymbol{\nabla}_j$ of quantum mechanics. This yields the elliptic operator

$$\mathbf{H}=\tfrac{1}{2}(\boldsymbol{\nabla}^i+A^i)(\boldsymbol{\nabla}_i+A_i)+\phi, \tag{2.3a}$$

$$=\tfrac{1}{2}\Delta+A^i\boldsymbol{\nabla}_i+\tfrac{1}{2}(\boldsymbol{\nabla}^iA_i+A^iA_i)+\phi, \tag{2.3b}$$

where Δ denotes the Laplacian. Then the generalized heat operator,

$$\mathbf{L}=\mathbf{H}-\frac{\partial}{\partial t}, \tag{2.4}$$

is the forward operator of a general Markov diffusion with unit diffusion matrix δ^{ij} drift $b^i(x,t)=-A^i(x,t)$ and creation/killing rate

$$c(x,t)\triangleq\tfrac{1}{2}(A^iA_i-\boldsymbol{\nabla}^iA_i)(x,t)+\phi(x,t). \tag{2.5}$$

See Ref. 23 for a study of Markov diffusions with creation or killing. The Green's function $G(x,s;y,t)$ associated to $\mathbf{L}$ is given by

$$\mathbf{L}_{y,t}G(x,s;y,t)=0, \quad t\geqslant s, \tag{2.6a}$$

$$G(x,s;y,s)=\delta(x-y), \tag{2.6b}$$

where the subscripts $\{y,t\}$ specify the variables upon which the operator $\mathbf{L}$ is acting. To ensure that $G(x,s;y,t)$ represents the transition density of a general Markov diffusion, $G(x,s;y,t)$ is also required to decay as $|y|\to\infty$.

Then, $x(t)$ is a reciprocal diffusion over $[0,T]$ in the class associated to the Hamiltonian (2.2) if given an arbitrary set of times $t_0=0<t_1<\cdots<t_N=T$, the joint probability density of $x(t_0),x(t_1),\ldots,x(t_N)$ can be expressed as

$$p(x_0,t_0;x_1,t_1;\ldots;x_N,t_N)=q(x_0,t_0;x_N,t_N)\prod_{k=0}^{N-1}G(x_k,t_k;x_{k+1},t_{k+1}), \tag{2.7}$$

where the end-point density $q(x_0,0;x_T,T)$ is positive and satisfies the normalization condition

$$\int\int q(x_0,0;x_T,T)G(x_0,0;x_T,T)dx_0\,dx_T=1. \tag{2.8}$$

Since the Green's function $G(x,s;y,t)$ is completely specified by the Hamiltonian $H(x,p,t)$, the expression (2.7) indicates that all diffusions associated to a given physical system differ only by the choice of end-point density $q(x_0,0;x_T,T)$. To verify that the finite joint densities (2.7) satisfy the Jamison conditions (2.1a)–(2.1b), note that for $s<t<u$, the three-point transition density $r(x,s;y,t;z,u)$ can be expressed as

$$r(x,s;y,t;z,u)=\frac{G(x,s;y,t)G(y,t;z,u)}{G(x,s;z,u)}. \tag{2.9}$$

Then (2.1b) can be verified by inspection, and the fact that $r(x,s;y,t;z,u)$ is a density in y is a consequence of the transition property,

$$G(x,s;z,u)=\int G(x,s;y,t)G(y,t;z,u)dy \tag{2.10}$$

of the heat kernel G.

The end-point density q appearing in (2.7) is related to the joint probability density of $x(0)$ and $x(T)$ through the relation

$$p(x_0,0;x_T,T)=q(x_0,0;x_T,T)G(x_0,0;x_T,T). \tag{2.11}$$

From the structure (2.7) for the finite joint densities, we deduce that when the interval of definition of a reciprocal diffusion is restricted from $[0,T]$ to a subinterval $[s,t]$ with $0<s<t<T$, the density $q(x,s;y,t)$ that needs to be applied to the new end points (s,t) is given by

$$q(x,s;y,t)=\int\int G(x_0,0;x,s)G(y,t;x_T,T)q(x_0,0;x_T,T)dx_0\,dx_T. \tag{2.12}$$

The expression (2.12) implies that $q(x,s;y,t)$ with $s\leqslant t$ satisfies the two evolution equations,

$$\mathbf{L}_{x,s}q(x,s;y,t)=0, \tag{2.13a}$$

$$\mathbf{L}^*_{y,t}q(x,s;y,t)=0, \tag{2.13b}$$

where $\mathbf{L}^*$ denotes the adjoint operator of $\mathbf{L}$.

Within the general class of reciprocal diffusions specified by the Hamiltonian $H(x,p,t)$, it was shown in Theorem 2.1 of Ref. 19 that the subclass of Markov diffusions has the feature that for any subinterval $[t,s]$ of $[0,T]$, the end-point density $q(x,s;y,t)$ admits the separable structure

$$q(x,s;y,t)=q_f(x,s)q_b(y,t), \tag{2.14}$$

where $q_f(x,t)$ and $q_b(y,t)$ obey, respectively, the forward and backward heat quations,

$$Lq_f(x,t)=0,\quad L^*q_b(x,t)=0, \tag{2.15}$$

with initial conditions $q_f(x_0,0)$ and $q_b(x_T,T)$, respectively.

The identities (2.7) and (2.12) imply that the density $\rho(x,t)$ of a reciprocal diffusion $x(t)$ can be expressed as

$$\rho(x,t)=q(x,t;x,t)=\int\int G(x_0,0;x,t)G(x,t;x_T,T)q(x_0,0;x_T,T)dx_0\,dx_T, \tag{2.16}$$

so that it is completely fixed by q. In the Markov case, this expression reduces to

$$\rho(x,t)=q_f(x,t)q_b(x,t), \tag{2.17}$$

which represents a modification due to Schrödinger of the standard representation for the density of a Markov diffusion, where instead of viewing ρ as the solution of either a forward or a backward heat equation, it is expressed as a product of components q_f and q_b propagating in both time directions. These two components describe the information about the diffusion process specified at each end of the interval $[0,T]$. In Schrödinger's attempt at reformulating quantum mechanics in terms of Markov diffusions, which is further elaborated in Refs. 6 and 7, the identity (2.17) is employed as a substitute for the usual representation,

$$\rho(x,t)=\psi(x,t)\psi^*(x,t), \tag{2.18}$$

for the density of a quantum process in terms of the wave function $\psi(x,t)$ generated by Schrödinger's equation. Unfortunately, as we shall see below, the potentials $\{A_i,\phi\}$ used to construct the wave function ψ are inconsistent with those employed to generate the matching Markov diffusion.

In Ref. 19, several important properties of reciprocal diffusions were derived, which are now summarized. We denote the mean position and the centered first- and second-order differences of the process $x(t)$ as

$$\bar{x}(t,h)=\tfrac{1}{2}(x(t+h)+x(t-h)), \tag{2.19a}$$

$$d^1x(t,h)=\tfrac{1}{2}(x(t+h)-x(t-h)), \tag{2.19b}$$

$$d^2x(t,h)=x(t+h)+x(t-h)-2x(t). \tag{2.19c}$$

Then, it was shown in Ref. 19 that the three-point transition density $r(\bar{x}-uh,t-h;x,t;\bar{x}+uh,t+h)$ of $x(t)=x$ given $x(t\pm h)=\bar{x}\pm uh$ can be approximated locally by a Gaussian distribution for $d^2x(t,h)$ with mean

$$E[d^2x^i|x(t\pm h)=\bar{x}\pm uh]=F^i(\bar{x},u,t)h^2+O(h^{5/2}), \tag{2.20}$$

and variance

$$E[d^2x^i\ d^2x^j|x(t\pm h)=\bar{x}\pm uh]=2h\delta^{ij}+O(h^{5/2}). \tag{2.21}$$

In relation (2.20), if

$$dA_{ij}=\frac{\partial A_j}{\partial x^i}-\frac{\partial A_i}{\partial x^j} \tag{2.22}$$

denotes the exterior derivative of A_i,

$$F_i(x,u,t)=dA_{ij}(x,t)u^j-\left(\frac{\partial\phi}{\partial x^i}+\frac{\partial A_i}{\partial t}\right)(x,t), \tag{2.23}$$

represents the force applied to a particle with position x and velocity u due to the potentials $\{A^i,\phi\}$. Thus (2.20) can be viewed as a stochastic form of Newton's law, since it states that the conditional mean acceleration,

$$a^i=E\left[\frac{d^2x^i}{h^2}\middle|x(t\pm h)=\bar{x}\pm uh\right], \tag{2.24}$$

for the process at time t equals the force based on the mean position $\bar{x}(t,h)$ and empirical velocity $u(t,h)=d^1x(t,h)/h$ estimated from the positions at times $t\pm h$. Note that this form of Newton's law is *noncausal*, since the conditioning is taken with respect to positions at times $t-h$ and $t+h$. From a physical point of view, we see that the local motion of a reciprocal diffusion is obtained by superposing the classical motion specified by the force F_i with some random fluctuations, which, according to the expression (2.21) for the conditional variance, have a size proportional to $h^{1/2}$. Note also that the definition (2.24) of the acceleration differs from the one employed by Nelson[9,10] in his derivation of Newton's law for Markov diffusions. See Ref. 24 for a detailed comparison of the two accelerations.

Let

$$M(a,b,t)\triangleq\ln\ q(a-b,t;a+b,t) \tag{2.25}$$

and

$$w_i(a,t)=\frac{1}{2}\frac{\partial M}{\partial b^i}\,(a,0,t), \tag{2.26a}$$

$$\pi_{ij}(a,t)=\frac{1}{4}\frac{\partial^2 M}{\partial b^i\partial b^j}\,(a,0,t), \tag{2.26b}$$

$$\tau_{ijk}(a,t)=\frac{1}{8}\frac{\partial^3 M}{\partial b^i\,\partial b^j\,\partial b^k}(a,0,t). \tag{2.26c}$$

Then, in addition to the above characterization for the mean acceleration, it was shown in Ref. 19 that the conditional density of the first difference $d^1x(t,h)$ given the mean position $\bar{x}(t,h)$, is locally Gaussian with mean

$$E[d^1x(t,h)|\bar{x}(t,h)=x]=v^i(x,t)h+O(h^2), \tag{2.27}$$

where

$$v^i(x,t)\triangleq -A^i(x,t)+w^i(x,t), \tag{2.28}$$

represents the *mean velocity* of the process, and with covariance

$$E[(d^1x^i-v^i(x,t)h)(d^1x^j-v^j(x,t)h)|\bar{x}(t,h)=x]=\delta^{ij}h/2+\pi^{ij}(x,t)h^2+o(h^2). \tag{2.29}$$

By analogy with the kinetic theory of gases, for which the $1/h$ term of the covariance expansion (2.29) is not present, we call $\pi^{ij}(x,t)$ the *stress tensor* of the Gaussian velocity distribution specified by (2.27) and (2.28).

An important difference between the stochastic Newton law and velocity distribution obtained above is that whereas the conditional distribution for d^2x specified by (2.20)–(2.21) is the same for all diffusions in the same reciprocal class, the velocity distribution given by (2.27)–(2.29) depends on the density function $q(x,s;y,t)$ through the functions $w^i(x,t)$ and $\pi^{ij}(x,t)$, so that different diffusions within a same reciprocal class will admit different conditional velocity distributions.

Finally, it was shown in Ref. 19 that reciprocal diffusions admit an infinite chain of conservation laws, which can be generated by considering the function $q(x,t;y,t)$ obtained by letting $s\to t$ in the end-point density of the reciprocal diffusion over $[s,t]$. The identities (2.13a)–(2.13b) imply $q(x,t;y,t)$ obeys the evolution equation

$$\frac{\partial q}{\partial t}(x,t;y,t)=(\mathbf{H}_{x,t}-\mathbf{H}^*_{y,t})q(x,t;y,t). \tag{2.30}$$

Then, the function

$$m(a,b,t)\triangleq q(a-b,t;a+b,t), \tag{2.31}$$

plays the role of generating function for the conservation laws. Specifically, by performing a Taylor series expansion of $m(a,b,t)$ in the vicinity of $b=0$ and taking into account the definitions (2.26a)–(2.26b) of w_i and π_{ij}, we find $m(a,b,t)$ admits the power series representation,

$$m(a,b,t)=\rho(a,t)\Bigg[1+2w_i(a,t)b^i+4(\pi_{ij}+w_iw_j)(a,t)\,\frac{b^ib^j}{2} +8(\tau_{ijk}+\pi_{ij}w_k+\pi_{ki}w_j+\pi_{jk}w_i+w_iw_jw_k)(a,t)\,\frac{b^ib^jb^k}{6}+\cdots\Bigg], \tag{2.32}$$

for small b. The chain of conservation laws of reciprocal diffusions is then obtained by performing the change of coordinates $x=a-b$ and $y=a+b$ and matching successive powers of b on both sides of (2.30). The constant term yields the law of mass conservation,

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla}^i(\rho v_i) = 0. \tag{2.33}$$

The linear terms in b^j give the conservation of momentum,

$$\frac{\partial}{\partial t}(\rho v_j) + \boldsymbol{\nabla}^i(\rho P_{ij}) = \rho F_j(x,v,t), \tag{2.34}$$

where F_j is the force defined in (2.23) and where, by analogy with fluid dynamics,

$$P_{ij}(x,t) \triangleq (\pi_{ij} + v_i v_j)(x,t), \tag{2.35}$$

is called the *flux of momentum tensor*. Finally, matching the quadratic terms in $b^j b^k$, we obtain the tensor form

$$\frac{\partial}{\partial t}(\rho P_{jk}) + \boldsymbol{\nabla}^i(\rho S_{ijk}) = \rho(dA_{ji}\, P^i{}_k + dA_{ki}\, P^i{}_j + f_j v_k + f_k v_j) \tag{2.36}$$

of the conservation of energy. In this expression,

$$f_j(x,t) = -\left(\frac{\partial A_j}{\partial t} + \frac{\partial \phi}{\partial x^j}\right)(x,t), \tag{2.37}$$

corresponds to the electric component (the part independent of v) of the force F_j, and if we introduce the tensor

$$\sigma_{ijk}(x,t) \triangleq \left(\tau_{ijk} - \frac{1}{4}\frac{\partial^2 A_i}{\partial x^j\, \partial x^k}\right)(x,t), \tag{2.38a}$$

$$S_{ijk}(x,t) \triangleq (\sigma_{ijk} + \pi_{ij} v_k + \pi_{ki} v_j + \pi_{jk} v_i + v_i v_j v_k)(x,t), \tag{2.38b}$$

represents the *flux of energy tensor*. Then, if we denote the internal energy by $E = \pi_j{}^j/2$,, and take the trace of (2.36) by using the skew symmetry of the tensor dA_{ij}, we obtain the scalar form

$$\frac{\partial}{\partial t}\left(\rho\left(E + \frac{1}{2} v_j v^j\right)\right) + \frac{1}{2}\boldsymbol{\nabla}^i(\rho S_{ij}{}^j) = \rho f_j v^j \tag{2.39}$$

of the energy conservation law of fluid mechanics, where the term $v_j v^j/2$ represents the kinetic energy.

The above procedure for generating the conservation laws of reciprocal diffusions makes clear that they usually form an infinite chain, since each successive law contains a divergence term involving the next conserved quantity in the chain. However for the Gaussian case, i.e., when

$$A_i(x,t) = A_{ij}(t)x^j, \quad \phi(x,t) = \tfrac{1}{2}\Phi_{ij}(t)x^i x^j, \tag{2.40}$$

are, respectively, linear and quadratic in x, and $\ln q(x_0,0;x_T,T)$ is a quadratic form of x_0 and x_T, the tensor $\sigma_{ijk}(x,t)$ given by (2.38a) is identically zero, so that S_{ijk} depends only on the previous conserved quantities in the chain. In this case, the chain closes after the first three laws. Specifically, in the Gaussian case, $\rho(x,t)$ and $v(x,t)$ admit the parametrization

$$\rho(x,t) = N(x_C(t), K_x(t)), \tag{2.41a}$$

$$v(x,t) = \dot{x}_C(t) + V(t)(x - x_C(t)), \tag{2.41b}$$

where $N(m,K)$ denotes a normal distribution with mean vector and covariance matrix K. Here $x_C(t)$ represents the classical trajectory in the absence of random fluctuations and $K_x(t)$ denotes the covariance matrix of $x(t)$. The stress tensor π_{ij} does not depend on x, and can be represented by an $n\times n$ matrix $\pi(t)$. Let

$$L_1(t)=A^T(t)-A(t), \tag{2.42a}$$

$$L_2(t)=-\Phi(t)-\frac{dA}{dt}(t), \tag{2.42b}$$

where $A(t)$ and $\Phi(t)$ are the $n\times n$ matrices representing the tensors A_{ij} and Φ_{ij} in the parametrization (2.40) of the covector and scalar potentials, and T denotes the matrix transpose. Then, the conservation laws (2.33), (2.34), and (2.36) can be expressed compactly[25] as

$$\frac{d\Omega}{dt}=\Lambda\Omega+\Omega\Lambda^T, \tag{2.43}$$

with

$$\Omega=\begin{bmatrix} K_x & K_xV \\ VK_x & \pi+VK_xV^T \end{bmatrix}, \tag{2.44a}$$

$$\Lambda=\begin{bmatrix} 0 & I_n \\ L_2 & L_1 \end{bmatrix}, \tag{2.44b}$$

which obviously forms a closed system.

III. CONSTRUCTION OF QUANTUM DIFFUSIONS

The general family of reciprocal diffusions contains two interesting and disjoint subclasses, the Markov and quantum diffusions, for which the chain of conservation laws closes after the first two. These two classes are characterized by the requirement that the functions $w_i(x,t)$ and $\pi_{ij}(x,t)$ given by (2.26a)–(2.26b) must satisfy the closure rules,

$$w_i(x,t)=\nabla_i S(x,t), \tag{3.1a}$$

$$\pi_{ij}(x,t)=\frac{\epsilon}{4}\nabla_i\nabla_j \ln \rho(x,t), \tag{3.1b}$$

where $S(x,t)$ is an arbitrary function, and where $\epsilon=1$ for Markov diffusions and $\epsilon=-1$ in the quantum case. Note that (3.1a) is satisfied whenever the exterior derivative of $w_i=v_i+A_i$ equals zero. Using this last observation, it is easy to verify that for the Gaussian case, the closure rules reduce to

$$L_1(t)=V(t)-V^T(t), \tag{3.2a}$$

$$\pi(t)=-\frac{\epsilon}{4}K_x^{-1}(t), \tag{3.2b}$$

where K_x, V, and L_1 are as defined in (2.41)–(2.42). By using the representation (2.43) of the conservation laws, we can also verify that if the closure rules (3.2) hold at one instant in time, at that instant we have

$$\frac{d}{dt}(L_1+V^T-V)=\frac{d}{dt}\left(\pi+\frac{\epsilon}{4}K_x^{-1}\right)=0, \tag{3.3}$$

so that the closure rules continue to hold for the complete time interval over which (2.43) admits a solution. In other words, once closed, the conservation laws remain closed.

For the non-Gaussian case, to discuss the consequences of the closure rules (3.1), it is convenient to rewrite the conservation laws (2.33), (2.34), and (2.36), which are expressed in Eulerian form, in the equivalent Lagrangian form

$$\frac{\partial\rho}{\partial t}+v_i\boldsymbol{\nabla}^i\rho+\rho\ \boldsymbol{\nabla}^i v_i=0, \tag{3.4a}$$

$$\rho\ \frac{\partial v_j}{\partial t}+\rho v_i\ \nabla^i v_j+\boldsymbol{\nabla}^i(\rho\pi_{ij})-\rho F_j=0, \tag{3.4b}$$

$$\rho\ \frac{\partial\pi_{jk}}{\partial t}+\rho v_i\ \nabla^i\pi_{jk}+\boldsymbol{\nabla}^i(\rho\sigma_{ijk})=\rho[(dA_{ji}-\boldsymbol{\nabla}_i v_j)\pi^i{}_k+(dA_{ki}-\boldsymbol{\nabla}_i v_k)\pi^i{}_j]. \tag{3.4c}$$

Then, if we introduce the function

$$R(x,t)=\tfrac{1}{2}\ln\ \rho(x,t), \tag{3.5}$$

and use (3.1a) to specify $S(x,t)$, it is easy to verify that under the closure rules (3.1a)–(3.1b), the first two conservation laws can be expressed in terms of R and S as

$$\frac{\partial R}{\partial t}+(\boldsymbol{\nabla}^i S-A^i)\boldsymbol{\nabla}_i R+\frac{1}{2}\ \boldsymbol{\nabla}^i(\boldsymbol{\nabla}_i S-A_i)=0, \tag{3.6}$$

$$\boldsymbol{\nabla}_j I(x,t)=0, \tag{3.7a}$$

with

$$I(x,t)\triangleq\frac{\partial S}{\partial t}+\frac{1}{2}\ (\boldsymbol{\nabla}^i S-A^i)(\boldsymbol{\nabla}_i S-A_i)+\phi+\frac{\epsilon}{2}\ (\boldsymbol{\nabla}^i R\ \boldsymbol{\nabla}_i R+\Delta R). \tag{3.7b}$$

The identity (3.7a) implies that $I(x,t)$ depends on t only, i.e., $I(x,t)=I(t)$. At this point, it is useful to note that for a fixed w_i, the relation (3.1a) specifies $S(x,t)$ only up to a function of t, say $f(t)$. This function contributes a term equal to $\dot{f}(t)$ to $I(t)$, which can be used to set $I(t)\equiv 0$. Thus, under the closure rules (3.1), we have shown that the first two conservation laws are equivalent to the coupled evolution equations (3.6) and (3.7b), with $I=0$, for R and S. Note that except for the addition of the term $-\epsilon\kappa/2$, with

$$\kappa\triangleq-(\boldsymbol{\nabla}^i R\ \boldsymbol{\nabla}_i R+\Delta R)=-\frac{\Delta\rho^{1/2}}{\rho^{1/2}}, \tag{3.8}$$

the equation $I(x,t)=0$ is identical to the Hamilton–Jacobi equation of classical mechanics.

In the Markov case, for which $\epsilon=1$, if we denote

$$q_f(x,t)=\exp(R-S)(x,t), \tag{3.9a}$$

$$q_b(x,t)=\exp(R+S)(x,t), \tag{3.9b}$$

it is easy to verify that Eq. (3.6) and (3.7b) can be rewritten as the decoupled forward and backward heat equations (2.15) for q_f and q_b. With this choice, the product

$$q_f(x,t)q_b(x,t)=\exp 2R(x,t)=\rho(x,t) \tag{3.10}$$

corresponds precisely to the identity (2.14) for the probability density of a Markov diffusion.

Similarly, for the quantum case, for which $\epsilon=-1$, if we introduce the wave function

$$\psi(x,t)=\exp(R+iS)(x,t), \tag{3.11}$$

the coupled equations (3.6) and (3.7b) correspond, respectively, to the real and imaginary parts of Schrodinger's equation,

$$i\,\frac{\partial\psi}{\partial t}=\mathbf{H}_Q\psi(x,t), \tag{3.12}$$

where we have set Planck's constant $\hbar=1$, and where the Hermitian operator,

$$\mathbf{H}_Q=\tfrac{1}{2}(-i\boldsymbol{\nabla}^i-A^j)(-i\boldsymbol{\nabla}_j-A_j)+\phi, \tag{3.13}$$

is obtained by applying the correspondence principle $p_j\leftrightarrow -i\boldsymbol{\nabla}_j$ of quantum mechanics to the Hamiltonian $H(x,p,t)$. The wave function $\psi(x,t)$ obtained in this manner satisfies

$$|\psi(x,t)|^2=\exp 2R(x,t)=\rho(x,t), \tag{3.14}$$

and is thus consistent with the probability density of the quantum diffusion we are considering.

Comparing the coupled evolution equations (3.6) and (3.7b) for $\epsilon=1$ and $\epsilon=-1$, one finds that the probability density ρ of a quantum diffusion with potentials $\{A_i,\phi\}$ is consistent with the density of a Markov diffusion with potentials $\{A_i,\phi'\}$, where

$$\phi'=\phi+\kappa, \tag{3.15}$$

with κ given by (3.8). This identification forms the basis for the reinterpretation of quantum mechanics based on Markov diffusions proposed by Schrödinger[5] and later refined by Zambrini[9] and Nagasawa.[10] In this respect, it is worth noting that the correction term κ relating the physical potential ϕ to the potential ϕ' of the matching Markov diffusion is identical, except for a factor of 2, to the "quantum potential" introduced by Bohm[12] in his causal formulation of quantum mechanics in terms of hidden variables (see Ref. 26 for comprehensive accounts of Bohm's theory). The factor of 2 arises because the correcting potential that must be applied to the stochastic Hamilton–Jacobi equation (3.7b) to transform the Markov motion ($\epsilon=1$) into a quantum one ($\epsilon=-1$) is twice as large as the correction needed to go from the classical motion ($\epsilon=0$) to the quantum motion. One problem associated with the introduction of a quantum potential is, of course, that it implies an action at a distance whereby two widely separated particles can affect each other instantaneously, thus violating the locality of classical physics, according to which the dynamics of each particle should be governed only by local force fields.

Nelson's stochastic mechanics[9–11] relies also on Markov diffusions. However, unlike Schrödinger's approach, which redefines the force fields to incorporate a quantum potential, it redefines the acceleration. Specifically, for a Markov diffusion $x(t)$, Nelson's stochastic acceleration takes the form

$$a_N^i(t)=\tfrac{1}{2}(D_-D_++D_+D_-)x^i(t), \tag{3.16}$$

where D_+ and D_- denote the mean forward and backward derivatives corresponding to $x(t)$. In flat space, and for an arbitrary tensor $T(x,t)$, these derivatives are defined as

$$D_+T(x(t),t)=\lim_{h\to 0}\frac{1}{h}E_t[T(x(t+h),t+h)-T(x(t),t)], \tag{3.17a}$$

$$D_-T(x(t),t)=\lim_{h\to 0}\frac{1}{h}E_t[T(x(t),t)-T(x(t-h),t-h)], \tag{3.17b}$$

where E_t denotes the conditional expectation given $x(t)$. It is shown in Ref. 24 [see Eq. (7.4)] that for a standard Markov diffusion with forward drift $b^i(x,t)$, which corresponds to setting $A^i=-b^i$ and $\phi=-(b^ib_i+\nabla^ib_i)/2$, and diffusion metric δ_{ij}, the acceleration $a_N^i(t)$ satisfies

$$a_N^i(t)=F^i(x(t),v(x(t),t),t)+\nabla^i\kappa(x(t),t), \tag{3.18}$$

where $F(x,v,t)$ is the force defined in (2.23),

$$v(x(t),t)=\tfrac{1}{2}(D_++D_-)x(t), \tag{3.19}$$

coincides with the mean velocity specified by (2.27), and κ is the quantum potential given in (3.8). Consequently, when Nelson's acceleration is evaluated for a Markov diffusion with modified potentials $\{A_i,\phi'\}$, we obtain

$$a_N^i(t)=F^i(x(t),v(x(t),t),t), \tag{3.20}$$

so that the acceleration equals the force associated to the unmodified potentials $\{A_i,\phi\}$. Thus, even though Nelson's stochastic mechanics employs exactly the same Markov diffusions as Schrodinger's theory, in the Newton law $ma=F$, where we have set $m=1$, the correction term associated to the quantum potential is shifted from the right to the left-hand side through a redefinition of the acceleration. Not surprisingly, it was discovered that Nelson's stochastic mechanics is nonlocal, a feature that, although it is viewed as a virtue by advocates of Bohm's theory (see Ref. 27 for a discussion of stochastic mechanics from a Bohmian viewpoint), led Nelson (Ref. 10, p. 127) to write "But the whole point (of the Markovian stochastic mechanics) was to construct a physically realistic picture of microprocesses, and a theory that violates locality is untenable."

The problem is, of course, that the conservation laws of Markov diffusions are not equivalent to Schrödinger's equation, and our objective here is to develop a stochastic mechanics, which instead of focusing on Markov diffusions, will apply to the quantum diffusions obtained by setting $\epsilon=-1$ in the closure rules (3.1). As a first step, we need to prove that such diffusions exist. Specifically, in the specification (2.7) for the reciprocal diffusions associated to a Hamiltonian with potentials $\{A_i,\phi\}$, the only element that does not depend on the physics of the problem is the end-point density $q(x,s;y,t)$. We need therefore to construct densities q such that the closure rules (3.1) hold with $\epsilon=-1$. In addition, since we seek to model quantum phenomena, it would be nice, if given a wave function $\psi(x,t)$ satisfying Schrödinger's equation, we could construct the matching q directly from ψ.

To elucidate the structure of the density $q(x,s;y,t)$ for quantum diffusions, consider the function $M(a,b,t)$ defined in (2.25). Taking into account the definition (2.26b) of $\pi_{ij}(a,t)$ and observing that

$$M(a,0,t)=\ln\,\rho(a,t)=2R(a,t), \tag{3.21}$$

the closure rule (3.1b) can be expressed as

$$\left(\frac{\partial^2 M}{\partial a^k\,\partial a^l}+\frac{\partial^2 M}{\partial b^k\,\partial b^l}\right)(a,0,t)=0. \tag{3.22}$$

This constraint is, of course, satisfied if

$$\left(\frac{\partial^2 M}{\partial a^k\,\partial a^l}+\frac{\partial^2 M}{\partial b^k\,\partial b^l}\right)(a,b,t)=0, \tag{3.23}$$

for all a and b in $\mathbb{R}^n$, where we recognize the Cauchy–Riemann conditions for an analytic function of the n complex variables $z^k=a^k+ib^k$.

Specifically, $M(a,b,t)$ can be viewed as the real part of an analytic function,

$$F(z,t)=M(a,b,t)+iN(a,b,t), \tag{3.24}$$

with $z=a+ib\in\mathbb{C}^n$, for which the Cauchy–Riemann conditions take the form

$$\frac{\partial M}{\partial a^k}=\frac{\partial N}{\partial b^k}, \tag{3.25a}$$

$$\frac{\partial M}{\partial b^k}=-\frac{\partial N}{\partial a^k}. \tag{3.25b}$$

These conditions imply (3.23). Furthermore, substituting (3.25b) inside the expression (2.26a) for w_k gives

$$2w_k(a,t)=\frac{\partial M}{\partial b^k}(a,0,t)=-\frac{\partial N}{\partial a^k}(a,0,t), \tag{3.26}$$

so that the closure rule (3.1a) is also satisfied with

$$2S(a,t)=-N(a,0,t). \tag{3.27}$$

To summarize, the end-point density $q(x,t;y,t)$ obtained by shrinking to zero the interval of definition $[s,t]$ of a reciprocal diffusion corresponds to a quantum diffusion, provided

$$q(x,t;y,t)=\exp M\left(\frac{y+x}{2},\frac{y-x}{2},t\right), \tag{3.28}$$

where $M(a,b,t)=\mathrm{Re}\,F(z,t)$ is the real part of an analytic function of z. Furthermore, from (3.21) and (3.27), the evaluation of $F(z,t)$ for $z=a+i0\in\mathbb{R}^n$ gives

$$F(a+i0,t)=M(a,0,t)+iN(a,0,t)=2(R(a,t)-iS(a,t))=2\ln\psi^*(a,t), \tag{3.29}$$

i.e., $F(z,t)$ can be viewed as obtained by analytical continuation of the function $2\ln\psi^*(a,t)$ defined over $\mathbb{R}^n$. Note that this is only possible as long as $\rho(a,t)=|\psi(a,t)|^2$ does not admit nodes, i.e., values of a for which the density is zero. When nodes are present, $\ln\psi^*(a,t)$ has singularities, so that a straightforward analytic continuation is not possible, although $F(z,t)$ can still be defined as a meromorphic function.

To analyze the effect of the nodes of $\rho(x,t)$ on the end-point density, let $\ln\psi(z,t)$ with $z=a+ib$ denote the analytical continuation of $\ln\psi(a,t)$ to $\mathbb{C}^n$. Then the expression (3.28) for the end-point density can be rewritten as

$$q(x,t;y,t)=\left|\psi\left(\frac{y+x}{2}-i\,\frac{y-x}{2},t\right)\right|^2, \tag{3.30}$$

so that whenever $\rho(x,t)$ has a node at $x=x_0$, $q(x,t;y,t)$ has a node at $x=y=x_0$. Note also that the structure (3.30) of the end-point density is the analog for quantum diffusions of the separable structure (2.14) of Markov diffusions.

Assuming at this point that a function $q(x,t;y,t)$ of the form (3.28) has been constructed, to obtain the end-point density $q(x,s;y,t)$ for an interval $[s,t]$ of nonzero length, we can either propagate the evolution equation (2.13a) backward in time, with initial condition $q(x,t;y,t)$, or propagate (2.13b) forward in time starting from $q(x,s;y,s)$. In both cases, this corresponds to propagating a heat equation in an unstable direction, i.e., we are trying to push back the heat toward its source. Consequently, solutions will usually exist only over a finite time interval, thus suggesting that quantum diffusions have generally a finite lifetime. In addition, although $q(x,t;y,t)$ given by (3.28) is always non-negative, for $s<t$, the solution $q(x,s;y,t)$ of (2.13a) or (2.13b) may become negative for some values of x and y, as will be shown in Sec. VII.

IV. GAUSSIAN PROCESSES

The construction procedure we have just outlined can be simplified further for the case when the potentials $\{A_i,\phi\}$ have the structure (2.40) and the wave function $\psi(x,t)$ is Gaussian, in which case the corresponding quantum diffusion is a Gaussian process. Specifically, following Ref. 10, Sec. 16, assume that

$$\ln \psi(x,t)=R(x,t)+iS(x,t), \tag{4.1a}$$

with

$$R(x,t)=-\tfrac{1}{2}(x-x_C(t))^T R(t)(x-x_C(t))+f_R(t), \tag{4.1b}$$

$$S(x,t)=\tfrac{1}{2}(x-x_C(t))^T S(t)(x-x_C(t))+x^T p_C(t)+f_S(t), \tag{4.1c}$$

where $f_R(t)$, $f_S(t)$ are functions of t only. $x_C(t)$ denotes the classical trajectory of the particle, and $p_C^i(t)=\dot{x}_C^i(t)+A^i(x_C,t)$ represents the momentum along this trajectory. In this case,

$$\rho(x,t)=|\psi(x,t)|^2 \tag{4.2}$$

is a Gaussian distribution with mean $x_C(t)$ and covariance matrix

$$K_x(t)=R^{-1}(t)/2. \tag{4.3}$$

Since $2\ln\psi^*(a,t)$ is quadratic in a, its analytical continuation is obtained by replacing a with $z=a+ib$, which gives

$$F(z,t)=-(z-x_C(t))^T R(t)(z-x_C(t))-i(z-x_C(t))^T S(t)(z-x_C(t))-2iz^T p_C(t)+f_F(t), \tag{4.4}$$

where $f_F(t)$ depends again on t only. Taking the real part, we find

$$M(a,b,t)=-(a-b-x_C(t))^T R(t)(a+b-x_C(t))+2b^T S(t)(a-x_C(t))+2b^T p_C(t)+f_M(t). \tag{4.5}$$

Substituting this expression inside the identities (2.26a)–(2.26b) for $w(a,t)$ and the stress tensor $\pi(a,t)$ gives

$$w(a,t)=p_C(t)+S(t)(a-x_C(t)), \tag{4.6a}$$

$$\pi(a,t)=\frac{R(t)}{2}. \tag{4.6b}$$

Clearly, π satisfies the closure rule (3.1b), and (4.6a) can be rewritten in terms of the mean velocity $v^i=w^i-A^i$ in the form (2.41a) with

$$V(t)=S(t)-A(t), \tag{4.7}$$

where $A(t)$ denotes the matrix representing the tensor A_{ij} in (2.40).

Next, the expression (3.28) for $q(x,t;y,t)$ yields

$$\ln q(x,t;y,t)=-\frac{1}{2}[(x-x_C(t))^T(y-x_C(t))^T]Q(t,t)\begin{bmatrix}x-x_C(t)\\ y-x_C(t)\end{bmatrix}$$
$$-[(x-x_C(t))^T(y-x_C(t))^T]\begin{bmatrix}p_C(t)\\ -p_C(t)\end{bmatrix}+f_q(t), \tag{4.8}$$

with

$$Q(t,t)=\begin{bmatrix}S(t) & R(t)\\ R(t) & -S(t)\end{bmatrix}. \tag{4.9}$$

Assume now that $q(x,s;y,t)$ has the structure

$$\ln q(x,s;y,t)=-\frac{1}{2}[(x-x_C(s))^T(y-x_C(t))^T]Q(s,t)\begin{bmatrix}x-x_C(s)\\ y-x_C(t)\end{bmatrix}$$
$$-[(x-x_C(s))^T(y-x_C(t))^T]p(s,t)+f_q(s,t), \tag{4.10a}$$

with

$$Q(s,t)=\begin{bmatrix}Q_{xx}(s,t) & Q_{xy}(s,t)\\ Q_{yx}(s,t) & Q_{yy}(s,t)\end{bmatrix}, \tag{4.10b}$$

$$p(s,t)=\begin{bmatrix}p_x(s,t)\\ p_y(s,t)\end{bmatrix}. \tag{4.10c}$$

By substituting this expression and the representation (2.40) of the potentials $\{A_i,\phi\}$ inside the heat equation (2.13a) for $q(x,s;y,t)$, we find it reduces to the ordinary differential equations,

$$-\frac{dQ}{ds}(s,t)=\begin{bmatrix}Q_{xx}-A^T(s)\\ Q_{yx}\end{bmatrix}[Q_{xx}-A(s) \quad Q_{xy}]+\begin{bmatrix}\Phi(s) & 0\\ 0 & 0\end{bmatrix}, \tag{4.11}$$

$$-\frac{dp}{ds}(s,t)=\begin{bmatrix}Q_{xx}\\ Q_{yx}\end{bmatrix}(p_x-A(s)x_C(s)-\dot{x}_C(s))-\begin{bmatrix}A^T(s)(p_x-A(s)x_C(s))-\Phi(s)x_C(s)\\ 0\end{bmatrix}, \tag{4.12}$$

where Φ is the matrix representing the tensor Φ_{ij} in (2.40). By observing that the position x_C and momentum p_C for the classical trajectory, satisfy Hamilton's equations,

$$\dot{x}_C=\frac{\partial H}{\partial p}=p_C-Ax_C, \tag{4.13a}$$

$$\dot{p}_C=-\frac{\partial H}{\partial x}=A^T(p_C-Ax_C)-\Phi x_C, \tag{4.13b}$$

it is easy to verify that the differential equation (4.12) is satisfied by

$$p_x(s,t)=p_C(s), \quad p_y(s,t)=-p_C(t). \tag{4.14}$$

Thus, once the classical trajectory has been evaluated, to specify the end-point density $q(x,s;y,t)$, we only need to solve the matrix Riccati equation (4.11) for $s \leqslant t$, with initial condition (4.9).

To illustrate the above results, we consider two simple examples: the minimum uncertainty wave packet and the coherent state of the harmonic oscillator.

Example 4.1: For a *free particle*, we have

$$A(x,t) = \phi(x,t) = 0, \tag{4.15}$$

so that the Green's function,

$$G(x,s;y,t) = \frac{1}{(2\pi(t-s))^{1/2}} \exp - \frac{(y-x)^2}{2(t-s)} \tag{4.16}$$

is the standard heat kernel. The wave function corresponding to a minimum uncertainty wave packet centered about the classical trajectory $x_C(t) = x_0 + v_0 t$ is given by

$$\psi(x,t) = \frac{1}{\pi^{1/4}(r+it/r)^{1/2}} \exp\left[- \frac{(x-x_0-ir^2v_0)^2}{2(r^2+it)} - \frac{r^2 v_0^2}{2} \right]. \tag{4.17}$$

The real and imaginary parts R and S of $\ln \psi$ have the form (4.1b)–(4.1c) with

$$R(t) = \frac{r^2}{r^4+t^2}, \quad S(t) = \frac{t}{r^4+t^2}, \tag{4.18}$$

and where the momentum $p_C(t) = v_0$ along the classical trajectory remains constant. The density $\rho(x,t)$ is therefore Gaussian, centered about $x_C(t)$, with standard deviation,

$$\sigma_x(t) = \frac{1}{\sqrt{2}} \left(r^2 + \frac{t^2}{r^2} \right)^{1/2}. \tag{4.19}$$

The momentum density, which is obtained by Fourier transforming $\psi(x,t)$, and squaring the resulting transform, is also Gaussian with mean v_0 and standard deviation,

$$\sigma_p(t) = \frac{1}{r\sqrt{2}}. \tag{4.20}$$

The position-momentum uncertainty product,

$$\sigma_x(t)\sigma_p(t) = \tfrac{1}{2}(1 + t^2/r^4)^{1/2}, \tag{4.21}$$

equals the Heisenberg lower bound of $\frac{1}{2}$ at $t=0$, which explains why this process is called a minimum uncertainty wave packet. The factor r^2 represents the ratio of the position and momentum standard deviations, i.e., their relative spreading, at $t=0$.

According to (4.7) and (4.6b), the mean velocity and stress tensor of the quantum diffusion modeling this process are given by

$$v(x,t) = v_0 + \frac{t(x-x_C(t))}{r^4+t^2}, \tag{4.22a}$$

$$\pi(x,t) = \frac{r^2}{2(r^2+t^2)}. \tag{4.22b}$$

Note that as $t\to\infty$, the mean velocity,

$$v(x,t)\approx v_0+(x-x_C(t))/t=(x-x_0)/t, \tag{4.23}$$

is obtained by modeling trajectories passing through x at time t as straight lines originating from x_0. Solving the Riccati equation (4.11) yields

$$Q(s,t)=\frac{1}{r^4+st}\begin{bmatrix} t & r^2 \\ r^2 & -s \end{bmatrix}, \tag{4.24}$$

which specifies $q(x,s;y,t)$.

Since both $q(x,s;y,t)$ and the Green's function $G(x,s;y,t)$ are Gaussian, the process $x(t)$ is Gaussian, so that it is entirely described by its mean and autocovariance functions. By combining the expressions (4.10) and (4.16) for q and G, we find that for $s<t$, the joint density of $x(s)$ and $x(t)$ is given by

$$p(x,s;y,t)=G(x,s;y,t)q(x,s;y,t)=N\left(\begin{bmatrix} x_C(s) \\ x_C(t) \end{bmatrix},\mathbf{P}(s,t)\right), \tag{4.25a}$$

where

$$\mathbf{P}(s,t)=\frac{1}{2}\begin{bmatrix} r^2+s^2/r^2 & r^2+st/r^2-(t-s) \\ r^2+st/r^2-(t-s) & r^2+t^2/r^2 \end{bmatrix}, \tag{4.25b}$$

denotes the covariance matrix of $x(s)$ and $x(t)$. Thus, if $z(t)=x(t)-x_C(t)$ represents the deviation of $x(t)$ with respect to the classical trajectory, $z(t)$ is Gaussian, with zero mean, and autocorrelation function

$$K(t,s)=E[z(t)z(s)]=\tfrac{1}{2}(r^2+ts/r^2-|t-s|). \tag{4.26}$$

Taking into account Newton's law and the characterization of Gaussian reciprocal diffusions given in Refs. 18 and 25, we find that over an arbitrary interval $[0,T]$, $z(t)$ satisfies the second-order stochastic differential equation,

$$\mathscr{L}_F z(t)=\xi(t), \tag{4.27a}$$

$$\mathscr{L}_F\triangleq-\frac{d^2}{dt^2}, \tag{4.27b}$$

with Dirichlet conditions

$$\begin{bmatrix} z(0) \\ z(T) \end{bmatrix}\sim N(0,\mathbf{P}(0,T)). \tag{4.28}$$

The driving noise $\xi(t)$, which is usually called the dual or conjugate process of $z(t)$, is a generalized Gaussian process independent of $z(0)$ and $z(T)$, with zero mean and autocorrelation

$$E[\xi(t)\xi(s)]=\mathscr{L}_F\delta(t-s). \tag{4.29}$$

The Green's function of $\mathscr{L}_F$ can be used to decompose the solution of (4.27)–(4.29) into a component depending only on the noise $\xi(t)$ and a component representing the effect of the boundary conditions, so that over $[0,T]$, $z(t)$ can be represented as

$$z(t)=B(t)+\frac{T-t}{T}\,z(0)+\frac{t}{T}\,z(T), \tag{4.30}$$

where $B(t)=W(t)-tW(T)/T$ is a Brownian bridge process, independent of $z(0)$ and $z(T)$. Since the interval length T is arbitrary, the quantum diffusion corresponding to a minimum uncertainty wave packet has an infinite lifetime. This can also be seen by noting that a stochastic model equivalent to the one obtained above is given by

$$z(t)=W(t)+z(0)(1-t/r^2), \tag{4.31}$$

where $W(t)$ is a Wiener process independent of $z(0)$. See Ref. 28, Sec. 5 for general results on the representation of scalar Gaussian reciprocal processes in terms of the Wiener process.

Example 4.2: The *harmonic oscillator* has for potentials,

$$A(x,t)=0, \quad \phi(x,t)=\frac{(\omega x)^2}{2}. \tag{4.32}$$

Since the Lagrangian $L(x,p,t)=p\dot{x}-H(x,p,t)$ is quadratic, the Green's function can be expressed (see Ref. 2, Sec. 3.5) as

$$G(x,s;y,t)=C(t-s)\exp-S_C(x,s;y,t), \tag{4.33a}$$

where

$$S_C(x,s;y,t)=\int L(x_C,\dot{x}_C,u)\,du \tag{4.33b}$$

denotes the action for the classical path linking $x(s)=x$ to $x(t)=y$, and $C(t-s)$ is a function of $t-s$. Evaluating S_C yields

$$S_C=\frac{\omega}{2\sin(\omega(t-s))}\,[(x^2+y^2)\cos(\omega(t-s))-2xy], \tag{4.34a}$$

and substituting (4.32a) inside expression (2.10) for the transition property of the Green's function, we can identify

$$C(t-s)=\left(\frac{\omega}{2\pi\,\sin(\omega(t-s))}\right)^{1/2}. \tag{4.34b}$$

An important property of the Green's function $G(x,s;y,t)$ is that, viewed as a function of y, it decays as $|y|\to\infty$ for $t-s<\pi/2\omega$, but for $(t-s)>\pi/2\omega$, it grows exponentially with y, so that the Green's function does not exist for intervals of length larger than $T=\pi/2\omega$, which represents one-quarter of the period of the harmonic oscillator.

The wave function corresponding to a coherent state centered about the classical trajectory $x_C(t)=l\cos(\omega t)$, where l denotes the oscillation amplitude, takes the form (4.1) with

$$R(t)=\omega, \quad S(t)=0, \tag{4.35}$$

and where the momentum along the classical trajectory is given by $p_C(t)=\dot{x}_C(t)=-l\omega\sin(\omega t)$. According to (4.7) and (4.6b), the mean velocity and stress tensor of the quantum diffusion modeling this process are given by

$$v(x,t)=p_C(t), \tag{4.36a}$$

$$\pi(x,t)=\omega/2. \tag{4.36b}$$

Note that since the mean velocity $v(x,t)$ does not depend on x, the wave packet does not undergo any deformation with time and retains its coherence, hence the name of the process. The solution of the Riccati equation (4.11) is given by

$$Q(s,t)=\frac{\omega}{\cos(\omega(t-s))}\begin{bmatrix}\sin(\omega(t-s)) & 1\\ 1 & \sin(\omega(t-s))\end{bmatrix}. \tag{4.37}$$

Both $q(x,s;y,t)$ and $G(x,s;y,t)$ are again Gaussian, so $x(t)$ is a Gaussian process. The joint density of $x(s)$ and $x(t)$ takes again the form (4.25a), with

$$\mathbf{P}(s,t)=\frac{1}{2\omega}\begin{bmatrix}1 & \gamma(t-s)\\ \gamma(t-s) & 1\end{bmatrix}, \tag{4.38a}$$

where

$$\gamma(t-s)=\cos(\omega(t-s))-\sin(\omega(t-s))=\frac{\cos(\omega(t-s)+\pi/4)}{\cos(\pi/4)}, \tag{4.38b}$$

denotes the correlation coefficient of $x(t)$ and $x(s)$. Note that for $\gamma(t-s)$ to be a correlation coefficient, its magnitude must be less than unity, which requires $t-s<\pi/2\omega$. Thus, the deviation $z(t)=x(t)-x_C(t)$ of $x(t)$ with respect to the classical trajectory $x_C(t)$ is Gaussian, with zero mean and autocorrelation function

$$K(t,s)=E[z(t)z(s)]=\frac{1}{2\omega}\frac{\cos(\omega(t-s)+\pi/4)}{\cos(\pi/4)}. \tag{4.39}$$

This process, which is called the *shifted cosine process*, was introduced by Carmichael, Massé, and Theodorescu,[29] while completing a classification of scalar stationary Gaussian reciprocal processes proposed earlier by Jamison.[30] In Ref. 18, it is shown that this process is defined over a finite interval of length $T=\pi/2\omega$, and satisfies the second-order stochastic differential equation,

$$\mathscr{L}_H z(t)=\xi(t), \tag{4.40a}$$

$$\mathscr{L}_H \triangleq -\frac{d^2}{dt^2}-\omega^2, \tag{4.40b}$$

with boundary condition

$$z(0)=-z(T)\sim N(0,1/(2\omega)), \tag{4.41}$$

where the driving noise $\xi(t)$ is a generalized Gaussian process independent of $z(0)$ and $z(T)$, with zero mean and autocorrelation

$$E[\xi(t)\xi(s)]=\mathscr{L}_H\delta(t-s). \tag{4.42}$$

The relation (4.40a) shows that the dynamics of the shifted cosine process are those of an oscillator subjected to random fluctuations $\xi(t)$. The noise $\xi(t)$ is not white but has a local correlation structure depending on the oscillator dynamics $\mathscr{L}_H$. The lifetime $\pi/(2\omega)$ of the shifted cosine process corresponds to only one-quarter of the period of the harmonic oscillator. To con-

struct a model valid for longer periods of time, since the ground state of the harmonic oscillator is stationary, it is natural to expect that its model should not depend on the choice of time origin. The boundary condition $z(\pi/(2\omega))=-z(0)$ therefore suggests the rule

$$z(t+\pi/(2\omega))=-z(t), \tag{4.43}$$

for extending $z(\cdot)$ to all times. However, this choice implies $z(t+n\pi/\omega)=z(t)$ for n integer, whereas Heisenberg's position operator satisfies $X(t+n\pi/\omega)=(-1)^n X(t)$. This difference, and in particular its effect on the evaluation of multitime quantum correlations, requires further analysis. □

V. POSITION-MOMENTUM UNCERTAINTY

Although the position-momentum uncertainty relations form a cornerstone of standard quantum mechanics, their role has been somewhat diminished in the development of Markovian stochastic mechanics.[31] This difference arises in part from difficulties in giving an operational definition to the momentum process.[32] Indeed, unlike the Hilbert space formulation of quantum mechanics, where position and momentum play completely symmetric roles, stochastic mechanics privileges position variables. While this last feature is retained by the stochastic mechanics of quantum diffusions described here, the position-momentum uncertainty relations will regain a key role. Specifically, we show they are a consequence of the closure rule (3.1b) with $\epsilon=-1$, and are thus characteristic of quantum diffusions.

As a starting point, consider the *empirical momentum* process,

$$p^k(t;h)=u^k(t;h)+A^k(x(t),t), \tag{5.1}$$

where $u(t;h)=d^1x(t;h)/h$ is the empirical velocity of the diffusion. The expression (2.27) for the conditional mean of $d^1x(t;h)$ given the mean position $\bar{x}(t;h)$ implies

$$E[p^k(t;h)|\bar{x}(t;h)=x]=v^k(x,t)+A^k(x,t)+o(1)=w^k(x,t)+o(1), \tag{5.2}$$

so that as $h\to 0$, the conditional mean of the *abstract momentum* process $p(t)$ given the position $x(t)$ can be defined as

$$E[p^k(t)|x(t)=x]\triangleq\lim_{h\to 0} E[p^k(t;h)|\bar{x}(t;h)=x]=w^k(x,t). \tag{5.3}$$

Taking into account the closure rule (3.1a) gives

$$E[p_k(t)]=\int w_k(x,t)\rho(x,t)dx=\int \psi^*(x,t)\nabla_k S(x,t)\psi(x,t)dx=\int \psi^*(x,t)(-i\ \nabla_k\psi(x,t))dx, \tag{5.4}$$

so that the usual correspondence principle,

$$p_k\leftrightarrow -i\nabla_k, \tag{5.5}$$

holds for this momentum definition.

The correlation matrix of the abstract momentum $p(t)$ is harder to define, since according to the characterization (2.27), (2.29) of the velocity distribution, the empirical momentum $p^k(t;h)$ has a size proportional to $h^{-1/2}$. However, following Ref. 2, p. 179, we can define it as the correlation of the empirical momentum evaluated for two successive infinitesimal time intervals. Specifically, we consider

$$p^k\left(t+\frac{h}{2};\frac{h}{2}\right)p^l\left(t-\frac{h}{2},\frac{h}{2}\right)=\left(\frac{dx_+^k}{h}+A^k\right)\left(\frac{dx_-^l}{h}+A^l\right), \tag{5.6}$$

where $dx_\pm=\pm(x(t\pm h)-x(t))/h$. Observing that the cross-product of the forward and backward differences d^+x and d^-x can be expressed in terms of the centered first- and second-order differences d^1x and d^2x as

$$dx_+^k\ dx_-^l=d^1x^k\ d^1x^l-\tfrac{1}{4}d^2x^k\ d^2x^l, \tag{5.7}$$

and using expressions (2.21) and (2.29) to evaluate the conditional covariances of d^2x and d^1x given the mean position $\bar{x}(t;h)$, we find

$$E[p^k(t+h/2;h/2)p^l(t-h/2,h/2)|\bar{x}(t;h)=x]=\pi^{kl}(x,t)+u^k(x,t)w^l(x,t)+o(1). \tag{5.8}$$

This implies

$$E[p^k(t)p^l(t)|x(t)=x]\triangleq\lim_{h\to 0}\ E[p^k(t+h/2;h/2)p^l(t-h/2,h/2)|\bar{x}(t;h)=x]$$

$$=\pi^{kl}(x,t)+w^k(x,t)w^l(x,t). \tag{5.9}$$

Taking into account the closure rules (3.1a)–(3.1b), it can then be checked that

$$\begin{aligned}E[p_k(t)p_l(t)]&=\int(\pi_{kl}+w_kw_l)(x,t)\rho(x,t)dx\\&=\int\psi^*(x,t)(-\tfrac{1}{2}\nabla_k\nabla_lR(x,t)+\nabla_kS(x,t)\nabla_lS(x,t))\psi(x,t)dx\\&=\int\psi^*(x,t)(-\nabla_k\nabla_l\psi(x,t))dx,\end{aligned} \tag{5.10}$$

so that we have again the usual correspondence principle,

$$p_kp_l\leftrightarrow(-i\nabla_k)(-i\nabla_l). \tag{5.11}$$

Note, however, that this correspondence depends on the unusual rule employed in (5.9) to evaluate the conditional correlation matrix of the momentum given the position.

From expressions (5.9) and (5.3) we see that the entries of the conditional covariance matrix $K_{p|x}(t)$ of the momentum $p(t)$ given the position $x(t)$ take the form

$$K_{p|x,kl}(x,t)=\mathrm{cov}(p_k(t),p_l(t)|x(t)=x)=\pi_{kl}(x,t). \tag{5.12}$$

Taking expectations, this implies

$$E[K_{p|x,kl}(x(t),t)]=\int\pi_{kl}(x,t)\rho(x,t)dx. \tag{5.13}$$

On the other hand, the covariance matrix $K_p(t)$ of $p(t)$ is given by

$$K_{p,kl}(t)=\mathrm{cov}(p_k(t),p_l(t))=\int[\pi_{kl}(x,t)+(\psi_k(x,t)-E[p_k(t)])(w_l(x,t)-E[p_l(t)])^T\rho(x,t)dx. \tag{5.14}$$

Comparing (5.13) and (5.14), we obtain

$$K_p(t) \geqslant E[K_{p|x}(t)], \tag{5.15}$$

which just expresses the fact that the knowledge of $x(t)$ reduces the momentum variance.

Our derivation of the position-momentum uncertainty relations relies on the following lemma, which is an adaptation of standard results of Bayesian estimation theory.

Lemma 5.1: Let X be a random vector of $\mathbb{R}^n$ with probability density $p(x)$. Its mean vector and covariance matrix are denoted by m and K, respectively, i.e.,

$$E[X^k] = m^k, \quad E[(X^k - m^k)(X^l - m^l)] = K^{kl}. \tag{5.16}$$

Then, if we consider the Fisher information matrix J with entries

$$J_{kl} = -E[\boldsymbol{\nabla}_k \boldsymbol{\nabla}_l \ln p(X)], \tag{5.17}$$

the matrix

$$\mathbf{P} = \begin{bmatrix} K & -I \\ -I & J \end{bmatrix} \tag{5.18}$$

is non-negative definite. If K is positive definite, this implies

$$J \geqslant K^{-1}. \tag{5.19}$$

Proof: Consider the random vectors $A = X - m$ and $B = \boldsymbol{\nabla} \ln p(X)$. Both have zero mean, A has covariance matrix K, and

$$E[A^k B_l] = E\left[(X^k - m^k) \frac{\partial}{\partial x^l} \ln p(X) \right] = \int (x^k - m^k) \left(\frac{\partial}{\partial x^l} \ln p(x) \right) p(x) dx$$

$$= -\int \frac{\partial}{\partial x^l} (x^k - m^k) p(x) dx = -\delta_l^k, \tag{5.20a}$$

$$E[B_k B_l] = E\left[\frac{\partial}{\partial x^k} \ln p(X) \frac{\partial}{\partial x^l} \ln p(X) \right] = \int \frac{\partial}{\partial x^k} \ln p(x) \frac{\partial}{\partial x^l} \ln p(x) p(x) dx$$

$$= -\int \frac{\partial^2}{\partial x^k \partial x^l} \ln p(x) p(x) dx = J_{kl}. \tag{5.20b}$$

The identities (5.20) indicate that the matrix $\mathbf{P}$ given by (5.18) is just the covariance matrix of A and B, and thus must be non-negative. In this covariance matrix, $J - K^{-1}$ is the Schur complement of the (2,2) block K, so that it is non-negative. □

The Lemma 5.1 can be combined with the quantum closure rule (3.1b) to derive the following result.

Theorem 5.1: If $x(t)$ is a quantum diffusion with position covariance matrix $K_x(t)$, it satisfies the matrix position-momentum uncertainty relation,

$$K_p(t) \geqslant E[K_{p|x}(t)] \geqslant \tfrac{1}{4} K_x^{-1}(t), \tag{5.21}$$

where the conditional covariance matrix $K_{p|x}(t)$ and the covariance matrix $K_p(t)$ are specified by (5.12) and (5.14), respectively.

Proof: Let $J(t)$ denote the Fisher information matrix corresponding to the quantum diffusion $x(t)$ with density $\rho(x,t)$. Taking into account (5.13), the closure rule (3.1b) implies

$$E[K_{p|x}(t)]=\tfrac{1}{4}J(t), \tag{5.22}$$

which, when combined with inequalities (5.15) and (5.19), yields (5.21). □

The key step in the above derivation was the use of the quantum closure rule to derive the equality (5.22). This implies that the uncertainty relation (5.21) is specific to quantum diffusions and may not hold for other reciprocal diffusions. Also, as expressed in (5.21), the position-momentum uncertainty relation is slightly stronger than the usual version, since it holds for the averaged conditional covariance matrix $E[K_{p|x}(x(t),t)]$ of the momentum, given the position.

VI. LOCALITY

An important test for evaluating the realism of stochastic formulations of quantum mechanics is whether such formulations preserve locality. Indeed, in spite of the existence of interpretations of quantum mechanics, such as Bohm's theory,[26] which are apparently nonlocal, when viewed as a set of computational rules for evaluating statistical averages, quantum mechanics is inherently local, in a sense that will be described below. Unfortunately, as was demonstrated in Ref. 10, Markovian stochastic mechanics does not have this property, and must therefore be rejected as a proper model of quantum phenomena. In contrast, we show that the new form of stochastic mechanics described here is local.

To demonstrate this fact, consider a general reciprocal diffusion,

$$x(t)=\begin{bmatrix} x_1(t) \\ x_2(t) \end{bmatrix}, \tag{6.1}$$

not necessarily of quantum type, but where the components $x_1(t)$ and $x_2(t)$ are dynamically uncoupled. This means that the Hamiltonian (2.2) admits the decomposition

$$H(x,p,t)=H_1(x_1,p_1,t)+H_2(x_2,p_2,t), \tag{6.2}$$

where $\{A_1(x_1,t),\phi_1(x_1,t)\}$ and $\{A_2(x_2,t),\phi_2(x_2,t)\}$ are the potentials affecting each of the diffusion components. From the form (6.2) of the Hamiltonian, we can deduce that the Green's function $G(x,s;y,t)$ corresponding to $\mathbf{H}$ can be factored as

$$G(x,s;y,t)=G_1(x_1,s;y_1,t)G_2(x_2,s;y_2,t), \tag{6.3}$$

where G_1 and G_2 are the Green's functions corresponding to $\mathbf{H}_1$ and $\mathbf{H}_2$, respectively. This structure can be used to derive the following result.

Lemma 6.1: Let $x(t)$ be a reciprocal diffusion with two dynamically uncoupled components $x_1(t)$ and $x_2(t)$. Then each component $x_1(t)$ or $x_2(t)$ considered separately is a reciprocal diffusion. Furthermore, if $x(t)$ is a quantum diffusion, its component $x_1(t)$ is of quantum type if and only if the function R and S given by (3.5) and (3.1a) admit the additive decomposition,

$$R(x,t)=R_1(x_1,t)+R_2(x_2,t), \tag{6.4a}$$

$$S(x,t)=S_1(x_1,t)+S_2(x_2,t), \tag{6.4b}$$

or equivalently if the wave function $\psi(s,t)$ decomposes multiplicatively as

$$\psi(x,t)=\psi_1(x_1,t)\psi_2(x_2,t). \tag{6.5}$$

Proof: Substituting (6.3) inside expression (2.7) for the joint density of $x(t_0)$, $x(t_1),\ldots,x(t_N)$ and integrating over the x_2 components, we find that the marginal joint density of $x_1(t_0),x_1(t_1),\ldots,x_1(t_N)$ can be expressed as

$$p_1(x_{10},t_0;x_{11},t_1;\ldots;x_{1N},t_N)=q_1(x_{10},t_0;x_{1N},t_N)\prod_{k=0}^{N-1} G_1(x_{1k},t_k;x_{1k+1},t_{k+1}), \tag{6.6}$$

where the end-point density $q_1(x_1,s;y_1,t)$ is given by

$$q_1(x_1,s;y_1,t)=\int G_2(x_2,s;y_2,t)q(x,s;y,t)dx_2\,dy_2, \tag{6.7}$$

with $x^T=[x_1^T,x_2^T]$ and $y^T=[y_1^T,y_2^T]$. The structure (6.6) of the finite joint densities of $x_1(t)$ indicates it is a reciprocal diffusion. However, if $x(t)$ is a quantum diffusion, there is no guarantee that $x_1(t)$ will also be of the quantum type. Specifically, consider the partition

$$v(x,t)=\begin{bmatrix} v_1(x,t) \\ v_2(x,t)\end{bmatrix}, \quad \pi(x,t)=\begin{bmatrix} \pi_{11}(x,t) & \pi_{12}(x,t) \\ \pi_{21}(x,t) & \pi_{22}(x,t)\end{bmatrix} \tag{6.8}$$

of the mean velocity and stress tensor in terms of their x_1 and x_2 components. According to the characterization (2.27) and (2.29) of the velocity distribution, the mean velocity $v_1^m(x_1,t)$ and stress tensor $\pi_{11}^m(x_1,t)$ for the marginal probability distribution of $x_1(\cdot)$ can be expressed as

$$v_1^m(x_1,t)=\int v_1(x,t)\rho_{2|1}(x_2,t|x_1,t)dx_2, \tag{6.9a}$$

$$\pi_1^m(x_1,t)=\int \pi_{11}(x,t)\rho_{2|1}(x_2,t|x_1,t)dx_2+\int (v_1(x,t)-v_1^m(x_1,t)) \times (v_1(x,t)-v_1^m(x_1,t))^T\rho_{2|1}(x_2,t|x_1,t)dx_2, \tag{6.9b}$$

where $\rho_{2|1}(x_2,t|x_1,t)$ denotes the conditional probability density of $x_2(t)$ given $x_1(t)$. Note that since the covector potential A_1 depends only on x_1,

$$v_1(x,t)-v_1^m(x_1,t)=w_1(x,t)-w_1^m(x_1,t). \tag{6.10}$$

Then if $x_1(t)$ is a quantum diffusion, w_1^m and π_1^m must satisfy the closure rules,

$$w_1^m(x_1,t)=\nabla_1 S_1(x_1,t), \tag{6.11a}$$

$$\pi_1^m(x_1,t)=\frac{-1}{4}\,\nabla_1\nabla_1^T \ln \rho_1(x_1,t), \tag{6.11b}$$

where $\rho_1(x_1,t)$ denotes the marginal probability density of $x_1(t)$ and ∇_1 is the gradient with respect to x_1. Substituting these closure rules and the closure rules for $x(t)$, we find that after integration by parts, (6.9b) can be rewritten as

$$0=\frac{1}{4}\int \nabla_1 \ln \rho_{2|1}(\nabla_1 \ln \rho_{2|1})^T\rho_{2|1}\,dx_2+\int (w_1-w_1^m)(w_1-w_1^m)^T\rho_{2|1}\,dx_2, \tag{6.12}$$

which implies

$$0=\nabla_1 \ln \rho_{2|1}=\nabla_1(R(x,t)-R_1(x_1,t)), \tag{6.13a}$$

$$0=w_1-w_1^m=\nabla_1(S(x,t)-S_1(x_1,t)), \tag{6.13b}$$

so that R and S admit the decomposition (6.4). □

Note that the conclusion that dynamically uncoupled components of quantum diffusions need not be quantum diffusions is consistent with the standard interpretation of quantum mechanics, which holds that statistically coupled components of a quantum process cannot be analyzed separately. It is also worth observing that the multiplicative structure of the decomposition (3.5) is preserved by the Schrödinger equation (or the equivalent conservation laws of quantum diffusions), so that if (3.5) holds for one t, it holds for all t.

Nevertheless, as indicated by Lemma 6.1, dynamically uncoupled components of quantum diffusions are reciprocal diffusions. This result is now employed to demonstrate locality. We use the fact that if $\psi(x,t)$ is the wave function of two dynamically decoupled, but possibly statistically coupled particles, quantum mechanics has the following locality property. Let $\mathbf{O}_1$ be a Hermitian operator involving only the position and momentum operators of $x_1(t)$. Then, since the Heisenberg representation $\mathbf{O}_1(t)$ of $\mathbf{O}_1$ depends only on the Hamiltonian H_1, the inner product,

$$\langle \psi(x,t), \mathbf{O}_1 \psi(x,t) \rangle, \tag{6.14}$$

is independent of the potentials $\{A_2, \phi_2\}$.

Theorem 6.1: Let $x(t)$ be a quantum diffusion constructed from a wave function with two dynamically uncoupled components $x_1(t)$ and $x_2(t)$. Then, the end-point density $q_1(x_1,s;y_1,t)$ of $x_1(t)$ does not depend on the potentials $\{A_2, \phi_2\}$ acting on $x_2(t)$.

Proof: The argument is patterned after that of Ref. 10, Theorem 23.1. Setting $s=t$ in (6.7), the end-point density of x_1 takes the form

$$\begin{aligned} q_1(a_1-b_1,t;a_1+b_1,t) &= \int \exp M(a_1,a_2,b_1,0,t)\,da_2 \\ &= \int \exp[M(a_1,a_2,b_1,0,t) - M(a_1,a_2,0,0,t)]\rho(a_1,a_2,t)\,da_2, \end{aligned} \tag{6.15}$$

where $\rho(x_1,x_2,t)$ is the joint density of $x_1(t)$ and $x_2(t)$. But in (6.15),

$$M(a_1,a_2,b_1,0,t) - M(a_1,a_2,0,0,t) = \mathrm{Re}[F(z_1,a_2,t) - 2\ln \psi^*(a_1,a_2,t)], \tag{6.16}$$

where $F(z_1,z_2,t)$ is the analytical continuation of $2\ln\psi^*(a_1,a_2,t)$. Since in expression (6.16), $z_2 = a_2 + i0$ is real, the analytic continuation needs to be performed only with respect to the z_1 variables, which requires taking derivatives of $2\ln\psi^*(a_1,a_2,t)$ with respect to the entries of a_1 only. Noting that $q_1(a_1-b_1,t;a_1+b_1,t)$ is non-negative real, by integrating (6.15) against an arbitrary function $f(a_1)$, we find

$$\int f(a_1) q_1(a_1-b_1,t;a_1+b_1,t)\,da_1 = \langle \psi(a_1,a_2,t), \mathbf{O}_1(b_1)\psi(a_1,a_2,t)\rangle, \tag{6.17}$$

where $\mathbf{O}_1(b_1)$ is Hermitian, so that the left-hand side of (6.17) does not depend on $\{A_2,\phi_2\}$. Since $f(a_1)$ is arbitrary, this implies that the end-point density $q_1(x_1,t;y_1,t)$ does not depend on the potentials $\{A_2,\phi_2\}$. □

To illustrate this result, we consider an example used by Nelson in Ref. 10, pp. 125–126 and Ref. 13 to demonstrate that his version of stochastic mechanics is nonlocal.

Example 6.1: Consider a quantum diffusion $x(t)$ with components $x_1(t)$ and $x_2(t)$, which correspond to the positions of two correlated but dynamically uncoupled particles, where the first particle is free and the second is a harmonic oscillator with frequency ω and rest position x_{20}. The initial wave function is given by

$$\psi(x,0)=\frac{1}{(2\pi)^{1/2}}\exp-\frac{1}{4}(x-x_0)^T K_x^{-1}(0)(x-x_0), \tag{6.18a}$$

with

$$K_x(0)=\begin{bmatrix}2 & 1\\ 1 & 1\end{bmatrix} \tag{6.18b}$$

and

$$x_0=\begin{bmatrix}x_{10}\\ x_{20}\end{bmatrix}, \tag{6.18c}$$

where the rest positions x_{10} and x_{20} of the two particles are assumed to be widely separated. Then, although $x_1(t)$ and $x_2(t)$ are statistically correlated, the locality property requires that the statistics of the $x_1(t)$ process should not depend on the frequency ω. This is due to the fact that, in the absence of any instantaneous action at a distance, the first particle does not know which frequency ω has been selected for the harmonic oscillator.

To verify that this is the case, note that since the Hamiltonian is quadratic and the initial wave function is Gaussian, the wave function remains Gaussian and can be expressed as

$$\psi(x,t)=\exp[-\tfrac{1}{2}(x-x_0)^T\Psi^{-1}(t)(x-x_0)+\alpha(t)], \tag{6.19}$$

where $\alpha(t)$ denotes a normalizing constant. Then the Schrödinger equation reduces to the Riccati equation,

$$i\frac{d\Psi}{dt}=-I_2+\Psi\Phi\Psi, \tag{6.20}$$

where

$$\Phi=\begin{bmatrix}0 & 0\\ 0 & \omega^2\end{bmatrix} \tag{6.21}$$

is the matrix representing the scalar potentials of the free particle and harmonic oscillator. Solving this equation with initial condition $2K_x(0)$ gives

$$\Psi(t)=\frac{1}{\beta(t)}\begin{bmatrix}(4+it)\beta(t)-4i\omega\,\sin(\omega t) & 2\\ 2 & 2\cos(\omega t)+\dfrac{i}{\omega}\sin(\omega t)\end{bmatrix}, \tag{6.22a}$$

with

$$\beta(t)=\cos(\omega t)+2i\omega\,\sin(\omega t). \tag{6.22b}$$

Then the real and imaginary parts $R(x,t)$ and $S(x,t)$ of $\ln\psi(x,t)$ take the form (4.1b)–(4.1c) with $x_C(t)=x_0$, $p_C(t)=0$, and

$$(2R(t))^{-1}=K_x(t)=\begin{bmatrix}2+\dfrac{t^2}{4} & \cos(\omega t)-\dfrac{t}{4\omega}\sin(\omega t)\\ \cos(\omega t)-\dfrac{t}{4\omega}\sin(\omega t) & \cos^2\omega t+\dfrac{1}{2\omega^2}\sin^2(\omega t)\end{bmatrix}, \tag{6.23}$$

$$K_x(t)S(t)=\begin{bmatrix} \dfrac{t}{4} & -\omega\,\sin(\omega t)-\dfrac{t}{4}\cos(\omega t) \\ -\dfrac{1}{4\omega}\sin(\omega t) & \left(\dfrac{1}{2\omega}-\omega\right)\sin(\omega t)\cos(\omega t) \end{bmatrix}. \tag{6.24}$$

Fourier transforming $\psi(x,t)$ and squaring the magnitude of the resulting transform, we also find that the momentum process $p(t)$ has a zero-mean Gaussian density with covariance matrix

$$K_p(t)=\frac{K_x^{-1}(t)}{4}+S(t)K_x(t)S(t). \tag{6.25}$$

Since $S(0)=0$, the process $x(t)$ has minimum uncertainty at $t=0$.

The end-point density $q(x,t;y,t)$ takes the form (4.8)–(4.9), and to complete the construction of the quantum diffusion corresponding to the wave function (6.19), we would need, in principle, to evaluate $q(x,s;y,t)$ by propagating the backward heat equation (2.13a). However, this computation is rather tedious. A simpler approach consists in observing from the characterization of Gaussian reciprocal diffusions in terms of their Newton law given in Ref. 18, that for an interval $[0,T]$ over which it is defined, $z(t)=x(t)-x_0$ is a solution of the second-order stochastic differential equation,

$$\mathscr{L}_F z_1(t)=\xi_1(t) \tag{6.26a}$$

$$\mathscr{L}_H z_2(t)=\xi_2(t), \tag{6.26b}$$

with Dirichlet boundary conditions

$$\begin{bmatrix} z(0) \\ z(T) \end{bmatrix}\sim N(0,\mathbf{P}), \tag{6.27a}$$

where

$$\mathbf{P}=\begin{bmatrix} K_x(0) & K(0,T) \\ K(T,0) & K_x(T) \end{bmatrix}. \tag{6.27b}$$

In this equation, the operators $\mathscr{L}_F$ and $\mathscr{L}_H$ are given by (4.27b) and (4.40b), respectively, and the noises $\xi_1(t)$ and $\xi_2(t)$ are two independent generalized Gaussian processes, independent of $z(0)$ and $z(T)$, with zero mean and autocorrelations

$$E[\xi_1(t)\xi_1(s)]=\mathscr{L}_F\delta(t-s), \tag{6.28a}$$

$$E[\xi_2(t)\xi_2(s)]=\mathscr{L}_H\delta(t-s). \tag{6.28b}$$

In (6.27b), $K(t,s)=E[z(t)z^T(s)]$ denotes the matrix autocorrelation of $z(t)$, which still remains to be determined.

In our analysis, the length T of the interval is selected as one-quarter of the period of the harmonic oscillator, i.e., $T=\pi/2\omega$. Then, the Green's functions of the operators $\mathscr{L}_F$ and $\mathscr{L}_H$ with homogeneous Dirichlet boundary conditions at $t=0$ and $t=T$ are given by

$$\Gamma_F(t,s)=\begin{cases} \left(1-\dfrac{t}{T}\right)s, & \text{for } t\geqslant s, \\ t\left(1-\dfrac{s}{T}\right), & \text{for } s\geqslant t, \end{cases} \tag{6.29}$$

and

$$\Gamma_H(t,s)=\begin{cases}\dfrac{1}{\omega}\cos(\omega t)\sin(\omega s), & \text{for } t\geqslant s,\\ \dfrac{1}{\omega}\sin(\omega t)\cos\,\omega s, & \text{for } s\geqslant t.\end{cases} \tag{6.30}$$

As shown in Ref. 18, the solution of the stochastic boundary value problem (6.26)–(6.28) can be expressed as

$$z_1(t)=I_1(t)+\frac{T-t}{T}\,z_1(0)+\frac{t}{T}\,z_1(T), \tag{6.31a}$$

$$z_2(t)=I_2(t)+\cos(\omega t)z_2(0)+\sin(\omega t)z_2(T), \tag{6.31b}$$

where

$$I_1(t)=\int_0^T \Gamma_F(t,s)\xi_1(s)ds, \tag{6.32a}$$

$$I_2(t)=\int_0^T \Gamma_H(t,s)\xi_2(s)ds, \tag{6.32b}$$

are two independent zero-mean Gaussian processes with covariances $\Gamma_F(t,s)$ and $\Gamma_H(t,s)$, respectively. This implies that $I_1(t)$ is a Brownian bridge process, i.e., $I_1(t)=W_1(t)-tW_1(T)/T$, where $W_1(\cdot)$ is a standard Wiener process. The only element missing in the above specification of $z(t)$ is the correlation matrix $K(0,T)$ of the end-point vectors $z(0)$ and $z(T)$. Evaluating the autocorrelation function of the solution $z(t)$ given by (6.31), and comparing with the expression (6.23) for $K_x(t)$ gives

$$E[z(0)z^T(T)]=K(0,T)=\begin{bmatrix}2-\dfrac{T}{2} & 0\\ 1 & -\dfrac{1}{2\omega}\end{bmatrix}, \tag{6.33}$$

from which we deduce that the autocorrelation of the process $z(t)$ is given by

$$K_1(t,s)=E[z_1(t)z_1(s)]=2+\frac{ts}{4}-\frac{|t-s|}{2}, \tag{6.34a}$$

$$K_{12}(t,s)=E[z_1(t)z_2(s)]=\cos(\omega s)-\frac{t}{4\omega}\sin(\omega s), \tag{6.34b}$$

$$K_2(t,s)=E[z_2(t)z_2(s)]=-\frac{1}{2\omega}\sin(\omega|t-s|)+\cos\,\omega t\,\cos\,\omega s+\frac{1}{2\omega^2}\sin\,\omega t\,\sin\,\omega s. \tag{6.34c}$$

From (6.34a), we see that the covariance function of the $x_1(t)=z_1(t)+x_{10}$ process is independent of the frequency ω of the harmonic oscillator, thus demonstrating locality.

It is also worth noting that the components $z_1(t)$ and $z_2(t)$, viewed as isolated processes, are not quantum diffusions. To verify this fact, note that according to Lemma 6.1, z_1 and z_2 are

zero-mean Gaussian reciprocal diffusions. Given such a diffusion with autocorrelation $K(t,s)$, it is shown in Ref. 18 that the matrix $V(t)$ parametrizing the mean velocity in (2.41b), and the stress tensor $\pi(t)$ can be expressed as

$$V(t)=\frac{1}{2}\left(\frac{\partial K}{\partial t}(t^+,t)+\frac{\partial K}{\partial t}(t^-,t)\right)K^{-1}(t,t), \tag{6.35a}$$

$$\pi(t)=\frac{1}{2}\left(\frac{\partial^2 K}{\partial t\,\partial s}(t^+,t)+\frac{\partial^2 K}{\partial t\,\partial s}(t^-,t)\right)-V(t)K(t,t)V^T(t). \tag{6.35b}$$

Applying these expressions to the autocorrelation functions K_1 and K_2 in (6.34a) and (6.34c) gives

$$V_1(t)=\frac{t/4}{2+t^2/4},\quad \pi_1(t)=\frac{1}{2(2+t^2/4)}=\frac{1}{2}K_{x_1}^{-1}(t), \tag{6.36a}$$

$$V_2(t)K_2(t,t)=\left(\frac{1}{2\omega}-\omega\right)\sin(\omega t)\cos(\omega t), \tag{6.36b}$$

$$\pi_2(t)=\left[2\left(\cos^2(\omega t)+\frac{1}{2\omega^2}\sin^2(\omega t)\right)\right]^{-1}=\frac{1}{2}K_{x_2}^{-1}(t). \tag{6.36c}$$

Thus, the stress tensors $\pi_i(t)$ with $i=1,2$ are proportional to the inverse covariances $K_{x_1}^{-1}(t)$, but the coefficient of proportionality is $\frac{1}{2}$, instead of $\frac{1}{4}$, as required by the closure rule (3.2b). □

Finally, it is worth noting that the reciprocity property of quantum diffusions can be viewed as locality in time, in the sense that given $x(t-h)$ and $x(t+h)$, the position $x(t)$ is conditionally independent of $x(s)$ for s outside the interval $[t-h,t+h]$, so that, in some sense, the stochastic mechanics of quantum diffusions achieves locality in both space and time.

VII. NEGATIVE PROBABILITIES

For all the quantum processes considered up to this point, such as the Gaussian processes of Sec. IV, the end-point density $q(x,s;y,t)$ of the quantum diffusion associated to the wave function $\psi(x,t)$ was always positive. Unfortunately, this property does not hold when $\rho(x,t)=|\psi(x,t)|^2$ has some nodes. To see this, note that the density $q(x,t;y,t)$ obtained from (3.27) is non-negative but takes zero values whenever $x=y=x_0$, where x_0 denotes an arbitrary node of $\rho(x,t)$. But the heat equation (2.13a) for $q(x,s;y,t)$ with $s<t$ implies that it satisfies the integral equation,

$$q(x,t;y,t)=\int G(z,s;x,t)q(z,s;y,t)dz. \tag{7.1}$$

In this expression, the Green's function $G(z,s;x,t)$, which is the transition density of a Markov diffusion with creation or killing, is positive for all z and x. Consequently, zero values on the left side of the above identity can only occur if the integrand $q(z,s;y,t)$ takes both negative and positive values. To illustrate this phenomenon, consider the excited states of the harmonic oscillator.

Example 7.1: The wave functions corresponding to the eigenstates of a harmonic oscillator with frequency ω are given by

$$\psi_n(x,t)=\left(\frac{\omega}{\pi}\right)^{1/4}\frac{1}{(2^n n!)^{1/2}}H_n(\omega^{1/2}x)\exp-\left[\frac{\omega x^2}{2}+i\omega\left(n+\frac{1}{2}\right)t\right], \tag{7.2}$$

where the $H_n(y)s$ are the Hermite polynomials. They satisfy the recursion

$$H_n(y)=2yH_{n-1}(y)-2(n-1)H_{n-2}(y), \tag{7.3a}$$

for $n\geqslant 2$, with

$$H_0(y)=1, \quad H_1(y)=2y. \tag{7.3b}$$

Since $\psi_n(x,t)$ depends on t only through its phase, the probability density $\rho_n(x,t)=\rho_n(x)=|\psi_n(x,t)|^2$ of each eigenstate is time invariant. In (7.2), $n=0$ represents the ground state of the harmonic oscillator, and $n\geqslant 1$ the excited states. Note that the ground state is obtained by setting $x_C(t)=0$ in the coherent state examined in Example 4.2. The excited states have nodes at the values of x corresponding to zeros of the Hermite polynomials $H_n(\omega^{1/2}x)$. For example, for the first two excited states, $\rho_1(x)$ has a node at $x=0$, and $\rho_2(x)$ has nodes at $x=\pm 1/(2\omega)^{1/2}$. This implies that the function

$$2\ln\ \psi_n^*(a,t)=-\omega a^2+2\ln\ H_n(\omega^{1/2}a)+f_n(t), \tag{7.4a}$$

with

$$f_n(t)=\frac{1}{2}\ln\left(\frac{\omega}{\pi}\right)-\ln(2^2n!)+i\omega(2n+1), \tag{7.4b}$$

has logarithmic singularities at these nodes. Consequently, the function

$$F_n(z,t)=-\omega z^2+2\ln\ H_n(\omega^{1/2}z)+f_n(t), \tag{7.5}$$

obtained by analytic continuation of $2\ln\ \psi^*(a,t)$ is meromorphic. Its real part,

$$M_n(a,b)=-\omega(a^2-b^2)+\ln[|H_n(\omega^{1/2}(a+jb))|^2]+f_{M,n}, \tag{7.6a}$$

with

$$f_{M,n}=\frac{1}{2}\ln\left(\frac{\omega}{\pi}\right)-\ln(2^2n!), \tag{7.6b}$$

has the feature of being time invariant. From (2.26b)–(2.26c), we find that the mean velocity and stress tensor of the quantum diffusions modeling the eigenstates of the harmonic oscillator take the form

$$v_n(a,t)=v_n(a)=0 \tag{7.7a}$$

$$\pi_n(a,t)=\pi_n(a)=\frac{\omega}{2}-\frac{1}{2}\frac{d^2}{da^2}\ln\ H_n(\omega^{1/2}a), \tag{7.7b}$$

for values of a that do not correspond to nodes of $\rho_n(a)$. The zero value of the mean velocity just reflects the stationarity of the eigenstates.

Then the expression (2.35) for the end-point density gives

$$q_n(x,t;y,t)=\left(\frac{\omega}{\pi}\right)^{1/2}P_n(x,y)\exp-\omega xy, \tag{7.8a}$$

where

$$P_n(x,y)=\frac{1}{2^n n!}\left|H_n\left(\omega^{1/2}\left(\frac{y+x}{2}+i\,\frac{y-x}{2}\right)\right)\right|^2 \tag{7.8b}$$

is a polynomial of degree $2n$ in x and y. In particular,

$$P_0(x,y)=1, \quad P_1(x,y)=\omega(x^2+y^2), \tag{7.9a}$$

$$P_2(x,y)=\tfrac{1}{8}\left[(4\omega yx-2)^2+4\omega^2(y^2-x^2)^2\right]. \tag{7.9b}$$

Note that $q_n(x,t;y,t)$ does not depend on t, and, as expected, $q_1(x,t;y,t)$ has a node at $x=y=0$ and $q_2(x,t;y,t)$ has nodes at $x=y\pm 1/(2\omega)^{1/2}$.

To solve the backward heat equation (2.13a) for $q_n(x,s;y,t)$, it is convenient to perform the transformation

$$q_n(x,s;y,t)=P_n(x,s;y,t)q_0(x,s;y,t), \tag{7.10}$$

where $q_0(x,s;y,t)$ is the end-point density for the ground state of the harmonic oscillator. It can be evaluated by setting $x_C(t)=p_C(t)$ in the expression obtained for the coherent oscillator of Example 4.2. This gives

$$q_0(x,s;y,t)=D(t-s)\exp\left[-\frac{\omega}{2\cos(\omega(t-s))}\left(\sin(\omega(t-s))(x^2+y^2)+2xy\right)\right], \tag{7.11a}$$

with

$$D(t-s)=\left(\frac{\omega}{\pi\cos(\omega(t-s))}\right)^{1/2}. \tag{7.11b}$$

Note that since the initial condition $q_0(x,t;y,t)$ does not depend on t, and the spatial part,

$$\mathbf{H}=\frac{1}{2}\left(\frac{d^2}{dx^2}+(\omega x)^2\right) \tag{7.12}$$

of the heat operator $\mathbf{L}_{x,s}$ is time invariant, $q_0(x,s;y,t)$ depends only on $t-s$. Under the transformation (7.10), the heat equation (2.13a) for q_n is transformed into the equation

$$\left(\frac{\partial}{\partial s}-\frac{1}{2}\frac{\partial^2}{\partial x^2}-\frac{\partial}{\partial x}\ln q_0(x,s;y,t)\,\frac{\partial}{\partial x}\right)P_n(x,s;y,t)=0, \tag{7.13}$$

for P_n with $s\leqslant t$. Since

$$\frac{\partial}{\partial x}\ln q_0(x,s;y,t)=\frac{\omega}{\cos(\omega(t-s))}\left(\sin(\omega(t-s))x+y\right) \tag{7.14}$$

is linear in x and y, and the initial condition $P_n(x,t;y,t)$ for this equation is a polynomial of degree $2n$, $P_n(x,s;y,t)$ remains a polynomial of degree $2n$ in x and y for all $s\leqslant t$. Matching the coefficients of like powers of x and y in (7.13), this equation can be transformed into a system of ordinary differential equations for the coefficients of P_n.

For the first excited state of the harmonic oscillator, we obtain

$$P_1(x,s;y,t)=\frac{\omega}{\cos^2(\omega(t-s))}\left[(x^2+y^2)+2xy\,\sin(\omega(t-s))-\frac{1}{2}\sin(2\omega(t-s))\right], \tag{7.15}$$

which even for small values of $t-s$ takes negative values in the vicinity of the node $x=y=0$ of $q_1(x,t;y,t)$.

Finally, since $q_n(x,t;y,t)$ does not depend on t, and the spatial part $\mathbf{H}$ of the heat operator $\mathbf{L}_{x,s}$ is time invariant, the end-point density $q_n(x,s;y,t)$ depends only on $t-s$. This implies that the

quantum diffusions modeling the excited states of the harmonic oscillator are all stationary, since their finite joint densities (2.7) are invariant under time shifts. □

The above example shows that, given a quantum process whose wave function $\psi(x,t)$ includes nodes, the end-point density $q(x,s;y,t)$ of the corresponding quantum diffusion must necessarily take negative values. Although this feature may appear troubling at first sight, it is not completely inconsistent with standard probability theory, provided that instead of selecting the Borel cylinder sets as the family of events associated to the finite joint densities (2.7), we select a smaller family of events E whose probability $P(E)$ satisfies $0 \leqslant P(E) \leqslant 1$. In other words, as was already argued from a physics perspective in Ref. 22, we can employ negative probabilities as an intermediate bookkeeping step, as long as all ''observable'' events have a positive probability, and provided the operations we perform respect the axioms of probability theory. In this respect, note that the set of ''observable'' events is highly restricted in quantum mechanics, since such events must concern quantities represented by commuting operators. For example, for the position and momentum processes, only events concerning the position only, or the momentum only, are observable. Since most operators do not commute, the emphasis in quantum mechanics is usually on marginal densities, such as for the position, or the momentum only. By contrast, the goal of stochastic mechanics in either Markovian or non-Markovian form, is to construct finite joint densities for the position process at successive times $t_1 \leqslant \cdots \leqslant t_i \leqslant \cdots \leqslant t_N$, even if the position operators $\{X(t_i), 1 \leqslant i \leqslant N\}$ in the Heisenberg representation do not commute.

The first attempt at accomplishing an objective of this type, at least in a limited way, dates back to the introduction by Wigner[20] of a joint density for the position and momentum of a particle at time t. Specifically, the Wigner distribution, which is defined as

$$W(x,p,t) = \frac{1}{2\pi} \int \psi\left(x + \frac{y}{2}, t\right) \psi^*\left(x - \frac{y}{2}, t\right) \exp - ipy \; dy, \tag{7.16}$$

has the feature that its marginals with respect x and p correspond to the position and momentum probability densities of quantum mechanics. However, an aspect of the Wigner distribution that some researchers find unappealing is that it takes negative values. For example, the Wigner distribution for the eigenstates of the harmonic oscillator is given by[21]

$$W_n(x,p,t) = \frac{(-1)^n}{\pi} L_n\left(\frac{4H}{\omega}\right) \exp\left(\frac{-2H}{\omega}\right), \tag{7.17a}$$

where

$$H(x,p) = \frac{p^2}{2} + \frac{(\omega x)^2}{2} \tag{7.17b}$$

is the harmonic oscillator's Hamiltonian, and $L_n(y)$ is the nth Laguerre polynomial. From the first few Laguerre polynomials,

$$L_0(y) = 1, \quad L_1(y) = 1 - y, \quad L_2(y) = 1 - 2y + y^2, \tag{7.18}$$

we see that while $W(x,p,t)$ is positive for the oscillator's ground state, it takes negative values for the excited states. The fact that the Wigner distribution can be negative inspired efforts to find distributions that would always be positive. However, it was later shown[20] that if, beyond the requirement that the marginals of $W(x,p,t)$ should coincide with the position and momentum densities, a few additional conditions are imposed, $W(x,p,t)$ is unique.

Note that the Wigner distribution is closely related to the end-point density $q(x,t;y,t)$ of quantum diffusions, since the inverse Fourier transform $w(x,z,t)$ of $W(x,p,t)$ with respect to p takes the form

$$w(x,z,t)=\psi(x+z/2,t)\,\psi^*(x-z/2,t), \tag{7.19}$$

which should be contrasted with the expression (3.27) for $q(x,t;y,t)$. Thus, the finite joint densities we have constructed for quantum diffusions can be viewed as extended Wigner distributions for the position variables at arbitrary times. Observe also that in the expression (2.7) for the finite joint densities, the only quantity that can be negative is the end-point density $q(x,s;y,t)$. The marginal densities $\rho(x,t)=q(x,t;x,t)$ are always non-negative, since by construction the density $q(x,t;y,t)$ given by (3.27) is always non-negative, and the three-point transition densities $r(x,s;y,t;z,u)$ with $s<t<u$ are also positive.

VIII. CONCLUSIONS

In this paper, we have presented a comprehensive reformulation of stochastic mechanics, which instead of using Markov diffusions, relies on a subclass of reciprocal diffusions, the quantum diffusions, whose conservation laws are equivalent to Schrödinger's equation. This new form of stochastic mechanics presents several advantages over earlier Markovian theories of Schrödinger or Nelson. First, it is not necessary to introduce a quantum potential in the Newton law satisfied by the diffusions in order to make their evolution consistent with Schrödinger's equation. The new mechanics is local, and the uncertainty principle arises naturally from the closure rules defining quantum diffusions.

In spite of the apparent agreement between quantum mechanics and the stochastic mechanics of quantum diffusions, the two theories have significant differences. Quantum mechanics is less ambitious than stochastic mechanics in the sense that it is primarily concerned with the evolution of marginal densities for the position or momentum variables of a physical system. No attempt is made at evaluating joint probability densities for the positions at different times, since, in general, the Heisenberg operators $X(t)$ and $X(s)$ representing the positions at different times t and s do not commute, so that these positions are not simultaneously observable. On the other hand, stochastic mechanics assigns joint probability densities $p(x_0,t_0;x_1,t_1;\ldots,x_N,t_N)$ to the positions at different times. These joint densities yield marginals for the position and velocity variables at a single time t, which are consistent with the rules of quantum mechanics, in the sense that the conservation laws for $\rho(x,t)$ and $v(x,t)$ are equivalent to Schrödinger's equation. However, the finite joint densities may themselves be devoid of physical significance, as evidenced by the fact that they can be negative. Through Newton's law, stochastic mechanics provides a nice interpretation of the relation existing between quantum and classical mechanics, but it represents a model rather than a physical theory.

The new stochastic mechanics sketched here is incomplete in several respects. First, many important quantum mechanics phenomena, such as interference, scattering, statistics of indistinguishable particles, or measurement theory, need to be given a stochastic formulation within the new theory. It would also be of interest to obtain a variational derivation of the closure rules (3.1a)–(3.1b) similar to the one proposed in Ref. 33 for Markovian stochastic mechanics, but possibly with a different action functional. Finally, as was noted in the discussion of the harmonic oscillator of Example 4.2, we need to examine how quantum diffusions with a finite lifetime can be combined to describe quantum processes over longer periods of time.

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Nonequilibrium fluctuation–dissipation relations for independent random rate processes with dynamical disorder

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A class of rate processes with dynamical disorder is investigated based on the two following assumptions: (a) the system is composed of a random number of particles (or quasiparticles) which decay according to a first-order kinetic law; (b) the rate coefficient of the process is a random function of time with known stochastic properties. The formalism of characteristic functionals is used for the direct computation of the dynamical averages. The suggested approach is more general than the other approaches used in the literature: it is not limited to a particular type of stochastic process and can be applied to any type of random evolution of the rate coefficient. We derive an infinity of exact fluctuation–dissipation relations which establish connections among the moments of the survival function and the moments of the number of surviving particles. The analysis of these fluctuation–dissipation relations leads to the unexpected result that in the thermodynamic limit the fluctuations of the number of particles have an intermittent behavior. The moments are explicitly evaluated in two particular cases: (a) the random behavior of the rate coefficient is given by a non-Markovian process which can be embedded in a Markovian process by increasing the number of state variables and (b) the stochastic behavior of the rate coefficient is described by a stationary Gaussian random process which is generally non-Markovian. The method of curtailed characteristic functionals is used to recover the conventional description of dynamical disorder in terms of the Kubo–Zwanzig stochastic Liouville equations as a particular case of our general approach. The fluctuation–dissipation relations can be used for the study of fluctuations without making use of the whole mathematical formalism. To illustrate the efficiency of our method for the analysis of fluctuations we discuss three different physicochemical and biochemical problems. A first application is the kinetic study of the decay of positrons or positronium atoms thermalized in dense fluids: in this case the time dependence of the rate coefficient is described by a stationary Gaussian random function with an exponentially decaying correlation coefficient. A second application is an extension of Zwanzig's model of ligand–protein interactions described in terms of the passage through a fluctuating bottle

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neck; we complete the Zwanzig's analysis by studying the concentration fluctuations. The last example deals with jump rate processes described in terms of two independent random frequencies; this model is of interest in the study of dielectric or conformational relaxation in condensed matter and on the other hand gives an alternative approach to the problem of protein–ligand interactions. We evaluate the average survival function in several particular cases for which the jump dynamics is described by two activated processes with random energy barriers. Depending on the distributions of the energy barriers the average survival function is a simple exponential, a stretched exponential, or a statistical fractal of the inverse power law type. The possible applications of the method in the field of biological population dynamics are also investigated. © *1996 American Institute of Physics.* [S0022-2488(96)02212-8]

I. INTRODUCTION

Rate processes with static or dynamic disorder are commonly encountered in nature.[1] A common approach to a first-order rate process with static disorder is based on the assumption that the observed survival (relaxation) function at time t, $\langle l(t)\rangle_{\text{static}}$ is an average of an exponential decay law $\exp(-Wt)$ with respect to the possible values of the rate coefficient W

$$\langle l(t)\rangle_{\text{static}}=\int_0^\infty \exp(-Wt)f(W)dW, \tag{1.1}$$

where $f(W)dW$ is the probability density of the rate coefficient. We note that the average survival function is simply the Laplace transform of the probability density $f(W)dW$ of the rate coefficient W. Such an approach has been used in the study of protein–ligand interactions in biochemistry;[2,3] in this case different conformational states of the protein have different activation barriers to rebinding, resulting in a statistical distribution of the rate coefficients. Similar approaches have been used for describing the combination processes of active intermediates in radiochemistry,[4] the extinction of fluorescence due to the direct energy transfer from excited donors to acceptors,[5–8] the description of dielectric relaxation,[8,9] for the random walk description of transport processes with static or temporal disorder,[10] and for the study of one-channel compound nuclear reactions,[11] or of linear viscoelasticity.[12]

The description of rate processes with dynamical disorder is more complicated. In this case the relaxation rate is a random function of time and the average (1.1) is replaced by

$$\langle l(t)\rangle_{\text{dynamic}}=\left\langle \exp\left(-\int_0^t W(t')dt'\right)\right\rangle_{\text{dynamic}}, \tag{1.2}$$

where the average can be reduced to the evaluation of a path integral over all possible trajectories $W=W(t')$, $t\geqslant t'\geqslant 0$

$$\langle l(t)\rangle_{\text{dynamic}}=\overline{\int\int} \exp\left(-\int_0^t W(t')dt'\right)\mathscr{P}[W(t')]D[W(t')], \tag{1.3}$$

where $\overline{\int\int}$ stands for the operation of path integration, $D[W(t')]$ is a suitable integration measure over the space of random rates $W(t')$, and

$$\mathscr{P}[W(t')]D[W(t')], \quad \text{with} \quad \overline{\int\int \mathscr{P}[W(t')]D[W(t')]} = 1 \tag{1.4}$$

is the probability density functional of the random rate coefficient $W(t')$. Equation (3) is a functional analog of the Laplace transform corresponding to the static disorder [Eq. (1)]. The evaluation of dynamical averages is much more difficult than the evaluation of static averages, mainly because the functional integral (3) can be computed only in a few particular cases; the major difficulty is due to the fact that for non-Gaussian processes we do not even have an appropriate definition for the integration measure $D[W(t')]$.

The first system with dynamical disorder studied in the literature is a simplified model for the line shape in magnetic resonance spectroscopy[13,14] suggested by Anderson and Kubo. This initial approach has been extended to other spectroscopical problems.[14–21] Similar rate processes with dynamical disorder have been used in connection with the study of earthquakes,[22] non-Gaussian diffusion,[23] the Taylor problem from hydrodynamics,[24] the description of transport processes in networks with dynamic percolation,[25] the Browniam motion description of very fast chemical processes without activation barriers,[26] the study of fluorescence depolarization[27] and of protein dynamics,[28] and in connection with the analysis of collective orientational relaxation in dense liquids.[29] In these studies most authors avoid the direct evaluation of the dynamical average (3) and use instead indirect methods such as the solving of certain stochastic Liouville equations.[1,30,31]

The approaches presented in the literature can be applied only to certain particular cases of stochastic processes, for instance, in the case of a Markovian or Gaussian behavior. A general treatment for the analysis of dynamical disorder for an arbitrary type of stochastic dependence is missing. The purpose of this article is to fill this gap in the literature and to derive an efficient method for evaluating the dynamical average for a rate process characterized by an arbitrary stochastic behavior. The initial motivation of our approach is the investigation of fluctuations for a model of ligand–protein interactions suggested by Zwanzig[32] and further studied by Wang and Wolynes.[33] The main sources of inspiration for our method are the initial Kubo approach[14] to the problem of line shape and the characteristic functional approaches used by the authors for the description of space and time-dependent colored noise,[34] of stochastic gravitational fluctuations,[35] and of fractal random processes.[36] The main advantage of our approach is its versatility and generality. It leads to an infinite number of fluctuation–dissipation relations which allow to study the fluctuations without using the whole mathematical apparatus of the theory.

The structure of the article is as follows. In Sec. II we give a general formulation of the problem. In Secs. III and IV a general approach for computing the dynamical averages is developed and the fluctuation–dissipation relations are derived. In Sec. V the moments of the survival function and of the number of surviving particles are explicitly derived for Markovian and stationary Gaussian processes. Sections VI, VII, and VIII deal with the application of the theory to three different problems from condensed matter physics and biochemistry. In Sec. IX the main results of the article are summarized and the possibilities of application to the theory in exobiology and biological population dynamics are pointed out. To make the body of the article easier the details of the computations are not presented in the text; they are given in Appendices A to D.

II. FORMULATION OF THE PROBLEM

We consider a system made up of a random number of independent particles or quasiparticles and assume that the rate of decomposition of a particle at a time between t and $t+dt$, $W(t)dt$, is a random function whose stochastic properties are characterized by the probability density functional (1.4) or by the corresponding characteristic functional

$$G[K(t')]=\left\langle \exp\left(i\int_0^t K(t')W(t')dt' \right) \right\rangle_{\text{dynamic}}$$
$$=\overline{\int\int} \exp\left(i\int_0^t K(t')W(t')dt' \right)\mathscr{P}[W(t')]D[W(t')], \tag{2.1}$$

where $K(t')$ is a suitable test function. The initial number N of particles is a random variable characterized by a probability

$$P(N,t=0), \quad \sum_N P(N,0)=1 \tag{2.2}$$

or by the corresponding generating function

$$g(z,t=0)=\sum_N z^N P(N,0), \quad |z|\leqslant 1, \tag{2.3}$$

where z is a complex variable with the absolute value at most equal to the unity.

The stochastic properties of the numbers $N(t_1),\ldots,N(t_m)$ of particles surviving at times $0\leqslant t_1\leqslant\cdots\leqslant t_m\leqslant t$ are characterized by an m-gate probability

$$P_m(N(t_m),t_m;\ldots;N(t_1),t_1), \tag{2.4}$$

with the normalization condition

$$\sum_{N_m}\cdots\sum_{N_1} P_m(N_m,t_m;\ldots;N_1,t_1)=1 \tag{2.5}$$

and

$$t_u=u\Delta t, \quad \Delta t=(t-t_0)/(m+1), \quad u=1,\ldots,m. \tag{2.6}$$

In the limit $m\to\infty$ ($\Delta t\to 0$), P_m becomes a probability functional which describes the stochastic properties of a random trajectory $N(t')$, $0\leqslant t'\leqslant t$

$$B[N(t');\quad 0\leqslant t'\leqslant t]=\lim_{\substack{m\to\infty\\(\Delta t\to 0)}} P_m(N_m,t_m;\ldots;N_1,t_1), \tag{2.7}$$

which obeys the normalization condition

$$\overline{\sum\sum} B[N(t');\quad 0\leqslant t'\leqslant t]=1, \tag{2.8}$$

where $\overline{\sum\sum}$ stands for a path sum which is a discrete analog of a path integral

$$\overline{\sum\sum}\cdots=\lim_{\substack{m\to\infty\\(\Delta t\to 0)}}\sum_{N(t_1)}\cdots\sum_{N(t_m)}\cdots. \tag{2.9}$$

In terms of the probability functional $B[N(t')]$ we can define the characteristic functional

$$\Xi[\mathscr{K}(t')]=\left\langle \exp\left(i\int_0^t \mathscr{K}(t')N(t')dt' \right) \right\rangle_{\text{dynamic}} = \overline{\sum\sum} \exp\left(i\int_0^t \mathscr{K}(t')N(t')dt' \right) B[N(t')]. \tag{2.10}$$

The central moments $\langle N(t_1)\cdots N(t_m)\rangle$ and the cumulants $\langle\langle N(t_1)\cdots N(t_m)\rangle\rangle$ of the number of surviving particles may be defined by the moment and cumulant expansions of $\Xi[\mathscr{K}(t')]$

$$\begin{aligned}\Xi[\mathscr{K}(t')]&=1+\sum_{m=1}^{\infty}\frac{i^m}{m!}\int_0^t\cdots\int_0^t \langle N(t_1')\cdots N(t_m')\rangle \mathscr{K}(t_1')\cdots\mathscr{K}(t_m')dt_1'\cdots dt_m' \\ &=\exp\left\{\sum_{m=1}^{\infty}\frac{i^m}{m!}\int_0^t\cdots\int_0^t \langle\langle N(t_1')\cdots N(t_m')\rangle\rangle \mathscr{K}(t_1')\cdots\mathscr{K}(t_m')dt_1'\cdots dt_m'\right\},\end{aligned} \tag{2.11}$$

that is, the central moments and the cumulants can be computed by evaluating the functional derivatives

$$\langle N(t_1)\cdots N(t_m)\rangle=(-i)^m\left.\frac{\delta^m\Xi[\mathscr{K}(t')]}{\delta\mathscr{K}(t_1)\cdots\delta\mathscr{K}(t_m)}\right|_{\mathscr{K}(t')=0}, \tag{2.12}$$

and

$$\langle\langle N(t_1)\cdots N(t_m)\rangle\rangle=(-i)^m\left.\frac{\delta^m \ln \Xi[\mathscr{K}(t')]}{\delta\mathscr{K}(t_1)\cdots\delta\mathscr{K}(t_m)}\right|_{\mathscr{K}(t')=0}. \tag{2.13}$$

On the other hand the rate process can be characterized by the moments of a realization of the survival function

$$l(t)=\exp\left(-\int_0^t W(t')dt'\right), \tag{2.14}$$

i.e., by the averages

$$\langle l(t_1)\cdots l(t_m)\rangle_{\text{dynamic}}=\overline{\int\int} l(t_1)\cdots l(t_m)\mathscr{P}[W(t')]D[W(t')]. \tag{2.15}$$

The aim of this article is to answer the following questions:

(1) Given the stochastic properties of the random rate coefficient and of the initial number of particles, which are the stochastic properties of the number of particles at any time?
(2) Which are the moments of the survival function $l(t)$?
(3) Is there any relationship between the moments of the survival function and the moments of the number of surviving particles?
(4) For which systems can the moments of the number of surviving particles and of the survival function be computed explicitly and which is the relationship between these functions and the experimentally accessible quantities?
(5) In order to answer these questions we should express the characteristic functional $\Xi[\mathscr{K}(t')]$ of the number of surviving particles in terms of the characteristic functional $G[K(t')]$ of the random rate coefficient. The main idea of our approach is to evaluate the dynamical average in Eq. (2.10) in two steps: first we consider a given realization of the random rate coefficient $W(t')$, $0\leqslant t'\leqslant t$ and average over all possible numbers of surviving particles which are

compatible with this realization; finally we average over all possible realizations of the random rate coefficient $W(t')$.

III. CHARACTERISTIC FUNCTIONAL APPROACH TO DYNAMICAL DISORDER

In this section we consider a realization $W(t')$, $0 \leqslant t' \leqslant t$ of the rate coefficient and try to evaluate the corresponding generating functional of the number of surviving particles. First we notice that for a given realization of the rate coefficient the dynamical disorder does not exist; we deal with an ordered random system with a time-dependent rate coefficient. The study of such systems is not necessarily related to the problem of dynamical disorder; such a study is also of interest on its own, for instance, in connection with the statistical description of the death process in mathematical demography[37] or for the study of radiochemical reactions.[4,38] We introduce the ordered characteristic functional

$$\Xi_{\text{ordered}}[.\mathscr{K}(t')|W(t')] = \left\langle \exp\left(i \int_0^t .\mathscr{K}(t')N(t')dt' \right) \right\rangle_{\text{ordered}}, \tag{3.1}$$

where the average $\langle \cdots \rangle_{\text{ordered}}$ is computed with respect to the number of surviving particles compatible with the realization $W(t')$ $0 \leqslant t' \leqslant t$. The characteristic functional $\Xi[.\mathscr{K}(t')]$ of the disordered process is simply given by

$$\Xi[.\mathscr{K}(t')] = \langle \Xi_{\text{ordered}}[.\mathscr{K}(t')|W(t')] \rangle_{\text{disorder}} = \overline{\int \int} \Xi_{\text{ordered}}[.\mathscr{K}(t')|W(t')] \mathscr{P}[W(t')] D[W(t')], \tag{3.2}$$

where the average $\langle \cdots \rangle_{\text{disorder}}$ is computed with respect to all possible values of the random function $W(t')$, $0 \leqslant t' \leqslant t$.

In Appendix A we show that the generating functional $\Xi_{\text{ordered}}[.\mathscr{K}(t')|W(t')]$ can be expressed in terms of the realization $l(t)$ of the survival function as

$$\Xi_{\text{ordered}}[.\mathscr{K}(t')|W(t')] = g\left\{ z = 1 + \int_0^t l(t').\mathscr{K}(t') \exp\left[i \int_0^{t'} .\mathscr{K}(6)d6 \right] dt', \quad t = 0 \right\}. \tag{3.3}$$

In order to compute the characteristic functional $\Xi[.\mathscr{K}(t')]$ for systems with dynamical disorder we express the generating function $g(z,0)$ corresponding to the probability $P(N,0)$ in terms of the initial factorial moments of the number of particles

$$F_m(t=0) = \langle N(N-1)\cdots(N-m+1) \rangle_{\text{dynamic}}(t=0) = \sum_N N(N-1)\cdots(N-m+1)P(N,0); \tag{3.4}$$

we have

$$F_m(0) = N_0(N_0-1)\cdots(N_0-m+1) \tag{3.5}$$

for an initial canonical ensemble and

$$F_m(0) = (\langle N_0 \rangle)^m, \tag{3.6}$$

for an initial grand canonical ensemble.

From the definition (2.3) of $g(z,0)$ it follows that

$$F_m(0)=d^m g(z,0)/dz^m|_{z=1} \tag{3.7}$$

and thus $g(z,0)$ can be expressed as a Taylor series

$$g(z,0)=1+\sum_{m=1}^{\infty}\frac{1}{m!}F_m(0)(z-1)^m. \tag{3.8}$$

By combining Eqs. (3.2), (3.3), and (3.8) the characteristic functional $\Xi[\mathscr{K}(t')]$ for systems with dynamical disorder can be expressed as

$$\Xi[\mathscr{K}(t')]=1+\sum_{m=1}^{\infty}\frac{(i)^m}{m!}F_m(0)\int_0^t\cdots\int_0^t \mathscr{K}(t_1')\cdots\mathscr{K}(t_m')\exp\left(i\sum_{u=1}^{m}\int_0^{t_u'}\mathscr{K}(\mathscr{6})d\mathscr{6}\right)$$
$$\times\langle l(t_1')\cdots l(t_m')\rangle dt_1'\cdots dt_m', \tag{3.9}$$

where $\langle l(t_1')\cdots l(t_m')\rangle$ are dynamical averages given by Eqs. (2.15). By combining Eqs. (3.9) and (3.10) and using the definition (2.1) of the characteristic functional $G[K(t')]$ of the rate coefficient we can express $\langle l(t_1')\cdots l(t_m')\rangle$ as

$$\langle l(t_1')\cdots l(t_m')\rangle=\overline{\int\int}\exp\left(-\sum_{u=1}^{m}\int_0^{t_u'}W(\mathscr{6})d\mathscr{6}\right)\mathscr{P}[W(t')]D[W(t')]$$
$$=G\left[K(t')=i\sum_{u=1}^{m}h(t_u'-t')\right], \tag{3.10}$$

where $h(x)$ is the usual Heaviside step function. By inserting Eqs. (3.10) into Eq. (3.9) we have

$$\Xi[\mathscr{K}(t')]=1+\sum_{m=1}^{\infty}\frac{i^m}{m!}F_m(0)\int_0^t\cdots\int_0^t\mathscr{K}(t_1')\cdots\mathscr{K}(t_m')$$
$$\times\exp\left(i\sum_{u=1}^{m}\int_0^{t_u'}\mathscr{K}(\mathscr{C})d\mathscr{C}\right)G\left[K(t')=i\sum_{u=1}^{m}h(t_u'-t')\right]dt_1'\cdots dt_m'. \tag{3.11}$$

Equation (3.11) is the main result of this article. It expresses the stochastic properties of the number of surviving particles in terms of the stochastic properties of the random rate coefficient $W(t')$, $0\leqslant t'\leqslant t$.

Combining Eqs. (2.12) and (2.13) and Eq. (3.11) we can compute the first two cumulants of the number of surviving particles. We assume that the initial distribution of the number of particles is given by equilibrium statistical mechanics. We get

$$\langle\langle N(t)\rangle\rangle=N_0\langle l(t)\rangle, \tag{3.12}$$

$$\langle\langle N(t_1)N(t_2)\rangle\rangle=N_0[\langle l(t_2^*)\rangle-\langle l(t_1)l(t_2)\rangle]+(N_0)^2\langle\langle l(t_1)l(t_2)\rangle\rangle \tag{3.13}$$

for an initial canonical ensemble and

$$\langle\langle N(t)\rangle\rangle=N_0\langle l(t)\rangle, \tag{3.14}$$

$$\langle\langle N(t_1)N(t_2)\rangle\rangle=\langle N_0\rangle\langle l(t_2^*)\rangle+\langle N_0\rangle^2\langle\langle l(t_1)l(t_2)\rangle\rangle \tag{3.15}$$

for an initial grand canonical ensemble. Here

$$\langle\langle l(t_1)l(t_2)\rangle\rangle = \langle l(t_1)l(t_2)\rangle - \langle l(t_1)\rangle\langle l(t_2)\rangle \tag{3.16}$$

is the second cumulant of the survival function for systems with dynamic disorder. We have

$$\langle\langle l(t_1)l(t_2)\rangle\rangle \geqslant 0, \quad t_1, t_2 \text{ finite}, \tag{3.17}$$

where the equality holds for systems without dynamical disorder. In both cases in the thermodynamic limit the relative fluctuation has the same asymptotic behavior

$$\rho_{\text{dynamic}}(t_1,t_2) \sim \left(\frac{\langle\langle l(t_1)l(t_2)\rangle\rangle}{\langle l(t_1)\rangle\langle l(t_2)\rangle} \right)^{1/2} \text{const} \quad \text{as} \quad N_0, \quad \langle N_0\rangle \to \infty. \tag{3.18}$$

Unlike in the case of ordered systems discussed in Appendix A for dynamical disorder the relative fluctuation of the number of particles does not decrease to zero but rather tends towards a constant value; in other words the fluctuations have an intermittent behavior.

The other moments and cumulants can be computed in a similar way, the complexity of computations increasing with the order of the moments. The computations are much simpler if we are interested in the analysis of fluctuations at a single time; in this case an infinity of fluctuation dissipation relations for all moments exist which are independent of the type of statistical ensemble which describes the initial state of the system. The derivation of these fluctuation–dissipation relations is presented in the following section.

IV. FLUCTUATION–DISSIPATION RELATIONS

We introduce the probability $P(N,t)$ of the number N of surviving particles at time t and the corresponding generating function

$$g(z,t) = \sum z^N P(N,t), \quad |z| \leqslant 1; \tag{4.1}$$

$P(N,t)$ can be expressed as an average of a functional Kronecker symbol over all possible trajectories $N(t')$, $0 \leqslant t' \leqslant t$

$$P(N,t) = \overline{\sum\sum B[N(t')]\delta^{(\text{funct})}_{N(t')N(t)}}, \tag{4.2}$$

where

$$\begin{aligned} \delta^{(\text{funct})}_{N(t')N(t)} &= \delta_{N(t)N(t')}, \quad \text{for} \quad t = t', \\ &= 0, \quad \text{for} \quad t \neq t' \end{aligned} \tag{4.3}$$

and $\delta_{NN'}$ is the usual numerical Kronecker symbol. By combining Eqs. (2.10) and (4.1) for $\Xi[\mathscr{K}(t')]$ and $g(z,t)$ and using Eqs. (4.2) and (4.3) we note that we have the relationship

$$g(z,t) = \Xi[i\mathscr{K}(t') = \delta(t-t')\ln z]. \tag{4.4}$$

By combining Eqs. (3.2), (3.10), (3.11), and (4.4) we obtain

$$g(z,t) = \overline{\int\int g(1+(z-1)l(t),0)\mathscr{P}[W(t')]D[W(t')]} = 1 + \sum_{m=1}^{\infty} \frac{1}{m!} F_m(0)\langle l^m(t)\rangle (z-1)^m, \tag{4.5}$$

where

$$\langle l^m(t)\rangle = \overline{\int\int} l^m(t)\mathscr{P}[W(t')]D[W(t')] \tag{4.6}$$

is the mth central moment of the survival function at time t. From Eqs. (2.14) and (4.6) we note that at one time all moments $\langle l^m(t)\rangle$ can be expressed in terms of the average value $\langle l(t)\rangle$, by replacing the instantaneous value of the rate coefficient $W(t')$ by $mW(t')$, $m=2,3,\ldots$.

$$\langle l^m(t)\rangle = \overline{\int\int} \exp\left(-m\int_0^t W(t')dt'\right)\mathscr{P}[W(t')]D[W(t')] = \langle l(t;W(t')\rightarrow mW(t'))\rangle. \tag{4.7}$$

On the other hand, by using Eq. (3.10) we can express the one-time moments of the survival function in terms of the characteristic functional $G[K(t')]$ of the random rate coefficient

$$\langle l^m(t)\rangle = G[K(t')=im]. \tag{4.8}$$

Now we note that the factorial moments of the number of particles at time t

$$F_m(t) = \langle N(N-1)\cdots(N-m+1)\rangle_{\text{dynamic}}(t) = \sum N(N-1)\cdots(N-m+1)P(N,t) \tag{4.9}$$

can be computed by differentiating the generating function $g(z,t)$

$$F_m(t) = d^m g(z,t)/dz^m|_{z=1}. \tag{4.10}$$

By differentiating Eq. (4.5) m times and making $z=1$ we come to

$$F_m(t) = F_m(0)\langle l^m(t)\rangle = F_m(0)\langle l(t,W(t')\rightarrow mW(t'))\rangle, \quad m=1,2,\ldots \tag{4.11}$$

Equations (4.11) are an infinity of fluctuation–dissipation relations which establish a connection between the average dissipative behavior of the rate process, expressed by the average survival function $\langle l(t;W(t')\rightarrow mW(t'))\rangle$ and all the factorial moments of the number of surviving particles, which express the fluctuation dynamics.

For applying the fluctuation–dissipation relations (4.11) we should be able to evaluate the average survival function $\langle l(t;W(t')\rightarrow mW(t'))\rangle$. If the cumulants of the random rate coefficient

$$\sigma_q(t_1,\ldots,t_q) = \langle\langle W(t_1)\cdots W(t_q)\rangle\rangle_{\text{dynamic}} \tag{4.12}$$

exist and are finite the characteristic functional $G[K(t')]$ can be expressed in the form of a cumulant expansion

$$G[K(t')] = \exp\left\{\sum_{q=1}^{\infty}\frac{i^q}{q!}\int_0^t\cdots\int_0^t \sigma_q(t_1,\ldots,t_q)K(t_1)\cdots K(t_q)dt_1\cdots dt_q\right\}. \tag{4.13}$$

By combining Eq. (4.13) with the expressions (4.8) for the one-time moments of the survival function and with the fluctuation–dissipation relations (4.11) we come to

$$F_m(t)/F_m(0) = \langle l^m(t)\rangle = \exp\left\{\sum_{q=1}^{\infty}\frac{(-m)^q}{q!}\int_0^t\cdots\int_0^t \sigma_q(t_1,\ldots,t_q)dt_1\ldots dt_q\right\}. \tag{4.14}$$

This is a general expression for the one-time moments of the number of surviving particles and of the survival function; for applying it we should evaluate the integrals and the series in the exponential.

In Appendix B we show how Eqs. (4.11)–(4.14) can be used for computing the central moments and the cumulants of the number of surviving particles.

V. EXACTLY SOLVABLE MODELS

In this section we consider two particular cases for which, at least in principle, the formal expressions (4.8) or (4.11) for the moments of the survival function can be explicitly evaluated.

In the first case we assume that the random rate coefficient $W(t')$ is a known function of a generally non-Markovian random vector $\mathbf{y}_1$ which can be embedded in a more complicated Markovian random process characterized by a higher dimensional random vector

$$\mathbf{x}=(\mathbf{y}_1,\mathbf{y}_2), \tag{5.1}$$

where $\mathbf{y}_2$ is the vector of the minimum number of additional random variables necessary for a Markovian description. The random rate coefficient $W(t')$ can be expressed as

$$W(t')=W(\mathbf{x}(t')=(\mathbf{y}_1(t'),\mathbf{y}_2(t'))=W(\mathbf{y}_1(t')). \tag{5.2}$$

The dynamical averages $\langle l^m(t)\rangle$ can be computed by evaluating the characteristic functional $G[K(t')]$ with the help of the method of curtailed characteristic functionals suggested by Lax[39] and Van Kampen.[40] The computations are presented in Appendix C. The moments of the survival function are equal to

$$\langle l^m(t)\rangle=\int \Lambda_m(\mathbf{x},t)d\mathbf{x}, \tag{5.3}$$

where m is a positive number, not necessarily an integer, and $\Lambda_m(\mathbf{x},t)$ is the solution of the evolution equation

$$\partial_t\Lambda_m(\mathbf{x},t)=\mathbb{L}\Lambda_m(\mathbf{x},t)-mW(\mathbf{x})\Lambda_m(\mathbf{x},t), \tag{5.4}$$

with the initial condition

$$\Lambda_m(\mathbf{x},0)=P(\mathbf{x},0) \quad \text{independent of} \quad m. \tag{5.5}$$

$P(\mathbf{x};0)$ is the probability density of the state vector at $t=0$ and $\mathbb{L}$ is a linear Markovian evolution operator. For a time-homogeneous Fokker–Planck process

$$\mathbb{L}\cdots=-\sum_q \partial_{x_q}[A_q(\mathbf{x})\cdots]+\sum_{q,q'} \partial^2_{x_qx_{q'}}[D_{qq'}(\mathbf{x})\cdots], \tag{5.6}$$

whereas for a pure jump Markovian process we have

$$\mathbb{L}P(\mathbf{x},t|\mathbf{x}_0,0)=\int [\mathscr{W}(\mathbf{x}'\rightarrow\mathbf{x})P(\mathbf{x}',t|\mathbf{x}_0,0)-\mathscr{W}(\mathbf{x}\rightarrow\mathbf{x}')P(\mathbf{x},t|\mathbf{x}_0,0)]d\mathbf{x}'. \tag{5.7}$$

Here $A_q(\mathbf{x})$ and $D_{qq'}(\mathbf{x})$ are probability drift and diffusion coefficients, respectively, and $\mathscr{W}(\mathbf{x}'\rightarrow\mathbf{x})d\mathbf{x}$ is the jump rate from a state $\mathbf{x}$ to a state with a random vector between $\mathbf{x}$ and $\mathbf{x}+d\mathbf{x}$.

To clarify the physical significance of the function $\Lambda_m(\mathbf{x},t)$ we introduce the logarithmic decrement of the survival function

$$\varepsilon(t)=-\ln\, l(t). \tag{5.8}$$

Borrowing a commonly used name from nuclear physics, we call the function $\varepsilon(t)$ the lethargy variable. We denote by

$$\phi(\varepsilon,\mathbf{x};t)d\varepsilon d\mathbf{x}, \quad \text{with} \quad \int\int \phi(\varepsilon,\mathbf{x};t)d\varepsilon\ d\mathbf{x}=1 \tag{5.9}$$

the probability that at time t the lethargy has a value between ε and $\varepsilon+d\varepsilon$ and that the state vector is between $\mathbf{x}$ and $\mathbf{x}+d\mathbf{x}$. In Appendix C we show that the function $\Lambda_m(\mathbf{x},t)$ can be expressed in terms of the Laplace transform of $\phi(\varepsilon,\mathbf{x};t)$ with respect to ε:

$$\tilde{\phi}(\beta,\mathbf{x};t)=\int_0^\infty \exp(-\beta\varepsilon)\phi(\varepsilon,\mathbf{x};t)d\varepsilon, \tag{5.10}$$

where β is the Laplace variable conjugated to ε. We have (see Appendix C)

$$\Lambda_m(\mathbf{x},t)=\tilde{\phi}(\beta=m,\mathbf{x};t), \tag{5.11}$$

that is, the function $\Lambda_m(\mathbf{x},t)$ is the Laplace transform of the lethargy-state vector joint probability density $\phi(\varepsilon,\mathbf{x};t)$ for $\beta=m$. From this physical interpretation of the function $\Lambda_m(\mathbf{x},t)$ it follows that the probability density

$$C(l,t)dl, \quad \text{with} \quad \int_0^1 C(l,t)dl=1 \tag{5.12}$$

of the survival function at time t can be expressed as

$$C(l,t)=\int\int \delta(l-\exp(-\varepsilon))\phi(\varepsilon,\mathbf{x};t)d\mathbf{x}\ d\varepsilon=l^{-1}\int \tilde{\phi}(-\ln l,\mathbf{x};t)d\mathbf{x}=l^{-1}\int \Lambda_{m=-\ln l}(\mathbf{x},t)d\mathbf{x}. \tag{5.13}$$

A second case for which the moments of the survival function can be explicitly evaluated corresponds to a time-homogeneous Gaussian behavior of the rate coefficient $W(t')$ for which the cumulants $\sigma_q(t_1,\ldots,t_q)$ are given by

$$\sigma_1=\langle W\rangle \quad \text{independent of} \quad t, \tag{5.14}$$

$$\sigma_2=\sigma(|t_1-t_2|)=\langle \Delta W(t_1)\Delta W(t_2)\rangle, \tag{5.15}$$

$$\sigma_q=0, \quad q>2. \tag{5.16}$$

Here $\langle W\rangle$ and $\langle \Delta W(t_1)\Delta W(t_2)\rangle$ are the average value and the absolute autocorrelation function of the rate coefficient, respectively. Due to the stationary character of the process the average rate $\langle W\rangle$ is independent of time and the autocorrelation function $\langle \Delta W(t_1)\Delta W(t_2)\rangle$ depends only on the absolute value of the difference of the two times, t_1 and t_2. In this case Eq. (4.14) becomes

$$F_m(t)/F_m(0)=\langle l^m(t)\rangle=\exp\{-m\langle W\rangle t+m^2\langle \Delta W^2(0)\rangle \mathscr{J}(t)\}, \tag{5.17}$$

where

$$\langle \Delta W^2(t)\rangle=\langle \Delta W^2(0)\rangle \tag{5.18}$$

is the stationary one-time dispersion of the rate coefficient

$$\mathscr{J}(t)=\int_0^t (t-\sigma)\mathscr{E}(|\sigma|)d\sigma \geqslant 0, \tag{5.19}$$

is a non-negative function of time and

$$\mathscr{E}(|t_1-t_2|)=\langle \Delta W(t_1)\Delta W(t_2)\rangle/\langle \Delta W^2(0)\rangle \tag{5.20}$$

is the relative correlation function of the rate coefficient.

The multitime moments and cumulants of the correlation function can be computed in a similar way. By applying Eq. (3.10) to the case of a stationary Gaussian process we obtain

$$\begin{aligned}\langle l(t_1)l(t_2)\rangle &= G[W(t')=(h(t_1-t')+h(t_2-t'))i] \\ &= \exp\Bigg\{-\langle W\rangle(t_1+t_2)+\tfrac{1}{2}\langle \Delta W^2(0)\rangle \int_0^t\int_0^t \mathscr{E}(|t_1'-t_2'|)[h(t_1-t_1') \\ &\quad + h(t_2-t_1')][h(t_1-t_2')+h(t_2-t_2')]dt_1'\,dt_2'\Bigg\}, \quad \text{with} \quad t_1,t_2\leqslant t. \end{aligned} \tag{5.21}$$

After lengthy algebraic manipulations the double integral in Eq. (5.21) can be expressed in terms of the function $j(t)$, resulting in

$$\langle l(t_1)l(t_2)\rangle=\exp\{-\langle W\rangle(t_1+t_2)+\langle \Delta W^2(0)\rangle[2\not{j}(t_1)+2\not{j}(t_2)-\not{j}(|t_1-t_2|)]\} \tag{5.22}$$

and

$$\begin{aligned}\langle\langle l(t_1)l(t_2)\rangle\rangle &= \exp\{-\langle W\rangle(t_1+t_2)+\langle \Delta W^2(0)\rangle[\not{j}(t_1)+\not{j}(t_2)]\} \\ &\quad \times\{\{\exp\{\langle \Delta W^2(0)\rangle[\not{j}(t_1)+\not{j}(t_2)-\not{j}(|t_1-t_2|)]\}-1\}. \end{aligned} \tag{5.23}$$

The first two cumulants of the number of surviving particles for initial canonical and grand canonical ensembles can be computed by combining the general equations (3.12)–(3.18) with Eqs. (5.17) and (5.22), (5.23). In the thermodynamic limit the relative fluctuation is given by

$$\rho_{\text{dynamic}}(t_1,t_2)=\{\exp\{\langle \Delta W^2(0)\rangle[\not{j}(t_1)+\not{j}(t_2)-\not{j}(|t_1-t_2|)]\}-1\}^{1/2}. \tag{5.24}$$

VI. POSITRON LIFETIME DISTRIBUTIONS IN DENSE FLUIDS

As a first application of the approach developed here, we consider the problem of the distribution of the lifetime of positrons or positronium atoms in dense fluids. A positron or a positronium atom thermalized in a dense fluid can become localized.[41] This type of localization is due to the interaction of the trapped particles with the environment, for instance, via the Fermi repulsion, and it is different from the usual Anderson localization typical for disordered systems.[42] Eventually the trapped particles decay due to the annihilation reaction with the neighboring electrons. With respect to this annihilation-self-trapping phenomenon it is not clear whether the positron actively creates a well in the fluid in which it localizes, or randomly visits favorable fluctuations. Density functional theory calculations[43] support the idea of a definite localized state for the trapped particle and under these circumstances one normally expects to have a well definite decay rate. This point of view is consistent with the ease with which experimentalists are able to assign specific annihilation rates to each decay mode. In contrast, quantum Monte Carlo calculations[44] show that substantial fluctuations occur in the neighborhood of a trapped particle resulting in a broad distribution of decay rates. These Monte Carlo simulations seem to contradict the experimental measurements which lead to single, definite decay rates.

To solve this contradiction Miller, Reese, and Worrell[45] (MRW) have recently suggested an approximate stochastic model with dynamical disorder. They have shown that the difference between the density functional and Monte Carlo calculations is due to a misinterpretation of the results of simulations in terms of a model with static disorder. Both the Monte Carlo and the density functional approaches are recovered as particular cases of the MRW dynamical stochastic

model.[45] In the MRW treatment the rate coefficient is a quantum mechanical operator $\hat{W}$ which depends on the electron density in the neighborhood of the trapped particle. The time-dependent instantaneous rate coefficient $W(t)$ is a quantum mechanical average

$$W(t)=\langle\psi(t)|\hat{W}|\psi(t)\rangle. \tag{6.1}$$

Due to the environmental fluctuations of the density the quantum mechanical average $W(t)$ is a fluctuating quantity that can be written in the form

$$W(t)=\langle W\rangle+\Delta W(t), \tag{6.2}$$

where $\langle W\rangle$ is a time-independent statistical average rate coefficient and $\Delta W(t)$ is the fluctuating part of $W(t)$.

The average survival function is given by

$$\langle l(t)\rangle=\exp(-\langle W\rangle t)\left\langle \exp\left(-\int_0^t \Delta W(t')dt'\right)\right\rangle. \tag{6.3}$$

To evaluate the dynamical average in Eq. (6.3) Miller, Reese, and Worrell[45] do not use the characteristic functional method suggested in this article. Instead they use a nonsystematic approximation based on two series expansions. They expand the exponential under the average brackets in a Taylor series and keep the first three terms, resulting in

$$\langle l(t)\rangle\cong\exp(-\langle W\rangle t)\left\{1+\frac{1}{2}\int_0^t\int_0^t\langle\Delta W(t_1')\Delta W(t_2')\rangle dt_1'\,dt_2'\right\}. \tag{6.4}$$

The next step is to take the logarithm of the average survival function and to approximate the logarithm containing the double integral by the first term from its Taylor expansion

$$\ln\langle l(t)\rangle\cong-\langle W\rangle t+\frac{1}{2}\int_0^t\int_0^t\langle\Delta W(t_1')\Delta W(t_2')\rangle dt_1'\,dt_2'. \tag{6.5}$$

The simplest assumption for the time dependence of the correlation function $\langle\Delta W(t_1)\Delta W(t_2)\rangle$ is an exponential decay

$$\langle\Delta W(t_1)\Delta W(t_2)\rangle=\langle\Delta W^2(0)\rangle\exp(-|t_1-t_2|/\bar{\tau}_W), \tag{6.6}$$

where $\bar{\tau}_W$ is a characteristic relaxation time for the regression of fluctuations. Equations (6.5) and (6.6) lead to

$$\ln\langle l(t)\rangle=-\langle W\rangle t+\langle W\rangle^2\zeta^2\bar{t}_W\{1-(\bar{\tau}_W/t)[1-\exp(-t/\bar{\tau}_W)]\}, \tag{6.7}$$

where

$$\zeta=\langle W^2(0)\rangle^{1/2}/\langle W\rangle. \tag{6.8}$$

Miller, Reese, and Worrell[45] have estimated the parameters entering Eq. (6.7) for the orthopositronium atom (o-Ps) in xenon at 340 °K and for the bare positron (e^+) at 300 °C. The result of this estimation is that for o-Ps the macroscopic relaxation time scale

$$\bar{t}_{\text{macro}}=1/\langle W\rangle \tag{6.9}$$

is much larger than the regression time of fluctuations $\bar{\tau}_W$: $\bar{t}_{\text{macro}}\gg\bar{\tau}_W$; in this case the fluctuations are very fast and the average survival function is practically exponential

$$\ln\langle l(t)\rangle \cong -\langle W\rangle t, \tag{6.10}$$

which corresponds to a definite effective relaxation rate $\langle W\rangle$. This behavior is a particular case of a general feature of the systems with dynamic disorder and very fast fluctuations.[1] For the bare positronium, however, the macroscopic and fluctuation time scales are less well separated and the average survival function is given by Eq. (6.7).

Now we investigate the MRW model from the point of view of our approach. First note that within the framework of our theory the MRW approximative equations (6.5) and (6.7) *are exact for a Gaussian and Markovian process*. According to Doob's theorem the only possible expression for the correlation function of a stationary Gaussian and Markovian process is the exponential form given by Eq. (6.6). Inserting Eq. (6.6) into Eq. (5.20) and using Eqs. (5.19) and (5.17) for $m=1$ we recover the MRW equation (6.7). If the stochastic process describing the behavior of the random rate coefficient $W(t')$ is close to a Gaussian process then the superior cumulants lead to small corrections in the expression of the average survival function [see the general non-Gaussian relationships (4.14)].

Examining the MRW derivation of Eq. (6.7) it follows that this equation is valid only if

$$\frac{1}{2}\int_0^t\int_0^t \langle \Delta W(t_1')\Delta W(t_2')\rangle dt_1'\, dt_2' = \langle W\rangle^2 \xi^2 t\bar{\sigma}_W\{1-(\bar{\sigma}_W/t)[1-\exp(-t/\bar{\sigma}_W)]\} \ll 1. \tag{6.11}$$

Indeed, only if this restriction is fulfilled are the series expansions used in Eqs. (6.4) and (6.5) justified. Our approach, however, shows that the restriction (6.11) is not necessary. For a stationary Gaussian and Markovian process the MRW equation (6.7) is exact for any values of the integral term in Eq. (6.11). Miller, Reese, and Worrell did not notice this relationship between their approach and the stationary Gaussian and Markovian processes. We do not know whether the actual random properties of the rate coefficient are accurately described by a stationary Gaussian and Markovian process. Note, however, that the standard description of stationary fluctuations is based on the use of such a process.[46] The broad range of validity of Eq. (6.7) is surprising but it is due to the fact that in the MRW derivation the errors due to the two series expansions in Eqs. (6.4) and (6.5) compensate each other.

The exponential or nonexponential structure of the average survival function is governed by the relationship between the macroscopic and the microscopic (fluctuation) time scales. From the MRW approach it follows that in the case of very rapid fluctuations the system behaves as if the dynamical disorder were missing. Our approach, however, shows that this is not the case. Applying the expression (5.24) for the relative fluctuation of the number of particles in the thermodynamic limit we obtain

$$\rho_{\text{dynamic}}(t_1,t_2) \sim \exp\{(\bar{\sigma}_W)^2\langle \Delta W^2(0)\rangle[2\min(t_1,t_2)/\bar{\sigma}_W - 1 - \exp(-|t_1-t_2|/\bar{\sigma}_W) + \exp(-t_1/\bar{\sigma}_W) + \exp(-t_2/\bar{\sigma}_W)] - 1\}^{1/2}, \quad \text{as} \quad N_0, \langle N_0\rangle \to \infty. \tag{6.12}$$

For large t_1, t_2 Eq. (6.12) takes a simpler form

$$\rho_{\text{dynamic}}(t_1,t_2) \sim \exp\{(\bar{\sigma}_W)\langle \Delta W^2(0)\rangle \min(t_1,t_2)\}, \quad t_1,t_2 \to \infty, \tag{6.13}$$

that is, the relative fluctuation increases exponentially to infinity. From Eqs. (6.12) and (6.13) we notice that the intermittent behavior of the fluctuations exists even if the fluctuations are very rapid. This is a surprising result which cannot be obtained by applying the MRW approach. It might be possible that the intermittent character of fluctuations of the number of particles can be observed experimentally.

The existence of dynamical disorder decreases the efficiency of the annihilation process. This is reflected in the fact that the decrease of the survival function given by Eq. (6.11) is slower than in the case when the fluctuations of the rate coefficient are missing. By using the method devel-

oped here, we can show that this slowing down effect due to the dynamical disorder is also present in the case of Gaussian, non-Markovian fluctuations of the rate coefficient for which the correlation function $\langle \Delta W(t_1)\Delta W(t_2)\rangle$ is generally nonexponential. If the dynamical disorder is missing we have $\langle \Delta W(t_1)\Delta W(t_2)\rangle = 0$, $\not{\gamma}(t)=0$ and Eqs. (5.17) lead to

$$\langle l^m(t)\rangle_{\text{ordered}} = (F_m(t)/F_m(0))_{\text{ordered}} = \exp(-m\langle W\rangle t). \tag{6.14}$$

As $\not{\gamma}(t)$ is generally non-negative by comparing Eqs. (120) with Eqs. (6.14) we obtain

$$\langle l^m(t)\rangle_{\text{ordered}} = (F_m(t)/F_m(0))_{\text{ordered}} \geqslant \langle l^m(t)\rangle_{\text{dynamic}} = (F_m(t)/F_m(0))_{\text{dynamic}}, \quad m=1,2,\ldots \tag{6.15}$$

The slowing down generated by the dynamical disorder affects not only the moments of the survival function but also the factorial moments of the number of particles.

VII. PASSAGE THROUGH A FLUCTUATING GEOMETRICAL BOTTLENECK

The model for the binding of a ligand to a protein molecule suggested by Zwanzig[32] is based on the following assumptions:

(1) The rate determining process is the passage of a ligand molecule through a geometrical bottleneck formed by the protein chain. The rate coefficient W is proportional to the area of the bottleneck

$$W(r) = \alpha r^2, \tag{7.1}$$

where r is the radius of the bottleneck and α is a positive coefficient with dimension $[\text{time}]^{-1}[\text{length}]^{-2}$.

(2) Due to the conformational fluctuations of the protein molecule the radius r of the bottleneck is a random variable which obeys a Langevin equation

$$dr/dt = -\lambda r + F(t), \tag{7.2}$$

in which λ is the rate of regression of a fluctuation in r and $F(t)$ is thermal (Gaussian white) noise. The stochastic properties of $F(t)$ are completely characterized by the cumulants

$$\langle\langle F(t)\rangle\rangle = 0, \quad \langle\langle F(t)F(t')\rangle\rangle = 2\lambda\theta\delta(t-t') \tag{7.3}$$

and

$$\langle\langle F(t_1)\ldots F(t_q)\rangle\rangle = 0, \quad q>2, \tag{7.4}$$

where θ is the second moment of the radius r

$$\theta = \langle r^2\rangle. \tag{7.5}$$

Using these two assumptions Zwanzig has computed the expression of the average survival function $\langle l(t)\rangle$ of the ligand molecules. In this section we complete the Zwanzig's analysis by evaluating the fluctuations of the number of ligand molecules. This is more than a simple academic exercise; indeed, even though the fluctuations are not easily experimentally accessible the theoretical investigation of their behavior would lead to the clarification of the nature of the process in the thermodynamic limit. We shall see in the following that, like in the case of positron trapping in fluids, the Zwanzig's model leads to an intermittent behavior.

Equation (7.2) shows that the radius of a bottleneck is a Markovian random variable. It follows that we can apply the Markovian approach developed in Sec. V. In this case the state

vector $\mathbf{x}$ is made up of one component $\mathbf{x}=(r)$. Reducing the Langevin description (7.2)–(7.4) to a Fokker–Planck description it turns out that the evolution operator $\mathbb{L}$ is given by

$$\mathbb{L}\cdots=\lambda\partial_r(r\cdots)+\lambda\theta\partial_{r^2}^2(\cdots), \tag{7.6}$$

which is a particular case of Eq. (5.6). The factorial moments of the number of surviving particles and the moments of survival functions can be derived by applying the fluctuation–dissipation relation (4.11). The details of computations are presented in Appendix D. By combining our formalism with the data available in the literature[32,47] we obtain

$$F_m(t)/F_m(0)=\langle l^m(t)\rangle=\mathscr{S}_m(t), \tag{7.7}$$

where

$$\mathscr{S}_m(t)=\left\{\frac{\lambda+2\alpha m\theta}{(\lambda^2+4\alpha m\theta\lambda)^{1/2}}\sinh[(\lambda^2+4\alpha m\theta\lambda)^{1/2}t]+\cosh[(\lambda^2+4\alpha m\theta\lambda)^{1/2}t]\right\}^{-1/2}\exp(\lambda t/2). \tag{7.8}$$

For $m=1$ Eqs. (7.7) and (7.8) reduce to the Zwanzig's expression for the average survival function. The expressions (7.7) and (7.8) for $m>1$ for the fluctuations of the survival function and of the number of ligand molecules are new.

The average rate coefficient is equal to

$$\langle W\rangle=\langle\alpha r^2\rangle=\alpha\theta. \tag{7.9}$$

In terms of $\langle W\rangle$ and λ the macroscopic time scale $\bar{t}_{\text{macro}}$ and the fluctuation time scale $\bar{\mathscr{C}}_{\text{fluct}}$ can be expressed as

$$\bar{t}_{\text{macro}}=1/\langle W\rangle=(\alpha\theta)^{-1},\quad \bar{\mathscr{C}}_{\text{fluct}}=1/\lambda. \tag{7.10}$$

The limit behavior of Eqs. (7.7) and (7.8) can be analyzed in terms of the ratio y of the two time scales

$$y=\bar{\mathscr{C}}_{\text{fluct}}/\bar{t}_{\text{macro}}=\alpha\theta/\lambda. \tag{7.11}$$

For $y\to\infty$ the fluctuations are slow, the disorder is static, and Eqs. (7.7) and (7.8) become

$$F_m(t)/F_m(0)=\langle l^m(t)\rangle\sim(1+2m\alpha\theta t)^{1/2},\quad m=1,2,\ldots,\quad y\to\infty. \tag{7.12}$$

In the opposite case of rapid fluctuations $y\to 0$ and the moments decrease exponentially in time

$$F_m(t)/F_m(0)=\langle l^m(t)\rangle\sim\exp(-m\alpha\theta t),\quad m=1,2,\ldots,\quad y\to 0. \tag{7.13}$$

The one-time central moments and the cumulants of the number of ligand molecules can be computed by using the relationships presented in Appendix B. To save space we give here only the expression of the one-time relative fluctuation

$$\rho(t)=\langle\Delta N^2(t)\rangle^{1/2}/\langle N(t)\rangle=[(1+\rho^2(0))\mathscr{S}_2(t)/(\mathscr{S}_1(t))^2-1+(1-\mathscr{S}_2(t)/\mathscr{S}_1(t))/\langle N(0)\rangle]^{1/2}$$
$$\sim[(1+\rho^2(0))\mathscr{S}_2(t)/(\mathscr{S}_1(t))^2-1]^{1/2},\quad \langle N(0)\rangle\to\infty. \tag{7.14}$$

Note that in the thermodynamic limit $\langle N(0)\rangle \to \infty$ the fluctuations are intermittent. To estimate the intensity of the intermittent behavior we analyze the asymptotic expressions for the factorial moments $F_m(t)$ and for the one-time relative fluctuation $\rho(t)$. For large time both $F_m(t)$ and $\rho(t)$ are exponentials

$$F_m(t)/F_m(0)=\langle l^m(t)\rangle \sim \frac{2(1+4my)^{1/4}}{1+(1+4my)^{1/2}} \exp\{-\tfrac{1}{2}\lambda t[(1+4my)^{1/2}-1]\},$$

$$t \gg 0, \tag{7.15}$$

$$\rho(t)\sim(1+\rho^2(0))^{1/2}R(y)\exp[\tfrac{1}{4}\lambda t Q(y)], \quad t\gg 0, \tag{7.16}$$

where

$$R(y)=\frac{(1+8y)^{1/8}[1+(1+4y)^{1/2}]}{(1+4y)^{1/4}[1+(1+8y)^{1/2}]^{1/2}\sqrt{2}}, \tag{7.17}$$

$$Q(y)=2(1+4y)^{1/2}-(1+8y)^{1/2}-1>0, \quad \text{for} \quad y>0. \tag{7.18}$$

As time increases the factorial moments $F_m(t)$ of the number of ligand molecules decrease exponentially to zero and the relative fluctuation $\rho(t)$ increases exponentially to infinity.

From Eqs. (7.15) we see that the effective exponential rate constant $W_{\text{eff}}(m)$ for the decay of fluctuations is a parabolic function of the moment index m. Equations (7.15) may be rewritten in the form

$$F_m(t)\sim\exp[-W_{\text{eff}}(m)t], \quad t\to\infty, \tag{7.19}$$

with

$$W_{\text{eff}}(m)=\tfrac{1}{2}\lambda[(1+4my)^{1/2}-1]\sim(m\alpha\lambda\theta)^{1/2}, \quad y\gg 1; \tag{7.20}$$

for $m=1$ Eq. (7.20) reduces to a relation derived by Zwanzig[32]

$$W_{\text{eff}}(1)\sim(\alpha\lambda\theta)^{1/2}, \quad y\gg 1. \tag{7.21}$$

As the relaxation rate λ of the radius fluctuations is inversely proportional to the viscosity η of the solvent[32,48] Eq. (7.21) leads to

$$W_{\text{eff}}(1)\sim\eta^{-1/2} \tag{7.22}$$

a relationship which is approximately consistent with the experimental data which can be fitted by the law[49]

$$W_{\text{eff}}(1)\sim\eta^{-K}, \quad \text{with} \quad 0.8>K>0.4. \tag{7.23}$$

A possible explanation of the existence of an exponent different from $\frac{1}{2}$ would be the fact that the fluctuations of the radius r of the bottleneck are actually non-Gaussian. The Gaussian behavior of a geometrical parameter of a polymeric chain is generally related to the description of the conformational fluctuations by a noncorrelated random walk.[50] For real polymers, however, the excluded volume effect necessarily leads to non-Gaussian behavior.[50] A generalization of the Zwanzig's model which provides a theoretical derivation of the experimental law (7.23) is based on the assumption that the non-Gaussian fluctuations can be described by using the fractional diffusion equation.[51] Details concerning this model will be given elsewhere. We mention that Wang and Wolynes[33] suggest a different explanation for the experimental law (7.23). They assume

that the fluctuations of the radius r are Gaussian but that the corresponding correlation function $\langle \Delta r(t_1)\Delta r(t_2)\rangle$ is a nonexponential function of the time interval t_1-t_2.

VIII. JUMP RATE PROCESSES AND RELAXATION

The third application of our approach is an exactly solvable model with dynamical disorder which can be used both in biochemistry and condensed matter physics. We assume that the random time evolution of the rate coefficient $W(t')$ can be described in terms of a jump process. For each jump a new value of W is randomly selected from a given probability density $f(W)dW$. The jump frequency is also a random function $\Omega(t')$ which obeys a similar dynamics. For each jump a new frequency Ω is picked up from another probability density $\xi(\Omega)d\Omega$. For this kind of model the random function $W(t')$ is generally non-Markovian. However the set (Ω,W) has a Markovian behavior characterized by the jump rate

$$\mathscr{W}(\Omega',W' \rightarrow \Omega,W)d\Omega\ dW\ \Delta t=\Omega'\xi(\Omega)f(W)d\Omega\ dW\ \Delta t, \tag{8.1}$$

where $\Delta t \rightarrow 0$ is the length of the time interval in which a jump occurs. This type of model is a particular case of the Markovian processes studied in Sec. V. The state vector $\mathbf{x}$ is given by

$$\mathbf{x}=(\Omega,W) \tag{8.2}$$

and the evolution operator $\mathbb{L}$ can be computed by inserting Eq. (8.1) into Eq. (5.7). Using the expression for $\mathbb{L}$ the evolution equations (5.4), (5.5), and (5.10) for $\Lambda_m(\Omega,W,t)=\tilde{\phi}(\beta=m,\Omega,W;t)$ become

$$\partial_t\tilde{\phi}(\beta,\Omega,W;t)=\xi(\Omega)f(W)\int\int \Omega'\tilde{\phi}(\beta,\Omega',W')d\Omega'\ dW'-(\Omega+\beta W)\tilde{\phi}(\beta,\Omega,W;t), \tag{8.3}$$

with the initial condition

$$\tilde{\phi}(\beta,\Omega,W;t=0)=P(\Omega,W,t=0)=\xi(\Omega)f(W). \tag{8.4}$$

Equation (182) can be solved by introducing the auxiliary function

$$b(\beta,t)=\int\int \Omega\tilde{\phi}(\beta,\Omega,W;t)d\Omega\ dW. \tag{8.5}$$

We express the integral in Eq. (8.3) in terms of $b(\beta,t)$ and integrate the resulting equation by assuming the function $b(\beta,t)$ is known. This gives

$$\tilde{\phi}(\beta,\Omega,W;t)=\xi(\Omega)f(W)\left[\exp(-(\Omega+\beta W)t)+\int_0^t b(\beta,t-t')\exp(-(\Omega+\beta W)t')dt'\right]. \tag{8.6}$$

Inserting Eq. (8.6) into Eq. (8.5) we obtain a linear integral equation for $b(\beta,t)$

$$b(\beta,t)=\langle l^{\beta}(t)\rangle_{\text{static}}\psi(t)+\int_0^t \langle l^{\beta}(t')\rangle_{\text{static}}\psi(t')b(\beta,t-t')dt', \tag{8.7}$$

where

$$\langle l^{\beta}(t)\rangle_{\text{static}}=\int_0^{\infty} l^{\beta}f(W)dW=\int_0^{\infty}\exp(-\beta Wt)f(W)dW \tag{8.8}$$

is the one-time fractional static moment of order β of the survival function $l(t)$ and

$$\psi(t)=\int_0^\infty \Omega\ \exp(-\Omega t)\xi(\Omega)d\Omega \tag{8.9}$$

is the static average of the probability density of the waiting time between two jumps. Combining Eqs. (5.3), (4.11), and (8.6) we can express the dynamic moments of the survival function and of the number of surviving particles in terms of the function $b(\beta,t)$

$$F_m(t)/F_m(0)=\langle l^m(t)\rangle=\langle l^m(t)\rangle_{\text{static}}\,\mathscr{S}(t)+\int_0^t b(m,t-t')\mathscr{S}(t')\langle l^m(t')\rangle_{\text{static}}\,dt', \tag{8.10}$$

where

$$\mathscr{S}(t)=\int_t^\infty \psi(t')dt'=\int_0^\infty \exp(-\Omega t)\xi(\Omega)d\Omega \tag{8.11}$$

is the probability that in a time interval of length t no jump processes occur. Equation (8.7) is a linear convolution equation in $b(\beta,t)$ which can be solved by using the Laplace transformation. We denote the Laplace transform of the real time variable t by an overbar

$$\bar{b}(\beta,s)=\int_0^\infty \exp(-st)b(\beta,t)dt, \quad \text{etc.}, \tag{8.12}$$

where s is the Laplace variable conjugated to the time t. We apply the Laplace transform to Eqs. (5.13) and (8.6)–(8.8), eliminate the function $b(\beta,s)$ from the resulting equations, and come back to the real time variable t. After lengthy calculations we get the following expressions for the probability density $C(l,t)$ of the survival function l at time t and for the dynamic averages $\langle l^m(t)\rangle$ and $F_m(t)$

$$C(l,t)=(2\pi i l)^{-1}\int d\beta\ \exp(\beta\ \ln\ l)\mathscr{L}^{-1}\times\left\{\left[\int\int \frac{\xi(\Omega)f(W)d\Omega\ dW}{\Omega+\beta W+s}\right]\Big/\left[\int\int \frac{(s+\beta W)\xi(\Omega)f(W)d\Omega\ dW}{\Omega+\beta W+s}\right]\right\}, \tag{8.13}$$

$$F_m(t)/F_m(0)=\langle l^m(t)\rangle=\mathscr{L}^{-1}\left\{\left[\int\int \frac{\xi(\Omega)f(W)d\Omega\ dW}{\Omega+mW+s}\right]\Big/\left[\int\int \frac{(s+mW)\xi(\Omega)f(W)d\Omega\ dW}{\Omega+mW+s}\right]\right\}, \tag{8.14}$$

where the complex integral over β is computed along a vertical line from the left hand side of the complex plane from $-i\infty$ to $+i\infty$ and $\mathscr{L}^{-1}$ denotes the inverse Laplace transformation with respect to the s variable conjugated to the real time.

The probability density $P(x,t)=P(\Omega,W,t)$ of the rates Ω and W at time t can be evaluated in a similar way. We have

$$P(\Omega,W,t)=\int \phi(\mathscr{E},\Omega,W;t)d\mathscr{E}=\tilde{\phi}(\beta=0,\Omega,W;t). \tag{8.15}$$

Combining Eq. (8.15) with the Laplace transform of Eq. (8.6) we obtain

$$P(\Omega,W,t)=\xi(\Omega)f(W)\mathscr{L}^{-1}[(s+\Omega)^{-1}(1-\bar{\psi}(s))^{-1}], \tag{8.16}$$

where

$$\bar{\psi}(s)=\int_0^\infty \exp(-st)\psi(t)dt=\int_0^\infty \frac{\Omega}{s+\Omega}\,\xi(\Omega)d\Omega \tag{8.17}$$

is the Laplace transform of the average probability density of the waiting time between two jumps.

The above equations allow us to express the dynamic averages $\langle l^m(t)\rangle$ and $F_m(t)$ in terms of static averages over the rates Ω and W. Equations (8.14) may be rewritten as

$$F_m(t)/F_m(0)=\langle l^m(t)\rangle=\langle l^m(t)\rangle_{\text{static}}\otimes\psi(t)\otimes\chi(t), \tag{8.18}$$

where $\langle l^m(t)\rangle_{\text{static}}$ is given by Eq. (8.18), $\otimes$ denotes the temporal convolution product, and the function $\chi(t)$ is given by

$$\chi(t)=\mathscr{L}^{-1}[(1-\varphi_m(s))^{-1}], \tag{8.19}$$

with

$$\varphi_m(s)=\int_0^\infty \exp(-st)\psi(t)\langle l^m(t)\rangle_{\text{static}}\,dt. \tag{8.20}$$

According to Eq. (8.18) the intermediate time behavior of the dynamical averages $\langle l^m(t)\rangle$ and $F_m(t)$ can be quite complicated; the large time behavior, however, is dominated by the most rapidly decreasing functions on the right hand side of Eq. (8.18). The asymptotic behavior of the static averages $\langle l^m(t)\rangle_{\text{static}}$ and $\psi(t)$ can be investigated by using the methods developed in the literature dealing with systems with static disorder.[10] On the other hand the behavior of $\chi(t)$ can be investigated by making an analogy with Lotka's theory of stable populations.[37,52] Equation (8.19) shows that the function $\chi(t)$ depends on the roots of the transcendental equation

$$\varphi_m(s)=\int_0^\infty \exp(-st)\psi(t)\langle l^m(t)\rangle_{\text{static}}\,dt=1. \tag{8.21}$$

Equation (8.21) has exactly the same form as the well-known Lotka equation for the intrinsic rate of growth from population dynamics.[37,52] By using this analogy it follows that Eq. (8.21) has a single real root $s=s_0$ which is nonpositive. We have[37,52]

$$s_0<0 \quad \text{if} \quad \varphi_m(0)<1 \quad \text{and} \quad s_0=0 \quad \text{if} \quad \varphi_m(0)=1. \tag{8.22}$$

Equation (30) can also have at most a countable number of complex roots $s_{\pm q}=u_q\pm iv_q$, $q=1,2,...$ with real parts u_q smaller or at most equal to the real root s_0 (Refs. 37 and 52)

$$u_q\leqslant s_0, \quad q=1,2,\ldots \tag{8.23}$$

If the complex roots are simple then $\chi(t)$ can be expressed as

$$\chi(t)=(I_0)^{-1}\exp(-|s_0|t)+2\sum_{q=1}^{\infty}\exp(-|u_q|t)\{[I_q^+\cos(v_qt)-I_q^-\sin(v_qt)]/[(I_q^+)^2+(I_q^-)^2]\}, \tag{8.24}$$

where

$$I_0=\int\int \frac{\Omega\xi(\Omega)f(W)}{(\Omega+mW)^2}\,d\Omega\;dW \tag{8.25}$$

and

$$I_q^{\pm}=\int\int \frac{\Omega\xi(\Omega)f(W)}{[(\Omega+mW-u_q)^2+v_q^2]^2}\begin{Bmatrix}(\Omega+mW-u_l)^2-v_l^2\\ 2(\Omega+mW-u_l)v_l\end{Bmatrix}d\Omega\;dW. \tag{8.26}$$

The expansion (8.24) is physically consistent only if the integrals (8.25) and (8.26) exist and are finite.

The constant $\varphi_m(0)$ can be expressed as

$$\varphi_m(0)=\int\int \frac{\Omega}{\Omega+mW}\,\xi(\Omega)f(W)d\Omega\;dW=\left\langle\frac{\Omega}{\Omega+mW}\right\rangle_{\text{static}}. \tag{8.27}$$

In most cases the average $\langle\Omega/(\Omega+mW)\rangle_{\text{static}}$ is smaller than unity and thus $s_0<0$ and

$$\chi(t)\sim(I_0)^{-1}\,\exp(-|s_0|t)\quad\text{as}\quad t\to\infty. \tag{8.28}$$

In this case the dynamical averages $\langle l^m(t)\rangle$ and $F_m(t)$ decrease to zero exponentially or faster. In some exceptional cases it may happen that $\langle\Omega/(\Omega+mW)\rangle_{\text{static}}=1$. In this situation there are two possibilities: if $1-\varphi_m(s)$ is analytic near $s=0$

$$1-\varphi_m(s)\sim s\quad\text{as}\quad s\to 0\quad\text{and}\quad\chi(t)\sim\text{const}\quad\text{as}\quad t\to\infty. \tag{8.29}$$

If Eq. (8.29) holds then the dynamical averages $\langle l^m(t)\rangle$ and $F_m(t)$ are completely determined by the static averages $\langle l^m(t)\rangle_{\text{static}}$. The second possibility is that $1-\varphi_m(s)$ is nonanalytic near $s=0$ so

$$1-\varphi_m(s)\sim s^a,\quad 1>a>0\quad\text{as}\quad s\to 0. \tag{8.30}$$

In this case the integrals (8.25) and (8.26) are infinite, the expansion (8.24) breaks down and the asymptotic behavior of $\chi(t)$ as $t\to\infty$ is given by

$$\chi(t)\sim t^{a-1}/\Gamma(a)\quad\text{as}\quad t\to\infty. \tag{8.31}$$

The asymptotic fractal time behavior of $\chi(t)$ may lead to an exotic (i.e., nonexponential) large time behavior for $\langle l^m(t)\rangle$ and $F_m(t)$.

As expected for very rare jumps the dynamical moments $\langle l^m(t)\rangle$ and $F_m(t)/F_m(0)$ are the same as the static averages

$$\langle l^m(t)\rangle=\langle l^m(t)\rangle_{\text{static}}. \tag{8.32}$$

In this case we have $\xi(\Omega)=\delta(\Omega)$ and Eq. (8.14) reduces to Eq. (8.8). In the other extreme of very frequent jumps we have $\xi(\Omega)=\delta(\Omega-\Omega')$, $\Omega'\to\infty$ and Eq. (8.14) becomes

$$F_m(t)/F_m(0)=\exp\left(-t\int Wf(W)dW\right)=\exp(-\langle W\rangle t)\quad\text{as}\quad t\to\infty. \tag{8.33}$$

Equation (8.33) is similar with Eqs. (6.9) and (7.13) derived in Secs. VI and VII.

It is easy to check that for the jump process considered here the fluctuations of the number of surviving particles are also intermittent. A straightforward calculation shows that the expression (7.14) for the one-time relative fluctuation remains valid provided that the functions $\mathscr{S}_{1,2}(t)$ are replaced by the functions $\langle l^m(t)\rangle$, $m=1,2$ given by Eq. (8.14).

A more detailed analysis requires knowledge of the probability densities $\xi(\Omega)$ and $f(W)$. We consider here only a few particular situations which may generate exotic relaxation. We assume the validity of the random activation energy model (RAEM[53,54]), i.e., that both the jump and the rate processes are activated phenomena corresponding to a random distribution of energy barriers. We have

$$\Omega(E)=\mu\ \exp(-E/kT), \quad W(E)=\nu\ \exp(-E/kT), \tag{8.34}$$

where the activation energy E may take any value between zero and infinity, the pre-exponential factors μ and ν are the maximum values of the rates Ω and W, respectively, k is the Boltzmann's constant, and T is the absolute temperature of the system. The activation energies corresponding to Ω and W are random variables selected from two different probability densities

$$\eta_{\Omega,W}(E)dE, \quad \text{with} \quad \int \eta_{\Omega,W}(E)dE=1. \tag{8.35}$$

Combining Eqs. (8.34) and (8.35) it follows that the probability densities $\xi(\Omega)$ and $f(w)$ of the rates Ω and W can be expressed as

$$\xi(\Omega)=\int \eta_{\Omega}(E)\,\delta[\Omega-\mu\ \exp(-E/kT)]dE, \tag{8.36}$$

$$f(W)=\int \eta_{W}(E)\,\delta[W-\nu\ \exp(-E/kT)]dE. \tag{8.37}$$

Depending on the choice of the probability densities $\eta_{\Omega,W}(E)dE$ we distinguish the following cases:

(1) We assume that the jump dynamics is Markovian, i.e., that the height of the energy barrier corresponding to the jump process is constant

$$\eta_{\Omega}(E)=\delta(E-E_{\Omega}) \tag{8.38}$$

and that the height of the energy barrier corresponding to the rate process is exponentially distributed

$$\eta_{W}(E)=(kT_{W})^{-1}\ \exp(-E/kT_{W}), \quad T_{W}\geqslant T. \tag{8.39}$$

The probability law (8.39) corresponds to a canonical distribution of energies ''frozen'' at the temperature T_0. This type of distribution was introduced almost sixty years ago in surface chemistry;[55] it has also been used in the study of transport processes in disordered systems.[10,53,54] In this case the dynamical moments $\langle l^{m}(t)\rangle$ and $F_m(t)$ and the relative fluctuation $\rho(t)$ are given by

$$F_{m}(t)/F_{m}(0)=\langle l^{m}(t)\rangle\ \frac{\Gamma(1+H)(m\nu t)^{-H}\ \exp(-\Omega_{0}t)}{1-H(\Omega_{0}/m\nu)^{H}B[H,1-H,m\nu/(\Omega_{0}+m\nu)]}, \quad t\to\infty, \tag{8.40}$$

$$\rho(t)\sim(1+\rho^{2}(0))^{1/2}\ \frac{1-H(\Omega_{0}/\nu)^{H}B[H,1-H,\nu/(\Omega_{0}+\nu)]}{\{\Gamma(1-H)[1-H(\Omega_{0}/2\nu)^{H}B[H,1-H,2\nu/(\Omega_{0}+2\nu)]]\}^{1/2}}\ (\nu t/2)^{H/2}$$
$$\times\exp(\tfrac{1}{2}\Omega_{0}t), \quad \text{as} \quad t\to\infty, \tag{8.41}$$

where

$$\Gamma(p)=\int_0^\infty t^{p-1}\,\exp(-t)dt,\quad B(p,q,x)=\int_0^x t^{p-1}(1-t)^{q-1}\,dt \tag{8.42}$$

are the complete gamma and the incomplete beta Eulerian integrals, respectively,

$$H=T/T_W\leqslant 1, \tag{8.43}$$

and

$$\Omega_0=\mu\,\exp(-E_\Omega/kT). \tag{8.44}$$

(2) The distribution of the height of jump barriers is given by a positive Gompertz law[10] with a characteristic energy E_0

$$\eta_\Omega(E)=(E_0)^{-1}\,\exp[E/E_0-\exp(E/E_0)-1] \tag{8.45}$$

and the probability density of the rate coefficient W is given by the exponential law (8.39). In this case the large time behavior of the dynamical moments $\langle l^m(t)\rangle$ and $F_m(t)$ is given by a stretched exponential

$$F_m(t)/F_m(0)=\langle l^m(t)\rangle\sim\Gamma(1+H)(m\nu)^{-H}\mu t^{1-H}\,\exp[-\sigma(\mu t)^\alpha], \tag{8.46}$$

where

$$\sigma=[1+kT/E_0]/(kT/E_0)^\alpha \tag{8.47}$$

and

$$\alpha=kT/(E_0+kT)\leqslant 1. \tag{8.48}$$

The one-time relative fluctuation diverges to infinity as $t\to\infty$ according to a positive stretched exponential

$$\rho(t)=\left(\frac{1+\rho^2(0)}{\mu\Gamma(1+H)}\right)^{1/2}(\nu/2)^{H/2}t^{-(1-H)/2}\,\exp[\tfrac{1}{2}\sigma(\mu t)^\alpha],\quad \text{as}\quad t\to\infty \tag{8.49}$$

(3) Both activation barriers are exponentially distributed; $\eta_W(E)$ is given by Eq. (218) and $\eta_\Omega(E)$ is given by a similar canonical distribution "frozen" at temperature T_Ω

$$\eta_\Omega(E)=(kT_\Omega)^{-1}\,\exp(-E/kT_\Omega),\quad T\leqslant T_\Omega\,. \tag{8.50}$$

We have

$$F_m(t)/F_m(0)=\langle l^m(t)\rangle\sim\Gamma(\mathscr{K}+1)\Gamma(H+1)(\mu/m\nu)^H(\mu t)^{-(H+\mathscr{K})},$$

$$\nu\gg\mu,\quad t\gg\mu^{-1}, \tag{8.51}$$

$$\rho(t)=\left(\frac{1+\rho^2(0)}{\Gamma(1+\mathscr{K})\Gamma(1+H)}\right)^{1/2}(\nu/2\mu)^{H/2}(\mu t)^{(H+\mathscr{K})/2},$$

$$\nu\gg\mu,\quad t\gg\mu^{-1}, \tag{8.52}$$

where

$$\mathscr{K}=T/T_\Omega\leqslant 1. \tag{8.53}$$

Thus the large time decrease of the dynamical moments $F_m(t)$ and $\langle l^m(t)\rangle$ is given by a statistical fractal law with an exponent $\mathscr{H}+H$ and the relative fluctuation increases to infinity according to a statistical fractal law with an exponent $\frac{1}{2}(\mathscr{H}+H)$.

The probability density $P(\Omega,W,t)$ of the rates Ω and W can be evaluated from Eq. (8.16). If the average time between two jumps

$$\langle t\rangle=\int_0^\infty t\psi(t)dt=\int_0^\infty \Omega^{-1}\xi(\Omega)d\Omega=\langle\Omega^{-1}\rangle_{\text{static}}, \tag{8.54}$$

exists and is finite, then

$$P(\Omega,W,t)\sim\xi(\Omega)f(W)/[\Omega\langle\Omega^{-1}\rangle_{\text{static}}] \quad \text{as} \quad t\to\infty. \tag{8.55}$$

If $\langle t\rangle$ is infinite then the state $\Omega=0$ acts as a trap and in the limit $t\to\infty$ the random jumps cease. We have

$$P(\Omega,W,t)\to\delta(\Omega)f(W) \quad \text{as} \quad t\to\infty. \tag{8.56}$$

For example, if the distribution of jump activation energies is given by the exponential law (8.50) then $\langle t\rangle=\infty$ and for $\Omega\neq 0$ the probability density $P(\Omega,W,t)$ decreases to zero according to an inverse power law

$$P(\Omega,W,t)\sim\frac{f(W)}{\Omega^{2-\mathscr{H}}}\frac{\sin(\pi\mathscr{H})}{\pi\Gamma(\mathscr{H})}t^{-(1-\mathscr{H})}, \quad \Omega\neq 0, \quad t\to\infty. \tag{8.57}$$

We have checked the validity of the asymptotic laws (8.46) and (8.51) by assuming that $\nu/\mu\sim 10$–10^2 and $H,\mathscr{H}\sim 0.5$–0.9. For this range of parameters the stretched exponential (8.46) and the inverse power law (8.51) describe the behavior of the tail of the average survival function for $0.15\text{–}-0.10\geqslant\langle l(t)\rangle\geqslant 0$ and 0.12–$0.08\geqslant P(l(t)\rangle\geqslant 0$, respectively.

Although the above analysis provides a mathematical description of dynamical disorder in terms of pure jump processes it does not clarify its physical significance. By rephrasing the pure jump model in a physical language, we distinguish three different features:

(1) There are two different types of dynamical processes: a first process, described in terms of the jump frequency Ω, is responsible for the occurrence of dynamical disorder, whereas the second is the rate process itself characterized by the random rate coefficient W.

(2) Although no direct relations concerning the relative values of the frequencies Ω and W are assumed, their statistical behavior is correlated due to their mechanism of change. For each new step two new values of the frequencies Ω and W are randomly selected from two different probability laws. For this assumption to be fulfilled it is necessary that the interaction process corresponding to a step is very strong, resulting in a loss of memory concerning the previous states of the system. Such an assumption, known in the literature as the ''strong collision hypothesis,'' has been commonly used in spectroscopy,[14–17] chemical kinetics,[56] and condensed matter physics.[10,21,23,57]

(3) The third assumption is the one concerning the random distribution of the rates Ω and W which describe activated phenomena with a random distribution of energy barriers. This assumption has been used in biochemistry,[2,3] chemical kinetics,[4] the structural or dielectric relaxation in glassy materials,[53] transport phenomena in disordered systems,[54] etc. For this assumption to be satisfied it is necessary that a state of local equilibrium exists, i.e., that besides the jump and rate processes taken explicitly into account there is another type of process which ensures the thermalization of the system. Besides, it is necessary that the particles involved in the rate process can exist in a large variety of different states, to which correspond different activation barriers.

For illustration we consider two possible applications of the theory. The first example is the problem of protein–ligand interactions which has already been mentioned earlier. In this context the jump model is a generalization of the model with static disorder suggested by Frauenfelder *et al.*[2,3] We assume that the passage from a conformation to another is not an instantaneous process but rather it is characterized by a distribution of time scales $\mathscr{C}_{\text{fluct}}=1/\Omega_u$ corresponding to different jump frequencies Ω_u, $u=1,2,...$. For this problem the strong collision assumption means that the interaction between the ligand and the protein is sufficiently strong that it leads to a conformational change of the protein which is relatively independent of the state of the protein molecule before the interaction. Although the constraints imposed by the model seem to be rather strong, they are less restrictive than the ones corresponding to the models with static disorder presented in the literature.[2,3]

A second possible application of the theory is the study of interactions between the collective orientational relaxation in dense fluids and the kinetics of chemical processes.[29] In this case the collective orientational relaxation is responsible for the occurrence of dynamical disorder and it plays a role which is similar to the role played by the process of conformational relaxation in protein dynamics. The chemical reaction plays the role of the rate process.

IX. COOPERATIVITY VERSUS STATISTICAL INDEPENDENCE FOR RANDOM RELAXATION RATES

A referee of this article has pointed out that our approach is based on the implicit assumption that all particles making up the system are controlled by the same realization of the random rate $W(t')$. In this section we investigate the general implications of this assumption and suggest an alternative approach of random relaxation processes for which the above-mentioned assumption does not hold anymore.

The assumption that the relaxation behavior of all particles is controlled by the same realization of the random rate $W(t')$ corresponds to a very strong cooperative behavior. As the above-mentioned referee has pointed out this cooperative behavior of all particles is the physical cause which generates the intermittent behavior of the process characterized by the general fluctuation–dissipation relations (4.11). We emphasize that this cooperative behavior is related only to the dynamical disorder and has nothing to do with the particles themselves which in the framework of our approach are otherwise supposed to be independent.

Although the cooperativity of a dynamical-disordered process is not an unreasonable assumption there is no guarantee that it is universally valid. In two of the three applications considered in this article, the positron lifetime distributions and the passage through a fluctuating geometrical bottleneck, one expects to have only a partial cooperative behavior, limited to the particles trapped in a given region of the fluid or to the number of particles passing through the same bottleneck. However, the theory developed in the preceding sections remains valid, provided that the number N_0 of particles is not the total number of particles from the system, but rather the number of the particles from a given cluster corresponding to a given region of the fluid or to a given bottleneck, respectively. Generally speaking, for such a system with partial cooperativity, in addition to the two averages considered in this article, over the sample fluctuations and over the dynamical disorder, we should consider an additional averaging, over the all possible numbers and sizes of the clusters. Concerning the jump process model investigated in Sec. VIII the cooperative or noncooperative behavior of dynamical disorder should be examined for each possible applications of the model.

We emphasize that the cooperative or noncooperative behavior of dynamical disorder does not influence the expressions for the average survival functions derived in this article; only the behavior of the fluctuations is influenced by the type of dynamical disorder considered. For illustration in this section we investigate the other extreme of complete statistical independence for which the fluctuations of the relaxation rates attached to the different particles are completely independent. In this case the average in definition (2.10) of the characteristic functional $\Xi[.\mathscr{K}(t')]$ of the

number of particles should be computed by taking into account all possible realizations of different random relaxation functions $W(t_1'),\ldots,W(t_N')$ which are assumed to be independent of each other. Equation (3.2) should be replaced by

$$\Xi[\mathscr{K}(t')]=\left\langle \exp\left(i\int_0^t \mathscr{K}(t')\langle N(t')\rangle_{\text{disorder}}\, dt' \right)\right\rangle, \tag{9.1}$$

where

$$\langle N(t')\rangle_{\text{disorder}}=N_0\left\langle \exp\left(-\int_0^{t'} W(t'')dt'' \right)\right\rangle_{\text{disorder}} \tag{9.2}$$

is a dynamical average of the type (3.10). The characteristic functional $\Xi[\mathscr{K}(t')]$ can be expressed by an expansion of the type (3.9)

$$\begin{aligned}\Xi[\mathscr{K}(t')]&=g\left\{ z=1+\int_0^t \langle l(t')\rangle_{\text{dynamic}} i\mathscr{K}(t')\exp\left[i\int_0^{t'} \mathscr{K}(\mathscr{C})d\mathscr{C}\right]dt',\quad t=0\right\}\\ &=1+\sum_{m=1}^{\infty}\frac{(i)^m}{m!}F_m(0)\int_0^t\cdots\int_0^t \mathscr{K}(t_1')\cdots\mathscr{K}(t_m')\\ &\quad\times\exp\left(i\sum_{u=1}^{m}\int_0^{t_u'}\mathscr{K}(\mathscr{C})d\mathscr{C}\right)\langle l(t_1')\rangle\cdots\langle l(t_m')\rangle dt_1'\cdots dt_m'.\end{aligned} \tag{9.3}$$

By following the same steps as in Secs. II–IV from Eq. (9.3) we can show that for independent fluctuations of the random rates $W(t_1'),\ldots,W(t')$ the two-time cumulants of the second order of the number of particles and the factorial cumulants $F_m(t)$ are given by

$$\langle\langle N(t_1)N(t_2)\rangle\rangle=N_0[\langle l(t_2^*)\rangle-\langle l(t_1)\rangle\langle l(t_2)\rangle] \tag{9.4}$$

and

$$F_m(t)=F_m(0)\langle l(t)\rangle^m. \tag{9.5}$$

We notice that, in contrast with the case of cooperative dynamical disorder, for independent fluctuating rates the cumulants of the second order of the number of particles depend on the first power of the total number N_0 of particles and not on the second power N_0^2. As a result in the thermodynamic limit $N_0\to\infty$ the relative fluctuation of the number of particles decreases to zero as $(N_0)^{-1/2}$ as $N_0\to\infty$, a situation which corresponds to a nonintermittent behavior.

The choice between these two limit approaches corresponding to correlated and noncorrelated fluctuations of the relaxation rates, respectively, should be done depending on the characteristics of the particular system studied. It may happen that for certain systems none of the two approaches developed in in this article may be used and thus the development of an averaging procedure corresponding to a partially correlated behavior may be necessary.

X. DISCUSSION

Dynamical disorder occurs when there is a partial overlapping between the time scales of two correlated random processes. In this article we have addressed two problems concerning systems with dynamical disorder, to which little attention has been paid in the literature:

(1) The elaboration of an efficient method for the direct evaluation of the dynamical averages and

(2) The study of fluctuations of the number of surviving particles for independent rate processes with dynamical disorder.

Our method of direct averaging is based on the use of characteristic functionals; within its framework the direct evaluation of means is less unpleasant and less formidable than has been claimed in the literature.[1] We have derived a general class of fluctuation–dissipation relations which can be used to evaluate all moments of the number of surviving particles in terms of the average survival function. For applying these fluctuation–dissipation relations it is not necessary to use the whole mathematical apparatus of the theory. Our approach can be used to evaluate not only the fluctuations of the number of particles but also the moments of the survival functions as well as other properties of the systems. It is more general than the indirect methods of averaging used in the literature, in particular it is not confined to a certain class of stochastic processes. For Markovian processes the method of stochastic Liouville equations[1,30,31] is recovered as a particular case of our approach.

A surprising result of our treatment is that for systems with dynamical disorder the fluctuations of the number of particles have an intermittent behavior. In the thermodynamic limit the relative fluctuation does not decrease to zero, but rather tends to a constant value. In all particular cases investigated the relative fluctuation diverges to infinity for large time. This type of behavior is very different from the equilibrium behavior of systems made up of independent particles for which the relative fluctuation decreases to zero in the thermodynamic limit as the reciprocal value of the square root of the number of particles.[58] An important consequence of the intermittent behavior is that for systems with dynamical disorder the fluctuations should play an important role even in the macroscopic limit, and should lead to observable macroscopic effects. These effects would be the stochastic analog of the macroscopic quantum effects.

Although this article is long, it does not exhaust the possibilities of the application of our method. A first generalization would be the development of a field theory in which the spatial distribution of the particles is taken into account. The development of this type of theory is of importance in connection with the measurement of large fluctuations corresponding to the intermittent behavior by means of light scattering.[59] A second generalization would be to the study of the interaction between an annihilation process and a generation process of the particles (or quasiparticles). In this case nonequilibrium steady states may occur for which the generation and annihilation processes compensate each other. For these processes the fluctuation–dissipation relations may serve as a basis for the derivation of a generalized thermodynamic description of nonequilibrium steady states by using the method suggested by Ross, Hunt, and Hunt.[60]

Another possible application is related to the analysis of new experimental techniques for the study of radical kinetics by applying external variable magnetic fields, for instance, the study of geminate recombination of radical pairs by means of the stimulated polarization of nuclei (SPN[61]).

The possibilities of application of the theory are not limited to the study of physical or chemical phenomena. The method can also be used in population dynamics for the analysis of the influence of environmental fluctuations on the growth of a population[62] or in exobiology for the evaluation of the probability of the existence of extraterrestrial life.[63]

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APPENDIX A: TIME-DEPENDENT, ORDERED SYSTEMS

For computing the generating functional $\Xi_{\text{ordered}}[\mathscr{K}(t')|W(t')]$ we come back to the discrete representation (2.6) of the time variable and notice that for a given realization of the rate coefficient $W(t')$, $0\leqslant t'\leqslant t$ the m-gate probability $P_m(N_m,t_m;\ldots;N_1,t_1)$ is a superposition of binomial distributions

$$P_m(N_m,t_m;\ldots;N_1,t_1)=\sum_{N_0} P(N_0,0)\,\frac{N_0!}{(N_0-N_1)!N_1!}\,(1-p_1)^{N_1}(p_1)^{N_0-N_1}\cdots\,\frac{N_{m-1}!}{(N_{m-1}-N_m)!N_m!}$$
$$\times(1-p_m)^{N_m}(p_m)^{N_{m-1}-N_m},\quad m\gg 1, \tag{A1}$$

where

$$p_u=W(u\Delta t)\Delta t,\quad u=1,\ldots,m \tag{A2}$$

is the probability of disappearance of a particle in a small time interval limited by the times $u\Delta t$ and $(u+1)\Delta t$. Equation (A1) has been derived by taking into account that the disappearance of a particle is a statistical process independent of the evolution of other particles and by making a balance of the surviving particles from time interval to time interval. The generating function of the m-gate probability $P_m(N_m,t_m;\ldots;N_1,t_1)$

$$\Xi_m(z_m,t_m;\ldots;z_1,t_1)=\sum_{N_m}\cdots\sum_{N_1}\prod_{u=1}^{m}(z_u)^{N_u}P_m(N_m,t_m;\ldots;N_1,t_1),$$
$$\text{with}\quad |z_u|\leqslant 1,\quad u=1,\ldots,m \tag{A3}$$

can be computed by a repeated application of the binomial summation formula. By combining Eqs. (2.3), (A1), and (A3) after some elementary algebraic manipulations we come to

$$\Xi_m(z_m,t_m;\ldots;z_1,t_1)=g(\varphi_m(z_1,\ldots,z_m),0), \tag{A4}$$

where

$$\varphi_m(z_1,\ldots,z_m)=p_1+z_1(1-p_1)p_2+z_1z_2(1-p_1)(1-p_2)p_3+\cdots+z_1\cdots z_{m-1}$$
$$\times(1-p_1)\cdots(1-p_{m-1})p_m+z_1\cdots z_m(1-p_1)\cdots(1-p_m) \tag{A5}$$

and $g(z,0)$ is the generating function of the initial distribution of particles [Eq. (2.3)].

Now we compare the definitions of the ordered characteristic functional $\Xi_{\text{ordered}}[\mathscr{K}(t')|W(t')]$ and of the m-gate generating function $\Xi_m(z_m,t_m,\ldots,z_1,t_1)$; the comparison shows that in the limit $\Delta t\to 0$ we have

$$\Xi_{\text{ordered}}[\mathscr{K}(t')|W(t')]=\lim_{\substack{\Delta t\to 0\\(m\to\infty)}}\Xi_m(z_u=\exp(i\mathscr{K}(u\Delta t)\Delta t),\quad u=1,\ldots,\ldots,m). \tag{A6}$$

By combining Eqs. (A2) and (A4)–(A6) we obtain the following expression for the ordered characteristic functional:

$$\Xi_{\text{ordered}}[\mathscr{K}(t')|W(t')]=g\left\{z=\int_0^t\mathscr{F}(t')\exp\left(i\int_0^{t'}K(\mathscr{C})d\mathscr{C}\right)dt'+l(t)\exp\left(i\int_0^t K(\mathscr{C})d\mathscr{C}\right),0\right\}, \tag{A7}$$

where

$$\mathcal{F}(t)=-[\partial l(t)/\partial t]=W(t)\exp\left(-\int_0^t W(t')dt'\right). \tag{A8}$$

Performing a partial integration in Eq. (A7) we come to Eq. (3.3).

The central moments $\langle N(t_1)\cdots N(t_m)\rangle_{\text{ordered}}$ and the cumulants $\langle\langle N(t_1)\cdots N(t_m)\rangle\rangle_{\text{ordered}}$ of the number of surviving particles for a given realization of the random rate coefficient are given by

$$\langle N(t_1)\cdots N(t_m)\rangle_{\text{ordered}}=(-i)^m\left.\frac{\delta^m\Xi_{\text{ordered}}[\mathcal{K}(t')]}{\delta\mathcal{K}(t_1)\cdots\delta\mathcal{K}(t_m)}\right|_{\mathcal{K}(t')=0} \tag{A9}$$

and

$$\langle\langle N(t_1)\cdots N(t_m)\rangle\rangle_{\text{ordered}}=(-i)^m\left.\frac{\delta^m\ln\Xi_{\text{ordered}}[\mathcal{K}(t')]}{\delta\mathcal{K}(t_1)\cdots\delta\mathcal{K}(t_m)}\right|_{\mathcal{K}(t')=0}. \tag{A10}$$

For an initial canonical ensemble we get the following expressions for the first two moments of the number of particles:

$$\langle\langle N(t)\rangle\rangle_{\text{ordered}}=\langle N(t)\rangle_{\text{ordered}}=N_0 l(t) \tag{A11}$$

and

$$\langle\langle N(t_1)N(t_2)\rangle\rangle_{\text{ordered}}=\langle N(t_1)N(t_2)\rangle_{\text{ordered}}-\langle N(t_1)\rangle_{\text{ordered}}\langle N(t_2)\rangle_{\text{ordered}}=N_0[l(t_2^*)-l(t_1)l(t_2)], \tag{A11$'$}$$

where

$$t_m^*=\max(t_1,\ldots,t_m). \tag{A12}$$

The relative fluctuation of the number of particles is equal to

$$\rho_{\text{ordered}}(t_1,t_2)=\left(\frac{\langle\langle N(t_1)N(t_2)\rangle\rangle_{\text{ordered}}}{\langle\langle N(t_1)\rangle\rangle_{\text{ordered}}\langle\langle N(t_2)\rangle\rangle_{\text{ordered}}}\right)^{1/2}=(N_0)^{-1/2}\left(\frac{l(t_2^*)}{l(t_1)l(t_2)}-1\right)^{1/2}. \tag{A13}$$

In the thermodynamic limit $\langle N_0\rangle\to\infty$ the relative fluctuation of the number of particles decreases to zero as $(N_0)^{-1/2}$, that is, in the thermodynamic limit the fluctuations are insignificant, i.e., they have a nonintermittent behavior.[58]

For an initial grand canonical ensemble the generating function $g(z,0)$ depends exponentially on $z-1$, all terms in the functional Taylor expansion of $\ln\Xi_{\text{ordered}}[\mathcal{K}(t')|W(t')]$ can be computed exactly, which allows the evaluation of all cumulants. After some calculus we come to

$$\langle\langle N(t_1)\cdots N(t_m)\rangle\rangle_{\text{ordered}}=m2^{1-m}l(t_m^*)\langle N_0\rangle. \tag{A14}$$

The relative fluctuation of the number of particles is given by an equation similar to Eq. (A13)

$$\rho_{\text{ordered}}(t_1,t_2)=(\langle N_0\rangle)^{-1/2}\left(\frac{l(t_2^*)}{l(t_1)l(t_2)}\right)^{1/2}. \tag{A15}$$

For an initial grand canonical ensemble in the thermodynamic limit $\langle N_0\rangle\to\infty$ the fluctuations are also nonintermittent.

APPENDIX B: MOMENTS AND CUMULANTS

The central moments of the number of particles, $\langle N^m(t)\rangle$, can be expressed in terms of the factorial moments by using the Stirling numbers of the second and first kind $\$_m^{(q)}$ and $S_m^{(q)}$, respectively,[34]

$$\$_m^{(q)}=\sum_{k=0}^{q}\frac{(-1)^{q-k}k^m}{k!(q-k)!}, \tag{B1}$$

$$S_m^{(q)}=\sum_{k=0}^{m-q}(-1)^k\frac{(m-1+k)!}{(m-q+k)!(q-1)!}\cdot\frac{(2m-q)!}{(m-q-k)!(m+k)!}\$_{m-q+k}^{(k)}. \tag{B2}$$

We have

$$\langle N^m(t)\rangle=\sum_{q=0}^{m}\$_m^{(q)}F_q(0)\langle l^q(t)\rangle=\sum_{q=0}^{m}\sum_{v=0}^{q}\$_m^{(q)}S_q^{(v)}\langle N^v(0)\rangle\langle l^q(t)\rangle. \tag{B3}$$

The one-time cumulants $\langle\langle N^m(t)\rangle\rangle_{\text{dynamic}}=C_m(t)$ can be computed in terms of the factorial moments by comparing the logarithm of Eq. (4.5) with an expansion of $\ln g(z,t)$ similar to the expansion used in Eq. (2.11) for the characteristic functional $\Xi[\mathscr{K}(t')]$. We obtain

$$C_m(t)=\sum_{m_1,m_2,\ldots}m!(-1)^{\Sigma m_v}(\Sigma m_v-1)!\prod_v(\langle N^v(t)\rangle/[(v!)^{m_v}m_v!])^{m_v}, \tag{B4}$$

where $\Sigma v m_v=m$ is a partition of the integer m into smaller integers $m_1,m_2,\ldots$, and $\langle N^v(t)\rangle$ are given by Eq. (B3).

APPENDIX C: CURTAILED CHARACTERISTIC FUNCTIONALS

Following Lax[39] and Van Kampen[40] the characteristic functional $G[K(t')]$ of the rate coefficient $W(t')$ can be expressed as an integral of a curtailed generating functional $\mathscr{G}[K(t');\mathbf{x}]$ over all possible values of the random vector $\mathbf{x}$

$$G[K(t')]=\int\mathscr{G}[K(t'),\mathbf{x}]d\mathbf{x}, \tag{C1}$$

where $\mathscr{G}[K(t'),\mathbf{x}]$ is the solution of the evolution equation

$$\partial_t\mathscr{G}[K(t'),\mathbf{x}]=\mathbb{L}\mathscr{G}[K(t'),\mathbf{x}]+iK(t)W(\mathbf{x})\mathscr{G}[K(t'),\mathbf{x}], \tag{C2}$$

with the initial condition

$$\mathscr{G}(t=0)=P(\mathbf{x},0). \tag{C3}$$

To compute the one-time moments of the survival function, $\langle l^m(t)\rangle$, we need to evaluate $\mathscr{G}[K(t'),\mathbf{x}]$ for a constant test function $K(t')=im$ [see Eq. (4.8)]. Combining Eqs. (4.8) and (C1)–(C3) yields Eqs. (5.3)–(5.5).

From Eqs. (2.14) and (5.8) it follows that the lethargy variable $\varepsilon(t)$ obeys a differential equation with random parameters

$$d\varepsilon(t)/dt=W(\mathbf{x}(t)),\quad\text{with}\quad\varepsilon(0)=0, \tag{C4}$$

where the random evolution of $\mathbf{x}(t)$ is determined by the evolution operator $\mathbb{L}$. From Eq. (C3) it follows that the probability density $\phi(\varepsilon,\mathbf{x};t)$ obeys the stochastic Liouville equation

$$\partial_t \phi(\varepsilon,\mathbf{x};t)+W(\mathbf{x})\partial_\varepsilon \phi(\varepsilon,\mathbf{x};t)=\mathbb{L}\phi(\varepsilon,\mathbf{x};t), \tag{C5}$$

with the initial condition

$$\phi(\varepsilon,\mathbf{x};t=0)=\delta(\varepsilon)P(\mathbf{x},0). \tag{C6}$$

Through Laplace transformation Eqs. (C5)–(C6) become

$$\partial_t \tilde{\phi}(\beta,\mathbf{x};t)=\mathbb{L}\tilde{\phi}(\beta,\mathbf{x};t)-\beta W(\mathbf{x})\tilde{\phi}(\beta,\mathbf{x};t), \tag{C7}$$

$$\tilde{\phi}(\beta,\mathbf{x};t=0)=P(\mathbf{x},0). \tag{C8}$$

By comparing Eqs. (5.4) and (5.5) with Eqs. (C7) and (C8) we obtain Eq. (5.11).

APPENDIX D: FLUCTUATING GEOMETRICAL BOTTLENECKS

We introduce the joint probability density of the number N of ligand molecules and of the radius r of the bottleneck

$$\mathscr{B}(N,r;t)dr, \quad \text{with} \quad \sum \int \mathscr{B}(N,r;t)dr=1. \tag{D1}$$

$\mathscr{B}(N,r;t)$ is the solution of a stochastic Liouville equation

$$\partial_t \mathscr{B}(N,r;t)=\alpha r^2[(N+1).\mathscr{B}(N+1;r;t)-N.\mathscr{B}(N,r;t)]+\lambda\,\partial_r[r.\mathscr{B}(N,r;t)]+\lambda\,\theta\partial^2_{r^2}[.\mathscr{B}(N,r;t)], \tag{D2}$$

with the initial and boundary conditions

$$\mathscr{B}(N,r;t=0)=P(N,0)(\pi\theta)^{-1/2}\exp(-r^2/4\theta), \tag{D3}$$

$$\partial_r \mathscr{B}(N,r=0;t)=0. \tag{D4}$$

The boundary condition (D4) expresses the fact the radius r of the bottleneck cannot be negative, whereas the initial condition (D3) corresponds to an initial equilibrium truncated Gaussian distribution which obeys the condition $r\geqslant 0$.

Introducing the marginal generating function

$$g^*(z,r,t)=\sum z^N \mathscr{B}(N,r;t), \quad |z|\leqslant 1. \tag{D5}$$

Equations (D2)–(D4) become

$$\partial_t g^*(z,r,t)=\alpha r^2(1-z)\partial_z g^*(z,r,t)+\lambda\,\partial_r[rg^*(z,r,t)]+\lambda\,\theta\partial^2_{r^2}[g^*(z,r,t)], \tag{D6}$$

$$g^*(z,r,t=0)=g(z,0)(\pi\theta)^{-1/2}\exp(-r^2/4\theta), \tag{D7}$$

$$\partial_r g^*(z,r=0,t)=0.$$

We express the factorial moments $F_m(t)$ in terms of the marginal generating function $g^*(z,r,t)$. We obtain

$$F_m(t)=\sum N(N-1)\cdots(N-m+1)\int \mathscr{B}(N,r;t)dr=\int F^*_m(r,t)dr, \tag{D8}$$

where the functions $F_m^*(r,t)$ are given by

$$F_m^*(r,t)=\partial^m g^*(z,r,t)/\partial z^m|_{z=1}. \tag{D9}$$

From Eqs. (D5)–(D7) and (D9) we get a set of partial differential equations in $F_m^*(r,t)$

$$\partial_t F_m^*(r,t)=-\alpha m r^2 F_m^*(r,t)+\lambda\partial_r[rF_m^*(r,t)]+\lambda\theta\partial_{r^2}^2[F_m^*(r,t)], \tag{D10}$$

with the initial and boundary conditions

$$F_m^*(r,0)=F_m(0)(\pi\theta)^{-1/2}\exp(-r^2/4\theta), \tag{D11}$$

$$\partial_r F_m^*(r=0,t)=0. \tag{D12}$$

Equation (D10) have the same formal structure as a differential equation used by Zwanzig[32] for the evaluation of the average survival function. An eigenfunction solution of the same type of equation has been given by Weiss[47] in a different physical context. Equation (D10) can be solved by searching for Gaussian solutions of the type

$$F_m^*(r,t)=A_m(t)\exp[-r^2 b_m(t)], \quad m=1,2,\ldots, \tag{D13}$$

which obviously are compatible with the initial and boundary conditions (D11) and (D12). Inserting Eqs. (D13) into Eqs. (D10)–(D12) we obtain a chain of ordinary differential equations in $A_m(t)$ and $b_m(t)$. Solving these differential equations and inserting the solutions into Eqs. (D13) we can compute the functions $F_m^*(r,t)$. The calculations are lengthy but standard. Substituting the expressions for $F_m^*(r,t)$ into Eqs. (D8) and using the fluctuation–dissipation relations (4.11) we come to Eqs. (7.7) and (7.8).

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Gauge invariant perturbations of black holes. I. Schwarzschild space–time

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We cast the perturbed Bianchi identities, in the Schwarzschild background, into a form involving only tetrad and coordinate gauge invariant Newman–Penrose field quantities. These quantities, which arise naturally in our approach, are gauge invariant quantities of spin-weight ± 2, ± 1, and 0. Some of the integrability conditions for the Bianchi identities then provide a system of six gauge invariant perturbation wave equations for the spin-weighted quantities. These wave equations are, respectively, the (spin-weight ± 2) Bardeen–Press equations, two new (spin-weight ± 1) gravitational wave equations, and two (spin-weight 0) Regge–Wheeler equations. Other integrability conditions provide the transformation identities that relate the field quantities to each other, and hence relate the various perturbation wave equations to one another. In particular, this method provides an alternative derivation of the transformations between the Bardeen–Press and Regge–Wheeler equations. The integrability conditions also allow us to relate the Bardeen–Press quantities of opposite spin-weight, and we investigate how this relationship compares with the Teukolsky–Starobinsky identities. Finally, we give a derivation of the gauge invariant Zerilli equation, and show how it is related to the fundamental equations mentioned above. © *1996 American Institute of Physics.* [S0022-2488(96)04601-4]

I. INTRODUCTION

Chandrasekhar,[1] and Sasaki and Nakamura,[2,3] have investigated the gravitational perturbations of the Schwarzschild space–time extensively. They have shown how the well-known Bardeen–Press[4] (BP) and Regge–Wheeler[5] (RW) equations are related to one another, and have provided transformations between the quantities that satisfy these equations. Their analysis is based on the transformation properties of some ordinary differential operators.

We wish to show that these results may be derived from the perturbed Bianchi identities in a gauge-independent manner, using the modified Newman–Penrose (compacted spin-coefficient) formalism.[6] We use a purely symbolic approach in order to make full use of the Einstein equations and their integrability conditions, which are embedded in the complete set of Newman–Penrose (NP) equations. The underlying structure that becomes evident, that is, our ability to derive a system of perturbation wave equations and the transformations between them, is due largely to the properties of the background space–time. We would surely not succeed in our aim, using a formalism that did not exploit all available information about the physical scenario.

We will model our approach to this problem on the much simpler case of electromagnetic perturbations to the Schwarzschild space–time. In this case the BP and RW equations arise quite naturally from the integrability conditions for the Maxwell equations. We show how transformations between the BP and RW equations may also be derived from the integrability conditions.

Our aim will then be to extend this approach to the gravitational case. The perturbed Bianchi identities, like the perturbed source-free Maxwell equations, are gauge invariant:

$$\mathscr{L}_u(R^a{}_{b[cd;e]}) = 0$$

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(see Lun[7]), where $R^a{}_{b[cd;e]}$ refers to the background space–time and u^a is an arbitrary vector field. Therefore the field quantities that arise naturally in our analysis are also gauge invariant. That is, our field quantities, like those in the electromagnetic case, are invariant under infinitesimal coordinate and infinitesimal Lorentz transformations. After identifying these quantities, the perturbed Bianchi identities may be cast into a form that resembles the Maxwell equations, involving only gauge-independent boost- and spin-weighted quantities (see Penrose and Rindler[6]). These quantities are related to the NP Weyl scalars and spin coefficients.

We will show how the integrability conditions for the perturbed Bianchi identities give rise to six wave equations for the gauge invariant quantities. These are the BP equations, two new equations for the quantities of spin-weight ± 1, and the (gauge invariant) RW equations. We will also demonstrate how the integrability conditions naturally relate the quantities of various spin-weight, and provide the transformations between the equations that govern them. For the transformations to proceed, we use a set of higher-order commutation relationships, which may be derived from the NP commutators. In this way, the transformation identities between the BP and RW equations arise naturally, and gauge independently, from the Bianchi identities. The Zerilli[8] equation, while not arising in the same way as the other perturbation equations, may be constructed and given gauge invariant meaning.

Because of the nontrivial nature of the constructions in this article, it is worthwhile highlighting the significant results from each section here.

Section II is devoted to analyzing the electromagnetic perturbations. The work presented in this section will be used as the model for our approach to the gravitational perturbations in Sec. III.

In Sec. III A we write the perturbed Bianchi identities (3.21)–(3.28) in a form involving only gauge invariant field quantities, which we define in (3.29). This is a major result in our analysis, the verification of which involves lengthy calculations, and also makes use of the perturbed Ricci identities.

Section III B is devoted to investigating the integrability conditions for the perturbed Bianchi identities. Here we find the spin-weight ± 2 (BP), ± 1, and 0 (RW) wave equations (3.38), (3.39), (3.46)–(3.49), and the transformation identities (3.40)–(3.43), (3.53)–(3.60). We also provide an alternative derivation of Price's[9] result, that $\mathrm{Im}(\Psi_{2B})$ is a RW quantity.

In Sec. III C we investigate the significant role played by the ∂_t Killing vector (3.66), which arises very naturally in our approach. The Killing vector is fundamental in relating the BP and RW equations, as well as relating the quantities of opposite spin-weight below.

In Secs. III D and III E we examine the transformations between the six wave equations. These require some higher-order commutation relationships. Since the transformations between the BP and RW equations are of particular interest, we consider these separately in Sec. III D.

In Sec. III F, we relate quantities of opposite spin-weight. The relationship between the BP quantities Ψ_{4B} and Ψ_{0B} is given in (3.108), and we investigate how this relationship compares with the Teukolsky–Starobinsky identities. A consequence of our results is that the solution of any one of the perturbation wave equations is sufficient to determine the other gauge invariant quantities (for $l \geqslant 2$), after resolving into spherical harmonics and specifying the time dependence.

Finally, in Sec. III G, we construct the Zerilli equation (3.115), and show how the Zerilli quantity is defined in terms of our gauge invariant RW quantity.

Some of our results have already appeared elsewhere: Fernandes and Lun.[10,11] Here we attempt to give an overview, extend the earlier work, and provide more of the detail. We adopt the usual convention of denoting perturbation quantities by a subscript B.

II. ELECTROMAGNETIC PERTURBATIONS: AN ILLUSTRATION

The Schwarzschild space–time may be described in the Newman–Penrose formalism using the null tetrad:

$$l^{\alpha}=\frac{1}{\Delta}\,(r^2,\Delta,0,0),\quad n^{\alpha}=\frac{1}{2r^2}\,(r^2,-\Delta,0,0),\quad m^{\alpha}=\frac{1}{r\sqrt{2}}\,(0,0,1,i\ \mathrm{cosec}\ \vartheta), \tag{2.1}$$

where $\Delta=r^2-2Mr$. Then

$$\begin{gathered}\kappa=\sigma=\lambda=\nu=\epsilon=\pi=\tau=\Phi_0=\Phi_1=\Phi_2=\Psi_0=\Psi_1=\Psi_3=\Psi_4=0,\\ \text{þ}\rho=\rho^2,\quad \text{þ}'\rho=-\rho\mu-\Psi_2,\quad \text{þ}\mu=\rho\mu+\Psi_2,\quad \text{þ}'\mu=-\mu^2,\\ \text{þ}\Psi_2=3\rho\Psi_2,\quad \text{þ}'\Psi_2=-3\mu\Psi_2,\\ \text{ð}\Psi_2=\text{ð}\mu=\text{ð}\rho=\text{ð}'\Psi_2=\text{ð}'\mu=\text{ð}'\rho=0,\end{gathered} \tag{2.2}$$

and

$$\rho=\bar{\rho}=-\frac{1}{r},\quad \mu=\bar{\mu}=-\frac{\Delta}{2r^3},\quad \alpha=-\beta=-\frac{\cot\vartheta}{2r\sqrt{2}},\quad \gamma=\frac{M}{2r^2},\quad \Psi_2=-\frac{M}{r^3}. \tag{2.3}$$

Thus

$$\text{þ}r=-\rho r,\quad \text{þ}'r=\mu r,\quad \text{ð}r=0. \tag{2.4}$$

The fundamental equations governing the electromagnetic perturbations are the perturbed Maxwell equations,[12] which, in the compacted spin-coefficient formalism, take the form

$$(\text{þ}-2\rho)\Phi_{1B}=\text{ð}'\Phi_{0B}, \tag{2.5}$$

$$(\text{þ}-\rho)\Phi_{2B}=\text{ð}'\Phi_{1B}, \tag{2.6}$$

$$(\text{þ}'+\mu)\Phi_{0B}=\text{ð}\Phi_{1B}, \tag{2.7}$$

$$(\text{þ}'+2\mu)\Phi_{1B}=\text{ð}\Phi_{2B}. \tag{2.8}$$

From the integrability conditions on the perturbed Maxwell equations, we obtain four wave equations in the following way. Operating on equation (2.8) with ð′ and on (2.6) with $(\text{þ}'+3\mu)$, using (2.2) and making use of the appropriate NP commutation relation to eliminate Φ_{1B}, we obtain

$$[(\text{þ}'+3\mu)(\text{þ}-\rho)-\text{ð}'\text{ð}]\Phi_{2B}=0. \tag{2.9}$$

On the other hand, acting on (2.5) with ð and on (2.7) with $(\text{þ}-3\rho)$, we recover

$$[(\text{þ}-3\rho)(\text{þ}'+\mu)-\text{ð}\text{ð}']\Phi_{0B}=0. \tag{2.10}$$

Similarly, from Eqs. (2.6) and (2.8), and (2.5) and (2.7), we have

$$[(\text{þ}-2\rho)(\text{þ}'+2\mu)-\text{ð}\text{ð}']\Phi_{1B}=0, \tag{2.11}$$

$$[(\text{þ}'+2\mu)(\text{þ}-2\rho)-\text{ð}'\text{ð}]\Phi_{1B}=0. \tag{2.12}$$

In fact, Eqs. (2.11) and (2.12) are identical, as can be seen by using the commutators $[\text{þ},\text{þ}']$ and $[\text{ð},\text{ð}']$.

It should be noted that these equations, when expanded in coordinates according to the tetrad given in (2.1), reduce to familiar forms: (2.11) and (2.12) are precisely the RW equation for electromagnetic perturbations, while (2.9) and (2.10) are, respectively, the spin-weight -1 and $+1$ BP equations.

The integrability conditions also give rise to six (complex) *transformation identities*. Applying $\eth$ to (2.6), we get

$$\eth\eth' \Phi_{1B} = \eth(\text{þ} - \rho)\Phi_{2B}. \tag{2.13}$$

A similar procedure on (2.8), (2.7), and (2.5) gives, respectively,

$$\eth'\eth \Phi_{2B} = \eth'(\text{þ}' + 2\mu)\Phi_{1B}, \tag{2.14}$$

$$\eth'\eth \Phi_{1B} = \eth'(\text{þ}' + \mu)\Phi_{0B}, \tag{2.15}$$

$$\eth\eth' \Phi_{0B} = \eth(\text{þ} - 2\rho)\Phi_{1B}. \tag{2.16}$$

Finally, using the appropriate commutation relations, we eliminate Φ_{1B} between equations (2.5) and (2.6), and between Eqs. (2.7) and (2.8), to relate the quantities of opposite spin-weight (also see Teukolsky and Press[13]):

$$(\text{þ} - 3\rho)(\text{þ} - \rho)\Phi_{2B} = \eth'\eth' \Phi_{0B}, \tag{2.17}$$

$$(\text{þ}' + 3\mu)(\text{þ}' + \mu)\Phi_{0B} = \eth\eth \Phi_{2B}. \tag{2.18}$$

Chandrasekhar[1] refers to the coordinate forms of Eqs. (2.17) and (2.18) as the Teukolsky–Starobinsky identities, and shows how these relations can be used to make the transformation between the wave equations (2.9) and (2.10) for Φ_{2B} and Φ_{0B}, respectively.

Now, Eqs. (2.13)–(2.16) also act as transformations between the various wave equations. To see this, resolve Φ_{0B}, Φ_{1B}, and Φ_{2B} into spin-weighted spherical harmonics in the usual way [see, for example, Penrose and Rindler,[6] Eq. (4.15.106)]. Equation (2.13) becomes

$$\Phi_{1B} = \frac{-2r^2}{l(l+1)}\,\eth(\text{þ} - \rho)\Phi_{2B}, \tag{2.19}$$

where $l \geqslant 1$ for electromagnetic radiation. Allow the RW operator,

$$[(\text{þ} - 2\rho)(\text{þ}' + 2\mu) - \eth\eth'],$$

to act on the quantity in (2.19). From (2.2), (2.4), and the NP commutators, one can prove an important commutation relation for weighted quantities of type (p,q):

$$[(\text{þ} - 2\rho)(\text{þ}' + 2\mu) - \eth\eth'][r^2\eth(\text{þ} - \rho)] = [r^2\eth(\text{þ} - 3\rho)][(\text{þ}' + 3\mu)(\text{þ} - \rho) - \eth'\eth]. \tag{2.20}$$

This higher-order commutator, when acting on Φ_{2B}, relates the RW and BP wave operators. Consequently, since Φ_{2B} satisfies the spin-weight -1 BP equation (2.9), we see that Φ_{1B} satisfies the RW equation (2.11):

$$[(\text{þ} - 2\rho)(\text{þ}' + 2\mu) - \eth\eth']\Phi_{1B} = -\frac{2r^2}{l(l+1)}\,\eth(\text{þ} - 3\rho)[(\text{þ}' + 3\mu)(\text{þ} - \rho) - \eth'\eth]\Phi_{2B} = 0.$$

Hence, from the relation (2.13) between Φ_{1B} and Φ_{2B}, the quantity Φ_{1B} automatically satisfies (the RW) equation (2.11) by virtue of (the BP) Eq. (2.9).

The converse also holds true. The following is the corresponding commutation relation for (p,q) quantities:

$$[(\text{þ}'+3\mu)(\text{þ}-\rho)-\text{ð}'\text{ð}][r^2\text{ð}'(\text{þ}'+2\mu)]=[r^2\text{ð}'(\text{þ}'+4\mu)][(\text{þ}-2\rho)(\text{þ}'+2\mu)-\text{ðð}']. \tag{2.21}$$

Given the RW equation (2.11) and the identity (2.14), which becomes

$$\Phi_{2B}=\frac{-2r^2}{l(l+1)}\,\text{ð}'(\text{þ}'+2\mu)\Phi_{1B}, \tag{2.22}$$

we derive the spin-weight -1 BP equation (2.9) for Φ_{2B}:

$$[(\text{þ}'+3\mu)(\text{þ}-\rho)-\text{ð}'\text{ð}]\Phi_{2B}=0,$$

by acting on (2.22) with the BP operator and using (2.21).

The identities (2.15) and (2.16) offer similar transformations between the spin-weight $+1$ BP equation (2.10) and the RW equation (2.12). Alternatively, one can simply apply the GHP[14] prime operator to the above equations. Thus, the given identities [(2.13)–(2.16)] between the Newman–Penrose Maxwell scalars may be viewed as transformations between the RW and BP equations.

The remaining integrability conditions yield no new useful information in the case of electromagnetic perturbations of the Schwarzschild space–time.

III. GRAVITATIONAL PERTURBATIONS

A. Rewriting the Bianchi identities

The fundamental equations for the gravitational perturbations are the (gauge invariant) perturbed Bianchi identities.[15] After linearization in the Schwarzschild background, they become

$$(\text{þ}'+4\mu)\Psi_{3B}=\text{ð}\Psi_{4B}+3\nu_B\Psi_2, \tag{3.1}$$

$$(\text{þ}'+3\mu)\Psi_{2B}+(\text{þ}'_B+3\mu_B)\Psi_2=\text{ð}\Psi_{3B}, \tag{3.2}$$

$$(\text{þ}-2\rho)\Psi_{3B}=\text{ð}'\Psi_{2B}+(\text{ð}'_B+3\pi_B)\Psi_2, \tag{3.3}$$

$$(\text{þ}-\rho)\Psi_{4B}=\text{ð}'\Psi_{3B}-3\lambda_B\Psi_2, \tag{3.4}$$

$$(\text{þ}-4\rho)\Psi_{1B}=\text{ð}'\Psi_{0B}-3\kappa_B\Psi_2, \tag{3.5}$$

$$(\text{þ}-3\rho)\Psi_{2B}+(\text{þ}_B-3\rho_B)\Psi_2=\text{ð}'\Psi_{1B}, \tag{3.6}$$

$$(\text{þ}'+2\mu)\Psi_{1B}=\text{ð}\Psi_{2B}+(\text{ð}_B-3\tau_B)\Psi_2, \tag{3.7}$$

$$(\text{þ}'+\mu)\Psi_{0B}=\text{ð}\Psi_{1B}+3\sigma_B\Psi_2. \tag{3.8}$$

The following (Ricci) identities relating the spin coefficients will also be useful:

$$\text{þ}'\lambda_B-\text{ð}'\nu_B=-2\lambda_B\mu-\Psi_{4B}, \tag{3.9}$$

$$\text{þ}\lambda_B-\text{ð}'\pi_B=\rho\lambda_B+\mu\bar{\sigma}_B, \tag{3.10}$$

$$\text{þ}\sigma_B-\text{ð}\kappa_B=2\sigma_B\rho+\Psi_{0B}, \tag{3.11}$$

$$\text{ð}\tau_B-\text{þ}'\sigma_B=\mu\sigma_B+\rho\bar{\lambda}_B, \tag{3.12}$$

$$\eth_B\rho+\eth\rho_B-\eth'\sigma_B=-\Psi_{1B}, \tag{3.13}$$

$$\eth\lambda_B-\eth'_B\mu-\eth'\mu_B=-\Psi_{3B}. \tag{3.14}$$

We note that only six of the twelve Ricci identities are required.

To put the Bianchi identities into a form that more closely resembles the Maxwell equations of the previous section, we define the following six quantities:

$$\xi_4:=\frac{12\Psi_2 r^4}{\Lambda}(\rho\text{þ}'+\mu\text{þ}-2\Psi_2)\Psi_{4B}, \tag{3.15}$$

$$\xi_3:=-\frac{12\Psi_2 r^4}{\Lambda}\eth'\eth\lambda_B, \tag{3.16}$$

$$\xi_2:=\frac{4r^4}{\Lambda}\eth\eth(\eth'\eth'_B-3\rho\lambda_B-3\mu\bar{\sigma}_B)\Psi_2, \tag{3.17}$$

$$\xi'_2:=\frac{4r^4}{\Lambda}\eth'\eth'(\eth\eth_B-3\mu\sigma_B-3\rho\bar{\lambda}_B)\Psi_2=\bar{\xi}_2, \tag{3.18}$$

$$\xi_1:=\frac{12\Psi_2 r^4}{\Lambda}\eth\eth'\eth'\sigma_B=\xi'_3, \tag{3.19}$$

$$\xi_0:=-\frac{12\Psi_2 r^4}{\Lambda}(\mu\text{þ}+\rho\text{þ}'+2\Psi_2)\Psi_{0B}=\xi'_4, \tag{3.20}$$

where, for convenience, we have written

$$\Lambda:=(l-1)l(l+1)(l+2),$$

and $l\geqslant 2$ for gravitational radiation. In fact, (3.15)–(3.20) are weighted quantities of (p,q) type $(-4,0)$, $(-2,0)$, $(0,0)$, $(0,0)$, $(2,0)$, and $(4,0)$, respectively. The quantities of opposite spin-weight are related by the GHP[14] prime operation. While they appear mysterious at first, these quantities arise naturally in the Bianchi identities. Importantly, each of (3.15)–(3.20) vanishes in the flat space–time limit, when $\Psi_2=0$. Note that there has been a minor change in the notation since Fernandes and Lun.[10,11]

With these definitions, the Bianchi identities (3.1)–(3.8) become

$$\left(1+\frac{12\Psi_2 r^4}{\Lambda}\eth'\eth\right)\eth\Psi_{4B}=(\text{þ}'+4\mu)\hat{\Psi}_{3B}, \tag{3.21}$$

$$\eth\hat{\Psi}_{3B}=(\text{þ}'+3\mu)\hat{\Psi}_{2B}+\frac{12\Psi_2 r^4}{\Lambda}\eth\eth(\text{þ}-2\rho)\Psi_{4B}, \tag{3.22}$$

$$\eth'\hat{\Psi}_{2B}=(\text{þ}-2\rho)\hat{\Psi}_{3B}, \tag{3.23}$$

$$\eth'\hat{\Psi}_{3B}=(\text{þ}-\rho)\Psi_{4B}, \tag{3.24}$$

$$\left(1+\frac{12\Psi_2 r^4}{\Lambda}\eth\eth'\right)\eth'\Psi_{0B}=(\text{þ}-4\rho)\hat{\Psi}_{1B}, \tag{3.25}$$

$$\eth'\hat{\Psi}_{1B}=(\text{þ}-3\rho)\hat{\Psi}'_{2B}+\frac{12\Psi_2 r^4}{\Lambda}\,\eth'\eth'(\text{þ}'+2\mu)\Psi_{0B}, \tag{3.26}$$

$$\eth\hat{\Psi}'_{2B}=(\text{þ}'+2\mu)\hat{\Psi}_{1B}, \tag{3.27}$$

$$\eth\hat{\Psi}_{1B}=(\text{þ}'+\mu)\Psi_{0B}, \tag{3.28}$$

where

$$\hat{\Psi}_{3B}:=\Psi_{3B}+\xi_3,\quad \hat{\Psi}_{2B}:=\Psi_{2B}+\xi_2,\quad \hat{\Psi}'_{2B}:=\Psi_{2B}+\xi'_2,\quad \hat{\Psi}_{1B}:=\Psi_{1B}+\xi_1. \tag{3.29}$$

By substituting the appropriate quantity, we can show that the identities (3.21)–(3.28) are identical to (3.1)–(3.8). For example, in Eq. (3.21), we use (3.16), (2.2), (2.4), and the commutator $[\text{þ}',\eth']$ followed by $[\text{þ}',\eth]$. The term involving $\text{þ}'\lambda_B$ is then rewritten according to the Ricci identity (3.9). After cancellation of terms and expansion in spin-weighted spherical harmonics, so that

$$\eth'\eth\eth'\nu_B=\frac{\Lambda}{4r^4}\,\nu_B,$$

we recover precisely (3.1).

Considerably more work is required to show that (3.2) can be written as (3.22). This is because we also use the perturbed NP commutator $[\text{þ}',\eth']_B$, since ξ_2 involves perturbed derivatives of Ψ_2. The identity (3.22) may be expanded immediately to give

$$\eth\Psi_{3B}=(\text{þ}'+3\mu)\Psi_{2B}+(\text{þ}'+3\mu)\xi_2-\eth\xi_3+\frac{12\Psi_2 r^4}{\Lambda}\,\eth\eth(\text{þ}-2\rho)\Psi_{4B}. \tag{3.30}$$

Now, using $[\text{þ}',\eth]$, (2.2), and (2.4),

$$(\text{þ}'+3\mu)\xi_2=\frac{4r^4}{\Lambda}\,\eth\eth(\text{þ}'+5\mu)[\eth'\eth'_B-3\rho\lambda_B-3\mu\bar{\sigma}_B]\Psi_2. \tag{3.31}$$

From $([\text{þ}',\eth']\Psi_2)_B$, we have

$$(\text{þ}'+\mu)\eth'_B\Psi_2+3\eth'_B(\mu\Psi_2)=\eth'\text{þ}'_B\Psi_2+(3\mu\bar{\tau}_B+3\rho\nu_B)\Psi_2. \tag{3.32}$$

Expanding the second term by the Liebniz rule, and rewriting the term $\eth'_B\mu$ according to the Ricci identity (3.14), we see that

$$(\text{þ}'+4\mu)\eth'_B\Psi_2=\eth'(\text{þ}'_B+3\mu_B)\Psi_2-3\Psi_2(\eth\lambda_B+\Psi_{3B}-\mu\bar{\tau}_B-\rho\nu_B). \tag{3.33}$$

So the first term in (3.31) is

$$\frac{4r^4}{\Lambda}\,\eth\eth(\text{þ}'+5\mu)\eth'\eth'_B\Psi_2=(\text{þ}'_B+3\mu_B)\Psi_2-\frac{12\Psi_2 r^4}{\Lambda}\,\eth\eth\eth'(\eth\lambda_B+\Psi_{3B}-\mu\bar{\tau}_B-\rho\nu_B). \tag{3.34}$$

From (2.2), (2.4), (3.9), and (3.12), the second part of (3.31) becomes, after a straightforward calculation

$$-\frac{12\Psi_2 r^4}{\Lambda}\,\eth\eth[\rho\eth'\nu_B+\mu\eth'\bar{\tau}_B-(2\rho\mu+\Psi_2)\lambda_B-\rho\Psi_{4B}]. \tag{3.35}$$

Hence, using (3.4),

$$(\text{þ}'+3\mu)\xi_2=(\text{þ}'_B+3\mu_B)\Psi_2-\frac{12\Psi_2 r^4}{\Lambda}\,\text{ð}\text{ð}[\text{ð}'\text{ð}\lambda_B+(\text{þ}-2\rho)\Psi_{4B}+2(\Psi_2-\rho\mu)\lambda_B]. \tag{3.36}$$

Now

$$\text{ð}\xi_3=-\frac{12\Psi_2 r^4}{\Lambda}\,\text{ð}\text{ð}'\text{ð}\text{ð}\lambda_B,$$

which becomes, using $[\text{ð},\text{ð}']$,

$$\text{ð}\xi_3=-\frac{12\Psi_2 r^4}{\Lambda}\,[\text{ð}\text{ð}\text{ð}'\text{ð}\lambda_B+2(\Psi_2-\rho\mu)\text{ð}\text{ð}\lambda_B]. \tag{3.37}$$

Combining all terms, and after a transparent cancellation, (3.30) becomes

$$(\text{þ}'+3\mu)\Psi_{2B}+(\text{þ}'_B+3\mu_B)\Psi_2=\text{ð}\Psi_{3B}.$$

The other Bianchi identities follow in a similar way, using the NP commutators, Eqs. (2.2) and (2.4), and the Ricci identities (3.9)–(3.14). For (3.26) we also require $[\text{þ},\text{ð}]_B$. Alternatively, we can apply the GHP prime to the analysis above.

An important feature of (3.29) is that they are fully gauge invariant (the proof of this result is given in the Appendix). In this way, the Bianchi identities (3.21)–(3.28) can be regarded as the gravitational analogs of the Maxwell equations of the previous section.

B. The integrability conditions for the Bianchi identities

The integrability conditions for the perturbed Bianchi identities (3.21)–(3.28) provide a set of six wave equations. The first two are well known: they are the BP equations. Operating with ð′ on (3.21) and $(\text{þ}'+5\mu)$ on (3.24), and using the appropriate NP commutation relation in conjunction with (2.2), we find

$$[(\text{þ}'+5\mu)(\text{þ}-\rho)-\text{ð}'\text{ð}-3\Psi_2]\Psi_{4B}=0. \tag{3.38}$$

Likewise, from (3.25) and (3.28), we get

$$[(\text{þ}-5\rho)(\text{þ}'+\mu)-\text{ð}\text{ð}'-3\Psi_2]\Psi_{0B}=0 \tag{3.39}$$

(cf. Chandrasekhar[1] and Bardeen and Press[4]). Equations (3.38) and (3.39) are the usual spin-weight -2 and $+2$ BP equations, respectively.

Before moving on to the remaining wave equations, it is necessary to establish some of the other integrability conditions, which, as will be shown, are transformation identities in the gravitational case. Operating on (3.23) with ð′ and on (3.24) with $(\text{þ}-3\rho)$, and using the NP commutators to eliminate $\hat{\Psi}_{3B}$, yields

$$(\text{þ}-3\rho)(\text{þ}-\rho)\Psi_{4B}=\text{ð}'\text{ð}'\hat{\Psi}_{2B}. \tag{3.40}$$

On the other hand, applying ð to (3.21), $(\text{þ}'+5\mu)$ to (3.22), and using the equation (3.38) for Ψ_{4B}, we get

$$(\text{þ}'+5\mu)(\text{þ}'+3\mu)\hat{\Psi}_{2B}=\text{ð}\text{ð}(\Psi_{4B}+\xi_4). \tag{3.41}$$

Analogously, from (3.25)–(3.28),

$$(\text{þ}'+3\mu)(\text{þ}'+\mu)\Psi_{0B}=\text{ð}\text{ð}\hat{\Psi}'_{2B}, \tag{3.42}$$

$$(\text{þ}-5\rho)(\text{þ}-3\rho)\hat{\Psi}'_{2B}=\text{ð}'\text{ð}'(\Psi_{0B}+\xi_0). \tag{3.43}$$

We are now in a position to derive the last four wave equations. Operating on (3.23) with $(\text{þ}'+4\mu)$ and on (3.22) with ð′, using [þ′,ð′], (2.2), and (2.4) we get

$$[(\text{þ}'+4\mu)(\text{þ}-2\rho)-\text{ð}'\text{ð}]\hat{\Psi}_{3B}=-\frac{12\Psi_2 r^4}{\Lambda}\,\text{ð}'\text{ð}\text{ð}(\text{þ}-2\rho)\Psi_{4B}.$$

From (3.24), and expanding in harmonics, we may rewrite this equation as

$$[(\text{þ}'+4\mu)(\text{þ}-2\rho)-\text{ð}'\text{ð}+3\Psi_2]\hat{\Psi}_{3B}=\frac{12\Psi_2\rho r^4}{\Lambda}\,\text{ð}'\text{ð}\text{ð}\Psi_{4B}. \tag{3.44}$$

Similarly, from (3.26) and (3.27):

$$[(\text{þ}-4\rho)(\text{þ}'+2\mu)-\text{ð}\text{ð}'+3\Psi_2]\hat{\Psi}_{1B}=-\frac{12\Psi_2\mu r^4}{\Lambda}\,\text{ð}\text{ð}'\text{ð}'\Psi_{0B}. \tag{3.45}$$

These equations simplify greatly if we resolve into spherical harmonics, use (3.21) and (3.25) to eliminate Ψ_{4B} and Ψ_{0B}, respectively, and the commutators [þ,þ′] and [ð,ð′]. They become

$$[(\text{þ}+(W-2)\rho)(\text{þ}'+4\mu)-\text{ð}\text{ð}'-3\Psi_2]\hat{\Psi}_{3B}=0, \tag{3.46}$$

$$[(\text{þ}'-(W-2)\mu)(\text{þ}-4\rho)-\text{ð}'\text{ð}-3\Psi_2]\hat{\Psi}_{1B}=0, \tag{3.47}$$

where

$$W:=\frac{6r^2\Psi_2}{(l-1)(l+2)-6r^2\Psi_2}.$$

So (3.44) and (3.45) may be expressed as wave equations for the gauge invariant spin-weight -1 and $+1$ quantities.

Now, acting on (3.22) with $(\text{þ}-3\rho)$ and on (3.23) with ð and using [þ,ð], we get

$$[(\text{þ}-3\rho)(\text{þ}'+3\mu)-\text{ð}\text{ð}']\hat{\Psi}_{2B}+\frac{12\Psi_2 r^4}{\Lambda}\,\text{ð}\text{ð}(\text{þ}-2\rho)(\text{þ}-2\rho)\Psi_{4B}=0.$$

Actually, $(\text{þ}-2\rho)(\text{þ}-2\rho)\equiv(\text{þ}-3\rho)(\text{þ}-\rho)$. Using (3.40) to eliminate Ψ_{4B} and again expanding in harmonics, we see that this becomes

$$[(\text{þ}-3\rho)(\text{þ}'+3\mu)-\text{ð}\text{ð}'+3\Psi_2]\hat{\Psi}_{2B}=0. \tag{3.48}$$

The last wave equation follows in a similar natural way from (3.26) and (3.27):

$$[(\text{þ}'+3\mu)(\text{þ}-3\rho)-\text{ð}'\text{ð}+3\Psi_2]\hat{\Psi}'_{2B}=0. \tag{3.49}$$

Equations (3.48) and (3.49) are the gauge invariant RW equations, after expansion in coordinates. The RW operators associated with these equations are identical, using the commutators [þ,þ′] and [ð,ð′]. However, the field quantities $\hat{\Psi}_{2B}$ and $\hat{\Psi}'_{2B}$ are distinct [with ξ_2 related to Ψ_{4B} via (3.40) and $\xi'_2=\bar{\xi}_2$ related to Ψ_{0B} via (3.42)]. We emphasize the difference between the two RW field

quantities here, since this will be important for the identities relating quantities of opposite spin-weight [see (3.101) and (3.102)]. Hence, the integrability conditions naturally provide two RW equations. Clearly, the imaginary quantities,

$$\hat{\Psi}_{2B}-\hat{\Psi}'_{2B}=2i\ \mathrm{Im}(\xi_2), \tag{3.50}$$

$$\hat{\Psi}_{2B}-(\overline{\hat{\Psi}'_{2B}})=2i\ \mathrm{Im}(\Psi_{2B}), \tag{3.51}$$

also satisfy the RW equation and are gauge invariant. This is an alternative way of obtaining Price's[9] result.

Thus, the six equations (3.38), (3.39), and (3.46)–(3.49) are the wave equations governing the gauge invariant spin-weight ± 2, ± 1, and 0 gravitational perturbation fields, and we shall view them as fundamental wave equations governing the evolution of gravitational perturbations in the Schwarzschild background.

Using the techniques outlined above and in the previous section, the perturbed Bianchi identities also give rise to the transformation identities below. First, we obtain a useful result by operating on (3.21) with $\eth'$:

$$[\eth'\eth+3\Psi_2]\Psi_{4B}=\eth'(\text{þ}'+4\mu)\hat{\Psi}_{3B}. \tag{3.52}$$

Acting on (3.21) with $\eth'\eth'\eth$, using $[\eth,\eth']$ to simplify the second term, and (3.52), it follows that

$$[\eth'\eth'\eth\eth-3\Psi_2(\Psi_2+2\rho\mu)]\Psi_{4B}=\eth'(\eth'\eth-3\Psi_2)(\text{þ}'+4\mu)\hat{\Psi}_{3B}. \tag{3.53}$$

The other identities follow similarly. They are

$$\eth\eth'\eth'\eth\hat{\Psi}_{3B}=\eth\eth'\eth'(\text{þ}'+3\mu)\hat{\Psi}_{2B}+3\Psi_2\eth(\text{þ}-2\rho)\Psi_{4B}, \tag{3.54}$$

$$\eth\eth\eth'\eth'\hat{\Psi}_{2B}=\eth\eth\eth'(\text{þ}-2\rho)\hat{\Psi}_{3B}, \tag{3.55}$$

$$\eth'\eth\eth\eth'\hat{\Psi}_{3B}=\eth'\eth\eth(\text{þ}-\rho)\Psi_{4B}, \tag{3.56}$$

$$[\eth\eth\eth'\eth'-3\Psi_2(\Psi_2+2\rho\mu)]\Psi_{0B}=\eth(\eth\eth'-3\Psi_2)(\text{þ}-4\rho)\hat{\Psi}_{1B}, \tag{3.57}$$

$$\eth'\eth\eth\eth'\hat{\Psi}_{1B}=\eth'\eth\eth(\text{þ}-3\rho)\hat{\Psi}'_{2B}+3\Psi_2\eth'(\text{þ}'+2\mu)\Psi_{0B}, \tag{3.58}$$

$$\eth'\eth'\eth\eth\hat{\Psi}'_{2B}=\eth'\eth'\eth(\text{þ}'+2\mu)\hat{\Psi}_{1B}, \tag{3.59}$$

$$\eth\eth'\eth'\eth\hat{\Psi}_{1B}=\eth\eth'\eth'(\text{þ}'+\mu)\Psi_{0B}. \tag{3.60}$$

The significance of these relations is two-fold. First, they are gauge invariant (that is, invariant under infinitesimal coordinate and infinitesimal tetrad transformations; see the Appendix). Second, together with (3.40)–(3.43), they provide the required transformations between the various wave equations. In this way they are precisely the gravitational analogs of the transformations (2.13)–(2.16), which arose from the perturbed Maxwell equations in the previous section.

C. The ∂_t Killing vector

It is important that the gauge invariant quantities ξ_4 and ξ_0 also satisfy the spin-weight -2 and $+2$ BP equations:

$$[(\text{þ}'+5\mu)(\text{þ}-\rho)-\eth'\eth-3\Psi_2]\xi_4=0, \tag{3.61}$$

$$[(\text{þ}-5\rho)(\text{þ}'+\mu)-\text{ð}\text{ð}'-3\Psi_2]\xi_0=0. \tag{3.62}$$

Since this result is significant for the development of the theory, it is worthwhile spending some time on it here before investigating our transformation identities more fully. Using the NP commutators, (2.2) and (2.4), one can prove the following commutation relations for weighted quantities of the general type (p,q):

$$\begin{aligned}(\text{þ}+n\rho)[r^4\Psi_2(\rho\text{þ}'+\mu\text{þ}+\tfrac{1}{2}(p+q)\Psi_2)]&=[r^4\Psi_2(\rho\text{þ}'+\mu\text{þ}+\tfrac{1}{2}(p+q+2)\Psi_2)](\text{þ}+n\rho),\\ (\text{þ}'+m\mu)[r^4\Psi_2(\rho\text{þ}'+\mu\text{þ}+\tfrac{1}{2}(p+q)\Psi_2)]&=[r^4\Psi_2(\rho\text{þ}'+\mu\text{þ}+\tfrac{1}{2}(p+q-2)\Psi_2)](\text{þ}'+m\mu),\\ \text{ð}[r^4\Psi_2(\rho\text{þ}'+\mu\text{þ}+\tfrac{1}{2}(p+q)\Psi_2)]&=[r^4\Psi_2(\rho\text{þ}'+\mu\text{þ}+\tfrac{1}{2}(p+q)\Psi_2)]\text{ð}.\end{aligned} \tag{3.63}$$

From these, we derive the following commutator for quantities of type $(-4,0)$:

$$\begin{aligned}&[(\text{þ}'+5\mu)(\text{þ}-\rho)-\text{ð}'\text{ð}-3\Psi_2][r^4\Psi_2(\rho\text{þ}'+\mu\text{þ}-2\Psi_2)]\\ &\quad=[r^4\Psi_2(\rho\text{þ}'+\mu\text{þ}-2\Psi_2)][(\text{þ}'+5\mu)(\text{þ}-\rho)-\text{ð}'\text{ð}-3\Psi_2].\end{aligned} \tag{3.64}$$

The above results are self-evident when ξ_4 is written in coordinate form:

$$\xi_4=\frac{12M}{\Lambda}\frac{\partial}{\partial t}\Psi_{4B}. \tag{3.65}$$

The operator

$$r^4\Psi_2(\rho\text{þ}'+\mu\text{þ}+\tfrac{1}{2}(p+q)\Psi_2) \tag{3.66}$$

corresponds to the ∂_t Killing vector of the background space–time for a quantity of type (p,q), and so commutes with the spin-weight -2 BP operator when $(p,q)=(-4,0)$.

The operator (3.66) plays an important role in our results, and, in fact, makes several appearances. For example, the quantity $\mathrm{Im}(\xi_2)$ in (3.50) reduces to

$$\mathrm{Im}(\xi_2)=\frac{12r^4}{\Lambda}\Psi_2(\rho\text{þ}'+\mu\text{þ})\mathrm{Im}(\Psi_{2B}), \tag{3.67}$$

or, in coordinates,

$$\mathrm{Im}(\xi_2)=\frac{12M}{\Lambda}\frac{\partial}{\partial t}\mathrm{Im}(\Psi_{2B}). \tag{3.68}$$

To see this, consider

$$\frac{\Lambda}{4r^4}\xi_2=\text{ð}\text{ð}'\text{ð}'_B\Psi_2-3\Psi_2(\rho\text{ð}\text{ð}\lambda_B+\mu\text{ð}\text{ð}\bar{\sigma}_B). \tag{3.69}$$

The first term on the right-hand side of (3.69) is

$$(\text{ð}\text{ð}'-2(\Psi_2-\rho\mu))\text{ð}\text{ð}'_B\Psi_2, \tag{3.70}$$

using $[\text{ð},\text{ð}']$. From $([\text{ð},\text{ð}']\Psi_2)_B$ and (2.2),

$$\text{ð}\text{ð}'_B\Psi_2=\text{ð}'\text{ð}_B\Psi_2+3\Psi_2[\rho(\mu_B-\bar{\mu}_B)+\mu(\bar{\rho}_B-\rho_B)]. \tag{3.71}$$

After substitution of (3.71), and commuting $\eth$ and $\eth'$, (3.70) reads

$$\eth'\eth'\eth\eth_B\Psi_2+3[\eth\eth'-2(\Psi_2-\rho\mu)][\rho(\mu_B-\bar{\mu}_B)+\mu(\bar{\rho}_B-\rho_B)]\Psi_2. \tag{3.72}$$

From the complex conjugate of (3.13), and (3.14), we may substitute for $\eth\overline{\sigma_B}$ and $\eth\lambda_B$ in the second term on the right-hand side of (3.69). The result is

$$-3\Psi_2\rho(\eth\eth'_B\mu+\eth\eth'\mu_B-\eth\Psi_{3B})-3\Psi_2\mu(\eth\eth'_B\rho+\eth\eth'\bar{\rho}_B+\eth\overline{\Psi}_{1B}). \tag{3.73}$$

Now, using $([\eth,\eth']\rho)_B$ and $([\eth,\eth']\mu)_B$, and after some cancellations, (3.69) becomes

$$\frac{\Lambda}{4r^4}\,\xi_2=\eth'\eth'\eth\eth_B\Psi_2-3\Psi_2\eth'(\rho\eth\bar{\mu}_B+\mu\eth\rho_B+\rho\eth_B\mu+\mu\eth_B\rho)-9\Psi_2^2\rho(\mu_B-\bar{\mu}_B)$$
$$-9\Psi_2^2\mu(\bar{\rho}_B-\rho_B)+3\rho\eth\Psi_{3B}-3\mu\eth\overline{\Psi}_{1B}. \tag{3.74}$$

Using (3.13) and the complex conjugate of (3.14), (3.74) simplifies to give

$$\frac{\Lambda}{4r^4}\,\xi_2=\eth'\eth'(\eth\eth_B-3\rho\overline{\lambda}_B-3\mu\sigma_B)\Psi_2+3\Psi_2[\rho(\eth\Psi_{3B}-\eth'\overline{\Psi}_{3B})+\mu(\eth'\Psi_{1B}-\eth\overline{\Psi}_{1B})$$
$$-3\rho\Psi_2(\mu_B-\bar{\mu}_B)-3\mu\Psi_2(\bar{\rho}_B-\rho_B)]. \tag{3.75}$$

The terms involving Ψ_{3B} and Ψ_{1B} may be rewritten according to (3.2), (3.6), and their complex conjugates. The expression (3.75) then simplifies greatly to give

$$\frac{\Lambda}{4r^4}\,\xi_2=\frac{\Lambda}{4r^4}\,\xi'_2+3\Psi_2(\rho\text{þ}'+\mu\text{þ})(\Psi_{2B}-\overline{\Psi}_{2B}). \tag{3.76}$$

Recalling that $\xi'_2=\bar{\xi}_2$, (3.67) is proved. So, in fact, it is no surprise that $\mathrm{Im}(\xi_2)$ is a RW quantity!

D. The transformations between the BP and RW equations

The (0,0) quantities $\hat{\Psi}_{2B}$ and $\hat{\Psi}'_{2B}$ are gauge invariant, and satisfy the RW equation. From (3.40)–(3.43) we have

$$\eth\eth'\eth'\hat{\Psi}_{2B}=\eth\eth(\text{þ}-3\rho)(\text{þ}-\rho)\Psi_{4B}, \tag{3.77}$$

$$\eth'\eth'\eth\eth(\Psi_{4B}+\xi_4)=\eth'\eth'(\text{þ}'+5\mu)(\text{þ}'+3\mu)\hat{\Psi}_{2B}, \tag{3.78}$$

$$\eth'\eth'\eth\eth\hat{\Psi}'_{2B}=\eth'\eth'(\text{þ}'+3\mu)(\text{þ}'+\mu)\Psi_{0B}, \tag{3.79}$$

$$\eth\eth\eth'\eth'(\Psi_{0B}+\xi_0)=\eth\eth(\text{þ}-5\rho)(\text{þ}-3\rho)\hat{\Psi}'_{2B}. \tag{3.80}$$

Taking (3.77) and resolving into spin-weighted spherical harmonics, we get

$$\hat{\Psi}_{2B}=\frac{4r^4}{\Lambda}\,\eth\eth(\text{þ}-3\rho)(\text{þ}-\rho)\Psi_{4B}. \tag{3.81}$$

Applying the RW operator,

$$[(\text{þ}-3\rho)(\text{þ}'+3\mu)-\eth\eth'+3\Psi_2]$$

to this quantity, we derive [again by making repeated use of the NP commutation relationships and Eqs. (2.2) and (2.4)] a commutation relation for quantities of (p,q) type $(-4,0)$,

$$[(\text{þ}-3\rho)(\text{þ}'+3\mu)-\text{ð}\text{ð}'+3\Psi_2][r^4\text{ð}\text{ð}(\text{þ}-3\rho)(\text{þ}-\rho)]$$
$$=[r^4\text{ð}\text{ð}(\text{þ}-5\rho)(\text{þ}-3\rho)][(\text{þ}'+5\mu)(\text{þ}-\rho)-\text{ð}'\text{ð}-3\Psi_2]. \tag{3.82}$$

Hence, assuming the spin-weight -2 BP equation (3.38), we have the RW equation (3.48),

$$[(\text{þ}-3\rho)(\text{þ}'+3\mu)-\text{ð}\text{ð}'+3\Psi_2]\hat{\Psi}_{2B}=0.$$

Conversely, from (3.78),

$$\Psi_{4B}+\xi_4=\frac{4r^4}{\Lambda}\,\text{ð}'\text{ð}'(\text{þ}'+5\mu)(\text{þ}'+3\mu)\hat{\Psi}_{2B}, \tag{3.83}$$

and we may derive the spin-weight -2 BP equation for $\Psi_{AB}+\xi_4$ from the RW equation, by operating on (3.83) with the BP operator,

$$[(\text{þ}'+5\mu)(\text{þ}-\rho)-\text{ð}'\text{ð}-3\Psi_2],$$

and making use of the following commutation relation for (0,0) quantities:

$$[(\text{þ}'+5\mu)(\text{þ}-\rho)-\text{ð}'\text{ð}-3\Psi_2][r^4\text{ð}'\text{ð}'(\text{þ}'+5\mu)(\text{þ}'+3\mu)]$$
$$=[r^4\text{ð}'\text{ð}'(\text{þ}'+7\mu)(\text{þ}'+5\mu)][(\text{þ}-3\rho)(\text{þ}'+3\mu)-\text{ð}\text{ð}'+3\Psi_2]. \tag{3.84}$$

Our commutators (3.82) and (3.84), like those in the electromagnetic case, relate the BP and RW wave operators. Similar results follow by applying the GHP prime operator to (3.81)–(3.84). They give the transformations between the spin-weight $+2$ BP equation (3.39) and the RW equation (3.49). Alternatively, (3.79) and (3.80) are the transformation identities in this case.

The identities (3.81) and (3.83), when written in coordinates, agree (up to multiplication by a constant) with the transformations that Chandrasekhar[1] and Sasaki and Nakamura[2,3] derived through a consideration of the theory of differential equations. When expanded in coordinates, (3.81) becomes

$$\Lambda\hat{\Psi}_{2B}=2\mathscr{L}^{\dagger}_{1}\mathscr{L}^{\dagger}_{2}\mathscr{D}_0\mathscr{D}_0(r^2\Psi_{4B}), \tag{3.85}$$

while (3.83) becomes

$$\left[\Lambda+12M\,\frac{\partial}{\partial t}\right]\Psi_{4B}=\frac{\Delta^2}{2r^6}\,\mathscr{L}_{-1}\mathscr{L}_0\mathscr{D}_0^{\dagger}\mathscr{D}_0^{\dagger}(r^4\hat{\Psi}_{2B}), \tag{3.86}$$

where

$$\mathscr{D}_0:=\frac{\partial}{\partial r}+\frac{r^2}{\Delta}\,\frac{\partial}{\partial t},\quad \mathscr{D}_0^{\dagger}:=\frac{\partial}{\partial r}-\frac{r^2}{\Delta}\,\frac{\partial}{\partial t},$$

$$\mathscr{L}_n:=\frac{\partial}{\partial\vartheta}-i\ \text{cosec}\ \vartheta\,\frac{\partial}{\partial\varphi}+n\ \cot\ \vartheta,$$

$$\mathscr{L}^{\dagger}_m:=\frac{\partial}{\partial\vartheta}+i\ \text{cosec}\ \vartheta\,\frac{\partial}{\partial\varphi}+m\ \cot\ \vartheta.$$

It should be noted that the constant $[\Lambda+12Mi\sigma]$, which appears in Chandrasekhar's results, occurs naturally in our equation (3.86) or (3.83), if a time dependence $e^{i\sigma t}$ is used. (To see agreement with the work of Chandrasekhar[1] and Sasaki and Nakamura,[2,3] recall that the radial part of the quantity $r^3\hat{\Psi}_{2B}$ satisfies the RW ordinary differential equation.)

E. Other transformations

The identities (3.53)–(3.60) provide the remaining transformations between the various gauge invariant perturbation quantities. The required commutators given below, which can be derived form the NP commutators and the relations (2.2) and (2.4), are rather complicated by comparison with (3.82) and (3.84). Their ordering here is purely for later convenience.

On quantities of (p,q) type (0,0):

$$[(\text{þ}'+4\mu)(\text{þ}-2\rho)-\text{ð}'\text{ð}+3\Psi_2][r^4\text{ðð}'\text{ð}'(\text{þ}'+3\mu)]$$
$$=[r^4\text{ðð}'\text{ð}'(\text{þ}'+5\mu)][(\text{þ}-3\rho)(\text{þ}'+3\mu)-\text{ðð}'+3\Psi_2]+3\mu r^4\Psi_2\text{ðð}'\text{ð}'. \quad (3.87)$$

On quantities of type $(-4,0)$:

$$[(\text{þ}'+4\mu)(\text{þ}-2\rho)-\text{ð}'\text{ð}+3\Psi_2][r^4\Psi_2\text{ð}(\text{þ}-2\rho)]$$
$$=[r^4\Psi_2\text{ð}(\text{þ}-3\rho)][(\text{þ}'+5\mu)(\text{þ}-\rho)-\text{ð}'\text{ð}-3\Psi_2]$$
$$-r^4\Psi_2\mu\text{ð}(\text{þ}-3\rho)(\text{þ}-\rho)+r^4\Psi_2\rho\text{ð}'\text{ðð}. \quad (3.88)$$

On quantities of type $(-2,0)$:

$$[(\text{þ}-3\rho)(\text{þ}'+3\mu)-\text{ðð}'+3\Psi_2][r^4\text{ðð}\text{ð}'(\text{þ}-2\rho)]$$
$$=[r^4\text{ðð}\text{ð}'(\text{þ}-4\rho)][(\text{þ}'+4\mu)(\text{þ}-2\rho)-\text{ð}'\text{ð}+3\Psi_2]-3\rho r^4\Psi_2\text{ðð}\text{ð}'. \quad (3.89)$$

On quantities of type $(-2,0)$:

$$[(\text{þ}'+5\mu)(\text{þ}-\rho)-\text{ð}'\text{ð}-3\Psi_2][r^4\text{ð}'(\text{ð}'\text{ð}-3\Psi_2)(\text{þ}'+4\mu)]$$
$$=[r^4\text{ð}'(\text{ð}'\text{ð}-3\Psi_2)(\text{þ}'+5\mu)][(\text{þ}'+4\mu)(\text{þ}-2\rho)-\text{ð}'\text{ð}+3\Psi_2]$$
$$+r^4\mu\text{ð}'\text{ð}'\text{ð}[(\text{þ}'+4\mu)(\text{þ}-2\rho)-\text{ð}'\text{ð}+3\Psi_2]$$
$$-3r^4\Psi_2(\text{þ}'+6\mu)[\rho\text{ð}'(\text{þ}'+4\mu)]+6\mu r^4\Psi_2(\rho\mu+2\Psi_2)\text{ð}'. \quad (3.90)$$

On quantities of type $(-4,0)$:

$$[(\text{þ}'+5\mu)(\text{þ}-\rho)-\text{ð}'\text{ð}-3\Psi_2][r^4\Psi_2(\Psi_2+2\rho\mu)]$$
$$=[r^4\Psi_2(\Psi_2+2\rho\mu)][(\text{þ}'+5\mu)(\text{þ}-\rho)-\text{ð}'\text{ð}-3\Psi_2]$$
$$+2r^4\Psi_2(2\Psi_2+\rho\mu)[(\text{þ}'+4\mu)\rho-\mu(\text{þ}-\rho)]-6r^4\Psi_2^2\rho\mu, \quad (3.91)$$

$$[(\text{þ}'+4\mu)(\text{þ}-2\rho)-\text{ð}'\text{ð}+3\Psi_2][r^4\text{ð}'\text{ðð}(\text{þ}-\rho)]$$
$$=[r^4\text{ð}'\text{ðð}(\text{þ}-3\rho)][(\text{þ}'+5\mu)(\text{þ}-\rho)-\text{ð}'\text{ð}-3\Psi_2]+3\rho r^4\Psi_2\text{ð}'\text{ðð}. \quad (3.92)$$

The identities (3.54) and (3.55), together with the commutators (3.87)–(3.89), provide the transformations between $\hat{\Psi}_{3B}$ and (the RW quantity) $\hat{\Psi}_{2B}$. For example, after resolving into spherical harmonics, (3.54) may be written as

$$\hat{\Psi}_{3B}=\frac{4r^4}{\Lambda}\,\eth\eth'\eth'(\text{þ}'+3\mu)\hat{\Psi}_{2B}+\frac{12\Psi_2 r^4}{\Lambda}\,\eth(\text{þ}-2\rho)\Psi_{4B}. \tag{3.93}$$

Applying the operator,

$$[(\text{þ}'+4\mu)(\text{þ}-2\rho)-\eth'\eth+3\Psi_2],$$

to this quantity, using the commutators (3.87) and (3.88), and the relationship (3.40) between $\hat{\Psi}_{2B}$ and Ψ_{4B}, we see that

$$\begin{aligned}&[(\text{þ}'+4\mu)(\text{þ}-2\rho)-\eth'\eth+3\Psi_2]\hat{\Psi}_{3B}\\&\quad=\frac{4r^4}{\Lambda}\,\eth\eth'\eth'(\text{þ}'+5\mu)[(\text{þ}-3\rho)(\text{þ}'+3\mu)-\eth\eth'+3\Psi_2]\hat{\Psi}_{2B}+\frac{12r^4}{\Lambda}\,\Psi_2\eth(\text{þ}-3\rho)\\&\qquad\times[(\text{þ}'+5\mu)(\text{þ}-\rho)-\eth'\eth-3\Psi_2]\Psi_{4B}+\frac{12r^4}{\Lambda}\,\rho\Psi_2\eth'\eth\eth\Psi_{4B}.\end{aligned} \tag{3.94}$$

From the RW and BP equations (3.48) and (3.38), (3.94) may be written as

$$[(\text{þ}'+4\mu)(\text{þ}-2\rho)-\eth'\eth+3\Psi_2]\hat{\Psi}_{3B}=\frac{12r^4}{\Lambda}\,\rho\Psi_2\eth'\eth\eth\Psi_{4B}. \tag{3.95}$$

Although the right-hand side of (3.93) also involves Ψ_{4B}, it would not be difficult to express it solely in terms of $\hat{\Psi}_{2B}$ (see below). So the identity (3.54) is the transformation from the RW equation (3.48) to the spin-weight -1 equation (3.44).

The transformation from $\hat{\Psi}_{3B}$ to $\hat{\Psi}_{2B}$ proceeds along similar, although much simpler, lines. We use the identity (3.55) with the commutator (3.89), followed by the identity (3.24).

The transformations between $\hat{\Psi}_{3B}$ and Ψ_{4B} are achieved through (3.53) and (3.56), using the commutators (3.90)–(3.92). For example, take (3.53):

$$[\Lambda-12r^4\Psi_2(\Psi_2+2\rho\mu)]\Psi_{4B}=4r^4\eth'(\eth'\eth-3\Psi_2)(\text{þ}'+4\mu)\hat{\Psi}_{3B}. \tag{3.96}$$

Applying the BP operator,

$$[(\text{þ}'+5\mu)(\text{þ}-\rho)-\eth'\eth-3\Psi_2],$$

to this, using (3.90) and (3.91), substituting the expressions (3.52) and (3.24) for $\eth'(\text{þ}'+4\mu)\hat{\Psi}_{3B}$ and $\eth'\hat{\Psi}_{3B}$, respectively, and using the spin-weight -1 equation (3.44), we find, after much cancellation,

$$[\Lambda-12r^4\Psi_2(\Psi_2+2\rho\mu)][(\text{þ}'+5\mu)(\text{þ}-\rho)-\eth'\eth-3\Psi_2]\Psi_{4B}=0. \tag{3.97}$$

Conversely, from (3.56) and (3.92), we derive the wave equation for $\hat{\Psi}_{3B}$ from the BP equation for Ψ_{4B} in a similar calculation:

$$\begin{aligned}&[(\text{þ}'+4\mu)(\text{þ}-2\rho)-\eth'\eth+3\Psi_2]\hat{\Psi}_{3B}\\&\quad=\frac{4r^4}{\Lambda}\,\eth'\eth\eth(\text{þ}-3\rho)[(\text{þ}'+5\mu)(\text{þ}-\rho)-\eth'\eth-3\Psi_2]\Psi_{4B}+\frac{12\rho\Psi_2 r^4}{\Lambda}\,\eth'\eth\eth\Psi_{4B}.\end{aligned} \tag{3.98}$$

At first sight, these transformations appear not to be as satisfying as the RW–BP transformations above. In particular, in the transformation (3.93) between $\hat{\Psi}_{2B}$ and $\hat{\Psi}_{3B}$, we are forced to use Ψ_{4B} as an intermediate. In (3.96), the quantity is not itself the BP quantity. We consider these two issues here.

If we wished, it would be quite straightforward to write the right-hand side of (3.54) or (3.93) purely in terms of $\hat{\Psi}_{2B}$. In fact, operating on (3.54) with

$$\left[1+\frac{12\Psi_2 r^4}{\Lambda}(\rho\text{þ}'+\mu\text{þ}-\Psi_2)\right],$$

we find

$$\begin{aligned}\text{ð}\text{ð}'\text{ð}'\text{ð}&\left[1+\frac{12\Psi_2 r^4}{\Lambda}(\rho\text{þ}'+\mu\text{þ}-\Psi_2)\right]\hat{\Psi}_{3B}\\ &=\text{ð}\text{ð}'\text{ð}'(\text{þ}+3\mu)\left[1+\frac{12\Psi_2 r^4}{\Lambda}(\rho\text{þ}'+\mu\text{þ})\right]\hat{\Psi}_{2B}+3\Psi_2\text{ð}(\text{þ}-2\rho)\\ &\quad\times\left[1+\frac{12\Psi_2 r^4}{\Lambda}(\rho\text{þ}'+\mu\text{þ}-2\Psi_2)\right]\Psi_{4B},\end{aligned} \tag{3.99}$$

using (3.63). The right-hand side of this is

$$\text{ð}\text{ð}'\text{ð}'(\text{þ}'+3\mu)\left[1+\frac{12\Psi_2 r^4}{\Lambda}(\rho\text{þ}'+\mu\text{þ})\right]\hat{\Psi}_{2B}+3\Psi_2\text{ð}(\text{þ}-2\rho)(\Psi_{4B}+\xi_4),$$

or, using the identity (3.78),

$$\left[\text{ð}\text{ð}'\text{ð}'(\text{þ}'+3\mu)\left[1+\frac{12\Psi_2 r^4}{\Lambda}(\rho\text{þ}'+\mu\text{þ})\right]+\frac{12\Psi_2 r^4}{\Lambda}\text{ð}\text{ð}'\text{ð}'(\text{þ}-4\rho)(\text{þ}'+5\mu)(\text{þ}'+3\mu)\right]\hat{\Psi}_{2B}. \tag{3.100}$$

There is no need to do any further work to prove that this transformation proceeds. The analysis presented above ensures that this identity gives the desired result.

The fact that (3.96) is not exactly the BP quantity is manifest in the calculation required to derive (3.97), where the terms from the left-hand side cancel with some from the right. Although this is not in keeping with the manner in which the other transformations (notably the transformations between the BP and RW quantities) proceed, it does, nonetheless, provide the correct result. We can isolate Ψ_{4B} in (3.96) by dividing by the factor $[\Lambda-12r^4\Psi_2(\Psi_2+2\rho\mu)]$. It would be more satisfying to put this transformation into a simpler form, and we hope to refine this part of our work at some future time.

The primed versions of the commutators (3.87)–(3.92) are required when treating the other transformations given by (3.57)–(3.60). These transformations follow directly.

F. Relating quantities of opposite spin-weight

Now, the identities (3.40)–(3.43) also relate Ψ_{4B} and Ψ_{0B}. We may derive, from our transformation identities, the following relationships in a straightforward way:

$$(\text{þ}-7\rho)(\text{þ}-5\rho)(\text{þ}-3\rho)(\text{þ}-\rho)\Psi_{4B}=\text{ð}'\text{ð}'\text{ð}'\text{ð}'(\Psi_{0B}+\xi_0)+(\text{þ}-7\rho)(\text{þ}-5\rho)\text{ð}'\text{ð}'(\xi_2-\xi_2'), \tag{3.101}$$

$$(\text{Þ}'+7\mu)(\text{Þ}'+5\mu)(\text{Þ}'+3\mu)(\text{Þ}'+\mu)\Psi_{0B}=\text{ððððð}(\Psi_{4B}+\xi_4)+(\text{Þ}'+7\mu)(\text{Þ}'+5\mu)\text{ðð}(\xi_2'-\xi_2). \tag{3.102}$$

These identities allow, say, Ψ_{0B} to be determined if Ψ_{4B} is known. From (3.42) and (3.43) we may derive the following useful higher-order equation for Ψ_{0B}:

$$(\text{Þ}-7\rho)(\text{Þ}-5\rho)(\text{Þ}'+3\mu)(\text{Þ}'+\mu)\Psi_{0B}=\text{ðð}\text{ð}'\text{ð}'(\Psi_{0B}+\xi_0). \tag{3.103}$$

Recall, from (3.67),

$$(\xi_2-\xi_2')=(\xi_2-\bar{\xi}_2)=\frac{12r^4}{\Lambda}\,\Psi_2(\rho\text{Þ}'+\mu\text{Þ})(\Psi_{2B}-\overline{\Psi}_{2B}). \tag{3.104}$$

Using the identity (3.40) and the complex conjugate of (3.42), we may write

$$\text{ð}'\text{ð}'(\Psi_{2B}-\overline{\Psi}_{2B})=(\text{Þ}-3\rho)(\text{Þ}-\rho)\Psi_{4B}-(\text{Þ}'+3\mu)(\text{Þ}'+\mu)\overline{\Psi}_{0B}. \tag{3.105}$$

Substituting this into (3.101), using the commutators (3.63), and the equation (3.103), we eliminate reference to the term $(\xi_2-\xi_2')$, to get

$$\begin{aligned}&(\text{Þ}-7\rho)(\text{Þ}-5\rho)(\text{Þ}-3\rho)(\text{Þ}-\rho)(\Psi_{4B}-\xi_4)\\&\quad=\text{ð}'\text{ð}'\text{ð}'(\Psi_{0B}+\xi_0)-3\Psi_2(\rho\text{Þ}'+\mu\text{Þ}+2\Psi_2)(\overline{\Psi}_{0B}+\bar{\xi}_0).\end{aligned} \tag{3.106}$$

Taking the complex conjugate of this expression yields

$$\begin{aligned}&(\text{Þ}-7\rho)(\text{Þ}-5\rho)(\text{Þ}-3\rho)(\text{Þ}-\rho)(\overline{\Psi}_{4B}-\bar{\xi}_4)\\&\quad=\text{ððððð}(\overline{\Psi}_{0B}+\bar{\xi}_0)-3\Psi_2(\rho\text{Þ}'+\mu\text{Þ}+2\Psi_2)(\Psi_{0B}+\xi_0).\end{aligned} \tag{3.107}$$

We may eliminate $\overline{\Psi}_{0B}+\overline{\xi}_0$ from these two expressions by operating on (3.106) with ðððð and on (3.107) with $3\Psi_2(\rho\text{Þ}'+\mu\text{Þ}+2\Psi_2)$, using (3.63), and adding. The final result is

$$\begin{aligned}&[\text{ðððððð}'\text{ð}'\text{ð}'-(3\Psi_2(\rho\text{Þ}'+\mu\text{Þ}+2\Psi_2))^2](\Psi_{0B}+\xi_0)\\&\quad=\text{ðððð}(\text{Þ}-7\rho)(\text{Þ}-5\rho)(\text{Þ}-3\rho)(\text{Þ}-\rho)(\Psi_{4B}-\xi_4)\\&\qquad+3\Psi_2(\rho\text{Þ}'+\mu\text{Þ}+2\Psi_2)(\text{Þ}-7\rho)(\text{Þ}-5\rho)(\text{Þ}-3\rho)(\text{Þ}-\rho)(\overline{\Psi}_{4B}-\bar{\xi}_4).\end{aligned} \tag{3.108}$$

After expanding in coordinates we get

$$\begin{aligned}&\left(\Lambda-12M\,\frac{\partial}{\partial t}\right)\Big[\mathscr{B}\Psi_{0B}-\mathscr{L}^{\dagger}_{-1}\mathscr{L}^{\dagger}_{0}\mathscr{L}^{\dagger}_{1}\mathscr{L}^{\dagger}_{2}\mathscr{D}_0\mathscr{D}_0\mathscr{D}_0\mathscr{D}_0(4r^4\Psi_{4B})\\&\qquad-12M\,\frac{\partial}{\partial t}\,\mathscr{D}_0\mathscr{D}_0\mathscr{D}_0\mathscr{D}_0(4r^4\overline{\Psi}_{4B})\Big]=0,\end{aligned} \tag{3.109}$$

where

$$\mathscr{B}:=\left[\Lambda^2-144M\,\frac{\partial^2}{\partial t^2}\right].$$

If we separate the variables, so that Ψ_{4B} and Ψ_{0B} may be expanded as

$$4r^4\Psi_{4B}=\int_{-\infty}^{\infty}\sum_{l=2}^{\infty}\sum_{m=-l}^{l}R^{lm}_{-2}(r,\sigma)Y^{lm}_{-2}(\theta,\varphi)e^{i\sigma t}\,d\sigma,$$
$$\Psi_{0B}=\int_{-\infty}^{\infty}\sum_{l=2}^{\infty}\sum_{m=-l}^{l}R^{lm}_{+2}(r,\sigma)Y^{lm}_{+2}(\theta,\varphi)e^{i\sigma t}\,d\sigma, \tag{3.110}$$

and if we assume $\bar{R}^{l-m}_{\pm 2}(r,-\sigma)=(-1)^m R^{lm}_{\pm 2}(r,\sigma)$, then we recover the usual Teukolsky–Starobinsky relationships (see, for example, Chandrasekhar[1]) from (3.109) or indeed (3.106). For example, using (cf. Newman and Penrose[16] and Penrose and Rindler[6])

$$\bar{Y}^{lm}_{s}=(-1)^{m+s}Y^{l-m}_{-s},\quad \eth'\eth'\eth'\eth' Y^{lm}_{+2}=\frac{\Lambda}{4r^4}\,Y^{lm}_{-2}, \tag{3.111}$$

(3.106) implies

$$\int_{-\infty}^{\infty}(\Lambda-12Mi\sigma)\sum_{l}\sum_{m}[\mathscr{D}_0\mathscr{D}_0\mathscr{D}_0\mathscr{D}_0R^{lm}_{-2}-\Lambda R^{lm}_{+2}+(-1)^m 12Mi\sigma\bar{R}^{l-m}_{+2}(r,-\sigma)]$$
$$\times Y^{lm}_{-2}e^{i\sigma t}\,d\sigma=0, \tag{3.112}$$

and the Teukolsky–Starobinsky identity follows.

A similar approach can be used to relate the quantities of spin-weight ± 1. Operating on (3.22) with $\eth$, using the commutator $[\text{þ}',\eth]$ and (3.27), we recover

$$\eth\eth\hat{\Psi}_{3B}=(\text{þ}'+4\mu)(\text{þ}'+2\mu)\hat{\Psi}_{1B}+(\text{þ}'+4\mu)\eth(\xi_2-\xi_2')+\frac{12\Psi_2 r^4}{\Lambda}\,\eth\eth\eth(\text{þ}-2\rho)\Psi_{4B}. \tag{3.113}$$

Also, from (3.26) and (3.23),

$$\eth'\eth'\hat{\Psi}_{1B}=(\text{þ}-4\rho)(\text{þ}-2\rho)\hat{\Psi}_{3B}+(\text{þ}-4\rho)\eth'(\xi_2'-\xi_2)+\frac{12\Psi_2 r^4}{\Lambda}\,\eth'\eth'\eth'(\text{þ}'+2\mu)\Psi_{0B}. \tag{3.114}$$

We could go further and simplify these expressions by substituting for Ψ_{4B} and Ψ_{0B} as we did for (3.54), however, this goes beyond our present needs.

The term $\xi_2-\xi_2'$ that appears in our results, exits due to the lack of symmetry in the identities (3.21)–(3.28). This is something one does not encounter when treating the electromagnetic case in the previous section (also see Teukolsky and Press[13]).

The results of Secs. III D–III F demonstrate why the six wave equations (3.38), (3.39), and (3.46)–(3.49) presented above can be viewed as master perturbation equations. The solution of any one of these equations for the appropriate gauge invariant quantity, determines all of the other gauge invariant quantities (3.29).

G. Another perturbation equation: The Zerilli equation

The Regge–Wheeler equation appears very naturally in our approach to the perturbation problem. The Zerilli equation may be found as well, however, it does not arise in the manner described above. Consider the equation

$$[(\eth\eth'+\Psi_2+2\rho\mu)^2(\text{þ}-3\rho)(\text{þ}'+3\mu)-((\eth\eth'+2\rho\mu-2\Psi_2)^2+9\Psi_2^2)(\eth\eth'+3\Psi_2)$$
$$-9\Psi_2^2(2\rho\mu-4\Psi_2)]Z=0, \tag{3.115}$$

where

$$(\eth\eth'+\Psi_2+2\rho\mu)Z=(\eth\eth'+\Psi+2\rho\mu)\hat{\Psi}_{2B}-\frac{24\Psi_2\rho r^4}{\Lambda}\,\eth\eth(\text{þ}-\rho)\Psi_{4B}\,. \tag{3.116}$$

To show that the equation holds, that is, that it follows from the fundamental equations (3.38), (3.39), (3.44), (3.45), (3.48), and (3.49), we require the following:

On quantities of type (0,0):

$$\begin{aligned}&[(\eth\eth'+\Psi_2+2\rho\mu)^2(\text{þ}-3\rho)(\text{þ}'+3\mu)-((\eth\eth'+2\rho\mu-2\Psi_2)^2+9\Psi_2^2)(\eth\eth'+3\Psi_2)\\&\quad-9\Psi_2^2(2\rho\mu-4\Psi_2)]\\&=[(\eth\eth'+\Psi_2+2\rho\mu)(\text{þ}-5\rho)(\text{þ}'+5\mu)+3\Psi_2(\mu(\text{þ}-3\rho)+\Psi_2-\rho(\text{þ}'+5\mu))\\&\quad-(\eth\eth'+2\rho\mu-5\Psi_2)(\eth\eth'+3\Psi_2)-18\Psi_2^2](\eth\eth'+\Psi_2+2\rho\mu),\end{aligned} \tag{3.117}$$

$$\begin{aligned}&[(\eth\eth'+\Psi_2+2\rho\mu)^2(\text{þ}-3\rho)(\text{þ}'+3\mu)-((\eth\eth'+2\rho\mu-2\Psi_2)^2+9\Psi_2^2)(\eth\eth'+3\Psi_2)\\&\quad-9\Psi_2^2(2\rho\mu-4\Psi_2)]\\&=(\eth\eth'+\Psi_2+2\rho\mu)^2[(\text{þ}-3\rho)(\text{þ}'+3\mu)-\eth\eth'+3\Psi_2]\\&\quad+6\Psi_2[3\rho\mu\Psi_2-(\Psi_2+2\rho\mu)(\eth\eth'+2\rho\mu+\Psi_2)].\end{aligned} \tag{3.118}$$

On quantities of type $(-4,0)$:

$$\begin{aligned}&[(\eth\eth'+\Psi_2+2\rho\mu)(\text{þ}-5\rho)(\text{þ}'+5\mu)+3\Psi_2(\mu(\text{þ}-3\rho)+\Psi_2-\rho(\text{þ}'+5\mu))\\&\quad-(\eth\eth'+2\rho\mu-5\Psi_2)(\eth\eth'+3\Psi_2)-18\Psi_2^2]\rho\Psi_2 r^4\eth\eth(\text{þ}-\rho)\\&=r^4\rho\Psi_2\eth\eth[(\eth'\eth+3\Psi_2)(\text{þ}-3\rho)-3\rho\Psi_2][(\text{þ}'+5\mu)(\text{þ}-\rho)-\eth'\eth-3\Psi_2]\\&\quad+r^4\Psi_2[3\Psi_2\rho\mu-(\eth\eth'+\Psi_2+2\rho\mu)(\Psi_2+2\rho\mu)]\eth\eth(\text{þ}-3\rho)(\text{þ}-\rho).\end{aligned} \tag{3.119}$$

Now, using the above commutation relations and the transformation identity (3.77), we can prove that Eq. (3.115) holds. In fact

$$\begin{aligned}&[(\eth\eth'+\Psi_2+2\rho\mu)^2(\text{þ}-3\rho)(\text{þ}'+3\mu)-((\eth\eth'+2\rho\mu-2\Psi_2)^2+9\Psi_2^2)(\eth\eth'+3\Psi_2)\\&\quad-9\Psi_2^2(2\rho\mu-4\Psi_2)]Z\\&=[(\eth\eth'+\Psi_2+2\rho\mu)(\text{þ}-5\rho)(\text{þ}'+5\mu)+3\Psi_2(\mu(\text{þ}-3\rho)+\Psi_2-\rho(\text{þ}'+5\mu))\\&\quad-(\eth\eth'+2\rho\mu-5\Psi_2)(\eth\eth'+3\Psi_2)-18\Psi_2^2](\eth\eth'+\Psi_2+2\rho\mu)Z\\&=(\eth\eth'+\Psi_2+2\rho\mu)^2[(\text{þ}-3\rho)(\text{þ}'+3\mu)-\eth\eth'+3\Psi_2]\hat{\Psi}_{2B}-\frac{24\rho\Psi_2 r^4}{\Lambda}\\&\quad\times\eth\eth[(\eth'\eth+3\Psi_2)(\text{þ}-3\rho)-3\rho\Psi_2][(\text{þ}'+5\mu)(\text{þ}-\rho)-\eth'\eth-3\Psi_2]\Psi_{4B}\equiv 0.\end{aligned}$$

From (3.41) and (3.78) we have seen how Ψ_{4B} can be expressed in terms of $\hat{\Psi}_{2B}$. Thus, we can write (3.116) so that it involves only Z and $\hat{\Psi}_{2B}$, thereby relating the Regge–Wheeler and Zerilli quantities directly. Acting on (3.116) with

$$\left[1+\frac{12r^4}{\Lambda}\,\Psi_2(\rho\text{þ}'+\mu\text{þ})\right],$$

we get

$$(\eth\eth'+\Psi_2+2\rho\mu)\left[1+\frac{12r^4}{\Lambda}\Psi_2(\rho\text{þ}'+\mu\text{þ})\right]Z$$
$$=(\eth\eth'+\Psi_2+2\rho\mu)\left[1+\frac{12r^4}{\Lambda}\Psi_2(\rho\text{þ}'+\mu\text{þ})\right]\hat{\Psi}_{2B}-\frac{24r^4}{\Lambda}\rho\Psi_2(\text{þ}-3\rho)\eth\eth$$
$$\times\left[1+\frac{12r^4}{\Lambda}\Psi_2(\rho\text{þ}'+\mu\text{þ}-2\Psi_2)\right]\Psi_{4B},$$

using (3.63) and the NP commutator $[\eth,\text{þ}]$. Together with (3.41), this implies

$$(\eth\eth'+\Psi_2+2\rho\mu)\left[1+\frac{12^4}{\Lambda}\Psi_2(\rho\text{þ}'+\mu\text{þ})\right]Z=(\eth\eth'+\Psi_2+2\rho\mu)\left[1+\frac{12r^4}{\Lambda}\Psi_2(\rho\text{þ}'+\mu\text{þ})\right]\hat{\Psi}_{2B}$$
$$-\frac{24r^4}{\Lambda}\rho\Psi_2(\text{þ}-3\rho)(\text{þ}'+5\mu)(\text{þ}'+3\mu)\hat{\Psi}_{2B}. \tag{3.120}$$

Since $\hat{\Psi}_{2B}$ satisfies the RW equation (3.48), we can use the commutator $[\text{þ},\text{þ}']$ to write the product $(\text{þ}-3\rho)(\text{þ}'+5\mu)(\text{þ}'+3\mu)$ in the second term on the right-hand side as a single $\text{þ}'$ derivative. This quantity, expanded in coordinates according to (2.1), can be shown to agree with Chandrasekhar's[1] Zerilli quantity, up to multiplication by a constant. Equation (3.115), when written down in coordinates, is precisely the Zerilli equation. Of course, acting on (3.116), with the prime operation, we have a Zerilli quantity related to $\hat{\Psi}'_{2B}$, and Ψ_{0B}. So, just as there are two RW equations, we may derive two Zerilli equations.

IV. DISCUSSION

Our approach to the linearized gravitational perturbations of the Schwarzschild black hole reveals a wealth of structure. The coordinate approach to the problem provided by Chandrasekhar[1] and Sasaki and Nakamura,[2,3] obscures, to a certain extent, how natural their results really are. Actually, the transformations between the BP and RW equations are only part of a broader picture.

As we have shown, the perturbed Bianchi identities may be cast into a form involving only tetrad and coordinate-gauge-independent quantities. The identities then give rise to a system of six wave equations for the (gauge invariant) perturbation field quantities of spin-weight 0, ±1, and ±2. Historically, the spin-weight 0 and ±2 equations have been the focus of much investigation (motivated by the desire to derive a RW-like equation in the Kerr case). We are now led to establish two new perturbation equations for the intermediate spin-weights. These spin-weight ±1 equations for the gravitational perturbations are quite distinct from the spin-weight ±1 (BP) equations in the electromagnetic case.

In fact, the fundamental perturbation wave equations are some of the integrability conditions for the perturbed Bianchi identities. Other integrability conditions also naturally give rise to (transformation) identities that allow us to transform from one wave equation to another, via some higher-order commutation relations. To an extent, the work presented here addresses the question of why the transformations of Sasaki and Nakamura[2,3] and Chandrasekhar[1] should work, and how they fit into the broader theory. Thus, we have been able to provide an explanation for their results, from the point of view of the integrability conditions for the linearized Einstein equations.

The RW equation naturally plays a central role in our analysis. The Zerilli equation is not natural in the sense described above, but may be constructed from our fundamental wave equations, and given gauge invariant meaning. The Zerilli quantities may be

expressed in terms of the RW quantities, as shown here, and in coordinate form in Chandrasekhar.[1] The gauge invariant approach of Moncrief,[17] using the Hamiltonian formalism with a perturbed metric, has the Zerilli equation as a centerpiece. An interesting question for future consideration is how to relate the present gauge invariant approach, where we use the modified Newman–Penrose formalism, to the results of Moncrief.[17]

The fact that there are two RW equations should not cause too much concern. In fact, this has been foreseen by Chandrasekhar,[1] although from another point of view. The difference between the two RW quantities $\hat{\Psi}_{2B}$ (associated with Ψ_{4B}) and $\hat{\Psi}'_{2B}$ (associated with Ψ_{0B}) is manifest throughout our analysis. In fact,

$$\frac{1}{2i}(\hat{\Psi}_{2B}-\hat{\Psi}'_{2B})=\mathrm{Im}(\xi_2)=\frac{12M}{\Lambda}\frac{\partial}{\partial t}\mathrm{Im}(\Psi_{2B}).$$

It is not surprising to discover that the imaginary part of our quantity ξ_2, which arises naturally in the Bianchi identities, can be written in this way. Suppose we wished to manufacture a gauge invariant quantity by adding a complete scalar to Ψ_{2B}. Since $\mathrm{Im}(\Psi_{2B})$ is gauge invariant, it is $\mathrm{Re}(\Psi_{2B})$ that must be modified. Thus, for $\hat{\Psi}_{2B}$ to be gauge invariant, we should expect $\mathrm{Im}(\xi_2)$ to be gauge invariant also, so as not to interfere with the gauge invariance of $\mathrm{Im}(\Psi_{2B})$. As we have shown, $\mathrm{Im}(\xi_2)$ is indeed gauge invariant and contains no new information.

It is worthwhile emphasizing the natural way in which the ∂_t Killing vector appears in our analysis, not only in the terms ξ_4 and ξ_0, but also in $\mathrm{Im}(\xi_2)$ above. It plays an important role in the identities relating the quantities of opposite spin-weight, as well as in the transformation identities (3.78) and (3.80).

Since $\mathrm{Im}(\xi_2)$ is nonzero in general, the identities (3.101) and (3.102) relating Ψ_{0B} and Ψ_{4B} are not as simple as one would infer from (for example) Chandrasekhar.[1] After some work, we can show that the Teukolsky–Starobinsky identities follow from our (more general) identities, if the NP scalars Ψ_{4B} and Ψ_{0B} satisfy certain conditions. The quantity Ψ_{0B} is uniquely determined by Ψ_{4B} (and vice versa) after Fourier analyzing the time dependence, and expanding in spherical harmonics.

An important feature of our results is that they are equally valid in the flat space–time limit, when $\Psi_2=0$ ($M=0$). Thus, in particular, our wave equations and transformation identities are the direct generalizations of their flat space–time forms to the Schwarzschild space–time.

The nonvacuum perturbations of Schwarzschild space–time may also be formulated using the approach presented above. It is not difficult to include source terms in the analysis, and, in fact, the associated NP quantities (Φ_{mnB}) are necessarily gauge invariant as well. The inclusion of source terms will be considered in a future paper.

We are prompted to ask whether the approach outlined in this paper can be generalized further to other Petrov type-D background metrics. In fact, we have shown that our approach can be extended to treat the perturbations of the Kerr and Reissner–Nordström space–times. In the Reissner–Nordström case (see Fernandes and Lun[18]), we have been able to rewrite the perturbed Maxwell equations and the perturbed Bianchi identities so that only canonical gauge invariant electromagnetic and gravitational field quantities are involved. In the Kerr case (see Fernandes and Lun[19]) the perturbed Bianchi identities can be cast into a form involving only gauge invariant field quantities. In both cases we have investigated the integrability conditions for these identities, and derived gauge invariant perturbation equations. These are coupled gauge invariant electromagnetic–gravitational perturbation equations in the Reissner–Nordström case.

Preliminary results suggest that a further extension to deal with the electromagnetic and gravitational perturbations of the Kerr–Newman space–time in a gauge invariant manner may be possible.

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APPENDIX: GAUGE INVARIANCE

Since Ψ_{0B} and Ψ_{4B} are (both tetrad and coordinate) gauge invariant, our results will be seen to be gauge invariant when we prove that the quantities

$$\hat{\Psi}_{2B},\ \hat{\Psi}'_{2B},\ \hat{\Psi}_{3B},\ \hat{\Psi}_{1B}$$

are gauge invariant. To prove this, consider a combined tetrad and coordinate-gauge transformation. Then (Lun[7])

$$\Psi_{2B}\mapsto\Psi_{2B}-(X\text{þ}+Y\text{þ}')\Psi_2,\quad \Psi_{3B}\mapsto\Psi_{3B}+3v\Psi_2,$$

$$\Psi_{1B}\mapsto\Psi_{1B}+3w\Psi_2,\quad \lambda_B\mapsto\lambda_B+\text{ð}'v,\quad \sigma_B\mapsto\sigma_B-\text{ð}w,$$

and

$$\text{ð}'_B\mapsto\text{ð}'_B+(\text{ð}'X+v)\text{þ}+(\text{ð}'Y+\bar{w})\text{þ}',$$

when acting on Ψ_2 [using (2.2)]. A quick calculation reveals that all coordinate-gauge terms (X,Y) and tetrad-gauge terms (v,w) disappear from our quantities when they are subjected to gauge transformations. So $\hat{\Psi}_{2B}$ is gauge independent, as are $\hat{\Psi}'_{2B}$, $\hat{\Psi}_{3B}$, and $\hat{\Psi}_{1B}$.

Hence, the quantities

$$\hat{\Psi}_{2B}-\hat{\Psi}'_{2B}=2i\ \mathrm{Im}(\xi_2),\quad \hat{\Psi}_{2B}-(\overline{\hat{\Psi}'_{2B}})=2i\ \mathrm{Im}(\Psi_{2B}),$$

are also gauge invariant.

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Cosmological models expressible as gradient vector fields

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Classes of cosmological models, for which Einstein's equations reduce to two-dimensional dynamical systems, are studied in the presence of stochastic perturbations using the steady state of the associated Fokker–Planck equations and Zeeman's notion of ϵ-stability. In all cases, a set of variables is found for which the dynamical systems are expressible as gradient vector flows, showing that the associated cosmologies are stochastically stable. Such models are also important in connection with application of catastrophy theory to cosmology. © *1996 American Institute of Physics.* [S0022-2488(96)01101-5]

I. INTRODUCTION

A common approach to cosmological modeling is to start from Einstein's field equations

$$R_{\alpha\beta}-\tfrac{1}{2}Rg_{\alpha\beta}+\Lambda g_{\alpha\beta}=\kappa T_{\alpha\beta} \tag{1}$$

in the usual notation, and use various simplifying assumptions, such as particular symmetries, to reduce these equations to a set of ordinary differential equations of the form

$$\frac{d\mathbf{x}}{dt}=\mathbf{v(x,c)}, \tag{2}$$

where $\mathbf{x}\in\mathbb{R}^N$ (N being the dimension of the system), $\mathbf{v}$ is the vector field defining the flow, and $\mathbf{c}\in\mathbb{R}^M$ are the control parameters of the system (with M the dimension of the parameter space). Starting from Eq. (2), it has recently been argued that almost all models currently employed in cosmology are fragile, in the sense that the presence of small physically plausible perturbations can qualitatively change their dynamical behavior.[1–5] This can clearly have important consequences both for the theoretical models commonly employed in cosmology and for the interpretation of the observational data. Interestingly, it turns out that perturbations whose existence in the cosmological context give rise to such fragility could have very different consequences if they are perceived as a source of stochasticity and if at the same time a new notion of stability proposed by Zeeman[6] is employed. Briefly, Zeeman's idea is to employ a coarser notion of equivalence class (instead of the usual one employed in deterministic dynamical systems theory which is defined in terms of topological conjugacy), such that the set of structurally stable systems are dense. More precisely, Zeeman starts with dissipative flows of the form (2) with the vector field $\mathbf{v}$ defined on an orientable manifold M. The dynamics of such systems can usually be understood in terms of attractors or some measures on them. As a result, the effect of ''noise'' may be understood in terms of forcing the dynamics to take place on a neighborhood of the original attractor, denoted by s say, and defined by the steady state of the Fokker–Planck equation for $\mathbf{v}$ with $\epsilon>0$ diffusion in the form

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$$\epsilon\nabla^2 s - \nabla\cdot(s\mathbf{v}) = 0. \tag{3}$$

Defined in this way, s can be looked upon as the smooth probability function on the manifold M, with its greatest values corresponding to locations where the orbit moves most slowly on the attractor. Zeeman defines two vector fields as ϵ-equivalent if their corresponding Fokker–Planck steady states defined by Eq. (3) are equivalent as functions. A vector field $\mathbf{v}$ is then said to be ϵ-stable if it has neighborhoods of ϵ-equivalent vector fields and stable if it is ϵ-stable for arbitrary small ϵ. The most important outcome of this scheme is that ϵ-stable systems are dense. This should be contrasted with the usual notion of structural stability, defined in terms of topological conjugacy, under which the structurally stable systems are not dense[7] in the set of systems of the type (2).

This method of stabilization was recently introduced in a cosmological setting[8] and applied to simple cosmological models expressible as one-dimensional flows. The framework is particularly useful for studying those aspects of the universe that are invariant under ϵ-perturbations. Our aim here is to extend that work by studying cosmological models that are expressible as two-dimensional gradient vector fields (GVFs).

Zeeman's procedure for stabilization can be of relevance in cosmology, particularly in the presence of viscosity (which makes the resulting flow dissipative). To find the steady state of the Fokker–Planck equation (3), however, is not an easy task for a general vector field, without resorting to numerical techniques. There is, however, one class of vector fields for which the steady state s can be easily evaluated analytically and these are the GVFs expressible in the form

$$\mathbf{v} = \nabla f, \quad f: M \to \mathbb{R}, \tag{4}$$

where we shall call f the *generating function* for $\mathbf{v}$.

In such cases, the *steady state* s can be shown to be of the form

$$s = s_0\, e^{f/\epsilon}, \tag{5}$$

where the constant s_0 is defined by the condition $\int_M s = 1$. Furthermore, it can be shown that GVFs are ϵ-stable.[6] As a result, it would be of interest to find the set of reductions of Einstein's field equations which can be expressed as dissipative GVFs (in the presence of viscosity), since in such cases structurally stable properties of these models in the presence of stochasticity may easily be obtained. Such GVFs are also of interest in applications of catastrophy theory to reductions of Einstein's field equations.[9] In the following we give a number of such two-dimensional reductions together with the corresponding steady states of their corresponding Fokker–Planck equation.

Many of the calculations of this article were checked by using various algebraic computing systems, such as CLASSI[10,11] written in the symbolic language SHEEP,[11,12] REDUCE,[13,14] and Maple.[15]

II. MATHEMATICAL PRELIMINARIES

In what follows, one shall have occasion to study dynamical systems which fit the general form

$$\dot{X} = Y, \quad \dot{Y} = aX^m + bY, \tag{6}$$

with $a, b, m \in \mathbb{R}$. We show here that it is always possible to find a transformation of variables which takes Eq. (6) into a GVF. We note in passing that it is trivial to show that the generalization of Eq. (6) with $\dot{X} = dY$, where d is a constant, is also reducible to a GVF. However, in all cosmological models we study $d = 1$ and so we introduce this simplification here.

Consider the change of variable $X = cZ^n$, where $c, n \in \mathbb{R}$. As we shall see later, X is essentially the cosmological scale factor and so assumes physically meaningful values when $X \geqslant 0$. Math-

ematically however it is often both possible and useful to extend the analysis to include $X<0$. Since $Z \propto X^{1/n}$, when $n<0$ the transformation is undefined for $X=0$ and, depending on the value of n, Z may not be defined when $X<0$. Again this is not a problem for physical values of X and Z but may hinder any mathematical analysis for $X<0$.

After transforming from X to Z, Eqs. (6) become

$$\dot{Z}=\frac{1}{cn}\,YZ^{1-n}, \quad \dot{Y}=ac^{m}Z^{mn}+bY. \tag{7}$$

For Eq. (7) to represent a GVF, we must have $\partial\dot{Z}/\partial Y=\partial\dot{Y}/\partial Z$, which implies

$$\frac{1}{cn}\,Z^{1-n}=ac^{m}mnZ^{mn-1}.$$

Hence choosing

$$n=\frac{2}{m+1}, \quad c=\left[\frac{(m+1)^{2}}{4am}\right]^{1/m+1} \tag{8}$$

the system (7) will be a GVF. We note that the definition of c places a further restriction on the transformation from X to Z, since for a general value of the exponent in Eq. (8) we must demand that the quantity in the square brackets is positive, though this restriction can be lifted when the exponent is a rational number with an odd denominator. So for a *generic* $m\in\mathbb{R}$, we should only consider cases where $am>0$, and the upper half-plane $Z\geqslant 0$.

After the change of variables, our dynamical system can be incorporated within the GVF form

$$\dot{Z}=\alpha qYZ^{q-1}, \quad \dot{Y}=\alpha Z^{q}+bY, \tag{9}$$

where

$$\alpha\equiv ac^{m}, \quad q\equiv mn=\frac{2m}{m+1}, \tag{10}$$

and such a system will have the generating function

$$f=\alpha YZ^{q}+\tfrac{1}{2}bY^{2}. \tag{11}$$

Now an important property of GVFs is that their ω-limit sets consist solely of critical points. An easy proof is to note that for the vector field $\mathbf{v}=\boldsymbol{\nabla} f$, the rate of change of f, i.e., $\dot{f}\equiv\boldsymbol{\nabla} f\cdot\mathbf{v}=|\boldsymbol{\nabla} f|^{2}$, which shows that f may be appropriately chosen as a Lyapunov function.[16] As a result, we shall confine ourselves to the analysis of f near the critical points of the dynamical system, since it is at such points that we should hope to see the pronounced effect of noise on the dynamical system's stability. An interesting case arises in a neighborhood of stable critical points, where the effect of noise is to replace the critical point with a peak in the graph of the steady state s, centered on the critical point.

Postponing the subject of critical points at infinity later, it can be seen that the only critical point which Eq. (9) admits that does not lie at infinity is at the origin. On solving the equation $\dot{Y}=0$, we find that the condition $\dot{Z}=0$ is

$$Y=-\frac{\alpha}{b}\,Z^{q}\Rightarrow\frac{\alpha^{2}}{b}\,qZ^{2q-1}=0.$$

We note that for the origin to be a critical point we must have $q>1/2$. When $q<1/2$ the origin is a singular point. We shall see that even when the origin is a singular point of Eq. (9) the behavior of trajectories near the origin may be analyzed in a manner similar to that used for critical points. When $q=1/2$ (or equivalently $m=1/3$) no critical point exists.

Since the dynamical system is not linearizable, we cannot use standard eigenvalue analysis to determine the stability near the origin. Instead our analysis must be somewhat artisan and will rely on piecing together information about the gradient of the trajectories within each quadrant, their behavior as they cross the Y- and Z-axes, and the use of polar coordinates centered on the origin to analyze the effects of perturbations on the radial coordinate.

Defining polar coordinates by

$$Y=r\ \cos\ \theta, \quad Z=r\ \sin\ \theta, \tag{12}$$

and taking care to restrict θ to $(0,\pi)$ when Z is restricted to the upper half-plane $Z>0$, Eqs. (9) become

$$\begin{aligned} \dot{r}&=\alpha(q+1)r^q\ \sin^q\ \theta\ \cos\ \theta+br\ \cos^2\ \theta, \\ \dot{\theta}&=\alpha r^{q-1}\ \sin^{q-1}\ \theta(q\ \cos^2\ \theta-\sin^2\ \theta)-b\ \sin\ \theta\ \cos\ \theta. \end{aligned} \tag{13}$$

In this coordinate system, provided the dynamical system is well-defined for all values of θ, a perturbation for which $\dot{r}\geqslant 0 \forall \theta$, implies that the origin is an unstable critical point, while if $\dot{r}\leqslant 0 \forall \theta$ the origin is a stable critical point. If the sign of $\dot{r}$ depends on θ the situation is more complicated, giving rise to the possibility of not only saddles and centers, but also behaviors typical of nonlinearizable systems, such as cusps. In such cases further investigation is needed to determine the behavior near the origin.

Studying the equation for $\dot{r}$, the stability near the origin can be seen to depend primarily on the value of q, which divides the nature of the origin into six categories.

(1) If $q>1$, the origin is a critical point. The term linear in r dominates near the origin, which will be a stable node if $b<0$, and an unstable node if $b>0$.

(2) When $q=1$, the system (9) is linear and standard eigenvalue techniques can be used to study the critical point. It is found that the eigenvectors of the dynamical system are always real and of opposite sign and the critical point is a saddle.

(3) For $\frac{1}{2}<q<1$, the origin is still a critical point and the term in r^q dominates near the origin. The factor $\sin^q\ \theta$ implies that for a general q we must restrict our analysis to the upper half-plane where $\sin\ \theta>0$. The sign of $\dot{r}$ is determined by the product $(q+1)\alpha\ \cos\ \theta$ and so must necessarily be opposite in the first and second quadrants.

(4) If $q=\frac{1}{2}$, the origin is neither a critical point nor a singular point, and so the question of stability does not make sense.

(5) For $q<\frac{1}{2}$, $q\neq -1$, the origin is a singular point. Again the term in r^q dominates the equations close to the origin, and so the sign of $\dot{r}$ is necessarily opposite in the first and second quadrants.

(6) When $q=-1$, the origin is singular and will be either ''stable'' or ''unstable'' depending on the sign of b.

To distinguish between the behaviors when the sign of $\dot{r}$ depends on θ, we can analyze the behavior of dZ/dY (or dY/dZ) in various quadrants, together with the symmetry of the dynamical system near the origin under reflection in the Z-axis. Moving anticlockwise from the first quadrant, if $\text{sign}(dZ/dY)=\{-+-+\}$ and the system is symmetric under reflection in the Y-axis, the origin behaves like a center; whereas if $\text{sign}(dZ/dY)=\{+-+-\}$, the origin is a saddle point. From Eq. (9) we find that near the origin,

$$\frac{dY}{dZ}=\frac{1}{q}\frac{Z}{Y}+\frac{b}{\alpha q}Z^{1-q}=\frac{1}{q}\tan\theta+\frac{b}{\alpha q}r^{1-q}\sin^{1-q}\theta \tag{14}$$

which shows that when $q<1$ the term in $\tan\theta$ dominates near the origin and $\mathrm{sign}(dY/dZ)$ is determined by the sign of q. For $q>1$, the nature of the critical point will depend on $\mathrm{sign}(b/\alpha q)$. [Strictly speaking, this is true for the upper half-plane only: if q is rational then the behavior in the lower half-plane also depends on the numerator of $1-q$. If this numerator is even, $\mathrm{sign}(dY/dZ)$ always has the same sign.]

Equation (14) also tells us about the behavior of trajectories near the axes, which allows us to distinguish between saddles and centers. When $q<1$, $dZ/dY\to\infty$ as $\theta\to 0$ or as $\theta\to\pi$ while $dZ/dY=0$ for $\theta=\pi/2$ or $\theta=3\pi/2$. When $q>1$, we still have $dY/dZ\to\infty$ as $Y\to 0$ and so trajectories still cross the Z-axis perpendicularly. But now $dY/dZ\to\infty$ as $Z\to 0$, and so trajectories close to the Y-axis must be parallel to the Y-axis.

Polar coordinates may also be used to analyze the behavior of f, in which f assumes the form

$$f=\alpha r^{q+1}\cos\theta\sin^{q}\theta+\tfrac{1}{2}br^{2}\cos^{2}\theta. \tag{15}$$

Hence if $q\geqslant -1$, f increases with r close to $r=0$, while for $q<-1$, f decreases with r, tending to infinity at the origin. In terms of the steady state s, since s is essentially $\exp(f)$, s will peak at the origin for either of the combinations $\{\alpha<0,\ q<1\}$ or $\{b<0,\ q>1\}$.

In the light of what has been developed in this section, we now turn to examine a class of cosmological models for which various subclasses fall into the description (6).

III. APPLICATIONS TO COSMOLOGY

A. Friedman-like models with bulk viscosity

We first consider a class of spatially homogeneous models with bulk viscosity, shear, curvature, and cosmological constant. In this case, the Raychaudhuri equation[17] subject to $\omega=0=\dot{u}$ takes the form

$$3\frac{\ddot{R}}{R}=-2\sigma^{2}-\frac{1}{2}(\mu+3\bar{P})+\Lambda, \tag{16}$$

where an overdot represents a derivative with respect to time, R is the mean cosmological scale factor, σ the shear scalar ($=\sqrt{\sigma_{\alpha\beta}\sigma^{\alpha\beta}}$), μ the energy density, and $\bar{P}=p-3\zeta(\dot{R}/R)$ the pressure in the presence of bulk viscosity, with $\zeta>0$ representing the coefficient of bulk viscosity. Recalling the conservation law

$$\dot{\mu}=-3(\mu+3\bar{P})\frac{\dot{R}}{R}, \tag{17}$$

and letting $\sigma^{2}=\Sigma^{2}/R^{6}$, which includes the Bianchi types I and V,[18] Eq. (16) can be integrated to give the generalized Friedman equation in the form

$$3\frac{\dot{R}^{2}}{R^{2}}=\frac{\Sigma^{2}}{R^{6}}-\frac{3k}{R^{2}}+\Lambda+\mu. \tag{18}$$

The resulting dynamics are simplified by the choice of an isothermal equation of state, $p=(\gamma-1)\mu$, $(1\leqslant\gamma\leqslant 2)$, and a change of variables[1,18] such that $X\equiv R^{D}$ with $D\equiv 3\gamma/2$, so that $3/2\leqslant D\leqslant 3$. Note that since $R\geqslant 0$, the physically meaningful values of X are $X\geqslant 0$. Substituting in Eqs. (16) and (18) we obtain the second order differential equation expressing the dynamics in presence of shear, bulk viscosity, curvature, and a nonzero cosmological constant, to be

$$\ddot{X}-\frac{3}{2}\,\zeta\dot{X}-\frac{D^2\Lambda}{3}\,X-\frac{D(D-3)}{3}\,X^{(D-6)/D}\Sigma^2+kD(D-1)X^{D-2/D}=0 \tag{19}$$

which can be expressed as the two-dimensional dynamical system

$$\dot{X}=Y,$$

$$\dot{Y}=\frac{D^2\Lambda}{3}\,X+\frac{D(D-3)}{3}\,X^{(D-6)/D}\Sigma^2-kD(D-1)X^{(D-2)/D}+\frac{3}{2}\,\zeta Y. \tag{20}$$

Now, if we set any two of the constants $\{k,\Lambda,\Sigma\}$ equal to zero, the system will have the form (6) and we know that a GVF exists to describe that cosmological model, which must then be ϵ-stable. We examine each of these three cases in turn.

Case I. Shear-free spatially flat models: For these models we set $k=\Sigma=0$ and Eq. (20) becomes

$$\dot{X}=Y,\quad \dot{Y}=\frac{D^2\Lambda}{3}\,X+\frac{3}{2}\,\zeta Y. \tag{21}$$

This has the form (6) with the following identifications:

$$a=\frac{D^2\Lambda}{3},\quad b=\frac{3}{2}\,\zeta,\quad m=1.$$

Since $m=1$, it is easily calculated that

$$n=1,\quad c=a^{-1/2}=\frac{1}{D}\,\sqrt{\frac{3}{\Lambda}},\quad q=1$$

and so the transformation between X and Z is well-defined for $\Lambda>0$. As a GVF the dynamical system is

$$\dot{Z}=D\sqrt{\frac{\Lambda}{3}}\,Y,\quad \dot{Y}=\frac{3}{2}\,\zeta Y+D\sqrt{\frac{\Lambda}{3}}\,Z. \tag{22}$$

As discussed earlier, when $q=1$ the origin is a critical point, whose nature is a saddle point.

In Fig. 1 is shown a graph of the full phase-plane of the GVF (22) for the particular choice of a radiation fluid ($D=2$) and with values of the parameters $\zeta=1$ and $\Lambda=1$. From our analysis we know that the general characteristics of the graph are not sensitive to the values of the parameters D, ζ, and Λ, within the physical constraints already imposed.

The generating function f in this case is

$$f=D\sqrt{\frac{\Lambda}{3}}\,YZ+\frac{3}{4}\,\zeta Y^2=D\sqrt{\frac{\Lambda}{3}}\,r^2\,\cos\,\theta\,\sin^2\,\theta+\frac{3}{4}\,\zeta r^2\,\cos^2\,\theta. \tag{23}$$

Figure 2 shows the plot of the steady state s for f given by Eq. (23), with the same values of D, ζ, and Λ as used in Fig. 1. In this, and other examples, we have absorbed the arbitrary constant of integration into the constant s_0 of Eq. (5).

Interpreting s as a measure of ''likelihood of state,'' we see that, as might have been expected, s tends to infinity in the direction of the unstable manifold. A bounded graph would result around a stable fixed point, but as we shall see later system (22) only admits a stable critical point at infinity. In order to study critical points at infinity, we need to use coordinates which compactify

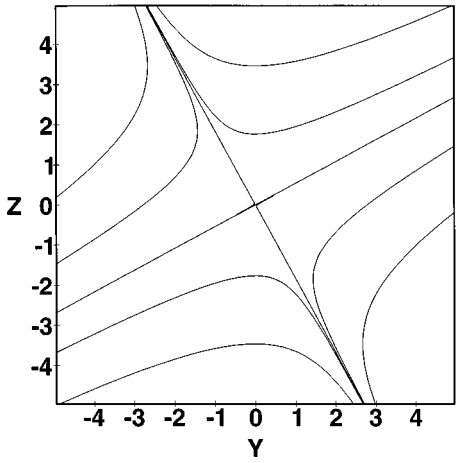

FIG. 1. The phase plane of dynamical system (22) with $\zeta=1$, $D=2$, and $\Lambda=1$.

the phase-space. One potential problem with this approach is that, in terms of the new coordinates, our dynamical system is no longer a GVF! Nevertheless, if the compactification is made sufficiently carefully, the stability analysis and the overall characteristics of the steady state s are unchanged. The application of compactification to study the critical point at infinity is dealt with in Sec. IV.

For a comparison with the more conventional approach to the stability of these cosmological models using structural stability, the reader is referred to the article of Golda *et al.*[19]

Case II. Shear-free models with no cosmological constant: Within the parameter-space allowed by the physics, these models have the richest structure of the three subclasses. Setting $\Sigma=\Lambda=0$ in Eqs. (20) we obtain

$$\dot{X}=Y, \quad \dot{Y}=\tfrac{3}{2}\zeta Y-kD(D-1)X^{(D-2)/D}. \tag{24}$$

In this case, we have the identifications

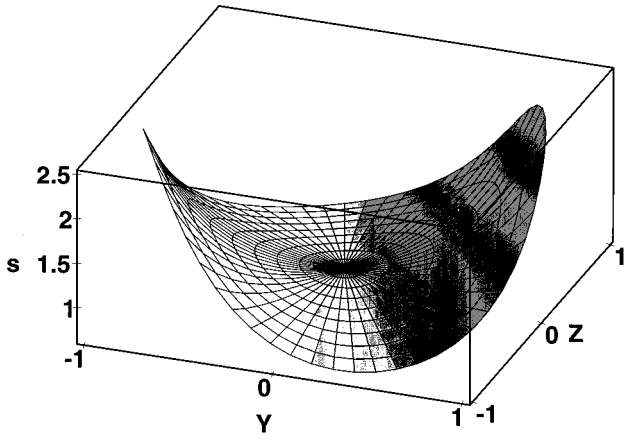

FIG. 2. The steady state function s for Fig. 1 plotted out to $r=1$.

$$a=-kD(D-1), \quad b=\frac{3}{2}\,\zeta, \quad m=\frac{D-2}{D},$$

which give us

$$n=\frac{D}{D-1}, \quad c=\left[-\frac{D-1}{kD^2(D-2)}\right]^{D/2(D-1)}.$$

Because of the exponent involved in the definition of c, the values of D which we consider in this case are restricted by the necessity that the quantity inside the square brackets of c must be positive. This implies that in general we can only consider fluids for which $D<2$ when $k=1$ and $D>2$ when $k=-1$. When $D=2$ (radiation) the transformation is singular and we must use a different transformation to obtain a GVF. This case is discussed later as case IId.

After the change of variables, the dynamical system assumes the form (9) with

$$q=\frac{D-2}{D-1}, \quad \alpha=-kD(D-1)\left[-\frac{D-1}{kD^2(D-2)}\right]^{(D-2)/2(D-1)}. \tag{25}$$

For a general q we can only study the dynamical system for this case in the half-plane $Z>0$. Given the values of D we are considering, we find that $q\in[-1,\frac{1}{2}]$.

Besides the radiation case ($q=0$), the range of q for these models incorporates four different behaviors. There are the special cases $q=1/2$ (stiff fluid) and $q=-1$ (dust). For the other cases, since we have chosen the quantity in the square brackets of Eq. (25) to be positive,

$$\text{sign}(\alpha)=\text{sign}(a)=-\text{sign}(k).$$

So for closed models, with $k=1$, $\alpha<0$, and $\dot{r}$ is negative in the first quadrant and positive in the second. For open models with $k=-1$, $\alpha>0$ and this situation is reversed.

Using the analysis of Eq. (14), since $q<1$ for all values of D under consideration, sign(dY/dZ) alternates, with the sign in the first quadrant being given by $\text{sign}(q)=\text{sign}(D-2)$.

Case IIa. $2<D<3$, $k=-1$: For these models $q>0$ and so we know that dZ/dY is positive in the first quadrant and negative in the second. The trajectories cross both the Y- and Z-axes perpendicularly, and since $\alpha>0$, Eqs. (13) tell us that trajectories will be traced in a clockwise direction. From these data, it can be deduced that the trajectories close to the origin will behave analogously to a saddle point.

Figure 3 presents, as an illustrative example, the upper phase plane for an open cosmology with $\zeta=1$, $D=5/2$, and $k=-1$. In the neighborhood of the origin, we see that the origin does behave as a saddle point, and that this is the only critical point in the phase plane.

Case IIb. $3/2<D<2$, $k=1$. Turning now to the closed models, the analysis is similar and (where the system is defined for $Z<0$) the system is symmetric under reflection in the Y-axis. As $q<1$, trajectories will meet both axes perpendicularly.

In Eqs. (9) we see that the change in sign of k and hence α means that $\dot{Y}$ will now be negative near $Y=0$ and trajectories will cross the Z-axis from right to left. However, since $\text{sign}(\dot{Y})=-\text{sign}(Y)$, Y will be increasing from the right and decreasing on the left. Piecing this together, the trajectories encircle the origin, and the origin acts as a center.

Figure 4 shows the phase plane near the origin for a closed cosmology, with $\zeta=1$, $D=1.9$, and $k=1$. Though we show only the physical upper half-plane, if we could extend the trajectories into the region $Z<0$, we would find that near the origin the trajectories are closed, confirming that the origin acts as a center.

From our earlier analysis we know that, since $q<1$, the steady state s cannot peak at the origin, and the form of s shown in a semicircle near the origin is plotted in Fig. 5, showing this instability.

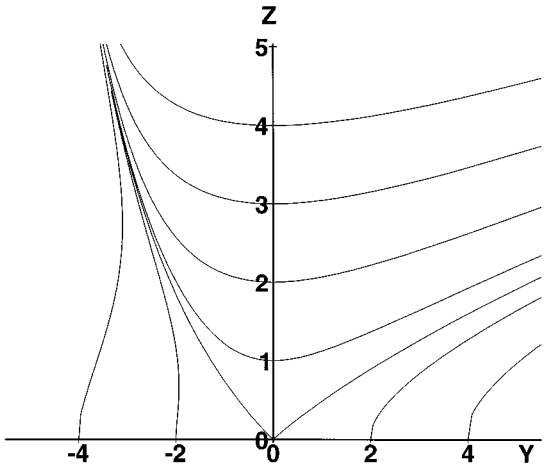

FIG. 3. Phase plane of the dynamical system given by Eqs. (9) and (25) with $\zeta=1$, $D=5/2$, and $k=-1$.

Case IIc. $D=3/2$ (Dust): For the special case of dust, when $D=3/2$ and $k=1$, we have $q=-1$, $\alpha=-9/8$ and Eq. (9) simplifies considerably to give

$$\dot{Z}=\tfrac{9}{8}YZ^{-2}, \quad \dot{Y}=\tfrac{3}{2}\zeta Y-\tfrac{9}{8}Z^{-1}. \tag{26}$$

Only integral powers of Z appear in this system, and much of the analysis for case IIb goes through unchanged: the trajectories are perpendicular to the axes, and must encircle the origin due to the signs of dZ/dY. However in Eq. (13), the vanishing of the first term for $\dot{r}$ implies that $\dot{r}>0$ in all four quadrants (since $b>0$), and the origin will be unstable. Given that the trajectories encircle the origin, it must be an unstable spiral. Figure 6 represents the upper half-plane for a cosmology with dust and $\zeta=1$. Though apparently qualitatively the same as Fig. 4, if the trajectories are extended to the lower half-plane we find that they do not close, but spiral around the origin as expected.

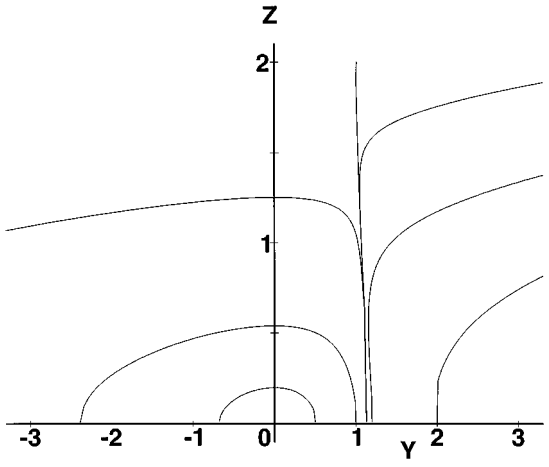

FIG. 4. Phase plane of the dynamical system given by Eqs. (9) and (25) with $\zeta=1$, $D=1.9$, and $k=1$.

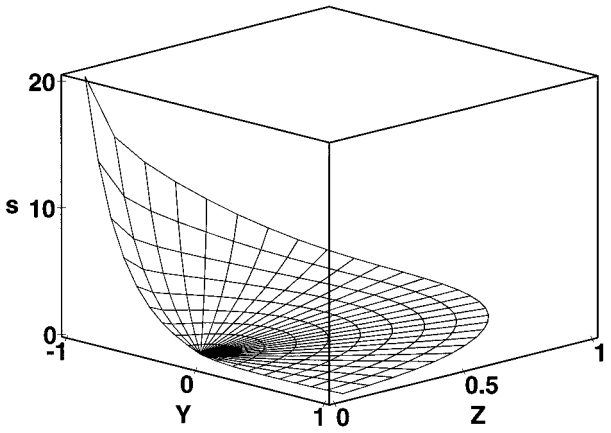

FIG. 5. The steady state function s for the dynamical system of Fig. 4, plotted out to $r=1$ in the upper half-plane.

Case IId. $D=2$ (Radiation): We consider the special case $D=2$ both because of its exceptional property from the mathematical point of view, and because of the physical interest of the fluid for which this value of D corresponds. In this case Eqs. (24) reduce to

$$\dot{X}=Y, \quad \dot{Y}=\tfrac{3}{2}\zeta Y-2k. \tag{27}$$

We may turn this system into a GVF by considering the linear transformation of variables $Y=\alpha Z+\beta X$, with α and β constants. It is found that the system in terms of X and Z will be a GVF provided the relation

$$\alpha^2=\beta(\tfrac{3}{2}\zeta-\beta)$$

holds. One choice of β which leads to particularly simple equations is[20]

$$\beta=\tfrac{6}{5}\zeta \Rightarrow \alpha=\tfrac{3}{5}\zeta.$$

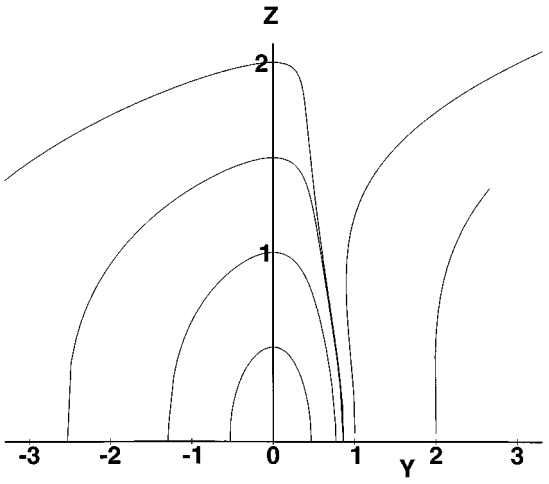

FIG. 6. Phase plane of the dynamical system given by Eqs. (9) and (25) with $\zeta=1$, $D=3/2$, and $k=1$ (dust).

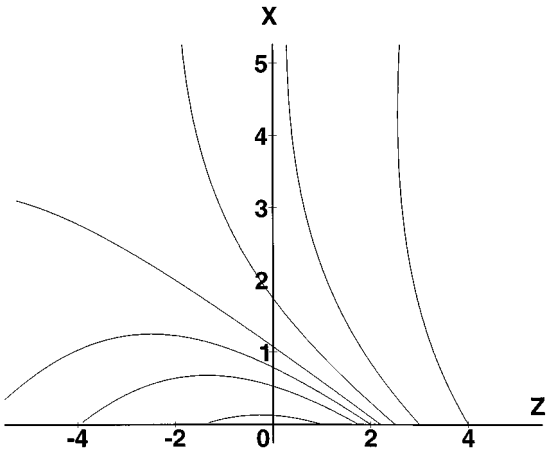

FIG. 7. Phase plane of the dynamical system given by Eqs. (9) and (25) with $\zeta=1$, $D=2$, and $k=1$ (radiation).

The dynamical system assumes the form

$$\dot{X}=\frac{3}{5}\,\zeta(2X+Z),\quad \dot{Z}=\frac{3}{10}\,\zeta(2X+Z)-\frac{10}{3}\,\frac{k}{\zeta}, \tag{28}$$

from which it is easily seen that there is *no* critical point at the origin. The generating function has the form

$$f=\frac{3}{20}\,\zeta(4X^2+4XZ+Z^2)-\frac{10}{3}\,\frac{k}{\zeta}\,Z.$$

For completeness the upper phase plane is shown as Fig. 7.

Case III. Flat models with shear and $\Lambda=0$: For these models we set $k=\Lambda=0$ in Eq. (20) to obtain

$$\dot{X}=Y,\quad \dot{Y}=\frac{3}{2}\,\zeta Y+\frac{D(D-3)}{3}\,\Sigma^2X^{(D-6)/D}. \tag{29}$$

This system takes the form (6) with the identifications

$$b=\frac{3}{2}\,\zeta,\quad a=\frac{1}{3}\,D(D-3)\Sigma^2,\quad m=\frac{D-6}{D}.$$

We calculate the values of the parameters in the GVF (9) to be

$$\alpha=\frac{1}{3}\,D(D-3)\Sigma^2\left[\frac{3(D-3)}{D^2(D-6)\Sigma^2}\right]^{D/2(D-3)},\quad q=\frac{D-6}{D-3}. \tag{30}$$

Again there is a slight restriction on the equation of state, since for a stiff fluid ($D=3$) this transformation is singular. Given $D\in[3/2,3)$, q takes values in the range $[3,\infty)$. In general, we are once more limited to considering the upper half-plane $Z>0$ because of the exponent of Z in the equation for $\dot{Z}$, which is negative for all values of D under consideration.

In Fig. 8 we plot the phase diagram for these cosmologies with $\zeta=1$, $\Sigma=1$, and $D=2$. The origin is seen to be an unstable cusp.

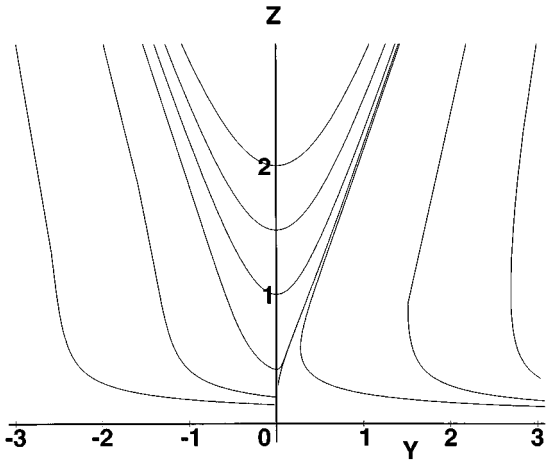

FIG. 8. The phase plane of the dynamical system (9) with Eq. (30) for $\zeta=1$, $D=2$, and $\Sigma=1$.

Referring to Eq. (15), the large value of q means that the term in r^2 dominates near the origin. Since $b>0$, we expect the origin to be unstable for all values of θ, which is indeed the case.

B. Novello–Rebouças space-times

As a second family of space-times, we consider a class of rotating dissipative cosmological models[21] whose line element is given by

$$ds^2=dt^2+2A(t,x)dt\ dy-F^2(t)dx^2-\tfrac{1}{2}A(t,x)dy^2-H^2(t)dz^2. \tag{31}$$

Making use of the algebra packages referred to in the Introduction it can be shown that the corresponding Einstein equations reduce to a set of seven differential equations. One of these implies that $F(t)H(t)$ is constant. Three of the rest define the energy density and the heat flux vector q^α. The remaining three space-diagonal equations can be reduced to the equations

$$\dot{X}=-2\sqrt{2}XY, \quad \dot{Y}=-\sqrt{2}(2Y^2+X^2), \tag{32}$$

where, in order to express the result as a GVF, the following change of variables have been used:

$$X=\frac{\dot{F}}{F}, \quad Y=\frac{1}{2\sqrt{2}}\frac{\dot{A}}{A} \tag{33}$$

in agreement with Ref. 9. The system has one critical point at $X=Y=0$ and the generating function

$$f=-\sqrt{2}X^2Y-\frac{2\sqrt{2}}{3}Y^3. \tag{34}$$

In polar coordinates, the sign of f is seen to change at $\theta=\pi/2$, and so the steady state again cannot be stable. This is confirmed by the phase plane shown in Fig. 9, where it is seen that the origin is a saddle point.

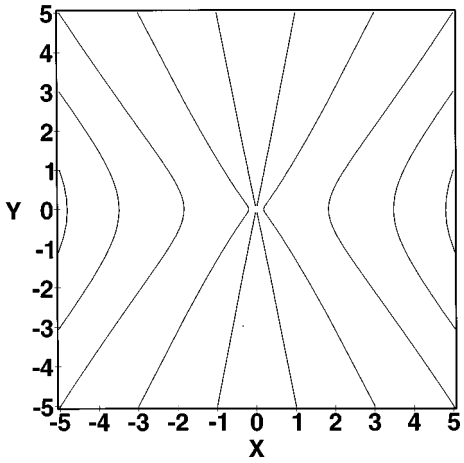

FIG. 9. The phase plane of dynamical system (32).

IV. CRITICAL POINTS AND STEADY STATES AT INFINITY

In this section we return briefly to the question of the link between the steady state function and the critical points of a GVF. Unfortunately in all the cases considered, the only critical point which occurs for finite Y and Z— namely the origin—has been shown to be unstable, and we therefore do not obtain the graph of the steady state s peaking at the critical point. This leaves the possibility of stable critical points at infinity, and in order to study these, we compactify the phase-space to a unit disk by defining new coordinates:

$$y \equiv \frac{Y}{\sqrt{1+Y^2+Z^2}}, \quad z \equiv \frac{Z}{\sqrt{1+Y^2+Z^2}}. \tag{35}$$

This transformation also has the useful property that it maps the straight lines $Y=mZ$ to the lines $y=mz$. The dynamical system in terms of y and z is no longer a GVF, however the transformation (35) does not destroy the nature of the critical points of the GVF for Y and Z.

We shall apply this technique to case I of the dynamical systems studied since, in addition to the bulk viscosity, it contains a nonzero cosmological constant. According to the cosmic no-hair conjecture, a cosmological model with a (positive) cosmological constant which does not recollapse and whose energy-momentum tensor obeys the energy conditions should tend towards de-Sitter space. However, a model with bulk viscosity can have $p<0$, and so the energy conditions do not in general hold, but it is instructive to study the phase plane at infinity for general ζ and see whether we recover de-Sitter space as a stable critical point in the limit $\zeta \to 0$.

de-Sitter space is characterized by having a scale factor which obeys $\dot{R}/R=\sqrt{\Lambda/3}$. On following through the various transformations from R and $\dot{R}$ to X, Y, and Z, it is remarkable that in terms of Y and Z, de-Sitter space corresponds to the line $Y=Z$ and by the properties of the transformation between $\{Y,Z\}$ and $\{y,z\}$, de-Sitter space corresponds to the line $y=z$. If the cosmic no-hair conjecture holds in this case, all models (which do not recollapse) should therefore tend to this line.

In terms of y and z the dynamical system (9) becomes

$$\dot{y} = \frac{3}{2}\,\zeta y(1-y^2) + D\sqrt{\frac{\Lambda}{3}}\,(1-2y^2)z, \quad \dot{z} = y\left(D\sqrt{\frac{\Lambda}{3}} - 2D\sqrt{\frac{\Lambda}{3}}\,z^2 - \frac{3}{2}\,\zeta yz \right). \tag{36}$$

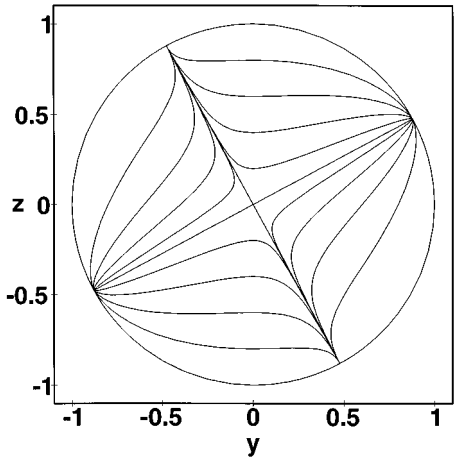

FIG. 10. The compact phase plane of dynamical system (36).

The critical points of this system occur at $y=z=0$ and at the two points

$$y=\frac{2}{3\zeta}\sqrt{\frac{\Lambda}{3}}\left(\frac{1}{z}-2z\right), \quad z^2=\frac{1}{2}+\frac{3\sqrt{3}\zeta}{2}\sqrt{16D^2\Lambda+27\zeta^2}, \tag{37}$$

which, as expected, do not correspond to de-Sitter space. Now in the limit $\zeta\to 0$, for which $z\to\pm\sqrt{\frac{1}{2}}$, both the numerator and denominator of y in Eq. (37) tend to zero. Hence to study the case with zero bulk viscosity we need to set $\zeta=0$ in Eq. (36) and determine the critical points anew. On performing the algebra we find the critical points at infinity are $y=z=\pm(1/\sqrt{2})$ and indeed correspond to the end state (with infinite scale factor) of de-Sitter space.

Finally, since we expect de-Sitter space to represent a stable critical point, we plot the compactified phase plane for $\zeta=1$, $D=2$, and $\Lambda=1$ and the steady state function s for Eq. (23) in terms of the compactified variables as Figs. 10 and 11, respectively. We see that the graph of s peaks at the stable critical points of the dynamical system.

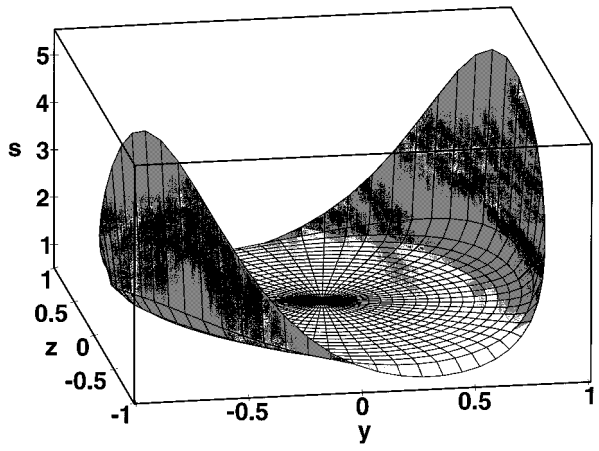

FIG. 11. The steady state function s for the generating function (23) plotted in terms of the compactified variables y and z.

V. CONCLUDING REMARKS

We have considered examples of two-dimensional reductions of Einstein's equations which are expressible as dissipative GVFs, with the aid of nonlinear transformations. The set of reductions of Einstein's equations so expressible are of interest as their ω-limit sets solely consist of critical points. In addition they allow the steady states of their corresponding Fokker–Planck equations to be readily found analytically. This is especially important in view of the fact that almost all the known exact reductions of Einstein field equations are fragile with respect to plausible physical perturbations. The steady states of the Fokker–Planck equations in these cases essentially define noisy neighborhoods of the original attractors which are structurally stable.[6] As a result such steady states are of importance for those features of the universe which are dissipative, as they give likelihood estimates for various features of the universe around such attractors, which are structurally stable. Furthermore, the presence of such steady states could be of relevance in ultimately resolving the question of natural measure on the initial state of the classical Universe—with quantum fluctuations acting as noise. Also, the set of reductions of Einstein's equations expressible as GVFs are important in connection with the applications of catastrophy theory to cosmology.

In the two-dimensional cases considered here the critical points which do not lie at infinity turn out not to be stable. In the majority of cases, the critical point is a saddle, resulting in decaying and exponentially expanding directions for the function s, corresponding dynamically to the directions of the stable and unstable manifolds. In this way the behavior of s is compatible with the dynamics of a distribution of initial states.

It has also been shown that the stable fixed points at infinity, and the form of the steady state function s in the neighborhood of these fixed points, can be examined by a careful compactification of the phase plane. In this case, s remains bounded in all directions, indicating the attracting nature of the fixed points in all directions.

It is also interesting to note that systems of coordinates which produce a GVF are not unique. This begs the question as to whether or not there might be an invariant property of the geometry of a space-time which defines whether or not it is possible to find a GVF that describes a cosmology. There are certainly cases (the most general case above with shear, curvature, and a cosmological constant, for example) which defeated our attempts to find a description in terms of a GVF. Perhaps a solution to this question might be found by the techniques used in Cartan's equivalence problem.[22]

The consideration of cosmological models expressible as GVFs is a first step in the application of Zeeman's notion of ϵ-stability to cosmology. The study of models not so expressible would involve extensive numerical calculations to which we hope to return in the future.

ACKNOWLEDGMENTS

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The Dirac equation in the Robertson–Walker space–time

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The Dirac equation is considered, via the Newman–Penrose formalism, in the context of the Robertson–Walker geometry. The solution of the equation, which contrary to the neutrino case is not directly separable, is reduced to the study of decoupled spatial and temporal equations. The spatial equations are explicitly integrated and show the existence of discrete energy levels in case of closed universe. Besides the neutrino, the time equation is discussed in limiting situations of the standard cosmology. © *1996 American Institute of Physics.* [S0022-2488(96)02701-4]

I. INTRODUCTION

In this paper we determine the solution of the Dirac wave equation in the curved space–time given by the Robertson–Walker metric. The formulation of the equation is done by the spinorial formalism of Newman and Penrose,[1] an account of which can be found in the books by Penrose and Rindler[2] and by Chandrasekhar.[3] Besides the physical interest, this study is motivated also by the fact that the Dirac equation is not directly separable as it happens in the massless case or in the context of the Kerr geometry.[4–6]

For what concerns the solution of the Dirac equation, the separation of the angular part is performed in a standard way[3] obtaining the Teukolsky-like equation for spin $\frac{1}{2}$ field admitting explicit solution.[7] The surviving coupled equations in the r,t variables which are not separable are treated by expressing the unknown wave function in terms of a known particular solution. This enables us to separate the r and t dependence in such a way that the resulting r-equation is independent of the mass of the particle. The price to be paid is, however, the fact that the final resulting t-equation comes out to be of second order. The possible values of the constant K^2 relative to the r,t separation, which are interpreted as giving the energy spectrum of the particle, are determined by the study of the radial equations corresponding in the case of a flat, closed and open universe. In each case the solutions of the equations are explicitly found. The set of values of K^2 reduces to a discrete set in the closed universe case.

The time equation, which depends explicitly on the dynamics of the underlying cosmological model, is discussed in connection with limiting situations of the standard cosmology. The present treatment covers the results relative to the neutrino case previously considered only in a special case.

II. THE DIRAC EQUATION

It is well known that the Dirac equation can be written in general relativity in terms of covariant derivatives and generalized Pauli matrices. In the context of the Newman–Penrose formalism the Dirac equation can be further expressed in terms of directional derivatives and spin coefficients (we will refer to Chandrasekhar's book[3] for notations, mathematical conventions, and development of the formalism).

Here we study the problem in the case of the Robertson–Walker space–time of metric

$$ds^2=dt^2-R^2(t)\left[\frac{dr^2}{1-ar^2}+r^2(d\theta^2+\sin^2\theta\, d\phi^2)\right] \quad (a=0,\pm 1). \tag{1}$$

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We choose the null-tetrad frame $\{l^i, n^i, m^i, m^{\star i}\}$ whose associated directional derivatives are given by

$$
\begin{aligned}
D &= l^i \partial_i = \frac{1}{\sqrt{2}} [\partial_t + R^{-1}\sqrt{1-ar^2}\,\partial_r], \\
\Delta &= n^i \partial_i = \frac{1}{\sqrt{2}} [\partial_t - R^{-1}\sqrt{1-ar^2}\,\partial_r], \\
\delta &= m^i \partial_i = \frac{1}{\sqrt{2} r R} [\partial_\theta + i \csc\theta \partial_\phi], \\
\delta^\star &= m^{\star i} \partial_i = \frac{1}{\sqrt{2} r R} [\partial_\theta - i \csc\theta \partial_\phi],
\end{aligned}
\tag{2}
$$

and whose corresponding nonzero spin coefficient are given by[7]

$$
\begin{aligned}
&\rho = -\frac{1}{\sqrt{2} r R}(r\dot{R} + \sqrt{1-ar^2}), \quad \beta = -\alpha = \frac{\cot\theta}{2\sqrt{2} r R}, \\
&\mu = \frac{1}{\sqrt{2} r R}(r\dot{R} - \sqrt{1-ar^2}), \quad \epsilon = -\gamma = \frac{R}{2\sqrt{2} R}.
\end{aligned}
\tag{3}
$$

The Dirac equations in the Newman–Penrose formalism are then[3]

$$
\begin{aligned}
&(D + \epsilon - \rho) F_1 + (\delta^\star - \alpha) F_2 = i \mu_\star G_1, \\
&(\Delta + \mu - \gamma) F_2 + (\delta - \alpha) F_1 = i \mu_\star G_2, \\
&(D + \epsilon - \rho) G_2 - (\delta - \alpha) G_1 = i \mu_\star F_2, \\
&(\Delta + \mu - \gamma) G_1 - (\delta^\star - \alpha) G_2 = i \mu_\star F_1,
\end{aligned}
\tag{4}
$$

where $\mu_\star \sqrt{2}$ is the mass of the particle. Owing to the special dependence of the directional derivatives and of the spin rotation coefficients on the variable ϕ, the ϕ dependence of the wave function can be assumed to be given by the usual factor $e^{im\phi}$ ($m = 0, \pm 1, \pm 2, \pm 3, \ldots$). With this assumption the Dirac equations become

$$
\begin{aligned}
&\sqrt{2} r R (D + \epsilon - \rho) F_1 + L^- F_2 = i \mu_\star r R G_1 \sqrt{2}, \\
&\sqrt{2} r R (\Delta + \mu + \epsilon) F_2 + L^+ F_1 = i \mu_\star r R G_2 \sqrt{2}, \\
&\sqrt{2} r R (D + \epsilon - \rho) G_2 - L^+ G_1 = i \mu_\star r R F_2 \sqrt{2}, \\
&\sqrt{2} r R (\Delta + \mu + \epsilon) G_1 - L^- G_2 = i \mu_\star r R F_1 \sqrt{2},
\end{aligned}
\tag{5}
$$

where it has been set $L^\pm = \partial_\theta \mp m \csc\theta + (1/2)\cot\theta$, the wave function depending now on the variables r, θ, t. Also, the θ dependence can be separated by setting

$$rR(t)F_1=H_1(r,t)S_1(\theta), \quad rR(t)F_2=H_2(r,t)S_2(\theta),$$
$$rR(t)G_1=H_2(r,t)S_1(\theta), \quad rR(t)G_2=H_1(r,t)S_2(\theta), \tag{6}$$

thus obtaining from Eqs. (5) the Teukolsky-like equations for spin $\frac{1}{2}$ field[3,4]

$$L^-S_2=-\lambda S_1, \quad L^+S_1=\lambda S_2, \tag{7}$$

and the equations in the r,t variables

$$DH_1+\epsilon H_1=\left(i\mu_\star-\frac{\lambda}{rR\sqrt{2}}\right)H_2, \quad \Delta H_2+\epsilon H_2=\left(i\mu_\star+\frac{\lambda}{rR\sqrt{2}}\right)H_1, \tag{8}$$

λ being the separation constant. The solution of the eigenvalue problem for S_1,S_2 that arises from Eqs. (7) gives $\lambda^2=(l+1)^2$ $(l=0,1,2,3,..)$ if $m=0$ and $\lambda^2=(l+\frac{1}{2})^2$ $(l=|m|,|m|+1,|m|+2,\ldots)$ if $|m|\geqslant 1$, the eigenfunctions S_1,S_2 being essentially the Tchebichef polynomials in the first case and the Jacobi polynomials in the second one.[7]

A straightforward inspection of the coupled equation (8) shows that the r,t dependences are not directly separable, namely that solutions of the form $H_1=R_1(r)T_1(t)$, $H_2=R_2(r)T_2(t)$ are not possible for Eq. (8) if at least $R_1\neq R_2$ or $T_1\neq T_2$. Furthermore, Eqs. (8) imply also that the wave function is subject to the constraints $H_1(0,t)=H_2(0,t)=0$.

III. SEPARATION OF TIME AND RADIAL EQUATIONS

In order to integrate Eqs. (8) we are first interested in the special solutions obtained by setting there $H^\pm=H_1=\pm H_2$. An explicit integration gives

$$H^\pm=\frac{K^\pm}{R(t)^{1/2}}\left(\frac{r}{1+\sqrt{1-ar^2}}\right)^{\mp\lambda}\exp(\pm i\sqrt{2}\mu_\star t) \quad (a=0,\pm 1), \tag{9}$$

$K^\pm$ being integration constants. Now we look for a general solution of the form

$$H_1=A(r,t)H^+, \quad H_2=B(r,t)H^+. \tag{10}$$

Since H^+ itself is a solution, Eqs. (8) imply for A,B the equations

$$DA=\left(i\mu_\star-\frac{\lambda}{rR\sqrt{2}}\right)(B-A), \quad \Delta B=-\left(i\mu_\star+\frac{\lambda}{rR\sqrt{2}}\right)(B-A). \tag{11}$$

To ease the calculation, instead of the r,t variables, we introduce now as independent variables

$$\tau=\tau(t)=\int_0^t\frac{dt}{R(t)}, \quad s=s(r)=\int_0^r\frac{dr}{\sqrt{1-ar^2}} \tag{12}$$

in terms of which the directional derivatives simplify to $D=(\partial_\tau+\partial_s)/(R\sqrt{2})$ and $\Delta=(\partial_\tau-\partial_s)/(R\sqrt{2})$. By further setting

$$2A=X(\tau,s)+Y(\tau,s), \quad 2B=X(\tau,s)-Y(\tau,s), \tag{13}$$

in Eq. (11), we obtain

$$X_\tau + Y_s = \frac{2\lambda}{r} Y, \quad Y_\tau + X_s = -2i\mu_* \sqrt{2} R Y, \tag{14}$$

from which the second-order equation for Y follows

$$Y_{\tau\tau} - Y_{ss} + 2\sqrt{2} i \mu_* R Y_\tau + 2\frac{\lambda}{r} Y_s + 2\left(\sqrt{2} i \mu_* R_\tau - \frac{\lambda r'}{r^2}\right) Y = 0 \tag{15}$$

that can be separated. Indeed if we put $Y(\tau,s) = A(s)T(\tau)$ in Eq. (15), we obtain

$$A'' - 2\frac{\lambda}{r} A' + \left(\frac{2\lambda r'}{r^2} + K^2\right) A = 0, \tag{16}$$

$$T'' + 2\sqrt{2} i \mu_* T' R + (2\sqrt{2} i \mu_* R' + K^2) T = 0, \tag{17}$$

K^2 being the separation constant. It is worth noting that Eq. (16) is independent of the mass of the particle. Once the Y solution is known, the X solution can be easily obtained from Eq. (14), which in its turn implies a wave function of the form

$$H_1(r,t) = \frac{H^+(r,t)}{2} \left\{ A(s)T(\tau) + \left[\frac{2\lambda}{r} A(s) - A'(s)\right] \int_0^\tau T d\tau + X(0,s) \right\}. \tag{18}$$

An analogous result holds for H_2. If, instead of (10), we assume $H_1 = AH^-$, $H_2 = BH^-$ we obtain the above equations with the substitutions $X \leftrightarrow Y$.

IV. RADIAL EQUATIONS

We discuss Eq. (16) separately according to the different values 0, $\pm\frac{1}{2}$ of a.

Case a=0: Equation (12) gives $r = s$. If we put $x = 2iKr$, $A = x^{2\lambda} e^{-\frac{1}{2}x} v(x)$ in Eq. (16), we find that v satisfies the confluent hypergeometric equation:

$$x v'' + (2\lambda - x) v' - \lambda v = 0, \tag{19}$$

whose solution[8] that is acceptable in $r = 0$ is $v = \Phi(\lambda; 2\lambda; x)$

Case a=1: From Eq. (12) we have $r = \sin s$. By setting $2x - 1 = \cos s$ and $A = [x(1-x)]^{1/2} f(x)$ in Eq. (16) we find for f the hypergeometric equation

$$x(1-x) f'' + (\tfrac{3}{2} + \lambda - 3x) f' + (K^2 - 1) f = 0, \tag{20}$$

whose acceptable solution (namely the one generating an H_1 solution which vanishes for $r = 0$) is

$$f(x) = (1-x)^{\lambda - 1/2} F(\lambda + \tfrac{1}{2} + K, \lambda + \tfrac{1}{2} - K; \lambda + \tfrac{1}{2}; 1 - x). \tag{21}$$

As a consequence of Eq. (16) we have that $A(s)$ is subject also to the constraint $A(\pi/2) = 0$. Therefore the solution (21) must be such that $f(\frac{1}{2}) = 0$ or

$$F(\lambda + \tfrac{1}{2} + K, \lambda + \tfrac{1}{2} - K; \lambda + \tfrac{1}{2}; \tfrac{1}{2}) = 0, \tag{22}$$

a condition which implies the existence of discrete values of K^2. A class of solutions of Eq. (22) is given by

$$K = K_n = 2n + \tfrac{1}{2} + \lambda, \quad (n = 0,1,2,3,\ldots). \tag{23}$$

Indeed, apart from a positive numerical factor, we have $F(-2n,2\lambda+1+2n;\lambda+\frac{1}{2};\frac{1}{2}) \equiv P_{2n}^{(\alpha,\alpha+1)}(0)$, $(\alpha=\lambda-\frac{1}{2})$. However, $P_{2n}^{(\alpha,\alpha+1)}(0)=bP_{2n+1}^{(\alpha,\alpha)}(0)+b'P_{2n-1}^{(\alpha,\alpha)}(0)=0$ by using the recurrence relations and the relation $P_n^{(\alpha,\beta)}(x)=(-1)^n P_n^{(\beta,\alpha)}(-x)$ for Jacobi's polynomials.[8]

Case $a=-1$*:* We have from Eq. (12) $r=\sinh s$. By setting $2x-1=\cosh s$ and $A(x)=(x(x-1))^{1/2}f(x)$ in Eq. (16) one obtains for f exactly Eq. (20) with the substitution $k\to ik$. Therefore the acceptable f is here $f=(1-x)^{\lambda-1/2}F(\lambda+\frac{1}{2}+iK,\lambda+\frac{1}{2}-iK;\lambda+\frac{1}{2};1-x)$.

V. TIME EVOLUTION AND INTERPRETATION

We first consider the neutrino case. By setting $\mu_*=0$, Eq. (17) becomes

$$T''+K^2T=0 \tag{24}$$

and its solution together with a suitable choice of $X(0,s)$ in Eq. (18) implies a time dependence of the H_1 wave function through the factor

$$R^{-1/2}\exp\left[\pm iK\int_0^t \frac{dt}{R}\right], \tag{25}$$

which apart from the present double sign is one of the neutrino cases previously studied.[7]

Therefore we interpret K^2 to represent the the energy of the neutrino because in Ref. 7 K^2 was the energy eigenvalue of the Scrhödinger equation to which the massless Dirac equation was reduced by means of the Chandrasekhar method. In general, both for massless and massive particles, we interpret K^2 as the gravitational interaction energy that is independent of the mass of the particle as a consequence of Eq. (16). By taking into account the result (23) there follows that in the case of a closed universe the energy of the particle contains a discrete spectrum. However, a numerical evaluation of these energy levels gives results that are beyond the present experimental sensitivity both for the neutrino as well for the electron.[7]

Besides the neutrino case, Eq. (17) can be solved, in principle, by giving an explicit $R(t)$ function representing the dynamics of the cosmological background.

An explicit analytical solution of Eq. (17) is not easy in general nor in the standard cosmology. Therefore we will consider Eq. (17) in some special physical situations all relative to the standard cosmology.

(a) Suppose $R(t)$ is given by the solution of the Friedmann–Einstein equation of the standard Cosmology relative to the case of a closed $(a=1)$ dominated matter universe with arbitrary $\Omega_0>1$, Ω_0 being the ratio of the energy density to the critical density today. In this case the scale factor $R(t)$ increases from 0 at $t=0$ to its maximum $R=R(t_{\max})$ and then collapses to zero at time $t=2t_{\max}$.[9] In correspondence of time intervals $t-t_{\max}$ small on cosmological scale, but great on microscopical level, we can assume $R'(\tau)=\dot{R}(t)R(t)\cong 0$, $R(t)\cong R$.

Under this assumption, Eq. (17) gives

$$T(t)\propto\exp[it(-\mu_*\sqrt{2}\pm\sqrt{2\mu_*^2+(k/R)^2})]. \tag{26}$$

(b) Another situation of interest is the one relative to the open $(a=-1)$ dominated matter Universe with $\Omega_0<1$ of the standard cosmology for time intervals relative to very large time t so that one can assume[9]

$$R(t)\cong R_0H_0t\cong R_0H_0e^{R_0H_0\tau}. \tag{27}$$

Therefore the asymptotic behavior of the solutions of Eq. (17) is given by $T(\tau)\cong\exp(-H_0R_0\tau)\cong t^{-1}$ and for $t\gg 1$ the H_1 time dependence is of the form [see Eqs. (9) and (18)]

$$t^{-1/2}e^{i\sqrt{2}\mu_* t}. \tag{28}$$

(c) Consider now the case of a cosmological model with $a=0$ and comparable contributions to the energy density from both matter and radiation. For large t, $R\sim t^{2/3}$ hence $R\sim\tau^2$ so that the asymptotic behavior of the solutions of Eq. (17) are now approximated by $T\sim\tau^{-2}\sim t^{-2/3}$ so that H_1 has the time dependence

$$t^{-1/3}e^{i\sqrt{2}\mu_* t}. \tag{29}$$

(d) Finally, consider the model of the points (a) and (b) for small t. We have $R\sim t^{2/3}\sim\tau^2$ for $a=\pm 1$.[9] The solutions of Eq. (17) are then approximated for small t by the solutions of Eq. (24) which imply now, for small t, the H_1 time behaviour

$$t^{-1/3}\exp(i\sqrt{2}t)\mu_*. \tag{30}$$

The fact that in the previous cases the t dependence of H_1 factors out is a consequence of the approximation done, while it is a general property for the neutrino case which is completely separable.[7]

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Geometrical aspect of topologically twisted two-dimensional conformal superalgebra

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We study the topologically twisted osp(2|2)⊕osp(2|2) conformal superalgebra. The algebra includes the Lagrangians which are intrinsic to the topological field theory and composed of fermionic generators. Studying the Lagrangians through a gauge system of osp(2|2)⊕osp(2|2), geometrical features inherent in the algebra are revealed: a moduli space associated with the algebra is derived and the crucial roles which the fermionic generators play in the moduli space are clarified. It is argued that there exists a specific relation between the topological twist and the moduli problem through a geometrical aspect of the algebra. © *1996 American Institute of Physics.* [S0022-2488(96)01702-4]

I. INTRODUCTION

In the recent progress of the quantum field theory (QFT), the detection of the cohomological field theory may be most the fascinating development. The theory is a kind of the topological QFT which deals with topological invariants, and has been pioneered by E. Witten.[1] We refer to the cohomological field theory as TFT in the present paper and will focus on it. The theory has some characteristic properties on the construction and has distinct framework. Therefore, many energetic researches in TFT have been done[2] and then TFT has been proved to be a real solid methodology in QFT. A few substantial problems associated with TFT still remain to be solved, however, for example, about the topological twist. In the conformal field theory (CFT), the topological twist of $N=2$ CFT is performed through a redefinition of the energy–momentum tensor of $N=2$ theory,[3] which generates the bosonic CFT models of vanishing central charge with hidden fermionic (topological) symmetry. In relation to the topological twisting mechanism, the different twistings of the same model yield the different moduli problems, respectively, which are related through the mirror symmetry[4] as the explicit example of twisting in general. For another example, the topological gauged WZW models[5] are composed of two different gauge fixing procedures from the same bosonic model, not necessarily twisting of the $N=2$ supersymmetry[6] of the Kazama–Suzuki model,[7] and in this case there surely exists the mirror symmetry.

There are two typical stand points for constructing TFT, i.e., topological twisting and BRST gauge fixing. Both approaches result in the so-called moduli problem.[8,9] In either case, the remarkable characteristic is that the Lagrangian is described as $\mathscr{L}=\{\mathscr{Q},\star\}$, where $\mathscr{Q}$ is the fermionic operator of nilpotency, i.e., the so-called topological symmetry. In terms of the ordinary QFT words, $\mathscr{L}$ is just composed of the BRST gauge fixing and the FP ghost terms, and the $\mathscr{Q}$ corresponds to the BRST operator. Because of the BRST-exact form of $\mathscr{L}$, every correlation function is independent of the coupling factor as a consequence of which the leading contribution to the path-integral is only the classical configuration of the fields, i.e., zero mode. This zero mode configuration is associated with some moduli space. In the BRST approach, the relation between the moduli problem and TFT may be comparatively clear owing to the intrinsic constructing procedure where some moduli problem can be settled as the gauge fixing condition. In the topological twisting formalism, the above relation is not much clearer, on the contrary. It seems that there has not been a common recognition on what the topological twist is really doing.

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In the present paper, we concentrate on $N=2$ finite-dimensional superalgebra in two dimensions, perform the topological twist on such a superalgebra, and show a characteristic property associated with the topological twist by discussing the twisted superalgebra, i.e., the so-called topological algebra, through a gauge system. First, a geometrical feature inherent in the algebra is revealed, and then it is argued that there exists a specific relation between the topological twist and the moduli problem through a geometrical aspect of the algebra.

In the next section, we decide on $\mathrm{osp}(2|2)\oplus\mathrm{osp}(2|2)$ as $N=2$ finite-dimensional superalgebra and perform the topological twist on $\mathrm{osp}(2|2)\oplus\mathrm{osp}(2|2)$, so that topological algebra is obtained. In Sec. III, three types of the TFT's Lagrangian are found in the topological algebra. One of the three types of Lagrangian is focused on, and the field configuration is investigated in the case of zero-limit of the coupling factor on the path-integral by considering a gauge system. It is shown that this configuration is indeed a moduli space of flat connections associated with the topological algebra, and this fact originates from vanishing Noether current. In Sec. IV, a geometrical aspect of the fermionic charges is discussed. Under the weak coupling limit, the total Lagrangian which is a linear combination of the three Lagrangians is regarded as the Laplacian operator on the moduli space, and the fermionic charges as Fredholm operators. Taking account of these facts, the moduli space which is obtained formally in Sec. III is made more visual. It is also shown that the index of these operators could be derived if proper support in the moduli space can be defined. Lastly, in Sec. IV, we discuss the triviality of the path-integral and obtain a nontrivial TFT's observable. The facts will support the argument developed in the present paper. In the final section, it is claimed that the algebra has a specific relation with the moduli problem and the same remark about the vanishing Noether current which plays a crucial role in the following discussions is mentioned.

II. PROCEDURE OF TOPOLOGICAL TWIST

A. $\mathrm{osp}(2|2)\oplus\mathrm{osp}(2|2)$ algebra

The first issue is the specification of $N=2$ finite-dimensional superalgebra in two dimensions on which the topological twist will be performed. The topological twist usually means the mixing of the representation space of the internal symmetry group of the supersymmetry with that of the symmetry group with respect to the space–time, i.e., spinor space. On manifolds, the latter symmetry is local. Consequently, the former symmetry must also be local. The situation is allowed in the case of the conformal supersymmetry alone. On the contrary, the other types of the super-extended algebra, that is, super-Poincaré or super-(anti-)de-Sitter, must not be adapted for the present case because it is not possible to deal with its internal symmetry as a purely geometrical object in contrast to the conformal case. In the first place, the topologically twisted super-Poincaré algebra is incomplete from the geometrical view point.[10,11]

What we are next interested in is the finite-dimensional conformal superalgebras. The finite-dimensional simple Lie superalgebras are fully investigated[12] and all the finite-dimensional conformal superalgebras in two dimensions are shown.[13] The four-types of all the algebras must be eliminated from the physical view point; s_2, $\mathrm{osp}(2,1|N)$, $\mathrm{su}(1,1|1,1)$, and $\mathrm{d}(1,2;\alpha)$.[13] The four-types are unsuitable also for the present case, either because there exists no anticommutator of the supercharges or because the supersymmetry is in the representations of integer spin. We will soon understand the reason why in the forthcoming contexts. After all, the possible finite-dimensional conformal superalgebras in two dimensions are then $\mathrm{osp}(N|2)$ $(N\geqslant 0)$, $\mathrm{su}(N|1,1)$ $(N\geqslant 2)$, f_4, and g_3. Moreover, it is the $N=2$ case that we are interested in. In this case, the remaining card is $\mathrm{osp}(2|2)$ alone. Therefore, $\mathrm{osp}(2|2)$ is the unique solution for performing the topological twist on finite-dimensional $N=2$ superalgebra in two dimensions.

The internal symmetry group of $\mathrm{Osp}(2|2)\otimes\mathrm{Osp}(2|2)$ in relation to (2,2) supersymmetry is $\mathrm{SO}(2)\otimes\mathrm{SO}(2)$, and $\mathrm{Osp}(2|2)$ is required to be compact so that its Cartan–Killing form is positive definite, while the super Lie group $\mathrm{Osp}(2|2)$ is generally not compact. $\mathrm{osp}(2|2)\oplus\mathrm{osp}(2|2)$ conformal superalgebra on which the twisting operation will be made to form a corresponding topologi-

cal algebra is then confined to the two-dimensional Lorentzian manifold with the local Lorentz metric in the light-cone coordinates: $g^{z\bar{z}}=g^{\bar{z}z}=-2, g_{z\bar{z}}=g_{\bar{z}z}=-\frac{1}{2}$, and $g^{zz}=g^{\bar{z}\bar{z}}=g_{zz}=g_{\bar{z}\bar{z}}=0$. This (2,2) superalgebra contains two types of complex Weyl spinorial charges Q, $\bar{Q}$; S, $\bar{S}$, where "$-$" means the Dirac conjugation $\bar{Q}=Q^{\dagger}\gamma^0$ in which $\gamma^0=i\sigma^2$ and incidentally $\gamma^1=\sigma^1$, $\gamma^5=-\gamma^0\gamma^1=\sigma^3$, or equivalently $\gamma^z=\gamma^0+\gamma^1$, $\gamma^{\bar{z}}=\gamma^0-\gamma^1$ in the light-cone coordinates. These supercharges are two component spinors, for example $Q=(Q_+,Q_-)^t$, where "$+,-$" mean spinor indices describing "left" and "right" moving, respectively, with respect to the local Lorentz coordinates $(z,\bar{z})$. These indices are raised and lowered by a metric in spinor space given by the charge conjugation matrix $C=\gamma^0$: $\eta^{+-}=\eta_{-+}=-1$, $\eta^{-+}=\eta_{+-}=1$, and $\eta^{++}=\eta^{--}=\eta_{++}=\eta_{--}=0$.

We can leave out the conjugate parts of the bracket bosonic relations with respect to the complex supercharges of osp(2|2)⊕osp(2|2) as follows:

$$
\begin{gathered}
[S,\ P_a]=\gamma_a Q,\quad [S,\ D]=-\tfrac{1}{2}S,\quad [S,\ M]=-\tfrac{1}{2}\gamma_5 S,\\
[Q,\ K_a]=-\gamma_a S,\quad [Q,\ D]=\tfrac{1}{2}Q,\quad [Q,\ M]=-\tfrac{1}{2}\gamma_5 Q,\\
[S,\ A]=-i\tfrac{1}{4}\gamma_5 S,\quad [S,\ V]=-i\tfrac{1}{4}S,\\
[Q,\ A]=-i\tfrac{1}{4}\gamma_5 Q,\quad [Q,\ V]=-i\tfrac{1}{4}Q.
\end{gathered}
\tag{2.1}
$$

If we want to get these conjugate parts of Eqs. (2.1), we must pay attention to the fact that the representation of the body so(2)⊕sp(2) of osp(2|2) is anti-Hermitian where the anti-Hermitian character of the representation of sp(2) actually leads to the positivity of the Cartan–Killing form of osp(2|2).

Ordinary (2,2) supersymmetry which is free from the central charges is the direct sum of (2,0) and (0,2), and the corresponding part in osp(2|2)⊕osp(2|2) reads

$$
\begin{aligned}
&\{Q_+,\bar{Q}_+\}=iP_z,\quad \{S_+,\bar{S}_+\}=-iK_z,\\
&\{Q_-,\bar{Q}_-\}=iP_{\bar{z}},\quad \{S_-,\bar{S}_-\}=-iK_{\bar{z}}.
\end{aligned}
\tag{2.2}
$$

While the super-extended conformal algebra has no central charge, there are mixing parts, instead, in the relations between the supercharges, and consequently the decomposition mentioned above does not exist. The mixing part of (2,0) and (0,2) in osp(2|2)⊕osp(2|2) is

$$
\begin{aligned}
&\{Q_+,\bar{S}_-\}=i(M-D)+2(A-V),\\
&\{Q_-,\bar{S}_+\}=i(M+D)+2(A+V),\\
&\{\bar{Q}_+,S_-\}=i(M-D)-2(A-V),\\
&\{\bar{Q}_-,S_+\}=i(M+D)-2(A+V).
\end{aligned}
\tag{2.3}
$$

The property will play an important role in the forthcoming contexts.

The bosonic generators of osp(2|2)⊕osp(2|2) are as follows: P_a, K_a, M, D, A, and V are translation, conformal-translation, Lorentz, Weyl, chiral so(2), and internal so(2), respectively. The finite two-dimensional conformal algebra composed of these bosonic generators alone is

$$[P_a, M]=\epsilon_{ab}P^b, \quad [P_a, D]=P_a, \quad [K_a, D]=-K_a,$$
$$[K_a, M]=\epsilon_{ab}K^b, \quad [K_a, P_b]=2(\epsilon_{ab}M-\delta_{ab}D), \tag{2.4}$$

where ϵ are $\epsilon^{z\bar{z}}=-\epsilon^{\bar{z}z}=-2$, $\epsilon_{z\bar{z}}=-\epsilon_{\bar{z}z}=\frac{1}{2}$, and $\epsilon^{zz}=\epsilon^{\bar{z}\bar{z}}=\epsilon_{zz}=\epsilon_{\bar{z}\bar{z}}=0$.

Lastly in the presentation of osp(2|2)⊕osp(2|2) algebra, let us comment on the naming of the generators of osp(2|2)⊕osp(2|2). In Sec. III where a pure gauge theory of osp(2|2)⊕osp(2|2) on two-dimensional manifold will be considered, the naming, for instance, P as translation, is perfectly formal. If not, the general coordinate transformations must exist in the system and then the theory may become empty as well as the ordinary 2-D conformal supergravity theories.[14]

B. Topological twist

We are now in a position to perform topological twisting of the algebra. Topological twist is usually a kind of mixing which results in identification of the representation space of internal symmetry group of $N=2$ supersymmetry with that of the local Lorentz group. It is easy to perform twisting of the algebra to get the topological algebra. Most of all what we have to do is to replace Q, $\bar{Q}$, S, and $\bar{S}$ with Q^+, Q^-, S^+, and S^-, respectively. The indices "+,−" are raised and lowered with the same metric as for the indices $\alpha;\beta$ of $C_{\alpha\beta}$ and Q_α. That is, the complex Weyl spinors $\varphi_\alpha, \bar{\varphi}_\alpha$ are substituted for $\varphi_\alpha{}^+, \varphi_\alpha{}^-$.

$$\varphi_\alpha=\frac{i}{\sqrt{2}}\,\varphi_a{}^+, \quad \bar{\varphi}_\alpha=\frac{i}{\sqrt{2}}\,\varphi_\alpha{}^-. \tag{2.5}$$

The remaining manipulations are as follows. The fermionic charges $Q^+=(Q_+{}^+, Q_-{}^+)^t$ have become ((0,0)-form, (0,1)-form), and $Q^-=(Q_+{}^-, Q_-{}^-)^t$ with ((1,0)-form, (0,0)-form), idem $S^\pm$. Then we have to modify the definitions of local Lorentz M and Weyl D generators so that the four (0,0)-form fermionic generators of supersymmetry have no charge with respect to these two bosonic generators. We have put the representation space accompanied with the internal symmetry group SO(2)⊗SO(2) upon the space of spinor. The modified M, D generators must be direct sums with so(2)⊕so(2) generators V and A, respectively. The solution to this constraint resolves into

$$\tilde{M}=M+2iV, \quad \tilde{D}=D+2iA. \tag{2.6}$$

These modified generators then satisfy the following relations:

$$[\Delta_\pm{}^\pm, \tilde{M}]=0, \quad [\Delta_\pm{}^\pm, \tilde{D}]=0, \tag{2.7}$$

where Δ means both Q and S.

There appear some problems about the closure of the modified algebra, however. The generators A and V have been put upon D and M, respectively, and the modified algebra which contains $\tilde{M}$ and $\tilde{D}$ must not contain A and V. In fact, the modified algebra contains subtle relations:

$$\{Q_-{}^+, S_+{}^-\}=i(\tilde{M}+\tilde{D})-4i(A+V),$$
$$\{Q_+{}^-, S_-{}^+\}=i(\tilde{M}-\tilde{D})+4i(A-V). \tag{2.8}$$

We can avoid the above relations (2.8) as in the following. Here it is necessary to omit another generator with regard to Eqs. (2.8), if this modified algebra still obeys the closure property for the generators of the gauge symmetry. In this point of view, the four fermionic generators $Q_+{}^-$, $Q_-{}^+$, $S_+{}^-$, and $S_-{}^+$ do not induce the gauge transformations generated by both $i(\tilde{M}+\tilde{D})-4i(A+V)$ and $i(\tilde{M}-\tilde{D})+4i(A-V)$. There are two alternatives, that is, the case in which the left chiral charges $Q_+{}^-$, $S_+{}^-$, P_z, and K_z vanish, or the case in which the right chiral charges $Q_-{}^+$, $S_-{}^+$,

P_z^-, and K_z^- vanish, without any compensation procedure, that is, all gauge fields and parameters of these four generators are assured to vanish. The second case is adapted here. In Sec. IV, it will be shown that a moduli space derived from either case is reduced to that associated with an intersection part of both cases.

The twisting procedure is explained in terms of the gauge fields of the corresponding symmetry osp(2|2)⊕osp(2|2). Let us introduce the gauge field **a**, which is Lie superalgebra-valued one-form of osp(2|2)⊕osp(2|2) in the form

$$\mathbf{a}_\mu = e^a_\mu P_a + f^a_\mu K_a + \omega_\mu M + b_\mu D + a_\mu A + v_\mu V + \bar{\psi}_\mu Q + \bar{Q}\psi_\mu + \bar{\phi}_\mu S + \bar{S}\phi_\mu , \tag{2.9}$$

as well as transformation parameter τ defined by

$$\tau = \xi^a_P P_a + \xi^a_K K_a + \lambda_l M + \lambda_d D + \theta_a A + \theta_v V + \bar{\varepsilon} Q + \bar{Q}\varepsilon + \bar{\kappa} S + \bar{S}\kappa . \tag{2.10}$$

Using the gauge fields and parameters, the above-mentioned topological twist and additional manipulations can be described as follows: Eqs. (2.6) mean

$$v_\mu = 2i\omega_\mu , \quad a_\mu = 2ib_\mu , \tag{2.11}$$

and elimination of the generators $Q_-{}^+$, $S_-{}^+$, P_z^-, and K_z^- means

$$\begin{gathered} \phi_{\mu+}{}^- = 0 = \psi_{\mu+}{}^- , \quad \kappa_+{}^- = 0 = \varepsilon_+{}^- , \\ e^{\bar{z}}_\mu = 0 = f^{\bar{z}}_\mu , \quad \xi^{\bar{z}}_P = 0 = \xi^{\bar{z}}_K . \end{gathered} \tag{2.12}$$

Under the conditions we are led to

$$\delta\phi_{\mu+}{}^+ \sim \delta\phi_{\mu-}{}^- , \quad \delta\psi_{\mu+}{}^+ \sim \delta\psi_{\mu-}{}^- . \tag{2.13}$$

Accordingly, we have the following identifications:

$$\begin{gathered} \psi_{\mu+}{}^+ = -\psi_{\mu-}{}^- \equiv -\psi_\mu , \quad \phi_{\mu+}{}^+ = -\phi_{\mu-}{}^- \equiv -\phi_\mu , \\ \varepsilon_+{}^+ = -\varepsilon_-{}^- \equiv -\varepsilon , \quad \kappa_+{}^+ = -\kappa_-{}^- \equiv -\kappa , \end{gathered} \tag{2.14}$$

which read without loss of generality

$$Q \equiv Q_+{}^+ + Q_-{}^- , \quad S \equiv S_+{}^+ + S_-{}^- . \tag{2.15}$$

Taking into account all these additional conditions with respect to the topological twist on the original osp(2|2)⊕osp(2|2), we get the gauge connection **a**,

$$\dot{\mathbf{a}}_\mu = e^z_\mu P_z + f^z_\mu K_z + \omega_\mu \tilde{M} + b_\mu \tilde{D} - \tfrac{1}{2}(Q_+{}^- \psi_{\mu-}{}^+ + S_+{}^- \phi_{\mu-}{}^+ + \psi_\mu Q + \phi_\mu S), \tag{2.16}$$

and transformation parameter τ,

$$\tau = \xi^z_P P_z + \xi^z_K K_z + \lambda_l \tilde{M} + \lambda_d \tilde{D} - \tfrac{1}{2}(Q_+{}^- \varepsilon_-{}^+ + S_+{}^- \kappa_-{}^+ + \varepsilon Q + \kappa S), \tag{2.17}$$

respectively.

After all, the generators in Eqs. (2.16) and (2.17) obey the following relations:

$$[S,\ P_z] = Q_+{}^- , \quad [Q_+{}^-,\ \tilde{D}] = Q_+{}^- , \quad [Q_+{}^-,\ \tilde{M}] = -Q_+{}^- ,$$

$$[Q,\ K_z] = -S_+{}^- , \quad [S_+{}^-,\ \tilde{D}] = -S_+{}^- , \quad [S_+{}^-,\ \tilde{M}] = -S_+{}^- ,$$

$$\{Q,Q_+{}^-\}=-2iP_z,\quad \{S,S_+{}^-\}=2iK_z,\quad \{Q,S\}=-4i\tilde{M},$$
$$[P_z,\ \tilde{M}]=-P_z,\quad [P_z,\ \tilde{D}]=P_z,$$
$$[K_z,\ \tilde{M}]=-K_z,\quad [K_z,\ \tilde{D}]=-K_z, \tag{2.18}$$

and the gauge connections (2.16) satisfy the following transformation rules:

$$\begin{aligned}
&\delta\psi_\mu=\partial_\mu\varepsilon,\\
&\delta\phi_\mu=\partial_\mu\kappa,\\
&\delta\psi_{\mu-}{}^+=\mathscr{D}_\mu\varepsilon_-{}^+ +\xi_P^z\phi_\mu+(\lambda_l-\lambda_d)\psi_{\mu-}{}^+-e_\mu^z\kappa,\\
&\delta\phi_{\mu-}{}^+=\mathscr{D}_\mu\kappa_-{}^+ -\xi_K^z\psi_\mu+(\lambda_l+\lambda_d)\phi_{\mu-}{}^+ +f_\mu^z\varepsilon,\\
&\delta e_\mu^z=\mathscr{D}_\mu\xi_P^z+(\lambda_l-\lambda_d)e_\mu^z-\frac{i}{4}(\varepsilon\psi_{\mu-}{}^+-\psi_\mu\varepsilon_-{}^+),\\
&\delta f_\mu^z=\mathscr{D}_\mu\xi_K^z+(\lambda_l+\lambda_d)f_\mu^z+\frac{i}{4}(\kappa\phi_{\mu-}{}^+-\phi_\mu\kappa_-{}^+),\\
&\delta\omega_\mu=\partial_\mu\lambda_l+\frac{i}{4}(\kappa\psi_\mu-\varepsilon\phi_\mu),\\
&\delta b_\mu=\partial_\mu\lambda_d,
\end{aligned} \tag{2.19}$$

where

$$\begin{aligned}
&\mathscr{D}_\mu\varepsilon_-{}^+=(\partial_\mu-\omega_\mu+b_\mu)\varepsilon_-{}^+,\quad \mathscr{D}_\mu\kappa_-{}^+=(\partial_\mu-\omega_\mu-b_\mu)\kappa_-{}^+,\\
&\mathscr{D}_\mu\xi_P^z=(\partial_\mu-\omega_\mu+b_\mu)\xi_P^z,\quad \mathscr{D}_\mu\xi_K^z=(\partial_\mu-\omega_\mu-b_\mu)\xi_K^z.
\end{aligned} \tag{2.20}$$

The field strengths in relation to the discarded right chiral charges $Q_-{}^+$, $S_-{}^+$, $P_{\bar{z}}$, and $K_{\bar{z}}$ all vanish as expected. The resultant algebra (2.18) can be referred to as the topological algebra.[10]

SO(2)⊗SO(2) symmetry still remains as global internal symmetry whose charge is the so-called ghost number, the generators of which are defined by $G\equiv 2i(A-V)$, $\tilde{G}\equiv 2i(A+V)$. Here G and $\tilde{G}$ satisfy the following relations:

$$\begin{aligned}
&[G,\ Q_+{}^+]=Q_+{}^+,\quad [G,S_+{}^+]=-S_+{}^+,\\
&[G,Q_+{}^-]=-Q_+{}^-,\quad [\tilde{G},S_+{}^-]=S_+{}^-,\\
&[\tilde{G},Q_-{}^-]=Q_-{}^-,\quad [\tilde{G},S_-{}^-]=-S_-{}^-,
\end{aligned} \tag{2.21}$$

where the other combinations are trivial. As a consequence of Eqs. (2.21), indeed, it is natural to regard these generators G, $\tilde{G}$ as the ghost number operators. Here $Q_\pm{}^\pm$ and $S_+{}^-$ increase the ghost number by one unit, while $Q_+{}^-$ and $S_\pm{}^\pm$ decrease it by the same quantity. The assignment is consistent with the relations (2.18) and (2.19).

In preparation for the forthcoming contexts, next the description of the coordinate indices in the relations (2.18) must be simplified. First of all, the local Lorentz coordinates are substituted for spinor indices of the supercharges as follows:

$$Q_+{}^- = 2Q_z, \quad S_+{}^- = 2S_z, \tag{2.22}$$

from the following relations of fermionic field φ:

$$\varphi_\alpha{}^\beta = \varphi_a(\gamma^a)_\alpha{}^\beta = \begin{matrix} + \\ - \end{matrix} \begin{pmatrix} 0 & 2 \\ 0 & 0 \end{pmatrix} \varphi_z \begin{matrix} + \\ - \end{matrix} + \begin{matrix} + \\ - \end{matrix} \begin{pmatrix} 0 & 0 \\ -2 & 0 \end{pmatrix} \varphi_{\bar{z}}, \tag{2.23}$$

where $\alpha(\beta)$ is "$+,-$" and "a" means "$z,\bar{z}$". The above supercharges are further substitutable as follows:

$$Q_z = q_z Q_c, \quad S_z = s_z S_c, \tag{2.24}$$

where q_z and s_z, carrying the chiral index, z, commute all generators in the algebra (2.18) and "c" means the "chiral". Here q_z and s_z are left chiral components of real vectors $q = (q_z, q_{\bar{z}})^t$, $s = (s_z, s_{\bar{z}})^t$, respectively. Therefore, Q_c and S_c are real generators. We then obtain a different description of the topological algebra (2.18):

$$[S,\ q^z P_z] = 2qQ_c, \quad [Q_c,\ \tilde{D}] = Q_c, \quad [Q_c,\ \tilde{M}] = -Q_c,$$

$$[Q,\ s^z K_z] = -2sS_c, \quad [S_c,\ \tilde{D}] = -S_c, \quad [S_c,\ \tilde{M}] = -S_c,$$

$$\{Q, Q_c\} = -\frac{i}{q} q^z P_z, \quad \{S, S_c\} = \frac{i}{s} s^z K_z, \quad \{Q, S\} = -4i\tilde{M},$$

$$[P_z,\ \tilde{M}] = -P_z, \quad [P_z,\ \tilde{D}] = P_z,$$

$$[K_z,\ \tilde{M}] = -K_z, \quad [K_z,\ \tilde{D}] = -K_z, \tag{2.25}$$

where $q = q^z q_z$ and $s = s^z s_z$.

We must note that the four generators $q^z P_z$, $s^z K_z$, Q_c, and S_c still behave as holomorphic one-forms because the real vectors q, s commute all generators in the algebra (2.25) and then the commutation relation with $\tilde{M}$ is still retained. It is a matter of course that, if two-manifold M^2 is Hermitian with no boundary, four generators $q^z P_z$, $s^z K_z$, Q_c, and S_c could behave as zero-forms, that is, they commute $\tilde{M}$, regarding $q^z(s^z)$ as the ordinary adjoint Dolbeault operator; $\partial^\dagger (= -*\partial *)$ which satisfies the relation $[\tilde{M}, \partial^\dagger] = -\partial^\dagger$. We must note that the scale dimensions can not be wiped out through $\partial^\dagger$, however.

III. REDUCTION TO MODULI SPACE

Let us introduce TFT Lagrangians in explanation of the derivation of a moduli space associated with the algebra (2.25):

$$\mathscr{L}_Q = \{Q, Q_c\}, \quad \mathscr{L}_S = \{S, S_c\}, \quad \mathscr{L}_{QS} = \{Q, S\}. \tag{3.1}$$

We see that the above relations are on two-manifold with boundary owing to the Stokes' theorem, and it is possible for the corresponding theory to be in the case of two-manifold without boundary. We can make the formulation on manifold without boundary by means of the inner product of the path-integrals as "in" and "out" states,[15,16] and then suppose that the manifold of the theory will be without boundary. Moreover, at the quantum level the three Lagrangians (3.1) are invariant under the symmetry generated by the topological algebra $A^\star$:

$$A^\star = P_z, K_z, \tilde{M}, \tilde{D}, Q, Q_c, S, S_c, \tag{3.2}$$

because, if the Lagrangian is the exact form of BRST-like operator $\mathcal{Q}$ of TFT, the path-integral of the $\mathcal{Q}$-exact form is trivial; $\langle \mathcal{Q}\text{-exact} \rangle = 0$. We will show that the moduli space associated with the algebra (2.25) can be derived just by focusing on the Lagrangian $\mathcal{L}_{QS}$ through a gauge system of $\mathrm{osp}(2|2) \oplus \mathrm{osp}(2|2)$ algebra.

It is well known that the configuration of the system results in a corresponding moduli space after the quantization in TFT. The reduction to a moduli space is a result of the weak coupling limit. Under the limit, the leading contribution could be given by zero mode, that is, the classical configuration which makes the Lagrangian vanish. We now suppose that there exists some proper observable which guarantee the nontriviality of the path-integral. Let us start with a vanishing Lagrangian condition. Therefore, we obtain

$$\mathcal{L}_{QS} = \{Q, S\} = -4i\tilde{M} = 0. \tag{3.3}$$

There exists a system Γ of the gauge fields (2.16) of the topological algebra (2.25). Let a Noether current which generates $\tilde{M}$ be $J_0^{\tilde{M}}$. From the condition (3.3), $dJ_0^{\tilde{M}} = 0$ on two-manifold M^2 without boundary can be derived. The condition means $J_0^{\tilde{M}}$ is constant on M^2 for arbitrary 2-D metric. Moreover, it is necessary to estimate the behavior of the path-integral defined on two-manifold with boundary under the zero coupling limit. We know that a path-integral on manifold with boundary can be regarded as a functional on boundary:

$$Z_{D_i}[\varphi] = \int_{\psi|_{\partial M^2} = \varphi} \mathcal{D}\psi e^{-S(\psi)} \quad (i = 1,2), \tag{3.4}$$

where $M^2 = D_1 \cup_{\partial M^2} D_2$. The boundary condition $\psi|_{\partial M^2} = \varphi$ could be confined in a delta function with a proper periodicity. The coupling factor independence of $Z_{D_i}[\varphi]$ is evident because the invariance of $Z_{D_i}[\varphi]$ under the gauge transformations by Q and S holds.[15] Therefore, we see that

$$Z_{D_i}[\varphi](\mathcal{O}) = \int \mathcal{D}\psi e^{-S(\psi)} \delta_p(\psi|_{\partial M^2} - \varphi)\mathcal{O} = 0, \tag{3.5}$$

where $\mathcal{O} = Q$- or S-exact and δ_p denotes a delta function with some proper periodicity. The characteristic (3.5) guarantees the coupling factor independence of $Z_{D_i}[\varphi]$ in a way similar to the case of no-boundary. Therefore, the zero coupling limit would induce the classical configuration which makes the Lagrangian vanish and then the condition $J_0^{\tilde{M}} = 0$ on boundary holds because the Lagrangian could be described as one-dimensional integration on ∂M^2; $\mathcal{L} = \int_{\partial M^2} J_0^{\tilde{M}}$. Consequently, the condition (3.3) is reduced to $J_0^{\tilde{M}} = 0$ on two-manifold without boundary. We then define a subconfiguration Γ_s which satisfies $J_0^{\tilde{M}} = 0$. The constraint $J_0^{\tilde{M}} = 0$ yields the following reduction of the configuration:

$$\Gamma \Rightarrow \Gamma_s. \tag{3.6}$$

Let us confine ourselves to investigation of the physical meaning of the reduction mentioned above just through the Noether current which is composed of the connections of original $\mathrm{Osp}(2|2) \otimes \mathrm{Osp}(2|2)$ ($\equiv \mathcal{G}$). To this aim, we will consider a pure gauge theory of $\mathrm{osp}(2|2) \oplus \mathrm{osp}(2|2)$, not supergravity theory. Therefore, the naming of the generators of $\mathrm{osp}(2|2) \oplus \mathrm{osp}(2|2)$, which is shown in Sec. II, is perfectly formal. If not, that is, the naming is meaningful, the general coordinate transformations must be induced, and then the theory becomes empty as in the case of the ordinary two-dimensional conformal supergravity gauge theory.

Let us start with considering the Yang–Mills action on two-dimensional manifold without boundary:

$$\mathscr{L}_{\mathrm{YM}_2}=\int_{M^2}|R_{\mathscr{G}}|^2*1, \tag{3.7}$$

where $*$ is Hodge star operator and $R_{\mathscr{G}}$ is a field strength two-form: $R_{\mathscr{G}}=R^A B I_{AB}$ in which I_{AB} is the Cartan–Killing matrix on the Lie algebra of $\mathscr{G}$. Here the norm $|R_{\mathscr{G}}|^2$ has been obtained by using the metric on M^2 and I_{AB}. It is of interest to argue that the integrand of Eq. (3.7) can be rewritten as $R^A\wedge *R^B I_{AB}$, together with the volume form of the metric $*1$. It is a matter of course that Eq. (3.7) is invariant with respect to the gauge symmetry $\mathscr{G}$ and has no general coordinate invariance. The time component of the Noether current in association with the symmetry generated by M then turns out to be

$$J^0_M=\frac{\partial \mathscr{L}_{\mathrm{YM}_2}}{\partial(\partial_0 \mathbf{a}^A_\mu)}\, G^A_M(\mathbf{a})_\mu = R^B L_{AB} G^A_M(\mathbf{a})_\mu, \tag{3.8}$$

where $G^A_M\ (\mathbf{a})_\mu$ is defined by

$$\delta_M \mathbf{a}^A_\mu=\lambda_M G^A_M(\mathbf{a})_\mu, \tag{3.9}$$

$\mathbf{a}$ is general form of the gauge connections, and $R^A=R^A_{01}$. We can now add the optional field strength components to the original current (3.8) owing to the ambiguity of the Noether current. We are free to choose the additional term:

$$\partial_\alpha(\theta^A R^{A\alpha\beta}), \tag{3.10}$$

where $\theta^A(x)$ zero-form is an arbitrary function which supplements the characteristics of J^0_M with respect to the paired field strength R^A. Here note that the summation convention for repeated indices does not apply to indices of θ and of exponent of statistical factor $(-)$ in the following equations. It is a matter of course that the conventional sum rule is alive for the indices except the exponent of θ.

For the purpose of determining the compensating factor $\theta^A(x)$ zero-form, we refer to Eq. (3.8) in which $G^A_M(\mathbf{a})_\mu$ is composed of the gauge transformation $\delta_\prime \mathbf{a}^A$ one-form as in Eq. (3.9), and surely correspond to $\theta^A(x)$ zero-form. Therefore, $\theta^A(x)$ zero-form must be constructed through the reduction procedure of $\delta\mathbf{a}^A$ one-form. That is, we need some map X:

$$X:\delta\mathbf{a}^A\ldots\text{one-form}\mapsto\theta^A\ldots\text{zero-form}. \tag{3.11}$$

The map X can indeed be chosen as

$$X\equiv\mathscr{D}^\dagger, \tag{3.12}$$

where $\mathscr{D}^\dagger$ is the adjoint exterior derivative operator:

$$\mathscr{D}^\dagger:\Omega^r(M^2)\to\Theta^{r-1}(M^2), \tag{3.13}$$

with $\mathscr{D}^\dagger=*\mathscr{D}*$ on the two-dimensional Lorentzian manifold without boundary. We then obtain $\theta^A(x)$ zero-form as follows:

$$\theta^A\equiv\mathscr{D}^\dagger\delta\mathbf{a}^A. \tag{3.14}$$

Accordingly, Eq. (3.10) is reduced to

$$\partial_\beta(\theta^A R^{A\beta\alpha})=(\partial_\beta\theta^A-(-)^{|B||A|}f_{BA}{}^C\theta^C\mathbf{a}^B_\beta)R^{A\beta\alpha}+\theta^A\mathscr{D}_\beta R^{A\beta\alpha}, \tag{3.15}$$

where

$$\mathscr{D}_\beta R^{A\beta\alpha}=\partial_\beta R^{A\beta\alpha}+(-)^{|B||C|}f_{BC}{}^{A}\mathbf{a}_\beta^B R^{C\beta\alpha}. \tag{3.16}$$

We next add Eq. (3.15) to J_M^0 which leads to

$$J_M^0=\sum_{A(\text{on }\theta)}^{\text{all}}[\Pi_{\mu=1}^{A(\text{on }\theta)}R^A+\theta^A\mathscr{D}_{\mu=1}R^A], \tag{3.17}$$

where

$$\Pi_{\mu=1}^{A(\text{on }\theta)}=(-)^{|B||A|}I_{AB}G_M^B(\mathbf{a})_1+\partial_1\theta^A-\sum_C^{\text{all}}(-)^{|B||A|}f_{BA}{}^{C}\theta^C\mathbf{a}_1^B, \tag{3.18}$$

and $\Sigma_{A(\text{on }\theta)}^{\text{all}}$ denotes a summation of the indices appearing in the exponent of θ. That is, we must sum up the indices A in Eq. (3.17) except for the indices appearing in the exponent of the statistical factor $(-)$. The index A of I_{AB} and f_{BA}^C in $\Pi_{\mu=1}^{A(\text{on }\theta)}$ obeys the conventional summation rule.

Our principal task is now to make the topological twist on the current J_M^0 (3.17) and set it upon the configuration Γ_s as a result of the weak coupling limit. Making the topological twist on J_M^0 leads us to the modified current $J_{\tilde{M}}^0$ where $\tilde{M}=M+2iV$. The zero field strengths of the current J_M^0 are removed through replacement of A by $A^\star$ (3.2), which means that the configuration is reduced to Γ. We then obtain the information for the limiting condition $J_{\tilde{M}}^0=0$ as follows:

$$R^{A^\star}=0, \quad \theta^{A^\star}=0. \tag{3.19}$$

Clearly, this solution (3.19) is not unique in the mathematical view point, but seems natural because of the independence of the specific space–time coordinate index: $\mu=1$.

The informations $R^{A^\star}=0$ and $\theta^{A^\star}=0$ obtained above play the roles of the constraints for the configuration Γ_s, which eventually lead to some moduli space. The number of the equivariant constraint $R^{A^\star}=0$ is equal to that of the fermionic connections with ghost number $\psi_\mu(-1)$, $\psi_{\mu^-}{}^+(1)$, $\phi_\mu(1)$, and $\phi_{\mu^-}{}^+(-1)$. Therefore, $R^{A^\star}=0$ can be regarded as the fixing condition of the so-called topological symmetry whose degree of freedom is equal to number of these fermionic connections, i.e., the so-called topological ghosts.

Let us next explain the physical meaning of the condition $\theta^{A^\star}=0$. The tangent of the connection space $\mathscr{A}$ can be decomposed[17] as follows:

$$T_a\mathscr{A}=\text{Im }\mathscr{D}\oplus\text{Ker }\mathscr{D}^\dagger, \tag{3.20}$$

where Im $\mathscr{D}$ one-form is the tangent in the gauge direction, while Ker $\mathscr{D}^\dagger$ one-form means the component orthogonal to the gauge orbit and $0=\theta^{A^\star}=\mathscr{D}^\dagger\delta\mathbf{a}^{A^\star}$ is natural gauge condition in which $\delta\mathbf{a}^{A^\star}$ is an infinitesimal variation of the connection $\mathbf{a}^{A^\star}$. The constraint $\theta^{A^\star}$, the number of which is equal to that of the generators of the gauge symmetry, is then regarded as the gauge fixing condition.

We can therefore claim that all the constraints $R^{A^\star}=0$, $\theta^{A^\star}=0$ which originate from $J_{\tilde{M}}^0=0$ indeed lead to a moduli space of flat connections:

$$\mathscr{M}_{\text{flat}}=\{R^{A^\star}=0\}/\mathscr{G}^\star. \tag{3.21}$$

The moduli space (3.21) is really associated with the topological algebra (2.25). The BRST gauge fixing is necessary, by way of parenthesis, for the detailed investigation of observables, correlation functions, and their geometrical meaning in TFT.[18,19] Incidentally, let us describe another repre-

sentation for the conditions (3.19). If the infinitesimal variation of the connection $\delta \mathbf{a}^{A^\star}$ is on Γ_s, the variations of $R^{A^\star}$ under $\delta \mathbf{a}^{A^\star}$ must also vanish. Linearized representation[20,21] of the flat connection equations yields

$$0 = *\delta R = *\mathscr{D}\delta \mathbf{a} = *\mathscr{D}**\delta \mathbf{a} = \mathscr{D}^\dagger * \delta \mathbf{a},$$
$$0 = \mathscr{D}^\dagger \delta \mathbf{a}. \tag{3.22}$$

If $\delta \mathbf{a}$ is the arbitrary variation on $\mathscr{M}_{\text{flat}}$, its Hodge dual $\star \delta \mathbf{a}$, which is still one-form only in the two-dimension, is also on $\mathscr{M}_{\text{flat}}$.

Let us next refer to the general coordinate transformations. In the ordinary $N=2$ conformal supergravity, all curvatures must vanish in full consonance with the general coordinate transformations as gauge symmetry generated by the conformal super group.[14] As a consequence, there exists no kinetic term, i.e., no dynamics of connection fields in the ordinary theory. In the present case, on the contrary, zero curvatures play the roles of the conditions which lead to the configuration of the fields. Accordingly, the general coordinate transformation $\delta_{gc}(\xi)$ is induced by these conditions. Here $\delta_{gc}(\xi)$ is expressed as

$$\delta_{gc}(\xi)\mathbf{a}_\mu^A = \sum_B \delta_B(\xi^\nu \mathbf{a}_\nu^B)\mathbf{a}_\mu^A + \xi^\nu R_{\nu\mu}^A. \tag{3.23}$$

The topological twist on Eq. (3.23) induces the replacement $A \to A^\star$, so that the zero field strengths associated with $A - A^\star$ are removed. Moreover, under the weak coupling limit, the resultant configuration is given by (3.19). Therefore, the transformation law (3.23) on $\mathscr{M}_{\text{flat}}$ is described as follows:

$$\delta_{gc}(\xi)\mathbf{a}_a^{A^\star} = \sum_{B^\star} \delta_{B^\star}(\xi^\nu \mathbf{a}_\nu^{B^\star})\mathbf{a}_\mu^{A^\star}. \tag{3.24}$$

In Eqs. (3.24), $\delta_{gc}(\xi)$ have been fixed in accordance with the thoroughly fixed gauge symmetry (3.21). It is then possible to argue that the configuration $\mathscr{M}_{\text{flat}}$ is a quotient not only in the sense of the gauge symmetry, but also in the sense of the diffeomorphism:

$$\sim / \mathscr{G}^\star \supset \sim / \text{Diff}_0. \tag{3.25}$$

IV. GEOMETRICAL MEANING OF FERMIONIC OPERATORS

In the last section, the moduli space $\mathscr{M}_{\text{flat}}$ (3.21) has been derived formally. It is possible to obtain more information on $\mathscr{M}_{\text{flat}}$ by studying a geometrical meaning of the fermionic operators of the algebra (2.25). In TFT, the operator δ_f of the BRST-like fermionic symmetry corresponds to the exterior derivative operator d on a moduli space where the ghost number corresponds to the form degree. In the topological Yang–Mills theory on four-manifolds,[1,8] for instance, the cotangent vector, i.e., one-form on the Yang–Mills instanton moduli space, is described as

$$\delta_f \mathbf{a} = \psi, \tag{4.1}$$

where $\mathbf{a}$ is a generic point in the moduli space and ψ is a topological ghost. In the present case, it is natural to regard the fermionic operators Q, S, $Q_c S_c$ as δ_f, because there exists the ghost number which has nothing to do with the gauge symmetry and, moreover, the fermionic operators generate the transformations with the ghost number, that is, they are the ghost number carriers. Whatever the gauge orbit may be collapsed under the zero coupling limit, the four fermionic operators can still remain as BRST-like operators on $\mathscr{M}_{\text{flat}}$. The operation on $\mathscr{M}_{\text{flat}}$ must be read off from the transformation rule (2.19). The existence of such operators on $\mathscr{M}_{\text{flat}}$ leads us to

consistent and interesting results. A space which we can regard as a moduli space will be equipped with some analytical, or in other words, differentiable structure, in general. It is well known, for instance, that the moduli space of 4-D (anti-) instantons is locally homeomorphic to a differentiable manifold under the appropriate conditions, and the complex structure of the (anti-) instanton moduli space corresponds to that of the base manifold.[11,22] It is a matter of course that the topological invariants of TFT, which are originated from the Donaldoson theory, must be integrals on certain analytical support of the moduli space.

We now suppose that the moduli space $\mathscr{M}_{\text{flat}}$ (3.21) has such an analytical support. This assumption is appropriate because the general discussion of flat connections shows that the moduli space of flat connections is regarded as a manifold. In the present case, it is possible to decompose $\mathscr{M}_{\text{flat}}$ locally into fermionic subspace $\mathscr{M}^f$ and bosonic subspace $\mathscr{M}^b$ as follows:

$$\mathscr{M}_{\text{flat}} \cong \mathscr{M}^{\text{f}} \otimes \mathscr{M}^b. \tag{4.2}$$

Accordingly, $\mathscr{M}_{\text{flat}}$ is regarded as a fiber bundle over the base space $\mathscr{M}^b$, which is described by using the following fibration:

$$\begin{array}{ccc} F & \rightarrow & \mathscr{M}_{\text{flat}} \\ & & \downarrow \pi \\ & & \mathscr{M}^b \end{array} . \tag{4.3}$$

Here F denotes a fiber parametrized by the ghost number. That is, $\mathscr{M}_{\text{flat}}$ is regarded as the Whitney sum bundle composed of the vector bundles; E_k with the ghost number $k(=-1,0,1)$:

$$\mathscr{M}_{\text{flat}} = E_{-1} \oplus E_0 \oplus E_1 . \tag{4.4}$$

Let us discuss a geometrical meaning of the fermionic operators in the present theory. In Sec III, the three TFT's Lagrangians have been set up in (3.1). While, under the weak coupling limit, we have induced the reduction to the moduli space $\mathscr{M}_{\text{flat}}$ by considering one of the three Lagrangians; $\mathscr{L}_{QS}$, all Lagrangians are adapted here. We introduce a total Lagrangian $\mathscr{L}_{\text{tot}}$ as a linear combination of the three Lagrangians:

$$\mathscr{L}_{\text{tot}} = \mathscr{L}_Q + \mathscr{L}_S + \mathscr{L}_{QS} . \tag{4.5}$$

Using the algebra (2.25), $\mathscr{L}_{\text{tot}}$ is also described as an anticommutator of two fermionic operators as follows:

$$\mathscr{L}_{\text{tot}} = \{\mathscr{QS}, \mathscr{QS}^\dagger\}, \tag{4.6}$$

where $\mathscr{QS} = Q + S_c$ and $\mathscr{QS}^\dagger = Q_c + S$. As can be seen from the relations (2.21), $\mathscr{QS}$ increases the ghost number by one unit, while $\mathscr{QS}^\dagger$ decreases it by the same quantity. Moreover, both $\mathscr{QS}$ and $\mathscr{QS}^\dagger$ are nilpotent. Under the weak coupling limit, $\mathscr{QS}$ and $\mathscr{QS}^\dagger$ can be regarded as operators on the fiber bundle $\mathscr{M}_{\text{flat}}$. To be precise, $\mathscr{QS}(\mathscr{QS}^\dagger)$ operates on the vector bundles E_k $(k=-1,0,1)$. The operation sequence of $\mathscr{QS}$ is

$$0 \xrightarrow{i} E_{-1} \xrightarrow{\mathscr{QS}_{-1}} E_0 \xrightarrow{\mathscr{QS}_0} E_1 \xrightarrow{\mathscr{QS}_1} 0, \tag{4.7}$$

where $E_{-1} = \{\psi, \phi^z\}$, $E_0 = \{\omega, b, e^z, f^z\}$, $E_1 = \{\psi^z, \phi\}$, $\mathscr{QS}_k$ $(k=-1,0,1) = \mathscr{QS}$, and i denotes inclusion. Therefore, we can regard the above sequence (4.7) as an elliptic complex, and $\mathscr{QS}$ as a Fredholm operator with $\mathscr{QS}^\dagger$ its adjoint. Accordingly, $\mathscr{L}_{\text{tot}}$ corresponds to the Laplacian operator.

It is possible to derive the index of the above elliptic complex as an additional result:

$$\mathrm{ind}(\mathcal{QS})=\sum_{k=-1}^{1}(-1)^k\mathrm{Harm}^k(\mathcal{M}_{\mathrm{flat}}\mathcal{QS})=0, \tag{4.8}$$

where $\mathrm{Harm}^k(\mathcal{M}_{\mathrm{flat}},\mathcal{QS})$ denotes the Kernel of $\{\mathcal{QS}_k,\mathcal{QS}_k^{\dagger}\}$.

The vanishing Lagrangian condition $\mathcal{S}_{\mathrm{tot}}=0$ means that the eigenvalues of the Laplacian operator must be zero. The facts seem to show that $\mathcal{M}_{\mathrm{flat}}$ is corresponding to the Kernels; $\mathrm{Harm}^k(\mathcal{M}_{\mathrm{flat}},\mathcal{QS})$. To see the contents of the Kernels, we describe the operator sequence (4.7) in terms of the components:

$$\phi^z\underset{S}{\overset{Q}{\rightleftharpoons}}f^z\overset{S_c}{\rightarrow}\phi,\quad \psi\overset{S}{\leftarrow}\omega\overset{Q}{\rightarrow}\phi,\quad \psi\overset{Q_c}{\leftarrow}e^z\underset{S}{\overset{Q}{\rightleftharpoons}}\psi^z,\quad b. \tag{4.9}$$

As can be seen from the sequences (4.9), four components e^z, f^z, ψ^z, and ϕ^z are not suitable for the Kernel of the Laplacian. In the above context, we have indicated that $\mathcal{S}_{\mathrm{tot}}$ is regarded as the Laplacian under the weak coupling limit and the vanishing Lagrangian condition leads us to the Kernels of the Laplacian. It is natural to expect that the Kernels correspond to $\mathcal{M}_{\mathrm{flat}}$. Consequently, we claim that the four components must not be in $\mathcal{M}_{\mathrm{flat}}$.

This statement is also supported by the following consideration. First of all, there are two closed loops in the sequences (4.9), which are composed of two sets (e^z,ψ^z), (f^z,ϕ^z):

$$\phi^z\underset{S}{\overset{Q}{\rightleftharpoons}}f^z,\quad e^z\underset{S}{\overset{Q}{\rightleftharpoons}}\psi^z. \tag{4.10}$$

The two components in each set circulate on its own loop by operation of Q and S. Any other components cannot reach the two loops by any operations. Moreover, the S-operation after the Q-operation (or Q after S) leads the component to itself and such a double operation of $S*Q$ (or $Q*S$) induces the transformation in the direction of the gauge orbit, because of the relation $[Q,S]=-4i\tilde{M}$. Therefore, the two closed loops are in the gauge orbit and are expected to be collapsed together with the gauge orbit on $\mathcal{M}_{\mathrm{flat}}$. The fact shows that e^z, f^z, ψ^z, and ϕ^z are not in the moduli space $\mathcal{M}_{\mathrm{flat}}$.

More detailed information of $\mathcal{M}_{\mathrm{flat}}$ is obtained through studying the geometrical meaning of the fermionic operators. It is clarified that the choice of the left-chiral part of the algebra (2.25) is rather meaningless for the purpose of the derivation of the moduli space and the intersection of the left- and right-chiral part is only effective. Therefore, $\mathcal{M}_{\mathrm{flat}}$ is reduced to $\mathcal{M}_0$:

$$\mathcal{M}_0=\{R^{A^{\star\star}}=0\}/\mathcal{G}^{A^{\star\star}}, \tag{4.11}$$

where $A^{\star\star}=\tilde{M},\tilde{D},Q,S$. We then claim that the moduli space intrinsic to the topologically twisted $\mathrm{osp}(2|2)\oplus\mathrm{osp}(2|2)$ is really $\mathcal{M}_0$.

A. Observable

We will see that there exists a TFT observable $\mathcal{O}$ which assures that the path-integral under consideration is nontrivial. Let us begin with introducing the following two forms:

$$\hat{\varrho}_\alpha=\varepsilon_v\hat{\varrho}_\alpha\quad(\alpha=0,1,). \tag{4.12}$$

Here ϵ_v denotes a two-form determined by a metric and $\hat{\varrho}_\alpha$ is a zero-form defined by

$$\hat{\varrho}_\alpha=\psi_\alpha\phi_\alpha. \tag{4.13}$$

The index α can be regarded as mere labels because the coordinate transformations are not considered. Therefore, we present a candidate for the nontrivial observable as in the following:

$$\mathcal{O}=\int_{M^2} d\mu\ \varrho_0\varrho_1 . \tag{4.14}$$

The behavior of ϱ_α under the gauge transformation δ_g (2.19) is written in the form

$$\delta_g\varrho_\alpha=(\partial_\alpha\epsilon)\phi_\alpha+\psi_\alpha\partial_\alpha\kappa=\acute{\epsilon}\phi_\alpha-\acute{\kappa}\psi_\alpha=\delta_{QS}\psi_\alpha , \tag{4.15}$$

where $\acute{\epsilon}=\partial_\alpha\epsilon$ and $\acute{\kappa}=\partial_\alpha\kappa$. Therefore, we see that

$$\begin{aligned}\delta_g\mathcal{O}=\int_{M^2} d\mu\ \delta_g(\varrho_0\varrho_1)&=\int_{M^2} d\mu\{(\delta_g\varrho_0)\varrho_1+\varrho_0(\delta_g\varrho_1)\}\\ &=\int_{M^2} d\mu\{(\delta_{QS}\omega_0)\varrho_1+\varrho_0(\delta_{QS}\omega_1)\}\\ &=\int_{M^2} d\mu\ \delta_{QS}(\omega_0\varrho_1+\varrho_0\omega_1-\omega_0\omega_1)\\ &=\delta_{QS}\int_{M^2} d\mu(\omega_0\varrho_1+\varrho_0\omega_1-\omega_0\omega_1).\end{aligned} \tag{4.16}$$

The above equation (4.16) shows that $\mathcal{O}$ is gauge invariant in the path-integral. Clearly, $\mathcal{O}$ is not dependent on a metric and includes the coupling $\psi_0\phi_0\psi_1\phi_1$. Therefore, we conclude that $\mathcal{O}$ is a nontrivial TFT's observable. The fact shows that the path-integral is not trivial and supports the present discussion from beginning to end.

V. SUMMARY AND REMARKS

First, we have investigated the topologically twisted osp(2|2)⊕osp(2|2) conformal superalgebra and derived the moduli space intrinsic to the twisted algebra. The algebra includes the appropriate TFT's Lagrangians composed of the fermionic charges Q, S, Q_c, and S_c. They lead us to the moduli space $\mathcal{M}_{\text{flat}}$ intrinsic to the algebra under the condition of the weak coupling limit. As a consequence of the investigation of the geometrical meaning of the fermionic charges, it is shown that $\mathcal{M}_{\text{flat}}$ is reduced to $\mathcal{M}_0$ associated with the intersection of the left- and right-chiral part of the topological algebra and is just a moduli space inherent in the algebra. As an additional result, the index of these fremionic operators is derived if some proper support in the moduli space can be defined. The facts which have been clarified in the above discussion show that the topological algebra has a specific relation with a moduli problem. It is claimed that a geometrical feature of the algebra is one of the interesting characteristics inherent in the topological twist. Therefore, we have succeeded in shedding some light upon the relation between the topological twist and the moduli problem through the geometrical aspect of the topological algebra.

Second, let us make a remark on the vanishing Noether current. Making use of the ambiguity of the Noether current, we are led to the relation (3.17) between the vanishing Noether current $J^0_{\tilde{M}}=0$ and the flat connection conditions $R^{A^\star}=0$, $\theta^{A^\star}=0$. In the conventional QFT, e.g., the quantum electro-dynamics, this ambiguity mentioned above plays an important role in association with avoiding one mass-less state to obtain a well-defined conserved charge while its physical role is not clarified in the case of the classical correspondent. In the present TFT, on the contrary, the classical theory has been obtained as the limiting case of the path-integral, and consequently the ambiguity argued above leads to the corresponding moduli problem.

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Heat kernel coefficients of the Laplace operator on the *D*-dimensional ball

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We present a very quick and powerful method for the calculation of heat kernel coefficients. It makes use of rather common ideas, as integral representations of the spectral sum, Mellin transforms, non-trivial commutation of series and integrals and skillful analytic continuation of zeta functions on the complex plane. We apply our method to the case of the heat kernel expansion of the Laplace operator on a D-dimensional ball with either Dirichlet, Neumann or, in general, Robin boundary conditions. The final formulas are quite simple. Using this case as an example, we illustrate in detail our scheme —which serves for the calculation of an (in principle) arbitrary number of heat kernel coefficients in any situation when the basis functions are known. We provide a complete list of new results for the coefficients B_3,..., B_{10}, corresponding to the D-dimensional ball with all the mentioned boundary conditions and $D=3,4,5$. © *1996 American Institute of Physics.*
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I. INTRODUCTION

An important issue for more than twenty years now has been to obtain explicitly the coefficients which appear in the short-time expansion of the heat kernel $K(t)$ corresponding to a Laplacian-like operator on a D-dimensional manifold $\mathcal{M}$. In mathematics this interest extends to basically all of Geometric Analysis, including in particular, the well-known connection that exists between the heat equation and the Atiyah-Singer index theorem,[1] but also analytic torsion, sharp inequalities of borderline Sobolev and Moser–Trudinger type, etc. In physics, the importance of that expansion is notorious in different domains of quantum field theory, where it is commonly known as the (integrated) Schwinger–De Witt proper-time expansion.[2,3] In this context, the heat-equation for an elliptic (in general pseudoelliptic) differential operator P and the corresponding zeta function $\zeta_P(s)$ has been realized to be a particularly useful tool for the determination of effective actions[4] and for the calculation of vacuum or Casimir energies[5] (a fundamental issue for understanding the vacuum structure of a quantum field theory). Here usually the derivative $\zeta_P'(0)$ of the zeta function[4] and its value at $s=-1/2$ (sometimes the principal part) are needed.[5,6]

In this paper we would like to exploit another property of the zeta function $\zeta_P(s)$ corresponding to an elliptic operator P, namely its well-known close connection with the heat kernel expansion. In spite of the fact that almost everybody is aware of such connection, its actual use in the

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literature has remained very scarce until now. If the manifold $\mathcal{M}$ has a boundary $\partial\mathcal{M}$, the coefficients B_n in the short-time expansion have both a volume and a boundary part.[7,8] It is usual to write this expansion in the form

$$K(t)\sim(4\pi t)^{-D/2}\sum_{k=0,1/2,1,\ldots}^{\infty}B_k t^k, \tag{1.1}$$

with

$$B_k=\int_{\mathcal{M}}dV b_n+\int_{\partial\mathcal{M}}dS c_n\,. \tag{1.2}$$

For the volume part very effective systematic schemes have been developed (see for example Refs. 9–11). The calculation of c_n, however, is in general more difficult. Only quite recently has the coefficient c_2 for Dirichlet and for Neumann boundary conditions been found.[12–17] Very new results on the coefficient $B_{5/2}$ for manifolds with totally geodesic boundaries will be given in Ref. 18.

When using the general formalism of Ref. 12 for higher-spin particles, Moss and Poletti[19,20] found a discrepancy with the direct calculations of D'Eath and Esposito[21] (see also Refs. 22–25). The latter results have been confirmed in Refs. 26,27, where a new systematic scheme for the calculation of c_2 has been designed in the context of the Hartle–Hawking wave-function of the universe and for the case when the whole set of basis functions is known[26,27]. Finally, very recently the discrepancy has been resolved completely[28] and now the results that are found using the general algorithm[29] are in agreement with those coming from the direct calculations[21–27].

The connection between the heat kernel expansion, Eq. (1.1) and the associated zeta function is established through the formulas[30]

$$\text{Res }\zeta(s)=\frac{B_{m/2-s}}{(4\pi)^{m/2}\Gamma(s)}, \tag{1.3}$$

for $s=m/2$, $(m-1)/2$, ..., $\frac{1}{2}$; $-(2l+1)/2$, for $l\in\mathbb{N}_0$, and

$$\zeta(-p)=(-1)^p p!\,\frac{B_{m/2+p}}{(4\pi)^{m/2}}, \tag{1.4}$$

for $p\in\mathbb{N}_0$. The aim of the present article is to show that these equations, (1.3) and (1.4), can actually serve as a very convenient starting point for the calculation of the coefficients B_k, even in the cases when the eigenvalues of the operator P under consideration are not known. The good knowledge in explicit zeta-function evaluations that have been accumulated in the past few years (for a review of many results in this respect, see Ref. 31) will allow us to elaborate a very competitive method of calculation of the heat kernel coefficients which makes use of rather common ingredients, such as integral representations of the spectral sum, Mellin transforms, non-trivial commutation of series and integrals and skillful analytic continuation of zeta functions on the complex plane.

To explain the method in detail we will consider the Laplace operator on the D-dimensional ball with Dirichlet, Neumann or (in general) Robin boundary conditions. Earlier investigations on the first few coefficients are due, for $D=1$, to Stewartson and Waechter ,[32] to Waechter in $D=2$[33] and to Kennedy[34,35] in up to $D=5$ dimensions. Concerning the four-dimensional ball, another rather large work is documented in Refs. 36,37, where the focus is in conformal deformations of the metrics, the four-ball being treated explicitly in the second of these papers (for recent results on the functional determinant of the Laplace operator on the three- and four-dimensional ball see

also Ref. 38). In these references the method was based on the use of Laplace transformations of the heat kernel $K(t)$ itself. In that method an intermediate cut off has to be introduced at some point—because one needs to consider the Laplace transform of a function which is singular at $t=0$. In contrast, in our approach it is the complex argument s of the zeta function of the Laplace operator which very neatly serves for the regularization of all sums (in just the usual way[31]).

The layout of the paper is as follows. In section II we briefly describe the eigenvalue problem of the massive Laplace operator on the ball and derive a representation of the associated zeta function in terms of a contour integral. We consider the *massive* Laplace operator because the analytical continuation procedure is slightly easier for the case of non-vanishing mass. In section III we describe how an analytical representation of the zeta function —valid in the strip $(1-N)/2<\Re s<1$— can be obtained for any N, restricting our considerations in this section to $D=3$ and to the case of Dirichlet boundary conditions. This representation will display very clearly the meromorphic structure of the zeta function. As is then shown in section IV, from this representation it is quite immediate to read off special properties, as the ones reflected by (1.3) and (1.4), in order to find the heat kernel coefficients. In section V we explain the small changes in the procedure that are necessary in order to treat Robin boundary conditions, in general. Finally, in section VI we study the modification to be introduced in the formulas for considering any arbitrary dimension D. In Appendix A we exhibit some technical details of the calculation and in appendices B, C and D we give explicit tables of the heat kernel coefficients for Dirichlet, Neumann and general Robin boundary conditions, for the dimensions $D=3,4,5$.

II. HEAT KERNEL COEFFICIENTS ON THE *D*-DIMENSIONAL BALL

As explained in the introduction, we are interested in the zeta function of the operator $(-\Delta+m^2)$ on the D-dimensional ball $B^D=\{x\in\mathbb{R}^D;|x|\leqslant R\}$ endowed with Dirichlet, Neumann or Robin boundary conditions. The zeta function is formally defined as

$$\zeta(s)=\sum_k \lambda_k^{-s}, \tag{2.1}$$

with the eigenvalues λ_k being determined through

$$(-\Delta+m^2)\phi_k(x)=\lambda_k\phi_k(x) \tag{2.2}$$

(k is in general a multiindex here), together with one of the three boundary conditions above. It is convenient to introduce a spherical coordinate basis, with $r=|x|$ and $D-1$ angles $\Omega=(\theta_1,...,\theta_{D-2},\varphi)$. In these coordinates, a complete set of solutions of Eq. (2.2) together with one of the mentioned boundary conditions may be given in the form

$$\phi_{l,m,n}(r,\Omega)=r^{1-D/2}J_{l+(D-2)/2}(w_{l,n}r)Y_{l+D/2}(\Omega), \tag{2.3}$$

with $J_{l+(D-2)/2}$ being Bessel functions and $Y_{l+D/2}$ hyperspherical harmonics.[39] The $w_{l,n}$ (>0) are determined through the boundary conditions by

$$J_{l+(D-2)/2}(w_{l,n}R)=0, \text{ for Dirichlet boundary conditions,}$$

$$\frac{u}{R}J_{l+(D-2)/2}(w_{l,n}R)+w_{l,n}J'_{l+(D-2)/2}(w_{l,n}r)\big|_{r=R}=0, \text{ for Robin boundary conditions.} \tag{2.4}$$

As is clear, the case $u=(1-D/2)$ of the (general) Robin boundary conditions corresponds to the Neumann boundary conditions. In this notations, using $\lambda_{l,n}=w_{l,n}^2+m^2$, the zeta function can be given in the form

$$\zeta(s)=\sum_{n=0}^{\infty}\sum_{l=0}^{\infty} d_l(D)(w_{l,n}^2+m^2)^{-s}, \tag{2.5}$$

where $w_{l,n}$ (>0) is defined as the n-th root of the l-th equation. Here the sum over n is extended over all possible roots $w_{l,n}$ on the positive real axis, and $d_l(D)$ is the number of independent harmonic polynomials, which defines the degeneracy of each value of l and n in D dimensions. Explicitly,

$$d_l(D)=(2l+D-2)\frac{(l+D-3)!}{l!(D-2)!}. \tag{2.6}$$

Furthermore, here and in what follows the prime will always mean derivative of the function with respect to its argument.

To distinguish in the notation among the different cases, we will use the indices D, N and R to denote Dirichlet, Neumann and Robin boundary conditions, respectively. Thus, we will write ζ_D, ζ_N and ζ_R for the corresponding zeta functions. Using for the moment the unified notation $\Phi_{l+(D-2)/2}(w_{l,n}R)=0$ for the boundary condition Eq. (2.4), it turns out that Eq. (2.5) may be written under the form of a contour integral on the complex plane,

$$\zeta(s)=\sum_{l=0}^{\infty} d_l(D)\int_{\gamma}\frac{dk}{2\pi i}(k^2+m^2)^{-s}\frac{\partial}{\partial k}\ln\Phi_{l+\,(D-2)/2}(kR), \tag{2.7}$$

where the contour γ runs counterclockwise and must enclose all the solutions of (2.4) on the positive real axis (for a similar treatment of the zeta function as a contour integral see Refs. 26,27,40). This representation of the zeta function in terms of a contour integral around some circuit γ on the complex plane, Eq. (2.7), is the *first step* of our procedure.

Depending on the value of the dimension D and on the boundary conditions chosen, the analysis of the zeta function, Eq. (2.7) —to be given below— will differ, but just in small details. For this reason, we will only describe at length the case of the three-dimensional ball with Dirichlet boundary condition. The derivation of the analogous results for the other boundary conditions and higher dimensions will then be clear, and shall be indicated only briefly.

III. A QUICK PROCEDURE FOR CALCULATING HEAT KERNEL COEFFICIENTS

As explained above, we will illustrate the procedure in the case of the three-dimensional ball with Dirichlet boundary conditions. For $D=3$ the degeneracy is $d_l(3)=2l+1$, so that the starting point of the calculation reads (we omit further indication of the dimension in the notation)

$$\zeta_D(s)=\sum_{l=0}^{\infty}(2l+1)\int_{\gamma}\frac{dk}{2\pi i}(k^2+m^2)^{-s}\frac{\partial}{\partial k}\ln J_{l+1/2}(kR). \tag{3.1}$$

As it stands, the representation (3.1) is valid for $\Re s>3/2$. However, we are interested in the properties of $\zeta_D(s)$ in the range $\Re s<0$ and thus, we need to perform the analytical continuation to the left domain of the complex plane. Before considering in detail the l-summation, we will first proceed with the k-integral alone.

The first specific idea is to shift the integration contour and place it along the imaginary axis. In order to avoid contributions coming from the origin $k=0$, we will consider (with $\nu=l+1/2$) the expression

$$\zeta_D^{\nu}=\int_{\gamma}\frac{dk}{2\pi i}(k^2+m^2)^{-s}\frac{\partial}{\partial k}\ln(k^{-\nu}J_{\nu}(kR)), \tag{3.2}$$

where the additional factor $k^{-\nu}$ in the logarithm does not change the result, for no additional pole is enclosed. One then easily obtains

$$\zeta_D^\nu = \frac{\sin(\pi s)}{\pi} \int_m^\infty dk (k^2 - m^2)^{-s} \frac{\partial}{\partial k} \ln(k^{-\nu} I_\nu(kR)) \tag{3.3}$$

valid in the strip $1/2 < \Re s < 1$. A similar representation valid for $m = 0$ has been given in Refs. 41,42.

As the *second step* of our method, we make use of the uniform expansion of the Bessel function $I_\nu(k)$ for $\nu \to \infty$ at $z = k/\nu$ fixed.[43] One has

$$I_\nu(\nu z) \sim \frac{1}{\sqrt{2\pi\nu}} \frac{e^{\nu\eta}}{(1+z^2)^{1/4}} \left[1 + \sum_{k=1}^\infty \frac{u_k(t)}{\nu^k} \right], \tag{3.4}$$

with $t = 1/\sqrt{1+z^2}$ and $\eta = \sqrt{1+z^2} + \ln[z/(1+\sqrt{1+z^2})]$. The first few coefficients are listed in Ref. 43, higher coefficients are immediate to obtain by using the recursion[43]

$$u_{k+1}(t) = \frac{1}{2} t^2 (1-t^2) u_k'(t) + \frac{1}{8} \int_0^t d\tau (1 - 5\tau^2) u_k(\tau), \tag{3.5}$$

starting with $u_0(t) = 1$. As is clear, all the $u_k(t)$ are polynomials in t. Furthermore, the coefficients $D_n(t)$ defined by

$$\ln\left[1 + \sum_{k=1}^\infty \frac{u_k(t)}{\nu^k} \right] \sim \sum_{n=1}^\infty \frac{D_n(t)}{\nu^n} \tag{3.6}$$

are easily found with the help of a simple computer program.

Now comes what can be considered as the *third step* of our method. By adding and subtracting N leading terms of the asymptotic expansion, Eq. (3.6), for $\nu \to \infty$, Eq. (3.3) may be split into the following pieces

$$\zeta_D^\nu = Z_D^\nu(s) + \sum_{i=-1}^N A_i^{\nu,D}(s), \tag{3.7}$$

with the definitions

$$Z_D^\nu(s) = \frac{\sin(\pi s)}{\pi} \int_{mR/\nu}^\infty dz \left[\left(\frac{z\nu}{R} \right)^2 - m^2 \right]^{-s} \frac{\partial}{\partial z} \times \left\{ \ln[z^{-\nu} I_\nu(z\nu)] - \ln\left[\frac{z^{-\nu}}{\sqrt{2\pi\nu}} \frac{e^{\nu\eta}}{(1+z^2)^{\frac{1}{4}}} \right] - \sum_{n=1}^N \frac{D_n(t)}{\nu^n} \right\}, \tag{3.8}$$

and

$$A_{-1}^{\nu,D} = \frac{\sin(\pi s)}{\pi} \int_{mR/\nu}^\infty dz \left[\left(\frac{z\nu}{R} \right)^2 - m^2 \right]^{-s} \frac{\partial}{\partial z} \ln(z^{-\nu} e^{\nu\eta}), \tag{3.9}$$

$$A_0^{\nu,D} = \frac{\sin(\pi s)}{\pi} \int_{mR/\nu}^\infty dz \left[\left(\frac{z\nu}{R} \right)^2 - m^2 \right]^{-s} \frac{\partial}{\partial z} \ln(1+z^2)^{-1/4}, \tag{3.10}$$

$$A_i^{\nu,D}=\frac{\sin(\pi s)}{\pi}\int_{mR/\nu}^{\infty}dz\left[\left(\frac{z\nu}{R}\right)^2-m^2\right]^{-s}\frac{\partial}{\partial z}\left(\frac{D_i(t)}{\nu^i}\right). \tag{3.11}$$

The essential idea is conveyed here by the fact that the representation (3.7) has the following important properties. First, by considering the asymptotics of the integrand in Eq. (3.8) for $z\to mR/\nu$ and $z\to\infty$, it can be seen that the function

$$Z_D(s)=\sum_{l=0}^{\infty}(2l+1)Z_D^{l+1/2}(s)$$

is analytic on the strip $(1-N)/2<\Re s<1$. For this reason, it gives no contribution to the residue of $\zeta_D(s)$ in that strip. Furthermore, for $s=-k,k\in\mathbb{N}_0$, $k<-1+N/2$, we have $Z(s)=0$ and, thus, it also yields no contribution to the values of the zeta function at these points. Together with Eqs. (1.3) and (1.4), this result means that the heat kernel coefficients are just determined by the terms $A_i^D(s)$ with

$$A_i^D(s)=\sum_{l=0}^{\infty}(2l+1)A_i^{l+1/2,D}(s). \tag{3.12}$$

As they stand, the $A_i^{\nu,D}(s)$ in Eqs. (3.9), (3.10) and (3.11) are well defined on the strip $1/2<\Re s<1$ (at least). And we will now show that the analytic continuation in the parameter s to the whole of the complex plane, in terms of known functions, can be performed. Keeping in mind that $D_i(t)$ is a polynomial in t, all the $A_i^{\nu,D}(s)$ are in fact hypergeometric functions, which is seen by means of the basic relation [44]

$${}_2F_1(a,b;c;z)=\frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)}\int_0^1 dt\,t^{b-1}(1-t)^{c-b-1}(1-tz)^{-a}.$$

Let us consider first in detail $A_{-1}^{\nu,D}(s)$, $A_0^{\nu,D}(s)$, and the corresponding $A_{-1}^{D}(s)$, $A_0^{D}(s)$. One finds immediately that

$$A_{-1}^{\nu,D}(s)=\frac{m^{-2s}}{2\sqrt{\pi}}Rm\,\frac{\Gamma\left(s-\frac{1}{2}\right)}{\Gamma(s)}{}_2F_1\left(-\frac{1}{2},s-\frac{1}{2};\frac{1}{2};-\left(\frac{\nu}{mR}\right)^2\right)-\frac{\nu}{2}m^{-2s}, \tag{3.13}$$

$$A_0^{\nu,D}(s)=-\frac{1}{4}m^{-2s}{}_2F_1\left(1,s;1,-\left(\frac{\nu}{mR}\right)^2\right)=-\frac{1}{4}m^{-2s}\left[1+\left(\frac{\nu}{mR}\right)^2\right]^{-s}, \tag{3.14}$$

where in the last equality we have used that ${}_2F_1(a,s;a;x)=(1-x)^{-s}$.

The next step is to consider the summation over l. For $A_{-1}^{\nu,D}(s)$ this is best done using a Mellin–Barnes type integral representation of the hypergeometric functions

$${}_2F_1(a,b;c;z)=\frac{\Gamma(c)}{\Gamma(a)\Gamma(b)}\,\frac{1}{2\pi i}\int_{\mathscr{C}}dt\,\frac{\Gamma(a+t)\Gamma(b+t)\Gamma(-t)}{\Gamma(c+t)}(-z)^t, \tag{3.15}$$

where the contour is such that the poles of $\Gamma(a+t)\Gamma(b+t)/\Gamma(c+t)$ lie to the left of it and the poles of $\Gamma(-t)$ to the right.[44] After interchanging the summation over l and the integration in (3.15), the result will be a Hurwitz zeta function, which is defined as

$$\zeta_H(s;v)=\sum_{l=0}^{\infty}(l+v)^{-s},\quad \Re s>1. \tag{3.16}$$

However, as is well known, one has to be very careful with this kind of manipulation with what has been realized and explained with great detail in Refs. 45–47. This point is of crucial importance (it has been the source of many errors in the literature over the past ten years[31]) and can be considered as the *fourth step* of our original procedure here. Applying the method, as described in the mentioned references, to $A^D_{-1}(s)$,

$$A^D_{-1}(s)=\sum_{l=0}^{\infty}(2l+1)\left[\frac{m^{-2s}}{2\sqrt{\pi}}Rm\frac{\Gamma(s-1/2)}{\Gamma(s)}{}_2F_1\left(-\frac{1}{2},s-\frac{1}{2};\frac{1}{2};-\left(\frac{l+1/2}{mR}\right)^2\right)-\frac{l+\frac{1}{2}}{2}m^{-2s}\right],$$

it turns out that we may interchange the Σ_l and the integral in Eq. (3.15) *only* if for the real part $\Re\mathscr{C}$ of the contour the condition $\Re\mathscr{C}<-1$ is satisfied. However, the argument $\Gamma(-1/2+t)\Gamma(s-1/2)/\Gamma(1/2+t)$ has a pole at $t=1/2$. Thus the contour $\mathscr{C}$ coming from $-i\infty$ must cross the real axis to the right of $t=1/2$, and then once more between 0 and 1/2 (in order that the pole $t=0$ of $\Gamma(-t)$ lies to the right of it), before going to $+i\infty$. That is, before interchanging the sum and the integral we have to shift the contour $\mathscr{C}$ over the pole at $t=1/2$ to the left, cancelling the (potentially divergent) second piece in $A^D_{-1}(s)$. Closing then the contour to the left, we end up with the following expression in terms of Hurwitz zeta functions

$$A^D_{-1}(s)=\frac{R^{2s}}{2\sqrt{\pi}\Gamma(s)}\sum_{j=0}^{\infty}\frac{(-1)^j}{j!}(mR)^{2j}\frac{\Gamma(j+s-1/2)}{s+j}\zeta_H(2j+2s-2;1/2). \tag{3.17}$$

For A^D_0 one only needs to use the binomial expansion in order to find

$$A^D_0(s)=-\frac{R^{2s}}{2\Gamma(s)}\sum_{j=0}^{\infty}\frac{(-1)^j}{j!}(mR)^{2j}\Gamma(s+j)\zeta_H(2j+2s-1;1/2). \tag{3.18}$$

The series are convergent for $|mR|<1/2$. These representations (3.17) and (3.18) show very clearly the analytic structure of $A^D_{-1}(s)$ and $A^D_0(s)$. As the *fifth* (and final) *step* of our procedure, we are left with the quite simple task of explictly evaluating this analytic structure, namely of finding its poles and some point values, and of adding all contributions together.

The point values $A^D_{-1,0}(-p)$,$p\in\mathbb{N}_0$—respectively their residues at $s=1/2$, $-(2l+1)/2$, $l\in\mathbb{N}_0$— necessary for the calculation of the associated heat kernel coefficients are immediate to obtain, using

$$\zeta_H(1+\epsilon,1/2)=\frac{1}{\epsilon}+\mathscr{O}(\epsilon^0),$$

$$\Gamma(\epsilon-n)=\frac{1}{\epsilon}\frac{(-1)^n}{n!}+\mathscr{O}(\epsilon^0). \tag{3.19}$$

However, before we can actually calculate (an in principle arbitrary number of) the heat kernel coefficients, we need to obtain analytic expressions for the $A^D_i(s)$, $i\in\mathbb{N}$. As is easy to see, they are similar to the ones for $A^D_{-1}(s)$ and $A^D_0(s)$ above. We need to recall only that $D_i(t)$, Eq. (3.6), is a polynomial in t,

$$D_i(t)=\sum_{a=0}^{i} x_{i,a}t^{i+2a}, \tag{3.20}$$

which coefficients $x_{i,a}$ are easily found by using Eqs. (3.5) and (3.6) directly, or either by using the direct recursion relations presented in appendix A. Thus the calculation of $A_i^{\nu,D}(s)$ is essentially solved through the identity

$$\int_{mR/\nu}^{\infty} dz\left[\left(\frac{z\nu}{R}\right)^2-m^2\right]^{-s}\frac{\partial}{\partial z}t^n=-m^{-2s}\frac{n}{2(mR)^n}\frac{\Gamma(s+n/2)\Gamma(1-s)}{\Gamma(1+n/2)}\nu^n\left[1+\left(\frac{\nu}{mR}\right)^2\right]^{-s-n/2}. \tag{3.21}$$

The remaining sum may be done as mentioned for A_0^D, and we end up with

$$A_i^D(s)=-\frac{R^{2s}}{\Gamma(s)}\sum_{j=0}^{\infty}\frac{(-1)^j}{j!}(mR)^{2j}\zeta_H(-1+i+2j+2s;1/2)\sum_{a=0}^{i}x_{i,a}\frac{(i+2a)\Gamma(s+a+j+i/2)}{\Gamma(1+a+i/2)}. \tag{3.22}$$

In summary we have obtained the analytic expression of all the asymptotic terms coming from expansion (3.4) in its most elementary form, which involves the very familiar Hurwitz zeta functions and Gamma functions only. Expressions (3.17), (3.18) and (3.22) constitute the explicit starting point for the calculation of an —in principle arbitrary— number of heat kernel coefficients in an extremely quick way.

IV. HEAT KERNEL COEFFICIENTS FOR DIRICHLET BOUNDARY CONDITIONS ON THE THREE-DIMENSIONAL BALL

Let us now see how the analysis in Sec. II can be used for a very effective calculation of the heat kernel coefficients. The dependence of the coefficients on the mass is already contained in the coefficients of the massless case through

$$K_m(t)=K_{m=0}(t)e^{-m^2t}$$

and for this reason we shall restrict ourselves to $m=0$. For the sums in (3.17), (3.18) and (3.22) this means that only $j=0$ will contribute.

We shall distinguish between the coefficients B_k with integer and half-integer index k, because the situation is actually different in both cases. In fact, corresponding to Eq. (1.3) (resp. Eq. (1.4)), the residue of (resp. the value of the function) ζ_D is needed.

Let us start with the case of integer index $k\in\mathbb{N}$, so that Res $\zeta_D(3/2-k)$ is to be calculated. In order that $Z_D(s)$ does not contribute, one has to choose $N=2k-1$ and thus only the asymptotic terms $A_j^D(s), j=-1,0,1,...,2k-1$, will provide some contribution. Furthermore, one may see very easily which terms in the different $A_j^D(s)$ contribute. An important feature is, that for $i=2n$, $n\in\mathbb{N}_0$, $A_i^D(s)$ does not contribute to B_k for $k\in\mathbb{N}$. The relevant residues are found to be

$$\text{Res } A_{-1}^D\left(\frac{3}{2}-k\right)=\frac{(-1)^{k-1}}{(k-1)!}\frac{R^{3-2k}}{2\sqrt{\pi}\Gamma(5/2-k)}\zeta_H\left(1-2k;\frac{1}{2}\right),$$

$$\text{Res } A_{2k-1}^D\left(\frac{3}{2}-k\right)=-\frac{R^{3-2k}}{2\Gamma(3/2-k)}\sum_{a=0}^{2k-1}x_{2k-1,a}\frac{(2k-1+2a)a!}{\Gamma(1/2+a+k)},$$

and for $n\in\mathbb{N}$, $n\leqslant k-1$, $k\leqslant 3n$,

$$\text{Res}\ A_{2n-1}\left(\frac{3}{2}-k\right)=\frac{(-1)^k R^{3-2k}}{\Gamma(3/2-k)}\zeta_H\left(1+2n-2k;\frac{1}{2}\right)\sum_{a=0}^{k-1-n} x_{2n-1,a}\frac{(-1)^{a+n}(2n+2a-1)}{(k-1-a-n)!},$$

whereas for $n\leqslant k-1$, $k>3n$, we have

$$\text{Res}\ A_{2n-1}\left(\frac{3}{2}-k\right)=\frac{(-1)^k R^{3-2k}}{\Gamma(3/2-k)}\zeta_H\left(1+2n-2k;\frac{1}{2}\right)\sum_{a=0}^{2n-1} x_{2n-1,a}\frac{(-1)^{a+n}(2n+2a-1)}{(k-1-a-n)!}.$$

From these results we readily obtain the heat kernel coefficients through

$$\text{Res}\ \zeta_D\left(\frac{3}{2}-k\right)=\text{Res}\sum_{l=0}^{k} A_{2l-1}^D\left(\frac{3}{2}-k\right)\equiv\frac{B_k}{(4\pi)^{3/2}\Gamma(3/2-k)}.$$

The coefficients up to B_{10} are listed in appendix B.

Let us now consider the calculation of the coefficients corresponding to half-integer index $B_{k+1/2}, k\in\mathbb{N}$. Here the value of $\zeta_D(3/2-k)$ is needed and one finds $N=2k$. It is apparent that the $A_i^D(s)$ with odd i, $i=2j-1$, $j\in\mathbb{N}_0$, do not contribute now. The relevant values of the $A_i^D(s)$ read

$$A_0^D(1-k)=-\frac{R^{2-2k}}{2}\zeta_H\left(1-2k;\frac{1}{2}\right),$$

$$A_{2k}^D(1-k)=(-1)^k(k-1)!R^{2-2k}\sum_{a=0}^{2k} x_{2k,a}\frac{a!}{(a+k-1)!},$$

and for $n\in\mathbb{N}$, $n\leqslant k-1$, $k\leqslant 3n+1$,

$$A_{2n}^D(1-k)=-2R^{2-2k}(k-1)!\zeta_H\left(1+2n-2k;\frac{1}{2}\right)\sum_{a=0}^{k-n-1} x_{2n,a}\frac{(-1)^{n+a}}{(k-n-a-1)!(a+n-1)!},$$

whereas for $n\leqslant k-1$, $k>3n+1$, we have

$$A_{2n}^D(1-k)=-2R^{2-2k}(k-1)!\zeta_H\left(1+2n-2k;\frac{1}{2}\right)\sum_{a=0}^{2n} x_{2n,a}\frac{(-1)^{n+a}}{(k-n-a-1)!(a+n-1)!}.$$

And from these results, we finally obtain

$$\zeta_D(1-k)=\sum_{n=0}^{k} A_{2n}(1-k)\equiv\frac{(-1)^{k-1}(k-1)!}{(4\pi)^{3/2}}B_{k+1/2}.$$

The heat kernel coefficients $B_{k+1/2}$ are listed in appendix B too. Using $\zeta_H(-n;q)=-B_{n+1}(q)/(n+1), n\in\mathbb{N}_0$, the results might have been given, equivalently, in terms of Bernoulli polynomials $B_{n+1}(q)$.

V. ROBIN BOUNDARY CONDITIONS ON THE THREE-DIMENSIONAL BALL

When Robin boundary conditions are imposed, using the same method of the preceding sections we can write the zeta function as

$$\zeta_R(s)=\sum_{l=0}^{\infty}(2l+1)\int_\gamma\frac{dk}{2\pi i}(k^2+m^2)^{-s}\frac{\partial}{\partial k}\ln\left[\frac{u}{R}J_{l+1/2}(kR)+kJ'_{l+1/2}(kR)\right] \tag{5.1}$$

and, in analogy with Eq. (3.3), we then consider

$$\zeta_R^\nu = \frac{\sin(\pi s)}{\pi} \int_m^\infty dk (k^2 - m^2)^{-s} \frac{\partial}{\partial k} \ln\left[k^{-\nu} \left(\frac{u}{R} I_\nu(kR) + k I'_\nu(kR) \right) \right]. \tag{5.2}$$

Employing the same idea as for Dirichlet boundary conditions, this time we have in addition the following uniform asymptotic expansion [43]

$$I'_\nu(\nu z) \sim \frac{1}{\sqrt{2\pi\nu}} \frac{e^{\nu\eta}(1+z^2)^{1/4}}{z} \left[1 + \sum_{k=1}^\infty \frac{v_k(t)}{\nu^k} \right], \tag{5.3}$$

with the $v_k(t)$ determined by

$$v_k(t) = u_k(t) + t(t^2-1)\left[\frac{1}{2} u_{k-1}(t) + t u'_{k-1}(t) \right].$$

In analogy with Eq. (3.6), we write

$$\ln\left[1 + \sum_{k=1}^\infty \frac{v_k(t)}{\nu^k} + \frac{u}{\nu} t \left(1 + \sum_{k=1}^\infty \frac{u_k(t)}{\nu^k} \right) \right] \sim \sum_{n=1}^\infty \frac{M_n(t)}{\nu^n}, \tag{5.4}$$

where the functions $M_n(t)$ are easily obtained. At this point we see already, that for Robin boundary conditions no additional calculation is necessary. Comparing the expansion (5.3) with (3.4) and introducing $A_i^R(s)$ for the contributions coming from the asymptotic terms, one has

$$A^R_{-1}(s) = A^D_{-1}(s), \quad A^R_0(s) = -A^D_0(s). \tag{5.5}$$

Furthermore, the functions $M_i(t)$ are of the form

$$M_i(t) = \sum_{a=0}^{2i} z_{i,a} t^{i+a} \tag{5.6}$$

(notice that here, in contrast with the case of Dirichlet boundary conditions, all powers between i and $3i$ are present). As a result, we find

$$A_i^R(s) = -\frac{R^{2s}}{\Gamma(s)} \sum_{j=0}^\infty \frac{(-1)^j}{j!} (mR)^{2j} \zeta_H(-1+i+2j+2s; 1/2) \sum_{a=0}^{2i} z_{i,a} \frac{(i+a)\Gamma(s+j+(i+a)/2)}{\Gamma(1+(i+a)/2)}. \tag{5.7}$$

One can show again that only the even indices i contribute to the residues of $\zeta_R(s)$, whereas the odd ones will contribute to the point values.

Restricting ourselves as before (see the comment in the previous section) to the massless case, the results for the heat kernel coefficients may now be read off from the formulas in the previous section. One has

$$\text{Res } A^R_{-1}\left(\frac{3}{2} - k \right) = \text{Res } A^D_{-1}\left(\frac{3}{2} - k \right),$$

$$\text{Res } A^R_{2k-1}\left(\frac{3}{2} - k \right) = -\frac{R^{3-2k}}{2\Gamma(3/2-k)} \sum_{a=0}^{4k-2} z_{2k-1,a} \frac{(2k-1+a)\Gamma(1+a/2)}{\Gamma(1/2+k+a/2)},$$

where the expressions for A^R_{2n-1} are found from the results in Sec. III, once $x_{2n-1,a}$ has been replaced with $z_{2n-1,2a}$. The coefficients for Neumann boundary conditions are given in appendix C, and for the general case (u arbitrary) in appendix D. For the point values the analogous formulas read

$$A^R_0(1-k) = -A^D_0(1-k),$$

$$A^R_{2k}(1-k) = (-1)^k R^{2-2k}(k-1)! \sum_{a=0}^{4k} z_{2k,a} \frac{(2k+a)\Gamma(1+a/2)}{2\Gamma(1+k+a/2)},$$

and once more the replacement of $x_{2n,a}$ with $z_{2n,2a}$ leads to the results for A^R_{2n}. The results for the heat kernel coefficients are summarized in appendices C and D.

VI. GENERALIZATION TO THE D-DIMENSIONAL BALL

As we will now explain, for the generalization of our results to the case of a D-dimensional ball almost no additional calculations are necessary. Let us discuss first the case of Dirichlet boundary condition. The starting point of the analysis is now

$$\zeta_D(s) = \sum_{l=0}^{\infty} d_l(D) \int_\gamma \frac{dk}{2\pi i} (k^2+m^2)^{-s} \frac{\partial}{\partial k} \ln J_{l+(D-2)/2}(kR). \tag{6.1}$$

It is easy to see that the above treatment for the individual terms of the l-series,

$$\zeta^\nu_D = \int_\gamma \frac{dk}{2\pi i} (k^2+m^2)^{-s} \frac{\partial}{\partial k} \ln J_\nu(kR) \tag{6.2}$$

remains valid, once we have set $\nu = l+(D-2)/2$. In order to use our procedure for the whole l-summation, what remains to be done is to substitute for the degeneracy $d_l(D)$ its value in powers of $l+(D-2)/2$, in order to find again expressions in terms of the Hurwitz zeta function $\zeta_H(s;(D-2)/2)$. Writing

$$d_l(D) = \sum_{\alpha=1}^{D-2} e_\alpha(D) \left(l + \frac{D-2}{2} \right)^\alpha, \tag{6.3}$$

the final results for $A^D_{-1}(s)$, $A^D_0(s)$ and $A^D_i(s)$, $i \in \mathbb{N}$, may be read off from Eqs. (3.17), (3.18) and (3.22). We find

$$A^D_{-1}(s) = \frac{R^{2s}}{4\sqrt{\pi}\Gamma(s)} \sum_{j=0}^{\infty} \frac{(-1)^j}{j!} (mR)^{2j} \frac{\Gamma(j+s-1/2)}{s+j} \left[\sum_{\alpha=1}^{D-2} e_\alpha(D) \zeta_H(2j+2s-1-\alpha;(D-2)/2) \right], \tag{6.4}$$

$$A^D_0(s) = -\frac{R^{2s}}{4\Gamma(s)} \sum_{j=0}^{\infty} \frac{(-1)^j}{j!} (mR)^{2j} \Gamma(s+j) \left[\sum_{\alpha=1}^{D-2} e_\alpha(D) \zeta_H(2j+2s-\alpha;(D-2)/2) \right], \tag{6.5}$$

$$A^D_i(s) = -\frac{R^{2s}}{2\Gamma(s)} \sum_{j=0}^{\infty} \frac{(-1)^j}{j!} (mR)^{2j} \left[\sum_{\alpha=1}^{D-2} e_\alpha(D) \zeta_H(-\alpha+i+2j+2s;(D-2)/2) \right] \times \sum_{a=0}^{i} x_{i,a} \frac{(i+2a)\Gamma(s+a+j+i/2)}{\Gamma(1+a+i/2)}. \tag{6.6}$$

We shall spare the reader the analogous results for Robin boundary conditions. They need not be given explicitly, since the procedure is absolutely clear by now. Let us just write down the relevant residues and point values of $\zeta_D(s)$ (the Robin case follows from the replacements explained in Sect. V). They read

$$\text{Res } A_{-1}^D\left(\frac{3}{2}-k\right)=\frac{(-1)^{k-1}}{(k-1)!}\frac{R^{3-2k}}{4\sqrt{\pi}\Gamma\left(\frac{5}{2}-k\right)}\sum_{\alpha=1}^{D-2}e_\alpha(D)\zeta_H\left(2-2k-\alpha;\frac{D-2}{2}\right),$$

for $n=1,\ldots,k-1$, $k>3n$,

$$\text{Res } A_{2n-1}\left(\frac{3}{2}-k\right)=(-1)^k\frac{R^{3-2k}}{2\Gamma(3/2-k)}\sum_{\alpha=1}^{D-2}e_\alpha(D)\zeta_H\left(2+2n-\alpha-2k;\frac{D-2}{2}\right)$$
$$\times\sum_{a=0}^{2n-1}(-1)^{n+a}x_{2n-1,a}\frac{2n+2a-1}{(k-1-n-a)!\Gamma(1/2+a+n)},$$

whereas for $k\leqslant 3n$, it reads

$$\text{Res } A_{2n-1}\left(\frac{3}{2}-k\right)=(-1)^k\frac{R^{3-2k}}{2\Gamma(3/2-k)}\sum_{\alpha=1}^{D-2}e_\alpha(D)\zeta_H\left(2+2n-\alpha-2k;\frac{D-2}{2}\right)$$
$$\times\sum_{a=0}^{k-n-1}(-1)^{n+a}x_{2n-1,a}\frac{(2n+2a-1)}{(k-1-n-a)!\Gamma(1/2+a+n)}.$$

For higher indices it is advisable to distinguish between D even and D odd. For D odd contributions arise for $n=k,\ldots,k+(D-3)/2$, and read

$$\text{Res } A_{2n-1}\left(\frac{3}{2}-k\right)=-\frac{R^{3-2k}}{4\Gamma(3/2-k)}e_{1+2n-2k}\sum_{a=0}^{2n-1}x_{2n-1,a}\frac{(2n+2a-1)(a+n-k)!}{\Gamma(1/2+a+n)},\tag{6.7}$$

whereas for D even the indices run from $n=k,\ldots,k+(D-4)/2$, and the results are

$$\text{Res } A_{2n}\left(\frac{3}{2}-k\right)=-\frac{R^{3-2k}}{2\Gamma(3/2-k)}e_{2+2n-2k}\sum_{a=0}^{2n}x_{2n,a}\frac{\Gamma(3/2-k+a+n)}{(a+n-1)!}.$$

Let us conclude with the list of point values. The leading asymptotics A_{-1}^D gives only contributions for $k=0$,

$$A_{-1}(0)=-\frac{1}{2}\sum_{\alpha=1}^{D-2}e_\alpha(D)\zeta_H\left(-\alpha-1;\frac{D-2}{2}\right).$$

Furthermore, for $n=1,\ldots,k-1$, we have

$$A_{2n}(1-k)=-R^{2-2k}(k-1)!\sum_{\alpha=1}^{D-2}e_\alpha(D)\zeta_H\left(-\alpha+2n+2-2k;\frac{D-2}{2}\right)$$
$$\times\sum_{a=0}^{2n}x_{2n,a}\frac{(-1)^{a+n}}{(a+n-1)!(k-1-a-n)!},$$

if $k>3n+1$, and if $k\leqslant 3n+1$

$$A_{2n}(1-k)=-R^{2-2k}(k-1)!\sum_{\alpha=1}^{D-2} e_\alpha(D)\zeta_H\left(-\alpha+2n+2-2k;\frac{D-2}{2}\right)$$
$$\times\sum_{a=0}^{k-n-1} x_{2n,a}\frac{(-1)^{a+n}}{(a+n-1)!(k-1-a-n)!}.$$

Finally, for D odd and for $n=k,...,k+(D-3)/2$,

$$A_{2n}(1-k)=\frac{1}{2}(-1)^k(k-1)!R^{2-2k}e_{1+2n-2k}\sum_{a=0}^{2n} x_{2n,a}\frac{(a+n-k)!}{(a+n-1)!},$$

whereas for D even the indices run from $n=k+1,...,k+(D-2)/2$, and the result reads

$$A_{2n-1}(1-k)=\frac{1}{4}(-1)^k(k-1)!R^{2-2k}e_{2n-2k}\sum_{a=0}^{2n-1} x_{2n-1,a}\frac{(2n-1+2a)\Gamma(1/2-k+a+n)}{\Gamma(1/2+a+n)}.$$

The formulas above simplify a bit if we write the degeneracy (2.6) under the form

$$d_l(D)=\frac{2}{(D-2)!}\left[\left(l+\frac{D-2}{2}\right)^2-\left(\frac{D}{2}-2\right)^2\right]\times\ldots\times\left(l+\frac{D-2}{2}\right),\ \text{for}\ \ D\ \ \text{odd},$$

$$d_l(D)=\frac{2}{(D-2)!}\left[\left(l+\frac{D-2}{2}\right)^2-\left(\frac{D}{2}-2\right)^2\right]\times\ldots\times\left(l+\frac{D-2}{2}\right)^2,\ \text{for}\ \ D\ \ \text{even},$$

so that $e_{2k}(D)=0$ for D odd and $e_{2k-1}(D)=0$ for D even, $k\in\mathbb{N}$.

Furthermore, one might use the following recursion for the coefficients $e_\alpha(D)$ appearing in the expression of the degeneracy $d_l(D)$, Eq. (6.3),

$$e_{2\alpha}(D+2)=\frac{1}{D(D-1)}\left[e_{2\alpha-2}(D)-\left(\frac{D}{2}-1\right)^2 e_{2\alpha}(D)\right],\ \text{for}\ \ D\ \ \text{even},$$

$$e_{2\alpha-1}(D+2)=\frac{1}{D(D-1)}\left[e_{2\alpha-3}(D)-\left(\frac{D}{2}-1\right)^2 e_{2\alpha-1}(D)\right],\ \text{for}\ \ D\ \ \text{odd},$$

where we have used the definitions $e_{-k}(D)=0$ for $k\in\mathbb{N}_0$ and $e_\alpha(D)=0$ for $\alpha>D-2$.

We have performed explicit calculations for $D=4$ and $D=5$. One has in these cases

$$d_l(4)=(l+1)^2,\quad e_1(4)=0,\quad e_2(4)=1,$$

$$d_l(5)=\tfrac{1}{3}(l+\tfrac{3}{2})[(l+\tfrac{3}{2})^2-\tfrac{1}{4}],\quad e_1(5)=-\tfrac{1}{12},\quad e_2(5)=0,\quad e_3(5)=\tfrac{1}{3}.$$

The results for the heat kernel coefficients are presented in appendices B, C and D.

VII. CONCLUSIONS

As promised in the introduction, we have developed in this paper a very convenient method in order to deal with the problem of the calculation of heat kernel coefficients corresponding to an arbitrary elliptic operator with any of the usual boundary conditions (Dirichlet, Neumann or Robin), with the only proviso that the behavior of some basis for its spectrum should be known (even if the eigenvalues themselves are actually unknown).

This is indeed a very common case in mathematical physics, what confers to our procedure a wide generality of application. Another fundamental characteristic of the method is its extreme simplicity, which comes in part from the quite strong background on zeta function computations that we have acquired during the last half a dozen years. This knowledge confers to the new method the same elegance that the procedure of zeta function regularization (including the analytic continuation techniques and non-trivial series commutation that it involves) has in itself.

Finally, we have tried our method with explicit examples and gave several tables of heat kernel coefficients that have been calculated here (with relative ease) for the first time. For the near future we envisage to investigate other physical applications where the method can prove useful.

Note: At the final stage of our analysis, P. Gilkey made us aware of related research by M. Levitin,[48] who has further developed the approach of Kennedy,[34,35] also with the aim of calculating higher-order heat kernel coefficients. We are indebted to M. Levitin for sending us his results, which have served as a very good check of our calculations. All results in common with his are in complete agreement.

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APPENDIX A: RECURSION RELATION FOR THE COEFFICIENTS $x_{i,a}$

In this appendix we present the recursion relations for the coefficients $x_{i,a}$, Eq. (3.20). For convenience let us introduce for $i \in \mathbb{N}$, $a=0,...,i$,

$$x_{i,a}=\frac{c_{i+1,a}}{2^{i+1}(i+2a)}.$$

Then, starting with $c_{1,0}=-1$, we find the following recursion relation,

$$c_{i,0}=(i-2)c_{i-1,0}-\frac{1}{2}\sum_{s=1}^{i-1} c_{i-s,0}c_{s,0},$$

$$c_{i,i-1}=(4-3i)c_{i-1,i-2}+\frac{1}{2}\sum_{s=1}^{i-1} c_{i-s,i-s-1}c_{s,s-1},$$

and for $a=1,..., i-2$, we have

$$c_{i,a}=(i-2+2a)(c_{i-1,a}-c_{i-1,a-1}) -\frac{1}{2}\sum_{s=1}^{i-1}\left(\sum_{j=\mathrm{Max}(0,1+a+s-i)}^{\mathrm{Min}(a,s-1)} c_{i-s,a-j}c_{s,j}-\sum_{j=\mathrm{Max}(0,a+s-i)}^{\mathrm{Min}(a-1,s-1)} c_{i-s,a-j-1}c_{s,j}\right).$$

This relation can be used very effectively for the calculation of the coefficients $x_{i,a}$.

APPENDIX B: HEAT KERNEL COEFFICIENTS FOR DIRICHLET BOUNDARY CONDITIONS

In this appendix we list our results for the heat kernel coefficients of the Laplace operator in three, four and five dimensions with Dirichlet boundary conditions. Here and in the following appendices, the first coefficients B_0,..., $B_{5/2}$ are listed for completeness and may also be found in Refs. 34,35 or derived from Ref. 12.

In three dimensions we have found that

$$B_0=\frac{3}{4}\pi R^3, \quad B_{1/2}=-2\pi^{3/2}R^2,$$

$$B_1=\frac{8\pi R}{3}, \quad B_{3/2}=-\frac{1}{6}\pi^{3/2},$$

$$B_2=-\frac{16\pi}{315R}, \quad B_{5/2}=-\frac{\pi^{3/2}}{120R^2},$$

$$B_3=-\frac{64\pi}{9009R^3}, \quad B_{7/2}=-\frac{47\pi^{3/2}}{20160R^4},$$

$$B_4=-\frac{202816\pi}{72747675R^5}, \quad B_{9/2}=-\frac{521\pi^{3/2}}{443520R^6},$$

$$B_5=-\frac{25426048\pi}{15058768725R^7}, \quad B_{11/2}=-\frac{9521\pi^{3/2}}{11531520R^8},$$

$$B_6=-\frac{90878576896\pi}{67689165418875R^9}, \quad B_{13/2}=-\frac{34344493\pi^{3/2}}{47048601600R^{10}}$$

$$B_7=-\frac{22835854180352\pi}{17531493843488625R^{11}}, \quad B_{15/2}=-\frac{36201091\pi^{3/2}}{47048601600R^{12}},$$

$$B_8=-\frac{1509389910845640704\pi}{10199647803203247138 75R^{13}}, \quad B_{17/2}=-\frac{153984929039\pi^{3/2}}{164481911193600R^{14}},$$

$$B_9=-\frac{1673450232605639069696\pi}{872477873086005760248675R^{15}}, \quad B_{19/2}=-\frac{13334525091737\pi^{3/2}}{10362360405196800R^{16}},$$

$$B_{10}=-\frac{6439850137321813453250 56\pi}{231206636367791526465898875R^{17}}.$$

In four dimensions the result is

$$B_0=\frac{1}{2}\pi^2R^4, \quad B_{1/2}=-\pi^{5/2}R^3,$$

$$B_1=2\pi^2R^2, \quad B_{3/2}=-\frac{11\pi^{5/2}R}{32},$$

$$B_2=-\frac{4\pi^2}{45}, \quad B_{5/2}=-\frac{35\pi^{5/2}}{4096R},$$

$$B_3=-\frac{464\pi^2}{45045R^2},\quad B_{7/2}=-\frac{911\pi^{5/2}}{196608R^3},$$

$$B_4=-\frac{107456\pi^2}{14549535R^4},\quad B_{9/2}=-\frac{827315\pi^{5/2}}{201326592R^5},$$

$$B_5=-\frac{23288576\pi^2}{3011753745R^6},\quad B_{11/2}=-\frac{158590273\pi^{5/2}}{32212254720R^7},$$

$$B_6=-\frac{20064545792\pi^2}{1933976154825R^8},\quad B_{13/2}=-\frac{630648945109\pi^{5/2}}{86586540687360R^9},$$

$$B_7=-\frac{492912963584\pi^2}{29464695535275R^{10}},\quad B_{15/2}=-\frac{70309732006867\pi^{5/2}}{5541538603991040R^{11}},$$

$$B_8=-\frac{37648078688043008\pi^2}{1204208713483264125R^{12}},\quad B_{17/2}=-\frac{1578924180477650401\pi^{5/2}}{624198908353550745 60R^{13}},$$

$$B_9=-\frac{887504373820227584\pi^2}{13409327181833639595R^{14}},\quad B_{19/2}=-\frac{1018264365864160946171\pi^{5/2}}{17976928560582261473280R^{15}},$$

$$B_{10}=-\frac{252629551155828479492096\pi^2}{161682962494959109416712 5R^{16}}.$$

Finally, in five dimensions we obtain

$$B_0=\frac{8\pi^2R^5}{15},\quad B_{1/2}=-\frac{4\pi^{5/2}R^4}{3},$$

$$B_1=\frac{32\pi^2R^3}{9},\quad B_{3/2}=-\pi^{5/2}R^2,$$

$$B_2=-\frac{128\pi^2R}{945},\quad B_{5/2}=\frac{17\pi^{5/2}}{360},$$

$$B_3=\frac{1216\pi^2}{45045R},\quad B_{7/2}=\frac{157\pi^{5/2}}{30240R^2},$$

$$B_4=\frac{235264\pi^2}{43648605R^3},\quad B_{9/2}=\frac{5\pi^{5/2}}{2464R^4},$$

$$B_5=\frac{779264\pi^2}{280598175R^5},\quad B_{11/2}=\frac{593\pi^{5/2}}{449280R^6},$$

$$B_6=\frac{91757946368\pi^2}{43074923448375R^7},\quad B_{13/2}=\frac{32815499\pi^{5/2}}{28229160960R^8},$$

$$B_7=\frac{22103738934272\pi^2}{10518896306093175R^9},\quad B_{15/2}=\frac{119034319\pi^{5/2}}{94097203200R^{10}},$$

$$B_8=\frac{53300366610079744\pi^2}{213978625242026163 75R^{11}},\quad B_{17/2}=\frac{798608979601\pi^{5/2}}{493445733580800R^{12}},$$

$$B_9=\frac{3818097875734148669 44\pi^2}{1118561375751289436216 25R^{13}},\quad B_{19/2}=\frac{146801666871373\pi^{5/2}}{62174162431180800R^{14}},$$

$$B_{10}=\frac{3181528278957943911219 2\pi^2}{6031477470464126777371275R^{15}}.$$

APPENDIX C: HEAT KERNEL COEFFICIENTS FOR NEUMANN BOUNDARY CONDITIONS

Here is a list of the results we have obtained for the heat kernel coefficients of the Laplace operator in three, four and five dimensions with Neumann boundary conditions. In three dimensions we have found

$$B_0=\frac{4}{3}\pi R^3,\quad B_{1/2}=2\pi^{3/2}R^2,$$

$$B_1=\frac{8\pi R}{3},\quad B_{3/2}=\frac{7}{6}\pi^{3/2},$$

$$B_2=\frac{16\pi}{9R},\quad B_{5/2}=\frac{47\pi^{3/2}}{60R^2},$$

$$B_3=\frac{6464\pi}{6435R^3},\quad B_{7/2}=\frac{3973\pi^{3/2}}{10080R^4},$$

$$B_4=\frac{14766656\pi}{31177575R^5},\quad B_{9/2}=\frac{5057\pi^{3/2}}{28160R^6},$$

$$B_5=\frac{2314167424\pi}{10756263375R^7},\quad B_{11/2}=\frac{2320069\pi^{3/2}}{27675648R^8},$$

$$B_6=\frac{1439468204288\pi}{13537833083775R^9},\quad B_{13/2}=\frac{11298472831\pi^{3/2}}{250925875200R^{10}},$$

$$B_7=\frac{369968178163712\pi}{5843831281162875R^{11}},\quad B_{15/2}=\frac{1718717967893\pi^{3/2}}{57211099545600R^{12}},$$

$$B_8=\frac{483665328253543669 76\pi}{1019964780320324713875R^{13}},\quad B_{17/2}=\frac{113384991528329\pi^{3/2}}{4511503849881600R^{14}},$$

$$B_9=\frac{7819802371259230453 76\pi}{1780567087930624000507 5R^{15}},\quad B_{19/2}=\frac{33839928581307889\pi^{3/2}}{1326382131865190400R^{16}},$$

$$B_{10}=\frac{1439243621677544005066342 4\pi}{2972656753300176768847271 25R^{17}}.$$

In four dimensions

$$B_0=\frac{1}{2}\pi^2R^4,\quad B_{1/2}=\pi^{5/2}R^3,$$

$$B_1=2\pi^2R^2,\quad B_{3/2}=\frac{41\pi^{5/2}R}{32},$$

$$B_2=\frac{116\pi^2}{45},\quad B_{5/2}=\frac{5861\pi^{5/2}}{4096R},$$

$$B_3=\frac{99472\pi^2}{45045R^2},\quad B_{7/2}=\frac{388657\pi^{5/2}}{393216R^3},$$

$$B_4=\frac{18334144\pi^2}{14549535R^4},\quad B_{9/2}=\frac{91095533\pi^{5/2}}{201326592R^5},$$

$$B_5=\frac{6269294336\pi^2}{15058768725R^6},\quad B_{11/2}=\frac{2096614963\pi^{5/2}}{32212254720R^7},$$

$$B_6=-\frac{1448614636544\pi^2}{13537833083775R^8},\quad B_{13/2}=-\frac{13041149176631\pi^{5/2}}{86586540687360R^9},$$

$$B_7=-\frac{38509398708224\pi^2}{100179964819935R^{10}},\quad B_{15/2}=-\frac{1498787760061463\pi^{5/2}}{5541538603991040R^{11}},$$

$$B_8=-\frac{75623979333176688 64\pi^2}{13246295848315905375R^{12}},\quad B_{17/2}=-\frac{23865356170241004641\pi^{5/2}}{624198908353550745 60R^{13}},$$

$$B_9=-\frac{30045051913611575296\pi^2}{3662211205122632662 5R^{14}},\quad B_{19/2}=-\frac{13525296643319409269778 7\pi^{5/2}}{2337000712875693991526 40R^{15}},$$

$$B_{10}=-\frac{30784375321962136705433 6\pi^2}{2309756607070844420238 75R^{16}}.$$

And, finally, in five dimensions

$$B_0=\frac{8\pi^2R^5}{15},\quad B_{1/2}=\frac{4\pi^{5/2}R^4}{3},$$

$$B_1=\frac{32\pi^2R^3}{9},\quad B_{3/2}=3\pi^{5/2}R^2,$$

$$B_2=\frac{1024\pi^2R}{135},\quad B_{5/2}=\frac{1873\pi^{5/2}}{360},$$

$$B_3=\frac{63296\pi^2}{6435R},\quad B_{7/2}=\frac{10121\pi^{5/2}}{1890R^2},$$

$$B_4=\frac{504064\pi^2}{61047R^3},\quad B_{9/2}=\frac{198463\pi^{5/2}}{55440R^4},$$

$$B_5=\frac{125689856\pi^2}{30879225R^5},\quad B_{11/2}=\frac{34154807\pi^{5/2}}{34594560R^6},$$

$$B_6=-\frac{56447170574848\pi^2}{157941385977375R^7},\quad B_{13/2}=-\frac{16602940093\pi^{5/2}}{14114580480R^8},$$

$$B_7=-\frac{945576485184512\pi^2}{281253911927625R^9},\quad B_{15/2}=-\frac{13550828636809\pi^{5/2}}{5721109954560R^{10}},$$

$$B_8=-\frac{2591040115278546288 64\pi^2}{5563444256292680257 5R^{11}},\quad B_{17/2}=-\frac{5379580705269259\pi^{5/2}}{1973782934323200R^{12}},$$

$$B_9=-\frac{4618067750093566203084 8\pi^2}{9587668935011052310425R^{13}},\quad B_{19/2}=-\frac{26403546772565576 17\pi^{5/2}}{9947865988988928 00R^{14}},$$

$$B_{10}=-\frac{1401638457879249954799616\pi^2}{3067757227347963641741 25R^{15}}.$$

APPENDIX D: HEAT KERNEL COEFFICIENTS FOR ROBIN BOUNDARY CONDITIONS

We conclude our list of results with the leading coefficients for general Robin boundary conditions for $D=3,4$ and 5.

In three dimensions, we have found

$$B_0=\frac{4\pi R^3}{3},\quad B_{1/2}=2\pi^{3/2}R^2,$$

$$B_1=-\frac{4\pi R}{3}(1+6u),\quad B_{3/2}=\frac{\pi^{3/2}}{6}(1+24u^2),$$

$$B_2=\frac{2\pi}{45R}(1-18u+60u^2-120u^3),\quad B_{5/2}=\frac{\pi^{3/2}}{60R^2}(2-15u+60u^2-120u^3+120u^4),$$

$$B_3=\frac{\pi}{45045R^3}(1633-12870u+46904u^2-107536u^3+144144u^4-96096u^5),$$

$$B_{7/2}=\frac{\pi^{3/2}}{10080R^4}(151-1008u+3612u^2-8400u^3+13440u^4-13440u^5+6720u^6),$$

$$B_4=\frac{\pi}{436486050R^5}(8243319-51363270u+169826940u^2-395830040u^3+676878800u^4$$
$$-835097120u^5+665121600u^6-266048640u^7),$$

$$B_{9/2}=\frac{\pi^{3/2}}{1774080R^6}(14639-80784u+249304u^2-556600u^3+976800u^4-1330560u^5$$
$$+1340416u^6-887040u^7+295680u^8),$$

$$B_5=\frac{\pi}{301175374500R^7}(3517532467-17760354570u+49945523040u^2-105573378240u^3$$
$$+182023225440u^4-259648898880u^5+295543449600u^6-252181862400u^7$$
$$+142779436800u^8-40794124800u^9).$$

In four dimensions, the results read

$$B_0=\frac{\pi^2R^4}{2},\quad B_{1/2}=\pi^{5/2}R^3,$$

$$B_1=-2\pi^2R^2(1+2u),\quad B_{3/2}=\frac{\pi^{5/2}R}{32}(9+32u+64u^2),$$

$$B_2=-\frac{4\pi^2}{45}(1+30u^3),$$

$$B_{5/2}=-\frac{\pi^{5/2}}{4096R}(59-224u+2048u^3-4096u^4),$$

$$B_3=-\frac{16\pi^2}{45045R^2}(75-286u+286u^2+858u^3-3003u^4+3003u^5),$$

$$B_{7/2}=-\frac{\pi^{5/2}}{393216R^3}(5807-21024u+29952u^2+7168u^3-110592u^4+196608u^5-131072u^6),$$

$$B_4=-\frac{32\pi^2}{14549535R^4}(11726-39368u+62016u^2-36176u^3-75582u^4+230945u^5-277134u^6$$
$$+138567u^7),$$

$$B_{9/2}=-\frac{\pi^{5/2}}{201326592R^5}(2961171-9105152u+14440448u^2-13142016u^3-458752u^4$$
$$+25427968u^5-46137344u^6+41943040u^7-16777216u^8),$$

$$B_5=-\frac{64\pi^2}{15058768725R^6}(6419236-17976600u+27448200u^2-28336920u^3+14866740u^4$$
$$+14709420u^5-49365705u^6+65189475u^7-47805615u^8+15935205u^9).$$

Finally, in five dimensions we have found

$$B_0=\frac{8\pi^2R^5}{15},\quad B_{1/2}=\frac{4\pi^{5/2}R^4}{3},$$

$$B_1=-\frac{8\pi^2R^3}{9}(5+6u),\quad B_{3/2}=\frac{\pi^{5/2}R^2}{3}(3+8u+8u^2),$$

$$B_2=\frac{4\pi^2R}{135}(-5+6u-60u^2-120u^3),\quad B_{5/2}=\frac{\pi^{5/2}}{360}(-17-240u^2+480u^4),$$

$$B_3=\frac{2\pi^2}{135135R}(87+13442u-35464u^2+61776u^3+48048u^4-96096u^5),$$

$$B_{7/2}=\frac{\pi^{5/2}}{7560R^2}(-88+483u-1806u^2+2940u^3-1680u^4-3360u^5+3360u^6),$$

$$B_4=\frac{\pi^2}{43648605R^3}(-539501+4050078u-12086660u^2+23878744u^3-23715952u^4$$
$$+1478048u^5+26604864u^6-17736576u^7),$$

$$B_{9/2}=\frac{\pi^{5/2}}{2661120R^4}(-18927+99616u-302720u^2+576048u^3-748704u^4+473088u^5+177408u^6$$
$$-591360u^7+295680u^8),$$

$$B_5=\frac{\pi^2}{903526123 50R^5}(-935536567+4964319990u-13111462800u^2+25019918880u^3$$
$$-34365190560u^4+32451298368u^5-12409401600u^6-12609093120u^7+20397062400u^8$$
$$-8158824960u^9).$$

This concludes our lists of explicit tables for the heat kernel coefficients. In the same way, results for any desired dimension D are very easy to obtain from the formulas in the text.

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On position and momentum operators in the q-oscillator algebra

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The aim of this paper is to study the position and momentum operators in q-deformed oscillator algebras. The natural form of the position operator is $X_p = q^{pN}(a^+ + a)q^{pN}$, where p is a real number. This operator is an operator representable by a Jacobi matrix. Using the theory of Jacobi matrices, the theory of classical moment problem and the theory of basic hypergeometric functions, it is shown that, depending on values of q and p, X_p can be unbounded symmetric operator [which has the deficiency indices (1,1) and, hence, is not self-adjoint, but has self-adjoint extensions], bounded self-adjoint operator with continuous simple spectrum or self-adjoint operator of trace class (therefore, with discrete spectrum with zero as the point of accumulation of eigenvalues). The connection of the q-deformed Heisenberg relation $PX - qXP = 1$ for the position and momentum operators with a q-deformation of the quantum harmonic oscillator is also considered. © *1996 American Institute of Physics.* [S0022-2488(96)04401-6]

I. INTRODUCTION

The q-oscillator appeared in the papers by Coon and others[1–3] devoted to dual resonance models. The q-oscillator relation can also be found in the papers by Feinsilver[4,5] on the Heisenberg–Weyl algebra. The q analog of the quantum harmonic oscillator, related to the quantum group $SU_q(2)$, was studied by Biedenharn[6] and Macfarland.[7] The papers by Biedenharn and Macfarlane initiated an extensive research of q-deformed oscillators and their different applications. There exists a good review on this subject by Damaskinsky and Kulish.[8] A big attention to q-oscillators is related to quantum groups appeared approximately ten years ago. Quantum groups and q oscillators led to a new development in mathematical and theoretical physics.

For the one-dimensional q oscillator, the theory was developed similar to that for the usual quantum harmonic oscillator (coherent states, linear representations, different realizations, and so on). As in the case of quantum groups, many things for the q-deformed oscillator differ from the corresponding items for the usual quantum oscillator. For example, in the q-deformed case we have not so good a connection of the creation and annihilation operators with the q-Heisenberg–Weyl algebra containing the position and momentum operators.

It is well known that the operators of canonical position $X = a^+ + a$ and of canonical momentum $P = i(a^+ - a)$ are self-adjoint operators with a continuous simple spectrum, coinciding with the real axis. (It would be more natural to use the words ''Hermitian operator,'' which is a synonym of ''self-adjoint operator.'' However, in our investigation below we extensively use the mathematical literature, where the words ''self-adjoint operator'' and the notion ''self-adjoint extensions'' are used. For this reason, we use the same words.) This is not the case for q-deformed oscillators.[9] It is natural for representations of quantum algebras and of q-deformed oscillator algebras that closures of unbounded symmetric operators are not self-adjoint operators.[10] Since the difference between symmetric and self-adjoint operators is very important for our study, we recall

these notions. Let A be a linear unbounded operator on a Hilbert space H. Suppose that the domain $D(A)$ of A is an everywhere dense subspace of H and A is a closed operator. If A would not be closed, then we could close it and obtain a closed operator. There are pairs v and v' of elements from H such that

$$\langle v|Au\rangle=\langle v'|u\rangle, \quad \text{for} \quad \text{all} \ \ u\in D(A).$$

We set $v'=A^*v$ and call A^* the operator conjugate to A. It is proved that A^* is defined on an everywhere dense subspace $D(A^*)$ of H [since $D(A)$ is everywhere dense in H]. The operator A^* is linear and closed. Moreover, $A^{**}=A$ if A is closed. The operator A is called symmetric if $A\subseteq A^*$, that is, $D(A)\subset D(A^*)$. If $A^*=A$, that is $D(A)=D(A^*)$, then A is called self-adjoint. If a symmetric operator is not self-adjoint, then it can have self-adjoint extensions. To know whether a symmetric operator A has self-adjoint extensions or not, there are the notion of deficiency indices (m,n) of A. If these indices are equal to each other, then A has self-adjoint extensions. Self-adjoint extensions are constructed with the help of deficiency subspaces. A detailed description of deficiency indices and deficiency subspaces can be found in Ref. 11.

The important fact is that different self-adjoint extensions of a symmetric operator can have different spectra. For example, it was shown in Ref. 12 that in a q-deformed Heisenberg algebra, symmetric operators appear that have self-adjoint extensions with nonoverlaping spectra, that is, their spectra have no common points. This can happen when their spectra are discrete. This means that we must be very careful when dealing with closed symmetric operators that are not self-adjoint. In order to avoid an ambiguity we must deal with self-adjoint operators. In other words, if a closed symmetric operator is not self-adjoint, then we must take an appropriate self-adjoint extension (of course, we must have some criterion explaining to us which self-adjoint extension we need; clearly, this criterion depend on a problem we must solve).

In this paper we study in detail the position and momentum operators in the q-oscillator algebra. These operators are operators representable by Jacobi matrices. Therefore, we can apply the theory of moment problem,[13] the theory of Jacobi matrices,[14] as well as the theory of basic hypergeometric functions.[15] The theory of Jacobi matrices reduces the spectral theory of the position operator to studying three-term recurrence relations. Solutions of these recurrence relations are q-orthogonal polynomials. Actually, values of these polynomials are coefficients of transition from the usual basis $|n\rangle$ to the basis that diagonalizes the position operator. An orthogonality relation for polynomials, which are solutions of an appropriate three-term recurrence relation, defines the spectral measure of the position operator under consideration. The transition coefficients that appear here are also called overlap coefficients for the corresponding bases. These coefficients are of independent interest, since they can have a certain physical meaning.

Depending on values of q, there appear different possibilities. Sometimes, the position operator is bounded and, therefore, its closure is a self-adjoint operator. In other cases, it is not bounded and then its closure is not a self-adjoint operator. But in the last cases it has the deficiency indices (1,1) and, therefore, has self-adjoint extensions. For some cases we found explicitly the corresponding deficiency subspaces.

In Sec. II we give some information on the second-order difference operators that are used below. These operators are, in fact, operators representable by Jacobi matrices. In Sec. III we discuss the position and momentum operators in q-deformed oscillator algebras. We explain there why we must consider the position operators in the form $X_p=q^{pN}(a^++a)q^{pN}$. Section IV is devoted to studying the operators X_p for $q<1$. In Sec. V we investigate the operators X_p at $q>1$. Section VI is devoted to consideration of the q-Heisenberg relation $PX-qXP=1$ for position and momentum operators. In our investigation we extensively use the theory of q-orthogonal polynomials and basic hypergeometric functions. The theory of these polynomials and hypergeometric functions, as well as the related notions and assertions, can be found in Ref. 15.

II. DIFFERENCE OPERATORS OF THE SECOND ORDER

Let V be the Hilbert space with the orthonormal basis $|n\rangle$, $n=0,1,2,\ldots$. Let L be a linear operator on V, acting upon basis elements as

$$L|n\rangle = a_n|n+1\rangle + b_n|n\rangle + c_n|n-1\rangle, \tag{1}$$

and let

$$|z\rangle = \sum_{n=0}^{\infty} p_n(z)|n\rangle, \tag{2}$$

be an eigenvector of L with an eigenvalue z: $L|z\rangle = z|z\rangle$. Then

$$L|z\rangle = \sum_{n=0}^{\infty} (p_n(z)a_n|n+1\rangle + p_n(z)b_n|n\rangle + p_n(z)c_n|n-1\rangle) = z\sum_{n=0}^{\infty} p_n(z)|n\rangle.$$

Equating coefficients at the vector $|n\rangle$, we obtain the recurrence relation for the coefficients from (2):

$$c_{n+1}p_{n+1}(z) + b_n p_n(z) + a_{n-1}p_{n-1}(z) = zp_n(z). \tag{3}$$

Since $p_{-1}(z)\equiv 0$, then setting $p_0(z)\equiv 1$, we have that this relation completely determines the coefficients $p_n(z)$. Moreover, $p_n(z)$ are polynomials in z of degree n.

Sometimes, vectors $\mathbf{v}=\Sigma_{n=0}^{\infty} v_n|n\rangle$ of V are represented as numerical sequences $(v_0, v_1, \ldots)$. In this case formula (1) can be written as

$$(L\mathbf{v})_n = a_{n-1}v_{n-1} + b_n v_n + c_{n+1}v_{n+1}.$$

Because of this, such operators L are called *second-order difference operators*.

Now let L be a symmetric operator. Then formula (1) is of the form

$$L|n\rangle = a_n|n+1\rangle + b_n|n\rangle + a_{n-1}|n-1\rangle, \tag{4}$$

and Eq. (3), determining eigenvectors, reduces to the recurrence relation

$$a_n p_{n+1}(z) + b_n p_n(z) + a_{n-1}p_{n-1}(z) = zp_n(z). \tag{5}$$

If the coefficients a_n and b_n are real, then all coefficients of the polynomials $p_n(z)$ are real.

We suppose that a_n and b_n are real and $a_n>0$. If the operator L is unbounded, then we denote the closure of L by $\bar{L}$. The operator $\bar{L}$ may not be self-adjoint. In this case, $\bar{L}$ has nonzero deficiency indices (m,k), which determine dimensions of deficiency subspaces. (The definitions of deficiency indices and deficiency subspaces, as well as their properties, can be found in Ref. 11.) If $(m,k)\neq(0,0)$, then to every complex number z, $\operatorname{Im} z\neq 0$, there correspond its deficiency subspaces. The following statements may be used for studying operators L representable by formula (4).

(a) Deficiency indices of the operator $\bar{L}$ are coinciding. Moreover, these indices are (0,0) or (1,1). In the first case the operator L is self-adjoint. In the second case L is not self-adjoint, however, it has self-adjoint extensions.

(b) Deficiency indices of $\bar{L}$ are (0,0) if and only if the series $\Sigma_{n=0}^{\infty}|p_n(z)|^2$ diverges for all complex z, $\operatorname{Im} z\neq 0$, where $p_n(z)$ are polynomials from (5). If deficiency indices are (1,1), then this series converges for all complex z, $\operatorname{Im} z\neq 0$.

(c) If deficiency indices are (1,1), then deficiency subspaces are one-dimensional. The deficiency subspace $N_{\bar{z}}$ corresponding to a complex number $\bar{z}$ is spanned by the vector

$$\sum_{n=0}^{\infty} p_n(z)|n\rangle,$$

where $p_n(z)$ are taken from formula (5).

To find whether or not the operator $\bar{L}$ is self-adjoint, we may use the following statements.[14]

(a) If the coefficients a_n and b_n from (4) are bounded, then the operator $\bar{L}$ is bounded and, therefore, self-adjoint.

(b) If b_n are any real numbers and a_n are such that $\Sigma_{n=0}^{\infty} a_n^{-1}=\infty$, then the operator $\bar{L}$ is self-adjoint.

(c) Let $|b_n|\leqslant C$, $n=0,1,2,...$, and let beginning with some positive integer j we have $a_{n-1}a_{n+1}\leqslant a_n^2$, $n\geqslant j$. If

$$\sum_{n=0}^{\infty} \frac{1}{a_n}<\infty, \tag{6}$$

then the operator $\bar{L}$ is not self-adjoint. If $\bar{L}$ is not a self-adjoint operator, then it has self-adjoint extensions. There are infinitely many self-adjoint extensions of $\bar{L}$. We refer the reader to Refs. 11 and 14 for a more detailed discussion of self-adjoint extensions.

Using the terminology of Ref. 14, we can say about the operator $\bar{L}$ the following. Let B be the operator $\bar{L}$ if it is self-adjoint or its self-adjoint extension if it is not self-adjoint. Let $E(\Delta)$ be the decomposition of the unity of the operator B. Then

$$E(\Delta)=\int_{\Delta} P(\lambda)d\rho(\lambda),$$

where $P(\lambda)$ are operators of generalized projections acting from the space $l^2([0,\infty),d_n)$ into the space $l^2([0,\infty),d_n^{-1})$. Here $d_n\geqslant 0$ and such that $\Sigma_{j=0}^{\infty} d_j^{-1}<\infty$. Note that $l^2([0,\infty),d_n)$ is the space of sequences $(a_0,a_1,a_2,...)$ such that $\Sigma_{n=0}^{\infty}|a_n|^2 d_n<\infty$. The operators $P(\lambda)$ are matrix operators with positive definite matrices $(\Phi_{jk}(\lambda))_{j,k=0}^{\infty}$, satisfying the condition[14]

$$\sum_{j,k=0}^{\infty} |\Phi_{jk}(\lambda)|^2 (d_j d_k)^{-1}\leqslant 1.$$

Moreover, we have

$$\Phi_{jk}(\lambda)=p_j(\lambda)p_k(\lambda)\Phi_{00}(\lambda), \quad j,k=0,1,2,\ldots .$$

Let $d\sigma(\lambda)=\Phi_{00}(\lambda)d\rho(\lambda)$. It is shown in Ref. 14 that

$$\int_{-\infty}^{\infty} p_j(\lambda)p_k(\lambda)d\sigma(\lambda)=\delta_{jk}, \quad j,k=0,1,2,\ldots . \tag{7}$$

If the operator $\bar{L}$ is bounded and self-adjoint, then we can set $d_n=1$, $n=0,1,2,...$, and polynomials $p_j(\lambda)$ are coefficients of transition from the orthonormal basis $|n\rangle$ to the basis that diagonalizes the operator $\bar{L}$ (overlap coefficients). If we know the overlap coefficients, then we know eigenvectors of the operator $\bar{L}$. If we know the orthogonality relation for polynomials that give overlap coefficients, then we know spectrum and spectral measure for $\bar{L}$. Namely, the spectral measure of $\bar{L}$ coincides with $d\sigma(\lambda)$.

In general cases, it is difficult to evaluate polynomials $p_n(\lambda)$. The problem of their evaluation is closely related to the theory of orthogonal polynomials and to the moment problem (see, for example, Refs. 13 and 14). They are evaluated for many representation operators of type (4) for

infinite-dimensional representations of simplest Lie groups [for the groups $SL(2,\mathbf{R})$, $SO_0(3,1)$] and for class 1 representations of high dimension Lie groups (see Ref 16 and references therein). In Ref. 9 they are evaluated for some operators of different realizations of the q-oscillator algebra.

III. POSITION AND MOMENTUM OPERATORS FOR q-OSCILLATOR

We consider the q oscillator given by the relations

$$aa^+ - qa^+a = 1, \quad [N,a^+] = a^+, \quad [N,a] = -a. \tag{8}$$

The Fock representation of this q oscillator acts on the Hilbert space V with the orthonormal basis $|n\rangle, n=0,1,2,...$, and is given by the formulas

$$a|n\rangle = \left(\frac{1-q^n}{1-q}\right)^{1/2}|n-1\rangle, \quad a^+|n\rangle = \left(\frac{1-q^{n+1}}{1-q}\right)^{1/2}|n+1\rangle. \tag{9}$$

It follows from here that $N|n\rangle = n|n\rangle$.

For this q oscillator and for q oscillators given by other formulas,[6–8] it is assumed that the position and momentum operators are given, up to a constant, by the formulas

$$X = a^+ + a, \quad P = i(a^+ - a) \tag{10}$$

(see, for example, Ref. 6). Different q oscillators are related to each other by some nonlinear transformations.[8] That is, in fact, we deal with the same associative algebra, but q-creation and q-annihilation operators (which, together with the number operator N generate a q oscillator), are taken in different manners. Therefore, in the frame of the q-oscillator algebra, the position and momentum operators can be taken in different ways, depending on choosing the generating elements a^+, a, N. If to analyze the position and momentum operators in different cases, then one can make the following assertion. The position and momentum operators in a frame of any q oscillator differ from operators (10), taken for the q oscillator (8), by the mutipliers q^{pN}, where p is a real number. This fact compels us to study spectral properties of the operators,

$$X_p = q^{pN}(a^+ + a)q^{pN}, \quad P_p = iq^{pN}(a^+ - a)q^{pN}, \quad p \in \mathbf{R}. \tag{11}$$

Let us note that since

$$q^{sN}a^+q^{-sN} = q^s a^+, \quad q^{sN}aq^{-sN} = q^{-s}a,$$

then the operators

$$X = q^{pN}a^+q^{sN} + q^{sN}aq^{pN}, \quad P = i\{q^{pN}a^+q^{sN} - q^{sN}aq^{pN}\}, \tag{12}$$

with $p,s \in \mathbf{R}$ reduce to the operators of the type (11). Remark that the multipliers q^{pN} and q^{sN} in (11) and (12) are taken in such a way that the operators X and P are symmetric. If $q \to 1$ then, up to a constant, operators (11) tend to the usual position and momentum operators of the one-dimensional quantum harmonic oscillator.

It is well known that for the usual quantum harmonic oscillator the closures of the operators $a^+ + a$ and $i(a^+ - a)$ are unbounded self-adjoint operators with a continuous spectrum. In this paper we study spectra of operators (11) for different values of p. It is easy to show that multiplying the basis elements $|n\rangle$ by i^n, $i = \sqrt{-1}$, we transform the matrix of the operator $X = q^{pN}(a^+ + a)q^{pN}$ into that of the operator $P = iq^{pN}(a^+ - a)q^{pN}$. Therefore, the operators P and X are simultaneously bounded or unbounded, self-adjoint or not self-adjoint. Moreover, both of

them have the same spectrum and simultaneously have self-adjoint extensions or not. They also have the same spectral measure. For this reason, we consider below only the operator $X=q^{pN}(a^{+}+a)q^{pN}$.

It follows from formulas (9) that for the operator $X_p=q^{pN}(a^{+}+a)q^{pN}$ we have

$$X_p|n\rangle=a_{p,n}|n+1\rangle+a_{p,n-1}|n-1\rangle,$$

$$a_{p,n}=q^{2p(n+1)}q^{-p}\left(\frac{1-q^{n+1}}{1-q}\right)^{1/2}. \tag{13}$$

IV. SPECTRA AND EIGENVECTORS FOR THE OPERATORS X_p AT $q<1$

We assume in this section that $0<q<1$. The following assertion is valid for operator (13).

Proposition 1: Let $0<q<1$. If $p\geqslant 0$ then the operator X_p is bounded and has a unique self-adjoint extension coinciding with its closure $\overline{X_p}$. Moreover, $\overline{X_p}$ is an operator of trace class. If $p<0$, then the operator X_p is unbounded. The deficiency indices of $\overline{X_p}$ in the last case are (1,1) and the operator $\overline{X_p}$ is not self-adjoint. It has infinitely many self-adjoint extensions.

Proof: For the numbers $a_{p,n}$ from formula (13) at $q<1$, we have

$$a_{p,n+1}/a_{p,n}\to q^{2p}, \quad \text{when } n\to+\infty. \tag{14}$$

Since $0<q<1$, then the operator X_p is bounded for $p\geqslant 0$. It also follows from (14) that $\Sigma_{n=0}^{\infty}|a_{p,n}|<\infty$, that is, $\overline{X_p}$ is an operator of trace class. This proves the first part of the proposition. It follows from formula (14) that the operator $\overline{X_p}$ is unbounded for $p<0$. To prove the second part of the proposition, we remark that the inequality,

$$(1-q^{n-1})(1-q^{n+1})\leqslant(1-q^{n})^2, \tag{15}$$

is valid. Really, removing the parentheses, we obtain from here that $q+q^{-1}\geqslant 2$. This inequality is correct for all real q and the equality is achieved at $q=1$. It follows from (15) that

$$a_{p,n-1}a_{p,n+1}\leqslant a_{p,n}^2, \quad \text{for all } n>0.$$

Besides, in this case we have

$$\sum_{n=0}^{\infty}\frac{1}{a_{p,n}}<\infty,$$

since

$$a_{p,n}/a_{p,n+1}\to q^{-2p}<1, \quad \text{if } n\to+\infty.$$

Therefore, by criterion (c) from Sec. II, the deficiency indices of the operator $\overline{X_p}$, $p<0$, are (1,1). The proposition is proved.

Let us investigate the spectrum of the operator $\overline{X_p}$ for different values of p. If $p<0$, then the operator $\overline{X_p}$ has deficiency indices (1,1). In this case, any self-adjoint extension X_p^{ext} of $\overline{X_p}$, constructed without outcoming from the carrier Hilbert space V in which the operators a^{+} and a act, has a purely discrete simple spectrum (see Ref. 14, Sec. 1 of Chap. 7). Moreover, there exists a function $g(z)$ from the space $\mathbf{U}$ such that the spectrum of the operator X_p^{ext} coincides with the set of zeros $\lambda_j (j=1,2,3,\ldots)$ of $g(z)$ and jumps

$$\mu_j=\sigma(\lambda_j+0)-\sigma(\lambda_j), \quad j=1,2,3,\ldots,$$

of the spectral function $\sigma(u)$ of X_p^{ext} are such that the following conditions are fulfilled:

$$\sum_{j=1}^{\infty} \frac{1}{\mu_j(1+\lambda_j^2)(g'(\lambda_j))^2} < \infty, \quad \sum_{j=1}^{\infty} \frac{1}{\mu_j(g'(\lambda_j))^2} = \infty$$

(see Ref. 13, Chap. 4), where $g'(z)=(d/dz)g(z)$. Here **U** is the space of entire real functions on **C** such that the following conditions are fulfilled: (a) all zeros λ_j of g are real; (b) the absolute convergent expansion,

$$\frac{1}{g(z)} = \sum_{j=1}^{\infty} \frac{1}{g'(\lambda_j)(z-\lambda_j)},$$

has a place; (c) all series $\Sigma_{j=1}^{\infty}\lambda_j^m/g'(\lambda_j)$, $m=0,1,2,...$, are convergent.

It follows from these assertions that the discrete spectrum of the operator $\overline{X_p}$ has the infinite point as the only point of accumulation.

Let $p>0$. Since $\overline{X_p}$ is a trace class operator, it has a purely discrete spectrum with zero as the only point of accumulation. It follows from the results of Refs. 17 and 18 that the spectrum is symmetric with respect to the point $x=0$, which also belongs to the spectrum. We derive from Theorem 3 in Ref. 18 that there exists the transcendental meromorphic function $G(z)$ with the expansion

$$G(z) = -A + \sum_{n=1}^{\infty} \frac{2A_n}{z^2-\alpha_n^2},$$

where $-\Sigma_n A_n \alpha_n^{-2} < \infty$, $A \leqslant 0$, and $A_n < 0$, $n=1,2,...$, such that the spectrum of $\overline{X_p}$ coincides with the set of points $x=0$ and $x=\pm 1/\alpha_n$, $n=1,2,...$. Clearly, the points $x=\pm 1/\alpha_n$, $n=1,2,...$, are poles of the function $G(1/z)$. Jumps of the spectral measure $\sigma(x)$ of $\overline{X_p}$ at these poles are equal to residues of the function $z^{-1}G(1/z)$ at these points.[18] They coincide with

$$\sigma(x+0)-\sigma(x-0) = -A_n\alpha_n^{-2} \quad (\text{for the poles } \pm\alpha_n^{-1}),$$

and $\sigma(+0)-\sigma(-0)=-A$. Of course, the function $G(z)$ is determined by the coefficients b_{pm} from (13). However, the expression for $G(z)$ in terms of $a_{p,m}$ is very complicated [see formula (2.7) in Ref. 18].

We considered spectra of the operators $\overline{X_p}$ for $p>0$ and $p<0$. Now we have to consider the spectrum of the operator $X_0=a^+ + a$. We have

$$X_0|n\rangle = a_n|n+1\rangle + a_{n-1}|n-1\rangle, \quad a_n = \{(1-q^{n+1})/(1-q)\}^{1/2}.$$

This operator is bounded. Therefore, its closure $\overline{X_0}$ is a bounded self-adjoint operator. A generalized vector,

$$|x\rangle = \sum_{n=0}^{\infty} P_n(x)|n\rangle \tag{16}$$

is an eigenvector of $\overline{X_0}$ corresponding to an eigenvalue x, $x \in \mathbf{R}$, if $P_n(x)$, $n=0,1,2,...$, satisfy the recurrence relation

$$(1-q^{n+1})^{1/2}P_{n+1}(x) + (1-q^n)^{1/2}P_{n-1}(x) = (1-q)^{1/2}xP_n(x), \tag{17}$$

and the initial conditions $P_{-1}(x)\equiv 0$, $P_0(x)\equiv 1$. The substitution,

$$P_n(x)=(q;q)_n^{-1/2}\hat{P}_n(x),$$

where

$$(a;q)_n=(1-a)(1-aq)(1-aq^2)\cdots(1-aq^{n-1}),$$

reduces this recurrence relation to the form

$$\hat{P}_{n+1}(x)+(1-q^n)\hat{P}_{n-1}(x)=(1-q)^{1/2}x\hat{P}_n(x).$$

It can be written down as

$$P'_{n+1}(y)+(1-q^n)P'_{n-1}(y)=2yP'_n(y), \tag{18}$$

where $y=\frac{1}{2}(1-q)^{1/2}x$ and $P'_n(y)\equiv P'_n(\frac{1}{2}(1-q)^{1/2}x)=\hat{P}_n(x)$.

Comparing relation (18) with recurrence relation (6.2) for the continuous q-Hermite polynomials $H_n(y|q)$ from Ref. 19, we conclude that

$$P'_n(y)=H_n(y|q),$$

that is

$$P_n(x)=(q;q)_n^{-1/2}H_n((1-q)^{1/2}x/2|q). \tag{19}$$

Thus, eigenvectors of the operator $X_0=a^+ +a$ are given by formula (16), where the polynomials $P_n(x)$ are determined by (19).

The orthogonality relation for the polynomials $H_n(y|q)$ is given by the formula

$$\int_{-1}^{1}H_n(y|q)H_m(y|q)(1-y^2)^{-1/2}\prod_{k=0}^{\infty}\{1-2(2y^2-1)q^k+q^{2k})\}dy=\frac{2\pi(q;q)_n}{(q;q)_\infty}\,\delta_{nm}$$

[see formula (6.6) in Ref. 19]. Therefore, polynomials (19) satisfy the orthogonality relation

$$\int_{-b}^{b}P_n(x)P_m(x)\sigma(x)dx=\delta_{nm}, \tag{20}$$

where $b=2/(1-q)^{1/2}$ and

$$\sigma(x)=\frac{(1-q)^{1/2}(q;q)_\infty}{2\pi}\,\frac{\Pi_{k=0}^{\infty}\{1-((1-q)x^2-2)q^k+q^{2k}\}}{(4-(1-q)x^2)^{1/2}}. \tag{21}$$

Formula (20) means that the spectrum of the operator $\overline{X_0}$ is simple and continuous. This spectrum completely covers the interval $(-b,b)$, $b=2/(1-q)^{1/2}$. The spectral measure of $\overline{X_0}$ coincides with $\sigma(x)dx$, where $\sigma(x)$ is given by formula (21).

When $q\to 1$, then the spectrum turns into the real line and polynomials $P_n(x)$ tend to the usual Hermite polynomials multiplied by a constant. This agree with results for the quantum harmonic oscillator. Now we can formulate the following theorem.

Theorem 1: If $p>0$, then the operator $\overline{X_p}$ has a discrete simple spectrum with zero as the only point of accumulation. If $p<0$, then all self-adjoint extensions of $\overline{X_p}$ (without outcoming from the Hilbert space V) have discrete simple spectra with infinity as the only point of accumulation. The operator $\overline{X_0}$ has a continuous simple spectrum that covers the interval $(-b,b)$, $b=2/(1-q)^{1/2}$.

Let

$$|x\rangle=\sum_{n=0}^{\infty} P_n(x)|n\rangle$$

be an eigenvector of the operator $X_p: X_p|x\rangle=x|x\rangle$. Then the polynomials $P_n(x)$ satisfy the recurrence relation,

$$q^{2pn}q^p(1-q^{n+1})^{1/2}P_{n+1}(x)+q^{2p(n-1)}q^p(1-q^n)^{1/2}P_{n-1}(x)=(1-q)^{1/2}xP_n(x),$$

and the initial conditions $P_{-1}(x)\equiv 0$ and $P_0(x)\equiv 1$. Making here the substitution

$$P_n(x)=\left(\prod_{i=0}^{n-1} q^{-2pi}\right)\left(\prod_{i=1}^{n}(1-q^i)^{-1/2}\right)\hat{P}_n(x),$$

we obtain for $\hat{P}_n(x)$ the recurrence relation,

$$\hat{P}_{n+1}(x)+q^{4p(n-1)}(1-q^n)\hat{P}_{n-1}(x)=\frac{(1-q)^{1/2}}{q^p}\,x\hat{P}_n(x). \tag{22}$$

We found explicit expressions for overlap polynomials $P_n(x)$ and the corresponding spectral measure for operator $X_0=a^+ + a$. Unfortunately, we could not find an explicit expression for these polynomials in the case of the operator $\overline{X_p}$ for arbitrary real p. But it is possible to find polynomials $P_n(x)$ for some particular cases. Let us find them for $p=\frac{1}{4}$. In this case for polynomials $\hat{P}_n(x)$ we have

$$\hat{P}_{n+1}(x)+q^{n-1}(1-q^n)\hat{P}_{n-1}(x)=cx\hat{P}_n(x),$$

where $c=(1-q)^{1/2}q^{-1/4}$. It is equivalent to the relation

$$P'_{n+1}(y)+q^{n-1}(1-q^n)P'_{n-1}(y)=yP'_n(y),$$

where $y=cx\equiv(q^{-1/2}-q^{1/2})^{1/2}x$ and $P'_n(y)=\hat{P}_n(x)$. This recurrence relation coincides with the recurrence relation for the discrete q-Hermite polynomials,

$$H_n(y;q)=\sum_{k=0}^{[n/2]}\frac{(q;q)_n}{(q^2;q^2)_k(q;q)_{n-2k}}(-1)^k q^{k(k-1)}y^{n-2k}, \tag{23}$$

from Refs. 20 and 21. Here $[n/2]$ is an integral part of the number $n/2$. Therefore, $\hat{P}_n(x)=H_n(cx;q)$, $c=(q^{-1/2}-q^{1/2})^{1/2}$, and

$$P_n(x)=q^{-n(n-1)/4}(q;q)_n^{-1/2}H_n((q^{-1/2}-q^{1/2})^{1/2}x;q). \tag{24}$$

It follows from results of Ref. 21 that the orthogonality relation for polynomials (23) is of the form

$$\sum_{j=1}^{\infty}\{H_m(q^j;q)H_n(q^j;q)+H_m(-q^j;q)H_n(-q^j;q)\}\frac{q^j}{2}\frac{(q^{2j+2};q)_\infty(q;q^2)_\infty}{(q^2;q^2)_\infty}$$
$$+\tfrac{1}{2}(q;q^2)_\infty H_m(1;q)H_n(1;q)=\delta_{mn}q^{n(n-1)/2}(q;q)_n.$$

Therefore, the orthogonality relation for polynomials (24) is

$$\sum_{j=1}^{\infty}\{P_m(c^{-1}q^j)P_n(c^{-1}q^j)+P_n(-c^{-1}q^j)P_n(-c^{-1}q^j)\}W_j+P_m(-c^{-1})P_n(-c^{-1})W_0=\delta_{mn}, \tag{25}$$

where $c=(q^{-1/2}-q^{1/2})^{1/2}$ and

$$W_j=\frac{c^{-1}q^j}{2}\,\frac{(c^{-2}q^{2j+2};q^2)_\infty(q;q^2)_\infty}{(q^2;q^2)_\infty}. \tag{26}$$

This means that the spectrum of the operator $\bar{X}_{1/4}$ is simple and discrete. Moreover, the spectrum coincides with the set of points,

$$\pm\frac{q^j}{(q^{-1/2}-q^{1/2})^{1/2}}, \quad j=0,1,2,\ldots\ . \tag{27}$$

It follows from (25) that the set of vectors,

$$|d_j\rangle=\sum_{n=0}^{\infty}P_n\left(\frac{q^j}{(q^{-1/2}-q^{1/2})^{1/2}}\right)W_j^{1/2}|n\rangle, \quad j=0,1,2,\ldots,$$

$$|d_{-j}\rangle\equiv\sum_{n=0}^{\infty}P_n\left(-\frac{q^j}{(q^{-1/2}-q^{1/2})^{1/2}}\right)W_j^{1/2}|n\rangle, \quad j=1,2,3,\ldots,$$

where W_j are given by formula (26), form a new orthonormal basis of the Hilbert space V and

$$\bar{X}_{1/4}|d_j\rangle=d_j|d_j\rangle\equiv\frac{q^j}{(q^{-1/2}-q^{1/2})^{1/2}}\,|d_j\rangle, \quad j=0,1,2,\ldots,$$

$$\bar{X}_{1/4}|d_{-j}\rangle=d_{-j}|d_{-j}\rangle\equiv-\frac{q^j}{(q^{-1/2}-q^{1/2})^{1/2}}\,|d_{-j}\rangle, \quad j=1,2,3,\ldots\ .$$

Now let us consider the operator X_p at $p=-\frac{1}{4}$. In this case we represent formula (13) in the form

$$X_{-1/4}|n\rangle=b_n|n+1\rangle+b_{n-1}|n-1\rangle, \quad b_n=q^{1/4}\left(\frac{q^{-n-1}-1}{1-q}\right)^{1/2}.$$

This operator is unbounded and $\bar{X}_{-1/4}$ is not a self-adjoint operator. Since the deficiency indices of $X_{-1/4}$ are (1,1), then deficiency subspaces for this operator are one dimensional. Moreover, the deficiency subspaces $N_{\bar{z}}$, $\mathrm{Im}\,z\neq0$, are defined by the generalized vectors

$$|z\rangle=\sum_{n=0}^{\infty}P_n(z)|n\rangle, \tag{28}$$

such that

$$(q^{-n-1}-1)^{1/2}P_{n+1}(z)+(q^{-n}-1)^{1/2}P_{n-1}(z)=(q^{-1/2}-q^{1/2})^{1/2}zP_n(z),$$

and the initial conditions $P_{-1}(z)\equiv0$ and $P_0(z)\equiv1$ are satisfied. Making the substitution

$$P_n(z)=\left(\prod_{i=1}^{n}(q^{-i}-1)^{-1/2}\right)\hat{P}_n(z),$$

we obtain for $\hat{P}_n(z)$ the relation

$$\hat{P}_{n+1}(z)+(q^{-n}-1)\hat{P}_{n-1}(z)=(q^{-1/2}-q^{1/2})^{1/2}z\hat{P}_n(z).$$

This recurrence relation coincides with recurrence relation (1.7) in Ref. 22 (if q^{-1} is replaced by $q,q>1$) for the continuous q-Hermite polynomials $h_n(z|q)=i^{-n}H_n(iz|q)$ when $q>1$. Therefore,

$$\hat{P}_n(z)=h_n((q^{-1/2}-q^{1/2})^{1/2}z/2|q^{-1})$$

and

$$P_n(z)=q^{n(n+1)/4}(q;q)_n^{-1/2}h_n(cz|q^{-1}),$$

where $c=(q^{-1/2}-q^{1/2})^{1/2}/2$. We derive from formula (3.2) in Ref. 22 that the orthogonality relation for these polynomials are

$$\int_{-\infty}^{\infty}P_m(c^{-1}\sinh u)P_n(c^{-1}\sinh u)d\sigma(u)=\delta_{mn},$$

where

$$d\sigma(u)=\frac{du}{(q;q)_\infty(\log q^{-1})\Pi_{j=1}^{\infty}(1+2q^j\cosh 2u+q^{2j})}. \tag{29}$$

The operator $\overline{X_{-1/4}}$ can be extended to be a self-adjoint operator defined on the subspace

$$D(\overline{X_{-1/4}})\oplus N_z\oplus N_{\bar{z}},$$

where $D(\overline{X_{-1/4}})$ is the domain of $\overline{X_{-1/4}}$ and z is any fixed complex number. A description of self-adjoint extensions of symmetric operators can be found in Ref. 11, Chap. 7. It would be interesting to know how spectral measures of self-adjoint extensions of $\overline{X_{-1/4}}$ are connected with measure (29).

V. SPECTRA AND EIGENVECTORS FOR THE OPERATORS X_p AT $q>1$

If $q>1$, then the operators X_p have the following properties.

Proposition 2: Let $q>1$. If $p\leqslant-\frac{1}{4}$ then X_p is a bounded operator and has a unique self-adjoint extension coinciding with its closure $\overline{X_p}$. If $p>-\frac{1}{4}$ then the operator X_p is unbounded and $\overline{X_p}$ has the deficiency indices (1,1). In the last case, the operator $\overline{X_p}$ has infinitely many self-adjoint extensions.

Proof: For the numbers $a_{p,n}$ from formula (13) at $q>1$, we have

$$\frac{a_{p,n+1}}{a_{p,n}}=q^{2p+1/2}\left(\frac{q^{-n-2}-1}{q^{-n-1}-1}\right)^{1/2}\to q^{2p+1/2},\quad \text{when } n\to+\infty.$$

Now our proposition is proved in the same way as Proposition 1.

Again, if $p>-\frac{1}{4}$ then any self-adjoint extension X_p^{ext} of X_p, constructed without outcoming from the carrier Hilbert space V, has a purely discrete spectrum and there exists a function $g(z)$ from the space $\mathbf{U}$ such that the spectrum of X_p^{ext} coincides with the set of zeros λ_j $(j=1,2,3,...)$ of $g(z)$. In this case, the spectrum of X_p^{ext} has the infinite point as the only point of accumulation.

If $p<-\frac{1}{4}$ then $\overline{X_p}$ is an operator of trace class. It has a purely discrete spectrum with zero as the only point of accumulation.

Let us consider the spectrum of $\overline{X_p}$ at $p=-\frac{1}{4}$. In this case

$$\overline{X_{-1/4}}|n\rangle=a_n|n+1\rangle+a_{n-1}|n-1\rangle, \quad a_n=q^{1/4}\left(\frac{1-q^{-n-1}}{q-1}\right)^{1/2}.$$

A generalized vector,

$$|x\rangle=\sum_{n=0}^{\infty} P_n(x)|n\rangle,$$

is an eigenvector of $\overline{X_{-1/4}}$ with the eigenvalue x, $x\in\mathbf{R}$, if $P_n(x)$, $n=0,1,2,...$, satisfy the recurrence relation,

$$(1-q^{-n-1})^{1/2}P_{n+1}(x)+(1-q^{-n})^{1/2}P_{n-1}(x)=(q^{1/2}-q^{-1/2})^{1/2}xP_n(x).$$

This recurrence relation is solved in the same way as relation (17) and we have

$$P_n(x)=(q^{-1};q^{-1})_n^{-1/2}H_n((q^{1/2}-q^{-1/2})^{-1/2}x/2|q^{-1}),$$

where $H_n(y|q^{-1})$ are the continuous q-Hermite polynomials, taken with the base q^{-1}. For polynomials $P_n(x)$ we have the orthogonality relation

$$\int_{-b}^{b} P_n(x)P_m(x)\sigma(x)dx=\delta_{nm},$$

where $b=2/(q^{1/2}-q^{-1/2})^{1/2}$ and

$$\sigma(x)=\frac{(q^{1/2}-q^{-1/2})^{1/2}(q^{-1};q^{-1})_\infty}{2\pi}\,\frac{\Pi_{k=0}^{\infty}\{1-((1-q^{-1})x^2-2)q^{-k}+q^{-2k}\}}{(4-(1-q^{-1})x^2)^{1/2}}. \tag{30}$$

This means that the spectrum of the operator $\overline{X_{-1/4}}$ is simple and continuous. This spectrum exactly covers the interval $(-b,b)$, $b=2/(q^{1/2}-q^{-1/2})^{1/2}$. The spectral measure of $\overline{X_{-1/4}}$ coincides with $\sigma(x)dx$, where $\sigma(x)$ is given by formula (30). So, we can formulate the following theorem.

Theorem 2: If $p<-\frac{1}{4}$ then the operator $\overline{X_p}$ has a discrete simple spectrum with zero as the only point of accumulation. If $p>-\frac{1}{4}$, then all self-adjoint extensions of $\overline{X_p}$ (without outcoming from the Hilbert space V) have discrete simple spectra with infinity as the only point of accumulation. The operator $\overline{X_{-1/4}}$ has a continuous simple spectrum, which covers the interval $(-b,b)$, $b=2/(q^{1/2}-q^{-1/2})^{1/2}$.

Let us find the spectrum and the spectral measure for the operator $\overline{X_p}$ at $p=-\frac{1}{2}$. In this case

$$\overline{X_{-1/2}}|n\rangle=a_n|n+1\rangle+a_{n-1}|n-1\rangle, \quad a_n=q^{-n/2}\,\frac{(1-q^{-n-1})^{1/2}}{(q-1)^{1/2}}.$$

Therefore, a generalized vector,

$$|x\rangle=\sum_{n=0}^{\infty} P_n(x)|n\rangle$$

is an eigenvector of $\overline{X_{-1/2}}$ with the eigenvalue x, $x \in \mathbf{R}$, if $P_n(x)$, $n=0,1,2,...$, satisfy the recurrence relation

$$q^{-n/2}(1-q^{-n-1})^{1/2}P_{n+1}(x)+q^{(-n+1)/2}(1-q^{-n})^{1/2}P_{n-1}(x)=(q-1)^{1/2}xP_n(x).$$

Making the substitution

$$P_n(x)=\left(\prod_{i=0}^{n-1} q^{i/2}\right)\left(\prod_{i=1}^{n}(1-q^{-i})^{-1/2}\right)\hat{P}_n(x),$$

we obtain for $\hat{P}_n(x)$ the relation

$$\hat{P}_{n+1}(x)+q^{-n+1}(1-q^{-n})\hat{P}_{n-1}(x)=(q-1)^{1/2}x\hat{P}_n(x).$$

This recurrence relation is solved in the same way as relation (22). We obtain $\hat{P}_n(x)=H_n((q-1)^{1/2}x;q^{-1})$ and

$$P_n(x)=q^{n(n-1)/4}(q^{-1};q^{-1})_n^{-1/2}H_n((q-1)^{1/2}x;q^{-1}), \tag{31}$$

where $H_n(y;q)$ are the discrete q-Hermite polynomials (23).

The orthogonality relation for polynomials (31) is of the form (25), but now $c=(q-1)^{1/2}$ and

$$W_j=\frac{(q-1)^{-1/2}q^{-j}}{2}\,\frac{((q-1)^{-1}q^{-2j-2};q^{-2})_\infty(q^{-1};q^{-2})_\infty}{(q^{-2};q^{-2})_\infty}. \tag{32}$$

Therefore, the spectrum of the operator $\overline{X_{-1/2}}$ is simple and discrete. This spectrum coincides with the set of points

$$\pm\frac{q^{-j}}{(q-1)^{1/2}}, \quad j=0,1,2,\dots\ .$$

The eigenvectors of $\overline{X_{-1/2}}$ are the vectors

$$|d_j\rangle\equiv\sum_{n=0}^{\infty} P_n\left(\frac{q^{-j}}{(q-1)^{1/2}}\right)W_j^{1/2}|n\rangle, \quad j=0,1,2,\dots,$$

$$|d_{-j}\rangle\equiv\sum_{n=0}^{\infty} P_n\left(-\frac{q^{-j}}{(q-1)^{1/2}}\right)W_j^{1/2}|n\rangle, \quad j=1,2,3,\dots,$$

where W_j are given by formula (32). For these vectors we have

$$\overline{X_{-1/2}}|d_j\rangle=d_{\pm j}|d_{\pm j}\rangle, \quad \text{where } d_{\pm j}=\pm q^{-j}/(q-1)^{1/2}.$$

For the operator $\overline{X_p}$ at $p=0$ we have

$$\overline{X_0}=\left(\frac{q^{n+1}-1}{q-1}\right)^{1/2}|n+1\rangle+\left(\frac{q^n-1}{q-1}\right)^{1/2}|n-1\rangle.$$

This operator is unbounded and $\overline{X_0}$ is not a self-adjoint operator. Deficiency subspaces of $\overline{X_0}$ are one dimensional. The deficiency subspaces of N_z^-, $\operatorname{Im} z\neq 0$, are defined by the generating vectors

$$|z\rangle=\sum_{n=0}^{\infty} P_n(z)|n\rangle, \tag{33}$$

such that

$$(q^{n+1}-1)^{1/2}P_{n+1}(z)+(q^n-1)^{1/2}P_{n-1}(z)=(q-1)^{1/2}zP_n(z).$$

Solving this recurrence relation we find that

$$P_n(z)=q^{-n(n+1)/4}(q^{-1};q^{-1})_n^{-1/2}h_n((q-1)^{1/2}z|q),$$

where $h_n(y|q)$ are continuous q-Hermite polynomials with the base $q>1$ (see Sec. IV). The operator $\overline{X_0}$ can be extended to be the self-adjoint operator defined on the subspace,

$$D(\overline{X_0})\oplus N_z\oplus N_{\bar{z}},$$

where $D(\overline{X_0})$ is the domain of the operator $\overline{X_0}$.

VI. q-HEISENBERG POSITION AND MOMENTUM OPERATORS

For any $p\in\mathbf{R}$, the position and momentum operators, given by formulas (11), do not satisfy the q-deformed Heisenberg relation,

$$PX-qXP=1. \tag{34}$$

Let us find the new q deformation of the quantum harmonic oscillator, which is compatible with the q-Heisenberg relation (34). We suppose that a, a^+, and N satisfy the relations

$$H(N)aa^+-G(N)a^+a=1, \tag{35}$$

$$[N,a]=-a, \quad [N,a^+]=a^+, \tag{36}$$

where $H(N)$ and $G(N)$ are functions of N that must be found. Let

$$X=f(N)a+g(N)a^+, \quad P=h(N)a-k(N)a^+. \tag{37}$$

We take into account that relations (36) mean that

$$q^{sN}aq^{-sN}=q^{-s}a, \quad q^{sN}a^+q^{-sN}=q^sa^+.$$

Then Eqs. (34) and (35) lead to the relations

$$\frac{f(N+1)}{f(N)}=q\,\frac{h(N+1)}{h(N)}, \quad \frac{g(N-1)}{g(N)}=q\,\frac{k(N-1)}{k(N)}, \tag{38}$$

$$\{h(N)g(N+1)+qf(N)k(N+1)\}aa^+-\{k(N)f(N-1)+qg(N)h(N-1)\}a^+a=1. \tag{39}$$

Therefore, in (37) we have

$$f(N)=k(N)=\tfrac{1}{2}q^{2N}, \quad h(N)=g(N)=\tfrac{1}{2}q^N, \tag{40}$$

and according to (39) for $H(N)$ and $G(N)$ from (35), we obtain the expressions

$$H(N)=\tfrac{1}{2}(q^{2N+1}+q^{4N+3}), \quad G(N)=\tfrac{1}{2}(q^{4N-2}+q^{2N}). \tag{41}$$

So, we obtained the q-deformed oscillator algebra defined by formulas (35), (36), and (41). The Fock representation of this algebra acts in the Hilbert space V with the orthonormal basis $|n\rangle$, $n=0,1,2,...$, such that $N|n\rangle=n|n\rangle$. For the operators a^+ and a we have

$$a^+|n\rangle=\sqrt{\phi(n+1)}|n+1\rangle, \quad a|n\rangle=\sqrt{\phi(n)}|n-1\rangle,$$

where

$$\phi(n)=\frac{G(n-1)!}{H(n-1)!}\left(\frac{1}{H(0)}+\sum_{j=1}^{n-1}\frac{H(j-1)!}{G(j)!}\right), \tag{42}$$

and the factorials are defined by the formula

$$F(j)!=F(j)F(j-1)\cdot\cdot F(2)F(1), \quad F(0)!=1.$$

Inserting (41) into (42) yields to

$$\phi(n)=\frac{2q^{-n}}{(1+q^{2n-2})(1+q^{2n})}\left(1+\frac{q^n-q^{-n+1}}{q-1}\right). \tag{43}$$

Let us note that

$$a^+a=\phi(N), \quad aa^+=\phi(N+1),$$

where $\phi(N)$ is given by formula (42) or (43).

The position and momentum operators (37) are not symmetric in our case if $q\in\mathbf{R}$. It can be shown that these operators can be symmetric only if q is a root of unity. We also remark that realizations of the operators P and X, satisfying relation (34), by self-adjoint operators was found by Schmüdgen.[23]

Note added in proof: After the submission of this manuscript, we learned that there are some papers[24–28] that are mostly overlapping the material in the first part of this paper. We would like to mention that A. Kempf discussed Heisenberg algebra different from ours in his seminal work.[29–30]

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Analytic continuation from empirical data: A direct approach to the stabilization problem

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Analytic continuation plays a key role in many problems in physics. A central problem is the implementation of a stabilized continuation from approximate numerical data specified on an interior segment γ within the holomorphy domain. The solution to that problem presented in this paper is expressed in terms of a Fredholm integral equation of the second kind which refers only to the physical region γ; in this latter respect it differs from other approaches to the same problem which are normally formulated on the boundary, and has the considerable advantage of dealing directly with the physically relevant functions. © *1996 American Institute of Physics.* [S0022-2488(96)01401-2]

I. INTRODUCTION

A problem which arises in many different contexts in physics is to continue a data function $D(z)$ away from its domain of definition γ,γ being that part of the physical region within which the measurements defining $D(z)$ have been performed. Although the data function $D(z)$ will normally be given as a set of values corresponding to a discrete set of measurements, it may, however, in certain circumstances be given in functional form as an approximate theoretical expression such as, for example, that derived in QCD using a perturbative asymptotic expansion (in this particular example the data region γ will in fact be outside the physical region). In either case $D(z)$ will represent approximate information and a knowledge of the associated uncertainty will form an essential ingredient in the analysis. Continuation could be meant in various ways but applies most commonly within the context of the analytic properties of a complex function to which the data relate. We shall suppose that the data region γ is located within the interior of the holomorphy domain and that the problem of interest is to effect a continuation away from γ by associating the data function $D(z)$, given on γ, with an analytic function $X(z)$.

The first and obvious point to be made is that the process of analytic continuation as described is a totally unstable one. Despite the fact that the continuation of an analytic function is uniquely defined throughout the holomorphy domain, nevertheless when dealing with the practical problem of implementing such a continuation numerically, unless some suitable stabilizing condition is introduced we are faced with a mathematically ill-posed problem. This is because, without such stabilization, infinitesimal changes in the input function $D(z)$ can lead to arbitrarily large differences in the output. The stabilization problem, which is thus a necessary part of the process of carrying out the analytic continuation, and is a general feature of all so-called inverse problems, is well understood and has been applied in many different contexts. The classical method, due to Tychonov,[1] is based on the use of compact sets $\mathscr{C}_{\mathscr{K}}$, defined on some function space $\mathscr{C}$ referred to as the control space. For example, taking the domain of holomorphy to be the unit disk, we could define $\mathscr{C}$ to be the space of boundary value functions $x(\phi)\equiv X(e^{i\phi})$. The functions $X(z)$ are uniquely determined by the corresponding boundary function $x(\phi)$: there is a continuous linear map $\mathscr{M}$ (the Cauchy integral) from $\mathscr{C}$ to the space of functions X. Tychonov's method is based on the assumption that one can find physical arguments to require that the functions in the control space, in this case the $x(\phi)$, should lie within one of some set of compact sets $\mathscr{C}_{\mathscr{K}}\subset\mathscr{C}$.

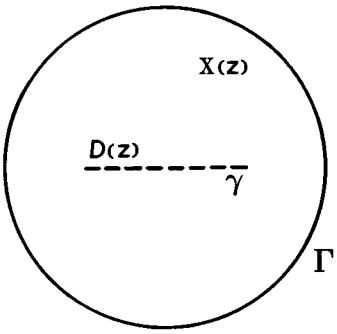

FIG. 1. The holomorphy domain of $X(z)$ and the data set γ where the data function $D(z)$ is given.

If we define the space $\mathscr{S}$ to consist, for example, of the L^2-functions defined on γ, then $\mathscr{C}$ is remote[2] from $\mathscr{S}$ but maps on to a subspace $\mathscr{M}(\mathscr{C})$ of $\mathscr{S}$ which consists of the restrictions $X^\gamma(z)$ to the segment γ, of the holomorphic functions defined by the boundary values $x(\phi)\in\mathscr{C}$. In the Tychonov procedure, stability is achieved through the restriction within $\mathscr{S}$ to $\mathscr{M}(\mathscr{C}_\mathscr{K})$, where $\mathscr{C}_\mathscr{K}\subset\mathscr{C}$ is compact. The continuity and bijectivity of $\mathscr{M}$ (the continuity and the uniqueness of the analytic continuation) together with the compactness of $\mathscr{C}_\mathscr{K}\subset\mathscr{C}$ ensures that the set $\mathscr{M}(\mathscr{C}_\mathscr{K})$ is also compact and that the inverse map $\mathscr{M}^{-1}$ from $\mathscr{M}(\mathscr{C}_\mathscr{K})$ to $\mathscr{C}_\mathscr{K}$ is also continuous. As well as that, and this is a key point, if the sets $\mathscr{C}_\mathscr{K}$ are convex, it ensures that within the subset $\mathscr{M}(\mathscr{C}_\mathscr{K})\subset$S there is a unique[3] nearest point[4] $X_Q^\gamma(z)$ to the data function $D(z)$. The corresponding boundary value $x_Q(\phi)\equiv\mathscr{M}^{-1}(X_Q^\gamma)\in\mathscr{C}_\mathscr{K}$ is usually referred to as the Tychonov regularized quasi-solution.

The practical difficulty with the Tychonov procedure is that actual physical constraints do not normally correspond to the restriction to compact sets $\mathscr{C}_\mathscr{K}$ in $\mathscr{C}$. Instead they are more likely to take the form of boundedness conditions producing a restriction in $\mathscr{C}$ to balls $\mathscr{C}_B$, $\|x\|\leqslant B$, which are not compact sets. Fortunately there is a useful role for ball conditions in implementing the program of stabilization using weak-star compactness. Why and how this works is explained in detail in Refs. 5 and 6, and in what follows we shall be dealing with physical constraints of this type.[7–9]

We begin by mapping the holomorphy domain onto the unit disk. The data set γ will be taken to be on the real axis, as shown in Fig. 1. We shall suppose that the data are given over a continuum γ, but the discussion may be readily adapted to apply to a discrete data set. For simplicity only real analytic functions are considered, which means that the data are values of a real function. The data will be denoted by $D(z)$, defined for $z\epsilon\gamma$, with corresponding errors $\epsilon(z)$, and the required function resulting from the analytic continuation will be represented by $X(z)$. In what follows $x(\phi)$ will denote a real function which may for example be $\Re e\ X(e^{i\phi})$, $\Im m\ X(e^{i\phi})$, $\partial\Im m\ X(e^{i\phi})/\partial\phi$, etc. Then $X(z)$ can be reconstructed from $x(\phi)$, for any point z within the disk, by a Schwarz–Villat type of representation expressed by an equation of the form

$$X(z)=d+\frac{1}{2\pi}\int_0^{2\pi}R(z_0;z,e^{i\phi})x(\phi)d\phi. \tag{1.1}$$

$R(z_0;z,e^{i\phi})$ takes the following forms, respectively, according as $x(\phi)$ is $\Re e\ X(e^{i\phi})$, $\Im m\ X(e^{i\phi})$ or $\partial\Im m\ X(e^{i\phi})/\partial\phi$,

$$\frac{e^{i\phi}+z}{e^{i\phi}-z},\quad \frac{2z\ \sin\ \phi}{1-2z\ \cos\ \phi+z^2}-\frac{2z_0\ \sin\ \phi}{1-2z_0\ \cos\ \phi+z_0^2},\quad 2\ln\frac{e^{i\phi}-z_0}{e^{i\phi}-z}. \tag{1.2}$$

The procedure is readily extended to include the case of the Cauchy kernel $e^{i\phi}/(e^{i\phi}-z)$, although in this case the boundary function $X(e^{i\phi})$ will no longer be real. The constant $d\equiv X(z_0)$ is a subtraction constant which arises from the need, in certain cases, to specify the value of $X(z)$ at one point z_0, usually chosen to be on the real axis, in order to fully determine the function $X(z)$. This occurs when, for example, out of the above alternatives, $x(\phi)$ is chosen to be $\Im m\ X(e^{i\phi})$ or $\partial\Im m\ X(e^{i\phi})/\partial\phi$. If $x(\phi)$ is chosen to be $\Re e\ X(e^{i\phi})$ or $X(e^{i\phi})$, then no subtraction is necessary and so d may be put equal to zero.

To obtain the quasi-solution $x_Q(\phi)$ for this problem, using bounded rather than compact sets to achieve stabilization, we consider the following two functionals:[6,10]

$$F_1[x]\equiv\delta=\frac{1}{2\pi}\int_0^{2\pi}(x(\phi))^2\sigma(\phi)d\phi, \tag{1.3}$$

$$F_2[X]\equiv\chi^2=\int_\gamma n(z)(X(z)-D(z))^2\,dz, \tag{1.4}$$

where $\sigma(\phi)$ is a suitably chosen positive weight function, and $n(z)\equiv(\epsilon(z))^{-2}$. We use the functional $F_2[X]\equiv\chi^2$ to provide a measure of the quality of fit of $X(z)$ to the given data $D(z)$, and any function X for which $F_2[X]\leqslant\chi_0^2$, where χ_0^2 is a suitably chosen constant, will be regarded as being compatible with the data $D(z)$ within the errors $\epsilon(z)$. Together, these two functionals—(1.3) allowing us to define a restriction within the space $\mathscr{C}$ of boundary value functions $x(\phi)$ to bounded sets $\mathscr{C}_B$, and (1.4) giving a measure of nearness to the data function $D(z)$ in terms of the prescribed errors $\epsilon(z)$—enable us to implement the stabilization procedure described above. What we do is to minimize $F_1[x]$ subject to the constraint $F_2[X]\leqslant\chi_0^2$ (although we could equally well have minimized F_2 with the restriction $F_1\leqslant\delta_0^2$). In fact the $x(\phi)$ which is constrained in this way, and the corresponding $X(z)$, may not represent the original function of interest but will more often correspond to the difference (discrepancy) when a trial function, usually depending on several parameters, has been subtracted from it. This procedure is explained in detail in Ref. 11.

To solve this stabilized problem of minimizing $F_1[x]$ subject to the data condition $F_2[X]\leqslant\chi_0^2$, the usual approach is to replace $X(z)$ in Eq. (1.4) by $x(\phi)$, using Eq. (1.1), so that F_2 becomes $F_2[x]$. One then constructs the functional $\mathscr{F}[x]\equiv F_1[x]+\lambda F_2[x]$, using a Lagrange multiplier λ, and then optimizes with respect to the function $x(\phi)$ by setting the Fréchet derivative of $\mathscr{F}[x]$ equal to zero,

$$\delta\mathscr{F}[x;y]\equiv\lim_{\alpha\to0}\frac{\partial}{\partial\alpha}\mathscr{F}[x(\phi)+\alpha y(\phi)]=0, \tag{1.5}$$

independently of the choice of function y. At the same time, bearing in mind that $\mathscr{F}[x]$ depends on the value of the subtraction constant d, and supposing that this value is not already determined by some other condition, we also optimize $\mathscr{F}$ with respect to d:

$$\frac{\partial\mathscr{F}}{\partial d}=0. \tag{1.6}$$

In this form the problem yields the required function $x(\phi)$ [which in turn defines $X(z)$ through Eq. (1.1)] as the solution to the following integral equation:

$$x(\phi)=\frac{\lambda}{\sigma(\phi)}\left\{G(z_0,\phi)+\frac{1}{2\pi}\int_0^{2\pi}K(z_0;\phi,\phi')x(\phi')d\phi'\right\}, \tag{1.7}$$

where

$$G(z_0;\phi)=\int_\gamma n(z')R(z_0;z',e^{i\phi})\left\{D(z')-\frac{1}{n_\gamma}\int_\gamma n(z'')D(z'')dz''\right\}dz', \tag{1.8}$$

$$K(z_0;\phi,\phi')=\frac{1}{n_\gamma}\int_\gamma n(z')R(z_0;z',e^{i\phi})dz'\int_\gamma n(z'')R(z_0;z'',e^{i\phi'})dz''$$
$$-\int_\gamma n(z')R(z_0;z',e^{i\phi})R(z_0;z',e^{i\phi'})dz' \tag{1.9}$$

and

$$n_\gamma\equiv\int_\gamma n(z')dz'. \tag{1.10}$$

The value of λ is determined using the condition $\chi^2=\chi_0^2$. The optimized value d_0 of the constant d, which is required in Eq. (1.1) to obtain the function $X(z)$, is given by

$$d_0=\frac{1}{n_\gamma}\int_\gamma dz'n(z')D(z')-\frac{1}{n_\gamma}\int_\gamma dz'n(z')\left\{\frac{1}{2\pi}\int_0^{2\pi}R(z_0;z',e^{i\phi})x(\phi)d\phi\right\}. \tag{1.11}$$

It is worth noting that, in this case, where we have optimized with respect to the subtraction constant d, the integral equation (1.7) is in fact independent of the subtraction point z_0. This follows from the fact that $R(z_0;z,e^{i\phi})$ can always be expressed in the form

$$R(z_0;z,e^{i\phi})\equiv R(z,e^{i\phi})-R(z_0,e^{i\phi}). \tag{1.12}$$

This is clear for the examples listed in Eq. (1.2), where the form of $R(z,e^{i\phi})$ in each case is obvious. Using Eq. (1.12) we can easily write $G(z_0;\phi)$ and $K(z_0;\phi,\phi')$ in a form which is manifestly independent of z_0:

$$G(z_0;\phi)\equiv G(\phi)=\int_\gamma dz'n(z')R(z',e^{i\phi})\{D(z')-\bar{D}\}, \tag{1.13}$$

$$K(z_0;\phi,\phi')=K(\phi,\phi')=\frac{1}{n_\gamma}\int_\gamma dz'n(z')R(z',e^{i\phi})\int_\gamma dz''n(z'')R(z'',e^{i\phi'})$$
$$-\int_\gamma dz'n(z')R(z',e^{i\phi})R(z',e^{i\phi'}), \tag{1.14}$$

where we have introduced $\bar{D}$ to represent the integral

$$\bar{D}\equiv\frac{1}{n_\gamma}\int_\gamma n(z')D(z')dz'. \tag{1.15}$$

[The term in $R(z_0,e^{i\phi})$ from the right-hand side of Eq. (1.12) has dropped out from Eqs. (1.13) and (1.14) since it does not depend on the integration variable and thus leaves a factor $\int dz'n(z')\{D(z')-\bar{D}\}$ which is zero.]

Another important result which holds in this case is that

$$\bar{X}\equiv\frac{1}{n_\gamma}\int_\gamma n(z')X(z')dz'=\bar{D}; \tag{1.16}$$

this follows directly from Eqs. (1.11) and (1.1).

It may happen that the value of $X(z)$ may be known at some point, not necessarily within the data range, for example at a physical threshold. If that point is chosen as the subtraction point, then the constant d is determined, say $d=d_1$. This is obviously an advantage and should improve the precision of the result for $X(z)$. In this fixed subtraction case we again obtain an integral equation identical in form with Eq. (1.7) but with $G(z_0;\phi)$ and $K(z_0;\phi,\phi')$ given by

$$G(z_0;\phi)=\int_\gamma n(z')R(z_0;z',e^{i\phi})(D(z')-d_1)dz' \tag{1.17}$$

$$K(z_0;\phi,\phi')=-\int_\gamma n(z')R(z_0;z',e^{i\phi})R(z_0;z',e^{i\phi'})dz'. \tag{1.18}$$

II. THE INTEGRAL EQUATION ON THE SEGMENT γ

In Sec. I we have summarized the usual approach to the stabilized analytic continuation problem. This is a necessary background to the primary purpose of the present paper which is to show that the integral equation (1.7), expressed in terms of the boundary values $x(\phi')$, may be replaced by an integral equation which applies to $X(z)$ directly and is written on the physically accessible data segment γ. It is convenient as well as elegant to be able to focus all one's attention on the data region without any explicit reference to the boundary function $x(\phi)$; it is also by no means obvious that it should be possible to do this, given the inherent instability of the analytic continuation from an open curve γ. In this section we show how this can be achieved, and derive the integral equation on γ for $X(z)$. Like Eq. (1.7) this is again a Fredholm equation of the second kind, the solution of which defines directly the analytic continuation away from the segment. The analytic continuation is discussed further in Sec. III where, in particular, an explicit expression is obtained for the continuation of $X(z)$ to the boundary.

If in Eq. (1.1) we substitute the right-hand side of Eq. (1.7) for $x(\phi)$, we obtain, after inserting the expressions (1.8) and (1.9) for $G(z_0;\phi)$, $K(z_0;\theta,\theta')$:

$$\begin{aligned}X(z)=d_0+\frac{\lambda}{2\pi}\int_0^{2\pi}\frac{d\phi}{\sigma(\phi)}R(z_0;z,e^{i\phi})\Bigg\{&\int_\gamma dz'n(z')R(z_0;z',e^{i\phi})(D(z')-\bar{D})\\&+\frac{1}{2\pi}\int_0^{2\pi}d\phi'\Bigg[\frac{1}{n_\gamma}\int_\gamma dz'n(z')R(z_0;z',e^{i\phi})\int_\gamma dz''n(z'')R(z_0;z'',e^{i\phi'})\\&-\int dz''n(z'')R(z_0;z'',e^{i\phi})R(z_0;z'',e^{i\phi'})\Bigg]x(\phi')\Bigg\}.\end{aligned} \tag{2.1}$$

We see now that we are in a position to carry out the ϕ' integration explicitly using Eq. (1.1); integrating $R(z_0;z'',e^{i\phi'})x(\phi')$ yields $X(z'')-d_0$ and so we have eliminated the boundary values $x(\phi')$ from Eq. (2.1), introducing instead the function $X(z'')$ defined on γ. The result is

$$\begin{aligned}X(z)=d_0+\frac{\lambda}{2\pi}\int_0^{2\pi}\frac{d\phi}{\sigma(\phi)}R(z_0;z,e^{i\phi})\Bigg\{&\int_\gamma dz'n(z')R(z_0;z',e^{i\phi})(D(z')-\bar{D})\\&+\frac{1}{n_\gamma}\int_\gamma dz'n(z')R(z_0;z',e^{i\phi})\int_\gamma dz''n(z'')(X(z'')-d_0)\\&-\int_\gamma dz''n(z'')R(z_0;z'',e^{i\phi})(X(z'')-d_0)\Bigg\}.\end{aligned} \tag{2.2}$$

This may be simplified, using Eq. (1.16), to the following form:

$$X(z)=d_0+\frac{\lambda}{2\pi}\int_0^{2\pi}\frac{d\phi}{\sigma(\phi)}\left\{R(z_0;z,e^{i\phi})\right.$$
$$\left.\times\int_\gamma dz'(z')R(z_0;z',e^{i\phi})(D(z')-X(z'))\right\}. \tag{2.3}$$

Notice that the d_0 which appears twice within the integral in Eq. (2.2) does not contribute, since the two corresponding terms cancel. To eliminate the other d_0 appearing at the beginning of the right-hand side of Eqs. (2.2) and (2.3), perhaps the most convenient way is again to use the result $X=D$ [Eq.(1.16)]. Inserting $X(z)$ from Eq. (2.3) into Eq. (1.16) gives

$$\bar{D}=d_0+\frac{\lambda}{2\pi}\int_0^{2\pi}\frac{d\phi}{\sigma(\phi)}\left\{\frac{1}{n_\gamma}\int_\gamma dz''n(z'')R(z_0;z'',e^{i\phi})\right.$$
$$\left.\times\int_\gamma dz'n(z')R(z_0;z',e^{i\phi})(D(z')-X(z'))\right\}. \tag{2.4}$$

This is now subtracted from Eq. (2.3) giving the result

$$X(z)=\bar{D}+\lambda\int_\gamma dz'n(z')\left(\mathscr{R}(z_0;z,z')-\frac{1}{n_\gamma}\int_\gamma dz''n(z'').\mathscr{R}(z_0;z'',z')\right)(D(z')-X(z')), \tag{2.5}$$

where we have defined $\mathscr{R}(z_0;z,z')$ by

$$\mathscr{R}(z_0;z,z')\equiv\frac{1}{2\pi}\int_0^{2\pi}\frac{d\phi}{\sigma(\phi)}R(z_0;z,e^{i\phi})R(z_0;z',e^{i\phi}). \tag{2.6}$$

If we now introduce the kernel $\mathscr{K}(z_0;z,z')$ defined by

$$\mathscr{K}(z_0;z,z')\equiv\mathscr{R}(z_0;z,z')-\frac{1}{n_\gamma}\int dz''n(z'').\mathscr{R}(z_0;z'',z'), \tag{2.7}$$

we obtain the following compact form of the integral equation for $X(z)$:

$$X(z)=\bar{D}+\lambda\int_\gamma dz'n(z').\mathscr{K}(z_0;z,z')D(z')-\lambda\int_\gamma dz'n(z').\mathscr{K}(z_0;z,z')X(z'). \tag{2.8}$$

There are several comments which may be made about this integral equation. The first is to observe that it may conveniently be expressed as an equation for $\mathscr{X}(z)\equiv X(z)-D(z)$, instead of for $X(z)$. In this case we have

$$\mathscr{X}(z)=(\bar{D}-D(z))-\lambda\int_\gamma dz'n(z').\mathscr{K}(z_0;z,z').\mathscr{X}(z'). \tag{2.9}$$

The second important point to make is that whereas $\mathscr{K}(z_0;z,z')$, defined by Eqs. (2.7), (2.6), and (1.12), is not independent of z_0, it is nevertheless possible to replace it in the integral equation

(2.8) by another kernel $\mathscr{K}(z,z')$ which is not only independent of the subtraction point z_0 but is also symmetric in z and z'. This is seen as follows. We first use Eqs. (2.7), (2.6), and (1.12) to write $\mathscr{K}(z_0;z,z')$ as

$$\mathscr{K}(z_0;z,z')=\frac{1}{2\pi}\int_0^{2\pi}\frac{d\phi}{\sigma(\phi)}\{R(z',e^{i\phi})-R(z_0,e^{i\phi})\}\{R(z,e^{i\phi})-\bar{R}(e^{i\phi})\}, \tag{2.10}$$

where, following an obvious notation, we have defined $\bar{R}(e^{i\phi})$ as

$$\bar{R}(e^{i\phi})\equiv\frac{1}{n_\gamma}\int_\gamma dz'n(z')R(z',e^{i\phi}). \tag{2.11}$$

Using again the fact that $\bar{X}-\bar{D}=0$, we obtain, after substituting Eq. (2.10) into Eq. (2.8),

$$X(z)=\bar{D}-\frac{\lambda}{2\pi}\int_0^{2\pi}\frac{d\phi}{\sigma(\phi)}\int_\gamma dz'n(z')R(z',e^{i\phi})\{R(z,e^{i\phi})-\bar{R}(e^{i\phi})\}\{X(z')-D(z')\}. \tag{2.12}$$

To make the kernel symmetric we can replace the factor $R(z',e^{i\phi})$ in the above equation by $R(z',e^{i\phi})-\bar{R}(e^{i\phi})$ without changing the value of the integral. We are now in a position to introduce a new kernel $\mathscr{K}(z,z')$, symmetric in z,z' and independent of z_0, defined as follows:

$$\mathscr{K}(z,z')=\frac{1}{2\pi}\int_0^{2\pi}\frac{d\phi}{\sigma(\phi)}\{R(z',e^{i\phi})-\bar{R}(e^{i\phi})\}\{R(z,e^{i\phi})-\bar{R}(e^{i\phi})\}. \tag{2.13}$$

Using $\mathscr{K}(z,z')$ we may write the integral equation in the following compact, manifestly z_0-independent and symmetric form:

$$X(z)=\bar{D}-\lambda\int_\gamma dz'n(z').\mathscr{K}(z,z')\{X(z')-D(z')\}. \tag{2.14}$$

The above result [Eq. (2.14)] relates to the situation where the subtraction constant d was not predetermined. The calculation leading to Eq. (2.14) incorporated a process of optimization with respect to d (leading to the optimal value d_0). The calculation in the fixed subtraction case, where the value $d=d_1$ of the subtraction constant at a specified point z_0 is known, is somewhat different. The integral equation for $X(z)$ is derived in the same way as above, but using Eqs. (1.17) and (1.18) for $G(z_0;\phi)$ and $K(z_0;\phi,\phi')$. The result in this case is

$$X(z)=d_1-\lambda\int_\gamma dz'n(z').\mathscr{R}(z_0,z,z')\{X(z')-D(z')\}. \tag{2.15}$$

The kernel of this integral equation is $\mathscr{R}(z_0;z,z')$, which is symmetric in z and z' but, as we would expect in this case, does depend on the subtraction point z_0.

As in the case of the integral equation for $x(\phi)$, the parameter λ has in each case to be determined from the condition $\chi^2=\chi_0^2$ [where χ^2 is defined in Eq. (1.4) and χ_0^2 is a given constant which specifies the precision of the data. We use the convexity of the functional χ^2 to impose the condition on the boundary $\chi^2=\chi_0^2$, rather than as an inequality $\chi^2\leqslant\chi_0^2$]. Notice that it is the same parameter λ which appears in the equations for $X(z)$ on the segment γ as in the equations on the boundary $x(\phi)$, so that the numerical value obtained for λ should be the same in either of the two approaches.

III. ANALYTIC CONTINUATION TO THE BOUNDARY

The integral equations (2.14) and (2.15) automatically provide an analytic continuation away from the integration region γ, since the domain of definition of $X(z)$ on the left-hand side of these equations is not restricted to γ. This procedure is often referred to as Nystrom continuation. We know that in general the analytic continuation from γ to the boundary will be unstable, in the sense that for two holomorphic functions which are close together on γ, even if these possess boundary values $x(\phi)$ on $|z|=1$ which are L^2, nevertheless the two corresponding functions $x(\phi)$ may be far apart. However, the functions $X(z)$ obtained as solutions to the integral equations are stable with respect to changes in $D(z)$ and, in fact, for any such solution $X(z)$, an explicit representation for the boundary value function $x(\phi)$ may be obtained. This is seen directly from Eq. (2.3) which has precisely the form of the generalized Schwarz–Villat representation given by Eq. (1.1) provided that we make the identification

$$x(\phi)=-\frac{\lambda}{\sigma(\phi)}\int_{\gamma}dz'n(z')R(z',e^{i\phi})\{X(z')-D(z')\}. \tag{3.1}$$

In deriving this we have used Eq. (1.12) for $R(z_0;z',e^{i\phi})$, and the relation $\bar{X}=\bar{D}$.

We may consider this representation, which gives the boundary function $x(\phi)$ in terms of the function $X(z)$ on the segment γ, as an *inverse Schwarz–Villat representation*. It is important to recognize that this inverse representation only applies in the very specific case of functions $X(z)$ which are solutions of the integral equations. Notice that the result depends on λ, the value of which has to be determined from the χ^2 condition. As an alternative to using Eq. (2.14) or (2.15) to perform an analytic continuation away from γ we can use Eq. (3.1) together with Eq. (1.1). Taken together these yield the function $X(z)$ at any point z within the unit disk.

In the case of a fixed subtraction constant d_1, the corresponding representation for $x(\phi)$ is

$$x(\phi)=-\frac{\lambda}{\sigma(\phi)}\int_{\gamma}dz'n(z')R(z_0;z',e^{i\phi})\{X(z')-D(z')\}. \tag{3.2}$$

As one would expect, this result is dependent on z_0 whereas Eq. (3.1) was not.

IV. CONCLUSION

We have been concerned in this paper with the problem of analytic continuation from approximate numerical data given on an interior segment, to the boundary of the domain of holomorphy. The usual approach to this problem leads, after a stabilization condition has been introduced, to an integral equation for the boundary values of the function. A representation of Schwarz–Villat type, Eq. (1.1), allows the value of the function $X(z)$ at any point in the holomorphy domain to be determined from the boundary values obtained from this integral equation. What we have shown here is that the same result can be achieved using an integral equation for $X(z)$ directly, the integration being over the physically accessible data segment γ instead of the boundary. We have derived these alternative integral equations and have shown that the solutions for $X(z)$ define an analytic continuation extending to the boundary. Like the other equations they are Fredholm equations of the second kind.

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On some representations of current algebras in two dimensions and their central extensions

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A class of unitary representations of the group of maps from a Riemannian manifold to a compact semisimple Lie group which are a modification of the so-called energy representations is considered. Their irreducibility is proved in any dimension $\geqslant 2$. This extends the known results of irreducibility for certain cases in dimension 2. Next, the corresponding algebra representations are studied and their irreducibility in dimension 2 is also proved. These are extended in a natural way to representations of certain central extensions of the algebras. Very explicit formulas are given, particularly on the two-dimensional torus, for the algebra extensions and the representations. © *1996 American Institute of Physics.* [S0022-2488(96)02801-3]

I. INTRODUCTION

Let G be a compact semisimple Lie group and X a Riemannian manifold. Consider the space $G^X \equiv \mathrm{Map}(X,G)$ of smooth maps from X to G, which send all points outside a compact set to the identity of G. This space is a group with respect to pointwise multiplication, i.e., $(g_1 g_2)(x) := g_1(x) g_2(x)$, $g_1, g_2 \in G^X$. When equipped with a Frechet-type topology, it becomes a topological group. The pointwise exponential map sends elements of the (infinite-dimensional) Lie algebra $C_0^\infty(X,\mathfrak{G}) \equiv \mathfrak{G}^X$, i.e., functions with values in the Lie algebra $\mathfrak{G}$ of G, to elements of G^X and this is a local homeomorphism. This can be used to give G^X the structure of an infinite-dimensional manifold modeled on the Frechet space $C_0^\infty(X,\mathfrak{G})$.

The simplest case is $X = S^1$, the so-called loop groups. These groups, their central extensions and the corresponding algebras (Kac–Moody algebras) have been thoroughly studied and the representation theory, at least of the so-called positive-energy representations, is quite complete. Among the vast literature on the subject we mention the monographs by Pressley and Segal[1] and by Mickelsson,[2] which also contain much information on the general case.

By contrast, the case $\dim X > 1$ is much less investigated. The main contributions to the representation theory date back to a period from the mid-1970s to the early 1980s. The first interesting irreducible unitary representations of these groups, the so-called energy representations, were constructed (in different settings) in papers by Albeverio and Høegh-Krohn,[3] Ismagilov,[4] and Gelfand, Graev, and Veršik.[5] Reference 4 contains the first proof of irreducibility of representations of this type for the case $\dim X \geqslant 5$ and $G = \mathrm{SU}(2)$. This result was extended in Refs. 5 and 6 to an arbitrary semisimple compact Lie group G and $\dim X = 4$. Later it was shown in Ref. 7 that irreducibility holds also for $\dim X = 3$ and under some conditions on the data, determining the representation, for $\dim X = 2$. The case $\dim X = 1$ is reducible.[7] Reference 5 contains a description of a modification of the energy representation, related to an arbitrary fixed subbundle of the cotangent bundle of X. Further in our paper we call such representations restricted energy representations. Irreducibility of the restricted energy representations is deduced in Ref. 5 from irreducibility of the corresponding energy representations. Thus, by putting together

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the results of Refs. 5–7, one can deduce irreducibility for $\dim X=3$ and under some conditions, for $\dim X=2$.

The present paper is devoted mainly to a study of the restricted energy representations of G^X and its algebra $\mathfrak{G}^X$, in particular in the case $\dim X=2$. Our interest in this case is motivated by several factors. First, we have made the observation that there is a direct proof of irreducibility in all cases when $\dim X>1$, which we present in Sec. II. Thus we extend the known results about irreducibility. Furthermore, our proof is simpler than the proof in Ref. 7 which would be required to treat, e.g., the case $\dim X=3$. Second, these are, in a sense, minimal representations—the infinite-dimensional Hilbert space is in a way ''smallest.'' The case of restricted energy representations for $\dim X=2$ admits a simpler (though equivalent) formulation where we work with Hilbert spaces of $\mathfrak{G}$-valued functions, instead of 1-forms and vector fields instead of subbundles. Third, the restricted energy representations, at least at the level of algebras, admit a very natural generalization to representations of certain central extensions of the algebras. In particular, for the case $\dim X=2$ these are central extensions and representations, determined by two vector fields. By contrast, the same scheme does not work for the usual energy representations. We should point out that Ref. 5 contains a hint of such a central extension and a representation at the group level. Finally, these representations when $\dim X=2$ have a certain ''one-dimensionality,'' in the sense that they are continuous with respect to a topology on $\mathfrak{G}^X$ which is determined by the uniform norms of the functions and of their directional derivatives (in the direction of the vector field). We hope that this may lead to the possibility of constructing new irreducible representations of loop groups.

We have tried to make this paper as self-contained as possible, in view of the fact that most of the material which we build on is probably not so well-known to a large mathematical physics audience. Therefore we begin Sec. II by a somewhat lengthy description of the energy representation and the restricted energy representation. Then we follow up by proving irreducibility. In Sec. III we derive the corresponding algebra representation. A similar formula given in the Appendix in Ref. 6 contains some errors. We have chosen a notation which is familiar to physicists and in which the formulas become rather simple. In this section we prove irreducibility of the algebra representations when $\dim X=2$, using irreducibility at the group level. This is not a trivial statement and the proof fails in dimensions higher than 2. In fact, quite possibly, it is not true. Section IV is devoted to certain central extensions of the algebras and their representations. In our approach these arise very naturally by making a simple generalization of the way the operators of the representation are defined. We describe as an example the case where X is the two-dimensional torus. There, considerations can be restricted to the dense subalgebra of Fourier polynomials and the formulas for the central extensions and the representations have a simple, purely algebraic form. A recent paper by Etingof and Frenkel[8] also considers central extensions of current groups and algebras in two dimensions. By translating our results into their language, we can provide candidates for irreducible representations of the extensions they construct. This will be treated elsewhere.

II. THE ENERGY REPRESENTATION AND THE RESTRICTED ENERGY REPRESENTATION

We begin by a brief description of the energy representation of the group G^X (see Refs. 5–7). Let $\Omega\equiv\Omega^1_0(X,\mathfrak{G})$ denote the space of compactly supported 1-forms on X with values in the Lie algebra $\mathfrak{G}$ of the group G and let $\mathscr{D}$ be its dual space, i.e., the space of $\mathfrak{G}$-valued generalized 1-forms. The bilinear form

$$(\omega_1,\omega_2):=\int_X(\omega_1(x),\omega_2(x))_x\rho(x)dx \tag{1}$$

is a scalar product on Ω. Here the measure dx is the volume form, determined by the Riemannian metric h, i.e., in local coordinates $dx = \sqrt{\det h}dx_1\cdots dx_n$ and ρ is a smooth everywhere positive density. (Except when $\dim X=2$, this density can be absorbed by redefining the metric.) The scalar product $(\omega_1,\omega_2)_x$ in each fiber x is given by the scalar product on T_xX^* induced from h and an Ad-invariant inner product on $\mathfrak{G}$, i.e., a multiple of the Killing form in each simple component of $\mathfrak{G}$. The space $\mathscr{D}$ becomes a (finite) measure space when equipped with the Gaussian measure μ with zero mean and covariance equal to the scalar product (1). In other words μ is the Gaussian measure corresponding to the heuristic expression $d\mu(f)=\exp[-1/2(f,f)]\Pi_{x\in X}\, df(x)$. The energy representation is realized in the space $L^2(\mathscr{D},\mu)$. First there is a natural (reducible) action V of G^X on Ω given by the pointwise adjoint action of G on $\mathfrak{G}$, namely for any $g\in G^X$ we define $(V(g)\omega)(x):=Ad_{g(x)}\omega(x)$. Note that due to the invariance of the Killing form, V leaves the inner product (1) invariant. Because of this the dual action $(V'(g)F)(\omega):=F(V(g^{-1})\omega)$, $F\in\mathscr{D}$, preserves the measure μ. This means that the operators $U_0(g)$ in $L^2(\mathscr{D},\mu)$ defined by

$$(U_0(g)\Phi)(F):=\Phi(V'(g^{-1})F),\quad \Phi\in L^2(\mathscr{D},\mu),\quad F\in\mathscr{D}$$

give a unitary representation of G^X. The reader may realize that $U_0(g)$ is nothing but the second quantized operator in the bosonic Fock space, corresponding to the one-particle operator $V(g)$.

At this point it is still not clear why one should consider $\mathfrak{G}$-valued 1-forms and not just $\mathfrak{G}$-valued functions, when all steps so far work for the latter case as well. The reason lies in the fact that the representation U_0 is reducible, as will be explained shortly, and the (irreducible) energy representation is obtained by modifying U_0 by a suitable 1-cocycle. A natural object of this type is the Maurer–Cartan cocycle (see below) which takes values precisely in the $\mathfrak{G}$-valued 1-forms.

The reducibility of U_0 can best be seen through the well-known Ito–Segal–Wiener canonical isomorphism between $L^2(\mathscr{D},\mu)$ and the Fock space $\oplus_{n=0}^{\infty}S^nH$ with H being the completion and complexification of Ω and S^nH being its nth symmetric tensor power. Up to unessential conventions, under this correspondence the constant function $1\in L^2$ goes to the scalar $1(\in S^0H)$ (the vacuum vector), the linear functions $\Phi_\omega(F):=iF(\omega)$ are sent to the elements $\omega\in H$ and the generalized Hermite polynomials (normal ordered products) $\Phi_{\omega_1}\cdots\Phi_{\omega_k}$: obtained from the ordinary products by the Gramm–Schmidt orthogonalization procedure go to the elements of the type $S^k(\omega_1\otimes\cdots\otimes\omega_k)$. It is evident that under this isomorphism of Hilbert spaces U_0 goes to the representation $\oplus_{n=0}^{\infty}S^nV$ which is reducible, e.g., leaves every n-particle subspace invariant.

Consider now the map $\beta:G^X\to\Omega$ which in matrix notations is defined as $\beta(g):=dg\ g^{-1}$. It satisfies the 1-cocycle condition $\beta(g_1g_2)=\beta(g_1)+g_1(\beta(g_2))g_1^{-1}=\beta(g_1)+V(g_1)\beta(g_2)$. The map β is known as the Maurer–Cartan cocycle. The energy representation is defined as follows:

$$(U(g)\Phi)(F):=\exp[iF(\beta(g))](U_0(g)\Phi)(F)=\exp[iF(\beta(g))]\Phi(V'(g^{-1})F). \tag{2}$$

The cocycle condition for β assures that this is a representation and its unitarity is obvious from the unitarity of U_0. Let us adopt the notation U_α for any representation defined as in Eq. (2) but with an arbitrary cocycle α in place of the Maurer–Cartan cocycle β.

The construction above can be generalized by considering, instead of smooth Riemannian metric h and weight ρ, objects which are piecewise smooth, i.e., such that are smooth outside a closed set of dx measure zero, bounded together with their first derivatives and bounded away from zero. In other words one can allow for jumps. This possibility is due to the fact (most easily seen from the Fock space realization of $L^2(\mathscr{D},\mu)$) that the set of distributions on X with singularity in some fixed subset with zero measure in X has μ measure zero.

Instead of the Maurer–Cartan cocycle β in Eq. (2), one could use a more general cocycle $E\beta$ where E is an invertible bounded operator on Ω (or rather the piecewise smooth category that generalizes it) which has to commute with the representation V. But V is a direct integral over X of mutually nonequivalent representations $Ad_{g(x)}$, so it is apparent that E has to be a (piecewise

smooth) function $E(x)$ where $E(x)$ for each $x \in X$ is a bounded invertible operator on $T_x X^* \otimes \mathfrak{G}$ which has to be a multiple of the identity on each simple component of $\mathfrak{G}$. This, however, is equivalent to redefining the inner product (1), and thus the Gaussian measure. Indeed, consider a measure μ_E with covariance $(E\omega_1, E\omega_2)$. The map sending $\exp[iF(\omega)] \in L^2(\mathscr{D}, \mu_E)$ to $\exp[iF(E\omega)] \in L^2(\mathscr{D}, \mu)$ (such functions form total sets in the respective L^2 spaces) is easily seen to preserve scalar products and it extends by linearity and continuity to a unitary equivalence between the representation U in the space $L^2(\mathscr{D}, \mu_E)$ and the representation $U_{E\beta}$ in the space $L^2(\mathscr{D}, \mu)$. Therefore the modification of the Maurer–Cartan cocycle just described can be absorbed by redefining h, ρ and the choice of invariant product in $\mathfrak{G}$.

In the present paper we are interested in a modification of the energy representation which is in a sense a singular version of the one described in the last paragraph. Consider a function $E(x)$ which takes values in the orthogonal projections in $T_x X^*$. Then $E\beta$ is again a cocycle for V. One cannot expect, however, the representation $U_{E\beta}$ to be irreducible in this case. Indeed, let $\Omega_E \oplus \Omega_{E^\perp}$ be the direct sum decomposition of Ω into the range of E and its orthogonal complement and $\mathscr{D}_E \oplus \mathscr{D}_{E^\perp}$ be the corresponding direct sum decomposition of the dual $\mathscr{D}$. The Gaussian measure μ is a product of the Gaussian measures on $\mathscr{D}_E$ and $\mathscr{D}_{E^\perp}$ corresponding to the inner products on Ω_E and $\Omega_{E^\perp}$ induced from Eq. (1) and there is a natural isomorphism $L^2(\mathscr{D}, \mu) \cong L^2(\mathscr{D}_E, \mu_E) \otimes L^2(\mathscr{D}_{E^\perp}, \mu_{E^\perp})$ which sends the representation $U_{E\beta}$ on $L^2(\mathscr{D}, \mu)$ to the tensor product of $U_{E\beta}$ on $L^2(\mathscr{D}_{\mathrm{E}}, \mu_{\mathrm{E}})$ and U_0 on $L^2(\mathscr{D}_{E^\perp}, \mu_{E^\perp})$. The second factor is reducible (see above) and therefore $U_{E\beta}$ is reducible as well. However, the first factor is irreducible as will be discussed in what follows. This is true in all cases when $E(x) \neq 0,1$, a.a. $x \in X$ and the result is independent of $\dim X$, quite contrary to the energy representation where the question of irreducibility is intricately tied to $\dim X$.[6,7] In particular, for $\dim X = 2$, one obtains an irreducible representation by fixing any piecewise smooth one-dimensional subbundle of TX^* and letting $E(x)$ be the projection onto this subbundle. We shall call representations obtained in this fashion, namely by a restriction to some fixed subbundle of TX^*, restricted energy representations.

Irreducibility or reducibility of the energy representation is tied to a specific property of the spectral measure of the representation when restricted to a certain Abelian subgroup. Namely, choose any Cartan subalgebra $\mathfrak{C} \subset \mathfrak{G}$ and let $\mathfrak{C}^X$ be the additive group of C_0^∞ maps from X to $\mathfrak{C}$. The pointwise exponential map is a homomorphism from $\mathfrak{C}^X$ to G^X and $W(a) := U(\exp a)$, $a \in \mathfrak{C}^X$ is a unitary representation of $\mathfrak{C}^X$. The orthogonal decomposition $\mathfrak{G} = \mathfrak{C} \oplus \mathfrak{C}^\perp$ induces a direct sum decomposition $\mathscr{D} = \mathscr{D}_{\mathfrak{C}} \oplus \mathscr{D}_{\mathfrak{C}^\perp}$ which gives rise to an isomorphism $L^2(\mathscr{D}, \mu) \cong L^2(\mathscr{D}_{\mathfrak{C}}, \mu_{\mathfrak{C}}) \otimes L^2(\mathscr{D}_{\mathfrak{C}^\perp}, \mu_{\mathfrak{C}^\perp})$; corresponding to it a tensor product decomposition of the representation $W = W' \otimes W''$, where

$$(W'(a)\Phi)(F) = \exp[iF(\beta \exp a)]\Phi(F), \quad F \in \mathscr{D}_{\mathfrak{C}},$$

$$(W''(a)\Phi)(F) = \Phi(V'(\exp(-a))F), \quad F \in \mathscr{D}_{\mathfrak{C}^\perp}.$$

Because $\mathfrak{C}^X$ is an Abelian subalgebra of the Lie algebra $\mathfrak{G}^X$, we have $\beta \exp a = da$, $a \in \mathfrak{C}^X$. The spectral measure of W' is the Gaussian measure on the dual space of $\mathfrak{C}^X$, i.e., the space of $\mathfrak{C}$-valued distributions on X (or equivalently the space of continuous characters on $\mathfrak{C}^X$), with zero mean and covariance given by the bilinear form (da_1, da_2) on $\mathfrak{C}^X$ where the inner product (1) is used. A sufficient condition for irreducibility of the energy representation is[6] that the Sobolev space obtained from $\mathfrak{C}^X$ by completing it with respect to the inner product (da_1, da_2) admits a Hilbert–Schmidt extension that does not contain linear combinations of δ-functions. (Strictly speaking, this has to be true for every open cube $Y \subset X$.)

Consider now a subbundle E of the cotangent bundle and the restricted energy representation corresponding to it. All the steps in the proof of irreducibility can be repeated without change, the only difference is that the spectral measure of the representation W' is the Gaussian measure with zero mean and covariance $(E\ da_1, E\ da_2)$ where by a slight abuse of notation we use $E(x)$ for the

orthogonal projection onto the subbundle E. The subbundle E can be specified by a distribution E' (of the same dimension) on X, i.e., a subbundle of the tangent bundle, e.g., by using the orthogonal decomposition $T_xX = E'(x) \oplus E'(x)^{\perp}$.

Lemma II.1: Let Y be an open cube in $\mathbb{R}^n$, $n>1$ (with compact closure) and let W be the completion of $C_0^{\infty}(Y)$ with respect to the norm

$$\|a\|^2 = \sum_{i=1}^{m} \int_Y \frac{\partial \bar{a}}{\partial x_i} \frac{\partial a}{\partial x_i} \rho_i(x) dx, \tag{3}$$

where $0<m<n$ is some fixed integer and $\rho_i(x)$, $i=1,\ldots,m$ are some smooth densities on Y, continuous and strictly positive on $\bar{Y}$. Then the space W admits a Hilbert–Schmidt extension which does not contain linear combinations of δ-functions.

Proof: A delta function δ_x on W, belonging to some extension of W, is an element of that extension with the property $(\delta_x, a) = a(x)$, $\forall a \in W$, where $(\ ,\ )$ is the inner product in W. (A more precise formulation would be through δ-sequences.) Due to the specific structure of the inner product in W, any δ-function contains as factors ordinary δ-functions δ_{x_j}, over those coordinates x_j with respect to which there is no differentiation in Eq. (3).

Let $\{\epsilon'_k\}$ be an orthonormal basis with respect to a "flat" inner product $(\ ,\ )'$ on W, i.e., one in which all ρ_i above are set to 1. Choose a square-summable sequence of positive numbers $\{\gamma_k\}$. Then the operator $\Gamma := \Sigma_k \gamma_k (\epsilon'_k, \cdot\ ) \epsilon'_k$ is strictly positive and Hilbert–Schmidt. Indeed, noting that $\|\epsilon'_k\|^2 \leqslant \sup_{i,x} \rho_i(x) \|\epsilon'_k\|'^2 = \sup_{i,x} \rho_i(x)$ and choosing a basis $\{\epsilon_j\}$ (with respect to $(\ ,)$), we have

$$\sum_j (\epsilon_j, \Gamma \epsilon_j) = \sum_j \sum_k \gamma_k (\epsilon_j, \epsilon'_k)(\epsilon'_k, \epsilon_j) = \sum_k \gamma_k \|\epsilon'_k\|^2 < \infty.$$

The basis $\{\epsilon'_k\}$ can be chosen as a product of bases on the Sobolev space $\mathring{W}_2^1(Y_m)$ (corresponding to the first m coordinates) and $(n-m)$ copies of L^2 spaces. The same product structure can be used when choosing the Hilbert–Schmidt operator Γ. Thus, picking up any of the last $(n-m)$ coordinates, it is enough to show that the corresponding L^2 space has a Hilbert–Schmidt extension that does not contain δ-functions. Let us take $\epsilon'_k := e^{ikx}$, $k \in \mathbb{Z}$ as basis functions in $L^2([0,2\pi], dx/2\pi)$ and let $\Gamma := (\epsilon'_0, \cdot\ ) \epsilon'_0 + \Sigma_{k \neq 0} (1/|k|)(\epsilon'_k, \cdot\ ) \epsilon'_k$. Summing up the series we find that Γ has a kernel $K(x,y) = 1 - 2 \ln|1 - e^{i(x-y)}|$. A δ-function $\delta(x-x_0)$ will be contained in the extension defined by Γ if its Γ-norm is finite, i.e., if $\int dx\, dy\ \delta(x-x_0)\delta(y-x_0)K(x,y) < \infty$, which obviously fails. This completes the proof for a single δ-function. For an arbitrary linear combination of δ-functions we must use the fact that in calculating the Γ-norm, the mixed terms of the form $\int dx\, dy\, \delta(x-x_0)\delta(y-x_1)K(x,y)$ are finite. □

The Lemma just proven together with the discussions of irreducibility above show that the following is true:

Proposition II.2: Let E' be an integrable piecewise smooth distribution on X and E the subbundle of T^*X determined by it. Then the restricted energy representation $U_{E\beta}$ corresponding to E is irreducible.

We need integrability of E' so that around each point in X we can find a coordinate map with the property that slices $(x_{m+1}, \ldots, x_n) = \text{const}$ are integral manifolds of E. Then our Lemma applies. The densities ρ_i in Eq. (3) are obtained from the overall density ρ in Eq. (1) and the components and determinant of the Riemannian metric h. As shown in Ref. 6, the restricted energy representation is irreducible in all cases when irreducibility holds for the energy representation. This is true because for any subbundle E and its orthogonal complement $E^{\perp}$ we have $U = U_{E\beta} \otimes U_{E^{\perp}\beta}$ and irreducibility of U implies irreducibility of the factors. In particular this means that the restricted energy representation is irreducible[7] for any G, h, ρ, and E when $\dim X \geqslant 3$. The only cases when irreducibility of $U_{E\beta}$ does not follow from irreducibility of U are in fact certain

cases when E' is a one-dimensional distribution on a two-dimensional manifold. Any one-dimensional distribution is integrable (locally, which is what we need), so the statement of Proposition II.2 is actually valid without the integrability assumption.

Without going into any detail we shall point out that the same property of the spectral measure which assures irreducibility is also sufficient to show nonequivalence of any two representations determined by two different sets of data.[5–7] More specifically we have the following extension of the results of Refs. 5–7, concerning this question:

Proposition II.3: Two restricted energy representations of G^X determined by two sets of data (E,h,ρ) and (E',h',ρ'), respectively, are equivalent if and only if $E=E'$ (a.e.) and the inner products on the space of sections of E induced by h and ρ and by h' and ρ', respectively, coincide.

III. THE LIE ALGEBRA REPRESENTATIONS. THE TWO-DIMENSIONAL CASE

In this section we give explicit formulas for the representations of the Lie algebra $\mathfrak{G}^X$ coming from restricted energy representations of G^X. We specialize the results to $\dim X=2$ and show irreducibility of the algebra representations in this case.

For a continuous representation U of G^X we define a (continuous) representation L of $\mathfrak{G}^X$ in the usual way:

$$L(a)\Phi := \lim_{t\to 0}\left(\frac{1}{t}\,(U(\exp ta)-\mathrm{Id})\Phi\right) \tag{4}$$

and the domain of $L(a)$ consists of those Φ for which the limit exists. By Stone's theorem unitarity and strong operator continuity of U imply that $iL(a)$ is self-adjoint.

Proposition III.1: Let X be two-dimensional and let U be either an irreducible energy representation or a restricted energy representation (which is always irreducible by Proposition II.2). Then the corresponding representation L of the Lie algebra $\mathfrak{G}^X$ is also irreducible.

Proof: Again we can choose an open submanifold $Y\subset X$ of full measure, diffeomorphic to the open disk and use the fact that $L^2(\mathscr{D},\mu)$ is the same for Y and X. As $\mathfrak{G}^Y\subset\mathfrak{G}^X$, it is enough to show irreducibility of L when restricted to $\mathfrak{G}^Y$. So we shall only consider X being an open disk in $\mathbb{R}^2$. The Hilbert spaces of our representations depend only on the Lie algebra of G and obviously so do the operators $L(a)$. We can replace G by its universal covering group, which is again a compact semisimple group. Suppose there exists a proper closed subspace invariant under all operators $L(a)$. By spectral theory it will also be invariant under $U(\exp a)$. By continuity of U and the fact that the invariant subspace is closed we could conclude that it is invariant with respect to all $U(g)$ and thus arrive at a contradiction, if we can show that the elements $\exp a$, $a\in\mathfrak{G}^X$ are dense in G^X. Any element of G^X is actually a based map $g:S^2\to G$, sending the south pole to the identity of G (recall that X is the open two-disk and that G^X consists of maps with compact support, i.e., maps which send all points outside a compact set to the identity). It is well known (cf. e.g., Ref. 9) that outside a so-called singular set, every element $g(x)$ of a simply connected compact group G can be represented uniquely as $\exp a_x$ and that the singular set is a closed subset of codimension not less than 3. Since we are mapping a two-dimensional manifold into G, by the transversallity theorem any map $g':S^2\to G$ can be made to avoid the singular set by an arbitrarily small perturbation and the perturbed map $g(x)$ can be written uniquely as $\exp a(x)$. (This is in fact the way $\pi_2(G)=0$ is shown, which is a necessary condition for the above to be true.) □

It is interesting to note that $\dim X=2$ is a critical dimension in this Proposition. For higher dimensions one cannot always avoid the singular set by a small perturbation and irreducibility of the algebra representation may fail.

The representation of $\mathfrak{G}^X$ defined by Eq. (4) takes a particularly simple form if one uses standard bosonic Fock space notations. Let us introduce for any $\omega\in\Omega$ the usual creation operator $B^*(\omega)$ and annihilation operator $B(\omega)$ which on an n-particle state act as follows:

$$B^*(\omega)(B^*(\omega_1)B^*(\omega_2)\cdots B^*(\omega_n)|0\rangle)=B^*(\omega)B^*(\omega_1)B^*(\omega_2)\cdots B^*(\omega_n)|0\rangle,$$

$$B(\omega)(B^*(\omega_1)B^*(\omega_2)\cdots B^*(\omega_n)|0\rangle)=\sum_{i=1}^{n}(\omega,\omega_i)B^*(\omega_1)\cdots B^*(\omega_{i-1})\times B^*(\omega_{i+1})\cdots B^*(\omega_n)|0\rangle.$$

As usual $(\,,\,)$ means the inner product (1). Let $L_0(a)$ be the second quantized operator, corresponding to $\omega(x)\to[a(x),\omega(x)]$:

$$L_0(a)B^*(\omega_1)B^*(\omega_2)\cdots B^*(\omega_n)|0\rangle=\sum_{i=1}^{n}B^*(\omega_1)\cdots B^*(\omega_{i-1})B^*([\omega,\omega_i])\times B^*(\omega_{i+1})\cdots B^*(\omega_n)|0\rangle.$$

With these notations the representation of the Lie algebra defined by Eq. (4) becomes

$$L(a)=L_0(a)+B^*(da)-B(da). \tag{5a}$$

Although the derivation is not very simple, the result is. One can check directly that this is a Lie algebra representation. Antihermiticity of the operators $L(a)$ is almost explicit. We can take as a domain of all $L(a)$ the subspace of finite sums of finite-number particle states. Of course we know *a priori* that $iL(a)$ are essentially self-adjoint as generators of strongly continuous one-parameter unitary groups.

We would like to point out that the simplicity of the action of $L(a)$ does not help much in understanding the problem of irreducibility. This can be appreciated if one considers the energy representation in the case $\dim X=1$, which is known to be reducible.[7] At the same time the formula for the algebra representation is entirely similar. In fact the only way we know of showing irreducibility of this type of representations of the algebra is by exponentiating the operators, i.e., going to the group representations.

The representation defined by Eq. (5) is extended almost without change to a representation of the complexified Lie algebra $\mathfrak{G}_{\mathbb{C}}^{X}$:

$$L(a)=L_0(a)+B^*(da)-B(d\bar{a}). \tag{5b}$$

($\bar{a}$ is a complex conjugation relative to the real algebra $\mathfrak{G}^X$.)

When $\dim X=2$ the restricted energy representations are specified by piecewise smooth one-dimensional distributions on X. Any distribution can be specified by a piecewise smooth nonzero vector field on X (as we allow piecewise smooth objects, nonorientable line bundles can also be represented by vector fields (with jumps)). The whole construction can easily be reformulated in terms of $\mathfrak{G}$-valued functions and vector fields acting on them without any reference to tangent and cotangent bundles and their subbundles. The one-particle Hilbert space can in this case be taken to be $L^2(X,dx;\mathfrak{G}_{\mathbb{C}})$ where dx is the Riemann–Lebesgue measure. Note that Za is an element of $L^2(X,dx;\mathfrak{G}_{\mathbb{C}})$ for any piecewise smooth vector field Z. Every piecewise smooth, a.e. nonzero vector field Z determines an irreducible representation of G^X and through Eq. (4) also an irreducible representation of $\mathfrak{G}^X$. For one and the same measure dx, different vector fields determine nonequivalent representations. Any rescaling of the measure is equivalent to an appropriate rescaling of the vector field. This possibility was discussed in the previous section. Here, however, this is true in the two-dimensional case due to the fact that we are dealing with $\mathfrak{G}$-valued functions and not $\mathfrak{G}$-valued 1-forms. Thus for any vector field Z as above and any Riemannian metric on X one obtains an irreducible representation of $\mathfrak{G}_{\mathbb{C}}$ in the bosonic Fock space over the one particle Hilbert space $L^2(X,dx;\mathfrak{G}_{\mathbb{C}})$ given by the formula

$$L(a)=L_0(a)+B^*(Za)-B(Z\bar{a}). \tag{6}$$

The operators $L(a)$ are anti-Hermitian for real a, which is evident from the formula.

Example: Let $X=S^1\times S^1$, with coordinates $(x,y)\in[0,2\pi)\times[0,2\pi)$ and the standard measure $(1/2\pi)dx\ dy$. Let $\{t_\alpha\}_{\alpha=1}^r$ be a basis in $\mathfrak{G}$, orthonormal with respect to the chosen invariant form on $\mathfrak{G}$ and $C_{\alpha\beta}^\gamma$ be the structure constants of $\mathfrak{G}$. Consider the linearly independent set of $\mathfrak{G}_{\mathbb{C}}$-valued functions $T_\alpha^{n,m}:=t_\alpha e^{i(nx+my)}$, $n,m\in\mathbb{Z}$. The linear span of this set is the so-called Fourier polynomial subalgebra, which is dense in $\mathfrak{G}_{\mathbb{C}}^X$. The commutator is obviously

$$[T_\alpha^{n,m},T_\beta^{k,l}]=\sum_{\gamma=1}^r C_{\alpha\beta}^\gamma T_\gamma^{n+k,m+l}.$$

Any piecewise smooth vector field can be written as $Z(x,y)=f(x,y)(\partial/\partial x)+g(x,y)(\partial/\partial y)$. An (unnormalized) basis in the Hilbert space of the representation will be given by vectors of the type

$$E^{n_1,m_1;n_2,m_2;\ldots;n_s,m_s}_{\alpha_1,\alpha_2,\ldots,\alpha_s}:=B^*(T_{\alpha_1}^{n_1,m_1})B^*(T_{\alpha_2}^{n_2,m_2})\cdots B^*(T_{\alpha_s}^{n_s,m_s})|0\rangle.$$

Denoting by $\hat{f}^{pq}$ and $\hat{g}^{pq}$ the Fourier coefficients of f and g, we obtain the following formula for the representation of the polynomial subalgebra:

$$\begin{aligned}L(T_\alpha^{n,m})E^{n_1,m_1;n_2,m_2;\ldots;n_s,m_s}_{\alpha_1,\alpha_2,\ldots,\alpha_s}=&\sum_{j=1}^s\sum_{\gamma=1}^r C_{\alpha\alpha_j}^\gamma E^{n_1,m_1;\ldots;n_{j-1},m_{j-1};n_j+n,m_j+m;n_{j+1},m_{j+1};\ldots;n_s,m_s}_{\alpha_1,\ldots,\alpha_{j-1},\alpha_\gamma,\alpha_{j+1},\ldots,\alpha_s}\\&+i\sum_{p,q=-\infty}^{\infty}(n\hat{f}^{pq}+m\hat{g}^{pq})E^{n+p,m+q;n_1,m_1;n_2,m_2;\ldots;n_s,m_s}_{\alpha,\alpha_1,\alpha_2,\ldots,\alpha_s}\\&-i\sum_{j=1}^s(n\hat{f}^{n_j-n,m_j-m}+m\hat{g}^{n_j-n,m_j-m})\\&\times\delta_{\alpha\alpha_j}E^{n_1,m_1;\ldots;n_{j-1},m_{j-1};n_{j+1},m_{j+1};\ldots;n_s,m_s}_{\alpha_1,\ldots,\alpha_{j-1},\alpha_{j+1},\ldots,\alpha_s}.\end{aligned}$$

The infinite sum, of course, is to be interpreted in the sense of convergence in the Hilbert space.

IV. A CENTRAL EXTENSION OF THE ALGEBRA AND ITS REPRESENTATIONS

The operators defined by Eq. (6) can be generalized by considering a complex vector field $Z=Z_1+iZ_2$. It is obvious that Eq. (6) still defines a linear map from $\mathfrak{G}_{\mathbb{C}}^X$ to the (unbounded) linear operators in H. It is also immediate that the operators $L(a)$ remain Hermitian when $a\in\mathfrak{G}^X$. There is no reason for these operators, however, to give a representation of the algebra. A straightforward calculation gives

$$L(a)L(b)-L(b)L(a)=L([a,b])+ic(a,b), \tag{7a}$$

where

$$c(a,b):=\frac{1}{i}[(Z\bar{b},Za)-(Z\bar{a},Zb)]. \tag{7b}$$

It is obvious that if Z is a real vector field we have $c(a,b)\equiv 0$ and Eq. (7a) expresses simply the fact that Eq. (6) defines a representation. In general, for $Z=Z_1+iZ_2$ we obtain

$$c(a,b)=2[(Z_1\bar{b},Z_2a)-(Z_1\bar{a},Z_2b)].$$

The functional $c:\mathfrak{G}_{\mathbb{C}}^{X} \times \mathfrak{G}_{\mathbb{C}}^{X} \to \mathbb{C}$ is bilinear antisymmetric and it is not difficult to check that it satisfies the cocycle condition

$$c([a,b],c)+c([c,a],b)+c([b,c],a)=0.$$

Thus Eqs. (7a) and (7b) show that when Z is a complex vector field, Eq. (6) defines a representation of a central extension $\tilde{\mathfrak{G}}_{\mathbb{C}}^{X}$ of the algebra $\mathfrak{G}_{\mathbb{C}}^{X}$, depending on the two vector fields $Z_{1,2}$. The Lie bracket in $\tilde{\mathfrak{G}}_{\mathbb{C}}^{X}$ is given by

$$[a,b]^{\sim}=[a,b]+c(a,b). \tag{8}$$

Formula (8) also gives an extension by $\mathbb{R}$ of the real algebra $\mathfrak{G}^{X}$. Note that we are working all the time with anti-Hermitian representations, so an element (a,α) should be represented by the operator $L(a)+i\alpha$. Not all choices of vector fields $Z_{1,2}$ give a nonzero cocycle c. A necessary and sufficient condition for $c\neq 0$ is $Z_1^* Z_2 - Z_2^* Z_1 \neq 0$, where Z_i^* are the formal adjoints with respect to the inner product in $L^2(X,dx)$. Any nonzero cocycle c of this type is nontrivial. Indeed, assuming the converse, i.e., that it is a coboundary of some 1-cochain c_1, we must have $c(a,b)=dc_1(a,b)=c_1([a,b])$. We can always find two functions $f_{1,2}\in C_0^{\infty}(X)$, such that $(Z_1 f_2, Z_2 f_1)-(Z_1 f_1, Z_2 f_2)\neq 0$. Then by fixing any $a_0\in\mathfrak{G}_{\mathbb{C}}$ and taking $a=f_1 a_0$, $b=f_2 a_0$, the right-hand side becomes zero while the left-hand side does not. This completes the argument.

The central extension does not depend separately on the two vector fields $Z_{1,2}$. Again, since we allow for the vector fields to be piecewise smooth we can fix some local coordinates and choose the integration measure dx to be just $dx\,dy$ in each coordinate patch (remember, that more general measures will not give us anything new, since this is equivalent to rescaling the vector fields). Let in the local coordinates

$$Z_i=f_i\frac{\partial}{\partial x}+g_i\frac{\partial}{\partial y}, \quad i=1,2.$$

Then, introducing the function $\varphi:=f_1 g_2 - f_2 g_1$ and using integration by parts we obtain

$$c(a,b)=2\left(a,\ \frac{\partial b}{\partial x}\frac{\partial \varphi}{\partial y}-\frac{\partial b}{\partial y}\frac{\partial \varphi}{\partial x}\right)+\text{possible boundary terms}.$$

In other words, up to integrals over one-dimensional submanifolds (the boundary terms), the central charge c can be written (for simplicity, let $\mathfrak{G}$ be simple) as

$$c(a,b)=\int_X \mathrm{Tr}(a\,db)\wedge d\varphi \tag{9}$$

for some (piecewise smooth) function φ. If we restrict ourselves to the smooth category, then Eq. (9) obviously defines a 2-cocycle. It depends only on the combination $a\,db$ as required by the general result of Ref. 1 (Prop. 4.2.8) about the universal central extension of $\mathfrak{G}^{X}$.

It is also worth pointing out that a representation, defined by Eq. (6), is invariant (in the sense of unitary equivalence) with respect to local phase transformations of the complex vector field Z. In other words, replacing $Z(x)$ by $e^{i\theta(x)}\,Z(x)$ leads to a representation which is unitarily equivalent to the initial one. This can be shown by introducing the unitary operator ($U(1)$ gauge transformation)

$$UB^*(\omega_1)B^*(\omega_2)\cdots B^*(\omega_n)|0\rangle = B^*(\omega_1')B^*(\omega_2')\cdots B^*(\omega_n')|0\rangle,$$

where $\omega_i'(x) = e^{i\theta(x)}\,\omega_i(x)$ and noticing that U intertwines the representation determined by $Z(x)$ and the one determined by $e^{i\theta(x)}\,Z(x)$. A straightforward computation shows that the combination $\varphi = f_1 g_2 - f_2 g_1$, which determines the central extension, is invariant with respect to such local phase transformations, as it should be.

Example: We consider again the example of the torus. Using the same notations as for the case of nonextended algebra and writing $\hat{f}_i^{pq}$, $\hat{g}_i^{p,q}$, $i=1,2$, $p,q\in\mathbb{Z}$ for the Fourier coefficients of the vector fields Z_i, $i=1,2$, we obtain the following expression for the central charge:

$$c(T_\alpha^{n,m}, T_\beta^{k,l}) = 2\,\delta_{\alpha\beta}(ln-km)\,\gamma_{n+k,m+l}, \tag{10}$$

where we have used the following definition:

$$\gamma_{n,m} := \sum_{p,q=-\infty}^{\infty} (\hat{f}_1^{pq}\hat{g}_2^{p+n,q+m} - \hat{g}_1^{pq}\hat{f}_2^{p+n,q+m}). \tag{11}$$

At this point we may forget about the way we obtained the numbers $\gamma_{n,m}$. Any infinite matrix will provide a central extension. If we introduce the notation $c_{nm,kl} := (ln-km)\,\gamma_{n+k,m+l}$, then the cocycle condition requires that

$$c_{n+s\ m+r,kl} + c_{nm,s+k\ r+l} + c_{k+n\ l+m,sr} = 0,$$

which can be checked directly. Thus we have the following central extension of the Fourier polynomial subalgebra on the torus:

$$[T_\alpha^{n,m}, T_\beta^{k,l}]^{\sim} = \sum_{\gamma=1}^{r} C_{\alpha\beta}^{\gamma} T_\alpha^{n+k,m+l} + 2\,\delta_{\alpha\beta}(ln-km)\,\gamma_{n+k,m+l}. \tag{12}$$

The representation of this algebra, determined by the two vector fields $Z_{1,2}$ has the following explicit expression:

$$\begin{aligned}
&L(T_\alpha^{n,m}) E^{n_1,m_1;n_2,m_2;\ldots;n_s,m_s}_{\alpha_1,\alpha_2,\ldots,\alpha_s} \\
&\quad = \sum_{j=1}^{s}\sum_{\gamma=1}^{r} C_{\alpha\alpha_j}^{\gamma} E^{n_1,m_1;\ldots;n_{j-1},m_{j-1};n_j+n,m_j+m;n_{j+1},m_{j+1};\ldots;n_s,m_s}_{\alpha_1,\ldots,\alpha_{j-1},\alpha_\gamma,\alpha_{j+1},\ldots,\alpha_s} \\
&\quad + i\sum_{p,q=-\infty}^{\infty} (n(\hat{f}_1^{pq} + i\hat{f}_2^{pq}) + m(\hat{g}_1^{pq} + i\hat{g}_2^{pq})) \\
&\quad \times E^{n+p,m+q;n_1,m_1;n_2,m_2;\ldots;n_s,m_s}_{\alpha,\alpha_1,\alpha_2,\ldots,\alpha_s} \\
&\quad - i\sum_{j=1}^{s} (n(\hat{f}_1^{n_j-n,m_j-m} - i\hat{f}_2^{n_j-n,m_j-m}) + m(\hat{g}_1^{n_j-n,m_j-m} - i\hat{g}_2^{n_j-n,m_j-m})) \\
&\quad \times \delta_{\alpha\alpha_j} E^{n_1,m_1;\ldots;n_{j-1},m_{j-1};n_{j+1},m_{j+1};\ldots;n_s,m_s}_{\alpha_1,\ldots,\alpha_{j-1},\alpha_{j+1},\ldots,\alpha_s}.
\end{aligned}$$

Once again, at this point we do not need to refer to any vector fields $Z_{1,2}$. We have an (infinite) matrix $\gamma_{n,m}$, which defines the central extension of the algebra and then we need to choose four l^2 sequences $\{\hat{f}_i^{pq}\}_{p,q=-\infty}^{\infty}$, $\{\hat{g}_i^{pq}\}_{p,q=-\infty}^{\infty}$, $i=1,2$, so that Eq. (11) holds. Then the formula above will give a representation of Eq. (12). Of course, not all different choices of $\{\hat{f}_i^{pq}\}_{p,q=-\infty}^{\infty}$, $\{\hat{g}_i^{pq}\}_{p,q=-\infty}^{\infty}$ will lead to nonequivalent representations, as pointed out before.

V. CONCLUDING REMARKS

There are a few important open problems concerning the discussed central extensions and their representations. First of all, we have not addressed the question of irreducibility of these representations. We believe that for generic choices of $Z_{1,2}$ irreducibility will still hold. Second, we have not treated the problem of integrability of the central extensions, i.e., when they correspond to central extensions of the group. Further, we only know that (anti)hermiticity holds, but we have not investigated whether the operators of the representation are actually essentially (anti) self-adjoint. Finally we have not studied the problem of exactly parametrizing the *nonequivalent* representations, corresponding to a given central extension.

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q-deformation of the Lorentz group

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We describe a q-deformation of the Lorentz group in terms of a q-deformation of the van der Waerden spinor algebra. © *1996 American Institute of Physics.* [S0022-2488(96)00502-0]

I. INTRODUCTION

Weak deformations which test the stability of quantum mechanics are of interest as a matter of principle. One deformation which has been the subject of considerable study results from the replacement of the commutators or anticommutators of dynamically conjugate operators by their q-commutators. As far as these studies have shown, there is no obstruction to the formulation of a ''q-quantum mechanics'' for finite systems.[1] In the field theoretic context, however, this is not a well-defined procedure and may lead to violation of the Poincaré group.[2]

In an alternative approach, one may begin with an explicit deformation of this group. We shall here examine the q-deformation of the Lorentz group by q-deforming its two-dimensional representation. Although the q-Lorentz group has already been studied by several authors,[3] the present treatment may be of interest as a simple modification of the van der Waerden calculus.

II. SPINOR ALGEBRA FOR LORENTZ GROUP

We shall first summarize the familiar spinor algebra for the Lorentz group. Let

$$\sigma^k=(\sigma^0,\vec{\sigma}),\quad \sigma^0=\begin{pmatrix}1&0\\0&1\end{pmatrix} \tag{2.1}$$

and

$$X=x_k\sigma^k=\begin{pmatrix}x_0+x_3 & x_1-ix_2\\ x_1+ix_2 & x_0-x_3\end{pmatrix}. \tag{2.2}$$

Then

$$\begin{gathered}\det X=x_0^2-\vec{x}^2=\eta^{kl}x_kx_l,\\ \eta^{kl}=\begin{pmatrix}1&&&\\&-1&&\\&&-1&\\&&&-1\end{pmatrix}.\end{gathered} \tag{2.3}$$

Here X is also Hermitian:

$$X=X^\dagger. \tag{2.4}$$

Let

$$X'=LXL^\dagger. \tag{2.5}$$

Then

$$(X')^{\dagger}=X'. \tag{2.6}$$

However, we shall now require

$$\det L=1. \tag{2.7}$$

Then

$$\det X'=\det X. \tag{2.8a}$$

or

$$(x_0^2-\vec{x}^2)'=x_0^2-\vec{x}^2. \tag{2.8b}$$

Here L has four complex matrix elements related by $\det L=1$. These are the six independent real parameters needed to describe a Lorentz transformation, and L is a two-dimensional representation of the Lorentz group.

Let ξ^A be a two-rowed basis for the two-dimensional representation, L,

$$\xi^A \rightarrow L^A{}_B \xi^B, \tag{2.9}$$

and η a basis for the conjugate representation

$$\eta^{\dot{A}} \rightarrow \bar{L}^{\dot{A}}{}_{\dot{B}} \eta^{\dot{B}}, \tag{2.10}$$

where the conjugate representation is distinguished by a dotted index. Likewise, let ξ be a two-rowed basis for L^{-1}:

$$\xi_A=(L^{-1})^B_A \xi_B\,. \tag{2.11}$$

Again there is a conjugate representation:

$$\chi_{\dot{A}} \rightarrow (\bar{L}^{-1})_{\dot{A}}{}^{\dot{B}} \chi_{\dot{B}}\,. \tag{2.12}$$

Then upper and lower indices behave in the usual way as contravariant and covariant, so that expressions like $\xi^A \xi_A$ are invariant.

The two-dimensional Levi–Civita symbol, ϵ_{AB}, may be used to define the determinant of L:

$$\epsilon_{AB} \det L = L^C{}_A L^D{}_B \epsilon_{CD}\,. \tag{2.13}$$

Since $\det L=1$,

$$\epsilon_{AB}=L^C{}_A L^D{}_B \epsilon_{CD}\,. \tag{2.14}$$

Therefore ϵ_{AB} is a covariant two-spinor that is taken into itself by spin transformations while

$$\epsilon_{AB} \xi^A \eta^B \tag{2.15}$$

is invariant.

Let us define ϵ^{AB} by

$$\epsilon^{AB}=\epsilon_{AB}\,. \tag{2.16}$$

Then

$$\epsilon^{AC}\epsilon_{BC}=\delta^A_B. \tag{2.17}$$

Also

$$\epsilon^{AB}=(L^{-1})^A{}_C(L^{-1})^B{}_D\epsilon^{CD}. \tag{2.18}$$

The spin tensors ϵ_{AB} and ϵ^{AB} provide ways of lowering and raising indices. Thus

$$\xi_B=\xi^A\epsilon_{AB}, \tag{2.19}$$

$$\xi^A=\epsilon^{AB}\xi_B, \tag{2.20}$$

and

$$\xi_A\eta^A=\xi^B\epsilon_{BA}\eta^A=-\eta^A\epsilon_{AB}\xi^B=-\eta_B\xi^B \tag{2.21}$$

if ξ and η commute. Therefore ϵ_{AB} serves as a two-dimensional metric.

One next introduces the matrices contravariant to $(\sigma^m_{A\dot{x}})$ with respect to ϵ:

$$(\bar{\sigma}^m)^{\dot{X}A}=\epsilon^{\dot{X}\dot{Y}}\epsilon^{AB}(\sigma^m)_{B\dot{Y}}. \tag{2.22}$$

Then if $(\sigma^m)_{B\dot{Y}}$ is the original set $(1,\vec{\sigma})$, defined in (2.1),

$$(\bar{\sigma}^m)^{\dot{X}A}=(1,-\vec{\sigma}) \tag{2.23}$$

The following relations are also useful:

$$\bar{\sigma}^m\sigma^n+\sigma^n\bar{\sigma}^m=2\eta^{nm}, \tag{2.24}$$

$$\mathrm{Tr}\ \bar{\sigma}^m\sigma^n=2\eta^{nm}, \tag{2.25}$$

or

$$(\bar{\sigma}^m)^{\dot{X}A}(\sigma_n)_{A\dot{X}}=2\delta^m_n \tag{2.26}$$

and

$$(\sigma_n)_{A\dot{X}}(\sigma^n)^{B\dot{Y}}=2\delta^B_A\delta^{\dot{Y}}_{\dot{X}}. \tag{2.27}$$

With the aid of the σ-matrices one may pass between the four-dimensional and spin representation

$$T^{A\dot{X}\,B\dot{Y}\ldots}{}_{C\dot{W}\ldots}=\sigma^{A\dot{X}}_a\sigma^{B\dot{Y}}_b\sigma^c_{C\dot{W}}T^{ab\ldots}{}_{c\ldots}, \tag{2.28}$$

and

$$T^{ab\ldots}{}_{c\ldots}=\sigma^a{}_{A\dot{X}}\sigma^b{}_{B\dot{Y}}\sigma_c{}^{C\dot{W}}T^{A\dot{X}\,B\dot{Y}\ldots}{}_{C\dot{W}\ldots}. \tag{2.29}$$

Any finite irreducible representation of L is equivalent to some spin representation which is separately symmetric in all dotted and undotted indices. Here $D(k,l)$ is the usual notation to describe $2k$ dotted and $2l$ undotted indices.

III. SPIN REPRESENTATION OF A VECTOR

In the notation just introduced, the vector x^a has the spin representation $X^{A\dot{X}}$ where

$$X^{A\dot{X}}=\sigma_a^{A\dot{X}}x^a, \tag{3.1}$$

$$2x^a=\sigma^a{}_{A\dot{X}}X^{A\dot{X}}. \tag{3.2}$$

If

$$X^{A\dot{X}}=\psi^A\bar{\psi}^{\dot{X}}, \tag{3.3}$$

then

$$2x^a=\psi\sigma^a\bar{\psi}. \tag{3.4}$$

The transformation of $X^{A\dot{X}}$ is given by

$$(X^{A\dot{X}})'=\psi'^A\bar{\psi}'^{\dot{X}}=(L^A{}_B\psi^B)(\bar{L}^{\dot{X}}{}_{\dot{Y}}\bar{\psi}\dot{Y})=L^A{}_B(\psi^B\bar{\psi}^{\dot{Y}})(L^\dagger)_{\dot{Y}}{}^{\dot{X}}=L^A{}_BX^{B\dot{Y}}(L^\dagger)_{\dot{Y}}{}^{\dot{X}} \tag{3.5}$$

or

$$X'=LXL^\dagger, \tag{3.6}$$

where

$$X=(X^{A\dot{X}})=x^a\sigma_a \tag{3.7}$$

so that we recover (2.5).

From (3.6) one may obtain the vector representation of L in the following familiar way. We have

$$\sum x'_a\sigma^a=\sum (L\sigma^bL^\dagger)x_b, \tag{3.8}$$

$$x'_b=\frac{1}{2}\sum (\mathrm{Tr}\ \bar{\sigma}_bL\sigma^cL^\dagger)x_c, \tag{3.9}$$

or the vector representation of L is

$$L_b{}^c=\tfrac{1}{2}\ \mathrm{Tr}\ \bar{\sigma}_bL\sigma^cL^\dagger \tag{3.10}$$

in terms of the spin representation of L.

IV. THE q-DEFORMATION OF THE LORENTZ GROUP

We base our work on the following q-deformation of the covariant Levi–Civita tensor:

$$\epsilon_q=\begin{pmatrix}0 & q^{-1/2}\\ -q^{1/2} & 0\end{pmatrix},\quad \epsilon_q^2=-1,\quad \epsilon_q\epsilon_q^t=\begin{pmatrix}q^{-1} & 0\\ 0 & q\end{pmatrix}. \tag{4.1}$$

Repeating (2.13) in terms of ϵ_q we define T, the q-deformed spin representation of L, as follows:

$$\epsilon_q\Delta_q=T^t\epsilon_qT \tag{4.2}$$

$$= T\epsilon_q T^t. \tag{4.3}$$

Here t means transpose, and Δ_q is by definition the q-determinant.

We know that these relations define the $\mathrm{GL}_q(2)$ group. That is, if

$$T = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \tag{4.4}$$

then (4.2) and (4.3) may be simultaneously satisfied only if the following relations hold:

$$\begin{gathered} ab = qba, \quad bc = cb, \quad ac = qca, \\ bd = qdb, \quad \Delta_q = ad - qbc, \quad cd = qdc, \end{gathered} \tag{4.5}$$

and

$$(\Delta_q, T_{kl}) = 0. \tag{4.6}$$

Here Δ_q is the q-determinant and (4.2) may be regarded as a definition of this determinant since

$$(\epsilon_q)_{AB} \det_q T = T^C{}_A T^D{}_B (\epsilon_q)_{CD} \tag{4.7}$$

$$= T_A{}^C T_B{}^D (\epsilon_q)_{CD} \tag{4.8}$$

as in (2.13).

The only restriction on the matrix L is (2.7). We shall now impose the corresponding condition on T. Then $\det_q T = 1$ and

$$\epsilon_q = T\epsilon_q T^t \tag{4.9}$$

$$= T^t \epsilon_q T. \tag{4.10}$$

Note also

$$\det_q T^t = \det_q T = 1. \tag{4.11}$$

We may now try to take over Eq. (2.5) with L replaced by T:

$$X' = TXT^\dagger, \quad \det_q T = 1. \tag{4.12}$$

The previous arguments no longer go through, however, since the matrix elements of T are noncommuting. In the limit $q = 1$, T approaches L, and (4.12) then describes a Lorentz transformation. However, (4.11) has the same meaning as (2.5) only in the $q = 1$ limit when the matrix elements (a,b,c,d) all commute and lie in the complex plane. In general (4.12) will have no classical meaning. Nevertheless a corresponding spinor algebra may again be constructed.

V. q-SPINORS

Except when explicitly otherwise indicated, let us now understand by ϵ the ϵ_q matrix. One may next define a contravariant ϵ by

$$\epsilon^{12} = q^{1/2}, \quad \epsilon^{21} = -q^{-1/2}, \quad \epsilon^{kk} = 0, \tag{5.1}$$

so that $\epsilon^{AB}(q) = \epsilon_{AB}(q^{-1})$ or

$$\epsilon^{AC}\epsilon_{BC}=\delta^{A}_{B}. \tag{5.2}$$

Then ϵ_{AB} is the metric in spin space and may be used to raise and lower indices. Thus if ξ_A is a covariant spinor, the corresponding contravariant spinor is

$$\xi^{B}=\epsilon^{BA}\xi_{A} \tag{5.3}$$

and

$$\xi_{A}=\xi^{C}\epsilon_{CA}. \tag{5.4}$$

By (4.7) ϵ_{AB} is an invariant tensor since

$$\epsilon_{AB}=T_{A}{}^{C}T_{B}{}^{D}\epsilon_{CD}. \tag{5.5}$$

Multiply (5.5) by $\xi^A\chi^B$. Then

$$\xi^{A}\epsilon_{AB}\chi^{B}=\xi^{C'}\epsilon_{CD}\chi^{D'}, \tag{5.6}$$

where

$$\xi^{C'}=\xi^{A}T_{A}{}^{C} \tag{5.7a}$$

$$\chi^{D'}=\chi^{B}T_{B}{}^{D}. \tag{5.7b}$$

The invariant quadratic forms (5.6) may also be written as follows:

$$\xi^{A}\epsilon_{AB}\chi^{B}=\xi_{B}\chi^{B}=\xi^{A}\tilde{\chi}_{A}, \tag{5.8}$$

where

$$\xi_{B}=\xi^{A}\epsilon_{AB}, \tag{5.9a}$$

$$\tilde{\chi}_{A}=\epsilon_{AB}\chi^{B}=\chi^{B}\epsilon^{t}_{BA}. \tag{5.10a}$$

By (5.2) the inverses of (5.9a) and (5.10a) are

$$\xi^{C}=\epsilon^{CB}\xi_{B} \tag{5.9b}$$

$$\chi^{C}=\tilde{\chi}_{A}\epsilon^{AC}. \tag{5.10b}$$

Given (5.7) and (5.9a) one finds

$$\xi'_{B}=\xi^{C}T_{C}{}^{A}\epsilon_{AB}. \tag{5.11}$$

By (5.9b)

$$\xi'_{B}=\epsilon^{CD}\xi_{D}T_{C}{}^{A}\epsilon_{AB}. \tag{5.12}$$

Denote the matrix $\|\epsilon^{CD}\|$ by $\hat{\epsilon}$ to distinguish it from $\|\epsilon_{CD}\|=\epsilon$. Then

$$\xi'_{B}=\xi_{D}(\hat{\epsilon}^{t}T\epsilon)^{D}{}_{B}. \tag{5.13}$$

However,

$$\hat{\epsilon}(q)=\epsilon(q^{-1})=-\epsilon^{t}(q) \tag{5.14}$$

and (5.13) becomes

$$\xi'_B=-\xi_D(\epsilon T\epsilon)^D{}_B. \tag{5.15}$$

By (4.9) or (4.10)

$$\epsilon T\epsilon=-(T^t)^{-1}. \tag{5.16}$$

Therefore

$$\xi'{}_B=\xi_D((T^t)^{-1})^D{}_B. \tag{5.17}$$

Note that $(T^t)^{-1}\neq(T^{-1})^t$ here. One checks that

$$\xi'{}_B\chi^{B'}=\xi_B\chi^B. \tag{5.18}$$

This invariant may be written as

$$\xi_A\chi^A=\epsilon_{BA}\xi^B\chi^A \tag{5.19}$$

$$=q^{-1/2}(\xi^1\chi^2-q\xi^2\chi^1). \tag{5.20}$$

Therefore the invariant equation

$$\xi_A\chi^A=0 \tag{5.21}$$

implies the invariance of the commutation rules

$$\xi^1\chi^2=q\xi^2\chi^1. \tag{5.22}$$

Just as in the Lorentz case, one must also make use of the conjugate representations. Corresponding to (5.7) and (5.17) one has

$$\bar{\xi}^{\dot{C}'}=\bar{\xi}^{\dot{A}}\bar{T}_{\dot{A}}{}^{\dot{C}} \tag{5.23}$$

and

$$\bar{\xi}'_B=\bar{\xi}_{\dot{D}}((\bar{T}^t)^{-1})^{\dot{D}}{}_{\dot{B}}, \tag{5.24}$$

where $\bar{\xi}^{\dot{A}}$ is the basis for $\bar{T}$, the conjugate representation, and the dot again indicates the conjugate representation. The conjugate is now in the SU_q (2) algebra, not in the complex plane.

An alternative procedure begins with (4.7) instead of (4.8). Then

$$\epsilon_{AB}=T^C{}_A\epsilon_{CD}T^D{}_B, \quad \xi^A\epsilon_{AB}\chi^B=(\xi^C\epsilon_{CD}\chi^D)', \tag{5.25}$$

where

$$\xi^{C'}=T^C{}_A\xi^A, \quad \chi^{D'}=T^D{}_B\chi^B, \tag{5.26}$$

instead of (5.7).

VI. THE σ_q MATRICES

Let us set

$$(\sigma_q^m)_{B\dot{Y}}=(1,\vec{\sigma}) \tag{6.1}$$

just as for the Lorentz case.

We now introduce the matrices contravariant to $(\sigma_q^m)_{B\dot{Y}}$ with respect to the metric ϵ_q:

$$(\bar{\sigma}_q^m)^{\dot{X}A}=\epsilon_q^{\dot{X}\dot{Y}}\epsilon_q^{AB}(\sigma_q^m)_{B\dot{Y}}. \tag{6.2}$$

Then

$$(\bar{\sigma}_q^m)^{\dot{X}A}=\begin{pmatrix} q & 0 \\ 0 & q^{-1}\end{pmatrix}\begin{pmatrix} 0 & -1 \\ -1 & 0\end{pmatrix}\begin{pmatrix} 0 & i \\ -i & 0\end{pmatrix}\begin{pmatrix} -q & 0 \\ 0 & q^{-1}\end{pmatrix}, \tag{6.3}$$

which satisfies the following relations:

$$(\bar{\sigma}_q^m)^{\dot{X}A}(\sigma_q^n)_{A\dot{X}}=2\,\eta^{mn}, \tag{6.4}$$

$$(\sigma_q^n)_{A\dot{X}}(\bar{\sigma}_{qn})^{\dot{Y}B}=2\,\delta_{\dot{X}}^{\dot{Y}}\delta_A^B, \tag{6.5}$$

where

$$\eta^{nm}=\begin{pmatrix} \frac{1}{2}(q+q^{-1}) & 0 & 0 & \frac{1}{2}(q-q^{-1}) \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ -\frac{1}{2}(q-q^{-1}) & 0 & 0 & -\frac{1}{2}(q+q^{-1}) \end{pmatrix}. \tag{6.6}$$

VII. THE q-SPIN REPRESENTATION OF VECTORS

Define the q-vector by

$$x_a=(\sigma_q)_a^{A\dot{X}}X_{A\dot{X}}, \tag{7.1}$$

where $X_{A\dot{X}}$ is the bispinor

$$X_{A\dot{X}}=\psi_A\bar{\psi}_{\dot{X}}. \tag{7.2}$$

Then

$$X_a=\psi(\sigma_q)_a\bar{\psi}. \tag{7.3}$$

The transformation of $X_{A\dot{X}}$ reads as follows:

$$X'_{A\dot{X}}=(T_A{}^B\psi_B)(\bar{T}_{\dot{X}}{}^{\dot{Y}}\bar{\psi}_{\dot{Y}})=T_A{}^B(\psi_B\bar{\psi}_{\dot{Y}})(T^\dagger)^{\dot{Y}}{}_{\dot{X}}, \tag{7.4}$$

where

$$\bar{T}_{\dot{X}}{}^{\dot{Y}}=(\bar{T}^t)^{\dot{Y}}{}_{\dot{X}}=(T^\dagger)^{\dot{Y}}{}_{\dot{X}}. \tag{7.5}$$

Then (7.4) may be written

$$X' = TXT^{\dagger}, \tag{7.6}$$

where $T^{\dagger}$ means the Hermitian adjoint matrix. This equation is formally the same as (3.6) with L replaced by T. In addition

$$\det_q T = \det L = 1, \tag{7.7}$$

but

$$\det_q X' \neq \det_q X, \tag{7.8}$$

unless $q=1$, since

$$\det_q AB \neq \det_q A \ \det_q B \tag{7.9}$$

unless

$$(A_{ij}, B_{kl}) = 0.$$

Although $\det_q X$ is not conserved, one may continue by rewriting (7.6) as follows,

$$\sum x^{a'}(\sigma_q)_a = T \sum x^a (\sigma_q)_a T^{\dagger}, \tag{7.10}$$

and solving to give the transformation equation for x^a:

$$x^{a'} = \sum T^a{}_b x^b, \tag{7.11}$$

where

$$T^a{}_b = \tfrac{1}{2} \ \mathrm{Tr} \ \bar{\sigma}_q^a T (\sigma_q)_b T^{\dagger}. \tag{7.12}$$

VIII. INVARIANTS AND IRREDUCIBLE REPRESENTATIONS[4]

Although the usual Lorentz interval, represented by $(\det X)^{1/2}$, is no longer invariant, there are of course new invariants belonging to the deformed group. Just as the invariants of the Lorentz group are the same as the invariants of the unimodular linear group SL(2), here they are the same as those of $\mathrm{SL}_q(2)$. The basic invariant may be expressed in terms of either the covariant or contravariant metric as follows:

$$\xi^A \epsilon_{AB} \chi^B = 0, \tag{8.1a}$$

$$\xi_A \hat{\epsilon}^{AB} \chi_B = 0, \tag{8.1b}$$

or

$$\xi^1 \chi^2 - q \xi^2 \chi^1 = 0, \tag{8.2a}$$

$$\xi_2 \chi_1 - q \xi_1 \chi_2 = 0. \tag{8.2b}$$

Take the special case $\xi = \chi$. Then

$$\chi_2 \chi_1 = q \chi_1 \chi_2 \tag{8.3}$$

and

$$\chi_1\chi_2\cdot\chi_2\chi_1=\chi_2\chi_1\cdot\chi_1\chi_2. \tag{8.4}$$

By the binomial theorem applied to (8.1)

$$\frac{(i\chi^t\epsilon\chi)^{2j}}{(2j)!}=\sum\ \tilde{V}(jm)V(jm)(-q)^m, \tag{8.5}$$

where

$$V(jm)=\frac{\chi_2^{j+m}\chi_1^{j-m}}{[(j+m)!(j-m)!]^{1/2}}\ \epsilon(q^{-1}|j+m), \tag{8.6}$$

$$\tilde{V}(jm)=\frac{\chi_1^{j+m}\chi_2^{j-m}}{[(j+m)!(j-m)!]^{1/2}}\ \epsilon(q|j-m), \tag{8.7}$$

and

$$\epsilon(q|n)=q^{n(n-1)/2}. \tag{8.8}$$

Therefore

$$e^{i\chi^t\epsilon\chi}=\sum\ \tilde{V}(jm)V(jm)(-q)^m=1. \tag{8.9}$$

The invariant terms of (8.5) may be written

$$Q(j)=\tilde{V}(j)C^j(-q)V(j), \tag{8.10}$$

where

$$C^j(q)=\begin{pmatrix} q^j & & \\ & \ddots & \\ & & q^{-j}\end{pmatrix}. \tag{8.11}$$

Here $\tilde{V}(jm)$ and $V(jm)$ are the $2j+1$-dimensional vectors which transform under T as

$$\tilde{V}'(jm)=\sum_{-j}^{j}\ \tilde{V}(jm')\tilde{D}^j(m'm), \tag{8.12}$$

$$V'(jm)=\sum_{-j}^{j}\ D^j(m,m')V(jm'). \tag{8.13}$$

One finds

$$\tilde{D}^j(m',m)=N^{jm}_{jm'}\ \frac{\epsilon(q|j-m)}{\epsilon(q|j-m')}\ q^{-j^2}\sum\ q^{\sigma}\left\langle \begin{matrix} j+m \\ j-m'-t\end{matrix}\right\rangle_{q^2}\left\langle \begin{matrix} j-m \\ t\end{matrix}\right\rangle_{q^2} b^{j-m'-t}a^{m+n'+t}d^tc^{j-m-t}. \tag{8.14}$$

Here

$$\left\langle \begin{matrix} n \\ s\end{matrix}\right\rangle=\frac{\langle n\rangle_q!}{\langle s\rangle_q!\langle n-s\rangle_q!},\quad \langle n_q\rangle=\frac{q^n-1}{q-1}, \tag{8.15}$$

where $\langle n \rangle$ is the basic integer.

These $2j+1$-dimensional vectors are the higher-dimensional spin tensors that correspond to the higher rank Lorentz tensors, and the invariants $Q(j)$ replace the Lorentz invariants such as the interval $(\det X)^{1/2}$.

To put (8.6) into correspondence with the bispinor of (7.2), one sets $j=\frac{1}{2}$ in (8.6) to obtain ψ^A, and then makes use of the conjugate representation in order to form $\chi^A \bar{\chi}^{\dot{X}}$.

With these results one may put the higher-dimensional representations of $\mathrm{SL}_q(2)$ into correspondence with the higher-dimensional representations of SL(2), or equivalently the Lorentz group.

IX. q-PENROSE TENSORS

With the aid of the ϵ-tensor, Penrose[5] showed how to decompose a reducible representation of the Lorentz group into its irreducible parts. As the q-analogue of his procedure we may propose relations such as the following:

$$F_{A\dot{X}B\dot{Y}}(q)=\epsilon_{AB}(q)\bar{\phi}_{\dot{X}\dot{Y}}(q)+\epsilon_{\dot{X}\dot{Y}}(q)\phi_{AB}(q) \tag{9.1}$$

and

$$F_{mn}(q)=F_{A\dot{X}B\dot{Y}}(q)\sigma_m^{A\dot{X}}(q)\sigma_n^{B\dot{Y}}(q). \tag{9.2}$$

When $q=1$, these are the Penrose relations for the decomposition of an antisymmetric tensor of the second rank. When $q=1$, ϵ is antisymmetric, the ϕ-spinors are symmetric, and F_{mn} is antisymmetric. The ϕ-spinors are the basis for the irreducible representations $D(0,1)$ and $D(1,0)$.

When $q\neq 1$ we shall still require

$$\epsilon^{\dot{X}\dot{Y}}(q)\bar{\phi}_{\dot{X}\dot{Y}}(q)=0 \quad \text{or} \quad q\bar{\phi}_{\dot{1}\dot{2}}(q)=\bar{\phi}_{\dot{2}\dot{1}}(q) \tag{9.3a}$$

and

$$\epsilon^{AB}(q)\phi_{AB}(q)=0 \quad \text{or} \quad q\phi_{12}(q)=\phi_{21}(q). \tag{9.3b}$$

When $q=1$, (9.3a) and (9.3b) are satisfied because of the symmetry of ϕ and antisymmetry of ϵ. When $q\neq 1$, these relations fix the symmetry of ϕ. Symmetry and antisymmetry are not preserved by $\mathrm{SL}_q(2)$ transformations. Equation (9.2) defines the q-analogue of a second-rank antisymmetric tensor.

Similarly we write for the q-Weyl tensor

$$W_{A\dot{W}B\dot{X}C\dot{Y}D\dot{Z}}(q)=\epsilon_{\dot{W}\dot{X}}(q)\epsilon_{\dot{Y}\dot{Z}}(q)W_{ABCD}(q)+\epsilon_{AB}(q)\epsilon_{CD}(q)\bar{W}_{\dot{W}\dot{X}\dot{Y}\dot{Z}}(q) \tag{9.4}$$

$$W_{mnrs}(q)=W_{A\dot{W}B\dot{X}C\dot{Y}D\dot{Z}}\sigma_m^{A\dot{W}}(q)\sigma_n^{B\dot{X}}(q)\sigma_r^{C\dot{Y}}(q)\sigma_s^{D\dot{Z}}(q), \tag{9.5}$$

where

$$\epsilon^{AB}(q)W_{ABCD}(q)=0 \quad \text{or} \quad qW_{12CD}=W_{21CD}, \tag{9.6a}$$

$$\epsilon^{CD}(q)W_{ABCD}(q)=0 \quad \text{or} \quad qW_{AB12}=W_{AB21}, \tag{9.6b}$$

$$\epsilon^{\dot{W}\dot{X}}(q)\bar{W}_{\dot{W}\dot{X}\dot{Y}\dot{Z}}(q)=0 \quad \text{or} \quad q\bar{W}b_{\dot{1}\dot{2}\dot{Y}\dot{Z}}=\bar{W}_{\dot{2}\dot{1}\dot{Y}\dot{Z}}, \tag{9.6c}$$

$$\epsilon^{\dot{X}\dot{Z}}(q)\bar{W}_{\dot{W}\dot{X}\dot{Y}\dot{Z}}(q)=0 \quad \text{or} \quad q\bar{W}_{\dot{W}\dot{X}\dot{1}\dot{2}}=\bar{W}_{\dot{W}\dot{X}\dot{2}\dot{1}}. \tag{9.6d}$$

When $q=1$, one has the Penrose decomposition of the Weyl tensor. When $q\neq 1$, the above relations describe a q-deformation of this tensor.

X. CHARGE CONJUGATION

The entire development in this paper is based on ϵ_q, the deformed Levi–Civita tensor defined by (4.4) and (4.10), where T is a two-dimensional representation of $SL_2(2)$. In an arbitrary $2j+1$-dimensional representation, D^j, these equations become[6]

$$(D^j)^t E^j D^j = D^j E^j (D^j)^t = E^j, \tag{10.1}$$

where

$$E^j(m,m') = (-q_1)^m \delta(m+m;0). \tag{10.2}$$

Then ϵ corresponds to the special case $j=\frac{1}{2}$ (E^j is undefined up to a factor).

Otherwise expressed

$$T^t E T = T E T^t = E \tag{10.3}$$

or E intertwines T^t and T^{-1}.

On the other hand the charge conjugation matrix of particle physics is defined with respect to the Lorentz transformation L by

$$L^t C L = C, \tag{10.4}$$

i.e., C intertwines L^t and L^{-1}.

Therefore E is the natural operator for q-charge conjugation and approaches C when T approaches L.

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A proof of polynomial identities of type $\widehat{sl(n)}_1 \otimes \widehat{sl(n)}_1 / \widehat{sl(n)}_2$

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We present a proof of polynomial identities related to finite analogs of the branching functions of the coset $\widehat{sl(n)}_1 \otimes \widehat{sl(n)}_1 / \widehat{sl(n)}_2$. © *1996 American Institute of Physics.* [S0022-2488(96)02102-5]

This paper is dedicated to the memory of Claude Itzykson

I. INTRODUCTION

Consider the affine algebra $\widehat{sl(n)}_\ell$, where $(n-1)$ is the rank and ℓ is the level.[1–3] Following Refs. 4 and 5, the branching functions of the coset

$$\mathscr{C}_{n,\ell_1,\ell_2} = \widehat{sl(n)}_{\ell_1} \otimes \widehat{sl(n)}_{\ell_2} / \widehat{sl(n)}_{\ell_1+\ell_2} \tag{1}$$

are characters of the highest weight modules (HWMs) of W_n algebras,[6] where W_2 is the Virasoro algebra.[7] We are interested in computing these branching functions.

A. *q*-series identities

An important observation, made independently in Ref. 8 in the context of affine algebras and in Ref. 9 in the context of branching functions, is that different approaches to computing the characters lead to completely different expressions for them. Equating different expressions of the same character leads to generalizations of the Rogers–Ramanujan identities. In the present work, we are interested in the identities related to the branching functions.

1. Boson–fermion identities

Because one side of these identities is generated using operators that obey bosonic commutation relations, while the other is generated using operators that obey fermionlike exclusion principles, these identities are also known as boson–fermion identities.

In Ref. 5, the branching functions of the coset $\mathscr{C}_{n,\ell_1,\ell_2}$ were obtained by counting certain configurations, known as *weighted paths*. These paths appear naturally in using the corner transfer matrix method to solve statistical mechanical models.[10] The expressions obtained are of the bosonic type. In the present work, we restrict our attention to the coset $\mathscr{C}_{n,1,1}$, and obtain expressions for the branching functions by counting the Ferrers graphs that appear in the crystal base description of the HWM's of $\widehat{sl(n)}_1$. The expressions obtained are of the fermionic type, and finitize the Lepowsky and Primc character formulas.[8]

2. Polynomial identities

In fact, we do not work directly in terms of the characters, which are formal infinite series. Instead, we work in terms of polynomials which depend on a parameter L, and reduce to the characters in the limit $L \to \infty$. In that sense, the identities we obtain are stronger than identities between characters.

Equating the expressions of Ref. 5, and those obtained in the present work, we obtain polynomial identities, one for each branching function of $\mathscr{C}_{n,1,1}$. For fixed n, there are $\mathscr{O}(n^2)$ such functions, and corresponding identities. These polynomial identities are generalizations of those considered by Schur in his approach to proving q-series identities.[11]

B. Two ways to count

Though the Ferrers graphs that we count are in one-to-one correspondence with the weighted paths, the expressions that we obtain are different from those of Ref. 5 because our approach to counting these objects is inherently different. We wish to outline the usual method of counting, in order to emphasize the contrast to ours.

1. Indirect counting: Sieving

In Ref. 5, the counting was achieved using a *sieving method* to obtain recurrence relations which can solved. The main idea of the sieving approach can be summarized as follows:[12]

Suppose one wishes to count the number of objects in a certain class P_0 which satisfy certain conditions.[13] This is typically a difficult problem, since the conditions satisfied by P_0 can be quite complicated. However, one can approach it *indirectly* as follows:

As a first step, one considers a larger class of objects Q_0, that includes P_0, but satisfies weaker conditions, and hence is easier to evaluate. Suppose one manages to do that. The next step would be to evaluate the difference $P_1 = Q_0 - P_0$, and subtract it to obtain $P_0 = Q_0 - P_1$ (hence the name *sieving*). However, evaluating P_1 *directly* is once again typically just as hard as the initial problem of evaluating P_0. Hence, it should also be evaluated in two steps: We consider a larger class of objects Q_1 that is easier to evaluate, and subtract that of the difference $P_2 = Q_1 - P_1$. We obtain $P_0 = Q_0 - Q_1 + P_2$. It is easy to see how the above procedure generalizes to give $P_0 = Q_0 - Q_1 + \cdots + Q_{\text{even}} - Q_{\text{odd}} + \cdots$.

The objects we are interested in—Ferrers graphs and paths—have dimensions. For larger i, P_i typically contains larger objects. If there are no restrictions on the dimensions of the objects being counted, then the above sieving procedure continues indefinitely. If there are such restrictions, then for sufficiently large i, the procedure terminates. Either way, the procedure amounts to writing a recurrence relation for the set $\{P_0, P_1, \ldots\}$ and solving it.

2. Direct counting: Sectoring

In contrast to the above, the approach used in this paper relies on a direct counting of the objects of interest. The main idea is to divide the set of all objects into sectors, each of which is easier to compute, and then to sum over all sectors. An outline of this approach is given below.

C. Outline of proof

(1) Given the set of graphs we wish to count, we propose to distinguish a certain subset to be called *parent graphs*. The remaining graphs are called *non-parents*.
(2) We propose a set of rules which reduces *any* non-parent graph uniquely to a parent graph by removing nodes from it. Using these rules we can decompose any non-parent graph into a parent graph plus a set of objects called *g-components*. The rules are such that a parent graph cannot be further reduced to another parent graph.

(3) We show that the above set of rules is invertible. Each non-parent can be uniquely obtained from a parent by attaching g-components. Consequently, the set of non-parents which reduce to a given parent may be regarded as the *descendants* of that parent.
(4) From the above, we classify the set of all graphs into sectors. Each sector contains precisely one parent plus its descendants.
(5) We show that, given a parent graph, the set of all its descendants is generated by a product over Gaussian polynomials.
(6) Since we know the explicit expression for the Gaussian polynomials in each sector, summing over all sectors, with the proper weighting which follows from the weight of the parent graph, we obtain the desired generating function of the graphs.

D. Plan of paper

In Sec. II, we outline a number of technical details related to weighted paths on the set of dominant integral weights of $\widehat{sl(n)}_2$, and recall the bosonic generating function as evaluated in Ref. 5. In Sec. III, we introduce the main objects of this paper, K-graphs, and discuss their properties. In Sec. IV, we describe the special set of K-graphs called parents. In Sec. V, we describe the graph components to be added to a parent to generate more general K-graphs, called descendants. In Sec. VI, we describe how the descendants are obtained from their parent, and why each graph is either a parent, or descends from a uniquely defined one. In Sec. VII, we evaluate the number of descendants of a certain parent. In Sec. VIII, we obtain fermionic expressions for the finite analogs of all branching functions of the coset $\mathscr{C}_{n,1,1}$. In Sec. IX we summarize our results to obtain the main theorem of this paper: polynomial identities for the finite analogs of the branching functions. This section also contains a discussion of our results.

II. PATHS

In this section, we consider weighted paths on the set of level-2 dominant integral weights of $\widehat{sl(n)}$, and recall their generating function as computed in Ref. 5.

A. Roots and weights

We start with some definitions from the theory of affine algebras.[1] Let Λ_i, α_i $(i=0,\ldots,n-1)$, and δ be the fundamental weights, the simple roots, and the null root of the affine Lie algebra $\widehat{sl(n)}$, respectively. The subscript i of Λ_i can be extended to $i \in \mathbb{Z}$ by setting $\Lambda_i = \Lambda_{i'}$ for $i \equiv i' \pmod n$. Let $\hat{i} = \Lambda_{i+1} - \Lambda_i$ $(i=0,\ldots,n-1)$ be the weights of the vector representation of $sl(n)$, and $\rho = \sum_{i=0}^{n-1} \Lambda_i$ be the Weyl vector.

Remark 1: For the rest of this work, we will simply use $a \equiv b$ to indicate $a \equiv b \pmod n$.

Let $P = \mathbb{Z}\Lambda_0 \oplus \cdots \oplus \mathbb{Z}\Lambda_{n-1} \oplus \mathbb{Z}\delta$ be the weight lattice.[1,2] There is an invariant bilinear form $(\cdot|\cdot)$ on P defined by

$$(\Lambda_i|\Lambda_j) = \min(i,j) - \frac{ij}{n}, \quad (\Lambda_i|\delta) = 1, \quad (\delta|\delta) = 0, \tag{2}$$

for $0 \leqslant i,j \leqslant n-1$.

We are not interested in the full weight lattice, but in certain restrictions of it:

Definition 1: (P_2^+) P_2^+ is the set of level-2 dominant integral weights, i.e., $P_2^+ = \{\Lambda_i + \Lambda_j | 0 \leqslant i \leqslant j \leqslant n-1\}$.

Examples of P_2^+ in the case of $n=2$, and 3 are shown in Fig. 1.

We can define paths on P_2^+ as follows:

Definition 2 (paths): For $L \in \mathbb{Z}_{\geqslant 0}$, we define a path p as $p = (\lambda_0, \ldots, \lambda_L)$ with all $\lambda_i \in P_2^+$ and $\lambda_{i+1} - \lambda_i \in \{\hat{0}, \hat{1}, \ldots, \widehat{n-1}\}$.

We are interested in particular sets of paths of length L defined by the following.

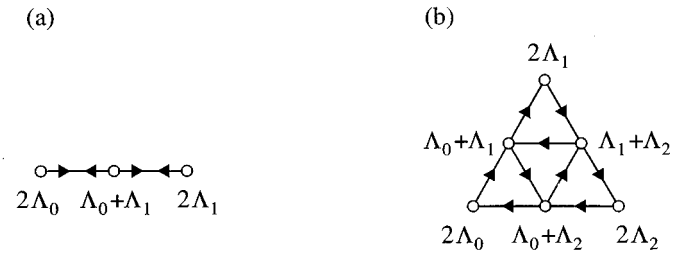

FIG. 1. Examples of the set P_2^+. A directed bond from λ to λ'($\lambda,\lambda' \in P_2^+$) indicates that a path can go from λ to λ'. (a) $n=2$, (b) $n=3$.

Definition 3: $[\mathscr{P}_L(\Lambda_i+\Lambda_j,\Lambda_k)]$.

$$\mathscr{P}_L(\Lambda_i+\Lambda_j,\Lambda_k)=\{p=(\lambda_0,\ldots,\lambda_L)\,|\,\lambda_0=\Lambda_i+\Lambda_j,\lambda_L=\Lambda_k+\Lambda_{i+j-k+L}\}. \tag{3}$$

For a path $p \in \mathscr{P}_L(\Lambda_i+\Lambda_j,\Lambda_k)$ we call $\Lambda_i+\Lambda_j,\Lambda_k$, and L its initial point, boundary, and length, respectively.

We note that $\mathscr{P}_L(\Lambda_i+\Lambda_j,\Lambda_k)$ is a finite analog (length L) of the set of $(\Lambda_k,\Lambda_{i+j-k})$-restricted paths of Ref. 14 and 15.

With the paths in $\mathscr{P}_L(\Lambda_i+\Lambda_j,\Lambda_k)$ we associate a special path $\bar{p}$ called the ground-state path, as follows:

Definition 4 (ground-state path $\bar{p}$):

$$\bar{p}=(\Lambda_k+\Lambda_{i+j-k},\Lambda_k+\Lambda_{i+j-k+1},\ldots,\Lambda_k+\Lambda_{i+j-k+L}) \in \mathscr{P}_L(\Lambda_k+\Lambda_{i+j-k},\Lambda_k).$$

Note that the initial point of the ground-state path may be different from that of the paths in $\mathscr{P}_L(\Lambda_i+\Lambda_j,\Lambda_k)$.

We can encode a path in terms of a sequence of integers as follows:

Definition 5 (sequence of integers): For a path $p=(\lambda_0,\ldots,\lambda_L) \in \mathscr{P}_L(\Lambda_i+\Lambda_j,\Lambda_k)$ we define a sequence of integers $\iota(p)=(\mu_0,\ldots,\mu_L)$, where $\hat{\mu}_\ell = \lambda_{\ell+1} - \lambda_\ell$, and where we have used $\lambda_{L+1}=\Lambda_k+\Lambda_{L+i+j-k+1}$. We denote the element μ_ℓ of $\iota(p)$ by $\iota(p)_\ell$.
Note that $\iota(\bar{p})$ of $\bar{p}$ in Definition 4 is given by $\iota(\bar{p})_\ell \equiv i+j-k+\ell$.

Example 1: The ground state path $\bar{p}$ associated to $\mathscr{P}_6(\Lambda_i+\Lambda_{-i},\Lambda_0)$ for $n=3$:

$$\bar{p}=(2\Lambda_0,\Lambda_0+\Lambda_1,\Lambda_0+\Lambda_2,2\Lambda_0,\Lambda_0+\Lambda_1,\Lambda_0+\Lambda_2,2\Lambda_0),$$

$$\iota(\bar{p})=(0,1,2,0,1,2,0).$$

Example 2: A path in $p^{(1)} \in \mathscr{P}_6(2\Lambda_0,\Lambda_1)$ for $n=3$:

$$p^{(1)}=(2\Lambda_0,\Lambda_0+\Lambda_1,\Lambda_0+\Lambda_2,\Lambda_1+\Lambda_2,\Lambda_0+\Lambda_1,\Lambda_0+\Lambda_2,\Lambda_1+\Lambda_2),$$

$$\iota(p^{(1)})=(0,1,0,2,1,0,2).$$

Example 3: A path in $p^{(2)} \in \mathscr{P}_6(2\Lambda_0,\Lambda_0)$ for $n=4$:

$$p^{(2)}=(2\Lambda_0,\Lambda_0+\Lambda_1,2\Lambda_1,\Lambda_1+\Lambda_2,2\Lambda_2,\Lambda_2+\Lambda_3,\Lambda_0+\Lambda_2),$$

$$\iota(p^{(2)})=(0,0,1,1,2,3,2).$$

B. Weighted paths

Let p be a path and $\bar{p}$ be the ground-state path associated to p, with integer sequences $\iota(p)=(\mu_0,\ldots,\mu_L)$ and $\iota(\bar{p})=(\bar{\mu}_0,\ldots,\bar{\mu}_L)$, respectively. We define an energy function E by the following.

Definition 6 (energy of a path):

$$E(p)=\sum_{\ell=1}^{L}\ell(\theta(\mu_{\ell-1}-\mu_\ell)-\theta(\bar{\mu}_{\ell-1}-\bar{\mu}_\ell)), \tag{4}$$

with θ the step function given by

$$\theta(\mu)=\begin{cases}0 & (\mu<0)\\ 1 & (\mu\geqslant 0).\end{cases} \tag{5}$$

1. Connection with cosets of affine algebras

Consider the coset $\mathscr{C}_{n,1,1}$. The branching functions corresponding to this coset can be defined as follows. Let $V(\Lambda)$ be an $\widehat{sl(n)}$ HWM with highest weight Λ, and let $|\Lambda\rangle$ be its highest weight vector. Consider the tensor product decomposition

$$V(\Lambda_k)\otimes V(\Lambda_{i+j-k})=\sum_{\Lambda\in P_2^+}\Omega_{\Lambda_k,\Lambda_{i+j-k},\Lambda}\otimes V(\Lambda). \tag{6}$$

Among all vectors in the tensor product on the left-hand side, $\Omega_{\Lambda_k,\Lambda_{i+j-k},\Lambda}$ is the space of highest weight vectors whose weights are equal to Λ mod $\mathbb{Z}\delta$. The connection between $\Omega_{\Lambda_k,\Lambda_{i+j-k},\Lambda}$, and $\mathscr{P}_L(\Lambda_i+\Lambda_j,\Lambda_k)$ is as follows: It has been shown in Ref. 14 that in the limit of $L\to\infty$, there is a bijection between the set of base vectors in $\Omega_{\Lambda_k,\Lambda_{i+j-k},\Lambda_i+\Lambda_j}$, and the set of paths in $\mathscr{P}_L(\Lambda_i+\Lambda_j,\Lambda_k)$. This implies that the paths of $\mathscr{P}_L(\Lambda_i+\Lambda_j,\Lambda_k)$ are characterized by weights. Under this bijection the ground-state path associated to $\mathscr{P}_L(\Lambda_i+\Lambda_j,\Lambda_k)$ is identified with $|\Lambda_k\rangle\otimes|\Lambda_{i+j-k}\rangle\in\Omega_{\Lambda_k,\Lambda_{i+j-k},\Lambda_k+\Lambda_{i+j-k}}$.

It turns out that the weight of a path can be expressed in terms of its energy function as

Definition 7: [weight of a path $p\in\mathscr{P}_L(\Lambda_i+\Lambda_j,\Lambda_k)$]

$$wt(p)=\Lambda_i+\Lambda_j-E(p)\,\delta. \tag{7}$$

2. Finite analogs of branching functions

Given the above considerations, we define finite analogs of the branching functions B_L for the coset $\mathscr{C}_{n,1,1}$ as the generating function of the weighted paths in $\mathscr{P}_L(\Lambda_i+\Lambda_j,\Lambda_k)$:

$$B_L(\Lambda_i+\Lambda_j,\Lambda_k)=\sum_{p\in\mathscr{P}_L(\Lambda_i+\Lambda_j,\Lambda_k)}q^{E(p)}. \tag{8}$$

C. Bosonic expressions

We are interested in expressions for the generating function $B_L(\Lambda_i+\Lambda_j,\Lambda_k)$. In Ref. 5, the following *bosonic* expression for $B_L(\Lambda_i+\Lambda_j,\Lambda_k)$ was obtained using recurrence relations based on the sieving method explained in Sec. I:

Theorem 1: Let $\lambda=\sum_{i=0}^{n-1}\lambda\hat{2}_i+\mathbb{Z}\delta\in P$, with all $\lambda_i\geqslant 0$ and $\sum_{i=0}^{n-1}\lambda_i=N$. For such λ set

$$\left[\!\left[\begin{matrix}N\\ \lambda\end{matrix}\right]\!\right]_q=\frac{(q)_N}{(q)_{\lambda_0}\cdots(q)_{\lambda_{n-1}}}, \tag{9}$$

with $(q)_m=\Pi_{k=1}^{m}(1-q^k)(m\geqslant 1)$ and $(q)_0=1$. Also, let $\mathscr{W}^{\cdot}$ denote the Weyl group of $\widehat{sl(n)}$ (see, e.g., Ref. 5, p. 91). Then

$$B_L(\Lambda_i+\Lambda_j,\Lambda_k)=q^{-|\Lambda_{i+j-k}|^2/2}\sum_{w\in\mathscr{W}^{\cdot}}(\det w)b_{L,i+j-k}(\Lambda_k+\Lambda_{i+j-k+L}+\rho-w(\Lambda_i+\Lambda_j+\rho)), \tag{10}$$

where

$$b_{L,i}(\lambda)=q^{|\lambda-\Lambda_{i+L}|^2/2}\begin{bmatrix}\begin{bmatrix}L\\ \lambda\end{bmatrix}\end{bmatrix}_q. \tag{11}$$

For proof we refer the reader to Ref. 5.

III. K-GRAPHS

Using matrices as intermediate structures, we give an alternative representation of the weighted paths on P_2^+ in terms of Ferrers graphs (or, equivalently, Young diagrams) which satisfy certain restrictions. We refer to these Ferrers graphs, which were introduced and extensively studied by the Kyoto school (see Refs. 14 and 16 and references therein), as K-graphs.

A. Interpolating matrices

In this subsection, we associate a matrix $M(p)$ with two rows to each path $p\in\mathscr{P}_L(\Lambda_i+\Lambda_j,\Lambda_k)$.

Definition 8 (domain wall): Let $\iota(p)=(\mu_0,\ldots,\mu_L)$ be the integer sequence of $p\in\mathscr{P}_L(\Lambda_i+\Lambda_j,\Lambda_k)$. If $\mu_{\ell}-\mu_{\ell-1}\equiv h_{\ell}+1 (0<h_{\ell}<n)$, we say that there is a domain wall in the sequence $\iota(p)$ of height h_{ℓ} at position ℓ.

Given a path p with N domain walls of heights $h_1,\ldots,h_N$ at the positions $x_1,\ldots,x_N$, respectively, we define the interpolating matrix $M(p)$ as follows:

Definition 9 (interpolating matrix):

$$M(p)=\begin{pmatrix}x_1 & (x_2-x_1) & \cdots & (x_N-x_{N-1})\\ h_1 & h_2 & \cdots & h_N\end{pmatrix}. \tag{12}$$

Example 4: The interpolating matrix of $p^{(2)}$ in Example 3 is

$$M(p^{(2)})=\begin{pmatrix}1 & 2 & 3\\ 3 & 3 & 2\end{pmatrix}.$$

B. K-graph representation of a path

Let p be a path and $M(p)$ its interpolating matrix of the form

$$M(p)=\begin{pmatrix}w_1 & w_2 & \cdots & w_N\\ h_1 & h_2 & \cdots & h_N\end{pmatrix}. \tag{13}$$

Consider a two-dimensional square lattice with an (x,y)-coordinate system. Set $W=w_1+\cdots+w_N$, $H=h_1+\cdots+h_N$. Starting from $(0,-H)$, we draw a polygon by moving w_1 steps to the right, then h_1 steps up, then w_2 steps to the right, etc., until we reach the point $(W,0)$. Connecting $(0,-H)$ and $(W,0)$ with the origin by straight line-segments, the resulting graph is *the Ferrers graph* or *Young diagram* corresponding to the original path [see Fig. 2(a)].

Definition 10 (K-graph): A Ferrers graph obtained from a path p on P_2^+, as described above, is called a K-graph.

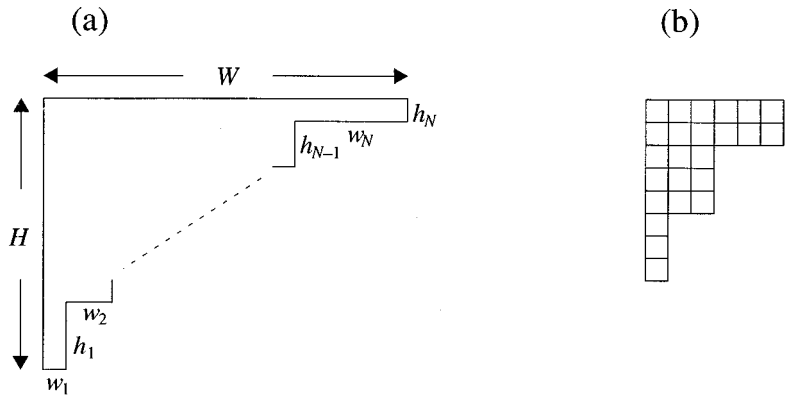

FIG. 2. (a) The general form of a K-graph. (b) A K-graph in $\mathscr{G}_6(2\Lambda_0,\Lambda_0)$ for $n=4$.

Definition 11: $(\mathscr{G}_L(\Lambda_i+\Lambda_j,\Lambda_k))$ $\mathscr{G}_L(\Lambda_i+\Lambda_j,\Lambda_k)$ is defined as the set of K-graphs corresponding to the set of path $\mathscr{P}_L(\Lambda_i+\Lambda_j,\Lambda_k)$.

Definition 12 (profile of a graph): The set of horizontal and vertical line segments used to construct a K-graph form the profile of a graph.

Example 5: The K-graph corresponding to the interpolating matrix of Example 4 is shown in Fig. 2(b).

Definition 13 (concave corner): A corner of the form ⌈.

Definition 14 (convex corner): A corner of the form ⌋.

Definition 15 (plain of width w): A horizontal line segment of w nodes (or boxes) marked by a concave corner to its left and convex corner to its right.

Definition 16 (cliff of height h): A vertical line segment of h nodes (or boxes) marked by a convex corner at its bottom and a concave corner at its top.

Notice that a cliff on a K-graph corresponds to a domain wall in the corresponding integer sequence.

Remark 2: From now on, we concentrate on K-graphs in $\mathscr{G}_L(2\Lambda_0,\Lambda_k)$, unless otherwise stated.

1. From a graph to its sequence of integers

For a graph $G\in\mathscr{G}_L(2\Lambda_0,\Lambda_k)$, we can recover the corresponding integer sequence $\iota(p)$ as follows. Let

$$M=\begin{pmatrix} w_1 & w_2 & \cdots & w_N \\ h_1 & h_2 & \cdots & h_N \end{pmatrix} \tag{14}$$

be the interpolating matrix corresponding to G. Set $H=h_1+\cdots+h_N$, and take the integer sequence $(0,1,2,\ldots,n-1,0,1,\ldots,n-1,0,1,\ldots)$ of length $H+L+1$. Starting from the left moving to the right, we now keep the first w_1 integers, then remove the next h_1 integers, then keep the next w_2 integers, remove the next h_2 integers, etc. The remaining sequence of exactly $L+1$ integers corresponds to $\iota(p)$.

2. From a graph to a path

To go from a graph $G\in\mathscr{G}_L(2\Lambda_0,\Lambda_k)$ to its corresponding path $p=(\lambda_0,\ldots,\lambda_L)$ on P_2^+ we simply first construct the sequence of integers $\iota(p)=(\mu_0,\ldots,\mu_L)$ as described above. We then compute $\lambda_{\ell+1}=\lambda_\ell+\hat{\mu}_\ell$ using $\lambda_0=2\Lambda_0$.

3. Conditions on $\mathcal{G}_L(2\Lambda_0, \Lambda_k)$

Among all K-graphs, those in $\mathcal{G}_L(2\Lambda_0, \Lambda_k)$ are characterized by the following conditions:

K1: $W \leqslant L$, with W the number of nodes in the first row.

K2: $H + k \equiv 0$, with H the number of nodes in the first column.

K3: $h_{i-1} + w_i + h_i \equiv 0$ and $0 < h_i < n$ for $1 \leqslant i \leqslant N$, with $h_0 = n$.

K1 is obvious. **K2** is obtained by considering the Lth component of $\iota(p)$ and the boundary condition. To obtain **K3**, suppose the ith cliff occurs at the rth position. We can assume $\lambda_r = \lambda_a + \Lambda_b, \lambda_{r-w_i} = \Lambda_a + \Lambda_{b-w_i}$ for some a, b. Now we have $\iota(p)_{r-1} \equiv b - 1$, $\iota(p)_{r-w_i} \equiv b - w_i$. Since there are cliffs at the rth and $(r-w_i)$-th position, we should have $\iota(p)_r \equiv a$ and $\iota(p)_{r-w_i} - 1 \equiv a - 1$. Thus we get $h_i \equiv a - b$, $h_{i-1} \equiv b - w_i - a$, which gives **K3**.

C. Fermionic expressions

We now wish to calculate the following sum.

$$F_L(\Lambda_i + \Lambda_j \Lambda_k) = \sum_{G \in \mathcal{G}_L(\Lambda_i + \Lambda_j, \Lambda_k)} q^{|G|/n}, \tag{15}$$

where $|G|$ denotes the number of nodes in G. Regarding the above, we have the following theorem.[14,16]

Theorem 2: Let p be a path in $\mathcal{P}_L(\Lambda_i + \Lambda_j, \Lambda_k)$ and $G(p)$ be the corresponding K-graph. The number of nodes of $G(p)$ is given by

$$|G| = \sum_{\ell=0}^{n-1} m_\ell, \tag{16}$$

where m_ℓ is determined from

$$(\Lambda_k + \Lambda_{i+j-k}) - wt(p) = \sum_{\ell=0}^{n-1} m_\ell \alpha_\ell. \tag{17}$$

Using

$$(\Lambda_i | \alpha_j) = \delta_{ij} \quad (i, j = 0, \ldots, n-1),$$

we obtain

$$m_l = (\Lambda_l | (\Lambda_k + \Lambda_{i+j-k}) - wt(p)) \quad (l = 0, \ldots, n-1).$$

Since we define the sum (15) in the "principal picture," i.e., each node has equal weight $1/n$, it is invariant under the Dynkin diagram automorphisms. Thus we can reduce the calculation of (15) to that of $F_L(\Lambda_0 + \Lambda_j, \Lambda_k)$. From now on, we hence assume $i = 0$.

Setting $(\Lambda_k + \Lambda_{j-k}) - (\Lambda_0 + \Lambda_j) = \Sigma_{\ell=0}^{n-1} \bar{m}_\ell \alpha_\ell$, we have $\Sigma_{\ell=0}^{n-1} \bar{m}_\ell = k(j-k)$ for $j \geqslant k$, $= (k-j)(n-k)$ for $j < k$. Calculating $|\Lambda_k|^2 + |\Lambda_{j-k}|^2 - |\Lambda_j|^2$ and comparing (15) with the bosonic expression, we obtain

$$F_L(\Lambda_0 + \Lambda_j, \Lambda_k) = q^{(|\Lambda_k|^2 + |\Lambda_{j-k}|^2 - |\Lambda_j|^2)/2} B_L(\Lambda_0 + \Lambda_j, \Lambda_k). \tag{18}$$

In the remainder of this paper we will compute a fermionic type of expression for F_L. Given (18) and the bosonic expression (10) for B_L, this gives rise to polynomial identities for the finite analogs of the branching functions of the coset $\mathcal{C}_{n,1,1}$.

IV. PARENTS

From the set of all K-graphs in $\mathcal{G}_L(2\Lambda_0,\Lambda_k)$ we select a subset of graphs to be called parent graphs, or simply parents. Let $\vec{m}^t=(m_1,\ldots,m_{n-1})\in(\mathbb{Z}_{\geqslant 0})^{n-1}$, such that

$$k+\sum_{i=1}^{n-1} i m_i \equiv 0, \tag{19}$$

and let M be the interpolating matrix of a graph $G\in\mathcal{G}_L(2\Lambda_0,\Lambda_k)$, with entries

$$M(p)=\begin{pmatrix} w_1 & w_2 & \cdots & w_N \\ h_1 & h_2 & \cdots & h_N \end{pmatrix}. \tag{20}$$

Definition 17 (*parent associated to* $\vec{m}$): G is the parent associated to $\vec{m}$ if

$$\begin{gathered} h_1,\ldots,h_{m_{n-1}}=n-1 \\ h_{m_{n-1}}+1,\ldots,b_{m_{n-1}+m_{n-2}}=n-2 \\ \vdots \\ h_{N-m_1+1},\ldots,h_N=1, \end{gathered} \tag{21}$$

with $N=\Sigma_{i=1}^{n-1} m_i$, and

$$h_{i-1}+w_i+h_i=2n, \quad 1\leqslant i\leqslant N, \tag{22}$$

where we recall that $h_0=n$.

Example 6: The K-graph of $p^{(2)}$ shown in Fig. 2(b) is the parent associated to $\vec{m}^t=(0,1,2)$.

A. The number of nodes of a parent graph

Let C be the Cartan matrix of $sl(n)$, i.e., $C_{ij}=2\delta_{i,j}-\delta_{i,j-1}-\delta_{i,j+1}(i,j=1,\ldots,n-1)$. The inverse of C is then given by the following formula:

$$(C^{-1})_{ij}=\begin{cases} \dfrac{i(n-j)}{n} & (i\leqslant j) \\ \dfrac{j(n-i)}{n} & (i>j). \end{cases}, \tag{23}$$

With this definition we have the following lemma:

Lemma 1: The number of nodes of the parent associated to $\vec{m}$ is given by $n\vec{m}^t C^{-1}\vec{m}$.

Though the proof of this statement is rather elementary, we need to take some care as some of the entries of $\vec{m}$ can actually be zero. In the following we use the notation $\langle i\rangle$ to denote $\Sigma_{j=1}^{i} m_{n-j}$. Clearly, $\langle i\rangle-\langle i-1\rangle=m_{n-i}$. We now compute the number of nodes of a parent $N(\vec{m})$ as follows:

$$N(\vec{m})=\sum_{i=1}^{N}\sum_{j=1}^{i} h_i w_j=\sum_{k=1}^{n-1}\sum_{i=1+\langle k-1\rangle}^{\langle k\rangle}\left(\sum_{\ell=1}^{k-1}\sum_{j=1+\langle \ell-1\rangle}^{\langle \ell\rangle}+\sum_{j=1+\langle k-1\rangle}^{i}\right) h_i w_j. \tag{24}$$

Now use (22) and $h_{1+\langle i-1\rangle}=\cdots=h_{\langle i\rangle}=n-i$ to get

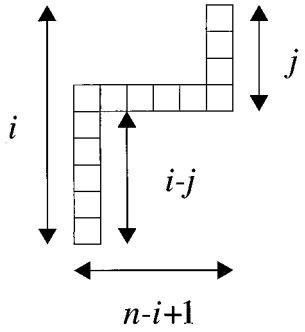

FIG. 3. An (i,j)-component.

$$N(\vec{m})=\sum_{k=1}^{n-1}\sum_{i=1+\langle k-1\rangle}^{\langle k\rangle}(n-k)\Bigg(\sum_{\ell=1}^{k-1}\sum_{j=1+\langle \ell-1\rangle}^{\langle \ell\rangle}\{2\ell-(h_{\langle \ell-1\rangle}-(n-\ell))\,\delta_{j,\langle \ell-1\rangle+1}\}$$
$$+\sum_{j=1+\langle k-1\rangle}^{i}\{2k-(h_{\langle k-1\rangle}-(n-k))\,\delta_{j,\langle k-1\rangle+1}\}\Bigg). \tag{25}$$

Finally, after some changes of variables, we obtain

$$N(\vec{m})=2\sum_{k=1}^{n-1}\sum_{\ell=1}^{k-1}\ell(n-k)m_k m_\ell+\sum_{k=1}^{n-1}(n-k)\sum_{i=1}^{m_{n-k}}\Bigg(2ik-\sum_{\ell=1}^{k}\sum_{j=1}^{m_{n-\ell}}(h_{\langle \ell-1\rangle}-(n-\ell))\,\delta_{j,1}\Bigg)$$
$$=2\sum_{k=1}^{n-1}\sum_{\ell=1}^{k-1}\ell(n-k)m_k m_\ell+\sum_{k=1}^{n-1}\sum_{i=1}^{m_{n-k}}k(n-k)(2i-1). \tag{26}$$

Summing over j and i this results in $n\vec{m}^{t}C^{-1}\vec{m}$.

V. *g*-COMPONENTS

Now that we have distinguished a subset of all K-graphs as parents, we wish to describe the minimal connected configuration of nodes that can be removed or added to a K-graph in $\mathcal{G}_L(2\Lambda_0,\Lambda_k)$ to obtain another K-graph in $\mathcal{G}_L(2\Lambda_0,\Lambda_k)$. Since, as we will see in Sec. VII, these configurations are generated by Gaussian polynomials, we call them *g*-components. Eventually, we will show that those graphs which are related by addition and removal of *g*-components belong to the same *sector*, and we will use this observation to relate any non-parent graph to a parent graph.

Definition 18: [(i,j)-component] For all $i=1,\ldots,n-1$, and all $j=1,\ldots,i$, we define an (i,j)-component as a connected configuration of n nodes, as shown in Fig. 3.

Some important characteristics of an (i,j)-component are the following.

G1 It consists of n nodes.

G2 It has total height i.

G3 It has total width $n-i+1$.

G4 It has (at most) two cliffs, one (the lower) of height $i-j$ and one (the upper) of height j.

We further note that for an (i,i)-component the lower cliff vanishes, resulting in a configuration with a single cliff.

Definition 19 (i-component): An (i,j)-component for arbitrary j is called an i-component.

Definition 20 (g-component): An (i,j)-component for arbitrary i and j is called a g-component.

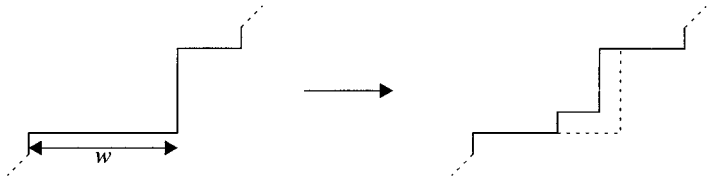

FIG. 4. Removing an (i,i)-component is only allowed when $w>2(n-i)$. The extra dotted lines in the resulting graph are to indicate the nodes which are removed.

We are now interested in the addition/removal of g-components to/from a K-graph. Clearly, in adding or removing a g-component to or from a K-graph in $\mathscr{G}_L(2\Lambda_0,\Lambda_k)$, we demand that the resulting graph is again a graph in $\mathscr{G}_L(2\Lambda_0,\Lambda_k)$. However, on top of this we impose one additional condition, which basically defines our sectors.

A. Removing an *i*-component

The removal of an (i,j)-component from a K-graph in $\mathscr{G}_L(2\Lambda_0,\Lambda_k)$ is allowed provided the following two conditions are satisfied:

R1 The resulting graph is again a K-graph in $\mathscr{G}_L(2\Lambda_0,\Lambda_k)$.

R2 If $j=i$ as in Fig. 4, we demand that $w>2(n-i)$.

Definition 21 (i-candidate): An i-component one is allowed to remove from a K-graph is called an i-candidate.

Since for any K-graph in $\mathscr{G}_L(2\Lambda_0,\Lambda_k)$ we have $h_{j-1}+w_j+h_j\equiv 0$, three kinds of candidates can occur.

(1) $b_{j-1}+w_j+h_j=n$ and $w_{j-1}>1$. In this case we can remove an $(h_{j-1}+h_j,h_j)$-component.
(2) $h_{j-1}+w_j+h_j=2n$ and $w_j>2(n-h_j)$. In this case we can remove an (h_j,h_j)-component.
(3) $h_{j-1}+w_j+h_j\geqslant 3n$. In this case we can remove an (h_j,h_j)-component.

Scanning the profile of a non-parent graph, several i-candidates may occur.

Definition 22 (leading i-candidate): The leading i-candidate is the down- and left-most i-candidate. (see Fig. 4.)

B. Attaching an *i*-component to a graph

Attaching an i-component to a K-graph in $\mathscr{G}_L(2\Lambda_0,\Lambda_k)$ is allowed provided the following conditions are satisfied:

A1 The resulting graph is again a K-graph in $\mathscr{G}_L(2\Lambda_0,\Lambda_k)$.

A2 We do not generate an i'-candidate, with $i'>i$.

Definition 23 (i-vacancy): An i-vacancy is a position on the profile such that one is allowed to attach an i-component.

An important statement about i-vacancies is the following. Given a sequence {cliff,plain,cliff} of dimensions h_{j-1},w_j,h_j such that $h_{j-1}+w_j+h_j=n$ and $h_{j-1}+h_j=i$, then the following holds:
Lemma 2: If $w_{j+1}=n-i$, the above sequence is not an i-vacancy.

To prove this, assume the above sequence is an i-vacancy. Hence we can attach an (i,h_j+1)-component as shown in Fig. 5(a). Note that in doing so the height of the jth cliff increases by 1 to $h_j'=h_j+1$, and the width of the $(j+1)$-th plain decreases by 1 to $w_{j+1}'=w_{j+1}-1=n-i-1$. Thus we compute

$$0<h_j'+w_{j+1}'+h_{j+1}=h_j+n-i+h_{j+1}\leqslant i+(n-i)+(n-1)=2n-1. \tag{27}$$

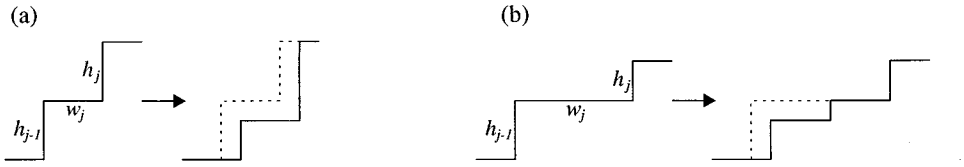

FIG. 5. (a) Attaching an $(h_{j-1}+h_j, h_j+1)$-component with $h_j \neq 1$. (b) Attaching an $(h_{j-1},1)$-component. The extra dotted lines in the resulting graphs are to indicate the profile before attaching the g-component.

Since $h'_j + w'_{j+1} + h_{j+1} \equiv n$, we conclude that $h'_j + w'_{j+1} + h_{j+1} = n$, and $h'_j + h_{j+1} = i+1$. However, these are the characteristics of an $(i+1)$-candidate. By the second condition for attaching i-components this contradicts our assumption that the initial sequence was an i-vacancy.

With the above lemma we note that two kinds of vacancies may occur. The first occurs if we have a sequence {cliff,plain,cliff} of dimensions h_{j-1}, w_j, h_j such that $h_{j-1}+w_j+h_j=n$ and $w_{j+1} > n-h_j-h_{j+1}$. In this case we can always attach an $(h_{j-1}+h_j, h_j+1)$-component, as shown in Fig. 5(a). The second occurs if we have a sequence {cliff,plain,cliff} of dimensions h_{j-1}, w_j, h_j such that $h_{j-1}+w_j+h_j \geqslant 2n$. In this case we can always attach an $(h_{j-1},1)$-component [see Fig. 5(b)].

VI. DESCENDANTS

In previous sections, we classified all admissible K-graphs into parents and non-parents. We need to show that each non-parent is a *descendant* of a unique parent. More precisely, we show the following.

(1) Given a non-parent graph, there is a reduction procedure, such that one can reduce it to a unique parent graph.
(2) The reduction procedure is reversible: given a parent graph, there is a composition procedure to recover the original non-parent graph.

Because the reduction procedure is reversible, any non-parent graph is a descendant of a unique parent graph. Thus the set of all admissible K-graphs can be divided into nonoverlapping sectors. Each sector contains and is labelled by a parent graph. Any admissible K-graph belongs to one and only one sector.

A. Reducing non-parent graphs

Given a non-parent K-graph, we can reduce it to a parent graph as follows.
Red0 Set $i=n-1$.
Red1 Search for the leading i-candidate and, if it exists, remove it.
Red2 Repeat the above step until no more i-candidates are found.
Red3 Set $i \to i-1$ and, if $i \geqslant 1$, repeat Red1–Red3.

To prove that a reduced graph is indeed a parent, we proceed as follows: Consider a profile with a sequence {cliff,plain,cliff} of dimensions h_{j-1}, w_j, h_j, respectively. Suppose that the part of the profile below the above sequence belongs to a parent, i.e., $h_{k-1}+w_k+h_k=2n$ and $h_{k-1} \geqslant h_k$ for $k=1,\ldots,j-1$. We wish to show that if the above sequence does not represent a candidate, it belongs to a parent. From Sec. V A we see that unless $h_{j-1}+w_j+h_j=2n$ and $w_j \leqslant 2(n-h_j)$ or $h_{j-1}+w_j+h_j=n$ and $w_{j-1}=1$, we always have a candidate.

In the first case we get $2n=h_{j-1}+w_j+h_j \leqslant h_{j-1}-h_j+2n$ and thus $h_{j-1} \geqslant h_j$. This is precisely the right sequence for a parent and we get $h_{k-1}+w_k+h_k=2n$ and $h_{k-1} \geqslant h_k$ for $k=1,\ldots,j$. The second case can, in fact, never occur. Since $h_{j-2}+w_{j-1}+h_{j-1}=2n$ and $h_{j-2}, h_{j-1} < n$ we find that $w_{j-1} > 1$.

B. Generating descendants from parents

Given the parent associated to $\vec{m}$, each cliff of height i plus the plain immediately to the right of this cliff forms an i-vacancy. Hence we have m_i i-vacancies. To obtain an arbitrary descendant of the parent under consideration, we proceed as follows.

Gen0 Set $i=1$.

Gen1 Set $j=1$.

Gen2 Attach $k_j^{(i)}$ i-components to the jth i-vacancy counted from the right.

Gen3 Set $j \to j+1$. If $j \leqslant m_i$, go to Gen2. If $j=m_j+1$, set $i \to i+1$, and if $i \leqslant n-1$, go to Gen1.

To properly interpret these rules, some important remarks need to be made. First, when we say "attach $k_j^{(i)}$ i-components to the jth i-vacancy," this should be understood as follows. Attaching an i-component to an i-vacancy has the effect of moving the vacancy to the right. Hence attaching the kth i-component means attaching an i-component to the image of the i-vacancy after attaching the $(k-1)$-th i-component. Second, it may occur that attaching an i-component to an i-vacancy does not have the effect of moving the i-vacancy to the right, but annihilates the vacancy. Hence, there are bounds on the numbers $k_j^{(i)}$. In the next section we will show that these bounds are as follows:

$$0 \leqslant k_{m_i}^{(i)} \leqslant \cdots \leqslant k_2^{(i)} \leqslant k_1^{(i)} \leqslant \ell_i, \tag{28}$$

with ℓ_i fixed by (31).

C. Reversibility

There remains the proof that our rules for attaching and removing g-components are reversible. This is true by construction.

VII. PROOF OF GAUSSIANS

In this section we prove that for the case of $\mathcal{G}_L(2\Lambda_0,\Lambda_k)$, the generating function for attaching the i-components to the parent graph associated to $\vec{m}$ is given by the Gaussian polynomial

$$\begin{bmatrix} \ell_i + m_i \\ m_i \end{bmatrix}_q, \tag{29}$$

where

$$\begin{bmatrix} N \\ m \end{bmatrix}_q = \begin{cases} \dfrac{(q)_N}{(q)_m (q)_{N-m}}, & 0 \leqslant m \leqslant N, \\ 0, \quad \text{otherwise}, \end{cases} \tag{30}$$

and

$$\vec{\ell} = C^{-1}(L\vec{e}_{n-1} + \vec{e}_r - 2\vec{m}), \tag{31}$$

and $\vec{e}_i$ the $(n-1)$-dimensional unit vector with entries $(\vec{e}_i)_j = \delta_{i,j}$ and with $0 < r \leqslant n$ fixed by

$$L - 2k \equiv r. \tag{32}$$

A. The $r=n$ case

To prove the above result we first treat the simpler case of $r=n$. In the next subsection we then show how to modify this to obtain (31) for general r.

We start with the following important fact, used extensively throughout this section:

Lemma 3: For $G \in \mathscr{G}_L(2\Lambda_0,\Lambda_k)$, let W be the number of nodes in the first row and h_N be the height of the Nth (uppermost) cliff [see Fig. 2(a)]. Then

$$W - h_N \equiv 2k. \tag{33}$$

We prove this by implementing the conditions K2 and K3 of Sec. III B 3, defining the K-graphs in $\mathscr{G}_L(2\Lambda_0,\Lambda_k)$. Recalling that W is the number of nodes in the first row of a K-graph, we have

$$W = \sum_{i=1}^{N} w_i \equiv -\sum_{i=1}^{N} (h_{i-1}+h_i) \equiv h_N - 2\sum_{i=1}^{N} h_i = h_N - 2H \equiv h_N + 2k, \tag{34}$$

which proves our claim.

1. i-strips

We are interested in the placement of the i-components. From the rules for placing the latter, it is natural to define m_i i-*strips* as follows:

S1 We define the i-strip as consisting of two regions: a principal region and a tail. The principal region is defined in terms of a top segment, a bottom segment, and a left and a right segment. The left and right segments will be called left and right terminal. We start by defining the principal region.

Consider the profile P_i of the K-graph after attaching all i'-components, with $i' = 1,2,\ldots,i-1$, but before attaching any component of height i or higher.

If the Nth (highest) cliff of P_i has height h_N, extend the *ceiling* of P_i by drawing a horizontal line of width $i - h_N$ starting from the top-right corner of the rightmost node of the top row of the graph, and extending to the right. This line will serve as a ceiling to the i-components that we will add shortly.

Consider the segment of P_i $2(n-i)$ columns to the right of the right-most cliff of height i. This will be the top segment of the i-strip. Let us denote this segment by P_i^0.

Now we proceed to define the bottom segment of the i-strip. Move P_i^0 to the left by $2(n-i)$ columns, and downward by i rows. Denote this shifted profile by P_i^1. This is the bottom segment that we are looking for.

Finally, close the figure formed by the top and bottom segments as follows: draw a plain of width $2(n-i)$ followed by a cliff of height i to the right (left) of P_i^0/P_i^1), called the right (left) terminal, respectively. As a result, we now have a region enclosed by P_i^0 ,P_i^1 and the left and right terminals. This defines the *principal region* of the first i-strip.

Next, we define the tail of the first i-strip as follows: Compute $M \equiv 0$ to be the largest integer such that $W + i - h_N + M \leq L$. The tail of the i-strip is a rectangle, of width M and height i, that we place to the right of the principal region in the first row.

The principal region plus the tail define the complete first i-strip. An example of the first 3-strip in a typical K-graph for $\widehat{sl(4)}$ is shown in Fig. 6(a).

S2 We draw the second i-strip by simply shifting the first i-strip to the left and down by $2(n-i)$ columns and i rows, respectively.

S3 We repeat the step S2 $(m_i - 1)$ times. That is, we define the $(j+1)$-th i-strip by translating the jth i-strip to the left by $2(n-i)$ columns and downwards by i rows. In Fig. 6(b) we have shown the construction of the 3-strips for a typical example of a K-graph for $\widehat{sl(4)}$.

By construction, adding the i-components corresponding to the jth i-vacancy (counted from the right) corresponds to filling the jth i-strip from left to right. In constructing an arbitrary descendant, we will not necessarily fill the complete jth i-strip. Furthermore, we will show below that the filling of the $(j+1)$-th strip is bound by the degree of filling of the jth strip. In particular, we will show that if the jth strip is filled with $k_j^{(i)}$ i-components, then the $(j+1)$-th strip cannot be

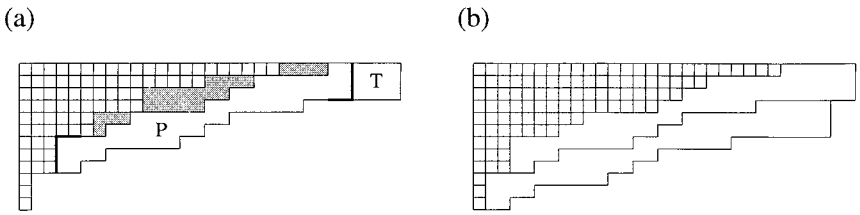

FIG. 6. (a) The construction of the first "3"-strip for a typical K-graph G. The part of G corresponding to the parent graph is drawn with open nodes/boxes and the (already) placed i'-components ($i'=1,2$) are shown in grey. The bold segments are the left–right terminals of the principal region (marked P). The tail of the strip is marked with T. (b) The two "3"-strips for the K-graph in (a).

filled with more than $k_j^{(i)}$ i-components. Since each i-component contains n nodes, and thus contributes a single factor q, we obtain the following expression for the generating function attaching the i-components:

$$G_i(q)=\sum_{k_1^{(i)}=0}^{\not{\ell}_i}\sum_{k_2^{(i)}=0}^{k_1^{(i)}}\cdots\sum_{k_{m_i}^{(i)}=0}^{k_{m_i-1}^{(i)}} q^{k_1^{(i)}+k_2^{(i)}+\cdots+k_{m_i}^{(i)}}. \tag{35}$$

Here the number $n\not{\ell}_i$ is the area (=number of nodes) of the first i-strip.

As defined above, G_i can be interpreted as the generating function of all partitions with largest part $\leqslant \not{\ell}_i$ and number of parts $\leqslant m_i$. Therefore

$$G_i(q)=\begin{bmatrix}\not{\ell}_i+m_i\\ m_i\end{bmatrix}_q. \tag{36}$$

Before ending this subsection, let us return to Lemma 3. We have stated above that attaching i-components corresponding to the right-most i-vacancy corresponds to filling the first i-strip. However, some caution needs to be taken, since in constructing the principal region of the first i-strip we have extended the profile of the K-graph by drawing a plain of width $i-h_N$ in the first row to the right of the Nth cliff. This clearly can only be done for all $i=1,\ldots,n-1$, if $L-W\geqslant n-1-h_N$. If L_s is the smallest possible value of L for which a K-graph of width W is possible, i.e.,

$$L_s=W+x,\quad 0\leqslant x\leqslant n-1, \tag{37}$$

with x fixed by (32), we have

$$x=L_s-W=(L_s-2k)-(W-2k)\equiv r-h_N, \tag{38}$$

where we have used Lemma 3 and the definition (32) of r. Since we require x to be at least $n-1-h_N$ we should thus have that $r=n$ or $n-1$. For simplicity we now assume $r=n$.

2. Calculation of $\not{\ell}_i$

To calculate the area of the first i-strip, we use the simple property that the area remains unchanged by deforming the strip by removing nodes from below and adding them from above.

We now choose to deform the i-strip such that its upper side corresponds to the profile of its parent graph, being labelled by $\vec{m}$. For the example of Fig. 6 this is shown in Fig. 7.

From this particular choice of deformation we can simply compute the area over n as

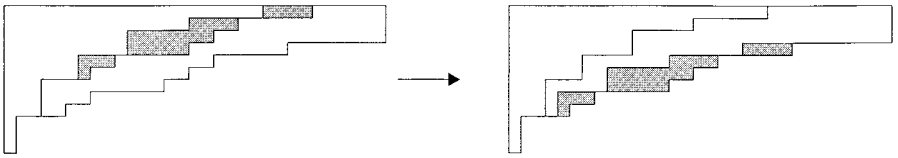

FIG. 7. The deformation of the first "3"-strip of the K-graph of Fig. 6, yielding the first "3"-strip of its parent graph.

$$\ell_i(r=n)=2\sum_{j=1}^{i-1} jm_{i-j}+i\left\lfloor\left(L+n-i-2\sum_{j=1}^{n-1} jm_{n-j}\right)\Big/ n\right\rfloor, \tag{39}$$

with $\lfloor x\rfloor$ denoting the integer part of x. Here the first term corresponds to the area of the principal region of the *deformed* i-strip and the second term to the area of the tail of the deformed strip. In particular, to compute the former we use the fact that it takes $(j+1)$ i-components to move an i-vacancy [of the type shown in Fig. 5(b)] upwards across a plain of width $2n-2i+j$ $(j\geqslant 1)$. To compute the latter, we compute $L-(W+i-h_N)$, using the result (33).

Recasting the definition (23) of the inverse Cartan matrix as

$$(C^{-1})_{i,j}=\frac{i(n-j)}{n}-\sum_{p=1}^{i-1}(i-p)\,\delta_{j,p} \tag{40}$$

and using the mod properties (19) and (32) we thus obtain

$$\ell_i(r=n)=\frac{iL}{n}-2\left(\sum_{j=1}^{n-1}\frac{i(n-j)}{n}-\sum_{j=1}^{i-1}(i-j)\right)m_j=L(C^{-1})_{n-1,i}-2(C^{-1}\vec{m})_i\,. \tag{41}$$

This proves (31) for $r=n$.

3. Proof of Gaussian form

It remains for us to prove that the filling of the $(j+1)$-th i-strip is bound by that of the jth i-strip.

Let us assume that we have placed $k_j^{(i)}$ i-components in the jth i-strip, and that the $k_j^{(i)}$-th component is an i-component of the form depicted in Fig. 8(a). Let us further assume that we have already filled the $(j+1)$-th strip with $k_j^{(i)}$ i-components (this is of course always possible). Since

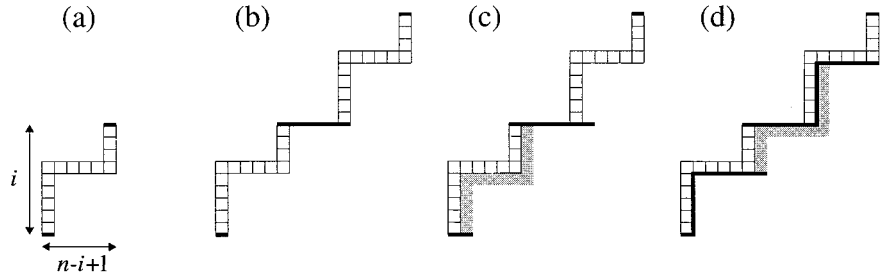

FIG. 8. (a) A typical i-component. The bold lines indicate part of the boundary of the i-strip. (b) The $k_j^{(i)}$-th i-component in both the jth and the $(j+1)$-th i-strip. (c) and (d) The two forbidden placements of an additional $(k_j^{(i)}+1)$-th i-component (shown in grey) in the $(j+1)$-th strip.

the $(j+1)$-th strip has identical shape as the jth strip, but is translated to the left and down by $2(n-i)$ columns and i rows, we have the configuration shown in Fig. 8(b).

Our claim is now that upon attaching the $k_j^{(i)}$-th i-component in the $(j+1)$-th strip we have annihilated the corresponding i-vacancy. To see this we consider two cases. Either the boundary separating the strips extends at least one more entry to the right, see Fig. 8(c), or the boundary progresses upwards as in Fig. 8(d). In the first case the lowest sequence {cliff,plain,cliff} could be an i-vacancy, but since the plain immediately above has width $n-i$, this is not the case thanks to Lemma 2. Hence placing the i-component in Fig. 8(c) as shown in grey is not allowed. In the second case, the middle sequence {cliff,plain,cliff} could be an i-vacancy, but again the plain immediately above has width $n-i$ and we can once more apply Lemma 2. Hence also the placement as shown in Fig. 8(d) is forbidden.

B. The general r case

As remarked at the end of Sec. VII A 1, only for $r=n$ and $n-1$ can we always draw a plain of width $i-h_N$ to the right of the Nth cliff without violating the condition $W+i-h_N \leqslant L$, for any i. If $L-2k \equiv r$, we can still do so for all $i \leqslant r$. Hence for these cases the principal region of the i-strips can still be defined as in Sec. VII A 1. However, for $i=r+a$ $(a>0)$, we have to reduce the principal region P by removing the part of P which would be occupied by the last a components to be attached, if P were to be completely filled from left to right. Of, course, in this case the tail no longer is a rectangle, but has a profile of two plains and two cliffs. An example of this reduction is shown in Fig. 9.

The above considerations lead to the following simple modification of (39):

$$\begin{aligned}
\ell_i &= 2\sum_{j=1}^{i-1} j m_{i-j} - \sum_{p=1}^{n-r-1} (n-r-p)\,\delta_{n-i,p} \\
&\quad + i\left\lfloor \left(L+n-i+\sum_{p=1}^{n-r-1} (n-r-p)\,\delta_{n-i,p} - 2\sum_{j=1}^{n-1} j m_{n-j} \right) \Big/ n \right\rfloor \\
&= 2\sum_{j=1}^{i-1} j m_{i-j} - \sum_{p=1}^{n-r-1} (n-r-p)\,\delta_{n-i,p} + \frac{i}{n}\left(L+n-r-2\sum_{j=1}^{n-1} j m_{n-j} \right) \\
&= \ell_i(r=n) + \left(\frac{i(n-r)}{n} - \sum_{p=1}^{n-r-1} (n-r-p)\,\delta_{n-i,p} \right) = \ell_i(r=n) + (C^{-1})_{r,i}\,, \qquad (42)
\end{aligned}$$

which proves the claim (31). Here we note that to obtain the first line of (42) one not only has to subtract the term $\Sigma_p (n-r-p)\,\delta_{n-i,p}$ to account for the reduction of the principal region, but also to add this same term within the $\lfloor . \rfloor$. This occurs since the effective length available for the tail of the i-strips has of course increased by the decrease of the principal region (see Fig. 9).

C. Fermionic form for $F_L(2\Lambda_0, \Lambda_k)$

We now have computed the number of nodes of the parent associated to $\vec{m}$ as well as the generating function for adding the g-components to this parent. Collecting these two results, we obtain the following expression for the generating function $F_L(2\Lambda_0, \Lambda_k)$ of K-graphs in $\mathscr{G}(2\Lambda_0, \Lambda_k)$:

Proposition 1:

$$F_L(2\Lambda_0, \Lambda_k) = \sum q^{\vec{m}^t C^{-1} \vec{m}} \prod_{i=1}^{n-1} \begin{bmatrix} \ell_i + m_i \\ m_i \end{bmatrix}, \qquad (43)$$

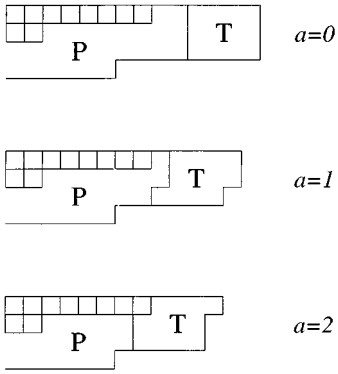

FIG. 9. Reduction of the 3-strips of Fig. 6. Recalling that $i=r+a$, we need for $i=3$ and $n=4$ to consider the cases $a=0,1,2$.

with $\vec{\ell}$ given by (31) and (32) and with the sum taken over all $\vec{m} \in (\mathbb{Z}_{\geqslant 0})^{(n-1)}$ satisfying $k+\Sigma_{i=1}^{n-1} i m_i \equiv 0$.

VIII. THE GENERAL CHARACTER

In this section we calculate $F_L(\Lambda_0+\Lambda_j \Lambda_k)$ for arbitrary $j(0 \leqslant j \leqslant n-1)$. As we have already mentioned in Sec. II, we count the weights in the principal picture, so that any fermionic form can be reduced to one of the above form.

First consider the following injection:

$$\begin{gathered} \mathscr{P}_L(\Lambda_0+\Lambda_j,\Lambda_k) \to \mathscr{P}_{L+j}(2\Lambda_0,\Lambda_k), \\ p=(\lambda_0,\ldots,\lambda_L) \mapsto p', \end{gathered} \tag{44}$$

where $p'=(2\Lambda_0,\Lambda_0+\Lambda_1,\ldots,\Lambda_0+\Lambda_{j-1},\lambda_0,\ldots,\lambda_L)$. In terms of K-graphs, we have

$$\begin{gathered} \mathscr{G}_L(\Lambda_0+\Lambda_j,\Lambda_k) \to \mathscr{G}_{L+j}(2\Lambda_0,\Lambda_k), \\ G \mapsto G'. \end{gathered} \tag{45}$$

Here G' is obtained from G by placing the rectangle of width j and height H' in the left-hand side of G (see Fig. 10), where, H being the height of G, H' is determined by $H'-H=0$ or $n-j$, $H' \in n\mathbb{Z}-k$. It is clear that the image under the injection (45) is the set of K-graphs in $\mathscr{G}_{L+j}(2\Lambda_0,\Lambda_k)$ having the lowest plain of width at least j.

Now let us recall that we have established the following bijection in the preceding sections:

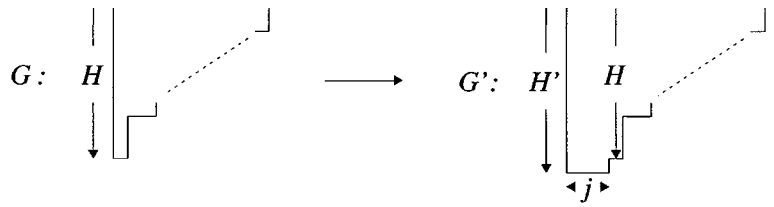

FIG. 10. Embedding of a K-graph in $\mathscr{G}_L(\Lambda_0+\Lambda_j,\Lambda_k)$ into $\mathscr{G}_{L+j}(2\Lambda_0,\Lambda_k)$.

$$\mathscr{P}_L(2\Lambda_0,\Lambda_k)\leftrightarrow\{(\vec{m},(F_1,\ldots,F_{n-1}))\}. \tag{46}$$

Here $\vec{m}^t=(m_1,\ldots,m_{n-1})$, satisfying (19), characterizes the parent graph, and F_i is the Ferrers graph of a partition with largest part $\leqslant \ell_i$ and number of parts $\leqslant m_i$. Regarding the image of the injection (45), the following question arises: How can we characterize K-graphs having the lowest plain of width at least j as elements in the right-hand side of the bijection (46)? The answer is given by the following.

Proposition 2: A K-graph in $\mathscr{G}_L(2\Lambda_0,\Lambda_k)$ has a lowest plain of width $w_1\geqslant j$, iff, for $n-j+1\leqslant i\leqslant n-1$, the smallest part in the Ferrers graph F_i has at least $i+j-n$ nodes.

To prove this, let G be such a K-graph, P its parent graph, and $M(G)$ and $M(P)$ the corresponding interpolating matrices. We write $M(G)$ as in (14) and $M(P)$ as

$$M(P)=\begin{pmatrix} c_0+c_1 & \cdots & c_{i-1}+c_i & \cdots & c_{N-1}+c_N \\ n-c_1 & \cdots & n-c_i & \cdots & n-c_N \end{pmatrix} \quad (c_0=0).$$

After removing g-components such that the first i columns of $M(G)$ equal $M(P)$, we must have that $w_{i+1}\geqslant j+c_i$.

We wish to prove the above assertion by induction on i. For $i=0$, the assertion is clear from the assumption of the proposition. Next, let us assume the assertion for $i-1$. Let us also assume that we have arrived at the minimal gap corresponding to $c_{i-1}+c_i$. In order to prove the assertion for i, we have to show that we can remove an $(n-c_i)$-component $j-c_{i-1}$ times strictly horizontally. This can indeed be shown through straightforward, though tedious, consideration of the profile, and the conditions on its various segments. Proposition 2 follows from the above statement.

Applying Proposition 2, we immediately obtain

$$F_L(\Lambda_0+\Lambda_j,\Lambda_k)=\sum q^{\vec{m}^tC^{-1}\vec{m}+Q}\prod_{i=1}^{n-1}\begin{bmatrix}\ell_i'+m_i\\ m_i\end{bmatrix}_q, \tag{47}$$

where

$$Q=\sum_{i=n-j+1}^{n-1}(i+j-n)m_i-\frac{j}{n}\sum_{i=1}^{n-1}im_i=-\vec{m}^tC^{-1}\vec{e}_{n-j},$$

$$\begin{aligned}\ell_i'&=\ell_i|_{L\to L+j}-(i+j-n)\theta(i+j-n),\\ &=[C^{-1}(L\vec{e}_{n-1}+\vec{e}_r+\vec{e}_{n-j}-2\vec{m})]_i.\end{aligned} \tag{48}$$

Here ℓ_i is defined in (31), and θ in (5).

In conclusion, we have the general form of the fermionic sum:

Theorem 3:

$$\begin{aligned}F_L(\Lambda_0+\Lambda_j,\Lambda_k)&=\sum q^{\vec{m}^tC^{-1}\vec{m}-\vec{m}^tC^{-1}\vec{e}_{n-j}}\prod_{i=1}^{n-1}\begin{bmatrix}\ell_i+m_i\\ m_i\end{bmatrix}_q,\\ \vec{\ell}&=C^{-1}(L\vec{e}_{n-1}+\vec{e}_r+\vec{e}_{n-j}-2\vec{m}),\end{aligned} \tag{49}$$

where the sum is taken over all $\vec{m}\in(\mathbb{Z}_{\geqslant 0})^{n-1}$ satisfying $k+\Sigma_{i=1}^{n-1}im_i\equiv 0$, and with r determined from $L+j-2k\equiv r$, $0<r\leqslant n$.

IX. SUMMARY AND DISCUSSION

In this paper we have presented a method to compute finite analogs of the branching functions of the coset

$$\widehat{sl(n)}_1 \otimes \widehat{sl(n)}_1 / \widehat{sl(n)}_2 . \tag{50}$$

Our approach, based on a direct counting of Ferrers graphs related to the crystal base formulation of the HWMs of $\widehat{sl(n)}$, leads to what are known as *fermionic polynomials*. This complements earlier results of Ref. 5 where the same finite analogs of branching functions were computed, and the result was expressed in terms of *bosonic polynomials*.

Equating these two results, as formulated in the Theorems 1 and 3, using Eq. (18), we obtain the main result of this paper:

Theorem 4: Let $\vec{m}$ and $\vec{e}_i$ be $(n-1)$-dimensional vectors with entries $(\vec{m})_i = m_i$ and $(\vec{e}_i)_j = \delta_{i,j}$, respectively. Also, let C be the Cartan matrix of $sl(n)$ and $\mathscr{W}$ the Weyl group of $\widehat{sl(n)}$. Defining the function $b_{L,i}$ as in (11), the following polynomial identity holds for all $j,k = 0,\ldots,n-1$:

$$\sum_{\vec{m} \in (\mathbb{Z}_{\geqslant 0})^{n-1}} q^{\vec{m}^t C^{-1} \vec{m} - \vec{m}^t C^{-1} \vec{e}_{n-j}} \prod_{i=1}^{n-1} \begin{bmatrix} (\vec{m} + C^{-1}(L\vec{e}_{n-1} + \vec{e}_r + \vec{e}_{n-j} - 2\vec{m}))_i \\ m_i \end{bmatrix}_q$$

$$= q^{(|\Lambda_k|^2 - |\Lambda'_j|^2)/2} \sum_{w \in \mathscr{W}} (\det w) b_{L,j-k}(\Lambda_k + \Lambda_{j-k+L} + \rho - w(\Lambda_0 + \Lambda_j + \rho)), \tag{51}$$

with $0 < r \leqslant n$ fixed by $L + j - 2k \equiv r$ and with the sum over $\vec{m}$ restricted by

$$\frac{k}{n} + (C^{-1}\vec{m})_{n-1} \in \mathbb{Z}. \tag{52}$$

Letting $L \to \infty$ we obtain the following q-series identities for the branching functions of the coset (50).

Corollary 1: Let Q be the root lattice and $\bar{\mathscr{W}}$ be the Weyl group of $sl(n)$. Then

$$q^{(|\Lambda_j|^2 - |\Lambda_k|^2)/2} \sum_{\vec{m} \in (\mathbb{Z}_{\geqslant 0})^{n-1}} \frac{q^{\vec{m}^t C^{-1} \vec{m} - \vec{m}^t C^{-1} \vec{e}_{n-j}}}{\Pi_{i=1}^{n-1} (q)_{m_i}}$$

$$= \frac{q^{|\Lambda_j + \rho|^2/2(n+2) - |\Lambda_k + \rho|^2/2(n+1)}}{(q)_\infty^{n-1}} \sum_{w \in \bar{\mathscr{W}}} (\det w) \Theta_{(n+2)(\bar{\Lambda}_k + \bar{\rho}) - (n+1) w(\bar{\Lambda}_j + \bar{\rho}), (n+1)(n+2)}(q), \tag{53}$$

with the sum over $\vec{m}$ again restricted by (52), and with $\Theta_{\lambda,\ell}$ defined by

$$\Theta_{\lambda,\ell}(q) = \sum_{\alpha \in Q} q^{\ell |\alpha - \lambda/\ell|^2/2}, \tag{54}$$

for $\lambda \in \Sigma_{i=1}^{n-1} \mathbb{C} \overline{\Lambda_i}$.

We note that the left-hand side of (53) coincides with the character expressions of Lepowsky and Primc[8] for the $\mathbb{Z}_n$-parafermion conformal field theory.

The polynomial identities (51) proven in this work are, strictly speaking, not new, since under level–rank duality they map onto identities related to the coset

$$\widehat{sl(2)}_{n-1} \otimes \widehat{sl(2)}_1 / \widehat{sl(2)}_n . \tag{55}$$

The latter were conjectured in Refs. 9 and 17, and proven in Refs. 18–20. However, the proof presented here is *intrinsically* of $\widehat{sl(n)}$ type, and we expect it admits generalization to the more general coset

$$\widehat{sl(n)}_\ell \otimes \widehat{sl(n)}_m / \widehat{sl(n)}_{\ell+m} . \tag{56}$$

Results related to general $\widehat{sl(2)}$-type cosets were discussed in Ref. 21. The fermionic character form for certain sectors of the higher-rank parafermions were proven in Ref. 22.

For the case of $\widehat{sl(2)}$, the paths considered in this paper admit yet another representation in terms of Ferrers graphs. These graphs, obeying entirely different conditions than our K-graphs, were introduced in Ref. 23. They are also more general, in the sense that they lead to character expressions for all $\widehat{sl(2)}$ cosets of type $\mathscr{C}_{2,\ell,1}$, including rational values of ℓ. Results for this type of coset have been discussed in Refs. 24 and 25.

NOTES ADDED:

After this work was completed, it was brought to our attention that the main concepts introduced in this work are analogous to, though intriguingly different from, concepts that are essential to the theory of modular representations of the symmetric group. (For the precise definition of some of the following terminology, see for example, the book by James and Kerber.[26]) In particular, our K-graphs of the coset $\mathscr{C}_{n,1,1}$ are known as n-regular Young diagrams, our *parent graphs* are analogous to *n-cores*, our Gaussian polynomials generate the analogs of *n-quotients*, our g-components are analogous to *hook–ribbons*, and our counting procedure is very much related to the evaluation of Kostka–Green–Foulkes polynomials. However, there are differences, due to the fact that our K-graphs obey additional conditions.

Now, to make things even more intriguing, we also learned that the conditions obeyed by our K-graphs are almost identical to, though stronger than, those obeyed by Young diagrams that parametrize irreducible representations of $sl(n)$ which remain irreducible under restriction to $sl(n-1)$. We hope to report on these interesting relationships in future publications.

In a recent preprint A. Schilling has given a recursive proof of fermionic forms for the cosets referred to in Eq. (56).[27]

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Type-I quantum superalgebras, q-supertrace, and two-variable link polynomials

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A new general eigenvalue formula for the eigenvalues of Casimir invariants, for the type-I quantum superalgebras, is applied to the construction of link polynomials associated with *any* finite dimensional unitary irrep for these algebras. This affords a systematic construction of new two-variable link polynomials associated with any finite dimensional irrep (with a real highest weight) for the type-I quantum superalgebras. In particular infinite families of nonequivalent two-variable link polynomials are determined in fully explicit form. © *1996 American Institute of Physics.* [S0022-2488(96)00802-8]

I. INTRODUCTION

Following the celebrated discovery by Jones[1] of the so-called Jones' link polynomial, there has been considerable interest in recent years in modern knot theory, which has been found to be closely related, through the quantum Yang–Baxter equation (QYBE), to various areas of physics such as solvable models and quantum field theories.[2,3] With the equally important discovery of quantum algebras during the same period by Drinfeld[4] and Jimbo[5] following the initiatives of the St. Petersberg group, it was soon realized by Reshetikhin[6] and Turaev[7] that quantum algebras provided a useful tool in constructing link polynomials. This idea was further developed in Refs. 8–10 where the authors proposed a simple systematic procedure for the construction of link polynomials arising from quantum bosonic algebras.

There were many attempts (see, e.g., Refs. 2, 11, and 12) to construct new two- or multi-variable link polynomials since the work of HOMFLY[13] and Kauffman[14] concerning two-variable extensions of the Jones link polynomial. The two-variable HOMFLY and Kauffman link polynomials arise from the minimal representations of A_n and B_n, C_n, D_n quantum algebras, respectively.

Subsequently, link polynomials arising from quantum superalgebras have been addressed by various authors.[15–20] Among all quantum superalgebras those of type-I, $\mathrm{U}_q[\mathrm{gl}(m|n)]$ and $\mathrm{U}_q[\mathrm{osp}(2|2n)]$, are particularly interesting because they possess one-parameter families of finite-dimensional unitary irreps even for generic q. The freedom of having extra parameters in the irreps opens up new and exciting possibilities in physics.[21] For the current case, the link polynomials from such representations will then also depend on these extra parameters, thus naturally yielding multi-variable link polynomials. We remark however that such multi-variable link polynomials are not related[22] to those arising from ''colored'' braids.[11]

For the case of quantum superalgebras, the situation is much more complicated than the bosonic case. The fundamental difficulty is the zero q-supertrace problem over typical irreps, so that the usual techniques developed for computing the eigenvalues of Casimir invariants for quantum bosonic algebras fail in this case. Due to this problem, only very few isolated examples of multi-variable link polynomials for quantum superalgebras have so far been known. These include the two-variable link polynomials[23] based on $\mathrm{U}_q[\mathrm{gl}(2|1)]$ and multi-variable ones[22] for a

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special class of representations of $U_q[gl(m|n)]$. In these examples, the authors only considered representations for which the above mentioned difficulty does not occur.

In this paper, we have succeeded in overcoming the above problem and obtain a well-defined q-supertrace formula which is applied to compute the eigenvalues of the Casimir invariants. These results are given in theorems 1, 2, and 3. However, the proof of the q-supertrace formulas are extremely lengthy and will be published in a separate paper.[32] Using these results, we are able to construct link polynomials associated with *any* finite dimensional unitary irrep of a type-I quantum superalgebra. Applied to one-parameter families of inequivalent finite dimensional irreps of $U_q[gl(m|n)]$ and $U_q[osp(2|2n)]$ for generic q, our method affords infinite families of nonequivalent two-variable link polynomials in fully explicit form.

This paper will be presented in the following order. After recalling some fundamentals in Sec. II, we give, in Sec. III an account of the atypicality indices and unitary irreps of $U_q(\mathcal{G})$. In Sec. IV we present three theorems concerning the computation of the q-supertraces and therefore the eigenvalues of Casimir invariants over typical irreps. Section V derives a spectral decomposition formula for the braid generator and its powers. A general method for constructing link polynomials is presented in Sec. VI and examples of two-variable link polynomials are illustrated in Sec. VII. In the last section, we give a brief discussion of our main results.

II. PRELIMINARIES

Let $\mathcal{G}$ be a type-I simple Lie superalgebra[24] with generators $\{e_i, f_i, h_i\}$ and let α_i, $i=0,1,\ldots,r$, be its simple roots with α_0 the unique odd simple root; here we choose the distinguished set of simple roots. (Superalgebras allow many inequivalent systems of simple roots. See Ref. 24. The relation between the different quantum superalgebras obtained by choosing different systems of simple roots is studied in Ref. 25.) Let $(,)$ be a fixed invariant bilinear form on H^*, the dual of the Cartan subalgebra H of $\mathcal{G}$. The quantum superalgebra $U_q(\mathcal{G})$ has the structure of a $\mathbf{Z}_2$-graded quasi-triangular Hopf algebra. Throughout the paper we will assume that q is generic, i.e., not a root of unity. We will not give the full defining relations of $U_q(\mathcal{G})$ here but mention that the simple raising and lowering generators of $U_q(\mathcal{G})$ obey more relations than just the usual q-Serre relations known from quantum bosonic algebras.[26–29] These necessary extra relations are referred to as "extra q-Serre relations." $U_q(\mathcal{G})$ has a coproduct Δ and antipode S given by

$$\Delta(q^{\pm h_i}) = q^{\pm h_i} \otimes q^{\pm h_i},$$

$$\Delta(e_i) = e_i \otimes q^{-h_i/2} + q^{h_i/2} \otimes e_i,$$

$$\Delta(f_i) = f_i \otimes q^{-h_i/2} + q^{h_i/2} \otimes f_i, \tag{1}$$

$$S(a) = q^{-h_\rho} \gamma(a) q^{h_\rho}, \quad a = e_i, f_i, h_i, \tag{2}$$

where γ is the principal anti-automorphism on $U_q(\mathcal{G})$ and ρ is the graded half-sum of positive roots of $\mathcal{G}$. We omit the formulas for the counit which are not needed here.

The algebra $U_q(\mathcal{G})$ is a quasitriangular graded Hopf algebra, which means the following. Let Δ' be the opposite coproduct so that $\Delta' = T\Delta$, where T is the graded twist map: $T(a \otimes b) = (-1)^{[a][b]} b \otimes a$, $\forall a, b \in U_q(\mathcal{G})$. Here $[a] \in \mathbf{Z_2}$ denotes the grading of element a: $[a]=0$ if a is even and $[a]=1$ if it is odd. Then Δ and Δ' are related by the universal R-matrix R in $U_q(\mathcal{G}) \otimes U_q(\mathcal{G})$ satisfying, among others, the relations

$$R\Delta(a) = \Delta'(a)R, \quad \forall a \in U_q(\mathcal{G}), \tag{3}$$

$$(I \otimes \Delta)R = R_{13}R_{12}, \quad (\Delta \otimes I)R = R_{13}R_{23}, \tag{4}$$

where if $R=\Sigma a_t\otimes b_t$ then $R_{12}=\Sigma a_t\otimes b_t\otimes 1$, $R_{13}=\Sigma a_t\otimes 1\otimes b_t$, etc. It follows from (4) that R satisfies the QYBE:

$$R_{12}R_{13}R_{23}=R_{23}R_{13}R_{12}. \tag{5}$$

Note that the multiplication rule for the tensor product is defined for homogeneous elements $a,b,c,d\in \mathrm{U}_q(\mathscr{G})$ by

$$(a\otimes b)(c\otimes d)=(-1)^{[b][c]}(ac\otimes bd). \tag{6}$$

It is a well established fact for quasitriangular Hopf algebras, that there exists a distinguished element[4]

$$u=\sum_t (-1)^{[t]}S(b_t)a_t, \tag{7}$$

where, as above, a_t and b_t are coordinates of the universal R-matrix. One can show that u has inverse

$$u^{-1}=\sum_t (-1)^{[t]}S^{-2}(b_t)a_t \tag{8}$$

and satisfies

$$S^2(a)=uau^{-1},\quad \forall a\in \mathrm{U}_q(\mathscr{G}),\quad \Delta(u)=(u\otimes u)(R^TR)^{-1}, \tag{9}$$

where $R^T=T(R)$. It is easy to check that

$$v=u^{-1}q^{-2h_\rho} \tag{10}$$

belongs to the center of $\mathrm{U}_q(\mathscr{G})$ and satisfies

$$\Delta(v)=(v\otimes v)(R^TR)^{-1}. \tag{11}$$

Moreover, on a finite dimensional irreducible module $V(\Lambda)$ with highest weight $\Lambda\in D^+$, the Casimir operator v takes the eigenvalue

$$\chi_\Lambda(v)=q^{(\Lambda,\Lambda+2\rho)}. \tag{12}$$

Note that the generators $\{e_i,f_i,q^{h_i},i=1,\ldots,r\}$ form generators of the quantum group $\mathrm{U}_q(\mathscr{G}_0)$, where $\mathscr{G}_0$ is the "even subalgebra" of $\mathscr{G}$. Specifically,

$$\mathscr{G}_0=u(1)\oplus \mathrm{sl}(m)\oplus \mathrm{sl}(n),\quad \text{for } \mathscr{G}=\mathrm{sl}(m|n),\quad m,n\geqslant 2,$$

$$\mathscr{G}_0=u(1)\oplus \mathrm{sl}(n),\quad \text{for } \mathscr{G}=\mathrm{sl}(1|n),\quad n\geqslant 2,$$

$$\mathscr{G}_0=u(1)\oplus \mathrm{sp}(2n),\quad \text{for } \mathscr{G}=\mathrm{osp}(2|2n). \tag{13}$$

Throughout we let $V_0(\Lambda)$ denote the finite dimensional irreducible $\mathrm{U}_q(\mathscr{G}_0)$ module with highest weight $\Lambda\in D^+$. We call

$$D_q^0(\Lambda)=\prod_{\beta\in\Phi_0^+}\frac{[(\Lambda+\rho,\beta)]_q}{[(\rho,\beta)]_q} \tag{14}$$

the q-dimension of the $U_q(\mathcal{G}_0)$ irrep $V_0(\Lambda)$, where Φ_0^+ denotes the set of even positive roots of $\mathcal{G}$. Here and in what follows we will adopt the notation

$$[x]_q=\frac{q^x-q^{-x}}{q-q^{-1}}. \tag{15}$$

III. ATYPICALITY INDICES AND FINITE-DIMENSIONAL UNITARY IRREPS

Let $K(\Lambda)$ be the Kac-module associated to $V(\Lambda)$. $K(\Lambda)$ is not necessarily irreducible. If it is, we have $V(\Lambda)=K(\Lambda)$ and refer to Λ and $V(\Lambda)$ as "typical." Recall that Λ is typical iff$(\Lambda+\rho,\beta)\neq 0$, $\forall\beta\in\Phi_1^+$, where Φ_1^+ is the set of odd positive roots of $\mathcal{G}$.

Let us remark that for typical modules the dimensions are easily evaluated to be $\dim V(\Lambda)=2^d\cdot\dim V_0(\Lambda)$, where d, which is equal to mn for $\mathrm{gl}(m|n)$ and $2n$ for $\mathrm{osp}(2|2n)$, is the number of odd positive roots. This formula is particularly useful in determining tensor product decompositions of typical modules.

Definition 1: The integer

$$a_\Lambda=|\overline{\Phi}_1^+(\Lambda)|,\quad \overline{\Phi}_1^+(\Lambda)=\{\beta\in\Phi_1^+|(\Lambda+\rho,\beta)=0\} \tag{16}$$

is called the "atypicality index" of $\Lambda\in D^+$. In particular, $a_\Lambda=0$ iff Λ is typical.

The type-I quantum superalgebras admit two types of unitary representations which may be described as follows. We make the simplifying assumption that $q>0$ (i.e., q is real and positive) and define a conjugation operation on the $U_q(\mathcal{G})$ generators by $e_i^\dagger=f_i$, $f_i^\dagger=e_i$, $h_i^\dagger=h_i$ which is extended uniquely to all of $U_q(\mathcal{G})$ such that $(xy)^\dagger=y^\dagger x^\dagger$, $\forall x,y\in U_q(\mathcal{G})$. We call π_Λ type (1) unitary if

$$\pi_\Lambda(x^\dagger)=\overline{\pi_\Lambda(x)},\quad \forall x\in U_q(\mathcal{G}) \tag{17}$$

and type (2) unitary if

$$\pi_\Lambda(x^\dagger)=(-1)^{[x]}\overline{\pi_\Lambda(x)},\quad \forall x\in U_q(\mathcal{G}), \tag{18}$$

where the overline denotes Hermitian matrix conjugation. The two types of unitary representations are in fact related via duality.

Lemma 1: Such unitary representations have the property that they are always completely reducible and the tensor product of two irreducible unitary representations of the same type reduces completely into irreducible unitary representations of the same type. Moreover the atypicality indices of the irreps occurring in this decomposition are less than or equal to the atypicality index of either component.

The finite dimensional irreducible unitary representations for all type-I quantum superalgebras have been classified in Refs. 30 and 31. For completeness we cite these classification results below. Let us first of all introduce some notation. For $\mathrm{gl}(m|n)$, we choose $\{\epsilon_i\}_{i=1}^m\cup\{\delta_j\}_{j=1}^n$ as a basis for H^* with $[\epsilon_i]=0$, $[\delta_j]=1$ and

$$(\epsilon_i,\epsilon_j)=\delta_{ij},\quad (\delta_i,\delta_j)=-\delta_{ij},\quad (\epsilon_i,\delta_j)=0. \tag{19}$$

Using this basis, any weight Λ may written as

$$\Lambda\equiv(\Lambda_1,\ldots,\Lambda_m|\overline{\Lambda_1},\ldots,\overline{\Lambda_n})\equiv\sum_{i=1}^m\Lambda_i\epsilon_i+\sum_{j=1}^n\overline{\Lambda_j}\delta_j \tag{20}$$

and the graded half-sum ρ of the positive roots is

$$2\rho=\sum_{i=1}^{m}(m-n-2i+1)\epsilon_i+\sum_{j=1}^{n}(m+n-2j+1)\delta_j. \tag{21}$$

For osp$(2|2n)$, choose $\{\epsilon_0\}\cup\{\epsilon_i\}_{i=1}^n$ as a basis for H^* with $[\epsilon_0]=1$, $[\epsilon_i]=0$ and

$$(\epsilon_0,\epsilon_0)=-1,\quad (\epsilon_i,\epsilon_j)=\delta_{ij},\quad \forall i,j=1,\ldots,n,\quad (\epsilon_0,\epsilon_i)=0. \tag{22}$$

In this case, any weight Λ may be expressed as

$$\Lambda\equiv(\overline{\Lambda}|\Lambda_1,\ldots,\Lambda_n)\equiv\overline{\Lambda}\epsilon_0+\sum_{i=1}^{n}\Lambda_i\epsilon_i \tag{23}$$

and the graded half-sum ρ of the positive roots is given by

$$\rho=\sum_{i=1}^{n}(n-i+1)\epsilon_i-n\epsilon_0. \tag{24}$$

Proposition 1: (*I*) *A given* $U_q[\mathrm{gl}(m|n)]$*-module* $V(\Lambda)$*, with* $\Lambda\in D_+$*, is type* (1) *unitary* iff: *(i)* $(\Lambda+\rho,\epsilon_m-\delta_n)>0$; *or (ii) there exists an odd index* $\omega\in\{1,2,\ldots,n\}$ *such that* $(\Lambda+\rho,\epsilon_m-\delta_\omega)=0=(\Lambda,\delta_\omega-\delta_n)$. *In the former case the given condition also enforces typicality on* $V(\Lambda)$*, while in the latter case all irreps are atypical.*
(*II*) *The* $U_q[\mathrm{gl}(m|n)]$*-module* $V(\Lambda)$*, with* $\Lambda\in D_+$*, is type* (2) *unitary* iff: *(i)* $(\Lambda+\rho,\epsilon_1-\delta_1)<0$; *or (ii) there exists an even index* $k\in\{1,2,\ldots,m\}$ *such that* $(\Lambda+\rho,\epsilon_k-\delta_1)=0=(\Lambda,\epsilon_1-\epsilon_k)$. *In the former case* $V(\Lambda)$ *is typical, while in the latter case it is atypical.*

Proposition 2: A given $U_q[\mathrm{osp}(2|2n])$*-module* $V(\Lambda)$ *is type* (1) *unitary* iff $(\Lambda,\alpha_0)\geqslant 0$, *where* α_0 *denotes the unique odd simple root, and type* (2) *unitary* iff *(i)* $(\Lambda+\rho,\epsilon_0+\epsilon_1)<0$; *or (ii) there exists an index* $k\in\{1,2,\ldots,n\}$ *such that* $(\Lambda+\rho,\epsilon_0+\epsilon_k)=0=(\Lambda,\epsilon_1-\epsilon_k)$; *or (iii)* $\Lambda=0$.

IV. q-SUPERTRACE AND EIGENVALUES OF CASIMIR INVARIANTS

Throughout this section we assume $V(\Lambda)$ is a fixed but arbitrary finite dimensional irreducible $U_q(\mathcal{G})$-module. Suppose $V(\nu)\subset V(\mu)\otimes V(\Lambda)$ is typical and let $P[\nu]$ denote the central projection of the tensor product module $V(\mu)\otimes V(\Lambda)$ onto its isotypic component $V(\nu)\equiv m_\nu V(\nu)\subset V(\mu)\otimes V(\Lambda)$ [that is $V(\nu)=V(\nu)\oplus\cdots\oplus V(\nu)$, m_ν copies]. We state the following q-supertrace formula:

Theorem 1: *For* $\mu,\ \nu\in D^+$ *typical,*

$$(I\otimes\mathrm{str})(I\otimes\pi_\Lambda(q^{-2h_\rho}))P[\nu]=(-1)^{[\nu]}m_\nu\frac{\chi_\mu(\Gamma_0)}{\chi_\nu(\Gamma_0)}\cdot\frac{D_q^0(\nu)}{D_q^0(\mu)}, \tag{25}$$

where $[\nu]$ *modulo* 2 *is the degree of the weight* ν, Γ_0 *is a central element of* $U_q(\mathcal{G}_0)$ *and* $\chi_\mu(\Gamma_0)$ *is the eigenvalue of* Γ_0 *on the* $U_q(\mathcal{G}_0)$*-module* $V_0(\mu)$:

$$\chi_\mu(\Gamma_0)=\prod_{\beta\in\Phi_1^+}\frac{[(\mu+\rho,\beta)]_q}{[(\rho,\beta)]_q}. \tag{26}$$

The proof of this theorem is very lengthy and detailed, and will be published elsewhere.[32]

Proposition 3: If the operator $c\in U_q(\mathcal{G})\otimes\mathrm{End}\,V(\Lambda)$ *satisfies* $\Delta_\Lambda(a)c=c\Delta_\Lambda(a)$, $\forall a\in U_q(\mathcal{G})$, *where* $\Delta_\Lambda=(I\otimes\pi_\Lambda)\Delta$, *then*

$$C_k^\Lambda=(I\otimes\mathrm{str})\{[I\otimes\pi_\Lambda(q^{-2h_\rho})]c^k\},\quad k\in\mathbf{Z}^+ \tag{27}$$

belong to the center of $U_q(\mathcal{G})$ *and thus form a family of Casimir invariants.*

An important example of c is given by

$$c=\frac{I\otimes I-R_\Lambda^T R_\Lambda}{q-q^{-1}}, \tag{28}$$

where $R_\Lambda=(I\otimes\pi_\Lambda)R$, with R the universal R-matrix.

Now assume $V(\mu)\otimes V(\Lambda)$ is completely reducible and write

$$V(\mu)\otimes V(\Lambda)=\oplus_\nu m_\nu V(\nu) \tag{29}$$

with now m_ν the multiplicity of the module $V(\nu)$ occurring in the tensor product. This always occurs when μ and Λ are unitary of the same type. Moreover, in such a case, each of the modules $V(\nu)$ is also unitary. If $c\in(I\otimes\pi_\Lambda)(Z\otimes Z)\Delta(Z)$ where Z is the center of $U_q(\mathcal{G})$, then one can deduce the following spectral decomposition for c and its powers c^k, $k\in\mathbf{Z}$:

$$c^k=\sum_\nu (\chi_\nu(c))^k P[\nu], \tag{30}$$

where $\chi_\nu(c)$ is the eigenvalue of c on $V(\nu)\subset V(\mu)\otimes V(\Lambda)$. Thus if c is given by the above example, then we have

$$\chi_\nu(c)=\frac{1-q^{C(\mu)+C(\Lambda)-C(\nu)}}{q-q^{-1}}, \tag{31}$$

where $C(\Lambda)\equiv(\Lambda,\Lambda+2\rho)$ denotes the eigenvalue of the second order Casimir invariant of $\mathcal{G}$.

With the aid of Theorem 1, we can determine the eigenvalues of the Casimir invariants C_k^Λ on a finite dimensional typical module $V(\mu)$ [notation as in Eq. (29)].

Theorem 2: *If* μ,ν *are all typical, then the eigenvalues of the Casimir invariants on* $V(\mu)$ *are given by*

$$\chi_\mu(C_k^\Lambda)=\sum_\nu (-1)^{[\nu]} m_\nu(\chi_\nu(c))^k \frac{\chi_\mu(\Gamma_0)}{\chi_\nu(\Gamma_0)}\cdot\frac{D_q^0(\nu)}{D_q^0(\mu)}, \quad k\in\mathbf{Z}. \tag{32}$$

Remark: Let $\{\lambda_i\}$ denote the set of distinct weights in $V(\Lambda)$ occurring with multiplicities m_{λ_i}. It can be shown that the above theorem may be extended to all finite dimensional modules $V(\mu)$, $\mu\in D^+$, by replacing ν,m_ν with $\mu+\lambda_i, m_{\lambda_i}$, respectively, and summing over λ_i. For more details see Ref. 33. The eigenvalue formula obtained in this way is referred to as the "extended eigenvalue formula" on $V(\mu)$, $\mu\in D^+$. Note that for generic μ, the extended eigenvalue formula determines a polynomial function on H^*. It is well defined if all $\mu+\lambda_i$ are typical but if some $\mu+\lambda_i$ is atypical it is necessary first to expand the right-hand side of the extended eigenvalue formula into a polynomial in order to avoid singularities.[33]

In the case of unitary $\mu\in D^+$ this latter problem can be overcome as follows. We set

$$\Phi_1^+(\lambda)=\{\beta\in\Phi_1^+|(\lambda+\rho,\beta)\neq 0\} \tag{33}$$

so that

$$|\Phi_1^+(\lambda)|+a_\lambda=|\Phi_1^+|. \tag{34}$$

Then we have the following.

Theorem 3: *The eigenvalues of the Casimir invariants on a unitary module* $V(\mu)$ *are given by*

$$\chi_\mu(C_k^\Lambda)=\sum_{\{\nu|a_\nu=a_\mu\}}(-1)^{[\nu]}m_\nu(\chi_\nu(c))^k\,\frac{\Pi_{\beta\in\Phi_1^+(\mu)}[(\mu+\rho,\beta)]_q}{\Pi_{\beta\in\Phi_1^+(\nu)}[(\nu+\rho,\beta)]_q}\cdot\frac{D_q^0(\nu)}{D_q^0(\mu)},\quad k\in\mathbf{Z}^+ \tag{35}$$

provided that $V(\Lambda)$, $V(\mu)$ *are unitary of the same type. Here the sum over* ν *is over* $V_0(\nu)\subset V_0(\mu)\otimes V(\Lambda)$ *and* m_ν *is the multiplicity of* $V_0(\nu)$ *in this space.*

For a given unitary module $V(\Lambda)$, the above formula is well defined for all unitary $\mu\in D^+$ of the same type.

V. DIAGONALIZATION OF THE BRAID GENERATOR

Let P be the graded permutation operator on $V(\Lambda)\otimes V(\Lambda)$ defined by $P(|x\rangle\otimes|y\rangle)=(-1)^{[x][y]}|y\rangle\otimes|x\rangle$, for all homogeneous $|x\rangle$, $|y\rangle\in V(\Lambda)$ and set

$$\sigma=PR\quad\in\mathrm{End}(V(\Lambda)\otimes V(\Lambda)). \tag{36}$$

Here and in what follows we regard elements of $\mathrm{U}_q(\mathcal{G})$ as operators on $V(\Lambda)$. Then (3) is equivalent to

$$\sigma\Delta(a)=\Delta(a)\sigma\quad\forall a\in\mathrm{U}_q(\mathcal{G}) \tag{37}$$

and (5) can be written as

$$(I\otimes\sigma)(\sigma\otimes I)(I\otimes\sigma)=(\sigma\otimes I)(I\otimes\sigma)(\sigma\otimes I). \tag{38}$$

It follows immediately that the operators $\sigma_i^\pm\in\mathrm{End}(V(\Lambda)^{\otimes M})$, $i=\{1,2,\ldots,M-1\}$ defined by

$$\sigma_i^\pm=\underbrace{I\otimes\cdots\otimes I}_{i-1}\otimes\sigma^\pm\otimes\underbrace{I\otimes\cdots\otimes I}_{M-i-1} \tag{39}$$

generate a nontrivial representation of the rank $(M-1)$ braid group B_M.

In the case when σ acts on $V(\Lambda)\otimes V(\Lambda)$ with $V(\Lambda)$ unitary, it can be shown that σ is self-adjoint and diagonalizable.[34] We remark however that only the type-I quantum superalgebras admit finite dimensional unitary irreps.

Similar to (29) we write,

$$V(\Lambda)\otimes V(\Lambda)=\oplus_\nu m_\nu V(\nu), \tag{40}$$

where again m_ν is the multiplicity of the module $V(\nu)$ occurring in the tensor product and each of the modules $V(\nu)$ is unitary. In view of the self-adjointness of σ, σ is diagonalizable on $V(\nu)\equiv m_\nu V(\nu)=V(\nu)\oplus\cdots\oplus V(\nu)$ (m_ν copies), regardless of the multiplicity. In fact it is possible to derive a spectral decomposition formula for σ, as in the case of quantum bosonic algebras.[10]

Recall that $\lim_{q\to1}\sigma=P$ and P is diagonalizable on $V(\Lambda)\otimes V(\Lambda)$ with eigenvalues ±1. Following Ref. 10, let $P[\pm]$ denote the projection operators defined by

$$P[\pm](V(\Lambda)\otimes V(\Lambda))=W_\pm, \tag{41}$$

where

$$W_\pm=\{w\in V(\Lambda)\otimes V(\Lambda)\,\Big|\,\lim_{q\to1}(\sigma\mp1)w=0\}. \tag{42}$$

Since σ is an $U_q(\mathcal{G})$-invariant each subspace $W_\pm$ determines a $U_q(\mathcal{G})$-module and $P[\pm]$ commute with the action of $U_q(\mathcal{G})$. As above $P[\nu]$ denotes the projection operator onto the modules $V(\nu)$; then obviously

$$P[\nu,\pm]=P[\pm]P[\nu]=P[\nu]P[\pm] \tag{43}$$

is the projection onto the isotypic component $\bar{V}(\nu)$ consisting of eigenvectors of σ with parities ± 1, respectively [i.e., the component of $V(\nu)$ in $W_\pm$, respectively].

The diagonalizability of σ, together with the fact that

$$\sigma^2=PRP\cdot R=R^TR=(v\otimes v)\Delta(v^{-1}), \tag{44}$$

implies the following spectral decomposition for σ and its powers:

$$\sigma^k=q^{-kC(\Lambda)}\sum_\nu q^{(k/2)C(\nu)}(P[\nu,+]+(-1)^kP[\nu,-]),\quad k\in\mathbf{Z}, \tag{45}$$

where as before $C(\lambda)\equiv(\lambda,\lambda+2\rho)$. It follows in particular that σ satisfies the polynomial identity

$$\prod_\nu (\sigma-q^{\frac{1}{2}C(\nu)-C(\Lambda)})(\sigma+q^{\frac{1}{2}C(\nu)-C(\Lambda)})=0 \tag{46}$$

which leads to the generalized skein relations for the corresponding link polynomials investigated below.

VI. LINK POLYNOMIALS

Let $\theta\in B_M$ be a word in the generators $\sigma_i^{\pm}$, $1\leqslant i\leqslant M-1$ and let $\hat{\theta}$ denote the link obtained by closing the braid. For the construction of link polynomials, the Markov trace ϕ plays an essential role. It is defined by

$$\text{(i)}\quad \phi(\theta\eta)=\phi(\eta\theta),\quad \forall\,\theta,\eta\in B_M,$$

$$\text{(ii)}\quad \phi(\theta\sigma_{M-1})=z\phi(\theta),\quad \phi(\theta\sigma_{M-1}^{-1})=\bar{z}\phi(\theta),\quad \forall\,\theta\in B_{M-1}\subset B_M. \tag{47}$$

Given such a Markov trace, it is well-known that one can define a link polynomial $L(\hat{\theta})$ through

$$L(\hat{\theta})=(z\bar{z})^{(M-1)/2}(\bar{z}z^{-1})^{e(\theta)/2}\phi(\theta),\quad \theta\in B_M, \tag{48}$$

where $e(\theta)$ is the sum of the exponents of the σ_i's appearing in θ. The functional $L(\hat{\theta})$ enjoys the following properties:

$$\text{(i)}\quad L(\widehat{\theta\eta})=L(\widehat{\eta\theta}),\quad \forall\,\theta,\eta\in B_M,$$

$$\text{(ii)}\quad L(\theta,\widehat{\sigma_{M-1}^{\pm 1}})=L(\hat{\theta}),\quad \forall\,\theta\in B_{M-1}\subset B_M \tag{49}$$

and is an invariant of ambient isotopy.

Proposition 4: The functional $\phi(\theta)$ defined by

$$\phi(\theta)=\frac{(\mathrm{tr}\otimes\mathrm{str}^{\otimes(M-1)})(I\otimes\Delta^{(M-1)}(q^{-2h_\rho})\theta)}{\dim V(\Lambda)}, \tag{50}$$

where tr *and* str *denote the trace and supertrace over $V(\Lambda)$, respectively, qualifies as a Markov trace with*

$$z=q^{(\Lambda,\Lambda+2\rho)},\quad \bar{z}=q^{-(\Lambda,\Lambda+2\rho)}. \tag{51}$$

Corollary 1: It follows that

$$L(\hat{\theta})=q^{-(\Lambda,\Lambda+2\rho)e(\theta)}\phi(\theta),\quad \theta\in B_M, \tag{52}$$

defines a link polynomial.

Now consider the family of Casimir invariants

$$C_k^{\Lambda}=(I\otimes \mathrm{str})[I\otimes \pi_{\Lambda}(q^{-2h_\rho})]\sigma^k. \tag{53}$$

Let ξ_k^{Λ} denote the eigenvalues of the invariants C_k^{Λ} on $V(\Lambda)$. In view of (45) and Theorem 2, one can deduce, for Λ typical, that they are given explicitly by

$$\xi_k^{\Lambda}=q^{-kC(\Lambda)}\sum_{\nu}\ (-1)^{[\nu]}q^{(k/2)C(\nu)}(m_\nu^{+}+(-1)^k m_\nu^{-})\ \frac{\chi_\Lambda(\Gamma_0)}{\chi_\nu(\Gamma_0)}\cdot\frac{D_q^0(\nu)}{D_q^0(\Lambda)}, \tag{54}$$

where $m_\nu^{\pm}$ are the multiplicities of $V(\nu)$ in $W_{\pm}$, respectively, so that

$$m_\nu=m_\nu^{+}+m_\nu^{-}. \tag{55}$$

Note: In the case that Λ is typical it necessarily follows that all $V(\nu)$ in the tensor product decomposition (40) are also typical so that (54) is always well defined (c.f. Lemma 1).

Theorem 4: *Consider the braid group B_M and a braid θ of the following general form:*

$$\theta=(\sigma_{i_1})^{k_1}(\sigma_{i_2})^{k_2}\cdots(\sigma_{i_{M-1}})^{k_{M-1}},\quad k_i\in\mathbf{Z} \tag{56}$$

with $\{i_1,i_2,\ldots,i_{M-1}\}$ an arbitrary permutation of $\{1,2,\ldots,M-1\}$. Then the following functional is a link polynomial

$$L(\hat{\theta})=q^{-(\Lambda,\Lambda+2\rho)\Sigma_{i=1}^{M-1}k_i}\prod_{i=1}^{M-1}\ \xi_{k_i}^{\Lambda}. \tag{57}$$

In the case that Λ is typical, ξ_k^{Λ} is given by (54).

VII. NEW TWO-VARIABLE LINK POLYNOMIALS

We will now apply the technique developed in previous sections to develop a general method for obtaining two-variable link polynomials corresponding to any real $\Lambda\in D^{+}$. Again we restrict to the type-I quantum superalgebras $\mathcal{G}=\mathrm{gl}(m|n)$ or $\mathcal{G}=\mathrm{osp}(2|2n)$.

Corresponding to any *real* $\Lambda\in D^{+}$ we have the one-parameter family of irreps

$$V(\Lambda_\alpha)\equiv V(\Lambda+\alpha\delta),\quad \alpha\in\mathbf{R},$$

$$\delta=\begin{cases}\displaystyle\sum_i\ \delta_i, & \text{for } \mathcal{G}=\mathrm{gl}(m|n)\\ \epsilon_0, & \text{for } \mathcal{G}=\mathrm{osp}(2|2n).\end{cases} \tag{58}$$

The module $V(\Lambda_\alpha)$ is typical and unitary for $|\alpha|$ sufficiently large. For example, for the case $\mathcal{G}=\mathrm{gl}(m|n)$, we have from Proposition 1 a type (1) unitary module for $\alpha>-(\Lambda+\rho,\epsilon_m-\delta_n)=n-1-(\Lambda,\epsilon_m-\delta_n)$, and a type (2) unitary module for $\alpha<-(\Lambda+\rho,\epsilon_1-\delta_1)=1-m-(\Lambda,\epsilon_1-\delta_1)$. Below we assume α belongs to this range (although the final formula for link polynomials should apply, by analytic continuation, to all real α).

Here we obtain a representation of the braid generator $\sigma \in \mathrm{End}[V(\Lambda+\alpha\delta)\otimes V(\Lambda+\alpha\delta)]$ and a formula for two variable link polynomials. Consider the $U_q(\mathscr{G}_0)$-module direct sum decomposition

$$V_0(\Lambda)\otimes K(\Lambda)=\oplus_{\nu} m_\nu V_0(\nu), \tag{59}$$

where $\mathscr{G}_0$ is the even subalgebra of $\mathscr{G}$ and $V_0(\Lambda)$ the maximal **Z**-graded component of $V(\Lambda)$. Then for $|\alpha|$ sufficient large (i.e., in the range considered above) we have the easily established decomposition

$$V(\Lambda+\alpha\delta)\otimes V(\Lambda+\alpha\delta)=\oplus_{\nu} m_\nu V(\nu+2\alpha\delta). \tag{60}$$

Note that this decomposition may be obtained solely from a knowledge of the $U_q(\mathscr{G}_0)$ modules occurring in $K(\Lambda)$ and $U_q(\mathscr{G}_0)$ tensor product rules. In principal this follows from the known characters of $K(\Lambda)$ and $V_0(\Lambda)$.

From our previous results we have the Casimir invariants

$$C_k^\Lambda=(I\otimes \mathrm{str})[I\otimes \pi_{\Lambda+\alpha\delta}(q^{-2h_\rho})]\sigma^k \tag{61}$$

which, from (54), take the following eigenvalues on $V(\nu+\alpha\delta)$:

$$\xi_k^\Lambda(q,\alpha)=q^{-kC(\Lambda+\alpha\delta)}\sum_{\nu}(-1)^{[\nu]}q^{(k/2)C(\nu+2\alpha\delta)}(m_\nu^+ +(-1)^k m_\nu^-)\,\frac{\chi_{\Lambda+\alpha\delta}(\Gamma_0)}{\chi_{\nu+2\alpha\delta}(\Gamma_0)}\cdot\frac{D_q^0(\nu)}{D_q^0(\Lambda)}, \tag{62}$$

where use has been made of the fact that $\alpha\delta$ is orthogonal to all even roots and $\Lambda+\alpha\delta$, $\nu+2\alpha\delta$ are all typical for α in the range considered.

Now for θ a braid of the general form (56), we arrive at at the link polynomial

$$L(\hat{\theta})=q^{-(\Lambda+\alpha\delta,\Lambda+\alpha\delta+2\rho)\Sigma_{i=1}^{M-1}k_i}\prod_{i=1}^{M-1}\xi_{k_i}^\Lambda(q,\alpha) \tag{63}$$

with $\xi_k^\Lambda(q,\alpha)$ given by (62). In this way we obtain a two-variable link polynomial corresponding to any real $\Lambda\in D^+$.

A. Two-variable link polynomials from $U_q[gl(m|n)]$

Following Ref. 35, we assume $m\geqslant n$ and for $0\leqslant N\leqslant mn$ we call a Young diagram $[\lambda]=[\lambda_1,\lambda_2,\ldots,\lambda_t]$, $\lambda_1\geqslant\lambda_2\cdots\geqslant\lambda_t\geqslant 0$ for the permutation group S_N (i.e., $\lambda_1+\lambda_2+\cdots+\lambda_t=N$) allowable, if it has at most n columns and m rows; i.e., $t\leqslant m$, $\lambda_i\leqslant n$. Associated with each such Young diagram $[\lambda]$ we define a weight of $gl(m|n)$

$$\Lambda_{[\lambda]}=(\dot{0}_{m-t},-\lambda_t,\cdots,-\lambda_1|\underbrace{t,\cdots,t}_{\lambda_t},\underbrace{t-1,\cdots,t-1}_{\lambda_{t-1}-\lambda_t},\cdots,\underbrace{1,\cdots,1}_{\lambda_1-\lambda_2},\underbrace{0,\cdots,0}_{n-\lambda_1}). \tag{64}$$

Using the basis $\{\epsilon_i,\delta_j\}$, the weight $\Lambda_{[\lambda]}$ may be expressed as

$$\Lambda_{[\lambda]}=-\sum_{i=1}^{t}\lambda_i\epsilon_{m-i+1}+t\sum_{j=1}^{\lambda_t}\delta_j+\sum_{s=1}^{t}(t-s)\sum_{j=\lambda_{t-s+1}}^{\lambda_{t-s}}\delta_j. \tag{65}$$

Let us consider the one-parameter family of finite-dimensional irreducible $U_q(gl(m|n))$-modules $V(\Lambda_\alpha)$ with highest weights of the form $\Lambda_\alpha=(0,...,0|\alpha,...,\alpha)\equiv(0|\dot{\alpha})=\alpha\delta$. [That is the case $\Lambda=(0|0)$.] These irreps $V(\alpha\delta)$ are unitary of type (1) if $\alpha>n-1$ and unitary of type (2) if $\alpha<1-m$. As mentioned above we assume real α satisfying one of these conditions, in which case $V(\alpha\delta)$ is also typical of dimension 2^{mn}.

We have the following decomposition of $V(\alpha\delta)$ into irreps of the even subalgebra $gl(m)\oplus gl(n)$:

$$V(\alpha\delta)=\bigoplus_{N=0}^{mn}\ \bigoplus_{[\lambda]\in S_N}V_0(\Lambda_{[\lambda]}+\alpha\delta), \tag{66}$$

where the summation is over allowed N-box Young diagrams. Note that the index N gives the **Z**-graded level of the irrep concerned. Alternatively we may simply write

$$V(\alpha\delta)=\bigoplus_{[\lambda]}V_0(\Lambda_{[\lambda]}+\alpha\delta). \tag{67}$$

The number of boxes N_λ in the Young diagram $[\lambda]$ then gives the level. We can deduce the tensor product decomposition

$$V(\alpha\delta)\otimes V(\alpha\delta)=\bigoplus_{[\lambda]}V(\Lambda_{[\lambda]}+2\alpha\delta). \tag{68}$$

The parity of the module $V(\Lambda_{[\lambda]}+2\alpha\delta)$ is $(-1)^{N_\lambda}$. The eigenvalue of the second-order Casimir on the irrep $V(\Lambda_{[\lambda]}+2\alpha\delta)$ can be shown to be

$$C(\Lambda_{[\lambda]}+2\alpha\delta)=2\sum_{i=1}^{t}\lambda_i(\lambda_i+1-2\alpha-2i)-2\alpha n(2\alpha+m),$$

$$C(\alpha\delta)=-\alpha n(\alpha+m). \tag{69}$$

Introduce the notation

$$\gamma_\alpha[\lambda]\equiv\frac{1}{2}C(\Lambda_{[\lambda]}+2\alpha\delta)-C(\alpha\delta)=2\sum_{i=1}^{t}\lambda_i(\lambda_i+1-2\alpha-2i)-\alpha n(3\alpha+m). \tag{70}$$

For θ a braid of the general form (56) we arrive at the two variable link polynomial

$$L(\hat{\theta})=q^{-n\alpha(\alpha+m)\Sigma_{i=1}^{M-1}k_i}\prod_{i=1}^{M-1}\xi_{k_i}(q,\alpha), \tag{71}$$

where now

$$\xi_k(q,\alpha)=\sum_{[\lambda]}(-1)^{(k-1)N_\lambda}q^{k\gamma_\alpha[\lambda]}\frac{\chi_{\alpha\delta}(\Gamma_0)}{\chi_{\Lambda_{[\lambda]}+2\alpha\delta}(\Gamma_0)}\cdot\frac{D_q^0(\Lambda_{[\lambda]}+2\alpha\delta)}{D_q^0(\alpha\delta)}. \tag{72}$$

In this formula, the sum is again over all allowable Young diagrams. This formula can be made fully explicit if we make use of the easily established result (which takes a bit of algebra)

$$\chi_{\alpha\delta}(\Gamma_0)\cdot\prod_{\beta\in\Phi_1^+}[(\rho,\beta)]_q=\prod_{i=1}^{m}\prod_{j=1}^{n}[i-j+\alpha]_q,$$

$$\chi_{\Lambda_{[\lambda]}+2\alpha\delta}(\Gamma_0)\cdot\prod_{\beta\in\Phi_1^+}[(\rho,\beta)]_q=\prod_{i=1}^{m}\prod_{j=1}^{n}[i-j-\lambda_i+2\alpha]_q\prod_{l=1}^{t}\frac{[\lambda_i-i-2\alpha+1-l]_q}{[\lambda_l+\lambda_i-i-2\alpha-l+1]_q},\tag{73}$$

where, in this last formula, it is implicitly understood that $\lambda_i=0$ for $m\geqslant i>t$. We thus obtain

$$\xi_k(q,\alpha)=\sum_{[\lambda]}(-1)^{(k-1)N_\lambda}q^{k\gamma_\alpha([\lambda])}\chi_\alpha([\lambda])D_q^0(\Lambda_{[\lambda]}),\tag{74}$$

where

$$\chi_\alpha([\lambda])\equiv\frac{\chi_{\alpha\delta}(\Gamma_0)}{\chi_{\Lambda_{[\lambda]}+2\alpha\delta}(\Gamma_0)}=\prod_{i=1}^{m}\prod_{j=1}^{n}\frac{[i-j+\alpha]_q}{[i-j-\lambda_i+2\alpha]_q}\prod_{l=1}^{t}\frac{[\lambda_l+\lambda_i-i-2\alpha+1-l]_q}{[\lambda_i-i-2\alpha+1-l]_q}.\tag{75}$$

As an illustration, let us consider some specific cases in the remaining part of this subsection.
Example (1): $U_q[gl(2|2)]$
The tensor product decomposition is

$$\begin{aligned}V(\alpha\delta)\otimes V(\alpha\delta)=V(0,0|2\alpha,2\alpha)\oplus V(0,-1|2\alpha+1,2\alpha)\oplus V(-1,-1|2\alpha+2,2\alpha)\oplus V(0,-2|2\alpha\\+1,2\alpha+1)\oplus V(-1,-2|2\alpha+2,2\alpha+1)\oplus V(-2,-2|2\alpha+2,2\alpha+2).\end{aligned}\tag{76}$$

We have in this case (using the Young diagram notation)

$$\begin{aligned}&\gamma_\alpha(\cdot)=-2\alpha^2,\quad \gamma_\alpha(\square)=-2\alpha(\alpha+1),\\&\gamma_\alpha(\square\square)=-2(\alpha^2+2\alpha-1),\quad \gamma_\alpha(\begin{smallmatrix}\square\\\square\end{smallmatrix})=-2(\alpha+1)^2,\\&\gamma_\alpha(\square\!\square\!\square)=-2\alpha(\alpha+3),\quad \gamma_\alpha(\begin{smallmatrix}\square\square\\\square\end{smallmatrix})=-2\alpha(\alpha+4),\\&D_q^0(\cdot)=1,\quad D_q^0(\square)=[2]_q^2,\quad D_q^0(\square\square)=[3]_q,\\&D_q^0(\begin{smallmatrix}\square\\\square\end{smallmatrix})=[3]_q,\quad D_q^0(\square\!\square\!\square)=[2]_q^2,\quad D_q^0(\begin{smallmatrix}\square\square\\\square\end{smallmatrix})=1,\end{aligned}\tag{77}$$

while the χ_α factors read

$$\begin{aligned}
\chi_\alpha(\cdot) &= \frac{[\alpha]_q^2[\alpha-1]_q[\alpha+1]_q}{[2\alpha]_q^2[2\alpha-1]_q[2\alpha+1]_q},\\
\chi_\alpha(\square) = \chi_\alpha(\begin{smallmatrix}\square\\\square\end{smallmatrix}) &= \frac{[\alpha]_q^2[\alpha-1]_q[\alpha+1]_q}{[2\alpha]_q^2[2\alpha-2]_q[2\alpha+2]_q},\\
\chi_\alpha(\square\!\square) = \chi_\alpha(\begin{smallmatrix}\square\\\square\\\square\end{smallmatrix}) &= \frac{[\alpha]_q^2[\alpha-1]_q[\alpha+1]_q}{[2\alpha+1]_q[2\alpha-1]_q[2\alpha-2]_q[2\alpha+2]_q},\\
\chi_\alpha(\begin{smallmatrix}\square\!\square\\\square\!\square\end{smallmatrix}) = \chi_\alpha(\cdot) &= \frac{[\alpha]_q^2[\alpha-1]_q[\alpha+1]_q}{[2\alpha]_q^2[2\alpha-1]_q[2\alpha+1]_q}.
\end{aligned} \tag{78}$$

It follows that

$$\begin{aligned}
\xi_k(q,\alpha) &= q^{k\gamma_\alpha(\cdot)}\chi_\alpha(\cdot)D_q^0(\cdot) + q^{k\gamma_\alpha(\begin{smallmatrix}\square\!\square\\\square\!\square\end{smallmatrix})}\chi_\alpha(\begin{smallmatrix}\square\!\square\\\square\!\square\end{smallmatrix})D_q^0(\begin{smallmatrix}\square\!\square\\\square\!\square\end{smallmatrix})\\
&\quad -(-1)^k\left[q^{k\gamma_\alpha(\square)}\chi_\alpha(\square)D_q^0(\square) + q^{k\gamma_\alpha(\begin{smallmatrix}\square\\\square\\\square\end{smallmatrix})}\chi_\alpha(\begin{smallmatrix}\square\\\square\\\square\end{smallmatrix})D_q^0(\begin{smallmatrix}\square\\\square\\\square\end{smallmatrix})\right]\\
&\quad +q^{k\gamma_\alpha(\square\!\square)}\chi_\alpha(\square\!\square)D_q^0(\square\!\square) + q^{k\gamma_\alpha(\begin{smallmatrix}\square\\\square\end{smallmatrix})}\chi_\alpha(\begin{smallmatrix}\square\\\square\end{smallmatrix})D_q^0(\begin{smallmatrix}\square\\\square\end{smallmatrix})\\
&= q^{-2k\alpha(\alpha+2)}\frac{(q^{4k\alpha}+q^{-4k\alpha})[\alpha+1]_q[\alpha-1]_q}{(q^\alpha+q^{-\alpha})^2[2\alpha+1]_q[2\alpha-1]_q}\\
&\quad -(-1)^k q^{-2k\alpha(\alpha+2)}\frac{(q^{2k\alpha}+q^{-2k\alpha})[2]_q^2}{(q^\alpha+q^{-\alpha})^2(q^{\alpha-1}+q^{-\alpha+1})(q^{\alpha+1}+q^{-\alpha-1})}\\
&\quad +\frac{q^{-2k(\alpha^2+\alpha+1)}(q^{2k\alpha}+q^{-2k\alpha})[3]_q(q^\alpha+q^{-\alpha})^2}{(q^{2\alpha-1}-q^{-2\alpha+1})(q^{2\alpha+1}-q^{-2\alpha-1})(q^{\alpha-1}+q^{-\alpha+1})(q^{\alpha+1}+q^{-\alpha-1})}.
\end{aligned} \tag{79}$$

Example (2): $U_q[gl(m|1)]$
We have the tensor product decomposition

$$V(\alpha\delta)\otimes V(\alpha\delta) = V(\dot{0}|2\alpha)\oplus V(\dot{0},-1|2\alpha+1)\oplus V(\dot{0},-1,-1|2\alpha+2)\oplus\cdots\oplus V(-\dot{1}|2\alpha+m). \tag{80}$$

In this case $D_q^0(\Lambda_{[\lambda]})$ reads

$$D_q^0(\Lambda_{[\lambda]}) = \prod_{i=1}^{t}\frac{[m+1-i]_q}{[t+1-i]_q} \equiv \frac{[m]_q!}{[m-t]_q![t]_q!} \tag{81}$$

and $\gamma_\alpha[\lambda]$, $\chi_\alpha([\lambda])$ reduce to, respectively,

$$\gamma_\alpha[\lambda] = -t(t-1)-\alpha(\alpha+2t),$$

$$\chi_\alpha([\lambda]) = \prod_{i=1}^{m}\frac{[i+\alpha-1]_q}{[i+2\alpha+t-1-\lambda_i]_q}. \tag{82}$$

The $\xi_k(q,\alpha)$ have the following form,

$$\xi_k(q,\alpha)=\sum_{t=0}^{m}$$

$$(-1)^{(k-1)t}q^{-k[t(t-1)+\alpha(\alpha+2t)]}\prod_{i=1}^{t}\frac{[m+1-i]_q[i+\alpha-1]_q}{[t+1-i]_q[i+2\alpha+t-2]_q}\prod_{i>t}^{m}\frac{[i+\alpha-1]_q}{[i+2\alpha+t-1]_q}. \tag{83}$$

B. Two-variable link polynomials from adjoint representation of $U_q[gl(2|1)]$

As another illustration of how the general formalism works it is instructive to consider the case $\Lambda=\psi$, $\psi=(1,0|-1)$ the highest weight of the adjoint representation of gl(2|1). This example is of interest since it affords the simplest example of a two-variable link polynomial in which a multiplicity occurs in the tensor product space.

First note that in this case $\epsilon_1-\epsilon_2$ is the single even positive root and $\epsilon_1-\delta_1,\epsilon_2-\delta_1$ are the two odd positive roots, from which we deduce that for any $\Lambda=(\Lambda_1,\Lambda_2|\Lambda_1)$

$$D_q^0[\Lambda]=[\Lambda_1-\Lambda_2+1]_q,\quad \chi_\Lambda(\Gamma_0)=[\Lambda_1+\overline{\Lambda_1}+1]_q[\Lambda_2+\overline{\Lambda_1}]_q. \tag{84}$$

For the Kac-module $K(\psi)$ we have the $U_q(\mathcal{G}_0)$-module ($\mathcal{G}_0=gl(2)\oplus u(1)$) decomposition (illustrated in terms of **Z**-graded levels):

$$K(\psi)=V_0(1,0|-1)\oplus V_0(1,-1|0)\oplus V_0(0,0|0)\oplus V_0(0,-1|1) \tag{85}$$

which is easily seen to be $2^2\cdot 2=8$ dimensional as required. Thus

$$\begin{aligned}V_0(\psi)\otimes K(\psi)&=V_0(1,0|-1)\otimes V_0(1,0|-1)\oplus V_0(1,0|-1)\otimes[V_0(1,-1|0)\oplus V_0(0,0|0)]\\&\quad\oplus V_0(1,0|-1)\otimes V(0,-1|1)\\&=V_0(2,0|-2)\oplus V_0(1,1|-2)\oplus V_0(2,-1|-1)\oplus 2V_0(1,0|-1)\\&\quad\oplus V_0(1,-1|0)\oplus V_0(0,0|0)\end{aligned} \tag{86}$$

which yields the tensor product decomposition:

$$\begin{aligned}V(\psi+\alpha\delta)\otimes V(\psi+\alpha\delta)&=V(2,0|2\alpha-2)\oplus V(1,1|2\alpha-2)\oplus V(2,-1|2\alpha-1)\oplus 2V(1,0|2\alpha-1)\\&\quad\oplus V(1,-1|2\alpha)\oplus V(0,0|2\alpha).\end{aligned} \tag{87}$$

It is seen that $V(1,0|2\alpha-1)$ occurs twice in the tensor product space. From the above **Z** gradation on $V_0(\psi)\otimes K(\psi)$ we obtain

$$(-1)^{[\nu]}=\begin{cases}-1, & \text{for } \nu=(2,-1|2\alpha-1),\quad (1,0|2\alpha-1)\\ 1, & \text{otherwise.}\end{cases} \tag{88}$$

In the $q\to 1$ limit the above tensor product module decomposes into symmetric and antisymmetric components (which determine the parities):

$$V(\psi+\alpha\delta)\otimes V(\psi+\alpha\delta)=W_+\oplus W_- \tag{89}$$

with

$$\begin{aligned}W_-&=V(1,1|2\alpha-2)\oplus V(2,-1|2\alpha-1)\oplus V(1,0|2\alpha-1)\oplus V(0,0|2\alpha),\\W_+&=V(2,0|2\alpha-2)\oplus V(1,0|2\alpha-1)\oplus V(1,-1|2\alpha).\end{aligned} \tag{90}$$

Note that there is one copy of $V(1,0|2\alpha-1)$ in each of these spaces. For the Casimirs we have

$$\tfrac{1}{2}C(\nu+2\alpha\delta)-C(\psi+\alpha\delta)=\begin{cases}-\alpha(\alpha+2), & \nu=(2,0|-2),(1,-1|0)\\ -(\alpha^2+1), & \nu=(1,0|-1)\\ -(\alpha^2+2\alpha+2), & \nu=(0,0|0)\\ -(\alpha^2-2\alpha+2), & \nu=(1,1|-2)\\ -\alpha^2+2, & \nu=(2,-1|-1).\end{cases} \tag{91}$$

Collecting together all of this information and substituting into (62) we arrive at

$$\begin{aligned}\xi_k^{\psi}(q,\alpha)=&q^{-k\alpha(\alpha+2)}\frac{[\alpha+1]_q[\alpha-1]_q[3]_q}{[2\alpha+1]_q[2\alpha-2]_q[2]_q}+q^{-k\alpha(\alpha+2)}\frac{[\alpha+1]_q[\alpha-1]_q[3]_q}{[2\alpha+2]_q[2\alpha-1]_q[2]_q}+(-1)^k\\ &\times q^{-k(\alpha^2+2\alpha+2)}\frac{[\alpha+1]_q[\alpha-1]_q}{[2\alpha+1]_q[2\alpha]_q[2]_q}+(-1)^k q^{-k(\alpha^2-2\alpha+2)}\frac{[\alpha+1]_q[\alpha-1]_q}{[2\alpha]_q[2\alpha-1]_q[2]_q}-\\ &(-1)^k q^{-k(\alpha^2-2)}\frac{[\alpha+1]_q[\alpha-1]_q[4]_q}{[2\alpha+2]_q[2\alpha-2]_q[2]_q}-(1+(-1)^k)q^{-k(\alpha^2+1)}\\ &\times\frac{[\alpha+1]_q[\alpha-1]_q}{[2\alpha+1]_q[2\alpha-1]_q}.\end{aligned} \tag{92}$$

C. Two-variable link polynomials from $U_q[osp(2|2n)]$

Consider the one-parameter family of 2^{2n}- dimensional irreducible $U_q[osp(2|2n)]$-modules $V(\Lambda_\alpha)$ with highest weights of form $\Lambda_\alpha=(\alpha|0,\ldots,0)\equiv\alpha\epsilon_0$ [and with lowest weight $\Lambda_\alpha^-=(\alpha-2n)\epsilon_0$]. $V(\alpha\epsilon_0)$ is unitary and typical provided that $\alpha<0$ or $\alpha>2n$. We therefore consider the tensor product module $V(\alpha\epsilon_0)\otimes V(\alpha\epsilon_0)$ with $\alpha<0$ or $\alpha>2n$ which decomposes as

$$V(\alpha\epsilon_0)\otimes V(\alpha\epsilon_0)=\bigoplus_{c=0}^{n}\bigoplus_{d=0}^{n-c}V(\Lambda_{c,d}) \tag{93}$$

with

$$\Lambda_{c,d}=(2\alpha-c-2d)\epsilon_0+\lambda_c,\quad \lambda_c=\sum_{i=1}^{c}\epsilon_i. \tag{94}$$

The decomposition (93) is obtained from known character formulae [c.f. Eq. (59)].

From the $\mathbf{Z}$ gradation on $V(\alpha\epsilon_0)$ we can deduce that the level of the module $V(\Lambda_{c,d})$ is equal to $c+2d$. Thus the parity of the module $V(\Lambda_{c,d})$ is $([1])^{c+2d}$. The Casimir eigenvalues read

$$\begin{aligned}C(\Lambda_{c,d})&=4(\alpha-d)(n+c+d-\alpha)-2c(c-1),\\ C(\alpha\epsilon_0)&=\alpha(2n-\alpha).\end{aligned} \tag{95}$$

For θ a braid of the general form (56) we thus arrive at the two variable link polynomial

$$L(\hat{\theta})=q^{-\alpha(2n-\alpha)\sum_{i=1}^{M-1}k_i}\prod_{i=1}^{M-1}\xi_{k_i}(q,\alpha), \tag{96}$$

where the $\xi_k(q,\alpha)$'s are given by

$$\xi_k(q,\alpha)=\sum_{c=0}^{n}\sum_{d=0}^{n-c}(-1)^{(k-1)(c+2d)}q^{k\gamma_\alpha}\frac{\chi_{\alpha\epsilon}(\Gamma_0)}{\chi_{\Lambda_{c,d}}(\Gamma_0)}\cdot\frac{D_q^0(\Lambda_{c,d})}{D_q^0(\alpha\epsilon)} \tag{97}$$

with

$$\gamma_\alpha\equiv\tfrac{1}{2}C(\Lambda_{c,d})-C(\alpha\epsilon). \tag{98}$$

After a bit algebra, we end up with

$$\chi_{\alpha\epsilon}(\Gamma_0)\cdot\prod_{\beta\in\Phi_1^+}[(\rho,\beta)]_q=\prod_{i=1}^{n}[2n+1-i-\alpha]_q[i-\alpha-1]_q,$$

$$\chi_{\Lambda_{c,d}}(\Gamma_0)\cdot\prod_{\beta\in\Phi_1^+}[(\rho,\beta)]_q=\prod_{i=1}^{n}[c+2d+2n+1-i-2\alpha-\delta_{i\leqslant c}]_q\cdot[c+2d+i-2\alpha-1+\delta_{i\leqslant c}]_q, \tag{99}$$

where $\delta_{i\leqslant c}$ equals 1 for $i\leqslant c$ and zero otherwise. We thus obtain

$$\xi_k(q,\alpha)=\sum_{c=0}^{n}\sum_{d=0}^{n-c}(-1)^{(k-1)(c+2d)}q^{k\gamma_\alpha}\chi_\alpha(c,d)\cdot D_q^0(\lambda_c), \tag{100}$$

where

$$\chi_\alpha(c,d)\equiv\frac{\chi_{\alpha\delta}(\Lambda_0)}{\chi_{\Lambda_{c,d}}(\Lambda_0)}=\prod_{i=1}^{n}\frac{[2n+1-i-\alpha]_q[i-\alpha-1]_q}{[c+2d+2n+1-i-2\alpha-\delta_{i\leqslant c}]_q[c+2d+i-2\alpha-1+\delta_{i\leqslant c}]_q},$$

$$D_q^0(\lambda_c)=\prod_{i<j}^{c}\frac{[2(n+2)-i-j]_q}{[2(n+1)-i-j]_q}\prod_{l=1}^{c}\frac{[2(n+2-l)]_q}{[2(n+1-l)]_q}. \tag{101}$$

VIII. DISCUSSION

We have demonstrated how link polynomials can be constructed associated with any finite-dimensional unitary irrep of a type-I quantum superalgebra. This is achieved by successfully overcoming a fundamental problem in computing the eigenvalues of Casimir invariants for the quantum superalgebras. Applying our results to one-parameter families of inequivalent irreps, we have been able to construct infinite families of nonequivalent two-variable link polynomials. Such two-variable link polynomials were previously known only for some isolated cases. For a class of braids, we have computed the link polynomials in fully explicit form.

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Structure of matrix manifolds and a particle model

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The decomposition of matrix manifolds into homogeneous spaces of certain groups is studied in some detail. The results are applied to the derivation of the internal structure of $\mathrm{SU}(2,2)\times\mathrm{SU}(m)$- and $P_4\times\mathrm{SU}(m)$-invariant particle models where the first (second) factor in the direct product represents external (internal) symmetry. © *1996 American Institute of Physics.* [S0022-2488(96)03302-1]

I. INTRODUCTION

The mathematical description of physical laws is based on observed symmetries and underlying geometry. An example is the Poincaré symmetry $P_4=T_4\times_s\mathrm{SO}(3,1)$, with the underlying space–time M_4, one of the homogeneous spaces of P_4, namely

$$M_4\cong T_4\cong P_4/\mathrm{SO}(3,1). \tag{1.1}$$

This fact inspired some physicists[1,2] to investigate other homogeneous spaces of the Poincaré group

$$\frac{P_4}{H_i}\cong\frac{P_4}{\mathrm{SO}(3,1)}\cdot\frac{\mathrm{SO}(3,1)}{H_i}, \quad H_i\subset\mathrm{SO}(3,1), \quad i=1,2,\ldots \tag{1.2}$$

for possible applicability in physics. For instance, the local coordinates on $\mathrm{SO}(3,1)/H_i$ can be interpreted as internal degrees of freedom of a relativistic particle. In this paper, we wish to combine an old idea[3] of describing the particle structure in complex space rather than in Minkowski space, with the investigation of the homogeneous spaces of the entire physical symmetry group, comprising both types of symmetries, internal as well as external.[4] We shall assume, in accordance with experiment, that the physical symmetry is the direct product $\mathrm{SU}(2,2)\times\mathrm{SU}(m)$ or $P_4\times\mathrm{SU}(m)\subset\mathrm{SU}(2,2)\times\mathrm{SU}(m)$ of external conformal or Poincaré and internal $\mathrm{SU}(m)$ symmetry (we keep m arbitrary to include such possibilities as $\mathrm{SU}(3)$, $\mathrm{SU}(3)\times\mathrm{SU}(2)\times\mathrm{U}(1)$, etc.). The Poincaré group P_4 is here considered as a subgroup of $\mathrm{SU}(2,2)$. The natural representation space for a direct product $GL(n,\mathbf{C})\times GL(m,\mathbf{C})$ is a complex matrix manifold $\mathbf{C}^{nm}$. In the case of $\mathrm{SU}(2,2)\times\mathrm{SU}(m)$ it will be $\mathbf{C}^{4m}$. In this space, both internal and external symmetries have a common geometrical basis in contrast to space–time, where only external symmetries are geometrized.

We shall consider homogeneous manifolds of $\mathrm{SU}(2,2)\times\mathrm{SU}(m)$ and $P_4\times\mathrm{SU}(m)$ in $\mathbf{C}^{4m}$ and show that there exists one and only one such manifold which admits a unique and consistent projection onto the compactified complex Minkowski space.

In the case of smaller $P_4\times\mathrm{SU}(m)$ symmetry we arrive at the homogeneous manifold

$$\frac{P_4\times\mathrm{SU}(m)}{\mathrm{SO}(2)\times\mathrm{SU}(m-2)}\cong\frac{P_4}{\mathrm{SO}(3,1)}\times\frac{\mathrm{SO}(3,1)\times\mathrm{SU}(m)}{\mathrm{SO}(2)\times\mathrm{SU}(m-2)}. \tag{1.3}$$

A particle structure in this model is described by a 5-dimensional real manifold $\mathrm{SO}(3,1)/\mathrm{SO}(2)$ and the manifold $\mathrm{SU}(m)/\mathrm{SU}(m-2)$, depending on the kind of internal symmetry.

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The structure of homogeneous submanifolds of $\mathbf{C}^{nm}$ with arbitrary n and m can be investigated, up to a certain point, without essential difficulties (Sections II–IV). This general case provides the theory of n complex m-vectors subject to certain invariance conditions and generalizes, in a certain sense, the theory of spinors (including bispinors, twistors etc.) to arbitrary dimensions. When the symmetry is the direct product of more than two groups, one has to generalize to ''tensor manifolds'' of tensors with more than two indices.[5] One can also consider supermatrices (supertensors) being representation spaces of direct products of supergroups and their decomposition into homogeneous structures.[6]

In the case of sets of vector fields, the general theory provides a classification of all possible invariance constraints.

In Sections V and VI, we derive the internal structure of $\mathrm{SU}(2,2)\times\mathrm{SU}(m)$-invariant particle models determined by the above-mentioned assumptions. This structure is described in terms of homogeneous spaces (like (1.3)). It remains to describe invariant dynamics and invariant differential operators in these spaces; these questions will be treated elsewhere.

II. MATRIX MANIFOLDS

Let us consider the set $\mathbf{C}^{nm}$ of all complex $n\times m$ matrices. The elements of this set may be viewed as arrays of m complex n-vectors (or m complex n-vectors) or, more geometrically, as homomorphisms $\mathrm{Hom}(\mathbf{C}^m,\mathbf{C}^n)$ of the vector spaces, i.e., linear maps $\mathbf{C}^m\to\mathbf{C}^n$. In the context of chosen bases in $\mathbf{C}^n$ and $\mathbf{C}^m$, the elements of $\mathbf{C}^{nm}$ will be represented by matrices indexed

$$M=\{m_{a\alpha}\}_{\substack{a=1,\ldots,n;\\ \alpha=1,\ldots,m}}\in\mathbf{C}^{nm}\cong\mathrm{Hom}(\mathbf{C}^m,\mathbf{C}^n).$$

The set $\mathbf{C}^{nm}\cong\mathrm{Hom}(\mathbf{C}^m,\mathbf{C}^n)$ decomposes in a natural way into submanifolds $\mathscr{O}_k^{(n,m)}$ of matrices (maps) of fixed rank k

$$\mathscr{O}_k^{(n,m)}:=\{M\in\mathbf{C}^{nm}:\mathrm{rank}M=k\}. \tag{2.1}$$

The decomposition is given by

$$\mathbf{C}^{nm}=\bigcup_{k=0}^{\min(n,m)}\mathscr{O}_k^{(n,m)},\quad \mathscr{O}_k^{(n,m)}\cap\mathscr{O}_l^{(n,m)}=\delta_{kl}\mathscr{O}_k^{(n,m)}. \tag{2.2}$$

A matrix of rank k is characterized by the fact that all subdeterminants (minors)

$$m\begin{pmatrix}\alpha_1 & \ldots, & \alpha_l\\ a_1 & \ldots, & a_l\end{pmatrix}:=\det\begin{bmatrix}m_{a_1\alpha_1} & \ldots & m_{a_1\alpha_l}\\ \vdots & & \\ \vdots & & \\ m_{a_l\alpha_1} & \ldots & m_{a_l\alpha_l}\end{bmatrix} \tag{2.3}$$

of order l higher than k vanish, and that there exists at least one nonvanishing subdeterminant of order k, say

$$m\begin{pmatrix}\alpha_1 & \ldots & \alpha_k\\ a_1 & \ldots & a_k\end{pmatrix}\neq 0. \tag{2.4}$$

Equation (2.4) determines a coordinate neighborhood on the manifold $\mathscr{O}_k^{(n,m)}$. There are $\binom{n}{k}\binom{m}{k}$ such neighborhoods according to the $\binom{n}{k}$ possibilities to choose k rows out of n rows, and the $\binom{m}{k}$ possibilities to choose k columns out of m columns.

Let us choose on $\mathscr{O}_k^{(n,m)}$ a neighborhood corresponding to a particular $k\times k$ square submatrix

$$K=\begin{bmatrix} m_{a_1\alpha_1} & \dots & m_{a_1\alpha_k} \\ \vdots & & \vdots \\ m_{a_k\alpha_1} & \dots & m_{a_k\alpha_k} \end{bmatrix}, \quad \det=K\neq 0, \tag{2.5}$$

where $a_1<a_2<\ldots<a_k$ and $\alpha_1<\alpha_2<\ldots<\alpha_k$ are some distinct k numbers from set $\{1,2,\ldots,n\}$ and $\{1,2,\ldots,m\}$, respectively. Denote the complementary ordered subsets by $a_{k+1}<\ldots<a_n$ and $\alpha_{k+1}<\ldots<\alpha_n$, respectively, and denote the complementary matrices by

$$A=\begin{bmatrix} m_{a_{k+1}\alpha_1} & \dots & m_{a_{k+1}\alpha_k} \\ \vdots & & \vdots \\ m_{a_n\alpha_1} & \dots & m_{a_n\alpha_k} \end{bmatrix}, \quad B=\begin{bmatrix} m_{a_1\alpha_{k+1}} & \dots & m_{a_1\alpha_m} \\ \vdots & & \vdots \\ m_{a_k\alpha_{k+1}} & \dots & m_{a_k\alpha_m} \end{bmatrix},$$

$$Y=\begin{bmatrix} m_{a_{k+1}\alpha_{k+1}} & \dots & m_{a_{k+1}\alpha_m} \\ m_{a_n\alpha_{k+1}} & \dots & m_{a_n\alpha_m} \end{bmatrix}. \tag{2.6}$$

Due to the fact that, on $\mathcal{O}_k^{(n,m)}$, $\det K \neq 0$ and all higher order subdeterminants vanish, we have, according to well known properties from linear algebra,

$$A=aK, \quad Y=aB, \quad B=Kb, \quad Y=Ab, \tag{2.7}$$

where

$$a=\{a^{a_i}_{a_j}\}_{\substack{i=1,\ldots,k \\ j=k+1,\ldots,n}} \quad b=\{b^{\alpha_i}_{\alpha_j}\}_{\substack{i=1,\ldots,k \\ j=k+1,\ldots,n}}. \tag{2.8}$$

These formulae express the fact that, in a $n\times m$ matrix of rank k, $n-k$ rows are linear combination of the remaining k rows.

The decomposition of $M \in \mathcal{O}_k^{(n,m)}$ into K, A, B, and Y is particularly simple in the neighborhood determined by $m(^{1,\ldots,k}_{1,\ldots,k})$. We have in this case

$$M=\begin{bmatrix} K & B \\ A & Y \end{bmatrix}. \tag{2.9}$$

It is sufficient to consider this particular case without loss of generality; the general formulae can be obtained by simply replacing the submatrices K, A, B, and Y in (2.9) by the general submatrices (2.5), (2.6). Due to invertibility of K ($\det K \neq 0$) we obtain from (2.7)

$$Y=aKb=AK^{-1}B. \tag{2.10}$$

These formulae, as well as formulae (2.7), describe the possible natural coordinate systems on $\mathcal{O}_k^{(n,m)}$ corresponding to the neighborhood $\det K \neq 0$. Coordinates a and b play a particularly important role because of their invariance properties. Coordinates a do not depend on the particular selection of columns (Greek indices), while coordinates b do not depend on the selection of rows (Latin indices).

The $(n-k)(m-k)$ dependent coordinates Y are functions of the $k^2+k(n-k)+k(m-k)$ independent coordinates, say K,A,B. The complex dimension of $\mathcal{O}_k^{(n,m)}$ is, therefore,

$$\dim\mathcal{O}_k^{(n,m)}=k(n+m-k). \tag{2.11}$$

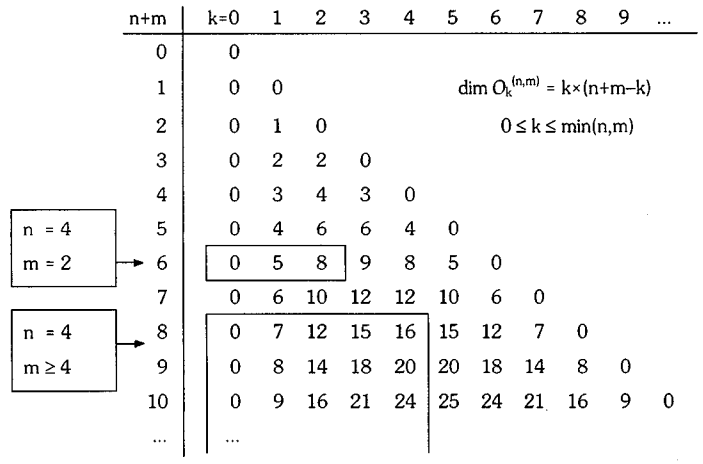

FIG. 1. Dimensions of matrix manifolds.

The manifold of the lowest dimension, corresponding to $k=0$, is a point $m_{a\alpha}=0$ for all $a=1,\ldots,n;\alpha=1,\ldots,m$. The next admissible dimension is already $n+m-1$. The dimension $k(n+m-k)$ of $\mathscr{O}_k^{(n,m)}$ appears fairly often in our considerations, so let us draw[7] the analogue of the Pascal triangle for the quantity

$$\begin{bmatrix} a \\ b \end{bmatrix} := b(a-b) \tag{2.12}$$

(see Figure 1). Dimensions of $\mathscr{O}_k^{(n,m)}$ appear here as $\left[\begin{smallmatrix} n+m \\ k \end{smallmatrix}\right]$. In the case $n=4$, $m\geqslant 4$ we have a decomposition

$$\mathbf{C}^{4m}=\mathscr{O}_0^{(4,m)}\cup\mathscr{O}_1^{(4,m)}\cup\mathscr{O}_2^{(4,m)}\cup\mathscr{O}_3^{(4,m)}\cup\mathscr{O}_4^{(4,m)} \tag{2.13}$$

with corresponding complex dimensions $k(4+m-k)$ with $k=1,\ldots,4$. The bounded region in Figure 1 displays possible dimensions; the right hand side of the triangle is cut out by the requirement $k\leqslant\min(n,m)$. The case $n=4,m=2$ is also indicated in Figure 1 since it corresponds to the Penrose model.[8] Definition (2.1–2) implies that each manifold $\mathscr{O}_l^{(n,m)}$ with $l<k$ lies in the boundary of $\mathscr{O}_k^{(n,m)}$ in the sense

$$\mathscr{O}_{(n,m)}^{l}\subset\bar{\mathscr{O}}_k^{(n,m)}, \quad l<k, \tag{2.14}$$

where the "bar" denotes closure in the topology induced on $\mathscr{O}_k^{(n,m)}$ from the natural topology in $\mathbf{C}^{nm}$. We can write therefore

$$\bar{\mathscr{O}}_k^{(n,m)}=\bigcup_{l=0}^{k}\mathscr{O}_l^{(n,m)}. \tag{2.15}$$

Each manifolds $\mathscr{O}_{(n,m)}^{l}$ has elements arbitrarily close to $\mathscr{O}:=\mathscr{O}_0^{(n,m)}$, and together they form a flag of manifolds[7] (see Figure 2) in the sense that $\bar{\mathscr{O}}_k^{(n,m)}\subset\bar{\mathscr{O}}_{k+1}^{(n,m)}$. All closed varieties $\bar{\mathscr{O}}_k^{(n,m)}$ meet at the point $\mathscr{O}$ and their tangent spaces at this point form a flag of spaces in the usual sense

$$\mathscr{O}=T_0\bar{\mathscr{O}}_0^{(n,m)}<T_0\bar{\mathscr{O}}_1^{(n,m)}<\ldots<T_0\bar{\mathscr{O}}_k^{(n,m)}<\ldots<T_0\mathscr{O}_{\min(n,m)}^{(n,m)}\cong\mathbf{C}_{nm} \tag{2.16}$$

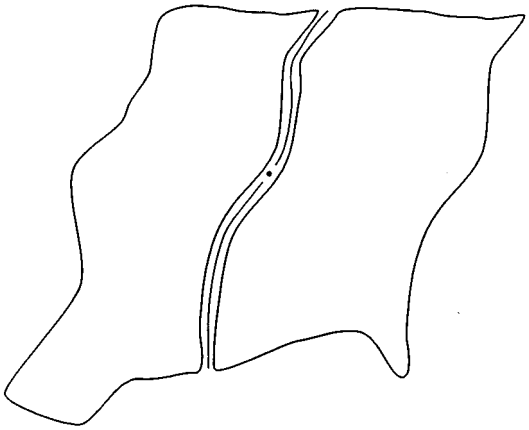

FIG. 2. Matrix manifolds form a "flag."

being an element of the flag manifold

$$F_{[_0^{n+m}],[_1^{n+m}],\ldots,[_{\min(n,m)}^{n+m}]}. \tag{2.17}$$

According to the interpretation of $\mathbf{C}^{(n,m)}$ as $\mathrm{Hom}(\mathbf{C}^m,\mathbf{C}^n)$, matrix M belonging to the submanifold $\mathscr{O}_k^{(n,m)}$ represents a homomorphism $\mathbf{C}^m\to\mathbf{C}^n$; its kernel $\mathrm{Ker}\ M$ is an $(m-k)$-dimensional subspace of $\mathbf{C}^m$ and its image $\mathrm{Im}\ M$ is a k-dimensional subspace of $\mathbf{C}^n$. This is particularly clear in the example of a matrix

$$M_0=\begin{bmatrix}\mathbb{1}_k & 0\\ 0 & 0\end{bmatrix}\in\mathscr{O}_k^{(n,m)}. \tag{2.18}$$

Thus, the canonical decomposition of a homomorphism gives in our case[7]

$$\mathbf{C}^m\xrightarrow{\pi}\mathbf{C}^m/\mathrm{Ker}\ M\xrightarrow{\iota}\mathrm{Im}\ M\xrightarrow{\epsilon}\mathbf{C}^n \tag{2.19}$$

(cf., Figure 3) where π is a canonical projection onto the coset space, ι is an isomorphism, and ε is an embedding. This suggests that, at least locally, manifold $\mathscr{O}_k^{(n,m)}$ may be decomposed into

$$\mathscr{G}_{m-k}^m\times GL(k,\mathbf{C})\times\mathscr{G}_k^n, \tag{2.20}$$

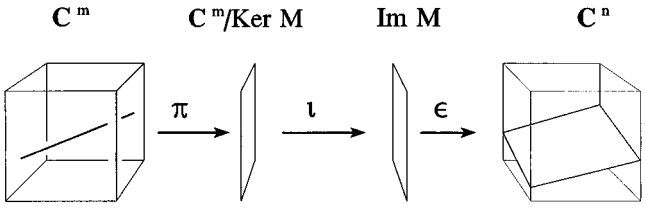

FIG. 3. Three maps.

where $\mathcal{G}^m_{m-k}$ and $\mathcal{G}^n_k$ are complex Grassman manifolds consisting of all $(m-k)$-dimensional subspaces in $\mathbf{C}^m$ and all k-dimensional subspaces in $\mathbf{C}^n$, respectively; group $\mathrm{GL}(k,\mathbf{C})$ is the k^2-dimensional set of all isomorphisms between the k-dimensional spaces $\mathbf{C}^m/\mathrm{Ker}\, M$ and $\mathrm{Im}\, M$.

However, globally manifold $\mathcal{O}^{(n,m)}_k$ cannot be trivialized into a direct product (2.20). Instead, one may consider $\mathcal{O}^{(n,m)}_k$ as a fiber bundle over $\mathcal{G}^m_{m-k}\times\mathcal{G}^n_k$ with the group $\mathrm{GL}(k,\mathbf{C})$ as the typical fiber. Including the natural projections of the Cartesian product of the two Grassman manifolds, we obtain the following diagram

$$\begin{array}{ccc} & \mathcal{O}^{(n,m)}_k & \\ {\scriptstyle\pi_1}\swarrow & \downarrow{\scriptstyle\pi} & \searrow{\scriptstyle\pi_2} \\ & \overset{(\mathrm{id},0)}{\mathcal{G}^m_{m-k}} \leftarrow \mathcal{G}^m_{m-k}\times\mathcal{G}^n_k \rightarrow \overset{(0,\mathrm{id})}{\mathcal{G}^n_k} & \end{array}$$

of three possible fiberings of manifold $\mathcal{O}^{(n,m)}_k$:

$$(\mathcal{O}^{(n,m)}_k,\mathcal{G}^m_{m-k}\times\mathcal{G}^n_k,\pi),\quad (\mathcal{O}^{(n,m)}_k,\mathcal{G}^m_{m-k},\pi_1),\quad (\mathcal{O}^{(n,m)}_k,\mathcal{G}^n_k,\pi_2)$$

where the projections are defined

$$\begin{aligned} \pi&:\mathcal{O}^{(n,m)}_k\to\mathcal{G}^m_{m-k}\times\mathcal{G}^n_k : M\to \mathrm{Ker}\ M\times \mathrm{Im}\ M \\ \pi_1&:\mathcal{O}^{(n,m)}_k\to\mathcal{G}^m_{m-k} : M\to \mathrm{Ker}\ M \\ \pi_2&:\mathcal{O}^{(n,m)}_k\to\mathcal{G}^n_k : M\to \mathrm{Im}\ M \end{aligned} \tag{2.21}$$

and the typical fibers are isomorphic to $\mathrm{GL}(k,\mathbf{C})$, $\mathbf{C}^{km}$, and $\mathbf{C}^{kn}$, respectively.

In local coordinates, Grassman manifolds $\mathcal{G}^m_{m-k}$ and $\mathcal{G}^n_k$ are parameterized by elements of the matrices a and b respectively, and the fiber $\mathrm{GL}(k,\mathbf{C})$ is parameterized by elements of the matrix K (cf., (2.10)). The fiber bundle $\mathcal{O}^{(n,m)}_k$ is not trivializable. In particular, it also contains all the topological singularities of the Grassman manifold in the base.

Remark: note that since the dimension of a complex Grassman manifold is $\dim\mathcal{G}^n_k = k(n-k)$, the complex dimension of $\mathcal{O}^{(n,m)}_k$ is, according to (2.20), equal to $k(m-k)+k(n-k)+k^2 = k(n+m-k)$, in a complete agreement with (2.11).

III. GROUP THEORETICAL DESCRIPTION OF MATRIX MANIFOLDS

Space $\mathbf{C}^{nm}\cong\mathrm{Hom}(\mathbf{C}^m,\mathbf{C}^n)$ is a natural representation space for the direct product $GL(n,\mathbf{C})\times GL(m,\mathbf{C})$:

$$M\to M' = gMh^{-1},\quad g\in GL(n,\mathbf{C}),\quad h\in GL(m,\mathbf{C}), \tag{3.1}$$

according to the commuting diagram

$$\begin{array}{ccc} \mathbf{C}^m & \overset{M}{\to} & \mathbf{C}^n \\ h\downarrow & & \downarrow g \\ \mathbf{C}^m & \overset{M'}{\to} & \mathbf{C}^n \end{array} \tag{3.2}$$

The manifolds $\mathscr{O}_k^{(n,m)}$ are orbits of $\mathrm{GL}(n,\mathbf{C})\times\mathrm{GL}(m,\mathbf{C})$. Indeed, a linear transformation of rows and columns does not change the rank of matrix. Moreover, the group $\mathrm{GL}(n,\mathbf{C})\times\mathrm{GL}(m,\mathbf{C})$ acts transitively on each $\mathscr{O}_k^{(n,m)}$. We can describe therefore the matrix manifolds $\mathscr{O}_k^{(n,m)}$ as homogeneous spaces[9] of the group $\mathrm{GL}(n,\mathbf{C})\times\mathrm{GL}(m,\mathbf{C})$:

$$\mathscr{O}_k^{(n,m)}=\frac{\mathrm{GL}(n,\mathbf{C})\times\mathrm{GL}(m,\mathbf{C})}{H_k^{(n,m)}}, \tag{3.3}$$

where $H_k^{(n,m)}$ is the isotropy group of the group $\mathrm{GL}(n,\mathbf{C})\times\mathrm{GL}(m,\mathbf{C})$ in $\mathscr{O}_k^{(n,m)}$. For the point

$$M_0=\begin{bmatrix}\mathbb{1}_k & 0\\ 0 & 0\end{bmatrix}\in\mathscr{O}_k^{(n,m)}$$

the isotropy group $H_k^{(n,m)}$ can be easily calculated

$$H_k^{(n,m)}=\begin{bmatrix}g_1 & g_2\\ 0 & g_1\end{bmatrix}\times\begin{bmatrix}g_1^{-1} & 0\\ h_2 & h_3\end{bmatrix}, \tag{3.4}$$

where $g_1\in\mathrm{GL}(k,\mathbf{C})$, $g_2\in\mathbf{C}^{k(n-k)}$, $g_3\in\mathrm{GL}(n-k,\mathbf{C})$, $h_2\in\mathbf{C}^{(m-k)k}$, $h_3\in\mathrm{GL}(m-k,\mathbf{C})$. We check the (complex) dimensions: $\dim\mathrm{GL}(n,\mathbf{C})\times\mathrm{GL}(m,\mathbf{C})/H_k^{(n,m)}=n^2+m^2-k^2-(n-k)^2-(m-k^2)-k(n-k)-k(m-k)=k(n+m-k)$.

Another, equivalent, group-theoretical description of $\mathscr{O}_k^{(n,m)}$ can be obtained by representing the Grassman manifolds appearing in the base of the fiber bundle $\mathscr{O}_k^{(n,m)}$ as homogeneous spaces of certain groups. There are two possibilities to represent a complex Grassman manifold as a homogeneous space:

$$\mathscr{G}_k^n\cong\frac{\mathrm{U}(n)}{\mathrm{U}(k)\mathrm{U}(n-k)}\cong\frac{\mathrm{GL}(n,\mathbf{C})}{H_k^n} \tag{3.5}$$

where H_k^n is a matrix group defined:

$$H_k^n=\left\{\begin{bmatrix}g_1 & g_2\\ 0 & g_3\end{bmatrix},\quad g_1\in\mathrm{GL}(k,\mathbf{C}),\quad g_2\in\mathbf{C}^{k(n-k)},\quad g_3\in\mathrm{GL}(n-k,\mathbf{C})\right\}. \tag{3.6}$$

It is important to notice that Grassman manifolds $\mathscr{G}_k^n$ and $\mathscr{G}_{m-k}^m$ of the base of the fiber bundle $\mathscr{O}_k^{(n,m)}$ are invariant under action of the groups $\mathbb{1}_n\times\mathrm{GL}(m,\mathbf{C})$ and $\mathrm{GL}(n,\mathbf{C})\times\mathbb{1}_m$, respectively, and transform into themselves under action of the groups $\mathrm{GL}(n,\mathbf{C})\times\mathbb{1}_m$ and $\mathbb{1}_n\times\mathrm{GL}(m,\mathbf{C})$, respectively. This follows immediately from the remark after formula (2.10) and (2.21) stating that the coefficients a (b) of linear combinations $A=aK$ $(B=Kb)$ do not depend on the columns (rows) of matrix M.

Let us consider, finally, the transformation properties of the local coordinates on $\mathscr{O}_k^{(n,m)}$ with respect to the group $\mathrm{GL}(n,\mathbf{C})\times\mathrm{GL}(m,\mathbf{C})$. For this purpose, to simplify the notation, we extend the $(n-k)\times k$ and $k\times(m-k)$ matrices a and b of (2.8) to the $n\times k$ and $k\times m$ matrices

$$a=\{a^{a_i}_{a_j}\}^{i=1,\ldots,k}_{j=1,\ldots,n},\qquad b=\{b^{a_i}_{\alpha_j}\}^{i=1,\ldots,k}_{j=1,\ldots,n} \tag{3.7}$$

by means of unit matrices

$$\{a^{a_i}_{a_j}\}=\{\delta^{a_i}_{a_j}\},\quad \{b^{\alpha_i}_{\alpha_j}\}=\{\delta^{\alpha_i}_{\alpha_j}\}\quad i,j=1,\ldots,k. \tag{3.8}$$

(We denote these extended matrices by the same letters; the context will always clarify whether we have to do with the original or the extended matrices.) With the help of the extended matrices we can combine relations (2.7), (2.11) into a single formula

$$M = aKb, \quad M \in \mathcal{O}_k^{(n,m)}, \quad \det K \neq \mathcal{O}. \tag{3.9}$$

Equation (3.1) takes, on $\mathcal{O}_k^{(n,m)}$, the form

$$M' = gaKbh^{-1} = a'K'b', \tag{3.10}$$

where K' is chosen so that $\det K \neq 0$ (this is always possible because transformation (3.1) does not change the rank of M). Matrices a' and b' have, in this neighborhood, the same functional dependence of the elements of M' as the matrices a and b have of the elements of M:

$$\begin{aligned} a' &= a(gMh^{-1}) = a(gM), \\ b' &= b(gMh^{-1}) = b(Mh^{-1}). \end{aligned} \tag{3.11}$$

The second parts of these equalities express the invariance of a and b with respect to $\mathbb{1}_n \times \mathrm{GL}(m,\mathbf{C})$ and $\mathrm{GL}(n,\mathbf{C}) \times \mathbb{1}_m$, respectively. (Cf., the remark after formula (2.6)). It is also useful to note the explicit form of the transformation law (3.11). For this purpose, we write equation $a = AK^{-1}$ as

$$a_{a_j}^{a_i} = \sum_{l=1}^{k} m_{a_j \alpha_l} (K^{-1})^{\alpha_l a_i} = \frac{m\begin{pmatrix} \alpha_1 \ldots & & \ldots \alpha_k \\ a_1 \ldots & a_{i-1} a_j a_{i+1} & \ldots a_k \end{pmatrix}}{m\begin{pmatrix} \alpha_1 & \ldots & \alpha_k \\ a_1 & \ldots & a_k \end{pmatrix}}, \tag{3.12}$$

where $i = 1, \ldots, k$ and $j = k+1, \ldots, n$. The same formula holds for a' in terms of M'

$$\begin{aligned} a'^{ai}_{aj} &= \frac{m'\begin{pmatrix} \alpha_1 \ldots & & \ldots \alpha_k \\ a_1 \ldots & a_{i-1} a_j a_{i+1} & \ldots a_k \end{pmatrix}}{m'\begin{pmatrix} \alpha_1 & \ldots & \alpha_k \\ a_1 & \ldots & a_k \end{pmatrix}} = \frac{gaKbh^{-1}\begin{pmatrix} \alpha_1 \ldots & & \ldots \alpha_k \\ a_1 \ldots & a_{i-1} a_j a_{i+1} & \ldots a_k \end{pmatrix}}{gaKbh-1\begin{pmatrix} \alpha_1 & \ldots & \alpha_k \\ a_1 & \ldots & a_k \end{pmatrix}} \\ &= \frac{ga\begin{pmatrix} \alpha_1 \ldots & & \ldots \alpha_k \\ a_1 \ldots & a_{i-1} a_j a_{i+1} & \ldots a_k \end{pmatrix}}{ga\begin{pmatrix} \alpha_1 & \ldots & \alpha_k \\ a_1 & \ldots & a_k \end{pmatrix}} \end{aligned} \tag{3.13}$$

where $i = 1, \ldots, k$ and $j = k+1, \ldots, n$. Analogously

$$b_{\alpha_j}^{\alpha_i} = \frac{m\begin{pmatrix} \alpha_1 \ldots & \alpha_{i-1} \alpha_j \alpha_{i+1} & \ldots \alpha_k \\ \alpha_1 \ldots & & \ldots \alpha_k \end{pmatrix}}{m\begin{pmatrix} \alpha_1 & \ldots & \alpha_k \\ a_1 & \ldots & a_k \end{pmatrix}} \tag{3.14}$$

and

$$b'^{\alpha_i}_{\alpha_j}=\frac{bh^{-1}\begin{pmatrix}\alpha_1\ldots & \alpha_{i-1}\alpha_j\alpha_{i+1} & \ldots\alpha_k\\ a_1\ldots & & \ldots a_k\end{pmatrix}}{bh^{-1}\begin{pmatrix}\alpha_1\ldots & \ldots & \alpha_k\\ a_1 & \ldots & a_k\end{pmatrix}}. \tag{3.15}$$

Relations (3.13) and (3.15) provide an alternative proof of the transformation properties of a and b and an explicit form of the transformation law. The second equation of (3.11) follows from the well known formula for subdeterminants of a product of matrices two A and B

$$AB\begin{pmatrix}j_1 & \ldots & j_l\\ i_1 & \ldots & i_l\end{pmatrix}=\sum_{\binom{n}{l}} A\begin{pmatrix}k_1 & \ldots & k_l\\ i_1 & \ldots & i_l\end{pmatrix}B\begin{pmatrix}j_1 & \ldots & j_l\\ k_1 & \ldots & k_l\end{pmatrix} \tag{3.16}$$

that is taken for the particular case $l=n$. Here the sum goes over all $\binom{n}{l}$ selections of l distinct numbers $k_1,\ldots,k_l$ between 1 and n.

Let us consider the infinitesimal form or the transformation law of the local coordinates. The infinitesimal version of (3.10) and (3.11) is

$$M'=M+\delta M,\quad a'=a+\delta a,\quad b'=b+\delta b, \tag{3.17}$$

with

$$\delta M=\delta g M+M\,\delta h^{-1}=i\sum_{k=1}^{r}\delta\lambda_k x_k M-i\sum_{k=1}^{s}\delta\mu_k M y_k \tag{3.18}$$

and

$$\delta a=\sum_{k=1}^{r}\delta\lambda_k\frac{\partial a(gM)}{\partial\lambda_k}\bigg|_{\lambda=0},\quad \delta b=\sum_{k=1}^{s}\delta\mu_k\frac{\partial b(Mh^{-1})}{\partial\mu_k}\bigg|_{\mu=0} \tag{3.19}$$

where

$$x_k=\frac{1}{i}\frac{\partial g}{\partial\lambda_k}\bigg|_{\lambda=0},\quad y_k=\frac{1}{i}\frac{\partial h}{\partial\mu_k}\bigg|_{\mu=0} \tag{3.20}$$

are generators of the factors $\mathrm{GL}(n,\mathbf{C})$ and $\mathrm{GL}(m,\mathbf{C})$ of the direct product $\mathrm{GL}(n,\mathbf{C})\times\mathrm{GL}(m,\mathbf{C})$ or of one of its subgroups, and $\lambda_1,\lambda_2,\ldots,\lambda_r$ and $\mu_1,\mu_2,\ldots,\mu_s$ are the corresponding parameters. Formula (3.18) for δM has already its final form; the formulae for δa and δb have yet to be expressed in terms of generators x_k and y_k. Differentiate equations $A'=a'K'$ and $B'=K'b'$ with respect to the corresponding parameters:

$$\begin{aligned}\frac{\partial A'}{\partial\lambda_k}&=\frac{\partial a'}{\partial\lambda_k}K'+a'\frac{\partial K'}{\partial\lambda_k},\\ \frac{\partial B'}{\partial\mu_k}&=\frac{\partial K'}{\partial\mu_k}b'+K'\frac{\partial b'}{\partial\mu_k}.\end{aligned} \tag{3.21}$$

This gives

$$\left.\frac{\partial a'}{\partial \lambda_k}\right|_{\lambda=0} = \left(\frac{\partial A'}{\partial \lambda_k} - a'\frac{\partial K'}{\partial \lambda_k}\right)_{\lambda=0} K^{-1} = i(x_k a - a x_k a),$$
$$\left.\frac{\partial b'}{\partial \mu_k}\right|_{\mu=0} = K^{-1}\left(\frac{\partial B'}{\partial \mu_k} - \frac{\partial K'}{\mu \lambda_k} b'\right)_{\mu=0} = -i(b y_k - b y_k b). \tag{3.22}$$

Substituting (3.22) into (3.19) we obtain finally

$$\delta a = i\sum_{k=1}^{r} \delta\lambda_k (x_k a - a x_k a),$$
$$\delta b = -i\sum_{k=1}^{s} \delta\mu_k (b y_k - b y_k b). \tag{3.23}$$

Similarly, one can easily show that

$$\left.\frac{\partial a'}{\partial \mu_k}\right|_{\mu=0} = \left.\frac{\partial b'}{\partial \lambda_k}\right|_{\lambda=0} = 0, \tag{3.24}$$

which confirms the transformation properties of a and b as exhibited in equation (3.11), and used explicitly in (3.19).

IV. REDUCTION OF SYMMETRY

Reduction of the symmetry $\mathrm{GL}(n,\mathbf{C})\times\mathrm{GL}(m,\mathbf{C})$ to a subgroup induces in general a decomposition of the matrix manifolds $\mathscr{O}_k^{(n,m)}$. Here, we shall consider only the case of the subgroup $\mathrm{SU}(n-p,p)\times\mathrm{SU}(m-q,q)$ determined by Hermitian metric tensors F_1 and F_2 (not necessarily diagonal), with $n-p$ and $m-q$ eigenvalues $+1$ respectively, and p and q eigenvalues -1 respectively. For simplicity of the following considerations, we shall assume that F_1 denotes Hermitian structure in the space $\mathbf{C}^n$ (two lower indices), while F_2 denotes Hermitian structure in the *dual* space $\mathbf{C}^{m*}$ (two upper indices).

Define the following invariants

$$I_n = \mathrm{Tr}\, r^n, \quad n = 1,2,\ldots, \tag{4.1}$$

where

$$r = F_2 M^* F_1 M \tag{4.2}$$

is an automorphism of $\mathbf{C}^m$ described by a non-commuting diagram

$$\begin{array}{ccc} \mathbf{C}^{m*} & \overset{M^*}{\leftarrow} & \mathbf{C}^{n*} \\ F_2\downarrow & & \uparrow F_1 \\ \mathbf{C}^m & \overset{M}{\rightarrow} & \mathbf{C}^m \end{array} \tag{4.3}$$

and where the Hermitian metric tensors F_1 and F_2 are considered as maps to the corresponding dual spaces. Clearly, the order of matrices in r can be changed by a cyclic permutation without causing change of the invariants.

One can easily show that the quantities I_n are indeed invariants of the group $\mathrm{SU}(n-p,p)\times\mathrm{SU}(n-q,q)$ and that they are real. Indeed, due to $g^*F_1g=F_1$ and $hF_2h^*=F_2$, we have

$$I'_n:=\mathrm{Tr}(r')^n=\mathrm{Tr}(F_2M'^*F_1M')^n=\mathrm{Tr}(F_2h^{-1}{}^*M^*g^*F_1gMh^{-1})^n=\mathrm{Tr}(F_2M^*F_1M)^n=I_n$$

and

$$I_n^*=\mathrm{Tr}(M^*F_1^*MF_2^*)^n=\mathrm{Tr}(F_2M^*F_1M)^n=I_n.$$

Another kind of invariant appears as coefficients J of the eigenvalue equation for the automorphism r

$$\det(r-\lambda)=\sum_{n=0}^{m}(-\lambda)^nJ_{m-n}=0, \tag{4.4}$$

where J's are defined

$$J_{m-n}=\frac{(-1)^n}{n!}\frac{d^n\det(r-\lambda)}{d\lambda^n}\bigg|_{\lambda=0}. \tag{4.5}$$

These invariants have the explicit form

$$J_n=\sum_{\binom{m}{n}} r\begin{pmatrix}\alpha_1,\alpha_2,\ldots,\alpha_n\\ \alpha_1,\alpha_2,\ldots,\alpha_n\end{pmatrix}, \tag{4.6}$$

where the summation extends over all $\binom{m}{n}$ possible selections of n distinct numbers α_i from the set $\{1,2,\ldots,m\}$.

There exists a relation between both types of invariants. In case $n=1$ the invariants coincide

$$J_1=I_1 \tag{4.7}$$

and for $n\geqslant 2$ the relation is

$$J_n=\frac{1}{n!}\sum_{\alpha_1}\sum_{\alpha_2}\cdots\sum_{\alpha_n} r\begin{pmatrix}\alpha_1,\alpha_2,\ldots,\alpha_n\\ \alpha_1,\alpha_2,\ldots,\alpha_n\end{pmatrix}=\frac{1}{n!}(-1)^{n-1}(n-1)I_n+\Phi_n(I_1,I_2,\ldots,I_{n-1}), \tag{4.8}$$

with some polynomial Φ_n of order less than n. Thus, only the first k invariants are independent on $\mathscr{O}_k^{(n,m)}$. Indeed, all determinants of order higher than k vanish on $\mathscr{O}_k^{(n,m)}$ and, therefore,

$$J_{k+r}=0,\quad r=1,2,\ldots. \tag{4.9}$$

Consequently, relation

$$\frac{1}{(k+r)!}(-1)^{k+r-1}(k+r-1)I_{k+r}+\Phi_{k+r}(I_1,I_2,\ldots,I_{k+r-1})=0\quad r=1,2,\ldots \tag{4.10}$$

provides a set of equations expressing the higher order invariants I_{k+r}, $r=1,2,\ldots$, in terms of I_1, $I_2,\ldots,I_k$. In particular

$$J_1=I_1,\quad 2J_2=I_1^2-I_2,\quad 6J_3=I_1^3-3I_1I_2+2I_3. \tag{4.11}$$

The invariants may be used to foliate the space; equations

$$I_n=\kappa_n, \quad n=1,2,\ldots,k \tag{4.12}$$

with constants κ_n satisfying certain compatibility conditions, determine a k-parametric family of $\mathrm{SU}(n-p,p)\times\mathrm{SU}(m-q,q)$-invariant submanifolds of space $\mathbf{C}^{nm}$. Their intersections with the $\mathrm{GL}(n,C)\times\mathrm{GL}(m,C)$-invariant submanifolds $\mathscr{O}_k^{(n,m)}$ provide a decomposition of $\mathscr{O}_k^{(n,m)}$ into a k-parametric family of $\mathrm{SU}(n-p)\times\mathrm{SU}(m-q)$–invariant submanifolds $\mathscr{O}_{(k,\kappa)}^{(n,m)}$ where $\kappa=\{\kappa_1,\kappa_2,\ldots,\kappa_k\}$. The analytic description of these sections is obtained by substituting (3.9) into (4.12):

$$I_l=\mathrm{Tr}(F_2b^*K^*a^*F_1aKb)^l=\mathrm{Tr}(f_2K^*f_1K)^l=\kappa_l^*, \quad l=1,2,\ldots,k, \tag{4.13}$$

where

$$f_1=a^*F_1a, \quad f_2=bF_2b^* \tag{4.14}$$

represent the metrics induced on the columns and rows of the matrix K from the metric tensors F_1 and F_2 on M.

The induced metric tensors f_1 and f_2 depend on the Grassman coordinates a and b respectively, on the choice of neighborhood, and on the choice of the representation of the initial metrics F_1 and F_2 on M. For the purpose of a general discussion we consider the induced metric $f(a)$ given by a $k\times k$ Hermitian matrix being a function of the $k(n-k)$ complex Grassman coordinates a. The signature of the induced metric is determined by the roots of the secular equation for f,

$$\det(f-\lambda\mathbb{1})=(-\lambda)^k+(-\lambda)^{k-1}\mathrm{Tr}\,f+\ldots+\det f=\sum_{i=0}^{k}(-\lambda)^ic_{k-i}=\prod_{i=1}^{k}(\lambda_i-\lambda)=0, \tag{4.15}$$

where, similarly as in (4.4)–(4.6),

$$c_i=\sum_{\binom{k}{i}} f\begin{pmatrix}a_1,a_2,\ldots,a_n\\ a_1,a_2,\ldots,a_n\end{pmatrix}, \quad i=1,2,\ldots,k, \tag{4.16}$$

where the sum runs over all $\binom{k}{i}$ possible selections of i distinct numbers from $\{1,2,\ldots,k\}$. Roots $\lambda_i(a)$, which determine the induced metric, are functions of the Grassman coordinates a and change as the a's vary over the Grassman manifold $\mathscr{G}_k^n$.

Not all eigenvalues can appear in the induced metric. The induced metric tensor on the k-plane in C^n may have different degree of degeneration. A triple (a,b,c) will denote signature of a pluses, b minuses, and c zeros of a $(a+b+c)$-dimensional space. Notation (a,b) means that $c=0$.

Consider first the planes with non-degenerate induced metric tensors. The number of positive (negative) roots cannot exceed the number of positive (negative) signs in the original metric. If the original signature in $\mathbf{C}^n$ is $(n-p,p)$ then the admissible signatures on k-dimensional planes in $\mathbf{C}^n$ are $(k-l,l)$, for some l satisfying the obvious relations

$$k-l\leqslant n-p, \quad l\leqslant p, \quad 0\leqslant l\leqslant k \tag{4.17}$$

or, jointly,

$$L_{\min}\leqslant l\leqslant L_{\max}, \tag{4.18}$$

where

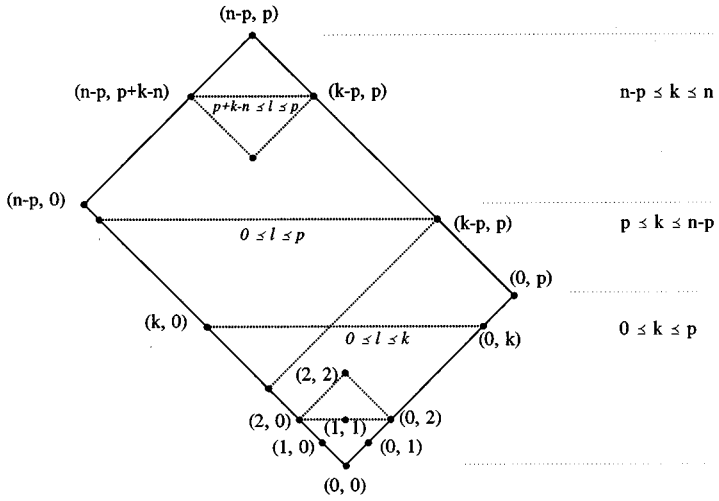

FIG. 4. The lattice of induced metric structures.

$$L_{\min}=\max\{0,k+p-n\}, \quad L_{\max}=\min\{p,k\}.$$

There are six different situations:

$$n-p\geqslant p \quad \text{and} \quad \begin{cases} 0\leqslant k\leqslant p \\ p\leqslant k\leqslant n-p, \\ n-p\leqslant k\leqslant n \end{cases} \quad \text{or} \quad n-p\leqslant p \quad \text{and} \quad \begin{cases} 0\leqslant k\leqslant n-p \\ n-p\leqslant k\leqslant p \\ p\leqslant k\leqslant n. \end{cases}$$

The three possibilities corresponding to $n-p\geqslant p$ are illustrated in Figure 4.

Also, degenerate metrics will appear for certain submanifolds of $\mathcal{G}_k^n$ corresponding to zero roots $\lambda_i(a)=0$ of equation (4.13). There will be zero roots of various orders ranging from 1 to k described by the vanishing of the first coefficients $c_i(a)$ in (4.15). Root $\lambda(a)$ of multiplicity r is described by r equations

$$c_{k-j}(a)=0, \quad j=0,1,\ldots,r-1. \tag{4.19}$$

Let us consider a zero root with multiplicity one. It always lies on the border between two roots of the opposite sign. The corresponding metric has signature $(k-l-1,l,1)$ and lies in $\mathcal{G}_k^n$ between two metrics differing by interchanging a positive with a negative sign, that is to say between $(k-l,l,0)$ and $(k-l-1,l+1,0)$ and may be obtain by replacing one plus of the first, or one minus of the second, by a zero.

The case of zero with multiplicity two is obtained by descending one step down to the $(k-2)$-dimensional hyperplane in $\mathbf{C}^n$ with the metric $(k-2-l,l,2)$, where now l varies $L_{\min}\leqslant l\leqslant L_{\max}-2$. Proceeding in this way we obtain, after r steps, a set of degenerate metrics of signatures

$$(k-r-l,l,r),$$

where l and r vary according to

$$L_{\min}\leqslant l\leqslant L_{\max-r}, \quad 0\leqslant r\leqslant L_{\max}-L_{\min}. \tag{4.20}$$

Summarizing, the Grassman manifold $\mathscr{G}_k^n$ decomposes into domains, each domain consisting of hyperplanes that have the same signature of the induced metric. There are $L_{\min}-L_{\max}+1$ such domains corresponding to non-degenerate metrics. They are separated by boundaries, each boundary consisting of those hyperplanes that have the same signature of the induced degenerate metric. The boundaries are determined by equations

$$c_{k-j}(a)=0, \quad j=0,1,\ldots,r-1, \quad r=1,2,\ldots,L_{\max}-L_{\min}.$$

The dimension of the boundaries decreases with r. These domains and their boundaries represent again a flag of manifolds of different dimensions meeting at the manifold with lowest dimension corresponding to $r_{\max}=L_{\min}-L_{\max}$. The latter consists of k-dimensional planes in $\mathbf{C}^n$ with induced degenerate metric of signature $(k-L_{\max},L_{\min},L_{\max}-L_{\min})$ (cf., (4.20)).

The situation is illustrated by Figure 4 (see also Ref. 7). The triangle represents a lattice $\mathscr{L}$ of metrics (i,j), the first (second) letter in the bracket denoting the number of positive (negative) signs. Lattice $\mathscr{L}$ becomes partially ordered set if we introduce the ordering relation

$$(i,j)\leqslant(i',j') \;\Leftrightarrow\; i\leqslant j' \text{ and } j\leqslant j'. \tag{4.21}$$

Let us assume that the original metric F_1 is $(n-p,p)$. The sublattice $\mathscr{L}(n-p,p)$ of all admissible induced metrics consists, according to (4.17), (4.18), of all those metrics which are in relation $\leqslant$ with the original metric $(n-p,p)$

$$\mathscr{L}(n-p,p):=\{(i,j)\in\mathscr{L}\,|\,(i,j)\leqslant(n-p,p)\}. \tag{4.22}$$

Let us pick up all the admissible metrics $\mathscr{R}^k$ which lie in the k-th row (counting from below), i.e., the row corresponding to $i+j=k$ and representing the set of non-degenerate admissible metrics induced on the k-dimensional planes from the original metric in $\mathbf{C}^n$

$$\mathscr{R}^k(n-p,p):=\{(i,j)\in\mathscr{L}(n-p,p)\,|\,i+j=k\}. \tag{4.23}$$

According to (4.20), all admissible metrics (degenerate and non-degenerate) lie in the triangle

$$\mathscr{L}^k:=\{(i,j)\in\mathscr{L}(n-p,p)\,|\,(i,j)\leqslant(i',j'),i'+j'=k\Rightarrow(i',j')\in\mathscr{R}^k\}. \tag{4.24}$$

They have to be completed up to k signs by an appropriate number of zeros. The number of metrics in the triangle $L^k(n-p,p)$ is

$$N_k^{(n-p,p)}=1+2+\ldots+(L_{\max}-L_{\min}+1)=\frac{1}{2}(L_{\max}-L_{\min}+1)(L_{\max}-L_{\min}+2). \tag{4.25}$$

Accordingly, Grassman manifold $\mathscr{G}_k^n$ decomposes into $N_k^{(n-p,p)}$ regions $\mathscr{G}_{k-r,l}^{(n-p,p)}$ of different signatures of induced metric tensors and of different dimensions

$$\mathscr{G}_k^n=\bigcup_r\bigcup_l\mathscr{G}_{k-r,l}^{(n-p,p)}, \tag{4.26}$$

where the l-summation is over the intervals indicated in (4.20). Manifold $\mathscr{O}_k^{(n,m)}$ decomposes into "chimneys" given by the inverse π^{-1} of the canonical projection π of (2.19) (cf., Figure 5)

$$\pi^{-1}(\mathscr{G}_{k-s,l_s}^{(m-q,q)}\times\mathscr{G}_{k-r,l_r}^{(n-p,p)}). \tag{4.27}$$

Introducing the invariance conditions $I_l=\kappa_l$, $l=1,\ldots,k$, we obtain finally a decomposition of the $\mathrm{SU}(n-p,p)\times\mathrm{SU}(m-q,q)$ invariant submanifolds $\mathscr{O}_k^{(n,m)}$ into domains corresponding to the various induced metrics.

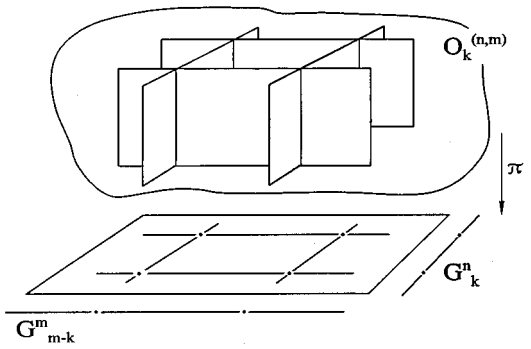

FIG. 5. Decomposition of a matrix manifold.

One may note that although the original metrics F_1 and F_2 are invariant under $\mathrm{SU}(n-p,p)\times\mathrm{SU}(m-q,q)$, the induced metrics f_1 and f_2 are not. This is due to the fact that the decomposition of the Grassman manifolds into subdomains depends upon the frame of reference.

V. THE MODEL

To construct a particle model one has to derive the structure of the space of internal parameters. The derivation is based on two plausible assumptions.

(1) The physical symmetry group is represented by the direct product $\mathrm{SU}(2,2)\times\mathrm{SU}(m)$ or its subgroup $P_4\times\mathrm{SU}(m)$. Group SU(2,2), the covering group of the conformal group, or its Poincaré subgroup P_4, represents the external symmetries, while SU(m) represents the internal symmetries, in accordance with experimental evidence. Representing the external symmetries by SU(2,2) (or one of its subgroups) provides a common geometrical basis $\mathbf{C}^{4m}$ for both internal and external symmetries in accordance with the idea to describe physical laws in complex vector spaces [3]. So far, it is not necessary to specify m; one can think, e.g., of SU(3) or $\mathrm{SU}(3)\times\mathrm{SU}(2)\times\mathrm{U}(1)$.

(2) The internal and external parameters of the particle are represented by local coordinates of an invariant homogeneous submanifold of the linear representation space $\mathbf{C}^{4m}$ of $\mathrm{SU}(2,2)\times\mathrm{SU}(m)$. This manifold has to satisfy the ''correspondence principle:'' it must admit a projection on the Minkowski space that is unique and consistent with the symmetry. We shall prove that there exists one and only one such a submanifold of $\mathbf{C}^{4m}$.

To find the manifold satisfying the above conditions we use decomposition (2.2), (2.13). For $n=4$, we have

$$\mathbf{C}^{4m}=\mathscr{O}_0^{(4,m)}\cup\mathscr{O}_1^{(4,m)}\cup\mathscr{O}_2^{(4,m)}\cup\mathscr{O}_3^{(4,m)}\cup\mathscr{O}_4^{(4,m)}$$

complemented with fiberings (2.20), (2.21). It follows immediately that the only submanifold containing $\mathscr{G}_2^4$ in the base is $\mathscr{O}_2^{(4,m)}$ with the local trivialization $\mathscr{G}_2^4\times\mathrm{GL}(2,\mathbf{C})\times\mathscr{G}_2^m$. It is well known that $\mathscr{G}_2^4$ is homeomorphic with the compactified complex Minkowski space $\mathscr{M}_4^{\mathbf{C}}$, the homeomorphism (and its inverse) being given by the relations

$$z_\mu=\frac{i\lambda}{2}\mathrm{Tr}\sigma_\mu a,\quad a=\frac{1}{i\lambda}z_\mu\tilde{\sigma}^\mu, \tag{5.1}$$

where a is a 2×2 complex matrix the entries of which are Grassman coordinates of two-dimensional hyperplanes in $\mathbf{C}^4$. According to (2.7), we have $A=aK$ and $Y=aB$. The explicit form of the Grassman coordinates is given by equations (3.12), (3.14) specified to the particular case $k=2$, $n=4$

$$a_j^1=\frac{m\begin{pmatrix}\alpha_1 & \alpha_2\\ j & 2\end{pmatrix}}{m\begin{pmatrix}\alpha_1 & \alpha 2\\ 1 & 2\end{pmatrix}},\quad a_j^2=\frac{m\begin{pmatrix}\alpha_1 & \alpha_2\\ 1 & j\end{pmatrix}}{m\begin{pmatrix}\alpha_1 & \alpha_2\\ 1 & 2\end{pmatrix}},\quad j=3,4, \tag{5.2}$$

where $\sigma_0=\mathbb{1}_2$ and σ_i, $i=1,2,3$, are Pauli matrices, $\tilde{\sigma}_i=\sigma_i$, $\tilde{\sigma}_0=-\sigma_0$. Parameter λ is a ''dimensional parameter'' with dimension of length and has to be introduced to relate the complex vector z_μ with the dimensionless ratios (5.2).

Following the remark after formula (2.10), coordinates a_j^k do not depend on the particular choice of (distinct) α_1 and α_2 from $\{1,2,\ldots,m\}$. This proves the uniqueness of the projection π_1.

To prove consistency with the group SU(2,2) (the a's do not transform with the respect to SU(m)), we have to investigate the transformation properties of the skew-symmetric forms appearing in (5.2)

$$m\begin{pmatrix}\alpha_1\alpha_2\\ a_1a_2\end{pmatrix}=m_{a_1\alpha_1}m_{a_2\alpha_2}-m_{a_1\alpha_2}m_{a_2\alpha_1}=\xi_{a_1}\eta_{a_2}-\xi_{a_2}\eta_{a_1}, \tag{5.3}$$

where $a_1,a_2=1,2,3,4$, and $\alpha_1,\alpha_2=1,2,\ldots,m$. Due to the fact that the ratios of the determinants appearing in (5.2) do not depend on particular selection of (α_1,α_2), we can drop for simplicity the second index, introducing temporarily the following notation

$$\xi_a=m_{a\alpha},\quad \eta_a=m_{a\beta},\quad a=1,2,3,4. \tag{5.4}$$

In the case of $n=4$, there are six skew-symmetric forms and they satisfy one obvious relation

$$\begin{aligned}0=\frac{1}{2}m\begin{pmatrix}\alpha_1 & \alpha_2 & \alpha_1 & \alpha_2\\ a_1 & a_2 & a_3 & a_4\end{pmatrix}&=\frac{1}{8}m\begin{pmatrix}\alpha_1 & \alpha_2\\ a_1 & a_2\end{pmatrix}\varepsilon_{a_1a_2a_3a_4}m\begin{pmatrix}\alpha_1 & \alpha_2\\ a_3 & a_4\end{pmatrix}\\ &=m\begin{pmatrix}\alpha_1 & \alpha_2\\ 1 & 2\end{pmatrix}m\begin{pmatrix}\alpha_1 & \alpha_2\\ 3 & 4\end{pmatrix}-m\begin{pmatrix}\alpha_1 & \alpha_2\\ 1 & 3\end{pmatrix}m\begin{pmatrix}\alpha_1 & \alpha_2\\ 2 & 4\end{pmatrix}\\ &=m\begin{pmatrix}\alpha_1 & \alpha_2\\ 1 & 2\end{pmatrix}m\begin{pmatrix}\alpha_1 & \alpha_2\\ 3 & 4\end{pmatrix}+m\begin{pmatrix}\alpha_1 & \alpha_2\\ 1 & 4\end{pmatrix}m\begin{pmatrix}\alpha_1 & \alpha_2\\ 2 & 3\end{pmatrix}.\end{aligned} \tag{5.5}$$

It is convenient to express these forms and the coordinates κ_μ in terms of Dirac γ-matrices. In the representation

$$\gamma_\mu=i\begin{bmatrix}0 & \sigma_\mu\\ -\tilde{\sigma}_\mu & 0\end{bmatrix},\quad \varepsilon=\begin{bmatrix}0 & 1 & 0 & 0\\ -1 & 0 & 0 & 0\\ 0 & 0 & 0 & 1\\ 0 & 0 & -1 & 0\end{bmatrix}\quad \gamma_5=\gamma_1\gamma_2\gamma_3\gamma_4,\quad \gamma_4=i\gamma_0, \tag{5.6}$$

we have the following forms

$$
\begin{aligned}
s &:= (\xi\varepsilon\eta) = m\begin{pmatrix}\alpha_1\alpha_2\\ 1\ 2\end{pmatrix} + m\begin{pmatrix}\alpha_1\alpha_2\\ 3\ 4\end{pmatrix},\\
p &:= (\xi\varepsilon\gamma_5\eta) = m\begin{pmatrix}\alpha_1\alpha_2\\ 1\ 2\end{pmatrix} - m\begin{pmatrix}\alpha_1\alpha_2\\ 3\ 4\end{pmatrix},\\
v_1 &:= (\xi\varepsilon\gamma_1\eta) = im\begin{pmatrix}\alpha_1\alpha_2\\ 1\ 3\end{pmatrix} - im\begin{pmatrix}\alpha_1\alpha_2\\ 2\ 4\end{pmatrix},\\
v_2 &:= (\xi\varepsilon\gamma_2\eta) = -m\begin{pmatrix}\alpha_1\alpha_2\\ 1\ 3\end{pmatrix} - m\begin{pmatrix}\alpha_1\alpha_2\\ 2\ 4\end{pmatrix},\\
v_3 &:= (\xi\varepsilon\gamma_3\eta) = -im\begin{pmatrix}\alpha_1\alpha_2\\ 1\ 4\end{pmatrix} - im\begin{pmatrix}\alpha_1\alpha_2\\ 2\ 3\end{pmatrix},\\
v_0 &:= (\xi\varepsilon\gamma_0\eta) = im\begin{pmatrix}\alpha_1\alpha_2\\ 1\ 4\end{pmatrix} - im\begin{pmatrix}\alpha_1\alpha_2\\ 2\ 3\end{pmatrix}.
\end{aligned}
\tag{5.7}
$$

Coordinates z_μ of the complex Minkowski space (see (5.1)) obtain a simple form

$$z_\mu = \lambda\frac{v_\mu}{s+p}. \tag{5.8}$$

Relation (5.5) now takes the form

$$s^2 - p^2 - v_\mu v^\mu = 0. \tag{5.9}$$

Recall that representation (5.6) is adapted to the neighborhood $m\left(\begin{smallmatrix}\alpha_1\alpha_2\\ 1\ 2\end{smallmatrix}\right) = \frac{1}{2}(s+p) \neq 0$ and in other neighborhoods, other representations must be used. Nevertheless, formulae (5.8) and (5.9) are independent of the representation. This becomes clear when one considers transformation properties with respect to the group SU(2,2). Let us consider an arbitrary representation of γ-matrices satisfying

$$
\begin{gathered}
\gamma_\mu\gamma_\nu + \gamma_\nu\gamma_\mu = 2g_{\mu\nu}, \quad \gamma_\mu^+ = \gamma_\mu,\\
\gamma_4 = i\gamma_0, \quad \gamma_5 = \gamma_1\gamma_2\gamma_3\gamma_4
\end{gathered}
\tag{5.10}
$$

(μ,ν=1,2,3,4) together with a skew-symmetric matrix ε satisfying

$$\varepsilon^T = -\varepsilon, \quad \varepsilon^2 = -1, \quad (\varepsilon\gamma_\mu)^T = -\varepsilon\gamma_\mu. \tag{5.11}$$

The infinitesimal generators of SU(2,2) in $\mathbf{C}^4$ can be rewritten in terms of the 4×4 matrices (5.10), as

$$d = \frac{-i}{2}\gamma_5, \quad p_\mu = i\lambda^{-1}\gamma_-\gamma_\mu, \quad k_\mu = -i\lambda\gamma_+\gamma_\mu, \quad m_{\nu\mu} = \frac{i}{4}[\gamma_\mu,\gamma_\nu], \quad \gamma_\pm = \frac{1}{2}(1\pm\gamma_5). \tag{5.12}$$

It is easy to check that these generators satisfy the well known commutation relations of the Lie algebra of SU(2,2)

$$
\begin{gathered}
[d,p_\mu]=ip_\mu, \quad [d,k_\mu]=-ik_\mu, \quad [d,m_{\mu\nu}]=0,\\
[p_\mu,p_\nu]=[k_\mu,k_\nu]=0, \quad [k_\mu,p_\nu]=2ig_{\mu\nu}d-2im_{\mu\nu},\\
[m_{\mu\nu},p_\lambda]=-ig_{\mu\lambda}p_\nu+ig_{\nu\lambda}p_\mu,\\
[m_{\mu\nu},k_\lambda]=-ig_{\mu\lambda}k_\nu+ig_{\nu\lambda}k_\mu,\\
[m_{\mu\nu},m_{\rho\lambda}]=i\{g_{\nu\rho}m_{\mu\lambda}+g_{\mu\lambda}m_{\nu\rho}-g_{\mu\rho}m_{\nu\lambda}-g_{\nu\lambda}m_{\mu\rho}\}.
\end{gathered}
\tag{5.13}
$$

Let us consider six forms

$$
s=(\xi\varepsilon\gamma_5\eta), \quad p=(\xi\varepsilon\gamma_5\eta), \quad v_\mu=(\xi\varepsilon\gamma_\mu\eta),
$$

with some factors $\xi,\eta\in\mathbf{C}^4$, prevailing the arbitrariness of representation of the γ's. The action of the generators (5.12) in $\mathbf{C}^4$ induces the following action of these generators on the bilinear asymmetric forms (5.12):

$$
\begin{array}{ccc}
ds=ip & dp=is & dv_\mu=0\\
p_\mu s=i\lambda^{-1}v_\mu & p_\mu p=i\lambda^{-1}v_\mu & p_\mu v_\lambda=i\lambda^{-1}g_{\mu\lambda}(s+p)\\
k_\mu s=i\lambda v_\mu & k_\mu p=i\lambda v_\mu & k_\mu v_\lambda=i\lambda^{-1}g_{\mu\lambda}(s-p)\\
m_{\mu\nu}s=0 & m_{\mu\nu}p=0 & m_{\mu\nu}v_\lambda=-ig_{\mu\lambda}v_\nu+ig_{\nu\lambda}v_\mu.
\end{array}
\tag{5.14}
$$

These transformation properties imply that a vector transforming properly under rotations must necessarily be of the following form

$$
z_\mu=f(s,p)v_\mu,
$$

where $f(s,p)$ is a function of scalar s and pseudoscalar p. This function can be determined by a further demand that the quantities z_μ transform properly under translations:

$$
z_\mu\to z'_\mu=z_\mu+a_\mu=(\mathbb{1}+ia^\nu p_\nu)z_\mu \;\Leftrightarrow\; p_\nu z_\mu=-ig_{\mu\nu}.
$$

Applying p_μ to $z_\mu=f(s,p)v_\mu$ we find that

$$
p_\mu z_\nu=i\lambda^{-1}\left(\frac{\partial f}{\partial p}-\frac{\partial f}{\partial s}\right)v_\mu v_\nu-\lambda^{-1}g_{\mu\nu}f(s,p)(s+p)=-ig_{\mu\nu}
$$

is satisfied only if

$$
\frac{\partial f}{\partial p}=\frac{\partial f}{\partial s}, \quad f(s,p)=\frac{\lambda}{s+p}.
$$

Notice that only translations and rotations are necessary to determine the form (5.8) in an arbitrary representation (5.10), (5.11) of the γ-matrices. The behavior with respect dilations and special conformal transformations follows as a consequence of (5.8). The complete set of infinitesimal transformations of z_μ under the full conformal group is

$$
dz_\mu=-iz_\mu, \quad p_\mu z_\lambda=-ig_{\mu\lambda}, \quad k_\mu z_\lambda=+ig_{\mu\lambda}z_\nu z^\nu-2iz_\mu z_\lambda, \quad m_{\mu\nu}z_\lambda=-ig_{\mu\lambda}z_\nu+ig_{\nu\lambda}z_\mu.
\tag{5.15}
$$

Thus, dilation d and rotations $m_{\mu\nu}$ are linear transformations, and, therefore, they act in the same way on the real and on the imaginary parts of the complex vector $z_\mu = x_\mu + iy_\mu$. Special conformal transformations are non-linear and, therefore, they mix x_μ and y_μ according to

$$\begin{aligned} k_\mu x_\lambda &= ig_{\mu\lambda}(x_\nu x^\nu - y_\nu y^\nu) - 2i(x_\mu x_\lambda - y_\mu y_\lambda), \\ k_\mu y_\lambda &= 2ig_{\mu\lambda} x_\nu y^\nu - 2i(x_\mu y_\lambda + y_\mu x_\lambda), \end{aligned} \tag{5.16}$$

Action of translations is also non-linear and (5.15) implies that the real part x_μ transforms like a vector $p_\mu x_\lambda = -ig_{\mu\lambda}$ whereas the imaginary part is translation invariant $p_\mu y_\lambda = 0$.

Transformation properties (5.15) prove that the condition of consistency of the projection (5.8) with the group is satisfied for the complex vector $z_\mu = x_\mu + iy_\mu$. The real and imaginary parts of $z_\mu = x_\mu + iy_\mu$ transform like vectors with respect to rotations and dilations. The fact that y_μ is invariant under translations, and x_μ transforms like a vector, suggests the interpretation of x_μ as the local coordinates of the center of mass and of y_μ as relative coordinates (coordinate differences) with respect to the center of mass. This interpretation corresponds to Yukawa's idea of bilocal theory.[10,11]

Relation (5.9) between the forms (5.7) provides a simple geometrical interpretation of the projection (5.8). Dividing (5.8) and (5.9) by s in the neighborhood $s \neq 0$ we obtain

$$z_\mu = \lambda \frac{v_\mu / s}{1 + p/s}, \quad \frac{v_\mu}{s} \cdot \frac{v^\mu}{s} + \frac{p^2}{s^2} = 1. \tag{5.17}$$

This suggests that formula (5.8) can be viewed as a complex stereographic projection of the complex hyperboloid (5.9) on the complex Minkowski space. SU(2,2)-transformations of the variables $\xi, \eta \in \mathbf{C}^4$ induce pseudoorthogonal $O(4,2)$-transformations of the bilinear skew-symmetric forms s, p, and v_μ (5.7). The last induce conformal transformations of the complex Minkowski coordinates z_μ by the intermediary of the complex stereographic projection of the complex hyperboloid (5.17) in the complex projective space $\mathbf{C}P^5$ with local coordinates p/s, v_μ/s, $\mu = 0,1,2,3$, onto the complex Minkowski space.

Let us go over now to the calculation of invariants of the theory. According to (4.13–14), we have to calculate invariants I_l for the particular metric tensors of SU(2,2) and SU(m) in $\mathbf{C}^{4m}$ and for the particular manifold $\mathcal{O}_2^{4m}$, i.e., for $k=2$, $l=1,2$. We shall use a mixed coordinate system consisting of the elements of the matrices K, a, B. Introducing the $2 \times m$ matrix

$$C = (K|B) = \{m_{a\alpha}\}_{\alpha = 1, \ldots, m}^{a = 1,2} \tag{5.18}$$

we can write

$$I_l = \mathrm{Tr}(F_2 C^* f_1 C)^l, \quad l = 1,2. \tag{5.19}$$

The metric for the group SU(m) is $F_2 = \mathbb{1}_m$. The invariant form of the group SU(2,2) is $(\xi^*, \gamma_4 \eta)$, as one can easily check by applying the generators (5.12) (note that $X_k(\xi\gamma\eta)^* = -(X_k(\xi\gamma\eta)^*)$. In representation (5.6) we have

$$F_1 = \gamma_4 = -\begin{bmatrix} 0 & \mathbb{1}_2 \\ \mathbb{1}_2 & 0 \end{bmatrix} \tag{5.20}$$

and the invariants take, on $\mathcal{O}_2^{4m}$, the form

$$I_l = \mathrm{Tr}(f_1 C C^*)^l, \quad l = 1,2, \tag{5.21}$$

where

$$f_1 = a^* F_1 a = -(a^* + a). \tag{5.22}$$

Note that the right hand side of (5.22) the original (2.8) (and not the extended) matrix a appears. With the help of homeomorphism (5.1) we can express the complex matrix a through the complex vector z_μ

$$-f_1 = a^* + a = -\frac{1}{i\lambda}\tilde{\sigma}^\mu(z_\mu^* - z_\mu) = \frac{2}{\lambda} y_\mu \tilde{\sigma}^\mu \tag{5.23}$$

and obtain

$$I_1 = -\frac{2}{\lambda} y_\mu \mathrm{Tr}\tilde{\sigma}^\mu CC^*,$$

$$I_2 = \frac{4}{\lambda^2} y_\mu y_\nu \mathrm{Tr}\tilde{\sigma}^\mu CC^* \tilde{\sigma}^\nu CC^*. \tag{5.24}$$

We denote

$$r_\mu = -\mathrm{Tr}\tilde{\sigma}^\mu CC^* = -\sum_{a=1}^{2}\sum_{\alpha=1}^{m} m_{\alpha a}^* (\tilde{\sigma}_\mu)^{\dot{a}b} m_b . \tag{5.25}$$

One can show that

$$\mathrm{Tr}\tilde{\sigma}_\mu CC^* \tilde{\sigma}_\nu CC^* = \sum_{a,b,c,d=1}^{2}\sum_{\alpha,\beta=1}^{m} m_{\alpha a}^* \tilde{\sigma}_\mu^{\dot{a}b} m_{b\beta} m_{\beta c}^* \tilde{\sigma}_\nu^{\dot{c}d} m_{d\alpha} = -\frac{1}{2} g_{\mu\nu} r_\lambda r^\lambda + r_\mu r_\nu . \tag{5.26}$$

Therefore the two invariants are in this case

$$I_1 = \frac{2}{\lambda} y_\mu r^\mu, \quad I_2 = \frac{4}{\lambda^2}\left\{ -\frac{1}{2} y_\mu y^\mu r_\nu r^\nu + (y_\mu r^\mu)^2 \right\}. \tag{5.27}$$

Instead of the invariants I_1 and I_2 we can use, equivalently, the invariants $y \cdot r = y_\mu r^\mu$, and $|y|^2 \cdot |r|^2 = y_\mu y^\mu r_\nu r^\nu$ and describe the decomposition of $\mathscr{C}^2_{(4,m)}$ into a two-parametric family of submanifolds by the two SU(2,2)$\times$SU(m)-invariant equations

$$y_\mu r^\mu = -c_{12}, \quad y_\mu y^\mu r_\nu r^\nu = c_1, \tag{5.28}$$

with some constants c_1 and c_{12}. We already know the transformation properties or y_μ with respect to SU(2,2) (cf., (5.15–16)). From these transformation properties it follows that $y_\mu y^\mu$ is Poincaré invariant. Let us now derive the transformation properties of r_μ. For this purpose we rewrite r_μ in terms of the γ-matrices in representation (5.6). According to definition (5.25) and notation (5.4), we have

$$r_\mu = -\sum_{a,b=1}^{2}\sum_{\alpha=1}^{m} m_{\alpha a}^* (\tilde{\sigma}_\mu)^{\dot{a}b} m_{b\alpha} = i(\xi^* \gamma_4 \gamma_\mu \gamma_+ \xi). \tag{5.29}$$

Applying now the infinitesimal SU(2,2) generators (5.12), we obtain

$$\begin{gathered} dr_\mu = i r_\mu, \quad p_\mu r_\lambda = 0, \quad m_{\mu\nu} r_\lambda = -i g_{\mu\lambda} r_\nu + i g_{\nu\lambda} r_\mu , \\ k_\mu r_\lambda = 2i\{ g_{\mu\lambda} r_\nu x^\nu + x_\mu r_\lambda - r_\mu x_\lambda - \varepsilon_{\mu\lambda\rho\nu} r^\rho y^\nu \}. \end{gathered} \tag{5.30}$$

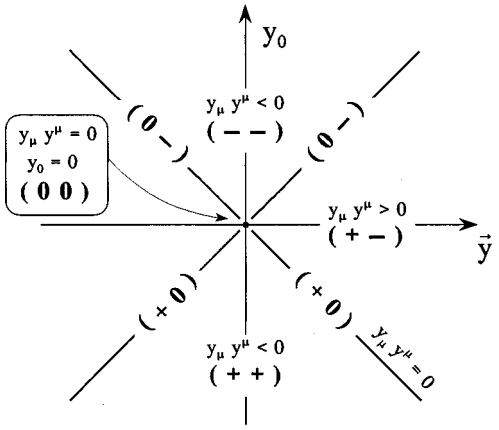

FIG. 6. Six label regions corresponding to six types of induced metric structure.

It follows that

$$p_\mu r_\lambda r^\lambda = m_{\mu\nu} r_\lambda r^\lambda = 0 \tag{5.31}$$

in accordance with (5.2).

Further reduction of the SU(2,2) symmetry to Poincaré symmetry causes appearance of another invariant, namely the Poincaré invariant $r_\lambda r^\lambda$. Consequently, there is a further decomposition of $\mathscr{O}^2_{(4,m)}$ into a three parameter family of submanifolds $\mathscr{O}^{2c}_{(4,m)}$ described by the equations

$$y_\mu y^\mu + c_{11} = y_\mu r^\mu + c_{12} = r_\mu r^\mu + c_{22} = 0. \tag{5.32}$$

Let us consider finally the decomposition of the Grassman manifold $\mathscr{G}^4_2$ into subdomains corresponding to different induced metrics. According to (4.18), the induced signatures are determined by the roots of the secular equation (4.15). In our case (cf., (5.20), (5.23))

$$f_1 = -\frac{2}{\lambda} y_\mu \tilde{\sigma}^\mu,$$

$$\lambda_{1,2} = \frac{1}{2}\mathrm{Tr} f_1 \pm \sqrt{\left(\frac{1}{2}\mathrm{Tr}\, f_1\right)^2 - \det f_1}, \tag{5.33}$$

$$\det f_1 = -\frac{4}{\lambda^2} y_\mu y^\mu, \quad \mathrm{Tr}\, f_1 = -\frac{4}{\lambda} y_0 .$$

According to the general scheme (4.20) and Figure 4, we have the following six domains corresponding to the six admissible metric types $(++)$, $(+-)$, $(--)$, $(+0)$, $(0-)$, (00) (see Figure 6):

$$\begin{array}{lllll}(++) & y_0<0 & y_\mu y^\mu<0 & \lambda_1>0 & \lambda_2>0,\\ (+\,0) & y_0<0 & y_\mu y^\mu=0 & \lambda_1=0 & \lambda_2>0,\\ (+-) & & y_\mu y^\mu>0 & \lambda_1<0 & \lambda_2>0,\\ (0-) & y_0>0 & y_\mu y^\mu=0 & \lambda_1<0 & \lambda_2=0,\\ (--) & y_0>0 & y_\mu y^\mu<0 & \lambda_1<0 & \lambda_2<0,\\ (0\,0) & y_0=0 & y_\mu y^\mu=0 & \lambda_1=0 & \lambda_2=0.\end{array} \tag{5.34}$$

VI. INTERNAL STRUCTURE

We have, so far determined the decomposition of $\mathscr{O}^2_{(4,m)}$ into $\mathrm{SU}(2,2)\times\mathrm{SU}(m)$ and $P_4\times\mathrm{SU}(m)$ invariant submanifolds $\mathscr{O}^{2C}_{(4,m)}$. To give a common description of both cases, we introduce the shorthand notation

$$c_{11}=-y_\mu y^\mu,\quad c_{12}=-y_\mu r^\mu,\quad c_{22}=-r_\mu r^\mu, \tag{6.1}$$

corresponding to condition (5.28), (5.32). In the conformally invariant case only c_{12} and $c_1=c_{11}c_{22}$ can be considered as constants. In the Poincaré-invariant case, all three quantities c_{11}, c_{12}, c_{22} can be considered as constants. Rewriting the second equation of (6.1) in the form

$$y_0=r_0^{-1}(\vec{y}\vec{r}+c_{12}) \tag{6.2}$$

and substituting it into the first, we obtain a second order equation for the coordinates y_1,y_2,y_3, of the vector $\vec{y}$ with coefficients depending on r_μ, $\mu=0,1,2,3$, and the constants c_{12}, c_1:

$$\vec{y}^2-\frac{(\vec{r}\vec{y}+c_{12})^2}{r_0^2}=\frac{c_1}{r_\mu r^\mu}. \tag{6.3}$$

By a proper transformation of the coordinates we can bring this equation into diagonal form

$$(y_1')^2+(y_2')^2+\frac{c_{22}}{r_0^2}(y_3')^2=-\frac{\det c}{c_{22}}, \tag{6.4}$$

which represents various types of second order surfaces in three dimensional space depending on the values of the coefficients appearing in (6.4).

To get better insight to the situation, we calculate the quantity $c_{22}=-r_\mu r^\mu$ in terms of the variables $m_{a\alpha}$, $a=1,2$, $\alpha=1,..,m$, (cf., (5.25)). The result is

$$c_{22}=-r_\mu r^\mu=2\sum_{\alpha_1,\alpha_2=1}^{m}\left|m\begin{pmatrix}\alpha_1 & \alpha_2\\ 1 & 2\end{pmatrix}\right|^2. \tag{6.5}$$

In the case of $\mathrm{SU}(m)$ internal symmetry ($q=0$), c_{22} is always positive. The value $c_{22}=0$ is excluded on $\mathscr{O}_2^{(4,m)}$ in domains $m\binom{\alpha_1\alpha_2}{1\ 2}\neq 0$ which we consider. Also

$$r_0=\sum_{a=1}^{2}\sum_{\alpha=1}^{m}|m_{a\alpha}|^2>0$$

is strictly positive. Due to these facts, the quadratic form (6.4) is positive definite and the condition that the surface is real is

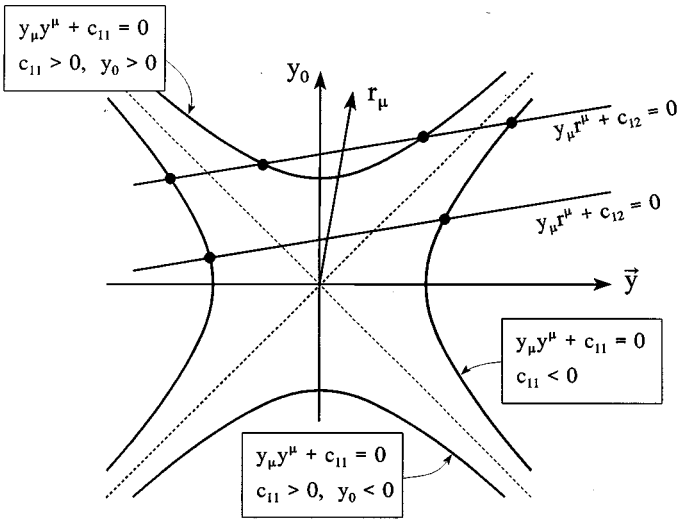

FIG. 7. Different values of the invariant **c**.

$$\det c = c_{11}c_{22} - c_{12}^2 = c_1 - c_{12}^2 < 2. \tag{6.6}$$

Otherwise we have to do with disjoint surfaces in the space of variables y_μ, $\mu = 0,1,2,3$ (see Figure 7). Let us note that $\det c$ is always negative when y_μ is space-like ($c_{11} < 0$).

We can solve equations (5.28), (5.32) with respect to $y = \sqrt{y_1^2 + y_2^2 + y_3^2}$ or $r = \sqrt{r_1^2 + r_2^2 + r_3^2}$ by eliminating y_0 or r_0 from the equations (cf., (6.1))

$$y^2 - y_0^2 + c_{11} = yr\ \cos\theta - y_0 r_0 + c_{12} = r^2 - r_0^2 + c_{22}. \tag{6.7}$$

The result is

$$y = \frac{c_{12} r\ \cos\theta \pm r_0 \sqrt{-\det c - c_{11} r^2\ \sin^2\theta}}{c_{22} + r^2 \sin^2\theta},$$

$$r = \frac{c_{12} y\ \cos\theta \pm y_0 \sqrt{-\det c - c_{22} y^2\ \sin^2\theta}}{c_{11} + y^2\ \sin^2\theta}, \tag{6.8}$$

with the reality conditions for the roots

$$\det c + c_{11} r^2 \sin^2\theta < 0 \quad \text{or} \quad \det c + c_{22} y^2 \sin^2\theta < 0. \tag{6.9}$$

The situation is particularly simple for the vector $r_i = 0$, $r_0 = \sqrt{c_{22}}$. In this case (cf., Eqs. (6.4), (6.8))

$$y = \sqrt{-\frac{\det c}{c_{22}}}$$

is an equation of a sphere S^2 with radius $\sqrt{-\det c / c_{22}}$. It is important to have also a coordinate free description of the spaces determined by the conditions (5.28) or (5.32) together with equations (5.25), (5.29). Here, we shall restrict ourselves to the Poincaré invariance. In this case one can

show that the submanifolds $\mathcal{O}_{2,c}^{(4,m)}$ are direct products of a real Minkowski space M_4 and a homogeneous space M^{int} of the group $\mathrm{SU}(3,1)\times\mathrm{SU}(m)$. To convince ourselves of this fact, we consider a point with coordinates $\mathring{m}_{a\alpha}$, $\mathring{y}_\mu$ satisfying the conditions

$$\mathring{y}_1=\mathring{y}_2=0, \quad \mathring{m}_{1\alpha}=0, \quad \mathring{m}_{2\alpha'}=0 \tag{6.10}$$

for $\alpha=2,3,\ldots,m$ and $\alpha'=3,4,\ldots,m$, and

$$\begin{gathered}\mathring{r}_i=-\mathring{m}^*_{\alpha a}(\tilde{\sigma}_i)^{\dot{a}b}\mathring{m}^*_{b\alpha}=0, \quad \mathring{r}_0=-\mathring{m}^*_{\alpha a}(\tilde{\sigma}_0)^{\dot{a}b}\mathring{m}^*_{b\alpha}=\sqrt{c_{22}},\\ (\mathring{y}_3)^2-(\mathring{y}_0)^2=-c_{11}, \quad \mathring{y}_0\mathring{r}_0=c_{12}, \quad \det c<0.\end{gathered} \tag{6.11}$$

This point satisfies conditions (5.32) and the isotropy group of this point is $\mathrm{SO}(2)\times\mathrm{SU}(m-2)$. Moreover, every point satisfying (5.32) can be reached from the point (6.10) by a transformation of $\mathrm{SO}(3,1)\times\mathrm{SU}(m)$. We can write therefore, globally,

$$\mathcal{O}_{2,c}^{(4,m)}=\frac{P_4}{\mathrm{SO}(3,1)}\times\frac{\mathrm{SO}(3,1)\times\mathrm{SU}(m)}{\mathrm{SO}(2)\times\mathrm{SU}(m-2)}, \tag{6.12}$$

where c denotes the three real parameters c_{ik} satisfying $\det c<0$. The first quotient $M_4=P_4/\mathrm{SO}(3,1)$ represents the real Minkowski space M_4 parameterized by coordinates $x_\mu=Re z_\mu$. This space is not affected by the invariance conditions (5.32) and it transforms into itself under dilations d, translations p_μ, and rotations $m_{\mu\nu}$. The internal space

$$M^{\text{int}}=\frac{\mathrm{SO}(3,1)\times\mathrm{SU}(m)}{\mathrm{SO}(2)\times\mathrm{SU}(m-2)} \tag{6.13}$$

can be viewed as the direct product of five-dimensional outer internal space $\mathrm{SO}(3,1)/\mathrm{SO}(2)$ parameterized by coordinates y_μ, r_μ subject to conditions (5.32) which does not depend on m and is invariant with respect to $\mathrm{SU}(m)$ and the inner internal space $\mathrm{SU}(m)/\mathrm{SU}(m-2)$. Both spaces are translation invariant.

In the case of the larger SU(2,2)-symmetry, the situation is more complicated due to the fact that special conformal transformations mix the variables x_μ, y_μ, r_μ (cf., e.g., (5.16)). The domains described by the admissible metrics $(++)$, $(+-)$, $(--)$ correspond to $c_{11}\neq 0$. The degenerate metrics $(+\,0)$, $(0\,-)$, and $(0\,0)$ correspond to $c_{11}=0$. The last one involves the additional condition $y_0=0$ so that the internal space reduces to one point.

One can give also a local geometrical interpretation of the internal space M^{int}. Indeed, $\mathrm{SO}(3,1)\times\mathrm{SO}(2)$ can be considered locally as the direct product of a three-dimensional hyperboloid H^3 and a two-dimensional sphere S^2. Vector r_μ moves on H^3 while y_μ moves on a 2-dimensional ellipsoid (see Figure 7). Similarly, vectors $m_{1\alpha}$ and $m_{2\alpha}$, $\alpha=1,\ldots,m$, move on a $(2m-1)$-dimensional sphere and on a sphere with two dimensions less, i.e. on S^{2m-3}, respectively (the second vector is additionally restricted by the length and the scalar product). We can consider, therefore, M^{int} locally as the direct product

$$M^{\text{int}}=S^2\times H^3\times S^{2m-1}\times S^{2m-3}. \tag{6.14}$$

Thus, the internal space in this $P_4\times\mathrm{SU}(m)$ invariant particle model is not compact due to the appearance of the homogeneous manifold $\mathrm{SO}(3,1)/\mathrm{SO}(2)$ in (6.13) or the hyperboloid H^3 in (6.14). The other factors $\mathrm{SU}(m)\times\mathrm{SU}(m-2)$ in (6.13), or $S^2\times S^{2m-1}\times S^{2m-3}$ in (6.14), are compact. Moreover, there is one factor which is independent on the number m and which has, therefore, a universal meaning.

For full physical interpretation, it remains to find the representations $\mathrm{SU}(2,2)\times\mathrm{SU}(m)$ and $P_4\times\mathrm{SU}(m)$ in the corresponding homogeneous spaces. We shall present the results in a separate publication.

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Planar coincidences for *N*-fold symmetry

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The coincidence problem for planar patterns with N-fold symmetry is considered. For the N-fold symmetric module with $N<46$, all isometries of the plane are classified that result in coincidences of finite index. This is done by reformulating the problem in terms of algebraic number fields and using prime factorization. The more complicated case $N\geqslant 46$ is briefly discussed and $N=46$ is described explicitly. The results of the coincidence problem also solve the problem of colour lattices in two dimensions and its natural generalization to colour modules. © *1996 American Institute of Physics.* [S0022-2488(95)01710-7]

I. INTRODUCTION

The concept of coincidence site lattices (CSLs) arises in the crystallography of grain and twin boundaries.[1] Different domains of a crystal do have a relationship: There is a sublattice common to both domains across a boundary, and this is the CSL. This can be seen as the intersection of a perfect lattice with a rotated copy of it where the set of points common to both forms a sublattice of finite index, the CSL. Up to now, CSLs have been investigated only for special cases, for example, for cubic or hexagonal crystals.[2] With the advent of quasicrystals infinitely many new cases arise: quasicrystals also have grain boundaries, and one should know the coincidence site quasilattices.[3,4] In a rather different context, multiple coincidences of families of one-dimensional (1D) quasicrystals have been applied in constructing quasicrystals with arbitrary symmetry (in higher dimensions).[5,6] An application of these results was made by Rivier and Lawrence[7] to crystalline grain boundaries, which themselves turn out to be quasicrystalline. This is an important example of the relevance of a coincidence quasilattice. The experimental evidence was provided indirectly by Sass, Tan and Balluffi in the 1970s,[8] but beautifully by the observations of growth of quasicrystalline grain at the grain boundary between two crystals by Cassada, Shiflet and Poon[9] and by Sidhom and Portier.[10] Gratias and Thalal,[11] on the other hand, used quasicrystal concepts in a different context to embed the two crystal grains adjacent to a grain boundary in a higher dimensional perfect lattice. So an extension of the CSL analysis to all discrete structures is desirable.

In this paper we give a unified treatment of the coincidence problem for planar structures with general N-fold rotation symmetry, extending previous[3,13] and parallel[12] work and putting it in a more general setting. This is what is needed for quasicrystalline T-phases that are quasiperiodic in a plane and periodically stacked in the third dimension. Icosahedral symmetry in 3D requires different methods and will be described separately.[14] Common to both is the necessity of an attack in two stages: not only do we have to find the coincidence isometries (the universal part of the problem), but also the specific modifications of the atomic surfaces (also called windows or acceptance domains) that are needed to describe the set of coinciding points.

In order to describe this scenario, we start with the coincidence problem of the square lattice $\mathbb{Z}^2$. The set of coincidence transformations for $\mathbb{Z}^2$ forms a group, the generators of which can be

given explicitly through their connection with Gaussian integers. Simultaneously, the so-called Σ-factor or coincidence index can be calculated for an arbitrary CSL isometry. Though this is not new, the approach we use here can be generalized to quasiperiodic planar patterns with N-fold symmetry. The description of this more general case and the tools necessary to tackle it is the main aim of this paper.

In two dimensions the classification of CSLs is the same as the classification of colour lattices with rotational symmetry (Ref. 15, Section 5.8). In that setting the Σ-factor or coincidence index is the number of colours and the different coloured sublattices are the different cosets of the CSL in the original lattice. This is because, as long as the symmetry group consists of 2D rotations, all members of the symmetry group commute with the CSL rotation, thus ensuring that the CSL is invariant under the symmetry group. For indecomposable groups in higher dimensions no non-trivial orthogonal transformation commutes with all symmetries so there is no longer this equivalence. The only non-trivial rotation groups of 2D lattices are C_3, C_4 and C_6. The prime numbers p for which there exist p-colour lattices with these symmetries are listed in Ref. 15, p. 76, and coincide with the sets of primes in the denominators of the Dirichlet series given at the end of Section IV for the cases $n=3$ and $n=4$. (Note that $N=2n$ for n odd and $N=n$ otherwise as will be explained later.) For non-lattices the solution of the CSL problem in 2D can be regarded as a classification of colour modules in the plane. An *r-colour n-module* is a pair of n-modules $(\mathscr{M},\mathscr{M}_1)$ such that $\mathscr{M}_1$ has index r in $\mathscr{M}$ and is invariant under the symmetry group of $\mathscr{M}$, but no other coset of $\mathscr{M}_1$ is (see Section III for a definition of n-modules). The colour of a point in $\mathscr{M}$ is then determined by its coset mod $\mathscr{M}_1$. In this light, the results of Sections III and VI can be interpreted as finding, for each n, the numbers r for which there are r-colour n-modules and what these n-modules are.

The paper is organized as follows. In Section II, we review the coincidence problem for the square lattice and formulate it in terms of Gaussian integers. This enables us to describe the group structure and the coincidence indices explicitly and to introduce the concepts needed for the generalization in Section III. There, the main structure is derived with the aid of the algebraic number theory of cyclotomic fields, followed by various worked out cases in Section IV. They include 8-, 10- and 12-fold symmetry, the most important cases for quasicrystalline T-phases, and thus cover all cases linked to quadratic irrationalities.[16] In Section V we then show, in an illustrative way, how to use the method for the eightfold symmetric Ammann–Beenker rhombus pattern and the tenfold symmetric Tübingen triangle tiling. We give an explicit formula for the necessary correction of the coincidence index. In Section VI we discuss certain details to be dealt with for $N\geqslant 46$, where the variety of modules rapidly increases though this does not affect the generality of our findings. The case $N=46$ ($n=23$) is presented in some detail. This is followed by some concluding remarks, while the two appendices cover further examples (Appendix A) and proofs of technical results used in Sections III and IV (Appendix B).

II. THE SQUARE LATTICE: A WARM-UP EXERCISE

Let us consider the CSL problem for the square lattice $\mathbb{Z}^2$. We focus on pure rotations first and deal with the easy extension to reflections later. Consider therefore a rotation [i.e., an element of the group $SO(2)=SO(2,\mathbb{R})$] and ask for the condition that it maps some lattice point to another one. Clearly, rotations through multiples of $\pi/2$ do this. They form the cyclic group C_4—an index 2 subgroup of D_4, the point group of $\mathbb{Z}^2$.

But there are more cases, as can already be seen from the growing number of lattice points on expanding circles, summarized in the coefficients of the theta-function of the lattice, cf. Ref. 17,

$$\Theta_{\mathbb{Z}^2}(x)=\sum_{q\in\mathbb{Z}^2} x^{|q|^2}=(\vartheta_3(x))^2=1+\sum_{M=1}^{\infty} r(M)x^M=1+4x+4x^2+4x^4+8x^5+\ldots\ . \qquad (1)$$

Here, $\vartheta_3(x)=\Sigma_{q\in\mathbb{Z}}x^{|q|^2}=1+2x+2x^4+2x^9+\ldots$ is Jacobi's theta-function and $r(M)$ denotes the number of integral solutions of the equation $a^2+b^2=M$, see Ref. 18 for details on $r(M)$. This number is only slowly increasing but is unbounded, so there is an infinite number of rotations that map one lattice point to another.

As is obvious (cf. Ref. 19 and references therein), the set of coincidence rotations (or CSL rotations) consists of all rotations R through angles φ with $\sin(\varphi)=a/m$ and $\cos(\varphi)=b/m$ rational, and hence is identical with the group $SO(2,\mathbb{Q})$. This requires integral solutions of the Diophantine equation

$$a^2+b^2=m^2, \tag{2}$$

where we need consider only the *primitive* solutions, i.e., $\gcd(a,b)=1$. They are, of course, given by the primitive Pythagorean triples.[18] For a primitive solution, the set of coinciding points forms a sublattice of $\mathbb{Z}^2$ of index m, whence $1/m$ is the fraction of lattice points coinciding. We call m the *coincidence index* of R, denoted by $\Sigma_{\mathbb{Z}^2}(R)$, or $\Sigma(R)$ for short. This index is often called the Σ-factor.[2,3,4]

A. The number of CSL rotations with given index

Without determining the rotations explicitly we can calculate their possible indices and the number of different rotations with each index as follows.

The number of *primitive* solutions of Eq. (2) can be derived from the well-known formula (cf. Ref. 18)

$$r(M)=4(d_1(M)-d_3(M)), \tag{3}$$

[where $d_k(M)$ counts the number of divisors of M of the form $4l+k$] for the total number of integer solutions of

$$a^2+b^2=M. \tag{4}$$

If we write $M=2^z M_1 M_3$, where M_1 and M_3 are maximal divisors of M composed of primes congruent to 1 or 3 (mod 4), respectively, then Eq. (3) can be equivalently expressed as

$$r(M)=\begin{cases}4d(M_1), & \text{if } M_3 \text{ is a square,}\\ 0, & \text{otherwise,}\end{cases} \tag{5}$$

where $d(M_1)$ counts *all* the divisors of M_1. When (as in our case) M is a square, the first alternative in Eq. (5) occurs. The number of primitive solutions, $r^*(m^2)$, of Eq. (2) can now be derived from the "input-output" principle (cf. Ref. 18, Thm 260) as

$$r^*(m^2)=r(m^2)-\sum_p r\left(\left(\frac{m}{p}\right)^2\right)+\sum_{p,p'} r\left(\left(\frac{m}{pp'}\right)^2\right)-\sum_{p,p',p''} r\left(\left(\frac{m}{pp'p''}\right)^2\right)+\cdots, \tag{6}$$

where p runs through all prime factors of m, pp' through all pairs of distinct prime factors of m, and so on. After substituting Eq. (5) on the right hand side of Eq. (6) and then counting the contributions of the factors of m one at a time, it can be seen that

$$r^*(m^2)=\begin{cases}4d^*(m), & \text{if } m \text{ has prime factors } \equiv 1(4) \text{ only,}\\ 0, & \text{otherwise,}\end{cases} \tag{7}$$

where $d^*(m)$ counts the square-free divisors of m. We note that the number of CSLs (as distinct from CSL rotations) of index m in the square lattice is a quarter this number, since each is itself a square lattice stabilized by the rotation group of the square (of order 4). (Note however that not every sublattice with square symmetry is a CSL.)

So far we have the following

Theorem 1: *The coincidence indices of the square lattice are precisely the numbers m with prime factors* $\equiv 1 \pmod 4$ *only. The number of coincidence rotations* $\hat{f}(m)$ *with a given index m is*

$$\hat{f}(m) = 4d^*(m), \tag{8}$$

and the number of CSLs with index m is

$$f(m) = d^*(m). \tag{9}$$

B. CSL rotations and Gaussian integers

We have settled the question of what numbers occur as coincidence indices of CSL rotations of $\mathbb{Z}^2$ and how many rotations there are with each index, but there is still more to be said.

We have seen that the set of CSL rotations forms a group [$SO(2,\mathbb{Q})$, in fact]. Let us introduce the notation

$$SOC(\mathbb{Z}^2) := \{R \in SO(2) \mid \Sigma(R) < \infty\} \tag{10}$$

for it. We shall investigate its structure and derive independent generators.

The most transparent proof of Eq. (3) (that given in Ref. 18) depends on factorization in the ring of Gaussian integers. By making direct use of this idea, we not only find independent generators for $SOC(\mathbb{Z}^2)$ but also have a method that readily generalizes to other lattices and modules.

To this end, we consider the lattice $\mathbb{Z}^2$ as the ring $\mathbb{Z}[i]$ of Gaussian integers, i.e., with $i = \sqrt{-1}$,

$$\mathbb{Z}[i] = \{a + ib \mid a,b \in \mathbb{Z}\}, \tag{11}$$

together with the (number theoretic) norm,

$$\mathrm{norm}(a+ib) = (a+ib)(a-ib) = |a+ib|^2. \tag{12}$$

The ring $\mathbb{Z}[i]$ consists of all algebraic integers in the cyclotomic field $\mathbb{Q}(i) = \{a + ib \mid a,b \in \mathbb{Q}\}$. The coincidence rotation problem is then equivalent to finding all numbers of norm 1 in $\mathbb{Q}(i)$ because rotation through an angle means multiplication with the corresponding complex number on the unit circle and a coincidence can only happen if this complex number is in $\mathbb{Q}(i)$.

Any such number can uniquely be written (up to units) as the quotient of two Gaussian integers,

$$e^{i\varphi} = \frac{\alpha}{\beta} = \frac{a+ib}{c+id}, \tag{13}$$

with coprime Gaussian integers α,β of identical norm, $\mathrm{norm}(a+ib) = \mathrm{norm}(c+id) = l$, say. Now, we can profit from unique factorization in $\mathbb{Z}[i]$ because any integer $\alpha \in \mathbb{Z}[i]$ divides its norm:

$$\alpha \mid \mathrm{norm}(\alpha). \tag{14}$$

Let $l = p_1^{\nu_1} \cdot \ldots \cdot p_r^{\nu_r}$ be the (unique) factorization of l of (13) into "ordinary" primes of $\mathbb{Z}$, called *rational primes* from now on. If any rational prime p_j stayed prime in $\mathbb{Z}[i]$ (i.e., did not split into

two Gaussian integers), which happens if $p_j \equiv 3\ (4)$, it would appear both in the numerator and the denominator of (13) which is inconsistent with coprimality. Thus such a rational prime cannot divide l.

A similar argument applies to the prime 2, which, although it splits as $2=i(1-i)^2$, also has only one Gaussian prime factor up to units. The remaining primes are $\equiv 1 \pmod 4$ and split as $p=\omega_p\overline{\omega}_p$ into two Gaussian integers. One of them appears in the numerator of (13), the other in the denominator, if $p|l$. Of course, the actual choice of ω_p is only unique up to units and up to taking the complex conjugate that reflects the point symmetry of the square lattice! One convenient choice for uniqueness (which we will now take) is a rotation angle in the interval $(0,\pi/4)$.

This, in fact, solves the above problem constructively: any CSL rotation can be written in the form

$$e^{i\varphi}=\epsilon\cdot\prod_{\mathscr{P}\ni p\equiv 1(4)}\left(\frac{\omega_p}{\overline{\omega}_p}\right)^{n_p}, \tag{15}$$

where $n_p\in\mathbb{Z}$, ϵ is a unit in $\mathbb{Z}[i]$ and $\mathscr{P}$ denotes the set of rational primes. Since the group of units in $\mathbb{Z}[i]$ is nothing but C_4, we find

$$SOC(\mathbb{Z}^2)\simeq C_4\times\mathbb{Z}^{(\aleph_0)} \tag{16}$$

and the generators are i (for C_4) and $\omega_p/\overline{\omega}_p$ for rational primes $p\equiv 1\ (4)$. By $\mathbb{Z}^{(\aleph_0)}$ we mean, as usual, the infinite Abelian group that consists of all *finite* integer linear combinations of the (countably many) generators. The coincidence index m is obviously 1 for the units in C_4 and $p=\mathrm{norm}(\omega_p)$ for the other generators because this counts the number of residue classes of the CSL in $\mathbb{Z}^2$. If the CSL rotation R is factorized as in Eq. (15), we thus find

$$\Sigma(R)=\prod_{\mathscr{P}\ni p\equiv 1(4)} p^{|n_p|}. \tag{17}$$

This solves the rotation part in principle, one can now work along the primes $p\equiv 1\ (4)$ to write down the generators explicitly, e.g.,

$$\frac{4+3i}{5},\ \frac{12+5i}{13},\ \frac{15+8i}{17},\ \frac{21+20i}{29},\ \frac{35+12i}{37},\ \frac{40+9i}{41},\ \text{etc},$$

where the number on the unit circle is shown in a form with denominator p and rotation angle in $(0,\pi/4)$. All other CSL rotations are obtained by combinations, and one can regain the formula of Theorem 1 for the number of them with index m. Since $d^*(m)$ is a multiplicative function [i.e., $d^*(m_1m_2)=d^*(m_1)d^*(m_2)$ for coprime m_1,m_2] and $d^*(p^r)=2$ for a prime power p^r $(r\geqslant 1)$, we obtain for $f(m)=d^*(m)$ the Dirichlet series generating function [18],

$$\Phi(s)=\sum_{m=1}^{\infty}\frac{d^*(m)}{m^s}=\prod_{p\equiv 1(4)}\left(1+\frac{2}{p^s}+\frac{2}{p^{2s}}+\cdots\right)=\prod_{p\equiv 1(4)}\frac{1+p^{-s}}{1-p^{-s}}, \tag{18}$$

and the Dirichlet series generating function for $\hat{f}(m)$ is $4\Phi(s)$.

Finally, the full group of CSL isometries, $OC(\mathbb{Z}^2)$, is the semidirect product of the rotation part $SOC(\mathbb{Z}^2)$ (normal subgroup) with the group $\mathbb{Z}_2$ generated by complex conjugation (=reflection in the x-axis):

$$OC(\mathbb{Z}^2)=SOC(\mathbb{Z}^2)\times_s\mathbb{Z}_2. \tag{19}$$

Here conjugation of a rotation through an angle φ by complex conjugation results in the inverse rotation through $-\varphi$. Let us give a brief justification of Eq. (19). Since $O(2)=SO(2)\times_s\mathbb{Z}_2$ (semidirect product) with the $\mathbb{Z}_2$ of Eq. (19), *any* planar isometry T with $\det(T)=-1$ can uniquely be written as the product

$$T=R(\varphi)\cdot T_x \tag{20}$$

of a rotation through φ with T_x, the reflection in the x-axis. But T_x leaves $\mathbb{Z}^2$ invariant, so T is a coincidence isometry if and only if $R(\varphi)$ is a coincidence rotation.

The calculation of coincidence indices is also simple in this case. The coincidence index for the reflection T_x is 1. For an arbitrary element of $OC(\mathbb{Z}^2)$, we either meet a rotation (where we know the result already) or use the factorization (20) again. Then, the coincidence index is identical with that of its rotation part, so Eq. (20) is all that is needed. This solves the coincidence problem for the square lattice completely, and we have the following.

Theorem 2: *The group of coincidence isometries of the square lattice* $\mathbb{Z}^2$ *is*

$$OC(\mathbb{Z}^2)\simeq O(2,\mathbb{Q})\simeq(C_4\times\mathbb{Z}^{(\aleph_0)})\times_s\mathbb{Z}_2\,. \tag{21}$$

This group is fully characterized by Eqs. (15), (16) and (19), and the coincidence index of an element (20) is given by Eqs. (17) and (15).

III. MORE GENERALITY: THE UNIQUE FACTORIZATION CASE

As briefly explained in the Introduction, the corresponding programme for a locally finite tiling $\mathcal{T}$ with N-fold symmetry (or rather for its set of vertex sites) consists of two steps, the first being the solution of the coincidence problem for the limit translation module $\mathcal{M}(\mathcal{T})$ of $\mathcal{T}$ (see Ref. 20 for details about this concept). For the moment, we consider only tilings with the property that the set of vertex sites of $\mathcal{T}$ is a subset of $\mathcal{M}(\mathcal{T})$, a condition we shall come back to in Section V. Furthermore, we assume $\mathcal{M}(\mathcal{T})$ to be what is termed an "N-lattice" in Ref. 21, but which we shall call an "n-module" (where $N=2n$ for n odd and $N=n$ otherwise) in line with the mathematical practice of reserving the word "lattice" for discrete subgroups. The *principal n-module* (the "standard N-lattice" of Ref. 21) is the additive subgroup of $\mathbb{R}^2$, generated by the vectors of the regular n-star,

$$(\cos(2\pi k/n),\sin(2\pi k/n)),\quad k=0,\ldots,n-1. \tag{22}$$

The other modules are the non-trivial subgroups of the principal module that are invariant under rotation about the origin through $2\pi/n$. Modules that differ only in scale and orientation are regarded as equivalent.

Because all modules are invariant under rotation through π (since if x is in the module then so is $-x$), an n-module with n odd is invariant not only under rotation through $2\pi/n$ but also through π/n. So n-modules and N-modules are the same. In view of this we shall assume throughout that n is either odd or divisible by 4, though this necessitates bearing in mind that for odd n an n-module has $2n$-fold symmetry. The opposite convention is used in Ref. 21, but the one used here is more convenient for expressing results about cyclotomic fields that we shall need later because it gives n the parity of the discriminant of the corresponding field.

The first stage of our analysis, occupying all but Section V, is to investigate coincidence rotations for modules and their associated coincidence site modules, which we designate CSMs.

A. Symmetric modules and cyclotomic fields

Viewed as complex numbers, the vectors (22) are ξ^k, where ξ is a primitive nth root of 1, and the modules are subsets of the cyclotomic field $K=\mathbb{Q}(\xi)$. The principal module is precisely the ring of integers $\mathcal{O}_K$ of K, since it is known that $\{1,\xi,\xi^2,\ldots,\xi^{\phi(n)-1}\}$ is a basis for the integers of K, where

$\phi(n)$, the Euler totient function of n, is the degree of K over $\mathbb{Q}$, cf. Chapter 9 of Ref. 22. The other modules are the ideals of $\mathcal{O}_K$ (to be defined later), modules being equivalent precisely when they belong to the same ideal class (defined in Section VI).

In this section, at the expense of discussing only 29 modules (see Refs. 25 and 21), we restrict attention to values of n for which all n-modules are equivalent. Because of the connection with algebraic number theory we call this the ''class number 1'' case and use the designation ''CN1'' to indicate results that are special to this case. (The reason behind this terminology is explained in Sec. VI. Briefly, it is the case when the nth cyclotomic field has class number number 1.) The class number 1 assumption simplifies the treatment in two ways:

(1) it is enough to solve the coincidence problem for the principal module $\mathcal{O}_K$ only, since all others are equivalent to it; and

(2) in the class number 1 case each integer in $\mathcal{O}_K$ has a factorization into irreducible integers that is unique apart from multiplying the factors by units. (Because of the unique factorization these irreducible integers can safely be called *primes* in the class number 1 case.)

Though a convenience, the restriction to class number 1 is by no means essential: with only minor modifications our method applies to any 2D module, as outlined in Section VI.

As in the previous section, a coincidence rotation that takes β to α, say $(\alpha,\beta\in\mathcal{O}_K)$ can be represented by the point $\gamma=\alpha/\beta$ on the unit circle. So the CSM problem amounts to finding the structure of the set of numbers γ in K with

$$|\gamma|=1 \tag{23}$$

(a subgroup of the multiplicative group of K).

The CSM associated with γ is $\mathcal{O}_K\cap\gamma\mathcal{O}_K=\mathrm{num}(\gamma)\mathcal{O}_K$, where $\mathrm{num}(\gamma)$, the numerator of γ, is given by

$$\mathrm{num}(\gamma)=\gcd(\nu\in\mathcal{O}_K\,|\,\nu/\gamma\in\mathcal{O}_K), \tag{24}$$

and is unique up to multiplication by a unit. In particular, $\mathrm{num}(\gamma)|\alpha$. The index of this module in the original module $\mathcal{O}_K$ is $\mathrm{norm}(\mathrm{num}(\gamma))$, the absolute norm of $\mathrm{num}(\gamma)$, (Ref. 22, 4.4 and Cor. 2.96). (Since units have norm 1 this is independent of the particular numerator chosen. All conjugates of the field K are complex, so norms of numbers in K are products of pairs of complex conjugates and hence positive.)

Equation (23) can be reformulated as an algebraic condition with the aid of the maximal real subfield L of K:

$$L:=\mathbb{Q}(\xi+\xi^{-1})=\mathbb{Q}\left(\cos\frac{2\pi}{n}\right). \tag{25}$$

It is known that when K has unique factorization L does too (see p. 231 of Ref. 27). As an extension of L, K has degree 2 and the set of conjugates over L of a number $\gamma\in K$ is just the complex conjugate pair $\{\gamma,\overline{\gamma}\}$. Consequently, the *relative norm* of γ over L, $\mathrm{norm}_{K/L}(\gamma)$, is given by

$$\mathrm{norm}_{K/L}(\gamma)=|\gamma|^2. \tag{26}$$

In this notation, the *absolute norm* of γ is $\mathrm{norm}(\gamma)=\mathrm{norm}_{K/\mathbb{Q}}(\gamma)$ and we have the relation

$$\mathrm{norm}_{K/\mathbb{Q}}(\gamma)=\mathrm{norm}_{L/\mathbb{Q}}(\mathrm{norm}_{K/L}(\gamma)). \tag{27}$$

Relative norms of integers in K are integers in L and norms of units are units. As in the previous section (where $L=\mathbb{Q}$), $\alpha|\mathrm{norm}_{K/L}(\alpha)=\alpha\overline{\alpha}$ for every integer α of K, so the only possible prime factors of α in K are those that divide $\mathrm{norm}(\alpha)$.

B. Cyclotomic numbers on the unit circle

When a planar module $\mathscr{M}$ intersects a rotated or reflected copy of itself in a submodule of finite index, the isometry (rotation or reflection) is again called a coincidence isometry. The set of coincidence isometries of $\mathscr{M}$ is denoted by $OC(\mathscr{M})$. It is again a group, with $SOC(\mathscr{M})$ being its subgroup of rotations. (These concepts can be put in a more general setting. Some slight extensions of them are already required for the examples in Appendix A, for example.)

In view of Eq. (26) and our representation of $SOC(\mathscr{O}_K)$ as the elements of K on the unit circle, we have

$$SOC(\mathscr{O}_K) \simeq \{\gamma \in K | \mathrm{norm}_{K/L}(\gamma) = 1\}. \tag{28}$$

To analyze the right hand side further we need some facts about the arithmetic of K and L. First, the units ϵ of K with $|\epsilon|=1$ are precisely the powers of ξ, though in general there are also infinitely many units not on the unit circle. (This follows, e.g., from Ref. 28, Lemma 1.6, and the last sentence of the remark following it.) Second, if a prime ϱ of L has two non-associated prime factors in K (i.e., their ratio is not a unit) then they can be taken as complex conjugates, ω and $\overline{\omega}$. This is because $\omega|\varrho$ implies $\overline{\omega}|\varrho$, so, if ω and $\overline{\omega}$ are not associates, $\omega\overline{\omega}$ is an integer in $\mathscr{O}_L$ dividing ϱ, hence is an associate of ϱ. (Here $\mathscr{O}_L$ is the ring of integers of L, of course.) Conversely, if ϱ is divisible by just the prime ω in K and no other (up to units), then, as $\overline{\omega}$ also divides ϱ, $\omega/\overline{\omega}$ must be a unit. Thus a prime $\omega \in \mathscr{O}_K$ divides a prime $\varrho \in \mathscr{O}_L$ with distinct factors if and only if $\overline{\omega}$ is not an associate of ω. By Eq. (26), $\mathrm{norm}_{K/L}(\omega) = \mathrm{norm}_{K/L}(\overline{\omega})$.

Now suppose that $\gamma \in K$ satisfies $\mathrm{norm}_{K/L}(\gamma)=1$ and write $\gamma=\alpha/\beta$, where α,β are integers of $\mathscr{O}_K$ with no common factor. Then

$$\mathrm{norm}_{K/L}(\alpha) = \mathrm{norm}_{K/L}(\beta) = \nu \in \mathscr{O}_L \tag{29}$$

and every prime factor of ν must factorize into two non-associated primes of K, one of which divides α only and the other β only. Since any such pair can be chosen to be complex conjugates, γ can be written as

$$\gamma = \epsilon \prod_k \left(\frac{\omega_k}{\overline{\omega}_k} \right)^{n_k}, \tag{30}$$

with ϵ a unit of K and the n_k's in $\mathbb{Z}$. Taking absolute values in (30) shows that $|\epsilon|=1$, whence ϵ is a root of unity. Different values of the n_k's give γ's with different prime factorizations, which are therefore not associates, and different roots of unity ϵ give different γ's within each set of associates. So in this more general situation we again have explicit presentations of $SOC(\mathscr{O}_K)$ and $OC(\mathscr{O}_K)$ almost identical to those for $SOC(\mathbb{Z}^2)$ and $OC(\mathbb{Z}^2)$ in the previous section. These are, for SOC,

$$SOC(\mathscr{O}_K) \simeq \langle \xi \rangle \underset{\{\omega,\overline{\omega}\} \in \Omega}{\times} \left\langle \frac{\omega}{\overline{\omega}} \right\rangle \simeq C_N \times \mathbb{Z}^{(\aleph_0)}, \tag{31}$$

where Ω is the set of complex conjugate pairs of non-associated primes in K (and $N=\mathrm{lcm}(n,2)$ as usual) and, for OC,

$$OC(\mathscr{O}_K) = SOC(\mathscr{O}_K) \times_s \langle \overline{\cdot} \rangle, \tag{32}$$

where $\overline{\cdot}$ is complex conjugation and its action on $SOC(\mathscr{O}_K)$ is clear.

The coincidence index of the typical rotation (30) of $SOC(\mathcal{O}_K)$ is the absolute norm of its numerator:

$$\prod_k \left(\mathrm{norm}_{K/\mathbb{Q}}(\omega_k)\right)^{|n_k|}. \tag{33}$$

For each prime pair $\{\omega,\overline{\omega}\}\in\Omega$ the common value $\mathrm{norm}(\omega)=\mathrm{norm}(\overline{\omega})$ is a rational prime power p^d. We call these prime powers the *basic indices* of $\mathcal{O}_K$ and the primes p themselves the *complex splitting primes* for K (because, in their factorization over K, they contain at least one complex conjugate pair of distinct primes). Then (31), (32) and (33) show the following.

Proposition 1: (CN1) An integer $m\in\mathbb{N}$ is a coincidence index if and only if it is a product of basic indices.

To find out what basic indices there are and count how many members of the group $SOC(\mathcal{O}_K)$ have a given index we need to determine how each rational prime p factorizes in the fields L and K. It will turn out that the basic indices are powers of distinct primes and that whether a power of p is a basic index (and what this power is) depends only on the residue class of p mod n.

C. Factorization of primes in algebraic number fields

Before considering K and L specifically we describe how primes factorize in a general algebraic number field extension $F(\alpha)\supset F$ of degree D. [We shall use the standard notation $F(\alpha)/F$ to denote such an extension. A detailed account of the material in this section can be found in Chapter 2 of Ref. 23].

Let $f(x)=0$ be the minimal equation satisfied by α with coefficients in F [so the degree of $f(x)$ is D] and let $\mathcal{O}$ and $\mathcal{O}'$ be the rings of integers of F and $F(\alpha)$.

An *ideal* of $\mathcal{O}$ is a subset $\mathbf{a}$ of $\mathcal{O}$ (non-empty and $\neq\{0\}$) such that $\alpha+\beta\in\mathbf{a}\ \forall\alpha,\beta\in\mathbf{a}$ and $\lambda\alpha\in\mathbf{a}$ $\forall\lambda\in\mathcal{O},\alpha\in\mathbf{a}$. We use the notation $(\alpha,\beta,\ldots)_{\mathcal{O}}$ to denote the smallest ideal containing $\alpha,\beta,\ldots$ (where these are numbers in $\mathcal{O}$). Ideals have a natural multiplication, defined by $\mathbf{ab}=(\alpha\beta|\alpha\in\mathbf{a},\beta\in\mathbf{b})_{\mathcal{O}}$ and $\mathcal{O}$ itself is the multiplicative identity. There is an infinite set of *prime ideals* in $\mathcal{O}$ and every ideal can be uniquely factorized into prime ideals.

Every ideal $\mathbf{a}$ in $\mathcal{O}$ extends to an ideal $(\mathbf{a})_{\mathcal{O}'}$ in $\mathcal{O}'$, but $\mathcal{O}'$ also has other ideals not of this form. For an ideal $\mathbf{a}'$ of $\mathcal{O}'$ the relative norm, $\mathrm{norm}_{F(\alpha)/F}(\mathbf{a}')$ is defined as $(\mathrm{norm}_{F(\alpha)/F}(\alpha)|\,\alpha\in\mathbf{a}')_{\mathcal{O}}$—an ideal of $\mathcal{O}$. Norms are completely multiplicative [i.e., $\mathrm{norm}(\mathbf{ab})=\mathrm{norm}(\mathbf{a})\mathrm{norm}(\mathbf{b})$]. Let $\mathbf{p}$ be a prime ideal in $\mathcal{O}$. Then $(\mathbf{p})_{\mathcal{O}'}$ factorizes into prime ideals in $\mathcal{O}'$ as

$$(\mathbf{p})_{\mathcal{O}'}=\mathbf{p}_1^{e_1}\ldots\mathbf{p}_g^{e_g}, \tag{34}$$

and for each $k=1,\ldots,g$,

$$\mathrm{norm}_{F(\alpha)/F}(\mathbf{p}_k)=\mathbf{p}^{d_k}, \tag{35}$$

where d_k is the *residue class degree* of $\mathbf{p}_k$. Taking norms of both sides of Eq. (34) shows that

$$d_1e_1+\cdots+d_ge_g=D. \tag{36}$$

For the special case of *normal* field extensions [i.e., extensions where $F(\alpha)$ contains not only α itself but also all other roots of $f(x)=0$] we have $e_1=\cdots=e_g$ and $d_1=\cdots=d_g$. So in this case

$$(\mathbf{p})_{\mathcal{O}'}=(\mathbf{p}_1\ldots\mathbf{p}_g)^e, \tag{37}$$

where each $\mathbf{p}_k$ has the same degree d, $d\cdot e\cdot g=D$ and without ambiguity we can define $\deg_{F(\alpha)}(\mathbf{p}):=\mathrm{d}$ and $e_{F(\alpha)}(\mathbf{p}):=\mathrm{e}$. Also $e_{F(\alpha)}(\mathbf{p})>1$ only for the finitely many primes $\mathbf{p}$ that divide the discriminant of the extension $F(\alpha)/F$. (Such primes are called *ramified*.)

Another special case is field extensions where α can be chosen so that $\mathcal{O}'=\mathcal{O}[\alpha]$ ($\mathcal{O}'$ has a *simple integral basis* over $\mathcal{O}$). In this case the factorization of a prime $\mathbf{p}$ of $\mathcal{O}$ into prime ideals of $\mathcal{O}'$ mimics the factorization of $f(x)$ into irreducible factors over the finite residue class field $\mathcal{O}/\mathbf{p}$. So if $\mathbf{p}$ factorizes as in Eq. (34) then

$$f(x)\equiv f_1(x)^{e_1}\ldots f_g(x)^{e_g}(\mathrm{mod}\ \mathbf{p}), \tag{38}$$

where each f_k is irreducible of degree d_k and distinct f_k's correspond to distinct primes $\mathbf{p}_k$. This provides a simple way of calculating the degrees and multiplicities of the prime factors of $\mathbf{p}$.

The three extensions we have to deal with—$K/\mathbb{Q}$, $L/\mathbb{Q}$ and K/L—are all normal and have simple integral bases, so all the above results apply to them. Also relative degrees are multiplicative: if p is a rational prime having a prime factor ϱ in $\mathcal{O}_L$, which in turn has a prime factor ω in $\mathcal{O}_K$ then

$$\deg_{K/\mathbb{Q}}(\omega)=\deg_{K/L}(\omega)\cdot\deg_{L/\mathbb{Q}}(\varrho). \tag{39}$$

In particular, $\deg_{K/L}(\omega)$ is the same for all prime factors ω in $\mathcal{O}_K$ of the same rational prime p.

The primes of $\mathcal{O}_K$ in the non-associated pairs $\{\omega,\overline{\omega}\}$ are precisely the unramified primes of relative degree 1 over $\mathcal{O}_L$. In view of (39) and the normality of K and L, Ω is the set of all pairs of distinct prime factors $\{\omega,\overline{\omega}\}$ in $\mathcal{O}_K$ that divide rational primes p with

$$\deg_L(p)=\deg_K(p)(=d,\ \text{say}), \tag{40}$$

and, for any such ω, the absolute norm [cf. (27) above] is

$$\mathrm{norm}(\omega)=p^d. \tag{41}$$

We have the following.

Proposition 2: (CN1) The complex splitting primes for K are the primes satisfying (40) and the basic indices of $\mathcal{O}_K$ are the powers p^d of these primes.

D. How to calculate the CSL group and its coincidence indices

Getting more explicit information about $SOC(\mathcal{O}_K)$ and its coincidence indices comes down to finding $\deg_L(p)$ and $\deg_K(p)$ for rational primes p. The following facts are sufficient to do this; we state them here and justify them in Appendix B.

To reiterate our notation: $K=\mathbb{Q}(\xi)$ and $L=\mathbb{Q}(\xi+\xi^{-1})$, where ξ is a primitive nth root of 1, and p is any rational prime.

Fact 1: If $p\nmid n$ then $\deg_K(p)$ is the smallest $d\in\mathbb{N}$ such that n divides p^d-1.

Fact 2: If $p\nmid n$ then $\deg_L(p)$ is the smallest $d\in\mathbb{N}$ such that n divides at least one of p^d+1 or p^d-1.

Fact 3: (a) If $n=p^r$, for some r, then p is not a complex splitting prime and $\deg_K(p)=1$.

(b) More generally, if $n=p^r n_1$ with $p\nmid n_1$ then p is a complex splitting prime in K if and only if it is a complex splitting prime in K_1 (the cyclotomic field of n_1th roots of unity). Moreover, $\deg_K(p)=\deg_{K_1}(p)$.

Although these facts alone clearly enable us to identify the complex splitting primes and calculate their degrees and multiplicities, it is nevertheless worth listing some general consequences of them.

Remark 1: These facts show that whether a prime p is a complex splitting prime of n and what its degree d is depend only on the residue class of p mod n.

Remark 2: Since, for a prime ω in $\mathcal{O}_K$ dividing p, $\mathrm{norm}(\omega)=p^d$, where $d=\deg_K(p)$, Fact 1 has the well-known consequence that $\mathrm{norm}(\omega)\equiv 1\ (\mathrm{mod}\ n)$ for every prime ω in $\mathcal{O}_K$ with $\omega\nmid n$. In particular, every coincidence index m with $\gcd(m,n)=1$ satisfies $m\equiv 1\ (\mathrm{mod}\ n)$.

Remark 3: When $p\nmid n$ is not a complex splitting prime, $\deg_K(p)=2\deg_L(p)$, so $\deg_K(p)$ is even. Facts 1, 2 and 3(a) show that, conversely, if n is an odd prime power then no prime p with $d=\deg_K(p)$ even is a complex splitting prime. This is because if $n\mid p^d-1=(p^{d/2}-1)(p^{d/2}+1)$ but $n\nmid p^{d/2}-1$ then, since $\gcd(p^{d/2}-1,p^{d/2}+1)=2$ (or 1 if $p=2$), $n\mid p^{d/2}+1$, so $\deg_L(p)=d/2$.

So, for n an odd prime power, p is a complex splitting prime if and only if $\deg_K(p)$ is odd and $p\nmid n$, and it is unnecessary to compute degrees over L in this case.

Remark 4: By Fact 1 the unramified primes with $\deg_K(p)=1$ (i.e., the primes that *split completely* in K) are precisely those $\equiv 1 \pmod n$. So these primes are always complex splitting primes.

Remark 5: Facts 1 and 2 show that, for primes $p\equiv -1 \pmod n$, $\deg_K(p)=2$ and $\deg_L(p)=1$, so these primes are never complex splitting primes. Consequently, for every n, the proportion of integers that are coincidence indices is 0.

In the next section we apply these facts and remarks to calculate coincidence indices of specific modules.

E. The number of coincidences with given index

Let $\hat{f}(m)=N\cdot f(m)$ be the number of elements of $SOC(\mathcal{O}_K)$ with index m. The computational convenience of representing $\hat{f}(m)$ this way arises from the fact that $f(m)$ is more fundamental: it is a multiplicative function of m and, as for the square lattice, it counts the CSMs with index m, since the rotation group of each module is the group of roots of unity in K and has order N. In the general case, $f(m)$ cannot be described as simply as in Eq. (9), but its Dirichlet series generating function does have a very simple expression in terms of the ζ-functions of the fields K and L. Also, for quite sizeable individual values of the index, the number of coincidence isometries can be calculated from (33) and knowledge of the identity, degrees and exponents of the complex splitting primes (or, equivalently, from the generating function).

From the decomposition (31) of $SOC(\mathcal{O}_K)$ and the function (33) it can be seen that $f(m)$ is multiplicative, i.e., $\gcd(m_1,m_2)=1$ implies $f(m_1m_2)=f(m_1)f(m_2)$. This makes its Dirichlet series,

$$\sum_{m=1}^{\infty}\frac{f(m)}{m^s}, \tag{42}$$

a convenient tool for studying f: it can be expressed[18] as an "Euler product,"

$$\prod_p\left(\sum_{r=1}^{\infty}\frac{f(p^r)}{p^{rs}}\right), \tag{43}$$

with one Euler factor for each prime p, and the individual Euler factors are straightforward to compute. [The series we obtain will all be absolutely convergent in the right half-plane $\mathrm{Re}(s)>1$ and extendable to meromorphic functions on the whole plane. For using the series formally to calculate individual values of f these analytic properties are irrelevant, but they play an essential rôle in calculating the asymptotic average value of f.]

Suppose the rational prime p is divisible by the pairs $\{\omega_1,\overline{\omega}_1\},\ldots,\{\omega_{g/2},\overline{\omega}_{g/2}\}$ of non-associated primes in K and that each ω_j has $\mathrm{norm}_{K/\mathbb{Q}}(\omega_j)=p^d$. Then $f(p^k)$ is the coefficient of p^{-ks} in

$$\left(\cdots+\frac{1}{p^{2ds}}+\frac{1}{p^{ds}}+1+\frac{1}{p^{ds}}+\frac{1}{p^{2ds}}+\cdots\right)^{g/2}, \tag{44}$$

the product of $g/2$ two-way infinite sums (one for each pair $\{\omega_j,\overline{\omega}_j\}$) each having one term for each value of the corresponding n_k in (33). (The symmetry of the sums arises from the fact that the index depends only on $|n_k|$, of course.) On summing the series this becomes

$$\left(\frac{1+p^{-ds}}{1-p^{-ds}}\right)^{g/2}. \tag{45}$$

Since $f(m)$ is multiplicative, for a general m it is the coefficient of m^{-s} in

$$\prod_{\mathscr{C}\ni p|m}\left(\frac{1+p^{-ds}}{1-p^{-ds}}\right)^{g/2}, \tag{46}$$

where $\mathscr{C}$ is the set of complex splitting primes for K, and the values of d and g are those appropriate to each individual prime p. This, in turn, is the coefficient of m^{-s} in the infinite product,

$$\Phi_K(s)=\prod_{p\in\mathscr{C}}\left(\frac{1+p^{-ds}}{1-p^{-ds}}\right)^{g/2}. \tag{47}$$

To express this more simply we introduce the Dedekind ζ-functions of number fields.[22,28] The ζ-function of a general algebraic number field F is the Dirichlet series generating function for the number of ideals $\mathbf{a}$ of $\mathscr{O}$ with $\mathrm{norm}(\mathbf{a})=m$, hence is given by

$$\zeta_F(s)=\sum_{\mathbf{a}}\frac{1}{\mathrm{norm}(\mathbf{a})^s}=\prod_{\mathbf{p}}\left(1-\frac{1}{\mathrm{norm}(\mathbf{p})^s}\right)^{-1}, \tag{48}$$

where $\mathbf{a}$ runs through all ideals of F and $\mathbf{p}$ through all prime ideals. When F is normal we can collect together prime ideals $\mathbf{p}$ dividing the same rational prime p to put the product on the right in the form

$$\prod_{p}\left(1-\frac{1}{p^{ds}}\right)^{-g}, \tag{49}$$

where, for each rational prime p, $d=\deg_{F/\mathbb{Q}}(p)$ and g is the number of prime ideals of F dividing it.

A particular case of this is

$$\zeta_{\mathbb{Q}}(s)=\sum_{m=1}^{\infty}\frac{1}{m^s}=\prod_{p}\left(1-\frac{1}{p^s}\right)^{-1}, \tag{50}$$

which is the Riemann ζ-function $\zeta(s)$ itself.

The following table compares the Euler factors of $\zeta_K(s)$ and $\zeta_L(2s)$ for each rational prime p, there being three cases to consider. (It follows from Lemma 3 of Ref. 24 and Prop. 2.15(b) of Ref.

28 that the third case, $e_K(p) \neq e_L(p)$, occurs for at most one prime p: the prime, if any, a power of which is equal to n.)

p	Field	Degree	Distinct prime factors	Euler factor
Complex splitting	K	d	g	$(1-p^{-ds})^{-g}$
	L	d	$g/2$	$(1-p^{-2ds})^{-g/2}$
Not complex splitting and $e_K(p)=e_L(p)$	K	d	g	$(1-p^{-ds})^{-g}$
	L	$d/2$	g	$(1-p^{-ds})^{-g}$
$e_K(p) \neq e_L(p)$	K	1	1	$(1-p^{-s})^{-1}$
	L	1	1	$(1-p^{-2s})^{-1}$

On taking the quotients of the Euler factors arising from K and L and comparing with Eq. (47), we see that

$$\frac{\zeta_K(s)}{\zeta_L(2s)} = \Phi_K(s)\left(1+\frac{1}{p^s}\right)^*, \tag{51}$$

the asterisk indicating that the second factor on the right is present only if n is a power of a prime p. So

$$CN1 \Rightarrow \Phi_K(s) = \begin{cases} (1+p^{-s})^{-1}\zeta_K(s)/\zeta_L(2s), & \text{if } n \text{ is a power of a prime } p; \\ \zeta_K(s)/\zeta_L(2s), & \text{if not.} \end{cases} \tag{52}$$

We summarize this in the following theorem.

Theorem 3: *Let n be one of the 29 numbers for which the cyclotomic field K of nth roots of unity has class number 1. Then the group of coincidence rotations of an n-fold symmetric module is the direct product of its finite rotation symmetry group C_N and countably many infinite cyclic groups, as in (31), and the full group of coincidence isometries is the extension of this by a reflection symmetry. The coincidence index of such an isometry is given by (33) and (30). The Dirichlet series generating function for*

$$f(m) = \{number\ of\ CSMs\ of\ index\ m\}, \tag{53}$$

$$= \frac{1}{N} \times \{number\ of\ coincidence\ rotations\ of\ index\ m\}, \tag{54}$$

is given by (52).

A principal use of a Dirichlet series is to find asymptotic formulæ for sum functions of its coefficients by means of residue calculus. In the present instance this technique shows, for example, that

$$\text{Number of CSMs of index} < X = \sum_{m<X} f(m) \sim X \cdot \{\text{residue of } \Phi_K(s) \quad \text{at } s=1\}. \tag{55}$$

In view of Eq. (52) this residue can be computed from known formulæ for the residues of ζ-functions at 1 and values of ζ-functions at 2. The value of the residue can be regarded as the "average number of CSMs" with a given arbitrarily chosen positive integer as index.

IV. EXAMPLES: $N=6$, 4, 10, 14, 8, AND 12

After the general derivation of the previous section, let us present some examples explicitly. We select those relevant to known crystals and quasicrystals. For each example we list the following

(a) The fields K and L and the degree $[K:\mathbb{Q}]$ of K over $\mathbb{Q}$.

(b) A table giving, for each residue class mod n containing primes p, $\deg_K(p)$ [and, if necessary, $\deg_L(p)$ too]. In the bottom line of the table [where $\deg_K(p)$ is given] the degrees of complex splitting primes are underlined. With each table is a comment describing which facts and remarks from the previous section were used to compute it.

(c) A list of the types of basic indices, using the notation that $p_{(a)}^b$ represents the bth powers of all primes congruent to a mod n.

(d) The Dirichlet series generating function of $f(m)$, given as a ratio of ζ-functions, as an Euler product and expanded explicitly as far as the 12th nonzero term. [The same notation as in (c) is used for the primes in the Euler product.]

(e) An explicit formula for $f(m)$ in the style of Eq. (9). In these formulæ e_p denotes the largest exponent e for which $p^e|m$.

(f) The average value of $f(m)$, as defined above.

The smallest coincidence indices can be read off as the denominators (with $s=1$) of the Dirichlet series, with the corresponding values of $f(m)$ as the numerators. All values of $f(m)$ for $m>1$ are even, reflecting the geometrical fact that the reverse of a coincidence rotation is also a coincidence rotation.

A. $n=3$, the triangular (or hexagonal) lattice

$$K=\mathbb{Q}(\sqrt{-3}),\quad L=\mathbb{Q},\quad [K:\mathbb{Q}]=2.$$

$p \pmod 3$	1	2	3	Computed using
$\deg_K(p)$	$\underline{1}$	2	1	Facts 1 and 3(a) and Remark 3.

Basic indices: $p_{(1)}$.

Dirichlet series:

$$\left(1+\frac{1}{3^s}\right)^{-1}\frac{\zeta_K(s)}{\zeta(2s)}=\prod\frac{1+p_{(1)}^{-s}}{1-p_{(1)}^{-s}}=1+\frac{2}{7^s}+\frac{2}{13^s}+\frac{2}{19^s}+\frac{2}{31^s}+\frac{2}{37^s}+\frac{2}{43^s}+\frac{2}{49^s}+\frac{2}{61^s}+\frac{2}{67^s}+\frac{2}{73^s}+\frac{2}{79^s}+\cdots.$$

Number of CSLs with index m:

$$f(m)=\begin{cases}\prod_{p|m}2, & \text{if } m \text{ is a product of basic indices;}\\ 0, & \text{otherwise.}\end{cases}$$

Average number of CSLs:

$$\frac{\sqrt{3}}{2\pi}\simeq 0.276.$$

B. $n=4$, the square lattice

$$K=\mathbb{Q}(i), \quad L=\mathbb{Q}, \quad [K:\mathbb{Q}]=2.$$

$p \pmod 4$	1	2	3
$\deg_L(p)$	1	1	1
$\deg_K(p)$	$\underline{1}$	1	2

Computed from Facts 1, 2 and 3(a).

Basic indices: $p_{(1)}$.
Dirichlet series:

$$\left(1+\frac{1}{2^s}\right)^{-1}\frac{\zeta_K(s)}{\zeta(2s)}=\prod\frac{1+p_{(1)}^{-s}}{1-p_{(1)}^{-s}}=1+\frac{2}{5^s}+\frac{2}{13^s}+\frac{2}{17^s}+\frac{2}{25^s}+\frac{2}{29^s}+\frac{2}{37^s}+\frac{2}{41^s}+\frac{2}{53^s}+\frac{2}{61^s}+\frac{4}{65^s}+\frac{2}{73^s}+\cdots .$$

Number of CSLs with index m:

$$f(m)=\begin{cases}\prod_{p|m} 2, & \text{if } m \text{ is a product of basic indices;}\\ 0, & \text{otherwise.}\end{cases}$$

Average number of CSLs:

$$\frac{1}{\pi}\simeq 0.318.$$

C. $n=5$, the tenfold module

$$K=\mathbb{Q}(e^{2\pi i/5}), \quad L=\mathbb{Q}(\sqrt{5}), \quad [K:\mathbb{Q}]=4.$$

$p \pmod 5$	1	2	3	4	5
$\deg_K(p)$	$\underline{1}$	4	4	2	1

Computed using Facts 1 and (3a) and Remark 3.

Basic indices: $p_{(1)}$.
Dirichlet series:

$$\left(1+\frac{1}{5^s}\right)^{-1}\frac{\zeta_K(s)}{\zeta_L(2s)}=\prod\left(\frac{1+p_{(1)}^{-s}}{1-p_{(1)}^{-s}}\right)^2=1+\frac{4}{11^s}+\frac{4}{31^s}+\frac{4}{41^s}+\frac{4}{61^s}+\frac{4}{71^s}+\frac{4}{101^s}+\frac{8}{121^s}+\frac{4}{131^s}+\frac{4}{151^s}+\frac{4}{181^s}+\frac{4}{191^s}+\cdots .$$

Number of CSMs with index m:

$$f(m)=\begin{cases}\prod_{p|m} 4e_p, & \text{if } m \text{ is a product of basic indices;}\\ 0, & \text{otherwise.}\end{cases}$$

Average number of CSMs:

$$\frac{5\log\tau}{\pi^2}\simeq 0.244.$$

D. $n=7$, the 14-fold module

$$K=\mathbb{Q}(e^{2\pi i/7}),\quad L=\mathbb{Q}(\cos(2\pi/7)),\quad [K:\mathbb{Q}]=6.$$

$p \pmod 7$	1	2	3	4	5	6	7
$\deg_K(p)$	$\underline{1}$	$\underline{3}$	6	$\underline{3}$	6	2	1

Computed using Facts 1 and 3(a) and Remark 3.

Basic indices: $p_{(1)}$, $p_{(2)}^3$, $p_{(4)}^3$.
Dirichlet series:

$$\left(1+\frac{1}{7^s}\right)^{-1}\frac{\zeta_K(s)}{\zeta_L(2s)}=\prod\left(\frac{1+p_{(1)}^{-s}}{1-p_{(1)}^{-s}}\right)^3\frac{(1+p_{(2)}^{-3s})(1+p_{(4)}^{-3s})}{(1-p_{(2)}^{-3s})(1-p_{(4)}^{-3s})}$$
$$=1+\frac{2}{8^s}+\frac{6}{29^s}+\frac{6}{43^s}+\frac{2}{64^s}+\frac{6}{71^s}+\frac{6}{113^s}+\frac{6}{127^s}+\frac{6}{197^s}$$
$$+\frac{6}{211^s}+\frac{12}{232^s}+\frac{6}{239^s}+\cdots .$$

Number of CSMs with index m:

$$f(m)=\begin{cases}\displaystyle\prod_{\substack{p\mid m\\ p\equiv 1(7)}}(4e_p^2+2)\prod_{\substack{p\mid m\\ p\not\equiv 1(7)}}2, & \text{if } m \text{ is a product of basic indices;}\\ 0, & \text{otherwise.}\end{cases}$$

Average number of CSMs:

$$\frac{343\sqrt{7}R}{256\pi^3}\simeq 0.240,$$

where R (the regulator of K) is given by

$$\frac{R}{4}=\log^2\left(2\cos\frac{2\pi}{7}\right)-\log\left(2\cos\frac{\pi}{7}\right)\log\left(2\cos\frac{3\pi}{7}\right)\simeq 0.525.$$

E. $n=8$, the eightfold module

$$K=\mathbb{Q}(e^{\pi i/4}),\quad L=\mathbb{Q}(\sqrt{2}),\quad [K:\mathbb{Q}]=4.$$

$p \pmod 8$	1	2	3	5	7
$\deg_L(p)$	1	1	2	2	1
$\deg_K(p)$	$\underline{1}$	1	$\underline{2}$	$\underline{2}$	2

Computed from Facts 1, 2 and 3(a).

Basic indices: $p_{(1)}$, $p_{(3)}^2$, $p_{(5)}^2$.
Dirichlet series:

$$\left(1+\frac{1}{2^s}\right)^{-1}\frac{\zeta_K(s)}{\zeta_L(2s)}=\prod\left(\frac{1+p_{(1)}^{-s}}{1-p_{(1)}^{-s}}\right)^2\frac{(1+p_{(3)}^{-2s})(1+p_{(5)}^{-2s})}{(1-p_{(3)}^{-2s})(1-p_{(5)}^{-2s})}$$
$$=1+\frac{2}{9^s}+\frac{4}{17^s}+\frac{2}{25^s}+\frac{4}{41^s}+\frac{4}{73^s}+\frac{2}{81^s}+\frac{4}{89^s}+\frac{4}{97^s}$$
$$+\frac{4}{113^s}+\frac{2}{121^s}+\frac{4}{137^s}+\cdots .$$

Number of CSMs with index m:

$$f(m)=\begin{cases}\displaystyle\prod_{\substack{p\mid m\\ p\equiv 1(8)}}4e_p\prod_{\substack{p\mid m\\ p\not\equiv 1(8)}}2, & \text{if } m \text{ is a product of basic indices;}\\ 0, & \text{otherwise.}\end{cases}$$

Average number of CSMs:

$$\frac{2\sqrt{2}\,\log(1+\sqrt{2})}{\pi^2}\simeq 0.253.$$

F. $n=12$, the 12-fold module

$$K=\mathbb{Q}(e^{\pi i/6}),\quad L=\mathbb{Q}(\sqrt{3}),\quad [K:\mathbb{Q}]=4.$$

$p \pmod{12}$	1	2	3	5	7	11
$\deg_L(p)$	1	1	1	2	2	1
$\deg_K(p)$	1	2	2	2	2	2

Computed from Facts 1 and 2 and the cases $n=3$ and $n=4$ using Fact 3(b).

Basic indices: $p_{(1)}$, $p_{(5)}^2$, $p_{(7)}^2$.
Dirichlet series:

$$\frac{\zeta_K(s)}{\zeta_L(2s)}=\prod\left(\frac{1+p_{(1)}^{-s}}{1-p_{(1)}^{-s}}\right)^2\frac{(1+p_{(5)}^{-2s})(1+p_{(7)}^{-2s})}{(1-p_{(5)}^{-2s})(1-p_{(7)}^{-2s})}$$
$$=1+\frac{4}{13^s}+\frac{2}{25^s}+\frac{4}{37^s}+\frac{2}{49^s}+\frac{4}{61^s}+\frac{4}{73^s}+\frac{4}{97^s}+\frac{4}{109^s}+\frac{4}{157^s}+\frac{8}{169^s}+\frac{4}{181^s}+\cdots .$$

Number of CSMs with index m:

$$f(m)=\begin{cases}\displaystyle\prod_{\substack{p\mid m\\ p\equiv 1(12)}}4e_p\prod_{\substack{p\mid m\\ p\not\equiv 1(12)}}2, & \text{if } m \text{ is a product of basic indices;}\\ 0, & \text{otherwise.}\end{cases}$$

Average number of CSMs:

$$\frac{\sqrt{3}\,\log(2+\sqrt{3})}{\pi^2}\simeq 0.231.$$

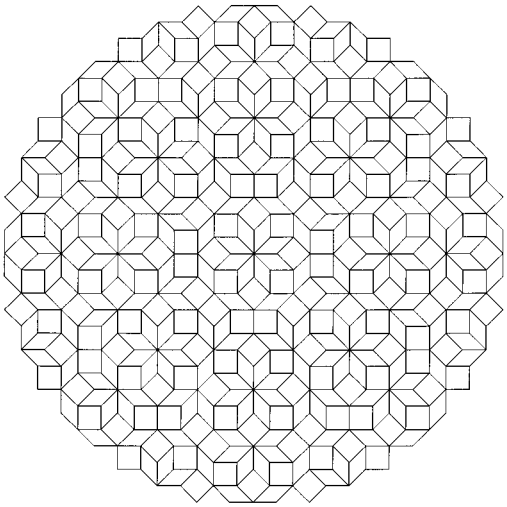

FIG. 1. Central patch of the exactly eightfold symmetric Ammann–Beenker tiling.

V. APPLICATION TO 2D QUASICRYSTALS

The reader might like to see at least one or two examples where we apply the above results to planar quasicrystals. For simplicity, we consider the eightfold symmetric Ammann–Beenker tiling and the decagonal Tübingen triangle tiling[29] here, while the slightly more complicated rhombic Penrose tiling is discussed in Appendix A.

A. The Ammann–Beenker tiling

Consider the eightfold symmetric Ammann–Beenker tiling of Fig. 1 and, in particular, the coincidence problem of its vertex points for rotations around the symmetry centre. The underlying module is the standard eightfold module of rank 4, usually obtained as projection of the hypercubic lattice $\mathbb{Z}^4$ to a suitably chosen 2D plane. This plane, and its perpendicular complement, are eigenspaces of an eightfold rotation.

The set of vertex sites of this tiling is just the subset of module points whose corresponding points in $\mathbb{Z}^4$ perpendicularly project into a certain regular octagonal window. It is clear then that a coincidence of vertex sites implies one in the module, but also the converse is true due to the way the tiling sites are distributed over the module.

A coincidence rotation can be lifted to 4-space whence it also affects the window. In fact, a coincidence point must have perpendicular projections both in the original and in the rotated window! But this results in a slight modification of the fraction of coinciding points, which has to be corrected by an acceptance factor A. This is nothing but the area ratio of the intersection of the rotated windows with the original window, see Fig. 2. For a coincidence rotation through φ, it turns out to be

$$A = 1 - \left(1 - \frac{1}{\sqrt{2}}\right) \sin(\hat{\psi}) \sin\left(\frac{\pi}{4} - \hat{\psi}\right), \tag{56}$$

where $\hat{\psi} \in [0, \pi/4)$ via

$$\hat{\psi} = \psi - \left\lfloor \frac{4\psi}{\pi} \right\rfloor \cdot \frac{\pi}{4} \tag{57}$$

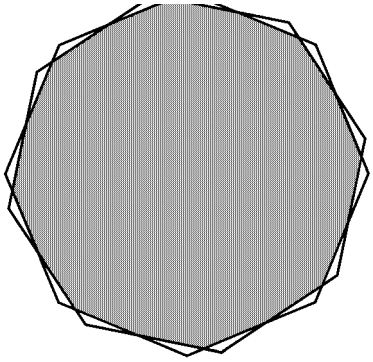

FIG. 2. Intersection of two acceptance domains that are rotated against each other.

and ψ, the rotation angle in perpendicular or internal space, is related to the angle $\varphi=2\arctan(a+b\sqrt{2})$ through an algebraic conjugation:

$$\psi=2\arctan(a-b\sqrt{2}). \tag{58}$$

The acceptance factor (56) is 1 for symmetry rotations and smaller otherwise, the minimal value being $A_{\min}\simeq 0.957$ at $\pi/8$. The set of coinciding points almost looks like an Ammann–Beenker pattern again, but some points are missing: the quantity $1-A$ is the frequency of such failures that were observed in Ref. 3. With a more complicated window, star-shaped say, the acceptance factor would also become more complicated: with some choices of window it can even be zero for certain angles. But we will not go into further details here.

B. The Tübingen triangle tiling

Let us now consider the coincidence problem for the vertices of the decagonal triangular tiling of Fig. 3. All vertex sites belong to the standard tenfold module that can be obtained by projection of the root lattice A_4 to a suitably chosen plane.[29] For simplicity, we consider the cartwheel tiling (which is singular) because it has full D_{10} symmetry in the sense that a D_{10} operation produces mismatches of density zero in the plane (along worms). We thus have coincidence fraction 1 in this case. Also, all other coincidences of the tenfold module are realized. As in the previous example, one has to correct the coincidence fraction, this time by rotating a decagon (the window of the vertex sites) and intersecting it with the original one. Let us give the correction formula in slightly more generality. If the window were a regular n-gon, the analogue of Eq. (56) would read

$$A=1-\left(\frac{\sin(\alpha/2)}{\sin(\alpha)}\right)^2 \sin(\hat{\psi})\sin(\alpha-\hat{\psi}), \tag{59}$$

where $\alpha=2\pi/n$, $\hat{\psi}=\psi-[n\psi/2\pi]\cdot 2\pi/n$, and ψ is related to φ via an algebraic conjugation.

In the present instance, this relation is that $\tan(\varphi/2)$ can be expressed in the form

$$\tan\frac{\varphi}{2}=(a+b\tau)\sin\frac{2\pi}{5}\quad (a,b\in\mathbb{Q}), \tag{60}$$

and then

$$\tan\frac{\psi}{2}=(a+b\tau')\sin\frac{4\pi}{5}, \tag{61}$$

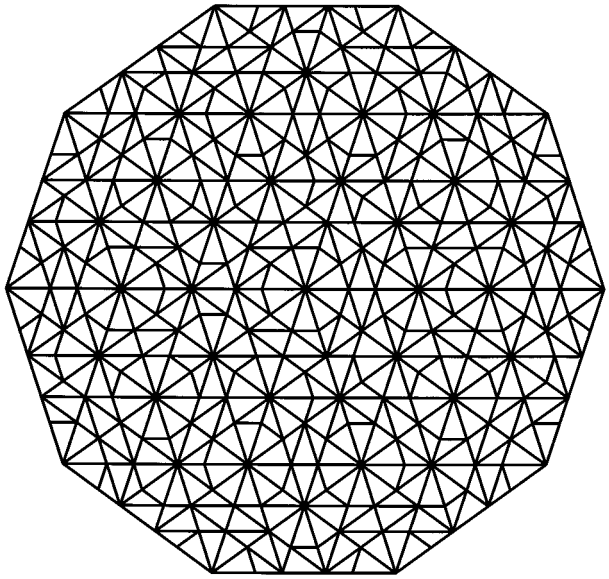

FIG. 3. Central patch of the cartwheel version of the tenfold symmetric triangle tiling.

where $\tau' = -1/\tau$ is the conjugate of τ in $\mathbb{Q}(\tau)$.

C. 12-fold symmetric tilings

As well as eight- and tenfold symmetries, twelvefold symmetry is of practical interest. Here the calculation of ψ is very similar to the eightfold case: given the angle

$$\phi = 2 \arctan(a + b\sqrt{3}) \tag{62}$$

in tiling space, one obtains the angle

$$\psi = 2 \arctan(a - b\sqrt{3}) \tag{63}$$

in internal space, which can be used with Eq. (59).

VI. BEYOND UNIQUE FACTORIZATION

In Section III, we restricted ourselves to the ''class number 1'' case, where there is essentially only one n-module. We now show how our method can be adapted to other cases, too. The smallest value of n to which Section III does not apply is 23 ($N=46$), mentioned in Ref. 21. Here, the corresponding cyclotomic field has class number 3, so there are three distinct modules with 46-fold symmetry. (The number of modules increases rapidly with n.[21,26])

A. Ideals and ideal classes

Let F be algebraic number field with ring of integers $\mathcal{O}$. The set of ideals of $\mathcal{O}$ can be extended to form a group by admitting *fractional ideals* of the form

$$\mathbf{ab}^{-1} = \{\gamma \,|\, \gamma\beta \in \mathbf{a} \forall \beta \in \mathbf{b}\}, \tag{64}$$

where **a** and **b** are ideals as defined in Section III. (A fractional ideal need not be a subset of $\mathcal{O}$.) The identity element of the group of fractional ideals is $\mathcal{O}$. A *principal ideal* is a fractional ideal of the form

$$(\gamma)_{\mathscr{O}}=\{\gamma\alpha\,|\,\alpha\in\mathscr{O}\}, \tag{65}$$

generated by the single number γ. When unique factorization into irreducible integers fails in F then some ideals must necessarily be non-principal. Two fractional ideals **a** and **b** are *equivalent* if $\mathbf{b}=\gamma\mathbf{a}$ for some $\gamma\in F$. The equivalence classes, called *ideal classes*, form a quotient group of the group of fractional ideals called the *ideal class group*, $H=H(F)$, which turns out to be finite. Its order is called the *class number*, $h(F)$. The identity element of H is the class of principal ideals.

The ideal classes inherit complex conjugation from F: each ideal class $C\in H$ has a complex conjugate class C. Complex conjugation is an automorphism of H of order 2.

B. Ideals as modules

Our definition of n-modules makes them ideals in the ring of integers of the nth cyclotomic field (and with any broader definition an n-module would certainly be equivalent to one of these). Multiplication by a complex number γ is equivalent to a combined rotation and scale change in the plane, so equivalent ideals certainly correspond to equivalent modules. Conversely, equivalent modules can be transformed into each other by multiplication by a complex number γ, and if both modules are subsets of an algebraic number field K then γ is in K and the corresponding ideals are equivalent.

So the set of n-modules up to equivalence corresponds to the class group of the nth cyclotomic field.

C. Coincidence rotations in the general case

With class number >1, n-modules are no longer all equivalent. So, for comprehensiveness, we need to consider not just $OC(\mathscr{O}_K)$ but also $OC(\mathbf{c})$ for an arbitrary ideal **c** of $\mathscr{O}_K$.

There are two problems to be overcome in extending our method to the general n-module:

(1) How to classify which of the products on the right of Eq. (30) give rise to numbers γ with $|\gamma|=1$ (when some ω_k's are non-principal ideals) and

(2) how to choose a representative of the reflection coset of OC, for modules not invariant under complex conjugation, and how to calculate coincidence indices of reflections from it.

In this subsection we address the first of these.

For the fractional ideal $\mathbf{a}\overline{\mathbf{a}}^{-1}$ to give rise to a number $\gamma\in K$ with $|\gamma|=1$ two conditions are necessary (and the conjunction of these conditions is also sufficient). They are

(A) $\mathbf{a}\overline{\mathbf{a}}^{-1}$ is principal, and

(B) for every δ such that $(\delta)_{\mathscr{O}}=\mathbf{a}\overline{\mathbf{a}}^{-1}$, $\delta\overline{\delta}=\epsilon\overline{\epsilon}$ for some unit ϵ of K.

Condition (B) arises because $\gamma=\epsilon\delta$ in Eq. (30) gives $\delta\overline{\delta}=\epsilon^{-1}\overline{\epsilon}^{-1}$. Condition (A) is tantamount to saying that the ideals **a** and $\overline{\mathbf{a}}$ are equivalent, in other words that **a** belongs to a class in H_1, the subgroup of H consisting of classes C with $C=\overline{C}$. It is easily checked that Condition (B) also depends only on the class of **a** and is preserved under multiplication and inversion of classes. For Condition (B) to be applicable at all **a** must belong to a class in H_1. Consequently Condition (B) is equivalent to **a** belonging to a class in a certain subgroup H_2 of H_1.

When Condition (B) is satisfied the numbers $\gamma=\xi\delta\epsilon^{-1}$, where ξ runs through the N roots of 1 in K, satisfy $|\gamma|=1$. In this case $\mathrm{num}(\gamma)$ is the ideal **a** and can still be defined exactly as in Eq. (24), provided that "gcd" is interpreted as meaning "the ideal generated by." Again $\mathbf{c}\cap\gamma\mathbf{c}=\mathrm{num}(\gamma)\mathbf{c}$ and the coincidence index associated with the rotation γ is $\mathrm{norm}(\mathrm{num}(\gamma))$ (independent of the ideal **c**). In the general case, when the ω's may be non-principal ideals, a member of the product group on the right of Eq. (31) is a pair (root of unity, fractional ideal of the form $\mathbf{a}\overline{\mathbf{a}}^{-1}$) and the argument of Sec. III shows that elements of $SOC(\mathbf{c})$ correspond precisely to those pairs with the class of **a** in H_2. Such pairs form a subgroup of finite index in the full product group. One can choose a set

of generators for this subgroup in much the same way as one chooses a basis for a lattice of finite index in a given lattice, and as in that case there is an infinite number of such bases and no canonical choice.

Although $SOC(\mathbf{c})$ has independent generators as a group, the set of coincidence indices in general no longer has independent generators as a semigroup.

D. Coincidence reflections in the general case

Our second problem was how to calculate indices of coincidence reflections for a module class in which no module is invariant under complex conjugation. Choose, for simplicity, a prime ideal $\mathbf{p}$ in the class (which is possible since every ideal class is known to contain infinitely many prime ideals). Then $\mathbf{p}\cap\overline{\mathbf{p}}=\mathbf{p}\overline{\mathbf{p}}$ has index norm($\mathbf{p}$) in $\mathbf{p}$. Every coincidence reflection of $\mathbf{p}$ has the form $\rho=\gamma\overline{\cdot}$ for some $\gamma\in\mathbb{C}$ with $|\gamma|=1$. Being a coincidence reflection on $\mathbf{p}$, $\rho(\alpha)=\beta$ for some $\alpha,\beta\in\mathbf{p}$. Hence $\gamma=\beta/\overline{\alpha}\in K$. The index of ρ is the index of $\mathbf{p}\cap\gamma\overline{\mathbf{p}}$ in $\mathbf{p}$ which is

$$\begin{cases} \mathrm{norm}(\mathrm{num}(\gamma))\mathrm{norm}(\mathbf{p}), & \text{if } \mathbf{p} \nmid \mathrm{num}(\gamma); \\ \mathrm{norm}(\mathrm{num}(\gamma))/\mathrm{norm}(\mathbf{p}), & \text{if } \mathbf{p} \mid \mathrm{num}(\gamma). \end{cases} \tag{66}$$

We note that there is a reflection of index 1 if and only if the class of $\mathbf{p}$ is in H_2 (when we can choose γ to be a generator of the fractional ideal $\mathbf{p}/\overline{\mathbf{p}}$) and that in that case (66) agrees with our previous way of calculating the index. When the class of $\mathbf{p}$ is not in H_2 the smallest reflection index is obtained by taking $(\gamma)=\mathbf{pa}/\overline{\mathbf{pa}}$, where $\mathbf{a}$ is the ideal of minimal norm such that the class of $\mathbf{pa}$ is in H_2. Of course, $OC(\overline{\mathbf{p}})$ is $OC(\mathbf{p})$ conjugated by reflection in the x-axis (corresponding isometries having the same index). We note that this is consistent with (66): just replace $\mathbf{p}$ and γ by their complex conjugates.

Theorem 4: *The group of coincidence rotations of a general n-fold symmetric module is the direct product of its finite rotation symmetry group C_N and countably many infinite cyclic groups which can be effectively computed and depend only on n. The index of any coincidence rotation so presented can be calculated explicitly. Any such module is equivalent to some prime ideal in the cyclotomic field of nth roots of unity, and in this form complex conjugation represents the coset of coincidence reflections whose indices can be computed from (66) (they depend not only on n but on the individual module). Such a module need not have exact reflection symmetry.*

The following table lists some statistics for the first few cyclotomic fields with $h>1$. We follow Washington[28] in listing fields with their degree, $\phi(n)$, as the primary order and n as the secondary order. For each field we give n,N,H,H_1,H_2, the smallest rotation index and the smallest reflection index of the non-principal modules (for the principal module it is always 1). In brackets after each index we give the number of different rotations or reflections with that index. For all fields on our list H_2 is the trivial subgroup consisting only of the identity element E of H. Also complex conjugation acts on the class group as multiplicative inversion for all these fields.

n	N	Degree	H	H_1	H_2	Min. rotation index		Min. reflection index of non-principal modules	
23	46	22	C_3	$\{E\}$	$\{E\}$	599	(22)	47	(11)
39	78	24	C_2	C_2	$\{E\}$	157	(24)	13	(2)
52	52	24	C_3	$\{E\}$	$\{E\}$	313	(24)	13	(1)
56	56	24	C_2	C_2	$\{E\}$	64	(2)	8	(2)
72	72	24	C_3	$\{E\}$	$\{E\}$	729	(2)	9	(1)
29	58	28	C_2^3	C_2^3	$\{E\}$	4931	(28)	59	(4)
31	62	30	C_9	$\{E\}$	$\{E\}$	5953	(30)	32 125	(1):order 9 (5):order 3

The two sets of figures in the last entry are due to the fact that non-principal modules with different orders in the class group of $\mathbb{Q}(e^{2\pi i/31})$ have different minimum reflection indices.

E. Another example: $N=46$

To illustrate the results of the previous subsection we treat in detail the case $n=23$ (with 46-fold symmetry). For this n, the class group H of K is $H=\{E,C,C^2\}$, where $C^3=E$ and $C=C^2$. Hence $H_1=\{E\}$ and therefore $H_2=\{E\}$ too. The methods of Section III show that the complex splitting primes are precisely those that are quadratic residues mod 23 and for these $\deg(p)=1$ or 11 according to whether $p\equiv 1 \bmod 23$ or not. The prime ideals $\mathbf{p}$ of $\mathcal{O}_K$ that divide a given rational prime p are either all principal or all non-principal [because the Galois group $\mathrm{Gal}(K/\mathbb{Q})$ permutes them transitively] and in the non-principal case fall into complex conjugate pairs of ideals, one from each of the classes C and C^2. We partition the set of pairs Ω into the sets Ω_1, Ω_2 as follows:

$$\Omega_1=\{\{\omega_1,\overline{\omega}_1\},\{\omega_2,\overline{\omega}_2\},\ldots\}, \tag{67}$$

$$\Omega_2=\{\{\mathbf{p}_1,\overline{\mathbf{p}_1}\},\{\mathbf{p}_2,\overline{\mathbf{p}_2}\},\ldots\}, \tag{68}$$

where the ω_i's are numbers (corresponding to principal ideals) and where in Ω_2 we have chosen $\mathbf{p}_i\in C$, $\overline{\mathbf{p}_i}\in C^2$ for each i. Finding all numbers of K on the unit circle is equivalent to finding all principal ideals with K/L-norm equal to $\mathcal{O}_L$. (The numbers γ are then the sets of associates of the generators of these ideals.) These ideals are precisely those of the form

$$\prod_l \left(\frac{\omega_l}{\overline{\omega}_l}\right)^{m_l}\prod_k \left(\frac{\mathbf{p}_k}{\overline{\mathbf{p}}_k}\right)^{n_k}, \tag{69}$$

with Σn_k divisible by 3 (since each $\mathbf{p}_k/\overline{\mathbf{p}_k}$ belongs to the class C^2 of order 3). This group of ideals has each $\omega_l/\overline{\omega}_l$ as an independent generator of the first factor, and a set of independent generators of the second factor can be chosen as follows:

$$(\mathbf{p}_1/\overline{\mathbf{p}_1})^3,\quad \overline{\mathbf{p}_1}\mathbf{p}_2/\mathbf{p}_1\overline{\mathbf{p}_2},\quad \overline{\mathbf{p}_2}\mathbf{p}_3/\mathbf{p}_2\overline{\mathbf{p}_3},\ldots\ . \tag{70}$$

Although this exhibits $SOC(\mathbf{c})$ as having independent generators as a group, the set of coincidence indices no longer has independent generators as a semigroup. Instead of basic coincidence indices one has the prime powers

$$p\ [p\equiv 1 \pmod{23}]\quad \text{and}\quad p^{11}\ [p\equiv 2,3,4,6,8,9,12,13,16,18 \pmod{23}],$$

which can be partitioned into two classes P_1 and P_2 (corresponding to Ω_1 and Ω_2) according to whether or not the prime ideals dividing p are principal. As examples:

$$599,691,829,59^{11},101^{11} \in P_1$$

and

$$47,139,277,461,967,2^{11},3^{11},13^{11},29^{11},31^{11},41^{11},71^{11},73^{11} \in P_2 .$$

These examples were computed using the observation (derived from the last paragraph of Chapter 1 of Ref. 28) that p factorizes into principal primes if and only if it factorizes into principal primes in $\mathbb{Q}(\sqrt{-23})$. A necessary and sufficient condition for this is the solubility of the Diophantine equation $6x^2+xy+y^2=p$.

The general product of these numbers has the form

$$m=p_1^{a_1}\cdots p_r^{a_r}(p_{r+1}^{11})^{a_{r+1}}\cdots(p_s^{11})^{a_s}\times\{P_1\text{-factors}\}, \tag{71}$$

where $p_1,\ldots,p_s^{11}$ are in P_2 with $p_1,\ldots,p_r\equiv 1 \pmod{23}$ and $p_{r+1},\ldots,p_s\not\equiv 1 \pmod{23}$. Now, for $k=r+1,\ldots,s$, define

$$\epsilon_k=\begin{cases}0, & \text{if } 3|a_k,\\ 1, & \text{if not.}\end{cases} \tag{72}$$

Then m is a coincidence index if and only if

$$a_1+\cdots+a_r+\epsilon_{r+1}+\cdots+\epsilon_s\neq 1. \tag{73}$$

[The reason for this is that in choosing a principal ideal giving index m we can arrange that Σn_k is divisible by 3 in (69) by changing the sign of some n_k's, provided at least two n_k's are not divisible by 3. Primes of degree 11 are divisible by only one pair of primes in K, but primes of degree 1 are divisible by 11 such pairs, so for these we can easily arrange that no n_k is divisible by 3.]

Consequently the first three rotation coincidence indices are 1, 599, 691, the smallest not composed entirely of primes $\equiv 1 \pmod{23}$ is $2^{11}47=96256$ and the smallest with no prime factors $\equiv 1 \pmod{23}$ is $2^{11}3^{11}=362797056$.

The Dirichlet series generating function of $f(m)$ can be found much as before, except that the contribution from non-principal ideals with K/L-norm equal to $\mathcal{O}_L$ must be omitted. This can be done using the three characters of the class group: we form three Dirichlet series (Hecke L-series), one for each character, by multiplying each norm in the series by the value of the character on its ideal. The required generating function is then the average of these three series.

For the principal character (identically equal to 1) the corresponding Dirichlet series is exactly as in Eq. (52), namely,

$$\left(1+\frac{1}{23^s}\right)^{-1}\frac{\zeta_K(s)}{\zeta_L(2s)}. \tag{74}$$

For a non-principal character χ the Euler factor for a prime p occurring in P_1 is exactly as in (44) and (45). For a prime p occurring in P_2, however, the Euler factor is

$$\left(\cdots+\frac{\eta}{p^{2ds}}+\frac{\eta^2}{p^{ds}}+1+\frac{\eta}{p^{ds}}+\frac{\eta^2}{p^{2ds}}+\cdots\right)^{g/2}=\left(\frac{1-2p^{-ds}}{1-p^{-ds}}\right)^{g/2}, \tag{75}$$

where $\eta^3=1$. Since this does not depend on which primitive cube root of unity η is, the Dirichlet series formed with the characters χ and $\overline{\chi}$ are the same, and we have

$$\sum_{m=1}^{\infty} \frac{f(m)}{m^s} = \frac{1}{3}\left(1+\frac{1}{23^s}\right)^{-1} \frac{\zeta_K(s)}{\zeta_L(2s)} \left\{1+2\prod_{p\in P_2}\left(\frac{1-2p^{-s}}{1+p^{-s}}\right)^{11}\prod_{q\in P_2}\left(\frac{1-2q^{-s}}{1+q^{-s}}\right)\right\},$$

where the first product is over the primes p in P_2 [which are $\equiv 1 \pmod{23}$] and the second is over the 11th powers q in P_2.

In line with earlier examples we give the first 12 nonzero terms:

$$1+\frac{22}{599^s}+\frac{22}{691^s}+\frac{22}{829^s}+\frac{22}{1151^s}+\frac{110}{2209^s}+\frac{22}{2347^s}+\frac{22}{2393^s}+\frac{22}{3037^s}$$

$$+\frac{22}{3313^s}+\frac{22}{3359^s}+\frac{22}{4463^s}+\cdots .$$

Note that this applies to all three modules.

For the principal module the reflection indices are the same as the rotation indices. For the two non-principal modules, however, the first three reflection indices are 47, 139, 277.

VII. CONCLUDING REMARKS

Let us summarize our results. We have solved the coincidence problem for planar patterns with N-fold symmetry by number theoretic methods. The first stage consisted of the analysis of lattices and modules in the plane where the coincidence indices are integers.

For various cases of interest we have given the solution explicitly, in particular describing the set of possible coincidence indices and the number of coincidence isometries with a given index. The method is described in sufficient detail to allow other examples along these lines to be worked out. This is relatively easy for $N<46$, but the complication increases astronomically for larger N as foreshadowed even in the example $N=46$, where the class number is only 3.

The second stage was the explicit investigation of discrete structures associated with a given module. Here, in the non-periodic case, the calculation of the coincidence ratio requires a non-integral correction factor. We have demonstrated its calculation in several examples.

Furthermore, the approach via algebraic number fields automatically yields sets of independent generators for the CSM group and therefore an explicit description of it. The group structure is interesting in itself because we deal here with infinite discrete groups that are countably generated and the structure of such groups is not at all obvious.

An obvious next step is to extend the investigation to $3D$ examples. This is not only an interesting extension of the technique, but may have concrete realizations. There are two cases to consider: first the T-phases, i.e., quasicrystals that have a unique quasiperiodic plane and are periodic in the third direction. The CSMs for rotations around the unique axis are the ones treated in this paper. CSMs around other axes occur only when special relations hold between the lattice constants in the plane and perpendicular to the plane, a result familiar from the hexagonal case.[2] There are also near-coincidences with small misfits between the two grains, but it is beyond our scope to deal with these. The second case is the icosahedral one, the only remaining non-crystalline symmetry in $3D$. Here we do not have such a powerful tool as the complex numbers and the structure of the CSM groups is more complicated, even the rotation part being non-Abelian in general. Some results are reported in Ref. 13 and will be described more fully in Ref. 14.

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APPENDIX A: OTHER ROTATION CENTRES

In the main text we have analyzed the standard situation of coincidence rotations around lattice (or module) points. Here we will briefly comment on rotations around other centres in the lattice case and on situations with more than one translation class of points.

1. $n=4$: the square lattice revisited

Another obvious rotation problem is that around the centre of a Delaunay cell of $\mathbb{Z}^2$, (1/2,1/2) say. This point represents the only class of deep holes of $\mathbb{Z}^2$, cf. Ref. 17, and has the entire point group D_4 of $\mathbb{Z}^2$ as site symmetry. It is obvious that the coincidence problem is equivalent to that of the point set Γ defined by

$$\Gamma=\{a+ib \,|\, a,b\in\mathbb{Z},\ \ a+b\ \ \text{odd}\}, \tag{A1}$$

which is obtained from $\mathbb{Z}^2-(1/2,1/2)$ by rotation through $\pi/4$ and dilation by $\sqrt{2}$.

Observe that (A1) can be rewritten as

$$\Gamma=\{\alpha\in\mathbb{Z}[i] \,|\, \alpha\not\equiv 0(1+i)\}, \tag{A2}$$

which solves the problem: as was shown in Sec. II, the coincidence rotations of $\mathbb{Z}^2$ can be factorized, the generators being $e^{i\varphi}=i$ (rotation through $\pi/2$) or of the form $e^{i\varphi}=\omega_p/\overline{\omega}_p$ with $N(\omega_p)=p\equiv 1\ (4)$, hence $\omega_p\not\equiv 0(1+i)$. The former still is a symmetry of Γ (index 1), and we also get the latter because both numerator and denominator are in Γ. Also, the reflection in the x-axis remains a coincidence operation of index 1. Summarizing:

$$OC(\Gamma)=OC(\mathbb{Z}^2), \tag{A3}$$

and the coincidence indices are unchanged.

2. $n=3$: the hexagonal packing

Consider the Voronoi complex of the triangular lattice—it is a packing made from regular hexagons—and let H be its vertex set. Let us consider rotations around the centre of a hexagon, which is a point of maximal site symmetry D_6. If we rotate the complex through $\pi/6$ and dilate by $\sqrt{3}$, then H can be characterized as

$$H=\{\alpha\in\mathbb{Z}[\varrho] \,|\, \alpha\not\equiv 0(1+\varrho)\} \tag{A4}$$

where $\varrho=(1+i\sqrt{3})/2$. Since $N(1+\varrho)=3$ and 3 is not a complex splitting prime in $\mathbb{Q}(\varrho)$, we find again all rotations and reflections that we had already for the triangular lattice:

$$OC(H)=OC(A_2), \tag{A5}$$

and also the indices remain unchanged.

3. $n=3$: coincidence definition revisited

Slightly different is the situation where we keep the entire set of lattice points, but rotate around the centre of a Delaunay cell: the latter is a triangle and its centre has only D_3 site symmetry. We rotate again through $\pi/6$ and dilate by $\sqrt{3}$, which gives the point set

$$G=\{\alpha\in\mathbb{Z}[\varrho]\,|\,\alpha\equiv 1(1+\varrho)\}. \tag{A6}$$

Here, a rotation through $\pi/3$ would change the congruence class of G from 1 to -1, so it is no longer a coincidence rotation. This reduces the torsion part of OC from C_6 to C_3, in agreement with the reduced site symmetry, while all other generators remain unchanged. In particular, the reflection in the x-axis leaves G invariant and the index formula applies for all remaining elements.

One might also consider possible variants of the coincidence concept here: a rotation through $\pi/3$ alone does not produce a coincidence for the set G, while the same rotation followed by a suitable *translation* can give a coincidence of index 1. The latter might be more important when the connection to grain boundary growth is considered. Indeed, especially in view of applications to nonperiodic discrete point sets, one might define (with obvious meaning)

$$\inf_{t\in\mathbb{R}^2}[P:P\cap(RP+t)], \tag{A7}$$

to be the coincidence index of an isometry R acting on a point set P. This gets rid of the dependence of the index on the rotation centre and comes closer to the idea of optimal fitting of grain fragments.

4. $n=5$: the rhombic Penrose tiling

A complication here is that the vertex sites of the rhombic Penrose tiling $\mathcal{T}$ fall into four different translation classes with respect to the uniquely defined limit translation module $\mathcal{M}(\mathcal{T})$, compare Refs. 29 and 20. We identify $\mathcal{M}(\mathcal{T})$ with the projection of the $4D$ root lattice A_4 into tiling space for definiteness. Then each point class has its own window of pentagonal shape. The windows come in two different sizes [related by a factor of $\tau=(1+\sqrt{5})/2$] and in pairs related by rotation through π, compare Ref. 29. The vertices of the rhombi are not points of the module $\mathcal{M}(\mathcal{T})$ (which also means that none of them is a ''standard'' rotation centre).

Let us now consider the coincidence problem of the set of vertex sites with all translation classes identified. To be explicit, we take the rhombic version of the cartwheel pattern where the rotation centre is not a rhombus vertex but coincides with the centre of a regular decagon filled with rhombi. This point is a representative of the fifth translation class, so far absent. The cartwheel tiling has D_{10} symmetry in the sense that any D_{10}-operation either maps the tiling upon itself (thus, in particular, the set of vertex sites) or produces at most a mismatch of density zero (along the well-known worms). All these operations thus have coincidence ratio 1. The corresponding rotation in window space maps windows to windows, because they appear in D_{10}-orbits around the origin. More than this, it maps translation classes of windows to translation classes of windows.

For other coincidence isometries, we first observe that the integral span of all vertex points is again a planar module of rank 4, in our explicit case the projection of the weight lattice A_4^*, the dual of A_4, into tiling space. This module is equivalent to $\mathcal{M}(\mathcal{T})$ and possesses therefore the same coincidence isometries, namely those described in Section III. Consequently, we find all these also as coincidence isometries of the rhombic cartwheel tiling. The coincidence ratio must now be corrected in a similar way to that of the Ammann–Beenker tiling in Sec. IV, but the window system requires a slightly more complicated calculation, which we will not present here.

Even more complicated would be the coincidence analysis for rotations around vertex points, in particular with various point classes distinguished. The methods needed are in principle those described for $n=3$ above, but details will not be given here.

5. $n=12$: a square-triangle tiling

Quasiperiodic square-triangle tilings are attractive for a number of reasons. We mention them because they can have 12-fold symmetry in the sense of mismatches of at most density zero under D_{12}-operations, see Ref. 30 for an example. There, all vertex points are in one translation class, so no problem occurs and we find all coincidence isometries of Section III. But for the correction factor due to window overlaps one encounters a new difficulty: the window is fractally shaped, and consequently we see no way of calculating this factor. It is left as an exercise for fractal readers.

APPENDIX B: PROOFS

Here we give the promised references and proofs of Facts 1–3 in Section III.

Fact 1**:** This is proved in Ref. 24 (Lemma 4) or Ref. 28 (Theorem 2.13) for example, but we sketch the proof here as it leads on naturally to the proof of Fact 2, which is less commonly found in the literature.

Let $\mathbf{P}$ be a prime factor of p in K. Since $p\nmid n$ the nth roots of 1 in K are distinct mod $\mathbf{P}$. [The most straightforward way to see this is from the identity

$$n=\prod_{k=1}^{n-1}(1-\xi^k), \tag{B1}$$

got by putting $x=1$ in $(x^n-1)/(x-1)$, and noting that every difference of roots of unity is an associate of $1-\xi^k$ for some k.] The residue class field $\mathbb{F}_{\mathbf{P}}=\mathbb{Z}[\xi]/\mathbf{P}$ is a finite field generated over $\mathbb{F}_p$ by the residue class ξ^* of ξ, and since distinct roots of unity are distinct mod $\mathbf{P}$, the order of ξ^* in $\mathbb{F}_{\mathbf{P}}$ is n. Every finite extension of $\mathbb{F}_p$ is normal with the cyclic Galois group generated by the *Frobenius automorphism* $x\mapsto x^p$, whose order is the degree d of the extension. Consequently the degree $[\mathbb{F}_{\mathbf{P}}:\mathbb{F}_p]$ is the smallest d with $\xi^{*p^d}=\xi^*$; that is, the smallest d with $n\mid(p^d-1)$. This establishes Fact 1, since $[\mathbb{F}_{\mathbf{P}}:\mathbb{F}_p]$ is the degree of the minimal polynomial satisfied by ξ mod p and hence is $\deg_K(p)$.

Fact 2**:** Analogously to the above proof, $\deg_L(p)$ is the degree d' of the residue class field extension $\mathbb{F}_{\mathbf{p}}/\mathbb{F}_p$, where $\mathbf{p}$ is the prime of L divisible by $\mathbf{P}$ and $\mathbb{F}_{\mathbf{p}}$ is the residue class field $\mathbb{Z}[\xi+\xi^{-1}]/\mathbf{p}$. Clearly $[\mathbb{F}_{\mathbf{P}}:\mathbb{F}_{\mathbf{p}}]\leqslant[K:L]=2$, so the d of Fact 1 is either d' or $2d'$. If d is odd then $d'=d$, the order of p mod n, and no power of p is congruent to -1 mod n.

To treat the case of even d we first note that if $\xi^{*k_1}+\xi^{*-k_1}=\xi^{*k_2}+\xi^{*-k_2}$ in $\mathbb{F}_{\mathbf{P}}$ (where $0\leqslant k_1,k_2<n$) then either $\xi^{*k_1}=\xi^{*k_2}$ or $\xi^{*k_1}=\xi^{*-k_2}$. This is because ξ^{*k_j},ξ^{*-k_j} are the two roots in x of

$$x^2-(\xi^{*k_j}+\xi^{*-k_j})x+1=0 \quad (j=1,2), \tag{B2}$$

and when the equations are the same the roots must match in some order. Now $d'=d/2$ if and only if $\mathbb{F}_{\mathbf{p}}$ is the unique subfield of index 2 in $\mathbb{F}_{\mathbf{P}}$, this being the fixed field of the element $x\mapsto x^{p^{d/2}}$ of order 2 in the Galois group of $\mathbb{F}_{\mathbf{P}}/\mathbb{F}_p$. So $d'=d/2$ if and only if

$$\xi^*+\xi^{*-1}=(\xi^*+\xi^{*-1})^{p^{d/2}}=\xi^{*p^{d/2}}+\xi^{*-p^{d/2}}, \tag{B3}$$

which requires $\xi^{*-1}=\xi^{*p^{d/2}}$ (equivalent to $n\mid p^{d/2}+1$), since $\xi^*\neq\xi^{*p^{d/2}}$. The exponent $d/2$ here is plainly minimal, since $n\mid p^a+1\Rightarrow n\mid p^{2a}-1$.

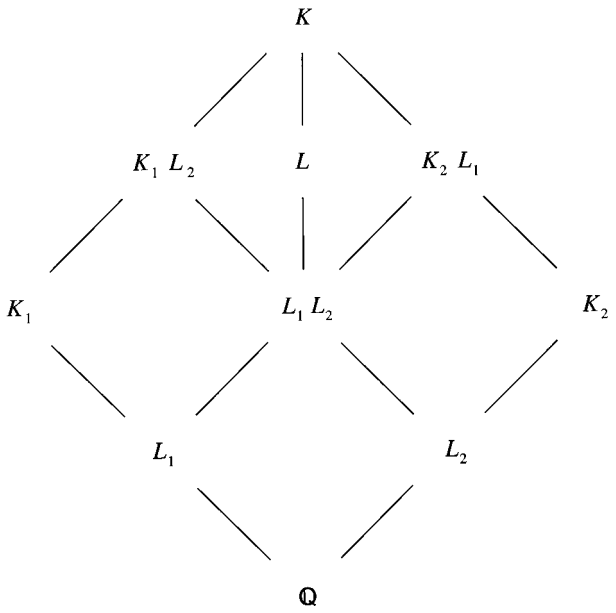

FIG. 4. Hasse diagram.

Fact 3: Part (a) is a result of the fact that when $n=p^r$ then p is totally ramified in K [that is, p is the $\phi(p^r)$th power of a degree 1 prime of K], see for example Ref. 24, Lemma 3. As a consequence $\deg_K(p)=1$ and p is not a complex splitting prime because it has only one prime factor in K.

For part (b) we refer to the Hasse diagram of field inclusions in Figure 4. Here K_1 and K_2 are the cyclotomic fields of n_1th and p^rth roots of unity and L_1 and L_2 their maximal real subfields. Then $K=K_1K_2$, the compositum of K_1 and K_2, and, since $p\nmid n_1$, $K_1\cap K_2=\mathbb{Q}$ (see Ref. 22 Thm. 9.52 or Ref. 28, Prop. 2.4). Let $\mathbf{p}=\mathbf{p}_K$ be a prime of K dividing p. For an arbitrary subfield F of K we denote by $\mathbf{p}_F$ the prime ideal of F that is divisible by $\mathbf{p}$.

Because p is unramified in L_1 and K_1 but totally ramified in K_2, it follows that $\mathbf{p}_{L_1}$ and $\mathbf{p}_{K_1}$ are totally ramified in K_2L_1 and K and, in particular,

$$\deg_{K_2L_1/L_1}(\mathbf{p}_{K_2L_1})=\deg_{K/K_1}(\mathbf{p}_K)=1. \tag{B4}$$

Consequently

$$\deg_{K/K_2L_1}(\mathbf{p})=\deg_{K_1/L_1}(\mathbf{p}_{K_1}). \tag{B5}$$

Now look at the fields L_1L_2, K_2L_1, L and K. Since $\mathbf{p}_{L_2}$ ramifies in K_2 but p is unramified in L_1, $\mathbf{p}_{L_1L_2}$ ramifies in K_2L_1 and hence in K. By Prop. 2.15(b) of Ref. 28, $\mathbf{p}_L$ is unramified in K, and hence $\mathbf{p}_{L_1L_2}$ ramifies in L. We now have

$$\deg_{L/L_1L_2}(\mathbf{p}_L)=\deg_{K_2L_1/L_1L_2}(\mathbf{p}_{K_2L_1})=1, \tag{B6}$$

whence

$$\deg_{K/L}(\mathbf{p})=\deg_{K/K_2L_1}(\mathbf{p}). \tag{B7}$$

Since $\mathbf{p_L}$ is unramified in K and $\mathbf{p}_{L_1}$ is unramified in K_1, Eqs. (B5) and (B7) imply that $\mathbf{p}_L$ factors into two primes of K if and only if $\mathbf{p}_{L_1}$ factors into two primes of K_1. Finally, $\deg_K(p) = \deg_{K_1}(p)$ is an immediate consequence of the fact that $\mathbf{p}_{K_1}$ is totally ramified in K.

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The identities of the algebraic invariants of the four-dimensional Riemann tensor

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It is well known that there are fourteen independent algebraic invariants of the four-dimensional Riemann tensor. Several authors have written down a set of fourteen independent invariants, but it is still not known how other invariants can be expressed in terms of these sets. This paper investigates this problem by looking for relationships between invariants of the Riemann tensor. Essentially the problem turns out to be analogous to finding relationships between the invariants of two 3×3 matrices, one of which is symmetric and trace-free and the other Hermitian. A number of identities between the invariants can be obtained simply by using a generalization of the Cayley–Hamilton theorem but others, which depend on the symmetry of the matrices, are considerably more complex. © *1996 American Institute of Physics.* [S0022-2488(96)03602-6]

I. INTRODUCTION

The classification of the Riemann tensor in general relativity has so far focused on the separate classifications of the Weyl tensor and the Ricci tensor. Many features of these classifications depend on properties of the algebraic invariants of both of these tensors. Any attempt to classify the Riemann tensor as a whole would also be expected to depend on the fourteen independent invariants of the Riemann tensor and the relationships between them. Over the past 50 years a number of papers have been directed towards understanding these invariants and relationships. In this time several different sets of fourteen invariants have been presented, including those by Narlikar and Karmarkar,[1] Géhéniau and Debever,[2] Greenberg,[3] Sobczyk,[4] and Sneddon.[5] The fact that a number of the sets proposed were deficient in some sense (see, for example, Sneddon[5] and Carminati and McLenaghan[6]) is an indication that this task is not as straightforward as it may seem. The main difficulty is that the relationships between the different invariants are not all that well understood. It is also the case that none of the sets proposed form a complete set of invariants. A complete set is a set of invariants $\{I_1,\ldots,I_k\}$ (which can be chosen to be homogeneous polynomial invariants) such that any other polynomial invariant can be expressed as a polynomial in $I_1,\ldots,I_k$, and none of the invariants in the set can be expressed as a polynomial function of the remainder (Penrose and Rindler,[7] Gurevich[8]). It would be expected[9] that any complete set would contain more than fourteen invariants, but that they would be connected by some algebraic relationships (syzygies).

In addition, if either the Weyl tensor or the Ricci tensor is algebraically special, the number of independent invariants will be less than in the algebraically general case. The precise number will depend on the algebraic types of these tensors.[6,10] In this case the number of independent invariants in any given set may be reduced, as some may become zero and there can be algebraic relationships between the remainder. It is possible that a set which contains fourteen independent invariants for algebraically general metrics may, for an algebraically special case, contain fewer independent invariants than the maximum allowed for that case. This cannot happen for a complete set. For such a set, in any algebraically special subcase, the number of independent invariants

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will be the maximum allowed for that case. The more recent papers of Carminati and McLenaghan[6] and Zakhary[10] (see also McIntosh and Zakhary[11]) have each produced a set of invariants with more than fourteen elements, with the knowledge that there will be relationships between them. Carminati and McLenaghan showed that for the perfect fluid and Einstein–Maxwell cases, their set will still contain the maximum number of independent invariants. Zakhary has shown that his set will have this property for any combination of Petrov type and Segre type. However, it does not follow that such a set will be complete. Zakhary has also shown which subset of his invariants will be independent in each of the algebraically special cases.

So far however the syzygies which must exist between the invariants in such sets have proved elusive and it is still an open question as to which would be the preferred set. As well as these considerations of the relationships between a (usually) small number of invariants in a complete set, there is the related problem of establishing the connection between any other invariant and those in the set. In other words, given a set containing fourteen independent invariants, how can any other invariant be expressed in terms of that set? Harvey[12] has produced a number of relationships between the invariants, but it turns out that these are not of the required type. It is the aim of this paper to find some new identities that will help provide a greater understanding of the nature of the relationships between the invariants. This may in turn lead to some insight into the relationship between the various sets of invariants that have been proposed and eventually to a complete set of invariants.

In Sec. II it is shown that the relationships given by Harvey can be written more simply in terms of the Weyl tensor and trace-free Ricci tensor and that, when $n=4$, the spinor form of many of them is actually a straightforward identity. Also one of the invariants used by Carminati and McLenaghan is expressed in a form which is consistent with the manner in which the invariants in Ref. 5 were presented. In Sec. III several identities are obtained which are valid for a pair of 3×3 matrices and a complete set of invariants is found for this case. Many of the invariants of the Riemann tensor can be expressed in terms of a pair of symmetric 3×3 matrices and in Sec. IV the results are specialized to this case. Again a complete set is obtained and it is shown how any of these invariants can be related to those in Ref. 5. In Sec. V the invariants of a trace-free symmetric matrix together with a Hermitian matrix are considered. This is precisely the situation for the Riemann tensor. A complete set has yet to be found in this case but it is shown how to obtain one further identity that could be used to express one of the 'extra' invariants of Carminati and McLenaghan in terms of those in Ref. 5. While it is possible to find several more identities of this nature, any practical use of these identities may be inhibited by their complexity.

Throughout it is assumed that the Weyl tensor and trace-free Ricci tensor are algebraically general. While the relationships obtained are still valid in the algebraically special cases, in some cases they may reduce to trivial identities. In these cases there may well be other relationships that are not valid in the algebraically general case. The notation used follows that of Sneddon.[5] The Riemann tensor R_{ijkl} can be written in terms of its irreducible parts, namely, the Weyl tensor C_{ijkl}, the trace-free Ricci tensor S_{ij} and the Ricci scalar R. If $n=4$, it is common to introduce Ψ_{ABCD} and $\Phi_{AB\dot{C}\dot{D}}$ the spinor equivalents of R_{ijkl} and S_{ij}, respectively.

For much of this work though, it is more convenient to work in the space of complex self-dual bivectors (see, for example, Buchdahl[13] or Cahen, Debever, and Defrise[14]). Buchdahl has referred to such quantities as ''rotors.'' This choice provides a reasonable compromise between the number of indices required by spinor quantities and the range of the indices (and the detailed symmetries) of the corresponding tensor quantities. Appendix A gives a summary of the main features of Buchdahl's work. Briefly, the dual of a skew-symmetric tensor f^{ij} is given by

$$*f^{ij} := \tfrac{1}{2}e^{ijkl}f_{kl},$$

where $e^{ijkl} := (1/\sqrt{-g})\epsilon^{ijkl}$. Then

$$F^A \leftrightarrow F^{ij} := \tfrac{1}{2}(f^{ij} - i\ *f^{ij})$$

is self-dual. Note that the skew-symmetric index pair is replaced by the single rotor index A which can take values from 1 to 3. (It will be clear from the context whether the indices $A,B,...$ are to be interpreted as spinor indices or rotor indices.) For the Weyl tensor, $*C^{ijkl} := \frac{1}{2}e^{ijmn}C_{mn}{}^{kl}$, $\overset{\pm}{C}{}^{ijkl} := \frac{1}{2}(C^{ijkl} \mp i\, *C^{ijkl})$ and the corresponding rotor quantities are

$$\Psi^{AB} \leftrightarrow \overset{+}{C}{}^{ijkl} \quad \text{and} \quad \dot{\overline{\Psi}}^{\dot{A}\dot{B}} \leftrightarrow \overset{-}{C}{}^{ijkl}.$$

For the trace-free Ricci tensor

$$\Gamma^{A\dot{B}} \leftrightarrow \tfrac{1}{2}(E^{ijkl} - i*E^{ijkl}),$$

where $E^{ijkl} := 2g^{[i[k}S^{l]j]}$.

The metric in this space is symmetric and is denoted by α_{AB}. Also needed are $e^{ABC} := (1/\sqrt{\alpha})\epsilon^{ABC}$ and $e_{ABC} := \sqrt{\alpha}\epsilon_{\mathrm{ABC}}$ where $\alpha := \det(\alpha_{AB})$. The trace of a matrix is denoted by square brackets (i.e., $[\Psi] := \Psi^{A}{}_{A}$). It follows that Ψ^{AB} is trace-free and symmetric, $\Gamma^{A\dot{B}}$ is Hermitian and $K := \Gamma\Gamma$ is symmetric. The trace-free part of K is denoted by L and its tensor equivalent has been referred to as the Plebanski tensor by McIntosh, Foyster and Lun.[15] With this notation, the invariants in Ref. 5 are given by

$$\begin{array}{cccc} & & [\Psi^2] & [\Psi^3] \\ [K] & [\Psi K] & [\Psi^2 K] & \\ [K^2] & [\Psi K^2] & & \\ [K^3] & & & \end{array} . \tag{1}$$

II. SOME COMMENTS ON EARLIER WORK

In 1987 Xu[16] obtained two identities relating the cubic invariants of the Riemann tensor. In a recent paper, Harvey[12] showed how these identities can be obtained easily by using the generalized Kronecker delta symbol. He then went on to find several identities between the quartic scalars. Although the identities of Xu were given in terms of R_{ijkl}, R_{ij}, and R, one of them at least came initially from a much simpler equation involving C_{ijkl}. In fact, each of the identities discussed by Harvey takes a much simpler form if it is written in terms of C_{ijkl} and S_{ij} rather than R_{ijkl} and R_{ij}. If $n=4$ and the identities are written of either spinor or bivector quantities, they simplify even further. In the case of the cubic identities this is not surprising as Xu made use of the spinor form to obtain these identities initially. This simplification occurs because the content of these identities is already ''built-in'' to the spinor and bivector formalisms and they either become trivial, or cannot be written at all in this form. Thus while these identities may be useful in simplifying terms in various action principles, they do not help in finding relationships between the invariants (1) and other invariants.

One further observation is worth noting before looking at these identities in detail. It is possible to construct eight cubic invariants from those in (1) together with R. The invariant $S^{i}{}_{j}S^{j}{}_{k}S^{k}{}_{i}$ is independent of these, and so there will be nine independent cubic invariants of the Riemann tensor. In their work on tensor polynomials, Fulling *et al.*[17] list only eight (algebraic) cubic invariants. Furthermore, Harvey's identities imply that not all of those will be independent. The reason for this discrepancy is that the scalars of Fulling *et al.* do not include those that could be obtained using e^{ijkl}. This quantity is of course available only in four dimensional spaces. Similar remarks apply to their quartic invariants.

The cubic identities discussed by Harvey are

$$\delta^{pqrst}_{abcde}R^{ab}{}_{pq}R^{cd}{}_{rs}R^{e}{}_{t} = 0 \tag{2}$$

and

$$\delta^{pqrstu}_{abcdef} R^{ab}{}_{pq} R^{cd}{}_{rs} R^{ef}{}_{tu} = 0, \tag{3}$$

and are valid for $n \leqslant 4$ and $n \leqslant 5$, respectively. Putting

$$R^{ab}{}_{cd} = C^{ab}{}_{cd} + 2\,\delta^{[a}{}_{[c} S^{b]}{}_{d]} + \tfrac{1}{12}\delta^{[a}{}_{c}\delta^{b]}{}_{d} R,$$

$$R^{a}{}_{b} = S^{a}{}_{b} + \tfrac{1}{4}\delta^{a}{}_{b} R$$

into (2) we get

$$\delta^{pqrst}_{abcde} C^{ab}{}_{pq} C^{cd}{}_{rs} S^{e}{}_{t} = 0. \tag{4}$$

This follows since, for $n=4$, terms involving δ^{aqrst}_{abcde} will disappear. The identity then reduces to

$$S^{a}{}_{b} C^{bcde} C_{acde} = 0. \tag{5}$$

(Since $S^{a}{}_{b}$ is independent of C^{abcd}, this identity is actually equivalent to the well-known identity $C^{bcde}C_{acde} = \frac{1}{4}\delta^{b}{}_{a} C^{cdef} C_{cdef}$.) Similarly, (3) is equivalent to

$$\delta^{pqrstu}_{abcdef} C^{ab}{}_{pq} C^{cd}{}_{rs} C^{ef}{}_{tu} = 0 \tag{6}$$

or

$$C^{a}{}_{c}{}^{b}{}_{d} C^{c}{}_{e}{}^{d}{}_{f} C^{e}{}_{a}{}^{f}{}_{b} = \tfrac{1}{2} C^{ab}{}_{cd} C^{cd}{}_{ef} C^{ef}{}_{gh}. \tag{7}$$

[For $n=4$, Eq. (4) is also needed to obtain Eq. (6) from Eq. (3).] This is the form in which Xu originally presented the identity and is likely to be more useful in establishing the type of identity needed to relate other invariants to (1). It is interesting to note that the identity (5) cannot even be written in the bivector form since it is impossible to construct any invariants that are of the correct degree in Ψ and Γ. Similarly, this identity cannot be written in terms of spinor quantities. The content of (5) is already included in these formalisms. Equation (7) on the other hand simply provides two different ways of writing the invariant $[\Psi^3]+[\overline{\Psi^3}]$.

Similar remarks apply to the identities for the quartic invariants. These may be written as

$$\delta^{pqrst}_{abcde} C^{ab}{}_{pq} S^{c}{}_{r} S^{d}{}_{s} S^{e}{}_{t} = 0, \tag{8}$$

$$\delta^{pqrstu}_{abcdef} C^{ab}{}_{pq} C^{cd}{}_{rs} S^{e}{}_{t} S^{f}{}_{u} = 0, \tag{9}$$

$$\delta^{pqrstuv}_{abcdefg} C^{ab}{}_{pq} C^{cd}{}_{rs} C^{ef}{}_{tu} S^{g}{}_{v} = 0, \tag{10}$$

$$\delta^{pqrstuvw}_{abcdefgh} C^{ab}{}_{pq} C^{cd}{}_{rs} C^{ef}{}_{tu} C^{gh}{}_{vw} = 0. \tag{11}$$

When expanded, these equations are considerably simpler than those given by Harvey. As in the case of Eq. (5), Eqs. (8) and (10) have no counterparts in the bivector form. Also, Eq. (9) can involve at most the invariants $[\Psi^2][K]$, $[\Psi^2 K]$, and $[\Psi\Gamma\Psi\Gamma]$. These invariants are actually independent, so (9) cannot express any new identity between them. Equation (11) though does give a useful identity. Each term in this equation will involve either $[\Psi^4]$ or $[\Psi^2]^2$. The Cayley–Hamilton theorem for the matrix Ψ can be used to prove the identity $[\Psi^4] = \frac{1}{2}[\Psi^2]^2$ and so, for $n=4$, (11) can result in (at most) the sum of this equation and its complex conjugate. It may also be noted that each of Eqs. (5) and (7) and the identities resulting from Eqs. (9) and (10) can be obtained from the single tensor identity

TABLE I. The comparison between the three sets of invariants.

Sneddon (Ref. 5)	Carminati and McLenaghan (Ref. 6)	Zakhary (Ref. 10)
R	R	R
$[\Psi^2]$	w_1	I
$[\Psi^3]$	w_2	J
$[K]$	r_1	I_6
⋯	r_2	I_7
$[K^2]$	r_3	I_8
$[K^3]$	⋯	⋯
$[\Psi K]$	m_1	K
$[\Psi^2 K]$	m_2	L
$[\Psi K^2]$	⋯	M
⋯	m_3	M_1
⋯	m_4	⋯
⋯	m_5	M_2

$$C^{[ab}{}_{ab}C^{cd}{}_{cf}\delta^{e]}{}_{g}=0 \tag{12}$$

after multiplication by appropriate tensor quantities. In other words, skew-symmetrization over five indices is sufficient to give each of these equations.

Carminati and McLenaghan[6] and Zakhary[10] have chosen sets of invariants that contain 16 and 17 real invariants, respectively. Some comments are now made on these sets. As indicated in Appendix A, there are some differences in notation which could result in a change in sign in the imaginary part of the invariant. Aside from this possibility, most of the invariants of Carminati and McLenaghan and Zakhary have an obvious counterpart in (1) and these are presented in Table I. Invariants that appear in the same row in this table are equivalent in the sense that they are proportional apart from an additive term involving invariants of lower degree. For example r_3, whose spinor form is $\Phi_{AB\dot{A}\dot{B}}\Phi^{B}{}_{C}{}^{\dot{B}}{}_{\dot{C}}\Phi^{C}{}_{D}{}^{\dot{C}}{}_{\dot{D}}\Phi^{DA\dot{D}\dot{A}}$, is proportional to $2[K^2]-3[K]^2$. The invariants of Carminati and McLenaghan that are not simply related to those of Sneddon can also be written in bivector form. To within a multiplicative constant, the correspondences are

Spinor form	Bivector form
$r_2:=\Phi_{AB\dot{A}\dot{B}}\Phi^{B}{}_{C}{}^{\dot{B}}{}_{\dot{C}}\Phi^{CA\dot{C}\dot{A}}$	$\Delta:=\frac{1}{6}e^{\dot{A}\dot{B}\dot{C}}e_{ABC}\Gamma^{A}{}_{\dot{A}}\Gamma^{B}{}_{\dot{B}}\Gamma^{C}{}_{\dot{C}}$
$m_3:=\Psi^{AB}{}_{CD}\Phi^{CD}{}_{A\dot{B}}\overline{\Psi}^{A\dot{B}}{}_{C\dot{D}}\Phi_{AB}{}^{C\dot{D}}$	$[\Psi\Gamma\overline{\Psi\Gamma}]$
$m_4:=\Psi_{A}{}^{B}{}_{DE}\Phi^{DE}{}_{A}{}^{\dot{B}}\overline{\Psi}_{B}{}^{\dot{C}}{}_{\dot{D}\dot{E}}\Phi_{B}{}^{CD\dot{E}}\Phi_{C}{}^{A}{}_{\dot{C}}{}^{\dot{A}}$	$e^{\dot{A}\dot{B}\dot{C}}e_{ABC}(\Psi\Gamma)^{A}{}_{\dot{A}}(\Gamma\overline{\Psi})^{B}{}_{\dot{B}}\Gamma^{C}{}_{\dot{C}}$
$m_5:=\Psi^{AB}{}_{CD}\Psi^{CD}{}_{EF}\Phi^{EF}{}_{\dot{E}\dot{F}}\overline{\Psi}^{\dot{E}\dot{F}}{}_{\dot{C}\dot{D}}\Phi_{AB}{}^{\dot{C}\dot{D}}$	$[\Psi^2\Gamma\overline{\Psi\Gamma}]$.

The choice of r_2 rather than $[K^3]$ is consistent with their requirement that the invariants be of lowest possible degree. The identity

$$2[K^3]-3[K][K^2]+[K]^3=6\det K=6\Delta^2. \tag{13}$$

shows that the two choices will be equivalent apart from an ambiguity in sign in Δ. This ambiguity does have some consequences, as will be seen later. [The real invariant Δ is the same as $\det(\Gamma^{A}{}_{\dot{B}})$ to within a phase factor.] The invariants m_3, m_4, and m_5 (four real invariants) are chosen instead of $[\Psi K^2]$ (two real invariants). Thus there must be two real identities connecting the invariants of this set.

Carminati and McLenaghan have also noted that the invariant

$$(C_{ade}{}^{b}-i{*}C_{ade}{}^{b})(C_{bfg}{}^{c}-i{*}C_{bfg}{}^{c})S^{de}S^{fg}S_{c}{}^{a}$$

can be factorized. Since it appears that the factorization was done initially using computer algebra, it may be of interest that it can also be done "by hand." In terms of Ψ and Γ, this invariant is proportional to

$$e^{\dot{A}\dot{B}\dot{C}}e_{ABC}\Psi^{A}{}_{E}\Gamma^{E}{}_{\dot{A}}\Psi^{B}{}_{D}\Gamma^{D}{}_{\dot{B}}\Gamma^{C}{}_{\dot{C}}.$$

In this expression, $e^{\dot{A}\dot{B}\dot{C}}\Gamma^{E}{}_{\dot{A}}\Gamma^{D}{}_{\dot{B}}\Gamma^{C}{}_{\dot{C}}$ is completely skew-symmetric in E, D, and C and so must be proportional to e^{EDC}. In fact, $e^{\dot{A}\dot{B}\dot{C}}\Gamma^{E}{}_{\dot{A}}\Gamma^{D}{}_{\dot{B}}\Gamma^{C}{}_{\dot{C}} = \Delta e^{EDC}$. The invariant then becomes $\Delta e_{ABC}e^{EDC}\Psi^{A}{}_{E}\Psi^{B}{}_{D}$ which is equal to $-\Delta\,[\Psi^2]$.

This same type of calculation can be used to write m_4 in terms of the trace of matrix products. We have

$$m_4 \propto e^{\dot{A}\dot{B}\dot{C}}e_{ABC}\Psi^{A}{}_{D}\Gamma^{D}{}_{\dot{A}}\Gamma^{B}{}_{\dot{D}}\overline{\Psi}^{\dot{D}}{}_{\dot{B}}\Gamma^{C}{}_{\dot{C}}$$

and can write $e_{ABC}\Gamma^{B}{}_{\dot{D}}\Gamma^{C}{}_{\dot{C}} = e_{\dot{E}\dot{D}\dot{C}}\Omega^{\dot{E}}{}_{A}$ where $\Gamma^{A}{}_{\dot{B}}\Omega^{\dot{B}}{}_{C} = \Delta\,\delta^{A}{}_{C}$. The characteristic equation for K, namely, $K^3-[K]K^2+(1/2)([K]^2-[K^2])K=(\det K)I$, showsthat

$$\Omega=\Delta^{-1}\overline{\Gamma}(K^2-[K]K+(1/2)([K]^2-[K^2])I).$$

After some further manipulation, we find

$$m_4\propto\Delta^{-1}([\Psi\Gamma\overline{\Psi\Gamma K}][K]-[\Psi\Gamma\overline{\Psi\Gamma}K^2]-(1/2)[\Psi\Gamma\overline{\Psi\Gamma}]([K]^2-[K^2])).$$

If m_3 is already known, the *extra* information provided by m_4 is $[\Psi\Gamma\overline{\Psi\Gamma K}][K]-[\Psi\Gamma\overline{\Psi\Gamma}K^2]$.

Finally, Zakhary[10] has shown that his set still has the correct number of independent invariants in each of the cases where either Ψ or Γ is algebraically special. In each case, by making use of the available tetrad freedom, he has shown how the components of the Weyl spinor and Ricci spinor can be constructed from these invariants.

III. INVARIANTS OF TWO 3×3 MATRICES

Initially we look for identities between invariants of two 3×3 matrices under similarity transformations. These results do not require any symmetry and so are given in terms of general matrices A and B. In this case there will be ten independent invariants (twenty if the matrices are complex) and one possible independent set is

$$\begin{array}{cccc} & [A] & [A^2] & [A^3] \\ [B] & [AB] & [A^2B] & \\ [B^2] & [AB^2] & [A^2B^2] & \\ [B^3] & & & \end{array}\quad . \tag{14}$$

Since skew-symmetrization over four indices must give zero, we have

$$A^{[A}{}_{A}B^{B}{}_{B}C^{C}{}_{C}\delta^{D]}{}_{E}=0$$

which can be expanded to give a matrix identity for A, B, and C. (This is similar to the manner in which Harvey used the generalized Kronecker delta and essentially gives a generalization of the Cayley–Hamilton theorem.) If C is replaced with B in this identity, the result is

$$AB^2+B^2A+BAB-[A]B^2-[B](AB+BA)+\tfrac{1}{2}([B]^2-[B^2])A$$

$$+([A][B]-[AB])B-([AB^2]-[B][AB]+\tfrac{1}{2}([A][B]^2-[A][B^2]))I=0. \tag{15}$$

Multiplying by A and taking the trace gives

$$2[A^2B^2]+[ABAB]-2[A][AB^2]-2[B][A^2B]-[AB]^2-\tfrac{1}{2}([A^2]-[A]^2)([B^2]-[B]^2)=0. \tag{16}$$

This equation effectively gives $[(AB)^2]$ in terms of the set (14). Several more identities can be obtained in this way. For example, the Cayley–Hamilton theorem for AB together with (16) and the identity $\det(AB) = \det A \det B$ will give an expression for $[(AB)^3]$ in terms of (14). However, there will still be some invariants that cannot be expressed in this way. (The invariant $[A^2B^2AB]$ seems to be resistant to this approach.) The possibility of using an identity involving skew-symmetrization over five indices is also unlikely to result in anything other than Eq. (15) and equations that can be found from it by simple substitutions (such as replacing A with A^2).

The set (14) together with $[A^2B^2AB]$ actually forms a complete set for the invariants of A and B. Any polynomial invariant of A and B can be expressed as a polynomial function of the elements of this set. To see this it is sufficient to consider invariants of the form $[A^iB^jA^k\cdots B^m]$ where each of the exponents $i,j,...$ has the value 1 or 2. (Any higher powers of A or B can be expressed in terms of lower powers by using the Cayley–Hamilton theorem.) The proof is essentially by induction on the degree d of the invariant. The case $d\leqslant 4$ is straightforward. If $d=5$ it is sufficient to consider $[A^2BAB]$. However, (15) can be used to show $[A^2BAB]\approx 0$, where the symbol ''$\approx$'' is used to indicate that the term on the left is equal to the term on the right plus ''a polynomial involving invariants of lower degree.'' If $d=6$ the terms to consider are $[ABABAB]$, $[A^2B^2AB]$, and $[B^2A^2BA]$. The first of these, $[(AB)^3]$, has already been dealt with and $[A^2B^2AB]$ is itself contained in the complete set. Equation (15) can now be used to show $[B^2A^2BA]\approx -[A^2B^2AB]$. For $d>6$ it is possible, by repeated use of (15) and its generalizations, to reduce any invariant to the form

$$[A^2B^2A^2B^2\cdots]+\text{''a polynomial involving invariants of lower degree.''}$$

For example,

$$[A^2B^2ABA\cdots]\approx -[A^2B^2A^2B\cdots]-[A^2B^3A^2\cdots]\approx -[A^2B^2A^2B\cdots].$$

These terms can be further reduced by using the expression for $A^4B^2+B^2A^4+A^2B^2A^2$ obtainable from (15). Thus

$$[A^2B^2A^2B\cdots]\approx -[A^4B^3\cdots]-[B^2A^4B\cdots]\approx 0.$$

The only time neither of these steps is successful in reducing the degree is for the terms $[A^2B^2AB]$ and $[B^2A^2BA]$ which have been dealt with above.

Finally, there must be a syzygy relating $[A^2B^2AB]$ to (14). It is most likely that this syzygy can be obtained by starting with

$$[C]^3-3[C][C^2]+2[C^3]=6\det C$$

and putting $C=A^2B^2AB$. This can be expected to give a cubic equation for $[A^2B^2AB]$.

IV. INVARIANTS THAT INVOLVE Ψ AND K

In the case of interest though, both Ψ and K are symmetric and Ψ is trace-free. In this case, as well as the relationship $[\Psi^2K^2\Psi K]\approx -[K^2\Psi^2K\Psi]$, we know that $[\Psi^2K^2\Psi K]$ and

$[K^2\Psi^2K\Psi]$ must be equal. Therefore $[\Psi^2K^2\Psi K]$ can be expressed as a polynomial function of the invariants (14) with A replaced by Ψ and B replaced by K. Thus the complete set in this case is

$$\begin{array}{cccc} & & [\Psi^2] & [\Psi^3] \\ [K] & [\Psi K] & [\Psi^2K] & \\ [K^2] & [\Psi K^2] & [\Psi^2K^2] & \\ [K^3] & & & \end{array} . \tag{17}$$

Since these invariants are not independent, it remains to find the identity connecting $[\Psi^2K^2]$ with the other invariants. In order to simplify the form of this identity we write it in terms of L, the trace-free part of K. (Ψ is already trace-free). We also introduce

$$\tilde{\Psi} := \Psi - uI - vL - wL^2$$

with u, v, and w chosen so that $[\tilde{\Psi}]$, $[\tilde{\Psi}L]$, and $[\tilde{\Psi}L^2]$ are all zero. This implies that

$$u = 2[L^2]([L^3][\Psi L] - [L^2][\Psi L^2])/([L^2]^3 - 6[L^3]^2),$$

$$v = ([L^2]^2[\Psi L] - 6[L^3][\Psi L^2])/([L^2]^3 - 6[L^3]^2),$$

$$w = -6([L^3][\Psi L] - [L^2][\Psi L^2])/([L^2]^3 - 6[L^3]^2).$$

The expressions for $[\tilde{\Psi}^2]$, $[\tilde{\Psi}^2L]$, $[\tilde{\Psi}^2L^3]$, and $[\tilde{\Psi}^3]$ in terms of $[\Psi^2]$ etc., are also needed. These are given in Appendix B. A basis can be chosen in which K is diagonal, and $\tilde{\Psi}^A{}_B$ and $L^A{}_B$ may be written as

$$\tilde{\Psi} = \begin{pmatrix} 0 & a & b \\ a & 0 & c \\ b & c & 0 \end{pmatrix} \quad \text{and} \quad L = \mathrm{diag}(\gamma_1, \gamma_2, -\gamma_1 - \gamma_2).$$

The expressions for $[\tilde{\Psi}^2]$, $[\tilde{\Psi}^2L]$, and $[\tilde{\Psi}^2L^2]$ in terms of a, b, c, and γ_i can be solved for a^2, b^2, and c^2 to give

$$a^2 = [2(2\gamma_1+\gamma_2)(\gamma_1+2\gamma_2)]^{-1}(-2[\tilde{\Psi}^2L^2] + 2(\gamma_1+\gamma_2)[\tilde{\Psi}^2L] + (2\gamma_1^2 + 3\gamma_1\gamma_2 + 2\gamma_2^2)[\tilde{\Psi}^2]),$$

$$b^2 = [2(\gamma_1-\gamma_2)(\gamma_1+2\gamma_2)]^{-1}(2[\tilde{\Psi}^2L^2] + 2\gamma_2[\tilde{\Psi}^2L] - (\gamma_1^2 + \gamma_1\gamma_2 + 2\gamma_2^2)[\tilde{\Psi}^2]),$$

$$c^2 = [2(\gamma_1-\gamma_2)(2\gamma_1+\gamma_2)]^{-1}(-2[\tilde{\Psi}^2L^2] - 2\gamma_1[\tilde{\Psi}^2L] + (2\gamma_1^2 + \gamma_1\gamma_2 + \gamma_2^2)[\tilde{\Psi}^2]).$$

These may now be substituted into $[\tilde{\Psi}^3]^2 = 36a^2b^2c^2$. In the resulting equation, terms involving γ_1 and γ_2 may be written in terms of $[L^2]$ and $[L^3]$. The result is the cubic equation

$$d_3[\tilde{\Psi}^2L^2]^3 + d_2[\tilde{\Psi}^2L^2]^2 + d_1[\tilde{\Psi}^2L^2] + d_0 = 0, \tag{18}$$

where

$$d_3 = -4,$$

$$d_2 = 5[L^2][\tilde{\Psi}^2],$$

$$d_1 = 2[L^2][\tilde{\Psi}^2L]^2 - 2[L^3][\tilde{\Psi}^2][\tilde{\Psi}^2L] - 2[L^2]^2[\tilde{\Psi}^2]^2,$$

$$d_0 = -\tfrac{4}{3}[L^3][\tilde{\Psi}^2L]^3 - \tfrac{1}{2}[\tilde{\Psi}^2][L^2]^2[\tilde{\Psi}^2L]^2 + \tfrac{2}{3}[\tilde{\Psi}^2]^2[L^2][L^3][\tilde{\Psi}^2L] + \tfrac{1}{4}[L^2]^3[\tilde{\Psi}^2]^3 + \tfrac{1}{18}([\tilde{\Psi}^2]^3[L^3]^2 + [\tilde{\Psi}^3]^2[L^2]^3) - \tfrac{1}{3}[\tilde{\Psi}^3]^2[L^3]^2.$$

If we substitute for $[\tilde{\Psi}^2]$, etc., in (18) we get

$$c_3[\Psi^2L^2]^3+c_2[\Psi^2L^2]^2+c_1[\Psi^2L^2]+c_0=0, \tag{19}$$

where

$$c_3=-4,$$

$$c_2=[\Psi L]^2+5[L^2][\Psi^2],$$

$$\begin{aligned}c_1=&2[L^2][\Psi^2L]^2+2[\Psi^2][\Psi L^2]^2-2[\Psi L][\Psi L^2][\Psi^2L]-2[L^3][\Psi^2][\Psi^2L]-2[L^2][\Psi^3]\\&\times[\Psi L^2]-[L^2][\Psi^2][\Psi L]^2+2[L^3][\Psi^3][\Psi L]-2[L^2]^2[\Psi^2]^2,\end{aligned}$$

$$\begin{aligned}c_0=&-\tfrac{4}{3}([L^3][\Psi^2L]^3+[\Psi^3][\Psi L^2]^3)+[\Psi^2L]^2[\Psi L^2]^2-\tfrac{1}{2}[L^2][\Psi^2]([L^2][\Psi^2L]^2+[\Psi^2]\\&\times[\Psi L^2]^2)+2[L^3][\Psi^3][\Psi^2L][\Psi L^2]-\tfrac{4}{9}[L^3][\Psi^3][\Psi L]^3+\tfrac{2}{3}[\Psi L]^2([L^3][\Psi^2][\Psi^2L]\\&+[L^2][\Psi^3][\Psi L^2])+\tfrac{1}{3}[\Psi L]([L^2]^2[\Psi^3][\Psi^2L]+[L^3][\Psi^2]^2[\Psi L^2])+\tfrac{2}{3}[L^2][\Psi^2]([L^3]\\&\times[\Psi^2][\Psi^2L]+[L^2][\Psi^3][\Psi L^2])-\tfrac{2}{3}[L^2][L^3][\Psi^2][\Psi^3][\Psi L]+\tfrac{1}{4}[L^2]^3[\Psi^2]^3\\&+\tfrac{1}{18}([L^3]^2[\Psi^2]^3+[L^2]^3[\Psi^3]^2)-\tfrac{1}{3}[L^3]^2[\Psi^3]^2.\end{aligned}$$

If required, the equations involving K can be obtained by putting $L=K-\frac{1}{3}[K]I$ in (19).

Equation (19) is valid for all trace-free symmetric matrices whether or not they are algebraically general. The fact that it is a cubic is perhaps not surprising, but it does mean that $[\Psi^2K^2]$ cannot be determined uniquely from the set (1). This is not the same as the situation when the characteristic polynomial for Ψ say is solved for its eigenvalues λ_i. In that case the different values simply amount to a relabeling of the principal directions. The different solutions of (19) however correspond to quite different relative alignments of the principal directions of Ψ and K. It is also difficult to think of an elegant method for obtaining this equation. The equation itself is not valid unless both Ψ and K are symmetric. This means that a simple approach of the type used to obtain (16) cannot be expected to be successful as those equations are valid for all matrices.

Thus (17) is a complete set for the invariants formed from Ψ and K and (19) is the syzygy connecting these invariants. Equations such as (15) can be used to write any other invariant as a function of these invariants. An alternative method for expressing other invariants in this way is to introduce the eigenvalues (λ_i and γ_i) and eigenvectors (with components $u_{(i)}{}^A$ and $v_{(i)}{}^A$) of Ψ and K. Even though the space is complex, in the algebraically general case the eigenvectors of each matrix can still be chosen to be orthonormal. In that case $\Psi^A{}_B=\Sigma_i\ \lambda_i u_{(i)}{}^A u_{(i)B}$ and $K^A{}_B=\Sigma_i\ \gamma_i v_{(i)}{}^A v_{(i)B}$. Also, the matrix $M_{ij}:=u_{(i)}{}^A v_{(j)A}$ will be orthogonal and can be calculated from the equations

$$\sum_{i,j}\ (\lambda_i)^m(\gamma_j)^n(M_{ij})^2=[\Psi^mK^n],\quad m=0,1,2,\quad n=0,1,2.$$

The ambiguities in sign can be resolved to the extent that any remaining uncertainty simply corresponds to changing the sign of one or more of the eigenvectors. [This approach also leads to an alternative derivation of (19).] Once M_{ij} is known it can be used to write down any invariant involving Ψ and K. In some sense, the six independent real invariants represented by M_{ij} can be seen as "replacing" the mixed invariants $[\Psi K]$, $[\Psi^2K]$, and $[\Psi K^2]$.

These considerations suggest that a classification scheme for the full Riemann tensor, and in particular the interaction between the Weyl tensor and the Ricci tensor, could be based on the manner in which the two sets of principal directions are aligned. It seems though that the number of possibilities could be considerable and the physical interpretation would need to be investigated. It should be noted that these questions of the interaction between the Weyl tensor and the Ricci tensor and their physical interpretation have recently been investigated by Haddow.[18] He looked at the specific cases of Einstein–Maxwell fields and perfect fluids and based his results on the manner in which the two sets of principal spinors were aligned.

V. INVARIANTS THAT INVOLVE Ψ AND Γ

The invariants that involve Γ are a little more difficult to deal with as they will involve both Ψ and $\bar{\Psi}$. However the work of the previous section does provide some assistance. The basis $\{v_{(i)}{}^{A}\}$ will also diagonalize the matrix $\Gamma^{A}{}_{\dot{B}}$. The diagonal elements μ_i will be real and will satisfy $(\mu_i)^2=\gamma_i$. We have $\Gamma^{A}{}_{\dot{B}} = \Sigma_i\ \mu_i v_{(i)}{}^{A}\bar{v}_{(i)\dot{B}}$ and it seems as though it would be possible to write down an expression for any invariant of Ψ and Γ. Some caution needs to be exercised here though as the μ_i are determined only to within a sign. Potentially there will be eight combinations of sign, but the value of Δ provides a little more information as it gives the sign of the product of the μ_i. Thus for each choice $\{\mu_1,\mu_2,\mu_3\}$ there will be another three equally valid choices, namely, $\{\mu_1,-\mu_2,-\mu_3\}$, $\{-\mu_1,-\mu_2,\mu_3\}$ and $\{-\mu_1,\mu_2,-\mu_3\}$. Any equation to be satisfied by one choice, must also be satisfied by the others. Thus any polynomial identity involving these invariants may well be of fourth degree or higher.

A simple example will illustrate this point. The combination $\sigma=\mu_1+\mu_2+\mu_3$ is an invariant, but cannot be determined uniquely from the invariants $[K]=\mu_1^2+\mu_2^2+\mu_3^2$, $\Delta=\mu_1\mu_2\mu_3$ and $[K^2]=\mu_1^4+\mu_2^4+\mu_3^4$. Even though σ is not the trace of Γ, one could imagine a diagonal matrix $\Sigma^{A}{}_{B}$ with diagonal elements μ_i. Then $[\Sigma]=\sigma$, $[\Sigma^2]=[K]$, $[\Sigma^4]=[K^2]$ and $\det\Sigma=\Delta$ and the Cayley–Hamilton theorem for this matrix can be used to show that

$$\sigma^4+[K]\sigma^2-8\Delta\sigma+2[K^2]-[K^2]^2=0. \tag{20}$$

This fourth degree polynomial is actually as much as we can find out about the invariant σ from $[K]$, $[K^2]$, and Δ. If $[K^3]$ was used (instead of Δ) the best that could be achieved would be an eighth degree polynomial, namely,

$$\sigma^8-4[K]\sigma^6+2(2[K^2]+[K]^2)\sigma^4+4([K]^3-2[K][K^2]-16\Delta^2)\sigma^2+(2[K^2]-[K]^2)^2=0,$$

where Δ^2 is given by (13). [The matrix Σ has no real significance, other than as an aid for obtaining equations such as (20).]

The appearance of (20) suggests it is unlikely there will be simple identities for invariants involving Γ. Those that might be sought initially are identities for the invariants mentioned in Sec. II that have been proposed by other authors. These are $[\Psi\Gamma\bar{\Psi}\Gamma]$, $[\Psi^2\Gamma\bar{\Psi}\Gamma]$, $[\Psi\Gamma\Psi\Gamma K]$, and $[\Psi\Gamma\Psi\Gamma K^2]$. As an example, an identity is found for $[\Psi\Gamma\bar{\Psi}\Gamma]$. In principle the same techniques can be used for others of these invariants, but the results are untidy.

We again make use of $\tilde{\Psi}$ and take $\Gamma=\mathrm{diag}(\mu_1,\mu_2,\mu_3)$. Then

$$[\tilde{\Psi}\Gamma\bar{\tilde{\Psi}}\bar{\Gamma}=2(\mu_1\mu_2 a\bar{a}+\mu_1\mu_3 b\bar{b}+\mu_2\mu_3 c\bar{c}).$$

If we put

$$\Sigma=\mathrm{diag}(2\mu_1\mu_2 a\bar{a},\ 2\mu_1\mu_3 b\bar{b},\ 2\mu_2\mu_3 c\bar{c}),$$

then

$$[\Sigma]=\sigma=[\tilde{\Psi}\Gamma\bar{\tilde{\Psi}}\bar{\Gamma}],$$

$$[\Sigma^2]=4(\gamma_1\gamma_2a^2\bar{a}^2+\gamma_1\gamma_3b^2\bar{b}^2+\gamma_2\gamma_3c^2\bar{c}^2),$$

$$[\Sigma^4]=16(\gamma_1^2\gamma_2^2a^4\bar{a}^4+\gamma_1^2\gamma_3^2b^4\bar{b}^4+\gamma_2^2\gamma_3^2c^4\bar{c}^4),$$

and

$$\det\Sigma=8\gamma_1\gamma_2\gamma_3(abc)(\bar{a}\bar{b}\bar{c})=\tfrac{2}{9}\Delta^2[\tilde{\Psi}^3][\bar{\tilde{\Psi}}^3].$$

The equation satisfied by σ is

$$\sigma^4+[\Sigma^2]\sigma^2-8(\det\Sigma)\sigma+2[\Sigma^4]-[\Sigma^2]^2=0, \tag{21}$$

and both $[\Sigma^2]$ and $[\Sigma^4]$ can be expressed in terms of the invariants (17). To accomplish this, equations can be obtained for a^2, b^2, and c^2, this time in terms of $X:=[\tilde{\Psi}^2]$, $Y:=[\tilde{\Psi}^2K]$, and $Z:=[\tilde{\Psi}^2K^2]$. It does not seem appropriate to make use of the trace-free part of K in this case. We find

$$a^2=[2(\gamma_2-\gamma_3)(\gamma_3-\gamma_1)]^{-1}(2Z-2(\gamma_1+\gamma_2)Y+(\gamma_1\gamma_2+\gamma_2\gamma_3+\gamma_1\gamma_3-\gamma_3^2)X),$$

$$b^2=[2(\gamma_1-\gamma_2)(\gamma_2-\gamma_3)]^{-1}(2Z-2(\gamma_3+\gamma_1)Y+(\gamma_1\gamma_2+\gamma_2\gamma_3+\gamma_1\gamma_3-\gamma_2^2)X),$$

$$c^2=[2(\gamma_3-\gamma_1)(\gamma_1-\gamma_2)]^{-1}(2Z-2(\gamma_2+\gamma_3)Y+(\gamma_1\gamma_2+\gamma_2\gamma_3+\gamma_1\gamma_3-\gamma_1^2)X).$$

These equations are substituted into the equations for $[\Sigma^2]$ and $[\Sigma^4]$ and terms involving γ_i are written in terms of $[K]$, $[K^2]$, and $[K^3]$. For example, f_{xx}, the numerator of the coefficient of XX in $[\Sigma^2]$, will be a symmetric function of γ_1, γ_2, and γ_3. It can be written in terms of $[K]$, $[K^2]$, and $[K^3]$ by first setting $\gamma_3=-\gamma_1-\gamma_2$ to find the term independent of $[K]$, then subtracting this from f_{xx}, dividing the result by $[K]$ and repeating the procedure. This can be carried out for all such coefficients. (The computer algebra package *Mathematica* proved indispensible at this point.) The results are

$$V^2[\Sigma^2]=f_{zz}Z\bar{Z}+f_{zy}(Z\bar{Y}+Y\bar{Z})+f_{zx}(Z\bar{X}+X\bar{Z})+f_{yy}Y\bar{Y}+f_{yx}(Y\bar{X}+X\bar{Y})+f_{xx}X\bar{X},$$

where

$$\begin{aligned}V^2:&=(\gamma_1-\gamma_2)^2(\gamma_2-\gamma_3)^2(\gamma_3-\gamma_1)^2\\&=\tfrac{1}{2}[L^2]^3-3[L^3]^2\\&=\tfrac{1}{2}[K^2]^3-3[K^3]^2+6[K][K^2][K^3]-\tfrac{7}{2}[K]^2[K^2]^2-\tfrac{4}{3}[K]^3[K^3]+\tfrac{3}{2}[K]^4[K^2]-\tfrac{1}{6}[K]^6\end{aligned} \tag{22}$$

and

$$f_{zz}=-4[K^2]^2+4[K][K^3],$$

$$f_{zy}=4[K^3][K^2]-2[K][K^2]^2-\tfrac{16}{3}[K]^2[K^3]+4[K]^3[K^2]-\tfrac{2}{3}[K]^5,$$

$$f_{zx}=2[K^3]^2+[K^2]^3-\tfrac{20}{3}[K][K^2][K^3]+3[K]^2[K^2]^2+\tfrac{8}{3}[K]^3[K^3]-\tfrac{7}{3}[K]^4[K^2]+\tfrac{1}{3}[K]^6,$$

$$f_{yy}=-4[K^3]^2+\tfrac{10}{3}[K][K^3][K^2]+\tfrac{10}{3}[K]^3[K^3]-\tfrac{10}{3}[K]^4[K^2]+\tfrac{2}{3}[K]^6$$

$$f_{yx}=-\tfrac{4}{3}[K^3][K^2]^2+[K]([K^2]^3-\tfrac{2}{3}[K^3]^2)+\tfrac{14}{3}[K]^2[K^3][K^2]-\tfrac{11}{3}[K]^3[K^2]^2-2[K]^4[K^3]$$
$$+\tfrac{7}{3}[K]^5[K^2]-\tfrac{1}{3}[K]^7,$$

$$f_{xx}=-\tfrac{1}{4}[K^2](\tfrac{14}{3}[K^3]^2+[K^2]^3)+\tfrac{11}{3}[K][K^3][K^2]^2-2[K]^2[K^2]^3+\tfrac{13}{18}[K]^2[K^3]^2$$
$$-\tfrac{11}{3}[K]^3[K^3][K^2]+\tfrac{17}{6}[K]^4[K^2]^2+\tfrac{8}{9}[K]^5[K^3]-\tfrac{7}{6}[K]^6[K^2]+\tfrac{5}{36}[K]^8.$$

The expression for $[\Sigma^4]$ has been obtained similarly and partial results are given in Appendix B. Neither of these expressions is particularly simple to deal with. It may be that these coefficients can be written more simply in terms of the trace of higher powers of K. For instance f_{zy} can be written as $4[K^3][K^2]-4[K][K^4]$. However, similar simplifications are not immediately apparent for the other terms.

We still need to use (B2) to get Eq. (21) in terms of the invariants (17) and also write $[\tilde{\Psi}\Gamma\bar{\tilde{\Psi}}\overline{\Gamma}]$ in terms of $[\Psi\Gamma\Psi\Gamma]$. The next step would be to eliminate $[\Psi^2K^2]$ which can be found from one of the solutions of the cubic (19). There will be three solutions of (19) and each one will give four solutions of (21). Thus the complete equation for $[\Psi\Gamma\Psi\Gamma]$ in terms of (1) can be expected to be of twelfth degree at least. In fact the presence of Z as well as Z in (21) means that the degree could be as high as 36.

Similar procedures can be used to find equations that will be satisfied by $[\Psi^2\Gamma\overline{\Psi\Gamma}]$, $[\Psi\Gamma\Psi\Gamma K]$, and $[\Psi\Gamma\Psi\Gamma K^2]$. Again, the degree of these equations may be as high as 36. Whether the degree is 12 or 36 it is higher than one may have expected. No doubt it is the complexity of these equations that has inhibited progress in the field.

VI. CONCLUSION

To date the nature of the relationships connecting the algebraic invariants of the Riemann tensor has been poorly understood. A number of new relationships have been proposed in this paper and, even though they should be amongst the simplest, they are more complex than may have been expected. The use of the bivector formalism makes some aspects of the problem a little more straightforward. It is shown that the invariants of other authors can also be expressed simply in terms of bivectors and much of the problem is then reduced to finding relationships between invariants (under similarity transformations) of two 3×3 matrices.

For invariants involving Ψ and K only, a complete set of invariants (17) has been found. Equation (19) is the syzygy connecting them and can be seen as an equation to obtain $[\Psi^2K^2]$ from (1). All other invariants involving Ψ and K can be written as polynomial functions of this set by using equations such as (15). Alternatively, any invariant can be written (at least in principle) in terms of the eigenvalues of Ψ and K and the rotation matrix, M_{ij}, which connects their eigenvectors. This would entail the solution of two cubic equations for the eigenvalues, a cubic equation for $[\Psi^2K^2]$, and a set of linear equations for the M_{ij}.

A complete set for invariants involving Ψ and Γ has yet to be found. On the other hand if μ_i, the diagonal elements of the diagonalized matrix $\Gamma^{A}{}_{\dot{B}}$, are known it would still be possible to write any invariant in terms of M_{ij} together with μ_i and the eigenvalues of Ψ. Ideally, each of the sets of invariants of Carminati and McLenaghan and Zakhary could be connected by (respectively) two or three real identities. Though this has not been accomplished, it has been shown how to obtain relationships connecting m_3, m_4, and m_5 with the invariants (1). Equation (21) is one such relationship for m_3 though the coefficients of σ^i in this equation are quite complicated. Similar procedures could be used to find relationships for m_4 and m_5.

Overall, one may have hoped for less complicated relationships between the invariants. It may be possible to find a complete set for invariants involving Ψ and Γ together with a set of syzygies that are not as complicated as (21). Clearly more work needs to be done to achieve this goal. Also, the possibility of a different approach should not be ruled out, but the present work offers no suggestion as to what form such an approach might take.

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APPENDIX A: ROTOR SPACE

This appendix summarises the main features needed from Buchdahl's work on rotor calculus.[13] In keeping with that work, and so as to avoid the likely confusion of spinor indices and rotor indices, the less common notation of using Greek letters for spinor indices has been adopted for this appendix. Also, Buchdahl uses a different definition for the dual of a bivector, namely, ${}^{\dagger}f^{kl}=-\frac{1}{2}ie^{klmn}f_{mn}$. However, the requirement for a bivector to be self-dual is equivalent to that used in the main text and so the content of the results will be unaffected. This requirement is also seen to be consistent with that of Penrose and Rindler when account is taken of their choice of $e_{0123}>0$ rather than $e^{1234}>0$.

In the same way that spinors and vectors are related by the matrices $\sigma_{k\mu\dot{\nu}}$, a self-dual bivector F_{kl} can be written in terms of a rotor ϕ^A by the equation

$$F_{kl}=\tfrac{1}{2}\tau_{Akl}\phi^A, \tag{A1}$$

where the connecting matrices τ_{Akl} are skew-symmetric and self-dual in the indices k and l. The covariant components ϕ_A are given by $\phi_A=\alpha_{AB}\phi^A$ where

$$\alpha_{AB}=\tfrac{1}{4}\tau_{Akl}\tau_B{}^{kl}$$

is the metric to be used in rotor space. This choice will ensure that $F_{kl}F^{kl}=\phi_A\phi^A$ and it follows that the inverse relation to (A1) is

$$\phi^A=\tfrac{1}{2}\tau^{Akl}F_{kl}.$$

The alternating symbol in rotor space, ϵ^{ABC}, can now be introduced together with $e^{ABC}:=(1/\sqrt{\alpha})\epsilon^{ABC}$ and $e_{ABC}:=\sqrt{\alpha}\epsilon_{ABC}$ where $\alpha:=\det(\alpha_{AB})$. It can also be shown that

$$\tau_{Ak}{}^{m}\tau_{Blm}=g_{kl}\alpha_{AB}-e_{ABC}\tau^{C}{}_{kl}$$

which can be seen as a defining relation for the τ-matrices. If ϕ^A is any rotor, its complex conjugate will be denoted by $\bar{\phi}^{\dot{A}}$ (or more simply by $\phi^{\dot{A}}$) and the bivector $\frac{1}{2}\tau_{\dot{A}kl}\phi^{\dot{A}}$ will be anti-self-dual.

The relationship between the Weyl tensor and Ψ^{AB} is given by

$$\Psi^{AB}=\tfrac{1}{4}\tau^{A}{}_{kl}\tau^{B}{}_{mn}C^{klmn}=\tfrac{1}{4}\tau^{A}{}_{kl}\tau^{B}{}_{mn}\overset{+}{C}{}^{klmn}. \tag{A2}$$

The matrix $\Gamma^{A\dot{B}}$ can be related directly to S_{kl} by

$$\Gamma^{A\dot{B}}=\tfrac{1}{2}\hat{T}^{A\dot{B}kl}S_{kl}. \tag{A3}$$

where $\hat{T}^{A\dot{B}kl}:=\tau^{Akm}\tau^{\dot{B}l}{}_{m}$ is trace-free and symmetric in k and l and Hermitian in A and $\dot{B}$. The inverse of (A3) is

$$S_{kl}=\hat{T}_{A\dot{B}kl}\Gamma^{A\dot{B}}.$$

Rotors can also be related directly to symmetric two-index spinors by using the connecting matrices $\lambda_{A\mu\nu} := \frac{1}{2}\tau_A{}^{kl} S_{kl\mu\nu}$. Here, $S^{kl\mu}{}_{\nu} := \sigma^{[k\mu\dot{\lambda}}\sigma^{l]}{}_{\nu\dot{\lambda}}$ is self-dual in k and l. Thus a rotor ϕ^A can be expressed in terms of a symmetric two-index spinor $f_{\mu\nu}$ by

$$\phi_A = \lambda_{A\mu\nu} f^{\mu\nu}. \tag{A4}$$

It can be shown that $\lambda_{A\mu\nu}\lambda^{A\alpha\beta} = 2\,\delta^{\alpha}{}_{(\mu}\delta^{\beta}{}_{\nu)}$ and so the inverse of (A4) is

$$f_{\mu\nu} = \tfrac{1}{2}\lambda_{A\mu\nu}\phi^A. \tag{A5}$$

It also follows that $f_{\mu\nu}f^{\mu\nu} = \frac{1}{2}\phi_A\phi^A$ and the λ-matrices satisfy

$$\lambda_{A\mu\alpha}\lambda_{B\nu}{}^{\alpha} = \epsilon_{\mu\nu}\alpha_{AB} + e_{ABC}\lambda^{C}{}_{\mu\nu}.$$

Equations (A4)–(A5) differ by a factor of 2 from those in Ref. 13. This difference will ensure that the spinor $\Psi_{\mu\nu\rho\sigma}$ obtained from Ψ^{AB} in this way will correspond to the usual choice of the Weyl spinor. There is however one further difference between this notation and the notation used by Carminati and McLenaghan. In their work, self-dual bivectors are associated with spinors with dotted indices. For example, their invariant w_1 (whose spinor form is $\Psi_{\mu\nu\rho\sigma}\Psi^{\mu\nu\rho\sigma}$) is equal to $\frac{1}{4}$ $\overset{-}{C}_{klmn}\overset{-}{C}{}^{klmn}$. In our notation it would be equal to $\frac{1}{4}\overset{+}{C}_{klmn}\overset{+}{C}{}^{klmn}$. The difference arises from a different realization of the connection matrices $\sigma_{k\mu\dot{\nu}}$ in terms of the Pauli matrices. (Compare for example the choice in Penrose and Rindler with that of Corson,[19] noting that Corson gives expressions for $\sigma_{k\dot{\nu}\mu}$, the transpose of $\sigma_{k\mu\dot{\nu}}$.) In fact, in the realization given by Penrose and Rindler, $S^{kl\mu\nu}$ as defined above is anti-self-dual. As a consequence, if an invariant such as $\Psi_{\mu\nu\rho\sigma}\Psi^{\mu\nu\rho\sigma}$ is expressed in terms of the components of the Riemann tensor, the different conventions will lead to expressions which are complex conjugates of each other.

APPENDIX B: ADDITIONAL EQUATIONS

This appendix contains some of the equations that were considered too lengthy for the main text. The first set of equations expresses invariants involving $\tilde{\Psi}$ in terms of those involving Ψ. These are

$$[\tilde{\Psi}^2] = [\Psi^2] - \tfrac{1}{2}V^{-2}([L^2]^2[\Psi L]^2 - 12[L^3][\Psi L][\Psi L^2] + 6[L^2][\Psi L^2]^2),$$

$$[\tilde{\Psi}^2 L] = [\Psi^2 L] + \tfrac{1}{2}V^{-2}([L^2][L^3][\Psi L]^2 - 2[L^2]^2[\Psi L][\Psi L^2] + 6[L^3][\Psi L^2]^2),$$

$$[\tilde{\Psi}^2 L^2] = [\Psi^2 L^2] + \tfrac{1}{2}V^{-2}((2[L^3]^2 - \tfrac{1}{2}[L^2]^3)[\Psi L]^2 + 2[L^2][L^3][\Psi L][\Psi L^2] - [L^2]^2[\Psi L^2]^2),$$

$$\begin{aligned}[\tilde{\Psi}^3] = [\Psi^3] &- \tfrac{1}{2}V^{-2}(6[L^2]([L^3][\Psi L] - [L^2][\Psi L^2])[\Psi^2] + 3([L^2]^2[\Psi L] \\ &- 6[L^3][\Psi L^2])[\Psi^2 L] - 18([L^3][\Psi L] - [L^2][\Psi L^2])[\Psi^2 L^2] + 4[L^3][\Psi L]^3 \\ &- 6[L^2][\Psi L^2][\Psi L]^2 + 12[\Psi L^2]^3),\end{aligned} \tag{B1}$$

where V is given by Eq. (22). In terms of K these equations become

$$\begin{aligned}[\tilde{\Psi}^2] = [\Psi^2] &- \tfrac{1}{2}V^{-2}(([K^2]^2 + 8[K][K^3] - 6[K]^2[K^2] + [K]^4)[\Psi K]^2 \\ &+ (-12[K^3] + 4[K][K^2])[\Psi K][\Psi K^2] + (6[K^2] + 2[K]^2)[\Psi K^2]^2),\end{aligned}$$

$$[\tilde{\Psi}^2K]=[\Psi^2K]-\tfrac{1}{2}V^{-2}((-[K^2][K^3]+\tfrac{1}{3}[K]^2[K^3]+[K]^3[K^2]-\tfrac{1}{3}[K]^5)[\Psi K]^2$$
$$+(2[K^2]^2+4[K][K^3]-8[K]^2[K^2]+2[K]^4)[\Psi K][\Psi K^2]$$
$$+(-6[K^3]+8[K][K^2]-2[K^3])[\Psi K^2]^2),$$

$$[\tilde{\Psi}^2K^2]=[\Psi^2K^2]-\tfrac{1}{2}V^{-2}((-2[K^3]^2+\tfrac{1}{2}[K^2]^3+\tfrac{14}{3}[K][K^2][K^3]-\tfrac{7}{2}[K]^2[K^2]^2$$
$$-2[K]^3[K^3]+\tfrac{17}{6}[K]^4[K^2]-\tfrac{1}{2}[K]^6)[\Psi K]^2+(-2[K^2][K^3]+2[K][K^2]^2$$
$$+\tfrac{14}{3}[K]^2[K^3]-6[K]^3[K^2]+\tfrac{4}{3}[K]^5)[\Psi K][\Psi K^2]+([K^2]^2-4[K][K^3]$$
$$+4[K]^2[K^2]-[K]^4)[\Psi K^2]^2),$$

$$[\tilde{\Psi}^3]=[\Psi^3]-\tfrac{1}{2}V^{-2}((6[K^2][K^3][\Psi K]-[K^2]^2[\Psi K^2]-3[K][K^2]^2[\Psi K]+6[K][K^3][\Psi K^2]$$
$$-8[K]^2[K^3][\Psi K]+6[K]^3[K^2][\Psi K]-[K]^5[\Psi K])[\Psi^2]+(3[K^2]^2[\Psi K]-18[K^3]$$
$$\times[\Psi K^2]+24[K][K^3][\Psi K]+6[K][K^2][\Psi K^2]-18[K]^2[K^2][\Psi K]+3[K]^4[\Psi K])$$
$$\times[\Psi^2K]+(-18[K^3][\Psi K]+18[K^2][\Psi K^2]+6[K][K^2][\Psi K]-6[K]^2[\Psi K^2])[\Psi^2K^2]$$
$$+(4[K^3]-4[K]^3)[\Psi K]^3+(-6[K^2]+18[K]^2)[\Psi K^2][\Psi K]^2-24[K][\Psi K][\Psi K^2]$$
$$+12[\Psi K^2]^3). \tag{B2}$$

The other set of equations is for $[\Sigma^4]$. $[\Sigma^4]$ is given by

$$V^4[\Sigma^4]=f_{zzz\bar{z}}ZZZ\bar{Z}+f_{zzz\bar{y}}(ZZZ\bar{Y}+ZYZ\bar{Z})+f_{zzz\bar{x}}(ZZZ\bar{X}+ZXZ\bar{Z})+f_{zzy\bar{y}}(ZZY\bar{Y}+YYZ\bar{Z})$$
$$+f_{zzy\bar{x}}(ZZY\bar{X}+YXZ\bar{Z})+f_{zzx\bar{x}}(ZZX\bar{X}+XXZ\bar{Z})+f_{zy\bar{z}}ZYZ\bar{Y}+f_{zy\bar{z}}(ZY\bar{Z}\bar{X}+ZX\bar{Z}\bar{Y})$$
$$+f_{zyy\bar{y}}(ZY\bar{Y}\bar{Y}+YYZ\bar{Y}+f_{zyy\bar{x}}(ZY\bar{Y}\bar{X}+YXZ\bar{Y}+f_{zyx\bar{x}}(ZY\bar{X}\bar{X}+XXZ\bar{Y})+f_{zx\bar{z}x}ZX\bar{Z}\bar{X}$$
$$+f_{zxy\bar{y}}(ZX\bar{Y}\bar{Y}+YYZ\bar{X})+f_{zxy\bar{x}}(ZX\bar{Y}\bar{X}+YX\bar{Z}\bar{X})+f_{zxx\bar{x}}(ZX\bar{X}\bar{X}+XXZ\bar{X})+f_{yyy\bar{y}}YY\bar{Y}\bar{Y}$$
$$+f_{yyy\bar{x}}(YY\bar{Y}\bar{X}+YX\bar{Y}\bar{Y})+f_{yyx\bar{x}}(YY\bar{X}\bar{X}+XX\bar{Y}\bar{Y})+f_{yx\bar{y}x}YX\bar{Y}\bar{X}$$
$$+f_{yx\bar{x}x}(YX\bar{X}\bar{X}+XX\bar{Y}\bar{X})+f_{xx\bar{x}x}XX\bar{X}\bar{X}. \tag{B3}$$

The coefficients f are given below. Only the part not involving $[K]$ is given. The full equations are available from the author.

$$f_{zzz\bar{z}}=-16[K^2](3[K^3]^2-[K^2]^3)+[K]\times\{\cdots\},$$

$$f_{zzz\bar{y}}=32[K^3]([K^3]^2-\tfrac{2}{3}[K^2]^3)+[K]\times\{\cdots\},$$

$$f_{zz\bar{z}x}=8[K^2]^2(2[K^3]^2-[K^2]^3)+[K]\times\{\cdots\},$$

$$f_{zzy\bar{y}}=8[K^3]^2[K^2]^2+[K]\times\{\cdots\},$$

$$f_{zzy\bar{x}}=\tfrac{16}{3}[K^3][K^2]^4+[K]\times\{\cdots\},$$

$$f_{zz\overline{xx}}=[K^2]^6+\tfrac{4}{9}[K^3]^2(3[K^3]^2-2[K^2]^3)+[K]\times\{\cdots\},$$

$$f_{zy\overline{zy}}=32[K^3]^2[K^2]^2+[K]\times\{\cdots\},$$

$$f_{zy\overline{zx}}=\tfrac{32}{3}[K^3][K^2]^4+[K]\times\{\cdots\},$$

$$f_{zy\overline{yy}}=-16[K^3]^3[K^2]+[K]\times\{\cdots\},$$

$$f_{zy\overline{yx}}=-\tfrac{16}{9}[K^3]^2(6[K^3]^2+5[K^2]^3)+[K]\times\{\cdots\},$$

$$f_{zy\overline{xx}}=-\tfrac{4}{3}[K^3][K^2]^2(2[K^3]^2+[K^2]^3)+[K]\times\{\cdots\},$$

$$f_{zx\overline{zx}}=4[K^2]^6+\tfrac{16}{9}[K^3]^2(3[K^3]^2-2[K^2]^3)+[K]\times\{\cdots\},$$

$$f_{zx\overline{yy}}=-\tfrac{8}{9}[K^3]^2(6[K^3]^2+5[K^2]^3)+[K]\times\{\cdots\},$$

$$f_{zx\overline{yx}}=-\tfrac{8}{3}[K^3][K^2]^2(2[K^3]^2+[K^2]^3)+[K]\times\{\cdots\},$$

$$f_{zx\overline{xx}}=-\tfrac{1}{2}[K^2]^7-\tfrac{2}{9}[K^3]^2[K^2](9[K^3]^2+[K^2]^3)+[K]\times\{\cdots\},$$

$$f_{yy\overline{yy}}=\tfrac{4}{9}[K^3]^2(12[K^3]^2+[K^2]^3)+[K]\times\{\cdots\},$$

$$f_{yy\overline{yx}}=\tfrac{16}{3}[K^3]^3[K^2]^2+[K]\times\{\cdots\},$$

$$f_{yy\overline{xx}}=\tfrac{2}{3}[K^3]^2[K^2](2[K^3]^2+[K^2]^3)+[K]\times\{\cdots\},$$

$$f_{yx\overline{yx}}=\tfrac{8}{3}[K^3]^2[K^2](2[K^3]^2+[K^2]^3)+[K]\times\{\cdots\},$$

$$f_{yx\overline{xx}}=\tfrac{1}{3}[K^3][K^2]^6-\tfrac{4}{27}[K^3]^3(3[K^3]^2-11[K^2]^3)+[K]\times\{\cdots\},$$

$$f_{xx\overline{xx}}=\tfrac{1}{16}[K^2]^8+\tfrac{1}{36}[K^3]^2[K^2]^2(17[K^3]^2+5[K^2]^3)+[K]\times\{\cdots\}. \tag{B4}$$

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Conformal Lorentz geometry revisited

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The group U(2,2) and its subgroup SU(2,2) were considered by Penrose in his study of the conformal compactification $\mathscr{M}$ of the Minkowski space M [R. Penrose and W. Rindler, *Spinors and Space-Time* (Cambridge University, Cambridge, 1986) and R. O. Wells, Jr., Bull. Am. Math. Soc. **I**, 2 (1979)]. The standard representation of SU(2,2) in $\mathbb{C}^4$ and in $\mathscr{M}$ are the corner stones of twistor theory, which was created by Penrose to the double purpose of obtaining new solutions of Einstein equations and new insights on gravitational radiation. We think that other representations of SU(2,2) or U(2,2) could also bring some information in relativity [see also, Barut O. Asjim, in *Noncompact Lie Groups and some of their Applications*, edited by E. A. Tanner and R. Wilson (Kluwer Academic, Dordrecht, 1994), p. 103] and, accordingly, we propose an extension of Penrose twistor program. In this paper we deal with a new U(2,2)-space, which we denote by W. We show first that the SU(2,2)-space $\mathscr{M}$ introduced by Penrose is isomorphic to U(2), endowed with an action of SU(2,2) given by *non-Abelian* homographic transformations. These transformations keep invariant the equation $\det(u-v)=0$, characterizing the pairs $(u,v)\in \mathrm{U}(2)\times\mathrm{U}(2)$ such that "u lies on the light-cone of v." By definition, our space W consists of all pairs $(u,v)\in \mathrm{U}(2)\times\mathrm{U}(2)$ satisfying the condition $\det(u-v)\neq 0$. The starting point of this article is the observation that W carries an SU(2,2)-invariant pseudo-Riemannian metric $L:=\mathrm{Tr}[(u-v)^{-1}\dot{u}\times(u-v)^{-1}\dot{v}]$, of signature (4,4). (W,L) is in fact an irreducible symmetric space in Cartan's sense, which is isomorphic to the quotient $\mathrm{SO}(2,4)/S[\mathrm{O}(1,1)\times\mathrm{O}(1,3)]$. As an irreducible symmetric space, it is an 8-dimensional Einstein space, whose Ricci tensor is proportional to the metric tensor. We study the geodesic paths of this space giving the general solutions in terms of initial data and studying the constants of motion. In particular we determine the geodesic paths which exhibit two periods. We also show that Mach's principle on inertial motions receives an explanation in our theory by considering the particular geodesic paths, for which one of the partners of an interacting pair is fixed and sent to infinity. In fact we study a dynamical system (W,L) which presents some formal and topological similarities with a system of two particles interacting gravitationally. (W,L) is the *only* conformally invariant relativistic two-point dynamical system. At the end we show that W can be naturally regarded as the base of a principal $\mathrm{GL}(2,\mathbb{C})$-bundle which comes with a natural connection. We study this bundle from differential geometric point of view. Physical interpretations will be discussed in a future paper. This text is an improvement of a previous version, which was submitted under the title "Hypertwistor Geometry." [See, K. Teleman, "Hypertwistor Geometry (abstract)," 14th International Conference on General Relativity and Gravitation, Florence, Italy, 1995.] The change of the title and many other improvements are due to the valuable comments of the referee, who also suggested the author to avoid hazardous interpretations. © *1996 American Institute of Physics.* [S0022-2488(96)03702-5]

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I. A NATURAL CONFORMAL STRUCTURE ON U(2)

The unitary group U(2) has an underlying structure of a compact 4-manifold, which is diffeomorphic to $S^1\times S^3$. The Minkowski space can be identified with the space M of 2×2 Hermitian matrices. For each $a\in \mathrm{U}(2)$ there is a Cayley map

$$C_a: M\to \mathrm{U}(2), \quad x\mapsto u=-a(I+ix)(I-ix)^{-1}.$$

The inverse is given by the formula $x=i(a-u)^{-1}(a+u)$ and is defined on the image of C_a, which is the subset U_a of U(2) consisting of all unitary matrices u satisfying $\det(a-u)\neq 0$ (the complement of the "light-cone" of a). Therefore, the images of the Cayley maps are open dense subsets of U(2).

Remark: The use of the Cayley maps enables us to give physical interpretations to objects in U(2) by passing to the Minkowski space. For instance, the relations

$$\det(u-v)=0; \quad \det\left(\frac{du}{dt}\right)=0; \quad \det\left(u^*\,\frac{du}{dt}\right)<0$$

characterize light intervals, light trajectories, and massive particle trajectories, respectively. Using the Cayley maps one can easily show that the space

$$W:=\{(u,v)\in \mathrm{U}(2)\times \mathrm{U}(2)\,|\det(u-v)\neq 0\}$$

is diffeomeorphic to the product $\mathrm{U}(2)\times M$. On the other hand, U(2) carries a conformally flat Lorentz metric, namely,

$$\rho:=-\det(u^*\,du),$$

and the group U(2,2) acts on U(2) through (non-Abelian) "homographic" transformations:

$$u\mapsto u':=(Au+B)(Cu+D)^{-1},$$

where A,B,C,D are 2×2-matrices such that

$$\begin{pmatrix} A & B\\ C & D\end{pmatrix}\in \mathrm{U}(2,2).$$

The action is not faithful, since matrices in the center Z of U(2,2) act by identity. The quotient $\mathrm{U}(2,2)/Z$ is isomorphic to SO(2,4) and, as an SO(2,4)-space, U(2) is isomorphic to the quadric $Q\subset \mathbb{P}^5(\mathbb{R})$ defined by the equation

$$x_1^2+x_2^2-x_3^2-x_4^2-x_5^2-x_6^2=0.$$

An isomorphism is given by the map

$$[x_1,x_2,x_3,x_4,x_5,x_6]\mapsto (x_1+ix_2)^{-1}\begin{pmatrix} x_3+ix_4 & x_5+ix_6\\ -x_5+ix_6 & x_3-ix_4\end{pmatrix}.$$

The above formula for the U(2,2)-action on U(2) implies that, for a path $u(\cdot)$ in U(2), we have

$$\frac{du'}{dt}=(AC^{-1}D-B)(Cu+D)^{-1}C\,\frac{du}{dt}\,(Cu+D)^{-1},$$

and it follows that

Remark 1: The conformal structure of U(2) *defined by the metric* ρ *is invariant under the action of* U(2,2)*, and that the Cayley maps are local conformal equivalences. Endowed with this structure,* U(2) *is a conformal compactification of the Minkowski space* M.

It is also worthwile to note that the isotropy subgroup at $-I$ is the subgroup of U(2,2) formed by the matrices

$$\frac{1}{2}\begin{pmatrix} ixg+g+(g^*)^{-1} & ixg+g-(g^*)^{-1} \\ -ixg+g-(g^*)^{-1} & -ixg+g+(g^*)^{-1} \end{pmatrix},$$

with $g\in \mathrm{GL}(2,\mathbb{C})$ and $x^*=x$.

II. CONFORMAL INVARIANTS

In this section we explain how ideas from the classical projective geometry can be extended in the non-Abelian context in order to obtain conformal invariants in our geometry.

If R is a (possibly noncommutative) ring with unit element, we can define the projective line over R to be the quotient $\mathbb{P}^1(R):=R_0^2/R^*$, where R^* denotes the multiplicative group of invertible elements and R_0^2 is the subset of R^2 consisting of pairs r,s with r or s invertible. R_0^2 is an R^*-space via the diagonal right action. R itself can be regarded as an affine line and can be embedded in $\mathbb{P}^1(R)$ via $u\mapsto[u,1]$. If $x=[r,s]\in\mathbb{P}^1(R)$, we say as usual that r and s are homogeneous coordinates of x.

For a system $(A,B,C,D)\in(R^*)^4$ with $(A^{-1}B-C^{-1}D)$ invertible, the corresponding ''conformal transformation''

$$[r,s]\mapsto[(Ar+Bs),\ (Cr+Ds)]$$

is not everywhere defined in general, but it is formally invertible.

In the classical (Abelian) projective geometry it is shown that the biratio associated with four points on the projective line is invariant under conformal transformations. If the four points lie on the affine line, the biratio is defined by

$$(u,v;u_1,v_1):=(u-u_1)(u_1-v)^{-1}(v-v_1)(v_1-u)^{-1}.$$

In the noncommutative case the expressions $(u-v)$, $(u,v;u_1,v_1)$ change under a conformal transformation according to the laws:

$$\begin{aligned}(u-v)&\mapsto(AC^{-1}D-B)(Cu+D)^{-1}C(u-v)(Cv+D)^{-1}\\ &=(AC^{-1}D-B)(Cv+D)^{-1}C(u-v)(Cu+D)^{-1},\end{aligned}$$

$$(u,v;u_1,v_1)\mapsto[(AC^{-1}D-B)(Cu+D)^{-1}C](u,v;u_1,v_1)[(AC^{-1}D-B)(Cu+D)^{-1}C]^{-1}$$

which shows that the biratio is still a *relative* invariant, i.e., invariant up to an inner automorphism of the ring.

The point is now that if R is a ring of matrices, the determinant and the trace of the biratio give *absolute* invariants, since det and Tr are conjugacy-invariant polynomials on the ring of matrices. Moreover, the relation of **harmonic conjugation** $(u,v;u_1,v_1)=-I$ is (absolute) invariant, as in the classical Abelian case.

Supposing now that u,u_1 and v,v_1 are points moving on two distinct or identical paths in U(2) and making u_1 or v_1 to approach u or v, we obtain as limits the following differential relative invariants:

$$I_1:=\dot{u}(u-v)^{-1}(v-v_1)(u-v_1)^{-1},\quad I_2:=\ddot{u}\dot{u}^{-1}-2\dot{u}(u-v)^{-1},\quad I_3:=(\dddot{u}-\tfrac{3}{2}\ddot{u}\dot{u}^{-1}\ddot{u})\dot{u}^{-1},$$

and

$$I_4 := \dot{u}(u-v)^{-1}\dot{v}(u-v)^{-1}.$$

Therefore

Remark 2: The traces and the determinants of I_1, I_2, I_3, *and* I_4 *are absolute invariants. In particular* $L := \mathrm{Tr}(I_4)$ *is an invariant pseudo-Riemannian metric on the subspace* W *of* $\mathrm{U}(2) \times \mathrm{U}(2)$ *consisting of all pairs* (u,v) *with* $\det(u-v) \neq 0$.

Remark 3:

1. *The expression* $\log(\det(I_4))$ *has a similar form with the Lagrange function of a system of two particles, interacting gravitationally according to Newton's Mechanics.*
2. *The relation* $I_4 = -I$ *is also invariant, hence it defines a conformally invariant subset of the tangent space* $T(W)$.

III. THE GEODESIC PATHS OF THE SPACE (W,L) AND THE CONSTANTS OF MOTION

In this section we determine explicitly the geodesics of the pseudo-Riemannian manifold W, and we find expressions which remain constant along a geodesic.

The Euler–Lagrange equations for the Lagrange function L can be written in the form

$$\ddot{u} = 2\dot{u}(u-v)^{-1}\dot{u}, \quad \ddot{v} = 2\dot{v}(v-u)^{-1}\dot{v}. \tag{1}$$

It is not difficult to verify that the solution of these equations corresponding to the initial data

$$u(0) = a, \quad \dot{u}(0) = a_1, \quad v(0) = b, \quad \dot{v}(0) = b_1 \tag{2}$$

is given by

$$u(t) = (a - b\alpha\tau)(I - \alpha\tau)^{-1}, \quad v(t) = (b + a\tau\beta)(I + \tau\beta)^{-1}, \tag{3}$$

where we have used the notations:

$$\alpha := (a-b)^{-1}a_1, \quad \beta := (a-b)^{-1}b_1, \quad \tau := k^{-1}\tanh(kt), \tag{4}$$

and k is any 2×2-matrix satisfying

$$k^2 = -\beta\alpha. \tag{5}$$

Note that the matrix τ is a function of t and k^2, which makes sense even when k is a singular matrix.

The initial data (2) must fulfill of course the conditions:

$$a,b \in \mathrm{U}(2); \quad \det(a-b) \neq 0; \quad ia^*a_1, \quad ib^*b_1 \in M,$$

the last two conditions meaning that ia^*a_1, ib^*b_1 must be Hermitian matrices. For instance, when $a = I, b = -I, ia_1, ib_1$ must be Hermitian matrices and k must be chosen such that $4k^2 = -b_1a_1$.

Notice now that a Cayley map $C_d : M \to \mathrm{U}(2)$ defines a chart

$$W \supset W_d \to M_d \subset M \times M$$

of our manifold W, which is also given by a homographic expression. The Lagrangian L, as well as the Euler–Lagrange equations (1) keep the same form, if we use the coordinates $x,y \in M$ induced by such a chart, instead of the U(2)-valued coordinates u,v. In particular the equations (3) giving the geodesic paths, as well as the formulas giving the parameters α,β,τ,k in dependence on

the initial data, will also have the same form. The only difference is that the initial data $a=x(0)$, $a_1=\dot{x}(0)$, $b=y(0)$, $b_1=\dot{y}(0)$ must be Hermitian matrices this time. For instance, for $a=0$, $b=a_1=I$, $b_1=-k^2$, we get

$$x=\tanh(kt)[k+\tanh(kt)]^{-1}, \quad y=[1+k\ \tanh(kt)]^{-1}.$$

We can write now the equations (3) in the form

$$u=b+(a-b)(I-\alpha\tau)^{-1}, \quad v=a-(a-b)(I+\tau\beta)^{-1},$$

and we get

$$\begin{aligned} \dot{u}&=(a-b)(I-\alpha\tau)^{-1}\alpha(I-k^2\tau^2)(I-\alpha\tau)^{-1},\\ \dot{v}&=(a-b)(I+\tau\beta)^{-1}(I-k^2\tau^2)\beta(I+\tau\beta)^{-1}, \end{aligned} \tag{6}$$

$$u-v=(a-b)(I-\alpha\tau)^{-1}(I+\alpha\tau^2\beta)(I+\tau\beta)^{-1}=(a-b)(I+\tau\beta)^{-1}(I+\tau\beta\alpha\tau)\beta(I-\alpha\tau)^{-1}. \tag{7}$$

On the other hand, since $k^2=-\beta\alpha$, we have the identities

$$I+\tau\beta\alpha\tau=I-k^2\tau^2, \quad I+\alpha\tau^2\beta=\alpha(\tau^2-k^{-2})\beta=\alpha(I-k^2\tau^2)\alpha^{-1}.$$

We obtain

$$(u-v)^{-1}\dot{v}(u-v)^{-1}\dot{u}=-(I-\alpha\tau)k^2(I-\alpha\tau)^{-1},$$

which shows that, for every geodesic path, it holds

$$(\mathrm{Tr}\ I_4)(u,v,\dot{u},\dot{v})=-\mathrm{Tr}\ k^2, \quad (\det I_4)(u,v,\dot{u},\dot{v})=\det k^4.$$

Put now $w:=(u-v)^{-1}$, $c:=(a-b)^{-1}$, and let us introduce the Hamiltonian coordinates

$$p:=w\dot{v}w, \quad q:=w\dot{u}w.$$

The equations (3) become

$$\begin{aligned} p&=-(I-\alpha\tau)k^2(I-k^2\tau^2)^{-1}\alpha^{-1}(I-\alpha\tau)c,\\ q&=(I-k^2\tau\alpha^{-1})\alpha(I-k^2\tau^2)^{-1}(I-k^2\tau\alpha^{-1})c, \end{aligned}$$

and easy computations show that the expressions

$$A=pu+qv, \quad B=p+q, \quad C=upu+vqv, \quad D=up+vq \tag{8}$$

are constant along every geodesic path. In fact these expressions are the constants of motion provided by Emmy Noether's theorem on conservations laws applied to the Lagrange function L and to the symmetry group SU(2,2) (see for instance Ref. 5).

From the last formulas one easily obtains

$$v(A-Bu)=(C-Du), \quad uA-C=(uB-D)v,$$

hence there exist (constant) homographic transformations mapping one partner into the other. For instance,

$$v=(C-Du)(A-Bu)^{-1}=(uB-D)^{-1}(uA-C).$$

Since A,B,C,D depend symmetrically on u and v, we obtain two other relations by permuting u and v. We can also see that u and v are solution of the (non-Abelian) quadratic equation (with constant coefficients)

$$u(AB-BD)u+u(BC-A^2)+(D^2-CB)u+(CA-DC)=0.$$

This can be interpreted in the following way: u and v are fixed points of the homographic transformation

$$u\mapsto((D^2-CB)u+(CA-DC))((BD-AB)u+(A^2-BC))^{-1},$$

whose coefficients are the entries of the matrix $\mathscr{M}^2$, where

$$\mathscr{M}:=\begin{pmatrix} -D & C \\ -B & A \end{pmatrix}.$$

This matrix belong to the Lie algebra of the group SU(2,2), because we always have

$$A^*+A=D^*+D=0, \quad B^*=C, \quad \mathrm{Tr}\,A=\mathrm{Tr}\,D.$$

The matrix $\mathscr{M}$ has an important geometrical interpretation. There is a well-known theorem of Élie Cartan asserting that, in any symmetric space and for any geodesic path g, there is a one-parameter group Γ_g of isometries (called **transvections**), which translate the points of g along g itself. In our case, we claim that the group Γ_g is formed by the matrices $\exp(t.\mathscr{M})$, $t\in\mathbb{R}$, where $\mathscr{M}$ is the matrix associated with the geodesic g as explained above. Indeed, from (8) we get easily that $u(\cdot)$ and $v(\cdot)$ satisfy the equation

$$\dot{u}=uBu-uA-Du+C. \tag{9}$$

On the other hand, the group $\{\exp(t.\mathscr{M})|t\in\mathbb{R}\}$ induces on U(2) a tangent vector field whose trajectories are precisely the solutions of the differential equation (9). Thus g is invariant under the transformations $\exp(t.\mathscr{M})$.

There is a second important geometric property of Cartan's symmetric spaces:

Proposition 4: In any symmetric space, each point m is an isolated fixed point of an involutive isometry I_m, which reverses the geodesic paths starting from m.

Using again non-Abelian projective geometry, we can easily find the isometry I_m. Let $m=(a,b)\in W$, and consider a geodesic $(u(\cdot),v(\cdot))$ satisfying the initial condition $u(0)=a$, $v(0)=b$. Using the formulas (3) we can easily verify that

$$(a,b,u(t),u(-t))=(a,b,v(t),v(-t))=-I.$$

Since, by definition, $I_m(u(t))=u(-t)$ and $I_m(v(t))=v(-t)$, we see that

Remark 5: The symmetry I_m maps any pair $(u,v)\in W$ into the pair (u',v') formed by the **harmonic conjugates** *of u and v with respect to the pair (a,b).*

We also notice that $u(\cdot)$ can be formally obtained from $v(\cdot)$ by performing the transformation $\tau\mapsto\tau':=k^{-2}\tau^{-1}$ in (3). (Note that in general this change does not correspond to a transformation of the parameter t.) For $\tau=\pm k^{-1}$, we get $\tau'=\tau$, hence

Remark 6: The two points $P_\pm$ obtained by replacing formally τ by $\pm k^{-1}$ in the equations (3) are also constants of motion. For any t, the partners $u(t),v(t)$ are harmonic conjugate with respect to the constant pair (P_+,P_-):

$$(P_+,P_-,u(t),v(t))=-I.$$

By (8), the matrix $\mathscr{M}$ is also given by the expression

$$\mathscr{M}=\begin{pmatrix} u & v \\ I & I \end{pmatrix}\begin{pmatrix} p & 0 \\ 0 & q \end{pmatrix}\begin{pmatrix} -I & u \\ -I & v \end{pmatrix}$$

and it follows that

$$\det \mathscr{M}=\det k^2.$$

On the other hand we obviously have

$$\mathrm{Tr}(\mathscr{M}^2)=\mathrm{Tr}(A^2+D^2-2BC)=2\ \mathrm{Tr}(k^2).$$

Note finally that, while A,B,C,D are uniquely determined by a given geodesic path and are invariant with respect to the translations along that path, the matrix k^2 also depends on the initial data.

IV. THE TOPOLOGICAL BEHAVIOR OF SOME GEODESIC PATHS

The group U(2,2) acts transitively on W. This implies that any geodesic path is equivalent to a geodesic path with initial data

$$a=I, \quad b=-I.$$

The isotropy group $H\subset \mathrm{U}(2,2)$ of $(I,-I)$ is

$$\left\{ \frac{1}{2}\begin{pmatrix} g+(g^*)^{-1} & g-(g^*)^{-1} \\ g-(g^*)^{-1} & g+(g^*)^{-1} \end{pmatrix} \middle| g\in \mathrm{GL}(2,\mathbb{C}) \right\},$$

hence it is isomorphic to $\mathrm{GL}(2,\mathbb{C})$.

The motion-equations (3) give in the case $a=I, b=-I$

$$u(t)=(2I+a_1\tau)(2I-a_1\tau)^{-1}, \quad v(t)=(-2I+\tau b_1)(2I+\tau b_1)^{-1}, \tag{10}$$

and the matrix $\mathscr{M}$ associated with such a geodesic becomes

$$\frac{1}{4}\begin{pmatrix} -b_1+a_1 & b_1+a_1 \\ -b_1-a_1 & b_1-a_1 \end{pmatrix}.$$

Since $4k^2=(ia_1)(ib_1)$ is a product of two Hermitian matrices, its eigenvalues are either real or complex conjugated to each other. This means that

Remark 7: The trace and the determinant of the matrix k^2 are, in all cases, real numbers.

These are the main invariants associated with a geodesic path. We shall first consider the case of two massive interacting particles, i.e., the case when

$$\det a_1<0, \quad \det b_1<0.$$

It follows $\det k^2>0$. Using the isotropy group H, we can transform the geodesic path (10) into a geodesic path with

$$a_1=iI, \quad b_1=i\ \mathrm{diag}(\lambda,\mu), \quad 4k^2=\mathrm{diag}(\lambda,\mu) \quad \text{with} \quad \lambda\in\mathbb{R}, \quad \mu\in\mathbb{R}.$$

In this case, the matrices $u(t),v(t)$ will remain diagonal, for any t. Let us consider the interesting case when both λ,μ are negative, and let us introduce the **real** matrix $h:=-ik$. Then

$$\tau=h^{-1}\ \tan(ht)=\mathrm{diag}(h_{11}^{-1}\ \tan(h_{11}t),h_{22}^{-1}\ \tan(h_{22}t)),$$

where $4h_{11}^2=-\lambda$, $4h_{22}^2=-\mu$. The first equation in (10) shows that $u(t)$ is a diagonal matrix with complex entries of module 1:

$$u_{jj}=(2h_{jj}+i\ \tan(h_{jj}t))(2h_{jj}-i\ \tan(h_{jj}t))^{-1},\quad j=1,2. \tag{11}$$

The above equations define a path in the torus $T^2=S^1\times S^1$, which is periodic when h_1/h_2 is rational, and is dense in T^2 otherwise. The same holds for the components $v_{11}(t)$, $v_{22}(t)$ of the diagonal matrix v, hence:

Remark 8: We have identified a class of geodesic paths which exhibit two periods $T_j=\pi/h_j$, in some similarity with the behavior of the geodesic paths in the Schwartzschild space.

From (10) we get the formula

$$(u-v)^{-1}=\frac{1}{2}\cos(2ht)+\frac{i}{4}(h^2+1)h^{-1}\sin(2ht)$$

which reminds on the classical formulae giving r^{-1} in Newton's and Schwartzschild's theories on planetary motions.

The case $b_1=0$ in (10) corresponds to a motion in which the partner v is fixed, $v=-I$, $k^2=0$, $\tau=t$ and $u=(2+it)(2-it)^{-1}I$. Using a Cayley chart which sends $-I$ to infinity in the Minkowski space, we obtain for the first partner u an **inertial** motion in the Minkowski space

$$x(t)=\tfrac{1}{2}t.$$

This case should be related to **Mach's principle**, asserting that inertial motions of particles u are produced by the attraction of particles v situated at infinity.

Let us discuss other classes of geodesics:
The condition $\det \dot{u}=0$ means that the particle u is moving with velocity 1, which is, conventionally, the light velocity. Taking in (10) a_1, b_1 such that $\det a_1=0$ (or $\det a_1=\det b_1=0$), we obtain solutions with the property that one component, (respectively, both components) are light trajectories.

When $\det a_1>0$, $\det b_1>0$, u and v are **tachions**. An example is given by the case

$$a_1=\begin{pmatrix}0 & i\\ i & 0\end{pmatrix},\quad b_1=\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix},\quad 4k^2=\begin{pmatrix}i & 0\\ 0 & -i\end{pmatrix}.$$

V. THE PRINCIPAL FIBER BUNDLE U(2,2)→*W*

The elements of U(2,2) define distinguished accelerated frames in the Minkowski space, which we call **twisted frames**. This class of frames should have a physical significance, expressing some internal symmetry properties of elementary particles. Therefore we think there is some interest to relate more deeply our previous results to the Lie group U(2,2).

We study first the principal fibre bundle U(2,2)→W which exhibits the pseudo-Riemannian manifold W as a homogeneous space:

We define the map P:U(2,2)→W by associating to each matrix

$$N=\begin{pmatrix}A & B\\ C & D\end{pmatrix}\in \mathrm{U}(2,2)$$

the image of $(I,-I)$ via the homographic transformation (also denoted by N) defined by N:

$$P(N):=(u,v),\quad u=(A+B)(C+D)^{-1},\quad v=(A-B)(C-D)^{-1}.$$

Put $K:=\left(\begin{smallmatrix}I & I\\ I & -I\end{smallmatrix}\right)$. With each point $(u,v)\in W$ and each $g\in \mathrm{GL}(2,\mathbb{C})$ we further associate the matrix

$$N(u,v,g):=\begin{pmatrix} h & g \\ uh & vg \end{pmatrix}K, \quad h:=-\tfrac{1}{2}(u-v)^{-1}v(g^*)^{-1}.$$

It follows $N(u,v,g)\in \mathrm{U}(2,2)$ and $N(u,v,g)(I,-I)=(u,v)$. Moreover, the map $W\times \mathrm{GL}(2,\mathbb{C})\ni(u,v,g)\mapsto N(u,v,g)\in \mathrm{U}(2,2)$ is a diffeomorphism and defines a global trivialization of the bundle $P:\mathrm{U}(2,2)\to W$. In particular, the group U(2,2) is diffeomeorphic to the product $W\times \mathrm{GL}(2,\mathbb{C})$.

The group U(2,2) carries a standard, bi-invariant pseudo-Riemannian metric

$$\sigma=\mathrm{Tr}[(N^{-1}dN)^2]=\mathrm{Tr}[(JN^*JdN)^2], \quad J:=\begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}.$$

The Lie algebra $L(\mathrm{U}(2,2))$ of U(2,2) has a nondefinite Hermitian structure and a corresponding pseudo-orthogonal decomposition

$$L(\mathrm{U}(2,2))=L(H)\oplus L(H)^{\perp},$$

where H is the isotropy group of $(I,-I)$.

It is convenient to transform all matrices under consideration according to the rule $N\mapsto N':=KNK^{-1}$. In this way we obtain a subgroup H' of the Lie group $(K\cdot \mathrm{U}(2,2)\cdot K^{-1})$, a fiber bundle $P':(K\cdot \mathrm{U}(2,2)\cdot K^{-1})\to W$, a distribution $D'=L(H')^{\perp}\subset T(K\cdot \mathrm{U}(2,2)\cdot K^{-1})$ and a pseudo-Riemannian metric $\sigma'=\mathrm{Tr}[(N'^{-1}dN')^2]$ on $(K\cdot \mathrm{U}(2,2)\cdot K^{-1})$. The corresponding trivialization of P' is given by $N'(u,v,g)=K\left(\begin{smallmatrix} h & g \\ uh & vg \end{smallmatrix}\right)$, and, using again the notation $w:=(u-v)^{-1}$, we get

$$N'^{-1}dN'=\mathrm{diag}(h,g)^{-1}\begin{pmatrix} dh+w\ du\ h & w\ dv\ g \\ -w\ du\ h & dg-w\ dv\ g \end{pmatrix}.$$

It can be easily seen now that the distribution D' can be defined by any of the two equivalent equations

$$dq=w\ dv\ g, \quad dh=-w\ du\ h.$$

Proposition 9: The principal fibration $P:\mathrm{U}(2,2)\to W$ is, up to a constant factor, a pseudo-Riemannian submersion.

Indeed, it is enough to prove that $P':K\cdot \mathrm{U}(2,2)\cdot K^{-1}\to W$ is a pseudo-Riemannian submersion. But the restriction of $\sigma'=\mathrm{Tr}[(N'^{-1}dN')^2]$ to D' is $2\,\mathrm{Tr}(w\ du\ w\ dv)$, which obviously coincides with twice the restriction to this distribution of the pull-back $[P']^*(L)$ of our Lagrangian L.

This mathematical result can be reformulated as follows:

Remark 10: The dynamical system defined by the Lagrange function $L:T(W)\to\mathbb{R}$ is equivalent with the dynamical system defined by the Lagrange function $\sigma=\mathrm{Tr}[(JN^*JdN)^2]$: $T(M_4(\mathbb{C}))\to\mathbb{R}$ and by the constraints

$$N^*JN=J, \quad dg=w\ dv\ g.$$

Note that

$$w:=g^{-1}(dg-w\ dv\ g)$$

is the connection form of the canonical connection in the principal fiber bundle $P:\mathrm{U}(2,2)\to W$; the corresponding curvature form is

$$\Omega=d\omega+\omega\wedge\omega=g^{-1}(u-v)^{-1}\ du\wedge(u-v)^{-1}\ dv\ g.$$

Since the principal bundle $P:\mathrm{U}(2,2)\to W$ is a sub-bundle of the principal bundle of pseudo-orthogonal tangent frames of (W,L), the form Ω gives also the curvature of the Levi–Civita connection of the pseudo-Riemannian space (W,L).

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Comment on Ricci collineations of static spherically symmetric spacetimes [J. Math. Phys. 35, 3005–3012 (1994)]

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We present a counter example to a theorem given by Amir *et al.* [J. Math. Phys. **35**, 3005–3012 (1994)]. We also comment on a misleading statement of the same reference. © *1996 American Institute of Physics.* [S0022-2488(96)04001-9]

In a recent paper, M. Jamil Amir *et al.*[1] have presented a detailed analysis of Ricci collineations (RC) for static, spherically symmetric spacetimes, with a special focus on the relationship between RC and isometries (KV). This has led the authors to the following theorem.

Theorem 1: *Spherically symmetric static spacetimes with a nonzero (and noninfinite) determinant of the Ricci tensor have RCs identical with the Killing vector, but when the determinant is zero there may be additional degrees of freedom, giving infinitely many RCs for each degree of freedom*.

We have found a counter example to this result. The metric for spherically symmetric static spacetimes can be written in the form[2]

$$ds^2=-e^{\nu(r)}\,dt^2+e^{\lambda(r)}\,dr^2+r^2(d\vartheta^2+\sin^2\,\phi\,d\phi^2). \tag{1}$$

The Ricci tensor for this metric is diagonal and can be written as $R_{00}=A(r)$, $R_{11}=B(r)$, $R_{22}=C(r)$, and $R_{33}=C(r)\sin^2\vartheta$. Let us consider the particular case in which $A(r)=C(r)=1$, which leads to the metric

$$\nu(r)=\frac{r^4}{8r_0^2}+h\,\ln\frac{r}{r_0}+k,\quad \lambda(r)=\nu(r)+2\ln\frac{r}{r_0}, \tag{2}$$

with

$$B(r)=2\,\frac{h+1}{r^2}, \tag{3}$$

where r_0, h, and k are constants.

From the equation for RC,

$$\pounds_\xi R_{ab}=0, \tag{4}$$

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we obtain

$$\xi^t_{,t}=0, \tag{5}$$

$$\xi^t_{,r}+B(r)\xi^r_{,t}=0, \tag{6}$$

$$\xi^t_{,\vartheta}+\xi^\vartheta_{,t}=0, \tag{7}$$

$$\xi^t_{,\phi}+\sin^2\vartheta\,\xi^\phi_{,t}=0, \tag{8}$$

$$B'(r)\xi^r+2B(r)\xi^r_{,r}=0, \tag{9}$$

$$B(r)\xi^r_{,\vartheta}+\xi^\vartheta_{,r}=0, \tag{10}$$

$$B(r)\xi^r_{,\phi}+\sin^2\vartheta\,\xi^\phi_{,r}=0, \tag{11}$$

$$\xi^\vartheta_{,\vartheta}=0, \tag{12}$$

$$\xi^\vartheta_{,\phi}+\sin^2\vartheta\,\xi^\phi_{,\vartheta}=0, \tag{13}$$

$$\cot\vartheta\,\xi^\vartheta+\xi^\phi_{,\phi}=0. \tag{14}$$

Equations (5) and (9) can be integrated, giving $\xi^t=\Sigma(r,\vartheta,\phi)$ and $\xi^r=K(t,\vartheta,\phi)B^{-1/2}$, respectively. Substituting these expressions into the ϑ-derivative of Eq. (6) we find that $K(t,\vartheta,\phi)=S_1(\vartheta,\phi)t+S_2(\vartheta,\phi)$. Using these results into (7) and (8), we obtain an expression for ξ:

$$\xi^t=\Sigma(r,\vartheta,\phi),\quad \xi^r=\frac{S_1(\vartheta,\phi)t+S_2(\vartheta,\phi)}{B^{1/2}}, \tag{15}$$

$$\xi^\vartheta=-\Sigma_{,\vartheta}t+\Gamma(r,\vartheta,\phi)\quad\text{and}\quad\xi^\phi=-\Sigma_{,\phi}t+\Psi(r,\vartheta,\phi). \tag{16}$$

Substitution of ξ into (6) and (10)–(14) enables us to completely determine the functions $\Sigma(r,\vartheta,\phi)$, $S_1(\vartheta,\phi)$, $S_2(\vartheta,\phi)$, $\Gamma(r,\vartheta,\phi)$, and $\Psi(r,\vartheta,\phi)$. Then,

$$\begin{aligned}
\xi^0&=-c_4\sqrt{2(h+1)}\,\ln r+c_0,\\
\xi^1&=\frac{c_4t+c_5}{\sqrt{2(h+1)}}\,r,\\
\xi^2&=c_1\sin\phi-c_2\cos\phi,\\
\xi^3&=(c_1\cos\phi+c_2\sin\phi)\cot\vartheta+c_3.
\end{aligned} \tag{17}$$

According to Theorem 1, (17) should represent an isometry; however, it is easy to see that ξ does not reduce to a KV unless $c_4=c_5=0$. This result invalidates the theorem stated above. Moreover, it is straightforward, but tedious, to show that the same condition is necessary for ξ to reduce to a Riemann collineation ($\pounds_\xi R^a_{bcd}=0$). Therefore (17) is a proper RC.

Next, we should like to make a remark on a misleading statement that appears in Amir *et al.*:[1] "... there is no reason, *a priori*, why a RC should be a KV or *vice versa*... ." It is easy to show that any KV is a RC. Indeed, Katzin *et al.*[3] have proved that a necessary and sufficient condition for a spacetime to admit a curvature collineation (CC) is

$$((\pounds_\xi g_{im})_{;j}+(\pounds_\xi g_{mj})_{;i}-(\pounds_\xi g_{ij})_{;m})_{;k}-((\pounds_\xi g_{km})_{;j}+(\pounds_\xi g_{mj})_{;k}-(\pounds_\xi g_{kj})_{;m})_{;i}=0. \tag{18}$$

Then, it is evident that a KV satisfies the above condition and, as it is well known, every CC is a RC.

The analysis of RC for the general case of static, spherically symmetric metrics, i.e., $A(r)$ and $C(r)$ arbitrary, is obviously more involved and its complete solution will be reported elsewhere. The study of RC for *nonstatic* spherically symmetric metrics gives interesting results which will be the subject of a subsequent publication.

Algebraic calculations of the present work have been checked with MAPLE V. The authors wish to thank the staff of the SUMA, the computational facility of the Faculty of Science (Universidad de Los Andes), for making this work possible.

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Erratum: Ricci collineations of static spherically symmetric spacetimes [J. Math. Phys. 35, 3005–3012 (1994)]

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We are grateful to R. Bertolotti, L. A. Nunez, U. Percoco, and J. Carot for pointing out a serious error in the statement of Theorem 1 of the above paper.[1] Counter examples to it are available in an earlier paper by two of us[2] (A.H.B. and A.Q.) as cases (Ia) and (IIyi). The correct statement is that ''Spherically symmetric static spacetimes with higher than minimal isometries and with a nonzero (and noninfinite) determinant of the Ricci tensor have RCs identical with the KVs of the spacetimes, but when the determinant is zero there may be additional degrees of freedom, giving infinitely many RCs for each degree of freedom.'' They also feel that the statement ''...there is no reason, *a priori*, why a RC should be a KV or vice versa...'' in our paper is misleading. Our intention was not to say that all KVs are not RCs, but that it is not *a priori obvious* that this is so. We agree that it can be proved easily enough and intuition does suggest it.

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Null surfaces, initial values, and evolution operators for spinor fields

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We analyze the initial value problem for spinor fields obeying the Dirac equation, with particular attention to the characteristic surfaces. The standard Cauchy initial value problem for first-order differential equations is to construct a solution function in a neighborhood of space and time from the values of the function on a selected initial value surface. On the characteristic surfaces the solution function may be discontinuous, so the standard Cauchy construction breaks down. For the Dirac equation the characteristic surfaces are null surfaces. An alternative version of the initial value problem may be formulated using null surfaces; the initial value data needed differs from that of the standard Cauchy problem. We study, in particular, the intersecting pair of characteristics $t=x$ and $t=-x$ (and supress the y and z dependence). In this case the values of separate components of the spinor function on the intersecting pair of null surfaces comprise the necessary initial value data. We present an expression for the construction of a solution from the null surface data; two analogs of the quantum mechanical Hamiltonian operator determine the evolution of the system. © *1996 American Institute of Physics.* [S0022-2488(96)02003-X]

I. INTRODUCTION

In this work we discuss the initial value problem for spinor fields obeying the free particle Dirac equation, with particular regard to characteristic surfaces. The standard Cauchy problem for a first-order partial differential equation is to use the values of the solution function on an initial value surface to determine the values of the function in a neighborhood of the surface.[1] The solution of the problem proceeds by showing how the initial value data and the differential equation determine all the time derivatives of the function on the initial surface and thus allow a power series development of the function for future times.

If the solution function has a discontinuity across some special surface, then the standard Cauchy problem cannot be solved using that surface for the initial value data. Such surfaces are called characteristic surfaces, or simply characteristics. The characteristics of the Dirac equation for a free particle in flat space are easily shown to be null surfaces. Thus, the discontinuities of the solution functions propagate at the velocity of light, independent of the mass parameter in the equations. The characteristics of Maxwell's equations, the Klein–Gordon equation, and the vacuum Einstein equations of general relativity are also all null surfaces.[1,2]

First, we briefly review the standard Cauchy problem for the Dirac equation. Then we obtain the characteristics (null surfaces), and, in particular, we study the pair of planar null surfaces $t=x$ and $t=-x$. For this pair of surfaces we solve the analog of the Cauchy problem, surpressing dependence on y and z. Initial data for this situation consists of the values of disparate components of the spinor function on the *pair* of null surfaces. We give a simple evolution operator expression

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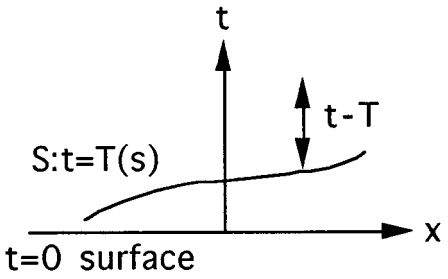

FIG. 1. Initial value surface for the Dirac equation.

in terms of null coordinates, which is a direct analog of the usual expression of quantum theory, except that *two* analogs of the Hamiltonian operator determine the evolution of the solution, that is, are generators of displacements in the null coordinates.[3–7] The result is remarkably similar to that obtained for the scalar field.[8]

II. DEVELOPMENT OF A SPINOR FUNCTION FROM A CONSTANT TIME SURFACE

Since the Dirac equation may be expressed in Hamiltonian form, the development of a solution from initial value data given on a constant time surface is one of the most familiar problems of physics.[9] We express the Dirac equation in Hamiltonian form as[10]

$$i\psi_{|t}(\mathbf{x},t)=[-i\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}+\beta m]\psi(\mathbf{x},t)=H\psi(\mathbf{x},t). \tag{1}$$

(We use units in which $\hbar=c=1$. The slash notation indicates differentiation with respect to the indicated variable, in this case time t.) We write a Taylor series expansion as

$$\psi(\mathbf{x},t)=\psi(\mathbf{x},t)_{t=0}+\psi_{|t}(\mathbf{x},t)_{t=0}t+\psi_{|t|t}(\mathbf{x},t)_{t=0}t^2/2+\cdots\ . \tag{2}$$

All of the time derivatives at $t=0$ may be readily obtained from the Dirac equation and the value of the spinor functions at $t=0$, which we call $h(\mathbf{x})$. When substituted in the series, these give the familiar result,

$$\psi(\mathbf{x},t)=\psi(\mathbf{x},t)_{t=0}+(-iH)\psi(\mathbf{x},t)_{t=0}t+(-iH)^2\psi(\mathbf{x},t)_{t=0}t^2/2+\cdots=e^{-iHt}h(\mathbf{x}). \tag{3}$$

The indicated exponential of the Hamiltonian operator is thereby seen as the finite time displacement operator.

III. CHARACTERISTICS OF THE DIRAC EQUATION

The characteristics of the Dirac equation are found in the standard way, as discussed in Ref. 1; since the Dirac equation is first order in time, the problem is particularly easy. We suppose that the initial value of the solution is given on a surface S, $t=T(\mathbf{x})$, by a four component spinor (see Fig. 1),

$$\psi(\mathbf{x},T(\mathbf{x}))=h(\mathbf{x}), \tag{4}$$

and that the solution is given by a Taylor series expansion,

$$\psi(\mathbf{x},t)=\psi(\mathbf{x},t)_{t=T}+\psi_{|t}(\mathbf{x},t)_{t=T}[t-T(\mathbf{x})]+\psi_{|t|t}(\mathbf{x},t)_{t=T}[t-T(\mathbf{x})]^2/2+\cdots\ . \tag{5}$$

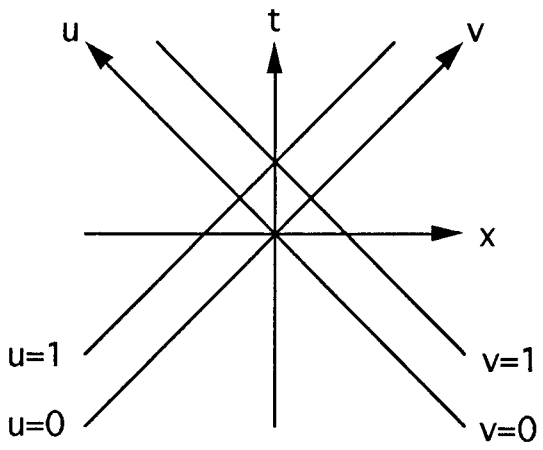

FIG. 2. The Cartesian coordinates t and x, and the null coordinate u and v.

To find the first time derivative in (5), we first express the gradient of the initial value function h in terms of ψ, as

$$\nabla h(\mathbf{x}) = \nabla \psi(\mathbf{x},t)_{t=T} + \psi_{|t}(\mathbf{x},t)_{t=T}\, \nabla T(\mathbf{x}). \tag{6}$$

From this and the Dirac equation (1) we may write an equation for the time derivative of ψ on S,

$$i[I - \boldsymbol{\alpha}\cdot\nabla T(\mathbf{x})]\psi_{|t}(\mathbf{x},t)_{t=T} = -i\boldsymbol{\alpha}\cdot\nabla h(\mathbf{x}) + \beta m h(\mathbf{x}). \tag{7}$$

This may be solved for the time derivative if the matrix in square brackets has an inverse. The determinant of that matrix is easily found to be

$$|I - \boldsymbol{\alpha}\cdot\nabla T(\mathbf{x})| = (1 - \nabla T(\mathbf{x})^2)^2. \tag{8}$$

Thus the condition that S be a characteristic is that the above quantity be zero, or

$$\nabla T(\mathbf{x})^2 = 1. \tag{9}$$

This equation states that the four-vector normal $(1,\nabla T)$ is a null vector, or that the characteristic is a null surface. It is the same as the characteristic equation for Maxwell's equations[2] and for the Klein–Gordon equation.[1,8] Note that the equation is independent of the mass parameter in the Dirac equation. The particular null surfaces that we will study in the remainder of this paper are

$$\begin{aligned} u &= t - x = 0, \quad u \text{ characteristic or null surface,} \\ v &= t + x = 0, \quad v \text{ characteristic or null surface} \end{aligned} \tag{10}$$

(see Fig. 2). These are easily seen to be solutions of (9).

IV. CONSTRUCTION OF A SOLUTION FUNCTION IN TERMS OF NULL COORDINATES

The covariant form of the Dirac equation is[10]

$$\gamma^\alpha i \frac{\partial}{\partial x^\alpha} \psi = m\psi. \tag{11}$$

We will study this using the null coordinates $u=t-x$ and $v=t+x$, and suppress dependence on y and z in all that follows.[11] Then the gamma matrices are $\gamma^u=\gamma^0-\gamma^1$ and $\gamma^v=\gamma^0+\gamma^1$. The Dirac equation and the gamma matrix algebra in terms of the null coordinates are

$$\left[\gamma^u i\,\frac{\partial}{\partial u}+\gamma^v i\,\frac{\partial}{\partial v}\right]\psi(u,v)=m\psi(u,v),$$
$$\frac{\gamma^u\gamma^v}{4}+\frac{\gamma^v\gamma^u}{4}=I,\quad (\gamma^u)^2=(\gamma^v)^2=0. \tag{12}$$

We define a pair of projection operators as

$$\Lambda_u=\frac{\gamma^u\gamma^v}{4},\quad \Lambda_v=\frac{\gamma^v\gamma^u}{4}. \tag{13}$$

From (12), the usual projection operator properties follow, that is

$$\Lambda_u+\Lambda_v=I,\quad \Lambda_u\Lambda_u=\Lambda_u,\quad \Lambda_v\Lambda_v=\Lambda_v,\quad \Lambda_v\Lambda_u=\Lambda_u\Lambda_v=0. \tag{14}$$

To analyze the Dirac equation on and near the null surfaces $u=0$ and $v=0$, we make an expansion in the mass m, since the solutions of the zero mass Dirac equation are functions of only u or only v. Thus, we write

$$\psi(u,v)=\psi^{(0)}(u,v)+m\psi^{(1)}(u,v)+m^2\psi^{(2)}(u,v)+\cdots. \tag{15}$$

Substitution of this into the Dirac equation gives the following set of iterative equations:

$$\left[\gamma^u i\,\frac{\partial}{\partial u}+\gamma^v i\,\frac{\partial}{\partial v}\right]\psi^{(0)}(u,v)=0,\quad \left[\gamma^u i\,\frac{\partial}{\partial u}+\gamma^v i\,\frac{\partial}{\partial v}\right]\psi^{(n)}(u,v)=\psi^{(n-1)}(u,v). \tag{16}$$

A solution of the zeroth-order equation is easy by inspection,

$$\psi^{(0)}(u,v)=\Lambda_u f(u)+\Lambda_v g(v). \tag{17}$$

Here the functions f and g are any differentiable 4-tuple functions of u and v; we will call these the generating functions. It is instructive to consider a representation of the gamma matrices in which the projection operators Λ are diagonal; then the Λ and the zeroth-order solution are

$$\Lambda_u=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&0&0\\0&0&0&0\end{pmatrix},\quad \Lambda_v=\begin{pmatrix}0&0&0&0\\0&0&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix},\quad \psi^{(0)}(u,v)=\begin{pmatrix}f_1(u)\\f_2(u)\\g_3(v)\\g_4(v)\end{pmatrix}. \tag{18}$$

Thus, only two components of f and two components of g enter the solution.

The first-order equation (16) is

$$\left[\gamma^u i\,\frac{\partial}{\partial u}+\gamma^v i\,\frac{\partial}{\partial v}\right]\psi^{(1)}(u,v)=\Lambda_u f(u)+\Lambda_v g(v). \tag{19}$$

Only a particular solution to this is needed since the homogeneous solution may be absorbed into the zeroth-order solution. We break the equation into u and v parts by premultiplying by γ^μ and using (12) to get

$$i\,\frac{\partial}{\partial v}\,\Lambda_u\psi^{(1)}(u,v)=\frac{1}{4}\,\gamma^u\Lambda_v g(v). \tag{20}$$

The right side of this is a function of v only, so the left side must be as well. Thus, we may write a solution by integration,

$$\Lambda_u\psi^{(1)}(u,v)=\frac{-i}{4}\,\gamma^u\Lambda_v\int_{v_0}^{v} g(v')dv'. \tag{21}$$

Here v_0 is an arbitrary parameter. In the same way we may obtain a similar expression for the v projection of the solution,

$$\Lambda_v\psi^{(1)}(u,v)=\frac{-i}{4}\,\gamma^v\Lambda_u\int_{u_0}^{u} f(u')du'. \tag{22}$$

The sum of (21) and (22) gives the complete first-order solution,

$$\psi^{(1)}(u,v)=\frac{-i}{4}\left[\gamma^u\Lambda_v\int_{v_0}^{v} g(v')dv'+\gamma^v\Lambda_u\int_{u_0}^{u} f(u')du'\right]. \tag{23}$$

The second-order equation (16) may now be written as

$$\left[\gamma^u i\,\frac{\partial}{\partial u}+\gamma^v i\,\frac{\partial}{\partial v}\right]\psi^{(2)}(u,v)=\frac{-i}{4}\left[\gamma^v\Lambda_u\int_{u_0}^{u} f(u')du'+\gamma^u\Lambda_v\int_{v_0}^{v} g(v')dv'\right]. \tag{24}$$

As before we premultiply by γ^μ to obtain, with the use of (13) and (14),

$$\frac{\partial}{\partial v}\,\Lambda_u\psi^{(2)}(u,v)=\frac{-1}{4}\,\Lambda_u\int_{u_0}^{u} f(u')du'. \tag{25}$$

Since the right side of this is a function of only u, we may write a particular solution by inspection,

$$\Lambda_u\psi^{(2)}(u,v)=\frac{-1}{4}\,(v-v_0)\Lambda_u\int_{u_0}^{u} f(u')du'. \tag{26}$$

In the same way we may obtain the v projection of the solution,

$$\Lambda_v\psi^{(2)}(u,v)=\frac{-1}{4}\,(u-u_0)\Lambda_v\int_{v_0}^{v} g(v')dv'. \tag{27}$$

Summing (26) and (27) we have the complete second-order solution,

$$\psi^{(2)}(u,v)=\frac{-1}{4}\left[(v-v_0)\Lambda_u\int_{u_0}^{u} f(u')du'+(u-u_0)\Lambda_v\int_{v_0}^{v} g(v')dv'\right]. \tag{28}$$

The procedure is now clear, and we may continue to all orders; the even orders are similar in form, and the odd orders are similar in form. The complete series solution is

$$\psi(u,v)=\sum_{n=0}^{\infty}\frac{[-(m^2/4)(v-v_0)\Gamma_u]^n}{n!}\left(1-\frac{im}{4}\gamma^v\Gamma_u\right)\Lambda_u f(u)$$
$$+\sum_{n=0}^{\infty}\frac{[-(m^2/4)(u-u_0)\Gamma_v]^n}{n!}\left(-\frac{im}{4}\gamma^u\Gamma_v\right)\Lambda_v g(v), \tag{29}$$

where the multiple integral operator Γ^n is defined as

$$\Gamma_u^n f(u)=\int_{u_0}^{u}du'\int_{u_0}^{u'}du''\cdots\int_{u_0}^{u^{n-1}}du^n\ f(u^n). \tag{30}$$

The series (29) may be readily summed to give a concise expression for the solution

$$\psi(u,v)=\exp\left[-\left(\frac{m^2}{4}\right)(v-v_0)\Gamma_u\right]\left(1-\frac{im}{4}\gamma^v\Gamma_u\right)\Lambda_u f(u)$$
$$+\exp\left[-\left(\frac{m^2}{4}\right)(u-u_0)\Gamma_v\right]\left(1-\frac{im}{4}\gamma^u\Gamma_v\right)\Lambda_v g(v). \tag{31}$$

This gives a solution of the free particle Dirac equation for any pair of generating functions f and g; the generating functions together have only four independent components, however, so this initial value data contains the same amount of information as that in the standard Cauchy problem.

V. INITIAL VALUES ON NULL SURFACES

The generating functions f and g are arbitrary functions, and are simply related to the initial values of the solution on the null surfaces, as we will now discuss. In this and the following section we set $u_0=v_0=0$ without loss of generality.

To get a relation between the initial values of the function ψ on the null surfaces and the generating functions f and g, we set $u=0$ and then $v=0$ in (31) and easily find

$$\psi_0(u,0)=\left(1-\frac{im}{4}\gamma^v\Gamma_u\right)\Lambda_u f(u)+\Lambda_v g(0),$$
$$\psi_0(0,v)=\left(1-\frac{im}{4}\gamma^u\Gamma_v\right)\Lambda_v g(v)+\Lambda_u f(0). \tag{32}$$

We wish to make a convenient choice for the values of $f(0)$ and $g(0)$; taking $u=v=0$ in (32), we see that

$$\psi_0(0,0)=\Lambda_u f(0)+\Lambda_v g(0). \tag{33}$$

Accordingly, we choose $f(0)=g(0)=\psi_0(0,0)$; then the quantities that appear in the evolution expression (31) are

$$\left(1-\frac{im}{4}\gamma^v\Gamma_u\right)\Lambda_u f(u)=\psi_0(u,0)-\Lambda_v\psi_0(0,0),$$
$$\left(1-\frac{im}{4}\gamma^u\Gamma_v\right)\Lambda_v g(v)=\psi_0(0,v)-\Lambda_u\psi_0(0,0). \tag{34}$$

Thus, the spinorial expressions in parentheses turn the arbitrary 4-tuple functions into the indicated initial data on the null surfaces. These expressions may be inverted if it is desired to obtain f and g,

$$\begin{aligned}\Lambda_u f(u) &= \left(1+\frac{im}{4}\,\gamma^v\Gamma_u\right)[\psi_0(u,0)-\Lambda_v\psi_0(0,0)],\\ \Lambda_v g(v) &= \left(1+\frac{im}{4}\,\gamma^u\Gamma_v\right)[\psi_0(0,v)-\Lambda_u\psi_0(0,0)].\end{aligned} \tag{35}$$

In terms of the initial values of the solution, the expression (31) now reads

$$\begin{aligned}\psi(u,v) &= \exp[-(m^2/4)(v-v_0)\Gamma_u](\psi_0(u,0)-\Lambda_v\psi_0(0,0))\\ &\quad+\exp[-(m^2/4)(u-u_0)\Gamma_v](\psi_0(0,v)-\Lambda_u\psi_0(0,0)).\end{aligned} \tag{36}$$

This is a complete expression for the evolution of the solution from its values on the pair of null surfaces $u=0$ and $v=0$. Note that only the *square* of the mass appears in the evolution operators.

The form of the solution in (36) is very similar to that obtained in Ref. 8 for scalar fields obeying the Klein–Gordon equation; the two exponential evolution operators are identical and only the forms of the initial data expressions are slightly different since the present one contains spin information. Thus, in terms of the null coordinates the dynamics of scalar and spinor fields is remarkably similar, much more so than in terms of the usual Cartesian coordinates.

VI. PLANE WAVES

We wish to verify the consistency of (36) for plane wave solutions of the Dirac equation. We will show that if the appropriate initial data functions are put into (36), then the solution function generated is the appropriate plane wave. We write a plane wave solution in Cartesian and null coordinates as

$$\psi(u,v)=e^{-i(Et-kx)}w(E,k)=e^{-i(\lambda u+\tau v)}w(\lambda,\tau). \tag{37}$$

Here w is the usual Dirac 4-tuple spin function and the null momenta are given by

$$\lambda=\frac{E+k}{2},\quad \tau=\frac{E-k}{2},\quad \lambda\tau=\frac{1}{4}(E^2-k^2)=\frac{m^2}{4}. \tag{38}$$

Thus, the appropriate initial value quantities that enter the evolution expression (36) are

$$\begin{aligned}\psi_0(u,0)-\Lambda_v\psi_0(0,0) &= (e^{-i\lambda u}-\Lambda_v)w(\lambda,\tau),\\ \psi_0(0,v)-\Lambda_u\psi_0(0,0) &= (e^{-i\tau v}-\Lambda_u)w(\lambda,\tau).\end{aligned} \tag{39}$$

We substitute these expressions into (36), abbreviating for convenience $B=-i\lambda$, $C=-i\tau$, $-m^2/4=BC$, and find

$$\begin{aligned}\psi(u,v) &= e^{BCv\Gamma_u}(e^{Bu}-\Lambda_v)w(\lambda,\tau)+e^{BCu\Gamma_v}(e^{Cv}-\Lambda_u)w(\lambda,\tau)\\ &= (e^{BCv\Gamma_u}e^{Bu}+e^{BCu\Gamma_v}e^{Cv})w(\lambda,\tau)-F_C(uv)w(\lambda,\tau).\end{aligned} \tag{40}$$

Here F_C denotes the function related to a constant generator, defined and evaluated as

$$F_C(uv)=\exp\left[-\left(\frac{m^2}{4}\right)v\Gamma_u\right]1=\exp\left[-\left(\frac{m^2}{4}\right)u\Gamma_v\right]1=\sum_{n=0}^{\infty}\frac{(-(m^2/4)uv)^n}{(n!)^2}. \tag{41}$$

Notice that this function is symmetric in u and v. The quantity in parentheses in (40) is straightforward to evaluate; we expand the exponentials in a double series as

$$(e^{BCv\Gamma_u}e^{Bu}+e^{BCu\Gamma_v}e^{Cv})=\sum_{n=0,j=0}^{\infty}\frac{(BCv\Gamma_u)^n}{n!}\frac{(Bu)^j}{j!}+\sum_{n=0,j=0}^{\infty}\frac{(BCu\Gamma_v)^j}{j!}\frac{(Cv)^n}{n!}. \tag{42}$$

It is easy to obtain the operation of Γ^n on powers of u,

$$\Gamma_u^n u^j=\frac{u^{j+n}}{(j+1)(j+2)\cdots(j+n)}. \tag{43}$$

We substitute this into (42) and rearrange summation indices to find

$$\begin{aligned}(e^{BCv\Gamma_u}e^{Bu}+e^{BCu\Gamma_v}e^{Cv})&=\sum_{n\leqslant k}^{\infty}\frac{(Cv)^n}{n!}\frac{(Bu)^k}{k!}+\sum_{n\geqslant k}^{\infty}\frac{(Cv)^n}{n!}\frac{(Bu)^k}{k!}\\&=\sum_{n=0,k=0}^{\infty}\frac{(Cv)^n}{n!}\frac{(Bu)^k}{k!}+\sum_{n=0}^{\infty}\frac{(CBuv)^n}{n!}\\&=e^{Bu+Cv}+F_c(uv).\end{aligned} \tag{44}$$

We now combine (40) and (44) to get the complete solution,

$$\psi(u,v)=e^{Bu+Cv}w(\lambda,\tau)=e^{-i(\lambda u+\tau v)}w(\lambda,\tau), \tag{45}$$

which is the correct plane wave solution. We have thus checked the consistency of a known solution with our formalism. Moreover, it follows that the evolution operator equation (36) will produce the correct solution in any case that may be expanded as a superposition of plane waves.

We note that the constant terms in the initial data expression (34) play a very important role in the formalism and cannot be ignored.

VII. RELATION TO THE HAMILTONIAN VIEWPOINT

The evolution operators in (36) are close symbolic analogs of the usual evolution operator in expression (3), as we will discuss in some detail.[12]

A Taylor series expansion in t of a function may be expressed symbolically as an exponential as follows:

$$\psi(\mathbf{x},t)=e^{(t-t_0)\partial/\partial t}\psi(\mathbf{x},t_0)\equiv\sum_{n=0}^{\infty}\frac{(t-t_0)^n}{n!}\,\psi_{|nt}(\mathbf{x},t)_{t=t_0}. \tag{46}$$

That is, the quantity in the exponent generates a time shift. In standard quantum mechanics the time derivative is related to the energy operator by $\partial/\partial t=-iE$. To define the dynamics the energy operator in terms of t is identified with the Hamiltonian operator H in terms of x. That is, a Schrödinger equation is postulated, with an operator equivalence,

$$\frac{\partial}{\partial t}=-iH. \tag{47}$$

Then for a wave function the Taylor series expression reads

$$\psi(\mathbf{x},t)=e^{-i(t-t_0)H}\psi(\mathbf{x},t_0), \tag{48}$$

which is the standard form for the time evolution operator, as in (3).

We can use the same procedure to obtain our result (36)—but only symbolically and up to a normalization and constant terms. We begin with an expression for a double Taylor series expansion of a function of u and v in analogy with (46),

$$\psi(u,v)=\tfrac{1}{2}\left[e^{(v-v_0)\partial/\partial v}\psi(u,v_0)+e^{(u-u_0)\partial/\partial u}\psi(u_0,v)\right]. \tag{49}$$

In analogy with the Schrödinger equation, we define the dynamics with the Klein–Gordon equation, which in terms of u and v is

$$\frac{\partial^2}{\partial u\ \partial v}\ \psi(u,v)=-\frac{m^2}{4}\ \psi(u,v), \tag{50}$$

which solutions of the Dirac equation must obey. In analogy with (47), this allows us to identify the v derivative operator with the following operator in terms of u:

$$\frac{\partial}{\partial v}=-\frac{m^2}{4}\left(\frac{\partial}{\partial u}\right)^{-1}\equiv-\frac{m^2}{4}\,\Gamma_u\,. \tag{51}$$

Substituting this into (49) we obtain (36)—if we do not concern ourselves about the normalization factor and the constant terms, which the symbolic derivation does not seem to explain.

In conclusion, our main result (36) presents the evolution of a spinor field in terms of two analogs of the Hamiltonian operator, and the dynamics of the spinor field is remarkably similar to that of the scalar field.[8]

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The monopole equations in topological Yang–Mills

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We twist the monopole equations of Seiberg and Witten and show how these equations are realized in topological Yang–Mills theory. A Floer derivative and a Morse functional are found and are used to construct a unitary transformation between the usual Floer cohomologies and those of the monopole equations. Furthermore, these equations are seen to reside in the vanishing self-dual curvature condition of an OSp(1|2)-bundle. Alternatively, they may be seen arising directly from a vanishing self-dual curvature condition on an SU(2)-bundle in which the fermions are realized as spanning the tangent space for a specific background. © *1996 American Institute of Physics.* [S0022-2488(96)00202-3]

I. INTRODUCTION

In this note, we will demonstrate how the monopole equations of Ref. 1 for an Abelian connection A and SU(2) doublet fermions arise in topological Yang–Mills (TYM) gauge theory[2] and in Floer theory[3] in particular. As we will see the process is remarkably simple. Along the way, we will develop a quantum mechanical system whose ground states have support on the fields which satisfy the twisted monopole equations. What is more, we will find that the inner products of representatives of the cohomology groups so constructed are formally equal to the Donaldson invariants.[4]

Consider the twisted version of the monopole equations. Let $\mathscr{T}$ denote the twisting map, $S^{\pm}$ the right/left spin bundles over a four-dimensional manifold, X, Λ^p the bundle of p-forms, and Λ^p_O the bundle of p-forms with odd Grassmann parity. Then for a spinor which in addition to being a section of S^+ is also a doublet of a rigid SU(2) (denoted by $\mathscr{S}$) so that $M=\sigma(S^+\otimes\mathscr{S})$, we have $\mathscr{T}:\sigma(S^+\otimes\mathscr{S})\to\Lambda^1_O$; likewise, [$P_{\pm}(\Lambda^2)=\Lambda^{2\pm}$ is the projection to (anti-)self-dual two-forms.], $\mathscr{T}:\sigma(S^-\otimes\mathscr{S})\to\Lambda^0_O\oplus\Lambda^{2+}_O$. With this as background, the equations we are interested in are

$$P_+(D\psi)=0, \quad D^*\psi=0, \quad F^+=iP_+(\bar{\psi}\wedge\psi), \tag{1}$$

where $\psi=\sigma(\Lambda^1_O\otimes L)$, D is the covariant exterior derivative given by the connection A on L, $P_+=\frac{1}{2}(I+*)$ is the self-dual projector, and the "bar" denotes complex conjugation. (A related set of equations but with bosons instead of fermions was obtained[5] from $N=4$ super Yang–Mills and further studied in Ref. 6.) In the notation of Ref. 1, the elliptic complex on which these twisted monopole equations are realized form the exact sequence

$$0\to\Lambda^0\overset{s}{\to}\Lambda^1\oplus(\Lambda^1_O\otimes L)\overset{t}{\to}\Lambda^{2+}\oplus(\Lambda^0_O\oplus\Lambda^{2+}_O)\to 0. \tag{2}$$

This complex defines the arena in which we will work in this paper. These equations stand on their own irrespective of our discussion in the previous paragraph; in particular, the value of $w_2(X)$.

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However, they may be viewed as arising from the twisting of the $N=2$ versions of the monopole equations on spin manifolds. It should be noted that, unlike TYM, the first equation cannot be obtained by smoothly varying the connection in the third equation.

In the next section we will see how the twisted monopole equations (1) arise by a reduction of a class of zero-action solutions of TYM to a $U(1)$ subgroup of the gauge group. Our intention is not to perform a duality transformation on or any addition (such as twisted $N=2$ hypermultiplets) to TYM as we would like to see these equations directly in the field space of the quantum field theory for the Donaldson invariants. In this way, we hope to be able to shed light on the connection between the Seiberg–Witten invariants[1,7–9] and those of Donaldson.[4] A step in this direction will be made in Sec. III. Some other directions spawned by this approach will be discussed in Sec. IV. Our conclusions may be found in Sec. V.

II. IN TOPOLOGICAL YANG–MILLS

Let us focus on obtaining the twisted monopole equations as a special minimum action condition in topological Yang–Mills theory on a G-bundle. For simplicity, we will take the structure group to be SU(2).

First, we realize that the Eqs. (1) cannot arise by breaking the gauge group to $U(1)$. Although breaking the gauge group in TYM is possible by adding

$$S_m \equiv \left\{ Q, \int_X \mathrm{Tr}(\psi \wedge * D\phi) \right\} + \int_X V(\phi) \tag{3}$$

to the action for TYM, the equations cannot be obtained in the low-energy effective theory as all fields are in the adjoint representation here. [Note that $V(\phi)$ is a Higgs potential for the BRST singlet field, which is bounded from below at zero. Although this explicitly introduces a metric (in a volume preserving, diffeomorphism invariant way), as long as V is zero in the low-energy effective field theory, we can ignore this effect.] It is presumably possible to add matter to the TYM theory so that the fermions which appear on the right-hand side (via a current–current coupling in the effective action) of Eq. (1) were not in the adjoint representation of the gauge group. However, a negative feature of that approach would be to take us outside of the field space of TYM, thus making it difficult to realize the connection with the Donaldson invariants. Thus, we now resort to the explicit breaking of the SU(2) gauge group.

As an *ansatz*, let us look for field configurations for which the TYM action[2] vanishes. Write the SU(2) generators as $J^a \equiv (J, \bar{J}, J^3)$, similarly for the sections of $\mathrm{ad}(G)$. [We will use the symbol $\mathscr{A}^a$, with gauge index a, to denote the SU(2) connection; while we will use $\underline{A} = \underline{\mathscr{A}^3}$ for the $U(1)$ connection, as in the previous section.] The following fields will vanish: $\mathscr{A}$, $\bar{\mathscr{A}}$, $\lambda, \bar{\lambda}, \phi^3, \chi^3, \eta^3$. We will in addition set $(\phi, \bar{\phi}) = (\nu, \bar{\nu})$, where for now ν is a complex constant. Note that the BRST transformations in this field-restricted sector are $[Q', A] = \psi^3$ and $\{Q', \psi^a\} = 0$.

After integrating out λ, the TYM action becomes

$$S = \int_X \left[\frac{1}{8} F^{3+} \wedge * F^{3+} + \frac{1}{8|\nu|^2} (\psi \wedge \bar{\psi}) \wedge * (\psi \wedge \bar{\psi}) - \bar{\chi} \wedge * D\psi - \chi \wedge * D\bar{\psi} + \bar{\eta} D * \psi - \eta D * \bar{\psi} \right]. \tag{4}$$

The first line in this expression may be written as

$$S_0 = \frac{1}{8} \int_X \left| F^{3+} + \frac{1}{\nu} P_+ (\bar{\psi} \wedge \psi) \right|^2, \tag{5}$$

so long as ν is pure imaginary. Then, invoking the χ, η-equations of motion, we see that the action is zero on nontrivial field equations which satisfy the twisted monopole equations (1) with $\psi \to |\nu|^{-1/2}\psi$.

Now that we have obtained the twisted monopole equations in Donaldson field space, we might impose them as semi-classical conditions on the polynomial invariants. Indeed, the parameter $|\nu|$ is best defined by the Donaldson invariant

$$\langle W_0 \rangle = \langle \tfrac{1}{2} \operatorname{Tr}(\phi^2) \rangle = \tfrac{1}{4} |\nu|^2, \tag{6}$$

where the brackets mean the evaluation on these special field configurations. For the map from $H_2(X)$ to $H^2(\mathscr{M})$, the observable, $\int_\Sigma W_2$, becomes

$$\left\langle \int_\Sigma W_2 \right\rangle = \left\langle \int_\Sigma \operatorname{Tr}\left(\frac{1}{2}\, \psi \wedge \psi + \phi F \right) \right\rangle = -2\pi |\nu| c_1(L)[\Sigma], \tag{7}$$

proportional to the first Chern class of the line bundle.

Having recovered the twisted monopole equations by hand from TYM, we now wonder why they should exist in the latter theory in the first place. Well, this is where the ''by-hand'' procedure we have just performed actually teaches us something. The first and third equations in (1) are nothing but the anti-self-dual condition in disguise. To see this, consider starting off with the equation $\mathscr{F}^+(\mathscr{A})=0$ for a SU(2) curvature with connection $\mathscr{A}$. Then write the connection as a particular background (A) plus a fluctuation $(\hat{\psi})$ via the expressions $\mathscr{A}^3 = A^3$, $(1/\sqrt{2})(\mathscr{A}^1 + i\mathscr{A}^2) = \hat{\psi}$ and $(1/\sqrt{2})(\mathscr{A}^1 - i\mathscr{A}^2) = \hat{\bar{\psi}}$; i.e., A^3 does not fluctuate while the other connection components do not have background parts. Upon substituting these expressions into the $\mathscr{F}^+ = 0$ equation, dropping the hats on the ψs, and changing their Grassmann parity we arrive at the first and third twisted monopole equations. Thus we see that it is not surprising that we obtained them in TYM.

III. IN FLOER COHOMOLOGY

We have seen how the twisted monopole equations appear as a minimum action configuration in TYM. We will now identify the analogous Floer cohomology condition. Then we will see that a unitary transformation exists which relates the Floer and monopole cohomologies so constructed. It is important that we will be working in the phase space of the Floer theory. As a point of reference recall that given a closed, orientable three-manifold, Y, the Floer cohomology operator is (t is an arbitrary real parameter)

$$Q_t = \int_Y \psi_i^a(x) \left(\frac{\delta}{\delta \mathscr{A}_i^a(x)} + \frac{1}{2}\, t \epsilon^{ijk} \mathscr{F}_{jka}(x) \right), \tag{8}$$

for which the representatives of the cohomology groups are the wavefunctionals, $\Psi[\mathscr{A}_i^a, \psi_i^a]$ which satisfy the condition $Q_t \Psi = Q_t^\dagger \Psi = 0$, where $\psi^\dagger = \overline{\chi}$.

As before, let $\mathscr{A} \equiv (\mathscr{A}^\pm, A)$ be the connection on the SU(2) bundle, G, over Y and take ψ^a to be the components of a section of the bundle $(\Lambda^1_O \otimes G)$. Choose the Morse function to be (see also Ref. 10)

$$W'[A,\psi] = \frac{1}{4\pi} \int_Y [A \wedge dA + i2\bar{\psi} \wedge D(A)\psi], \tag{9}$$

and based on $Q = \int_Y \psi_i^a \delta / \delta \mathscr{A}_i^a$ define the exterior derivative

$$Q_t' = e^{-2\pi t W'[A,\psi]} Q e^{2\pi t W'[A,\psi]}$$

$$= \int_Y \left[\psi_i^1 \frac{\delta}{\delta \mathscr{A}_i^1} + \psi_i^2 \frac{\delta}{\delta \mathscr{A}_i^2} + \psi_i^3 \left(\frac{\delta}{\delta A_i} + \frac{1}{2} t \epsilon^{ijk} F_{jk}(A) - 2it \epsilon^{ijk} (\bar{\psi}_j(x) \psi_k(x)) \right) \right]. \quad (10)$$

Clearly, a solution of $Q_t' \Psi'[\mathscr{A}_i^a, \psi_i^a] = 0$ is any $\Psi'[A,\psi]$ which has support only on Eq. (1) written on $X = Y \times \mathbb{R}$,

$$F_{0i}^+ = \epsilon_{ijk} \bar{\psi}^j \psi^k, \quad (11)$$

in the gauge $\mathscr{A}_0^a = \psi_0^a = 0$.

The Hamiltonian whose vacuum states include solutions to the twisted monopole equations will take the form $H' = \frac{1}{2}\{Q', Q'^\dagger\}$. After some straightforward algebra, one finds the new Hamiltonian on the states $\Psi'[A, \psi]$ takes the form

$$H' = 2 \int_Y (F_{0i}^+ - \epsilon_{ijk} \bar{\psi}_j \psi_k)^\dagger (F_{0i}^+ - \epsilon_{imn} \bar{\psi}_m \psi_n). \quad (12)$$

Comparing this Hamiltonian to the Floer Hamiltonian, we note some interesting differences. First, only the Abelian component of the gauge fields play a role. Next, the fermionic partners appear in a fashion which does not preserve ghost number. Note also that none of the fermions have appropriate kinetic contributions. All of these features are consistent with the fact that the twisted monopole equations are simply rewritings of the self-dual curvature condition.

The question remains how to extract the solution Ψ' from the Floer cohomology. That is, we seek a W such that given a Floer representative Ψ,

$$\Psi[A_i^a, \psi_i^a] = e^{-2\pi t W[\mathscr{A}_i^a, \psi_i^a]} \Psi'[A, \psi]. \quad (13)$$

It is not hard to see that such a functional is given by

$$W[\mathscr{A}_i^a, \psi_i^a] \equiv -\frac{1}{4\pi} \int_Y \mathrm{Tr} \left(\mathscr{A} d \mathscr{A} + \frac{2}{3} \mathscr{A}^3 \right) + W'[A, \psi]. \quad (14)$$

Here, the first term in W is recognized as the SU(2) Chern–Simons action. The virtue of the construction (13) is that it allows us to conjecture that given $X \equiv X_l \cup_Y X_r$, where X_l and X_r are manifolds whose boundaries are diffeomorphic to Y but have opposite orientation, the inner products are related by

$$\langle \Psi | \Psi \rangle = \langle \Psi' | \Psi' \rangle. \quad (15)$$

It is reasonable to presume that the Ψ' are representatives of a Floer homology group but for spectral flows governed by the monopole equations and are obtained from the Seiberg–Witten invariants via surgery. In that case, we conjecture that this equality will unlock the formal relationship between those invariants and the Donaldson polynomials.

IV. OTHER DIRECTIONS

Apart from the obvious solutions to the usual Floer homology condition, namely Ψs which have support only on $\delta / \delta A_i^a(x) + \frac{1}{2} t \epsilon^{ijk} \mathscr{F}_{jka}(x) = 0 \leftrightarrow \mathscr{F}_{0ia}^+ = 0$, another simple solution is evident. If the condition

$$\mathscr{F}_{0ia}^+ = \kappa f_{abc} \epsilon_{ijk} \psi^{jb} \chi^{kc} \quad (16)$$

is met, then $Q_t = Q_t^\dagger = 0$ for any κ. However, this solution is not compatible with Eq. (1) due to the presence of the structure constants and the fact that ψ and χ are canonically conjugate to each other. Beyond this, our methodology in the last section may be extended to construct other cohomologies.

Our procedure suggests another direction to explore. As we discussed before, we do not want to add topological matter to TYM in order to obtain the monopole equations as this would spoil the direct connection with the self-dual curvatures of Donaldson theory. Now, in principle, TYM exists for an arbitrary structure group. With this in mind, we are led to introduce a group which has both bosonic and fermionic generators; i.e., a supergroup. For simplicity, let us take the group to be OSp(1|2) with graded commutators:

$$
\begin{aligned}
[J_a,\ J_b] &= \epsilon_{abc} J^c, \\
[J_a,\ Q_\alpha] &= -i\tfrac{1}{2}(\gamma_a)_\alpha{}^\beta Q_\beta, \\
\{Q_\alpha, Q_\beta\} &= i(\gamma_a)_{\alpha\beta} J^a.
\end{aligned}
\tag{17}
$$

As these equations suggest, $J_a(Q_\alpha)$ are Grassmann even(odd) generators with $\alpha=1,2$ and the J_a forming a SU(2) subgroup. The (γ^a) are three-dimensional Clifford matrices: $\gamma^a \in (\sigma^3, -\sigma^1, \sigma^2)$. We introduce a connection one-form on the OSp(1|2)-bundle over X,

$$
\mathbf{A} = \mathscr{A}^a J_a + \Upsilon^\alpha Q_\alpha, \tag{18}
$$

where the two-component Grassmann odd field Υ^α is (ψ^1, ψ^2). Its curvature two-form is

$$
\begin{aligned}
\mathscr{F} &= \hat{F}^a J_a + f^\alpha Q_\alpha, \\
\hat{F}^a &= F^a(\mathscr{A}) J_a + i\tfrac{1}{2}(\gamma^a)_{\alpha\beta} \Upsilon^\alpha \wedge \Upsilon^\beta J_a, \\
f^\alpha &= D(\mathscr{A})\Upsilon^\alpha = d\Upsilon^\alpha - \tfrac{1}{2}\mathscr{A}^a \wedge \Upsilon^\beta (\gamma_a)_\beta{}^\alpha,
\end{aligned}
\tag{19}
$$

where $F(\mathscr{A})$ is the usual curvature of a SU(2)-bundle. It then follows that the self-dual curvature equations become

$$
\mathscr{F}^+ = 0 \Rightarrow \begin{cases} F^{+a}(\mathscr{A}) = -i\tfrac{1}{2}(\gamma^a)_{\alpha\beta} P_+(\Upsilon^\alpha \wedge \Upsilon^\beta), \\ P_+(D(\mathscr{A})\Upsilon^\alpha) = 0. \end{cases} \tag{20}
$$

By enlarging the principle bundle we have incorporated the monopole equations into a single vanishing self-dual curvature equation.

V. CONCLUSION

We have realized the twisted version of the monopole equations[1] in the fields space of topological Yang–Mills. In addition, we have identified a unitary transformation between the respective cohomologies and were led to conjecture an equivalence between the Donaldson invariants and those which follow from the spectral flows governed by the monopole equations. Our method suggests a number of generalizations, including the appearance of the monopole equations in a self-dual curvature condition on a super-bundle. In addition, we have found that the twisted monopole equations arise directly from vanishing self-dual curvature condition on an SU(2)-bundle in which the fermions are realized as spanning the tangent space for a specific background, that background being one in which only the connection in the Abelian direction is non-zero and

its tangent space is null. In this vein, the fermions in the equations span the tangent space to the point zero which is the background value of the connections in the compliment of the $U(1)$ subgroup.

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Generalization of the Calogero–Cohn bound on the number of bound states

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It is shown that for the Calogero–Cohn-type upper bounds on the number of bound states of a negative spherically symmetric potential $V(r)$, in each angular momentum state, that is, bounds containing only the integral $\int_0^\infty |V(r)|^{1/2}\,dr$, the condition $V'(r)\geqslant 0$ is not necessary, and can be replaced by the less stringent condition $(d/dr)[r^{1-2p}(-V)^{1-p}]\leqslant 0$, $\frac{1}{2}\leqslant p<1$, which allows oscillations in the potential. The constants in the bounds are accordingly modified, depend on p and l, and tend to the standard value for $p=\frac{1}{2}$. © *1996 American Institute of Physics.* [S0022-2488(96)00302-2]

I. INTRODUCTION

Among the numerous bounds on the number of bound states in a potential, or more generally the moments of the eigenvalues, physicists prefer those given by semi-classical expressions. Often these are only valid in the strong coupling limit and the price to pay to convert them into strict bounds is to multiply them by some appropriate numerical factor. In the case of the bound of Calogero and Cohn, who assume monotonicity of the potential, it is a factor two. What we shall show in this paper is that the requirement of monotonicity of the potential can be considerably weakened if one is ready to replace this factor two by a correspondingly larger one. This will broaden the field of application of the bound.

For a regular and spherically symmetric potential $V(r)$, which is purely attractive and non-decreasing ($V'\geqslant 0$), and vanishes at infinity, Calogero[1] and Cohn[2] have shown that in the S-wave, the number of bound states for the radial Schrödinger equation

$$\varphi''+E\varphi=V\varphi, \quad r\in[0,\infty), \quad \varphi(0)=0, \tag{1}$$

admits the upper bound

$$n_0\leqslant \frac{2}{\pi}\int_0^\infty |V(r)|^{1/2}\,dr. \tag{2}$$

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By regular potentials, we mean those which are less singular than r^{-2} at the origin, and go to zero faster than r^{-2} at infinity. More precisely, they satisfy the condition[3,4]

$$\int_0^\infty r|V(r)|dr<\infty. \tag{3}$$

In what follows, we always assume that this condition is satisfied.

Recently, the bound has been generalized to higher angular momenta by taking into account the effect of the centrifugal potential $l(l+1)/r^2$, $l\geqslant 0$. One finds then, again, with the same conditions on the potential, namely (3) and $V'\geqslant 0$, the upper bound[5]

$$n_l\leqslant 1+\frac{2}{\pi}\left[\int_0^\infty |V|^{1/2}\,dr-\sqrt{\left(\frac{\pi}{2}\right)^2+l(l+1)}\right], \tag{4}$$

which reduces to (2) for $l=0$.

For negative values of l, $-\frac{1}{2}<l\leqslant 0$, and again with the previous conditions on V, one has now[5]

$$n_l\leqslant \frac{1}{\sqrt{2(2l+1)}}\int_0^\infty |V|^{1/2}\,dr. \tag{5}$$

Making $l=0$ here, we do not get the Calogero–Cohn constant $2/\pi$, but $\sqrt{2}/2$, which is slightly larger. The above bound is singular for $l=-\frac{1}{2}$, and we shall see that this cannot be avoided.

With no condition on the potential, except (3), we have the general Bargmann bound[3,6]

$$n_l\leqslant \frac{1}{(2l+1)}\int_0^\infty r|V(r)|\,dr. \tag{6}$$

This bound also has been generalized, again with no condition on potential except (3), to a large family of bounds[7]

$$n_l\leqslant \frac{C_p}{(2l+1)^{2p-1}}\int_0^\infty |r^2V|^p\,\frac{dr}{r}, \tag{7}$$

where p is a free parameter, $1\leqslant p\leqslant\frac{3}{2}$, and

$$C_p=\frac{(p-1)^{p-1}\Gamma(2p)}{p^p\Gamma^2(p)}. \tag{8}$$

Making $p\downarrow 1$, we get the Bargmann bound (6), as expected. In (6) and (7), we have tacitly assumed V to be negative everywhere. If the potential changes sign, then we should replace in (6) and (7) V by its negative part V_-.

Now, the question arises whether one could fill the gap between (7), valid for $1\leqslant p\leqslant\frac{3}{2}$, and (2), (4), and (5), where we have the integral of $|V(r)|^p$, with $p=\frac{1}{2}$. In short, whether one could find, with some condition on the potential—similar to the Calogero–Cohn condition $V'\geqslant 0$—such that one would have a bound similar to (7) for $\frac{1}{2}\leqslant p\leqslant 1$. The answer is in the affirmative. Indeed, assuming again V to be negative everywhere, and

$$\frac{d}{dr}\,[r^{1-2p}(-V)^{1-p})]\leqslant 0,\quad \tfrac{1}{2}\leqslant p\leqslant 1, \tag{9}$$

one can show that[8]

$$n_l \leqslant \frac{p}{(1-p)^{1-p}(2l+1)^{2p-1}} \int_0^\infty (-r^2V)^p \frac{dr}{r}. \tag{10}$$

We should remark here that again, for $p=1$, (9) imposes no condition on the potential, and (10) gives us then the Bargmann bound (6), as expected. On the other hand, for $p=\frac{1}{2}$, we obtain the Calogero–Cohn condition $V' \geqslant 0$, but then (10) goes to (5) with $l=0$, which is slightly larger than (2), as we have noticed before.

For p strictly inside the interval $(\frac{1}{2},1)$, the potential may have oscillations while staying everywhere negative. As examples, we give just the two following ones:[9]

$$V_1 = -r^{(2p-1)/(1-p)} e^{-r/(1-p)}; \tag{11}$$

$$V_2 = -r^{(2p-1)/(1-p)} \{[1+\tfrac{1}{2}(\sin r + \cos r)]e^{-r}\}^{1/(1-p)}. \tag{12}$$

It is easily seen that V_1, which vanishes at the origin, has a minimum before going to zero at $r=\infty$, whereas V_2 oscillates indefinitely while going to zero at $r=\infty$. Both satisfy (9).

The purpose of the present paper is to show that, in fact, condition (9) leads to a Calogero–Cohn-type bound, for all $p \in [\frac{1}{2},1)$, that is, a bound containing the integral $\int_0^\infty \sqrt{|V|}dr$, but, of course, with a different constant than $2/\pi$. This would be much more satisfactory for strong attractive potentials since we know that, in the limit $\lambda \to \infty$, the number of bound states of λV, for any fixed $l \geqslant 0$, has the asymptotic behavior[10,11]

$$n_l = \frac{\lambda^{1/2}}{\pi} \int_0^\infty |V_-|^{1/2}\, dr + \text{smaller terms}, \tag{13}$$

with no condition on V other than the finiteness of the integral.

II. GENERAL PROOF OF A CALOGERO–COHN-TYPE BOUND

Since we assume in general (3), we must have $\lim r^2V(r)=0$ as $r \to 0$ or $r \to \infty$. Now, (9) can be written

$$\frac{d}{dr}\{[r^2(-V)]^{1-p}/r\} = -q(r), \tag{14}$$

where q is some positive function, and the function inside the bracket on the l.h.s. vanishes at infinity. Assuming $q(r)$ to be integrable there, which is quite natural, and solving the differential equation (14) for V, together with $V(\infty)=0$, we obtain

$$V(r) = -r^{(2p-1)/(1-p)} \left(\int_r^\infty q(t)dt \right)^{1/(1-p)}. \tag{15}$$

The only condition to be imposed on $q(r)$, besides being positive and integrable for $r>0$, is that (3) must be satisfied. As examples, we can take $q(t)=e^{-t}$ or $q(t)=(1+\sin t)e^{-t}$, and we obtain, respectively, (11) and (12).

We have now to deal with the radial Schrödinger at zero energy

$$\varphi_l'' = \left[V(r) + \frac{l(l+1)}{r^2} \right] \varphi_l \tag{16}$$

together with $\varphi_l(0)=0$, and the well-known nodal theorem,[3] which asserts that the number of bound states $n_l(V)$ is equal to the number of nodes (zeros) of $\varphi_l(r)$ on the real r-axis, origin excepted. The potential being given by (15), we can now use the Liouville transformation

$$r\to Z=r^{1/2(1-p)}, \quad \varphi\to\psi(Z)=Z^{(2p-1)/2}\varphi(r(Z)). \tag{17}$$

The change of variable is one-to-one, and applies $r\in[0,\infty)$ on $Z\in[0,\infty)$, $r=0$ corresponding to $Z=0$. The change of function is such that to $\varphi(r=0)=0$ corresponds $\psi(Z=0)=0$. After the transformation, (16) becomes ($\dot{} = d/dZ$)

$$\ddot{\psi}(Z)=\left[\tilde{V}(Z)+\frac{L(L+1)}{Z^2}\right]\psi(Z) \tag{18}$$

together with $\psi(0)=0$, where

$$\tilde{V}(Z)=-4(1-p)^2\left(\int_r^\infty q(t)dt\right)^{1/(1-p)}\Bigg|_{r=Z^{2(1-p)}}, \tag{19}$$

and

$$L=L(l,p)=-\tfrac{1}{2}+(1-p)(2l+1). \tag{20}$$

We see that we again have to deal with a Schrödinger equation at zero energy, in the variable Z, with Dirichlet condition at the origin, and a potential $\tilde{V}(Z)$ which is now attractive and increasing, together with the centrifugal term $L(L+1)/Z^2$. Moreover, the zeros of ψ on the positive Z-axis are in one-to-one correspondence with those of $\varphi(r)$ on the positive r-axis. It follows that the number of bound states is the same for (16) as for (18). However, the advantage of (18) is that we can now use the bounds (4) or (5), according to the value of $L\geqslant 0$, or $-\frac{1}{2}<L\leqslant 0$. We would then get bounds which contain $\int_0^\infty|\tilde{V}(Z)|^{1/2}\,dZ$. This, expressed in terms of the variable r, is exactly $\int_0^\infty|V(r)|^{1/2}\,dr$, and we obtain the desired result. In review, we have the following.

Theorem 1: Under the condition (9) on the potential, we have

$$n_l\leqslant 1+\frac{2}{\pi}\left[\int_0^\infty|V(r)|^{1/2}\,dr-\sqrt{\left(\frac{\pi}{2}\right)^2+L(L+1)}\right], \tag{21}$$

if L, given by (20), is $\geqslant 0$, and

$$n_l\leqslant\frac{1}{\sqrt{2(2L+1)}}\int_0^\infty|V(r)|^{1/2}\,dr, \tag{22}$$

if $L\in(-\frac{1}{2},0]$. The first case corresponds to $l\geqslant(2p-1)/4(1-p)$, and the second to $-\frac{1}{2}<l\leqslant(2p-1)/4(1-p)$. We should remark here that when $l=0$, we have $L=\frac{1}{2}-p$, which is negative, except for $p=\frac{1}{2}$, and so, we must use in general (22). If $l=0$, and $p=\frac{1}{2}$, i.e., the Calogero–Cohn case, we have the bound (2), and do not have to use (22).

III. DIRECT PROOF OF THE GENERALIZED BOUND (22)

We consider the S-wave, described by Eq. (1). Suppose that there are n_0 bound states. This means that $\varphi_0(r)$ has n_0 nodes $0<r_1<\cdots<r_{n_0}<\infty$. We assume now the potential satisfies the following conditions:

$$V(r)\leqslant 0, \quad [-r^{-\nu}V(r)]'\leqslant 0 \quad \text{for some} \quad \nu\geqslant 0. \tag{23}$$

We have now the following.

Lemma 1: If V satisfies (23), the same is true for $-V(r)(r-r_k)^{-\nu}$ for $r>r_k$. Indeed, we have

$$|V(r)|(r-r_k)^{-\nu}=[|V(r)|r^{-\nu}]\left(\frac{r}{r-r_k}\right)^{\nu},$$

and both factors are decreasing for $r\geqslant r_k$. □

Now, from the Bargmann bound (6) with $l=0$, we have

$$1\leqslant\int_{r_k}^{r_{k+1}}(r-r_k)|V(r)|dr.$$

Taking $\rho_k=r-r_k$, this can be written

$$1\leqslant\int_0^{r_{k+1}-r_k}\rho_k W(\rho_k)d\rho_k, \tag{24}$$

where $W(\rho_k)=V(\rho_k+r_k)$. Restricting ourselves to the interval (r_k,r_{k+1}), and dropping the index k, let us define

$$I(\rho)=\int_0^{\rho}\sqrt{|W(\rho')|}d\rho'. \tag{25}$$

If V satisfies (23), Lemma 1 shows that $|W(\rho)|\rho^{-\nu}$ is also decreasing. Therefore

$$I(\rho)=\int_0^{\rho}\sqrt{|W(\rho')|\rho'^{-\nu}}\rho'^{\nu/2}d\rho'\geqslant\sqrt{\rho^{-\nu}|W(\rho)|}\times\frac{\rho^{1+\nu/2}}{1+\nu/2}=\rho\,\frac{\sqrt{|W(\rho)|}}{1+\nu/2}. \tag{26}$$

Now using this inequality, together with (24) and $dI/d\rho=\sqrt{|W(\rho)|}$, we obtain

$$1\leqslant\int_0^{r_{k+1}-r_k}[\rho\sqrt{|W(\rho)|}]\sqrt{|W(\rho)|}d\rho\leqslant\left(1+\frac{\nu}{2}\right)\int_0^{r_{k+1}-r_k}I(\rho)\,\frac{dI}{d\rho}\,d\rho$$
$$=\frac{1}{2}\left(1+\frac{\nu}{2}\right)[I(r_{k+1}-r_k)]^2.$$

Therefore

$$1\leqslant\frac{\sqrt{\nu+2}}{2}\,I(r_{k+1}-r_k)=\frac{\sqrt{\nu+2}}{2}\int_{r_k}^{r_{k+1}}\sqrt{|V(r)|}dr. \tag{27}$$

Adding up these inequalities for all the intervals, we end up with

$$n_0\leqslant\frac{\sqrt{\nu+2}}{2}\int_0^{\infty}|V|^{1/2}\,dr. \tag{28}$$

In order to apply this inequality to our potential satisfying (9), we just have to put $\nu=(2p-1)/(1-p)$. When p varies between $\frac{1}{2}$ and 1, ν varies between 0 and ∞. In any case, we obtain finally

$$n_0\leqslant\frac{1}{2\sqrt{1-p}}\int_0^{\infty}|V(r)|^{1/2}\,dr \tag{29}$$

which is the desired result. □

Let us remark here that, for $p=1$, the r.h.s. of (29) is infinite. Indeed, condition (9) for $p=1$ puts no restriction on the potential. And with no restriction on the potential, the only bound which is valid in general is the Bargmann bound (6), which contains the integral of $|V|$ instead of $|V|^{1/2}$. As is well known,[3,6] the Bargmann bound can be saturated by n_0 negative δ-potentials with suitable strengths and locations:

$$V(r)=-\sum_{k=1}^{n_0} g_k \delta(r-r_k) \tag{30}$$

and such a potential gives zero in the r.h.s. of (29). It follows that the singularity at $p=1$ in front of the integral in (29) cannot be avoided. We can summarize the results in the following

Theorem 2: For a purely attractive potential satisfying the condition (23) for some $\nu \geqslant 0$, the number of S-wave bound states satisfies the bound

$$n_0 \leqslant \frac{\sqrt{\nu+2}}{2} \int_0^\infty |V|^{1/2}\, dr. \tag{31}$$

IV. IMPROVEMENT OF THE GENERALIZED BOUND (22)

If $L=L(l,p)\in(-\frac{1}{2},0)$ we have the following operator inequality due to the local uncertainty principle:[12]

$$-\frac{d^2}{dz^2}+\frac{L(L+1)}{z^2} \geqslant -(2L+1)^2 \frac{d^2}{dz^2}. \tag{32}$$

Hence the number of bound states of the operator associated to (18) is bounded above by the number of bound states of $(-2L+1)^2 d^2/dz^2+\tilde{V}(z)$. Applying the Calogero–Cohn bound to this operator we find

$$n_l \leqslant \frac{1}{2L+1}\frac{2}{\pi}\int_0^\infty |V(r)|^{1/2}\, dr. \tag{33}$$

Together with (22) we therefore have the following.

Theorem 3: Under the condition (9) on the potential and if $L\in(-1/2,0]$, we have

$$n_l \leqslant C_L \int_0^\infty |V(r)|^{1/2}\, dr, \tag{34}$$

where

$$C_L=\min\left(\frac{1}{2L+1}\frac{2}{\pi}, \frac{1}{\sqrt{2(2L+1)}}\right). \tag{35}$$

If the potential satisfies condition (23) for some $V \leqslant 0$, the number of S-wave bound states satisfies the bound

$$n_0 \leqslant C_\nu \int_0^\infty |V(r)|^{1/2}\, dr \tag{36}$$

with

$$C_\nu = \min\left(\frac{\nu+2}{\pi}, \frac{\sqrt{\nu+2}}{2} \right). \tag{37}$$

In particular

$$C_\nu = \begin{cases} \dfrac{\nu+2}{\pi}, & \text{if } \nu < \nu_C := \dfrac{\pi^2-8}{4} \\ \dfrac{\sqrt{\nu+2}}{2}, & \text{if } \nu_C \leqslant \nu < \infty \end{cases}. \tag{38}$$

We note that $\lim_{\nu\to 0} C_\nu = 2/\pi$ so that we recover in the limit $\nu \to 0$ the optimal bound.

V. THE CASE $0 > \nu > -2$

From (31), we see that if the r.h.s. is less than 1, then there is no bound state. It is easy to see that this holds not only for $\nu > 0$, but also for $0 > \nu > -2$. In other words, if the absolute value of the potential decreases faster than $r^{-|\nu|}$, $0 > \nu > -2$, then the condition

$$\frac{\sqrt{\nu+2}}{2} \int_0^\infty |V(r)|^{1/2}\, dr < 1 \tag{39}$$

guarantees the absence of bound states. As an example, we can consider the Yukawa potential $V = -g \exp(-\mu r)/r$. Here, $\nu = -1$, and the constant in front of the integral becomes $\frac{1}{2}$, which is smaller than the Calogero constant $2/\pi$. However, we must remember that all this is derived from the Bargmann bound, and therefore we cannot do better than that. Also, generalization to n bound states for $\nu < 0$ is impossible because Lemma 1 no longer holds. So the interest of $\nu < 0$ is rather limited.

VI. THE CALOGERO'S SUFFICIENT CONDITION

Here, we would like to see how good the constant C_ν is in front of (36). For this purpose, we consider the simple power-potential

$$V(r) = -\lambda r^\nu \theta(1-r). \tag{40}$$

Now, a sufficient condition of Calogero[13] states that, for a purely attractive potential, if there exists an R such that

$$\frac{1}{R} \int_0^R r^2 |V(r)|\, dr + R \int_R^\infty |V(r)|\, dr \geqslant 1, \tag{41}$$

then there is at least one bound state. Here R is arbitrary and can be chosen at will. Applying (41) to (40), and maximizing with respect to R, we find that it is sufficient to have

$$\lambda \geqslant \lambda_1 = (\nu+2)\left[\frac{2(\nu+2)}{\nu+3} \right]^{1/(\nu+1)}. \tag{42}$$

Now, assume that the r.h.s. of (36) is too large, and that C_ν can be replaced by a better (smaller) constant $\tilde{C}_\nu$. Applying now (36), with $n_0 = 1$ and the better constant $\tilde{C}_\nu$ to our potential (40), we find that we must have $\tilde{C}_\nu \sqrt{\lambda_1} \int_0^1 r^{\nu/2}\, dr \geqslant 1$, that is

$$\tilde{C}_\nu \geqslant \frac{(\nu+2)}{2\sqrt{\lambda_1}} > \left(\frac{\sqrt{\nu+2}}{2}\right)\left[\frac{\nu+3}{2(\nu+2)}\right]^{1/2(\nu+1)}. \tag{43}$$

It is easily seen (see Appendix) that the factor $[(\nu+3)/2(\nu+2)]^{1/2(\nu+1)}$ is an increasing function of ν and goes to 1 as $\nu\to\infty$.

On the other hand the function

$$\frac{\pi}{2}\frac{1}{\sqrt{\nu+2}}\left[\frac{\nu+3}{2(\nu+2)}\right]^{1/2(\nu+2)}$$

is a decreasing function of ν (see Appendix). Therefore this example shows that our constant C_ν is not too bad, and that it cannot be improved by more than a factor

$$[(\nu_C+3)/2(\nu_C+2)]^{1/2(\nu_C+1)} = \left[\frac{1}{2}+\frac{2}{\pi^2}\right]^{2/(\pi^2-4)} \simeq 0.887.$$

We should note here that the Schrödinger equation with the potential (40) can be solved exactly at zero energy. The regular solution is $\varphi = \sqrt{r}J_{L+1/2}(\sqrt{\lambda}Z)$, where $Z=r^{1+\nu/2}/(1+\nu/2)$, and $L=-\nu/2(2+\nu)$. The exact value of λ for which the first bound state appears is given by $\varphi'(r=1)=0$. This is a transcendental equation whose solution is not simple, and needs numerical computation. In principle, this exact value of λ could be used instead of λ_1 of the Calogero's sufficient condition.

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APPENDIX

We must show that the derivative of $F(\nu)=[(\nu+3)/(\nu+2)]^{1/2(\nu+1)}$ is positive, which amounts to the same thing for the derivative of $G(\nu)=\log F(\nu)$. Now, if we write $H(\nu)=2(\nu+1)^2G'(\nu)$, we have

$$H(\nu)=\frac{1}{\nu+2}-\frac{2}{\nu+3}-\log\frac{\nu+3}{2(\nu+2)} \tag{A1}$$

and, therefore,

$$H'(\nu)=(\nu+1)\left[\frac{1}{(\nu+2)^2}-\frac{1}{(\nu+3)^2}\right]>0. \tag{A2}$$

It follows that $H(\nu)$ is increasing for $\nu\geqslant 0$. Now,

$$H(0)\equiv 2G'(0)=\log(\tfrac{4}{3})-\tfrac{1}{6}>0. \tag{A3}$$

Therefore, $H(\nu)$ is positive for $\nu\geqslant 0$, and the same is true for $G'(\nu)$. □

Similarly, we consider the derivative of $\tilde{G}(\nu)=-\frac{1}{2}\log(\nu+2)+G(\nu)$. If we write $\tilde{H}(\nu)=2(\nu+1)^2\tilde{G}'(\nu)$, we find

$$\tilde{H}(\nu)=-\frac{(\nu+1)^2}{\nu+2}+H(\nu), \tag{A4}$$

and, therefore

$$\tilde{H}'(\nu)=-\frac{(\nu+1)(\nu+3)}{(\nu+2)^2}+H'(\nu)=(\nu+1)\left[-\frac{1}{\nu+2}-\frac{1}{(\nu+3)^2}\right]<0. \tag{A5}$$

Since $\tilde{H}(0)=\log\frac{4}{3}-\frac{2}{3}<0$, it follows that $\tilde{H}(\nu)<0$ for all $\nu\geqslant 0$.

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Group theoretical foundations of fractional supersymmetry

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Fractional supersymmetry denotes a generalization of supersymmetry which may be constructed using a single real generalized Grassmann variable, $\theta=\bar{\theta}, \theta^n=0$, for arbitrary integer $n=2,3,\ldots$. An explicit formula is given in the case of general n for the transformations that leave the theory invariant, and it is shown that these transformations possess interesting group properties. It is shown also that the two generalized derivatives that enter the theory have a geometric interpretation as generators of left and right transformations of the fractional supersymmetry group. Careful attention is paid to some technically important issues, including differentiation, that arise as a result of the peculiar nature of quantities such as θ. © *1996 American Institute of Physics.* [S0022-2488(96)01902-6]

I. INTRODUCTION

Supersymmetry has been a popular and fruitful area of research for at least twenty years. Study of it in space-time of one dimension, time, has given rise to the important topic of supersymmetric quantum mechanics (see Refs. 1–3 for reviews). The most primitive version of supersymmetric quantum mechanics is one that involves the use of a single real Grassmann number θ such that

$$\theta=\bar{\theta}, \quad \theta^2=0. \tag{1.1}$$

As a result the theory possesses a natural $\mathbb{Z}_2$-grading and a single generator Q of its supersymmetry transformations which obeys $Q^2=-\partial_t$. The distinctive features of supersymmetric theories which possess such a $\mathbb{Z}_2$-grading can be seen by referring to various papers.[4–9] The term fractional supersymmetry is currently being applied to a class of generalizations of supersymmetry in one dimension. Our work on fractional supersymmetry can be presented most straightforwardly by creating theories with $\mathbb{Z}_n$-grading by generalization of theories with $\mathbb{Z}_2$-grading. Thus we consider theories involving a single real (generalized) Grassmann number θ which obeys

$$\theta=\bar{\theta}, \quad \theta^n=0, \quad n=2,3,4,\ldots, \tag{1.2}$$

in which the generator Q of the generalized ('fractional') supersymmetry transformations that leave such a theory invariant obeys

$$Q^n=-\partial_t. \tag{1.3}$$

The last result accounts loosely for the use of the term 'fractional' as an identifier of the theory.

The generalization from ordinary to fractional supersymmetry not only has intrinsic interest but may also be expected to produce interesting new models in classical and quantum mechanics. There have been a large number of studies of fractional supersymmetry in recent years.[10–18] Some of these deal with a complex Grassmann variable θ such that $\theta^n=0$. Others employ N different copies of θ which obey (1.2), thus developing N-extended fractional supersymmetry. Fractional supersymmetry is contrasted below with a distinct class of generalizations of basic, or $\mathbb{Z}_2$ -graded, supersymmetry, those which possess parasupersymmetry. There has been a great deal of attention

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given recently to work in this field[19–26] and often these papers contain thinking also relevant to fractional supersymmetry. We believe that the whole area promises both activity and progress in the future.

This paper discusses two important aspects of fractional supersymmetry. First, we discuss the fact that the fractional supersymmetry transformations that describe the invariance properties of the $\mathbb{Z}_n$-graded theory form a group G_n. Second, we elucidate certain fundamental technical matters stemming from unfamiliar features of the algebra. Two areas need attention. One concerns differentiation with respect to θ; the other is the situation surrounding families of multiplicative rules of the type

$$\epsilon\theta = q^{-1}\theta\epsilon, \quad q = \exp(2\pi i/n), \tag{1.4}$$

involving a Grassmann number θ, its associated transformation parameter ϵ and dynamical variables of Grassmann type. In the former there are difficulties of principle, which we treat; in the latter it is a matter of demonstrating a coherent rationale behind the formulation and the consistency of results like (1.4) within it.

We give explicit formulas for the elements of the group G_n of transformations that should leave any $\mathbb{Z}_n$-graded theory invariant, and related proofs. Once the status of derivatives with respect to θ is established, we turn to the objects of generalized covariant derivative type that enter (up to now in an *ad hoc* way) into a theory possessing fractional symmetry. We show that these have the interesting geometrical interpretation of being the generators of the left and right actions of the fractional supersymmetry group G_n (as is the case for ordinary supersymmetry[27]).

We have introduced into our discussion a quantity $q = \exp(2\pi i/n)$ which obeys

$$q^n = 1. \tag{1.5}$$

To provide some appropriate comment, we recall that fractional symmetry aims at a generalization of supersymmetry. The latter when quantized, involves one boson and one fermion variable, and requires use of a 2×2 matrix representation of the fermion. We plan a generalization (see (4.3), (4.1) for $n=3$ or (7.2) below), which retains the boson and replaces the fermion by some more general object, cf. (1.1) and (1.2). Two classes of variables, which can be represented by matrices in an n-dimensional vector space are known to us. The parafermions[28,29] are one of these; use of them leads down a path of interest, but not the one we are able to usefully follow at the moment, toward parasupersymmetry. We follow the other path. The q-deformed harmonic oscillator[30–32] possesses commutation relations in terms of its a and $a^\dagger$ variables that make sense, not only for $q \in R$, but also $q \in C$, when (1.5) applies. In this situation, a and $a^\dagger$ are represented (for each n) by $n\times n$ matrices. Since for $n=2$ we get back in this way to a description of fermions, it is clear that we are talking about generalizations of these. By looking at the $n=3$ case and beyond one can see that the generalizations are distinct from parafermions. We are not yet in a position to push satisfactorily the quantization of our theory to a point where the implied interpretation is present in a consistent well-understood way, but we are describing a plausible scenario for it.

For reasons of notational simplicity and clarity, we present first our ideas for the $\mathbb{Z}_3$-graded case, the first non-trivial generalization of the basic supersymmetry. This already requires that most of the central issues of the $\mathbb{Z}_n$ case be treated seriously. The paper contains seven sections. Section II contains introductory material for G_3 including its group law, and the reasons behind expressions such as (1.4). Section III derives the formula for the transformations of G_n. Section IV discusses the problem of defining derivatives with respect to θ, leading into section V which shows how the usual derivatives Q and D enter crucially into the construction of a Lagrangian theory with G_3 invariance. Section VI establishes Q and D as the generators of the left and right

actions of G_3 by introducing a suitable exponentiation of the first order formulas. Section VII extends our results for $n=3$ to the general case and includes the proof of the exponentiation for general n.

II. FRACTIONAL SUPERSYMMETRY TRANSFORMATIONS: THE CASE OF G_3

The simplest version of ordinary supersymmetry deals with the transformation

$$t'=t+\tau+i\epsilon\theta, \quad \theta'=\theta+\epsilon. \tag{2.1}$$

This $\mathbb{Z}_2$-graded theory contains a time variable t and a parameter τ of grade zero, and a real Grassmann number θ and parameter ϵ of grade one. Thus

$$\theta=\bar{\theta}, \quad \theta^2=0; \quad \epsilon=\bar{\epsilon}, \quad \epsilon^2=0; \quad \theta\epsilon=-\epsilon\theta. \tag{2.2}$$

We consider generalization to a situation involving a single real Grassmann variable θ, such that $\theta=\bar{\theta}$, $\theta^n=0$, $n=2,3,4\ldots$, within a theory that possesses $\mathbb{Z}_n$-grading; the case $n=3$ provides the simplest non-trivial generalization of ordinary supersymmetry. Without loss of generality, we take θ to have grade one in the $\mathbb{Z}_3$-grading, and to obey

$$\theta=\bar{\theta}, \quad \theta^3=0. \tag{2.3}$$

The $\mathbb{Z}_3$-generalization of (2.1) is then given by

$$t\to t'=t+\tau+\xi(\epsilon,\theta), \quad \theta\to\theta'=\theta+\epsilon, \tag{2.4}$$

where

$$\xi(\epsilon,\theta)=q(\epsilon\theta^2+\epsilon^2\theta), \tag{2.5}$$

t and τ are as in (2.1), ϵ is a real grade one parameter, such that $\epsilon=\bar{\epsilon}, \epsilon^3=0$,

$$\epsilon\theta=q^{-1}\theta\epsilon, \tag{2.6}$$

and q is a complex cube-root of unity. For definiteness we take $q=\exp(2\pi i/3)$; replacing q by q^{-1} in (2.5) and (2.6) would modify only slightly the appearance of the expressions written below, but not their content. Equation (2.6) ensures that the two terms of (2.5), in addition to being of overall grade zero, are real, *e.g.*

$$q\overline{\epsilon\theta^2}=q^{-1}\theta^2\epsilon=q^{-1}q^2\epsilon\theta^2=q\epsilon\theta^2.$$

The fact that (2.4) describes a group G_3 of transformations is easy to check. Applying two transformations $g=(\tau,\epsilon)$ and $g'=(\tau',\epsilon')$ to (t,θ) we find $g''=g'g$ with parameters

$$\epsilon''=\epsilon'+\epsilon, \quad \tau''=\tau'+\tau+q(\epsilon'\epsilon^2+\epsilon'^2\epsilon)\equiv\tau'+\tau+\xi(\epsilon',\epsilon), \tag{2.7}$$

where, in analogy with (2.6), we have

$$\epsilon'\epsilon=q^{-1}\epsilon\epsilon'. \tag{2.8}$$

In fact, we may view (2.4) as the (left) action of the element $g\in G_3$ on a $\mathbb{Z}_3$-graded physical 'manifold' M, of 'coordinates' (t,θ), given by

$$g:(t,\theta)\mapsto(t'\theta'), \quad \theta'=\theta+\epsilon, \quad t'=t+\tau+\xi(\epsilon,\theta); \tag{2.9}$$

likewise, we may view (2.7) as describing the left action of $g'=(\tau',\epsilon')$ on the G_3 group itself.

The unit and inverse elements are given by (0,0) and $(-\tau,-\epsilon)$. The associativity of the group law $g''(g'g)=(g''g')g$ is easily checked, and, in fact, it follows from a two-cocycle condition

$$\xi(\epsilon'',\epsilon')+\xi(\epsilon''+\epsilon',\epsilon)=\xi(\epsilon'',\epsilon'+\epsilon)+\xi(\epsilon',\epsilon), \tag{2.10}$$

in which $\epsilon,\epsilon',\epsilon''$ are the grade one parameters of three transformations performed in succession, and which holds for the $\xi(\epsilon',\epsilon)$ given in (2.7) provided that

$$\epsilon''\epsilon'=q^{-1}\epsilon'\epsilon, \quad \epsilon'\epsilon=q^{-1}\epsilon\epsilon'. \tag{2.11}$$

As is well known (see, *e.g.* Ref. 33), two-cocycles are associated with central extensions of a Lie group . In their Lie algebra formulation they correspond to a curvature two-form (which is symmetric rather than antisymmetric in the case of supersymmetry, see Ref. 27). The structure of the fractional supersymmetry group opens the possibility of extending these concepts to a (here) ternary algebra by introducing a 'curvature' three-form (cf. Ref. 12).

To exhibit the origin of (2.6), (2.8) and (2.11), we observe that in any context where such results arise, there is a natural ordering of the entities of non-zero grading that enter it. It will further be seen that this ordering determines consistently (and always according to the same pattern) the powers of q that enter the required multiplicative relations. In the case of group multiplication, the above ordering (in *symbolic* notation $\epsilon'>\epsilon>\theta$) requires

$$\epsilon'\epsilon=q^{-1}\epsilon\epsilon', \quad \epsilon\theta=q^{-1}\theta\epsilon \tag{2.12}$$

used above. To these, we add the result $\epsilon'\theta=q^{-1}\theta\epsilon'$ (see below). For all three, one passes from the lexical order to the opposite one by using relations that use the same power of q, here q^{-1}, in the same places. In the discussion of associativity, the ordering $\epsilon''>\epsilon'>\epsilon$ similarly implies the results (2.11) used above, and in addition $\epsilon''\epsilon=q^{-1}\epsilon\epsilon''$.

Similarly, if we had elected to write our fractional supersymmetry transformation as

$$\theta'=\theta+\eta, \quad t'=t+\tau+q^2(\eta\theta^2+\eta^2\theta), \tag{2.13}$$

the reality of t' would now imply

$$\eta\theta=q\theta\eta, \tag{2.14}$$

and, for the ordering $\eta'>\eta>\theta$, the same rule would govern matters but with the power q as in (2.14), and in $\eta'\eta=q\eta\eta'$. However, (2.13) is equivalent to

$$\theta'=\theta+\eta, \quad t'=t+\tau+q(\theta^2\eta+\theta\eta^2), \tag{2.15}$$

so that we prefer the ordering $\theta>\eta>\eta'$, and write

$$\theta\eta=q^{-1}\eta\theta, \quad \eta\eta'=q^{-1}\eta'\eta, \quad \theta\eta'=q^{-1}\eta'\theta. \tag{2.16}$$

This is now in full conformity with the other examples discussed. Further, just as our discussion related to $\epsilon'>\epsilon>\theta$ is appropriate to the case of left transformations, the passage involving (2.15) and $\theta>\eta>\eta'$ is seen to be similarly suited to the discussion of right translations. The results (2.15) and (2.16) are indeed so employed in section VI.

One consequence of results of the type (2.8) is in the form of q-deformed binomial expansions. For example,

$$(\epsilon'+\epsilon)^m=\sum_{t=0}^{r}\begin{bmatrix} m \\ t \end{bmatrix}\epsilon'^t\epsilon^{m-t}. \tag{2.17}$$

The braced object here is the q-analogue of the ordinary binomial coefficient, in which ordinary factorials, *e.g.* $m!$, are replaced by

$$[m]!=[m][m-1]\cdots[1], \quad [m]\equiv\frac{1-q^m}{1-q}=1+q+\cdots+q^{m-1}. \tag{2.18}$$

It is easy to see and well-known that (2.17) indeed follows by use of (2.8). Results such as (2.17) are employed in section III.

We append our notation for q-deformed exponentials for use in sections VI and VII. We write

$$\exp(q^k;X)=\sum_{m=0}^{\infty}\frac{1}{[m;q^k]!}X^m, \tag{2.19}$$

for suitable k, where

$$[m;q^k]!=[m;q^k]\cdots[2;q^k][1], \quad [m;q^k]\equiv\frac{1-q^{km}}{1-q^k}. \tag{2.20}$$

In this notation $[m]$ in (2.18) is $[m;q]$.

III. THE TRANSFORMATION FORMULA FOR G_n

We now extend the work done in the previous section on G_3 to the $\mathbb{Z}_n$-graded case which employs a single real Grassmann number θ and an associated parameter ϵ with the properties

$$\theta=\bar{\theta}, \quad \theta^n=0; \quad \epsilon=\bar{\epsilon}, \quad \epsilon^n=0; \quad \epsilon\theta=q^{-1}\theta\epsilon. \tag{3.1}$$

It is understood that no power of θ or ϵ lower than the n-th can vanish.

We retain the general structure (2.4) for G_n but seek, for the cocycle ξ, a formula of the type

$$\xi(\epsilon',\epsilon)=\sum_{r=1}^{n-1}c_r\epsilon'^r\epsilon^{n-r}q^{\omega(r)},$$

$$q=\exp(2\pi i/n), \quad n=2,3,4,\ldots, \tag{3.2}$$

so that $q^n=1$ replaces $q^3=1$ in previous work. Also, the exponent of q shown in (3.2) namely

$$\omega(r)=\frac{1}{2}r(n-r), \tag{3.3}$$

ensures using (2.8) that each term of (3.2) is real if c_r is real. We set $c_1=1$, and rewrite (3.2) as

$$\xi(\epsilon',\epsilon)=\sum_{r=1}^{n-1}d_r\epsilon'^r\epsilon^{n-r}. \tag{3.4}$$

We must determine the numbers d_r in such a way that (2.10) is satisfied, so that when ξ is given by (3.2) and (3.3), eq. (2.4) has the required G_n group multiplication properties. First we note that the terms on the two sides of (2.10) that are independent of ϵ agree. Then, with the aid of results like (2.17), we can show that consideration of the terms of (2.10) linear in ϵ allow us to determine all the d_r as multiples of d_1. Explicitly we find $d_r=d_{n-r}$ and

$$\frac{d_r}{d_1}=\frac{[n-1]!}{[r]![n-r]!}, \quad r=1,2,\ldots,n-1. \tag{3.5}$$

Now that (3.4) is fully determined by (3.5) we must prove that (2.10) is identically satisfied. Thus, we use (3.4), (3.5) and (2.17) to obtain

$$\xi(\epsilon'',\epsilon'+\epsilon)=\sum_{r=1}^{n-1}\sum_{s=0}^{n-r}\frac{\epsilon''^{r}\epsilon'^{s}\epsilon^{n-r-s}d_1[n-1]!}{[r]![s]![n-r-s]!}. \tag{3.6}$$

We now observe that $\xi(\epsilon',\epsilon)$ differs only slightly from what will provide the $r=0$ of the r.h.s. of (3.6). In fact, we can write

$$\xi(\epsilon'',\epsilon'+\epsilon)+\xi(\epsilon',\epsilon)=\sum_{r=0}^{n}\sum_{s=0}^{n-r}\frac{\epsilon''^{r}\epsilon'^{s}\epsilon^{n-r-s}d_1[n-1]!}{[r]![s]![n-r-s]!}-d_1(\epsilon''^{n}+\epsilon'^{n}+\epsilon^{n})/[n]. \tag{3.7}$$

Here, in order to make a tractable double sum we have added and subtracted certain ill-defined terms. The procedure is necessary to expedite the key step of our proof. In this, we reverse the order of summations in (3.7) obtaining

$$\sum_{r=0}^{n}\sum_{s=0}^{r}=\sum_{s=0}^{n}\sum_{r=s}^{n}=\sum_{s=0}^{n}\sum_{u=0}^{n-s},$$

where a shift in the variable of summation r to $u=r-s$ has also been made. The result so obtained for the left side of (2.10) can now be shown to agree exactly with the analogue of (3.7) obtained by direct calculation of the r.h.s. of (2.19), completing the required demonstration.

The remaining ingredients of the group multiplication laws for G_n are attended to immediately. Indeed, an additional calculation to prove associativity is not needed, since the cocycle property guarantees it.

IV. DERIVATIVES WITH RESPECT TO θ

We want to move from the description of the group properties of the fractional supersymmetry transformation towards the construction of actions and dynamical systems that possess invariance properties relative to them. This requires a geometrical understanding of the derivatives $\partial/\partial\theta$, and of objects in the theory of covariant derivative type. Let us go back to G_3, again as a good example, aiming in particular to expose and treat the conceptual difficulties that occur in discussing reality properties of $\partial/\partial\theta$. It is sufficient for the purposes of this section, although not of course for the eventual construction of Lagrangian theories, to work with scalar, *i.e.* grade zero real superfields f, whose expansion in powers of θ involves three real terms (see *e.g.* Refs. 11, 15, 16, and 18)

$$f=x+q\alpha\theta+q\beta\theta^2=\bar{f}=x+q^2\theta\alpha+q^2\theta^2\beta, \tag{4.1}$$

in which x is a grade zero (bosonic) variable, and the variables α and β are of grades two and one. The reality of f expressed by (4.1) implies the properties

$$\theta\beta=q\beta\theta,\quad \theta\alpha=q^{-1}\alpha\theta. \tag{4.2}$$

Comparing (4.1) with (2.5) now seen to be of scalar superfield nature, we see that β, of grade one, is related like ϵ to θ, so that $\beta>\theta$, and α, of grade two, is likewise related to ϵ^2, so that $\alpha<\theta$. The latter implies that we should adopt the rule $\beta\alpha=q^{-1}\alpha\beta$, although in this section no call for any such result is made.

To prepare the ground for our discussion of derivatives in the $\mathbb{Z}_3$ case, we recall briefly the case of basic supersymmetry and $\mathbb{Z}_2$-grading (eq. (1.1)) for which a real scalar field has the expansion

$$f = x + i\theta\phi = x - i\phi\theta. \tag{4.3}$$

It is normal to use the left spinorial derivative so that

$$\frac{\partial f}{\partial \theta} = \partial f \equiv \partial_L f = i\phi, \tag{4.4}$$

and to employ $\partial\theta/\partial\theta = 1$ and

$$\theta\partial + \partial\theta = 1 \tag{4.5}$$

to do routine manipulations. Since (4.4) is not real for real f there is no case for viewing ∂ as a real entity. However one did not consider using such an idea as a guide towards (4.5). Equation (4.5) is valid because it holds when applied to an arbitrary superfield f. In fact, the right spinorial derivative ∂_R can be consistently viewed as a conjugate to ∂_L via

$$\overline{\partial_L f} \equiv \overline{\frac{\partial f}{\partial \theta}} \equiv f \frac{\overleftarrow{\partial}}{\partial \theta} = \partial_R f, \tag{4.6}$$

which agrees trivially with

$$\partial_L f = i\phi, \quad \partial_R f = -i\phi.$$

Similarly, by application to arbitrary f it follows that the conjugate of (4.5),

$$\partial_R\theta + \theta\partial_R = 1,$$

makes good sense.

Returning to the $\mathbb{Z}_3$ case, we see that to compute $\partial f/\partial\theta \equiv \partial f \equiv \partial_L f$ and $\partial_R f$, we need the $\mathbb{Z}_3$-analogue of (4.5) to treat the θ^2 terms of (4.1). We begin by postulating

$$\frac{\partial\theta}{\partial\theta} = 1 \tag{4.7}$$

and a result of the type

$$\partial\theta = a\theta\partial + b, \tag{4.8}$$

in which $a, b \in C$. Equation (4.7) is certainly natural. We discuss whether it can or needs to be modified (it doesn't) below. When (4.8) is applied to 1, then (4.7) implies $b = 1$. Applied to θ, eq. (4.8) yields

$$(\partial\theta^2) = (1 + a)\theta. \tag{4.9}$$

Then, using (4.1), we get

$$\frac{\partial f}{\partial \theta} = \partial_L f = q^2\alpha + q^2(1 + a)\theta\beta, \tag{4.10}$$

which is not real for real f. To complete the specification of (4.8), we stipulate that it must be true when applied to an arbitrary scalar superfield. It is easy to see that it does so if

$$1 + a + a^2 = 0. \tag{4.11}$$

Thus we find two solutions for a; the two corresponding candidates for the derivative with respect θ are both used in the literature and, as we see below, essential. If $a=q$, we shall write ∂ for the derivative that obeys

$$\frac{\partial\theta}{\partial\theta}=1, \quad \partial\theta=q\,\theta\partial+1, \quad [\partial,\theta]_q=1. \tag{4.12}$$

If $a=q^{-1}$, we write δ, and

$$\frac{\delta\theta}{\delta\theta}=1, \quad \delta\theta=q^{-1}\theta\delta+1, \quad [\delta,\theta]_{q^{-1}}=1. \tag{4.13}$$

Also $\partial\delta=q^{-1}\delta\partial$ (or $[\partial,\delta]_{q^{-1}}=0$). Both derivatives hereby introduced are acting from the left. Neither has any natural reality properties that can be uncovered without reference to their partner right derivatives. The above is sufficient for our own intended applications. However, variations in the literature exist, and are often associated with implicit assumptions hinting at reality properties of ∂. If one uses (4.8) with or without (4.7) and without reference to the requirement that, applied to an arbitrary superfield, it holds true, one might try to complete specification of (4.8) by demanding that its correctness ensures the correctness of its adjoint. However, if one assumes ∂ is in some sense real (which we do not believe to be a tenable view) then (4.8) implies successively

$$\begin{gathered}\theta\partial=\bar{a}\partial\theta+\bar{b},\\ a\,\theta\partial=a\bar{a}\partial\theta+a\bar{b}, \text{ calling for } a\bar{a}=1,\\ \partial\theta=a\,\theta\partial-a\bar{b},\end{gathered}$$

reproducing (4.8) when $b=-a\bar{b}$. The choice $b=1$, the natural choice, implies $a=-1$, and we are forced back to the $\mathbb{Z}_2$-supersymmetry result as the only non-trivial possibility. If one tries a choice like $a=q$, then $b=iq^{1/2}r, r\in R$, so that

$$\partial\theta=q\,\theta\partial+irq^{1/2}.$$

Application of this result to an arbitrary real scalar f fails to give an identity. Also so does *any* attempt to view $c\partial$ as a conjugate to ∂, for $c\in C$.

In fact, it is sensible to view ∂_R as the conjugate of ∂. Since doing so is independent of whether one is looking at ∂ or δ, it is sufficient to give details for the former. Thus we shall employ here (4.12) and (4.10). We take $\partial_R\theta=(\theta(\overleftarrow{\partial}/\partial\theta))=1$ and, from (4.9), by conjugation, deduce

$$(\partial_R\theta^2)\equiv\left(\theta^2\frac{\overleftarrow{\partial}}{\partial\theta}\right)=(q^2+1)\,\theta.$$

Then, from (4.1), we obtain

$$\partial_R f=\left(f\frac{\overleftarrow{\partial}}{\partial\theta}\right)=q\alpha+q\beta(1+q^2)\,\theta=\overline{\partial_L f}, \tag{4.14}$$

where (4.2) and (4.10) for $\partial f\equiv\partial_L f$ have been used. Similarly, a consistent picture for δ,δ_R emerges. So, in summary, if on rare occasions one needs a conjugate for ∂, one may not use any multiple of ∂, although ∂_R serves perfectly well. Neither δ nor δ_R are satisfactory candidates for the rôle of the conjugate of ∂. We note in passing that the fact that a variable and the derivative

with respect to it cannot be made *simultaneously* real (or hermitian) is a known feature of noncommutative geometry and has been discussed in completely different contexts (see, *e.g.* Ref. 34).

We note that the result

$$q\partial_L\partial_R f=\partial_R\partial_L f,$$

treated with care, also makes sense, but forbear from appending any remark about ordering.

We return finally to (4.7). It is not obviously wrong to let $(\partial\theta)=c, c\in C$, but (4.7) clearly remains the natural choice. With ∂_R, rather than any multiple of ∂, seen as the true conjugate of ∂, we are not aware of any compelling reason for using $c\neq 1$.

V. COVARIANT DERIVATIVE OBJECTS

The derivatives ∂ and δ discussed feature in the literature on fractional supersymmetry in the definition (see *e.g.* Refs. 11, 15, and 18) of the important quantities

$$Q=\partial_\theta+q\theta^2\partial_t, \tag{5.1}$$

$$D=\delta_\theta+q^2\theta^2\partial_t; \tag{5.2}$$

Q produces the first order generalized supersymmetry transformation. We then write

$$\delta_{(\epsilon)}f=\epsilon Qf. \tag{5.3}$$

Equation (5.3) implies the superfield component transformations

$$\begin{aligned}\delta_{(\epsilon)}x&=q^2\epsilon\alpha,\\ \delta_{(\epsilon)}\alpha&=-q\epsilon\beta,\\ \delta_{(\epsilon)}\beta&=\epsilon\dot{x}.\end{aligned} \tag{5.4}$$

We note that the 'θ^2 component' of f changes by a total time derivative. Proceeding from this remark towards the construction of actions, we realize that D has been defined in (5.2) and in relation to (5.1) in such a way that Df has the same transformation law as f. It follows that the same philosophy that worked for supersymmetry may, in principle, be applied to the construction of actions with the correct invariance properties under generalized supersymmetry transformations. We just take the 'θ^2 component' of a suitable product, of the correct dimensions, of superfields such as $f,\dot{f},Df$ etc. For example (*cf.* Refs. 15, 16, and 18)

$$S=\int dt\,\frac{1}{2}q\dot{f}Df|_{\theta^2}=\int dtL, \tag{5.5}$$

$$L=\frac{1}{2}\dot{x}\dot{x}+\frac{1}{2}q^2\dot{\beta}\alpha-\frac{1}{2}q\dot{\alpha}\beta. \tag{5.6}$$

Exposition of the canonical formalism that stems from (5.6) is neither problem free in quantum mechanics, nor in existence at all at the present time to our knowledge in classical mechanics. We may expect, as is the case in $\mathbb{Z}_2$-supersymmetry where symmetric Poisson brackets are associated with anticommutators, that both formalisms, classical (fractional pseudomechanics) and quantum, are closely related. There are various issues, in fractional supersymmetry, however, indicating that a braided structure may be needed and that it may require further study.

The important rôles of Q and D having been put into evidence, we note that Df will transform like f provided that

$$\delta_{(\epsilon)}D=D\delta_{(\epsilon)}, \tag{5.7}$$

or

$$\epsilon Q D = D \epsilon Q. \tag{5.8}$$

Since (2.6) implies $\theta^2 \epsilon = q^2 \epsilon \theta^2$, and hence

$$qD\epsilon = \epsilon D,$$

we deduce that (5.7) requires

$$DQ = qQD, \quad [D,Q]_q = 0. \tag{5.9}$$

The consistency of (5.8) as an operator identity demands that, when applied to an arbitrary f, it gives a superfield identity. The choice (5.2) shows this to be satisfied.

To conclude, we note the further well-known results (*cf.* Refs. 11, 15, and 18)

$$D^3 = -\partial_t, \quad Q^3 = -\partial_t, \tag{5.10}$$

which are most easily seen as identities by applying them to arbitrary f.

VI. LEFT AND RIGHT TRANSFORMATIONS

What governed the choices (5.1), (5.2)? In the case of (5.1) the application of ϵQ to (t,θ) does reproduce (2.4) to *first* order in ϵ. This however does not allow ∂ to be preferred to δ in (5.1), nor conversely. Once (5.1) has been chosen, as seems sensible enough, it is quite easy to find a derivative in the form (5.2) that satisfies (5.8). However, this choice has a deep geometrical interpretation. In fact, we now show that Q and D can be regarded as the generators of the left and right actions of the group G_3 on the physical 'manifold' M of (2.9), and that (5.8) expresses the fact that left and right actions commute. This geometrical picture is a nontrivial generalisation of one that applies to ordinary supersymmetry where, of course, both actions are linear.

Let us denote the parameters of the left and right transformations of G_3 as ϵ and η. Thus $\epsilon > \theta > \eta$, as discussed in section two, and hence

$$\epsilon\theta = q^{-1}\theta\epsilon, \quad \theta\eta = q^{-1}\eta\theta. \tag{6.1}$$

We define the left and right actions $L_{(\epsilon)}$ and $R_{(\eta)}$ by

$$L_{(\epsilon)}: \theta \mapsto \theta' = \epsilon + \theta, \quad t \mapsto t' = t + \tau + q(\epsilon\theta^2 + \epsilon^2\theta), \tag{6.2}$$

$$R_{(\eta)}: \theta \mapsto \theta' = \theta + \eta, \quad t \mapsto t' = t + \tau + q(\theta^2\eta + \theta\eta^2), \tag{6.3}$$

which agree with (2.4) and (2.15). It is a non-trivial result that these transformations may be written as exponentials of the generators Q and D respectively

$$L(\epsilon)t = \exp(q^{-1}; \epsilon Q)t, \tag{6.4}$$

$$R_{(\eta)}t = \exp(q; \eta D)t, \tag{6.5}$$

where we have used the notation of (2.19). The proof, which due to the ordering necessarily involves distinct deformed exponentials, is given below. The commutativity of the two actions implies

$$[\epsilon Q, \eta D] = 0. \tag{6.6}$$

This requires the consequences

$$D\epsilon = q^{-1}\epsilon D, \quad \eta Q = q^{-1} Q\eta \tag{6.7}$$

of (6.1), and a hitherto unused relation

$$\epsilon\eta = q^{-1}\eta\epsilon. \tag{6.8}$$

Then (6.6) is seen to imply (5.8).

To prove (6.4), we use (2.19) in the form

$$\exp(q^{-1};\epsilon Q) = 1 + \epsilon Q + \epsilon Q \epsilon Q/[2;q^{-1}]. \tag{6.9}$$

A simple computation using $\epsilon\theta = q^{-1}\theta\epsilon$ and $(\partial\theta^2) = [2;q]\theta$ gives us (6.4); the proof depends crucially on the former and on the occurrence of ∂ rather than δ in the definition (5.1) of Q.

We prove (6.5) in the same way, noting again how critically the success of the proof depends on the actual arrangement of details involving θ, δ, η and $\exp(q;\eta D)$.

VII. SUPERFIELDS, DERIVATIVES AND q-EXPONENTIATION FOR G_n

We have already given in section III the definition of the transformation of the group G_n when

$$\theta = \bar{\theta}, \quad \theta^n = 0; \quad \epsilon = \bar{\epsilon}, \quad \epsilon^n = 0; \quad \theta\epsilon = q\epsilon\theta. \tag{7.1}$$

In general we expect most features of the $\mathbb{Z}_3$ - graded theory that are discussed above to allow fairly direct extension to the $\mathbb{Z}_n$ theory. We will indicate some of these briefly in this section, without examining in much detail how the general case may yield a theory significantly richer in content.

In place of (4.1), we have the expansion of the real scalar superfield

$$f = x + \sum_{r=1}^{n-1} q^{\omega(r)}\psi_r\theta^{n-r} = \bar{f} = x + \sum_{r=1}^{n-1} q^{-\omega(r)}\theta^{n-r}\psi_r, \tag{7.2}$$

where the power $\omega(r)$ of $q = \exp(2\pi i/n)$ is chosen to make all terms in f all real; it is given by (3.3). Moreover, in place of (4.2), we now have

$$\theta\psi_r = q^r\psi_r\theta, \quad r = 1,\ldots,n-r; \tag{7.3}$$

in the $\mathbb{Z}_3$ case, α and β of (4.1) would be written as ψ_2 and ψ_1 to conform with (7.2).

The discussion of derivatives, via (7.1) and

$$\partial\theta = a\,\theta\partial + 1, \tag{7.4}$$

yields more possibilities, for a must now obey

$$1 + a + a^2 + \cdots + a^{n-1} = 0. \tag{7.5}$$

We thus write ∂_r for the derivative which obeys

$$\partial_r\theta = q^r\theta\partial_r + 1, \quad r = 1,2,\ldots,n-1. \tag{7.6}$$

Our previous ∂ and δ correspond to ∂_1 and ∂_{n-1}. We will continue to use the former notation because we do not describe any context that involves crucial use of ∂_r for $r \neq 1$ or $r \neq n-1$. We note, in particular, the direct consequences of (7.6)

$$(\partial\theta^s) = [s]\theta^{s-1}, \quad (\delta\theta^s) = q^{1-s}[s]\theta^{s-1}, \quad s = 1,2,\ldots,n-1. \tag{7.7}$$

Here δ directly involves $(1-q^{-s})/(1-q^{-1})$, which we have expressed in terms of $[s]$, defined by (2.18).

The definitions (5.1) and (5.2) of Q,D in section V are now modified to read

$$Q=\partial_1+c_1q^{\omega(1)}\theta^{n-1}\partial_t\equiv\partial+c_1q^{\omega(1)}\theta^{n-1}\partial_t, \tag{7.8}$$

$$D=\partial_{n-1}+c_1q^{-\omega(1)}\theta^{n-1}\partial_t\equiv\delta+c_1q^{-\omega(1)}\theta^{n-1}\partial_t, \tag{7.9}$$

where $\omega(1)$ is given by (3.3) and a suitable normalization of the real number c_1 is fixed for general n. We note that Q, so defined, does generate correctly the first order term of the G_n-transformation for a parameter ϵ related to θ via (7.1). Also

$$\delta_{(\epsilon)}\psi_1=\epsilon\dot{x} \tag{7.10}$$

indicates that we can still follow the usual way of obtaining invariant actions from the θ^{n-1} components of suitable superfields. Further (5.8) again holds. But in place of (5.9), we use n-th powers (thereby fixing the normalization of c_1): the $\mathbb{Z}_n$ theory is of fractional supersymmetry with fractions $1/n$, of course.

Finally, it is to be expected that the exponentiation results of section VI carry over into the general theory. We rewrite then in general notation

$$L_{(\epsilon)}t\mapsto t'=\exp(q^{-1};\epsilon Q)t, \tag{7.11}$$

$$R_{(\eta)}t\mapsto t'=\exp(q;\eta D)t, \tag{7.12}$$

where

$$\theta\epsilon=q\epsilon\theta,\quad \eta\theta=q\theta\eta,\quad \eta\epsilon=q\epsilon\eta. \tag{7.13}$$

To prove the extension (7.11) of (6.4) to the $\mathbb{Z}_n$-graded theory we need to recover

$$L_{(\epsilon)}:t\to t'=t+\sum_{r=1}^{n-1}d_r\epsilon^r\theta^{n-r}, \tag{7.14}$$

where d_r is given by (3.5), as the expansion of (7.11)

$$L_{(\epsilon)}t=t+\sum_{r=1}^{n}\frac{1}{[r;q^{-1}]!}(\epsilon Q)^rt, \tag{7.15}$$

where Q is given by (7.8). The first order term, which comes from the action of ϵQ on t is clearly correct:

$$d_1\epsilon\theta^{n-1}=(\epsilon Q)t, \tag{7.16}$$

since $d_1=c_1q^{\omega(1)}$.

This is the first key element of a proof, by induction, that the individual terms of (7.14) and (7.15) coincide. We therefore assume this for $r=1,2,\ldots,k$ and seek, on the basis of that assumption, to prove it for $r=k+1$. This requires us to show that

$$d_{k+1}\epsilon^{k+1}\theta^{n-k-1}=\frac{1}{[k+1;q^{-1}]}(\epsilon Q)d_k\epsilon^k\theta^{n-k}. \tag{7.17}$$

Only the term $\partial_1\equiv\partial$ of Q contributes. The formula $\partial\epsilon^k=q^{-k}\epsilon^k\partial$ then prepares for the use of (7.7), and we can see that (7.17) is an equality provided that

$$\frac{1}{[k+1;q]} = \frac{q^{-k}}{[k+1;q^{-1}]}. \tag{7.18}$$

It is easy to show that (7.18) is true, and the proof is complete.

Proof of (7.12) proceeds similarly. We remark that the exponentials in (7.11) and (7.12) are necessarily different because of the use of the different derivatives ∂ and δ in the definitions (7.8) and (7.9) of Q and D.

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Zeta-regularization of the $O(N)$ nonlinear sigma model in D dimensions

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The $O(N)$ nonlinear sigma model in a D-dimensional space of the form $R^{D-M}\times T^M$, $R^{D-M}\times S^M$, or $T^M\times S^P$ is studied, where R^M, T^M, and S^M correspond to flat space, a torus, and a sphere, respectively. Using zeta-regularization and the $1/N$ expansion, the corresponding partition functions—for deriving the free energy—and the gap equations are obtained. In particular, the free energy at the critical point on $R^{2q+1}\times S^{2p+2}$ vanishes in accordance with the conformal equivalence to the flat space R^D. Numerical solutions of the gap equations at the critical coupling constants are given for several values of D. The properties of the partition function and its asymptotic behavior for large D are discussed. In a similar way, a higher-derivative nonlinear sigma model is investigated, too. The physical relevance of our results is discussed. © *1996 American Institute of Physics.* [S0022-2488(96)02002-6]

I. INTRODUCTION

Zeta-regularization[1] (for a review see Ref. 2) is a very powerful and elegant method for regularizing the divergences that appear in quantum field theory. Many applications have been found, from the calculation of the vacuum energy density or Casimir energy corresponding to varied configurations (different fields, space–times, boundaries), to its application in wetting/nonwetting phenomena in actual condensed matter and solid state systems, to the analysis of phase transitions coming from the study of effective potentials in several contexts, topological mass generation, Bose–Einstein condensation phenomena, evaluation of the partition function in string and p-brane theories, etc.[2] From a more mathematical point of view, the method has allowed the computation of the basic operator tr log $(\Box+X)$ on a curved manifold, which is very important in quantum gravity and cosmology.

In this paper we will study the zeta-function regularization of the $O(N)$ nonlinear sigma model in an arbitrary number, D, of dimensions and on spaces of the form $R^{D-M}\times T^M$, $R^{D-M}\times S^M$, and $T^M\times S^P$. In flat space–time this model has a large number of different applications (see Ref. 3 for a review), in particular, in the theory of critical phenomena and solid state physics. For example, such a three-dimensional model, which is known to be renormalizable in this case, may be used in condensed matter physics as an effective field theory of the two-dimensional quantum antiferromagnet.[4] In particular, the $O(N)$ nonlinear sigma model on $S^1\times R^2$ may be applied to describe the low-temperature properties of the quantum antiferromagnet.[5] Recently, in connection with the study of higher-dimensional conformal theories,[6] where one can use

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well-known $2d$ conformal field theory techniques, such a model has been considered in three-dimensional curved space–time.[6] The critical properties of the model were also discussed.

Here we will extend this important analysis, by studying the $O(N)$ nonlinear sigma model in topologically nontrivial spaces of constant curvature in arbitrary dimension D. Using zeta-function regularization and the $1/N$ expansion techniques we will obtain the partition function and the gap equation in each of the cases considered, and also numerical solutions of the gap equations for some spaces. The asymptotic behavior in the limit $D\to\infty$ will be considered, too. Finally, a higher-derivative generalization of the $O(N)$ nonlinear sigma model will be introduced, and the corresponding zeta-function on a flat but topologically nontrivial space will be obtained. Numerical solutions of the gap equations in this last model, for different values of D, will be discussed, too. The relevant partition function and gap equations are presented in Secs. II and III, while the applications to $R^{D-M}\times T^M$ and $R^{D-M}\times S^M$ appear in Secs. IV and V, respectively. Our higher-derivative model is introduced in Sec. VI. In the conclusion we comment on the relevance of our results and discuss future perspectives. The appendix is devoted to the calculation of the necessary zeta functions for the spaces under consideration.

II. THE $O(N)$ NONLINEAR SIGMA MODEL IN D DIMENSIONS: PARTITION FUNCTION

Let us consider an arbitrary D-dimensional space of constant (or zero) curvature. It is well known that the scalar conformally invariant D'Alembertian operator on such a manifold is

$$-\Box+\xi R, \tag{2.1}$$

where $\xi=(D-2)/4(D-1)$. In what follows we use Euclidean space notations. The partition function of the $O(N)$ nonlinear sigma model in D dimensions we will be interested in is given as follows:

$$Z[g]=\int \mathscr{D}\phi\mathscr{D}\sigma\,\exp\left\{-\frac{1}{2\lambda}\int d^Dx\sqrt{g}[\,\phi^i(-\Box+\xi R)\phi^i+\sigma(\phi^{i2}-1)]\right\}, \tag{2.2}$$

where ϕ^i are scalars in curved space–time, $i=1,\ldots,N$, $\xi=(D-2)/4(D-1)$ is the conformal coupling, σ is an auxiliary scalar introduced in order to keep the constraint $\phi^i(x)\phi^i(x)=1$, coming from the condition of $O(N)$-invariance, and λ is the coupling constant. Note that σ has no dynamics, as it just plays the role of a Lagrange multiplier. Observe also that we have chosen to work with the conformally invariant operator $-\Box+\xi R$, in order to better understand the conformally invariant properties of the model.

The theory (2.2) was extensively studied in Ref. 7 in three-dimensional curved space–time at its nontrivial fixed point. In particular it was shown, in the large-N limit, that such a model is an example of a conformal field theory at a nontrivial fixed point. Investigation of this theory in different spaces of constant curvature has suggested that what distinguishes a given model is not curvature, but the conformal class of its metric.

Our purpose here will be to study the theory in D-dimensional curved space–times of constant curvature near the nontrivial fixed point in the $1/N$ expansion. What is even more important, we will analyze, in addition to the large-N limit, some situations involving the limit $D\to\infty$, which is relevant to dimensional dependence investigations in a number of quantum systems.[8,9] Numerical solutions to the gap equations will also be given.

It is convenient to rescale $\phi\to\sqrt{\lambda}\,\phi$. Then

$$Z[g]=\int \mathscr{D}\phi\mathscr{D}\sigma\,\exp\left\{-\int d^Dx\sqrt{g}\left[\frac{1}{2}\,\phi^i(-\Box+\xi R+\sigma)\phi^i-\frac{\sigma}{2\lambda}\right]\right\}, \tag{2.3}$$

where the mass dimensions of the fields and parameters are

$$[\phi]=\frac{D-2}{2},\quad [\sigma]=2,\quad \left[\frac{1}{\lambda}\right]=D-2,\quad [\xi]=0, \tag{2.4}$$

and the dependence of Z on the metric $g_{\mu\nu}$ is explicitly shown. Note that sometimes it is convenient to rewrite the partition function (2.3) as explicitly regularized. In particular, if one uses a cutoff Λ for regularizing, it may be adequate to do the change $1/\lambda(\Lambda)\to\Lambda^{D-2}/\lambda(\Lambda)$ in order to work with a dimensionless $\lambda(\Lambda)$.

The aim is to study the above theory in the large-N limit keeping, as usual, $N\lambda$ fixed as $N\to\infty$. The space–time dimension D will be arbitrary. Integrating out the first $N-1$ components of ϕ and rescaling the Nth component ϕ_N to $\sqrt{(N-1)/2}\phi_N$, and $[(N-1)/2]\lambda$ to λ, we obtain

$$Z[g]=\int \mathscr{D}\phi_N\mathscr{D}\sigma\,\exp\Bigg(-\frac{N-1}{2}\Bigg\{\mathrm{Tr}\,\log(-\Box+\xi R+\sigma) + \frac{1}{2}\int d^Dx\sqrt{g}\Bigg[\phi_N(-\Box+\xi R+\sigma)\phi_N-\frac{\sigma}{2\lambda}\Bigg]\Bigg\}\Bigg). \tag{2.5}$$

III. THE GAP EQUATIONS

Since we shall deal with manifolds of constant curvature, we will look for a uniform saddle point: $\sigma(x)=m^2$, $\phi_N(x)=b$. Extremizing the action (2.5) with respect to $\phi_N(x)$ maintaining $\sigma(x)$ fixed, and the other way around, we obtain the *gap equations*

$$(-\Box+\xi R+m^2)b=0,\quad G(x,x;m^2,g)+b^2-1/\lambda=0, \tag{3.1}$$

where

$$G(x,x;m^2,g)=\langle x|(-\Box+\xi R+m^2)^{-1}|x\rangle \tag{3.2}$$

is the two-point Green's function at equal points. Once the solutions to these equations have been found, it is sensible to evaluate the free-energy density W at the saddle point to leading order in $1/N$

$$W[g,\lambda]=\frac{N}{2}\left[\mathrm{Tr}\,\log(-\Box+\xi R+m^2)-\int d^Dx\sqrt{g}\,\frac{m^2}{\lambda}\right]. \tag{3.3}$$

Applying zeta-function regularization one defines

$$G(x,x;m^2,g)=\lim_{s\to1}G(x,x;m^2,g;s)\propto\lim_{s\to1}\langle x|\zeta_{\mathscr{M}}(s)|x\rangle,$$
$$\mathrm{Tr}\,\log(-\Box+\xi R+m^2)\propto-\zeta'_{\mathscr{M}}(0). \tag{3.4}$$

Here $\zeta_{\mathscr{M}}(s)$ is the spectral zeta-function of the operator $-\Box+\xi R+m^2$ on the space–time $\mathscr{M}$ under consideration, i.e.

$$\zeta_{\mathscr{M}}(s)=\mathrm{Tr}(-\Box+\xi R+m^2)^{-s}. \tag{3.5}$$

The proportionality factors, not explicitly written in (3.4) are determined, in each case, by the normalization of the physical states, and they have such a form that the dimensionalities match.

By heat-kernel series analysis, it is known that the short-distance divergences of this two-point Green's function depend in general on the curvature of the space–time, except for the leading pole which is independent of g and, therefore, present in all cases. As a result, in flat space–times with nontrivial topology such as T^D or $R^{D-M}\times T^M$, this singular behavior will be the same as in the flat

space R^D. That is why it is natural to study R^D first. According to this reasoning, the critical value of λ, at which the theory becomes finite, will be the same for all these space–times.

The gap equations in the space–time R^D, after momentum cutoff regularization, read

$$m^2 b = 0, \quad b^2 = \left[\frac{\Lambda}{\lambda(\Lambda)} - G_\Lambda(x,x;m^2,g) \right]. \tag{3.6}$$

Here $G_\Lambda(x,x;m^2,g)$ means the Green's function obtained when setting a cutoff Λ on the norm of the integrated momentum. Studying their solutions, one finds that, for $b=m=0$,

$$\frac{\Lambda}{\lambda_c(\Lambda)} = \int^{(\Lambda)} \frac{d^D k}{(2\pi)^D} \frac{1}{k^2} = \frac{1}{(4\pi)^{D/2}\Gamma\left(\frac{D}{2}\right)} \frac{\Lambda^{D-2}}{\frac{D}{2}-1}, \quad \text{if } D>2, \tag{3.7}$$

and, for $b=0$, $m\neq 0$,

$$\frac{\Lambda}{\lambda_c(\Lambda)} - \frac{\Lambda}{\lambda(\Lambda)} = m^2 \int^{(\Lambda)} \frac{d^D k}{(2\pi)^D} \frac{1}{k^2(k^2+m^2)} = -\frac{m^{D-2}}{(4\pi)^{D/2}} \Gamma\left(1-\frac{D}{2}\right) + \epsilon(\Lambda), \tag{3.8}$$

where $\epsilon(\Lambda)$ are terms vanishing as $\Lambda\to\infty$. Since $\Gamma(1-D/2)<0$ for odd $D>1$, this indicates the unphysical character of the solution when $\lambda<\lambda_c$. A more detailed study shows that $\lambda=\lambda_c$ is a critical value separating two different phases.

In the same space–time, when using zeta-function regularization the second gap equation becomes

$$b^2 = \lim_{s\to 1} \left[\frac{1}{\lambda(s)} - G(x,x;m^2,g;s) \right], \tag{3.9}$$

where

$$G(x,x;m^2;g,s) = \int \frac{d^D k}{(2\pi)^D} \frac{1}{(k^2+m^2)^s} = \frac{m^{D-2s}}{(4\pi)^{D/2}} \frac{\Gamma(s-D/2)}{\Gamma(s)}. \tag{3.10}$$

Following the line of thinking of Ref. 7, we set the values $m=b=0$ from the discussion in cutoff regularization, and realize that now the only consistent way out is

$$\lim_{s\to 1} \frac{1}{\lambda_c(s)} = 0, \tag{3.11}$$

which gives the critical value of λ in this regularization.

In curved space–times without boundaries, heat-kernel expansion gives

$$
\begin{aligned}
&G_\Lambda(x,x;m^2,g)\\
&\quad=\int_{1/\tilde{\Lambda}^2}^{\infty} dt\langle x|e^{-t(-\Box+\xi R+m^2)}|x\rangle\\
&\quad=\begin{cases}
\dfrac{1}{(4\pi)^{D/2}}\left[\dfrac{a_0}{D/2-1}\,\tilde{\Lambda}^{D-2}+\dfrac{a_2}{D/2-2}\,\tilde{\Lambda}^{D-4}+\cdots+\dfrac{a_{D-1}}{1/2}\,\tilde{\Lambda}^2\right]+f_1(\Lambda),\\
\quad \text{for odd } D,\\
\dfrac{1}{(4\pi)^{D/2}}\left[\dfrac{a_0}{D/2-1}\,\tilde{\Lambda}^{D-2}+\dfrac{a_2}{D/2-2}\,\tilde{\Lambda}^{D-4}+\cdots+a_{D-4}\tilde{\Lambda}^2+a_{D-2}\,\log\,\tilde{\Lambda}^2\right]+f_2(\Lambda),\\
\quad \text{for even } D,
\end{cases}
\end{aligned}
\tag{3.12}
$$

where $f_1(\Lambda)$ and $f_2(\Lambda)$ are terms that become finite when $\Lambda\to\infty$ and where, for consistency, we have taken $\tilde{\Lambda}^2=[\Gamma(D/2)]^{(D-2)/2}\Lambda^2$. As usual, the a_{2n}'s stand for the even Seeley–Gilkey coefficients,[10] and we have taken into account that $a_{2n+1}=0$ in the absence of boundaries. Since $a_0=1$, for the first D's we immediately obtain

D	divergences of $G_\Lambda(x,x;m^2,g)$
3	$\dfrac{1}{(4\pi)^{3/2}}\,2\tilde{\Lambda}$
4	$\dfrac{1}{(4\pi)^2}\,(\tilde{\Lambda}^2+a_2\,\log\,\tilde{\Lambda}^2)$
5	$\dfrac{1}{(4\pi)^{5/2}}\left(\dfrac{2}{3}\,\tilde{\Lambda}^3+2a_2\tilde{\Lambda}\right)$
6	$\dfrac{1}{(4\pi)^3}\left(\dfrac{1}{2}\,\tilde{\Lambda}^3+a_2\tilde{\Lambda}^2+a_2\,\log\,\tilde{\Lambda}^2\right)$
7	$\dfrac{1}{(4\pi)^{7/2}}\left(\dfrac{2}{5}\,\tilde{\Lambda}^5+\dfrac{2}{3}\,a_2\tilde{\Lambda}^3+2a_4\tilde{\Lambda}\right)$

The $D=3$ result does not depend on $a_2,a_4,...$, and is thus independent of the curvature. In consequence, it is the same for any three-dimensional space without boundaries and therefore it is enough to find it in R^3. For conformally flat manifolds of any D, the property $R=0$ makes $a_2,a_4,...$ vanish with the same consequence, i.e., we can get by with the critical values in R^D. This fact will be used in the study of $R^{D-M}\times T^M$.

When $R\neq 0$ in $D>3$, a particular study of every particular situation is called for. In spaces of constant positive curvature, such as spheres or some products of R^D by spheres, the first gap equation reads $(\xi R+m^2)b=0$ with $R>0$, and admits no other solution than $b=0$. From the second equation, $\Lambda/\lambda(\Lambda)=G_\Lambda(x,x;m^2,g)$, where the divergent parts of the r.h.s. as $\Lambda\to\infty$ are given by (3.12). Next, we form the difference between the $m=0$ and the $m>0$ cases:

$$
\frac{\Lambda}{\lambda_{m=0}(\Lambda)}-\frac{\Lambda}{\lambda(\Lambda)}=\frac{1}{(4\pi)^{D/2}}\left[\frac{a_2(m=0)-a_2(m)}{D/2-2}\,\tilde{\Lambda}^{D-4}+\frac{a_4(m=0)-a_4(m)}{D/2-4}\,\tilde{\Lambda}^{D-6}+\cdots\right].
\tag{3.13}
$$

To obtain $a_{2n}(m)$ from $a_{2n}(m=0)$ is just a matter of replacing $\xi\to\xi+m^2/R$ in every expression of these coefficients. As an example we consider $D=5$, whose divergences appear in the preceding table. Since $a_2(m=0)=(\xi-\frac{1}{6})R$, $a_2(m=0)-a_2(m)=m^2$ independently of the value of R. After dividing by Λ we obtain

$$\frac{1}{\lambda_{m=0}(\Lambda)}-\frac{1}{\lambda(\Lambda)}=\frac{1}{(4\pi)^{5/2}}\frac{\pi^{3/4}}{8}2m^2. \tag{3.14}$$

This equality stops making sense if $\lambda<\lambda_{m=0}$, which can be interpreted by regarding $\lambda_{m=0}=\lambda_c$ as the critical value separating two phases. Since this was obtained by setting $b=0$ and $m=0$, those are the values we shall set for computing $1/\lambda_c$ in zeta-regularization.[7]

IV. $R^{D-M}\times T^M$

Putting the adequate normalization factors, the Green's function, and the free energy at the critical value of λ read

$$\begin{aligned} G(x,x;m^2,g;s=1)&=\frac{1}{(2\pi)^{D-M}\rho^M}\,\zeta_{R^{D-M}\times T^M}(1),\\ \frac{W}{N}&=-\frac{1}{2}\left(\frac{\rho}{2\pi}\right)^{D-M}\zeta_{R^{D-M}\times T^M}(0). \end{aligned} \tag{4.1}$$

After calculating the zeta function for our operator on this space–time (see the Appendix), we can write

$$\zeta_{R^{D-M}\times T^M}(s)=\frac{\pi^{D/2}}{\Gamma(s)}\left(\frac{2\pi}{\rho}\right)^{-2s+D-M}\left[I_M\left(s-\frac{D-M}{2},\frac{\rho m}{2\pi}\right)+\left(\frac{\rho m}{2\pi}\right)^{D-2s}\Gamma\left(s-\frac{D}{2}\right)\right]. \tag{4.2}$$

The second term tells us that the singularities at $s=0,1$ are present only when D is even, independently of M. Here $I_M(s-(D-M)/2,\rho m/2\pi)$ is an integral of the type

$$I_M(z,\alpha)=\int_0^\infty dt\,t^{z-M/2-1}e^{-t\alpha^2}\left[\theta^M\left(\frac{\pi}{t}\right)-1\right], \tag{4.3}$$

where $\theta(x)$ is the Jacobi function

$$\theta(x)=\sum_{n=-\infty}^{\infty}e^{-\pi x n^2}. \tag{4.4}$$

The key point is that the integrand is well behaved around $t=0$, causing no new pole at $z=M/2$ (i.e., at $s=D/2$). Further, I_M can be expanded into a Dirichlet series, which reads

$$I_M\left(s-\frac{D-M}{2},\frac{\rho m}{2\pi}\right)=2^{D/2-s}\left(\frac{\rho m}{2\pi}\right)^{D-2s}\sum_{l=1}^{M}\binom{M}{l}2^{l+1}\sum_{\vec{n}\in(\mathbb{N}^*)^l}\frac{K_{D/2-s}(\rho m|\vec{n}|_l)}{(\rho m|\vec{n}|_l)^{D/2-s}}, \tag{4.5}$$

where K is the modified Bessel function and $|\vec{n}|_l$ stands for the Euclidean norm of $\vec{n}=(n_1,\ldots,n_l)$.

The particular cases we will calculate are those of odd $D=2d+3$, $M=1$. Under these conditions the Bessel functions involved are just

$$K_{D/2-1}(x)=K_{d+1/2}(x)=\sqrt{\frac{\pi}{2x}}\,e^{-x}\sum_{k=0}^{d}\frac{(d+k)!}{k!(d-k)!}\frac{1}{(2x)^k},$$

and we may interchange the summations to obtain

$$\xi_{R^{2d+2}\times T^1}(1)=\pi^{d+3/2}\left(\frac{2\pi}{\rho}\right)^{2d}\left(\frac{\rho m}{2\pi}\right)^{2d+1}\left[2^{d+2}\sqrt{\pi}\sum_{k=0}^{d}\frac{(d+k)!}{k!(d-k)!2^k}\frac{Li_{d+1+k}(e^{-\rho m})}{(\rho m)^{d+1+k}}+\Gamma\left(-d-\frac{1}{2}\right)\right],$$

$$\zeta'_{R^{2d+2}\times T^1}(0)=\pi^{d+3/2}\left(\frac{2\pi}{\rho}\right)^{2d+2}\left(\frac{\rho m}{2\pi}\right)^{2d+3}\times\left[2^{d+3}\sqrt{\pi}\sum_{k=0}^{d+1}\frac{(d+1+k)!}{k!(d+1-k)!2^k}\frac{Li_{d+2+k}(e^{-\rho m})}{(\rho m)^{d+2+k}}+\Gamma\left(-d-\frac{3}{2}\right)\right], \tag{4.6}$$

where Li is the polylogarithm function. Setting $d=0$ ($D=3$), these formulas reproduce, as should be expected, the ones in Ref. 7.

We look at the solutions of the gap equations for the critical value $1/\lambda_c=0$. The chances are the following:

(1) $m=0$, $b\neq 0$. This leads to

$$b^2=-\frac{\pi^{d+3/2}}{(2\pi)^{2d+3}}\frac{1}{\rho^{2d+1}}4\sqrt{\pi}\,\frac{(2d)!}{d!}\,\zeta(2d+1).$$

When $d=0$, the rhs diverges and no solution can exist. For $d>0$, $\zeta(2d+1)>0$ and there is a sign conflict which prevents the appearance of any solution on this side.

(2) $m>0$, $b=0$. Now we are posed with solving

$$\sum_{k=0}^{d}\frac{(d+k)!}{k!(d-k)!2^k}(\rho m)^{d-k}Li_{d+1+k}(e^{-\rho m})+(\rho m)^{2d+1}\frac{\Gamma(-d-1/2)}{2^{d+2}\sqrt{\pi}}=0. \tag{4.7}$$

Only $d=0$ admits a relatively simple analytic solution because Li_1 is the only polylogarithm that can be trivially expressed in terms of elementary functions. In that case one obtains (see also Refs. 7 and 11) $(\rho m)_c=2\log\tau$, with $\tau=(1+\sqrt{5})/2$, i.e., $(\rho m)_c\simeq 0.9624$. Of course, it is also possible to find this same value by numerically solving the above equation for $d=0$, and this is precisely what we do for the next d's. Afterwards, the value found is replaced into (4.6) and (4.1), so as to find the free energy W. We thus arrive at

d	$(\rho m)_c$	$W/N[\rho m=(\rho m)_c]$
0	0.9624	−0.1530
1	no solution	
2	2.1775	−0.0441
3	no solution	
4	3.5504	−0.0561
5	no solution	
6	3.6841	−2.2634

The figure for W/N when $d=0$ coincides with the numerical value of $-(2/5\pi)\zeta(3)$, derived in Ref. 7 with the help of polylogarithm identifies from Ref. 12. The rest of the values are the first (and possibly only) solutions found after scanning a reasonable positive range.

We can now study the asymptotic behaviors of these expressions for M (and D) and/or $\alpha[=\rho m/(2\pi)]$ going to infinity. Two cases will be considered: (i) $\alpha \gg 1$ and M bounded, with $M-D$ fixed, and (ii) $\alpha \gg 1$ and $M \gg 1$ with $\alpha/M \to$const, again with $M-D$ finite.

Let us start with the first case. As everywhere the dependence on M is through $D-M$, it is enough to study $I_M(\tau,\alpha)$, where $\tau = s-(D-M)/2$ with $s=0$ or $s=1$. From the behavior

$$K_{D/2-s}(2\pi\alpha|\vec{n}|) \sim \left(\frac{\pi}{4\pi\alpha|\vec{n}|}\right)^{1/2} e^{-2\pi\alpha|\vec{n}|}, \tag{4.8}$$

we easily obtain that

$$I_M(\tau,\alpha) \sim \pi^{s-D/2}\alpha^{(D-1)/2-s}\sum_{l=1}^{M}\binom{M}{l} 2^l Li^{(l)}_{(d+1)/2-s}(e^{-2\pi\alpha}), \tag{4.9}$$

where $Li_P^{(l)}(x)$ denotes the generalized polylogarithm, for which we have

$$Li_P^{(l)}(x) = \sum_{n_1,\ldots,n_l=1}^{\infty} \frac{x^{\sqrt{n_1^2+\cdots+n_l^2}}}{\sqrt{n_1^2+\cdots+n_l^2}^P} \sim \frac{x^{\sqrt{l}}}{\sqrt{l}^P} + \mathcal{O}\left(\frac{x^{\sqrt{l+3}}}{\sqrt{l+3}^P}\right), \quad x \ll 1. \tag{4.10}$$

Taking this into account, we obtain

$$I_M\left(s-\frac{D-M}{2},\alpha\right) \leqslant 2\pi^{s-D/2}\alpha^{(D-1)/2-s}M^2 e^{-2\pi\alpha}. \tag{4.11}$$

We can now consider M to be large, of course, but never competing with α or the above expression loses its sense. In order to deal with both limits at the same time, we must consider the case (ii). From the well-known behavior of $K_\nu(\nu z)$ for constant z and $\nu \to \infty$, by calling

$$u_l = \lim_{\alpha,D\to\infty} \frac{2\pi\alpha\sqrt{l}}{D/2-s} \equiv \text{const}, \quad v_l = \eta(u_l) = \sqrt{1+u_l^2} + \log\frac{u_l}{1+\sqrt{1+u_l^2}} \equiv \text{const}, \tag{4.12}$$

we obtain

$$I_M\left(s-\frac{D-M}{2},\alpha\right) \sim \frac{\sqrt{2}}{(1+u_1^2)^{1/4}}\left(\frac{u_1}{2}\right)^{D/2-s}\left(\frac{D}{2}-s\right)^{D/2-s+1} e^{-(D/2-s)v_1}. \tag{4.13}$$

V. $R^{D-M}\times S^M$

The Green's function and the Tr log contribution to the free energy are now

$$G(x,x;m^2,g;1) = \frac{1}{(2\pi)^{D-M}a^M}\,\zeta_{R^{D-M}\times S^M}(1), \tag{5.1}$$

and

$$\frac{W}{N} = \frac{1}{2}\left(\frac{a}{2\pi}\right)^{D-M}\zeta'_{R^{D-M}\times S^M}(0), \tag{5.2}$$

respectively, where a is the radius of the sphere. Here we will consider the massless case only. By our discussion on gap equations, in $D=5$ $1/\lambda_c = G(x,x;0,g,1)$. Therefore, in these conditions,

$\zeta_{R^{5-M}\times S_M}(1)$ for $m=0$ tells us the critical value of λ. Another reason for the $m=0$ choice, apart from simplicity, is that the $M=D-1$ case is conformally equivalent to $R^D-\{0\}$, and, then, $m=0$ corresponds also to solutions for critical λ.

Taking the conformal coupling and the known form of the Riemann scalar for the sphere, we follow a method analogous to Ref. 13 (see also Ref. 14) to construct the required zeta-function, which is

$$\zeta_{R^{D-M}\times S^M}(s)=2a^{2s-D+m}\pi^{(D-M)/2}\frac{\Gamma(s-(D-M)/2)}{\Gamma(s)}\begin{cases}\Sigma_\alpha(p,2s-D+M), & \text{for } M=2p+2,\\ \Sigma_\beta(p,2s-D+M), & \text{for } M=2p+1,\end{cases} \tag{5.3}$$

where

$$\Sigma_\alpha(p,2z)=\frac{1}{(2p+1)!}\sum_{k=0}^{p}(-1)^k\alpha_k(p-1)\zeta_H\left(-2p+2k+2z-1,\frac{1}{2}\right),$$
$$\Sigma_\beta(p,2z)=\frac{1}{(2p)!}\sum_{k=0}^{p-1}(-1)^k\beta_k(p-2)\zeta_R(-2p+2k+2z), \tag{5.4}$$

ζ_H and ζ_R denote the Hurwitz and Riemann zeta-functions, and the α_k and β_k coefficients are

$$\alpha_0(j)=1,\quad \alpha_k(j)=\sum_{0\leqslant i_1<\cdots<i_k\leqslant j}\left(i_1+\frac{1}{2}\right)\cdots\left(i_k+\frac{1}{2}\right),\quad k\geqslant 1,$$
$$\beta_0(j)=1,\quad \beta_k(j)=\sum_{0\leqslant i_1<\cdots<i_k\leqslant j}(i_1+1)\cdots(i_k+1),\quad k\geqslant 1. \tag{5.5}$$

Our notation is just slightly different from that in Ref. 13. In fact $\alpha_k(p-1)=1/2^k\alpha_k^{\mathrm{CC}}(p-1)$ and $\beta_k(p-2)=\beta_k^{\mathrm{CC}}(p-1)$, where CC stands for the coefficients employed in Ref. 13. These coefficients enable one to write

$$d(M,l)=\sum_{k=0}^{k_{\max}(M)}(-1)^k\mathscr{A}_k(M)\left(l+\frac{M-1}{2}\right)^{M-1-2k}, \tag{5.6}$$

where $\mathscr{A}_k(M)=2/(2p+1)!\,\alpha_k(p-1)$ and $k_{\max}(M)=p$ for $M=2p+2$, while $\mathscr{A}_k(M)=2/(2p)!\,\beta_k(p-2)$ and $k_{\max}(M)=p-1$ for $M=2p+1$.

In order to study the Green's function and the Tr log contribution to the free energy we need to evaluate the above zeta-function at $s=1$ and its derivative at $s=0$. Such quantities will be expressed in terms of

$$\Sigma'_\alpha(p,2z)=\frac{1}{(2p+1)!}\sum_{k=0}^{p}(-1)^k\alpha_k(p-1)\zeta'_H\left(-2p+2k+2z-1,\frac{1}{2}\right),$$
$$\Sigma'_\beta(p,2z)=\frac{1}{(2p)!}\sum_{k=0}^{p-1}(-1)^k\beta_k(p-2)\zeta'_R(-2p+2k+2z), \tag{5.7}$$

and the results will follow. Then, we have the following cases.

(1) Even $D-M=2q$:

(a) $M=2p+2$:

$$\zeta_{R^{2q}\times S^{2p+2}}(1+\varepsilon)=\pi^q\frac{(-1)^{q-1}}{(q-1)!}2a^{-2q+2}\left\{\left[\frac{1}{\varepsilon}+\gamma+\psi(q)+2\log(a\mu)\right]\Sigma_\alpha(p,-2q+2)+2\Sigma'_\alpha(p,-2q+2)\right\}+O(\varepsilon),$$

$$\zeta'_{R^{2q}\times S^{2p+2}}(0)=\pi^q\frac{(-1)^q}{q!}2a^{-2q}\{[\gamma+\psi(q+1)+2\log(a\mu)]\Sigma_\alpha(p,-2q)+2\Sigma'_\alpha(p,-2q)\}. \tag{5.8}$$

As usual, μ is a parameter with mass dimension, introduced by redefining $\zeta_{\mathscr{M}}^{-\Box+\xi R}(s)$ as $\mu^{-2s}\zeta_{\mathscr{M}}^{(-\Box+\xi R)/\mu^2}(s)$, which renders the log arguments dimensionless.

(b) $M=2p+1$:

$$\zeta_{R^{2q}\times S^{2p+1}}(1)=\pi^q\frac{(-1)^{q-1}}{(q-1)!}2a^{-2q+2}2\Sigma'_\beta(p,-2q+2),$$

$$\zeta'_{R^{2q}\times S^{2p+1}}(0)=\pi^q\frac{(-1)^q}{q!}2a^{-2q}2\Sigma'_\beta(p,-2q). \tag{5.9}$$

The absence of terms with primeless Σ_β is a consequence of the location of the real zeros of ζ_R.

(2) Odd $D-M=2q+1$.

(a) $M=2p+2$:

$$\zeta_{R^{2q+1}\times S^{2p+2}}(1)=0,\quad \zeta'_{R^{2q+1}\times S^{2p+2}}(0)=0. \tag{5.10}$$

This vanishing follows from known properties of $\zeta_H(x,\frac{1}{2})$ and, as a result of (5.2),

$$W/N=0. \tag{5.11}$$

(b) $M=2p+1$:

$$\zeta_{R^{2q+1}\times S^{2p+1}}(1)=\pi^{q+1/2}\Gamma\left(-q+\frac{1}{2}\right)\frac{2a^{-2q+1}}{(2p)!}\Sigma_\beta(p,-2q+1),$$

$$\zeta'_{R^{2q+1}\times S^{2p+1}}(0)=\pi^{q+1/2}\Gamma\left(-q-\frac{1}{2}\right)\frac{2a^{-2q-1}}{(2p)!}\Sigma_\beta(p,-2q-1). \tag{5.12}$$

When studying the four kinds of sums (5.4) and (5.7) for $p\to\infty$ and finite $2z$ of the type $-2q-1,-2q,-2q+1,-2q+2$, one has to consider the behaviors of the α_k and β_k coefficients, which vary within the ranges

$$\alpha_0(p-1)=1,\ldots,\alpha_p(p-1)=\frac{\Gamma^2(p+1/2)}{\pi},$$

$$\beta_0(p-2)=1,\ldots,\beta_{p-1}(p-2)=[(p-1)!]^2, \tag{5.13}$$

and also satisfy

$$\alpha_k(p-1)\sim\beta_k(p-2)\sim\frac{p^{3k}}{3^k k!},\quad \text{as } p\to\infty. \tag{5.14}$$

For the β_k coefficients, this property was already observed in Ref. 13.

We must also take into account the following asymptotics:

$$\begin{gathered}\zeta_R(-(2n+1))\sim(-1)^{n+1}\,\frac{2(2n+1)!}{(2\pi)^{2n+1}},\\ \zeta_H(-(2n+1),\tfrac{1}{2})\sim-\zeta_R(-(2n+1)),\\ \xi_R'(-(2n+1))\sim-\zeta_R(-(2n+1))\log n,\\ \zeta_H'(-(2n+1),\tfrac{1}{2})\sim\zeta_R'(-(2n+1)),\end{gathered}\tag{5.15}$$

which are valid for $n\gg1$, and follow from known results about the gamma, Riemann and Hurwitz zeta-functions.

We show, as an example, the case of $\Sigma_\beta(p,-2q+1)$. Including the prefactor $1/(2p)!$, we denote the terms in that sum by $\Sigma_\beta(p,-2q+1)=(-1)^{p+q}\Sigma_{k=0}^{p-1}t_k$, where, as one may check for large p,$0<t_0<\cdots<t_{p-1}$. Therefore

$$|\Sigma_\beta(p,-2q+1)|<pt_{p-1}.\tag{5.16}$$

Combining the information we have with the Stirling approximation for the factorial (or Γ) functions, we obtain

$$pt_{p-1}=p\,\frac{2(2q+1)!}{(2\pi)^{2q+2}!}\,\zeta(2q+2)\,\frac{[(p-1)]^2}{(2p)!}\sim\frac{(2q+1)!\zeta(2q+2)}{2^{2q+1}\pi^{2q+3/2}}\,\frac{p^{-1/2}}{2^{2p}}.\tag{5.17}$$

As a result,

$$\begin{gathered}\Sigma_\beta(p,-2q+1)\to0,\quad\text{for any finite positive } q,\\ p\to\infty.\end{gathered}\tag{5.18}$$

The other three types of sum have the same property but, since the proof is of similar nature, the details are omitted. In consequence,

$$\begin{gathered}\zeta_{R^{D-M}\times T^M}(1)\to0,\\ \zeta'_{R^{D-M}\times T^M}(0)\to0,\\ M\to\infty,\quad\text{finite }(D-M),\end{gathered}\tag{5.19}$$

i.e., the two-point Green's function at equal points and the Tr log contribution to the free-energy vanish in this case of the $D\to\infty$ limit. The importance of that limit lies in the chance of using the space–time dimension as a perturbation parameter in field theory, with the advantage that it is then possible to obtain nonperturbative results in the coupling constants,[9] such as Green's functions for quantum fields in the Ising limit. In this spirit, expansions in inverse powers of the dimension have proven quite useful in atomic physics.[15]

The $m>0$ case is mathematically more involved. A possible way out is the construction of a power series in am by combining the preceding results with a simple binomial expansion. Such a method leads to

$$\zeta_{R^{D-M}\times S^M}(s)=2a^{2s-D+M}\,\frac{\pi^{(D-M)/2}}{\Gamma(s)}\sum_{k=0}^{\infty}\frac{(-1)^k}{k!}\,(am)^{2k}\Gamma\left(s+k-\frac{D-M}{2}\right)$$
$$\times\begin{cases}\Sigma_\alpha(p,2s+2k-D+M), & \text{for } M=2p+2,\\ \Sigma_\beta(p,2s+2k-D+M), & \text{for } M=2p+1.\end{cases}\tag{5.20}$$

A. A calculation in $R^2\times S^3$

For S^3 the degeneracy of each spherical mode [see (A14)] is just $(l+1)^2$. After applying standard Mellin-transform techniques, we end up by writing the zeta-function as follows:

$$\zeta_{R^2\times S^3}(s)=\frac{\pi^{3/2}a^{2(s-1)}}{\Gamma(s)}\left[-\frac{1}{2}\,(am)^{5/2-s}\Gamma\left(s-\frac{5}{2}\right)-\frac{1}{2}\,J_3^{(0)}(s-1,am)+J_3^{(1)}(s-1,am),\right],\tag{5.21}$$

where

$$J_M^{(0)}(z,\alpha)=\int_0^\infty dt\,t^{z-M/2-1}e^{-t\alpha^2}\left[\theta\left(\frac{\pi}{t}\right)-1\right],$$
$$J_M^{(1)}(z,\alpha)=\int_0^\infty dt\,t^{z-M/2-1}e^{-t\alpha^2}\,\frac{d}{dt}\,\theta\left(\frac{\pi}{t}\right).\tag{5.22}$$

Although not exactly like (4.3), these integrals may also be written as Dirichlet series involving modified Bessel functions. Furthermore, for $M=3$ such Bessel functions are expressible by finite series, and it is then possible to interchange the summations finally arriving at finite sums of polylogarithm functions. In this way, we obtain

$$\zeta_{R^2\times S^3}(1)=2\pi^2\left[-\frac{1}{3}\,(am)^{3/2}-(am)^3\left(\frac{Li_2(e^{-2\pi am})}{(2\pi am)^2}+\frac{Li_3(e^{-2\pi am})}{(2\pi am)^3}\right)+\pi^2 am\,Li_{-2}(e^{-2\pi am})\right],$$
$$\zeta'_{R^2\times S^3}(0)=4\pi^2\left[\frac{1}{15}\,(am)^{5/2}-(am)^5\left(\frac{Li_3(e^{-2\pi am})}{(2\pi am)^3}+3\,\frac{Li_4(e^{-2\pi am})}{(2\pi am)^4}+3\,\frac{Li_5(e^{-2\pi am})}{(2\pi am)^5}\right)\right.$$
$$\left.+\pi^2(am)^3Li_{-1}(e^{-2\pi am})\right].\tag{5.23}$$

Since we are in $D=5$, λ_c must be the value of λ satisfying the second gap equation for $b=0$, $m=0$, i.e.,

$$\frac{1}{\lambda_c}=G(x,x;0,g)=\frac{1}{(2\pi)^2a^3}\,\zeta_{R^2\times S^3}(1)\Big|_{m=0}=-\frac{1}{16\pi^3a^3}\,Li_3(1)=-\frac{1}{16\pi^3a^3}\,\zeta_R(3).$$

Next, we replace $1/\lambda$ with this critical value and solve numerically the second gap equation for $b=0$ only. The critical value obtained for am is

$$(am)_c=2.2689.$$

Calculating $\zeta'_{R^2\times S^3}(0)$ at $am=(am)_c$, we find the finite contribution to the free energy density at the critical point:

$$\frac{W}{N}=-\frac{1}{2}\left(\frac{a}{2\pi}\right)^2\zeta'_{R^2\times S^3}(0)=-0.7773.$$

B. Application to $T^M\times S^P$

The zeta-function in this space may be written

$$\zeta_{T^M\times S^P}(s)=\left(\frac{2\pi}{\rho}\right)^{-2s}\delta^{-s}\sum_{n_1,\ldots,n_M}\sum_{l}d(P,l)\left\{\frac{1}{\delta}(n_1^2+\cdots+n_M^2)+\delta\left[\left(l+\frac{P-1}{2}\right)^2+a^2m^2\right]\right\}^{-s},\tag{5.24}$$

where we are using the notation

$$\delta=\frac{\rho}{2\pi a},\tag{5.25}$$

and $d(P,l)$ is the degeneracy of the lth P-dimensional spherical mode (A14). In the $m=0$ case, using (5.6) this is put in the way

$$\zeta_{T^M\times S^P}(s)=\left(\frac{2\pi}{\rho}\right)^{-2s}\delta^{-s}\sum_{k=0}^{k_{\max}(P)}(-1)^k\mathscr{A}_k(P)\sum_{n_1,\ldots,n_M}\sum_{l}\left(l+\frac{P-1}{2}\right)^{P-1-2k}$$
$$\times\left[\frac{1}{\delta}(n_1^2+\cdots+n_M^2)+\delta\left(l+\frac{P-1}{2}\right)^2\right]^{-s}.\tag{5.26}$$

For odd P, $(P-1)/2$ is an integer and simple properties under dual transformations $\delta\to 1/\delta$ in the sense of Sec. IV in the second reference of Ref. 6 may appear, after making the replacements explained there. It is quite clear that if P is even, there can be no such invariance—in whatever sense. However, it can be achieved considering antiperiodic (instead of periodic) field solutions, which lead to the change $n_i\to n_i+\frac{1}{2}$, and making some further alterations. In particular, for $M=1$, $P=2$, $d(2,l)=2(l+\frac{1}{2})$ and $l+(P-1)/2=l+\frac{1}{2}$. As a result, one can then put

$$\zeta_{T^1\times S^2}(s)\propto\sum_{n,l}\left(l+\frac{1}{2}\right)\left[\frac{1}{\delta}\left(n+\frac{1}{2}\right)^2+\delta\left(l+\frac{1}{2}\right)^2\right]^{-s}.$$

Then, the ensuing free energy will be invariant if one cares to replace the ordinary δ-derivative with the ''fractional-derivative'' from Ref. 6. In a similar way, by adequately modifying the definition of the free energy, we may get the $\delta\to 1/\delta$ invariance in higher dimensions.

Combining the general forms of the previous calculations we find

$$\zeta_{T^M\times S^P}(s)=\frac{\pi^{M/2}(2\pi/\rho)^{-2s}}{\Gamma(s)}\sum_{l=0}^{\infty}d(P,l)\left[I_M\left(s,\frac{\rho}{2\pi}m(P,l)\right)+\left(\frac{\rho}{2\pi}m(P,l)\right)^{M-2s}\Gamma\left(s-\frac{M}{2}\right)\right],\tag{5.27}$$

where

$$m(P,l)\equiv\sqrt{\frac{1}{a^2}\left(l+\frac{P-1}{2}\right)^2+m^2}.\tag{5.28}$$

After expanding I_M into a Dirichlet series of modified Bessel functions, we realize that for $P\to\infty$ this part may be neglected because it is exponentially vanishing. Calling $\zeta^{(\infty)}_{T^M\times S^P}(s)$ the rest, one obtains

$$\zeta^{(\infty)}_{T^M\times S^N}(s)\sim \frac{2a^{2s}\left(\frac{\rho}{a}\right)^M}{(4\pi)^{M/2}}\frac{\Gamma\left(s-\frac{M}{2}\right)}{\Gamma(s)}\times\begin{cases}\Sigma_\alpha(p,2s-M), & \text{for } P=2p+2,\\ \Sigma_\beta(p,2s-M), & \text{for } P=2p+1,\end{cases} \tag{5.29}$$

which is, up to a constant, the zeta-function for $R^M\times S^P$ with $m=0$, whose properties have already been considered.

VI. HIGHER-DERIVATIVE $O(N)$ NONLINEAR SIGMA MODEL IN $R^{D-M}\times T^M$

It is interesting to observe that the model (2.2) may be easily generalized to have higher-derivative terms. In order not to have to study higher-derivative conformally invariant operators, we limit ourselves to $R^{D-M}\times T^M$, which is relatively simple due to its conformal flatness. Then we may write

$$Z[g]=\int \mathscr{D}\phi\mathscr{D}\sigma\,\exp\left\{-\frac{1}{2\lambda}\int d^Dx\sqrt{-g}\,[\,\phi^i\Box^2\phi^i+\sigma(\,\phi^{i2}-1)]\right\}. \tag{6.1}$$

Repeating all the steps in Sec. I, we obtain

$$W[g,\lambda]=\frac{N}{2}\left[\mathrm{Tr}\,\log(\Box^2+\sigma)-\int d^Dx\sqrt{g}\,\frac{m^2}{\lambda}\right]. \tag{6.2}$$

The Green's function and the Tr log part of the above expression are directly linked to the associated zeta-function, which admits the following power expansion in $\rho\sigma^{1/4}$:

$$\begin{aligned}\zeta^{(\Box^2+\sigma)}_{R^{D-M}\times T^M}(s)=&\frac{\pi^{D-M}}{\Gamma(s)}\,\sigma^{(D-M)/4-s}\left[\frac{\sqrt{\pi}}{2^{(D-M)/2}}\frac{\Gamma(s-(D-M)/4)}{\Gamma((D-M+2)/4)}\right.\\ &+\frac{\sqrt{\pi}}{2^{2s-1}}\sum_{k=0}^{\infty}\frac{(-1)^k}{k!}\frac{\Gamma(2s+2k-(D-M)/2)}{2^{2k}\Gamma(s+k+\frac{1}{2})}\\ &\left.\times Z_M\left(2s+2k-\frac{D-M}{2}\right)\left(\frac{\rho\sigma^{1/4}}{2\pi}\right)^{4s+4k-D+M}\right],\end{aligned} \tag{6.3}$$

where Z_M is the usual Epstein zeta-function. This function has poles at $s=D/4-k$, $k=0,1,2,...$, with the exception (if they coincide) of $s=0,-1,-2,...$, where it is finite.

Mathematically speaking, this object is harder to deal with than an ''ordinary'' zeta-function (i.e., one for a second-order operator). It can also be expressed by a series of hypergeometric functions:

$$\begin{aligned}\zeta^{(\Box^2+\sigma)}_{R^{D-M}\times T^M}(s)=&\frac{\pi^{D-M}}{2^{(D-M)/2}\Gamma(s)}\left(\frac{2\pi}{\rho}\right)^{D-M-4s}\frac{\Gamma(s-(D-M)/4)\Gamma(s-(D-M)/4+\frac{1}{2})}{\Gamma(s+\frac{1}{2})}\\ &\times\sum_{\vec{n}\in Z^M}{}_2F_1\left(s-\frac{D-M}{4},s-\frac{D-M}{4}+\frac{1}{2},s+\frac{1}{2};-\left(\frac{\rho\sigma^{1/4}}{2\pi}\right)^4(\vec{n}^2)^{-2}\right)\\ &\times(\vec{n}^2)^{(D-M)/2-2s},\end{aligned} \tag{6.4}$$

or by the integral representations

$$\zeta_{R^{D-M}\times T^M}^{(\Box^2+\sigma)}(s)=\frac{\pi^{(D+1)/2}\sigma^{s/2+1/4}}{2^{3s-1/2}\Gamma(s)}\left(\frac{2\pi}{\rho}\right)^{D-M-6s-1}\left[\mathscr{T}_{D,M}\left(s,\frac{\rho\sigma^{1/4}}{2\pi}\right)\right.$$
$$\left.+\left(\frac{\rho\sigma^{1/4}}{2\pi}\right)^{D-6s-1}\frac{\Gamma(4s+1-D/2)}{2^{(D+1)/2-3s}\Gamma(-2s+2+D/2)}\right], \tag{6.5}$$

where

$$\mathscr{T}_{D,M}(s,\alpha)=\sum_{l=1}^{M}\binom{M}{l}2^l\sum_{\vec{n}\in(\mathbb{N}^*)^l}\int_0^\infty dt\,t^{3s-(D+1)/2}J_{s+1/2}(\alpha^2 t)e^{-(\pi/t)|\vec{n}|_l^2}. \tag{6.6}$$

Here J is the first species Bessel function.

A different strategy is to regard $\Box^2+\sigma$ as $(\Box+i\sigma^{1/2})(\Box-i\sigma^{1/2})$. Then,

$$\tfrac{1}{2}\mathrm{Tr}\,\log(\Box^2+\sigma)=\tfrac{1}{2}[\mathrm{Tr}\,\log(\Box+i\sigma^{1/2})+\mathrm{Tr}\,\log(\Box-i\sigma^{1/2})]$$
$$=-\left(\frac{\rho}{2\pi}\right)^{D-M}\mathrm{Re}\;\zeta_{R^{D-M}\times T^{M'}}^{(\Box+i\sigma^{1/2})}(0). \tag{6.7}$$

Taking advantage of the calculation in Sec. IV for $-\Box+m^2$ when $D=2d+3$, we arrive at the following expression for the finite part of $(W/N)(\rho\sigma^{1/4})$:

$$-\frac{1}{(4\pi)^{d+3/2}}\left\{2^{d+3}\sqrt{\pi}\sum_{k=0}^{d+1}\frac{(d+1+k)!}{k!(d+1-k)!2^k}(\rho\sigma^{1/4})^{d+1-k}\right.$$
$$\left.\times\mathrm{Re}[i^{(d+1-k)/2}Li_{d+2+k}(e^{-i^{1/2}p\sigma^{1/4}})]+\Gamma\left(-d-\frac{3}{2}\right)(\rho\sigma^{1/4})^{2d+3}\;\mathrm{Re}[i^{d+3/2}]\right\}. \tag{6.8}$$

Observing that the values at the critical point have to coincide with the extremals of W/N as a function of $\rho\sigma^{1/4}$, these points are found by numerical examination of (6.8).

d	min of $-\frac{1}{2}(\rho/2\pi)^{2d+2}\zeta'_{R^{2d+2}\times T^1}(0)$	$(\rho\sigma^{1/4})$
1	1.65	−0.1459
2	2.36	−0.1088

For $d=0$, 3, and 4 no solution has appeared, while for $d=5$ we obtain 3.03 and −0.3141. Comparing with numerical estimates for the model (2.2) on the same background, we see that the properties of the higher-derivative model (6.1) are drastically different.

VII. CONCLUSIONS

In the present paper, using zeta-function regularization, we have calculated the free vacuum energy (or Casimir energy) for the D-dimensional $O(N)$ nonlinear sigma model on some spaces with constant curvature. Explicit expressions for the free energy have been obtained at the critical point (when the gap equations have been used) and also in noncritical regime (when the gap equations have not been used). For all those spaces with $D=3,4$, the explicit expressions for the free energy may be easily used in studies of the quantum antiferromagnet.[5] Moreover, for $2<D<4$ it is known[16] that the $O(N)$ model in R^D possesses an order–disorder phase transition and hence its free energy may be very useful for studying dual properties. In this respect, the generalization to curved backgrounds is of interest.

In particular, we have shown [see Eq. (5.10)] that the free energy of the model in $R^{2q+1}\times S^{2p+2}$ vanishes. This generalizes the corresponding result of Ref. 7 in $R^1\times S^2$, and shows

that in D dimensions the free energy at the critical point for $R^{2q+1}\times S^{2p+2}$ is the same as that for R^D, in accordance with the conformal equivalence between both manifolds.

From another viewpoint, for the development of connections of two-dimensional conformal field theory (which is a very powerful tool) with higher dimensional models, it is important to study the modular properties of such theories.[6] In Sec. V B we have checked dual invariance in Cardy's sense for $m=0$ and antiperiodic modes in $S^1\times S^2$. Hence, the higher-dimensional $O(N)$ model may serve as a very useful toy model for studying dual symmetries, which have become quite popular in recent studies of strings and supersymmetric QCD.

Finally let us note that the D-dimensional $O(N)$ nonlinear sigma model may be considered as a toy model of quantum field theory in a Kaluza–Klein framework for studying the question of spontaneous compactification, for example. As usual, Kaluza–Klein theories are not renormalizable. However, in the model under discussion we may still use the $1/N$-expansion in order to control somehow the quantum corrections.

Observe also that in addition to the $1/N$-expansion one can calculate the free energy as an expansion in inverse powers of the dimension. Such calculations in frames of the toy model under consideration may be useful in atomic physics.[15]

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APPENDIX: ON THE CALCULATION OF ZETA-FUNCTIONS

1. General considerations

Let $\mathscr{M}$ be a space–time of the type $R^{D-M}\times\mathscr{M}^M$, $D>M$, with the operator $-\Box+m^2+\xi R$ acting on the whole manifold. Since $-\Box = -\Box_{R^{D-M}} - \Box_{\mathscr{M}^M}$, the spectrum has the form $p^2+\lambda_n+m^2+\xi R$, $p\in R^{D-M}$, $\lambda_n \in \mathrm{Sp}(-\Box_{\mathscr{M}^N})$. Then, the global zeta-function on $\mathscr{M}=R^{D-M}\times\mathscr{M}^M$ is defined as

$$\zeta_{R^{D-M}\times\mathscr{M}^M}(s)=\int d^{D-M}p \sum_{\substack{n:\\ \lambda_n\in \mathrm{Sp}(-\Box_{\mathscr{M}^M})}} (p^2+\lambda_n+m^2+\xi R)^{-s}. \tag{A1}$$

Such a definition is purely mathematical, i.e., the usual physical factors coming from state normalization are here absent. Notice that each momentum integration is introducing a further mass dimension. The arbitrary mass scale μ, typically supplied in order to render the function dimensionless, is not present either. All these elements may be included at a later stage.

After doing the p-integrations, this zeta-function can be written in terms of the one for $\mathscr{M}^N$

$$\zeta_{R^{D-M}\times\mathscr{M}^M}(s)=\pi^{(D-M)/2}\,\frac{\Gamma(s-(D-M)/2)}{\Gamma(s)}\,\zeta_{\mathscr{M}^M}\left(s-\frac{D-M}{2}\right), \tag{A2}$$

with

$$\zeta_{\mathscr{M}^M}(z)=\sum_{\substack{n:\\ \lambda_n\in \mathrm{Sp}(-\Box_{\mathscr{M}^M})}} (\lambda_n+m^2+\xi R)^{-z}, \tag{A3}$$

where possible degeneracies must be accounted for into this sum.

First, we make the following hypothesis: only the Γ function has singularities at $s-(D-M)/2$, $s=0$, 1—and, obviously, these poles can be encountered for even $D-M$ only—while $\zeta_{\mathscr{M}^M}$ and

its derivative are finite at these points. Such an assumption is right when $\mathcal{M}^M = T^M$ for odd D, or $\mathcal{M}^M = S^M$ for the massless case. Using the expansion of the Γ functions, both around their poles and around regular points, we obtain the generic results:

(1) Even $D-M=2q$:

$$\zeta_{R^{2q}\times\mathcal{M}^M}(1+\varepsilon)=\pi^q\frac{(-1)^{q-1}}{(q-1)!}\left\{\left[\frac{1}{\varepsilon}+\psi(q)+\gamma\right]\zeta_{\mathcal{M}^M}(-q+1)+\zeta'_{\mathcal{M}^M}(-q+1)\right\}+O(\varepsilon),$$
$$\zeta'_{R^{2q}\times\mathcal{M}^M}(0)=\pi^q\frac{(-1)^q}{q!}\{[\psi(q)+\gamma]\zeta_{\mathcal{M}^M}(-q)+\zeta'_{\mathcal{M}^M}(-q)\}. \tag{A4}$$

(2) Odd $D-M=2q+1$:

$$\zeta_{R^{2q+1}\times\mathcal{M}^M}(1)=\pi^{q+1/2}\Gamma(-q+\tfrac{1}{2})\zeta_{\mathcal{M}^M}(-q+\tfrac{1}{2}),$$
$$\zeta'_{R^{2q+1}\times\mathcal{M}^M}(0)=\pi^{q+1/2}\Gamma(-q-\tfrac{1}{2})\zeta_{\mathcal{M}^M}(-q-\tfrac{1}{2}). \tag{A5}$$

When, on the contrary, $\zeta_{\mathcal{M}^M}(z)$ has poles at $z=s-(D-M)/2$, $s=0,1$, this function has to be Laurent-expanded around these singularities before taking the limits $s\to 0,1$, and a somewhat different calculation is required in every particular case.

2. Zeta-function on T^M

We study the torus only. Once we have the zeta-function on T^M, we can find the one on $\zeta_{R^{D-M}\times\mathcal{M}^M}$ by application of (A2). So, when looking at $\zeta_{T^N}(z)$ we will have in mind the arguments $z=s-(D-M)/2$, $s=0,1$.

For simplicity we take all the radii equal and with value ρ. Then

$$\zeta_{T^M}(z)=\left(\frac{2\pi}{\rho}\right)^{2z}Z_M\left(z,\frac{\rho m}{2\pi}\right), \tag{A6}$$

where

$$Z_M(z,a)=\sum_{n_1,\ldots,n_M=-\infty}^{\infty}(n_1^2+\cdots+n_M^2+a^2)^{-z} \tag{A7}$$

is an Epstein zeta-function with inhomogeneous term. After Mellin-transforming we obtain

$$\zeta_{T^M}(z)=\left(\frac{2\pi}{\rho}\right)^{-2z}\frac{1}{\Gamma(z)}\int_0^\infty dt\,t^{z-1}e^{-t(\rho m/2\pi)^2}\theta^M\left(\frac{t}{\pi}\right). \tag{A8}$$

The Jacobi theta function $\theta(x)$, given by (4.4), has the property

$$\theta(x)=\frac{1}{\sqrt{x}}\,\theta\left(\frac{1}{x}\right). \tag{A9}$$

Taking advantage of this, we separate the part which diverges at $t=0$, i.e., the $n=0$ contribution in the θ function, and write

$$\xi_{T^M}(z)=\left(\frac{2\pi}{\rho}\right)^{-2z}\frac{\pi^{M/2}}{\Gamma(z)}\left\{\int_0^\infty dt\,t^{z-M/2-1}e^{-t(\rho m/2\pi)^2}\left[\theta^M\left(\frac{\pi}{t}\right)-1\right]+\left(\frac{\rho m}{2\pi}\right)^{M-2z}\Gamma\left(z-\frac{M}{2}\right)\right\}$$
$$\equiv\left(\frac{2\pi}{\rho}\right)^{-2z}\frac{\pi^{M/2}}{\Gamma(z)}\left\{I_M\left(z,\frac{\rho m}{2\pi}\right)+\left(\frac{\rho m}{2\pi}\right)^{M-2z}\Gamma\left(z-\frac{M}{2}\right)\right\}. \tag{A10}$$

Now the t-integral, that [in accordance with (4.3)] we have called $I_M(z,\rho m/2\pi)$, contains no small-t singularity. This expression has the additional advantage that its second term exhibits the poles of this function at $z=M/2,(M-1)/2,\ldots$. After writing θ^M as a binomial expansion (in the $n=0$ term of θ and the rest of the summatory), we use the integral representation

$$\int_0^\infty dt\,t^{\nu-1}e^{-a/t-bt}=2\left(\frac{a}{b}\right)^{\nu/2}K_\nu(2\sqrt{ab}) \tag{A11}$$

and end up with the Dirichlet series

$$I_M\left(z,\frac{\rho m}{2\pi}\right)=2^{M/2-z}\left(\frac{\rho m}{2\pi}\right)^{M-2z}\sum_{l=1}^{M}\binom{M}{l}2^{l+1}\sum_{n_1,\ldots,n_l=1}^{\infty}\frac{K_{M/2-z}(\rho m\sqrt{n_1^2+\cdots+n_l^2})}{(\rho m\sqrt{n_1^2+\cdots+n_l^2})^{M/2-z}}. \tag{A12}$$

These results, combined with (A2), give rise to (4.2) and (4.5) for $\zeta_{R^{D-M}\times T^M}(s)$.

3. Zeta-function on S^M

The same method is employed to derive the expressions in $\zeta_{R^{D-M}\times S^M}(s)$ from the ones for S^M. Taking into account the known spectrum of the D'Alembertian on S^M, the Riemann curvature on this space, and the conformal coupling value of ξ, we readily obtain the eigenvalues of our operator and construct its zeta-function,

$$\zeta_{S^M}(z)=\sum_{l=0}^{\infty}d(M,l)\left[\frac{1}{a^2}\left(l+\frac{M-1}{2}\right)^2+m^2\right]^{-z}, \tag{A13}$$

with degeneracies (see e.g. Ref. 17)

$$d(M,l)=\frac{(l+M-2)!}{l!(M-1)!}(2l+M-1)=\binom{l+M-2}{l}\frac{l+(M-1)/2}{(M-1)/2}. \tag{A14}$$

Setting $m=0$ one obtains

$$\zeta_{S^M}(z)=\frac{2a^{2z}}{M-1}\sum_{l=0}^{\infty}\binom{l+M-2}{l}\left(l+\frac{M-1}{2}\right)^{1-2z}$$
$$=\begin{cases}\dfrac{2a^{2z}}{(2p+1)!}\displaystyle\sum_{k=0}^{p}(-1)^k\alpha_k(p-1)\zeta_H\left(-1+2z-2p+2k,p+\frac{1}{2}\right), & \text{for } M=2p+2,\\ \dfrac{2a^{2z}}{(2p)!}\displaystyle\sum_{k=0}^{p-1}(-1)^k\beta_k(p-2)\zeta_H(2z-2p+2k,p), & \text{for } M=2p+1,\end{cases} \tag{A15}$$

with the α_k and β_k coefficients as written in (5.5). The Hurwitz functions in (A15) may be reexpressed with the help of the identities

$$\zeta_H\left(z,p+\frac{1}{2}\right)=\zeta_H\left(z,\frac{1}{2}\right)-\sum_{n=0}^{p-1}\left(n+\frac{1}{2}\right)^{-z},\quad \zeta_H\left(z,\frac{1}{2}\right)=(2^z-1)\zeta_R(z),$$
$$\zeta_H(z,p)=\zeta_R(z)-\sum_{n=1}^{p-1}n^{-z}. \tag{A16}$$

Afterwards, taking advantage of the properties

$$\sum_{k=0}^{p}(-1)^k\alpha_k(p-1)\left(n+\frac{1}{2}\right)^{2(p-k)}=0,\quad \text{when } 0\leqslant n\leqslant p-1,$$
$$\sum_{k=0}^{p-1}(-1)^k\beta_k(p-2)(n+1)^{2(p-1-k)}=0,\quad \text{when } 0\leqslant n\leqslant p-2, \tag{A17}$$

we may put

$$\zeta_{S^M}(z)=\begin{cases}2a^{2z}\Sigma_\alpha(p,2z), & \text{for } M=2p+2,\\ 2a^{2z}\Sigma_\beta(p,2z), & \text{for } M=2p+1,\end{cases} \tag{A18}$$

where the $\Sigma_\alpha(p,2z)$ and $\Sigma_\beta(p,2z)$ are the ones defined by (5.4). Observing those finite sums, one locates the singularities of $\zeta_{S^M}(z)$, which come from the pole of $\zeta_H(x,a)$ or $\zeta_R(x)$ at $x=1$:

$$z=1,2,\ldots,p+1,\quad \text{for } N=2p+2,$$
$$z=\tfrac{3}{2},\tfrac{5}{2},\ldots,p+\tfrac{1}{2},\quad \text{for } N=2p+1.$$

As a result, we realize that at the points we are interested in, i.e., $z=s-(D-M)/2$, $s=0$, 1, $\zeta_{S^M}(z)$ is finite and we may therefore apply (A4) and (A5), thus obtaining the values of $\zeta_{R^{D-M}\times S^M}(1)$, $\zeta'_{R^{D-M}\times S^M}(0)$ given in Sec. V.

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Complete sets of non-self-adjoint observables: An unbounded approach

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The notion of completeness of a set $\mathscr{S}$ of compatible observables represented by maximal symmetric operators is discussed directly in terms of unbounded operators. In contrast with what happens for self-adjoint observables, the present framework forces us to involve some partial algebraic structures such as the partial GW^*-algebra generated by $\mathscr{S}$. In this way the previous approaches based on von Neumann algebras and on O^*-algebras are generalized. © *1996 American Institute of Physics.* [S0022-2488(96)00402-1]

I. INTRODUCTION

In the last two decades there has been a growing interest in quantum problems where symmetric but non-self-adjoint observables are involved.[1–5] This is basically motivated by the following two facts.

First, in the analysis of open quantum mechanical systems,[1,6,7] which frequently exhibit an irreversible behavior, the dynamics is represented, in general, by a one-parameter semigroup of contractions which is, in turn, generated, in the most favorable situation, by a symmetric operator.

Second, the quantum mechanical axiom of repeatability, which forces us to represent observables by projection-valued (PV) measures, is violated in many quantum mechanical experiments which are unrepeatable for their own nature.[5] A quite extensive literature is concerned with problems of this kind, such as the repeated or inexact measurements (localization measurements), e.g., Refs. 8–10 or the position measurements of the photon, e.g., Refs. 11, 12, etc. The quantum measurements are, in all these cases, described by positive-operator-valued (POV) measures which are not necessarily PV.[13,14] As is known, the operator determined, via the corresponding integral representation,[15] by a POV measure defined on the line (i.e., an observable), when it exists, is symmetric but not necessarily self-adjoint, hence to general quantum measurements on the line there correspond symmetric observables. (The statistical apparatus based on POV measures finds even technical applications, e.g., in quantum communication systems[16]).

The role played by POV measures and by dynamical semigroups is not, however, the only reason for considering symmetric observables. They, indeed, occur in many other situations:

(1) the neutral (hence observable) scalar field in (Wightman) quantum field theory provides an example of a set of not necessarily self-adjoint but symmetric operators defined on a common dense and invariant domain;
(2) the limit of (bounded) self-adjoint observables is in general a non-self-adjoint observable;[17]
(3) generalized symmetries[18,19] are represented by semigroups of isometries generated by maximal symmetric observables.

Finally, it is worth mentioning that also in the usual formulation of quantum mechanics non-self-adjoint observables may occur: for instance, the momentum operator on the half-line is maximal symmetric but not self-adjoint.

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Of course, in the case of self-adjoint observables it is possible to deal indifferently with the operators or with the corresponding spectral measures or, still, with the one-parameter groups of unitary operators that they generate, because of the mathematical equivalence stated by the spectral theorem and by Stone's theorem. For symmetric operators the relations are no longer so simple (for an exhaustive discussion we refer to Ref. 15) and some new mathematical difficulties appear when we try to express, in this more general framework, concepts and problems which play a relevant role in the traditional formulation of quantum mechanics.

One of them is certainly that of a rigorous description of Dirac's concept of a complete set of commuting observables (CSCO) which has an almost 35-year-old history, starting from the pioneering Jauch's paper.[20] Therein observables were considered as (possibly) unbounded *self-adjoint* operators in Hilbert space and the full discussion was then carried out in terms of the Abelian von Neumann algebra generated by the PV measures associated to the self-adjoint observables via the spectral theorem (which, as is known, establishes a one-to-one correspondence between PV measures and self-adjoint operators).

In a previous paper,[18] we studied the notion of a CSCO when the observables are represented by unbounded symmetric operators in Hilbert space. This is certainly not the most general situation, but it corresponds to the reasonable requirement that to each observable it corresponds sufficiently many vectors with finite expectation value. On the contrary, there is no loss of generality in the assumption that these symmetric operators are maximal (each symmetric operator has, indeed, a maximal extension). Under these assumptions we were able to define the strong commutativity of a family of maximal symmetric observables via the semigroups of isometries they generate. With methods which parallel those in Ref. 20, we considered the von Neumann algebra generated by these semigroups. This von Neumann algebra is no longer Abelian, but only *semi-Abelian*;[18] nevertheless a notion of maximality can be introduced also in this case.

On the other hand, in Ref. 21, the completeness of a set of commuting self-adjoint observables was discussed directly in terms of unbounded operators. More precisely, the properties of the CSCO were described there in terms of O^*-algebras theory;[22] the concept of SV^* algebra[23] was used and the connections with the bounded approach developed in Ref. 20 were discussed. For other approaches to commutation properties, see Refs. 24 and 25.

In this paper we will present a study parallel to that in Ref. 21, in the case where the observables are represented by symmetric but non-self-adjoint observables. However, as we shall see in Sec. IV, the transition from the self-adjoint observables description of a CSCO to the present case involves partial algebraic structures.[26–31] Actually, with the help of the recently developed formalism of *partial GW^*-algebras* (partial GW^*-algebras are, in a sense, the *unbounded* analog of von Neumann algebras),[31] both the bounded approach[20] and its unbounded generalization[21] are naturally embedded in the present scheme to include non-self-adjoint observables as well.

In any case, when dealing with unbounded operators, unavoidable problems of domain arise. In typical situations one supposes that the operators involved in the physical problem constitute an O^*-algebra. There are, however, very simple instances which do not fit into this algebraic framework. This depends, in general, on the fact that the involved operators do not admit an *invariant* domain or, even if they do, this domain is not the most natural for practical purposes. For these reasons, J. P. Antoine and W. Karwowski[26] introduced *partial O^*-algebras*, whose study has been then deepened also by other authors.[27–31] As said before, also in our investigation on the unbounded description of complete sets of compatible symmetric observables (for the sake of simplicity we consider also in this paper only maximal symmetric observables), these partial *-algebras will play a relevant role. In our discussion, we will also emphasize some domain problems which arise independently of how nicely the operators behave. As discussed in Ref. 29, in fact, the different possible choices of the domain is the main motivation for the appearing of partial O^*-algebras also for families of strongly commuting normal operators.

In Sec. III we reformulate in a suitable form some results of Ref. 18 and discuss the possible definitions of compatibility and completeness.

We show in Sec. IV that a set of strongly commuting non-self-adjoint observables admit always a common dense and invariant domain where they, obviously, generate an O^*-algebra. Moreover, the algebraic commutativity, which is a specific feature of a CSCO in the self-adjoint case, is preserved also in the non-self-adjoint case on this domain. (It is perhaps worth mentioning the fact that the algebraic commutativity is a very weak condition which does not imply compatibility, as Nelson's example, cf. Sec. IV, shows also in the self-adjoint case.)

We prove, furthermore, that a set of compatible observables generates a partial GW^*-algebra on an appropriate domain. However, in this case, the minimal partial GW^*-algebra containing the von Neumann algebra of the corresponding semigroups is no more Abelian as in the self-adjoint case. Incidentally, the above discussion shows that partial algebraic structures provide a quite natural framework where some quantum theoretical application can be conveniently cast and that they are not so rare or exotic as their mathematical aspects could lead to think.

We discuss, finally, a Nelson-type physical example and some regularity properties of a family of compatible observables.

II. PRELIMINARIES

Let $\mathscr{H}$ be a complex Hilbert space and $\mathscr{D}$ a dense subspace of $\mathscr{H}$. We denote, as usual, by $\mathscr{L}^\dagger(\mathscr{D},\mathscr{H})$ the set of all (closable) linear operators X in $\mathscr{H}$ such that $\mathscr{D}(X)=\mathscr{D}$, $\mathscr{D}(X^*)\supseteq\mathscr{D}$. The set $\mathscr{L}^\dagger(\mathscr{D},\mathscr{H})$ is a partial *-algebra, with respect to the following operations: the usual sum X_1+X_2, the scalar multiplication λX, the involution $X\mapsto X^\dagger\equiv X^*\restriction\mathscr{D}$, and the partial multiplication $X_1\square X_2 = X_1^\dagger{}^* X_2$, defined whenever $X_2\in R(X_1)$, that is, iff $X_2\mathscr{D}\subset\mathscr{D}(X_1^\dagger{}^*)$ and $X_1^*\mathscr{D}\subset\mathscr{D}(X_2^*)$. A partial O^*-algebra on $\mathscr{D}$ is a partial *-subalgebra $\mathfrak{M}$ of $\mathscr{L}^\dagger(\mathscr{D},\mathscr{H})$, that is, $\mathfrak{M}$ is a subspace of $\mathscr{L}^\dagger(\mathscr{D},\mathscr{H})$, containing the identity and such that $X^\dagger\in\mathfrak{M}$ whenever $X\in\mathfrak{M}$ and $X_1\square X_2\in\mathfrak{M}$ for any $X_1,X_2\in\mathfrak{M}$ if $X_2\in R(X_1)$. As for $\mathscr{L}^\dagger(\mathscr{D},\mathscr{H})$ itself, it is the largest partial O^*-algebra on the domain $\mathscr{D}$.

As usual,[22] we put

$$\mathscr{L}^\dagger(\mathscr{D})=\{X\in\mathscr{L}^\dagger(\mathscr{D},\mathscr{H});X\mathscr{D}\subset\mathscr{D}\ \text{ and }\ X^*\mathscr{D}\subset\mathscr{D}\}. \tag{1}$$

Then $\mathscr{L}^\dagger(\mathscr{D})$ is a *-algebra with the involution $X\mapsto X^\dagger$. A *-subalgebra of $\mathscr{L}^\dagger(\mathscr{D})$ with identity operator is called an O^*-algebra on $\mathscr{D}$.

In addition, for any †-invariant subset of $\mathscr{L}^\dagger(\mathscr{D},\mathscr{H})$, we define the sets

$$\hat{\mathscr{D}}(\mathfrak{M})\equiv\bigcap_{X\in\mathfrak{M}}\mathscr{D}(\bar{X}),\quad \mathscr{D}^*(\mathfrak{M})\equiv\bigcap_{X\in\mathfrak{M}}\mathscr{D}(X^*), \tag{2}$$

so that $\mathscr{D}\subset\hat{\mathscr{D}}(\mathfrak{M})\subset\mathscr{D}^*(\mathfrak{M})$. The full closure of $\mathfrak{M}$ is the set $\hat{\mathfrak{M}}=\{\bar{X}\restriction\hat{\mathscr{D}}(\mathfrak{M});\ X\in\mathfrak{M}\}$. The partial O^*-algebra $\mathfrak{M}$ is called *fully closed* if $\mathscr{D}=\hat{\mathscr{D}}(\mathfrak{M})$ and *self-adjoint* if $\mathscr{D}=\mathscr{D}^*(\mathfrak{M})$.

We will often consider on $\mathscr{L}^\dagger(\mathscr{D},\mathscr{H})$ the *strong* *-topology (shortly s^*-topology) defined by the seminorms

$$X\in\mathscr{L}^\dagger(\mathscr{D},\mathscr{H})\to\max\{\|Xf\|,\|X^\dagger f\|\},\quad f\in\mathscr{D}.$$

This topology plays a relevant role in the study of *commutants* and *bicommutants* of subsets of $\mathscr{L}^\dagger(\mathscr{D},\mathscr{H})$.

The *weak unbounded commutant*[23] $\mathfrak{M}'_\sigma$ of a †-invariant subset of $\mathscr{L}^\dagger(\mathscr{D},\mathscr{H})$ is defined as

$$\mathfrak{M}'_\sigma=\{X\in\mathscr{L}^\dagger(\mathscr{D},\mathscr{H})\mid(Af,X^\dagger g)=(Xf,A^\dagger g)\,\forall A\in\mathfrak{M},\ \forall f,g\in\mathscr{D}\}. \tag{3}$$

Its bounded part $\mathfrak{M}'_w=\mathfrak{M}'_\sigma\cap\mathscr{B}(\mathscr{H})$ is called the *weak bounded commutant* of $\mathfrak{M}$, where $\mathscr{B}(\mathscr{H})$ denotes the set of bounded linear operators in $\mathscr{H}$.

A fully closed partial O^*-algebra $\mathfrak{M}$ with the properties $\mathfrak{M} = \mathfrak{M}''_{w\sigma}$ and $\mathfrak{M}'_w\mathscr{D}\subseteq\mathscr{D}$ is called a *partial GW*-algebra*.

The main problem, when a †-invariant subset $\mathfrak{R}$ of $\mathscr{L}^\dagger(\mathscr{D},\mathscr{H})$ is given, is how to construct a partial GW^*-algebra containing $\mathfrak{R}$. Of course, the definition itself suggests looking at bicommutants; there are, however, as expected when dealing with unbounded operators, several problems with domains. The following result, that we will use later, provides the answer.

Proposition 2.1: Let $\mathfrak{R}$ be a †-invariant subset of $\mathscr{L}^\dagger(\mathscr{D},\mathscr{H})$. Then the following statements are equivalent:

(1) $\widehat{\mathfrak{R}''_{w\sigma}}$ is a partial GW^*-algebra on $\hat{\mathscr{D}}(\mathfrak{R}''_{w\sigma})$.
(2) $\mathfrak{R}''_{w\sigma} = [(\mathfrak{R}'_w)']^{s^*} = \{X \in \mathscr{L}^\dagger(\mathscr{D},\mathscr{H}); X \text{ is affiliated with } (\mathfrak{R}'_w)'\}$.
(3) $\mathfrak{R}'_w\hat{\mathscr{D}}(\mathfrak{R}''_{w\sigma}) = \hat{\mathscr{D}}(\mathfrak{R}''_{w\sigma})$.

Then, as is clear from the above discussion, a partial GW^*-algebra $\mathfrak{M}$ is a fully closed partial *-algebra which coincides with the s^*-closure of its bounded part $\mathfrak{M}_b$. This is, indeed, a possible alternative definition. For further details we refer to Refs. 30–32.

III. COMPATIBLE OBSERVABLES AND COMPLETENESS

As well as in Ref. 18, we will use Naimark's theory of extensions of symmetric operators in Hilbert space $\mathscr{H}$ to a *larger* Hilbert space $\tilde{\mathscr{H}}\supset\mathscr{H}$ and the related extensions of a POV measure $B(\Theta)$ [$\Theta \in \mathscr{B}(\mathbb{R}^n)$—the family of Borel sets in $\mathbb{R}^n$) in $\mathscr{H}$ to a PV measure $E(\Theta)$ in $\tilde{\mathscr{H}}$.[15,33] We will use also the extension of a semigroup of isometries $V(t)$ in $\mathscr{H}$ to a group $U(t)$ of unitary operators in $\tilde{\mathscr{H}}$.[15,18,34]

For reader's convenience, we give here first some useful statements, analogous to those presented in Ref. 18. In view of their physical meaning, discussed in the Introduction, we will often term self-adjoint or maximal symmetric operators as self-adjoint or maximal symmetric *observables*.

Let us now consider the maximal symmetric operators S_i and their generalized (i.e., POV) spectral measures $\{B_i(\Delta),\ i=1,\ldots,n;\ \Delta\in\mathscr{B}(\mathbb{R})\}$.

Definition 3.1: Let $\mathscr{S}=\{S_1,\ldots,S_n\}$ be a set of maximal symmetric operators. The set $\mathscr{S}$ is called *strongly commuting* if every pair S_i, S_j of elements of $\mathscr{S}$ commute strongly, i.e., the isometry semigroups that S_i and S_j, respectively, generate commute.

Definition 3.2: The operators $S_1,\ldots,S_n$ are called *operationally compatible*, if there exists a POV measure $B(\Theta)$, $\Theta \in \mathscr{B}(\mathbb{R}^n)$ (called the joint spectral measure) such that for any n-tuple $\Delta_1,\ldots,\Delta_n\in\mathscr{B}(\mathbb{R})$ one has $B_i(\Delta_i)=B(\mathbb{R}\times\cdots\times\Delta_i\times\ \mathbb{R}\times\cdots\times\mathbb{R})$.

Lemma 3.3: Let $\{S_1,\ldots,S_n\}$ be operationally compatible maximal symmetric observables in $\mathscr{H}$. Then $S_1,\ldots,S_n$ admit self-adjoint extensions $A_1,\ldots,A_n$, respectively, in one and the same larger Hilbert space $\tilde{\mathscr{H}}$, and A_i commute pairwise strongly, i.e., their spectral projections commute.

Lemma 3.4: Let $\{S_1,\ldots,S_n\}$ be a set of strongly commuting maximal symmetric observables in $\mathscr{H}$. There exist self-adjoint extensions $A_1,\ldots,A_n$ in one and the same larger Hilbert space $\tilde{\mathscr{H}}$ which commute pairwise strongly.

The link between operational compatibility of observables and commutativity of the representing operators is provided by the following.

Proposition 3.5: For a set $\{S_1,\ldots,S_n\}$ of maximal symmetric operators the statements

(i) $S_1,\ldots,S_n$ commute pairwise strongly (i.e., via the generated semigroups) and
(ii) $S_1,\ldots,S_n$ are operationally compatible

are equivalent.

Proof: We only sketch the proof of (ii)⇒(i). Set $B(\Delta_1,\ldots,\Delta_n)$ for the joint spectral measure of $S_1,\ldots,S_n$. Lemma 3.3 implies the existence of strongly commuting self-adjoint extensions A_i,

$i=1,2,\ldots,n$, in one and the same larger space $\tilde{\mathscr{H}}$. Set $U(t_1,\ldots,t_n)=\Pi_{k=1}^{n}\exp(it_kA_k)$; an application of Proposition 2.7 of Ref. 18 shows that for the semigroups of isometries $V_i(t_i)$ generated by S_i one has

$$V_i(t_i)\subset U(0,\ldots,0,t_i,0,\ldots,0).$$

Then $V_i(t_i)$, $i=1,2\ldots,n$ mutually commute.□

From now on, we will use the term *compatible* for a set $\{S_1,\ldots,S_n\}$ of observables satisfying (i) or (ii) of Proposition 3.5.

A physical example of this situation is provided (see Ref. 18) by the three components of the momentum operator considered on the positive coordinate semi-axes.

In Ref. 18 we made use, for the study of the completeness of a set of compatible observables, of the notion of *semi-Abelian* von Neumann algebra whose definition we repeat here for the reader's convenience.

Definition 3.6: Let $\mathfrak{N}$ be a von Neumann algebra; we say that $\mathfrak{N}$ is *semi-Abelian* if $\mathfrak{N}$ contains two subalgebras $\mathfrak{U}$ and $\mathfrak{B}$ (the component algebras of $\mathfrak{N}$) with the following properties

(a) $\mathfrak{U}$ and $\mathfrak{B}$ are Abelian,
(b) $\mathfrak{U}\cup\mathfrak{B}$ generates $\mathfrak{N}$,
(c) $\mathfrak{U}=\mathfrak{B}^*$,
(d) $\mathfrak{U}=\mathfrak{U}''$ (resp., $\mathfrak{B}=\mathfrak{B}''$).

Moreover, we say that $\mathfrak{N}$ is maximal semi-Abelian if for anyone of its component algebras, e.g., $\mathfrak{U}$, the equation $\mathfrak{U}=\mathfrak{U}'$ results.

Remark 3.7: In the corresponding definition given in Ref. 18, the condition (d) was omitted. There is no loss of generality in this assumption, since $\mathfrak{U}$, its weak closure, $[\mathfrak{U}]^w$, and $\mathfrak{U}''$ are all component algebras of $\mathfrak{N}$. Still, in Ref. 18 the definition of maximality was given by means of the equality $[\mathfrak{U}]^w=\mathfrak{U}'$, but as is easy to see, the equality $[\mathfrak{U}]^w=\mathfrak{U}'$ implies that $\mathfrak{U}''=\mathfrak{U}'$ and so the maximality in the sense given in Definition 3.6 implies the maximality in the sense of Ref. 18. The converse implication is obvious. Therefore the two definitions are equivalent.

If $\mathscr{S}=\{S_1,S_2,\ldots,S_n\}$ is a set of strongly commuting maximal symmetric operators, then, as shown in Ref. 18, we can consider the von Neumann algebra $\mathfrak{N}$ generated by the isometry semigroups $\{V_1,\ldots,V_n\}$, corresponding respectively to $\{S_1,\ldots,S_n\}$, and by their adjoints $\{V_1^*,\ldots,V_n^*\}$. (We will call $\mathfrak{N}$ the von Neumann algebra generated by $\mathscr{S}$). Then by Definition 3.6, $\mathfrak{N}$ is a semi-Abelian von Neumann algebra, with component algebras $\mathfrak{U}=\{V_1,\ldots,V_n\}''$ and $\mathfrak{B}=\mathfrak{U}^*$. It is worth remarking that $\{V_1,\ldots,V_n\}''$ need not be a *-algebra and that $\mathfrak{N}$ does not coincide, contrary to the self-adjoint case, with the von Neumann algebra generated by the generalized spectral families (i.e., the POV measures) of the operators $S_1,\ldots,S_n$.[35]

Remark 3.8: In Ref. 18 the analysis of the completeness was carried out taking into account the structure of the Abelian component $\mathfrak{U}$ rather than that of the whole algebra $\mathfrak{N}$. For this reason the use of semi-Abelian von Neumann algebras seems to be unnecessary. We prefer to maintain it here for coherence with the language of Ref. 18. One relevant remark is in order: it seems that *many* von Neumann algebras are semi-Abelian. For instance if $\mathfrak{N}$ is generated by two bounded self-adjoint operators A and B, then $\mathfrak{N}$ is semi-Abelian ($\mathfrak{U}$ can be taken to be the Abelian algebra generated by $A+iB$). For this reason $\mathscr{B}(\mathscr{H})$ itself is semi-Abelian when $\mathscr{H}$ is separable, since one may choose A and B as generating two maximal Abelian von Neumann algebras with trivial intersection. We leave the question as to whether there are *non*-semi-Abelian von Neumann algebras and a detailed analysis of the whole question to a future paper.

In Ref. 18 we gave the following definition of complete set of compatible observables (CSCO).

Definition 3.9: A set $\mathscr{S}=\{S_1,\ldots,S_n\}$ of strongly commuting maximal symmetric operators is said to be a CSCO if the semi-Abelian von Neumann algebra generated by $\mathscr{S}$ is maximal.

Adopting the same notations as before, we will now show that this definition of CSCO is close to Dirac's original concept.

Proposition 3.10: If the set $\mathscr{S}=\{S_1,S_2,\ldots,S_n\}$ is a CSCO, then for any maximal symmetric observable S_{n+1} strongly commuting with $\{S_1,S_2,\ldots,S_n\}$, the contraction semigroup V_{n+1} corresponding to S_{n+1} belongs to $\mathfrak{U}=\{V_1,\ldots,V_n\}''$.

Proof: Let $\mathscr{S}=\{S_1,S_2,\ldots,S_n\}$ be a CSCO and $\mathscr{V}=\{V_1,\ldots,V_n\}$; then $\mathscr{S}$ generates a maximal semi-Abelian algebra[18] with component subalgebra $\mathfrak{U}$ equal to $\mathscr{V}''$. Then for the semigroup V_{n+1} corresponding to an additional element S_{n+1} compatible with S_i, $1\leqslant i\leqslant n$, one has $V_{n+1}(t)\in\mathfrak{U}'=\mathfrak{U}$. □

Remark 3.11: The converse of the above proposition is not true, in general. However, we may consider $\mathfrak{U}$ as a component algebra of $\mathfrak{N}=(\mathfrak{U}\cup\mathfrak{U}^*)''$; then, clearly, $\mathfrak{N}'\subset\mathfrak{U}'$ and $\mathfrak{U}'\supset\mathfrak{U}$. Under the additional condition that $\mathfrak{N}'\backslash\mathfrak{U}$ is not empty, if we suppose that $\mathfrak{U}\neq\mathfrak{U}'$, we can find a bounded self-adjoint operator $X\in\mathfrak{U}'\backslash\mathfrak{U}$ (it suffices to take $X\in\mathfrak{N}'\backslash\mathfrak{U}$). For this X one necessarily has $e^{itX}\notin\mathfrak{U}$, for any t. So, X does not commute strongly with $\{S_1,S_2,\ldots,S_n\}$.

IV. THE ALGEBRAIC STRUCTURE OF COMPATIBLE OBSERVABLES

In this section we prove the existence of a domain of C^∞-vectors (dense and invariant) for a CSCO and we show that it generates, in a natural way, a partial algebraic structure on this domain.

Proposition 4.1: Let $\mathscr{S}=\{S_1,\ldots,S_n\}$ be a set of strongly commuting maximal symmetric operators in $\mathscr{H}$. Then there exists in $\mathscr{H}$ a common dense domain $\mathscr{D}$ such that $S_i(\mathscr{D})\subset\mathscr{D}$ for any $i=1,\ldots,n$.

Proof: Let $V_k(t_k)$, $k=1,2,\ldots,n$, be the strongly continuous one-parameter semigroups of isometries corresponding to S_k. Then $V_k(t_k)$ and $V_j(t_j)$ commute, for any k and j. For any $\Phi\in\mathscr{H}$ and $f\in C_0^\infty(\mathbb{R}_+^n)$, where $\mathbb{R}_+^n=\Pi_i^n\{x:x\geqslant 0\}$, define $V(t)=\Pi_k V_k(t_k)$ and set

$$\Phi_f=\int_{\mathbb{R}_+^n} f(t)V(t)\Phi\ dt,$$

where $dt:=dt_1\cdots dt_n$.

Denote as $\mathscr{D}_{\mathscr{S}}$ the set of all linear combinations of Φ_f. Then $\mathscr{D}_{\mathscr{S}}$ is dense in $\mathscr{H}$. Indeed, let $i(t)$ be a function of $C_0^\infty(\mathbb{R}_+^n)$, whose support is contained in the set $K:=\{t=(t_1,\ldots,t_n):|t|\leqslant 1,t_k>0\}$ and with $\int_K i(t)dt=1$. For $\epsilon>0$ we put $i_\epsilon(t)=\epsilon^{-n}i(t/\epsilon)$. Then we have

$$\|\Phi_{i_\epsilon}-\Phi\|=\left\|\int_{\mathbb{R}_+^n} i_\epsilon(t)(V(t)\Phi-\Phi)dt\right\|\leqslant\int_{\mathbb{R}_+^n} i_\epsilon(t)dt\ \sup_{t\in\epsilon K}\|V(t)\Phi-\Phi\|\to 0,$$

as $\epsilon\to 0$ since each V_k is strongly continuous.

We will now prove that each S_i, $i=1,\ldots,n$, leaves $\mathscr{D}_{\mathscr{S}}$ invariant.

For each $f\in C_0^\infty(\mathbb{R}_+^n)$, we can define a linear operator $U(f)$ by

$$U(f)\Phi=\Phi_f,\quad \Phi\in\mathscr{H}.$$

Then $U(f)$ is bounded and $\|U(f)\|\leqslant\|f\|_1$ (the L^1-norm on $\mathbb{R}_+^n$).
A simple computation shows that

$$V(t)U(f)\Phi=U(f_t)\Phi,\quad \forall\Phi\in\mathscr{H},$$

where $f_t(s)=f(s-t)$. Then,

$$iS_j\Phi_f = \lim_{t_j\to 0} \frac{V_j(t_j)-\mathbb{I}}{t_j}\,\Phi_f = \lim_{t_j\to 0} \frac{U(f_{t_{[j]}}-f\,)}{t_j}\,\Phi,$$

where $t_{[j]}=(0,\ldots,t_j,\ldots,0)$.
Now,

$$\left\| \frac{U(f_{t_{[j]}}-f\,)}{t_j}\,\Phi + U(\partial_j f\,)\Phi \right\| \leqslant \left\| \frac{f_{t_{[j]}}-f}{t_j} + \partial_j f \right\|_1 \|\Phi\| \to 0$$

because of the existence of $\partial_j f$ in the L^1-sense for $f\in C_0^\infty(\mathbb{R}^n_+)$. □

Lemma 4.2: Let S be a maximal symmetric operator in $\mathscr{H}$ and A a self-adjoint extension of S in a larger Hilbert space $\tilde{\mathscr{H}}$; then

$$D(S^k)=\mathscr{H}\cap D(A^k), \quad k=1,2\ldots,$$

and

$$S^k f = A^k f, \quad \forall f\in D(S^k).$$

Thus

$$\mathscr{D}^\infty(S)=\mathscr{H}\cap\mathscr{D}^\infty(A).$$

Proof: Clearly

$$\mathscr{H}\cap D(A^k)=\{f\in\mathscr{H}\cap D(A^{k-1}):A^{k-1}f\in D(A)\}. \tag{4}$$

Since S is maximal symmetric and A extends S, then

$$D(S)=\mathscr{H}\cap D(A) \tag{5}$$

and

$$Sf=Af, \quad \forall f\in D(S).$$

To proceed by induction assume that

$$D(S^{k-1})=\mathscr{H}\cap D(A^{k-1}) \tag{6}$$

and

$$S^{k-1}f=A^{k-1}f, \quad \forall f\in D(S^{k-1}). \tag{7}$$

Then from (4), (6), and (7), we obtain

$$\mathscr{H}\cap D(A^k)=\{f\in D(S^{k-1}):S^{k-1}f\in D(A)\}. \tag{8}$$

The statement then follows from the fact that for any k: $\operatorname{Ran} S^{k-1}\subseteq\mathscr{H}$. The equality $S^k f=A^k f$, $\forall f\in D(A^k)$ is now evident. □

Proposition 4.3: Let $\mathscr{S}=\{S_1,\ldots,S_n\}$ be a set of compatible maximal symmetric operators. Let

$$\mathscr{D}^\infty(\mathscr{S})=\bigcap_{i=1}^n \mathscr{D}^\infty(S_i),$$

where $\mathscr{D}^\infty(S_i)=\cap_{k\geqslant 1}D(S_i^k)$. Then the following statements hold:

(i) $\mathscr{D}^\infty(\mathscr{S})$ is a common invariant dense domain for all the elements of $\mathscr{S}$.
(ii) $S_iS_jf=S_jS_if\forall f\in\mathscr{D}^\infty(\mathscr{S})$.
(iii) If one, at least, of the operators $S_i\in\mathscr{S}$ is not essentially self-adjoint on $\mathscr{D}^\infty(\mathscr{S})$, then the Nelson operator $\Delta=\Sigma_{i=1}^n S_i^2[\mathscr{D}^\infty(\mathscr{S})$ cannot be essentially self-adjoint.

Proof: (i) By Lemma 4.1, $\mathscr{D}^\infty(\mathscr{S})$ is dense and it is clearly a common domain for all elements of $\mathscr{S}$. It remains to prove the invariance. Let $\mathscr{A}=\{A_1,\ldots,A_n\}$ be the family of commuting self-adjoint operators extending $\mathscr{S}=\{S_1,\ldots,S_n\}$ to a common larger Hilbert space $\tilde{\mathscr{H}}$ (Lemma 3.3). Then by Lemma 4.2 we obtain

$$\mathscr{D}^\infty(\mathscr{S})=\mathscr{H}\cap\mathscr{D}^\infty(\mathscr{A}),$$

where $\mathscr{D}^\infty(\mathscr{A})=\cap_{i=1}^n\mathscr{D}^\infty(A_i)$; by Ref. 21, Proposition 2.1 $\mathscr{D}^\infty(\mathscr{A})$ is left invariant by A_i, $i=1,\ldots,n$.
(ii) Part (ii) follows immediately from the strong commutativity of the set $\mathscr{A}$ extending $\mathscr{S}$.
(iii) Suppose, on the contrary, that Δ is essentially self-adjoint on $\mathscr{D}^\infty(\mathscr{S})$. Then, from Ref. 36, p. 351, all the elements of $\mathscr{S}$ would be essentially self-adjoint on the same domain. □

Remark 4.4: In Ref. 21 it was proved also that if all elements of $\mathscr{S}$ are self-adjoint, then Δ is essentially self-adjoint on $\mathscr{D}^\infty(\mathscr{S})$.

We notice also that for $n=1$, Proposition 4.3 says that any maximal symmetric operator has a dense set of C^∞ vectors. This is a particular case of Proposition 1.6.1 of Ref. 22. Furthermore, for $n>1$ and compatible $S_1,\ldots,S_n$, Proposition 4.3 asserts the existence of a common dense set of C^∞-vectors for all S_i.

Making use of the previous proposition and by some simple topological considerations, we obtain the following.

Proposition 4.5: The set $\mathscr{S}$ generates a closed Abelian O^*-algebra $\mathfrak{U}(\mathscr{S})$ on $\mathscr{D}^\infty(\mathscr{S})$.

Proof: Were $\mathfrak{U}(\mathscr{S})$ not closed on $\mathscr{D}^\infty(\mathscr{S})$, then it would admit a closure $\tilde{\mathfrak{U}}(\mathscr{S})$ to a larger domain $\tilde{\mathscr{D}}^\infty(\mathscr{S})$. This domain would be invariant for each S_i, $i=1,\ldots,n$, and therefore

$$\tilde{\mathscr{D}}^\infty(\mathscr{S})\subseteq\mathscr{D}^\infty(S_i)$$

for $i=1,\ldots,n$. This contradicts the assumption. □

Clearly, apart from closedness, the same statement remains true on the domain $\mathscr{D}_{\mathscr{S}}$ defined in the proof of Proposition 4.1.

The following lemma generalizes to maximal symmetric operators a well-known statement which holds true for self-adjoint ones. The proof is completely analogous and is therefore omitted.

Lemma 4.6: Let $V(t)$, $t\geqslant 0$, be the isometry semigroup generated by a maximal symmetric operator S. If $X\in\mathfrak{B}(\mathscr{H})$ commutes with $V(t),\forall t\geqslant 0$, then

$$X:D(S^n)\to D(S^n)\quad\forall n=1,2,\ldots,$$

and

$$S^nXf=XS^nf\quad\forall f\in D(S^n).$$

Thus X leaves $\mathscr{D}^\infty(S)$ invariant and commutes with the O^*-algebra generated by S on $\mathscr{D}^\infty(S)$.

Proposition 4.7: Let $\mathscr{S}=\{S_1,\ldots,S_n\}$ be a set of compatible maximal symmetric operators. Let $\mathfrak{N}$ be the von Neumann algebra generated by the isometry semigroups $\{V_1(t_1),\ldots V_n(t_n)\}$ and by their adjoints [where $V_i(t_i)$ is the semigroup generated by S_i]. Then $\mathfrak{N}''_{w\sigma}$ is a partial GW^*-algebra on $\mathscr{D}^\infty(\mathscr{S})$. Moreover, $\mathfrak{N}''_{w\sigma}$ is the minimal partial GW^*-algebra on $\mathscr{D}^\infty(\mathscr{S})$ containing $\mathscr{S}$.

Proof: From Ref. 31, Corollary 4.15, $\widehat{\mathfrak{N}''_{w\sigma}}$ is a partial GW^*-algebra on $\widehat{\mathscr{D}(\mathfrak{N}''_{w\sigma})}$, where

$$\widehat{\mathscr{D}(\mathfrak{N}''_{w\sigma})} = \bigcap_{X \in \mathfrak{N}''_{w\sigma}} D(\bar{X}).$$

By Lemma 4.6, $\mathscr{S} \subset \mathfrak{N}''_{w\sigma}$ [or, also, $\mathfrak{U}(\mathscr{S}) \subset \mathfrak{U}''_{w\sigma}$] and thus we obtain

$$\mathscr{D}^\infty(\mathscr{S}) \subseteq \widehat{\mathscr{D}(\mathfrak{N}''_{w\sigma})} = \bigcap_{X \in \mathfrak{N}''_{w\sigma}} D(\bar{X}) \subset \bigcap_{X \in \mathfrak{U}(\mathscr{S})} D(\bar{X}) \subset \mathscr{D}^\infty(\mathscr{S}),$$

where the last inclusion follows from Proposition 4.5.

Therefore, $\mathfrak{N}''_{w\sigma}$ is fully closed. To prove the second part, recall that by 2.1, we have

$$\mathfrak{N}''_{w\sigma} = [\mathfrak{N}]^{\natural *} = \{X \in \mathscr{L}^\dagger(\mathscr{D}, \mathscr{H}); \bar{X}\, \eta \mathfrak{N}\},$$

where $\bar{X}\, \eta \mathfrak{N}$ means that $\bar{X}$ is affiliated with $\mathfrak{N}$. Since (Lemma 4.6) $\mathfrak{N}$ is the smallest von Neumann algebra to which all S_is are affiliated, for any other partial GW^*-algebra $\mathfrak{R}$ containing $\mathscr{S}$ we would have $\mathfrak{R}_b \supset \mathfrak{N}$ and therefore $[\mathfrak{N}]^{\natural *} \subset [\mathfrak{R}_b]^{\natural *} = \mathfrak{R}$. This implies that $\mathfrak{N}''_{w\sigma}$ is the minimal partial GW^*-algebra containing all S_is. □

Remark 4.8: The previous proposition implies, clearly, that $\mathfrak{N}''_{w\sigma}$ is the minimal partial GW^*-algebra containing the Abelian O^*-algebra $\mathfrak{U}(\mathscr{S})$. Nevertheless, $\mathfrak{N}''_{w\sigma}$ is not Abelian, in general. This fact contrasts, evidently, the well-known situation of bounded operator algebras. If $\mathscr{S}$ consists only of self-adjoint operators, then as shown in Ref. 21, $\mathfrak{N}''_{w\sigma}$ is then an Abelian SV^*-algebra on $\mathscr{D}^\infty(\mathscr{S})$ and it is an O^*-algebra itself. This depends, essentially, on the fact that $\mathfrak{U}(\mathscr{S})$ is standard (i.e., each symmetric element is essentially self-adjoint) (Ref. 23, Proposition 6.4).

Proposition 4.9: For the partial GW^*-algebra $\mathfrak{N}''_{w\sigma}$ generated by $\mathscr{S}$ there exist two partial subalgebras $\mathfrak{U}^{(1)}$ and $\mathfrak{B}^{(1)}$ (called the component partial algebras) such that

(a) $\mathfrak{B}^{(1)} = \mathfrak{U}^{(1)\dagger}$;
(b) $\mathfrak{U}^{(1)} \subseteq (\mathfrak{U}_b^{(1)})'_\sigma$ (where $\mathfrak{U}_b^{(1)}$ denotes the bounded part of $\mathfrak{U}^{(1)}$);
(c) $\mathfrak{N}''_{w\sigma}$ is the smallest partial GW^*-algebra on $\mathscr{D}^\infty(\mathscr{S})$ containing $\mathfrak{U}^{(1)} \cup \mathfrak{B}^{(1)}$.

In this case we say that $\mathfrak{N}''_{w\sigma}$ is *semi-Abelian*.

Proof: Let $\mathfrak{N}$ be the semi-Abelian von Neumann algebra generated by $\mathscr{S}$. Then $\mathfrak{N}$ has two component algebras $\mathfrak{U}$ and $\mathfrak{B}$ satisfying the conditions of Definition 3.6. Set $\mathfrak{U}^{(1)} = \mathfrak{U}''_{w\sigma}$ and $\mathfrak{B}^{(1)} = \mathfrak{U}^{(1)\dagger}$.

First we show that $\mathfrak{U}^{(1)}$ is a partial algebra (in the sense that if $X \square Y$ is well defined for some $X, Y \in \mathfrak{U}^{(1)}$, then $X \square Y \in \mathfrak{U}^{(1)}$).

Indeed, because of Lemma 4.6, we have $\mathfrak{U}'_w \mathscr{D}^\infty(\mathscr{S}) = \mathscr{D}^\infty(\mathscr{S})$. For this reason, for any $X \in \mathfrak{U}''_{w\sigma}$ and $C \in \mathfrak{U}'_w$, $XCf = \bar{C}Xf$, $\forall f \in \mathscr{D}^\infty(\mathscr{S})$, results. Therefore, if $X, Y \in \mathfrak{U}^{(1)}$ and $X \square Y$ is well defined, we obtain, for any $C \in \mathfrak{U}'_w$ and $f, g \in \mathscr{D}^\infty(\mathscr{S})$,

$$\begin{aligned}\langle (X \square Y) f, C^\dagger g \rangle &= \langle X^\dagger * Y f, C^\dagger g \rangle \\ &= \langle Yf, X^\dagger C^\dagger g \rangle = \langle Yf, C^* X^\dagger g \rangle = \langle \bar{C} Y f, X^\dagger g \rangle = \langle YCf, X^\dagger g \rangle \\ &= \langle Cf, Y^* X^\dagger g \rangle = \langle Cf, Y^\dagger \square X^\dagger g \rangle.\end{aligned}$$

Hence $X \square Y \in \mathfrak{U}''_{w\sigma} = \mathfrak{U}^{(1)}$.

The statement (b) follows from the fact that $\mathfrak{U} \subseteq \mathfrak{U}'_w$ implies $\mathfrak{U}''_{w\sigma} \subseteq \mathfrak{U}'_\sigma$ and from the equality $\mathfrak{U} = \mathfrak{U}''_{ww} = (\mathfrak{U}''_{w\sigma})_b$.

To prove (c), let us consider another partial GW^*-algebra $\mathfrak{P}$ containing $\mathfrak{U}^{(1)} \cup \mathfrak{B}^{(1)}$; then, $\mathfrak{P}_b \supset \mathfrak{N}$, where $\mathfrak{P}_b$ denotes the bounded part of $\mathfrak{P}$. Since $\mathfrak{N}$ is the smallest von Neumann algebra containing $\mathfrak{U} \cup \mathfrak{B}$, then $\mathfrak{N}''_{w\sigma} = [\mathfrak{N}]^{\prime *} \subset [\mathfrak{P}_b]^{\prime *} = \mathfrak{P}$.□

Remark 4.10: The condition (b), i.e., $\mathfrak{U}^{(1)} \subseteq (\mathfrak{U}_b^{(1)})'_\sigma$, does not imply that $\mathfrak{U}^{(1)}$ is Abelian but only that $\mathfrak{U}_b^{(1)}$ is Abelian. We recall that a partial algebra $\mathfrak{U}^{(1)}$ is Abelian if for $X, Y \in \mathfrak{U}^{(1)}$ such that $X \square Y$ is well defined, also $Y \square X$ is well defined and $X \square Y = Y \square X$. This is, indeed, a quite strong requirement.

In the self-adjoint case, the standardness[21] of the corresponding SV^*-algebra $\mathfrak{N}''_{w\sigma}$ implies the equality $\mathfrak{U}^{(1)} = (\mathfrak{U}_b^{(1)})'_\sigma$ and therefore the Abelianness of both $\mathfrak{U}^{(1)}$ and $\mathfrak{N}''_{w\sigma}$.

Making use of the previous proposition, one can easily prove the following.

Proposition 4.11: The partial GW^*-algebra $\mathfrak{M}$ generated by $\mathscr{S}$ is semi-Abelian if, and only if, its bounded part $\mathfrak{M}_b$ is a semi-Abelian von Neumann algebra whose component algebras can be taken to be the bounded parts of $\mathfrak{U}^{(1)}$ and $\mathfrak{B}^{(1)}$.

Definition 4.12: Let $\mathfrak{M}$ be a semi-Abelian partial GW^*-algebra on $\mathscr{D}$. We say that $\mathfrak{M}$ is *maximal* semi-Abelian if $\mathfrak{M}$ is not properly contained in any other semi-Abelian partial GW^*-algebra on $\mathscr{D}$.

The following proposition shows the complete equivalence of the *bounded* and unbounded approaches to the problem of complete sets of compatible observables as in the self-adjoint case.[21]

Proposition 4.13: Let $\mathfrak{N}$ be the von Neumann algebra generated by a set $\mathscr{S}$ of strongly commuting maximal symmetric operators. The following statements are equivalent:

(i) $\mathfrak{N}$ is a maximal semi-Abelian von Neumann algebra;
(ii) $\mathfrak{N}''_{w\sigma}$ is a maximal semi-Abelian partial GW^*-algebra on $\mathscr{D}^\infty(\mathscr{S})$.

Proof: (i)⇒(ii) Let $\mathfrak{R} \supset \mathfrak{N}''_{w\sigma}$ be a partial GW^*-algebra on $\mathscr{D}^\infty(\mathscr{S})$. Then its bounded part $\mathfrak{R}_b$ is semi-Abelian and contains $\mathfrak{N}$; this implies that $\mathfrak{R}_b = \mathfrak{N}$ and so $\mathfrak{R} = \mathfrak{N}''_{w\sigma}$.

(ii)⇒(i) If $\mathfrak{O}$ is a semi-Abelian von Neumann algebra containing $\mathfrak{N}$, then $\mathfrak{O}''_{w\sigma}$ is a semi-Abelian partial GW^*-algebra on $\mathscr{D}^\infty(\mathscr{S})$ which contains $\mathfrak{N}''_{w\sigma}$, by construction. Then $\mathfrak{O}''_{w\sigma} = \mathfrak{N}''_{w\sigma}$ and therefore $\mathfrak{O} = \mathfrak{N}$. □

Propositions 4.7, 4.9, and 4.13 express precisely what we mean when we say that a CSCO (consisting, in general, of non-self-adjoint observables) gives rise naturally to a partial algebraic structure. In the self-adjoint case (bounded or unbounded setting) one considers the unitary groups U_i generated by the self-adjoint observables A_i, $i = 1,2,\ldots,n$. Clearly the von Neumann algebra $\mathfrak{N}$ generated by U_i, $i = 1,2,\ldots,n$, is Abelian, as well as the smallest GW^*-algebra generated by the CSCO which, moreover coincides with an Abelian O^*-algebra. Furthermore, Proposition 4.13 exhibits the density of the semi-Abelian von Neumann algebra generated by the non-self-adjoint observables S_i, $i = 1,\ldots,n$, in the corresponding partial GW^*-algebra. This fact generalizes the similar result obtained in Ref. 21 in the self-adjoint case.

We conclude this section with a discussion on the relations between strong commutativity of observables and their algebraic commutativity on a dense domain. We begin with discussing a Nelson-type example which arises from a concrete physical situation.

Example: Consider a particle which moves in a finite-size crystal medium and has different masses m_1, m_2, m_3 along the coordinate axes x, y, z, due to the many-body system effects. Thus one has a quantum mechanical particle moving in a potential well with infinitely high walls along the boundary $\partial\Omega$ of a three-dimensional connected domain Ω. For the operators p^2 and E corresponding, respectively, to the squared momentum and to the energy, one has

$$p^2 = p_x^2 + p_y^2 + p_z^2,$$

$$E=\frac{p_x^2}{2m_x}+\frac{p_y^2}{2m_y}+\frac{p_z^2}{2m_z},$$

where

$$p_x^2=-\hbar^2\frac{\partial^2}{\partial x^2},\quad p_y^2=-\hbar^2\frac{\partial^2}{\partial y^2},\quad p_z^2=-\hbar^2\frac{\partial^2}{\partial z^2}.$$

The operators p^2 and E are defined on the following domain $\mathscr{D}$ of C^∞-functions with Dirichlet's boundary condition

$$\{u\in C^\infty(\overline{\Omega}):u\restriction\partial\Omega=0\}.$$

Let $C_0^\infty(\Omega)$ denote the set of all infinitely differentiable functions with compact support in Ω. As known,[37] the Friedrichs self-adjoint extensions, $\widetilde{p_0^2}$ and $\widetilde{E_0}$, where

$$p_0^2=(p^2)\restriction C_0^\infty(\Omega),\quad E_0=E\restriction C_0^\infty(\Omega),$$

commute strongly if and only if Ω is a parallelepiped with sides parallel to the coordinate axes. Furthermore, p^2 and E are essentially self-adjoint on $\mathscr{D}$ and for the closures $\overline{E}$ and of $\overline{p^2}$ one has $\overline{E}=\widetilde{E_0}$, $\overline{p^2}=\tilde{p}_0^2$.[37] The operators $\overline{E}$ and $\overline{p^2}$ are considered to represent, respectively, the physical observables of energy and squared momentum.

Suppose now that Ω is not a parallelepiped. Then $S_1\equiv\overline{E}$ and $S_2\equiv\overline{p^2}$ commute on $\mathscr{D}_S=C_0^\infty(\Omega)$ but the groups, V_1 and V_2, corresponding respectively, to S_1 and S_2, do not generate an Abelian von Neumann algebra (considered as a special instance of the semi-Abelian case). Thus S_1 and S_2 are not compatible.[37] Moreover we check that there are no self-adjoint extensions $S_1^+\supset S_1$ and $S_2^+\supset S_1$ in some bigger Hilbert space $\mathscr{H}^+\supset\mathscr{H}$ which commute strongly. Assume on the contrary that

$$E^+(\Delta)G^+(\Delta')=G^+(\Delta')E^+(\Delta) \tag{9}$$

holds for the extensions of the generalized spectral measures $E(\Delta)$ and $G(\Delta')$ of S_1 and S_2 correspondingly. The restriction $S_1^+\restriction\mathscr{H}$ is defined on $L=\{\varphi\in\mathscr{H}:S_1^+\varphi\in\mathscr{H}\}$. Since S_1 is the minimal closed extension of S_1, then $S_1\subset S_1^+$. Moreover since $G(S_1^+)\cap\mathscr{H}\times\mathscr{H}$ [where $G(S_1^+)$ denotes the graph of S_1^+] is closed and S_1 is self-adjoint, one has $S_1^+\restriction\mathscr{H}=S_1$. Due to the invariance of L under the self-adjoint operator S_1^+ and since $S_1^+\restriction\mathscr{H}$ is also self-adjoint, it follows for the orthogonal projection $P:\mathscr{H}^+\to\mathscr{H}$ that $PS_1^+=S_1^+P$. Hence S_1^+ is an orthogonal sum $S_1^+=S_1\oplus S_1^\perp$ and similarly $S_2^+=S_2\oplus S_2^\perp$. Then Eq. (9) would imply strong commutativity of S_1 and S_2, which contradicts the choice of Ω.

Due to the equivalence of strong commutativity and operational commutativity (Proposition 3.5) one restates the above result as follows: for $E(\Delta)$ and $G(\Delta)$ there is no joint POV measure $M(\Delta\times\Delta')$, $\Delta\times\Delta'\subseteq R^1\times R^1$ such that $M(\Delta\times R^1)=F(\Delta)$ and $M(R^1\times\Delta')=G(\Delta')$.

In view of this kind of counterexample, we discuss below sufficient conditions for a set $\mathscr{S}=\{S_i,i\in I\}$ of algebraically commuting maximal symmetric observables to be compatible.

Let all $S_j\in\mathscr{S}$ be defined on a common invariant and dense domain $\mathscr{D}_S\in\mathscr{H}$. Without loss of generality, we suppose that $i\in\rho(S_j)\forall j=1,\ldots,n$. With this choice, we may introduce the skew-symmetric operators $T_j=iS_j$, $j\in I$, and denote $\mathscr{D}_{i,j}^{n,m}=(1-\epsilon_iT_i)^n(1-\epsilon_jT_j)^m\mathscr{D}_S$, $\epsilon_i,\epsilon_j>0$.

We say that $\mathscr{S}$ is a regular set on $\mathscr{D}_S$ if for every pair of observables S_i, $S_j\in\mathscr{S}$ and any $\epsilon_i>0$, $\epsilon_j>0$ there exists an integer $N>0$ such that for all integers n, $m>N$, $\mathscr{D}_{i,j}^{n,m}$ is dense in $\mathscr{H}$.

Proposition 4.14: Let $\mathscr{S}$ be a regular set of maximal symmetric observables S_j, $j=1,2,\ldots,m$, commuting algebraically, i.e., $S_jS_k=S_kS_j$ on a common dense and invariant domain $\mathscr{D}_S$. Then the semigroups V_j corresponding to S_j commute and the von Neumann algebra $\mathfrak{N}$ generated by $\{V_j : j\in I\}$ is semi-Abelian.

Proof: It is sufficient to check that V_i, V_j for $i\neq j$ commute and thus they generate one of the Abelian component algebras of $\mathfrak{N}$. In the following we set

$$\left(1-\frac{t_j}{n}\,T_j\right)^n \equiv R(t_j,n)\equiv R_{j,n},$$

thus omitting the t_j dependence as unessential for the argument. Recall that, due to the maximality of S_j, one has $\mathrm{Ran}(1-\epsilon_jT_j)=\mathscr{H}$. Furthermore, according to Hille–Yosida theorem on semigroups,[38] for any $\epsilon_j>0$, $(1-\epsilon_jT_j)^{-1}$ is bounded and

$$\lim_{n\to\infty}\left(1-\frac{t_j}{n}\,T_j\right)^n \equiv \lim_{n\to\infty} R_{j,n}^{-1}f=V_j(t)f$$

in the norm topology for $f\in D(T_j)$. Set $g_i\equiv R_{i,n}f$ where $f\in\mathscr{D}_S$. The commutativity assumption written for any power $n=k$, $l=1,2,\ldots$, in $R_{i,n}, R_{j,n}$, implies

$$R_{i,k}R_{j,l}f=R_{j,l}R_{i,k}f, \quad f\in\mathscr{D}_S.$$

Hence,

$$R_{i,k}R_{j,l}R_{i,k}^{-1}g_i=R_{j,l}g_i,$$

i.e.,

$$R_{j,l}R_{i,k}^{-1}g_i=R_{i,k}^{-1}R_{j,l}g_i.$$

A repetition of the argument using this time $R_{j,l}g_i=g_j$ gives

$$R_{i,k}^{-1}R_{j,l}^{-1}g_j=R_{j,l}^{-1}R_{i,k}^{-1}g_j, \tag{10}$$

where $g_j\in\mathscr{D}_{i,j}^{n,m}$

Due to the regularity of $\mathscr{S}$ and to the boundedness of $R_{m,n}^{-1}$ (since each S_m is maximal), the last equation holds for an arbitrary vector in $\mathscr{H}$. Since the commutativity property is preserved by taking strong limits of operators, then Eq. (10) implies that V_i, V_j commute. □

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Topological sectors and measures on moduli space in quantum Yang–Mills on a Riemann surface

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Previous path integral treatments of Yang–Mills on a Riemann surface automatically sum over principal fiber bundles of all possible topological types in computing quantum expectations. This paper extends the path integral formulation to treat separately each topological sector. The formulation is sufficiently explicit to calculate Wilson line expectations exactly. Further, it suggests two new measures on the moduli space of flat connections, one of which proves to agree with the small-volume limit of the Yang–Mills measure. © *1996 American Institute of Physics.* [S0022-2488(96)00803-5]

I. INTRODUCTION

In Refs. 1 and 2, we use the path integral formalism to evaluate quantum expectations of Wilson lines in the Yang–Mills theory on $G=\mathrm{SU}(N)$ product bundles over Riemann surfaces of any genus. Other approaches to these expectations include Sengupta's stochastic quantization of Ref. 3 and Blau and Thompson's use of the Nikolai map to simplify the gauge-fixed path integral in Ref. 4. Witten, in Ref. 5, derives these expectations combinatorially and via a Hilbert-space approach using axioms of quantum field theory for any simple Lie group G. He notes that these results, by contrast with an approach based on Verlinde's formula, automatically sum over all topological types. In the more recent treatment of Ref. 6, he describes how to modify his Hilbert space approach to treat separately each topological sector. Likewise, in Refs. 7 and 8, Sengupta extends the stochastic quantization to nonsimply connected G in a manner which treats separately each topological sector.

In this paper, we analyze the path integral formulation of Yang–Mills on a principal G-bundle of fixed topological type. While doing so, we augment Witten's results on the partition function by including the insertion of Wilson lines. These agree with Sengupta's recent results. Our main focus, however, is on the path integral itself. There is a recognized scarcity of field theories wherein the path integral can be evaluated (or interpreted) nonperturbatively to obtain something approaching a well-defined measure on configuration space. With the present extension of the detailed account of how to perform such an evaluation (in a manifestly gauge-invariant fashion), we hope to contribute to the eventual rigorous understanding of gauge-theoretic path integration.

As an immediate benefit, in addition to the above-mentioned extension of Witten's results, we obtain new measures on the moduli space of flat connections. For genus $g\geqslant 1$, the moduli space, $\mathscr{M}$ of (irreducible) flat connections is a finite-dimensional manifold. Witten uses the small-volume limit of Yang–Mills to compute the volume of $\mathscr{M}$, which he shows agrees with that defined by the symplectic volume form on $\mathscr{M}$. In Ref. 9, Forman extends this agreement to one between measures on $\mathscr{M}$. Our approach suggests two new measures on $\mathscr{M}$. We show that one of these, which was arrived at independently by King and Sengupta in Ref. 10, is equivalent to the small-volume limit of the Yang–Mills measure.

This paper is organized as follows: Section II gives a brief summary of results for $G=\mathrm{SU}(N)$ product bundles. Section III describes the modifications required to keep track of individual

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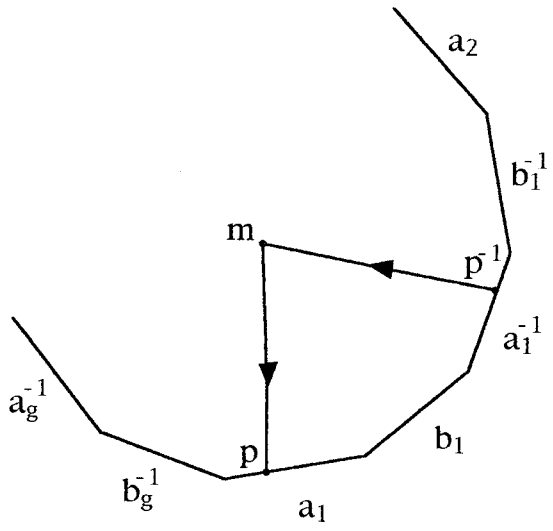

FIG. 1. A typical radial path.

topological sectors in treating bundles with nontrivial topology. Section IV introduces the new measures on $\mathscr{M}$ and compares them with the small-volume limit of the Yang–Mills measure.

II. REVIEW OF THE PRODUCT CASE

Let P be a principal bundle with symmetry group G over a Riemann surface M with a base point $m \in M$. Let $\mathscr{A}$ denote the space of connections on P, and let $\mathscr{G}_m$ denote the group of gauge transformations which are the identity on the fiber over m. In Ref. 2, we describe $\mathscr{A}/\mathscr{G}_m$ as itself a principal bundle with affine-linear fiber over $\mathrm{Path}^{2g} G$, the space of $2g$-tuples of paths in G subject to the following relation on the $4g$ endpoint values $\{\alpha_i(0),\alpha_i(1),\beta_i(0),\beta_i(1)\}_{i=1}^{g}$:

$$\prod_{i=1}^{g} \alpha_i(0)\beta_i(1)^{-1}\alpha_i(1)^{-1}\beta_i(0)=\mathbf{1}. \tag{1}$$

Here, successive factors multiply from the right, and $g \geqslant 1$. The projection ξ: $\mathscr{A}/\mathscr{G}_m \to \mathrm{Path}^{2g} G$ is obtained from holonomy about a certain one-parameter family of closed paths in M determined by a choice of fundamental domain and $2g$ generators $\{a_i,b_i\}_{i=1}^{g}$ of $\pi_1(M)$; the unusual naming of the components of the elements of $\mathrm{Path}^{2g} G$ reflects this genesis. In the genus-0 case, the base space is simply ΩG, the space of based loops in G.

As the holonomies giving rise to ξ enter into the account of topological sectors, we review them in more detail here. Let D be a fundamental domain for M and consider a family of paths from the base point m to the boundary ∂D of D such that every point of M except m lies on exactly one such path. Call these radial paths. Let p be a point of an edge of ∂D corresponding to a generator of the fundamental group of M, and let $p^{-1} \in \partial D$ denote the point corresponding to p in the identification of the edges of ∂D. Consider, for a given connection A, the holonomy of the closed path originating at m, following the radial path to p and returning from the radial path through p^{-1}. See Fig. 1. Relative to a fixed point on the fiber over m, this holonomy determines an element of G which we denote by $\alpha_i(p)$ if p is in the edge corresponding to the generator a_i [$\beta_i(p)$ if the corresponding generator is b_i]. As p varies along its edge, $a_i(p)$ describes a path in G. The $2g$-tuple of such paths in G described as p moves among the edges corresponding to

generators is $\xi([A]) \in \mathrm{Path}^{2g} G$. The endpoint relation reflects the fact that the radial paths to the vertices of ∂D are each traversed twice. In particular, the concatenation of paths whose holonomy is $\Pi_{i=1}^{g} \alpha_i(0)\beta_i(1)^{-1}\alpha_i(1)^{-1}\beta_i(0)$ is a contractible path containing no area, so the holonomy is the identity in accordance with Eq. (1). The fiber of ξ is the affine-linear space $\ker P_r$ of Lie-algebra-valued one-forms which vanish in the radial direction.

In this picture, the path integral for the expectation of some function on $\mathscr{A}/\mathscr{G}_m$, in the Yang–Mills measure μ, is an iterated integral over the linear fibers and the base $\mathrm{Path}^{2g} G$. The integral over the fibers is Gaussian. Performing this integral yields a path integral expression for the push-down measure $\xi_*(\mu)$. The main result of Ref. 2 is that $\xi_*(\mu)$ is the product of Wiener measures on the components $\{\alpha_i, \beta_i\}$ of the elements of $\mathrm{Path}^{2g} G$, conditioned to satisfy the endpoint relation of Eq. (1). This measure is computed by integrating products of heat kernels on G. For example, when $g=1$, the partition function Z is given by

$$Z = \int H(\alpha(0)^{-1}\alpha(1); 2\rho_a) H(\beta(0)^{-1}\beta(1); 2(\rho - \rho_a)),$$

where the integral is over all possible values of $\alpha(0)$, $\alpha(1)$, and $\beta(0)$, and $\beta(1)$ is determined by the relation $\alpha(0)\beta(1)^{-1}\alpha(1)^{-1}\beta(0) = \mathbf{1}$. Here, H is the heat kernel, ρ is the total area of the surface, and ρ_a is the area bounded by the pair of paths whose holonomies determine $\alpha(0)$ and $\alpha(1)$. The convolution property of the heat kernel reduces this expression to

$$Z = \int H((\beta(0)^{-1}\alpha(1)^{-1}\beta(0)\alpha(1); 2\rho)\ \ d\beta(0) d\alpha(1).$$

More generally, for genus $g \geqslant 1$,

$$Z = \int H\left(\prod_{i=1}^{g} x_i y_i x_i^{-1} y_i^{-1}; 2\rho \right)\ dx\ dy. \tag{2}$$

Since

$$H(x;t) = \sum_{\mu}\ (\dim\ \mu)\chi_\mu(x) e^{-2c(\mu)}, \tag{3}$$

where χ_μ is the character of the representation μ, and c denotes the quadratic Casimir, the partition function is the sum

$$Z = \sum_{\mu}\ \frac{e^{-4c_\mu \rho}}{(\dim\ \mu)^{2g-2}}\ .$$

All sums are over the irreducible representations of G. The induction step in reducing the integral expression of Eq. (2) to the above sum is given by a pair of integral (orthogonality) relations among the characters:

$$\int\ \chi_\mu(wxyx^{-1}y^{-1}) dy = \frac{\chi_\mu(wx)\chi_\mu(x^{-1})}{\dim\ \mu},$$

and

$$\int\ \chi_\mu(wx)\chi_\mu(x^{-1}) dx = \frac{\chi_\mu(w)}{\dim\ \mu}\ .$$

This formalism also treats the insertion of Wilson lines. For example, the expectation of an unknotted Wilson line, in the representation μ, given by the trace of holonomy about a noncontractible, homotopically nontrivial loop C, is

$$\langle \mathscr{W}_\mu \rangle = \frac{1}{Z}\int \chi_\mu(x_1) H\left(\prod_{i=1}^{g} x_i y_i x_i^{-1} y_i^{-1}; 2\rho \right) dx\ dy.$$

As a sum over characters, this is

$$\langle \mathscr{W}_\mu \rangle = \frac{1}{Z} \sum_\nu D_{\mu\nu\nu} \frac{e^{-4c_\nu \rho}}{(\dim\ \nu)^{2g-2}},$$

where $D_{\mu\nu\nu}$ is the Clebsch–Gordan coefficient: $\chi_\mu(x)\chi_\nu(x) = \Sigma D_{\mu\nu\sigma}\chi_\sigma(x)$.

To make sense of the path integral, we restricted connections in $\mathscr{A}$ to have finite Yang–Mills action and to satisfy a continuity restriction. Without a refinement of this restriction, bundles P of different topological types are indistinguishable. Thus, although nominally we treated only product bundles, our results, when naively extended to non-simply-connected symmetry groups, correspond to a sum over all topological types.

III. SEPARATING THE TOPOLOGICAL SECTORS

To sort out the topological sectors in the case where G is not simply-connected and $g \geqslant 1$, let $\tilde{G}$ be the covering group of G. Then $G = \tilde{G}/\Gamma$, where Γ is a subgroup $\{\mathbf{1}, u_1, \cdots, u_n\}$ of the finite center of the simply-connected Lie group $\tilde{G}$. The topological type of P can be characterized as follows: Consider holonomy by a flat connection about contractible paths in M. As elements of G, these must be the identity. However, if we lift to $\tilde{G}$, these holonomies, though equal to each other, can be any element u of Γ. This element defines the topological type of P.

The description in Sec. II of ξ goes through as before to yield the same endpoint relation for $\mathrm{Path}^{2g}\ G$. However, if we attempt to lift from G to $\tilde{G}$, the holonomy of the right-hand side of the relation in Eq. (1) will be replaced by the element u of Γ labeling the topological type of P. This follows from the fact that the concatenation contains no area (so the holonomy is the same as for a flat connection) and is contractible. We have thus proven the required refinements of the main theorems of Refs. 1 and 2:

Theorem 3.1: *On a principal fiber bundle of topological type u, $\mathscr{A}/\mathscr{G}_m$ is itself a fiber bundle with projection ξ and affine-linear fiber. The base space $\mathrm{Path}^{2g}\ \tilde{G}$ consists of all 2g-tuples of paths in $\tilde{G}$, subject to the relation*

$$\prod_{i=1}^{g} \alpha_i(0)\beta_i(1)^{-1}\alpha_i(1)^{-1}\beta_i(0) = u. \tag{4}$$

Theorem 3.2: *The push-down measure $\xi_*(\mu)$ is the product of Wiener measures on the components of each element of $\mathrm{Path}^{2g}\ \tilde{G}$, conditioned to satisfy Eq. (4).*

These allow us to calculate the partition function and the expectation of Wilson lines on a bundle of type u over a surface of genus g. For example, the calculation of the partition function for a bundle of type u on the torus ($g=1$) begins as before:

$$Z(u) = \int H(\alpha(0)^{-1}\alpha(1); 2\rho_a) H(\beta(0)^{-1}\beta(1); 2(\rho - \rho_a)).$$

Now, however, $\beta(1)$ is determined by the relation $\alpha(0)\beta(1)^{-1}\alpha(1)^{-1}\beta(0) = u$. Thus,

$$Z(u)=\int H(\beta(0)^{-1}\alpha(1)^{-1}\beta(0)\alpha(1)u^{-1};2\rho)d\beta(0)d\alpha(1).$$

More generally, for genus $g\geqslant 1$,

$$Z(u)=\int H\left(\prod_{i=1}^{g} x_i y_i x_i^{-1} y_i^{-1} u^{-1};2\rho\right) dx\ dy.$$

In all these expressions the integrals are over copies of $\tilde{G}$ and H is the heat kernel on $\tilde{G}$. Decomposing H as a sum of characters (of representations of $\tilde{G}$) according to Eq. (3),

$$Z(u)=\sum_{\mu} \frac{e^{-4c_\mu \rho}}{(\dim\ \mu)^{2g-2}} \frac{\chi_\mu(u^{-1})}{(\dim\ \mu)}. \tag{5}$$

This agrees with Witten's results from Ref. 6 (Sec. 4) except for a constant factor depending on G and g but not on ρ.

Incorporating Wilson lines given by parallel transport about the radial paths used to define ξ is as straightforward as in the product case. For instance, the expectation of the Wilson line $\chi_\sigma(\alpha_i(p))$, given by the trace of holonomy about a noncontractible, homologically nontrivial loop, is

$$\begin{aligned}\langle \chi_\sigma(\alpha_i(p))\rangle &= \frac{1}{Z(u)}\int \chi_\sigma(x) H\left(\prod_{i=1}^{g} x_i y_i x_i^{-1} y_i^{-1} u^{-1};2\rho\right) dx\ dy \\ &= \sum_{\mu} D_{\sigma\mu\mu} \frac{e^{-4c_\mu\rho}}{(\dim\ \mu)^{2g-2}} \frac{\chi_\mu(u^{-1})}{(\dim\ \mu)}.\end{aligned}$$

By contrast, the expectation of a Wilson line coming from a contractible loop is

$$\begin{aligned}\langle \chi_\sigma(\alpha_i(p_1)^{-1}\alpha_i(p_2))\rangle &= \frac{1}{Z(u)}\int \chi_\sigma(\bar{x}) H(\bar{x};2\rho_a) \\ &\quad \times H\left(\bar{x}^{-1}\prod_{i=1}^{g} x_i y_i x_i^{-1} y_i^{-1} u^{-1};2(\rho-\rho_a)\right) d\bar{x}\ dx\ dy \\ &= \sum_{\mu\nu} D_{\sigma\mu\nu} \frac{e^{-4c_\nu(\rho-\rho_a)} e^{-4c_\mu\rho_a}}{(\dim\ \nu)^{2g-2}} \frac{(\dim\ \mu)}{(\dim\ \nu)} \frac{\chi_\nu(u^{-1})}{(\dim\ \nu)},\end{aligned}$$

where ρ_a is the area enclosed by the contractible loop.

Given the ability to disentangle the topological sectors, it is an amusing exercise to compute the expected value of the topology of a random bundle. That is, let $f:\Gamma\to R$, and, viewing f as a map from topological sectors to the reals, define its Yang–Mills expectation taken over bundles of all topological types (G and g are fixed) by

$$\langle f\rangle = \sum_{u\in\Gamma} f(u)Z(u) \Big/ \sum_{u\in\Gamma} Z(u). \tag{6}$$

To evaluate this expression, re-write Eq. (5) as

$$Z(u)=\sum_{\mu} \frac{e^{-4c_\mu\rho}}{(\dim\ \mu)^{2g-2}} \lambda_\mu(u^{-1}),$$

where $\lambda_\mu(u)\equiv\chi_\mu(u)/\dim\mu$. Note that λ_μ is a character for the representation μ of Γ. Let $\mathrm{Rep}\,\tilde{G}$ denote the set of equivalence classes of irreducible representations of $\tilde{G}$, and, for fixed $\alpha\in\mathrm{Rep}\,\tilde{G}$, let $(\mathrm{Rep}\,\tilde{G})_\alpha$ denote the set of representations which agree with α on Γ. Expanding $f:\Gamma\to R$ in characters as $f(u)=\Sigma_{\alpha\in\mathrm{Rep}\,\tilde{G}}f_\alpha\lambda_\alpha(u)$, and letting $\alpha=0$ denote the trivial representation of $\tilde{G}$, we shall prove

Corollary 3.2.1:

$$\langle f\rangle=\sum_{\alpha\in\mathrm{Rep}\,\tilde{G}} f_\alpha\left(\sum_{\mu\in(\mathrm{Rep}\,\tilde{G})_\alpha}\frac{e^{-4c_\mu\rho}}{(\dim\mu)^{2g-2}}\Big/\sum_{\mu\in(\mathrm{Rep}\,\tilde{G})_0}\frac{e^{-4c_\mu\rho}}{(\dim\mu)^{2g-2}}\right).$$

Proof: The character λ_μ satisfies the orthogonality relation

$$\sum_{u\in\Gamma}\lambda_\mu(u)\lambda_\nu(u^{-1})=\begin{cases}\#\Gamma, & \text{if } \lambda_\mu(u)=\lambda_\nu(u) \text{ for all } u\in\Gamma,\\ 0, & \text{otherwise.}\end{cases}$$

Thus the α th component of the numerator in Eq. (6) is

$$\sum_{u\in\Gamma}\lambda_\alpha(u)Z(u)=\sum_{\mu\in\mathrm{Rep}\,\tilde{G}}\frac{e^{-4c_\mu\rho}}{(\dim\mu)^{2g-2}}\sum_{u\in\Gamma}\lambda_\alpha(u)\lambda_\mu(u^{-1})$$
$$=\#\Gamma\sum_{\mu\in(\mathrm{Rep}\,\tilde{G})_\alpha}\frac{e^{-4c_\mu\rho}}{(\dim\mu)^{2g-2}}.$$

Moreover, $1=\lambda_0(u)$, so the denominator in Eq. (6) is the same expression with α replaced by 0.□

Remark 3.1: Since $(\mathrm{Rep}\,\tilde{G})_0=\mathrm{Rep}\,G$, the evaluation of the denominator proves the statement that naively applying the results of Refs. 1 and 2 to topologically nontrivial bundles is equivalent to summing over topologies.

Remark 3.2: Let $G=\mathrm{SO}(3)=\mathrm{SU}(2)/\Gamma$ for $\Gamma=\{\mathbf{1},-\mathbf{1}\}$, and $f(\pm\mathbf{1})=\pm1$. Labeling the irreducible representations of SU(2) by their dimensions, which span the positive integers, the odd-integer representations of SU(2) are trivial on Γ, while the even-integer representations are not [that is, $\lambda_n(-\mathbf{1})=(-1)^{n+1}$]. With the conventions of Ref. 1, the Casimir is $c(\mu)=\frac{1}{8}(n^2-1)$. Thus, the expected value of the topology of an SO(3)-bundle is

$$\langle f\rangle=\sum_{n\ \mathrm{even}}\frac{e^{-(1/2)(n^2-1)\rho}}{n^{2g-2}}\Big/\sum_{n\ \mathrm{odd}}\frac{e^{-(1/2)(n^2-1)\rho}}{n^{2g-2}}.$$

IV. MEASURES ON THE MODULI SPACE OF FLAT CONNECTIONS

Let $\mathscr{M}_m$ denote the space of flat connections modulo gauge transformations. As Witten describes in Ref. 5, there is a natural symplectic form ω on $\mathscr{M}_m$ which defines a measure $\mu_\omega=[1/\#Z(G)](\omega^n/n!)$. Here $n=\frac{1}{2}\dim\mathscr{M}_m$. Sengupta has shown in Ref. 9 that the small-volume limit of the Yang–Mills measure μ on $\mathscr{A}/\mathscr{G}_m$ described above defines, at least in genus 0, a second measure μ_0 on $\mathscr{M}_m$. Witten shows these two measures agree on the total volume of $\mathscr{M}_m$, and in Ref. 10 Forman shows that, in fact, $\mu_\omega=\mu_0$.

The picture of $\mathscr{A}/\mathscr{G}_m$ as a bundle over $\mathrm{Path}^{2g}\,\tilde{G}$ suggests a new measure on $\mathscr{M}_m$. First note that two points of $\mathscr{M}_m$ cannot lie in the same fiber, as there is no 1-form $\tau\in\ker P_r$ for which $D_A\tau=0$. Thus, the restriction of ξ to $\mathscr{M}_m$, henceforth denoted $\xi|_{\mathscr{M}_m}$, is invertible. Moreover, $\xi(\mathscr{M}_m)=\{\boldsymbol{\gamma}\in\mathrm{Path}^{2g}\,\tilde{G}:\ \gamma_i \text{ is constant}\}$. [This is another way of saying that $\mathscr{M}_m$ may be viewed as the representations of $\pi_1(M)$ on $\tilde{G}$]. In short, $\xi|_{\mathscr{M}_m}$ provides an isomorphism between $\mathscr{M}_m$ and $\tilde{G}_z^{2g}$, the space of constant $2g$-tuples in $\mathrm{Path}^{2g}\,\tilde{G}$. In Theorem 4.2 of Ref. 2, we exhibited a global section $\sigma:\mathrm{Path}^{2g}\,G\to\mathscr{A}/\mathscr{G}_m$. Here we note the restriction of σ to $\tilde{G}_z^{2g}$ is $\xi|_{\mathscr{M}_m}^{-1}$. This is an

immediate consequence of the fact that, in a given fiber, the connection A representing a point in the image of σ is determined up to gauge transformation by the condition that $\langle F_A, D_A\tau\rangle$ vanishes for all $\tau \in \ker P_r$.

To define a measure on $\mathscr{M}_m$, use the Haar measure on G to define a measure on $\tilde{G}_z^{2g}$ and then use σ to push this measure forward to $\mathscr{M}_m$. In detail, the Haar measure on G defines a measure μ_H on $\tilde{G}_z^{2g}$ which is the product of Haar measures on the components of $\tilde{G}^{2g}$, conditioned to satisfy the endpoint relation. That is,

$$\mu_H(x_1,y_1,\ldots,x_g,y_g)=\delta\left(\prod_{i=1}^{g} x_i y_i x_i^{-1} y_i^{-1} z^{-1}\right) dx\ dy,$$

where δ denotes the Dirac delta distribution massed at the identity of $\tilde{G}$.

Under the isomorphism $\xi|_{\mathscr{M}}, \mu_H$ defines a measure μ_ξ on $\mathscr{M}_m$. As a measure on functions on $\mathscr{M}_m$, μ_ξ is given as:

$$\int_{\mathscr{M}_m} f\mu_\xi = \int_{\tilde{G}^{2g}} f\circ\sigma(\mathbf{x},\mathbf{y})\mu_H. \tag{7}$$

Note that the right-hand side is an obvious measure to define on $\mathscr{M}_m$ viewed as representations of $\pi_1(M)$. This measure may be normalized to define $\langle f\rangle_{\mu_\xi}$, the expectation of a function on $\mathscr{M}_m$.

In Ref. 11, King and Sengupta arrive at the measure μ_ξ by a construction analogous to the construction of ξ reviewed in Sec. II. (They, however, restrict from the outset to connections representing elements of $\mathscr{M}_m$.) They then argue directly that $\mu_\xi=\mu_\omega$. Here, by contrast, we will show that $\mu_\xi=\mu_0$. More precisely,

Theorem 4.1: *Up to normalization, $\mu_\xi=\mu_0$ on functions which are analytic along the fibers of $\mathscr{A}/\mathscr{G}_m$.*

Proof: We shall show $\lim_{p\to 0}\langle f\rangle_\mu = \langle f|_{\mathscr{M}_m}\rangle_{\mu_\xi}$. Writing out the path integral expression for $\langle f\rangle_\mu$ and performing the Gaussian integral over the fibers yields

$$\langle f\rangle_\mu = \frac{1}{Z}\int_{\mathrm{Path}^{2g}\tilde{G}} \hat{f}(\boldsymbol{\gamma})\xi_*(\mu)(\boldsymbol{\gamma}),$$

where $\hat{f}$ is obtained from $f(\sigma(\boldsymbol{\gamma})+\tau)$ by performing the Gaussian integral over $\tau\in\ker P_r$. Since $\xi_*(\mu)$ is the product of Wiener measures, and the latter are determined by their behavior on cylinder sets, we may assume, without loss of generality, that $\hat{f}(\boldsymbol{\gamma})$ depends on α_i and β_i evaluated at points p_{ij} and q_{ik}, respectively, where $j=1,2,...,m_i$ and $k=1,2,...,n_i$ (and $i=1,2,...,g$). Then, as in the examples of Sec. II,

$$\begin{aligned}\langle f\rangle_u &= \langle \hat{f}(\alpha_1(p_{11}),\alpha_1(p_{12}),\ldots,\beta_g(q_{gn_g}))\rangle_{\xi*(\mu)}\\ &= \frac{1}{Z}\int \hat{f}(x_{11},x_{12},\ldots,y_{gn_g})\prod_{j=1}^{m_i+1} H(x_{i(j-1)}^{-1}x_{ij};\Delta t_{ij})\\ &\quad\times\prod_{k=1}^{n_i+1} H(y_{i(k-1)}^{-1}y_{ik};\Delta s_{ik})\,\delta\left(\prod_{i=1}^{g} x_{i0}y_{i(n_i+1)}^{-1}x_{i(m_i+1)}^{-1}y_{i0}z^{-1}\right)\prod_{i,j,k} dx_{ij}\ dy_{ik},\end{aligned} \tag{8}$$

where $\Delta t_{i0}=0$, Δt_{ij} is twice the area between the radial loops through p_{ij} and $p_{i(j-1)}$ and Δs_{ik} is defined similarly. As ρ approaches 0, so do Δt_{ij} and Δs_{ik}. However, as Δt approaches 0, $H(x;\Delta t)$ becomes a delta function massed at x. Thus, if we may take the limit prior to integrating,

$$\lim_{\rho\to 0}\langle f\rangle_\mu=\frac{1}{Z}\int \hat{f}(x_{11},x_{12},\ldots,y_{gn_g})\prod_{j=1}^{m_i+1}\delta(x_{i(j-1)}^{-1}x_{ij})$$
$$\times\prod_{k=1}^{n_i+1}\delta(y_{i(k-1)}^{-1}y_{ik})\,\delta\left(\prod_{i=1}^{g}x_{i0}y_{i(n_i+1)}^{-1}x_{i(m_i+1)}^{-1}y_{i0}z^{-1}\right)\prod_{i,j,k}dx_{ij}\,dy_{ik}.$$

Performing the integrations over x_{ij} and y_{ik} for $j,k\neq 0$ changes all the x_{ij}'s and y_{ik}'s to x_{i0}'s and y_{i0}'s, respectively, leaving

$$\lim_{\rho\to 0}\langle f\rangle_\mu=\frac{1}{Z}\int_{\tilde{G}^{2g}}\hat{f}(x_{10},x_{10},\ldots,y_{g0})\,\delta\left(\prod_{i=1}^{g}x_{i0}y_{i0}^{-1}x_{i0}^{-1}y_{i0}z^{-1}\right)\prod_i dx_{i0}\,dy_{i0}. \tag{9}$$

The right-hand side is exactly $(1/Z)\int \hat{f}|_{\xi(\mathscr{M}_m)}\mu_H$. The assumption we made about interchanging limit and integration is

$$\lim_{t\to 0}\int f(x)H(y^{-1}x;t)dx=\int f(x)\,\delta(y^{-1}x)dx.$$

That each side is equal to $f(y)$ follows from the definition of the heat kernel (and the continuity in t of solutions of the heat equation) on the left and the definition of the distribution δ on the right. We thus have

$$\lim_{\rho\to 0}\langle f\rangle_\mu=\frac{1}{Z}\int \hat{f}|_{\xi(\mathscr{M}_m)}\mu_H.$$

According to Eq. (7), we must now show

$$\lim_{\rho\to 0}\hat{f}=f|_{\mathscr{M}_m}\circ\sigma. \tag{10}$$

First, note that if f constant along the fibers, that is, if $f(\sigma(\gamma)+\tau)=f\circ\sigma$, then, for any ρ, $\hat{f}=f\circ\sigma$. More generally, if $f(\sigma(\gamma)+\tau)$ is an nth order polynomial in τ, then $\hat{f}$ is an nth order polynomial in ρ, whose constant term is $f\circ\sigma$. This follows from standard manipulations of Gaussian integrals and the fact that, in two dimensions, the area ρ plays the role of the coupling constant. Thus, for f polynomial, or, more generally, analytic, in τ, Eq. (10) holds (with the convergence being uniform); hence, up to normalization, $\mu_\xi=\mu_0$ on analytic functions. □

Remark 4.1: The restriction to analytic functions of the fiber is not terribly severe. In most field theory, polynomials are sufficient. Moreover, the freedom in choosing the fundamental domain is sufficient to ensure that a large class of Wilson lines may be realized as function which are *constant* on each fiber.

Theorem 4.1 provides a new proof of Forman's generalization of Sengupta's result:

Corollary 4.1.1: The small-volume limit of μ is supported on $\mathscr{M}_m$.

Observe that only the restriction of f to $\mathscr{M}_m$ enters into the above calculation of $\langle f\rangle_{\mu_0}$. Specifically, let χ_R be the indicator function of a measurable set $R\subset\mathscr{A}/\mathscr{G}_m$ for which $R\cap\mathscr{M}_m=\emptyset$, and let χ_R^{smooth} be a smooth, non-negative function which is 1 on R and has support in the complement of $\mathscr{M}_m$. Now, let $\{\chi_R^n\}$ be a sequence of analytic functions converging uniformly to χ_R^{smooth}. Then, by the theorem, $\langle\chi_R^n\rangle_{\mu_0}=\langle\chi_R^n|_{\mathscr{M}_m}\rangle_{\mu_\xi}$. By the construction of the sequence, there is some N such that χ_R^n vanishes on $\mathscr{M}_m$ for all $n>N$. Hence, $\langle\chi_R^{\text{smooth}}\rangle_{\mu_0}=0$ and thus $\langle\chi_R\rangle=0$.

Remark 4.2: We have assumed the existence of the sequence $\{\chi_R^n\}$. If $\mathscr{A}/\mathscr{G}_m$ were a finite-dimensional manifold, the Stone–Weierstrass Theorem would ensure the existence of such a sequence, but at present the ''proof'' of the corollary is a heuristic argument.

Comparing the arguments to $\hat{f}$ in Eqs. (8) and (9) shows that one effect of going to the small-volume limit is to project from $\mathrm{Path}^{2g}\ \tilde{G}$ to $\tilde{G}_z^{2g}$ by evaluating each component path at $t=0$. Denote this evaluation map by e: $\mathrm{Path}^{2g}\ \tilde{G}\to\tilde{G}_z^{2g}$. This projection suggests another measure μ_e on $\mathscr{M}_m$ which is the push-forward of μ by the projection from $\mathscr{A}/\mathscr{G}_m$ to $\mathscr{M}_m$ given by $\sigma\circ e\circ\xi$. That is,

$$\mu_e=\sigma_* e_* \xi_*(\mu).$$

As σ is an isomorphism and $\xi_*(\mu)$ is the product of Wiener measures described in Sec. III, the only new feature is the effect of pushing forward by e. This means integrating using the Wiener measures with fixed left endpoints. The derivation of Eq. (2), with minor modifications to work in a fixed topological sector and to integrate only over right end-points, leads to

$$\langle f\rangle_{\mu_e}=\frac{1}{Z}\int\ f\circ\sigma(x_1,\ldots y_g)H\left(\prod_{i=1}^{g}\ x_i y_i x_i^{-1}y_i^{-1};2\rho\right)\ dx_i\ dy_i\,.$$

Comparing this with $\langle f\rangle_{\mu\xi}$ [cf. Eq. (7)], it is clear that, up to normalization,

$$\mu_e=\frac{H(\Pi_{i=1}^{g}x_i y_i x_i^{-1}y_i^{-1};2\rho)}{\delta(\Pi_{i=1}^{g}x_i y_i x_i^{-1}y_i^{-1};2\rho)}\ \mu_\xi\,.$$

The measure μ_e is thus a new measure on $\mathscr{M}_m$ which agrees with μ_ξ only in the limit as ρ approaches 0.

V. CONCLUSION

We have extended the path integral formulation of Yang–Mills on Riemann surfaces to treat each topological sector separately. The result is in agreement with Witten's approach and is sufficiently explicit to compute quantum expectations of a large class of Wilson lines. It also provides a new measure on $\mathscr{M}_m$, the moduli space of flat connections.

There are many routes to defining measures on $\mathscr{M}_m$. The symplectic form ω on $\mathscr{M}_m$ and the small-volume limit of μ define the measures μ_ω and μ_0, respectively. The view of $\mathscr{A}/\mathscr{G}_m$ as a bundle over $\mathrm{Path}^{2g}\ G$ suggests the measures μ_ξ and μ_e. However, this apparent profusion of measures on $\mathscr{M}_m$ is in fact a pair of measures. Combining Theorem 4.1 with Forman's result:

$$\mu_\xi=\mu_0=\mu_\omega\,.$$

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On the time decay of a wave packet in a one-dimensional finite band periodic lattice

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Nonstationary Schrödinger equation with a periodic finite band potential $p(x)$ is considered. The Green's function $G(x,x',t)$ of this equation is investigated when $t\to\infty$. Asymptotics for $G(x,x',t)$ are specified. It is shown that for large "velocities" $v=(x-x')/t$ the principal term in asymptotics of $G(x,x',t)$, $t\to\infty$ coincides with the Green's function for $p=0$. The principal term in the asymptotics of $G(x,x',t)$ in the case $v\to\infty$ is equal to a sum of Green's functions of unperturbed problems for particles whose masses are equal to effective masses of the Hill operator under investigation. © *1996 American Institute of Physics.* [S0022-2488(96)02901-2]

I. INTRODUCTION

We consider the Cauchy problem for nonstationary Schrödinger equations:

$$u'=-iHu,\quad H=-\frac{d^2}{dx^2}+p(x),\quad u(x,0)=u_0(x) \tag{1.1}$$

in $L_2(0,1)$, with the real 1-periodic N-band potential $p(x)$, $p\in L_1(0,1)$. The Green's function $G(x,x',t)$ of the problem (1.1) is a nucleus of an integral operator $\exp(-itH)$. We specify the asymptotics of the Green's function $G(x,x',t)$ (as announced in Ref. 1) using the results of Ref. 2. Asymptotics of the Green's function for the heat equation was obtained in Ref. 3 and the case of the wave equation was covered in Ref. 4. The scattering theory for the operator H and its perturbations was studied in Refs. 5–7.

We will prove that the Green's function $G(x,x',t)$ is equal to a sum of N integrals along N spectral bands. We find asymptotics of every integral using the stationary phase method. Using Ref. 2 we see that there exists no more than two stationary points on every bounded spectral band and just one point on the infinite band. This statement allows us to simplify asymptotics found in Ref. 1.

Corollaries are obtained for the cases of large and small velocities $v=(x-x')/t$.

(1) Let $v\to\infty$, $t\to\infty$. Then the principal term in the asymptotic expansion of $G(x,x',t)$ coincides with $G^0(x,x',t)$ which is a Green's function for the unperturbed case $p=0$.

(2) Let $v\to 0$, $t\to\infty$. Then the principal term in the asymptotic expansion of $G(x,x',t)$ is equal to a sum of Green's functions $G_l^0(x,x',t)$, $l=1,\ldots,2N+1$ of the operators $H_l^0=-(2\mu_l)^{-1}d^2/dx^2$, $l=1,2,\ldots,2N+1$. Here we denote by μ_l the effective mass at the corresponding end of a spectral band.

Using the asymptotics of the Green's function $G(x,x',t)$ the following asymptotic relations as $v\to\infty$ are obtained:

$$\int_{x'}^{x'+2a}|G(x,x',t)|^2dx'=\frac{1}{\pi t}\left[\sum_{l=1}^{2N+1}|\mu_l||\Psi(x,s_l)|^2+O(t^{-1})\right],\quad x\in X,\quad x'\in X', \tag{1.2}$$

$$\int_x^{x+2a} dx \int_{x'}^{x'+2a} |G(x,x',t)|^2 dx' = \frac{2}{\pi t}\left[\sum_{l=1}^{2N+1} |\mu_l| + O(t^{-1})\right], \quad x \in X, \quad x' \in X', \qquad (1.3)$$

where X, X' are compact sets, μ_l is the effective mass, and $\Psi(x,s_l)$ is a normalized Floquet–Bloch function at the lth end of a spectral band, $l=1,\ldots,2N+1$. Relations (1.2) and (1.3) show that the principal term in the asymptotics of the probability for a particle to get from the segment $[x',x'+2a]$ to the point x or to the segment $[x,x+2a]$ does not depend at large times on $x' \in X'$ or $x' \in X'$, $x \in X$, respectively.

II. MAIN RESULTS

Notations and definitions necessary for the formulation of the main results are introduced. As it is known the spectrum σ of the N-band Hill operator H is absolutely continuous and consists of a sequence of bands $\sigma(n)=[s_{2n-1},s_{2n}]$, $n=1,\ldots,N$ and $\sigma(N+1)=[s_{2N+1},+\infty)$, $\sigma=\cup_{n=1}^{N+1}\sigma(n)$. We call the interval $(-\infty,s_1)$, (s_{2n},s_{2n+1}), $s_{2n}\leqslant s_{2n+1}$, $n=1,\ldots,N$ gaps in the spectrum of the operator H. If a gap degenerates, i.e., if $s_{2n}=s_{2n+1}$ then we say that the corresponding bands $\sigma(n)$ and $\sigma(n+1)$ merge.

We denote by $\mathbf{E}$ the spectral surface of the operator H. We can get it from the two copies of the spectral plane $\mathbf{C}\backslash\sigma$, cut by spectral bands, the upper side of the nth band of the first leave $\mathbf{E}_1$ being identified with the lower side of the nth band of the second leave $\mathbf{E}_2$ (we call it on an upper side σ_n^+). A lower side of the nth band of the leave $\mathbf{E}_1$ is identified with its upper side of the leave $\mathbf{E}_2$ (we call it lower side σ_n^-), $\sigma^{\pm}=\cup_{n=1}^{N+1}\sigma_n^{\pm}$.

Consider on the upper side σ_1^+ in the neighborhood of the point s_1 a function $k(E)=\arccos F(E)$, where $F(E)$ is the Lyapunov function for the Hill operator H. The function $k(E)$ can be analytically continued on $\mathbf{E}$ so that $\mathbf{E}$ is one-to-one mapped on a Riemann surface $\mathbf{K}$ described in Refs. 5 and 6. In particular images $\Sigma_{\pm n}$ of bands $\sigma_n^{\pm}$ in this mapping are as follows:

$$\Sigma_n = k(\sigma_n^+) = [\pi(n-1)+0, \pi n - 0], \quad \Sigma_{-n} = k(\sigma_n^-) = -\Sigma_n, \quad n=1,\ldots,N, \qquad (2.1)$$

$$\Sigma_{N+1} = k(\sigma_{N+1}^+) = [\pi N + 0, +\infty), \quad \Sigma_{-N-1} = k(\sigma_{N+1}^-) = -\Sigma_{N+1}, \quad \mathbf{R}_* = \cup_{-N-1}^{N+1}\Sigma_n. \qquad (2.2)$$

We denote

$$\Sigma(n) = \Sigma_n \cup \Sigma_{-n}, \quad n=1,\ldots,N+1. \qquad (2.3)$$

From the theorem of decomposition for the Hill operator in the form[5,6] it follows that for the Green's function of problem (1.1) there is a formula:

$$G(x,x',t) = \int_{\mathbf{R}_*} g(x,x',k,t)\,dk, \quad t>0, \qquad (2.4)$$

$$g(x,x',k,t) = (2\pi)^{-1} \exp(-itE(k))\Psi^+(x,k)\Psi^-(x',k), \qquad (2.5)$$

where $\Psi^{\pm}(x,k)$ are normalized Floquet–Bloch functions. Hence we get

$$G(x,x',t) = \sum_{n=1}^{N+1} I_n(x,x',t), \qquad (2.6)$$

$$I_n(x,x',t) = \int_{\Sigma(n)} g(x,x',k,t)\,dk, \quad n=1,\ldots,N+1, \qquad (2.7)$$

where the function $E(k)$ and consequently the function $g(x,x',k,t)$ is analytic in k in a (small) neighborhood of $\Sigma(n)$. Further on we assume that $v \geqslant 0$. A case when $v \leqslant 0$ is similar.

We obtain asymptotics of the integral $I_n(x,x',t)$ as $t \to \infty$ using the stationary phase method. To do it we have to analyze the following equation for stationary points of the integral $I_n(x,x',t)$:

$$E_k'(k) = v, \quad k \in \Sigma(n), \quad n = 1,\ldots,N+1. \tag{2.8}$$

First we analyze the function $E_k'(k)$. As

$$E_k'(-k) = -E_k'(k), \quad E_{kk}''(-k) = E_{kk}''(k), \quad k \in \mathbf{R}_*, \tag{2.9}$$

it is enough to learn a behavior of functions E_k', E_{kk}'' on Σ_n, $n = 1,\ldots,N+1$ to analyze Eq. (2.8). Using the results obtained in Ref. 4 we describe this behavior which is as follows:

Proposition II.1: (1) On a finite band Σ_n, $n = 1,\ldots,N$, the function $E_k'(k)$ at first strictly monotonously increases being equal to zero at the left end $\pi(n-1)+0$ and reaching its maximum at a point k_n which lies just inside the band Σ_n. Then $E_k'(k)$ strictly monotonously decreases and is equal to zero at the right end $\pi n - 0$.

(2) On the last infinite band the function $E_k'(k)$ strictly monotonously increases from zero to infinity.

From Proposition II.1 and Eq. (2.9) follows that the function E_k', maps a set $\Sigma(n)$ to $V_n = [-E_k'(k_n), E_k'(k_n)]$, $n = 1,\ldots,N$, and $V_{N+1} = \mathbf{R}$. In Ref. 2 it is also shown that the function E_{kk}'' on Σ_n, $n = 1,\ldots,N$ decreases strictly monotonously and is equal to zero in the point k_n. Hence

$$E_n^{(3)} = E_{kkk}'''(k_n) = -|E_{kkk}'''(k_n)|, \quad n = 1,\ldots,N. \tag{2.10}$$

Let us describe as a corollary a result of the analysis of Eq. (2.8).

Lemma II.1: (1) Equation (2.8) for $v \geqslant 0$ has on $\Sigma(n)$, $n = 1,\ldots,N$,
(a) two solutions $a_{2n-1}, a_{2n} \in \Sigma_n$, $a_{2n-1} < a_{2n}$ if $v < E_k'(k_n)$,
(b) one solution $a_{2n-1} = a_{2n} = k_n$ if $v = E_k'(k_n)$,
(c) no solutions if $v > E_k'(k_n)$.
(2) Equation (2.8) on $\Sigma(N+1)$ has just one solution for any $v \geqslant 0$.

If in Lemma II.1 the parameter $v = 0$ then $E_k'(k) = 0$ in four points on $\Sigma(n)$, $n = 1,\ldots,N$, and in two points on $\Sigma(N+1)$. However, because of the identifications on $\mathbf{K}$ and equivalence relations there are only two different points or one point, respectively.

Denote

$$X^{\pm}(x,k) = \Psi^{\pm}(x,k)\exp(\mp ikx), \quad X(x,x',k) = X^{+}(x,k)X^{-}(x',k). \tag{2.11}$$

Here $X^{\pm}(x,k)$ are 1-periodical functions,[8] $X^{\pm}(x+1,k) = X^{\pm}(x,k)$, $x \in \mathbf{R}$, $k \in \mathbf{K}$.

Now we formulate the main result.

Theorem II.1: *(1) Let $n = 1,\ldots,N$ and $t \to \infty$. Then uniformly in $x,x' \in \mathbf{R}$ we have*
(a) if a number $\delta > 0$ and v obeys the inequalities $0 \leqslant v \leqslant E_k'(k_n) - \delta$, then

$$I_n(x,x',t) = \frac{1}{\sqrt{2\pi i t}} \sum_{l=2n-1,2n} \sqrt{(E_{kk}''(a_l))^{-1}}\, \exp[it(va_l - E(a_l))][X(x,x',a_l) + O(t^{-1})]. \tag{2.12}$$

(b) If $v \geqslant E_k'(k_n) + \delta$ for some $\delta > 0$ then for any real m:

$$I_n(x,x',t) = O(t^{-m}). \tag{2.13}$$

(2) Let $n=N+1$, $t\to\infty$. Then uniformly in $x,x'\in\mathbf{R}$ we have

$$I_{N+1}(x,x',t)=(1/\sqrt{2\pi itE''_{kk}(a_{2N+1})}\exp\{it[va_{2N+1}-E(a_{2N+1})]\}[X(x,x',a_{2N+1})+O(t^{-1})]. \tag{2.14}$$

Here and later we define a main branch of the square root if it is not fixed.

Asymptotics of the Green's function $G(x,x',t)$ for given $v\neq E'_k(k_n)$, $n=1,\ldots,N$ is a sum of Eq. (2.14) and formulas (2.12) with numbers n for which the condition $0\leqslant v\leqslant E'_k(k_n)-\delta$ holds true.

We describe corollaries which follow from Theorem II.1.

Corollary II.1: Let the assumptions of Theorem II.1 be true and $v\to\infty$. Then as $t\to\infty$ we have asymptotics uniform in $x,x'\in\mathbf{R}$:

$$I_n(x,x',t)=O(t^{-1}),\quad n=1,\ldots,N, \tag{2.15}$$

where m is any real number and

$$I_{N+1}(x,x',t)=\frac{1}{2\sqrt{\pi it}}\exp\left[\frac{itv^2}{4}(1+O(v^{-2}))\right](1+O(v^{-1})+O(t^{-1})). \tag{2.16}$$

We see that the principal term in the asymptotics (2.16) coincides with the well known formula:

$$G^0(x,x',t)=\frac{1}{2\sqrt{\pi it}}\exp\left(\frac{itv^2}{4}\right). \tag{2.17}$$

Corollary II.2: Let the conditions of Theorem II.1 be satisfied and also $v\to 0$. Then as $t\to\infty$ we have asymptotics uniform in $x,x'\in\mathbf{R}$:

$$\begin{aligned}I_n(x,x',t)=&\frac{1}{\sqrt{2\pi it}}\sum_{l=2n-1,2n}\sqrt{\mu_l}\exp it[-s_l+\pi v[l/2]+\mu_l v^2/2+O(v^3)]\\&\times[X(x,x',s_l)+O(t^{-1})+O(v)],\quad n=1,\ldots,N,\end{aligned} \tag{2.18}$$

where $[l/2]$ is the entire of $l/2$ and

$$\begin{aligned}I_{N+1}(x,x',t)=&\frac{\sqrt{\mu_{2N+1}}}{\sqrt{2\pi it}}\exp[it[-s_{2N+1}+\pi vN+\mu_{2N+1}v^2/2+O(v^3)]]\\&\times[X(x,x',s_{2N+1})+O(t^{-1})+O(v)].\end{aligned} \tag{2.19}$$

In Ref. 1 Theorem II.1 and Corollaries II.1 and II.2 were announced but a number of terms in the sum in Eq. (2.12) and in Eq. (2.14), i.e., a number of solutions of Eq. (2.8) on $\Sigma(n)$ was not known exactly except in the cases $v\to 0$ and $v\to\infty$. We can now show that there are just two terms in the sum in Eq. (2.12) and one term in Eq. (2.14) because it was proven in Ref. 2 that the function $E'_k(k)$ is convex for $k>0$.

Integrating asymptotics of $G(x,x',t)$ for $x\in X$, $x'\in X'$ which is a sum of Eq. (2.18), $n=1,\ldots,N$ and Eq. (2.19) we get the asymptotic relations (1.2) and (1.3) using Eqs. (2.11) and (3.6).

Let us now consider a case of the confluence of the stationary points a_{2n-1}, $a_{2n}\in\Sigma(n)$. Let $\alpha=E'_k(k_n)-v$ be a small positive parameter and $a_{2n-1}(\alpha)$, $a_{2n2n}(\alpha)$ be solutions of Eq. (2.8) in $\Sigma(n)$. Let Ai be the Airy function. The following statement is proved.

Theorem II.2: *Let $\alpha<\delta$, and δ be a sufficiently small positive number. Then if $t\to\infty$ we have an asymptotics uniform in x,x', α:*

$$I_n(x,x',t)=(t|E_n^{(3)}|/2)^{-1/3}\exp[it[vk_n-E_n+O(\alpha^{3/2})]][\mathrm{Ai}(z_n)[X(x,x',k_n)+O(\alpha^{1/2})] - i(t|E_n^{(3)}|/2)^{-1/3}\mathrm{Ai}'(z_n)[X_k'(x,x',k_n)+O(\alpha^{1/2})]+O(t^{-1})], \tag{2.20}$$

where

$$z_n=z_n(t,\alpha)=-\alpha t^{2/3}(|E_n^{(3)}|/2)^{-1/3}(1+O(\alpha^{1/2})). \tag{2.21}$$

If $\alpha=0$ we have

$$I_n(x,x',t)|_{\alpha=0}=(t|E_n^{(3)}|/2)^{-1/3}\exp[it(vk_n-E_n)]\{\mathrm{Ai}(0)X(x,x',k_n) - i(t|E_n^{(3)}|/2)^{-1/3}\mathrm{Ai}'(0)X_k'(x,x',k_n)+O(t^{-1})\}. \tag{2.22}$$

We get another theorem which is more convenient when α is fixed.

Theorem II.3: *Let α be a sufficiently small number, $\alpha\to 0$, so that $\alpha t^{2/3}\to\infty$. Then there is asymptotics:*

$$I_n(x,x',t)=\frac{1}{2\sqrt{\pi t}}(\alpha|E_n^{(3)}|/2)^{-1/4}\exp[it(vk_n-E_n+O(\alpha^{3/2}))] \times\left[X(x,x',k_n)\cos\left(\frac{2}{3}t(|E_n^{(3)}|/(2\alpha^3))^{-1/2}(1+O(\alpha^{1/2}))+\frac{\pi}{4}\right) + O(\alpha^{1/2})+O(t^{-1}\alpha^{-3/2})\right]. \tag{2.23}$$

III. PRELIMINARIES

Let us consider the solutions $\varphi(x,E)$ and $\theta(x,E)$ of the equation

$$-y''+p(x)y=Ey,\quad E\in\mathbf{C} \tag{3.1}$$

under the conditions $\theta(0,E)=\varphi'(0,E)=1$, $\theta_x'(0,E)=\varphi(0,E)=0$. The functions $\varphi(x,E)$, $\theta(x,E)$, their derivatives, and the Lyapunov function $F(E)=[\theta(1,E)+\varphi_x'(1,E)]/2$ are the entire functions of E, real on the real axis. An asymptotics for the function $F(E)$ when $E\to\infty$ provided $\int_0^1 p(x)dx=0$ is as follows (see Ref. 8):

$$F(E)=\cos\sqrt{E}+O(\exp(\mathrm{Im}\sqrt{E})/E). \tag{3.2}$$

A function $\sqrt{F^2(E)-1}$, a branch being determined by the condition $\sqrt{F^2(E)-1}>0$, $E<s_1$, $E\in\mathbf{E}_1$, is an analytical function in $\mathbf{E}$ (see Ref. 5). In every nondegenerate gap there is just one (simple) zero ζ_n, $n=1,\ldots,N$ of the function $F'(E)$.

The function $k(E)$ mentioned above is a one-to-one mapping of $\mathbf{E}$ to the surface $\mathbf{K}$, which is a complex plane with vertical excised slits $\gamma_n=(\pi n+i\epsilon_n,\pi n-i\epsilon_n)$. The positive numbers ϵ_n are determined from the equalities

$$sh\,\epsilon_n=|\sqrt{F^2(\zeta_n)-1}|,\quad n=1,\ldots,N, \tag{3.3}$$

and a slit γ_{-n} is symmetrical to the slit γ_n with respect to the imaginary axis, $n=1,\ldots,N$. The right-hand side of the slit γ_n is identified to the left-hand side of the slit γ_{-n}, $n=\pm 1,\ldots,\pm N$. The

image of the first leave $\mathbf{E}_1$ is the upper half $\mathbf{K}_+=\{k\in\mathbf{K},\mathrm{Im}\,k>0\}$ of the surface $\mathbf{K}$, the image of the second leave being a lower part, $\mathbf{K}_-=\overline{\mathbf{K}_+}$. The function $k(E)$ maps the zeroth gap $(-\infty,s_1)$ to the upper half of the imaginary axis. The gap $(s_{2n},s_{2n+1})\subset\mathbf{E}_1$ is mapped to the identified upper halfs of the slits γ_n, γ_{-n}, the gap $(s_{2n},s_{2n+1})\subset\mathbf{E}_2$ being mapped to lower halfs of the slits γ_n, γ_{-n}, $n=1,\ldots,N$. An energy E and quasimomentum k are connected by the relations[5,6]

$$\cos k(E)=F(E),\quad \sin k(E)=i\sqrt{F^2(E)-1},\quad E_k'(k)=-\sin k/F'(E), \tag{3.4}$$

where $E(k)$ is a function reverse to the function $k(E)$.

As it is shown in Ref. 8 for any $E\in\mathbf{E}_1\backslash\sigma$ there is a single number $m^{\pm}(E)=[\varphi'(1,E)-\theta(1,E)\pm 2i\sin k]/(2\varphi(1,E)$ so that

$$\psi(x,E)=\theta(x,E)+m^{\pm}(E)\varphi(x,E)\in L_2(0,\pm\infty). \tag{3.5}$$

Normalized Floquet–Bloch solutions are determined as follows:

$$\Psi^{\pm}(x,k)=\psi^{\pm}(x,k)/N(E),$$

$$N(E)=\left[\int_0^1\psi^+(x,E)\psi^-(x,E)dx\right]^{1/2},\quad E=E(k), \tag{3.6}$$

where a branch of the square root is chosen so that on the spectrum we have $N(E)>0$. The properties of the functions (3.6) can be found in Refs. 5 and 6.

Let us introduce a set $\mathbf{K}_\delta=\{k\in\mathbf{K},|k-k(s_l)|>\delta,l=1,\ldots,2N+1\}$, $\delta>0$, $k(s_l)=\pi[l/2]+(-1)^{l+1}(0)$. Further on we shall need asymptotics when $|k|\to\infty$ (see Refs. 5 and 6):

$$E(k)=k^2+O(k^{4/3}),\quad k\in\mathbf{K}, \tag{3.7}$$

$$E(k)=k^2+O(1),\quad k\in\mathbf{K}_\delta. \tag{3.8}$$

Last asymptotics may be differentiated, i.e., we have as $|k|\to\infty$,

$$E_k'(k)=2k+O(k^{-1}),\quad k\in\mathbf{K}_\delta, \tag{3.9}$$

$$E_{kk}''(k)=2+O(k^{-1}),\quad k\in\in\mathbf{K}_\delta. \tag{3.10}$$

In a neighborhood of points $k(s_l)$, $l=1,\ldots,2N+1$, the function $E(k)$ has the following form:

$$E(k)=(k-k(s_l))^2/(2\mu_l)+O((k-k(s_l))^4),\quad l=1,\ldots,2N+1, \tag{3.11}$$

where the effective masses

$$\mu_l=1/E_{kk}''(k)|_{k=k(s_l)},\quad l=1,\ldots,2N+1. \tag{3.12}$$

For the functions $X^{\pm}(x,k)$ (see Eq. (2.11)) we have[6,8]

$$X(x,x',k)=1+O(k^{-1}),\quad k\in\mathbf{K}_\delta, \tag{3.13}$$

$$|X^{\pm}(x,k)|\leqslant C,\quad x\in\mathbf{R},\quad k\in\mathbf{R}_*. \tag{3.14}$$

IV. THE PROOF OF THE MAIN THEOREM

In this section we consider the cases $0 \leqslant v \leqslant E_k'(k_n) - \delta$ and $v \geqslant E_k'(k_n) + \delta$, $\delta > 0$. At first we describe those results on the stationary phase method which we shall need (see for instance Ref. 9).

Proposition IV.1: Let $M=[-\epsilon,\epsilon]$, $\epsilon>0$, be a finite segment and $f \in C_0^\infty(M)$, $S \in C^\infty(M)$, S be a real function. Then

(1) If the function $S(k)$ has on M a single nondegenerate stationary point $k=0$, i.e., $S'(0)=0$, $S''(0)\neq 0$ then as $t\to\infty$ the following asymptotics is true:

$$I(t)=\int_M f(k)\exp(itS(k))dk=\sqrt{\frac{2\pi}{t|S''(0)|}}\exp\left[itS(0)+i\,\frac{\pi}{4}\,\operatorname{sgn} S''(0)\right][f(0)+O(t^{-1})]. \tag{4.1}$$

(2) If $\min_{k\in M}|S'(k)|>0$ then for any real m we have $I(t)=O(t^{-m})$ as $t\to\infty$.

Now we start proving Theorem II.1. Note that $\Sigma(n)$ i.e., a contour of integration in the integral $I_n(x,x',t)$ is a closed curve because of the identifications on **K**. In a neighborhood of the contour of integration the functions $E(k)$ and $X(x,x',k)$ are analytic (see Refs. 5 and 6). From Eqs. (2.5), (2.7), and (2.11) we have

$$I_n(x,x',t)=\frac{1}{2\pi}\int_{\Sigma(n)} X(x,x',k)\exp(itS(k))dk, \quad S(k)=vk-E(k). \tag{4.2}$$

According to Lemma II.1 by solving Eq. (2.8) we get two stationary points a_{2n-1},a_{2n} on $\Sigma(n)$ if $|v|<|E_k'(k_n)|$ or there is none of them if $|v|>|E_k'(k_n)|$. It is easy to check that in the neighborhoods of the points a_{2n-1},a_{2n} all the conditions of Proposition IV.1(1) are satisfied. Outside these neighborhoods we use Proposition IV.1(2). Hence we get formula (2.12). One should only take into consideration that

$$|E_{kk}''(a_l)|^{-1/2}\exp\left[-i\,\frac{\pi}{4}\operatorname{sgn} E_{kk}''(a_l)\right]=\sqrt{(E_k''(a_l))^{-1}}/\sqrt{i}, \quad l=1,\ldots,2N.$$

If $v > E_k'(k_n)$ then the asymptotics (2.13) follows from Lemma II.1(c), Proposition IV.1(2).

We can consider the case $n=N+1$ the same way.

Let us now prove corollaries from Theorem II.1. At first we let $v\to\infty$ and consider Corollary II.1. From Eqs. (2.8) and (3.9) we have

$$v=E_k'(a_{2N+1})=2a_{2N+1}+O(1/a_{2N+1}). \tag{4.3}$$

For large v, Eq. (4.3) is equivalent to the asymptotics

$$a_{2N+1}=\frac{v}{2}\,(1+O(v^{-2})), \quad v\to\infty. \tag{4.4}$$

Hence and from Eq. (3.8) we find

$$E(a_{2N+1})=\frac{v^2}{4}\,(1+O(v^{-2})), \quad v\to\infty. \tag{4.5}$$

From Eqs. (3.10), (3.13), and (4.4) it follows

$$E_{kk}''(a_{2N+1})=2+O(v^{-1}), \quad X(x,x',a_{2N+1})=1+O(v^{-1}), \quad v\to\infty. \tag{4.6}$$

Hence and from Eqs. (2.11), (4.4), and (4.5) follows Eq. (2.16).

We now prove Corollary II.2. Let $v \to 0$. Then from Eqs. (2.1), (2.8), and (3.12) we have

$$v = E_k'(a_{2n-1}) = (a_{2n-1} - \pi(n-1))/\mu_{2n-1} + O((a_{2n-1} - \pi(n-1))^2), \quad n = 1,\ldots,N. \quad (4.7)$$

Hence it follows that

$$a_{2n-1} = \pi(n-1) + v\mu_{2n-1} + O(v^2), \quad v \to \infty, \quad n = 1,\ldots,N, \quad (4.8)$$

and therefore

$$E(a_{2n-1}) = s_{2n-1} + O(v^3), \quad E_{kk}''(a_{2n-1}) = 1/\mu_{2n-1} + O(v),$$

$$X(x,x',a_{2n-1}) = X(x,x',s_{2n-1}) + O(v), \quad n = 1,\ldots,N. \quad (4.9)$$

Hence and from Eqs. (2.12) and (4.8) we get the first term in the sum (2.18). The second term in Eq. (2.18) and the asymptotics (2.19) are obtained the same way.

V. THE CASE OF MERGING STATIONARY POINTS

At first we describe well-known results on asymptotics for a case of merging stationary points. Let a function $S(k,\alpha)$ have two close simple saddle points on M when α is small. Let us consider an integral:

$$I(t,\alpha) = \int_M f(k) \exp itS(k,\alpha)\, dk \quad (5.1)$$

by small α. Let us introduce

Condition A_1: the functions $F(k)$ and $S(k,\alpha)$ are holomorphic in k, α when k is in a neighborhood of M and $|\alpha| < \delta$.

Condition A_2: $S_k'(0,0) = S_{kk}''(0,0) \neq 0, S_{kkk}'''(0,0) \neq 0$.

It is known[9] that under conditions A_1 and A_2 for small $\alpha \neq 0$ the equation $S_k'(k,\alpha) = 0$ has just two nondegenerate saddle points, $a_1(\alpha)$ and $a_2(\alpha)$ such that $a_1(0) = a_2(0) = 0$. The functions $a_1(\alpha)$ and $a_2(\alpha)$ are analytic of $\sqrt{\alpha}$ by small α and for $l = 1,2$ we have

$$a_l(\alpha) = \sqrt{2S_{k\alpha}''(0,0)/S_{kkk}'''(0,0)} \times \left(1 + \sum_{m>0} c_m \alpha^{m/2}\right). \quad (5.2)$$

The values a_1 and a_2 differ by choosing a sign of the square root. Let $0 < a_2(\alpha) < c\sqrt{\alpha}$, $c > 0, \sqrt{\alpha} > 0$ as $\alpha > 0$.

We now introduce the definitions

$$A(\alpha) = (S_1(\alpha) + S_2(\alpha))/2, \quad B(\alpha) = (3/4)^{2/3}(S_1(\alpha) - S_2(\alpha))^{2/3}, \quad (5.3)$$

$$z(\alpha) = -t^{2/3}B(\alpha), \quad (5.4)$$

where $S_l(\alpha) = S(a_l(\alpha),\alpha)$, $l = 1,2$. Let us also introduce the functions

$$T(\alpha) = \sum_{l=1,2} Q_l(\alpha) f_l(\alpha), \quad D(\alpha) = B(\alpha)^{-1/2} \sum_{l=1,2} (-1)^{l+1} Q_l(\alpha) f_l(\alpha), \quad (5.5)$$

where

$$Q_l(\alpha)=\sqrt{(-1)^l 2(B(\alpha))^{1/2}/S''_{kk}(k,\alpha)}|_{k=a_l},\quad f_l(\alpha)=f(a_l(\alpha)). \tag{5.6}$$

There is a statement (see Ref. 9).

Proposition V.1: Let the conditions A_1 and A_2 be satisfied. Then if $t\to\infty$, $|\alpha|<\delta$, δ being a sufficiently small number, then the integral (5.1) has an asymptotics uniform in α:

$$I(t,\alpha)=\pi t^{-1/3}\exp[itA(\alpha)][T(\alpha)\mathrm{Ai}(z)+it^{-1/3}D(\alpha)\mathrm{Ai}'(z)+O(t^{-1})]. \tag{5.7}$$

It is not difficult to check that the conditions of Proposition V.1 are satisfied for the integral $I_n(x,x',t)$, $n=1,\ldots,N$. Therefore there is an asymptotic:

$$I_n(x,x',t)=\pi t^{-1/3}\exp[itA(\alpha)][T_n(\alpha)\mathrm{Ai}(z_n)+it^{-1/3}D_n(\alpha)\mathrm{Ai}'(z_n)+O(t^{-1})], \tag{5.8}$$

uniform in α, $|\alpha|<\delta$. Here we have

$$A_n(\alpha)=(S_{2n-1}(\alpha)+S_{2n}(\alpha))/2,\quad B_n(\alpha)=(3/4)^{2/3}(S_{2n}(\alpha)-S_{2n-1}(\alpha))^{2/3}, \tag{5.9}$$

$$z_n(t,\alpha)=-t^{2/3}B_n(\alpha), \tag{5.10}$$

where $S_l(\alpha)=S(k,\alpha)|_{k=a_l(\alpha)}=[vk-E(k)]|_{k=a_l}$, $l=2n-1,2n$. For $T_n(x,x',\alpha)$ and $D_n(x,x',\alpha)$ we get the formulas:

$$T_n(x,x',\alpha)=(2\pi)^{-1}\sum_{l=2n-1,2n}Q_l(\alpha)X(x,x',a_l(\alpha)), \tag{5.11}$$

$$D_n(x,x',\alpha)=(2\pi)^{-1}B_n^{-1/2}(\alpha)\sum_{l=2n-1,2n}(-1)^{l+1}Q_l(\alpha)X(x,x',a_l(\alpha)), \tag{5.12}$$

where

$$Q_l(\alpha)=\sqrt{2(-1)^{l+1}(B_n(\alpha))^{1/2}/E''_{kk}(a_l(\alpha))},\quad l=2n-1,2n, \tag{5.13}$$

In order to investigate the asymptotics (5.8) when α tends to zero we need

Lemma V.1: For $n=1,\ldots,N$ and small $\alpha=E'(k_n)-v$ there are the following asymptotics:

$$A_n(\alpha)=vk_n-E_n+O(\alpha^{3/2}), \tag{5.14}$$

$$B_n(\alpha)=\alpha(|E_n^{(3)}|/2)^{-1/3}(1+O(\alpha^{1/2})), \tag{5.15}$$

$$T_n(x,x',\alpha)=(\pi)^{-1}(|E_n^{(3)}|/2)^{-1/3}[X(x,x',k_n)+O(\alpha^{1/2})], \tag{5.16}$$

$$D_n(x,x',\alpha)=-(\pi)^{-1}(|E_n^{(3)}|)^{-2/3}[X'_k(x,x',k_n)+O(\alpha^{1/2})]. \tag{5.17}$$

Proof: Let us expand a function $S(k,\alpha)=vk-E(k)$ in a neighborhood of the point $k=k_n$. We obtain [see Eq. (2.10)]

$$S(k,\alpha)=vk_n-E_n-\alpha(k-k_n)+|E_n^{(3)}|(k-k_n)^3/3!+O((k-k_n)^4). \tag{5.18}$$

Hence we get

$$\alpha=|E^{(3)}|(a_l(\alpha)-k_n)^2/2+O((a_l(\alpha)-k_n)^3) \tag{5.19}$$

as $S'_k(a_l(\alpha))=0$, $l=2n-1,2n$. Solving Eq. (5.19) we obtain

$$a_l(\alpha)-k_n=(-1)^l\alpha^{1/2}(|E_n^{(3)}|/2)^{-1/2}+O(\alpha),\quad l=2n-1,2n. \tag{5.20}$$

Putting Eq. (5.20) into Eq. (5.18) we have for $k=a_l(\alpha)$:

$$S_l(\alpha)=S(s_l(\alpha))=vk_n-E_n-\tfrac{2}{3}(-1)^l\alpha^{3/2}(|E_n^{(3)}|/2)^{-1/2}+O(\alpha^2). \tag{5.21}$$

Hence and from Eq. (5.9) we get Eqs. (5.14) and (5.15).

We obtain Eq. (5.16). From Eq. (5.18) we see that $E_k''(a_l(\alpha))=-S_{kk}''(a_l(\alpha))=-|E_n^{(3)}|(a_l(\alpha)-k_n)+O((a_l(\alpha)-k_n)^2)$. Using Eq. (5.20) we find

$$E_{kk}''(a_l(\alpha))=-(-1)^l\alpha^{1/2}(2|E_n^{(3)}|)^{1/2}(1+O(\alpha^{1/2})),\quad l=2n-,2n. \tag{5.22}$$

It is not difficult to check that from Eqs. (5.13), (5.15), and (5.22) it follows

$$Q_l(\alpha)=(|E_n^{(3)}|/2)^{-1/3}(1+O(\alpha^{1/2})). \tag{5.23}$$

As $X(x,x',al(\alpha))=X(x,x',k_n)+X_k'(x,x',k_n)(a_l(\alpha)-k_n)+O((a_l(\alpha)-k_n)^2)$, $l=2n-1,2n$ we obtain [see Eq. (5.20)]

$$X(x,x',a_l(\alpha))=X(x,x',k_n)+(-1)^l\alpha^{1/2}(|E_n^{(3)}|/2)^{-1/2}X_k'(x,x',k_n)+O(\alpha),\quad l=2n-1,2n. \tag{5.24}$$

From Eqs. (5.11), (5.23), and (5.24) follows Eq. (5.16) as $X(x,x',k_n)$ is a periodic function.

Let us now consider $D_n(x,x',\alpha)$ in a neighborhood of the point $\alpha=0$. Transforming Eq. (5.12) and using Eqs. (5.15) and (5.23) we get Eq. (5.17) taking into consideration Eq. (5.24). Lemma V.1 is proved.

To prove Theorem II.2 one should put Eqs. (5.14)–(5.17) into Eqs. (5.8) and (5.10). Then we get Eqs. (5.20) and (5.21).

Remark that from Eq. (5.15) it follows that $B_n(0)=0$ and therefore [see Eq. (5.10)] $z_n(0)=0$. Hence and from Eq. (2.20) we obtain Eq. (2.22). Theorem II.2 is proved.

Let us turn to the proof of Theorem II.3. At first we describe asymptotics of the Airy functions and their derivatives (see for instance Ref. 9)

$$\mathrm{Ai}(-z)=\frac{1}{\sqrt{\pi}}z^{-1/4}\left[\cos\left(\frac{2}{3}z^{3/2}+\frac{\pi}{4}\right)+O(z^{-3/2})\right],\quad z\to\infty, \tag{5.25}$$

$$\mathrm{Ai}'(-z)=\frac{1}{\sqrt{\pi}}z^{1/4}\left[\sin\left(\frac{2}{3}z^{3/2}+\frac{\pi}{4}\right)+O(z^{-3/2})\right],\quad z\to\infty. \tag{5.26}$$

Hence from Eq. (2.21) it follows that when $\alpha t^{2/3}\to\infty$ we have

$$\begin{aligned}\mathrm{Ai}(z_n)=&\frac{1}{\sqrt{\pi}}t^{-1/6}\alpha^{-1/4}(|E_n^{(3)}|/2)^{1/12}(1+O(\alpha^{1/2}))\\&\times\left[\cos\left[\frac{2}{3}t\alpha^{3/2}(|E_n^{(3)}|/2)^{-1/2}(1+O(\alpha^{1/2}))+\frac{\pi}{4}\right]+O(t^{-1}\alpha^{-3/2})\right],\end{aligned} \tag{5.27}$$

$$\mathrm{Ai}'(z_n)=\frac{1}{\sqrt{\pi}}\,t^{1/6}\alpha^{1/4}(|E_n^{(3)}|/2)^{-1/12}(1+O(\alpha^{1/2}))$$
$$\times\left[\sin\left[\frac{2}{3}\,t\alpha^{3/2}(|E_n^{(3)}|/2)^{-1/2}(1+O(\alpha^{1/2}))+\frac{\pi}{4}\right]+O(t^{-1}\alpha^{-3/2})\right]. \tag{5.28}$$

The statement of Theorem II.3 follows Eq. (2.20).

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Variational formulation of a moment problem quantization method

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The eigenvalue moment method (EMM) has proven to be an effective technique for generating converging lower and upper bounds to the bosonic ground state energy of singular, strongly coupled, quantum systems. Application of EMM theory requires an appropriate linearization of the highly nonlinear Hankel–Hadamard (HH) moment determinant constraints for the $(n+1)\times(n+1)$ Hankel matrices $\mathscr{M}^n[\mathbf{u}] \equiv \hat{M}_0^n + \Sigma_{i=1}^{m_s}\hat{M}_i^n u(i)$, dependent on the *missing moment* variables $\{u(i)\}\equiv\mathbf{u}$. We propose an alternate variational formulation utilizing the functions $\mathrm{Det}(\mathscr{M}^{n+1}[\mathbf{u}])/\mathrm{Det}(\mathscr{M}^n[\mathbf{u}])$, which we prove to be locally convex over the missing moment subset satisfying the HH positivity conditions $\mathrm{Det}(\mathscr{M}^\nu[\mathbf{u}])>0$, for $\nu\leqslant n$. Additional features of this variational formulation facilitate its application to important problems such as the octic, sextic, and quartic anharmonic oscillators.
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I. INTRODUCTION

The eigenvalue moment method (EMM) is a general procedure for generating converging lower and upper bounds to the ground state energy of Schrödinger Hamiltonians.[1–3] It is a nonperturbative and highly accurate method that utilizes fundamental theorems in mathematics (moment problems),[4,5] mathematical physics (positivity properties of physical bound states),[6] and operations research (optimization methods such as linear programming).[7] Its intrinsic Fourier space representation structure defines a systematic multiscale approach suitable for solving strongly coupled singular perturbation type systems. Unlike some bounding methods that require semibounded Hamiltonians or identification of a positive definite decomposition ($H=H_0+V$, where V is positive definite),[8–10] the EMM approach is independent of such preconditions. In contrast to some recently developed basis-dependent bounding methods,[11,12] EMM is explicitly independent of any basis set specification. All of these properties suggest that EMM may offer an important alternative to other methods for yielding precise eigenenergies through converging bounds.

Many one- and two-dimensional problems have been solved through EMM theory, including the well-known quadratic Zeeman effect for superstrong magnetic fields.[3] Its extension to larger systems such as the spinless Coulombic three body problem with $J=0$ (a three-dimensional system), for approximate/exact coequal masses (i.e., Ps^-),[13] will require more efficient computational schemes, such as that made possible through the variational formulation developed in this work.

A. Overview of EMM

The basic structure of the EMM formalism, as outlined below through a generic one-dimensional parity invariant example, begins with the transformation of the Schrödinger equation (with a rational fraction potential),

$$-\frac{d^2\Psi}{dx^2}+V(x)\Psi(x)=E\Psi(x), \tag{1.1}$$

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into a Stieltjes moment equation representation of the form

$$u(p)=\hat{M}_E(p,0)+\sum_{i=1}^{m_s}\hat{M}_E(p,i)u(i), \tag{1.2}$$

for $p\geqslant 0$. The latter expresses the linear dependence on the $(u(1),\ldots,u(m_s))$ moments (designated the *missing moments*), through energy-dependent coefficients obtainable algebraically or numerically. Through an implicit normalization, the missing moments are limited to the m_s-dimensional hypercube, $[0,1]^{m_s}$. The m_s index is related to the differential equation order for the Fourier transformed Schrödinger equation.

Quantization of the ground state energy proceeds by constraining the missing moments and energy parameter variable to satisfy the highly nonlinear Hankel–Hadamard (HH) determinental inequalities:

$$\Delta_{m,n}[u]>0, \quad m=0, \quad 1 \quad \text{and} \quad n\geqslant 0; \tag{1.3a}$$

where

$$\Delta_{m,n}[u]\equiv \mathrm{Det}(\mathscr{M}^{m,n}(u)), \tag{1.3b}$$

and the $(n+1)\times(n+1)$ Hankel matrices are defined by $(\mathscr{M}^{m,n}(u))_{i,j}\equiv u(m+i+j)$, for $0\leqslant i,j\leqslant n$. These constraints follow from the positivity of the bosonic ground state wavefunction, $\Psi_{\mathrm{gr.}}(x)>0$,[6] and the well-known Moment Problem theorems for positive functions.[4,5] In particular, the HH inequalities are necessary and sufficient [within the context of Eq. (1.2)] to characterize a positive measure.

The missing moment solution set to Eq. (1.3a), for $m+2n\leqslant N$, is denoted by $\mathscr{U}_E^N$. It is convex.[2,3] The index N denotes the maximum moment order used in the corresponding HH determinants $(u(\nu),0\leqslant\nu\leqslant N)$. Let $\mathscr{U}_{E,n}^m$ denote the missing moment solution set satisfying $\Delta_{m,\nu}[u]>0$ for fixed m and all $\nu\leqslant n$. It is also convex. Let $n[N]$ and $m[N]$ (0 or 1) refer to the unique elements of the decomposition $N\equiv 2n[N]+m[N]$, then $\mathscr{U}_E^N \equiv \mathscr{U}_{E,n[N]}^{m[N]}\cap\mathscr{U}_{E,n[N-1]}^{m[N-1]}$.

The focus of the computational implementation of EMM is to determine, for a given E parameter value, the existence or nonexistence of $\mathscr{U}_E^N$. The energy values associated with existing solution sets define an open interval (E_N^L,E_N^U), which, in turn, through the end points, define the converging lower and upper bounds to the ground state energy, $E_N^L\leqslant E_g\leqslant E_N^U$.

One of the more successful approaches for solving the highly nonlinear HH inequalities makes use of linear programming (LP) to quickly *cut* up the unit m_s hypercube into either the null set, or a finite polytope containing the solution set.[2,3] Either of these outcomes establishes the nonexistence or existence of $\mathscr{U}_E^N$, respectively. This approach yielded excellent bounds for the superstrong quadratic Zeeman effect.[3] However, because many linear inequalities (*cuts*) must be stored, this approach may not be appropriate for larger systems. Variational approaches do not have this difficulty and as such have been the focus of much recent work.

B. Variational formulations

A first attempt at defining an alternate variational formulation[14] involved the globally convex function $(\mathbf{u}\equiv(u(1),\ldots,u(m_s)))$,

$$F_E^n[\mathbf{u}]\equiv \mathrm{Min}_{m=0,1}\,\lambda^{m,n}[\mathbf{u}], \tag{1.4}$$

where $\lambda^{m,n}[\mathbf{u}]$ is the smallest eigenvalue of the $\mathscr{M}^{m,n}$ Hankel matrix.[15,16] We refer to $F_E^n[\mathbf{u}]$ as the *Volcano function* for its suggestive graphical representation in the context of the sextic anharmonic oscillator problem.[16] Gradient methods can be used to determine the global maximum of the *Volcano* function, $V_n(E)=\mathrm{Max}_{\mathbf{u}}F_E^n[\mathbf{u}]$, enabling the determination of the energy feasibility inter-

val, (E_N^L, E_N^U), through the relation $V_n(E)>0$.[14] However, because the *Volcano* function is continuous and piecewise differentiable (corresponding to the degenerate intersection of varying Hankel matrix eigenvalue surfaces) this overall approach is very delicate to implement for multidimensional problems. Furthermore, the calculation of the Hankel eigenvalues can be costly. For all of these reasons, the gradient/variational analysis of the Volcano function is not suitable for large systems.

Despite the above, we have been able to formulate an alternate gradient/variational approach with many exceptional features. The present approach involves a hierarchy of locally convex functions on which gradient methods are implemented.

From the definition of the HH determinental constraints the nonlinear convex solution sets satisfy the subset relations:

$$[0,1]^{m_s} \supset \mathscr{U}_E^0 \supset \mathscr{U}_E^1 \supset \cdots \supset \mathscr{U}_E^N . \tag{1.5}$$

Utilizing gradient optimization methods, the sequence of locally convex functions,

$$\mathscr{D}_{n[\nu]}^{m[\nu]}[\mathbf{u}], \quad \text{for } \nu = 0,1,\ldots, \tag{1.6a}$$

where

$$\mathscr{D}_n^m[\mathbf{u}] = \frac{\Delta_{m,n}[u]}{\Delta_{m,n-1}[u]}, \tag{1.6b}$$

can be used to systematically locate a convex subset within the previous one, $\mathscr{U}_E^\nu \to \mathscr{U}_E^{\nu+1}$. Specifically (for fixed E), starting at an arbitrary point, $\mathbf{u} \in [0,1]^{m_s}$, gradient iteration/optimization on $\mathscr{D}_0^0$ will generate a point, $\mathbf{u}_0$, lying in $\mathscr{U}_E^0$. A subsequent gradient iteration/optimization with respect to $\mathscr{D}_0^1$ will define a new point in $\mathscr{U}_E^1$, and so forth. In general, at the point $\mathbf{u}_N \in \mathscr{U}_E^N$, gradient iteration with respect to $\mathscr{D}_{n[N+1]}^{m[N+1]}$, restricted to the $\mathscr{U}_E^N$ set, will either generate a point in $\mathscr{U}_E^{N+1}$ or yield a nonpositive maximum. The latter establishes that the particular E value chosen is not in the feasible energy interval (E_{N+1}^L, E_{N+1}^U).

The $\mathscr{D}_n^m$ functions are simply the diagonal entries appearing in the LU decomposition of the associated Hankel matrix,

$$\mathscr{M}^{m,n}[u] \equiv \mathscr{L}^{m,n}[u]\mathscr{D}^{m,n}[u](\mathscr{L}^{m,n}[u])^t, \tag{1.7a}$$

where $\mathscr{L}$ is a lower triangular matrix with unit diagonals and $\mathscr{D}^{m,n}$ corresponds to the diagonal matrix,

$$\mathscr{D}^{m,n}[u] \equiv \begin{pmatrix} \mathscr{D}_0^m[u] & 0 & 0 & \cdots \\ 0 & \mathscr{D}_1^m[u] & 0 & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \mathscr{D}_n^m[u] \end{pmatrix}. \tag{1.7b}$$

They are easily obtained. In the Appendix we prove that they are locally convex. This is an important property that removes any multimaxima concerns in implementing the aforementioned gradient optimization. Also, the gradient vector, $\partial_{u_i}\mathscr{D}_n^m[\mathbf{u}]$, is easily computed without having to do any numerical differencing. As such, this overall variational program defines an efficient approach for studying large systems. We present this alternate LU-EMM gradient method in the context of three one-dimensional problems: the octic, sextic, and quartic anharmonic oscillators. The more difficult case is presented first (the octic) in order to define the underlying theory. The

sextic results are presented in the tables with minimal discussion. The quartic anharmonic problem affords some interesting graphical illustrations, highlighting the essentials of the theory.

II. IMPORTANT PROPERTIES OF THE LU-EMM VARIATIONAL FORMULATION

From Eq. (1.7), which denotes the LU decomposition of the symmetric Hankel matrices, and the determinental relation $\mathrm{Det}(\mathscr{M}^{m,n})=\Pi_{\nu=0}^{n}\mathscr{D}_n^m$, one may replace the standard HH determinental positivity constraints with positivity constraints for the LU diagonals:

$$\mathscr{D}_n^m[\mathbf{u}]>0, \tag{2.1}$$

for $m=0,1$ and $n\geqslant 0$. For future reference, we rewrite the Hankel matrices as explicit functions of the missing moments ($\mathbf{u}\equiv(u(1),u(2),\ldots,u(m_s))$),

$$(\mathscr{M}^{m,n}[\mathbf{u}])_{i,j}\equiv\hat{M}_E(m+i+j,0)+\sum_{l=1}^{m_s}\hat{M}_E(m+i+j,l)u(l), \tag{2.2a}$$

for $0\leqslant i,j\leqslant n$. In abbreviated matrix notation we have

$$\mathscr{M}^{m,n}[\mathbf{u}]\equiv\hat{M}_{E;0}^{m}+\sum_{l=1}^{m_s}\hat{M}_{E;l}^{m}u(l), \tag{2.2b}$$

where the expressions are defined by their relative appearance in Eq. (2.2a).

Despite the fact that the diagonal functions are ratios of successive HH determinants, $\mathscr{D}_n^m[\mathbf{u}]\equiv\mathrm{Det}(\mathscr{M}^{m,n}[\mathbf{u}])/\mathrm{Det}(\mathscr{M}^{m,n-1}[\mathbf{u}])$, and therefore singular, they nevertheless have some very important properties. Clearly, they are infinitely differentiable at any nonsingular point. In the following discussion, all energy, E, dependencies are implicitly assumed.

A. Local convexity property for $\mathscr{D}_n^m[\mathbf{u}]$

We prove in the Appendix that the LU diagonal $\mathscr{D}_n^m[\mathbf{u}]$, for $n\geqslant 0$, regarded as a function of the missing moment variables, exists (is finite) and is a convex function (not necessarily of uniform signature) on the open convex subset $\mathscr{U}_{n-1}^m\equiv\{\mathbf{u}|\mathscr{D}_\nu^m[\mathbf{u}]>0,\ 0\leqslant\nu\leqslant n-1,\ \text{and}\ 0<u(i)<1,\ 1\leqslant i\leqslant m_s\}$.

B. Simple expression for $\nabla\mathscr{D}_n^m[\mathbf{u}]$

In the Appendix we derive a convenient closed form expression for the gradient vector of the diagonal functions:

$$\partial_{u_l}\mathscr{D}_n^m[\mathbf{u}]=\langle\mathscr{V}^{m;n}[\mathbf{u}]|\hat{M}_l^m|\mathscr{V}^{m;n}[\mathbf{u}]\rangle, \tag{2.3}$$

for $1\leqslant l\leqslant m_s$, where the $\mathscr{V}^{m;n}$ vectors are automatically generated through the LU decomposition. Indeed, as shown by Handy[17] (and discussed in the Appendix), the usual LU decomposition of a symmetric matrix, $\mathscr{M}$, is equivalent to considering the set of *generalized orthogonal vectors* satisfying $\langle\mathscr{V}^i|\mathscr{M}|\mathscr{V}^j\rangle=\delta_{i,j}$, where the components of the ith vector satisfy $\mathscr{V}_{j<i}^i\neq 0$, $\mathscr{V}_i^i=1$, and $\mathscr{V}_{j>i}^i=0$.

C. Singularities of $\mathscr{D}_n^m[\mathbf{u}]$

The singularities of the diagonal functions do not pose any difficulties if restricted to the $\mathscr{U}_n^m$ subsets. Specifically, from $[0,1]^{m_s}\supset\mathscr{U}_0^m\cdots\supset\mathscr{U}_n^m$, it follows that all of the diagonal functions

$\mathscr{D}^m_{\nu\leqslant n}[\mathbf{u}]$ are positive and convex on $\mathscr{U}^m_n$. Also, none of them can become singular at the boundary of $\mathscr{U}^m_n$ (when approached from within the set) since a differentiable positive convex function cannot be singular at a finite point.

The convex function $\mathscr{D}^m_{n+1}[\mathbf{u}]$ can become singular on the boundary of $\mathscr{U}^m_n$, since it can have a nonuniform signature on $\mathscr{U}^m_n$. Even then, if it becomes singular, it can only do so by becoming negatively infinite. That is, if $|\mathscr{D}^m_{n+1}[\mathbf{u}\rightarrow\mathbf{u}_\beta]|\rightarrow\infty$, for $\mathbf{u}_\beta\in$Boundary $(\mathscr{U}^m_n)$ and $\mathbf{u}\in\mathscr{U}^m_n$, then $\mathscr{D}^m_{n+1}[\mathbf{u}\rightarrow\mathbf{u}_\beta]\rightarrow-\infty$. This is also a consequence of the convexity property of the diagonal functions and the boundedness of the subsets in question, since a convex function can become negatively infinite at a finite point. The graphical representation for the quartic anharmonic oscillator illustrates these results.

The gradient optimization implementation of the proposed LU-EMM variational formulation always seeks to maximize the $\mathscr{D}^m_{n+1}$ function over the $\mathscr{U}^m_n$ subset. As such, one is always moving away from singularities. Therefore, in conclusion, the singularities of the LU diagonals do not affect the numerical implementation of the LU-EMM variational gradient optimization approach.

The preceding results were based on the local convexity property of the LU-diagonal functions, and the boundedness of the subsets in question. An alternate proof that the $\mathscr{D}^m_{\nu\leqslant n}[\mathbf{u}]$ diagonal, restricted to the $\mathscr{U}^m_n$ subset, cannot become positively infinite at the boundary follows from the eigenvalue-interlacing theorem for symmetric matrices. Let $\mathscr{M}^{\nu\leqslant n}$ denote the upper left hand $(1+\nu)\times(1+\nu)$ submatrices for the symmetric matrix $\mathscr{M}^n$. Assume that for some $k<n$, $\mathrm{Det}(\mathscr{M}^{\nu<k})>0$ and $\mathrm{Det}(\mathscr{M}^k)=0$. Then $\mathrm{Det}(\mathscr{M}^{k+1})\leqslant 0$. To prove this, let λ^ν_i denote the ith eigenvalue for the $\mathscr{M}^\nu$ matrix. From the eigenvalue interlacing theorem, $\lambda^{\nu+1}_i\leqslant\lambda^\nu_i\leqslant\lambda^{\nu+1}_{i+1}$, for $i=0,\ldots,\nu$, it follows that all of the eigenvalues of $\mathscr{M}^{\nu<k}$ are positive, while the smallest eigenvalue of $\mathscr{M}^k$ is zero. Accordingly, the matrix $\mathscr{M}^{k+1}$ can have only one nonpositive eigenvalue.

Let us now assume that the preceding matrices correspond to the Hankel, missing moment-dependent, matrices (the m index is implicit) $\mathscr{M}^{\nu\leqslant n}[\mathbf{u}]$, and that $\mathbf{u}\in\mathscr{U}_n$ (the convex set on which all the indicated Hankel matrices have positive determinants). Let us approach the boundary of $\mathscr{U}_n$ from a particular direction within the set, $\mathbf{u}\rightarrow\mathbf{u}_\beta$. Let k (as used above) refer to the first submatrix to have a zero determinant at $\mathbf{u}_\beta$. Then from the eigenvalue interlacing property, as well as the fact that one is approaching the boundary from within the set $\mathscr{U}_n$, and the continuity of the determinant function with respects to the moment variables, it follows that $\mathrm{Det}(\mathscr{M}^{k+1}(\mathbf{u}_\beta))=0$.

With respects to successive determinant ratios of the form

$$\frac{\mathrm{Det}\,\mathscr{M}^{k+1}[\mathbf{u}]}{\mathrm{Det}\,\mathscr{M}^k[\mathbf{u}]}=\frac{\Pi^{k+1}_{i=0}\lambda^{k+1}_i[\mathbf{u}]}{\Pi^k_{i=0}\lambda^k_i[\mathbf{u}]}, \tag{2.4}$$

upon recognizing the positivity of the eigenvalues and $0<\lambda^{k+1}_i[\mathbf{u}]/\lambda^k_i[\mathbf{u}]\leqslant 1$, for $0\leqslant i\leqslant k$ (as long as $\mathbf{u}$ lies within the open set $\mathscr{U}_n$), then

$$\mathrm{Lim}_{\mathbf{u}\rightarrow\mathbf{u}_\beta}\left(\frac{\mathrm{Det}\,\mathscr{M}^{k+1}[\mathbf{u}]}{\mathrm{Det}\,\mathscr{M}^k[\mathbf{u}]}\right)=0, \tag{2.5}$$

or a finite positive number.

This confirms the same conclusion reached through the local convexity property for such determinant ratios (with positive numerator and denominator determinants). Only the ratio $\mathrm{Det}\,\mathscr{M}^{n+1}[\mathbf{u}]/\mathrm{Det}\,\mathscr{M}^n[\mathbf{u}]$ over the $\mathscr{U}_n$ set, involving a nonpositive numerator determinant, can have singularities along the boundary. Even then, these must be negative infinity singularities.

Despite the simplicity of the previous results based on the eigenvalue interlacing theorem, it is the local convexity property for the LU diagonals, as defined above, that is most important with respects to the overall LU-EMM variational formalism. Not only does local convexity tame the

singularities, but it also ensures the absence of multimaxima concerns in implementing the gradient optimization program summarized in the Introduction and further discussed in the ensuing sections.

III. THE OCTIC ANHARMONIC OSCILLATOR

Consider the Schrödinger octic anharmonic potential problem:

$$-\frac{d^2\Psi}{dx^2}+[mx^2+gx^8]\Psi(x)=E\Psi(x). \tag{3.1}$$

Define the Hamburger moments by $\mu(p)\equiv\int_{-\infty}^{+\infty}dx\ x^p\Psi(x)$. Upon multiplying both sides of Eq. (3.1) by x^p and integrating by parts, there results the moment equation:

$$\mu(p+8)=g^{-1}[-m\mu(p+2)+E\mu(p)+p(p-1)\mu(p-2)], \tag{3.2}$$

for $p\geqslant 0$.

The ground state wave function must be symmetric. This allows us to simplify the previous equation and work with the even-order Hamburger moments: $\mu(2\rho)\equiv u(\rho)$, where the latter are Stieltjes moments, $u(\rho)=\int_0^{+\infty}dy\ y^\rho(\Psi(\sqrt{y})/\sqrt{y})$ (i.e., $y\equiv x^2$). Accordingly, the corresponding Stieltjes moment equation is

$$u(p+4)=g^{-1}[-mu(p+1)+Eu(p)+2p(2p-1)u(p-1)], \tag{3.3}$$

for $p\geqslant 0$. The energy, E, appears as a variable parameter.

The Stieltjes moment equation corresponds to a linear finite difference equation of effective degree four. Thus, upon initializing the moments $\{u(0),u(1),u(2),u(3)\}$ one may generate all of

TABLE I. LU-EMM gradient bounds: x^2+x^8.

$N_{\max}$	E_{lower}	E_{upper}
8	1.42	1.56
9	1.4298	1.5138
10	1.482 72	1.5138
11	1.484 895 6	1.501 368
12	1.484 895 6	1.491 978 732
13	1.490 137 117 68	1.491 837 069 36
14	1.490 851 097 385 6	1.491 769 071 292 8
15	1.490 851 097 385 6	1.491 135 669 296 8
16	1.490 902 320 329 6	1.491 064 526 319 0
17	1.491 009 376 282 6	1.491 064 526 319 0
18	1.491 011 030 783 7	1.491 034 193 799 0
19	1.491 011 494 044 0	1.491 021 222 510 4
20	1.491 018 303 970 5	1.491 021 222 510 4
21	1.491 019 617 313 5	1.491 021 134 954 2
22	1.491 019 617 313 5	1.491 020 057 429 3
23	1.491 019 727 342 4	1.491 019 960 603 8
24	1.491 019 881 294 9	1.491 019 960 603 8
25	1.491 019 883 674 2	1.491 019 915 397 8
26	1.491 019 883 674 2	1.491 019 897 632 6
27	1.491 019 893 584 7	1.491 019 897 493 0
28	1.491 019 895 265 2	1.491 019 897 375 7
29	1.491 019 895 265 2	1.491 019 895 856 2
30	1.491 019 895 454 3	1.491 019 895 732 1

TABLE II. LU-EMM gradient bounds: x^2+x^6.

$N_{\max}$	E_{lower}	E_{upper}
6	1.31	1.51
7	1.3802	1.4602
8	1.409 78	1.460 15
9	1.423 38	1.460 15
10	1.423 748 685 05	1.437 720 906 95
11	1.434 926 462 57	1.437 720 906 95
12	1.435 233 851 451 80	1.436 407 518 091 40
13	1.435 245 588 118 20	1.435 691 581 441 25
14	1.435 557 783 444 33	1.435 687 121 508 02
15	1.435 601 758 385 98	1.435 683 241 366 10
16	1.435 601 758 385 98	1.435 627 832 939 62
17	1.435 621 575 046 74	1.435 627 572 194 08
18	1.435 623 674 048 31	1.435 627 212 365 24
19	1.435 623 709 431 48	1.435 624 770 926 56
20	1.435 624 431 248 12	1.435 624 760 311 60
21	1.435 624 576 036 05	1.435 624 760 311 59
22	1.435 624 577 878 80	1.435 624 627 633 20
23	1.435 624 609 224 08	1.435 624 626 140 57
24	1.435 624 617 343 99	1.435 624 625 802 24
25	1.435 624 617 343 99	1.435 624 619 458 56
26	1.435 624 618 485 86	1.435 624 619 331 69
27	1.435 624 618 934 16	1.435 624 619 331 69
28	1.435 624 618 938 13	1.435 624 619 025 59
29	1.435 624 618 977 49	1.435 624 619 018 60
30	1.435 624 619 000 92	1.435 624 619 017 77

TABLE III. LU-EMM gradient bounds: x^2+x^4.

$N_{\max}$	E_{lower}	E_{upper}
5	1.115	1.460
6	1.346 15	1.4462
7	1.367 160 5	1.436 195
8	1.367 160 5	1.400 987 405
9	1.390 501 064 45	1.400 987 405
10	1.390 710 791 261 00	1.392 703 195 965 50
11	1.392 025 778 365 97	1.392 623 499 777 33
12	1.392 234 980 859 94	1.392 611 545 349 09
13	1.392 234 980 859 94	1.392 385 606 655 60
14	1.392 346 443 948 73	1.392 384 100 397 64
15	1.392 347 573 642 20	1.392 353 598 674 02
16	1.392 349 682 403 34	1.392 352 935 920 53
17	1.392 351 179 021 24	1.392 352 903 385 36
18	1.392 351 179 021 24	1.392 351 748 061 40
19	1.392 351 628 562 96	1.392 351 742 370 99
20	1.392 351 629 701 04	1.392 351 654 738 81
21	1.392 351 630 452 18	1.392 351 646 977 10
22	1.392 351 639 871 39	1.392 351 646 977 10
23	1.392 351 639 942 45	1.392 351 641 789 93
24	1.392 351 641 457 38	1.392 351 641 752 97
25	1.392 351 641 475 11	1.392 351 641 611 08
26	1.392 351 641 475 11	1.392 351 641 551 26
27	1.392 351 641 525 37	1.392 351 641 551 25
28	1.392 351 641 525 62	1.392 351 641 530 80
29	1.392 351 641 529 76	1.392 351 641 530 80
30	1.392 351 641 530 06	1.392 351 641 530 77

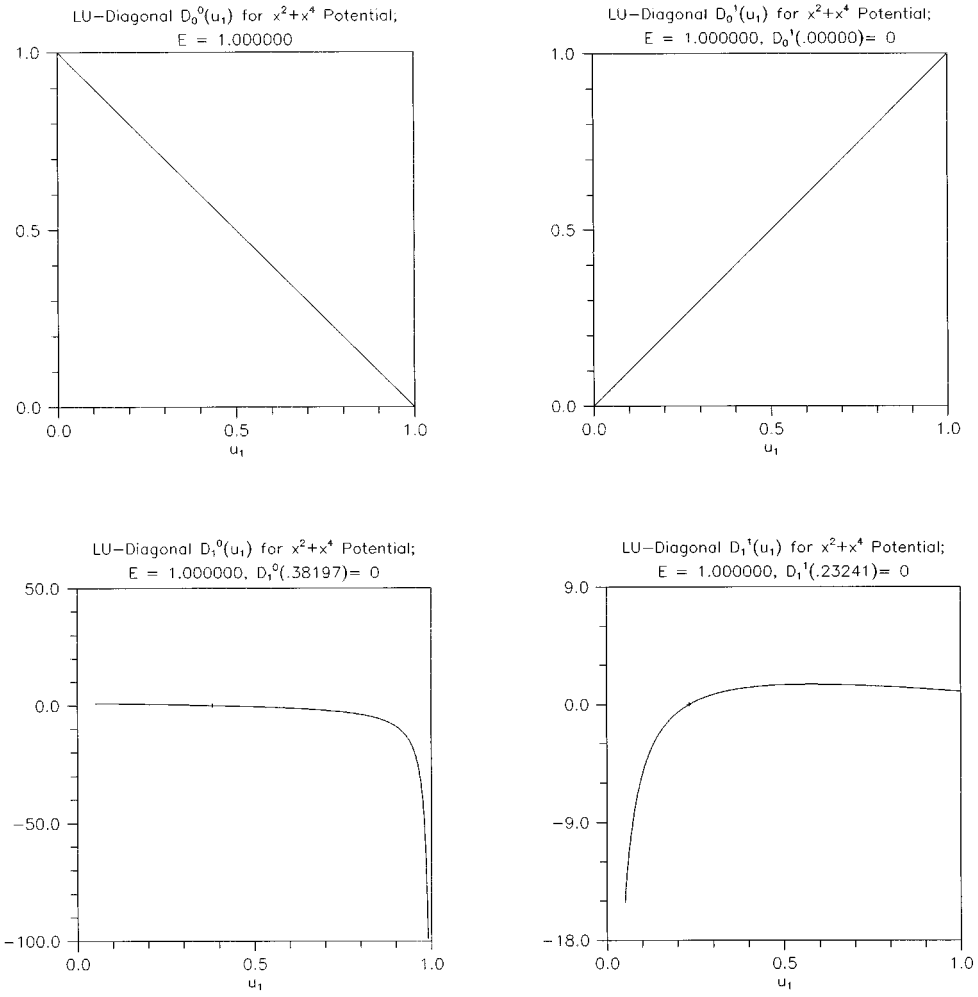

FIG. 1. LU-diagonal functions for quartic anharmonic oscillator, $E=1$.

the remaining moments. The initialization moments are referred to as *missing moments*. The linear dependence of the moments on the missing moments may be expressed through the relation

$$u(p)=\sum_{i=0}^{3} M_E(p,i)u(i), \tag{3.4}$$

where the energy-dependent coefficients $M_E(p,i)$ are numerically or algebraically obtainable and satisfy the *initialization* conditions $M_E(i,j)\equiv\delta_{i,j}$, for $0\leqslant i,j\leqslant 3$.

The homogeneous character of the moment equation requires the imposition of an additional normalization condition. One choice is

$$\sum_{i=0}^{3} u(i)=1. \tag{3.5}$$

Upon solving for $u(0)$, we may reexpress the linear dependence of the moments upon the unconstrained missing moments by

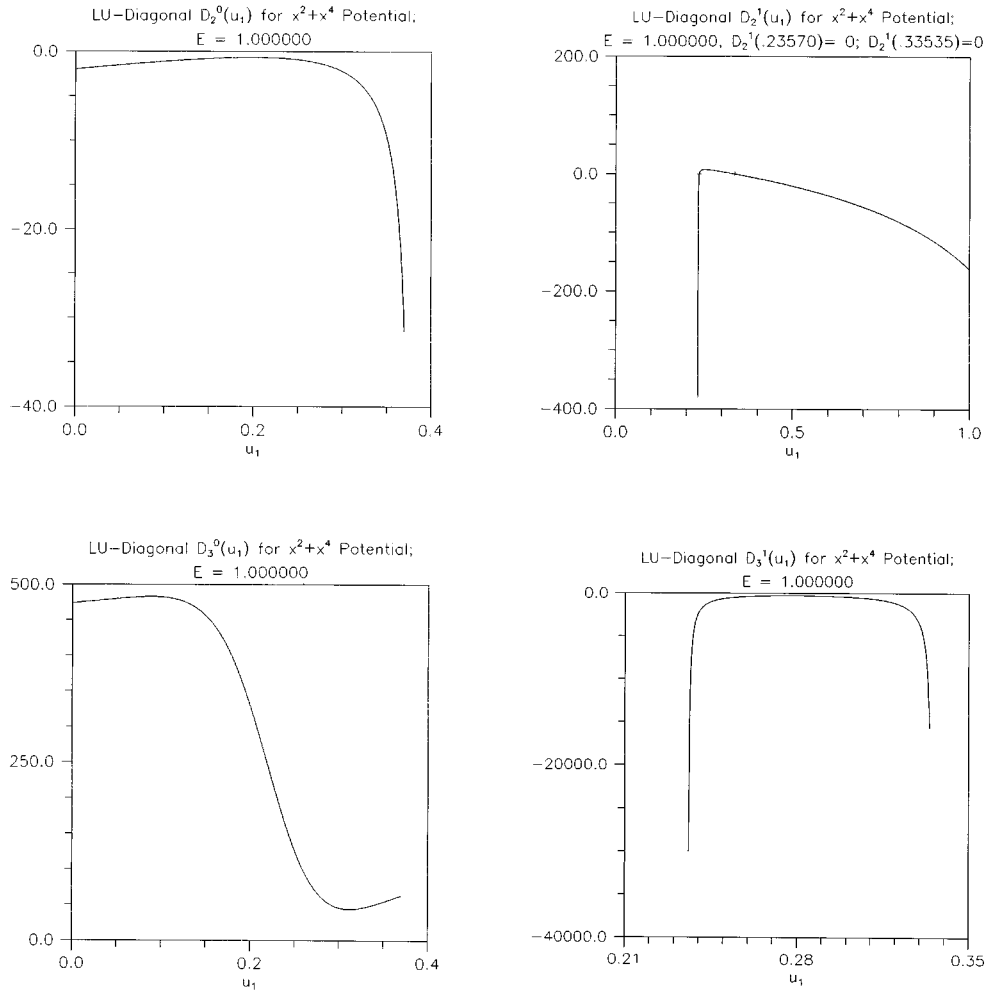

FIG. 1 (*Continued.*)

$$u(p)=\sum_{i=0}^{3}\hat{M}_E(p,i)\hat{u}(i), \tag{3.6}$$

where $\hat{u}(0)\equiv 1$ and $\hat{u}(i)\equiv u(i)$ for $i=1,2,3$. The associated coefficients satisfy $\hat{M}_E(p,0)=M_E(p,0)$ and $\hat{M}_E(p,i)=M_E(p,i)-M_E(p,0)$, for $i=1,2,3$.

Quantization of the ground state energy is achieved by imposing the positivity constraints on the LU diagonals of the Hankel matrices, as indicated in the previous sections. This is a consequence of the positivity of the ground state wave function. The first two LU-diagonal functions to be considered, $\mathscr{D}_{n[0]}^{m[0]}$ and $\mathscr{D}_{n[1]}^{m[1]}$, are defined by $\mathscr{D}_0^0=u(0)=1-u(1)-u(2)-u(3)$ and $\mathscr{D}_0^1=u(1)$, respectively.

From the positivity of the ground state wave function and the adopted normalization condition, it follows that $0<u(0)<1$, as well as $0<u(i=1,2,3)<1$. The last set of relations corresponds to restricting the unconstrained missing moments to the unit cube: $\mathbf{u}=(u(1),u(2),u(3))\in[0,1]^3\equiv\mathscr{C}^3$. This restriction also satisfies the requirement $u(0)<1$ as well as $\mathscr{D}_0^1>0$. In order to satisfy $0<u(0)$, we may take $\mathbf{u}\equiv(\rho,\rho,\rho)$, where $u(0)=1-3\rho>0$. An appropriate choice is $\rho=\frac{1}{4}$. Note that the point $(\frac{1}{4},\frac{1}{4},\frac{1}{4})\in\mathscr{U}_E^1\subset\mathscr{U}_E^0$.

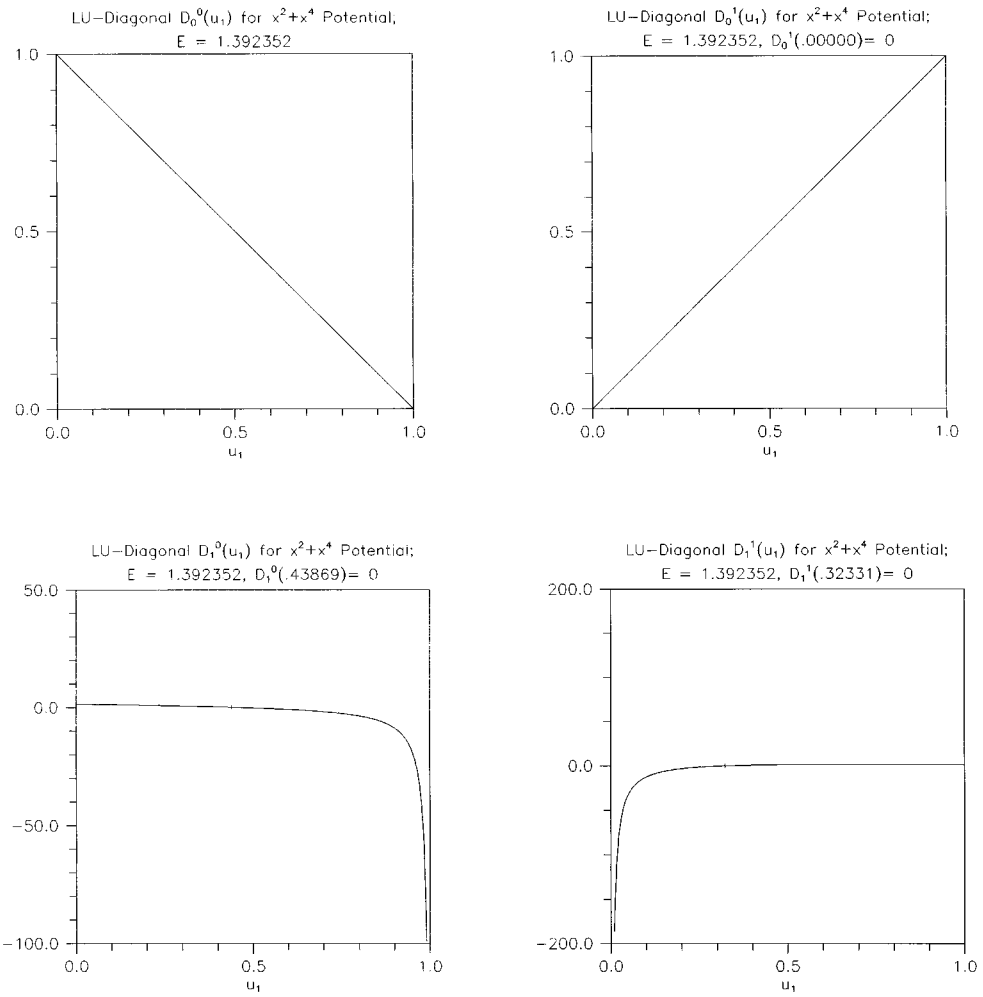

FIG. 2. LU-diagonal functions for quartic anharmonic oscillator, $E=1.392\,352$.

Starting at the point $(\frac{1}{4},\frac{1}{4},\frac{1}{4})$, for a given fixed E and maximum moment order N, we implement a gradient iteration ansatz of the form

$$\mathbf{u}_{l+1}=\mathbf{u}_l+s_l\boldsymbol{\nabla}\mathscr{D}_1^0[E,\mathbf{u}_l], \tag{3.7}$$

to determine the maximum of $\mathscr{D}_{n[2]}^{m[2]}[\mathbf{u}] \equiv \mathscr{D}_1^0[\mathbf{u}]$ over the set $\mathscr{U}_E^1$. If any iterate satisfies $\mathscr{D}_1^0[\mathbf{u}_{l*}]>0$, then it establishes the existence of the subset $\mathscr{U}_E^2$. If the gradient iterates converge to a nonpositive maximum, $\mathscr{D}_1^0[\mathbf{u}_\infty]\leqslant 0$, then it establishes the nonexistence of $\mathscr{U}_E^2$. Given the former possibility, one then continues to perform a gradient optimization for locating the maximum of the LU diagonal $\mathscr{D}_{n[3]}^{m[3]}[\mathbf{u}] \equiv \mathscr{D}_1^1[\mathbf{u}]$ restricted to the $\mathscr{U}_E^2$ subset. Of course, the starting iterate point is $\mathbf{u}_{l*}$. If the ensuing gradient iteration points yield positive $\mathscr{D}_1^1$ values, then they must correspond to points in $\mathscr{U}_E^3$, establishing the existence of the subset. If the gradient iterates identify a nonpositive maximum, then $\mathscr{U}_E^3$ does not exist. The entire process continues up to order N. In this manner one determines if the chosen E value is physically feasible or not, thereby eventually determining the feasibility energy interval (E_N^L,E_N^U).

The above procedure corresponds to a constrained gradient optimization method. When the gradient iterates hit the boundary of the corresponding subset, one must define a new gradient

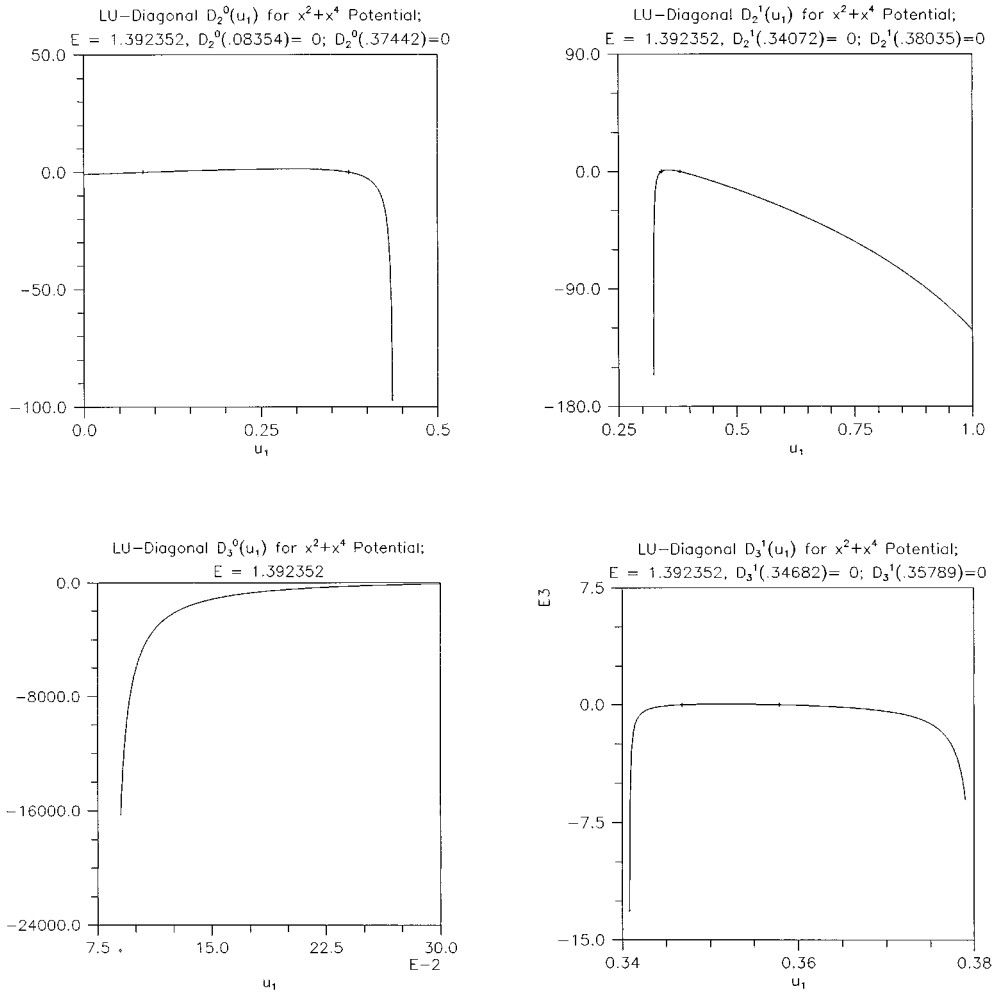

FIG. 2 (*Continued.*)

iteration direction consistent with the inward normal vectors to the intersected boundary. These inward normal vectors are either the inward normal vectors to the $[0,1]^3$ cube, or the gradient vectors for the LU diagonal functions defining the intersected boundary. The details for implementing this may be found elsewhere.[18]

The application of the above gradient procedure was done with respect to the octic anharmonic oscillator. The ground state energy results are given in Table I and reproduce the same bounds obtained through the traditional, linear programming based, EMM procedure, as it should. The LU-EMM gradient method was also applied to the sextic anharmonic oscillator [i.e., replace the gx^8 term in Eq. (3.1) by gx^6]. The results also duplicated the bounds generated by the traditional EMM approach. These are cited in Table II.

IV. THE QUARTIC ANHARMONIC OSCILLATOR

The quartic anharmonic oscillator is defined by the equation

$$-\frac{d^2\Psi}{dx^2}+[x^2+gx^4]\Psi(x)=E\Psi(x). \tag{4.1}$$

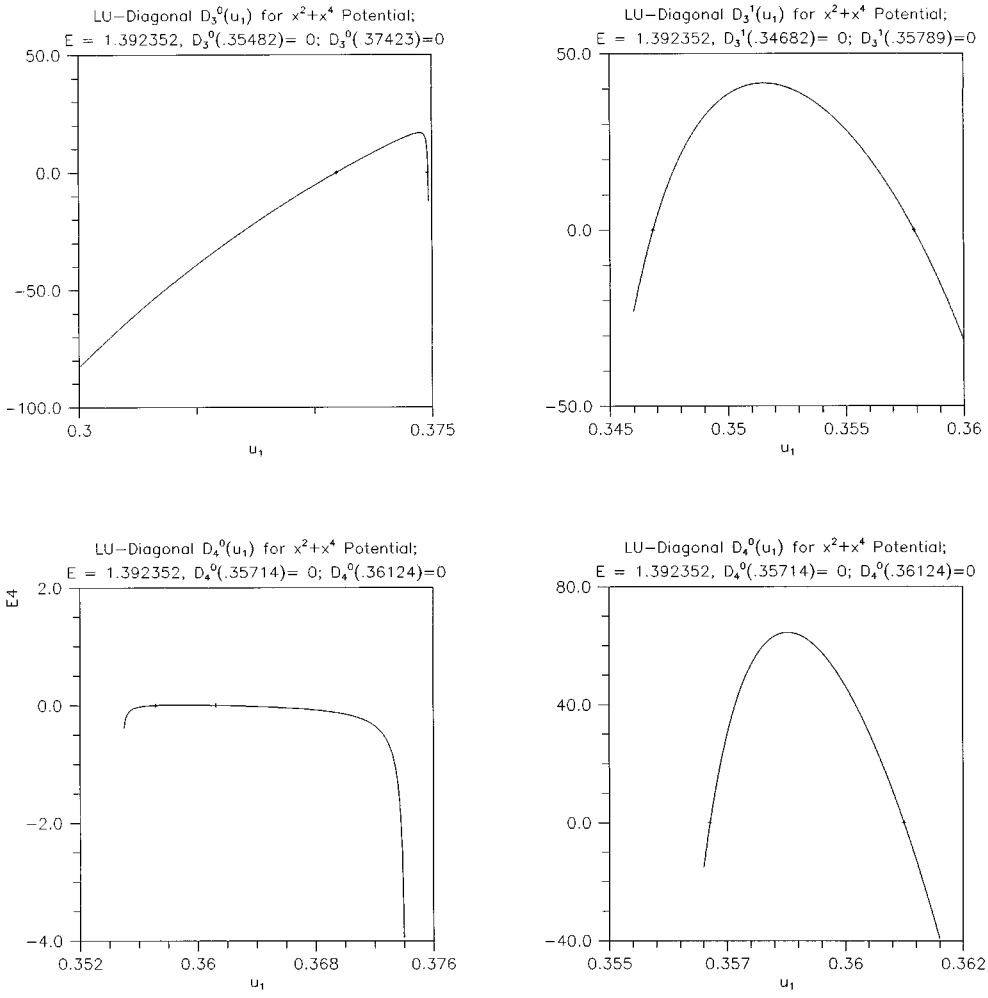

FIG. 2 (*Continued.*)

The corresponding Stieltjes moment equation for the symmetric states is given by

$$u(p+2)=g^{-1}[-u(p+1)+Eu(p)+2p(2p-1)u(p-1)], \tag{4.2}$$

for $p\geqslant 0$. This corresponds to a one-*missing moment* problem, since upon imposing the normalization $u(0)+u(1)=1$ [or $u(0)=1-u(1)$], only one initialization moment variable, $u(1)$, is required. The implementation of the LU-Gradient technique for this case yields the ground state energy bounds quoted in Table III. These results also concur with the linear programming based EMM approach. We also illustrate in Figs. 1 and 2 the first few diagonal functions $\{\mathscr{D}_0^0,\mathscr{D}_0^1,\mathscr{D}_1^0,\mathscr{D}_1^1,$ etc.$\}$, for the energy value $E=1$ as well as the physical ground state energy, $E_{\text{ground}}=1.392\,351\,641\,53$ (rounded off to 1.392 352). In both cases, we note that the convexity properties discussed in the preceding sections are satisfied. That is, the $\mathscr{D}_n^m$ function is convex within the *positivity* interval $\mathscr{T}_{n-1}^m\equiv\mathscr{U}_{n-1}^m$ on which all the lower-order diagonal functions $(\mathscr{D}_\nu^m,\nu\leqslant n-1)$ are positive. In Fig. 1, the last convex functions plotted are $\mathscr{D}_2^0$ and $\mathscr{D}_3^1$, which are both negative (within the region depicted), and therefore confirm the unphysical nature of the

value $E=1$. Convexity disappears when the intervals of positivity, $\mathscr{T}_n^m$, do not exist, as reflected by the nonconvex nature of $\mathscr{D}_3^0$ (for $E=1$) based on the uniformly nonpositive signature of $\mathscr{D}_2^0$ on the $\mathscr{T}_1^0$ interval.

For the (more physical) case $E=1.392\,352$, we see that the $\mathscr{D}_n^m$ functions depicted have positive regions and remain convex over the appropriate intervals.

A final observation consistent with the convex nature of the $\mathscr{D}_n^m s$ (over the appropriate intervals) is the singular behavior $\mathrm{Lim}_{u_1\to u_\beta}\mathscr{D}_n^m[u_1]\to -\infty$, when the singular boundary point, u_β, is approached from within the corresponding $\mathscr{U}^{2n+m-1}$ set. Recall that $\mathscr{U}^N$ (the intersection of all the $\mathscr{T}_n^m$ intervals for $m+2n\leqslant N$) is the convex set on which all the relevant diagonal functions are positive, $\mathscr{U}^N\equiv\{\mathscr{D}_n^m[u]>0 \,|\, 2n+m\leqslant N$ and $n\geqslant 0$, $m=0$ or $1\}$. Therefore, on the set $\mathscr{U}^{N-1}$ the function $\mathscr{D}_{n[N]}^{m[N]}[u]$ can have arbitrary signature.

ACKNOWLEDGMENTS

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Discussions with Professor Andre Mezincescu are gratefully acknowledged.

APPENDIX: GENERALIZED ORTHOGONAL VECTORS

A convenient alternate formulation[17] to the standard LU matrix decomposition of a symmetric $(D+1)\times(D+1)$ matrix, $\mathscr{M}$ (with matrix element indices initialized at 0), is to consider generating a complete set of generalized orthogonal vectors corresponding to

$$\langle \mathscr{V}^i | \mathscr{M} | \mathscr{V}^j \rangle = \mathscr{D}_i \delta_{i,j}\,, \tag{A1a}$$

for $0\leqslant i,j\leqslant D$, where the vector components satisfy

$$\mathscr{V}_i^i \equiv 1 \quad \text{and} \quad \mathscr{V}_k^i \equiv 0, \quad \text{for } k=i+1,i+2,\ldots,D. \tag{A1b}$$

It is shown in Ref. 17 that the vectors in question can be generated according to the recursion relation:

$$\mathscr{V}_k^l = -\mathscr{D}_k^{-1}\left[\sum_{j=k+1}^{l}\left[\sum_{i=0}^{k}\mathscr{V}_i^k \mathscr{M}_{i,j}\right]\mathscr{V}_j^l\right], \tag{A2}$$

for $k=l-1,l-2,\ldots,0$. Observe that once the vector $\mathscr{V}^l$ is generated, one can then calculate $\mathscr{D}_l$ as given from Eq. (A1a) or, equivalently, $\mathscr{D}_l = \Sigma_{i=0}^{l}\mathscr{M}_{l,i}\mathscr{V}_i^l$. We reemphasize one immediate but important point: as long as $\mathscr{D}_l\neq 0$, for $0\leqslant l\leqslant L$, then $\mathscr{D}_{L+1}$ exists.

From Ref. 17 the determinant is given by $\mathrm{Det}(\mathscr{M})=\Pi_{i=0}^{D}\mathscr{D}_i$. Clearly, a zero determinant is associated with one of the $\mathscr{D}_i$ becoming zero. This, in turn, limits the generation of the $\mathscr{V}$ vectors. Specifically, if $\mathscr{D}_{k=0,\ldots,l-1}\neq 0$, we can only generate the vector set $\{\mathscr{V}^i \,|\, 0\leqslant i\leqslant l\}$.

Two immediately relevant properties follow from Eq. (A1b). If the set of vectors $\{\mathscr{V}^i \,|\, 0\leqslant i\leqslant l\}$ exists, then any vector $\mathscr{A}$ with components $\mathscr{A}_k=0$, for $k>l$, can be written as $\mathscr{A}=\Sigma_{i=0}^{l}c_i\mathscr{V}^i$. Furthermore, if $\mathscr{A}_l=1$, then $c_l=1$.

1. Derivative formula for $\mathscr{D}_i[\mathbf{u}]$

Let us now assume a $\mathbf{u}$ dependence for the symmetric matrix $\mathscr{M}$ of the form $(\mathbf{u}\equiv(u_1,\ldots,u_\nu))$ $\mathscr{M}[\mathbf{u}]\equiv\hat{M}_0+\Sigma_{i=1}^{\nu}\hat{M}_i u_i$, where the $\hat{M}$ matrix coefficients are u independent. Let us define

$$\mathscr{D}_k[\mathbf{u}] = \langle \mathscr{V}^k[\mathbf{u}] | \mathscr{M}[\mathbf{u}] | \mathscr{V}^k[\mathbf{u}] \rangle. \tag{A3}$$

As long as $\mathscr{D}_{k=0,\ldots,l-1}[\mathbf{u}]\neq 0$, then all of these functions, as well as $\mathscr{D}_l$, are differentiable. The derivative for each of these functions is given by

$$\partial_{u_j}\mathscr{D}_k[\mathbf{u}]=\langle\mathscr{T}^k[\mathbf{u}]|\hat{M}_j|\mathscr{T}^k[\mathbf{u}]\rangle,\quad \text{for } j\geq 1. \tag{A4}$$

The proof is immediate. All that is needed is to prove that

$$\langle\partial_{u_j}\mathscr{T}^k[\mathbf{u}]|.\mathscr{M}[\mathbf{u}]|\mathscr{T}^k[\mathbf{u}]\rangle=0. \tag{A5}$$

This follows from the fact that $\partial_{u_j}\mathscr{T}^k$ is completely spanned by the vector set $\{\mathscr{T}^i|0\leq i\leq k-1\}$ and each of these, in turn, is orthogonal to the vector $\mathscr{M}[\mathbf{u}]\mathscr{T}^k$, from Eq. (A1). In greater detail,

$$\partial_{u_j}\mathscr{T}^k[\mathbf{u}]=\sum_{i=0}^{k-1} d_i^j[\mathbf{u}]\mathscr{T}^i[\mathbf{u}], \tag{A6}$$

since $\partial_{u_j}\mathscr{T}_i^k[\mathbf{u}]=0$, for all j and components $i\geq k$. However, from Eq. (A1) we must have $\langle\mathscr{T}^i[\mathbf{u}]|.\mathscr{M}[\mathbf{u}]|\mathscr{T}^k[\mathbf{u}]\rangle=0$, for $i=0,\ldots,k-1$. Equation (A5) then follows, and, in turn, Eq. (A4) is obtained.

2. Proof of local convexity property for $\mathscr{D}_i[\mathbf{u}]$

Let us now assume that we restrict all $\{\mathscr{D}_k[\mathbf{u}]|0\leq k\leq l\}$ to a region, $\mathscr{U}$, in which each of the functions is positive and differentiable. Then each of these, as well as $\mathscr{D}_{l+1}$, is a convex function on $\mathscr{U}$. To prove this, it suffices to show that within the neighborhood of an arbitrary point $\mathbf{v}\in\mathscr{U}$, the tangent plane for $\mathscr{D}_k[\mathbf{u}]$ (at $\mathbf{v}$) is greater than the function itself (except at $\mathbf{v}$):

$$\mathscr{D}_k[\mathbf{v}]+\sum_{j=1}^{\nu}(u_j-v_j)\partial_{v_j}\mathscr{D}_k[\mathbf{v}]\geq\mathscr{D}_k[\mathbf{u}]. \tag{A7}$$

From Eq. (A3) and the assumed dependence $\mathscr{M}[\mathbf{u}]\equiv M_0+\Sigma_{i=1}^{\nu}M_iu_i$, the LHS of Eq. (A7) is equal to $\langle\mathscr{T}^k[\mathbf{v}]|.\mathscr{M}[\mathbf{u}]|\mathscr{T}^k[\mathbf{v}]\rangle$; so Eq. (A7) becomes

$$\langle\mathscr{T}^k[\mathbf{v}]|.\mathscr{M}[\mathbf{u}]|\mathscr{T}^k[\mathbf{v}]\rangle\geq\langle\mathscr{T}^k[\mathbf{u}]|.\mathscr{M}[\mathbf{u}]|\mathscr{T}^k[\mathbf{u}]\rangle. \tag{A8}$$

To prove Eq. (A8) we take note of the fact that each of the vectors $\mathscr{T}^k[\mathbf{v}]$, for $k=0,\ldots,l+1$ can be decomposed into

$$\mathscr{T}^k[\mathbf{v}]=\sum_{i=0}^{l+1}c_i^k[\mathbf{u}]\mathscr{T}^i[\mathbf{u}], \tag{A9}$$

for fixed $\mathbf{v}$ and arbitrary $\mathbf{u}$. That is, at each $\mathbf{u}\in\mathscr{U}$ we can define a new decomposition with respect to the generalized orthogonal vectors for the point $\mathbf{u}$. In particular, because $\mathscr{T}_k^k[\mathbf{v}]=1$ and $\mathscr{T}_{i>k}^k[\mathbf{v}]=0$, as well as $\mathscr{T}_k^k[\mathbf{u}]=1$ and $\mathscr{T}_{i>k}^k[\mathbf{u}]=0$, it then follows that $c_i^k[\mathbf{u}]=0$ if $i>k$, while $c_k^k[\mathbf{u}]=1$. From this it then follows that

$$\langle\mathscr{T}^k[\mathbf{v}]|.\mathscr{M}[\mathbf{u}]|\mathscr{T}^k[\mathbf{v}]\rangle=\sum_{i=0}^{k}(c_i^k[\mathbf{u}])^2\mathscr{D}_i[\mathbf{u}] \tag{A10}$$

or

$$\langle\mathscr{T}^k[\mathbf{v}]|.\mathscr{M}[\mathbf{u}]|\mathscr{T}^k[\mathbf{v}]\rangle=\mathscr{D}_k[\mathbf{u}]+\sum_{i=0}^{k-1}(c_i^k[\mathbf{u}])^2\mathscr{D}_i[\mathbf{u}]. \tag{A11}$$

The summation over $i=0,\ldots,k-1$ is positive (even for the case $k=l+1$), since we have assumed to be working in a region $\mathscr{U}$ within which the functions $\{\mathscr{D}_k[\mathbf{u}]|1\leqslant k\leqslant l\}$ are all positive. Thus, Eq. (A7) is valid, and the functions $\{\mathscr{D}_k[\mathbf{u}]|0\leqslant k\leqslant l+1\}$ are all convex.

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Geometric phase for isotopic spin coherent states

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The concept of geometric phase for a closed circuit in the ray space is applied to the manifold of generalized coherent states defined as the eigenstates of isotopic spin charges. The geometry of the state manifold is elucidated through a calculation of the Gaussian curvature. © *1996 American Institute of Physics.*
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I. INTRODUCTION

The subject of geometric phase has acquired significant attention since its discovery by Berry.[1] Although in the initial formulation the adiabatic theorem was required to ensure that the transported state returns to its original state (apart from a phase factor) so that the evolution in ray space is periodic, it was immediately realized that this phase depends only on the closed curve in the projective Hilbert space of rays and the geometric phase can be formulated entirely in terms of geometric structures on this space.[2–6] At a fundamental level, it is analogous to the angle through which a vector turns if it is parallel transported through a closed loop back to the starting point and is therefore determined by the curvature of the state space in that region.

The object of our article is to study the geometric phase and Gaussian curvature for the case where the charge concerned is non-Abelian, e.g., the isotopic spin.[7] This is motivated by the fact that in strong interactions isotopic spin is indeed a conserved quantity and therefore a calculation of the geometric phase keeping this restriction in mind should naturally be undertaken. Preliminary studies[8] with Abelian charge[9,10] indicate that the phase in question do depend on the charge.

The relevant geometric object to study is the symplectic two-form σ.[11,12] In order to construct σ we need to introduce a smooth parametrization of the state space. This is most conveniently done in terms of coherent states.[13–15] For the present purpose we confine ourselves to the generalized coherent states for isotopic spin. Although the isotopic spin coherent states are not conventional, it can be parametrized smoothly and a metric can be introduced in the projective Hilbert space (ray space). In this case we see that though the charge concerned is non-Abelian, the metric appears to be in the isothermal form very convenient for the calculation of the Gaussian curvature of the state space.

The article is organized as follows. In Sec. II A we review some of the properties of generalized coherent states[7] that are relevant to our study. In Sec. II B we introduce the notion of symplectic two-form (or phase two-form) whose integral will yield the geometric phase that we need and in Sec. III we study the geometric phase and Gaussian curvature for generalized coherent states.

II. REVIEW OF GENERALIZED COHERENT STATES AND THE SYMPLECTIC TWO-FORM

A. Generalized coherent states

We introduce bosonic creation and annihilation operators,

$$\mathbf{a}\equiv(a_1,a_2,a_3), \quad \mathbf{a}^\dagger\equiv(a_1^\dagger,a_2^\dagger,a_3^\dagger) \tag{2.1}$$

satisfying the commutation relations

$$[a_i,\ a_j^\dagger]=\delta_{ij}, \quad [a_i,\ a_j]=0=[a_i^\dagger,\ a_j^\dagger]. \tag{2.2}$$

The total number operator is given by

$$N=N_1+N_2+N_3=\mathbf{a}^\dagger.\mathbf{a}, \tag{2.3}$$

satisfying the commutation relations

$$\begin{gathered}[N_i,\ a_j]=-\delta_{ij}a_j,\quad [N_i,\ a_j^\dagger]=\delta_{ij}a_j^\dagger,\quad [N_i,\ N_j]=0,\\ [N,\ \mathbf{a}]=-\mathbf{a},\quad [N,\ \mathbf{a}^\dagger]=\mathbf{a}^\dagger,\end{gathered} \tag{2.4}$$

where

$$N_i=a_i^\dagger a_i,\quad i=1,2,3. \tag{2.5}$$

The isospin operators are given by

$$I_k=-i\epsilon_{klm}a_l^\dagger a_m \tag{2.6}$$

satisfying the usual commutation relations

$$\begin{gathered}[I_j,\ I_k]=i\epsilon_{jkl}I_l,\\ [I_j,\ a_k]=i\epsilon_{jkl}a_l,\\ [I_j,\ a_k^\dagger]=i\epsilon_{jkl}a_l^\dagger\end{gathered} \tag{2.7}$$

such that

$$\mathbf{I}^2=N^2+N-A^\dagger A, \tag{2.8}$$

where

$$A=a_ia_i,\quad A^\dagger=a_i^\dagger a_i^\dagger. \tag{2.9}$$

A and $A^\dagger$ satisfy the commutation relations

$$\begin{gathered}[A,\ A^\dagger]=4N+6,\\ [N,\ A]=-2A,\quad [N,\ A^\dagger]=2A^\dagger,\\ [\mathbf{I},\ A]=0=[\mathbf{I},\ A^\dagger].\end{gathered} \tag{2.10}$$

From the above equations (2.10) it is evident that $A^\dagger$ creates a pair in an isosinglet. Therefore, states which are eigenstates of N, $\mathbf{I}^2$, and I_3 belonging, respectively, to eigenvalues $(l+2n)$, $l(l+1)$, and m, are given by

$$|l,m:l+2n\rangle=Q_{l,n}(A^\dagger)^n\mathscr{Y}_m^l(\mathbf{a}^\dagger)|0\rangle, \tag{2.11}$$

where

$$Q_{l,n}=\left[\frac{2^l(n+l)!}{(2n+2l+1)!n!}\right]^{1/2} \tag{2.12}$$

is the normalization constant. The solid harmonics[16] $\mathscr{Y}^{l}_{m}(\mathbf{a}^{\dagger})$ are homogeneous polynomials of degree l in the components of the vector operator $\mathbf{a}^{\dagger}$, viz. $a^{\dagger}_{0}[\equiv a^{\dagger}_{3}]$ and $a^{\dagger}_{\pm}[\equiv (a^{\dagger}_{2}\pm ia^{\dagger}_{3})/\sqrt{2}]$ and are given by

$$\mathscr{Y}^{l}_{m}(\mathbf{a}^{\dagger})=(-1)^{m}[(2l+1)(l+m)!(l-m)!]^{1/2}$$
$$\times\sum_{k=0}\frac{(-1)^{k}2^{-k-m/2}}{(l-m-2k)!(k+m)!k!}(a^{\dagger}_{0})^{l-m-2k}(a^{\dagger}_{+})^{k+m}(a^{\dagger}_{-})^{k}$$

for $m\geqslant 0$. For $m<0$, one uses $\mathscr{Y}^{l}_{-m}(\mathbf{x})=\mathscr{Y}^{l}_{m}(\mathbf{x}^{*})$. It is easily checked that $\mathscr{Y}^{l}_{m}(\mathbf{a}^{\dagger})|0\rangle$ is an eigenstate of the operators $\mathbf{I}^{2}$ and I_{3} belonging to eigenvalues $l(l+1)$ and m, respectively. Since $A^{\dagger}$ commutes with $\mathbf{I}$ and creates a pair in an isosinglet, $(A^{\dagger})^{n}$ increases the number of Bosons by $2n$ without changing the isospin quantum numbers.

Isotopic spin coherent states (or generalized coherent states) being eigenstates of the commuting set of $\mathbf{I}^{2}$, I_{3} and $\mathbf{A}$, are obtained from the isospin decomposition of conventional coherent states as

$$|\xi;l,m\rangle=V_{l}(|\xi|)\sum_{n=0}^{\infty}\left[\frac{2^{l}(n+l)!}{(2n+2l+1)!n!}\right]^{1/2}\xi^{n}|l,m;l+2n\rangle \tag{2.13}$$

such that

$$A|\xi;l,m\rangle=\xi|\xi;l,m\rangle, \tag{2.14}$$

where ξ is a complex number ($\xi=\xi_{1}+i\xi_{2}$). The normalization factor $V_{l}(|\xi|)$ is given by

$$V_{l}(|\xi|)=[\phi_{l}(|\xi|^{2})]^{-1/2},$$

with

$$\phi_{l}(x^{2})=\frac{j_{l}(-ix)}{(-ix)^{l}}=2^{l}\sum_{n=0}^{\infty}\frac{(n+l)!}{(2n+2l+1)!n!}x^{2n}, \tag{2.15}$$

j_{l} being the spherical bessel function.

The scalar product of two isotopic spin coherent states is given by

$$\langle\xi;l,m|\xi';l',m'\rangle=\delta_{ll'}\delta_{mm'}\left[\frac{\phi_{l}(\xi^{*}\xi')}{\phi_{l}(|\xi|^{2})\phi_{l}(|\xi'|^{2})}\right]^{1/2}. \tag{2.16}$$

These coherent states form a complete set with a measure. We can write the completeness relation as

$$\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\int\frac{d^{2}\xi}{2\pi}\Phi_{l}(|\xi|)|\xi;l,m\rangle\langle\xi;,l,m|=1,$$

where

$$\Phi_{l}(x)=\phi_{l}(x^{2})k_{l}(x)x^{l+1},$$

and $k_{l}(x)$ is a spherical modified Bessel function.

B. The symplectic two-form and the metric

We consider a smoothly parametrized space of normalized state vectors $\psi(\xi)$ with

$$\xi=(\xi_1,\xi_2,\ldots,\xi_N)\in R^N.$$

The symplectic two-form σ is defined as

$$\sigma=\sigma_{ij}(\xi)d\xi_i\wedge d\xi_j, \tag{2.17}$$

where the antisymmetric tensor σ_{ij} is given by

$$\sigma_{ij}=\mathrm{Im}\left(\frac{\partial\psi}{\partial\xi_i},\frac{\partial\psi}{\partial\xi_j}\right). \tag{2.18}$$

The symplectic two-form (2.17) has the following properties: (1) $d\sigma=0$ (d standing for exterior differentiation); (2) σ is invariant under a local gauge transformation:

$$\psi(\xi)\rightarrow\psi'(\xi)=e^{i\alpha(\xi)}\,\psi(\xi). \tag{2.19}$$

These properties follow immediately from the fact that locally

$$\sigma=d\beta,$$

where

$$\beta=\beta_i(\xi)d\xi_i=-i\left(\psi(\xi),\frac{\partial\psi(\xi)}{\partial\xi_i}\right)d\xi_i \tag{2.20}$$

and under a local gauge transformation

$$\beta\rightarrow\beta'=\beta+d\alpha. \tag{2.21}$$

Thus σ is truly a ray space object. The quantity

$$\gamma(\mathscr{C}=\partial s)=\int_S\sigma \tag{2.22}$$

is the geometric phase associated with a state vector carried around the closed curve $\mathscr{C}$.

A metric may be introduced by observing that the quantity D defined through[12]

$$D^2[\tilde{\psi}_1,\ \tilde{\psi}_2]=\inf_{\delta,\gamma}\|\psi_1e^{i\delta}-\psi_2e^{i\gamma}\|=2-2|(\psi_1,\psi_2)|, \tag{2.23}$$

where the double bars represent the norm and the tilde represents a ray, has all the properties of a distance function in the projective Hilbert space. The metric in a given state space is then obtained by writing

$$D^2[\tilde{\psi}(\xi+d\xi),\ \tilde{\psi}(\xi)]=g_{ij}(\xi)d\xi_i\,d\xi_j \tag{2.24}$$

and expanding the left-hand side up to quadratic term in $d\xi$. We remark that the metric $g_{ij}(\xi)$ can be expressed as

$$g_{ij}=\gamma_{ij}(\xi)-\beta_i(\xi)\beta_j(\xi), \tag{2.25}$$

where the symmetric tensor γ_{ij} is given by

$$\gamma_{ij}=\mathrm{Re}\left(\frac{\partial\psi}{\partial\xi_i},\frac{\partial\psi}{\partial\xi_j}\right) \tag{2.26}$$

and $\beta_i(\xi)$ is as defined in Eq. (2.20).

The symplectic two-form is naturally related to a metric in the following way. The generalized coherent states[13] parametrize the points in some quotient space having the structure of a Kähler manifold with complex coordinate η_α. The Kähler metric $g_{\alpha\beta}$ then determines the symplectic structure through the relation[17,18]

$$\sigma=ig_{\alpha\beta}\,d\eta_\alpha^*\wedge d\eta_\beta. \tag{2.27}$$

III. GEOMETRIC PHASE FOR ISOTOPIC SPIN COHERENT STATES

We now proceed to investigate the geometric properties for the isotopic spin coherent states. We observe that both the metric g_{ij} and the two-form σ can be easily calculated from the overlap function

$$\langle\xi;l,m|\xi';l,m\rangle=\frac{\phi_l(\xi^*\xi')}{[\phi_l(|\xi|^2)\phi_l(|\xi'|^2)]^{1/2}}, \tag{3.1}$$

by noticing that

$$\beta_i(\xi)=-i\,\frac{\partial}{\partial\xi_i'}\,\langle\xi;l,m|\xi';l,m\rangle|_{\xi'=\xi}, \tag{3.2}$$

$$\gamma_{ij}(\xi)+i\sigma_{ij}(\xi)=\frac{\partial}{\partial\xi_i}\frac{\partial}{\partial\xi_j'}\,\langle\xi;l,m|\xi';l,m\rangle|_{\xi'=\xi}. \tag{3.3}$$

Inserting Eq. (3.1) in Eq. (3.3), we obtain

$$\gamma_{11}=\frac{1}{4}\frac{\phi_{l+2}(|\xi|^2)|\xi|^2}{\phi_l(|\xi|^2)}+\frac{1}{2}\frac{\phi_{l+1}(|\xi|^2)}{\phi_l(|\xi|^2)}-\frac{1}{4}\frac{[\phi_{l+1}(|\xi|^2)]^2\xi_1^2}{[\phi_l(|\xi|^2)]^2},$$

$$\gamma_{22}=\frac{1}{4}\frac{\phi_{l+2}(|\xi|^2)|\xi|^2}{\phi_l(|\xi|^2)}+\frac{1}{2}\frac{\phi_{l+1}(|\xi|^2)}{\phi_l(|\xi|^2)}-\frac{1}{4}\frac{[\phi_{l+1}(|\xi|^2)]^2\xi_2^2}{[\phi_l(|\xi|^2)]^2},$$

$$\gamma_{12}=\gamma_{21}=-\frac{1}{4}\frac{[\phi_{l+1}(|\xi|^2)]^2\xi_1\xi_2}{[\phi_l(|\xi|^2)]^2}, \tag{3.4}$$

$$\sigma_{11}=0=\sigma_{22},$$

$$\sigma_{12}=-\sigma_{21}=\frac{1}{4}\frac{\phi_{l+2}(|\xi|^2)|\xi|^2}{\phi_l(|\xi|^2)}+\frac{1}{2}\frac{\phi_{l+1}(|\xi|^2)}{\phi_l(|\xi|^2)}-\frac{1}{4}\frac{[\phi_{l+1}(|\xi|^2)]^2|\xi|^2}{[\phi_l(|\xi|^2)]^2}.$$

From the above results we can obtain the symplectic structure. We take ξ_1 and ξ_2 (the real and imaginary parts of ξ) as smooth parameters in the state space. From Eq. (3.4) it is clear that σ_{ij} has only one independent component. Therefore, the symplectic two-form is given by

$$\sigma=2\sigma_{12}\,d\xi_1\wedge d\xi_2=\left[\frac{1}{2}\frac{\phi_{l+2}(|\xi|^2)|\xi|^2}{\phi_l(|\xi|^2)}+\frac{\phi_{l+1}(|\xi|^2)}{\phi_l(|\xi|^2)}-\frac{1}{2}\frac{[\phi_{l+1}(|\xi|^2)]^2|\xi|^2}{[\phi_l(|\xi|^2)]^2}\right]d\xi_1\wedge d\xi_2. \tag{3.5}$$

The geometric phase for a circular curve of radius $s=|\xi|$ centered at the origin can be obtained from Eq. (3.5):

$$\gamma=\int_s \sigma=\pi|\xi|^2\,\frac{\phi_{l+1}(|\xi|^2)}{\phi_l(|\xi|^2)}=-\pi|\xi|\,\frac{I_{l+3/2}(-|\xi|)}{I_{l+1/2}(-|\xi|)}, \tag{3.6}$$

where ϕ_l is given by Eq. (2.15) and I_l is the modified Bessel function of order l.

In the limit of small circles,

$$\frac{I_{l+3/2}(-|\xi|)}{I_{l+1/2}(-|\xi|)}\approx-\frac{|\xi|}{2l+3}$$

and we have

$$\gamma\approx\frac{\pi|\xi|^2}{2l+3}, \tag{3.7}$$

which shows that the phase acquired after a complete circle decreases as the isotopic spin increases.

For large circles, i.e., for large $|\xi|$,

$$\frac{I_{l+3/2}(-|\xi|)}{I_{l+1/2}(-|\xi|)}\approx-1$$

and we have

$$\gamma\approx\pi|\xi|, \tag{3.8}$$

showing that for large circles the phase is independent of isotopic spin. Inserting Eq. (3.1) in Eq. (3.2) we obtain

$$\begin{aligned}\beta_1(\xi)&=\frac{1}{2}\,\frac{\phi_{l+1}(|\xi|^2)\xi_2}{\phi_l(|\xi|^2)},\\ \beta_2(\xi)&=-\frac{1}{2}\,\frac{\phi_{l+1}(|\xi|^2)\xi_1}{\phi_l(|\xi|^2)}.\end{aligned} \tag{3.9}$$

From Eqs. (2.25), (3.4), and (3.9) we find

$$g_{ij}=E(|\xi|)\,\delta_{ij}=E(s)\,\delta_{ij}, \tag{3.10}$$

where $s=|\xi|$ and

$$E(s)=\frac{1}{4}\,\frac{\phi_{l+2}(s^2)s^2}{\phi_l(s^2)}+\frac{1}{2}\,\frac{\phi_{l+1}(s^2)}{\phi_l(s^2)}-\frac{1}{4}\,\frac{[\phi_{l+1}(s^2)]^2s^2}{[\phi_l(s^2)]^2}. \tag{3.11}$$

The above formula for g_{ij} could also be easily arrived at by the use of Eq. (2.27). The metric is in the very convenient isothermal form. We look upon ξ_1 and ξ_2 as orthogonal coordinates with $\sqrt{E}d\xi_1$ and $\sqrt{E}d\xi_2$ being the elements of length and σ essentially is the element of area.

The Gaussian curvature K for a metric in the isothermal form is given by a very simple formula.[19] In our case, it takes the form

$$K=-\frac{1}{2Es}\frac{d}{ds}\left(s\frac{d}{ds}\ln E\right). \tag{3.12}$$

Inserting Eq. (3.11) in Eq. (3.12) and after simplification we obtain

$$K=4-4\frac{\phi_{l+2}(s^2)\phi_l(s^2)}{[\phi_{l+1}(s^2)]^2}-\left[4\frac{\phi_{l+3}(s^2)\phi_l(s^2)}{[\phi_{l+1}(s^2)]^2}+28\frac{\phi_{l+2}(s^2)}{\phi_{l+1}(s^2)}-8\frac{[\phi_{l+2}(s^2)]^2\phi_l(s^2)}{[\phi_{l+1}(s^2)]^3}\right]s^2+\cdots . \tag{3.13}$$

We now investigate the behavior of K near the origin. When s is very small, we have from Eq. (3.13),

$$K=\frac{8}{2l+5}-8\left[\frac{12l^2+73l+109}{(2l+7)(2l+5)^2}\right]s^2+\cdots , \tag{3.14}$$

which for a few values of l behaves as follows:

$$\begin{aligned} l=0:&\quad K=\tfrac{8}{5}-|\tfrac{872}{175}s^2+\cdots ,\\ l=1:&\quad K=\tfrac{8}{7}-\tfrac{1552}{441}s^2+\cdots ,\\ l=2:&\quad K=\tfrac{8}{9}-\tfrac{2424}{891}s^2+\cdots . \end{aligned} \tag{3.15}$$

From the quadratic behavior of K near the origin it is evident that the space is flat for small s and the geometric phase for small circles is proportional to s^2, i.e., $|\xi|^2$.

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Quantum chaos in the group-theoretical picture

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The dynamical-group approach is developed and applied to investigate the problems of controllability and quantum chaos in two fundamental models of the matter–radiation interaction. It provides a new insight into the dynamics of nonstationary quantum process of the interaction between two-level atoms and a single-mode radiation field without and with the feedback. A sequence of transitions from the quasiperiodicity to chaos has been numerically observed for two-level atoms interacting with a self-consistently generated radiation field. The unitary irreducible representations of the SU(2) group of dynamical symmetry in a noncanonical parametrization is constructed, allowing one to use the results for describing the time evolution of any driven quantum system with the underlying SU(2) symmetry. © *1996 American Institute of Physics.* [S0022-2488(96)01102-X]

I. INTRODUCTION

In studying the time evolution of driven quantum systems, the natural question is how one can attain a desirable state of a system under consideration from a given initial state. In physics of field–matter interactions, it may be formulated, for example, as follows. Is it possible to use specifically crafted laser pulses to achieve coherent control of atomic or molecular dynamics? From this point of view the evolution problem may be regarded as a control problem.

Let our objective be to transfer a quantum dynamical system from an initial state $x(t_0)$ to a desired state $x(t)$ in the time $t-t_0$. Depending on the tasks considered, the variable $x(t)$ may be a Heizenberg operator, a state vector, a density matrix, etc. The control problem on the finite interval $[t,t_0]$ is to design the vector function $\mathbf{u}(t)=\{u_1,\ldots,u_n\}$ (belonging to a class of admissible controls) that allows us to synthesize the time evolution operator $U_{\mathbf{u}}(t,t_0)$ providing the mapping

$$x_{\mathbf{u}}(t_0) \xrightarrow{U_{\mathbf{u}}(t,t_0)} x_{\mathbf{u}}(t), \tag{1.1}$$

under the condition that it satisfies the operator equation

$$i\hbar \frac{d}{dt} U(t,t_0)=H[\mathbf{u}(t)]U(t,t_0), \quad U(t_0,t_0)=I. \tag{1.2}$$

Since the evolution equation (1.2) can be regarded as a differential equation in the group of dynamical symmetry,[1–3] it is natural to use group-theoretical methods as for the analysis of general questions of controllability of driven quantum systems[4,5] as for finding the solution of the evolution equation in terms of the control functions $u_j(t)$ and the structure constants of the Lie algebra generated by the Hamiltonian $H(t)$. The group-theoretical strategy has been successfully applied to describe the time evolution of numerous physical model systems in different disciplines, extending from classical mechanics to physics of elementary particles (see, for example, Refs. 6–13 and references therein). As to the control problems for driven quantum systems, the dynamical-symmetry approach has been developed by one of the authors (S.V.P.) for the general analytical description of the coherent population control in multilevel quantum systems[14] and then applied

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for controlling population dynamics in semiclassical models of externally driven three-level atoms[15] and for controlling atom-field dynamics in fully quantum, stationary and nonstationary models of interaction between atoms and cavity radiation fields.[16]

In recent years, another fundamental aspect of the evolution problem has attracted considerable interest. The question is which controls $\mathbf{u}(t)$ may lead to unpredictable behavior of a quantum dynamical system in the sense of deterministic chaos. Despite the large amount of efforts devoted to the question, how classical chaos might manifest itself in a quantum case, the answer is still far from clear (for a review of the status of the subject, see, for example Ref. 17).

The purpose of this paper is to develop the concept of dynamical symmetry to examine in a unified manner as problems of controllability of quantum evolution as questions of quantum manifestations of classical deterministic chaos in the atom-field systems. The simplest, and, in the same time, most fundamental system for studying matter-radiation dynamics is a single two-level atom interacting with a single mode of an electromagnetic field. The SU(2) group is a basic group of dynamical symmetry for this interaction.

The organization of the paper is as follows. We begin in Sec. II with a brief review of the theory of quantum time evolution on the dynamical Lie groups. In Sec. III we present a general description of the evolution of an arbitrarily driven quantum system with underlying SU(2) dynamical symmetry. In particular, we construct the unitary irreducible representations of the SU(2) in a noncanonical parametrization that will be used in the next sections. In Sec. IV we consider the system without any feedback between atoms and a field and show numerically that atomic behavior may be more or less complicated (depending on the type of field polarization and on the ratio of the driving frequencies), but it is always fully controlled in the sense of lacking of sensitive dependence on initial conditions. In Sec. V we consider atoms interacting with a self-consistently generated electromagnetic field. It is shown that the group-theoretical picture provides further insight into the dynamics of such a process. In particular, it is discovered, by directly computing the largest Lyapunov exponent, the sequence of transitions from quasiperiodicity to chaos (as the coupling strength increases) with chaotic regimes, alternating among quasiperiodic regimes. Section VI is devoted to concluding remarks.

II. QUANTUM TIME EVOLUTION ON THE DYNAMICAL LIE GROUPS

Let the Hamiltonian, H, of a quantum dynamical system be the linear form on the generators, $\{L_j, j=1,2,\ldots,n\}$, of an n-dimensional Lie algebra L,

$$H(t)=\sum_{j=1}^{n} u_j(t)L_j, \tag{2.1}$$

where u_j are the linearly independent complex-valued functions of a real independent variable t (some of them can be null). The generators satisfy the commutation relations

$$[L_j,L_k]=\sum_{l=1}^{n} c_{jk}^{l}L_l, \tag{2.2}$$

where c_{jk}^{l} are structure constants. For any quantum system with the Hamiltonian (2.1), there exists the time evolution operator that obeys the Schrödinger equation,

$$i\hbar\,\frac{d}{dt}\,U(t)=H(t)U(t), U(0)=I. \tag{2.3}$$

The time evolution of the system is described by the one-parameter family $U(t)$ of unitary transformations defined on the Hilbert space of the system's state vectors. It is a space where a representation of the dynamical Lie group G, connected with the dynamical Lie algebra L, acts.

It follows from the Frobenius theorem,[18] that there exists a neighborhood of $t=0$, in which the solution of the Eq. (2.3) can be written as

$$U(t)=\prod_{j=1}^{n}(\exp g_j(t)L_j), \quad g_j(0)=0, \tag{2.4}$$

if the generators L_j's satisfy Eq. (2.2). Substituting the solution (2.4) into Eq. (2.3) and using the Baker–Campbell–Hausdorff formula,

$$e^A B e^{-A}=B+[A,B]+\tfrac{1}{2}[A,[A,B]]+\cdots, \quad A,B\in\{L_j\}, \tag{2.5}$$

Wei and Norman[3] obtained a set of nonlinear ordinary differential equations for the functions g's,

$$u_k(t)=i\hbar\sum_{l=1}^{n}\xi_{kl}\dot{g}_l, \quad k=1,2,\ldots,n. \tag{2.6}$$

Since the elements ξ_{kl} of the transform matrix ξ are analytic functions of the g's, $\det\xi$ is an analytic function of g's. On the other hand, $\xi(t=0)=I$, and hence $\det\xi(t=0)\neq 0$. Therefore a neighborhood of $t=0$ exists in which $\det\xi(t)\neq 0$. We now can write (2.6) as

$$i\hbar\dot{g}_k=\sum_{l=1}^{n}\eta_{kl}u_l, \tag{2.7}$$

where $\eta\equiv\xi^{-1}$. Since $\det\eta\neq 0$, we are assured of the neighborhood of $t=0$, where the solution of Eq. (2.7) exists and is unique.

It is worthwhile to emphasize that the equations (2.7) depend only on the structure of the dynamical Lie algebra L. Based on some well-known results in the theory of the Lie algebras, Wichmann, Wei, and Norman[2,3] have pointed out the reduction principles for the evolution problem (2.3). They can be summarized as follows.

(1) If the dynamical Lie algebra L, generated by the Hamiltonian $H(t)$, is commutative, then the solution of Eq. (2.3) is trivial,

$$U(t)=\exp\left(-i\hbar^{-1}\int_0^t H(\tau)d\tau\right). \tag{2.8}$$

(2) For a solvable Lie algebra L there exists a basis and its ordering in which η forms a triangular matrix, and the set (2.7) can be resolved in quadratures. The solution (2.4) is globally valid for all solvable Lie algebras.

(3) The representation by the product of one-parameter subgroups (2.4) is globally valid for the real simple three-dimensional Lie algebra with the following commutation relations in the spherical basis,

$$[L_-,L_+]=2\alpha L_0, \quad [L_0,L_\pm]=\pm L_\pm, \quad L_0=L_0^\dagger, \quad L_+=L_-^\dagger, \tag{2.9}$$

where $\alpha=-1$ for SU(2) algebra and $\alpha=+1$ for SU(1,1) algebra.

(4) Let L be a finite-dimensional Lie algebra. Then by the Levi–Mal'tsev theorem, it can be decomposed into a semidirect sum,

$$L=S\oplus R, \tag{2.10}$$

of its unique radical R and a semisimple subalgebra S. The splitting (2.10) gives rise to the corresponding decomposition of the Hamiltonian (2.1),

$$H=H_S+H_R, \quad H_S\in S, \quad H_R\in R, \tag{2.11}$$

to the decomposition of Eq. (2.3),

$$i\hbar\,\frac{d}{dt}\,U_S=H_SU_S, \quad i\hbar\,\frac{d}{dt}\,U_R=(U_S^{-1}H_RU_S)U_R, \tag{2.12}$$

and to the decomposition of its solution (2.4),

$$U=U_SU_R. \tag{2.13}$$

(5) Let S be a finite-dimensional semisimple Lie algebra. Then, by the structure theorem, it can be uniquely decomposed into the direct sum,

$$S=\sum_{j=1}^{m}\oplus S_j, \tag{2.14}$$

of its simple ideals S_j. It follows from (2.14) that

$$H_S=H_1+H_2+\cdots+H_m, \tag{2.15}$$

$$U_S=U_1U_2\cdots U_m, \tag{2.16}$$

with U_j satisfies the equation

$$i\hbar\,\frac{d}{dt}\,U_j=H_jU_j, \quad j=1,2,\ldots,m. \tag{2.17}$$

Thus, the structural properties of the dynamical Lie algebras make it possible to reduce a high-dimensional evolution problem (2.3) to solving evolution subproblems (2.12) and/or (2.17) of smaller dimensions (in the sense mentioned above).

III. GENERAL DESCRIPTION OF THE QUANTUM TIME-EVOLUTION OF A DRIVEN SU(2) SYSTEM

In a variety of physical problems SU(2) appears to be a group of dynamical symmetry. It is well known[3,6,7] that the set of three equations for the SU(2) group parameters (2.7) can be reduced to a single second-order differential equation. The form of this governing equation depends on the choice of the basis and its exponential ordering. The right choice of parametrization of the dynamical group is especially important if we must explicitly solve the governing equation for a given physical Hamiltonian.

The Hermitian Hamiltonian of a quantum system with the SU(2) dynamical symmetry can be cast in the general form,

$$H(t)=u_0(t)R_0+u^*(t)R_-+u(t)R_+, \tag{3.1}$$

where R_0 and $R_\pm$ are the generators that satisfy the commutation relations (2.9) with $\alpha=-1$. If we choose the following noncanonical parametrization of SU(2):

$$U=\exp\left[\left(g_0-i\int_0^t u_0(\tau)d\tau\right)R_0\right]\exp\,g_-R_-\,\exp\,g_+R_+, \tag{3.2}$$

then the system (2.7) can be reduced to the governing equation of a comparatively simple form,

$$\ddot{g}-\left(\frac{\dot{u}}{u}+iu_0\right)\dot{g}+|u|^2g=0, \quad g(0)=1, \quad \dot{g}(0)=0, \tag{3.3}$$

where

$$g\equiv\exp(g_0/2). \tag{3.4}$$

We can now express the rest of the SU(2) group parameters in terms of the function g,

$$g_-=ig\dot{g}u^{-1}\exp\left(-i\int_0^t u_0\,d\tau\right), \tag{3.5}$$

$$\dot{g}_+=-iug^{-2}\exp\left(i\int_0^t u_0\,d\tau\right). \tag{3.6}$$

It follows from Eq. (3.4) that real and imaginary parts of g are not independent. It is convenient to introduce the parameter

$$\tilde{g}\equiv g_-/g. \tag{3.7}$$

Every SU(2) group element in the parametrization (3.2) can now be described by a pair of complex numbers g and $\tilde{g}$ obeying the condition

$$|g|^2+|\tilde{g}|^2=1, \tag{3.8}$$

where $|\cdots|$ denotes the modulus of a complex number. All the formulas (3.3)–(3.8) are valid within any representation of SU(2).

Using the well-known expressions for the matrix elements R_0 and $R_\pm$ in the standard basis,

$$|j,m\rangle, \quad m=-j,-j+1,\ldots,j \tag{3.9}$$

(see, for example, Ref. 19), we construct after some algebra the unitary irreducible representations of SU(2) in the chosen noncanonical parametrization (3.2),

$$U^{(j)}_{m'm}=\exp\left(-im'\int_0^t u_0\,d\tau\right)\sum_{l=-j}^{j}\left[\frac{(j-m')!(j-m)!}{(j+m')!(j+m)!}\right]^{1/2}$$
$$\times\frac{(j+l)!}{(j-l)!(l-m)!(l-m')!}\,g^{m+m'}(\tilde{g})^{l-m'}(-\tilde{g}^*)^{l-m}. \tag{3.10}$$

Up to now we said nothing about physical nature of a system with the SU(2) dynamical symmetry. All the results of this section are valid, of course, for any quantum system with such a symmetry. Since we are going to demonstrate a variety of regimes of behavior, which are possible for a driven SU(2) system, it is natural to choose, as an example, a simplest one. We shall deal in the next sections with the fundamental semiclassical model of field–matter interactions, namely, with a two-state system driven by a radiation field. This model is usually adopted in magnetic resonance,[20] optical resonance,[21,22] and quantum acoustics.[6] For definiteness, we shall speak about a two-level atom interacting with a time-varying electric field, both in a prescribed way and in a self-consistent way. It will be demonstrated further that the time evolution in the group-theoretical picture is radically different in these cases.

IV. ATOM-FIELD INTERACTION WITHOUT ANY FEEDBACK

A. Two-level atoms in a prescribed, circularly polarized field

Let us write a circularly polarized light as

$$\mathbf{E}(t)=E_0\epsilon(t)(\mathbf{i}\cos\omega t+\mathbf{j}\sin\omega t), \tag{4.1}$$

where E_0 is the constant amplitude of the electric field strength and $\epsilon(t)$ is the dimensionless variable representing the amplitude modulation that has here the simple form

$$\epsilon(t)=\sin\omega' t. \tag{4.2}$$

The time-dependent Hamiltonian of a two-level atom, interacting with the field (4.1) and (4.2), is given by

$$H(t)=\hbar\omega_0 R_0+\tfrac{1}{2}\hbar\Omega_0\epsilon(t)(R_- e^{i\omega t}+R_+ e^{-i\omega t}), \tag{4.3}$$

where ω' is the modulation frequency and ω is the carrier frequency of the wave, which is mismatched, in general, from the exact atomic resonance frequency ω_0 by $\Delta\equiv\omega_0-\omega$. Here

$$\Omega_0\equiv dE_0/\hbar \tag{4.4}$$

is the constant part of the Rabi frequency and d is the transition electric dipole moment. The SU(2) generators have the familiar form in the 2×2 matrix representation,

$$R_0=\frac{1}{2}\begin{vmatrix}1 & 0\\ 0 & -1\end{vmatrix},\quad R_-=\begin{vmatrix}0 & 0\\ 1 & 0\end{vmatrix},\quad R_+=\begin{vmatrix}0 & 1\\ 0 & 0\end{vmatrix}. \tag{4.5}$$

Factorizing the time-evolution operator as

$$U=\exp(-i\omega t R_0)U', \tag{4.6}$$

we obtain the following evolution equation:

$$i\hbar\frac{d}{dt}U'=H'(t)U', \tag{4.7}$$

with the transformed Hamiltonian

$$H'(t)=\hbar\,\Delta R_0+\tfrac{1}{2}\hbar\Omega_0\epsilon(t)(R_-+R_+). \tag{4.8}$$

The evolution matrix (4.6) is found in an explicit form from the general expression (3.10) for the unitary irreducible representations of SU(2) in the noncanonical parametrization (3.2):

$$U=\begin{pmatrix}e^{-i\omega_0 t/2} & 0\\ 0 & e^{i\omega_0 t/2}\end{pmatrix}\begin{pmatrix}g & -\tilde{g}^*\\ \tilde{g} & g^*\end{pmatrix}. \tag{4.9}$$

The governing SU(2) group parameter g satisfies the following equation that results from Eqs. (3.3), (4.2), and (4.8):

$$\ddot{g}-(\omega'\cot\omega' t+i\Delta)\dot{g}+\left(\frac{\Omega_0\sin\omega' t}{2}\right)^2 g=0,\quad g(0)=1,\quad \dot{g}(0)=0. \tag{4.10}$$

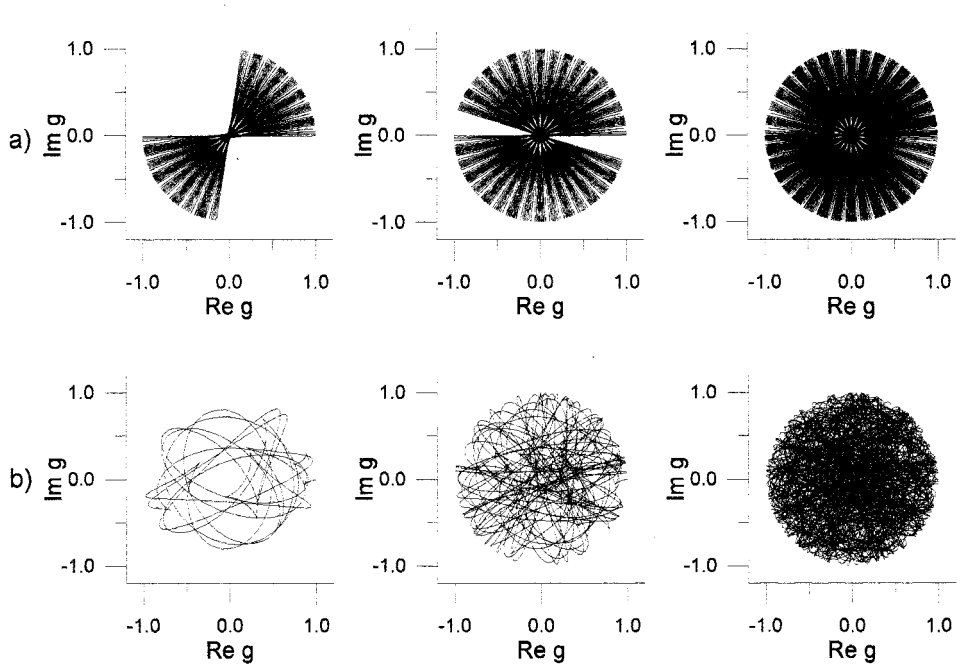

FIG. 1. Stroboscopic two-dimensional phase portraits of a two-level atom driven by a nonresonant, prescribed, laser field with incommensurate carrier, ω, and modulation, ω', frequencies in the case of (a) circular polarization and (b) linear polarization. The parameters used are $\Delta=0.023$, $\omega=1$, $\omega'=0.201$, and $\Omega=5$.

The solution for the probabilities of finding our two-level system in lower $|-\rangle$ and in upper $|+\rangle$ states at time t in terms of their values at the initial time $t=0$ is given by

$$\begin{bmatrix} P_+(t) \\ P_-(t) \end{bmatrix} = \begin{pmatrix} |g|^2 & |\tilde{g}|^2 \\ |\tilde{g}|^2 & |g|^2 \end{pmatrix} \begin{bmatrix} P_+(0) \\ P_-(0) \end{bmatrix}. \tag{4.11}$$

It follows from (4.11) that the squared modulus of the SU(2) group parameter, $|g(t)|^2$, has the sense of the initial-state population probability in the case $P_\alpha(0)=1$, $\alpha=\pm$.

Equation (4.10), governing the dynamical evolution of a two-level atom in an inexhaustible circularly polarized external field (4.1) with harmonic amplitude modulation (4.2), has been numerically integrated using a scaled dimensionless time $\tau=\omega_0 t$. The strength of coupling between an atom and the external field is characterized by the dimensionless parameter

$$\Omega \equiv \Omega_0/2\omega_0 .$$

We have studied different aspects of the atomic dynamics in the group-theoretical picture. Such indicators of motion as (1) the squared modulus $|g(t)|^2$, (2) the power spectrum of g, and (3) the motion in the phase plane $\mathrm{Re}\, g - \mathrm{Im}\, g$, have been numerically calculated for an initially unexcited atom.

All the results show that the time evolution is regular for a circularly polarized field, both with commensurate and with incommensurate driving frequencies ω and ω'. The power spectrum for the nonresonant excitation ($\Delta=0.023$, $\Omega=5$), with the incommensurate frequencies $\omega=1$ and $\omega'=0.201$, shows many δ-like peaks, as in the case of quasiperiodic motion. We only represent here the two-dimensional stroboscopic phase portraits of a two-level atom driven under the same conditions [Fig. 1(a)]. In other words, we plot trajectories in the plane $\mathrm{Re}\, g - \mathrm{Im}\, g$ for the different

values of the integration time growing from the left to the right.

It should be pointed out that the frequencies ω and ω' are assumed to be incommensurate, if the period between successive phase coincidence of the functions $\cos \omega t$ and $\cos \omega' t$ is much longer that the interval of integration. In the case $\omega=1$ and $\omega'=0.201$, the period of incommensurability is equal to 2000π, and the maximal integration interval is 512.

B. Two-level atoms in a prescribed, linearly polarized field

Writing the field in the form

$$\mathbf{E}(t)=E_0\epsilon(t)\mathbf{x}\cos\ \omega t, \tag{4.12}$$

with

$$\epsilon(t)=\sin\ \omega' t, \tag{4.13}$$

the Hamiltonian can be cast as

$$H(t)=\hbar\omega_0 R_0+\tfrac{1}{2}\hbar\Omega_0\epsilon(t)\cos\ \omega t(R_-+R_+). \tag{4.14}$$

The time-evolution matrix and the solution for the transition probabilities has the same form as in the case of circular polarization, i.e. (4.9) and (4.11), respectively. However, the group parameter g now satisfies the equation

$$\ddot{g}-(\omega'\ \cot\ \omega' t-\omega\ \tan\ \omega t+i\omega_0)\dot{g}+\left(\frac{\Omega_0\ \sin\ \omega' t\ \cos\ \omega t}{2}\right)^2 g=0. \tag{4.15}$$

We have numerically calculated all the relevant characteristics (1), (2), and (3) for an initially unexcited atom. In addition to the irregular temporal behavior of the squared modulus of the solution of Eq. (4.15), we have the broadened power spectrum of this solution. The larger is the coupling coefficient, Ω, the more broadband is the spectrum. As for incommensurate and commensurate driving frequencies, the whole allowed phase plane $\mathrm{Re}\, g-\mathrm{Im}\, g$ is occupied by the motion, apparently in an irregular way. We plot in Fig. 1(b) the two-dimensional stroboscopic phase portraits of a two-level atom driven by nonresonant linearly polarized external field with incommensurate driving frequencies.

The analytical results for an externally driven quantum system with the underlying SU(2) dynamical symmetry can be resumed as follows. Its time evolution is governed by a single second-order ordinary differential equation in four real variables. However, real and imaginary parts of the complex variable g are not independent. They can be connected with each other by means of Eq. (3.4). In addition, we have the conservation law that it follows from Eqs. (3.5), (3.7), and (3.8). For the Hamiltonians (4.3) or (4.8), it has the form

$$|g|^2+\left(\frac{2|\dot{g}|}{\Omega_0\epsilon}\right)^2=1. \tag{4.16}$$

This leaves two independent real variables, and by the Poincaré–Bendixson theorem[23] therefore precludes any possibility of chaos for an externally driven SU(2) system.

The explicit form of the time-evolution matrix for any driven SU(2) system is defined by its matrix elements (3.10). The problem of population control of two-level systems, interacting with a prescribed modulated external field, is resolved by Eq. (4.11), with g satisfying Eq. (4.10) or Eq. (4.15).

We can summarize our numerical results for the externally driven two-level system as follows. If the external field is circularly polarized, the atomic dynamics is (independent on whether the

driving frequencies are incommensurate or not) regular, in the sense that (a) the oscillations of the initial-state population probability are periodic, (b) the power spectrum of this variable shows δ-like peaks, and (c) the motion in the phase plane is nonergodic. If the external field is linearly polarized, the atomic dynamics is (independent on whether the driving frequencies are incommensurate or not) irregular, in the sense that (a) the oscillations of the initial-state population probability is not periodic, (b) the power spectrum of this variable is broadband, and (c) the motion in the pseudophase plane is ergodic.

In any case, the time evolution is not fully chaotic, since the characteristic Lyapunov exponents are always nonpositive for a two-level atom in a prescribed field.

V. QUANTUM CHAOS IN THE ATOM-FIELD SYSTEM WITH THE FEEDBACK

As it was shown in the preceding section, the equation for the SU(2) group parameter, governing the time evolution of a two-level atom in a prescribed external field, does not admit truly chaotic motion. Atomic behavior may be more or less regular, depending on the type of field polarization and on the ratio of the two driving frequencies, but it always implies the Lyapunov characteristic exponents to be nonpositive.

Let us now take into account the feedback effects of atoms on the radiation field. It may be done by the different ways. In the Belobrov–Zaslavski–Tartakovski model,[24–26] the radiation field is treated semiclassically from the outset, and the analysis of the time evolution of the coupled atom-field system is based on the well-known Maxwell–Bloch equations. In the other model,[27,28] we have *ab initio* a quantized single-mode field, and the dynamics of the system is governed by the Heizenberg equations. To obtain the c-number equations for the expectation values of the relevant operators, one has to make some sort of their factorization approximation. It has been shown for both models the atom-field system with the feedback exhibits chaotic time evolution for the sufficiently large coupling strength.[24–28]

Further insight into the dynamics of the process of atom-field interaction with the feedback can be obtained in the group-theoretical picture developed in the preceding sections.

Here we will consider $E(t)\equiv E_0\epsilon(t)$ as the field generated by a two-level atom enclosed in a single-mode lossless cavity. The classical Maxwell equation in the dipole and the slowly varying envelope approximations is written as

$$\ddot{\epsilon}+\omega^2\epsilon=-\Omega_0\omega\langle R_+ + R_-\rangle, \tag{5.1}$$

where ϵ is the dimensionless time-varying part of the field E, $\Omega_0\equiv dE_0/\hbar$, ω is the radiation frequency, and $\langle\cdots\rangle$ denotes the quantum expectation value of the relevant operator. The atomic Hamiltonian is given by Eq. (4.8) with the substitution ω_0 for Δ.

In the group-theoretical picture, the dynamics of the coupled atom-field system is governed by two ordinary differential equations of the second order:

$$\ddot{g}-\left(\frac{\dot{\epsilon}}{\epsilon}+i\omega_0\right)\dot{g}+\left(\frac{\Omega_0\epsilon}{2}\right)^2 g=0, \tag{5.2}$$

$$\ddot{\epsilon}+\omega^2\epsilon\pm 4\frac{\omega}{\epsilon}\,\mathrm{Im}(g^*\dot{g})=0, \tag{5.3}$$

with the initial conditions

$$g(0)=1,\quad \dot{g}(0)=0,\quad \epsilon(0)=1,\quad \dot{\epsilon}(0)=0. \tag{5.4}$$

The upper (lower) sign in Eq. (5.3) refers to the atom that is initially in the ground (excited) state. To obtain Eqs. (5.2)–(5.4), we used the governing equation for the SU(2) dynamical group (3.3) in the parametrization (3.2) and its two-dimensional irreducible unitary representation (4.9).

The set (5.2)–(5.4) describes two coupled oscillators. Physically, it means that the field mode ϵ determines via (5.2) the atomic motion on the phase plane $\mathrm{Re}\, g - \mathrm{Im}\, g$, while the atom, in turn, acts as a source for the field via Eq. (5.3). For numerical integration, it is convenient to introduce the alternative set of the first-order equations instead of the second-order ones (5.2) and (5.3). Supposing the atom to be initially in the ground state, we obtain

$$\dot{g} = -\frac{i\Omega_0}{2}\,\epsilon G, \tag{5.5}$$

$$\dot{G} = i\omega_0 G - \frac{i\Omega_0}{2}\,\epsilon g, \tag{5.6}$$

$$\dot{\epsilon} = -\omega \mathscr{P}, \tag{5.7}$$

$$\mathscr{P} = \omega\epsilon - 2\Omega_0\, Re(g^* G). \tag{5.8}$$

This equations possess two integrals of motions. The first one,

$$gg^* + GG^* = \mathrm{const}, \tag{5.9}$$

immediately follows from Eq. (3.8). It is simply conservation of total probability for the undamped two-level system. The second integral,

$$\omega_0(gg^* - GG^*) - \frac{\omega}{2}\,(\epsilon^2 + \mathscr{P}^2) + \Omega_0\epsilon(gG^* + g^*G) = \mathrm{const}, \tag{5.10}$$

results from the conservation of total energy for the combined atom-field system with the items in (5.10) describing the atomic, field, and interaction energies, respectively.

Since real and imaginary parts of the complex group parameter g are not independent; we have the set of ordinary differential equations (5.2) and (5.3), or alternatively, (5.5)–(5.8) in five real variables and two conservation laws, (5.9) and (5.10). As it is well known by the Poincaré–Bendixson theorem,[23] we must have three independent variables as a necessary condition for a dynamical system to be chaotic.

The quantitative characteristics of chaotic motion are the Lyapunov exponents for the trajectory. For an N-dimensional set of first-order differential equations there are N, possibly nondistinct, Lyapunov exponents,[29,30]

$$\lambda(\mathbf{Q}_0, \Delta\mathbf{q}_0) = \lim_{\substack{t\to\infty \\ \|\Delta\mathbf{q}_0\|\to 0}} \frac{1}{t} \ln \frac{\|\Delta\mathbf{q}(\mathbf{Q}_0, t)\|}{\|\Delta\mathbf{q}_0\|}, \tag{5.11}$$

where $\Delta\mathbf{q}$ is the vector in the phase space having the components $\{\Delta q_j, j = 1,\ldots,N\}$ and the norm $\|\Delta\mathbf{q}\|$. In Eq. (5.11), $\Delta\mathbf{q}_0$ and $\Delta\mathbf{q}(\mathbf{Q}_0, t)$ denote the separation between two initially adjacent trajectories at the initial moment $t = 0$ and at time t, respectively, and $\mathbf{Q}_0$ is the initial position. In general, the ordinary limit may not exist, and, therefore, λ should be defined as a limit superior.[31] If, at least, one of the Lyapunov exponents, is positive, trajectories, starting close together in phase, separate exponentially as time grows. This very sensitive dependence on initial conditions is one of the main indicators of chaos.

We have numerically calculated the largest Lyapunov exponent λ_m for different values of the coupling strength Ω using the fourth-order Runge–Kutta method. Here λ_m has been calculated in the following range of the values of the coupling strength: $0 < \Omega < 10$. As it is evident in Fig. 2, the largest Lyapunov exponent is not a monotonic function of Ω. It demonstrates as the domains of

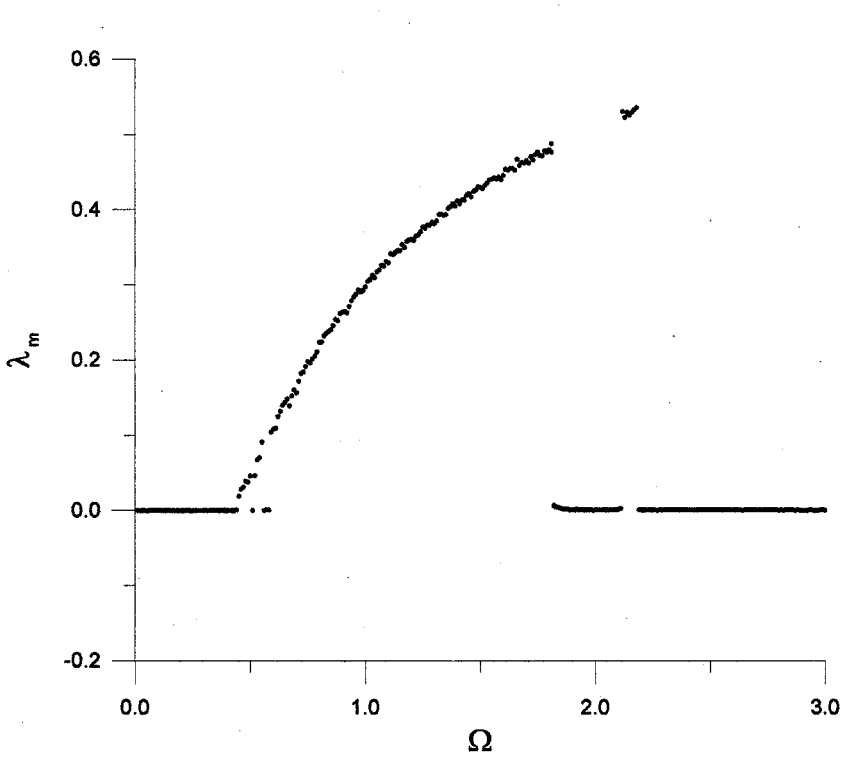

FIG. 2. The largest Lyapunov exponent λ_m for the set of differential equations (5.5)–(5.8), describing the coupled atom-field system with the feedback, as a function of the coupling strength Ω.

positive values those of negligibly small (zero) values. Let us, at first, consider three intervals of nonchaotic motion with (a) $0<\Omega<0.5$; (b) $1.8<\Omega<2.1$; and (c) $2.2<\Omega<10$.

Within all three ranges of Ω we have $\lambda_m \simeq 0$, however, the motion in the plane $\mathrm{Re}\, g - \mathrm{Im}\, g$ is shown to be quite distinct for the intervals (a), (b), and (c). In Fig. 3 we depict the stroboscopic two-dimensional phase portraits of the coupled atom-field system in the domains of quasiperiodic motion for (a) $\Omega=0.3$ and (b) $\Omega=1.9$. These portraits are the two-dimensional projections of the five-dimensional phase space of the system on the plane $\mathrm{Re}\, g - \mathrm{Im}\, g$ for the different values of the integration time growing from the left to the right. Figure 4(a) shows the same for $\Omega=2.3$. As Ω increases, but remaining within one of the intervals (a), (b), and (c), it is apparent that the motion in the phase plane $\mathrm{Re}\, g - \mathrm{Im}\, g$ becomes less localized, and the trajectories become wandering. Whereas for Ω from the range (a) the motion is localized inside the narrow ring, where $|g|^2 \approx 1$, it occupies more volume in the phase plane for Ω from the ranges (b) and (c).

It is evident in Fig. 2 that the largest Lyapunov exponent becomes positive for two ranges of Ω. The first transition to chaos occurs when the coupling strength reaches a threshold value of the order of $\Omega \simeq 0.5$. The first abrupt transition to a quasiperiodic motion takes places when Ω reaches the value in the neighborhood of 1.8. The second transition to chaos takes place suddenly when the coupling strength Ω is in the neighborhood of 2.1. The second chaotic regime of oscillations in the coupled atom-field system seems to be much shorter than the first one, and persists until $\Omega \simeq 2.2$.

The power spectra have been calculated for different values of the coupling strength. As is usual, the spectra demonstrates a few δ-like peaks for all three intervals of quasiperiodic motion, and become broadband in the cases of chaotic regimes.

Representative two-dimensional phase portraits of the system with the coupling strength

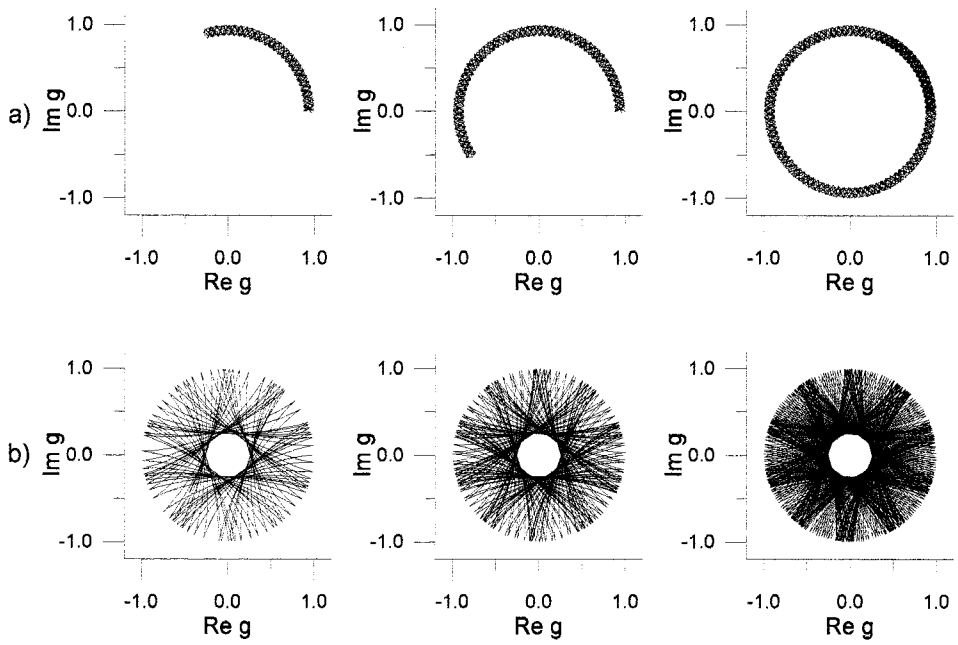

FIG. 3. Stroboscopic two-dimensional phase portraits of the coupled atom-field system oscillating in the quasiperiodic regime ($\lambda_m \simeq 0$) with (a) $\Omega=0.3$ and (b) $\Omega=1.9$ under the resonance condition, $\omega=\omega_0$.

$\Omega=1.36$, which gives the positive largest Lyapunov exponent of the order of $\lambda_m \simeq 0.4$, are shown in Fig. 4(b) for three different time moments.

In summary, we have numerically observed a nontrivial sequence of transitions from quasiperiodicity to chaos in the coupled atom-field system with the feedback. The quantitative criterion of chaos, the largest Lyapunov exponent, does not increase monotonically with the coupling strength. The sequence of the transitions is clearly seen in Fig. 2, with two chaotic regimes alternating among three regular regimes. As far as we know, the alternating regimes of chaos and periodicity was not found in coupled atom-field models.[24–28] Our results are rather reminiscent of the classic Lorenz attractor (see, for example, Ref. 32).

VI. CONCLUSION

We have shown that the dynamical-symmetry approach is a useful tool for treating the dynamics of quantum systems as from the point of view of the problem of controlling quantum evolution and as from the standpoint of the problem of quantum chaos. Applying this method to the system of two-level atoms interacting with an electromagnetic field, we have provided a new insight into the dynamics of such a process. In particular, a sequence of transitions from the quasiperiodicity to chaos has been numerically observed for a two-level atom interacting with a self-consistently generated radiation field.

We have focused attention on this atom-field system because it appears to be the simplest and the most fundamental model for studying interaction between matter and radiation. Since the group-theoretical approach is based on symmetry properties of the governing Hamiltonian, it is applicable to a variety of physical situations. In particular the results obtained in this paper can be used (with a slight modification) for describing the time evolution of any driven quantum system with the underlying SU(2) dynamical symmetry.

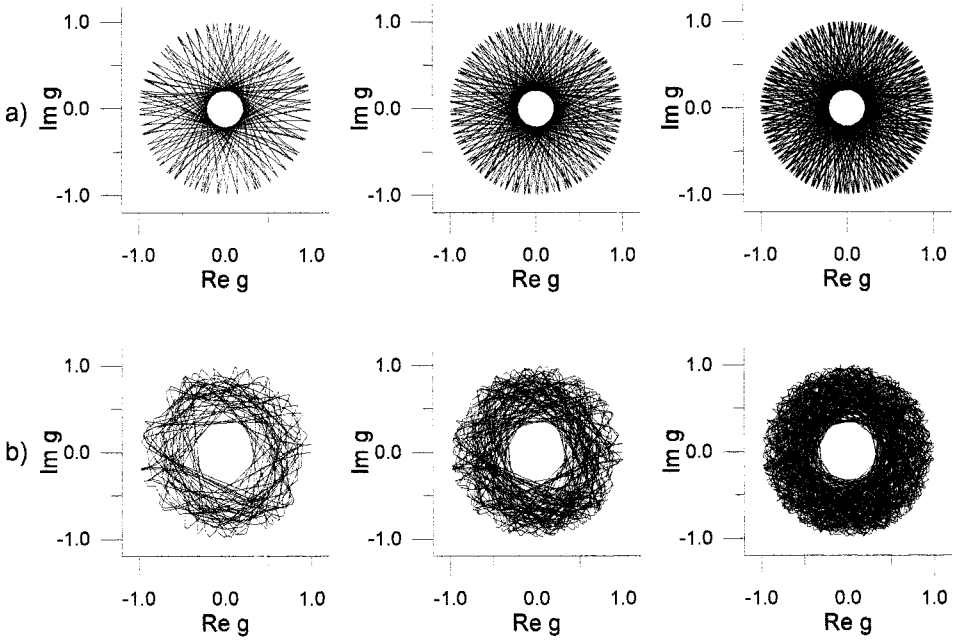

FIG. 4. Stroboscopic two-dimensional phase portraits of the coupled atom-field system oscillating in (a) the quasiperiodic regime ($\lambda_m \simeq 0$) with $\Omega=2.3$ and in (b) the chaotic regime ($\lambda_m \simeq 0.4$), with $\Omega=1.36$ under the resonance condition, $\omega=\omega_0$.

ACKNOWLEDGMENT

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Geometric phase, bundle classification, and group representation

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The line bundles that arise in the holonomy interpretations of the geometric phase display curious similarities to those encountered in the statement of the Borel–Weil–Bott theorem of the representation theory. The remarkable relationship between the mathematical structure of the geometric phase and the classification theorem for complex line bundles provides the necessary tools for establishing the relevance of the Borel–Weil–Bott theorem to Berry's adiabatic phase. This enables one to define a set of topological charges for arbitrary compact connected semisimple dynamical Lie groups. These charges signify the topological content of the phase. They can be explicitly computed. In this paper, the problem of the determination of the parameter space of the Hamiltonian is also addressed. It is shown that, in general, the parameter space is either a flag manifold or one of its submanifolds. A simple topological argument is presented to indicate the relation between the Riemannian structure on the parameter space and Berry's connection. The results about the fiber bundles and group theory are used to introduce a procedure to reduce the problem of the nonadiabatic (geometric) phase to Berry's adiabatic phase for cranked Hamiltonians. Finally, the possible relevance of the topological charges of the geometric phase to those of the non-Abelian monopoles is pointed out. © *1996 American Institute of Physics.* [S0022-2488(96)03502-7]

I. INTRODUCTION

In the past ten years, since the revival of the geometric phase,[1,2] by Berry,[3] the subject has attracted the attention of many physicists. The main reason for the unusual popularity of this remarkably simple subject, particularly among the theoretical physicists, has been its rich mathematical and physical foundations.

Recently, it was shown that the two holonomy interpretations of Berry's phase were linked via the theory of universal bundles.[4,5] This remarkable coincidence of the physics of geometric phase and the mathematics of fiber bundles enables one to set up a convenient framework to analyze the nonadiabatic phase.[5] In the present paper, the results of[5] are briefly reviewed and their generalization to arbitrary finite-dimensional unitary systems are presented.

In Sec. II, it is shown how the study of the standard example of a spin in a processing magnetic field directs one to the Borel–Weil–Bott (BWB) theorem of the representation theory of compact semisimple Lie groups. In Sec. III, the relation of the BWB theorem to the phenomenon of a geometric phase is discussed in a general setting. Section IV is devoted to a discussion of the relation of Berry's connection and the Riemannian geometry of the parameter space. Section V includes the discussion of the reduction of the nonadiabatic phase problem to the adiabatic one for the cranked Hamiltonians. Section VI consists of a short account on the classification of the

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parameter spaces and the topology of non-Abelian monopoles. Section VII includes the conclusions.

II. BUNDLE CLASSIFICATION AND THE HOLONOMY INTERPRETATIONS OF THE GEOMETRIC PHASE

There are two mathematical interpretations of Berry's (adiabatic) phase. These are due to Simon[6] and Aharonov and Anandan.[7] I shall refer to these two approaches by ''BS'' and ''AA,'' which are the abbreviations of ''Berry–Simon'' and ''Aharonov–Anandan,'' respectively.

In the BS approach, one constructs a line bundle L over the space M of the parameters of the system. Then, L is endowed with a particular connection that reproduces Berry's phase as the holonomy of the closed loop in the parameter space.

Let us consider a quantum mechanical system whose evolution is governed by a parameter-dependent Hamiltonian:

$$H=H(x), \quad x\in M.$$

Assume that for all $x\in M$ the spectrum of $H(x)$ is discrete and that there are no level crossings. Then, locally one can choose a set of orthonormal basic eigenstate vectors $\{|n,x\rangle\}$. As functions of x, $|n,x\rangle$ are smooth and single valued. By definition, they satisfy

$$H(x)|n,x\rangle=E_n(x)|n,x\rangle, \tag{1}$$

where $E_n(x)$ are the corresponding energy eigenvalues. The Hamiltonian is made explicitly time dependent by interpreting time t as the parameter of a curve,

$$C:[0,T]\ni t\to x(t)\in M, \tag{2}$$

and setting

$$H(t):=H(x(t)), \quad t\in[0,T]. \tag{3}$$

Then, each closed curve C in M defines a periodic Hamiltonian with period T. I shall discuss only the evolution of nondegenerate cyclic states with period T.

Under the adiabatic approximation the initial eigenstates undergo cyclic evolutions.[3] If $|\psi_n(t)\rangle$ denotes the evolving state vector, i.e., the solution of the Schrödinger equation:

$$H(t)|\psi_n(t)\rangle=i\,\frac{d}{dt}\,|\psi_n(t)\rangle$$

$$|\psi_n(0)\rangle:=|n,x(0)\rangle, \tag{4}$$

then

$$|\psi_n(T)\rangle\langle\psi_n(T)|\simeq|\psi_n(0)\rangle\langle\psi_n(0)|. \tag{5}$$

After a cycle is completed, the state vector gains a phase factor that consists of a dynamical ($e^{i\omega}$) and a geometric ($e^{i\gamma}$) part,

$$|\psi_n(T)\rangle=e^{i(\omega+\gamma)}|\psi_n(0)\rangle, \tag{6}$$

where

$$\omega := -\int_0^T E_n(x(t))dt,$$

and

$$e^{i\gamma} := \exp\left(\oint_C A\right), \tag{7}$$

$$A := -\langle n,x|d|n,x\rangle = -\langle n,x|\,\frac{\partial}{\partial x^\mu}\,|n,x\rangle dx^\mu. \tag{8}$$

The one-form A is known as Berry's connection one-form.[3]

In Ref. 6, Simon showed that A could be interpreted as a connection one-form on a (spectral) line bundle L over M,

$$\mathbb{C}\to L\to M, \tag{9}$$

whose fibers are given by the energy eigenrays in the Hilbert space $\mathscr{H}$,

$$L_x := \{z|n,x\rangle \;:\; z\in\mathbb{C}\}. \tag{10}$$

Thus, in the BS approach, Berry's phase is identified with the holonomy of the loop $C\subset M$ defined by the connection one-form A of Eq. (8).

In the AA approach one considers a complex line bundle E, or alternatively, the associated $U(1)$-principal bundle, over the projective Hilbert space $P(\mathscr{H})=\mathbb{C}P^N$, $N:=\dim(\mathscr{H})-1$:

$$\mathbb{C}\to E\to\mathscr{P}(\mathscr{H}). \tag{11}$$

The fibers over the points $\eta=|\eta\rangle\langle\eta|$ of $\mathscr{P}(\mathscr{H})=\mathbb{C}P^N$ are the corresponding rays:

$$E_\eta := \{z|\eta\rangle \;:\; z\in\mathbb{C}\}, \tag{12}$$

in the Hilbert space $\mathscr{H}$. (The topological structure of E is determined by the topological structure of $\mathbb{C}P^N$. In particular, a natural local trivialization is given by adopting the standard homogeneous local coordinate charts for $\mathbb{C}P^N$. The associated transition functions of E are determined from those of $\mathbb{C}P^N$ similarly. See Sec. IV for an alternative characterization of the topology of E.)

The AA connection one-form $\mathscr{A}$ (Ref. 7) is then viewed as a connection one-form on E and the geometric phase is identified with the corresponding holonomy of loops,

$$\mathscr{C}:[0,T]\ni t\to\eta(t)\in\mathscr{P}(\mathscr{H}), \tag{13}$$

in $\mathscr{P}(\mathscr{H})$. In the adiabatic approximation one approximates $\eta(t)$ by $\psi_n(t)$ of Eq. (4).

These two interpretations of Berry's phase turn out to be linked via the theory of *universal bundles*. It is shown in Refs. 4 and 5 that E (with $N\to\infty$) is indeed the universal classifying line bundle,[8–10] and as a result of the classification theorem for complex line bundles,[9,8,11] every complex line bundle can be obtained as a pullback bundle from E. In particular, there is a smooth map,

$$f:M\to\mathscr{P}(\mathscr{H}), \tag{14}$$

such that

$$L=f^*(E). \tag{15}$$

The map f is simply given by

$$f(x):=|n,x\rangle\langle n,x|. \tag{16}$$

Furthermore, the fact that the phase is obtained from either of A or $\mathscr{A}$ is a consequence of the theory of *universal connections*.[12,13] In fact, the AA connection $\mathscr{A}$ is precisely the universal connection, which yields all connections on all complex line bundles as pullback connections. In particular, Berry's connection on L is given by

$$A=f^*(\mathscr{A}). \tag{17}$$

These results are exploited in Ref. 5 to explore the quantum dynamics of Berry's original example:

$$H(x)=b\mathbf{x}\cdot\mathbf{J}, \quad \mathbf{x}\in S^2\subset\mathbb{R}^3, \tag{18}$$

where b is the Larmor frequency, $\mathbf{x}$ is the direction of the magnetic field, and $\mathbf{J}=(J_i)$, $i=1,2,3$, are the generators of rotations, $J_i\in so(3)=su(2)$. In Ref. 5, it is shown that if one considers the case of precessing magnetic field, i.e., precessing $\mathbf{x}$ about a fixed axis, then one can promote Simon's construction to the nonadiabatic case, namely, define a nonadiabatic analog of Berry's connection and identify the nonadiabatic phase with its holonomy. This can be done in general unless the frequency of precession, ω, becomes equal to b. In the northern hemisphere the nonadiabatic connection $\tilde{A}$ is given by

$$\tilde{A}=ik(1-\cos\,\tilde{\theta})d\phi, \tag{19}$$

where k labels an eigenvalue of $H(x)$ (alternatively an eigenvalue of J_3), and

$$\cos\,\tilde{\theta}:=\frac{\cos\,\theta-\nu}{\sqrt{\nu^2-2\nu\,\cos\,\theta+1}}, \tag{20}$$

$$\nu:=\frac{\omega}{b}. \tag{21}$$

Here (θ,ϕ) are the spherical coordinates $(\theta\in[0,\pi))$, and ν is the "slowness parameter".[14] The adiabatic limit is characterized by $\nu\to 0$. In this limit $\tilde{A}$ approaches to Berry's connection,

$$A=ik(1-\cos\,\theta)d\phi. \tag{22}$$

Note that unlike the adiabatic case $(\nu\to 0)$, the cyclic states in the more general nonadiabatic case cannot be approximated by the eigenstates of the initial Hamiltonian. They are given as the eigenstates of the unitary time evolution operator at time T. This operator does not generally commute with the initial Hamiltonian, and they do not share simultaneous eigenstates.

The topology of a line bundle on S^2 is determined by its first Chern number,

$$c_1:=\frac{i}{2\pi}\int_{S^2}\Omega, \tag{23}$$

where Ω is the curvature two-form. For line bundles, the curvature two-form is obtained from the connection one-form by taking its ordinary exterior derivative.[15] A simple calculation shows that taking $\Omega=d\tilde{A}$ results in

$$c_1=-2k, \quad \text{for } \nu<1. \tag{24}$$

This is quite remarkable since the fact that c_1 is an integer agrees with the fact that k is a half-integer. The first statement is an algebraic topological result, whereas the second is related to group theory. One of the best known mathematical results that links these two disciplines is the celebrated Borel–Weil–Bott (BWB) theorem.[16–19]

Equation (24) may also be viewed as an example of a topological quantization of angular momentum. In the language of magnetic monopoles, which are relevant to the adiabatic case, $k=-c_1/2$ corresponds to the product of the electric and magnetic charges.[20,21]

III. BOREL–WEIL–BOTT THEOREM AND THE BERRY–SIMON LINE BUNDLES

The BWB theorem constructs all the finite-dimensional irreducible representations (irreps.) of semisimple compact Lie groups from the irreps. of their maximal tori. The construction is as follows.

Let G be a semisimple compact Lie group and T be a maximal torus. Let $\mathscr{G}$ and Υ be the Lie algebras of G and T, respectively. G can be viewed as a principal bundle over the quotient space G/T:[22]

$$T\rightarrow G\rightarrow G/T. \tag{25}$$

The homogeneous space G/T can be shown to have a canonical complex structure.[17] Since T is Abelian, its irreps. are one dimensional.[22] Thus, each irrep. Λ of T defines an associated complex line bundle L_Λ to (25):

$$\mathbb{C}\rightarrow L_\Lambda\rightarrow G/T. \tag{26}$$

Now, consider a Λ whose corresponding line bundle L_Λ is an ample (positive) line bundle. Then L_Λ has the structure of a holomorphic line bundle. BWB theorem asserts that all the irreps. of G are realized on the spaces of holomorphic sections of ample (positive) line bundles, L_Λ. In particular, the space $\mathscr{H}_\Lambda$ of the holomorphic sections of L_Λ provides the irrep. of G with maximal weight Λ.[18,17,19]

The simplest nontrivial example of the application of the BWB theorem is for $G=\mathrm{SU}(2)$. In this case, $T=U(1)=S^1$ and $G/T=S^2=\mathbb{C}P^1$. The bundle (25) is the Hopf bundle:[22]

$$U(1)=S^1\rightarrow SU(2)=S^3\rightarrow S^2. \tag{27}$$

Λ takes non-negative half-integers. It is usually denoted by j in QM. It is common knowledge that $j=0,\ \frac{1}{2},1,...,$ yield all the irreps. of SU(2) and that the j representation has dimension $2j+1$. The dimension of the space $\mathscr{H}_\Lambda$ can be given by an index theorem.[18,16] For SU(2), it is obtained by the Riemann–Roch theorem in the context of the theory of Riemann surfaces. The result is

$$\dim(\mathscr{H}_\Lambda)=c(L_\Lambda)=1+c_1(L_\Lambda), \tag{28}$$

where c and c_1 denote the total and first Chern numbers of L_Λ. This means that one must have

$$c_1(L_\Lambda)=2j. \tag{29}$$

Combining (24) and (29), one recovers the line bundle L_Λ as Simon's line bundle L of (9) for $k=-j$.

In the rest of this section, I shall try to show that there is a general relationship between the constructions used in the BWB theorem and those encountered in BS interpretation of Berry's phase. To proceed in this direction, let us consider the generalization of (18) to an arbitrary compact semisimple Lie group, namely, consider

$$H(x)=\epsilon\sum_{i=1}^{d} x^i J_i\,, \quad (x^i)\in\mathbb{R}^d-\{0\}. \tag{30}$$

Here J_i are the generators of G and ϵ is a constant with the dimension of energy. Since $H(x)$ is assumed to be Hermitian, J_i must be represented by Hermitian matrices. In other words, the group G is in a unitary representation. In this sense, the example of $G=U(N)$ plays a universal role. (This reminds one of the Peter–Weyl theorem.[19,22])

The system described by Eq. (30) is studied in Refs. 23 and 24. In Ref. 23, it is argued that, in general, there are unitary operators $U(t)$ that diagonalize the instantaneous Hamiltonian:

$$H(t)=U(t)H_D(t)U(t)^\dagger. \tag{31}$$

In view of Eq. (3), one has

$$U(t)=U(x(t)), \tag{32}$$

where

$$x(t)=(x^i(t))\in\mathcal{G}-\{0\}=\mathbb{R}^d-\{0\}, \tag{33}$$

are the points of the loop in the parameter space. In fact, one can show that the parameter space "is not" $\mathbb{R}^d-\{0\}$, but a submanifold of this space, namely the flag manifold G/T.

To see this, let me first introduce the root system of $\mathcal{G}$ associated with Υ and the corresponding Cartan decomposition:

$$\mathcal{G}_{\mathbb{C}}=\Upsilon_{\mathbb{C}}\oplus_\alpha\mathcal{G}_\alpha\,, \tag{34}$$

where the subscript $\mathbb{C}$ means *complexification* and α stand for the roots. Let l denote the rank of $\mathcal{G}$, $\{H_i\}_{i=1,2,\ldots,l}$ and E_α be bases of Υ and $\mathcal{G}_\alpha$, respectively.[25,22,18,17] Then, one has

$$\begin{gathered}[H_i\,,\,H_j]=0, \quad [H_i\,,\,E_\alpha]\propto E_\alpha\,, \quad [E_\alpha\,,\,E_{-\alpha}]\propto H_\alpha\in\Upsilon,\\ [E_\alpha\,,\,E_\beta]\propto E_{\alpha+\beta}\,, \qquad \text{for} \quad \beta\neq-\alpha.\end{gathered} \tag{35}$$

Any group element can be obtained as a product of the exponentials of the generators of the algebra. In particular,

$$U(t)=\exp\left[i\sum_\alpha \chi_\alpha(t)E_\alpha\right]\exp\left[i\sum_i \chi_i(t)H_i\right]. \tag{36}$$

Since any diagonal element commutes with H_i's, it belongs to Υ. Hence, one has

$$H_D(t)=\sum_i b_i(t)H_i\,. \tag{37}$$

Substituting Eq. (37) in Eq. (36) and using the resulting equation to simplify Eq. (31), one obtains

$$H(t)=\exp\Big(i\sum_{\alpha}\chi_{\alpha}(t)E_{\alpha}\Big)H_D(t)\exp\Big(-i\sum_{\alpha}\chi_{\alpha}(t)E_{\alpha}\Big) \tag{38}$$

$$=\exp\Big(i\sum_{\alpha>0}[z_{\alpha}(t)E_{\alpha}+z_{\alpha}^{*}(t)E_{-\alpha}]\Big)H_D(t)$$

$$\times\exp\Big(-i\sum_{\alpha>0}[z_{\alpha}^{*}(t)E_{\alpha}+z_{\alpha}(t)E_{-\alpha}]\Big). \tag{39}$$

In Eqs. (38) and (39), $\chi_{\alpha}\in\mathbb{R}$ and $z_{\alpha}\in\mathbb{C}$ are time-dependent parameters. It is shown in Ref. 23 that, in general, the geometric phase is given in terms of χ_{α}'s, or alternatively in terms of z_{α}'s, and it does not depend on $H_D(t)$. It is not difficult to see that indeed χ_{α} correspond to the coordinates of the points of the flag manifold G/T. Alternatively, one can use the complex coordinates z_{α}. This is reminiscent of the fact that G/T has a canonical complex structure.[17] This completes the proof of the claim that the true parameter space of the system described by (30) is G/T, or a submanifold of G/T. I will come back to this point in Sec. VI. The fact that G/T can be viewed as embedded in $\mathscr{G}$ is useful because it allows one to work with the global Cartesian coordinates systems on $\mathscr{G}=\mathbb{R}^d$.[24] A natural embedding of G/T is provided by taking a regular (nondegenerate) element H_0 of Υ and considering the adjoint action of G on $\mathscr{G}$. The orbit corresponding to H_0 is a copy of G/T. Thus, one might note that in Eq. (30),

$$x=(x^i)\in G/T\subset\mathbb{R}^d. \tag{40}$$

The fact that the phase information is encoded in $U(t)$ of Eq. (31) can be used to simplify the problem, namely one can restrict to the case where the $H_D(t)=H_D(0)=H_0$ is kept constant, i.e.,

$$H_D=\sum_i b_iH_i=:H_0\in\Upsilon,\quad b_i=\text{const.} \tag{41}$$

The Hilbert space $\mathscr{H}$ of the quantum state vectors provides the representation space. It can be decomposed into irrep. spaces. I shall assume that $\mathscr{H}$ (or the subspace of $\mathscr{H}$ relevant to the geometric phase) corresponds to an irrep. with maximal weight Λ.[18] The weights are the simultaneous eigenvectors of H_i's.[25] They are conveniently denoted by $|\lambda_1,...,\lambda_l\rangle$, or collectively by $|\lambda\rangle$, where

$$H_i|\lambda\rangle=\lambda_i|\lambda\rangle,\quad \forall i=1,\ldots,l. \tag{42}$$

Clearly, the weight vectors $|\lambda\rangle$ are the eigenstate vectors of the initial Hamiltonian. Here, I have set $U(0)=1$ in Eq. (31).[23] In general, this can be achieved by appropriately choosing the maximal torus T. Thus, one has

$$H(x(0))=H_D=H_0 \tag{43}$$

and

$$H_D|\lambda\rangle=\sum_{i=1}^{l}b_i\lambda_i|\lambda\rangle. \tag{44}$$

Making the dependence of $H_D(H_0)$ on the initial point $x_0:=x(0)$ explicit, one can write Eq. (44) in the form

$$H_0(x_0)|\lambda,x_0\rangle = E_\lambda(x_0)|\lambda,x_0\rangle, \quad E_\lambda(x_0) := \sum_{i=1}^{l} b_i \lambda_i(x_0). \tag{45}$$

The weight vectors $|\lambda,x_0\rangle$ are precisely the eigenvectors $|n,x_0\rangle$ of the instantaneous Hamiltonian $H_0(x_0)$. Since x_0 can be chosen arbitrarily, one can simply drop the subscript "0," i.e., replace x_0 by x and $H_0(x_0)$ by $H(x)$.

The BS line bundle, in this case, is obtained as the pullback bundle from the universal classifying bundle E,

$$L_\lambda^{\mathrm{BS}} := f^*(E), \tag{46}$$

induced by the map

$$f: M \ni x \to |\lambda,x\rangle\langle\lambda,x| \in \mathscr{P}(\mathscr{H}) \subset \mathbb{C}P^\infty.$$

Recalling some basic facts about the flag manifolds and their relation to projective spaces,[18] one finds that, in fact, L_λ^{BS} corresponds to the line bundle L_Λ of the BWB theorem, if the weight vector $|\lambda,x_0\rangle$ is chosen to be the maximal weight Λ of the representation. First, let us recall[18,17] that flag manifolds are projective varieties, i.e., there exist embeddings of M into $\mathbb{C}P^\infty$,

$$i: M \hookrightarrow \mathbb{C}P^\infty. \tag{47}$$

Indeed, one can obtain $M = G/T$ as a unique closed orbit of the action of G on $\mathscr{P}(\mathbb{C}^{N+1}) = \mathbb{C}P^N$, for some $(N+1)$-dimensional irrep. (Ref. 18, Sec. 23.3). The line bundle L_Λ is then the restriction (pullback under the identity map) of E:

$$L_\Lambda = i^*(E). \tag{48}$$

Let $|v_0\rangle$ be a nonzero vector in the representation (Hilbert) space of the Λ representation of $G, G_{\mathbb{C}}$ be the complexification of G, and consider the map

$$\Phi: G_{\mathbb{C}} \to \mathscr{P}(\mathscr{H}),$$

defined by

$$\Phi(\tilde{g}) := [U(\tilde{g})|v_0\rangle] = U(\tilde{g})|v_0\rangle\langle v_0|U(\tilde{g})^\dagger. \tag{49}$$

Here $U(\tilde{g})$ is the representation of $\tilde{g} \in G_{\mathbb{C}}$ and $[U(\tilde{g})|v_0\rangle]$ denotes the ray passing through $U(\tilde{g})|v_0\rangle$. Φ is clearly not one to one. Let P be the closed subgroup of $G_{\mathbb{C}}$ defined by

$$P := \{\tilde{h} \in G_{\mathbb{C}} \ : \ U(\tilde{h})|v_0\rangle = c|v_0\rangle, \quad \text{for some } c \in \mathbb{C}-\{0\}\}. \tag{50}$$

By construction the map Φ induces a one-to-one map on $G_{\mathbb{C}}/P$:

$$\hat{\Phi}: G_{\mathbb{C}}/P \to \mathscr{P}(\mathscr{H}). \tag{51}$$

Now, let us choose

$$|v_0\rangle := |\Lambda,x_0\rangle, \tag{52}$$

and denote by B the *Borel subgroup* of $G_{\mathbb{C}}$ generated by H_i and $E_{\alpha>0}$. Then, $B \subset P$ and consequently $G_{\mathbb{C}}/P$ is a compact submanifold (subvariety) of $G_{\mathbb{C}}/B$. However, one has the identity

$$G_{\mathbb{C}}/B = G/T,$$

where by equality I mean the diffeomorphism of homogeneous spaces.[17] Thus, in general, $G_{\mathbb{C}}/P \subset G/T$.

The extreme case is when $P=B$, i.e., $M=G_{\mathbb{C}}/P=G/T$. However, in general, B may be a proper subgroup of P, in which case the parameter manifold can be restricted to the submanifold $G_{\mathbb{C}}/P$ of G/T. This depends on the representation, i.e., on Λ.

Let us consider the general case, i.e., $M=G_{\mathbb{C}}/P$. The basic vectors $|\lambda,x\rangle$ are parametrized by the points of $G_{\mathbb{C}}/P \subset G/T$ and the map f of (16) becomes

$$f: G_{\mathbb{C}}/P \ni x \to |\lambda,x\rangle\langle\lambda,x| \in \mathscr{P}(\mathscr{H}). \tag{53}$$

In view of the fact that $G_{\mathbb{C}}/P \subset G/T$, one may work with the representative of $x=[g] \in G/T$ rather than $x=[\tilde{g}] \in G_{\mathbb{C}}/P$ for the parameters x. The next logical step is to compare the map $\hat{\Phi}$ of (51) with f. Let $x \in M \subset G/T$; then every eigenstate vector $|\lambda,x\rangle$ can be obtained by the action of G on a nonzero vector. In particular, there is a $g_x \in G$ such that

$$|\lambda,x\rangle = U(g_x)|\lambda,x_0\rangle. \tag{54}$$

Combining Eqs. (52), (53), (54), and specializing to $\lambda=\Lambda$, one finds

$$f(x) = U(g_x)|v_0\rangle\langle v_0|U(g_x) = [U(g_x)|v_0\rangle]. \tag{55}$$

Recalling the procedure according to which x is assigned to represent the parameter (40) of the system (30), one can identify $[g_x] \in G_{\mathbb{C}}/P \subset G/T$ with x, i.e.,

$$U(g_x) \equiv U(x),$$

and consequently,

$$f(x) = [U(x)|v_0\rangle] = \hat{\Phi}(x). \tag{56}$$

For the special case of $P=B$, the map $\hat{\Phi}$ becomes the map i of (47). Thus, according to Eqs. (48) and (56), the following identity is established:

$$L_\Lambda = f^*(E). \tag{57}$$

Equation (57) is valid generally, i.e., even when $P \neq B$. In this case, $M=G_{\mathbb{C}}/P$ is a proper submanifold of G/T, and the role of the embedding i of Eq. (47) is played by

$$i': M \hookrightarrow G/T \overset{i}{\hookrightarrow} \mathbb{C}P^\infty.$$

Comparing Eq. (57) with Eq. (46), one arrives at the desired result, namely that the bundle L_Λ of the BWB theorem is identical to the BS bundle L_Λ^{BS}. In particular, the dimension of the irrep., i.e., the Hilbert space $\mathscr{H}$ is given by the number of the linearly independent holomorphic sections of L_Λ^{BS}. The latter is a topological invariant of L_Λ^{BS}.

It is well known that the topology of a complex line bundle is uniquely determined by its first Chern class $\hat{c}_1$.[26,5] $\hat{c}_1$ is represented by a closed differential two-form on M. It can be characterized by a set of $[p:=\dim H_2(M,\mathbb{Z})]$ integers by integrating it over p compact two-dimensional submanifolds of M, which are called the 2-cells of M. For example, if $G=\mathrm{SU}(2)$, $M=S^2$ and the space S^2 is the only 2-cell. Therefore, $\hat{c}_1$ is determined by a single integer c_1 via Eq. (23).

In general, the following modification of Eq. (23) provides the necessary integers,

$$c_1^a = \hat{c}_1(\sigma_a) := \frac{i}{2\pi}\int_{\sigma_a} \Omega, \tag{58}$$

where σ_a is the ath 2-cell ($a=1,\ldots,p$), c_1^a is the first Chern number associated with σ_a, and Ω is the curvature two-form of the line bundle.

For the case of the BWB–BS line bundle, c_1^a determine the irreps. On the other hand, the irreps. are given by the maximal weight Λ of the representation. The latter can be written as a linear combination of the so-called *fundamental weights* (Ref. 18, Sec. 14.1), with non-negative integer coefficients. Let us denote these by Λ_b, $b=1,\ldots,l$. Then,

$$\Lambda=\sum_{b=1}^{l} k_b\Lambda_b, \quad k_b\in\mathbb{Z}^+\cup\{0\}. \tag{59}$$

This means that to determine the k_b's and hence the irrep. one needs precisely l "independent" first Chern numbers. These are obtained by integrating (58) over the 2-cells of G/T. The 2-cells are l copies of S^2 that correspond to the canonical SU(2) subgroups of G. These are generated by the triplets of the generators $(E_\alpha,E_{-\alpha},H_\alpha)$, where α's are the l simple roots of $\mathscr{G}$, and E_α and H_α are as in Eq. (35). Denoting these $SU(2)$ subgroups and their maximal tori by G_a and T_a, respectively, the 2-cells are given by

$$\sigma_a:=G_a/T_a=SU(2)/U(1)=S^2. \tag{60}$$

The restriction of the curvature two-form Ω on σ_a yields Berry's curvature two-form.[3] Integrating these two-forms on σ_a gives rise to l identities of the form (24). Incidentally, in view of the relevance of the system of Eq. (18) to magnetic monopoles[21] (30) corresponds to a generalized magnetic monopole whose charge has a vectorial character with integer components. I shall return to the discussion of monopoles in Sec. VI.

IV. BERRY'S CONNECTION AND THE RIEMANNIAN GEOMETRY OF THE PARAMETER MANIFOLD

One of the rather interesting facts about the geometric phase is that the AA connection $\mathscr{A}$ is related to the Fubini–Study metric on the projective space $\mathbb{C}P^N$.[27] In the language of fiber bundles, the Riemannian geometry of a manifold X means the geometry of its tangent bundle TX. In particular, the Riemannian metric (the Levi–Civita connection) is a metric (resp., a connection) on TX. The statement that the AA connection is related to the Riemannian geometry of $\mathbb{C}P^N$ is equivalent to say that the universal (AA) bundle,

$$E:\mathbb{C}\to E\to\mathbb{C}P^N,$$

is related to the tangent bundle,

$$T\mathbb{C}P^N:\mathbb{C}^N\to T\mathbb{C}P^N\to\mathbb{C}P^N.$$

This is easy to show topologically. The precise relation is demonstrated in the form of the following identity:

$$\mathrm{Det}[T\mathbb{C}P^N]=E^*\otimes E^*, \tag{61}$$

where Det means the determinant bundle:

$$\mathrm{Det}[T\mathbb{C}P^N]:=\underbrace{T\mathbb{C}P^N\wedge\cdots\wedge T\mathbb{C}P^N}_{N\ \text{times}},$$

$\wedge$ stands for the wedge product of the vector bundles, E^* is the dual line bundle to E, and $\otimes$ is the tensor product.[8] To see the validity of Eq. (61), it is sufficient to examine the first Chern classes of both sides. In fact, since $\mathbb{C}P^N$ has a single 2-cell, namely $\mathbb{C}P^1=S^2$, one can simply compare the first Chern numbers. It is well known[10] that

$$c_1(E)=-1. \tag{62}$$

Furthermore, for any vector bundle V,

$$\hat{c}_1[\text{Det } V]=\hat{c}_1[V]. \tag{63}$$

Also, it is not difficult to show that

$$c_1(T\mathbb{C}P^N)=c_1(T\mathbb{C}P^1)=\chi(S^2)=2, \tag{64}$$

where χ stands for the Euler–Poincaré characteristic. Equations (63) and (64) imply that

$$c_1[\text{Det } T\mathbb{C}P^N]=2.$$

The last equality, together with the fact that

$$c_1(E^*)=-c_1(E)$$

and Eq. (62), are sufficient to establish the validity of Eq. (61).

The existence of this relationship between the AA connection and the Riemannian metric on $\mathbb{C}P^N$ has triggered the investigation of a similar pattern in the BS approach.[28] In Ref. 28, the authors discuss the case of a general Hamiltonian with a dynamical group G and a parameter space G/H, where H is a closed subgroup of symmetries of the Hamiltonian. The analysis presented above seems to include all these cases. In the following section, I will show that the system of Eq. (30) has a universal character. In other words, all the cases discussed in Ref. 28 can be reduced to the one given by (30). In all these cases the parameter space, G/H, is a submanifold of $FU(m):=U(m)/T^m$, $T^m:=[U(1)]^m$, which is itself embedded into $\mathbb{C}P^\infty$. Hence, the results of Ref. 28 are expected because (i) the BS bundle (connection) is the pullback (restriction) of the universal bundle E; and (ii) E is related to $T\mathbb{C}P^N$, via Eq. (61).

V. REDUCTION OF THE NONADIABATIC PHASE TO THE ADIABATIC PHASE FOR THE CRANKED HAMILTONIANS

Let us consider an arbitrary $m\times m$ Hamiltonian H acting on $\mathscr{H}=\mathbb{C}^m$. H can be viewed as an element of the (real) vector space of all complex $m\times m$-dimensional Hermitian matrices. It is very easy to compute the real dimension of this space and find out that it is equal to m^2. Thus, H can be written as a linear combination of m^2 linearly independent Hermitian matrices. Incidentally, the generators J_i of $U(m)$ form a set of m^2 such matrices. This simply indicates that one can always express H in the form of Eq. (30). This may be seen as a realization of the Peter–Weyl theorem.[19] The particular representation of H given by Eq. (30) with $G=U(m)$ for some $m\in\mathbb{Z}^+$ might not be a practical choice. For example, the quadratic Hamiltonian,

$$H=\sum_{i,j=1}^{3} Q_{ij}\sigma_i\otimes\sigma_j,$$

with σ_i being Pauli matrices,[28,29] is more manageable in this form than in the form of Eq. (30), with J_i chosen to be the generators of $U(4)$. However, in principle, one can always use the linear representation, Eq. (30).

Actually, one can use the generators of $SU(m)$ rather than $U(m)$. This is emphasized in Ref. 23. It can be directly justified by recalling that the (m^2-1) generators of $SU(m)$ are also linearly independent, and these together with the $(m\times m)$ identity matrix I provide a basis for the space of $(m\times m)$ Hermitian matrices. The Hamiltonian H can then be written as a linear combination in this basis. Clearly, the term proportional to I does not contribute to the geometric phase. This is often used as an indication of the geometric nature of Berry's phase.[30]

An advantage of the linear representation is that it allows one to use the knowledge about the universal bundles and BWB theorem directly. In particular, in some cases, it is possible to obtain the nonadiabatic analog of the BS line bundle and the connection A. The first example of this is presented in Ref. 5. In this section, I will show that since the above argument does not refer to the adiabaticity of the system, one can always reduce the Hamiltonian to the linear form. Moreover, if the time dependence of the corresponding linear Hamiltonian is realized by cranking of the initial Hamiltonian along a fixed direction,[24] then one can obtain a nonadiabatic analog $\tilde{A}$ of Berry's connection A as a pullback connection one-form. The geometric phase is then identified with the associated holonomy of the loops in the space of parameters. This is remarkable because it means that, as far as the geometric phase is concerned, one does not need the full solution of the Schrödinger equation. The essential ingredient is the function F that induces $\tilde{A}$ as a pullback one-form from the adiabatic connection one-form A.

Wang[24] has presented a procedure that essentially computes F. Nevertheless, he does not even label this function, nor does he implement the idea of universal bundles. Let us see how the conditions introduced in Ref. 5 are realized in for cranked Hamiltonians. These conditions are the following.

(1) The cyclic states are the eigenstates of a Hermitian operator $\tilde{H}$ that depends parametrically on the points of the parameter manifold M, i.e., the cyclic states are eigenstates of $\tilde{H}(x_0)$ with $x_0=x(t=0)$.

(2) $\tilde{H}$ is related to the Hamiltonian according to

$$\tilde{H}(x)=H(F(x))=(HoF)(x), \tag{65}$$

where $F:M\to M$ is some smooth function, such that in the adiabatic limit, F approaches the identity map.

Let us first see how the first condition is fulfilled for any periodic Hamiltonian. According to a result of Floquet theory,[31] the time evolution operator for any periodic Hamiltonian is of the form

$$\mathscr{U}(t)=Z(t)e^{it\tilde{H}}, \tag{66}$$

where $\tilde{H}$ is a time-independent Hermitian operator and Z is a periodic unitary operator with the same period as the Hamiltonian, i.e.,

$$Z(t+T)=Z(t), \quad Z(0)=1. \tag{67}$$

Clearly, one has

$$\mathscr{U}(T)=e^{iT\tilde{H}}, \tag{68}$$

which justifies the first condition. The second condition can be seen to hold for the cranked Hamiltonians, either by referring to the work of Wang[24] or following the argument used in the discussion of the transformation of the Hamiltonian into the linear form. The latter is quite straightforward. One simply starts by realizing that since $\tilde{H}$ is Hermitian, it can also be written in the linear form:

$$\tilde{H}(x_0)=\sum_{i=1}^{d}\tilde{x}_0^i J_i\,, \tag{69}$$

where $\tilde{x}_0:=(\tilde{x}_0^i)\in M$ must depend on the Hamiltonian (30), and consequently on $C\subset M$. However, for the cranked Hamiltonians the time dependence of the Hamiltonian is governed by the action of a one-parameter subgroup of G, i.e., the operator $U(t)$ of Eq. (32) is given by

$$U(t):=\exp[i\omega t n_\alpha E_\alpha],\quad \text{with } n_\alpha=\text{const},$$

where ω and (n_α) are called the cranking rate and direction, respectively. It is clear that for such systems $\tilde{x}_0$ can only depend on the initial Hamiltonian and thus on x_0. The function F is defined by

$$\tilde{x}_0=:F(x_0). \tag{70}$$

The only problem is that in some cases, depending on the value of the slowness parameter $\nu(\omega)$, F may be discontinuous or even multivalued. This happens in the case of Eq. (18) for $\nu=\omega/b=1$. But in the generic case F is smooth and the second condition holds as well. The nonadiabatic analog of the BS line bundle is then given by

$$\tilde{L}:=F^*(L). \tag{71}$$

It is endowed with the nonadiabatic connection one-form,

$$\tilde{A}:=F^*(A). \tag{72}$$

For completeness, let me briefly review the arguments of Ref. 5, which lead to Eqs. (71) and (72). The basic idea is that the existence of $\tilde{H}$ that satisfies Eq. (69) allows one to imitate Berry's treatment of the adiabatic systems. The energy eigenstate vectors $|n,x\rangle$ are replaced by the eigenstate vectors $|\tilde{n},x\rangle$ of $\tilde{H}(x)$. In view of Eq. (65), these are given by

$$|\tilde{n},x\rangle=|n,\tilde{x}\rangle=|n,F(x)\rangle. \tag{73}$$

The nonadiabatic line bundle $\tilde{L}$ is obtained from the universal line bundle E via the nonadiabatic analog of the map f of Eq. (14). Denoting the latter by $\tilde{f}:M\to\mathscr{P}(\mathscr{H})$, one has

$$\tilde{f}(x):=|\tilde{n},x\rangle\langle\tilde{n},x|=|n,F(x)\rangle\langle n,F(x)|=(foF)(x).$$

Then, using the functorial property of the pullback operation, one shows that

$$\tilde{L}=\tilde{f}^*(E)=(foF)^*(E)=(F^*of^*)(E)=F^*(L), \tag{74}$$

where in the last equality Eq. (15) is used. This proves Eq. (71). The proof of Eq. (72) is identical. An important observation is that unlike $|n,x_0\rangle$, the initial state vectors $|\tilde{n},x_0\rangle$ undergo exact cyclic evolutions.

VI. MORE ON PARAMETER SPACES AND MONOPOLES

In the discussion of the the relation between the BS connection and the Riemannian structure on the parameter space, the parameter space is taken to be $M=G/H$, for some arbitrary closed subgroup H of G.[28] It can be shown that all these cases are included in the analysis of the linear system Eq. (30).

In Sec. III, I argued that depending on the (maximal weight Λ of the) irrep. of G, M is of the form $G_{\mathbb{C}}/P\subset G/T$, where P is defined by Eq. (50). Let us consider the Weyl chamber $\mathscr{W}$ of Υ^*

with respect to which the positive and the negative roots are distinguished.[18] If Λ happens to lie on at least one of the walls of $\mathscr{W}$, then B is a proper subgroup of P, otherwise $P=B$. The universal character of the linear Hamiltonian is also realized, in that all the homogeneous spaces of G can be obtained as $G_{\mathbb{C}}/P$ by choosing Λ appropriately. In fact, this is the basic idea of the classification of the compact homogeneous spaces of semisimple Lie groups. Therefore, in principle, one should be able to reproduce the results of[28] using the relation of Berry's phase to the theory of universal bundles.

Let us consider the group $G=\mathrm{SU}(3)$ in its defining (standard) representation. SU(3) is of rank $l=2$. So any irrep. is given by two integers. The standard representation is itself a fundamental representation, namely $(k_1=1,\ k_2=0)$.[18] The maximal weight is on a wall of $\mathscr{W}$ and the Borel subgroup of upper triangular matrices in $SL(3,\mathbb{C})=\mathrm{SU}(3)_{\mathbb{C}}$ is a proper subgroup of P. The subgroup P of $SL(3,\mathbb{C})$ consists of the elements of the form

$$\begin{bmatrix} * & * & * \\ * & * & * \\ 0 & 0 & * \end{bmatrix},$$

where $*$ are complex numbers.[18] The parameter space is $M=SL(3,\mathbb{C})/P=\mathrm{SU}(3)/\mathrm{U}(2)=\mathbb{C}P^2=\mathscr{P}(\mathscr{H})$. It is interesting to see that in this case the parameter space M and projective Hilbert space $\mathscr{P}(\mathscr{H})$ are identical. In fact, this is true for all $\mathrm{SU}(N+1)$ groups. The defining representation corresponds to $(k_1=1,\ k_2=\cdots=k_N=0)$ and the parameter space is $M=\mathrm{SU}(N+1)/\mathrm{U}(N)=\mathbb{C}P^N=\mathscr{P}(\mathscr{H})$. Therefore, the inducing map f maps $\mathbb{C}P^N$ to itself for all $N>1$.

The situation is different for the octet representation of SU(3). In this case one has $k_1=k_2=1$. Λ lies in the interior of $\mathscr{W}$, $P=B$, and the parameter space is the full flag manifold $M=\mathrm{SU}(3)/\mathrm{U}(1)\times\mathrm{U}(1)$. The map f maps M into $\mathscr{P}(\mathscr{H})=\mathbb{C}P^7$. [Note that this representation is eight dimensional, i.e., the representation space for $SL(3,\mathbb{C})$ is $\mathbb{C}^8$. Hence, $\mathscr{H}=\mathbb{C}^8$.]

For $G=\mathrm{SU}(2)$, it is well known that the system of Eq. (18) is related to the magnetic monopoles.[21] The relation of monopoles to the gauge theories and their generalization to arbitrary compact semisimple gauge groups have been studied in the late 1970s.[20] These generalized monopoles are called *non-Abelian* or *multimonopoles* for general groups and *color monopoles* for $SU(3)$.[32] They are topologically classified by an associated set of l integers, where l is the rank. These are called the *topological charges* of the monopole and they are defined as elements of the second homotopy group $\pi_2(G/H)$, where H is the group of the symmetries of a ground state of the Higgs fields (a minimum of Higgs potential).[20] For $G=SU(3)$, there are two possibilities. Either

$$\text{(I)}\quad H=U(2)\quad \text{or}\quad \text{(II)}\quad H=T=U(1)\times U(1).$$

These cases have been studied in almost every article written on this subject, e.g. see Refs. 33, 20 and references therein.

If G is simply connected, then a result of algebraic topology indicates that

$$\pi_2(G/H)=\pi_1(H).$$

Applying this result to $G=\mathrm{SU}(3)$, one finds

$$\text{(I)}\quad \pi_2(\mathrm{SU}(3)/\mathrm{U}(2))=\pi_1(\mathrm{U}(2))=\mathbb{Z},$$

$$\text{(II)}\quad \pi_2(\mathrm{SU}(3)/\mathrm{U}(1)\times\mathrm{U}(1))=\pi_1(\mathrm{U}(1)\times\mathrm{U}(1))=\mathbb{Z}\oplus\mathbb{Z}.$$

Thus, for (I) and (II) one has, respectively, one and two topological charges. This is precisely the case with the topological charges of the geometric phase defined earlier. The same correspondence holds for arbitrary compact, connected semisimple Lie groups.

The possible relevance of the topological charges of monopoles to the representations of the group have been conjectured by Goddard *et al.*.[34] Although the analysis of the present paper does not prove their conjecture, it provides a formula for the topological charges as integrals of the first Chern class, defined by Berry's connection, over the 2-cells σ_a of Sec. III. There is a simple topological explanation for the correspondence of the topological charges of the monopoles and those of the geometric phase. This can be summarized in the identity

$$\pi_2(G/H)=H_2(G/H,\mathbb{Z}),$$

where $H_2(\cdot,\mathbb{Z})$ denotes the second homology group. This identity is a consequence of *Hurewicz theorem*,[35] where one uses the fact that $\pi_1(G/H)=H_1(G/H)=0$. The 2-cells σ_a are indeed the generators of $H_2(G/T,\mathbb{Z})$. For $H\neq T$, some of them may be smashed to a point, as is the case for $G=\mathrm{SU}(3)$ and $H=\mathrm{U}(2)$.

VII. CONCLUSION

The relationship between the phenomenon of Berry's phase and the Borel–Weil–Bott theorem is a direct consequence of the application of the universal bundles in the Aharonov–Anandan definition of the geometric phase. This relationship is appealing, not only because it links quantum mechanics to yet another central mathematical result, but also because it offers a better understanding of the theoretical foundations of geometric phases. The implications of the fact that the A–A bundles are indeed the universal bundles of mathematics for the study of nonadiabatic phases is a typical indication of the importance of this observation.

The identification of the mathematical structures used in the holonomy interpretations of the geometric phase with those employed in the Borel–Weil–Bott theorem sheds light on a number of unresolved issues. Among these are the determination of the appropriate parameter space and the relation between the geometry of the parameter space and the geometric structure of the phase. The BWB theorem leads to the introduction of a set of topological charges, which determine the topology of the BS line bundles and thus encompass all the topological content of the phase. These charges seem to be related to, if not identical with, the topological charges of non-Abelian monopoles. The integral nature of these charges is a consequence of the topological properties of the first Chern class. The latter is essentially the reason for the quantization of the charges of the monopoles.

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Note added in proof: The material presented in this paper is also relevant to the subject of Ref. 36. The author wishes to thank the referee for informing him of this reference.

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Essential spectrum of the Dirac Hamiltonian for a spin 1/2 neutral particle with an anomalous magnetic moment in an asymptotically constant magnetic field

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The both lower and upper estimates of the lower bound λ_0^2 of the essential spectrum $\sigma_{ess}(H^2)$ of the square of the Dirac Hamiltonian H for a spin 1/2 neutral particle with an anomalous magnetic moment in an asymptotically constant magnetic field are obtained. It is found that in a restricted case, $\lambda_0^2 \leqslant m^2$, where m is the mass of the particle. Moreover, it is proven that $\sigma_{ess}(H^2)=[\lambda_0^2,\infty)$. In particular, in the case where the space dimension d is odd and $d \geqslant 3$, $\sigma_{ess}(H)=(-\infty,-\lambda_0]\cup[\lambda_0,\infty)$. In the case where $d=2$ and 3, $\sigma_{ess}(H)$ is exactly identified. © *1996 American Institute of Physics.* [S0022-2488(96)01302-4]

I. INTRODUCTION

From the experimental data on the existence of anomalous magnetic moment λ and electric dipole moment for the Dirac particle[1] the study of the Dirac equations with nonminimal interactions seems to be important. In fact, for electrically neutral hadrons, e.g. neutrons, the interaction of λ with an external field becomes significant on the security of the nuclear energy.[2] However, the number of articles devoted to the study of this problem is small. In some special cases exact solutions for the Dirac equation for this particle are obtained[2,3] and the 0-energy ground states are obtained for the Dirac Hamiltonian for this particle in electric fields.[4–6] In Ref. 7 some results on particles with anomalous moments and further references are contained.

For the spin 1/2 Schrödinger operator $\tilde{H}(a)$, which is given by the square of the Dirac operator $D(a)$ with minimal interaction in R^d, the following results are known: Let $a(x)=\Sigma_{j=1}^d a_j(x)dx^j$ be a real 1-form called a vector potential and $b=da=\Sigma b_{jk}dx^j \wedge dx^k$, $b_{jk}=\partial a_k/\partial x^j-\partial a_j/\partial x^k$, be the magnetic field. Assume that b is asymptotically constant, i.e. $b_{jk}(x)\to\Lambda_{jk}$ as $|x|\to\infty$ for some constant matrix $\Lambda=(\Lambda_{jk})$. We denote by $\sigma(A)$ (resp. $\sigma_{ess}(A)$) the spectrum (resp. essential spectrum) of an operator A and use the unit system where $\hbar=c=e=1$.

Theorem1.1: *(Shigekawa Ref. 8) (i) Assume that 0 is an eigenvalue of* Λ. *Then*

$$\sigma(\tilde{H}(a))=\sigma_{ess}(\tilde{H}(a))=[0,\infty).$$

(ii) Assume that 0 *is not an eigenvalue of* Λ. *Let* $\pm i\lambda_1, \ldots, \pm i\lambda_n$, $(\lambda_j>0)$ *be eigenvalues of* Λ. *Then*

$$\sigma_{ess}(\tilde{H}(a))=\left\{\sum_{j=1}^n 2k_j\lambda_j \middle| k_j\in Z_+\right\},$$

where $Z_+=\{0,1,2,\ldots\}$.

(iii) In the even dimensional cases,

$$\sigma_{ess}(D(a)+m\tau)=\{\sqrt{m^2+\lambda}\,|\,\lambda\in\sigma_{ess}(\tilde{H}(a)\restriction\ker(\tau-1))\}$$

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$$\cup\{-\sqrt{m^2+\lambda}\,|\,\lambda\in\sigma_{ess}(\tilde{H}(a)\restriction\ker(\tau+1))\},$$

where m is the mass of the particle and τ is the grading operator associated to $D(a)$. This result holds for $\sigma_{ess}(\cdot)$ replaced by $\sigma(\cdot)$.

Before Ref. 8, though only in two and three dimensions, but in more general case, Helffer *et al.* have been proved a similar result.[9] We remark that by the part (iii) of Theorem 1.1, $\inf\sigma((D(a)+m\tau)^2)\geqslant m^2$.

In this article, we investigate the essential spectrum of the square of the Dirac Hamiltonian H for a spin 1/2 electrically neutral particle with an anomalous magnetic moment in an arbitrary dimensional asymptotically constant magnetic field. We denote by m the mass of the particle ($m\geqslant 0$). One of the results obtained in this article is that in a restricted case, $\inf\sigma(H^2)\leqslant m^2$ holds. (See, Theorem 3.2.)

The plan of this article is as follows. In Section II, we define H and prove three propositions. In Section III, we prove our main theorems. In Section IV, we treat the case where the space dimension $d=2$ or 3. In Section V, we give some discussions.

II. DEFINITION AND PROPOSITIONS

In this section we define the Dirac Hamiltonian H for a spin 1/2 neutral particle with an anomalous magnetic moment $\lambda\in R\backslash\{0\}$ in a d-dimensional magnetic field $B=(b_{jk})$, $j,k=1,...,d$. Here, $d\in N$ and $d\geqslant 2$. Then we prove three propositions.

The Dirac equation for the particle interacting with an electromagnetic field $F=(F_{\mu\nu})$, $\mu,\nu=0,1,\ldots,d$, is given by

$$\left(\sum_{\mu=0}^{d}\gamma^{\mu}p_{\mu}-m\right)\phi=\lambda\sum_{\mu,\nu=0}^{d}s^{\mu\nu}F_{\mu\nu}\phi,$$

where $p_{\mu}=i\partial/\partial x^{\mu}$, γ^{μ} are the gamma matrices (γ^0 is Hermitian and γ^k anti-Hermitian) satisfying

$$[\gamma^{\mu},\gamma^{\nu}]_{+}=2g^{\mu\nu},\quad \mu,\nu=0,1,\ldots,d,$$

with g the Minkowski metric such that

$$g^{00}=1,\quad g^{kk}=-1,\quad k=1,\ldots,d,\quad \text{and others components}=0,$$

and

$$s^{\mu\nu}=\frac{i}{4}[\gamma^{\mu},\gamma^{\nu}],\quad \mu,\nu=0,1,\ldots,d.$$

Here, $[A,B]_{+}=AB+BA$, $[A,B]=AB-BA$. The vector space on which γ^{μ}'s act is taken to be C^r, with $r=2^{d/2}$ for d even and $r=2^{(d+1)/2}$ for d odd. Define the Dirac Hamiltonian H by

$$H=-\sum_{k=1}^{d}\gamma^0\gamma^k p_k+\lambda\gamma^0\sum_{\mu,\nu=0}^{d}s^{\mu\nu}F_{\mu\nu}+m\gamma^0$$

acting in $L^2(R^d;C^r)$. We consider the case where there exists no electric field:

$$F_{0k}=-F_{k0}=0,\quad k=1,\ldots,d.$$

We have

$$F_{jk}=-F_{kj}=b_{jk},\quad j,k=1,\ldots,d.$$

Hence we have

$$H=-\sum_{k=0}^{d}\gamma^0\gamma^k p_k+i\lambda\gamma^0\sum_{j<k}\gamma^j\gamma^k b_{jk}+m\gamma^0.$$

In this article we consider the case where B is asymptotically constant, i.e.

$$b_{jk}(x)\to\Lambda_{jk}\quad\text{as}\quad|x|\to\infty \tag{1}$$

for some constant matrix $\Lambda=(\Lambda_{jk})$. Throughout this article, assume that all b_{jk} are bounded real valued functions and Lebesgue measurable. Then H is a selfadjoint operator with the domain $D(H)=\oplus^r W_{2,1}(R^d)$, where $W_{2,1}(R^d)$ is the L^2-Sobolev space of order 1. By making an orthogonal transformation, we may assume that Λ is of the form

$$\Lambda=\begin{pmatrix}
0 & h_1 & & & & & & \\
-h_1 & 0 & & & & & 0 & \\
 & & \ddots & & & & & \\
 & & & 0 & h_n & & & \\
 & & & -h_n & 0 & & & \\
 & & & & & 0 & & \\
 & 0 & & & & & \ddots & \\
 & & & & & & & 0
\end{pmatrix}, \tag{2}$$

where $h_j>0$, $0\leqslant n\leqslant[d/2]$. Here $[\cdot]$ denotes the Gauss symbol. Let $h_j=0$ for $j=n+1,\ldots,[d/2]$. Then H can be decomposed as follows:

$$H=H_0+B_0,$$

where

$$H_0=-\sum_{k=1}^{d}\gamma^0\gamma^k p_k+i\lambda\gamma^0\sum_{j=1}^{n}\gamma^{2j-1}\gamma^{2j}h_j+m\gamma^0,$$

$$B_0=i\lambda\gamma^0\sum_{j<k}\gamma^j\gamma^k(b_{jk}-\Lambda_{jk}).$$

In the rest of this section, we prove three propositions.

Proposition 2.1: B_0 is H_0-compact. In particular, $\sigma_{ess}(H)=\sigma_{ess}(H_0)$.

Proof: Let

$$S=-\sum_{k=1}^{d}\gamma^0\gamma^k p_k.$$

We have $S^2=-\Delta$ with the domain $D(S^2)=\oplus^r W_{2,2}(R^d)$, where $W_{2,2}(R^d)$ is the L^2-Sobolev space of order 2. By Eq. (1), for all $j,k=1,\ldots,d$, $b_{jk}-\Lambda_{jk}$ is S^2-compact (see, e.g. Sec. 10.3 in Ref. 10). Since $b_{jk}-\Lambda_{jk}$ is S-bounded with S-bound 0, by Theorem 9.11 in Ref. 10, $b_{jk}-\Lambda_{jk}$ is S-compact. Therefore, $i\lambda\gamma^0\gamma^j\gamma^k(b_{jk}-\Lambda_{jk})$ and so B_0 is S-compact. Moreover, since S is H_0-bounded, B_0 is H_0-compact. □

As for the essential spectrum of H, Proposition 2.1 allows us to concentrate our attention on the case where the magnetic field is a constant one.

Proposition 2.2: $\sigma_{ess}(H^2)=\sigma_{ess}(H_0^2)$.

Proof: This proposition follows immediately from Proposition 2.1. □

Proposition 2.3: Let d be odd and

$$\Gamma=(-i)^{d(d+1)/2}\gamma^1\cdots\gamma^d.$$

Then

$$[H,\Gamma]_+=0 \quad on \quad D(H).$$

Proof: By direct computations. □

Proposition 2.3 shows that in the case where d is odd, H has a supersymmetric quantum mechanical structure.

III. THEOREMS

We state the main theorem in this article.

Theorem 3.1: *Assume that the magnetic field B is asymptotically constant and*

$$\lim_{|x|\to\infty}(b_{jk}(x))=\Lambda,$$

where Λ is a constant matrix defined by Eq. (2). Let

$$\lambda_0^2=\inf\sigma_{ess}(H^2),$$

$$\lambda_+^2=\min\left\{\left(m+\lambda\sum_{j=1}^n\epsilon_j h_j\right)^2\middle|\epsilon_j=\pm1,\ j=1,\ldots,n\right\},$$

$$\lambda_-^2=\lambda_+^2-\lambda^2\max_{j=1,\ldots,n}\{h_j^2\},$$

where $\lambda_0,\ \lambda_+\geqslant0$. Then we have

$$\lambda_-^2\leqslant\lambda_0^2\leqslant\lambda_+^2.$$

Moreover

$$\sigma_{ess}(H^2)=[\lambda_0^2,\infty).$$

In particular, if B is a constant magnetic field, then

$$\sigma(H^2)=[\lambda_0^2,\infty).$$

Proof: By Proposition 2.2, we prove this theorem in the case where B is a constant magnetic field, i.e. $B_0=0$. Let $\hat{H}$ be the Fourier transform of H. We have

$$\hat{H}=-\sum_{k=1}^d\gamma^0\gamma^k p_k+m\gamma^0+i\lambda\gamma^0\sum_{j=1}^n\gamma^{2j-1}\gamma^{2j}h_j,$$

where $p=(p_1,\ldots,p_d)\in R^d$. The operator $F:L^2(R^d;C^r)\to L^2(R^d;C^r)$ given by

$$F\begin{pmatrix} f_1 \\ \vdots \\ f_r \end{pmatrix}(p)=\begin{pmatrix} (2\pi)^{-d/2}\int_{R^d} e^{-ip\cdot y} f_1(y)dy \\ \vdots \\ (2\pi)^{-d/2}\int_{R^d} e^{-ip\cdot y} f_r(y)dy \end{pmatrix}, \quad \text{for } \begin{pmatrix} f_1 \\ \vdots \\ f_r \end{pmatrix} \in L^2(R^d;C^r)$$

is unitary and give a constant fiber direct integral decomposition of $L^2(R^d;C^r)$ over R^d with fiber C^r. Let

$$H_p=-\sum_{k=1}^{d} \gamma^0\gamma^k p_k+m\gamma^0+i\lambda\gamma^0\sum_{j=1}^{n} \gamma^{2j-1}\gamma^{2j}h_j$$

be a $r\times r$-matrix valued function in $p\in R^d$. Then

$$\hat{H}=\int_{R^d}^{\oplus} H_p dp.$$

Thus, by the general theory of constant fiber direct integral (see, e.g. Ref. 11),

$$\sigma(\hat{H}^2)=\{\lambda\in R|\ \text{for all } \epsilon>0, |\{p\in R^d|\sigma(H_p^2)\cap(\lambda-\epsilon,\lambda+\epsilon)\neq\varnothing\}|>0\},$$

where $|\cdot|$ denotes the Lebesgue measure on R^d. Therefore, we set $\lambda_0^2(p)=\min\sigma(H_p^2)$ and prove that $\lambda_0^2(p)$ is continuous in $p\in R^d$ with $\lambda_0^2(p)\to\infty$ as $|p|\to\infty$ and that

$$\lambda_-^2\leqslant \inf_{p\in R^d}\lambda_0^2(p)\leqslant\lambda_+^2. \tag{3}$$

Let

$$A_p=-\sum_{k=1}^{d} \gamma^0\gamma^k p_k,$$

$$B=i\lambda\gamma^0\sum_{j=1}^{n} \gamma^{2j-1}\gamma^{2j}h_j+m\gamma^0.$$

Then, we have $H_p=A_p+B$. We remark that

$$[\gamma^0\gamma^j,\gamma^0\gamma^k]_+=2\delta^{jk}, \quad \text{for all } j,k\geqslant 1;$$

$$[\gamma^0\gamma^k,\gamma^0\gamma^{2j-1}\gamma^{2j}]_+=\begin{cases} 2\gamma^{2j} & \text{if } k=2j-1, \\ -2\gamma^{2j-1} & \text{if } k=2j, \\ 0 & \text{otherwise;} \end{cases}$$

$$[\gamma^0,\gamma^0\gamma^{2j-1}\gamma^{2j}]=0, \quad \text{for all } j\geqslant 1;$$

$$[\gamma^0\gamma^{2j-1}\gamma^{2j},\gamma^0\gamma^{2k-1}\gamma^{2k}]=0 \quad \text{for all } j,k\geqslant 1.$$

Therefore, we have

$$A_p^2=\sum_{j=1}^{d} p_j^2$$

and

$$[A_p,B]_+=2i\lambda\sum_{j=1}^{n}(\gamma^{2j-1}p_{2j}-\gamma^{2j}p_{2j-1})h_j.$$

Hence

$$[A_p,B]_+^2=4\lambda^2\sum_{k=1}^{n}(p_{2k-1}^2+p_{2k}^2)h_k^2.$$

Therefore, $[A_p,B]_+$'s eigenvalues are $\pm 2|\lambda|\sqrt{\Sigma_{k=1}^{n}(p_{2k-1}^2+p_{2k}^2)h_k^2}$. Moreover, since γ^0, $i\gamma^0\gamma^1\gamma^2,\ldots,i\gamma^0\gamma^{2n-1}\gamma^{2n}$ are simultaneously diagonalizable,

$$\sigma(B^2)=\left\{\left(m+\lambda\sum_{j=1}^{n}\epsilon_j h_j\right)^2\middle|\epsilon_j=\pm 1\right\}.$$

We denote by $\langle\cdot,\cdot\rangle$ the standard inner product of C^r and set $\|f\|=\sqrt{\langle f,f\rangle}$ for $f\in C^r$. By the min-max principle, we have

$$\begin{aligned}\lambda_0^2(p)&=\inf_{\|f\|=1}\langle H_p^2 f,f\rangle\\&\geqslant\inf_{\|f\|=1}\langle(A_p^2+B^2)f,f\rangle+\inf_{\|f\|=1}\langle[A_p,B]_+f,f\rangle\\&=\sum_{j=1}^{d}p_j^2+\min_{\epsilon_j=\pm1}\left\{\left(m+\lambda\sum_{j=1}^{n}\epsilon_j h_j\right)^2\right\}-2|\lambda|\sqrt{\sum_{k=1}^{n}(p_{2k-1}^2+p_{2k}^2)h_k^2}\\&=\sum_{j=1}^{d}p_j^2+\lambda_+^2-2|\lambda|\sqrt{\sum_{k=1}^{n}(p_{2k-1}^2+p_{2k}^2)h_k^2}.\end{aligned}\tag{4}$$

Hence

$$\begin{aligned}\inf_{p\in R^d}\lambda_0^2(p)&=\inf_{r\geqslant 0}\inf_{|p|^2=r^2}\lambda_0^2(p)\\&\geqslant\inf_{r\geqslant 0}[r^2+\lambda_+^2-2|\lambda|\sqrt{r^2\max_{j=1,\ldots,n}\{h_j^2\}}]\\&=\inf_{r\geqslant 0}[(r-|\lambda|\sqrt{\max_{j=1,\ldots,n}\{h_j^2\}})^2+\lambda_+^2-\lambda^2\max_{j=1,\ldots,n}\{h_j^2\}]\\&=\lambda_+^2-\lambda^2\max_{j=1,\ldots,n}\{h_j^2\}=\lambda_-^2.\end{aligned}$$

We prove that $\inf_{p\in R^d}\lambda_0^2(p)\leqslant\lambda_+^2$. We can take a vector $f\in C^r$ such that $\|f\|=1$, $\gamma^0 f=f$,

$$i\gamma^0\gamma^{2j-1}\gamma^{2j}f=\nu_j f,\quad\text{for } j=1,\ldots,n,\tag{5}$$

where $\nu_j=1$ or -1 and $(m+\lambda\Sigma\nu_j h_j)^2=\min\{(m+\lambda\Sigma\epsilon_j h_j)^2|\epsilon_j=\pm1\}=\lambda_+^2$. Then, we have

$$Bf=\left(m+\lambda\sum_{j=1}^{n}\nu_j h_j\right)f$$

and, since $[A_p,\gamma^0]_+=0$ and $\gamma^0 f=f$,$\langle A_p f,f\rangle=0$. Hence we have

$$\langle H_p^2 f,f\rangle=\sum_{j=1}^{d}p_j^2+\left(m+\lambda\sum_{j=1}^{n}\nu_j h_j\right)^2\geqslant\inf_{\|g\|=1}\langle H_p^2 g,g\rangle=\lambda_0^2(p).$$

Thus,

$$\lambda_+^2\geqslant\inf_{p\in R^d}\lambda_0^2(p).$$

Therefore we have proved Eq. (3). Note that $\{f\in C^r|\|f\|=1\}$ is a compact set. Then we can easily prove that $\lambda_0^2(p)=\inf_{\|f\|=1}\langle H_p^2 f,f\rangle$is continuous in $p\in R^d$. By Eq. (4), we have $\lambda_0^2(p)\to\infty$ as $|p|\to\infty$. Consequently, we obtain the desired result. □

The following theorem is immediately obtained by Theorem 3.1.

Theorem 3.2: *Suppose that*

$$2m\geqslant\left|\lambda\sum_{j=1}^{n}\nu_j h_j\right|$$

with ν_j defined by Eq. (5). Then

$$\inf\sigma_{ess}(H_0^2)\leqslant m^2.$$

Proof: By the assumption, we have

$$m^2\geqslant\left(m+\lambda\sum_{j=1}^{n}\nu_j h_j\right)^2=\lambda_+^2.$$

Hence, by Theorem 3.1, we obtain the desired result. □

Remark: In the case where

$$2m\geqslant|\lambda|\sum_{j=1}^{n}h_j,$$

the assumption in Theorem 3.2 holds. (Note that $h_j\geqslant 0$ for all j.) This means that in an asymptotically constant magnetic field with the constant *small* at infinity, $\inf\sigma_{ess}(H_0^2)\leqslant m^2$.

In the case where d is odd, using Proposition 2.3, we can identify on the essential spectrum of H.

Theorem 3.3: *Consider the case where d is odd ($d\geqslant 3$). Assume the same assumptions and use the same notations, $\lambda_0,\lambda_+,\lambda_-$, as in Theorem 3.1. Let*

$$S=\begin{cases}(-\infty,-|\lambda_-|]\cup[|\lambda_-|,\infty), & if\ \lambda_-^2>0,\\ R, & if\ \lambda_-^2\leqslant 0,\end{cases}$$

$$s=(-\infty,-\lambda_+]\cup[\lambda_+,\infty),\quad M=(-\infty,-m]\cup[m,\infty).$$

Then

$$S \supset \sigma_{ess}(H) = (-\infty, -\lambda_0] \cup [\lambda_0, \infty) \supset s.$$

In particular, under the same assumption in Theorem 3.2, we have

$$S \supset \sigma_{ess}(H) = (-\infty, -\lambda_0] \cup [\lambda_0, \infty) \supset s \supset M.$$

Proof: The operator

$$\Gamma = (-i)^{d(d+1)/2} \gamma^1 \cdots \gamma^d$$

is unitary and, by Proposition 2.3, we have $\Gamma^* H \Gamma = -H$. Hence we have

$$\sigma_{ess}(H) = \{\pm\sqrt{\mu} \mid \mu \in \sigma_{ess}(H^2)\} = (-\infty, -\lambda_0] \cup [\lambda_0, \infty).$$

The rest of conclusions immediately follows from Theorems 3.1 and 3.2. □

IV. SPECIAL CASES

In the case where $n=1$, i.e. Λ's nonzero eigenvalues are only $\pm i h_1$ $(h_1 > 0)$, we can explicitly calculate λ_0. Of course, if $d=2$ and 3, this holds always. We denote h_1 by h for simplicity.

Theorem 4.1: *Assume that Λ's nonzero eigenvalues are only $\pm ih$ $(h \geqslant 0)$. Let*

$$\lambda_0 = \max\{m - |\lambda h|, 0\}.$$

Then

$$\sigma_{ess}(H^2) = [\lambda_0^2, \infty).$$

Moreover, if d is odd,

$$\sigma_{ess}(H) = (-\infty, -\lambda_0] \cup [\lambda_0, \infty).$$

Proof: In a way similar to the one in the proof of Theorem 3.1, we can prove this theorem. In this case we can obtain the exact value of $\lambda_0^2(p)$, the minimum eigenvalue of H_p^2. We have

$$H_p^2 = \sum_{j=1}^{d} p_j^2 + m^2 + \lambda^2 h^2 + 2im\lambda \gamma^1 \gamma^2 h + 2i\lambda \gamma^1 h p_2 - 2i\lambda \gamma^2 h p_1$$

and

$$(2im\lambda \gamma^1 \gamma^2 h + 2i\lambda \gamma^1 h p_2 - 2i\lambda \gamma^2 h p_1)^2 = 4\lambda^2 h^2 (m^2 + p_2^2 + p_1^2).$$

Hence, H_p^2's eigenvalues are

$$\sum_{j=1}^{d} p_j^2 + m^2 + \lambda^2 h^2 \pm 2|\lambda h| \sqrt{m^2 + p_2^2 + p_1^2}.$$

Thus

$$\lambda_0^2(p) = \sum_{j=1}^{d} p_j^2 + m^2 + |\lambda h|^2 - 2|\lambda h| \sqrt{m^2 + p_1^2 + p_2^2}$$

$$= \sum_{j=3}^{d} p_j^2 + (\sqrt{m^2 + p_1^2 + p_2^2} - |\lambda h|)^2.$$

Therefore,

$$\inf_{p\in R^d} \lambda_0^2(p)=\begin{cases}(m-|\lambda h|)^2 & \text{if } m>|\lambda h|\\ 0 & \text{otherwise.}\end{cases}$$

Consequently, we obtain the desired results. □

In the rest of this section, we consider the case where $d=2$. By Theorem 4.1, we have $\sigma_{ess}(H^2)=[\lambda_0^2,\infty)$. In this case, we can prove the next theorem.

Theorem 4.2: *Let $d=2$ and $\pm ih$ be the nonzero eigenvalues of Λ. Then*

$$\sigma_{ess}(H)=(-\infty,-m-\lambda h]\cup[m-\lambda h,\infty).$$

Proof: Let σ^j, $j=1, 2, 3$, be the Pauli's spin matrices. In this case, we can set that $\gamma^0=\sigma^3$, $\gamma^1=i\sigma^1$, $\gamma^2=-i\sigma^2$. Then we have

$$H_0=\sigma^2 p_1+\sigma^1 p_2+m\sigma^3-\lambda h.$$

We know that

$$\sigma(\sigma^2 p_1+\sigma^1 p_2+m\sigma^3)=(-\infty,-m]\cup[m,\infty).$$

Hence we obtain the desired result. □

V. DISCUSSIONS

In this article, we have investigated the essential spectrum of the Dirac Hamiltonian H for a spin 1/2 neutral particle with an anomalous magnetic moment in an asymptotically constant magnetic field. Our results are quite different from those on the essential spectrum of a spin 1/2 Schrödinger operators $\tilde{H}(a)=D(a)^2$ in an asymptotically constant magnetic field.

It is well known that in even dimensional cases, the lower bound of the spectrum $\sigma((D(0)+m\tau)^2)$ of the square of the free Dirac Hamiltonian $D(0)+m\tau$ is equal to m^2, where m is the mass of the particle, and that the lower bound of $\sigma((D(a)+m\tau)^2)$ for the Dirac Hamiltonian $D(a)+m\tau$ with minimal interaction is greater than or equal to m^2. (See, Theorem 1.1 and Ref. 8.) Hence, we have $\inf\sigma((D(a)+m\tau)^2)\geqslant\inf((D(0)+m\tau)^2)=m^2$. On the other hand, in an asymptotically constant magnetic field with the constant *small*, the lower bound of $\sigma(H^2)$ of the square of the Dirac Hamiltonian H with the nonminimal interaction through the Pauli term is smaller than or equal to m^2. (See, Theorems 3.1 and 3.2.) We have a question: When does $\inf\sigma(H^2)\leqslant m^2$ hold?

Another phenomenon is as follows. In the case where 0 is not an eigenvalue of Λ, $\sigma_{ess}(\tilde{H}(a))$ is a discrete set. Hence, all the points of it are an eigenvalue of $\tilde{H}(a)$. On the other hand, for an arbitrary H with an asymptotically constant magnetic field, $\sigma_{ess}(H^2)$ is not a discrete set (it is a half line). Another question arises: When is $\sigma_{ess}(H^2)$ a discrete set?

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Classical mechanics with lapse

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Mechanics is developed over a differentiable manifold as space of possible positions. Time is considered to fill a one-dimensional Riemannian manifold, so having the metric as lapse. Then the system is quantized with covariant instead of partial derivatives in the Schrödinger operator. © *1996 American Institute of Physics.* [S0022-2488(96)01402-4]

I. INTRODUCTION

In General Relativity, the differential quotient between proper time and coordinate time is called lapse function. In the present article, this notion is used for an arbitrary classical mechanical system. Space is considered as n-dimensional Riemannian space V_n and time is considered as 1-dimensional Riemannian space V_1. Then the square of the lapse function turns out to be the metric of this V_1. Possible applications and comparison with other approaches found in the literature will be shown in section VI below.

Let us consider a mechanical system. The space of all possible positions shall be the n-dimensional differentiable manifold M_n. It is endowed with local coordinates $q^i, i=1,\ldots n$. Most of all mechanical systems have the property that M_n is a subset of $\mathrm{R}^m \times (S^1)^{n-m}$, so that the first m coordinates are Cartesian ones and the remaining are periodic ones (i.e., angles). Here, R denotes the space of reals, Z the space of integers, and the one-dimensional torus S^1 can be defined as factor space $S^1=\mathrm{R}/\mathrm{Z}$. But in general, M_n cannot be covered by one single coordinate system. The time is denoted by t, and d/dt will be denoted by a dot. So, $\dot{q}^i$ is the velocity of a moving particle $q^i(t)$. Therefore, the velocity at time t is an element of the tangent space $T_x M_n$ of M_n at $x=q^i(t)$. The tangent bundle TM_n is the union of all tangent spaces.

Contrarily to the usual procedure we now introduce the lapse function $N(t)$ which shall be an arbitrary positive function. (Here and below all functions shall have the necessary differentiability properties.) The proper time τ is defined by

$$\tau = \int N(t)dt. \tag{1}$$

It is uniquely determined up to an integration constant, i.e., without specifying the point where $\tau=0$. The space of all possible times is a connected oriented one-dimensional Riemannian space V_1 with coordinate $x^1=t$ and metric $g_{11}=N^2(t)$. The orientation is chosen such that increasing time leads into the future. So, Eq. (1) represents the proper time τ as proper length within this V_1.

Remark: The definition is chosen such that proper time does not *depend on the velocity, so we do not cover relativistic effects.*

Each positive function $N(t)$ defines a gauge, and results should not depend on it. In this manner, we define the following gauge-invariant quantity, the proper velocity v^i

$$v^i = \frac{1}{N}\dot{q}^i. \tag{2}$$

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We have to prove that v^i does not depend on the special choice of N; this follows from Eqs. (1),(2) via the equation

$$v^i = \frac{dq^i}{d\tau}.$$

The action I is the integral of a Lagrangian L

$$I = \int L\,dt \tag{3}$$

and is supposed to be a coordinate-, gauge-, and T-invariant quantity. T-invariance means that I does not change if the orientation of V_1 is reversed. The range of integration in Eq. (3) is a connected subset of V_1, i.e., any fixed time-interval; but we do not specify now which kind of interval is used.

We restrict ourselves to first-order Lagrangians, i.e., L is a function

$$L: TM_n \mathrm{x}\, V_1 \to \mathrm{R}\,. \tag{4}$$

The next three steps are done by plausible arguments, not by proofs.

First, the explicit t-dependence ($t \in V_1$) of L, Eq. (4), is compatible with gauge-invariance of I only for the case that the t-dependence of L is via $N(t)$ only, i.e.,

$$L = L(q^i, \dot{q}^i, N). \tag{5}$$

Second, the coordinate- and gauge-invariance of I requires the following form of L

$$L = G(q^i, v^i) \cdot N, \tag{6}$$

where G is a certain scalar; this becomes plausible from Eqs. (1),(2),(3).

Third, we assume that G can be developed into powers of v^i

$$G = \sum_{k=0}^{\infty} \alpha^{(k)}_{i_1,\ldots i_k}(q^i) v^{i_1} \cdots v^{i_k} \tag{7}$$

with certain tensors $\alpha^{(k)}_{\ldots}$. Here, and below, the Einstein sum convention is to be applied. Then it follows from T-invariance, that only even values k give a nonvanishing contribution to Eq. (7).

The simplest nontrivial example for Eq. (7) is the case that only $k=0$ and $k=2$ give contributions. To meet the usual notation we define

$$V = -\alpha^{(0)}(q^i), h_{ij} = 2\alpha^{(2)}_{ij}(q^i). \tag{8}$$

Inserting Eqs. (7),(8) into Eq. (6) we get

$$L = (\tfrac{1}{2} h_{ij} v^i v^j - V) \cdot N. \tag{9}$$

Without loss of generality, h_{ij} is assumed to be a symmetric tensor in M_n. Here, the coordinate-, gauge-, and T-invariance of I, Eqs. (3),(9) is immediately seen; so we also could have taken Eq. (9) as a definition of L.

To give the Lagrangian Eq. (9) the structure defined by Eq. (5) we insert Eq. (2) into Eq. (9) and get

$$L = \tfrac{1}{2} g_{ij} \dot{q}^i \dot{q}^j - V \cdot N, \tag{10}$$

where we used the definition

$$g_{ij}=\frac{1}{N}\cdot h_{ij}\,. \tag{11}$$

Next, we introduce the momentum p_i by

$$p_i=\frac{\partial L}{\partial \dot{q}^i}. \tag{12}$$

From Eq. (10) we get

$$p_i=g_{ij}\dot{q}^j. \tag{13}$$

It holds: the momentum is gauge-invariant. This is proven by the fact that from Eqs. (2),(11,(13) one gets

$$p_i=h_{ij}v^j. \tag{14}$$

From Eqs. (12),(13) we get

$$\frac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^j}=g_{ij}\,, \tag{15}$$

where g_{ij} depends on q^i and N only. The analogous gauge-invariant equation to Eq. (15) reads

$$\frac{\partial p_i}{\partial v^j}=h_{ij} \tag{16}$$

and h_{ij} depends on q^i only.

Remark: One could use Eqs. (12),(15) also for the general case L, Eqs. (6),(7); but then g_{ij} would in general depend on the velocities, too. If g_{ij} is interpreted as metric, then this would be the step from Riemannian to Finslerian geometry. A typical example of Finslerian geometry appears, if the term with $k=4$ in Eq. (7) is allowed to appear.

Let us introduce the Hamiltonian

$$H=p_i\dot{q}^i-L. \tag{17}$$

The canonical equations make sense only for the case that the velocities can be expressed as functions of the coordinates, momenta, and time. Looking at Eq. (13) one can see that this takes place if and only if g_{ij} is a regular matrix. So, we assume this to be the case in the following and denote the inverse matrix to g_{ij} by g^{ij}. From Eq. (11) it follows that also h_{ij} is invertible. The inverse matrix to h_{ij} is denoted by h^{ij}. It holds

$$g^{ij}=N\cdot h^{ij}. \tag{18}$$

From Eq. (13) we get

$$\dot{q}^i=g^{ij}p_j\,. \tag{19}$$

We insert Eqs. (10),(18),(19) into Eq. (17) and get

$$H=\tfrac{1}{2}g^{ij}p_ip_j+V\cdot N, \tag{20}$$

which can also be written as $H=(\frac{1}{2}h^{ij}p_ip_j+V)\cdot N$. The canonical equations are

$$\dot{q}^i=\frac{\partial H}{\partial p_i} \tag{21}$$

and

$$\dot{p}_i=-\frac{\partial H}{\partial q^i}. \tag{22}$$

Equation (21) is equivalent to Eq. (19), whereas Eq. (22) represents the equation of motion; in the next section we discuss it in more detail.

II. THE EQUATION OF MOTION

The acceleration is $a^i=\ddot{q}^i$. In general, the equation of motion expresses the acceleration as function of coordinates, velocity, and time. To get this structure, we insert Eqs. (13),(20) into Eq. (22). After some calculus we get

$$a^i=\frac{\dot{N}}{N}\dot{q}^i-V^{\cdot,i}\cdot N-\dot{q}^j\dot{q}^k\Gamma^i_{jk}, \tag{23}$$

where $V^{\cdot,i}=g^{ij}V_{,j}$ and Γ denotes the Christoffel affinity (which is the same both for g_{ij} and h_{ij}). As usual, $\langle\langle,i\rangle\rangle$ is an abbreviation for the partial derivative with respect to the coordinate $\langle\langle q^i\rangle\rangle$.

We can give three results immediately: First, for N and V being constant, the equation of motion is just the geodesic equation in the M_n with Riemannian metric g_{ij}. Second, for N and g_{ij} being constant, the equation of motion reads $0=a^i+V^{\cdot,i}$ and equals the classical equation of motion in the potential V. Third, using gauge-invariant quantities, we can write the equation of motion as

$$0=\frac{dv^i}{d\tau}+\Gamma^i_{jk}v^jv^k+h^{ij}V_{,j}. \tag{24}$$

The first two terms of the r.h.s. represent the covariant derivative of the proper velocity with respect to proper time.

In the next step we consider, independently of the Hamiltonian, under which condition the action I [Eq. (3)] has a stationary value. One should expect that the same equation of motion appears, but this is not fully trivial to show.

The corresponding Euler–Lagrange equation to the action I reads

$$0=\frac{\partial L}{\partial q^i}-\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}^i}\right). \tag{25}$$

With Eq. (12) we get

$$\dot{p}_i=\frac{\partial L}{\partial q^i}. \tag{26}$$

Comparing with Eq. (22) we have to show that

$$\frac{\partial H}{\partial q^i} = -\frac{\partial L}{\partial q^i}. \tag{27}$$

Looking at Eq. (17) one could get the impression that Eq. (27) can be fulfilled for a constant product $p_i \dot{q}^i$ only, but this impression is wrong, because in the l.h.s., H is a function $H(q^i, p_i, N)$ but in the r.h.s., L is a function $L(q^i, \dot{q}^i, N)$. And so, with H [Eq. (20)] and L [Eq. (10)], the validity of Eq. (27) can be proven.

III. THE LOWER-DIMENSIONAL CASES

Let us consider the simplifications for the lower-dimensional cases. For $n=1$, one knows that the Riemannian space V_1 is flat, and so the Lagrangian Eq. (9) reduces to $L=[(m/2)\,v^2 - V(x)]\cdot N(t)$ with $q^1 = x, v^1 = v$ and $h_{11} = m = const. \neq 0$. With $N=1$ this is the usual point particle in a potential V.

For $n=2$, the Riemannian space $V_2 = (M_2, h_{ij})$ need not to be flat, but it is always conformally flat. So one can always find local coordinates such that the Lagrangian Eq. (9) can be written as

$$L = \left[\frac{m}{2}v^2 + \frac{M}{2}w^2 - W(x,y)\right]\cdot S(x,y)\cdot N(t) \tag{28}$$

with $q^2 = y, v^2 = w$ and $h_{22} = M = const. \neq 0$ and $W \cdot S = V$ as additional relations. $S \neq 0$ is the suitably chosen conformal factor.

For $n \geqslant 3$, however, a V_n need not to be conformally flat, and so, in general, the usual kinetic term with constant masses can be reached neither by a coordinate nor by a conformal transformation.

IV. QUANTIZATION

The usual quantization procedure is to substitute p_k by $i\hbar\,(\partial/\partial q^k)$ in the Hamiltonian to come from the function to the operator. If we make this in our approach, then gauge-invariance is automatically ensured, because both q^k and p_k are gauge-invariant quantities. (To prevent misunderstandings, we explicitly say: i is an index $\in \{1, \ldots n\}$ if written in index position, and it is the imaginary unit otherwise.) But to ensure coordinate-invariance, the partial derivative is not sufficient. The most natural way to circumvent this difficulty is to use the covariant derivative with the same Γ as before. Then ∇_k denotes the covariant derivative with respect to q^k.

The world function is denoted by ψ, it is a function

$$\psi : M_n \to \mathrm{C}\,, \tag{29}$$

where C denotes the set of complex numbers.

The energy of the system is $E = H/N$. It is a gauge–invariant scalar, and it is constant along classical trajectories: $dE/dt = 0$ which follows from Eqs. (20),(21),(22).

So we get the Schrödinger equation $\hat{H}\psi = E \cdot N \cdot \psi$ with $\psi = \psi(q^i)$ and

$$\hat{H} = -\tfrac{1}{2}\hbar^2 g^{ij}\nabla_i \nabla_j + V \cdot N. \tag{30}$$

The zero energy Schrödinger equation simply reads

$$\hbar^2 \Box \psi = 2V\psi, \tag{31}$$

where $\Box$ denotes the D'Alembertian with respect to the metric h_{ij}, i.e., $\Box = h^{ij}\nabla_i \nabla_j$, whereas the general Schrödinger equation can be obtained from this one by a suitable redefinition of V.

To circumvent the explicit calculation of the Christoffel affinities we apply the following formula

$$\Box = \frac{1}{\sqrt{h}} \partial_i \sqrt{h} h^{ij} \partial_j , \tag{32}$$

where $h = |\det h_{ij}| \neq 0$.

Remark: One should observe that the form used here is surely the simplest possible way to get a coordinate–invariant Schrödinger equation; however, it is not the only possible one which goes over to the classical Schrödinger equation (i.e., that one with partial derivatives) if h_{ij} becomes constant. Indeed, one could use the conformally invariant operator $\Box_c = \Box - \xi R$ instead of $\Box$, where R is the curvature scalar of the metric h_{ij} and $\xi = (n-2)/4(n-1)$. Only for $n \leqslant 2$ one has $\Box_c = \Box$; for $n = 2$ because of $\xi = 0$, and for $n = 1$ because of $R = 0$. But even for $n \geqslant 3$ one can cover this variant by a suitable redefinition of V.

Let us briefly say what happens for the lower-dimensional cases. For $n = 1$, one simply uses coordinates such that $h_{11} = 1$ and one gets the usual equation. For $n = 2$, however, it is a little more involved. We employ the fact that h_{ij} is conformally flat and so it can be written as $h_{ij} = \sqrt{h}\, \eta_{ij}$ where η_{ij} is a matrix in diagonal form where all diagonal elements are $\in \{+1, -1\}$. η^{ij} is the inverse to η_{ij}; and, by construction, they coincide. Then we insert Eq. (32) into Eq. (31) and get

$$\hbar^2 \eta^{ij} \partial_i \partial_j \psi = 2 \sqrt{h} V \psi. \tag{33}$$

The l.h.s. represents the flat-space D'Alembertian, and the factor $\sqrt{h}$ in the r.h.s. can be absorbed by a redefinition of V.

For $n \geqslant 3$, however, it requires special circumstances to get the Schrödinger equation in the form of a flat-space D'Alembertian.

V. SOLUTIONS OF THE SCHRÖDINGER EQUATION

From the full set of solutions of the Schrödinger equation (31) we are essentially interested in those solutions which correspond to the classical solutions of the system (21),(22). To this end we apply the WKB-approximation and insert the ansatz

$$\psi = a \cdot \exp(iS/\hbar), \tag{34}$$

into Eq. (31) and get

$$\hbar^2 \Box a + i\hbar (2 a_{,k} S^{,k} + a \Box S) - a S_{,k} S^{,k} = 2aV, \tag{35}$$

where $S^{,k} = h^{jk} S_{,j}$. From Eq. (34) we have the situation that now two functions (a, S) represent one function (ψ). So we are free to put an additional relation as calibration. It turns out that the following calibration is useful: we set for a moment $\hbar = 0$, insert this into Eq. (35) and use the resulting equation

$$S_{,k} S^{,k} + 2V = 0 \tag{36}$$

as natural calibration. This is the usual classical limit.

Before we proceed we must be sure that Eq. (36) possesses solutions. If the metric h_{ij} has indefinite signature, then this is trivial. Let h_{ij} be of definite signature; without loss of generality it shall be positively definite, for, otherwise, simply V has to change its sign. In regions where $V \leqslant 0$, Eq. (36) has solutions, but in regions with $V > 0$ it does not have any solutions. One should remember here, that we have redefined V such that the whole system has zero energy. So, $V > 0$

corresponds to a negative kinetic energy; the latter is impossible for a positively definite metric h_{ij}. We get as the result: the calibration of Eq. (36) is possible if and only if classical motion takes place there.

Now we insert Eq. (36) into Eq. (35) and get

$$0=\hbar\Box a+2ia_{,k}S^{,k}+ia\Box S. \tag{37}$$

To proceed, there exist different possibilities: first, one again neglects the term with $\hbar$, second, one requires a to be a slowly varying amplitude such that $\Box a$ is negligible in comparison with $\Box S$, or, third, one thinks of a and S as real functions and so Eq. (37) splits into real and imaginary parts. It is not so essential which of these three arguments are applied, because all of them give rise to the equation

$$0=2a_{,k}S^{,k}+a\Box S. \tag{38}$$

Equation (38) can be solved as follows: let $S(q^i)$ be a solution of Eq. (36) with $S_{,k}\neq 0$. There exists no time in the system, but we can introduce a time T by requiring that $d/dT = S^{,k}\partial_k$. With $b=\ln a^2$, Eq. (38) now reads

$$\frac{db}{dT}=-\Box S, \tag{39}$$

which can be integrated along the trajectories of T. In an afterwards-interpretation one can identify T with τ, $S^{,k}$ with v^k and $S_{,k}$ with p_k; this turns out to be compatible with the classical (= nonquantum) equations. But this alone does not suffice: from Eq. (39) one calculates the function $a(q^i)$ and inserts it together with $S(q^i)$ into Eq. (37). Then the WKB-approximation turns out to yield results close to the exact solution only for the case that indeed, $|\hbar\Box a|$ is negligible in comparison to $|a\Box S|$. So one can check in which region the semiclassical approach makes sense.

VI. CONCLUSION

Classical mechanics, as is usually presented, e.g. in Refs. 1 and 2, uses essentially vector spaces as space of possible positions. Then one has the duality between coordinates and momenta (which we do loose here) and can build a symplectic manifold. Furthermore, one has usually a constant mass tensor (which means a constant matrix h_{ij} in our notation).

Both points are generalized in the present paper. The present approach is inspired by work on Hamiltonian quantum cosmology, e.g. Ref. 3, where the space of possible positions is the set of all possible spatial geometries (called superspace). The set of all possible spatial geometries turns out to be neither a vector space nor is the matrix h_{ij} a constant one. Even, if one restricts to the minisuperspace which corresponds to homogeneous spatial geometries, one does not get a vector space. Example: The set of all homogeneous 3-spaces of Bianchi-type IX [i.e., there exists a transitive subgroup of the isometry group isomorphic to $SO(3)$] which is a manifold with boundary, the interior is composed of points corresponding to spaces whose isometry group is 3-dimensional, and the boundary points are formed by spaces with 4-dimensional isometry group (i.e., the axially symmetric Bianchi-type IX models), and the edge (the boundary of the boundary) consists of one line which itself corresponds to the isotropic 3-spheres with 6-dimensional isometry group. (Concerning details to this point see e.g. Ref. 4).

If M_n is such a manifold with boundary, then a trajectory is simply mirrored at the boundary.

Here we carefully distinguish between co- and contravariant tensor indices, and the Einstein sum convention is used in its strong version: summation over double indices takes place only for the case that one of them is in upper (= contravariant) and the other in lower (= covariant) position. It is a nice additional check of the formulas that the necessity to write the Σ–sign never appeared.

The essential result of the present paper is to show that up to dimension two, the Schrödinger equation comes out with the flat-space D'Alembertian whereas for higher dimensions, it requires a special structure of the action to have this property. This has the following consequence for quantum cosmology: All models with one- or two-dimensional minisuperspace can be written with the flat-space D'Alembertian in the Schrödinger equation (which is called Wheeler de Witt equation here), whereas for higher-dimensional minisuperspace models, e.g. Ref. 5, this property requires a special structure of the underlying system.

Reformulated for the classical (i.e., nonquantized) system one can state: A system with one or two degrees of freedom has always a kinetic energy which can be written as sum of terms of the type $\pm(m/2)\,v^2$ with positive constant values m, whereas for three or higher dimension this need not to be the case.

The kind of introducing the covariant derivative in Eq. (30) instead of the partial one is the mathematical background of the (today widely accepted) solution of the so-called factor-ordering problem, which filled many papers on quantum cosmology in the eighties, see Ref. 6 which is a bibliography of papers on the topic.

We always wrote velocities with upper (contravariant) and momenta with lower (covariant) index; this is more than a purely notational arbitrariness, moreover, it is the only adequate form from the differential geometric point of view.

A geometric description of nonrelativistic quantum mechanics has already been carried out by Kuchař[7] in 1980. He uses a degenerate metric (i.e., a metric with vanishing determinant), so that he needs additional considerations to relate the co- and the contravariant components of it. He solves the factor-ordering problem by writing the Laplacian covariant with respect to this degenerate metric. Contrary to our approach (see also Ref. 5 for more details), he uses Dirac's constraint quantization.

Section 7.2 of Ref. 8 develops classical mechanics in parametrized form. In this form, it becomes time-reparametrization invariant just as General Relativity is coordinate-invariant. Their approach takes velocities and momenta on the same footing (both are covariantly written vectors).

The book[9] by Zeh reviews many aspects of the *direction* of time. In subsection 5.2.1 of that book, also the reparametrization invariance of time is mentioned, Zeh relates this property to Mach's principle (regarding time). Reference 10 presents a geometrization of classical mechanics by use of a symplectic structure. Reference 11 discusses the recovering of time and the deduction of the Wheeler de Witt equation in quantum cosmology.

An application of the present approach (the present article is a revised version of the unpublished Potsdam-Report No. 93/10 from January 1993) can be found in section V A of Ref. 12, where it is used to deduce the Wheeler de Witt equation for the Starobinsky cosmological model. For further generalizations see e.g. Ref. 13.

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Solvable (nonrelativistic, classical) *n*-body problems on the line. II

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A solvable n-body problem is exhibited, which features equations of motion of Newtonian type, $m_j\ddot{x}_j=F_j$, $j=1,\ldots,n$, with "forces" F_j that are linear and quadratic in the particle velocities, $F_j=\dot{x}_j\{\Sigma_{k=1}^{n}[f_{jk}^{(1)}(\mathbf{x})+\dot{x}_k f_{jk}^{(2)}(\mathbf{x})]\}$, and depend highly nonlinearly on the positions $x_k\equiv x_k(t)$, $k=1,\ldots,n$, of the n "particles" on the line. Explicit expressions of the functions $f_{jk}^{(i)}(\mathbf{x})$, in terms of elliptic functions, are given; they contain $n+4$ arbitrary constants, in addition to the n "masses" m_k and to n arbitrary functions $g_k(x_k)$. Special cases in which the elliptic functions reduce to trigonometric or rational functions are of course included. The technique whereby this model has been arrived at entails that its initial-value problem is *solvable by quadratures* [for any n and arbitrary initial data $\mathbf{x}(0)$ and $\dot{\mathbf{x}}(0)$]. A discussion of the actual behavior of the solution, and of special cases, is postponed to future papers. © *1996 American Institute of Physics.* [S0022-2488(96)01802-3]

I. INTRODUCTION

In a previous paper a technique was discussed, to identify solvable n-body problems on the line, characterized by equations of motion of Newtonian type,

$$m_j\ddot{x}_j=F_j, \quad j=1,\ldots,n, \tag{1.1}$$

with the "forces" F_j (appropriately) given functions of the "particle coordinates" x_k and of their velocities $\dot{x}_k$. It is a general feature of these models to be *solvable by quadratures*. Several examples were exhibited for $n=2,3,4,5$, with the forces F_j explicitly given in terms of elementary functions.[1]

The purpose and scope of this paper is to exhibit a model of this kind, solvable for *arbitrary* n, with forces $F_j(\mathbf{x},\dot{\mathbf{x}})$ explicitly given in terms of *elliptic functions*. The model is described in the following section, and future work to analyze its behavior is outlined in the last section.

Let us complete this introductory section with a brief review of the technique exploited here to uncover (or, equivalently, to manufacture) solvable models.[1,2] The basic idea is to start from a function that lives in a finite-dimensional functional space, being representable as a linear superposition of, say, n basic functions $s_m(x)$ ("seeds"):

$$f(x,t)=\sum_{m=1}^{n} c_m(t)s_m(x). \tag{1.2}$$

Here x is the "space" coordinate, and t the "time" coordinate. It is then generally possible[2] to exhibit an *explicit* relation between the n coefficients $c_m(t)$ and the n values, $f_j(t)$, that the function $f(x,t)$ takes at the n points $x_j(t)$ ("nodes"):

$$f_j(t)=f[x_j(t),t]. \tag{1.3}$$

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Hence it is also generally possible to relate, in this manner, a simple (and completely controllable) time evolution of, say, the coefficients $c_m(t)$, to a more complicated (but possibly more interesting; for instance, interpretable as an n-body problem) evolution of the quantities $f_j(t)$ and/or $x_j(t)$. There are several ways in which this can be done, which have been variously explained in the literature and have led to the identification of various classes of solvable many-body problems (see Refs. 1, 2 and the literature quoted there). The approach used in this paper is a direct application of that described in detail in the first paper of this series;[1] and let us reemphasize that the main novel feature here is the *explicit* exhibition of solvable equations of motion of Newtonian type involving *elliptic functions*.

II. THE MODEL

These solvable models are characterized by the equations of motion (1.1), with forces $F_j(\mathbf{x},\dot{\mathbf{x}})$ given by the formula[1]

$$F_j(\mathbf{x},\dot{\mathbf{x}})=\dot{x}_j\left\{-g_j'(x_j)+\sum_{k=1}^{n} D_{jk}(\mathbf{x})[m_k\dot{x}_k+g_k(x_k)]\right\}. \tag{2.1}$$

The n functions $g_j(x)$ are arbitrary, and the $(n\times n)$-matrix $D_{jk}(\mathbf{x})$ (which in fact provides a finite-dimensional representation of the differential operator[2]) is given by the following formulas:

$$D_{jk}(\mathbf{x})=\delta_x^{(k)}(x_j;\mathbf{x}), \tag{2.2}$$

where $\delta_x^{(k)}(x_j;\mathbf{x})$ is the x-derivative of the function $\delta^{(k)}(x;\mathbf{x})$ with respect to x, evaluated at $x=x_j$. (Of course here and throughout this paper $\mathbf{x}$ is the n-vector of components x_k, $k=1,\ldots,n$). The ''interpolational'' function $\delta^{(k)}(x;\mathbf{x})$ is defined, in terms of the scalar variable x and n-vector $\mathbf{x}$, by the formula

$$\delta^{(k)}(x;\mathbf{x})=\Delta(x_1,\ldots,x_{k-1},x,x_{k+1},\ldots,x_n)/\Delta(x_1,\ldots,x_n), \tag{2.3}$$

where

$$\Delta(\mathbf{x})=\det[s_j(x_k);j,k=1,\ldots,n], \tag{2.4}$$

and the ''seeds'' $s_j(x)$ are n functions whose choice remains our privilege, except for the requirement that they be linearly independent. This condition is necessary and sufficient to exclude that $\Delta(\mathbf{x})$ vanish identically; of course $\Delta(\mathbf{x})$ might vanish for some special values of $\mathbf{x}$, thereby implying that the forces $F_j(\mathbf{x},\dot{\mathbf{x}})$ become singular for some special configurations of the n-body system [see (2.1)–(2.4)].

The solution of the initial-value problem is then given[1] by the quadrature

$$m_j\int_{x_j(0)}^{x_j(t)} dy\left[-g_j(y)+\sum_{k=1}^{n} c_k s_k(y)\right]^{-1}=t, \quad j=1,\ldots,n, \tag{2.5}$$

of course followed by an inversion [to express $x_j(t)$ in terms of t, rather than t in terms of $x_j(t)$; at this stage singularities may of course emerge]. The n constants c_k are defined in terms of the initial data $\mathbf{x}(0),\dot{\mathbf{x}}(0)$ by the linear algebraic system

$$\sum_{k=1}^{n} c_k s_k[x_j(0)]=m_j\dot{x}_j(0)+g_j[x_j(0)], \quad j=1,\ldots,n. \tag{2.6}$$

As indicated above, the main novelty of this paper is the involvement of *elliptic functions*, in a context which allows *explicit* computations based on certain remarkable identities satisfied by these functions (see the Appendix). Indeed we now choose the n seeds

$$s_j(x)=\exp(\alpha x)\varphi(a_0,x-a_j), \quad j=1,\ldots,n, \tag{2.7}$$

where the $n+1$ constants α and a_j, $j=1,\ldots,n$, are arbitrary (except for the requirement that the a_j's be all different, $a_j\neq a_k \bmod(2\omega_1,2\omega_2)$, where ω_1 and ω_2 are the semiperiods associated with $\varphi(a_0,z)$, see below), and the function $\varphi(a_0,z)$ is defined as follows:

$$\varphi(a_0,z)=\sigma(a_0+z)/[\sigma(a_0)\sigma(z)]. \tag{2.8}$$

Here $\sigma(z)$ is the Weierstrass sigma-function,[3] which is of course completely characterized by its two ''primitive semiperiods'' ω_1 and ω_2; and a_0 is also an arbitrary constant, except for the condition $a_0\neq 0 \bmod(2\omega_1,2\omega_2)$, which is of course necessary and sufficient to guarantee that $\sigma(a_0)\neq 0$. We report for convenience some properties of $\sigma(z)$ and other elliptic functions in the Appendix.

Using the formulas (A3) and (A5) one obtains from (2.1), after some elementary, if tedious, calculations, the following expression for the forces $F_j(\mathbf{x},\dot{\mathbf{x}})$:

$$F_j(\mathbf{x},\dot{\mathbf{x}})=\dot{x}_j\sum_{k=1}^{n}[f_{jk}^{(1)}(\mathbf{x})+\dot{x}_k f_{jk}^{(2)}(\mathbf{x})], \tag{2.9a}$$

$$f_{jk}^{(1)}(\mathbf{x})=\delta_{jk}[-g_j'(x_j)+g_j(x_j)u_j(\mathbf{x})]+(1-\delta_{jk})g_k(x_k)v_{jk}(\mathbf{x}), \tag{2.10a}$$

$$f_{jk}^{(2)}(\mathbf{x})=\delta_{jk}m_j u_j(\mathbf{x})+(1-\delta_{jk})m_k v_{jk}(\mathbf{x}), \tag{2.10b}$$

$$u_j(\mathbf{x})=\alpha+\zeta[A_0(X)]-\zeta(x_j-a_j)+\sum_{s=1,s\neq j}^{n}[\zeta(x_j-x_s)-\zeta(x_j-a_s)], \tag{2.11a}$$

$$\begin{aligned} v_{jk}(x)=&[\sigma(x_j-x_k)]^{-1}\{\sigma[x_j-x_k+A_0(X)]/\sigma[A_0(X)]\}\\ &\cdot\exp[\alpha(x_j-x_k)][A(x_k)/A(x_j)][S_j(\mathbf{x})/S_k(\mathbf{x})], \end{aligned} \tag{2.11b}$$

$$X=n^{-1}\sum_{j=1}^{n}x_j, \tag{2.12}$$

$$A_0(X)=a_0+nX-\sum_{j=1}^{n}a_j=a_0+\sum_{j=1}^{n}(x_j-a_j), \tag{2.13}$$

$$A(x)=\prod_{r=1}^{n}\sigma(x-a_r), \tag{2.14}$$

$$S_j(\mathbf{x})=\prod_{s=1,s\neq j}^{n}\sigma(x_j-x_s). \tag{2.15}$$

The zeta-function $\zeta(z)$ which enters in (2.11a) is defined in the Appendix, where some of its properties are also reported; it is of course assumed that it is characterized by the same two semiperiods $\omega_{1,2}$ as $\sigma(z)$.

III. OUTLOOK

Due to the richness implied by the presence of the $n+2$ free parameters α and a_m, $m=0,1,\ldots,n$, even in the simplest case in which the elliptic functions $\sigma(z)$ resp. $\zeta(z)$ reduce merely to z resp. z^{-1} [see (A11c)], the model (1.1) with (2.9)–(2.15) requires considerable elaboration to analyze in detail the behavior of its solutions; although it should be emphasized that (at least) *in this case, the quadrature needed to solve the initial-value problem can be explicitly performed in terms of elementary functions* [provided $\alpha=0$ and simple choices are also made for the functions $g_k(x)$; for instance the choice $g_k(x)=$rational functions would do; see (2.5), (2.7), (2.8), and (A11c)]. Hence we postpone to future papers an analysis of the actual behavior of the solutions of the model introduced in this paper, as well as a discussion of its relation with other models, such as the beautiful relativistic "RS-model" due to S. N. Rujsenaars and H. Schneider,[4] which features equations analogous[5] to (1.1) with (2.9a) and $f_{jk}^{(1)}(\mathbf{x})=0$ [note that this condition can be easily enforced by choosing $g_k(x)=0$, $k=1,\ldots,n$; see (2.10a)]. Let us however end by noting that the model considered in this paper (which is solvable by quadratures) does not appear to overlap with the RS-model (which is a completely integrable Hamiltonian system), except in some very degenerate case.[6]

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APPENDIX: ELLIPTIC FUNCTIONS

In this Appendix we report some useful formulas satisfied by the Weierstrass sigma function $\sigma(z)$ and by other elliptic functions:[3]

$$\sigma(z)=z\prod_{j,k}{}'(1-z/\omega_{jk})\exp[z/\omega_{jk}+\tfrac{1}{2}(z/\omega_{jk})^2], \tag{A1a}$$

$$\omega_{jk}=2j\omega_1+2k\omega_2. \tag{A1b}$$

The product in (A1a) runs over all integers (positive, negative, and vanishing), except for $j=k=0$ (the prime appended to the product symbol is a reminder of this exclusion). As it is clear from these formulas, the sigma function is completely characterized by its two "primitive semiperiods" ω_1 and ω_2; it is an entire function, and its quasiperiodicity is displayed by the formula

$$\sigma(z+2\omega_{1,2})=-\sigma(z)\exp[2\eta_{1,2}(z+\omega_{1,2})], \tag{A2a}$$

where the complementary quantities $\eta_{1,2}$ are defined via the Weierstrass zeta-function (see below),

$$\eta_{1,2}=\zeta(\omega_{1,2}), \tag{A2b}$$

and satisfy the relation $\eta_1\omega_2-\eta_2\omega_1=\mathrm{i}\pi/2$.

The two primitive semiperiods ω_1 and ω_2 must of course have different phases, so that the numbers ω_{jk}, see (A1b), do not all lie on a straight line in the complex plane. The sigma function is odd, $\sigma(-z)=-\sigma(z)$; it is real if ω_1 is real and ω_2 imaginary.

There holds for the sigma function the following determinantal identity:[7]

$$\varphi(a,z)=\sigma(a+z)/[\sigma(a)\sigma(z)], \tag{A3a}$$

$$\varphi_{jk}(a)=\varphi(a,x_j-y_k), \tag{A3b}$$

$$\det[\varphi_{jk}(a);j,k=1,\ldots,n]=\left\{\sigma\left[a+\sum_{r=1}^{n}(x_r-y_r)\right]\Big/\sigma(a)\right\}$$
$$\cdot\left\{\prod_{1\leqslant j<k\leqslant n}[\sigma(x_j-x_k)\sigma(y_k-y_j)]\right\}\Big/\left[\prod_{j,k=1}^{n}\sigma(x_j-y_k)\right], \tag{A3c}$$

as well as the related identity[8]

$$\prod_{j=1}^{n}[\sigma(z-x_j)/\sigma(z-y_j)]=\sum_{r=1}^{n}\varphi(a,z-y_r)\cdot\left[\prod_{m=1}^{n}\sigma(y_r-x_m)\right]\Big/\left[\prod_{s=1,s\neq r}^{n}\sigma(y_r-y_s)\right], \tag{A4a}$$

with

$$a=\sum_{j=1}^{n}(y_j-x_j)\neq 0. \tag{A4b}$$

In these formulas the $2n$ numbers x_j,y_j are arbitrary (but different, or else the formulas may require the taking of appropriate limits); and in (A3) [but not in (A4), see (A4b)] a is also arbitrary, except for the condition $a\neq 0 \bmod(2\omega_1,2\omega_2)$, which is necessary and sufficient to exclude the vanishing of $\sigma(a)$, $\sigma(a)\neq 0$.

We also report the definition of the Weierstrass zeta-function,

$$\zeta(z)=\sigma'(z)/\sigma(z). \tag{A5}$$

This function is also odd, $\zeta(-z)=-\zeta(z)$; it is meromorphic, with simple poles at $z=0 \bmod(2\omega_1,2\omega_2)$; and its quasiperiodicity is displayed by the formula

$$\zeta(z+2\omega_{1,2})=\zeta(z)+2\eta_{1,2}. \tag{A6}$$

There holds the following identities:[9]

$$\prod_{k=1}^{n}[\sigma(z-x_k)/\sigma(z-y_k)]=\sum_{r=1}^{n}[\zeta(z-y_r)-\zeta(x_j-y_r)]$$
$$\cdot\left[\prod_{m=1}^{n}\sigma(y_r-x_m)\right]\Big/\left[\prod_{s=1,s\neq r}^{n}\sigma(y_r-y_s)\right],\quad j=1,\ldots,n. \tag{A7a}$$

Here again the $2n$ numbers x_j,y_j are arbitrary (but different), except for the condition [note the difference from (A4b)]

$$\sum_{j=1}^{n}(x_j-y_j)=0. \tag{A7b}$$

Finally we report the definition of the Weierstrass $\mathscr{P}$-function:

$$\mathscr{P}(z)=-\zeta'(z). \tag{A8}$$

Hence $\mathscr{P}(z)$ is even, $\mathscr{P}(-z)=\mathscr{P}(z)$, meromorphic with double poles at $z=0 \bmod(2\omega_1,2\omega_2)$,

$$\mathscr{P}(z)=z^{-2}+\sum_{j,k}{}'[(z-\omega_{jk})^{-2}-\omega_{jk}^{-2}], \tag{A9}$$

and doubly-periodic:

$$\mathscr{P}(z+\omega_{jk})=\mathscr{P}(z), \quad j,k=\text{integers}. \tag{A10}$$

Of course in these formulas ω_{jk} is defined by (A1b), and the sum in (A9) has the same range as the product in (A1a).

All these elliptic functions become elementary in the degenerate cases in which one or both semiperiods diverge:

$$\omega_1=\infty, \quad \omega_2=\mathrm{i}\pi\lambda/2; \quad \sigma(z)=\lambda\ \sinh(z/\lambda)\exp(-\tfrac{1}{6}z^2/\lambda^2),$$

$$\zeta(z)=-\tfrac{1}{3}z/\lambda^2+\lambda^{-1}\ \coth(z/\lambda), \quad \mathscr{P}(z)=\{\lambda^2[\tfrac{1}{3}+\sinh(z/\lambda)]\}^{-2}; \tag{A11a}$$

$$\omega_1=\pi\lambda/2, \quad \omega_2=\mathrm{i}\infty; \quad \sigma(z)=\lambda\ \sin(z/\lambda)\exp(\tfrac{1}{6}z^2/\lambda^2),$$

$$\zeta(z)=\tfrac{1}{3}z/\lambda^2+\lambda^{-1}\ \cot(z/\lambda), \quad \mathscr{P}(z)=\{\lambda^2[-\tfrac{1}{3}+\sin(z/\lambda)]\}^{-2}; \tag{A11b}$$

$$\omega_1=\infty, \quad \omega_2=\mathrm{i}\infty; \quad \sigma(z)=z, \quad \zeta(z)=z^{-1}, \quad \mathscr{P}(z)=z^{-2}. \tag{A11c}$$

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Statistical mechanics of the deformable droplets on Riemannian surfaces: Applications to reptation and related problems

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The statistical mechanics treatment of the Laplace–Young-type problems developed for the flat surfaces is generalized to the case of surfaces of constant negative curvature and connected with them to Riemannian surfaces. Obtained results are mainly used to supply an additional support of the quantum Hall effect (QHE) analogy employed in recent work [J. Phys. **4**, 843 (1994)], which provides theoretical justification of the tube concept used in polymer reptation models. As a byproduct, close links between QHE, quantum chaos, and the non-Abelian Chern–Simons quantum mechanics are indicated. © *1996 American Institute of Physics.* [S0022-2488(96)02502-1]

I. INTRODUCTION

In the previous paper, Ref. 1, the statistical mechanics of the Laplace–Young (LY) and related equations on flat surfaces was considered. At the classical level the LY equation can be written as

$$H=\frac{\Delta p}{2\sigma}, \tag{1.1}$$

where H is the mean curvature of surface, σ is the surface tension, while Δp is the pressure difference. In three dimensions, (1.1) can be obtained by minimization of the following functional:

$$F_3=\sigma A-\Delta p V, \tag{1.2}$$

where A is the area of surface and V is its volume. Evidently, there is a two-dimensional analog of F_3, as was shown in Ref. 1. In two dimensions one can write

$$F_2=\sigma L-\Delta p\ S, \tag{1.3}$$

where L is the length of a closed contour while S is the area enclosed by this contour. If $\mathbf{r}(\tau)=\{x(\tau),y(\tau)\}$ is the spatial position of the contour segment characterized by the contour position τ, then F_2 can be rewritten as

$$F_2[\mathbf{r}(\tau)]=\sigma\int_0^L d\tau\sqrt{\left(\frac{dx}{d\tau}\right)^2+\left(\frac{dy}{d\tau}\right)^2}-\frac{\Delta p}{2}\left|\int_0^L d\tau\left(x\,\frac{dy}{d\tau}-y\,\frac{dx}{d\tau}\right)\right|. \tag{1.4}$$

The statistical mechanics can be developed by considering a path integral of the type

$$Z(\Delta p,\sigma)=\int_{\mathbf{r}(0)=\mathbf{r}(N)} D[\mathbf{r}(\tau)]\exp\{-\beta F_2[\mathbf{r}(\tau)]\}, \tag{1.5}$$

where β is the usual Boltzmann's factor. Traditionally, e.g., see Ref. 2, the "nonrelativistic" analog of (1.4) is studied, i.e.,

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$$F_2[\mathbf{r}(\tau)]=\frac{1}{l}\int_0^L d\tau\left(\frac{d\mathbf{r}}{d\tau}\right)^2-\frac{\Delta p}{2}\int_0^L d\tau\left(x\frac{dy}{d\tau}-y\frac{dx}{d\tau}\right), \tag{1.6}$$

corresponding to the ''motion'' of the nonrelativistic ''particle'' of ''mass'' $m=2/l$ (where l is the Kuhn's length) in the constant ''magnetic'' field characterized by the vector potential $\mathbf{A}=\{-(\Delta p/2)y,(\Delta p/2)x\}$.

The detailed analysis of both (1.4) and (1.6) performed in Ref. 1 shows that these two problems are closely related so that the solution of one of them facilitates a solution of the other. In view of that, it is sufficient to study only the statistical mechanics based on (1.6).

In this paper the situation is going to be complicated by inclusion of the disorder-type random potential that is to be added to the functional F_2. This complication is motivated by the results of Ref. 3, where the existence of the tube in the reptation theory of deGennes, Doi, and Edwards (DDE),[4,5] was investigated using the analogy with QHE. The individual tube cross section can be obtained by analyzing the path integral based on functional (1.6), where, instead of pressure parameter Δp, another parameter is used, as described below and in Ref. 3. On another hand, the traditionally used idea of reptation comes from analysis of static and dynamic models of chains trapped in the array of obstacles,[4–10] i.e. one usually considers some particular chain moving among other chains motion of which is considered to be frozen. The coarse grained motion of this selected chain is being modeled by the primitive path (chain), which at some scale acts as if it is Gaussian. Because of this, it is natural to select the longitudinal and the transversal directions of motion of such a primitive chain so that the transversal conformational statistics of such a chain is described with help of the path integral based on (1.6). In Ref. 3, the notion of a single tube was extended to allow the interactions between the tubes. The interactions are of a topological nature. They affect the very existence of an individual tube. It was shown, that, because of these interactions, the individual tube may or may not exist. The quantum Hall effect (QHE) analogy developed in Ref. 3 allowed to replace the complicated picture of polymer–polymer interactions by the much better studied model of classical disks (tube cross sections) ''living'' in a plane and interacting with each other via the Coulombic-like potential. Such a statistical system, known as one component plasma (OCP), can undergo a phase transition so that in one of the phases one has ''frozen'' a two-dimensional lattice of disks, while in the other one has a sort of liquid-like state, where the concept of tube loses its meaning. If ρ is the polymer (monomer) concentration while a is the tube radius, then in the ''frozen'' phase Eq. (4.35) of Ref. 3 provides $\rho a=\text{const}$. This result is in excellent agreement with the most recent Monte Carlo[11] and the real experimental[12] data.

In the light of this agreement, the analogy with QHE is developed further in this paper by considering the stability of an individual tube against perturbations caused by the random obstacles. In QHE this problem is known as a problem of explaining the robustness of QHE against various kinds of two-dimensional disorders.[13] Although the reptation theory is the main theme of this work, some obtained results can be used to explain other phenomena as well, e.g. suppression of the first-order phase transitions on surfaces of constant negative curvature, etc.

This work is organized as follows. In Sec. II known results related to static conformational properties of polymer chains trapped in the regular array of obstacles and on the Bethe lattice are reanalyzed. In Sec. III it is demonstrated, *without any approximations*, that the continuum limit of the equation of motion, known as the Smoluchowski equation,[10] is also the usual diffusion equation on the surface of constant negative curvature known as tractrix.[14] Moreover, by means of changes of variables, the same equation can be recast without any approximations (as compared with Ref. 15) into the form that describes the diffusion on the Lobachevsky plane. It is shown that the solutions of the Smoluchowski equation and the diffusion equation on the Lobachesky plane produce *the same* results in the *whole range* of permissible changes of variables and *not* only in some limit, as defined in Ref. 15. In Sec. IV it is explained why it is necessary to consider the Riemannian surfaces instead of the Lobachevsky plane. In short, it is motivated by the necessity first to consider the classical motion in the chaotic billiards (e.g., arrays of obstacles with some

periodic boundary conditions imposed) and then, second, to consider the quantum mechanical analog of such billiards.[16] Some results related to this section are presented in the Appendix. In Sec. V the ''magnetic'' field (the area constraint) is included into consideration to model the tube cross section and some qualitative (semiclassical) analysis of the existence and stability of a tube in such environment is discussed. Unlike the flat case, described by Eq. (1.6), where for any finite Δp the corresponding quantum mechanical problem has an infinite spectrum of bound states, in the present case the spectrum may have only finite (or even zero!) number of bound states. This fact provides an independent (complementary to Ref. 3) mechanism by which the tube can be destroyed. In Sec. VI, more systematic (fully quantum mechanical) mathematical treatment of the results presented in Sec. V is developed. The same treatment could also be used to explain the suppression of the first-order phase transitions on surfaces of constant negative curvature. Section VII is devoted to the discussion that is meant to demonstrate the universality of the QHE-like tube model concept used in reptation theory. Close connections between QHE, quantum chaos, and the non-Abelian Chern–Simons quantum mechanics are indicated in this section.

II. POLYMER CHAIN IN AN ARRAY OF OBSTACLES. REVIEW OF KNOWN RESULTS AND ADDITIONAL DEVELOPMENTS

The De Gennes–Doi–Edwards (DDE) reptation model[4,5] is based on the assumption that in dense polymer melt the motion of an individual polymer chain of length N takes place inside a tube created by the instantaneous configuration of other chains. By definition, the tube diameter $a \ll N$ so that the chain ''reptates'' along the tube in an essentially one-dimensional fashion. Because the existence of a tube is accepted in DDE theory axiomatically, the problem of its justification remains (see, however, Ref. 3). One of the most popular ways of justifying the tube model lies in considering the conformational properties (static and dynamic) of a chain trapped in an array of fixed obstacles.[4–10]

In this paper only the static case is going to be discussed. To this purpose, let us imagine first a *regular* lattice of obstacles localized at the vertices of a lattice. Let us place a polymer chain into such an environment and consider how the conformational properties of this chain are affected by the presence of obstacles. For simplicity, and without loss of generality, it is assumed that the chain interacts with obstacles only via δ-like short range repulsive potential.

The conformational properties of polymer chain in the external field V are described with help of end-to-end distribution function $G(\mathbf{r},\mathbf{r}';N)$, which obeys the equation of ''motion''[17] given by

$$\left(\frac{\partial}{\partial N}-\frac{l}{2d}\,\nabla_{\mathbf{r}}^2+V(\mathbf{r})\right)G(\mathbf{r},\mathbf{r}';N)=\delta(\mathbf{r}-\mathbf{r}')\,\delta(N), \tag{2.1}$$

where l is Kuhn's step length. The question arises of how to modify (2.1) in order to account for the periodicity of the lattice. In case of d dimensions, if $\mathbf{a}_n$ is some arbitrary lattice period, then it is always possible to write

$$\mathbf{a}_n=\sum_{i=1}^{d} n_i\mathbf{e}_i\,, \tag{2.2}$$

where n_i are some integers (positive or negative) while $\mathbf{e}_i$ are elementary periods (lattice spacings). Obviously, the potential V now should be also a periodic function, i.e.,

$$V(\mathbf{r}+\mathbf{a}_n)=V(\mathbf{r}). \tag{2.3}$$

The question remains of how (2.1) should be modified in view of periodicity of the potential V reflected in (2.3)? The famous Bloch theorem[18] provides an answer. Here, some details are provided that are essential for the rest of our discussion. To begin, let us assume that the distribution function G can be written as

$$G(\mathbf{r},\mathbf{r}';N)=\sum_n e^{\epsilon_n N}\Psi_n(\mathbf{r})\Psi_n^*(\mathbf{r}'), \tag{2.4}$$

so that the function $\Psi_n(\mathbf{r})$ obeys a stationary Schrödinger-like equation,

$$\left[\epsilon_n-\frac{l}{2d}\,\nabla_{\mathbf{r}}+V(\mathbf{r})\right]\Psi_n(\mathbf{r})=0. \tag{2.5}$$

In case the potential V is a periodic function, the solution to Eq. (2.5) can be sought in the form[18]

$$\Psi(\mathbf{r})=e^{i\mathbf{k}\cdot\mathbf{r}}\Psi_{\mathbf{k}}(\mathbf{r}), \tag{2.6}$$

where $\mathbf{k}$ is determined by the boundary conditions

$$\Psi(\mathbf{r}_i+L_i\mathbf{e}_i)=\Psi(\mathbf{r}_i) \tag{2.7}$$

or

$$e^{\pm ik_iL_i}=1, \tag{2.8}$$

L_i being the size of the lattice in the ith direction. Combining Eqs. (2.5) and (2.6) produces

$$\nabla_{\mathbf{r}}^2\Psi_{\mathbf{k}}+2i\mathbf{k}\cdot\nabla_{\mathbf{r}}\Psi_{\mathbf{k}}-\frac{2d}{l}\left(\epsilon(\mathbf{k})+V(\mathbf{r})+\frac{l\mathbf{k}^2}{2d}\right)\Psi_{\mathbf{k}}=0. \tag{2.9}$$

For $\mathbf{r}\neq\mathbf{a}_n$, by construction, we have $V(\mathbf{r})=0$. Let, moreover, $\mathbf{r}\rightarrow i\mathbf{r}$, so that (2.9) can be rewritten as

$$\nabla_{\mathbf{r}}^2\tilde{\Psi}_{\mathbf{k}}-2\mathbf{k}\cdot\nabla\mathbf{r}\tilde{\Psi}_{\mathbf{k}}+E(\mathbf{k})\tilde{\Psi}_{\mathbf{k}}=0, \tag{2.10}$$

where $E(\mathbf{k})$ is defined by (2.9). Alternatively, one can rewrite (2.10) (for $\mathbf{r}\neq\mathbf{a}_n$) as follows:

$$\frac{\partial}{\partial N}\,\tilde{\Psi}_{\mathbf{k}}(\mathbf{r},N)=\nabla_{\mathbf{r}}^2\tilde{\Psi}_{\mathbf{k}}-2\mathbf{k}\cdot\nabla_{\mathbf{r}}\tilde{\Psi}_{\mathbf{k}}. \tag{2.11}$$

The regular lattice used above is a very crude approximation of the environment that the individual polymer chain encounters in the polymer melt.

It is believed[8–10] that this environment is being better modeled by placing our polymer chain on a Cayley tree (or Bethe) lattice. The standard recursion-type arguments produce then in the continuum limit the diffusion equation for the end-to-end distribution function in the form given by[10]

$$\frac{\partial P}{\partial N}=D\,\frac{\partial^2 P}{\partial r^2}-c\,\frac{\partial}{\partial r}\,P, \tag{2.12}$$

where $D=2pq$, $c=q-p$, $p=z^{-1}$, $q=1-p$, and z is believed to be a coordination number of the regular lattice, e.g., see Refs. 6 and 10, or Bethe lattice, e.g., see Refs. 8 and 9. Evidently, Eqs. (2.11) and (2.12) look mathematically very similar. The only difference they have lies in the fact

that Eq. (2.11) is multidimensional while Eq. (2.12) is not (which is of no surprise for Bethe lattice-type of calculations). Both equations should be supplemented with boundary conditions. In the continuum limit they are given [for (2.12)] by

$$P(r,0)=\delta(r), \quad D\left.\frac{\partial P(r,N)}{\partial r}\right|_{r=0}-cP(r,N)=0. \tag{2.13}$$

The mathematical treatment of (2.12) (with $c=0$) supplemented with boundary conditions of the type given by (2.13), was discussed in detail in Ref. 19. Because of this, this work is mainly concentrated on (2.12), thus ignoring boundary conditions. This is permissible because, as it follows from analysis given in Ref. 19, once the solution of (2.12) with $P(r,0)=\delta(r)$ is known, the boundary problem of the type given by (2.13) can be solved as well.

The direct and transparent correspondence between Eqs. (2.11) and (2.12) is obtained above without recourse to the conformal mapping, the Lobachevsky plane, etc., as discussed in Ref. 15, and is based on use of the Bloch theorem only.[18] Moreover, Eq. (2.12) is not restricted to its use in the periodic array of obstacles.[15,20–22] Indeed, it was first obtained in the classical paper by de Gennes [e.g., see Eqs. (II.4) and (II.5) of Ref. 4] based on different arguments. Whence, I just demonstrated, that the periodicity of the lattice is not essential in developing the reptation model. This statement will be further elaborated below in connection with chaoticity in classical and quantum billiards. Toward this goal, it is useful to provide a somewhat different mathematical interpretation of Eq. (2.12). This is accomplished in the next section.

III. SMOLUCHOWSKI EQUATION ON THE LOBACHEVSKY PLANE

Following Ref. 10, let us call Eq. (2.12) as Smoluchowski (or rather Smoluchowski–de Gennes) equation. As is usual in mathematical physics, it is convenient to rewrite (2.12) in the dimensionless form. To this purpose, let us rescale $N\rightarrow\alpha\tau$ and $r\rightarrow\beta x$ so that, in terms of such rescaled variables, one obtains

$$\frac{1}{\alpha}\frac{\partial}{\partial\tau}P(\tau,x)=\frac{D}{\beta^2}\frac{\partial^2}{\partial x^2}P-\frac{c}{\beta}\frac{\partial}{\partial x}P. \tag{3.1}$$

If now one chooses $\alpha=D/c^2$, $\beta=D/c$, then Eq. (3.1) acquires the form

$$\frac{\partial}{\partial\tau}P(\tau,x)=\frac{\partial^2}{\partial x^2}P-\frac{\partial}{\partial x}P. \tag{3.2}$$

Although (3.2) has a correct dimensionless form it, nevertheless, is incomplete for the following reasons. In (2.12) both D and c are dimensionless while both N and r have dimensionality of length. Thus, it is implicitly assumed in (2.12) that both N and r are being measured in terms of the effective step length l [e.g., see (2.1)] and that the length l is of order of lattice spacing s. Under this condition (2.12), taken from Ref. 10, holds. If, however, $l\neq s$, then the adjustments should be made, which are discussed below.

Let us now pose the following question: is it possible to rewrite (3.2) in the form of the diffusion equation on some curved manifold?

The answer to this question turns out to be affirmative. Indeed, on a curved manifold the diffusion equation can be written as

$$\frac{\partial}{\partial\tau}P=\frac{1}{\sqrt{g}}\partial_\alpha(g^{\alpha\beta}\sqrt{g}\partial_\beta P), \tag{3.3}$$

where $g_{\alpha\beta}$ is the induced metric tensor of this manifold, $\alpha,\beta=1-d$, $g^{\alpha\beta}$ is its inverse, while g is the determinant of the metric $g_{\alpha\beta}$. Following the same arguments as in Refs. 3 and 15, let us restrict ourselves by the case of two-dimensional manifolds. Indeed, in the polymer melts we can always choose an arbitrary plane that crosses the melt. In this plane we can study the *projection* of our three-dimensional random walk. According to Ref. 10, Eq. (2.12) is independent of the dimensionality of the underlying lattice (which enters only through the coordination number z). Because in Ref. 15 the planar regular array was studied, it is convenient to compare our results with that of Ref. 15, thus considering only two-dimensional manifolds. Additional reasons for studying the two-dimensional case can be found in Ref. 3 and also will become apparent from the development presented below.

In the two-dimensional case let us consider the first fundamental form of the surface given by[14]

$$ds^2=dr^2+e^{-2r}\,dx^2, \tag{3.4}$$

i.e., we have $g_{rr}=1$, $g_{xx}=e^{-2r}$, $g_{rx}=g_{rx}=0$, and $g=e^{-2r}$. From here we obtain $g^{rr}=1$, $g^{xx}=e^{+2r}$, so that

$$\frac{1}{\sqrt{g}}\,\partial_\alpha(g^{\alpha\beta}\sqrt{g}\partial_\beta\cdots)=e^r\,\frac{\partial}{\partial r}\left(e^{-r}\,\frac{\partial}{\partial r}\cdots\right)+e^r\,\frac{\partial}{\partial x}\left(e^r\,\frac{\partial}{\partial x}\cdots\right). \tag{3.5}$$

If the function P is independent of x [not to be confused with x in (3.2)], then we obtain, by combining (3.3) and (3.5), equation (2.12) in the original variables. Whence, the above arguments had just demonstrated, that *(2.12) is diffusion equation on a curved manifold.*

Let us now examine closer what is the nature of a manifold that is described by (3.4). To this purpose, let us introduce a new variable $y=e^r$ so that $dy=e^r\,dr$ and, whence,

$$ds^2=dr^2+e^{-2r}\,dx^2=\frac{dy^2+dx^2}{y^2}. \tag{3.6}$$

In the mathematical literature the metric given by the last of Eqs. (3.6) is known as a hyperbolic metric.[14] The Poincaré model consists of a subset of the complex plane C, defined by

$$H=\{z=x+iy\in C|y>0\}, \tag{3.7}$$

supplemented with the hyperbolic metric, Eq. (3.6), on H. As it was known already to Poincaré,[23] the geometry of motions in H is that on the Lobachevsky plane. Because metrics given by Eqs. (3.4) and (3.6) are interconnected, the metric defined by (3.4) is called horocyclical[24] and, accordingly, the coordinate system in this metric is called horocyclic.[14] It is instructive to understand better the geometrical meaning of the horocyclical coordinates. To this purpose let us recall some elementary facts from the differential geometry of surfaces. Following Ref. 25, let us consider the surfaces of revolution of constant Gaussian curvature. Such surfaces can be described in the parametric form, given by

$$x=r\,\cos\,\varphi,\quad y=r\,\sin\,\varphi,\quad z=f(r), \tag{3.8}$$

so that the first fundamental form of such a surface is given by

$$ds^2=(1+f'^2)dr^2+r^2\,d\varphi^2, \tag{3.9}$$

where $f'=df/dr$. By means of transformation,

$$du=\sqrt{1+f'^2}\,dr, \tag{3.10}$$

Eq. (3.9) can be brought into the form

$$ds^2 = du^2 + G(u)d\varphi^2, \tag{3.11}$$

$G = r^2(u)$.

If K is constant Gaussian curvature, then it can be shown[25] that

$$K = -\frac{1}{\sqrt{G}}\frac{d^2\sqrt{G}}{du^2}. \tag{3.12}$$

For $K<0$, the solution of (3.12) is given by

$$\sqrt{G} = C_1 e^{u/b} + C_2 e^{-u/b}, \tag{3.13}$$

where $-b^2 = K$ and C_1, C_2 are some constants of integration. Now, if we choose $C_1 = 0$ and $b = 1$, then we arrive back at (3.4). Whence, both metrics, (3.4) and (3.6), describe surfaces of constant Gaussian curvature equal to -1. The first fundamental form (3.4) [or its equivalent (3.11)] describes the surface of revolution known as tractrix.[14,25] It is essentially a conical surface that cannot be embedded (rigorously speaking[14]) into $3d$ space. To conclude this discussion, it is helpful to consider transformation from the H plane to the unit circle, given by the mapping[24]

$$w = \frac{z-i}{z+i}, \quad z \in H. \tag{3.14}$$

If $w = u + iv$, then it can be shown that $u^2 + v^2 \leqslant 1$, so that the first fundamental form can be written as

$$ds^2 = \frac{4(du^2 + dv^2)}{[1-(u^2+v^2)]^2}. \tag{3.15}$$

The transformation given by (3.14) is isometric, i.e. it preserves the distance d that in H (or in the unit disk) is defined by

$$\cosh d(z,z') = 1 + \frac{|z-z'|^2}{2\,\mathrm{Im}\,z\;\mathrm{Im}\,z'}. \tag{3.16}$$

In analyzing this result, it is useful to remember that the usual Euclidean distance in the complex C plane is given by

$$d_E(z,z') = |z-z'|. \tag{3.17}$$

With the help of d just defined, the solution of (2.12) (without account of boundary effects) in the H plane can be found, e.g. see Ref. 24, and is given by

$$P_H(z,z',\tau) = \frac{1}{2(2\pi\tau)^{1/2}}\, e^{-\tau/4}\int_{d(z,z')}^{\infty} dx\, \frac{x e^{-x^2/4\tau}}{\sqrt{\cosh x - \cosh d(z,z')}}. \tag{3.18}$$

This result coincides with that obtained in Ref. 15 [e.g., see Eq. (3.10) of Ref. 15] in a completely different way. The same result can also be obtained with use of the metric of the unit disk (3.15), as explained in great detail in Ref. 26 (e.g., see p. 3586 of this reference).

In the case of a unit disk, Eq. (3.3) can be presented as follows:[26,31]

$$\frac{1}{4}\,\nabla^2_{r,\varphi}P(r,\varphi;\tau)=\frac{1}{(1-r^2)}\,\frac{\partial}{\partial\tau}\,P(r,\varphi;\tau), \tag{3.19}$$

where use has been made of psendospherical coordinates: $u=\sinh\theta\cos\varphi$, $v=\sinh\theta\sin\varphi$ ($0<\theta<\infty$, $0<\varphi\leqslant 2\pi$) in (3.15) and the Laplacian $\nabla^2_{r,\varphi}$ is given in these coordinates by [$r=\tanh(\theta/2)$]

$$\nabla^2_{r,\varphi}=\frac{\partial^2}{\partial r^2}+\frac{1}{r}\,\frac{\partial}{\partial r}+\frac{1}{r^2}\,\frac{\partial^2}{\partial\varphi^2}\,. \tag{3.20}$$

For additional details, please see Sec. VII. The comparison between our (3.19) and (3.6) of Ref. 15 allows one to restore the missing scale factors [as discussed below (3.2)]. With this remark, to restore this missing scale factors it is useful to rewrite (3.15) in the following way:[27]

$$ds^2=\frac{4R^4(du^2+dv^2)}{(R^2-u^2-v^2)^2}, \tag{3.21}$$

where, instead of canonical $R=1$, an arbitrary dimensionless curvature parameter R is chosen. Comparison between this result and (3.6) of Ref. 15 produces $R^2\simeq s^2/l^2$ (if N is measured in units of l). This fact is going to be used below.

IV. FROM THE LOBACHEVSKY PLANE TO THE RIEMANN SURFACE

In statistical mechanics, it is common to use the periodic boundary conditions. In case of a plane, use of periodic boundary conditions effectively converts it to the torus,[28] i.e. the surface of genus one. Now, the entire complex plane plus the point at infinity is equivalent to the Riemann sphere (via stereographic projection).[27] The question arises as to what surface can be related to H?

Let us begin with some elementary observations. Following Arnold (e.g., see Ref. 29, Appendix 1), let us consider a classical billiard made of a square inside of which there is a small circle (a hole). The particle in such a billiard can scatter from the walls and from the circle (hole) and motion of such a particle is believed to be chaotic. This is so because, according to Arnold, the topology of such a billiard is the same as that for the sphere with two handles that can be obtained by gluing together two toruses, each of which having a hole, along the circumference of these holes. Notice that such a surface cannot be obtained if instead of toruses with holes we would have two spheres, each having a hole.[14]

Whence, the major building block of any higher genus surface consists of a sphere with three punctures and any Riemann surface of genus $g>1$ is just a collection of trice punctured spheres along with a gluing prescription,[24] which is used for their assembly. In case of Arnold's ''double torus,'' we have the first example of a surface of a constant negative curvature so that the nearby classical trajectories tend to diverge during their evolution,[29,30] which is the main characteristic of the chaotic behavior.

It is important at this moment to realize that the appearance of a constant negative curvature surface that is seemingly compact is *not* in contradiction with the statement made in Sec. III about the constant negative surfaces that cannot be embedded into three-dimensional Euclidean space. This will become apparent upon reading the rest of this section.

The example, just described, can be easily generalized. Indeed, following Ref. 24 (e.g., see Cr. 5, Sec. 5.3), let us construct a finite square lattice of m^2 copies of the Arnold's square. By gluing these squares together it is possible to insert yet another k holes into this lattice thus forming a surface of genus

$$g=1+\frac{m^2+k}{2}, \tag{4.1}$$

$k \in \{0,2,\ldots,2m\}$ if m is even or $k \in \{1,3,5,\ldots 2m-1\}$ if m is odd. Whence, using Eq. (4.1) for $m=1$ one obtains $g=2$, in agreement with Arnold. The above example demonstrates that polymer chain (or rather its two-dimensional projection) ''lives'' on a two-dimensional surface of genus g. Because every Riemann surface can be visualized as a sphere with g handles,[14,24] we have to conclude *that the problem of finding the distribution function for the polymer chain trapped in an array of obstacles is equivalent to finding the distribution function for the free chain but on the Riemannian surface of genus* $g \gg 1$. To understand better the connection between the manifolds of constant negative curvature and the flat plane domains with punctures, reading of the Appendix at this time is the most helpful. To complete this presentation, it is necessary to make a connection between the Poincaré H plane model and the Riemannian surfaces of genus g. To this purpose, it is useful again to recall that the usual torus can be obtained by identifying the opposite sides of a square in the plane. Evidently, the plane $\mathbf{R}^2$ can be covered without gaps by squares, and if Γ is a discrete translation (i.e., the matrix that belongs to translation group Γ), then a given square Sq can be thought of as an image of some fundamental square $\hat{S}q$, i.e. $Sq=\Gamma\hat{S}q$. Because of this, the torus can be defined as a quotient: $\mathbf{R}^2/\Gamma$.[14] Analogously, let Γ now be a group of translations in the H plane, such that some fundamental domain $G \in H$ with help of the action of Γ covers (tessellates) the entire H so that the Riemamann surface M is just the quotient H/Γ. Every higher genus g Riemann surface can be constructed from the fundamental $4g\text{-}gon \in H$ sides of which are geodesics, i.e. ''straight'' (or horocyclical) lines in H[24] (e.g., genus two surface requires an octagon, etc.,[16,31] supplemented with the appropriate group of translations Γ in H). It can be shown[32] that Γ is represented by 2×2 matrices, which belong to the group $SL(2,R)/\{\pm 1\}=PSL(2,R)$. $\{\pm 1\}$ factor is a 2×2 identity matrix responsible for reflections (recall the Lorentz group). If $z \in H$ and $\gamma \in SL(2,R)$ with chosen sign (e.g. ''+''), then

$$\gamma z = \frac{az+b}{cz+d}. \tag{4.2}$$

For compact Riemann surfaces $M=H/\Gamma$ it can be shown[33] that tr $\gamma>2$, which amounts to dilatations: $z \to e^{\delta}z$, where δ is some constant. Transformations given by (4.2) leave the metric (3.16) invariant, i.e. they are isometries. Because of this fact, the solution P_H given by (3.18), is also invariant with respect to the action of γ and, whence, is the same for all compact surfaces H/Γ. This explains a relative success in use of P_H, as advocated in Ref. 15. DDE theory, however, assumes not only the existence of a primitive path whose conformational statistics is being described by P_H,[9,10] but also the existence of a tube through which the primitive path reptates.[4,5] As it was noticed in Ref. 5 (also see Ref. 3 for additional details), the existence of a tube can be modeled by considering the problem of statistics of random walks that enclose a constant area. In the present case the situation is complicated by the fact that we have to consider, instead of planar walks, the walks on Riemannian surfaces in the presence of an area constraint. This represents the subject of the next section.

V. POLYMER CHAIN IN AN ARRAY OF OBSTACLES IN THE PRESENCE OF A TUBE. QUALITATIVE TREATMENT

In Ref. 1, an extensive study of random walks on flat surfaces in the presence of an area constraint is presented, while in Ref. 3 it was shown how this flat problem is related to the theory of reptation, on one hand, and to the formalism used to describe the quantum Hall effect, on the other. Because of this, it is essential for the reader to consult with the above references for details related to statistics of planar configurations. Here only the most essential facts needed for further uninterrupted development are provided. In this paper the emphasis is made mainly on applications related to DDE reptation theory. The necessary transcription for the Laplace–Young (LY) type of problems, discussed in detail for the case of flat surfaces in Ref. 1, should become obvious upon reading of this section and, whence, is not elaborated in detail in this paper.

It is convenient to subdivide this section into subsections in order to explain better the physics of the problem.

A. Statistical mechanics of interacting tubes

The classical DDE reptation model[4,5] is based on the axiomatic assumption that in a dense polymer melt there are "tubes" (which can appear and disappear) through which the primitive chain crawls[3,4,6–10] in an essentially one-dimensional fashion. The existence of tubes in melts can be easily understood if the analogy with diffusion models in simple liquids is used.[34] In the case of simple liquids, thermal fluctuations cause formation of vacancies inside the liquid so that diffusion (or viscosity) is facilitated by their presence. Because the process of formation of vacancies is surface tension mediated, solutions of the LY equation $H=\Delta p/2\sigma$, where H is mean curvature, Δp is the pressure difference, and σ is surface tension[1] yield only round spheres of the average size of the host molecule in a simple liquid case. In the case of polymers, the molecules are extremally elongated, so that one should use the cylindrical shape solutions to the L-Y equation.

The Doi and Edwards reptation model[5] describes the conformations of a polymer chain trapped inside such a cylindrical tube. The size of a tube is determined with help of the distribution function $G(\mathbf{r},\mathbf{r}',N)$, which obeys the following equation of "motion:"

$$\left(\frac{\partial}{\partial n}-\frac{l}{2d}\,\nabla_{\mathbf{r}}^2+\frac{w^2}{6}\,(x^2+y^2)\right)G(\mathbf{r},\mathbf{r}';N)=\delta(\mathbf{r}-\mathbf{r}')\,\delta(N), \tag{5.1}$$

to be compared with Eq. (2.1), here $\mathbf{r}=\{x,y,z\}$. The parameter w is determined from the condition

$$\langle x^2+y^2\rangle=\frac{l}{w}=a^2, \tag{5.2}$$

where the tube cross section $\sim a^2$ is considered to be a phenomenological parameter of the theory and $\langle\cdots\rangle$ denotes the statistical average performed with the help of $G(\mathbf{r},\mathbf{r}';N)$, as usual.[17]

Following Ref. 3, let us imagine an arbitrary plane that crosses the polymer melt and let us concentrate our attention on the distribution of just defined cross sections in this imaginary plane. Because of the natural cutoff given by the Kuhn's length l, the requirement $a^2>l^2$ should be imposed. Let A be an area of an imaginary plane and let n_t be the number of tubes (or, rather, their cross sections) that cross this plane.

If the surface density $\hat{\rho}$ is defined by

$$\hat{\rho}=\frac{n_t}{A}, \tag{5.3}$$

then the Wigner–Seitz radius r_{w-z} can also be introduced via

$$\pi r_{w-z}^2=\frac{1}{\hat{\rho}}. \tag{5.4}$$

Evidently, $2r_{w-z}$ represents an average distance between the centers of two neighboring tubes. Use of Eq. (5.4) facilitates an introduction of a filling fraction ν, defined by

$$\nu=\left(\frac{a}{r_{w-z}}\right)^2=\pi a^2\hat{\rho}. \tag{5.5}$$

By construction, $\nu\leqslant 1$. Because both a^2 and $\hat{\rho}$ depend ultimately on the polymer (monomer) concentration ρ, the previous equation can also be rewritten as

$$\nu = \pi a^2(\rho)\hat{\rho}(\rho), \tag{5.6}$$

where both a^2 and $\hat{\rho}$ are some, in general unknown, functions of ρ. In view of (5.3), it is expected, however, that $\hat{\rho}(\rho) \propto \rho$.

Suppose now that there is some interaction between the cross sections (disks) in the plane so that the gas of disks can be either in a ''solid'' (ordered lattice) or in a ''liquid'' (or ''gas'') state. In the last case a ''liquid'' of uniform density may occur so that an initially well-defined tube radius $\sqrt{a^2}$ may lose its meaning. Like in the theory of liquid–gas transitions (based on the Ising model), it is reasonable to anticipate, that if instead the solid–liquid transition takes place, it will be characterized by ν^*, which is some model-dependent (usually known) number, $0 \leqslant \nu^* \leqslant 1$. If this number is known, (5.6) can be rewritten as

$$\nu^* = \pi a^2(\rho^*)\hat{\rho}(\rho^*). \tag{5.7}$$

The last equation implicitly determines the critical polymer (monomer) density ρ^*. This density determines the experimentally observed transition from the reptation-like (solid phase) to the Rouse-like (liquid phase) viscoelastic regime.[35] In Ref. 3, the interaction between the cross sections was caused by the topological effects of entanglements. In the absence of such a topological mechanism of interactions between the cross sections, they are always stable in the case of flat surfaces. This is caused by the fact that oscillator-like potential in (5.1) for arbitrary small w still produces a countable infinity of discrete energy levels, making the tube stable.

The situation changes dramatically if, instead of flat surfaces, Eq. (5.1) is treated on the Riemannian surfaces of constant negative curvature.

B. Statistical mechanics of charged particles on curved manifolds. Semiclassical treatment

The harmonic oscillator model described by (5.1) can be understood also from the point of view of the magnetic analogy discussed in great detail in Refs. 1 and 3.

The Bloch equation for the density matrix $\rho(\mathbf{r},\mathbf{r}';\beta)$ for the spinless electron of mass m and charge $e=1$ in the magnetic field B can be written in a standard way,[36] as

$$-\frac{\partial}{\partial\beta}\rho = \hat{H}\rho. \tag{5.8}$$

The above equation is supplemented by the initial condition:

$$\rho(\mathbf{r},\mathbf{r}';\beta\to 0) = \delta(\mathbf{r}-\mathbf{r}'), \tag{5.9}$$

where $\beta=(K_BT)^{-1}$. For the constant magnetic field perpendicular to x-y plane, (5.8) acquires the form

$$\left(\frac{\partial}{\partial\beta} - \frac{1}{2m}\nabla_r^2 + \frac{B}{2mi}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) + \frac{B^2}{8m}(x^2+y^2)\right)\rho = 0. \tag{5.10}$$

In view of (5.1), the corresponding polymer problem is obtained by making the following replacement: $\beta \rightleftarrows N$, $1/m = l/2d$, $B^2/8m \rightleftarrows w^2/6$, $d=3$, and considering only the states that have the total angular momentum equal to zero. Because for the harmonic oscillator the path integral is quadratic in the field variables,[37] the semiclassical treatment of the path integral produces the exact result anyway. This observation is helpful because it allows us to obtain solutions to the quantum mechanical problem using methods of classical mechanics. This remains to be true, even for the curved manifolds,[38] and, therefore, it is instructive to get a feeling of the problem at the classical level first.

To this purpose, following Ref. 38, [Eq. (4.2)], the (semi)classical Lagrangian L for the particle of mass $m=2$ and charge $e=1$ moving on the H plane in the presence of the magnetic field B can be written as follows:

$$L=\frac{R^2}{y^2}\,(\dot{x}^2+\dot{y}^2)-\frac{b\dot{x}}{y}-\frac{1}{16R^2}. \tag{5.11}$$

Here use has been made of R^2 defined after (3.21), and $b=BR^2$. Proceeding from the Lagrangian to the Hamiltonian in a standard way and introducing the canonical action-angle variables produces Bohr–Sommerfield quantization condition, which yields the energy spectrum given by

$$E_n=\frac{1}{4R^2}\left[\frac{1}{4}+b^2-\left(n+\frac{1}{2}-b\right)^2\right]. \tag{5.12}$$

Consider now this expression in the limit of $R^2\to\infty$ (i.e., large distance between the obstacles). In this limit (5.12) reduces to the familiar Landau result:

$$E_n=\frac{B}{2}\left(n+\frac{1}{2}\right), \tag{5.13}$$

discussed in great detail in the previous work, Ref. 1. At the same time, by requiring E_n to be non-negative, one obtains the constraint on the magnetic field:

$$n\leqslant|b|-\tfrac{1}{2}. \tag{5.14}$$

This constraint indicates that, unlike the flat case given by (5.13), where for any $B>0$ the spectrum E_n is non-negative countable infinity, on the manifold of constant negative curvature the field strength B should exceed a certain threshold, e.g. $B\geqslant 1/2R^2$ (for $n=0$), in order for the discrete spectrum, and, whence, for the tube to exist. The size of the tube $\sim a$ is determined by the condition (e.g., see Ref. 38, p. 191 and take into account that their a is our R, etc.),

$$\frac{a}{R}=\operatorname{arctanh}\frac{\sqrt{B^2-4|c|}}{B}, \tag{5.15}$$

and also, according Ref. 38 [e.g., see Eqs. (4.9) and (4.11) of this reference] there is an additional relation:

$$b-2R^2\sqrt{c}=n+\tfrac{1}{2}, \tag{5.16}$$

where the constant c is related to the period of motion along the circular orbit. Combining Eqs. (5.14) and (5.16), one obtains $c=0$ for $n=0$. Use of this result in (5.15) indicates that in this case $a\to\infty$, i.e. the tube does not exist. For the tube to exist, one must require that $a/R\leqslant 1$, i.e. that the size of the tube be less (or equal) to the distance between the obstacles. In this case, using (5.15) and (5.16), one obtains an estimate:

$$\tanh 1\simeq\sqrt{\frac{n+\frac{1}{2}}{b}}\sqrt{\frac{2b-n-\frac{1}{2}}{b}}. \tag{5.17}$$

For $n=0$, this produces

$$b\,\tanh 1\simeq\sqrt{b-\tfrac{1}{4}} \tag{5.18}$$

or

$$b \simeq 0.86(1 \pm 0.643). \tag{5.19}$$

For compact Riemannian surfaces, b cannot have an arbitrary value and should be quantized as well.[40,41] Using the results of Refs. 39–41, one obtains

$$b = \frac{f}{2(g-1)}, \tag{5.20}$$

where $f = 0, \pm 1, \pm 2, \ldots$. Using (4.1) one can rewrite (5.20) as

$$b = \frac{f}{m^2 + k}. \tag{5.21}$$

In view of the results of Sec. V A, it is appropriate to make an identification: $m^2 + k \simeq n_t$, so that by combining Eqs. (5.19) and (5.21), one obtains

$$\frac{f}{n_t} \simeq 0.86(1 \pm 0.643). \tag{5.22}$$

Let $A = f\pi a^2$ so that (5.3) can be rewritten as $\pi \hat{\rho} a^2 = n_t/f$. Combining this result with Eqs. (5.5) and (5.22) produces an estimate for ν^*: $\nu^* \approx 0.708$. The obtained result is too high, as compared with an earlier result $\nu^* \approx 0.0286$ (e.g., see Ref. 3). This can be easily explained by looking at Eq. (5.5). Indeed, if $r_{w-z} \approx 2a \approx R$, then $0.25 < \nu \leqslant 1$. Obviously, the tube is well defined only if $a < R$ and $r_{w-z} \gg a$ (i.e., the tubes are well separated), so that the estimate just obtained is too crude. In addition, this estimate is based on the assumption that the tubes do not interact. The interaction between the tubes can be introduced analogously to the flat case discussed in Ref. 3. Such a generalization would lead us to the non-Abelian version of the Chern–Simons quantum Hall effect[42,43] picture of reptation developed earlier in Ref. 3. The additional compelling arguments in favor of the non-Abelian generalization of the model developed in Ref. 3 are presented in Sec. VII. In the meantime, in anticipation of these generalizations, more systematic mathematical treatment of the results just obtained is desirable since the results presented so far are only semiclassical. It is given in the next section.

VI. SELBERG TRACE FORMULA AND THE LAPLACE–YOUNG-TYPE EQUATIONS ON RIEMANNIAN SURFACES: APPLICATIONS TO REPTATION AND RELATED PROBLEMS

In order to study systematically the problems discussed in previous sections at the quantum level, it is helpful at this time to provide a summary of the results related to random walks in the plane in the presence of an area constraint. (e.g., see Ref. 1 for more details).

A. Review of the flat case results

The probability $P(A,N)$ for the random walk to length N to enclose a given area A could be defined as

$$P(A,N) = \frac{Z(A,N)}{Z(0,N)}, \tag{6.1}$$

where

$$Z(A,N)=\int d\mathbf{r}\; G(\mathbf{r}_1=\mathbf{r}_2=\mathbf{r},N|A) \tag{6.2}$$

and

$$G(\mathbf{r},\mathbf{r}',N|A)=\int_{\mathbf{r}(0)=\mathbf{r}}^{\mathbf{r}(N)=\mathbf{r}'} D[\mathbf{r}(\tau)]\,\delta\left(A-\frac{1}{2}\left|\int_0^N d\tau\left(x\,\frac{dy}{d\tau}-y\,\frac{dx}{d\tau}\right)\right|\right)\exp\left\{-\frac{1}{l}\int_0^N d\tau\left(\frac{d\mathbf{r}}{d\tau}\right)\right\}^2. \tag{6.3}$$

Because the area A cannot exceed $N^2/4\pi$ (i.e., the area of the circle that has a perimeter length equal to N), the normalization condition for $P(A,N)$ is given by

$$\int_0^{N^2/4\pi} dA\; P(A,N)=1. \tag{6.4}$$

Using (6.4), the mean area $\langle A\rangle$ can now be defined as

$$\langle A\rangle=\int_0^{N^2/4\pi} dA\; AP(A,N). \tag{6.5}$$

In case of the Laplace–Young (LY)-type problem, one has to replace $(1/l)\int_0^N d\tau(d\mathbf{r}/d\tau)^2$ in the exponent of (6.3) by $\sigma\int_0^1 d\tau\sqrt{(d\mathbf{r}/d\tau)^2}$, where $(d\mathbf{r}/d\tau)^2=(dx/d\tau)^2+(dy/d\tau)^2$ and σ is the bare surface tension. In Ref. 1 it was shown that the LY and the random walk [e.g., see Eq. (6.3)] problems are inter-related. Therefore, it is sufficient to study mainly the problem defined by Eq. (6.3). In case if there is a pressure difference Δp (inflated vesicles), the average area is given by

$$\langle A\rangle=\frac{\partial}{\partial\Delta p}\ln\int_0^{N^2/4\pi} dA\; e^{A\,\Delta p}P(A,N). \tag{6.6}$$

By comparing Eqs. (6.2), (6.3), and (6.6), one may naively think that integration over the area A leads to the removal of the δ-function constraint, thus causing us to study the partition function given by

$$Z(\Delta p,N)=\int d\mathbf{r}\; G(\mathbf{r},=\mathbf{r}_2=\mathbf{r},N|\Delta p), \tag{6.7}$$

where

$$G(\mathbf{r},\mathbf{r}',N|\Delta p)=\int_{\mathbf{r}(0)=\mathbf{r}}^{\mathbf{r}(N)=\mathbf{r}'} D[\mathbf{r}(\tau)]\exp\left\{-\frac{1}{l}\int_0^N d\tau\left(\frac{d\mathbf{r}}{d\tau}\right)^2+\frac{\Delta p}{2}\left|\int_0^N d\tau\left(x\,\frac{dy}{d\tau}-y\,\frac{dx}{d\tau}\right)\right|\right\}. \tag{6.8}$$

Calculations performed in Ref. 1 indicate that, at least for finite N,

$$\int_0^{N^2/4\pi} dA\; e^{A\,\Delta p}P(A,N)\neq Z(\Delta p,N). \tag{6.9}$$

Moreover, the lhs is finite for all finite values of N and Δp while the rhs can be even divergent (e.g., see the discussion about the rhs given in Ref. 44). Because, however, the average area given by (6.6), involves ratios, the infinities may not be so harmful. This is indeed the case for small enough Δp's [e.g., see Eq. (6.13) below].

In (5.2), the mean size of the tube $\sim a$ is defined. *Evidently, with the appropriate choice of* Δp *in (6.8) it is possible to claim that* $a^2\approx\langle A\rangle$. In the previous paper, Ref. 1, it was explicitly

demonstrated that the geometric area defined in (6.3) and the algebraic area [i.e., the same as in (6.3) but without the modulus sign] actually lead to the same kind of expressions for $Z(A,N)$. Because of this very important fact, many simplifications can be made. Indeed, using a representation of the propagator (6.8) in terms of eigenfunctions, e.g. see (2.4), one can rewrite (6.7) in the standard form of a partition function [e.g., see (4.4) of Ref. 1]:

$$Z(\Delta p,N)=\sum_{n=0}^{\infty} g_n e^{-N\epsilon_n}, \tag{6.10}$$

where g_n is the degeneracy factor. Whence, to calculate $Z(\Delta p,N)$ it is sufficient to know the energy levels ϵ_n and the degeneracy factors g_n. Both of these were calculated in Ref. 1 (and references therein) so that here I provide only the final result (e.g., see p. 3047 of Ref. 44),

$$Z(\Delta p,N)=\frac{x}{\sin x}, \tag{6.11}$$

where $x=(\Delta p/2)Nl$. The average area can be calculated now according to (6.6), i.e. one obtains

$$\langle A\rangle=\frac{1}{\Delta p}-\frac{Nl}{2}\cot\frac{\Delta p\ Nl}{2}. \tag{6.12}$$

For small Δp's this result can be simplified to

$$\langle A\rangle\simeq\tfrac{1}{12}\,\Delta p(Nl)^2\simeq\Delta p a^2 l^2, \tag{6.13}$$

and this result should be compared with Eq. (5.2).

Extension of the result (6.10) to curved manifolds is known in the mathematical literature[24,33] as a special case of Selberg's trace formula. For the constant ''magnetic'' field on compact Riemannian surfaces of genus g, this formula was obtained by many authors.[38,39,45–48] Whence, there is no need here to go into many details that can be found in the literature. Nevertheless, to facilitate the reader's understanding of this literature, it is essential to provide some key elements of these treatments, which are needed for proper understanding of the final new results presented in this section. The key general reference on Selberg's trace formula is the paper by McKean,[33] which is highly recommend for proper understanding of the subsequent material.

B. Automorphic forms and tensors on Riemannian surfaces

Traditionally, these subjects are known in physical literature in connection with the string theory[46] or with chaotic systems.[16,31,39] Here known results are used to study new physically relevant problems.

Following Ref. 47, the time-independent Schiödinger equation for the nonrelativistic particle of mass m, charge e ''living'' in the H plane in the presence of magnetic field B is given by

$$\left[-\frac{\hbar^2}{2m}y^2\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)-i\hbar\,\frac{eB}{m}\,y\,\frac{\partial}{\partial x}+\frac{e^2B^2}{2m}\right]\Psi_n=E_n\Psi_n. \tag{6.14}$$

This result should be compared with (5.10). The comparison indicates the different choice of gauge in (6.14), as compared to (5.10). The choice of gauge in (6.14) coincides with that suggested by Landau[1] for the analogous flat problem. Putting in (6.14), $\hbar=1=e$, with the rest of identifications the same as in (5.10) converts (6.14) into the corresponding polymer problem. In view of the discussion following Eqs. (3.2), (3.21), and (5.11), Eq. (6.14) can be rewritten as[40]

$$\left[-y^2\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)-2iby\,\frac{\partial}{\partial x}+b^2\right]\Psi_n=\epsilon_n\Psi_n, \tag{6.15}$$

where $\epsilon_n = 4R^2 E_n$. As was discussed in Ref. 40, on compact Riemannian manifolds, the ''magnetic'' field b can take only values prescribed by (5.21). For simplicity, only the case when b is integer is considered. A more general situation, when b is rational, is considered in Ref. 41. Such a restriction is fortunately not too severe because the result (5.12) is not affected by this limitation.

As in the planar case discussed in Ref. 3, it is convenient to introduce a complex variable $z = x + iy$ and to rewrite (6.15) in terms of z, taking into account that

$$\frac{\partial}{\partial \bar{z}} = \frac{1}{2}\left(\frac{\partial}{\partial x} - i\,\frac{\partial}{\partial y}\right) \quad \text{and} \quad \frac{\partial}{\partial z} = \frac{1}{2}\left(\frac{\partial}{\partial x} + i\,\frac{\partial}{\partial y}\right). \tag{6.16}$$

By definition, function $f(z)$ is automorphic if

$$f(\gamma z) = f(x), \tag{6.17}$$

where the product γz is defined in (4.2). The above definition can be extended by introducing the automorphic form of weight (p,q), with p,q being integers, via

$$f(\gamma z) = (cz + d)^p (c\bar{z} + d)^q f(z). \tag{6.18}$$

In this definition the phase factor is chosen to be equal to unity[44] and, whence, it is not explicitly written. Equation (6.18) allows one to define a scalar product in the Hibbert space, which is defined on H/Γ,[46–48] i.e. if f_1 and f_2 are two functions that have the property described by (6.18), then

$$\langle f_1 | f_2 \rangle = \int_{H/\Gamma} \frac{d^2 z}{y^2}\, y^p y^q \bar{f}_1 f_2. \tag{6.19}$$

Thus, the defined scalar product allows one to introduce an analog of the Fourier series, which in this case is called the Poincaré series. If function $h(z)$ is decaying at infinity fast enough, then any automorphic form of weight (p,q) can be presented in the form[46,48]

$$f_h(z,\bar{z}) = \sum_{\gamma \in \Gamma} (cz + d)^p (c\bar{z} + d)^q h(\gamma z). \tag{6.20}$$

C. Selberg trace formula

Using the results just obtained, let, in particular, $K_b^\tau(z,z')$ be a Riemann surface H/Γ analog of the density matrix ρ defined by (5.8), then, in view of (6.20), it can be presented in a form[47]

$$K_b^\tau(z,z') = \sum_{\gamma \in \Gamma} \left(\frac{c\bar{z}' + d}{cz' + d}\right)^b \left(\frac{z - \gamma \bar{z}'}{\gamma z' - \bar{z}}\right)^b g_b^\tau(z, \gamma z'), \tag{6.21}$$

where $g_b^\tau(z, \gamma z')$ has two parts: discrete (bound states) and continuous (scattering states).[24,33,48] For compact Riemann surfaces, the whole spectrum is, rigorously speaking, discrete,[24] nevertheless, the subdivision just described can be made anyway.[33,39,48] This is so because, as it is argued in Ref. 48, the ''truly discrete'' part of the spectrum remains *unchanged* for *both* compact and noncompact (e.g., leaky toruses[16]) Riemann surfaces. Use of the compact surfaces is more advantageous because it is easier to define the magnetic field B on such surfaces,[40] and, in addition, in this case B is quantized. The explicit form of g_b^τ is rather complicated in general.[45,47] In view of (6.10), it is more useful to calculate the Selberg trace given by

$$\theta(\tau) = \int_{H/\Gamma} \frac{d^2 z}{y^2}\, K_b^\tau(z,\bar{z})_{\text{discr}} = (g-1) \sum_{0 \leqslant n < b - 1/2} (2b - 2n - 1) e^{-\tau(2nb + b - n^2 - n)}, \tag{6.22}$$

where the last result is taken from Ref. 48 [e.g., see Eqs. (27)–(29) and (47)]. In view of Eq. (5.12), this result can be rewritten in the usual units as follows:

$$\theta(N)\simeq\frac{g-1}{4R^2}\sum_{0\leqslant n<b-1/2}(2BR^2-2n-1)\exp\{-NE_n\},\tag{6.23}$$

where E_n is the same as in Eq. (5.12).
For $R\to\infty$, and in view of (5.12), one obtains a standard flat plane result:[1,2]

$$\theta(N)\propto\frac{B}{\sin(BN/2)},\tag{6.24}$$

which is also in accord with (6.11) (up to an unimportant constant). For finite R, this is, of course, no longer true, so that a qualitative analysis of Sec. V can be used.

The result given by Eq. (6.23) provides justification to the semiclassical results, Eqs. (5.12) and (5.14), discussed in Sec. V. In addition, as a byproduct, one can easily obtain some results related to suppression of the first-order phase transitions on surfaces of constant negative curvature. Indeed, let $B\propto\Delta p$; then, according to Eq. (6.23) the droplet may exist only if $\Delta p\ R^2\geqslant\frac{3}{2}$ [since $\theta(N)$ cannot be negative]. For small enough R's the droplets can become more and more unstable and disappear by breaking into smaller and smaller pieces. This fact explains why even large spills of oil from tankers eventually disappear in a stormy sea (where R's are sufficiently small).

VII. DISCUSSION: THE INEVITABILITY OF THE QHE INTERPRETATION OF REPTATION THEORY

A polymer chain in the array of obstacles is traditionally believed to be an adequate model, which explains reptation.[4,6–10] Extension of this model presented in the previous sections is also able to explain (qualitatively) the transition from the reptation (facilitated by the tube formation) to the Rouse regime (which does not require the tube) in the way, which, at first sight, looks very different from that developed in Ref. 3. It is argued here that this is actually *not* the case and that the physical picture developed in this work is consistent with that presented earlier in Ref. 3.

A. Connection with the Calogero–Sutherland model

To begin, let us return once again to Eqs. (3.19) and (3.20). Let us recall that the distance element ds^2 on the sphere of constant radius R is given by $ds^2=R^2(d\theta^2+\sin^2\theta\,d\varphi^2)$. Analogously, for the pseudoshere (hyperboloid) the distance element is given by $ds^2=R^2(d\theta^2+\sinh^2\theta\,d\varphi^2)$. In terms of θ, φ coordinates, Eqs. (3.19) and (3.20) can now be rewritten as[26,31]

$$\left(\frac{1}{\sinh\theta}\frac{\partial}{\partial\theta}\left(\sinh\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sinh^2\theta}\frac{\partial^2}{\partial\varphi^2}\right)P(\theta,\varphi;\tau)=R^2\frac{\partial}{\partial\tau}P(\theta,\varphi;\tau).\tag{7.1}$$

Assuming, as before, that the distribution function P is φ independent, the above equation can be reduced to

$$\hat{L}P(x-x';\tau)\equiv\left(\frac{d^2}{dx^2}+\coth^2 x\frac{d}{dx}\right)P(x-x';\tau)=R^2\frac{\partial}{\partial\tau}P(x-x';\tau),\tag{7.2}$$

where $x\equiv\theta$. Evidently, the distribution function $P(x;\tau)$ can be found if the eigenvalue problem for the operator $\hat{L}$ is solved. In connection with this eigenvalue problem, let us consider now a seemingly unrelated eigenvalue problem related to the "particle" in the potential $q^2\sinh^{-2}x$, with q being some adjustable constant. This eigenvalue problem can be formulated, as usual, as

$$\hat{H}\varphi_n \equiv \left[-\frac{1}{2}\frac{d^2}{dx^2} + q^2 \sinh^{-2} x \right] \varphi_n = E_n \varphi_n . \tag{7.3}$$

If can be shown[49] that the function

$$\varphi_0 = (\sinh x)^{\mu} \tag{7.4}$$

is the solution of (7.3) with the eigenvalue $E_0 = -\mu^2 2$, provided that $\mu(\mu-1) = 2q^2$. This function is non-normalizable since it is increasing for $x \to \infty$. Whence, E_0 does not belong to the spectrum of the operator $\hat{H}$. Following Ref. 49, upon substitution of $\varphi_n = \varphi_0 \phi_n$ into (7.3), it is being converted into the equation

$$\hat{L}\phi_n = -(\mu^2 + n^2)\phi_n , \tag{7.5}$$

where the operator $\hat{L}$ is *the same* as in (7.2). Whence, (7.2) and (7.5) have *the same eigenfunctions*. The one-body Hamiltonian $\hat{H}$ defined by Eq. (7.3) can be easily generalized to the many-body case and is known in the literature as the Calogero–Sutherland (CS) Hamiltonian.[49,50] It is given by[51]

$$\hat{H}_{\mathrm{CS}} = -\sum_{i=1}^{n} \frac{1}{2}\frac{d^2}{dx_i^2} + \alpha \sum_{i<j}^{n} \frac{\omega^2}{\sinh^2(x_i - x_j)\omega}, \tag{7.6}$$

where n is the number of particles in the (one-dimensional!) system and α and ω are some constants. For $\omega \to 0$, Eq. (7.6) is known as the Calogero Hamiltonian.

To use the CS Hamiltonian in the reptation problem, several issues need to be resolved. First, (7.2) describes the ''motion'' of an individual primitive chain (so far in the absence of the ''magnetic field''). For noninteracting chains the total Hamiltonian should be evidently just a sum of one-body Hamiltonians. Therefore, naively, the total Hamiltonian $\hat{H}^T$ should look like

$$\hat{H}^T = \sum_{i=1}^{n} \left[-\frac{1}{2}\frac{d^2}{dx_i^2} + \frac{q^2}{\sinh^2 x_i} \right] + \hat{H}_{\mathrm{int}} . \tag{7.7}$$

Second, from Ref. 3, it is known, however, that the interaction between the tubes (cross sections) is of topological nature so that $\hat{H}_{\mathrm{int}}$ cannot have a small parameter and is to be considered as just a perturbation. Third, since the eigenvalue problem for the many-body CS Hamiltonian can be solved exactly,[50–52] the eigenvalues and eigenfunctions of this model are known. As was noticed already in Ref. 52, to find these eigenfunctions and eigenvalues it is sufficient to know only the two-body scattering phase shift. Because the two-body problem is always reducible to the one-body problem, we are effectively coming back to Eq. (7.3) [and, whence, to (7.2)]. More rigorous arguments explaining this fact can be found in Ref. 49. Fourth, as was rigorously demonstrated in Ref. 51 (also see Ref. 53), the wave functions of the CS and Knizhnik–Zamolodchikov (KZ) equations are practically the same. This fact was implicitly present already in Ref. 52. In Ref. 3 it was demonstrated that the Laughlin wave function [e.g., see Eq. (3.24) of Ref. 3] can be also obtained with help of the KZ equation [e.g., see Eqs. (5.2) and (5.3) of the same reference]. Whence, we are coming inevitably to the conclusion *that the CS Hamiltonian (perhaps with an extra quadratic term to account for the "magnetic" field[54]), can be also used to describe the interacting tube model developed in* Ref. 3. This statement provides a missing link between the results of Ref. 3 and that known from polymer physics.[4–10]

In Ref. 3 the Abelian variant of Chern–Simons quantum mechanics was actually discussed, while use of the KZ equation requires, in general, use of the non-Abelian quantum mechanics.[42,43] Nevertheless, as was already argued in Ref. 3, the actual final results do not change so that the

arguments presented above remain valid. Since the CS Hamiltonian is widely known in the theory of chaotic/disordered systems,[55,56] the results outlined above provide yet another application for the CS models.

B. Landau diamagnetism in the presence of impurities, and the topological origin of the robustness of the QHE: Applications to reptation

Consider once again a one ''electron'' problem described by the Hamiltonian given by (5.1). In the theory of QHE, such a type of problem with additional random potential $\hat{V}$ was known for some time. The most comprehensive solution of such a problem for various types of disorder was obtained in Ref. 57. This solution, however, ''does not illumine the question of robustness of the QHE. It does not either clarify what is exactly meant by localization in the presence of magnetic field'' (e.g., see p. 688 of Ref. 58).

The peculiarity of the situation is well summarized in the review paper by Pruisken.[13] On one hand, in the absence of a magnetic field, even in the presence of very weak disorder, all electronic states are localized in two dimensions, i.e. conductivity is zero. On another hand, in the presence of a rather strong magnetic field the conductivity reappears and, moreover, the value of Hall conductivity is *independent* of the degree of disorder.

Using polymer's language, the above situation can be restated as follows. In the absence of an area constraint, the propagator P_H given by (3.18) produces for the square of end-to-end distance (or the square of the radius of gyration), the result[9]

$$\langle R_g^2\rangle = \frac{z}{z-2}\,\frac{\sqrt{2\pi}}{8}\,l\sqrt{N}, \tag{7.8}$$

to be compared with the usual free Gaussian chain case: $\langle R_g^2\rangle = lN/6$. If time is identified with N, then the diffusion coefficient D in the last case can be estimated as $D\sim d\langle R_g^2\rangle/dN = \text{const}$, while in the first case $D\sim d\langle R_g^2\rangle/dN \sim 1/\sqrt{N}$. Because the diffusion and the conductivity are connected via the Einstein relation,[59] it is obvious that the result (7.8) leads to localization (i.e., an absence of ''conductivity''). At the same time, according to the main postulates of DDE reptation theory the statistics of the primitive path for large N should be Gaussian-like,[5,35] i.e. ''conduction'' should take place.

Using the results of Sec. IV, the following conclusions could be drawn. First, the classical motion of the fictitious particle in an Arnold-type billiard is chaotic. Moreover, the dynamical systems of such a type that evolve on surfaces of constant negative curvature are known as an Anosov type.[60] These Anosov-type systems are known to be robust with respect to perturbations.[30] Using the results of the appendix, it should be obvious that this robustness takes place in the ''quantum'' case too, because the short time asymptotic expansions are insensitive to the way the holes in the plane are distributed. Second, in Secs. V and VI, it was demonstrated that the presence of the ''magnetic'' field changes the propagator P_H (3.18) into that given by (6.21). The last one has both the scattering (''continuous'') and the bound (''discrete'') parts and the ''continuous'' part is *not* the same as that given by (3.18) (for more details, e.g., see Refs. 45 and 47). It would be of interest to calculate $\langle R_g^2\rangle$ using the continuous part of K_b^τ defined by (6.21). Even if one can succeed in doing so, the calculation cannot be considered as complete, because, so far, in the presentation given above the tube–tube interactions are not included. There is, however, a better way to look at the localization problem. It is discussed in the next section.

C. Related problems

The localization described above takes place for Gaussian (i.e., fully flexible) chains. If instead the Dirac chains[1] are used, then the localization no longer takes place, as was shown recently in the context of QHE in Ref. 61. The local rigidification of the initially flexible chains in

the polymer melt happens due to the topological and geometrical constraints.[62] In the context of the problems discussed in this paper, it would be necessary to study spinors and Dirac-type equations on Riemann surfaces.[63] These problems are similar to that studied in the theory of superstrings.[64] Connections between CS and $c=1$ conformal field theory were recently discussed in Ref. 65, while in Ref. 66 connections between CS and two-dimensional QCD were established. These results are also supported by the discovered connection between CS and two-dimensional Yang–Mills theory.[67]

Finally, the metric (3.15) is similar to that discussed in connection with the gravitational Aharonov–Bohm effect.[68,69] This observation is very helpful because of a wealth of accumulated knowledge about the gravitational analog of QHE.[70–73]

Note added: When this paper was completed, another two very important papers came to my attention. First, in the paper Gutkin[74] a very detailed connection between the polygonal billiards and the Riemannian surfaces is given, which is helpful for better understanding of Sec. IV. Second, another application of the ideas discussed in this work can be inferred from reading of the recently published Ref. 75.

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APPENDIX: SHORT TIME HEAT KERNEL EXPANSIONS AND THE CURVATURE EFFECTS

Although the spectrum of the heat equation in the plane is well known, it is much less known that the spectrum of the heat equation studied in the restricted polygonal domain with holes exhibits rather remarkable properties. Following Ref. 76, let us consider the simplest case of the heat equation for the propagator G, given by

$$\frac{\partial G}{\partial t}=\nabla_{\mathbf{r}}^2 G(\mathbf{r},\mathbf{r}',t), \tag{A1}$$

in a planar circular domain Ω. Define now the trace of G via

$$\theta(t)=\int\int_{\Omega} d\mathbf{r}\; G(\mathbf{r},\mathbf{r},t), \tag{A2}$$

then for small t it can be shown that $\theta(t)$ is given by the following universal expansion:

$$\theta(t)\simeq\frac{|\Omega|}{4\pi t}-\frac{L}{8(\pi t)^2}+\frac{1}{6}+O(t^{1/2}), \tag{A3}$$

where $|\Omega|$ is the area of a circular domain while L is the total perimeter length. In case if, instead of a circular domain, we would choose an annulus (i.e., a circular domain with a hole) then, it could be shown that

$$\theta(t)\simeq\frac{|\Omega|}{4\pi t}-\frac{L}{8(\pi t)^2}-\frac{1}{6}+O(t^{1/2}). \tag{A4}$$

The change is sign [$\frac{1}{6}$ in (A3) vs $-\frac{1}{6}$ in (A4)] has a profound effect. Indeed, already Kac[77] has shown that for small t's and ''smooth'' polygons with r holes one can write the following asymptotic result:

$$\theta(t) \simeq \frac{|\Omega|}{4\pi t} - \frac{L}{8(\pi t)^{1/2}} + \frac{1}{6}(1-r) + O(t^{1/2}), \tag{A5}$$

so that for $r=0$ we obtain (A3) while for $r=2$ we obtain (A4). Following McKean and Singer,[78] it can be shown that for smooth Riemannian open two-dimensional manifolds with a compact one-dimensional boundary, the short time asymptotic expansion of $\theta(t)$ is given by

$$\theta(t) \simeq \frac{|\Omega|}{4\pi t} - \frac{L}{8(\pi t)^{1/2}} + \frac{1}{6}(1-g) + O(t^{1/2}), \tag{A6}$$

where g is the number of handles (or genus) of the surface. Whence, by comparing (A5) and (A6), one is led to the conclusion that Arnold's billiard, discussed in Sec. IV, at least locally, behaves as the Riemannian surface of genus two, as claimed in the main text.

Following Dowker,[20] it is also instructive to consider a propagator for a planar regular triangular lattice of obstacles. For such an array of obstacles the short time asymptotic expansion of $\theta(t)$ is given by

$$\theta(t) \simeq \frac{|\Omega|}{4\pi t} \pm \frac{1}{2}. \tag{A7}$$

This result cannot be compared directly with that given by (A6). Instead, another formula by McKean and Singer[78] should be used:

$$\theta(t) \simeq \frac{\text{area}}{4\pi t} + \frac{1-h}{3}, \tag{A8}$$

which is valid for smooth manifolds without a boundary. Comparison between (A7) and (A8) indicates that $h \approx 2$. A more accurate comparison is not possible, unfortunately, in view of some minor errors in Dowker's work, (e.g., see Ref. 22 for a more complete analysis).

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On a nonlinear stationary problem arising in transport theory

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In this article a nonlinear one-dimensional stationary transport equation with general boundary conditions is considered where an abstract boundary operator relates the incoming and the outgoing fluxes. Existence results are proved in the case where the collision operator is of the Hammerstein type. In particular, it is shown that these results remain valid for multidimensional geometry with vacuum boundary conditions. Sufficient conditions are given in terms of collision frequency and scattering kernel assuring the existence and uniqueness of solutions. The article ends with the discussion of the case of multiplying boundary conditions. © *1996 American Institute of Physics.* [S0022-2488(95)00607-6]

I. INTRODUCTION

In this article we are concerned with the existence and uniqueness results of the transport equation

$$\xi \frac{\partial \psi}{\partial x}(x,\xi)+\sigma(x,\xi,\psi(x,\xi))+\lambda\psi(x,\xi)=\int_{-1}^{1}\kappa(x,\xi,\xi',\psi(x,\xi'))d\xi' \tag{1.1}$$

under general boundary conditions where $x\in[-a,\ a]$ for a parameter $0<a<\infty$ and $\xi\in[-1,1]$. This equation describes the transport of particles (neutrons, photons, molecules of gas, etc.) in a plane parallel domain with a width of $2a$ mean free paths. The unknown of this equation is a scalar function $\psi(x,\xi)$ which represents the number (or probability) density of gas particles having the position x and the direction cosine of propagation ξ. (The variable ξ may be thought of as the cosine of the angle between the velocity of particles and the x-direction.) The functions $\sigma(.,.,.)$ and $\kappa(.,.,.,.)$ are nonlinear functions of ψ and are called, respectively, the collision frequency and the scattering kernel.

The transport equation was considered in different fields of mathematical physics to describe transport processes of particles. Thus, in kinetic theory of gas where we must describe the interaction of gas molecules with the solid walls bounding the region where the gas flows, the theoretical problem is to relate the distribution function of molecules leaving a solid surface to the distribution of the molecules arriving at the same surface. However, the boundary conditions which describe this interaction are very complex because the reaction of a gas molecule with a wall is so complicated and determined by many competing factors as to appear random and then their mathematical precise formulation is very controversial (c.f. Ref. 1). Nevertheless, a model which is often used consists of supposing that a part of the outgoing flux is re-emitted in a deterministic way (specular reflexion), whereas the other part is re-emitted in random directions (diffuse reflections).

In our framework, the boundary conditions are modeled by

$$\psi_{|\Gamma^-}=H\psi_{|\Gamma^+}, \tag{1.2}$$

where Γ^- (resp. Γ^+) is the incoming (resp. outgoing) part of the phase space boundary, $\psi_{|\Gamma^-}$ (resp. $\psi_{|\Gamma^+}$) is the restriction of ψ to Γ^- (resp. Γ^+), and H is a linear bounded operator from a suitable

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function space on Γ^+ to a similar one on Γ^-. The known classical boundary conditions (vacuum boundary, specular reflections, periodic, diffuse reflexions, generalized and mixed type boundary conditions[2–6]) are special examples of our general framework.

The purpose of the present article is to discuss the *existence and uniqueness* results of the equation (1.1) supplemented with *general boundary conditions* (1.2) in one-dimensional geometry where an abstract boundary operator H relates the outgoing flux to the incoming one. We recall that for linear transport equation the existence and uniqueness theory is well known in a general context (see, for instance, Ref. 7 or 8, Ch. 11 and 12).

For purely absorbing walls, i.e., $H=0$, this problem has been considered by C. V. Pao,[9] in the space of continuous functions. In Sec. IV we extend Pao's results to general boundary conditions and Lp-spaces in one-dimensional context.

To conclude this Introduction let us briefly discuss the content of this paper. We start with a preliminary part (Sec. II) where we fix the different notations and introduce the function spaces used in the sequel. Thus, we define the streaming operator and the boundary conditions in a rather general setting and present some preliminary results. In Sec. III we investigate the boundary value problem (1.1)–(1.2) in the case where $\sigma(.,.,.)=0$ and $\kappa(x,\xi,\xi',\psi(x,\xi'))=k(\xi,\xi')f(\xi,\xi',\psi(x,\xi'))$. Existence results are given (Theorems 3.1, 3.2, 3.5, and 3.6) for a large class of scattering kernels $k(.,.)$ and functions $f(.,.,.)$. The multidimensional case is also considered with purely absorbing walls. The analysis is *essentially based on new compactness* results obtained in Refs. 10 and 11 and Schauder's fixed point theorem. Section IV is devoted to the existence and uniqueness results for the problem (1.1)–(1.2). The main results of this section are Theorems 4.1 and 4.2 (where the global and the local problems are considered). In Sec. V, we discuss briefly how to extend the results of Secs. III and IV to multiplying boundary conditions.

II. CHOICE OF FUNCTIONAL FRAMEWORK

We shall treat the problem (1.1)–(1.2) in the following functional setting.

Now let $X_p:=L_p[(-a,a)\times(-1,1),dxd\xi]$, $1\leqslant p<\infty$, and

$$X_p^o:=L_p[\{-a\}\times(-1,0),|\xi|d\xi]\times L_p[\{a\}\times(0,1),|\xi|d\xi]:=X_{1,p}^o\times X_{2,p}^o$$

equipped with the norm:

$$\|\psi^o;X_p^o\|=[\|\psi_1^o;X_{1,p}^o\|^p+\|\psi_2^o;X_{2,p}^o\|^p]^{1/p}=\left[\int_{-1}^0|\psi(-a,\xi)|^p|\xi|d\xi+\int_0^1|\psi(a,\xi)|^p|\xi|d\xi\right]^{1/p};$$

$$X_p^i:=L_p[\{-a\}\times(0,1),|\xi|d\xi]\times L_p[\{a\}\times(-1,0),|\xi|d\xi]:=X_{1,p}^i\times X_{2,p}^i$$

equipped with the norm:

$$\|\psi^i;X_p^i\|=[\|\psi_1^i;X_{1,p}^i\|^p+\|\psi_2^i;X_{2,p}^i\|^p]^{1/p}=\left[\int_0^1|\psi(-a,\xi)|^p|\xi|d\xi+\int_{-1}^0|\psi(a,\xi)|^p|\xi|d\xi\right]^{1/p}.$$

We define the partial Sobolev space W_p by

$$W_p=\left\{\psi\in X_p \quad \text{such that} \quad \xi\frac{\partial\psi}{\partial x}\in X_p\right\}.$$

It is well known that any function ψ in W_p has traces on $\{-a\}$ and $\{a\}$ in X_p^o and X_p^i (see Ref. 7 or 8). They are denoted, respectively, by ψ^o and ψ^i and represent the outgoing and the incoming fluxes (''o'' for outgoing and ''i'' for incoming).

Let H be the following boundary operator:

$$\begin{cases} H: X_p^o \to X_p^i, \\ u \to Hu, \\ Hu = \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}, \end{cases}$$

where $H_{11} \in \mathscr{L}(X_{1,p}^o; X_{1,p}^i)$, $H_{12} \in \mathscr{L}(X_{2,p}^o; X_{1,p}^i)$, $H_{21} \in \mathscr{L}(X_{1,p}^o; X_{2,p}^i)$ and $H_{22} \in \mathscr{L}(X_{2,p}^o; X_{2,p}^i)$.

We define the free streaming operator T_H by

$$\begin{cases} T_H: D(T_H) \subset X_p \to X_p, \\ \psi \to T_H \psi(x,\xi) = -\xi \dfrac{\partial \psi}{\partial x}(x,\xi), \\ D(T_H) = \{\psi \in W_p \quad \text{such that} \quad H\psi^o = \psi^i\}, \end{cases}$$

where $\psi^o = (\psi_1^o, \psi_2^o)[resp. \psi^i = (\psi_1^i, \psi_2^i)]$ is in X_p^o (resp. X_p^i).

It is well known (see Ref. 10, Section 1) that for $\|H\| \leqslant 1$, $\{\lambda \in \mathbf{C}/\mathrm{Re}\,\lambda > 0\} \subset \rho(T_H)$, where $\rho(T_H)$ stands for the resolvent set of T_H. For more informations concerning the operator T_H we refer to Ref. 10.

We end this section by giving an elementary estimate which plays an essential role in the proofs of the results discussed below.

Proposition 2.1: Assume that $\|H\| \leqslant 1$. Then, for all λ such that $\mathrm{Re}\,\lambda > 0$, we have

$$\|(\lambda - T_H)^{-1}\| \leqslant \frac{1}{\mathrm{Re}\,\lambda}. \tag{2.1}$$

◇

For the reader's convenience, let us first recall the following:

Let X be an arbitrary real or complex Banach space; X^* denotes its dual space. For each $x \in X$ define

$$\mathscr{T}(x) = \{x^* \in X^* : \|x^*\|^2 = \|x\|^2 = \langle x, x^* \rangle\}.$$

Let $x \in X$, $\mathscr{T}(x)$ is nonempty by Hahn–Banach theorem. A linear operator A with domain and range both in X is called dissipative if for every $x \in D(A)$ there is a $x^* \in \mathscr{T}(x)$ such that $\mathrm{Re}\langle Ax, x^* \rangle \leqslant 0$.

Let (Ω, Σ, μ) be a measure space and $X = L_p(\Omega, \Sigma, d\mu)$ with $(1 \leqslant p < \infty)$, $\mathscr{T}(0) = \{0\}$ and for $0 \neq u \in X$, $\mathscr{T}(u)$ has solely one element, that is,

$$\mathscr{T}(u) = \{\|u\|^{2-p} |u|^{p-2} u\} \quad \text{for } 1 < p < \infty.$$

For $p = 1$, in order to show the dissipativity of the operator A it is sufficient to show that $\mathrm{Re}\langle Au, s_0(u) \rangle \leqslant 0$ for all u in $D(A)$ where

$$s_0(u)(x) = \begin{cases} 1 & \text{when } u(x) > 0, \\ 0 & \text{when } u(x) = 0, \\ -1 & \text{when } u(x) < 0. \end{cases}$$

Proof of Proposition 2.1: Let us first show that T_H is dissipative on X_p for $p \in [1, \infty)$. To this end we treat separately the cases $p = 1$ and $1 < p < \infty$.

(i) Let $1 < p < \infty$ and consider $\psi \in D(T_H)$; we have

$$\langle T_H\psi, |\psi|^{p-2}\psi\rangle = \int_{-a}^{a}\int_{-1}^{1} |\psi|^{p-2}\psi\left(-\xi\frac{\partial\psi}{\partial x}\right)(x,\xi)dxd\xi.$$

Taking into account the fact that $\xi(\partial/\partial x)(|\psi|^p)=p|\psi|^{p-2}\psi\xi(\partial\psi/\partial x)$, we may write

$$\langle T_H\psi, |\psi|^{p-2}\psi\rangle = -\frac{1}{p}\int_{-a}^{a}\int_{-1}^{1}\xi\frac{\partial}{\partial x}(|\psi|^p)dxd\xi = \frac{1}{p}[\|\psi^i\|^p_{X_p^i} - \|\psi^0\|^p_{X_p^0}] \leq 0 \quad \text{(because } \|H\|\leq 1\text{)}.$$

(ii) Consider now the case $p=1$. Let $\psi\in D(T_H)$; then we have

$$\begin{aligned}\langle T_H\psi, s_0(\psi)\rangle &= -\int_{-a}^{a}\int_{-1}^{1}\xi\frac{\partial}{\partial x}(\psi)(x,\xi)s_0(\psi)(x,\xi)dxd\xi \\ &= -\int_{-a}^{a}\int_{-1}^{1}\xi\frac{\partial}{\partial x}|\psi|dxd\xi = [\|\psi^i\|_{X_1^i} - \|\psi^0\|_{X_1^0}] \leq 0 \quad \text{(because } \|H\|\leq 1\text{)}.\end{aligned}$$

Therefore, one concludes that T_H is dissipative on $X_p(1\leq p<\infty)$.

Now, consider $\psi\in D(T_H)$ and let $\varphi=\lambda\psi-T_H\psi$ (Re $\lambda>0$):

$$\begin{aligned}\text{Re }\lambda\|\psi\|^2 = \text{Re }\lambda\langle\psi,\psi^*\rangle &= \text{Re}(\lambda\langle\psi,\psi^*\rangle) \\ &\leq \text{Re}[\lambda\langle\psi,\psi^*\rangle - \langle T_H\psi,\psi^*\rangle] \quad \text{(because } T_H \text{ is dissipative)} \\ &= \text{Re}\langle\varphi,\psi^*\rangle \leq \|\varphi\|\|\psi\|.\end{aligned}$$

Consequently, $\|\psi\|\leq\|\varphi\|/\text{Re }\lambda$, which completes the proof. Q.E.D.

III. TRANSPORT EQUATIONS INVOLVING HAMMERSTEIN OPERATORS

Here and throughout this article, we use the definitions and notations introduced above. As stated in the Introduction we shall prove several existence results for the problem (1.1)–(1.2) in the situation where $\sigma(.,.,.)=0$ and $\kappa(x,\xi,\xi',\psi(x,\xi'))=k(\xi,\xi')f(\xi,\xi',\psi(x,\xi'))$. The functions $k(.,.)$ and $f(.,.,.)$ will be made precise below. Our analysis is essentially based on new compactness results obtained in Refs. 10–12.

A. Slab geometry

In this paragraph we assume that the boundary operator H satisfies the estimate $\|H\|\leq 1$. Let us consider the following boundary value problem:

$$\begin{cases}\lambda\psi+\xi\dfrac{\partial\psi}{\partial x}(x,\xi) = \displaystyle\int_{-1}^{1}k(\xi,\xi')f(x,\xi',\psi(x,\xi'))d\xi', \\ \psi^i = H(\psi^0), \quad \text{Re }\lambda>0,\end{cases} \tag{3.1}$$

where $x\in[-a,\ a]$, ξ and $\xi'\in[-1,\ 1]$ while f is a measurable function defined by

$$\begin{cases} f:\Omega\times\mathbf{C}\to\mathbf{C}, \\ (t,u)\to f(t,u)\end{cases}$$

with $\Omega=[-a,\ a]\times[-1,\ 1]$. We denote by K the linear bounded operator

$$\begin{cases} K: X_p \to X_p, \\ \psi \to \displaystyle\int_{-1}^{1} k(\xi,\xi')\psi(x,\xi')d\xi', \end{cases}$$

where the scattering kernel $k:(-1,1)\times(-1,1)\to\mathbf{R}$ is assumed to be measurable.

Let $r>0$; we denote by S_r the ball $S_r = \{\psi \in X_p, \|\psi\|_{X_p} \leqslant r\}$.

For our subsequent analysis, the following definitions are required.

Definition 3.1:[12] A bounded operator K, defined as above, is said to be regular if its restriction to $L_p(-1,1)$ is compact. ◇

Definition 3.2: We say that $f:\Omega\times\mathbf{C}\to\mathbf{C}$ satisfies the Carathéodory conditions (C) provided that

$$(C) \quad \begin{cases} t \to f(t,u) & \text{is measurable on } \Omega \text{ for all } u \in \mathbf{C}, \\ u \to f(t,u) & \text{is continuous on } \mathbf{C} \text{ for almost all } t \in \Omega. \end{cases}$$

◇

If f satisfies the Carathéodory condition, then we define an operator $\mathscr{N}$, called the Nemytskii operator on the set of functions $\psi:\Omega\to\mathbf{C}$ by $(\mathscr{N}\psi)(x,\xi)=f(x,\xi,\psi(x,\xi))$ for every $(x,\xi)\in\Omega$.

In Lp-spaces, the Nemytskii operator has been extensively studied (cf., e.g., Ref. 13 and the bibliography therein). We now quote a result (Proposition 3.1) which states a basic fact for the theory of these operators in Lp-spaces.

Proposition 3.1: (Ref. 14, p. 35) If the operator $\mathscr{N}$ acts from $L_p(\Omega)$ to $L_q(\Omega)$ with $1\leqslant q<\infty$, then $\mathscr{N}$ is continuous and takes bounded sets into bounded sets. ◇

Throughout this subsection we suppose

$$\begin{cases} K \text{ is regular on } X_p, \\ 1<p<\infty, \\ f \text{ satisfies the condition } (C). \end{cases}$$

Theorem 3.1: Suppose that the operator $\mathscr{N}$ acts from X_p into X_p. Then for each $r>0$ there is $\lambda_0>0$ such that the problem (3.1) has at least one solution on S_r for all λ satisfying $\mathrm{Re}\,\lambda>\lambda_0$. ◇

Proof: Let λ be a complex number. It is clear that if $\mathrm{Re}\,\lambda>0$, $\lambda\in\rho(T_H)$ (cf. Sec. II) and consequently, the problem (3.1) may be transformed into

$$\begin{cases} \psi = F(\lambda)\psi, \\ \psi^i = H(\psi^0), \end{cases}$$

where $F(\lambda)=(\lambda-T_H)^{-1}K\mathscr{N}$.

Let $r>0$. According to (2.1) and the Proposition 3.1 we obtain for every $\psi\in S_r$

$$\|F(\lambda)\psi\| \leqslant \|(\lambda-T_H)^{-1}\|\|K\|\|\mathscr{N}(\psi)\| \leqslant \frac{\|K\|M(r)}{\mathrm{Re}\,\lambda}, \tag{3.2}$$

where $M(r)$ denotes the upper bound of $\mathscr{N}$ on S_r. Hence, by setting $\lambda_0=\|K\|M(r)/r$, for $\mathrm{Re}\,\lambda>\lambda_0$, (3.2) shows that $F(\lambda)$ maps S_r into itself. On the other hand, Proposition 3.1 and Ref. 10, Theorem 2.1, imply that $F(\lambda)$ is completely continuous on S_r. Now, by using Schauder's theorem, one concludes that $F(\lambda)$ has at least one fixed point $\psi^*\in D(T_H)\cap S_r$ and the proof is complete. Q.E.D.

The next corollary is a slightly more general form of the previous theorem.

Corollary 3.1: Suppose that there is a positive number α and a measurable function $\beta:\Omega\to[0,\infty)$ in X_p such that

$$|f(x,\xi,\psi(x,\xi))|\leqslant|\beta(x,\xi)|+\alpha|\psi(x,\xi)| \quad \forall(x,\xi)\in\Omega \text{ and } \psi\in X_p. \tag{3.3}$$

Then for each $r>0$ there is $\lambda_0>0$ such that the problem (3.1) has at least one solution on S_r for all λ satisfying $\mathrm{Re}\,\lambda>\lambda_0$. ◇

Proof: Thanks to (3.3), $\mathscr{N}$ is continuous on X_p and takes bounded sets into bounded sets (cf. Ref. 14, Theorem 5.2, p. 35). Now the rest of the proof may be sketched in a similar way to that of the Theorem 3.1. The details are therefore omitted. Q.E.D.

Remark 3.1: The hypothesis (3.3) is a sufficient condition which guarantees that $\mathscr{N}$ is continuous and bounded from X_p into X_p. In fact, this condition is not only sufficient but also necessary for $\mathscr{N}$ to map X_p into X_p (see, for instance, Ref. 14, p. 35). ◇

Theorem 3.2: Suppose that f satisfies the condition (3.3). Then for each $r>0$ and $\lambda\in\rho(T_H)$ there is $\mu>0$ such that the problem

$$\begin{cases} \lambda\psi+\xi\dfrac{\partial\psi}{\partial x}(x,\xi)=\mu\displaystyle\int_{-1}^{1}k(\xi,\xi')f(x,\xi',\psi(x,\xi'))d\xi', \\ \\ \psi^i=H(\psi^0) \end{cases} \tag{3.4}$$

has at least one solution $\psi^*\in D(T_H)\cap S_r$ verifying $\|\psi^*\|=r$. ◇

Proof: As in Corollary 3.1, $\mathscr{N}$ is continuous on X_p and maps bounded sets into bounded sets. This together with Ref. 10, Theorem 2.1, implies that the map $F(\lambda):=(\lambda-T_H)^{-1}K\mathscr{N}$ is completely continuous on X_p. Let $r>0$ and denote by

$$G(\psi)=\begin{cases} r\dfrac{F(\lambda)(\psi)}{\|F(\lambda)(\psi)\|} & \text{if } \psi\in S_r \text{ and } F(\lambda)(\psi)\neq 0, \\ 0 \quad \text{if } \psi\in S_r \text{ and } F(\lambda)(\psi)=0. \end{cases}$$

G is also completely continuous and takes the convex set S_r into itself. Hence by Schauder's theorem G has a fixed point ψ^*, i.e., $G\psi^*=\psi^*$. Clearly, $\|\psi^*\|=r$. Setting $\mu=r/\|F(\lambda)\psi^*\|$, we obtain $(\lambda-T_H)^{-1}K\mathscr{N}(\psi^*)=\mu^{-1}\psi^*$. Consequently, $\psi^*\in D(T_H)\cap S_r^+$ and

$$\lambda\psi^*+\xi\frac{\partial\psi^*}{\partial x}(x,\xi)=\mu\int_{-1}^{1}k(\xi,\xi')f(x,\xi',\psi^*(x,\xi'))d\xi',$$

which achieves the proof. Q.E.D.

The remainder of this section is devoted to the existence of positive solutions of the problem (3.1). Let X_p^+ denote the positive cone of the Banach space X_p. A bounded operator $A:X_p\to X_p$ is called positive if and only if $A(X_p^+)\subset X_p^+$ (and also if and only if $\psi\leqslant\varphi$ implies $A\psi\leqslant A\varphi$).

Let us now assume the positivity of the boundary operator H. As a consequence of this assumption the operator $(\lambda-T_H)^{-1}$ is positive on X_p for all $\lambda>0$ (cf. Ref. 10, p. 57). Finally, for all $r>0$, we define the set S_r^+ by $S_r^+:=S_r\cap X_p^+$.

Theorem 3.3: Suppose that K is positive and $\mathscr{N}$ acts from X_p into X_p with $\mathscr{N}(X_p^+)\subset X_p^+$. Then for each $r>0$ there is $\lambda_0>0$ such that the problem (3.1) has at least one solution on S_r^+ for all $\lambda>\lambda_0$. ◇

In the same way, we have also the following.

Theorem 3.4: Suppose that K is positive and $\mathscr{N}$ acts from X_p into X_p with $\mathscr{N}(X_p^+)\subset X_p^+$. Then for each $r>0$ and $\lambda>0$ there is $\mu>0$ such that the problem (3.4) has at least one solution $\psi^*\in D(T_H)\cap S_r^+$ verifying $\|\psi^*\|=r$. ◇

The proof of the Theorem 3.3 (resp. Theorem 3.4) may be modeled very closely after the proof of the Theorem 3.1 (resp. Theorem 3.2). We replace solely the set S_r by S_r^+ and $\lambda \in \rho(T_H)$ by $\lambda > 0$.

B. Multidimensional geometry

In this paragraph we shall show that the results of the previous subsection are also valid for multidimensional geometry with vacuum boundary conditions, $H=0$. In fact, the free-streaming operator T_0 (i.e., $H=0$) is defined by

$$\begin{cases} T_0 : D(T_0) \subset L_p(D\times V) \to L_p(D\times V), \\ \psi \to T_0\psi(x,v) = -v\,\dfrac{\partial \psi}{\partial x}(x,v), \\ D(T_0) = \left\{ \psi \in L_p(D\times V) \;\Big/\; v\,\dfrac{\partial \psi}{\partial x} \in L_p(D\times V), \psi_{|\Gamma^-} = 0 \right\}, \end{cases}$$

$(x,v) \in D\times V$, where the configuration space D is an open and bounded subset of R^N, $N \geqslant 1$, the velocity space V is an arbitrary open subset of R^N while the set Γ^- is given by $\Gamma^- = \{(x,v) \in \partial D \times V / v \text{ is ingoing at } x \in \partial D\}$, and finally $\psi_{|\Gamma^-}$ denotes the restriction of ψ to Γ^-.

It is well known that $\rho(T_0) \supset \{\lambda \in \mathbf{C}/\mathrm{Re}\,\lambda > 0\}$ and for $\mathrm{Re}\,\lambda > 0$, $\|(\lambda - T_0)^{-1}\| \leqslant 1/\mathrm{Re}\,\lambda$ (see, for instance, Ref. 7 or 12).

Now we consider the problem

$$\begin{cases} \lambda\psi + v\,\dfrac{\partial \psi}{\partial x}(x,v) = \displaystyle\int_V k(v,v')f(x,v',\psi(x,v'))dv', \\ \psi_{|\Gamma^-} = 0, \quad \mathrm{Re}\,\lambda > 0, \end{cases} \tag{3.5}$$

where f is defined as in the previous paragraph with $\Omega = D\times V$. The function $k(.,.)$ is the kernel of a bounded operator K defined on $L_p(D\times V)$ by $\psi \to \int_V k(v,v')\psi(x,v')dv'$. *We assume that the restriction of K to $L_p(V)$ is compact*.

Theorem 3.5: Suppose that the operator $\mathscr{N}$ acts from $L_p(D\times V)$ into $L_p(D\times V)$. Then for each $r>0$ there is $\lambda_0 > 0$ such that the problem (3.5) has at least one solution on S_r for all λ satisfying $\mathrm{Re}\,\lambda > \lambda_0$. ◇

Proof: Note that for λ such that $\mathrm{Re}\,\lambda > 0$ the problem (3.5) may be transformed into

$$\psi = F(\lambda)\psi, \quad \psi_{|\Gamma^-} = 0,$$

with $F(\lambda) = (\lambda - T_H)^{-1} K\mathscr{N}$.

The remainder of the proof is similar to that of Theorem 3.1. We must solely replace Ref. 10, Theorem 2.1, by Ref. 12, Lemma 2.1. ◇

Again by using Ref. 12, Lemma 2.1, and following the same strategy as in the proof of Theorem 3.2, we can establish the following result:

Theorem 3.6: Suppose that f fulfills the condition (3.3). Then for each $r>0$ and $\lambda \in \rho(T_0)$, there is $\mu > 0$ such that the problem

$$\begin{cases} \lambda\psi + v\,\dfrac{\partial \psi}{\partial x}(x,v) = \mu \displaystyle\int_v k(v,v')f(x,v',\psi(x,v'))dv', \\ \psi_{|\Gamma^-} = 0, \end{cases} \tag{3.6}$$

has at least one solution $\psi^* \in D(T_0) \cap S_r$ verifying $\|\psi^*\| = r$. ◇

It is well known that T_0 generates a positive strongly continuous semigroup on $L_p(D \times V)$ (cf. Ref. 12), so $(\lambda - T_0)^{-1}$ is a positive operator on $L_p(D \times V)$. If, further, we suppose that K and $\mathscr{N}$ are also positive on $L_p(D \times V)$. Then the use of Ref. 12, Lemma 2.1, together with Schauder's theorem and the reasoning above makes it easy to deduce the following corollary.

Corollary 3.2: Let r be a real number satisfying $r > 0$. Then

(i) there is $\lambda_0 > 0$ such that the problem (3.5) has at least one solution on S_r^+ for all λ satisfying $\mathrm{Re}\,\lambda > \lambda_0$, and

(ii) for any $\lambda > 0$ there is $\mu > 0$ such that the problem (3.6) has at least one solution $\psi^* \in D(T_0) \cap S_r$ verifying $\|\psi^*\| = r$. ◇

We close this section by pointing out that the results obtained in this section are open for $p = 1$.

IV. EXISTENCE AND UNIQUENESS RESULTS

Consider again the problem (1.1)–(1.2) which can be rewritten as

$$\begin{cases} (\lambda - T_H)\psi(x,\xi) = f(x,\xi,\psi(x,\xi)), \\ \psi \in D(T_H), \quad \mathrm{Re}\,\lambda > 0, \end{cases} \tag{4.1}$$

where

$$\begin{cases} f(x,\xi,\psi) = f_1(x,\xi,\psi) + f_2(x,\xi,\psi), \\ f_1(x,\xi,\psi) = -\sigma(x,\xi,\psi(x,\xi)), \\ f_2(x,\xi,\psi) = \displaystyle\int_{-1}^{1} \kappa(x,\xi,\xi',\psi(x,\xi'))\,d\xi'. \end{cases} \tag{4.2}$$

In the following, we shall give some sufficient conditions on the functions $\sigma(.,.,.)$ and $\kappa(.,.,.,.)$ which guarantee the existence of a unique solution of the problem (4.1). To this purpose, we make the following assumptions.

(H_1): $\sigma(x,\xi,\psi)$ is defined for $x \in [-a, a]$, $\xi \in [-1, 1]$, $\psi \in X_p$ with values in X_p, and there is a function $\rho(x,\xi)$ satisfying

$$\rho_1 := \operatorname*{ess-sup}_{(x,\xi) \in [-a,\, a] \times [-1,\, 1]} |\rho(x,\xi)| < \infty,$$

such that

$$|\sigma(x,\xi,\psi_1) - \sigma(x,\xi,\psi_2)| \leqslant |\rho(x,\xi)|\,|\psi_1 - \psi_2| \quad \text{for all } \psi_1, \psi_2 \text{ in } X_p. \tag{4.3}$$

(H_2): $\kappa(x,\xi,\xi',\psi)$ is defined for $x \in [-a, a]$, $\xi,\ \xi' \in [-1, 1]$, $\psi \in X_p$ with values in $L_p([-a, a] \times [-1, 1] \times [-1, 1], dx\,d\xi\,d\xi')$, and there exists a function $\chi(x,\xi,\xi')$ satisfying

$$\chi_1 := \left\{ \int_{-1}^{1} \operatorname*{ess-sup}_{x \in [-a,a]} \left(\int_{-1}^{1} |\chi(x,\xi,\xi')|^q d\xi' \right)^{p/q} \right] d\xi \Bigg\}^{1/p} < \infty \quad \text{for } 1 < p < \infty,$$

$$\chi_2 := \left\{ \int_{-1}^{1} \left(\operatorname*{ess-sup}_{x \in [-a,a], \xi \in [-1,1]} |\chi(x,\xi,\xi')| \right) d\xi \right\} < \infty \quad \text{if } p = 1,$$

such that

$$|\kappa(x,\xi,\xi',\psi_1)-\kappa(x,\xi,\xi',\psi_2)|\leqslant|\chi(x,\xi,\xi')||\psi_1-\psi_2| \quad \text{for all } \psi_1,\psi_2 \text{ in } X_p. \tag{4.4}$$

Under the hypotheses (H_1) and (H_2) we may define a mapping F from X_p into itself by

$$(F\psi)(x,\xi)=f(x,\xi,\psi(x,\xi)) \quad \forall\,\psi\in X_p, \tag{4.5}$$

where f is defined in (4.2). The following lemma shows that F is Lipschitz continuous in X_p.

Lemma 4.1: Assume that (H_1) and (H_2) hold. Then the mapping F satisfies

$$\|F(\psi_1)-F(\psi_2)\|_{X_p}\leqslant 2[(\rho_1)^p+(\chi_1)^p]^{1/p}\|\psi_1-\psi_2\|_{X_p} \quad \text{for all } \psi_1,\psi_2 \text{ in } X_p \tag{4.6}$$

$(1<p<\infty)$ and

$$\|F(\psi_1)-F(\psi_2)\|_{X_1}\leqslant(\rho_1+\chi_2)\|\psi_1-\psi_2\|_{X_1} \quad \text{for all } \psi_1,\psi_2 \text{ in } X_1 \text{ for } p=1. \tag{4.7}$$

Proof: Let ψ_1 and ψ_2 be two elements of X_p. Using (4.5) we may write

$$|F(\psi_1)(x,\xi)-F(\psi_2)(x,\xi)|=|f(x,\xi,\psi_1)-f(x,\xi,\psi_2)|.$$

Now, by (H_1) and (H_2) we have

$$|F(\psi_1)-F(\psi_2)|\leqslant|\rho(x,\xi)||\psi_1-\psi_2|+\int_{-1}^{1}|\chi(x,\xi,\xi')||\psi_1-\psi_2|d\xi'. \tag{4.8}$$

Let us first consider the case $1<p<\infty$.

The use of the inequality $(|a+b|)^p\leqslant 2^p(|a|^p+|b|^p)$ and Holder's inequality gives

$$\begin{aligned}
|F(\psi_1)-F(\psi_2)|^p&\leqslant 2^p\left[|\rho(x,\xi)|^p|\psi_1-\psi_2|^p+\left(\int_{-1}^{1}|\chi(x,\xi,\xi')||\psi_1-\psi_2|d\xi'\right)^p\right]\\
&\leqslant 2^p\left[(\rho_1)^p|\psi_1-\psi_2|^p+\left(\int_{-1}^{1}|\chi(x,\xi,\xi')|^q d\xi'\right)^{p/q}\left(\int_{-1}^{1}|\psi_1-\psi_2|^p d\xi'\right)\right]\\
&\leqslant 2^p\left[(\rho_1)^p|\psi_1-\psi_2|^p+\operatorname*{ess-sup}_{x\in[-a,a]}\left\{\left(\int_{-1}^{1}|\chi(x,\xi,\xi')|^q d\xi'\right)^{p/q}\right\}\right.\\
&\quad\left.\times\left(\int_{-1}^{1}|\psi_1-\psi_2|^p d\xi'\right)\right].
\end{aligned}$$

Therefore, Fubini's theorem gives

$$\begin{aligned}
\|F(\psi_1)-F(\psi_2)\|_{X_p}^p\leqslant 2^p\left[(\rho_1)^p\|\psi_1-\psi_2\|_{X_p}^p+\int_{-1}^{1}\operatorname*{ess-sup}_{x\in[-a,a]}\left\{\left(\int_{-1}^{1}|\chi(x,\xi,\xi')|^q d\xi'\right)^{p/q}\right\}\right.\\
\left.\times d\xi\|\psi_1-\psi_2\|_{X_p}^p\right].
\end{aligned}$$

Consequently,

$$\|F(\psi_1)-F(\psi_2)\|_{X_p}\leqslant 2[(\rho_1)^p+(\chi_1)^p]^{1/p}\|\psi_1-\psi_2\|_{X_p},$$

which proves (4.6).

Let $p=1$. After integrating both sides of Eq. (4.8) with respect to x and ξ, we obtain

$$\begin{aligned}\int_{-a}^{a}\int_{-1}^{1}|F(\psi_1)-F(\psi_2)|dxd\xi &\leqslant \rho_1\|\psi_1-\psi_2\|_{X_1}+\int_{-a}^{a}\int_{-1}^{1}\operatorname*{ess-sup}_{\xi\in[-1,1]}|\chi(x,\xi,\xi')|dxd\xi'\int_{-1}^{1}|\psi_1-\psi_2|d\xi' \\ &\leqslant \rho_1\|\psi_1-\psi_2\|_{X_1}+\|\psi_1-\psi_2\|_{X_1}\int_{-1}^{1}\operatorname*{ess-sup}_{(x,\xi)\in[-a,a]\times[-1,1]}|\chi(x,\xi,\xi)|dxd\xi \\ &\leqslant (\rho_1+\chi_2)\|\psi_1-\psi_2\|_{X_1},\end{aligned}$$

which implies (4.7) and completes the proof. Q.E.D.

Let $g(.,.)$ be any function in X_p, and set

$$\phi(x,\xi)=f(x,\xi,g(x,\xi))$$

so that $\phi(x,\xi)=F(g)(x,\xi)$. Consider the problem

$$\begin{cases}\lambda\psi+\xi\dfrac{\partial\psi}{\partial x}=\phi, \\ \psi^{i}=H\psi^{0}, \quad \operatorname{Re}\lambda>0.\end{cases} \tag{4.9}$$

Since $\operatorname{Re}\lambda>0$, then $\lambda\in\rho(T_H)$ and therefore the problem (4.9) has a unique solution $\psi=(\lambda-T_H)^{-1}\phi$ in $D(T_H)$.

Now we are in a position to prove the following result:

Theorem 4.1: Assume that the hypotheses (H_1) and (H_2) hold. Then, for λ satisfying $\operatorname{Re}\lambda>2[(\rho_1)^p+(\chi_1)^p]^{1/p}$ $(1<p<\infty)$, the problem (4.1) has a unique solution $\psi(x,\xi)$ in $D(T_H)$.

For $p=1$, the same result holds if $\operatorname{Re}\lambda>(\rho_1+\chi_2)$.

Proof: Let $g\in X_p(1<p<\infty)$ be given and let ψ in $D(T_H)$ be the unique solution of the problem (4.9) (see above). Then, we have

$$(\lambda-T_H)\psi=\phi=F(g).$$

However, $\operatorname{Re}\lambda>0$. Hence the operator $(\lambda-T_H)$ is invertible and

$$\psi=(\lambda-T_H)^{-1}F(g). \tag{4.10}$$

The use of Proposition 2.1 allows us to write for any g_1,g_2 in X_p

$$\begin{aligned}\|(\lambda-T_H)^{-1}F(g_1)-(\lambda-T_H)^{-1}F(g_2)\|_{X_p} &\leqslant \frac{1}{\operatorname{Re}\lambda}\|F(g_1)-F(g_2)\|_{X_p} \\ &\leqslant \frac{2[(\rho_1)^p+(\chi_1)^p]^{1/p}}{\operatorname{Re}\lambda}\|g_1-g_2\|_{X_p}.\end{aligned}$$

Therefore, for $\operatorname{Re}\lambda>2[(\rho_1)^p+(\chi_1)^p]^{1/p}$, the operator $(\lambda-T_H)^{-1}F$ is a contraction mapping on X_p. It follows from the contraction mapping principle that (4.10) has a unique fixed point ψ^*, i.e.,

$$\psi^*=(\lambda-T_H)^{-1}F(\psi^*).$$

This implies that $\psi^*\in D(T_H)$ and $(\lambda-T_H)(\psi^*)=F(\psi^*)$, i.e., ψ^* is the solution of the problem (4.1).

For $p=1$, the same calculations as above conduct to the equation

$$\|(\lambda-T_H)^{-1}F(g_1)-(\lambda-T_H)^{-1}F(g_2)\|_{X_1}\leqslant\left[\frac{\rho_1+\chi_2}{\mathrm{Re}\,\lambda}\right]\|g_1-g_2\|_{X_1}.$$

Now, a similar reasoning as previously gives the result and completes the proof. Q.E.D.

Remark 4.1: (a) In case σ contains a linear part, that is, $\sigma(x,\xi,\psi)=\sigma_1(x,\xi)\psi+\sigma_2(x,\xi,\psi)$ where $\sigma_1(x,\xi)$ is essentially bounded in $[-a,\ a]\times[-1,\ 1]$ and $\sigma_2(x,\xi,\psi)$ satisfies (H_1), then the existence and uniqueness of a solution stated in Theorem 4.1 remain true since $\sigma_1(x,\xi)$ is also Lipschitz continuous. Observe that in this case λ must satisfy $\mathrm{Re}\,\lambda>-\lambda^*$ where

$$\lambda^*=\operatorname*{ess-inf}_{(x,\xi)\in[-a,\ a]\times[-1,\ 1]}\mathrm{Re}(\sigma_1(x,\xi)).$$

(b) In case $F(\psi)=K(\psi)$ where K is a bounded linear operator on X_p, then it is Lipschitz continuous with Lipschitz constant $\|K\|$. Thus Theorem 4.1 is an extension to the linear case. On the other hand, if $F(\psi)=K(\psi)+F_0(\psi)$, where F_0 is Lipschitz continuous, then so is $F(\psi)$ and the result remains true. ◇

Remark 4.2: We have seen that under the hypotheses of the Theorem 4.1, $(\lambda-T_H)^{-1}F$ is a contraction mapping, for suitable λ in $\rho(T_H)$, on the Banach space X_p $(1\leqslant p<\infty)$. Let ψ_0 be a given function in X_p and define the sequence ψ_n successively by

$$\psi_n=(\lambda-T_H)^{-1}F(\psi_{n-1}),\quad n=1,2,\ldots,$$

where $\lambda\in\rho(T_H)$.

Therefore, the sequence $\{\psi_n\}$ converges to the unique solution $\psi(x,\xi)$ of the problem (4.1) for all λ such that $\mathrm{Re}\,\lambda>2[(\rho_1)^p+(\chi_1)^p]^{1/p}$ if $1<p<\infty$ and $\mathrm{Re}\,\lambda>[\rho_1+\chi_2]$ for $p=1$. Moreover,

$$\|\psi_n-\psi\|_{X_p}\leqslant\frac{\tau}{\mathrm{Re}\,\lambda+\tau}\left(\frac{\tau}{\mathrm{Re}\,\lambda}\right)^{n-1}\|\psi_1-\psi\|_{X_p},\tag{4.11}$$

where

$$\tau=\begin{cases}2[(\rho_1)^p+(\chi_1)^p]^{1/p}, & \text{if } 1<p<\infty,\\ [\rho_1+\chi_2], & \text{if } p=1.\end{cases}$$

The estimate (4.11) follows immediately from the standard proof of the contraction mapping principle and the fact that $\tau/\mathrm{Re}\,\lambda$ is the contraction constant of the operator $(\lambda-T_H)^{-1}F$. ◇

In the hypotheses (H_1) and (H_2) the functions $\sigma(.,.,.)$ and $\kappa(.,.,.,.)$ are assumed to satisfy some global Lipschitz conditions on X_p. In case (4.3) and (4.4) hold only for ψ_1 and ψ_2 in some neighborhood of the origin of X_p, we may modify σ and κ away from the origin, so that they satisfy Lipschitz conditions on the hole space X_p, and then establish the existence of a unique ''local solution'' to the problem (4.1).

Let r be a non-negative real number and denote by S_r the set

$$S_r=\{\psi\in X_p,\|\psi\|_{X_p}\leqslant r\}.$$

Assume that

$$(H_3)\begin{cases}\text{for some } r>0,\\ |\sigma(x,\xi,\psi_1)-\sigma(x,\xi,\psi_2)|\leqslant|\rho(x,\xi)||\psi_1-\psi_2| \quad (\forall\,\psi_1,\psi_2\in S_r),\\ |\kappa(x,\xi,\xi',\psi_1)-\kappa(x,\xi,\xi',\psi_2)|\leqslant|\chi(x,\xi,\xi')||\psi_1-\psi_2| \quad (\forall\,\psi_1,\psi_2\in S_r),\end{cases}$$

where $\rho(x,\xi)$ and $\chi(x,\xi,\xi')$ satisfy the same hypotheses as in (H_1) and (H_2).

Then we have the following.

Theorem 4.2: Assume that (H_3) holds for some $r>0$. Then, the problem (4.1) has a unique solution ψ^* in $D(T_H)$ for any λ such that $\mathrm{Re}\,\lambda>4[(\rho_1)^p+(\chi_1)^p]^{1/p}$ $(1<p<\infty)$. Moreover, this solution exists so long as $\|\psi^*\|_{X_p}\leqslant r$.

For $p=1$, the same result holds if $\mathrm{Re}\,\lambda>2(\rho_1+\chi_2)$. ◇

Proof: Define a mapping Q from X_p to X_p $(1<p<\infty)$ by

$$Q(\psi)=\begin{cases} f(x,\xi,\psi), & \text{if } \|\psi\|\leqslant r,\\ f\left(x,\xi,r\,\dfrac{\psi}{\|\psi\|}\right), & \text{if } \|\psi\|>r. \end{cases}$$

Then Q is an extension of f from S_r to the hole space X_p. Now, let ψ_1, ψ_2 in X_p $(1<p<\infty)$. A simple calculations give

$$\|Q(\psi_1)-Q(\psi_2)\|_{X_p}\leqslant \frac{2[(\rho_1)^p+(\chi_1)^p]^{1/p}}{\mathrm{Re}\,\lambda}\,\|R(\psi_1)-R(\psi_2)\|_{X_p},$$

where R is the radial retraction mapping from X_p on S_r defined by

$$R(\psi)=\begin{cases} \psi & \text{if } \|\psi\|\leqslant r,\\ r\,\dfrac{\psi}{\|\psi\|} & \text{if } \|\psi\|>r. \end{cases}$$

Clearly, R satisfies $\|R(\psi_1)-R(\psi_2)\|_{X_p}\leqslant 2\|\psi_1-\psi_2\|_{X_p}$ for all ψ_1,ψ_2 in X_p (cf. Ref. 15). Therefore, we have

$$\|Q(\psi_1)-Q(\psi_2)\|_{X_p}\leqslant \frac{4[(\rho_1)^p+(\chi_1)^p]^{1/p}}{\mathrm{Re}\,\lambda}\,\|\psi_1-\psi_2\|_{X_p}.$$

Consider now the problem

$$\begin{cases} (\lambda-T_H)\psi=Q(\psi),\\ \psi\in D(T_H), \quad \mathrm{Re}\,\lambda>0. \end{cases}$$

It follows from the proof of Theorem 4.1 that for $\mathrm{Re}\,\lambda>4[(\rho_1)^p+(\chi_1)^p]^{1/p}$, the preceding problem has a unique solution ψ^* in X_p.

For $p=1$ the same calculations as previously leads to

$$\|Q(\psi_1)-Q(\psi_2)\|_{X_1}\leqslant 2\,\frac{\rho_1+\chi_2}{\mathrm{Re}\,\lambda}\,\|\psi_1-\psi_2\|_{X_1},$$

which gives the desired result. Q.E.D.

V. MULTIPLYING BOUNDARY CONDITIONS

The aim of this section is to show that the results of Secs. III and IV hold also for multiplying boundary conditions. To this purpose, in all that follows, we shall assume that the boundary operator H verifies the estimate $\|H\|>1$. Let us first point out a few preliminary facts.

Let $\lambda_0=-\lambda^*+(1/2a)\mathrm{Log}(\|H\|)$ and define $\Gamma_{\lambda_0}:=\{\lambda\in\mathbf{C}/\mathrm{Re}\,\lambda>\lambda_0\}$. As it has been proven, (cf., Ref. 11), the resolvent set of the operator T_H, $\rho(T_H)$, contains Γ_{λ_0}.

Remark 5.1: Unlike in Sec. II, generally the strip $0<\mathrm{Re}\,\lambda\leqslant\lambda_0$ is not included in the resolvent set of T_H. However, with additional hypotheses on the boundary operator H, we can obtain more information about its structure (see Ref. 11). ◇

We note that the crucial arguments in the previous analysis (Secs. III and IV) are the estimate (2.1) and the compactness results obtained in Ref. 10 for the class of regular collision operators K. So, in order to extend the previous results to multiplying boundary conditions, we must first establish the analogous of these arguments to the case of multiplying boundary conditions. Let us remark that the compactness results used above hold true even if $\|H\|>1$ for all $\lambda\in\Gamma_{\lambda_0}$ (cf., Ref. 11, Theorem 3.1) while the lemma below, proven in Ref. 11, gives the analogous of the estimate (2.1) for $\lambda\in\Gamma_{\lambda_0}$.

Lemma 5.1: (Ref. 11, Proposition 3.1) Let H be a multiplying bounded boundary operator. Then there exists $\lambda_0\in\mathbf{R}$ such that for $\mathrm{Re}\,\lambda>\lambda_0$, we have

$$\|(\lambda-T_H)^{-1}\|\leqslant\frac{\nu}{\mathrm{Re}\,\lambda-\lambda_0},\tag{5.1}$$

where ν is a non-negative constant. ◇

Now we are in a position to assert that the results obtained in Sec. III A remain valid if instead of considering $\|H\|\leqslant 1$, we suppose $\|H\|>1$. Their proofs may be modeled very closely after those of these results. It suffices to replace the statement $\lambda\in\rho(T_H)$ by $\lambda\in\Gamma_0$, Eq. (2.1) by (5.1), and Ref. 10, Theorem 2.1, by Ref. 11, Theorem 3.1.

In the same way Theorems 4.1 and 4.2 hold also true for multiplying boundary conditions with $\mathrm{Re}\,\lambda>\max(\lambda_0,\ 2\nu[(\rho_1)^p+(\chi_1)^p]^{1/p})$ if $1<p<\infty$ and $\mathrm{Re}\,\lambda>\max(\lambda_0,\nu[\rho_1+\chi_2])$ if $p=1$. For the proofs, we must solely replace the statement $\mathrm{Re}\,\lambda>0$ by $\lambda\in\Gamma_0$ and Eq. (2.1) by (5.1).

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An elegant solution of the *n*-body Toda problem

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The solution of the classical open-chain n-body Toda problem is derived from an ansatz and is found to have a highly symmetric form. The proof requires an unusual identity involving Vandermonde determinants. The explicit transformation to action-angle variables is exhibited. © *1996 American Institute of Physics.* [S0022-2488(96)02103-9]

The Toda chain is one of the paradigmatic examples of an integrable many-body system of interacting particles. The discovery of its conserved integrals of motion[1,2] and its subsequent solution[3–5] were important steps in the development of the theory of integrable systems.[6] An almost universal feature of analytical studies of the Toda system is the use of the Lax pair formalism. In this paper, an alternative derivation of the solution of the classical open-chain n-body Toda system is given.

The derivation proceeds essentially from an ansatz about the form of the solution and therefore lacks the power and generality of the Lax pair treatment. The solution, however, has an elegant structure that is not evident in previous representations. More, it can be interpreted as the classical canonical transformation from the Toda system to a free theory. This is an important clue to constructing the classical and quantum solutions by a sequence of elementary canonical transformations.[7] Following the successful solution of the three-body Toda problem with this approach,[8] work is in progress on the classical and quantum open-chain n-body problems.

The Hamiltonian for the $(n+1)$-body open chain Toda system is

$$H=\frac{1}{2}\sum_{k=1}^{n+1} p_k^2+\sum_{k=1}^{n} e^{q_k-q_{k+1}}. \tag{1}$$

The arguments of the exponential potentials can be interpreted as expressions for the root vectors of A_n in the Cartan basis.[5] A coordinate transformation will put the root vectors into the Chevalley basis and separate out the motion of the center of mass. The transformation is given by

$$\begin{aligned} q_1 &\mapsto q_1+\frac{q_{n+1}}{n+1}, \\ q_k &\mapsto -q_{k-1}+q_k+\frac{q_{n+1}}{n+1} \quad (2\leqslant k\leqslant n), \\ q_{n+1} &\mapsto -q_n+\frac{q_{n+1}}{n+1}, \\ p_k &\mapsto \frac{1}{n+1}\left(\sum_{j=k}^{n}(n+1-j)p_j-\sum_{j=1}^{k-1} jp_j\right)+p_{n+1}, \quad (1\leqslant k\leqslant n), \end{aligned} \tag{2}$$

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$$p_{n+1}\mapsto \frac{-1}{n+1}\left(\sum_{j=1}^{k-1} jp_j\right)+p_{n+1}.$$

The transformed Hamiltonian is

$$H^a=\frac{1}{2(n+1)}\left(\sum_{k=1}^{n} k(n+1-k)p_k^2+\sum_{k=2}^{n}\sum_{j=1}^{k-1} 2j(n+1-k)p_jp_k\right)$$
$$+\frac{n+1}{2}\,p_{n+1}^2+e^{2q_1-q_2}+\sum_{k=2}^{n-1} e^{2q_k-q_{k-1}-q_{k+1}}+e^{2q_n-q_{n-1}}. \tag{3}$$

This leads to the equations of motion,

$$\begin{aligned}\ddot{q}_1&=-e^{2q_1-q_2},\\ \ddot{q}_k&=-e^{2q_k-q_{k-1}-q_{k+1}}\quad(2\leqslant k\leqslant n-1),\\ \ddot{q}_n&=-e^{2q_n-q_{n-1}}.\end{aligned} \tag{4}$$

The solution of these equations has the remarkably simple form

$$e^{-q_m}=\sum_{j_1<\cdots<j_m}^{n+1} f_{j_1}\cdots f_{j_m}\Delta^2(j_1,\ldots,j_m)e^{(\mu_{j_1}+\cdots+\mu_{j_m})t}, \tag{5}$$

where $\Delta^2(j_1,\ldots,j_m)$ is the square of the Vandermonde determinant,

$$\Delta^2(j_1,\ldots,j_m)=\prod_{j_i<j_k}(\mu_{j_i}-\mu_{j_k})^2, \tag{6}$$

and f_k and μ_k are arbitrary constants, satisfying

$$\begin{aligned}\prod_{k=1}^{n+1} f_k&=\Delta^{-2}(1,\ldots,n+1),\\ \sum_{k=1}^{n+1}\mu_k&=0.\end{aligned} \tag{7}$$

(There are additional constraints on the range of the f_k if one requires the q_m be real.) The solution has $2n$ free parameters, as required. The solution in the original variables is determined from the transformation (2) to be composed of ratios of these solutions times a factor for the center of mass motion.

To derive the solution, make the ansatz

$$e^{-q_m}=\sum_{j_1<\cdots<j_m}^{n+1} f_{j_1\cdots j_m}e^{(\mu_{j_1}+\cdots+\mu_{j_m})t}, \tag{8}$$

where the μ_k are arbitrary real numbers. Note that this ansatz defines a variable,

$$e^{-q_{n+1}}=f_{1\cdots n+1}e^{(\mu_1+\cdots+\mu_{n+1})t}. \tag{9}$$

Such a variable might naturally appear in the final equation of (4) to give $\ddot{q}_n = -e^{2q_n - q_{n-1} - q_{n+1}}$. That this variable does not appear can be interpreted as meaning that one has set $q_{n+1}=0$. This ultimately is the origin of the restrictions (7) on the f_k and μ_k. The equation for $\ddot{q}_1$ is also of the form of the others if there is a $q_0=0$. The open-chain Toda system thus has fixed end points in this sense. The ansatz and solution are compatible with the slightly more general problem, where $e^{-q_{n+1}} = ce^{\kappa t}$. Then, in the solution, one would have $\Pi_{k=1}^{n+1} f_k = c\Delta^{-2}(1,\ldots,n+1)$ and $\Sigma_{k=1}^{n+1}\mu_k=\kappa$.

Consider e^{-q_m}. Differentiating twice and multiplying by e^{-q_m} leads to

$$-\ddot{q}_m e^{-2q_m} = e^{-q_m}\partial_t^2 e^{-q_m} - (\partial_t e^{-q_m})^2. \tag{10}$$

But from the equations of motion, $-\ddot{q}_m e^{-2q_m} = e^{-q_{m-1}-q_{m+1}}$ (using $q_0=0=q_{n+1}$). Substituting the ansatz into the resulting equation gives $(2\leqslant m\leqslant n-1)$

$$\sum_{\substack{j_1<\cdots<j_m \\ k_1<\cdots<k_m \\ j_1<k_1}}^{n+1} f_{j_1\cdots j_m} f_{k_1\cdots k_m} \left(\sum_{i=1}^{m}\mu_{j_i} - \sum_{i=1}^{m}\mu_{k_i}\right)^2 \exp\left(\left(\sum_{i=1}^{m}\mu_{j_i} + \sum_{i=1}^{m}\mu_{k_i}\right)t\right)$$

$$= \sum_{\substack{j_1<\cdots<j_{m-1} \\ k_1<\cdots<k_{m+1}}}^{n+1} f_{j_1\cdots j_{m-1}} f_{k_1\cdots k_{m+1}} \exp\left(\left(\sum_{i=1}^{m-1}\mu_{j_i} + \sum_{i=1}^{m+1}\mu_{k_i}\right)t\right). \tag{11}$$

The equation for $m=1$ is

$$\sum_{j_1<j_2}^{n+1} f_{j_1} f_{j_2} (\mu_{j_1}-\mu_{j_2})^2 e^{(\mu_{j_1}+\mu_{j_2})t} = \sum_{j_1<j_2}^{n+1} f_{j_1 j_2} e^{(\mu_{j_1}+\mu_{j_2})t}. \tag{12}$$

The equation for $m=n$ involves $f_{j_1\cdots j_n}$, where $1\leqslant j_1<\cdots<j_n\leqslant n+1$. As one is choosing n integers out of $n+1$, this is more succinctly labeled by $f_{\hat{r}}$, where r is the integer that is not in the set. Similarly, $f_{\widehat{rs}}$ means the two integers $r\neq s$ do not appear, and the indices of f are the remaining $n-1$ integers. With this notation, the equation for $m=n$ is

$$\sum_{r<s}^{n+1} f_{\hat{r}} f_{\hat{s}} (-\mu_r+\mu_s)^2 \exp\left(\left(-\mu_r-\mu_s+2\sum_{k=1}^{n+1}\mu_k\right)t\right) = \sum_{r<s}^{n+1} f_{\widehat{rs}} \exp\left(\left(-\mu_r-\mu_s+\sum_{k=1}^{n+1}\mu_k\right)t\right). \tag{13}$$

Assume the μ_k are all distinct and that they have no accidental degeneracies in their linear combinations, such as $\mu_{j_1}+\mu_{j_2}=\mu_{j_3}+\mu_{j_4}$. The asymptotic behavior of the exponentials can be used to equate like terms in the sums. The degenerate cases can be recovered later by continuity in the μ_k. Let

$$f_{j_1\cdots j_m} = f_{j_1}\cdots f_{j_m}\Delta^2(j_1,\ldots,j_m), \tag{14}$$

where the f_{j_k} are (so far) arbitrary constants and $\Delta^2(j_1,\ldots,j_m)$ is the square of the Vandermonde determinant (6). With this definition, the $m=1$ equation (12) is easily verified. The $m=n$ equation (13) is satisfied if the constraints (7) on the f_k and μ_k are imposed. The proof that Eq. (11) is satisfied reduces to a hierarchy of identities for Vandermonde determinants.

On the left-hand side of (11), there are two sets of indices $\{j_\alpha\}$ and $\{k_\beta\}$. Since $j_1<k_1$, at most, they can have $m-1$ indices in common. The asymptotic behavior of the exponential is given by a sum over the μ_i indexed by the combined set $S=\{j_\alpha,k_\beta\}$. Different partitions of S into sets $\{j_\alpha\}$

and $\{k_\beta\}$ $(j_1<k_1)$ will have the same asymptotic behavior. The number of such terms will depend on the number of distinct indices between the two sets, and these constitute separate cases. Let $2r$ denote the number of distinct indices.

Consider the case $r=1$, labeling the common indices $s_1,\ldots,s_{m-1}$ and the distinct ones j_1 and k $(j_1<k)$. There is a unique term on both sides of (11) with the asymptotic behavior given by this set of indices, and one has

$$f_{j_1 s_1\cdots s_{m-1}} f_{\{k s_1\cdots s_{m-1}\}}(\mu_{j_1}-\mu_k)^2 = f_{s_1\cdots s_{m-1}} f_{\{j_1 k s_1\cdots s_{m-1}\}}, \tag{15}$$

where the curly brackets indicate that the indices should be arranged in increasing order. Using (14), the constant factors f_i cancel and one has a relation between Vandermonde determinants,

$$\Delta^2(j_1,s_1,\ldots,s_{m-1})\Delta^2(k,s_1,\ldots,s_{m-1})(\mu_{j_1}-\mu_k)^2 = \Delta^2(s_1,\ldots,s_{m-1})\Delta^2(j_1,k,s_1,\ldots,s_{m-1}). \tag{16}$$

Using the relation

$$\Delta^2(k,s_1,\ldots,s_{m-1}) = \Delta^2(s_1,\ldots,s_{m-1})\prod_{i=1}^{m-1}(\mu_k-\mu_{s_i})^2 \tag{17}$$

and its relatives, the dependence on the common indices is seen to cancel and one is left with the identity

$$(\mu_{j_1}-\mu_k)^2 = \Delta^2(j_1,k). \tag{18}$$

It is a general feature for all r that the dependence on the constant factors and the common indices cancels on both sides, so without loss of generality one can focus on the distinct indices alone. Reindex the set S of distinct indices by the integers 1 to $2r$. Partition S into two sets $\alpha=\{1,\alpha_2,\ldots,\alpha_r\}$ and $\beta=\{\beta_1,\ldots,\beta_r\}$ and denote the collection of such partitions $P_{\alpha\beta}$. Separately partition S into sets $\gamma=\{\gamma_1,\ldots,\gamma_{r-1}\}$ and $\delta=\{\delta_1,\ldots,\delta_{r+1}\}$, calling the collection of partitions $P_{\gamma\delta}$. Denote $\Delta^2(\alpha;r)=\Delta^2(1,\alpha_2,\ldots,\alpha_r)$, and similarly for the rest. The number r of indices involved in the Vandermonde determinant is made explicit to reduce confusion. Both sides of Eq. (11) will be equal if the following identity between Vandermonde determinants holds:

$$\sum_{P_{\alpha\beta}} \Delta^2(\alpha;r)\Delta^2(\beta;r)\left(\sum_\alpha \mu_\alpha-\sum_\beta \mu_\beta\right)^2 = \sum_{P_{\gamma\delta}} \Delta^2(\gamma;r-1)\Delta^2(\delta;r+1). \tag{19}$$

It seems likely that this identity has a group theoretical interpretation, but in its absence, the identity can be proved inductively as follows.[9] Divide both sides by $\Delta^2(S;2r)$. This gives the equation

$$\sum_{P_{\alpha\beta}} \frac{(\Sigma_\alpha\mu_\alpha-\Sigma_\beta\mu_\beta)^2}{\Pi_{\alpha,\beta}(\mu_\alpha-\mu_\beta)^2} = \sum_{P_{\gamma\delta}} \frac{1}{\Pi_{\gamma,\delta}(\mu_\gamma-\mu_\delta)^2}. \tag{20}$$

Denote the left-hand side of the equation by L_r and the right-hand side by R_r. The equation $L_1=R_1$ holds trivially. Assume that $L_{r-1}=R_{r-1}$. The inductive step will be made by considering the pole structure of L_r and R_r. Since L_r and R_r are analytic functions of the μ_i without zeros, if they can be shown to have the same residue at all of their poles, they must be equal.

Choose two indices from the set S, neither equal to 1, and let their associated μ_i be labeled z and a. (The index 1 is special because it has a preferred role in the partitioning. Which of the original μ_i is associated to the index 1 is, however, arbitrary, so one can investigate the pole

structure at the μ_i missed here by reindexing the set S.) Let S' denote the set S with these two indices removed, and let $\alpha',\beta',\gamma',\delta'$ denote partitions of S' as defined above, with r replaced by $r-1$.

Consider the residue of L_r at $z=a$. L_r has a double pole at $z=a$ if $z\in\alpha$ and $a\in\beta$ or *vice versa*. In the former case, the residue is computed to be

$$\operatorname*{Res}_{z=a} L_r|_{z\in\alpha,a\in\beta}=\frac{2}{\Pi_{S'}(a-\mu_{S'})^2}\sum_{P_{\alpha'\beta'}}\left(\frac{1}{\Sigma_{\alpha'}\mu_{\alpha'}-\Sigma_{\beta'}\mu_{\beta'}}-\sum_{\beta'}\frac{1}{a-\mu_{\beta'}}\right)\frac{(\Sigma_{\alpha'}\mu_{\alpha'}-\Sigma_{\beta'}\mu_{\beta'})^2}{\Pi_{\alpha',\beta'}(\mu_{\alpha'}-\mu_{\beta'})^2}. \tag{21}$$

In the alternative case $z\in\beta,a\in\alpha$, the residue is

$$\operatorname*{Res}_{z=a} L_r|_{z\in\beta,a\in\alpha}=\frac{2}{\Pi_{S'}(a-\mu_{S'})^2}\sum_{P_{\alpha'\beta'}}\left(-\frac{1}{\Sigma_{\alpha'}\mu_{\alpha'}-\Sigma_{\beta'}\mu_{\beta'}}-\sum_{\alpha'}\frac{1}{a-\mu_{\alpha'}}\right)\times\frac{(\Sigma_{\alpha'}\mu_{\alpha'}-\Sigma_{\beta'}\mu_{\beta'})^2}{\Pi_{\alpha',\beta'}(\mu_{\alpha'}-\mu_{\beta'})^2}. \tag{22}$$

Adding these, the residue of L_r at $z=a$ is

$$\operatorname*{Res}_{z=a} L_r=-\frac{2L_{r-1}}{\Pi_{S'}(a-\mu_{S'})^2}\sum_{S'}\frac{1}{a-\mu_{S'}}. \tag{23}$$

The residue at $z=a$ of R_r is similarly composed of terms where $z\in\gamma,a\in\delta$ and *vice versa*. The full residue is

$$\operatorname*{Res}_{z=a} R_r=-\frac{2R_{r-1}}{\Pi_{S'}(a-\mu_{S'})^2}\sum_{S'}\frac{1}{a-\mu_{S'}}. \tag{24}$$

This is seen to equal the residue of L_r at $z=a$, given $L_{r-1}=R_{r-1}$. Since this result holds for all pairs of the original μ_i, one concludes that $L_r=R_r$ and the induction is complete.

To exhibit the solution (5) as a canonical transformation from (3) to a Hamiltonian independent of coordinates, one must introduce final coordinates and momenta and find a relation between them and the f_j and μ_k so that the transformation is canonical. It is clear that one can redefine f_j by an overall constant,

$$f_j=e^{\bar{x}_j}\tilde{f}_j. \tag{25}$$

The arguments of the exponentials then define the final coordinates,

$$x_j=\mu_j t+\bar{x}_j. \tag{26}$$

There should only be n independent degrees of freedom, and the coordinate $x_{n+1}=-\Sigma_{i=1}^{n}x_i$ is not independent because it is related to the others by the constraints (7). It is useful, however, to introduce a temporary form of the final Hamiltonian,

$$\tilde{H}=\frac{1}{2}\sum_{i=1}^{n+1}\mu_i^2. \tag{27}$$

The μ_j are not the momenta conjugate to x_j because if the constraint $\mu_{n+1}=-\Sigma_{i=1}^{n}\mu_i$ were eliminated, the wrong $\dot{x}_j$ would follow from Hamilton's equations. It is necessary to introduce n momenta k_j conjugate to the x_j, so that $\dot{x}_j=\partial\tilde{H}/\partial k_j=\mu_j$. The relation between k_j and μ_j is found to be

$$k_j=\mu_j-\mu_{n+1}=\mu_j+\sum_{i=1}^{n}\mu_i, \tag{28}$$

or in reverse ($j\neq n+1$),

$$\begin{aligned}\mu_j&=k_j-\frac{1}{n+1}\sum_{i=1}^{n}k_i,\\ \mu_{n+1}&=-\frac{1}{n+1}\sum_{i=1}^{n}k_i.\end{aligned} \tag{29}$$

The final Hamiltonian is then

$$\tilde{H}=\frac{n}{2(n+1)}\sum_{j=1}^{n}k_j^2-\frac{1}{n+1}\sum_{i<j}k_ik_j. \tag{30}$$

The next step is to find an equation for the evolution of the original momenta. This is easily done by taking a time derivative of the solution (5),

$$e^{-q_m}=\sum_{j_1<\cdots<j_m}^{n+1}\tilde{f}_{j_1}\cdots\tilde{f}_{j_m}\Delta^2(j_1,\ldots,j_m)e^{x_{j_1}+\cdots+x_{j_m}}, \tag{31}$$

to find

$$-\dot{q}_me^{-q_m}=\sum_{j_1<\cdots<j_m}^{n+1}\tilde{f}_{j_1}\cdots\tilde{f}_{j_m}\Delta^2(j_1,\ldots,j_m)(\mu_{j_1}+\cdots+\mu_{j_m})e^{x_{j_1}+\cdots+x_{j_m}}. \tag{32}$$

Using Hamilton's equations with the Hamiltonian (3), one can express $\dot{q}_m$ in terms of the momenta as

$$\dot{q}_m=\frac{1}{(n+1)}\left[m(n+1-m)p_m+\sum_{i=1}^{m-1}i(n+1-m)p_i+\sum_{i=m+1}^{n}m(n+1-i)p_i\right]. \tag{33}$$

The result is

$$\begin{aligned}&\frac{-1}{(n+1)}\left[m(n+1-m)p_m+\sum_{i=1}^{m-1}i(n+1-m)p_i+\sum_{i=m+1}^{n}m(n+1-i)p_i\right]e^{-q_m}\\ &\quad=\sum_{j_1<\cdots<j_m}^{n+1}\tilde{f}_{j_1}\cdots\tilde{f}_{j_m}\Delta^2(j_1,\ldots,j_m)(\mu_{j_1}+\cdots+\mu_{j_m})e^{x_{j_1}+\cdots+x_{j_m}}.\end{aligned} \tag{34}$$

Finally, by requiring that the Poisson brackets be preserved under the transformation, one can determine the $\tilde{f}_j$ in terms of the k_i's. The result is that ($j\neq n+1$)

$$\tilde{f}_j=(-1)^{j-1}k_j^{-1}\prod_{i\neq j}^{n}(k_j-k_i)^{-1},$$
$$\tilde{f}_{n+1}=\prod_{i=1}^{n}k_i^{-1}. \tag{35}$$

One confirms that the f_j satisfy the constraint (7). (Note that the maximal symmetry is evident in terms of the μ_i's, since $k_j=\mu_j-\mu_{n+1}$ and $k_j-k_i=\mu_j-\mu_i$.) The proof that this is the correct form for the f_j follows by constructing the Poisson brackets and collecting like exponentials. Conditions are quickly found that the f_j must be particular products of differences between momenta. It is then seen that there are no additional requirements.

Using (29) and (35) in (31) and (34) gives the explicit canonical transformation between the open-chain n-body Toda Hamiltonian in the Chevalley basis (3) and a Hamiltonian (30) that is independent of coordinates. The reduction to action-angle variables is essentially complete. From this point, one can attempt to construct a product of elementary canonical transformations that produces this full transformation. This has been done for the three-body system[8] and work is in progress on the n-body system. The value of such a product is that, when it is found in the quantum system, it allows the construction of integral representations of the eigenfunctions of the system.

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$N=4$ super KdV hierarchy in $N=4$ and $N=2$ superspaces

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We present the results of further analysis of the integrability properties of the $N=4$ supersymmetric Korteweg–de Vries (KdV) equation deduced earlier by two of us [F. Delduc and E. Ivanov, Phys. Lett. B **309**, 312 (1993)] as a Hamiltonian flow on $N=4$ SU(2) superconformal algebra in the harmonic $N=4$ superspace. To make this equation and the relevant Hamiltonian structures more tractable, we reformulate it in the ordinary $N=4$ and further in $N=2$ superspaces. In $N=2$ superspace it is represented by a coupled system of evolution equations for a general $N=2$ superfield and two chiral and antichiral superfields, and involves two independent real parameters, a and b. We construct a few first bosonic conserved charges in involution, of dimensions from 1 to 6, and show that they exist only for the following choices of the parameters: (i) $a=4$, $b=0$; (ii) $a=-2$, $b=-6$; (iii) $a=-2$, $b=6$. The same values are needed for the relevant evolution equations, including $N=4$ KdV itself, to be bi-Hamiltonian. We demonstrate that the above three options are related via SU(2) transformations and actually amount to the SU(2) covariant integrability condition found in the harmonic superspace approach. Our results provide a strong evidence that the unique $N=4$ SU(2) super KdV hierarchy exists. Upon reduction to $N=2$ KdV, the above three possibilities cease to be equivalent. They give rise to the $a=4$ and $a=-2$ $N=2$ KdV hierarchies, which thus prove to be different truncations of the single $N=4$ SU(2) KdV one. © *1996 American Institute of Physics.* [S0022-2488(96)03002-1]

I. INTRODUCTION

The Korteweg–de Vries (KdV) hierarchy and its supersymmetric extensions were the subject of many studies for the last several years. Besides supplying nice examples of integrable systems, they bear a deep relation to conformal field theory, 2D gravity, matrix models, etc. One of the remarkable properties of these systems is that they are related, via the second Hamiltonian structure, to the classical (super)conformal algebras: Virasoro algebra in the bosonic case and $N\geqslant 1$ superconformal ones in the case of $N\geqslant 1$ superextended hierarchies.[1–14] Generalized KdV type systems related to W_n algebras and their supersymmetric extensions also received a great deal of attention (see, e.g., Ref. 15 and references therein).

Up to now, supersymmetric KdV hierarchies have been constructed for $N=1$, 2, 3, and 4, based on the above mentioned relation to superconformal algebras.[3–14] An interesting peculiarity is that, beginning with $N=2$, the supersymmetric KdV equations turn out to be integrable (give rise to the whole hierarchy or, in other words, have an infinite number of conservation laws in involution) only for special choices of the parameters in the Hamiltonian. There exist only three integrable $N=2$ KdV hierarchies: the $a=4$, $a=-2$, and $a=1$ ones,[8–10] with a a parameter entering into the $N=2$ KdV Hamiltonian, despite the fact that for any value of a the related $N=2$ super KdV possesses $N=2$ SCA as the second Hamiltonian structure. The generalized $N=2$ KdV system associated with $N=2$ W_3 algebra ("$N=2$ super Boussinesq hierarchy") has similar properties as established in Refs. 16 and 15. For the $N=3$ super KdV equation associated with $N=3$ SCA the requirement of integrability also strictly fixes the value of a free parameter in the Hamiltonian,[13]

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though the existence of the whole hierarchy in this case has not yet been proven (the Lax pair representation has not been found). Only a few higher order conservation laws in involution have been constructed. Nevertheless the existence of such quantities is highly nontrivial and provides strong evidence in favor of the integrability of the associated $N=3$ super KdV.

Another higher N extension of $N=2$ super KdV, the $N=4$ one, has been constructed in Ref. 14. We proceeded from the $N=4$ SU(2) (''small'') superconformal algebra[17] as the second Hamiltonian structure. This extension is, in a sense, more economic than the $N=3$ one, because $N=4$ SU(2) SCA by its component currents content is a natural generalization of $N=2$ SCA. Like $N=2$ SCA, it contains only currents with canonical dimensions: a dimension 2 conformal stress tensor, four dimension 3/2 fermionic currents and three dimension 1 affine su(2) currents. $N=3$ SCA includes an extra current with a subcanonical dimension 1/2.[17] Both $N=4$ SU(2) and $N=2$ SCAs belong to the family of u(N) Knizhnik–Bershadsky superconformal algebras (which are nonlinear in general, starting with $N=3$).

In our construction[14] we used the formalism of $N=4$, 1D harmonic superspace (HSS) as the most natural one for representing $N=4$ SU(2) SCA in a manifestly supersymmetric form. We found that the general superfield $N=4$ KdV Hamiltonian, H_3, consists of two pieces. One is an integral over the whole $N=4$ HSS and the second is an integral over an analytic subspace of this HSS, containing half the number of odd coordinates. This second piece involves a set of SU(2) breaking constants which are naturally combined into a symmetric rank 4 SU(2) spinor c^{ilkj} (symmetric traceless rank 2 tensor). We did not construct a Lax pair for the $N=4$ KdV equation, but instead addressed the question of the existence of higher order conserved quantities, like in the $N=3$ KdV case.[13] We found that such quantities exist and, hence, that $N=4$ KdV can lead to an integrable hierarchy, provided (i) the SU(2) breaking tensor is expressed as a square of some constant real SU(2) vector $a^{ij}=a^{ji}$, $(i,j=1,2)$, and (ii) the norm of the latter is proportional to the reciprocal of the level of the affine su(2) subalgebra of $N=4$ SU(2) SCA

$$c^{ijkl}=\tfrac{1}{3}(a^{ij}a^{kl}+a^{ik}a^{jl}+a^{il}a^{jk}), \tag{1.1}$$

$$|a|^2\equiv -a^{ij}a_{ij}=\frac{20}{k}. \tag{1.2}$$

We also showed that under these restrictions the $N=4$ KdV equation is bi-Hamiltonian, i.e., it possesses a first Hamiltonian structure, the relevant Hamiltonian being the dimension 4 conserved charge H_4 (next in dimension to H_3). We considered a reduction to the $N=2$ case and found that, under a certain embedding of U(1) subalgebra in SU(2), the $a=4$ integrable version[8] of $N=2$ KdV comes out.

In Ref. 14 we limited ourselves to the construction of the dimension 4 higher order conserved charge. On the other hand, it is known that in the $N=2$ case the even dimension bosonic conserved charges exist only for the $a=4$ hierarchy.[8,9] As pointed out in Ref. 14, to learn whether the other two $N=2$ hierarchies admit an extension to $N=4$, perhaps under different restrictions on the parameters a^{ij}, the construction of the dimension 5 conserved charge for $N=4$ KdV would be crucial. In the $N=2$ case it exists for all three super KdV hierarchies and is given by different expressions in every case.[9] It is very complicated to construct such a quantity directly in HSS. At the same time, for $N=2$ superfield computations there exist powerful computer methods based on the package ''Mathematica.''[18] Keeping this in mind, it is tempting to reformulate $N=4$ super KdV in terms of $N=2$ superfields.

This is one of the main purposes of the present paper. We rewrite the $N=4$ super KdV in $N=2$ superspace as a coupled system of equations for a general dimension 1 superfield (this is just the $N=2$ KdV superfield) and dimension 1 chiral and antichiral conjugated superfields. This system involves two independent parameters which are the components of the SU(2) breaking tensor c^{ijkl} in a fixed SU(2) frame. We explicitly construct the dimension 5 and 6 conserved charges for this

system (beside reproducing in the $N=2$ formalism the charges found in Ref. 14). They exist if and only if the restrictions (1.1), (1.2) hold. This is a very strong indication that $N=4$ KdV, with conditions (1.1), (1.2), gives rise to an integrable hierarchy and that the latter is unique. One more argument in favor of the integrability is that under the same restrictions on the parameters the $N=4$ super KdV system is bi-Hamiltonian. In this article we check this property also for the evolution equations associated with other conserved charges. One more new result of this article is the observation that two inequivalent reductions of the same $N=4$ KdV to the $N=2$ one are possible. They depend on how the U(1) symmetry of the latter is embedded into the original SU(2) group. One of these reductions was described in Ref. 14 and it leads to the $a=4$, $N=2$ KdV. The second one yields the $a=-2$, $N=2$ KdV. Thus these two different $N=2$ KdV hierarchies prove to originate from the single higher symmetry $N=4$ KdV hierarchy.

The paper is organized as follows. In Sec. II we recall, with some further comments, the basic points of our construction of $N=4$ super KdV in $N=4$, 1D HSS. In Sec. III we rewrite $N=4$ KdV in ordinary $N=4$, 1D superspace and then in $N=2$ superspace, and show the possibility of two different reductions to $N=2$ super KdV. In Sec. IV the dimension 4, 5, and 6 conserved charges are constructed and shown to exist only with the restrictions (1.1), (1.2). Concluding remarks are collected in Sec. V. Two appendices contain some technical details.

II. $N=4$ KdV IN 1D HARMONIC SUPERSPACE

Here we recapitulate the salient features of $N=4$ super KdV equation in the harmonic superspace formulation basically following Ref. 14. We use a slightly different notation and add some comments.

A. $N=4$ SU(2) SCA

We started in Ref. 14 with the $N=4$ SU(2) superconformal algebra. In ordinary $N=4$, 1D superspace with coordinates

$$Z^M \equiv (x, \theta^i, \bar{\theta}_j), \quad (i,j=1,2), \tag{2.1}$$

this SCA is represented by the dimension 1 supercurrent $V^{ij}(Z)=V^{ji}(Z)$, $(V^{ij})^\dagger=\epsilon_{ik}\epsilon_{jl}V^{kl}$, satisfying the constraints (see, e.g., Ref. 19):

$$D^{(i}V^{jk)}=0, \quad \bar{D}^{(i}V^{jk)}=0. \tag{2.2}$$

Here

$$D_i=\frac{\partial}{\partial\theta^i}-\frac{i}{2}\bar{\theta}_i\frac{\partial}{\partial x}, \quad \bar{D}^i=-\frac{\partial}{\partial\bar{\theta}_i}+\frac{i}{2}\theta^i\frac{\partial}{\partial x}, \quad \{D_i,\bar{D}^j\}=i\delta_i^j\partial, \quad \{D_i,D_j\}=0, \tag{2.3}$$

the SU(2) indices i,j are raised and lowered by the antisymmetric tensors $\epsilon^{ij},\epsilon_{ij}(\epsilon^{ij}\epsilon_{jk}=\delta^i_k$, $\epsilon_{12}=-\epsilon^{12}=1)$ and $(i_1\ldots i_n)$ means symmetrization (with the factor $1/n!$). It is straightforward to check that the constraints (2.2) leave in V^{ij} only the following independent superfield projections

$$V^{ij}, \quad \xi^k=D^iV^k_i, \quad \bar{\xi}^k=-\bar{D}^iV^k_i, \quad T=\bar{D}^iD^kV_{ik}. \tag{2.4}$$

The θ independent parts of these projections, $w^{ij}(x),\zeta^l(x),\overline{\zeta^l}(x),T(x)$, up to inessential rescalings coincide with the currents of $N=4$ SU(2) SCA: the SU(2) triplet of spin 1 currents generating SU(2) affine Kac–Moody subalgebra, a complex doublet of spin 3/2 currents and the spin 2 conformal stress-tensor, respectively. Superfield Poisson brackets between the $N=4$ SU(2) supercurrents leading to the classical $N=4$ SU(2) SCA for these component currents will be presented below.

The same $N=4$ SU(2) supercurrent admits an elegant reformulation in the $N=4$, 1D harmonic superspace.

The latter is defined as an extension of $\{Z^M\}$ by the harmonic variables $u_i^{\pm}$ describing a 2-sphere $\sim$SU(2)/U(1)

$$\{Z^M\} \Rightarrow \{Z^M, u^{+i}, u^{-j}\},$$

$$u^{+i}u_i^- = 1, \quad u_i^+ u_j^- - u_i^- u_j^+ = \epsilon_{ij} \tag{2.5}$$

(see Refs. 20 and 21 for details of the harmonic superspace approach).

In what follows we will need the derivatives in harmonic variables which are given by

$$D^{++} \equiv \partial^{++} = u^{+i} \frac{\partial}{\partial u^{-i}}, \quad D^{--} \equiv \partial^{--} = u^{-i} \frac{\partial}{\partial u^{+i}},$$

$$D^0 = [D^{++}, D^{--}] = u^{+i} \frac{\partial}{\partial u^{+i}} - u^{-i} \frac{\partial}{\partial u^{-i}}. \tag{2.6}$$

The operator D^0 measures the U(1) charge of functions on the harmonic superspace. This charge is defined as the difference between the numbers of the $+$ and $-$ indices. The preservation of this U(1) charge is one of the basic postulates of the harmonic superspace approach. It expresses the fact that the harmonic variables belong to the sphere S^2 (actually contain two independent parameters) and the harmonic superfields are functions on this sphere as well. Let us notice that this U(1) charge commutes with the automorphism SU(2) group which acts on the doublet indices i,j.

Also, instead of $D^i, \bar{D}^j$ we will use their projections on $u^{\pm i}$

$$D^{\pm} = D^i u_i^{\pm}, \quad \bar{D}^{\pm} = \bar{D}^i u_i^{\pm}. \tag{2.7}$$

Nonvanishing (anti)commutators of these projections with themselves and with the harmonic derivatives D^{++}, D^{--} are

$$\{D^-, \bar{D}^+\} = i\partial, \quad \{D^+, \bar{D}^-\} = -i\partial, \tag{2.8}$$

$$[D^{++}, D^-] = D^+, \quad [D^{--}, D^+] = D^- \ \text{(and c.c.)}. \tag{2.9}$$

We define now the $N=4$, 1D harmonic superfield $V^{++}(Z,u)$ subjected to the constraints

$$D^+ V^{++} = 0, \quad \bar{D}^+ V^{++} = 0, \tag{2.10}$$

$$D^{++} V^{++} = 0. \tag{2.11}$$

[Their consistency stems from the fact that the differential operators in (2.10), (2.11) are mutually (anti)commuting.] The harmonic constraint (2.11) implies that V^{++} is a homogeneous function of degree 2 in u^{+i}

$$V^{++}(Z,u) = V^{ij}(Z) u_i^+ u_j^+. \tag{2.12}$$

Then, in view of the arbitrariness of u^{+i}, u^{+j}, the constraints (2.10) imply for V^{ij} the original constraints (2.2). Thus the superfield V^{++} obeying (2.10), (2.11) represents the $N=4$ SU(2) conformal supercurrent in the harmonic $N=4$ 1D superspace (see also Ref. 22).

The constraints (2.10) can be viewed as Grassmann analyticity conditions covariantly eliminating in V^{++} the dependence on half of the original Grassmann coordinates, namely, on their u^- projections $\theta^- = \theta^i u_i^-$, $\bar{\theta}^- = \bar{\theta}^i u_i^-$. So V^{++} is an *analytic* harmonic superfield living on an analytic subspace containing only the u^+ projections of $\theta^i, \bar{\theta}^i$

$$\{\zeta^M\} = \{z, \theta^+, \bar{\theta}^+, u^+, u^-\},$$

$$z = x - \frac{i}{2}(\theta^+\bar{\theta}^- + \theta^-\bar{\theta}^+), \quad \theta^\pm = \theta^i u_i^\pm, \quad \bar{\theta}^\pm = \bar{\theta}^i u_i^\pm. \tag{2.13}$$

This harmonic analytic superspace is closed under the action of $N=4$, 1D supersymetry [and actually under the transformations of the whole $N=4$ SU(2) SCA, see below]. Thus, one may construct additional superinvariants as integrals over this superspace. This opportunity will be exploited when constructing the $N=4$ super KdV Hamiltonian and higher order conserved quantities.

In the analytic basis $\{z, \theta^\pm, \bar{\theta}^\pm, u_i^\pm\}$ the covariant spinor derivatives $D^+, \bar{D}^+$ are reduced to the partial derivatives

$$D^+ = -\frac{\partial}{\partial\theta^-}, \quad \bar{D}^+ = -\frac{\partial}{\partial\bar{\theta}^-},$$

and the conditions (2.10) indeed become Grassmann Causchy–Riemann conditions stating the independence of V^{++} on $\theta^-, \bar{\theta}^-$ in this basis

$$V^{++} = V^{++}(\zeta).$$

Now the irreducible components $w^{ij}(x), \zeta^l(x), \bar{\zeta}^l(x), T(x)$ naturally appear in the $\theta^+, \bar{\theta}^+$ expansion of V^{++} as the result of solving the harmonic constraint (2.11). The analyticity-preserving harmonic derivative D^{++} in the analytic basis, when acting on analytic superfields, is given by the expression

$$D^{++} = \partial^{++} - i\theta^+\bar{\theta}^+\partial_z,$$

and using this expression in Eq. (2.11) yields

$$V^{++}(\zeta) = w^{ij}u_i^+u_j^+ - \tfrac{2}{3}\theta^+\xi^k u_k^+ + \tfrac{2}{3}\bar{\theta}^+\bar{\xi}^k u_k^+ + \theta^+\bar{\theta}^+(i\partial w^{ik}u_i^+u_k^- + \tfrac{1}{3}T), \tag{2.14}$$

where the numerical coefficients are inserted for agreement with the definition (2.4).

It is easy to implement the superconformal $N=4$ SU(2) group as a group of transformations in analytic superspace (2.13). Actually, there exist two different realizations of this group in the superspace (2.13)[23,24] which yield as their closure the "large" $N=4$ SO(4)×U(1) superconformal group.[25,26] The realization for which just V^{++} serves as the supercurrent can be written in the following concise form[24]

$$\delta z = (\partial^{--}D^{++} - 2)\lambda, \quad \delta\theta^+ = i\frac{\partial}{\partial\bar{\theta}^+}D^{++}\lambda, \quad \delta\bar{\theta}^+ = -i\frac{\partial}{\partial\theta^+}D^{++}\lambda,$$

$$\delta u_i^+ = (D^{++}\partial\lambda)u_i^- \equiv (D^{++}\Lambda^0)u_i^-, \quad \delta u_i^- = 0. \tag{2.15}$$

Here, the analytic function $\lambda(\zeta)$ satisfies the harmonic constraint

$$(D^{++})^2\lambda(\zeta) = 0 \tag{2.16}$$

and collects all the parameters of $N=4$ SU(2) superconformal transformations

$$\lambda(\zeta)=\lambda+\lambda^{(ij)}u_i^+u_j^-+\theta^+\varepsilon^i u_i^-+\bar{\theta}^+\bar{\varepsilon}^i u_i^-+i\theta^+\bar{\theta}^+\partial\lambda^{(ij)}u_i^-u_j^-, \tag{2.17}$$

$\lambda(z),\varepsilon^i(z),\bar{\varepsilon}^i(z),\partial\lambda^{(ij)}(z)$ being, respectively, the parameters of the conformal, supersymmetry and SU(2) affine transformations.

This realization of the $N=4$ SU(2) superconformal group is fully determined by the requirement that the harmonic derivative D^{++} transforms as

$$\delta D^{++}=-(D^{++}\Lambda^0)D^0. \tag{2.18}$$

The transformation law of V^{++} is almost uniquely fixed from the preservation of the harmonic constraint (2.11):

$$\delta V^{++}\simeq V^{++\prime}(\zeta')-V^{++}(\zeta)=2\Lambda^0V^{++}-\frac{k}{2}D^{++}\partial\Lambda^0, \tag{2.19}$$

where k is a free parameter (its meaning will become clear soon).

In what follows we will never actually need to know the explicit coordinate structure of the analytic superspace and how V^{++} is expressed there. We will only make use of the constraints (2.10), (2.11) and of some important consequences of them, e.g.,

$$(D^{--})^3V^{++}=0,\quad D^-(D^{--})^2V^{++}=\bar{D}^-(D^{--})^2V^{++}=0, \tag{2.20}$$

and those quoted in Appendix A.

After we have represented the $N=4$ SU(2) supercurrent as a harmonic superfield V^{++}, it remains to write the Poisson bracket between two V^{++}'s which yields the $N=4$ SU(2) SCA Poisson brackets for the component currents. Surprisingly, this superfield Poisson bracket is almost uniquely determined by dimensionality and compatibility with the constraints (2.10), (2.11). It reads

$$\{V^{++}(1),V^{++}(2)\}=\mathscr{D}^{(++|++)}\Delta(1-2),$$

$$\mathscr{D}^{(++|++)}\equiv(D_1^+)^2(D_2^+)^2\left(\left[\left(\frac{u_1^+u_2^-}{u_1^+u_2^+}\right)-\frac{1}{2}D_2^{--}\right]V^{++}(2)-\frac{k}{4}\partial_2\right), \tag{2.21}$$

where $\Delta(1-2)=\delta(x_1-x_2)(\theta^1-\theta^2)^4$ is the ordinary 1D $N=4$ superspace delta function and

$$(D^+)^2\equiv D^+\bar{D}^+.$$

We refer to Ref. 21 for more details on harmonic distributions. Note that the harmonic singularity in the rhs of (2.21) is fake: it is cancelled after decomposing the harmonics $u_2^{\pm i}$ over $u_1^{\pm i}$ with making use of the completeness relation (2.5) and the general formula (A6) from Appendix A.

Using the algebra of spinor and harmonic derivatives and also the completeness condition (2.5), one can check that the rhs of (2.21) is consistent with the constraints (2.10), (2.11) with respect to both sets of arguments and antisymmetric under the interchange $1\Leftrightarrow2$. Note that we should require the preservation of the harmonic U(1) charge independently for the points 1 and 2 in order to guarantee that both sets of harmonic variables $u_{1i}^{\pm}$ and $u_{2i}^{\pm}$ parametrize the corresponding internal spheres S^2.

To be convinced that (2.21) gives rise to the correct Poisson brackets for the component currents, we deduce from (2.21) the Poisson brackets of SU(2) affine Kac–Moody currents. After simple algebraic manipulations we obtain for $w^a\equiv\sigma_i^{aj}w_j^i$ the familiar relation:

$$\{w^a(1),w^b(2)\}=\epsilon^{abc}w^c(2)\,\delta(1-2)-\frac{k}{2}\,\delta^{ab}\partial_2\delta(1-2). \tag{2.22}$$

All other currents can also be checked to satisfy the structure relations of $N=4$ SU(2) SCA. We see that the central charge k in (2.21) is the level of the affine su(2) subalgebra.

It is straightforward to rewrite the Poisson structure (2.21) in ordinary $N=4$, 1D superspace. There it looks much more complicated: it involves intricate combinations of SU(2) indices, etc. We will quote it in the next section as an intermediate step in the derivation of the $N=2$ superfield form of this structure.

Finally, we point out that the Poisson structure (2.21) allows us to write the $N=4$ superconformal transformation law of the supercurrent in the following basis-independent form

$$\delta^* V^{++}(\zeta')=4i\int [d\zeta^{-2}]\lambda(\zeta)\{V^{++}(\zeta),V^{++}(\zeta')\}\Rightarrow \tag{2.23}$$

$$\begin{aligned}\delta^* V^{++}(\zeta')=&2(\partial\lambda)V^{++}+(2\lambda-D^{--}D^{++}\lambda)\partial V^{++}-(D^{++}\partial\lambda)D^{--}V^{++}\\&+i(D^-D^{++}\lambda)\bar{D}^-V^{++}-i(\bar{D}^-D^{++}\lambda)D^-V^{++}-\frac{k}{2}\,D^{++}\partial^2\lambda,\end{aligned} \tag{2.24}$$

where $[d\zeta^{-2}]=dz[du]D^-\bar{D}^-$ is the measure of integration over the analytic superspace (the integral over harmonics is defined in the standard way: $\int[du]1=1$ and the integral of any symmetrized product of harmonics is vanishing[20]). It is easy to see that this variation obeys the defining constraints (2.10), (2.11). In the analytic basis of the harmonic superspace, it becomes the active form of the variation (2.19). The coefficient before the inhomogeneous term in (2.19) has been chosen for consistency with the fundamental Poisson structure (2.21). Note that in deriving (2.24) from (2.23) and (2.21) we essentially exploited the identity (A6) from Appendix A.

It is interesting to note that the Poisson bracket (2.21) can be used to introduce the notion of primarity for analytic harmonic $N=4$ superfields. Namely, let us consider a generalization of V^{++}, the analytic superfields $L^{+l}(D^0L^{+l}=lL^{+l})$ subjected to the same harmonic constraint (2.10)

$$D^{++}L^{+l}=0$$

(they can be chosen real for $l=2n$). The homogeneous $N=4$ SU(2) superconformal transformation law of L^{+l} unambiguously follows from the preservation of this constraint

$$\delta L^{+l}=l\Lambda^0L^{+l}.$$

This law can be equivalently reproduced by a formula of the type (2.23), with the following Poisson bracket between V^{++} and L^{+l}

$$\{V^{++}(1),\,L^{+l}(2)\}=\frac{1}{2}\,(D_1^+)^2(D_2^+)^2\left(\left[l\left(\frac{u_1^+u_2^-}{u_1^+u_2^+}\right)-D_2^{--}\right]L^{+l}(2)\Delta(1-2)\right). \tag{2.25}$$

This bracket can be viewed as the manifestly supersymmetric definition of $N=4$ SU(2) primarity for the constrained analytic superfields L^{+l} (at the classical level). It would be of interest to know whether one can define appropriate Poisson brackets between the superfields L^{+l} so that they form, together with (2.21) and (2.25), a closed algebra providing an extension (perhaps, nonlinear) of $N=4$ SU(2) SCA.

B. $N=4$ super KdV

To deduce the super KdV equation with the second Hamiltonian structure given by the $N=4$ SU(2) SCA in the form (2.21) we need to construct the relevant Hamiltonian of the dimension 3. The only requirement we impose *a priori* is that of $N=4$, 1D supersymmetry. The most general dimension 3, $N=4$ supersymmetric Hamiltonian H_3 one may construct out of V^{++} consists of two pieces

$$H_3=\int [dZ]V^{++}(D^{--})^2V^{++}-i\int [d\zeta^{-2}]c^{-4}(u)(V^{++})^3. \tag{2.26}$$

Here $[dZ]=dx[du]D^-\bar{D}^-D^+\bar{D}^+$ is the integration measure of the full harmonic superspace. We see that the U(1) invariance of the integral over analytic subspace requires the inclusion of the harmonic monomial $c^{-4}(u)=c^{ijkl}u_i^-u_j^-u_k^-u_l^-$ which explicitly breaks SU(2) symmetry. The coefficients c^{ijkl} belong to the dimension 5 spinor representation of SU(2), i.e., form a symmetric traceless rank 2 tensor, and completely break the SU(2) symmetry, unless c^{-4} is of the special form

$$c^{-4}(u)=(a^{-2}(u))^2, \quad a^{-2}(u)=a^{ij}u_i^-u_j^- . \tag{2.27}$$

After taking off the harmonics this condition becomes Eq. (1.1). In this case, the symmetry breaking parameter belongs to the dimension 3 (vector) representation of SU(2), and thus has U(1) as a little group. We point out that the presence of the trilinear term in the Hamiltonian is unavoidable if one hopes to eventually obtain an integrable super KdV equation (it should be reduced in some limit to the $N=2$ super KdV family which is integrable only providing the relevant Hamiltonian contains a trilinear term). Thus one necessary condition for the integrability of $N=4$ super KdV is that SU(2) is broken, at least down to its U(1) subgroup.

Using the Hamiltonian (2.26), we construct the relevant evolution equation:

$$V_t^{++}=\{H,V^{++}\}. \tag{2.28}$$

After some rather tedious but straightforward computations, it may be cast into the following form:

$$V_t^{++}=i(D^+)^2\left\{\frac{k}{2}D^{--}V_{xx}^{++}-\left[V^{++}(D^{--})^2V^{++}-\frac{1}{2}(D^{--}V^{++})^2\right]_x-\frac{3}{20}kA^{-4}(V^{++})_x^2 + \frac{1}{2}A^{-6}(V^{++})^3\right\}. \tag{2.29}$$

Here A^{-4} and A^{-6} are differential operators on the 2-sphere $\sim$SU(2)/U(1)

$$A^{-4}=\sum_{N=1}^{4}(-1)^{N+1}c^{2N-4}\frac{1}{N!}(D^{--})^N,$$

$$A^{-6}=\frac{1}{5}\sum_{N=0}^{4}(-1)^Nc^{2N-4}\frac{(5-N)}{(N+1)!}(D^{--})^{N+1}. \tag{2.30}$$

We have used the notation:

$$c^{2N-4}=\frac{(4-N)!}{4!}(D^{++})^Nc^{-4}, \quad N=0,\ldots,4. \tag{2.31}$$

Equation (2.29) is the $N=4$ SU(2) super KdV equation we sought for. It is easy to check that its rhs satisfies the same constraints (2.10), (2.11) as the lhs. One might bring (2.29) into a more explicit form using the algebra (2.8), (2.9) [the first term takes then the familiar form $-(k/2)V^{++}_{xxx}$], but for technical reasons it is convenient to keep the analytic subspace projector $(D^+)^2$ in front of the curly brackets in (2.29). The Hamiltonian (2.26) and Eq. (2.29) can be rewritten in ordinary $N=4$ superspace (Sec. III), but they look there very intricate, like the Poisson bracket (2.21). For instance, the second term in (2.26) would involve explicit θ's, so that it would be uneasy to see that it is supersymmetric. Thus harmonic superspace seems to provide the most appropriate framework for a manifestly $N=4$ supersymmetric formulation of $N=4$ super KdV equation. The last comment concerns the presence of the $N=4$ SU(2) SCA central charge k in (2.29). Making in (2.29) the rescalings $t\to bt$, $V^{++}\to b^{-1}V^{++}$, $c\to bc$, we can in principle change this parameter to any nonzero value. However, in order to have a clear contact with the original $N=4$ SU(2) Poisson structure (2.21), for the time being we prefer to leave $N=4$ super KdV in its original form.

C. Conserved charges

As was mentioned in the Introduction, the $N=2$ super KdV equation is integrable only for $a=4, -2, 1$. Since the SU(2) breaking tensor c^{ijkl} is a direct analog of the $N=2$ KdV parameter a (and is reduced to it upon the reduction $N=4\to N=2$, see Sec. III), one may expect that the $N=4$ super KdV equation is integrable only when certain restrictions are imposed on this tensor. To see which kind of restrictions arises, in Ref. 14 we required the existence of nontrivial conserved charges for (2.29) which are in involution with the Hamiltonian (2.26). Here we recall the results of that analysis.

Conservation of the dimension 1 charge:

$$H_1=\int [d\zeta^{-2}]V^{++} \tag{2.32}$$

imposes no condition on the parameters of the Hamiltonian.

A charge with dimension 2 exists only provided the condition (2.27) ((1.1)) holds. It reads:

$$H_2=i\int [d\zeta^{-2}]a^{-2}(V^{++})^2. \tag{2.33}$$

The conservation of this charge implies a stringent constraint on a^{ij}, namely

$$s\equiv a^{+2}a^{-2}-(a^0)^2=\frac{1}{2}\,a^{ij}a_{ij}=-\frac{10}{k}, \tag{2.34}$$

where

$$a^{+2}=D^{++}a^0=\tfrac{1}{2}(D^{++})^2a^{-2}=a^{ij}u^+_iu^+_j\,.$$

This is just the second condition (1.2) quoted in the Introduction. Note that with the convention (2.27) this condition implies for a^{ik} the following reality properties

$$(a^{ik})^\dagger=-\epsilon_{ij}\epsilon_{kl}a^{kl}\Leftrightarrow(a^{12})^\dagger=a^{12},\quad (a^{11})^\dagger=-a^{22}. \tag{2.35}$$

Assuming that the central charge k is an integer [if we restrict ourselves to unitary representations of the SU(2) Kac–Moody algebra[27]], Eq. (2.34) means that a^{ij} parametrizes some sphere $S^2\sim$SU(2)/U(1), such that the reciprocal of its radius is *quantized*. It is interesting to explicitly find the evolution equation produced by H_2 through the Hamiltonian structure (2.21)

$$V^{++}_{t'}=3\{H_2,V^{++}\}\Rightarrow \tag{2.36}$$

$$V^{++}_{t'}=\frac{i}{2}\,(D^+)^2\{k\tilde{A}^{-2}V^{++}_x-3\tilde{A}^{-4}(V^{++})^2\},$$

$$\tilde{A}^{-2}=a^0D^{--}-\tfrac{1}{2}a^{+2}(D^{--})^2,$$

$$\tilde{A}^{-4}=a^{-2}D^{--}-\tfrac{1}{3}a^0(D^{--})^2+\tfrac{1}{18}a^{+2}(D^{--})^3, \tag{2.37}$$

[the factor 3 in (2.36) was chosen for further convenience]. This equation is the first nontrivial one in the conjectured $N=4$ KdV hierarchy. As was recently noticed,[28] the $N=2$ counterpart of this equation can be interpreted as a ''disguised'' form of the $N=2$ supersymmetric extension of the nonlinear Schrödinger equation (NLS). Thus, it is natural to expect that Eq. (2.37) is related in an analogous way to the $N=4$ extended NLS.

The last conserved charge we constructed in Ref. 14 is a dimension 4 one H_4 (the dimension 3 conserved charge is the $N=4$ KdV Hamiltonian itself). H_4 exists under the same restrictions (2.27), (2.34) [or, equally, (1.1), (1.2)] on c^{ijkl} and reads:

$$H_4=\int [dZ]a^{-2}V^{++}(D^{--}V^{++})^2+\frac{i}{6}\int [d\zeta^{-2}]\left[\frac{7}{6}\,(a^{-2})^3(V^{++})^4-ka^{-2}(V^{++}_x)^2\right]. \tag{2.38}$$

It is curious that it yields the same $N=4$ KdV equation (2.29) via the first Hamiltonian structure associated with the Poisson bracket

$$\{V^{++}(1),V^{++}(2)\}_{(1)}=i\beta\left(a^0(1)-a^{+2}(1)\,\frac{u^-_1u^+_2}{u^+_1u^+_2}\right)(D^+_1)^2(D^+_2)^2\Delta(1-2). \tag{2.39}$$

Here, β is an arbitrary real constant. This bracket is related to the original one (2.21) by the shift

$$V^{++}\to V^{++}+i\beta a^{+2}(u). \tag{2.40}$$

Taking as a new Hamiltonian

$$H_{(1)}=-i\,\frac{9k}{4\beta}\,H_4, \tag{2.41}$$

we reproduce (2.29) as the Hamiltonian flow:

$$V^{++}_t=\{H_{(1)},V^{++}\}_{(1)}. \tag{2.42}$$

This comes about in a very nontrivial way, since both the new Poisson bracket (2.39) and the new Hamiltonian (2.41) are proportional to the SU(2) breaking parameter a^{ij}, while the super KdV equation (2.29) includes terms containing no dependence on a^{ij}. The key point is that these terms appear in (2.42) multiplied by the factor

$$-\frac{k}{10}\,s=-\frac{k}{20}\,a^{ij}a_{ij},$$

which is independent of harmonic coordinates $u^\pm$ and is constrained to be 1 from the condition (2.34).

Thus the conditions (2.27) and (2.34) [(1.1), (1.2)] are necessary not only for the existence of the first nontrivial conservation laws for Eq. (2.29), but also for it to be bi-Hamiltonian. This property persists for the evolution equations associated with other conserved charges. For instance, with respect to the structure (2.39) Eq. (2.37) with a^{ik} constrained by (1.2) has H_3 as the Hamiltonian.

The presence of the bi-Hamiltonian structure and the existence of nontrivial conserved charges are indications that $N=4$ KdV equation (2.29) with the restrictions (2.27), (2.34) [(1.1), (1.2)] is integrable, i.e., gives rise to a whole $N=4$ super KdV hierarchy. Clearly, in order to prove this, one should, before all, either find the relevant Lax pair or prove the existence of an infinite number of conserved charges of the type given above (e.g., by employing recursion relations implied by the bi-Hamiltonian property[1,11]). Unfortunately, at present it is a very nontrivial and technically complicated problem to analyze these issues in full generality in the framework of harmonic superspace. Even the direct construction of the next, dimension 5 charge H_5, turned out to be too intricate. In Sec. III we will reformulate $N=4$ KdV in $N=2$ superspace where powerful computer methods for such calculations have been developed. One thing which can be proven in a relatively simple way in the framework of the HSS formalism is that Eq. (2.27) [Eq. (1.1)] is a necessary condition for the existence of higher-order conserved charges for (2.29). We end the present section with the proof.

First of all, it is clear that after the reduction to $N=2$ such charges should become those of the integrable $N=2$ super KdV equations (see Sec. III for details of this reduction). Any such charge of dimension, say, l is known to contain in the integrand a term $\sim V^l$, where V is the $N=2$ super KdV superfield ($N=2$ superconformal stress-tensor).[8,9] These terms can only be obtained by reduction of analytic integrals of the form

$$\sim \int [d\zeta^{-2}] b^{-2(l-1)} (V^{++})^l, \tag{2.43}$$

where

$$b^{-2(l-1)} = b^{i_1 \dots i_{2(l-1)}} u^-_{i_1} \dots u^-_{i_{2(l-1)}}. \tag{2.44}$$

If the corresponding charge is to be conserved, the highest order contribution to the time derivative of (2.43) [coming from the third order term in the rhs of (2.29)] should vanish separately. A simple analysis shows that it is possible if and only if

$$b^{-2(l-1)} \sim (a^{-2})^{l-1}, \quad c^{-4} = (a^{-2})^2. \tag{2.45}$$

Note that in our previous paper[14] an erroneous statement that this condition is necessary only for $l=2n$ was made.

III. $N=4$ KdV IN $N=2$ SUPERSPACE

A. $N=4$ KdV and $N=4$ SU(2) SCA in ordinary $N=4$ superspace

We first rewrite Eq. (2.29) in ordinary $N=4$ superspace, where it is expressed as an equation for the superfield $V^{ij}(Z)$ constrained by Eqs. (2.2). A straightforward calculation, that makes use of the identities given in Appendix A, yields

$$\begin{aligned} V^{ij}_t = & \left\{ -\frac{1}{2} k V^{ij}_{xx} - 2 V^{(il}_x V^{j)}_l + \frac{2i}{3} T V^{ij} - \frac{4i}{9} \xi^{(i} \bar{\xi}^{j)} - \frac{3}{10} (c^{klf(i} V_{kl} V^{j)}_f)_x + \frac{3}{10} k c^{klf(i} V_{klx} V^{j)}_f \right. \\ & \left. - \frac{i}{10} k c^{ijkl} \left(T V_{kl} + \frac{4}{3} \xi_{(k} \bar{\xi}_{l)} \right) \right\}_x - \frac{3}{10} c^{klfg} V_{kl} V_{fg} V^{ij}_x - \frac{3}{5} c^{klfg} V_{kl} (V^i_f V^j_g)_x \\ & - \frac{i}{5} c_{klf(i} (B^{j)}_k V_{lf} + V^{j)}_k B_{lf}). \end{aligned} \tag{3.1}$$

Here,

$$B^{ij} \equiv TV^{ij} + \tfrac{8}{3}\xi^{(i}\bar{\xi}^{j)}, \tag{3.2}$$

the irreducible superfield projections $\xi^k, \bar{\xi}^l, T$ were defined in (2.4) and the subscript "x" corresponds as before to x-derivative. We have verified that both sides of Eq. (3.1) respect the constraints (2.2).

It is also straightforward to rewrite the Poisson bracket (2.21) in ordinary $N=4$ superspace

$$\{V^{ij}(Z_1), V^{kl}(Z_2)\} = -\mathscr{D}^{(ij|kl)}\Delta(1-2), \tag{3.3}$$

$$\mathscr{D}^{(ij|kl)} = \frac{1}{4}\left\{\left[iV^{ik}D^{jl}\partial + \frac{1}{3}V^{ik}\epsilon^{jl}D^4 + \frac{i}{2}\partial V^{kl}D^{ij} + \frac{1}{6}(\bar{\xi}^k\epsilon^{il}D^2\bar{D}^j + \xi^k\epsilon^{il}\bar{D}^2D^j) \right.\right.$$
$$\left.\left. + \frac{i}{4}k\left(\epsilon^{jl}D^{ik}\partial^2 - \frac{i}{3}\epsilon^{ik}\epsilon^{jl}D^4\partial\right)\right] + (k\leftrightarrow l)\right\} + (i\leftrightarrow j). \tag{3.4}$$

Here

$$D^{ij} \equiv D^{(i}\bar{D}^{j)}, \quad D^2 \equiv D^iD_i, \quad \bar{D}^2 \equiv \bar{D}_i\bar{D}^i, \quad D^4 \equiv D^{ij}D_{ij}, \tag{3.5}$$

and the differential operator (3.4) is evaluated at the point Z_2.

The $N=4$ KdV Hamiltonian (2.26) and the other conserved charges presented in the previous section can also be appropriately rewritten. However, it is not very enlightening to do so, because, as was already said above, only those pieces of these charges which live in the whole harmonic superspace retain a manifestly supersymmetric form after passing to the standard $N=4$ superspace [e.g., the integrand in the first term in (2.26) becomes $\sim V^{ij}V_{ij}$]. The ordinary $N=4$ superspace form of the analytic harmonic superspace pieces explicitly includes θ's. Below we will rewrite these conserved quantities via $N=2$ superfields, so that both kinds of terms will be represented as integrals over the same $N=2$ superspace without explicit θ's in the integrands.

B. From $N=4$ to $N=2$

To make a reduction to $N=2$ superspace, we split the $N=4$, 1D superspace (2.1) as follows

$$\{Z^M\} = (x, \theta, \bar{\theta}) \otimes (\eta, \bar{\eta}) \equiv \{Z^\mu\} \otimes (\eta, \bar{\eta}) \tag{3.6}$$

with

$$\theta \equiv \theta^1, \quad \bar{\theta} \equiv \bar{\theta}_1, \quad \eta \equiv \theta^2, \quad \bar{\eta} \equiv \bar{\theta}_2. \tag{3.7}$$

We also split the set of covariant spinor derivatives into those acting in $N=2$ SS $\{Z^\mu\}$ and those acting on the extra spinor coordinates $\eta, \bar{\eta}$

$$D_1 \equiv D, \quad \bar{D}^1 \equiv \bar{D}, \quad D_2 \equiv d, \quad \bar{D}^2 = \bar{d},$$
$$\{D, \bar{D}\} = i\partial, \quad \{d, \bar{d}\} = i\partial, \tag{3.8}$$

(all other anticommutators are vanishing). Then we put the constraints (2.2) into the form

$$DV^{22} = 0, \quad dV^{11} = 0, \quad dV^{12} = \tfrac{1}{2}DV^{11}, \quad dV^{22} = 2DV^{12}, \tag{3.9}$$

$$\bar{D}V^{11}=0, \quad \bar{d}V^{22}=0, \quad \bar{d}V^{12}=-\tfrac{1}{2}\bar{D}V^{22}, \quad \bar{d}V^{11}=-2\bar{D}V^{12}. \tag{3.10}$$

The first equations in the sets (3.9) and (3.10) are most essential. They tell us that the superfields V^{11} and $V^{22}=(V^{11})^{\dagger}$ are chiral and anti-chiral in the $N=2$ superspace. The remainder of constraints and their consequences

$$d\bar{d}V^{12}=\bar{D}DV^{12}, \quad d\bar{d}V^{11}=iV^{11}_{x}, \quad \bar{d}dV^{22}=iV^{22}_{x}, \tag{3.11}$$

serve to express all the coefficient $N=2$ superfields in the $\eta,\overline{\eta}$ expansion of V^{12}, V^{11}, and V^{22} in terms of spinor and ordinary derivatives of the lowest order $N=2$ superfields

$$V(Z^{\mu})\equiv V^{12}(Z^{M})\big|_{\eta=0}, \quad \Phi(Z^{\mu})\equiv V^{11}(Z^{M})\big|_{\eta=0}, \quad \overline{\Phi}(Z^{\mu})\equiv V^{22}(Z^{M})\big|_{\eta=0}, \tag{3.12}$$

$$\bar{D}\Phi=0, \quad D\overline{\Phi}=0. \tag{3.13}$$

Note that $V(Z^{\mu})$ is not constrained by (3.9), (3.10).

Thus, by going to $N=2$ superspace we have explicitly solved the constraints (2.2) in terms of an unconstrained $N=2$ superfield V and a pair of conjugate chiral and anti-chiral $N=2$ superfields $\Phi,\overline{\Phi}$. Now it is clear how to obtain the $N=2$ superfield form of Eq. (3.1). Its rhs obeys the same constraints (2.2) as the lhs, so one should express all the $N=4$ spinor derivatives in the former through $N=2$ spinor derivatives, by using the constraints in the form (3.9), (3.10). Then one puts $\eta=\overline{\eta}=0$ in both sides of the equations obtained. Some useful relations are

$$\xi^{1}=-\frac{3}{2}DV^{11}, \quad \xi^{2}=-3DV^{12}, \quad \bar{\xi}^{1}=-3\bar{D}V^{12},$$

$$\bar{\xi}^{2}=-\frac{3}{2}\bar{D}V^{22}, \quad T=3[D,\bar{D}]V^{12}. \tag{3.14}$$

The last step needed to put $N=4$ KdV in a convenient $N=2$ superfield form consists of choosing an appropriate frame with respect to the global SU(2) that acts on both the doublet indices in (3.1) and the doublet indices of the $N=4$ superspace Grassmann coordinates. It is easy to show that this frame can always be chosen so that only two real components in the SU(2) breaking tensor c^{iklj} are nonzero

$$c^{1212}\equiv\frac{5}{6}a, \quad c^{1111}=c^{2222}\equiv\frac{5}{6}b, \quad c^{1112}=c^{2221}=0 \tag{3.15}$$

(the numerical factors were introduced for further convenience). Note that this is still true if c^{ijkl} is bilinear in the constant vector a^{ik} in accord with Eq. (2.27). In this important case

$$c^{ijkl}=\tfrac{1}{3}(a^{ij}a^{kl}+a^{ik}a^{jl}+a^{il}a^{jk}). \tag{3.16}$$

For three independent SU(2) fixations of a^{ik}

$$\text{(a)}\ \ a^{11}=a^{22}=0, \quad a^{12}\neq 0; \quad \text{(b)}\ \ a^{12}=0, \quad a^{11}=a^{22}\neq 0;$$

$$\text{(c)}\ \ a^{12}=0, \quad a^{11}=-a^{22}\neq 0, \tag{3.17}$$

the components of c^{ijkl} satisfy (3.15). The values of a and b are given by

$$\text{(a)}\ \ a=\tfrac{4}{5}a^{12}a^{12}, \quad b=0; \quad \text{(b)}\ \ a=\tfrac{2}{5}a^{11}a^{11}, \quad b=3a$$

$$\text{(c)}\quad a=-\tfrac{2}{5}a^{11}a^{22},\quad b=-3a. \tag{3.18}$$

As we will see below, only these choices of the SU(2) frame allow an unambiguous reduction to $N=2$ KdV.

The whole tensor c^{ijkl} [or a^{ik} in the case (2.27),(3.16)] can be restored by an appropriate SU(2) rotation. It is instructive to describe how these SU(2) rotations, which are manifest in the original $N=4$ superspace, are realized on $N=2$ superfields $V,\Phi,\bar{\Phi}$

$$\begin{aligned}
\delta^*V&=-\lambda_0\left(\theta\frac{\partial}{\partial\theta}-\bar{\theta}\frac{\partial}{\partial\bar{\theta}}\right)V+\lambda_+[\Phi+D(\theta\Phi)]-\lambda_-[\bar{\Phi}-\bar{D}(\bar{\theta}\bar{\Phi})],\\
\delta^*\Phi&=\lambda_0\left(2-\theta\frac{\partial}{\partial\theta}+\bar{\theta}\frac{\partial}{\partial\bar{\theta}}\right)\Phi+\lambda_-\bar{D}(\bar{\theta}V),\\
\delta^*\bar{\Phi}&=\lambda_0\left(-2-\theta\frac{\partial}{\partial\theta}+\bar{\theta}\frac{\partial}{\partial\bar{\theta}}\right)\bar{\Phi}+\lambda_+D(\theta V).
\end{aligned} \tag{3.19}$$

For completeness, we also give the transformation properties of the superfields under the second complex supersymmetry, implicit in the $N=2$ superfield notation

$$\begin{aligned}
\delta^*V&=\tfrac{1}{2}\epsilon^2D\Phi+\tfrac{1}{2}\bar{\epsilon}_2\bar{D}\bar{\Phi},\\
\delta^*\Phi&=2\bar{\epsilon}_2\bar{D}V,\quad \delta^*\bar{\Phi}=2\epsilon^2DV.
\end{aligned} \tag{3.20}$$

After these preparatory steps and choosing, for convenience, $k=2$ henceforth, we deduce the $N=4$ SU(2) KdV equation in an $N=2$ superfield form as the following system of coupled evolution equations

$$\begin{aligned}
V_t=&-V_{xxx}+3i([D,\bar{D}]VV)_x-\frac{i}{2}(1-a)([D,\bar{D}]V^2)_x-3aV_xV^2+\frac{1}{4}(a-4)(\Phi_x\bar{\Phi}-\bar{\Phi}_x\Phi)_x\\
&+\frac{i}{2}(a-1)(D\Phi\bar{D}\bar{\Phi})_x-\frac{3}{2}a(V\Phi\bar{\Phi})_x+\frac{1}{8}b(\Phi^2-\bar{\Phi}^2)_{xx}-\frac{3}{4}b[V(\Phi^2+\bar{\Phi}^2)]_x\\
&+\frac{i}{2}b[D,\bar{D}][V(\Phi^2-\bar{\Phi}^2)],
\end{aligned} \tag{3.21}$$

$$\begin{aligned}
\Phi_t=&-\Phi_{xxx}-\frac{5}{4}b\Phi_x\Phi^2-\bar{D}[6i(DV\Phi)_x-i(a+2)D(V\Phi)_x]\\
&+\bar{D}D\left[3ia\left(V^2\Phi+\frac{1}{4}\Phi^2\bar{\Phi}\right)+ib(V\bar{\Phi})_x+ib\left(V^2\bar{\Phi}+\frac{1}{4}\bar{\Phi}^2\Phi\right)\right],
\end{aligned} \tag{3.22}$$

$$\begin{aligned}
\bar{\Phi}_t=&-\bar{\Phi}_{xxx}-\frac{5}{4}b\bar{\Phi}_x\bar{\Phi}^2+D[6i(\bar{D}V\bar{\Phi})_x-i(a+2)\bar{D}(V\bar{\Phi})_x]\\
&+D\bar{D}\left[3ia\left(V^2\bar{\Phi}+\frac{1}{4}\bar{\Phi}^2\Phi\right)-ib(V\Phi)_x+ib\left(V^2\Phi+\frac{1}{4}\Phi^2\bar{\Phi}\right)\right].
\end{aligned} \tag{3.23}$$

We have explicitly checked that Eqs. (3.21)–(3.23) are covariant under the second hidden supersymmetry (3.20). It is also obvious from the form of Eqs. (3.22), (3.23) that they are consistent with the $N=2$ chirality properties of $\Phi,\bar{\Phi}$.

Proceeding in a similar way, one can rewrite the second and first Poisson bracket structures (2.21) and (2.39) in terms of the $N=2$ superfields

$$\{V^A(1),V^B(2)\}=\mathscr{D}^{AB}\Delta^{(2)}(1-2), \tag{3.24}$$

$$\mathscr{D}^{11}=\frac{1}{4}\left(iV\partial+i\partial V-\bar{D}VD-DV\bar{D}+\frac{k}{4}[D,\bar{D}]\partial\right)$$

$$\mathscr{D}^{12}=\frac{1}{4}(i\partial\Phi+2\Phi\bar{D}D-D\Phi\bar{D}),\quad \mathscr{D}^{13}=\frac{1}{4}(i\partial\bar{\Phi}+2\bar{\Phi}D\bar{D}-\bar{D}\bar{\Phi}D),$$

$$\mathscr{D}^{21}=\frac{1}{4}(2\Phi D\bar{D}+D\Phi\bar{D}),\quad \mathscr{D}^{23}=\left(VD\bar{D}+DV\bar{D}-\frac{k}{4}D\bar{D}\partial\right)$$

$$\mathscr{D}^{31}=\frac{1}{4}(2\bar{\Phi}\bar{D}D+\bar{D}\bar{\Phi}D),\quad \mathscr{D}^{32}=\left(V\bar{D}D+\bar{D}VD+\frac{k}{4}\bar{D}D\partial\right),$$

$$\mathscr{D}^{22}=\mathscr{D}^{33}=0 \tag{3.25}$$

$$\{V^A(1),V^B(2)\}_{(1)}=\mathscr{D}^{AB}_{(1)}\Delta^{(2)}(1-2), \tag{3.26}$$

$$\mathscr{D}^{11}_{(1)}=-\frac{1}{4}\beta a^{12}\partial,\quad \mathscr{D}^{12}_{(1)}=\frac{i}{2}\beta a^{11}\bar{D}D,\quad \mathscr{D}^{13}_{(1)}=\frac{i}{2}\beta a^{22}D\bar{D},$$

$$\mathscr{D}^{21}_{(1)}=\frac{i}{2}\beta a^{11}D\bar{D},\quad \mathscr{D}^{22}_{(1)}=0,\quad \mathscr{D}^{23}_{(1)}=i\beta a^{12}D\bar{D},$$

$$\mathscr{D}^{31}_{(1)}=\frac{i}{2}\beta a^{22}\bar{D}D,\quad \mathscr{D}^{32}_{(1)}=i\beta a^{12}\bar{D}D,\quad \mathscr{D}^{33}_{(1)}=0. \tag{3.27}$$

In these formulas we made use of the condensed notation

$$V^A\equiv(V,\Phi,\bar{\Phi})$$

and defined the $N=2$ superspace delta function by

$$\Delta^{(2)}(1-2)\equiv(d_2\bar{d}_2\Delta(1-2))\big|_{\eta=\bar{\eta}=0}.$$

The differential operators $\mathscr{D}^{AB},\mathscr{D}^{AB}_{(1)}$ are evaluated at the second point of $N=2$ superspace.

Using the relation between the $N=4$ and $N=2$ superspace integration measures

$$[dZ]=\mu^{(2)}[du]d\bar{d},\quad [d\zeta^{-2}]=-\mu^{(2)}[du][(\theta\bar{\theta}d\bar{d}-1)u^-_1u^-_2+\theta du^-_1u^-_1+\bar{\theta}\bar{d}u^-_2u^-_2], \tag{3.28}$$

with

$$\mu^{(2)}\equiv dx\ d\theta\ d\bar{\theta}=dx\ D\bar{D}, \tag{3.29}$$

and the constraints (3.9),(3.10), it is also easy to get the $N=2$ superfield form of the $N=4$ KdV Hamiltonian (2.26)

$$H_3=\int\mu^{(2)}\left\{8\bar{D}V\,DV+2i\Phi_x\bar{\Phi}+\frac{i}{3}a(V^3+6V\Phi\bar{\Phi})+ib(V\Phi^2+V\bar{\Phi}^2)\right\}. \tag{3.30}$$

Note that each of the three parts of (3.30), viz. those with the coefficients a and b and the remainder, are separately invariant with respect to the hidden supersymmetry transformations (3.20). At the same time, only the first piece (containing no dependence on a and b) respects the invariance under the SU(2) transformations (3.19) [it comes from the first integral in the original

expression (2.26)]. Applying (3.19) to the terms proportional to a and b, one can restore all five components of the initial SU(2) breaking tensor c^{iklj}. These will appear with appropriate $N=4$ superinvariant combinations of $V,\Phi,\bar{\Phi}$ and derivatives of the latter.

It is a straightforward exercise to rederive Eqs. (3.21)–(3.23) as the evolution equations with respect to the $N=2$ superfield Hamiltonian structure (3.24),(3.25),(3.30)

$$V_t^A = \mathscr{D}^{BA}\,\frac{\delta H_3}{\delta V^B}. \tag{3.31}$$

As was mentioned in Sec. II, the same $N=4$ super KdV equation, provided the constraints (1.1), (1.2) hold (their form in the $N=2$ notation will be discussed in the next subsection), can be regarded as an evolution equation with respect to the first Poisson structure (2.39),(3.26) with H_4 as the Hamiltonian, Eq. (2.42). In $N=2$ superfield language, this form of $N=4$ KdV is as follows

$$V_t^A = -\,i\,\frac{9}{2\beta}\,\mathscr{D}^{BA}_{(1)}\,\frac{\delta H_4}{\delta V^B}. \tag{3.32}$$

The $N=2$ superfield form of the conserved charge H_4 (2.38) will be given below (Sec. IV).

C. Reduction to $N=2$ super KdV and the integrability conditions

The first line of Eq. (3.21), up to unessential redefinitions, is just the rhs of $N=2$ super KdV equation,[8,9] with the parameter a related to the SU(2) breaking tensor of $N=4$ super KdV as

$$a = \tfrac{6}{5}c^{1212}. \tag{3.33}$$

Thus, the reduction to $N=2$ KdV is obtained by putting

$$\Phi = \bar{\Phi} = 0 \tag{3.34}$$

in Eqs. (3.21)–(3.23). As a result of the reduction, one gets

$$V_t = -V_{xxx} + 3i([D,\bar{D}]VV)_x - \frac{i}{2}\,(1-a)([D,\bar{D}]V^2)_x - 3aV_xV^2. \tag{3.35}$$

This equation is related to the standard form of $N=2$ KdV equation given in Refs. 8 and 9 via the redefinitions

$$V=\tilde{V},\quad \partial_x = i\tilde{\partial}_x,\quad \partial_t = -i\tilde{\partial}_t,\quad D=\tfrac{1}{2}(D_1+iD_2),\quad \bar{D}=-\tfrac{1}{2}(D_1-iD_2),$$
$$D_1^2 = D_2^2 = \tilde{\partial}_x. \tag{3.36}$$

We should point out that the above reduction is consistent because Eqs. (3.22) and (3.23) are homogeneous in $\Phi,\bar{\Phi}$ and, for this reason, condition (3.34) together with Eq. (3.35) yield a particular solution of the original set (3.21)–(3.23). The superfield V satisfies Eq. (3.35) and is unconstrained otherwise. All the conserved charges of $N=4$ KdV become conserved charges of $N=2$ KdV in the reduction limit.

This is not the case for any *other* choice of the SU(2) frame beside those leading to (3.15). This is because for nonzero c^{1112} and c^{2221} there appear extra pieces in the equations for $\Phi,\bar{\Phi}$, that *do not vanish* after the reduction (3.34). For example, for Eq. (3.22) these pieces are as follows

$$\Delta\Phi_t = -\tfrac{2}{5}ic^{1112}\bar{D}D[3VV_x + 4V^3]. \tag{3.37}$$

In this case, the reduction to $N=2$ KdV is inconsistent, because the superfield V becomes constrained in the $N=2$ KdV limit [the rhs of Eq. (3.37) should vanish after imposing (3.34)]. To avoid confusion, we mention that the systems associated with these other choices of the SU(2) frame are simply other ''SU(2) gauges'' of the same $N=4$ super KdV equation. They can be rotated into Eqs. (3.21)–(3.23) by an appropriate SU(2) transformation. Only in the $N=2$ KdV limit, where SU(2) covariance gets broken, different choices of the SU(2) frame turn out to lead to inequivalent systems.

Now let us see which values of a correspond to the restrictions (2.27),(2.34) [or (1.1),(1.2)] that are required for $N=4$ KdV to be integrable. According to the reasonings just mentioned, only three directions of the SU(2) vector a^{ij}, summarized in Eq. (3.17), allow for an unambigous reduction to $N=2$ super KdV. Indeed, only under this choice the components

$$c^{1112}=-(c^{2221})^{\dagger}=a^{11}a^{12}$$

are zero. Then, substituting the relations (3.17) into (2.34) we find three cases for which $N=4$ super KdV in the $N=2$ superfield form (3.21)–(3.23) is expected to be integrable

$$\text{(a)}\ \ a=4,\quad b=0;\quad \text{(b)}\ \ a=-2,\quad b=-6;\quad \text{(c)}\ \ a=-2,\quad b=6. \tag{3.38}$$

In the full $N=4$ case these possibilities are all equivalent since they are related by SU(2) rotations. Nevertheless, they yield inequivalent systems upon the reduction (3.34). Remarkably, *these are precisely two integrable $N=2$ KdV hierarchies, the $a=4$ and $a=-2$ $N=2$ KdVs.*[8,9]

Thus, the single $N=4$ SU(2) super KdV equation (2.29) [or its equivalent forms (3.1) and (3.21)–(3.23)] with the restrictions (2.27) and (2.34) [(1.1),(1.2)] embodies as particular solutions two of the three integrable inequivalent $N=2$ super KdV equations. Below we will explicitly construct the $N=2$ superfield form of the dimension 5 and 6 conserved charges for $N=4$ KdV and show that they exist only for the values of the parameters a and b listed in Eq. (3.38). This is a strong evidence that a unique $N=4$ SU(2) KdV hierarchy exists, yielding by reduction the $a=4$ and $a=-2$, $N=2$ KdV hierarchies (3.34). Reversing the argument, we conclude that only these two $N=2$ KdV hierarchies can be promoted to the $N=4$ SU(2) KdV hierarchy. It is worth noting that in this respect the latter is complementary to the $N=3$ super KdV one[13] which yields, upon the reduction to $N=2$ superspace, the $a=1$, $N=2$ KdV.

In the rest of this section we discuss how to recover the restrictions (1.2), (1.1) directly at the level of the $N=2$ superfield formulation, starting from the $N=2$ superfield system (3.21)–(3.23), with the parameters a and b restricted to the values (3.38) by some reasoning (e.g., coming from the study of higher-order conserved quantities). The only extra assumption will be that the parameters a and b correspond to a SU(2) fixed form of some constant tensor c^{iklj} in accordance with the definition (3.15). In other words, we assume that the system (3.21)–(3.23) still ''remembers'' about its manifestly SU(2) covariant and $N=4$ supersymmetric origin.

First of all, computing two independent invariants of c^{iklj},

$$\mathscr{A}\equiv c^{ijkl}c_{ijkl},\quad \mathscr{B}\equiv c^{ik}{}_{jl}c^{jl}{}_{ft}c^{ft}{}_{ik},$$

for three options in (3.38), we find that in all cases the invariants take the same values

$$\mathscr{A}=\tfrac{2}{3}\,10^2,\quad \mathscr{B}=-\tfrac{2}{9}\,10^3, \tag{3.39}$$

from which it follows that the above choices represent the same tensor c_0^{iklj} in different SU(2) frames (up to possible discrete reflection-type transformations of c^{ikjl}). Further, according to the Lemma proved in Appendix B, the necessary and sufficient conditions for c^{ijkl} to have the special form (1.1) are the following two:

$$\mathscr{A}^3=6.\mathscr{B}^2,\quad \mathscr{B}<0. \tag{3.40}$$

The values (3.39) satisfy these criterions, from which follows the constraint (1.1) for c_0^{iklj}. From (1.1) and (3.15) we find

$$a=\tfrac{2}{5}(2a^{12}a^{12}+a^{11}a^{22}),\quad b=\tfrac{6}{5}a^{11}a^{11}=\tfrac{6}{5}a^{22}a^{22},\quad a^{12}a^{11}=a^{12}a^{22}=0. \tag{3.41}$$

Then, for the three options in (3.38), we have the following solutions for a^{ik}

$$\text{(a)}\ \ a^{12}=\pm\sqrt{5},\quad a^{11}=a^{22}=0;\quad \text{(b)}\ \ a^{12}=0,\quad a^{11}=a^{22}=\pm i\sqrt{5};$$

$$\text{(c)}\ \ a^{12}=0,\quad a^{11}=-a^{22}=\pm\sqrt{5}. \tag{3.42}$$

In all these three cases

$$|a|^2=-a^{ij}a_{ij}=2(a^{12}a^{12}-a^{11}a^{22})=10 \tag{3.43}$$

that is precisely the constraint (1.2) at $k=2$. Note that the reconstruction of the vector a^{ik} from the known c_0^{ijkl} is unique modulo some reflections of a^{ik}, as is seen from the explicit solution (3.42).

Finally, we note that, when analyzing the integrability properties of $N=4$ super KdV in the $N=2$ superfield formulation, we actually do not need to keep track of all these subtleties concerning the relation between c^{ijkl} and a^{ik}, etc. One can forget about the $N=4$ superfield origin of the system (3.21)–(3.23) and view it as some two-parameter extension of $N=2$ KdV equation. Then the specific values (3.38) of the parameters a and b come out as the values at which this system possesses higher-order conserved charges and is bi-Hamiltonian (see the next section). Of course, in order to see that the three options in Eq. (3.38) are actually equivalent to each other, one should take into account the fact that the system (3.21)–(3.23) respects a hidden SU(2) symmetry, or, eqivalently, admits a manifestly $N=4$ supersymmetric and SU(2) covariant description discussed in Sec. II. The above discussion was aimed just at carefully clarifying the links between this latter description and the $N=2$ superfield one.

IV. CONSERVED CHARGES IN THE $N=2$ SUPERFIELD FORMULATION

In this section we put into an $N=2$ superfield form all the $N=4$ super KdV conserved charges given in Ref. 14 and Sec. II and present two new ones: H_5 and H_6. We find that all these charges exist under the same restrictions (3.38) which, as was discussed in the end of the previous section, actually amount to the original constraints (1.1), (1.2).

A. The charges H_1 and H_2

In order to find the $N=2$ superfield representation of the conserved charges initially written as integrals over $N=4$ HSS and its analytic subspace, we proceed in the same way that was used to get the $N=2$ superfield form of H_3, Eq. (3.30). Namely, we make use of the relations (3.28) and (3.9),(3.10) and do the harmonic integrals in the end.

The charge H_1 (2.32) is of the same form as in the $N=2$ KdV case

$$H_1=-2\int \mu^{(2)}V. \tag{4.1}$$

Starting with H_2, nontrivial contributions of the superfields $\Phi,\overline{\Phi}$ come out

$$H_2=\frac{4i}{3}\int \mu^{(2)}\left\{a^{12}\left(V^2+\frac{1}{2}\,\Phi\overline{\Phi}\right)-a^{11}V\overline{\Phi}-a^{22}V\Phi\right\}. \tag{4.2}$$

Like in H_3, three terms in (4.2) are separately invariant under the hidden supersymmetry (3.20) but are mixed by the SU(2) transformations (3.19). Assuming for the moment that the coefficients

a^{ik} are *arbitrary*, we have checked the conservation of (4.2) with respect to Eqs. (3.21)–(3.23), both "by hand" and using the computer, and found $(H_2)_t$ to vanish under the following conditions

$$\begin{aligned} &\text{(a)}\quad a=4, \quad b=0, \quad a^{12}\neq 0, \quad a^{11}=a^{22}=0;\\ &\text{(b)}\quad a=-2, \quad b=-6, \quad a^{12}=0, \quad a^{11}=a^{22}\neq 0;\\ &\text{(c)}\quad a=-2, \quad b=6, \quad a^{12}=0, \quad a^{11}=-a^{22}\neq 0. \end{aligned} \tag{4.3}$$

Keeping in mind the discussion in the end of the previous section [see Eqs. (3.42)], these solutions, up to relative scaling factors, precisely correspond to the conditions (1.1), (1.2) found from the computations in HSS.

This is the appropriate place to give the $N=2$ superfield form of the evolution equation (2.37) associated with the Hamiltonian H_2. It can be obtained either by a direct transition to $N=2$ superfields in (2.37) or using the $N=2$ Poisson structure (3.24), (3.25)

$$V^A_{t'}=3\mathscr{D}^{BA}\frac{\delta H_2}{\delta V^B}. \tag{4.4}$$

Both these equivalent ways yield the same $N=2$ superfield system

$$\begin{aligned} V_{t'}&=a^{12}(i[D,\bar D]V-2V^2-\Phi\overline{\Phi})_x+a^{11}(\tfrac{1}{2}\overline{\Phi}_{xx}+2(V\overline{\Phi})_x+i[D,\bar D](V\overline{\Phi}))\\ &\quad -a^{22}(\tfrac{1}{2}\Phi_{xx}-2(V\Phi)_x+i[D,\bar D](V\Phi)),\\ \Phi_{t'}&=i\bar D D\{a^{12}(\Phi_x+4V\Phi)-2a^{11}(V_x+V^2+\tfrac{1}{2}\Phi\overline{\Phi})-\tfrac{3}{2}a^{22}\Phi^2\},\\ \overline{\Phi}_{t'}&=-iD\bar D\{a^{12}(\overline{\Phi}_x-4V\overline{\Phi})-2a^{22}(V_x-V^2-\tfrac{1}{2}\Phi\overline{\Phi})+\tfrac{3}{2}a^{11}\overline{\Phi}^2\}. \end{aligned} \tag{4.5}$$

This system can be derived in one more way, via the first Poisson structure (3.26),(3.27) with H_3 as the Hamiltonian. However, this is possible only under the constraints (1.1),(1.2). Requiring the equations

$$V^A_{t'}=\mathscr{D}^{BA}_{(1)}\frac{\delta H_3}{\delta V^B} \tag{4.6}$$

to coincide, up to an overall renormalization factor, with Eqs. (4.5) immediately leads to the restrictions (4.3) and, hence, to (1.1),(1.2). Thus, like in the case of the $N=4$ KdV equation, the system (4.5) is bi-Hamiltonian only provided the basic conditions (1.1),(1.2) hold. Of course, these conditions can also be deduced by demanding H_3 to be conserved with respect to Eqs. (4.5) with for the moment arbitrary coefficients a^{ik}, viz.

$$\{H_2,H_3\}=0. \tag{4.7}$$

Clearly, this is equivalent to demanding H_2 to be conserved with respect to $N=4$ KdV Eqs. (3.21)–(3.23).

Finally, we observe that in the $N=2$ KdV limit (3.34) H_2 is nonzero for the option (a) in (4.3) and identically vanishes in the two other cases. As we will see, this property persists for the $N=4$ KdV charges H_4 and H_6. It reflects the fact that the even dimension bosonic conserved quantities exist only for the $a=4$, $N=2$ KdV, but not for the $a=-2$ one.[9]

B. The charges H_4, H_5, and H_6

We have found the $N=2$ superfield form of the conserved charge H_4 in two ways: first starting from the harmonic superspace expression (2.38) and, second, constructing the most general dimension 4 expression directly in $N=2$ superspace and then checking under which restrictions on the coefficients it is conserved with respect to Eqs. (3.21)–(3.23) (in doing this, we made use of the computer). Both ways lead to the same answer.

Proceeding in the first way and representing H_4 as

$$H_4=\int \mu^{(2)}(\mathscr{H}_4^I+\mathscr{H}_4^{II}+\mathscr{H}_4^{III}), \tag{4.8}$$

where the three pieces in the integrand precisely correspond to the three terms in the expression (2.38), we get

$$\mathscr{H}_4^I=-\frac{4}{3}\left\{a^{12}(4VDV\bar{D}V-VD\Phi\bar{D}\bar{\Phi})+a^{11}\left(2\bar{\Phi}\bar{D}VDV+\frac{i}{4}\bar{\Phi}^2\Phi_x\right)\right.$$
$$\left.+a^{22}\left(2\Phi\bar{D}VDV-\frac{i}{4}\Phi^2\bar{\Phi}_x\right)\right\},$$

$$\mathscr{H}_4^{II}=\frac{i}{36}\left\{\frac{2}{5}(2(a^{12})^3+3a^{12}a^{11}a^{22})(8V^4+3\Phi^2\bar{\Phi}^2+24V^2\Phi\bar{\Phi})+4(a^{11})^2a^{12}(\bar{\Phi}^3\Phi+6V^2\bar{\Phi}^2)\right.$$
$$+4(a^{22})^2a^{12}(\Phi^3\bar{\Phi}+6V^2\Phi^2)-8(a^{11})^3V\bar{\Phi}^3-\frac{8}{5}(4(a^{12})^2a^{11}+(a^{11})^2a^{22})(4V^3\bar{\Phi}$$
$$\left.+3\bar{\Phi}^2\Phi V)-8(a^{22})^3V\Phi^3-\frac{8}{5}(4(a^{12})^2a^{22}+(a^{22})^2a^{11})(4V^3\Phi+3\Phi^2\bar{\Phi}V)\right\},$$

$$\mathscr{H}_4^{III}=\frac{4i}{9}\left\{a^{11}V_x\bar{\Phi}_x+a^{22}V_x\Phi_x-a^{12}\left(V_xV_x+\frac{1}{2}\Phi_x\bar{\Phi}_x\right)\right\}. \tag{4.9}$$

On the other hand, the results of the second calculation can be summarized as follows:

$$\hat{H}_4=\int \mu^{(2)}\left(a_1V^4+ia_2V^3\Phi+ia_3V^3\bar{\Phi}+3a_1V^2\Phi\bar{\Phi}+\frac{3a_1}{8}\Phi^2\bar{\Phi}^2+i\frac{5a_3}{4}V\Phi^3+i\frac{3a_2}{4}V\Phi^2\bar{\Phi}\right.$$
$$+i\frac{3a_3}{4}V\Phi\bar{\Phi}^2+i\frac{5a_2}{4}V\bar{\Phi}^3-i\frac{3a_1}{2}V^2[D,\bar{D}]V+i\frac{3a_2}{2}V_xV\Phi-\frac{3a_2}{2}[D,\bar{D}]VV\Phi$$
$$-i\frac{3a_3}{2}V_xV\bar{\Phi}-\frac{3a_3}{2}[D,\bar{D}]VV\bar{\Phi}-i\frac{3a_1}{2}VD\Phi\bar{D}\bar{\Phi}-i\frac{3a_2}{4}\bar{\Phi}\Phi\Phi_x+i\frac{3a_3}{4}\Phi\bar{\Phi}\bar{\Phi}_x$$
$$\left.+\frac{a_1}{2}VV_{xx}-i\frac{a_2}{2}V\Phi_{xx}-i\frac{a_3}{2}V\bar{\Phi}_{xx}+\frac{a_1}{4}\Phi\bar{\Phi}_{xx}\right), \tag{4.10}$$

where in Table I we listed the values of the coefficients and parameters a and b for which the charge (4.10) is conserved. We stress that there are only these three solutions. Substituting into Eqs. (4.9) the values (3.42) of a^{ij} which correspond to three different choices of the parameters a and b in Table I, we find that the relevant H_4 and $\hat{H}_4$ differ (modulo full derivatives) merely by unessential scaling factors. These factors are not fixed by requiring the conservation of the $N=4$ KdV charges in the $N=2$ superfield formalism and can always be chosen so as to achieve the full

TABLE I. Coefficients in $\hat{H}_4$.

	a_1	a_2	a_3
$a=4,\ b=0$	1	0	0
$a=-2,\ b=-6$	0	$-1/2$	$-1/2$
$a=-2,\ b=6$	0	1/2	$-1/2$

coincidence between H_4 and $\hat{H}_4$. Thus, the independent $N=2$ superfield calculation entirely confirms the conclusions about H_4 made in our previous paper[14] in the framework of the HSS formalism.

Having at our disposal the explicit $N=2$ superfield form of H_4 we can check the first Hamiltonian structure representation (3.32) for $N=4$ KdV system (3.21)–(3.23). Like in the case of the set (4.5), the necessary conditions for the existence of such a representation are the above constraints on the parameters a and b. Actually, an alternative and technically more simple way to obtain (4.10) with the coefficients from Table I is to start from the most general $N=2$ superfield expression for $\hat{H}_4$ and to require it to reproduce Eqs. (3.21)–(3.23) via the Poisson structure (3.26), (3.27).

Note that for the second and third lines in Table I, the charge H_4 identically vanishes in the $N=2$ KdV limit (3.34) in accordance with the absence of the even dimension bosonic conserved charges for the $a=-2$, $N=2$ KdV hierarchy.

Let us now present the conserved charge H_5. As was already mentioned, it is a very complicated technical problem to construct it directly in the harmonic superspace formalism. This becomes feasible in the $N=2$ superfield approach due to the possibility to use a computer. We start from the most general dimension 5 $N=2$ superfield expression for H_5 with undetermined coefficients and then examined the restrictions imposed on these coefficients by the conservation condition $(H_5)_t=0$. Like in the case of the lower-dimension charges, we have found only three solutions listed in Table II:

$$
\begin{aligned}
H_5=\int \mu^{(2)}\Big\{ & \frac{i}{4}\,\Phi\overline{\Phi}_{xxx}-V[D,\bar{D}]V_{xx}-ia_1V^2V_{xx}+2iV[D,\bar{D}]V[D,\bar{D}]V+ia_2V\Phi\Phi_{xx} \\
& +\frac{ia_2}{2}\,V\Phi_x\Phi_x+ia_3V\Phi_{xx}\overline{\Phi}+ia_4V\Phi_x\overline{\Phi}_x+ia_3V\Phi\overline{\Phi}_{xx}-2VD\Phi_x\bar{D}\overline{\Phi}+2VD\Phi\bar{D}\overline{\Phi}_x \\
& +ia_2V\overline{\Phi\Phi}_{xx}+\frac{ia_2}{2}\,V\overline{\Phi}_x\overline{\Phi}_x+2a_4V^3[D,\bar{D}]V+\frac{3ia_2}{2}\,V^2\Phi\Phi_x+\frac{3a_2}{2}\,V[D,\bar{D}]V\Phi^2 \\
& +\frac{3ia_4}{2}\,V^2\Phi_x\overline{\Phi}-\frac{3ia_4}{2}\,V^2\Phi\overline{\Phi}_x+3a_4V[D,\bar{D}]V\Phi\overline{\Phi}-12DV\bar{D}V\Phi\overline{\Phi}-\frac{3ia_2}{2}\,V^2\overline{\Phi\Phi}_x \\
& +\frac{3a_2}{2}\,V[D,\bar{D}]V\overline{\Phi}^2-\frac{ia_2}{4}\,\overline{\Phi}_x\Phi^3-\frac{3ia_3}{4}\,\Phi^2\overline{\Phi\Phi}_x+\frac{ia_2}{4}\,\Phi_x\overline{\Phi}^3-ia_5V^5-ia_2V^3\Phi^2 \\
& -5ia_5V^3\Phi\overline{\Phi}-ia_2V^3\overline{\Phi}^2-ia_6V\Phi^4-\frac{ia_2}{2}\,V\Phi^3\overline{\Phi}-ia_7V\Phi^2\overline{\Phi}^2-\frac{ia_2}{2}\,V\Phi\overline{\Phi}^3-ia_6V\overline{\Phi}^4\Big\}.
\end{aligned}
\tag{4.11}
$$

Thus, H_5 exists under the same restrictions (3.38) on the $N=4$ KdV parameters a and b [or their manifestly SU(2) covariant form (1.1), (1.2)] as in the previous cases. After reduction to

TABLE II. Coefficients in H_5.

	a_1	a_2	a_3	a_4	a_5	a_6	a_7
$a=4,\ b=0$	3	0	−2	−4	16/5	0	6
$a=-2,\ b=6$	−2	−5	3	1	6/5	35/8	9/4
$a=-2,\ b=-6$	−2	5	3	1	6/5	35/8	9/4

$N=2$ super KdV by setting $\Phi=\bar{\Phi}=0$, H_5 is reduced to the 5 dimension conserved charges of the $a=4$ and $a=-2$, $N=2$ KdV hierarchies, respectively, for the first line and the last two lines in Table II.

It is interesting to see how this conserved charge looks in the original manifestly $N=4$ supersymmetric formulation. It is a matter of straightforward though somewhat cumbersome computation to find that the following $N=4$ superfield expression yields (4.11) after passing to $N=2$ superfields and imposing the constraint (1.2)

$$H_5=\frac{1}{2}\int [dZ]\left[\frac{1}{4}(D^{--}V^{++})^4+i(D^{--}V^{++})^2(D^-)^2V^{++}+\frac{15}{4}(a^{-2})^2(D^{--}V^{++})^2(V^{++})^2 - \frac{1}{2}(D^{--}V_x^{++})^2\right]+\frac{i}{4}\int [d\zeta^{-2}]\left[\frac{63}{100}(a^{-2})^4(V^{++})^5-5(a^{-2})^2(V_x^{++})^2V^{++}\right]. \tag{4.12}$$

The last conserved charge we have explicitly constructed is H_6. Once again, it exists only for the above three choices of the $N=4$ KdV parameters. We present it here only for the choice $a=4$, $b=0$ since the expressions for the two other choices are very long and complicated. Of course, they can be obtained from the $a=4$, $b=0$ expression via finite SU(2) rotations.

This charge H_6 reads

$$\begin{aligned}H_6=\int \mu^{(2)}\{&6\bar{\Phi}_{xxxx}\Phi+12VV_{xxxx}-240i\ \bar{D}V_xDV_xV-120i[D,\bar{D}]V_{xx}V^2+60i\ V\bar{D}\bar{\Phi}D\Phi_{xx}\\
&+60i\ V\bar{D}\bar{\Phi}_xD\Phi_x+60i\ V\bar{D}\bar{\Phi}_{xx}D\Phi-240i\ \bar{D}VDV\bar{\Phi}_x\Phi-240i\ \bar{D}VDV_x\bar{\Phi}\Phi\\
&-60[D,\bar{D}]V[D,\bar{D}]V\bar{\Phi}\Phi-120[D,\bar{D}]V[D,\bar{D}]VV^2+240i[D,\bar{D}]VV\bar{\Phi}_x\Phi\\
&+120i[D,\bar{D}]VV_x\bar{\Phi}\Phi+120i[D,\bar{D}]V_xV\bar{\Phi}\Phi-15\bar{\Phi}^2(\Phi_x)^2+30\bar{\Phi}\bar{\Phi}_{xx}\Phi^2+15(\bar{\Phi}_x)^2\Phi^2\\
&+240\ V^2\bar{\Phi}_{xx}\Phi+120\ V^3V_{xx}+480\ VV_x\bar{\Phi}_x\Phi+360\ VV_{xx}\bar{\Phi}\Phi+180(V_x)^2\bar{\Phi}\Phi\\
&+1440i\ \bar{D}VDVV\bar{\Phi}\Phi-45i[D,\bar{D}]V\bar{\Phi}^2\Phi^2-720i[D,\bar{D}]VV^2\bar{\Phi}\Phi-240i[D,\bar{D}]VV^4\\
&+90\ V\bar{\Phi}^2\Phi\Phi_x-90\ V\bar{\Phi}\bar{\Phi}_x\Phi^2+240\ V^3\bar{\Phi}\Phi_x-240\ V^3\bar{\Phi}_x\Phi+20\ \bar{\Phi}^3\Phi^3+360\ V^2\bar{\Phi}^2\Phi^2\\
&+480\ V^4\bar{\Phi}\Phi+64i\ V^5\}.\end{aligned} \tag{4.13}$$

Finally, we wish to stress that all the conserved charges H_n, $n=1,...6$, are in involution with respect to both Poisson brackets

$$\{H_n,H_m\}=\{H_n,H_m\}_{(1)}=0. \tag{4.14}$$

This property can be easily deduced from the bi-Hamiltonian nature of the conjectural $N=4$ KdV hierarchy. The bi-Hamiltonian structure can be expressed as the following general recursion relation (up to relative scaling factors between the conserved charges)

$$\mathscr{D}^{AB}\frac{\delta H_n}{\delta V^A}=\mathscr{D}^{AB}_{(1)}\frac{\delta H_{n+1}}{\delta V^A}. \tag{4.15}$$

We have explicitly checked (4.15) for all H_n presented above, limiting ourselves, for simplicity, to the case $a=4$, $b=0$ and keeping in mind that the other two integrable cases can be generated from this one by SU(2) transformations (3.19). Actually, as we already mentioned, *postulating* the relations (4.15) gives an alternative method to construct higher-order conservation laws, even more simple than the direct method we resorted to in this section. We do not foresee any reason why the construction procedure of these laws based on the relations (4.15) should terminate at any finite step. Both the existence of the nontrivial conserved charges H_2, H_4, H_5, and H_6 and the above bi-Hamiltonian property are strong indications that the $N=4$ super KdV equation with the restrictions (1.1), (1.2) produces the whole $N=4$ super KdV hierarchy and so is integrable. In order to rigorously prove this, it is of primary importance to find the appropriate Lax representation. We believe that in the $N=2$ superfield formalism this problem will be simpler than in the harmonic superspace formulation and can be solved along the lines of Refs. 10, 11, and 28.

V. CONCLUSION

As the main goal of the present work, we have obtained the $N=4$ super KdV equation of Ref. 14 in an $N=2$ superfield form and studied the question of its integrability in this approach. We reproduced the results of Ref. 14 and constructed two new conserved bosonic quantities for $N=4$ super KdV, the dimension 5 and 6 ones H_5 and H_6. They were found to exist under the same restrictions on the SU(2) breaking parameters (1.1), (1.2) as the lower dimension charges given in Ref. 14. The bi-Hamiltonian structure of the $N=4$ KdV equation was extended to the whole set of evolution equation associated with the Hamiltonians H_n that have been constructed. Requiring the existence of this structure gives rise to the same conditions (1.1), (1.2) on the parameters. These results suggest that the unique integrable $N=4$ SU(2) KdV hierarchy exists, with the choice of the SU(2) breaking parameters as in Eqs. (1.1), (1.2). The $N=2$ superfield formulation allowed us also to show that two inequivalent reductions to $N=2$ KdV are possible. They yield, respectively, the integrable $a=4$ and $a=-2$ cases of $N=2$ KdV. Thus the single $N=4$ SU(2) KdV hierarchy incorporates as particular solutions two of the three $N=2$ KdV hierarchies.

Among the problems for future study, besides the construction of a Lax pair representation for the $N=4$ SU(2) KdV, let us mention a generalization to the case of the ''large'' $N=4$ superconformal algebra[25,26] with the affine subalgebra so(4)$\times$u(1). The related $N=4$ super KdV hierarchy is expected to embrace both the $N=4$ SU(2) and $N=3$ KdV ones as particular cases. Also, it would be interesting to construct generalized $N=4$ super KdV systems associated with nonlinear W type extensions of $N=4$ superconformal algebras. One of possible ways to define such extensions was mentioned in Sec. II A.

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APPENDIX A: USEFUL IDENTITIES

In this appendix we collect a number of useful identities.

First of all, we present some consequences of the constraints (2.2) and their harmonic superspace version (2.10), (2.11):

$$D^iV^{kl}=-\tfrac{1}{3}(\epsilon^{ik}\xi^l+\epsilon^{il}\xi^k),\quad \bar{D}^iV^{kl}=\tfrac{1}{3}(\epsilon^{ik}\bar{\xi}^l+\epsilon^{il}\bar{\xi}^k), \tag{A1}$$

$$D^i\bar{D}^j V^{kl} = -\frac{i}{2}(\epsilon^{jk}V_x^{il}+\epsilon^{jl}V_x^{ik}) - \frac{1}{6}(\epsilon^{il}\epsilon^{jk}+\epsilon^{ik}\epsilon^{jl})T, \tag{A2}$$

$$D^i D^j V^{kl} = \bar{D}^i\bar{D}^j V^{kl} = 0, \tag{A3}$$

$$D^- V^{++} = -\frac{2}{3}\xi^k u_k^+ , \quad \bar{D}^- V^{++} = \frac{2}{3}\bar{\xi}^k u_k^+ , \tag{A4}$$

$$(D^-)^2 V^{++} = -\frac{i}{2} D^{--} V_x^{++} - \frac{1}{3} T. \tag{A5}$$

When deducing Eqs. (2.29) and (2.37) from the harmonic superspace Poisson structure (2.21) and rewriting the latter in ordinary $N=4$ superspace, one needs to decompose the objects given in terms of one set of harmonic variables, say $u_i^{\pm}$, over another set, $v_i^{\pm}$, using the completeness condition (2.5). The general decomposition formula for some object bilinear in harmonics,

$$S^{++}(u) \equiv S^{ik}u_i^+ u_k^+$$

[S^{++} can stand, e.g., for V^{++} or $(D^+)^2 = D^+\bar{D}^+$], is as follows

$$S^{++}(u) = S^{++}(v)(v^-u^+)^2 + \tfrac{1}{2}(D_v^{--})^2 S^{++}(v)(v^+u^+)^2 - D_v^{--}S^{++}(v)(v^-u^+)(v^+u^+). \tag{A6}$$

Analogous relations for other harmonic projections of S^{ik}, namely S^{+-} and S^{--}, can be obtained by applying D_u^{--} to both sides of Eq. (A6) and making use of the harmonic differentiation rules

$$D^{--}u_i^+ = u_i^- , \quad D^{--}u_i^- = 0.$$

APPENDIX B: LEMMA

In this appendix we prove the following Lemma.

Lemma: Let c^{iklj} be an arbitrary rank 4 symmetric SU(2) spinor subjected to the reality condition

$$(c^{iklj})^\dagger = \epsilon_{ii'}\epsilon_{kk'}\epsilon_{ll'}\epsilon_{jj'}c^{i'k'l'j'}.$$

The necessary and sufficient conditions for it to be a square of some real rank 2 symmetric SU(2) spinor a^{ik},

$$c^{ijkl} = \tfrac{1}{3}(a^{ij}a^{kl}+a^{ik}a^{jl}+a^{il}a^{jk}), \quad (a^{ik})^\dagger = -\epsilon_{il}\epsilon_{kj}a^{lj}, \tag{B1}$$

are the following ones

$$(I)\ \mathscr{A}^3 = 6\ \mathscr{B}^2, \quad (II)\ \mathscr{B} < 0; \quad (\mathscr{A} \equiv c^{ijkl}c_{ijkl}, \quad \mathscr{B} \equiv c^{ik}{}_{jl}c^{jl}{}_{ft}c^{ft}{}_{ik}). \tag{B2}$$

Proof: The proof is simpler in the vector notation, with c^{ikjl} represented by a real traceless symmetric rank 2 tensor and a^{ik} by a real vector

$$c^{iklj} \Rightarrow c^{\mu\nu} = \frac{1}{2}c^{ij}{}_{kl}(\sigma^\mu)_i^k(\sigma^\nu)_j^l, \quad a^{ik} \Rightarrow a^\mu = \frac{1}{\sqrt{2}}a^i{}_k(\sigma^\mu)_i^k; \quad (\mu,\nu\ldots = 1,2,3)$$

$$\mathscr{A} = c^{\mu\nu}c^{\mu\nu}, \quad \mathscr{B} = -c^{\mu\nu}c^{\nu\rho}c^{\rho\mu}.$$

Here, $(\sigma^\mu)_k^l$ are Pauli matrices.

In this notation, the relation (B1) amounts to

$$c^{\mu\nu}=a^{\mu}a^{\nu}-\tfrac{1}{3}\delta^{\mu\nu}(a^{\rho}a^{\rho}). \tag{B3}$$

Then the necessity of (B2) immediately follows from computing the invariants $\mathscr{A}$ and $\mathscr{B}$ for the tensor (B3)

$$\mathscr{A}=\tfrac{2}{3}(a^2)^2, \quad \mathscr{B}=-\tfrac{2}{9}(a^2)^3, \quad a^2\equiv a^{\mu}a^{\mu}>0.$$

In order to show that (B2) is also sufficient for $c^{\mu\nu}$ to be representable in the form (B3), let us go to the frame where $c^{\mu\nu}$ is a diagonal traceless matrix with the following nonzero entries

$$c^{11}=\lambda_1, \quad c^{22}=\lambda_2, \quad c^{33}=-(\lambda_1+\lambda_2), \tag{B4}$$

λ_1,λ_2 being arbitrary for the moment. After substituting this into the first of conditions (B2) we get the equation

$$(\lambda_1-\lambda_2)^2(\lambda_1+2\lambda_2)(2\lambda_1+\lambda_2)=0, \tag{B5}$$

which has the following nonzero roots

$$\text{(a)}\ \ \lambda_1=\lambda_2; \quad \text{(b)}\ \ \lambda_1=-2\lambda_2; \quad \text{(c)}\ \ \lambda_2=-2\lambda_1. \tag{B6}$$

The inequality in (B2) takes the form

$$\lambda_1\lambda_2(\lambda_1+\lambda_2)<0 \tag{B7}$$

and restricts the solutions (B6) in the following way

$$\text{(a)}\ \ \lambda_1<0, \quad \text{(b)}\ \ \lambda_1>0, \quad \text{(c)}\ \ \lambda_1<0. \tag{B8}$$

Now it is an elementary exercise to see that these three solutions correspond to three different choices of the vector a^{μ} in (B3) (up to the reflection $a^{\mu}\to -a^{\mu}$)

$$\text{(a)}\ \ a^{\mu}=(0,0,\sqrt{3|\lambda_1|}); \quad \text{(b)}\ \ a^{\mu}=\left(\sqrt{\frac{3}{2}\,|\lambda_1|},0,0\right); \quad \text{(c)}\ \ a^{\mu}=(0,\sqrt{3|\lambda_1|},0).$$

This proves the sufficiency of the conditions (B2).

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A formula for obtaining new hereditary symmetries and new integrable equations

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In this paper we give a simple formula to obtain hereditary symmetries related to the isospectral eigenvalue problem of integrable equations. Using this formula, (i) we prove that eigenfunctions of hereditary strong symmetry are symmetries for the whole hierarchy, which improves the result of Fokas and Anderson [J. Math. Phys. **23**, 1066 (1982)]; (ii) we find new integrable equations; and (iii) we give strong symmetries of these new integrable equations and various equations for eigenfunctions of the isospectral eigenvalue problems. © *1996 American Institute of Physics.* [S0022-2488(96)01202-9]

I. INTRODUCTION

As is well known, there is a deep connection between certain integrable nonlinear evolution equations in $1+1$ dimensions and certain linear isospectral eigenvalue *equations*.[1–3] The isospectral eigenvalue equation algorithmically implies a certain linear integrodifferential operator Φ called the strong symmetry (or the recursion operator). This operator plays a central role in the understanding of the algebraic–geometrical structure of integrable evolution equations. Some important results about the recursion operator can be found in Refs. 4–6. Moreover, if an operator Φ has an algebraic–geometrical property called hereditary, then the equations $u_t=K_n=\Phi^n u_x$ possess the Lax pairs $\Phi\sigma=\lambda\sigma$, $\sigma_t=K_{nu}\sigma$, so finding new hereditary symmetry is equivalent to finding new integrable equations.

Therefore, many authors have found various methods to find strong symmetries. Two general and algorithmic methods are the following:

(1) Fokas and Amderson proved that a linear isospectral eigenvalue problem gives rise to a strong *symmetry*.[7]
(2) Fuchssteiner showed that Bäcklund transformations yield transformations between strong symmetries, thus they generate a class of strong symmetries from a *given*.[8]

The first method is useful only when the isospectral eigenvalue problem is found and these two methods are tedious. It is not easy to find explicitly strong symmetry using the above methods.

In Ref. 9, Strampp pointed that for certain nonlinear integrable equations

$$u_t=K(u), \tag{1.1}$$

their Lax pairs can be transformed into

$$\Phi(u)\sigma=\mu\sigma, \quad \sigma_t=K_u\sigma, \tag{1.2}$$

respectively, where Φ is a strong hereditary symmetry operator of (1.1), K_u is the Gateaux derivative of K with respect to u, and μ is a constant. In fact, for an equation such as the KdV equation, the Schrödinger equation, there exists an explicit relationship between Φ and the Hamiltonian operator θ,[7]

$$\theta\Phi^+=\Phi\theta, \tag{1.3}$$

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where Φ^+ denotes the adjoint of Φ, Using the result in Ref. 7 σ is a symmetry for the whole hierarchy

$$u_t = K_n = \Phi^n K(u), \quad n = 1,2,\ldots . \tag{1.4}$$

But for an equation such as Burgers equation, the relation (1.3) does not exist, and we cannot use the result in Ref. 7 to prove that σ is a symmetry for the whole hierarchy (1.4).

In Sec. III regarding the linear isospectral eigenvalue equation as a Miura transformation we prove a property about hereditary symmetry and prove that the eigenfunctions of hereditary strong symmetries are symmetries for the whole hierarchy, which improve the result in Ref. 7. In Sec. IV we give a formula to obtain strong symmetries of equations which the eigenfunctions of isospectral eigenvalue problems satisfy. Using this formula we also construct a new class of integrable equations (4.5); these equations have strong symmetries and Lax pair and can also be treated as the symmetry constraints of the original equations. Section V gives some examples. We obtain strong symmetries of nonlinear equations for eigenfunctions in Lax pairs of Burgers equation, the KdV equation, the Schrödinger equation, and the Harry Dym equation and construct new integrable equations.

II. BASIC NOTIONS

We consider an evolution equation

$$u_t = K(u) \tag{2.1}$$

on a normed space M of vector-valued functions on the real line, K is a suitable C^∞ vector field on M. We also assume the space of smooth vector fields on M is some space V of C^∞ functions on the real line vanishing rapidly at $\pm\infty$.

The derivative of $K(u)$ in the direction v is denoted by $K_u(u)[v]$ and can be calculated by

$$K_u(u)[v] = \left.\frac{\partial K(u+\mu v)}{\partial \mu}\right|_{\mu=0}. \tag{2.2}$$

A function σ is a symmetry of (2.1) if

$$\sigma_t = K_u \sigma.$$

An operator-valued function $\Phi(u)$ is called a strong *symmetry*[10] (or recursion operator in the terminology of Ref. 11) for (2.1) if

$$\frac{\partial \Phi}{\partial t} = [K_u, \Phi] \equiv K_u \Phi - \Phi K_u, \tag{2.3}$$

where $\partial\Phi/\partial t$ is the total derivative and u satisfies (2.1). Φ maps symmetries of (2.1) onto symmetries of (2.1). Obviously, if Eq. (2.1) has a strong symmetry Φ, then it has a Lax pair

$$\Phi(u)w = \mu w, \quad w_t = K_u w.$$

An operator-valued function $\Phi(u)$ is called a hereditary *symmetry*[10,12] if

$$\Phi_u[\Phi v]w - \Phi_u[\Phi w]v = \Phi(\Phi_u[v]w - \Phi_u[w]v) \tag{2.4}$$

is valid for any functions $v, w \in M$.

It is well known that If $\Phi(u)$ is a hereditary and strong symmetry for (2.1), then Φ is a strong symmetry for the following equations:

$$u_t=(\Phi(u))^nK(u),\quad n=0,1,2\ldots, \tag{2.5}$$

that is, (2.5) inherits its strong symmetry from (2.1).

III. HEREDITARY SYMMETRY AND LAX PAIR

In what follows, let Ω be the algebra of operator valued function on V which has no zero divisors.

We consider the eigenvalue problem of the hereditary symmetry which does not depend on time t explicitly.

$$\Phi(u)\sigma=\mu\sigma. \tag{3.1}$$

Proposition 3.1: Suppose (a) Φ is a nonconstant hereditary symmetry, (b) (3.1) is equivalent to $u=f(\sigma,\mu)$, (c) $\Phi(u), T^{-1}\Phi-\Phi T^{-1}\in\Omega(T\equiv f_\sigma)$ (or $\Phi, T\in\Omega$), then

$$\Phi_u[\sigma]=T^{-1}\Phi-\Phi T^{-1}. \tag{3.2}$$

Proof: Substituting $u=f(\sigma,\mu)$ into (3.1) we obtain an identity

$$\Phi(f(\sigma,\mu))\sigma\equiv\mu\sigma.$$

Taking the Gateaux derivative with respect to σ in two sides we have

$$\Phi_u[\cdot]\sigma=-\Phi T^{-1}+\mu T^{-1}. \tag{3.3}$$

On the other hand, Φ is a hereditary symmetry operator, and we get an identity from (2.4)

$$\Phi_u[\Phi\sigma]-\Phi_u[\Phi\cdot]\sigma=\Phi(\Phi_u[\sigma]-\Phi_u[\cdot]\sigma). \tag{3.4}$$

Substituting (3.3) into (3.4) yields

$$(\mu-\Phi)(\Phi_u[\sigma]-T^{-1}\Phi+\Phi T^{-1})=0,$$

and we get (3.2) because Ω has no zero divisors.

Lemma 3.2: Under the assumption of Proposition 3.1 and

$$T^{-1}K=K_u\sigma, \tag{3.5}$$

then

$$T^{-1}K_n=K_{nu}\sigma,\quad n=0,1,2,\ldots,$$

where $K_n=\Phi^nK$.

Proof: We prove it by induction. When $n=m+1$, we find

$$T^{-1}K_n=T^{-1}\Phi K_m=(\Phi_u[\sigma]+\Phi T^{-1})K_m=\Phi_u[\sigma]K_m+\Phi K_{mu}\sigma=(\Phi K_m)_u\sigma=K_{(m+1)u}\sigma.$$

Theorem 3.3: *Under the assumption of Proposition 3.1 and σ the symmetry of (2.1), if u is a solution of (2.5), then*

$$\sigma_t=K_{nu}\sigma;$$

that is, σ is a symmetry of (2.5).

Proof:

$$\sigma_t = T^{-1}u_t = T^{-1}K_n .$$

Using Lemma 3.2,

$$\sigma_t = K_{nu}\sigma.$$

Remark 1: Almost all well-known integrable equations $K = u_x$, and then the condition (3.5) in Lemma 3.2 and the condition "σ is a symmetry of $u_t = u_x$" in Theorem 3.3 are satisfied automatically.

Remark 2: Let V be equal to the space of those fast decreasing functions or the space of those C^∞ functions vanishing rapidly at $-\infty$. Let $\Omega(D, D^{-1})$ denote the algebra of operator-valued functions on V generated by functions of the following type:

$$u \to D, \quad u \to D^{-1}, \quad u \to f(u^{(n)}), \quad u \to g(u^{(-n)}),$$

where f and g are allowed to be arbitrary entire analytic functions, and where $u^{(n)}$ are $u^{(-n)}$ are the nth derivative and the nth integral of u. It was proved that $\Omega(D, D^{-1})$ has no zero *divisors*.[12]

In many cases, to check (3.2), we may check the the following identity directly:

$$T\Phi_u[\sigma]T = \Phi(u)T - T\Phi(u).$$

Formula (3.2) has some applications. Section IV uses it to give new hereditary symmetry and new integrable equations. Many integrable equations possess two sets of symmetries, called K-symmetries and *τ-symmetries*.[13] Recently Lou used inverse strong symmetry to find new *symmetries*,[14,15] and this formula also played a central role in obtaining the Lie algebra of these *symmetries*.[16,17]

Now we turn to the usual Lax pair of (2.5),

$$L(u)\psi = \lambda\psi, \tag{3.6a}$$

$$\psi_t = A_n\psi, \tag{3.6b}$$

where $L(u)$ and A_n are certain linear differential operators.

Theorem 3.4: *Suppose (a) Φ is an nonconstant hereditary symmetry; (b) the isospectral eigenvalue problem (3.6a) is equivalent to*

$$u = p(\psi, \lambda); \tag{3.7}$$

and (c) there exists an invertible transformation

$$\sigma = h(\psi) \tag{3.8}$$

to convert (3.6a) into (3.1) where μ is a constant related to λ, with σ a symmetry of (2.1). (d) Φ, $\sigma_u\Phi - \Phi\sigma_u \in \Omega$ (or $\Phi, \psi_u, \sigma_\psi \in \Omega$). Then (3.6) is transformed to

$$\Phi(u)\sigma = \mu\sigma, \quad \sigma_t = K_{nu}\sigma. \tag{3.9}$$

Proof: Because

$$T \equiv u_\sigma = u_\psi\psi_\sigma ,$$

we can use Theorem 3.3 to prove this theorem easily.

IV. NEW HEREDITARY SYMMETRY AND NEW INTEGRABLE EQUATION

A. Eigenfunction equation

Under the assumption of Theorem 3.4, Theorem 3.4 gives a method to obtain hereditary symmetry. In fact, from the result in Refs. 7 and 8 we know that $T^{-1}\Phi T$ is a hereditary symmetry iff Φ is a hereditary symmetry and $T^{-1}\Phi T$ is a strong symmetry of

$$\sigma_t = K_u(f(\sigma,\lambda))\sigma \tag{4.1}$$

iff Φ is a strong symmetry of (2.1). From (3.2)

$$\Psi(\sigma) = T^{-1}\Phi T = \Phi_u[\sigma]T + \Phi(u) = \Phi_u[\sigma]u_\psi\psi_\sigma + \Phi(u). \tag{4.2}$$

We need not calculate the inverse operator T^{-1} by using this formula, which is very useful in calculating hereditary symmetry. Similarly, a strong hereditary symmetry of the equation

$$\psi_t = A_1(p(\psi))\psi = p_\psi^{-1}K(p(\psi)) \tag{4.3}$$

is

$$\Psi_2 = \psi_\sigma[\Phi_u[\sigma]u_\psi\psi_\sigma + \Phi(u)]\sigma_\psi = \psi_\sigma[\Phi_u[\sigma]u_\psi + \Phi(u)\sigma_\psi]. \tag{4.4}$$

Remark: For most equations having the relation (1.3)

$$\sigma = \theta G_\lambda, \tag{4.4$'$}$$

where G_λ is the gradient of λ which is calculated from the isospectral eigenvalue *problem* (3.6a).[7] ■

Konopelchenko first found that (4.3) is an integrable *equation*;[18] he calls (4.3) an eigenfunction equation.

B. Constraints equation

Under the assumption of Proposition 3.1, formula (3.2) tell us to construct other new integrable equations about u:

$$u_t = \sigma(u,\mu). \tag{4.5}$$

where σ only satisfies (3.1). It should be noted that we do not require u to satisfy any other equations here!

In fact (3.2) is just the definition that $\Phi(u)$ is a strong symmetry of (4.5), so (4.5) has the Lax pair

$$\Phi(u)w = \lambda w, \quad w_t = \sigma_u w. \tag{4.6}$$

Substituting $u = f(\sigma,\mu)$ into (4.5) we get the equation of σ,

$$f_t(\sigma,\mu) = \sigma; \tag{4.7}$$

(4.2) is its strong symmetry.

Furthermore, if an isospectral eigenvalue problem (3.6a) can be transformated into (4.6a) by the transformation $\sigma = h(\psi)$, then we have the integrable equation of ψ,

$$f_t(h(\psi),\mu) = h(\psi), \tag{4.8}$$

which has a strong symmetry with the form (4.4).

Remark: Eq. (4.5) can be regarded as the symmetry (u_t and σ) constraints of the equation which possesses strong symmetry Φ and symmetry σ,[19] so we call it the constraints equation. Equations (4.5) and (4.8) also possess K symmetries and τ *symmetries*.[17] Equation (4.8) is connected with the equations studied in Refs. 14, 15, and 19.

Using the formulas given here we can get strong symmetries of various equations in Refs. 14 and 15 and others. In Sec. V, for instance, we study some important equations.

V. EXAMPLES AND APPLICATIONS

(A) Burgers equation[9,20]

$$u_t = K(u) = u_{xx} + u u_x . \tag{5.1}$$

An isospectral eigenvalue problem for (5.1) is given by

$$\psi_x + \frac{u}{2}\psi = \lambda\psi, \tag{5.2a}$$

where the eigenfunction ψ evolves in time according to the equation

$$\psi_t = \left(\lambda^2 - \frac{u^2}{4} - \frac{u_x}{2}\right)\psi. \tag{5.2b}$$

By using the transformation

$$\sigma = \psi_x , \tag{5.3}$$

we obtain

$$\Phi(u)\sigma = \lambda\sigma, \quad \sigma_t = K_u\sigma, \tag{5.4}$$

where

$$\Phi = D + \frac{u}{2} + \frac{u_x}{2} D^{-1}, \quad D = \frac{\partial}{\partial x}, \quad DD^{-1} = D^{-1}D = 1.$$

From Theorem 3.3, ψ_x is a symmetry for the whole hierarchy

$$u_t = \Phi^n u_x .$$

We find σ satisfies

$$\sigma_t = 2\lambda\sigma_x + \sigma_{xx} - \frac{4\sigma\sigma_x}{D^{-1}\sigma} + \frac{2\sigma^3}{(D^{-1}\sigma)^2}. \tag{5.5}$$

It has a strong hereditary symmetry

$$\Psi_1 = D + \lambda - 2(\ln D^{-1}\sigma)_{xx}D^{-1} - 2(\ln D^{-1}\sigma)_x ; \tag{5.6}$$

furthermore,

$$\psi_t = 2\lambda\psi_x + \psi_{xx} - \frac{2\psi_x^2}{\psi}. \tag{5.7}$$

Its strong hereditary symmetry is

$$\Psi_2 = D + \lambda - \frac{2\psi_x}{\psi}. \tag{5.8}$$

(B) The KdV equation

$$u_t = K_1(u) = \Phi(u) u_x = u_{xxx} + 6uu_x, \tag{5.9}$$

where

$$\Phi = D^2 + 4u + 2u_x D^{-1}$$

is a strong hereditary symmetry.

Its Lax pair is

$$\psi_{xx} + u\psi = \lambda\psi, \quad \psi_t = (2u + 4\lambda)\psi_x - u_x\psi. \tag{5.10}$$

Let

$$\sigma = (\psi^2)_x, \tag{5.11}$$

then (5.10) becomes

$$\Phi\sigma = 4\lambda\sigma, \quad \sigma_t = K_u\sigma, \tag{5.12}$$

where σ is a symmetry of the whole hierarchy $u_t = \Phi^n u_x$, that is, its Lax pair

$$\psi_{xx} + u\psi = \lambda\psi, \quad \psi_t = B_n\psi_x - \frac{B_{nx}}{2}\psi$$

is transformed into

$$\Phi\sigma = 4\lambda\sigma, \quad \sigma_t = K_{nu}\sigma.$$

The eigenfunction σ in the Lax pair (5.12) satisfies

$$\sigma_t = \sigma_{xxx} + 6\lambda\sigma_x - \left(\frac{3\sigma^2}{2D^{-1}\sigma}\right)_{xx}. \tag{5.13}$$

A strong hereditary symmetry of this equation is

$$\Psi_1 = D^2 + 4u + 2u_x D^{-1} + (4\sigma + 2\sigma_x D^{-1})(-D^2 + \lambda - u)\frac{D^{-1}}{2D^{-1}\sigma}, \tag{5.14}$$

where

$$u = \lambda - \frac{2\sigma_x D^{-1}\sigma - \sigma^2}{4(D^{-1}\sigma)^2}. \tag{5.15}$$

Φ also is a strong symmetry of the following new integrable equation for u:

$$u_t = \sigma, \tag{5.16}$$

with σ defined in (5.15). Equation (5.14) is just a strong symmetry of the new integrable equation about σ which also defined by (5.16) with u defined by (5.15).

The ψ of the Lax pair (5.10) *satisfies*[18]

$$\psi_t=\psi_{xxx}+6\lambda\psi_x-3\frac{\psi_{xx}\psi_x}{\psi}. \tag{5.17}$$

One of its strong hereditary symmetries is

$$\Psi_2=D^2-2\frac{\psi_x}{\psi}D+4\lambda-\frac{\psi_{xx}}{\psi}-\frac{2\psi_x^2}{\psi^2}-4\psi_xD^{-1}\left(\frac{1}{\psi}\right)_{xx}; \tag{5.18}$$

(5.18) is also a strong symmetry of the new integrable equation

$$\left(\frac{\psi_{xx}}{\psi}\right)_t=-2\psi\psi_x. \tag{5.19}$$

This equation was first studied in Ref. 19 and it can be transformed into sinh-Gordon *equation,*[19] here we give its strong symmetry.

(C) The Schrödinger equation

$$u_t=K_1=\Phi u_x \tag{5.20}$$

with

$$u=\begin{pmatrix}q\\ r\end{pmatrix},\quad \Phi(u)=i\begin{pmatrix}D-2qD^{-1}r & -2qD^{-1}q\\ 2rD^{-1}r & -D+2rD^{-1}q\end{pmatrix};$$

the corresponding Lax pair is

$$\begin{aligned}&\psi_{1x}=\lambda\psi_1+q\psi_2,\quad \psi_{2x}=-\lambda\psi_2+r\psi_1,\\ &\psi_{1t}=(2i\lambda^2-iqr)\psi_1+i(q_x+2\lambda q)\psi_2,\\ &\psi_{2t}=i(-r_x+2\lambda r)\psi_1-i(2\lambda^2-qr)\psi_2.\end{aligned} \tag{5.21}$$

Taking the transformation

$$\sigma=\begin{pmatrix}\psi_1^2\\ \psi_2^2\end{pmatrix}, \tag{5.22}$$

(5.21) becomes

$$\Phi\sigma=2i\lambda\sigma,\quad \sigma_t=K_{1u}\sigma, \tag{5.23}$$

where σ is a symmetry for the whole hierarchy $u_t=\Phi^n u_x$. A strong hereditary symmetry of the eigenfunction equation about σ is

$$\Psi_1(\sigma)=i\begin{pmatrix}a_{11} & a_{12}\\ a_{21} & a_{22}\end{pmatrix} \tag{5.24}$$

with

$$a_{11}=\sigma_1D^{-1}\frac{r}{\sqrt{\sigma_1\sigma_2}}\left(\frac{\sigma_{1x}}{\sigma_1}-D\right)+\lambda-\frac{\sigma_{1x}}{2\sigma_1}+D,$$

$$a_{12}=\sigma_1 D^{-1}\frac{q}{\sqrt{\sigma_1\sigma_2}}\left(\frac{\sigma_{2x}}{\sigma_2}-D\right)-\frac{q\sqrt{\sigma_1}}{\sqrt{\sigma_2}},$$

$$a_{21}=-\sigma_2 D^{-1}\frac{r}{\sqrt{\sigma_1\sigma_2}}\left(\frac{\sigma_{1x}}{\sigma_1}-D\right)-\frac{r\sqrt{\sigma_2}}{\sqrt{\sigma_1}},$$

$$a_{22}=-\sigma_2 D^{-1}\frac{q}{\sqrt{\sigma_1\sigma_2}}\left(\frac{\sigma_{2x}}{\sigma_2}-D\right)-\lambda+\frac{\sigma_{2x}}{2\sigma_2}-D,$$

where

$$q=\frac{\sigma_{1x}-2\lambda\sigma_1}{2\sqrt{\sigma_1\sigma_2}},\quad r=\frac{\sigma_{2x}+2\lambda\sigma_2}{2\sqrt{\sigma_1\sigma_2}}. \tag{5.25}$$

$\Phi(u)$ is a strong symmetry of the following integrable equation about u;

$$q_t=\sigma_1,\quad r_t=\sigma_2, \tag{5.26}$$

with σ_1,σ_2 defined in (5.25). Furthermore, (5.24) is a strong symmetry of the integrable equation (5.26) about σ with (q,r) defined in (5.25).

A strong hereditary symmetry of the eigenfunction equation about ψ is

$$i\begin{pmatrix}\psi_1 D^{-1}\frac{r}{\psi_2}\left(\frac{\psi_{1x}}{\psi_1}-D\right)+\lambda+D & \psi_1 D^{-1}\frac{q}{\psi_1}\left(\frac{\psi_{2x}}{\psi_2}-D\right)-q\\ -\psi_2 D^{-1}\frac{r}{\psi_2}\left(-D+\frac{\psi_{1x}}{\psi_1}\right)+r & \psi_2 D^{-1}\frac{q}{\psi_1}\left(D-\frac{\psi_{2x}}{\psi_2}\right)-\lambda-D\end{pmatrix}, \tag{5.27}$$

where

$$q=\frac{\psi_{1x}-\lambda\psi_1}{\psi_2},\quad r=\frac{\psi_{2x}+\lambda\psi_2}{\psi_1}. \tag{5.28}$$

Equation (5.27) is also a strong symmetry of the new integrable equation about ψ

$$q_t=\psi_1^2,\quad r_t=\psi_2^2. \tag{5.29}$$

(D) The Harry Dym equation:

$$u_t=K(u)=2(1+u)_{xx}^{-1/2}, \tag{5.30}$$

arising as the integrability condition of the following equations:

$$\begin{aligned}&\psi_{xx}+(1+u)\lambda^2\psi=0,\\ &\psi_t=-4(1+u)^{-3/2}\psi_{xxx}-2\left((1+u)^{-3/2}\right)_x\psi_{xx}.\end{aligned} \tag{5.31}$$

By using the transformation

$$\sigma=(\psi^2)_{xxx} \tag{5.32}$$

(5.32) becomes

$$\Phi(u)\sigma=-2\lambda^2\sigma,\quad \sigma_t=K_u\sigma, \tag{5.33}$$

where

$$\Phi(u)=\tfrac{1}{2}D^3(1+u)^{-1/2}D^{-1}(1+u)^{-1/2}. \tag{5.34}$$

Its inverse operator is

$$\Phi^{-1}(u)=2(1+u)D^{-2}+u_xD^{-3}; \tag{5.35}$$

(5.34) and (5.35) are two strong symmetries. σ is a symmetry for the whole hierarchy $u_t=\Phi^nK(u)$. Two strong symmetries corresponding to the equation of σ in (5.33) are

$$\begin{aligned}\Psi_1(\sigma)=&-\frac{1}{4}\,[D^3v^3\sigma D^{-1}v+D^3vD^{-1}v^3\sigma]\left[\frac{2D^{-3}\sigma D^{-1}+2D^{-1}\sigma D^{-3}-2D^{-2}\sigma D^{-2}}{4(D^{-3}\sigma)^2}\right.\\&\left.-\frac{(2D^{-1}\sigma D^{-3}\sigma-(D^{-2}\sigma)^2)D^{-3}}{2(D^{-3}\sigma)^3}\right]+\frac{1}{2}\,D^3vD^{-1}v,\\ \Psi_1^{-1}(\sigma)=&[2\sigma D^{-2}+\sigma_xD^{-3}]\left[\frac{2D^{-3}\sigma D^{-1}+2D^{-1}\sigma D^{-3}-2D^{-2}\sigma D^{-2}}{4(D^{-3}\sigma)^2}\right.\\&\left.-\frac{(2D^{-1}\sigma D^{-3}\sigma-(D^{-2}\sigma)^2)D^{-3}}{2(D^{-3}\sigma)^3}\right]+2(1+u)D^{-2}+u_xD^{-3},\end{aligned} \tag{5.36}$$

where

$$u=-1-\frac{(\sqrt{D^{-3}\sigma})_{xx}}{\lambda^2\sqrt{D^{-3}\sigma}},\quad v=(1+u)^{-1/2}. \tag{5.37}$$

Equations (5.34) and (5.35) are two strong symmetries of the integrable equation of u

$$u_t=\sigma(u) \tag{5.38}$$

with σ defined in (5.37). On the other hand, (5.36) are two strong symmetries of the integrable equation (5.38) of σ.

Two strong hereditary symmetries for the eigenfunction equation about ψ are

$$\begin{aligned}\Psi_2(\psi)=&-\frac{D^3}{8\psi}\left[(D^3v^3(\psi^2)_{xxx}D^{-1}v+D^3vD^{-1}v^3(\psi^2)_{xxx})\left(-\frac{D^2}{\lambda^2\psi}+\frac{\psi_{xx}}{\lambda^2\psi}\right)+\frac{1}{2}\,D^3D^{-1}v\right],\\ \Psi_2^{-1}(\psi)=&\frac{D^{-3}}{2\psi}\left[(2(\psi^2)_{xxx}+(\psi^2)_{xxxx}D^{-3})\left(-\frac{D^2}{\lambda^2\psi}+\frac{\psi_{xx}}{\lambda^2\psi^2}\right)-\frac{2\psi_{xx}\psi_x}{\lambda^2\psi}-\frac{2\psi_{xxx}}{\lambda^2}-\frac{4\psi_{xx}}{\lambda^2}\,D\right],\end{aligned} \tag{5.39}$$

where $v=(-\psi_{xx}/\lambda^2\psi)^{-1/2}$.

Equations (5.39) are also two strong symmetries of the new integrable equation

$$\left(\frac{\psi_{xx}}{\psi}\right)_t=-\lambda^2(\psi^2)_{xxx}. \tag{5.40}$$

VI. CONCLUSION

In this paper, we give a formula for obtaining hereditary strong symmetries of nonlinear equations for eigenfunctions and the constraints equation. Using this formula we prove that eigenfunctions of hereditary strong symmetries are symmetries for the whole hierarchy. Applying the strong symmetries given here we can easily obtain K symmetries and τ symmetries and their Lie algebraic structure of eigenfunction equations (4.1), (4.3), and constraints equations (4.5).[21,22] At last, the Darboux transformations (DTs) of (3.6) give the Bäcklund transformations (BTs) for the eigenfunction equations (4.3). For example, associated with the KdV equation (5.9) there exists a DT[23]

$$u[1]=u+2(\ln\ \psi_1)_{xx}, \tag{6.1}$$

$$\psi[1]=\psi_x-\frac{\psi_{1x}}{\psi_1}\ \psi, \tag{6.2}$$

where ψ_1 is the fixed solution of (5.10) with $\lambda=\lambda_1$, then (6.2) becomes a BT for Eq. (5.14), in particular (5.14) has a auto-BT

$$\psi[1]=\frac{1}{\psi}.$$

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Soliton solutions and gauge equivalence for the problem of Zakharov–Shabat and its generalizations

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In a paper by Takhtadjan and Faddeev [*Hamiltonian approach to the soliton theory* (in Russian) (Nauka, Moskov, 1986)] the *N*-soliton solutions, related to the nonlinear Schrödinger equation (NSE), are given. A generalization of this approach allows us to apply it not only to the NSE, but to the whole hierarchy of the Zakharov–Shabat problem, to the quadratic bundle problem, and to the ones gauge equivalent to them [where one can find, for example, the Heisenberg ferromagnet equation, the relativistic Mikhailov model (which, in appropriate reduction, is equivalent to the massive Thirring model), the derivative nonlinear Schrödinger equation (which is equivalent to the derivative Landau–Lifshitz equation), etc.]. We have used an appropriate reduction, giving us interesting, from a physical point of view, results. Thus we manage to obtain the soliton solutions for the whole hierarchy of the quadratic bundle problem (free and under reduction) and for the ones gauge equivalent to it. This result was first announced in previous articles by Vaklev, but here we manage to solve the determinants given there and to present the searched result as simple fractions of products of numerical differences. © *1996 American Institute of Physics.* [S0022-2488(96)02802-9]

I. PRELIMINARIES

One can find the *N*-soliton solution for the particular case of the nonlinear Schrödinger equation in Ref. 1. An equivalent modification of the same method could be applied to any nonlinear evolution equation (NLEE) from the whole hierarchy of the Zakharov–Shabat system. Here we shall use a generalization of the approach used in Ref. 1. By means of that we also manage to obtain the *N*-soliton solutions of all NLEEs related to the quadratic bundle problem[3,8–10]

$$[2D_x+q_0(x,t)+\lambda q(x,t)+r(x,t)-\lambda^2]v(x,t,\lambda)=0, \tag{1}$$

where D_x, q_k, $k=0,1$, and r are of the form

$$D_x:=\frac{i}{2}\,\sigma_3 d_x, \quad q_k:=\begin{pmatrix} 0, & q_k^+ \\ q_k^-, & 0 \end{pmatrix},$$

$$q(x,t):=q_1(x,t), \quad r(x,t):=-\tfrac{1}{2}q^+(x,t)q^-(x,t).$$

(One can see that the Zakharov–Shabat system follows from Eq. (1) imposing $q=0$ and setting the spectral parameter $\mu=\lambda^2$.)

In this article we use the so-called "Expansion over 'squared solutions' method" (EOSSM).[11–13] This method allows us to examine simultaneously the whole classes of NLEE's related to the corresponding auxiliary linear problems. If one does the same in the Lax approach, he has to look for a great number of Lax pairs working separately equation by equation. The EOSSM unifies the result of such an activity and allows to write it in a complete form. For example the whole class of NLEE's related to the problem (1) can be written as[3,10–13]

$$i\Sigma\mathbb{Q}_t+F(\Lambda)\mathbb{Q}=0, \tag{2}$$

where (here we follow the notations of Ref. 5 with some insignificant modifications):

$$\Lambda:=\begin{pmatrix} Z_{10}, & 1+Z_1 \\ \Lambda_0, & Z_{01} \end{pmatrix}, \quad \Sigma:=\sigma_0\times\sigma_3,$$

$$\mathbb{Q}(x,t):=\begin{pmatrix} q \\ q_0 \end{pmatrix}, \quad \Lambda_0:=D_x+r+Z_0,$$

$$Z_{kl}:=\frac{i}{2}\,q_k(x,t)\left(\int_x^{\infty}dy+\int_x^{-\infty}dy\right)\langle q_l,[\sigma_3,\cdot\,]_-\rangle, \quad k,l=0,1,$$

$$Z_k:=Z_{kk}, \quad [X,Y]_{\pm}:=XY\pm YX, \quad X,Y\in gl(n,c),$$

$$\langle X,Y\rangle=\tfrac{1}{2}\ \mathrm{tr}\ XY, \quad X,Y\in gl(2,c),$$

and $F(\lambda)$ is the dispersion law of the form

$$F(\lambda)=\sum_{l=-k}^{c} f_l\lambda^l, \quad k,c\in\mathbb{R}_1, \quad k,c<\infty. \tag{3}$$

The results obtained by means of Lax approach correspond to the ones given here at a fixed value of the dispersion law (3). In order to obtain, for example, the soliton solutions of the relativistic Mikhailov model[8,14] we fix it $F(\lambda)=\lambda^{-2}$:

$$h_{1,x,t}+m^2h_1-2ih_1h_2h_{1,x}=0,$$

$$h_{2,x,t}+m^2h_2+2ih_1h_2h_{2,x}=0.$$

[It is equivalent (in case of an appropriate reduction)[3] to the massive Thirring model.] The derivative nonlinear Schrödinger equation (DNSE)

$$i\nu_t+\nu_{xx}+i\epsilon(|\nu|^2\nu)_x=0$$

is gauge equivalent [see Sec. V, Eq. (35)] to the one obtained by the choice of the dispersion law $F(\lambda)=\lambda^2$. It is gauge equivalent as well to the derivative Landau–Lifshitz equation (DLLE)

$$S_t-\frac{i}{2}\,[S,S_{xx}]_-+\frac{1}{4\omega^2}\,(S_x)^2=0$$

(see, e.g., Ref. 5 and the references given there). In order to obtain these results, we have to impose the reduction

$$q_0=0 \tag{4}$$

to the problem (1). In this case the new problem has some symmetry properties leading to evenness of the dispersion law (3). Thus the corresponding class of NLEE's related to problem (3) under (4) can be given as

$$i\sigma_3 q_{1,t}+F(\Lambda_1)q_1=0, \quad \Lambda_1:=(1+Z_1)(D_x+r),$$
$$F(\lambda^2):=\sum_{l=-\tilde{k}}^{\tilde{c}} f_{2l}\lambda^{2l}, \quad \tilde{k},\tilde{c}\in\mathbb{R}_1, \quad \hat{k},\tilde{c}<\infty. \tag{5}$$

(We note that if Λ in Eq. (2) is taken in power two, Λ_1 in Eq. (5) corresponds to power one.)

We would like to note that the topic of the presented work has been developing very intensively. Many papers appear and many new results are given. For example, in Ref. 15 new results for the MNLS equation were obtained. A part of them can be found here by setting the dispersion law (3):[5]

$$F(\lambda^2)=-4\lambda^4+8\omega^2\lambda^2-4\omega^4.$$

(The corresponding NLEE is given in Sec. V.) In the points of the spectrum $\lambda_j^{\pm}=\pm i\omega$ the used[5] transformation is singular. We have to evaluate there the whole quantities separately. That is why the results given in Ref. 15 differ from the ones given in Ref. 8 and from the ones presented here. It is difficult for us to quote all the results. The new point in the presented paper is that by means of EOSSM we obtain results not only for a fixed value of the dispersion function, but for the whole class of NLEEs (2,5).

II. SOLITON SOLUTIONS

One can draw some analogy between the Zakharov–Shabat problem and the problem of the quadratic bundle (1). The results in both cases are close. As we have mentioned, the results for the Zakharov–Shabat problem follows by setting $q=0$ and $\mu=\lambda^2$. We would like to note that some of the quantities used here are changed and others are absent. That is why the limit has to be performed carefully.

The Jost solutions $\boldsymbol{\psi}$ and $\boldsymbol{\phi}$ corresponding to the problem (1) are built as usual:

$$\boldsymbol{\psi}(x,t,\lambda):=(\boldsymbol{\psi}^-,\boldsymbol{\psi}^+)(x,t,\lambda):=\psi(x,t,\lambda)\exp(i\lambda^2 x\sigma_3),$$
$$\boldsymbol{\phi}(x,t,\lambda):=(\boldsymbol{\phi}^-,\boldsymbol{\phi}^+)(x,t,\lambda):=\phi(x,t,\lambda)\exp(i\lambda^2 x\sigma_3);$$
$$\lim_{x\to\infty}\boldsymbol{\psi}(x,t,\lambda)=\sigma_0, \quad \lim_{x\to-\infty}\boldsymbol{\phi}(x,t,\lambda)=\sigma_0, \tag{6}$$

where ψ and ϕ are solutions of (1) and σ_0 is $gl(2)$ unit matrix. For these solutions the following representations are valid:[8–10]

$$\boldsymbol{\psi}^{\pm}(x,t,\lambda)=e^{\pm}\pm\sum_{j=1}^{N}\frac{\zeta_j^{\mp}(x,t)}{\lambda_j^{\mp}-\lambda}\boldsymbol{\psi}_j^{\mp}(x,t)+\frac{1}{2\pi i}\int_{\Gamma}\frac{d\kappa}{\kappa-\lambda}\rho^{\mp}(t,\kappa)\boldsymbol{\psi}^{\mp}(x,t,\kappa)\exp\mp 2i\kappa^2 x, \tag{7}$$

where we note by

$$\zeta_j^{\pm}(x,t):=c_{0j}^{\pm}\exp\pm i[2(\lambda_j^{\pm})^2 x-F(\lambda_j^{\pm})t],$$
$$c_{0j}^{\pm}:=\left.\frac{b^{\pm}(t,\lambda)}{\frac{da^{\pm}(\lambda)}{d\lambda}}\right|_{\lambda=\lambda_j^{\pm},t=0}, \quad \boldsymbol{\psi}_j^{\pm}(x,t):=\boldsymbol{\psi}^{\pm}(x,t,\lambda_j^{\pm}), \tag{8}$$
$$e^+:=\begin{pmatrix}0\\1\end{pmatrix}, \quad e^-:=\begin{pmatrix}1\\0\end{pmatrix}, \quad \rho^{\pm}:=\frac{b^{\pm}(t,\lambda)}{a^{\pm}(\lambda)}.$$

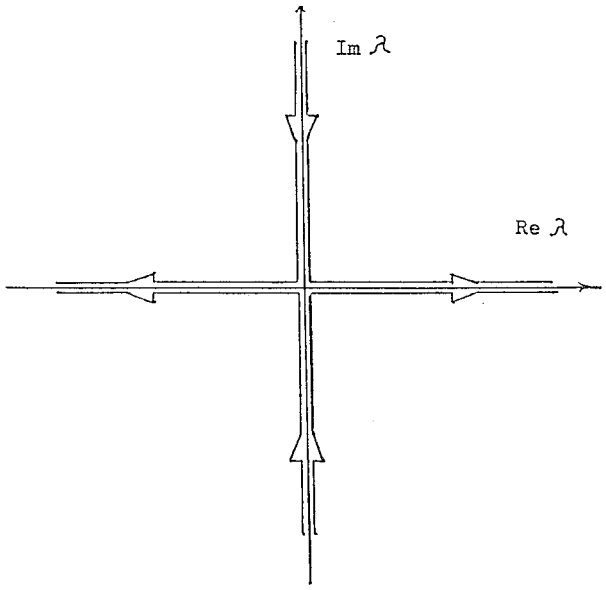

FIG. 1. The contour Γ.

By means of $a^{\pm},b^{\pm}$ we denote the reflection coefficients for the quadratic bundle (1). The continuous spectrum of Zakharov–Shabat problem coincides with the line: Im $\mu=0$, since for problem (1) the same spectrum is given by the contour Γ: Im $\lambda^2=0$ (see Fig. 1). The simple roots $\lambda_j^{\pm}$ (at which $a^{\pm}(\lambda_j^{\pm})=0$), $\lambda_j^{\pm}\notin\Gamma$ give the discrete spectrum of problem (1).

We remind that for ϕ from Eq. (6) is correct:

$$\phi_j^{\pm}(x,t)=\pm b_j^{\pm}(t)\psi_j^{\pm}(x,t),$$

where [compare Eq. (8)] $\phi_j^{\pm}$ is $\phi^{\pm}$ at the point $\lambda_j^{\pm}$. If we define

$$b_j^{\pm}(t)=b^{\pm}(\lambda,t)|_{\lambda=\lambda_j^{\pm}},$$

we can write

$$b_j^{\pm}(t)=b_{j0}^{\pm}\exp\pm iF(\lambda_j^{\pm})t,$$

where F is the dispersion law for problem (1), $b_{j0}^{\pm}$ are complex constants.

In the case of a reflectionless potential since

$$\rho^{\pm}=0, \tag{9}$$

the representations (7) turn into an algebraic system of $2N$ equations for the $2N$ quantities $\boldsymbol{\psi}_k^{\pm}$ [Eq. (8)]. Due to the Cramer formulas one obtains the N-soliton solution $\boldsymbol{\psi}$ of the problem of the quadratic bundle (1) in the form

$$\boldsymbol{\psi}(x,t,\lambda)=\sigma_0+\frac{\sigma_3}{|K|}\sum_{j=1}^{N}\begin{pmatrix}\sum_{s=1}^{N}\frac{\zeta_s^-}{\omega_{js}^+}|K_{(s)}^-|, & |K_{(j)}^-|\\ |K_{(j)}^+|, & \sum_{s=1}^{N}\frac{\zeta_s^+}{\omega_{js}^-}|K_{(s)}^+|\end{pmatrix}(x,t)\begin{pmatrix}\frac{\zeta_j^+(x,t)}{\lambda_j^+-\lambda}, & 0\\ 0, & \frac{\zeta_j^-(x,t)}{\lambda_j^--\lambda}\end{pmatrix}$$

$$= \sigma_0 - \frac{\sigma_3}{|K|}\sum_{j=1}^{N}\begin{pmatrix} \sum_{s=1}^{N}\frac{\zeta_s^-}{\omega_{js}^+}|K_{(s)}^-|, & |K_{(j)}^-| \\ |K_{(j)}^+|, & \sum_{s=1}^{N}\frac{\zeta_s^+}{\omega_{js}^-}|K_{(s)}^+| \end{pmatrix}(x,t)\begin{pmatrix} \zeta_j^+, & 0 \\ 0, & \zeta_j^- \end{pmatrix}(x,t)$$

$$\times\left[\frac{1}{\lambda}+\frac{1}{\lambda^2}\begin{pmatrix}\lambda_j^+, & 0\\ 0, & \lambda_j^-\end{pmatrix}+o\left(\frac{1}{\lambda^2}\right)\right]. \tag{10}$$

In the relations (10) we have used the notations (compare Refs. 6 and 7)

$$K_{i,l}^{\pm} := \delta_{i,l} - \zeta_l^{\pm}\sum_{s=1}^{N}\frac{\zeta_s^{\mp}}{\omega_{is}^{\pm}\omega_{ls}^{\pm}}, \quad \omega_{kj}^{\pm} := \pm(\lambda_k^{\pm}-\lambda_j^{\mp});$$

$$K_{(j)i,l}^{\pm} := K_{i,l}^{\pm} - \delta_{l,j}(K_{i,j}^{\pm}-1), \tag{11}$$

$$|X| := \det X, \quad X \in gl(2,c).$$

It remains to give explicitly the determinants $|K|$ and $|K_{(j)}^{\pm}|$ in order to have the result in an explicit form. {One can see here, because of the symmetry properties of the summarized quantities entering in determinant $|K|$ [see Eq. (14)], that it does not depend on "$\pm$."} We have obtained them from definition (11) using their expansion over the principal minors. The terms entering the expansion can be simplified applying the Binet–Cauchy formula to them. We succeeded to solve these determinants explicitly. (We have solved also the ones used in Ref. 7; in spite of that it concerns another case which we shall examine further.) The result for the case of the Zakharov–Shabat problem coincides with those in Ref. 1 and repeats the ones given in Refs. 5, 8, and 10 for the one soliton solutions in case (1). For the N-soliton solutions, when $N \geqslant 2$, the result is new. We use the known from the linear algebra formula [compare with formula (II.8.49) of Ref. 1]:

$$\begin{vmatrix} \frac{1}{a_{i_1}+b_{j_1}}, & \ldots, & \frac{1}{a_{i_1}+b_{j_n}} \\ \vdots & \ddots & \vdots \\ \frac{1}{a_{i_n}+b_{j_1}}, & \ldots, & \frac{1}{a_{i_n}+b_{j_n}} \end{vmatrix} = \prod_{k<l=1}^{n}(a_{i_k}-a_{i_l})(b_{j_k}-b_{j_l})\prod_{m,s=1}^{n}(a_{i_m}+b_{j_s})^{-1},$$

where $i_1,\ldots,i_n,j_1,\ldots,j_n$ can be different increasing number sets. Thus we have (compare Refs. 6 and 7)

$$|\Theta_{j_1,\ldots,j_n}^{\pm i_1,\ldots,i_n}| := \begin{vmatrix} \frac{1}{\omega_{i_1 j_1}^{\pm}}, & \ldots, & \frac{1}{\omega_{i_1 j_n}^{\pm}} \\ \vdots & \ddots & \vdots \\ \frac{1}{\omega_{i_n j_1}^{\pm}}, & \ldots, & \frac{1}{\omega_{i_n j_n}^{\pm}} \end{vmatrix} = (\pm 1)^n \prod_{k<l=1}^{n}(\lambda_{i_k}^{\pm}-\lambda_{i_l}^{\pm})(\lambda_{j_l}^{\mp}-\lambda_{j_k}^{\mp})\prod_{m,s=1}^{n}(\lambda_{i_m}^{\pm}-\lambda_{j_s}^{\mp})^{-1},$$

$$|\Theta_{j_1,\ldots,j_n}^{\pm i_1,\ldots,i_n}| = |\Theta_{i_1,\ldots,i_n}^{\mp j_1,\ldots,j_n}|. \tag{12}$$

For the determinant of the difference, we have obtained

$$|\Theta^{\pm i_1,\ldots,i_n}_{p_1,\ldots,p_n}-\Theta^{\pm j\ldots,j}_{p_1,\ldots,p_n}|=\prod_{k=1}^{n}\left(1-\frac{\omega^{\pm}_{i_k p_k}}{\omega^{\pm}_{j p_k}}\right)|\Theta^{\pm i_1,\ldots,i_n}_{p_1,\ldots,p_n}|. \tag{13}$$

By means of the relations (12) and (13) from the definition (11) one obtains

$$|K|(x,t)=\sum_{k=0}^{N}(-1)^{N-k}\sum_{\substack{i_1<\cdots<i_{N-k}=1\\ p_1<\cdots<p_{N-k}=1}}^{N}\prod_{s=1}^{N-k}(\zeta^{\pm}_{i_s}\zeta^{\mp}_{p_s})(x,t)|\Theta^{\pm i_1,\ldots,i_{N-k}}_{p_1,\ldots,p_{N-k}}|^2,$$

$$|K^{\pm}_{(j)}|(x,t)=\sum_{k=1}^{N}(-1)^{N-k}\sum_{\substack{i_1<\cdots<i_{N-k}=1\\ i\neq j\\ p_1<\cdots<p_{N-k}=1}}^{N}\prod_{s=1}^{N-k}(\zeta^{\pm}_{i_s}\zeta^{\mp}_{p_s})(x,t)\left(1-\frac{\omega^{\pm}_{i_s p_s}}{\omega^{\pm}_{j p_s}}\right)|\Theta^{\pm i_1,\ldots,i_{N-k}}_{p_1,\ldots,p_{N-k}}|^2,$$

$$\sum_{i_1<\cdots<i_{N-k}=1}^{N}\Bigg|_{k=N}(\cdots):=\prod_{s=1}^{N-k}(\cdots)\Bigg|_{k=N}:=1. \tag{14}$$

We have expansions of $\boldsymbol{\psi}$ for $\lambda\gg 1$:

$$\boldsymbol{\psi}^{d}(x,t,\lambda)=\sigma_0-\frac{i}{\lambda}\,\sigma_3\int_x^{\infty}dy\langle q_1,q_0\rangle(y,t)+o\left(\frac{1}{\lambda}\right),$$

$$\boldsymbol{\psi}^{a}(x,t,\lambda)=\frac{1}{2\lambda}\,q_1+\frac{1}{2\lambda^2}\left[q_0(x,t)+i\sigma_3 q_1(x,t)\int_x^{\infty}dy\langle q_1,q_0\rangle(y,t)\right]+o\left(\frac{1}{\lambda^2}\right),$$

where, as it is known,

$$X^{d}:=\tfrac{1}{2}\sigma_3[\sigma_3,X]_{+},\quad X^{a}:=\tfrac{1}{2}\sigma_3[\sigma_3,X]_{-}.$$

Thus we have the potentials q_0,q from this expansion and Eq. (10) for the case of the quadratic bundle problem (1):

$$\begin{aligned}q_0&=\frac{2}{|K|}\sum_{j=1}^{N}\begin{pmatrix}0, & \zeta^{-}_j|K^{-}_{(j)}|\\ \zeta^{+}_j|K^{+}_{(j)}|, & 0\end{pmatrix}\left[\begin{pmatrix}\lambda^{+}_j, & 0\\ 0, & -\lambda^{-}_j\end{pmatrix}+\frac{\Sigma_{k,l=1}^{N}\dfrac{\zeta^{\pm}_l\zeta^{\mp}_k}{\omega^{\pm}_{lk}}|K^{\pm}_{(l)}|}{|K|}\right],\\ q&=-\frac{2}{|K|}\,\sigma_3\sum_{j=1}^{N}\begin{pmatrix}0, & \zeta^{-}_j|K^{-}_{(j)}|\\ \zeta^{+}_j|K^{+}_{(j)}|, & 0\end{pmatrix}\end{aligned} \tag{15}$$

in an explicit form. The quantities $|K|$ and $|K^{\pm}_{(j)}|$ are given explicitly by Eqs. (12) and (14). Thus we have represented the result in a form of simple fractions of numerical differences.

III. THE REDUCTION CASE

In order to investigate the solutons of DNSE, its gauge equivalent DLLE, etc., we have to use the quadratic bundle problem (1) under the reduction (4).

One can see[5] that in case of reduction,

$$q_0=\omega\sigma_3 q,\quad \omega\in\mathbb{C},$$

to problem (1) it leads to

$$\psi(x,t,\lambda)=\sigma_3\psi(x,t,-\lambda)\sigma_3 \rightarrow \boldsymbol{\psi}(x,t,-\lambda)=\mp\sigma_3\boldsymbol{\psi}(x,t,\lambda).$$

Thus if $\lambda_\pm$ belongs to the discrete spectrum of Eq. (1), then so do $-\lambda_\pm$. This is not true for Eq. (7) in general. Due to these symmetry properties of the coefficients entering Eq. (7) and of the trivial fact

$$\frac{1}{\lambda-\lambda_j^\pm}-\frac{1}{\lambda+\lambda_j^\pm}=\frac{2\lambda_j^\pm}{\lambda^2-(\lambda_j^\pm)^2},\quad \frac{1}{\lambda-\lambda_j^\pm}+\frac{1}{\lambda+\lambda_j^\pm}=\frac{2\lambda}{\lambda^2-(\lambda_j^\pm)^2}$$

the new representation, in the case of reflectionless potential (9) and reduction (4), has the form

$$\boldsymbol{\psi}^\pm(x,t,\lambda)=e^\pm\pm 2\sum_{j=1}^{N}\frac{\zeta_j^\mp(x,t)}{(\lambda_j^\mp)^2-\lambda^2}\,l_j^\mp(\lambda)\boldsymbol{\psi}_j^\mp(x,t), \tag{16}$$

where $\zeta_j^\pm$ and $\boldsymbol{\psi}_j^\pm$ are given again by Eq. (8) and

$$l_j^+(\lambda):=\begin{pmatrix}\lambda_j^+, & 0\\ 0, & \lambda\end{pmatrix},\quad l_j^-(\lambda):=\begin{pmatrix}\lambda, & 0\\ 0, & \lambda_j^-\end{pmatrix}.$$

[We would like to note that for convenience we have denoted the solution of problem (1) under reduction (4) by the same letter as it was done in relations (7); but as we have mentioned above these solutions in general differ.]

From the representation (16) one derives (we shall not repeat the calculations since it was done in Ref. 7):

$$\begin{aligned}\boldsymbol{\psi}(x,t,\lambda)=\sigma_0+2\sigma_3\sum_{j=1}^{N}&\begin{pmatrix}\dfrac{1}{|M^-(x,t)|}, & 0\\ 0, & \dfrac{1}{|M^+(x,t)|}\end{pmatrix}\\ &\times\begin{pmatrix}2(\lambda_j^+)^2\displaystyle\sum_{s=1}^{N}\frac{\zeta_s^-|M_{(s)}^-|}{\Delta_{js}^+}, & \lambda|M_{(j)}^-|\\ \lambda|M_{(j)}^+|, & 2(\lambda_j^-)^2\displaystyle\sum_{s=1}^{N}\frac{\zeta_s^+|M_{(s)}^+|}{\Delta_{js}^-}\end{pmatrix}(x,t)\\ &\times\begin{pmatrix}\dfrac{\zeta_j^+(x,t)}{(\lambda_j^+)^2-\lambda^2}, & 0\\ 0, & \dfrac{\zeta_j^-(x,t)}{(\lambda_j^-)^2-\lambda^2}\end{pmatrix},\quad \Delta_{ij}^\pm:=\pm[(\lambda_i^\pm)^2-(\lambda_j^\mp)^2].\end{aligned} \tag{17}$$

The new point here is that we manage to solve explicitly the determinants entering the given expressions. The determinants $|M^\pm|$ and $|M_{(j)}^\pm|$ in Eq. (17) are given by [compare relations (12) and (14)]

$$|M^\pm|(x,t)=\sum_{k=0}^{N}(-4)^{N-k}\sum_{\substack{i_1<\cdots<i_{N-k}=1\\ p_1<\cdots<p_{N-k}=1}}^{N}\prod_{s=1}^{N-k}(\zeta_{i_s}^\pm\zeta_{p_s}^\mp)(x,t)(\lambda_{p_s}^\mp)^2|\Xi_{p_1,\ldots,p_{N-k}}^{\pm i_1,\ldots,i_{N-k}}|^2,$$

$$|M^{\pm}_{(j)}|(x,t)=\sum_{k=1}^{N}(-4)^{N-k}\sum_{\substack{i_1<\cdots<i_{N-k}=1\\ i\neq j\\ p_1<\cdots<p_{N-k}=1}}^{N}\prod_{s=1}^{N-k}(\zeta^{\pm}_{i_s}\zeta^{\mp}_{p_s})(x,t)(\lambda^{\mp}_{p_s})^2\left(1-\frac{\Delta^{\pm}_{i_s p_s}}{\Delta^{\pm}_{j p_s}}\right)|\Xi^{\pm i_1,\ldots,i_{N-k}}_{p_1,\ldots,p_{N-k}}|^2,$$

$$\Xi^{\pm i_1,\ldots,i_n}_{j_1,\ldots,j_n}=\Xi^{\mp j_1,\ldots,j_n}_{i_1,\ldots,i_n}:=\begin{pmatrix}\frac{1}{\Delta^{\mp}_{i_1 j_1}}, & \ldots, & \frac{1}{\Delta^{\mp}_{i_1 j_n}}\\ \vdots, & \ddots & \vdots\\ \frac{1}{\Delta^{\mp}_{i_n j_1}} & \ldots, & \frac{1}{\Delta^{\mp}_{i_n j_n}}\end{pmatrix},$$

$$|\Xi^{\pm i_1,\ldots,i_n}_{p_1,\ldots,p_n}|^2=\prod_{l<m=1}^{n}[(\lambda^{\pm}_{i_l})^2-(\lambda^{\pm}_{i_m})^2]^2[(\lambda^{\mp}_{p_l})^2-(\lambda^{\mp}_{p_m})^2]^2\prod_{k,s=1}^{n}[(\lambda^{\pm}_{i_k})^2-(\lambda^{\mp}_{p_s})^2]^{-2}.$$

Here and further we shall denote by p the potential q for the problem (1) under reduction (4). The result is given by[7]

$$p(x,t)=4\sum_{j=1}^{N}\begin{pmatrix}0, & -\frac{\zeta^{-}_j|M^{-}_{(j)}|}{|M^{-}|}\\ \frac{\zeta^{+}_j|M^{+}_{(j)}|}{|M^{+}|}, & 0\end{pmatrix}(x,t). \tag{18}$$

One can see that we have represented the result in a form of simple fractions of numerical differences.

IV. REGULARITY AND ASYMPTOTIC BEHAVIOR

Going over to the N-soliton solution case, we impose (see Refs. 6 and 7)

$$\begin{aligned}&\lambda_j^2:=(\lambda_j^{+})^2:=m_j+im_j^1,\quad (\lambda_j^{-})^2=\overline{\lambda_j^2},\\ &F(\lambda_j^{\pm})=F_j\pm iF_j^1,\quad \arg c_{0j}^{+}c_{0j}^{-}\neq(2k+1)\pi.\end{aligned} \tag{19}$$

The case of reduction (4) conserves the conditions for $(\lambda_j^{\pm})^2$ and $F(\lambda_j^{\pm})$ changing the last one for $c_{0j}^{\pm}$, into

$$\arg c_{0j}^{+}c_{0j}^{-}+2\arg\lambda_j^{\pm}\neq(2k+1)\pi. \tag{20}$$

One obtains the asymptotic behavior of the solutions q_0, q [Eq. (15)], and p [Eq. (18)] analyzing the behavior of the corresponding products of $\zeta_k^{\pm}$ forming their entries. We define the velocities

$$v_j:=\frac{F_j^1}{2m_j^1}. \tag{21}$$

Let us observe the investigated quantities "tracing them" by fixed velocity v_h, namely

$$x-v_ht=c,\quad c=\text{const}\in\mathbb{R}_1. \tag{22}$$

We choose the numeration of the points of the discrete spectrum so that the velocities v_j [Eq. (21)] to be ordered in the following way:

$$v_1<v_2<\cdots<v_N.$$

This allows one to evaluate that

$$\lim_{\substack{j<h\\ x-v_ht=c\\ x,t\to-\infty}}\zeta_j^{\pm}=\infty,\qquad \lim_{\substack{j>h\\ x-v_ht=c\\ x,t\to-\infty}}\zeta_j^{\pm}=0;\qquad \lim_{\substack{j<h\\ x-v_ht=c\\ x,t\to\infty}}\zeta_j^{\pm}=0,\qquad \lim_{\substack{j>h\\ x-v_ht=c\\ x,t\to\infty}}\zeta_j^{\pm}=\infty.$$

Thus from the relations (14), one obtains

$$\lim_{t,x\to-\infty}|K(x,t)|=\lim_{t,x\to-\infty}\left[(-1)^h\prod_{s=1}^{h}\zeta_s(x,t)|\Theta^{\pm 1,\ldots,h}_{1,\ldots,h}|^2+(-1)^{h-1}\prod_{s=1}^{h-1}\zeta_s(x,t)|\Theta^{\pm 1,\ldots,h-1}_{1,\ldots,h-1}|^2\right],$$

$$\lim_{t,x\to\infty}|K(x,t)|=\lim_{t,x\to\infty}\left[(-1)^{N-h+1}\prod_{s=h}^{N}\zeta_s(x,t)\left|\Theta^{\pm h,\ldots,N}_{h,\ldots,N}\right|^2+(-1)^{N-h}\prod_{s=h+1}^{N}\zeta_s(x,t)|\Theta^{\pm h+1,\ldots,N}_{h+1,\ldots,N}|^2\right],$$

$$\lim_{t,x\to-\infty}\sum_{j=1}^{N}(\lambda_j^{\pm})^a(\zeta_j^{\pm}|K^{\pm}_{(j)}|)(x,t)=\lim_{t,x\to-\infty}(-1)^{h-1}\zeta_h^{\pm}(x,t)\sum_{\substack{j=1\\ i_1<\cdots<i_{h-1}=1\\ i\neq j}}^{h}(\lambda_j^{\pm})^a\times\prod_{s=1}^{h-1}\zeta_s(x,t)\left(1-\frac{\omega^{\pm}_{i_ss}}{\omega^{\pm}_{js}}\right)|\Theta^{\pm i_1,\ldots,i_{h-1}}_{1,\ldots,h-1}|^2,$$

$$\lim_{t,x\to\infty}\sum_{j=1}^{N}(\lambda_j^{\pm})^a(\zeta_j^{\pm}|K^{\pm}_{(j)}|)(x,t)=\lim_{t,x\to\infty}(-1)^{N-h}\zeta_h^{\pm}(x,t)\sum_{\substack{j=h\\ i_1<\cdots<i_{N-h}=h\\ i\neq j}}^{N}(\lambda_j^{\pm})^a\times\prod_{s=h+1}^{N}\zeta_s(x,t)\left(1-\frac{\omega^{\pm}_{i_{s-h}s}}{\omega^{\pm}_{js}}\right)|\Theta^{\pm i_1,\ldots,i_{N-h}}_{h+1,\ldots,N}|^2,$$

$$\zeta_k=\zeta_k^{+}\zeta_k^{-},\quad a=0,1,\quad x-v_ht=c,$$

$$\Theta^{\pm 1,\ldots,h-1}_{1,\ldots,h-1}|_{h=1}:=\Theta^{\pm h+1,\ldots,N}_{h+1,\ldots,N}|_{h=N}:=1. \tag{23}$$

The sums, entering the last two relations (23), can be calculated explicitly. We have done it due to the properties of the Vandermonde determinants and the explicit form of these given by Eq. (12) (see Appendices A and B):

$$\sum_{\substack{j=1\\ i_1<\cdots<i_{h-1}=1\\ i\neq j}}^{h}(\lambda_j^{\pm})^a\prod_{k=1}^{h-1}\left(1-\frac{\omega^{\pm}_{i_kk}}{\omega^{\pm}_{jk}}\right)|\Theta^{\pm i_1,\ldots,i_{h-1}}_{1,\ldots,h-1}|^2=\left(\lambda_h^{\pm}\mp 2i\sum_{\alpha=1}^{h-1}m_\alpha^1\right)^a\prod_{l=1}^{h-1}\left(1-\frac{\omega^{\pm}_{ll}}{\omega^{\pm}_{hl}}\right)^2|\Theta^{\pm 1,\ldots,h-1}_{1,\ldots,h-1}|^2,$$

$$\sum_{\substack{j=h \\ i_1<\cdots<i_{N-h}=h \\ i\neq j}}^{h} (\lambda_j^{\pm})^a \prod_{k=h+1}^{N} \left(1-\frac{\omega^{\pm}_{i_{k-h}k}}{\omega^{\pm}_{jk}}\right) |\Theta^{\pm i_1,\ldots,i_{N-h}}_{h+1,\ldots,N}|^2$$

$$= \left(\lambda_h^{\pm} \mp 2i \sum_{\alpha=h+1}^{N} m_\alpha^1\right)^a \prod_{l=h+1}^{N} \left(1-\frac{\omega^{\pm}_{ll}}{\omega^{\pm}_{hl}}\right)^2 |\Theta^{\pm h+1,\ldots,N}_{h+1,\ldots,N}|^2, \quad a=0,1. \tag{24}$$

Now we apply the results (23) and (24) to q [Eq. (15)], imposing condition (22):

$$\lim_{\substack{t,x\to-\infty \\ x-v_h t=c}} q^{\pm}(x,t) = \mp 2 \prod_{k=1}^{h-1} \left(\frac{\lambda_h^{\mp}-\lambda_k^{\mp}}{\lambda_h^{\mp}-\lambda_k^{\pm}}\right)^2 \lim_{\substack{t,x\to-\infty \\ x-v_h t=c}} \frac{\zeta_h^{\mp}(x,t)}{1+\dfrac{1}{4\ \mathrm{Im}^2\ \lambda_h} \Pi_{k=1}^{h-1} \left|\dfrac{\lambda_h-\lambda_k}{\lambda_h-\overline{\lambda_k}}\right|^4 \zeta_h(x,t)},$$

$$\lim_{\substack{t,x\to\infty \\ x-v_h t=c}} q^{\pm}(x,t) = \mp 2 \prod_{k=h+1}^{N} \left(\frac{\lambda_h^{\mp}-\lambda_k^{\mp}}{\lambda_h^{\mp}-\lambda_k^{\pm}}\right)^2 \lim_{\substack{t,x\to\infty \\ x-v_h t=c}} \frac{\zeta_h^{\mp}(x,t)}{1+\dfrac{1}{4\ \mathrm{Im}^2\ \lambda_h} \Pi_{k=h+1}^{N} \left|\dfrac{\lambda_h-\lambda_k}{\lambda_h-\overline{\lambda_k}}\right|^4 \zeta_h(x,t)}. \tag{25}$$

[For convenience we use simultaneously both ways of definition of $\lambda_k^{\pm}$, given by relation (19).]

In case of reduction (4) the asymptotic behavior of $p^{\pm}$ looks like

$$\lim_{\substack{t,x\to-\infty \\ x-v_h t=c}} p^{\pm}(x,t) = \mp 4 \lim_{\substack{t,x\to-\infty \\ x-v_h t=c}} \frac{\Pi_{l=1}^{h-1} \left[\dfrac{(\lambda_h^{\mp})^2-(\lambda_l^{\mp})^2}{(\lambda_h^{\mp})^2-(\lambda_l^{\pm})^2}\right]^2 \zeta_h^{\mp}(x,t)}{1+\dfrac{(\lambda_h^{\pm})^2}{(m_h^1)^2} \Pi_{l=1}^{h-1} \left|\dfrac{\lambda_h^2-\lambda_l^2}{\lambda_h^2-\overline{\lambda_l^2}}\right|^4 \zeta_h(x,t)},$$

$$\lim_{\substack{t,x\to\infty \\ x-v_h t=c}} p^{\pm}(x,t) = \mp 4 \lim_{\substack{t,x\to\infty \\ x-v_h t=c}} \frac{\Pi_{l=h+1}^{N} \left[\dfrac{(\lambda_h^{\mp})^2-(\lambda_l^{\mp})^2}{(\lambda_h^{\mp})^2-(\lambda_l^{\pm})^2}\right]^2 \zeta_h^{\mp}(x,t)}{1+\dfrac{(\lambda_h^{\pm})^2}{(m_h^1)^2} \Pi_{l=h+1}^{N} \left|\dfrac{\lambda_h^2-\lambda_l^2}{\lambda_h^2-\overline{\lambda_l^2}}\right|^4 \zeta_h(x,t)}. \tag{26}$$

The expression giving the asymptotic behavior of q_0 [Eq. (15)] is not simple. That is why in the majority of papers the reduction (4) was imposed.

One can see that the asymptotic behavior of q and p, Eqs. (25) and (26), reminds one of the one soliton solutions with some changed $\zeta_k^{\pm}$ [Eq. (8)]. As a matter of fact, only $b_k^{\pm}$ changes [see the comment of notations (8)]. It is so because the discrete spectrum $\{\lambda_k^{\pm}\}$ does not change.

Using the functionals generating the infinite series of conservation quantities related to the problem (1) in case (9) one derives

$$\left.\frac{da^{\pm}(\lambda)}{d\lambda}\right|_{\lambda=\lambda_h^{\pm}} = \mp \frac{i}{2\ \mathrm{Im}\ \lambda_h} \prod_{h\neq k=1}^{N} \frac{\lambda_h^{\pm}-\lambda_k^{\pm}}{\lambda_h^{\pm}-\lambda_k^{\mp}}, \quad q_0\neq 0, \tag{27}$$

$$\left.\frac{da^{\pm}(\lambda^2)}{d\lambda}\right|_{\lambda=\lambda_h^{\pm}} = \mp\frac{i\lambda_h^{\pm}}{m_h^1}\prod_{h\neq k=1}^{N}\frac{(\lambda_h^{\pm})^2-(\lambda_k^{\pm})^2}{(\lambda_h^{\pm})^2-(\lambda_k^{\mp})^2}, \quad q_0=0.$$

If we put relation (27) in definition (8) for $\zeta_h^{\pm}$, we can write

$$\begin{aligned}\zeta_h^{\pm}(x,t) &= \prod_{h\neq k=1}^{N}\frac{\lambda_h^{\pm}-\lambda_k^{\mp}}{\lambda_h^{\pm}-\lambda_k^{\pm}}\,\zeta_{1h}^{\pm}(x,t), \quad q_0\neq 0,\\ \zeta_h^{\pm}(x,t) &= \prod_{h\neq k=1}^{N}\frac{(\lambda_h^{\pm})^2-(\lambda_k^{\mp})^2}{(\lambda_h^{\pm})^2-(\lambda_k^{\pm})^2}\,\zeta_{1h}^{\pm}(x,t), \quad q_0=0.\end{aligned} \tag{28}$$

The quantities $\zeta_{1h}^{\pm}$ in relation (28) are $\zeta_h^{\pm}$ taken at $N=1$. They form the one soliton solutions for the quadratic bundle problem (1) [free or under reduction (5)] satisfying conditions (19) and (20), respectively.

We define as usual:

$$x_h, x_{0h} = \frac{1}{2m_h^1}\ln\sqrt{|b_{h0}^{+}b_{h0}^{-}|};$$

$$\eta_h^{\mp}, \eta_{0h}^{\pm} = \frac{1}{2}\arg\frac{b_{h0}^{\mp}}{b_{h0}^{\pm}} + (2k+1)\,\frac{\pi}{2}, \quad k=0,\pm 1,\ldots .$$

Thus in case of the quadratic bundle (1) with $q_0\neq 0$, we obtain

$$\begin{aligned}\Delta x_h &:= \frac{1}{m_h^1}\left(\sum_{k=h+1}^{N}\ln\left|\frac{\lambda_h-\overline{\lambda_k}}{\lambda_h-\lambda_k}\right| - \sum_{k=1}^{h-1}\ln\left|\frac{\lambda_h-\overline{\lambda_k}}{\lambda_h-\lambda_k}\right|\right),\\ \Delta\eta_h^{\pm} &= \mp 2\left(\sum_{k=h+1}^{N}\arg\frac{\lambda_h-\overline{\lambda_k}}{\lambda_h-\lambda_k} - \sum_{k=1}^{h-1}\arg\frac{\lambda_h-\overline{\lambda_k}}{\lambda_h-\lambda_k}\right).\end{aligned} \tag{29}$$

In case of reduction (5) (compare Ref. 8)

$$\begin{aligned}\Delta x_0 h &:= \frac{1}{m_h^1}\left(\sum_{k=h+1}^{N}\ln\left|\frac{\lambda_h^2-\overline{\lambda_k^2}}{\lambda_h^2-\lambda_k^2}\right| - \sum_{k=1}^{h-1}\ln\left|\frac{\lambda_h^2-\overline{\lambda_k^2}}{\lambda_h^2-\lambda_k^2}\right|\right),\\ \Delta n_0 h^{\pm} &= \mp 2\left(\sum_{k=h+1}^{N}\arg\frac{\lambda_h^2-\overline{\lambda_k^2}}{\lambda_h^2-\lambda_k^2} - \sum_{k=1}^{h-1}\arg\frac{\lambda_h^2-\overline{\lambda_k^2}}{\lambda_h^2-\lambda_k^2}\right).\end{aligned} \tag{30}$$

One can obtain the result of Ref. 8 imposing the reduction (4), an additional reduction to q, and setting $F(\lambda)=\lambda^{-2}$ in the problem of the quadratic bundle (1). Because of the reduction (4), a pair of eigenvalues corresponds to the one soliton solution; that is why the result of Ref. 8 follows from Eq. (30) putting $N=2$. Our result concerns the general case (not only the one studied in Ref. 8, and not only for $N=2$). We note again that the result (29) is related only to q; for q_0 (as mentioned above) the result is different and complicated. This trouble does not appear in the case of reduction (4).

In order to obtain the one component equations (nonlinear Schrödinger equation, DNSE, DLLE, MNLS, etc.), we impose an additional reduction:

$$q^{*\pm} = -q^{\mp}, \quad p^{*\pm} = -p^{\mp}, \tag{31}$$

which leads to

$$\arg\, c_0^+ c_0^- = 0.$$

This reduction cancels the imaginary part in the denominators of the one soliton solutions in the case $q_0 \neq 0$, but in the case $q_0 = 0$ remains a constant:

$$\pm \frac{i \arg \lambda_j^{\pm}}{2m_h^1}.$$

V. GAUGE TRANSFORMED CASE

Let $\tilde{g}$ be a solution of the Zakharov–Shabat problem in the point $\mu = \mu_0$, and g a solution of problem (1) in the point $\lambda = \lambda_0$. Then the auxiliary linear problems

$$(i\tilde{S}d_x - \mu)\tilde{v}_g(x,t,\mu) = 0,$$

$$[iSd_x + (\lambda - \lambda_0)S' + \lambda_0^2 - \lambda^2]v_g(x,t,\lambda) = 0,$$

where

$$\tilde{S} := Ad_{\tilde{g}^{-1}}\sigma_3, \quad S := Ad_{g^{-1}}\sigma_3, \quad S' := Ad_{g^{-1}}q,$$

$$(2D_x + q)\tilde{g} = 0, \quad (2D_x + q_0 + \lambda_0 q + r - \lambda_0^2)g = 0, \tag{32}$$

$$\tilde{v}_g := \tilde{g}^{-1}\tilde{v}, \quad v_g := g^{-1}v$$

are gauge equivalent to the problems of Zakharov–Shabat and Eq. (1), respectively. We also have that in the case of reduction (4) the problems

$$\left[iS^0 d_x + \frac{i(\lambda_0 - \lambda)}{2\lambda_0} S_x^0 + \lambda_0^2 - \lambda^2\right] v_{g0}(x,t,\lambda) = 0,$$

$$[2D_x + (\lambda + i\omega\sigma_3)\tilde{q} - \lambda^2]\tilde{v} = 0,$$

where

$$(2D_x + \lambda_0 q + r - \lambda_0^2)g_0 = 0, \quad S^0 := Ad_{g_0^{-1}}\sigma_3, \quad v_{g0} := g_0^{-1}v,$$

$$\tilde{v} := \left(\exp\, i\sigma_3 \int_x^{\infty} dy\; r\right) v, \quad \tilde{q} := \left(\exp\, 2i\sigma_3 \int_x^{\infty} dy\; r\right) q \tag{33}$$

are gauge equivalent to problem (1) under reduction (4).[2,5,16] (For convenience we do not use the more general case studied in Ref. 5.)

One can derive by means of the explicit form of $\tilde{\psi}$ and ψ [Eq. (10) and Eq. (14)], that $\tilde{S}$ and S [Eq. (32)] have the form

$$\tilde{S}(x,t)=\left[\sigma_3+\frac{1}{|\tilde{K}|}\sum_{j=1}^{N}\begin{pmatrix}\dfrac{\tilde{\zeta}_j^-(x,t)}{\mu_j^-}, & 0\\ 0, & \dfrac{\tilde{\zeta}_j^+(x,t)}{\mu_j^+}\end{pmatrix}\right.$$
$$\left.\times\begin{pmatrix}-\Sigma_{s=1}^{N}\dfrac{\tilde{\zeta}_s^+}{\tilde{\omega}_{js}^-}|\tilde{K}_{(s)}^+|, & |\tilde{K}_{(j)}^-|\\ |\tilde{K}_{(j)}^+|, & -\Sigma_{s=1}^{N}\dfrac{\tilde{\zeta}_s^-}{\tilde{\omega}_{js}^+}|\tilde{K}_{(s)}^-|\end{pmatrix}(x,t)\right]\tilde{g}(x,t),$$

$$S(x,t)=\left[\sigma_3+\frac{1}{|K|}\sum_{j=1}^{N}\begin{pmatrix}\dfrac{\zeta_j^-(x,t)}{\lambda_j^--\lambda_0}, & 0\\ 0, & \dfrac{\zeta_j^+(x,t)}{\lambda_j^+-\lambda_0}\end{pmatrix}\right.$$
$$\left.\times\begin{pmatrix}-\Sigma_{s=1}^{N}\dfrac{\zeta_s^+}{\omega_{js}^-}|K_{(s)}^+|, & |K_{(j)}^-|\\ |K_{(j)}^+|, & -\Sigma_{s=1}^{N}\dfrac{\zeta_s^-}{\omega_{js}^+}|K_{(s)}^-|\end{pmatrix}(x,t)\right]g(x,t).$$

The quantities $\tilde{g}$ and g are defined as

$$\tilde{g}(x,t)=\tilde{\boldsymbol{\psi}}(x,t,0),\quad g(x,t)=\boldsymbol{\psi}(x,t,\lambda_0)\exp(-i\lambda_0 x\sigma_3),\tag{34}$$

where $\tilde{\boldsymbol{\psi}}$, are the Jost solutions for the Zakharov–Shabat problem and $\boldsymbol{\psi}$ are taken from Eq. (10). The gauge transformed potential S' [Eq. (32)] is obtained by

$$g^{-1}(x,t)=\boldsymbol{\psi}^{-1}(x,t,\lambda_0)=\sigma_0-\frac{\sigma_3}{|K|}\sum_{j=1}^{N}\begin{pmatrix}\dfrac{\zeta_j^-(x,t)}{\lambda_j^--\lambda_0}, & 0\\ 0, & \dfrac{\zeta_j^+(x,t)}{\lambda_j^+-\lambda_0}\end{pmatrix}$$
$$\times\begin{pmatrix}\Sigma_{s=1}^{N}\dfrac{\zeta_s^+}{\omega_{js}^-}|K_{(s)}^+|, & |K_{(j)}^-|\\ |K_{(j)}^+|, & \Sigma_{s=1}^{N}\dfrac{\zeta_s^-}{\omega_{js}^+}|K_{(s)}^-|\end{pmatrix}(x,t),$$

$q(x,t)$ [Eq. (15)] and $g(x,t)$ [Eq. (34)]. The last potential S^0 [Eq. (33)] can be written as

$$S^0(x,t)=\Bigg[\sigma_3+2\sum_{j=1}^{N}\begin{pmatrix}\dfrac{\zeta_j^-(x,t)}{(\lambda_j^-)^2-\lambda_0^2}, & 0\\ 0, & \dfrac{\zeta_j^+(x,t)}{(\lambda_j^+)^2-\lambda_0^2}\end{pmatrix}$$
$$\times\begin{pmatrix}-2(\lambda_j^-)^2\Sigma_{s=1}^{N}\dfrac{\zeta_s^+}{\Delta_{js}^-}|M_{(s)}^+|, & \lambda_0|M_{(j)}^-|\\ \lambda_0|M_{(j)}^+|, & -2(\lambda_j^+)^2\Sigma_{s=1}^{N}\dfrac{\zeta_s^-}{\Delta_{js}^+}|M_{(s)}^-|\end{pmatrix}(x,t)$$
$$\times\begin{pmatrix}\dfrac{1}{|M^+|}, & 0\\ 0, & \dfrac{1}{|M^-|}\end{pmatrix}(x,t)\Bigg]g_0(x,t),$$

where

$$g_0(x,t):=\psi(x,t,\lambda_0)|_{q_0=0}\exp(-i\lambda_0 x\sigma_3).$$

Thus we have the soliton solutions of the NLEEs[5]

$$i\mathbb{S}^t+F(\Lambda_g)\mathbb{S}=0$$

and in the case of reduction (4),

$$i\sigma_3\tilde{q}_t+F(\tilde{\Lambda})\tilde{q}=0,\quad iS_t^0+\tfrac{1}{2}F(\Lambda_{\kappa g})[\sigma_3,S^0]_-=0. \tag{35}$$

We have used the notations (5), (32), (33), and

$$\Lambda_g:=\begin{pmatrix}\tilde{Z}_{10}+\lambda_0\sigma_0, & \sigma_0+\tilde{Z}_1\\ \tilde{\Lambda}_0+Z-2\lambda_0\tilde{Z}_{10}, & \tilde{Z}_{01}-2\lambda_0\tilde{Z}_1-\lambda_0\sigma_0\end{pmatrix},$$

$$\mathbb{S}:=\begin{pmatrix}-\frac{1}{2}[\sigma_3,S]_-\\ \langle\sigma_3,S\rangle S'\end{pmatrix},\quad \mathbb{S}^t:=\begin{pmatrix}-S_t\\ \frac{1}{2}[S,S_t']_-\end{pmatrix},$$

$$\tilde{\Lambda}:=(D_x+\omega^2)(1+\tilde{Z}),\quad \Lambda_{\kappa g}=\left(1+\frac{Z}{\lambda_0^2}\right)(\tilde{\Lambda}_0+\lambda_0^2),$$

$$\tilde{\Lambda}_0:=\frac{i}{4}[S,d_x]_-,\ \frac{i}{4}[S^0,d_x\cdot]_-,\quad \tilde{Z}:=\frac{1}{2}(\tilde{Z}^+ +\tilde{Z}^-),$$

$$Z:=\tfrac{1}{2}(Z^+ +Z^-),\quad Z_{\alpha\beta}:=\tfrac{1}{2}(Z_{\alpha\beta}^+ +Z_{\alpha\beta}^-),\quad \alpha,\beta=0,1,$$

$$\tilde{Z}^{\pm}:=i\tilde{q}\int_x^{\pm\infty}dy\langle\tilde{q},[\sigma_3,\cdot]_-\rangle,\quad Z_1^{\pm}:=iS'\int_x^{\pm\infty}dy\langle S',[S,\cdot]_-\rangle,$$

$$Z^{\pm}:=-\frac{i}{4}S_x\int_x^{\pm\infty}dy\langle S_y,[S,\cdot]_-\rangle,-\frac{i}{4}S_x^0\int_x^{\pm\infty}dy\langle S_y^0,[S^0,\cdot]_-\rangle,$$

$$\tilde{Z}_{10}^{\pm}:=\frac{1}{2}\,S'\int_x^{\pm\infty}dy\langle S_y,[S,\cdot]_-\rangle,\quad \tilde{Z}_{01}^{\pm}:=\frac{1}{2}\,S_x\int_x^{\pm\infty}dy\langle S',[S,\cdot]_-\rangle.$$

(The NLEEs given in Ref. 5 are more complicated because as mentioned, we studied a more general case, which is gauge equivalent to the one presented here.)

We would like to give an example related to the dispersion law:

$$F(\lambda^2)=-4\lambda^4+8\omega^2\lambda^2-4\omega^4,$$

given in Sec. I. One obtains from the first Equation (35) under reduction (31),

$$\tilde{q}:=\begin{pmatrix}0, & u\\ -\epsilon u^*, & 0\end{pmatrix},$$

the following NLEE:

$$iu_t+u_{xx}+i\epsilon(|u|^2u)_x+2\epsilon\omega^2|u|^2u=0.$$

(We note[5] that λ^{2n} in the dispersion law leads to $\tilde{\Lambda}^n$ in Eq. (35).) The equation given in Ref. 15,

$$iu_t+u_{xx}+i(|u|^2u)_x+2\rho|u|^2u=0,$$

can be obtained from the above equation setting

$$\omega=\pm\sqrt{\rho},\quad \rho>0,\quad \omega=\pm i\sqrt{\rho},\quad \rho<0,\quad \epsilon=1.$$

As mentioned in Sec. I, the used transformation in Ref. 5 is singular in the points of the spectrum

$$\lambda_j^{\pm}=\pm i\omega$$

because

$$\lambda=\pm\sqrt{\mu^2+\omega^2}$$

vanishes in those points [see formula (4.3) in Ref. 5]. So we have $\lambda_j^{\pm}\in\Gamma$ (one can see that $0,\ \pm i\omega\in\Gamma$) but, as we required, $\lambda_j^{\pm}\notin\Gamma$ have to be realized.

Finally we would like to note that among the NLEEs [Eq. (35)], one can find the relativistic Mikhailov model mentioned in the beginning (equivalent, in an appropriate reduction, to the massive Thirring model), the DNSE and its gauge equivalent—DLLE, etc.[4,5]

APPENDIX A: WANDERMONDE-TYPE DETERMINANTS

Let us denote by W_n the Wandermonde determinant

$$W_n:=\begin{vmatrix}a_1^{n-1}, & a_1^{n-2}, & \ldots, & 1\\ a_2^{n-1}, & a_2^{n-2}, & \ldots, & 1\\ \vdots & \vdots & \ddots & \vdots\\ a_n^{n-1}, & a_n^{n-2}, & \ldots, & 1\end{vmatrix}=\prod_{j<k=1}^{n}(a_j-a_k),\quad \prod_{j<k=1}^{N}(\cdots)\big|_{n=1}:=1.$$

One can prove that

$$\tilde{W}_n := \begin{vmatrix} a_1^n, & a_1^{n-2}, & a_1^{n-3}, & \ldots, & 1 \\ a_2^n, & a_2^{n-2}, & a_2^{n-3}, & \ldots, & 1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_n^n, & a_n^{n-2}, & a_n^{n-3}, & \ldots, & 1 \end{vmatrix} = \left(\sum_{i=1}^{n} a_i \right) W_n . \tag{A1}$$

The proof of relation (A1) can be carried out by induction. Indeed, one can easily check it for $n=1,2,3$. Let us have it satisfied for some $n=k$. Developing W_{k+1} over the first column we derive

$$\begin{aligned} \left(\sum_{i=1}^{k+1} a_i \right) W_{k+1} &= \left(\sum_{i=1}^{k+1} a_i \right) [a_1^k W_k^{(1)} - a_2^k W_k^{(2)} + \cdots + (-1)^{k-1} a_k^k W_k^{(k)} + (-1)^k a_{k+1}^k W_k^{(k+1)}] \\ &= a_1^{k+1} W_k^{(1)} - a_2^{k+1} W_k^{(2)} + \cdots + (-1)^{k-1} a_k^{k+1} W_k^{(k)} + (-1)^k a_{k+1}^{k+1} W_k^{(k+1)} \\ &\quad + \left(\sum_{\substack{i=1 \\ i \neq 1}}^{k+1} a_i \right) a_1^k W_k^{(1)} - \left(\sum_{\substack{i=1 \\ i \neq 2}}^{k+1} a_i \right) a_2^k W_k^{(2)} + \cdots + (-1)^{k-1} \left(\sum_{\substack{i=1 \\ i \neq k}}^{k+1} a_i \right) a_k^k W_k^{(k)} \\ &\quad + (-1)^k \left(\sum_{\substack{i=1 \\ i \neq k+1}}^{k+1} a_i \right) a_{k+1}^k W_k^{(k+1)}, \end{aligned}$$

where we have denoted by

$$W_k^{(s)} := \begin{vmatrix} a_1^{k-1}, & a_1^{k-2}, & a_1^{k-3}, & a_1^{k-4}, & \ldots, & 1 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{s-1}^{k-1}, & a_{s-1}^{k-2}, & a_{s-1}^{k-3}, & a_{s-1}^{k-4}, & \ldots, & 1 \\ a_{s+1}^{k-1}, & a_{s+1}^{k-2}, & a_{s+1}^{k-3}, & a_{s+1}^{k-4}, & \ldots, & 1 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{k+1}^{k-1}, & a_{k+1}^{k-2}, & a_{k+1}^{k-3}, & a_{k+1}^{k-4}, & \ldots, & 1 \end{vmatrix} . \tag{A2}$$

One can see that the first $k+1$ terms give us $\tilde{W}_{k+1}$. We see that relation (A1) is satisfied by definition for the second $k+1$ terms. This gives

$$\left(\sum_{i=1}^{k+1} a_i \right) W_{k+1} = \tilde{W}_{k+1} + a_1^k \tilde{W}_k^{(1)} - a_2^k \tilde{W}_k^{(2)} + \cdots + (-1)^{k-1} a_k^k \tilde{W}_k^{(k)} + (-1)^k a_{k=1}^k \tilde{W}_k^{(k+1)},$$

where by analogy with definitions of W_n, Eqs. (A1) and (A2), we denote

$$\tilde{W}_k^{(s)} := \begin{vmatrix} a_1^k, & a_1^{k-2}, & a_1^{k-3}, & a_1^{k-4}, & \ldots, & 1 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{s-1}^k, & a_{s-1}^{k-2}, & a_{s-1}^{k-3}, & a_{s-1}^{k-4}, & \ldots, & 1 \\ a_{s+1}^k, & a_{s+1}^{k-2}, & a_{s+1}^{k-3}, & a_{s+1}^{k-4}, & \ldots, & 1 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{k+1}^k, & a_{k+1}^{k-2}, & a_{k+1}^{k-3}, & a_{k+1}^{k-4}, & \ldots, & 1 \end{vmatrix} .$$

Thus the second $k+1$ terms in the above sum become zero because they are in fact the development of the determinant

$$\begin{vmatrix} a_1^k, & a_1^k, & a_1^{k-2}, & \ldots, & 1 \\ a_2^k, & a_2^k, & a_2^{k-2}, & \ldots, & 1 \\ a_3^k, & a_3^k, & a_3^{k-2}, & \ldots, & 1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{k+1}^k, & a_{k+1}^k, & a_{k+1}^{k-2}, & \ldots, & 1 \end{vmatrix} = 0$$

over the first column, which concludes the proof.

APPENDIX B: EXPLICIT CALCULATIONS OF SOME DETERMINANTS

Let us calculate

$$(\mathrm{lhs}) = \sum_{\substack{i_1<\cdots<i_{n-1}=s_1 \\ i\neq j=s_1 \\ p_1<\cdots<p_{n-1}=\mathrm{fix.}}}^{s_n} \prod_{l=1}^{n-1} \left(\frac{\lambda_j^{\pm} - \lambda_{i_l}^{\pm}}{\lambda_j^{\pm} - \lambda_{p_l}^{\mp}} \right) \left| \Theta_{p_1,\ldots,p_{n-1}}^{\pm i_1,\ldots,i_{n-1}} \right|^2$$

$$= \sum_{\substack{k=1 \\ p=\mathrm{fix.}}}^{n} \frac{\Pi_{l=1, l\neq k}^{n} (\lambda_{s_k}^{\pm} - \lambda_{s_l}^{\pm})}{\Pi_{m=1}^{n-1} (\lambda_{s_k}^{\pm} - \lambda_{p_m}^{\mp})} \left| \Theta_{p_1,\ldots,p_{n-1}}^{\pm s_1,\ldots,s_{k-1},s_{k+1},\ldots,s_n} \right|^2 = \sum_{k=1}^{n} \prod_{m=1}^{n-1} (\lambda_{s_k}^{\pm} - \lambda_{p_m}^{\mp})$$

$$\times \prod_{l=1}^{k-1} (\lambda_{s_k}^{\pm} - \lambda_{s_l}^{\pm}) \prod_{l=k+1}^{n} (\lambda_{s_k}^{\pm} - \lambda_{s_l}^{\pm}) \frac{\Pi_{\substack{1\leq l<m<n \\ l,m\neq k}} (\lambda_{s_l}^{\pm} - \lambda_{s_m}^{\pm})^2 (\lambda_{p_\alpha}^{\mp} - \lambda_{p_\beta}^{\mp})^2}{\Pi_{m=1}^{n-1} (\lambda_{s_k}^{\pm} - \lambda_{p_m}^{\mp})^2 \Pi_{\substack{1\leq l\leq n \\ l\neq k \\ 1\leq\alpha\leq n-1}} (\lambda_{s_l}^{\pm} - \lambda_{p_\alpha}^{\mp})^2}.$$

One can derive it by means of the relations

$$\sum_{l<m=1}^{n} (a_l - a_m) = \prod_{l=1}^{k-1} (a_l - a_k) \prod_{l=k+1}^{n} (a_k - a_l) \prod_{\substack{l<m=1 \\ l,m\neq k}}^{n} (a_l - a_m),$$

$$\prod_{m=1}^{n-1} (a_k - b_m) = (a_k)^{n-1} - (a_k)^{n-2} \sum_{s=1}^{n-1} b_s + \cdots + (-1)^{n-2} a_k \sum_{s_1<\cdots<s_{n-2}=1}^{n-1} \prod_{l=1}^{n-2} b_{s_l}$$

$$+ (-1)^{n-1} \prod_{l=1}^{n-2} b_l; \tag{B1}$$

$$\prod_{\substack{l<m=1 \\ l,m\neq k}}^{n} (a_l - a_m) = W_{n-1}^{(k)},$$

where $W_{n-1}^{(k)}$ was defined by Eq. (A2) (in our case $a_k := \lambda_k^{\pm}$). Thus we derive

$$(\mathrm{lhs}) = \sum_{k=1}^{n} \frac{\Pi_{l<m=s_1}^{s_n} (\lambda_l^{\pm} - \lambda_m^{\pm}) \Pi_{\alpha<\beta=p_1}^{p_{n-1}} (\lambda_\alpha^{\mp} - \lambda_\beta^{\mp})^2}{\Pi_{1\leq\alpha\leq n-1}^{1\leq l\leq n} (\lambda_{s_l}^{\pm} - \lambda_{p_\alpha}^{\mp})^2} (-1)^{k-1} \Bigg[(\lambda_{s_k})^{n-1} - (\lambda_{s_k})^{n-2} \sum_{m=1}^{n-1} \lambda_{p_m}^{\mp}$$

$$+ \cdots + (-1)^{n-2} \lambda_{s_k}^{\pm} \sum_{m_1<\cdots<m_{n-2}=p_1}^{p_{n-1}} \lambda_{m_1}^{\mp},\ldots,\lambda_{m_{n-2}}^{\mp} + (-1)^{n-1} \lambda_{p_1}^{\mp},\ldots,\lambda_{p_{n-1}}^{\mp} \Bigg] W_{n-1}^{(k)}$$

$$=\frac{\Pi_{l<m=s_1}^{s_n}(\lambda_l^{\pm}-\lambda_m^{\pm})\Pi_{\alpha<\beta=p_1}^{p_{n-1}}(\lambda_\alpha^{\mp}-\lambda_\beta^{\mp})^2}{\Pi_{p_1\leqslant\alpha\leqslant p_{n-1}}^{s_1\leqslant l\leqslant s_n}(\lambda_l^{\pm}-\lambda_\alpha^{\mp})^2}\,W_n$$

$$=\frac{\Pi_{l<m=s_1}^{s_n}(\lambda_l^{\pm}-\lambda_m^{\pm})^2\Pi_{1\leqslant\alpha<\beta\leqslant n-1}(\lambda_{p_\alpha}^{\mp}-\lambda_{p_\beta}^{\mp})^2}{\Pi_{p_1\leqslant\alpha\leqslant p_{n-1}}^{s_1\leqslant l\leqslant s_n}(\lambda_l^{\pm}-\lambda_\alpha^{\mp})^2}=\prod_{l=1}^{n-1}\left(\frac{\lambda_{s_n}^{\pm}-\lambda_{s_l}^{\pm}}{\lambda_{s_n}^{\pm}-\lambda_{p_l}^{\mp}}\right)^2|\Theta_{p_1,\ldots,p_{n-1}}^{\pm s_1,\ldots,s_{n-1}}|^2.$$

Here we have used that

$$\sum_{k=1}^{n}(-1)^{k-1}(\lambda_{s_k}^{\pm})^{n-\nu}W_{n-1}^{(k)}=\begin{vmatrix}(\lambda_1^{\pm})^{n-\nu}, & (\lambda_1^{\pm})^{n-2}, & \ldots, & 1\\ (\lambda_2^{\pm})^{n-\nu}, & (\lambda_2^{\pm})^{n-2}, & \ldots, & 1\\ \vdots & \vdots & \ddots & \vdots\\ (\lambda_n^{\pm})^{n-\nu}, & (\lambda_n^{\pm})^{n-2}, & \ldots, & 1\end{vmatrix}=\theta(2-\nu)W_n,$$

$$\theta(x):=0,\quad x\leqslant 0,\quad \theta(x):=1,\quad x>0.$$

In the same way one obtains

$$\sum_{\substack{i_1<\cdots<i_{n-1}=s_1\\ i\neq j=s_1\\ p_1<\cdots<p_{n-1}=\text{fix.}}}^{s_n}\lambda_j^{\pm}\prod_{l=1}^{n-1}\left(\frac{\lambda_j^{\pm}-\lambda_{i_l}^{\pm}}{\lambda_j^{\pm}-\lambda_{p_l}^{\mp}}\right)|\Theta_{p_1,\ldots,p_{n-1}}^{\pm i_1,\ldots,i_{n-1}}|^2$$

$$=\sum_{k=1}^{n}\frac{\Pi_{l<m=s_1}^{s_n}(\lambda_l^{\pm}-\lambda_m^{\pm})\Pi_{\alpha<\beta=p_1}^{p_{n-1}}(\lambda_\alpha^{\mp}-\lambda_\beta^{\mp})^2}{\Pi_{p_1\leqslant\alpha\leqslant p_{n-1}}^{s_1\leqslant l\leqslant s_n}(\lambda_l^{\pm}-\lambda_\alpha^{\mp})^2}(-1)^{k-1}\lambda_{s_k}^{\pm}\Bigg[(\lambda_{s_k})^{n-1}-(\lambda_{s_k})^{n-2}\sum_{m=1}^{n-1}\lambda_{p_m}^{\mp}$$

$$+\cdots+(-1)^{n-2}\lambda_{s_k}^{\pm}\sum_{m_1<\cdots<m_{n-2}=p_1}^{p_{n-1}}\lambda_{m_1}^{\mp},\ldots,\lambda_{m_{n-2}}^{\mp}+(-1)^{n-1}\lambda_{p_1}^{\mp}\cdots\lambda_{p_{n-1}}^{\mp}\Bigg]W_{n-1}^{(k)}$$

$$=\frac{\Pi_{l<m=s_1}^{s_n}(\lambda_l^{\pm}-\lambda_m^{\pm})\Pi_{\alpha<\beta=p_1}^{p_{n-1}}(\lambda_\alpha^{\mp}-\lambda_\beta^{\mp})^2}{\Pi_{p_1\leqslant\alpha\leqslant p_{n-1}}^{s_1\leqslant l\leqslant s_n}(\lambda_l^{\pm}-\lambda_\alpha^{\mp})^2}\left[\tilde{W}_n-\left(\sum_{m=1}^{n-1}\lambda_{p_m}^{\mp}\right)W_n\right]$$

$$=\frac{\Pi_{l<m=s_1}^{s_n}(\lambda_l^{\pm}-\lambda_m^{\pm})\Pi_{\alpha<\beta=p_1}^{p_{n-1}}(\lambda_\alpha^{\mp}-\lambda_\beta^{\mp})^2}{\Pi_{p_1\leqslant\alpha\leqslant p_{n-1}}^{s_1\leqslant l\leqslant s_n}(\lambda_l^{\pm}-\lambda_\alpha^{\mp})^2}\left[\sum_{m=1}^{n}\lambda_{s_m}^{\pm}-\sum_{m=1}^{n-1}\lambda_{p_m}^{\mp}\right]W_n$$

$$=\frac{\Pi_{l<m=s_1}^{s_n}(\lambda_l^{\pm}-\lambda_m^{\pm})^2\Pi_{p_1\leqslant\alpha<\beta\leqslant p_{n-1}}(\lambda_\alpha^{\mp}-\lambda_\beta^{\mp})^2}{\Pi_{p_1\leqslant\alpha\leqslant p_{n-1}}^{s_1\leqslant l\leqslant s_n}(\lambda_l^{\pm}-\lambda_\alpha^{\mp})^2}\left[\lambda_{s_n}^{\pm}-\sum_{m=1}^{n-1}(\lambda_{s_m}^{\pm}-\lambda_{p_m}^{\mp})\right]$$

$$=\left(\lambda_{s_m}^{\pm}\mp\sum_{m=1}^{n-1}\omega_{s_m p_m}^{\pm}\right)\prod_{l=1}^{n-1}\left(\frac{\lambda_{s_n}^{\pm}-\lambda_{s_l}^{\pm}}{\lambda_{s_n}^{\pm}-\lambda_{p_l}^{\mp}}\right)^2|\Theta_{p_1,\ldots,p_{n-1}}^{\pm s_1,\ldots,s_{n-1}}|^2.$$

Let us calculate as well

$$\sum_{\substack{i_1<\cdots<i_{n-1}=s_0\\ i\neq j=s_0\\ p_1<\cdots<p_{n-1}=\text{fix.}}}^{s_{n-1}} \prod_{l=1}^{n-1}\left(\frac{\lambda_j^{\pm}-\lambda_{i_l}^{\pm}}{\lambda_j^{\pm}-\lambda_{p_l}^{\mp}}\right)\left|\Theta_{p_1,\ldots,p_{n-1}}^{\pm i_1,\ldots,i_{n-1}}\right|^2$$

$$=\sum_{\substack{k=0\\ p=\text{fix.}}}^{n-1}\frac{\prod_{s_l=0}^{s_{n-1}}{}_{s_l\neq s_k}(\lambda_{s_k}^{\pm}-\lambda_{s_l}^{\pm})}{\prod_{m=p_1}^{p_{n-1}}(\lambda_{s_k}^{\pm}-\lambda_m^{\mp})}\left|\Theta_{p_1,\ldots,p_{n-1}}^{\pm s_0,\ldots,s_{k-1},s_{k+1},\ldots,s_{n-1}}\right|^2$$

$$=\sum_{k=0}^{n-1}(-1)^{k-1}\prod_{m=1}^{n-1}(\lambda_{s_k}^{\pm}-\lambda_{p_m}^{\mp})\prod_{l=s_0}^{s_{k-1}}(\lambda_l^{\pm}-\lambda_k^{\pm})\prod_{l=s_{k+1}}^{s_{n-1}}(\lambda_{s_k}^{\pm}-\lambda_l^{\pm})$$

$$\times\frac{\prod_{\substack{l,m\neq k\\ p_1\leqslant\alpha<\beta\leqslant p_{n-1}}}^{s_0\leqslant l<m\leqslant s_{n-1}}(\lambda_l^{\pm}-\lambda_m^{\pm})^2(\lambda_\alpha^{\mp}-\lambda_\beta^{\mp})^2}{\prod_{m=1}^{n-1}(\lambda_{s_k}^{\pm}-\lambda_{p_m}^{\mp})^2\prod_{\substack{s_l\neq s_k\\ p_1\leqslant\alpha\leqslant p_{n-1}}}^{s_0\leqslant l\leqslant s_{n-1}}(\lambda_l^{\pm}-\lambda_\alpha^{\mp})^2}$$

$$=\sum_{k=0}^{n-1}\frac{\prod_{s_0\leqslant l<m=s_{n-1}}(\lambda_l^{\pm}-\lambda_m^{\pm})\prod_{p_1\leqslant\alpha<\beta\leqslant p_{n-1}}(\lambda_\alpha^{\mp}-\lambda_\beta^{\mp})^2}{\prod_{p_1\leqslant\alpha\leqslant p_{n-1}}^{s_0\leqslant l\leqslant s_{n-1}}(\lambda_l^{\pm}-\lambda_\alpha^{\mp})^2}(-1)^{k-1}$$

$$\times\Bigg[(\lambda_{s_k})^{n-1}-(\lambda_{s_k})^{n-2}\sum_{m=1}^{n-1}\lambda_{p_m}^{\mp}+\cdots+(-1)^{n-2}\lambda_{s_k}^{\pm}$$

$$\times\sum_{m_1<\cdots<m_{n-2}=p_1}^{p_{n-1}}\lambda_{m_1}^{\mp},\ldots,\lambda_{m_{n-2}}^{\mp}+(-1)^{n-1}\lambda_{p_1}^{\mp},\ldots,\lambda_{p_{n-1}}^{\mp}\Bigg]\mathbf{W}_{n-1}^{(k)}$$

$$=\frac{\prod_{l<m=s_0}^{s_{n-1}}(\lambda_l^{\pm}-\lambda_m^{\pm})\prod_{\alpha<\beta=p_1}^{p_{n-1}}(\lambda_\alpha^{\mp}-\lambda_\beta^{\mp})^2}{\prod_{p_1\leqslant\alpha\leqslant p_{n-1}}^{s_0\leqslant l\leqslant s_{n-1}}(\lambda_l^{\pm}-\lambda_\alpha^{\mp})^2}\mathbf{W}_n$$

$$=\frac{\prod_{l<m=s_0}^{s_{n-1}}(\lambda_l^{\pm}-\lambda_m^{\pm})^2\prod_{p_1\leqslant\alpha<\beta\leqslant p_{n-1}}(\lambda_\alpha^{\mp}-\lambda_\beta^{\mp})^2}{\prod_{p_1\leqslant\alpha\leqslant p_{n-1}}^{s_0\leqslant l\leqslant s_{n-1}}(\lambda_l^{\pm}-\lambda_\alpha^{\mp})^2}.$$

Here we have denoted by $\mathbf{W}_{n-1}^{(k)}$ and $\mathbf{W}_n$ the same determinants as $W_{n-1}^{(k)}$ and W_n, in which instead of $\lambda_{s_1}^{\pm},\ldots,\lambda_{s_n}^{\pm}$ one must put $\lambda_{s_0}^{\pm},\ldots,\lambda_{s_{n-1}}^{\pm}$. In a similar way one obtains

$$\sum_{\substack{i_1<\cdots<i_{n-1}=s_0\\ i\neq j=s_0\\ p_1<\cdots<p_{n-1}=\text{fix.}}}^{s_{n-1}}\lambda_j^{\pm}\prod_{l=1}^{n-1}\left(\frac{\lambda_j^{\pm}-\lambda_{i_l}^{\pm}}{\lambda_j^{\pm}-\lambda_{p_l}^{\mp}}\right)\left|\Theta_{p_1,\ldots,p_{n-1}}^{\pm i_1,\ldots,i_{n-1}}\right|^2$$

$$=\sum_{\substack{k=0\\ p=\text{fix.}}}^{n-1}(-1)^{k-1}\lambda_{s_k}^{\pm}\frac{\prod_{l=s_0}^{s_{n-1}}{}_{l\neq k}(\lambda_{s_k}^{\pm}-\lambda_l^{\pm})}{\prod_{m=p_1}^{p_{n-1}}(\lambda_{s_k}^{\pm}-\lambda_m^{\mp})}\left|\Theta_{p_1,\ldots,p_{n-1}}^{\pm s_0,\ldots,s_{k-1},s_{k+1},\ldots,s_{n-1}}\right|^2$$

$$=\frac{\prod_{l<m=s_0}^{s_{n-1}}(\lambda_l^{\pm}-\lambda_m^{\pm})\prod_{\alpha<\beta=p_1}^{p_{n-1}}(\lambda_\alpha^{\mp}-\lambda_\beta^{\mp})^2}{\prod_{p_1\leqslant\alpha\leqslant p_{n-1}}^{s_0\leqslant l\leqslant s_{n-1}}(\lambda_l^{\pm}-\lambda_\alpha^{\mp})^2}\lambda_{s_k}^{\pm}\Bigg[(\lambda_{s_k})^{n-1}-(\lambda_{s_k})^{n-2}\sum_{m=1}^{n-1}\lambda_{p_m}^{\mp}$$

$$
\begin{aligned}
&+\cdots+(-1)^{n-2}\lambda_{s_k}^{\pm}\sum_{m_1<\cdots<m_{n-2}=p_1}^{p_{n-1}}\lambda_{m_1}^{\mp},\ldots,\lambda_{m_{n-2}}^{\mp}+(-1)^{n-1}\lambda_{p_1}^{\mp},\ldots,\lambda_{p_{n-1}}^{\mp}]\mathbf{W}_{n-1}^{(k)}\\
&=\frac{\Pi_{l<m=s_0}^{s_{n-1}}(\lambda_l^{\pm}-\lambda_m^{\pm})\Pi_{\alpha<\beta=p_1}^{p_{n-1}}(\lambda_\alpha^{\mp}-\lambda_\beta^{\mp})^2}{\Pi_{p_1\leqslant\alpha\leqslant p_{n-1}}^{s_0\leqslant l\leqslant s_{n-1}}(\lambda_l^{\pm}-\lambda_\alpha^{\mp})^2}\left[\tilde{\mathbf{W}}_n-\left(\sum_{m=1}^{n-1}\lambda_{p_m}^{\mp}\right)W_n\right]\\
&=\frac{\Pi_{l<m=s_0}^{s_{n-1}}(\lambda_l^{\pm}-\lambda_m^{\pm})\Pi_{\alpha<\beta=p_1}^{p_{n-1}}(\lambda_\alpha^{\mp}-\lambda_\beta^{\mp})^2}{\Pi_{p_1\leqslant\alpha\leqslant p_{n-1}}^{s_0\leqslant l\leqslant s_{n-1}}(\lambda_l^{\pm}-\lambda_\alpha^{\mp})^2}\left[\sum_{m=0}^{n-1}\lambda_{s_m}^{\pm}-\sum_{m=1}^{n-1}\lambda_{p_m}^{\mp}\right]W_n\\
&=\frac{\Pi_{l<m=s_0}^{s_{n-1}}(\lambda_l^{\pm}-\lambda_m^{\pm})^2\Pi_{p_1\leqslant\alpha<\beta\leqslant p_{n-1}}(\lambda_\alpha^{\mp}-\lambda_\beta^{\mp})^2}{\Pi_{p_1\leqslant\alpha\leqslant p_{n-1}}^{s_0\leqslant l\leqslant s_{n-1}}(\lambda_l^{\pm}-\lambda_\alpha^{\mp})^2}\left[\lambda_{s_0}^{\pm}-\sum_{m=1}^{n-1}(\lambda_{s_m}^{\pm}-\lambda_{p_m}^{\mp})\right]\\
&=\left[\lambda_{s_0}^{\pm}-\sum_{m=1}^{n-1}(\lambda_{s_m}^{\pm}-\lambda_{p_m}^{\mp})\right]\prod_{l=1}^{n-1}\left(\frac{\lambda_{s_0}^{\pm}-\lambda_{s_l}^{\pm}}{\lambda_{s_0}^{\mp}-\lambda_{p_l}^{\mp}}\right)^2|\Theta_{p_1,\ldots,p_{n-1}}^{\pm s_1,\ldots,s_{n-1}}|^2.
\end{aligned}
$$

Thus we have obtained the results

$$
\sum_{\substack{i_1<\cdots<i_{n-1}=s_1\\ i\neq j=s_1\\ p_1<\cdots<p_{n-1}=\text{fix.}}}^{s_n}\prod_{l=1}^{n-1}\left(1-\frac{\omega_{i_lp_l}^{\pm}}{\omega_{jp_l}^{\pm}}\right)|\Theta_{p_1,\ldots,p_{n-1}}^{\pm i_1,\ldots,i_{n-1}}|^2=\prod_{l=1}^{n-1}\left(1-\frac{\omega_{s_lp_l}^{\pm}}{\omega_{s_np_l}^{\pm}}\right)^2|\Theta_{p_1,\ldots,p_{n-1}}^{\pm s_1,\ldots,s_{n-1}}|^2, \tag{B2}
$$

$$
\begin{aligned}
&\sum_{\substack{i_1<\cdots<i_{n-1}=s_1\\ i\neq j=s_1\\ p_1<\cdots<p_{n-1}=\text{fix.}}}^{s_n}\lambda_j^{\pm}\prod_{l=1}^{n-1}\left(1-\frac{\omega_{i_lp_l}^{\pm}}{\omega_{jp_l}^{\pm}}\right)|\Theta_{p_1,\ldots,p_{n-1}}^{\pm i_1,\ldots,i_{n-1}}|^2\\
&\quad=\left(\lambda_{s_n}^{\pm}\mp\sum_{\alpha=1}^{n-1}\omega_{s_\alpha p_\alpha}^{\pm}\right)\prod_{l=1}^{n-1}\left(1-\frac{\omega_{s_lp_l}^{\pm}}{\omega_{s_np_l}^{\pm}}\right)^2|\Theta_{p_1,\ldots,p_{n-1}}^{\pm s_1,\ldots,s_{n-1}}|^2,
\end{aligned} \tag{B3}
$$

$$
\sum_{\substack{i_1<\cdots<i_{n-1}=s_0\\ i\neq j=s_0\\ p_1<\cdots<p_{n-1}=\text{fix.}}}^{s_{n-1}}\prod_{l=1}^{n-1}\left(1-\frac{\omega_{i_lp_l}^{\pm}}{\omega_{jp_l}^{\pm}}\right)|\Theta_{p_1,\ldots,p_{n-1}}^{\pm i_1,\ldots,i_{n-1}}|^2=\prod_{l=1}^{n-1}\left(1-\frac{\omega_{s_lp_l}^{\pm}}{\omega_{s_0p_l}^{\pm}}\right)^2|\Theta_{p_1,\ldots,p_{n-1}}^{\pm s_1,\ldots,s_{n-1}}|^2, \tag{B4}
$$

and

$$
\begin{aligned}
&\sum_{\substack{i_1<\cdots<i_{n-1}=s_0\\ i\neq j=s_0\\ p_1<\cdots<p_{n-1}=\text{fix.}}}^{s_{n-1}}\lambda_j^{\pm}\prod_{l=1}^{n-1}\left(1-\frac{\omega_{i_lp_l}^{\pm}}{\omega_{jp_l}^{\pm}}\right)|\Theta_{p_1,\ldots,p_{n-1}}^{\pm i_1,\ldots,i_{n-1}}|^2\\
&\quad=\left(\lambda_{s_0}^{\pm}\mp\sum_{\alpha=1}^{n-1}\omega_{s_\alpha p_\alpha}^{\pm}\right)\prod_{l=1}^{n-1}\left(1-\frac{\omega_{s_lp_l}^{\pm}}{\omega_{s_0p_l}^{\pm}}\right)^2|\Theta_{p_1,\ldots,p_{n-1}}^{\pm s_1,\ldots,s_{n-1}}|^2.
\end{aligned} \tag{B5}
$$

We also have [see Eq. (B1)] the relation

$$\prod_{m=1}^{n-1} b_m(a_k-b_m)=\prod_{m=1}^{n-1} b_m\Bigg[a_k^{n-1}-a_k^{n-2}\sum_{s=1}^{n-1} b_s+\cdots+(-1)^{n-2}a_k\sum_{s_1<\cdots<s_{n-2}=1}^{n-1}\prod_{l=1}^{n-2} b_{s_l}$$
$$+(-1)^{n-1}\prod_{s=1}^{n-1} b_s\Bigg].$$

Thus by analogy with Eqs. (B2), (B3), and (B4) one writes

$$\sum_{\substack{i_1<\cdots<i_{n-1}=s_1\\ i\neq j=s_1\\ p_1<\cdots<p_{n-1}=\text{fix.}}}^{s_n}\prod_{l=1}^{n-1}(\lambda_{p_l}^{\mp})^2\left(1-\frac{\Delta_{i_lp_l}^{\pm}}{\Delta_{jp_l}^{\pm}}\right)\left|\Xi_{p_1,\ldots,p_{n-1}}^{\pm i_1,\ldots,i_{n-1}}\right|^2=\prod_{l=1}^{n-1}(\lambda_{p_l}^{\mp})^2\left(1-\frac{\Delta_{s_lp_l}^{\pm}}{\Delta_{s_np_l}^{\pm}}\right)^2\left|\Xi_{p_1,\ldots,p_{n-1}}^{\pm s_1,\ldots,s_{n-1}}\right|^2,$$

$$\sum_{\substack{i_1<\cdots<i_{n-1}=s_1\\ i\neq j=s_0\\ p_1<\cdots<p_{n-1}=\text{fix.}}}^{s_{n-1}}\prod_{l=1}^{n-1}(\lambda_{p_l}^{\mp})^2\left(1-\frac{\Delta_{i_lp_l}^{\pm}}{\Delta_{jp_l}^{\pm}}\right)\left|\Xi_{p_1,\ldots,p_{n-1}}^{i_1,\ldots,i_{n-1}}\right|^2=\prod_{l=1}^{n-1}(\lambda_{p_l}^{\mp})^2\left(1-\frac{\Delta_{s_lp_l}}{\Delta_{s_0p_l}^{\pm}}\right)^2\left|\Xi_{p_1,\ldots,p_{n-1}}^{\pm s_1,\ldots,s_{n-1}}\right|^2.$$

The result is obtained in the same way as it was done when proving Eqs. (B2), (B3), (B4), and (B5) and by means of substitution of a_k with $(\lambda_k^{\pm})^2$ and b_k with $(\lambda_k^{\mp})^2$.

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Instability proof for Einstein–Yang–Mills solitons and black holes with arbitrary gauge groups

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We prove that static, spherically symmetric, asymptotically flat soliton and black hole solutions of the Einstein–Yang–Mills equations are unstable for arbitrary gauge groups, at least for the ''generic'' case. This conclusion is derived without explicit knowledge of the possible equilibrium solutions. © *1996 American Institute of Physics.* [S0022-2488(96)02902-8]

I. INTRODUCTION

In several recent papers[1–4] we have studied important aspects of the Einstein–Yang–Mills (EYM) system for arbitrary gauge groups. In particular, we investigated the classification and properties of spherically symmetric EYM solitons (magnetic structure, Chern–Simons numbers) and a generalization of the Birkhoff theorem for the non-Abelian case. We also worked out the generalization of the first law of black hole physics (Bardeen–Carter–Hawking formula), allowing for additional Higgs and dilaton fields.[5,6] For other studies of these and related topics, we refer to Refs. 7–10.

In the present paper, we prove that static, spherically symmetric, asymptotically flat solutions of the EYM equations are unstable for any gauge group, if they are ''generic'' (defined in Sec. II). In a recent letter,[11] we have already sketched how we arrived at this result for solitons. Here we present details of the proof and extend it to black holes. We also discuss some further mathematical issues involved.

This general instability was expected since the Bartnik–McKinnon solutions[12] for the gauge group SU(2) and the related black hole solutions[13–15] are unstable.[16–19] A mathematical proof of this expectation presents, however, quite a challenge, since one cannot rely on any knowledge of the possible solutions (apart from regularity and boundary conditions).

Our strategy is based on the study of the pulsation equations, describing linear radial perturbations of the equilibrium solutions, and involves the following main steps: First we show that the frequency spectrum of a class of radial perturbations is determined by a coupled system of radial, respectively, one-dimensional ''Schrödinger equations.'' Negative parts in the spectrum of the effective Hamiltonian imply linear instability. With the help of suitably constructed trial functions, it is then proven that the spectrum contains always a negative part (for ''generic'' solutions).

We have recently used a similar procedure to establish the instability of the gravitating, regular sphaleron solutions of the SU(2) EYM–Higgs system with a SU(2) Higgs doublet,[20] which have been constructed numerically in Ref. 21. Our results contain, as a special case, the conclusion of Ref. 22 for the gauge group SU(2). Here, we analyze the regular SU(2) case further. We show that the effective Hamiltonian for ''sphaleron-like'' perturbations has the form of a ''deuteron'' Hamiltonian.

The paper is organized as follows: In Sec. II we recall some basic facts and equations of our previous work,[2,4] which will be needed in the present analysis. In Sec. III we then derive the linearized perturbation equations for solitons and black holes and bring them into a convenient, partially decoupled form. The resulting eigenvalue problem is discussed in Sec. IV and in Sec. V

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we show the existence of unstable perturbations. The ''deuteron'' interpretation for the unstable modes of a SU(2) soliton is presented in Sec. VI. In the Appendix, we elaborate on mathematical issues, related to the self-adjointness of the effective Hamiltonian and the connection between the negative part in its spectrum and unstable solutions of the perturbation equations.

II. SPHERICALLY SYMMETRIC EYM FIELDS

We begin with a convenient description of gauge fields with spherical symmetry (for derivations see Ref. 2).

Let us fix a maximal torus T of the gauge group G with corresponding integral lattice I (=kernel of the exponential map restricted to the Lie algebra LT of the torus T). In addition, we choose a basis S of the root system R of real roots. The corresponding fundamental Weyl chamber,

$$K(S)=\{H\in LT\,|\,\alpha(H)>0, \quad \text{for all} \quad \alpha\in S\}, \tag{2.1}$$

plays an important role in what follows.

To a spherically symmetric gauge field there belongs a canonical element $H_\lambda \in I\cap\overline{K(S)}$, which characterizes the corresponding principal bundle $P(M,G)$ over the space–time manifold M, admitting a SU(2) action. If the configuration is also regular at the origin, H_λ is restricted to a small, finite subset of $I\cap\overline{K(S)}$, which is described in Ref. 4. In the present discussion, we exclude (for technical reasons) the possibility that H_λ lies on the boundary of the fundamental Weyl chamber. The term ''generic'' always refers to fields for which the classifying element H_λ is contained in the *open* Weyl chamber $K(S)$.

The SU(2) action on $P(M,G)$ by bundle automorphisms induces an action on the base manifold M. A SU(2) invariant connection in $P(M,G)$ defines an invariant connection in the sub-bundle over each single orbit of the action on M. By Wangs theorem, the induced connections are described by a linear map $\Lambda: L\mathrm{SU}(2)\to LG$, which depends (at least locally) smoothly on the orbit and satisfies

$$\Lambda_1=[\Lambda_2,\Lambda_3], \quad \Lambda_2=[\Lambda_3,\Lambda_1], \quad \Lambda_3=-H_\lambda/4\pi, \tag{2.2}$$

where $\Lambda_k:=\Lambda(\tau_k)$ and $2i\tau_k$ are the Pauli matrices. These equations imply that $\Lambda_+:=\Lambda_1+i\Lambda_2$ lies in the following direct sum of root spaces L_α of $LG_{\mathbb{C}}$:

$$\Lambda_+\in \bigoplus_{\alpha\in S(\lambda)} L_\alpha, \quad S(\lambda):=\{\alpha\in R_+\,|\,\alpha(H_\lambda)=2\}, \tag{2.3}$$

where R_+ denotes the set of positive roots in R (relative to the basis S). In the generic case $S(\lambda)$ turns out to be a basis of a root system contained in R (see Appendix A of Ref. 4).

The LG-valued functions $\Lambda_\pm$ on the orbit space determine part of the connection on $P(M,G)$. Before we give a parametrization of the YM potential in a convenient gauge, we fix our conventions in parametrizing the Lorentz metric on M and introduce some further notation. We use standard Schwarzschild-like coordinates and set

$$ds^2=-NS^2\,dt^2+N^{-1}\,dr^2+r^2(d\vartheta^2+\sin^2\vartheta\,d\varphi^2), \tag{2.4}$$

where the metric functions $N=:1-2m/r$ and S depend only on r and t.

A suitably normalized $\mathrm{Ad}(G)$-invariant scalar product on LG will be denoted by $\langle\cdot,\cdot\rangle$. We use the same symbol for the Hermitian extension to $LG_{\mathbb{C}}$ (linear in the second argument), and $|\cdot|$ means the corresponding norm. Note that the original $\mathrm{Ad}(G)$-invariance extends on $LG_{\mathbb{C}}$ to

$$\langle X,[Z,Y]\rangle+\langle[c(Z),X],Y\rangle=0, \tag{2.5}$$

where c is the conjugation in $LG_{\mathbb{C}}$.

In Ref. 2, it is shown that the gauge potential A can be chosen to have the form

$$A=\tilde{A}+\hat{A}, \tag{2.6}$$

with

$$\hat{A}=\Lambda_2\, d\vartheta+(\Lambda_3\cos\vartheta-\Lambda_1\sin\vartheta)d\varphi \tag{2.7}$$

and

$$\tilde{A}=\tilde{\mathscr{A}}\, dt+\tilde{\mathscr{B}}\, dr, \tag{2.8}$$

where $\tilde{\mathscr{A}}$ and $\tilde{\mathscr{B}}$ commute with H_λ (i.e., with Λ_3). Since H_λ is assumed to be generic, its centralizer is the infinitesimal torus LT. Hence, $\tilde{\mathscr{A}}$ and $\tilde{\mathscr{B}}$ are LT valued and $\tilde{A}$ is thus Abelian.

For the example of the gauge group SU(2), H_λ is an integer multiple of $4\pi\tau_3$: $H_\lambda=4\pi k\tau_3$ with $k\in\mathbb{Z}$, and the only solutions of (2.2) are $\Lambda_1=\Lambda_2=0$, $\Lambda_3=k\tau_3$, and

$$\Lambda_1=w\tau_1-\tilde{w}\tau_2,\quad \Lambda_2=\pm\tilde{w}\tau_1\pm w\tau_2,\quad \Lambda_3=\pm\tau_3. \tag{2.9}$$

The gauge potential A contains a ''trivial,'' Abelian part, which decouples from the EYM equations. To demonstrate this, let us first construct a convenient decomposition of LT. For a given potential we restrict the sum in Eq. (2.3) to the smallest subset Σ of $S(\lambda)$, for which

$$\Lambda_+\in \bigoplus_{\alpha\in\Sigma\subset S(\lambda)} L_\alpha. \tag{2.10}$$

Since every root space L_α is $\mathrm{Ad}(T)$-invariant, and since the residual gauge group of the potential A is just the torus T, the subset Σ is unique and depends only on the invariant connection. With the help of Σ we now split LT:

$$LT=\langle\Sigma\rangle\oplus\langle\Sigma\rangle^\perp, \tag{2.11}$$

where $\langle\Sigma\rangle$ denotes the linear span of Σ. The decomposition (2.11) is *independent* of the chosen $\mathrm{Ad}(G)$-invariant scalar product[4] and satisfies

$$[\langle\Sigma\rangle^\perp,\Lambda_+]=0. \tag{2.12}$$

This property motivates us to set

$$\tilde{\mathscr{A}}=a+\mathscr{A},\quad \tilde{\mathscr{B}}=b+\mathscr{B},\quad \Lambda_3=\Lambda_{3\perp}+\Lambda_{3\|}, \tag{2.13}$$

with $a,b,\Lambda_{3\perp}\in\langle\Sigma\rangle^\perp$ and $\mathscr{A},\mathscr{B},\Lambda_{3\|}\in\langle\Sigma\rangle$. For our instability proof we adopt the following (mixed) gauge:

$$\mathscr{A}\equiv 0,\quad b\equiv 0,\quad \lim_{r\to\infty} a=0. \tag{2.14}$$

If we now insert the parametrizations (2.4), (2.6)–(2.8), (2.13), and (2.14) into the EYM equations, we obtain a system of partial differential equations for the metric functions N, S and the YM amplitudes $\Lambda_\pm,\mathscr{B}$. As noted above and as Eq. (2.12) indicates, the equation for a decouples. Specializing the results of Ref. 2 (and using slightly different notation), they read as follows.

The Einstein equations give two constraint equations for the r derivative (denoted by a dash) and the t derivative (denoted by a dot) of m,

$$m' = \frac{\kappa}{2}\{NG + r^2 p_\theta\}, \quad \dot{m} = \frac{\kappa}{2} NH \tag{2.15}$$

($\kappa := 8\pi \times$ Newton's gravitation constant), and the (rr) equation reduces to

$$\frac{S'}{S} = \frac{\kappa}{r} G, \tag{2.16}$$

where

$$G = \tfrac{1}{2}\{(NS)^{-2}|\dot{\Lambda}_+|^2 + |\Lambda'_+ + [\mathscr{B}, \Lambda_+]|^2\}, \tag{2.17}$$

$$H = \mathrm{Re}\langle \dot{\Lambda}_+ , \Lambda'_+ + [\mathscr{B}, \Lambda_+]\rangle, \tag{2.18}$$

$$p_\theta = \frac{1}{2r^4}\{|\hat{\mathscr{F}}_\parallel|^2 + |\check{\mathscr{F}}_\parallel|^2 + |P_\perp|^2 + |Q_\perp|^2\}, \tag{2.19}$$

with

$$\hat{\mathscr{F}}_\parallel = \frac{i}{2}[\Lambda_+ , \Lambda_-] - \Lambda_{3\parallel}, \quad \check{\mathscr{F}}_\parallel = \frac{r^2}{S}\dot{\mathscr{B}} \tag{2.20}$$

and

$$P_\perp = \Lambda_{3\perp}, \quad Q_\perp = -\frac{r^2}{S} a'. \tag{2.21}$$

The YM equations decompose into

$$\frac{2}{NS}\left(\frac{r^2}{S}\dot{\mathscr{B}}\right)^{\cdot} + [\Lambda_+ , \Lambda'_- + [\mathscr{B}, \Lambda_-]] + [\Lambda_- , \Lambda'_+ + [\mathscr{B}, \Lambda_+]] = 0, \tag{2.22}$$

$$\frac{1}{S}\left(\frac{1}{NS}\dot{\Lambda}_+\right)^{\cdot} - \frac{1}{S}(NS\{\Lambda'_+ + [\mathscr{B}, \Lambda_+]\})' - N[\mathscr{B}, \Lambda'_+ + [\mathscr{B}, \Lambda_+]] + \frac{i}{r^2}[\hat{\mathscr{F}}_\parallel, \Lambda_+] = 0, \tag{2.23}$$

$$2\left(\frac{r^2}{S}\dot{\mathscr{B}}\right)' + \frac{1}{NS}\{[\Lambda_+ , \dot{\Lambda}_-] + [\Lambda_- , \dot{\Lambda}_+]\} = 0. \tag{2.24}$$

The Abelian electric part of the potential satisfies

$$Q_\perp = -\frac{r^2}{S} a' = \mathrm{const} \quad (\in \langle\Sigma\rangle^\perp), \tag{2.25}$$

and hence decouples.

Equation (2.24) is the Gauss constraint. For static solutions, all time derivatives disappear, $\mathscr{B}$ can be gauged away, and the basic equations simplify considerably. [For the Bartnik–McKinnon solutions, Λ is of the form (2.9) with $\tilde{w} = 0$, $\Lambda_{3\parallel} = \Lambda_3 = \tau_3$, and $\tilde{A} = 0$ in (2.6).]

III. PERTURBATION EQUATIONS

In this section we study time-dependent perturbations of a given static, asymptotically flat solution of the coupled EYM equations (2.15), (2.16), and (2.22)–(2.25). Regular solutions are "purely magnetic" [$\tilde{A}=0$ in (2.6)] with vanishing YM charge ($P_\perp = Q_\perp = 0$ and $\lim_{r\to\infty} \hat{\mathscr{F}}_\parallel = 0$). Unfortunately, this is not yet proven with satisfactory weak fall-off conditions, but there is strong evidence for this (see Refs. 4 and 23 for partial results.) The perturbation equations we derive also hold for black holes, if their gauge potentials A have the form

$$A = a\ dt + \hat{A}, \tag{3.1}$$

with

$$a(r) = Q_\perp \int_r^\infty \frac{S}{y^2}\, dy, \tag{3.2}$$

for a constant vector $Q_\perp$ in $\langle\Sigma\rangle^\perp$ [i.e., $\mathscr{A}=\mathscr{B}=0$ in Eq. (2.13)]. We call such gauge fields "essentially magnetic."

From now on, $\Lambda_\pm$, N, S, etc. refer to an essentially magnetic equilibrium solution and time-dependent perturbations are denoted by $\delta\Lambda_\pm$, $\delta\mathscr{B}$, etc. All basic equations are linearized around the equilibrium solution. In order to decouple the perturbation δa, we impose the additional constraint $\delta Q_\perp = 0$.

First, we linearize the right-hand sides of the Einstein equations (2.15) and (2.16). Since $\mathscr{B}$ and $\dot{\Lambda}_\pm$ vanish for the equilibrium solution, the first-order variation of the source G is

$$\delta G = \mathrm{Re}\langle \Lambda_+', \delta\Lambda_+' \rangle - \mathrm{Re}\langle \Lambda_+', [\Lambda_+, \delta\mathscr{B}] \rangle. \tag{3.3}$$

Here, the last term vanishes, because the property (2.5) of the scalar product implies

$$-2\ \mathrm{Re}\langle \Lambda_+', [\Lambda_+, \delta\mathscr{B}] \rangle = \langle [\Lambda_+, \Lambda_-'] + [\Lambda_-, \Lambda_+'], \delta\mathscr{B} \rangle, \tag{3.4}$$

and the YM equation (2.22) for the equilibrium solution shows that

$$[\Lambda_+, \Lambda_-'] + [\Lambda_-, \Lambda_+'] = 0. \tag{3.5}$$

Thus,

$$\delta G = \mathrm{Re}\langle \Lambda_+', \delta\Lambda_+' \rangle. \tag{3.6}$$

The only first-order variation for p_θ comes from $\delta|\hat{\mathscr{F}}_\parallel|^2 = 2\langle \hat{\mathscr{F}}_\parallel, \delta\hat{\mathscr{F}}_\parallel \rangle$. Using

$$\delta\hat{\mathscr{F}}_\parallel = \frac{i}{2}[\Lambda_+, \delta\Lambda_-] - \frac{i}{2}[\Lambda_-, \delta\Lambda_+] \tag{3.7}$$

[see Eq. (2.20)], we have

$$\delta p_\theta = \frac{1}{r^4}\, \mathrm{Re}\langle i[\hat{\mathscr{F}}_\parallel, \Lambda_+], \delta\Lambda_+ \rangle. \tag{3.8}$$

Now we can work out the variation of the first Einstein equation in (2.15). With (3.6), (3.8), and (2.16) for the equilibrium solution, we find

$$\delta m' = -\frac{S'}{S}\,\delta m + \frac{\kappa}{2}\left\{ N\ \mathrm{Re}\langle \Lambda_+', \delta\Lambda_+'\rangle + \mathrm{Re}\left\langle \frac{i}{r^2}\,[\hat{\mathscr{F}}_\parallel, \Lambda_+], \delta\Lambda_+ \right\rangle \right\}. \tag{3.9}$$

For the commutator in the last term we use the unperturbed YM equation (2.23), i.e.

$$\frac{i}{r^2}\,[\hat{\mathscr{F}}_\parallel, \Lambda_+] = N\,\frac{S'}{S}\,\Lambda_+' + N'\Lambda_+' + N\Lambda_+'', \tag{3.10}$$

whence

$$\delta m' = -\frac{S'}{S}\,\delta m + \frac{S'}{S}\left\{ \frac{\kappa}{2}\,N\ \mathrm{Re}\langle \Lambda_+', \delta\Lambda_+\rangle \right\} + \left\{ \frac{\kappa}{2}\,N\ \mathrm{Re}\langle \Lambda_+', \delta\Lambda_+\rangle \right\}' \tag{3.11}$$

or

$$(\delta m\ S)' = \left\{ \frac{\kappa}{2}\,NS\ \mathrm{Re}\langle \Lambda_+', \delta\Lambda_+\rangle \right\}'. \tag{3.12}$$

Therefore, δm must be of the form

$$\delta m = \frac{\kappa}{2}\,N\ \mathrm{Re}\langle \Lambda_+', \delta\Lambda_+\rangle + \frac{f(t)}{S}, \tag{3.13}$$

where $f(t)$ is a function of t alone. This function is determined by considering the variation of the second Einstein equation in (2.15), which gives

$$\delta\dot{m} = \frac{\kappa}{2}\,N\ \mathrm{Re}\langle \Lambda_+', \delta\dot{\Lambda}_+\rangle. \tag{3.14}$$

Thus, we have also

$$\delta m = \frac{\kappa}{2}\,N\ \mathrm{Re}\langle \Lambda_+', \delta\Lambda_+\rangle + g(r), \tag{3.15}$$

with a function $g(r)$ of r alone. By comparing (3.13) and (3.15), we arrive at the remarkably simple result,

$$\delta m = \frac{\kappa}{2}\,N\ \mathrm{Re}\langle \Lambda_+', \delta\Lambda_+\rangle, \tag{3.16}$$

which generalizes an observation already made in Ref. 16.

The variation of the Einstein equation (2.16) is immediately obtained with (3.6),

$$\delta\left(\frac{S'}{S}\right) = \frac{\kappa}{r}\,N\ \mathrm{Re}\langle \Lambda_+', \delta\Lambda_+'\rangle. \tag{3.17}$$

Also, before linearizing the YM equations, we introduce a suitable decomposition of Λ_+ and $\delta\Lambda_+$. To do so, we choose a base element e_α of the root spaces L_α and expand the unperturbed Λ_+ as well as its perturbation $\delta\Lambda_+$:

$$\Lambda_+ = \sum_{\alpha\in\Sigma} w_\alpha e_\alpha, \quad \delta\Lambda_+ = \sum_{\alpha\in\Sigma} \delta w_\alpha e_\alpha. \tag{3.18}$$

Then, we have

$$\delta\Lambda_{\pm} = \delta X_{\pm} \pm i\ \delta Y_{\pm} \tag{3.19}$$

with

$$\delta X_{+} = \sum_{\alpha\in\Sigma}\ \mathrm{Re}(\delta w_{\alpha})e_{\alpha}, \quad \delta Y_{+} = \sum_{\alpha\in\Sigma}\ \mathrm{Im}(\delta w_{\alpha})e_{\alpha}, \tag{3.20}$$

and the corresponding expansion for δX_{-} and δY_{-} with e_{α} replaced by $c(e_{\alpha})\in L_{-\alpha}$, because $\delta\Lambda_{-}=c(\delta\Lambda_{+})$ and thus

$$\delta X_{-} = c(\delta X_{+}), \quad \delta Y_{-} = c(\delta Y_{+}). \tag{3.21}$$

We call $\delta X_{\pm}, \delta Y_{\pm}$ the ''real'' (or ''gravitational'') and ''imaginary'' (or ''sphaleron-like'') parts of the perturbations $\delta\Lambda_{\pm}$. It was shown in Ref. 4 that the unperturbed Λ_{+} can be chosen to have only a *real* part.

This decomposition will lead to a significant decoupling of the perturbation equations. Note, in particular, that the variations δm and δp_{θ} in (3.8) and (3.16) depend only on the real part δX_{+}:

$$\delta m = \frac{\kappa}{2}\, N\langle \Lambda_{+}', \delta X_{+}\rangle, \tag{3.22}$$

$$\delta p_{\theta} = \frac{1}{r^4}\,\langle i[\hat{\mathscr{F}}_{\|}, \Lambda_{+}], \delta X_{+}\rangle. \tag{3.23}$$

We consider now the first variation of the YM equation (2.23). Its decomposition into real and imaginary parts yields

$$\begin{aligned} -\frac{1}{NS^2}\ \delta\ddot{X}_{+} = &-N\delta X_{+}'' - \frac{(NS)'}{S}\ \delta X_{+}' - \frac{i}{r^2}\,[\Lambda_{+}, \delta\hat{\mathscr{F}}_{\|}] \\ &+ \frac{i}{r^2}\,[\hat{\mathscr{F}}_{\|}, \delta\Lambda_{+}] - \delta N\ \Lambda_{+}'' - \delta\left(\frac{(NS)'}{S}\right)\Lambda_{+}' \end{aligned} \tag{3.24}$$

and

$$\begin{aligned} -\frac{1}{NS^2}\ \delta\ddot{Y}_{+} = &-N\{\delta Y_{+}'' + i[\Lambda_{+}, \delta\mathscr{B}]' + i[\Lambda_{+}', \delta\mathscr{B}]\} \\ &- \frac{(NS)'}{S}\,\{\delta Y_{+}' + i[\Lambda_{+}, \delta\mathscr{B}]\} + \frac{i}{r^2}\,[\hat{\mathscr{F}}_{\|}, \delta Y_{+}]. \end{aligned} \tag{3.25}$$

The third term on the right-hand side of (3.24) is indeed real and can be written, using (3.7), as

$$\frac{i}{r^2}\,[\Lambda_{+}, \delta\hat{\mathscr{F}}_{\|}] = \frac{1}{r^2}\,\mathrm{ad}(\Lambda_{+})\mathrm{ad}(\Lambda_{-})\,\delta X_{+}. \tag{3.26}$$

Equation (3.24) can be simplified further. From (3.22) and the equilibrium equation (3.10), we deduce

$$-\delta N\Lambda_+''=\frac{2}{r}\ \delta m\ \Lambda_+''=\kappa N\ \mathrm{Re}\langle\Lambda_+',\delta X_+\rangle\Lambda_+''=\kappa\ \mathrm{Re}\langle\Lambda_+',\delta X_+\rangle\left\{-\frac{(NS)'}{S}\ \Lambda_++\frac{i}{r^2}\ [\hat{\mathscr{F}}_\parallel,\Lambda_+]\right\},$$

and the Einstein equations (2.15) and (2.16) give

$$-\delta\frac{(NS)'}{S}=-\frac{2}{r^2}\ \delta m+\kappa r\ \delta p_\theta. \tag{3.27}$$

If we use here (3.22) and (3.23), we see that the last two terms in (3.24) can be expressed as follows:

$$-\delta N\ \Lambda_+''-\delta\frac{(NS)'}{S}\ \Lambda_+'=\frac{1}{NS^2}\left\{-\Lambda_+'\kappa r\mu^2\left\{\frac{(NS)'}{S}+\frac{N}{r}\right\}\langle\Lambda_+',\delta X_+\rangle+\Lambda_+'\kappa\ \frac{\mu^2}{r}\right.$$
$$\left.\times\langle[i\hat{\mathscr{F}}_\parallel,\Lambda_+],\delta X_+\rangle+[i\hat{\mathscr{F}}_\parallel,\Lambda_+]\kappa\ \frac{\mu^2}{r}\ \langle\Lambda_+',\delta X_+\rangle\right\}, \tag{3.28}$$

where

$$\mu^2:=\frac{NS^2}{r^2}. \tag{3.29}$$

Inserting these expressions into (3.24) gives the following pulsation equation for the real amplitude δX_+ of the YM field:

$$\delta\ddot{X}_++U_{XX}\ \delta X_+=0, \tag{3.30}$$

where the operator U_{XX} is given by

$$U_{XX}=p_*{}^2+\mu^2\ \mathrm{ad}(i\hat{\mathscr{F}}_\parallel)-\mu^2\ \mathrm{ad}(\Lambda_+)\mathrm{ad}(\Lambda_-)-\Lambda_+\kappa\mu^2\{1-\kappa r^2p_\theta\}\langle\Lambda_+',\cdot\rangle$$
$$+\Lambda_+'\kappa\ \frac{\mu^2}{r}\ \langle[i\hat{\mathscr{F}}_\parallel,\Lambda_+],\cdot\rangle+[i\hat{\mathscr{F}}_\parallel,\Lambda_+]\kappa\ \frac{\mu^2}{r}\ \langle\Lambda_+',\cdot\rangle, \tag{3.31}$$

and p_* denotes the differential operator,

$$p_*=-iNS\ \frac{\partial}{\partial r}. \tag{3.32}$$

It is remarkable that the perturbations $\delta Y_\pm$ and $\delta\mathscr{B}$ do not appear in (3.30) and that the back reaction of gravitation on δX_+ can be described by an effective potential [the last three terms in (3.31)].

Equation (3.25) can easily be brought into the form

$$\delta\ddot{Y}_++U_{YY}\ \delta Y_++U_{Y\mathscr{B}}\sqrt{N}r\ \delta\mathscr{B}=0, \tag{3.33}$$

where

$$U_{YY}=p_*{}^2+\mu^2\ \mathrm{ad}(i\hat{\mathscr{F}}_\parallel), \tag{3.34}$$

$$U_{Y\mathscr{B}}=p_*\mu\ \mathrm{ad}(\Lambda_+)+\mu\ \mathrm{ad}(p_*\Lambda_+). \tag{3.35}$$

We have thus achieved a partial decoupling, because neither δX_+ nor the metric perturbations appear in (3.33).

We proceed with the linearization of the YM equation (2.22). The variation of the last two terms is

$$-[\Lambda_+,[\Lambda_-,\delta\mathscr{B}]]+[\Lambda_+,\delta\Lambda'_-]-[\Lambda'_-,\delta\Lambda_+]+\text{conjugate}, \tag{3.36}$$

which leads (with $\delta\Lambda_\pm=\delta X_\pm \pm i\,\delta Y_\pm$) to

$$-\{[\Lambda_+,[\Lambda_-,\delta\mathscr{B}]]+i[\Lambda_+,\delta Y'_-]+i[\Lambda'_-,\delta Y_+]\}+\{[\Lambda_+,\delta X'_-]-[\Lambda'_-,\delta X_+]\}+\text{conjugate}.$$

Here, the terms in the first curly bracket are in LT, while those in the second are in iLT. The latter are compensated by their conjugates, and we find

$$\sqrt{N}r\,\delta\ddot{\mathscr{B}}+U_{\mathscr{B}\mathscr{B}}\sqrt{N}r\,\delta\mathscr{B}+U_{\mathscr{B}Y}\;\delta Y_+=0, \tag{3.37}$$

with

$$U_{\mathscr{B}\mathscr{B}}=-\mu^2\;\mathrm{ad}(\Lambda_+)\mathrm{ad}(\Lambda_-), \tag{3.38}$$

$$U_{\mathscr{B}Y}=-\mu\;\mathrm{ad}(\Lambda_-)p_*+\mu\;\mathrm{ad}(p_*\Lambda_-). \tag{3.39}$$

At this point, we collect the results obtained so far as follows: Let

$$\Phi=\begin{pmatrix}\phi_Y\\ \phi_{\mathscr{B}}\end{pmatrix}=\begin{pmatrix}\delta Y_+\\ \sqrt{N}r\,\delta\mathscr{B}\end{pmatrix}, \tag{3.40}$$

then (3.33) and (3.37) can be written as a 2×2 matrix equation,

$$\ddot{\Phi}+U\Phi=0, \tag{3.41}$$

with

$$U=\begin{pmatrix}U_{YY} & U_{Y\mathscr{B}}\\ U_{\mathscr{B}Y} & U_{\mathscr{B}\mathscr{B}}\end{pmatrix}. \tag{3.42}$$

The operators in this matrix are given in Eqs. (3.34), (3.35), (3.38), and (3.39).

The perturbation equations (3.30) and (3.41) do not include the Gauss constraint (2.24), whose linearization is easily found to be

$$\partial_t\left\{p_*\,\frac{1}{\mu}\,\phi_{\mathscr{B}}+\mathrm{ad}(\Lambda_-)\,\phi_Y\right\}=0. \tag{3.43}$$

The role of this constraint will be discussed below.

In concluding this section, we emphasize once more that the perturbation equations also hold for black holes, if these are assumed to be of an essentially magnetic type [see Eq. (3.1)]. We also would like to note that a comprehensive discussion of the pulsation equations for the SU(2) YM–Higgs sphaleron can be found in Ref. 24.

IV. TRANSFORMATION TO A HYPERBOLIC SYSTEM

A look at the second-order differential operator U shows that it is not elliptic and, thus, the system (3.41) of partial differential equations is not hyperbolic. With the help of the Gauss constraint (3.43) it is, however, possible to derive a hyperbolic system for the subspace of physical perturbations orthogonal to a space of pure gauge modes. This reformulation of the perturbation equations will turn out to be very useful for several purposes.

We need first some notation. It is natural to introduce the following scalar product for $LG_{\mathbb{C}}$-valued functions on $(r_0,\infty)\subset\mathbb{R}_+$:

$$\langle\phi|\psi\rangle=\int_{r_0}^{\infty}\langle\phi,\psi\rangle dr_*, \tag{4.1}$$

with the weighted measure

$$dr_*=\frac{dr}{NS}.$$

For a black hole, the lower limit r_0 is the radius of the horizon and for a regular solution it is zero. The operators U_{XX} and U are symmetric with respect to this scalar product on a dense domain of L^2 functions. This can be seen easily, using

$$\langle\phi|p_*\psi\rangle=\langle p_*\phi|\psi\rangle, \tag{4.2}$$

for smooth functions, which vanish at r_0, and

$$\langle\phi|\mathrm{ad}(Z)\psi\rangle=-\langle\mathrm{ad}(c(Z))\phi|\psi\rangle, \tag{4.3}$$

for arbitrary $LG_{\mathbb{C}}$-valued functions ϕ, ψ, Z in L^2 [see (2.5)].

A "gauge mode" Φ_G is, by definition, a perturbation of the form

$$\Phi_G=-i\mathscr{G}\chi, \tag{4.4}$$

where $\mathscr{G}$ is the linear operator,

$$\mathscr{G}\chi=\begin{pmatrix}-\mathrm{ad}(\Lambda_+)\chi\\(1/\mu)p_*\chi\end{pmatrix}, \tag{4.5}$$

and χ is a $\langle\Sigma\rangle_{\mathbb{C}}$-valued function. Note that such variations arise if (2.6) is subjected to (T-valued) gauge transformations $g=\exp(-\epsilon\chi)$. Equation (2.7) and (2.8) show that this induces the infinitesimal transformation,

$$\Lambda_+\to\Lambda_+-\mathrm{ad}(\Lambda_+)\chi,\quad \sqrt{N}r.\mathscr{B}\to\sqrt{N}r.\mathscr{B}-i\,\frac{1}{\mu}\,p_*\chi. \tag{4.6}$$

It is not surprising that the following identity holds:

$$U\mathscr{G}=0, \tag{4.7}$$

whence

$$U\Phi_G=0. \tag{4.8}$$

"Physical perturbations" Φ_P satisfy, by definition,

$$\tilde{\mathscr{G}}\Phi_P=0, \tag{4.9}$$

where $\tilde{\mathscr{G}}$ is the linear operator,

$$\tilde{\mathscr{G}}\Phi=p_*\,\frac{1}{\mu}\,\phi_{\mathscr{B}}+\mathrm{ad}(\Lambda_-)\phi_Y. \tag{4.10}$$

The component ϕ_Y is assumed to have values in the subspace (2.10) of $LG_{\mathbb{C}}$ and $\phi_{\mathscr{B}}$ has to be $\langle\Sigma\rangle_{\mathbb{C}}$-valued. Hence, physical perturbations are, by definition, those for which the curly bracket in (3.43) vanishes.

Roughly speaking, a physical perturbation is orthogonal to all gauge modes. More precisely, *modulo boundary terms* we have

$$i\langle\Phi_P|\Phi_G\rangle=\langle\Phi_P|\mathscr{G}\chi\rangle=\langle\tilde{\mathscr{G}}\Phi_P|\chi\rangle=0, \tag{4.11}$$

which follows easily with Eqs. (4.2) and (4.3).

The identity

$$\tilde{\mathscr{G}}U=0, \tag{4.12}$$

which can be verified by direct calculation, is related to the Gauss constraint,

$$\partial_t\tilde{\mathscr{G}}\,\Phi=0, \tag{4.13}$$

in the following way: Assume Eq. (4.13) is satisfied for $t=t_0$, then the dynamical equation (3.41) implies that (4.13) is satisfied for all times. Indeed, we conclude with (4.12) that

$$\partial_t^2(\tilde{\mathscr{G}}\Phi)=\tilde{\mathscr{G}}(\partial_t^2\Phi)=-\tilde{\mathscr{G}}(U\Phi)=0. \tag{4.14}$$

As a corollary we have a solution of (3.41), which lies initially in the physical subspace (4.9) and satisfies initially the Gauss constraint (4.13), will satisfy the ''strong'' Gauss constraint (4.9) for all times. For physical perturbations we can thus use this strong form to bring Eq. (3.41) to a hyperbolic form. After some manipulations, one finds

$$U=\{p_*{}^2+V\}-\mathscr{G}\mu^2\tilde{\mathscr{G}}, \tag{4.15}$$

where

$$V=\begin{pmatrix} V_{YY} & V_{Y\mathscr{B}} \\ V_{\mathscr{B}Y} & V_{\mathscr{B}\mathscr{B}} \end{pmatrix} \tag{4.16}$$

is the following (matrix-valued) potential:

$$V_{YY}=\mu^2K^2+\mu^2\ \mathrm{ad}(i\hat{\mathscr{F}}_{\parallel}), \tag{4.17}$$

$$V_{Y\mathscr{B}}=2(p_*\mu)K_+ +2\mu\ \mathrm{ad}(p_*\Lambda_+), \tag{4.18}$$

$$V_{\mathscr{B}Y}=-2(p_*\mu)K_- +2\mu\ \mathrm{ad}(p_*\Lambda_-), \tag{4.19}$$

$$V_{\mathscr{B}\mathscr{B}}=\mu^2K^2-\frac{(p_*{}^2\mu)}{\mu}, \tag{4.20}$$

with

$$K^2=-\mathrm{ad}(\Lambda_+)\mathrm{ad}(\Lambda_-), \tag{4.21}$$

$$K_\pm=\pm\mathrm{ad}(\Lambda_\pm). \tag{4.22}$$

Modulo the strong Gauss constraint $\tilde{\mathscr{G}}\Phi=0$, Eq. (3.41) is thus equivalent to

$$\partial_t^2\Phi=-\{p_*{}^2+V\}\Phi. \tag{4.23}$$

This system is clearly hyperbolic. We emphasize that this new system implies the strong Gauss constraint for all times, if it is satisfied initially: $\tilde{\mathscr{G}}\Phi|_{t_0} = \tilde{\mathscr{G}}\,\partial_t\Phi|_{t_0} = 0$. The argument runs as follows: As a result of (4.8), (4.15), and (4.23), $\tilde{\mathscr{G}}\Phi$ satisfies the hyperbolic equation

$$\partial_t{}^2(\tilde{\mathscr{G}}\Phi) = -\tilde{\mathscr{G}}\mathscr{G}\mu^2(\tilde{\mathscr{G}}\Phi) = -\left\{p_*\,\frac{1}{\mu^2}\,p_* + K^2\right\}\mu^2(\tilde{\mathscr{G}}\Phi). \tag{4.24}$$

Uniqueness of the Cauchy problem for the hyperbolic system (4.24), with appropriate boundary conditions at r_0, then implies our claim.

We specialize now to harmonic perturbations proportional to $e^{-i\omega t}$ and obtain for the amplitude of Φ, denoted by the same letter, the two eigenvalue problems:

$$U\Phi = \omega^2\Phi \tag{4.25}$$

and

$$\{p_*{}^2 + V\}\Phi = \omega^2\Phi. \tag{4.26}$$

The second equation has the form of a (vector-valued) Schrödinger equation.

In the next section, we prove that the spectrum of U has a nonempty negative part (which is presumably discrete), by constructing a smooth trial function $\delta\Phi$ for which $\langle\delta\Phi|U|\delta\Phi\rangle$ is strictly negative. This implies that the operator $p_*{}^2 + V$ also has a negative part in the spectrum. This can be seen as follows:

If we can show that there exists a smooth function χ, such that

$$i\tilde{\mathscr{G}}\,\delta\Phi = \tilde{\mathscr{G}}\mathscr{G}\chi = \left\{p_*\,\frac{1}{\mu^2}\,p_* + K^2\right\}\chi, \tag{4.27}$$

then we have a decomposition,

$$\delta\Phi = \delta\Phi_P - i\mathscr{G}\chi, \tag{4.28}$$

into smooth physical and gauge components. Using also (4.8), we have

$$\langle\delta\Phi|U|\delta\Phi\rangle = \langle\delta\Phi_P|U|\delta\Phi_P\rangle = \langle\delta\Phi_P|p_*{}^2 + V|\delta\Phi_P\rangle < 0, \tag{4.29}$$

which would imply our claim.

Since $\tilde{\mathscr{G}}\mathscr{G}$ is a positive operator and since $i\tilde{\mathscr{G}}\,\delta\Phi$ is smooth, we expect on the basis of elliptic existence and regularity theorems that (4.27) indeed has a smooth solution. This is one of several mathematical points that will be discussed in the Appendix. Another issue will be, whether the operator $p_*{}^2 + V$ is essentially self-adjoint on a dense domain of smooth functions, which satisfy the boundary conditions implied by the physics of the problem. This will be analyzed in Sec. VI and in the Appendix.

The relation between the operators U and $Q := p_*{}^2 + V$, given explicitly in (4.15), can be summarized (on a formal level) as follows: As a result of (4.7) and (4.15), both operators split relative to the decomposition of the L^2 space of perturbations into physical and gauge degrees of freedom, $L^2 = \mathscr{H}_P \oplus \mathscr{H}_G$, and their restrictions satisfy

$$Q|_{\mathscr{H}_P} = U|_{\mathscr{H}_P}, \quad U|_{\mathscr{H}_G} = 0, \quad Q|_{\mathscr{H}_G} = \mathscr{G}\mu^2\tilde{\mathscr{G}}|_{\mathscr{H}_G} \geqslant 0.$$

The last inequality follows from

$$\langle\Phi_G|\mathscr{G}\mu^2\tilde{\mathscr{G}}|\Phi_G\rangle = \langle\tilde{\mathscr{G}}\Phi_G|\mu^2|\tilde{\mathscr{G}}\Phi_G\rangle,$$

for $\Phi_G \in \mathscr{H}_G$. In particular, the negative part of the spectra of U is contained in that of Q and the discrete spectra of the two operators coincide.

V. INSTABILITY OF GENERIC EYM SOLUTIONS

We are now ready to establish the main point of this paper: For a given solution with $\Lambda_+ = \Sigma_{\alpha\in\Sigma} w_\alpha e_\alpha$, we construct a one-parameter family of field configurations $\Lambda_{(\tau)+}$, $\mathscr{B}_{(\tau)}$, such that $\langle \delta\Phi | U | \delta\Phi\rangle < 0$ for the variation

$$\delta\Phi = \begin{pmatrix} \delta\phi_Y \\ \delta\phi_{\mathscr{B}} \end{pmatrix} = \begin{pmatrix} -i\ \partial_\tau \Lambda_{(\tau)+}|_{\tau=0} \\ \sqrt{N} r \partial_\tau \mathscr{B}_{(\tau)}|_{\tau=0} \end{pmatrix}. \tag{5.1}$$

The families we consider are of the form

$$\Lambda_{(\tau)+} = \mathrm{Ad}(\exp(\tau Z))\{\Lambda_+ \cos(\tau) + iT_+ \sin(\tau)\}, \tag{5.2}$$

$$\mathscr{B}_{(\tau)} = -\tau Z', \tag{5.3}$$

where T_+ is a real element in the subspace (2.10), satisfying

$$[T_+, T_-] = -2i\Lambda_{3\|}, \tag{5.4}$$

and Z is a $\langle\Sigma\rangle$-valued function of r with

$$\lim_{r\to r_0,\infty} \mathrm{ad}(\Lambda_+) Z = iT_+, \quad \text{supp } Z' \subset (r_0, \infty). \tag{5.5}$$

If Σ is not empty such an element T_+ always exists (see Appendix A of Ref. 4). A function Z with the required properties can be found if

$$\lim_{r\to r_0,\infty} w_\alpha \neq 0, \quad \text{for all } \alpha \in \Sigma. \tag{5.6}$$

This can be seen as follows: Let $\{h_\alpha\}_{\alpha\in\Sigma}$ be the dual basis of $2\pi\Sigma$ and put

$$Z = \sum_{\alpha\in\Sigma} Z_\alpha h_\alpha, \quad T_+ = \sum_{\alpha\in\Sigma} T_\alpha e_\alpha \tag{5.7}$$

and

$$Z_\alpha = \begin{cases} -T_\alpha / w_\alpha(r_0), & \text{for } r < r_0 + (1-\epsilon), \\ -T_\alpha / w_\alpha(\infty), & \text{for } r > r_0 + (1+\epsilon), \end{cases} \tag{5.8}$$

for an $\epsilon > 0$. Then, both conditions in (5.5) are satisfied.

For a regular (uncharged) solution, condition (5.6) is fulfilled and Σ is not empty.[4] Thus, a family (5.2), (5.3) *always* exists for solitons.

We note some properties of the families above. For the gauge group SU(2), these are closely related to families studied by other authors.[25] The equilibrium solution is clearly obtained for $\tau = 0$. Applying a gauge transformation with $g = \exp(\tau Z)$, we obtain

$$\Lambda_{(\tau)+} \to \Lambda_+ \cos(\tau) + iT_+ \sin(\tau), \quad \mathscr{B}_{(\tau)} \to 0. \tag{5.9}$$

The first variations of (5.2) and (5.3) are

$$\delta\phi_Y = i\ \mathrm{ad}(\Lambda_+)Z + T_+, \quad \delta\phi_{\mathscr{B}} = -i\,\frac{1}{\mu}\,p_* Z, \tag{5.10}$$

and these satisfy by construction the desired boundary conditions,

$$\lim_{r\to r_0,\infty} \delta\phi_Y = 0, \qquad \lim_{r\to r_0,\infty} \delta\phi_{\mathscr{B}} = 0. \tag{5.11}$$

[$\delta\phi_{\mathscr{B}}$ has even compact support in (r_0,∞)]. Since an equilibrium solution satisfies

$$p_*\Lambda_+|_{r_0} = p_*\Lambda_+|_\infty = 0, \tag{5.12}$$

we also have

$$\lim_{r\to r_0,\infty} p_*\ \delta\phi_Y = 0. \tag{5.13}$$

This choice of trial functions fulfills our goal: $\delta\Phi$ is normalizable and $\langle\delta\Phi|U|\delta\Phi\rangle$ is finite and turns out to be strictly negative.

The first of these two points is simple. Since $\delta\phi_{\mathscr{B}}$ in (5.10) has compact support, we have to check only whether

$$\int_{r_0}^{\infty} |\delta\phi_Y|^2\,\frac{dr}{NS} < \infty. \tag{5.14}$$

By construction,

$$\delta\phi_Y = \begin{cases} \displaystyle\sum_{\alpha\in\Sigma} T_\alpha\left(\frac{w_\alpha}{w_\sigma(r_0)} - 1\right)e_\alpha, & \text{for } r < r_0 + (1-\epsilon), \\ \displaystyle\sum_{\alpha\in\Sigma} T_\alpha\left(\frac{w_\alpha}{w_\alpha(r_\infty)} - 1\right)e_\alpha, & \text{for } r > r_0 + (1-\epsilon). \end{cases} \tag{5.15}$$

Hence, the integrand has a finite limit for $r\to r_0$ (even for extreme black hole solutions). Since N and S both approach one at infinity, the integral is finite if $\Lambda_+ - \Lambda_+(\infty)$ converges to zero faster than $r^{-1/2}$.

The calculation of $\langle\delta\Phi|U|\delta\Phi\rangle$ is somewhat tedious. Considerable simplifications occur by separating a gauge mode in $\delta\Phi$:

$$\delta\Phi = \delta\tilde{\Phi} - i\mathscr{G}Z, \tag{5.16}$$

with

$$\delta\tilde{\Phi} = \begin{pmatrix} T_+ \\ 0 \end{pmatrix}, \quad \mathscr{G}Z = \begin{pmatrix} -\mathrm{ad}(\Lambda_+)Z \\ \dfrac{1}{\mu}\,p_* Z \end{pmatrix}. \tag{5.17}$$

We stress that neither $\delta\tilde{\Phi}$ nor $\mathscr{G}Z$ are normalizable. Nevertheless, we have $U\mathscr{G}Z = 0$, and thus (5.16) and (5.17) give (with a slight abuse of notation)

$$\begin{aligned} \langle\delta\Phi|U|\delta\Phi\rangle &= \langle\delta\tilde{\Phi}|U|\delta\tilde{\Phi}\rangle + i\langle\mathscr{G}Z|U\delta\tilde{\Phi}\rangle = \langle\delta\tilde{\Phi}|U|\delta\tilde{\Phi}\rangle + i\langle U\mathscr{G}Z|\delta\tilde{\Phi}\rangle + \langle\mathrm{ad}(p_*\Lambda_+)Z, T_+\rangle|_{r_0}^{\infty} \\ &= \langle\delta\tilde{\Phi}|U|\delta\tilde{\Phi}\rangle. \end{aligned} \tag{5.18}$$

The boundary term does not contribute because of Eq. (5.12). From this, we obtain the intermediate result,

$$\langle \delta\Phi | U | \delta\Phi \rangle = \int_{r_0}^{\infty} \mu^2 \langle T_+ , \mathrm{ad}(i\hat{\mathscr{F}}_\parallel) T_+ \rangle dr_* = 2 \int_{r_0}^{\infty} \mu^2 \langle \hat{\mathscr{F}}_\parallel , \Lambda_{3\parallel} \rangle dr_* , \tag{5.19}$$

where we have used (2.5) and the property (5.4) of T_+.

Finally, we show that the last term has a definite sign:

$$2 \int_{r_0}^{\infty} \mu^2 \langle \hat{\mathscr{F}}_\parallel , \Lambda_{3\parallel} \rangle dr_* = - \int_{r_0}^{\infty} |p_* \Lambda_+|^2 + 2\mu^2 |\hat{\mathscr{F}}_\parallel|^2 \, dr_* . \tag{5.20}$$

After a partial integration, we find with the unperturbed YM equation (2.23),

$$\int_{r_0}^{\infty} |p_* \Lambda_+|^2 \, dr_* = - i \langle p_* \Lambda_+ , \Lambda_+ \rangle |_{r_0}^{\infty} - \int_{r_0}^{\infty} \mu^2 \langle \Lambda_+ , \mathrm{ad}(i\hat{\mathscr{F}}_\parallel) \Lambda_+ \rangle dr_* . \tag{5.21}$$

The boundary term vanishes because of Eq. (5.12), and since

$$2 |\hat{\mathscr{F}}_\parallel|^2 = \langle \hat{\mathscr{F}}_\parallel , i[\Lambda_+ , \Lambda_-] - 2\Lambda_{3\parallel} \rangle = \langle \Lambda_+ , \mathrm{ad}(i\hat{\mathscr{F}}_\parallel) \Lambda_+ \rangle - 2 \langle \hat{\mathscr{F}}_\parallel , \Lambda_{3\parallel} \rangle , \tag{5.22}$$

we have established the crucial result,

$$\langle \delta\Phi | U | \delta\Phi \rangle = - \langle p_* \Lambda_+ | p_* \Lambda_+ \rangle - 2 \langle \mu \hat{\mathscr{F}}_\parallel | \mu \hat{\mathscr{F}}_\parallel \rangle = - \int_{r_0}^{\infty} \left\{ N |\Lambda_+'|^2 + \frac{2}{r^2} |\hat{\mathscr{F}}_\parallel|^2 \right\} S \, dr . \tag{5.23}$$

This expression is clearly finite and strictly negative.

One can show that expression (5.23) is also equal to the second variation of the Schwarzschild mass for the one-parameter family (5.2), (5.3). [This is the way we arrived originally at the variation (5.10).] For a systematic discussion of the relation between variational principles for the spectra of radial pulsations and second variations of the total mass, we refer to Ref. 26.

In summary, we have proven (apart from technical subtleties) that static, spherically symmetric, asymptotically flat solutions of the EYM equations are unstable. More precisely, we have established the following.

Theorem 1: *A generic, regular solution is* unstable, *if the (magnetic) YM charge vanishes (i.e., if* $\lim_{r\to\infty} \Lambda(r)$ *is a homomorphism from L*SU(2) *to LG) and if asymptotically* $\Lambda_+ - \Lambda_+(\infty) \sim r^{-\alpha}$ *with* $\alpha > \frac{1}{2}$.

For a black hole (with horizon at r_h and $\Lambda_+ = \Sigma_{\alpha\in\Sigma} w_\alpha e_\alpha$), the assumptions are somewhat more restrictive and ''trivial'' solutions have to be excluded. We call a generic, essentially magnetic solution ''trivial'' if either Σ is empty or each amplitude ω_α is constant. These are clearly just the Reissner–Nordström solutions.

Theorem 2: *A generic, essentially magnetic, nontrivial black hole solution is* unstable, *if* $\lim_{r\to r_h,\infty} w_\alpha \neq 0$ *for all* $\alpha \in \Sigma$ *and if asymptotically* $\Lambda_+ - \Lambda_+(\infty) \sim r^{-\alpha}$ *with* $\alpha > \frac{1}{2}$.

We would like to stress that we were able to draw this conclusion, assuming only weak asymptotic conditions for the solutions. In particular, the fall-off condition is mild and is certainly fulfilled for the Bartnik–McKinnon and the related black hole solutions, as was shown rigorously in Ref. 27. The same is true for the regular solutions, which have been found numerically by Künzle for the group SU(3).[23] (For both types, the exponent α is equal to unity.)

VI. SPHALERON-LIKE INSTABILITIES AS BOUND STATES OF A FICTITIOUS DEUTERON PROBLEM

We now address the question whether the operator $p_*^2 + V$ in the eigenvalue problem (4.26) is essentially self-adjoint on a dense domain of smooth functions, which satisfy the boundary conditions implied by the physics of the problem. That this is indeed the case will be shown in the present section for SU(2) solitons. The discussion of the general case is deferred to the Appendix.

For regular SU(2) solutions, it turns out that the eigenvalue equation (4.26) can be interpreted as a fictitious deuteron problem for a neutron–proton potential, consisting of a central part, a tensor force, and a spin-orbit coupling. All parts are determined by the unperturbed soliton and can be shown to be bounded. The corresponding Schrödinger operator is thus essentially self-adjoint on the subspace of smooth functions with compact support and self-adjoint on the Sobolev space $H^2(\mathbb{R}^3)$. These facts will be used later in an analysis of the instabilities, implied by the existence of bound states (see the Appendix).

In order to bring the operator $p_*^2 + V$ to a standard Schrödinger form, we introduce the new radial coordinate,

$$\rho(r) = \int_0^r \frac{dy}{NS}, \tag{6.1}$$

in terms of which $p_* = -id/d\rho$. Since μ^2 behaves like $1/\rho^2$ near the origin, we separate from the potential (4.16) the singular term

$$V(\rho) = \frac{J^2}{\rho^2} + \tilde{V}(\rho), \tag{6.2}$$

where

$$J^2 = \begin{pmatrix} K^2(0) & 2iK_+(0) \\ -2iK_-(0) & K^2(0)+2 \end{pmatrix}, \tag{6.3}$$

and the remainder $\tilde{V}$ is bounded.

For a generic soliton, the eigenvalues of J^2 are equal to $j(j+1)$ with $j = k \pm 1$, whereby the integer k runs through a (strictly) positive, finite set. This set always contains $k=1$ and is uniquely determined by $\Lambda_3 = \Lambda_{3\|}$.

In a representation in which J^2 is diagonal, J^2/ρ^2 thus describes the central barriers of a finite set of partial waves.

We now discuss in detail the equations for the gauge group SU(2). For this group, only S and D waves occur in Eq. (4.26). In the variable ρ and with the parametrization

$$\Lambda_+ = w\tau_+ = w(\tau_1 + i\tau_2), \quad \Lambda_3 = \tau_3,$$

and

$$\begin{pmatrix} \phi_Y \\ \phi_{\mathscr{B}} \end{pmatrix} = \frac{u_S}{\sqrt{3}} \begin{pmatrix} \tau_+ \\ \tau_3 \end{pmatrix} + \frac{u_D}{\sqrt{6}} \begin{pmatrix} -\tau_+ \\ 2\tau_3 \end{pmatrix}, \tag{6.4}$$

the eigenvalue equation (4.26) takes the form

$$\left\{ -\frac{d^2}{d\rho^2} + \frac{1}{\rho^2}\begin{pmatrix} 0 & 0 \\ 0 & 6 \end{pmatrix} + \tilde{V} \right\} \begin{pmatrix} u_S \\ u_D \end{pmatrix} = \omega^2 \begin{pmatrix} u_S \\ u_D \end{pmatrix}. \tag{6.5}$$

For the potential $\tilde{V}$ we find

$$\tilde{V} = \frac{1}{3}\begin{pmatrix} \tilde{V}_{SS} & \tilde{V}_{SD} \\ \tilde{V}_{DS} & \tilde{V}_{DD} \end{pmatrix}, \tag{6.6}$$

where

$$\tilde{V}_{SS} = \{\mu''/\mu + 8(\mu w)' + 6\mu^2 w^2\} - 2\mu^2(1-w^2), \tag{6.7}$$

$$\tilde{V}_{SD} = \sqrt{2}\{\mu''/\mu + 2(\mu w)'\} + \sqrt{2}\mu^2(1-w^2), \tag{6.8}$$

$$\tilde{V}_{DS} = \tilde{V}_{SD}, \tag{6.9}$$

$$\tilde{V}_{DD} = 2\{\mu''/\mu - 4(\mu w)' + 3\mu^2 w^2 - 9/\rho^2\} - \mu^2(1-w^2), \tag{6.10}$$

and a *dash* denotes a derivative *with respect to* ρ.

It is amusing and helpful to note that this coupled eigenvalue problem has the same form as the Schrödinger equation for the relative motion of a two-body proton–neutron system with the three standard terms $V_C(r)$ (central potential), $V_T(r)\mathbf{S}_{12}$ (tensor interaction) and $V_{LS}(r)\mathbf{L}\cdot\mathbf{S}$ (spin-orbit interaction). For total angular momentum $J=1$ and total spin $S=1$, the possible orbital angular momenta are $L=1$ and $L=0,2$. Because of parity conservation, the P wave decouples from the S and D waves. The remaining equation, describing coupled S and D waves, reads, in suitable units,

$$\left\{ -\frac{d^2}{dr^2} + \frac{1}{r^2}\begin{pmatrix} 0 & 0 \\ 0 & 6 \end{pmatrix} + \begin{pmatrix} V_C & \sqrt{8}V_T \\ \sqrt{8}V_T & V_C - 2V_T - 3V_{LS} \end{pmatrix} \right\} \begin{pmatrix} u_S \\ u_D \end{pmatrix} = E \begin{pmatrix} u_S \\ u_D \end{pmatrix}. \tag{6.11}$$

These equations have first been derived by Rarita and Schwinger.[28] Our eigenvalue problem (6.5) is clearly just a special case of (6.11) and we can, by identification, express the three potentials in terms of the functions N,S,w of the Bartnik–McKinnon solutions.

We present numerical results elsewhere (also see Ref. 29) and emphasize here only, that with this interpretation the mathematical nature of our eigenvalue problem is automatically settled, because the perturbation $\tilde{V}$ is completely harmless. We come back to this in the Appendix, where we also discuss the operator corresponding to the strong Gauss constraint.

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APPENDIX A: ESSENTIAL SELF-ADJOINTNESS OF THE EFFECTIVE HAMILTONIAN

For black holes, the operator $Q = p_*^2 + V$ in (4.15), with the expressions (4.17)–(4.20) for the matrix-valued potential V, is effectively a standard Schrödinger operator on the whole real line (see Ref. 17), and is thus essentially self-adjoint on C^∞ functions with compact support. (The potential V is bounded for black holes.) For solitons, we can use Weyl's limit point–limit circle criterion (see Ref. 30, Sec. X.1 or Ref. 31) for the first two terms of the operator,

$$Q = -\frac{d^2}{d\rho^2} + \frac{J^2}{\rho^2} + \tilde{V}(\rho) \tag{A1}$$

[see (6.2) and (6.3)]. Since $\tilde{V}$ is bounded, the Rellich–Kato theorem implies that the domains of (essential) self-adjointness are not changed by this additive term.

Another method that will be used later is to lift Q to a Schrödinger operator H_Q on $\mathbb{R}^3$ and to use powerful results for these kind of operators. In Sec. VI we showed how this can be achieved if the gauge group is SU(2): H_Q can then be chosen to be of the standard form for a deuteron problem. This operator is essentially self-adjoint on $C_0^2(\mathbb{R}^3)\otimes\mathbb{C}^4$ and self-adjoint on the Sobolev space $H^2(\mathbb{R}^3)\otimes\mathbb{C}^4$ (see, e.g., Ref. 30, Sec. X 2). Restricting these domains to the subspace of S and D waves, provides the domains we are interested in for the original operator Q. For instance, Q is essentially self-adjoint on

$$\mathscr{D}(Q) = \{(u_S, u_D) \,|\, u_S \in C_0^\infty[0,\infty), u_S(0) = 0; u_D \in C_0^\infty(0,\infty)\}. \tag{A2}$$

Although we have not yet generalized this construction to arbitrary gauge groups, the generalization of $\mathscr{D}(Q)$ is obvious: The S waves have to be restricted as in (A2) and the higher waves have to lie in $C_0^\infty(0,\infty)$. We also note at this point that the variation (5.10) lies in the domain of definition of the self-adjoint extension of $(Q, \mathscr{D}(Q))$.

If we would restrict the S waves also to $C_0^\infty(0,\infty)$, the operator Q would not be essentially self-adjoint. For each S wave sector, it would actually have a one-parameter family of self-adjoint extensions. The self-adjoint extension, given above, is just the Friedrichs extension, and one can show that it is the only one that is compatible with the strong Gauss constraint (4.9).

The existence and smoothness problems in connection with Eq. (4.27) can also be solved by lifting the equation to $\mathbb{R}^3$ and using standard existence and regularity theorems for elliptic operators on $\mathbb{R}^3$. [The details can easily be worked out for $G = \mathrm{SU}(2)$.]

APPENDIX B: SPECTRAL PROPERTIES AND UNSTABLE PERTURBATIONS

In Sec. IV it was shown that the perturbation equations for even parity perturbations are equivalent to the hyperbolic system,

$$\partial_t^2 \Phi = -Q\Phi. \tag{B1}$$

We also recall that these equations imply the propagation of the strong Gauss constraint. As a main point of this paper we proved that the self-adjoint operator Q, restricted to the subspace of physical states, satisfying the strong Gauss constraint, has a nonempty negative spectral part. This fact implies, of course, that there are unstable Hilbert space solutions of (B1). We just have to choose the initial data Φ_0 such that $E_Q(-\infty,0)\,\Phi_0 \neq 0$, where $E_Q(\cdot)$ denotes the projection valued measure belonging to Q (see below). It is even possible to choose $\Phi_0 \in C_0^\infty$, because the smooth functions with compact support are dense in the Hilbert space L^2.

The question now arises whether such a Hilbert space solution is even a (classical) solution of the system of partial differential equations (B1), in other words, whether the Hilbert space solutions with $\Phi_0 \in C_0^\infty$ are automatically smooth. For black holes, the positive answer to this question is contained in a paper by Wald.[32] His analysis does, however, not directly apply to solitons, because he assumed that space is a *complete* Riemannian manifold.

A direct attack of the problem on the half-line $(0,\infty)$ is again difficult. Once more, a way out is lifting the problem to $\mathbb{R}^3$,

$$\partial_t^2 \Phi = -H_Q \Phi, \tag{B2}$$

where the analysis of Ref. 32 applies. We showed earlier, how this can be done for SU(2). Since the required smoothness properties certainly do not depend on the gauge group, it is not worthwhile to elaborate further on this. We would like, however, to present here a simplified version of Wald's argument.

Consider a hyperbolic system on $\mathbb{R}\times\mathbb{R}^n$ of the form (B2) with a smooth elliptic operator A (instead of H_Q), which is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$. For systems of this kind, a lot is known about the Cauchy problem (a standard reference is Ref. 33). In particular, one knows (see Theorem 23.2.2 in Vol. III of Ref. 33), that the Cauchy problem with initial data Φ_0, $\dot{\Phi}_0 \in C_0^\infty(\mathbb{R}^n)$ has a unique solution in $C^\infty(\mathbb{R}\times\mathbb{R}^n)$, which for any fixed time t is in $C_0^\infty(\mathbb{R}^n)$. This smooth solution must agree with the Hilbert space solution of the Cauchy problem because the latter is also unique.

Let us now assume that the spectrum $\sigma(A)$ of A has a nonempty intersection $\sigma(A)_-$ with $(-\infty,0)$. We also assume that $\sigma(A)$ is bounded from below (this is the case for $A=H_Q$). The Hilbert space solution of the Cauchy problem can easily be expressed in terms of the projection valued measure $E(\cdot)$ belonging to A. It suffices, for what follows, to take as initial data $\Phi|_{t=0}=\Phi_0$, $\partial_t\Phi|_{t=0}=0$. Then, the corresponding Hilbert space solution of

$$\ddot{\Phi}_t = -A\Phi_t \tag{B3}$$

is

$$\Phi_t = E(\{0\})\Phi_0 + \int_{(0,\infty)} \cos(t\sqrt{\lambda})\,dE(\lambda)\Phi_0 + \int_{\sigma(A)_-} \cosh(t\sqrt{-\lambda})\,dE(\lambda)\Phi_0, \tag{B4}$$

as can easily be verified. Note, in particular, that $\Phi_{t=0}=E(\mathbb{R})\Phi_0=\Phi_0$, as required.

With standard rules (see, e.g., Ref. 34, Chap. 13), we obtain from this,

$$\langle\Phi_0|\Phi_t\rangle = \|E(\{0\})\Phi_0\|^2 + \int_{(0,\infty)} \cos(t\sqrt{\lambda})\,d\mu_{\Phi_0}(\lambda) + \int_{\sigma(A)_-} \cosh(t\sqrt{-\lambda})\,d\mu_{\Phi_0}(\lambda) \tag{B5}$$

and

$$\|\Phi_t\|^2 \geqslant \int_{\sigma(A)_-} \cosh(t\sqrt{-\lambda})\,d\mu_{\Phi_0}(\lambda), \tag{B6}$$

where μ_{Φ_0} is the finite measure $\langle\Phi_0|E(\cdot)\Phi_0\rangle$ on $\mathbb{R}$, whose support is contained in $\sigma(A)$. As emphasized above, we can choose Φ_0 such that $(\text{supp}\ \mu_{\Phi_0})\cap\sigma(A)_-$ is nonempty. Then (B5) and (B6) imply that both quantities on the left diverge exponentially. This exponential grows translates to an average exponential grows of the *classical* solution of the hyperbolic system for smooth initial data with compact support.

These considerations conclude our instability proof.

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Collapsing regions and black hole formation

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Up to a conjecture in Riemannian geometry, we significantly strengthen a recent theorem of Eardley by proving that a compact region in an initial data surface that is collapsing sufficiently fast in comparison to its surface-to-volume ratio must contain a future trapped region. In addition to establishing this stronger result, the geometrical argument used does not require any asymptotic or energy conditions on the initial data. It follows that if such a region can be found in an asymptotically flat Cauchy surface of a spacetime satisfying the null-convergence condition, the spacetime must contain a black hole with the future trapped region therein. Further, up to another conjecture, we prove a strengthened version of our theorem by arguing that if a certain function (defined on the collection of compact subsets of the initial data surface that are themselves three-dimensional manifolds with boundary) is not strictly positive, then the initial data surface must contain a future trapped region. As a byproduct of this work, we offer a slightly generalized notion of a future trapped region as well as a new proof that future trapped regions lie within the black hole region. © *1996 American Institute of Physics.* [S0022-2488(96)00103-0]

I. INTRODUCTION

Given an initial data set for the gravitational field[1] (Σ, g_{ab}, K_{ab}) associated with a Cauchy surface in an asymptotically flat spacetime, can we tell whether gravitational collapse has proceeded to such a point that a black hole has formed in that spacetime? In principle, the answer is yes: Given a complete description of the matter fields in the spacetime (i.e., their initial data and evolution equations), then using Einstein's equation, evolve the initial data to reconstruct the entire spacetime and then see whether the spacetime has a nonempty black-hole region and, if so, whether and where it intersects Σ. In practice, however, carrying out this construction is a highly nontrivial task, even in the vacuum case and even when done numerically.[2]

While there is currently no simple algorithm for determining from an initial data set whether a black hole has formed, if a future trapped region exists in Σ, it must lie within the black-hole region, provided the spacetime satisfies the null-convergence condition.[3–5] Recall that a closed subset C of Σ having the structure of a three-manifold with smooth (or at least C^2) boundary, bounded away from spatial infinity, is said to be a future trapped region if the convergence of the future-directed null geodesics orthogonal to ∂C and outward directed (in the sense that the projection of null geodesic tangent vectors on C into Σ point outward from C) is non-negative everywhere on ∂C.[4] Denoting the induced metric on ∂C by h_{ab}, the mean extrinsic curvature[6] of ∂C in Σ by H, and the extrinsic curvature of Σ in the spacetime by K_{ab}, C is a future trapped region if

$$H \leqslant K_{ab} h^{ab} \tag{1.1}$$

on ∂C. Likewise, the total future trapped region of Σ (being the closure of the union of all future trapped regions in Σ) along with its boundary $\mathscr{A}$ (the future apparent horizon, on which $H = K_{ab} h^{ab}$), is contained within the black-hole region (under the same conditions as before).[7] So, in initial data sets with a non-empty total future trapped region, gravitational collapse has proceeded sufficiently far so that black holes have formed.

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Are there any simple conditions that guarantee the existence of a future trapped region in an initial data set? Thorne's ''hoop conjecture'' offers a test of this type: If a body of mass M is sufficiently compact so that a hoop of circumference $4\pi M$ can encircle the body no matter how it is rotated there about, then the body must be contained within a horizon.[8,9] While a precise version of this conjecture remains to be proven, Schoen and Yau have proven that an initial data set containing a region Ω with sufficient matter density must contain a future or past apparent horizon.[10] This interesting result has the slight weaknesses that its requirement on the matter content is so strict that arbitrarily small vacuum regions in Ω are not allowed and that, as a time-symmetric theorem, we cannot conclude that the apparent horizon must be a future horizon. (Of course, this last criticism can be avoided by restricting oneself to initial data sets that do not contain past trapped regions.) Further, a number of necessary conditions and sufficient conditions have been found for spherically symmetric initial data sets.[11] More recently, using Jang's equation and its properties as established by Schoen and Yau,[12] Eardley has recently provided a remarkably simple proof of the following theorem.[13,14]

Theorem (Eardley). Fix an asymptotically flat initial data set for the gravitational field[1] (Σ, g_{ab}, K_{ab}) satisfying the dominant-energy condition. If there exists a compact region $\Omega \subset \Sigma$ such that $K_{ab}(g^{ab}-n^a n^b)$ is no less than the surface-to-volume ratio of Ω for all unit vectors n^a everywhere on Ω, then Σ must contain an apparent horizon.

Were the apparent horizon a *future* apparent horizon, then, as noted, the conditions of this theorem would guarantee that gravitational collapse has proceeded sufficiently far that a black-hole region has formed. Unfortunately, as given, the theorem alone does not allow one to draw this conclusion as it suffers from the same problem of Schoen and Yau's theorem[10] in that the possibility that all such horizons will be past apparent horizons has not been eliminated. However, the time-asymmetry in the hypotheses of Eardley's theorem ($K^a{}_a$ is strictly positive on Ω indicating that the region is collapsing ''on average'') is a strong indication that there should be a future apparent horizon somewhere in Σ.

By changing our viewpoint, Eardley's theorem suggests an alternative argument having the advantage of producing a strengthened version of the above theorem under weaker hypotheses. In particular, we can now show that Σ must in fact contain a future apparent horizon. Further, this argument has an entirely geometric character, which is to be compared to Eardley's argument, which, through the use of Jang's equation, has an analytic character.

To begin, notice that the induced metric h^{ab} on a two-surface $\mathscr{S} \subset \Sigma$ can be written as $h^{ab}=g^{ab}-n^a n^b$, where n^a is either of the two unit-normal vectors to $\mathscr{S}$. Therefore, the hypothesis of the above theorem guarantees that, on $\mathscr{S}$, $K_{ab}h^{ab}$ is bounded from below by the surface-to-volume ratio of Ω, which we denote by $\sigma(\Omega)$. Notice that this bound is independent of the two-surface in Ω. This suggests that if there exists a region in Ω (having the structure of a three-manifold with boundary) whose boundary's mean extrinsic curvature H is bounded above by $\sigma(\Omega)$, then Eq. (1.1) would hold on the boundary, and hence the region would be a future trapped region.

Does such a region exist in Ω? The appearance of the surface-to-volume ratio σ in Eardley's theorem suggests that we study this quantity as function on the collection of regions C in Ω. Consider a region $C \subset \Omega$ that is ''nearly degenerate'' in the sense that it is either flat like a pancake of thickness r, thin like a cigar of radius r, or small like a sphere of radius r. Then, we expect (as in the flat space case) that $\sigma(C) \approx \text{const}/r$, for r sufficiently small, showing that regions that are nearly degenerate in the sense that they are small in one or more dimensions have very large surface-to-volume ratios. This suggests that there is some sufficiently well-behaved region in Ω having minimal surface-to-volume ratio. In fact, we conjecture that there always exists a region $\hat{C} \subset \Omega$, having the structure of a differentiable manifold with boundary, that minimizes σ over such regions $C \subset \Omega$. (See conjecture 1 in Sec. IV.) Remarkably, it then follows that $H \leqslant \sigma(\Omega)$ on any open subset of $\partial\hat{C}$ where the surface is C^2, i.e., on the portion having a well-defined and continuous extrinsic curvature. (The proof of this fact is given in Sec. II.)

Putting this all together, we have

$$H \leqslant \sigma(\Omega) \leqslant K_{ab} h^{ab} \tag{1.2}$$

on the open subset of $\partial\hat{C}$ that is C^2, where the first inequality is a consequence of the minimizing property of $\hat{C}$ and the second follows by hypothesis. Were $\partial\hat{C}$ everywhere C^2, then $\hat{C}$ would be a future trapped region. As explained in Sec. IV, this is not always the case. However, it is expected that $\partial\hat{C}$ is sufficiently well-behaved so that Eq. (1.2) holds over a sufficiently large subset of $\partial\hat{C}$ that $\hat{C}$ is indeed a future trapped region, in the sense that it must lie in the black-hole region of the spacetime. In particular, we conjecture that $\partial\hat{C}$ is everywhere C^{2-} (see below) and C^2 everywhere except on a closed set $\mathscr{Z}$ of measure zero. (See Sec. IV for the statement and discussion of this conjecture.) Therefore, although Eq. (1.1) may not hold everywhere on $\partial\hat{C}$, it does hold on $\partial\hat{C}\backslash\mathscr{Z}$, which, with the fact that the surface is C^{2-}, is sufficient to guarantee the region is trapped. (See theorem 5 in Sec. V B.) This proves the following strengthened version of Eardley's theorem.

Theorem 1. Fix an initial data set for the gravitational field[1] (Σ, g_{ab}, K_{ab}) and fix a subset $\Omega \subset \Sigma$ that is a compact three-manifold with C^2 boundary. If $K_{ab}h^{ab}$ is no less than the surface-to-volume ratio of Ω for all rank 2 orthogonal projection maps[15] $h^a{}_b$ everywhere on Ω, then there exists a future trapped region in Ω, provided conjecture 1 (stated in Sec. IV) holds for (Ω, g_{ab}).

Denoting the eigenvalues of $K^a{}_b$ by (k_1, k_2, k_3), ordered so that $k_1 \leqslant k_2 \leqslant k_3$, it is worth noting that the minimum of $K_{ab}h^{ab}$ over all rank 2 orthogonal projection maps[15] $h^a{}_b$ is precisely $k_1 + k_2$. Therefore, the sole condition of theorem 1 is that the sum of the two lesser principal (extrinsic) curvatures be no less than the surface-to-volume ratio of Ω, everywhere on Ω.

We can now assert (assuming conjecture 1) that if such a region Ω exists in a Cauchy surface of an asymptotically flat spacetime[4] satisfying the null-convergence condition,[3] the spacetime must contain a black hole with the future trapped region therein.

Comparing the two theorems, we see that while neither locates the future apparent horizon, theorem 1 does tell us some subset of Ω, namely $\hat{C}$, is contained within the future apparent horizon. Further, we see that theorem 1 dispenses with the asymptotic and energy conditions that were needed by Eardley because of their use in Schoen and Yau's analysis of Jang's equation.

The remainder of this work is organized as follows. In Sec. II, we prove the lemma providing the bound $H \leqslant \sigma(\Omega)$ on $\partial\hat{C}$. In Sec. III, we review Eardley's argument and then present a strengthened version of theorem 1. In Sec. IV, we state and discuss the two conjectures in Riemannian geometry needed for this work. In Sec. V, we offer a new proof that future trapped regions are trapped, which is then modified to establish the same result for our weaker notion a future trapped region, and then we discuss the possibility of further extending the notion of a future trapped region. Lastly, in Sec. VI, we discuss the strengths and weakness of our results.

Our conventions are those of Ref. 4 with the notable exception that our sign convention for the extrinsic curvature of our initial data surfaces is such that positive K is associated with collapse in the sense that it measures the *convergence* of future-directed geodesic normals to the surface. On the other hand, H measures the *divergence* of the outward geodesic normals to the surface of a region within an initial data surface.

Recall that a map between manifolds is said to be C^{k-} if the mapping is C^{k-1} and its $(k-1)$-order derivatives of the functions defining the mapping are locally Lipschitz.[5,16] Thus, a C^{2-} embedded surface is C^1 and the derivative of the embedding map is locally Lipschitz.

It proves very convenient to make the following definitions. Given a manifold N (possibly with boundary), define $\mathscr{C}^k(N)[\mathscr{C}^{k-}(N)]$ to be the collection of compact subsets of N having the structure of a manifold with C^k (C^{k-}) boundary. It is useful to keep in mind that

$$\mathscr{C}^0(N)\supset\mathscr{C}^{1-}(N)\supset\mathscr{C}^1(N)\supset\mathscr{C}^{2-}(N)\supset\mathscr{C}^2(N)\supset\cdots. \tag{1.3}$$

Elements of $\mathscr{C}^k(N)$ and $\mathscr{C}^{k-}(N)$ need not be connected, i.e., they can have many connected components. Further, if $\Omega\in\mathscr{C}^k(N)$, then $\Omega\in\mathscr{C}^k(\Omega)$, and, similarly, if $\Omega\in\mathscr{C}^{k-}(N)$, then $\Omega\in\mathscr{C}^{k-}(\Omega)$.

Lastly, for a map $\phi:A\to B$, $\phi[A]$ denotes the image of A in B, $A\backslash B$ denotes the set of elements in A that are not in B, and A denotes the closure of A.

II. PROOF THAT $H\leqslant\sigma(\Omega)$ ON $\partial\hat{C}$

Denote the surface area, volume, and surface-to-volume ratio of a region $C\in\mathscr{C}^1(\Sigma)$ by $A(C)$, $V(C)$, and $\sigma(C)=A(C)/V(C)$, respectively. More explicitly,

$$A(C)=\int_{\partial C}\epsilon_{ab}, \tag{2.1a}$$

$$V(C)=\int_{C}\epsilon_{abc}, \tag{2.1b}$$

where ϵ_{abc} is the volume element constructed from g_{ab} and ϵ_{ab} is the volume element constructed from the metric h_{ab} induced on ∂C by g_{ab}.

Lemma 1. Fix a pair (Ω,g_{ab}), where Ω is a compact three-dimensional manifold with C^1 boundary and g_{ab} is a smooth Riemannian metric on Ω. If $\hat{C}\in\mathscr{C}^1(\Omega)$ is such that $\sigma(\hat{C})\leqslant\sigma(C)$ for all $C\in\mathscr{C}^1(\Omega)$ and O is an open subset of $\partial\hat{C}$ where the surface is C^2, then $H\leqslant\sigma(\hat{C})\leqslant\sigma(\Omega)$ on O, where H is the mean extrinsic curvature[6] of $\partial\hat{C}$. If, further, O is in the interior of Ω, then $H=\sigma(\hat{C})$ on O.

Proof. The idea of the proof is simple: We calculate σ as a function along certain well-behaved curves in $\mathscr{C}^1(\Omega)$ containing $\hat{C}$, calculate its derivative at $\hat{C}$, and then use the fact that $\hat{C}$ minimizes σ in $\mathscr{C}^1(\Omega)$.

Although there are many curves in $\mathscr{C}^1(\Omega)$, by which we mean one-parameter family of regions $C_\lambda\in\mathscr{C}^1(\Omega)$, for simplicity, we shall restrict ourselves to families arising from a smooth deformation of a region $C\in\mathscr{C}^1(\Omega)$ in the sense that $C_\lambda=\phi_\lambda[C]$ for some one-parameter family of maps $\phi_\lambda:\Omega\to\Omega$ such that ϕ_λ is a diffeomorphism between Ω and $\phi_\lambda[\Omega]$, with ϕ_0 being the identity map on Ω. Our requirement that Ω and $\phi_\lambda[\Omega]$ be diffeomorphic is sufficient to guarantee that $\partial(\phi_\lambda[C])=\phi_\lambda[\partial C]$, which makes the following calculations easier than they would be otherwise.

A particularly simple class of such deformations, which is sufficient for our purposes, are those associated with the flows of fixed vector fields on Ω.[16] [That is, given a fixed vector field ξ^a, for $p\in\Omega$, $\phi_\lambda(p)$ is the point along the integral curve of ξ^a containing p a parameter distance λ from p.] In order that these deformations be well defined on all of Ω for some positive λ, it is necessary to restrict ourselves to vector fields that are inward pointing everywhere on $\partial\Omega$ (where we consider vectors tangent to $\partial\Omega$ as inward pointing, so $\xi^k n_k\leqslant 0$ everywhere on $\partial\Omega$, where n^k is the unit outward normal to $\partial\Omega$). Otherwise, a point $p\in\partial\Omega$ where ξ^a is strictly outward pointing would be mapped "out of" Ω, and hence the deformation constructed from it would not be defined for any positive λ, no matter how small. A deformation ϕ_λ constructed from an inward pointing vector field is well defined for all $\lambda\geqslant 0$ and is a diffeomorphism between Ω and $\phi_\lambda[\Omega]$.

Fix any inward pointing vector field ξ^a whose support intersects ∂C within O and construct its one-parameter family of deformations ϕ_λ. Evaluating A and V on $C_\lambda=\phi_\lambda[C]$ using Eqs. (2.1), differentiating with respect to λ, and then evaluating at $\lambda=0$, we find that

$$A'(C)=\int_O H(\xi^k n_k)\epsilon_{ab}, \tag{2.2a}$$

$$V'(C)=\int_O (\xi^k n_k)\epsilon_{ab}, \tag{2.2b}$$

where H is the mean extrinsic curvature of ∂C and n^k is the outward unit normal to ∂C. Differentiating the equality $\sigma(C_\lambda)=A(C_\lambda)/V(C_\lambda)$, evaluating at $\lambda=0$, and using Eqs. (2.2), we find that

$$\sigma'(C)=\frac{1}{V(C)}\int_O (H-\sigma(C))(\xi^k n_k)\epsilon_{ab}. \tag{2.3}$$

Using this equation, we now establish our bound on H.

We begin with the case where O is in the interior of Ω. Fix any point $p \in O$. To show that $H(p)=\sigma(\hat{C})$, suppose, for contradiction, that $H(p)>\sigma(\hat{C})$. Then, using the facts that p is in the interior of Ω and H is continuous at p, it is not difficult to show that there exists an open neighborhood $\underline{N}$ of p and a vector field ξ^a such that: (1) the support of ξ^a is $\bar{N}$; (2) $\partial\hat{C}$ is C^2 on $\bar{N}\cap\partial\hat{C}$; (3) $(\bar{N}\cap\partial\Omega)=\emptyset$; (4) $(H-\sigma(\hat{C}))>0$ on $N\cap\partial\hat{C}$; (5) $(\xi^k n_k)<0$ on $N\cap\partial\hat{C}$. Notice that ξ^a, being zero on $\partial\Omega$, is inward pointing, so the one-parameter family of deformations ϕ_λ constructed from ξ^a is defined for all $\lambda\geqslant 0$. Using Eq. (2.3), we see that $\sigma'(\hat{C})<0$, which is impossible as otherwise, for sufficiently small λ, the region $\phi_\lambda[\hat{C}]$ would have a smaller surface-to-volume ratio than $\hat{C}$. Similarly, if $H(p)<\sigma(\hat{C})$, there exists an open neighborhood N of p and a vector field ξ^a satisfying the above except with the inequalities in (4) and (5) both reversed. Using Eq. (2.3), we again find that $\sigma'(\hat{C})<0$, which is again a contradiction. Therefore, $H(p)=\sigma(\hat{C})$, as claimed.

Otherwise, fix any point $p \in O$. To show that $H(p)\leqslant\sigma(\hat{C})$, suppose, for contradiction, that $H(p)>\sigma(\hat{C})$. Then, there exists an open neighborhood $\underline{N}$ of p and a vector field ξ^a satisfying the above with (3) replaced by: (3') ξ^a is inward pointing on $\bar{N}\cap\partial\Omega$. Again the one-parameter family of deformations ϕ_λ constructed from ξ^a is defined for all $\lambda\geqslant 0$. Using Eq. (2.3), we see that $\sigma'(\hat{C})<0$, which is contradicts the minimality of σ at $\hat{C}$. Therefore, $H(p)\leqslant\sigma(\hat{C})$, as claimed.

Lastly, that $\sigma(\hat{C})\leqslant\sigma(\Omega)$ follows simply from the facts that $\hat{C}$ minimizes σ over $\mathscr{C}^1(\Omega)$ and $\Omega \in \mathscr{C}^1(\Omega)$. This completes the proof of lemma 1. □

III. STRENGTHENING THEOREM 1

We begin with two definitions. First define the scalar field κ on Σ by setting

$$\kappa(p)=\min_{h^a{}_b}(K_{ab}h^{ab}), \tag{3.1}$$

for each $p \in \Sigma$, where the minimum is over the set of all rank 2 orthogonal projection maps[15] $h^a{}_b$ at p. That is, $\kappa(p)$ is the sum of the two lesser principal (extrinsic) curvatures at p. Second, for any continuous function f on Σ, define the function W_f on $\mathscr{C}^1(\Sigma)$ by setting

$$W_f(C)=\int_C f\epsilon_{abc}, \tag{3.2}$$

for each $C \in \mathscr{C}^1(\Sigma)$. Note that with $f=1$, $W_1(C)=V(C)$.

The idea behind the proof of theorem 1 was to use the properties of the region that minimizes the surface-to-volume ratio σ on $\mathscr{C}^1(\Omega)$. Noting that $\sigma=A/V=A/W_1$, one way to proceed in

generalizing theorem 1 is to analyze the properties of the region that minimizes A/W_κ on $\mathscr{C}^1(\Omega)$. Assuming the relevant generalized version of conjecture 1 holds, it can be shown that there is a future trapped region in Ω provided that $A(\Omega)/W_\kappa(\Omega)\leqslant 1$ and κ is non-negative (and not everywhere zero) on Ω. However, such an argument must fail if κ is negative somewhere on Ω since, by choosing regions with large area in regions where κ is negative, we can find $C \in \mathscr{C}^1(\Sigma)$ for which the ratio $A(C)/W_\kappa(C)$ is negative and as large as we wish (i.e., A/W_κ has no finite lower bound in this case). The fact that κ cannot be even slightly negative on small subsets of Ω makes this route unattractive, so we take an alternative path suggested by the argument Eardley used in proving his theorem.

A. Eardley's argument

Fix an asymptotically flat initial data set for the gravitational field[1] (Σ, g_{ab}, K_{ab}) with sources satisfying the dominant energy condition. Schoen and Yau have shown that such an initial data set does not contain an apparent horizon (either future or past) if and only if there exists a scalar field f satisfying Jang's equation everywhere on Σ.[12] Eardley's argument is that certain initial data are inheritly incompatible with the existence of a global solution of Jang's equation, and therefore a (future or past) apparent horizon must be present. This argument goes as follows.

Defining

$$h^a = \frac{D^a f}{\sqrt{1 + D^m f D_m f}}, \tag{3.3}$$

where D_a is the derivative operator on Σ associated with g_{ab}, Jang's equation takes the simple form

$$D_a h^a = K_{ab}(g^{ab} - h^a h^b). \tag{3.4}$$

Noting that $h^m h_m < 1$ everywhere, define the scalar field $\tilde{\kappa}$ on Σ by setting

$$\tilde{\kappa}(p) = \inf_{|x|<1} (K_{ab}(g^{ab} - x^a x^b)), \tag{3.5}$$

at each point $p \in \Sigma$, where the infimum is over all vectors x^a at p with $x^m x_m < 1$. (By continuity, the value of $\tilde{\kappa}$ is unchanged if we modify its definition by taking the minimum over all vectors x^a at p with $x^m x_m \leqslant 1$.) Using the fact that for $x^a \neq 0$

$$K_{ab}(g^{ab} - x^a x^b) = (1 - x^m x_m) K_{ab} g^{ab} + (x^m x_m) K_{ab}(g^{ab} - x^a x^b / (x^m x_m)), \tag{3.6}$$

it is not difficult to show that

$$\tilde{\kappa} = \min(K^a{}_a, \kappa) \leqslant \kappa \tag{3.7}$$

at each point. Define the function $\tilde{S}$ on $\mathscr{C}^1(\Sigma)$ by setting

$$\tilde{S}(C) = A(C) - W_{\tilde{\kappa}}(C), \tag{3.8}$$

for each $C \in \mathscr{C}^1(\Sigma)$.

If a global solution of Jang's equation exists, it follows that

$$D_a h^a \geqslant \tilde{\kappa}, \tag{3.9}$$

everywhere on Σ. Integrating Eq. (3.9) over any region $C \in \mathscr{C}^1(\Sigma)$ and using the fact that $h^k n_k < 1$ everywhere on ∂C, where n^k is the outward unit normal to ∂C, we find that

$$\tilde{S}(C)>0. \tag{3.10}$$

That is, $\tilde{S}$ is a strictly positive function on $\mathscr{C}^1(\Sigma)$. Therefore, if there exists a region $\Omega \in \mathscr{C}^1(\Sigma)$ with $\tilde{S}(\Omega)\leqslant 0$, a global solution of Jang's equation cannot exist, and, thus, by Schoen and Yau's results, a (future or past) apparent horizon must be present within Σ.

In this argument, we see that the function $\tilde{S}$ on $\mathscr{C}^1(\Sigma)$ arises rather naturally. This suggests that we should attempt to strengthen the above result by showing that when there exists $\Omega \in \mathscr{C}^1(\Sigma)$ with $\tilde{S}(\Omega)\leqslant 0$ a future trapped region must exist within Ω (without the need for any asymptotic or stress-energy conditions). However, it turns out that we can do a little better using the function S on $\mathscr{C}^1(\Sigma)$, defined by

$$S(C)=A(C)-W_{\kappa}(C), \tag{3.11}$$

for each $C \in \mathscr{C}^1(\Sigma)$, rather than $\tilde{S}$. Since $\tilde{\kappa}\leqslant\kappa$, it follows that $S(C)\leqslant\tilde{S}(C)$, and, hence, if $\tilde{S}(\Omega)\leqslant 0$, then $S(\Omega)\leqslant 0$. So a future trapped region theorem using $\tilde{S}$ follows from such a theorem for S. (See theorem 3, below).

It is worth noting that for many initial data sets, S and $\tilde{S}$ will coincide. Using the facts that $K^a{}_a=k_1+k_2+k_3$ and $\kappa=k_1+k_2$, it follows that $\tilde{\kappa}<\kappa$ if and only if K_{ab} is negative definite ($K_{ab}x^a x^b<0$ for all non-zero x^a), and $\tilde{\kappa}=\kappa$ otherwise. Therefore, if K_{ab} is nowhere negative definite on Σ, i.e., nowhere is the surface positively expanding in all directions, then $S(C)=\tilde{S}(C)$ for all $C \in \mathscr{C}^1(\Sigma)$.

B. New argument

Our first notable property of S is that any region $\hat{C} \in \mathscr{C}^2(\Sigma)$ that is a stationary point of S is a future trapped region.

Theorem 2. If $\hat{C} \in \mathscr{C}^2(\Sigma)$ is a stationary point of S (in the sense that $S'(\hat{C})=0$ for all smooth variations of C), then $\hat{C}$ is a future trapped region.

Proof. Fix any region $C \in \mathscr{C}^2(\Sigma)$ and any open subset O of ∂C. Then, for all smooth vector fields ξ^a whose support intersects ∂C within O

$$S'(C)=\int_O (H-\kappa)(\xi^k n_k)\epsilon_{ab}\,. \tag{3.12}$$

Therefore, repeating the argument used in lemma 1 and using the fact that $\hat{C}$ is in the interior of Σ (as Σ has no boundary), we find that $H=\kappa$ on $\partial\hat{C}$. However, as $\kappa\leqslant K_{ab}h^{ab}$ on $\partial\hat{C}$, where h^{ab} is the metric induced on $\partial\hat{C}$, $H\leqslant K_{ab}h^{ab}$ on $\partial\hat{C}$. Therefore, $\hat{C}$ is a future trapped region. □

Note that if $\hat{C} \in \mathscr{C}^2(\Sigma)$ is a local minimum of S in the sense that there is an open set $N\subset\Sigma$ such that $S(\hat{C})\leqslant S(C)$ for all $C \in \mathscr{C}^2(\Sigma)$ with $C\subset N$, then $\hat{C}$ is a stationary point of S. Further, for momentarily static initial data sets ($K_{ab}=0$ on Σ), $\kappa=0$ on Σ, so S is simply the surface area of C. Therefore, in this case, the problem of finding stationary points of S is exactly the problem of finding surfaces whose area is stationary (in the sense of theorem 2), e.g., minimal two-surfaces.[17]

Since finding stationary points of S is a difficult task, it is desirable to have an alternate condition that guarantees the existence of a future trapped region. Mimicking the proof of theorem 1, we fix a region $\Omega \in \mathscr{C}^2(\Sigma)$ and then analyze the properties of a region that minimizes S on $\mathscr{C}^1(\Omega)$. If $S(\Omega)>0$, S may not have a minimum on $\mathscr{C}^1(\Omega)$. To see this, note that as there exist regions with arbitrarily small surface areas and volumes, $\inf_{\mathscr{C}^1(\Omega)}(S)\leqslant 0$. Yet, for an initial data set with $\kappa\leqslant 0$ (as is the case for a maximal hypersurface), there is no region $\hat{C} \in \mathscr{C}(\Omega)$ that attains the infimum (being zero) as any such region necessary has $S(\hat{C})\geqslant A(\hat{C})>0$. However, for any region

Ω with $S(\Omega)\leqslant 0$, we conjecture that S does have a minimum on $\mathscr{C}^1(\Omega)$. (In fact, we conjecture that the minimizing region $\hat{C}$ is a member of $\mathscr{C}^{2^-}(\Omega)$ and has further nice differentiable properties. See conjecture 2 in Sec. IV.) The idea behind this conjecture is that if $\inf_{\mathscr{C}^1(\Omega)}(S)<0$ (which is guaranteed to be the case if $S(\Omega)<0$), a sequence of regions C_i with $S(C_i)$ approaching this infimum cannot become degenerate in the sense that their volumes go to zero or their areas become infinite, while if $\inf_{\mathscr{C}^1(\Omega)}(S)=0$, then $S(\Omega)=0$, so Ω itself is a minimizing region. Note that $\inf_{\mathscr{C}^1(\Omega)}(S)$ must be finite as

$$\inf_{\mathscr{C}^1(\Omega)}(S)\geqslant -\max_{\Omega}(\kappa)V(\Omega); \tag{3.13}$$

a lower bound that holds even if κ is negative somewhere on Ω. This is to be compared to the difficulty in establishing a similar result for the surface-to-volume ratio function σ and lack of any finite lower bound on A/W_κ when κ is negative somewhere on Ω. Using these ideas, the following theorem shows that if S is not strictly positive on $\mathscr{C}^2(\Sigma)$, then Σ must contain a future trapped region.

Theorem 3. If $S(\Omega)\leqslant 0$ for some $\Omega \in \mathscr{C}^2(\Sigma)$, then there exists a future trapped region in Ω, provided conjecture 2 (stated in Sec. IV) holds for (Ω, g_{ab}).

Proof. By conjecture 2, there exists $\hat{C} \in \mathscr{C}^{2^-}(\Omega)$ that minimizes S on $\mathscr{C}^1(\Omega)$ and further $\partial\hat{C}$ is C^2 on $\partial\hat{C}\backslash\mathscr{Z}$, where $\mathscr{Z}$ is a closed set of measure zero. Therefore, for all one-parameter family of deformations constructed from an inward pointing vector field on Ω whose support intersects $\partial\hat{C}$ where the surface is C^2, we have $0\leqslant S'(\hat{C})$. Using Eq. (3.12), with $C=\hat{C}$ and repeating the argument used in lemma 1, we find that $H\leqslant\kappa$ on $\partial\hat{C}\backslash\mathscr{Z}$. However, as $\kappa\leqslant K_{ab}h^{ab}$ on all of $\partial\hat{C}$, where h^{ab} is the metric induced on $\partial\hat{C}$, $H\leqslant K_{ab}h^{ab}$ on $\partial\hat{C}\backslash\mathscr{Z}$. Therefore, $\hat{C}$ is a future trapped region. □

Note that if $\kappa\leqslant 0$ on Σ (as is the case for maximal hypersurfaces), then there is no region Ω meeting the condition of theorem 3 as $S(\Omega)\geqslant A(\Omega)>0$. Further, the condition of Eardley's theorem and theorem 1 that $\sigma(\Omega)\leqslant\min_\Omega(\kappa)$ implies that $A(\Omega)\leqslant\min_\Omega(\kappa)V(\Omega)\leqslant W_\kappa(\Omega)$ and, therefore, $S(\Omega)\leqslant 0$, which is the sole condition of theorem 3. Therefore, theorem 3 is stronger than theorem 1, which is stronger than Eardley's theorem.

It is interesting to note that $S(C)$ can be expressed as a pure surface integral by introducing any vector field ζ^a on Σ (or merely on Ω) having the property that $D_a\zeta^a=\kappa$, where D_a is the derivative operator associated with the metric g_{ab}. With this, we have

$$S(C)=\int_{\partial C}(1-\zeta^k n_k)\epsilon_{ab}\,. \tag{3.14}$$

For instance, a particularly simple choice of ζ^a is that given by taking $\zeta^a=D^a\phi$ for a scalar field ϕ. Then, ϕ must be a solution of Poisson's equation $D_aD^a\phi=\kappa$ and can be fixed uniquely by fixing boundary data for ϕ on $\partial\Omega$ (e.g., $\phi=0$ on $\partial\Omega$) or a boundary condition on ϕ at infinity (though whether this can always be accomplished is more subtle). We will not pursue this formulation any further here as nothing new seems to be gained from this viewpoint.

In theorems 1 and 3, we have restricted ourselves to regions Ω with C^2 boundary for the sake of simplicity, and we expect that both theorems hold under weaker conditions. It would seem that the weakest differentiability condition that should be imposed is that for which it makes sense for a region to speak of a region being future trapped.

IV. TWO GEOMETRICAL CONJECTURES

The relevance of theorems 1 and 3 rests heavily upon the following two conjectures, which we believe to be true.

Conjecture 1. Fix a pair (Ω, g_{ab}), where Ω is a compact three-dimensional manifold with C^2 boundary and g_{ab} is a smooth Riemannian metric on Ω. There exists $\hat{C} \in \mathscr{C}^{2-}(\Omega)$ such that $\sigma(\hat{C}) \leqslant \sigma(C)$ for all $C \in \mathscr{C}^1(\Omega)$.[In other words, σ has a minimum on $\mathscr{C}^1(\Omega)$ and a minimizing region is a member of $\mathscr{C}^{2-}(\Omega)$.] Further, $\partial\hat{C}$ is C^2 everywhere except on the closed set of measure zero given by $\partial\mathscr{W}$, where $\mathscr{W} = (\partial\Omega \cap \partial\hat{C})$ (and $\partial\mathscr{W}$ is constructed viewing $\mathscr{W}$ as a subset of either $\partial\Omega$ or $\partial\hat{C}$).

Conjecture 2. Fix a triple (Ω, g_{ab}, κ), where Ω is a compact three-dimensional manifold with C^2 boundary, g_{ab} is a smooth Riemannian metric on Ω, and κ is a smooth scalar field on Ω. If $S(\Omega) \leqslant 0$, then there exists $\hat{C} \in \mathscr{C}^{2-}(\Omega)$ such that $S(\hat{C}) \leqslant S(C)$ for all $C \in \mathscr{C}^1(\Omega)$.[In other words, S has a minimum on $\mathscr{C}^1(\Omega)$ and a minimizing region is a member of $\mathscr{C}^{2-}(\Omega)$.] Further, $\partial\hat{C}$ is C^2 everywhere except on the closed set of measure zero given by $\partial\mathscr{W}$, where $\mathscr{W} = (\partial\Omega \cap \partial\hat{C})$ (and $\partial\mathscr{W}$ is constructed viewing $\mathscr{W}$ as a subset of either $\partial\Omega$ or $\partial\hat{C}$).

Note that although $\partial\mathscr{W}$ is by its definition a closed subset of $\partial\hat{C}$, its being a set of measure zero does not appear to be guaranteed as there exist boundaries of positive measure.

In conjectures 1 and 2, we have asserted that the surface $\partial\hat{C}$ is a C^{2-} submanifold that is almost everywhere C^2. It is too much to expect that $\partial\hat{C}$ will be everywhere C^2 as we expect a discontinuity in its mean extrinsic curvature H where $\partial\hat{C}$ "first intersects" $\partial\Omega$, i.e., on $\partial\mathscr{W}$. To see this, suppose conjectures 1 and 2 are true. Then, write $\partial\hat{C}$ as the disjoint union of three sets as follows

$$\partial\hat{C} = (\partial\hat{C} \backslash \mathscr{W}) \cup (\mathscr{W} \backslash \partial\mathscr{W}) \cup (\partial\mathscr{W}). \tag{4.1}$$

As $\partial\hat{C} \backslash \mathscr{W}$ is in the interior of Ω, $H = \sigma(\hat{C})$ and $H = \kappa$ in conjectures 1 and 2, respectively. However, as $\partial\hat{C}$ coincides with $\partial\Omega$ on the open set $\mathscr{W} \backslash \partial\mathscr{W}$, H will equal the mean extrinsic curvature of $\partial\Omega$ on $\mathscr{W} \backslash \partial\mathscr{W}$. Therefore, in general, we expect that H will suffer a discontinuity on $\partial\mathscr{W}$. So, as H will not always be C^2, $\partial\hat{C}$ will not always be C^2. However, note that this argument suggests that the lack in continuity in the second-order partial derivatives defining the surface arise from mere jumps and not divergences. It is this property that suggests that the surface is C^{2-}.

While we shall not attempt to do so here, conjectures 1 and 2 can probably be proven using the ideas and techniques of geometric measure theory.[18] Very roughly, we consider a subset $\mathscr{V}(\Omega)$ of $\mathscr{C}^{1-}(\Omega)$ whose members are sufficiently well-behaved that they have finite volume and surface area (using the Hausdorff measure). One then argues that S is a continuous function (in some natural topology) on $\mathscr{V}(\Omega)$ and that the subset of $\mathscr{V}(\Omega)$ defined by those $C \in \mathscr{V}(\Omega)$ such that $S(C) \leqslant S(\Omega)$ is compact. It then follows immediately that there is a region $\hat{C} \in \mathscr{V}(\Omega)$ that achieves the minimal value of S on this set. The last step would be to establish that $\hat{C}$ is actually a member of $\mathscr{C}^{2-}(\Omega)$ and C^2 on $\partial\hat{C} \backslash \partial\mathscr{W}$ (and that $\partial\mathscr{W}$ is a set of measure zero). We leave the task of showing that these steps can actually be completed open for investigation.

V. FUTURE TRAPPED REGIONS ARE TRAPPED

Although there exists theorems showing that future trapped regions must lie within the black hole region of the spacetime, the arguments, as given, require that their surfaces be everywhere C^2.[4,5] Here, we show that the same result holds for regions with boundaries that are not quite this smooth, and so deserve to be called future trapped regions. To make our method of proof clear, we first cover the case where the surface of the region is everywhere C^2. After this, we modify the proof to accommodate our more general regions. We then discuss the possibility of further generalizations.

While our method of proof is similar to the existing proofs for smooth regions, there is a notable difference in the final derived contradiction. The Hawking and Ellis argument ends with the contradiction that the area of ∂C is no less than the area of $\partial J^+(C) \cap \mathscr{I}^+$, which, being at infinity, is infinite. The Wald argument ends with the contradiction that the future expansion of the

null generators of $\partial J^+(C)$ is non-positive on ∂C and yet positive near $\mathscr{I}^+$. Here, we end with the contradiction that there are null generators of $\partial J^+(C)$ extending beyond $\mathscr{I}^+$ that possess a point conjugate to ∂C on $\mathscr{I}^+$.

Actually, it should be noted that the Wald argument contains a slight error in that the local cross-sections of $\mathscr{I}^+$ constructed need not have the requisite differentiability properties in order that nearby cross-sections of $\partial J^+(C)$ have strictly positive future expansion. A simple counterexample is provided by a smooth closed region C in a flat spatial hypersurface Σ in Minkowski spacetime with the property that all of C lies to one side of a flat plane $\mathscr{P}$ in Σ except for a closed region $\partial C \cap \mathscr{P}$ having a non-empty interior (as a subset of $\mathscr{P}$). Then, it is not difficult to see that the null generators of $\partial J^+(C)$ having past endpoint on $\partial C \cap \mathscr{P}$ intersect $\mathscr{I}^+$ and have zero expansion everywhere. Of course, the Wald argument can easily be fixed by introducing an area type argument, or by adopting the method of theorem 4, which can be viewed as such a fix as it has much of its inspiration from the Wald argument.

Our notion of asymptotic flatness is that given in Ref. 4. We denote the manifolds of the "physical" and "unphysical" spacetime by M and M', respectively. We remind the reader that $M = M' \backslash (J^+(i^0) \cup J^-(i^0))$, where i^0 is the point representing spatial infinity. Therefore, $\partial M = (i^0 \cup \mathscr{I}^+ \cup \mathscr{I}^-)$, where $\mathscr{I}^\pm = (\partial J^\pm(i^0)) \backslash i^0$ are future and past null infinity.

Furthermore, the theorems we prove are for strongly asymptotically predictable spacetimes,[4] which are simply those asymptotically flat spacetimes for which there exists an open globally hyperbolic subset V of M' containing $\overline{J^-(\mathscr{I}^+) \cap M}$ (where the closure is as a subset of M'). Note that $\partial M \subset V$. It can be shown that all globally hyperbolic asymptotically flat spacetimes are strongly asymptotically predictable. Further, the globally hyperbolic asymptotic region V can be chosen so that it contains all of M and an asymptotically flat Cauchy surface Σ for M together with spatial infinity i^0 is a Cauchy surface for V. Therefore, the requirement that a subset C of Σ be closed and bounded away from infinity (so there exists a neighborhood of i^0 disjoint from C) is equivalent to the condition that C be closed as a subset of $\Sigma' = (\Sigma \cup i^0)$.

A. Regions whose surfaces are C^2

Theorem 4. Fix a smooth strongly asymptotically predictable spacetime[4] satisfying the null-convergence condition.[3] Let Σ' be a smooth asymptotically flat Cauchy surface for V and let $C \subset (\Sigma' \cap M)$ be a future trapped region in the sense that C is a closed subset of Σ', ∂C is C^2, and the convergence of the outward future-directed null normals to ∂C is everywhere non-negative. Then, $(C \cap J^-(\mathscr{I}^+)) = \emptyset$. [That is, $C \subset (\Sigma' \cap B)$, where B is the black-hole region of the spacetime.]

Proof. In the following, all of our constructions are carried out solely within the asymptotic globally hyperbolic region V. Therefore, statements regarding the openness or closedness of sets refer to these properties in V alone. Since C does not contain i^0 (as C is a subset of M), $J^+(C)$ does not contain i^0. Further, $J^+(C)$ is closed, since C is a closed subset of Σ'. (See exercise 8 from chapter 8 of Ref. 4.) Therefore, there is a neighborhood of i^0 disjoint from $J^+(C)$.

Suppose, for contradiction, that $(C \cap J^-(\mathscr{I}^+)) \neq \emptyset$. Then, $(J^+(C) \cap \mathscr{I}^+) \neq \emptyset$, and, hence, $(J^+(C) \cap I^+(i^0)) \neq \emptyset$. It then follows that $(\partial J^+(C) \cap I^+(i^0)) \neq \emptyset$. To see this, fix any point $p \in (J^+(C) \cap I^+(i^0))$. Then, as there exists a timelike curve γ from i^0 to p [which must lie entirely within $I^+(i^0)$] and there exists an open neighborhood of i^0 disjoint from the closed set $J^+(C)$, the curve γ must leave $J^+(C)$ and therefore intersect $\partial J^+(C)$, showing that $(\partial J^+(C) \cap I^+(i^0)) \neq \emptyset$.

Recall that if p is any point on a null generator of $\partial J^+(C)$ whose past endpoint on ∂C has an open neighborhood on which ∂C is C^2, there must not be a point conjugate to ∂C between ∂C and p.[4,5] Pick a point $p \in (\partial J^+(C) \cap I^+(i^0))$ and a null generator ν of $\partial J^+(C)$ containing p. Then ν cannot possess a point conjugate to ∂C in M (with respect to either the physical or unphysical metric) nor on $\mathscr{I}^+$ (with respect to the unphysical metric). However, in the physical portion of the

spacetime M, it follows from the null Raychaudhuri equation and the null-convergence condition that the (physical) future convergence of the null generators of $\partial J^+(C)$ is not only non-negative on ∂C, it is non-negative everywhere to the future.[4,5] Furthermore, if such a generator has positive convergence $\rho_0>0$ at some point, then it must possess a conjugate point within an affine parameter time $2/\rho_0$ thereafter, provided the generator can be extended this far. Therefore, as ν is future complete in the physical metric in M (as it intersects $\mathscr{I}^+$), the (physical) convergence along ν must be zero in M. Therefore, in the infinitesimal sense, the physical area of a bundle of outgoing future-directed null rays orthogonal to ∂C is constant along ν (in M). In terms of the unphysical metric, this area is that given by the physical area multiplied by the square of the conformal factor. As this conformal factor is zero on $\mathscr{I}^+$, it follows that ν possesses a point conjugate to ∂C where it intersects $\mathscr{I}^+$ (with respect to the unphysical metric), which is a contradiction. □

B. Regions whose surfaces are not quite C^2

The problem with the proof of theorem 4 when ∂C is not everywhere C^2 is that it may happen that because of our choice of p in the last paragraph, ν may have its past endpoint at a place on ∂C where the surface is not C^2, thus making the final conjugate point argument inapplicable. When ∂C is everywhere C^{2-} and C^2 on $\partial C\backslash\mathscr{Z}$, where $\mathscr{Z}$ is a closed set of measure zero, although we do not have complete freedom in what choice to make for p, it turns out we can always find one so that the past endpoint of its associated null generator has a neighborhood within ∂C on which the surface is C^2, i.e., its past endpoint is somewhere on $\partial C\backslash\mathscr{Z}$. The idea is that it is impossible for only the generators of $\partial J^+(C)$ with past endpoint on $\mathscr{Z}$ to make it beyond $\mathscr{I}^+$ as there are not "enough of them" to make up a "local piece" of $\partial J^+(C)$, as $\mathscr{Z}$ is a set of measure zero in ∂C.

We capture this idea using the notion of Hausdorff measure.[18] On a differentiable manifold N with Riemannian metric, for any two points a and b in N, define $d(a,b)$ to be the greatest lower bound on the lengths of C^1 curves in N connecting a to b [so (N,d) is a metric space]. For any subset $S\subset N$, set $\mathrm{diam}(S)=\sup_{a,b\in S}(d(a,b))$. Then, for any subset $A\subset N$ and numbers k and $\delta>0$, set

$$\mathscr{H}^k_\delta(A)=\inf\sum_j \nu_k\left(\frac{\mathrm{diam}(S_j)}{2}\right)^k, \tag{5.1}$$

where ν_k is the volume of a unit-ball in flat $\mathbb{R}^k$ when k is a non-negative integer (so $\nu_0=1$, $\nu_1=2$, $\nu_2=\pi$, $\nu_3=4\pi/3$, etc.) and an arbitrary positive constant otherwise, and where the infimum is taken over all countable coverings $\{S_j\}$ of A (i.e., $A\subset\cup_j S_j$) with $\mathrm{diam}(S_j)\leqslant\delta$. With this, the $\mathscr{H}^k$-measure of a set A is defined as

$$\mathscr{H}^k(A)=\lim_{\delta\to 0}\mathscr{H}^k_\delta(A). \tag{5.2}$$

This limit is well defined (although possibly infinite) as $\mathscr{H}^k_\delta(A)$ is non-decreasing in δ. It is worth noting that if $\mathscr{H}^k(A)<\infty$ then $\mathscr{H}^m(A)=0$ for all $m>k$. It can be shown that if A is a k-dimensional C^1 embedded submanifold of N with $k\leqslant\dim(N)$, then $\mathscr{H}^k(A)$ corresponds to the usual "volume" of this submanifold. For instance, in the case $\dim(N)=3$, $\mathscr{H}^1(A)$ is the length of a one-dimensional submanifold A, $\mathscr{H}^2(A)$ is the area of a two-dimensional submanifold A, and $\mathscr{H}^3(A)$ is the volume of a three-dimensional submanifold A.

With this, we say a subset A of a differentiable manifold N has $\mathscr{H}^k$-measure zero if $\mathscr{H}^k(A)=0$. It can be shown that this notion is independent of which Riemannian metric is chosen, and, therefore, whether a subset of a (paracompact) manifold has $\mathscr{H}^k$-measure zero is dependent solely upon the set. In the case where $k=\dim(N)$, $\mathscr{H}^k$-measure zero is identical to the usual

Lebesgue notion of measure zero on a differential manifold. Furthermore, if f is a locally Lipschitz map from the manifold N to another differentiable manifold, it follows that if $\mathscr{H}^k(A)=0$, then $\mathscr{H}^k(f[A])=0$.

Using these concepts, we can now prove that our generalized future trapped regions are indeed trapped.

Theorem 5. Fix a smooth strongly asymptotically predictable spacetime[4] satisfying the null-convergence condition.[3] Let Σ' be a smooth asymptotically flat Cauchy surface for V and let $C\subset(\Sigma'\cap M)$ be a future trapped region in the sense that C is a closed subset of Σ', ∂C is everywhere C^{2-} and, on $\partial C\backslash\mathscr{Z}$, ∂C is C^2 and the convergence of the outward future-directed null normals to ∂C is non-negative, where $\mathscr{Z}$ is a closed set of measure zero. Then, $(C\cap J^-(\mathscr{I}^+))=\emptyset$.[That is, $C\subset(\Sigma'\cap B)$, where B is the black-hole region of the spacetime.]

Proof. Suppose, for contradiction, that $(C\cap J^-(\mathscr{I}^+))\neq\emptyset$. Then, using the same argument as in theorem 4, it again follows that $(\partial J^+(C)\cap I^+(i^0))\neq\emptyset$. We claim that there exists $p\in(\partial J^+(C)\cap I^+(i^0))$ with an associated null generator ν having past endpoint on $\partial C\backslash\mathscr{Z}$, an open subset of ∂C where the surface is C^2. We show this by arguing that there are not enough generators with past endpoint on $\mathscr{Z}$ to make up $\partial J^+(C)$ in $I^+(i^0)$ as follows.

First, the subset $\tilde{\mathscr{Z}}$ of $\partial J^+(C)$ consisting of those points with null generators having past endpoint on $\mathscr{Z}$ has $\mathscr{H}^3$-measure zero. To see this, denote by $\mathscr{K}$ the subset of TV (the tangent bundle associated with V) consisting of all pairs (p,k^a) where $p\in\partial C$ and k^a is an outward future-directed null vector normal to ∂C at p. Using the fact that ∂C is C^{2-}, it follows that there exists a locally Lipschitz map from $\partial C\times\mathbb{R}$ onto $\mathscr{K}\subset TV$. Next, since $\partial J^+(C)\backslash C$ is generated by null geodesics with past endpoint on ∂C and future-directed outgoing tangent vector normal to ∂C, we see that $\partial J^+(C)\backslash C$ is a subset of the projection of $\exp(\mathscr{K})$ onto V (where exp is the smooth diffeomorphism from TV to TV defined by the geodesic flow on TV). As both exp and the projection map are smooth, it follows that $\partial J^+(C)\backslash C$ is a subset of the image of a subset of $\partial C\times\mathbb{R}$ under a locally Lipschitz map. Therefore, since $\mathscr{Z}\times\mathbb{R}$ has $\mathscr{H}^3$-measure zero as a subset of $\partial C\times\mathbb{R}$ (which follows from the fact that $\mathscr{Z}$ has $\mathscr{H}^2$-measure zero as a subset of ∂C) and since $\tilde{\mathscr{Z}}$ is a subset of the image of a subset of $\mathscr{Z}\times\mathbb{R}$ under a locally Lipschitz map, it follows that $\tilde{\mathscr{Z}}$ has $\mathscr{H}^3$-measure zero in V. (Note that it is in the establishment of this result that we use the fact ∂C is C^{2-} and not merely C^1.)

Next, pick any point $q\in(\partial J^+(C)\cap I^+(i^0))$ and an open neighborhood O of q with $O\subset I^+(i^0)$. Using the fact that $\partial J^+(C)$ is an achronal C^{1-} embedded three-dimensional submanifold of V (see proposition 6.3.1 of Ref. 5), it follows that $\partial J^+(C)\cap O$ has positive $\mathscr{H}^3$-measure. (To see this, note that we can choose O so that it is diffeomorphic to an open subset of $\mathbb{R}^4$ with $\partial J^+(C)\cap O$ corresponding to the graph of a C^{1-} function of three variables.) Therefore, as the subset of $\partial J^+(C)$ consisting of generators with past endpoint on $\mathscr{Z}$ has $\mathscr{H}^3$-measure zero, it follows that there must exist a point $p\in\partial J^+(C)\cap O$ with an associated null generator ν that has past endpoint on $\partial C\backslash\mathscr{Z}$. (In fact, there are many such points.)

Arguing as we did in theorem 4 shows that ν contains a point conjugate to ∂C (with respect to the unphysical metric) where ν intersects $\mathscr{I}^+$ (being between ∂C and p), which is a contradiction. □

C. Possible generalizations

In extending the notion of a future trapped region, we have restricted ourselves to regions C with C^{2-} surfaces that are further C^2 everywhere except on a closed set of measure zero. We have done this because this is both what we expect of the surfaces constructed (conjectures 1 and 2) and these are regions for which we can carry through all the relevant arguments (theorems 3 and 5). However, a much greater extension seems possible. For instance, it is plausible that the notion of a future trapped region can be extended to regions with surfaces that are merely C^{2-}. Such a surface is twice differentiable everywhere except on a set of measure zero $\mathscr{Z}$. If the convergence of a family of future-directed outgoing null geodesics orthogonal to a surface can be defined on

$\partial C \backslash \mathscr{Z}$ and the conjugate point argument used in theorem 5 can be applied to the generators with past endpoint on $\partial C \backslash \mathscr{Z}$, the notion of a future trapped region with a C^{2-} surface would be a well-defined concept.

However, it would seem that the best notion of a region being future trapped would not involve any differentiability conditions. For example, consider the analogous problem of what we mean by a closed region C in flat space having a surface S that is everywhere locally convex. Here, we have a precise notion that imposes no differentiability conditions on the surface: For each point $p \in S$ there is a neighborhood N in S such that $(1-\lambda)x+\lambda y \in C$ for all $x,y \in N$ and $\lambda \in [0,1]$. (That is, the convex hull of N is a subset of C.) Likewise, we say the surface of a region C is locally concave if it is locally convex when viewed as the surface of the closure of the complement of C. Note that this flat space notion has a natural generalization to curved spaces: We call the surface S of a closed region C locally convex if for each point $p \in S$ there is a neighborhood N in S and a convex normal neighborhood U containing N such that for all points $x,y \in N$ the geodesic from x to y (within U, being unique) lies within C. In the C^2 case, the above implies the the extrinsic curvature H_{ab} of S is positive semi-definite.

We want a geometric condition that, in the C^2 case, leads to the bound $H=H^a{}_a \leqslant K_{ab}h^{ab}$. Surely, such a notion would be based on a demand that the areas of all local cross sections of $\partial J^+(C)$ are non-increasing to the future (at least sufficiently near ∂C). The problem is to capture this idea in a well-defined sense. For instance, one needs for $\partial J^+(C)$ to be sufficiently well-behaved so that the surface areas of suitable cross-sections are well-defined. This is probably not such a problem as $\partial J^+(C)$ is an embedded C^{1-} submanifold for any set C. Then, to show that such regions are indeed trapped, an area-type argument similar to that used by Hawking and Ellis would probably be the most natural method to use. However, how is one to show that the areas of cross-sections are non-increasing to the future when the null Raychaudhuri equation cannot be implemented? Clearly, some subtlety is needed here.

Note that a naive condition such as ∂C being everywhere C^{1-} and, on $\partial C \backslash \mathscr{Z}$, ∂C is C^2 and the convergence of the outward future-directed null normals to ∂C is non-negative, where $\mathscr{Z}$ is a closed set of measure zero, is insufficient. A simple counterexample is provided by taking C to be a solid cube in a flat spatial hypersurface in Minkowski spacetime. Here, ∂C is everywhere C^{1-} and, except along the edges and vertices (a closed set $\mathscr{Z}$ of measure zero), the surface is C^∞ and the convergence of the outward future-directed null normals to ∂C is zero. However, C is clearly "visible" from $\mathscr{I}^+$, i.e., it is not trapped. In the proof of theorem 5, the problem with such surfaces is that one does not have a one-to-one correspondence between the null generators of $\partial J^+(C)$ and ∂C, and, as a result, the portion of $\partial J^+(C)$ consisting of the generators having past endpoint on $\mathscr{Z}$ has positive $\mathscr{H}^3$-measure. For example, at a vertex, an entire "octant's worth" of null generators of $\partial J^+(C)$ intersect ∂C at a single point. In this case, all null generators of $\partial J^+(C)$ that do make it beyond $\mathscr{I}^+$ have past endpoints on $\mathscr{Z}$.

Lastly, one might expect that a differentiability condition that would be sufficient to establish that a region C is future trapped is that ∂C is everywhere C^1 and C^2 on an open dense subset D of ∂C (with the convergence of the outward future-directed null normals being non-negative on D). In fact, this was the approach first taken herein, but was abandoned because of a difficulty. The idea is that if a null generator ν associated with a point $p \in (J^+(C) \cap I^+(i^0))$ has its past endpoint on D, the argument proceeds as in theorem 4, while if not, then it would seem that we could find a point arbitrarily near p in $(J^+(C) \cap I^+(i^0))$ with an associated generator having past endpoint on D. (After all, D is dense in ∂C.) While this may be true, proving it appears to be difficult. For instance, although one might expect that there would exist a neighborhood of $\nu \cap \partial C$ (within ∂C) such that all null generators with past endpoint thereon remain on $\partial J^+(C)$ long enough to enter $I^+(i^0)$, it turns out that this need not be the case if we just use the fact that ∂C is C^1. Whether this does hold when the additional conditions on ∂C are used is not clear.

VI. DISCUSSION

Theorems 1 and 3 provide us with simple tests for the existence of future trapped regions within an initial data set, but how effective are they?

First, the conditions of theorems 1 and 3 are quite strong in the following sense. Recall that theorem 1 requires that $\min_{\Omega}(\kappa) \geqslant \sigma(\Omega)$ (as does Eardley's theorem). Using the fact that κ is the sum of the two lesser principal (extrinsic) curvatures (k_1, k_2, k_3), it is not difficult to show that $K^a{}_a = k_1 + k_2 + k_3 \geqslant \frac{3}{2}\kappa \geqslant \frac{3}{2}\sigma(\Omega) > 0$ everywhere on Ω, showing that this region is everywhere contracting "on average." However, if $K^a{}_a$ is non-negative, κ need not be positive. This shows that the region Ω is more than contracting "on average." Indeed, on a maximal hypersurface ($K^a{}_a = 0$ everywhere on Σ), $\kappa \leqslant 0$ (with equality only where $K_{ab} = 0$) everywhere on Σ. In this respect, the condition of theorem 1 (and Eardley's theorem) is quite strong. While theorem 3 merely requires that $S(\Omega) \leqslant 0$, so κ need not be positive on all of Ω, κ still must be positive over a sufficiently large subset of Ω in order to meet this condition.

Second, while both theorems give sufficient conditions for the existence of future trapped regions, neither condition is necessary. This is easily seen by constructing a momentarily static initial data set (so $K_{ab} = 0$, and hence $\kappa = 0$, on Σ) that contains a minimal two-surface bounding a compact region C. This region C is future (and past) trapped and yet, as $S(C) = A(C)$ is positive, the condition of neither theorem 1 nor 3 is met.

Third, neither theorem is very sensitive to the "local" existence of a future trapped region in the following sense. Suppose we have a future trapped surface S such that both families of future-directed orthogonal null congruences have strictly positive convergence on S. Construct a three-dimensional region Ω by "thickening" S a small distance r within an initial data surface containing S. Then, for r sufficiently small, Ω is a future trapped region. However, for sufficiently small r, $\sigma(\Omega)$ will be larger than $\inf_{\Omega}(\kappa)$ and $S(\Omega)$ will be positive, and hence neither theorem enables us to deduce that Ω itself is a future trapped region.

Fourth, the conditions of theorems 1 and 3 are quite robust in the sense that if we have a region Ω that satisfies the condition of either theorem with strict inequality and then deform it to create a new region Ω' by "pushing" very thin fingers of the surface of Ω into Ω (in arbitrarily complex ways), then, provided our fingers are sufficiently thin, the surface area, volume, and the integral of κ for Ω' will be sufficiently near those of Ω so that the conditions of both theorems will be met for Ω'. More generally, if we construct Ω' by excising sufficiently thin regions from Ω, both theorems guarantee the existence of a future trapped region within Ω'. This is perhaps somewhat surprising at first given that Ω' can be topologically quite complex. However, noting that the mean curvature of the portions of the surface of Ω' created by excising "very thin fingers" is very large and negative, we realize that $\hat{C}$ less the thin regions is nearly a future trapped region—all that is needed is a bit of adjusting near the edges where the excised region intersects $\hat{C}$.

Fifth, and last, theorems 1 and 3 do have a slight advantage in numerical search for the existence of future trapped regions as the calculation of $\sigma(\Omega)$ or $S(\Omega)$ requires only the calculation of a surface area and a volume integral, which are not as sensitive to numerical inaccuracies that would arise in calculating the mean extrinsic curvature H of a two-surface in Σ to test whether the surface is future outer trapped [i.e., testing whether the condition given by Eq. (1.1) holds on the boundary].

So, while theorems 1 and 3 do offer tests for the existence of future trapped regions, their inability to detect the existence of future trapped regions in some instances, e.g., in initial data sets associated with maximal hypersurfaces and "thin" future trapped regions, leads us to wonder whether stronger tests of the type considered here can be devised to give sufficient conditions for the existence of future trapped regions.

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[1] Here, Σ is an orientable three-manifold (without boundary), representing the Universe at a given time; g_{ab} is a Riemannian metric on Σ, giving the intrinsic geometry of Σ as induced by the spacetime metric; and K_{ab} is a symmetric tensor, giving the extrinsic curvature of Σ in the spacetime.

[2] P. Anninos *et al.*, Event Horizons of Numerical Black Holes, article gr-qc/9412056 on gr-qc@xxx.lanl.gov archive (to appear in the proceedings of the Seventh Marcel Grossmann Meeting on General Relativity, edited by R. Ruffini and M. Keiser, World Scientific, 1995).

[3] A spacetime with Ricci tensor R_{ab} is said to satisfy the null-convergence condition if $R_{ab}k^a k^b \geqslant 0$ for all null k^a.

[4] R. M. Wald, *General Relativity* (University of Chicago, Chicago, 1984).

[5] S. W. Hawking and G. F. R. Ellis, *The Large-Scale Structure of Space-time* (Cambridge University, Cambridge, England, 1973).

[6] Actually, this is a slight abuse in terminology in that H is the trace of extrinsic curvature of the two-surface in the three-manifold and not one-half this value. (The latter quantity is the mean value of the two principal curvatures.)

[7] This assumes that the future apparent horizon $\mathscr{H}$ has the structure of a sufficiently smooth manifold. See, e.g., Proposition 12.2.5 of Ref. 4

[8] K. Thorne, in *Magic without Magic: John Archibald Wheeler*, edited by J. R. Klauder (W. H. Freeman, San Francisco, 1972). It should be remembered that the imprecision in Thorne's hoop conjecture is intentional; making it precise is part of the problem. [What is meant by M? What is meant by a hoop encircling the body? Is the horizon a black-hole event horizon or a (future) apparent horizon?]

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[15] We call a tensor $h^a{}_b$, acting on a vector space V with metric g_{ab}, a rank 2 orthogonal projection map if h_{ab} is symmetric, $h^a{}_b = h^a{}_c h^c{}_b$, and $h^a{}_a = 2$, where indices are raised and lowered with g_{ab}. The trace condition on $h^a{}_b$ ensures that $h^a{}_b$ maps V onto a two-dimensional vector subspace of itself, i.e., its rank is two. It is not difficult to show that with $\dim(V) = 3$, there exists a unique (up to sign) unit vector n^a such that $h^{ab} = g^{ab} - n^a n^b$. Further, any such unit vector n^a defines a unique rank 2 orthogonal projection map in this way. While perhaps more complicated than it could be otherwise, this statement of the theorem follows the spirit of its proof.

[16] Y. Choquet-Bruhat, C. DeWitt-Morette, and M. Dillard-Bleick, *Analysis, Manifolds and Physics, Part I: Basics* (North Holland, New York, 1989).

[17] R. Osserman, *A Survey of Minimal Surfaces* (Dover, New York, 1986).

[18] H. Federer, *Geometric Measure Theory* (Springer-Verlag, New York, 1969). See also F. Morgan, *Geometric Measure Theory: A Beginner's Guide* (Academic, San Diego, 1988) and F. J. Almgren, Jr., *Plateau's Problem: An Invitation to Varifold Geometry* (Benjamin, New York, 1966).

Radiation-dominated quantum Friedmann models

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Radiation-filled Friedmann–Robertson–Walker universes are quantized according to the Arnowitt–Deser–Misner formalism in the conformal-time gauge. Unlike previous treatments of this problem, here both closed and open models are studied, only square-integrable wave functions are allowed, and the boundary conditions to ensure self-adjointness of the Hamiltonian operator are consistent with the space of admissible wave functions. It turns out that the tunneling boundary condition on the universal wave function is in conflict with self-adjointness of the Hamiltonian. The evolution of wave packets obeying different boundary conditions is studied, and it is generally proven that all models are nonsingular. Given an initial condition on the probability density under which the classical regime prevails, it is found that a closed universe is certain to have an infinite radius, a density parameter $\Omega=1$ becoming a prediction of the theory. Quantum stationary geometries are shown to exist for the closed universe model, but oscillating coherent states are forbidden by the boundary conditions that enforce self-adjointness of the Hamiltonian operator. © *1996 American Institute of Physics.* [S0022-2488(96)02503-5]

I. INTRODUCTION

The lack of a consistent quantum theory of the full gravitational field and its sources has stimulated the development of quantum cosmology, a less complete but more tractable method to investigate the influence of quantum effects on the evolution of the universe. The primordial universe, when presumably curvatures and densities approach the Planck scale, is believed to be the privileged scenario in which the quantum aspects of gravity are expected to become important or even dominant. In its broadest sense, quantum cosmology consists in ''freezing out'' all but a finite number of degrees of freedom of the gravitational field plus its sources (through imposition of symmetry requirements) and then quantizing the remaining ones. This procedure, initiated by DeWitt,[1] is expected to provide some general insights on what an acceptable quantum theory of gravity should be like, although it cannot be strictly valid and is open to criticism.[2] Such a line of attack has been extensively explored to quantize Friedmann–Robertson–Walker (FRW) universes with varying matter content, such as a scalar field,[3–6] radiation,[7–9] a spinor field,[10] dust,[9,11–14] or a Rarita–Schwinger field.[15]

The present paper is dedicated to a further study of the quantum theory of a radiation-filled FRW universe. Differently from previous investigations of this system,[7–9] here we discuss both closed and open models, deal only with normalizable wave functions, and pay full attention to the domain of self-adjointness of the Hamiltonian operator. We follow the Arnowitt–Deser–Misner (ADM) genuine canonical quantization method.[16] In this approach one has to solve the constraint equations at the classical level and go over to a reduced phase space spanned by independent canonical variables alone, and this process demands a definite choice of time. Although often leading to complicated and time-dependent Hamiltonians, this formalism has the great advantage

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of reducing the problem to one of standard quantum mechanics, enabling one to make full use of the powerful theory of linear operators in Hilbert space. In our treatment the time variable is chosen as conformal time, as this enormously simplifies the form of the Hamiltonian operator, making the quantum dynamics exactly soluble. Further reasons for choosing conformal time are given in Ref. 8.

After the ADM reduction of phase space, only one degree of freedom remains, which is taken to be the scale factor R. Since R is restricted to positive values, it becomes necessary to impose boundary conditions on the wave functions belonging to the domain of the Hamiltonian operator to ensure its self-adjointness. For the simplest of such boundary conditions, the time evolution of wave packets of the Gaussian type is worked out, and it is shown in full generality for the first time that both the closed and open models are nonsingular. It is remarked that in the context of the ADM quantization the so-called tunneling boundary condition on the universal wave function is in conflict with self-adjointness of the Hamiltonian operator, or, equivalently, with unitarity of the quantum evolution. This is not an artifact of the particular quantization scheme adopted here, since the ADM and Wheeler–DeWitt descriptions are equivalent for the model at hand.[7] An initial condition such that the probability density is sharply concentrated at $R=0$ and under which the classical regime sets in is considered. In the closed case, under such an extreme initial condition the probability of finding any finite radius for the universe vanishes. Therefore a density parameter $\Omega=1$ becomes a prediction of the model, without neither sacrificing the requirement of square integrability on the wave functions nor imposing boundary conditions inconsistent with the space of admissible state vectors. A physically questionable aspect of the initial condition adopted is pointed out, however. Stationary quantum geometries are shown to exist for the closed model, but the existence of oscillating coherent states of the geometry is precluded by the boundary conditions required to enforce self-adjointness of the Hamiltonian operator, a result at variance with previous findings.[9]

The layout of this paper is as follows. In Sec. II the classical model is specified and the ADM reduction of phase space[7] is briefly reviewed. In Sec. III the problem of the necessary boundary conditions to ensure self-adjointness of the Hamiltonian operator is considered, and the respective propagators are written down when the two simplest of such boundary conditions are adopted. In Sec. IV the motion of wave packets obeying different boundary conditions is obtained in closed form, and it is verified that the singularity is avoided in all cases. A special initial condition under which the quantum model is forced into the classical regime is discussed, and the consequences for the case of a closed universe are considered. Stationary quantum geometries are taken up in Sec. V, with particular emphasis on how the restricted domain of self-adjointness of the Hamiltonian operator influences such states. Section VI is devoted to some final comments.

II. DYNAMICS OF THE CLASSICAL MODEL

The line element for a homogeneous and isotropic universe can be written in the FRW form (we take $c=1$)

$$ds^2=g_{\nu\lambda}\,dx^{\nu}\,dx^{\lambda}=-N(t)^2\,dt^2+R(t)^2\sigma_{ij}dx^i\,dx^j, \tag{2.1}$$

where σ_{ij} denotes the metric for a 3-space of constant curvature $k=+1$, 0, or -1, corresponding to spherical, flat, or hyperbolic space-like sections, respectively.

The matter content will be taken to be a perfect fluid, and Schutz's canonical formulation of the dynamics of a relativistic fluid in interaction with the gravitational field will be employed.[17] The degrees of freedom ascribed to the fluid are five scalar potentials $\varphi,\alpha,\beta,\theta,S$ in terms of which the four-velocity of the fluid is written as

$$U_{\nu}=\frac{1}{\mu}\,(\varphi_{,\nu}+\alpha\beta_{,\nu}+\theta S_{,\nu}), \tag{2.2}$$

where μ is the specific enthalpy. By means of the normalization condition

$$g_{\nu\lambda}U^{\nu}U^{\lambda}=-1, \tag{2.3}$$

one can express μ in terms of the velocity potentials. The action for the gravitational field plus the perfect fluid is

$$S=\int_M d^4x\sqrt{-g}^{(4)}R+2\int_{\partial M}d^3x\sqrt{h}h_{ij}K^{ij}+\int_M d^4x\sqrt{-g}p, \tag{2.4}$$

in units such that $c=16\pi G=1$. In Eq. (2.4), p is the pressure of the fluid, ${}^{(4)}R$ is the scalar curvature derived from the space–time metric $g_{\nu\lambda}$, h_{ij} is the 3-metric on the boundary ∂M of the 4-manifold M, and K^{ij} is the second fundamental form of the boundary.[18] The surface term is necessary in the path-integral formulation of quantum gravity in order to rid the Einstein–Hilbert Lagrangian of second-order derivatives. Variations of the pressure are computed from the first law of thermodynamics.

Compatibility with the homogeneous space–time metric is guaranteed by taking all of the velocity potentials of the fluid as functions of t only. We shall take $p=(\gamma-1)\rho$ as an equation of state for the fluid, where γ is a constant and ρ is the fluid's energy density (we shall eventually put $\gamma=\frac{4}{3}$). In the geometry characterized by (2.1), the appropriate boundary condition for the action principle is to fix the initial and final hypersurfaces of constant time. The second fundamental form of the boundary becomes $K_{ij}=-\dot{h}_{ij}/2N$. As described in its full details in Ref. 7, after inserting the metric (2.1) into the action (2.4), using the equation of state, computing the canonical momenta and employing the constraint equations to eliminate the pair (θ,p_θ), what remains is a reduced action in the Hamiltonian form

$$S_r=\int dt\{\dot{R}p_R+\dot{\varphi}p_\varphi+\dot{S}p_S-N\mathscr{H}\}, \tag{2.5}$$

where an overall factor of the spatial integral of $(\det\sigma)^{1/2}$ has been discarded, since it has no effect on the equations of motion. The super-Hamiltonian $\mathscr{H}$ is given by

$$\mathscr{H}=-\left(\frac{p_R^2}{24R}+6kR\right)+p_\varphi^{\gamma}R^{-3(\gamma-1)}e^{S}. \tag{2.6}$$

The lapse N plays the role of a Lagrange multiplier, and upon its variation it is found that the super-Hamiltonian $\mathscr{H}$ vanishes. This is a constraint, revealing that the phase space contains redundant canonical variables.

According to the ADM presciption, in order to perform a bonafide canonical quantization, one must go over to a reduced phase space spanned by independent canonical variables alone. This can be achieved by first making a choice of time and then solving the super-Hamiltonian constraint equation $\mathscr{H}=0$ for the canonical variable conjugate to the time chosen in the first step. This ensures that the final action preserves its canonical form, and the Hamiltonian in the reduced phase space is identical to the canonical variable whose Poisson bracket is unity with whatever was chosen as time, but now expressed as a function of the remaining independent canonical variables.[16] In the conformal-time gauge $N=R$ (that is, henceforward t denotes conformal time), and for $\gamma=\frac{4}{3}$ (radiation) this procedure leads to the very simple reduced action[7]

$$S_r=\int dt\left\{\dot{R}p_R-\left(\frac{p_R^2}{24}+6kR^2\right)\right\}. \tag{2.7}$$

Only one degree of freedom is left, namely the scale factor R, and the Hamiltonian in the reduced phase space is

$$H=\frac{p_R^2}{24}+6kR^2. \tag{2.8}$$

Hamilton's equations of motion lead immediately to

$$\ddot{R}+kR=0. \tag{2.9}$$

The solution for $R(t)$ can be written as

$$R(t)=R_0\begin{cases}\sin t, & \text{if } k=+1,\\ t, & \text{if } k=0,\\ \sinh t, & \text{if } k=-1,\end{cases} \tag{2.10}$$

with a suitable choice for the origin of conformal time t. The standard cosmic time τ is related to conformal time by

$$d\tau=R\ dt; \tag{2.11}$$

hence

$$\tau=R_0\begin{cases}1-\cos t, & \text{if } k=1,\\ t^2/2, & \text{if } k=0,\\ \cosh t-1, & \text{if } k=-1,\end{cases} \tag{2.12}$$

with the convention that $\tau=0$ when $t=0$. In the spatially flat case ($k=0$), for instance, one recovers the usual behavior $R=C\tau^{1/2}$ for the scale factor.[19] It is seen that Hamilton's principle based on the reduced action (2.7) gives rise to the same equations of motion as those obtained by first varying the full action (2.4) and then simplifying them through the use of the space–time symmetries of homogeneity and isotropy and of the equation of state $p=\rho/3$. Such a consistency check is indispensable if quantization in minisuperspace is to have any meaning at all.

III. QUANTIZATION, SELF-ADJOINTNESS, AND BOUNDARY CONDITIONS

The remarkably simple form of the Hamiltonian (2.8) makes it possible to find exact results for the cosmic evolution at the quantum level. The quantum dynamics is not so straightforward as one might think at first sight because the scale factor R is restricted to the domain $R>0$, so that the minisuperspace quantization in the R representation deals only with wave functions defined on the half-line $(0,\infty)$. It is well known that in such circumstances one usually has to impose boundary conditions on the allowed wave functions, otherwise the relevant operators will not be self-adjoint, the most important of all operators being the Hamiltonian, which must be self-adjoint in order that the time evolution be unitary. The need to impose boundary conditions to ensure self-adjointness has been long recognized by practitioners of the ADM formalism as applied to quantum cosmology.[3,11] Very recently, it has also been seen to have nontrivial cosmological implications in the Wheeler–DeWitt approach.[20] What does not appear to have been duly emphasized is that self-adjointness conditions depend on the set of allowed state vectors. It has been argued by adherents of the many-worlds interpretation[8] and of the pilot-wave formulation[21] of quantum theory that non-normalizable wave functions are unavoidable in quantum cosmology. Irrespective of whether their arguments are physically well founded or not, what we want to stress here is that the self-adjointness conditions must be consistent with the point of view adopted, if the results obtained are to be regarded as trustworthy.

As follows from the substitution $p_R \to -id/dR$, the Hamiltonian operator associated with the classical Hamiltonian function (2.8) is (we take $\hbar=1$)

$$\hat{H}=-\frac{1}{24}\frac{d^2}{dR^2}+6kR^2, \tag{3.1}$$

defined on the half-line $(0,\infty)$. The condition for $\hat{H}$ to be symmetric (which, in turn, is a necessary condition for $\hat{H}$ to be self-adjoint) is

$$(\psi_1,\hat{H}\psi_2)=(\hat{H}\psi_1,\psi_2) \tag{3.2}$$

or

$$\int_0^\infty \psi_1^*(R)\,\frac{d^2\psi_2}{dR^2}\,dR=\int_0^\infty \frac{d^2\psi_1^*}{dR^2}\,\psi_2(R)dR, \tag{3.3}$$

where the asterisk stands for the complex conjugate. Integrating by parts twice, this leads to

$$\left(\psi_1^*\,\frac{d\psi_2}{dR}-\frac{d\psi_1^*}{dR}\,\psi_2\right)(\infty)=\left(\psi_1^*\,\frac{d\psi_2}{dR}-\frac{d\psi_1^*}{dR}\,\psi_2\right)(0). \tag{3.4}$$

If both ψ and its derivative are square integrable, the left-hand side of (3.4) vanishes, and we are left with

$$\left(\psi_1^*\,\frac{d\psi_2}{dR}-\frac{d\psi_1^*}{dR}\,\psi_2\right)(0)=0. \tag{3.5}$$

Then it can be shown[22] that to ensure the validity of this condition it is necessary and sufficient that the domain of $\hat{H}$ be restricted to those wave functions such that

$$\psi'(0)=\alpha\psi(0), \tag{3.6}$$

with $\alpha\in(-\infty,\infty]$. This generic boundary condition was explicitly taken into account in Ref. 11 and implicitly used in the simplest cases $\alpha=0$ and $\alpha=\infty$ in Ref. 7, in which only square-integrable wave functions were considered acceptable.

If the potential is unbounded from below, the Hamiltonian may possess eigenstates $\psi\in L^2(0,\infty)$ such that ψ' is not square integrable. In this case, or if non-normalizable wave functions are allowed, the correct condition for symmetry of the Hamiltonian is Eq. (3.4), and as such it has been recently employed in Ref. 20. However, in Ref. 8 non-square-integrable wave functions were argued to be necessary in quantum cosmology, but, inconsistently with this point of view, Eq. (3.6) was imposed on the allowed wave functions to allegedly enforce self-adjointness of the Hamiltonian operator. As a consequence of demanding that the initial wave function when $t=0$ be perfectly localized at the singularity $R=0$, Tipler[8] was led to a universal wave function of the form

$$\psi(R,t)=\left[\frac{3i}{4L_{\rm P}\sin t}\right]^{1/2}\exp\left[\left(\frac{3\pi}{4i}\right)(\cot t)\left(\frac{R}{L_{\rm P}}\right)^2\right]\equiv A(t)\exp[iB(t)R^2], \tag{3.7}$$

where $L_{\rm P}$ denotes the Planck length, and that satisfies the boundary condition (3.6) for $\alpha=0$. Since this wave function is not square integrable, it should obey Eq. (3.4), that is,

$$\lim_{R\to\infty}[4iA^*BR]=0, \tag{3.8}$$

which is not satisfied because both $A(t)$ and $B(t)$ are different from zero. Therefore, a wave function of the form (3.7) cannot represent a possible state of the universe. This means that Tipler's initial condition on the wave function of the universe, together with his imposition of boundary condition (3.6) with $\alpha=0$, are in conflict with the requirement that $\hat{H}$ be a self-adjoint operator, and this renders the conclusions of Ref. 8 invalid.

In the present work we shall deal only with square integrable wave functions, so that the set of admissible states in the R representation is the Hilbert space $L^2(0,\infty)$. Therefore, the domain of self-adjointness of the Hamiltonian operator is restricted to those wave functions that obey (3.6). For the sake of simplicity, here we shall address ourselves only to the cases $\alpha=0$ and $\alpha=\infty$, that is, the boundary conditions we shall be concerned with are

$$\psi'(0,t)=0 \tag{3.9a}$$

or

$$\psi(0,t)=0. \tag{3.9b}$$

Both of these conditions refer to what happens to a wave packet when it hits the singularity $R=0$. The boundary condition (3.9b) was advocated by DeWitt to keep wave packets away from the singularity, but, in general, it is not powerful enough to prevent wave functions from becoming concentrated in the neighborhood of $R=0$.[23] As a matter of fact, it has been argued[11] that DeWitt's boundary condition is just not relevant to the issue of quantum gravitational collapse.

The time development of the models is fully determined once one is in possession of the propagator or the Green's function. Let $G(x,y,t)$ be the propagator for the problem in the usual Hilbert space $L^2(-\infty,\infty)$. Then the propagator for the problem in the restricted Hilbert space $L^2(0,\infty)$ is

$$G^{(a)}(R,R',t)=G(R,R',t)+G(R,-R',t), \tag{3.10}$$

if the boundary condition is (3.9a), or

$$G^{(b)}(R,R',t)=G(R,R',t)-G(R,-R',t), \tag{3.11}$$

if the boundary condition is (3.9b), as noted by several authors.[24,8,25]

The general Green's function for the Hamiltonian (3.1) on the usual Hilbert space $L^2(-\infty,\infty)$ is

$$G(x,y,t)=\left[\frac{6\sqrt{k}}{\pi i\,\sin(\sqrt{k}t)}\right]^{1/2}\exp\left\{\frac{6i\sqrt{k}}{\sin(\sqrt{k}t)}\left[(x^2+y^2)\cos(\sqrt{k}t)-2xy\right]\right\}, \tag{3.12}$$

as one immediately obtains from the expression of the propagator for the harmonic oscillator[26] by setting $m=12$ and $\omega=\sqrt{k}$. In the limiting case $k=0$ the well-known free-particle propagator is regained, whereas for $k=-1$ all one has to do is make use of the simple formulas $\cos(it)=\cosh t$ and $\sin(it)=i\sinh t$. The latter case corresponds to the quantum mechanics of a particle in an inverted oscillator potential, studied extensively in Ref. 27.

In the quantum cosmology à la Hartle–Hawking–Vilenkin–Linde, an essential role is played by initial or boundary conditions. One of these is the so-called tunneling boundary condition,[28,29] according to which the wave function of the universe must consist only of outgoing modes at singular boundaries of superspace. In our present context this amounts mathematically to

$$J=\frac{i}{2}\left(\psi^*\frac{\partial\psi}{\partial R}-\psi\frac{\partial\psi^*}{\partial R}\right)_{R=0}>0, \tag{3.13}$$

where J is the probability current density. However, from (3.6) it follows immediately that $J=0$ because α is a real number. One is forced to conclude that, at least for this minisuperspace model, the tunneling boundary condition cannot be implemented because it is irreconcilable with self-adjointness of the Hamiltonian operator or, equivalently, unitarity of the time evolution. Furthermore, since the ADM and Wheeler–DeWitt descriptions are equivalent for the present model,[7] this difficulty is not an artifact of the particular quantization scheme adopted here.

IV. EVOLUTION OF THE QUANTUM MODELS

We shall now dedicate some paragraphs to the description of the main features of the dynamical evolution of our quantum cosmological models. This will be done by first following the time development of wave packets and then by studying the effect of imposing a very special initial condition.

A. Motion of wave packets

Let us start by working out the dynamical evolution of representative initial wave packets. The first initial state to be considered is the one described at $t=0$ by the normalized wave function

$$\psi_0^{(a)}(R)=\left(\frac{8\sigma}{\pi}\right)^{1/4}e^{-\beta R^2}, \tag{4.1}$$

where $\beta=\sigma+ip$ with p real and $\sigma>0$, corresponding to the boundary condition (3.9a).

The initial wave function (4.1) is an even function of R, so that

$$\begin{aligned}\psi^{(a)}(R,t)&=\int_0^\infty G^{(a)}(R,R',t)\psi_0^{(a)}(R')dR'\\&=\int_0^\infty G(R,R',t)\psi_0^{(a)}(R')dR'+\int_0^\infty G(R,-R',t)\psi_0^{(a)}(R')dR'\\&=\int_{-\infty}^\infty G(R,R',t)\psi_0^{(a)}(R')dR'.\end{aligned} \tag{4.2}$$

Inserting the propagator (3.12) and the initial wave function (4.1) into (4.2) and performing the Gaussian integration, one finds

$$\begin{aligned}\psi^{(a)}(R,t)=&\left(\frac{8\sigma}{\pi}\right)^{1/4}\left\{\frac{6\sqrt{k}}{\cos(\sqrt{k}t)[\beta\tan(\sqrt{k}t)-6i\sqrt{k}]}\right\}^{1/2}\\&\times\exp\left\{\frac{6i\sqrt{k}}{\tan(\sqrt{k}t)}\left(1+\frac{6i\sqrt{k}}{\cos^2(\sqrt{k}t)[\beta\tan(\sqrt{k}t)-6i\sqrt{k}]}\right)R^2\right\}.\end{aligned} \tag{4.3}$$

An important quantity is the expectation value of the scale factor

$$\langle\hat{R}\rangle_t^{(a)}=\int_0^\infty R|\psi^{(a)}(R,t)|^2\,dR, \tag{4.4}$$

which can be readily computed from the wave function (4.3). We find

$$\langle\hat{R}\rangle_t^{(a)}=\frac{1}{12}\sqrt{\frac{2}{\pi\sigma}}\begin{cases}\sqrt{\sigma^2\sin^2 t+(6-p\tan t)^2\cos^2 t}, & \text{if } k=+1,\\ \sqrt{\sigma^2t^2+(6-pt)^2}, & \text{if } k=0,\\ \sqrt{\sigma^2\sinh^2 t+(6-p\tanh t)^2\cosh^2 t}, & \text{if } k=-1.\end{cases}\tag{4.5}$$

Notice that, in all cases, $\langle\hat{R}\rangle_t^a$ never vanishes. For $k=0$ or $k=-1$ and $p>0$, the expectation value of the scale factor initially decreases, reaches a minimum value, and then grows steadily without limit, whereas if $p<0$ there is a continuous expansion without bound. As expected, for large t the highest expansion rate belongs to the hyperbolic model ($k=-1$). For $k=1$ the universe oscillates between a minimum and a maximum radius. An interesting interpretation of this behavior in terms of reflection of parts of the wave packet as they hit the origin $R=0$ can be found in Ref. 11.

It should be stressed that the previous results establish that, at the quantum level, the singularity is avoided in all cases (that is, $k=0,\pm1$), according to the following reasonable criterion:[11,30] the quantum system is singular at a certain instant if $\langle\psi|\hat{f}|\psi\rangle=0$ for any quantum observable $\hat{f}$ whose classical counterpart f vanishes at the classical singularity, ψ being any state of the system at the instant under consideration. For FRW models the relevant quantum observable is $\hat{f}=\hat{R}$, since $R=0$ defines the classical singularity. This criterion is in consonance with the usage in quantum cosmology. Indeed, since $\hat{R}$ is a positive operator on $L^2(0,\infty)$, if $\langle\hat{R}\rangle_t=0$ then $\psi(t)$ is sharply peaked at $R=0$, and a strong peak in the wave function at a certain classical configuration is regarded in quantum cosmology as a prediction of the occurrence of such a configuration.[29]

We now turn our attention to the boundary condition (3.9b). As an initial wave function let us choose

$$\psi_0^{(b)}(R)=\left(\frac{128\sigma^3}{\pi}\right)^{1/4}Re^{-\beta R^2}.\tag{4.6}$$

Taking advantage of the odd character of this wave function, we can write

$$\psi^{(b)}(R,t)=\int_0^\infty G^{(b)}(R,R',t)\psi_0^{(b)}(R')dR'=\int_{-\infty}^\infty G(R,R',t)\psi_0^{(b)}(R')dR'.\tag{4.7}$$

Insertion of (4.6) and (3.12) into (4.7) yields

$$\psi^{(b)}(R,t)=\left(\frac{128\sigma^3}{\pi}\right)^{1/4}\left[\frac{216ik^{3/2}}{\sin^3(\sqrt{k}t)}\right]^{1/2}\left[\beta-\frac{6i\sqrt{k}}{\tan(\sqrt{k}t)}\right]^{-3/2}R$$
$$\times\exp\left\{\frac{6i\sqrt{k}}{\tan(\sqrt{k}t)}\left(1+\frac{6i\sqrt{k}}{\cos^2(\sqrt{k}t)[\beta\tan(\sqrt{k}t)-6i\sqrt{k}]}\right)R^2\right\}.\tag{4.8}$$

The expectation value of the scale factor is found to be

$$\langle\hat{R}\rangle_t^{(b)}=2\langle\hat{R}\rangle_t^{(a)},\tag{4.9}$$

so that there is no singularity for boundary condition (3.9b) either.

As a matter of fact, we have shown only that the states evolving from (4.1) or (4.6) are such that $\langle\hat{R}\rangle_t$ never vanishes. Incomplete analyses like ours of the quantum gravitational collapse problem have been made before.[7,9] This is insufficient, however, because in order to establish that the quantum cosmological models are nonsingular one has to prove that $\langle\hat{R}\rangle_t\neq0$ for *any* evolving state $\psi(t)$ for which $\langle\hat{R}\rangle_t$ is defined. A somewhat indirect proof of this will be given below.

Classically, the presence of the singularity at $t=0$ makes it physically mandatory to restrict the conformal time t to positive values. The absence of singularity at the quantum level makes such a

restriction unnecessary, so that $-\infty<t<\infty$ and the quantum cosmological models are not naturally endowed with an origin of time. This kind of situation is also encountered in dust-filled FRW models in the cosmic-time gauge.[11]

B. Special initial condition

Having a quantum dynamical framework to describe the evolution of the universe is not enough to explain its present state, one has to face the problem of initial conditions, the gist of modern quantum cosmology. In the path-integral approach to quantum cosmology, both the Hartle–Hawking and the Vilenkin–Linde proposals appear to suffer from vagueness and lack of generality, and can hardly be said to lead unambiguously to a unique universal wave function.[29] In the present minisuperspace model the Vilenkin–Linde tunneling boundary condition is not even implementable, as we have seen in Sec. III.

With this in mind, we proceed tentatively to examine the outcome of imposing initial conditions on the probability density associated with the universal wave function. We content ourselves with discussing the extreme situation $\sigma\to\infty$, in which case $|\psi_0|^2$ becomes sharply concentrated around $R=0$:

$$\lim_{\sigma\to\infty}|\psi_0^{(a)}(R)|^2=\delta(R). \tag{4.10}$$

Under such circumstances the universe starts with certainty from the singularity $R=0$, so that (4.10) may be regarded as the condition for a quantum explosive birth of the universe, or what might be called a quantum big bang. For σ sufficiently large Eq. (4.5) reduces to

$$\langle\hat{R}\rangle_t\approx\frac{1}{12}\sqrt{\frac{2\sigma}{\pi}}\begin{cases}\sin t, & \text{if } k=+1,\\ t, & \text{if } k=0,\\ \sinh t, & \text{if } k=-1,\end{cases} \tag{4.11}$$

so that the classical regime sets in—compare the above equation with (2.10).

Now for the promised proof that $\langle\hat{R}\rangle_t\neq0$ for any evolving state $\psi(t)$, implying that our quantum cosmological models are nonsingular. If $\langle\hat{R}\rangle_{t_1}=0$ for some t_1, then $|\psi(R,t_1)|^2=\delta(R)$. Suppose that $\psi(R,t)$ with $t>t_1$ is a state evolved from $\psi(R,t_1)$ taken as an initial condition. By letting $\sigma\to\infty$, it follows from (4.11) that $\langle\hat{R}\rangle_t=\infty$. Therefore, no state with a finite expectation value of the scale factor can arise from $\psi(R,t_1)$. Since quantum mechanics is time reversible, no state $\psi(R,t_0)$ with $t_0<t_1$ and finite $\langle\hat{R}\rangle_{t_0}$ can evolve to $\psi(R,t_1)$, which proves that $\langle\hat{R}\rangle_t\neq0$ for all evolving states $\psi(t)$ for which the expectation value of the scale factor is finite.

Let us focus our attention particularly on the closed model ($k=+1$), the only one for which the following considerations are meaningful. In our present treatment, which deals only with normalized wave functions, the probability $P(R<R_1;t)$ that at time t the radius of the universe is smaller than a given radius R_1 is given by

$$\begin{aligned}P(R<R_1;t)^{(a)}&=\int_0^{R_1}|\psi^{(a)}(R,t)|^2\,dR\\ &=\left(\frac{8\sigma}{\pi}\right)^{1/2}\left[\frac{36}{\cos^2 t[\sigma^2\tan^2 t+(6-p\tan t)^2]}\right]^{1/2}\\ &\quad\times\int_0^{R_1}\exp\left\{-\frac{72\sigma R^2}{\cos^2 t[\sigma^2\tan^2 t+(6-p\tan t)^2]}\right\}dR.\end{aligned} \tag{4.12}$$

With the change of variable,

$$x=\frac{\sqrt{72\sigma}}{\cos t[\sigma^2 \tan^2 t+(6-p \tan t)^2]^{1/2}} R, \tag{4.13}$$

one gets

$$P(R<R_1;t)^{(a)}=\frac{2}{\sqrt{\pi}} \int_0^{R_*} e^{-x^2} dx, \tag{4.14}$$

where

$$R_*=\frac{\sqrt{72\sigma}}{\cos t[\sigma^2 \tan^2 t+(6-p \tan t)^2]^{1/2}} R_1. \tag{4.15}$$

Notice that $R_* \to 0$ as $\sigma \to \infty$, hence $P(R<R_1;t)=0$ for an explosive quantum beginning of the universe. This leads to the prediction that the density parameter Ω equals unity in the limit of a truly explosive birth of the universe. Such a prediction was called ''inflation without inflation'' by Tipler,[8] but here it is derived without having to resort to non-normalizable wave functions.

If the initial wave function is chosen as (4.6), corresponding to the boundary condition (3.9b), Eq. (4.9) shows that if σ is sufficiently large the classical regime takes over. For the closed model one readily finds

$$P(R<R_1;t)^{(b)}=\frac{4}{\sqrt{\pi}} \int_0^{R_*} x^2 e^{-x^2} dx. \tag{4.16}$$

Again, in the limit $\sigma \to \infty$ the probability that at time t the radius of the universe is smaller than a given radius R_1 is zero. Note that as $\sigma \to \infty$ the wave packet (4.6) also satisfies (4.10), thus providing a concrete illustration of the fact that an initial wave function whose associated probability density is concentrated entirely at $R=0$ can be harmonized with the boundary condition (3.9b). Besides, the prediction $\Omega=1$ does not appear to be sensitive to boundary conditions of the type (3.6) on the wave function itself, but to result exclusively from the condition (4.10) that its modulus squared be sharply concentrated at $R=0$ when $t=0$. An initial condition on the wave function itself that gives rise to $\Omega=1$ is known,[8] but then one has to give up the square integrability requirement, and the resulting universal wave function does not belong to the domain of self-adjointness of the Hamiltonian operator, as remarked in Sec. III.

Unfortunately, this state of affairs is still physically dubious. The inevitable singularity makes the restriction $t \geqslant 0$ *dynamically* obligatory in classical cosmology. On the other hand, it is only the *imposition* of the initial condition $|\psi_0(R)|^2=\delta(R)$ that makes the instant $t=0$ so especially distinguished as to induce the restriction $t \geqslant 0$ upon the quantized model too. This is so because no unitary evolution from an earlier time could have led to such a perfectly localized state at $t=0$. This questionable feature is also present in Tipler's treatment,[8] in which use is made of non-normalizable wave functions. Although inconclusive, our tentative considerations were intended to suggest that it may be physically reasonable to impose initial conditions on some probability distribution engendered by the wave function rather than on the universal wave function itself.

V. QUANTUM STATIONARY GEOMETRIES

In the case of the closed FRW model, the Hamiltonian operator (3.1) possesses square-integrable eigenfunctions. Consider the normalized wave functions

$$\psi_n(R)=\left(\frac{\sqrt{48}}{\sqrt{\pi}2^n n!}\right)^{1/2} H_n(\sqrt{12}R)\exp(-6R^2), \tag{5.1}$$

where H_n denotes the nth Hermite polynomial. They satisfy

$$\hat{H}\psi_n = (n + \tfrac{1}{2})\psi_n , \tag{5.2}$$

where n is a non-negative integer. For even n the wave functions (5.1) satisfy both Eq. (5.2) and the boundary condition (3.9a), whereas for odd n they obey both Eq. (5.2) and the boundary condition (3.9b). The effect of the boundary conditions is to exclude either even or odd eigenfunctions. This does not agree with Ref. 9, where no boundary conditions are imposed on the wave functions belonging to the domain of $\hat{H}$, with the result that all values for n are allowed. For a universe in any of the stationary states (5.1), nothing changes with time. This is a purely quantum effect since radiation-filled FRW universes do not possess classical static solutions.

A more significant effect of imposing self-adjointness boundary conditions is the preclusion of oscillating coherent states, that is, nondispersive Gaussian wave packets whose center oscillates just like a solution to the classical equations of motion. From the general form of such wave functions,[31] one recognizes at once that the general boundary condition (3.6) cannot be satisfied, even if the real parameter α is allowed to be time dependent. It is clear, therefore, that a coherent state such that the classical solution (2.10) emerges as the expectation value of the scale factor does not exist, in contradiction with the findings in Ref. 9.

VI. CONCLUDING REMARKS

In this paper we dealt with square-integrable wave functions only, that is, we limited ourselves to the orthodox framework of quantum mechanics in Hilbert space. Interpretational controversies apart, it is in this arena that the requirement of self-adjointness on the quantum observables is most naturally justified and easily understood. Accordingly, being careful about domains of operators becomes a necessity in quantum cosmology, and in the case of radiation-filled FRW universes the simplest boundary conditions required to enforce self-adjointness of $\hat{H}$ were taken into account. Initial or boundary conditions introduced with the purpose of selecting a unique wave function are customarily unrelated to the former, although on occasion this has been the object of confusion in the literature. Sometimes, however, these two types of boundary conditions interfere with each other, as we pointed out in Sec. III.

An important distinction should be emphasized between the classical and quantum cosmologies discussed in this paper. An origin of time comes into being *dynamically* in classical gravity due to the inevitable singularity, while no origin of time occurs naturally in quantum gravity, except if *induced* by a choice of initial conditions. On the other hand, admitting the hypothesis that a suitable initial condition exists, it is open to doubt whether it should be imposed on the wave function itself or on some probability distribution derived thereof.

Our treatment differs from the one based upon consideration of conformal fluctuations about a given geometry. Apart from lack of application of boundary conditions to ensure self-adjointness, there is a physically more important difference. In Ref. 9 fluctuations are discussed about a *specific* FRW classical solution of Einstein's equations, whereas the ADM approach considers fluctuations that encompass all possible universes of the FRW kind. Although these standpoints may be classically undistinguishable, they are not necessarily equivalent in the quantum realm. This raises the question of what the relation between these approaches is and which, if any, is appropriate from the physical point of view, a study we reserve for the future.

We have circumscribed our analysis to radiation as the cause of curvature, that is, to a matter content consisting of a perfect fluid with polytropic index $\gamma = \frac{4}{3}$. It can be shown[32] that in the conformal-time gauge the form of the classical equation of motion of all Friedmann models with any γ fluid as a source can be reduced to that of a harmonic oscillator after a suitable change of variables. This suggests the possibility of extending the previous quantum treatment to cosmological models whose matter content is a perfect fluid with an arbitrary polytropic index. This is presently under investigation.

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Uniqueness of zero surface gravity SU(2) Einstein–Yang/Mills black holes

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In this paper we prove that the only spherically symmetric black hole solution to the SU(2) Einstein–Yang/Mills equations that has zero temperature at the event horizon is the extreme Reissner–Nordström solution. No assumptions are made on the signs of the metric coefficients, save that the metric has Lorentz signature. © *1996 American Institute of Physics.* [S0022-2488(96)02803-2]

I. INTRODUCTION

Black holes having a degenerate horizon, that is, vanishing surface gravity, $\kappa=0$, are called extremal. In view of Hawking's celebrated formula (see Ref. 1),

$$\kappa=2\pi\tau,$$

where τ is the temperature at the horizon, this implies that such black holes have zero horizon temperature, and thus do not radiate; (however, see Refs. 2 and 3). The quantum mechanical stability of extremal black holes makes them very interesting objects, in various contexts. First, they are natural candidates for the final states of the evaporation process. Second, the scattering of quantum fields off extremal black holes can be described entirely within the semiclassical approximation, and this allows one to analyze the information loss in black hole evaporation without confronting the problem of unknown Plank-scale physics.[4] Finally, it was suggested in Ref. 5 that extreme black holes resemble, in a certain sense, elementary particles—in fact, it was recently shown in Ref. 6 that extremal black holes can be identified with elementary string excitations.

In Ref. 7 it was shown that the only black-hole solution of the static, spherically symmetric, coupled Einstein–Yang/Mills (EYM) equations [with SU(2) gauge group], which has zero surface gravity, is the extreme Reissner–Nordström (ERN) solution. More precisely, if the Einstein metric is written in the form

$$ds^2=-A(r)B(r)^{-2}\,dt^2+A^{-1}(r)dr^2+r^2(d\theta^2+\sin^2\theta\,d\phi^2), \tag{1.1}$$

and the SU(2) Yang/Mills field is (cf. Refs. 7–10)

$$F=w'(r)\tau_1\,dr\wedge r\,d\theta+w'(r)\tau_2 dr\wedge(\sin\theta\,d\phi)-(1-w^2(r))\tau_3\,d\theta\wedge(\sin\theta\,d\phi), \tag{1.2}$$

where τ_1,τ_2,τ_3 form a basis for the Lie algebra su(2), then if

$$\lim_{r\searrow\bar{r}}A(r)=0=\lim_{r\searrow\bar{r}}A'(r),\quad A(r)\geqslant 0,\quad \text{for } r>\bar{r}, \tag{1.3}$$

the metric must be the ERN metric; namely $A(r)=[(r-1)/r]^2$, $B(r)\equiv 1$, $w(r)\equiv 0$, and the Yang–Mills curvature 2-form takes values in the Lie algebra u(1). It was also proved in Ref. 7 that for the metric (1.1), the surface gravity $\kappa=0$ if and only if A' vanishes at the black hole horizon $\bar{r}$.

In this paper we shall strengthen the above result, so as to also apply to the interior of a black hole. Namely, we will prove that if (A,w) is a smooth solution of the EYM equations, defined for $r>\bar{r}$, such that A is positive for some large r, and if

$$\lim_{r\searrow\bar{r}} A(r)=0=\lim_{r\searrow\bar{r}} A'(r), \tag{1.4}$$

then again the metric (1.1) is the ERN metric, $w(r)\equiv 0$, and the Yang/Mills curvature 2-form lies in u(1); cf. Theorem 3.1 The proof of this result is *much* more difficult than the proof in Ref. 7, because $A(r)$ is not assumed to be positive for $r>\bar{r}$.

Finally, we remark that it was proved in Ref. 10; (also see Ref. 11), that if $A(\bar{r})=0$ and $A'(\bar{r})\neq 0$, then the singularity in the metric at $r=\bar{r}$ can be transformed away by a "Kruskal-like" change of coordinates in which the YM field remains well behaved. Moreover, it was proved in Ref. 12 that for the ERN solution, the metric singularity at $r=\bar{r}$ can also be transformed away. It thus follows from our result here that for *any* SU(2) spherically symmetric EYM black hole solution with event horizon at $r=\bar{r}>0$, the singularity in the metric at $r=\bar{r}$ can be transformed away by a change of coordinates, whereby the YM field remains well behaved.

II. PRELIMINARIES

As discussed elsewhere, (cf. Refs. 8 and 9), the static, spherically symmetric EYM equations, with gauge group SU(2) can be written in the form

$$rA'+(1+2w'^2)A=1-\frac{u^2}{r^2}, \tag{2.1}$$

$$r^2Aw''+\left[r(1-A)-\frac{u^2}{r}\right]w'+w(1-w^2)=0, \tag{2.2}$$

$$\frac{B'}{B}=\frac{2w'^2}{r}, \tag{2.3}$$

where

$$u(r)=1-w^2(r). \tag{2.4}$$

Since (2.1) and (2.2) do not involve B, we can use these to obtain A and w, and then use (2.3) to find B. Here $w(r)$ is the connection coefficient that determines the Yang–Mills curvature 2-form; see Refs. 8 and 9. If we write

$$\Phi(A,w,r)=r(1-A)-\frac{u^2}{r}, \tag{2.5}$$

then (2.1) and (2.2) can be written in the more compact form

$$rA'+2w'^2A=\Phi/r, \tag{2.6}$$

$$r^2Aw''+\Phi w'+w(1-w^2)=0. \tag{2.7}$$

If $(A(r),w(r))$ is a specific solution of (2.1),(2.2), then we write $\Phi(r)=\Phi(A(r),w(r),r)$.

III. THE THEOREM

In this section we shall prove the following theorem.

Theorem 1: Let $(A(r),w(r))$ be a smooth solution of (2.1) and (2.2), satisfying

$$\lim_{r\searrow\bar{r}} A(r)=0=\lim_{r\searrow\bar{r}} A'(r), \tag{3.1}$$

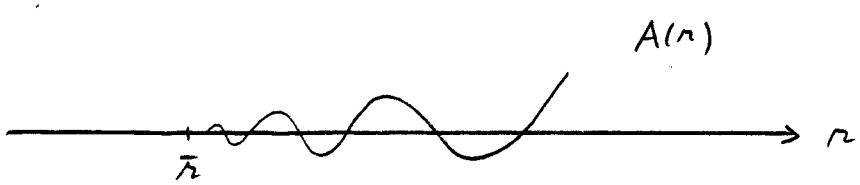

FIG. 1. A oscillates.

for some $\bar{r}\geqslant 0$, and assume $A(r_1)>0$ for some $r_1>\max(\bar{r},1)$. Then (A,w) is the extreme Reissner–Nordström (ERN) solution; namely,

$$A(r)=\left(\frac{r-1}{r}\right)^2, \quad w(r)\equiv 0. \tag{3.2}$$

Remarks:

(1) If (3.2) holds, then from (2.3) we have $B(r)\equiv 1$.

(2) Theorem 1 was proved in Ref. 7 under the additional hypothesis that $A(r)\geqslant 0$ for $r>\bar{r}$. We show here that the theorem is still true under the far weaker hypothesis $A(r_1)>0$ for some $r_1>\max(1,\bar{r})$.

Proof of Theorem 1: There are three cases to consider; namely, for $\bar{r}\geqslant 0$, the following occurs.

Case (i). There is a sequence $r_n\searrow\bar{r}$ such that

$$(-1)^n A(r_n)>0. \tag{3.3}$$

In this case we say that *A oscillates*; cf. Fig. 1.

Case (ii). $A(r)<0$ for $r>\bar{r}$, r near $\bar{r}$; cf. Fig. 2.

Case (iii). $A(r)>0$ for $r>\bar{r}$, r near $\bar{r}$.

As mentioned above, a proof of the Theorem in case (iii) was given in Ref. 7, under the additional hypothesis that $A(r)\geqslant 0$ for $r>\bar{r}$.

We shall prove that neither of the cases (i) or (ii) can occur, and that if case (iii) occurs, the solution is the ERN solution. The proof is further divided into two subcases; namely either the solution (A,w) is "smooth up to the boundary;" i.e., $(A,w)\in(C^1\times C^2)[\bar{r},\bar{r}+\epsilon)$ for some $\epsilon>0$, or (A,w) is not smooth at $\bar{r}$. The following proposition is subsumed by Theorem 1. The simple proof is given here in order to demonstrate that the difficulties occur when neither A nor w is assumed to be smooth at $\bar{r}$.

Proposition 2: Suppose that $(A,w)\in(C^1\times C^2)[\bar{r},\bar{r}+\epsilon)$ for some $\epsilon>0$. If (3.1) holds, then $\bar{r}=1$, and the solution is the ERN solution (3.2).

Before giving the proof, we shall need a preliminary result.

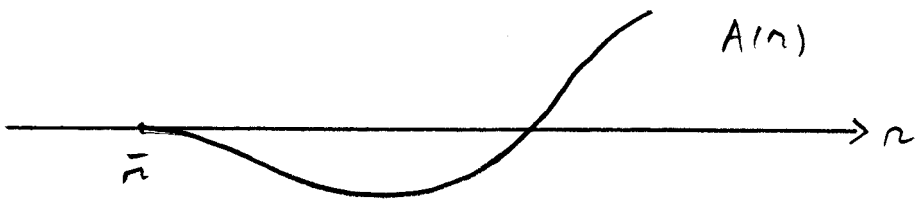

FIG. 2. $A<0$ near $\bar{r}$.

Lemma 3: If (A,w) is a solution of the EYM equations defined in an open interval about r_0, and if we have $w^2(r_0)\leqslant 1$, $A'(r_0)=0$ and $A(r_0)<0$, then $r_0<1$.

Proof: If $r_0\geqslant 1$, then from (2.1) we obtain the contradiction

$$0>(1+2w'^2(r_0))A(r_0)=1-\frac{u^2(r_0)}{r_0^2}\geqslant 0.$$

■

Proof of Proposition 2: If $\bar{r}=0$, then (as in Ref. 10) expanding A and w in Taylor polynomials gives

$$A(r)=A_0+A_1r+O(r^2),$$

$$w(r)=w_0+w_1r+O(r^2),$$

and we easily obtain from (2.1) and (2.2) that $A_0=1$. Thus, $A(0)=1$ and this violates (3.1). If $\bar{r}>0$, then from (2.6) we see $\Phi(\bar{r})=0$ so (2.5) gives $\bar{r}^2=\bar{u}^2$, where

$$\bar{u}=1-\bar{w}^2, \quad \bar{w}=\bar{w}(\bar{r}). \tag{3.4}$$

From (2.7) we conclude $\bar{u}\bar{w}=0$, so since $\bar{r}>0$, we obtain $\bar{w}=0$, and thus $\bar{r}=1$. Now $A(r_1)>0$, $A(1)=0$, so $\min A(r)$ in the interval $[1,r_1]$ cannot be negative, in view of Lemma 3; hence $A(r)\geqslant 0$ on $1\leqslant r\leqslant r_1$. To invoke the results of Ref. 7, we must show that $A(r)\geqslant 0$ for all $r>1$. To do this, suppose that r_2 was the first zero of A, $r_2>r_1$. If $w^2(r_2)\leqslant 1$, then from (2.1) we find $A'(r_2)>0$, so $A(r)<0$ for some $r<r_2$, r near r_2, and this is impossible. If $w^2(r_2)>1$, then $w^2(r_3)>1$, and $A(r_3)>0$ for some $r_3<r_2$, r_3 near r_2. If $(ww')(r_3)>0$, it was shown in Ref. 10, Proposition 2.2, that w' tends to infinity for some $r>r_3$, thereby violating the smoothness assumption. If $(ww')(r_3)<0$, it was shown in Ref. 10, Proposition 2.3, that $A(\bar{r})>0$, thereby violating (3.1). If $(ww')(r_3)=0$, then $w'(r_3)=0$, so (2.2) implies the contradiction $(uw)(r_3)=0$. Thus $A(r)>0$ if $r>r_1$, so $A(r)\geqslant 0$ if $r>\bar{r}$; hence the results of Ref. 7 apply to show (A,w) is the ERN solution. ■

Remark: One case in which Proposition 2 applies is the following; namely, suppose that $(A(r),w(r))$ is the solution of (2.6) and (2.7), defined for $r>\bar{r}$, where $A(\bar{r})=0$, and $A(r)>0$ for $r>\bar{r}$, r near $\bar{r}$. Then by Ref. 10, Theorems 3.4 and 3.7, the solution can be extended to be smooth at $\bar{r}$, if $\bar{r}>0$, and if $\bar{r}=0$, $A(0)=1$; hence Proposition 2 applies. Thus, *in proving Theorem 1, we may assume that either case (i) or case (ii), above, hold. That is, we may assume that either there is a sequence* $r_n\searrow\bar{r}$ *such that (3.3) holds, or else that* $A(r)<0$ *for* r *near* $\bar{r}$, $r>\bar{r}$.

In what follows, we shall assume only that

$$(A,w)\in(C^1\times C^2)(\bar{r},\bar{r}+\epsilon),$$

for some $\epsilon>0$; this case is far more difficult.

Notes. (1) We do not assume that A or w is smooth at $\bar{r}$, nor do we assume that our solution is regular, as in Ref. 10.

(2) The proof given in this paper is considerably more difficult than that in Ref. 10 because since we allow A to change signs for r near $\bar{r}$, the curve $(w(r),w'(r))$ can *a priori* be "all over" the $w-w'$ plane. That is, both A and w can oscillate unboundedly and w' can be unbounded. We shall, in fact, show that none of the above can occur; this will require that we "systematically" rule out all such pathological behavior.

(3) In what follows, we assume that (A,w) is not the ERN solution, and we shall prove that (3.1) leads to a contradiction.

Proof of Theorem 1: We begin with the following lemma.

Lemma 4: There does not exist a sequence $r_n\searrow\bar{r}$ satisfying $w(r_n)^2=1$.

Proof: Suppose that the contrary holds. Then, by passing to a subsequence if necessary, we may assume, without loss of generality, that $w(r_n)=1$, and $w'(r_n)\geqslant 0$, for $n=1,2,\ldots$. We claim that for each n, $A(r_n)\leqslant 0$. To see this, suppose that $A(r_n)>0$. Then, if $w'(r_n)=0$, it follows by uniqueness that $w(r)\equiv 1$ and $A(r)=1+c/r$ for some constant c. This violates (1.2). Thus, we may assume that $w'(r_n)>0$. It follows that the orbit enters the region $w>1$, $w'>0$, for $r>r_n$, r near r_n, with $A(r)>0$. From Ref. 10, Proposition 2.2, it follows that w' tends to infinity for some $r>\bar{r}$, so the solution cannot be smooth. This contradiction proves our claim; i.e. $A(r_n)>0$. Now, since $u(r_n)=0$, (2.1) gives

$$r_n A'(r_n)+A(r_n)=-2(Aw'^2)(r_n)+1,$$

and since $A(r_n)\leqslant 0$, we have

$$r_n A'(r_n)+A(r_n)\geqslant 1.$$

But this cannot hold for large n, in view of (3.1). ■

Corollary 5: There is an $\tilde{r}>\bar{r}$ such that $w^2(r)\neq 1$ if $\bar{r}<r<\tilde{r}$.

In view of this corollary, we may assume that precisely one of the following holds:

$$w(r)>1, \quad \text{if } \bar{r}<r<\tilde{r}, \tag{3.5}$$

$$w(r)<-1, \quad \text{if } \bar{r}<r<\tilde{r}, \tag{3.6}$$

or

$$-1<w(r)<1, \quad \text{if } \bar{r}<r<\tilde{r}. \tag{3.7}$$

In order to consider these cases, we shall need some preliminary results. We begin by noting that from (2.1), we have

$$rA'+A+2Aw'^2=1-\frac{u^2}{r^2}\leqslant 1. \tag{3.8}$$

Also, given any $\delta>0$, (3.1) shows that for r near $\bar{r}$, $rA'(r)+A(r)>-\delta$, and so from (3.8),

$$2Aw'^2\leqslant 1+\delta. \tag{3.9}$$

Thus we have the following.

Lemma 6: There is an $\epsilon>0$ such that

$$A(r)w'^2(r)\leqslant 1, \quad \text{if } \bar{r}<r<\bar{r}+\epsilon. \tag{3.10}$$

Thus Aw'^2 is bounded from above if r is near $\bar{r}$. Our first goal is the show that Aw'^2 is bounded (Proposition 10); as a first step in this direction we have the following.

Lemma 7: Let $\bar{r}>0$, and assume that $w(r)$ is bounded for r near $\bar{r}$. Then $(Aw'^2)(r)$ is bounded for r near $\bar{r}$.

Proof: Assume that the result is false. In view of (3.10), we may assume that there is a sequence $r_n\searrow\bar{r}$ such that $(Aw'^2)(r_n)\to-\infty$. But from (2.1), we see that if $\bar{r}>0$ and w is bounded, it follows that Aw'^2 is bounded in view of (3.1). ■

Lemma 8: Let $\bar{r}\geqslant 0$, and assume that there is an $\epsilon>0$ such that if r is close to $\bar{r}$,

$$(Aw'^2)(r)\leqslant -\tfrac{1}{2}-\epsilon. \tag{3.11}$$

Then Aw'^2 has a negative limit at $\bar{r}$ (which may equal $-\infty$), $A(r)$ is negative for r near $\bar{r}$, and $w'^2(r)\to\infty$ as $r\searrow\bar{r}$.

Proof: Let

$$f=Aw'^2; \tag{3.12}$$

then (cf. Refs. 9 and 10) f satisfies the equation

$$rf'+\left(2f+\frac{\Phi}{r}\right)w'^2+2\frac{u}{r}ww'=0. \tag{3.13}$$

Since $A(r)\to 0$, as $r\searrow\bar{r}$, we see $w'^2(r)\to\infty$. Also, for r near $\bar{r}$,

$$2f+\frac{\Phi}{r}=2f+1-A-\frac{u^2}{r^2}\leqslant -2\epsilon-A-\frac{u^2}{r^2}<-\epsilon-\frac{u^2}{r^2}\leqslant-\epsilon. \tag{3.14}$$

We shall now show that

$$f'(r)>0, \quad \text{if } r \text{ is near } \bar{r}. \tag{3.15}$$

To do this, we only consider those r for which $\bar{r}<r<\tilde{r}$ [c.f. (3.5)–(3.7)].

Suppose first that for all such r, the sequence $\{w^2(r)\}$ is bounded. Then from (3.14), we have, at such r,

$$\left(2f+\frac{\Phi}{r}\right)w'^2+2\frac{u}{r}ww'<-\epsilon w'^2-\frac{u^2}{r^2}w'^2+\frac{2u}{r}ww'. \tag{3.16}$$

If $(u/r)w'\to 0$, as $r\searrow\bar{r}$, then (3.14) shows that $(2f+\Phi/r)w'^2+(2u/r)ww'<0$, so from (3.13) we conclude that (3.15) holds. On the other hand, if $\underline{\lim}_{r\searrow\bar{r}}|(u/r)w'|>0$, then as $\{w(r)\}$ is bounded and $|w'(r)|\to\infty$, we see from (3.16) that (3.15) holds. Thus, (3.15) holds if $\{w^2(r)\}$ is bounded near $\bar{r}$.

Suppose now that $w^2(r_n)\to\infty$ for some sequence $r_n\searrow\bar{r}$; we shall show that for large n, (3.15) holds. Thus, if $w^2(r_n)\to\infty$, we have, at $r=r_n$,

$$\begin{aligned}-\frac{u^2}{r_n^2}w'^2+2\frac{u}{r_n}ww' &= \frac{-u}{r_n^2}[uw'^2-2ww'r_n]\\ &= \frac{-u}{r_n^2}[(1-w^2)w'^2-2ww'r_n]\\ &< \frac{-u}{r_n^2}\left[-\frac{w^2}{2}w'^2-2ww'r_n\right],\end{aligned} \tag{3.17}$$

if n is large. Let $x_n=w(r_n)w'(r_n)$; then $x_n^2\to\infty$, and if $h(x_n)=-x_n^2/2-2x_nr_n$, then if $x_n\to+\infty$, $h(x_n)=(x_n/2)(-x_n+4r_n)\to-\infty$ [since $u(r_n)\to-\infty$], while if $x_{n_k}\to-\infty$ for some subsequence $\{n_k\}$, then $h(x_{n_k})=(-x_{n_k}/2)(x_{n_k}-4r_{n_k})\to-\infty$. Thus, (3.17) and (3.16) show that (3.15) holds, at x_{n_k}, so that (3.15) is valid. Thus $\lim_{r\searrow\bar{r}}f(r)$ exists and is $\leqslant-\frac{1}{2}$, so $A(r)$ is negative for r near $\bar{r}$, and $w'^2(r)\to\infty$ as $r\searrow\bar{r}$. This completes the proof of Lemma 8. ■

Lemma 9: Let $\bar{r}=0$; then $(Aw'^2)(r)$ is bounded for r near 0.

Proof: Suppose Aw'^2 is not bounded near $r=0$. Then, in view of Lemma 6, Aw'^2 is not bounded from below, so we can find a sequence $r_n\searrow 0$ such that $(Aw'^2)(r_n)\leqslant-\frac{1}{2}-\epsilon$, for some

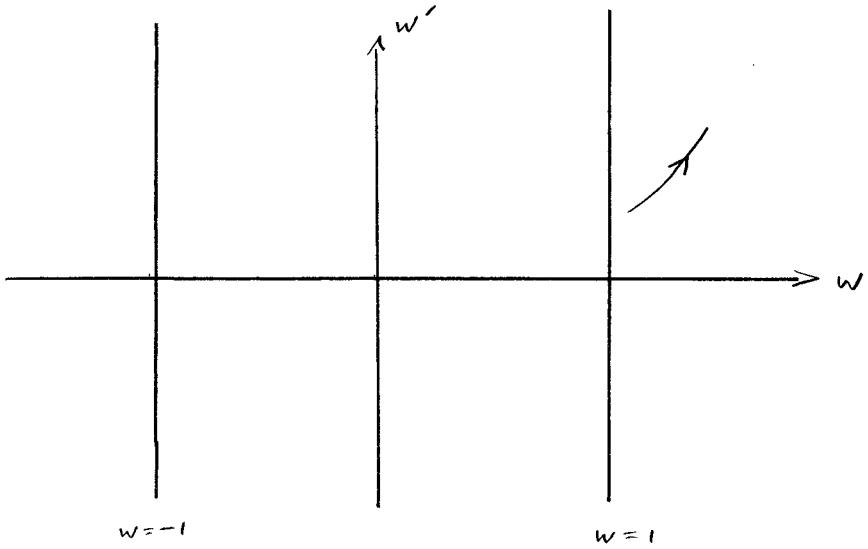

FIG. 3. w is bounded near $r=0$.

$\epsilon>0$. By the last lemma, Aw'^2 has a negative limit at $r=0$, and as Aw'^2 is unbounded near $r=0$, we see that $(Aw'^2)(r)\to-\infty$ as $r\searrow 0$. Thus, from the last lemma, we have

$$A(r)<0, \quad \text{for } r \text{ near } 0, \tag{3.18}$$

$$w'(r) \text{ is of one sign for } r \text{ near } 0, \tag{3.19}$$

$$\lim_{r\searrow 0} w'^2(r)=\infty. \tag{3.20}$$

Next, from (2.1) $\lim_{r\searrow 0}[u^2/r^2 + 2(Aw'^2)(r)] = 1$, and as $Aw'^2\to-\infty$, we see

$$\lim_{r\searrow 0} \frac{u^2(r)}{r^2}=\infty. \tag{3.21}$$

Thus $r^2/u^2\to 0$ as $r\searrow 0$, so

$$\lim_{r\searrow 0} \frac{2(Aw'^2)(r)}{u^2/r^2}=-1. \tag{3.22}$$

Since (3.21) holds, we have

$$-\frac{\Phi}{r}=-1+A+\frac{u^2}{r^2}>\frac{u^2}{2r^2} \quad \text{for } r \text{ near } 0. \tag{3.23}$$

Now, in view of (3.19) and (3.20), either $\lim_{r\searrow 0} w'(r) = +\infty$ or $\lim_{r\searrow 0} w'(r) = -\infty$. Then, in either case $\lim_{r\searrow 0} w(r)$ exists. Suppose first that $\lim_{r\searrow 0} w'(r) = \infty$ [the case where $w'(r)\to-\infty$ will be discussed below]. We consider r in the range $0=\bar{r}<r<\tilde{r}$; cf. (3.5)–(3.7). Then there are three possibilities: $w(r)$ is bounded, $\lim_{r\searrow 0} w(r) = -\infty$, or $\lim_{r\searrow 0} w(r) = +\infty$. Note first that since $w'(r)\to\infty$, if $w(r)\to+\infty$, then w is bounded near 0; cf. Fig. 3. Thus

we shall suppose that

$$\lim_{r\searrow 0} w'(r)=\infty, \tag{3.24}$$

and either

$$\lim_{r\searrow 0} w(r)=-\infty, \tag{3.25}$$

or

$$w(r) \text{ is bounded near } r=0; \tag{3.26}$$

we shall obtain a contradiction in both cases.

Now for r near 0, we have, from (2.7) and (3.23),

$$rAw''=\frac{-\Phi}{r}\,w'-\frac{u}{r}\,w>\frac{u^2}{2r^2}\,w'-\frac{u}{r}\,w\geqslant\frac{1}{4}\,\frac{u^2}{r^2}\,w', \tag{3.27}$$

because (3.25) or (3.26) holds. That is, if (3.26) holds, then (3.21) implies

$$\frac{u^2}{4r^2}\,w'-\frac{u}{r}\,w=\frac{u}{4r}\left[\frac{u}{r}\,w'-4w\right]>0, \quad \text{if } r \text{ is near } 0,$$

while if (3.25) holds, then since $w=o(u)$,

$$\frac{u^2}{4r^2}\,w'-\frac{u}{r}\,w=\frac{u}{4r}\left[\frac{(1-w^2)}{r}\,w'-4w\right]>0.$$

Thus, for r near 0, (3.27) and (3.22) give, for r near 0,

$$-w''\geqslant\frac{1}{4}\,\frac{u^2}{(-Ar^2)}\,w'=\frac{1}{4}\,\frac{u^2}{r^2}\left(\frac{1}{-Aw'^2}\right)\frac{w'^3}{r}\geqslant\frac{c^2}{r}\,w'^3,$$

where c is a positive constant. Now let $0<t<s$, where s is near 0. Then, from (3.28) we obtain

$$\frac{1}{2}\left[\frac{1}{w'^2(t)}-\frac{1}{w'^2(s)}\right]=-\frac{1}{2}\,\frac{1}{w'^2(r)}\bigg|_t^s=\int_t^s\frac{w''}{w'^2}\,dr\geqslant c^2\int_t^s\frac{dr}{r}=c^2\,\ln\frac{s}{t},$$

so that

$$\frac{1}{2}\left[\frac{1}{w'^2(t)}-\frac{1}{w'^2(s)}\right]\geqslant c^2\,\ln\frac{s}{t}. \tag{3.28}$$

Now let $t\to 0$; then the left side of (3.28) is bounded [because of (3.20)], but the right side tends to ∞. This contradiction shows that the lemma holds if (3.24), and either (3.25) or (3.26) holds.

Now suppose that

$$\lim_{r\searrow 0} w'(r)=-\infty, \tag{3.29}$$

and either

$$\lim_{r\searrow 0} w(r)=\infty, \tag{3.30}$$

or (3.25) holds; we shall indicate how to obtain a contradiction. [It is easy to see that if (3.29) holds then $\lim_{r\searrow \bar r} w(r)\neq -\infty$.] In this case we obtain, from (2.7), (3.23), and (3.29),

$$rAw''\leqslant \frac{u^2}{2r^2}\,w'-\frac{u}{r}\,w\leqslant \frac{u^2}{4r^2}\,w',$$

if r is near 0, so that, using (3.22),

$$-w''\leqslant \frac{1}{4}\,\frac{u^2}{(-Ar^3)}\,w'=\frac{1}{4}\left[\frac{u^2/r^2}{-Aw'^2}\right]\frac{w'^3}{r}\leqslant c^2\,\frac{w'^3}{r},$$

so $w''\geqslant(-c^2/r)w'^3$, and thus $(-w''/w'^3)\geqslant c^2/r$. If we again integrate from t to s, we get

$$\frac{1}{2}\,\frac{1}{w'^2(r)}\bigg|_t^s \geqslant c^2\,\lim\frac{s}{t},$$

and letting $t\to 0$ gives a contradiction, as before. This completes the proof of Lemma 9. ■

We next have the following.

Proposition 10: $(Aw'^2)(r)$ is bounded if r is near $\bar r$.

Proof: From Lemma 9, we may assume that $\bar r>0$. Now choose r such that $\bar r<r<\tilde r$, where $\tilde r$ is defined in Corollary 5. Thus, as we have shown above, (3.5)–(3.7) are valid. Now if $w(r)$ is bounded, then Lemma 7 implies that Aw'^2 is bounded near $\bar r$. Thus, we may assume that w is unbounded near $\bar r$, so that for $\bar r<r<\tilde r$, either $w(r)>1$ or $w(r)<-1$. Since the proofs are similar in both cases, we shall restrict attention to the case $w(r)>1$ for $\bar r<r<\tilde r$.

Thus, assume that w is unbounded near $\bar r$, and $w(r)>1$ for $\bar r<r<\tilde r$. Now suppose that Aw'^2 is not bounded for r near $\bar r$. Then, as in the proof of Lemma 9, $\lim_{r\searrow \bar r}(Aw'^2)(r)=-\infty$, and (3.18)–(3.20) are valid. Thus, from (3.19), we conclude that $\lim_{r\searrow \bar r} w(r)$ exists; hence

$$\lim_{r\searrow \bar r} w(r)=+\infty. \tag{3.31}$$

Also, the orbit cannot stay in the region $w'>0$ for r near $\bar r$, for otherwise it would follow that w is bounded near $\bar r$; cf. Fig. 3. Thus the orbit enters the region $w'<0$, and in view of (3.19), we may assume that $w'(r)<0$ if r is near $\bar r$; cf. Fig. 4. In view of (3.19) we have

$$\lim_{r\searrow \bar r} w'(r)=-\infty. \tag{3.32}$$

From (2.7) we can write

$$Aw''w'^2+\frac{\Phi}{r^2}\,w'^3+\frac{uw}{r^2}\,w'^2=0. \tag{3.33}$$

Now, from (2.1),

$$rA'+A+2Aw'^2=1-\frac{u^2}{r^2},$$

so that for r near $\bar r$, since $\bar r>0$,

$$(Aw'^2)\ \text{ is well approximated by }\ -c_1^2w^4, \tag{3.34}$$

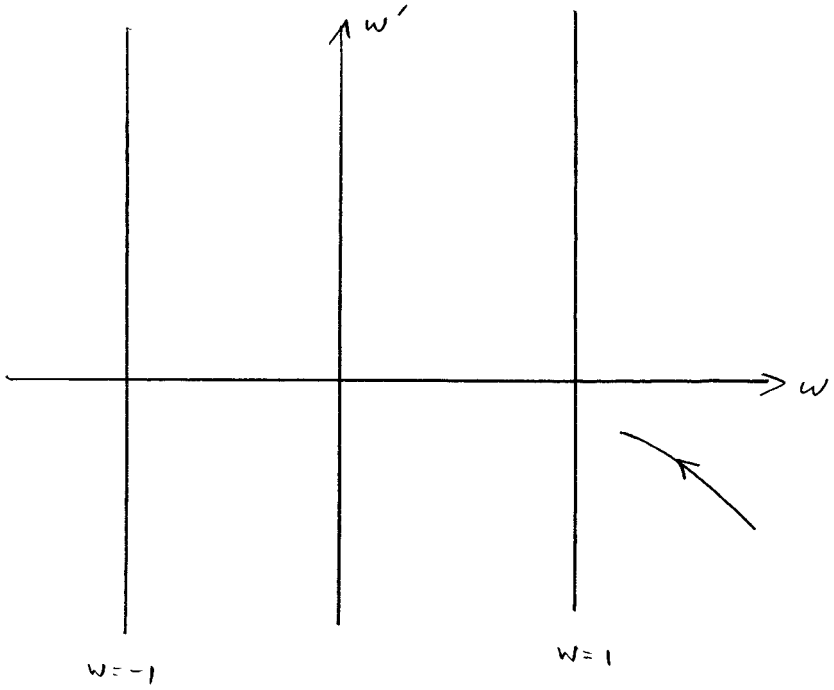

FIG. 4. $w'<0$ for r near 0.

for some constant $c_1^2 \neq 0$. Also,

$$\frac{\Phi}{r^2} w'^3 + \frac{uw}{r^2} w'^2 = \frac{1}{r} w'^3 - \frac{A}{r} w'^3 - \frac{u^2}{r^3} w'^3 + \frac{uw}{r^2} w'^2,$$

and as $\bar{r} > 0$, we see that for r near $\bar{r}$,

$$\left(\frac{\Phi}{r^2} w'^3 + \frac{uw}{r^2} w'^2 \right) \text{ is well approximated by } -c_2^2 w^4 w'^3, \tag{3.35}$$

for some constant $c_2^2 \neq 0$. Thus, for r near $\bar{r}$, solutions of (3.33) are well approximated by the equation

$$-c_1^2 w^4 w'' - c_2^2 w^4 w'^3 = 0, \tag{3.36}$$

or, writing $c^2 = (c_2/c_1)^2$, (3.36) becomes

$$w'' + c^2 w'^3 = 0, \tag{3.37}$$

where c is a nonzero constant. Now the solution of (3.37) satisfying (3.32) is

$$w'(r) = -\frac{1}{\sqrt{2c^2}} \frac{1}{\sqrt{r - \bar{r}}}, \quad r > \bar{r},$$

which implies that $w(r)$ is bounded near $\bar{r}$, contrary to (3.31). This contradiction completes the proof of Proposition 10. ■

Proposition 10 yields a few useful corollaries. First, if we define $v(r)$ by (cf. Ref. 8)

$$v(r)=(Aw')(r), \tag{3.38}$$

then v satisfies the equation

$$v'+\frac{2w'^2}{r}v+\frac{uw}{r^2}=0. \tag{3.39}$$

Corollary 11: $\lim_{r\searrow\bar{r}} v(r)=0$.

Proof: $v^2(r)=A(r)(Aw'^2(r))\to 0$ as $r\searrow\bar{r}$. ■

Corollary 12: $w(r)$ is bounded for r near $\bar{r}$, and if $\bar{r}=0$, then $\lim w^2(r)=1$.

Proof: Consider Eq. (2.1): the left side is bounded near $\bar{r}$ so that u^2/r^2 is also bounded near $\bar{r}$. If $\bar{r}>0$ then u^2 is bounded, so w is bounded near $\bar{r}$, while if $\bar{r}=0$, then $w^2(r)\to 1$ as $r\searrow\bar{r}$. ■

We shall now consider the case where w' is bounded near $\bar{r}$.

Proposition 13: Assume that there is an $M>0$ such that $|w'(r)|\leqslant M$ for r near $\bar{r}$, then Theorem 1 holds.

To prove this proposition, we shall need a lemma.

Lemma 14: If w' is bounded near $\bar{r}$, then

$$A \text{ is of one sign near } \bar{r}, \tag{3.40}$$

$$w' \text{ is of one sign near } \bar{r}, \tag{3.41}$$

and

$$\lim_{r\searrow\bar{r}}\frac{u^2}{r^2}=1. \tag{3.42}$$

Proof: First note that w' bounded near $\bar{r}$ implies that w is uniformly continuous near $\bar{r}$, so that $\lim_{r\searrow\bar{r}} w(r)=\bar{w}$ exists. Next, since w' is bounded near $\bar{r}$, (2.1) shows that $\lim_{r\searrow\bar{r}}(u^2/r^2)=1$, so (3.42) holds and

$$\frac{u}{r}\to\pm 1, \quad \text{as } r\searrow\bar{r}. \tag{3.43}$$

Now writing (3.39) in the form

$$r^2v'+2w'^2vr+uw=0, \tag{3.44}$$

we see that if $\bar{w}\neq 0$, $\lim_{r\searrow\bar{r}} rv'(r)=\pm\bar{w}\neq$, so v' is of one sign near $\bar{r}$, and using Corollary 11, v is of one sign near $\bar{r}$, so (3.40) and (3.41) hold. On the other hand, if $\bar{w}=0$, (3.42) implies that $\bar{r}=1$, so from (3.39), we have $v'(1)=0$ and $v''(1)\neq 0$. Thus v is again of one sign near $\bar{r}$ so (3.40) and (3.41) hold. ■

We can now give the following.

Proof of Proposition 13: The last-lemma implies that A is of one sign near $\bar{r}$. If $A>0$ near $\bar{r}$, then the result in Ref. 7 (cf. the remark after the proof of Proposition 2), shows that (A,w) is the ERN solution. Thus we may assume that

$$A(r)<0, \quad \text{if } r \text{ is near } \bar{r}, \tag{3.45}$$

and we shall show that this leads to a contradiction.

First, suppose that $\bar{w}=0$. Then from (3.42), we see that $\bar{r}=1$, and as in the proof of Proposition 2, the solution must be the ERN solution. Thus, we may assume that

$$\bar{w}\neq 0. \tag{3.46}$$

Let $\bar{r}<r_2<r_3$ where r_3 is near $\bar{r}$. We consider two cases:

$$\bar{u}\bar{w}\neq 0 \tag{3.47}$$

or

$$\bar{u}\bar{w}=0. \tag{3.48}$$

Using (2.7),

$$\int_{r_2}^{r_3} r^2 A w''\, dr+\int_{r_2}^{r^3}\Phi w'\, dr+\int_{r_2}^{r_3} uw\, dr=0. \tag{3.49}$$

Suppose first that (3.47) holds. Then

$$\int_{r_2}^{r_3} r^2 A w''\, dr=r^2 A w'\Big|_{r_2}^{r_3}-\int_{r_2}^{r_3}(r^2A)'w'\, dr,$$

and letting $r_2\searrow\bar{r}$ gives, for some intermediate point ξ,

$$\int_{\bar{r}}^{r_3} r^2 A w''=r_3^2 A(r_3)w'(r_3)-[\xi^2 A'(\xi)+2\xi A(\xi)]w'(\xi)(r_3-\bar{r}),$$

so that

$$\int_{r_2}^{r_3} r^2 A w''\, dr=o(r_3-\bar{r}). \tag{3.50}$$

Similarly, since $\Phi(r)=r-rA-u^2/r\to 0$ as $r\searrow\bar{r}$ [in view of (3.42)], we have, for some intermediate point η,

$$\lim_{r_2\searrow\bar{r}}\int_{r_2}^{r_3}\Phi w'\, dr=\int_{\bar{r}}^{r_3}\Phi w'\, dr=(\Phi w')(\eta)(r_3-\bar{r})=o(r_3-\bar{r}). \tag{3.51}$$

Finally, we have, for some intermediate point ζ,

$$\lim_{r_2\searrow\bar{r}}\int_{r_2}^{r_3} uw\, dr=\int_{\bar{r}}^{r_3} uw\, dr=(uw)(\eta)(r_3-\bar{r})=O(r_3-\bar{r}), \tag{3.52}$$

where the constant is nonzero, in view of (3.47). Taking the limit $r_2\searrow\bar{r}$ in (3.49), and using (3.50)–(3.51) gives the contradiction

$$o(r_3-\bar{r})=O(r_3-\bar{r}).$$

Now suppose that (3.48) holds. In view of (3.46), this means $\bar{u}=0$ so (3.42) implies $\bar{r}=0$. Thus, $\bar{w}=\pm 1$, and, for definiteness, suppose that $\bar{w}=1$ (the proof for $\bar{w}=-1$ is similar, and will be omitted). As above, (3.49) gives

$$\int_0^{r_3} r^2 A w''\, dr = r_3^2 A(r_3) w'(r_3) - \int_0^{r_3} (r^2 A'(r) + 2rA(r)) w'(r) dr.$$

But

$$r_3^2 A'(r_3) w'(r_3) = o(r_3^3)$$

[since $A(r_3) = o(r_3)$], and for some intermediate point ξ,

$$\int_0^{r_3} (r^2 A' + 2rA(r)) w'(r) dr = (\xi^2 A'(\xi) + 2\xi A(\xi))(w(r_3) - w(0)) = o(r_3^3);$$

thus

$$\int_0^{r_3} r^2 A w'' dr = o(r_3^3). \tag{3.53}$$

Similarly, for some intermediate point η,

$$\int_0^{r_3} \Phi w'\, dr = (\Phi w')(\eta) r_3 = o(r_3^3), \tag{3.54}$$

because

$$\Phi(r) = r\left(1 - \frac{u^2}{r^2} - A\right) = r(rA' + 2Aw'^2) = o(r_3^2).$$

However, for some intermediate point ζ, we have

$$\int_0^{r_3} uw\, dr = \int_0^{r_3} \frac{u}{r}\, wr\, dr = \frac{u(\zeta)}{\zeta}\, w(\zeta)\, \frac{r_3^2}{2} = O(r_3^2),$$

and this gives a contradiction, in view of (3.53) and (3.54). This completes the proof of Proposition 13. ■

In view of this last result, *we may assume in what follows that*

$$w'(r) \text{ is unbounded for } r \text{ near } \bar{r}. \tag{3.55}$$

Our strategy for completing the proof of Theorem 1 is to first show that Theorem 1 holds, provided that both $A(r)$ and $w'(r)$ are of one sign (not necessarily the same), for r near $\bar{r}$, and then to prove that this assumption is always valid.

Proposition 15: Assume that $w'(r)$ and $A(r)$ each are of one sign for r near $\bar{r}$; then Theorem 1 holds.

Proof: As we have remarked earlier, we may assume that (3.45) holds, and also in view of Proposition 13, we may also assume that (3.55) holds. We shall show that our assumptions lead to a contradiction.

First recall that since Aw'^2 is bounded near $\bar{r}$, it follows from Corollary 12 that for r near $\bar{r}$, w is bounded, and if $\bar{r}=0$, then $w^2(r)\to 1$. Furthermore, as w' is of one sign near $\bar{r}$, $\bar{w} = \lim_{r\searrow \bar{r}} w(r)$ exists and is finite. We assume for definiteness that

$$w'(r) > 0, \quad \text{for } r \text{ near } \bar{r}; \tag{3.56}$$

if $w' < 0$ near $\bar{r}$, the proof is similar.

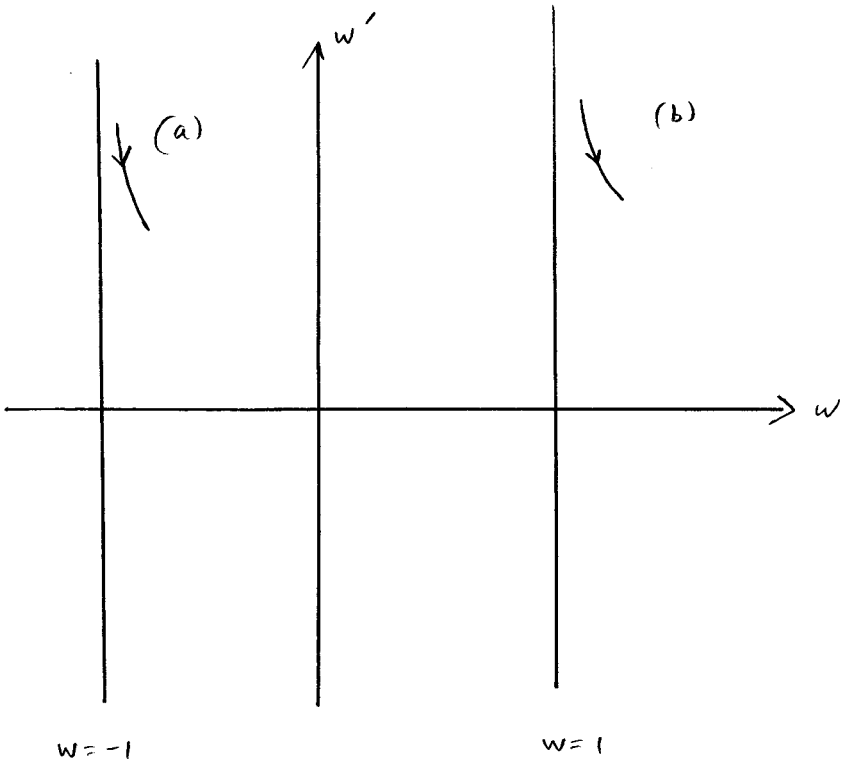

FIG. 5. $w'>0$, w^2 near 1, for r near $\bar{r}$.

The proof is now divided into two cases: $\bar{r}=0$ and $\bar{r}>0$.

Case 1. $\bar{r}=0$. Since $\lim_{r\searrow 0} w^2(r) = 1$, (3.56) implies that for r near 0, either (a) $-1<w(r)<0$, or (b) $1<w(r)<1+\epsilon$, for some small $\epsilon>0$; cf. Fig. 5. Now from Corollary 11, $v(0)=0$, and from (3.19), $v'(r)>0$, for r near 0, and $v'(0)\geqslant 0$. This implies that $v(r)>0$ for r near 0, and this is impossible because $A<0$ and $w'>0$.

Case 2. $\bar{r}>0$. Since w has a finite limit at $\bar{r}$, it follows from (2.1) that $\lim_{r\searrow 0}(Aw'^2)(r) = -L$, where $L\geqslant 0$. If $L>0$, then $w'^2\to\infty$ as $r\searrow\bar{r}$, and (3.56), together with (3.39) shows that $v'(\bar{r})>0$, for r near $\bar{r}$, which is impossible, as we have just seen. Thus we may assume that $L=0$.

If $-1\leqslant\bar{w}\leqslant 0$, or $\bar{w}\geqslant 1$, then (3.19) and (3.39) show that $v'(r)>0$ for r near $\bar{r}$ so that if $\epsilon>0$ is small, we have, for some intermediate point ξ,

$$v(\bar{r}+\epsilon)=v(\bar{r}+\epsilon)-v(\bar{r})=\epsilon v'(\xi)>0,$$

and this is a contradiction. Thus, we can assume that $\bar{w}<-1$, or $0<\bar{w}<1$. Now as $L=0$, (2.6) implies that $\Phi(\bar{r})=0$, so $\bar{u}=\bar{r}$. Also, from Refs. 8 and 9,

$$\Phi'(\bar{r})=\frac{2u^2}{\bar{r}^2}+2Aw'^2+\frac{4uww'}{\bar{r}},$$

so that $\Phi'(\bar{r})>0$. Thus $\Phi(r)>0$ for $r>\bar{r}$, r near $\bar{r}$, so (2.6) implies that $A'(r)>0$ for r near $\bar{r}$, and hence as $A(\bar{r})=0$, we get the contradiction $A(r)>0$ for r near $\bar{r}$. This completes the proof of Proposition 15. ■

Now in view of Corollary 5, we may assume that for r near $\bar{r}$, one of the following must hold:

$$\begin{aligned} &\text{(I)} \quad w^2(r)<1,\\ &\text{(II)} \quad w(r)>1,\\ &\text{(III)} \quad w(r)<-1. \end{aligned}$$

Our objective is to show that in each of these cases, both $A(r)$ and $w'(r)$ have fixed signs for r near $\bar{r}$. Then Proposition 15 will complete the proof of Theorem 1. We begin with the most difficult case; namely the following.

Case I: $w^2(r)<1$ for r near $\bar{r}$.

In order to carry out our program in this case, we shall first rule out "infinite rotation" of the orbit $(w(r),w'(r))$ about the origin. There are two cases to consider; namely

$$\lim_{r\searrow\bar{r}} w(r)=0, \quad \text{and } w' \text{ is not of one sign near } \bar{r}, \tag{3.57}$$

or

$$-1\leqslant \underline{\lim_{r\searrow\bar{r}}}\, w(r)\leqslant 0\leqslant \overline{\lim_{r\searrow\bar{r}}}\, w(r)\leqslant 1 \tag{3.58}$$

and

$$\underline{\lim_{r\searrow\bar{r}}}\, w(r)<\overline{\lim_{r\searrow\bar{r}}}\, w(r);$$

cf. Figs. 6 and 7.

Proposition 16: It is impossible for (3.57) to hold.

Proof: Define $Q'(r)=2w'^2/r$, $Q(r_1)=0$. Then, $Q(r)<0$ if $\bar{r}\leqslant r<r_1$ and (2.1) can be written as

$$(re^Q A)'=\left(1-\frac{u^2}{r^2}\right)e^Q. \tag{3.59}$$

Also, $|re^{Q(r)}A(r)|\leqslant|rA(r)|$, so that

$$re^{Q(r)}A(r)\to 0, \quad \text{as } r\searrow\bar{r}. \tag{3.60}$$

Now if $\bar{r}-1/\bar{r}\geqslant 0$, then (3.57) and (3.59) imply that for r near $\bar{r}$, $(re^QA)'\geqslant 0$, so that for such r,

$$re^{Q(r)}A(r)=re^{Q(r)}A(r)-\bar{r}e^{Q(\bar{r})}A(\bar{r})=(\xi e^{Q(\xi)}A(\xi))'>0,$$

for some intermediate point ξ. It follows that $A(r)>0$ for r near $\bar{r}$, and this is contrary to our assumptions; cf. the remark after the proof of Proposition 2.

If $\bar{r}-1/r<0$, then a similar argument shows that $A(r)<0$ for r near $\bar{r}$. Thus from (2.7), if $w'(r)=0$, then $w''(r)>0$, for $0<w(r)<1$, and $w''(r)<0$, if $-1<w(r)<0$; cf. Fig. 8. Thus, $w'(r)$ is of one sign for r near $\bar{r}$, contrary to our assumption (3.57). This completes the proof of Proposition 16. ■

We now turn to the remaining case; namely (3.58). To handle, this case, we first note that

$$\bar{r}>0, \tag{3.61}$$

if (3.58) holds. Indeed, (3.58) implies that we can find a sequence $r_n\searrow\bar{r}$ such that $w(r_n)=0$. Then (2.1) gives

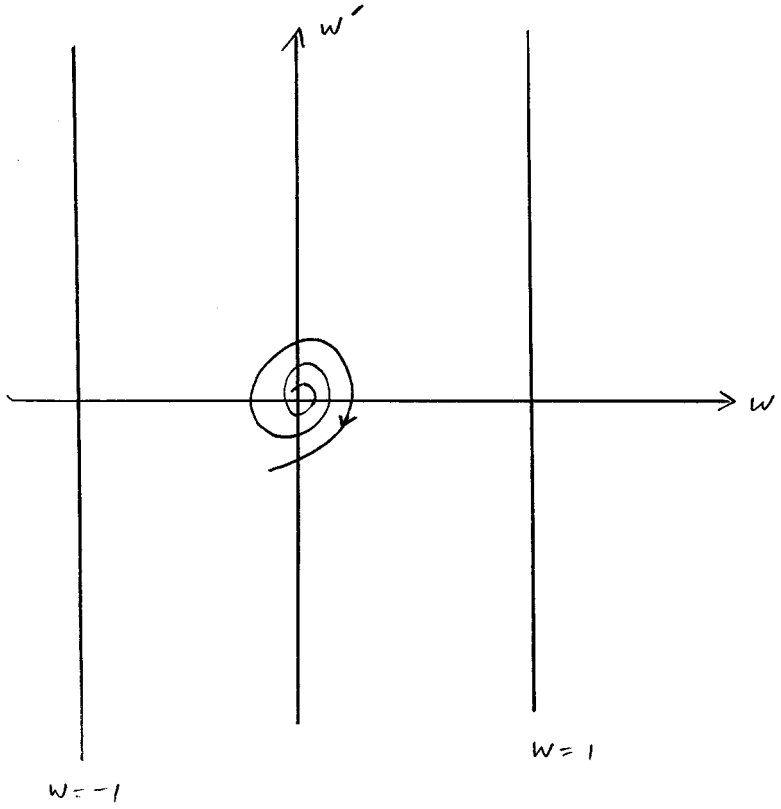

FIG. 6. The case where (3.57) holds.

$$r_n A'(r_n) + (1 + 2w'^2(r_n))A(r_n) = 1 - \frac{1}{r_n^2},$$

and since the left side is bounded (Proposition 10), it follows that $\{1/r_n^2\}$ is also bounded, and this proves (3.61).

Proposition 17: It is impossible for (3.58) to hold.

Proof: If (3.58) holds, then we can find an ϵ,

$$0 < \epsilon < \tfrac{1}{4},$$

such that either $\overline{\lim}_{r \searrow \bar{r}} w(r) > 2\epsilon$, or $\underline{\lim}_{r \searrow \bar{r}} w(r) < -2\epsilon$. Without loss of generality, let us assume that the former inequality holds; cf. Fig. 9.

Thus there exist sequences of points $\{a_n\}$ and $\{b_n\}$, such that

$$b_n > a_n > b_{n+1} > \bar{r}, \quad b_n \to \bar{r}, \tag{3.62}$$

$$w(a_n) = 0, \quad w(b_n) = 2\epsilon, \tag{3.63}$$

and if $a_n < r < b_n$, then

$$w(a_n) < w(r) < w(b_n), \tag{3.64}$$

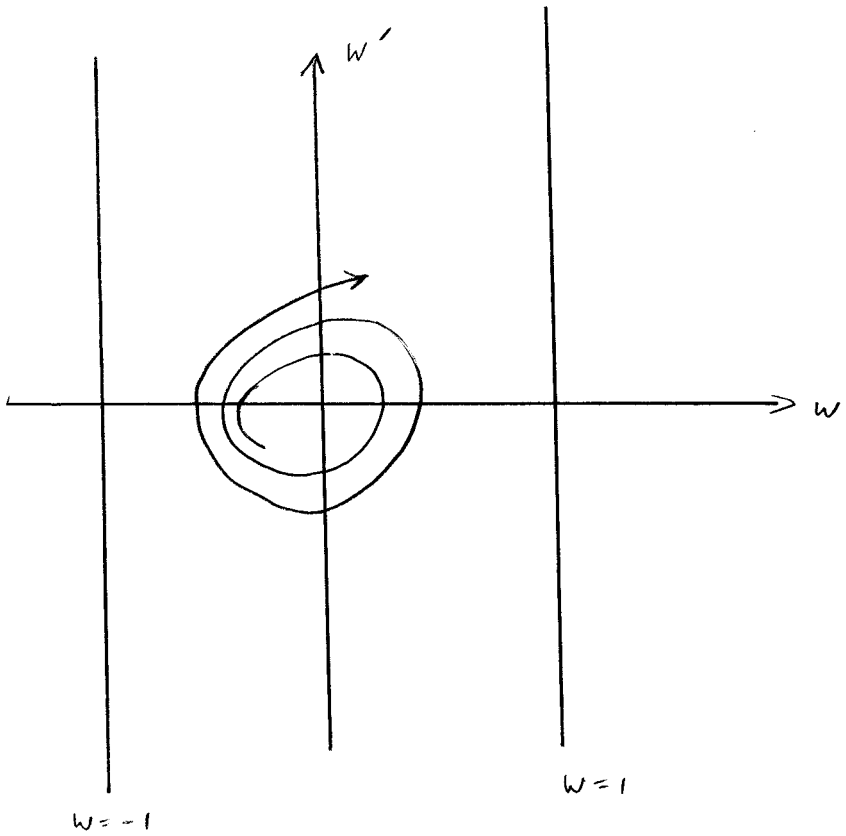

FIG. 7. The case where (3.58) holds.

and finally,

$$w'(r)>0; \tag{3.65}$$

see Fig. 9. We note that the intervals $[a_n,b_n]$ are all disjoint from each other.

Lemma 18: There exist $\delta>0$, $\eta>0$, and an integer $N>0$, and sequences $\{c_n\}$, $\{d_n\}$, defined for $n\geqslant N$,

$$a_n\leqslant c_n<d_n\leqslant b_n, \tag{3.65}$$

such that if r satisfies $c_n\leqslant r\leqslant d_n$, then

$$A(r) \quad \text{is of one sign,} \tag{3.66}$$

$$|\phi(r)|\geqslant\eta, \tag{3.67}$$

$$w(d_n)-w(c_n)\geqslant\delta. \tag{3.68}$$

Before giving the proof, we shall need a few lemmas. We begin with the following easy result.

Lemma 19: Suppose $\Phi(A(r),w(r),r)\equiv\Phi(r)\neq 0$ on $I=[a,b]$, where $a>0$. Then A can have at most one zero on I.

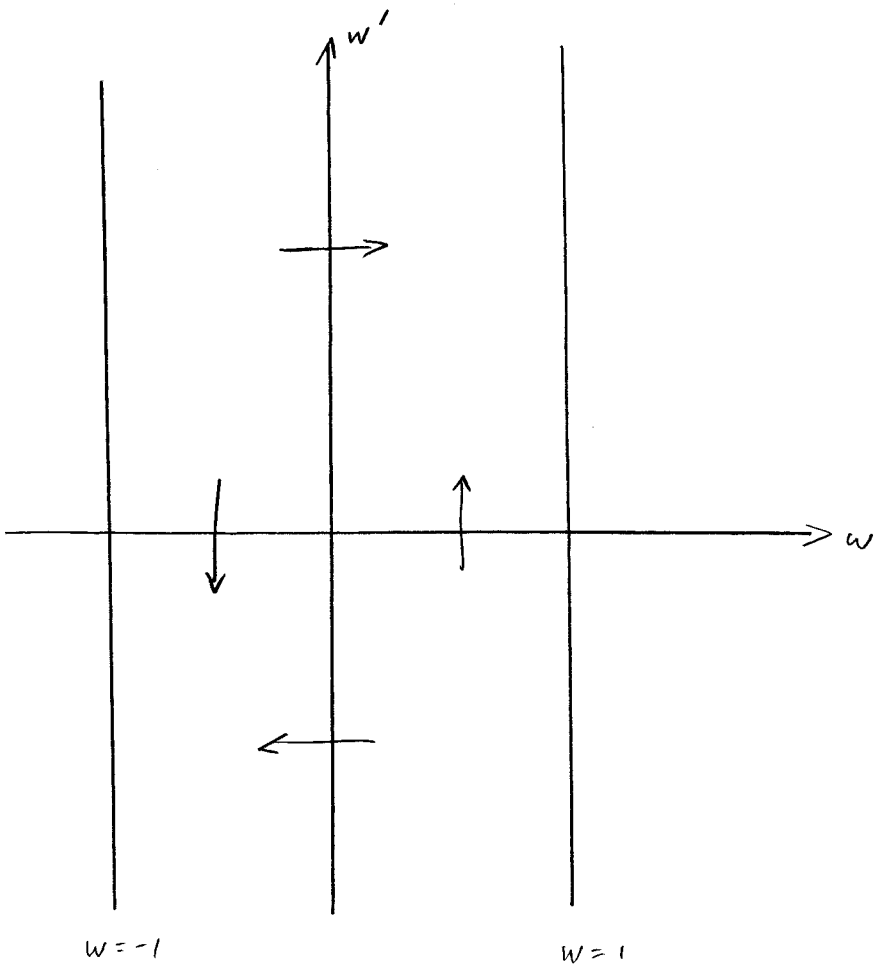

FIG. 8. w' is of one sign near $\bar{r}$.

Proof: From (2.6), if $A(r)=0$ for some $r\in I$, we see $rA'(r)=\Phi(r)/r\neq 0$. Thus A' is of one sign, and this implies that A can have at most one zero on I. ■

Lemma 20: Suppose $\Phi(A(r),w(r),r)\equiv\Phi(r)\neq 0$ on the interval $I=$[a,b], where $a>0$, and that $w(a)=0$, $w(b)=2\epsilon>0$. Then there exist numbers c,d, $a\leqslant c<d\leqslant b$ such that $w(d)-w(c)\geqslant\epsilon/2$, and A has one sign on $[c,d]$.

Proof: We break the proof up into two cases; namely, $A(a)A(b)\neq 0$ and $A(a)A(b)=0$.

Case 1. $A(a)A(b)\neq 0$.

If $\operatorname{sgn}A(a)=\operatorname{sgn}A(b)$, then set $c=a$, $d=b$, and the result holds in view of Lemma 19. If $\operatorname{sgn}A(a)\neq\operatorname{sgn}A(b)$, choose z such that $w(z)=\epsilon$, $a<z<b$. If $A(z)\neq 0$, then in view of Lemma 19, one of the following must hold; namely, either $A(a)A(z)>0$ or $A(z)A(b)>0$. In the first case, choose $c=a$, $d=z$, and in the second case, choose $c=z$, $d=b$. If $A(z)=0$, choose $z'\in I$ with $w(z')=3\epsilon/2$. Then $A(z')\neq 0$, and we proceed as before to reach the desired conclusion; this completes the proof in case 1.

Case 2. $A(a)A(b)=0$.

In view of Lemma 19, we cannot have both $A(a)=0$ and $A(b)=0$. Thus suppose $A(a)=0$, $A(b)\neq 0$; (the proof in the other case is similar). Now choose $z\in I$, z near a, such that $A(z)\neq 0$,

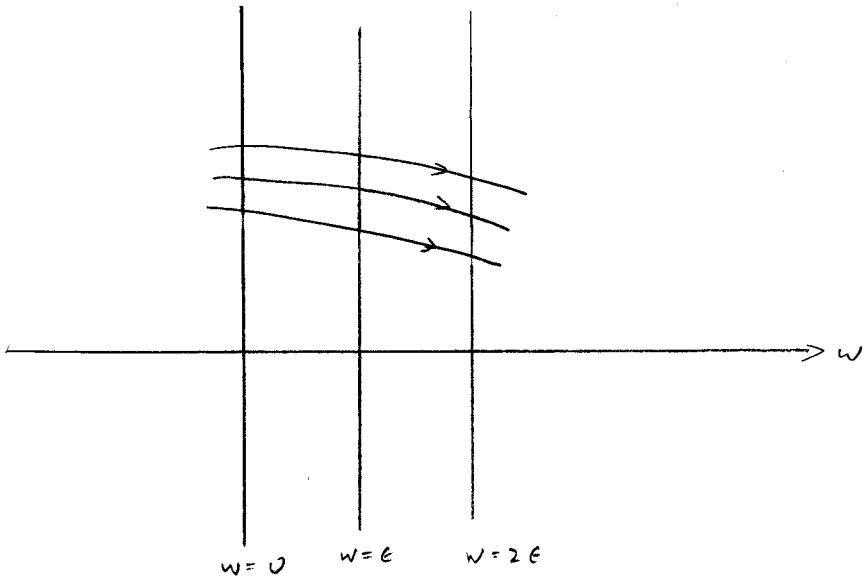

FIG. 9. $\overline{\lim}_{r\searrow \bar{r}} w(r) > 2\epsilon$.

and apply the result in Case 1 to the situation where a is replaced by z. This proves Lemma 20.■

Proof of Lemma 18: We break the proof up into three cases: $\bar{r}>1$, $\bar{r}<1$, $\bar{r}=1$.

Suppose first that $\bar{r}>1$. Then set

$$\bar{r}-\frac{1}{\bar{r}}=2\eta,$$

where $\eta>0$. Since $\lim_{r\searrow \bar{r}} A(r) = 0$, then if $r>\bar{r}$,

$$\Phi(A,w,r)=r-rA-\frac{u^2}{r}>r-rA-\frac{1}{r}>\bar{r}-\frac{1}{\bar{r}}-rA.$$

Thus there exists a σ, $0<\sigma<\epsilon$ such that if $0<r-\bar{r}<\sigma$, then

$$\Phi(A,w,r)>\eta. \tag{3.69}$$

Now we only consider those n for which $b_n<\bar{r}+\sigma$; [cf. (3.62)]. Then with $I_n=[a_n,b_n]$, we apply Lemma 20 to conclude that (3.65)–(3.68) hold, with $\delta=\epsilon/2$.

Suppose now that $\bar{r}<1$. Then set

$$\bar{r}-\frac{1}{\bar{r}}=-2\eta,$$

where $\eta>0$. Since

$$\Phi(A,w,r)=r-\frac{u^2}{r}-rA,$$

and $rA(r)\to 0$ as $r\searrow \bar{r}$, and $u(r)=1-w^2(r)$, we see that we can find a $\sigma>0$ such that if $0<r-\bar{r}<\sigma$, and $0<w<\sigma$,

$$\Phi(A,w,r)<-\eta. \tag{3.70}$$

Again, we only consider those n for which $b_n<\bar{r}+\sigma$. Now as $0\leqslant w(r)\leqslant 2\epsilon$ if $a_n\leqslant r\leqslant b_n$, we choose b_n' such that $w(b_n')=\min(\sigma,2\epsilon)$. Then $\Phi(r)<-\eta$ on the interval $[a_n,b_n']$. Another application of Lemma 20 shows that we can achieve (3.65)–(3.68).

Finally, consider the case $\bar{r}=1$. Consider w satisfying $\epsilon\leqslant w\leqslant 2\epsilon$. Then for these w,

$$1-\frac{u^2}{r}\geqslant 1-(1-\epsilon^2)^2\equiv 2\eta>0,$$

since $\epsilon<1/4$. Thus, if r is sufficiently close to 1, say $0<r-1<\sigma$, then $\Phi(A,w,r)>\eta$. Taking n so large that $b_n<\bar{r}+\sigma$, and defining c_n by $w(c_n)=\epsilon$, and setting $d_n=b_n$, we see that Lemma 20 again applies, and we can achieve (3.65)–(3.68). This completes the proof of Lemma 18. ■

We now can give the following proof.

Proof of Proposition 17: From Lemma 18, we see that we have infinitely many intervals, $J_n=[c_n,d_n]\subset[a_n,b_n]$, where (3.66)–(3.68) hold on J_n. We now consider two cases.

Case a. For infinitely many intervals J_n,

$$(A\Phi)(r)>0, \quad \text{if } r\in J_n. \tag{3.71}$$

Case b. For all but a finite number of intervals J_n,

$$(A\Phi)(r)<0 \quad \text{if } r\in J_n. \tag{3.72}$$

The proof is somewhat involved, so before giving the details, we shall discuss the strategy. The basic idea is to show that there is a $\zeta>0$ such that

$$d_n-c_n\geqslant\zeta; \tag{3.73}$$

then since $\bar{r}<a_n\leqslant c_n<d_n\leqslant b_n$ and $b_n\to\bar{r}$, (3.73) would give the desired contradiction. Now, in order to carry out this program, we need the following fundamental lemma.

Lemma 21. Let $0<\bar{r}<\alpha<\beta<2\bar{r}$, and assume that (A,w) is a solution of (2.1), (2.2) on $J_+=[\alpha,\beta]$ or $J_-=[-\beta,-\alpha]$. Assume too that on this interval, $w^2(r)<1$,

$$0<|(Aw'^2)(\bar{r})|<L \tag{3.74}$$

and

$$|\Phi(r)|\geqslant\eta, \tag{3.75}$$

for some positive constants L and η. Then

$$|\beta-\alpha|\geqslant\zeta>0, \tag{3.76}$$

where ζ is a constant depending only on $\bar{r}$, L, η, and

$$\Delta\equiv|w(\beta)-w(\alpha)|. \tag{3.77}$$

Proof: Assume first that we are on J_+, and that on J_+ both

$$w'>0 \tag{3.78}$$

and

$$A\Phi>0. \tag{3.79}$$

Define the constant m by

$$m=\max\left(\frac{1}{\eta},\frac{16\bar{r}^2L}{\eta\Delta}\right). \tag{3.80}$$

We claim that

$$\text{if } r\in J_+ \quad \text{and} \quad w'(r)\geqslant m, \quad \text{then} \quad w''(r)<0. \tag{3.81}$$

To see this, we have from (2.7),

$$r^2Aw''+\Phi w'+uw=0,$$

and as $|\Phi w'|>1$ and $|uw|<1/2$ on J_+, it follows that $\operatorname{sgn}(\Phi w'+uw)=\operatorname{sgn}\Phi w'=\operatorname{sgn}\Phi$; thus $\operatorname{sgn}w''=\operatorname{sgn}(-A\Phi)<0$, and this proves (3.85). It follows from this that

$$\text{if } \tilde{r}\in J_+ \quad \text{and} \quad w'(\tilde{r})\leqslant m, \quad \text{then } w'(r)<m \quad \text{for } r>\tilde{r}, \quad r\in J_+. \tag{3.82}$$

Now define ξ by

$$w(\xi)=\frac{w(\alpha)+w(\beta)}{2}.$$

Then if for some $\tilde{r}\in J_+$, $\tilde{r}\leqslant\xi$, we have $w'(\tilde{r})\leqslant m$, then $w'(r)\leqslant m$ for all $r\geqslant\tilde{r}$. In this case, we would have, for some intermediate point θ,

$$|\beta-\alpha|\geqslant|\beta-\tilde{r}|=\frac{|w(\beta)-w)(\tilde{r})|}{|w'(\theta)|}\geqslant\frac{\Delta/2}{m}=\zeta,$$

and this would prove the result. Thus, *we may assume that*

$$w'(r)\geqslant m, \quad \text{for all } r\in J_+, \quad r\leqslant\xi. \tag{3.83}$$

We will show that this leads to a contradiction.

We first claim that

$$\frac{w''}{w'^2}<\frac{-\Phi w'}{2r^2Aw'^2}, \quad \text{if} \quad r\in J_+. \tag{3.84}$$

Indeed, (2.7) gives

$$\frac{-w''}{w'^2}=\frac{\Phi w'+uw}{r^2Aw'^2}>\frac{\Phi w'}{2r^2Aw'^2}, \tag{3.85}$$

because $|\Phi w'|>1$, and $|uw|<\frac{1}{2}$ imply that $\operatorname{sgn}(\Phi w'+uw)=\operatorname{sgn}(\Phi w')$. Thus using (3.78), $\operatorname{sgn}[(\Phi w'+uw)/r^2Aw'^2]=\operatorname{sgn}[\Phi w'/A]=\operatorname{sgn}w'>0$, and this gives (3.84).

Next, we show

$$\frac{-\Phi w'}{2r^2Aw'^2}\leqslant-c^2w'(r), \quad \text{if } r\in J_+, \quad r\leqslant\xi, \tag{3.86}$$

where

$$c^2=\frac{\eta}{8\bar{r}^2L}. \tag{3.87}$$

To see this we have, for $r\in J_+$, $r\leqslant\xi$,

$$\frac{\Phi w'}{2r^2Aw'^2}=\left|\frac{\Phi w'}{2r^2Aw'^2}\right|\geqslant\frac{\eta w'}{2r^2L}\geqslant\frac{\eta w'}{8\bar{r}^2L}, \tag{3.88}$$

since $r\leqslant\xi<\beta\leqslant 2\bar{r}$, and this gives (3.86).

Now if $r\in J_+$, $r\leqslant\xi$, (3.84) and (3.88) give

$$\frac{w''}{w'^2}\leqslant -c^2w'.$$

Integrating this from α to ξ gives

$$-\frac{1}{w'(\xi)}<\frac{1}{w'(\alpha)}-\frac{1}{w'(\xi)}\leqslant -c^2(w(\xi)-w(\alpha))=-\frac{c^2\Delta}{2},$$

so that $w'(\xi)<2/c^2\Delta=16\bar{r}^2L/\eta\Delta\leqslant m$, and this contradicts (3.83). Thus the lemma is proved if we are on J_+, and both (3.78) and (3.79) hold.

Now suppose that we are on J_-, and both (3.78), and (3.79) hold. It is clear that in this case the same proof works; we merely substitute $-\beta$ for α and $-\alpha$ for β.

Next, consider the case where $w'<0$, (on J_+ or J_-), and (3.79) holds. Note that if (A,w) is a solution of (2.1), (2.2), then so is $(A,-w)$. Also, if (A,w) satisfies the hypotheses of the lemma, so does $(A,-w)$; this shows that the case $w'<0$ is reduced to the case $w'>0$.

Finally, suppose that $A\phi<0$, on J (where $J=J_+$ or J_-). We extend the functions A and w to $-J$ by defining

$$(A(-r),w(-r))=(A(r),w(r)),\quad r\in J.$$

Since $\Phi(-r)=-\Phi(r)$, we see that $A\Phi>0$ on $-J$. Thus, applying what we have already proved to $-J$ gives that $(-A,-w)$ satisfies the conclusions of the lemma, and hence so does (A,w). This completes the proof of Lemma 21. ■

We now return to the proof of Proposition 17. For this, we shall use Lemmas 18 and 21. Thus, choose n so large that $b_n<2\bar{r}$; cf. (3.62). Now we apply Lemma 21 to the intervals $J_n=[c_n,d_n]$; the hypotheses of Lemma 21 are valid because of Proposition 10, and (3.65)–(3.67), of Lemma 18. We conclude that for large n, $d_n-c_n\geqslant\zeta$, where ζ is independent of n. Thus for large n, $b_n-a_n\geqslant\zeta$, and this contradicts (3.62). The proof of Proposition 17 is complete. ■

We now return to the proof of Theorem 1. For this, recall that from Corollary 5, we have that for r near $\bar{r}$, one of the following must hold: either $w^2(r)<1$, or $w(r)>1$, or $w(r)<-1$. In view of Propositions 16 and 17, the orbit $(w(r),w'(r))$ cannot have infinite rotation about (0,0); thus for r near r, we may assume that the orbit does not cross $w=0$. We shall show that in all of the above cases both A and w' are each of fixed sign for r near $\bar{r}$, and then Proposition 15 will complete the proof of Theorem 1.

To carry out this program, we first note that for r near $\bar{r}$, we cannot have both $A(r)=0=w'(r)$. Indeed, for r near $\bar{r}$, our above remarks imply that $(uw)(r)\neq 0$, so that (2.2) implies that not both $A(r)$ and $w'(r)$ can be zero. Similarly, not both $A(r)$ and $A'(r)$ can be zero for some $r>\bar{r}$, since if this were so, (2.6) implies $\Phi(r)=0$ so (2.7) would give the contradiction $(uw)(r)=0$.

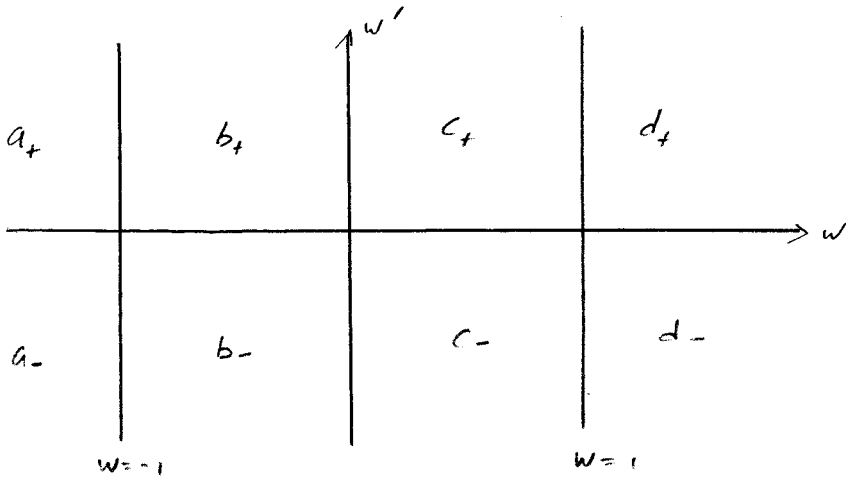

FIG. 10. $a \cup b \cup c \cup d$.

Now let us denote the region $w<-1$ by $a=a_+\cup a_-$ (cf. Fig. 10); the region $-1<w<0$ by $b=b_+\cup b_-$; the region $0<w<1$ by $c_+\cup c_-$; and the region $1<w$ by $d_+\cup d_-$. For r near $\bar{r}$, we may assume that the orbit lies in precisely one of the regions a, b, c, or d.

Lemma 22: If $v(s)=0$, for s near $\bar{r}$, then $(uwv')(s)<0$.

Proof: If s is near $\bar{r}$, then $(uw)(s)\neq 0$, by our above remarks. Thus from (3.39),

$$(uwv')(s)=-\frac{u^2(s)w^2(s)}{s^2}<0,$$

and this proves the lemma. ■

We can now complete the proof of Theorem 1. Namely, if r is near $\bar{r}$, then we have $(uw)(r)\neq 0$. Thus the last lemma shows that v changes sign at every zero. Since v can have at most one sign change in each of the regions a, b, c, or d, A, and w' can have at most one sign change between them. Thus for r near $\bar{r}$, A and w' each are of fixed sign. As we have noted above, Proposition 15 completes the proof of Theorem 1. ■

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Conformal gauge theory of (2+1)-dimensional gravity

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A conformal gauge theory of (2+1)-dimensional gravity is developed within a fiber-bundle structure. Here gravitational field variables are triads and Lorentz gauge potentials, both introduced under a nonlinear realization, which leads to a spontaneous break of symmetry. The most general gravitational Lagrangian density is given in a quadratic form of the conformal invariant gauge fields. We also obtain the Poincaré gauge theory in vacuum. In a weak-field limit the gravitational field equations for a static and spinless point-like source, are naturally reduced to the Newtonian case. © *1996 American Institute of Physics.* [S0022-2488(96)01502-6]

I. INTRODUCTION

Models with lower-dimensional gravity have demonstrated considerable attention recently, with the purpose to study gravity as a field theory. We remind that Einstein's theory of general relativity (GR) has no Newtonian limit and no dynamical degrees of freedom in (2+1) dimensions,[1–3] but it has nontrivial global structures. At the classical level analogies between Yang–Mills (YM) gauge theory and GR have long been studied, under their common basic geometrical setting. A conformally invariant gauge theory in (2+1) dimensions is equivalent to a YM gauge theory of the conformal group in three dimensions, with a Chern–Simons action. This means that conformal gravity is finite and exactly soluble.[4]

We recall that when we look for a space–time gauge model for gravity, it is necessary to investigate the features of space–time gauge-like characteristics, because on any differentiable manifold there is the bundle of affine frames, naturally defined, whose structural group is the affine linear group $AL(n,\mathscr{R})$. In particular, for the space–time case, the requirement of Lorentz frames reduces $AL(n,\mathscr{R})$ to the Poincaré group (P_4). Gravitational gauge theories for the P_4 group have been extensively studied as alternative theories for gravity. The structure of P_4 gauge field equations for gravity, and their Einsteinian content, under duality conditions for the sourceless case, was first pointed out by Baekler *et al.*[5]

A YM gravitational model for the P_4 group, under an Inonu–Wigner contraction of the gauge fields, has been pointed out before. In that case, the absence of metric for the group manifold, because P_4 is not a semisimple group, does not allow one to establish a Lagrangian density in this theory. Such a problem has been circumvented by means of Lie algebra invariants.[6] The disagreements to a P_4 gauge model for gravity may be justified by two main reasons: it is not a Lagrangian gauge theory under gauge-like conditions, and if one tries to quantize it, vertices are not well defined.[7] However, in spite of the absence of a group metric, a$(2-d)$ gauge theory for the Poincaré group can be constructed.[8] We notice that a Poincaré (2+1)-dimensional gauge theory for gravity was also developed recently by Kawai,[9] where has been shown among other things that solutions of the vacuum Einstein equation satisfy gravitational field equations in the vacuum of the Poincaré theory.

In a previous paper we have pointed out that the inclusion of a source in the rotational sector of a YM theory for gravity with the group P_4, violates the conservation law of Einstein's tensor.[10] The purpose of the present paper is to develop a conformal gauge theory of (2+1)-dimensional gravity, and analyze the aspects of this approach in two cases: a Poincaré gauge theory properly, which is obtained as a subtheory of the conformal case, and afterward Newton's theory of gravity in a spinless weak-field limit.

II. FIBER-BUNDLE STRUCTURE WITH CONFORMAL SYMMETRY

Here we consider a gauge model in a fiber bundle $P=(M,G)$, where M is the base-manifold (Minkowski space–time) and G is the conformal group. The $\mathscr{G}$ algebra of G is a vector space, given by the direct sum $\mathscr{G}=\mathscr{R}\oplus\mathscr{T}\oplus\mathscr{C}\oplus\mathscr{D}$, where $\mathscr{R}$ and $\mathscr{T}$ are, respectively, the rotational and translation sectors of $\mathscr{G}$, $\mathscr{C}$ is the conformal sector, and $\mathscr{D}$ is the sector related to dilatations. Differential forms are written in a coordinate basis $\{dx^{\mu}\}$ in space–time and are valued in the $\mathscr{G}$ algebra. Since G is a semisimple group, it allows us to write a gauge Lagrangian density in this approach. In the present paper the space–time metric is $g_{\mu\nu}$ and the group metric is η_{ab}. Greek indices are referred to space–time and have the range $\mu,\nu,...,0,1,2$ and Latin indices have the respective ranges $A,B,...=0,1,2,4,6$, and $a,b,...=0,1,2$.

A. Preliminary review on conformal transformations

In special relativity (SR) the invariance of the space–time interval $ds^2=dx_{\mu}\,dx^{\mu}=ds'^2$ ensures the constancy of the speed of light, and the equivalence between inertial frames of reference. SR transformations of coordinates between two frames are Lorentz transformations added by translations $x'^{\mu}=\Lambda^{\mu}_{\nu}x^{\nu}+a^{\mu}$, which characterizes the inhomogeneous Lorentz group (Poincaré group). If we extend the condition $ds^2=ds'^2=0$, we see that the following transformations are also possible: (a) dilatations, $x'^{\mu}=x^{\mu}+\epsilon x^{\mu}$; (b) special conformal transformations, which are generated by an inversion $(x'^{\mu}=k^2x^{\mu}/x^{\nu}x_{\nu})$, a translation and another inversion $x'^{\mu}=x^{\mu}+\alpha^{\mu}x^2-2x^{\mu}\alpha x$. Thus, the generalization of SR transformations in (3+1) dimensions of the Poincaré group is given by a 15-parameter group, the conformal group SO(4,2). Conformal invariance has been considered in physics for the first time by Bateman,[11] pointing out the covariance of Maxwell's equations under conformal transformations. Afterward it was enhanced that massive particles are not invariant under conformal transformations, and in 1972 Barut, Rolf, and Haugen[12] developed a theory, including concepts of conformal invariance for mass and charge. Later, Wess[13] pointed out the conformal invariance of the stress-energy tensor, which is the source of a gauge field theory. The main characteristic of the conformal group is that it encompasses a set of general transformations that preserve the speed of light. In (2+1) dimensions this group has ten parameters (three rotations L, three translations P, three conformal transformations K, and one dilatation D), and it is denoted by the SO(3,2) group.

Differential group generators are $M_{AB}=-i(\eta_A\partial_B-\eta_B\partial_A)$, or in the $\mathscr{R}^3$ space,

$$p_a=-i\partial_a,\quad l_{ab}=x_bp_a-x_ap_b,\quad d=x^ap_a,\quad k_a=(2x_ax^b-x^2\delta^b_a)p_b, \tag{2.1}$$

and the action of operators in a matter field is given below for each case:

$$\begin{gathered} L_{ab}\Psi=l_{ab}\Psi+\Sigma_{ab}\Psi,\quad P_a\Psi=p_a\Psi,\\ K_a\Psi=k_a\Psi+\kappa_a\Psi-2x^b(g_{ab}\Delta-\Sigma_{ab}\Psi),\quad D\Psi=d\Psi+\Delta\Psi, \end{gathered} \tag{2.2}$$

where Σ_{ab}, Δ, and κ_a represent the respective generators of each sector of the conformal group. The commutation relations for the conformal group with generators J_{AB} are in the $\mathscr{R}^5$ space the usual ones of orthogonal groups, and become in the $\mathscr{R}^3$ space,

$$\begin{gathered} \frac{1}{i}[L_{ab},L_{cd}]=\eta_{ad}L_{bc}-\eta_{ac}L_{bd}-\eta_{bd}L_{ac}+\eta_{bc}L_{ad},\\ \frac{1}{i}[L_{ab},P_c]=\eta_{bc}P_a-\eta_{ac}P_b,\quad \frac{1}{i}[L_{ab},K_c]=\eta_{bc}K_a-\eta_{ac}K_b,\quad \frac{1}{i}[L_{ab},D]=0,\\ \frac{1}{i}[P_a,P_b]=0,\quad \frac{1}{i}[P_a,K_b]=-2(\eta_{ab}D+L_{ab}),\quad \frac{1}{i}[P_a,D]=-P_a, \end{gathered} \tag{2.3}$$

$$\frac{1}{i}[K_a,K_b]=0, \quad \frac{1}{i}[K_a,D]=K_a, \quad \frac{1}{i}[D,D]=0.$$

B. $\mathscr{G}$-valued connection and curvature forms

The covariant derivative for the conformal group algebra is defined by

$$D_\mu\Psi=\{\partial_\mu+i(\tfrac{1}{2}A_\mu^{ab}[L]L_{ab}+A_\mu^a[K]K_a+A_\mu^a[P]P_a+A_\mu[D]D)\}\Psi, \tag{2.4}$$

where

$$A_\mu=\tfrac{1}{2}A_\mu^{ab}[L]L_{ab}+A_\mu^a[P]P_a+A_\mu^a[K]K_a+A_\mu[D]D \tag{2.5}$$

is the connection form, transformed according to $A_\mu\to g^{-1}A_\mu g+ig^{-1}\,\partial_\mu g$, where $g\in G$. The curvature form is the covariant derivative of the connection $\mathbf{A}$: $\mathbf{\Omega}=\mathbf{dA}+[\mathbf{A},\mathbf{A}]$, and under the action of the group element g it is transformed by $\mathbf{\Omega}\to g^{-1}\mathbf{\Omega}g$. In the $\mathscr{R}^5$ space we have $\Omega_{\mu\nu}=\frac{1}{2}\Omega_{\mu\nu}^{AB}J_{AB}$, where

$$\Omega_{\mu\nu}^{AB}=\partial_\mu A_\nu^{AB}-\partial_\nu A_\mu^{AB}-(A_{C\mu}^A A_\nu^{CB}-A_{C\nu}^A A_\mu^{CB}). \tag{2.6}$$

In the $\mathscr{R}^3$ space $\mathbf{\Omega}$ has the components

$$\Omega_{\mu\nu}=\Omega_{\mu\nu}^{ab}[L]L_{ab}+\Omega_{\mu\nu}^a[P]P_a+\Omega_{\mu\nu}^a[K]K_a+\Omega_{\mu\nu}[D]D, \tag{2.7}$$

where

$$\begin{aligned}\Omega_{\mu\nu}^{ab}[L]=&\partial_\mu A_\nu^{ab}[L]-\partial_\nu A_\mu^{ab}[L]-(A_{c\mu}^a[L]A^{cb}[L]-A_{c\mu}^a[L]A_\mu^{cb}[L])+2(A_\mu^a[P]A_\nu^b[K]\\&-A_\mu^b[P]A_\nu^a[K])-2(A_\nu^a[P]A_\mu^b[K]-A_\nu^b[P]A_\mu^a[K]),\end{aligned} \tag{2.8}$$

$$\begin{aligned}\Omega_{\mu\nu}^a[P]=&\partial_\mu A_\nu^a[P]-\partial_\nu A_\mu^a[P]-(A_{c\mu}^a[L]A_\nu^c[P]-A_{c\nu}^a[L]A_\mu^c[P])\\&+(A_\mu^a[P]A_\nu[D]-A_\nu^a[P]A_\mu[D]),\end{aligned} \tag{2.9}$$

$$\begin{aligned}\Omega_{\mu\nu}^a[K]=&\partial_\mu A_\nu^a[K]-\partial_\nu A_\mu^a[K]-(A_{c\mu}^a[L]A_\nu^c[K]-A_{c\nu}^a[L]A_\mu^c[K])\\&+(A_\mu^a[K]A_\nu[D]-A_\nu^a[K]A_\mu[D]),\end{aligned} \tag{2.10}$$

$$\Omega_{\mu\nu}[D]=\partial_\mu A_\nu[D]-\partial_\nu A_\mu[D]+2(A_\mu^a[P]A_{a\nu}[K]-A_\nu^a[P]A_{a\mu}[K]). \tag{2.11}$$

C. Triads

Gauge theories of gravity differ from the usual YM theory because they contain a strong relation to space–time, i.e., the fiber space is isomorphic to the tangent space–time. Such a isomorphism is represented by the solder form $S=P_a h_\mu^a\,dx^\mu$, whose components in (2+1) dimensions are the triads, where P_a are generators of translations. In the case where space–time is a simple transformation of coordinates of the tangent space T_xM, the triads are given by $h_\mu^a=\partial_\mu x^a$, and we do not have a true gravitational field generated by triads, but instead, we have fictitious forces like the centrifugal force and the Coriolis force. However, if h_μ^a are not integrable, we can define a true gravitational field that does not vanish under a particular choice of coordinates. Triads allow us to obtain dual physical quantities like (v^μ,v^a) that are related by $v^\mu=h_a^\mu v^a$ and $v_\mu=h_\mu^a v_a$. By the same reason the metric η_{ab} is "projected" onto the base manifold by the triads $g_{\mu\nu}=\eta_{ab}h_\mu^a h_\nu^b$. The field associated to these triads is the torsion field, whose components are $T_{lm}^k=h_l^\mu h_m^\nu(\partial_\mu h_\nu^k-\partial_\nu h_\mu^k)-h_l^\mu A_{ml}^k+h_m^\mu A_{l\mu}^k$, where A_μ^{kl} is the Lorentz potential.

Inclusion of the above fields in a Lorentz theory is not usual in gauge theories in general. The potential in a gauge theory is such that $\partial_\mu \to \partial_\mu + iA_\mu$ with $A_\mu \to g^{-1}A_\mu g + ig^{-1}\,\partial_\mu g$, where the triad field leads to $\partial_\mu \to \partial_\mu$ and $h_\mu \to g^{-1}h_\mu g$. An argument to consider h^a_μ as a potential of the theory is that in a gauge theory for the group of translations the triads are given by the Kibble prescription[14] $h^a_\mu = \delta^a_\mu + B^a_\mu$, where B^a_μ is the gauge potential. This implies that dynamical properties of triads must be the same ones of the gauge potential. At a first view we could assume the potential in the form $\mathbf{\Gamma} = \mathbf{A} + \mathbf{S}$ and the field would become $\mathbf{\Omega} = \mathbf{R} + \mathbf{T} = D_{\mathbf{\Gamma}}\mathbf{\Gamma} = D_{\mathbf{A}}\mathbf{A} + D_{\mathbf{A}}\mathbf{S}$. However, the best way to include triads in this approach is by means of a nonlinear realization of the conformal group. The procedure is to extend the definition of triads to the form $h^a_\mu = D_\mu x^a$, where D_μ is a generalized group covariant derivative in a nonlinear realization.

D. Nonlinear realization

A simple reason to consider a nonlinear realization is to reduce the gauge symmetry of G to a subsymmetry H in a situation of spontaneous break of symmetry. This is the case of a conformal symmetry that must be broken down in order to be applied to the real world. Moreover, we employ this argument with the purpose to obtain a representation where some potentials are transformed covariantly. The first step is to define a "reduction matrix" $(L_\phi)_{\alpha\beta}$, whose elements are field variables.

Salam and Strathdee[15] pointed out that for a gauge theory with potentials $A_{\mu i}$, the nonlinear derivative operator can be split up into covariant terms $D_\mu \psi = (\partial_\mu + iB_{\mu a}M^a)\psi$ and $D_\mu \phi_b = B_{\mu b}$, where $B_{\mu a}$ are the potentials in the algebra $\mathscr{H}$, $B_{\mu b}$ are the potentials in the algebra $\mathscr{G} - \mathscr{H}$, and ϕ_b are fields of the reduction matrix.

Following Salam–Strathdee's suggestion, we assume that for the conformal group we have $L_\phi = \exp[P + i\phi K - i\sigma D]$, and then we define the new potentials

$$\omega^{ij}_\mu = L_\phi^{-1}A^{ij}_\mu[L]L_\phi - iL_\phi^{-1}\,\partial_\mu L_\phi, \quad \omega^i_\mu = L_\phi^{-1}A^a_\mu[P]L_\phi - L_\phi^{-1}\,\partial_\mu L_\phi, \tag{2.12}$$

$$\bar{\omega}^i_\mu = L_\phi^{-}A^a_\mu[K]L_\phi - iL_\phi^{-1}\,\partial_\mu L_\phi, \quad \omega_\mu = L_\phi^{-1}A_\mu[D]L_\phi - iL_\phi^{-1}\,\partial_\mu L_\phi. \tag{2.13}$$

Thus, the covariant derivative becomes $D_\mu \psi = \{\partial_\mu + \frac{1}{2}A^{ab}{}_\mu[L]L_{ab}]\}\psi$, and for the field derivatives we obtain $D_\mu x^a = \omega^a_\mu$, $D_\mu \phi^a = \bar{\omega}^a_\mu$, $D_\mu \sigma = -\omega_\mu$, which lead to the transformation laws

$$\begin{gathered} \omega^{ij}{}_\mu \to h\omega^{ij}{}_\mu h^{-1} - ih\,\partial_\mu h^{-1}\,L^{ij}, \\ \omega^i_\mu \to h\omega^i_a h^{-1}, \quad \bar{\omega}^i_\mu \to h\bar{\omega}^i_\mu h^{-1}, \quad \omega_\mu \to h\omega_\mu h^{-1}. \end{gathered} \tag{2.14}$$

This means that the potentials ω^i_μ, $\bar{\omega}^i_\mu$ and ω_μ are transformed covariantly. Besides, we identify in the equation for ω^a_μ the definition of triads, in such a way that in this representation they are given by $h^a_\mu \equiv \omega^a_\mu$. Moreover, the new fields are now defined by $F_{\mu\nu} = L_\phi^{-1}G_{\mu\nu}L_\phi$, and they are written in terms of the new potentials according to

$$f^{ab}{}_{\mu\nu} = \partial_\mu \omega^{ab}_\nu - \partial_\nu \omega^{ab}_\mu - (\omega^a_{c\mu}\omega^{cb}_\nu - \omega^a_{c\nu}\omega^{cb}_\mu) + 2(\omega^a_\mu \bar{\omega}^b_\nu - \omega^b_\mu \bar{\omega}^a_\nu - \omega^a_\nu \bar{\omega}^b_\mu + \omega^b_\nu \bar{\omega}^a_\mu), \tag{2.15}$$

$$T^a{}_{\mu\nu} = \partial_\mu \omega^a_\nu - \partial_\nu \omega^a_\mu - (\omega^a_{c\mu}\omega^c_\nu - \omega^a_{c\nu}\omega^c_\mu) + (\omega^a_\mu \omega_\nu - \omega^a_\nu \omega_\mu), \tag{2.16}$$

$$t^a{}_{\mu\nu} = \partial_\mu \bar{\omega}^a_\nu - \partial_\nu \bar{\omega}^a_\mu - (\omega^a_{c\mu}\bar{\omega}^c_\nu - \omega^a_{c\nu}\bar{\omega}^c_\mu) - (\bar{\omega}^a_\mu \omega_\nu - \bar{\omega}^a_\nu \omega_\mu), \tag{2.17}$$

$$F_{\mu\nu} = \partial_\mu \omega_\nu - \partial_\nu \omega_\mu + 2(\omega^a_\mu \bar{\omega}_{a\nu} - \omega^a_\nu \bar{\omega}_{a\mu}). \tag{2.18}$$

E. Relations to space–time

For a vector field V^k the covariant derivative is now $D_l V^k = \omega_l^{\nu} \omega_{\mu}^k \, D_{\nu} V^{\mu}$, thus we can define an affine connection $\Gamma_{\lambda\nu}^{\mu}$ in such a way that $D_{\nu} V^{\mu} = \partial_{\nu} V^{\mu} + \Gamma_{\lambda\nu}^{\mu} V^{\lambda}$ and, moreover, $A^k{}_{l\mu} = -\Gamma_{\lambda\mu}^{\nu} \omega_{\nu}^k \omega_l^{\lambda} - \omega_{\nu}^k \, \partial_{\mu} \omega_l^{\nu}$. After multiplying both sides of this expression by $\omega_{\lambda}^l \omega_k^{\nu}$, we get

$$\Gamma_{\lambda\mu}^{\nu} = -A^k{}_{l\mu} \omega_{\lambda}^l \omega_k^{\nu} - \omega_{\lambda}^l \, \partial_{\mu} \omega_l^{\nu} . \tag{2.19}$$

If we now define $T_{\mu\nu}^{\lambda} = \omega_k^{\lambda} T^k{}_{\mu\nu}$, we are led to

$$T_{\mu\nu}^{\lambda} = \Gamma_{\mu\nu}^{\lambda} - \Gamma_{\nu\mu}^{\lambda} + \delta_{\mu}^{\lambda} \omega_{\nu} - \delta_{\nu}^{\lambda} \omega_{\mu} , \tag{2.20}$$

which generalizes the torsion tensor. We also obtain that

$$\Gamma^{\lambda}{}_{\mu\nu} = \{^{\lambda}_{\mu\nu}\} + K^{\lambda}{}_{\mu\nu} + D^{\lambda}{}_{\mu\nu} , \tag{2.21}$$

where the first term represents the Christoffel symbols $\{^{\lambda}_{\mu\nu}\} = 1/2 g^{\lambda\xi} (\partial_{\mu} g_{\xi\nu} + \partial_{\nu} g_{\xi\mu} - \partial_{\xi} g_{\mu\nu})$, the second term in the above equation is the contorsion tensor,

$$K_{\mu\nu}^{\lambda} = -\tfrac{1}{2} (T^{\lambda}{}_{\mu\nu} - T_{\mu}{}^{\lambda}{}_{\nu} - T_{\nu}{}^{\lambda}{}_{\mu}), \tag{2.22}$$

and the third one is related to dilatations

$$D_{\lambda\mu\nu} = g_{\mu\nu} \omega_{\lambda} - g_{\lambda\nu} \omega_{\mu} . \tag{2.23}$$

The projection on space–time of the field components $f_{\mu\nu}^{ab}$, given in Eq. (2.15), is now

$$f_{\mu\nu}^{\lambda\rho} = \omega_a^{\lambda} \omega_b^{\rho} f_{\mu\nu}^{ab} = R^{\lambda\rho}{}_{\mu\nu} + (\delta_{\mu}^{\lambda} \omega_b^{\rho} \, \bar{\omega}_{\nu}^b - \delta_{\mu}^{\rho} \omega_a^{\lambda} \, \bar{\omega}_{\nu}^a - \delta_{\nu}^{\lambda} \omega_b^{\rho} \, \bar{\omega}_{\mu}^b + \delta_{\nu}^{\rho} \omega_a^{\lambda} \, \bar{\omega}_{\mu}^a), \tag{2.24}$$

where the first term above stands for the Riemann tensor,

$$R_{\rho\mu\nu}^{\lambda} = \partial_{\mu} \Gamma_{\rho\nu}^{\lambda} - \partial_{\nu} \Gamma_{\rho\mu}^{\lambda} + \Gamma_{\sigma\nu}^{\lambda} \Gamma_{\rho\nu}^{\sigma} - \Gamma_{\sigma\mu}^{\lambda} \Gamma_{\rho\nu}^{\sigma} , \tag{2.25}$$

and the remaining terms in Eq. (2.24) are concerning special conformal transformations.

III. FIELD EQUATIONS

We can derive now the field equations for a conformal theory, taking into account the corresponding potentials and fields obtained before. We want to establish a general gauge theory of (2+1)-dimensional gravity with conformal symmetries, which is reduced to a Newtonian theory in the limit $c \to \infty$, but keeping in mind that we must assume an invariant action.

A. Gauge Lagrangian structure

In YM gauge theories the invariant Lagrangian density is $\mathscr{L} = F^{\mu\nu} F_{\mu\nu}$, however, in a conformal theory, since all sectors of $\mathscr{G}$ constitute independent subalgebras, we can extend the Lagrangian density to the form $\mathscr{L} = \mathscr{L}_L + \mathscr{L}_P + \mathscr{L}_K + \mathscr{L}_D$, with $\mathscr{L}_L$, $\mathscr{L}_P$, $\mathscr{L}_K$, and $\mathscr{L}_D$ all quadratic in the potentials f, T, t and F, respectively. Otherwise, for the rotational sector we have an analogous relation to the Riemann–Ricci relation,

$$f_{\mu\nu}^{ab} = \omega_{\mu}^a f_{\nu}^b - \omega_{\nu}^a f_{\mu}^b - \omega_{\mu}^b f_{\nu}^a + \omega_{\nu}^b f_{\mu}^a - \tfrac{1}{2} (\omega_{\mu}^a \omega_{\nu}^b - \omega_{\nu}^a \omega_{\mu}^b) f, \tag{3.1}$$

where $f = \omega_c^{\rho} f_{\rho}^c$, which points out that the most general Lagrangian in the rotational sector will be given in terms of f_{ν}^b instead of terms in $f_{\mu\nu}^{ab}$. Hence, the fields that must be taken into account in the Lagrangian density are

$$P^{kl}=\omega^{\sigma l}\omega^{\rho}_{a}(\partial_{\rho}\omega^{ak}_{\sigma}-\partial_{\sigma}\omega^{ak}_{\rho}-\omega^{a}_{cp}\omega^{ck}_{\sigma}+\omega^{a}_{c\sigma}\omega^{ck}_{\rho})+2(\omega^{\sigma l}\bar{\omega}^{k}_{\sigma}+\omega^{\sigma}_{\alpha}\bar{\omega}^{\alpha}_{\sigma}\eta^{kl}), \tag{3.2}$$

$$T^{k}{}_{lm}=\omega^{\alpha}_{l}\omega^{\beta}_{m}(\partial_{\alpha}\omega^{k}_{\beta}-\partial_{\beta}\omega^{k}_{\alpha})-\omega^{k}{}_{m\alpha}\omega^{\alpha}_{l}+\omega^{k}{}_{l\alpha}\omega^{\alpha}_{m}+\delta^{k}_{l}\omega^{\alpha}_{m}\omega_{\alpha}-\delta^{k}_{m}\omega^{\alpha}_{l}\omega_{\alpha}, \tag{3.3}$$

$$t^{k}{}_{lm}=\omega^{\alpha}_{l}\omega^{\beta}_{m}[\partial_{\alpha}\bar{\omega}^{k}_{\beta}-\partial_{\beta}\bar{\omega}^{k}_{\alpha}-(\omega^{k}_{c\alpha}\bar{\omega}^{c}_{\beta}-\omega^{k}{}_{c\beta}\bar{\omega}^{c}_{\alpha})-(\bar{\omega}^{k}_{\alpha}\omega_{\beta}-\bar{\omega}^{k}_{\alpha}\omega_{\alpha})], \tag{3.4}$$

$$F_{kl}=\omega^{\rho}_{k}\omega^{\sigma}_{l}(\partial_{\rho}\omega_{\sigma}-\partial_{\sigma}\omega_{\rho})+2(\omega^{\rho}_{l}\bar{\omega}_{k\rho}-\bar{\omega}_{l\rho}\omega^{\rho}_{k}). \tag{3.5}$$

Partial Lagrangian densities are then

$$\mathscr{L}_{L}=a_{1}E^{kl}E_{kl}+a_{2}I^{kl}I_{kl}+a_{3}P, \tag{3.6}$$

$$\mathscr{L}_{P}=2\,f^{klm}f_{klm}+\beta v^{k}v_{k}+\gamma a^{klm}a_{klm}, \tag{3.7}$$

$$\mathscr{L}_{K}=\mu g^{klm}g_{klm}+\nu u^{k}u_{k}+\rho b^{klm}b_{klm}, \tag{3.8}$$

$$\mathscr{L}_{D}=bF^{kl}F_{kl}, \tag{3.9}$$

where a_1, a_2, a_3, b, β, γ, μ, ν, and ρ are arbitrary coefficients. In the above equations we have defined the traceless and symmetric components of **T**, its trace and its antisymmetrical components, given, respectively, by

$$f^{klm}=\tfrac{1}{2}\,(T^{klm}+T^{klm})+\tfrac{1}{4}\,(\eta^{mk}v^{l}+\eta^{ml}v^{k})-\tfrac{1}{2}\,\eta^{kl}v^{m}, \tag{3.10}$$

$$v_{k}=T^{l}{}_{lk}, \tag{3.11}$$

$$a_{klm}=\tfrac{1}{3}\,(T_{klm}+T_{mkl}+T_{lmk}). \tag{3.12}$$

In an analogous manner we have for **t**,

$$g^{klm}=\tfrac{1}{2}\,(t^{klm}+t^{lkm})+\tfrac{1}{4}\,(\eta^{mk}u^{l}+\eta^{ml}u^{k})-\tfrac{1}{2}\,\eta^{kl}u^{m}, \tag{3.13}$$

$$u^{k}=t^{l}{}_{lk}, \tag{3.14}$$

$$b_{klm}=\tfrac{1}{3}\,(t_{klm}+t_{mkl}+t_{lmk}), \tag{3.15}$$

and finally for **P**,

$$I^{kl}=\tfrac{1}{2}\,(P^{kl}+P^{lk})-\tfrac{1}{3}\,\eta^{kl}P, \tag{3.16}$$

$$E^{kl}=\tfrac{1}{2}\,(P^{kl}-P^{lk}), \tag{3.17}$$

$$P=P^{k}_{k}. \tag{3.18}$$

The total action is now

$$I=\int\sqrt{g}(\mathscr{L}_{L}+\mathscr{L}_{P}+\mathscr{L}_{K}+\mathscr{L}_{D}+g\mathscr{L}_{M})\;d^{3}x, \tag{3.19}$$

where $g=\det(g_{\mu\nu})$, $\mathscr{L}_{M}$ is the Lagrangian density of the matter field, and the integral is taken in the whole (2+1) space-time.

B. Field equation from $\delta I / \delta \omega^i_\mu = 0$

The field equations are derived here according to the usual procedure of Lagrangian theories, i.e. by means of $\delta I = 0$, from Eq. (3.19). This yields

$$\partial_\nu \frac{\partial(\sqrt{g}\mathscr{L})}{\partial[\partial_\nu A_\mu]} - \frac{\partial(\sqrt{g}\mathscr{L})}{\partial A_\mu} = 0, \tag{3.20}$$

where A_μ is each one of the potentials in our approach. Thus, we have four field equations. Equation (3.20) then becomes for ω^i_μ,

$$\omega_{\mu j} \frac{1}{\sqrt{g}} \frac{\partial\sqrt{g}}{\partial\omega^i_\mu} \mathscr{L}_c + \omega_{\mu j} \frac{\partial\mathscr{L}_c}{\partial\omega_i} - \omega_{\mu j} \frac{\partial_\nu\sqrt{g}}{\sqrt{g}} \frac{\partial\mathscr{L}_c}{\partial(\partial_\nu\omega^i_\mu)} - \omega_{\mu j}\partial_\nu \frac{\partial\mathscr{L}_c}{\partial(\partial_\nu\omega^i_\mu)} = -T_{ij}, \tag{3.21}$$

where we have considered the energy-momentum tensor in the form

$$T_{ij} = \omega_{\mu j} \frac{1}{\sqrt{g}} \frac{\delta\sqrt{g}\mathscr{L}_M}{\delta\omega^i_\mu}. \tag{3.22}$$

Taking into account that $\mathscr{L}_c = \mathscr{L}_L + \mathscr{L}_P + \mathscr{L}_K + \mathscr{L}_D$, the field equation (3.21) turns into

$$\begin{aligned} &-2D^k\bar{F}_{ijk} + 2v^k\bar{F}_{ijk} + 2H_{ij} + 4\bar{F}_{ilj}\omega^l + 4J_{[ik][jl]}P^{kl} + 4J^{[lk]}{}_{[lj]}P_{ki} - 2J^{[il]}{}_{[jl]}P \\ &+ 4J^{[ik]}{}_{[jl]}\omega^\sigma_l\bar{\omega}_{k\sigma} + 2\bar{f}_{kj}{}^m t^k{}_{im} + 4F_j{}^l F_{il} - 3F^{jl}\omega^\rho_l\bar{\omega}_{i\rho} - \eta_{ij}\mathscr{L}_c = T_{ij}, \end{aligned} \tag{3.23}$$

where

$$D^k\bar{F}_{ijk} = \omega^{\mu k}\,\partial_\mu\bar{F}_{ijk} + \omega^m{}_{j\mu}\bar{F}_{imk} + \omega^m{}_{k\mu}\bar{F}_{ijm} + \omega^m{}_{i\mu}\bar{F}_{mjk}, \tag{3.24}$$

$$\bar{F}_{ijk} = \alpha(f_{ijk} - f_{ikj}) + \beta(\eta_{ij}v_k - \eta_{ik}v_j) + 2\gamma a_{ijk}, \tag{3.25}$$

$$H_{ij} = \bar{F}_{kj}{}^m T^k{}_{im} - \tfrac{1}{2}\bar{F}_i{}^{lm}T_{jlm}, \tag{3.26}$$

$$J_{ijkl} = 2a_3\eta_{ik}\eta_{jl}P + 2a_1\eta_{ik}E_{jl} + 2a_2\eta_{ik}I_{jl}, \tag{3.27}$$

$$\bar{f}_{klm} = \mu(g_{klm} - g_{kml}) + \nu(\eta_{kl}u_m - \eta_{km}v_l) + 2\rho b_{klm}. \tag{3.28}$$

Since the fields are transformed covariantly the only derivative to be considered is the covariant derivative, and then the potentials $\bar{\omega}_{kj}$ and ω_l are also covariantly transformed. As as consequence, we conclude that Eq. (3.23) is covariant under transformations of the conformal group, as desired.

C. Field equation from $\delta I / \delta \omega^{ij}{}_\mu = 0$

The field equation derived from Eq. (3.20) for the potential $\omega^{ij}{}_\mu$ is

$$\omega_{\mu k'} \frac{\partial\mathscr{L}_c}{\partial\omega^{ij}{}_\mu} - \omega_{\mu k'} \frac{\partial_\nu\sqrt{g}}{\sqrt{g}} \frac{\partial\mathscr{L}_c}{\partial(\partial_\nu\omega^{ij}{}_\nu)} - \omega_{\mu k'}\partial_\nu \frac{\partial\mathscr{L}_c}{\partial(\partial_\nu\omega^{ij}{}_\mu)} = S_{ijk'}, \tag{3.29}$$

where $S_{ijk'}$ is the spin density, which is defined by

$$S_{ijk'} = \frac{-\omega_{\mu k'}}{\sqrt{g}} \frac{\delta\sqrt{g}\mathscr{L}_M}{\delta\omega^{ij}{}_\mu}. \tag{3.30}$$

This yields

$$2D^{l}J_{[ij][kl]}+(\tfrac{4}{3}\,t_{k}^{\,[lm]}-\delta_{k}^{\,[l}v^{m]}+a_{k}^{\,lm})J_{[ij][lm]}+H_{ijk}+2(\eta_{k}^{\,[l}\omega^{m]}J_{[ij][kl]}+G_{ijk}=S_{ijk}, \tag{3.31}$$

where

$$D^{l}J_{[ij][kl]}=\omega^{\mu l}(\partial_{\mu}J_{[ij][kl]}+\omega^{m}{}_{i\mu}J_{[mj][kl]}+\omega^{m}{}_{j\mu}J_{[im][kl]}+\omega^{m}{}_{k\mu}J_{[ij][ml]}+\omega^{m}{}_{l\mu}J_{[ij][km]}), \tag{3.32}$$

$$H_{ijk}=\alpha(t_{kji}-t_{kij})+\beta(\eta_{jk}v_{i}-\eta_{il}v_{j})+4\gamma a_{ijk}, \tag{3.33}$$

$$G_{ijk}=\mu\omega_{\mu k}\bar{\omega}^{\mu m}(g_{mji}-g_{mij})+\nu\omega_{\mu l}\bar{\omega}^{\mu m}(\eta_{jm}u_{i}-\eta_{im}u_{j})+4\rho b_{ijm}\omega_{k}^{\mu}\bar{\omega}_{\mu}^{m}, \tag{3.34}$$

$$J_{ijkl}=a_{1}\eta_{ik}E_{jl}+a_{2}\eta_{ik}I_{jl}+a_{3}\eta_{ik}\eta_{jl}P. \tag{3.35}$$

By inspection we see that Eq. (3.31) is also covariant under gauge transformations.

D. Field equation from $\delta I/\delta\bar{\omega}_{\mu}^{i}=0$

Equation (3.20) for the potential $\bar{\omega}_{\mu}^{i}$ is written in the form

$$\omega_{\mu j}\frac{\partial\mathscr{L}_{c}}{\partial\bar{\omega}_{\mu}^{i}}-\omega_{\mu j}\frac{\partial_{\nu}\sqrt{g}}{\sqrt{g}}\frac{\partial\mathscr{L}_{c}}{\partial\,\partial_{\nu}\bar{\omega}_{\mu}^{j}}-\omega_{\mu j}\partial_{\nu}\frac{\partial\mathscr{L}}{\partial(\partial_{\nu}\bar{\omega}_{\mu}^{i})}=-K_{ij}, \tag{3.36}$$

where

$$K_{ij}=\frac{\omega_{\mu j}}{\sqrt{g}}\frac{\delta\mathscr{L}\sqrt{g}}{\delta\bar{\omega}_{\mu}^{i}}. \tag{3.37}$$

This leads to

$$-2\,D^{k}\bar{f}_{ijk}+2v^{k}\bar{f}_{ijk}-\bar{f}_{i}^{\,lm}(\tfrac{4}{3}\,t_{k[lm]}+a_{jlm}+\eta_{j[l}v_{m]}+4J^{[ik]}{}_{[kj]})+8F_{ji}=K_{ij}, \tag{3.38}$$

where

$$D^{k}\bar{f}_{ijk}=\omega^{\mu k}(\partial_{\mu}\bar{f}_{ijk}+\omega^{m}{}_{j\mu}\bar{f}_{imk}+\omega^{m}{}_{k\mu}\bar{f}_{ijm}+\omega^{m}{}_{i\mu}\bar{f}_{mjk}), \tag{3.39}$$

$$\bar{f}_{ilm}=\mu(g_{ilm}-g_{iml})+\nu(\eta_{il}u_{m}-\eta_{im}u_{l})+\rho b_{ilm}, \tag{3.40}$$

$$J_{ijkl}=a_{1}\eta_{ik}E_{jl}+a_{2}\eta_{ik}I_{jl}+a_{3}\eta_{ik}\eta_{jl}P. \tag{3.41}$$

Notice that Eq. (3.38) is also covariant under conformal transformations.

E. Field equation from $\delta I/\delta\omega_{\mu}=0$

In an analogous way to the preceding cases we obtain the conformal covariant equation,

$$-2\,D^{k}F_{jk}+2v^{k}F_{jk}-F^{lm}(\tfrac{4}{3}\,t_{j[lm]}+a_{jlm}+\eta_{j[l}v_{m]})-2F^{l}{}_{j}\omega_{l}+H_{kj}{}^{k}+G_{jk}{}^{k}=D_{j}, \tag{3.42}$$

where

$$D^{k}F_{jk}=\omega^{\mu k}\,\partial_{\mu}F_{jk}+\omega^{m}{}_{j\mu}F_{mk}+\omega^{m}{}_{k\mu}F_{jm}, \tag{3.43}$$

$$H_{ijk}=\alpha(t_{kji}-t_{kij})+\beta(\eta_{jk}v_i-\eta_{ik}v_j)+4\gamma a_{ijk}, \tag{3.44}$$

$$G_{ijk}=\mu\omega_{\mu k}\bar{\omega}^{\mu m}(g_{mji}-g_{mij})+\nu\omega_{\mu k}\bar{\omega}^{\mu m}(\eta_{jm}u_i-\eta_{im}u_j)+4\rho b_{ijm}\omega^{\mu}_{k}\bar{\omega}^{m}_{\mu}. \tag{3.45}$$

IV. LINEARIZED FIELD EQUATIONS

A. Weak-field approach

Now we examine the gravitational field equations (3.23), (3.31), (3.38), and (3.42) in the weak-field limit, i.e. in the case where $a^{i}_{\mu}=\omega^{i}_{\mu}-\delta^{i}_{\mu}$, and $\omega^{ij}{}_{\mu}$, $\bar{\omega}^{i}_{\mu}$, and ω_{μ} are so small that it suffices to take into account only linear terms in a^{i}_{μ}, $\omega^{ij}{}_{\mu}$, $\bar{\omega}^{i}_{\mu}$, and ω_{μ}. In such a procedure we can neglect the distinction between Greek indices and Latin indices $a,b,...$, since geometric quantities are now projected on the base-manifold by trivial triads $h^{a}_{\mu}=\delta^{a}_{\mu}$. In this case the space–time metric is

$$g_{\mu\nu}=\eta_{\mu\nu}+h_{\mu\nu}, \tag{4.1}$$

where $h_{\mu\nu}=a_{\mu\nu}+a_{\nu\mu}$. The field equation (3.23) thus becomes

$$-2\,\partial^{\lambda}F_{\mu\nu\lambda}=T_{\mu\nu}, \tag{4.2}$$

and the field equations (3.31), (3.38), and (3.42) are now, respectively,

$$2\,\partial^{\rho}J_{[\lambda\mu][\nu\rho]}+H_{\lambda\mu\nu}=S_{\lambda\mu\nu}, \tag{4.3}$$

$$-2\,\partial^{\rho}\bar{f}_{\mu\nu\rho}+4J^{[\mu\rho]}{}_{[\rho\nu]}+8F_{\nu\mu}=K_{\mu\nu}, \tag{4.4}$$

$$-2\,\partial^{\nu}F_{\mu\nu}+H_{\mu\nu}{}^{\nu}=D_{\mu}. \tag{4.5}$$

To make clear the contribution of the metric tensor in the above field equations, we rewrite these equations, considering that

$$-A_{ij\mu}=\Delta_{ij\mu}+K_{ij\mu}+D_{ij\mu}, \tag{4.6}$$

where $\Delta_{ij\mu}$ are Ricci rotation coefficients,

$$\Delta_{ij\mu}=\tfrac{1}{2}\,\omega^{k}_{\mu}(C_{ijk}-C_{jik}-C_{kij}), \tag{4.7}$$

with

$$C_{ijk}=\omega^{\nu}_{j}\omega^{\lambda}_{k}(\partial_{\nu}\omega_{i\lambda}-\partial_{\lambda}\omega_{i\nu}). \tag{4.8}$$

Notice that in Eq. (4.6), $K_{ij\mu}$ is the contortion and $D_{ij\mu}$ is an additional term related to dilatations, i.e. $D_{ij\mu}=\omega_{j\mu}\omega_{\nu i}\omega^{\nu}-\omega_{i\mu}\omega_{\nu j}\omega^{\nu}$. With the above results we are led to

$$-f_{ij\mu\nu}=R_{ij\mu\nu}(\{\ \})+f_{ij\mu\nu}(K)+f_{ij\mu\nu}(D), \tag{4.9}$$

where

$$R_{ij\mu\nu}(\{\ \})=\partial_{\mu}\Delta_{ij\nu}-\partial_{\nu}\Delta_{ij\mu}-\Delta_{i}{}^{k}{}_{\mu}\Delta_{jk\nu}+\Delta_{i}{}^{k}{}_{\nu}\Delta_{jk\mu}=\omega_{i\lambda}\omega^{\rho}_{j}R^{\lambda}_{j\mu\nu}(\{\ \}), \tag{4.10}$$

$$f_{ij\mu\nu}(K)=\boldsymbol{\nabla}_{\mu}K_{ij\nu}-\boldsymbol{\nabla}_{\nu}K_{ij\mu}-K_{i}{}^{k}{}_{\mu}K_{jk\nu}+K_{i}{}^{k}{}_{\nu}K_{jk\mu}, \tag{4.11}$$

$$f_{ij\mu\nu}(D)=\bar{\boldsymbol{\nabla}}_{\mu}D_{ij\nu}-\bar{\boldsymbol{\nabla}}_{\nu}D_{ij\mu}-D_{i}{}^{k}{}_{\mu}D_{jk\nu}+D_{i}{}^{k}{}_{\nu}D_{jk\mu}. \tag{4.12}$$

Here $\nabla_\mu K_{ij\nu}$ represents the covariant derivative with respect to the Ricci coefficients for Latin indices, and the covariant derivative with respect to the Levi-Civitá connection $\{^i_{jk}\}$, for Greek indices. Also, $\bar{\nabla}_\mu D_{ij\nu}$ is the covariant derivative with respect to $\Delta_{ij\mu}+K_{ij\mu}$ for Latin indices, and the covariant derivative related to the Levi-Civitá connection, for Greek indices. Moreover, each irreducible part of P^{kl} given in Eq. (3.2) can be divided in three parts, in such a way that the fields J_{ijkl} of Eqs. (3.27), (3.35), and (3.41) may be expressed in the form

$$J_{ijkl}=J_{ijkl}(\{\ \})+J_{ijkl}(K)+J_{ijkl}(D). \tag{4.13}$$

In particular, we also have

$$J_{ijkl}(\{\ \})=2a_2\,\eta_{ik}R_{jl}(\{\ \})+2\left(a_3-\frac{al_2}{3}\right)\eta_{lk}\eta_{jl}R(\{\ \}) \tag{4.14}$$

and

$$\partial^\rho J_{[\lambda\mu][\nu\rho]}(\{\ \})=\partial^\rho\Bigg[a_2(\eta_{\lambda\nu}R_{\mu\rho}-\eta_{\lambda\rho}R_{\mu\nu}-\eta_{\mu\nu}R_{\lambda\rho}+\eta_{\mu\rho}R_{\lambda\nu})+\left(a_3-\frac{a_2}{3}\right)$$
$$\times(\eta_{\lambda\nu}\eta_{\mu\rho}-\eta_{\lambda\rho}\eta_{\mu\nu}-\eta_{\mu\nu}\eta_{\lambda\rho}+\eta_{\mu\rho}\eta_{\lambda\nu})R(\{\ \})\Bigg]. \tag{4.15}$$

We now consider Einstein's tensor in the form $G_{ij}=R_{ij}-\frac{1}{2}\eta_{ij}R$, where $G=-R/2$ and the Bianchi identity $\nabla^\rho G_{\mu\rho}=0$, which becomes now $\partial^\rho G_{\mu\rho}=0$. This yields

$$2\,\partial^\rho J_{[\lambda\mu][\nu\rho]}(\{\ \})=-a_2(\partial_\lambda G_{\mu\nu}-\partial_\mu G_{\lambda\nu})-8\left(a_3+\frac{a_2}{6}\right)\eta_{\nu[\lambda}\partial_{\mu]}G. \tag{4.17}$$

The K component then becomes $f_{ij\mu\nu}(K)=\partial_\mu K_{ij\nu}-\partial_\nu K_{ij\mu}$, which leads to

$$E_{\mu\nu}(K)=-\tfrac{2}{3}\,\partial_\sigma t^\sigma{}_{[\mu\nu]}-\tfrac{1}{2}\,\partial_\sigma a^\sigma{}_{\mu\nu}-\tfrac{1}{2}\,\partial_{[\nu}v_{\mu]}, \tag{4.18}$$

$$I_{\mu\nu}(K)=\tfrac{2}{3}\,\partial_\sigma t^\sigma{}_{(\mu\nu)}-\tfrac{2}{3}\,\partial_\sigma t_{\mu\nu}{}^\sigma-\tfrac{1}{2}\,\partial_{(\nu}v_{\mu)}+\tfrac{1}{6}\,\eta_{\mu\nu}\,\partial_\sigma v^\sigma, \tag{4.19}$$

where the brackets denote antisymmetrization and the parentheses denote symmetrization. We also see that the term $P(K)$ that appears in the expressions of J_{ijkl} becomes now $P(K)=-2\,\partial_\rho v^\rho$. Also, after some algebraic manipulation we obtain for the term in a_1 in the equations for J_{ijkl},

$$-2\,\partial^\rho J_{[\lambda\mu][\nu\rho]}(K)=\eta_{\nu[\mu}\partial_\rho\,\partial_\sigma t^{\rho\sigma}{}_{\lambda]}+\tfrac{2}{3}\,\partial_\mu\,\partial_\sigma t^\sigma{}_{[\lambda\nu]}-\tfrac{2}{3}\,\partial_\lambda\,\partial_\sigma t^\sigma{}_{[\mu\nu]}+\tfrac{1}{2}\,\eta_{\nu[\mu}\partial_{\lambda]}\,\partial_\sigma v^\sigma$$
$$+\tfrac{1}{2}\,(\partial_\nu\,\partial_{[\mu}v_{\lambda]}+\eta_{\nu[\lambda}\Box v_{\mu]})+\partial_\sigma\,\partial_{[\mu}a_{\lambda]\nu}{}^\sigma, \tag{4.20}$$

where we have considered the properties

$$t_{\sigma\mu\nu}+t_{\nu\sigma\mu}+t_{\mu\nu\sigma}=0,\quad t_{\sigma(\mu\nu)}=-\tfrac{1}{2}\,t_{\mu\nu\sigma}. \tag{4.21}$$

Similarly, for the term in a_2 we obtain

$$-2\,\partial^\rho J_{[\lambda\mu][\nu\rho]}(K)=\eta_{\nu[\mu}\partial_\rho\,\partial_\sigma t^{\rho\sigma}{}_{\lambda]}+\partial_\mu\,\partial_\sigma t_{\lambda\nu}{}^\sigma-\partial_\lambda\,\partial_\sigma t_{\mu\nu}{}^\sigma+\tfrac{1}{6}\,\eta_{\nu[\mu}\partial_{\lambda]}\,\partial_\sigma v^\sigma$$
$$+\tfrac{1}{2}\,(\partial_\nu\,\partial_{[\mu}v_{\lambda]}+\eta_{\nu[}\Box v_{\mu]}), \tag{4.22}$$

and finally, the D component of Eq. (4.12) becomes now in this approximation,

$$f_{ij\mu\nu}(D)=\partial_\mu D_{ij\nu}-\partial_\nu D_{ij\mu}, \tag{4.23}$$

which leads to

$$E_{\mu\nu}(D)=\partial_{[\nu}\omega_{\mu]}, \tag{4.24}$$

$$I_{\mu\nu}(D)=\partial_{(\nu}\omega_{\mu)}-\tfrac{1}{3}\,\eta_{\mu\nu}\,\partial^\rho\omega_\rho, \tag{4.25}$$

$$P(D)=4\,\partial_\rho\omega^\rho, \tag{4.26}$$

$$2\,\partial^\rho J_{[\lambda\mu][\nu\rho]}(D)=(\eta_{\nu[\lambda}\Box\omega_{\mu]}+\eta_{\nu[\mu}\partial_{\lambda]}\,\partial^\rho\omega_\rho+\partial_\nu\,\partial_{[\mu}\omega_{\lambda]}), \tag{4.27}$$

$$2\,\partial^\rho J_{[\lambda\mu][\nu\rho]}(D)=(\eta_{\nu[\lambda}\Box\omega_{\mu]}+\tfrac{1}{3}\,\eta_{\nu[\mu}\partial_{\lambda]}\,\partial^\rho\omega_\rho+\partial_\nu\,\partial_{[\mu}\omega_{\lambda]}). \tag{4.28}$$

The field equations are then

$$-2\,\partial^\lambda F_{\mu\nu\lambda}=T_{\mu\nu}, \tag{4.29a}$$

$$Z_{\lambda\mu\nu}=-S_{\lambda\mu\nu}, \tag{4.29b}$$

$$W_{\mu\nu}=K_{\mu\nu}, \tag{4.29c}$$

$$X_\mu=D_\mu, \tag{4.29d}$$

where

$$\begin{aligned}Z_{\lambda\mu\nu}=&\,a_2(\partial_\lambda G_{\mu\nu}-\partial_\mu G_{\lambda\nu})+8\left(a_3+\frac{a_2}{6}\right)\eta_{\nu[\lambda}\partial_{\mu]}G+(a_1+a_2)\,\eta_{\nu[\mu}\partial_\rho\,\partial_\sigma t^{\rho\sigma}{}_{\lambda]}\\&+\tfrac{1}{3}\,[\partial_\mu\partial_\sigma\{2a_1t^\sigma{}_{[\lambda\nu]}+3a_2t_{\lambda\nu}{}^\sigma\}-\partial_\lambda\partial_\sigma\{2a_1t^\sigma{}_{[\mu\nu]}+3a_2t_{\mu\nu}{}^\sigma\}]+\tfrac{1}{6}\,(3a_1+a_2\\&-48a_3)\,\eta_{\nu[\mu}\partial_{\lambda]}\,\partial_\sigma v^\sigma+\tfrac{1}{2}\,(a_1+a_2)\{\partial_\nu\,\partial_{[\mu}v_{\lambda]}+\eta_{\nu[\lambda}\Box v_{\mu]}\}+a_1\partial_\sigma\,\partial_{[\mu}a_{\lambda]\nu}{}^\sigma+(a_1+a_2)\\&\times(\eta_{\nu[\mu}\Box\omega_{\lambda]}+\partial_\nu\partial_{[\lambda}\omega_{\mu]})+\tfrac{1}{3}\,(3a_1+a_2-48a_3)\,\eta_{\nu[\lambda}\partial_{\mu]}\,\partial^\rho\omega_\rho+H_{\lambda\mu\nu},\end{aligned} \tag{4.30}$$

$$W_{\mu\nu}=-2\,\partial^\rho\bar{f}_{\mu\nu\rho}+8F_{\nu\mu}+J^{[\mu\rho]}{}_{[\rho\nu]}, \tag{4.31}$$

$$X_\mu=-2\,\partial^\nu F_{\mu\nu}+\bar{F}^\nu{}_{\mu\nu}. \tag{4.32}$$

B. Related equations between gravitational sources

Since gravitational sources are linked to conservation laws, these relations define the maximum degree of freedom we possess to choose sources, and they allow us to obtain important conclusions in the present approach. Indeed, if we differentiate Eq. (4.29a) and use the fact that $F_{\mu\nu\lambda}$ is antisymmetric in $(\nu\lambda)$, we obtain that $\partial^\nu T_{\mu\nu}=0$, which is the conservation law of the energy-momentum tensor in the linearized form for a weak gravitational field. Similarly, differentiating Eq. (4.29b) and keeping in mind that $H_{\lambda\mu\nu}=F_{\nu\mu\lambda}$, we obtain

$$\partial^\nu F_{\nu\mu\lambda}=T_{[\mu\nu]}=\partial^\nu S_{\lambda\mu\nu}, \tag{4.33}$$

which relates the spin tensor to the energy-momentum tensor (Tetrode's formula).

Conformal theory also yields an equation for the conformal field,

$$\partial^{\nu}K_{\mu\nu}=2S_{\mu\rho}{}^{\rho}+4D_{\mu}, \tag{4.34}$$

and another equation for the dilatation field,

$$\partial^{\mu}D_{\mu}=T. \tag{4.35}$$

From Eqs. (4.33)–(4.35) we conclude that at first-order approximation the following occurs

(i) For gravitational sources with nonsymmetrical energy-momentum tensor the spin is necessarily non-null.

(ii) For gravitational sources whose energy-momentum tensor is not traceless the dilatation source is necessarily non-null.

(iii) Either, if the field has spin or if the dilatation field is non-null, the conformal source is also non-null.

(iv) The only manner to annihilate the conformal source is to take a symmetric and traceless energy-momentum tensor.

(v) If the trace of the energy-momentum tensor is non-null, both conformal and dilatation sources are also non-null.

(vi) The conservation law for the energy-momentum tensor and Tetrode's formula are not affected by additional symmetries.

(vii) Elimination of dilatation symmetry does not ensure one the possibility to eliminate the conformal field, and by the same reason, the elimination of the conformal sector does not ensure one the possibility to eliminate the dilatation source.

C. Field equation for $h_{\mu\nu}$

Since we desire to verify the consistency of the present approach in space–time, we must derive an equation for the perturbations $h_{\mu\nu}$ on the metric. For that we simplify the field equations (4.29) by introducing the quantity $\bar{h}_{\mu\nu}$, and that satisfies the conditions

$$\partial^{\nu}\bar{h}_{\mu\nu}=0, \quad \bar{h}_{\mu\nu}=h_{\mu\nu}-\tfrac{1}{2}\,\eta_{\mu\nu}h. \tag{4.36}$$

This results for the Einstein tensor $G_{\mu\nu}=-1/2\Box\bar{h}_{\mu\nu}$. Its is also convenient to decompose Eq. (4.29a) in symmetrical and antisymmetrical parts, according to

$$-3\alpha\,\partial^{\lambda}t_{\mu\nu\lambda}-2\beta(\eta_{\mu\nu}\,\partial^{\lambda}v_{\lambda}-\partial_{(\mu}v_{\nu)})=T_{(\mu\nu)}, \tag{4.37a}$$

$$2\alpha\,\partial^{\lambda}t_{\lambda[\mu\nu]}+2\beta\partial_{[\mu}v_{\nu]}-4\gamma\,\partial^{\lambda}a_{\mu\nu\lambda}=T_{[\mu\nu]}. \tag{4.37b}$$

Also, if we take the trace of Eq. (4.37a) we obtain $T=-4\beta\,\partial^{\lambda}v_{\lambda}$. Hence, we have an isolated equation for $h_{\mu\nu}$ when we symmetrize Eq. (4.29b) in $(\mu\nu)$ and take its divergence in λ: $\partial^{\lambda}Z_{\lambda(\mu\nu)}=-\partial^{\lambda}S_{\lambda(\mu\nu)}$.

With the formulas below,

$$\partial^{\lambda}(\eta_{\mu\nu}\partial_{\rho}\,\partial_{\sigma}t^{\rho\sigma}{}_{\lambda}-\tfrac{1}{2}\,\eta_{\nu\lambda}\,\partial_{\rho}\sigma\,t^{\rho\sigma}{}_{\mu}-\tfrac{1}{2}\,\eta_{\mu\lambda}\partial_{\rho}\,\partial_{\sigma}t^{\rho\sigma}{}_{\nu})=0, \tag{4.38a}$$

$$\partial^{\lambda}(\partial_{\sigma}\partial_{(\mu}t_{\nu)\lambda}{}^{\sigma}-\Box\partial_{\sigma}t_{\mu\nu}{}^{\sigma})=\frac{1}{3\alpha}\left(\Box T_{(\mu\nu)}-\frac{1}{2}\,(\eta_{\mu\nu}\Box-\partial_{\mu}\partial_{\nu})T+2\partial^{\lambda}\,\partial^{\rho}\partial_{(\mu}S_{\nu)\lambda\rho}\right), \tag{4.38b}$$

$$\partial^{\lambda}[\tfrac{1}{12}\,(3a_1+a_2+48a_3)(\eta_{\mu\nu}\partial_{\lambda}\,\partial_{\sigma}v^{\sigma}-\partial_{\mu}\partial_{\nu}\,\partial_{\sigma}v^{\sigma})+\tfrac{1}{4}\,(a_1+a_2)(\eta_{\mu\nu}\Box-\partial_{\mu}\partial_{\nu})\partial_{\sigma}v^{\sigma}]$$
$$=\frac{a_2+24a_3}{24\beta}\,(\eta_{\mu\nu}\Box-\partial_{\mu}\partial_{\nu})T, \tag{4.38c}$$

$$\partial^{\lambda}\left[\tfrac{1}{12}(3a_1+a_2+48a_3)(\eta_{\mu\nu}\partial_{\lambda}\,\partial_{\sigma}\omega^{\sigma}-\partial_{\mu}\partial_{\nu}\,\partial_{\sigma}\omega^{\sigma})+\tfrac{1}{4}(a_1+a_2)(\eta_{\mu\nu}\Box-\partial_{\mu}\partial_{\nu})\partial_{\sigma}\omega^{\sigma}\right]$$
$$=\frac{a_2+24a_3}{6\beta}(\eta_{\mu\nu}\Box-\partial_{\mu}\partial_{\nu})\partial^{\sigma}\omega_{\sigma}, \tag{4.38d}$$

we can simplify the form of our field equation if we choose a gauge for ω_{σ} that is similar to the Lorentz gauge: $\partial^{\sigma}\omega_{\sigma}=0$. In this case our field equation becomes

$$-a_2\Box^2\bar{h}_{\mu\nu}+\frac{2(a_2+6a_3)}{3}(\eta_{\mu\nu}\Box-\partial_{\mu}\partial_{\nu})\Box\bar{h}=T^{(\mathrm{ef})}_{\mu\nu}, \tag{4.39}$$

where $T^{(\mathrm{ef})}_{\mu\nu}$ is an effective symmetric energy-momentum tensor,

$$T^{(\mathrm{ef})}_{\mu\nu}=T_{(\mu\nu)}-2\,\partial^{\lambda}S_{\lambda(\mu\nu)}-\frac{a_2+24a_3}{12\beta}(\eta_{\mu\nu}\Box-\partial_{\mu}\partial_{\nu})T-\frac{2a_2}{3\alpha}$$
$$\times\left[\Box T_{(\mu\nu)}-\tfrac{1}{2}(\eta_{\mu\nu}\Box-\partial_{\mu}\partial_{\nu})T+2\partial^{\lambda}\partial^{\rho}\,\partial_{(\mu}S_{\nu)\lambda\rho}\right]. \tag{4.40}$$

It is important to notice that the parameters a_1 and γ, and also the conformal and dilatation sectors, are not present in Eq. (4.39). This points out that, *at a first approximation*, the dilatation sector and the conformal sector do not intervene in the structure of space–time.

V. SOLUTIONS AND SUBTHEORIES

A. Geometric solutions

Let us consider the field due to a spinless point source located at the origin of coordinates, where $T_{\mu\nu}$ is given by

$$T_{\mu\nu}=\begin{cases}Mc^2\delta^2(\mathbf{r}), & \mu=\nu=0,\\ 0, & \text{otherwise},\end{cases} \tag{5.1}$$

with $\mathbf{r}=(x^1,x^2)$. In this case $T^{(\mathrm{ef})}_{\mu\nu}$ has the components

$$T^{(\mathrm{ef})}_{00}=Mc^2\{\delta^2(\mathbf{r})+(P+Q)\Delta\,\delta^2(\mathbf{r})\},$$
$$T^{(\mathrm{ef})}_{0\alpha}=T^{(\mathrm{ef})}_{\alpha 0}=0, \tag{5.2}$$
$$T^{(\mathrm{ef})}_{\alpha\beta}=Mc^2(P-Q)(\partial_{\alpha}\partial_{\beta}-\delta_{\alpha\beta}\Delta)\,\delta^2(\mathbf{r})\quad(\alpha=1,2),$$

with $\Delta=(\partial_1)^2+(\partial_2)^2$, $P=-(a_2+24a_3)/12\beta$, and $Q=-a_2/3\alpha$. The equation for $\bar{h}$ is

$$(B+2C)\Box^2\bar{h}=-Mc^2\delta^2(\mathbf{r})-2Mc^2P\,\Delta\,\delta^2(\mathbf{r}), \tag{5.3}$$

where $B=-a_2$ and $C=2(a_2+6a_3)/3$. The above equation can be solved by the Fourier integration method, and yields

$$\bar{h}(\mathbf{k})=-\frac{(2\pi)Mc^2}{(B+2C)k^4}-\frac{(4\pi)Mc^2P}{(B+2C)k^2}, \tag{5.4}$$

$$\bar{h}(\mathbf{r})=-\frac{Mc^2}{(B+2C)}\left[\frac{r^2\,\ln r}{4\pi}\right]-\frac{2Mc^2P}{(B+2C)}\left[\frac{\ln r}{2\pi}\right]+C_1r^2+C_2, \tag{5.5}$$

where C_1 and C_2 are integration constants. The equation for $\bar{h}_{00}$ thus becomes

$$B\Box^2\bar{h}_{00}=-\frac{Mc^2C}{(B+2C)}\,\delta^2(\mathbf{r})-\frac{2Mc^2CP}{(B+2C)}\,\Delta\delta^2(\mathbf{r})+Mc^2\delta^2(\mathbf{r})$$
$$+Mc^2P\;\Delta\delta^2(\mathbf{r})+Mc^2Q\;\Delta\delta^2(\mathbf{r}), \tag{5.6}$$

and has the solution

$$\bar{h}_{00}(\mathbf{k})=\left[-\frac{Mc^2C}{(B+2C)B}+\frac{Mc^2}{B}\right]\frac{2\pi}{k^4}+\left[-\frac{2Mc^2PC}{(B+2C)B}+\frac{Mc^2P}{B}+\frac{Mc^2Q}{B}\right]\frac{2\pi}{k^2}. \tag{5.7}$$

Since $h_{00}=\bar{h}_{00}+\bar{h}$, we get

$$h_{00}(\mathbf{r})=\frac{Mc^2(3\alpha+4\beta)}{24\pi\alpha\beta}\ln r-\frac{Mc^2(a_2+6a_3)}{4\pi a_2(a_2+24a_3)}\,r^2\ln r+C_3r^2+C_4, \tag{5.8}$$

for $\alpha\beta a_2(a_2+24a_3)\neq 0$. If we assume $a_2,a_3\to\infty$, we obtain in particular for Eq. (5.8),

$$h_{00}(\mathbf{r})=\frac{Mc^2(3\alpha+4\beta)}{24\pi\alpha\beta}\ln r+C_5r^2+C_6. \tag{5.9}$$

B. Relation to the Newtonian theory

If we consider the classical motion of a spinless particle in the field of a spinless gravitational source, then at first order the particle's motion is given by the equation $d^2\mathbf{r}/dt^2=-\partial U/\partial\mathbf{r}$, where $U=-c^2h_{00}/2$. Thus, with a convenient choice of parameters, we derive the Newtonian solution from Eq. (5.8). Such a solution, with the conditions

$$3\alpha+4\beta=-\frac{96\alpha\beta\pi G}{c^4},\quad a_2+6a_3=0,\quad C_3=0, \tag{5.10}$$

satisfies Newton's equation for the source given in Eq. (5.1):

$$\Delta U=4\pi GM\delta^2(\mathbf{r}). \tag{5.11}$$

In similar way we can derive the Newtonian limit from the solution (5.9), with the conditions

$$3\alpha+4\beta=-\frac{96\alpha\beta\pi G}{c^4},\quad C_5=0. \tag{5.12}$$

In this limit the equation for $\bar{h}$ can be written in the form

$$\Delta[(B+2C)\Delta\bar{h}+2Mc^2P\delta^2(\mathbf{r})]=0 \tag{5.13}$$

in the sourceless case and

$$(B+2C)\Delta\bar{h}+2Mc^2P\delta^2(\mathbf{r})=\psi(\mathbf{r}) \tag{5.14}$$

if a source is considered, where $\Delta\psi(\mathbf{r})=0$. Then, the equation for $\bar{h}_{00}$ becomes, in the sourceless case,

$$\Delta\left[B\Delta\bar{h}_{00}+\frac{2Mc^2CP}{B+2C}\,\delta^2(\mathbf{r})-Mc^2(P+Q)\,\delta^2(\mathbf{r})\right]=0, \tag{5.15}$$

and, with the inclusion of a source,

$$B\,\Delta\bar{h}_{00}+\frac{2Mc^2CP}{B+2C}\,\delta^2(\mathbf{r})-Mc^2(P+Q)\,\delta^2(\mathbf{r})=\phi(\mathbf{r}), \tag{5.16}$$

where $\Delta\phi(\mathbf{r})=0$. If we choose the particular solution $\psi(\mathbf{r})=\phi(\mathbf{r})=0$, we obtain from the above equation the Newtonian gravitational equation,

$$\Delta U=4\pi GM\,\delta^2(\mathbf{r}). \tag{5.17}$$

C. Relation to the Poincaré theory

From the results obtained in Sec. III and from the field equation for $F_{\mu\nu}$, we conclude that we are not led to a Poincaré gauge theory by means of an appropriate choice of sources, fields and integration constants. This is due to the fact that $\mathbf{T}\neq 0$, in general, in the Poincaré limit, which means that D_μ, $F_{\mu\nu}$, and ω_μ are both non-null. Moreover, since the covariant derivative is expressed in terms of $A^{ij}{}_\mu$ (and, in consequence, it is also expressed in terms of the potential ω_μ), then a whole Poincaré theory does not emerge as a natural limit from the conformal theory.

However, outside matter, we can assume vanishing sources, in such a way that we can obtain from Eq. (3.38) a particular solution $\bar{f}_{ilm}=0$, yielding $G_{ijk}=0$. If this result is replaced in Eq. (3.42), we are led to the particular solution $F^{lm}=0$. This points out that the Poincaré gauge theory in vacuum can be obtained from a choice of gauge $\omega_\mu=\overset{+}{\omega}_\mu=0$, and it leads to the field equations

$$-2\,D^k\bar{F}_{ijk}+2u^k\bar{F}_{ijk}+2H_{ij}+4\bar{F}_{ilj}\omega^l+4J_{[ik][jl]}P^{kl}+4J^{[lk]}{}_{[lj]}P_{ki}-2J^{[il]}{}_{[jl]}P-\eta_{ij}\mathscr{L}_c=T_{ij}, \tag{5.18}$$

$$2\,D^lJ_{[ij][kl]}+(\tfrac{4}{3}\,t_k{}^{[lm]}-\delta_k^{[l}v^{m]}+a_k{}^{lm}J_{[ij][lm]}+H_{ijk}+2(\eta_k{}^{[l}\omega^{m]}J_{[ij][kl]}=S_{ijk}. \tag{5.19}$$

The above equations have been derived already by Kawai.[9]

D. Comments on the Einsteinian limit

Einstein's theory of GR is not derivable here as a subtheory. This is due to the fact that such a theory can only be obtained with the inclusion of linear terms of fields in the Lagrangian density. Otherwise, we remind that GR is not a conformal invariant theory,[16] because the above field terms are not invariant under conformal transformations.[10] Hence, the Einsteinian limit cannot be obtained from a conformal gauge theory of gravity.

VI. CONCLUDING REMARKS

Here we developed a conformal theory for (2+1)-dimensional gravity, which is similar to YM gauge theories and that has a Newtonian limit. This approach has the following characteristics.

(i) The framework was developed in a fiber bundle with the (2+1) Minkowski space–time as a base manifold, whose structural group is the conformal group with ten generators. The group algebra manifold is the direct sum of the sectors of rotations, translations, dilatations, and special conformal transformations.

(ii) We have considered a nonlinear realization of the gauge fields in order to obtain a break of symmetry and to get a theory applicable to the physical space–time, with triads being the potential in the sector of translations.

(iii) We have assumed a Lagrangian density that is quadratic in the fields, in order to maintain the invariance of these fields under conformal transformations, and also, to verify a similarity between this approach and YM gauge theories.

(iv) The affine connection is generalized here to $\Gamma^\lambda{}_{\mu\nu}=\{{}^\lambda_{\mu\nu}\}+K^\lambda{}_{\mu\nu}+D^\lambda{}_{\mu\nu}$, where $D_{\lambda\mu\nu}=g_{\mu\nu}\omega_\lambda-g_{\lambda\nu}\omega_\mu$ is defined in the dilatation sector.

(v) The field equations are given by Eqs. (3.23), (3.31), (3.38), and (3.42).

(vi) At a first approximation the field equations are given by Eqs. (4.29).

(vii) Gravitational sources whose energy-momentum tensor is traceless, necessarily maintain the nullity of a conformal source.

(viii) Either, if the field has spin or if the dilatation source is non-null, then the gravitational source will be also non-null.

(ix) The unique way to annihilate both sectors of dilatations and conformal transformations is to assume a symmetric, traceless, and spinless energy-momentum tensor;

(x) The conservation law of the energy-momentum tensor and Tetrode's formula are not affected by additional symmetries.

(xi) At a first approximation the sectors of dilatations and conformal transformations do not affect the structure of space–time.

(xii) The Newtonian theory is obtained here as a particular limit of a spinless weak field;

(xiii) The Poincaré theory in vacuum is also obtained as a subtheory, however, inside matter, the sectors of dilatations and conformal transformations are not annihilated.

(xiv) Since GR is not conformally invariant, it cannot be derived here as a subtheory.

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On the solutions of the CP^1 model in (2+1) dimensions

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We use the methods of group theory to reduce the equations of motion of the CP^1 model in (2+1) dimensions to sets of two coupled ordinary differential equations. We decouple and solve many of these equations in terms of elementary functions, elliptic functions, and Painlevé transcendents. Some of the reduced equations do not have the Painlevé property. The existence of a Lax pair, making the model integrable, is hence very unlikely, even though it possesses many properties of integrable systems (such as stable ''numerical solitons''). © *1996 American Institute of Physics.* [S0022-2488(96)03202-X]

I. INTRODUCTION

Over the past few years, it has become clear that many physical processes can be described well in terms of various partial nonlinear differential equations. The areas providing such equations range from solid state physics, hydrodynamics, and particle physics to biophysics and biochemistry. As the equations are nonlinear, in general, they are hard to solve; in fact, so far no general method of solving these equations is known and each equation has to be treated on its own. However, a particular class of equations, which are derived from the so-called integrable models can be solved using some very general techniques[1] (inverse scattering methods, Bäcklund transformations,...). These equations are very special and their solutions have very special properties. Many of these equations have solutions that are localized in space and propagate at a constant speed. Such solutions, usually called solitons, or extended structures in general, have received a lot of attention in recent years. However, most of these equations depend on two space (or space–time) variables and, as such, can only describe phenomena that are quasi-two-dimensional. When they involve more variables, either all variables come in a very nonsymmetric way, or the models are very special.

Most applications in nature involve three spatial dimensions, and in many applications all spatial variables come on an equal footing. When the applications involve, for example, particle physics or relativity, the underlying models are Lorentz covariant. Such models are, generally, nonintegrable and the methods mentioned above do not apply. On the other hand, some of them can be studied numerically. Such studies have involved full simulations of similar models in (2+1) dimensions or simulations of various reduced models (i.e., approximations to the original models). Some of these studies[2] have found that even though the models were not integrable, the behavior of their extended structures resembled the behavior that was expected had the models been integrable (i.e., the structures preserved their shapes well, there was little radiation, etc.) Moreover, the approximate methods[3] gave results that were virtually indistinguishable from the results of full simulations. Hence we feel that the behavior of integrable models may not be that unusual; other models, which, strictly speaking, are not integrable, may be ''almost'' so. Their

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extended structures show very little difference from what might be expected had the models been integrable. Moreover, various approximate methods work well and may be used to provide some insight to the behavior of the solutions of the full equations.

Most of the results, which involve models in (2+1) dimensions, were obtained in the so-called CP^1 model [also called the S^2 or $O(3)$ model] and its modifications.[2] This model, in its original version[4] is probably the simplest model in (2+1) dimensions, which is relativistically covariant and which admits the existence of localized soliton-like solutions.

The CP^1 σ model is defined by the Lagrangian density,

$$\mathscr{L}_\sigma = \tfrac{1}{4}(\partial^\mu \boldsymbol{\phi})\cdot(\partial_\mu \boldsymbol{\phi}), \tag{1.1}$$

together with the constraint $\boldsymbol{\phi}\cdot\boldsymbol{\phi}=1$. The Euler–Lagrange equations derived from (1.1) are

$$\partial^\mu\ \partial_\mu \boldsymbol{\phi} + (\partial^\mu \boldsymbol{\phi}\cdot\partial_\mu \boldsymbol{\phi})\,\boldsymbol{\phi} = \mathbf{0}. \tag{1.2}$$

The model can be modified by the addition of further terms to the Lagrangian density. The terms that have been studied the most extensively involve the (2+1)-dimensional analog of the "Skyrme" term[5] and various "potential" terms.[2,6] They were added, primarily, to stabilize the soliton-like structures. In the original model the soliton-like structures were not really stable; any perturbation would induce their shrinking or expanding, which they could do without any cost of energy, due to the conformal invariance of the pure CP^1 model. Apart from curing the shrinking and inducing also weak forces between soliton-like structures, the additional forces had little effect on the dynamics of these structures. Moreover, the affects of nonintegrability of these models were also not that different from similar effects in the pure CP^1 case. Hence, the dynamics of these models was described well by the dynamics of the CP^1 case. The same was true when one looked at the approximate methods.[7]

These observations suggest that a lot can be learned from looking at exact solutions of the CP^1 model using the group theoretical method of symmetry reduction.[8–10] This method exploits the symmetry of the original equations to find solutions invariant under some subgroup of the symmetry group (the classic example one can give here involves seeking solutions in two dimensions that are rotationally invariant). The method puts all such attempts on a unified footing, and it has been applied with success to many equations. The method leads to equations whose solutions represent specific solutions of the full equations; the solutions are determined locally and the method does not tell us whether these solutions are stable or not with respect to any perturbations.

In our case we would like to apply this method to looking for solutions of the original CP^1 model; from the remarks made above we can hope that these solutions will also be approximate solutions of the modified models. Their stability is harder to predict; but again, guided by the experience from the numerical simulations we hope that, at least, some of them will be stable with respect to small perturbations.

In order to perform the symmetry reductions of the pure CP^1 model in (2+1) dimensions we have to decide what variable to use. To avoid having to use the constrained variables ($\boldsymbol{\phi}$), it is convenient to use the W formulation of the model that involved the stereographic projection of the sphere $\boldsymbol{\phi}\cdot\boldsymbol{\phi}=1$ onto the complex plane. In this formulation, instead of using the ϕ fields, we express all the dependence on ϕ in terms of their stereographic projection onto the complex plane W. The ϕ fields are then related to W by

$$\phi^1 = \frac{W+W^*}{1+|W|^2}, \quad \phi^2 = i\,\frac{W-W^*}{1+|W|^2}, \quad \phi^3 = \frac{1-|W|^2}{1+|W|^2}. \tag{1.3}$$

In this formulation the Lagrangian density becomes

$$L=\frac{\partial_\mu W\ \partial^\mu W^*}{(1+|W|^2)^2}, \tag{1.4}$$

where * denotes complex conjugation.

To perform our analysis it is convenient to use the polar version of the W variables; i.e. to put $W=R\exp(i\psi)$ and then study the equations for R and ψ. The advantage of this approach is that the equations become simple; the disadvantage comes from having to pay attention that R is real and ψ should be periodic with a period of 2π. (If the period is not 2π then the solution may become multivalued, etc.) Thus, if we find solutions that do not obey these restrictions, then these solutions, however interesting they may be, cannot, in general, be treated as solutions of the original model.

The equations for R and ψ take the form

$$\partial_{tt}\psi-\partial_{xx}\psi-\partial_{yy}\psi+2\frac{(1-R^2)}{R(1+R^2)}\,(\partial_t\psi\ \partial_t R-\partial_x\psi\ \partial_x R-\partial_y\psi\ \partial_y R)=0 \tag{1.5}$$

and

$$\partial_{tt}R-\partial_{xx}R-\partial_{yy}R-\frac{R(1-R^2)}{(1+R^2)}\,(\partial_t\psi\ \partial_t\psi-\partial_x\psi\ \partial_x\psi-\partial_y\psi\partial_y\psi)$$
$$-\frac{2R}{(1+R^2)}\,((\partial_t R)^2-(\partial_x R)^2-(\partial_y R)^2)=0. \tag{1.6}$$

Note that if we put $R=1$ the second equation is automatically satisfied and the first one reduces to

$$\partial_{tt}\psi-\partial_{xx}\psi-_{yy}\psi=0, \tag{1.7}$$

i.e., the linear wave equation for the phase ψ.

In section II we determine the symmetry group of Eqs. (1.5) and (1.6). In the following section we present coupled pairs of reduced ordinary differential equations (ODEs) for all two-dimensional subgroups of the symmetry group. Sections IV and V are devoted to the presentation of explicit solutions. We finish the paper with a short discussion of the derived solutions, their relation to the solutions known before, and their physical relevance.

II. THE SYMMETRY GROUP AND ITS SUBGROUPS

The symmetry group of the system (1.5) and (1.6) can be calculated using standard methods.[8–10] We actually made use of a MACSYMA package[11] that provides a simplified and partially solved set of determining equations.

Solving those, we find that the symmetry group has the structure of a direct product, namely,

$$G\sim \mathrm{SIM}(2,1)\otimes \mathrm{SU}(2), \tag{2.1}$$

where SIM(2,1) is the similitude group of (2+1)-dimensional Minkowski space (the Poincaré group extended by dilations). The group SU(2) rotates the components of the fields among each other.

The corresponding Lie algebras, sim(2,1) and $su(2)$, can be represented by vector fields acting on R and ψ and the space–time coordinates. A suitable basis is given by two Lorentz boosts K_1 and K_2, one rotation L, three translations P_0, P_1, and P_2, one dilation D, and three $su(2)$ generators X, Y, and Z. We have

$$K_1=-(x\partial_t+t\partial_x),\quad K_2=-(y\partial_t+t\partial_y),\quad L=-x\partial_y+y\partial_x,$$
$$P_0=\partial_t,\quad P_1=\partial_x,\quad P_2=\partial_y,\quad D=t\partial_t+x\partial_x+y\partial_y, \tag{2.2}$$

$$X=\frac{1}{2}\left(\left(R-\frac{1}{R}\right)\sin\,\psi\partial_\psi+(R^2+1)\cos\,\psi\partial_R\right),$$
$$Y=\frac{1}{2}\left(\left(R-\frac{1}{R}\right)\cos\,\psi\partial_\psi-(R^2+1)\sin\,\psi\partial_R\right), \tag{2.3}$$
$$Z=\partial_\psi.$$

Our aim is to obtain solutions of Eqs. (1.5) and (1.6) by the method of symmetry reduction.[8–10] In practice, we shall require that solutions are invariant under a two-dimensional subgroup of the symmetry group G. This will reduce the original partial differential equations (1.5) and (1.6) to a system of ODEs. Subalgebras of sim(2,1) were classified in Ref. 12. A two-dimensional algebra $\{\hat{A},\hat{B}\}$ can be either Abelian, $[\hat{A},\hat{B}]=0$, or solvable non-Abelian, $[\hat{A},\hat{B}]=\hat{A}$. Subalgebras of the direct sum $\mathrm{sim}(2,1)\oplus su(2)$ can be obtained by the Goursat "twist" method.[13,14]

The result is the following. There exist ten parametric classes of Abelian subalgebras, represented by

$$\{\hat{A}+aZ,\quad \hat{B}+bZ\}, \tag{2.4}$$

with $a,b\in\mathbb{R}$, Z as in (2.3), and $\{\hat{A},\hat{B}\}$ equal to one of the following pairs:

$$\{K_1,P_2\};\quad \{D,K_2+L\};\quad \{K_2+L,P_0-P_1\};\quad \{P_2,P_0-P_1\};\quad \{L,P_0\};$$
$$\{P_1,P_2\};\quad \{P_0,P_1\};\quad \{D,K_1\};\quad \{D,L\};\quad \{D-K_1,P_0-P_1\}. \tag{2.5}$$

Further, there exist 15 parametric classes of non-Abelian two-dimensional subalgebras represented by

$$\hat{A}+cZ,\hat{B},\quad c\in\mathbb{R}, \tag{2.6}$$

where $\{\hat{A},\hat{B}\}$ is one of the pairs:

$$\{K_1,K_2+L\};\quad \{D,P_2\};\quad \{K_1,P_0-P_1\};\quad \{D,P_0-P_1\};\quad \{K_1+\epsilon P_2,P_0-P_1\};$$
$$\{D+\epsilon(K_2+L),P_0-P_1\};\quad \{D,P_0\};\quad \{D+aK_1,K_2+L\};\quad \{D+aK_1,P_2\};$$
$$\{D-K_1+\epsilon(P_0-P_1),K_2+L\};\quad \{D+K_2+\epsilon(P_0+P_2),P_1\};\quad \{D+aL,P_0\}; \tag{2.7}$$
$$\{D+aK_1,P_0-P_1\};\quad \{D+K_1+\epsilon(P_0+P_1),P_0-P_1\};\quad \{D+\tfrac{1}{2}K_1,K_2+L+\epsilon(P_0+P_1)\},$$

with $a\in\mathbb{R}$ and $\epsilon=\pm1$.

III. THE REDUCED EQUATIONS

For each subgroup (2.4) and (2.6) we find three invariants, ξ, R, and F, using standard methods.[8–10] In terms of these we express the two functions R and ψ of (1.5) and (1.6) as

$$R=R(\xi),\quad \psi=\alpha(x,y,t)+F(\xi),\quad \xi=\xi(x,y,t), \tag{3.1}$$

TABLE I. Subalgebras leading to second order equations and the quantities figuring in the reduced equations [see (3.1),...,(3.7) in the text].

No	Algebra	ξ	α	p	g	h	s	l	m	B
1	K_1+aZ, P_2+bZ	$\sqrt{(t^2-x^2)}$	$by-a\ \operatorname{arctanh}\frac{x}{t}$	$-\frac{1}{\xi}$	$\frac{1}{\xi}$	0	0	$-\left(b^2+\frac{a^2}{\xi^2}\right)$	0	$2(b^2\xi^2+a^2)$
2	$P_0+aZ, L+bZ$	$\sqrt{x^2+y^2}$	$bt+a\ \arctan\frac{y}{x}$	$-\frac{1}{\xi}$	$\frac{1}{\xi}$	0	0	$-\left(b^2-\frac{a^2}{\xi^2}\right)$	0	$2(b^2\xi^2-a^2)$
3	K_1+aZ, K_2+L	$\sqrt{t^2-x^2-y^2}$	$-a\ \ln\lvert x+t\rvert$	$\frac{-2}{\xi}$	$\frac{1}{\xi^2}$	0	0	0	0	0
4	K_2+aZ, P_0-P_2	x	$-a\ \ln\lvert y+t\rvert$	0	1	0	0	0	0	0
5	$D+aZ, P_0-P_1$	$\frac{t+x}{y}$	$a\ \ln\lvert t+x\rvert$	$\frac{-2}{\xi}$	$\frac{1}{\xi^2}$	0	0	0	0	0
6	$K_1+\epsilon P_2+aZ$, P_0-P_1	$y\epsilon+\operatorname{arctanh}\frac{x}{t}$ $+\frac{1}{2}\ln\lvert t^2-x^2\rvert$	$a\epsilon y$	0	1	a	0	a^2	0	0
7	$D+\epsilon(K_2+L)+aZ$, P_0-P_1	$\frac{2y}{t+x}+2\epsilon\ \ln\lvert\frac{t+x}{2}\rvert$	$-a\ \ln\lvert\frac{t+x}{2}\rvert$	0	1	0	0	0	0	0
8	$D+aK_1+bZ$, P_0-P_1	$\frac{x+t}{2}y^{(a-1)}$, $a\neq 1$,	$\frac{1}{2}\ b\ \ln\lvert y\rvert$	$\frac{2-a}{a-1}\frac{1}{\xi}$	$\xi^{(2-a)/(a-1)}$	$\frac{b}{2(a-1)}\frac{1}{\xi}$	$\frac{-b}{2(a-1)^2}\frac{1}{\xi^2}$	$\frac{b^2}{4(a-1)^2}\frac{1}{\xi^2}$	0	0
9	$D+K_1+\epsilon(P_0+P_1)$ $+aZ$, P_0-P_1	$e^{x+t}y^{-2\epsilon}$, $\epsilon=\pm 1$	$\frac{a\epsilon}{2}(x+t)$	$-\frac{1+2\epsilon}{2\epsilon}\frac{1}{\xi}$	$\xi^{-(1+2\epsilon)/2\epsilon}$	0	0	0	0	0
10	$P_1+aZ; P_2+bZ$	t	$by+ax$	0	1	0	0	$-(b^2+a^2)$	0	$2(b^2+a^2)$
11	$D+aZ, P_2$	$\frac{x}{t}$	$a\ \ln t$	$-\frac{2\xi}{\xi^2-1}$	$\frac{1}{\xi^2-1}$	$-\frac{a\xi}{\xi^2-1}$	$-\frac{a}{\xi^2-1}$	$\frac{a^2}{\xi^2-1}$	0	$2a^2$
12	$D+K_1+\epsilon(P_0+P_1)$ $+aZ, P_2$	$t+x-\epsilon\ln\lvert t-x\rvert$	$\frac{a}{2}\ln\lvert t-x\rvert$	0	1	$-\frac{\epsilon a}{4}$	0	0	0	$\frac{a^2}{8}$
13	$D+aZ, P_0$	$\arctan\frac{y}{x}$	$a\ \ln\sqrt{x^2+y^2}$	0	1	0	0	a^2	0	$-2a^2$
14	$D+aL+bZ, P_0$	$\frac{1}{2}\ln(x^2+y^2)-\frac{1}{a}\arctan\frac{y}{x}$	$\frac{b}{a}\arctan\frac{y}{x}$	0	1	$-\frac{b}{1+a^2}$	0	$\frac{b^2}{1+a^2}$	0	$-2\frac{b^2a^2}{(1+a^2)^2}$

TABLE I. (*Continued.*)

No	Algebra	ξ	α	p	g	h	s	l	m	B
15	P_2+aZ, P_0+bZ	x	$by+at$	0	1	0	0	(b^2-a^2)	0	$2(a^2-b^2)$
16	$D+aK_1+bZ, P_2,$	$\dfrac{(t+x)^{a+1}}{(t-x)^{1-a}}$ $a\geqslant 0,\ a\neq 1,$	$\dfrac{b}{1+a}\ln\lvert t-x\rvert$	$-\dfrac{1}{\xi}$	$\dfrac{1}{\xi}$	$\dfrac{b}{2\xi(a^2-1)}$	0	0	0	$\dfrac{b^2}{2(a^2-1)^2}$
17	$D+aZ, K_2+L+bZ$	$\dfrac{(t^2-x^2-y^2)^{1/2}}{x+t}$	$-b\,\dfrac{y}{t+x}+a\,\ln\lvert t+x\rvert$	0	1	$\dfrac{-a}{\xi}$	0	b^2	$\dfrac{a}{\xi^2}$	$2\left(\dfrac{a^2}{\xi^2}-b^2\right)$
		$\dfrac{(x^2+y^2-t^2)^{1/2}}{x+t}$	$-b\,\dfrac{y}{t+x}+a\,\ln\lvert t+x\rvert$	0	1	$\dfrac{-a}{\xi}$	0	$-b^2$	$\dfrac{a}{\xi^s}$	$2\left(\dfrac{a^2}{\xi^2}+b^2\right)$
18	$D+aZ, K_1+bZ$	$\arctan\dfrac{(t^2-x^2-y^2)^{1/2}}{y}$	$-b\,\operatorname{arctanh}\dfrac{x}{t}+\dfrac{a}{2}\lvert t^2-x^2\rvert$	0	1	$-\dfrac{a}{\tan\xi}$	0	b^2-a^2	$-\dfrac{a}{\sin^2\xi}$	$2\left(\dfrac{a^2}{\sin^2\xi}+b^2\right)$
		$\operatorname{arctanh}\dfrac{(x^2+y^2-t^2)^{1/2}}{y}$	$-b\,\operatorname{arctanh}\dfrac{x}{t}+\dfrac{a}{2}\lvert x^2-t^2\rvert$	0	1	$-\dfrac{a}{\tanh\xi}$	0	a^2-b^2	$\dfrac{-a}{\sinh^2\xi}$	$2\left(\dfrac{a^2}{\sinh^2\xi}-b^2\right)$
19	$D+aZ, L+bZ$	$\arctan\dfrac{(x^2+y^2-t^2)^{1/2}}{t}$	$-b\,\arctan\dfrac{y}{x}+\dfrac{a}{2}\ln\sqrt{x^2+y^2}$	0	1	$-\dfrac{a}{\tan\xi}$	0	$-a^2-b^2$	$\dfrac{a}{\sin^2\xi}$	$2\left(\dfrac{a^2}{\sin^2\xi}+b^2\right)$
		$\operatorname{arctanh}\dfrac{(t^2-x^2-y^2)^{1/2}}{t}$	$-b\,\arctan\dfrac{y}{x}+\dfrac{a}{2}\ln\sqrt{x^2+y^2}$	0	1	$-\dfrac{a}{\tanh\xi}$	0	a^2+b^2	$\dfrac{a}{\sinh^2\xi}$	$2\left(\dfrac{a^2}{\sinh^2\xi}-b^2\right)$
20	$D-K_1+aZ,$ P_0-P_1+bZ	$\dfrac{\sqrt{x+t}}{y}$	$at-\dfrac{a}{2}(x+t)+\dfrac{b}{2}\ln\lvert x+t\rvert$	$-\dfrac{2}{\xi}$	$\dfrac{1}{\xi^2}$	$-\dfrac{a}{2\xi^2}$	0	$-\dfrac{ab}{\xi^4}$	$\dfrac{a}{2\xi^4}$	$2\left(\dfrac{a^2}{4\xi^2}+ab\right)$
21	$D+aK_1+bZ,$ K_2+L	$\dfrac{1}{t^2-x^2-y^2}(t+x)^{2/(1-a)},$ $a\neq\pm 1,$	$\dfrac{b}{1-a}\ln\lvert x+t\rvert$	$\dfrac{1}{2}\dfrac{3+a}{a+1}\dfrac{1}{\xi}\xi^{-(3+a)/(2a+2)}$		$\dfrac{b}{a+1}\dfrac{1}{2\xi}$	0	0	$\dfrac{b(1-a)}{4(a+1)^2}\dfrac{1}{\xi^2}$	$\dfrac{b^2}{2(a+1)^2}\xi^{(1-a)/(1+a)}$
22	$D-K_1+\epsilon(P_0-P_1)+aZ,$ K_2+L	$\dfrac{x^2+y^2-t^2}{2(x+t)}-\dfrac{\epsilon}{2}\ln\lvert x+y\rvert,$ $\epsilon=\pm 1$	$\dfrac{a}{2}\ln\lvert x+t\rvert$	ϵ	$e^{\epsilon\xi}$	$-\dfrac{\epsilon a}{2}$	0	0	$\dfrac{a}{2}$	$\dfrac{a^2e^{-2\epsilon\xi}}{2}$
23	$D+\frac{1}{2}K_1+aZ,$ $K_2+L+\epsilon(P_0+P_1)$	$\dfrac{6(t-x)+(t+x)^3+6\epsilon y(t+x)}{[(t+x)^2+4\epsilon y]^{3/2}}$	$a\,\ln\lvert(t+x)^2+4\epsilon y\rvert$	$\dfrac{5}{3}\dfrac{-\xi}{1-\xi^2}$	$\dfrac{1}{1-\xi^2}^{5/6}$	$\dfrac{2}{3}\dfrac{a\xi}{1-\xi^2}$	$\dfrac{4}{9}\dfrac{a}{1-\xi^2}$	$-\dfrac{4}{9}\dfrac{a^2}{1-\xi^2}$	$\dfrac{2a}{9(1-\xi^2)^2}$	$\dfrac{8a^2}{9}(1-\xi^2)^{-1/3}$

TABLE II. Subalgebras leading to first order equations and quantities figuring in the reduced equations [see (3.13),...,(3.17)].

No	Algebra	ξ	α	$\Delta\xi$	$(\nabla\xi)^2$	$\Delta\alpha$	$(\nabla\alpha,\nabla\xi)$	$(\nabla\alpha)^2$
24	P_2+aZ, P_0-P_1+bZ	$x+t$	$-bx+ay$	0	0	0	b	$-b^2-a^2$
25	K_2+L+aZ, P_0-P_1+bZ	$x+t$	$bt-\dfrac{2ay+by^2}{2(x+t)}$	0	0	$\dfrac{b}{x+t}$	b	$b^2-\dfrac{a^2}{\xi^2}$
26	$D+K_1+bZ, K_2+L$	$x+t$	$\dfrac{b}{2}\ln\lvert t^2-x^2-y^2\rvert$	0	0	$\dfrac{b}{t^2-x^2-y^2}$	$\dfrac{b(t+x)}{t^2-x^2-y^2}$	$\dfrac{b^2}{t^2-x^2-y^2}$
27	$D-K_1+bZ, K_2+L$	$\dfrac{x+t}{t^2-x^2-y^2}$	$\dfrac{b}{2}\ln\lvert t+x\rvert$	$-2\dfrac{(x+t)}{(t^2-x^2-y^2)^2}$	0	0	$-b\dfrac{(t+x)}{(t^2-x^2-y^2)^2}$	0
28	$D+K_1+bZ, P_2$	$x+t$	$\dfrac{b}{2}\ln\lvert t-x\rvert$	0	0	0	$\dfrac{b}{t-x}$	0
29	$D+K_1+bZ, P_0-P_1$	$x+t$	$\alpha=b\ln\lvert y\rvert$	0	0	$\dfrac{b}{y^2}$	0	$-\dfrac{b^2}{y^2}$

where α and ξ are given for each subalgebra in Tables I and II. Derivatives with respect to the variable ξ will be denoted by dots. We introduce the two invariant operators Δ and ∇^2 by setting

$$\Delta f = f_{tt} - f_{xx} - f_{yy}, \quad (\nabla f, \nabla g) = f_t g_t - f_x g_x - f_y g_y, \tag{3.2}$$

and consider three cases separately.

(1) $(\nabla\xi)^2 \neq 0$. We put

$$\frac{\Delta\xi}{(\nabla\xi)^2} = -p = -\frac{\dot{g}}{g}, \quad \frac{(\nabla\alpha, \nabla\xi)}{(\nabla\xi)^2} = h, \quad \frac{\Delta\alpha}{(\nabla\xi)^2} = s, \quad \frac{(\nabla\alpha)^2}{(\nabla\xi)^2} = l, \tag{3.3}$$

with $g = g(\xi)$, $h = h(\xi)$, $s = s(\xi)$, and $l = l(\xi)$.

For further use we also introduce

$$m = \dot{h} - \frac{\dot{g}}{g} h - s \tag{3.4}$$

and

$$B = 2\frac{h^2 - l}{g^2}. \tag{3.5}$$

The two PDEs (1.5) and (1.6) now reduce to

$$\ddot{F} + 2\dot{R}\dot{F}\frac{(1-R^2)}{R(1+R^2)} - \frac{\dot{g}}{g}\dot{F} + 2\frac{(1-R^2)}{R(1+R^2)}\dot{R}h + s = 0, \tag{3.6}$$

$$\ddot{R} - \frac{2R}{1+R^2}\dot{R}^2 - \frac{R(1-R^2)}{1+R^2}\dot{F}^2 - \frac{\dot{g}}{g}\dot{R} - 2\frac{R(1-R^2)}{1+R^2}\dot{F}h - \frac{R(1-R^2)}{1+R^2}l = 0. \tag{3.7}$$

For each algebra the functions (3.3) are given in Table I.

In order to solve the above system, we must decouple its two equations. Putting $\dot{F} + h = V$ we first rewrite Eq. (3.6) as

$$\dot{V} + 2\dot{R}\frac{(1-R^2)}{R(1+R^2)}V - \frac{\dot{g}}{g}V - m = 0, \tag{3.8}$$

with m as in Eq. (3.4).

For $m = 0$ we solve (3.6) and obtain

$$\dot{F} = A\frac{(1+R^2)^2}{R^2}g(\xi) - h, \quad A = \text{const.} \tag{3.9}$$

Next, we substitute $\dot{F}$ into Eq. (3.7) and obtain a second-order ODE for $R(\xi)$,

$$\ddot{R} - \frac{2R}{1+R^2}\dot{R}^2 - \frac{\dot{g}}{g}\dot{R} - A^2g^2\frac{(1-R^2)(1+R^2)^3}{R^3} + \frac{R(1-R^2)}{1+R^2}(h^2 - l) = 0. \tag{3.10}$$

For $m \neq 0$, Eq. (3.8) is inhomogeneous. We can still decouple it by putting

$$\dot{F} = \frac{Um}{\dot{U}} - h \tag{3.11}$$

$$\dot{U}=\frac{mR^2}{(R^2+1)^2 g}. \tag{3.12}$$

Using Eq. (3.11), we can rewrite (3.7) as a third-order ODE for the auxiliary function $U(\xi)$. If we can solve it we obtain $R(\xi)$ from (3.12). However, in this paper we restrict our attention to the case of $m(\xi)=0$.

(2) $(\nabla\xi)^2=0$, $\Delta\xi=0$, $(\nabla\alpha,\nabla\xi)\neq 0$. The reduced equations decouple immediately and we have

$$(\nabla\alpha,\nabla\xi)\,\frac{(1-R^2)}{R(1+R^2)}\,\dot{R}=-\frac{1}{2}\,\Delta\alpha, \quad (\nabla\alpha,\nabla\xi)\dot{F}=-\frac{1}{2}\,(\nabla\alpha)^2. \tag{3.13}$$

For $(\nabla\alpha,\nabla\xi)\neq 0$ we can integrate directly to obtain

$$\frac{R}{R^2+1}=C\,\exp\left\{-\frac{1}{2}\int\frac{\Delta\alpha}{(\nabla\alpha,\nabla\xi)}\,d\xi\right\}, \tag{3.14}$$

$$F=-\frac{1}{2}\int\frac{(\nabla\alpha)^2}{(\nabla\alpha,\nabla\xi)}\,d\xi+F_0. \tag{3.15}$$

For $(\nabla\alpha,\nabla\xi)=0$ we must have also $\Delta\alpha=0$, $(\nabla\xi)^2=0$. Then $R(\xi)$ and $F(\xi)$ are arbitrary functions of ξ. In particular, this is true for $\alpha=0$.

(3) $(\nabla\xi)^2=0$, $\Delta\xi\neq 0$. We obtain two equations that are easy to solve:

$$F'+2\frac{(1-R^2)R'}{R(1+R^2)}\,\frac{(\nabla\alpha_1\nabla\xi)}{\Delta\xi}=-\frac{\Delta\alpha}{\Delta\xi}, \tag{3.16}$$

$$-2\frac{(\nabla\alpha_1\nabla\xi)}{\Delta\xi}F'+\frac{1+R^2}{R(1-R^2)}\,R'=\frac{(\nabla\alpha)^2}{\Delta\xi}. \tag{3.17}$$

IV. ANALYSIS OF SECOND-ORDER ODE

A. General comments

In order to obtain explicit solutions, we need to solve the ODE (3.10) for the function $R(\xi)$. This equation is in the class analyzed by Painlevé and Gambier;[15–17] namely, it is of the form

$$\ddot{y}=f(\dot{y},y,x), \tag{4.1}$$

where f is rational in $\dot{y}$ and y and analytical in x. If this equation has the Painlevé property (no movable singularities other than poles), then it can be transformed into one of the 50 standard equations listed, e.g., by Ince.[17] The Painlevé test[18,19] provides us with necessary (but not sufficient) conditions for Eq. (4.1) to have the Painlevé property. The solution is expanded about an arbitrary point x_0 in the complex x plane in a Laurent series,

$$y(x)=\sum_{k=0}^{\infty} a_k\tau^{k+p}, \quad \tau=x-x_0, \tag{4.2}$$

where p is required to be an integer (a negative one if we are interested in points where the solution itself has a pole). The coefficients are obtained from a recursion relation of the form

$$P_k a_k=h_k(x_0,a_0,a_1,\ldots,a_{k-1}). \tag{4.3}$$

Since (4.2) is supposed to represent a general solution, it must depend on two constants; x_0 and a_r for some non-negative r, called a resonance value. This occurs if the function P_r satisfies $P_r=0$. Then a_r is arbitrary and we have a consistency condition, the "resonance condition," $h_r(x_0,a_0,a_1,\ldots,a_{r-1})=0$ (which must be satisfied identically in x_0). If the above conditions are satisfied, the Painlevé test is passed and (4.2) represents a two-parameter family of formal solutions (locally, within the radius of convergence of the series).

Turning our attention to Eq. (3.10), we note that the cases $A\neq 0$ and $A=0$ must be treated separately.

B. The case $A\neq 0$

The Painlevé test applied directly fails immediately since a balance between the most singular terms occurs for $p=-\frac{1}{2}$, i.e. we have a movable square root branch point. To remedy this problem we put

$$R(\xi)=\sqrt{-U(\xi)} \tag{4.4}$$

and obtain

$$\ddot{U}=\dot{U}^2\left[\frac{1}{2U}+\frac{1}{U-1}\right]+2A^2g^2\,\frac{(1+U)(1-U)^3}{U}+\dot{U}\,\frac{\dot{g}}{g}+2(h^2-l)\,\frac{U(1+U)}{(U-1)}. \tag{4.5}$$

We can now choose a new variable η to be

$$\eta=\int g(\xi)d\xi, \tag{4.6}$$

and transform Eq. (4.5) into

$$\ddot{U}=\dot{U}^2\left[\frac{1}{2U}+\frac{1}{U-1}\right]+2A^2\,\frac{(1+U)(1-U)^3}{U}+B\,\frac{U(1+U)}{(U-1)}, \tag{4.7}$$

with B as in (3.5).

For $B=$const this is Eq. PXXXVIII listed, e.g., by Ince.[17] It has a first integral K that we use to write a first-order equation for U:

$$\dot{U}^2=-4A^2U^4+4KU^3+(8A^2-2B-8K)U^2+4KU-4A^2. \tag{4.8}$$

Since we have $A\neq 0$, we can rewrite (4.8) as

$$(\dot{U})^2=-4A^2(U-U_1)(U-U_2)(U-U_3)(U-U_4), \tag{4.9}$$

where the constant roots of the right-hand side of (4.9) U_i, $i=1,\ldots,4$ can be expressed in terms of the constants A, B, and K.

Equation (4.9) has elementary algebraic and trigonometric solutions, as well as solutions that resemble solitary waves or kink-like structures (in the symmetry variable η) in the case of multiple roots. If all U_i are distinct, then the solutions of (4.8) involve elliptic functions.[20] Explicit solutions will be presented in the next section.

If B in Eq. (4.7) is not constant, we proceed differently. We again introduce a new independent variable,

$$\eta=\exp\int g\,d\xi, \tag{4.10}$$

and transform Eq. (4.5) into

$$\ddot{U}=\dot{U}^2\left[\frac{1}{2U}+\frac{1}{U-1}\right]-\frac{\dot{U}}{\eta}+\frac{2A^2}{\eta^2}(1-U)^2\left(\frac{1}{U}-U\right)+2\frac{h^2-l}{g^2\eta^2}\frac{U(U+1)}{U-1}. \tag{4.11}$$

For

$$2\frac{h^2-l}{g^2\eta^2}=\delta=\text{const}, \tag{4.12}$$

this is the equation for the fifth Painlevé transcendent.

The values of $m=0$ and $B\neq$const occur for the cases 1 and 2 from Table I, and we actually have

$$\eta=\xi, \quad \delta=2\left(b^2\pm\frac{a^2}{\eta^2}\right), \tag{4.13}$$

so $\delta=$const requires $a=0$.

Hence, we obtain the solutions

$$\begin{gathered}U(\xi)=P_V(\alpha,\beta,\gamma,\delta;\xi),\\ \alpha=-\beta=2A^2, \quad \gamma=0, \quad \delta=2b^2,\end{gathered} \tag{4.14}$$

for equations describing the group reductions 1 and 2 (of Table I) in the case when $a=0$.

For $b=0$, in the cases of these two reductions we have $B=2a^2=$const, and we obtain solutions in terms of Eq. (4.8).

If δ in Eq. (4.12) is not constant, then Eq. (4.5) does not have the Painlevé property and we were not able to integrate it in terms of known functions.

C. The case $A=0$, $B=$const

The transformation (4.4) can also be performed for the case $A=0$. We use the first integral to write our equation as

$$\begin{gathered}\dot{U}^2=4K(U-U_1)(U-U_2),\\ U_{1,2}=L+1\pm\sqrt{L(L+2)}, \quad L=\frac{B}{4K}, \quad K\neq 0.\end{gathered} \tag{4.15}$$

For $K=0$, we find a solution immediately; namely, we have

$$U=U_0e^{\pm\sqrt{-2B}\eta}, \quad B\leqslant 0. \tag{4.16}$$

On the other hand, for $A=0$ in Eq. (3.10), the Painlevé expansion (4.2) gives us $p=-1$ for the leading (most singular) power. Hence, the transformation (4.4) is not required and so we can transform Eq. (3.10) directly into one of the standard forms.

We put

$$R=-i\frac{Z(\eta)+\mu(\xi)}{Z(\eta)-\mu(\xi)}, \quad \eta=\eta(\xi), \quad \mu\neq 0, \quad \dot{\eta}\neq 0, \tag{4.17}$$

and obtain

$$\ddot{Z}=\frac{\dot{Z}^2}{Z}-\frac{1}{\dot{\eta}}\left(\frac{\ddot{\eta}}{\dot{\eta}}-\frac{\dot{g}}{g}\right)\dot{Z}+\frac{1}{\dot{\eta}^2\mu}\left(\ddot{\mu}-\frac{\dot{\mu}^2}{\mu}-\frac{\dot{g}}{g}\dot{\mu}\right)Z+\frac{h^2-l}{4\dot{\eta}^2\mu^2}\frac{Z^4-\mu^4}{Z}. \tag{4.18}$$

If B of Eq. (3.5) is constant we can choose η as in Eq. (4.6), set $\mu=1$, and obtain the equation

$$\ddot{Z}=\frac{\dot{Z}^2}{Z}+\frac{B}{8}\left(\frac{Z^4-1}{Z}\right). \tag{4.19}$$

This equation can be integrated directly for $B=0$. For $B\neq 0$ it has a first integral K in terms of which we obtain a first-order ODE,

$$\dot{Z}^2=\frac{B}{8}(Z^2-Z_1^2)(Z^2-Z_2^2),\quad Z_{1,2}^2=-K\pm\sqrt{K^2-1}. \tag{4.20}$$

Again, we have elliptic function solutions. They are, however, not new. Since R is real (and non-negative) we must require that

$$Z=e^{i\sigma(\eta)},\quad \text{for } \mu=1, 0\leqslant\eta<2\pi. \tag{4.21}$$

The relation between the function $\sigma(\eta)$ and $U(\eta)$ of Eq. (4.7) is

$$\sqrt{-U(\eta)}=\left|\frac{\sin\sigma}{1-\sin\sigma}\right|. \tag{4.22}$$

For $B\neq$const we use the variable (4.10), again set $\mu=1$, and reduce Eq. (4.18) to

$$\ddot{Z}=\frac{\dot{Z}^2}{Z}-\frac{1}{\eta}\dot{Z}+\frac{h^2-l}{4g^2\eta^2}\frac{Z^4-1}{Z}. \tag{4.23}$$

For δ, defined by (4.12), being constant ($\delta=\delta_0$), Eq. (4.23) is a special case of the third Painlevé transcendent $P_{\mathrm{III}}(\alpha,\gamma,\beta,\delta;\eta)$ and so we have as a solution of Eq. (4.23),

$$Z=P_{\mathrm{III}}\left(0,0,\frac{\delta_0}{8},-\frac{\delta_0}{8};\eta\right). \tag{4.24}$$

This equation is, however, not new; it can be transformed into solution (4.14) by making use of relations between special cases of P_{V} and P_{III}.

Again, for δ not constant, Eq. (4.23) does not have the Painlevé property and we are not able to solve it.

D. Comments on the Painlevé analysis and integrability of model

For $A\neq 0$, Eq. (4.5) passes the Painlevé test for $U(x_0)\to\infty$ for any functions $g(\xi)$ and $h^2(\xi)-l(\xi)$. Indeed, we find $p=-1$ in the expansion (4.2). A resonance is obtained for $k=1$; the resonance condition is satisfied and so the coefficient a_1 is a free constant (as is x_0). We did not investigate the other two possible pole type irregularities, namely, $U(x_0)\to 0$, or $U(x_0)\to 1$.

The Painlevé test only checks whether certain necessary conditions are satisfied. If an equation of the type (4.1) does actually have the Painlevé property (as opposed to merely passing the Painlevé test), then it can be transformed into a standard form by a Möbius transformation (with variable coefficients),

$$y(\xi)=\frac{\alpha(\xi)U(\eta(\xi))+\beta(\xi)}{\delta(\xi)U(\eta(\xi))+\rho(\xi)},\quad \eta=\eta(\xi),\quad \alpha\rho-\beta\delta=\pm 1. \tag{4.25}$$

Equation (4.5) is already, to a large extent, standardized. Indeed, the coefficient of $\dot{U}^2$ has poles at $U=0$, 1, and ∞. This puts the equation into Ince's class IV and the residues have the correct values. Hence, we have $\alpha=\rho=1$, $\beta=\delta=0$ in Eq. (4.25). The only remaining permitted transformation is that of the independent variable. We have shown above that Eq. (4.5) can be reduced to the elliptic function equation if and only if B in Eq. (4.7) is constant. It can be transformed into the equation for the P_{V} transcendent if and only if its coefficients satisfy

$$\frac{d}{d\xi}\left(\frac{h^2-l}{g^2}\right)-2\left(\frac{h^2-l}{g^2}\right)g=0. \tag{4.26}$$

In all other cases the equation (4.5) cannot be transformed into a standard form, and hence it does not have Painlevé property.

The situation is exactly the same for $A=0$. Equation (3.10) passes the Painlevé test and is transformed into Eq. (4.18) by a Möbius transformation. The coefficient of $\dot{Z}^2$ has poles at $Z=0$ and $Z\to\infty$ with the correct residues. Hence, only $Z(\xi)\to\alpha(\xi)Z(\eta(\xi))$ is permitted. Equation (4.18) is of Ince's type II and has the Painlevé properties if and only if Eq. (4.26) is satisfied.

Thus we have shown that Eq. (4.5) has the Painlevé property if and only if the coefficients satisfy $B=$const, or if they satisfy Eq. (4.26).

V. EXPLICIT SOLUTIONS

We have reduced the original system (1.5) and (1.6) for the function

$$W=\mathrm{R}e^{i\psi}, \tag{5.1}$$

to one of the pairs of equations {(3.9),(3.10)}, {(3.14),(3.15)}, or (3.16), (3.17).

Let us first look at the pair {(3.9),(3.10)}. Equation (3.9) provides $F(\xi)$ by a quadrature, once Eq. (3.10) is solved. In Sec. IV we have further reduced Eq. (3.10). Using Eq. (4.4) we replace equations for $R(\xi)$ by equations for $U(\xi)$, where $U(\xi)$ must satisfy $U(\xi)\leqslant 0$.

As mentioned above, the algebras 1 and 2 of Table I lead to solutions of the form (4.14), i.e. the fifth Painlevé transcendent $P_{\mathrm{V}}(\xi)$, for $a=0$, $b\neq 0$.

Algebras 1–23 lead to the elliptic function equation (4.9) for $m=0$, $A\neq 0$, $B=$const and to Eq. (4.15) for $m=0$, $A=0$, $B=$const, $K\neq 0$. In both cases, elementary solutions are obtained in the case of multiple roots of the polynomial on the right-hand side of the equation.

Many excellent discussions of solutions of the elliptic function equation exist in the literature. We mention an article by Wadati on wave propagation in nonlinear lattices,[21] as well as the "Handbook" of Byrd and Friedman.[20] That notwithstanding, in order to keep this article readable and self-contained, and to specify the values and ranges of parameters occurring in our problem, we shall present nonsingular solutions of Eqs. (4.9) and (4.15) explicitly.

The character of the solution depends crucially on the sign of B in Table I. [B is defined in (3.5).] We have $B>0$ for algebras,

$$\begin{gathered}
1\ \ (b=0,a\neq 0),\quad 10\ \ (a^2+b^2\neq 0),\quad 11\ \ (a\neq 0),\quad 12\ \ (a\neq 0),\\
15\ \ (a^2>b^2),\quad 16\ \ (b\neq 0),\\
17\ \ (a=0,b\neq 0,x^2+y^2-t^2>0),\quad 18\ \ (a=0,b\neq 0,x^2+y^2-t^2>0),\\
19\ \ (a=0,b\neq 0,x^2+y^2-t^2>0);
\end{gathered} \tag{5.2}$$

$B<0$ for algebras,

$$2\ \ (b=0,a\neq 0),\quad 13\ \ (a\neq 0),\quad 14\ \ (ab\neq 0),\quad 15\ \ (a^2-b^2<0),$$

$$17\ \ (a=0,b\neq 0,t^2-x^2-y^2>0),\quad 18\ \ (a=0,b\neq 0,t^2-x^2-y^2>0), \tag{5.3}$$

$$19\ \ (a=0,b\neq 0,t^2-x^2-y^2>0).$$

In all other cases with $m=0$ we have $B=0$

Let us first run through all elementary functions solutions, remembering that the independent variable is η given in Eq. (4.6).

Localized solutions are obtained precisely for the algebras (5.2). From Eq. (4.15) (i.e., $A=0$) we obtain a kink in $R(\xi)$ where ξ and function $h(\xi)$ are read from Table I. Two situations are to be considered.

I. $A=0$, $L=-2$, $K<0$, $B>0$

The solution is the following:

1.

$$R=\pm\tanh\frac{1}{2}\sqrt{\frac{B}{2}}\,(\eta-\eta_0),\quad F=-\int h(\eta)d\eta+F_0. \tag{5.4}$$

II. $A\neq 0$, $B>4(A^2-K)>0$, $K<0$

Equation (4.9) ($A\neq 0$) leads to solitary wave (''bump''- or ''well''-type solutions) for the function $U(\eta)$ in the following four cases:

2. $U_4=U_3=U_2<U\leqslant U_1<0$,

$$U=U_2+\frac{U_1-U_2}{1+(U_1-U_4)^2A^2(\eta-\eta_0)^2}. \tag{5.5}$$

Equation (5.5) represents an ''algebraic bump.''

3. $U_4\leqslant U<U_3=U_2=U_1<0$

$$U=U_1-\frac{U_1-U_4}{1+(U_1-U_4)^2A^2(\eta-\eta_0)^2}. \tag{5.6}$$

This is an ''algebraic well.''

4. $U_4<U_3=U_2<U\leqslant U_1<0$

$$U=U_2+\frac{(U_1-U_2)(U_2-U_4)}{(U_1-U_4)\cosh^2 A\sqrt{(U_1-U_2)(U_2-U_4)}(\eta-\eta_0)-(U_1-U_2)}. \tag{5.7}$$

Equation (5.7) is an ''exponential bump.''

5. $U_4\leqslant U\leqslant U_3=U_2<U_1<0$

$$U=U_2-\frac{(U_1-U_2)(U_2-U_4)}{(U_1-U_4)\cosh^2 A\sqrt{(U_1-U_2)(U_2-U_4)}(\eta-\eta_0)-(U_2-U_4)}. \tag{5.8}$$

This is an ''exponential well.''

Further elementary solutions of Eq. (4.9) are trigonometrically periodic.

6. $U_4=U_3<U_2\leqslant U\leqslant U_1<0$, $K<0$, $B>4(A^2-K)>0$

$$U=U_3+\frac{(U_1-U_3)(U_2-U_3)}{U_2-U_3+(U_1-U_2)\cos^2 A\sqrt{(U_1-U_3)(U_2-U_3)}(\eta-\eta_0)}. \tag{5.9}$$

This type of solution also occurs only for the algebras (5.2)

7. $U_4 \leqslant U \leqslant U_3 < U_2 = U_1$

$$U = U_1 - \frac{(U_1-U_4)(U_1-U_3)}{U_1-U_3+(U_3-U_4)\cos^2 A\sqrt{(U_1-U_4)(U_1-U_3)}(\eta-\eta_0)}. \tag{5.10}$$

This solution can occur in the case of algebras (5.2) for $U_1<0$, i.e. all roots negative. It can also occur for $U_3<0<U_2=U_1$, and this allows us to have $B\leqslant 0$, Thus, solutions (5.10) can occur for all algebras (and variables ξ) 1–23 in Table I. Notice, however, that they are periodic, rather than localized, in the variable η.

The remaining solutions are periodic and expressed in terms of Jacobi elliptic functions. We have the following.

8. $A=0$, $K>0$, $B<-8K<0$, $U_2 \leqslant U \leqslant U_1 < 0$

$$U = \frac{U_1U_2}{U_2+(U_1-U_2)\mathrm{sn}^2(\sqrt{-(U_2K/2)}(\eta-\eta_0),k)}, \quad k^2=\frac{U_1-U_2}{(-U_2)}. \tag{5.11}$$

This occurs for the algebras (5.3).

9. $A=0$, $K<0$, $B>-8K>0$, $U_2<U_1 \leqslant U \leqslant 0$

$$R = \sqrt{-U_1}\,\mathrm{sn}\sqrt{\frac{U_2K}{2}}\,(\eta-\eta_0,k), \quad k^2=\frac{U_1}{U_2}. \tag{5.12}$$

The algebras concerned are those of Eq. (5.2).

10. $A\neq 0$, $U_4 \leqslant U \leqslant U_3 < U_2 < U_1$

$$U = \frac{U_1(U_3-U_4)\mathrm{sn}^2[\beta(\eta-\eta_0),k]+U_4(U_1-U_3)}{(U_3-U_4)\mathrm{sn}^2[\beta(\eta-\eta_0),k]+U_1-U_3},$$
$$k^2=\frac{(U_1-U_2)}{(U_1-U_3)}\frac{(U_3-U_4)}{(U_2-U_3)}, \quad \beta=A\sqrt{(U_1-U_3)(U_2-U_4)}. \tag{5.13}$$

This can occur for $U_1<0$; then we must have $B>4(A^2+(-K))>0$, i.e. the algebras (5.2). It can also occur for $U_3<U_4<0<U_2<U_1$, then all of the algebras 1–23 of Table I can occur.

11. $A\neq 0$, $U_4<U_3<U_2 \leqslant U \leqslant U_1<0$

$$U = \frac{U_4(U_1-U_2)\mathrm{sn}^2[\beta(\eta-\eta_0),k]+U_1(U_2-U_4)}{(U_1-U_2)\mathrm{sn}^2[\beta(\eta-\eta_0),k]+U_2-U_4}, \tag{5.14}$$

with k^2 and β as in Eq. (5.13). we must have $B>4(A^2+(-K))>0$ and hence algebras (5.2).

12. $A\neq 0$, $U_4<U<U_1$, $U_{2,3}=p\pm iq$, $q>0$

$$U = \frac{[CU_4-DU_1]\mathrm{cn}[\beta(\eta-\eta_0),k]+DU_1+CU_4}{(C-D)\mathrm{cn}[\beta(\eta-\eta_0),k]+C+D},$$
$$C=(U_1-p)^2+q^2, \quad D=(U_4-p)^2+q^2, \tag{5.15}$$
$$k^2=\frac{(U_1-U_4)^2-(C-D)^2}{4CD}, \quad \beta=2A(CD)^{1/4}.$$

This situation can occur for all algebras 1–23 of Table I.

13. $A=0$, $K=0$, $B<0$. We obtain the solution (4.16) for algebras (5.3) with ξ as given in Table I [and η given by Eq. (4.6)].

The algebras No. 24–29 of Table II correspond to variables ξ such that $(\nabla\xi)^2=0$ and hence to first-order ODEs. The solutions are readily obtained and we just list them:

$$\text{No. 24:}\quad R=R_0,\psi=ay-bx+\frac{a^2+b^2}{2b}(x+t)+\psi_0,\quad b\neq 0, \tag{5.16}$$

$$\text{No. 25:}\quad R=c\sqrt{x+t}\pm\sqrt{c^2(x+t)-1},\quad \psi=\frac{b}{2}(t-x)-\frac{(a+by)^2}{2b(x+t)}+\psi_0, \tag{5.17}$$

$$\text{No. 26:}\quad R=c\sqrt{x+t}\pm\sqrt{c^2(x+t)-1},\quad \psi=b\,\ln\sqrt{\frac{|t^2-x^2-y^2|}{|x+t|}}+\psi_0, \tag{5.18}$$

$$\text{No. 27:}\quad R=R_0,\quad \psi=\frac{b}{2}\ln|x+t|+\psi_0; \tag{5.19}$$

No. 28 and 29 provide nonconstant solutions only for $b=0$. Then $F(\xi)$ and $R(\xi)$ are arbitrary functions of $\xi=x+t$.

All solutions presented so far are group invariant solutions in the standard sense of the words.[8–10]

Let us mention that the PDEs (1.5) and (1.6) can be reduced to ODEs of the form (3.6) and (3.7), by the transformation (3.1), where ξ and α are any functions satisfying Eq. (3.3). The restriction is that p, h, s, and l must be functions of ξ. Group theory generates solutions of these equations by the requirement that F and ξ in (3.1) be invariants of subgroups of the symmetry group. However, other solutions may exist, corresponding, e.g., to so-called "null variables,"[22,23] to "conditional symmetries,"[24,25] or simply generated by the "direct method" of Clarkson and Kruskal.[26]

Let us just give some examples of such variables.

First, a few words about null variables and the corresponding solutions. Consider a variable ξ satisfying

$$(\nabla\xi)^2=\Delta\xi=0. \tag{5.20}$$

The equations for $F(\xi)$ and $R(\xi)$ reduce to Eq. (3.13). As mentioned in Sec. III, if we also have

$$(\nabla\alpha,\nabla\xi)=(\nabla\alpha)^2=\Delta\alpha=0 \tag{5.21}$$

(e.g., for $\alpha=$const), then $F(\xi)$ and $R(\xi)$ are arbitrary functions. We have already encountered this situation for $\xi=x+t$, however, Eq. (5.20) have more general solutions,[22,23] that can be written in terms of Riemann invariants.

Indeed, let us put

$$\xi=H(\sigma),\quad \sigma=(\mathbf{a},\mathbf{x})=a_0t-a_1x-a_2y,\quad (\mathbf{a},\mathbf{a})=0, \tag{5.22}$$

where $\mathbf{a}$ is a light-like vector, depending on ξ [i.e., Eq. (5.22) defines ξ implicitly]. It is easy to check that ξ of Eq. (5.22) satisfies Eq. (5.20) for any choice of the function H and light-like vector $\mathbf{a}(\xi)$. The function $H(\sigma)$ can be chosen to be $H(\sigma)=\sigma$ with no loss of generality, since $F(\xi)$ and $R(\xi)$ are themselves arbitrary. Thus, we can replace Eq. (5.22) by

$$\xi=a_0(\xi)t-a_1(\xi)x-a_2(\xi)y,\quad \mathbf{a}^2=0. \tag{5.23}$$

Choosing $\mathbf{a}$ to be constant, we recover the variable $\xi=x+t$ (up to a Lorentz transformation). Other choices give different results, which become explicit if we can solve the algebraic equation (5.23). For example, choose

$$\mathbf{a}=(1,\xi,\sqrt{1-\xi^2}). \tag{5.24}$$

Solving Eq. (5.23) for ξ, we obtain

$$\xi=\frac{(1+x)t\pm\sqrt{(1+x)^2+y^2-t^2}}{(1+x)^2+y^2}. \tag{5.25}$$

Choosing $F(\xi)$ and $R(\xi)$ appropriately, e.g. $F(\xi)$ constant and $R(\xi)$ with compact support, we obtain a localized solution (localized in the variable ξ).

An example of a ''conditionally invariant'' solution is obtained by putting

$$\psi=\psi(\xi),\quad R=R(\xi),\quad \xi=\sqrt{\frac{x^2+y^2}{x^2-t^2}}. \tag{5.26}$$

We have $\alpha(x,y,t)=0$ and

$$p=\frac{\dot{g}}{g}=-\frac{1}{\xi},\quad g=\frac{1}{\xi},\quad h=s=l=m=0,\quad B=0, \tag{5.27}$$

in Eqs. (3.6) and (3.7). These values could hence be added to those in Table I.

VI. COMMENTS AND CONCLUSIONS

Inserting the variables ξ and α of Table I into the formulas of Sec. V, we obtain a great variety of exact analytic solutions.

Some of our solutions are (possibly up to phase factors, contained in the variable α) really solutions of the 1+1-, or 2+0-dimensional CP^1 model. Thus, algebras 1, 11, 12, and 16 provide solutions, depending essentially only on x and t. Similarly, algebras 2, 13, and 14 provide essentially static solutions (independent of t). A sizable literature exists on static solutions.[27–31] Particularly interesting solutions of this type are obtained for algebra 2 when we have $\xi=\sqrt{x^2+y^2}$, and we take $b=0$. We obtain elliptic function solutions (5.11) and (5.15) as well as the elementary solution (4.16), or, more explicitly,

$$W=W_0(x^2+y^2)^{n/2}e^{in\phi}, \tag{6.1}$$

where $a=n$ is an integer (and ϕ is the azimuthal angle in the xy plane). This can be identified as an ''n-soliton solution'' (or instanton) and it has finite energy.[4] Our static solutions are not new: they are to be found, e.g., among those obtained by Purkait and Ray, or earlier.[27–31]

The same algebra gives rise to a very different type of solution. If we take $b\neq 0$, $a=0$ we express $R(\xi)$ in terms of the Painlevé transcendent P_{V}, as in Eq. (4.14). The phase is $\psi=bt+\psi_0$ so that we have a global rotation of spins in the horizontal plane. To our knowledge, this type of solution is new.

Algebra 14 introduces a ''helical''-type variable ξ. Solution (4.16) in this case is

$$W=R_0(x^2+y^2)^{ab/2(1+a^2)}e^{-b/(1+a^2\ \arctan\ y/x)}e^{ib\phi/a}. \tag{6.2}$$

This solution is multivalued, even for the b/a integer. This type of variable and solution could be pertinent in condensed matter applications, concerning, e.g., critical phenomena in multilayered films.

In general, our method provides us with "local solutions," not necessarily defined for all of $\mathbb{R}^+$. The solutions are not necessarily single valued and they can have singularities for real values of the variable ξ. Moreover, in view of the existence of the light cone, it is sometimes necessary to consider space-like and time-like regions of space–time separately, since solutions in these regions may differ. Typical examples of this phenomenon are provided by algebras 17, 18, and 19. We list two variables ξ in Table I for each of these, one valid for $t^2-x^2-y^2>0$, the other for $x^2+y^2-t^2>0$. In all cases we restrict to $a=0$, in order to have $m=0$ in the table. The simplest solutions are given by Eq. (4.16) for $B<0$ and (5.4) for $B>0$.

In the case of algebra 17, the corresponding solutions are

$$\begin{aligned} W&=R_0 e^{\epsilon b\sqrt{t^2-x^2-y^2}/(x+t)} e^{-iby/(x+t)}, \quad t^2-x^2-y^2>0,\\ W&=\tanh\frac{b}{2}\left(\frac{\sqrt{x^2+y^2-t^2}}{x+t}-\xi_0\right) e^{-iby/(x+t)}, \quad t^2-x^2-y^2<0. \end{aligned} \tag{6.3}$$

The two solutions can be connected on the cone, however, their derivatives will be discontinuous in any case.

Similarly, for algebra 18 of Table I we find the elementary solutions,

$$\begin{aligned} W&=R_0 e^{b\ \arctan\sqrt{t^2-x^2-y^2}/y} e^{-ib\ \operatorname{arctanh}\ x/t}, \quad t^2-x^2-y^2>0,\\ W&=\tanh\frac{b}{2}\left[\operatorname{arctanh}\frac{\sqrt{x^2+y^2-t^2}}{y}-\xi_0\right] e^{-ib\ \operatorname{arctanh}\ x/t}, \quad x^2+y^2-t^2>0. \end{aligned} \tag{6.4}$$

Finally, for algebra 19 of Table I, we have

$$\begin{aligned} W&=\tanh\frac{b}{2}\left(\arctan\frac{\sqrt{x^2+y^2-t^2}}{t}-\xi_0\right) e^{-ib\ \arctan/x}, \quad x^2+y^2-t^2>0,\\ W&=W_0 e^{b\ \operatorname{arctanh}\sqrt{t^2-x^2-y^2}/t} e^{-ib\ \arctan\ y/x}, \quad t^2-x^2-y^2>0. \end{aligned} \tag{6.5}$$

In many soliton-like problems in field theory, we are interested in solutions that are regular in $\mathbb{R}^+$, i.e., which are valid at all times (though this condition is sometimes relaxed a bit) and which are defined for $-\infty<x<\infty$, $-\infty<y<\infty$. Among them particularly important are those whose energy is finite (as they describe localized "soliton-like" field structures). If we restrict our attention to such field configurations, we see that we should consider the energy density for our fields. As the energy density is given by

$$\rho=\frac{|W_t|^2+|W_x|^2+|W_y|^2}{[1+|W|^2]^2}, \tag{6.6}$$

we see that this gives us

$$\rho=\frac{(\xi_t^2+\xi_x^2+\xi_y^2)\dot{R}^2}{[1+R^2]^2}+\frac{(\psi_t^2+\psi_x^2+\psi_y^2)R^2}{[1+R^2]^2}, \tag{6.7}$$

where ψ is given as in (3.1) and $\dot{R}=dR/d\xi$. We can rewrite $(\psi_t^2+\psi_x^2+\psi_y^2)=(\alpha_t^2+\alpha_x^2+\alpha_y^2)+\dot{F}^2(\xi_t^2+\xi_x^2+\xi_y^2)+2\dot{F}(\xi_t\alpha_t+\xi_x\alpha_x+\xi_y\alpha_y)$ and then substitute the expression for F given by (3.9) (when $m=0$).

To get the total energy we should integrate ρ over all space,

$$E=\int \rho \, dx \, dy. \tag{6.8}$$

To perform this integration, in some cases, we can replace the integration over x and y by an integration over ξ and another conveniently chosen variable (which may have a finite or an infinite range). Thus in the cases of algebras 2, 3, and 19 of the Table I, we can use ξ and an angle, while in the cases of 1, 4, 11, 12, 15, and 16, ξ involves only x, and as our variables of integration we can use ξ and y. Clearly, in these latter cases the total energy of any nontrivial solution is infinite.

The most extreme case corresponds to the algebra 10. In this case $\xi=t$, energy density is independent of x and y, and so the total energy is infinite. In this case ϕ^3 of (1.3) is given by $\phi^3=(1-R^2(\xi))/(1+R^2(\xi))$ and is independent of x and y, while ϕ^1 and ϕ^2 depend on x and y only through α. Thus, treating ϕ^i as components of a spin vector field (of unit length) we see that this solution describes very coherent movements of spins that move up and down in phase for all x and y and whose movements in the horizontal plane are modulated by α and $F(t)$.

Similar spin wave interpretations can be given to other solutions. In particular, this is the case when the symmetry variable is more complicated than in the cases mentioned above. One can think of applications in condensed matter physics, the theory of nematic liquid crystals, etc., and even in cosmology. In some of such systems the orientation of $\boldsymbol{\phi}$ does not matter; such cases can be described by a larger class of our solutions. At the same time we can consider $W(x,y,t)$ as a Landau–Ginzburg field that arises in many applications in condensed matter physics [as can be checked, the Landau–Ginzburg equation is very similar to the equation derived from (1.4)]. Indeed, at least one version of the Landau–Ginzburg equation has been treated using the group theoretical techniques applied in this paper. The context was that of magnetic phenomena in external fields.[32]

However, returning to the field theory soliton-like applications, in which case the reductions 2, 3, 17, 18, and 19 are particularly relevant, we note that using an angular variable of integration makes it more likely that a given solution will describe a time evolution of a field configuration of finite energy.

Clearly it would be desirable to analyze further the physical implications of this and other solutions. We hope to be able to report on this in the near future.

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A duality for endomorphisms of von Neumann algebras

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We consider endomorphisms of von Neumann algebras: Let M be a von Neumann algebra, represented on a Hilbert space $\mathscr{H}$, and let M' be the corresponding commutant. Let $\alpha\in\mathrm{End}(M)$ be given, and suppose M has a cyclic vector in $\mathscr{H}$, such that the corresponding state leaves α invariant. Then there is a ''dual'' completely positive mapping β on M' which we find and describe: Each of the two α and β has an associated spectral group, and we show that the group for β is contained in that for α. We consider the following three restrictions on α: i) α is a shift on M, ii) α is strongly ergodic, and iii) α is ergodic. We give spectral theoretic conditions on α (using the two groups described above) to fall into each of the three classes. We also show that the two groups are *conjugacy invariants*, and we discuss the case of *cocycle conjugacy*. © *1996 American Institute of Physics.* [S0022-2488(96)02603-6]

I. INTRODUCTION

Let M be a von Neumann algebra, and let $\alpha:M\to M$ be an endomorphism. A special case of this, of course, is when α is an automorphism, in which case $\alpha(M)=M$. (We will assume that α is *unital*, i.e., that $\alpha(1)=1$. If α is then also assumed *normal*, then $\ker(\alpha)$ is a two-sided closed ideal in M. So, if M is a factor, then α must be 1–1. In the motivating discussion below, we will therefore *assume* that α is 1–1. Then, of course, α is an automorphism iff $\alpha(M)=M$). If there is no subalgebra N of M, other than $\mathbb{C}1$, such that α restricted to N is an automorphism, then we say that α is a *shift*. This shift property is clearly equivalent to the condition

$$\cap_{k=1}^{\infty}\alpha^k(M)=\mathbb{C}1, \tag{1.1}$$

so the shifts are the endomorphisms which is on the ''opposite extreme'' from the automorphisms. They were defined and studied systematically first in Ref. 1 and many results, examples and applications followed in the papers,[2–7] to mention only a few. Several recent papers (see e.g., Refs. 1, 8–11) have dealt with the case $M=\mathscr{B}(\mathscr{H})$ for $\mathscr{H}$ a separable Hilbert space; and others with the case when M is the von Neumann hyperfinite II_1-factor (see e.g.,[12–14]). For the first case, we have structure theoretic results on the conjugacy classes, and their classification; but still only for special restricted types of shifts. For the second case, there are remarkable results on special examples, but here we are further away from structure theoretic results and classification. The basic ideas start with Refs. 15 and 10. But while these papers are concerned with one-parameter semigroups, the focus here is on single endomorphisms. Our constructions use standard tools from Refs. 16–23. We also extend earlier work from Ref. 6. (See also Ref. 24 for one of the early approaches to endomorphisms.)

The present paper nonetheless deals with the general setting, while still motivated both by our own earlier work on $\mathscr{B}(\mathscr{H})$ (see especially Ref. 7) and also by the Powers–Price results for *binary shifts* on the hyperfinite II_1-factor (see especially Refs. 2 and 3). The more concrete areas of application of the present abstract endomorphism theory are to states in quantum statistical mechanics (see Refs. 25 and 26), and to the harmonic analysis of fractal-limit measures (see Ref. 27). The framework of Ref. 23 is also general and includes both of these applications.

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By an *endomorphism* α of a von Neumann algebra M, $\alpha \in \mathrm{End}(M)$, we mean a homomorphism of M which preserves the unit 1 and the *-operation, i.e., $\alpha(1)=1$ and $\alpha(X^*)=\alpha(X)^*$, $\forall X \in M$. For the case $M=\mathscr{B}(\mathscr{H})$, Powers [1] showed that, if there is a normal invariant pure state ω on M, i.e., $\omega\circ\alpha=\omega$, then the conjugacy classes of shifts are labeled by an integral valued index n, specifically the commutant of $\alpha(\mathscr{B}(\mathscr{H}))$ is of the form M_n where M_n is the type I_n-factor, i.e., the n by n complex matrices.

Examples of endomorphisms abound in von Neumann algebra theory (see e.g., Refs. 13 and 12). In fact, R. Longo[13] showed that for *any* inclusion $N \subset M$ of properly infinite von Neumann algebras, there is a "canonical" $\alpha \in \mathrm{End}(M)$ such that $\alpha(M) \subset N$. Specifically, if J_M, J_N denote the associated modular conjugations (of M resp., N), then the formula

$$\alpha(X)=\mathrm{Ad}(\Gamma)(X):=\Gamma X \Gamma^*, \quad \forall X \in M$$

satisfies the stated conditions when Γ is defined as the product $\Gamma:=J_N J_M$. Moreover, Longo showed that the "canonical" endomorphism $\mathrm{Ad}(\Gamma)$ of M is well defined up to inner automorphism of N.

Let R be von Neumann's hyperfinite II_1 factor. Continuing from a question in Ref. 13 Jones (in Ref. 12) determines the (Jones) index $[R:\beta(R)]$ of an endomorphism $\beta \in \mathrm{End}(R)$ which is constructed in turn from a unitary element $U \in R$, and a *shift* (endomorphism) $\sigma: R \to R$, such that

$$\beta=\lim_{n\to\infty}\mathrm{Ad}(U\sigma(U)\cdots\sigma^n(U)).$$

The study from Ref. 13 was continued in a different direction by M. Choda in Refs. 28 and 29. Choda gets information on the Jones-index $[M:N]$ instead from estimates on a certain entropy which she introduces.

We say that two α, $\alpha' \in \mathrm{End}(M)$ are *conjugate* if there is a $\beta \in \mathrm{Aut}(M)$ such that $\alpha'=\beta\circ\alpha\circ\beta^{-1}$, and we say that they are *co-cycle conjugate* if there is a unitary $U \in M$, such that α' and $\mathrm{Ad}(U)\circ\alpha$ are conjugate. (Here, $\mathrm{Ad}(U)$ denotes the inner automorphism, $\mathrm{Ad}(U)(X)=UXU^{-1}$, $\forall X \in M$). As noted in Ref. 6 for the $\mathscr{B}(\mathscr{H})$ case, there is, for each n, just one *co-cycle-conjugacy class* of shifts. But for other factors M, even the cocycle conjugacy classes are relatively poorly understood, and we *do not have complete invariants*.

In general the conjugacy classes in $\mathrm{End}(M)$ are not amenable to classification. Even for $M=\mathscr{B}(\mathscr{H})$ we show in Ref. 6 that the conjugacy classes form a non-smooth space in the sense of Dixmier; see Ref. 20. But in Ref. 7 we isolate specific sections (relative to a new group action) in the "space" of all conjugacy classes.

The present paper has one new invariant which is based on spectral theory. It applies to the general case when M is represented on a Hilbert space $\mathscr{H}$, and there is a unit vector Ω in the same $\mathscr{H}$ such that the corresponding state $\omega=\langle\Omega|\cdot\Omega\rangle$ satisfies $\omega\circ\alpha=\omega$ on M, where α denotes the given endomorphism, and $\langle\cdot|\cdot\rangle$ is the inner product on $\mathscr{H}$. Even when we don't have this condition satisfied *initially*, we show that there is an associated and related system which has the property; but it will be for a different (albeit related) von Neumann algebra and an induced endomorphism. A second main issue in our paper is that of exhibiting explicit conditions on a given $\alpha \in \mathrm{End}(M)$ that it be a *shift* (in the sense of Powers, i.e., $\cap_{k=1}^{\infty}\alpha^k(M)=\mathbb{C}1$). Our results are based on a duality between $\alpha \in \mathrm{End}(M)$, and an associated *completely positive* mapping $\beta: M' \to M'$ where M' denotes the commutant.

We illustrate this last point with the following observation regarding representations π of the *Cuntz algebra* $\mathscr{O}_n$, where $n>1$ is given and finite. Recall[30] that $\mathscr{O}_n$ is the (simple) C^*-algebra on the relations,

$$s_i^* s_j=\delta_{ij}1, \text{and} \sum_{i=1}^{n} s_i s_i^*=1; \tag{1.2}$$

and, moreover, that $\sigma \in \mathrm{End}(\mathcal{O}_n)$ is the canonical shift

$$\sigma(a) := \sum_{i=1}^{n} s_i a s_i^*, \forall a \in \mathcal{O}_n. \tag{1.3}$$

Let $\pi \in \mathrm{Rep}(\mathcal{O}_n, \mathcal{H})$, i.e., a representation of $\mathcal{O}_n$ on $\mathcal{H}$, and set $\mathfrak{A}_k = \pi(\sigma^k(\mathcal{O}_n))'$. We shall suppose that π has a *cyclic vector* $\Omega \in \mathcal{H}$, and we set $\omega = \langle \Omega | \cdot \Omega \rangle$. We say that π is *periodic of period* k if

$$\pi(\sigma^k(s_i^*))\Omega \in \mathfrak{A}_k \Omega,$$

$\forall i = 1, \ldots, n$. If $M =: \pi(\sigma^k(\mathcal{O}_n))''$, then $M' = \mathfrak{A}_k$, and σ induces an endomorphism $\alpha \in \mathrm{End}(M)$. We refer to Refs. 7 and 6 for details on $\mathrm{Rep}(\mathcal{O}_n, \mathcal{H})$. The constructions are motivated by Refs. 31 and 32 and the techniques are drawn from Refs. 33–35 and to some extent Refs. 36 and 37.

The concept of *periodic representations* of $\mathcal{O}_n$ is from Ref. 7 where it plays a crucial role in our analysis of the conjugacy classes of $\mathrm{End}(\mathcal{B}(\mathcal{H}))$, when $\mathcal{H}$ is a given separable Hilbert space. In that case (as we also note in Proposition V below), we are interested in *irreducible* representations of $\mathcal{O}_n$, but the periodicity property (1.6) is in fact useful more generally (see also Refs. 26, 38–42 for related ideas).

Proposition I.1: Let $\pi \in \mathrm{Rep}(\mathcal{O}_n, \mathcal{H})$ with cyclic vector Ω, and set $\omega = \langle \Omega | \cdot \Omega \rangle$. Suppose π is periodic with period k, and let $M =: \pi(\sigma^k(\mathcal{O}_n))''$. Let

$$\alpha(\pi(\sigma^k(a))) = \pi(\sigma^{k+1}(a)) \tag{1.4}$$

$\forall a \in \mathcal{O}_n$. Then there is $\alpha \in \mathrm{End}(M)$, and $\beta: M' \to M'$, completely positive, such that

$$\omega(\beta(A)X) = \omega(A\alpha(X)) \forall A \in M', \forall X \in M. \tag{1.5}$$

Proof: Let $S_i := \pi(s_i)$. and let $\alpha(X) = \Sigma_{i=1}^n S_i X S_i^*$. Then $\alpha(X)$ is defined for all $X \in \mathcal{B}(\mathcal{H})$, and we see that it leaves M invariant, restricts to $\pi(\sigma^k(\mathcal{O}_n))$ and is given by the stated formula (1.4). By assumption (periodicity) there are elements $L_i \in M' = \mathfrak{A}_k$ such that

$$\pi(\sigma^k(s_i^*))\Omega = L_i^* \Omega, \forall i = 1, \ldots, n. \tag{1.6}$$

For $b \in \mathcal{O}_n$, set $X = \pi(\sigma^k(b))$, and for $A \in M'$, set

$$\beta(A) := \sum_{i=1}^{n} L_i A L_i^*. \tag{1.7}$$

Then

$$\begin{aligned}
\omega(\beta(A)X) &= \sum_{i=1}^{n} \langle \Omega | L_i A L_i^* X \Omega \rangle \\
&= \sum_i \langle L_i^* \Omega | A X L_i^* \Omega \rangle \\
&= \sum_i \langle \pi(\sigma^k(s_i^*))\Omega | A X \pi(\sigma^k(s_i^*))\Omega \rangle \\
&= \sum_i \omega(A \pi(\sigma^k(s_i b s_i^*)))
\end{aligned}$$

$$= \omega(A\pi(\sigma^{k+1}(b))) = \omega(A\alpha(\pi(\sigma^k(b)))$$
$$= \omega(A\alpha(X)),$$

which is the desired conclusion. Note that when $A=1$ in $\mathfrak{A}_k = M'$ then we get the invariance, $\omega\circ\alpha=\omega$, holding on M. □

Note that from the Cuntz relations (1.2) it follows that the mapping $\beta: M' \to M'$ in (1.5) satisfies $\beta(1)=1$, and also that it is completely positive. (For more details on β in the general case, see Lemma IV below.)

II. ERGODICITY

The setting is a given endomorphism α on a von Neumann algebra M. It is assumed throughout that M acts on a fixed Hilbert space $\mathscr{H}$ containing a cyclic vector Ω, $\|\Omega\|=1$, such that the state $\omega = \langle\Omega|\cdot\Omega\rangle$ satisfies $\omega\circ\alpha=\omega$ on M.

Let the data $(M,\omega,\mathscr{H},\Omega)$ be given as stated, and let $\alpha \in \mathrm{End}(M)$ be such that $\omega\circ\alpha=\omega$. Let $Q \in M$ be the *support projection* for ω viewed as a state on M. Then it follows that

$$Q \leqslant \alpha(Q) \leqslant \cdots \leqslant \alpha^k(Q) \leqslant \cdots,$$

so that the limit

$$\lim_{k\to\infty} \alpha^k(Q) = Q_\infty \tag{2.1}$$

exists in M, as projections of a von Neumann algebra form a complete lattice. Clearly $\alpha(Q_\infty)=Q_\infty$. We shall say that the given system is in *reduced form* if $Q_\infty=1$ in M; and we note that it is no essential restriction on the system if we assume at the outset that it be in reduced form: Indeed, suppose it were not in reduced form. Then replace M with $Q_\infty M Q_\infty$, and $\mathscr{H}$ with $Q_\infty(\mathscr{H})$. We then have $(Q_\infty M Q_\infty)' = M' Q_\infty$, and the vector $\Omega = Q_\infty\Omega$ will also be cyclic for $Q_\infty M Q_\infty$ on $Q_\infty(\mathscr{H})$. Finally α induces an endomorphism α_∞ of $Q_\infty M Q_\infty$, i.e., $\alpha_\infty \in \mathrm{End}(Q_\infty M Q_\infty)$, by

$$\alpha_\infty(Q_\infty X Q_\infty) = Q_\infty \alpha(X) Q_\infty, \tag{2.2}$$

$\forall X \in M$, which is just the *restriction* of α to the subalgebra $Q_\infty M Q_\infty \subset M$. Finally, of course, Q_∞ serves as the identity element in $Q_\infty M Q_\infty$, and it acts as the identity operator on $Q_\infty(\mathscr{H})$. In the sequel, we shall assume therefore that a given system, as specified, *is in reduced form*. If it is not, it may be replaced with the canonically restricted system (which is in reduced form) without loss of generality.

It is known[43,44] that every isometry in a given Hilbert space decomposes uniquely as an orthogonal sum of a unitary operator and a shift operator. We now study this decomposition for the isometry W which was introduced above. But first:

Definitions II.1: Let M be a von Neumann algebra and let $\alpha \in \mathrm{End}(M)$ be given such that $\alpha(1)=1$. Following Powers,[1] we say that α is a *shift* if $\cap_{k=1}^{\infty} \alpha^k(M) = \mathbb{C}1$. Let W be an isometry on a Hilbert space $\mathscr{H}$. Following Wold (see Refs. 43 and 44), we make the *orthogonal decomposition* $\mathscr{H} = \mathscr{H}_u \oplus \mathscr{H}_s$ where

$$\mathscr{H}_u = \cap_{k=1}^{\infty} W^k \mathscr{H}, \tag{2.3}$$

and

$$\mathscr{H}_s = \sum_{k=0}^{\infty} W^k N(W^*) \tag{2.4}$$

with $N(W^*)=\{\xi \in \mathscr{H}: W^*\xi=0\}$, and the distinct spaces $W^kN(W^*)$ mutually orthogonal. The restriction $W|_{\mathscr{H}_u}$ is *unitary*, and the space $N(W^*)$ is *wandering* (referring to the orthogonality) for W. The decomposition is called the *Wold decomposition*, and it is unique as specified.

If $\omega(\cdot)=\langle\Omega|\cdot\Omega\rangle$ is a state on M, corresponding to a cyclic vector Ω, and if $\omega\circ\alpha=\omega$, then

$$W(X\Omega):=\alpha(X)\Omega, \quad \forall X\in M \tag{2.5}$$

defines an *isometry* on $\mathscr{H}$, and $\Omega \in \mathscr{H}_u$. We say that W is an *essential shift* on $\mathscr{H}$ if $\mathscr{H}_u=\mathbb{C}\Omega$, i.e., if the unitary subspace for the decomposition is one-dimensional.

It is generally difficult to verify if a given $\alpha \in \mathrm{End}(M)$ is a *shift* in the sense of Powers. But if there is also a given invariant state $\omega=\langle\Omega|\cdot\Omega\rangle$ as described above, then we have the following result (with a partial converse).

Proposition II.2: Let $(M,\omega,\mathscr{H},\Omega)$ be as described and let $\alpha \in \mathrm{End}(M)$ be given such that $\omega=\langle\Omega|\cdot\Omega\rangle$ satisfies $\omega\circ\alpha=\omega$ on M, and assume further that the system is in reduced form. Then, if the isometry W from (2.5) is given to be an essential shift, then it follows that α is an shift on M in the sense of Powers.

Proof: Let

$$X\in M^\infty:=\cap_{k=1}^{\infty}\alpha^k(M) \tag{2.6}$$

be given. Then $X\Omega \in \mathscr{H}_u$, and we are assuming that $\mathscr{H}_u=\mathbb{C}\Omega$. It follows that

$$X\Omega=\omega(X)\Omega$$

.

If $Q \in M$ denotes the support projection for the state ω on M, then we get

$$QXQ=\omega(X)Q$$

.

Applying α to both sides yields

$$\alpha(Q)\alpha(X)\alpha(Q)=\omega(X)\alpha(Q).$$

But $\alpha|_{M^\infty} \in \mathrm{Aut}(M^\infty)$ and $\omega(\alpha^{-1}(X))=\omega(X)$. Replacing X with $\alpha^{-1}(X) \in M^\infty$ yields

$$\alpha(Q)X\alpha(Q)=\omega(X)\alpha(Q),$$

and by iteration

$$\alpha^k(Q)X\alpha^k(Q)=\omega(X)\alpha^k(Q)$$

for $\forall k=1,2,\ldots$. Since the system is in reduced form, $\lim_{k\to\infty}\alpha^k(Q)=1$, and it follows that $X=\omega(X)1$, proving that $M^\infty=\mathbb{C}1$ which is the defining property for α to be a shift on M. □

In Corollary X below we shall show that, if (α,M) is a strongly ergodic shift, then $\mathscr{H}_u=\mathbb{C}\Omega$, i.e., the corresponding *isometry* W must then have one-dimensional unitary part. In any case, the dimension of $\mathscr{H}_u$ is a *conjugacy invariant* for the strongly ergodic endomorphisms of von Neumann algebras.

III. SPECTRAL THEORY

The next result gives the spectral decomposition for a given $\alpha \in \mathrm{End}(M)$ with the stated properties:

Theorem III.1: Let M be a von Neumann algebra acting on a Hilbert space $\mathscr{H}$, and let $\Omega \in \mathscr{H}$ be a cyclic vector with the corresponding state ω given on $\mathscr{B}(\mathscr{H})$ by

$$\omega(A)=\langle \Omega | A\Omega \rangle, \quad A \in \mathscr{B}(\mathscr{H}).$$

Let $\alpha \in \mathrm{End}(M)$ be given and assume $\omega \circ \alpha = \omega$ on M, and moreover that α is strongly ergodic. Let

$$M^{\infty} := \cap_{k=1}^{\infty} \alpha^k(M), \tag{3.1}$$

and let $W: \mathscr{H} \to \mathscr{H}$ be the *isometry* defined by

$$W(A\Omega) := \alpha(A)\Omega, \quad \forall A \in M. \tag{3.2}$$

Let

$$\mathscr{H}^{\infty} := \mathscr{H}_u = \cap_{k=1}^{\infty} R(W^k) \tag{3.3}$$

be the unitary part in the Wold decomposition of W on $\mathscr{H}$, and let $E(\cdot)$ be the corresponding orthogonal spectral resolution-measure of $W|_{\mathscr{H}^{\infty}}$. For $\xi \in \mathscr{H}^{\infty}$, $\|\xi\|=1$, let $d\mu(z) := \|E(dz)\xi\|^2$ be the corresponding measure on $\mathbb{T}$. Then there is a μ measurable function $b: \mathbb{T} \to M$, $\|b(z)\| \leqslant 1$, such that

$$\int_{\mathbb{T}} \langle b(z)\Omega | \xi \rangle b(z)\Omega \, d\mu(z) = \xi \tag{3.4}$$

and $\alpha(b(z)) = z b(z)$ a.e. on $\mathbb{T}$. In particular, if $W\xi = \lambda \xi$, for some $\lambda \in \mathbb{T}$, then there is a single element $b \in M$, $\|b\| \leqslant 1$ such that

$$b\Omega = \xi \text{ and } \alpha(b) = \lambda b. \tag{3.5}$$

The above result yields the spectral decomposition for the *unitary part* of the Wold decomposition for the isometry W which is associated to a given $\alpha \in \mathrm{End}(M)$ as stated. But, in the present form, the theorem is difficult to apply as the cyclic vector Ω which is given for M at the outset is typically not separating. Specifically if M' is the commutant, then $[M'\Omega]$ is a proper subspace of $\mathscr{H}$. The projection onto this subspace will be denoted Q in the sequel.

Proof: We first supply some preliminaries in this section and the following two, and then we return to the proof again in Section VII below.

Lemma III.2: Let M, $\mathscr{H}$, Ω, $\alpha \in \mathrm{End}(M)$, and W be as specified in the theorem, and let $W^*: \mathscr{H} \to \mathscr{H}$ be the co-isometry given by

$$\langle W^*\xi | \eta \rangle = \langle \xi | W\eta \rangle, \quad \forall \xi, \eta \in \mathscr{H}. \tag{3.6}$$

Then there is a completely positive mapping $\beta: M' \to M'$ on the commutant such that $\beta(1)=1$, $\omega \circ \beta = \omega$, and

$$W^*(A\Omega) = \beta(A)\Omega, \quad \forall A \in M'. \tag{3.7}$$

Proof: For $A \in M'$ and $X \in M$, we have

$$\langle W^*(A\Omega) | X\Omega \rangle = \langle A\Omega | W(X\Omega) \rangle = \langle A\Omega | \alpha(X)\Omega \rangle$$

which, in the state $\omega(\cdot) = \langle \Omega | \cdot \Omega \rangle$, amounts to the identity

$$\langle W^*(A\Omega) | X\Omega \rangle = \omega(A^* \alpha(X)). \tag{3.8}$$

For the algebras M and M', we will use the subscript $+$ denoting the respective positive elements, and we claim that, if $A \in M'_+$ and $X \in M_+$, then

$$\omega(A\alpha(X)) \leqslant \|A\|\omega(X). \tag{3.9}$$

But then the Segal Radon–Nikodym theorem[25] yields the existence of some $B \in M'_+$ such that

$$\omega(A\alpha(X)) = \omega(BX) \tag{3.10}$$

for all $X \in M$. To prove (3.9), we iterate the Cauchy–Schwarz estimate as follows: Let $A \in M'_+$ and $X \in M_+$. Then

$$\begin{aligned}
\omega(A\alpha(X)) &= \omega(A\alpha(X)^{1/2}\alpha(X)^{1/2}) \\
&\leqslant \omega((A\alpha(X)^{1/2})^2)^{1/2}\omega(\alpha(X))^{1/2} \\
&= \omega(A^2\alpha(X))^{1/2}\omega(X)^{1/2} \leqslant \omega(A^4\alpha(X))^{1/4}\omega(X)^{\frac{1}{2}+\frac{1}{4}} \\
&\leqslant \cdots \\
&\leqslant \omega(A^{2^n}\alpha(X))^{2^{-n}}\omega(X)^{\frac{1}{2}+\frac{1}{4}+\cdots+\frac{1}{2^n}} \\
&\leqslant \|A^{2^n}\|^{2^{-n}}\|X\|^{2^{-n}}\omega(X)^{\frac{1}{2}+\cdots+\frac{1}{2^n}}.
\end{aligned}$$

Passing to the limit $(n\to\infty)$, and using the spectral radius formula, we get the expression $\|A\|\omega(X)$ on the right hand side, and the desired estimate (3.9) follows from this. Let $B \in M'_+$ be the corresponding element serving as a Segal Radon–Nikodym derivative (see Refs. 45 and 25). Returning to (3.8) and (3.10), we get

$$\langle W^*(A\Omega)|X\Omega\rangle = \langle B\Omega|X\Omega\rangle,$$

and this now holds for all $X \in M$. Since Ω is cyclic for M, and therefore separating for M', we have the identity

$$W^*(A\Omega) = B\Omega \text{ in } \mathscr{H}, \tag{3.11}$$

and with $B \in M'$ uniquely defined. Moreover the assignment $\beta: A \mapsto B$ defines a positive mapping of M' into itself with the properties listed in the lemma. But the argument may be repeated with the tensor factor M_n ($=$ all the n by n complex matrices), and we conclude that $\beta(A) := B$ is indeed *completely positive*. Setting $X = 1$ in M we conclude that $\omega \circ \beta = \omega$ holds on M'. □

When M, ω and $\mathscr{H}$ are given as in the theorem, and $\alpha \in \mathrm{End}(M)$, we shall say that the completely positive mapping $\beta: M' \to M'$ from Lemma III is the *dual mapping*, and the duality may be expressed in the identity

$$\omega(A\alpha(X)) = \omega(\beta(A)X) \tag{3.12}$$

valid for $\forall A \in M'$ and $\forall X \in M$.

IV. A COVARIANCE RELATION

The following is basic for the further analysis in the rest of the paper:

Lemma IV.1: Let $(M, \omega, \mathscr{H}, \Omega)$ be as in the theorem. Let $\alpha \in \mathrm{End}(M)$ be given and let β be the corresponding dual mapping of M'.

(i) Then there is a contractive operator $T: \mathscr{H} \to \mathscr{H}$ such that

$$TAW=\beta(A) \tag{4.1}$$

holds for all $A \in M'$ as an operator identity on $\mathscr{H}$.

(ii) Moreover we have the identity $T=W^*$ on $\mathscr{H}$ when W^* is viewed as a co-isometry. Specifically, we have for all $\xi \in N(W^*)=(W.\mathscr{H})^{\perp}$ that $T\xi=0$.

(iii) $W_uQ=QW_u$ where $Q \in M$ is the support projection of $\omega=\langle\Omega|\cdot\Omega\rangle$ on M.

Remark IV.2: Since W is an isometry on $\mathscr{H}$, $\mathscr{H}$ decomposes orthogonally as $\mathscr{H}=N(W^*) \oplus W.\mathscr{H}$, and if T is contractive on $\mathscr{H}$ and extending W^*, then there must be a contractive operator $C:N(W^*)\to\mathscr{H}$ such that

$$T(\xi_1+W\xi_2)=C\xi_1+\xi_2 \tag{4.2}$$

for $\forall\,\xi_1 \in N(W^*)$ and $\forall\,\xi_2 \in \mathscr{H}$. (We will show below that, in this case, in fact this operator C will be zero.)

Proof of Lemma IV.1: Recall W is the isometry on $\mathscr{H}$ given by

$$W(X\Omega):=\alpha(X)\Omega, \quad \forall X\in M. \tag{4.3}$$

To show that a contractive operator T can be found subject to (4.1), it is enough to check that the estimate

$$\|\beta(A)\xi\|\leqslant\|AW\xi\| \tag{4.4}$$

holds for $A \in M'$ and $\xi \in \mathscr{H}$. Since Ω is cyclic, we may restrict to vectors ξ of the form $\xi=X\Omega$ for $X \in M$. Then

$$\begin{aligned}\|\beta(A)X\Omega\|^2&=\omega((\beta(A)X)^*\beta(A)X)\\&=\omega(\beta(A)^*\beta(A)X^*X)\\&\leqslant\omega(\beta(A^*A)X^*X)\\&=\omega(A^*A\alpha(X^*X))\\&=\omega(A^*A\alpha(X)^*\alpha(X))\\&=\omega((A\alpha(X))^*A\alpha(X))\\&=\|AW(X\Omega)\|^2,\end{aligned}$$

which is the desired estimate (4.4). Note we are *not* claiming that

$$M'W.\mathscr{H}=\text{ span}\,\{\mathrm{AW}\xi:\mathrm{A}\in\mathrm{M}',\xi\in\mathscr{H}\}$$

is a dense subspace in $\mathscr{H}$, but T is defined on this subspace by

$$TAW\xi:=\beta(A)\xi\forall A\in M',\forall\,\xi\in\mathscr{H} \tag{4.5}$$

and then extended trivially on the orthogonal complement in $\mathscr{H}$. This is the desired conclusion (4.1) from (i).

Proof of (ii): The assertion in (ii) of Lemma IV is that the contractive operator C from (4.2) which defines the extension T of W^* must be the zero operator. To prove this, let $\xi_1 \in M(W^*)$, $\xi_2 \in \mathscr{H}$, $\|\xi_2\|=1$, and $p \in \mathbb{C}$, be given. Using the contractive property, we get

$$\|T\xi_1\|^2+2\mathrm{Re}(p\langle T\xi_1|\xi_2\rangle)\leqslant\|\xi_1\|^2.$$

Since this holds for $\forall p \in \mathbb{C}$, we conclude that $T\xi_1 = 0$. But $\xi_1 \in N(W^*)$, so $T\xi_1 = C\xi_1 = 0$ which is the desired conclusion in (ii).

Part (iii) of the lemma for the unitary part of the Wold decomposition follows from the results in Section VI below.

Definitions IV.3: Let M, ω, $\mathscr{H}$, Ω be as stated, and let $\alpha \in \mathrm{End}(M)$ satisfy $\omega \circ \alpha = \omega$. Let $\beta: M' \to M'$ be the dual completely positive mapping on the commutant M'. We say that the system is *strongly ergodic* if the only normal functionals φ on M' satisfying

$$\varphi(\beta(A)) = \varphi(A) \quad \text{for} \quad \forall A \in M' \tag{4.6}$$

are of the form

$$\varphi(A) = \text{const.} \times \omega(A), \quad \forall A \in M'. \tag{4.7}$$

We say that the system M, ω, α is *ergodic* if it is as specified, and if the subalgebra

$$M^\alpha = \{X \in M : \alpha(X) = X\} \tag{4.8}$$

is one-dimensional, i.e., if it is of the form $M^\alpha = \mathbb{C}1$ where 1 is the identity element in M.

The following result relates the concepts and definitions above:

Lemma IV.4: Let $(M, \omega, \mathscr{H}, \Omega)$ and $\alpha \in \mathrm{End}(M)$ be as specified: in particular, $\omega \circ \alpha = \omega$ on M is assumed. Suppose the system is in reduced form, and also that it is strongly ergodic. Then it follows that it is ergodic.

Proof: Let $\beta: M' \to M'$ be the dual completely positive mapping on the commutant M', and let $X \in M^\alpha$ be given. Then define the functional φ_X on M' by

$$\varphi_X(A) = \omega(XA), \quad \forall A \in M'.$$

We then have (4.6) satisfied as

$$\varphi_X(\beta(A)) = \omega(X\beta(A)) = \omega(\alpha(X)A) = \omega(XA) = \varphi_X(A), \quad \forall A \in M'.$$

Since the system is assumed strongly ergodic, it follows that φ_X satisfies (4.7), and in fact

$$\varphi_X(A) = \omega(XA) = \omega(X)\omega(A) \quad \text{for} \quad \forall A \in M'.$$

Introducing the support projection $Q \in M$, i.e., Q is the projection on $\mathscr{H}$ onto the closed subspace $[M'\Omega] \subset \mathscr{H}$, we conclude that

$$QXQ = \omega(X)Q.$$

Applying α^k, $k = 1, 2, \ldots$ to this, we get

$$\alpha^k(Q)X\alpha^k(Q) = \omega(X)\alpha^k(Q),$$

and passing to the limit $k \to \infty$,

$$Q_\infty X Q_\infty = \omega(X)Q_\infty. \tag{4.9}$$

Since the system is in reduced form, we have $Q_\infty = 1$, so the last formula (4.9) amounts to the assertion $X \in \mathbb{C}1$. We have shown that $M^\alpha = \mathbb{C}1$ which is the desired conclusion, i.e., (α, M) is ergodic. □

V. AN EXAMPLE

The present paper was motivated by our earlier study of endomorphisms of $\mathscr{B}(\mathscr{H})$, Refs. 6 and 7 and we found that the methods had potential also for the case when $\mathscr{B}(\mathscr{H})$ is replaced with a general von Neumann factor (see Refs. 2 and 3).

The following result shows that, for the example in Proposition I, the above definitions are closely connected (but, of course, for the general case of an endomorphism of a von Neumann algebra, the concepts are distinct).

Proposition V.1: Let $\pi \in \mathrm{Rep}(\mathscr{O}_n, \mathscr{H})$ be a cyclic representation and suppose it is periodic of period $k \in \{0,1,2, \dots\}$. Let α_k be the induced endomorphism from Proposition I.1, i.e.,

$$\alpha_k \in \mathrm{End}(\pi(\sigma^k(\mathscr{O}_n))'') \tag{5.1}$$

as specified in (1.4). Then the following three conditions are equivalent:

(i) α_k is strongly ergodic on $M_k := \pi(\sigma^k(\mathscr{O}_n))''$.

(ii) π is irreducible, i.e., $\pi(\mathscr{O}_n)' = \mathbb{C}1$.

(iii) The endomorphism $\alpha_\pi \in \mathrm{End}(\mathscr{B}(\mathscr{H}))$ given by

$$\alpha_\pi(A) := \sum_{i=1}^{n} \pi(s_i) A \pi(s_i^*), \quad \forall A \in \mathscr{B}(\mathscr{H}) \tag{5.2}$$

is ergodic.

Proof: The proof of this result is contained in Ref. 7 Section 6, and Lemma 7.8, and the present paper is motivated by this important special case. Starting with α_k as in (i) above and a cyclic vector $\Omega \in \mathscr{H}$ satisfying (1.6), we define the state $\omega = \langle \Omega | \cdot \Omega \rangle$. Since the equivalence (ii) $\Leftrightarrow$ (iii) is straightforward, we consider states φ such that for $\lambda \in \mathbb{R}_+$ we have

$$\lambda \varphi(X^*X) \leqslant \omega(X^*X) \quad \text{for} \quad \forall X \in \mathscr{O}_n .$$

Applying this to elements X of the form

$$\sum_i c_i (\pi(\sigma^k(s_i^*)) - L_i^*)$$

(as well as higher order monomials) we find that the GNS-representation π_φ of $\mathscr{O}_n$ is also periodic of period k, and the restricted state $\varphi|_{\mathfrak{A}_k}$ is $\beta(\cdot)$ invariant where β (as in (1.7)) is given by $\beta(A) = \Sigma_i L_i A L_i^*$, $\forall A \in \mathfrak{A}_k = \pi(\sigma^k(\mathscr{O}_n))' = M_k'$. The equivalence (i) $\Leftrightarrow$ (ii) follows from this. In fact Ref. 7, Section 6 shows that, up to scale, there is a unique β-invariant linear functional on $\mathfrak{A}_k$, not just a unique (up to scale) *positive* functional.

VI. EIGENVECTORS IN $\mathscr{H}$ AND EIGENELEMENTS IN M

We now return to the general case, and focus on the interplay between the Hilbert space and the von Neumann algebra in connection with our spectral theory.

Proposition VI.1: Let $\alpha \in \mathrm{End}(M)$ be given, and let M, ω, $\mathscr{H}$, Ω be as specified in Theorem Theorem 3.1. The system is assumed strongly ergodic. In particular, we have $\omega \circ \alpha = \omega$ on M, and an isometry W on $\mathscr{H}$ given by

$$W(X\Omega) = \alpha(X)\Omega \quad \text{for} \quad X \in M. \tag{6.1}$$

Let $\xi_1 \in \mathscr{H}$, $\xi_1 \neq 0$, be given such that, for some $\lambda \in \mathbb{C}$, $|\lambda| = 1$, we have $W\xi_1 = \lambda \xi_1$. Then it follows that there is an $X_1 \in M$ such that $\alpha(X_1) = \lambda X_1$, $X_1\Omega = \xi_1$ and $\|X_1\| \leqslant \|\xi_1\|$.

Remark VI.2: Let α, M, ω, W, $\mathscr{H}$, Ω be as stated in the proposition. In addition to the assumption of strong ergodicity, suppose also that the system is in reduced form. Then for every $\lambda \in \sigma(W) \cap \mathbb{T}$, we have $\lambda \in \sigma(W)$, and the element $X \in M$, satisfying $X\Omega = \xi_1$ and $\alpha(X) = \lambda X$, for a solution to $W\xi_1 = \lambda\xi_1$, may be chosen *unitary*, i.e., $X^*X = XX^* = 1$. To see this, note that a solution X as in the proposition must also satisfy $\alpha(X^*X) = X^*X$ and $\alpha(XX^*) = XX^*$, but the only fixed points for α are $\mathbb{C}1$.

Proof of Proposition VI.1: It is no essential restriction to assume $\|\xi_1\| = 1$ for the given eigenvector. Let

$$K := \{X \in M : \|X\| \leqslant 1, \quad X\Omega = \xi_1\} \tag{6.2}$$

and note that this set is w^*-compact and convex in M. Our first goal is to show that K is non-empty. The operator T from Lemma IV satisfies $TW\xi_1 = \xi_1$, and since $W\xi_1 = \lambda\xi_1$, we get $T\xi_1 = \lambda\xi_1$. Since $\|T\| \leqslant 1$, this implies that $T^*\xi_1 = \lambda\xi_1$. We claim that the state $\varphi(\cdot) := \langle \xi_1 | \cdot \xi_1 \rangle$ is β-invariant on M' when β denotes the *dual completely positive mapping* on M'. Indeed, let $A \in M'$, and use Lemma IV again as follows

$$\varphi(\beta(A)) = \langle \xi_1 | TAW\xi_1 \rangle = \langle T^*\xi_1 | AW\xi_1 \rangle = \langle \lambda\xi_1 | \lambda A\xi_1 \rangle = |\lambda|^2 \langle \xi_1 | A\xi_1 \rangle = \varphi(A)$$

and this is the desired invariance on M' for the state $\varphi = \langle \xi_1 | \cdot \xi_1 \rangle$; i.e., $\varphi \circ \beta = \varphi$ holds on M'. But the system is assumed strongly ergodic and we conclude that the two states φ and $\omega = \langle \Omega | \cdot \Omega \rangle$ must agree on M'. Specifically

$$\langle \xi_1 | A\xi_1 \rangle = \langle \Omega | A\Omega \rangle \tag{6.3}$$

and $\|A\Omega\| = \|A\xi_1\|$ holds for all $A \in M'$. The mapping $A\Omega \mapsto A\xi_1$ is therefore a well defined isometry from the subspace $[M'\Omega] = Q\mathscr{H}$ into $\mathscr{H}$ and it commutes with M'. From a theorem of Krein and Phillips (see Refs. 46, 47 and 48) we conclude that there is a contractive extension $X : \mathscr{H} \to \mathscr{H}$ of the partial isometry, defined initially only on $Q(\mathscr{H})$, and the extension may be chosen to also commute with M'. We have $X \in M'' = M$, $\|X\| \leqslant 1$, and $X\Omega = \xi_1$. So X is an element in the set K. But this set is also invariant under the mapping $\lambda^{-1}\alpha(\cdot)$, i.e., $\lambda^{-1}\alpha(X) \in K$ for all $X \in K$. To see that $\lambda^{-1}\alpha(X) \in K$, note that $\lambda^{-1}\alpha(X)\Omega = \lambda^{-1}W(X\Omega) = \lambda^{-1}W\xi_1 = \lambda^{-1}\lambda\xi_1 = \xi_1$ for all $X \in K$. We now apply the Schauder-Tychonoff fixed-point theorem to the restriction $\lambda^{-1}\alpha(\cdot)|_K$ (see Ref. 49 pp. 161–163 and Ref. 50 pp. 453–456) and conclude the existence of some $X_1 \in K$ such that $\lambda^{-1}\alpha(X_1) = X_1$, and it is clear that this solution X_1 has the properties which are listed in the conclusion of the proposition.

To apply the fixed-point theorem we must check of course that $\alpha(\cdot)$ is w^*-continuous on K. In the event that α is already normal at the outset, this is automatic. From Refs. 6 and 4 and 5 we know that if M is type I then the endomorphism α will automatically be normal.

For the general case, we proceed as follows: Let $\{X_j\}$ be an indexed net of elements in K such that $X_j \to X$ in the w^*-topology. Then we must show that for all ξ, $\eta \in \mathscr{H}$,

$$\langle \xi | \alpha(X_j)\eta \rangle \underset{j \to \infty}{\to} \langle \xi | \alpha(X)\eta \rangle. \tag{6.4}$$

This is easy in the event that $\eta \in R(W)$, i.e., $\eta = W\zeta$ for some $\zeta \in \mathscr{H}$. For then

$$\alpha(X_j)\eta = \alpha(X_j)W\zeta = WX_j\zeta,$$

and (as $j \to \infty$) we have,

$$\langle \xi | \alpha(X_j)\eta \rangle = \langle W^*\xi | X_j\zeta \rangle \to \langle W^*\xi | X\zeta \rangle = \langle \xi | WX\zeta \rangle = \langle \xi | \alpha(X)W\zeta \rangle = \langle \xi | \alpha(X)\eta \rangle$$

which is the asserted convergence (6.4), in this special case.

The remaining cases may be reduced to checking vectors $\eta \in N(W^*)$, and using the von Neumann BT-theorem (see Ref. 51 p. 106). We may represent the vector η in the form $\eta = AC\Omega$ where $A \in M'$ and C is an (unbounded) operator affiliated with M'. Since each $X_j \in K$, we get

$$\alpha(X_j)\eta = \alpha(X_j)AC\Omega = AC\alpha(X_j)\Omega = ACWX_j\Omega = ACW\xi_1 = \lambda AC\xi_1$$

and this last vector is independent of the index j for the net. So there is no convergence problem in this case. □

VII. PROOFS

In this section we return to the proof of Theorem III.1.

Proof of Theorem III.1: Let the system $(M,\omega,\mathscr{H},\Omega)$ be given as in the statement of the theorem. It is assumed that

$$\omega = \langle\Omega|\cdot\Omega\rangle \text{ satisfies } \omega\circ\alpha = \omega \text{ on } M, \tag{7.1}$$

and that α is strongly ergodic. Hence α induces an isometry on $\mathscr{H}$ given by (6.1). We must show that every

$$\xi \in \mathscr{H}_u = \cap_{k=1}^{\infty} W^k\mathscr{H}, \tag{7.2}$$

$\|\xi\| = 1$ with spectral measure μ has a generalized eigenfunction expansion as stated in (3.4) of the theorem, and given by some L^∞-function, $b(\cdot):\mathbb{T}\to M$, such that $z\mapsto b(z)\Omega$ is a measurable field of generalized eigenvectors for the unitary operator $W|_{\mathscr{H}_u}$ (restricted to the ξ-cyclic subspace, of course). Moreover the assertion is that the measurable field $b(\cdot)$ with values in M can be chosen such that

$$\alpha(b(z)) = zb(z), \quad \text{a.e. } z\in\mathbb{T}. \tag{7.3}$$

Recall that if ξ is in fact an eigenvector of W, then the result follows from Proposition VI above. It remains therefore to consider only the case where the spectral measure $\mu(\cdot)$ of ξ is continuous on $\mathbb{T}$. From the spectral theorem, we may choose a generalized eigenfunction expansion $\{v(z)\}_{z\in\mathbb{T}}$ in the form

$$\int_{\mathbb{T}} \langle v(z)|\xi\rangle v(z)\,d\mu(z) = \xi. \tag{7.4}$$

The compact convex set K corresponding to the one (6.2) above will now be a subset of elements in $L^\infty(\mathbb{T},M)$ such that $X(z)\Omega = v(z)$ a.e. $z, \|X(\cdot)\|_{L^\infty} \leqslant 1$. If $X(\cdot)$ is in K, then the element $Y(z) := z^{-1}\alpha(X(z))$ will also be in K and the Schauder–Tychonoff theorem[49] applies provided we check that $K \neq \varnothing$. But we have the field $v(\cdot)$ from (7.4), and the functional φ on M' may be defined now as follows: for $A \in M'$, set

$$\varphi(A) := \int_{\mathbb{T}} \langle v(z)|Av(z)\rangle\,d\mu(z). \tag{7.5}$$

Let $\beta: M'\to M'$ be the completely positive mapping which is dual to α on M. Then

$$\varphi(\beta(A)) = \int \langle v(z)|\beta(A)v(z)\rangle\,d\mu(z)$$

$$= \int \langle v(z) | TAWv(z) \rangle d\mu(z)$$

$$= \int \langle zv(z) | zAv(z) \rangle d\mu(z)$$

$$= \int \langle v(z) | Av(z) \rangle d\mu(z)$$

$$= \varphi(A),$$

where Lemma IV was used again in line two of the calculation. Using the strong ergodicity, we get that the mapping (for $A \in M'$):

$$1 \otimes A\Omega \mapsto Av(z)$$

is isometric from a subspace in $L^2(\mathbb{T},\mathscr{H})$ into $L^2(\mathbb{T},\mathscr{H})$, and it commutes with the action of $L^\infty(\mathbb{T}) \otimes M'$. We extend it (using Krein's theorem, see Refs. 47 and 46) to a contractive mapping of $L^2(\mathbb{T},\mathscr{H})$ commuting with the same algebra. But the extended mapping is then an element in $L^\infty(\mathbb{T},M)$; i.e., it is given as an operator on $L^2(\mathbb{T},\mathscr{H})$ by $\xi \mapsto \xi'$ where $\xi'(z) = X(z)\xi(z)$, a.e. $z \in \mathbb{T}$, and $X: \mathbb{T} \to M$ is a vector valued L^∞-function on $\mathbb{T}$. Since $X(z)\Omega = v(z)$ a.e. on $\mathbb{T}$, we conclude that X is an element in the set K. The fixed-point theorem applies, and the proof is concluded. □

VIII. INVARIANTS

Let $\alpha \in \mathrm{End}(M)$, and let M be represented on a Hilbert space $\mathscr{H}$ with cyclic vector Ω, such that

$$\omega := \langle \Omega | \cdot \Omega \rangle \text{ satisfies } \omega \circ \alpha = \omega \text{ on } M, \tag{8.1}$$

and suppose the system is in reduced form. Let $W: \mathscr{H} \to \mathscr{H}$ be the isometry,

$$W(X\Omega) := \alpha(X)\Omega, \quad \forall X \in M, \tag{8.2}$$

and let

$$W = W_u \oplus W_s \tag{8.3}$$

be the corresponding Wold decomposition with W_u (resp., W_s) the unitary (resp., the shift) part. For the spectrum we have $\sigma(W) \cap \mathbb{T} = \sigma(W_u)$, and we now show that this set is a *conjugacy invariant*.

Corollary VIII.1: Let M be a von Neumann algebra on a Hilbert space $\mathscr{H}$, and let $\alpha_1, \alpha_2 \in \mathrm{End}(M)$ be as specified above; i.e., we assume there are cyclic vectors Ω_1, Ω_2 in $\mathscr{H}$ such that $\omega_i = \langle \Omega_i | \cdot \Omega_i \rangle$ satisfy $\omega_i \circ \alpha_i = \omega_i$ $(i = 1,2)$, and we assume both are strongly ergodic. Let W_1 and W_2 be the corresponding isometries. If α_1 and α_2 are conjugate, then it follows that

$$\sigma(W_1) \cap \mathbb{T} = \sigma(W_2) \cap \mathbb{T}. \tag{8.4}$$

Proof: Let $\gamma \in \mathrm{Aut}(M)$ be such that $\alpha_2 = \gamma \circ \alpha_1 \circ \gamma^{-1}$, and let $\lambda_1 \in \sigma(W_1) \cap \mathbb{T}$. Let $\xi_1 \in \mathscr{H}$ satisfy $\|\xi_1\| = 1$, $W_1\xi_1 = \lambda_1\xi_1$. By Proposition VI, there is an $X_1 \in M$ such that $\|X_1\| \leqslant 1$, $X_1\Omega_1 = \xi_1$, and $\alpha_1(X_1) = \lambda_1 X_1$. It follows that then $\alpha_2(\gamma(X_1)) = \lambda_1\gamma(X_1)$ and setting $\xi_2 = \gamma(X_1)\Omega_2$, we get $W_2\xi_2 = \lambda_1\xi_2$. We claim that $\xi_2 \neq 0$, so $\lambda_1 \in \sigma(W_2) \cap \mathbb{T}$, proving that the two sets $\sigma(W_i) \cap \mathbb{T}$ $(i = 1,2)$ must coincide. From Lemma 4.4 we conclude that both systems are

in fact ergodic. From $\alpha_1(X_1)=\lambda_1 X_1$ we get $\alpha_1(X_1^* X_1)=X_1^* X_1$ so $X_1^* X_1$ must be in $\mathbb{C}1$. But $\omega_1(X_1^* X_1)=1$ from the construction. Hence $X_1^* X_1=1$; i.e., X_1 is an isometry. But then $\gamma(X_1)^*\gamma(X_1)=1$, so

$$\|\xi_2\|^2=\omega_2(\gamma(X_1)^*\gamma(X_1))=1$$

which was the desired property.

For the continuous spectrum the argument is very similar. Let $\delta\subset\sigma(W_1)\cap\mathbb{T}$ be a Borel set of positive spectral measure relative to some vector $\xi_1\in\mathscr{H}$, $\|\xi_1\|=1$. From Theorem III, we get an M-valued function on $\mathbb{T}$, $b(z)$ such that $\alpha_1(b(z))=zb(z)$, and $b(z)^*b(z)=1$ for all z in the subset $\delta\subset\mathbb{T}$. But then

$$\alpha_2(\gamma(b(z)))=z\gamma(b(z)), \tag{8.5}$$

and the integral resolution (3.4) from Theorem III yields a vector $\neq 0$ in the spectral subspace of the unitary part of W_2 corresponding to the same set δ. It follows that $\sigma(W_1)\cap\mathbb{T}=\sigma(W_2)\cap\mathbb{T}$ which is the conclusion in the corollary. □

IX. TWO SUBGROUPS OF THE TORUS $\mathbb{T}$

We now return to the duality between the systems (β,M') and (α,M) where $\alpha\in\mathrm{End}(M)$ is given and β is the dual mapping in M'. We show that there is a spectral group for each of the two systems, and that the β-group is a subgroup of the α-group (inside $\mathbb{T}$).

Theorem IX.1: Let $\alpha\in\mathrm{End}(M)$ where M is a von Neumann algebra represented on a Hilbert space $\mathscr{H}$ with cyclic vector Ω such that the corresponding state $\omega=\langle\Omega|\cdot\Omega\rangle$ satisfies $\omega\circ\alpha=\omega$ on M. Assume the system is both in reduced form and also strongly ergodic. Let W be the associated isometry (see (8.2) for definition), and let

$$S:=\sigma(W)\cap\mathbb{T}. \tag{9.1}$$

Then we have the following properties satisfied:

(i)

$$S=\{\lambda\in\mathbb{T}:\exists X\in M,\quad X\ \textit{uniitary},\ \ s.t.\,\alpha(X)=\lambda X\}. \tag{9.2}$$

(ii) Defining

$$G=\{X\in M:X\ \textit{unitary},\ \exists\lambda\in S\,\text{s.t.}\,\alpha(X)=\lambda X\}, \tag{9.3}$$

then for each $\lambda\in S$ the corresponding $X\in G$ is unique up to scale, i.e., two solutions X_1, X_2 in G corresponding to the same $\lambda\in S$ must be related by $X_2=zX_1$ for some $z\in\mathbb{T}$.

(iii) S is a group.

(iv) The assignment

$$(\lambda\in S)\mapsto(X_\lambda\in G)\ \ \text{from}\ \ S\ \ \text{to}\ \ G \tag{9.4}$$

is a co-cycle representation; i.e., when the assignment is specified, there is a mapping $\zeta:S\times X\to\mathbb{T}$ such that

$$\zeta(\lambda_1\lambda_2,\lambda_3)\zeta(\lambda_1,\lambda_2)=\zeta(\lambda_1,\lambda_2\lambda_3)\zeta(\lambda_2,\lambda_3)\quad\forall\lambda_1,\lambda_2,\lambda_3\in S, \tag{9.5}$$

specifically

$$X_{\lambda_1}X_{\lambda_2}=\zeta(\lambda_1,\lambda_2)X_{\lambda_1\lambda_2}\quad\text{for}\ \ \lambda_1,\lambda_2\in S. \tag{9.6}$$

(v) The isometry W from (8.2) depends on the choice of cyclic vector Ω, but $S=\sigma(W)\cap\mathbb{T}$ is independent of the choice of Ω.

(vi) Let β be the dual completely positive mapping from Lemma IV.1, i.e., $\beta: M'\to M'$ satisfying

$$\omega(\beta(A)X)=\omega(A\alpha(X))$$

for $\forall A\in M'$ and $\forall X\in M$ where M' denotes the commutant. Define

$$S(\beta)=\{\lambda\in\mathbb{T}:\exists A\in M' \text{ s.t. } \beta(A)=\lambda A \text{ and } A^*AQ=AA^*Q=Q\} \tag{9.7}$$

where $Q\in M$ is the support projection of ω on M. Then $S(\beta)$ is a subgroup of the group S in (9.1).

Proof: (i)–(ii) First note that if $\lambda\in\mathbb{T}$ and $\alpha(X)=\lambda X$ for some $X\in M$, then $\xi=X\Omega$ in $\mathscr{H}$ satisfies $W\xi=\lambda\xi$. So if $\xi\neq 0$ in $\mathscr{H}$, then it follows that $\lambda\in\sigma(W)$. Since $\lambda\in\mathbb{T}$ by assumption, we have λ in the spectrum of the unitary part W_u from the Wold decomposition (8.3) of W. But X can be chosen *unitary* since both X^*X and XX^* are in

$$M^\alpha=\{Y\in M:\alpha(Y)=Y\} \tag{9.8}$$

and $M^\alpha=\mathbb{C}1$ from an application of Lemma IV. Hence pick X unitary, and note that then both $\xi_1=X\Omega$ and $\xi_2=X^*\Omega$ will be unit-vectors (in particular $\neq 0$), and $W\xi_1=\lambda\xi_1$ and $W\xi_2=\overline{\lambda}\xi_2$. Hence $\lambda^{-1}=\overline{\lambda}\in S$.

(iii) If $\lambda_1,\lambda_2\in S$ and $X_1, X_2\in G$ are associated unitaries, then

$$\alpha(X_1X_2)=\alpha(X_1)\alpha(X_2)=(\lambda_1\lambda_2)X_1X_2.$$

Since X_1X_2 is also a unitary in M, we conclude that $\lambda_1\lambda_2\in S$, and the unitary X_1X_2 may serve as an associated element in G from (9.3).

(iv) The conclusions we stated in (iv) follow from the facts from (i)–(iii), and a second application of Lemma IV.4, specifically using that (see (9.8)) $M^\alpha=\mathbb{C}1$. The existence of the cocycle $\zeta: S\times S\to\mathbb{T}$ amounts to making a central extension $\tilde{G}$ from G in (9.3) as follows:

$$\tilde{G}:=S\times G, \text{ and } (\lambda_1,X_1)\cdot(\lambda_2,X_2)=(\lambda_1\lambda_2,\zeta(\lambda_1,\lambda_2)X_1X_2). \tag{9.9}$$

Note that the cocycle property (9.5) for ζ is equivalent to the assignment (9.9) defining a group multiplication on the set $S\times G$.

(v) Since, for $\lambda\in S=\sigma(W)\cap\mathbb{T}$, we may pick the eigenvectors ξ for $W\xi=\lambda\xi$ in the form $\xi=X\Omega$, with $X\in M$ unitary, and $\alpha(X)=\lambda X$; it follows that $X\Omega_1\neq 0$ *for every other choice* of cyclic vector Ω_1 in $\mathscr{H}$, and the conclusion (v) follows from this.

(vi) Let $S(\beta)$ be the set defined in (9.7). From Ref. 52 Theorem 2.2, we conclude that $S(\beta)$ is a subgroup of $\mathbb{T}$ (with complex multiplication). If Q is the support projection (from the statement of (vi) above) then we apply Ref. 52 to QMQ and commutant $M'Q$ now acting on $Q\mathscr{H}$. (Note that Ref. 52 applies only to this restricted system, but not to the initially given global system based on $\alpha\in\mathrm{End}(M)$. The fact that Ω is generally not separating is important.)

Let $A\in M'$ be such that $\beta(A)=\lambda A$ and $AA^*Q=A^*AQ=Q$, and $\lambda\in\mathbb{T}$. Then the vector $A\Omega$ is also cyclic for M on $\mathscr{H}$. Using Lemma IV.1 (i) we get

$$T(A\Omega)=TAW\Omega=\beta(A)\Omega=\lambda(A\Omega).$$

But by (ii) in Lemma IV, we have $T=W^*$, so the vector $\xi=A\Omega$ satisfies $W^*\xi=\lambda\xi$, and therefore $W\xi=\overline{\lambda}\xi$. But this means that $\overline{\lambda}=\lambda^{-1}\in S$ (the group from (iii) above), and therefore $\lambda\in S$ by (iii). We have proved that $S(\beta)$ is a group, and in fact a subgroup of S. □

X. SHIFTS ON VON NEUMANN ALGEBRAS

In Proposition II we introduced, for a given $\alpha \in \mathrm{End}(M)$ with a cyclic vector Ω such that $\omega = \langle \Omega | \cdot \Omega \rangle$ satisfies $\omega \circ \alpha = \omega$, a canonical isometry W on the Hilbert space on which M is represented. We showed in Theorem IX.1 that the isometry W, its unitary part, and the corresponding spectral groups are independent of the choice of cyclic vector. In Proposition II.2 we showed that α must be a shift on M if W is an essential shift on $\mathscr{H}$. Here we show that if α is assumed strongly ergodic, then the converse implication also holds.

Corollary X.1: Let M be a von Neumann algebra with cyclic vector Ω in a Hilbert space, and let $\alpha \in \mathrm{End}(M)$. Suppose the state $\omega = \langle \Omega | \cdot \Omega \rangle$ satisfies $\omega \circ \alpha = \omega$ on M and furthermore that the system is in reduced form, and α is strongly ergodic. If α is a shift in the sense of Powers, then it follows that the space $\mathscr{H}_u$ from the Wold decomposition is *one-dimensional.*

Proof: We have already noted that the converse implication holds as well. We are now assuming that

$$M^\infty = \cap_{k=1}^\infty \alpha^k(M) \tag{10.1}$$

is one-dimensional. Let W be the induced isometry from (8.2), and let

$$\mathscr{H}_u = \cap_{k=1}^\infty W^k \mathscr{H}. \tag{10.2}$$

Then $W|_{\mathscr{H}_u}$ is unitary, and $\alpha|_{M^\infty}$ is an automorphism. We now show that $\mathscr{H}_u$ is one-dimensional. Suppose first λ is in the point spectrum of $W|_{\mathscr{H}_u}$. Then it follows from Proposition VI that for some $X \in M$ we have $\alpha(X) = \lambda X$. But then $X \in M^\infty = \mathbb{C}1$ and we conclude that $\lambda = 1$. Suppose instead $\xi \in \mathscr{H}_u$ has continuous spectrum relative to the spectral resolution of $W|_{\mathscr{H}_u}$. From Theorem Theorem 3.1 we then get a measurable field $\mathbb{T} \to M$, $x \mapsto b(z) \in M$ on the support of the spectral measure for ξ such that $\alpha(b(z)) = z b(z)$. But $b(z) \in M^\infty = \mathbb{C}1$ so there can be no point in the support other than $z = 1$. Hence we need only show that

$$\mathscr{H}_0 := \{\xi \in \mathscr{H} : W\xi = \xi\} \tag{10.3}$$

is one-dimensional. If $\xi_0 \in \mathscr{H}_0$ is given, we get from Proposition VI.1 an element $X_0 \in M^\alpha$ (i.e., $\alpha(X_0) = X_0$) such that $X_0 \Omega = \xi_0$. But we proved, in Lemma IV.4, that α must be ergodic, so $X_0 \in \mathbb{C}1$, and $\xi_0 = X_0 \Omega \in \mathbb{C}\Omega$. This ends the proof that $\mathscr{H}_u = \mathbb{C}\Omega$ which is the asserted conclusion. □

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Superposition formulas for pseudounitary matrix Riccati equations

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The purpose of this article is to derive a superposition formula for the pseudounitary matrix Riccati equation of dimension $N \geqslant 2$. The superposition formula will be written in closed form in terms of five particular solutions satisfying certain well-specified conditions defining a fundamental set. Examples will be studied in order to show how the superposition formula works and how it can be used in numerical calculations. © *1996 American Institute of Physics.* [S0022-2488(96)01703-8]

I. INTRODUCTION

Let us consider a system of n first-order (real or complex) ordinary differential equations

$$y^{\mu} = \eta^{\mu}(y^1,\ldots,y^n,t), \quad 1 \leqslant \mu \leqslant n. \tag{1}$$

If the system is linear, then we can write the general solution as a linear combination of n particular solutions.

A generalization of the concept of linear superposition is that of a fundamental set of solutions. Thus, the system (1) has a fundamental set of solutions if its general solution can be written as a function of m particular solutions and n significant constants. Using vector notation, we write

$$\vec{y}(t) = \vec{F}(\vec{y}_1(t),\ldots,\vec{y}_m(t),c_1,\ldots,c_n). \tag{2}$$

If the system (1) is nonlinear and formula (2) exists, we shall call it a ''nonlinear superposition formula.''

Necessary and sufficient conditions for a fundamental set of solutions to exist for a system of nonlinear ordinary differential equations (NLODE) were presented by Sophus Lie (see, e.g., Ref. 1) and can be summed up as follows.

The system (1) allows a superposition formula (SF) (2) if and only if:

(1) The system has the form

$$y^{\mu} = \sum_{k=1}^{r} Z_k(t)\, \eta_k^{\mu}(\vec{y}). \tag{3}$$

(2) The vector fields

$$X_k = \sum_{\mu=1}^{n} \eta_k^{\mu}(\vec{y})\, \frac{\partial}{\partial y^{\mu}}, \quad 1 \leqslant k \leqslant r, \tag{4}$$

generate a finite-dimensional Lie algebra L:

$$[X_k,\, X_l] = \sum_{j=1}^{r} C_{kl}^{j} X_j, \quad r < \infty. \tag{5}$$

The number of solutions m in a fundamental set then satisfies

$$n \cdot m \geqslant r. \tag{6}$$

For $n=1$ only one nonlinear equation satisfies Lie's criterion, namely the Riccati equation

$$\dot{y} = Z_1(t) + Z_2(t)y + Z_3(t)y^2. \tag{7}$$

The SF in this case (well known long before Lie's work) is

$$y = \frac{cy_2(y_1-y_3) - y_1(y_2-y_3)}{c(y_1-y_3) - (y_2-y_3)}. \tag{8}$$

For $n \geqslant 2$ the situation is incomparably richer and a classification of systems of NLODEs with SFs is equivalent to a classification of Lie algebras that can be realized by vector fields in n dimensions [see Eq. (4)].

Such a classification, without further restrictions, is an unmanagable task. What has been performed is a classification of all indecomposable systems of NLODEs with SFs. These are systems from which it is not possible to split off a subsystem that itself has a SF. The classification of indecomposable systems of NLODEs with SFs was related[2] to a solved problem, namely that of classifying transitive primitive Lie algebras.[3–6] Many specific indecomposable systems of NLODEs with SFs were constructed.[7–11]

In particular, it was shown[2] that various types of matrix Riccati equations (MRE)

$$\dot{W} = A + WB + CW + WDW, \tag{9}$$

$W \in F^{m\times l}$, $A \in F^{m\times l}$, $B \in F^{l\times l}$, $C \in F^{m\times m}$, $D \in F^{l\times m}$, where $F=\mathbb{C}$ or $\mathbb{R}$ and A,B,C,D are given matrix functions of t, do have a nonlinear SF. Equation (9) is associated with a pair of Lie algebras, $L_0 \subseteq L$, where L is simple and L_0 is an irreducible maximal parabolic subalgebra of L. We also consider the corresponding Lie groups $G_0 = \exp L_0$, $G = \exp L$, and the homogeneous space $M \sim G/G_0$. The Lie group G will act transitively and primitively on M. The group G_0 is the isotropy group of the origin in M. The simple Lie algebra L is the one figuring in Lie's theorem, L_0 is the subalgebra of fields vanishing at the origin.

The SF (2) then has the general form

$$W(t) = g(t) \cdot U, \tag{10}$$

where U is a constant matrix (representing the initial conditions). Equation (10) represents the nonlinear action of the group G on the space M. When M is realized as a Grasmannian of k-planes, the components of $W(t)$ are identified as affine coordinates on M.

In particular, for MREs (9), the formula (10) reduces to

$$W(t) = (g_{11}(t)U + g_{12}(t))(g_{21}(t)U + g_{22}(t))^{-1}, \tag{11}$$

where $g_{\mu\nu}$ are matrices of the appropriate dimensions.

The above considerations bring out the physical interest of NLODEs with SFs. Lie's original result essentially states that the right-hand side of Eq. (1) must lie in a finite-dimensional Lie algebra [see Eq. (4)]. This condition is imposed[12] on Bäcklund transformations in the theory of completely integrable infinite-dimensional Hamiltonian systems.[13] For equations in the AKNS hierarchy,[14] the algebra is $\mathrm{sl}(2,\mathbb{R})$ or $\mathrm{sl}(2,\mathbb{C})$ and indeed the corresponding Bäcklund transformations have the form of Riccati equations (in each independent variable).

The MREs occur as Bäcklund transformations for multifield equations, such as those occurring in the σ-model[15,16] or n-dimensional generalizations of the sine-Gordon equations.[17] The

particular type of MRE that occurs depends on which σ-model is considered. In the case under consideration, the matrices W, subject to the MRE (9), will be pseudo-Hermitian [see Eq. (15) below], certainly a case of interest in the context of unitary σ-models.

The MREs related to the Lie groups $\mathrm{SL}(N,\mathbb{R})$ and $\mathrm{SP}(2N,\mathbb{R})$ were studied in earlier publications.[7–9]

The purpose of this article is to obtain SFs for the pseudounitary MRE, i.e., the case when we take G as the group $\mathrm{SU}(N,N)$.

II. PSEUDOUNITARY MATRIX RICCATI EQUATIONS AND FUNDAMENTAL SETS OF SOLUTIONS

A. The equation

Let us realize the Lie algebra $\mathrm{su}(N,N)$ and the Lie group $\mathrm{SU}(N,N)$ by matrices X and g, satisfying

$$XK+KX^{\dagger}=0, \quad gKg^{\dagger}=K, \quad K=\begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix},$$

$$X\in \mathrm{sl}(2N,\mathbb{C}), \quad g\in \mathrm{SL}(2N,\mathbb{C}), \tag{12}$$

respectively, where the cross denotes Hermitian conjugation.

Let us consider the maximal parabolic subgroup $G_p\subseteq \mathrm{SU}(N,N)$ of matrices g_p satisfying (12) and having the form

$$g_p=\begin{pmatrix} g_{11} & 0 \\ g_{21} & g_{22} \end{pmatrix}, \tag{13}$$

and construct the homogeneous space

$$M\sim G/G_p\,. \tag{14}$$

We can do this in terms of a Grassmanian of isotropic planes with affine coordinates given by the matrix W, satisfying

$$W+W^{\dagger}=0, \quad W\in \mathbb{C}^{N\times N}. \tag{15}$$

The action of $\mathrm{SU}(N,N)$ on M is then given by

$$W'=(g_{11}W+g_{12})(g_{21}W+g_{22})^{-1} \tag{16}$$

and is both transitive and primitive. The origin in M is the point $W=0$ and its isotropy group is indeed G_p of Eq. (13).

We can also use redundant "homogeneous" coordinates on M,

$$\begin{pmatrix} X \\ Y \end{pmatrix}\sim\begin{pmatrix} XG_0 \\ YG_0 \end{pmatrix}, \quad X^{\dagger}Y+Y^{\dagger}X=0, \tag{17}$$

$$X,Y\in \mathbb{C}^{N\times N}, \quad G_0\in GL(N,\mathbb{C}), \tag{18}$$

in which the action of $\mathrm{SU}(N,N)$ is linear:

$$\begin{pmatrix} X' \\ Y' \end{pmatrix}=\begin{pmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{pmatrix}\begin{pmatrix} X \\ Y \end{pmatrix}. \tag{19}$$

We have

$$W=XY^{-1}, \quad \det Y\neq 0. \tag{20}$$

Following the general theory[2] as outlined in the Introduction, we now write the pseudounitary matrix Riccati equation and the corresponding general form of the superposition formula, respectively, as

$$\dot{W}(t)=A+WB+B^{\dagger}W+WDW, \tag{21}$$

where

$$W+W^{\dagger}=0, \quad A+A^{\dagger}=0, \quad D+D^{\dagger}=0, \quad A,B,D,W\in\mathbb{C}^{N\times N} \tag{22}$$

and

$$W=(g_{11}U+g_{12})(g_{21}U+g_{22})^{-1}, \tag{23}$$

where

$$U+U^{\dagger}=0, \quad g_{12}g_{11}^{\dagger}+g_{11}g_{12}^{\dagger}=0, \quad g_{22}g_{21}^{\dagger}+g_{21}g_{22}^{\dagger}=0, \quad g_{12}g_{21}^{\dagger}+g_{11}g_{22}^{\dagger}=I_N. \tag{24}$$

The matrix U is constant, the others can be functions of t.

Equation (23) turns into a superposition formula, once the coefficients $g_{ik}(t)$ are expressed in terms of m known solutions. Let us first show that this can be done and that for $N\geqslant 2$ we have $m=5$.

B. The fundamental set of solutions

Lie's lower bound (6) on the number m of solutions in a fundamental set in the present case boils down to the following. We can view Eq. (23) for given solutions W_i and the corresponding initial conditions U_i as algebraic equations for the unknowns $g_{ik}(t)$. Their number is $r=4N^2-1=\dim[\mathrm{SU}(N,N)]$. Each solution provides $n=N^2$ real equations for these unknowns. Thus, Eq. (6) implies $m\geqslant 4$ for $N\geqslant 2$ and $m\geqslant 3$ for $N=1$. The case $N=1$ corresponds to a scalar Riccati equation for which the condition $m\geqslant 3$ is saturated (we have $m=3$). For $N\geqslant 2$ this is not so, i.e., the $4N^2$ equations given by four solutions are not linearly independent and hence do not determine $g(t)$ unambiguously.

In general, m is the minimal number of initial conditions U_i (and hence of solutions W_i) for which the joint stabilizer in the group G is the identity transformation. In the case under consideration, we require that the equations

$$U_i=(g_{11}U_i+g_{12})(g_{21}U_i+g_{22})^{-1}, \quad i=1,\ldots,m, \tag{25}$$

should imply

$$\begin{aligned} g_{11}&=g_{22}=\lambda I,\\ g_{12}&=g_{21}=0. \end{aligned} \tag{26}$$

Let us note that the $\mathrm{SU}(N,N)$ matrix $g(t)$ can be replaced by

$$g'(t)=g(t)h^{-1}, \quad h\in\mathrm{SU}(N,N), \tag{27}$$

where h is a constant matrix. We can use h to standardize the initial data matrices U_i into some convenient form.

Theorem 1: A fundamental set of solutions for the pseudounitary matrix Riccati equation (21) with $N \geqslant 2$ consists of five solutions with initial condition matrices $U_i = -U_i^\dagger$ satisfying

(1)

$$\begin{gathered} \det(U_1 - U_k) \neq 0, \quad k = 2,\ldots,5, \\ \det(U_2 - U_k) \neq 0, \quad k = 3,4,5. \end{gathered} \tag{28}$$

(2) The matrix is positive definite.

$$\begin{gathered} i(U_3 - U_2)(U_3 - U_1)^{-1}(U_1 - U_2) \equiv (h_0^\dagger h_0)^{-1}, \\ h_0 \in \mathbb{C}^{N \times N}, \quad \det h_0 \neq 0. \end{gathered} \tag{29}$$

(3) The matrix anharmonic ratios

$$R_a = (U_a - U_2)(U_a - U_1)^{-1}(U_3 - U_1)(U_3 - U_2)^{-1}, \quad a = 4,5, \tag{30}$$

do not have any common nontrivial invariant eigenspaces and all eigenvalues of R_4 are distinct.

Proof: If the above conditions are satisfied, the matrix, $h \in \mathrm{SU}(N,N)$

$$h = \begin{pmatrix} h_1 h_0 & 0 \\ 0 & h_1 h_0 \end{pmatrix} \begin{pmatrix} I & -U_2 \\ -i(U_3 - U_2)(U_3 - U_1)^{-1} & i(U_3 - U_2)(U_3 - U_1)^{-1} U_1 \end{pmatrix}, \tag{31}$$

used as g in (16), will transform $U_1,\ldots,U_5$ into

$$\begin{gathered} U_1^s \to \infty, \quad U_2^s = 0, \quad U_3^s = iI_N, \\ U_4^s = i\Lambda = i\ \mathrm{diag}(\lambda_1,\ldots,\lambda_N), \quad U_5^s = i\Omega, \end{gathered} \tag{32}$$

where $i\Omega$ is skew-Hermitian and has no common invariant subspaces with Λ, i.e., is not block diagonal. The unitary matrix h_1 is the one that diagonalizes the skew-Hermitian matrix $ih_0 R_4 h_0^{-1}$ [R_4 is defined by Eq. (30)].

Now, let us show that the joint stabilizer of the matrices (32) is only the identity transformation in Eq. (25). Indeed, Eq. (25) for U_i^s, $i = 1,2,3$, implies $g_{21} = 0$, $g_{12} = 0$, $g_{22} = g_{11}$. For U_4^s we obtain $g_{11} = \mathrm{diag}(e^{i\phi_1},\ldots,e^{i\phi_N})$, $0 \leqslant \phi_i < 2\pi$. Finally, the relation $g_{11}\Omega = \Omega g_{11}$ implies $g_{11} = \lambda I_N$ QED.

Comment: In order to be completely general, we should choose $U_3^s = iI_{p,q}$ with $p,q \in \mathbf{Z}^>$ and $p + q = N$. With this choice, the condition (29) is no longer necessary. The number of solutions needed is still five. Theorem 1, thus modified, defines a dense subset of the set of 5-tuples of skew-Hermitian matrices.

III. THE SUPERPOSITION FORMULA

We can derive the superposition formula, following the steps outlined in Theorem 1.

Let us assume that we know five solutions, $W_1(t),\ldots,W_5(t)$, corresponding to the initial data U_i^s of Eq. (32). Using Eq. (23) we find

$$W_1 = g_{11} g_{21}^{-1}, \quad W_2 = g_{12} g_{22}^{-1}, \quad W_3 = (ig_{11} + g_{12})(ig_{21} + g_{22})^{-1}, \tag{33}$$

and hence

$$W=[g_{11}Ug_{11}^{-1}+iW_2(W_3-W_2)^{-1}(I-W_3W_1^{-1})]$$
$$\times[W_1^{-1}g_{11}Ug_{11}^{-1}+i(W_3-W_2)^{-1}(I-W_3W_1^{-1})]^{-1}. \tag{34}$$

In order to determine g_{11} we make use of the remaining two solutions W_4 and W_5. From Eq. (34) we have

$$g_{11}Ug_{11}^{-1}=i(I-WW_1^{-1})^{-1}(W-W_2)(W_3-W_2)^{-1}(I-W_3W_1^{-1})\equiv iQ(W). \tag{35}$$

We put

$$g_{11}=g_sg_d, \tag{36}$$

where g_d is some diagonal matrix and g_s is a matrix that diagonalizes $iQ(W_4)$, i.e., its columns are the eigenvectors of $iQ(W_4)$. Hence, g_s is known, up to a common factor for each column. This ambiguity is absorbed into the matrix g_d.

Finally, the diagonal matrix g_d is determined from the last solution by solving the system of linear algebraic equations

$$g_d\Omega=g_s^{-1}(I-W_5W_1^{-1})^{-1}(W_5-W_2)(W_3-W_2)^{-1}(I-W_3W_1^{-1})g_sg_d. \tag{37}$$

Notice that we never need the solution $W_1(t)$ that is singular for $t=0$, but only the matrix $W_1^{-1}(t)$ that is well defined if we choose $W_1^{-1}(0)=0$.

We have arrived at the following result:

Theorem 2: The general solution $W(t)$ of the pseudounitary matrix Riccati equation (21) is given by the superposition formula (34) in terms of five particular solutions, satisfying the initial conditions specified in Theorem 1. The matrix g_{11} is given by Eq. (36) and the constant matrix U is related to the initial condition matrix $W(0)$ by a matrix linear fractional transformation with constant coefficients.

Comment: If we choose the initial conditions for $W_1,\ldots,W_5$ to satisfy Eq. (32), then we have directly $W(0)=U$ for any solution $W(t)$ that we wish to construct.

As mentioned above, we do not need the solution $W_1(t)$, but its inverse $V_1=W_1^{-1}$. This matrix satisfies a dual pseudounitary matrix Riccati equation, namely,

$$\dot{V}=-VAV-BV-VB^{\dagger}-D,$$
$$V_1(0)=0. \tag{38}$$

In homogeneous coordinates (17), $V_1(0)$ and $W_1(0)$ correspond to $\binom{I}{0}$ and $\binom{0}{I}$, respectively.

One possible application of the superposition formula (34) is to use it for numerical calculations. Thus, the needed five particular solutions can be generated numerically from well-chosen initial conditions for a given pseudounitary matrix Riccati equation. The matrix $g_{11}(t)$ can then be calculated once and for all and stored in a data bank. Then, we can calculate as many different solutions as we wish, using Eq. (34). The input solutions can be chosen to be smooth functions of t for $0\leqslant t\leqslant t_M$, where t_M is some chosen finite time. For other values of U, solutions may have poles in the same region. The superposition formula will provide these singularities and make it possible to pinpoint them with great precision. This procedure was adapted earlier[18,19] for matrix Riccati equations based on $\mathrm{SL}(2N,\mathbb{R})$ and $\mathrm{SP}(2N,\mathbb{R})$.

Examples for $\mathrm{SU}(N,N)$ matrix Riccati equations will be considered in Sec. IV below.

IV. EXAMPLES

Let us consider the pseudounitary MRE (21). The fundamental set of solutions for $N\geqslant 2$ will consist of five solutions. Let us choose the initial condition matrices to be

$$W_1^{-1}(0)=0, \quad W_2(0)=0, \quad W_3(0)=iI, \quad W_4(0)=i\ \mathrm{diag}(1,2,\ldots,N),$$
$$W_5(0)=\begin{pmatrix} 0 & i & & 0 & \\ i & 0 & i & & \\ & i & 0 & i & \\ 0 & & & \ddots & i \\ & & & i & 0 \end{pmatrix}. \tag{39}$$

We then calculate $Q(W_4)$ of Eq. (35) and use its eigenvectors as columns of g_s^{-1} [see Eq. (36)]. The matrix g_d is normalized so that we have $(g_d)_{11}=1$.

The five solutions corresponding to these initial conditions will be found using a fourth-order Runge–Kutta (R–K) algorithm. The MRE is rewritten in vector form

$$\dot{W}_k=f_k(t,\mathbf{W}), \quad k=1,\ldots,N(N+1)/2. \tag{40}$$

Here $N(N+1)/2$ is the number of independent complex elements in the matrix W. One then applies the Kutta–Simpson formula

$$W_{k,i+1}=W_{k,i}+\tfrac{1}{6}(p_k+2q_k+2r_k+s_k),$$
$$k=1,\ldots,N(N+1)/2, \tag{41}$$

where

$$p_k=hf_k(t_i,\mathbf{W}_i), \quad q_k=hf_k(t_i+0.5h,\mathbf{W}_i+0.5\mathbf{p}),$$
$$r_k=hf_k(t_i+0.5h,\mathbf{W}_i+0.5\mathbf{q}), \quad s_k=hf_k(t_i+h,\mathbf{W}_i+\mathbf{r}),$$
$$h=t_{i+1}-t_i. \tag{42}$$

The vectors $\mathbf{W}_i$ and $\mathbf{W}_{i+1}$ are the results of two consecutive iterations i and $i+1$, and their components are $W_{k,i}$ and $W_{k,i+1}$, respectively. The increment h is constant.

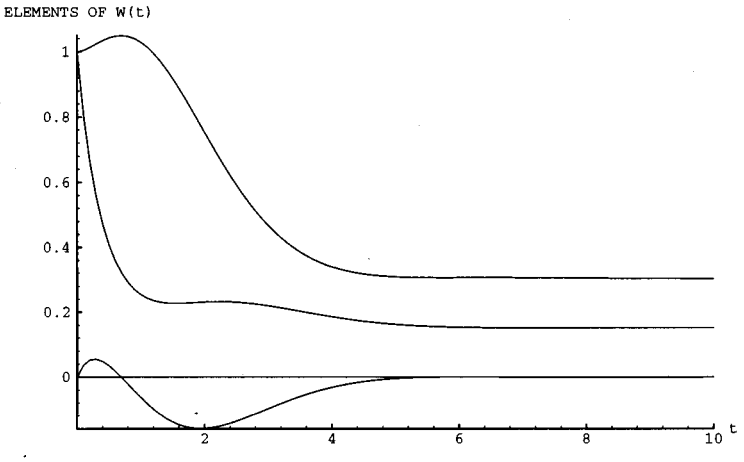
The first example corresponds to the following 2×2 coefficients

$$A=\begin{pmatrix} 0 & 0 \\ 0 & \dfrac{i}{4} \end{pmatrix}, \quad B=C^{\dagger}=\begin{pmatrix} 0 & -\frac{1}{2} \\ 1 & -\frac{3}{4} \end{pmatrix}, \quad D=\begin{pmatrix} 0 & 0 \\ 0 & i \end{pmatrix}. \tag{43}$$

Figure 1(a) shows the graph of the independent elements of one of the solutions of the fundamental set obtained using the R–K method with an increment of $\Delta t=0.1$ s. The initial condition is $W(0)=iI$. We note that the real part of the nondiagonal element is zero for all t. This is because we have, in our particular case, the proprieties that $A^*=-A$, $D^*=-D$, $B^*=B$, $C^*=C$, and $W^*(0)=-W(0)$. The MRE then gives $W^*(t)=-W(t)$ so that $W(t)$ is a purely imaginary matrix if its initial condition is one. We have also done the calculations for the initial condition

$$W(0)=\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tag{44}$$

using both methods: R–K and superposition. The agreement was found to be of four to eight significant digits.



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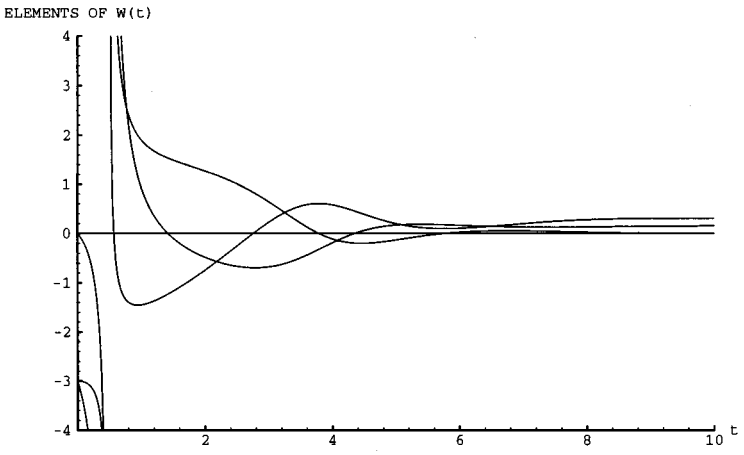

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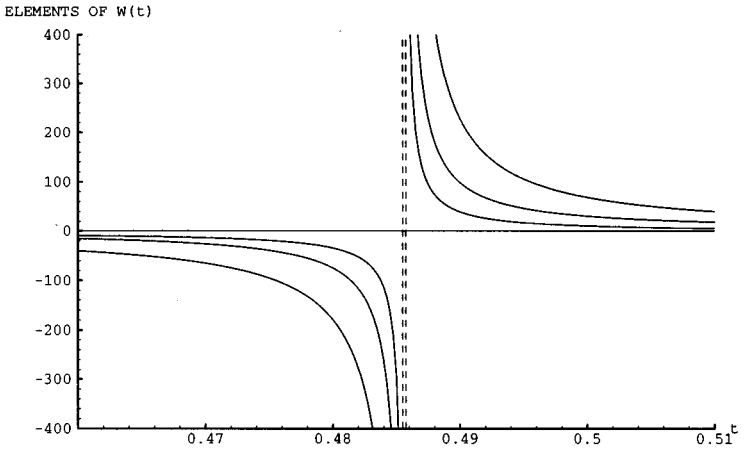

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FIG. 1. The independent elements of solutions obtained with coefficients (43): Real part of W_{12} and imaginary part of W_{11}, W_{12}, and W_{22}. (a) Runge–Kutta solution using increment $\Delta t=0.1$ and initial condition $W(0)=iI$. (b) Superposition solution using increment $\Delta t=0.025$ and initial condition $W(0)=-3iI$. (c) The same solution as (b) using increment $\Delta t=0.00025$.

Figure 1(b) shows a solution obtained using the superposition formula. The initial condition is $W(0)=-3iI$ and the increment is $\Delta t=0.025$ s. We note the singular point between $t=0$ s and $t=1$ s. In order to obtain the R–K solution after the singularity, we used the dual equation (38) with initial condition $V(0)=(-3iI)^{-1}=(i/3)I$ whose solution does not show a singularity before $t=1$. We were then able to calculate the inverse of the R–K solution at a time t past the singularity. The agreement with R–K is two to five significant digits for points before the singularity ($t\leqslant 0.4$ s) and one to five significant digits after ($t\geqslant 0.6$ s). Finally, Fig. 1(c) shows a closer look at the singularity. Here the calculations were done using $\Delta t=0.00025$. This graph makes it possible to locate the singularity around $t=0.485$ s.

The next example, a 3×3 case, involves the following coefficients:

$$A=\begin{pmatrix} -i & 1 & 1 \\ -1 & i\sin 2t & 1 \\ -1 & -1 & i \end{pmatrix}, \quad B=C^{\dagger}=\begin{pmatrix} 0 & \cos 2t & 0 \\ 1 & i & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad D=\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & i \end{pmatrix}. \tag{45}$$

Figure 2(a) shows some of the independent elements of the solution $W(t)$ found using the R–K method with the initial condition $W(0)=iI$ and an increment $\Delta t=0.01$. The calculations were also done with the initial condition

$$W(0)=\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix} \tag{46}$$

using both methods: R–K and superposition. The agreement between the two methods was found to be five to eight significant digits.

Figure 2(b) shows some of the independent elements of the solution $W(t)$ found using the superposition method with initial condition $W(0)=-iI(\Delta t=0.01)$. We note the singularity occurring between $t=0$ s and $t=1$ s. The same method as previously was used to compare our results from both methods. The agreement before the singularity ($t\leqslant 0.6$ s) is three to nine significant digits compared to three to seven significant digits after ($t\geqslant 0.65$ s). Finally, Fig. 2(c) shows a closer look at the singularity. Here the calculations were done using $\Delta t=0.001$. This graph makes it possible to locate the singularity around $t=0.624$ s.

V. CONCLUSIONS

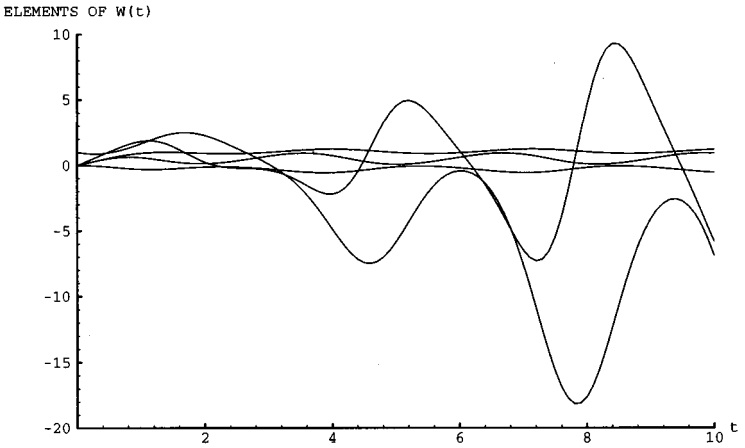
The main result of this paper is the SF (34) with $g_{11}(t)$ evaluated using Eqs. (35)–(37).

The SF can be used to investigate properties of the solution space of a given pseudounitary MRE.

In Sec. IV we have shown that the SF can also be used as a method for calculating solutions numerically. One of the purposes of including these examples is to show that a set of five smooth solutions, with no singularities on the considered interval of the real time axis, can be superposed to produce singular solutions (see the poles on Figs. 1 and 2). The SF makes it very easy to pinpoint singularities of solutions occurring in real time. Indeed, we can use our data bank of smooth solutions to approach a singularity from both sides with arbitrary precision.

Earlier studies of other types of matrix Riccati equations have shown that the SF becomes particularly efficient for large matrices ($N\geqslant 10$), but this is not the place to illustrate the computer science aspects of superposition formulas. Here, we have chosen the lowest meaningful dimensions ($N=2,3$) and one case with constant coefficients, the other with variable periodic ones.

We mention that MRE with constant coefficients [constant matrices A,B,D in Eq. (21)] allow for constant solutions, obtained by solving the algebraic equation



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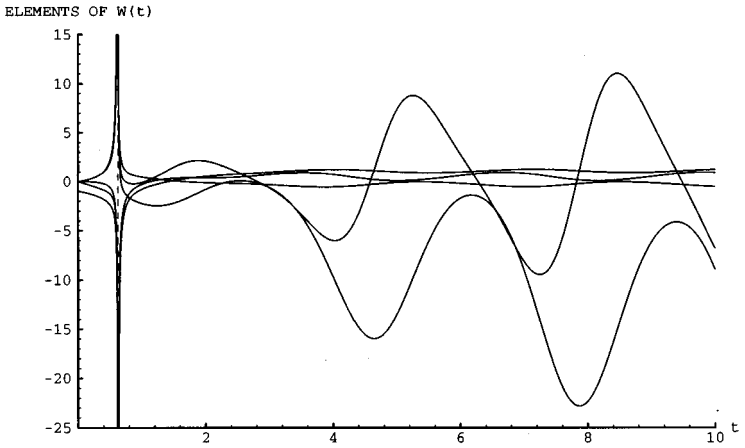

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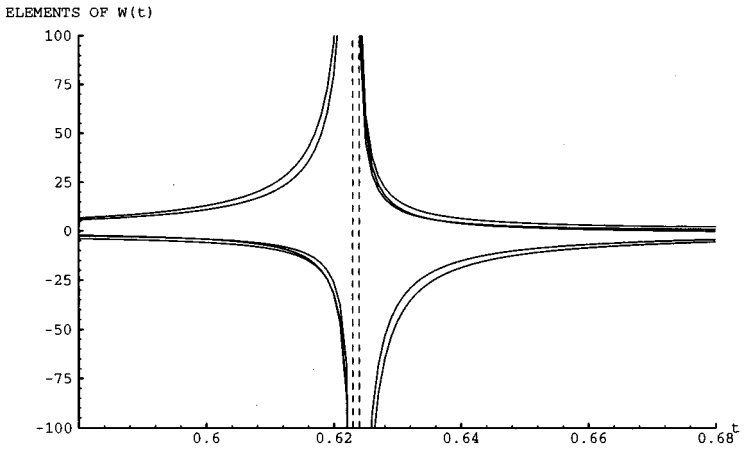

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FIG. 2. Some independent elements of solutions obtained with coefficients (45): Real part of W_{13} and W_{23} and imaginary part of W_{11}, W_{12}, and W_{23}. (a) Runge–Kutta solution using increment $\Delta t=0.01$ and initial condition $W(0)=iI$. (b) Superposition solution using increment $\Delta t=0.01$ and initial condition $W(0)=-iI$. (c) The same solution as (b) using increment $\Delta t=0.001$.

$$A+WB+B^{\dagger}W+WDW=0. \tag{47}$$

These can be used as input solutions in the SF. For instance, in the first example of Sec. IV, Eq. (43), the MRE has four different stationary solutions. However, only two of them, appropriately chosen, satisfy conditions (28) of Theorem 1 and can be used in the SF. One of them,

$$W_1=\frac{i}{2}(-3+\sqrt{13})\begin{pmatrix}1 & 0\\ 0 & \frac{1}{2}\end{pmatrix}, \tag{48}$$

actually serves as a global attractor: for $t\to\infty$ all solutions converge to this constant one. This is also demonstrated by our numerical calculation (see Fig. 1).

Finally, we comment on physical applications of pseudounitary matrix Riccati equations. We can perform a Cayley–Klein transformation

$$G=(I+W)(I-W)^{-1} \tag{49}$$

and the matrix G is unitary, i.e., Eq. (15) implies

$$GG^{\dagger}=I. \tag{50}$$

The unitary matrix G then satisfies a related pseudounitary Riccati equation

$$\dot{G}=\tilde{A}+G\tilde{B}+\tilde{C}G+G\tilde{D}G \tag{51}$$

with

$$\begin{aligned}&\tilde{A}=(A-B-B^{\dagger}+D)/2, \quad \tilde{B}=(A+B-B^{\dagger}-D)/2,\\ &\tilde{C}=(A-B+B^{\dagger}-D)/2, \quad \tilde{D}=(A+B+B^{\dagger}+D)/2.\end{aligned} \tag{52}$$

The Bäcklund transformations of the unitary σ-model then have the form

$$\begin{aligned}\frac{\partial G}{\partial x}&=R_1+GS_1+T_1G+GU_1G,\\ \frac{\partial G}{\partial y}&=R_2+GS_2+T_2G+GU_2G,\end{aligned} \tag{53}$$

where the model itself arises as a compatibility condition for the above two matrix Riccati equations. Our superposition formula Eq. (34) still applies even though G (and all solutions) depend on two independent variables x,y.

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Deformations of density functions in molecular quantum chemistry

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We generalize the use of the local scaling transformation developed by E. S. Kryachko and E. V. Ludeña to molecules in order to deform density functions. The connection with the Jacobian problem is clearly made, and we solve that problem using a formalism introduced by J. Moser. As a consequence, we can control the density information contained in a wave function, in some sense, at the same time as we keep particular regularity and behavior assumptions in the wave function (in particular concerning the symmetries of the wave function). The principal aim of the paper is to develop a correct mathematical background for further utilization in connection with density functional theory. Theoretical implications and numerical aspects are also discussed. © *1996 American Institute of Physics.* [S0022-2488(96)04301-7]

I. INTRODUCTION

This paper is motivated by the mathematical modelization, in molecular quantum chemistry, of an N electron system for a molecule with fixed nuclei. The N electron system is described by the following Hamiltonian H:

$$H=-\sum_{i=1}^{N}\Delta_i+\sum_{i=1}^{N}v(\mathbf{r}_i)+\sum_{1\leqslant i<j\leqslant N}\frac{1}{r_{ij}} \tag{1}$$

where Δ_i denotes the Laplacian with respect to the ith space variable $\mathbf{r}_i$, $r_{ij}=|\mathbf{r}_i-\mathbf{r}_j|$, and v is the external potential (real valued).

This Hamiltonian acts on $L^2_A(\mathbb{R}^{3N})$, the space of square integrable complex valued functions $\Psi(\mathbf{r}_1,...,\mathbf{r}_N)$ and where the index A denotes the antisymmetry with respect to the variables $\mathbf{r}_i\in\mathbb{R}^3$. Such a function is called a *state* or a *wave function* in quantum chemistry (spin is omitted for simplicity of presentation).

More generally we denote $\|f\|_p=(\int|f|^p)^{1/p}$ and $L^p(\mathbb{R}^n)=\{f:\mathbb{R}^n\to\mathbb{C}\mid\|f\|_p<\infty\}$. Furthermore $H^1(\mathbb{R}^{3N})=\{\Psi\in L^2(\mathbb{R}^{3N})|\forall i,\ \nabla_i\Psi\in L^2(\mathbb{R}^{3N})\}$ and $H^1_A(\mathbb{R}^{3N})$ is the restriction to antisymmetric functions. We denote also $\|\Psi\|^2_{H^1}=\|\Psi\|^2_2+\Sigma_i\|\nabla_i\Psi\|^2_2$.

For a state Ψ in $H^1_A(\mathbb{R}^{3N})$ we define the energy

$$E[\Psi]=\langle\Psi,H\Psi\rangle, \tag{2}$$

where $\langle .,.\rangle$ denotes the scalar product on $L^2(\mathbb{R}^{3N})$. A fundamental problem in quantum chemistry is to determine E_0, the minimum of the energy $E[\Psi]$ for $\Psi\in H^1_A(\mathbb{R}^{3N})$ with constraint $\langle\Psi,\Psi\rangle=1$.

To a state $\Psi\in L^2_A(\mathbb{R}^{3N})$ we associate its *density* ρ_Ψ by

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$$\rho_\Psi(\mathbf{r}) = N \int_{\mathbb{R}^{3(N-1)}} |\Psi(\mathbf{r},\mathbf{r}_2,\ldots,\mathbf{r}_N)|^2 d\mathbf{r}_2 \cdots d\mathbf{r}_N \tag{3}$$

and we denote $\Psi \mapsto \rho$ if $\rho = \rho_\Psi$.

Lieb proved in Ref. 1 (like Harriman[2]) that $\psi \mapsto \rho$ is continuous from $H^1_A(\mathbb{R}^{3N})$ *onto* I_1^N where

$$I_1^N = \left\{ \rho \in L^1(\mathbb{R}^3) \,\middle|\, \rho \geqslant 0, \quad \int \rho = N, \rho^{1/2} \in H^1(\mathbb{R}^3) \right\}. \tag{4}$$

This allows him to define (see Levy[3] or Lieb[1])

$$E[\rho] = \inf\{E[\Psi] \,|\, \Psi \mapsto \rho, \Psi \in H^1_A(\mathbb{R}^{3N})\} \tag{5}$$

which satisfies

$$E_0 = \inf\{E[\rho] \,|\, \rho \in I_1^N\}. \tag{6}$$

So he obtained a mathematical formulation of the density functional theory introduced by Hohenberg and Kohn.[4]

In Ref. 5 we have obtained a parametrization of the set $\{\Psi, \Psi \mapsto \rho\}$ by a decomposition theorem of the wave functions (a generalization of the approach of Zumbach and Maschke[6]). So we have a formal way to consider the minimization given by formula (5). However we do not have an explicit formula for $E[\rho]$; thus the minimization (6) is still not easy.

In a series of articles (see Petkov *et al.*,[7] Kryachko *et al.*[8–12]), Kryachko and Ludeña have proposed and developed an alternative method, the local scaling transformation, based on deformation of density functions. (See also March and Young.[13]) For instance, in Ref. 12, a first step consists in considering the transverse problem to (5), i.e., to minimize the energy with respect to the density. More precisely, given two densities ρ_0, ρ and a state Ψ_0 such that $\Psi_0 \mapsto \rho_0$, the problem is to construct a deformation which transforms Ψ_0 into a state Ψ_ρ of density ρ and then to minimize the energy $E[\Psi_\rho]$ with respect to ρ. If ρ_1 realizes the minimum, one then computes $\Psi_{\rho 1}$ the state of density ρ_1 which realized the minimum $E[\Psi_{\rho 1}]$. The second step is the minimization of the energy at fixed density ρ_1 (starting from the wave function $\Psi_{\rho 1}$). The algorithm is then to iterate those two steps. In fact if Ψ_0 is sufficiently closed to the exact state corresponding to the minimum E_0 then $E[\Psi_{\rho 1}]$ may already be a good approximation of E_0.

Note that if we are able to generate all the physical densities from ρ_0 with explicit deformations then the energy $E[\Psi_\rho]$ which depends on ρ and Ψ_0, corresponds to an exact density functional when Ψ_0, a generating state, is fixed.

Our aim in this paper is to obtain some deformations which transform Ψ_1 of density ρ_1, into Ψ_0 a state of a given density ρ_0.

First we formalize mathematically the concept of deformation via the so-called Jacobian problem. We denote $|D\mathbf{f}| = |\det(\partial f_i / \partial x_j)|$ the Jacobian of $\mathbf{f}$.

Definition I.1: Let ρ_0 and ρ_1 be two positive functions from $\mathbb{R}^3$ into $\mathbb{R}^+$. The Jacobian problem associated to ρ_0, ρ_1 consists of finding a C^1-diffeomorphism $\mathbf{f}: \mathbb{R}^3 \to \mathbb{R}^3$ such that

$$\forall \mathbf{x} \in \mathbb{R}^3, \quad \rho_0(\mathbf{x}) = |D\mathbf{f}(\mathbf{x})| \rho_1(\mathbf{f}(\mathbf{x})). \tag{7}$$

We then denote $\rho_0 = \mathbf{f} * \rho_1$.

Note that if $\rho_0 = \mathbf{f} * \rho_1$ and $\Psi_1 \mapsto \rho_1$ then $\Psi_0 = \hat{\mathbf{T}}_f(\Psi_1)$ solves our problem (i.e., $\Psi_0 \mapsto \rho_0$), where $\hat{\mathbf{T}}_f$ is the unitary operator on $L^2_A(\mathbb{R}^{3N})$ defined by

$$\hat{\mathbf{T}}_f(\Psi)(\mathbf{r}_1,\ldots,\mathbf{r}_N) = \prod_{i=1}^{N} |D\mathbf{f}(\mathbf{r}_i)|^{1/2} \Psi(\mathbf{f}(\mathbf{r}_1),\ldots,\mathbf{f}(\mathbf{r}_N)). \tag{8}$$

(This operator is introduced by Petkov, Stoitsov, and Kryachko[7] for particular **f**.) In fact in our first article[5] we obtained for each density ρ an explicit deformation $\mathbf{f}_\rho$ from $\mathbb{R}^3$ onto $[0,1]^3$ such that $\mathbf{f}_\rho * \mathrm{N} = \rho$ (in the measure sense), where here N denotes the constant density equal to N on $[0,1]^3$. Thus $\mathbf{f} = \mathbf{f}_{\rho 1}^{-1} o \mathbf{f}_{\rho 0}$ satisfies $\rho_0 = \mathbf{f} * \rho_1$. Note that it was one of the solutions proposed by Moser[14] in order to solve the Jacobian problem.

However, although this solution is explicit (up to the inversion of $\mathbf{f}_{\rho 1}$), we do not control well the regularity of the deformation $\mathbf{f}_\rho$ when ρ has singularities (which is always the case for molecular systems[15]), and we were not able to have more than two invariant points (see below) by this method.

But in order to define the energy $E[\Psi] = \langle \Psi, H\Psi \rangle$, we want the H^1 stability of the operator $\hat{\mathbf{T}}_f$; i.e., if Ψ is in H^1 then $\hat{\mathbf{T}}_f(\Psi)$ must be in H^1.

Actually there exist several results concerning the Jacobian problem (see in particular Refs. 14, 16–19). However, they do not solve the problem in a way that allows us to apply them in quantum chemistry, first because they almost always consider the Jacobian problem on a bounded domain and in regular cases, and second because we would like to obtain deformations that preserve the geometry of the molecule.

For instance, if we consider a molecule with P atoms, then we want the position of the P atoms be *invariant* under the deformation. Furthermore, following physical studies, we choose to characterize the geometry of the densities at this P singular position (the cusps conditions, see Kato,[15] Pack and Byers Brown[20]) and at infinity (exponential fall-off condition; see Refs. 21 and 22) as follows.

We denote $\mathbf{r} = (\mathrm{r}, \mathrm{w})$ in the spherical coordinates ($w \in S^2$ and $r \geqslant 0$), and $\mathbf{u}_r = \mathbf{r}/r$ the radial unit vector.

Definition I.2 (cusp): We say that $\rho: \mathbb{R}^3 \to \mathbb{R}^+$ *has a cusp in* $\mathbf{0}$ *if*

(i) in the neighborhood of $r = 0$,

$$\rho(r,w) = a + b(w)r + o(r) \tag{9}$$

with $a > 0$ *and* b *is a real continuous function on the sphere* S^2 *and* $o(r)$ *is uniform with respect to* $w \in S^2$;

(ii) $\nabla\rho$ *is bounded (where* ∇ *is the gradient in Euclidian coordinates).*

ρ also has a cusp in $\mathbf{x} \in \mathbb{R}^3$ *if* $\rho(\mathbf{r}+\mathbf{x})$ *has a cusp in* $\mathbf{r} = \mathbf{0}$.

Definition I.3 (exponential fall-off): We say that a function $\rho: \mathbb{R}^3 \to \mathbb{R}^+$ *has an exponential fall-off (at infinity) if, when* $r = |\mathbf{r}| \to \infty$,

$$\rho(r,w) = C(w) r^\beta e^{-\alpha r} + o(r^\beta e^{-\alpha r}) \tag{10}$$

where $\alpha < 0$, $\beta \in \mathbb{R}$, $C(w) \in C^0(S^2, \mathbb{R}_+^*)$ *and* $o(r^\beta e^{-\alpha r})$ *uniform with respect to* $w \in S^2$.

Note that for the exponential fall-off condition, we could have stated as for the cusp condition statement (ii), which in this case would have been ∇_ρ / ρ bounded at infinity. In fact the results of the paper can be extended to other types of cusp conditions and asymptotic behaviors.

In order to solve the Jacobian problem we use a method introduced by Moser[14] which linearizes the problem.

In the second section we rapidly recall this process and give some simple lemmas in order to obtain invariant points.

In the next section we show our principal theorem (Theorem III.1) where we construct a C^1-deformation $\mathbf{f}$ which transports a density ρ_0 into a density ρ_1 adapted to the geometry given below. In this theorem we precisely control the behavior of $\mathbf{f}$ near the cusps and at infinity.

In the fourth section we study the stability of the transformation $\hat{\mathbf{T}}_f$ under the symmetries induced by the point group of a given molecule. In particular we show how to obtain a transformation that conserves the classes of symmetries of dimension one.

In the last section we check the H^1-stability for the transformation $\hat{\mathbf{T}}_f$ [in order that if $\Psi \in H^1_A(\mathbb{R}^{3N})$, then $\hat{\mathbf{T}}_f\Psi$ be of finite energy], and we state a decomposition theorem (Theorem V.1) for the wave function. We then consider the practical point of view. More precisely, for a general exponential fall-off of the densities, we are not able to give an explicit construction of the deformation **f**. But with reasonable assumptions on the fall-off we show how to recover **f** using only the procedure of Moser. Thus the method developed by Kryachko and Ludeña can be numerically generalized for any molecule in order to approximate its fundamental energy E_0, or for other purposes.[11,9]

The results of this paper are usually stated in the space $\mathbb{R}^3$ but they can be easily generalized to $\mathbb{R}^n$.

II. MOSER'S PROCEDURE

A. Linearization of the Jacobian problem

We now recall one of the procedures described in Moser[14] and Dacorogna and Moser[17] for solving the Jacobian problem associated to ρ_0 and ρ_1. We shall hereafter refer to it as *Moser's procedure*. We present it in $\mathbb{R}^n$ and then deal with existence results.

Let $\rho_i : \mathbb{R}^n \to \mathbb{R}^*_+$, $i=0,1$, be two continuous non-negative functions satisfying $\int \rho_0 = \int \rho_1$. Regularity assumptions will be made precise later when needed.

Moser introduces a path of densities $(\rho_t), t \in [0,1]$, as follows:

$$\rho_t(\mathbf{x}) = (1-t)\rho_0(\mathbf{x}) + t\rho_1(\mathbf{x}). \tag{11}$$

He then considers the problem of finding for all $t \in [0,1]$ a function $\mathbf{f}_t$ such that

$$\rho_0 = \mathbf{f}_t * \rho_t \tag{12}$$

and with initial conditions

$$\mathbf{f}_0(\mathbf{x}) = \mathbf{x}, \quad \mathbf{x} \in \mathbb{R}^n. \tag{13}$$

Instead of searching for $\mathbf{f}_t$ such that (12) be true, Moser looks for equivalent equations only in terms of the flux $X_t : \mathbb{R}^n \to \mathbb{R}^n$, related to $\mathbf{f}_t$ by

$$\frac{d\mathbf{f}_t}{dt} = \mathbf{X}_t(\mathbf{f}_t), \quad \mathbf{x} \in \mathbb{R}^n, \quad t \in [0,1]. \tag{14}$$

We can then recover $\mathbf{f}_t$ by exponentiation of $\mathbf{X}_t$.

We recall how to obtain the equations in terms of $\mathbf{X}_t$ only, as detailed in Dacorogna and Moser.[17] Let $J_t = |D\mathbf{f}_t|$. By derivation of $\rho_0 = J_t \rho_t(\mathbf{f}_t)$ with respect to t, we obtain

$$0 = \dot{J}_t \rho_t(\mathbf{f}_t) + J_t \dot{\rho}_t(\mathbf{f}_t) + J_t \langle \nabla \rho_t(\mathbf{f}_t), \dot{\mathbf{f}}_t \rangle. \tag{15}$$

After division by J_t, and with $\mathbf{x} = \mathbf{f}_t(\mathbf{r})$, we have

$$\rho_0(\mathbf{x}) - \rho_1(\mathbf{x}) = \frac{\dot{J}_t}{J_t}(\mathbf{r})\rho_t(\mathbf{x}) + \nabla \rho_t(\mathbf{x}) \mathbf{X}_t(\mathbf{x}). \tag{16}$$

Furthermore by differentiation of $(d/dt)\mathbf{f}_t = \mathbf{X}_t(\mathbf{f}_t)$, we obtain

$$\frac{d}{dt} D\mathbf{f}_t = D\mathbf{X}_t(\mathbf{f}_t) D\mathbf{f}_t \tag{17}$$

which gives $\dot{J}_t = \mathrm{div}(\mathbf{X}_t)(\mathbf{f}_t)J_t$, where $\mathrm{div}(\mathbf{X}_t)$ denotes the divergence of the vector field $\mathbf{X}_t$. Finally we have a linear equation in terms of $\mathbf{X}_t$ only,

$$\mathrm{div}(\rho_t \mathbf{X}_t) = \rho_0 - \rho_1. \tag{18}$$

Note that more generally denoting $\rho(x,t) = \rho_t(x)$ and $\mathbf{X}(x,t) = \mathbf{X}_t(x)$ we obtain the conservation equation

$$\frac{\partial \rho}{\partial t} + \mathrm{div}(\rho \mathbf{X}) = 0.$$

We can choose $\mathbf{V}$ as a solution of $\mathrm{div}(\mathbf{V}) = \rho_0 - \rho_1$ and then take

$$\mathbf{X}_t(\mathbf{x}) = \frac{\mathbf{V}(\mathbf{x})}{\rho_t(\mathbf{x})}. \tag{19}$$

The Jacobian problem (7) is then formally equivalent to Eq. (14) with initial condition (13) and where $\mathbf{X}_t$ is given by (18) (see Ref. 17 in the bounded case). In order to obtain a solution of the Jacobian problem, we must now show an existence result for (14) and (13) on the whole space $\mathbb{R}^n$.

The following theorem will be applied to $\mathbf{X}_t = \mathbf{V}/\rho_t$. We make a strong hypothesis on $\mathbf{X}_t$ (i.e., it vanishes at infinity), and in the following sections we shall see how this particular case can be used.

Theorem II.1: *Let K be a finite set of $\mathbb{R}^n$ (eventually $K=0$). Let $\mathbf{X} \in C^0([0,1]\times\mathbb{R}^n, \mathbb{R}^n)$ [we denote $\mathbf{X}_t(\mathbf{x})$ where $t \in [0,1]$ and $x \in \mathbb{R}^n$]. We suppose that $\mathbf{X}$ is of class C^1 on $[0,1]\times(\mathbb{R}^n - K)$. (More precisely, for instance, on some open set of $\mathbb{R}^{n+1}$ that contains $[0,1]\times(\mathbb{R}^n - K)$.) We suppose furthermore that*

(i) $\forall \mathbf{x} \in K,\ \forall t \in [0,1],\ \mathbf{X}_t(\mathbf{x}) = 0$;

(ii) $\sup_{t\in[0,1]} |\mathbf{X}_t(\mathbf{r})| \to 0$ *when* $|r| \to \infty$;

(iii) $\|D\mathbf{X}_t(\mathbf{x})\|$ *(matrix norm) is bounded on* $[0,1]\times(\mathbb{R}^n - K)$.

Then the system (14), (13) has a unique solution $\mathbf{f}_t$ which is for all $t \in [0,1]$ a C^1-diffeomorphism from $\mathbb{R}^n - K$ onto itself, a homeomorphism on $\mathbb{R}^n$, and lets K be invariant. Furthermore $\|D\mathbf{f}_t\|$ and $\|D\mathbf{f}_t^{-1}\|$ are bounded.

Proof: We first treat the case K empty, and $\mathbf{X}_t$ regular. The proof is classical using the fixed point theorem as follows. For $T \in [0,1]$, let $E(T)$ be the set of functions $\mathbf{f} \in C^0([0,T]\times\mathbb{R}^n, \mathbb{R}^n)$ such that, when $|\mathbf{x}| \to \infty$,

$$\sup_{t\in[0,T]} |\mathbf{f}_t(\mathbf{x}) - \mathbf{x}| \to 0. \tag{20}$$

We denote indifferently $\mathbf{f}(t,\mathbf{x})$ or $\mathbf{f}_t(\mathbf{x})$. The space $E(T)$ is then metric complete for the distance

$$d(\mathbf{f},\mathbf{g}) = \sup_{t\in[0,T],\mathbf{x}\in\mathbb{R}^n} |\mathbf{f}_t(\mathbf{x}) - \mathbf{g}_t(\mathbf{x})|. \tag{21}$$

Let $\mathbf{g} \in E(T)$, t-independent $(\mathbf{g}(t,\mathbf{x}) = \mathbf{g}(\mathbf{x}))$. Let Γ be defined on $E(T)$ by

$$\Gamma(\mathbf{f})(t,\mathbf{x}) = \mathbf{g}(\mathbf{x}) + \int_0^t \mathbf{X}_s(\mathbf{f}_s(\mathbf{x}))ds. \tag{22}$$

From (ii) we obtain that Γ is well defined from $E(T)$ into itself. Furthermore $d(\Gamma(\mathbf{f}_1),\Gamma(\mathbf{f}_2)) \leqslant T\eta d(\mathbf{f}_1,\mathbf{f}_2)$ where $\nu = \sup_{t,\mathbf{x}} \|D\mathbf{X}_t(\mathbf{x})\|$. Thus Γ is contractant for T small enough, and we obtain the existence of a fixed point $\mathbf{f}_t$ on $t \in [0,T]$, using $\mathbf{g} = \mathbf{f}_0 = \mathrm{Id}$. Then using $\mathbf{g} = \mathbf{f}_T$ we obtain the same existence on $[T,2T]$, etc.

We also have that $\mathbf{f}_t$ is a C^1-diffeomorphism because it is the exponentiation of the flux X_t. More precisely, we have for all t,t_1,t_2,t_3 in [0,1],

$$\mathbf{f}_{t_2,t_3} o \mathbf{f}_{t_1,t_2} = \mathbf{f}_{t_1,t_3},$$

$$\mathbf{f}_{t,t} = Id,$$

where $\mathbf{f}_{t_1,t_2}(\mathbf{x})$ is the value at time t_2 of the solution of (14) that starts from $\mathbf{x}$ at time t_1. Thus $\mathbf{f}_t = \mathbf{f}_{t,0}$ is invertible on the all space $\mathbb{R}^n$.

Finally for the general case the result is the same using the restriction of the set $E(T)$ to the functions $\mathbf{f}_t$ such that $\mathbf{f}_t(\mathbf{x}) = \mathbf{x}$ for $\mathbf{x} \in K$. We only lose regularity on K. Also classical estimations give $\|D\mathbf{f}_t\| \leqslant \mathbf{e}^{\eta t}$ and a similar bound for $\|D\mathbf{f}_t^{-1}\|$. ■

B. Invariant points

We show here a simple way to obtain some invariant points [i.e., $\mathbf{f}(\mathbf{x}_i) = \mathbf{x}_i$, $\forall i = 1,\ldots,P$] while solving the Jacobian problem. The following method seems more constructive than the one presented in Ref. 17 for instance, where they treat the invariant points as border points. (However, Theorem III.1 gives lesser regularity than Ref. 17.)

A sufficient condition for having $\mathbf{f}(\mathbf{a}) = \mathbf{a}$ is to search $\mathbf{f}_t$ such that $\forall t \in [0,1]$, $\mathbf{f}_t(\mathbf{a}) = \mathbf{a}$. In terms of $\mathbf{X}_t$ this condition becomes

$$\forall t \in [0,1], \quad \mathbf{X}_t(\mathbf{a}) = \mathbf{0}. \tag{23}$$

So we need to find a solution $\mathbf{U}(\mathbf{x})$ of

$$\operatorname{div}(\mathbf{U}) = g, \tag{24}$$

$$\mathbf{U}(\mathbf{a}) = \mathbf{0} \tag{25}$$

where $g: \mathbb{R}^n \to \mathbb{R}$ is a given function.

But considering the linearity of the divergence operator, it remains to prove the following lemma.

Lemma II.1: Let $(\mathbf{a}_j, \mathbf{b}_j)_j = 1 \cdots \mathrm{P}$ *be a finite set of pairs of points of* $\mathbb{R}^n$, *with distinct* (a_j). *There exists* $\mathbf{X}$ *a regular vector field on* $\mathbb{R}^n$, *of compact support, such that* $\operatorname{div}(\mathbf{X}) = \mathbf{0}$ *and* $\forall j = 1,\ldots,P$, $\mathbf{X}(\mathbf{a}_j) = \mathbf{b}_j$.

Proof: We only need to prove the following result: for all $\epsilon > 0$, there exists $\mathbf{X}$, C^∞-regular on $\mathbb{R}^n$, such that $\operatorname{supp}(\mathbf{X}) \subset [-\epsilon,\epsilon]^n$, $\operatorname{div}(\mathbf{X}) = 0$ and $\mathbf{X}(\mathbf{0}) = \mathbf{c}$ where $\mathbf{c} = (\mathbf{c}_1,\ldots,\mathbf{c}_n)$ is a given vector of $\mathbb{R}^n$.

To construct $\mathbf{X} = (X_1,\ldots,X_n)$ we can, for instance, choose

$$X_1(x_1,\ldots,x_n) = \phi_1(x_1)\phi_2'(x_2)\cdots\phi_n'(x_n), \tag{26}$$

$$X_2(x_1,\ldots,x_n) = \phi_1'(x_1)\phi_2(x_2)\phi_3'(x_3)\cdots\phi_n'(x_n), \tag{27}$$

$$\vdots \tag{28}$$

$$X_n(x_1,\ldots,x_n) = -(n-1)\phi_1'(x_1)\cdots\phi_{n-1}'(x_{n-1})\phi_n(x_n), \tag{29}$$

where ϕ_j, $j = 1,\ldots,n$, are C^∞ functions on $\mathbb{R}$ with support included in $[-\epsilon,\epsilon]$ and such that $\phi_j(0) = c_j$, $j = 1,\ldots,n-1$, $\phi_n(0) = -[c_n/(n-1)]$ and $\phi_j'(0) = 1$, $j = 1,\ldots,n$. ■

The following lemma will be used in Theorem III.1. We restrict ourselves to the case $n = 3$, for simplicity of presentation.

Lemma II.2: Suppose that $\mathrm{div}(\mathbf{W})=0$, *where* $\mathbf{W}$ *is a regular vector field on* $\mathbb{R}^3$. *Let* $M^k=\mathrm{D}^k\mathbf{W}(0)$, *the differential of order* k of $\mathbf{W}$ *in* $\mathbf{0}$. *Let* $\epsilon>0$. *Then there exists a* C^∞*-regular vector field* $\mathbf{V}$ *on* $\mathbb{R}^3$ *such that* $\mathrm{supp}(\mathbf{V})\subset \mathrm{B}(\mathbf{0},\epsilon)$, $\mathrm{div}(\mathbf{V})=0$, *and* $\forall k=0,1,2: \mathrm{D}^k\mathbf{V}(\mathbf{0})=M^k$.

Proof: The proof is similar; we can, for instance, construct V using a linear combination of vector fields like $\mathbf{X}$ in the previous lemma. ■

III. GLOBAL EXISTENCE RESULT

In this section, we first construct a deformation which solves the Jacobian problem near each cusp, then we do the same in a neighborhood of the infinity, and finally in the remaining compact domain where there will be no more constrains. The final deformation will be obtained composing the three previous deformations.

A. Jacobian problem near a cusp

Proposition III.1: Let ρ_0,ρ_1 *be two functions in* $C^\infty(\mathbb{R}^3\backslash\{\mathbf{0}\},\mathbb{R}_+^*)\cap C^0(\mathbb{R}^3,\mathbb{R}_+^*)$, *and let* $\epsilon>0$. *Then there exists a* C^0*-diffeomorphism* $\mathbf{f}$ *which has the form* $\mathbf{f}(\mathbf{x})=f(r,w)\mathbf{u}_r$ *and such that*

(i) $\mathbf{f}$ *is a* C^∞*-diffeomorphism on* $\mathbb{R}^3\backslash\{\mathbf{0}\}$, differentiable in $\mathbf{0}$ and $\mathbf{f}(\mathbf{0})=(\mathbf{0})$;

(ii) $\mathbf{f}$ *solves the Jacobian problem* $\rho_0=\mathbf{f}*\rho_1$ *on a neighborhood of the origin*;

(iii) $\mathbf{f}$ *is the identity function on* $\mathbb{R}^3\backslash B(\mathbf{0},\epsilon)$

Proof: Using Moser's procedure, if we define

$$U(r,w)=\frac{1}{r^2}\int_0^r(\rho_0(s,w)-\rho_1(s,w))s^2ds, \tag{30}$$

then the radial vector field $\mathbf{U}=U(r,w)\mathbf{u}_r$ satisfies

$$\mathrm{div}(\mathbf{U})=\frac{1}{r^2}\frac{\partial}{\partial r}[r^2U(r,w)]=\rho_0-\rho_1.$$

Note that if we solve $d\mathbf{f}_t/dt=\mathbf{X}_t(\mathbf{f}_t)$ directly by Theorem II.1, we do not obtain regularity for $\mathbf{f}_1$ at $\mathbf{x}=\mathbf{0}$.

But we can remark that the solution of

$$\frac{d\mathbf{f}_t}{dt}=\mathbf{X}_t(\mathbf{f}_t) \tag{31}$$

with $\mathbf{X}_t=\mathbf{U}_t/\rho_t$ is given by the implicit equation

$$\int_0^{f_t(r,w)}\rho_t(s,w)s^2ds=\int_0^r\rho_0(s,w)s^2ds. \tag{32}$$

To see this, first we have

$$\frac{d}{dt}f_t(r,w)=\frac{\int_0^{f_t(r,w)}(\rho_0(s,w)-\rho_1(s,w))s^2ds}{f_t(r,w)^2\rho_t(f_t(r,w),w)}. \tag{33}$$

Now if we put for $i=0,1$:

$$R_i(r,w)=\int_0^r\rho_i(s,w)s^2ds \tag{34}$$

and $R_t=(1-t)R_0+tR_1$, then

$$\frac{d}{dt}\left[R_t(f_t(r,w),w)\right]=f_t(r,w)^2\rho_t(f_t(r,w),w)\,\frac{d}{dt}\,f_t(r,w)+(R_1-R_0)(f_t(r,w),w)$$

which is zero because of (33). Thus (32) is proved.

By implicit function theorem equation (32) defines uniquely $f_t(r,w)$ on a neighborhood of $\mathbf{0}$, say $B(\mathbf{0},\epsilon_1)$, and for $t\in[0,1]$ (one can find ϵ_1 such that $0<\epsilon_1<\epsilon$ because of the continuity assumption made on the ρ_i's). Furthermore $f_t(0)=0$ and $f_t\in C^\infty(B(\mathbf{0},\epsilon_1)\backslash\{\mathbf{0}\})$. Note that we cannot solve (32) on $\mathbb{R}^3$ because we do not necessarily have for all w:

$$\int_0^{+\infty}\rho_t(s,w)s^2ds=\int_0^{+\infty}\rho_0(s,w)s^2ds. \tag{35}$$

We have already proved that f_t is in $C^0(B(\mathbf{0},\epsilon_1))$. But in fact if $a_t=\rho_t(\mathbf{0})$ we obtain by straightforward calculus that

$$f_t(r,w)=\left(\frac{a_0}{a_t}\right)^{1/3}r+o(r) \tag{36}$$

uniformly with respect to t and w, and thus $\mathbf{f}=\mathbf{f}_1$ is differentiable in $\mathbf{0}$.

Now using (36) we deduce that for every $\epsilon_1>0$ there exists $\epsilon_0>0$ such that $\forall t\in[0,1]:\mathbf{f}_t(B(\mathbf{0},\epsilon_0))\subset B(\mathbf{0},\epsilon_1)$. We then define $\tilde{U}=U\Psi$ where Ψ is a radial C^∞ function such that $\Psi(\mathbf{x})=1$ for $\mathbf{x}\in B(\mathbf{0},\epsilon_1)$, $\Psi(\mathbf{x})=0$ for $\mathbf{x}\in\mathbb{R}^3\backslash B(\mathbf{0},2\epsilon_1)$, and $0\leqslant\Psi\leqslant1$ otherwise. Let $\tilde{\mathbf{f}}_t$ be the radial solution of

$$\frac{d}{dt}\,\tilde{\mathbf{f}}_t=\tilde{\mathbf{X}}_t(\tilde{\mathbf{f}}_t) \tag{37}$$

with $\tilde{\mathbf{X}}_t=\tilde{\mathbf{U}}/\rho_t$ and initial condition $\tilde{\mathbf{f}}_0=Id$ (see Lemma II.1 for the existence of $\tilde{\mathbf{f}}_t$). Then $\mathbf{f}_t$ and $\tilde{\mathbf{f}}_t$ are radial solutions of the same equation on $B(\mathbf{0},\epsilon_0)$ and thus are equal on this set. Because $\tilde{\mathbf{X}}_t$ is regular on $\mathbb{R}^3-\{\mathbf{0}\}$ this $\tilde{\mathbf{f}}_t$ satisfies the properties (i) and (ii) of the proposition.

Finally, using that $|\tilde{\mathbf{X}}_t(\mathbf{x})|\leqslant C|\mathbf{x}|$ (for some constant $C>0$) we can deduce by *a priori* estimations that $e^{-Ct}r\leqslant\tilde{f}_t(r,w)\leqslant e^{Ct}r$. Thus we have $\tilde{\mathbf{f}}^{-1}(B(\mathbf{0},2\epsilon_1))\subset B(\mathbf{0},\epsilon)$ with a choice of ϵ_1 such that $2\epsilon_1=e^{-C}\epsilon$. Then (iii) follows. ■

Now if we suppose that ρ_0 and ρ_1 have cusps in $\mathbf{0}$ we can prove that the diffeomorphism $\mathbf{f}$ constructed in proposition III.1 is C^1 on $\mathbb{R}^3$ and we can precisely determine the behavior of $\mathbf{f}$ near $\mathbf{0}$.

Proposition III.2: Let ρ_0,ρ_1 be two functions with cusps in zero (see definition I.2):

$$\rho_i(r,w)=a_i+b_i(w)r+o(r). \tag{38}$$

Then the diffeomorphism $\mathbf{f}$ *constructed in proposition III.1 is C^1 on $\mathbb{R}^3$ and admits the following behavior in zero:*

$$f(r,w)=\lambda_0r+\lambda_1(w)r^2+o(r^2) \tag{39}$$

[with $o(r^2)$ uniform in w], where

$$\lambda_0=\left(\frac{a_0}{a_1}\right)^{1/3}, \tag{40}$$

$$4\lambda_1(w)=\frac{b_0(w)}{a_0}\,\lambda_0-\frac{b_1(w)}{a_1}\,\lambda_0^2. \tag{41}$$

Proof: First we check the C^1 regularity in $\mathbf{0}$, by showing that the differential $D\mathbf{f}(\mathbf{x})\to\lambda_0 Id$ when $\mathbf{x}\to\mathbf{0}$. We know that $\nabla\rho_i$ are bounded near $\mathbf{0}$; thus

$$\frac{\partial(\rho_0-\rho_1)}{\partial r},\ \frac{1}{r}\frac{\partial(\rho_0-\rho_1)}{\partial\theta},\quad \frac{1}{r\sin(\theta)}\frac{\partial(\rho_0-\rho_1)}{\partial\phi}$$

are bounded near $\mathbf{0}$. On the other hand, using spherical coordinates we have

$$D\mathbf{f}(\mathbf{x})=U^T\begin{bmatrix}\frac{\partial f}{\partial r} & \frac{1}{r}\frac{\partial f}{\partial\theta} & \frac{1}{r\sin(\theta)}\frac{\partial f}{\partial\phi}\\ 0 & f/r & 0\\ 0 & 0 & f/r\end{bmatrix}U, \tag{42}$$

where the matrix U is unitary and given by $U=[\mathbf{u}_r,\mathbf{u}_\theta,\mathbf{u}_\phi]$. Thus we have only to verify that

$$\lim_{r\to0^+}\frac{\partial f}{\partial r}(r,w)=\lim_{r\to0^+}\frac{f(r,w)}{r}=\lambda_0 \tag{43}$$

(uniformly in w) and that

$$\lim_{r\to0^+}\frac{1}{r}\frac{\partial f}{\partial\theta}(r,w)=\lim_{r\to0^+}\frac{1}{r\sin(\theta)}\frac{\partial f}{\partial\phi}(r,w)=0. \tag{44}$$

For instance, by differentiation of (32) at $t=1$, we obtain

$$\frac{\partial f}{\partial r}(r,w)f(r,w)^2\rho_1(f(r,w),w)=r^2\rho_0(r,w) \tag{45}$$

and thus we prove (43). We can obtain (44) in the same way, using Eq. (32) at $t=1$ anew.

Finally the behavior (40) is obtained by straightforward calculus. ■

B. Jacobian problem at infinity

For the Jacobian problem at infinity we have a similar proposition, except that we can no longer prove it with Moser's procedure (at least with Theorem II.1). We mention also Greene and Shiohama[18] for the Jacobian problem in the non-compact case.

Proposition III.3: Let ρ_0,ρ_1 be two functions of $C^\infty(\mathbb{R}^3,\mathbb{R}_+^*)\cap L^1(\mathbb{R}^3)$. We suppose furthermore that ρ_0 satisfies the following condition when $R\to\infty$:

$$\int_R^{+\infty}\rho_0(t,w)t^2dt=o(1) \tag{46}$$

uniformly with respect to $w\in S^2$. Let $R>0$ and $\epsilon>0$. Then there exists $R_1>R$ and a radial-like function $\mathbf{f}(\mathbf{x})=f(r,w)\mathbf{u}_r$ such that

(i) $\mathbf{f}$ *is a C^∞-diffeomorphism on $\mathbb{R}^3$;*

(ii) $\mathbf{f}$ *is the solution on $\mathbb{R}^3\backslash B(\mathbf{0},R_1)$ of the Jacobian problem*

$$\rho_0=\mathbf{f}^*\rho_1, \tag{47}$$

(iii) $\mathbf{f}$ *is the identity function on $B(\mathbf{0},R)$.*

We first need a lemma. (In some sense we modify ρ_0 in $\tilde{\rho}$. There are similarities with the proof of Lemma 11 of Dacorogna.[16])

Lemma III.1: Let ρ_0,ρ_1 be two functions of $C^\infty(\mathbb{R}^3,\mathbb{R}_+^*)\cap L^1(\mathbb{R}^3)$, with ρ_0 satisfying relation (46). Let $R>0$. Then there exists $R_1>R$ and $\widetilde{\rho}\in C^\infty(\mathbb{R}^3,\mathbb{R}_+^*)$ such that

(i) $\widetilde{\rho}=\rho_0$, $r\geqslant R_1$,

(ii) $\widetilde{\rho}=\rho_1$, $r\leqslant R$,

(iii) $\int_R^{+\infty}\widetilde{\rho}(s,w)s^2ds=\int_R^{+\infty}\rho_1(s,w)s^2ds, \forall w$.

Proof: First we choose $R_1>R$ such that $\forall w$,

$$C_1(w)=\int_R^{+\infty}\rho_1(s,w)s^2ds-\int_{R_1}^{+\infty}\rho_0(s,w)s^2ds>0.$$

Let $\epsilon>0$ and ϕ_1^ϵ be a C^∞ function such that $0\leqslant\phi_1^\epsilon\leqslant 1$ and

$$\phi_1^\epsilon(r)=1, \quad r\leqslant R,$$

$$\phi_1^\epsilon(r)=0, \quad r\geqslant R+\epsilon.$$

Similarly let ϕ_0^ϵ be a C^∞ function such that $0\leqslant\phi_0^\epsilon\leqslant 1$ and

$$\phi_0^\epsilon(r)=0, \quad r\leqslant R_1-\epsilon,$$

$$\phi_0^\epsilon(r)=1, \quad r\geqslant R_1,$$

and choose $\epsilon>0$ such that for every w:

$$\int_R^{R_1}s^2(\phi_1^\epsilon(s)\rho_1(s,w)+\phi_0^\epsilon(s)\rho_0(s,w))ds<C_1(w).$$

Finally let k be a non-negative C^∞ function such that $\mathrm{supp}(k)=[R,R_1]$ and $\int_R^{R_1}k(s)s^2\,ds=1$. We define

$$\widetilde{\rho}(r,w)=\phi_1^\epsilon\rho_1(r,w)+\phi_0^\epsilon\rho_0(r,w)+C_2(w)k(r).$$

Then it suffices to define $C_2(w)$ by

$$C_2(w)=C_1(w)-\int_R^{R_1}s^2(\phi_1^\epsilon(s)\rho_1(s,w)+\phi_0^\epsilon(s)\rho_0(s,w))ds. \tag{48}$$

■

Proof of Proposition III.3: We define $f(r,w)$ by the implicit equation:

$$\int_{f(r,w)}^{+\infty}\rho_1(s,w)s^2ds=\int_r^{+\infty}\widetilde{\rho}(s,w)s^2ds. \tag{49}$$

This equation has a solution because from the previous lemma we now have

$$\int_0^{+\infty}\rho_1(s,w)s^2ds=\int_0^{+\infty}\widetilde{\rho}(s,w)s^2ds. \tag{50}$$

The solution is C^∞ because of the implicit function theorem, and furthermore by construction of $\widetilde{\rho}$ we have

$$f(r,w)=r \quad \forall r\leqslant R,\forall w. \tag{51}$$

Then $\mathbf{f}=f\mathbf{u}_r$ solves the Jacobian problem $\rho_0=\widetilde{\rho}=\mathbf{f}*\rho_1$ for $r\geqslant R_1$. ■

In the case we have an exponential fall-off at infinity we can precisely determine the behavior of **f**.

Proposition III.4: Let ρ_0,ρ_1 be two functions as in Proposition III.3 and with exponential fall-off (see definition I.3) when $r\to\infty$:

$$\rho_i(r,w)\sim C_i(w)r^{\beta_i}e^{-\alpha_i r}. \tag{52}$$

Then the solution of proposition III.3, $f(r,w)$, is defined for r large enough by

$$\int_{f(r,w)}^{\infty}\rho_1(t)t^2dt=\int_r^{\infty}\rho_0(t)t^2dt \tag{53}$$

and admits the following asymptotic when $r\to\infty$:

$$f(r,w)=Ar+B\,\log\,r+C(w)+o(1), \tag{54}$$

where

$$A=\frac{\alpha_0}{\alpha_1},\quad B=-\frac{(\beta_1-\beta_0)}{\alpha_1},\quad C(w)=\frac{1}{\alpha_1}\log\left(A^{2+\beta_1}\frac{C_1(w)}{C_0(w)}\right)$$

[and where $o(1)$ is uniform in w].

Proof: We only have to show the asymptotic for $r\to\infty$. Let us forget the index w for clarity. First we have

$$C_1\int_{f(r)}^{\infty}t^{\beta_1+2}e^{\alpha_1 t}dt\sim C_0\int_r^{\infty}t^{\beta_0+2}e^{\alpha_0 t}dt. \tag{55}$$

We recall that when $r\to\infty$ and for $\alpha>0$:

$$\int_r^{+\infty}t^m e^{-\alpha t}dt\sim\frac{1}{\alpha}r^m e^{-\alpha r}. \tag{56}$$

Thus at infinity

$$C_1 f(r)^{\beta_1+2}e^{-\alpha_1 f(r)}\sim C_0 r^{\beta_0+2}e^{-\alpha_0 r}. \tag{57}$$

Applying the logarithm, we deduce that $\alpha_1 f(r)\sim\alpha_0 r$. Let us denote $g(r)=\alpha_1 f(r)-\alpha_0 r$. We have

$$e^{g(r)}\sim\frac{C_1}{C_0}A^{\beta_1+2}r^{\beta_1-\beta_0} \tag{58}$$

from what we deduce $g(r)=\log\{(C_1/C_0)A^{\beta_1+2}r^{\beta_1-\beta_0}\}+o(1)$. ■

C. Global result

We deal here with the general case. We want to solve the Jacobian problem on $\mathbb{R}^3$, for densities (ρ_0,ρ_1) with cusps and exponential fall-off.

Lemma III.2: Let $\rho\in C^{\infty}(\mathbb{R}^3,\mathbb{R})$, of compact support included in $[-R,R]^3(R>0)$, and such that

$$\int_{\mathbb{R}^3}\rho=0. \tag{59}$$

Then there exists a vector field $\mathbf{V}\in C^\infty(\mathbb{R}^3,\mathbb{R}^3)$ *of support included in* $[-R,R]^3$ *and such that* $\mathrm{div}(\mathbf{V})=\rho$ *on* $\mathbb{R}^3$.

Proof: Let $g\in C^\infty(\mathbb{R},\mathbb{R})$ such that $g(x)=0$ for $x\leqslant -R$ and $g(x)=1$ for $x\geqslant R$. Thus $\mathrm{supp}(g')\subset[-R,R]$. Let

$$V_1(x,y,z)=\int_{-\infty}^{x}\rho(x',y,z)dx'-g(x)\int_{-\infty}^{+\infty}\rho(x',y,z)dx',$$

$$V_2(x,y,z)=g'(x)\int_{-\infty}^{+\infty}\int_{-\infty}^{y}\rho(x',y',z)dx'dy'-g'(x)g(y)\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\rho(x',y',z)dx'dy',$$

$$V_3(x,y,z)=g'(x)g'(y)\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{z}\rho(x',y',z')dx'dy'dz'.$$

Then $\mathbf{V}=(V_1,V_2,V_3)$ is a solution. ■

Theorem III.1: *Let* $K=\{\mathbf{x}_1,\ldots,\mathbf{x}_P\}$ *be P distinct points of* $\mathbb{R}^3$, *and* $R>0$ *such that* $K\subset B(\mathbf{0},R)$. *Let* ρ_0,ρ_1 *be two functions of* $C^\infty(\mathbb{R}^3-K,\mathbb{R}_+^*)$, *with cusps in each* x_j *(see definition I.2) and exponential fall-off at infinity (see definition I.3), and such that*

$$\int_{\mathbb{R}^3}\rho_0=\int_{\mathbb{R}^3}\rho_1.$$

Then there exists a solution $\mathbf{f}$ *of the Jacobian problem*

$$\rho_0=\mathbf{f}*\rho_1 \tag{60}$$

which is a C^1*-diffeomorphism on* $\mathbb{R}^3$ *and a* C^∞*-diffeomorphism on* $\mathbb{R}^3-K$ *onto itself, that lets K be invariant, with behavior near the cusps given precisely by Eq. (39) and defined on* $\mathbb{R}^3\backslash B(\mathbf{0},R_1)$ *(for some* $R_1>R$*) as in Proposition III.4.*

Proof: We solve separately the Jacobian problem near the infinity, then near the nuclei, and finally on a compact set where the cusp and infinity problems will disappear. More precisely, using Proposition III.3 we can deform ρ_1 in ρ_2 (by a C^∞-regular $\mathbf{f}_1$) such that $\rho_2=\rho_0$ outside a ball $B(\mathbf{0},R_1)(R_1>R)$ and such that f_1 be the identity function inside the ball $B(\mathbf{0},R)$ that contains K. For $\mu>0$ let us denote $V_\mu=\cup_j B(\mathbf{x}_j,\mu)$. Also, using Proposition III.1 around each nuclei, we can deform ρ_2 in ρ_3 (using a deformation $\mathbf{f}_2$) such that $\rho_3=\rho_0$ on a neighborhood V_{μ_1} of the nuclei $(0<\mu_1<\mu)$, and such that $\mathbf{f}_2$ be the identity function outside $V_\mu\subset B(\mathbf{0},R)$. If we choose R and μ such that $B(\mathbf{x}_j,\mu)\cap\mathrm{B}(\mathbf{x}_k,\mu)=\varnothing$, $\forall j\neq k$, and such that $V_\mu\subset B(\mathbf{0},R)$. We have $\rho_3=\rho_0$ near the nuclei and near infinity, with $\rho_3=\mathbf{f}_2*\rho_2=\mathbf{f}_2*(\mathbf{f}_1*\rho_1)=(\mathbf{f}_1\circ\mathbf{f}_2)*\rho_1$.

We have yet to solve $\rho_0=\mathbf{f}_3*\rho_3$. Using Lemma III.2, there exists $\mathbf{V}\in\mathrm{C}^\infty(\mathbb{R}^3,\mathbb{R}^3)$ such that $\mathrm{div}(\mathbf{V})=\rho_0-\rho_3$ on $\mathbb{R}^3$. Thus we use Lemma II.2 in order to obtain a regular $\mathbf{W}$ such that $\mathrm{div}(\mathbf{W})=\rho_0-\rho_3$ on $\mathbb{R}^3$ and with $\mathrm{D}^k\mathbf{W}(\mathbf{x}_j)=0$ for $k=0,1,2$ and $\mathbf{x}_j\in\mathrm{K}$.

We then define for $t\in[0,1]$:

$$\mathbf{U}_t=\frac{\mathbf{W}}{(1-t)\rho_0+t\rho_3}.$$

In order to clarify the proof we consider the case $\mathbf{x}_j=\mathbf{0}$. We have $\mathbf{U}_t(r,w)=O(r^3)$ uniformly in w (when $r\to 0$). Furthermore as we know that $\nabla\rho_t$ is bounded near each cusp we also obtain that $\mathrm{D}\mathbf{U}_t(r,w)=o(r)$ [using for instance Eq. (42)] and in particular $\mathbf{U}_t$ is C^1 on $\mathbb{R}^3$. Thus by Moser's procedure and Theorem II.1, we obtain a deformation $\mathbf{f}_3$ such that $\rho_0=\mathbf{f}_3*\rho_3$. Furthermore, by easy calculation we can verify that

$$\mathbf{f}_3(r,w)=r\mathbf{u}_r+O(r^3)$$

uniformly in w, when $r\to 0$.

Hence if we define $\mathbf{f}=\mathbf{f}_1 o \mathbf{f}_2 o \mathbf{f}_3$ then $\mathbf{f}$ is a C^1-diffeomorphism satisfying to $\rho_0=\mathbf{f}*\rho_1$ and the behavior of $\mathbf{f}$ near the cusps is given by the behavior of $\mathbf{f}_2$ (see Proposition III.2), and the behavior of $\mathbf{f}$ at infinity is given by $\mathbf{f}_1$ (see Proposition III.4). ■

Corollary III.1: Furthermore if $\nabla\rho_t/\rho_t$ *are bounded* $(i=0,1)$ *then in theorem III.1* $\|D\mathbf{f}\|$ *and* $\|D\mathbf{f}^{-1}\|$ *are also bounded.*

Proof: The study at infinity is similar to the study near a cusp in Proposition III.2. ■

Remark III.1: In Theorem III.1, if we relax the hypothesis of exponential fall-off at infinity, using only the hypothesis of proposition III.3, then the same result holds but off course without known behavior at infinity.

IV. SYMMETRIES

For a given set of fixed nuclei $K=\{\mathbf{y}_1,...,\mathbf{y}_P\}$ we consider the point group, denoted G, as the set of orthonormal transformations $Q\in O(3)$ that lets the set the molecule invariant.[23] Typically if we look for a solution of $H\Psi=E\Psi$ we usually want furthermore that Ψ belongs to a class of symmetry of the group G.

In this section we study the following problem. Given Γ a class of symmetry of the group G, find a deformation $\mathbf{f}:\mathbb{R}^3\to\mathbb{R}^3$ that solves the Jacobian problem $\rho_0=\mathbf{f}*\rho_1$ and furthermore such that if $\Psi_1\in\Gamma$ (with $\Psi_1\mapsto\rho_1$) then $\Psi_0=\hat{\mathbf{T}}_f\Psi_1\in\Gamma$. In fact we want the stability of the operator $\hat{\mathbf{T}}_f$ with respect to the geometry of the state under study.

Note that in the case that Ψ belongs to a class of symmetry of dimension one, we have for all $Q\in G$, $\hat{Q}\Psi=\lambda(Q)\Psi$ with $\lambda(Q)\in\mathbb{C}$, $|\lambda(Q)|=1$, and where $\hat{Q}$ is the operator on $L^2_A(\mathbb{R}^{3N})$ defined by

$$(\hat{Q}\Psi)(\mathbf{x}_1,\ldots,\mathbf{x}_N)=\Psi(Q^{-1}\mathbf{x}_1,\ldots,Q^{-1}\mathbf{x}_N).$$

We then deduce easily that

$$\forall Q\in G,\quad \rho_\Psi(Q\mathbf{x})=\rho_\Psi(\mathbf{x}). \tag{61}$$

Theorem IV.1 (symmetry): *Let* $K=\{y_1,\ldots,y_P\}$ *be a nonlinear set of nuclei (i.e., distinct and nonaligned points of* $\mathbb{R}^3$*), and* G *its associated finite point group. We suppose that* ρ_0,ρ_1 *are two density functions that satisfy the hypothesis of Theorem III.1 (with cusps in each* $\mathbf{y}_i$*) and also the symmetry conditions (61). Then there exists a solution* $\mathbf{f}$ *of the Jacobian problem* $\rho_0=\mathbf{f}*\rho_1$ *satisfying the conclusion of Theorem III.1, and furthermore such that for any class of symmetry* Γ *of* G, $\hat{\mathbf{T}}_f(\Gamma)\subset(\Gamma)$.

In particular when the class of symmetry Γ is of dimension one, we have solved our problem because the symmetry conditions (61) are satisfied for wave functions in Γ. A more general study will be done elsewhere.

Proof of Theorem IV.1: We assume that the invariant point of the group G is at the origin of $\mathbb{R}^3$. Although the infinite behavior of the densities may thus be changed, it can be easily shown that this does not affect the final result of the theorem.

Lemma IV.1: Suppose

$$\forall Q\in G,\quad \mathbf{f} o Q=Q o \mathbf{f}.$$

Then $\hat{\mathbf{T}}_f(\Gamma)=(\Gamma)$ *for any class of symmetry* Γ.

Proof: Let d be the dimension of the class of symmetry Γ. First note that $\hat{\mathbf{T}}_f\hat{Q}=\hat{Q}\hat{\mathbf{T}}_f$.In the case $d=1$, for $\Psi\in\Gamma$ we have for any $Q\in G$, $\hat{Q}\Psi=\lambda(Q)\Psi$ thus $\hat{Q}(\hat{\mathbf{T}}_f\Psi)=\lambda(Q)(\hat{\mathbf{T}}_f\Psi)$ which proves that $\hat{\mathbf{T}}_f\Psi\in\Gamma$. When $d>1$ and $\Psi\in\Gamma$, we know that $\Psi\in\mathrm{Vect}\{\Psi_1,...,\Psi_d\}$ with $\hat{Q}\Psi_i=\Sigma_j c_{i,j}(Q)\Psi_j$ and where $\{c_{i,j}(Q)\}$ are the matrix coefficients of the representation Γ in the basis set (Ψ_i). As in the

case $d=1$ we obtain that $\hat{Q}(\hat{\mathbf{T}}_f\Psi_i)=\Sigma_j c_{i,j}(Q)\hat{\mathbf{T}}_f\Psi_j$. Hence $(\hat{\mathbf{T}}_f\Psi_i)_i$ admits the same matrix representation as the $(\Psi_i)_i$, and thus belongs to Γ. Thus, $\hat{\mathbf{T}}_f\Psi\in\Gamma$ by linearity. ■

Lemma IV.2 (infinity): The deformation $\mathbf{f}^{(1)}=\mathbf{f}$ *obtained in Proposition III.3 commutes with the elements of* G.

Proof: First note that the density $\tilde{\rho}$ constructed in Lemma III.1 satisfies the symmetry conditions (61). Let us denote $\mathbf{f}(\mathbf{x})=f(r,w)\mathbf{u}_r(w)$ in spherical coordinates. Then $f(r,w)$ is also defined by

$$\int_0^{f(r,w)}\rho_1(s,w)s^2ds=\int_0^r\tilde{\rho}(s,w)s^2ds.$$

Let $Q\in G$. Because $Q\mathbf{0}=\mathbf{0}$, we can naturally define Qw by $Q(r,w)=(r,Qw)$ and we obtain that $f(r,Qw)=f(r,w)$ and $Q\mathbf{u}_r(w)=\mathbf{u}_r(Qw)$. Then $\mathbf{f}oQ(r,w)=\mathbf{f}(r,Qw)=f(r,w)\mathbf{u}_r(Qw)$, and this is also $Qo\mathbf{f}$(r,w). ■

We can now suppose that $\rho_0=\rho_1$ on $\mathbb{R}^3\backslash B(\mathbf{0},R)$, and we study the solution of the Jacobian problem near the cusps.

For simplicity of presentation, we denote the relation $Q(\mathbf{y}_j)=\mathbf{y}_k$ by $Q(j)=k$.

First for a given j we define a solution $\mathbf{f}_j$ of the Jacobian problem $\rho_0=\mathbf{f}_j*\rho_1$ inside some $B_j=B(\mathbf{y}_j,\epsilon_1)$ exactly as in the proof of Theorem III.1, the function $\mathbf{f}_j$ being the identity on some $\mathbb{R}^3\backslash B(\mathbf{y}_j,\epsilon)$, $\epsilon>\epsilon_1$ [with disjoint sets $B(\mathbf{y}_k,\epsilon)$, $k=1,\ldots,P$].

Now if k is in the cycle generated by j, i.e., if there exists Q in G such that $k=Q(j)$, we then define $\mathbf{f}_k$ by

$$\mathbf{f}_k=Q\mathbf{f}_jQ^{-1}. \tag{62}$$

We then reiterate the same construction for each cycle of K and obtain the following lemma.

Lemma IV.3 (cusps): Let $B_j=B(\mathbf{y}_j,\epsilon_1)$, $Q\in G$.

(i) The $(\mathbf{f}_j)$ *are well defined by Eq. (62), and commute:* $\mathbf{f}_k\,o\,\mathbf{f}_l=\mathbf{f}_l\,o\,\mathbf{f}_k$.

(ii) If $k=Q(j)$ *and* $\rho_0=\mathbf{f}_j*\rho_1$ *on* B_j, *then* $\rho_0=\mathbf{f}_k*\rho_1$ *on* B_k.

(iii) Let $\mathbf{f}^{(2)}=\mathbf{f}_1o\cdots o\mathbf{f}_P$, then $Q\mathbf{f}^{(2)}=\mathbf{f}^{(2)}Q$.

Proof: (i) We have to show that if $Q_0(j)=Q_1(j)=k$ with Q_0, $Q_1\in G$, then $Q_0\mathbf{f}_jQ_0^{-1}=Q_1\mathbf{f}_jQ_1^{-1}$. Let $Q=Q_0^{-1}Q_1$. We have $Q(j)=j$ and we want to show $\mathbf{f}_jQ=Q\mathbf{f}_j$. Note that by construction $\mathbf{f}_j$ satisfies

$$\int_0^{f_j(r_j,w_j)}\rho_1(s,w_j)s^2ds=\int_0^{r_j}\tilde{\rho}_0(s,w_j)s^2ds \tag{63}$$

where we have denoted $\mathbf{f}_j=f_j(r_j,w_j)\mathbf{u}_{r_j}(w_j)$ in spherical coordinates (r_j,w_j) centered in $\mathbf{y}_j$, and where $\tilde{\rho}_0=\rho_0$ on $B(\mathbf{y}_j,\epsilon_1)$ ($\tilde{\rho}_0$ will otherwise satisfies similar properties as in Lemma IV.2). It is then easy to verify, using $Q(j)=j$, that $\rho_1(Q(r_j,w_j))=\rho_1(r_j,w_j)$ and thus for $\tilde{\rho}_0$. In a similar way as for Lemma IV.2, if we define Qw_j such that $Q(r_j,w_j)=(r_j,Qw_j)$ (since $\mathbf{0}$ and $\mathbf{y}_j$ are both invariant by Q), we obtain $f_j(r_j,w_j)=f_j(r_j,Qw_j)$ and $Q\mathbf{u}_{r_j}(w_j)=\mathbf{u}_{r_j}(Qw_j)$; thus $\mathbf{f}_jQ=Q\mathbf{f}_j$. Commutation comes from the fact that $B(\mathbf{y}_k,\epsilon)\cap B(\mathbf{y}_l,\epsilon)=\varnothing$ for $k\neq l$.

(ii) $\mathbf{f}_k*\rho_1=|D\mathbf{f}_k|\rho_1(\mathbf{f}_k)$. From $\mathbf{f}_kQ=Q\mathbf{f}_j$ we deduce that $|D\mathbf{f}_k|(Q)=|D\mathbf{f}_j|$. Then $(\mathbf{f}_k*\rho_1)(Q)=|D\mathbf{f}_j|\rho_1(\mathbf{f}_kQ)=|D\mathbf{f}_j|\rho_1(Q\mathbf{f}_j)=|D\mathbf{f}_j|\rho_1(\mathbf{f}_j)=\mathbf{f}_j*\rho_1=\rho_0$; hence $\mathbf{f}_k*\rho_1=\rho_0$.

(iii) Thus $Q\mathbf{f}^{(2)}=\mathbf{f}_{Q(1)}o\cdots o\mathbf{f}_{Q(P)}Q$; but Q is one-to-one and lets $K=\{\mathbf{y}_1,\ldots,\mathbf{y}_P\}$ globally invariant, and the $(\mathbf{f}_j)$ are commuting. Hence $\mathbf{f}_{Q(1)}o\cdots o\mathbf{f}_{Q(P)}=\mathbf{f}_1o\cdots o\mathbf{f}_P=\mathbf{f}^{(2)}$. ■

Construction of $\mathbf{f}^{(3)}$: We have yet to solve the Jacobian problem $\rho_0=\mathbf{f}*\rho_1$ where now ρ_0,ρ_1 are equal around each cusp and outside some ball $B(\mathbf{0},R)$, and satisfy the symmetry conditions (61). The following construction shows how to do this by a symmetrization process on the field $\mathbf{X}_t$ used in Theorem III.1.

Let $\mathbf{V}$ be the solution of $\mathrm{div}(\mathbf{V})=\rho_0-\rho_1$ as in Lemma III.2, and compensated by a regular function so that $\mathrm{D}^k\mathbf{V}(\mathbf{y}_j)=0$ for $k=0,1,2$. Let $\mathbf{X}_t=\mathbf{W}/\rho_t$, where

$$\mathbf{W}=\frac{1}{|G|}\sum_{Q\in G} Q\mathbf{V}Q^{-1} \tag{64}$$

and where $|G|$ denotes the cardinal of G. Then note that for all $Q\in G$, $\mathbf{X}_tQ=Q\mathbf{X}_t$ [this is true for $\mathbf{W}$, and $\rho_t(\mathrm{Q}\mathbf{x})=\rho_t(\mathbf{x})$]. We have also $\mathrm{div}(Q\mathbf{V}Q^{-1})=\mathrm{div}(\mathbf{V})(Q^{-1})=(\rho_0-\rho_1)(Q^{-1})=\rho_0-\rho_1$; thus $\mathrm{div}(\mathbf{W})=\rho_0-\rho_1$. By integration of $\mathbf{X}_t$ we obtain $\mathbf{f}_t$, solution of the Jacobian problem $\rho_0=\mathbf{f}_t*\rho_t$.

We can also claim that $\mathbf{f}_tQ=Q\mathbf{f}_t$ for all $t\in[0,1]$, because both $\mathbf{f}_tQ$ and $Q\mathbf{f}_t$ satisfy the same differential equation with same initial condition.

Hence $\mathbf{f}^{(3)}=\mathbf{f}_{\{t=1\}}$ is a solution that commutes with any $Q\in G$. The cusp and infinite behaviors are unchanged by $\mathbf{f}^{(3)}$, by construction.

Finally, the solution for Theorem IV.1 is obtained by composition of the three previous functions, i.e., $\mathbf{f}^{(1)}o\,\mathbf{f}^{(2)}o\,\mathbf{f}^{(3)}$. ■

V. APPLICATIONS

A. Stability H^1 for the operator $\hat{T}_f$

We recall the definition of a linear operator on $L^2(\mathbb{R}^{3N})$ which has been introduced in Ref. 7 (see also Ref. 5).

Definition V.1: If f is a C^1*-diffeomorphism from* $\mathbb{R}^3-K$ *onto itself, where K is finite, we define the linear operator* $\hat{\mathbf{T}}_f$ *from* $L^2(\mathbb{R}^{3N})$ *onto itself by*

$$(\hat{\mathbf{T}}_f\Psi)(\mathbf{x}_1,\ldots,\mathbf{x}_N)=\prod_{i=1}^{N}|\mathrm{D}\mathbf{f}(\mathbf{x}_i)|^{1/2}\Psi(\mathbf{f}(\mathbf{x}_1),\ldots,\mathbf{f}(\mathbf{x}_N)). \tag{65}$$

Note that $\hat{\mathbf{T}}_f$ is a tensor product of N identical (unitary) operators: $\hat{\mathbf{T}}_f=\hat{\mathbf{t}}_f\otimes\cdots\otimes\hat{\mathbf{t}}_f$ where $(\hat{\mathbf{t}}_f\phi)(\mathbf{x})=|D\mathbf{f}(\mathbf{x})|^{1/2}\phi(\mathbf{f}(\mathbf{x}))$.

Proposition V.1: $\hat{\mathbf{T}}_f$ *is an invertible unitary operator of* $L^A_2(\mathbb{R}^{3N})$*, i.e., for all* $\Psi\in L^2_A(\mathbb{R}^{3N})$

$$\int_{R^{3N}}|\hat{\mathbf{T}}_f\Psi|^2=\int_{R^{3N}}|\Psi|^2 \tag{66}$$

and $(\hat{\mathbf{T}}_f)^{-1}=\hat{\mathbf{T}}_{f^{-1}}$.

Proof: Immediate, using the change of variables theorem. ■

Lemma V.1: Let f be a C^1*-diffeomorphism from* $\mathbb{R}^3-K$ *onto itself where K is finite, and let* $q(\mathbf{x})=|\mathrm{Df}(\mathbf{x})|$. *We suppose furthermore that*

(i) $\exists C\geqslant 0,\ \forall\mathbf{x},\ |\nabla q(\mathbf{x})|\leqslant \mathrm{Cq}(\mathbf{x})$;

(ii) *the differential* $\mathrm{D}\mathbf{f}(\mathbf{x})$ *has bounded coefficients on* $\mathbb{R}^3$.

Then $\hat{\mathbf{T}}_f$ *is continuous for the* H^1*-norm, and in particular* $\forall\Psi\in H^1(\mathbb{R}^{3N})$, $\hat{T}_f\Psi\in H^1(\mathbb{R}^{3N})$.

Proof: We just showed that $\hat{\mathbf{t}}_f$ is stable on $H^1(\mathbb{R}^3)$. In the distributional sense on $\mathbb{R}^3-K$ and for $\psi\in H^1(\mathbb{R}^3)$, we have

$$\nabla(\hat{\mathbf{t}}_f\psi)=\frac{1}{2}\frac{\nabla q(\mathbf{x})}{q(\mathbf{x})}\hat{\mathbf{t}}_f\psi+\mathrm{D}\mathbf{f}^{\mathrm{T}}(\mathbf{x})\hat{\mathbf{t}}_f(\nabla\psi). \tag{67}$$

\Note that the second member is in $L^2(\mathbb{R}^3)$ using (i) and (ii). This equality is still true in the distributional sense on $\mathbb{R}^3$, because $\hat{\mathbf{t}}_f\psi$ is in $L^2(\mathbb{R}^3)$. Estimations for the H^1-norm can then be obtained. ■

The following justifies our interest in obtaining a peculiar behavior of the solution of the Jacobian problem at infinity.

Proposition V.2: Let ρ_0,ρ_1 be two densities chosen as in Theorem III.1 and such that $\nabla\rho_i/\rho_i$ be bounded for $i=0,1$. Let $\mathbf{f}$ be a solution of the Jacobian problem as in Theorem III.1. Then $\hat{\mathbf{T}}_f$ *and* $(\hat{\mathbf{T}}_f)^{-1}$ *are both H^1-stable.*

Proof: From Corollary III.1 we have $D\mathbf{f}$ and $D\mathbf{f}^{-1}$ bounded. Then from $q=|D\mathbf{f}|=\rho_0/\rho_1(\mathbf{f})$ we have by differentiation that

$$\frac{\nabla q}{q}=\frac{\nabla\rho_0}{\rho_0}-D\mathbf{f}^{\mathsf{T}}\,\frac{\nabla\rho_1}{\rho_1}, \tag{68}$$

and thus is bounded. Thus, $\nabla q_1/q_1$ is bounded, where $q_1=|D(\mathbf{f}^{-1})|=1/q(\mathbf{f}^{-1})$. ■

B. Decomposition theorem

The following theorem is similar to Theorem 3.1 stated in Ref. 5, but with regularity H^1.

Theorem V.1: *Let $K=\{\mathbf{x}_1,...,\mathbf{x}_P\}\subset\mathbb{R}^3$ and ρ_0,ρ_1 be two density functions on $\mathbb{R}^3$, as in theorem III.1 and such that $\nabla\rho_i/\rho_i$ be bounded for $i=0,1$. Let $\Psi_0\in H^1_A(\mathbb{R}^{3N})$. Then $\Psi_0\mapsto\rho_0$ if and only if $\exists\mathbf{f}$ a C_1-diffeomorphism, with $D\mathbf{f}(\mathbf{x})$ and $Df(\mathbf{x})^{-1}$ bounded, and $\exists\Psi_1\in H^1_A(\mathbb{R}^{3N})$,*

$$\begin{cases}\Psi_0=\hat{\mathbf{T}}_f\Psi_1\\ \Psi_1\mapsto\rho_1\\ \rho_0=\mathbf{f}*\rho_1\end{cases}$$

Proof: If $\Psi_0\mapsto\rho_0$ then choose $\mathbf{f}$ a solution of the Jacobian problem $\rho_0=\mathbf{f}*\rho_1$ given by Theorem III.1, and $\Psi_1=(\hat{\mathbf{T}}_f)^{-1}\Psi_0$. We know that $\Psi_0\in H^1_A(\mathbb{R}^{3N})$ by Proposition V.2. Conversely, from $\Psi_0=\hat{\mathbf{T}}_f\Psi_1$ we obtain $\rho_{\Psi_0}=\mathbf{f}*\rho_{\Psi_1}$; thus $\rho_{\Psi_0}=\mathbf{f}*\rho_1=\rho_0$. ■

Note that a choice of $\mathbf{f}$ solution of $\rho_0=\mathbf{f}*\rho_1$ uniquely determines the wave function Ψ_1.

1. Expression for the energy

For the energy terms, we have also similar formula as in our previous paper.[5] We first recall the definition of the 2-density:

$$d^2_\Psi(\mathbf{x}_1,\mathbf{x}_2)=\frac{N(N-1)}{2}\int_{\mathbb{R}^{3N-6}}|\Psi(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3,\ldots,\mathbf{x}_N)|^2 d\mathbf{x}_3\cdots d\mathbf{x}_N \tag{69}$$

and of the first order reduced density matrix (1−RDM):

$$D^1_\Psi(\mathbf{x}_1,\mathbf{x}_1')=N\int_{\mathbb{R}^{3N-3}}\Psi(\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N)\Psi(\mathbf{x}_1',\mathbf{x}_2,\ldots,\mathbf{x}_N)d\mathbf{x}_2\cdots d\mathbf{x}_N. \tag{70}$$

If $\Psi_0=\hat{\mathbf{T}}_f\Psi_1$ and $q=|D\mathbf{f}|$ then (see Refs. 8 and 13):

$$d^2_{\Psi_0}(\mathbf{x}_1,\mathbf{x}_2)=q(\mathbf{x}_1)q(\mathbf{x}_2)d^2_{\Psi_1}(\mathbf{f}(\mathbf{x}_1),\mathbf{f}(\mathbf{x}_2)), \tag{71}$$

$$D^1_{\Psi_0}(\mathbf{x}_1,\mathbf{x}_1')=q(\mathbf{x}_1)^{1/2}q(\mathbf{x}_1')^{1/2}D^1_{\Psi_1}(\mathbf{f}(\mathbf{x}_1),\mathbf{f}(\mathbf{x}_1')). \tag{72}$$

Various expressions for the energy $E[\hat{\mathbf{T}}_f\Psi_1]$ can then be obtained. For instance, let us denote $\mathbf{g}=\mathbf{f}^{-1}$, $\mathbf{p}=[\nabla(q^{1/2})]/q^{1/2}$, $\overline{\mathbf{p}}=\mathbf{p}(\mathbf{g})$, $\overline{\mathrm{D}\mathbf{f}}=\mathrm{D}\mathbf{f}(\mathbf{g})$, and $(\cdot,\cdot)$ for the scalar product. Let $\Psi_1\in H^1_A(\mathbb{R}^{3N})$ and $\rho_1=\rho_{\Psi_1}$. Then by elementary calculations, with H given by relation (1), we can separate the information in f and in Ψ_1 as follows:

$$E[\hat{\mathbf{T}}_f\Psi_1]=\int_{\mathbb{R}^3}|\overline{\mathbf{p}}|^2\rho_1+\int_{\mathbb{R}^3}(\overline{\mathbf{p}},\overline{\mathrm{D}\mathbf{f}}^{\mathsf{T}}\nabla\rho_1)+N\int_{\mathbb{R}^{3N}}|\overline{\mathrm{D}\mathbf{f}}(\mathbf{x}_1)^{\mathsf{T}}\nabla_{x_1}\Psi_1(\mathbf{x}_1,\ldots,\mathbf{x}_N)|^2d\mathbf{x}_1\cdots d\mathbf{x}_N$$
$$+\int_{\mathbb{R}^3}v(\mathbf{g})\rho_1+\int_{\mathbb{R}^6}\frac{d^2_{\Psi_1}(\mathbf{x}_1,\mathbf{x}_2)}{|\mathbf{g}(\mathbf{x}_1)-\mathbf{g}(\mathbf{x}_2)|}\,d\mathbf{x}_1d\mathbf{x}_2\,. \tag{73}$$

2. Deformed Hamiltonian

We can also write $E[\hat{\mathbf{T}}_f\Psi]=\langle\Psi,H_f\Psi\rangle$ where $H_f=\hat{\mathbf{T}}_f^{-1}H\hat{\mathbf{T}}_f$ is the ''deformed'' Hamiltonian and is given by the analytic formula

$$H_f=\sum_{i=1}^{N}-\Delta_f(i)+\sum_{i=1}^{N}v(\mathbf{g}(\mathbf{x}_i))+\sum_{1\leqslant i<j\leqslant N}\frac{1}{|\mathbf{g}(\mathbf{x}_i)-\mathbf{g}(\mathbf{x}_j)|}, \tag{74}$$

where $\mathbf{g}=\mathbf{f}^{-1}$ and $\Delta_f(i)$ is the operator Δ_f applied on $\mathbf{x}_i$, with

$$\Delta_f=\frac{\Delta q_1(\mathbf{g})}{q_1(\mathbf{g})}+\sum_{j=1,2,3}\left\{\Delta f_j(\mathbf{g})+2\left(\frac{\nabla q_1(\mathbf{g})}{q_1(\mathbf{g})},\nabla f_j(\mathbf{g})\right)\right\}\partial_j+\sum_{j,k=1,2,3}(\nabla f_j(\mathbf{g}),\nabla f_k(\mathbf{g}))\partial_j\partial_k, \tag{75}$$

where we have denoted $\mathbf{f}=(f_1,f_2,f_3)$, $q_1=|\mathrm{D}\mathbf{f}|^{1/2}$, and $\nabla=(\partial_1,\partial_2,\partial_3)$ in the inner basis of $\mathbb{R}^3$ (compare with the expression given in Ref. 8, page 666.)

C. Propositions for a numerical resolution

1. The general scheme

We indicate here how to solve numerically the Jacobian problem in $\mathbb{R}^3$ with P invariant points $\{\mathbf{x}_1,\ldots,\mathbf{x}_P\}$ for two classical types of density representations (Slater type and Gaussian type). Of course it would be possible to consider other representations of the density functions. With some hypothesis on the behavior at infinity, we can use directly the Moser's procedure with $\mathbf{X}_t=\mathbf{V}/\rho_t$ and where $\mathbf{V}$ is the solution of $\mathrm{div}(\mathbf{V})=\rho_0-\rho_1$ given in Lemma III.2 and corrected by Lemma II.1 so that $\mathbf{V}(\mathbf{x}_i)=\mathbf{0}$ (and if possible with a symmetrized $\mathbf{X}_t$ as for the construction of $\mathbf{f}^{(3)}$ in the proof of Theorem IV.1). So we do not have to construct radial solutions around cusps or at infinity; in particular we do not use Lemma III.1 for instance. Hence, in these specific cases, we only use a linear algorithm to calculate the flux $\mathbf{X}_t$.

We remind the reader that $\mathbf{X}_t=\mathbf{V}/\rho_t$ and

$$\mathrm{D}\mathbf{X}_t=\frac{\mathrm{D}\mathbf{V}}{\rho_t}-\mathbf{X}_t\otimes\frac{\nabla\rho_t}{\rho_t}. \tag{76}$$

Thus, in order to apply Theorem II.1, we shall require that the density functions be such that

(i) $|\mathbf{V}/\rho_t|=o(1)$ when $\mathbf{x}\to\infty$ (uniform in $t\in[0,1]$);
(ii) $\nabla\rho_i/\rho_i$ and $\|\mathrm{D}\mathbf{V}/\rho_t\|$ bounded (uniformly in $t\in[0,1]$ and $\mathbf{x}\in\mathbb{R}^3$).

The final step is then the integration of $d\mathbf{f}_t/dt=\mathbf{X}_t(\mathbf{f}_t)$ over $t\in[0,1]$, which we do not discuss here (see Remark 3 of Sec. III D).

2. Use of a Slater-type basis set

In the case we want to expand the densities in a Slater-type basis set, i.e., with basis functions of the form $r^m e^{-\alpha\tau}$ around each nuclei, a density ρ is assumed to have the following form:

$$\rho(\mathbf{x})=\sum_{i=1}^{P}\sum_{j=1}^{M_i} P_{i,j}(r_i)e^{-\alpha_{i,j}r_i}, \tag{77}$$

where $r_i=|\mathbf{x}-\mathbf{x}_i|$ is the Euclidian distance between $\mathbf{x}$ and the nuclei $\mathbf{x}_i$, $\alpha_{i,j}>0$ and for simplicity we assume that $P_{i,j}$ is polynomial.

We first state a more general lemma that ensures a correct infinite behavior.

Lemma V.2: Suppose that ρ_0,ρ_1 are regular except eventually on $K=\{\mathbf{x}_1,...,\mathbf{x}_P\}$ (with $\nabla\rho_i$ bounded) and satisfy, when $|\mathbf{x}|\to\infty$, to

$$\rho_0(\mathbf{x})\sim\rho_1(\mathbf{x})\sim C(w)r^{\beta}\mathbf{e}^{-\alpha r}, \tag{78}$$

$$\rho_0(\mathbf{x})-\rho_1(\mathbf{x})=o(r^{\beta-1}\mathbf{e}^{-\alpha r}) \tag{79}$$

and furthermore to

$$|\nabla\rho_0| \quad \textit{and} \quad |\nabla\rho_1|=O(r^{\beta}e^{-\alpha r}), \tag{80}$$

$$\nabla(\rho_0-\rho_1)=o(r^{\beta-1}e^{-\alpha r}). \tag{81}$$

Take $\mathbf{V}$ as in Lemma III.2 [eventually locally modified so that $\mathbf{V}(\mathbf{x}_i)=0$]. If $\int\rho_0=\int\rho_1$, then

(i) $|\mathbf{V}/\rho_t|=o(1)$, *and $\nabla\rho_t/\rho_t$ and $\|\mathrm{D}\mathbf{V}/\rho_t\|$ are bounded*;
(ii) $\hat{\mathbf{T}}_f$ *and its inverse are both H^1-stable.*

Proof: We just give a sketch of proof for $|\mathbf{V}/\rho_t|=o(1)$. For the function g of Lemma III.2 we can suppose that $\mathrm{supp}(g)\subset[-1,1]$. First note that if $|f(\mathbf{r})|\leqslant Cr^{\gamma}e^{-\alpha r}$ ($\alpha>0,C>0$), then, with $r=(x^2+y^2+z^2)^{1/2}$,

(a) $\int_{-\infty}^{+\infty}|f(x',y,z)|dx'\leqslant C_2 r^{\gamma+1/2}e^{-\alpha r}$, for $|x|\leqslant 1$,
(b) $\int_{x}^{+\infty}|f(x',y,z)|dx'\leqslant (C/\alpha)r^{\gamma+1/2}e^{-\alpha r}$, for $x\geqslant 1$

(for some constant $C_2>0$ independent of γ and α; the case $\int_{-\infty}^{x}|f|dx'$, $x\leqslant -1$ is similar).

From these bounds and using Eq. (79) it follows that, with $\mathbf{V}=(\mathrm{V}_1,\mathrm{V}_2,\mathrm{V}_3)$, we have $|V_1(\mathbf{x})|=o(r^{\beta-1/2}e^{-\alpha r})$. In particular $V_1/\rho_t=o(r^{-1/2})=o(1)$. Thus using (a) and (b) anew we can show that $V_2(\mathbf{x})=o(r^{\beta}e^{-\alpha r})$ at infinity; thus $V_2/\rho_t=o(1)$.

Finally for V_3, when $z\to-\infty$ and $|x|,|y|\leqslant 1$, the bound comes from the bound of V_2. The case $z\to+\infty$ is similar because $\int(\rho_0-\rho_1)=0$ and $V_3(x,y,z)=-V_3(x,y,-z)$. ■

Thus in the case we are working with densities expanded in a Slater-type basis set as in Eq. (77) we see easily that a necessary and sufficient condition for the application of the above Lemma is just that

$$\rho_0(\mathbf{x})\sim\rho_1(\mathbf{x}), \quad |\mathbf{x}|\to\infty. \tag{82}$$

We also have for $k=0,1$

$$\rho_k(\mathbf{x})\sim r^m e^{-\alpha r}\left(\sum_{i=1}^{P_0} c_i^{(k)}e^{-\alpha\langle x,x_i\rangle}\right), \tag{83}$$

where (α,m) correspond, respectively, to the minimum of the coefficients $(\alpha_{i,j})$ and to the maximum of the degrees of the $(P_{i,j})$, and with the corresponding coefficients $c_i^{(k)}$. Hence $\rho_0 \sim \rho_1$ if and only if $c_i^{(0)} = c_i^{(1)}$ for all $i = 1,\ldots,P_0$.

In order to use Lemma III.2, we want also to be able to quickly integrate the following integrals:

$$\int_{-\infty}^{x} \rho_i(x',y,z)dx',$$

$$\int_{-\infty}^{+\infty}\int_{-\infty}^{y} \rho_i(x',y',z)dx'dy',$$

$$\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{z} \rho_i(x',y',z')dx'dy'dz'.$$

But drawback of the above Slater basis set is that the integration is not immediate. So we consider also the use of a Gaussian basis set.

3. Use of a Gaussian basis set

Denoting $\mathbf{x}=(x,y,z)$ and $r^2 = x^2+y^2+z^2$, we choose the Gaussian basis set $x^p y^q z^r e^{-\alpha r^2}$ where p,q,r are non-negative integers and $\alpha > 0$. The final form of a function ρ is thus assumed to be

$$\rho(\mathbf{x}) = \sum_{i=1}^{P}\sum_{j=1}^{M} P_{i,j}(x,y,z)e^{-\alpha_{i,j}|\mathbf{x}-\mathbf{x}_i|^2}, \tag{84}$$

where $P_{i,j}(x,y,z)$ are polynomials (such that ρ be strictly non-negative on $\mathbb{R}^3$). For calculation of the integrals we have to integrate $\int_{-\infty}^{x} t^m e^{-\alpha t^2} dt$ for a finite number of pairs (m,α). Thus we need only a fast integration program for

$$I(x) = \int_{-\infty}^{x} e^{-t^2} dt. \tag{85}$$

(Chemists have already developed and computed fast algorithms for such integrals, for *ab initio* programs.)

The densities ρ_0, ρ_1 developed in this basis set have the following asymptotic behavior when $r = |\mathbf{x}| \to \infty$ (for $k = 0,1$):

$$\rho_k(\mathbf{x}) \sim \sum_{i=1}^{P_0} P_i^{(k)}(\mathbf{x}) e^{-\alpha|\mathbf{x}-\mathbf{x}_i|^2}, \tag{86}$$

where the (P_i) are homogeneous polynomial of order q, for some $q \in \mathbb{N}$ and where $>$a is the smallest of the $\alpha_{i,j}$. [It is not equivalent to a $P(\mathbf{x})e^{-\alpha r^2}$, in general]. In order that (I) and (II) be satisfied we can then show that it is sufficient to have

$$\rho_0(x) \sim \rho_1(\mathbf{x}), \quad |\mathbf{x}| \to \infty. \tag{87}$$

This is realized if and only if $P_i^{(0)} = P_i^{(1)}$, for all $i = 1,\ldots,P_0$.

D. Remarks

(1) For solving the divergence problem, $\mathrm{div}(\mathbf{V})=\rho_0-\rho_1$, we could be tempted to use the solution of the Laplacian problem $\Delta u=\rho_0-\rho_1$, i.e., $u=-(1/4\pi|x|)*(\rho_0-\rho_1)$ (where $*$ stands for the convolution product), and then take $\mathbf{V}=\nabla u$ plus eventually a rotational term as in Ref. 17.

The problem is that ∇u has an asymptotic behavior with terms of the form $1/|\mathbf{x}|^n$ which we were not able to eliminate by a simple rotational. We recall that in the case the densities have an exponential fall-off, we also want $\mathbf{V}$ to have an exponential fall-off. Use of Dacorogna and Moser's procedure,[17] even after scaling $\mathbb{R}^3$ to the ball, lead to hardly constructible solutions (the densities vanishes at the border).

(2) Exact density functions have a Slater type decreasing at infinity, so the Gaussian basis set appears as a bad representation of the densities.

However, we think it is not so important for numerical purpose because the process of solving the Jacobian problem is mainly to determine a deformation $\mathbf{f}$ and then to apply $\hat{\mathbf{T}}_f$ to a wave function Ψ_1. The minimization of the energy $E[\Psi_2]$ where $\Psi_2=\hat{\mathbf{T}}_f\Psi_1$ can be done with respect to parameters put in ρ_2, with ρ_1 a given fictive density and $\mathbf{f}$ a solution of $\rho_2=\mathbf{f}*\rho_1$ taken as in Sec. V C.

Because we impose that $\rho_1\sim\rho_2$ at infinity [$\mathbf{f}(\mathbf{x})\sim\mathbf{x}$ at infinity] the infinite behavior of Ψ_2 can only be improved by another choice of Ψ_1. But the main numerical hope of the above process is to obtain a good representation around the molecule via density optimization.

(3) The procedure of Moser is a linearization procedure. Thus when $\rho_0-\rho_1$ is small, and with $\mathbf{V}$ a solution of $\mathrm{div}\,\mathbf{V}=\rho_0-\rho_1$ satisfying (I) and (II) in Sec. V C, we can take the approximation $\mathbf{f}_{\mathrm{app}}(\mathbf{x})=\mathbf{x}+\mathbf{h}(\mathbf{x})$ where $\mathbf{h}=\mathbf{V}/\rho_1$, and together with an approximated Jacobian $J_{\mathrm{app}}=\rho_0/\rho_1(\mathbf{f}_{\mathrm{app}})$ we may define analytically an approximate $\hat{\mathbf{T}}_{f\,\mathrm{app}}$. Thus the integration of $\mathbf{X}_t$ can be avoided for small deformations (or closed densities).

(4) One of the problem of the LST procedure proposed by Kryachko, Ludeña, and co-workers is the calculation and minimization of the energy because the expression for $\Psi_2=\hat{\mathbf{T}}_f\Psi_1$ is not analytically integrable in general. A fully numerical program then must be used, which in general is not easy. Use of a Monte Carlo procedure is under study.

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Localization in single Landau bands

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We consider a single-band approximation to the random Schrödinger operator in an external magnetic field. The random potential is taken to be constant on unit squares and i.i.d. on each square with a bounded distribution. We prove that the eigenstates corresponding to energies at the edges of the Landau band are localized. This is an important ingredient in the theory of the Quantum Hall Effect. © *1996 American Institute of Physics.* [S0022-2488(96)03403-1]

I. INTRODUCTION

We consider a two-dimensional infinite system of noninteracting electrons moving in a uniform magnetic field of strength B and a random potential V. In the symmetric gauge the vector potential is given by $A(x)=[(B/2)x_2,-(B/2)x_1]$, $x=(x_1,x_2)\in\mathbb{R}^2$ and the Hamiltonian is

$$H=(-i\nabla-A(x))^2+V(x). \tag{1.1}$$

The effect of the random potential is to broaden the Landau levels into bands. When the potential is bounded and the magnetic field is strong enough these bands do not overlap. It is generally expected that the states lying near the edges of the bands are exponentially localized and the corresponding spectrum is pure point.[1,2] Near the center of the bands the situation is more controversial. One possibility is that there exist truly extended states in some finite-energy range. Instead, it could happen that the localization length remains finite for all energies, except for one value, where it diverges (e.g., like a power law).[3–5] This picture is essential for understanding the occurrence of plateaus in the conductivity as a function of the magnetic field measured in Quantum Hall experiments. In this connection, Kunz[6] has shown that the localization length must be infinite for at least one energy in each band, assuming that the states with energy at the edges of the bands are exponentially localized.

Rigorous results on random Schrödinger operators with magnetic fields are still rare. A few exact results concerning the density of states have been obtained.[7–11] In the present paper we address the problem of proving that the energies at the edges of the bands correspond to localized states. For the random potential we choose a model already considered in previous works in the absence of magnetic field.[12,13] The two-dimensional plane is decomposed into unit squares, on each of which the potential is taken to be constant. The values of the potential on the squares are i.i.d.s with a bounded probability distribu-

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tion are stated in Sec. II. When the magnetic field is strong it is reasonable to consider only the projections of the Hamiltonian onto each Landau level and to neglect the cross terms. The Hamiltonian restricted to the nth level is

$$H_n = B(2n+1)P_n + P_n V P_n, \tag{1.2}$$

where P_n denotes the projection onto the level. The term $B(2n+1)P_n$ comes from the decomposition of the purely kinetic part of (1.1) and can be dropped as it modifies the energy only by a constant. Note that the resulting Hamiltonian is a random integral operator instead of a differential operator and that the kernels of P_n are known explicitly.

Our main result is that, for the Hamiltonian H_n, the states at the edges of the corresponding band are exponentially localized. For simplicity in this paper, we restrict ourselves to the case $n=0$. Our proof depends on a modification of a theorem of Von Dreifus and Klein.[14] This theorem is only stated here and the proof is given in a companion paper,[15] which deals with the easier case when the distribution of the random potential is unbounded, e.g., Gaussian. In this paper we concentrate on the case when the distribution is bounded.

We now describe the main features of our analysis. In Sec. II we prove (see Lemma 2.3) that it is enough to show that, because of the special form of the Hamiltonian, the wave function decays exponentially on the lattice. This simplification enables us to use the methods of Spencer,[16] Von Dreifus and Klein[14] for lattice models. However, the fact that the model is formulated in the continuum makes the model considerably more difficult to analyze and nontrivial modifications are required, because the relevant Green's identity (3.3) is more difficult to handle. These are described in Sec. III. This section also contains the basic step in the proof of localization, Theorem 3.1, which as in Ref. 14 reduces to two main conditions (P1) and (P2). The proof of this theorem, which does not depend on the boundedness of the potential, can be found in Ref. 15. In Sec. IV we verify the conditions (P1) and (P2). The condition (P1) is an estimate of the type first proved by Wegner[17] on the probability that an energy E lies within some small distance from the spectrum of the Hamiltonian for a finite box. This requires bounds on the integrated density of states in finite boxes. Our Hamiltonian, when restricted to a finite box, turns out to be a Hilbert–Schmidt operator. Therefore the spectrum has an accumulation point at zero that requires an adaptation of Wegner's argument. This feature is intimately related to the fact that the original Laudau levels are infinitely degenerate. Condition (P2) states that there exist a length scale L such that the Green's function for a box of size L decays exponentially fast, with a high probability depending on L. For bounded potentials the usual proofs in the absence of a magnetic field use the fact that the density of states is exponentially small near the band edge. These are the so-called Lifshitz tails. Here we verify (P2) directly using a Combes–Thomas argument[18] and the explicit form of the eigenfunctions of P_0. The main part of the paper is concerned with this problem.

While this paper was being written we received a preprint by Combes and Hislop[19] with similar results, and recently W.-M. Wang also obtained results along the same lines.[20] We wish to compare briefly these papers with the present one.

In Refs. 19 and 20, localization is proved for the Hamiltonian (1.1) in the case where the random potential V is sufficiently smooth. Mathematical techniques of percolation theory and microlocal analysis are used (also see Ref. 21). The regime studied is that of large magnetic field, that is, the magnetic length ($\approx 1/\sqrt{B}$) has to be smaller than the characteristic length over which the potential varies. In this situation the one-band problem is well approximated by the classical effective Hamiltonian $(2n+1)B+V(x)$. As a consequence the problem is mapped onto a percolation problem for the equipotential lines of $V(x)$. As far as we know this physical picture goes back to Ref. 22.

In contrast, the effective Hamiltonian used in this paper for the single band problem is $P_n V P_n$, and therefore the kinetic energy that is contained in P_n is not quenched. As a consequence our main theorem holds for arbitrary strength of the magnetic field (for the single band). In particular, localization at the band edges occurs even when the magnetic length is large with

respect to the characteristic length of variation of V, that is, when the percolation picture loses its validity. Of course, we have neglected the interband coupling, and if that is taken into account a condition on the strength of B would be necessary. However, it is not clear what the optimal condition would be. We remark that in the present study the random potential is of a different kind from that in Refs. 19 and 20 since it is discontinuous.

II. THE HAMILTONIAN

Let ω_n, $n\in\mathbb{Z}^2$ be i.i.d. random variables with distribution given by a probability measure μ with supp $\mu=X=[a,b]$, a compact interval in $\mathbb{R}$. We let $\Omega = X^{\mathbb{Z}^2}$ and $\mathbb{P} = \Pi_{n\in\mathbb{Z}^2}\mu$. For $m\in\mathbb{Z}^2$ let τ_m be the measure preserving automorphism of Ω defined by

$$(\tau_m\omega)_n=\omega_{n-m}. \tag{2.1}$$

The group $\{\tau_m : m\in\mathbb{Z}^2\}$ is ergodic for the probability measure $\mathbb{P}$.

Let $\mathscr{H}=L^2(\mathbb{R}^2)$ and let $\mathscr{H}_0$ be the eigenspace corresponding to the lowest eigenvalue (first Landau level) of the Hamiltonian H_0 defined in (1.1). Let P_0 be the orthogonal projection onto $\mathscr{H}_0$. The Hamiltonian for our model is the operator on $\mathscr{H}_0$, given by

$$H(\omega)=P_0V(\cdot,\omega)=P_0V(\cdot,\omega)P_0, \tag{2.2}$$

where $\omega\in\Omega$ and

$$V(x,\omega)=\sum_{n\in\mathbb{Z}^2}\mathbf{1}_{\Lambda_1(n)}(x)\omega_n, \tag{2.3}$$

$\Lambda_1(n)$ being the square of the unit side centered at n,

P_0 is an integral operator with kernel

$$P_0(x,y)=\frac{2\kappa}{\pi}\exp[-\kappa|x-y|^2+2i\kappa x\wedge y], \tag{2.4}$$

where $\kappa=B/4$. Since we shall be using both the Euclidean norm and the maximum norm on $\mathbb{R}^2$, we shall use the following convention:

$$|x|=(x_1^2+x_2^2)^{1/2},\quad \|x\|=\max(|x_1|,|x_2|),$$

and for $L>0$ and $x\in\mathbb{R}^2$,

$$B(x,L)=\{y\in\mathbb{R}^2:|y-x|\leqslant L\},\quad \Lambda_L(x)=\{y\in\mathbb{R}^2:\|y-x\|\leqslant \tfrac{1}{2}L\}.$$

Let $\{U_y : y\in\mathbb{R}^2\}$ be the family of unitary operators on $\mathscr{H}$ corresponding to the magnetic translations:

$$(U_yf\ )(x)=e^{2i\kappa y\wedge x}f(x+y). \tag{2.5}$$

Then for $n\in\mathbb{Z}^2$,

$$U_nH(\omega)U_n^{-1}=H(\tau_n\omega). \tag{2.6}$$

Note that $[P_0,U_y]=0$ for all $y\in\mathbb{R}^2$, so that $U_y\mathscr{H}_0\subset\mathscr{H}0$. Also $U_{y_1}U_{y_2} = e^{2i\kappa y_z\wedge y_1}U_{y_1+y_2}$. The ergodicity of $\{\tau_m : m\in\mathbb{Z}^2\}$ and Eq. (2.6) together imply that the spectrum of $H(\omega)$ and its components are nonrandom (see, for example, Carmona and Lacroix, Theorem V.2.4); it is easy to prove that almost surely the spectrum of $H(\omega)$ is equal to X (cf. Ref. 23).

Lemma 2.1: For P-almost all $\omega\in\Omega$,

$$\sigma(H(\omega))=X. \tag{2.7}$$

Proof: For $\psi\in.\mathscr{H}_0$,

$$a\|\psi\|^2\leqslant\langle\psi,H(\omega)\psi\rangle\leqslant b\|\psi\|^2,$$

and therefore

$$\sigma(H(\omega))\subset X.$$

To prove the reverse inclusion, it is sufficient to prove that[24] for each $E\in X$ and for all $\delta>0$ there exist $\Omega'\subset\Omega$ with $\mathbb{P}(\Omega')>0$ and $\psi\in.\mathscr{H}_0$ with $\|\psi\|=1$, such that for all $\omega\in\Omega'$, $\|(H(\omega)-E)\psi\|<\delta$. Let $E\in X$ and $\psi\in.\mathscr{H}_0$ with $\|\psi\|=1$. For $R>0$, let $\psi_R=P_0\mathbf{1}_{B(0,R)}\psi$. Since $\|\psi-\psi_R\|\leqslant\|\mathbf{1}_{B(0,R)^c}\psi\|$, we can choose R large enough such that $\|\psi_R\|>1/2$. Let $\Omega'=\{\omega:|V(x,\omega)-E|<1/2\delta,\forall x\in B(0,2R)\}$ then clearly $\mathbb{P}(\Omega')>0$. Now

$$\begin{aligned}\|(H(\omega)-E)\psi_R\|^2&=\|P_0(V(\cdot,\omega)-E)P_0\mathbf{1}_{B(0,R)}\psi\|^2\\&\leqslant\|(V(\cdot,\omega)-E)P_0\mathbf{1}_{B(0,R)}\psi\|^2\\&\leqslant\int_{B(0,2R)}dx(V(x,\omega)-E)^2|\psi_R(x)|^2+\int_{B(0,2R)^c}dx(V(x,\omega)-E)^2|\psi_R(x)|^2.\end{aligned} \tag{2.8}$$

If $\omega\in\Omega'$ for the first integral in (2.8), we have

$$\int_{B(0,2R)}dx(V(x,\omega)-E)^2|\psi_R(x)|^2\leqslant\frac{1}{4}\,\delta^2\|\psi_R\|^2\leqslant\frac{1}{4}\,\delta^2. \tag{2.9}$$

We now estimate the second integral in (2.8),

$$|\psi_R(x)|^2=\left(\int_{B(0,R)}dy\;P_0(x,y)\psi(y)\right)^2\leqslant\int_{B(0,R)}dy|P_0(x,y)|^2, \tag{2.10}$$

using the Schwarz inequality and $\|\psi\|=1$. If $x\in B(0,2R)^c$ and $y\in B(0,R)$,

$$|P_0(x,y)|^2\leqslant\frac{4\kappa^2}{\pi^2}\exp[-\kappa R^2-\kappa|x-y|^2], \tag{2.11}$$

so that we have, for the second integral in (2.8),

$$\begin{aligned}\int_{B(0,2R)^c}dx(V(x,\omega)-E)^2|\psi_R(x)|^2&\leqslant\frac{4(b-a)^2\kappa^2}{\pi^2}\,e^{-\kappa R^2}\int_{B(0,R)^c}dx\int_{B(0,R)}dy\;e^{-\kappa|x-y|^2}\\&\leqslant\frac{4(b-a)^2\kappa^2R^2}{\pi}\,e^{-\kappa R^2}\int_{\mathbb{R}^2}dx\;e^{-\kappa|x|^2}<\frac{1}{4}\,\delta^2,\end{aligned} \tag{2.12}$$

if R is sufficiently large. □

The next lemma describes the generalized eigenfunctions of $H(\omega)$. It is proved in Ref. 15 (see Theorem 2.3 and Lemma 6.2) in the case where X may be unbounded.

Lemma 2.2: For almost every $E \in X$ with respect to the spectral measure of H, there exists ψ, a polynomially bounded C^∞ function on $\mathbb{R}^2$ such that $H\psi = E\psi$ and $P_0\psi = \psi$. Moreover, if $\psi \in \mathscr{H}_0$ then E is in the pure-point spectrum of H.

The object of this paper is to prove that almost surely the generalized eigenfunctions of H corresponding to points of X near its edges are localized, in the sense that they decay exponentially and therefore those points are in the pure-point spectrum. The next definition makes precise what is meant by exponential decay.

Definition: $\psi: \mathbb{R}^2 \to \mathbb{R}$ decays exponentially with a rate greater or equal to m if

$$\limsup_{x \to \infty} \frac{\ln|\psi(x)|}{|x|} \leqslant -m. \tag{2.13}$$

The main result of this paper is the following theorem, which is proved in Sec. IV.

Theorem 2.3: If the probability measure corresponding to the i.i.d. random variables ω_n is absolutely continuous with respect to the Lebesgue measure and its density ρ satisfies a Lipshitz condition of order $\sigma > 0$ and supp $\rho = [a,b]$, where $-\infty < a < b < \infty$, then there is a $\Delta > 0$ and $m > 0$, such that almost surely $[a, a+\Delta] \cup [b-\Delta, b]$ is in the pure-point spectrum of H and the corresponding eigenfunctions of H decay with a rate greater or equal to m.

The last lemma of this section provides an important simplifying feature in our proof of localization. It shows that to prove that an eigenfunction decays exponentially it is sufficient to prove that its average on unit squares decays exponentially.

Lemma 2.4: If ψ is a generalized eigenfunction of H and

$$\limsup_{\substack{n \to \infty \\ n \in \mathbb{Z}^2}} \frac{\ln\langle \mathbf{1}_{\Lambda_1(n)}, |\psi| \rangle}{|n|} \leqslant -m, \tag{2.14}$$

then ψ decays exponentially with rate greater or equal to m.

Proof: If ψ is a generalized eigenfunction of H then, by Lemma 2.2, $\psi \in C^\infty$ and is polynomially bounded, $|\psi(x)| < C(1+|x|)^t$, say. If ψ satisfies (2.14) then, given $\epsilon > 0$, we can choose R such that for $n \in \mathbb{Z}^2$ with $|n| > R - 1/\sqrt{2}$,

$$\int_{\Lambda_1(n)} |\psi(x)| dx \leqslant e^{-(m-\epsilon)|n|}. \tag{2.15}$$

Since $\psi = R_0\psi$, for all $x \in \mathbb{R}^2$,

$$\begin{aligned} |\psi(x)| &\leqslant \frac{2\kappa}{\pi} \int_{\mathbb{R}^2} e^{-\kappa|x-y|^2} |\psi(y)| dy \\ &= \frac{2\kappa}{\pi} \int_{|y| \leqslant R} e^{-\kappa|x-y|^2} |\psi(y)| dx + \frac{2\kappa}{\pi} \int_{|y|>R} e^{-\kappa|x-y|^2} |\psi(y)| dy \\ &= \frac{2\kappa}{\pi} (I_1 + I_2). \end{aligned} \tag{2.16}$$

For the first term, we have

$$I_1 \leqslant C(1+|R|)^t \pi R^2 e^{-\kappa(|x|-R)^2}. \tag{2.17}$$

We now obtain an exponential bound on the second term,

$$I_2 \leqslant \sum_{\substack{n\in\mathbb{Z}^2\\ |n|>R-1/\sqrt{2}}} \int_{\Lambda_1(n)} e^{-\kappa|x-y|^2}|\psi(y)|dy$$

$$\leqslant \sum_{\substack{n\in\mathbb{Z}^2|x-n|\leqslant 1\\ |n|>R-1}} \int_{\Lambda_1(n)} e^{-\kappa|x-y|^2}|\psi(y)|dy$$

$$+ \sum_{\substack{n\in\mathbb{Z}^2|x-n|>1\\ |n|>R-1}} \int_{\Lambda_1(n)} e^{-\kappa|x-y|^2}|\psi(y)|dy = I_3 + I_4. \tag{2.18}$$

Now

$$I_3 \leqslant \sum_{n\in\mathbb{Z}^2|x-n|\leqslant 1} e^{-(m-\epsilon)|n|} \leqslant 4e^{-(m-\epsilon)(|x|-1)} \tag{2.19}$$

and

$$I_4 \leqslant \sum_{n\in\mathbb{Z}^2} e^{-(m-\epsilon)|n|} e^{-\kappa(|x-n|-1)^2}$$

$$\leqslant e^{-(m-\epsilon)|x|} \sum_{n\in\mathbb{Z}^2} e^{(m-\epsilon)|x-n|} e^{-\kappa(|x-n|-1)^2}$$

$$\leqslant e^{-(m-\epsilon)|x|} \sum_{n\in\mathbb{Z}^2} e^{(m-\epsilon)(|n|+1)} e^{-\kappa(|n|-2)^2} \leqslant C' e^{-(m-\epsilon)|x|}. \tag{2.20}$$

□

III. THE METHOD

In this short section we describe our method. Our proof is based on the paper of Von Dreifus and Klein[14] (also see Refs. 25 and 16). Here we give a summary of the main differences. The details can be found in Ref. 15.

The main tool in Refs. 14, 25, and 16 are the local Hamiltonians, the Hamiltonian restricted to bounded regions by Dirichlet boundary conditions, and the corresponding Green's functions. For $\Lambda\subset\mathbb{R}^2$, here we define the local Hamiltonian H_Λ on $L^2(\Lambda)$ by

$$H_\Lambda = P_\Lambda V_\Lambda P_\Lambda^*, \tag{3.1}$$

where $P_\Lambda = \mathbf{1}_\Lambda P_0$ and $V_\Lambda = V\mathbf{1}_\Lambda$. V is also truncated to ensure that for disjoint regions the corresponding local Hamiltonians are stochastically independent. We note that for bounded Λ, H_Λ is a Hilbert–Schmidt operator and its spectrum $\sigma(H_\Lambda)$ has an accumulation point at the origin.

For $\lambda \notin \sigma(H_\Lambda)$ let

$$G_\Lambda(E) = (H_\Lambda - E)^{-1}. \tag{3.2}$$

If ψ is an eigenfunction of H with eigenvalue $E \notin \sigma(H_\Lambda)$, then using the resolvent identity, we have for $x\in\Lambda$ [cf. Eq. (3.12) in Ref. 15]

$$\psi(x) = -(G_\Lambda(E)(P_\Lambda V P_{\Lambda^c}^* + P_\Lambda V_{\Lambda^c} P_\Lambda^*)\psi)(x). \tag{3.3}$$

Most of the complexity in adapting the proofs of Ref. 14 to this model comes from the fact that H is not a local operator. (3.3) contains terms that couple points in Λ to points outside. However,

because of the form of the kernel of P_0, the coupling is bounded by a Gaussian. The Green's function $G_\Lambda(E)$ does not have a kernel in this case. We therefore have to modify the definition of regularity.

Definition: Let $m>0$, $0<\beta<1$, $E\in\mathbb{R}$ and $\frac{1}{2}<s<1$. A square $\Lambda_L(x)$ is (ω,m,β,E,s) regular if
(RA), $d(E,\sigma(H_{\Lambda_L}(x)))>\frac{1}{2}e^{-L^\beta}$;
(RB), for all $\phi\in L_2(\Lambda_L(x))$,

$$\langle \mathbf{1}_{\Lambda_1(x)}, |G_{\Lambda_L(x)}(E)\mathbf{1}_{\tilde{\Lambda}_L(x)}\phi|\rangle < e^{-mL}\|\mathbf{1}_{\tilde{\Lambda}_L(x)}\phi\|,$$

where $\tilde{\Lambda}_L(x) = \Lambda_L(x)\backslash\Lambda_{\tilde{L}}(x)$ and $\tilde{L} = L - L^s$.

In order to state the theorem that is used in proving localization, we need to define the following two conditions: Let $E_0\in\mathbb{R}\backslash\{0\}$ and fix $\beta\in(0,1)$, $s\in(\frac{1}{2},1)$ and $p>2$. We shall say that L satisfies condition (P1) if the following occurs.

(P1) There exists $q>4p+12$ and $0<\eta<\frac{1}{2}|E_0|$, such that for all $L_1\geqslant L$ and all $E\in(E_0-\eta,E_0+\eta)$,

$$\mathbb{P}\{d(E,\sigma(H_{\Lambda_{L_1}(0)}))<e^{-L_1^\beta}\}<L_1^{-q};$$

and we shall say that L satisfies condition (P2) if the following occurs.

(P2) There exists $\gamma\in(0,1)$ and $m>L^{\gamma-1}$, such that

$$\mathbb{P}\{\Lambda_L(0) \text{ is } (\omega,m,\beta,E_0,s) \text{ regular}\}\geqslant 1-L^{-p}.$$

The following theorem is Theorem 4.1 in Ref. 15.

Theorem 3.1: There exists $L_0(\beta,s,p,q)$ such that if there is an $L\geqslant L_0$ that satisfies both conditions (P1) and (P2) then there is a $\Delta(L,\beta,s,\eta)>0$ so that almost surely, for $E_0\neq 0$, $\sigma(H)\cap(E_0-\Delta,E_0+\Delta)$ is in the pure-point spectrum and the corresponding eigenfunctions decay with mass greater or equal to m.

The proof of this theorem can be split up in two parts: one in which condition (P2) is iterated to pairs of larger and larger blocks and one in which the iterated condition is shown to imply exponential decay. Because of Lemma 2.4 it is sufficient to iterate on squares centered on points of $\mathbb{Z}^2$. This is very important in adapting the method of Ref. 14, which is for lattice Hamiltonians, to our model, which is for a continuous system, because it allows us to add probabilities.

Another difference between condition (P2) and the corresponding condition in Ref. 14 is the dependence of m on L. In most cases one checks (P2) by proving that the density of states decays very fast near the edges of the spectrum (Lifshitz tails). In this paper we check (P2) directly and this requires that we weaken (P2) to allow m to depend on L.

IV. PROOF OF LOCALIZATION

In this final section we shall show that the conditions of Theorem 3.1 are satisfied, thus establishing that the eigenfunctions corresponding to points near the edges of X are localized (Theorem 2.3).

From now on we shall assume that the probability measure μ is absolutely continuous with respect to the Lebesgue measure on $\mathbb{R}$ and has a density ρ that satisfies a Lipshitz condition of order σ.

There exist $\sigma>0$ and $K>0$ such that

$$|\rho(x)-\rho(y)|\leqslant K|x-y|^\sigma, \tag{4.1}$$

for all $x,y\in[a,b]$. This implies that that ρ is bounded, and therefore

$$\mu[c,d]<K'(d-c). \tag{4.2}$$

In the next ten lemmas (Lemmas 4.1–4.10) we shall assume that $0<a<b$, but we emphasize that this is not necessary for the final result. Let

$$N_\Lambda^>(V,E)=\#\{j:\lambda_\Lambda^{(j)}(V)\geqslant E\}, \tag{4.3}$$

where

$$\lambda_\Lambda^{(1)}(V)\geqslant\lambda_\Lambda^{(2)}(V)\geqslant\lambda_\Lambda^{(3)}(V)\geqslant\cdots\geqslant 0$$

are the eigenvalues of H_Λ. Note that since this operator is Hilbert–Schmidt, $N_\Lambda^>(V,E)$ is finite for $E>0$. We have the following simple scaling law for $N_\Lambda^>(V,E)$: If $t>0$,

$$N_\Lambda^>(tV,tE)=N_\Lambda^>(V,E). \tag{4.4}$$

Throughout this section we shall use a simplified notation. We let $H_L = H_{\Lambda_L(0)}$, $G_L = G_{\Lambda_L(0)}$, $V_L = V_{\Lambda_L(0)}$, $P_L = P_{\Lambda_L(0)}$, $\Lambda_L=\Lambda_L(0)$, $\tilde{\Lambda}_L=\tilde{\Lambda}_L(0)$, $\Lambda_1=\Lambda_1(0)$, and $\mathscr{H}_L=L^2(\Lambda_L(0))$. The following lemma will be required for condition (P1) and for part (RA) of the regularity condition in (P2). The proof is a modification of Wegner.[17]

Lemma 4.1: There exists a constant $C>0$ such that for $E>a>0$ and $0<\epsilon<\frac{1}{2}E$,

$$\mathbb{P}(d(E,\sigma(H_L))<\epsilon)\leqslant CL^4\epsilon^{\min(1,\sigma)}.$$

Proof: We first note that $V_\Lambda^{1/2}P_\Lambda^*$ is Hilbert–Schmidt since it has a square integrable kernel and therefore H_Λ is trace class. Also,

$$\text{trace } H_\Lambda=\int_\Lambda dx\int_\Lambda dy|P_0(x,y)|^2V(y). \tag{4.5}$$

Now, since $N_\Lambda^>(V,E)$ is the number of eigenvalues greater than E, it is smaller than the sum of $\lambda_\Lambda^{(i)}(V)/a$:

$$\begin{aligned}N_\Lambda^>(V,E)\leqslant a^{-1}\text{ trace } H_\Lambda&=a^{-1}\int_\Lambda dx\int_\Lambda dy|P_0(x,y)|^2V(y)\\&\leqslant a^{-1}b\int_{\mathbb{R}^2}dx\int_\Lambda dy|P_0(x,y)|^2\\&\leqslant 2(\pi a)^{-1}b\kappa|\Lambda|.\end{aligned} \tag{4.6}$$

By (4.4),

$$\mathbb{E}(N_\Lambda^>(V,E-\epsilon)-N_\Lambda^>(V,E+\epsilon))=\mathbb{E}\left(N_\Lambda^>\left(\frac{EV}{E-\epsilon},E\right)-N_\Lambda^>\left(\frac{EV}{E+\epsilon},E\right)\right). \tag{4.7}$$

Writing (4.7) explicitly, we get

$$\mathbb{E}(N_\Lambda^>(V,E-\epsilon)-N_\Lambda^>(V,E+\epsilon))=\prod_{n\in\Gamma}\left(1-\frac{\epsilon}{E}\right)\int_{Ea/(E-\epsilon)}^{Eb/(E-\epsilon)}d\omega_n\ \rho\left(\left(1-\frac{\epsilon}{E}\right)\omega_n\right)N_\Lambda^>(V,E)$$
$$-\prod_{n\in\Gamma}\left(1+\frac{\epsilon}{E}\right)\int_{Ea/(E+\epsilon)}^{Eb/(E+\epsilon)}d\omega_n\ \rho\left(\left(1+\frac{\epsilon}{E}\right)\omega_n\right)N_\Lambda^>(V,E), \tag{4.8}$$

where $\Gamma=\{n\in\mathbb{Z}^2:\Lambda_1(n)\cap\Lambda_L\neq 0\}$ If we order Γ in some way we can then write (4.8) as

$$\mathbb{E}(N_\Lambda^>(V,E-\epsilon)-N_\Lambda^>(V,E+\epsilon))=\sum_j\left(\prod_{i<j}\left(1-\frac{\epsilon}{E}\right)\int_{Ea/(E-\epsilon)}^{Eb/(E-\epsilon)}d\omega_{n_i}\ \rho\left(\left(1-\frac{\epsilon}{E}\right)\omega_{n_i}\right)\right.$$
$$\times\left(\prod_{i>j}\left(1+\frac{\epsilon}{E}\right)\int_{Ea/(E+\epsilon)}^{Eb/(E+\epsilon)}d\omega_{n_i}\ \rho\left(\left(1+\frac{\epsilon}{E}\right)\omega_{n_i}\right)\right)\int d\omega_{n_j}$$
$$\times\left(\left(1-\frac{\epsilon}{E}\right)\mathbf{1}_{E/(E-\epsilon)[a,b]}(\omega_{n_j})\rho\left(\left(1-\frac{\epsilon}{E}\right)\omega_{n_j}\right)-\left(1+\frac{\epsilon}{E}\right)\right.$$
$$\left.\left.\times\mathbf{1}_{E/(E+\epsilon)[a,b]}(\omega_{n_j})\rho\left(\left(1+\frac{\epsilon}{E}\right)\omega_{n_j}\right)\right)N_\Lambda^>(V,E). \right. \tag{4.9}$$

Thus

$$\mathbb{E}(N_\Lambda^>(V,E-\epsilon)-N_\Lambda^>(V,E+\epsilon))$$
$$\leq 2(\pi a)^{-1}b\kappa|\Lambda|^2\int d\omega\left|\left(1-\frac{\epsilon}{E}\right)\mathbf{1}_{E/(E-\epsilon)[a,b]}(\omega)\rho\left(\left(1-\frac{\epsilon}{E}\right)\omega\right)\right.$$
$$\left.-\left(1+\frac{\epsilon}{E}\right)\mathbf{1}_{E/(E+\epsilon)[a,b]}(\omega)\rho\left(\left(1+\frac{\epsilon}{E}\right)\omega\right)\right|$$
$$\leq 2(\pi a)^{-1}b\kappa|\Lambda|^2\left(\frac{2\epsilon}{E}+\int_{aE/(E-\epsilon)}^{bE/(E+\epsilon)}\left|\rho\left(\left(1-\frac{\epsilon}{E}\right)\omega\right)-\rho\left(\left(1+\frac{\epsilon}{E}\right)\omega\right)\right|d\omega\right.$$
$$\left.+\frac{E}{E+\epsilon}\,\mu\left(a,a\,\frac{E+\epsilon}{E-\epsilon}\right)+\frac{E}{E-\epsilon}\,\mu\left(b\,\frac{E-\epsilon}{E+\epsilon},b\right)\right)$$
$$\leq C|\Lambda|^2e^{\min(1,\sigma)}, \tag{4.10}$$

where we have used (4.1), (4.2), and $a\leq E\leq b$. Note that the constant C is independent of E. Now

$$\mathbb{P}(d(E,\sigma(H_L))<\epsilon)\leq\sum_i\ \mathbb{P}(\lambda_i\in(E-\epsilon,E+\epsilon))\leq\mathbb{E}(N_{\Lambda_L}^>(V,E-\epsilon)-N_{\Lambda_L}^>(V,E+\epsilon))$$
$$\leq CL^4e^{\min(1,\sigma)}. \tag{4.11}$$

□

We shall see later that it is sufficient to prove (P1) and part (RA) of (P2). The remaining lemmas will be used to prove part (RB) of (P2).

We first use a Combes–Thomas[18]-type argument to obtain an upper bound for $\langle\mathbf{1}_{\Lambda_1},|G_L\mathbf{1}_{\tilde{\Lambda}_L}\phi|\rangle$.

Lemma 4.2: There exists $C>0$ and $L_0>0$ such that if $0<\epsilon<1$ and $L>L_0$; then

$$\mathbb{P}\left(\langle \mathbf{1}_{\Lambda_1}, |G_L \mathbf{1}_{\tilde{\Lambda}_L}\phi|\rangle < \frac{C}{\epsilon}\, e^{-C\epsilon L}\|\mathbf{1}_{\tilde{L}_L}\phi\|, \forall\, \phi \in \mathscr{H}_L\right) \geqslant \mathbb{P}(d(E,\sigma(H_L)) \geqslant \epsilon). \tag{4.12}$$

Proof: Let U be the operator on $\mathscr{H}_L$ defined by $(Uf)(x) = e^{x_0\cdot x} f(x)$, where $x_0 \in \mathbb{R}^2$ with $|x_0|<1$ and let

$$Q = UH_L U^{-1} - H_L\,. \tag{4.13}$$

Then Q has a kernel $Q(x,y)$, where

$$Q(x,y) = (e^{x_0\cdot(x-y)} - 1)H_L(x,y), \tag{4.14}$$

$H_L(x,y)$ being the kernel of H_L. Therefore

$$|(Q\phi)(x)| \leqslant \frac{2\kappa b}{\pi} \int |e^{x_0\cdot(x-y)} - 1| e^{-(\kappa/2)|x-y|^2} |\phi(y)|\, dy. \tag{4.15}$$

Since

$$\begin{aligned} |e^{x_0\cdot(x-y)} - 1| e^{-(\kappa/4)|x-y|^2} &\leqslant |x_0\cdot(x-y)| e^{|x_0\cdot(x-y)|} e^{-(\kappa/4)|x-y|^2} \\ &\leqslant |x_0||x-y| e^{|x_0||x-y|} e^{-(\kappa/4)|x-y|^2} \\ &\leqslant |x_0| e^{2|x-y|} e^{-(\kappa/4)|x-y|^2} \leqslant e^{1/2\kappa^{1/2}} |x_0|, \end{aligned} \tag{4.16}$$

we have

$$|(Q\phi)(x)| \leqslant (T|\phi|)(x)|x_0|$$

where T is the operator with kernel $T(x,y) = (2\kappa b/\pi) e^{1/2\kappa^{1/2}} e^{-(\kappa/4)|x-y|^2}$. Thus

$$\|Q\phi\| \leqslant \||T|\phi|\|\ \ |x_0| \leqslant \|T\|\ \ |x_0|\ \ \|\phi\|, \tag{4.17}$$

and therefore $\|Q\| \leqslant K|x_0|$.

Let E satisfy $d(E,\sigma(H_L)) \geqslant \epsilon$ and choose x_0 such that $|x_0| < \epsilon/(2K)$, so that $\|Q\| \leqslant \frac{1}{2}\epsilon$. Then, by (4.13),

$$\|UG_L(E)U^{-1}\| = \|(H_L + Q - E)^{-1}\| < \frac{2}{\epsilon}. \tag{4.18}$$

Now we split up $\tilde{\Lambda}_L$ into four parts:

$$\tilde{\Lambda}_L = \bigcup_{i=1}^{4} \tilde{\Lambda}_L^{(i)},$$

where $\tilde{\Lambda}_L^{(i)} = \{x : x \in \tilde{\Lambda}, e_i \cdot x \geqslant |x|/\sqrt{2}\}$ and $e_1=(1,0)$, $e_2=(-1,0)$, $e_3=(0,1)$, and $e_4=(0,-1)$. We have

$$\langle \mathbf{1}_{\Lambda_1}, |G_L \mathbf{1}_{\tilde{\Lambda}_L}\phi|\rangle \leqslant \sum_{i=1}^{4} \langle \mathbf{1}_{\Lambda_1}, |G_L \mathbf{1}_{\tilde{\Lambda}_L^{(i)}}\phi|\rangle. \tag{4.19}$$

Now

$$\begin{aligned}\langle \mathbf{1}_{\Lambda_1}, |G_L \mathbf{1}_{\tilde{\Lambda}_L^{(1)}} \phi| \rangle &= \langle \mathbf{1}_{\Lambda_1}, U^{-1} | U G_L U^{-1} U \mathbf{1}_{\tilde{\Lambda}_L^{(1)}} \phi| \rangle \\ &\leqslant \| U^{-1} \mathbf{1}_{\Lambda_1} \| \| U G_L U^{-1} \| \| U \mathbf{1}_{\tilde{\Lambda}_L^{(1)}} \| \| \mathbf{1}_{\tilde{\Lambda}_L} \phi \| \\ &\leqslant \frac{2}{\epsilon} \| U^{-1} \mathbf{1}_{\Lambda_1} \| \| U \mathbf{1}_{\tilde{\Lambda}_L^{(1)}} \| \| \mathbf{1}_{\Lambda_L} \phi \|. \end{aligned} \tag{4.20}$$

Clearly,

$$\| U^{-1} \mathbf{1}_{\Lambda_1} \| \leqslant e^{\epsilon/2\sqrt{2}K} < K', \tag{4.21}$$

and by choosing $x_0 = (-\epsilon/2\sqrt{2}K, 0)$ we get

$$\| U \mathbf{1}_{\tilde{\Lambda}_L^{(1)}} \psi \|^2 = \int_{\tilde{\Lambda}_L^{(1)}} e^{2x_0 \cdot x} |\psi(x)|^2 \, dx \leqslant e^{-(\epsilon/4K)(L-L^s)} \| \psi \|^2, \tag{4.22}$$

from which it follows that

$$\| U \mathbf{1}_{\tilde{\Lambda}_L^{(1)}} \| \leqslant e^{-(\epsilon/8K)(L-L^s)} < e^{-(\epsilon/9K)L}, \tag{4.23}$$

for L sufficiently large. Thus, using (4.20)–(4.23) we get

$$\langle \mathbf{1}_{\Lambda_1}, |G_L \mathbf{1}_{\tilde{\Lambda}_L^{(1)}} \phi| \rangle < \frac{2K'}{\epsilon} \, e^{-(\epsilon/9K)L} \| \mathbf{1}_{\tilde{\Lambda}_L} \phi \|, \tag{4.24}$$

and similarly for $i = 2,3,4$. Therefore

$$\langle \mathbf{1}_{\Lambda_1}, \ |G_L \mathbf{1}_{\tilde{\Lambda}_L} \phi| \rangle < \frac{8K'}{\epsilon} \, e^{-(\epsilon/9K)L} \| \mathbf{1}_{\tilde{\Lambda}_L} \phi \|. \tag{4.25}$$

□

The proof of part (RB) of (P2) is now reduced to estimating $\mathbb{P}(d(E, \sigma_L(H_L)) < \epsilon)$. However, the estimate (4.1) is not good enough and we have to obtain a better one.

We shall make use of the explicit form of the following basis functions for $\mathscr{H}_0$. For $m \in \mathbb{N}$ and $x \in \mathbb{R}^2$ let

$$u_m(x) = \frac{(2\kappa)^{(1/2)(m+1)}}{(\pi m!)^{1/2}} (x_1 - i x_2)^m e^{-\kappa |x|^2}. \tag{4.26}$$

Then $\{u_m : m \in \mathbb{N}\}$ is an orthonormal basis for $\mathscr{H}_0$. Note that since U_y commutes with P_0, $\{U_y u_m : m \in \mathbb{N}\}$ is also an orthonormal basis for $\mathscr{H}_0$. We also have that if $m \neq n$, then

$$\int_{B(0,r)} \overline{u_m}(x) u_n(x) dx = 0, \tag{4.27}$$

so that if

$$\phi = \sum_{m=0}^{\infty} c_m u_m,$$

then

$$\int_{B(0,r)} |\phi(x)|^2\, dx = \sum_{m=0}^{\infty} |c_m|^2 \int_{B(0,r)} |u_m(x)|^2\, dx. \tag{4.28}$$

Lemma 4.3: If $0 \leqslant r \leqslant d$ and $m \in \mathbb{N}$, then

$$\int_{B(0,d)\setminus B(0,r)} |u_m(x)|^2\, dx \geqslant (e^{-2\kappa r^2} - e^{-2\kappa d^2}) \int_{B(0,r)} |u_m(x)|^2\, dx. \tag{4.29}$$

Proof: A straightforward calculation gives

$$\int_{B(0,d)\setminus B(0,r)} |u_m(x)|^2\, dx = \sum_{k=0}^{m} \left\{ \frac{(2\kappa r^2)^k}{k!}\, e^{-2\kappa r^2} - \frac{(2\kappa d^2)^k}{k!}\, e^{-2\kappa d^2} \right\} \tag{4.30}$$

and

$$\int_{B(0,r)} |u_m(x)|^2\, dx = 1 - \sum_{k=0}^{m} \frac{(2\kappa r^2)^k}{k!}\, e^{-2\kappa r^2}. \tag{4.31}$$

For fixed $t \geqslant 0$, we define $F(s)$ for $s \geqslant t$ by

$$F(s) = \sum_{k=0}^{m} \frac{s^k}{k!}\, e^{-s} - \left(1 - \sum_{k=0}^{m} \frac{t^k}{k!}\, e^{-t} \right) e^{-s}. \tag{4.32}$$

Then the statement of the lemma is equivalent to the following: If $s \geqslant t \geqslant 0$, then $F(s) \leqslant F(t)$. Now

$$\begin{aligned} F'(s) &= e^{-s} \left(-\frac{s^m}{m!} + \sum_{k=m+1}^{\infty} \frac{t^k}{k!}\, e^{-t} \right) \\ &= \frac{e^{-s}}{m!} \left(-s^m + t^m e^{-t} \sum_{k=1}^{\infty} \frac{t^k m!}{(k+m)!} \right) \\ &\leqslant \frac{e^{-s}}{m!} \left(-s^m + t^m e^{-t} \sum_{k=1}^{\infty} \frac{t^k}{k!} \right) \leqslant \frac{e^{-s}}{m!} (-s^m + t^m) \leqslant 0. \end{aligned} \tag{4.33}$$

□

In the remaining lemmas we shall prove that the part (RB) of (P2) is satisfied. From Lemma 4.2 with $\epsilon = L^{\delta-1}$ and $m = 2L^{(1/2\delta-1)}$, we get, for L sufficiently large

$$\mathbb{P}(\langle \mathbf{1}_{\Lambda_1}, |G_L \mathbf{1}_{\tilde{\Lambda}_L} \phi| \rangle < e^{-mL} \|\mathbf{1}_{\tilde{\Lambda}_L} \phi\|, \quad \forall \phi \in \mathscr{H}_L) \geqslant \mathbb{P}(d(E, \sigma(H_L)) \geqslant L^{\delta-1}).$$

Now, if $E > b - \epsilon$, the inequality $H_L \leqslant (b - 2\epsilon)\mathbf{1}$ implies that $d(E, \sigma(H_L)) > \epsilon$. Therefore, it is enough to prove that for L sufficiently large with probability greater than $1 - 1/2L^p$,

$$H_L \leqslant \left(b - \frac{2}{L^{1-\delta}} \right) \mathbf{1}. \tag{4.34}$$

We shall proceed in the following way.

Let $0 < \delta < 1/4$ and put $\epsilon_L = 4L^{-1/2+\delta}$. For each configuration, $\omega \in \Omega$ and for $A \subset \mathbb{R}^2$ let

$$A^+ = \{x \in A : V_L(x,\omega) > b - \epsilon_L\},$$

$$A^- = \{x \in A : V_L(x,\omega) \leqslant b - \epsilon_L\}.$$

Let t be a fixed number, such that $\kappa t > 768$. We shall say that a configuration $\omega \in \Omega$ satisfies the condition (C1) if the following holds

(C1) There is a set of regions $\{B_i\}$ with $\#\{B_i\} \leqslant L^2$, such that
(i) $\Lambda_L^+ \subset \cup_i B_i$,
(ii) diam $B_i \leqslant 2t \ln L$, and
(iii) $d(B_i, B_j) \geqslant \sqrt{t \ln L}$.

Let τ be a fixed number such that $16\kappa\tau^4 < 1$. We shall say that a configuration satisfies (C2) if the following occurs.

(C2) For each $k \in \Lambda_L \cap \mathbb{Z}^2$, we can find a ball D_k, center k, and radius ρ_k, where $(\tau^2/2)(\ln L)^{1/2} \leqslant \rho_k \leqslant \tau^2 (\ln L)^{1/2}$, with a surrounding annulus $\widetilde{D}_k$ of width $\tau(\ln L)^{1/4}$, such that $\widetilde{D}_k \cap \Lambda_L^+ = \emptyset$.

We shall first prove (Lemmas 4.4–4.8) that for configurations that satisfy (C1) and (C2) simultaneously, (4.34) holds. Then in Lemmas 4.9 and 4.10 we show that such configurations occur with probability greater than $1 - 1/2L^p$.

For a configuration that satisfies (C1), we let $B_i^{(j)} = \{x \in \mathbb{R}^2 : d(x, B_i) < (j/8)\sqrt{t \ln L}\}$ for $j = 1,2,3,4$. If $\phi \in \mathscr{H}$ we write ϕ_i for the restriction $\phi | B_i^{(2)}$.

In the following lemma we shall prove that on subsets of $B_i^{(1)}$, $P_0\phi$ can be approximated by $P_0\phi_i$.

Lemma 4.4: There exists L_0 such that if $L > L_0$ then, for all configurations that satisfy (C1), for all i, for all $\phi \in \mathscr{H}$ with $\|\phi\| \leqslant 1$, and for all $A \subset B_i^{(1)}$,

$$\left| \int_A |(P_0\phi)(x)|^2 \, dx - \int_A |(P_0\phi_i)(x)|^2 \, dx \right| < \frac{1}{L^4}. \tag{4.35}$$

Proof: Let $x \in B_i^{(1)}$; then

$$\begin{aligned} |(P_0\phi)(x) - (P_0\phi_i)(x)| &= \left| \int_{\mathbb{R}^2 \setminus B_i^{(2)}} P_0(x,x')\phi(x') dx' \right| \\ &\leqslant \left(\int_{\mathbb{R}^2 \setminus B_i^{(2)}} |P_0(x,x')|^2 \, dx' \right)^{1/2} \\ &= \frac{2\kappa}{\pi} \left(\int_{\mathbb{R}^2 \setminus B_i^{(2)}} e^{-2\kappa|x-x'|^2} \, dx' \right)^{1/2} \\ &\leqslant \frac{2\kappa}{\pi} \left(e^{-(\kappa t/64)\ln L} \int_{\mathbb{R}^2} e^{-\kappa|x-x'|^2} \, dx' \right)^{1/2} \\ &= 2\sqrt{\frac{\kappa}{\pi}} \frac{1}{L^{\kappa t/128}} \leqslant 2\sqrt{\frac{\kappa}{\pi}} \frac{1}{L^6}. \end{aligned} \tag{4.36}$$

Thus

$$\begin{aligned} ||(P_0\phi)(x)|^2 - |(P_0\phi_i)(x)|^2| &= (|(P_0\phi)(x)| + |(P_0\phi_i)(x)|)\,||(P_0\phi)(x)| - |(P_0\phi_i)(x)|| \\ &\leqslant 2\sqrt{\frac{\kappa}{\pi}} \frac{1}{L^6} (|(P_0\phi)(x)| + |(P_0\phi_i)(x)|). \end{aligned} \tag{4.37}$$

Now for L large enough,

$$\int_A |P_0\phi(x)|dx \leq |A|^{1/2}\|P_0\phi\| \leq |A|^{1/2}\|\phi\| \leq |A|^{1/2} < L, \tag{4.38}$$

and similarly,

$$\int_A |(P_0\phi_i)(x)| \leq |A|^{1/2}\|\phi_i\| \leq |A|^{1/2}\|\phi\| < L. \tag{4.39}$$

Therefore

$$\int_A |(P_0\phi)(x)|^2 - |(P_0\phi_i)(x)|^2|dx < 4\sqrt{\frac{\kappa}{\pi}}\frac{1}{L^5} < \frac{1}{L^4}, \tag{4.40}$$

for L sufficiently large. □

Lemma 4.5: There exists L_0 such that if $L > L_0$ then, for all configurations that satisfy (C1), for all i, for all $\phi \in \mathscr{H}$ with $\|\phi\| \leq 1$, and for all A and C subsets of $\mathbb{R}^2$ such that $B_i^{(3)} \subset C \subset A$,

$$\left| \int_A |(P_0\phi_i)(x)|^2 \, dx - \int_C |(P_0\phi_i)(x)|^2 \, dx \right| < \frac{1}{L^4}. \tag{4.41}$$

Proof: It is sufficient to prove the lemma for $A = \mathbb{R}^2$ and $C = B_i^{(3)}$,

$$\begin{aligned} |(P_0\phi_i)(x)| &\leq \frac{2\kappa}{\pi} \int_{B_i^{(2)}} e^{-\kappa|x-x'|^2} |\phi_i(x')| dx' \\ &\leq \frac{2\kappa}{\pi} \left(\int_{B_i^{(2)}} e^{-2\kappa|x-x'|^2} \, dx' \right)^{1/2} \\ &\leq \frac{2\kappa}{\pi} \left(\int_{B_i^{(2)}} e^{-2\kappa\{d(x,B_i^{(2)})\}^2} \, dx' \right)^{1/2} \\ &= \frac{2\kappa}{\pi} |B_i^{(2)}|^{1/2} e^{-\kappa\{d(x,B_i^{(2)})\}^2} \leq L e^{-\kappa\{d(x,B_i^{(2)})\}^2}, \end{aligned} \tag{4.42}$$

for L large enough. If $x \in \mathbb{R}^2 \setminus B_i^{(3)}$, $d(x, B_i^{(2)}) > \frac{1}{8}\sqrt{t \ln L}$. Also, we can find a ball B of radius L such that $B_i^{(3)} \subset B$. Let $\widetilde{B}$ be a ball of radius $2L$ concentric with B. Now

$$\begin{aligned} \int_{\mathbb{R}^2 \setminus B_i^{(3)}} |(P_0\phi_i)(x)|^2 \, dx &\leq \int_{\mathbb{R}^2 \setminus \widetilde{B}} |(P_0\phi_i)(x)|^2 \, dx + \int_{\widetilde{B} \setminus B_i^{(3)}} |(P_0\phi_i)(x)|^2 \, dx \\ &\leq 2\pi L^2 \int_{2L}^{\infty} e^{-2\kappa(r-L)^2} r \, dr + 4\pi L^4 e^{-(\kappa/32)\ln L} \\ &= \frac{\pi L^2}{2\kappa} e^{-2\kappa L^2} + \frac{4\pi}{L^{\kappa t/32 - 4}} < \frac{1}{L^4}, \end{aligned} \tag{4.43}$$

for L sufficiently large. □

In the next two lemmas we obtain an upper bound for the integral of $|(P_0\phi)(x)|^2$ over that part of B_i where $V_L(x,\omega) > b - \epsilon_L$ as a fraction of the integral over $B_i^{(4)}$.

If a configuration satisfies both (C1) and (C2), for each i we let K_i be the smallest subset of $\Lambda_L \cap \mathbb{Z}^2$, such that

$$B_i^{(3)} \subset \bigcup_{k \in K_i} D_k \subset B_i^{(4)}.$$

Then $\#K_i \leqslant C \ln L$. Note that the D_k's are not disjoint.

Lemma 4.6: There exists L_0 such that if $L > L_0$ then, for all configurations that satisfy both (C1) and (C2), for all i and for all $\phi \in \mathscr{H}$ with $\|\phi\| \leqslant 1$,

$$\int_{B_i^+} |(P_0\phi_i)(x)|^2 \, dx \leqslant \left(1 - \frac{1}{L^{1/4}}\right) \int_{B_i^{(4)}} |(P_0\phi_i)(x)|^2 \, dx + \frac{1}{L^4}. \tag{4.44}$$

Proof: Let

$$P_0\phi_i = \sum_{m=0}^{\infty} c_m U_{-k} u_m, \tag{4.45}$$

where $k \in K_i$. Since for each $k \in K_i$, $B_i^{(4)-} \supset \widetilde{D}_k$,

$$\begin{aligned} \int_{B_i^{(4)-}} |(P_0\phi_i)(x)|^2 \, dx &> \int_{\widetilde{D}_k} |(P_0\phi_i)(x)|^2 \, dx \\ &= \sum_{m=0}^{\infty} |c_m|^2 \int_{\widetilde{D}_k} |u_m(x-k)|^2 \, dx \\ &\geqslant \{e^{-2\kappa\rho_k^2} - e^{-2\kappa(\rho_k + \sqrt{\rho_k})^2}\} \sum_{m=0}^{\infty} |c_m|^2 \int_{D_k} |u_m(x-k)|^2 \, dx, \end{aligned} \tag{4.46}$$

by (4.28) and Lemma 4.3. Thus

$$\int_{B_i^{(4)-}} |(P_0\phi_i)(x)|^2 \, dx \geqslant \frac{1}{L^{2\kappa\tau^4}} (1 - e^{-\rho_L}) \int_{D_k} |(P_0\phi_i)(x)|^2 \, dx, \tag{4.47}$$

where $\rho_L = \kappa\tau^2 (\ln L)^{1/2}$. Summing over K_i and dividing by $\#K_i$, we get

$$\int_{B_i^{(4)-}} |(P_0\phi_i)(x)|^2 \, dx \geqslant \frac{1}{L^{2\kappa\tau^4}} (1 - e^{-\rho_L}) \frac{1}{\#K_i} \int_{B_i^{(3)}} |(P_0\phi_i)(x)|^2 \, dx. \tag{4.48}$$

By Lemma 4.5 and using $\#K_i < C \ln L$ we have for L large enough,

$$\int_{B_i^{(4)-}}|(P_0\phi_i)(x)|^2\,dx \geqslant \frac{1}{L^{2\kappa\tau^4}}\left(\frac{1-e^{-\rho_L}}{C\,\ln L}\right)\left(\int_{B_i^{(4)}}|(P_0\phi_i)(x)|^2\,dx-\frac{1}{L^4}\right)$$
$$\geqslant \frac{1}{L^{2\kappa\tau^4}}\,\frac{1}{2C\,\ln L}\int_{B_i^{(4)}}|(P_0\phi_i)(x)|^2\,dx-\frac{1}{L^4}$$
$$\geqslant \frac{1}{L^{1/8}}\,\frac{1}{2C\,\ln L}\int_{B_i^{(4)}}|(P_0\phi_i)(x)|^2\,dx-\frac{1}{L^4}$$
$$\geqslant \frac{1}{L^{1/4}}\int_{B_i^{(4)}}|(P_0\phi_i)(x)|^2\,dx-\frac{1}{L^4}. \tag{4.49}$$

Now

$$\int_{B_i^{+}}|(P_0\phi_i)(x)|^2\,dx=\int_{B_i^{(4)+}}|(P_0\phi_i)(x)|^2\,dx$$
$$=\int_{B_i^{(4)}}|(P_0\phi_i)(x)|^2\,dx-\int_{B_i^{(4)-}}|(P_0\phi_i)(x)|^2\,dx$$
$$\leqslant\left(1-\frac{1}{L^{1/4}}\right)\int_{B_i^{(4)}}|(P_0\phi_i)(x)|^2\,dx+\frac{1}{L^4}. \tag{4.50}$$

□

Lemma 4.7: There exists L_0 such that if $L>L_0$ then, for all configurations that satisfy both (C1) and (C2), for all i and for all $\phi\in\mathscr{H}$ with $\|\phi\|\leqslant 1$,

$$\int_{B_i^{+}}|(P_0\phi)(x)|^2\,dx\leqslant\left(1-\frac{1}{L^{1/2}}\right)\int_{B_i^{(4)}}|(P_0\phi)(x)|^2\,dx+\frac{4}{L^4}. \tag{4.51}$$

Proof: Let $\psi=P_0\phi$ so that $P_0\psi=\psi$ and $\|\psi\|\leqslant\|\phi\|\leqslant 1$,

$$|(P_0\psi_i)(x)|\leqslant\int_{B_i^{(2)}\setminus B_i}|P_0(x,x')||\psi(x')|dx'+\int_{B_i}|P_0(x,x')||\psi(x')|dx'$$
$$\leqslant\left(\int_{B_i^{(2)}\setminus B_i}|P_0(x,x')|^2\,dx'\right)^{1/2}\left(\int_{B_i^{(2)}\setminus B_i}|\psi(x')|^2\,dx'\right)^{1/2}$$
$$+\left(\int_{B_i}|P_0(x,x')|^2\,dx'\right)^{1/2}\left(\int_{B_i}|\psi(x')|^2\,dx'\right)^{1/2}$$
$$\leqslant\left(\frac{2\kappa}{\pi}\right)^{1/2}\left(\int_{B_i^{(2)}\setminus B_i}|\psi(x')|^2\,dx'\right)^{1/2}+\frac{2\kappa}{\pi}\,|B_i|^{1/2}e^{-\kappa\{d(x,B_i)\}^2}. \tag{4.52}$$

Therefore, if L is large enough,

$$|(P_0\psi_i)(x)|^2\leqslant\frac{2\kappa}{\pi}\int_{B_i^{(2)}\setminus B_i}|\psi(x')|^2\,dx'+Le^{-\kappa\{d(x,B_i)\}^2}. \tag{4.53}$$

Hence

$$\int_{B_i^{(4)}\setminus B_i^{(1)}}|(P_0\psi_i)(x)|^2\,dx\leqslant\frac{2\kappa}{\pi}\,|B_i^{(4)}\setminus B_i^{(1)}|\int_{B_i^{(2)}\setminus B_i}|\psi(x')|^2\,dx'+L\int_{B_i^{(4)}\setminus B_i^{(1)}}e^{-\kappa\{d(x,B_i)\}^2}\,dx. \tag{4.54}$$

The last term is less than

$$\frac{L^2}{L^{(\kappa t)/64}}<\frac{1}{L^4}.$$

Using this bound and $B_i^{(2)}\setminus B_i\subset B_i^{(4)-}$,

$$\int_{B_i^{(4)}\setminus B_i^{(1)}}|(P_0\psi_i)(x)|^2\,dx\leqslant\frac{2\kappa}{\pi}\,B_i^{(4)}\setminus B_i^{(1)}|\int_{B_i^{(4)-}}|\psi(x')|^2\,dx'+\frac{1}{L^4}. \tag{4.55}$$

Now

$$\begin{aligned}\left|\int_{B_i^{(4)}}|\psi(x)|^2\,dx-\int_{B_i^{(4)}}|(P_0\psi_i)(x)|^2\,dx\right|&\leqslant\left|\int_{B_i^{(1)}}|\psi(x)|^2\,dx-\int_{B_i^{(1)}}|(P_0\psi_i)(x)|^2\,dx\right|\\&\quad+\int_{B_i^{(4)}\setminus B_i^{(1)}}|\psi(x)|^2\,dx+\int_{B_i^{(4)}\setminus B_i^{(1)}}|(P_0\psi_i)(x)|^2\,dx\\&\leqslant\frac{1}{L^4}+\int_{B_i^{(4)-}}|\psi(x)|^2\,dx+\int_{B_i^{(4)}\setminus B_i^{(1)}}|(P_0\psi_i)(x)|^2\,dx\\&\qquad\text{using Lemma 4.4 and } B_i^{(4)}\setminus B_i^{(1)}\subset B_i^{(4)-},\\&\leqslant\left(1+\frac{2\kappa}{\pi}\,|B_i^{(4)}\setminus B_i^{(1)}|\right)\int_{B_i^{(4)-}}|\psi(x)|^2\,dx+\frac{2}{L^4}.\end{aligned} \tag{4.56}$$

Thus, writing $A=(2\kappa/\pi)|B_i^{(4)}\setminus B_i^{(1)}|$,

$$\begin{aligned}\int_{B_i^{(4)}}|(P_0\psi_i)(x)|^2\,dx&\leqslant(1+A)\int_{B_i^{(4)-}}|\psi(x)|^2\,dx+\int_{B_i^{(4)}}|\psi(x)|^2\,dx+\frac{2}{L^4}\\&=(2+A)\int_{B_i^{(4)}}|\psi(x)|^2\,dx-(1+A)\int_{B_i^{+}}|\psi(x)|^2\,dx+\frac{2}{L^4}.\end{aligned} \tag{4.57}$$

Hence by Lemma 4.6,

$$\begin{aligned}\int_{B_i^{+}}|(P_0\psi_i)(x)|^2\,dx&\leqslant\left(1-\frac{1}{L^{1/4}}\right)(2+A)\int_{B_i^{(4)}}|\psi(x)|^2\,dx\\&\quad-\left(1-\frac{1}{L^{1/4}}\right)(1+A)\int_{B_i^{+}}|\psi(x)|^2\,dx+\frac{3}{L^4}.\end{aligned} \tag{4.58}$$

Therefore, by using Lemma 4.4 and rearranging the inequality, we get

$$\left(1+(1+A)\left(1-\frac{1}{L^{1/4}}\right)\right)\int_{B_i^{+}}|\psi(x)|^2\,dx\leqslant\left(1-\frac{1}{L^{1/4}}\right)(2+A)\int_{B_i^{(4)}}|\psi(x)|^2\,dx+\frac{4}{L^4}. \tag{4.59}$$

Thus

$$\int_{B_i^+}|\psi(x)|^2\,dx \leqslant \frac{(1-1/L^{1/4})(2+A)}{(1-1/L^{1/4})(2+A)+1/L^{1/4}}\int_{B_i^{(4)}}|\psi(x)|^2\,dx+\frac{4}{L^4}$$
$$\leqslant\left(1-\frac{1}{L^{1/2}}\right)\int_{B_i^{(4)}}|\psi(x)|^2\,dx+\frac{4}{L^4}, \tag{4.60}$$

for L sufficiently large. □

Lemma 4.8: There exists $L_1>0$ such that for all $L>L_1$ and for all configurations that satisfy both (C1) and (C2),

$$H_L\leqslant\left(b-\frac{2}{L^{1-\delta}}\right)\mathbf{1}. \tag{4.61}$$

Proof: Let $\phi\in\mathscr{H}_L$ with $\|\phi\|$. Then

$$\begin{aligned}
\langle\phi,H_L\phi\rangle&=\langle\phi,P_LV_LP_L^*\phi\rangle\\
&=\langle P_L^*\phi,V_LP_L^*\phi\rangle\\
&=\langle P_0\phi,V_LP_0\phi\rangle\\
&=\int_{\Lambda_L}V(x)|(P_0\phi)(x)|^2\,dx\\
&\leqslant(b-\epsilon_L)\int_{\Lambda_L^-}|(P_0\phi)(x)|^2\,dx+b\int_{\Lambda_L^+}|(P_0\phi)(x)|^2\,dx\\
&\leqslant(b-\epsilon_L)\int_{\Lambda_L\setminus(\cup B_i^{(4)})}|(P_0\phi)(x)|^2\,dx+(b-\epsilon_L)\sum_i\int_{B_i^{(4)-}}|(P_0\phi)(x)|^2\,dx\\
&\quad+b\sum_i\int_{B_i^{(4)+}}|(P_0\phi)(x)|^2\,dx\\
&\leqslant(b-\epsilon_L)\int_{\Lambda_L\setminus(\cup B_i^{(4)})}|(P_0\phi)(x)|^2\,dx+\sum_i\left\{(b-\epsilon_L)\int_{B_i^{(4)}}|(P_0\phi)(x)|^2\,dx\right.\\
&\quad\left.+\epsilon_L\int_{B_i^+}|(P_0\phi)(x)|^2\,dx\right\}\\
&\leqslant(b-\epsilon_L)\int_{\Lambda_L\setminus(\cup B_i^{(4)})}|(P_0\phi)(x)|^2\,dx+\sum_i\left((b-\epsilon_L)+\epsilon_L\left(1-\frac{1}{L^{1/2}}\right)\right)\\
&\quad\times\int_{B_i^{(4)}}|(P_0\phi)(x)|^2\,dx+\frac{4\epsilon_L}{L^4}L^2,
\end{aligned}$$

by the previous lemma. Thus

$$\langle \phi, H_L \phi \rangle \leqslant (b - \epsilon_L L^{-1/2}) \int_{\Lambda_L \cup (\cup_i B_i^{(4)})} |(P_0 \phi)(x)|^2 dx + \frac{4\epsilon_L}{L^2}$$

$$\leqslant (b - \epsilon_L L^{-1/2}) \|P_0 \phi\|^2 + \frac{4\epsilon_L}{L^2}$$

$$\leqslant (b - \epsilon_L L^{-1/2}) \|\phi\|^2 + \frac{4\epsilon_L}{L^2}$$

$$\leqslant \left(b - \frac{\epsilon_L}{2L^{1/2}} \right) = \left(b - \frac{2}{L^{1-\delta}} \right).$$

□

Now we come to the main probabilistic estimate. The next two lemmas will be used in establishing that the configurations that satisfy (C1) and (C2) simultaneously occur with probability greater than $1-1/2L^p$.

Lemma 4.9: Let $\alpha>0$ and $p>0$. Then for all L sufficiently large, if $\alpha \ln L < a_L^2 < L^{1/4}$,

$$\mathbb{P}\left(\exists x \in \Lambda_L \cap \mathbb{Z}^2 : \#(B(x,a_L) \cap (\mathbb{Z}^2)^+) > \frac{1}{4} d_L^{1/2} \right) < \frac{1}{4L^p}.$$

Proof:

$$\mathbb{P}\left(\exists x \in \Lambda_L \cap \mathbb{Z}^2 : \#(B(x,a_L) \cap (\mathbb{Z}^2)^+) > \frac{1}{4} a_L^{1/2} \right) \leqslant \sum_{x \in \Lambda_L \cap \mathbb{Z}^2} \mathbb{P}\left(\#(B(x,a_L) \cap (\mathbb{Z}^2)^+) > \frac{1}{4} a_L^{1/2} \right)$$

$$\leqslant L^2 \sum_{n=n_0}^{N} \binom{N}{n} \epsilon_L^n, \tag{4.62}$$

where $n_0 = [a_L^{1/2}/4]$ and $N = \#(B(x,a_L) \cap \mathbb{Z}^2) \leqslant \gamma a_L^2$. Now $\binom{N}{n} \leqslant N^n/n! \leqslant (Ne/n)^n$, so that

$$\sum_{n=n_0}^{N} \binom{N}{n} \epsilon_L^n < \frac{1}{1-(N_{e\epsilon_L}/n_0)} \left(\frac{N_{e\epsilon_L}}{n_0} \right)^{n_0}. \tag{4.63}$$

The result now follows from

$$\frac{N_{e\epsilon_L}}{n_0} \leqslant \frac{4\gamma a_L^2 e L^{-1/2+\delta}}{[a_L^{1/2}/4]} \leqslant 16\gamma e L^{-1/4+\delta}. \tag{4.64}$$

□

Lemma 4.10: Let $\alpha>0$ and $p>0$. Then for all L sufficiently large, if $\alpha \ln L < a_L^2 < L^{1/4}$, the probability that for every $x \in \Lambda_L \cap \mathbb{Z}^2$, there exists $r_x \in (a_L/2, a_L - \sqrt{a_L})$, such that

$$(B(x, r_x + \sqrt{a_L}) \setminus B(x, r_x)) \cap (\mathbb{R}^2)^+ = \emptyset,$$

is greater than $1-1/4L^p$.

Proof: Suppose there exists $x \in \Lambda_L \cap \mathbb{Z}^2$ such that for all $r \in (a_L/2, a_L - \sqrt{a_L})$,

$$(B(x, r + \sqrt{a_L}) \setminus B(x, r)) \cap (\mathbb{R}^2)^+ \neq \emptyset.$$

Then each of the the concentric annuli,

$$B(x,a_L)\backslash B(x,a_L-\sqrt{a_L}),\quad B(x,a_L-\sqrt{a_L})\backslash B(x,a_L-2\sqrt{a_L}),\ldots,$$

$$B(x,a_L-([\sqrt{a_L}/2]-1)\sqrt{a_L})\backslash B(x,a_L-[\sqrt{a_L}/2]\sqrt{a_L}),$$

contains a point of $(\mathbb{R}^2)^+$, so that at least every other annulus contains a point of $(\mathbb{Z}^2)^+$. Therefore

$$\#(B(x,a_L)\cap\mathbb{Z}^2_+)>[\sqrt{a_L}/4].$$

By Lemma 4.9 this has a probability less than $1/4L^p$. □

We are going to apply this lemma in two instances: one to decouple regions of size $O(\ln L)$ and another for regions of size $O((\ln L)^{1/2})$ to get the over-spill of the wave function.

Proposition 4.11: There exists $L_1>0$ such that all $L>L_1$ satisfy (P1) and (P2) for each $E\in(b-L^{-\delta},b]$.

Proof: Putting $\epsilon = e^{-L^\beta}$ in Lemma 4.1 we get for $E>a>0$,

$$\mathbb{P}(d(E,\sigma(H_L))<e^{-L^\beta})\leqslant CL^4e^{-L^{\beta\,\min(1,\sigma)}}. \tag{4.65}$$

It follows from (4.65) that L satisfies (P1) if sufficiently large. (4.65) also shows that there is $L_1>0$ such that if $L>L_1$,

$$\mathbb{P}\left(d(E,\sigma(H_L))>\frac{1}{2}\,e^{-L^\beta}\right)\geqslant 1-\frac{1}{2L^p}.$$

It is then sufficient to prove that if $m=2L^{\gamma-1}$, where $\gamma=1/2\delta$, then

$$\mathbb{P}(\langle\mathbf{1}_{\Lambda_1}|G_L(E)\mathbf{1}_{\tilde{\Lambda}_L}\phi|\rangle<e^{-mL}\|\mathbf{1}_{\tilde{\Lambda}_L}\phi\|,\quad\forall\phi\in\mathscr{H}_L)\geqslant 1-\frac{1}{2L^p}.$$

From Lemma 4.2 with $\epsilon=L^{\delta-1}$, we get for L sufficiently large,

$$\mathbb{P}(\langle\mathbf{1}_{\Lambda_1},|G_L\mathbf{1}_{\tilde{\Lambda}_L}\phi|\rangle<e^{-mL}\|\mathbf{1}_{\tilde{\Lambda}_L}\phi\|,\quad\forall\phi\in\mathscr{H}_L)\geqslant\mathbb{P}(d(E,\sigma(H_L))\geqslant L^{\delta-1}).$$

If $E>b-\epsilon$, then $H_L\leqslant(b-2\epsilon)\mathbf{1}$ implies that $d(E,\sigma(H_L))>\epsilon$. Therefore it is enough to prove that for L sufficiently large with probability greater than $1-1/2L^p$,

$$H_L\leqslant\left(b-\frac{2}{L^{1-\delta}}\right)\mathbf{1}.$$

Let $a_L=t\ln L$ and let $\{x_i:\ i=1,\ldots,N\}$ be the points of $\Lambda_L\cap\mathbb{Z}^2$ so that $N\leqslant L^2$. By Lemma 4.10, with probability greater than $1-1/4L^p$ for each i, we can find $r_i\in(a_L/2,a_L-\sqrt{a_L})$ such that

$$(B(x_i,r_i+\sqrt{a_L})\backslash B(x_i,r_i))\cap(\mathbb{R}^2)^+=\emptyset.$$

Let

$$A_i=B(x_i,r_i)$$

and

$$\tilde{A}_i=B(x_i,r_i+\sqrt{a_L}).$$

Let $B_1=A_1$ and for $1<i\leqslant N$ let

$$B_i = A_i \setminus \cup_{j<i} \widetilde{A}_j ;$$

if $B_i = \emptyset$ it is ignored. Then for all $1 < i \leqslant N$,

$$\text{diam } B_i \leqslant \text{diam } A_i = 2r_i \leqslant 2a_L ,$$

and if $i > j$, since $B_j \subset A_j$ and $B_i \subset \widetilde{A}_j^c$,

$$d(B_i, B_j) > d(\widetilde{A}_j^c, A_j) = \sqrt{a_L}.$$

If $x \in \Lambda_L^+$, let i_x be the smallest i such that $x \in A_i$. Then $x \notin \cup_{j<i_x} \widetilde{A}_j$, therefore $x \in B_{i_x}$. Thus $\Lambda_L^+ \subset \cup_i B_i$. So we have proved that with probability $> 1 - 1/4L^p$ condition (C1) is satisfied. By applying Lemma 4.10 again, this time with $a_L = \tau^2 (\ln L)^{1/2}$, we see that with probability $> 1 - 1/4L^p$, condition (C2) is satisfied. Thus, with probability $> 1 - 1/2L^p$ both conditions (C1) and (C2) are satisfied and Lemma 4.8 gives the required result. □

We are now ready to prove the main theorem of this paper, Theorem 2.3.

Proof of Theorem 2.3: We remove the condition $a > 0$ and let

$$\widetilde{\omega}_n = \omega_n + 1 - a,$$

so that the probability measure corresponding to the random variable $\widetilde{\omega}_n$ has support equal to $[1,c]$, where $c = b - a + 1$. Let

$$\widetilde{V}(x,\omega) = \sum_{n \in \mathbb{Z}^2} \mathbf{1}_{\Lambda_1(n)} \widetilde{\omega}_n ,$$

and

$$\widetilde{H} = P_0 \widetilde{V} P_0 .$$

Let $\delta \in (0,1/4)$ and let $L > \max(L_0, L_1)$, where L_0 is as in Theorem 3.1 and L_1 is as in Proposition 4.11. Then there an $m > 0$, and for each $E \in [c - L^{-\delta}, c]$ there is a $\Delta_E > 0$ and $\Omega_E \subset \Omega$ with $\mathbb{P}(\Omega_E) = 1$, such that for $\omega \in \Omega_E$, $[1,c] \cap [E - \Delta_E, E + \Delta_E]$ is in the pure-point spectrum of $\widetilde{H}$ and the corresponding eigenfunctions decay with rate greater or equal to m. Let

$$\Omega' = \bigcap_{E \in [c - L^{-\delta}, c] \cap \mathbf{Q}} \Omega_E ;$$

then $\mathbb{P}(\Omega') = 1$ and for $\omega \in \Omega'$, $[c - L^{-\delta}, c]$ is in the pure-point spectrum of $\widetilde{H}$ and the corresponding eigenfunctions decay with mass greater or equal to m. Now the eigenfunctions of H with eigenvalues in $[c - L^{-\delta}, c]$ are eigenfunctions of $\widetilde{H}$ with eigenvalues in $[b - L^{-\delta}, b]$. Thus, it follows that almost surely $[b - L^{-\delta}, b]$ is in the pure-point spectrum of H and the corresponding eigenfunctions of H decay with mass greater or equal to m. Similarly, one can prove the same result for $[a, a + L^{-\delta}]$. □

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Spontaneous symmetry breaking in the SO(3) gauge theory to discrete subgroups

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In this paper we give a systematical description of the possible symmetry breakings in the SO(3)-gauge theory and show an algorithmical method to construct SU(2)- or SO(3)-invariant Higgs potentials in an arbitrary irreducible representation using regular graphs. We close our paper with the explicit construction of the Lagrangian of the simplest SO(3)$\rightarrow A_4$ theory. © *1996 American Institute of Physics.* [S0022-2488(96)00304-0]

I. INTRODUCTION

A very interesting area of today's theoretical physics is the study of the so-called discrete gauge theories (discrete Yang–Mills theories).[1–3] A familiar way to construct such theories is to break down the continuous symmetry of a usual gauge theory using Higgs mechanism. However, if we want to give an explicit example of such a symmetry breaking we need to solve two nontrivial problems.

First, how could we produce invariant polynomials of the initial gauge group in an arbitrary representation? This is a very difficult problem of the theory of group invariants and we cannot answer the question generally even in the very simple case of SU(2).

Our second problem is to find a representation of the initial gauge group G for a given subgroup $H\subset G$ which possesses the symmetry breaking $G\rightarrow H$. Generally this is an algebraic geometrical question, because we can equivalently say that we must find points on the zero variety of the G-invariant polynomial having given stabilizer subgroup H under the action of G.

In the case of the group SU(2) we were able to develop a simple method using regular graphs to make SU(2)- [and of course SO(3)-] invariant polynomials.

Because the subgroups of the group SO(3) have contacts with regular two- and three-dimensional polyhedra, using simple methods from the theory of group representations we can list all possible stabilizer subgroups in an arbitrary irreducible representation of the group SO(3).

II. STATEMENT OF THE PROBLEM

If we want to break down the symmetry in a given gauge theory with gauge group G we need to give explicitly a so-called Higgs-potential V which is a polynomial in the Higgs scalar fields and satisfies the following conditions:

(i) V is invariant under the action of the group G in a given representation;
(ii) V is bounded;
(iii) the self-interactions of the scalar fields induced by the polynomial V are renormalizable.

If we want to break the gauge symmetry to a given subgroup of the gauge group G we need some more information about the polynomial V. Our starting point is the familiar Lagrangian:

$$\mathscr{L}=-\tfrac{1}{4}F_a^{\mu\nu}F^a_{\mu\nu}+(D^\mu\Phi)^\star(D_\mu\Phi)-V(\Phi). \tag{1}$$

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Here $V:\mathbf{k}^n\to\mathbf{R}$ is a polynomial that satisfies the above properties ($\mathbf{k}$ denotes $\mathbf{C}$ or $\mathbf{R}$). We can fix the minimum of the polynomial V to be zero. Let $Z(V=0)$ denote the zero variety of V; so a vacuum state of the theory is given by $A^a_\mu=0$ and $\Phi=\Phi_0\in Z(V=0)$. Using the potential V we can ''break the symmetry spontaneously down,'' which means that the vacuum state [which is a point in $Z(V=0)$] has no more the whole dynamical symmetry (the group G) but a subgroup H of G only. This subgroup H has the property that its elements stabilize the vacuum state (i.e., $H\Phi_0=\Phi_0$). So this subgroup H is the *stabilizer subgroup* of the point $\Phi_0\in Z(V=0)$. We are interested in such situations when this group is *discrete*. Now we are in position to give a precise formulation of our problem.

Let us consider the field theory (1) with symmetry group G. [We assume that this group is an algebraic subgroup of some GL ($\mathbf{k}^m$).] Then let us take a discrete subgroup of it. Also take a representation $\rho:G\to\mathrm{GL}(\mathbf{k}^n)$ of the group G. We are searching for polynomials $V:\mathbf{k}^n\to\mathbf{R}$ which satisfy the following conditions:

(i) V is invariant under the action ρ of G on $\mathbf{k}^n$;
(ii) V is bounded;
(iii) and $Z(V=0)$ has a subset with stabilizer subgroup $H\subset G$.

We have omitted the condition of renormalizability because this is a simple restriction of the degree of the polynomial V.

In the case $G=\mathrm{SO}(3)$ we can solve the problem generally: We are able to list all possible symmetry violation and can show a simple algorithmical method to construct Higgs potentials in arbitrary high-dimensional Higgs representations. Let us see how to do this!

III. CONSTRUCTION OF INVARIANT POLYNOMIALS

Let j be an integer or half-integer number and let us take the space of all homogeneous complex polynomials $p_{2j}(x,y)$ having two variables and homogeneous degree $2j$. This space is naturally identified with $\mathbf{C}^{2j+1}$. By the aid of the canonical two-dimensional representation of SU(2) we can describe a $(2j+1)$-dimensional representations as follows. If $\left(\begin{smallmatrix}\alpha & \beta\\ -\overline{\beta} & \overline{\alpha}\end{smallmatrix}\right)\in\mathrm{SU}(2)$, the transformation of a vector $(x,y)\in\mathbf{C}^2$ is given by

$$x\to\alpha x+\beta y,\quad y\to-\overline{\beta x}+\overline{\alpha y}.$$

Using these equations we obtain the transformation rule of a homogeneous polynomial:

$$\sum_{n=0}^{2j}a_n x^n y^{2j-n}\to\sum_{n=0}^{2j}a_n(\alpha x+\beta y)^n(-\overline{\beta x}+\overline{\alpha y})^{2j-n}.$$

Clearly this is a $(2j+1)$-dimensional representation of the group SU(2). The irreducibility of this representation is due to the fact that in the two-dimensional representation of the SU(2) there are not SU(2)-invariant polynomials. Let λ_n denote the roots of the polynomial $p_{2j}(x,1)$. Now we can write

$$\sum_{n=0}^{2j}a_n x^n y^{2j-n}=a_{2j}\prod_{n=1}^{2j}(x-\lambda_n y).$$

Definition: Let k,l be positive integer numbers. The graph $\mathscr{G}$ is called *k-regular oriented graph of order l* if it has l vertices, in every vertex converge k edges, and every edge has an orientation.

For example, Fig. 1 shows a four-regular oriented graph of order 5. Now let $\mathscr{G}$ be a k-regular oriented graph of order $2j$. We order to $\mathscr{G}$ an expression:

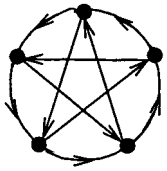

FIG. 1. An example: four-regular graph of order 5.

$$a_{2j}^{k}\prod_{(mn)}(\lambda_m-\lambda_n). \tag{2}$$

Here the product $\Pi_{(mn)}$ is understood as the product (2) has to involve a factor $\lambda_m-\lambda_n$ if in its graph there is an edge of the form seen in Fig. 2. (We can connect two verticies with more than one edge; in this situation we count the edges with multiplicity.)

On a graph of order $2j$ the permutation group S_{2j} acts as naturally transposing the vertices of the graph. This gives the symmetrization of the expression (2).

Proposition 1: The expression

$$\frac{1}{|S_{2j}|}\,a_{2j}^{k}\sum_{\pi\in S_{2j}}\prod_{(mn)}(\lambda_{\pi(m)}-\lambda_{\pi(n)}) \tag{3}$$

is invariant under the action of SU(2). ◇

Let σ_n denote the nth elementary symmetric polynomial with variables $\lambda_1,\ldots,\lambda_{2j}$. The expression (3) is clearly symmetric in $\lambda_1,\ldots,\lambda_{2j}$, so it is uniquely expressible as a polynomial in $\sigma_1,\ldots,\sigma_{2j}$. However, using the well-known relations between the roots and coefficients of a polynomial, $\sigma_n=(-1)^n a_{2j-n}/a_{2j}$, we have the result that (3) is an SU(2)- (or, if j is an integer, an SO(3)-) invariant polynomial of the form $f(a_0,\ldots,a_{2j})$ of homogeneous degree k.

The easy proof is left to the reader.

One can use this method very effectively if one has a computer [because of the symmetrization of the expression (2)]. We have computed some invariants of SU(2). Now we show only the seven-dimensional invariant of degree 2 illustrated in Fig. 3.

IV. CLASSIFICATION OF SYMMETRY VIOLATIONS OF THE SO(3)-THEORY

Now we turn to our second problem to classify all possible symmetry breaking in the SO(3)-gauge theory. Let $G\subset\mathrm{SO}(3)$ be a subgroup and its trivial representation given by $g\to 1\in\mathrm{GL}(1,\mathbf{R})=\mathbf{R}^*$, $g\in G$. We say that $G\subset\mathrm{SO}(3)$ is a maximal subgroup of the group SO(3) if there is no subgroup $H\subset\mathrm{SO}(3)$ satisfying $G\subset H$. The clue of the description is the following simple proposition.

Proposition 2: Let ρ:SO(3)$\to$GL(V) be an irreducible representation of the group SO(3) and let G its maximal subgroup. If the direct decomposition of ρ according to G contains the trivial representation of G, then in V there is a subspace W_G whose points are stabilized by the group G. Moreover, the dimension of W_G is equal to the multiplicity of the trivial representation of G in ρ. ◇

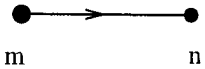

FIG. 2. A typical part of a graph.

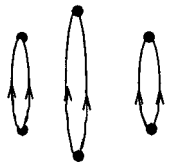

FIG. 3. $6a_3^2-16a_2a_4+40a_1a_5-240a_0a_6$; two-regular graph of order 6 and its SU(2)-invariant polynomial.

The straightforward verification of Proposition 2 is left to the reader. So if the subgroup G satisfies the condition of Proposition 2 the only thing that we need to do is to determine the characters of the group G in the representation ρ. But this is not difficult. First, if we take a review of the (discrete) subgroups of SO(3) we find that these groups are closely related to well-known geometrical objects: These groups are the symmetry groups of the two- and three-dimensional regular polyhedra. If we take into account this fact we are able to construct these groups as a set of rotations under which the adequate regular polyhedron remains invariant (but not pointwise).

However, if we know these rotations we can easily give the characters of the subgroup G in the representation ρ since

$$\chi_j(\phi)=\frac{\sin(j+\frac{1}{2})\phi}{\sin(\phi/2)}.$$

Here j denotes the weight of the representation ρ.

If the group is not maximal, i.e., there exists a subgroup H such that $G\subset H\subset \mathrm{SO}(3)$, then we need to consider the multiplicity of the trivial representation of G, resp. of H. If the multiplicity of the trivial G-representation is bigger than the multiplicity of the trivial H-representation, then there are points in V whose stabilizer subgroup is the not-maximal subgroup G. Leaving some technical details we get in summary the Appendix.

V. THE SO(3)→A_4 THEORY

The time has come to examine explicitly a not-usual symmetry violation. Using the Appendix we can see that it is possible to violate the SO(3)-gauge symmetry to its non-Abelian subgroup A_4 using seven-dimensional Higgs representation. We choose for this procedure the potential showed in Fig. 3. The seven-dimensional representation is constructed by the above polynomial method and is the seven-dimensional complex irreducible representation of the group SO(3), too. First we need to find a seven-dimensional *real* irreducible subspace $\mathbf{R}^7$ of $\mathbf{C}^7$ which gives the *real* representation of the SO(3). It is not difficult to see that a simple basis of this real subspace is given by the polynomials which satisfy the functional equation

$$p(x,y)=-\overline{p(}-\overline{y,x)}. \tag{4}$$

If we want to obtain an orthogonal real representation, we need to multiply the vectors satisfying (4) by certain numerical factors and obtain

$$\frac{i}{\sqrt{120}}(x^6+y^6);\quad \frac{1}{\sqrt{120}}(x^6-y^6),$$

$$\frac{1}{\sqrt{20}}(x^5y+xy^5);\quad \frac{i}{\sqrt{20}}(x^5y-xy^5), \tag{5}$$

$$\frac{i}{\sqrt{8}}(x^4y^2+x^2y^4);\quad \frac{1}{\sqrt{8}}(x^4y^2-x^2y^4),$$

$$\frac{1}{\sqrt{3}}x^3y^3.$$

In this basis the polynomial illustrated in Fig. 3 has the simple form

$$a_0^2+a_1^2+a_2^2+a_3^2+a_4^2+a_5^2+a_6^2,$$

which shows that this polynomial is bounded. Now we turn to our next question: how to find the coordinates of the A_4 vacuum. The group A_4, the fourth alternating group, has two generators denoted by a, b. Clearly, our points need to be in the linear space $\mathbf{R}^7\cap\mathrm{Ker}(\rho(a)-\mathrm{Id})\cap\mathrm{Ker}(\rho(b)-\mathrm{Id})$ and have to be normed. After constructing the seven-dimensional representation of a and b we obtain the two possible vacuum states in the basis (5):

$$\pm\frac{1}{\sqrt{270}}\begin{pmatrix}\sqrt{120}\\0\\0\\5\sqrt{6}\\0\\0\\0\end{pmatrix}. \tag{6}$$

Now we can write up the Lagrangian of the simplest $\mathrm{SO}(3)\to A_4$ theory:

$$\mathscr{L}=-\tfrac{1}{4}F_i^{\mu\nu}F^i_{\mu\nu}+(D^\mu\Phi)^\star(D_\mu\Phi)-\lambda(\Phi_0^2+\cdots+\Phi_6^2-1)^2. \tag{7}$$

Using (6) and (7) together we are able to study this ''exotic'' non-Abelian discrete gauge theory.

VI. CONCLUSIONS

In our paper we have studied the SO(3)-gauge theory. We have developed a general method to construct SO(3)-invariant polynomials and have given a systematical description of the possible symmetry violations in the SO(3) theory. Our results are important because it is possible that a general discrete gauge theory in two space–time dimensions possesses a strange field theoretical symmetry, the so-called quantum symmetry.[2,3] With the aid of explicit examples such as the $\mathrm{SO}(3)\to A_4$ model we can study this question very effectively.

APPENDIX: LIST OF STABILIZER SUBGROUPS

The following Appendix shows the stabilizer subgroups of the group SO(3) in an arbitrary $(2j+1)$-dimensional irreducible representation.

The representation of weight j contains the following stabilizer subgroups systematically:

• if j is even and $j\geqslant 4$, then

$$\mathbf{1},\mathbf{Z}_2\oplus\mathbf{Z}_2,\mathbf{Z}_3,\ldots,\mathbf{Z}_j,D_3,\ldots,D_j,\mathrm{O}(2),\mathrm{SO}(3),$$

• if j is odd and $j\geqslant 5$, then

$$\mathbf{1},\mathbf{Z}_2\oplus\mathbf{Z}_2,\mathbf{Z}_3,\ldots,\mathbf{Z}_j,D_3,\ldots,D_j,\mathrm{SO}(2),\mathrm{SO}(3).$$

Beyond these the not systematical groups are shown in Table I.

TABLE I. The not systematical stabilizer subgroups in the low-dimensional irreducible representations of the group SO(3).

dim ρ	1	3	5	7	9	11	13	15	17	19
H	SO(3)	SO(2) SO(3)	$\mathbf{Z}_2\oplus\mathbf{Z}_2$ O(2) SO(3)	$\mathbf{1}$ A_4 $\mathbf{Z}_3$ D_3 SO(2) SO(3)	S_4		A_4 S_4 A_5	A_4	S_4	A_4 S_4
dim ρ	21	23	25	27	29	31	33	35	37	39
H	A_4 S_4 A_5	A_4	A_4 S_4	A_4 S_4	A_4 S_4	A_4 S_4 A_5	A_4 S_4 A_5	A_4 S_4	A_4 S_4 A_5	A_4 S_4
dim ρ	41	43	45	47	49	51	53	55	57	59
H	A_4 S_4 A_5	A_4 S_4 A_5	A_4 S_4 A_5	A_4 S_4	A_4 S_4 A_5	A_4 S_4 A_5	A_4 S_4 A_5	A_4 S_4 A_5	A_4 S_4 A_5	A_4 S_4

The higher-dimensional representations one can simply list:

• if $j\geqslant 30$ and is even, the stabilizer subgroups in the $(2j+1)$-dimensional representations are

$$\mathbf{1},\mathbf{Z}_2\oplus\mathbf{Z}_2,\mathbf{Z}_3,\ldots,\mathbf{Z}_j,D_3,\ldots,D_j,A_4,A_5,S_4,\mathrm{O}(2),\mathrm{SO}(3),$$

• if $j\geqslant 31$ and is odd, then we obtain

$$\mathbf{1},\mathbf{Z}_2\oplus\mathbf{Z}_2,\mathbf{Z}_3,\ldots,\mathbf{Z}_j,D_3,\ldots,D_j,A_4,A_5,S_4,\mathrm{SO}(2),\mathrm{SO}(3).$$

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A q-deformation of the Coulomb problem

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The algebra of observables of $SO_q(3)$-symmetric quantum mechanics is extended to include the inverse $1/R$ of the radial coordinate and used to obtain eigenvalues and eigenfunctions of a q-deformed Coulomb Hamiltonian. © *1996 American Institute of Physics.* [S0022-2488(96)02203-8]

I. INTRODUCTION

Much work has been done recently to explore the $SO_q(3)$-symmetric quantum mechanics developed in Refs. 1 and 2. In particular, much is known about the q deformations of the harmonic oscillator. The other nontrivial soluble problem in ordinary quantum mechanics is the Coulomb problem, but for that one needs some notion of an inverse radius. Weich[3] considered a q-deformed Coulomb potential, defining $1/R$ in a manner dependent upon a particular Hilbert space representation. This differs from the more standard ''wave-function'' type approaches used in investigations of the oscillator (Refs. 4–6, for example).

Here we approach this problem by defining $1/R$ as an actual element of the algebra of observables, thereby achieving representation independence. Since $X^2=R^2$ is already defined, we can then also define R as well as all of its integral powers. A study of the action of momentum operators on powers of R then helps to bring out the interpretation of these operators as symmetric q derivatives.

Using this definition of $1/R$, a self-adjoint q deformation of the Coulomb Hamiltonian can be found, which shares the n^2-fold degeneracy of the undeformed Hamiltonian for the q analog of bound states. As in Refs. 3 and 7, we obtain a Balmer-type spectrum for these states with

$$E_n=-\left(\frac{\alpha}{[n]_q}\right)^2, \tag{1}$$

where the symmetric q analog of n is defined as

$$[n]_q=\frac{q^n-q^{-n}}{q-q^{-1}}. \tag{2}$$

In addition, we also obtain positive-energy wave functions and a candidate q-Coulomb S matrix.

The paper is structured as follows. After a brief review of $SO_q(3)$-symmetric quantum mechanics (Sec. II), we set up the formalism for dealing with the q-Coulomb problem (Secs. III–V), which is then treated in Sec. VI. The detailed proofs of some statements made in the text are deferred to the five Appendices.

II. $SO_q(3)$-SYMMETRIC QUANTUM MECHANICS

We build upon the algebra of observables as it is defined in Refs. 5 and 3. The q-deformed metric and Levi-Cività tensors are defined as follows:

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$$\gamma^{ij}\equiv\gamma_{ij}\equiv\begin{bmatrix}0&0&\frac{1}{\sqrt{q}}\\0&1&0\\\sqrt{q}&0&0\end{bmatrix},\quad \epsilon_1{}^{ij}\equiv\epsilon_{ij}{}^1\equiv\begin{bmatrix}0&\frac{1}{\sqrt{q}}&0\\-\sqrt{q}&0&0\\0&0&0\end{bmatrix},$$

$$\epsilon_2{}^{ij}\equiv\epsilon_{ij}{}^2\equiv\begin{bmatrix}0&0&-1\\0&\frac{1}{\sqrt{q}}-\sqrt{q}&0\\1&0&0\end{bmatrix},\quad \epsilon_3{}^{ij}\equiv\epsilon_{ij}{}^3\equiv\begin{bmatrix}0&0&0\\0&0&\frac{1}{\sqrt{q}}\\0&-\sqrt{q}&0\end{bmatrix}.$$

These give rise to an R matrix:

$$\tilde{R}{}^{ij}_{kl}=q\,\delta^i_k\delta^j_l-\epsilon_a{}^{ij}\epsilon_{kl}{}^a+\left(\frac{1}{q}-1\right)\gamma^{ij}\gamma_{kl},$$

which is a solution to the Yang–Baxter equation,

$$\tilde{R}{}^{ij}_{ab}\tilde{R}^{bk}_{cn}\tilde{R}^{ac}_{lm}=\tilde{R}^{jk}_{de}\tilde{R}^{id}_{lf}\tilde{R}^{fe}_{mn},$$

and has the inverse

$$\tilde{R}{}^{-1\,ij}_{kl}=\frac{1}{q}\,\delta^i_k\delta^j_l-\epsilon_a{}^{ij}\epsilon_{kl}{}^a+(q-1)\,\gamma^{ij}\gamma_{kl}.$$

We use the metric and Levi-Cività tensors to define scalar and vector products as for the undeformed tensors: $A\cdot B=\gamma^{ij}A_iB_j$ and $[A\times B]_k=\epsilon_k{}^{ij}A_iB_j$.

$\mathscr{A}^X_{R^3_q}$ is the $\mathrm{SO}_q(3)$-covariant*-algebra defined by the generators X_1,X_2,X_3 subject to the relations

$$[X\times X]_k=0$$

and

$$X_i^*=\gamma^{ij}X_j.$$

$X^2\equiv X\cdot X$ is then real and central in this algebra. In the $q=1$ limit, X_1 and X_3 correspond to $(1/\sqrt{2})(X\pm iY)$, while X_2 is Z. The space of wave functions in harmonic-oscillator treatments of $\mathrm{SO}_q(3)$-symmetric quantum mechanics is an appropriate subspace of $\mathscr{A}^X_{R^3_q}$.

One also considers an $\mathrm{SO}_q(3)$-covariant*-algebra $\mathscr{D}^X_{R^3_q}$ of operators on $\mathscr{A}^X_{R^3_q}$, whose generators are the X_i, derivative operators $\overline{\partial_i}$, and a scaling operator μ. The X_i act on $\mathscr{A}^X_{R^3_q}$ by left multiplication. μ is defined such that $\mu(1)=1$; and for all $f\in\mathscr{A}^X_{R^3_q}$, $\mu(X_if)=qX_i\mu(f)$. $\overline{\partial_i}$ is defined such that $\overline{\partial_i}(1)=0$; and for all $f\in\mathscr{A}^X_{R^3_q}$,

$$\overline{\partial_i}(X_jf)=\left[\gamma_{ij}+\frac{1}{q}\,\tilde{R}^{kl}_{ij}X_k\overline{\partial_l}\right]f.$$

The generators of $\mathscr{D}^X_{R^3_q}$ then obey the relations

$$\mu X_i = q X_i \mu, \quad \mu \overline{\partial_i} = \frac{1}{q} \overline{\partial_i} \mu,$$

$$\partial \overline{\ _i X_j} = \gamma_{ij} + \frac{1}{q} \widetilde{R}^{kl}_{ij} X_k \overline{\partial_l}, \quad [\overline{\partial} \times \overline{\partial}]_k = 0.$$

One also defines an inverse of μ:

$$\mu^{-1} = \mu[1 + q^{-2}(1-q^2) X \cdot \overline{\partial} + q^{-3}(1-q)^2 X^2 \overline{\partial^2}].$$

In addition, there is a conjugate set of derivative operators in $\mathscr{D}^X_{R^3_q}$,

$$\partial_i \equiv \mu^2[\overline{\partial_i} + (q^{-2} - q^{-1}) X_i \overline{\partial^2}].$$

∂_i then satisfy the relations

$$[\partial \times \partial]_k = 0$$

and

$$\partial_i X_j = \gamma_{ij} + q \widetilde{R}^{-1\,kl}_{\ \ ij} X_k \partial_l .$$

The * operation on μ and $\overline{\partial_i}$ is defined as $\mu^* \equiv q^{-3}\mu^{-1}$ and $(\overline{\partial_i})^* \equiv -q^3 \gamma^{ij} \partial_j$.

Neither triplet of derivative operators has a subalgebra isomorphic to $\mathscr{A}^X_{R^3_q}$, but a linear combination of the two does. This linear combination is then the triplet of q-momentum operators,

$$P_i = \frac{\partial_i + q^{-3} \overline{\partial_i}}{i(1 + q^{-3})}.$$

Then $(P_i)^* = \gamma^{ij} P_j$, $[P \times P]_k = 0$, and P^2 is a real scalar that commutes with the P_i.

The X_i and P_j satisfy q-deformed versions of the Heisenberg relations:

$$i(P_a X_b - q \widetilde{R}^{-1\,cd}_{\ \ ab} X_c P_d) = \mu^{-1} \left(\gamma_{ab} W + \frac{q-1}{qK} \epsilon_{ab}{}^m L_m \right)$$

and

$$-i(X_a P_b - q \widetilde{R}^{-1\,cd}_{\ \ ab} P_c X_d) = q^3 \mu \left(\gamma_{ab} W + \frac{q-1}{qK} \epsilon_{ab}{}^m L_m \right),$$

where $W \equiv \mu[1 + q^{-2}(1-q) X \cdot \overline{\partial}]$ is a real scalar, $L_i \equiv (1/q)\mu[X \times \overline{\partial}]_i$, and

$$K \equiv q - 1 + 1/q. \tag{3}$$

The L_i and W generate a q-deformed angular momentum algebra. Vectors Z_i (such as the X_i, ∂_j, and P_k) satisfy the following relations with L_i and W, generalizing the role of the L_i as generators of rotations:

$$L_i Z_j = -\epsilon_i{}^{cd} \epsilon_{dj}{}^e Z_c L_e + \epsilon_{ij}{}^a Z_a W,$$

$$L \cdot Z = Z \cdot L = 0,$$

$$W Z_j = K Z_j W - (K-1) \epsilon_j{}^{rs} Z_r L_s .$$

In addition, Z^2 commutes with the L_i and W. The L_i and W also satisfy the following relations:

$$L^2=\frac{W^2-1}{K-1}$$

and

$$[L\times L]_k=L_kW=WL_k\,.$$

$\mathscr{A}^X_{R^3_q}$ modulo powers of X^2 can be shown to be a direct sum, indexed by non-negative integers l, of irreducible representations of the angular momentum algebra. The lth representation is then $(2l+1)$ dimensional, and W is a Casimir operator with eigenvalue

$$w_l=\frac{q^{l+1}+q^{-l}}{q+1}. \tag{4}$$

For $q=1$, the eigenvalue of L^2 in the lth representation becomes the familiar $l(l+1)$.

As a last preliminary result, the momentum operators can be expressed in terms of W, μ, and X^2:

$$X^2P_i=\frac{1}{iK(q-1/q)(q-1)}\left[\frac{1}{q}\,X_iW\mu^{-1}-WX_i\mu^{-1}+q^2X_iW\mu-qWX_i\mu\right], \tag{5}$$

and

$$X^2P^2=\frac{1}{K^2(q-1/q)^2}\left[\frac{(q+1)^2}{q}\,W^2-q\mu^2-2-\frac{1}{q}\,(\mu^{-1})^2\right]. \tag{6}$$

These identities will be essential for calculations in the representation we will introduce later.

III. DEFINITION OF 1/*R*

$1/R$ is already a well-defined concept in the space of undeformed, complex functions on $\mathbb{R}^3$. Its essential properties are that it is a real, scalar function and that $X^2(1/R)^2=(1/R)^2X^2=1$. The simplest generalization of these properties is then to define $1/R$ to be a real, scalar corepresentation of $\mathrm{SO}_q(3)$. $\hat{\mathscr{A}}^X_{R^3_q}$ is then the * algebra generated by the X_i and $1/R$, where the X_i obey the same relations as in $\mathscr{A}^X_{R^3_q}$, $1/R$ commutes with the X_i, and

$$X^2\left(\frac{1}{R}\right)^2=1. \tag{7}$$

$\hat{\mathscr{D}}^X_{R^3_q}$ is the $\mathrm{SO}_q(3)$-covariant * algebra of operators on $\hat{\mathscr{A}}^X_{R^3_q}$, where we add $1/R$ to the generators of $\mathscr{D}^X_{R^3_q}$. For this definition to be complete we must have a set of relations involving $1/R$, μ, and the derivatives. These must be consistent with the relations between $1/R$ and the X_i. Clearly, since $1/R$ has dimensions of an inverse length, we should have

$$\mu\,\frac{1}{R}=q^{-1}\,\frac{1}{R}\,\mu.$$

Equation (7) allows us to find $\partial_i(1/R)$. Indeed, from

$$\partial_i X^2 \left(\frac{1}{R}\right)^2 = \partial_i(1) = 0,$$

it follows from the algebra of $\mathscr{D}^X_{R^3_q}$ that

$$\partial_i X^2 = (q^{-1}+1)X_i + q^2 X^2 \partial_i .$$

Thus,

$$(q^{-1}+1)X_i \frac{1}{R^2} + q^2 X^2 \partial_i \left(\frac{1}{R^2}\right) = 0,$$

and therefore

$$\partial_i \left(\frac{1}{R^2}\right) = -q^{-2}(q^{-1}+1)\frac{1}{R^4} X_i . \tag{8}$$

Note that we are using the notation that if $A \in \hat{\mathscr{D}}^X_{R^3_q}$, and $f \in \hat{\mathscr{A}}^X_{R^3_q}$, then $A(f) \in \hat{\mathscr{A}}^X_{R^3_q}$ is the result of evaluating the effect of A on f, whereas $Af \in \hat{\mathscr{D}}^X_{R^3_q}$ is the product of A and f as operators.

The simplest solution for $\partial_i(1/R)$ is

$$\partial_i \frac{1}{R} = q^{-1}\frac{1}{R}\partial_i - q^{-2}\frac{1}{R^3} X_i . \tag{9}$$

Repeated application of Eq. (9) indeed gives (8). Similarly, one finds that

$$\overline{\partial}_i \frac{1}{R} = q \frac{1}{R}\overline{\partial}_i - q^2 \frac{1}{R^3} X_i . \tag{10}$$

Equation (9) must be checked for consistency with the algebra of $\hat{\mathscr{A}}^X_{R^3_q}$ before we can conclude that $\hat{\mathscr{D}}^X_{R^3_q}$ is a consistent operator algebra. In particular, we must show that $\partial_i[(1/R)f] = \partial_i[f(1/R)]$, and $\partial_i[X^2(1/R^2)] = \partial_i[(1/R^2)X^2] = 0$. In addition, if $1/R$ is truly a scalar, it should commute with the L_i and W. The proofs that these conditions are satisfied are given in Appendix A.

Having defined $1/R$, we can now also define the q-deformed radius $R \equiv (1/R)X^2$. This has the following commutation relation with ∂_i:

$$\partial_i R = \partial_i \frac{1}{R} X^2 = \left[q^{-1}\frac{1}{R}\partial_k - q^{-2}\frac{1}{R^3} X_k\right] X^2 = q^{-1}\frac{1}{R}[(q^{-1}+1)X_i + q^2 X^2 \partial_i] - q^{-2}\frac{1}{R} X_i$$

$$= q^{-1}\frac{1}{R} X_i + qR\partial_i .$$

Induction over positive and negative n gives

$$\partial_i R^n = q^{-1}(n)_q R^{n-2} X_i + q^n R^n \partial_i ,$$

where

$$(n)_q \equiv \frac{q^n - 1}{q - 1}$$

is the asymmetric q analog. One can, in fact, develop a theory using ∂ or $\overline{\partial}$ as momentum operators and rewrite q-deformed harmonic oscillator theories in the language of R and integral powers of R. However, since ∂^2 and $\overline{\partial^2}$ are not self-adjoint, we will concentrate on the action of the P_i on elements of $\hat{\mathscr{H}}^X_{R^3_q}$.

IV. SEPARATION OF VARIABLES

Using the formalism developed in Sec. III, we can now consider the q analog of the separation of variables problem for the kinetic term of the Hamiltonian. To this end we first introduce q analogs of spherical harmonics. These are defined, up to a—for us irrelevant—normalization as elements $Y^{\,l}_{qm}$ of $\hat{\mathscr{H}}^X_{R^3_q}$ that obey the following two conditions.

(i) Left multiplication of $Y^{\,l}_{qm}$ by L^2 or by L_2 yields $Y^{\,l}_{qm}$ multiplied by a real eigenvalue; or, in other words, $Y^{\,l}_{qm}$ is an ''eigenfunction'' of both L^2 and L_2.

(ii) All $Y^{\,l}_{qm}$ commute with μ.

For illustration, we give the explicit expressions of $Y^{\,l}_{qm}$ for $l=0,1,2$,

$$Y^{\,0}_{q0} = 1, \quad Y^{\,1}_{q-1} = \frac{1}{R} X_1, \quad Y^{\,1}_{q0} = \frac{1}{R} X_2,$$

$$Y^{\,1}_{q1} = \frac{1}{R} X_3, \quad Y^{\,2}_{q-2} = \frac{1}{R^2} X_1{}^2, \quad Y^{\,2}_{q-1} = \frac{1}{R^2} X_1 X_2,$$

$$Y^{\,2}_{q0} = \frac{1}{R^2}\left[qX_1X_3 - \left(\sqrt{q} + \frac{1}{\sqrt{q}} \right) X_2X_2 + \frac{1}{q} X_3X_1 \right],$$

$$Y^{\,2}_{q1} = \frac{1}{R^2} X_2X_3, \quad Y^{\,2}_{q2} = \frac{1}{R^2} X_3{}^2.$$

Now, by multiplying Eqs. (5) and (6) on the left by K/R and K/R^2, respectively, we obtain

$$KP_i = \frac{1}{i[q-(1/q)](q-1)} \frac{1}{R}\left[\frac{1}{q} X_i W\mu^{-1} - WX_i\mu^{-1} + q^2 X_i W\mu - qWX_i\mu \right], \tag{11}$$

and

$$K^2P^2 = \frac{1}{[q-(1/q)]^2} \frac{1}{R^2}\left[\frac{(q+1)^2}{q} W^2 - q\mu^2 - 2 - \frac{1}{q}(\mu^{-1})^2 \right]. \tag{12}$$

Since μ commutes with the $Y^{\,l}_{qm}$ and W commutes with powers of R, if we expand functions in terms of $R^n Y^{\,l}_{qm}$, Equation (12) is ready made for calculating their momentum squared,

$$K^2P^2R^nY^{\,l}_{qm} = \frac{1}{[q-(1/q)]^2} \frac{1}{R^2}\left[\frac{(q+1)^2}{q} w_l^2 - q^{2n+1} - 2 - q^{-2n-1} \right] R^nY^{\,l}_{qm}$$
$$= \frac{q^{2l+1} + q^{-2l-1} - q^{2n+1} - q^{-2n-1}}{[q-(1/q)]^2} R^{n-2}Y^{\,l}_{qm}.$$

In terms of the symmetric q analog of n of Eq. (2), we can write this in the simplified form,

$$K^2P^2R^nY_{qm}^{\ l}=-[n+l+1]_q[n-l]_qR^{n-2}Y_{qm}^{\ l}. \tag{13}$$

This is a clear generalization of the result from ordinary real calculus that

$$\mathbf{\Delta}[r^nY_{lm}(\theta,\phi)]=(n+l+1)(n-1)r^{n-2}Y_{lm}(\theta,\phi),$$

and it is the main result of this section.

Equation (11) is not nearly as useful as its counterpart because the action of the X_i on $Y_{qm}^{\ l}$ is nontrivial. However, for powers of R, one can obtain the simple result that

$$iKP_i(R^n)=[n]_qR^{n-2}X_i=[n]_qR^{n-1}\frac{X_i}{R}. \tag{14}$$

V. THE FREE PARTICLE

Let us consider a system with the Hamiltonian,

$$H=K^2P^2,$$

with the convenient normalization factor K^2 determined by Eq. (3). Then the Schrödinger equation for this system is the q-deformed Helmholtz equation,

$$K^2P^2\psi=k^2\psi.$$

The solutions to this are of the form $j_{[q]l}(kR)Y_{qm}^{\ l}$ and $n_{[q]l}(kR)Y_{qm}^{\ l}$, where $j_{[q]l}$ and $n_{[q]l}$ are, respectively, the q-spherical Bessel and Neumann functions,

$$j_{[q]l}(x)=\sum_{n=0}^{\infty}\frac{(-1)^n[2n+2l]_q!!}{[2n]_q!![2n+2l+1]_q!}x^{2n+l}, \tag{15}$$

$$n_{[q]l}(x)=-\sum_{n=0}^{l-1}\frac{[2l-2n]_q!}{[2n]_q!![2l-2n]_q!!}x^{2n-l-1}+(-1)^{l+1}\sum_{n=l}^{\infty}\frac{(-1)^n[2n-2l]_q!!}{[2n]_q!![2n-2l]_q!}x^{2n-l-1}, \tag{16}$$

where for non-negative integers n,

$$[n]_q!\equiv\begin{cases}\Pi_{k=1}^{n}[k]_q, & n>0,\\ 1, & n=0,\end{cases} \tag{17}$$

and

$$[2n]_q!!\equiv\begin{cases}\Pi_{k=1}^{n}[2k]_q, & n>0\\ 1, & n=0.\end{cases} \tag{18}$$

That Eqs. (15) and (16) give rise to solutions is easily seen by applying Eq. (13). This eliminates the zeroth element, and then reindexing gives the desired result, as would be the case for the $q=1$ differential equation.

We can also obtain a q-deformed generalization of the Rayleigh formulas, which provide an alternative definition of these Bessel and Neumann functions. This will be a more convenient form for obtaining q-spherical Hankel functions,

$$h_{[q]l}^{(1)}(x)\equiv j_{[q]l}(x)+in_{[q]l}(x), \tag{19}$$

and

$$h^{(1)}_{[q]2}(x) \equiv j_{[q]l}(x) - i n_{[q]l}(x), \tag{20}$$

corresponding to incoming and outgoing spherical waves. These results are discussed in Appendix B.

It is interesting to note that, because the P_i do not commute, it is not possible to have a plane wave with definite momentum, as in ordinary quantum mechanics. The best we could do is specify the component of the momentum in the direction of propagation. Since, moreover, P_2, for example, does not commute with L_2, the problem of expanding even these quasiplane waves as a sum of $R^n Y^{\ l}_{qm}$ terms is nontrivial.

VI. THE q-COULOMB PROBLEM

In ordinary quantum mechanics, the Coulomb Hamiltonian is

$$H = \frac{p^2}{2m} - \frac{\alpha}{r};$$

or if we rescale this by $2m$ and incorporate the mass into α,

$$H = p^2 - \frac{2\alpha}{r}.$$

There are several possible ways to q-deform this. We are interested in a self-adjoint Hamiltonian that preserves the properties of the ordinary Hamiltonian that make it amenable to finding eigenfunctions. That is to say, we require the existence of a q-deformed Lenz vector that commutes with the q-deformed Hamiltonian, so that there continue to be degeneracies between solutions with different angular momentum quantum numbers.

Following Ref. 3, we define our q-deformed Coulomb Hamiltonian to be

$$H = K^2 P^2 - \alpha q \left(\frac{1}{R}\, \mu + \mu^* \, \frac{1}{R} \right),$$

which is clearly self-adjoint [for convenience, the normalization of the kinetic term has again been chosen with a prefactor K^2 determined by Eq. (3)]. Noting that $\mu^* = q^{-3}\mu^{-1}$, this can be written in the simpler form,

$$H = K^2 P^2 - \alpha \, \frac{1}{R} \, (q\mu + q^{-1}\mu^{-1}). \tag{21}$$

This Hamiltonian also commutes with the Lenz vector,

$$A_k \equiv \frac{[W, iKP_k]}{K-1} + \frac{\alpha X_k}{R} = iK(P_k W - (P \times L)_k) + \frac{\alpha X_k}{R}.$$

The Lenz vector along with the angular momentum operators then generate the algebra given in Ref. 3.

If we write the eigenvalues E of the Hamiltonian (21) in the form

$$E = -\left(\frac{\alpha}{[\gamma]_q} \right)^2, \tag{22}$$

then the corresponding ''eigenfunctions'' are (see Appendix C for their derivation)

$$\psi_{\gamma lm}=\sum_{p=0}^{\infty} A_p(\gamma)R^l\left(\frac{\alpha q^{\gamma}R}{[\gamma]_q}\right)^p \exp_q\left(\frac{-q^{l+1+p-\gamma}\alpha R}{[\gamma]_q}\right)Y^{\ l}_{qm}, \tag{23}$$

with

$$A_p(\gamma)=q^{pl+(1/2)p(p+1)}\,\frac{(1-q^2)^p(q^{2(l+1-\gamma)};q^2)_p}{(q^2;q^2)_p}\,\frac{(q^{2(l+1-\gamma)};q^2)_p}{(q^{2(2l+2)};q^2)_p}\,\frac{(q^{4(l+1)};q^4)_p}{(q^{2(l+1)};q^2)_p}. \tag{24}$$

Here

$$(a;u)_p\equiv\begin{cases}\Pi_{m=0}^{p-1}(1-au^m), & p=1,2,3,\ldots,\\ 1, & p=0,\end{cases} \tag{25}$$

is the q-deformed Pochhammer symbol,[7] with $u=q^2$ and q^4 in Eq. (24), and

$$\exp_q(x)=\sum_{n=0}^{\infty}\frac{x^n}{[n]_q!} \tag{26}$$

is the q-deformed exponential, where we have used the notation of Eq. (17). q^{γ} is obtained in terms of the energy E from the quadratic equation (22). This has two solutions:

$$q^{-\gamma_{\pm}}=\frac{\eta\pm\sqrt{\eta^2-E}}{\sqrt{-E}}, \tag{27}$$

with η given by

$$\eta=\frac{(q^{-1}-q)\alpha}{2}. \tag{28}$$

(We assume $q<1$ to ensure convergence; had we instead set $q>1$, we would have to everywhere change $q\to q^{-1}$.)

Note that for a given energy, we actually only have one solution since if we write the solutions as a power series in R, the difference equation admits only one solution that behaves as R^l for small R. Whether we write it in terms of γ_+ or γ_- simply gives us two expressions for the same result.

In ordinary quantum mechanics, a decaying exponential multiplied by a polynomial in the radial coordinate is normalizable and gives rise to a bound state. Something very similar happens in the $q\neq 1$ limit. Consider the wave function (23), which is a sum of terms, each of which is a non-negative power of R multiplying a q exponential of the form $\exp_q(-c_q(p)R)$. As can be seen from (23), the $c_q(p)$ become independent of p as $q\to 1$, thus reproducing the usual result. Then we define a bound state in the q-deformed case to be a wave function of the type (23) for which the sum over p truncates at the finite value $p=n-l-1$. On account of the factor $(q^{2(l+1-\gamma)};q^2)_p$ in the numerator of (24), such a truncation occurs if γ equals a positive integer $n>l$. From Eq. (22), we then obtain the q-Balmer formula, and we find the corresponding wave functions given by (23) and (24). The q-Balmer formula already appears in Refs. 3 and 7. In Ref. 3, as noted in the Introduction, the operator $1/R$ is treated differently. This difference is reflected in our wave functions.

In principle, these same wave functions (23) should also cover the continuum part of the spectrum, and one should be able to extract an S-matrix from them. How to do this in a rigorous fashion remains to be seen. Here we consider the candidate S matrix suggested by Eq. (24),

$$S_l^{(q)}(E)=(1-q^2)^{(\gamma_- -\gamma_+)}\,\frac{\Gamma_{q^2}(l+1-\gamma_+)}{\Gamma_{q^2}(l+1-\gamma_-)}=\prod_{n=0}^{\infty}\,\frac{1-q^{2(l+1-\gamma_-+n)}}{1-q^{2(l+1-\gamma_++n)}},\tag{29}$$

where the q-gamma function is defined as in Ref. 8:

$$\Gamma_{q^2}(x):=\frac{(q^2;q^2)_\infty}{(q^{2x};q^2)_\infty}\,(1-q^2)^{1-x}.\tag{30}$$

The S matrix (29) appears to have all the right features.

(A) For $q\to 1$ this S matrix reproduces the familiar Coulomb S matrix. In this limit the prefactor goes to unity, as can be seen from Eq. (27), and the q-gamma functions become precisely the ordinary gamma functions that appear in the ordinary Coulomb S matrix.

(B) For integer $\gamma_+\geqslant l+1$, $S_l^{(q)}(E)$ has a pole corresponding to a q-Balmer state. Both the location and the residue of this pole differ from those of its ordinary ($q=1$) Balmer limit.

(C) As can be seen from Eqs. (29) and (27) the branch point of $S_l^{(q)}(E)$, the scattering threshold, is now located at $E=\eta^2$, with η given in Eq. (28) and not at $E=0$, as in the ordinary case. This is the most dramatic departure from the ordinary case: the scattering region starts at $E=\eta^2$. For $q=1$ this reduces to the expected threshold $E=0$.

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APPENDIX A: PROPERTIES OF 1/*R*

We have already satisfied $\partial_i[X^2(1/R^2)]=0$. The definition Eq. (9) of $\partial_i(1/R)$ also satisfies the other half of the second constraint,

$$\partial_i\,\frac{1}{R^2}=q^{-2}\,\frac{1}{R^2}\,\partial_i-q^{-2}(q^{-1}+1)\,\frac{1}{R^4}\,X_i,$$

$$\partial_i\left(\frac{1}{R^2}\,X^2\right)=\left[q^{-2}\,\frac{1}{R^2}\,\partial_i+q^2X^2\partial_i\right](1)-q^{-2}(q^{-1}+1)\,\frac{1}{R^2}\,X_i=0.$$

Trivially, $\partial_i 1(1/R)=\partial_i(1/R)1=\partial_i(1/R)$. Suppose that

$$\partial_i f\,\frac{1}{R}==\partial_i\,\frac{1}{R}\,f,$$

where $f\in\hat{\mathscr{A}}^X_{R_q^3}$. Then

$$\begin{aligned}
\partial_i X_j f\,\frac{1}{R} &= [\,\gamma_{ij} + q\widetilde{R}^{-1}{}^{kl}_{ij} X_k \partial_l] f\,\frac{1}{R} \\
&= \gamma_{ij} f\,\frac{1}{R} + q\widetilde{R}^{-1}{}^{kl}_{ij} X_k \partial_l\,\frac{1}{R}\,f \\
&= \gamma_{ij} f\,\frac{1}{R} + q\widetilde{R}^{-1}{}^{kl}_{ij} X_k \left(q^{-1}\,\frac{1}{R}\,\partial_l - q^{-2}\,\frac{1}{R^3}\,X_l \right) f \\
&= \gamma_{ij} f\,\frac{1}{R} - q^{-2}\delta_i^k \delta_j^l\,\frac{1}{R^3}\,X_k X_l f + q^{-1}\epsilon_a{}^{kl}\epsilon_i{}^{ja} X_k X_l f\,\frac{1}{R^3} \\
&\quad - q^{-1}(q-1)\gamma^{kl}\gamma_{ij}\,\frac{1}{R^3}\,X_k X_l f + \frac{1}{R}\,\widetilde{R}^{-1}{}^{kl}_{ij} X_k \partial_l f \\
&= q^{-1}\gamma_{ij} f\,\frac{1}{R} + \frac{1}{R}\,\widetilde{R}^{-1}{}^{kl}_{ij} X_k\,\partial_l f - q^{-2}\,\frac{1}{R^3}\,X_i X_j f,
\end{aligned}$$

where we used the fact that $\epsilon_a{}^{kl} X_k X_l = 0$. At the same time,

$$\partial_i\,\frac{1}{R}\,X_j f = \left(q^{-1}\,\frac{1}{R}\,\partial_i - q^{-2}\,\frac{1}{R^3}\,X_i \right) X_j f = q^{-1}\,\frac{1}{R}[\,\gamma_{ij} + q\widetilde{R}^{-1}{}^{kl}_{ij} X_k \partial_l] f - q^{-2}\,\frac{1}{R^3}\,X_i X_j f = \partial_i X_j\,f\,\frac{1}{R}.$$

We must also show that

$$\partial_i\,\frac{1}{R}\,f\,\frac{1}{R} = \partial_i f\,\frac{1}{R}\,\frac{1}{R}$$

in order to complete this inductive proof. However, this is trivial, having assumed that $\partial_i f(1/R) = \partial_i (1/R) f$. Thus, $\hat{\mathscr{H}}^X_{R^3_q}$ and $\hat{\mathscr{D}}^X_{R^3_q}$ are consistently defined.

If $1/R$ is truly a scalar, it should commute with the L_i and W. This is indeed true:

$$W = \mu[1 + q^{-2}(1-q) X \cdot \overline{\partial}],$$

$$X \cdot \frac{1}{R} = \gamma^{ij} X_i \overline{\partial j}\,\frac{1}{R} = \gamma^{ij} X_i \left[q\,\frac{1}{R}\,\overline{\partial_j} - q^2\,\frac{1}{R^3}\,X_j \right] = q\,\frac{1}{R}\,X \cdot \overline{\partial} - q^2\,\frac{1}{R},$$

$$\begin{aligned}
W\,\frac{1}{R} &= \mu\left[\frac{1}{R} + (q^{-2} - q^{-1}) \left(q\,\frac{1}{R}\,X \cdot \overline{\partial} - q^2\,\frac{1}{R} \right) \right] \\
&= \mu\left[q\,\frac{1}{R} + q\,\frac{1}{R}\,(q^{-2} - q^{-1}) X \cdot \overline{\partial} \right] \\
&= \frac{1}{R}\,\mu[1 + (q^{-2} - q^{-1}) X \cdot \overline{\partial}] \\
&= \frac{1}{R}\,W,
\end{aligned}$$

$$L_i = \mu q^{-1}[X \times \overline{\partial}]_i,$$

$$[X \times \overline{\partial}]_i\,\frac{1}{R} = \epsilon_i{}^{jk} X_j \overline{\partial_k}\,\frac{1}{R} = \epsilon_i{}^{jk} X_j \left[q\,\frac{1}{R}\,\overline{\partial_k} - q^2\,\frac{1}{R^3}\,X_k \right] = q\,\frac{1}{R}\,\epsilon_i{}^{jk} X_j \overline{\partial_k} = q\,\frac{1}{R}\,[X \times \overline{\partial}]_i,$$

$$L_i\,\frac{1}{R} = \mu q^{-1}[X \times \overline{\partial}]_i\,\frac{1}{R} = \mu q\,\frac{1}{R}\,q^{-1}[X \times \overline{\partial}]_i = \frac{1}{R}\,\mu q^{-1}[X \times \overline{\partial}]_i = \frac{1}{R}\,L_i.$$

APPENDIX B: q-DEFORMED RAYLEIGH FORMULAS

Let D be the symmetric q derivative:

$$Df(x)\equiv\frac{f(qx)-f(q^{-1}x)}{(q-q^{-1})x}. \tag{B1}$$

Acting on monomials,

$$Dx^n=[n]_q x^{n-1}. \tag{B2}$$

Let us define the following q generalizations of some common functions by replacing factorials with q-deformed factorials in their Taylor expansions:

$$\exp_q(x)\equiv\sum_{n=0}^{\infty}\frac{x^n}{[n]_q!}, \tag{B3}$$

$$\cos_q(x)\equiv\sum_{n=0}^{\infty}\frac{(-1)^n x^{2n}}{[2n]_q!}, \tag{B4}$$

$$\sin_q(x)\equiv\sum_{n=0}^{\infty}\frac{(-1)^n x^{2n+1}}{[2n+1]_q!}. \tag{B5}$$

Then $\exp_q(ix)=\cos_q(x)+i\,\sin_q(x)$.

The q-deformed Rayleigh formulas,

$$j_{[q]l}(x)=(-x)^l\left(\frac{1}{x}D\right)^l\left(\frac{\sin_q(x)}{x}\right), \tag{B6}$$

$$n_{[q]l}(x)=(-x)^l\left(\frac{1}{x}D\right)^l\left(\frac{-\cos_q(x)}{x}\right), \tag{B7}$$

can then be proved by induction after noting that

$$j_{[q]0}(x)=\frac{\sin_q(x)}{x} \tag{B8}$$

and

$$n_{[q]0}x=-\frac{\cos_q(x)}{x}. \tag{B9}$$

The q-deformed spherical Hankel functions are

$$h^{(1)}_{[q]l}(x)\equiv j_{[q]l}(x)+in_{[q]l}(x), \tag{B10}$$

and $h^{(2)}_{[q]l}(x)$ is just the complex conjugate of $h^{(1)}_{[q]l}(x)$. Since $(-x)^l[(1/x)D]^l$ is a linear operator, it follows that $h^{(1)}_{[q]l}$ should satisfy

$$h^{(1)}_{[q]l}(x)=(-x)^l\left(\frac{1}{x}D\right)^l\left(\frac{-i\,\exp_q(ix)}{x}\right).$$

One can show by induction that

$$h^{(1)}_{[q]l}(x)=\sum_{n=0}^{l} q^{(1/2)[l(l+1)-n(n+1)]}\,\frac{i^{n-l-1}[l+n]_q!}{[2n]_q!![l-n]_q!}\,\frac{\exp_q(iq^n x)}{x^{n+1}}, \tag{B11}$$

satisfies this Rayleigh formula for all l. Thus, these functions must equal the Hankel functions.

The powers of q that appear both inside and outside the q exponential arise because

$$\begin{aligned} D(x^k\,\exp_q(\alpha x)) &= [k]_q x^{k-1}\,\exp_q(\alpha q x)+\alpha q^{-k}x^k\,\exp_q(\alpha x)\\ &= [-k]_q x^{k-1}\,\exp_q\!\left(\alpha\,\frac{1}{q}\,x\right)+\alpha q^k x^k\,\exp_q(\alpha x). \end{aligned}$$

This results from the q-deformed arithmetic in which

$$[n+k]_q=q^n[k]_q+q^{-k}[n]_q=q^{-n}[k]_q+q^k[n]_q. \tag{B12}$$

It appears to be a common trend of solutions to self-adjoint q-deformed Hamiltonians that they can be expressed as a series of the form $\Sigma_n A_n \exp_q(q^n x)$.

APPENDIX C: q-COULOMB HAMILTONIAN EIGENVALUE PROBLEM

Let $\beta=\sqrt{-E}$ and $[\gamma]_q=\alpha/\beta$. In order to obtain a difference equation for the A_p, we need to express $(H+\beta^2)\psi$ as a series of the form $\Sigma_p B_p \exp_q(q^p x)$, where B_p is a function of the A_p.

If we simply apply $(H+\beta^2)$ to any term of ψ using Eq. (13), we get

$$\begin{aligned} (H+\beta^2)R^{l+p}\,\exp_q(-q^s\beta R)Y^{\,l}_{qm} &= -\sum_{n=0}^{\infty}\frac{[n+p+2l+1]_q[n+p]_q}{[n]_q!}\,(-q^s\beta)^n R^{n+p+l-2}Y^{\,l}_{qm}\\ &\quad -\alpha\sum_{n=0}^{\infty}\frac{(q^{n+l+p-1}+q^{-n-l-p-1})}{[n]_q!}\,(-q^s\beta)^n R^{n+p+l-1}Y^{\,l}_{qm}\\ &\quad +\beta^2 R^{l+p}\,\exp_q(-q^s\beta R)Y^{\,l}_{qm}. \end{aligned}$$

If we decompose $[n+p+2l+1]_q[n+p]_q$, we get terms proportional to $[n]_q[n-1]_q$, $q^{-n}[n]_q$, and q^{-2n}. By resumming these terms, we can rewrite them as powers of R times exponentials. We wish to rewrite the entire equation in terms of functions of the form $R^{l+p-m}\exp_q(-q^{s+m}\beta R)Y^{\,l}_{qm}$, where m is an integer and s is a function of p. Then we can obtain a difference equation for the coefficients of these functions. In the following, we assume that $s=-l-1-p+\gamma$. The only terms that need to be rewritten are then

$$\left(K^2P^2-\alpha\,\frac{1}{R}\,q^{-1}\mu^{-1}\right)R^{l+p}\,\exp_q(-q^{-l-1-p+\gamma}\beta R)Y_{qm}^{\ l}$$

$$=-\sum_{n=0}^{\infty}\frac{[n+2l+p+1]_q[n+p]_q}{[n]_q!}\,(q^{l+1+p-\gamma}\beta)^nR^{n+l+p-2}Y_{qm}^{\ l}-[\gamma]_q\beta\sum_{n=0}^{\infty}\frac{q^{n+l+p+1}}{[n]_q!}$$

$$\times(-q^{l+1+p-\gamma}\beta)^nR^{n+l+p-1}Y_{qm}^{\ l}$$

$$=-\sum_{n=0}^{\infty}([n+2l+p+1]_q[n+p]_q-q^{-1+n+\gamma}[n]_q[\gamma]_q)\,\frac{(-q^{l+1+p-\gamma}\beta)^n}{[n]_q!}\,R^{n+l+p-2}Y_{qm}^{\ l}$$

$$=-\sum_{n=0}^{\infty}\{(q^{2p+2l+2}+1-q^{2\gamma})[n]_q[n-1]_q+q^{-2n}[p+2l+1]_q[p]_q+q^{-n}[n]_q$$

$$\times(-q^{1+\gamma}[\gamma]_qq^{p+2l+1}[p]_q+q^{1+p}[2l+2+p]_q)+q^{-2n}[p+2l+1]_q[p]_q\}$$

$$\times\frac{(-q^{l+1+p-\gamma}\beta)^n}{[n]_q!}\,R^{n+l+p-2}Y_{qm}^{\ l}$$

$$=\beta^2(q^{2l+2+2p}-q^{2l+2+2p-2\gamma}-q^{4l+4p+4-2\gamma})R^{l+p}\,\exp_q(-q^{-l-1-p+\gamma}\beta R)$$

$$\times Y_{qm}^{\ l}-\beta(q^{l+p+1}[\gamma]_q-q^{2p+3l+1-\gamma}[p]_q-q^{l+2p+1-\gamma}[2l+p+2]_q)R^{l+p-1}$$

$$\times\exp_q(-q^{-l-p+\gamma}\beta R)Y_{qm}^{\ l}-[p+2l+1]_q[p]_qR^{l+p-2}$$

$$\times\exp_q(-q^{-l-p+1+\gamma}\beta R)Y_{qm}^{\ l}.$$

Thus,

$$(H+\beta^2)R^{l+p}\,\exp_q(-q^{-l-p-1+\gamma}\beta R)Y_{qm}^{\ l}$$

$$=q^{2l+2p+2-\gamma}[2]_{q^{-l-p-1}}[l+p+1-\gamma]_q(q^{-1}-q)\beta^2R^{l+p}$$

$$\times\exp_q(-q^{-l-1-p+\gamma}\beta R)Y_{qm}^{\ l}+(q^{2p+3l+1-\gamma}[p]_q$$

$$+q^{l+2p+1-\gamma}[2l+p+2]_q-[2]_{q^{l+p+1}}[\gamma]_q)\beta R^{l+p-1}$$

$$\times\exp_q(-q^{-l-p+\gamma}\beta R)Y_{qm}^{\ l}-[p+2l+1]_q[p]_qR^{l+p-2}$$

$$\times\exp_q(-q^{-l-p+1+\gamma}\beta R)Y_{qm}^{\ l}.$$

If we sum over p from 0 to ∞, we can obtain the desired difference equation. We normalize the wave functions so that $A_0=1$. Then

$$A_1=q^{l+1}\beta\,\frac{[2]_{q^{l+1}}[l+1-\gamma]_q}{[2l+2]_q},$$

and for $p>0$,

$$\{[p+2l+3]_q[p+2]_q\}A_{p+2}=q^{2l+2p+2-\gamma}[2]_{q^{l+p+1}}[l+p+1-\gamma]_q(q^{-1}-q)\beta^2A_p$$

$$+(q^{2p+3l+3-\gamma}[p+1]_q+q^{l+2p+3-\gamma}[2l+p+3]_q$$

$$-[2]_{q^{-l-p-2}}[\gamma]_q)\beta A_{p+1}.$$

Equation (24) is then a solution to this difference equation. Thus the theorem is proved.

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Reduced SL(2,*R*) WZNW quantum mechanics

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The SL(2,*R*) WZNW→Liouville reduction leads to a nontrivial phase space on the classical level both in 0+1 and 1+1 dimensions. To study the consequences in the quantum theory, the quantum mechanics of the 0+1-dimensional, point particle version of the constrained WZNW model is investigated. The spectrum and the eigenfunctions of the obtained (rather nontrivial) theory are given, and the physical connection between the pieces of the reduced configuration space is discussed in all the possible cases of the constraint parameters. © *1996 American Institute of Physics.* [S0022-2488(96)00903-0]

I. INTRODUCTION

In the past several years the Toda models have been studied intensively. In these field theories scalar fields are coupled to each other by certain special exponential terms, in a way that corresponds to a simple Lie algebra. The Toda models can be considered as generalizations of the Liouville theory, which is of particular interest since it appears in many problems of physics and mathematics. An interesting means of deriving and studying the remarkable properties—integrability, conformal invariance and *W*-algebraic symmetry—of the Toda models is offered by the observation that the Toda theories can be obtained by a suitable reduction of the Wess–Zumino–Novikov–Witten (WZNW) model.[1] The WZNW model is a theory of a field that takes its values from a Lie group G, and the reduction procedure, by imposing appropriate (first class) constraints, associates it to a Toda theory that corresponds to the Lie algebra of G. In the case $G=\mathrm{SL}(2,R)$, the reduced theory is nothing but the Liouville theory.

However, the connection between the WZNW and Toda models is more intricate. A closer look at the reduction procedure shows that it yields not exactly the Toda theory but a richer structure; the Toda theory arises only as a component, a subsystem of it. This aspect was first noticed in Ref. 2. To study the precise relation of the Toda models to the WZNW ones a recent work examined the SL(2,*R*) WZNW→Liouville reduction from the phase space point of view.[3] The authors considered the classical SL(2,*R*) WZNW model, imposed the appropriate constraints, and described the reduction of the phase space under the constraints. They found that the reduced phase space contains two subsystems (nonintersecting open submanifolds) that admit a clear physical interpretation. On both subsets the reduced WZNW theory leads to the Liouville theory locally, but these two copies of Liouville theories are not independent. The connection between them comes from a ''border line,'' a lower-dimensional surface in the reduced phase space connecting them. For a better understanding of the situation, the authors of Ref. 3 carried out a similar analysis on the 0+1 dimensional, point mechanical analogue of the SL(2,*R*) WZNW model. This can be thought of as the space-independent version, the ''zero mode sector'' of the WZNW model. In Ref. 3 it was found that, depending on the signs of the constraint parameters, one can arrive at two different types of reduced theories. In both cases the phase space reduces into two locally independent parts. The difference is that when the constraint parameters have equal signs the two halves are disconnected, there is no ''border line'' between them. As a result a classical motion cannot touch both parts. Actually, though the reduced Hamiltonian is not of the usual form of the sum of a kinetic and a potential term, the system behaves as if the two halves of the reduced

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one-dimensional configuration space were separated by an infinitely high potential barrier. On the other hand, if the signs of the constraint parameters are opposite, then an analogue of an infinitely deep potential well characterizes the situation. In this case the two ''half-worlds'' are connected; a motion can cross the point that separates the two halves of the reduced configuration space. Moreover, the negative energy motions will oscillate between the two parts. In Ref. 3 it is concluded that it is not enough to give the (global) reduced theory in the local coordinates of the reduced phase space. The arising two components of the reduced theory seem to be independent while actually they may have a physical connection, a correlated behavior which can be discovered only from the global point of view. [Reference 3 also contains results about the SL(n,R) point particle model and discovers some similar properties for $n>2$ as well.]

These are the features of the classical theories. What happens on the quantum level? Because of the expected difficulties of quantizing the SL(2,R) WZNW model it is useful to examine the point particle version. Turning to the masspoint theory the following questions arise naturally: what kind of relation connects the two half-worlds in the quantum theory? Are there any oscillating motions quantum mechanically when the the constraint parameters are of opposite sign? Similarly we may ask if in the case of coinciding signs the separation remains or a tunneling is allowed. Moreover, in the first case one may expect negative energy bound states. Are they really present? In this paper we solve the quantum theory of the masspoint version, and thus we can answer whether our expectations based on the classical behavior hold. While, as a consequence of its rather nontrivial characteristics, the point particle problem is interesting in itself, its properties are expected to shed a light on the field theoretical case, just as it happened on the classical level.[3]

The paper is organized as follows. In Secs. II and III we present the classical mechanics of the SL(2,R) masspoint before, resp. after, imposing the point mechanical form of the WZNW $\rightarrow$Liouville constraints. The quantum mechanics of the unconstrained and the constrained systems are established in Sec. IV. The reduced system splits into two parts in a symmetric way, and in Sec. V we give the eigenfunctions on one such part. In Sec. VI we investigate the orthogonality and the completeness properties of these ''half-eigenfunctions.'' The connection between the two parts is examined in Sec. VII. In Sec. VIII, we discuss the coordinate independence of the definition of the constrained system. In Sec. IX we give the conclusions of the paper. The outline of the larger proofs and calculations belonging to the statements of Sec. VI is presented in the Appendix.

II. THE CLASSICAL MECHANICS OF THE UNCONSTRAINED THEORY

The SL(2,R) WZNW model is defined by the following action:

$$S_0=\frac{m}{4\pi}\int d\sigma\, d\tau\, \mathrm{Tr}[(g^{-1}\partial_\tau g)^2-(g^{-1}\partial_\sigma g)^2]+m'\int d^3x\,\epsilon^{ijk}\,\mathrm{Tr}(g^{-1}\partial_i g g^{-1}\partial_j g g^{-1}\partial_k g), \tag{1}$$

where σ and τ coordinate a two-dimensional Minkowski space, and g is an SL(2,R)-valued function of σ and τ being periodic in σ with period 2π. The coefficients of the first term, the action of the SL(2,R) sigma model, and the second, a topological term called the Wess–Zumino term, are denoted by $m/4\pi$ and m', respectively. The point particle version, i.e., the physics of the zero modes of the field theory (1) is defined by restricting the configurations to the space-independent ones $g=g(\tau)$ only. Then the action reduces to

$$S=\frac{m}{2}\int d\tau\,\mathrm{Tr}[(g^{-1}\partial_\tau g)^2]. \tag{2}$$

The motion of the point particle is a function $g:R\rightarrow$SL(2,R); we can see that the Wess–Zumino term does not contribute to the masspoint version. The theory posesses left and right translation

symmetries under the transformations $g\mapsto hg$, $g\mapsto gh^{-1}$, $h\in \mathrm{SL}(2,R)$, and the corresponding conserved quantities are $J=\dot{g}g^{-1}$ and $\tilde{J}:=g^{-1}\dot{g}$, taking their values in sl(2,R), the Lie algebra of SL(2,R).

The equation of motion following from the action (2) is $(g^{-1}\dot{g})^{\cdot}=0$. Its solution is $g(t)=g(0)e^{At}$, where $A\in \mathrm{sl}(2,R)$ is a kind of initial data specified by the initial conditions as $A=g(0)^{-1}\dot{g}(0)$. The solution can also be written in the form $g(t)=g(0)[\cosh(rt)\mathbf{1}+[\sinh(rt)/r]A]$ with $r^2=\frac{1}{2}\mathrm{Tr}[A^2]$. This formula also holds for $\mathrm{Tr}[A^2]<0$ with r being imaginary and for $\mathrm{Tr}[A^2]=0$ with $\cosh(rt)\to 1$, $\sinh(rt)/r\to t$. The $r^2<0$ solutions are closed because of their trigonometrical time dependence and the $r^2\geqslant 0$ motions are open.

To study the canonical structure of the theory let us consider a parametrization of SL(2,R) $g(\xi^i)$, $i=1,2,3$. The Lagrangian, the canonical momenta, and the Hamiltonian are

$$L(\xi,\dot{\xi})=\frac{m}{2}\,h_{kl}(\xi)\dot{\xi}^k\dot{\xi}^l,\quad p_k=\frac{\partial L}{\partial\dot{\xi}^k}=mh_{kl}\dot{\xi}^l,\quad \mathscr{H}(\xi,p)=\frac{1}{2m}\,h^{kl}p_kp_l, \tag{3}$$

where $h_{kl}(\xi)=\mathrm{Tr}[g^{-1}\partial_k g g^{-1}\partial_l g]$ is the metric tensor on SL(2,R).

Easily, the value of the Hamiltonian on a solution of the equation of motion is equal to the value of the Lagrangian, thus the energy of a motion is $E=(m/2)\mathrm{Tr}[A^2]=mr^2$. Consequently, the motions with negative energy are the closed ones and the motions with non-negative energy are the open ones.

Let us turn to a special parametrization, namely the one which is based on the Gauss decomposition:

$$\begin{pmatrix}\alpha & \beta\\ \gamma & \delta\end{pmatrix}=\begin{pmatrix}1 & a\\ 0 & 1\end{pmatrix}\begin{pmatrix}1/\delta & 0\\ 0 & \delta\end{pmatrix}\begin{pmatrix}1 & 0\\ c & 1\end{pmatrix}. \tag{4}$$

This parametrization describes any $\left(\begin{smallmatrix}\alpha & \beta\\ \gamma & \delta\end{smallmatrix}\right)\in \mathrm{SL}(2,R)$ except those having $\delta=0$. With $\delta=\xi^1$, $a=\xi^2$, and $c=\xi^3$, $\{h_{kl}\}$ is of the form

$$\{h_{kl}\}=\begin{pmatrix}2/\delta^2 & 0 & 0\\ 0 & 0 & \delta^2\\ 0 & \delta^2 & 0\end{pmatrix}. \tag{5}$$

Calculating the Hamiltonian in this parametrization yields

$$\mathscr{H}(\delta,a,c,p_\delta,p_a,p_c)=\frac{1}{4m}\,\delta^2p_\delta^2+\frac{1}{m}\,\frac{p_ap_c}{\delta^2}. \tag{6}$$

Expression (6) shows that a and c are cyclic coordinates since $\mathscr{H}$ is independent of them. This is an advantage of using the parameters δ,a,c. Later we will see that this parametrization fits very well for our further considerations. That is why in the following we will work in these coordinates.

III. THE CONSTRAINED MODEL ON THE CLASSICAL LEVEL

Now we impose the constraints that reduce the SL(2,R) WZNW theory to the Liouville one. For space-independent configurations they read

$$\mathrm{Tr}[e_{12}\dot{g}g^{-1}]=\mu,\quad \mathrm{Tr}[e_{21}g^{-1}\dot{g}]=\nu, \tag{7}$$

where $e_{12}=\left(\begin{smallmatrix}0 & 1\\ 0 & 0\end{smallmatrix}\right)$ and $e_{21}=\left(\begin{smallmatrix}0 & 0\\ 1 & 0\end{smallmatrix}\right)$. Expressing (7) in the δ,a,c parametrization gives

$$p_a=m\mu,\quad p_c=m\nu. \tag{8}$$

As p_a and p_c are constants of the unrestricted motion we see that the constraints mean nothing else but a special choice of some of the initial conditions. This is a general feature of first class constraints; that these constants of motion happen to be canonical momenta is the real advantage of the parameters δ,a,c.

The reduced phase space can be obtained by factorizing the complete phase space by the gauge transformations these first class constraints generate. The action of these gauge transformations is

$$g\mapsto e^{\theta_L e_{12}} g e^{\theta_R e_{21}} = \begin{pmatrix} 1 & \theta_L \\ 0 & 1 \end{pmatrix} g \begin{pmatrix} 1 & 0 \\ \theta_R & 1 \end{pmatrix} \tag{9}$$

(see Ref. 3) where θ_L and θ_R are the two parameters of the transformations. This symmetry transformation acts on a and c as $a\mapsto a+\theta_L$, $c\mapsto c+\theta_R$, while it leaves δ, p_δ, p_a, and p_c invariant. Thus the factorization simply means that δ and p_δ parametrize the reduced phase space.

Any motion $\delta(t),p_\delta(t)$ allowed by the constrained dynamics corresponding to the constraint parameters μ and ν can be obtained by taking a solution $\delta(t)$, $a(t)$, $c(t)$, $p_\delta(t)$, p_a, p_c of the unconstrained theory where $p_a=m\mu$ and $p_c=m\nu$. Roughly speaking we just have to omit $a(t)$ and $c(t)$. The coordinate $\delta\in R$ survives the reduction, thus one may consider it as the coordinate of the one-dimensional configuration space of the reduced theory. The constrained dynamics is governed by the Hamiltonian

$$H(\delta,p_\delta)=\frac{1}{4m}\,\delta^2 p_\delta^2+ms\,\frac{1}{\delta^2}, \tag{10}$$

where $s=\mu\nu$.

Until now we have found the Gauss decomposition a very appropriate way of introducing coordinates on the group SL(2,*R*) to reach the canonical structure of the reduced system. Now let us face the problematic side of this approach.

The topology of SL(2,*R*) is not R^3 but $R^2\times S^1$, consequently it cannot be covered by a single parametrization. In the case of the Gauss decomposition the signal of this is that the Gauss decomposition works only for $\delta\neq 0$ and the elements $\left(\begin{smallmatrix}\alpha & \beta\\ \gamma & 0\end{smallmatrix}\right)$ are left out. As a result the canonical coordinates δ, a, c, p_δ, p_a, and p_c parametrize only two nonintersecting open submanifolds, two ''open halves'' of the whole phase space, corresponding to the two regions $-\infty<\delta<0$ and $0<\delta<\infty$. In particular, the point $\delta=0$ is left out from the reduced configuration space. In the meantime, extracted from the solution of the equation of motion, the time dependence of δ is of the form $\delta(t)=C_1\sinh(rt)/r+C_2\cosh(rt)$, where C_1 and C_2 are arbitrary constants. Thus we can see that there exist motions that cross the $\delta=0$ surface in the whole phase space, for example, for imaginary values of r oscillations occur between the regions $\delta>0$ and $\delta<0$. Furthermore, for such a motion p_δ tends to infinity as the particle reaches $\delta=0$. This can be seen from $p_\delta(t)=2m\dot{\delta}/\delta^2$, the connection between p_δ and the smoothly varying quantity $\dot{\delta}$ [cf. (3) and (5)]. Hence the coordinates δ,p_δ of the reduced phase space seem to be able to describe only those parts of a motion when $\delta(t)\neq 0$; they cannot give an account of how the particle moves across $\delta=0$.

Fortunately we can overcome these difficulties. First, let us complete the reduced configuration space by mapping the points $\left(\begin{smallmatrix}\alpha & \beta\\ \gamma & 0\end{smallmatrix}\right)$ of the configuration space of the unconstrained system to the point $\delta=0$ of the reduced configuration space, just as we have mapped the points $\left(\begin{smallmatrix}\alpha & \beta\\ \gamma & \delta\neq 0\end{smallmatrix}\right)$ to δ. Second, let the recipe to follow a motion through $\delta=0$ be to fit the quantity $\delta^2 p_\delta$. This recipe is clear from the unconstrained point of view: we simply fit $\dot{\delta}$ here. By these tricks we can eliminate the disadvantage of working with only one parametrization instead of covering SL(2,*R*) with more than one patch. Clearly, the canonical formalism of the unconstrained system also owes the problem of the missing $\delta=0$. Nevertheless, the solution given here for the reduced system applies in a straightforward way for the unconstrained one, too.

We will see that the $\delta=0$ problem also arises in the quantum theory. There it appears as an irregular singularity of the Hamiltonian at $\delta=0$ and the challenge will be to define the quantum theory on the whole configuration space despite this singularity.

Finally let us introduce a canonical transformation which transforms the constrained Hamiltonian to a form of a sum of a kinetic and a potential term. This can be achieved by the following transformation:

$$x:=\sqrt{2}\ \ln\ \delta, \tag{11}$$

$$p_x:=\frac{1}{\sqrt{2}}\ \delta p_\delta. \tag{12}$$

The resulting Hamiltonian is

$$H_x(x,p_x)=\frac{1}{2m}\ p_x^2+mse^{-\sqrt{2}x}. \tag{13}$$

The price we have to pay for having such a nice Hamiltonian is that by (11) we restricted ourselves to $\delta>0$ only. [Or, because of the $\delta\leftrightarrow-\delta$ symmetry of the system, we restricted ourselves to $\delta<0$, if writing $-\delta$ instead of δ in (11).] Remarkably, the logarithmic connection between x and δ is the point mechanical analogue of the one that relates the field of the reduced SL(2,*R*) WZNW theory to the Liouville field ϕ in the field theoretical case.[2]

With the aid of (13) it is easy to analyze the three qualitatively different situations arising. If $s>0$, then the potential increases exponentially as we travel to the negative x direction. Thus for all the allowed motions with positive energies there is a turning point when moving to the negative direction towards $x=-\infty$ ($\delta=0$). In this case there is no possibility for the masspoint to cross the border $\delta=0$. For $s=0$ we have a free particle moving along the x axis. Now the ''point'' $x=-\infty$ ($\delta=0$) cannot be reached in a finite time interval so the masspoint cannot cross the border even in this case. In the case $s<0$ an exponentially deep potential valley attracts the particle towards the negative direction. What's more, the time needed to reach $x=-\infty$ happens to be finite. This shows that for $s<0$ the particle may cross the border $\delta=0$.

IV. THE QUANTUM THEORY

Let us define the quantum mechanics of the point particle SL(2,*R*) WZNW theory via canonical quantization. We use the coordinates δ, a, and c and work in the coordinate representation. The wave functions are then complex-valued functions defined for all $\delta\in R\backslash\{0\}$, $a\in R$, and $c\in R$. We define the scalar product as

$$(\Psi_1,\Psi_2):=\int \Psi_1^*\Psi_2\sqrt{-h}\ d\delta\ da\ dc. \tag{14}$$

Here h denotes the determinant of the matrix $\{h_{kl}\}$ in the δ,a,c parametrization [cf. (5)]. The measure in this integral is the usual one used on curved manifolds. It also ensures that if we adopt the usual left and right transformations for the wave functions,

$$[D_L(h)\Psi](g):=\Psi(h^{-1}g),\quad [D_R(h)\Psi](g):=\Psi(gh),\quad g,h\in \mathrm{SL}(2,R), \tag{15}$$

then the scalar product is also invariant. This property is inevitable if we want the left and right symmetries of the classical theory to be present on the quantum level as well. Observe that these natural requirements led to the appearance of a nontrivial weight function $\rho(\delta):=\sqrt{-h}=\sqrt{2}|\delta|$ in the integral (14).

In coordinate representation the canonical momenta are defined as partial derivations with respect to the corresponding coordinates if the configuration space is flat. For curved configuration spaces this definition does not give symmetric operators because of the presence of the weight function in the scalar product. Symmetricity and the requirement $[\hat{\xi}_k, \hat{p}_l]=i\hbar\delta_{kl}$ meet in the definition $\hat{p}_k:=(\hbar/i)(\partial_k+\frac{1}{2}\partial_k \ln\sqrt{-h})$ (see Ref. 4, for example). In our case this gives $\hat{p}_\delta:=(\hbar/i)[\partial_\delta+1/(2\delta)]$, $\hat{p}_a:=(\hbar/i)\partial_a$, and $\hat{p}_c:=(\hbar/i)\partial_c$.

The classical Hamiltonian (6) does not offer a unique way to define the quantum Hamiltonian because an ordering ambiguity is present. It is $(-\hbar^2/2m$ times) the Laplacian,

$$\Delta\Psi=\frac{1}{\sqrt{-h}}\frac{\partial}{\partial\xi^i}\left(\sqrt{-h}h^{ij}(\xi)\frac{\partial}{\partial\xi^j}\Psi\right), \tag{16}$$

which proves to suit all our requirements: to be symmetric, to be coordinate invariant, to be invariant under the left–right transformations (this is satisfied because the metric tensor itself is left–right invariant), and to offer an ordering of the classical Hamiltonian (see Ref. 4 as well). After determining Δ in the δ,a,c parametrization we arrive at our Hamiltonian:

$$(\hat{\mathscr{H}}\Psi)(\delta,a,c):=-\frac{\hbar^2}{4m}\frac{1}{|\delta|}\partial_\delta(|\delta|^3\partial_\delta\Psi(\delta,a,c))-\frac{\hbar^2}{m}\frac{1}{\delta^2}\partial_a\partial_c\Psi(\delta,a,c). \tag{17}$$

We mention that we have not defined the wave functions at $\delta=0$ and the operators $\hat{\delta}$, $\hat{p}_\delta$, and $\hat{\mathscr{H}}$ are apparently ill defined at $\delta=0$. These singularities are only coordinate artifacts here. This won't be the case for the reduced system as we will see soon.

Now let us consider the quantum analogue of the constraints and see what the reduction yields. We impose the constraints on the quantum level as

$$\hat{p}_a\Psi=m\mu\Psi, \quad \hat{p}_c\Psi=m\nu\Psi \tag{18}$$

[cf. (8)]. It is very easy to find the wave functions that satisfy (18): they are of the form

$$\Psi(\delta,a,c)=\psi(\delta)e^{(i/\hbar)(m\mu a+m\nu c)}. \tag{19}$$

Remarkably, the action of the operators $\hat{\delta}$, $\hat{p}_\delta$, and $\hat{\mathscr{H}}$ on a wave function of this form touches only its δ-depending part. This makes it possible to work with $\psi(\delta)$ instead of $\Psi(\delta,a,c)$ and to consider the one-dimensional quantum mechanics driven by a Hamiltonian $\hat{H}$:

$$(\hat{H}\psi)(\delta)=-\frac{\hbar^2}{4m}\frac{1}{|\delta|}\partial_\delta(|\delta|^3\partial_\delta\psi(\delta))+ms\frac{1}{\delta^2}\psi(\delta) \tag{20}$$

together with the scalar product

$$(\psi_1,\psi_2):=\int\psi_1^*\psi_2\rho(\delta)d\delta. \tag{21}$$

Therefore in the following we investigate the properties of this one-dimensional quantum system. [The classical H corresponding to this $\hat{H}$ is just (10) as we expect.] Here we witness how the decoupling of the variables a,c from the system happens on the quantum level.

The wave functions (19) are not square integrable in the SL(2,*R*) sense. This is a natural consequence of the constraints that decrease the degrees of freedom by two. We will require square integrability ''in the reduced sense,'' i.e., with respect to the scalar product (21).

The one-dimensional problem we arrived at is quite an unusual one. The Hamiltonian is not a

$$\psi \mapsto -b^2\psi'' + V\psi \tag{22}$$

type (with a real constant b and a potential function V) and a nontrivial weight function is present in the scalar product. It would be very convenient if our system could be transformed to an ''ordinary'' one with a Hamiltonian of the form (22) and with no weight function. This can be achieved by an appropriate transformation of δ to a new variable $x=x(\delta)$, accompanied by a change of $\psi(\delta)$ to a new wave function $\chi(x)$ via $\psi(\delta)=f(\delta)\chi(x(\delta))$ with a certain function f. How $\hat{H}$ transforms under such a transformation can be read off from the transformation of the Schrödinger equation. The requirements fix uniquely how to choose x and χ; the result is

$$x=\sqrt{2}\,\ln\,\delta, \quad \psi(\delta)=\frac{1}{\delta}\,\chi(x), \tag{23}$$

$$(\hat{H}_x\chi)(x)=-\frac{\hbar^2}{2m}\,\chi''(x)+\left(\frac{\hbar^2}{4m}+mse^{-\sqrt{2}x}\right)\chi(x). \tag{24}$$

This transformation is just the quantum analogue of (11) and (13). (The additional constant in the potential term of $\hat{H}_x$ is due to the ordering procedure we maintained at the definition of the quantum Hamiltonian.) Unfortunately the problem is the same as well: it works only for the positive half of the configuration space (or the negative one, if exploiting the symmetry $\delta\leftrightarrow-\delta$). Nevertheless, $\hat{H}_x$ will be very useful in understanding the physics encoded in $\hat{H}$.

V. EIGENFUNCTIONS ON THE HALF-CONFIGURATION SPACE

To get a first impression about the spectrum of $\hat{H}$, the ''potential valley'' of the case $s<0$ suggests carrying out the Bohr–Sommerfeld quantization procedure. However, if one considers the phase space area $\oint p_\delta\,d\delta$ for a classical bound motion, it turns out that this integral diverges at $\delta\approx 0$. Thus the Bohr–Sommerfeld quantization is impossible. The reason behind this is that $\hat{H}$ is not bounded from below if $s<0$. To see this let us consider a square integrable wave function ψ and define $\psi_\lambda(\delta):=\lambda\psi(\lambda\delta)$. The ψ_λs are normalized to 1; by inspecting the scaling properties of the two terms of $\hat{H}$ [cf. (20)] one finds that the expectation value of $\hat{H}$ in a state ψ_λ tends to $-\infty$ if we let λ increase to ∞.

Fortunately the eigenvalues and eigenfunctions of $\hat{H}$ can be determined exactly in all the cases $s>0$, $s=0$, and $s<0$. To do this we have to solve the equation $\hat{H}\psi=E\psi$ as a differential equation of second order. This equation has three singular points: $\delta=\pm\infty$, which are regular singular points, and $\delta=0$, which is an irregular singular point. Consequently one has to solve this equation restricted to the domains $\delta\in R^+$ and $\delta\in R^-$, respectively, and then fit together the obtained ''half-eigenfunctions.'' Because of the symmetry $\delta\leftrightarrow-\delta$ it is enough to work on R^+. The restriction of $\hat{H}$ to R^+ will be denoted by $\hat{H}_+$.

In the case $s<0$ the eigenvalue equation can be transformed to the Bessel equation

$$z^2w''+zw'+(z^2-\nu^2)w=0 \tag{25}$$

by the substitutions $z=k/\delta$ and $\psi(\delta)=\delta^{-1}w(k/\delta)$, where $\nu^2=1-4mE/\hbar^2$ and $k=\sqrt{-4m^2s/\hbar^2}$. The two linearly independent solutions of (25), existing for any complex value of ν, are $J_\nu(z)$ and $Y_\nu(z)$ (for the conventions and properties concerning the Bessel functions, cf. Ref. 5). Similarly, for $s>0$ the transformation $z=\kappa/\delta$ and $\psi(\delta)=\delta^{-1}w(\kappa/\delta)$ leads to the modified Bessel equation

$$z^2w''+zw'-(z^2+\nu^2)w=0 \tag{26}$$

with ν^2 being the same as above and $\kappa=\sqrt{4m^2s/\hbar^2}$. Now the two solutions of (26) are the modified Bessel functions $I_\nu(z)$ and $K_\nu(z)$. In the case $s=0$ the transformation (23) is the most useful. The eigenfunctions of $\hat{H}_x$ are $\exp(\pm iKx)$, where $K=\sqrt{2mE/\hbar^2-1/2}$ [cf. (24)]. In the variable δ they read

$$\frac{1}{\delta}\, e^{\pm i\sqrt{2}K \ln \delta}. \tag{27}$$

In the cases $s>0$ and $s=0$ $\hat{H}_x$ is bounded from below. The corresponding condition on the energy eigenvalues is $E\geqslant\hbar^2/4m$. For $s=0$ it means that K is a non-negative real number. In the case $s>0$ the condition gives $\nu^2\leqslant 0$, causing that only the functions $I_{iu}(z)$ and $K_{iu}(z)$, $u\in R$, mean energy eigenfunctions. For $s<0$ the Bessel functions with real indexes lead to $E\leqslant\hbar^2/4m$ and the imaginary indexes correspond to $E>\hbar^2/4m$.

To get more acquainted with the eigenfunctions let us carry out a simple check of our physical picture that is based on $\hat{H}_x$. In the cases $s>0$ and $s<0$, the potential term of $\hat{H}_x$ decreases exponentially to zero as x tends to ∞. Consequently we expect that for $x\to\infty$ the eigenfunctions with $E\geqslant\hbar^2/4m$ behave as plane waves. (For $s=0$ this expectation is satisfied trivially.) To see whether this is the case we make use of the $z\approx 0$ behavior of $J_{iu}(z)$ and $I_{iu}(z)$, which is $J_{iu}(z)\approx I_{iu}(z)\sim z^{iu}$. The connection between the variables x and z is $z=\text{const}\exp(-x/\sqrt{2})$ so we can see that in the variable x J_{iu} and I_{iu} are asymptotically plane waves. The momentum corresponding to them is $p=-\hbar u/\sqrt{2}$. Considering that, for $x\to\infty$, $V(x)$ tends not to zero but to $\hbar^2/4m$ and quoting the connection between $\nu=iu$ and E we find that the expectation "kinetic energy$=p^2/2m$" is satisfied as well. The two other eigenfunctions, Y_{iu} and K_{iu}, are linear combinations of J_{iu} and J_{-iu}, resp. I_{iu} and I_{-iu}. Thus they also behave the way we expect from our physical picture.

VI. ORTHOGONALITY AND COMPLETENESS

It will be important to form a complete orthogonal system from the half-eigenfunctions, an orthogonal basis in $L^2(R^+,\rho)$. In the case $s=0$ this is simple: the set $\{\exp(\pm iKx)|K\in[0,\infty)\}$ is a complete orthogonal system [in the variable $x\in(-\infty,\infty)$]. Therefore the same can be said about the functions (27) in the variable δ in $L^2(R^+,\rho)$. For $s<0$ there exist several independent choices of a complete orthogonal system. The different bases can be indexed by a $p\in(0,2]$. The corresponding eigenvectors [given in the transformed form $w(z)$] are

$$\begin{gathered} J_q(z), \quad q=p,p+2,p+4,\ldots, \\ \cos\left(\frac{\pi}{2}p\right)J_0(z)+\sin\left(\frac{\pi}{2}p\right)Y_0(z), \\ e^{-i\theta_p(u)}J_{iu}(z)+e^{i\theta_p(u)}J_{-iu}(z), \quad u\in(0,\infty), \end{gathered} \tag{28}$$

where

$$e^{i\theta_p(u)}=\frac{\cos\left(\frac{\pi}{2}p\right)\sinh\left(\frac{\pi}{2}u\right)+i\,\sin\left(\frac{\pi}{2}p\right)\cosh\left(\frac{\pi}{2}u\right)}{\sqrt{\cos^2\left(\frac{\pi}{2}p\right)\sinh^2\left(\frac{\pi}{2}u\right)+\sin^2\left(\frac{\pi}{2}p\right)\cosh^2\left(\frac{\pi}{2}u\right)}} \tag{29}$$

(see the Appendix and Ref. 6). For the case $s>0$ only one complete orthogonal system can be built from the functions $I_{iu}(z)$ and $K_{iu}(z)$, namely, the set

$$\{K_{iu}(z)|u\in[0,\infty)\} \tag{30}$$

(cf. the Appendix and Ref. 6).

What makes the difference that in the cases $s=0$ and $s>0$ the eigenbasis is unique, while for $s<0$ there are infinitely many complete orthogonal systems? The answer is in the self-adjointness of $\hat{H}_+$. For this reason we determine the deficiency index of $\hat{H}_+$. Here $\hat{H}_+$ is a differential operator of second order with real coefficients and two singular points $\delta=0$ and $\delta=\infty$. Its deficiency index is equal to the number of its orthogonal square integrable eigenfunctions corresponding to a *nonreal* eigenvalue (cf. Ref. 7) (the deficiency index does not depend on the eigenvalue chosen). In the case $s>0$ the deficiency index is zero, because, for a fixed nonreal ν^2, neither of the two linearly independent eigenfunctions—$I_\nu(z)$ and $K_\nu(z)$ in the variable z—is square integrable (cf. the Appendix and Ref. 6). In the case $s<0$ J_ν is square integrable while Y_ν is not (we can choose Re $\nu>0$ without loss of generality). Thus in this case the deficiency index is 1. For $s=0$ the deficiency index is 0, which can be seen most easily in the variable x.

Now, starting with the case $s<0$, we recall a theorem of Ref. 7, which states that if the deficiency index is 1, then the operator has several self-adjoint extensions. Reference 7 also gives a condition for the different domains of definition of the different self-adjoint extensions. For $\hat{H}_+$ this condition says that a function $\psi(\delta)$ lying in the domain of definition of a self-adjoint extension (has to be smooth enough, cf. Ref. 7, and) has to satisfy

$$\lim_{\delta\to 0}\left[\delta^3\left(\psi^*\frac{dU_\nu^\vartheta}{d\delta}-\frac{d\psi^*}{d\delta}U_\nu^\vartheta\right)\right]=\lim_{\delta\to\infty}\left[\delta^3\left(\psi^*\frac{dU_\nu^\vartheta}{d\delta}-\frac{d\psi^*}{d\delta}U_\nu^\vartheta\right)\right], \tag{31}$$

where

$$U_\nu^\vartheta(\delta)=\frac{1}{\delta}J_\nu\left(\frac{k}{\delta}\right)+e^{i\vartheta}\frac{1}{\delta}J_\nu^*\left(\frac{k}{\delta}\right) \tag{32}$$

with a $\vartheta\in[0,2\pi)$ and a $\nu\in C\backslash R$, Re $\nu>0$. Together ϑ and ν index the different self-adjoint extensions.

Then if one examines which eigenfunctions are included in the domain of definition of a self-adjoint extension indexed by an arbitrarily chosen value of ϑ and ν, a straightforward if lengthy calculation shows that these eigenfunctions are exactly the ones that form one of the complete orthogonal systems (28). The number p which characterizes this system is expressed by ϑ and ν as

$$p=\mathrm{Re}\ \nu+\frac{2}{\pi}\arcsin\left(\frac{\sinh\left(\frac{\pi}{2}\,\mathrm{Im}\ \nu\right)\sin\left(\frac{\vartheta}{2}\right)}{\sqrt{\sinh^2\left(\frac{\pi}{2}\,\mathrm{Im}\ \nu\right)\sin^2\left(\frac{\vartheta}{2}\right)+\cosh^2\left(\frac{\pi}{2}\,\mathrm{Im}\ \nu\right)\cos^2\left(\frac{\vartheta}{2}\right)}}\right)\quad(\mathrm{mod}\ 2). \tag{33}$$

Hence the multiplicity of the eigenbases originates in the multiple self-adjoint extensions of the differential operator $\hat{H}_+$.

In the cases $s>0$ and $s=0$ the deficiency index is zero. The appropriate theorem of Ref. 7 states that then the operator is self-adjoint. Consequently, the domain of definition is unique. All the eigenfunctions (or, more precisely, all the wave packets superposed from the eigenfunctions—remember that for both $s>0$ and $s=0$ all the eigenfunctions are non-normalizable) are lying in the domain of definition so the eigenbasis is unique as well [up to linear equivalence, i.e., except from trivial phase factors or, in the case $s=0$, choosing two linear combinations of $\exp(iKx)$ and $\exp(-iKx)$ instead of $\exp(iKx)$ and $\exp(-iKx)$].

VII. THE EIGENFUNCTIONS ON THE WHOLE CONFIGURATION SPACE

To investigate the eigenfunctions of the full system the task is to sew together the half-eigenfunctions and build up a complete orthogonal system of ''whole eigenfunctions'' (in the following: eigenfunctions). In usual quantum mechanical systems, i.e., with a Hamiltonian of the form (22) and with no weight function in the scalar product, the conditions for fitting parts of an eigenfunction together are the continuity of the eigenfunction and the continuity, or in special cases a given jump, of its (space) derivative. Now we cannot expect that such conditions work. In fact, the $\delta\to 0$ behavior of the half-eigenfunctions proves to be $\delta^{-1/2}\cos(k/\delta+\text{const})$ in the case $s<0$, $\delta^{-1}\exp(\pm i\sqrt{2}K\ln\delta)$ if $s=0$, and $\delta^{-1/2}\exp(-\kappa/\delta)$ if $s>0$. Thus this kind of fitting together is impossible. The situation is not better in the variable x either; the half-eigenfunctions tend to 0 in the limit $x\to-\infty$ in the cases $s<0$ and $s>0$, while for $s=0$ they behave as $\exp(\pm iKx)$. This infinite growth or decrease and infinitely rapid oscillating behavior of the half-eigenfunctions originates in the irregular singularity of the Hamiltonian at $\delta=0$.

Fortunately, the probability current is finite at $\delta\to 0$. It is this quantity we are able to fit. However, in our case the probability current is not of the usual form. By deriving the continuity equation for the probability density from the Schrödinger equation the probability current proves to be

$$\frac{\hbar}{2\sqrt{2}mi}\,|\delta|^3\left(\psi^*\,\frac{d\psi}{d\delta}-\frac{d\psi^*}{d\delta}\,\psi\right). \tag{34}$$

Any ψ can be expressed as a linear combination of eigenfunctions φ_k, which makes it possible to decompose the probability current as a sum of

$$\frac{\hbar}{2\sqrt{2}mi}\,|\delta|^3\left(\varphi_k^*\,\frac{d\varphi_l}{d\delta}-\frac{d\varphi_k^*}{d\delta}\,\varphi_l\right). \tag{35}$$

It can be verified that in each case $s<0$, $s=0$, or $s>0$ such a quantity has a well-defined finite limit for $\delta\to 0$ so the probability current is also finite at $\delta\to 0$.

We do not fit the probability current directly but carry out an equivalent procedure. In fact, fitting the probability current of the half-eigenfunctions is to ensure that the norm of a whole wave function does not change in time. The latter is equivalent to the self-adjointness of the whole Hamiltonian. We know that the eigenfunctions of a self-adjoint Hamiltonian are orthogonal. Conversely, a complete orthogonal system of the eigenfunctions of the Hamiltonian as a differential operator defines a self-adjoint Hamiltonian from the differential operator on an everywhere-dense set in $L^2(R,\rho)$, which is our purpose. That is why it is enough, while it is more interesting as well, to build up complete orthogonal systems out of the eigenfunctions instead of fitting the probability current.

Let us start with the case $s<0$. An eigenfunction $\Phi(\delta)$ is generally of the form

$$\alpha\varphi(-\delta)\quad\text{if}\quad\delta<0,\qquad\beta\varphi(\delta)\quad\text{if}\quad\delta>0, \tag{36}$$

where φ is a half-eigenfunction defined on R^+. From this it follows immediately that at most two linearly independent eigenfunctions can correspond to an eigenvalue in a (whole) eigenbasis. Another important observation is that if a value p corresponds to φ, the index of the half-eigenbasis φ is a member of, this p characterizes Φ as well. Now let us suppose that a complete orthogonal system of eigenfunctions does not include two linearly independent eigenfunctions that correspond to the same eigenvalue *and* have the same value p. (Later we will examine the other case as well, i.e., when one can find two such eigenfunctions in the system.) In this case there must be at least one eigenfunction in this eigenbasis with a different p. Otherwise we do not have

completeness: there exist functions that are orthogonal to any basis vector but are not identically zero; such an example is a whole eigenfunction that is not included in the basis but has the same value p.

For two eigenfunctions having different ps $(\,,\,)_+$ and $(\,,\,)_-$, the restriction of their scalar product to the positive, resp. negative, half of the configuration space are not zero, consequently they are orthogonal only if one of them is of the form

$$\text{const}\begin{cases}\varphi(-\delta) & \text{if } \delta<0,\\ \lambda\varphi(\delta) & \text{if } \delta>0,\end{cases} \tag{37}$$

and the other is of the form

$$\text{const}\begin{cases}-\lambda^*\varphi(-\delta) & \text{if } \delta<0,\\ \varphi(\delta) & \text{if } \delta>0,\end{cases} \tag{38}$$

(with a different φ but) with the same complex λ from the set $\{|\lambda|\leqslant 1$, if $|\lambda|=1$, then arg $\lambda\in[0,\pi)\}$. Let p_1 denote the value p of the eigenfunction of the first form and p_2 denote the p of the other one. The other eigenfunctions with p_1 also must have the form (37) (with the same λ) and the other eigenfunctions with p_2 also must have the form (38), in order to be orthogonal to these two eigenfunctions. These forms ensure that the further eigenfunctions are orthogonal to each other as well. Orthogonality also excludes the existence of any eigenfunctions in the eigenbasis having a p other than p_1 or p_2.

To examine completeness, first let us see whether an arbitrary function ψ_1 from $L^2(R,\rho)$ having the form (37) (where now φ is not a half-eigenfunction but an arbitrary half-function) can be spanned by these eigenfunctions. It is easy to see that this requirement is equivalent to that the restriction of the eigenfunctions with p_1 to R^- have to form a complete half-eigenbasis (a ψ_1 is orthogonal to the eigenfunctions with p_2, hence only the eigenfunctions with p_1 contribute to it). After a similar treatment of the ψ_2's of the form (38) we conclude that a complete system must consist of each of the eigenfunctions with p_1 [that have the form (37)] and each of the eigenfunctions with p_2. Then if any $\psi\in L^2(R,\rho)$ can be given as a sum of a ψ_1 and a ψ_2, then completeness is reached. With the notation

$$\psi(\delta)=\begin{cases}\psi_-(-\delta), & \delta<0,\\ \psi_+(\delta), & \delta>0,\end{cases} \tag{39}$$

the sum of the functions

$$\psi_1(\delta):=\begin{cases}\dfrac{1}{1+|\lambda|^2}\,(\psi_-(-\delta)+\lambda^*\psi_+(-\delta)), & \delta<0,\\ \dfrac{\lambda}{1+|\lambda|^2}\,(\psi_-(\delta)+\lambda^*\psi_+(\delta)), & \delta>0,\end{cases} \tag{40}$$

and

$$\psi_2(\delta):=\begin{cases}\dfrac{-\lambda^*}{1+|\lambda|^2}\,(-\lambda\psi_-(-\delta)+\psi_+(-\delta)), & \delta<0,\\ \dfrac{1}{1+|\lambda|^2}\,(-\lambda\psi_-(\delta)+\psi_+(\delta)), & \delta>0,\end{cases} \tag{41}$$

is ψ, thus the completeness of the considered system of eigenfunctions, which we shall denote by (p_1,p_2,λ), is proven. We remark that the above decomposition of ψ is a generalization of the decomposition of a function to a sum of an even and an odd function, which is actually the case $\lambda=1$.

Now let us turn to the other case, i.e., when the complete orthogonal system of whole eigenfunctions includes two linearly independent eigenfunctions with a same value p and corresponding to the same eigenvalue. In this case the other eigenfunctions must be of this p as well, otherwise they cannot be orthogonal to both of these eigenfunctions. Furthermore, the eigenvalues of the eigenbasis must be identical with the eigenvalues of the half-eigenbasis p and must be doubly degenerated: in the case of a simply degenerated or missing eigenvalue any (other) eigenfunction corresponding to this eigenvalue is orthogonal to each eigenfunction from the system, which is in contradiction with completeness. The constants α and β [see (36)] for the eigenfunctions of the system can be arbitrary, the only requirement is that for each eigenvalue the corresponding two eigenfunctions be linearly independent. The concrete values of these αs and βs are not important, they only embody a choice of two basis vectors in a two-dimensional linear subspace. Remarkably, such an eigenbasis is linearly equivalent to a one which, in the spirit of our notation, can be denoted by (p,p,λ) (the equivalence holds for an arbitrary λ). Based on this observation one can prove completeness the same way as for a system (p_1,p_2,λ).

We see that in contrast to the eigenbases (p_1,p_2,λ) considered earlier, these latter eigenbases are characterized by a single number p. Each of the different eigenbases (p_1,p_2,λ) and p means a different self-adjoint extension of the Hamiltonian as a differential operator.

For $s>0$ and $s=0$ the method to establish an eigenbasis is the same as for an eigenbasis with a single p in the case $s<0$. The difference is that now one starts with only one half-eigenbasis. Consequently, one arrives at only one eigenbasis (up to linear equivalence). As a result in these cases the self-adjoint Hamiltonian is unique.

That for $s<0$ two different half-eigenbases are needed in general for one eigenbasis may seem unusual. However, this situation is just an analogue of the case of the operator $-\partial^2/\partial x^2$ on the interval $[-\pi,\pi]$. If one wants to build up the eigenfunctions $\sin[(n/2)(x+\pi)]$, $n=1,2,...$ of $-\partial^2/\partial x^2$ from its half-eigenfunctions, defined on $[0,\pi]$ and $[-\pi,0]$, he/she will find that two different half-eigenbases are needed to do this, one for the eigenfunctions with even ns and one for odd ns (cf. Ref. 6).

In spite of the unusual form of the Hamiltonian and the presence of the nontrivial weight function, the $\hat{H}_x$ form of the Hamiltonian enables us to give the physical interpretation of the results to some extent.

In the case $s<0$ we expect that the two half-configuration spaces are in physical connection; the particle can cross the border $\delta=0$. Simple calculations show that this expectation is satisfied for the self-adjoint extensions (p_1,p_2,λ): there is a probability flow from one half to the other one. Consider for example a wave function $\psi=c_1\psi_1+c_2\psi_2$ where ψ_1 and ψ_2 are eigenfunctions, one having p_1 and the other having p_2. Though $(d/dt)(\psi,\psi)=0$, $(d/dt)(\psi,\psi)_+ = -(d/dt)(\psi,\psi)_- \neq 0$ for generic c_1 and c_2. Another transparent possibility to show the physical connectedness of the two halves is that one can easily find examples for a solution of the (time dependent) Schrödinger equation where the expectation value of the coordinate operator $\hat{\delta}$ is oscillating in time between a positive and a negative value. However, in the case of the self-adjoint extensions p, the two halves behave as two closed, independent subsystems. The reason is that for these eigenbases the restriction of the eigenfunctions on a half-configuration space is a half-eigenbasis, causing that $\hat{H}$ decouples to two self-adjoint half-operators.

The cases $s>0$ and $s=0$ are similar to the $s<0$, p one. The Hamiltonian is simply a pair of two self-adjoint half-Hamiltonians, the two parts of the configuration space being physically independent. This result is in accord with the naive pictures of the $s>0$ and $s=0$ systems based on $\hat{H}_x$. For $s>0$ we can think of an exponentially increasing and thus infinitely wide potential wall separating the two half-worlds. No wonder that we find no tunneling from one side to the other.

The situation is similar to the quantum mechanics of the system with the potential

$$V(x)=\begin{cases}0 & \text{if } |x|>a,\\ \infty & \text{if } |x|<a,\end{cases} \tag{42}$$

where it is meaningful to speak about the quantum mechanics of the system on the whole configuration space, yet there is no physical connection between the two allowed parts. In the case $s=0$ we have two free theories, both on an infinitely large configuration space (understood in the variable x). We may argue that under such circumstances a wave packet starting from one side (e.g., the $\delta>0$ one) cannot reach the other side in a finite time period. We cannot say anything stronger concerning interpretation: these are the limits we are forced into.

VIII. COORDINATE INDEPENDENCE

The reduced quantum system, as we saw, posesses several unusual properties. It is natural to ask whether these features are only artifacts, caused by the special coordinate system which was used for the definition of the reduced system. Therefore it is worth examining the possibility of defining the system in a coordinate-independent way.

The Hamiltonian of the unconstrained quantum theory, a multiple of the Laplacian of the manifold SL(2,*R*), and the scalar product (14) are in fact coordinate invariant. Consequently the question reduces to whether the constraints can be given a coordinate-independent form. In Sec. IV the constraints were imposed through the canonical momentum operators. The definition $\hat{p}_k:=(\hbar/i)(\partial_k+\frac{1}{2}\partial_k \ln\sqrt{-h})$ does not define a covariant quantity because h is not a coordinate invariant scalar. That is why it is recommended to impose the constraints independently of the canonical momentum operators.

In the spirit of the Lie derivative, let us introduce the following derivation operators:

$$(L_A\Psi)(g)=\frac{d}{ds}\,\Psi(e^{As}g)\bigg|_{s=0},\quad (R_A\Psi)(g)=\frac{d}{ds}\,\Psi(ge^{As})\bigg|_{s=0} \tag{43}$$

for any $A\in \mathrm{sl}(2,R)$. The definitions of L_A and R_A do not need any coordinate system. Nevertheless, if expressing them using the coordinates δ, a, and c one finds that $L_{e_{12}}=\partial_a$ and $R_{e_{21}}=\partial_c$. Thus we obtained a coordinate-independent reformulation of the constraints (18).

One can feel the need for checking whether the operators $(\hbar/im)L_{e_{12}}$ and $(\hbar/im)R_{e_{21}}$ are really the quantum equivalents of the classical quantities $\mathrm{Tr}[e_{12}\dot{g}g^{-1}]$ and $\mathrm{Tr}[e_{21}g^{-1}\dot{g}]$. The following heuristic argument makes this relation visible.

We consider a wave packet which is in some sense the most similar to a classical trajectory, determine the expectation value of $(\hbar/im)L_{e_{12}}$ and $(\hbar/im)R_{e_{21}}$, and compare it to $\mathrm{Tr}[e_{12}\dot{g}g^{-1}]$, resp. $\mathrm{Tr}[e_{21}g^{-1}\dot{g}]$, computed on the classical trajectory the wave packet is similar to. In the case of the free quantum mechanics on a three-dimensional Euclidean space, the Gaussian wave packet

$$\text{const}\int d^3\underline{k}\,e^{-1/(2\sigma^2)(\underline{k}-\underline{k}_0)^2}e^{i\underline{k}(\underline{x}-\underline{x}_0)} \tag{44}$$

is in some sense the best wave mechanical analogue of a classical trajectory. It is well localized both in position and in momentum—around the position $\underline{x}_0$ and the wave vector $\underline{k}_0$. In the case of SL(2,*R*) an appropriate analogue of (44) can be defined (for the details see Ref. 6). From the time development of this wave packet one can extract the motion of the peak of the wave packet. The needed classical quantities can be determined and prove to be equal to the corresponding quantum expectation values, as expected.[6]

We saw that both the unconstrained system and the constraints are actually coordinate independent. After defining a system in a coordinate-independent way, one can use concrete param-

etrizations to examine its properties. Turning to the concrete situation, all the properties explored in the coordinates δ, a, and c are valid everywhere $\delta \neq 0$. For example, the wave functions are scalars so the infinite growth and infinitely rapid oscillating of the eigenfunctions is a coordinate-independent fact, since this is the behavior of the eigenfunctions not *at* but *around* the invalid point $\delta=0$.

IX. CONCLUSIONS

We investigated the properties of the point particle version of the reduced SL(2,*R*) WZNW model both on the classical and the quantum levels, for all the possible values of the constraint parameters. We found that the quantum theory exhibits an analogous behavior to the classical one. The cases where the two parts are disconnected classically lead to two independent systems on the quantum level as well, and in the cases where the half-systems have a physical connection, this connection can also be found in the quantum theory. The only exception is that there is a possibility for a classically connected case to be disconnected quantum mechanically. This is possible because not only one quantum theory corresponds to a classically connected case. Several self-adjoint extensions of the Hamiltonian exist, including special ones where the two half-systems turn out to be independent.

Classical mechanically bounded motions exist, with arbitrary large negative energies, in the connected cases. The disconnected cases do not allow bounded motions and energy is bounded from below. These properties are also reflected on the quantum level. It is remarkable that the quantum theory is formally consistent irrespective of the values of the constraint parameters, while in the connected cases it leads to systems with a Hamiltonian not bounded from below (no matter which self-adjoint extension is chosen). Recently a method was proposed to discuss quantum mechanical systems that exhibit such a behavior.[8] The method implements the concept of Wilson renormalization. It would be interesting to carry out such an analysis for the system studied here. Nevertheless, the method of Ref. 8 means a kind of distortion of the system, which is not the purpose here as here we are interested in the properties of the original system for we want to obtain indications how the quantum theory of the corresponding field theory behaves. In Sec. III we have found classical space-independent configurations with arbitrary large negative energy in the connected cases. This and the quantum properties of the masspoint version make it quite possible that the energy is essentially not bounded from below in the quantum field theory.

That the energy is not bounded from below is not the only nontrivial property of the connected case. The most striking result of our analysis is the existence of several self-adjoint extensions corresponding to one classical system. There is no principle, physical or mathematical, to choose one out of them as the ''real'' one. The origin of this behavior is the strong singularity at the border which separates the two half-systems. This singularity is not present on the unconstrained level. It is a consequence of the characteristics of the constraints. As this singularity can also be observed in the classical reduced field theory version,[3] we expect to face the problem of the nonunique self-adjoint energy operator on the quantum level, i.e., in the quantum field theory of the reduced SL(2,*R*) WZNW model as well.

The method applied here to present the quantum mechanics of the reduced system was canonical quantization (supplemented by a coordinate independent approach). Because of the nontrivial properties found it would be interesting to examine this system by using other tools, geometric quantization or functional integration, and see how these methods give account of the characteristics of the theory.

Additionally we remark that recently a paper carried out an analysis of the relativistic quantum mechanics of a free particle on the SL(2,*R*) manifold.[9] The problem studied there is independent of the one presented here. Clearly, in Ref. 9 the group SL(2,*R*) plays the role of the (curved) *space–time* the particle exists in, while in our case SL(2,*R*) is the (configuration) *space* of the unconstrained system.

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APPENDIX: ORTHOGONALITY AND COMPLETENESS

In the Appendix we give the outline of how the statements concerning orthogonality and completeness of the half-eigenbases can be derived. For further technical details, see Ref. 6.

To find the possible orthogonal systems of the half-eigenfunctions the scalar product of the half-eigenfunctions is to be studied. This can be done by using the following formula of Ref. 10;

$$\int_a^b A_\mu(z)B_\nu(z)\,\frac{dz}{z}=\frac{1}{\nu^2-\mu^2}\,[z(A_\mu(z)B'_\nu(z)-A'_\mu(z)B_\nu(z))]_a^b \tag{A1}$$

($A,B=J$, Y, I or K) and by using the $z\approx 0$ and $z\approx\infty$ asymptotics of $J_\nu(z)$, $Y_\nu(z)$, $I_\nu(z)$, and $K_\nu(z)$. After determining the scalar products of the half-eigenfunctions one can start to build orthogonal systems out of them and arrives at (28) and (30) in the cases $s<0$, resp. $s>0$.

We demonstrate the proof of completeness of the half-eigensystems on the case $s<0$, $p=2$ (for the treatment of the cases $p\neq 2$ or $s>0$ only straightforward modifications are needed). Let us show that $S_N(x_1,x_2)+I_N(x_1,x_2)$ tends to $\delta(x_1-x_2)$ as $N\to\infty$, where

$$S_N(x_1,x_2)=\sum_{q=p}^{N}\sqrt{2}qJ_q(z_1)J_q(z_2), \tag{A2}$$

$$I_N(x_1,x_2)=\int_0^{N+1/2}\frac{du\;u}{2\sqrt{2}\,\sinh\,\pi u}\,[J_{iu}(z_1)+J_{-iu}(z_1)][J_{iu}(z_2)+J_{-iu}(z_2)], \tag{A3}$$

$z_i=k\,\exp(-x_i/\sqrt{2})$, $i=1,2$. After simple manipulations the contour of the integral can be deformed into a half circle with radius $N+\frac{1}{2}$, lying in the half-plane $\mathrm{Im}\,u<0$ of the complex u-plane. By doing this the contour passes through some poles of the integrand, thus the residue of these poles have to be taken into account. The contribution of these residues happens to be $-S_N(x_1,x_2)$. The large-N behavior of the new integral can be evaluated with the aid of the asymptotics of the integrand. The result is $\sin[(N+\frac{1}{2})/\sqrt{2}](x_1-x_2)]/\pi(x_1-x_2)$, which tends to $\delta(x_1-x_2)$.

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Commutator expansion. II. Relativistic reduced Green's functions and the Lamb shift calculation

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This is a continuation of an earlier paper [J. Math. Phys. **34**, 5509 (1993)]. A projection operator technique is introduced in the Lamb shift calculation in order to manage spurious infrared divergences. The method provides an efficient tool to exhibit factors of the field in the commutator expansion of the Lamb shift. Mass eigenfunction expansion concepts developed elsewhere provide the setting for the new technique. As a by-product of our method, relativistic reduced Green's functions are found to appear in a natural way. The method may prove useful, since reduced Green's functions are simpler than the full Green's functions, and behave like constant operators as regards the parameter integrals. © *1996 American Institute of Physics.* [S0022-2488(96)00404-7]

I. INTRODUCTION

We expand on earlier work inspired by a paper of Erickson and Yennie. In keeping with our earlier notation, the Erickson and Yennie paper[1] will still be referred to simply as I. For short we shall refer to our own previous work[2] as II. The notation ''Sec. I,'' ''Sec. II,'' etc., shall refer to the parts of the present paper. Both papers are concerned with the self-energy operator Σ for an electron in an external potential:

$$\Sigma=\frac{\alpha}{4\pi^3 i}\int\frac{d^4k}{k^2}\,\gamma_\mu\,\frac{1}{\not\Pi-\not k-m}\,\gamma^\mu,$$
$$\not\Pi\equiv\gamma^\mu(i\partial_\mu-qA_\mu). \tag{1}$$

We can separate Σ into a sum of terms $\Sigma=\Sigma_{\rm I}+\Sigma_{\rm II}+\Sigma_{\rm III}+\Sigma_{\rm IV}$ as follows:

$$\Sigma_{\rm I}=\frac{\alpha}{4\pi^3 i}\int d^4k\int_0^1 dz\,\gamma_\mu\,\frac{xm}{D^2}\,\gamma^\mu, \tag{2}$$

$$\Sigma_{\rm II}=\frac{\alpha}{4\pi^3 i}\int d^4k\int_0^1 dz(1-z)\,\gamma_\mu\not\Pi\,\frac{1}{D^2}\,\gamma^\mu, \tag{3}$$

$$\Sigma_{\rm III}=\frac{\alpha}{4\pi^3 i}\int d^4k\int_0^1 dzz\,\gamma_\mu\left[\not\Pi;\frac{1}{D}\right]\frac{1}{D}\,\gamma^\mu, \tag{4}$$

and

$$\Sigma_{\rm IV}=-\frac{\alpha}{4\pi^3 i}\int d^4k\int_0^1 dzz\,\gamma_\mu\left[\gamma^\lambda;\frac{1}{D}\right]\Pi_\lambda\,\frac{1}{D}\,\gamma^\mu,$$
$$D=-(\not k-z\not\Pi)^2-z(1-z)\not\Pi\not\Pi+zx^2m^2, \tag{5}$$

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and expand each separately in a ''commutator series.'' Each term in such a series has a representation as a single integral over a virtual electron mass squared parameter. From II, Eqs. (36)–(38), the lowest $(p=0)$ terms in the commutator series are

$$\Sigma_{\mathrm{I}}(0)=\frac{\alpha}{4\pi}\, m\int_1^\infty du\ \frac{u-1}{u^2}\ \gamma_\mu\ \frac{\rho}{\Delta}\ \gamma^\mu, \tag{6}$$

$$\Sigma_{\mathrm{II}}(0)=\frac{\alpha}{4\pi}\int_1^\infty du\ \frac{u^2-1}{2u^3}\ \gamma_\mu \not{\Pi}\ \frac{\rho}{\Delta}\ \gamma^\mu, \tag{7}$$

$$\Sigma_{\mathrm{III}}(0)=0, \tag{8}$$

and

$$\Sigma_{\mathrm{IV}}(0)=-\frac{\alpha}{2\pi m^2}\int_1^\infty du\left(\frac{u^2-1}{2u}-\ln(u)\right)\gamma_\mu\ \frac{1}{\Delta}\,[\Pi_\lambda;\not{\Pi}]\ \frac{1}{\Delta}\ \Pi^\lambda\ \frac{1}{\Delta}\ \gamma^\mu,$$
$$\left(\frac{u^2-1}{2u}-\ln(u)\right)=\frac{(u-1)^3}{6}+O((u-1)^4), \tag{9}$$

in which $\rho\equiv\not{\Pi}\not{\Pi}/m^2$ is the electron ''mass squared'' operator, and $1/\Delta=1/(u-\rho)$ is the Green's function of the iterated Dirac equation. All terms in the commutator expansion have similar one-dimensional integral representations involving the virtual electron mass squared parameter u. Also, all terms are already renormalized with subtraction point $p_\mu\, p^\mu=0$, and are both ultraviolet and infrared finite. The infrared convergence in Eq. (9) is evidenced by the behavior of the integrand at $u=1$: poles of the Green's functions $1/\Delta$ at $u=1$ are offset by zeros of the factor $((u^2-1)/2u-\ln(u))=O((u-1)^3)$. Although not a true expansion in powers of the field in the sense of I, the commutator expansion does have the virtue that we can treat the general term, thereby providing a window on the higher-order effects in the Lamb shift.

II. REARRANGEMENT

After forming an expectation value, we try to simplify Eq. (6), Eq. (7), and Eq. (9), by replacing Green's functions $1/\Delta$ by simple c-numbers $1/(u-1)$. In I this is achieved by moving Green's functions to the outside, where they can act on the state and become c-numbers. Errors for this involve commutators that in general produce factors of the field representing higher-order effects. The identity $[\Pi_\mu;\,\Pi_\nu]=-iqF_{\mu\nu}$ provides the basic mechanism for this. Spurious and mutually canceling infrared divergences are generated in this process by repeated use of the formula $[O;\,1/\Delta]=(1/\Delta)[O;\,\rho](1/\Delta)$, a formula that increases the apparent order of the pole at $u=1$.

We shall here introduce a technique that lets us avoid altogether working with infrared divergences. As a byproduct of our method, we find that relativistic reduced Green's functions appear in a natural way. Our method may be useful, since reduced Green's functions are quite a bit simpler than the full Green's function, and reduced Green's functions do not participate in the u-integration.

Our technique involves the introduction of projection operators.[3] We write $\cdots\rangle=\cdots P\rangle$, where P is the projector onto the entire degeneracy subspace of the particular state $\rangle$ being perturbed. The projection operators are then moved to the Green's functions. The Green's functions are thereby converted to c-numbers via the identity $(1/\Delta)P=[1/(u-1)]P$. Commutator correction terms for this are evaluated by means of the formula (II, Eq. 90):

$$[O;\,P]=K[O;\,\rho]P+P[O;\,\rho]K, \tag{10}$$

which does not increase the order of the pole at $u=1$. In this equation K is the relativistic reduced Green's function,[4] a simple constant as regards the u-dependence. In a typical situation, for which the operator O in Eq. (10) is either $O=\Pi_\lambda$ or $O=\gamma_\mu$, a factor of the field appears through the commutator $[O;\ \rho]$. In general, commutator corrections still describe higher-order effects.

To illustrate, let us transform the expectation value $\langle\gamma_\mu(\rho/\Delta)\gamma^\mu\rangle$ associated with the integrand of Eq. (6) in order to convert the operator ρ/Δ into the c-number $1/(u-1)$:

$$\begin{aligned}\left\langle \gamma_\mu \frac{\rho}{\Delta}\ \gamma^\mu \right\rangle &= \left\langle \gamma_\mu \frac{\rho}{\Delta}\ \gamma^\mu P \right\rangle \\ &= \left\langle \gamma_\mu \frac{\rho}{\Delta}[\gamma^\mu;\ P] + \gamma_\mu \frac{1}{u-1} P\gamma^\mu \right\rangle \\ &= \left\langle \gamma_\mu \frac{\rho}{\Delta}[\gamma^\mu;\ P] + \gamma_\mu \frac{1}{u-1}[P;\ \gamma^\mu] + \gamma_\mu \frac{1}{u-1}\ \gamma^\mu \right\rangle \\ &= \left\langle \gamma_\mu\left(\frac{\rho}{\Delta} - \frac{1}{u-1}\right)[\gamma^\mu;\ P] + \frac{4}{u-1} \right\rangle .\end{aligned}$$

The first step here uses the basic property $\rangle = P\rangle$ of the projection operator P. Also, the relations $\rho P = P$ and $(1/\Delta)P = [1/(u-1)]P$ were needed. Recall from II that ρ, $1/\Delta$, K, and $\not{\Pi}$ are mutually commuting operators. Using Eq. (10), the calculation may be continued as

$$\left\langle \gamma_\mu \frac{\rho}{\Delta}\ \gamma^\mu \right\rangle = \left\langle \gamma_\mu\left(\frac{\rho}{\Delta} - \frac{1}{u-1}\right)K[\gamma^\mu;\ \rho] + \frac{4}{u-1} \right\rangle . \tag{11}$$

In this equality we exploit the property $K\rangle = 0$. This is the reason only the first term of Eq. (10) was needed. Finally, we may exhibit an additional factor of the field by exploiting the identity $\langle K = 0$ to write $\langle\gamma^\mu K = \langle[\gamma^\mu;\ K]$:

$$\begin{aligned}\left\langle \gamma_\mu \frac{\rho}{\Delta}\ \gamma^\mu \right\rangle &= \left\langle [\gamma_\mu;\ K]\left(\frac{\rho}{\Delta} - \frac{1}{u-1}\right)[\gamma^\mu;\ \rho] + \frac{4}{u-1} \right\rangle \\ &= -\left\langle [\gamma_\mu;\ \rho]K^2\left(\frac{\rho}{\Delta} - \frac{1}{u-1}\right)[\gamma^\mu;\ \rho] + \frac{4}{u-1} \right\rangle ,\end{aligned}$$

in which the last line follows by expanding the commutator $[\gamma_\mu;\ K]$ as [II, Eq. (93)]

$$[O;\ K] = K[O;\ \rho]K - K^2[O;\ \rho]P - P[O;\ \rho]K^2. \tag{12}$$

At this point we have

$$\left\langle \gamma_\mu \frac{\rho}{\Delta}\ \gamma^\mu \right\rangle = -\left\langle [\gamma_\mu;\ \rho]K^2\left(\frac{\rho}{\Delta} - \frac{1}{u-1}\right)[\gamma^\mu;\ \rho] + \frac{4}{u-1} \right\rangle . \tag{13}$$

We have here converted the factor ρ/Δ into the c-number $1/(u-1)$, and have encountered certain commutator correction terms. To estimate the order of magnitude of such terms, we introduce nominal order estimates reflecting the behavior after the u-integration, estimated for bound states. In the language of the Coulomb potential, these estimates are

$$[\gamma^\mu;\ \rho] = O((Z\alpha)^3), \quad K = O\left(\frac{1}{(Z\alpha)^2}\right), \quad [\gamma^\mu;\ P] = O(Z\alpha), \tag{14}$$

$$1-\rho=O((Z\alpha)^2).$$

The further order estimate $(\rho/\Delta-1/(u-1))=O((Z\alpha)^2\ln((Z\alpha)^2))$ is valid in Eq. (13) where only a single factor of $(\rho/\Delta-1/(u-1))$ occurs. Note, however, that this estimate is ''context sensitive.'' See the Appendix where context sensitive behavior for factors of $(1/\Delta-1/(u-1))$ is discussed. The rule for factors of $(1/\Delta-1/(u-1))$ is: one factor contributes $O((Z\alpha)^2\ln((Z\alpha)^2))$; two or more factors collectively always contribute $O((Z\alpha)^2)$! Also, it should be remarked that the u-integration will, in general, produce complicated functions of $Z\alpha$. Our nominal order estimate simply describes the lowest-order effects present.

The nominal order estimate $O((Z\alpha)^3\ln((Z\alpha)^2))$ applies to the correction terms in Eq. (11). The final transformation $\langle\gamma^\mu K=\langle[\gamma^\mu;K]$ noted above and eventually leading to Eq. (13) brings the nominal order up to $O((Z\alpha)^4\ln((Z\alpha)^2))$, the lowest-order effect present in the contribution of $\Sigma_{\rm I}(0)$ to the Lamb shift. The effect of the c-number term $4/(u-1)$ in Eq. (13) is simply to renormalize the mass. We drop this term in going over from our present subtraction point $p_\mu p^\mu=0$ to a final subtraction point $p_\mu p^\mu=m^2$ on the physical mass shell.

By using almost all the same steps, we can obtain a result that parallels Eq. (13):

$$\left\langle \gamma_\mu \not{M}\frac{\rho}{\Delta}\gamma^\mu\right\rangle=\left\langle -[\gamma_\mu;\rho]\not{M}K^2\left(\frac{\rho}{\Delta}-\frac{1}{u-1}\right)[\gamma^\mu;\rho]-\frac{2\not{M}}{u-1}\right\rangle. \tag{15}$$

Again, the correction term for changing the Green's function to a c-number is $O((Z\alpha)^4\ln((Z\alpha)^2))$ and this is the lowest-order effect contained in the contribution of $\Sigma_{\rm II}(0)$ to the Lamb shift. The term $-2\not{M}/(u-1)$ is a charge renormalization term and is dropped in going over to a subtraction point on the physical mass shell.

Corresponding to Eqs. (13) and (15) we have

$$\langle\Sigma_{\rm IR}(0)\rangle=\frac{\alpha}{\pi m^3}\left\langle qF_{\mu\nu}\gamma^\nu K\frac{\ln(1-\rho)}{\rho}qF^{\mu\lambda}\gamma_\lambda\right\rangle \tag{16}$$

and

$$\langle\Sigma_{\rm IIR}(0)\rangle=\frac{\alpha}{\pi m^4}\left\langle qF_{\mu\nu}\gamma^\nu\not{M}K\left\{\frac{(1+\rho)\ln(1-\rho)}{2\rho^2}+\frac{1}{2\rho}\right\}qF^{\mu\lambda}\gamma_\lambda\right\rangle. \tag{17}$$

The subscript R signifies dropping renormalization effects. In these equations the integral over the virtual mass squared parameter, u, has been performed explicitly. Also, the identities

$$[\gamma_\mu;\rho]=-\frac{2iq}{m^2}F_{\mu\nu}\gamma^\nu \tag{18}$$

and

$$K^2(1-\rho)=K \tag{19}$$

were needed.

For more complicated expressions there is an advantage in making the replacement

$$\frac{1}{\Delta}\rightarrow\left(\frac{1}{\Delta}-\frac{1}{u-1}\right)+\frac{1}{u-1}$$

throughout, and then moving the projection operators to the factors $(1/\Delta-1/(u-1))$, where they are annulled. Only the commutator correction terms for this move survive. These are provided by the identities

$$\left(\frac{1}{\Delta}-\frac{1}{u-1}\right)OP=\left(\frac{1}{\Delta}-\frac{1}{u-1}\right)[O;\ P] \tag{20}$$

and

$$PO\left(\frac{1}{\Delta}-\frac{1}{u-1}\right)=[P;\ O]\left(\frac{1}{\Delta}-\frac{1}{u-1}\right). \tag{21}$$

This approach is used in the following calculation needed to evaluate $\langle\Sigma_{\mathrm{IV}}(0)\rangle$:

$$\begin{aligned}\left\langle \gamma_\mu \frac{1}{\Delta}[\Pi_\lambda;\ \not{A}]\frac{1}{\Delta}\Pi^\lambda\frac{1}{\Delta}\gamma^\mu\right\rangle=&\left\langle P\gamma_\mu\left(\frac{1}{\Delta}-\frac{1}{u-1}\right)[\Pi_\lambda;\ \not{A}]\left(\frac{1}{\Delta}-\frac{1}{u-1}\right)\Pi^\lambda\left(\frac{1}{\Delta}-\frac{1}{u-1}\right)\gamma^\mu P\right\rangle\\&+\left\langle P\gamma_\mu\left(\frac{1}{\Delta}-\frac{1}{u-1}\right)[\Pi_\lambda;\ \not{A}]\left(\frac{1}{\Delta}-\frac{1}{u-1}\right)\Pi^\lambda\frac{1}{u-1}\gamma^\mu P\right\rangle\\&+\left\langle P\gamma_\mu\left(\frac{1}{\Delta}-\frac{1}{u-1}\right)[\Pi_\lambda;\ \not{A}]\frac{1}{u-1}\Pi^\lambda\left(\frac{1}{\Delta}-\frac{1}{u-1}\right)\gamma^\mu P\right\rangle\\&+\left\langle P\gamma_\mu\left(\frac{1}{\Delta}-\frac{1}{u-1}\right)[\Pi_\lambda;\ \not{A}]\frac{1}{u-1}\Pi^\lambda\frac{1}{u-1}\gamma^\mu\right\rangle\\&+\left\langle \gamma_\mu\frac{1}{u-1}[\Pi_\lambda;\ \not{A}]\left(\frac{1}{\Delta}-\frac{1}{u-1}\right)\Pi^\lambda\left(\frac{1}{\Delta}-\frac{1}{u-1}\right)\gamma^\mu P\right\rangle\\&+\left\langle \gamma_\mu\frac{1}{u-1}[\Pi_\lambda;\ \not{A}]\left(\frac{1}{\Delta}-\frac{1}{u-1}\right)\Pi^\lambda\frac{1}{u-1}\gamma^\mu P\right\rangle\\&+\left\langle \gamma_\mu\frac{1}{u-1}[\Pi_\lambda;\ \not{A}]\frac{1}{u-1}\Pi^\lambda\left(\frac{1}{\Delta}-\frac{1}{u-1}\right)\gamma^\mu P\right\rangle\\&+\left\langle \gamma_\mu\frac{1}{u-1}[\Pi_\lambda;\ \not{A}]\frac{1}{u-1}\Pi^\lambda\frac{1}{u-1}\gamma^\mu\right\rangle.\end{aligned} \tag{22}$$

Projection operators have here been exhibited explicitly where they will be needed. The next step is to move the projection operators to the factors $(1/\Delta-1/(u-1))$ and process the commutator correction terms. The final result is

$$\begin{aligned}&\left\langle \gamma_\mu\frac{1}{\Delta}[\Pi_\lambda;\ \not{A}]\frac{1}{\Delta}\Pi^\lambda\frac{1}{\Delta}\gamma^\mu\right\rangle\\&=\left\langle [\rho;\gamma_\mu]K\left(\frac{1}{\Delta}-\frac{1}{u-1}\right)[\Pi_\lambda;\ \not{A}]\left(\frac{1}{\Delta}-\frac{1}{u-1}\right)K[\Pi^\lambda;\ \rho]\frac{1}{u-1}K[\rho;\ \gamma^\mu]\right\rangle\\&+\left\langle [\rho;\ \gamma_\mu]K\left(\frac{1}{\Delta}-\frac{1}{u-1}\right)[\Pi_\lambda;\ \not{A}]\left(\frac{1}{\Delta}-\frac{1}{u-1}\right)\Pi^\lambda\left(\frac{1}{\Delta}-\frac{1}{u-1}\right)K[\gamma^\mu;\ \rho]\right\rangle\\&+\left\langle [\rho;\ \gamma_\mu]K\left(\frac{1}{\Delta}-\frac{1}{u-1}\right)[\Pi_\lambda;\ \not{A}]\left(\frac{1}{\Delta}-\frac{1}{u-1}\right)K[\Pi^\lambda;\ \rho]\frac{1}{u-1}\gamma^\mu\right\rangle\\&+\left\langle [\rho;\ \gamma_\mu]K\left(\frac{1}{\Delta}-\frac{1}{u-1}\right)[\Pi_\lambda;\ \not{A}]\left(\frac{1}{\Delta}-\frac{1}{u-1}\right)\Pi^\lambda\frac{1}{u-1}K[\gamma^\mu;\ \rho]\right\rangle\end{aligned}$$

$$
\begin{aligned}
&+\left\langle [\rho;\ \gamma_\mu]K\left(\frac{1}{\Delta}-\frac{1}{u-1}\right)[\Pi_\lambda;\ \not{A}]\ \frac{1}{u-1}\ \Pi^\lambda\left(\frac{1}{\Delta}-\frac{1}{u-1}\right)K[\gamma^\mu;\ \rho]\right\rangle\\
&+\left\langle \gamma_\mu\ \frac{1}{u-1}\ [\Pi_\lambda;\ \not{A}]\left(\frac{1}{\Delta}-\frac{1}{u-1}\right)K[\Pi^\lambda;\ \rho]\ \frac{1}{u-1}\ K[\rho;\ \gamma^\mu]\right\rangle\\
&+\left\langle \gamma_\mu\ \frac{1}{u-1}\ [\Pi_\lambda;\ \not{A}]\left(\frac{1}{\Delta}-\frac{1}{u-1}\right)\Pi^\lambda\left(\frac{1}{\Delta}-\frac{1}{u-1}\right)K[\gamma^\mu;\ \rho]\right\rangle\\
&+\left\langle [\rho;\ \gamma_\mu]K\left(\frac{1}{\Delta}-\frac{1}{u-1}\right)[\Pi_\lambda;\ \not{A}]\ \frac{1}{u-1}\ \Pi^\lambda\ \frac{1}{u-1}\ \gamma^\mu\right\rangle\\
&+\left\langle \gamma_\mu\ \frac{1}{u-1}\ [\Pi_\lambda;\ \not{A}]\left(\frac{1}{\Delta}-\frac{1}{u-1}\right)K[\Pi^\lambda;\ \rho]\ \frac{1}{u-1}\ \gamma^\mu\right\rangle\\
&+\left\langle \gamma_\mu\ \frac{1}{u-1}\ [\Pi_\lambda;\ \not{A}]\left(\frac{1}{\Delta}-\frac{1}{u-1}\right)\Pi^\lambda\ \frac{1}{u-1}\ K[\gamma^\mu;\ \rho]\right\rangle\\
&+\left\langle \gamma_\mu\ \frac{1}{u-1}\ [\Pi_\lambda;\ \not{A}]\ \frac{1}{u-1}\ \Pi^\lambda\left(\frac{1}{\Delta}-\frac{1}{u-1}\right)K[\gamma^\mu;\ \rho]\right\rangle\\
&+\left\langle \frac{1}{u-1}\ [\Pi_\lambda;\ -2\not{A}]\ \frac{1}{u-1}\ \Pi^\lambda\ \frac{1}{u-1}\right\rangle. \qquad (23)
\end{aligned}
$$

The nominal order of magnitude of these terms is estimated using the rules mentioned above. Reading down from the top, the nominal orders of magnitude in the language of the Coulomb potential are: first term, $(Z\alpha)^8$; next four terms, $(Z\alpha)^7$; then a $(Z\alpha)^7 \ln((Z\alpha)^2)$ term; then a $(Z\alpha)^6$ term and four $(Z\alpha)^6 \ln((Z\alpha)^2)$ terms. The last term, although of order $(Z\alpha)^3$ by the rules enunciated above, will be found to be order $(Z\alpha)^4$ if nonrelativistic expressions are substituted. Only this last term contributes to the lowest-order Lamb shift. We may evaluate its contribution by substituting into Eq. (9), and find

$$\langle \Sigma_{\mathrm{IV}} \rangle = -\frac{\alpha}{8\pi m^2}\langle q \not{j} \rangle + \cdots, \quad \not{j} \equiv \gamma^\mu j_\mu, \qquad (24)$$

in which j_μ is the source current of the external field, and $\cdots$ signifies contributions of the omitted higher-order terms.

III. CONCLUSION

The projection operator technique introduced here has provided an efficient means of exhibiting factors of the field in the commutator expansion of the basic Lamb shift expression corresponding to the one-photon self-energy diagram. With this greater efficiency one naturally may expect eventually to achieve a greater accuracy in the calculated value of this important quantity.

By our method the infrared divergences complicating the expansions in I are bypassed altogether: all of our expressions are both infrared and ultraviolet finite. The infrared finiteness is evidenced through the appearance of reduced Green's functions. This appearance of reduced Green's functions in relativistic QED is quite surprising, since reduced Green's functions have hitherto typically been associated with nonrelativistic Rayleigh–Schrodinger perturbation theory!

The setting for the projection operator technique is provided by the mass eigenfunction expansion concepts referred to above and in II. It is this setting that lets us talk about relativistic reduced Green's functions associated with an eigenvalue spectrum of mass squared values. It is expected that the mass eigenfunction expansion concepts will prove useful in QED beyond the

present example. Applications to other bound state problems are envisioned, for example to radiative corrections associated with two-photon self-energy diagrams, and to recoil corrections in hydrogen. Also, positronium calculations may benefit from the new method.

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This work is dedicated to the late Professor Donald R. Yennie.

APPENDIX: A ''CONTEXT SENSITIVE'' ORDER OF MAGNITUDE ESTIMATE

We discuss here nominal order estimates for factors of $(1/\Delta - 1/(u-1))$. Consider II, Eqs. (36) and (38). The pth term of the commutator expansion is proportional to the integral

$$\int_1^\infty du(u-1)^{2p+2}\int_0^1 d\xi\,\frac{(1-\xi)^{p+1}}{(p+1)!}\,\frac{\xi^p}{(1+\xi(u-1))^2}\,\frac{N}{\Delta}\,(\tilde{B}_\Delta)^p, \tag{A1}$$

whose behavior near $Z\alpha=0$ we want to investigate. We have set $d=2$, the number of denominators in the original space time integral for $\Sigma_{\rm I}$, $\Sigma_{\rm II}$, $\Sigma_{\rm III}$, and $\Sigma_{\rm IV}$ [see Eqs. (2)–(5)]. We need to perform the symmetric insertions implied by the factor $(\tilde{B}_\Delta)^p$, replace $1/\Delta$ by a sum of two terms as follows:

$$\frac{1}{\Delta}\to\left(\frac{1}{\Delta}-\frac{1}{u-1}\right)+\frac{1}{u-1},$$

and expand. We start with $2+2p$ Green's functions in $(N/\Delta)(\tilde{B}_\Delta)^p$. Under the substitution

$$\frac{1}{\Delta}\to\left(\frac{1}{\Delta}-\frac{1}{u-1}\right)+\frac{1}{u-1}$$

the total number of both $(1/\Delta-1/(u-1))$ factors and $1/(u-1)$ factors in each term of the expanded $(N/\Delta)(\tilde{B}_\Delta)^p$ remains equal to $2+2p$. The result of substituting and expanding is a sum of terms involving integrals of the form

$$I\equiv\int_1^\infty du(u-1)^{2p+2+a}\int_0^1 d\xi\,\frac{(1-\xi)^{p+1}}{(p+1)!}\,\frac{\xi^{p+a}}{(1+\xi(u-1))^{2+a+b}}\left(\frac{1}{\Delta}-\frac{1}{u-1}\right)^n\left(\frac{1}{u-1}\right)^{2+2p-n}, \tag{A2}$$

except that the factors $(1/\Delta-1/(u-1))^n$ are in general separated by ''constant operators,'' operators independent of u and ξ. The parameters (a,b) have values as follows: (0,0) for $\Sigma_{\rm I}$; (0,1) for $\Sigma_{\rm II}$; and (1,0) for $\Sigma_{\rm III}$ and $\Sigma_{\rm IV}$.

The factor $(u-1)^{2p+2+a}$ in Eq. (A2) exhibits a zero at $u=1$ that offsets the poles of the factors

$$\left(\frac{1}{\Delta}-\frac{1}{u-1}\right)^n\left(\frac{1}{u-1}\right)^{2+2p-n}.$$

Accordingly, the u-integral converges and the pth term in the commutator expansion is infrared finite. Indeed, for $a=1$ ($\Sigma_{\rm III}$ and $\Sigma_{\rm IV}$) there is an extra factor of $(u-1)$ beyond what is needed for convergence. This allowed us to perform one commutator using the identity $[O;\,1/\Delta]=(1/\Delta)[O;\,\rho]1/\Delta$ in order to arrive at Eq. (9), a step that increased the order of the pole, making it match the order of the zero. The following discussion assumes that the order of the pole exactly matches the order of the zero, either because $a=0$ or because one commutator has been performed. Note that all requisite symmetric insertions must be carried out before performing a

commutator. See II, Sec. III. With this in mind, the total number of both $(1/\Delta-1/(u-1))$ factors and $1/(u-1)$ factors in each term can be written $2+2p+a$, and Eq. (A2) goes over into

$$I\equiv\int_0^1 d\xi\,\frac{(1-\xi)^{p+1}\xi^{p+a}}{(p+1)!}\int_1^\infty du\,\frac{1}{(1+\xi(u-1))^{2+a+b}}\left(\frac{-(1-\rho)}{u-\rho}\right)^n, \tag{A3}$$

an equation that incorporates the identity

$$\left(\frac{1}{\Delta}-\frac{1}{u-1}\right)=\frac{-(1-\rho)}{(u-\rho)(u-1)}.$$

We start out treating the case in which the factors $(-(1-\rho)/(u-\rho))$ occur together without intervening constant operators. For $n=1$, $(a,b)=(0,0)$, we have

$$\int_1^\infty du\,\frac{1}{(1+\xi(u-1))^2}\frac{1}{(u-\rho)}=-\frac{1}{(1+\xi(\rho-1))}-\frac{\ln(1-\rho)}{(1+\xi(\rho-1))^2}-\frac{\ln(\xi)}{(1+\xi(\rho-1))^2}, \tag{A4}$$

and for $n=1$, $(a,b)=(0,1)$ or $(1,0)$:

$$\int_1^\infty du\,\frac{1}{(1+\xi(u-1))^3}\frac{1}{u-\rho}=-\frac{1}{2(1+\xi(\rho-1))}-\frac{1}{(1+\xi(\rho-1))^2}-\frac{\ln(1-\rho)}{(1+\xi(\rho-1))^3}-\frac{\ln(\xi)}{(1+\xi(\rho-1))^3}. \tag{A5}$$

In either case after supplying a factor $-(1-\rho)$, we find the lowest-order term present to be $O((Z\alpha)^2\ln((Z\alpha)^2))$. This establishes the nominal order estimate for a single factor of $(1/\Delta-1/(u-1))$.

To determine the behavior for a second factor of $(1/\Delta-1/(u-1))$, we start by differentiating Eqs. (A4) and (A5) with respect to ρ. For $(a,b)=(0,0)$, $n=2$, we find

$$\int_1^\infty du\,\frac{1}{(1+\xi(u-1))^2}\frac{1}{(u-\rho)^2}=\frac{\xi}{(1+\xi(\rho-1))^2}+\frac{1}{1-\rho}\frac{1}{(1+\xi(\rho-1))^2}+\frac{2\xi\ln(1-\rho)}{(1+\xi(\rho-1))^3}+\frac{2\xi\ln(\xi)}{(1+\xi(\rho-1))^3}, \tag{A6}$$

and for $(a,b)=(0,1)$ or $(1,0)$, $n=2$:

$$\int_1^\infty du\,\frac{1}{(1+\xi(u-1))^3}\frac{1}{(u-\rho)^2}=\frac{\xi}{2(1+\xi(\rho-1))^2}+\frac{2\xi}{(1+\xi(\rho-1))^3}+\frac{1}{1-\rho}\frac{1}{(1+\xi(\rho-1))^3}+\frac{3\xi\ln(1-\rho)}{(1+\xi(\rho-1))^4}+\frac{3\xi\ln(\xi)}{(1+\xi(\rho-1))^4}. \tag{A7}$$

Next we multiply by $(-(1-\rho))^2$. The lowest-order term in the resultant expression arises from the $1/(1-\rho)$ factors in Eqs. (A6) and (A7). These terms become $O((Z\alpha)^2)$, and this is the collective effect of two factors of $(1/\Delta-1/(u-1))$ in lowest order.

We can investigate the effect of further factors of $(1/\Delta-1/(u-1))$ by carrying out further differentiations with respect to ρ, and then multiplying by higher powers of $(-(1-\rho))$. When these steps are carried out the increasing powers of $(Z\alpha)^2$ due to the additional factors of $(-(1-\rho))$ are exactly offset by the increased negative powers of $1/(1-\rho)$ that arise from the differentiation. The

result is that further factors of $(1/\Delta - 1/(u-1))$ lead to no further increase in the lowest-order present. All additional factors beyond two collectively contribute the same $O((Z\alpha)^2)$ lowest-order behavior!

Next we have to deal with the terms for which some of the factors in $(1/\Delta - 1/(u-1))^n$ are separated from each other by constant operators. Here we make use of the mass eigenfunction expansion of the Green's function to write (see II, Sec. X)

$$\left(\frac{1}{\Delta} - \frac{1}{u-1}\right) = \sum_{\rho_A \neq 1} \frac{-(1-\rho_A)}{(u-\rho_A)(u-1)} P_A . \tag{A8}$$

When this is substituted for $(1/\Delta - 1/(u-1))$ we encounter in place of Eq. (A3) c-number integrals of the general form

$$I = \int_0^1 d\xi \, \frac{(1-\xi)^{p+1}\xi^{p+a}}{(p+1)!} \int_1^\infty du \, \frac{1}{(1+\xi(u-1))^{2+a+b}} \times \frac{(-(1-\rho_A))^{i_A}}{(u-\rho_A)^{i_A}} \frac{(-(1-\rho_B))^{i_B}}{(u-\rho_B)^{i_B}} \cdots \frac{(-(1-\rho_Z))^{i_Z}}{(u-\rho_Z)^{i_Z}}, \tag{A9}$$

in which i_A is the number of occurrences of a particular eigenvalue ρ_A, and similarly for the other exponents. We have

$$i_A + i_B + \cdots + i_Z = n, \tag{A10}$$

when there are n factors of $(1/\Delta - 1/(u-1))$.

For simplicity we shall treat here only the case $(a,b)=(0,0)$, and assume that only two eigenvalues occur, each exactly once. The principles illustrated by this and the above examples are sufficient to handle the more general cases. The relevant u-integral is

$$\int_1^\infty du \, \frac{1}{(1+\xi(u-1))^2} \frac{1}{(u-\rho_A)} \frac{1}{(u-\rho_B)} = \frac{\xi}{\Delta_A \Delta_B} + R_\xi \ln(\xi) - R_A \ln(1-\rho_A) - R_B \ln(1-\rho_B). \tag{A11}$$

The meaning of the symbols is

$$\Delta_A = 1 + \xi(\rho_A - 1), \quad \Delta_B = 1 + \xi(\rho_B - 1), \quad R_\xi = \xi\left(\frac{1}{\Delta_A^2}\frac{1}{\Delta_B} + \frac{1}{\Delta_A}\frac{1}{\Delta_B^2}\right),$$

$$R_A = \frac{1}{\rho_A - \rho_B}\frac{1}{\Delta_A^2}, \quad R_B = -\frac{1}{\rho_A - \rho_B}\frac{1}{\Delta_B^2}.$$

The quantities R_ξ, R_A, and R_B are the residues of the integrand at the three poles: $u = -(1-\xi)/\xi$, $u = \rho_A$, and $u = \rho_B$. We have the following important ''residue identity:''

$$R_\xi + R_A + R_B = 0. \tag{A12}$$

It will be noted that the two residues R_A and R_B are separately $O(1/(Z\alpha)^2)$, while R_ξ is $O(1)$. The residue identity (A12) expresses the cancellation of the $O(1/(Z\alpha)^2)$ effects from the sum $R_A + R_B$. After multiplication by $(1-\rho_A)\,(1-\rho_B)$ we find that the lowest-order contributions in Eq. (A11) come from the two terms $-R_A \ln(1-\rho_A)$ and $-R_B \ln(1-\rho_B)$. These will separately contribute $O((Z\alpha)^2 \ln((Z\alpha)^2))$ to the final result, but when added give a higher-order contribution of $O((Z\alpha)^2)$. To see this, we introduce a set of quantities Λ_A of order unity defined through the equation

$$1-\rho_A \equiv (Z\alpha)^2 \Lambda_A . \tag{A13}$$

Then $\ln(1-\rho_A)=\ln((Z\alpha)^2)+\ln(\Lambda_A)$, and Eq. (A11) becomes

$$\int_1^\infty du \, \frac{1}{(1+\xi(u-1))^2} \frac{1}{(u-\rho_A)} \frac{1}{(u-\rho_B)}$$

$$= \frac{\xi}{\Delta_A \Delta_B} - \frac{\xi}{\Delta_A \Delta_B} \ln((Z\alpha)^2) + R_\xi \ln(\xi) - R_A \ln(\Lambda_A) - R_B \ln(\Lambda_B), \tag{A14}$$

whose lowest-order terms will contribute $O((Z\alpha)^2)$ after multiplication by $(1-\rho_A)\,(1-\rho_B)$, the $O((Z\alpha)^2 \ln((Z\alpha)^2))$ effects having dropped out because of the effect of the residue identity (A12). We conclude that two factors of $(1/\Delta - 1/(u-1))$ still collectively contribute $O((Z\alpha)^2)$, when separated by constant operators.

[1] G. W. Erickson and D. R. Yennie, Ann. Phys. **35**, 271 (1965).
[2] L. Hostler, J. Math. Phys. **34**, 5509 (1993).
[3] See II, Sec. X.
[4] The definition is

$$K \equiv \sum_{\rho_A \neq 1} \frac{P_A}{1-\rho_A}$$

(see II, Sec. X). The ρ_A represent the distinct eigenvalues of the ''mass squared'' operator, ρ. The projector onto the entire degeneracy subspace belonging to ρ_A is represented by P_A. The state $\rangle$ being perturbed has eigenvalue 1. For simplicity, the projector onto the degeneracy subspace of $\rangle$ is represented by just P.

Dually charged mesoatom on the space of constant negative curvature

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The discrete spectrum solutions corresponding to dually charged mesoatom on the space of constant negative curvature are obtained. The discrete spectrum of energies is finite and vanishes when the magnetic charge of the nucleus exceeds the critical value. © *1996 American Institute of Physics.* [S0022-2488(96)01603-9]

I. INTRODUCTION

The behavior of atomlike systems in curved backgrounds were studied by many authors (see, for example, Refs. 1–10 and references cited there). Many papers were devoted to calculations of the curvature-induced energy-level shifts within the framework of the perturbation theory.

In this paper we consider the ''motion'' of massive charged scalar particle (meson) in the field of static dually charged nucleus on the space of constant negative curvature. We find the discrete spectrum solutions of the Klein–Gordon equation [see formulas (3.29) and (3.31)]. The discrete spectrum of the mesoatom is finite. The largest principle number N_0 [see (3.26)] depends on the radius of curvature a and the magnetic charge g_m. For sufficiently small values of a or large values of g_m the discrete spectrum is empty.

It should be noted that the expression for the energy levels [formula (3.24) of this paper] was obtained earlier in Ref. 8. However, the expressions for N_0 and the wave functions in Ref. 8 are wrong.[10]

II. THE MODEL

We consider the space–time $R\times L^3(a)$ with the metric

$$g=c^2dt\otimes dt-\gamma=g_{\mu\nu}(x)dx^\mu\otimes dx^\nu, \tag{2.1}$$

where

$$L^3(a)\equiv\{z|z=(z^0,\vec{z})\in R^4,z^0>0,(z^0)^2-(\vec{z})^2=a^2\} \tag{2.2}$$

is three-dimensional space of constant negative curvature (a is radius of curvature) with the canonical metric

$$\gamma=\gamma_{ij}(\vec{x})dx^i\otimes dx^j=a^2[d\chi\otimes d\chi+\sinh^2\chi(d\theta\otimes d\theta+\sin^2\theta\, d\varphi\otimes d\varphi)], \tag{2.3}$$

$0<\chi<+\infty$ ($a\sinh\chi=|\vec{z}|$).

We consider a static dually charged nucleus with the electric charge $(-Ze)$ and a magnetic charge g_m, placed in the coordinate origin $\chi=0$. Let $U\subset L^3(a)$ be a domain with the trivial cohomology group $H^2(U,R)=0$ and $\{\chi=0\}\notin U$. The electromagnetic four-potential A_μ on $R\times U$, corresponding to the nucleus, has the following form:

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$$A = A_\mu dx^\mu = \left(- \frac{Ze}{a} \right) (\coth \chi - 1) dt + \mathscr{A}, \tag{2.4}$$

where

$$\mathscr{F} = d\mathscr{A} = g_m \sin \theta \, d\theta \wedge d\varphi \tag{2.5}$$

is the strength of the electromagnetic field, corresponding to the magnetic charge g_m. The relation (2.5) is correct, since due to $H^2(U,R)=0$ any closed two-form on U is exact, i.e., $d\mathscr{F}=0$ entails the existence of $\mathscr{A}$ such that $d\mathscr{A}=\mathscr{F}$. For $U = U_\pm$, where

$$U_\pm = L^3(a) \backslash \left\{ \theta = \frac{\pi}{2} \pm \frac{\pi}{2} \right\}, \tag{2.6}$$

the one-form on $U = U_\pm$,

$$\mathscr{A} = \mathscr{A}^\pm = g_m (\pm 1 - \cos \theta) d\varphi, \tag{2.7}$$

satisfies the relation (2.5).

A massive charged scalar particle (meson), moving in the field of the static dually charged nucleus, has the following action:

$$S[\varphi] = \frac{1}{c} \int_{M_*} d^4x (-\det g_{\mu\nu})^{1/2} \{ \hbar^2 g^{\mu\nu} (\overline{D_\mu(A^*)\varphi_*}) (D_\nu(A^*)\varphi_*) - m_0^2 c^2 \overline{\varphi}_* \varphi_* \}, \tag{2.8}$$

where $D_\mu = D_\mu(A^*) \equiv \nabla_\mu + (ie/\hbar c) A^*_\mu$, ∇_μ is covariant derivative, corresponding to the metric (2.1); the symbol $*=\pm$ and $A = A^\pm$ is a result of substitution of $\mathscr{A}^\pm$ from (2.7) to (2.4); m_0 is mass of the scalar particle and e is its charge (opposite in sign to the nucleus charge). The pair of functions

$$\varphi_\pm : M_\pm = R \times U_\pm \to C \tag{2.9}$$

satisfies the overlapping condition

$$\varphi_+(t,\vec{x}) = \Omega(\vec{x}) \varphi_-(t,\vec{x}), \tag{2.10}$$

$\vec{x} \in U_+ \cup U_-$, where

$$\Omega : U_+ \cup U_- \to U(1) \tag{2.11}$$

is a smooth overlapping function. The scalar particle (meson) wave function is a smooth section of a vector C-bundle with the base $R \times (L^3(a) \backslash \{\chi = 0\})$. This section is defined by the pair of functions (2.9), satisfying the condition (2.10). (The function $\varphi_\pm$ is the representation of the function $\varphi | M_\pm$ in the local trivialization over $M_\pm$.)

The action (2.8) is correctly defined, i.e., the right-hand side of (2.8) does not depend on the choice of the symbol $*=\pm$ (or equivalently on the choice of local trivialization) if the function Ω (2.11) satisfies the following relation on $U_+ \cup U_-$:

$$\mathscr{A}^+ = \mathscr{A}^- + i \frac{\hbar c}{e} \Omega^{-1} \, d\Omega \tag{2.12}$$

[$\mathscr{A}^\pm$ are defined in (2.7)]. It follows from the relations (2.7) and (2.12) that such a function does exist if and only if the Dirac quantization condition is satisfied:[11]

$$q \equiv e g_m / \hbar c = 0, \pm \tfrac{1}{2}, \pm \tfrac{3}{2}, \ldots \ . \tag{2.13}$$

In this case

$$\Omega = \exp[-2iq(\varphi - \varphi_0)], \tag{2.14}$$

where $\varphi_0 = \text{const}$.

Varying the action (2.8), we obtain the following equation of motion:

$$[\hbar^2 g^{\mu\nu} (\overline{D_\mu(A^*)})(D_\nu(A^*)) + m_0^2 c^2] \varphi_* = 0. \tag{2.15}$$

The Lagrangian, corresponding to the action (2.8), has the following form:

$$L(\varphi, v) = \int_{U_*} d^3\vec{x} (\det \ \gamma_{ij})^{1/2} \left\{ \frac{\hbar^2}{c^2} \left| v_* + \frac{ie}{\hbar} V \varphi_* \right|^2 - \hbar^2 \gamma^{ij} \right.$$
$$\left. \times (\overline{D_i(\mathscr{A}^*)\varphi_*})(D_j(\mathscr{A}^*)\varphi_*) - m_0^2 c^2 \overline{\varphi}_* \varphi_* \right\}, \tag{2.16}$$

where $V \equiv (-Ze)(\coth \chi - 1)/a$, $v_+(\vec{x}) = \Omega v_-(\vec{x})$. The Lagrangian (2.16) is a continuous mapping

$$L : H \times H \to R, \tag{2.17}$$

where $H \times H \cong TH$ and TH is tangent vector bundle over the Hilbert space H. This Hilbert space is the configuration space of the Lagrange system. It consists of smooth sections of the monopole vector C-bundle over $L^3(a) \setminus \{\chi = 0\}$ satisfying the restriction

$$\int_{U_*} d^3\vec{x} (\det \ \gamma_{ij})^{1/2} \{ \overline{\varphi}_* \varphi_* (1 + V^2) + \gamma^{ij} \overline{(D_i(\mathscr{A}^*)\varphi_*)} (D_j(\mathscr{A}^*)\varphi_*) \} < +\infty. \tag{2.18}$$

The scalar product in H is the following:

$$(\psi, \varphi) \equiv \int_{U_*} d^3\vec{x} (\det \ \gamma_{ij})^{1/2} \{ \overline{\psi}_* \varphi_* (1 + V^2) + \gamma^{ij} \overline{(D_i(\mathscr{A}^*)\psi_*)} (D_j(\mathscr{A}^*)\varphi_*) \}, \tag{2.19}$$

$* = \pm$. Strictly speaking, H is the completion of the pre-Hilbert space [with scalar product (2.19)] of smooth sections with compact support in $U_+ \cup U_-$. (H is the modified Sobolev space.) The field equation (2.15) is equivalent to the Euler–Lagrange equations for the Lagrange system (L, H).

III. THE DISCRETE SPECTRUM SOLUTIONS

We seek solutions of the equation of motion (2.15) in the following form:

$$\varphi(t, \vec{x}) = \exp(-iEt/\hbar) F(\vec{x}), \tag{3.1}$$

where $E \in C$ and $F \in H$. The substitution of (3.1) into (2.15) leads to the following relation:

$$\left\{ [\varepsilon + Z\alpha(\coth \chi - 1)]^2 + \frac{1}{\sinh^2 \chi} \frac{\partial}{\partial \chi} \left(\sinh^2 \chi \frac{\partial}{\partial \chi} \right) + \frac{1}{\sinh^2 \chi} \Delta_q^* - \mu^2 \right\} F_* = 0, \tag{3.2}$$

where

$$\varepsilon \equiv Ea/\hbar c, \quad \mu \equiv m_0 ac/\hbar, \quad \alpha \equiv e^2/\hbar c, \tag{3.3}$$

and

$$\Delta_q^* = \beta^{ij} D_i(\mathscr{A}^*) D_j(\mathscr{A}^*) \tag{3.4}$$

is the "monopole Laplace operator"[12] on the two-dimensional sphere S^2 (β is the canonical metric on S^2), written in the local trivialization over S^2_*, $*=\pm$, where $S^2_\pm = S^2 \setminus \{\theta = \pi/2 \pm \pi/2\}$. The operator Δ_q acts on the sections of the monopole vector C-bundle over S^2. For $q=0$ it coincides with the Laplace operator on S^2. The spectrum of Δ_q is well known,[12,13] it is discrete,

$$\Delta_q Y_{qlm} = [-l(l+1)+q^2] Y_{qlm}, \tag{3.5}$$

where

$$l = |q|, |q|+1, \ldots, \quad m = -l, -l+1, \ldots, l, \tag{3.6}$$

and Y_{qlm} are monopole spherical harmonics.[13] For the sake of completeness the explicit expression for Y_{qlm} is presented in the Appendix. The relation (3.5) follows from the representation for Δ_q (Ref. 13):

$$-\hbar^2 \Delta_q = (\vec{L}_q)^2 - \hbar^2 q^2. \tag{3.7}$$

In (3.7) $\vec{L}_q$ is the modified (monopole) momentum operator[13]

$$(L_q^j)^* = \varepsilon_{jkl} z^k \left(-i\hbar \frac{\partial}{\partial z^l} + \frac{e}{c} \mathscr{A}_l^* \right) - \hbar q \frac{z^j}{|z|}, \tag{3.8}$$

$j=1,2,3$, where $\mathscr{A}_i^\pm$ are the components of the one-form (2.7) in z-coordinates [see (2.2)]

$$\mathscr{A}^\pm = \mathscr{A}_t^\pm dz^i = \frac{g_m \varepsilon_{ij3} z^i \, dz^j}{|z|(z^3 \pm |z|)}. \tag{3.9}$$

The components of the operator (3.8) satisfy the commutation relations

$$[L_q^k, L_q^l] = i\hbar \varepsilon_{klj} L_q^j. \tag{3.10}$$

The monopole harmonics Y_{qlm} form a complete orthonormal set (on S^2) of the eigenfunctions of the operators $(\vec{L}_q)^2$ and L_q^3:

$$[(\vec{L}_q)^2 - \hbar^2 l(l+1)] Y_{qlm} = 0, \tag{3.11}$$

$$[L_q^3 - \hbar m] Y_{qlm} = 0, \tag{3.12}$$

where l and m satisfy (3.6). The equality (3.5) follows from the relations (3.7) and (3.10).

Let F be an eigenfunction of the operators $(\vec{L}_q)^2$ and L_q^3. Then

$$F_*(\chi, \theta, \varphi) = Q(\chi)(Y_{qlm})_*(\theta, \varphi). \tag{3.13}$$

Substituting (3.13) into (3.2) and taking into account (3.5), we obtain

$$\left\{ [\varepsilon + Z\alpha(\coth \chi - 1)]^2 + \frac{1}{\sinh^2 \chi} \frac{\partial}{\partial \chi} \left(\sinh^2 \chi \frac{\partial}{\partial \chi} \right) - \frac{1}{\sinh^2 \chi} [l(l+1) - q^2] - \mu^2 \right\} Q = 0. \tag{3.14}$$

The inclusion $F \in H$ is equivalent to the convergence of the integral

$$\int_0^\infty d\chi \, \sinh^2 \chi \left\{ |Q|^2 \left(1 + \frac{1}{\sinh^2 \chi} \right) + |\partial_\chi Q|^2 \right\} < +\infty \tag{3.15}$$

[this condition follows from (2.18) and (3.13)].

We introduce a new variable x,

$$x = 2/(\coth \chi + 1) \tag{3.16}$$

($0<x<1$ for $\chi>0$). Then Eq. (3.14), written in x-variable,

$$\frac{d^2Q}{dx^2} + \frac{2}{x}\frac{dQ}{dx} + \frac{1}{4x^2(1-x)^2}\{[\varepsilon x + 2Z\alpha(1-x)]^2 - \mu^2 x^2 - 4[l(l+1) - q^2](1-x)\}Q = 0, \tag{3.17}$$

has a generalized hypergeometric form.[14] The standard procedure (see, for example, Ref. 14) gives the substitution

$$Q = x^{-1/2+\kappa}(1-x)^{1/2+\lambda/2} v, \tag{3.18}$$

leading to the hypergeometric equation for the function $v = v(x)$

$$x(1-x)\frac{d^2v}{dx^2} + [1 + 2\kappa - (2 + 2\kappa + \lambda)x]\frac{dv}{dx} + [Z\alpha\varepsilon - (\kappa + \tfrac{1}{2})^2 - (Z\alpha)^2 - \lambda(\kappa + \tfrac{1}{2})]v = 0, \tag{3.19}$$

where

$$\lambda = \sqrt{\mu^2 + 1 - \varepsilon^2}, \quad \kappa = \sqrt{(l + \tfrac{1}{2})^2 - (Z\alpha)^2 - q^2}, \tag{3.20}$$

and $\sqrt{re^{i\phi}} \equiv r^{1/2}e^{i\phi/2}$, $-\pi < \phi \leqslant \pi$. Here and below we put the following restriction on Z: $Z\alpha < \frac{1}{2}$.

The solution of (3.19) may be expressed in terms of hypergeometric functions

$$v(x) = d_+ F(A_+, B_+, C_+, x) + d_- x^{-2\kappa} F(A_-, B_-, C_-, x), \tag{3.21}$$

where d_+, d_- are arbitrary constants and

$$A_\pm = \pm\kappa + \tfrac{1}{2}[\lambda + 1 - \sqrt{\lambda^2 + 4Z\alpha(\varepsilon - Z\alpha)}],$$

$$B_\pm = \pm\kappa + \tfrac{1}{2}[\lambda + 1 + \sqrt{\lambda^2 + 4Z\alpha(\varepsilon - Z\alpha)}],$$

$$C_\pm = \pm 2\kappa + 1.$$

Using the asymptotic formulas for the hypergeometric functions[14] (for $x \to 0$ and $x \to 1$), we find that the function Q, defined by (3.18) and (3.21), satisfies the restriction (3.15), if and only if $d_- = 0$ and

$$A_+ = -n, \tag{3.22}$$

$n = 0,1,2,\ldots$. In this case

$$v(x)=\text{const } P_n^{(2\kappa,\lambda)}(1-2x), \tag{3.23}$$

where $P_n^{(\alpha,\beta)}(z)$ is the Jacobi polynomial[14] (see also Appendix).

Solving Eq. (3.22), we obtain

$$\varepsilon=Z\alpha+N\,\frac{[\mu^2+1-N^2-(Z\alpha)^2]^{1/2}}{[N^2+(Z\alpha)^2]^{1/2}}, \tag{3.24}$$

where

$$N=n+\kappa+\tfrac{1}{2} \tag{3.25}$$

is the principal quantum number satisfying the inequality

$$N<N_0\equiv(Z\alpha)^{1/2}[(\mu^2+1)^{1/2}-Z\alpha]^{1/2}. \tag{3.26}$$

Thus, there exists only a finite number of normalizable solutions of the equation of motion (2.15) that have the form (3.1) and are eigenfunctions of the operators $(\vec{L}_q)^2$ and L_q^3. These solutions are the discrete spectrum solutions.

It follows from the definitions (3.20) and (3.25) and the inequalitiy (3.26) that the discrete spectrum is absent for $N_0\leqslant\frac{1}{2}$. For $N_0>\frac{1}{2}$ it is also absent if

$$|q|\geqslant|q|_0=(N_0)^2-N_0+(Z\alpha)^2 \tag{3.27}$$

and exists if $|q|<|q|_0$. In this case $\varepsilon=\varepsilon(N)=\varepsilon(N(n,l,|q|))$, where the principal quantum number N is defined in (3.25) and

$$l=|q|,\ldots,l_0(|q|),\quad n=0,\ldots,n_0(l,|q|). \tag{3.28}$$

In (3.28)

$$l_0(|q|)\equiv\max\{l|l-|q|=0,1,\ldots;l(l+1)-q^2<|q|_0\},$$

$$n_0(l,|q|)\equiv\max\{n|n=0,1,\ldots;n+\kappa+\tfrac{1}{2}<N_0\}$$

[the relations for l_0 and n_0 follow from the inequality (3.26)].

In the initial notations we have the following expression for the energy spectrum:

$$E=\frac{Ze^2}{a}+N\,\frac{[m_0^2c^4+(1-N^2-(Z\alpha)^2)(\hbar^2c^2/a^2)]^{1/2}}{[N^2+(Z\alpha)^2]^{1/2}}, \tag{3.29}$$

where $N<N_0(a)$, $N_0(a)>\frac{1}{2}$, and $|q|<|q|_0=|q|_0(a)$.

Due to (3.29),

$$Ze^2/a<E<m_0c^2. \tag{3.30}$$

The meson wave function, corresponding to the set of quantum numbers (n,l,m) is

$$\varphi=C\,\exp(-iEt/\hbar)\left(\frac{2}{\coth\chi+1}\right)^{-1/2+\kappa}\exp[-\chi(1+\lambda)]P_n^{(2\kappa,\lambda)}\left(\frac{\coth\chi-3}{\coth\chi+1}\right)Y_{qlm}, \tag{3.31}$$

where C is constant and n, l, and m satisfy the restrictions (3.28) and (3.6) correspondingly; $\kappa=\kappa(l,|q|)$ and $\lambda=\lambda(E,a)$ are defined in (3.20).

Now we show that the parameter E is the energy, corresponding to the meson wave function, appropriately normalized. The energy functional, corresponding to the Lagrangian (2.16), is

$$\mathscr{E}(\varphi,v)=\int_{U_*} d^3\vec{x}(\det\ \gamma_{ij})^{1/2} \times\left\{\frac{\hbar^2}{c^2}\ \overline{v}_*v_*-\frac{e^2}{c^2}\ V^2\overline{\varphi_*}\varphi_*+\hbar^2\gamma^{ij}\overline{(D_i(\mathscr{A}^*)\varphi_*)}(D_j(\mathscr{A}^*)\varphi_*)+m_0^2c^2\overline{\varphi_*}\varphi_*\right\}. \tag{3.32}$$

The energy is conserved on the solutions of the equation of motion (2.15): $\mathscr{E}=\mathscr{E}(\varphi(t),\dot{\varphi}(t))=$const. The Lagrangian (2.16) is invariant under the $U(1)$-transformations: $\varphi\mapsto\varphi^s=\exp(-ise/\hbar)\varphi$. Due to E. Noether's theorem we have $Q=Q(\varphi(t),\dot{\varphi}(t))=$const, where

$$Q(\varphi,v)=\int_{U_*} d^3\vec{x}(\det\ \gamma_{ij})^{1/2}\{i\hbar(\overline{\varphi_*}v_*-\overline{v_*}\varphi_*)-2eV\overline{\varphi_*}\varphi_*\} \tag{3.33}$$

is the charge functional ($Q:H\times H\to R$). Using (2.15) and (3.1), we get $\mathscr{E}=EQ/e$. The physical normalization of the wave function $Q=Q(\varphi(t),\dot{\varphi}(t))=e$ entails $\mathscr{E}=E$. So, E is the energy of the scalar particle (meson).

Let us consider the flat-space limit: $a\to+\infty$. In this case $|q|_0$, $N_0\to+\infty$ and the discrete spectrum (3.29) contains an infinite number of levels for all values of q. For $q=0$ and $a\to+\infty$ the formulas (3.29) and (3.31) coincide with the well-known relations (see, for example, Ref. 14).

For $a\sim10^{28}$ cm (present cosmological scale), $Z=1$, and $m=m_{\pi^+}$ (the mass of π^+-meson) we have $N_0\sim10^{20}$ and $|q|_0\sim10^{40}$.

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APPENDIX: MONOPOLE SPHERICAL HARMONICS

Here we present the explicit expressions for the monopole spherical harmonics Y_{qlm}, $l=|q|,|q|+1,...$, $m=-l,-l+1,\ldots,l$; Y_{qlm} are smooth sections of the monopole vector C-bundle over the sphere S^2. In the local trivialization over $S^2_\pm=S^2\setminus\{\theta=\pi/2\pm\pi/2\}$ the sections Y_{qlm} are represented by the complex-valued functions on $S^2_\pm$:

$$(Y_{qlm})_\pm=M_{qlm}P_n^{(\alpha,\beta)}(\cos\ \theta)\exp(i(m\pm q)\varphi), \tag{3.34}$$

where

$$\alpha=-q-m,\quad \beta=q-m,\quad n=l+m, \tag{3.35}$$

and $P_n^{(\alpha,\beta)}(x)$ is Jacobi polynomial

$$P_n^{(\alpha,\beta)}(x)=\frac{(-1)^n}{2^n n!}\ (1-x)^{-\alpha}(1+x)^{-\beta}\ \frac{d^n}{dx^n}\left[(1-x)^{\alpha+n}(1+x)^{\beta+n}\right]$$

$$=\frac{\Gamma(n+\alpha+1)}{n!\Gamma(\alpha+1)}\ F(-n,n+\alpha+\beta+1,\alpha+1,(1-x)/2)$$

(M_{qlm} are constants).

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Recursively minimally-deformed oscillators

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A recursive deformation of the boson commutation relation is introduced. Each step consists of a minimal deformation of a commutator $[a,a^\dagger]=f_k(\cdots;\hat{n})$ into $[a,a^\dagger]_{q_{k+1}}=f_k(\cdots;\hat{n})$, where $\cdots$ stands for the set of deformation parameters that f_k depends on, followed by a transformation into the commutator $[a,a^\dagger]=f_{k+1}(\cdots,q_{k+1};\hat{n})$ to which the deformed commutator is equivalent within the Fock space. Starting from the harmonic oscillator commutation relation $[a,a^\dagger]=1$ we obtain the Arik–Coon and Macfarlane–Biedenharn oscillators at the first and second steps, respectively, followed by a sequence of multiparameter generalizations. Several other types of deformed commutation relations related to the treatment of integrable models and to parastatistics are also obtained. The ''generic'' form consists of a linear combination of exponentials of the number operator, and the various recursive families can be classified according to the number of free linear parameters involved, that depends on the form of the initial commutator. © *1996 American Institute of Physics.* [S0022-2488(96)02403-6]

I. INTRODUCTION

The study of deformed oscillators has already yielded a plethora of formal results and applications, but the attempts to introduce some order in the rich and varied choice of deformed commutation (quommutation) relations studied by different authors has so far achieved limited success. Of particular interest in this respect are the treatments due to Jannussis *et al.*,[1,2] Daskaloyannis,[3,4] McDermott and Solomon,[5] and Meljanac *et al.*[6]

The following is a partial list of deformations that have been studied.

(1) The Arik–Coon oscillator[7]

$$[a,a^\dagger]_q\equiv aa^\dagger-qa^\dagger a=1.$$

(2) The Macfarlane–Biedenharn oscillator[8,9]

$$[a,a^\dagger]_q=q^{-\hat{n}}$$

that has independently been proposed by Sun and Fu.[10]

(3) The Chakrabarti–Jagannathan oscillator[11]

$$[a,a^\dagger]_p=q^{-\hat{n}}.$$

(4) The Calogero–Vasiliev oscillator[12]

$$[a,a^\dagger]=1+2\nu(-1)^{\hat{n}},$$

which for $2\nu=p-1$ is the Chaturvedi–Srinivasan parabose oscillator of order p.[13]

(5) The Brzeziński–Egusquiza–Macfarlane oscillator[14]

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$$[a,a^\dagger]=q^{-\hat{n}}[1+2\nu(-1)^{\hat{n}}].$$

(6) Macfarlane's q-deformed Calogero–Vasiliev oscillator[15]

$$aa^\dagger-q^{\pm(1+2\nu K)}a^\dagger a=[[1+2\nu K]]q^{\mp(\hat{n}+\nu-\nu K)},$$

where $K=(-1)^{\hat{n}}$ and $[[x]]=(q^x-q^{-x})/(q-q^{-1})$.

In the present contribution we introduce a notion of minimal deformation, that, along with the well known flexibility exhibited by the presentation of the quommutation relations within the Fock space, enables a recursive deformation procedure to be formulated, generating the various types of deformed oscillators listed above, thus yielding a certain classification principle. Moreover, the procedure proposed yields a multiparameter generalization of the quommutation relations and suggests that the "generic" structure involves sums of exponentials of the number operator.

II. EQUIVALENCE OF QUOMMUTATORS AND COMMUTATORS

Let a and $a^\dagger$ be two mutually conjugate operators and let $\hat{n}$ satisfy the commutation relations $[a,\hat{n}]=a$ and $[\hat{n},a^\dagger]=a^\dagger$. It follows that $\hat{n}$ commutes with $a^\dagger a$ and with $aa^\dagger$. Furthermore, let

$$a\alpha(\hat{n})a^\dagger-a^\dagger\beta(\hat{n})a=\gamma(\hat{n}), \tag{1}$$

where $\alpha(l)$, $\beta(l)$, and $\gamma(l)$ are given functions such that $\alpha(l)$ does not vanish for integral and non-negative l. This quommutation relation contains the form studied by McDermott and Solomon,[5] in which $\alpha(\hat{n})=\gamma(\hat{n})=1$. It is a symmetrized version of that studied by Meljanac *et al.*[6] [corresponding to $\alpha(\hat{n})=1$], to which it is easily shown to be equivalent. The transformations introduced below take place within a Fock space representation that is assumed to exist, possessing a nondegenerate ground state that satisfies $a|0\rangle=0$. At least within this representation it is rather likely that the form introduced by McDermott and Solomon[5] is sufficiently general. The nondegeneracy requirement of the ground state has recently been relaxed by several authors[16–18] who introduced a doubly degenerate ground state that was found useful in the context of discussing intermediate statistics. We shall not pursue this extension. From the assumptions specified above it follows that

$$a^\dagger|k\rangle=\sqrt{F(k+1)}|k+1\rangle \tag{2}$$

and

$$a|k+1\rangle=\sqrt{F(k+1)}|k\rangle, \tag{3}$$

where

$$F(k)=\sum_{i=0}^{k-1}\frac{\gamma(i)\beta(i)\beta(i+1)\cdots\beta(k-1)}{\alpha(i+1)\alpha(i+2)\cdots\alpha(k)\beta(k-1)}. \tag{4}$$

Hence, $aa^\dagger=F(\hat{n}+1)$, $a^\dagger a=F(\hat{n})$ and the quommutator $[a,a^\dagger]_Q\equiv aa^\dagger-Qa^\dagger a$ is

$$[a,a^\dagger]_Q=\frac{\gamma(\hat{n})}{\alpha(\hat{n}+1)}+\sum_{i=0}^{\hat{n}-1}\frac{\gamma(i)\beta(i)\beta(i+1)\cdots\beta(\hat{n}-1)}{\alpha(i+1)\alpha(i+2)\cdots\alpha(\hat{n})}\left(\frac{1}{\alpha(\hat{n}+1)}-\frac{Q}{\beta(\hat{n}-1)}\right), \tag{5}$$

where Q is arbitrary, but will usually be chosen to be equal to unity, and where the appearance of the number operator within the upper summation limit (as well as within the summand) has a well defined meaning when applied to any Fock state.

Consider the following example. Let

$$aa^\dagger - a^\dagger q^{\hat{n}+1} a = 1,$$

i.e., $\alpha(\hat{n})=1$, $\beta(\hat{n}) = q^{\hat{n}+1}$, $\gamma(\hat{n})=1$. This is equivalent to

$$[a,a^\dagger]=1+(q^{\hat{n}}-1)\sum_{j=0}^{\hat{n}-1} q^{[j(2\hat{n}-j-1)]/2}.$$

The quommutation relation obtained for $q=-1$, i.e., $aa^\dagger - a^\dagger(-1)^{\hat{n}+1}a = 1$, can be transformed with the aid of the identity

$$\sum_{j=0}^{2k} (-1)^{[(j-1)j]/2}=1$$

into the equivalent form $[a,a^\dagger] = (-1)^{\hat{n}}$, whose significance was discussed by Quesne and Vansteenkiste.[19]

As a further example we consider the q-deformed Calogero–Vasiliev oscillator, proposed by Macfarlane.[15] This oscillator can be transformed into

$$[a,a^\dagger]_Q=\frac{1}{2(q-q^{-1})}\{q^{\hat{n}}(q-Q)(q^{2\nu}+1)+q^{-\hat{n}}(Q-q^{-1})(q^{-2\nu}+1)$$
$$+(-q)^{\hat{n}}(Q+q)(q^{2\nu}-1)+(-q)^{-\hat{n}}(Q+q^{-1})(1-q^{-2\nu})\}. \tag{6}$$

This can be done either by starting from the quommutator quoted in the Introduction and applying the procedure illustrated above, or, more simply, using the expressions for $aa^\dagger$ and for $a^\dagger a$ presented by Macfarlane.[15] In either case, the expression obtained is written separately for $\hat{n}$ even and for $\hat{n}$ odd, and the two expressions are combined with coefficients of the form $\frac{1}{2}(1+(-1)^{\hat{n}})$ and $\frac{1}{2}(1-(-1)^{\hat{n}})$, respectively. Some further minor rearrangement yields Eq. (6), that consists of a linear combination of four exponentials in $\hat{n}$ (three, if Q is chosen to be equal to q, q^{-1}, $-q$, or $-q^{-1}$).

Another ''exotic'' quommutator is[20,21]

$$aa^\dagger - \frac{q^{\hat{n}+2}+1}{q(q^{\hat{n}}+1)}\,a^\dagger a = 1$$

i.e., $\alpha(\hat{n})=1$, $\beta(\hat{n}) = (q^{\hat{n}+3}+1)/[q(q^{\hat{n}+1}+1)]$, $\gamma(\hat{n})=1$. In this case,

$$[a,a^\dagger]_Q=1+\frac{q^{n+1}(q-Q)+1-qQ}{q^2-1}\,(1-q^{-\hat{n}}),$$

which, for $q=Q$ reduces to the Macfarlane–Biedenharn oscillator $[a,a^\dagger]_q = q^{-\hat{n}}$.

III. RECURSIVE DEFORMATION OF THE HARMONIC OSCILLATOR

In the following we will be interested in what appears to be a somewhat more restricted framework. Starting from $[a,a^\dagger]=f_0(\hat{n})$ let us assume that at the kth step of a recursive procedure to be fully explicated below we have obtained the commutation relation

$$[a,a^\dagger]=f_k(\hat{n}).$$

We define the next minimal deformation to be

$$[a,a^\dagger]_{q_{k+1}}=f_k(\hat{n}).$$

This minimally-deformed relation implies that, in the Fock-space representation,

$$a^\dagger|l\rangle=\sqrt{F_{k+1}(l+1)}|l+1\rangle$$

and

$$a|l+1\rangle=\sqrt{F_{k+1}(l+1)}|l\rangle,$$

where

$$F_{k+1}(l)=\sum_{i=0}^{l-1} q_{k+1}^i f_k(l-1-i). \tag{7}$$

It follows that

$$[a,a^\dagger]=f_{k+1}(\hat{n}),$$

where

$$f_{k+1}(\hat{n})\equiv F_{k+1}(\hat{n}+1)-F_{k+1}(\hat{n}).$$

This recurrence relation can also be written in the form

$$f_{k+1}(\hat{n})=\sum_{i=0}^{\hat{n}} q_{k+1}^{\hat{n}-i}(f_k(i)-f_k(i-1))$$

provided that we define $f_k(-1)\equiv 0$. From the recurrence relation it follows that if $\lim_{q_1\to 1,q_2\to 1,\ldots,q_k\to 1} f_k(l)=1$ for $l=0,1,\ldots$, then $\lim_{q_1\to 1,q_2\to 1,\ldots,q_{k+1}\to 1} f_{k+1}(l)=1$. In other words, for all k, if $f_k(\hat{n})$ is a deformation of unity, so is $f_{k+1}(\hat{n})$.

It will be convenient to define

$$\Phi_k(l)=\sum_{\substack{0\leqslant i_1,i_2,\ldots,i_k \\ (i_1+i_2+\cdots+i_k=l-k+1)}} q_1^{i_1}q_2^{i_2}\cdots q_k^{i_k},$$

which is easily shown to satisfy the limiting property

$$\lim_{q_1\to 1,q_2\to 1,\cdots,q_k\to 1}\Phi_k(l)=\binom{l}{k-1}.$$

Note that

$$\Phi_1(l)=q_1^l,$$

$$\Phi_2(l)=\frac{q_1^l-q_2^l}{q_1-q_2}=\frac{q_1^l}{q_1-q_2}+\frac{q_2^l}{q_2-q_1},$$

$$\Phi_3(l)=\frac{q_1^l}{(q_1-q_2)(q_1-q_3)}+\frac{q_2^l}{(q_2-q_1)(q_2-q_3)}+\frac{q_3^l}{(q_3-q_1)(q_3-q_2)},$$

or, in general,

$$\Phi_k(l)=\sum_{i=1}^{k} \frac{q_i^l}{\Pi_{m=1}^{k}{}'(q_i-q_m)},$$

the prime indicating that $m\neq i$.

Let us now take

$$f_0(l)=\begin{cases}1 & \text{for} \quad l\geqslant 0,\\ 0 & \text{for} \quad l<0,\end{cases}$$

i.e., start from the conventional harmonic oscillator commutation relation, $[a,a^\dagger]=1$. With this initial value it can be shown that for $k\geqslant 1$

$$f_k(\hat{n})=\sum_{j=0}^{k-1}(-1)^{k-1-j}\binom{k-1}{j}\Phi_k(\hat{n}+j)=\sum_{i=1}^{k}\omega_{k,i}q_i^{\hat{n}}, \tag{8}$$

where $\omega_{k,i}=\Pi_{m=1}^{k}{}'[(q_i-1)/(q_i-q_m)]$. Applying the residue theorem to the function

$$f(z)=\frac{(z-1)^l}{\Pi_{m=1}^{k}(z-q_m)}$$

we obtain

$$\sum_{i=1}^{k}\frac{(q_i-1)^l}{\Pi_{m=1}^{k}{}'(q_i-q_m)}=\begin{cases}1, & l=k-1,\\ 0, & 0\leqslant l<k-1.\end{cases} \tag{9}$$

The case $l=k-1$ yields

$$\sum_{i=1}^{k}\omega_{k,i}=1,$$

which clarifies the significance of Eq. (8), suggesting that the coefficients $\omega_{k,i}$, $i=1,2,\ldots,k$, are the weights in an appropriate average. Substituting Eq. (8) in Eq. (7) we obtain, for $k\geqslant 1$,

$$F_{k+1}(l)=\sum_{i=1}^{k}\frac{(q_i-1)^{k-1}}{\Pi_{m=1}^{k+1}{}'(q_i-q_m)}(q_i^l-q_{k+1}^l)=\sum_{i=1}^{k+1}\frac{(q_i-1)^{k-1}}{\Pi_{m=1}^{k+1}{}'(q_i-q_m)}q_i^l,$$

where use was made of the identity $\Sigma_{m=1}^{k+1}[(q_i-1)^{k-1}/\Pi_{m=1}^{k+1}{}'(q_i-q_m)]=0$ that corresponds to $l=k-2$ in Eq. (9). Using the latter identity once more, we obtain the equivalent form

$$F_k(l)=\sum_{i=1}^{k}\omega_{k,i}[l]_{q_i}, \tag{10}$$

where $[l]_{q_i}=(q_i^l-1)/(q_i-1)$ is the Jackson q_i-(basic) integer. $F_k(l)$ is the weighted average of the Jackson q deformations of the integer l, in the k different bases $q_1,q_2,\ldots,q_k$. Thus, $F_1(l)=(q_1^l-1)/(q_1-1)$, $F_2(l)=(q_1^l-q_2^l)/(q_1-q_2)=(q_1^l-1)/(q_1-q_2)+(q_2^l-1)/(q_2-q_1)$, etc.

Using the Jackson q-derivative ${}_qD_x g(x)\equiv[g(qx)-g(x)]/x(q-1)$ we introduce the multiparameter q-derivative

$$ {}_{q_1 q_2 \cdots q_k}D_x \equiv \sum_{i=1}^{k} \omega_{k,i}\ {}_{q_i}D_x , $$

which is a weighted average over the corresponding Jackson q_i-derivatives. In particular, the Macfarlane–Biedenharn q-derivative is a weighted average over Jackson q-derivatives with respect to q and q^{-1}, i.e.,

$$ {}_{q}\overline{D_x} = \omega_q\ {}_{q}D_x + \omega_{q^{-1}}\ {}_{q^{-1}}D_x , $$

where $\omega_q = (q-1)/(q-q^{-1}) = q^{1/2}/(q^{1/2}+q^{-1/2})$ and $\omega_{q^{-1}} = q^{-1/2}/(q^{1/2} + q^{-1/2})$. The multiparameter q-derivative satisfies

$$ {}_{q_1 q_2 \cdots q_k}D_x x^l = F_k(l) x^{l-1}, $$

that enables the introduction of a corresponding q-exponential.

Thus, the minimal deformation of the conventional harmonic oscillator

$$ [a, a^\dagger] = 1, $$

is the relation

$$ [a, a^\dagger]_{q_1} = 1, $$

which is due to Arik and Coon.[7] It is easily found that $F_1(l) = [l]_{q_1} \equiv (q_1^l - 1)/(q_1 - 1)$ and $f_1(\hat{n}) = q_1^{\hat{n}}$, i.e., the Arik–Coon oscillator is equivalent with

$$ [a, a^\dagger] = q_1^{\hat{n}}. \tag{11} $$

This equivalence had been pointed out by Kumari *et al.*[22] Equation (11) suggests that the Arik–Coon oscillator gets more and more classical, with increasing $\hat{n}$, for $q_1 < 1$, and more and more quantal for $q_1 > 1$. In other, more picturesque words, we have an ''energy dependent Planck's constant.'' This feature was discussed in Refs. 23 and 24, where it was referred to as the Tamm–Dancoff cutoff.

Continuing, we consider the minimal deformation of Eq. (11), i.e., $[a, a^\dagger]_{q_2} = q_1^{\hat{n}}$. This is the Chakrabarti–Jagannathan[11] two parameter oscillator, which for $q_1 = q_2^{-1}$ reduces to the Macfarlane–Biedenharn[8,9] oscillator. The equivalent commutation relation is

$$ [a, a^\dagger] = f_2(\hat{n}), \tag{12} $$

where

$$ f_2(\hat{n}) = \Phi_2(\hat{n}+1) - \Phi_2(\hat{n}). $$

When $q_1 = q_2^{-1}$ this expression reduces to the commutator $[a, a^\dagger] = (q_1^{(\hat{n}+1/2)} + q_1^{-(\hat{n}+1/2)})/(q_1^{1/2} + q_1^{-1/2})$, that (with a slight change of notation) was noted by Floreanini and Vinet.[25]

The equivalence between $[a, a^\dagger]_{q_2} = q_1^{\hat{n}}$ and $[a, a^\dagger] = f_2(\hat{n})$, and the fact that $f_2(\hat{n})$ is symmetric in q_1 and q_2, implies the well-known equivalence of $[a, a^\dagger]_{q_1} = q_2^{\hat{n}}$ and $[a, a^\dagger]_{q_2} = q_1^{\hat{n}}$. It is perhaps appropriate to emphasize that the latter equivalence, like the former, is only valid within the Fock space.

The minimal deformation of Eq. (12) yields $[a, a^\dagger]_{q_3} = f_2(\hat{n})$, which can be written in the equivalent commutator form

$$[a,a^\dagger]=f_3(\hat{n}), \tag{13}$$

where

$$f_3(\hat{n})=\Phi_3(\hat{n}+2)-2\Phi_3(\hat{n}+1)+\Phi_3(\hat{n}).$$

Continuing the recursion we note that since $f_k(\hat{n})$ is a symmetric polynomial in $q_1,q_2,\ldots,q_k$ [cf. Eq. (8)], it follows that the k relations

$$[a,a^\dagger]_{q_i}=f_{k-1}(q_1,q_2,\ldots,q_{i-1},q_{i+1},\ldots,q_k;\hat{n}), \quad i=1,2,\ldots,k$$

are all satisfied simultaneously with $[a,a^\dagger]=f_k(q_1,q_2,\ldots,q_k;\hat{n})$. Here, the dependence on the parameters is shown explicitly.

The present multiparameter deformation refers to a single coordinate, unlike the multiparameter quantum groups associated with the n-dimensional quantum space quommutation relations.[26–28]

At the kth step of the recursion we obtain a commutator which is equal to a linear combination of k exponentials of the number operator, with coefficients that are fixed by the construction formulated. We shall now consider a more general starting point, involving a commutator that is equal to some polynomial in the number operator. It will be found that once the number of recursions exceeds the degree of the polynomial, the resulting commutator is again equal to a sum of exponentials, but now with a greater flexibility in the choice of the coefficients.

Taking

$$f_0(l)=\begin{cases}\alpha_{0,1}l+\alpha_{0,0}, & \text{for } l\geqslant 0,\\ 0, & \text{for } l<0,\end{cases}$$

i.e., $[a,a^\dagger]=\alpha_{0,1}\hat{n}+\alpha_{0,0}$, we obtain

$$f_1(\hat{n})=\alpha_{1,0}+\alpha_{1,1}q_1^{\hat{n}}$$

where $\alpha_{1,0}=\alpha_{0,1}/(1-q_1)$ and $\alpha_{1,1}=\alpha_{0,0}-\alpha_{0,1}/(1-q_1)$. Thus,

$$[a,a^\dagger]=1+2\nu q_1^{\hat{n}} \tag{14}$$

is the first recursion of the relation $[a,a^\dagger]=f_0(\hat{n})$ with

$$f_0(l)=\begin{cases}(1-q_1)l+(1+2\nu) & \text{for } l\geqslant 0,\\ 0 & \text{for } l<0.\end{cases}$$

In particular, the Calogero–Vasiliev oscillator corresponds to Eq. (14) with $q_1=-1$. The second recursion yields

$$[a,a^\dagger]=f_2(\hat{n})=\alpha_{2,1}q_1^{\hat{n}}+\alpha_{2,2}q_2^{\hat{n}}, \tag{15}$$

where $\alpha_{2,1}=\alpha_{1,1}[(q_1-1)/(q_1-q_2)]$ and $\alpha_{2,2}=\alpha_{1,0}+\alpha_{1,1}[(q_2-1)/(q_2-q_1)]$. For $q_1=q^{-1},q_2=-q^{-1},q_3=q,\alpha_{2,1}=1,\alpha_{2,2}=2\nu$, the minimal deformation of Eq. (15) is the Brzeziński–Egusquiza–Macfarlane oscillator.[14]

The third recursion yields

$$f_3(\hat{n})=\alpha_{3,1}q_1^{\hat{n}}+\alpha_{3,2}q_2^{\hat{n}}+\alpha_{3,3}q_3^{\hat{n}},$$

where

$$\alpha_{3,1}=\frac{\alpha_{2,1}}{q_1-q_3}(q_1-1), \qquad \alpha_{3,2}=\frac{\alpha_{2,2}}{q_2-q_3}(q_2-1),$$

$$\alpha_{3,3}=\frac{(q_3-q_2)\alpha_{2,1}+(q_3-q_1)\alpha_{2,2}}{(q_3-q_1)(q_3-q_2)}(q_3-1),$$

etc.

Starting from a quadratic expression in the number operator

$$f_0(l)=\begin{cases}\alpha_{0,2}l^2+\alpha_{0,1}l+\alpha_{0,0}, & \text{for } l\geqslant 0\\ 0, & \text{for } l<0\end{cases}$$

we obtain

$$f_1(\hat{n})=\alpha_{1,1}q_1^{\hat{n}}+\alpha_{1,2}\hat{n}+\alpha_{1,3},$$

where

$$\alpha_{1,1}=\frac{q_1(\alpha_{0,2}+\alpha_{0,1})+(\alpha_{0,2}-\alpha_{0,1})}{(q_1-1)^2}+\alpha_{0,0},$$

$$\alpha_{1,2}=\frac{2\alpha_{0,2}}{1-q_1},$$

$$\alpha_{1,3}=\frac{q_1(\alpha_{0,2}+\alpha_{0,1})+(\alpha_{0,2}-\alpha_{0,1})}{(q_1-1)^2},$$

and

$$f_2(\hat{n})=\alpha_{2,1}q_1^{\hat{n}}+\alpha_{2,2}q_2^{\hat{n}}+\alpha_{2,3}$$

with appropriately defined coefficients. The next recursion yields

$$f_3(\hat{n})=\alpha_{3,1}q_1^{\hat{n}}+\alpha_{3,2}q_2^{\hat{n}}+\alpha_{3,3}q_3^{\hat{n}},$$

where the coefficients $\alpha_{3,1}$, $\alpha_{3,2}$, and $\alpha_{3,3}$, that can be expressed in terms of $\alpha_{0,0}$, $\alpha_{0,1}$, and $\alpha_{0,2}$, can be chosen to agree with the coefficients of the q-deformed Calogero–Vasiliev oscillator, Eq. (6), provided that Q is chosen to have one of the four values for which Eq. (6) reduces to a sum of three exponentials, say $Q=q$, and q_1, q_2, and q_3 are chosen to be q^{-1}, $-q$, and $-q^{-1}$, respectively.

Thus, starting with $f_0(\hat{n})$ that is a polynomial of degree k in $\hat{n}$ we obtain, upon performing the recursive minimal deformation procedure, polynomials of decreasing degrees in $\hat{n}$ combined with linear combinations of exponentials in $\hat{n}$. After k steps we obtain just a linear combination of exponentials, but the original kth degree polynomial allows a corresponding number of coefficients in the linear combination to be chosen at will.

IV. NORMAL ORDERING RELATIONS AND MULTIPARAMETER DEFORMED STIRLING NUMBERS

To derive a normal-ordering formula for the pair of operators a and $a^\dagger$ satisfying $[a,a^\dagger]_q=f(\hat{n})$ we first use the identity

$$[AB,C]_{q_1q_2}=A[B,C]_{q_2}+q_2[A,C]_{q_1}B$$

to derive the relation

$$[a^l,a^\dagger]_{q^l}=\{l(\hat{n})\}a^{l-1}, \tag{16}$$

where $\{l(\hat{n})\}\equiv\Sigma_{i=0}^{l-1}q^{l-1-i}f(\hat{n}+i)$. For $f(\hat{n})=1$ we obtain $\{l(\hat{n})\}_1=[l]_{q_1}=(q_1^l-1)/(q_1-1)$, that for $q_1=1$ is equal to l. For $f(\hat{n})=q_1^{\hat{n}}$ we have $\{l(\hat{n})\}_2=q_1^{\hat{n}}[[l]]_{q_1,q_2}$ where $[[l]]_{q_1,q_2}=(q_1^l-q_2^l)/(q_1-q_2)$.

Now, taking $q=q_{k+1}$ and $f(\hat{n})=f_k(\hat{n})$ [Eq. (8)] we obtain, for $k\geqslant 1$,

$$\{l(\hat{n})\}_{k+1}=\sum_{i=1}^{k}(q_i)^{\hat{n}}\,\frac{q_i^l-q_{k+1}^l}{q_i-q_{k+1}}\,\omega_{k,i}.$$

Thus, $\{l(\hat{n})\}_{k+1}$ is a multiparameter, operator-valued deformation of the integer l.

Using Eq. (16) we obtain that the coefficients in the normal ordering formula

$$(a^\dagger a)^m=\sum_{l=1}^{m}(a^\dagger)^l C_{m,l}(\hat{n})a^l \tag{17}$$

satisfy the initial condition $C_{1,1}(\hat{n})=1$ and the recurrence relation

$$C_{m+1,l}(\hat{n})=q^{l-1}C_{m,l-1}(\hat{n}+1)+\{l(\hat{n})\}_k C_{m,l}(\hat{n}).$$

In the appropriate limits this relation reduces to the Stirling, q-Stirling, and operator-valued q-Stirling coefficients, cf. Ref. 29.

The normally-ordered form of an expression of the type $(a^\dagger a)^m$ is not invariant with respect to the different equivalent commutation and quommutation relations that the corresponding pair of operators a and $a^\dagger$ satisfies. Starting from the commutation relation $[a,a^\dagger]=f_k(\hat{n})$, we obtain

$$[a^l,a^\dagger]=\overline{\{l(\hat{n})\}}_k,$$

where $\overline{\{l(\hat{n})\}}_k=\Sigma_{i=0}^{l-1}f_k(\hat{n}+i)=\Sigma_{i=1}^{k}\omega_{k,i}[l]_{q_i}$ and $[l]_{q_i}=(q_i^l-1)/(q_i-1)$. Hence, a normal ordering expansion of the form of Eq. (17) is obtained, with the coefficient satisfying the recurrence relation

$$\overline{C}_{m+1,l}(\hat{n})=\overline{C}_{m,l-1}(\hat{n}+1)+\overline{\{l(\hat{n})\}}_k\overline{C}_{m,l}(\hat{n}).$$

Thus, the Arik–Coon quommutation relation gives rise to the q-Stirling numbers as the coefficients in the normally-ordered expansion, but if the (equivalent) commutation relation $[a,a^\dagger]=q^{\hat{n}}$ is used to effect the normal ordering, the coefficients are operator valued. As an illustration consider $(a^\dagger a)^2$, which, in terms of the Arik–Coon quommutator is given by

$$(a^\dagger a)^2=q(a^\dagger)^2a^2+a^\dagger a,$$

whereas in terms of the equivalent commutator becomes

$$(a^\dagger a)^2=(a^\dagger)^2a^2+a^\dagger q^{\hat{n}}a.$$

These two normally-ordered expressions are related to one another via the identity $q^{\hat{n}}=(q-1)a^\dagger a+1$.

V. THE INVERSE PROBLEM

The following inverse problem may sometimes be of interest: Given a commutator of some form, can it be transformed into a quommutator that, in some sense, is of simpler form? To motivate this problem we recall that the normal ordering problem for the Arik–Coon oscillator $[a,a^\dagger]_q=1$ yields the q-Stirling numbers as coefficients, whereas the equivalent commutator relation, $[a,a^\dagger] = q^{\hat{n}}$, yields a normal ordering expansion with a new type of $\hat{n}$ dependent (''operator valued'') q-Stirling numbers. Given the latter commutator, we may wish to obtain the equivalent quommutator that, in this case, yields a simpler normal-ordering formula.

Thus, given $[a,a^\dagger]=\phi(\hat{n})$, where $\phi(0)=1$, it can be shown straightforwardly that $aa^\dagger-a^\dagger\beta(\hat{n})a=1$, where

$$\beta(\hat{n})=\frac{\sum_{i=1}^{\hat{n}+1}\phi(i)}{\sum_{i=0}^{\hat{n}}\phi(i)}.$$

As an example we take $\phi(\hat{n}) = q^{\hat{n}}$ that yields $\beta(\hat{n})=q$, thus reproducing the Arik–Coon quommutator.

A somewhat different inverse problem involves the transformation of

$$[a,a^\dagger]=\phi(\hat{n})$$

into the equivalent form

$$[a,a^\dagger]_Q=\Phi(\hat{n}),$$

choosing Q so as to make $\Phi(\hat{n})$ as simple as possible, for a given $\phi(\hat{n})$. Since in the above quommutation relation $\alpha(\hat{n})=\beta(\hat{n})=1$, we obtain

$$\Phi(\hat{n})=\phi(\hat{n})+(1-Q)\sum_{i=0}^{\hat{n}-1}\phi(i),$$

[cf. Eq. (5)]. Thus, $\phi(\hat{n}) = q^{\hat{n}}$ yields

$$\Phi(\hat{n})=q^{\hat{n}}\left(\frac{q-Q}{q-1}\right)+\frac{Q-1}{q-1}.$$

The ''best choice'' is very clear in this case, i.e., $Q=q$, yielding $\Phi(\hat{n})=1$.

Taking

$$\phi(\hat{n})=\alpha q_1^{\hat{n}}+\beta q_2^{\hat{n}}$$

we obtain

$$\Phi(\hat{n})=\alpha q_1^{\hat{n}}\left(\frac{q_1-Q}{q_1-1}\right)+\beta q_2^{\hat{n}}\left(\frac{q_2-Q}{q_2-1}\right)+\alpha\,\frac{Q-1}{q_1-1}+\beta\,\frac{Q-1}{q_2-1}.$$

In this case we have two equally good choices of Q, i.e., $Q=q_1$ and $Q=q_2$. The former yields

$$[a,a^\dagger]_{q_1}=\Phi(\hat{n})=\beta\left(\frac{q_2-q_1}{q_2-1}\right)q_2^{\hat{n}}+\left(\alpha+\beta\,\frac{q_1-1}{q_2-1}\right).$$

For the special case $\phi(\hat{n}) = 1 + 2\nu p^{\hat{n}}$ we obtain $\sum_{i=0}^{l-1}\phi(i)=l+2\nu(p^l-1)/(p-1)$, so, setting $Q=p$ it follows that $\Phi(\hat{n})=1+2\nu+(1-p)\hat{n}$. Hence, $[a,a^\dagger] = 1 + 2\nu p^{\hat{n}}$ is equivalent with

$[a,a^\dagger]_p=1+2\nu+(1-p)\hat{n}$. Taking $p=-1$ we obtain that $[a,a^\dagger]=1+2\nu(-1)^{\hat{n}}$ is equivalent with $\{a,a^\dagger\}=1+2\nu+2\hat{n}$, cf. Ref. 30. The latter is related to the realization of $osp(n/2,R)$ in terms of parabosons, presented by Palev.[31]

VI. NON-FOCK SPACE REPRESENTATIONS OF THE DEFORMED COMMUTATION RELATIONS

The equivalence between quommutators and corresponding commutators, presented in Sec. II, is a central ingredient of the recursive minimal deformation procedure introduced in Sec. III. It was noted in Sec. II that the transformation proposed is being carried out within the Fock space representation. Deformed oscillator algebras are known to have additional, non-Fock space, representations[32,33] that are characterized by the existence of a Casimir operator with nontrivial eigenvalues.[34,35] We stress that there is no reason to expect these non-Fock space representations to be the same for different ways of writing the commutation relation that are equivalent within the Fock space. While we do not wish to delve into a detailed analysis of these non-Fock space representations for the different algebras discussed, the following general observations indicate some of the features to be expected.

The algebra $[a,a^\dagger]=f_k(\hat{n})=F_k(\hat{n}+1)-F_k(\hat{n})$ has a Casimir operator

$$C_k=F_k(\hat{n})-a^\dagger a.$$

This can be shown by noting that $[C_k,a^\dagger]=[F_k(\hat{n})-F_k(\hat{n}-1)]a^\dagger-a^\dagger[a,a^\dagger]=0$. In the Fock-space representation a state $|0\rangle$ exists, for which the relation $a|0\rangle=0$ is satisfied. Furthermore, since $F_k(\hat{n})|0\rangle=F_k(0)|0\rangle$ and $F_k(0)\equiv 0$, it follows that within this representation C_k has eigenvalue 0. The non-Fock representations are characterized by nonvanishing eigenvalues of the Casimir operator.

The minimal deformation of the algebra just discussed, $[a,a^\dagger]_{q_{k+1}}=f_k(\hat{n})$, has a Casimir operator as well, i.e., $\widetilde{C}_k=\mu_k(\hat{n})-\nu_k(\hat{n})a^\dagger a$, where $\mu_k(\hat{n})$ and $\nu_k(\hat{n})$ should be determined so as to satisfy the condition $[\widetilde{C}_k,a^\dagger]=0$. By adding a suitable constant one can set $\mu_k(0)=0$, so that the Casimir operator vanishes on the Fock space representation. To determine $\mu_k(\hat{n})$ and $\nu_k(\hat{n})$ we note that

$$[\widetilde{C}_k,a^\dagger]=[\mu_k(\hat{n})-\mu_k(\hat{n}-1)-\nu_k(\hat{n})f_k(\hat{n}-1)]a^\dagger+[\nu_k(\hat{n}-1)-q_{k+1}\nu_k(\hat{n})](a^\dagger)^2a.$$

A sufficient condition for the vanishing of $[\widetilde{C}_k,a^\dagger]$ is

$$\mu_k(\hat{n})-\mu_k(\hat{n}-1)=\nu_k(\hat{n})f_k(\hat{n}-1), \tag{18}$$

$$\nu_k(\hat{n})=q_{k+1}^{-1}\nu_k(\hat{n}-1). \tag{19}$$

From Eq. (19) we obtain $\nu_k(\hat{n})=q_{k+1}^{-\hat{n}}$, where the normalization $\nu_k(0)=1$ [which is consistent with the choice $\mu_k(0)=0$ made above] was chosen. Consequently, Eq. (18) becomes a recurrence relation for $\mu_k(\hat{n})$, i.e., $\mu_k(\hat{n})=\mu_k(\hat{n}-1)+q_{k+1}^{-\hat{n}}f_k(\hat{n}-1)$. This recurrence relation, along with the initial condition $\mu_k(0)=0$, is satisfied by

$$\mu_k(\hat{n})=\sum_{i=1}^{\hat{n}} q_{k+1}^{-i}f_k(i-1).$$

For $f_k(\hat{n})=\Sigma_{i=1}^{k}\omega_{k,i}q_i^{\hat{n}}$, cf. Eq. (8), we obtain

$$\mu_k(\hat{n})=q_{k+1}^{-\hat{n}}\sum_{j=1}^{k+1}\omega_{k+1,j}[\hat{n}]_{q_j}=q_{k+1}^{-\hat{n}}F_{k+1}(\hat{n}),$$

where the last equality follows from Eq. (10). It follows that

$$\widetilde{C}_k = q_{k+1}^{-\hat{n}}[F_{k+1}(\hat{n}) - a^\dagger a] = q_{k+1}^{-\hat{n}} C_{k+1}.$$

The Casimir operators introduced can be used to investigate the non-Fock space representations of the various deformed oscillators presented, along the lines of Refs. 32–35.

VII. CONCLUSIONS

A recursive minimal deformation of a commutator into a quommutator, followed by a transformation of the resulting quommutator into a new commutator, to which it is equivalent within the corresponding Fock space, has been introduced. The familiar deformed oscillators have been obtained at appropriate steps of this recursive construction, along with multiparameter generalizations that would be difficult to guess otherwise. This recursive scheme provides a classification of the existing deformed oscillators. The multiparameter generalizations may appeal to investigators who would like to use the deformed oscillator framework in order to fit molecular or nuclear vibrational spectra, and in similar contexts in which further flexibility would be useful. To what extent they offer hints of further fundamental developments remains to be seen.

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Quantization of a loop extended SU(2) affine Kac–Moody algebra

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A quantization of a Lie bialgebra structure on a loop extended $\widehat{\mathrm{SU}}(2)$ algebra is considered. An asymptotic expansion for *R*-matrix is given. © *1996 American Institute of Physics.* [S0022-2488(96)03003-X]

I. INTRODUCTION

It is known that there is a closer relation between the representation theory of Kac–Moody algebras and quantum groups. The most interesting model in which both of these structures appears is the two-dimensional Wess–Zumino–Witten (WZW) model.[1] The representation theory of quantum groups allows one to compute the duality matrices in the WZW model.[2] In Refs. 3 and 4 it was shown that the exchange algebra for chiral fields in the WZW model can be expressed in terms of quantum groups. In this paper we use the idea of quantization of Lie bialgebras.[5,6] We show that in the WZW model, a Lie bialgebra structurer can be constructed in a natural way. By quantizing this Lie bialgebra we obtain a noncocommutative bialgebra, i.e., a Hopf algebra without an antipode. This bialgebra may be thought of as a generalization of a Yangian algebra.[5,6]

II. A LIE BIALGEBRA STRUCTURE

We consider the WZW model on a cylinder over an arbitrary, semisimple, compact Lie group *G*. The field $g(t,\sigma)$ is a mapping from the cylinder to *G*. After introducing complex coordinates on the cylinder, we split the field $g(t,\sigma)$ into holomorphic and antiholomorphic parts $g(t,\sigma)=u(z)v(\overline{z})$. The holomorphic current is defined by $J(z)=-k\partial_z u(z)u^{-1}(z)$. Passing by the transformation $w=\exp z$ to the complex plane we expand $J(w)$ in the Laurent series

$$J(w)=\sum J_a^m w^{-m-1}\tau^a,$$

where $\{\tau^a\}$ denotes the basis of the Lie algebra of *G* with the structure constants f_{abc}. The basis is assumed to satisfy the orthornormality condition $\mathrm{Tr}(\tau^a\tau^b)=\delta^{a,b}$. The Poisson brackets between the currents are[1]

$$\{J_a(w),J_b(\widetilde{w})\}=2\pi i f_{abc}J_c(w)\delta(w-\widetilde{w})-2\pi i k\delta'(w-\widetilde{w})\delta_{a,b}. \tag{1}$$

When we define the matrix $C(\lambda,\mu)=[1/(\lambda-\mu)]\Sigma\tau^a\otimes\tau^a$ and denote $J_1(w)=\Sigma J_a(w)\tau^a\otimes 1$, $J_2(w)=\Sigma J_a(w)1\otimes\tau^a$, *Eq.* (1) *can be written as*

$$\{J_1(w),J_2(\widetilde{w})\}=2\pi i[C(\lambda,\mu),\lambda J_1(w)+\mu J_2(w)]\delta(w-\widetilde{w})-2\pi i k\delta'(w-\widetilde{w})\sum \tau^a\otimes\tau^a. \tag{2}$$

Because of the existence of $\delta'(w-\widetilde{w})$ in (2) it is difficult to deal with it. We rewrite (2) in a more convenient form. To do this we extend the Poisson–Lie structure (1) written in terms of J_a^m

$$\{J_a^m,J_b^n\}=f_{abc}J_c^{m+n}+m\delta_{m+n,0}\delta_{a,b}k \tag{3}$$

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by two variables k,l with the following Poisson brackets

$$\{k,J_a^m\}=0, \quad \{k,l\}=0, \quad \{l,J_a^m\}=mJ_a^m. \tag{4}$$

Next we define the extended current J as

$$J=\sum J_a^m\tau_m^a+kd+lc,$$

where $\{\tau_m^a,c,d\}$ is a basis of an untwisted affine Kac–Moody algebra $\hat{g}$.[7] The generalization of the matrix $C(\lambda,\mu)$ is the operator

$$\Omega(\lambda,\mu)=\frac{1}{\lambda-\mu}\left(\sum \tau_m^a\otimes\tau_{-m}^a+c\otimes d+d\otimes c\right).$$

For $J_1=\Sigma J_a^m(\tau_m^a\otimes 1)+k(d\otimes 1)+l(c\otimes 1)$, $J_2=1\otimes J$ Eq. (2) becomes

$$\{J_1,J_2\}=[\Omega(\lambda,\mu),\lambda J_1+\mu J_2]. \tag{5}$$

The operator $\Omega(\lambda,\mu)\in\hat{g}[\lambda]\otimes\hat{g}[\lambda]$ where by $\hat{g}[\lambda]$ we denoted the loop extension of $\hat{g}$ and formally identify the algebras $\hat{g}[\lambda]\otimes\hat{g}[\lambda]\simeq\hat{g}\otimes\hat{g}[\lambda,\mu]$. The operator $\Omega(\lambda,\mu)$ satisfies the classical Yang–Baxter equation[5] and this implies the Jacobi identity for the lhs of (5).

Let us denote by $\hat{g}^*$ the Poisson–Lie algebra given by (3) and (4). On $\hat{g}^*[\lambda]$ we define a mapping δ^* as

$$\delta^*(J(\lambda^n))=\{\Omega^*(\lambda,\mu),J_1(\lambda^n)+J_2(\mu^n)\}, \tag{6}$$

where in this case we denoted by $J_1(\lambda^n)=\Sigma(J_a^m\lambda^n\otimes 1)\tau_m^a+(k\lambda^n\otimes 1)d+(l\lambda^n\otimes 1)c, J_2(\mu^n)=1\otimes J(\mu^n)$ and $\Omega^*(\lambda,\mu)=[1/(\lambda-\mu)](\Sigma J_a^m\otimes J_a^{-m}+k\otimes l+l\otimes k)$. It is easy to check that the pair $(\hat{g}^*[\lambda],\delta^*)$ is the Lie bialgebra.[5] This Lie bialgebra is dual to $(\hat{g}[\lambda],\delta)$ where the cocommutator δ can be defined by using (5). Let us write the explicit form of (6) for $n=0,\pm 1$

$$\delta^*(J_a^m)=0, \quad \delta^*(k)=0, \quad \delta^*(l)=0,$$

$$\delta^*(J_a^m\lambda)=\sum f_{abc}J_b^{m-n}\otimes J_c^n+m(J_a^m\otimes k-k\otimes J_a^m),$$

$$\delta^*(k\lambda)=0, \quad \delta^*(l\lambda)=-\sum mJ_a^m\otimes J_a^{-m}, \tag{7}$$

$$\delta^*(J_a^m\lambda^{-1})=-\sum f_{abc}J_b^{m-n}\lambda^{-1}\otimes J_c^n\mu^{-1}-m(J_a^m\lambda^{-1}\otimes k\mu^{-1}-k\lambda^{-1}\otimes J_a^m\mu^{-1}),$$

$$\delta^*(k\lambda^{-1})=0, \quad \delta^*(l\lambda^{-1})=\sum mJ_a^m\lambda^{-1}\otimes J_a^{-m}\mu^{-1}.$$

The parameters $(J_a^m,k,\ J_a^m\lambda^{\pm 1},k\lambda^{\pm 1})$ generate two subalgebras $\hat{g}'^*[\lambda]_\pm$. The quantization of these Lie bialgebras can be provided independently. But the construction of an R-matrix needs a quantization of a Lie bialgebra structure on $\hat{g}^*[\lambda]$, i.e., $\hat{g}'^*[\lambda]$ with added $l\lambda^n$ generators. We will show it on the example of the $(\widehat{SU}_2'^*[\lambda]_\pm,\ \delta^*)$ Lie bialgebras.

III. THE QUANTUM ($\widehat{SU}_2'^*$ [λ] ALGEBRA

The definition of a quantization of Lie bialgebras can be found in Refs. 5 and 6. Because we consider an infinite-dimensional Lie algebra and as we will see the antipodal mapping does not exist, we modify the definition. Namely, by a quantization of the ($\widehat{SU}_2'^*[\lambda]_{\pm}$, δ^*) Lie bialgebras we will mean a bialgebra $(\hat{A}_{\pm}'^*, \Delta, \varepsilon)$ with the basis $(Q^m_{a,\pm N}, k_{\pm N})m \in Z, N \geqslant 0, a = 1,2,3$ a coassociative comultiplication Δ and a counit ε, satisfying the asymptotic conditions

$$\lim_{h\to 0} Q^m_{a,N} = J^m_a \lambda^N, \quad \lim_{h\to 0} k_N = k\lambda^N, \quad \lim_{h\to 0} -\frac{1}{2h}(\Delta - \Delta') = \delta^*,$$

where by Δ' we denoted the transposed comultiplication and h is a quantum parameter which may be identified with the Planck's constant. We will also need later the quantum operators l_N which have the asymptotic behavior $\lim_{h\to 0} l_N = l\lambda^N$. The detailed analysis of these operators and the role which they play in $A^*_{\pm}$ we will leave for a future work. The quantum algebra $(A'^*_{\pm}, \Delta, \varepsilon)$ is generated by $(Q^m_{a,0}, k_0, Q^m_{a,1}, k_1)$. The defining relations for this algebra are

$$\begin{aligned}
&[Q^m_{a,0}, Q^n_{b,0}] = f_{abc} Q^{m+n}_{c,0} + m\,\delta_{m+n,0}\delta_{a,b} k_0, \\
&[Q^m_{n,0}, Q^n_{b,1}] = f_{abc} Q^{m+n}_{c,1} + m\,\delta_{m+n,0}\delta_{a,b} k_1, \\
&[Q^m_{a,1},[Q^n_{b,0}, Q^r_{c,1}]] - [Q^m_{a,0}[Q^n_{b,1}, Q^r_{c,1}]] \\
&= 2h^2 k_0^2 \Big(r(m-n)\,\delta_{a,b} Q^{m+n+r}_{c,0} + n(r-m)\,\delta_{a,c} Q^{m+n+r}_{b,0} + m(n-r)\,\delta_{b,c} Q^{m+n+r}_{a,0} \Big) \\
&\quad - h^2 f_{abc} mnr\,\delta_{m+n+r,0}\; k_0^3 - h^2 (m+n+r) f_{abc} k_0 \sum Q^{m+n+r-s}_{d,0} Q^s_{d,0} \\
&\quad - h^2 k_0 \sum \left(f_{bcd} s\{Q^{n+r-s}_{a,0}, Q^{m+s}_{d,0}\} + f_{cad} s\{Q^{m+r-s}_{b,0}, Q^{n+s}_{d,0}\} + f_{abd} s\{Q^{m+n-s}_{c,0}, Q^{r+s}_{d,0}\} \right),
\end{aligned} \tag{8}$$

where $\{a,b\}$ denotes $ab + ba$. The comultiplication and the counit read

$$\begin{aligned}
&\Delta(Q^m_{a,0}) = Q^m_{a,0} \otimes 1 + 1 \otimes Q^m_{a,0}, \quad \Delta(k_0) = k_0 \otimes 1 + 1 \otimes k_0, \\
&\Delta(Q^m_{a,1}) = Q^m_{a,1} \otimes 1 + 1 \otimes Q^m_{a,1} - h \sum f_{abc} Q^{m-n}_{b,0} \otimes Q^n_{c,0} - hm(Q^m_{a,0} \otimes k_0 - k_0 \otimes Q^m_{a,0}), \\
&\Delta(k_1) = k_1 \otimes 1 + 1 \otimes k_1, \\
&\varepsilon(Q^m_{a,0}) = 0, \quad \varepsilon(k_0) = 0, \quad \varepsilon(Q^m_{a,1}) = 0, \quad \varepsilon(k_1) = 0.
\end{aligned} \tag{9}$$

To avoid divergences we have restricted our considerations to the compact form of the $\widehat{SU}_2'^*$ algebra.[7] As can be seen from (9) the comultiplication Δ is not cocommutative. One may ask whether there exists an operator R having the property

$$R\Delta(Q^m_{a,N}) = \Delta'(Q^m_{a,N}) R.$$

To answer this question we have to quantize the ($\widehat{SU}_2'^*[\lambda]_-$, ϕ^*) Lie bialgebra. The quantum algebra $(A'^*_-, \Delta, \varepsilon)$ is generated by operators $(Q^m_{a,0}, k_0, Q^m_{a,-1}, k_{-1})$. Unfortunately, the formulas

for a comultiplication and the commutation relations in $A'_-{}^*$ are infinite series in h. The comultiplication and commutation relations for $Q^m_{a,0}, k_0$ are the same as in (8) and (9). The remaining formulas read

$$[Q^m_{a,0}, Q^n_{b,-1}] = f_{abc} Q^{m+n}_{c,-1} + m\,\delta_{m+n,0}\delta_{a,b} k_{-1} + h^2 m(m+n) f_{abc} k^2_{-1} Q^{m+n}_{c,-1} - h^2 \frac{1}{3} m^3 \delta_{m+n,0}\delta_{a,b} k^3_{-1}$$
$$+ h^2 \frac{2}{3} m\,\delta_{a,b} k_{-1} \sum Q^{m+n-r}_{c,-1} Q^r_{c,-1} - h^2 \frac{1}{3} m k_{-1} \sum \{Q^{m+n-r}_{a,-1}, Q^r_{b,-1}\} + O(h^3),$$

$$\Delta(Q^m_{a,-1}) = Q^m_{a,-1} \otimes 1 + 1 \otimes Q^m_{a,-1} + h \sum f_{abc} Q^{m-r}_{b,-1} \otimes Q^r_{c,-1} + hm(Q^m_{a,-1} \otimes k_{-1} - k_{-1} \otimes Q^m_{a,-1})$$
$$+ h^2 \frac{1}{6} \sum f_{abc} f_{cde} (\{Q^r_{b,-1}, Q^s_{d,-1}\} \otimes Q^{m-r-s}_{e,-1} + Q^{m-r-s}_{e,-1} \otimes \{Q^r_{b,-1}, Q^s_{d,-1}\})$$
$$+ h^2 \sum f_{abc} r(Q^r_{b,-1} \otimes k_{-1} Q^{m-r}_{c,-1} - Q^{m-r}_{b,-1} k_{-1} \otimes Q^r_{c,-1}) - h^2 m^2$$
$$\times (Q^m_{a,-1} k_{-1} \otimes k_{-1} + k_{-1} \otimes k_{-1} Q^m_{a,-1}) + O(h^3),$$

$$\Delta(k_{-1}) = k_{-1} \otimes 1 + 1 \otimes k_{-1},$$

$$\varepsilon(Q^m_{a,-1}) = 0, \quad \varepsilon(k_{-1}) = 0. \tag{10}$$

Although, we cannot give defining relations for $\hat{A}'_-{}^*$ similar to (8), we will write an asymptotic expansion for $\Delta(Q^m_{a,-N})$, it has the form

$$\Delta(Q^m_{a,-N}) = Q^m_{a,-N} \otimes 1 + 1 \otimes Q^m_{a,-N} + h \sum_{n=0}^{N} (f_{abc} Q^{m-r}_{b,n-1-N} \otimes Q^r_{c,-n}$$
$$+ m(Q^m_{a,-n} \otimes k_{n-1-N} - k_{n-1-N} \otimes Q^m_{a,-n})) + O(h^2). \tag{11}$$

Using the coassociativity property of a comultiplication one can determine the higher order terms in h but the formulas are not unique. Using the homomorphism property of a comultiplication one can deduce also the commutation relations between $A'_+{}^*$ and $A'_-{}^*$. The simplest formula reads

$$[Q^m_{a,1}, Q^n_{b,-1}] = f_{abc} Q^{m+n}_{c,0} + m\,\delta_{m+n,0}\delta_{a,b} k_0 - h^2 \frac{1}{3} m k_0 \sum \{Q^{m+n-r}_{a,-1}, Q^r_{b,-1}\}$$
$$- h^2 k_{-1} \sum r\{Q^{m-r}_{b,0}, Q^{n+r}_{a,-1}\} + h^2 \frac{2}{3} m\,\delta_{a,b} k_0 \sum Q^{m+n-r}_{c,-1} Q^r_{c,-1}$$
$$+ h^2 \delta_{a,b} k_{-1} \sum r\{Q^{m-r}_{c,0}, Q^{n+r}_{c,-1}\} + h^2 m^2 f_{abc} k_0 k_{-1} Q^{m+n}_{c,-1}$$
$$+ h^2 \frac{2}{3} \sum f_{abc} Q^r_{d,-1} Q^s_{d,-1} Q^{m+n-r-s}_{c,0} - h^2 \frac{1}{3} \sum f_{abc}$$
$$\times (Q^r_{c,-1} Q^s_{d,0} Q^{m+n-r-s}_{b,-1} + Q^{m+n-r-s}_{b,-1} Q^s_{d,0} Q^r_{c,-1}) + O(h^3).$$

Having defined the quantum algebras $A'^{*}_{\pm}$ we are able to write down the asymptotic expansion for the R-matrix. To do this we introduce the operators l_N with the property $[l_N, Q^m_{a,M}] = mQ^m_{a,M+N} + O(h)$. As an example that such operators really exist we give an explicit form of the comultiplication for l_N in the simplest case $N = 0, \pm 1$:

$$\Delta(l_0) = l_0 \otimes 1 + 1 \otimes l_0, \quad \Delta(l_1) = l_1 \otimes 1 + 1 \otimes l_1 + h \sum m Q^m_{a,0} \otimes Q^{-m}_{a,0},$$

$$\Delta(l_{-1}) = l_{-1} \otimes 1 + 1 \otimes l_{-1} - h \sum m Q^m_{a,-1} \otimes Q^{-m}_{a,-1}$$

$$+ h^2 \frac{1}{3} \sum m f_{abc} (Q^{-m-r}_{b,-1} \otimes Q^m_{a,-1} Q^r_{c,-1} - Q^m_{a,-1} Q^{-m-r}_{b,-1} \otimes Q^r_{c,-1})$$

$$- h^2 \sum m^2 (Q^m_{a,-1} k_{-1} \otimes Q^{-m}_{a,-1} + Q^m_{a,-1} \otimes Q^{-m}_{a,-1} k_{-1}) + O(h^3).$$

The R-matrix for A^* has the following expansion:

$$R = 1 \otimes 1 - 2h \sum_{N=0}^{\infty} (Q^m_{a,N} \otimes Q^{-m}_{a,-N-1} + l_N \otimes k_{-N-1} + k_N \otimes l_{-N-1}) + O(h^2).$$

In the classical limit $(1/4h)(R - R') \to \Omega^*(\lambda, \mu)$.

IV. CONCLUSIONS

We considered a quantization of two Lie bialgebras $(\widehat{SU}'_2{}^*[\lambda]_{\pm}, \delta^*)$. In the $(\widehat{SU}'_2{}^*[\lambda]_+$ case the relations (8) and (9) define $\hat{A}'^{*}_{\pm}$ uniquely and the results are exact. Unfortunately, in the $(\widehat{SU}'_2{}^*[\lambda]_-$ case we were able to give only asymptotic formulas. In addition the formula (10) for comultiplication is not unique. For example, if we define a comultiplication Δ by

$$\Delta(Q^m_{a,-1}) = Q^m_{a,-1} \otimes 1 + 1 \otimes Q^m_{a,-1} + h \sum f_{abc} Q^{m-r}_{b,-1} \otimes Q^r_{c,-1} + hm(Q^m_{a,-1} \otimes k_{-1} - k_{-1} \otimes Q^m_{a,-1})$$

$$+ h^2 \frac{1}{6} \sum f_{abc} f_{cde} (\{Q^r_{b,-1}, Q^s_{d,-1}\} \otimes Q^{m-r-s}_{e,-1} + Q^{m-r-s}_{e,-1} \otimes \{Q^r_{b,-1}, Q^s_{d,-1}\})$$

$$+ h^2 \sum f_{abc} r (Q^r_{b,-1} \otimes Q^{m-r}_{c,-1} k_{-1} - k_{-1} Q^{m-r}_{b,-1} \otimes Q^r_{c,-1}) - h^2 m^2 (k_{-1} \otimes Q^m_{a,-1} k_{-1}$$

$$+ k_{-1} Q^m_{a,-1} \otimes k_{-1}) + h^2 \frac{1}{3} m^2 (Q^m_{a,-1} \otimes k^2_{-1} + k^2_{-1} \otimes Q^m_{a,-1} + 2 Q^m_{a,-1} k_{-1} \otimes k_{-1} + 2 k_{-1}$$

$$\otimes Q^m_{a,-1} k_{-1}) + h^2 \frac{1}{3} \sum f_{abc} r (Q^{m-r}_{b,-1} Q^r_{c,-1} \otimes k_{-1} + k_{-1} \otimes Q^{m-r}_{b,-1} Q^r_{c,-1} + Q^{m-r}_{b,-1}$$

$$\otimes k_{-1} Q^r_{c,-1} + Q^{m-r}_{b,-1} k_{-1} \otimes Q^r_{c,-1} + Q^r_{c,-1} k_{-1} \otimes Q^{m-r}_{b,-1} + Q^r_{c,-1} \otimes k_{-1} Q^{m-r}_{b,-1}) + O(h^3), \tag{12}$$

we obtain another quantization of the $\widehat{SU}'_2{}^*[\lambda]_-$ Lie bialgebra. As can be checked, there is a nonlinear transformation which connects these two comultiplications,

$$Q^m_{a,-1} \to Q^m_{a,-1} + h^2 \frac{1}{3} k_{-1} \sum f_{abc} r Q^{m-r}_{b,-1} Q^r_{c,-1} + h^2 \frac{1}{3} m^2 k^2_{-1} Q^m_{a,-1} + O(h^3).$$

The appearance of the parameter λ in this theory may seem strange. To find a physical interpretation for this parameter it would be natural to consider the WZW model over a loop group as in, Ref. 8.

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Quantum scattering theory in light of an exactly solvable model with rearrangement collisions

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We present an exactly solvable quantum field theory which allows rearrangement collisions. We solve the model in the relevant sectors and demonstrate the orthonormality and completeness of the solutions, and construct the S-matrix. In light of the exact solutions constructed, we discuss various issues and assumptions in quantum scattering theory, including the isometry of the Möller wave matrix, the normalization and completeness of asymptotic states, and the nonorthogonality of basis states. We show that these common assertions are not obtained in this model. We suggest a general formalism for scattering theory which overcomes these and other shortcomings and limitations of the existing formalisms in the literature. © *1996 American Institute of Physics.* [S0022-2488(96)01602-5]

I. INTRODUCTION

Quantum scattering has been an important subject of study since the early days of quantum physics. Unfortunately, while we have a reasonable understanding and intuition for simple scattering problems, such as single channel scattering, we cannot say the same for more general scattering problems such as multichannel scattering, rearrangement collisions, field theoretic scattering, problems where bound states appear, and the like. There have been many attempts to generalize scattering theory to deal with more complicated cases. However, the literature in this field, though vast, is highly implicit and not constructive. Most authors that have dealt with the problem have carried over the intuition developed from the study of single channel potential scattering. This intuition, while quite adequate for simple problems, is ill-equipped to deal with more complicated scattering problems. Therefore it is important to examine the common claim by some authors, for example, Haag,[1,2] that their formalism is general enough to encompass complicated scattering problems, as well as field theory. Unfortunately, most such formalisms are based largely on previous results from potential scattering. Furthermore, even when these problems are addressed in quantum mechanical scattering, field theoretic scattering remains problematical. Many papers, such as the paper by Gell-Mann and Goldberger,[3] treat field theoretic scattering as somewhat of an afterthought, without much development from first principles, or such as the papers by Van Hove,[4] treat it as a case for discussion. The first clear development of field theoretic scattering from first principles was the seminal paper by Lehmann, Symanzik, and Zimmerman (LSZ).[5] However, the LSZ formalism is not applicable in many cases, for example, collisions in which stable bound states appear. This is, in fact, pointed out by the authors themselves.

All this leads to the question: how many of our results and assumptions, and how much of our intuition can we carry over from simple single channel potential scattering to more complicated scattering situations? To attempt to answer this question, we will construct an exactly solvable sector for a quantum field theory. This model has a three particle sector, and allows rearrangement collisions. We will use the solutions of this model, along with previous results, to point out where the existing formalism has defects and shortcomings.

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Our model, which we shall call the rearrangement model, is an elaboration of the Lee model,[6] and the cascade model,[7] but with extra particles and couplings chosen in such a way as to allow rearrangement collisions. The couplings of the model are $B \leftrightarrow C\phi$ and $D \leftrightarrow C\theta$. This model has a sector, which we shall call the rearrangement sector, $B\theta \leftrightarrow C\theta\phi \leftrightarrow D\phi$, in which rearrangement collisions can take place. The model can be applied directly to physical problems involving rearrangement collisions. We shall, however, leave the applications to subsequent work.

This model is interesting because it is a very simple one, and yet contains the essence of many phenomena that can take place in an interacting system. It displays the following characteristics:

(1) New states can appear, which have no corresponding states in the original Hamiltonian.
(2) The thresholds and continuous spectra shift, and the spectra of H and H_0 are *not* the same. Furthermore, the continuous spectra are shifted by different amounts.
(3) Genuine rearrangement collisions can take place. We have the subadditivity of the spectra: the spectra in the higher sectors is the sum of all the spectra in the lower sectors, with possible additional terms.

We will construct the solutions of this model, and then, in light of the solutions we have constructed, will examine various assumptions and assertions made in the literature about quantum scattering theory. In particular, we will focus on four key points, that of the isometry[1] of the Möller wave matrix,[8] the normalization[1] and completeness[9] of the asymptotic states, and the nonorthogonality of the physical $B\theta$, $C\theta\phi$, and $D\phi$ states.[10,11] We shall show that these assertions are not obtained in this model. We also comment on the use of the (renormalized) free Hamiltonian in the literature,[1,3,9,10,12] rather than the correct prescription, which is to use the isospectral comparison Hamiltonian (see Sec. VIII).

The plan of this work is as follows. We start with a review of scattering theory in both the single channel and multiple channel cases. In the next three sections, we introduce the Hamiltonian of the rearrangement model, show how explicit solutions can be found for this model in the rearrangement sector, and verify that the solutions obtained are, in fact, solutions to our model. We then show that the solutions obtained are orthonormal and complete. The Möller matrix and the comparison Hamiltonian are written down, and we show that the comparison Hamiltonian is isospectral with the full Hamiltonian, but not with the free Hamiltonian. Then we calculate the S-matrix of the system in this sector, demonstrate its unitarity, and calculate its eigenphases. In Sec. XII, we present a general formalism for scattering theory which overcomes the shortcomings and limitations of the existing formalisms in the literature. In Sec. XIII we discuss scattering theory and its relation to the solutions that we constructed, and to previous work. Finally, in Sec. XIV, we summarize our work and present our conclusions.

II. THE SINGLE CHANNEL FORMALISM

For our purposes, it makes no difference whether we use the time dependent or time independent formalisms of scattering theory. We are concerned with the assumptions and results that are obtained from the formalisms, and they remain essentially the same in both cases. We shall therefore restrict ourselves to the time dependent formalism in Secs. III and IV. We follow the treatment of Newton[13] for both sections.

The discussion in Secs. III and IV is supposed to be very general. In fact, even though the method described deals with the nonrelativistic region, ''the formalism set up is such that, provided there exists a consistent relativistic quantum field theory, the transition to the relativistic domain is relatively simple.''[14] However, we find that even in such a simple model as our rearrangement model, these anticipations are *not* fulfilled. This formalism leads to wrong and contradictory results, as will be discussed in Sec. XIII.

We wish to solve the Schrödinger equation

$$i\frac{\partial}{\partial t}\Psi(t)=H\Psi(t). \tag{2.1}$$

We split H into a free Hamiltonian and an interaction Hamiltonian,

$$H=H_0+H'. \tag{2.2}$$

We assume that this split can be carried out: we shall consider the case of rearrangement collisions later. We define four Green's functions:

$$\left(i\frac{\partial}{\partial t}-H_0\right)G^{\pm}(t)=\mathbf{1}\delta(t), \tag{2.3a}$$

$$\left(i\frac{\partial}{\partial t}-H\right)\mathcal{G}^{\pm}(t)=\mathbf{1}\delta(t) \tag{2.3b}$$

with the initial conditions

$$G^{+}(t)=\mathcal{G}^{+}(t)=0, \quad t<0, \tag{2.4a}$$

$$G^{-}(t)=\mathcal{G}^{-}(t)=0, \quad t>0. \tag{2.4b}$$

G^{+} and $\mathcal{G}^{+}$ are therefore the advanced Green's functions, and G^{-} and $\mathcal{G}^{-}$ are the retarded Green's functions.

These may be solved formally, yielding

$$G^{+}(t)=-i\,e^{-iH_0t}\theta(t), \tag{2.5a}$$

$$G^{-}(t)=i\,e^{-iH_0t}\theta(-t), \tag{2.5b}$$

$$\mathcal{G}^{+}(t)=-i\,e^{-iHt}\theta(t), \tag{2.5c}$$

$$\mathcal{G}^{-}(t)=i\,e^{-iHt}\theta(-t). \tag{2.5d}$$

Let $\Psi_0(t)$ be a state vector satisfying the free Schrödinger equation. The operator G^{+} can then be used to express the state vector $\Psi_0(t')$ for any time t' later than t, in terms of its value at $t'=t$,

$$\Psi_0(t')=iG^{+}(t'-t)\Psi_0(t). \tag{2.6}$$

$\Psi_0(t')$ then satisfies the free Schrödinger equation for $t'>t$, and $\Psi_0(t')\to\Psi_0(t)$ when $t'\to t$.

Therefore,

$$\lim_{t\to 0^{+}} G^{+}(t)=\lim_{t\to 0^{+}} \mathcal{G}(t)=-i\mathbf{1}, \tag{2.7a}$$

$$\lim_{t\to 0^{-}} G^{-}(t)=\lim_{t\to 0^{-}} \mathcal{G}^{-}(t)=i\mathbf{1}. \tag{2.7b}$$

Similarly, for $t'>t$ we can write

$$\Psi(t')=i\mathcal{G}^{+}(t'-t)\Psi(t) \tag{2.8}$$

and for $t'<t$ we have

$$\Psi_0(t')=-iG^{-}(t'-t)\Psi_0(t), \tag{2.9a}$$

$$\Psi(t')=-i\mathscr{G}^{-}(t'-t)\Psi(t). \tag{2.9b}$$

We now wish to define "in" and "out" states. We start by defining

$$\Psi_0(t)\equiv iG^{+}(t-t')\Psi(t'), \tag{2.10}$$

whose time development for $t>t'$ is governed by the free Hamiltonian, but which at time t_0 was equal to $\Psi(t_0)$. We now let the time t' approach $\pm\infty$. Then, for the case of $t\to+\infty$, we have the out state, and for the case of $t\to-\infty$, we have the in state. In terms of the in and out states, the equations for $\Psi(t)$ are

$$\Psi(t)=\Psi_{\text{in}}(t)+\int_{-\infty}^{+\infty}dt'\ \mathscr{G}^{+}(t-t')H'\Psi_{\text{in}}(t') \tag{2.11a}$$

$$=\Psi_{\text{out}}(t)+\int_{-\infty}^{+\infty}dt'\ \mathscr{G}^{-}(t-t')H'\Psi_{\text{in}}(t'). \tag{2.11b}$$

Note that these are retarded and advanced Green's functions for the *whole system*. These are *not* the same functions as those that appear in a (time ordered) Dyson series which are, instead, time ordered *particle propagators*. Note also that for every state in the continuous spectrum of H_0, and only for such states, these formulas define a corresponding state in the spectrum of H.

If we insert Eq. (2.9b) in Eq. (2.11a), we find

$$\Psi(t)=\Omega^{(+)}\Psi_{\text{in}}(t), \tag{2.12}$$

where

$$\Omega^{(+)}=\mathbf{1}-i\int_{-\infty}^{+\infty}dt'\ \mathscr{G}^{+}(t-t')H'G^{-}(t'-t)=\mathbf{1}-i\int_{-\infty}^{+\infty}dt\ \mathscr{G}^{+}(-t)H'G^{-}(t) \tag{2.13}$$

is called the wave operator or the Möller matrix. We can similarly define $\Omega^{(-)}$.

Because H' is Hermitian, Eq. (2.13) gives us the relation

$$\Psi_{\text{in}}(t)=\Omega^{(+)^{\dagger}}\Psi(t), \tag{2.14a}$$

and similarly

$$\Psi_{\text{out}}(t)=\Omega^{(-)^{\dagger}}\Psi(t). \tag{2.14b}$$

Then, Eq. (2.12) and Eqs. (2.14) give us the relations

$$\Psi_{\text{in}}(t)=\Omega^{(+)^{\dagger}}\Omega^{(+)}\Psi_{\text{in}}(t), \tag{2.15a}$$

$$\Psi_{\text{out}}(t)=\Omega^{(-)^{\dagger}}\Omega^{(-)}\Psi_{\text{out}}(t). \tag{2.15b}$$

We now consider the possibility that the free states $\Psi_{\text{in}}(t)$ and $\Psi_{\text{out}}(t)$ span the entire Hilbert space, i.e., they are complete. From this assumption, we conclude that $\Omega^{(+)}$ and $\Omega^{(-)}$ are isometric,

$$\Omega^{(+)^{\dagger}}\Omega^{(+)}=\Omega^{(-)^{\dagger}}\Omega^{(-)}=\mathbf{1}. \tag{2.16}$$

This does not, however, mean that the Ω's are unitary: we cannot conclude from Eq. (2.15a) that Eq. (2.16) holds with its factors reversed.

Furthermore, granted the assumption that the Ψ_{in} and Ψ_{out} each form complete sets, we conclude that

$$H\Omega^{(\pm)}=\Omega^{(\pm)}H_0. \tag{2.17}$$

When there are bound states in the spectrum of H, we proceed as follows. Let $\Psi_0(E,\alpha)$ be the eigenstates of the free Hamiltonian with eigenvalue E, and α be the set of variables necessary to remove any degeneracy. Then, the completeness of these states can be written as a resolution of the identity

$$\mathbf{1}=\sum_{\alpha}\int_0^{\infty} dE\ \Psi_0(E,\alpha){\Psi_0}^{\dagger}(E,\alpha). \tag{2.18}$$

We again emphasize that we do not know whether the states of H_0 are complete, *a priori*. We are simply proceeding under that assumption. We then insert this into the product $\Omega\Omega^{\dagger}$ to get

$$\Omega\Omega^{\dagger}=\Omega\int_0^{\infty} dE\sum_{\alpha}\ \Psi_0(E,\alpha){\Psi_0}^{\dagger}(E,\alpha)\Omega^{\dagger}=\int_0^{\infty} dE\sum_{\alpha}\ \Psi(E,\alpha)\Psi^{\dagger}(E,\alpha)=\mathbf{1}-\Lambda. \tag{2.19}$$

Λ is called the unitary deficiency of Ω. From the completeness of the set of all states, bound and scattering, of H,

$$\Lambda=\sum_{n}\ \Psi_{bd}^{(n)}\Psi_{bd}^{(n)^{\dagger}}. \tag{2.20}$$

Thus, Λ projects onto the space spanned by the bound states of H. If H has no bound states, then $\Omega^{(+)}$ and $\Omega^{(-)}$ are unitary. Both H and H_0 are Hermitian; therefore, the Hermitian conjugate of Eq. (2.17) gives

$$H_0\Omega^{\dagger}=\Omega^{\dagger}H. \tag{2.21}$$

We now let both sides of Eq. (2.21) act on $\Psi(E,\alpha)$ to get

$$H_0\Omega^{\dagger}\Psi(E,\alpha)=E\Omega^{\dagger}\Psi(E,\alpha), \tag{2.22}$$

which shows that if E is in the spectrum of H but not in the spectrum of H_0 then

$$\Omega^{\dagger}\Psi(E,\alpha)=0,$$

and so

$$\Omega^{\dagger}\Lambda=0. \tag{2.23}$$

Thus, the range of the operators $\Omega^{(\pm)}$ is not the entire Hilbert space. Instead, these operators map the whole space onto the subspace spanned by the continuum eigenstates of H. We cannot reach the subspace spanned by the bound states of H, and therefore, cannot construct an inverse operator for the whole space. The closest that we can come is to use the operators $\Omega^{(\pm)^{\dagger}}$ which are inverses of $\Omega^{(\pm)}$ on the subspace of states spanned by the scattering states of H, and which annihilate the subspace of bound states of H.

Assuming that the asymptotic states are complete, we construct the S-matrix in the following manner. We use Eqs. (2.15b) and (2.12) to write the out state in terms of the in state,

$$\Psi_{\text{out}}(t)=\Omega^{(-)}\Omega^{(+)}\Psi_{\text{in}}(t), \tag{2.24}$$

which defines for us the S-matrix

$$S \equiv \Omega^{(-)^\dagger} \Omega^{(+)}. \tag{2.25}$$

The S-matrix can be shown to be unitary and isometric. See Newton[13] for details; note, however, that S is only unitary when Ω is unitary. (This point is not clearly stated in Newton, or in the literature.)

Some mathematical questions about convergences arise in the above. Conventionally, in the Schrödinger picture (the one in which we are currently working), one demands that (see Newton[13] for details)

$$\lim_{t \to -\infty} [\Psi(t) - \psi_{\text{in}}(t)] \Rightarrow 0, \tag{2.26a}$$

$$\lim_{t \to +\infty} [\Psi(t) - \psi_{\text{out}}(t)] \Rightarrow 0, \tag{2.26b}$$

$$\lim_{t \to -\infty} \psi_{\text{in}}(0) \Rightarrow \Psi(0) \equiv \Omega^{(+)} \psi_{\text{in}}(0), \tag{2.26c}$$

where $\Rightarrow$ denotes the strong limit.

We will find, in our model, that if we construct the asymptotic in and out states correctly, these limits will be satisfied; however, the states will not be orthonormal or complete. On the other hand, if we make the usual assumptions of scattering theory, namely that the asymptotic states are orthonormal and complete, then these limits will not be satisfied.

III. THE MULTIPLE CHANNEL FORMALISM

The above formalism is only adequate for simple single channel cases. For more general scattering problems, such as rearrangement collisions, we must generalize the formalism. We shall again follow Newton.[13]

We want to split up the Hamiltonian into two pieces: one piece, H_a, that is left when the two initial fragments are taken far apart, and the remaining piece, H_a'. We can then go through the same development of $\Psi(t)$ from $\Psi_{\text{in}}(t)$ as above. However, there is a difficulty that occurs for the development for the distant future. If rearrangements or breakups can occur, then it is possible that the ''channel'' Hamiltonian in the future is different than the channel Hamiltonian in the past.

The various possibilities for an n-particle system are handled by defining a partition of them into k clusters, denoted by a_k. Given a partition a, we define H_a by allowing all distances between clusters to independently tend to infinity. Therefore, H_a will contain only interactions that are internal to clusters, but none between them. Then, H_a' is defined by the requirement that $H = H_a + H_a'$, and therefore, for any two partitions a and b, we have

$$H = H_a + H_a' = H_b + H_b'. \tag{3.1}$$

To each partition, there will correspond Green's functions given by

$$\left(i \frac{\partial}{\partial t} - H_a \right) G^{\pm}{}_a(t) = \mathbf{1} \delta(t), \tag{3.2}$$

with the same boundary conditions as Eqs. (2.4). If H_a, after removing the kinetic energy of the center of mass motion and of the centers of mass of its clusters, has at least one bound state, it is called an arrangement channel. When this condition on H_a does not hold, the channel is not of interest as an initial or final scattering state. If H_a has more than one bound state, then each of

them defines a separate channel, and therefore, in each channel the clusters are in a specific bound state but moving freely relative to one another. The channel consisting of the entire n-cluster partition is the channel 0 because then $H_a = H_0$.

Now consider the space of each arrangement channel a, which we shall denote by $\mathscr{H}_a$. Then, if a has m fragments, each state in $\mathscr{H}_a$ will have m groups of bound particles. This means that unless the channel a is the entire n-fragment arrangement channel, $\mathscr{H}_a$ will not be the whole Hilbert space: the ionized eigenstates of H_a will be missing. Furthermore, as each $\mathscr{H}_a$ is defined by different channel Hamiltonians, H_a, the $\mathscr{H}_a$'s are generally not orthogonal to each other. In fact, "the complete set of basis functions is not linearly independent and, of course, not orthonormal."[15]

It will be convenient to define the orthogonal projections P_a onto the channel spaces, $\mathscr{H}_a$. In other words, we define

$$P_a^2 = P_a, \quad P_a^\dagger = P_a, \quad P_a \mathscr{H}_a = \mathscr{H}_a, \tag{3.3}$$

with the null space of P_a defined as the space spanned by the ionized eigenstates of H_a. P_a projects states from the full Hilbert space $\mathscr{H}$ to the channel spaces $\mathscr{H}_a$. Obviously, for the n-cluster arrangement channel, we have $P_0 = \mathbf{1}$.

We now wish to define in and out states. We first define an a state, which is a state that develops according to H_a but is in $\mathscr{H}_a$,

$$\left(i \frac{\partial}{\partial t} - H_a \right) \Psi_a(\alpha, t) = 0, \tag{3.4}$$

where the label α contains all the other information including the arrangement channel (even though including the arrangement channel in α is redundant for $\Psi_a(\alpha,t)$, it is convenient for other purposes).

We then define $\Psi^{(+)}(\alpha,t)$ as a state in $\mathscr{H}$ that develops according to H,

$$\left(i \frac{\partial}{\partial t} - H \right) \Psi^{(+)}(\alpha, t) = 0, \tag{3.5}$$

and for which there exists an a state such that

$$\lim_{t \to -\infty} (\Psi_a(\alpha,t), \Psi^{(+)}(\alpha,t)) = 1. \tag{3.6}$$

Therefore, the state $\Psi_a(\alpha,t)$ is the in state $\Psi_{\text{in}}(\alpha,t)$ in relation to the state $\Psi^{(+)}(\alpha,t)$. Equation (3.6) demands that the probability of finding the system in state $\Psi_a(\alpha,t)$ in the remote past approach 1, and therefore, it is equivalent to

$$\Psi_a^{(+)} \underset{t \to -\infty}{\Rightarrow} \Psi_a(\alpha,t) \tag{3.7a}$$

or

$$\int dt\; iG_a^+(t-t') \Psi^{(+)}(\alpha,t') \underset{t \to -\infty}{\Rightarrow} \Psi_{\text{in}}(\alpha,t), \tag{3.7b}$$

with the double arrow denoting the strong limit.

Similarly,

$$\int dt'(-i)G_a^-(t-t')\Psi^{(-)}(\alpha,t') \underset{t\to-\infty}{\Rightarrow} \Psi_{\text{out}}(\alpha,t). \tag{3.8}$$

Exactly analogous to Eqs. (2.11), we can now write

$$\Psi^{(+)}(\alpha,t)=\Psi_{\text{in}}(\alpha,t)+\int_{-\infty}^{+\infty}dt'\ \mathscr{G}^+(t-t')H_a'\Psi_{\text{in}}(\alpha,t'), \tag{3.9a}$$

$$\Psi^{(-)}(\alpha,t)=\Psi_{\text{out}}(\alpha,t)+\int_{-\infty}^{+\infty}dt'\ \mathscr{G}^-(t-t')H_a'\Psi_{\text{out}}(\alpha,t'). \tag{3.9b}$$

We can now define the Möller matrices, and the S-matrix. The Möller matrices are defined by

$$\Psi^{\pm}(\alpha,t)=\Omega_a^{(\pm)}\Psi_a(\alpha,t), \tag{3.10}$$

with only those states Ψ_a admitted which are in $\mathscr{H}_a$. On the orthogonal complement (i.e., the ionized eigenstates of H_a) $\Omega^{(\pm)}$ is defined to be zero,

$$\Omega^{(\pm)}P_a=\Omega^{(\pm)}.$$

Then, on the space $\mathscr{H}_a$, using Eq. (3.9a), we find

$$\Omega_a^{(+)}=P_a+K_a^{(+)},$$

$$K_a^{(+)}=-i\int_{-\infty}^{\infty}dt\ \mathscr{G}^+(-t)H_a'G^-{}_a(t)P_a=-i\int_{-\infty}^{0}dt\ e^{iHt}H_a'\ e^{-iH_at}P_a,$$

and therefore,

$$\Omega_a^{(+)}=\lim_{t\to-\infty}e^{iHt}\ e^{-iH_at}P_a. \tag{3.11}$$

We can similarly find, on $\mathscr{H}_a$, that

$$\Omega_a^{(-)}=\lim_{t\to\infty}e^{iHt}\ e^{-iH_at}P_a. \tag{3.12}$$

The range of $\Omega_a^{(+)}$ is the space of all full states that develop from arrangement channel a, and the range of $\Omega_a^{(-)}$ is the space of all full states that develop into arrangement channel a. Let us call these ranges $\mathscr{R}_a^{(+)}$ and $\mathscr{R}_a^{(-)}$, and their respective orthogonal projections $Q_a^{(+)}$ and $Q_a^{(-)}$. The Möller matrices $\Omega^{(\pm)}$ map $\mathscr{H}_a$ onto $\mathscr{R}_a^{\pm}$, and from Eqs. (3.10) we find that on $\mathscr{R}_a^{(+)}$ and $\mathscr{R}_a^{(-)}$, respectively,

$$\Psi_a(\alpha,t)=\Psi_{\text{in}}(\alpha,t)=\Omega^{(+)^\dagger}\Psi^{(+)}(\alpha,t)=\Psi_{\text{out}}(\alpha,t)=\Omega^{(-)^\dagger}\Psi^{(-)}(\alpha,t). \tag{3.13}$$

Therefore, because the $\Psi_a(\alpha,t)$ span the space $\mathscr{H}_a$, we find that the Möller matrices $\Omega_a^{(\pm)}$ are partially isometric from the space $\mathscr{H}_a$, i.e.,

$$\Omega_a^{(\pm)^\dagger}\Omega_a^{(\pm)}=P_a. \tag{3.14}$$

Similarly, the $\Omega_a^{(\pm)^\dagger}$ are partially isometric from the ranges $\mathscr{R}_a^{(\pm)}$ of the $\Omega^{(\pm)}$, i.e.,

$$\Omega_a^{(\pm)}\Omega_a^{(\pm)^\dagger}=Q_a^{(\pm)}, \tag{3.15}$$

which defines the $Q_a^{(\pm)}$. The full states developing from or into any arrangement channel are orthogonal to each other as can be seen by direct evaluation of the inner products of asymptotic states. ''If the two arrangement channels are different, then there must be at least one particle for which the 'overlap' of the two states was negligible in the remote past because it belonged to a different fragment. Hence that inner product must vanish for all times.''[16]

A major point of difference with our results from the rearrangement model is the statement, ''note that the same argument shows that the inner product

$$(\Psi_b(\beta,t),\Psi_a(\alpha,t)) \tag{3.16}$$

approaches zero as $t\to\pm\infty$ (for $a\neq b$). But since $H_a\neq H_b$, it is not independent of t and hence it does not generally vanish for *finite* times'' (emphasis added).[16] In the rearrangement model, this is untrue: we show in Sec. VII that our states are all orthogonal to each other.

From the Schrödinger equation, one can write

$$H\Omega_a^{(\pm)}=\Omega_a^{(\pm)}H_a, \tag{3.17}$$

which means that Ω intertwines H and H_a. This again is a major difference with the rearrangement model, because we show in Sec. VII that Ω intertwines H and H_C, where H_C is the comparison Hamiltonian, which has the same spectrum as H; here, H_a does not have the same spectrum as H.

Our channel definitions could also include the single cluster arrangement channel, which is the channel of all the n-particle bound states of H. If we define Λ to be the orthogonal projection onto that subspace, then for all a we have

$$Q_a^{(\pm)}\Lambda=0. \tag{3.18}$$

Now, every nonbound state must be decomposable into states that arise from, or go into, one of the other arrangements. Therefore, we assume

$$\Lambda+\sum_a Q_a^{(\pm)}=\mathbf{1}, \tag{3.19}$$

which is known as asymptotic completeness.

Using Eqs. (3.12), (3.17), and (3.19), we may then define a unitary S-matrix,

$$\Psi^{(+)}(\alpha,t)\underset{t\to-\infty}{\Rightarrow}\Psi_{\text{out}}(t)=\sum_b S_{ba}\Psi_a(\alpha,t), \tag{3.20}$$

where

$$S_{ba}=\Omega_b^{(-)^\dagger}\Omega_a^{(+)}. \tag{3.21}$$

The mathematical questions of convergence are the same here as for the single channel case, as in Eqs. (2.26).

IV. THE REARRANGEMENT MODEL

To keep contact with earlier work, we shall use a combination of the notations of Refs. 7 and 17, as far as possible. We consider a quantum field theory with five distinct fields, B, C, D, θ, and ϕ, and the corresponding particles (no antiparticles).

The nonzero commutators are

$$[B,B^\dagger]=[D,D^\dagger]=[C,C^\dagger]=1,$$
$$[\theta(\omega),\theta^\dagger(\omega')]=\delta(\omega'-\omega),\quad [\phi(\nu),\phi^\dagger(\nu')]=\delta(\nu'-\nu). \tag{4.1}$$

Note that θ and ϕ are labeled by continuum parameters, $0<\omega,\nu<\infty$, while B, C, and D are treated as single modes ("infinitely heavy").[18] We choose to use the energy as our variable, rather than momentum, because this makes the model much simpler, and more physically transparent. We want a total Hamiltonian for the system which allows the transitions

$$B\leftrightarrow C\phi$$

and

$$D\leftrightarrow C\theta.$$

Therefore, we choose our Hamiltonian to be

$$H=H_0+V, \tag{4.2}$$

where

$$H_0=m_B B^\dagger B+m_D D^\dagger D+\int d\omega\ \omega\theta^\dagger(\omega)\theta(\omega)+\int d\nu\ \nu\phi^\dagger(\nu)\phi(\nu) \tag{4.3}$$

and

$$V=\int d\omega\ f(\omega)\theta(\omega)CD^\dagger+\int d\omega\ f^*(\omega)\theta^\dagger(\omega)C^\dagger D+\int d\nu\ g(\nu)\phi(\nu)CB^\dagger$$
$$+\int d\nu\ g^*(\nu)\phi^\dagger(\nu)C^\dagger B. \tag{4.4}$$

This Hamiltonian has three constants of motion apart from itself. They are

$$C_1=B^\dagger B+C^\dagger C+D^\dagger D, \tag{4.5a}$$

$$C_2=B^\dagger B+\int d\nu\ \phi^\dagger(\nu)\phi(\nu), \tag{4.5b}$$

$$C_3=D^\dagger D+\int d\omega\ \theta^\dagger(\omega)\theta(\omega). \tag{4.5c}$$

Therefore, no transitions can occur between sectors labeled by different values of these quantum numbers. Let us start by enumerating the stable sectors. The first such sector is the vacuum and has $C_1=C_2=C_3=0$. The next three are: $C_1=1$, $C_2=0$, $C_3=0$; $C_1=0$, $C_2=1$, $C_3=0$; and $C_1=0$, $C_2=0$, $C_3=1$. These correspond to the states C, ϕ, and θ, respectively. Finally, there is the sector with $C_1=0$, $C_2=1$, $C_3=1$; it corresponds to a state $\theta\phi$.

The three lowest nontrivial sectors are

$$C_1=1,\quad C_2=1,\quad C_3=0, \tag{4.6a}$$

$$C_1=1,\quad C_2=0,\quad C_3=1, \tag{4.6b}$$

$$C_1=1,\quad C_2=1,\quad C_3=1. \tag{4.6c}$$

These correspond to $B\leftrightarrow C\phi$, $D\leftrightarrow C\theta$, and $B\theta\leftrightarrow C\theta\phi\leftrightarrow D\phi$, respectively. The last of these is the sector in which rearrangement collisions can take place, and as mentioned before, we shall call this the rearrangement sector.

Our strategy for solving the model in the rearrangement sector will be to first construct the solutions of the two lowest nontrivial sectors, Eqs. (4.6a) and (4.6b) (which are exactly analogous to the Lee model), and then use these solutions to express the rearrangement sector equations.

V. SOLVING THE MODEL

We start by constructing the solutions for the $B\leftrightarrow C\phi$ and $D\leftrightarrow C\theta$ sectors. These are exactly the same as the Lee model, so the solutions are simple. We shall denote noninteracting (''bare'') states by single bras and kets ($\langle,\rangle$), and interacting states (''dressed'' or ''physical'') by double bras and kets ($\langle\langle,\rangle\rangle$).

The equations we need to solve for the continuum solutions are

$$H|\lambda\rangle\rangle=\lambda|\lambda\rangle\rangle \tag{5.1a}$$

in the $B\leftrightarrow C\phi$ sector, and

$$H|\mu\rangle\rangle=\mu|\mu\rangle\rangle \tag{5.1b}$$

in the $D\leftrightarrow C\theta$ sector.

We define

$$\alpha(z)\equiv z-m_D-\int_0^\infty d\omega\,\frac{|f(\omega)|^2}{z-\omega}, \tag{5.2}$$

$$\beta(z)\equiv z-m_B-\int_0^\infty d\nu\,\frac{|g(\nu)|^2}{z-\nu}, \tag{5.3}$$

$$\rho_{\lambda,B}(\nu)\equiv\langle C\phi(\nu)|\lambda\rangle\rangle, \tag{5.4}$$

$$\rho_{\mu,D}(\omega)\equiv\langle C\theta(\omega)|\mu\rangle\rangle, \tag{5.5}$$

$$\sigma_{\lambda,B}\equiv\langle B|\lambda\rangle\rangle, \tag{5.6}$$

$$\sigma_{\mu,D}\equiv\langle D|\mu\rangle\rangle. \tag{5.7}$$

For shorthand, we will write $\alpha(\lambda)$ for $\alpha(\lambda+i\epsilon)$ and $\alpha^*(\lambda)$ for $\alpha(\lambda-i\epsilon)$, and similarly for $\beta(\lambda)$. In terms of these, the solutions are

$$\rho_{\lambda,B}(\nu)=\delta(\lambda-\nu)+\frac{g^*(\nu)\sigma_{\lambda,B}}{\lambda-\nu+i\epsilon}, \tag{5.8a}$$

$$\rho_{\mu,D}(\omega)=\delta(\mu-\omega)+\frac{f^*(\omega)\sigma_{\mu,D}}{\mu-\omega+i\epsilon}, \tag{5.8b}$$

$$\sigma_{\lambda,B}=\frac{g(\lambda)}{\beta(\lambda)}, \tag{5.8c}$$

$$\sigma_{\mu,D}=\frac{f(\mu)}{\alpha(\mu)}. \tag{5.8d}$$

If $\alpha(z)$ develops zeros then we have additional discrete states. Similarly, if $\beta(z)$ develops zeros then again we have additional discrete states. For our purposes, we shall always assume that both $\alpha(z)$ and $\beta(z)$ have exactly one zero each, which are denoted by M_D and M_B, respectively. There is no loss of generality if we use this assumption because the extension to more than one zero is trivial. The equations for the discrete states are

$$H|M_B\rangle\rangle = M_B|M_B\rangle\rangle \tag{5.9a}$$

in the $B\leftrightarrow C\phi$ sector, and

$$H|M_D\rangle\rangle = M_D|M_D\rangle\rangle \tag{5.9b}$$

in the $D\leftrightarrow C\theta$ sector. We define

$$\rho_B(\nu)\equiv\langle C\phi(\nu)|M_B\rangle\rangle, \tag{5.10}$$

$$\rho_D(\omega)\equiv\langle C\theta(\omega)|M_D\rangle\rangle, \tag{5.11}$$

$$\sqrt{Z_B}\equiv\langle B|M_B\rangle\rangle, \tag{5.12}$$

$$\sqrt{Z_D}\equiv\langle D|M_D\rangle\rangle. \tag{5.13}$$

In terms of these, the normalized solutions are

$$\rho_B(\nu)=\sqrt{Z_B}\,\frac{g^*(\nu)}{M_B-\nu}, \tag{5.14a}$$

$$\rho_D(\omega)=\sqrt{Z_D}\,\frac{f^*(\omega)}{M_D-\omega}, \tag{5.14b}$$

$$Z_B=\left[1+\int d\nu\,\frac{|g(\nu)|^2}{(M_B-\nu)^2}\right]^{-1}, \tag{5.14c}$$

$$Z_D=\left[1+\int d\omega\,\frac{|f(\omega)|^2}{(M_D-\omega)^2}\right]^{-1}, \tag{5.14d}$$

where the last two are obtained by imposition of the orthonormality condition. Note that these solutions, Eqs. (5.8) and (5.14), form a complete orthonormal set.

Now, we use these solutions to construct the solutions in the rearrangement sector. In this sector we will have four sorts of solutions. The first will correspond to the physical $|C\theta(\omega)\phi(\nu)\rangle\rangle$ sector, the second to the physical $|D\phi(\nu)\rangle\rangle$, the third to the physical $|B\theta(\omega)\rangle\rangle$, and the last to one or more dynamically generated bound states, which we shall denote by $|M_A\rangle\rangle$. Which solution is obtained will depend on whether we put the delta functions (which represent the plane wave parts of our solutions) in our solutions. If we put none, we get the discrete states.

We wish to solve the eigenvalue equation

$$H|E\rangle\rangle = E|E\rangle\rangle. \tag{5.15}$$

We expand Eq. (5.15) in terms of $\theta^\dagger(\omega)|\lambda\rangle\rangle$, $\theta^\dagger(\omega)|M_B\rangle\rangle$, $\phi^\dagger(\nu)|\mu\rangle\rangle$, and $\phi^\dagger(\nu)|M_D\rangle\rangle$. By acting on these states with the Hamiltonian, and using Eqs. (5.1) and (5.9) we get

$$(E-\lambda-\omega)\langle\langle\lambda|\theta(\omega)|E\rangle\rangle = f^*(\omega)\langle\langle\lambda|C^\dagger D|E\rangle\rangle, \tag{5.16a}$$

$$(E-M_B-\omega)\langle\langle M_B|\theta(\omega)|E\rangle\rangle=f^*(\omega)\langle\langle M_B|C^\dagger D|E\rangle\rangle, \tag{5.16b}$$

$$(E-\mu-\nu)\langle\langle \mu|\phi(\nu)|E\rangle\rangle=g^*(\nu)\langle\langle \mu|C^\dagger B|E\rangle\rangle, \tag{5.16c}$$

$$(E-M_D-\nu)\langle\langle M_D|\phi(\nu)|E\rangle\rangle=g^*(\nu)\langle\langle M_D|C^\dagger B|E\rangle\rangle. \tag{5.16d}$$

We need to evaluate the unknown matrix elements on the right-hand side of Eqs. (5.16). We solve for these elements by inserting H in them, commuting it on one side, and letting it act on $|E\rangle\rangle$ on the other. For example, we can solve for $\langle\langle\lambda|C^\dagger D|E\rangle\rangle$ in the following manner:

$$\langle\langle\lambda|C^\dagger DH|E\rangle\rangle=E\langle\langle\lambda|C^\dagger D|E\rangle\rangle\Rightarrow\langle\langle\lambda|\{HC^\dagger D+[C^\dagger D,H]\}|E\rangle\rangle=E\langle\langle\lambda|C^\dagger D|E\rangle\rangle. \tag{5.17}$$

We now let H in the first term of Eq. (5.17) act on $\langle\langle\lambda|$, and evaluate the commutator in the second term. We proceed similarly for the other three equations and, when all the dust settles, get

$$\begin{aligned}(E-\lambda-m_D)\langle\langle\lambda|CD^\dagger|E\rangle\rangle=&\int d\omega\ f(\omega)\langle\langle\lambda|\theta(\omega)|E\rangle\rangle-\sigma_{\lambda,B^*}\Bigg[\int d\omega\ f(\omega)\\&\times\Bigg\{\int d\lambda'\ \sigma_{\lambda',B}\langle\langle\lambda'|\theta(\omega)|E\rangle\rangle+\sqrt{Z_B}\langle\langle M_B|\theta(\omega)|E\rangle\rangle\Bigg\}\\&+\int d\nu\ g(\nu)\Bigg\{\int d\mu'\ \sigma_{\mu',D}\langle\langle\mu'|\phi(\nu)|E\rangle\rangle\\&+\sqrt{Z_D}\langle\langle M_D|\phi(\nu)|E\rangle\rangle\Bigg\}\Bigg],\end{aligned} \tag{5.18a}$$

$$\begin{aligned}(E-M_B-m_D)\langle\langle M_B|CD^\dagger|E\rangle\rangle=&\int d\omega\ f(\omega)\langle\langle M_B|\theta(\omega)|E\rangle\rangle-\sqrt{Z_B}\Bigg[\int d\omega\ f(\omega)\\&\times\Bigg\{\int d\lambda'\ \sigma_{\lambda',B}\langle\langle\lambda'|\theta(\omega)|E\rangle\rangle+\sqrt{Z_B}\langle\langle M_B|\theta(\omega)|E\rangle\rangle\Bigg\}\\&+\int d\nu\ g(\nu)\Bigg\{\int d\mu'\ \sigma_{\mu',D}\langle\langle\mu'|\phi(\nu)|E\rangle\rangle\\&+\sqrt{Z_D}\langle\langle M_D|\phi(\nu)|E\rangle\rangle\Bigg\}\Bigg],\end{aligned} \tag{5.18b}$$

$$\begin{aligned}(E-\mu-m_B)\langle\langle\mu|CB^\dagger|E\rangle\rangle=&\int d\nu\ g(\nu)\langle\langle\mu|\phi(\nu)|E\rangle\rangle-\sigma_{\mu,D^*}\Bigg[\int d\omega\ f(\omega)\\&\times\Bigg\{\int d\lambda'\ \sigma_{\lambda',B}\langle\langle\lambda'|\theta(\omega)|E\rangle\rangle+\sqrt{Z_B}\langle\langle M_B|\theta(\omega)|E\rangle\rangle\Bigg\}\\&+\int d\nu\ g(\nu)\Bigg\{\int d\mu'\ \sigma_{\mu',D}\langle\langle\mu'|\phi(\nu)|E\rangle\rangle\\&+\sqrt{Z_D}\langle\langle M_D|\phi(\nu)|E\rangle\rangle\Bigg\}\Bigg],\end{aligned} \tag{5.18c}$$

$$(E-M_D-m_B)\langle\langle M_D|CB^\dagger|E\rangle\rangle=\int d\nu\ g(\nu)\langle\langle M_D|\phi(\nu)|E\rangle\rangle-\sqrt{Z_D}\Bigg[\int d\omega\ f(\omega)$$

$$\times\left\{\int d\lambda'\,\sigma_{\lambda',B}\langle\langle\lambda'|\theta(\omega)|E\rangle\rangle+\sqrt{Z_B}\langle\langle M_B|\theta(\omega)|E\rangle\rangle\right\}$$
$$+\int d\nu\, g(\nu)\left\{\int d\mu'\ \sigma_{\mu',D}\langle\langle\mu'|\phi(\nu)|E\rangle\rangle\right.$$
$$\left.+\sqrt{Z_D}\langle\langle M_D|\phi(\nu)|E\rangle\rangle\right\}\Bigg]. \tag{5.18d}$$

We first solve for the physical $|C\theta(\omega)\phi(\nu)\rangle\rangle$ states. We start by inverting Eqs. (5.16) and putting in the requisite delta functions. Note that we may put the product of two delta functions because this is an infinitely degenerate (double) continuum, which cannot be specified by just E; rather, we have to label the state with the variables E and n, with the n variable representing the division of energy between the θ and ϕ particles. We then substitute these into the first term of each of Eqs. (5.18), and solve for the unknown matrix elements. Having found them, we put them into Eqs. (5.16) to find our solutions. Defining

$$b^C(E,n,\lambda,\omega)\equiv\langle\langle\lambda|\theta(\omega)|E,n\rangle\rangle, \tag{5.19a}$$

$$b_F^C(E,n,M_B,\omega)\equiv\langle\langle M_B|\theta(\omega)|E,n\rangle\rangle, \tag{5.19b}$$

$$d^C(E,n,\mu,\nu)\equiv\langle\langle\mu|\phi(\nu)|E,n\rangle\rangle, \tag{5.19c}$$

$$d_F^C(E,n,M_D,\nu)\equiv\langle\langle M_D|\phi(\nu)|E,n\rangle\rangle, \tag{5.19d}$$

we get

$$b^C(E,n,\lambda,\omega)=\delta(E-\lambda-n)\rho_{n,D}(\omega)-\frac{f^*(\omega)}{(E-\lambda-\omega+i\epsilon)}\frac{\sigma_{\lambda,B*}}{\alpha(E-\lambda)}K_C(E,n), \tag{5.20a}$$

$$b_F^C(E,n,M_B,\omega)=-\frac{f^*(\omega)}{(E-M_B-\omega+i\epsilon)}\frac{\sqrt{Z_B}}{\alpha(E-M_B)}K_C(E,n), \tag{5.20b}$$

$$d^C(E,n,\mu,\nu)=\delta(\mu-n)\rho_{E-n,B}(\nu)-\frac{g^*(\nu)}{(E-\mu-\nu+i\epsilon)}\frac{\sigma_{\mu,D*}}{\beta(E-\mu)}K_C(E,n), \tag{5.20c}$$

$$d_F^C(E,n,M_D,\nu)=-\frac{g^*(\nu)}{(E-M_D-\nu+i\epsilon)}\frac{\sqrt{Z_D}}{\beta(E-M_D)}K_C(E,n), \tag{5.20d}$$

where

$$K_C(E,n)=\frac{g(E-n)f(n)}{\beta(E-n)\alpha(n)}\frac{1}{\gamma(E)}, \tag{5.21}$$

$$\gamma(E)=\frac{Z_D}{\beta(E-M_D)}+\int d\mu\,\frac{|f(\mu)|^2}{|\alpha(\mu)|^2}\frac{1}{\beta(E-\mu)} \tag{5.22a}$$

$$=\frac{Z_B}{\alpha(E-M_B)}+\int d\lambda\,\frac{|g(\lambda)|^2}{|\beta(\lambda)|^2}\frac{1}{\alpha(E-\lambda)}. \tag{5.22b}$$

The last equality follows from Eqs. (A10).

We now solve for the physical $|D\phi(\nu)\rangle\rangle$ sector. We must again start by inverting Eqs. (5.16), but this time need to put just the one requisite delta function in Eq. (5.16d). We put these equations in Eqs. (5.18), and solve for the unknown matrix elements putting in another delta function in Eq. (5.18a) when inverting because now we must account for the zero of $\alpha(E-\lambda)$ at M_D. We then put these results in Eqs. (5.16). Defining

$$b^D(E,\lambda,\omega)\equiv\langle\langle\lambda|\,\theta(\omega)|E\rangle\rangle, \tag{5.23a}$$

$$b_F^D(E,M_B,\omega)\equiv\langle\langle M_B|\,\theta(\omega)|E\rangle\rangle, \tag{5.23b}$$

$$d^D(E,\mu,\nu)\equiv\langle\langle\mu|\,\phi(\nu)|E\rangle\rangle, \tag{5.23c}$$

$$d_F^D(E,M_D,\nu)\equiv\langle\langle M_D|\,\phi(\nu)|E\rangle\rangle, \tag{5.23d}$$

we get

$$b^D(E,\lambda,\omega)=\rho_D(\omega)\,\delta(E-\lambda-M_D)-\frac{f^*(\omega)}{(E-\lambda-\omega+i\epsilon)}\,\frac{\sigma_{\lambda,B*}}{\alpha(E-\lambda)}\,K_D(E), \tag{5.24a}$$

$$b_F^D(E,M_B,\omega)=-\frac{f^*(\omega)}{(E-M_B-\omega+i\epsilon)}\,\frac{\sqrt{Z_B}}{\alpha(E-M_B)}\,K_D(E), \tag{5.24b}$$

$$d^D(E,\mu,\nu)=-\frac{g^*(\nu)}{(E-\mu-\nu+i\epsilon)}\,\frac{\sigma_{\mu,D*}}{\beta(E-\mu)}\,K_D(E), \tag{5.24c}$$

$$d_F^D(E,M_D,\nu)=\rho_{E-M_D,B}(\nu)-\frac{g^*(\nu)}{(E-M_D-\nu+i\epsilon)}\,\frac{\sqrt{Z_D}}{\beta(E-M_D)}\,K_D(E), \tag{5.24d}$$

where

$$K_D(E)=\frac{\sqrt{Z_D}}{\gamma(E)}\,\frac{g(E-M_D)}{\beta(E-M_D)}, \tag{5.25}$$

and $\gamma(E)$ is the same as that defined in Eqs. (5.22).

In exactly the same way, we can find the solutions for the physical $|B\theta(\omega)\rangle\rangle$ sector. They are

$$b^B(E,\lambda,\omega)=-\frac{f^*(\omega)}{(E-\lambda-\omega+i\epsilon)}\,\frac{\sigma_{\lambda,B*}}{\alpha(E-\lambda)}\,K_B(E), \tag{5.26a}$$

$$b_F^B(E,M_B,\omega)=\rho_{E-M_B,D}(\omega)-\frac{f^*(\omega)}{(E-M_B-\omega+i\epsilon)}\,\frac{\sqrt{Z_B}}{\alpha(E-M_B)}\,K_B(E), \tag{5.26b}$$

$$d^B(E,\mu,\nu)=\rho_B(\nu)\,\delta(E-\mu-M_B)-\frac{g^*(\nu)}{(E-\mu-\nu+i\epsilon)}\,\frac{\sigma_{\mu,D*}}{\beta(E-\mu)}\,K_B(E), \tag{5.26c}$$

$$d_F^B(E,M_D,\nu)=-\frac{g^*(\nu)}{(E-M_D-\nu+i\epsilon)}\,\frac{\sqrt{Z_D}}{\beta(E-M_D)}\,K_B(E), \tag{5.26d}$$

where

$$K_B(E)=\frac{\sqrt{Z_B}}{\gamma(E)}\,\frac{f(E-M_B)}{\alpha(E-M_B)}, \tag{5.27}$$

and $\gamma(E)$ is the same as that defined in Eq. (5.22).

Finally, we wish to solve for any dynamically generated discrete states. In this case, we put no delta functions anywhere. When we follow the procedure of putting Eqs. (5.16) in Eqs. (5.18) and solving for the unknown matrix elements, we find that the only way to satisfy all the equations is if $\gamma(E)$ has zeros. Denoting these zeros by M_A, we find the discrete state solutions:

$$b^A(M_A,\lambda,\omega)=-\frac{f^*(\omega)}{(M_A-\lambda-\omega)}\,\frac{\sigma_{\lambda,B*}}{\alpha(M_A-\lambda)}\,K_A(M_A), \tag{5.28a}$$

$$b_F^A(M_A,M_B,\omega)=-\frac{f^*(\omega)}{(M_A-M_B-\omega+i\epsilon)}\,\frac{\sqrt{Z_B}}{\alpha(M_A-M_B)}\,K_A(M_A), \tag{5.28b}$$

$$d^A(M_A,\mu,\nu)=-\frac{g^*(\nu)}{(M_A-\mu-\nu)}\,\frac{\sigma_{\mu,D*}}{\beta(M_A-\mu)}\,K_A(M_A), \tag{5.28c}$$

$$d_F^A(M_A,M_D,\nu)=-\frac{g^*(\nu)}{(M_A-M_D-\nu+i\epsilon)}\,\frac{\sqrt{Z_D}}{\beta(M_A-M_D)}\,K_A(M_A). \tag{5.28d}$$

where $K_A(M_A)$ is now an arbitrary normalization factor which is fixed, when demonstrating completeness, to be $\sqrt{d\gamma(E)/dE|_{E=M_A}}$ (see the discussion after Eq. (7.18)). For our purposes, without loss of generality, we assume that there is only one zero of $\gamma(E)$, denoted by M_A, and thus only one dynamically generated discrete state. The extension to more than one discrete state is trivial.

In each of Eqs. (5.20), (5.24), (5.26), and (5.28) the superscript refers to the sector that the solution is in, and the subscript F refers to solutions expanded in the discrete state part of the Lee Model sectors. Furthermore, we have anticipated future developments by fixing the arbitrary constants accompanying the delta functions in Eqs. (5.20), (5.24), and (5.26). We do this by demanding that Eq. (6.3a) and Eq. (6.3b), or their equivalents for the other two sectors, give the same result, and that the solutions be orthonormal.

VI. VERIFICATION OF THE SOLUTIONS

We now proceed to verify that Eqs. (5.20), (5.24), (5.26), and (5.28) are each solutions to our problem. To do this, we first transform our solutions into the bare state basis; i.e., in terms of the noninteracting states $|C\theta(\omega)\phi(\nu)\rangle$, $|B\theta(\omega)\rangle$, and $|D\phi(\nu)\rangle$, using the completeness of the lower sector solutions. With the expansion coefficients in the physical $|C\theta(\omega)\phi(\nu)\rangle\rangle$ sector defined in the following manner (with the coefficients for the other sectors defined similarly):

$$|E,n\rangle\rangle\equiv C^C(E,n,\omega,\nu)|C\theta(\omega)\phi(\nu)\rangle+B^C(E,n,\omega)|B\theta(\omega)\rangle+D^C(E,n,\nu)|D\phi(\nu)\rangle, \tag{6.1}$$

where

$$\Psi^C(E,n,\omega,\nu)\equiv\begin{pmatrix} C^C(E,n,\omega,\nu)\\ D^C(E,n,\nu)\\ B^C(E,n,\omega)\end{pmatrix} \tag{6.2}$$

and

$$C^C(E,n,\omega,\nu)\equiv\langle C\theta(\omega)\phi(\nu)|E,n\rangle\rangle,$$

$$B^C(E,n,\omega)\equiv\langle B\theta(\omega)|E,n\rangle\rangle,$$

$$D^C(E,n,\nu)\equiv\langle D\phi(\nu)|E,n\rangle\rangle,$$

we have

$$C^C(E,n,\omega,\nu)=\int d\lambda_{\rho\lambda,B}(\nu)b^C(E,n,\lambda,\omega)+\rho_B(\nu)b_F^C(E,n,M_B,\omega), \tag{6.3a}$$

$$=\int d\mu\ \rho_{\mu,D}(\omega)d^C(E,n,\mu,\nu)+\rho_D(\omega)d_F^C(E,n,M_D,\nu), \tag{6.3b}$$

$$D^C(E,n,\nu)=\int d\mu\ \sigma_{\mu,D}d^C(E,n,\mu,\nu)+\sqrt{Z_D}d_F^C(E,n,M_D,\nu), \tag{6.3c}$$

$$B^C(E,n,\omega)=\int d\lambda\ \sigma_{\lambda,B}b^C(E,n,\lambda,\omega)+\sqrt{Z_B}b_F^C(E,n,M_B,\omega), \tag{6.3d}$$

with similar equations for the other three sectors (e.g., for the physical $|D\phi(\nu)\rangle\rangle$ sector, we would replace $C^C(E,n,\omega,\nu)$ by $C^D(E,\omega,\nu)$, $b^C(E,n,\lambda,\omega)$ by $b^D(E,\lambda,\omega)$, etc.). A good check that we have solved our equations correctly is to verify that Eqs. (6.3a) and (6.3b) give the same result. This is indeed completely trivial if we use Eq. (A14).

For the physical $|C\theta(\omega)\phi(\nu)\rangle\rangle$ sector in the bare basis, we get

$$\begin{aligned}C^C(E,n,\omega,\nu)=&\rho_{n,D}(\omega)\rho_{E-n,B}(\nu)\\&-K_C(E,n)\frac{f^*(\omega)g^*(\nu)}{(E-\omega-\nu+i\epsilon)}\left\{\int d\lambda\ \frac{|\sigma_{\lambda,B}|^2}{(E-\lambda-\omega+i\epsilon)\alpha(E-\lambda)}\right.\\&+\int d\mu\ \frac{|\sigma_{\mu,D}|^2}{(E-\mu-\nu+i\epsilon)\beta(E-\mu)}+\frac{Z_B}{\alpha(E-M_B)(E-M_B-\omega+i\epsilon)}\\&\left.+\frac{Z_D}{\beta(E-M_D)(E-M_D-\nu+i\epsilon)}\right\},\end{aligned} \tag{6.4a}$$

$$\begin{aligned}D^C(E,n,\nu)=&\frac{f(n)}{\alpha(n)}\rho_{n,D}(\omega)-K_C(E,n)g^*(\nu)\left\{\int d\mu\ \frac{|\sigma_{\mu,D}|^2}{(E-\mu-\nu+i\epsilon)\beta(E-\mu)}\right.\\&\left.+\frac{Z_D}{\beta(E-M_D)(E-M_D-\nu+i\epsilon)}\right\},\end{aligned} \tag{6.4b}$$

$$\begin{aligned}B^C(E,n,\omega)=&\frac{g(E-n)}{\beta(E-n)}\rho_{E-n,B}(\nu)-K_C(E,n)f^*(\omega)\left\{\int d\lambda\ \frac{|\sigma_{\lambda,B}|^2}{(E-\lambda-\omega+i\epsilon)\alpha(E-\lambda)}\right.\\&\left.+\frac{Z_B}{\alpha(E-M_B)(E-M_B-\omega+i\epsilon)}\right\}.\end{aligned} \tag{6.4c}$$

For the physical $|D\phi(\nu)\rangle\rangle$ sector in the bare basis, we get

$$C^D(E,\omega,\nu)=\rho_D(\omega)\rho_{E-M_D,B}(\nu)-K_D(E)\frac{f^*(\omega)g^*(\nu)}{(E-\mu-\nu+i\epsilon)}\left\{\int d\lambda\ \frac{|\sigma_{\lambda,B}|^2}{(E-\lambda-\omega+i\epsilon)\alpha(E-\lambda)}\right.$$

$$+\int d\mu\,\frac{|\sigma_{\mu,D}|^2}{(E-\mu-\nu+i\epsilon)\beta(E-\mu)}+\frac{Z_B}{\alpha(E-M_B)(E-M_B-\omega+i\epsilon)}$$
$$+\frac{Z_D}{\beta(E-M_D)(E-M_D-\nu+i\epsilon)}\Bigg\}, \tag{6.5a}$$

$$D^D(E,\nu)=\sqrt{Z_{D\rho E-M_D,B}}(\nu)-K_D(E)g^*(\nu)\Bigg\{\int d\mu\,\frac{|\sigma_{\mu,D}|^2}{(E-\mu-\nu+i\epsilon)\beta(E-\mu)}$$
$$+\frac{Z_D}{\beta(E-M_D)(E-M_D-\nu+i\epsilon)}\Bigg\}, \tag{6.5b}$$

$$B^D(E,\omega)=\rho_D(\omega)\sigma_{E-M_D,B}-K_D(E)f^*(\omega)\Bigg\{\int d\lambda\,\frac{|\sigma_{\lambda,B}|^2}{(E-\lambda-\omega+i\epsilon)\alpha(E-\lambda)}$$
$$+\frac{Z_B}{\alpha(E-M_B)(E-M_B-\omega+i\epsilon)}\Bigg\}. \tag{6.5c}$$

For the physical $|B\theta(\omega)\rangle\rangle$ sector in the bare basis, we get

$$C^B(E,\omega,\nu)=\rho_B(\nu)\rho_{E-M_B,D}(\omega)-K_B(E)\,\frac{f^*(\omega)g^*(\nu)}{(E-\omega-\nu+i\epsilon)}\Bigg\{\int d\lambda\,\frac{|\sigma_{\lambda,B}|^2}{(E-\lambda-\omega+i\epsilon)\alpha(E-\lambda)}$$
$$+\int d\mu\,\frac{|\sigma_{\mu,D}|^2}{(E-\mu-\nu+i\epsilon)\beta(E-\mu)}+\frac{Z_B}{\alpha(E-M_B)(E-M_B-\omega+i\epsilon)}$$
$$+\frac{Z_D}{\beta(E-M_D)(E-M_D-\nu+i\epsilon)}\Bigg\}, \tag{6.6a}$$

$$D^B(E,\nu)=\rho_B(\nu)\sigma_{E-M_B,D}-K_B(E)g^*(\nu)\Bigg\{\int d\mu\,\frac{|\sigma_{\mu,D}|^2}{(E-\mu-\nu+i\epsilon)\beta(E-\mu)}$$
$$+\frac{Z_D}{\beta(E-M_D)(E-M_D-\nu+i\epsilon)}\Bigg\}, \tag{6.6b}$$

$$B^B(E,\omega)=\sqrt{Z_{B\rho E-M_B,D}}(\omega)-K_B(E)f^*(\omega)\Bigg\{\int d\lambda\,\frac{|\sigma_{\lambda,B}|^2}{(E-\lambda-\omega+i\epsilon)\alpha(E-\lambda)}$$
$$+\frac{Z_B}{\alpha(E-M_B)(E-M_B-\omega+i\epsilon)}\Bigg\}. \tag{6.6c}$$

Finally, for the discrete states, we get

$$C^A(M_A,\omega,\nu)=-K_A(M_A)\,\frac{f^*(\omega)g^*(\nu)}{M_A-\omega-\nu}\Bigg\{\int d\lambda\,\frac{|\sigma_{\lambda,B}|^2}{(M_A-\lambda-\omega)\alpha(M_A-\lambda)}$$
$$+\int d\mu\,\frac{|\sigma_{\mu,D}|^2}{(M_A-\mu-\nu)\beta(M_A-\mu)}+\frac{Z_B}{\alpha(M_A-M_B)(M_A-M_B-\omega+i\epsilon)}$$
$$+\frac{Z_D}{\beta(M_A-M_D)(M_A-M_D-\nu+i\epsilon)}\Bigg\}, \tag{6.7a}$$

$$D^A(M_A,\nu)=-K_A(M_A)g^*(\nu)\Bigg\{\int d\mu\ \frac{|\sigma_{\mu,D}|^2}{(M_A-\mu-\nu)\beta(M_A-\mu)} + \frac{Z_D}{\beta(M_A-M_D)(M_A-M_D-\nu+i\epsilon)}\Bigg\}, \tag{6.7b}$$

$$B^A(M_A,\omega)=-K_A(M_A)f^*(\omega)\Bigg\{\int d\lambda\ \frac{|\sigma_{\lambda,B}|^2}{(M_A-\lambda-\omega)\alpha(M_A-\lambda)} + \frac{Z_B}{\alpha(M_A-M_B)(M_A-M_B-\omega+i\epsilon)}\Bigg\}. \tag{6.7c}$$

We now verify that Eqs. (6.4), (6.5), (6.6), and (6.7) are each solutions of our model. To do this, we explicitly write down the analogs of Eqs. (5.16) in the bare basis, plug in each set of solutions in turn, and verify that the equations are satisfied. A straightforward analysis shows that the following equations must be satisfied in the bare basis (we have written them for the physical $|C\theta(\omega)\phi(\nu)\rangle\rangle$ sector, i.e., with the variable n—for the other sectors the variable n is, of course, missing):

$$(E-\omega-\nu)C(E,n,\omega,\nu)=g^*(\nu)B(E,n,\omega)+f^*(\omega)D(E,n,\nu), \tag{6.8a}$$

$$(E-m_B-\omega)B(E,n,\omega)=\int d\nu\ g(\nu)C(E,n,\omega,\nu), \tag{6.8b}$$

$$(E-m_D-\nu)D(E,n,\nu)=\int d\omega\ f(\omega)C(E,n,\omega,\nu). \tag{6.8c}$$

Putting each of Eqs. (6.4), (6.5), (6.6), and (6.7) in turn into Eqs. (6.8), or their equivalents for the other sectors, and using Eq. (A14), we find that each of these sets of solutions satisfies the equations. Incidentally, a glance at Eqs. (6.8) immediately shows why we could not have solved the problem directly rather than the somewhat convoluted method we went through: the integral equations are not separable, and are quite intractable.

VII. ORTHONORMALITY AND COMPLETENESS

We now proceed to verify orthonormality and completeness of the solutions Eqs. (6.4), (6.5), (6.6), and (6.7). We start by verifying orthonormality for the diagonal components beginning with the scalar product $(\Psi^{C^\dagger}(E',n',\omega,\nu),\Psi^C(E,n,\omega,\nu))$, which is given by

$$\begin{aligned}\int d\omega\ d\nu\Psi^{C^\dagger}(E',n',\omega,\nu)\Psi^C(E,n,\omega,\nu)&\\ =\int d\omega\ d\nu\ C^{C*}(E',n',\omega,\nu)C^C(E,n,\omega,\nu)+\int d\omega\ B^{C*}(E',n',\omega)B^C(E,n,\omega)&\\ +\int d\nu\ D^{C*}(E',n',\nu)D^C(E,n,\nu).&\end{aligned} \tag{7.1}$$

We now use Eqs. (6.3) to write this as

$$\int d\omega\, d\nu\, \Psi^{C^\dagger}(E',n',\omega,\nu)\Psi^{C}(E,n,\omega,\nu)$$
$$= \int d\omega\, d\nu \Big[\int d\lambda'\ \rho^*_{\lambda',B}(\nu) b^{C^*}(E',n',\lambda',\omega) + \rho^*_B(\nu) b^{C^*}_F(E',n',M_B,\omega) \Big]$$
$$\times \Big[\int d\lambda\ \rho_{\lambda,B}(\nu) b^{C}(E,n,\lambda,\omega) + \rho_B(\nu) b^{C}_F(E,n,M_B,\omega) \Big]$$
$$+ \int d\omega \Big[\int d\lambda'\ \sigma^*_{\lambda',B} b^{C^*}(E',n',\lambda',\omega) + \sqrt{Z_B} b^{C^*}_F(E',n',M_B,\omega) \Big]$$
$$\times \Big[\int d\lambda\ \sigma_{\lambda,B} b^{C}(E,n,\lambda,\omega) + \sqrt{Z_B} b^{C}_F(E,n,M_B,\omega) \Big] + \int d\nu\ D^{C^*}(E',n',\nu) D^{C}(E,n,\nu). \tag{7.2}$$

We then do the integrals over λ and λ' to find

$$\int d\omega\, d\nu\, \Psi^{C^\dagger}(E',n',\omega,\nu)\Psi^{C}(E,n,\omega,\nu) = \int d\lambda\ d\omega\ b^{C^*}(E',n',\lambda,\omega) b^{C}(E,n,\lambda,\omega)$$
$$+ \int d\omega\ b^{C^*}_F(E',n',M_B,\omega) b^{C}_F(E,n,M_B,\omega)$$
$$+ \int d\nu\ D^{C^*}(E',n',\nu) D^{C}(E,n,\nu). \tag{7.3}$$

Defining

$$L_1(E',n') \equiv \frac{f^*(n')g^*(E'-n')}{\alpha^*(n')\beta^*(E'-n')}, \quad L_2(E,n) \equiv \frac{f(n)g(E-n)}{\alpha(n)\beta(E-n)}, \tag{7.4}$$

we find that the sum of the first two integrals is

$$\delta(E-E')\delta(n-n') - \delta(E'-n'-E+n)\ \frac{f^*(n')f(n)}{\alpha^*(n')\alpha(n)} + L_1(E',n')L_2(E,n)$$
$$\times \left\{ \frac{1}{\gamma^*(E')\alpha^*(E'-E+n)} + \frac{1}{\gamma(E)\alpha(E-E'+n')} \right\} + \frac{L_1(E',n')L_2(E,n)}{\gamma^*(E')\gamma(E)}$$
$$\times \left\{ \frac{-Z_B}{\alpha^*(E'-M_B)\alpha(E-M_B)} - \int d\lambda\ \frac{|\sigma_{\lambda,B}|^2}{\alpha^*(E'-\lambda)\alpha(E-\lambda)} \right\} \tag{7.5}$$

while the third integral gives

$$\delta(E'-n'-E+n)\ \frac{f^*(n')f(n)}{\alpha^*(n')\alpha(n)} - L_1(E',n')L_2(E,n)$$
$$\times \left\{ \frac{1}{\gamma^*(E')\alpha^*(E'-E+n)} + \frac{1}{\gamma(E)\alpha(E-E'+n')} \right\} + \frac{L_1(E',n')L_2(E,n)}{\gamma^*(E')\gamma(E)}$$
$$\times \left\{ \frac{Z_D}{\beta(E-M_D)\alpha^*(E'-E+M_D)} + \frac{Z_D}{\beta^*(E'-M_D)\alpha(E-E'+M_D)} \right.$$

$$+\int d\mu' \frac{|\sigma_{\mu',D}|^2}{\beta^*(E'-\mu')\alpha(E-E'+\mu')}+\int d\mu \frac{|\sigma_{\mu,D}|^2}{\beta(E-\mu)\alpha^*(E'-E-\mu)}\Bigg\}. \tag{7.6}$$

Adding Eqs. (7.5) and (7.6) together, and doing the integrals by combining them into a single contour integral (which evaluates simply to its residues), we find that the only term left is $\delta(E'-E)\,\delta(n'-n)$, which is just as required.

We can similarly show that

$$\begin{aligned}\int d\omega\, d\nu\, \Psi^{D^\dagger}(E',\omega,\nu)\Psi^D(E,\omega,\nu) &= \int d\lambda\, d\omega\, b^{D*}(E',\lambda,\omega)b^D(E,\lambda,\omega)\\ &\quad+\int d\omega\, b_F^{D*}(E',M_B,\omega)b_F^D(E,M_B,\omega)\\ &\quad+\int d\nu\, D^{D*}(E',\nu)D^D(E,\nu)=\delta(E'-E)\end{aligned} \tag{7.7}$$

and

$$\begin{aligned}\int d\omega\, d\nu\, \Psi^{B^\dagger}(E',\omega,\nu)\Psi^B(E,\omega,\nu) &= \int d\lambda\, d\omega\, b^{B*}(E',\lambda,\omega)b^B(E,\lambda,\omega)\\ &\quad+\int d\omega\, b_F^{B*}(E',M_B,\omega)b_F^B(E,M_B,\omega)\\ &\quad+\int d\nu\, D^{B*}(E',\nu)D^B(E,\nu)=\delta(E'-E).\end{aligned} \tag{7.8}$$

Finally,

$$\Psi^{A^\dagger}(M_A,\omega,\nu)\Psi^A(M_A,\omega,\nu)=1. \tag{7.9}$$

Now we take up the off-diagonal elements. For

$$\begin{aligned}\int d\omega\, d\nu\, \Psi^{C^\dagger}(E',n',\omega,\nu)\Psi^D(E,\omega,\nu) &= \int d\lambda\, d\omega\, b^{C*}(E',n',\lambda,\omega)b^D(E,\lambda,\omega)\\ &\quad+\int d\omega\, b_F^{C*}(E',n',M_B,\omega)b_F^D(E,M_B,\omega)\\ &\quad+\int d\nu\, D^{C*}(E',n',\nu)D^D(E,\nu),\end{aligned} \tag{7.10}$$

we find that the third integral exactly cancels the sum of the first two, giving us 0. We can similarly show that

$$\int d\omega\, d\nu\, \Psi^{C^\dagger}(E',n',\omega,\nu)\Psi^B(E,\omega,\nu)=0, \tag{7.11}$$

$$\int d\omega\, d\nu\, \Omega^{C^\dagger}(E',n',\omega,\nu)\Psi^A(M_A,\omega,\nu)=0, \tag{7.12}$$

$$\int d\omega\, d\nu\, \Psi^{D^\dagger}(E',\omega,\nu)\Psi^B(E,\omega,\nu)=0, \tag{7.13}$$

$$\int d\omega\, d\nu\, \Psi^{D^\dagger}(E',\omega,\nu)\Psi^{A}(M_A,\omega,\nu)=0, \tag{7.14}$$

$$\int d\omega\, d\nu\, \Psi^{B^\dagger}(E',\omega,\nu)\Psi^{A}(M_A,\omega,\nu)=0. \tag{7.15}$$

Therefore, the set of solutions we found, Eqs. (6.4), (6.5), (6.6), and (6.7) are orthonormal.

We now consider completeness. We wish to show that

$$\begin{aligned}&\int dE\, dn\, \Psi^{C}(E,n,\omega,\nu)\Psi^{C^\dagger}(E,n,\omega',\nu')+\int dE\, \Psi^{D}(E,\omega,\nu)\Psi^{D^\dagger}(E,\omega',\nu')\\&+\int dE\, \Psi^{B}(E,\omega,\nu)\Psi^{B^\dagger}(E,\omega',\nu')+\Psi^{A}(M_A,\omega,\nu)\Psi^{A^\dagger}(M_A,\omega',\nu')\\&=\begin{pmatrix}\delta(\nu-\nu')\delta(\omega-\omega') & 0 & 0\\ 0 & \delta(\nu-\nu') & 0\\ 0 & 0 & \delta(\omega-\omega')\end{pmatrix}.\end{aligned} \tag{7.16}$$

Let us start with the diagonal elements. The (1,1) element of the matrix is

$$\begin{aligned}&\int dE\, dn\, C^{C}(E,n,\omega,\nu)C^{C^*}(E,n,\omega',\nu')+\int dE\, C^{D}(E,\omega,\nu)C^{D^*}(E,\omega',\nu')\\&+\int dE\, C^{B}(E,\omega,\nu)C^{B^*}(E,\omega',\nu')+C^{A}(M_A,\omega,\nu)C^{A^*}(M_A,\omega',\nu').\end{aligned} \tag{7.17}$$

These integrals are most easily done in the following manner. The first term can be rewritten, using Eqs. (6.3), as

$$\begin{aligned}&\int dE\, dn\, C^{C}(E,n,\omega,\nu)C^{C^*}(E,n,\omega',\nu')\Big\{\int d\lambda'\, \rho^{*}_{\lambda',B}(\nu')b^{C^*}(E,n,\lambda',\omega')\\&+\rho^{*}_{B}(\nu')b^{C^*}_{F}(E,n,M_B,\omega')\Big\}\\&=\int dE\, dn\Big\{\int d\lambda\, \rho_{\lambda,B}(\nu)b^{C}(E,n,\lambda,\omega)+\rho_{B}(\nu)b^{C}_{F}(E,n,M_B,\omega)\Big\}.\end{aligned} \tag{7.18}$$

One then rewrites subsequent terms in Eq. (7.17) in a similar fashion as Eq. (7.18). Since the integrals are exceedingly tedious, we describe how they are done, and leave it to the interested reader to verify our results. The integrals over n are done with the help of Eq. (A15). Then, the integrals over E are done by converting them into contour integrals. When all the contour integrals are combined it is found that they add together into one large contour integral (plus the noncontributing circle at infinity), which evaluates simply to its residues. These residues exactly cancel the other pieces in the expression, leaving over one or more delta functions for the diagonal terms, and nothing for the off-diagonal ones. For convenience, the branch cuts and poles of the function $1/\gamma(z)$, where z is a complex integration variable in the contour integral, are shown in Figs. 1, 2, and 3.

One finds that the (1,1) term is $\delta(\omega-\omega')\delta(\nu-\nu')$. In doing this, one has to fix $K_A(M_A)=\sqrt{d\gamma(E)/dE|_{E=M_A}}$, which fixes the unknown normalization constant in Eqs. (5.28). One can similarly show that the (2,2) and the (3,3) terms are $\delta(\nu-\nu')$ and $\delta(\omega-\omega')$, respectively.

For the off-diagonal terms, one proceeds similarly and finds that they are all zero. Thus, our set of solutions, namely, Eqs. (6.4), (6.5), (6.6), and (6.7) is a complete orthonormal set of solutions of our model in this sector.

VIII. THE MÖLLER MATRIX AND THE COMPARISON HAMILTONIAN

The matrix (with continuous eigenvalues) of the eigenfunctions, including any discrete solutions, gives us the generalized Möller matrix by virtue of the results already demonstrated on orthonormality and completeness.[7] It is given by

$$\Omega(E,n,\omega,\nu)=(\Psi^C(E,n,\omega,\nu),\Psi^D(E,\omega,\nu),\Psi^B(E,\omega,\nu),\Psi^A(M_A,\omega,\nu)) \tag{8.1}$$

with the components

$$\begin{pmatrix} C^C(E,n,\omega,\nu) & C^D(E,\omega,\nu) & C^B(E,\omega,\nu) & C^A(M_A,\omega,\nu) \\ D^D(E,n,\nu) & D^D(E,\nu) & D^B(E,\nu) & D^A(M_A,\nu) \\ B^C(E,n,\omega) & B^D(E,\omega) & B^B(E,\omega) & B^A(M_A,\omega) \end{pmatrix}. \tag{8.2}$$

It has the properties of being unitary:

$$\Omega\Omega^\dagger=\mathbf{1}, \tag{8.3a}$$

$$\Omega^\dagger\Omega=\mathbf{1}, \tag{8.3b}$$

and of diagonalizing the full Hamiltonian H,

$$H\Omega=\Omega H_C, \tag{8.4a}$$

$$\Omega^\dagger H\Omega=H_C, \tag{8.4b}$$

where H_C is called the comparison Hamiltonian. It can be calculated in the following manner. First, we use the eigenvalue equations to write

$$H\Omega(E,n,\omega,\nu)=(E\Psi^C(E,n,\omega,\nu),E\Psi^D(E,\omega,\nu),E\Psi^B(E,\omega,\nu),M_A\Psi^A(M_A,\omega,\nu)), \tag{8.5}$$

and then act on Eq. (8.5) with $\Omega^\dagger$ from the left, and make use of the orthonormality relations to get

$$\Omega^\dagger H\Omega=\begin{pmatrix} E\,\delta(E-E')\,\delta(n-n') & 0 & 0 & 0 \\ 0 & E\,\delta(E-E') & 0 & 0 \\ 0 & 0 & E\,\delta(E-E') & 0 \\ 0 & 0 & 0 & M_A \end{pmatrix}=H_C. \tag{8.6}$$

To compare H_C with the free Hamiltonian H_0, we rewrite H_C, putting $E=n+\tau$ for the (1,1) element, $E=M_D+\tau$ for the (2,2) element, and $E=M_B+\tau$ for the (3,3) element, and similarly for E'. Thus, H_C becomes

$$\begin{pmatrix} (n+\tau)\,\delta(\tau-\tau')\,\delta(n-n') & 0 & 0 & 0 \\ 0 & (M_D+\tau)\,\delta(\tau-\tau') & 0 & 0 \\ 0 & 0 & (M_B+\tau)\,\delta(\tau-\tau') & 0 \\ 0 & 0 & 0 & M_A \end{pmatrix}. \tag{8.7}$$

The free Hamiltonian H_0 is

$$\begin{pmatrix} (\omega+\nu)\,\delta(\omega-\omega')\,\delta(\nu-\nu') & 0 & 0 \\ 0 & (m_D+\nu)\,\delta(\nu-\nu') & 0 \\ 0 & 0 & (m_B+\omega)\,\delta(\omega-\omega') \end{pmatrix}. \tag{8.8}$$

Comparing H_C and H_0, we see that we can identify H_C with H_0 if we include *both* mass and wave function renormalization terms in the interaction, and ignore the discrete M_A state in H_C. The mass renormalization means that we must add a quantity Δ to H_0, where Δ is

$$\Delta=\begin{pmatrix} 0 & 0 & 0 \\ 0 & (M_D-m_D)\,\delta(\nu-\nu') & 0 \\ 0 & 0 & (M_B-m_B)\,\delta(\omega-\omega') \end{pmatrix}. \tag{8.9}$$

The structure of our solutions, Eqs. (6.4), (6.5), and (6.6), immediately tells us that we must have a wave function (and consequent coupling constant) renormalization.

Thus, the fields B, C, D, θ, and ϕ have the wave function renormalizations

$$B\to\sqrt{\beta'}B=\frac{1}{\sqrt{Z_B}}\,B, \tag{8.10a}$$

$$D\to\sqrt{\alpha'}D=\frac{1}{\sqrt{Z_D}}\,D, \tag{8.10b}$$

$$C\to C, \tag{8.10c}$$

$$\theta\to\theta, \tag{8.10d}$$

$$\phi\to\phi. \tag{8.10e}$$

Because there are no proper vertex corrections, the coupling constant renormalizations reflect the wave function renormalizations[7]

$$f(\omega)\to\sqrt{Z_D}f(\omega), \tag{8.11}$$

$$g(\nu)\to\sqrt{Z_B}g(\nu). \tag{8.12}$$

Furthermore, as there are no divergences in this problem, the coupling constant and wave function renormalizations are inessential, and the mass renormalization making $H_0+\Delta$ identifiable with H_C is essential only in this sector. These renormalizations are sufficient for higher sectors as well. The only change in the higher sectors is due to the mass renormalizations which alter the continuum thresholds from m_D and m_B to M_D and M_B, respectively, but leave everything else unaffected.

Notice that while H_C and H_0 have the same structure (as long as α and β both have zeros, and γ does not), they have different spectra. Only the double continuum $0<n<E<\infty$ is coextensive; the $D\phi$ and $B\theta$ continua are renormalized downwards from m_D to M_D and from m_B to M_B, respectively. Notice also that, contrary to conventional wisdom,[1,3,12] the Möller matrix intertwines the full Hamiltonian H with H_C, *not* with H_0. However, H_C and H do have the same spectrum.

In addition, if we take the unitary transformation of H_C in reverse, we can convert the comparison Hamiltonian to the full Hamiltonian

$$\Omega H_C\Omega^{\dagger}=H, \tag{8.13}$$

and just as in the cascade model of Ref. 7, we find that *the notion of an interaction is basis dependent*.

IX. THE *S*-MATRIX

We have obtained one set of solutions to our problem, namely, Eqs. (6.4)–(6.7). We can, of course, obtain another set in which the singular operators of the form $(E-\omega-\nu+i\epsilon)^{-1}$ (which give the in states) in Eqs. (6.4)–(6.6) are changed to $(E-\omega-\nu-i\epsilon)^{-1}$ (which give the out states), while Eqs. (6.7) remain unchanged. Let us denote these solutions, and quantities associated with them, with a prime. This new set also furnishes a Möller matrix,

$$\Omega' = (\Psi^{C'}(E,n,\omega,\nu),\Psi^{D'}(E,\omega,\nu),\Psi^{B'}(E,\omega,\nu),\Psi^{A}(M_A,\omega,\nu)), \tag{9.1}$$

which satisfies the same properties as the original Möller matrix, that of unitarity:

$$\Omega'\Omega'^{\dagger} = \mathbf{1}, \tag{9.2a}$$

$$\Omega'^{\dagger}\Omega' = \mathbf{1}, \tag{9.2b}$$

and of diagonalizing H,

$$H\Omega' = \Omega' H_C, \tag{9.3a}$$

$$\Omega'^{\dagger} H \Omega' = H_C. \tag{9.3b}$$

The set of states, Eqs. (6.4)–(6.7) are such that

$$\lim_{t\to-\infty} e^{iH_C t}\, e^{-iHt}\Psi^{C}(E,n,\omega,\nu) = \begin{pmatrix} \delta(n-\omega)\,\delta(E-\omega-\nu) \\ 0 \\ 0 \end{pmatrix}, \tag{9.4a}$$

$$\lim_{t\to-\infty} e^{iH_C t}\, e^{-iHt}\Psi^{D}(E,\omega,\nu) = \begin{pmatrix} 0 \\ \sqrt{Z_\Delta}\,\delta(E-M_D-\nu) \\ 0 \end{pmatrix}, \tag{9.4b}$$

$$\lim_{t\to-\infty} e^{iH_C t}\, e^{-iHt}\Psi^{B}(E,\omega,\nu) = \begin{pmatrix} 0 \\ 0 \\ \sqrt{Z_B}\,\delta(E-M_B-\omega) \end{pmatrix}, \tag{9.4c}$$

$$\lim_{t\to-\infty} e^{iH_C t}\, e^{-iHt}\Psi^{A}(M_A,\omega,\nu) = \Psi^{A}(M_A,\omega,\nu), \tag{9.4d}$$

of which the first three are the plane wave ideal eigenstates of the comparison Hamiltonian. However, notice that there is the need for a *wave function renormalization* in $\Psi^{D}(E,\omega,\nu)$ and $\Psi^{B}(E,\omega,\nu)$, and that the *threshold is renormalized* in these two cases (i.e., $m_B\to M_B$ and $m_D\to M_D$). Clearly, these states are the in states in our problem. This is again analogous to the cascade model of Ref. 7.

For $t\to+\infty$ for these in states we have

$$\lim_{t\to+\infty} e^{iH_C t}\, e^{-iHt}\Psi^{C}(E,n,\omega,\nu)$$

$$= \begin{pmatrix} \delta(E-\omega-\nu)\left[\delta(n-\omega)\,\dfrac{\alpha^*(n)\beta^*(E-n)}{\alpha(n)\beta(E-n)} + \dfrac{2\pi i}{\gamma(E)}\,\dfrac{f(n)g(E-n)}{\alpha(n)\beta(E-n)}\,\dfrac{f^*(\omega)g^*(\nu)}{\alpha(\omega)\beta(\nu)}\right] \\ \dfrac{2\pi i}{\gamma(E)}\,\dfrac{f(n)g(E-n)}{\alpha(n)\beta(E-n)}\,Z_D\,\delta(E-M_D-\nu)\,\dfrac{g^*(\nu)}{\beta(\nu)} \\ \dfrac{2\pi i}{\gamma(E)}\,\dfrac{f(n)g(E-n)}{\alpha(n)\beta(E-n)}\,Z_B\,\delta(E-M_B-\omega)\,\dfrac{f^*(\omega)}{\alpha(\omega)} \end{pmatrix}, \tag{9.5a}$$

$$\lim_{t\to+\infty} e^{iH_C t}\, e^{-iHt}\Psi^D(E,\omega,\nu) = \begin{pmatrix} 2\pi i\,\delta(E-\omega-\nu)\,\dfrac{\sqrt{Z_D}}{\gamma(E)}\,\dfrac{g(E-M_D)}{\beta(E-M_D)}\,\dfrac{f^*(\omega)g^*(E-\omega)}{\alpha(\omega)\beta(E-\omega)} \\ \sqrt{Z_D}\,\delta(E-M_D-\nu)\left[\dfrac{\beta^*(\nu)}{\beta(\nu)} + \dfrac{2\pi i}{\gamma(E)}\,Z_D\,\dfrac{|g(\nu)|^2}{\beta(\nu)\beta(\nu)}\right] \\ \sqrt{Z_B}\,\delta(E-M_B-\omega)\,\dfrac{2\pi i}{\gamma(E)}\,Z_B\,\dfrac{|f(\omega)|^2}{\alpha(\omega)\alpha(\omega)} \end{pmatrix}, \tag{9.5b}$$

$$\lim_{t\to+\infty} e^{iH_C t}\, e^{-iHt}\Psi^B(E,\omega,\nu) = \begin{pmatrix} 2\pi i\,\delta(E-\omega-\nu)\,\dfrac{\sqrt{Z_B}}{\gamma(E)}\,\dfrac{f(E-M_B)}{\alpha(E-M_B)}\,\dfrac{f^*(\omega)g^*(E-\omega)}{\alpha(\omega)\beta(E-\omega)} \\ \sqrt{Z_D}\,\delta(E-M_D-\nu)\,\dfrac{2\pi i}{\gamma(E)}\,Z_D\,\dfrac{|g(\nu)|^2}{\beta(\nu)\beta(\nu)} \\ \sqrt{Z_B}\,\delta(E-M_B-\omega)\left[\dfrac{\alpha^*(\omega)}{\alpha(\omega)} + \dfrac{2\pi i}{\gamma(E)}\,Z_B\,\dfrac{|f(\omega)|^2}{\alpha(\omega)\alpha(\omega)}\right] \end{pmatrix}, \tag{9.5c}$$

$$\lim_{t\to+\infty} e^{iH_C t}\, e^{-iHt}\Psi^A(M_A,\omega,\nu) = \Psi^A(M_A,\omega,\nu). \tag{9.5d}$$

[The limits in Eqs. (9.4) and Eqs. (9.5) are understood for multiplication by smooth functions of ω or ν or both, as the case may be.]

The out states behave in an analogous but opposite fashion to the in states. They behave simply for $t\to+\infty$, but have a complicated structure as $t\to-\infty$. Furthermore, the in states at $t\to-\infty$ and the out states at $t\to+\infty$ are identical. Therefore, we can define an S-matrix, and can compute it in one of several ways. For example, we can compute it using

$$\Psi_{\text{scattered}} = \lim_{t\to\infty}(\Psi(t)-\Psi(-t)), \tag{9.6}$$

or we can take the scalar product of the in and out states

$$(\Psi',\Psi) = S. \tag{9.7}$$

Both methods, of course, give the same answer.

The method of the inner products is cleaner and more aesthetically satisfying so we shall follow it for the calculation. The results are easily checked by doing the calculation by the other methods.

Schematically, the S-matrix looks like (the ''+'' subscript means an in state and the ''−'' subscript means an out state)

$$S=\begin{pmatrix} -\langle\langle C\theta\phi|C\theta\phi\rangle\rangle_+ & -\langle\langle C\theta\phi|D\phi\rangle\rangle_+ & -\langle\langle C\theta\phi|B\theta\rangle\rangle_+ & -\langle\langle C\theta\phi|M_A\rangle\rangle \\ -\langle\langle D\phi|C\theta\phi\rangle\rangle_+ & -\langle\langle D\phi|D\phi\rangle\rangle_+ & -\langle\langle D\phi|B\theta\rangle\rangle_+ & -\langle\langle D\phi|M_A\rangle\rangle \\ -\langle\langle B\theta|C\theta\phi\rangle\rangle_+ & -\langle\langle B\theta|D\phi\rangle\rangle_+ & -\langle\langle B\theta|B\theta\rangle\rangle_+ & -\langle\langle B\theta|M_A\rangle\rangle \\ \langle\langle M_A|C\theta\phi\rangle\rangle_+ & \langle\langle M_A|D\phi\rangle\rangle_+ & \langle\langle M_A|B\theta\rangle\rangle_+ & \langle\langle M_A|M_A\rangle\rangle \end{pmatrix}. \quad (9.8)$$

Let us start with the (1,1) component of S. We wish to calculate

$$\begin{aligned} {}_C\langle\langle E',n',\text{out}|E,n,\text{in}\rangle\rangle_C &= \int d\omega\, d\nu\, C^{C'*}(E',n',\omega,\nu)C^C(E,n,\omega,\nu) \\ &\quad + \int d\omega\, B^{C'*}(E',n',\omega)B^C(E,n,\omega) \\ &\quad + \int d\nu\, D^{C'*}(E',n',\nu)D^C(E,n,\nu). \end{aligned} \quad (9.9)$$

We rewrite Eq. (9.9) in terms of the lower sector physical states using Eqs. (6.3) to get

$$\begin{aligned} &\int d\omega\, d\nu \Big[\int d\lambda'\, \rho'^{*}_{\lambda',B}(\nu)b^{C'*}(E',n',\lambda',\omega)+\rho'^{*}_B(\nu)b^{C'*}_F(E',n',M_B,\omega)\Big] \\ &\times\Big[\int d\lambda\, \rho_{\lambda,B}(\nu)b^C(E,n,\lambda,\omega)+\rho_B(\nu)b^C_F(E,n,M_B,\omega)\Big] \\ &+\int d\omega\Big[\int d\lambda'\, \sigma'_{\lambda',B}b^{C'*}(E',n',\lambda',\omega)+\sqrt{Z_B}b^{C'*}_F(E',n',M_B,\omega)\Big] \\ &\times\Big[\int d\lambda\, \sigma_{\lambda,B}b^C(E,n,\lambda,\omega)+\sqrt{Z_B}b^C_F(E,n,M_B,\omega)\Big]+\int d\nu\, D^{C'*}(E',n',\nu)D^C(E,n,\nu). \end{aligned} \quad (9.10)$$

Doing the integrals over λ in Eq. (9.10) we get

$$\begin{aligned} &\int d\lambda\, d\lambda'\, \frac{\beta^*(\lambda)}{\beta(\lambda)}\,\delta(\lambda-\lambda')\int d\omega\, b^{C'*}(E',n',\lambda',\omega)b^C(E,n,\lambda,\omega)+\int d\omega\, b^{C'*}_F \\ &\quad\times(E',n',M_B,\omega)b^C_F(E,n,M_B,\omega)+\int d\nu\, D^{C'*}(E',n',\nu)D^C(E,n,\nu). \end{aligned} \quad (9.11)$$

The sum of the first and second integrals gives

$$\begin{aligned} &\delta(E-E')\Big\{\delta(n-n')\,\frac{\beta^*(E-n)\alpha^*(n)}{\beta(E-n)\alpha(n)}+\frac{2\pi i}{\gamma(E)}\,\frac{g(E-n)f(n)}{\beta(E-n)\alpha(n)}\,\frac{g^*(E-n')f^*(n')}{\beta(E-n')\alpha(n')}\Big\} \\ &\quad-\delta(E'-n'-E+n)\,\frac{\beta^*(E-n)f^*(n')f(n)}{\beta(E-n)\alpha(n')\alpha(n)}+\frac{g^*(E'-n')f^*(n')g(E-n)f(n)}{\beta(E'-n')\alpha(n')\beta(E-n)\alpha(n)} \\ &\quad\times\Big\{\frac{1}{\gamma(E)\alpha(E-E'+n')}+\frac{1}{\gamma(E')\alpha(E'-E+n)}\Big\} \\ &\quad+\frac{1}{\gamma(E')\gamma(E)}\,\frac{g^*(E'-n')f^*(n')g(E-n)f(n)}{\beta(E'-n')\alpha(n')\beta(E-n)\alpha(n)} \end{aligned}$$

$$\times\left\{-\int d\lambda\left|\sigma_{\lambda,B}\right|^2\frac{1}{\alpha(E'-\lambda)\alpha(E-\lambda)}-\frac{Z_B}{\alpha(E'-M_B)\alpha(E-M_B)}\right\},\tag{9.12}$$

and the third integral gives

$$\begin{aligned}
&\delta(E'-n'-E+n)\,\frac{\beta^*(E-n)f^*(n')f(n)}{\beta(E-n)\alpha(n')\alpha(n)}-\frac{g^*(E'-n')f^*(n')g(E-n)f(n)}{\beta(E'-n')\alpha(n')\beta(E-n)\alpha(n)}\\
&\quad\times\left\{\frac{1}{\gamma(E)\alpha(E-E'+n')}+\frac{1}{\gamma(E')\alpha(E'-E+n)}\right\}+\frac{1}{\gamma(E')\gamma(E)}\\
&\quad\times\frac{g^*(E'-n')f^*(n')g(E-n)f(n)}{\beta(E'-n')\alpha(n')\beta(E-n)\alpha(n)}\left\{\frac{1}{2}\int d\mu|\sigma_{\mu,D}|^2\,\frac{1}{\beta(E-\mu)}\right.\\
&\quad\times\left(\frac{1}{\alpha^*(E'-E+\mu)}+\frac{1}{\alpha(E'-E+\mu)}\right)\\
&\quad+\frac{1}{2}\int d\mu'|\sigma_{\mu',D}|^2\,\frac{1}{\beta(E'-\mu')}\left(\frac{1}{\alpha^*(E-E'+\mu')}+\frac{1}{\alpha(E-E'+\mu')}\right)+\frac{Z_D}{2\beta(E-M_D)}\\
&\quad\times\left(\frac{1}{\alpha^*(E'-E+M_D)}+\frac{1}{\alpha(E'-E+M_D)}\right)\\
&\quad\left.+\frac{Z_D}{2\beta(E'-M_D)}\left(\frac{1}{\alpha^*(E-E'+M_D)}+\frac{1}{\alpha(E-E'+M_D)}\right)\right\}.
\end{aligned}\tag{9.13}$$

Adding Eqs. (9.12) and (9.13), and converting the sum of the integrals to contour integrals (which evaluate to their residues and cancel the other terms with them inside the curly brackets), we are left with

$$\begin{aligned}
{}_C\langle\langle E',n',\text{in}|E,n,\text{out}\rangle\rangle_C=\delta(E-E')\Big\{&\delta(n-n')\,\frac{\beta^*(E-n)\alpha^*(n)}{\beta(E-n)\alpha(n)}\\
&+\frac{2\pi i}{\gamma(E)}\,\frac{g(E-n)f(n)}{\beta(E-n)\alpha(n)}\,\frac{g^*(E-n')f^*(n')}{\beta(E-n')\alpha(n')}\Big\}.
\end{aligned}\tag{9.14}$$

In a similar fashion, we can do all the other S-matrix elements. They are

$${}_D\langle\langle E',\text{out}|E,\text{in}\rangle\rangle_D=\delta(E-E')\left\{\frac{\beta^*(E-M_D)}{\beta(E-M_D)}+\frac{2\pi iZ_D}{\gamma(E)}\,\frac{|g(E-M_D)|^2}{\beta(E-M_D)\beta(E-M_D)}\right\},\tag{9.15}$$

$${}_B\langle\langle E',\text{out}|E,\text{in}\rangle\rangle_B=\delta(E-E')\left\{\frac{\alpha^*(E-M_B)}{\alpha(E-M_B)}+\frac{2\pi iZ_B}{\gamma(E)}\,\frac{|f(E-M_B)|^2}{\alpha(E-M_B)\alpha(E-M_B)}\right\},\tag{9.16}$$

$${}_A\langle\langle M_A|M_A\rangle\rangle_A=1,\tag{9.17}$$

$${}_B\langle\langle E',\text{out}|E,\text{in}\rangle\rangle_D=2\pi i\,\delta(E'-E)\,\frac{\sqrt{Z_D}\sqrt{Z_B}}{\gamma(E)}\,\frac{f^*(E-M_B)g(E-M_D)}{\alpha(E-M_B)\beta(E-M_D)},\tag{9.18}$$

$${}_D\langle\langle E',\text{out}|E,\text{in}\rangle\rangle_B=2\pi i\,\delta(E'-E)\,\frac{\sqrt{Z_D}\sqrt{Z_B}}{\gamma(E)}\,\frac{f(E-M_B)g^*(E-M_D)}{\alpha(E-M_B)\beta(E-M_D)},\tag{9.19}$$

$$ {}_D\langle\langle E',\text{out}|E,n,\text{in}\rangle\rangle_C = 2\pi i\,\delta(E'-E)\,\frac{\sqrt{Z_D}}{\gamma(E)}\,\frac{g(n)f(E-n)}{\alpha(n)\beta(E-n)}\,\frac{g^*(E-M_D)}{\beta(E-M_D)}, \tag{9.20} $$

$$ {}_C\langle\langle E',n',\text{out}|E,\text{in}\rangle\rangle_D = 2\pi i\,\delta(E'-E)\,\frac{\sqrt{Z_D}}{\gamma(E)}\,\frac{g^*(n')f^*(E-n')}{\alpha(n')\beta(E-n')}\,\frac{g(E-M_D)}{\beta(E-M_D)}, \tag{9.21} $$

$$ {}_B\langle\langle E',\text{out}|E,n,\text{in}\rangle\rangle_C = 2\pi i\,\delta(E'-E)\,\frac{\sqrt{Z_B}}{\gamma(E)}\,\frac{g(n)f(E-n)}{\alpha(n)\beta(E-n)}\,\frac{f^*(E-M_B)}{\alpha(E-M_B)}, \tag{9.22} $$

$$ {}_C\langle\langle E',n',\text{out}|E,\text{in}\rangle\rangle_B = 2\pi i\,\delta(E'-E)\,\frac{\sqrt{Z_B}}{\gamma(E)}\,\frac{g^*(n')f^*(E-n')}{\alpha(n')\beta(E-n')}\,\frac{f(E-M_B)}{\alpha(E-M_B)}, \tag{9.23} $$

$$ {}_A\langle\langle M_A|E,n,\text{in}\rangle\rangle_C = 0, \tag{9.24} $$

$$ {}_C\langle\langle E',n',\text{out}|M_A\rangle\rangle_A = 0, \tag{9.25} $$

$$ {}_A\langle\langle M_A|E,\text{in}\rangle\rangle_D = 0, \tag{9.26} $$

$$ {}_D\langle\langle E',\text{out}|M_A\rangle\rangle_A = 0, \tag{9.27} $$

$$ {}_A\langle\langle M_A|E,\text{in}\rangle\rangle_B = 0, \tag{9.28} $$

$$ {}_B\langle\langle E',\text{out}|M_A\rangle\rangle_A = 0. \tag{9.29} $$

X. UNITARITY OF THE *S*-MATRIX

We can almost trivially show that the S-matrix that we have obtained is unitary. In equations, we wish to show that

$$ SS^\dagger = 1. \tag{10.1} $$

Let us calculate the (1,1) term in $SS^\dagger$. It is

$$ \begin{aligned} SS^\dagger_{(1,1)} = {} & \delta(E-E')\int dn''\left[\delta(n-n'')\,\frac{\beta^*(E-n)\alpha^*(n)}{\beta(E-n)\alpha(n)} + \frac{2\pi i}{\gamma(E)}\,\frac{f^*(n'')f(n)g^*(E-n'')g(E-n)}{\alpha(n'')\alpha(n)\beta(E-n'')\beta(E-n)}\right] \\ & \times\left[\delta(n'-n'')\,\frac{\beta(E-n')\alpha(n')}{\beta^*(E-n')\alpha^*(n')} - \frac{2\pi i}{\gamma^*(E)}\,\frac{f(n'')f^*(n')g(E-n'')g^*(E-n')}{\alpha^*(n'')\alpha^*(n')\beta^*(E-n'')\beta^*(E-n')}\right] \\ & - \frac{(2\pi i)^2}{|\gamma(E)|^2}\,\delta(E-E')\,\frac{f(n)g(E-n)}{\alpha(n)\beta(E-n)}\,\frac{f^*(n')g^*(E-n')}{\alpha^*(n')\beta^*(E-n')} \\ & \times\left[Z_D\,\frac{|g(E-M_D)|^2}{|\beta(E-M_D)|^2} + Z_B\,\frac{|f(E-M_B)|^2}{|\alpha(E-M_B)|^2}\right]. \end{aligned} \tag{10.2} $$

Doing the integral in Eq. (10.2) with the help of Eq. (A15) we find that the result is $\delta(E-E')\,\delta(n-n')$, exactly as desired. The rest of the terms are done in the same way. We find

$$ SS^\dagger_{(2,2)} = \delta(E-E'), \tag{10.3} $$

$$ SS^\dagger_{(3,3)} = \delta(E-E'), \tag{10.4} $$

$$SS^{\dagger}_{(4,4)}=1, \tag{10.5}$$

with all other terms in $SS^{\dagger}$ being zero, as required. Thus $SS^{\dagger}=\mathbf{1}$. In the same way, we can also show that $S^{\dagger}S=\mathbf{1}$, and therefore, our S-matrix is unitary.

XI. EIGENPHASES OF THE *S*-MATRIX

The interesting case for the S-matrix is when $E>0$ so that all channels are open. The S-matrix must satisfy

$$S\zeta=\tau\zeta, \tag{11.1}$$

where $|\tau|^2=1$, for some ζ. This is equivalent to the following relations (where we ignore the discrete A channel, as it is decoupled from everything else, and suppress $\delta(E-E')$)

$$\tau-\frac{\beta^*(E-n)\alpha(n)}{\beta(E-n)\alpha(n)}\,\zeta_n=\frac{2\pi i}{\gamma(E)}\,\frac{f(n)g(E-n)}{\alpha(n)\beta(E-n)}\left\{\int dn'\,\frac{f^*(n')g^*(E-n')}{\alpha(n')\beta(E-n')}\,\zeta_{n'}+\sqrt{Z_D}\,\frac{g^*(E-M_D)}{\beta(E-M_D)}\,\zeta_D+\sqrt{Z_B}\,\frac{f^*(E-M_B)}{\alpha(E-M_B)}\,\zeta_B\right\}, \tag{11.2a}$$

$$\tau-\frac{\beta^*(E-M_D)}{\beta(E-M_D)}\,\zeta_D=\frac{2\pi i}{\gamma(E)}\,\sqrt{Z_D}\,\frac{g(E-M_D)}{\beta(E-M_D)}\left\{\int dn'\,\frac{f^*(n')g^*(E-n')}{\alpha(n')\beta(E-n')}\,\zeta_{n'}+\sqrt{Z_D}\,\frac{g^*(E-M_D)}{\beta(E-M_D)}\,\zeta_D+\sqrt{Z_B}\,\frac{f^*(E-M_B)}{\alpha(E-M_B)}\,\zeta_B\right\}, \tag{11.2b}$$

$$\tau-\frac{\alpha^*(E-M_B)}{\alpha(E-M_D)}\,\zeta_B=\frac{2\pi i}{\gamma(E)}\,\sqrt{Z_B}\,\frac{f(E-M_B)}{\alpha(E-M_B)}\left\{\int dn'\,\frac{f^*(n')g^*(E-n')}{\alpha(n')\beta(E-n')}\,\zeta_{n'}+\sqrt{Z_D}\,\frac{g^*(E-M_D)}{\beta(E-M_D)}\,\zeta_D+\sqrt{Z_B}\,\frac{f^*(E-M_B)}{\alpha(E-M_B)}\,\zeta_B\right\}. \tag{11.2c}$$

We now define the unimodular quantities

$$\tau(n)\equiv\frac{\beta^*(E-n)\alpha^*(n)}{\beta(E-n)\alpha(n)}, \tag{11.3a}$$

$$\tau_D\equiv\frac{\beta^*(E-M_D)}{\beta(E-M_D)}, \tag{11.3b}$$

$$\tau_B\equiv\frac{\alpha^*(E-M_B)}{\alpha(E-M_B)}. \tag{11.3c}$$

These are the basic equations. We can solve them for continuum values or for discrete values of the eigenphase shifts. Let us start with the continuum values. We invert Eq. (11.2a) and put a delta function on the right-hand side along with the appropriate normalization. We then multiply both sides of the equation by

$$\frac{f^*(n)g^*(E-n)}{\alpha(n)\beta(E-n)}$$

and integrate over n to get

$$\left\{1-\frac{2\pi i}{\gamma(E)}\int\frac{|f(l)|^2|g(E-l)|^2}{|\alpha(l)|^2|\beta(E-l)|^2}\frac{\tau(l)}{\tau-\tau(l)+i\epsilon}\right\}\int dn'\,\frac{f^*(n')g^*(E-n')}{\alpha(n')\beta(E-n')}\,\zeta_{n'}$$
$$=\frac{f^*(\tau)g^*(\tau)}{\alpha(\tau)\beta(\tau)}+\frac{2\pi i}{\gamma(E)}\int\frac{|f(l)|^2|g(E-l)|^2}{|\alpha(l)|^2|\beta(E-l)|^2}\frac{\tau(l)}{\tau-\tau(l)+i\epsilon}$$
$$\times\left\{\sqrt{Z_D}\,\frac{g^*(E-M_D)}{\beta(E-M_D)}\,\zeta_D+\sqrt{Z_B}\,\frac{f^*(E-M_B)}{\alpha(E-M_B)}\,\zeta_B\right\}. \tag{11.4}$$

Defining

$$\Sigma\equiv 1-\frac{2\pi i}{\gamma(E)}\,Z_D\,\frac{|g(E-M_D)|^2}{|\beta(E-M_D)|^2}\,\frac{\sigma_D}{\sigma-\sigma_D}-\frac{2\pi i}{\gamma(E)}\,Z_B\,\frac{|f(E-M_B)|^2}{|\alpha(E-M_B)|^2}\,\frac{\sigma_B}{\sigma-\sigma_B}, \tag{11.5}$$

we invert Eqs. (11.2b) and (11.2c) to solve for the term in the curly braces on the right-hand side of Eq. (11.4), namely,

$$\sqrt{Z_D}\,\frac{g^*(E-M_D)}{\beta(E-M_D)}\,\zeta_D+\sqrt{Z_B}\,\frac{f^*(E-M_B)}{\alpha(E-M_B)}\,\zeta_B,$$

and find

$$\sqrt{Z_D}\,\frac{g^*(E-M_D)}{\beta(E-M_D)}\,\zeta_D+\sqrt{Z_B}\,\frac{f^*(E-M_B)}{\alpha(E-M_B)}\,\zeta_B=\left(\frac{1}{\Sigma}-1\right)\int dn'\,\frac{f^*(n')g^*(E-n')}{\alpha(n')\beta(E-n')}\,\zeta_{n'}. \tag{11.6}$$

We now define

$$\chi(\tau)=1-\frac{2\pi i}{\gamma(E)\Sigma}\int dl\,\frac{|f(l)|^2|g(E-l)|^2}{|\alpha(l)|^2|\beta(E-l)|^2}\,\frac{\tau(l)}{\tau-\tau(l)+i\epsilon}, \tag{11.7}$$

and use this to combine Eqs. (11.4) and (11.6), and find

$$\int dn'\,\frac{f^*(n')g^*(E-n')}{\alpha(n')\beta(E-n')}\,\zeta_{n'}+\sqrt{Z_D}\,\frac{g^*(E-M_D)}{\beta(E-M_D)}\,\zeta_D+\sqrt{Z_B}\,\frac{f^*(E-M_B)}{\alpha(E-M_B)}\,\zeta_B$$
$$=\frac{1}{\chi(\tau)\Sigma}\,\frac{f^*(\tau)g^*(\tau)}{\alpha(\tau)\beta(E-\tau)}. \tag{11.8}$$

Therefore, our continuum solutions are

$$\zeta_n=\sqrt{\tau'}\,\delta(\tau-\tau(n))+\frac{2\pi i}{\gamma(E)}\,\frac{f(n)g(E-n)}{\alpha(n)\beta(E-n)}\,\frac{1}{(\tau-\tau(n)+i\epsilon)\chi(\tau)\Sigma}\,\frac{f^*(\tau)g^*(E-\tau)}{\alpha(\tau)\beta(E-\tau)}, \tag{11.9a}$$

$$\zeta_D=\frac{2\pi i}{\gamma(E)}\,\sqrt{Z_D}\,\frac{g(E-M_D)}{\beta(E-M_D)}\,\frac{1}{(\tau-\tau_D+i\epsilon)\chi(\tau)\Sigma}\,\frac{f^*(\tau)g^*(E-\tau)}{\alpha(\tau)\beta(E-\tau)}, \tag{11.9b}$$

$$\zeta_B=\frac{2\pi i}{\gamma(E)}\,\sqrt{Z_B}\,\frac{f(E-M_B)}{\alpha(E-M_B)}\,\frac{1}{(\tau-\tau_B+i\epsilon)\chi(\tau)\Sigma}\,\frac{f^*(\tau)g^*(E-\tau)}{\alpha(\tau)\beta(E-\tau)}. \tag{11.9c}$$

To investigate the spectrum of τ, we use the method of Ref. 7. We define the following quantities, taking advantage of their being unimodular:

$$e^{2i\theta(n)} \equiv \tau(n), \tag{11.10a}$$

$$e^{2i\theta_D} \equiv \tau_D, \tag{11.10b}$$

$$e^{2i\theta_B} \equiv \tau_B, \tag{11.10c}$$

$$e^{2i\delta} \equiv \tau. \tag{11.10d}$$

We then put these definitions in Eqs. (11.9), and see that $\tau(n)=e^{2i\theta(n)}$ ranges continuously along a unit circle in the complex plane from $\theta=\theta(0)$ to $\theta=\theta(E)$.

In addition, these solutions are continuum normalized:

$$\int dn\ \zeta_n(\tau'-i\epsilon)\zeta_n(\tau+i\epsilon)+\zeta_D(\tau'-i\epsilon)\zeta_D(\tau+i\epsilon)+\zeta_B(\tau'-i\epsilon)\zeta_B(\tau+i\epsilon)=\delta(\tau'-\tau), \tag{11.11}$$

and will be complete if there are no discrete zeros of $\chi(\tau)$. If there are, they will have to be included in the completeness identity. We now find the number of discrete zeros of $\chi(\tau)$, i.e., the number of discrete eigenphase shifts of our S-matrix.

We define

$$\tau \equiv \frac{1+ix}{1-ix}, \qquad \tau(n) \equiv \frac{1+ix(n)}{1-ix(n)},$$
$$\tau_D \equiv \frac{1+ix_D}{1-ix_D}, \qquad \tau_B \equiv \frac{1+ix_B}{1-ix_B},$$

put these in Eq. (11.7), and take real and imaginary parts to get

$$-\frac{1}{2}\int dl\ \frac{|f(l)|^2|g(E-l)|^2}{|\alpha(l)|^2|\beta(E-l)|^2}\frac{x(1+x(l))}{x-x(l)+i\epsilon}=\mathrm{Im}\left(\frac{\gamma(E)}{2\pi i}\right)-\frac{1}{2}\frac{x(1+x_D)}{x-x_D}Z_D\frac{|g(E-M_D)|^2}{|\beta(E-M_D)|^2}$$
$$-\frac{1}{2}\frac{x(1+x_B)}{x-x_B}Z_B\frac{|f(E-M_B)|^2}{|\alpha(E-M_B)|^2}, \tag{11.12a}$$

$$-\frac{1}{2}\int dl\ \frac{|f(l)|^2|g(E-l)|^2}{|\alpha(l)|^2|\beta(E-l)|^2}=\mathrm{Re}\left(\frac{\gamma(E)}{2\pi i}\right)-\frac{1}{2}Z_D\frac{|g(E-M_D)|^2}{|\beta(E-M_D)|^2}-\frac{1}{2}Z_B\frac{|f(E-M_B)|^2}{|\alpha(E-M_B)|^2}. \tag{11.12b}$$

We observe that Eq. (11.12b) is an identity, by means of Eq. (A15). To find the number of zeros of $\chi(\tau)$, we multiply both sides of Eq. (11.12a) by $(x-x_D)(x-x_B)$. We then find that the highest power of x appearing in Eq. (11.12a) is x^3, barring any higher powers contributed by the integral. Therefore, there are at least three discrete zeros of $\chi(\tau)$, and thus, at least three discrete solutions which will have to be included in the completeness identity, Eq. (11.11).

XII. A GENERAL FORMALISM FOR SCATTERING THEORY

In this section, we describe an approach due to Sudarshan and collaborators,[19–25] which takes a very different view of scattering problems, and is quite different in spirit. It is essentially immune to many of the problems that occur in the conventional approaches in the literature. The idea is that one always works with the complete set of eigenstates of the full Hamiltonian H properly labeled. This set, by definition, is both orthonormal and complete. The matrix made up of these eigenstates is the Möller matrix. This Möller matrix, again by definition, will diagonalize the full Hamiltonian giving the comparison Hamiltonian.

In other words, we have a Hamiltonian for the system H. We wish a physical interpretation of this object as a scattering system. One starts by considering the complete set of states for H, which we denote as $\psi_\alpha(E)$, where E is the energy of the eigenstate, and α contains everything else necessary to uniquely specify the state such as spin, channel, etc. Then,

$$H\psi_\alpha(E)=E_\alpha\psi_\alpha(E). \tag{12.1}$$

Form the generalized Möller matrix W, by defining

$$W_{E,\alpha}\equiv\psi_\alpha(E).$$

Therefore,

$$HW=WH_C, \tag{12.2}$$

where the implied integration is of the Stielje type—i.e., we sum over any discrete indices, and integrate over any continuous ones. Because we have assumed that the set of eigenstates of H is complete, this Möller matrix has the property that

$$\Omega\Omega^\dagger=\mathbf{1}, \quad \Omega^\dagger\Omega=\mathbf{1}. \tag{12.3}$$

It is thus isometric and unitary, as long as we ensure that the spectra of H and H_C are the same, and the spectrum multiplicity is properly preserved. The only caveat here is that not all formally Hermitian Hamiltonians have a complete set of eigenstates. However, all ''reasonable'' Hamiltonians will have a such complete set.

Now, one normally wants an interpretation of a scattering system in terms of asymptotic states. The point here is that, to get such an interpretation, we should use H_C, not H_0. We must set up a correspondence between the set of eigenstates of H_C with H, because unlike H_0, we are guaranteed that H and H_C are isospectral. Any asymptotic conditions (such as the strong convergence properties of Eqs. (2.26)) should be expressed using H_C, not H_0. Thus, it is H_C, not H_0, which is the proper starting point for any perturbative scheme. Furthermore, as indicated by our model, we should endeavor to construct a perturbative scheme to calculate the full states, not the asymptotic ones, because we cannot say, with any confidence, what the appropriate conditions are on the asymptotic states (see Sec. XIII for details). In addition, note another advantage of this formalism. Any, and all, shifts in the thresholds and spectrum of H (such as a mass renormalization) are automatically taken care of by this procedure.

Finally, it is worth remarking that, in general, W and H_C are not going to be analytic in the coupling constants. Therefore, the procedure that one occasionally sees in the literature of splitting H into H_C+V' is not very useful, and not very constructive. Both H_C and V' will be complicated functions of the coupling constants, and will have all sorts of renormalization factors appearing.

If we are interested in working perturbatively, then we must set up the system carefully. We give here an analysis of Sudarshan.[26] Consider a quantum system defined in a Hilbert space $\mathscr{H}$ with the Hamiltonian split in the usual way:

$$H=H_0+V, \tag{12.4}$$

in which we already know the ideal eigenstates for the continuum, and the proper eigenvectors for the discrete states. The ideal states are, of course, not normalizable and we must take proper linear combinations of them to get states that are square integrable, and in $\mathscr{H}$. Then, we set up a correspondence between eigenstates of H and eigenstates of H_0, in such a manner that

$$H\psi_\lambda=\lambda\psi_\lambda, \tag{12.5a}$$

$$H_0\psi_{0\lambda}=\lambda\psi_{0\lambda}\,. \tag{12.5b}$$

Therefore,

$$(1-G_0(\lambda)V)\psi_\lambda=\psi_{0\lambda}\,, \tag{12.6a}$$

$$G_0(\lambda)(\lambda-H_0)=\mathbf{1}, \tag{12.6b}$$

where G_0 is the free Green function. From this we can write

$$\psi_\lambda=(1-G_0(\lambda)V)^{-1}\psi_{0\lambda}\,, \tag{12.7}$$

thus defining for us a possible Möller matrix Ω' given by

$$\Omega'=(1-G_0V)^{-1}. \tag{12.8}$$

Now this Ω' is a possible Möller matrix in the sense that it intertwines H and H_0:

$$H\Omega'=\omega' H_0\,. \tag{12.9}$$

Unfortunately, it is not very useful because it is not necessarily unitary, or even isometric. One must renormalize it correctly so as to get a unitary operator. Furthermore, H and H_0 are not isospectral. Consider the full Green function $\mathcal{G}(\lambda)$:

$$\mathcal{G}(\lambda)=\frac{1}{\lambda-H+i\epsilon}=(1-G_0(\lambda)V)^{-1}G_0(\lambda). \tag{12.10}$$

While, at first glance, it would seem that G_0 and $\mathcal{G}$ have the same singularities, this is not necessarily true. First, $\mathcal{G}$ can have additional singularities from the first factor $(1-G_0(\lambda)V)^{-1}$ in Eq. (12.10). These can come from bound states produced by the interaction, and more importantly, from continuum states in which one or more of the particles is composite so that its mass gets shifted. Second, $\mathcal{G}$ can have some of its singularities cancelled when this factor vanishes. Therefore, $\mathcal{G}$ and G_0 are not necessarily isospectral, in general. In other words, the statement that ''perturbations vanish at infinity'' is not valid generally. Rather, this näive asymptotic condition is not generally fulfilled. This shows us why Ω' failed to be unitary: the new spectra produced by $(1-G_0(\lambda)V)^{-1}$ do not appear with a canonical weight. As advertised, we correct this problem by defining a renormalized Ω given by

$$\Omega=(1-G_0V)^{-1}D^{-1}, \tag{12.11a}$$

where

$$D^2=(1-VG_0^+)^{-1}(1-G_0V)^{-1}. \tag{12.11b}$$

However, since this new Ω is unitary, it connects H with an isospectral and diagonal Hamiltonian. We have already seen that this associated diagonal Hamiltonian cannot be H_0. Rather, it is a different object, which we call the comparison Hamiltonian H_C. For further details, and concrete examples of this formalism applied to several models, such as the Lee model, the separable potential model, and the Cascade model, see Ref. 26. In these models, one can explicitly see these various effects such as shifts in the continuous spectra, the deletion of spectra from H_0 to get the spectra of H, and the augmentation of spectra in H_0 to get the spectra of H.

XIII. PUTTING THE "GENERIC" FORMALISMS TO THE TEST

There are many different approaches to quantum scattering in the literature. The most familiar of these is potential scattering. Others include the LSZ formalism, the "almost local" formalism, and the Lax–Phillips formalism. Lax–Phillips[27] theory is outside the scope of this work.

The well-known LSZ formalism,[5] extended by Mohan,[28] postulates the convergence of the matrix elements of interacting fields to the matrix elements of free fields. However, the formalism does not apply in many cases. For example, as noted by LSZ themselves, it is inapplicable to problems in which stable bound states exist. Trouble occurs when this point is forgotten, and the formalism is extended into areas where it is inapplicable. The "almost local" formalism due to Haag,[1] Ruelle,[9] Ekstein,[10] Jauch,[12] Araki,[29] and others tries to be general enough to consider complicated problems.[1] Its basic idea is that it is possible to construct asymptotic ingoing and outgoing states as strong limits in Hilbert space, if a certain "spacelike asymptotic condition" is verified by the vacuum expectation values of products of field operators:[9] the so called almost local operators.[1]

We shall restrict our attention to the conventional, and quite "generic" formalism, as reviewed earlier in Secs. II and III; as mentioned before, the LSZ formalism is *not applicable* to situations where stable bound states are present, such as our model. We will compare these results to the results obtained from the rearrangement model.

Conventional formalisms for quantum scattering theory have the following protocol for generic scattering systems:

(1) They do not use the comparison Hamiltonian.
(2) The asymptotic states are orthonormal.[1,9,13]
(3) The completeness of the asymptotic states is postulated.[1,13]
(4) For the case of potential scattering only, the Möller matrix is isometric but not necessarily unitary.[1,13]
(5) The eigenstates of the exact Hamiltonian are never considered.

We shall take up these points one by one, and put them to the test by comparing them to the results explicitly obtained from our model.

(1) It is essential when taking the limits $\lim_{t\to\pm\infty} e^{iHt}\, e^{-iH_0 t}\Psi$, where Ψ is either a wave function or a field operator, that the continuous spectra of H and H_0 coincide. If they did not there would be wild oscillations while taking the limit, and the limit would not exist. It is for this purpose that H_0 is mass-renormalized to H_0'. However, in general, this is still not enough. It is perfectly possible, if there are bound states or unstable particles in the spectrum of H, that no amount of tinkering with H_0 will make its spectrum coincide with H. This can be seen by inspection of Eqs. (8.7) and (8.8). No amount of renormalization of H_0 can give us the discrete M_A state present in H_C, but this may be ignored because M_A is a discrete point eigenvalue. On the other hand, we do have the possibility of a continuous spectrum in H corresponding to the scattering states involving physical B or D particles.

However, unlike H and H_0, H and H_C are guaranteed to be isospectral because H_C is obtained by diagonalizing H. Therefore, it is H_C, and not H_0, that is the proper starting point for any scattering scheme, perturbative or otherwise. The method for obtaining the correct spectrum of H by perturbation theory is discussed in the work of Sudarshan, Chiu, and Bhamathi.[30] In simple cases such as when stable bound states are not present, or field theory with no bound states or unstable particles, H_C can be identified with the renormalized H_0, as noted in Sec. VIII.

In fact, even in cases where (formally) no splitting is made, i.e., no explicit mention or use is made of an H_0, there is still the implicit use of H_0 because, commonly, asymptotic particles are defined as solutions of free particle equations like the Klein–Gordon equation.

(2) Both formalisms assert the orthonormality of the asymptotic states, and the result is supposed to be generic. In Eqs. (9.4), we have obtained the asymptotic states of the rearrangement

model according to both formalisms. Yet, as we can see from a glance at the Haag–Ruelle asymptotic wave functions, Eqs. (9.4), the asymptotic states computed according to their rules do not form an orthonormal set. This point should not cause confusion. Our full states, namely, Eqs. (6.4), (6.5), (6.6), and (6.7) are, indeed, all orthonormal to each other, as was shown in Sec. VII. As a result, we have orthonormal sets of in and out states. However, when we calculate the Haag–Ruelle-type asymptotic states according to either of the formalisms, we find that they are not orthonormal. This lack of orthonormality stems from a factor of the wave function renormalization constant that appears in each of the asymptotic wave functions. This factor is essential: if it were not present, the interacting states would not be orthonormal.

(3) As mentioned earlier, Ruelle extends Haag's work by postulating the completeness of the in and out states.[9] This is also postulated in simple potential scattering.[13] This postulate is necessary to prove that the S-matrix is unitary. Again, simply by inspection of Eqs. (9.4), we can see that the asymptotic states of the rearrangement model, according to these two formalisms, are not complete. Again, this point should not cause confusion. Our full states, Eqs. (6.4), (6.5), (6.6), and (6.7) are complete, as was shown in Sec. VII. As a result, our in and out states form complete sets. However, the set of Haag–Ruelle-type asymptotic states calculated according to either of the two formalisms is *not* complete.

(4) In potential scattering the Möller matrix Ω can be defined using the full interacting wave functions so that it is isometric even in the presence of bound states.[1] We see that the Haag–Ruelle asymptotic solutions, Eqs. (9.4), obtained by the use of Ω, are certainly not orthonormal, whereas the original interacting wave functions were; therefore, the Möller matrix computed by their rules is not isometric, i.e., it is not norm preserving. However, the generalized Möller matrix that we defined in Eq. (8.1) is not only isometric, but unitary.

(5) It is important to note that even though these asymptotic wave functions are neither orthonormal nor complete, they still lead to the correct S-matrix, as can be verified by calculating it using Eq. (9.6). If we had insisted upon the asymptotic wave functions being orthonormal and complete, we would have gotten the wrong S-matrix.

(6) Notice that because of this lack of orthonormality and completeness in the exact asymptotic states, the strong limits of Eqs. (2.26) are satisfied. Namely,

$$\lim_{t\to-\infty}[\Psi(t)-\psi_{\text{in}}(t)]\Rightarrow 0, \tag{13.1a}$$

$$\lim_{t\to+\infty}[\Psi(t)-\psi_{\text{out}}(t)]\Rightarrow 0, \tag{13.1b}$$

$$\lim_{t\to-\infty}\psi_{\text{in}}(0)\Rightarrow\Psi(0)\equiv\Omega^{(+)}\psi_{\text{in}}(0) \tag{13.1c}$$

are automatically satisfied. This can be seen easily in the following way. For the first two equations above, the expression on the left-hand side is just the requisite full wave function, but with the delta function part removed. When we now take the norm and then take the limit, the remainder cancels giving zero. Similarly, the third equation above can be shown to be satisfied.

On the other hand, if we had insisted that the asymptotic states *are* orthonormal and complete, the wave function renormalization constants would have been missing from the asymptotic states. Thus, the delta function pieces would not have cancelled between the full and asymptotic states, and therefore, these pieces would contribute, and we would get a nonzero result. Thus, in this case, the strong limit would not hold.

(7) It is important to note that the reason that all these problems occur is that the full states are never considered. Most formalisms in the literature try to set up the problem in terms of the

asymptotic states, and are thus forced to make assumptions regarding their properties and behavior. These assumptions are not necessarily correct in general, as is amply demonstrated by the rearrangement model, and other models such as the cascade model.[7]

All this points out the importance of the correct normalization of the state vectors, a point already considered by DeWitt.[31] However, his work was restricted to the case of no bound states. The question of the correct description of the asymptotic states was also considered by Van Hove in his papers on the description of ''persistent interactions.''[4] However, as noted in those papers, the formalism developed there does not deal with cases involving bound states, and does not deal with field theoretic scattering except for a few comments at the end.

In the multichannel case (such as rearrangement collisions), in the ''channel Hamiltonian'' formalism, the statement is made that the basis states of one group of channels are not orthogonal to the others[10,11,13] because they are eigenstates of different free Hamiltonians. As we can see, in our model, the physical states $C\theta\phi$, $D\phi$, and $B\theta$ are strictly orthogonal to each other. Evidently, this problem arises due to the use of ''channel Hamiltonians'' in the formalism. It is our belief that the method of splitting up the interaction differently depending on which channel one is considering is fundamentally flawed because ''every channel can be distinguished and is observable independently in experiments. This means that these channels should be orthogonal to each other.''[32] One method for ensuring orthonormality is given in Ref. 32; however, this method still suffers from the flaws pointed out above.

It is straightforward to see the problems caused by this lack of orthogonality. We are instructed, in these formalisms, to begin with asymptotic states. Let us first consider the channel Hamiltonian formalism. Then, the asymptotic states are the eigenstates of the channel Hamiltonian in the sector we are considering. As an example, let us consider

$$|M_B\theta(\omega)\rangle\rangle \rightarrow |M_D\phi(\nu)\rangle\rangle, \tag{13.2}$$

where M_B is the physical B particle and M_D is the physical D particle. We immediately notice, even before we consider any scattering, that the $|M_B\theta(\omega)\rangle\rangle$ state is not orthogonal to the $|M_D\phi(\nu)\rangle\rangle$ state, as can be seen by inspection of Eqs. (5.10), (5.11), (5.12), (5.13), and (5.14). In other words, two experimentally distinct channels are not orthogonal to each other. This will clearly lead to the wrong S-matrix elements because it says that even if there is no scattering, there is a nonzero probability that the $|M_B\theta(\omega)\rangle\rangle$ state will turn into the $|M_D\phi(\nu)\rangle\rangle$ state. We cannot even argue that the two states are ''asymptotically orthonormal''[10] because they clearly are not. This can easily be seen by observing that both $|M_B\theta(\omega)\rangle\rangle$ and $|M_D\phi(\nu)\rangle\rangle$ have expansion coefficients in the ''bare'' $|C\theta(\omega)\phi(\nu)\rangle$ sector. Therefore, as these states are neither orthonormal nor complete, we cannot have an isometric or unitary S-matrix, since orthonormality is necessary for isometry, and completeness for unitarity. However, we have constructed a set of orthonormal (and complete) solutions for our system, a feat that many authors[33] tacitly assume is not possible, and have a perfectly isometric and unitary S-matrix.

These problems with the S-matrix can be verified by explicit calculation. Since the calculation is tedious, we describe the method, and leave it to the interested reader to verify the results. Our interest is in the scattering of physical states, and so we must start by reexpressing the Hamiltonian, Eqs. (4.3) and (4.4), in terms of the operators which create the *physical* B and D particles. We denote these operators by $\mathscr{B}$ and $\mathscr{D}$, respectively. They are found by inspection of Eqs. (5.10), (5.11), (5.12), (5.13), and (5.14), which are the wave functions for the physical particles. To find the expressions for these operators, we promote the states $|C\phi(\nu)\rangle$, $|C\theta(\omega)\rangle$, $|B\rangle$, and $|D\rangle$ to operators, all acting on the vacuum, and read off the expansions for the operators $\mathscr{B}$ and $\mathscr{D}$. In other words,

$$\mathscr{B}^\dagger = \int d\nu\ \rho_B(\nu) C^\dagger \phi^\dagger(\nu) + \sqrt{Z_B} B^\dagger, \tag{13.3a}$$

$$\mathscr{D}^\dagger = \int d\omega\ \rho_D(\omega) C^\dagger \theta^\dagger(\omega) + \sqrt{Z_D} D^\dagger. \tag{13.3b}$$

We reexpress the Hamiltonian in terms of these operators, which can be split into various channel Hamiltonians, from which the S-matrix is calculated.

We can go even further than this. Consider the state $|M_B\theta(\omega)\rangle\rangle$, which is a product state of the physical B particle and a free θ particle. If we wanted the asymptotic state corresponding to this then, by the Haag–Ruelle protocol, we should find that the components of this state are only in the $|C\theta\phi\rangle$ and $|B\theta\rangle$ sectors, with no admixture of the $|D\phi\rangle$ state. However, we can use our exact solutions to calculate this asymptotic state. We will find that this assertion will not hold true.

To calculate the asymptotic state, we take the limit

$$\lim_{t\to-\infty} e^{iH_C t}\, e^{-iHt} |M_B\theta(\omega)\rangle\rangle. \tag{13.4}$$

Inserting a complete set of states, we have

$$\begin{aligned}
&\int dE\ dn \lim_{t\to-\infty} e^{iH_C t}\, e^{-iHt} |E,n\rangle\rangle\langle\langle E,n|M_B\theta(\omega)\rangle\rangle \\
&\quad + \int dE\ dn \lim_{t\to-\infty} e^{iH_C t}\, e^{-iHt} |E\rangle\rangle_D{}^D\langle\langle E|M_B\theta(\omega)\rangle\rangle \\
&\quad + \int dE\ dn \lim_{t\to-\infty} e^{iH_C t}\, e^{-iHt} |E\rangle\rangle_B{}^B\langle\langle E|M_B\theta(\omega)\rangle\rangle.
\end{aligned} \tag{13.5}$$

Expanding each of the physical states, $|E,n\rangle\rangle$, $|E\rangle\rangle_D$, and $|E\rangle\rangle_B$ in terms of the bare states $|C\theta(\omega)\phi(\nu)\rangle$, $|B\theta(\omega)\rangle$, and $|D\phi(\nu)\rangle$, and taking the limit, it is immediately obvious that the expansion coefficients in the $|D\phi(\nu)\rangle$ sector are not zero.

As a physical example, consider the case of a proton bound to a fixed nucleus by a potential V_P, and bombarded by a neutron which interacts with the proton and the nucleus through the potentials V_{PN} and V_N, respectively.[32] The total Hamiltonian of the system is

$$H = K_P + K_N + V_P + V_N + V_{PN}, \tag{13.6}$$

where K_P and K_N are the kinetic energy of the proton and the neutron, respectively. The initial state, denoted by $\Phi_{1,i}$, is given by

$$H_1 \Phi_{1,i} = E_i \Phi_{1,i}, \tag{13.7}$$

where

$$H = H_1 + V_1, \tag{13.8a}$$

$$H_1 = K_P + K_N + V_P, \tag{13.8b}$$

$$V_1 = V_{PN} + V_N. \tag{13.8c}$$

Therefore, the initial state $\Phi_{1,i}$ is a product of a bound proton, $\phi_P^B(E_i^B)$, and of a free neutron (represented by a plane wave), $u_N(E_i - E_i^B)$, where E_i^B is the binding energy of the proton.

Several possible reactions can occur giving rise to different final products. Let us consider four such reactions.

(1) Elastic or inelastic collisions. The proton remains bound to the nucleus, and the neutron is free after the collision. Therefore, the Hamiltonian is divided in the same manner as above.

(2) Exchange scattering. The neutron knocks out the bound proton and becomes bound to the nucleus. The Hamiltonian is then divided as

$$H = H_2 + V_2, \tag{13.9a}$$

$$H_2 = K_P + K_N + V_N, \tag{13.9b}$$

$$V_2 = V_{PN} + V_P. \tag{13.9c}$$

Therefore, the final state is

$$H_2 \Phi_{2,f} = E_f \Phi_{2,f}, \tag{13.10a}$$

$$\Phi_{2,f} = u_P(E_f - E_f^B)\,\phi_N^B(E_f^B). \tag{13.10b}$$

(3) Ionization. The neutron knocks out the bound proton and both are free after the collision. The Hamiltonian is then divided as

$$H = H_3 + V_3, \tag{13.11a}$$

$$H_3 = K_P + K_N, \tag{13.11b}$$

$$V_3 = V_{PN} + V_P + V_N. \tag{13.11c}$$

Therefore, the final state is

$$H_3 \Phi_{3,f} = E_f \Phi_{3,f}, \tag{13.12a}$$

$$\Phi_{3,f} = u_P(E_f^P)\,u_N(E_f - E_f^P). \tag{13.12b}$$

(4) Pickup. The proton and the neutron become bound and form a deuteron. The Hamiltonian is then divided as

$$H = H_4 + V_4, \tag{13.13a}$$

$$H_4 = K_P + K_N + V_{PN}, \tag{13.13b}$$

$$V_4 = V_P + V_N. \tag{13.13c}$$

Therefore, the final state is

$$H_4 \Phi_{4,f} = E_f \Phi_{4,f}, \tag{13.14a}$$

$$\Phi_{4,f} = u_c(X, E_f - E_f^B)\,\phi_{PN}^B(r, E_f^B). \tag{13.14b}$$

Here, X is the center of mass coordinate of the deuteron, and r is the internal coordinate of the deuteron.

The final states given by Eqs. (13.10), (13.12), and (13.14), are eigenstates of different free Hamiltonians. Thus, in general, they are not orthogonal to each other, and the concomitant problems follow.

The reason that these methods do not work properly is that the basis used is one in which bound-state eigenfunctions of the Hamiltonians that bind each fragment are multiplied by plane

TABLE I. Comparison of the properties of the rearrangement model to various scattering formalisms.

Property	Conventional formalism	Rearrangement model
Asymptotic states normalized?	Yes	No
Asymptotic states orthogonal?	Yes	Yes
Asymptotic states complete?	Yes	No
Ω isometric?	Yes	No
S-matrix unitary?	Yes	Yes
Strong limit satisfied?	No	Yes
H_C used?	No	Yes
Additional property for the multiple channel case		
Physical states orthogonal	No	No Yes

waves for the fragment motion.[13] In our model, because we have made no breakup, we get the physically reasonable result that the wave functions of the bound states are always orthogonal to the scattering states, and that the basis states of different channels are explicitly orthogonal to each other. We do not have to worry about making the explicit assumption that as the separation between the fragments goes to infinity, the overlap becomes negligible. This assumption may or may not be true, and leads to the problems with ''persistent interactions'' considered by Van Hove.[4]

We compare the results from the conventional formalism with those from the rearrangement model in Table I.

In addition, even when it is not stated explicitly in the literature, it is often assumed that the spectra of the bound states and the scattering (continuum) states do not overlap. However, it is possible to construct models in which the spectra of one or more bound states overlap with the continuum.[34,35] Therefore, this assumption is not necessarily true, and will in general depend upon the details of the model under consideration. It is also possible to construct two different potentials which can lead to the same S-matrix with, in one case, redundant poles unnecessary for completeness, and in the other case, with the same poles being absolutely necessary for completeness.[36,37] This points out the need for resisting the temptation to identify the poles of the S-matrix with physical bound states of the system.

More importantly, no authors have as yet worried about the evident normalization problem with the asymptotic states because they are always assumed to be normalized. These states are not normalized in the rearrangement model, and consequently, assuming orthonormality of the asymptotic states, in general, is very dangerous. In addition, we notice that in this model even though the asymptotic states are not normalized, the interacting states are.

One approach that tries to avoid all these problems, especially in the cases of unstable particles and bound states, is that of analytic continuation[7,19,23,24,38,39] of the state space $\mathscr{H}$ into a generalized vector space $\mathscr{G}$. This has already been done for the case of the Lee model by Sudarshan, Chiu, and Gorini,[19] Parravicini, Gorini, and Sudarshan,[20] and Böhm.[40] For instance, with this method, one can identify resonances and redundant poles, and study the decay of a metastable quantum system. It can also be used for many other things, such as studying the Khalfin observation that the decay of a metastable system with an energy spectrum bounded from below can never be strictly exponential.[41] See the above references for details.

XIV. SUMMARY AND CONCLUSION

In this work, we constructed a model that allows rearrangement collisions. We explored the spectra and the complete set of orthonormal (ideal) eigenfunctions of this rearrangement model in the rearrangement sector. Because of the structure of the effective Hamiltonian in this sector, we were able to solve the model exactly. In a similar fashion as for the cascade model,[7] we find that

the spectra can be interpreted as a B particle with energy $M_B<0$ coupled to a θ particle with energy ω, $0<\omega<\infty$; a D particle with energy $M_D<0$ coupled to a θ particle with energy ν, $0<\nu<\infty$; and a C particle of energy 0 coupled to θ and ϕ particles with energies ω and ν, $0<\omega,\nu<\infty$. We see that the interacting field theory has a particle interpretation.

Both the B and the D particles suffer mass renormalizations, and these mass renormalizations alter the threshold of the $B\theta$ and $D\phi$ continua, respectively. In Eqs. (6.5b) and (6.6c), we also see the presence of both the mass and wave function renormalizations of the B and D particles in the plane wave parts of their respective wave functions.

We have throughout emphasized the importance of using the comparison Hamiltonian (the diagonalized form of the effective Hamiltonian) because it is isospectral with the full Hamiltonian. Its spectrum differs from that of the free Hamiltonian by the alteration of the $B\theta$ and $D\phi$ continua, and by the addition of a discrete A state. These effects are nonperturbative and, as emphasized in Ref. 7, can only be handled by a renormalized perturbation scheme in which H_C, not H_0, is taken as the starting point.

Our results are surprising when compared to what we would expect from conventional scattering theory. We find that while the interacting state vectors are normalized, the asymptotic states are not. Moreover, the asymptotic states are neither orthonormal nor complete because of the presence of the wave function renormalization factors in the physical $D\phi$ and $B\theta$ sectors. We note that this lack of orthonormality and completeness is absolutely necessary. If we construct the S-matrix from these states, we get the correct result (i.e., it is the same S-matrix as the one constructed from the full state). On the other hand, if we did not allow the wave function renormalization factors because of our demand that the asymptotic states be orthonormal and complete, we would get the wrong S-matrix. Furthermore, for the strong limits [Eqs. (2.26)] to hold, we must again make sure to have these nonorthonormal and noncomplete states. We also find that our physical $C\theta\phi$, $D\phi$, and $B\theta$ states, while being the basis states for different channels, are strictly orthogonal to each other. Further, the Möller matrix, as defined in the literature is not isometric: it does not preserve the norm of the states. However, we defined a generalized Möller matrix which is not only isometric, but unitary. All these results are contrary to the usual formalisms of quantum scattering theory.

More generally, we argued that the correct procedure, for any Hamiltonian H, is to take its complete set of eigenstates, and an associated isospectral comparison Hamiltonian, H_C. The matrix of normalized eigenfunctions of H constitutes the generalized Möller matrix, which is unitary and intertwines H and H_C.

This model is a very simple one. However, even this simple model is enough to show the problems with conventional perturbation theory, and the conventional formulations of scattering theory. It is clearly necessary in the light of this model, and previous work on the existence of redundant poles in the scattering amplitude[36,37] and the presence of discrete solutions degenerate in energy with the scattering continuum,[34,35] that a fundamental reexamination be made of some of the postulates and assumptions of conventional quantum scattering theory.

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APPENDIX: SOME USEFUL FORMULAS

The following formulas are very useful for the calculations in the main text. By our definitions in Sec. VI we have the following ranges for our variables:

$$0\leqslant\lambda\leqslant\infty, \tag{A1}$$

$$0\leqslant\mu\leqslant\infty, \tag{A2}$$

$$0 \leqslant n \leqslant \infty, \tag{A3}$$

with E being free to run over all values.

We then have the easily proved identities

$$|g(\lambda)|^2 = \frac{1}{2\pi i}\,[\beta(\lambda) - \beta^*(\lambda)], \tag{A4}$$

$$|f(\mu)|^2 = \frac{1}{2\pi i}\,[\alpha(\mu) - \alpha^*(\mu)], \tag{A5}$$

$$\frac{|g(\lambda)|^2}{|\beta(\lambda)|^2} = -\frac{1}{2\pi i}\left[\frac{1}{\beta(\lambda)} - \frac{1}{\beta^*(\lambda)}\right], \tag{A6}$$

$$\frac{|f(\mu)|^2}{|\alpha(\mu)|^2} = -\frac{1}{2\pi i}\left[\frac{1}{\alpha(\mu)} - \frac{1}{\alpha^*(\mu)}\right], \tag{A7}$$

$$\frac{|g(E-\lambda)|^2}{|\beta(E-\lambda)|^2} = -\frac{1}{2\pi i}\left[\frac{1}{\beta(E-\lambda)} - \frac{1}{\beta^*(E-\lambda)}\right] - Z_B\,\delta(E-\lambda-M_B), \tag{A8}$$

$$\frac{|f(E-\mu)|^2}{|\alpha(E-\mu)|^2} = -\frac{1}{2\pi i}\left[\frac{1}{\alpha(E-\mu)} - \frac{1}{\alpha^*(E-\mu)}\right] - Z_D\,\delta(E-\mu-M_D). \tag{A9}$$

Equations (A8) and (A9) follow because $E-\lambda$ and $E-\mu$ can be less than zero, and thus pick up singularities at $M_B<0$ and $M_D<0$, respectively. On the other hand, λ and μ are always greater than or equal to zero, and so cannot pick up any singularities.

Another useful identity is

$$\gamma(E) = \int d\lambda\,\frac{|g(\lambda)|^2}{|\beta(\lambda)|^2}\,\frac{1}{\alpha(E-\lambda)} + \frac{Z_B}{\alpha(E-M_B)}, \tag{A10a}$$

$$= \int d\mu\,\frac{|f(\mu)|^2}{|\alpha(\mu)|^2}\,\frac{1}{\beta(E-\mu)} + \frac{Z_D}{\beta(E-M_D)}. \tag{A10b}$$

We can easily show this by means of the contours in Figs. 1 and 2. If we convert the integral in Eq. (A10a) into a contour integral by using Eq. (A6), we get

$$\left(-\frac{1}{2\pi i}\right)\int_{C_1} dz\,\frac{1}{\beta(z)\alpha(E-z)} + \frac{Z_B}{\alpha(E-M_B)}, \tag{A11}$$

with the contour shown in Fig. 1. Then, we make a change of variables from z to $E-z$ to get

$$\left(-\frac{1}{2\pi i}\right)(-1)\int_{C_4} dz\,\frac{1}{\alpha(z)\beta(E-z)} + \frac{Z_B}{\alpha(E-M_B)}, \tag{A12}$$

with the contour shown in Fig. 2. Now we deform the contour C_4 and write it as the contour C_3 plus the circle at infinity, while picking up the contributions from the residues of the integrand. Note that the circle at infinity gives no result, so we have

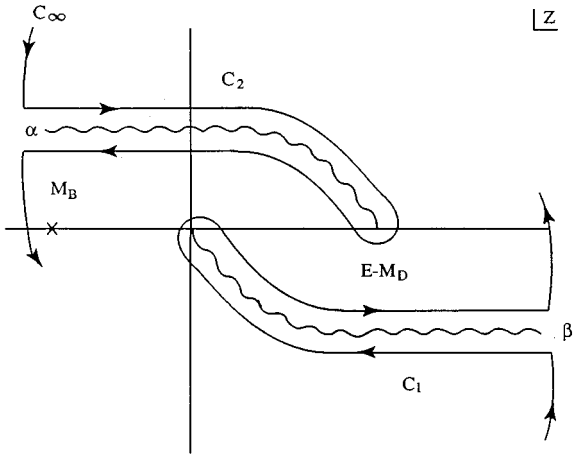

FIG. 1. Contour for Eq. (A10a).

$$\left(-\frac{1}{2\pi i}\right)(-1)(-1)\int_{C_3} dz\,\frac{1}{\alpha(z)\beta(E-z)}+\left(-\frac{1}{2\pi i}\right)(-1)(2\pi i)\,\frac{Z_D}{\alpha(E-M_D)}$$
$$+\left(-\frac{1}{2\pi i}\right)(-1)(-1)(2\pi i)\,\frac{Z_B}{\alpha(E-M_B)}+\frac{Z_B}{\alpha(E-M_B)}. \tag{A13}$$

The $\sqrt{Z_B}$ terms cancel, and the first two terms are Eq. (A10b), by definition. Therefore, Eq. (A10a) is equal to Eq. (A10b), and the identity is established.

We can similarly show that

$$\int d\lambda\,\frac{|g(\lambda)|^2}{|\beta(\lambda)|^2}\,\frac{1}{\alpha(E-\lambda)}\,\frac{1}{(\lambda-\nu+i\epsilon)}=\int d\mu\,\frac{|f(\mu)|^2}{|\alpha(\mu)|^2}\,\frac{1}{\beta(E-\mu)}\,\frac{1}{(E-\mu-\nu+i\epsilon)}$$

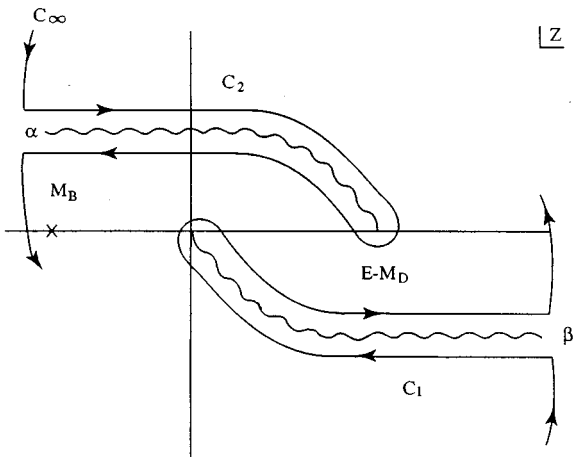

FIG. 2. Contour for Eq. (A10b).

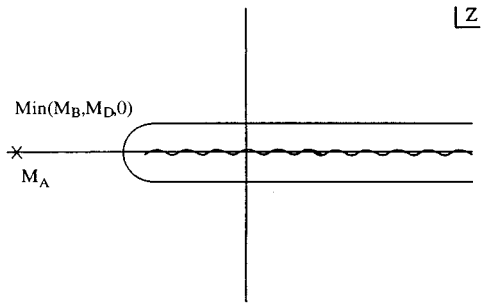

FIG. 3. Contour for the function $1/\gamma(z)$.

$$-\frac{1}{\alpha(E-\nu)\beta(\nu)}+\frac{Z_D}{\beta(E-M_D)(E-M_D-\nu+i\epsilon)}$$
$$-\frac{Z_B}{\alpha(E-M_B)(E-M_B-i\omega+i\epsilon)}. \tag{A14}$$

Using Eqs. (A7), (A8), and (A10) we can get another useful formula:

$$\int dn\,\frac{|f(n)|^2|g(E-n)|^2}{|\alpha(n)|^2|\beta(E-n)|^2}=\frac{\gamma(E)-\gamma^*(E)}{(-2\pi i)}-Z_D\frac{|g(E-M_D)|^2}{|\beta(E-M_D)|^2}-Z_B\frac{|f(E-M_B)|^2}{|\alpha(E-M_B)|^2}. \tag{A15}$$

Finally, in Fig. 3, we display the branch cuts and poles of $1/\gamma(z)$ which are used in showing the completeness of our solution set.

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Remarks on the quantization of gauge theories

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The methods of reduced phase space quantization and Dirac quantization are examined in a simple gauge theory. It is pointed out that care needs to be exercised in implementing the reduced phase space quantization method properly. © *1996 American Institute of Physics.* [S0022-2488(96)02903-1]

I. INTRODUCTION

A gauge theory is regarded in the canonical framework as a system with first class constraints.[1] In the classical analysis according to Dirac, the Hamiltonian H is the canonical one H_c plus an arbitrary linear combination of the first class constraints ϕ_i. This means that the classical trajectories involve arbitrary functions of time: the Lagrange multipliers λ_i. So a given physical state does not correspond to a unique set of canonical variables on the phase space Γ. This problem can be circumvented in either of two ways.

(i) Gauge-fixing constraints χ_i are introduced, one for each ϕ_i, such that they are preserved in time, i.e.

$$\{H,\chi_i\}\simeq 0,$$

and the matrix $C_{ij}=\{\phi_i,\chi_j\}$ is nonsingular. (This then becomes a theory with second class constraints.) Thus the λ_i's are fixed so that evolutions from initial states on the submanifold Γ^* defined by $\phi_i=\chi_i=0$ are unique. (For future reference, we will denote by $\Gamma^{*\prime}$ the constraint surface $\phi_i=\chi_i=0$, and provided $\det C\neq 0$ everywhere on the surface we will denote it by Γ^* and refer to it as the reduced phase space.)

(ii) Since the λ_i's bring in the arbitrary time dependence, all points on an orbit $\mathcal{O}$ generated by the gauge generators ϕ_i must be regarded as physically equivalent. So if $\hat{\Gamma}$ is the constraint surface $\phi_i=0$, then the true dynamical trajectories lie on $\tilde{\Gamma}\equiv\hat{\Gamma}/\sim$, where $\sim$ is the equivalence relation $P\sim P'$ if $P,\ P'\in\mathcal{O}$.

The surface Γ^* is diffeomorphic to $\tilde{\Gamma}$ provided the surface $\chi_i=0$ intersects each orbit in $\hat{\Gamma}$ exactly once. This condition on the gauge-fixing constraints χ_i is a prerequisite for the equivalence of the two approaches. For the first case, the condition of invertibility of the matrix C_{ij} ensures that *locally* the $\chi_i=0$ surface intersects $\hat{\Gamma}$ only once, but not necessarily globally. It is here that one has to be careful in choosing the gauge fixing constraints. This point has bearing on the quantization of a gauge theory, since quantum theory is sensitive to the global properties of the phase space to be quantized.

These two approaches have their counterparts in the quantization of gauge theories.

Method A: Reduced Phase Space Quantization—fix the gauge to obtain the space Γ^* and define the Poisson bracket structure on this as the Dirac brackets on the original phase space Γ. Γ^* so equipped is called the reduced phase space. It can then be directly quantized, which involves the finding of a commutator algebra representation for Poisson brackets. (This process can be complicated because the reduced phase space Γ^* is not always topologically trivial.) So here one quantizes *after* reducing the phase space.

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Method B: Dirac Quantization—canonically quantize the original phase space Γ (which is usually $\mathbf{R}^{2N}$) and then impose the gauge constraints as operator conditions on the physical quantum states:

$$\hat{\phi}_i \psi_{\text{phys}} = 0.$$

These are sometimes referred to as supplementary conditions. This is quantization *before* reduction.

Notice that method A depends manifestly on a choice of gauge-fixing constraints χ_i and there is a vast freedom in this choice, in general. An immediate question is whether method A applied with two different choices of the χ_i's gives equivalent quantum theories. Method B, on the other hand, is manifestly independent of any choice of gauge. If the two methods give equivalent quantum theories, then the manifest gauge invariance of method B reflects the gauge independence of method A applied for a class of χ_i's which ensure proper capturing of the reduced phase space. The discussion of the possible equivalence of Γ^* and $\tilde{\Gamma}$ has a crucial role to play in the equivalence of the quantum theories obtained by these two methods.

These matters are illustrated in the present work in the context of a very simple toy model gauge theory.

The model considered is described in the first section of the paper. In the second section we deal with its quantization by method A and the third section, method B. The choice of constraints and a discussion of a condition for the equivalence of these two methods is discussed in the fourth section. A discussion of and conclusions from the lessons learned from the exercise comprise the fifth section. An Appendix is included, giving a short review of the geometric quantization technique used in the quantization of the reduced phase space, along with the details of the calculations for the present case.

II. THE TOY MODEL

We consider the phase space $\mathbf{R}^4$ with canonical coordinates q^1, q^2, p_1, p_2, and the constraints

$$\phi \equiv q^{12} + q^{22} + p_1^2 + p_2^2 - R^2 = 0 \tag{1.1}$$

and

$$\chi \equiv p_2 = 0. \tag{1.2}$$

Suppose we regard the constraint ϕ as the gauge generator or the first class constraint and χ as the gauge-fixing condition. The constraint surface $\Gamma^{*\prime}$ is thus the 2-sphere S^2. The matrix

$$C \equiv \{\phi, \chi\} = \begin{pmatrix} 0 & 2q^2 \\ -2q^2 & 0 \end{pmatrix} \tag{1.3}$$

is nonsingular, provided $q^2 \neq 0$. This immediately shows that reduced phase space cannot be $\Gamma^{*\prime}$. Let us proceed, nevertheless, and see how to obtain the true reduced phase space Γ^*.

The Poisson bracket $\{\cdot,\cdot\}$ on $\mathbf{R}^4$ must be modified to the Dirac bracket $\{\cdot,\cdot\}^*$ on the constraint surface. This is given by

$$\{f,g\}^* = \{f,g\} - \sum_{i,j} \{f,\xi_i\} C^{-1}_{ij} \{\xi_j, g\}, \tag{1.4}$$

where ξ_i is a second class constraint and $f, g \in C^\infty(\mathbf{R}^4)$. The Dirac brackets of the canonical coordinates are

$$\{q^1,q^2\}=-\frac{p_1}{q^2},\quad \{q_1^1,p_1\}=1,\quad \{q^2,p_1\}=-\frac{q^1}{q^2}, \tag{1.5}$$

the rest being zero. Introducing the standard coordinates (θ',ϑ') on the sphere $S^2\sim\Gamma^{*\prime}$, (q^i,p_i) can be parametrized as

$$q^1=R\ \sin\ \theta'\ \cos\ \varphi',\quad p_1=R\ \sin\ \theta'\ \sin\ \varphi',\quad q^2=R\ \cos\ \theta', \tag{1.6}$$

where $0\leqslant\theta'\leqslant\pi$ and $0\leqslant\varphi'\leqslant2\pi$. This is singular at $\theta'=\pi/2$, which corresponds to the singularity of the Dirac brackets (1.6) at $q^2=0$, at the equator of the sphere. The Dirac bracket, which is also the induced 2-form from $\mathbf{R}^4$, is

$$\{f,g\}^*=\frac{1}{R^2\ \sin\ \theta'\ \cos\ \theta'}\left(\frac{\partial f}{\partial\theta'}\frac{\partial g}{\partial\varphi'}-\frac{\partial f}{\partial\varphi'}\frac{\partial g}{\partial\theta'}\right), \tag{1.7}$$

defines a symplectic form on $\Gamma^{*\prime}$ minus the equator: the constraint surface $\Gamma^{*\prime}$ is *not* the reduced phase space. The reason for this, as shall be demonstrated below, is that the set of points on $\Gamma^{*\prime}$ are not in 1–1 correspondence, with the set of inequivalent orbits of ϕ on the surface $\hat{\Gamma}\equiv\phi=0$. Also, reduced phase space on which the above Dirac bracket defines a symplectic structure must be obtained by a gauge-fixing condition that selects *one* point from each orbit $\mathcal{O}$. The χ of Eq. (1.2) does not satisfy this criterion. This is now shown explicitly.

The orbits $\mathcal{O}$ are the integral curves of the Hamiltonian vector fields corresponding to ϕ, which are described by the differential equations,

$$\dot{x}=\{x,\phi\},\quad \Rightarrow\dot{q}_i=2p_i,\quad \dot{p}_i=-2q_i,\quad i=1,2. \tag{1.8}$$

The general solution is

$$q_i(t)=A_i\ \cos(2t-\alpha_i),\quad p_i(t)=-A_i\ \sin(2t-\alpha_i), \tag{1.9}$$

with $A_i>0$, i.e. circles of radii A_i in the q_i-p_i planes, with initial conditions specified by the four parameters (A_i,α_i). Not all such sets specify distinct orbits: if the set (A_i,α_i) lies on the orbit generated from the set (A_i',α_i') then the two sets describe the same orbit. This happens when $A_i=A_i'\neq0$ and $\alpha_i'-\alpha_i=2\tau-2n\pi$ for some $t=\tau$, for each i. If either of the A_i's is zero, then there is only one orbit. So distinct orbits can be represented by

$$\begin{aligned} q^1&=A_1\ \cos(2t-\varphi),\quad p_1=-A_1\ \sin(2t-\varphi),\\ q^2&=A_2\ \cos(2t),\quad p_2=-A_2\ \sin(2t), \end{aligned} \tag{1.10}$$

where $0\leqslant\varphi\leqslant2\pi$ and $A_i\neq0$. (Note that $A_2=0$ corresponds to just *one* orbit for all values of φ.)

Now if an orbit $\mathcal{O}$ lies on $\hat{\Gamma}$, we also have $A_1^2+A_2^2=R^2$, so that we can write

$$A_1=R\ \sin\left(\frac{\theta}{2}\right),\quad A_2=R\ \cos\left(\frac{\theta}{2}\right), \tag{1.11}$$

with $0\leqslant\theta\leqslant\pi$. The orbits lying on $\hat{\Gamma}$ are thus parametrized by the two angles $\theta\in[0,\pi]$ and $\varphi\in[0,2\pi]$, so that the space of orbits is $\tilde{\Gamma}=S^2$.

The reduced phase space Γ^* is obtained by a gauge choice $\chi=0$, which cuts each of the above orbits once. The surface $p_2=0$ intersects the orbits (1.10) at the points $t=n\pi/2$ if $A_2\neq0$ and at $q_2=0$ for all t when $A_2=0$. Now $q_2=0$ represents one orbit, as discussed earlier. Note that this is the South Pole ($\theta=\pi$) of the space of orbits $\tilde{\Gamma}$. But the other orbits are intersected *twice*, i.e. at $q_2=\pm A_2$, corresponding to the upper and lower hemispheres of the constraint surface $\Gamma^{*\prime}$. This

means that while the *equator* ($q_2=0$) maps to the South Pole, *both* the hemispheres ($q_2=\pm A_2$) map to the rest of the sphere $\tilde{\Gamma}$: this means we are double counting. So to get the correct reduced phase space, we must restrict q_2 to be positive (say), so that θ' lies in $[0,\pi/2]$, which is the upper hemisphere alone. Now we get the reduced phase space as $\Gamma^*=S^2$, on which the Dirac bracket (1.7) actually defines the Poisson bracket:

$$\{f,g\}^*=\frac{4}{R^2\sin\theta}\left(\frac{\partial f}{\partial\theta}\frac{\partial g}{\partial\varphi}-\frac{\partial f}{\partial\varphi}\frac{\partial g}{\partial\theta}\right), \tag{1.12}$$

which is the standard one on a sphere of radius $R/2$, with the usual coordinate singularity at the poles. The symplectic structure induced from that on R^4 gives the same result, of course.

So the reduced phase space Γ^* of the system is S^2 after choosing as the gauge-fixing condition (1.2), *together* with the requirement that each gauge orbit is counted as cut only once.

We now proceed to quantize this system by the two methods A and B outlined in the Introduction.

II. METHOD A: QUANTIZATION OF THE REDUCED PHASE SPACE

Here we have a phase space, S^2, that is not a cotangent bundle, and so canonical methods of quantization cannot be applied. To quantize this, we use the technique of geometric quantization.[2] A quick review of this, as well as the calculations for S^2, are provided in the Appendix.

The sphere is quantizable only if the radius satisfies the Weil integrality condition: $R^2=2N\hbar$, $N\in\mathbf{Z}$ [cf. Eq. (A15) in the Appendix].

Working in the complex coordinates $(z,\overline{z})$ obtained by stereographic projection through the North Pole, the operator corresponding to an observable f satisfying the quantizability condition (A29) is given by

$$\hat{f}=\frac{2\hbar}{R^2}(1+|z|^2)^2(\partial_{\bar{z}}f\partial_z-\partial_z f\partial_{\bar{z}})-(1+|z|^2)\overline{z}\,\partial_{\bar{z}}f+f \tag{2.1}$$

[cf. Eq. (A18)]. This acts on $(N+1)$-dimensional Hilbert space of sections that are locally given by polynomials in z of order at most N.

There is a natural physical interpretation of this system. The phase space S^2 can be interpreted as describing the classical dynamics of the spin degrees of freedom of a particle, represented by a vector $\mathbf{J}$ in $\mathbf{R}^3$ such that $\mathbf{J}^2=j^2$. The magnitude of $\mathbf{J}$ is preserved and the equations of motion are understood as being of first order in the time derivatives. The components J_1, J_2, and J_3 are given in terms of the holomorphic coordinates on the sphere of radius j by

$$\begin{aligned} J_1&=j\ \frac{z+\overline{z}}{1+|z|^2},\\ J_2&=-ij\ \frac{z-\overline{z}}{1+|z|^2},\\ J_3&=j\,\frac{|z|^2-1}{1+|z|^2}, \end{aligned} \tag{2.2}$$

and they satisfy the Lie algebra, $\{J_a,J_b\}=\epsilon_{abc}J_c$, of SU(2). Upon quantizing, the integrability condition (A15) gives

$$j=\frac{N\hbar}{2},\quad N\in\mathbf{Z}^+, \tag{2.3}$$

and the spin operators are

$$\hat{J}_1=\frac{\hbar}{2}\,[(1-z^2)\partial_z+Nz],\quad \hat{J}_2=i\,\frac{\hbar}{2}\,[(1+z^2)\partial_z-Nz],\quad \hat{J}_3=\frac{\hbar}{2}\,[2z\partial_z-N]. \tag{2.4}$$

The Hilbert space is $(N+1)$ dimensional. One can see that $\Sigma\hat{J}_i^2=(\hbar^2/4)N(N+2)=j/\hbar(j/\hbar+1)$. This is therefore just the standard quantum theory of an elementary particle with spin $j/\hbar$, which can take half-integral values. One can also recover the Pauli matrices as the representation of the J_i's in the basis $(1,z,\ldots,z^N)$.

III. METHOD B: DIRAC QUANTIZATION

The constrained phase space Γ is now quantized by the Dirac method. Of the two second class constraints (1.1) and (1.2), one, in this case ϕ, is chosen to be the gauge-generating first class constraint while the other (χ in this case) is a gauge-fixing condition that plays no essential part in this scheme. Now one quantizes $\mathbf{R}^4$ by the canonical method, i.e., by the association of operators,

$$q^\alpha\rightarrow\hat{q}^\alpha=q^\alpha, \tag{3.1}$$

$$p_\alpha\rightarrow\hat{p}_\alpha=\frac{\hbar}{i}\,\frac{\partial}{\partial q^\alpha}, \tag{3.2}$$

which act on a Hilbert space of square-integrable wave functions $\Psi(q^1,q^2)$. Of these, only those represent physical states that are gauge invariant. So the operator corresponding to the gauge constraint must annihilate these state vectors (supplementary condition):

$$\hat{\phi}\Psi(q^1,q^2)=0, \tag{3.3}$$

$$\Rightarrow\left[q^{12}+q^{22}-\hbar^2\left(\frac{\partial^2}{\partial q^{12}}+\frac{\partial^2}{\partial q^{22}}\right)-R^2\right]\Psi=0, \tag{3.4}$$

which gives

$$\Psi(q^1,q^2)=(\text{const})e^{-(q^{12}+q^{22})/2}H_n(q^1)H_m(q^2), \tag{3.5}$$

with

$$R^2=2N\hbar, \tag{3.6}$$

where $N=n+m+1$ and n and m are non-negative integers. The radius is thus quantized as even multiples of $\hbar$, and since for each $R^2=2N\hbar$ there are N possible states, the Hilbert space is N dimensional.

The functions $f(q^\alpha,p_\alpha)$ in $\mathbf{R}^4$ that correspond to physical observables are those that commute with the gauge generator (the so-called first class observables in Dirac's terminology), i.e.,

$$\{\phi,f\}=0,\quad \Rightarrow q^1\,\frac{\partial f}{\partial p_1}-p_1\,\frac{\partial f}{\partial q^1}+q^2\,\frac{\partial f}{\partial p_2}-p_2\,\frac{\partial f}{\partial q^2}=0. \tag{3.7}$$

In the variables $z^\alpha=q^\alpha+i\,\delta^{\alpha b}p_b$, we have

$$(z^\alpha\partial_{z^\alpha}-\overline{z^\alpha}\,\partial_{\overline{z^\alpha}})f(z^\alpha,\overline{z^\alpha})=0, \tag{3.8}$$

$$\Rightarrow f(z^\alpha,\overline{z^b})=(z^\alpha)^{k_\alpha}(\overline{z^b})^{k_b}, \tag{3.9}$$

with

$$\sum_{\alpha} k_{\alpha} = \sum_{b} k_{b}\,.$$

For the corresponding quantum operators to be well defined, considerations such as that of self-adjointness may further restrict this class.

For the sake of comparison with the results of the previous section, let us look at the $SU(2)$ algebra generated by the following combinations of quadratic operators of the type $z^i\overline{z^j}$:

$$J_1 = \tfrac{1}{4}\,(z^1\overline{z^2} + z^2\overline{z^1}), \quad J_2 = \frac{1}{4i}\,(z^2\overline{z^1} - z^1\overline{z^2}), \quad J_3 = \tfrac{1}{4}\,(z^1\overline{z^1} + z^2\overline{z^2}). \tag{3.10}$$

Quantization, $J_i \to \hat{J}_i$, is achieved by $z^{\alpha} \to \hat{z}^{\alpha}$ and

$$\sum_{\alpha} \hat{J}_{\alpha}^2 = \frac{1}{16}\,(q^{\alpha 2} + p_{\alpha}^2)^2 + \frac{1}{4}\,(i\hbar)^2 = \left(\frac{R^2}{4}\right)^2 - \frac{\hbar^2}{4} = \hbar^2\left(\frac{N^2}{4} - \frac{1}{4}\right) = \hbar^2\left(\frac{N}{2} - \frac{1}{2}\right)\left(\frac{N}{2} + \frac{1}{2}\right). \tag{3.11}$$

If this corresponds to $\hbar^2 j(j+1)$, we get $j = (N-1)/2$, the standard result. In comparison, geometric quantization gave an $(N+1)$-dimensional Hilbert space for spin $N/2$. This slight discrepancy can be rectified by incorporating the metaplectic correction to geometric quantization (see, for example, Ref. 3), whereupon the two quantization schemes match exactly.

In the present instance, we find that Dirac quantization gives results equivalent to the quantization of the reduced phase space. In particular, the quantization of the parameter R, which resulted from the Weil integrability condition in the last section, appears here as a result of the normalizability of the wave functions.

A. Choice of constraints

When a system with second class constraints can be regarded as a gauge theory, half the constraints can be chosen as first class and generate gauge transformations, and the rest are gauge-fixing conditions. When there are only two second class constraints as in the example considered here, one may choose either as the gauge generator. The choices may give different theories. Dirac quantization requires no *a priori* criterion for the choice of the first class (gauge) constraints. Suppose, in the example considered here, that instead of ϕ one chose χ as the gauge generator, and let ϕ be the gauge-fixing condition. The constraint surface $\Gamma^{*\prime}$ and the singular Dirac brackets remain unaltered. The orbits $\mathcal{O}$ are in this case the lines $q^2(t) = q^2(0) + t$, and again the gauge choice $\phi = 0$ intersects these at two places: $q^2(t) = \pm q^2(0)$. So the reduced phase space Γ^* is again an S^2: the upper hemisphere of $\Gamma^{*\prime}$ with the (singular) equator mapped to the South Pole; quantization by method A is the same as before. However, in method B, the physical states are obtained by imposing the constraint condition

$$\hat{\chi}\Psi(q^1, q^2) = 0, \quad \Rightarrow \frac{\partial}{\partial q^2}\,\Psi(q^1, q^2) = 0, \tag{3.12}$$

i.e. Ψ is a function of q^1 alone. The Hilbert space is infinite dimensional and quantizable observables are general functions of q^1, p_1, and p_2. This quantization is manifestly different from that obtained previously. On the other hand, suppose we make a different gauge choice: $\chi' \equiv q^2 = 0$. Γ^* is the surface $q^2 = p_2 = 0$, which is R^2, and the Dirac quantization discussed in the beginning of the section gives the usual quantization on this, so that methods A and B give equivalent results. So here we see that method A gives different quantizations for different gauge choices.

This source of this ''discrepancy'' can be traced to the observation made in the Introduction regarding the intersection of the gauge-fixing surfaces with the gauge orbits. In the first case considered here, we carefully obtained the reduced phase space as $S^3/S^1=S^2$, and chose a gauge that selected one 2-sphere for every R. In the second case, though we were careful in considering only one intersection of the surfaces generated by the gauge choice $\phi=0$ with the gauge orbits $\mathcal{O}$, *not all orbits are cut*. A gauge choice that intersects *all* the gauge orbits is $\chi'=0$. So in the former case, one was artificially truncating the true phase space by an inappropriate gauge choice, and thereby obtained a different dynamical system.

Now the Dirac quantization method makes no reference to any gauge fixing and is determined once the gauge generators (ϕ_i's) are specified and a supplementary condition is imposed to ensure that the Hilbert space so constructed is associated with the true phase space $\tilde{\Gamma}$. Quantization of the reduced phase space Γ^* can be expected to give equivalent results only when Γ^* is diffeomorphic (symplectically) to $\tilde{\Gamma}$. So the gauge-fixing constraints χ_i must satisfy not only the condition $\det\{\phi_i,\chi_j\}\neq 0$, which ensures the selection of one point from each gauge orbit *locally*, but also that the resultant reduced phase space Γ^* be diffeomorphic to the space $\tilde{\Gamma}$ of orbits. This point may seem obvious in retrospect, but in practice one may miss it getting a resultant quantum theory, which may be consistent but not reflect gauge independence.

IV. DISCUSSION AND CONCLUSIONS

In the context of a simple gauge theory, viz. S^2 as a phase space, we have analyzed and compared two methods of quantization, viz. quantization of the reduced phase space and Dirac quantization, and examined a condition for their equivalence.

Another observation refers to quantizability itself. As is well known, in geometric quantization there exists a condition on the phase space for quantizability: the Weil integrability condition must be satisfied if the prequantum bundle is to exist. In the case of S^2 this restricts the radius to discrete values. This slightly counterintuitive result is not merely a peculiarity of the geometric approach. As shown in the present example, this quantizability condition reappears though in a different guise—it is a result of the physical Hilbert space being well defined (square integrability of the wave functions). This shows that the quantizability condition is related to the global topological properties of the phase space.

The comparison of quantizable observables shows that there exists a restricted class of classical observables that can be consistently quantized. Conditions of self-adjointness and operator commutativity with the gauge generators must also hold rigorously.

Gauge theories are encountered in many contexts, and in particular cases, either method of quantization may prove convenient. We have not considered the possible difficulties in applying either of these methods, but assuming they have been tided over, one needs to be careful about capturing the true phase space of the Dirac approach (method B) in the reduced phase space of method A. Further, restrictions may be encountered in parameters entering the theory via the constraints, for example, R in the present example.

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APPENDIX: GEOMETRIC QUANTIZATION ON S^2

This is a brief review of geometric quantization and its application to the quantization of S^2.

The classical phase space Γ is a $2n$-dimensional symplectic manifold. The symplectic form ω defines a Poisson algebra $\mathcal{A}$ of observables, which are C^∞ functions on Γ. In formulating a quantization, i.e. a map from $\mathcal{A}$ to the set $\mathcal{Q}$ of operators acting on a Hilbert space $\mathcal{H}$, the basic guidelines were spelt out by Dirac.

(i) The map $\mathcal{A}\to\mathcal{Q}$ is linear.
(ii) Constants are mapped to multiples of the identity operator.
(iii) For classical observables, $f_i\in\mathcal{A}$ and the corresponding quantum operators $\hat{f}_i\in\mathcal{Q}$,

$$[\hat{f}_1,\hat{f}_2]=k\hat{f}_3,\quad f_3=\{f_1,f_2\},$$

where $\{\cdot,\cdot\}$ is the Poisson bracket and $[\cdot,\cdot]$ is the commutator. k is some constant, canonically $i\hbar$.

Geometric quantization typically achieves this in two stages. The first stage, called ''prequantization'' involves finding such a map. The prequantum Hilbert space is, however, too large to be a physically reasonable quantum description. The wave functions depend on all the phase space variables, so that the standard Schrödinger description is not obtained, even in the case of $\mathbf{R}^{2N}$. Also, group representations of elementary systems turn out to be reducible. Hence, we need stage two of geometric quantization, which is the choice of a polarization of the manifold.

The ''prequantum'' operator corresponding to $f\in C^{\infty}(\Gamma)$ is constructed as follows: in local Darboux coordinates, (q^a,p_a),

$$\omega=dp_a\wedge dq^a, \tag{A1}$$

$$=d(p_a\,dq^a), \tag{A2}$$

so that the symplectic potential is

$$\theta=p_a\,dq^a. \tag{A3}$$

The Hamiltonian vector field X_f corresponding to f is

$$X_f=\frac{\partial f}{\partial p_a}\,\partial_{q^a}-\frac{\partial f}{\partial q^a}\,\partial_{p_a} \tag{A4}$$

and

$$\theta(X_f)=p_a\,\frac{\partial f}{\partial p_a}. \tag{A5}$$

Then the operator representation of f is

$$\hat{f}=-i\hbar X_f+\theta(X_f)+f. \tag{A6}$$

This acts on sections of a complex line bundle $\mathcal{B}$ over Γ, the connection potential on which is $\theta/\hbar$ (the curvature being $\omega/\hbar$). A compatible Hermitian structure $(\cdot,\cdot)$ must be defined on it. Now,

$$\hat{f}=-i\hbar\,\nabla x_f+f, \tag{A7}$$

where $\nabla x_f=X_f-(i/\hbar)\,\theta(X_f)$. Such a line bundle exists if and only if ω satisfies the Weil integrality condition.[4] This might restrict the class of classical phase spaces that can be quantized in this approach. One way of stating this condition, for a simply connected manifold, is that the integral of $\omega/\hbar$ over any closed, oriented two-dimensional submanifold of Γ is an integral multiple of 2π.

Stage two of geometric quantization involves the choice of a polarization P of the manifold. Sections of $\mathcal{B}$ constant along the polarization form the quantum Hilbert space $\mathcal{H}_Q$. If the vector fields X_m are tangent to P at a point m on Γ, then a section $s:\Gamma\to\mathcal{B}$ is said to be polarized if

$$\nabla_{x_m}s=0. \tag{A8}$$

Thus, s is a function of only n variables. So, if (s,s) is the Hermitian product on $\mathscr{B}$, the Hilbert space $\mathscr{H}_Q$ consists of polarized sections s such that

$$\langle s,s\rangle = \int_\Gamma (s,s)\,\omega^n < \infty. \tag{A9}$$

In this scheme, only those observables can be directly quantized that preserve the polarization: if s is a polarized section, so must $\hat{f}s$ be, meaning if X is a vector field tangent to P then we must have

$$\boldsymbol{\nabla}_X(\hat{f}s) = f(\boldsymbol{\nabla}_X s) - i\hbar\ \boldsymbol{\nabla}_{[X,X_f]}s = 0,$$

i.e. $[X,X_f]$ must also be tangent to P.

Further refinements such as half-density quantization and metaplectic corrections are not considered here as this level is sufficient for the case in hand.

This is applied to S^2 in the following.

The 2-sphere is a symplectic manifold on which the measure, in spherical coordinates (θ,ϕ),

$$\omega = \frac{R^2}{4}\sin\,\theta\ d\theta\wedge d\phi \tag{A10}$$

(where $R/2$ is the radius) serves as the symplectic form corresponding to the Poisson bracket (1.12). It is more convenient to look upon S^2 as a Kähler manifold with holomorphic coordinates z_i obtained by stereographic projection through the North (South) Poles:

$$z_n = \cot\left(\frac{\theta}{2}\right)e^{i\phi}, \quad z_s = \tan\left(\frac{\theta}{2}\right)e^{-i\phi}.$$

So it is covered by two charts, U_n and U_s, both isomorphic to the complex plane $\mathbf{C}$. Note that $z_n = 1/z_s$. Working in the northern chart, $z \in U_n \approx \mathbf{C}$, the symplectic form is

$$\omega_n = -i\,\frac{R^2}{2}\,(1+|z|^2)^{-2}\ dz\wedge d\bar{z}. \tag{A11}$$

The symplectic potential is

$$\theta_n = -i\,\frac{R^2}{2}\,(1+|z|^2)^{-1}\bar{z}\,dz. \tag{A12}$$

The prequantum line bundle $\mathscr{B}$, which is locally $U_i\times\mathbf{C}$, must have a curvature $\omega/\hbar$. This means that the transition function c_{ns} (on the overlap $U_n\cap U_s$) must be given by

$$\theta_s - \theta_n = i\hbar d\,\ln c_{ns}, \tag{A13}$$

which gives

$$c_{ns} = z^{R^2/2\hbar}. \tag{A14}$$

This is well defined only for $R^2/2\hbar \in \mathbf{Z}$. This, of course, is the Weil integrability condition:

$$\int_{S^2}\frac{\omega}{\hbar} = 2N\pi \Rightarrow R^2 = 2N\hbar, \quad N\in\mathbf{Z}. \tag{A15}$$

The Hamiltonian vector field corresponding to a function $f(z,\bar{z})$ is

$$X_f=\frac{2i}{R^2}(1+|z|^2)^2(\partial_{\bar{z}}f\ \partial_z-\partial_z f\ \partial_{\bar{z}}) \tag{A16}$$

and

$$\theta(X_f)=(1+|z|^2)\bar{z}\,\partial_{\bar{z}}f. \tag{A17}$$

So the quantum operator corresponding to f is

$$\hat{f}=\frac{2\hbar}{R^2}(1+|z|^2)^2(\partial_{\bar{z}}f\ \partial_z-\partial_z f\ \partial_{\bar{z}})-(1+|z|^2)\bar{z}\,\partial_{\bar{z}}f+f. \tag{A18}$$

A natural choice of polarization is the Kähler polarization (on S^2 there exist no real polarizations) spanned by the Hamiltonian vector fields generated by the holomorphic coordinates,

$$X_z=-\frac{2i}{R^2}(1+|z|^2)^2\partial_{\bar{z}}. \tag{A19}$$

There then exists a scalar K in the neighborhood of each point, such that the symplectic potential θ given by (A17) can be expressed as

$$\theta=-i\ \partial_z K, \tag{A20}$$

where $K=(R^2/2)\ln(1+|z|^2)$. This potential annihilates the vectors (A19), i.e., $\theta(X_z)=0$, and is said to be adapted to the polarization. The polarized sections of $\mathscr{B}$ satisfy

$$\nabla_{X_z}s(z,\bar{z})=0, \tag{A21}$$

$$\Rightarrow\partial_{\bar{z}}s=0. \tag{A22}$$

So $\mathscr{H}_Q$ consists of holomorphic sections of $\mathscr{B}$. In order that the wave functions be well defined on all of S^2, they must be well defined in the overlap region $U_n\cap U_z$, where they are related by

$$\psi_n=c_{ns}\psi_s,$$

i.e.,

$$\psi_s\left(\frac{1}{z}\right)=z^{-N}\psi_n(z). \tag{A23}$$

So $\psi(z)$ must be a polynomial in z of order at most N. $\mathscr{H}_Q$ is therefore spanned by the set $1,z,\ldots,z^N)$ and is $(N+1)$ dimensional. Given the scalar K of (A20), the Hermitian structure on $\mathscr{B}$ can then be chosen to be

$$(s,s)=\bar{s}\,s e^{-K/\hbar}. \tag{A24}$$

So the inner product on the Hilbert space is given by

$$\langle\psi,\psi\rangle=\int_C\bar{\psi}\,\psi(1+|z|^2)^{-N}\omega=\int_C\bar{\psi}\,\psi(1+|z|^2)^{-N-2}\,dz\,d\bar{z}. \tag{A25}$$

A similar result holds for the chart U_s.

Quantizable observables $f(z,\overline{z})$ in this scheme must satisfy $[X_z, X_f] \in P$. Now

$$[X_z, X_f] = \frac{2i}{R^2}\frac{\partial}{\partial z}\left((1+|z|^2)^2\frac{\partial f}{\partial \overline{z}}\right)X_z + \frac{2i}{R^2}\frac{\partial}{\partial \overline{z}}\left((1+|z|^2)^2\frac{\partial f}{\partial \overline{z}}\right)X_{\overline{z}}. \tag{A26}$$

For this to belong to the polarization, the second term must vanish, i.e.,

$$\frac{\partial}{\partial \overline{z}}\left((1+|z|^2)^2\frac{\partial f(z,\overline{z})}{\partial \overline{z}}\right) = 0, \tag{A27}$$

$$\Rightarrow f(z,\overline{z}) = \frac{h_1(z)+\overline{z}h_2(z)}{1+|z|^2}, \tag{A28}$$

where h_1 and h_2 are functions of z alone. For such an observable to be well defined on all of S^2, one requires that it have the same value in both charts:

$$\frac{h_1(z)+\overline{z}h_2(z)}{1+|z|^2} = \frac{h_1'(z')+\overline{z'}h_2'(z')}{1+|z'|^2},$$

which gives

$$h_1'(z) = zh_2(1/z), \quad h_2'(z) = zh_1(1/z),$$

where the prime denotes the Southern chart. These must be well defined for all z. Further, restriction to real functions alone gives a general observable in the form

$$f(z,\overline{z}) = \frac{a+bz+\overline{b}\overline{z}+c|z|^2}{1+|z|^2}, \tag{A29}$$

where the constants a and c are real and b is complex. Dynamics in this theory can be dictated by a Hamiltonian chosen from this class of observables. This completes the quantization of S^2.

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Directly interacting massless particles—A twistor approach

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Twistor phase spaces are used to provide a general description of the dynamics of a finite number of directly interacting massless spinning particles, forming a closed relativistic massive and spinning system with an internal structure. A Poincaré invariant canonical quantization of the so obtained twistor phase space dynamics is performed. © *1996 American Institute of Physics.* [S0022-2488(96)03603-X]

I. INTRODUCTION

It is possible that ''elementary'' massive particles such as electron, proton, neutron, etc. should be regarded as bound states of a *finite* number of massless and spinning interacting parts.

In order to investigate such a possibility we develop in this paper a general formalism with its roots in the Twistor Theory of Penrose[1] and in the Theory of Action at a Distance in Relativistic Particle Dynamics (in its instantaneous form).[2]

Somewhat similar attempts to classify elementary particles employing the Twistor Theory but without any explicit mention of the Theory of Action at a Distance in Relativistic Particle Dynamics (R.a-a-a-d), have been made before by Hughston[3] and Popovich.[4] Certain other developments in the same direction appeared in papers written by Perjès *et al.*[5,6] and Sparling.[7]

The quantum version of R.a-a-a-d in connection with the Twistor Theory seems to be implicit in an example worked out by Hughston.[8]

The framework we are presenting is, however, from the very beginning completely in accordance with R.a-a-a-d. Classical states, which correspond to relativistic quantum bound states of a massive and spinning composite particle, are represented by points in a finite-dimensional ''twistor phase space.'' The description is purely Hamiltonian. The suggested quantization procedure is simultaneously canonical and Poincaré invariant. The arising canonically conjugated quantum mechanical operators represent ''square roots'' of the null momenta and ''square roots'' of the ''positions'' attributed to (the classical limit of) the massless constituents forming a massive system.

Exploring the idea of instantaneous relativistic action at a distance[2] in the phase space of two twistors we have shown previously[9] how a free massive, spinning point-like particle may be thought of as a relativistic rigid rotator (endowed with intrinsic spin) composed of two massless spinning parts. The term ''instantaneous'' refers to the rest frame defined by the total time-like four-momentum of the rigid rotator itself. The present paper may be regarded as an extension and generalization of the same idea. In its very rough state the idea appeared in our report[10] from 1979.

The work is organized as follows: First, in the next section some results from the Twistor Theory are reformulated in a way that exhibits how they tie in with a relativistic, classical, finite-dimensional phase space mechanics of a massless particle with helicity. Ten Poincaré covariant functions fulfilling Poisson bracket algebra of the Poincaré group and a function corresponding to the helicity operator are identified.[1]

These well-known results in new clothes are generalized in Sec. III, where a twistor phase space of a massive spinning system composed of an arbitrary finite number of massless parts is introduced.

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Again, ten Poincaré covariant functions fulfilling Poisson bracket algebra of the Poincaré group are identified. Four functions representing the (real) position four-vector of the total massive spinning system are also identified.[3]

A fundamental set of Poincaré scalar functions forming a closed finite Poisson bracket subalgebra is identified. These functions serve as generators (eigenvalues of their quantum mechanical counterparts are tentatively identified with such quantum numbers as electric charge, baryon number etc.) of the internal symmetries.

A general formula for the four functions representing the Pauli–Lubański spin four-vector is derived.

A general formula for the function representing the square of the relativistic spin in terms of the generators of the internal symmetries is found.

It is discovered that, provided the relativistic spin does not vanish, the components of the position four-vector of the total system do not Poisson commute [see (3.27)].

A certain class of Poincaré scalar functions in the twistor phase space is selected. Functions in this class, when used as generators of motion, produce canonical flows, which in Minkowski space describe a finite number of mutually interacting spinning massless particles forming a closed freely moving massive and, in general, spinning relativistic system.

The so obtained relativistic dynamics constitutes our general dynamical principle.

In the last section this classical phase space dynamics is canonically quantized in a way that corresponds to the real polarization of the twistor phase space.[11] A Poincaré invariant scalar product, on the space of functions representing quantum states of the massive spinning system composed of a finite number of massless parts, is introduced.

The following notation will be used.

Latin letters with lower case Latin indices will denote four-vectors and four-tensors. Lower case Greek letters with upper case Latin indices (either primed or unprimed) will denote spinors. Upper case Latin letters with lower case Greek indices will denote nonprojective twistors. Lower case Latin indices within round brackets are used to number the different massless parts and in this way label the internal degrees of freedom. A bar over a letter or over an expression denotes complex conjugation. The usual summation convention over repeated indices is assumed throughout. The physical units are so chosen that $c=\hbar=1$. The signature of the metric g_{ij} in Minkowski space is taken to be $+---$. The fully antisymmetric alternating four-tensor will be denoted by ϵ_{ijkl}.

II. THE ELEMENTARY TWISTOR PHASE SPACE

There are no new results in this section except from the way they are presented.

We introduce the notion of a twistor-phase space **Tp**, which will be regarded as a space of classical states arising as a limit of some corresponding (not yet specified) quantum mechanical description of a massless particle with helicity. The value of such a quantum mechanical helicity is supposed to arise as an eigenvalue of some appropriate (not yet specified) quantum mechanical helicity operator. In the classical limit this quantum mechanical helicity operator should then correspond to a real valued function on **Tp**. Therefore the classical helicity (being a limit of a quantum mechanical operator whose eigenvalues are discrete) is not a discrete variable. In addition, following Penrose[1] and Hughston,[3] ten real valued Poincaré covariant functions (corresponding to the generators of the Poincaré algebra) on **Tp** are identified as (classical) physical observables.

Definition 1: A nonprojective twistor space **T** is a four-dimensional complex vector space (i.e., $C^4 \cong R^8$) endowed with the isometry group SU(2,2).

Remark 1: SU(2,2) is to be identified with (the universal covering of) the so-called conformal group of the compactified Minkowski space and it contains as one of its subgroups (the universal covering of) the Poincaré group, which, in turn, contains as one of its subgroups (the universal

covering of) the Lorentz group, i.e. SL(2,C). As is well known, the Poincaré group is the isometry group of the physical Minkowski space.

In order to see how vectors in **T** are related to physical Minkowskian quantities (such as angular and linear four-momenta, position four-vectors, and Poincaré invariant scalars), it is convenient to choose a basis in **T** in a very special way. A vector in **T** given with respect to such a basis is called a nonprojective twistor. With respect to any such twistor basis, the SU(2,2) metric is nondiagonal.

Definition 2: A nonprojective twistor Z^α and the corresponding (twistor) complex conjugated twistor Z_α may thus be represented by two Weyl spinors and their conjugates:

$$Z^\alpha=(\omega^A,\pi_{A'}),\quad \overline{Z_\alpha}=(\overline{\pi_A},\overline{\omega^{A'}}). \tag{2.1}$$

Remark 2: Such a spinor representation of a nonprojective twistor and its twistor conjugate also explicitly shows how the Poincaré group acts on **T**. Coordinates of the two spinors represented by $\pi_{A'}$ and ω^A are covariant with respect to the (identity connected part of the) Lorentz group, while four-translations T^a act only on the ''ω'' spinor parts of the twistor Z and its (twistor) complex conjugate[1] $\overline{Z}$.

Definition 3: The elementary twistor phase space **Tp** is spanned by R^8, in which each point is labeled by a nonprojective twistor and its twistor complex conjugate. Further, **Tp** is equipped with an SU(2,2) invariant symplectic structure[3,12,13] defined by the following canonical Poisson bracket relations:

$$\{Z^\alpha,\overline{Z_\beta}\}=i\,\delta^\alpha_\beta,\quad \{Z^\alpha,Z^\beta\}=\{\overline{Z_\alpha},\overline{Z_\beta}\}=0, \tag{2.2}$$

which, when written out in terms of spinors, reads as

$$\{\omega^A,\overline{\pi_B}\}=i\,\delta^A_B,\quad \{\pi_{B'},\overline{\omega^{A'}}\}=i\,\delta^{A'}_{B'}, \tag{2.3}$$

$$\{\omega^A,\omega^B\}=\{\omega^A,\pi_{A'}\}=\{\pi_{A'},\pi_{B'}\}=\{\pi_{A'},\overline{\pi_B}\}=0, \tag{2.4}$$

$$\{\overline{\omega_{A'}},\overline{\omega^{B'}}\}=\{\overline{\omega^{A'}},\overline{\pi_A}\}=\{\overline{\pi_A},\overline{\pi_B}\}=\{\omega^A,\overline{\omega^{B'}}\}=0. \tag{2.5}$$

Remark 3: Points in **Tp** represent classical states of (the classical limit of) a massless particle with (any value of its) helicity.

Lemma 1: If the linear four-momentum P_a and the angular four-momentum $M_{ab}=-M_{ba}$ of a massless particle (Penrose's abstract index notation[14] is used throughout the paper when appropriate) are defined[1] by the following set of Poincaré covariant functions on **Tp**:

$$P_a:=\pi_A\overline{\pi_A}, \tag{2.6}$$

$$M_{ab}:=i\,\overline{\omega}_{(A'}\pi_{B')}\epsilon_{AB}-i\,\omega_{(A}\overline{\pi}_{B)}\epsilon_{A'B'}, \tag{2.7}$$

then the canonical Poisson brackets (2.3)–(2.5) imply that P_a and M_{ab} fulfill the Poisson bracket relations of the Poincaré algebra:[3]

$$\{P_a,P_b\}=0, \tag{2.8}$$

$$\{M_{ab},P_c\}=2g_{c[a}P_{b]}, \tag{2.9}$$

$$\{M_{ab},M_{cd}\}=2(g_{c[a}M_{b]d}+g_{d[b}M_{a]c}). \tag{2.10}$$

Proof, which we omit, is just a tedious but straightforward computation. Penrose's blob notation[15] may be useful for this.

Remark 4: The above Poisson bracket relations define the momentum mapping for the action of the Poincaré group on **Tp**.

Remark 5: A point in **Tp** carries more information about the classical state of a massless particle than just information about its linear and angular four-momenta. It also defines its helicity and its phase.

Lemma 2: The helicity (state) function is given by[1]

$$s = \tfrac{1}{2}\,(Z^{\alpha}\overline{Z_{\alpha}}) = \tfrac{1}{2}\,(\omega^{A}\overline{\pi_{A}} + \pi_{A'}\overline{\omega^{A'}}), \tag{2.11}$$

which may be easily deduced if in the definition of the Pauli–Lubański spin four-vector:

$$S^{a} := \tfrac{1}{2}\,\epsilon^{abcd}P_{b}M_{cd}, \tag{2.12}$$

the expressions in (2.6)–(2.7) and the spinor version of ϵ^{abcd} are inserted. The result in (2.11) follows from a simple spinor algebra calculation,[13] which yields

$$S^{a} = sP^{a}. \tag{2.13}$$

Remark 6: Note that the massless particle's helicity function s coincides with one-half of the SU(2,2) norm of the corresponding nonprojective twistor.

III. THE GENERAL TWISTOR PHASE SPACE

A generalization of the results presented in the previous section opens some new ways for applications of the Twistor Theory and of the R.a-a-a-d.

Namely, it becomes possible to formulate a general dynamical principle, which, according to our interpretations and identifications, describes a closed massive and, in general, spinning system composed of a finite number of mutually interacting massless and spinning parts.

A direct product of any number of **Tp** may be used to define a (reducible) phase space for a massive spinning relativistic particle built up out of the massless ones. In such a direct product **Tp**(**n**) of n ($n \geqslant 2$) copies of the elementary twistor phase space **Tp** we exclude all points on all diagonals, i.e., each point in **Tp**(**n**) represents a state of n massless particles with their four-momenta pointing at n noncoinciding null directions.

Generalizing Definition 3 of the previous section, we let the symplectic structure on the product twistor phase space **Tp**(**n**) be given by the following set of canonical conformally invariant Poisson brackets:

Definition 4:

$$\{Z^{\alpha}_{(i)}, \overline{Z}_{\beta(j)}\} = i\,\delta^{\alpha}_{\beta}\delta_{(i)(j)}, \quad \{Z^{\alpha}_{(i)}, Z^{\beta}_{(j)}\} = \{\overline{Z}_{\alpha(i)}, \overline{Z}_{\beta(j)}\} = 0, \quad (i),(j) = 1,2,\ldots,n, \tag{3.1}$$

where the index within brackets labels the n distinct massless parts.

Lemma 3: If the linear and angular four-momenta functions of the massive and spinning particle, formed by the n massless spinning constituents, are defined by

$$\mathscr{P}_{a} := \pi_{A'(i)}\overline{\pi}_{A(i)}, \tag{3.2}$$

$$\mathscr{M}_{ab} := i\,\overline{\omega}_{(j)(A'}\pi_{B')(j)}\epsilon_{AB} - i\,\omega_{(j)(A}\overline{\pi}_{B)(j)}\epsilon_{A'B'}, \tag{3.3}$$

then the canonical commutation relations in (3.1) imply

$$\{\mathscr{P}_{a}, \mathscr{P}_{b}\} = 0, \tag{3.4}$$

$$\{\mathscr{M}_{ab}, \mathscr{P}_{c}\} = 2g_{c[a}\mathscr{P}_{b]}, \tag{3.5}$$

$$\{\mathscr{M}_{ab},\mathscr{M}_{cd}\}=2(g_{c[a}\mathscr{M}_{b]d}+g_{d[b}\mathscr{M}_{a]c}), \tag{3.6}$$

which, as should be expected, again represents Poisson bracket algebra of the Poincaré group.

Remark 7: Using the canonical (conformally covariant) twistor coordinates [on the $8n$- (real) dimensional twistor phase space], we note that they may be used to form $2n^2-n$ real-valued Poincaré scalar functions. n^2 of these are also conformally [i.e., SU(2,2)] invariant.

Definition 5: The n^2 real-valued SU(2,2) invariant scalars are represented by real and imaginary parts of the following functions:

$$a_{(i)(j)}:=Z^{\alpha}_{(i)}\overline{Z}_{\alpha(j)}, \quad \overline{a}_{(i)(j)}=a_{(j)(i)}, \tag{3.7}$$

while the remaining Poincaré invariant scalars are represented by real and imaginary parts of

$$m_{(i)(j)}:=I_{\alpha\beta}Z^{\alpha}_{(i)}Z^{\beta}_{(j)}=\epsilon^{C'D'}\pi_{D'(i)}\pi_{C'(j)}=-m_{(j)(i)}, \tag{3.8}$$

$$\overline{m}_{(i)(j)}:=I^{\alpha\beta}\overline{Z}_{\alpha(i)}\overline{Z}_{\beta(j)}=\epsilon^{CD}\overline{\pi}_{D(i)}\overline{\pi}_{C(j)}=-\overline{m}_{(j)(i)}, \tag{3.9}$$

where ϵ^{AB}, $\epsilon^{A'B'}$ denote the metric in the Weyl spinor space, or equivalently $I^{\alpha\beta}$ and $I_{\alpha\beta}$ denote the so-called infinity twistor and its dual.[1,13]

Lemma 4: From the canonical commutation relations in (3.1) it almost trivially follows that

$$\{a_{(i)(j)},Z^{\alpha}_{(k)}\}=-i\delta_{(j)(k)}Z^{\alpha}_{(i)}, \quad \{a_{(i)(j)},\overline{Z}_{\alpha(k)}\}=i\delta_{(i)(k)}\overline{Z}_{\alpha(j)}, \tag{3.10}$$

$$\{m_{(i)(j)},Z^{\alpha}_{(k)}\}=0, \quad \{\overline{m}_{(i)(j)},Z^{\alpha}_{(k)}\}=2iI^{\alpha\mu}\overline{Z}_{\mu[(i)}\delta_{(j)](k)}, \tag{3.11}$$

$$\{m_{(i)(j)},\overline{Z}_{\alpha(k)}\}=2iI_{\mu\alpha}Z^{\mu}_{[(i)}\delta_{(j)](k)}, \quad \{\overline{m}_{(i)(j)},\overline{Z}_{\alpha(k)}\}=0. \tag{3.12}$$

Lemma 5: As shown by Hughston,[3] the real four-vector-valued function on $\mathbf{Tp}(\mathbf{n})$ representing, in the Minkowski space, position four-vector of the total system (composed of n massless parts) is given by

$$X^a=X^{AA'}:=\frac{\mathscr{M}^{ab}\mathscr{P}_b}{m^2}+\frac{l}{m^2}\mathscr{P}^a, \tag{3.13}$$

where

$$l:=-\tfrac{1}{2}(i\omega^{A}_{(i)}\overline{\pi}_{A(i)}-i\pi_{A'(i)}\overline{\omega}^{A'}_{(i)}), \tag{3.14}$$

and where

$$m^2:=\mathscr{P}_a\mathscr{P}^a=m_{(i)(j)}\overline{m}_{(i)(j)}, \tag{3.15}$$

or equivalently by[3]

$$X^a=i\frac{1}{m^2}[\overline{m}_{(i)(j)}\omega^{A}_{(i)}\pi^{A'}_{(j)}-m_{(i)(j)}\overline{\omega}^{A'}_{(i)}\overline{\pi}^{A}_{(j)}]. \tag{3.16}$$

Now it is a straightforward task to calculate the following Poincaré invariant and Poincaré covariant Poisson bracket commutation relations that will be needed in the sequel.

Lemma 6: First we note that from the conformally invariant canonical Poisson bracket relations (3.1), it follows that the $2n^2-n$ scalars in (3.7)–(3.9) form a Poincaré invariant closed algebra of Poisson brackets:

$$\{a_{(i)(j)},a_{(k)(l)}\}=ia_{(k)(j)}\delta_{(i)(l)}-ia_{(i)(l)}\delta_{(j)(k)},\quad \{a_{(i)(j)},m_{(k)(l)}\}=2im_{(i)[(k)}\delta_{(l)](j)}, \tag{3.17}$$

$$\{a_{(i)(j)},\overline{m}_{(k)(l)}\}=2i\overline{m}_{(j)[(k)}\delta_{(l)](i)},\quad \{m_{(i)(j)},m_{(k)(l)}\}=\{\overline{m}_{(i)(j)},m_{(k)(l)}\}=0, \tag{3.18}$$

which may easily be proved by the help of Lemma 4.

Lemma 7: From the fact that $m_{(i)(j)}$, $\overline{m}_{(i)(j)}$, and $a_{(i)(j)}$ are Poincaré scalar functions, it trivially follows that they commute with all the generators of the Poincaré algebra:

$$\{a_{(i)(j)},\mathscr{P}_a\}=\{a_{(i)(j)},\mathscr{M}_{ab}\}=0, \tag{3.19}$$

$$\{m_{(i)(j)},\mathscr{P}_a\}=\{m_{(i)(j)},\mathscr{M}_{ab}\}=\{\overline{m}_{(i)(j)},\mathscr{P}_a\}=\{\overline{m}_{(i)(j)},\mathscr{M}_{ab}\}=0. \tag{3.20}$$

Lemma 8: The following commutation relations are also easily deduced from the canonical commutations relations in (3.1):

$$\{a_{(i)(j)},l\}=0 \tag{3.21}$$

$$\{m_{(i)(j)},l\}=m_{(i)(j)}. \tag{3.22}$$

Lemma 9: From (3.13) and (3.17)–(3.22) it now follows that

$$\{a_{(i)(j)},X^a\}=\frac{1}{m^2}\mathscr{P}^a\{a_{(i)(j)},l\}=0, \tag{3.23}$$

$$\{m_{(i)(j)},X^a\}=\frac{1}{m^2}\mathscr{P}^a\{m_{(i)(j)},l\}=\frac{1}{m^2}\mathscr{P}^a m_{(i)(j)}, \tag{3.24}$$

$$\{\mathscr{P}_b,X^a\}=\delta^a_b, \tag{3.25}$$

$$\left\{\frac{1}{2}\mathscr{P}_b\mathscr{P}^b,X^a\right\}=\mathscr{P}^a. \tag{3.26}$$

Lemma 10: Similarly, we obtain that

$$\{X^a,X^b\}=\frac{1}{m^4}\epsilon^{abcd}\mathscr{S}_c\mathscr{P}_d, \tag{3.27}$$

where the Pauli–Lubański four-vector $\mathscr{S}^a$ is defined as in (2.12), i.e. by

$$\mathscr{S}^a:=\tfrac{1}{2}\epsilon^{abcd}\mathscr{P}_b\mathscr{M}_{cd}. \tag{3.28}$$

Lemma 11: Expressing the right-hand side of (3.28) in terms of spinors defining the corresponding twistors, we obtain

$$2\mathscr{S}^a=2\mathscr{S}^{AA'}=\overline{m}_{(i)(j)}\omega^A_{(i)}\pi^{A'}_{(j)}+m_{(i)(j)}\overline{\omega}^{A'}_{(i)}\overline{\pi}^{A}_{(j)}+a_{(i)(j)}\overline{\pi}^{A}_{(i)}\pi^{A'}_{(j)}, \tag{3.29}$$

which, after some spinor algebra manipulations, may be rewritten as

$$2\mathscr{S}^{AA'}=[2a_{(i)(j)}-\delta_{(i)(j)}a_{(k)(k)}]\overline{\pi}^{A}_{(i)}\pi^{A'}_{(j)}=2a_{(i)(j)}\overline{\pi}^{A}_{(i)}\pi^{A'}_{(j)}-a_{(i)(i)}\overline{\pi}^{A}_{(j)}\pi^{A'}_{(j)}. \tag{3.30}$$

Remark 8: The formula in (3.30) is also valid for $n=1$ and reproduces the result[1] of Lemma 2. For $n=2$ it appeared in Tod's doctoral dissertation.[18] However, the author of this paper has never come across the general formula in (3.30), which is valid for any (finite) natural number n.

Lemma 12: From the above lemma (Lemma 11) it follows that the square of the value of the total spin s^2 (for $n>2$) is a function of the invariants in (3.7)–(3.9) (i.e., is a function of the generators of the internal symmetries), given by

$$-4m^2s^2:=4\mathscr{S}^a\mathscr{S}_a=(a_{(j)(j)})^2m^2+4a_{(j)(j)}a_{(u)(v)}\overline{m}_{(u)(k)}m_{(k)(v)}+4a_{(j)(k)}a_{(u)(v)}\overline{m}_{(j)(u)}m_{(k)(v)}\,. \tag{3.31}$$

Remark 9: For $n=2$ and $n=3$ the formula (3.31) agrees with those previously derived by Perjès, Hughston, and Sparling. The general formula above is, however, valid for any (finite) natural number $n\geqslant 2$. As far as we know this formula has not been derived before.

Proposition 1: As explained in the Introduction we wish to regard a closed massive and spinning system as composed of a finite number of interacting massless parts. For this reason we notice that any function of the form

$$H:=\tfrac{1}{2}\mathscr{P}_b\mathscr{P}^b+g(a_{(j)(k)},m_{(l)(m)},\overline{m}_{(n)(r)}), \tag{3.32}$$

where g is a positive real-valued function of the invariants in (3.7)–(3.9), generates a canonical flow in **Tp**(**n**), which in the Minkowski space describes a set of n mutually interacting massless particles. This follows from direct calculations, which produce the following equations of the motion:

$$\dot{X}^a=\{H,X^a\}=\mathscr{P}^a\left(1+\frac{1}{m^2}\frac{\partial g}{\partial m^{(i)(k)}}\,m_{(i)(k)}+\frac{1}{m^2}\frac{\partial g}{\partial \overline{m}^{(i)(k)}}\,\overline{m}_{(i)(k)}\right), \tag{3.33}$$

$$\dot{\pi}_{A'(k)}=\{H,\pi_{A'(k)}\}=-i\,\frac{\partial g}{\partial a^{(j)(k)}}\,\pi_{A'(j)}\,,\quad \dot{\mathscr{P}}^a=\{H,\mathscr{P}^a\}=0, \tag{3.34}$$

$$\dot{a}_{(k)(j)}=\{H,a_{(k)(j)}\}=i\,\frac{\partial g}{\partial a^{(j)(l)}}\,a_{(k)(l)}-i\,\frac{\partial g}{\partial a^{(l)(k)}}\,a_{(l)(j)}-2i\,\frac{\partial g}{\partial \overline{m}^{(k)(l)}}\,\overline{m}_{(l)(j)}+2i\,\frac{\partial g}{\partial m^{(j)(l)}}\,m_{(k)(l)}\,. \tag{3.35}$$

Remark 10: Note that the assumption in (3.32), stating that g is a function of the generators $a_{(i)(j)}$ (which are conformal scalars), makes the motion of the massless parts nontrivial (i.e., changes their null momenta during the motion). All functions g, which depend on $m_{(i)(j)}$ and their complex conjugates only, produce a motion of the massless parts that is trivial in the Minkowski space.

Assumption 1: From now on we assume that g is a function of the conformal invariants $a_{(i)(j)}$ only:

$$g=g(a_{(j)(k)}). \tag{3.36}$$

Proposition 2: Under this condition the equations of motion generated by the canonical flow in the twistor phase space simplify and read as

$$\dot{X}^a=\{H,X^a\}=\mathscr{P}^a, \tag{3.37}$$

$$\dot{\pi}_{A'(k)}=\{H,\pi_{A'(k)}\}=-i\,\frac{\partial g}{\partial a^{(j)(k)}}\,\pi_{A'(j)};\quad \dot{\mathscr{P}}^a=\{H,\mathscr{P}^a\}=0, \tag{3.38}$$

$$\dot{a}_{(k)(j)}=\{H,a_{(k)(j)}\}=i\,\frac{\partial g}{\partial a^{(j)(l)}}\,a_{(k)(l)}-i\,\frac{\partial g}{\partial a^{(l)(k)}}\,a_{(l)(j)}\,. \tag{3.39}$$

Remark 11: From (3.37) it follows that the parameter labeling points on the curves of the canonical flow generated by H with g such as in (3.36) is linearly related to the proper time of the total system.

If such a function g vanishes (or degenerates to a real number) then the function H and the function $\frac{1}{2}\,m^2$ are identical (modulo an additive real number) forming just one constant of the free motion generated by H.

For nontrivial such g the functions H and $\frac{1}{2}\,m^2$ correspond to two different mutually commuting but *a priori* unrelated constants of the motion generated by H.

Remark 12: The above equations of motion have been explicitly solved[9] for $n=2$ and for $g=s^2$. Such a motion describes a massive relativistic rigid rotator composed of two directly interacting massless spinning particles.

Assumption 2: Due to the fact that the parameter labeling the curves of the canonical flow generated by H is linearly related to the proper time of the total system, we make an additional ''physical'' assumption that for any nontrivial g such as in (3.36) the constant of the motion given by the value of the function H is proportional (modulo an additive real number r) to the value of the constant of the motion $\frac{1}{2}\,m^2$. The proportionality constant k is larger than one-half and approaches one-half when the function g approaches zero (modulo an additive real number r):

$$H=km^2+r,\quad k>\frac{1}{2}. \tag{3.40}$$

A posteriori this amounts to a ''constraint:''

$$m^2=\frac{g-r}{(k-\frac{1}{2})}. \tag{3.41}$$

The imposition of such a ''constraint'' seems perhaps somewhat unnecessary at this stage but may be motivated by the fact that after quantization we wish to interpret ratios of the arising possibly discrete eigenvalues of $\hat{H}$ [for some specific choices of g in (3.36)] as ratios of the squares of the quantized masses.

IV. QUANTIZATION

A nonstandard,[11] as opposed to the standard procedure introduced by Penrose,[1] canonical twistor quantization is obtained by means of a natural prescription á la Dirac,[16,17] given by

$$\hat{\omega}^A_{(i)}:=-\frac{\partial}{\partial\overline{\pi}^{(i)}_A},\quad \hat{\bar{\omega}}^{A'}_{(i)}:=\frac{\partial}{\partial\pi^{(i)}_{A'}}, \tag{4.1}$$

$$\hat{\bar{\pi}}_{A(i)}:=\overline{\pi}_{A(i)},\quad \hat{\pi}_{A'(i)}:=\pi_{A'(i)}\,. \tag{4.2}$$

The Poisson brackets relations in (3.1) will hereby be replaced by the corresponding commutators, turning the classical twistor phase space dynamics of massless particles into its quantum mechanical analog.

So, by the use of (4.1)–(4.2) the linear four-momentum functions in (3.2), the angular four-momentum functions in (3.3), the scalar functions in (3.7)–(3.9) turn into the corresponding operators:

$$\hat{\mathscr{P}}_a := \overline{\pi}_{A(i)} \pi_{A'(i)}, \tag{4.3}$$

$$\hat{\mathscr{M}}^{ab} := i \pi^{A'}_{(i)} \frac{\partial}{\partial \pi^{(i)}_{B'}} \epsilon^{AB} + i \overline{\pi}^{A}_{(i)} \frac{\partial}{\partial \overline{\pi}^{(i)}_{B}} \epsilon^{A'B'}, \tag{4.4}$$

$$\hat{a}_{(i)(j)} := - \overline{\pi}_{A(j)} \frac{\partial}{\partial \overline{\pi}^{(i)}_{A}} + \pi_{A'(i)} \frac{\partial}{\partial \pi^{(j)}_{A'}}, \quad \hat{m}_{(i)(j)} := \pi^{A'}_{(i)} \pi_{A'(j)}, \quad \hat{\bar{m}}_{(i)(j)} := \overline{\pi}^{A}_{(i)} \overline{\pi}_{A(j)}. \tag{4.5}$$

The Poisson bracket relations in (3.4)–(3.6) ensure that operators in (4.3) and (4.4) obey commutation relations of the Poincaré algebra. In addition, all the Poisson bracket commutation relations in (3.10)–(3.12), (3.17)–(3.27) turn into the corresponding operator commutators.

All functions on $\mathbf{Tp}(\mathbf{n})$ become (at least formally) operator-valued functions of the canonical differential operators in (4.1) and of the multiplicative operators in (4.2). Of course, this may lead to problems: Ordering problems, nonlocality of the operators arising from functions on $\mathbf{Tp}(\mathbf{n})$ in which the ''ω'' parts appear in the denominator, etc.

The multiplicative operators in (4.2) define a Poincaré invariant $4n$ real-dimensional configuration vector space Π spanned by n Weyl spinors and their complex conjugates.

The above (formally) defined operator-valued functions of the canonical operators in (4.1)–(4.2) act on the infinitely dimensional space Γ of complex-valued ''wave'' functions defined on Π.

A Poincaré invariant scalar product on the space of complex-valued functions on Π we tentatively define as

$$\langle f_1 | f_2 \rangle := \int [\overline{f_1}(\overline{\pi}_{B(i)}, \pi_{B'(i)}) f_2(\pi_{B'(i)}, \overline{\pi}_{B(i)})] d\pi^{A'}_{(j)} \wedge d\pi_{A'(j)} \wedge d\overline{\pi}^{A}_{(k)} \wedge d\overline{\pi}_{A(k)}. \tag{4.6}$$

The subspace $\mathfrak{N}$ of Γ consisting of functions having finite norms with respect to this scalar product defines a Hilbert space of quantum states of the massive spinning composite particle.

The quantized version of our general dynamical principle now reads as the following.

Find common eigenvalues and eigenfunctions of a maximal set of Hermitian mutually commuting operators containing the following subset (N refers to the normal ordering of terms):

$$\hat{\mathscr{P}}_a = \overline{\pi}_{A(i)} \pi_{A'(i)}, \tag{4.7}$$

$$\hat{H} = \tfrac{1}{2} \hat{m}^2 + N(g(\hat{a}_{(i)(j)})), \tag{4.8}$$

$$S_z = - \frac{1}{m} \hat{\mathscr{S}}^a n_a = - \frac{1}{m} \hat{\mathscr{S}}^{AA'} n_{AA'} = \frac{1}{2} (\hat{a}_{(i)(j)} \overline{\pi}^{A}_{(i)} \pi^{A'}_{(j)} + \overline{\pi}^{A}_{(i)} \pi^{A'}_{(j)} \hat{a}_{(i)(j)}) n_{AA'} - \frac{1}{4} (\hat{a}_{(i)(i)} \overline{\pi}^{A}_{(j)} \pi^{A'}_{(j)} + \overline{\pi}^{A}_{(j)} \pi^{A'}_{(j)} \hat{a}_{(i)(i)}) n_{AA'}. \tag{4.9}$$

$$\hat{m}^2 \hat{s}^2 := - \hat{\mathscr{S}}^a \hat{\mathscr{S}}_a = - \tfrac{1}{4} (\hat{a}_{(j)(j)})^2 m^2 - N(\hat{a}_{(j)(j)} \hat{a}_{(u)(v)} \overline{m}_{(u)(k)} m_{(k)(v)}) - N(\hat{a}_{(j)(k)} \hat{a}_{(u)(v)} \overline{m}_{(j)(u)} m_{(k)(v)}), \tag{4.10}$$

where m denotes an eigenvalue of the mass and n_a is any space-like unit four-vector orthogonal to the time-like direction defined by $\hat{\mathscr{P}}_a$. In other words, n^a represents a ''z-axis'' direction.

From the assumption 2 and general group theoretical considerations, it follows that eigenvalues of the mass squared $\hat{m}^2$ are proportional (up to an additive real number) to the eigenvalues of

$N(g(\hat{a}_{(i)(j)}))$ (which is assumed to be Hermitian). Moreover, the eigenvalues of the square of the spin $\hat{s}^2$ and of $\hat{S}_z$ assume the usual values, i.e., $j(j+1)$ and $j_z=-j\ldots\ldots,j$, with j being a positive integral number or a positive half-integral number.

For each choice of g one can choose among the operators in (4.5) a maximal set of mutually commuting ones that also commute with $N(g(\hat{a}_{(i)(j)}))$. The eigenvalues of these additional operators may be identified with the internal degrees of freedom of the total system. To each set of eigenvalues of the mutually commuting internal operators and to each set of the mutually commuting external operators' eigenvalues (the mass, j, j_z, total four-momentum of the system) there corresponds a state function in $\mathfrak{N}$ that may be calculated (at least in principle) using methods from nonrelativistic quantum mechanics.

As an example consider the relativistic rigid rotator composed of two ($n=2$) massless constituents with helicity.[9] To quantize it we note that the external commuting observables may be chosen as

$$\hat{\mathscr{P}}_a=\overline{\pi}_{A(1)}\pi_{A'(1)}+\overline{\pi}_{A(2)}\pi_{A'(2)}, \tag{4.11}$$

$$\hat{H}=\tfrac{1}{2}\hat{m}^2+\hat{s}^2, \tag{4.12}$$

$$\begin{aligned}\hat{\mathscr{S}}^a n_a=\mathscr{S}^{AA'}n_{AA'}=&\tfrac{1}{4}(\hat{a}_{(1)(1)}-\hat{a}_{(2)(2)})(\overline{\pi}^A_{(1)}\pi^{A'}_{(1)}-\overline{\pi}^A_{(2)}\pi^{A'}_{(2)})n_{AA'}+(\overline{\pi}^A_{(1)}\pi^{A'}_{(1)}\\&-\overline{\pi}^A_{(2)}\pi^{A'}_{(2)})n_{AA'}\,\tfrac{1}{4}(\hat{a}_{(1)(1)}-\hat{a}_{(2)(2)})+\tfrac{1}{2}(\hat{a}_{(1)(2)}\overline{\pi}^A_{(1)}\pi^{A'}_{(2)}\\&+\overline{\pi}^A_{(1)}\pi^{A'}_{(2)}\hat{a}_{(1)(2)})n_{AA'}+\tfrac{1}{2}(\hat{a}_{(2)(1)}\overline{\pi}^A_{(2)}\pi^{A'}_{(1)}+\overline{\pi}^A_{(2)}\pi^{A'}_{(1)}\hat{a}_{(2)(1)})n_{AA'},\end{aligned} \tag{4.13}$$

$$\hat{s}^2=\tfrac{1}{4}(\hat{a}_{(1)(1)}-\hat{a}_{(2)(2)})^2+\tfrac{1}{2}(\hat{a}_{(1)(2)}\hat{a}_{(2)(1)}+\hat{a}_{(2)(1)}\hat{a}_{(1)(2)}), \tag{4.14}$$

while internal symmetry operators are given, e.g., by

$$\hat{a}_{(1)(1)},\quad \hat{a}_{(2)(2)}. \tag{4.15}$$

In the rigid rotator case the eigenvalues of the square of the mass are proportional to $j(j+1)$, i.e., proportional to the eigenvalues of the square of the spin. In addition, the states (eigenfunctions) of the rigid rotator are labeled by the eigenvalues of the Euler operators in (4.15).

To find these relativistic rigid rotator eigenfunctions, $f(\pi^{A'}_{(1)},\pi^{A'}_{(2)},\overline{\pi}^A_{(1)},\overline{\pi}^A_{(2)})$ in $\mathfrak{N}$ is a much harder task and will not be pursued in this paper.

V. CONCLUSIONS AND REMARKS

If ''elementary'' particles such as e.g., electron, proton, neutron, etc. may be regarded as bound states of a *finite* number of massless spinning parts, then twistor theory combined with the idea of relativistic action at a distance provide a very powerful tool for construction of such models.

In such approaches, as shown in this paper, particle aspects of Penrose's twistor formalism should be emphasized, as opposed to the standard treatments where field aspects are at the front.

The nonstandard quantization procedure in (4.1)–(4.2) implies that we lose some of the results of conventional twistor theory, such as the twistor description of massless free fields in terms of holomorphic sheaf cohomology, the scalar product on such fields, geometrization of the concept of positive frequency of the field and the relationship between conformal curvature and the twistor ''position'' (twistor variables) and ''momentum'' (complex conjugates of the twistor variables) operators.[19]

What we gain is that the real dimension of the relativistic configuration space of massless spinning particles is one-half the real dimension of the configuration space obtained by means of the conventional holomorphic twistor quantization.[1] Further, the configuration space obtained in our paper may be given a clear physical interpretation. Wave functions on such a configuration space define quantum states in (the ''square root'' of) the linear four-momentum representation of the massless parts. However, in our opinion the most important gain is the fact that using our formulation we are able to treat *interacting* massless spinning particles (not fields), forming a closed composite bound system.

To apply our ideas to concrete physical systems is, at the moment, hampered by the fact that there are, as yet, no indications in the model how the function g in (3.36) should be chosen.

Nevertheless, the general principle presented in this paper seems to comply with the Twistor Programme announced by Penrose.[20]

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A solvable *N*-body problem in the plane. I

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We introduce and discuss an n-body problem *in the plane*, characterized by equations of motion of Newtonian type, $\ddot{\vec{r}}_j = \Sigma_{k=1}^{n} \vec{F}_{jk}$, $j=1,..,n$, with given ''forces'' $\vec{F}_{jk}$ having the following characteristics: $\vec{F}_{jk}$ depends only on $\vec{r}_j, \vec{r}_k, \dot{\vec{r}}_j, \dot{\vec{r}}_k$ (i.e., only ''one-body'' and ''two-body'' forces are present); $\vec{F}_{jk}$ behaves as a (two-dimensional) vector under rotations in the plane (i.e., the model is ''rotation-invariant''); for $j=k, \vec{F}_{jk}$ is linear in $\vec{r}_j$ and $\dot{\vec{r}}_j$; for $j \neq k$, $\vec{F}_{jk} = |\vec{r}_j - \vec{r}_k|^{-2} \vec{f}_{jk}$ with $\vec{f}_{jk}$ a homogeneous polynomial of third degree in $\vec{r}_j, \vec{r}_k, \dot{\vec{r}}_j, \dot{\vec{r}}_k$ (hence $\vec{F}_{jk}$ is homogeneous of degree one in $\vec{r}_j, \vec{r}_k, \dot{\vec{r}}_j, \dot{\vec{r}}_k$); $\vec{F}_{jk}$ contains linearly 8 arbitrary (''coupling'') constants. The n-body problem is solvable for arbitrary n and for arbitrary values of the 8 coupling constants; its solutions display a rich phenomenology. If the 8 coupling constants are suitably restricted, the model is translation-invariant, and/or Hamiltonian; of course, when it is Hamiltonian, it is integrable; indeed in some case a Hamiltonian function can be explicitly displayed, as well as the corresponding Lax pair. © *1996 American Institute of Physics.*
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I. INTRODUCTION

In this paper we introduce the n-body problem in the plane characterized by the equations of motion of Newtonian type

$$\ddot{\vec{r}}_j = \sum_{k=1}^{n} \vec{F}_{jk}, \quad j=1,\ldots,n, \tag{1.1}$$

with

$$\vec{F}_{jk} = (\alpha + \alpha' \hat{z}\wedge)\dot{\vec{r}}_j + (\beta + \beta' \hat{z}\wedge)\vec{r}_j \quad \text{for } j=k, \tag{1.2a}$$

$$\vec{F}_{jk} = r_{jk}^{-2} \vec{f}_{jk} \quad \text{for } j \neq k, \tag{1.2b}$$

with

$$\vec{f}_{jk} = 2[\dot{\vec{r}}_j(\dot{\vec{r}}_k \cdot \vec{r}_{jk}) + \dot{\vec{r}}_k(\dot{\vec{r}}_j \cdot \vec{r}_{jk}) - \vec{r}_{jk}(\dot{\vec{r}}_j \cdot \dot{\vec{r}}_k)] + (\lambda + \lambda' \hat{z}\wedge)\{(\dot{\vec{r}}_j + \dot{\vec{r}}_k)[r_j^2 - (\vec{r}_j \cdot \vec{r}_k)]$$
$$- \vec{r}_j[\vec{r}_k \cdot (\dot{\vec{r}}_j + \dot{\vec{r}}_k)] + \vec{r}_k[\vec{r}_j \cdot (\dot{\vec{r}}_j + \dot{\vec{r}}_k)]\} + (\mu + \mu' \hat{z}\wedge)\{\vec{r}_j[r_j^2 - 2(\vec{r}_j \cdot \vec{r}_k)] + \vec{r}_k r_j^2\}. \tag{1.3}$$

Throughout this paper a superimposed arrow denotes (two-dimensional) vectors in the plane; but we use for convenience for them a ''three-dimensional'' notation, denoting by $\hat{z}$ the unit vector orthogonal to the plane, and by the symbol $\wedge$ the usual three-dimensional vector

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product. Hence $\hat{z}\equiv(0,0,1)$, and, for instance, $\vec{r}_j\equiv(x_j,y_j,0)$, $\hat{z}\wedge\vec{r}_j=(-y_j,x_j,0)$. We also employ the convenient short-hand notation $\vec{r}_{jk}\equiv\vec{r}_j-\vec{r}_k$, and of course $r_{jk}^2\equiv\vec{r}_{jk}\cdot\vec{r}_{jk}=x_{jk}^2+y_{jk}^2=(x_j-x_k)^2+(y_j-y_k)^2$.

The n-body model (1.1)–(1.3) is solvable for arbitrary n and for arbitrary values of the 8 (real) ''coupling'' constants $\alpha,\alpha',\beta,\beta',\lambda,\lambda',\mu,\mu'$: the n ''particle coordinates'' $\vec{r}_j(t)$, corresponding to arbitrary initial data $\vec{r}_k(0),\dot{\vec{r}}_k(0)$, $k=1,\ldots,n$, coincide (see below) with the n roots of an explicitly known (time-dependent, complex) polynomial and their time-evolution can therefore be analyzed rather transparently (although, given the generality of this model, the phenomenology of the motions it entails is quite rich). This finding is remarkable, in view of the dearth of solvable n-body models in more than one dimension; yet it obtains via quite a simple extension (by complexification) of a one-dimensional model whose solvability had been pointed out almost two decades ago.[1] The interest of the model (1.1)–(1.3) is moreover enhanced by the fact that, provided the coupling constants are appropriately restricted, it is Hamiltonian (and then, of course, completely integrable); indeed in some cases a Hamiltonian function can be explicitly displayed, as well as a corresponding Lax pair (drawing, again, on results which have been known for quite some time[2]).

To advertise the richness and neatness of this model it might perhaps be mentioned that this two-dimensional extension was noticed in the course of a personal revisitation of known one-dimensional models,[1] motivated by a request[3] to indicate the *simplest yet nontrivial* integrable model which could be taught to first-year students of mechanics (but of course *all* solvable models are in some sense *trivial*!).

In Sec. II we briefly discuss the invariance properties of the equations of motion (1.1)–(1.3), and the motion they entail in some special case for the center-of-mass of the system. In Sec. III we indicate how this model has been obtained, and how it is solved. In Sec. IV we discuss the behavior of the solutions; the phenomenology being quite rich, this section is by far the longest, and it is subdivided into several subsections to treat separately various different cases, including those in which the system is translation-invariant or Hamiltonian. A concluding Sec. V outlines future directions of research.

II. INVARIANCE PROPERTIES AND CENTER-OF-MASS MOTION

In this brief section we discuss the invariance properties of the equations of motion (1.1)–(1.3), and the motion they entail in some special case for the center-of-mass $\vec{R}$ of the system,

$$\vec{R}=n^{-1}\sum_{j=1}^{n}\vec{r}_j\,. \tag{2.1}$$

The system (1.1)–(1.3) is autonomous, since we assume the 8 quantities $\alpha,\alpha',\beta,\beta',\lambda,\lambda',\mu,\mu'$ to be time-independent (although it should be noted that the technique of solution would also work if these quantities were time-dependent). Hence it is invariant under time-translation, $t\to t+t_0$.

The system (1.1)–(1.3) is also invariant under scale-transformation of the particle coordinates $\vec{r}_j$, namely under the transformation $\vec{r}_j\to c\vec{r}_j$, with c an arbitrary constant.

In the special case in which all 8 coupling constants vanish, $\alpha=\alpha'=\beta=\beta'=\lambda=\lambda'=\mu=\mu'=0$, the system (1.1)–(1.3) is moreover invariant under time rescaling, $t\to at$ with a an arbitrary constant; and in this special case, since $\vec{F}_{jk}=-\vec{F}_{kj}$ [see (1.2)–(1.3)], the center-of-mass (2.1) moves freely: $\ddot{\vec{R}}=0$. In view of its remarkable simplicity this case (which is Hamiltonian and of course integrable, and allows the *explicit* display of its Hamiltonian structure, including its Lax representation) is discussed in some detail below (see Sec. IV F).

In the slightly less special case in which only the coupling constants α and α' do not vanish ($\beta=\beta'=\lambda=\lambda'=\mu=\mu'=0$), the system (1.1)–(1.3) is clearly invariant under space translations ($\vec{r}_j\to\vec{r}_j+\vec{b}$; $j=1,..,n$; $\vec{b}=$arbitrary constant two-dimensional vector in the plane). In this case the center-of-mass $\vec{R}(t)$, see (2.1), evolves according to the linear equation

$$\ddot{\vec{R}}=(\alpha+\alpha'\hat{z}\wedge)\dot{\vec{R}}, \tag{2.2a}$$

so that (see below)

$$\vec{R}(t)=\vec{R}(0)+(\alpha^2+\alpha'^2)^{-1}\cdot[\dot{\vec{R}}(0)\{\alpha[\exp(\alpha t)\cos(\alpha' t)-1]+\alpha'\ \exp(\alpha t)\sin(\alpha' t)\}$$
$$+\hat{z}\wedge\dot{\vec{R}}(0)\{-\alpha'[\exp(\alpha t)\cos(\alpha' t)-1]+\alpha\ \exp(\alpha t)\sin(\alpha' t)\}]. \tag{2.2b}$$

In fact, the motion of the center-of-mass can be explicitly displayed also in the general case (generic values of all 8 coupling constants); see below.

Finally, and most importantly, the system (1.1)–(1.3) is invariant under rotations in the plane ($x_j\to x_j\cos\theta-y_j\sin\theta$, $y_j\to x_j\sin\theta+y_j\cos\theta$; $j=1,..,n$; θ arbitrary time-independent angle of rotation). This is an essential feature to interpret this system as a genuine n-body problem in the plane.

III. THE ORIGIN OF THE MODEL AND ITS SOLUTION

Almost two decades ago it was shown[1] that the one-dimensional n-body problem characterized by the equations of motion

$$\ddot{z}_j=\alpha_1\dot{z}_j+\beta_0+\beta_1 z_j+\sum_{k=1,k\neq j}^{n}(z_j-z_k)^{-1}.\{2\dot{z}_j\dot{z}_k+(\dot{z}_j+\dot{z}_k)(\lambda_0+\lambda_1 z_j)$$
$$+\lambda_2(\dot{z}_j z_k+\dot{z}_k z_j)z_j+\mu_{-1}+\mu_0 z_j+\mu_1 z_j^2+\mu_2 z_j^2 z_k\} \tag{3.1}$$

is *solvable*, since the motion of these n ''particle coordinates'' $z_j(t)$ may be identified with the motion of the n zeros of the polynomial solution $\psi(z,t)$,

$$\psi(z,t)=\prod_{j=1}^{n}[z-z_j(t)], \tag{3.2a}$$

of the *linear* partial differential equation

$$\psi_{tt}-(\lambda_0+\lambda_1 z+\lambda_2 z^2)\psi_{zt}+\tfrac{1}{2}(\mu_{-1}+\mu_0 z+\mu_1 z^2+\mu_2 z^3)\psi_{zz}-[\alpha_1-(n-1)\lambda_2 z]\psi_t$$
$$+[\beta_0+\beta_1 z-(n-1)\mu_2 z^2]\psi_z-[\tfrac{1}{2}n(n-1)(\mu_1-\mu_2 z)+n\beta_1]\psi=0, \tag{3.3}$$

identified by the initial data implied by (3.2a),

$$\psi(z,0)=\prod_{j=1}^{n}[z-z_j(0)], \tag{3.4a}$$

$$\psi_t(z,0)=-\psi(z,0)\sum_{j=1}^{n}\{\dot{z}_j(0)/[z-z_j(0)]\}. \tag{3.4b}$$

Since this solution is a polynomial in z of degree n,

$$\psi(z,t)=z^n+\sum_{m=1}^{n} c_m(t)z^{n-m}, \tag{3.2b}$$

to find it, it is generally necessary and sufficient to solve the linear system of ordinary differential equations satisfied by the coefficients $c_m(t)$, $m=1,..,n$, as implied by (3.2b) and (3.3). If all the ''coupling constants'' α_1, β_0, β_1, λ_0, λ_1, λ_2, μ_{-1}, μ_0, μ_1, and μ_2 are time-independent, as we assume hereafter, the solution of this system is an easy algebraic task; indeed in some cases it can be performed in closed form (see below). The solution of the n-body problem (3.1) is thus reduced to finding the zeros $z_j(t)$ of a known time-dependent polynomial in z of degree n.[1]

The potentialities of this approach, both as a source of solvable n-body problems on the line, and of related mathematical results, have been amply explored and reviewed in a number of papers.[4] And, as it is natural in any investigation that involves the zeros of a polynomial, the idea to extend the analysis from the real axis to the complex plane was also explored. In this manner solvable n-body problems in the plane (rather than on the line) can of course be generated. But these models did not appear to qualify as genuine n-body problems in the plane, because their equations of motion generally are not invariant under rotations of the frame of reference in the plane.[4]

The progress reported in this paper originates from a simple observation: if one focuses on the subcase of (3.1) characterized by the restrictions

$$\beta_0=\lambda_0=\lambda_2=\mu_0=\mu_2=\mu_3=0, \tag{3.5a}$$

so that the equations of motion read

$$\ddot{z}_j=(\alpha+\mathrm{i}\alpha')\dot{z}_j+(\beta+\mathrm{i}\beta')z_j+\sum_{k=1,k\neq j}^{n}(z_j-z_k)^{-1}$$
$$\cdot\{2\dot{z}_j\dot{z}_k+(\lambda+\mathrm{i}\lambda')(\dot{z}_j+\dot{z}_k)z_j+(\mu+\mathrm{i}\mu')z_j^2\}, \tag{3.6}$$

then the system is clearly invariant under rescaling of the dependent variables $z_j, z_j\to cz_j$, and in particular under the transformation

$$z_j\to z_j'=\exp(\mathrm{i}\theta)z_j. \tag{3.7a}$$

Note that, to write (3.6) in more explicit form, we have introduced the real and imaginary parts of the nonvanishing coupling constants, by setting

$$\alpha_1=\alpha+\mathrm{i}\alpha', \quad \beta_1=\beta+\mathrm{i}\beta', \quad \lambda_1=\lambda+\mathrm{i}\lambda', \quad \mu_1=\mu+\mathrm{i}\mu', \tag{3.5b}$$

of course now with the 8 ''coupling constants'' $\alpha,\alpha',\beta,\beta',\lambda,\lambda',\mu,\mu'$ all real.

But if one now interprets the real and imaginary parts of z_j,

$$z_j=x_j+\mathrm{i}y_i, \tag{3.8a}$$

as the x- and y-components of a two-vector $\vec{r}_j$ in the plane,

$$\vec{r}_j\equiv(x_j,y_j,0), \tag{3.8b}$$

then clearly the transformation (3.7a) corresponds to a rotation in the plane:

$$\vec{r}_j\to\vec{r}_j'=(x_j',y_j',0), \tag{3.7b}$$

$$x_j'=x_j\cos\theta-y_j\sin\theta, \tag{3.7c}$$

$$y_j' = x_j \sin\theta + y_j \cos\theta. \tag{3.7d}$$

Hence the subclass (3.6) yields, via the complexification (3.8a), a rotation-invariant model. And indeed *it is easily seen that, via the position (3.8), the equations of motion (3.6) coincide with (1.1)–(1.3).*

This argument explains the origin of the *n*-body model in the plane characterized by the rotation-invariant equations of motion (1.1)–(1.3), and of course it also entails that its solution is provided, via (3.8), by the *n* zeros of the polynomial (3.2b), namely by the formula [see (3.2a, b)]

$$\prod_{j=1}^{n} [z - z_j(t)] = z^n + \sum_{m=1}^{n} c_m(t) z^{n-m}, \tag{3.9}$$

with

$$c_m(t) = c_m^{(+)} \exp[\nu_m^{(+)} t] + c_m^{(-)} \exp[\nu_m^{(-)} t], \tag{3.10}$$

$$\nu_m^{(\pm)} = \tfrac{1}{2}\{\alpha + \lambda(n-m) + i[\alpha' + \lambda'(n-m)] \pm \Delta_m\}, \tag{3.11}$$

$$\begin{aligned}\Delta_m^2 = {} & [\alpha + \lambda(n-m)]^2 - [\alpha' + \lambda'(n-m)]^2 + 4\beta m + 2\mu m(2n-m-1) \\ & + i\{2[\alpha + \lambda(n-m)][\alpha' + \lambda'(n-m)] + 4\beta' m + 2\mu' m(2n-m-1)\},\end{aligned} \tag{3.12}$$

$$c_m^{(\pm)} = \pm[\dot{c}_m(0) - \nu_m^{(\mp)} c_m(0)]/\Delta_m. \tag{3.13}$$

These relations follow of course from the linear partial differential equation [see (3.3) and (3.5)]

$$\psi_{tt} - \lambda_1 z \psi_{zt} + \tfrac{1}{2}\mu_1 z^2 \psi_{zz} - \alpha_1 \psi_t + \beta_1 z \psi_z - [\tfrac{1}{2} n(n-1)\mu_1 + n\beta_1]\psi = 0, \tag{3.14}$$

which entails, via (3.2b)

$$\ddot{c}_m - [\alpha_1 + \lambda_1(n-m)]\dot{c}_m - m[\beta_1 + \tfrac{1}{2}\mu_1(2n-m-1)]c_m = 0. \tag{3.15}$$

As for the initial data, $c_m(0)$ and $\dot{c}_m(0)$, they are related to the initial positions $\vec{r}_j(0)$ and velocities $\dot{\vec{r}}_j(0)$ of the *n* particles in the plane, via (3.8), which of course also imply

$$\dot{z}_j = \dot{x}_j + i\dot{y}_j, \quad j = 1,..,n, \tag{3.16a}$$

$$\dot{\vec{r}} \equiv (\dot{x}_j, \dot{y}_j, 0), \quad j = 1,..,n, \tag{3.16b}$$

and via the relations implied by (3.9):

$$\sum_{m=1}^{n} c_m(0) z^{n-m} = -z^n + \prod_{j=1}^{n} [z - z_j(0)], \tag{3.17a}$$

$$\sum_{m=1}^{n} \dot{c}_m(0) z^{n-m} = -\sum_{j=1}^{n} \dot{z}_j(0) \prod_{k=1, k\neq j}^{n} [z - z_k(0)], \tag{3.17b}$$

which of course entail

$$c_1(0) = -\sum_{j=1}^{n} z_j(0), \tag{3.18a}$$

$$c_2(0)=\sum_{j,k=1;j\neq k}^{n} z_j(0)z_k(0), \tag{3.18b}$$

$$c_3(0)=-\sum_{j,k,l=1;j\neq k,k\neq l,l\neq j}^{n} z_j(0)z_k(0)z_l(0) \tag{13.8c}$$

and so on, as well as

$$\dot{c}_1(0)=-\sum_{j=1}^{n} \dot{z}_j(0), \tag{3.19a}$$

$$\dot{c}_2(0)=2\sum_{j,k=1;j\neq k}^{n} \dot{z}_j z_k(0), \tag{3.19b}$$

$$\dot{c}_3(0)=-3\sum_{j,k,l=1;j\neq k,k\neq l,l=j}^{n} \dot{z}_j(0)z_k(0)z_l(0)\cdots . \tag{3.19c}$$

Let us emphasize that the key to the solution is the formula (3.9), that provides a *one-to-one (nonlinear) transformation* between the n (complex) ''particle coordinates'' $z_j(t)$ [see (3.8)], which evolve according to (3.6) namely (1.1)–(1.3), and the n (complex) ''collective coordinates'' $c_m(t)$, which evolve according to (3.15), namely (3.10)–(3.13) with (3.17). These latter formulas are of course quite explicit and very simple.

Note in particular that the center-of-mass coordinate $\vec{R}(t)$, see (2.1), is simply related to the collective coordinate $c_1(t)$:

$$\vec{R}(t)\equiv(-n\ \mathrm{Re}[c_1(t)],-n\ \mathrm{Im}[c_1(t)],0); \tag{3.20}$$

hence its time evolution can be read directly from (3.10)–(3.13) (with $m=1$).

Simple and explicit as the time evolution (3.10)–(3.13) is, it is quite rich, and it implies, via (3.9) and (3.8), an even richer gamut of possible behaviors for the particle coordinates $\vec{r}_j(t)$. Several possibilities are surveyed in the following section. A more complete analysis is postponed to a future paper.

IV. MOTIONS IN THE PLANE AND SPECIAL MODELS

In this section we survey tersely the various possible motions of n particles in the plane, whose time evolution is determined by the equations of motion (1.1)–(1.3). As we have seen in the previous section, they in fact coincide, via the identification (3.8), with the motions in the complex plane of the n zeros $z_j(t)$ of the time-dependent polynomial of degree n in z whose expression is displayed in the right-hand-side of (3.9), with its time-dependent coefficients $c_m(t)$ given explicitly by (3.10)–(3.13) and, in terms of the initial positions $\vec{r}_j(0)$ and velocities $\dot{\vec{r}}_j(0)$ of the n particles in the plane, by (3.17) [with (3.16) and (3.8)].

In particular, we analyze the behavior of the system as $t\to+\infty$, and also as $t\to-\infty$, assuming it starts from given initial data at $t=0$. Of course the most important factor which determines the long-time behavior of the system are the real parts of the quantities $\nu_m^{(\pm)}$, see (3.11)–(3.12). Hence we set

$$\nu_m^{(\pm)}=\rho_m^{(\pm)}+\mathrm{i}\gamma_m^{(\pm)}, \quad m=1,..,n, \tag{4.1}$$

of course with $\rho_m^{(\pm)}$ and $\gamma_m^{(\pm)}$ real:

$$\rho_m^{(\pm)} = \tfrac{1}{2}[\alpha + \lambda(n-m) \pm \delta_m^{(+)}], \tag{4.2a}$$

$$\gamma_m^{(\pm)} = \tfrac{1}{2}[\alpha' + \lambda'(n-m) \pm \delta_m^{(-)}], \tag{4.2b}$$

where of course [see (3.11)–(3.12)]

$$\Delta_m = \delta_m^{(+)} + \mathrm{i}\delta_m^{(-)}, \tag{4.3a}$$

$$\delta_m^{(\pm)} = \{[(a_m^2 + b_m^2)^{1/2} \pm a_m]/2\}^{1/2} \geqslant 0, \tag{4.3b}$$

$$a_m = [\alpha + \lambda(n-m)]^2 - [\alpha' + \lambda'(n-m)]^2 + 2m[2\beta + \mu(2n-m-1)], \tag{4.3c}$$

$$b_m = 2\{[\alpha + \lambda(n-m)][\alpha' + \lambda'(n-m)] + m[2\beta' + \mu'(2n-m-1)]\}. \tag{4.3d}$$

A. The generic case

In this subsection we analyze (on the basis of the results of Appendix A, that should be read now, before proceeding any further) the behavior of the system in the generic case, when the 8 (real) coupling constants $\alpha,\alpha',\beta,\beta',\lambda,\lambda',\mu,\mu'$ have generic values (namely, we assume that these 8 coupling constants do not satisfy any of the equalities, which characterize instead the special cases discussed below).

Let us now consider the values of the $2n$ quantities $\rho_m^{(\pm)}$, $m=1,..,n$; since we are looking at the generic case, we assume they are *all* different, and we call ρ_+ the largest of these $2n$ real numbers and m_+ the corresponding value of m (of course $1 \leqslant m_+ \leqslant n$); likewise we call ρ_- the smallest of these $2n$ real numbers, and m_- the corresponding value of $m (1 \leqslant m_- \leqslant n)$:

$$\rho_m^{(\pm)} \leqslant \rho_+, \quad m=1,..,n; \quad \rho_{m_+}^{(+)} = \rho_+, \tag{4.4a}$$

$$\rho_m^{(\pm)} \geqslant \rho_-, \quad m=1,..,n; \quad \rho_{m_-}^{(-)} = \rho_-. \tag{4.4b}$$

The behavior of the system as $t \to \infty$ is mainly determined by the value of ρ_+ (and of m_+ if ρ_+ is positive); likewise the behavior as $t \to -\infty$ is mainly determined by the value of ρ_- (and of m_- if ρ_- is negative). Indeed if ρ_+ is negative, $\rho_+ < 0$, as $t \to \infty$ *all* n particles tend to the origin; and this happens for *all* initial conditions. In this case, of course, ρ_- is also negative, $\rho_- < 0$; then, as $t \to -\infty$, generally $n - m_-$ particles tend to the origin and m_- escape to infinity, namely they came in from a large distance in the remote past (but there exist special systems which display a different behavior, for instance some of the m_- particles might approach a periodic trajectory in a finite region of the plane rather than going to, or rather coming from, infinity; see Appendix A). This behavior corresponds to a *generic* set of initial conditions; a different behavior occurs for the *special* set of initial data characterized by the condition $c_{m_-}^{(-)} = 0$.

If instead ρ_+ is positive, $\rho_+ > 0$, as $t \to \infty$ generally m_+ particles escape to infinity and $n - m_+$ tend to the origin (but again there are special systems that yield a richer behavior: if there is more than a single value of m, in the interval $1 \leqslant m \leqslant n$, for which ρ_m attains its maximal value ρ_+, then some particles also tend to a periodic circular trajectory, see Appendix A); and again this outcome emerges from generic initial data (the exception, as discussed above, is the case when $c_{m_+}^{(+)} = 0$). As for the behavior as $t \to -\infty$: if ρ_- is also positive, $\rho_- > 0$, *all* particles tend to (or rather, in the remote past, came from) the origin (for arbitrary initial data); if ρ_- is negative, $\rho_- < 0$, generally m_- particles tend to (or rather, in the remote past, came from) infinity and $n - m_-$ tend to (i.e., came from) the origin (but other behaviors are also possible in special cases, see Appendix A).

This completes the outline of the behavior of solutions of the completely generic system of type (1.1)–(1.3), characterized by 8 coupling constants which do not satisfy any of the equalities

that characterizes the (more, or less) special cases considered below (or other special cases, which shall be discussed in future papers). This analysis has looked mainly at the motions that correspond to generic initial data. In some cases, some of which have been indicated above but without delving into any detailed analysis, there are (more, or less) special initial data which determine motions with some qualitative difference from the generic case. This may happen if the initial data cause some of the quantities $c_m^{(+)}, c_m^{(-)}$ to vanish [see (3.10), (3.13), (3.17)]. Note that the vanishing of *all* these quantities, $c_m^{(+)}=c_m^{(-)}=0$, $m=1,..,n$, is necessary and sufficient for the system to be at equilibrium (no time-evolution); but, as implied by (3.9) or (3.17), the only equilibrium configuration, for the generic system under present consideration, is the rather unphysical one with all particles piled up at the origin (systems with nontrivial equilibrium configurations are discussed in Sec. IV G).

Let us now continue, in the same vein, to survey the types of motion associated with the system (1.1)–(1.3), but now for values of the 8 coupling constants $\alpha,\alpha',\beta,\beta',\lambda,\lambda',\mu,\mu'$ which are restricted by the requirement to satisfy some equalities.

B. Models featuring a limit cycle

The first model we consider is the borderline case which falls between the two possibilities considered above, namely the case in which the quantity ρ_+, defined as above [see (4.4a)], vanishes:

$$\rho_+=0. \tag{4.5}$$

Note that this entails essentially a single (algebraic) constraint to be satisfied by the 8 coupling constants. Let us moreover assume that, except for (4.5), the system is generic, in particular such that $\rho_m^{(+)}<\rho_+$, for $m=1,..,n$ and $m\neq m_+$ (and *a fortiori* $\rho_m^{(-)}<\rho_+$ for $m=1,..,n$). It is then clear (see Appendix A) that, in the remote future ($t\to\infty$), $n-m_+$ particles tend to the origin, and m_+ approach (exponentially in time) the circular (limit-cycle) trajectories

$$\tilde{z}_k(t)=\exp(2\pi ik/m_+)(-c_{m_+})^{1/m_+}\exp(i\gamma_{m_+}t/m_+), \quad k=1,..,m_+. \tag{4.6}$$

Two comments about this formula are now in order.

Note first of all that, for notational convenience, we use here the standard rule to identify a two-dimensional vector in the plane by the complex number that corresponds to it via the identification (3.8). Clearly, via this identification, (4.6) describes a circular ring of m_+ equispaced particles which rotates uniformly around the origin.

Second, the notation $\tilde{z}_k(t)$ has been introduced to emphasize two important points: in the first place, the ''particle coordinates'' $z_j(t)$ do not coincide with the quantities $\tilde{z}_k(t)$, they only approach them (exponentially fast) as $t\to\infty$; and second, m_+ of the n ''particle coordinates'' $z_j(t)$, $j=1,..,n$, approach asymptotically the m_+ quantities $\tilde{z}_k(t)$, $k=1,..,m_+$ [see (4.6)]; but to ascertain whether, say, $z_1(t)$ tends to the origin or to one of the quantities $\tilde{z}_k(t)$, and in such a case to which one, a more detailed analysis of the motion is required than that given here (indeed, the choice between these different options depends nontrivially upon the initial data).

This behavior of the system as $t\to\infty$ emerges essentially out of any initial data; but of course for the subset of initial data such that $c_{m_+}^{(+)}$ vanishes, $c_{m_+}^{(+)}=0$, the limit circle (4.6) shrinks to the origin, so that for this subset of initial data all n particles tend to the origin as $t\to\infty$.

For the behavior of the system as $t\to-\infty$, the analysis given in the preceding Sec. IV A is applicable (of course, with $\rho_-<0$).

There clearly exists a plethora of other, non-completely-generic, models; for instance it might happen that, for some value of m, $\nu_m^{(+)}=\nu_m^{(-)}$, in which case the formula (3.10) would have to be

modified in a well-known manner. We forsake here the investigation of these possibilities, as well as the others hinted at above, and proceed to analyze some more special, and perhaps more interesting, cases.

C. Models with confined and with periodic motions

Let us now consider the model with

$$\alpha=0, \quad \lambda=0, \quad \beta'=0, \quad \mu'=0. \tag{4.7}$$

These 4 conditions, together with the 3 inequalities

$$\alpha'^2-2n[2\beta+(n-1)\mu]\geqslant 0, \tag{4.8a}$$

$$[\alpha'+(n-1)\lambda']^2-4[\beta+(n-1)\mu]\geqslant 0, \tag{4.8b}$$

$$(\alpha'+n\lambda')^2-(\lambda'^2+2\mu)^{-1}[\lambda'(\alpha'+n\lambda')+2\beta+(2n-1)\mu]^2\geqslant 0, \tag{4.8c}$$

are sufficient to guarantee that all the exponents $\nu_m^{(\pm)}$ be imaginary:

$$\nu_m^{(\pm)}=i\gamma_m^{(\pm)}, \tag{4.9a}$$

$$\gamma_m^{(\pm)}=\tfrac{1}{2}[\alpha'+\lambda'(n-m)]\pm\tfrac{1}{2}\{[\alpha'+\lambda'(n-m)]^2-2m[2\beta+(2n-m-1)\mu]\}^{1/2}. \tag{4.9b}$$

Note that the 3 inequalities (4.8) guarantee that, for all values of m, $1\leqslant m\leqslant n$, the argument of the square root in the right-hand-side of (4.9b) is non-negative, so that $\gamma_m^{(\pm)}$, as given by this formula, is real.

It is then clear that, under these conditions, the system (1.1)–(1.3) [which features now, see (4.7), the 4 arbitrary constants α', β, λ', and μ, restricted by the 3 inequalities (4.8)], yields, from *any* initial data, *trajectories which remain confined* to a finite region of the plane: see (3.9), (3.10), and (4.9). It is moreover clear that there are special initial conditions for which the motion is *completely periodic*, with period, say, $T=2\pi n!/\gamma_{m'}^{(+)}$ (or $T=2\pi n!/\gamma_{m'}^{(-)}$); they emerge of course from initial data such that, of all the $2n$ constants $c_m^{(\pm)}$, $m=1,..,n$, see (3.10)–(3.13) and (3.17), only $c_{m'}^{(+)}$ (or only $c_{m'}^{(-)}$) does not vanish.

This analysis applies of course if the values of the 4 nonvanishing coupling constants α', β, λ', and μ are generic. The system might behave differently for special values of these constants, for instance, if one or more of the $2n$ quantities $\gamma_m^{(\pm)}$, $m=1,..,n$, vanish; in such a case there would exist an equilibrium configuration different from the (unphysical) one in which all the particles pile up at the origin (see Sec. IV G). Let us mention here only the remarkable special case in which, from *any* initial data, there emerges a *completely periodic* trajectory. It is easily seen that this happens if the following 3 conditions hold [in addition to (4.7)]:

$$\alpha'+n\lambda'=0, \tag{4.10a}$$

$$2\beta+(2n-1)\mu=0, \tag{4.10b}$$

$$(1+2\mu/\lambda'^2)^{1/2}=p/q, \quad q>0, \tag{4.10c}$$

with p and q two *arbitrary integers* (q positive); we assume here that $|p|$ neither equals q, nor is divisible by q (unless $q=1$). Indeed it is easily seen that, in such a case,

$$\gamma_m^{(\pm)}=2\pi m(-q\mp p)/T', \quad m=1,..,n, \tag{4.11a}$$

with

$$T' = 4\pi q/\lambda', \tag{4.11b}$$

implying, see (4.9a) and (3.10) [and of course (3.9) and (3.8)], that in this case *all* trajectories, emerging from *any* initial data, are periodic with period $T = T' n!$. We are of course assuming here that λ' does not vanish, so that T is finite; this entails that also α' does not vanish, see (4.10a). Other cases which also feature completely periodic trajectories for any initial data, but with $\alpha' = \lambda' = 0$ respectively $\alpha' \neq 0, \lambda' = 0$, are discussed at the end of Secs. IV D, respectively, IV E.

D. Hamiltonian models

In this subsection we consider the models (1.1)–(1.3) in the special case

$$\alpha = \alpha' = \lambda = \lambda' = 0. \tag{4.12}$$

What makes these models worthy of focused attention is, that the corresponding equations for the coefficients $c_m(t)$ then read [see (3.15)],

$$\ddot{c}_m - m[\beta_1 + \tfrac{1}{2}\mu_1(2n - m - 1)]c_m = 0; \tag{4.13}$$

hence the evolution of these quantities is obviously, indeed trivially, *Hamiltonian*. But the transformation (3.9) among the ''particle coordinates'' $z_j(t)$ and the ''collective coordinates'' $c_m(t)$, as all *point* transformations, is certainly *canonical*. Hence the equations of motion (3.6) with (4.12) are certainly also *Hamiltonian* (how to write *in explicit form* the corresponding Hamiltonian function is discussed in a separate paper[8]).

It might appear that this argument only applies in the real domain, namely only if β_1 and μ_1 are real [implying $\beta' = \mu' = 0$; see (3.5b)], and $z_j(t)$ and $c_m(t)$ are also real; which would exclude the possibility to conclude that the two-dimensional system (1.1)–(1.3) with (4.12) is Hamiltonian. But the Hamiltonian structure can be generally extended from the real to the complex (i.e., two-dimensional) case, as we show in Appendix B.

The case with β_1 and μ_1 real, namely [see (3.5b)]

$$\beta' = \mu' = 0, \tag{4.14}$$

and moreover with

$$2\beta + \mu(2n - 1) = 0, \tag{4.15a}$$

$$\mu > 0, \tag{4.15b}$$

deserves however to be singled out, because it is again characterized by *completely periodic trajectories*, with period $T = 2\pi(2/\mu)^{1/2} n!$, for *any* initial data, since in this case [see (3.9)–(3.12)]

$$\nu_m^{(\pm)} = \pm i(\mu/2)^{1/2} m, \quad m = 1, .., n. \tag{4.16}$$

E. Translation-invariant models

As we indicated in Sec. II, the equations of motion (1.1)–(1.3) are translation-invariant if

$$\beta = \beta' = \lambda = \lambda' = \mu = \mu' = 0. \tag{4.17}$$

In this subsection we discuss these models. Note that in this case the equations of motion entail that a particle is acted upon by a nonvanishing force, and contributes by its presence to the force acting on other particles, *only if it moves* [with a nonvanishing velocity; except possibly at the

instant of a collision: see (1.1)–(1.3) with (4.17)]. Hence, in the context of the initial-value problem, only particles whose initial velocities $\dot{\vec{r}}_j(0)$ do not vanish, need to be taken into account; particles whose initial velocities vanish can simply be ignored.

In this case the solution of the initial-value problem is of course still yielded by (3.9) with (3.8), but the time-evolution of the coefficients $c_m(t)$ now reads [see (3.15)]

$$c_m(t)=c_m(0)+(\alpha+\mathrm{i}\alpha')^{-1}\dot{c}_m(0)\{\exp[(\alpha+\mathrm{i}\alpha')t]-1\}. \tag{4.18}$$

The initial values $c_m(0),\dot{c}_m(0)$ are still related to the initial positions $\vec{r}_j(0)$ and velocities $\dot{\vec{r}}_j(0)$ of the n particles in the plane via (3.17) [with (3.8) and (3.16)]. In fact, it is easily seen that these formulas may be combined to yield the following more compact prescription:[1] *the complex coordinates* $z_j(t)$ *are the* n *roots of the equation in* z,

$$\sum_{j=1}^{n}\dot{z}_j(0)/[z-z_j(0)]=(\alpha+\mathrm{i}\alpha')/\{\exp[(\alpha+\mathrm{i}\alpha')t]-1\}. \tag{4.19}$$

Let us now discuss the motion of the n particles in the plane entailed by these formulas; the main parameter determining its character is the value of α (in particular its sign).

We consider first the case of positive α, $\alpha>0$. Then, as $t\to\infty$, one of the particles escapes to infinity, and $n-1$ remain confined, and approach (exponentially in time, $O(\exp[-\alpha t])$) $n-1$ fixed positions, whose configuration depends on the initial positions and velocities [they are the $n-1$ zeros of the polynomial $\Sigma_{m=1}^{n}\dot{c}_m(0)z^{n-m}$]. The trajectory of the particle that tends to infinity coincides *asymptotically*, as $t\to\infty$, with that of the center-of-mass multiplied by n, $\vec{r}_j(t)\approx n\vec{R}(t)$ [see (3.18)] or, more explicitly [and in complex notation; see (3.8)], $z_j(t)\approx -c_1(t)\approx -(\alpha+\mathrm{i}\alpha')^{-1}\dot{c}_1(0)\exp[(\alpha+\mathrm{i}\alpha')\mathrm{t}]$; note that we indicate here with $\vec{r}_j(t)$, and correspondingly $z_j(t)$, the coordinate of the jth particle, identified as the (single) one that escapes to infinity (which one of the n particles is subject to such a fate depends nontrivially on the initial data). Note that the asymptotic motion of the escaping particle in straight or spiraling depending whether α' does or does not vanish.

The outcome we have described is obtained for a generic set of initial data; but there are special sets of initial data that entail a different outcome. Indeed a necessary and sufficient condition in order for this asymptotic outcome to emerge, is the condition [on the initial data; see (3.17b)] $\dot{c}_1(0)\neq 0$, which corresponds simply to the requirement that the center-of-mass of the system not be initially [hence, throughout the motion: see (3.18) and (4.18)] at rest. If instead that happens, namely if $\dot{c}_1(0)=\dot{c}_1(t)=0$, but $\dot{c}_2(0)\neq 0$, then, as $t\to\infty$, $n-2$ particles remain in a finite region of the plane and tend there to fixed positions, and 2 escape to infinity moving asymptotically in opposite directions (consistently with the center-of-mass being at rest), according to the asymptotic formulas $\tilde{z}_{\pm}(t)\approx\pm[-c_2(t)]^{1/2}$, $c_2(t)\approx(\alpha+\mathrm{i}\alpha')^{-1}\dot{c}_2(0)\exp[(\alpha+\mathrm{i}\alpha')\mathrm{t}]$. And the arguments holds further: if the initial data are such that [see (3.17b)] $\dot{c}_m(0)=0$ for $m=1,2,..,m'-1$, and $\dot{c}_{m'}(0)\neq 0$, then, as $t\to\infty$, $n-m'$ remain confined and m' escape to infinity. Specifically, the $n-m'$ particles which remain confined tend asymptotically, as $t\to\infty$, to the $n-m'$ zeros of the polynomial in z,

$$\sum_{n=m'}^{n}\dot{c}_m(0)z^{n-m}=0; \tag{4.20a}$$

while those which escape to infinity approach asymptotically the m' outgoing spiraling trajectories

$$\tilde{z}_k(t)=\exp(2\pi\mathrm{i}k/m')[-\dot{c}_m(0)]^{1/m'}\ \exp[(\alpha+\mathrm{i}\alpha')t/m'],\quad k=1,..,m'. \tag{4.20b}$$

As $t \to -\infty$, all n particles approach instead asymptotically [up to corrections $O(\exp[\alpha t])$] the configuration associated via (3.8) with the n (complex) roots of the polynomial equation in z,

$$z^n + \sum_{m=1}^{\infty} c_m(-\infty) z^{n-m} = 0, \tag{4.21a}$$

with [see (4.18)]

$$c_m(-\infty) = c_m(0) - (\alpha + i\alpha')^{-1} \dot{c}_m(0). \tag{4.21b}$$

This concludes our analysis of the behavior of the system (1.1)–(1.3) with (4.17) and $\alpha > 0$. Qualitatively the motion can be summarized as follows: in the remote past, the n particles are *almost at rest* at some positions (which could of course be arbitrarily assigned); the fact that they are not completely at rest is of course essential, so that they do interact and take part in the motion (if they are *completely at rest*, they remain so throughout time and can simply be ignored). Then the particles begin to move, and $n-1$ of them always remain in a finite region of the plane, approaching asymptotically, in the remote future, fixed positions; while one of them shoots off to infinity, along a straight (if $\alpha' = 0$) or spiraling (if $\alpha' \neq 0$) trajectory. This outcome corresponds to the generic case; in special cases (corresponding to special initial, at $t = 0$, or asymptotic as $t \to -\infty$, conditions), $n - m'$ particles remain always in a finite region of the plane, approaching asymptotically, as $t \to \infty$, a configuration (fixed by the initial data) there, and m' shoot eventually off to infinity along outgoing (straight or spiraling) trajectories, approaching asymptotically equispaced positions on a (fixed or rotating) circle of exponentially diverging radius.

This ends our discussion of the $\alpha > 0$ case. The $\alpha < 0$ need not be discussed, since the analysis is essentially identical to that of the $\alpha > 0$ case, except for the exchange of $t \to \infty$ with $t \to -\infty$ and vice versa.

We end this subsection with an analysis of the $\alpha = 0$ case (with $\alpha' \neq 0$; the $\alpha = \alpha' = 0$ case is treated in the following subsection). In this case, the time evolution of $c_m(t)$ is still given by (4.18) (of course with $\alpha = 0$); hence *from any initial data*, the systems always evolves *completely periodically*, with period $T = 2\pi n!/\alpha'$.

F. The simplest model: Its behavior, its Hamiltonian structure

In this subsection we discuss the model characterized by vanishing values of *all* coupling constants, $\alpha = \alpha' = \beta = \beta' = \lambda = \lambda' = \mu = \mu' = 0$, so that the equations of motion in the plane read [see (1.1)–(1.3)]

$$\ddot{\vec{r}}_j = 2 \sum_{k=1, k \neq j}^{n} [\dot{\vec{r}}_j (\dot{\vec{r}}_k \cdot \vec{r}_{jk}) + \dot{\vec{r}}_k (\dot{\vec{r}}_j \cdot \vec{r}_{jk}) - \vec{r}_{jk} (\dot{\vec{r}}_j \cdot \dot{\vec{r}}_k)] / r_{jk}^2, \tag{4.22a}$$

or equivalently, in complex notation [see (3.8) and (3.6)],

$$\ddot{z}_j = 2 \sum_{k=1, k \neq j}^{n} \dot{z}_j \dot{z}_k / (z_j - z_k). \tag{4.22b}$$

This is the ''simplest model'' within the class (1.1)–(1.3); although, in terms of the behavior of the solutions (see below), perhaps the simplest case is that considered at the end of the preceding Sec. IV E.

It is easily seen that the time-evolution of the n complex coordinates $z_j(t)$ is now given by the n roots of the equation in z,[1]

$$\sum_{j=1}^{n} \dot{z}_j(0)[z-z_j(0)]^{-1}=t^{-1}, \tag{4.23}$$

and that in this case the center-of-mass, whose *complex* coordinate we denote here by Z [see (2.1) and (3.8)],

$$Z(t)=n^{-1}\sum_{j=1}^{n} z_j(t), \tag{4.24}$$

moves freely:

$$\ddot{Z}(t)=0, \tag{4.25a}$$

$$Z(t)=Z(0)+\dot{Z}(0)t. \tag{4.25b}$$

If the initial conditions are such that the (time-independent) velocity, $\dot{Z}(t)=\dot{Z}(0)$, of the center-of-mass does not vanish, the system (4.22) evolves as follows: as $t\to\pm\infty$, $n-1$ particles approach asymptotically $n-1$ fixed locations [whose configuration depend on the initial conditions, being in fact given by the $n-1$ roots of the function of z appearing in the left-hand-side of (4.23)], while one of them shoots off to infinity, approaching asymptotically [up to corrections $O(t^{-1})$] the free trajectory

$$\tilde{z}(t)=n\dot{Z}(0)t+\sum_{j=1}^{n} \dot{z}_j(0)z_j(0)/[n\dot{Z}(0)]+\sum_{j=1}^{n} \dot{z}_j(0)z_j(0)/[n\dot{Z}(0)]. \tag{4.26}$$

Hence the system looks *on the whole* exactly the same in the remote future as in the remote past (''solitonic behavior''). Note however that the particle that escapes to infinity in the remote future need not be the same one that came in from infinity in the remote past, and moreover that, through the motion, some particles may change location (''game of musical chairs'': the locations of the chairs are given, the identity of their occupants may change, from the time $t=-\infty$ when the particles wander off in the plane, to the time $t=+\infty$ when they sit down again).

In the special case in which the initial data entail that the center-of-mass velocity vanishes, then as $t\to\pm\infty$ only $n-2$ particles tend to finite locations, and 2 emerge to infinity (but they do not move as free particles; see below). And if the initial data are further specialized by requiring them to satisfy additional conditions, the number of particles that escape to infinity increases. Since this phenomenon is analogous (albeit not identical, due to the symmetrical behavior now as $t\to+\infty$ and $t\to-\infty$) to the case discussed in the preceding subsection, we detail here directly the general outcome: if $\dot{c}_m(0)=0$ for $m=1,2,..,m'-1$, and $\dot{c}_{m'}(0)\neq 0$, then, as $t\to\pm\infty$, $n-m'$ particles tend asymptotically to fixed locations, given by the $n-m'$ zeros $\tilde{z}_k$ of the following polynomial of degree $n-m'$ in $\tilde{z}$,

$$\sum_{m=m'}^{n} \dot{c}_m(0)\tilde{z}^{n-m}=0, \quad \tilde{z}=\tilde{z}_k, \quad k=m'+1,m'+2,..,n, \tag{4.27a}$$

while m' particles go to infinity approaching [up to corrections $O(t^{-1})$] the asymptotic stellar trajectories

$$\tilde{z}_k(t)=\exp(2\pi ik/m')[-\dot{c}_{m'}(0)t]^{1/m'}, \quad j=1,..,m'. \tag{4.27b}$$

Here, of course, the quantities $\dot{c}_m(0)$, $m=1,..,n$, are related to the initial data via (3.17b). Again, as $t\to\pm\infty$, each particle coordinate $z_j(t)$ approaches one of the quantities $\tilde{z}_k$ so defined; but to ascertain which $z_j(t)$ approach which $\tilde{z}_k(t)$ (as $t\to-\infty$, and as $t\to+\infty$), a more detailed analysis is required, since this depends nontrivially on the initial data.

The system (4.22) is clearly a special case of those considered in Sec. IV D; hence it is certainly Hamiltonian. But in this case a Hamiltonian function can be explicitly exhibited:

$$H(\mathbf{q},\mathbf{p})=\sum_{j=1}^{n}\exp(ap_j)\prod_{k=1,k\neq j}^{n}(q_j-q_k)^{-1}. \tag{4.28}$$

Here the constant a is nonvanishing ($a\neq0$), but otherwise arbitrary. Indeed, it is easily seen that the standard Hamiltonian equations,

$$\dot{q}_j=\partial H/\partial p_j\,,\quad \dot{p}_j=-\partial H/\partial q_j\,, \tag{4.29}$$

yield

$$\dot{q}_j=a\,\exp(ap_j)\prod_{k=1,k\neq j}^{n}(q_j-q_k)^{-1},\quad j=1,..,n, \tag{4.30a}$$

and [after using (4.30a)]

$$\dot{p}_j=a^{-1}\sum_{k=1,k\neq j}^{n}(\dot{q}_j+\dot{q}_k)/(q_j-q_k),\quad j=1,..,n. \tag{4.30b}$$

Differentiating (the logarithm of) (4.30a) with respect to time and using (4.30b) one easily gets

$$\ddot{q}_j=2\sum_{k=1,k\neq j}^{n}\dot{q}_j\dot{q}_k/(q_j-q_k),\quad j=1,..,n. \tag{4.31}$$

But this equation coincides with (4.22b) if one identifies q_j with the *complex* variable z_j, $q_j=z_j$, $j=1,..,n$. The justification for so doing, and, most importantly, the prescription detailing how to obtain in this manner a Hamiltonian structure for the real two-dimensional vector system (4.22a), are implied by the results reported in Appendix B.

The Hamiltonian evolution equations (4.31) are merely a special case of those associated[2] (in the real domain) to the beautiful integrable relativistic one-dimensional n-body problem discovered by S.N.M. Ruijsenaars and H. Schneider.[5] Hence one can take over the known $(n\times n)$-matrix Lax pair,[2]

$$L_{jk}=\delta_{jk}\dot{q}_j+(1-\delta_{jk})(\dot{q}_j\dot{q}_k)^{1/2}, \tag{4.32a}$$

$$A_{jk}=-(1-\delta_{jk})(\dot{q}_j\dot{q}_k)^{1/2}/(q_j-q_k), \tag{4.32b}$$

which, as can be easily verified, yields, via the Lax $(n\times n)$-matrix equation,[6]

$$\dot{\mathbf{L}}=[\mathbf{L},\mathbf{A}], \tag{4.33}$$

precisely the evolution equations (4.31). And of course the two-dimensionalization of this Lax equation via complexification [$q_j=z_j$, and see (3.8)] is a trivial matter.

There also exist several other Hamiltonians which produce the same evolution equations (4.31).[8]

G. Models with nontrivial equilibrium and rotating configurations

Let us now return to the *general* model (1.1)–(1.3), to investigate the subcases when there exist nontrivial equilibrium configurations, namely time-independent solutions of (1.1)–(1.3),

$$\vec{r}_j(t)=\vec{\overline{r}}_j, \quad \dot{\vec{r}}_j(t)=0, \quad j=1,..,n, \tag{4.34a}$$

or equivalently [see (3.8)],

$$z_j(t)=\overline{z_j}, \quad \dot{z}_j(t)=0, \quad j=1,..,n, \tag{4.34b}$$

with the quantities $\overline{z_j}$ not all vanishing [we consider trivial, and indeed ''unphysical'', see (1.2b), the ''equilibrium configuration'' $\overline{z_j}=0$, $j=1,\ldots n$, which corresponds, see (3.9) as well as (3.10) and (3.13), to $c_m(t)=0$, $m=1,\ldots,n$].

It is clear [see (3.9), (3.10), and (3.13)] that a necessary and sufficient condition for this to happen is that, for some value $m=\overline{m}$, $1\leqslant\overline{m}\leqslant n$, either $\nu_{\overline{m}}^{(+)}$ or $\nu_{\overline{m}}^{(-)}$ (or both $\nu_{\overline{m}}^{(+)}$ and $\nu_{\overline{m}}^{(-)}$) vanish:

$$\nu_{\overline{m}}^{(+)}=0 \quad \text{or} \quad \nu_{\overline{m}}^{(-)}=0, \quad 1\leqslant\overline{m}\leqslant n. \tag{4.35}$$

Via (3.11)–(3.12) [or, more transparently, directly from (3.15) and (3.5b)], it is generally seen that this requirement entails the following two conditions:

$$(2n-\overline{m}-1)\mu+2\beta=0, \tag{4.36a}$$

$$(2n-\overline{m}-1)\mu'+2\beta'=0. \tag{4.36b}$$

These conditions constrain only the values of the coupling constants β,β',μ,μ'; indeed the other 4 coupling constants, $\alpha,\alpha',\lambda,\lambda'$, play no role at equilibrium, since the corresponding forces vanish when the particles are at rest, see (1.2)–(1.3).

Let us then assume that the constraints (4.36) do hold, for some value $\overline{m}$, $1\leqslant\overline{m}\leqslant n$. Then clearly the equilibrium configuration is characterized by the condition that all other coefficients $c_m(t)$ vanish,

$$c_m(t)=0, \quad m=1,..,n, \quad m\neq\overline{m} \tag{4.37a}$$

[see (3.9)]. Hence the equilibrium configuration is identified by the condition [see (3.9)]

$$\prod_{k=1}^{n}(z-\overline{z_k})=z^n+c_{\overline{m}}z^{n-\overline{m}}, \tag{4.37b}$$

with $c_{\overline{m}}$ an arbitrary complex constant, and, say [see (3.13)]

$$c_{\overline{m}}=c_{\overline{m}}^{(+)}, \quad c_{\overline{m}}^{(-)}=0. \tag{4.37c}$$

This constant can be rescaled away from (4.37b), by replacing z with cz and $\overline{z_k}$ with $c\overline{z_k}$, $z\to cz$, $\overline{z_k}\to c\overline{z_k}$, with $c=(c_{\overline{m}})^{1/\overline{m}}$. This freedom corresponds to the rotation and rescaling invariance of the model (1.1)–(1.3), which of course entail that, if $z_j=\overline{z_j}$, $j=1,\ldots,n$, is an equilibrium configuration, $z_j'=c\overline{z_j}$, $j=1,..,n$, with c any complex number, is also an equilibrium configuration. One may therefore conclude that the equilibrium configurations of the model (1.1)–(1.3) with (4.36) are provided, as usual via (3.8), and *up to rotations and rescalings*, by the solutions $\overline{z_k}$ of the polynomial equation in z,

$$z^n+z^{n-\overline{m}}=z^{n-\overline{m}}(1+z^{\overline{m}})=0, \tag{4.38}$$

implying of course

$$z_{\overline{k}} = \exp[\mathrm{i}(2k+1)\pi/\overline{m}), \quad k=1,\ldots,\overline{m}, \tag{4.39a}$$

$$z_{\overline{k}} = 0, \quad k=\overline{m}+1,\overline{m}+2,\ldots,n. \tag{4.39b}$$

Only two cases, therefore, must be considered, if one excludes as ''unphysical'' any configuration with more than one particle sitting at the origin [see (1.2b)]: the case $\overline{m}=n$, in which all n particles sit equispaced on a circle centered at the origin, and the case $\overline{m}=n-1$, in which one particle sits alone at the origin and $n-1$ sit equispaced on a circle centered at the origin. Both configurations display, of course, circular symmetry; and they are ''universal'', namely independent of the values of the coupling constants that characterize the different models (1.1)–(1.3); provided, of course, these coupling constants satisfy the condition (4.36), with $\overline{m}=n$ or $\overline{m}=n-1$. Note that in each case there are in fact $n!$ different configurations, corresponding to the different possible allocations of the n particle positions z_j to the equilibrium positions $\overline{z_k}$.

These equilibrium configurations cannot be completely stable, due to the circular and scale symmetries. Indeed it is clear that the equilibrium configuration (4.39) is a special case of the more general solution of the equations of motion (1.1)–(1.3) with (4.36) which reads, via (3.8),

$$\tilde{z_k}(t) = [-c_{\overline{m}}(t)]^{1/\overline{m}}\overline{z_k}, \quad k=1,\ldots,n, \tag{4.40a}$$

with $\overline{z_k}$ given by (4.39) and

$$c_{\overline{m}}(t) = c_{\overline{m}}(0) + \dot{c}_{\overline{m}}(0)[\alpha+\lambda(n-\overline{m})+\mathrm{i}\alpha'+\mathrm{i}\lambda'(n-\overline{m})]^{-1} \cdot [\exp\{[\alpha+\lambda(n-\overline{m})+\mathrm{i}\alpha'+\mathrm{i}\lambda'(n-\overline{m})]t\}-1]. \tag{4.40b}$$

Clearly this configuration of the system has $n-\overline{m}$ particles sitting at the origin (thus one might view only the two cases $\overline{m}=n$ and $\overline{m}=n-1$ as ''physically acceptable''), and $\overline{m}$ sitting equispaced on a circle (centered at the origin, with arbitrary initial radius and orientation), which itself rotates uniformly and expands or shrinks over time. Again, there are $n!$ such solutions, which differ merely in the one-to-one matching of the n particle coordinates $z_j(t)$ with the n quantities $\tilde{z_k}(t)$, see (4.40a).

Of course an additional element of possible instability of the equilibrium configuration (4.39), or, more generally, of the ''merry-go-round'' configuration (4.40), arises from the possibility that a perturbation excite other ''nonlinear modes,'' namely that it induce other coefficients $c_m(t)$, with $m \neq \overline{m}$, to become different from zero. Whether such a perturbation would then grow or decay depends of course on the sign of the quantities $\rho_m^{(\pm)}$, see (3.10) and (4.1)–(4.3).

A study of the behavior of the system (1.1)–(1.3) in the neighborhood of its equilibrium configuration (4.39) could of course be done in the standard manner,[1] by linearizing the equations of motion (1.1)–(1.3) around this equilibrium configuration via the position, say,

$$z_j(t) = \overline{z_j} + \epsilon\zeta_j(t), \quad j=1,\ldots,n, \tag{4.41}$$

with ϵ a small parameter. In this manner one is then led, in a well-known manner,[1] to identify ''remarkable matrices,'' whose eigenvalues and eigenvectors are known. We forsake here any further discussion of this topic.

Let us end this subsection by noting that (4.40a), with $c_{\overline{m}}(t)$ defined by (3.10)–(3.13) [rather than (4.40b)], provides a circularly symmetrical solution to (1.1)–(1.3) for the *general* case with 8 arbitrary coupling constants [namely, even if the conditions (4.36) do not hold].

H. First-order evolution equations

In this subsection we mention that the results described above (see, in particular, Sec. III) imply of course the possibility to also solve the models characterized by equations of motion *of first order*,

$$\dot{\vec{r}}_j=(\beta+\beta'\hat{z}\wedge)\vec{r}_j+\sum_{k=1,k\neq j}^{n} r_{jk}^{-2}(\mu+\mu'\hat{z}\wedge)\{\vec{r}_j[r_j^2-2(\vec{r}_j\cdot\vec{r}_k)]+\vec{r}_k r_j^2\}, \tag{4.42}$$

which might also be of applicative interest (perhaps in fluid dynamics). Suffice here to note that, via the mapping (3.8)–(3.9), they correspond to the equations

$$\dot{c}_m-m[\beta+\mathrm{i}\beta'+\tfrac{1}{2}(2n-m-1)(\mu+\mathrm{i}\mu')]c_m=0, \tag{4.43a}$$

implying

$$c_m(t)=c_m(0)\exp[m\{\beta+\tfrac{1}{2}(2n-m-1)\mu+\mathrm{i}[\beta'+\tfrac{1}{2}(2n-m-1)\mu']\}t]. \tag{4.43b}$$

I. One-dimensional motions

In this subsection we mention briefly the possibility that the model (1.1)–(1.3) allow motions which are essentially one-dimensional. It is clear that a necessary condition for this to be possible is the vanishing of all primed coupling constants,

$$\alpha'=\beta'=\lambda'=\mu'=0. \tag{4.44}$$

It is then clear that, if the initial conditions are characterized by an *aligned configuration*,

$$\vec{r}_j(0)=\vec{u}+s_j(0)\vec{v}, \quad j=1,\ldots,n, \tag{4.45a}$$

$$\dot{\vec{r}}_j(0)=\dot{s}_j(0)\vec{v}, \quad j=1,\ldots,n, \tag{4.45b}$$

with $\vec{u}$ and $\vec{v}$ two arbitrary 2-vectors in the plane, then the motion maintains, at least for some time, such *aligned configuration*,

$$\vec{r}_j(t)=\vec{u}+s_j(t)\vec{v}, \quad j=1,\ldots,n, \tag{4.46}$$

and it reproduces results which have been known for quite some time.[1] Even in this case there is, however, a possibility that the motion become two-dimensional when two particles collide and are then scattered, generally in opposite directions in the plane, away from the straight line which characterized their one-dimensional motion.

V. OUTLOOK

The interest of the *n*-body models considered in this paper originates from the dearth of *solvable* examples of *n*-body motion *in the plane*, besides the trivial case of purely harmonic oscillators, or other cases obtained by complexification from solvable one-dimensional *n*-body problems, whose relevance is however moot if they lack the property of rotation invariance, which is crucial for a proper interpretation of such evolutions as representing the motion of particles in the plane. The interest of the models treated in this paper is moreover underscored by the richness of the motions they entail, remarkably combined with the simplicity of the solution technique. This is displayed by the various cases discussed in the preceding section; the presentation of a more complete analysis remains as a task for the future.

As part of that analysis, let us mention that the consideration of special motions associated with symmetrical configurations opens several possibilities, including the identification of new solvable one-dimensional models, which might then again yield two-dimensional models via complexification. These extensions can be pursued as applications of the technique of ''duplication'',[7] but with the additional possibility now to consider multiring circularly-symmetrical configurations. We postpone such treatments to future papers.

Three avenues of future research appear especially interesting: at least in the case of Hamiltonian motions, the consideration of quantal versions of these models; the limit cases obtained by letting the number n of particles diverge, including continuum configurations corresponding to two-dimensional motions of (suitably interacting) strings in the plane; and the ambitious hope to find, by appropriate extensions of the techniques employed in this paper, interesting n-body problems which are solvable in three-dimensional space.

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APPENDIX A: ASYMPTOTIC BEHAVIOR OF THE ZEROS OF A POLYNOMIAL WHOSE COEFFICIENTS DEPEND EXPONENTIALLY ON A DIVERGING PARAMETER

Let $z_j(t)$, $j=1,..,n$, be the n zeros of a polynomial of degree n in z whose coefficients depend exponentially on t:

$$[z_j(t)]^n+\sum_{m=1}^{n} c_m(t)[z_j(t)]^{n-m}=0, \quad j=1,\ldots,n, \tag{A1}$$

$$c_m(t)=\overline{c_m}\,\exp[(\rho_m+\mathrm{i}\gamma_m)t], \quad m=1,\ldots,n. \tag{A2}$$

The *constants* $\overline{c_m}$ are n arbitrary (nonvanishing) *complex* numbers, and the *constants* ρ_m,γ_m are $2n$ arbitrary *real* numbers; n is an arbitrary positive integer, $n\geqslant 2$.

We now formulate, and then prove, the following

Proposition: As the real parameter t tends to (positive) infinity, $t\to\infty$,

$$z_j(t)=z_j^{(+)}(t)\{1+O(\exp[-p_j t])\}, \tag{A3a}$$

$$z_j^{(+)}(t)=\widetilde{z}_j(t)\exp(q_j t), \tag{A3b}$$

$$\widetilde{z_j}(t)=\overline{z_j}\,\exp(\mathrm{i}r_j t). \tag{A3c}$$

Here the superscript ''plus'' on $z_j^{(+)}(t)$ serves to distinguish this quantity from $z_j(t)$ [clearly $z_j^{(+)}(t)$ is the ''dominant part'' of $z_j(t)$ as $t\to\infty$], and also as a reminder that we are investigating the behavior as $t\to+\infty$ (an analogous superscript should be attached to $\widetilde{z}_j(t)$ and $\overline{z_j}$; it is omitted to simplify the notation). The n complex *constants* $\overline{z_j}$, and the $3n$ *real* numbers $p_j>0$, q_j and r_j, are given by the following prescriptions.

Identify on a Cartesian plane the n points with discrete abscissas $m=1,..,n$ and ordinates ρ_m, and in addition the origin (abscissa $m=0$, ordinate $\rho_0=0$). Draw the (clearly unique and continuous, if generally segmented) curve, which is the *upper envelope* of the $\frac{1}{2}n(n+1)$ segments connecting pairwise these $n+1$ points (see the example with $n=7$ in Fig. 1); hereafter we refer to this segmented line as the *upper curve*. Associate *to each segment of this upper curve* the following

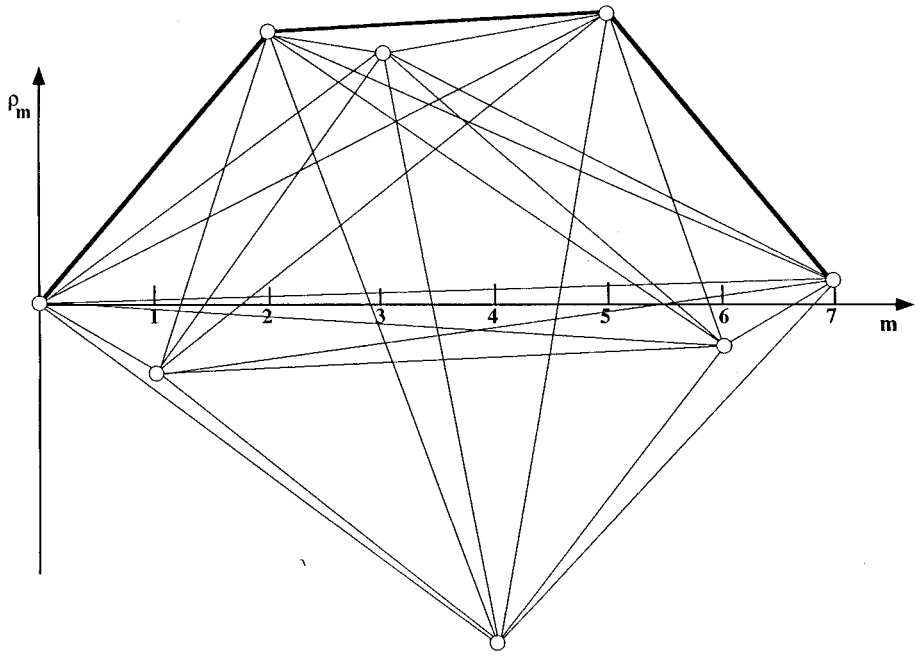

FIG. 1. The ''upper curve'' is bolded (see text for explanation).

numbers (the index s labels subsequent segments of this curve, from left to right): $m_s^{(-)}$ and $m_s^{(+)}$ are the values of m that identify the beginning and the end of the segment s (so that $m_1^{(-)}=0$, $m_s^{(+)}=m_{s+1}^{(-)}, m_S^{(+)}=n$, where S is the number of segments that make up the *upper curve*);

$$n_s=m_s^{(+)}-m_s^{(-)} \tag{A4}$$

(hence n_s is the number of points that lie below the segment s, increased by one, see Fig. 1; of course $\Sigma_{s=1}^{S} n_s=n$);

$$z^{(s)}=[-\overline{c}_{m_s^{(+)}}/\overline{c}_{m_s^{(-)}}]^{1/n_s} \tag{A5}$$

(with the convention $\overline{c}_0=1$),

$$q^{(s)}=[\rho_{m_s^{(+)}}-\rho_{m_s^{(-)}}]/[m_s^{(+)}-m_s^{(-)}], \tag{A6}$$

$$r^{(s)}=[\gamma_{m_s^{(+)}}-\gamma_{m_s^{(-)}}]/[m_s^{(+)}-m_s^{(-)}], \tag{A7}$$

$$p^{(s)}=\inf_{m=1,..,n;m\neq m_s^{(+)},m_s^{(-)}} [(\{[m-m_s^{(-)}]\rho_{m_s^{(+)}}+[m_s^{(+)}-m]\rho_{m_s^{(-)}}\}/[m_s^{(+)}-m_j^{(-)}])-\rho_m]. \tag{A8}$$

Note that the last formula implies that $p^{(s)}$ is positive, $p^{(s)}>0$, since the *straight line* defined, as a function of the variable m, by the expression $\{[m-m_s^{(-)}]\rho_{m_s^{(+)}}+[m_s^{(+)}-m]\rho_{m_s^{(-)}}\}/[m_s^{(+)}-m_s^{(-)}]$, which clearly goes through the points $(m_s^{(-)},\rho_{m_s^{(-)}})$ and $(m_s^{(+)},\rho_{m_s^{(+)}})$, is, by construction, *above* all other points (m,ρ_m) with $m\neq m_s^{(-)},m_s^{(+)}$. (See Fig. 1, and note that we assume here to be in the *generic case*, thereby excluding that three or more of the $n+1$ points identified

above lie on one and the same straight line; the exceptional cases when this instead happens are discussed below.) Then, to each segment s, are associated n_s asymptotic values $z_j^{(+)}(t)$ [see (A3a)], with the following identification of the parameters in (A3):

$$z_{\overline{j}}=z^{(s)}\exp(2\pi i\nu/n_s),\quad \nu=1,\ldots,n_s, \tag{A9}$$

$$p_j=p^{(s)},\quad q_j=q^{(s)},\quad r_j=r^{(s)}. \tag{A10}$$

To sum up: as $t\to\infty$, the dominant terms $z_j^{(+)}(t)$ in the asymptotic behavior of the n zeros $z_j(t)$ [see (A3a)] are divided into S families (where S is the number of segments that constitute the *upper curve*); each family includes n_s values which, in the complex plane, lie *equispaced* on a circle centered at the origin [see (A3), (A9), and (A5)], whose radius varies proportionally to $\exp(q^{(s)}t)$ [see (A3), (A10), and (A6)], and which rotates with constant velocity as entailed by the factor $\exp(ir_jt)$ in (A3b) [see (A10) and (A7)]. The radius of the circle diverges to infinity or converges to zero (in either case, exponentially), depending on whether the segment s has positive or negative slope [see (A10) and (A6)]; it is constant if the segment s is horizontal [so that $q^{(s)}$ vanishes, see (A6)]. Note that, in the case of *positive* slope, namely when the radius of the circle *diverges* exponentially as $t\to\infty$, so that the corresponding zeros $z_j(t)$ spiral to infinity, they may, or may not, actually approach their dominant parts $z_j^{(+)}(t)$, see (A3); this of course depends on the behavior of the *difference* $z_j(t)-z_j^{(+)}(t)$, which is $O(\exp\{[q^{(s)}-p^{(s)}]t\})$ [see (A3) and (A10)], hence which vanishes or diverges depending on whether $p^{(s)}$ is larger or smaller than $q^{(s)}$ [see (A8) and (A6)]. The zero $z_j(t)$ does of course approach, as $t\to\infty$, its dominant parts $z_j^{(+)}(t)$, if $z_j^{(+)}(t)$ does not diverge as $t\to\infty$, namely whenever $q_j\leqslant 0$.

As mentioned above, this outcome describes (completely) the situation in the *generic case* in which no point (m,ρ_m) lies on the segment joining two other points, say (m_1,ρ_{m_1}) and (m_2,ρ_{m_2}). If instead this is the case *for a point on the upper curve* [as it would for instance happen in the case of Fig. 1 if ρ_3 were a bit larger, so that the the point $(3,\rho_3)$ would lie exactly on the segment joining $(2,\rho_2)$ and $(5,\rho_5)$], then the formula (A3) remains valid with the same definition of q_j and also (essentially; but see below) of p_j [see (A3a,b) and (A5)–(A7)], while the definition (A3c) of $\tilde{z}_j(t)$ is instead replaced by a new one, as we now indicate.

But let us note first that the n_s quantities $\tilde{z}_j(t)$ defined by (A3c), (A9), and (A5) are in fact the n_s nonvanishing roots of the algebraic equation in $\tilde{z}$

$$c_{\overline{m_s^{(-)}}}\exp(i\gamma_{m_s^{(-)}}t)\tilde{z}^{n-m_s^{(-)}}+c_{\overline{m_s^{(+)}}}\exp(i\gamma_{m_s^{(+)}}t)\tilde{z}^{n-m_s^{(+)}}=0 \tag{A11}$$

[see (A4), (A5), and (A9)]. This is the equation applicable in the generic case considered above. A more general prescription to cover *all* possible cases requires the following supplementary rule: if the *upper curve* contains Σ_s points $(m_s^{(\sigma)},\rho_{m_s^{(\sigma)}})$, $\sigma=1,..,\Sigma_s$, which lie, in the Cartesian (m,ρ_m) plane, on the *same* segment s, of course with

$$m_s^{(1)}=m_s^{(-)},m_s^{(\Sigma_s)}=m_s^{(+)},m_s^{(-)}\leqslant m_s^{(\sigma)}\leqslant m_s^{(+)}, \tag{A12}$$

then the n_s dominant values $z_j^{(+)}(t)$, see (A3a), belonging to the family associated with this segment s, have parameters p_j and q_j still defined by (A9) and (A6)–(A8) [albeit with the smallest value in the definition (A8) of $p^{(s)}$ taken only over the values of m *different from every one of the values* $m_s^{(\sigma)}$, $\sigma=1,..,\Sigma_s$]; but the quantities $\tilde{z}_j(t)$, see (A3a,b), instead of being given by (A3c) [or, equivalently, as the n_s roots of (A11)], are now the n_s roots of the algebraic equation in $\tilde{z}$,

$$\sum_{\sigma=1}^{\Sigma_s} c_{\overline{m_s^{(\sigma)}}}\exp(i\gamma_{m_s^{(\sigma)}}t)[\tilde{z}]^{m_s^{(+)}-m_s^{(\sigma)}}=0. \tag{A13}$$

The fact that this equation has indeed n_s roots is implied by (A4) and (A12). Note that the general case considered here includes the generic case treated above, since (A11) is the special case of (A13) with $\Sigma_s=2$.

This completes the formulation of the *Proposition*. Before proceeding to prove it, let us note that, since obviously the shape of the *upper curve* is mainly determined by the value of the largest value ρ_+ attained by the n parameters ρ_m, the *Proposition* entails the following

Corollary: The behavior as $t\to\infty$ of the zeros $z_j(t)$, see (A1)–(A2), is mainly determined by the single parameter

$$\rho_+=\sup_{m=1,..,n}[\rho_m], \tag{A14}$$

and, if ρ_+ is *non-negative*, by the value m_+ (or the values $m_+^{(\sigma)}$, see below) at which ρ_m attains its maximal value ρ_+.

Indeed, if ρ_+ is *negative*, $\rho_+<0$, then as $t\to\infty$ all n zeros $z_j(t)$ converge (exponentially fast) to zero, $z_j(t)\to 0$, $j=1,..,n$.

If instead ρ_+ *vanishes*, $\rho_+=0$, then as $t\to\infty$, some of the zeros neither converge to zero nor escape to infinity, and the remaining ones (if any) converge to zero. Specifically, if $\rho_m=0$ for $m=m_+^{(\sigma)}$ and $\rho_m<0$ for $m\neq m_+^{(\sigma)}$, with $\sigma=1,..,\Sigma$ and $m_+^{(\sigma)}\leqslant m_+^{(\Sigma)}\equiv m_+$, then, as $t\to\infty, n-m_+$ of the n zeros $z_j(t)$ converge (exponentially fast) to zero, and m_+ of them approach (exponentially fast) the m_+ roots of the algebraic equation in $\tilde{z}$

$$[\tilde{z}]^{m_+}+\sum_{\sigma=1}^{\Sigma}\tilde{c}_{m_+^{(\sigma)}}\exp(i\gamma_{m_+^{(\sigma)}}t)[\tilde{z}]^{m_+-m_+^{(\sigma)}}=0. \tag{A15}$$

Note that, if $\Sigma=1$, these m_+ roots are given by the explicit formula

$$\tilde{z}_k(t)=\exp(2\pi ik/m_+)(-\overline{c_{m_+}})^{1/m_+}\exp(i\gamma_{m_+}t/m_+),\quad k=1,\ldots,m_+. \tag{A16}$$

Finally, if ρ_+ is *positive*, $\rho_+>0$, some of the n zeros $z_j(t)$ escape to infinity as $t\to\infty$. Specifically, if $\rho_m=\rho_+>0$ for $m=m_+$ and $\rho_m<\rho_+$ for $m\neq m_+$ (namely, if the maximal, positive, value ρ_+ is attained only at the single value m_+ of the index m), then, as $t\to\infty, m_+$ of the n zeros $z_j(t)$ escape (exponentially fast) to infinity and $n-m_+$ converge (exponentially fast) to zero. If instead, more generally, $\rho_m=\rho_+>0$ for $m=m_+^{(\sigma)}$ and $\rho_m<\rho_+$ for $m\neq m_+^{(\sigma)}$, with $\sigma=1,..,\Sigma$ and $m_-\equiv m_+^{(1)}\leqslant m_+^{(\sigma)}\leqslant m_+^{(\Sigma)}\equiv m_+$, then, as $t\to\infty, m_-$ of the n zeros $z_j(t)$ escape (exponentially fast) to infinity, $n-m_+$ converge (exponentially fast) to zero, and m_+-m_- approach (exponentially fast) the m_+-m_- roots of the algebraic equation in $\tilde{z}$

$$\sum_{\sigma=1}^{\Sigma}\tilde{c}_{m_\sigma^{(+)}}\exp[i\gamma_{m_\sigma^{(+)}}t][\tilde{z}]^{m_+-m_+^{(\sigma)}}=0. \tag{A17}$$

This more general case differs from the previous one iff $\Sigma\geqslant 2$; and of course if $\Sigma=2$ (so that $m_1^{(+)}=m_-$ and $m_2^{(+)}=m_+$), the m_+-m_- roots of this equation are given by the explicit formula

$$\tilde{z}_k(t)=\exp[2\pi ik/(m_+-m_-)][-\tilde{c}_{m_+}/\overline{c_{m_-}}]^{1/(m_+-m_-)}\exp[i(\gamma_{m_+}-\gamma_{m_-})t/(m_+-m_-)],$$
$$k=1,\ldots,m_+-m_-. \tag{A18}$$

This concludes the formulation of the *Corollary*, whose proof is obvious enough not to require any additional elaboration here. Let us rather proceed and prove the above *Proposition*. The basic idea is to assume that, as $t\to\infty$, *two* of the $n+1$ terms in the polynomial $\Sigma_{m=0}^{n}c_m(t)z^{n-m}$ [see (A1); and note that hereafter we set, for convenience, $c_0(t)=1$, entailing the validity of (A2) also

for $m=0$, with $\overline{c_0}=1$ and $\rho_0=\gamma_0=0$) are of the same order and dominate over all others. Hence our proof entails the identification of such pairs and the demonstration that they indeed dominate, and the derivation thereby of the results detailed in the above *Proposition*.

Let us then assume that the two terms with, say, $m=m_1$ and $m=m_2$ (with $m_2>m_1$) are of the same order and dominate over all others (as $t\to\infty$), so that by setting

$$z=\tilde{z}\exp(qt) \tag{A19}$$

with

$$\rho_{m_1}+(n-m_1)q=\rho_{m_2}+(n-m_2)q \tag{A20}$$

we can conveniently rewrite Eq. (A1) as follows:

$$c_{m_1}\exp(i\gamma_{m_1}t)\tilde{z}^{n-m_1}+\overline{c_{m_2}}\exp(i\gamma_{m_2}t)\tilde{z}^{n-m_2}=-\sum_{m=0;m\neq m_1,m_2}^{n}\overline{c_m}\exp(i\gamma_m t)\exp(-p_m t)\tilde{z}^{n-m} \tag{A21}$$

with

$$p_m=\rho_{m_1}+q(m-m_1)-\rho_m\,. \tag{A22}$$

From (A20) (which corresponds of course to the condition that the two selected terms are of the *same* order as $t\to\infty$) we get

$$q=(\rho_{m_2}-\rho_{m_1})/(m_2-m_1), \tag{A23}$$

hence, via (A22),

$$p_m=\{[(m-m_1)\rho_{m_2}+(m_2-m)\rho_{m_1}]/(m_2-m_1)\}-\rho_m\,. \tag{A24}$$

It is now clear that the expression in the left-hand-side of (A21) dominates, as $t\to\infty$, over every term in the right-hand-side, provided the quantities p_m, see (A24), are *positive*, $p_m>0$, for all values of $m\neq m_1,m_2$. Since the term inside the curly bracket in the right-hand-side of (A24) represents, as a function of m, the *straight line* that goes, in the Cartesian plane (m,ρ_m), through the two points (m_1,ρ_{m_1}) and (m_2,ρ_{m_2}), it is clear that this condition is satisfied in the generic case (see the formulation of the *Proposition* above), iff $m_1=m_s^{(-)}$ and $m_2=m_s^{(+)}$. With such a choice we clearly get (A6) from (A23), as well as, from (A21),

$$c_{m_s^{(-)}}\exp[i\gamma_{m_s^{(-)}}t]\tilde{z}^{n-m_s^{(-)}}+\overline{c_{m_s^{(+)}}}\exp[i\gamma_{m_s^{(+)}}t]\tilde{z}^{n-m_s^{(+)}}=O(\exp[-p^{(s)}t]) \tag{A25}$$

with (A8). Clearly this last formula, via (A4), entails (A3b,c) with (A5) and (A7).

The *Proposition* is thereby proved in the generic case. Extending this proof to the general case (see above) is, we trust, sufficiently easy to justify leaving this task as an easy exercise for the diligent reader.

Two final remarks.

In the formulations of the *Proposition* and of its *Corollary*, we have, for simplicity, assumed that none of the coefficients $c_m(t)$ in (A1) vanish identically [see the first sentence after (A2)]. Of course it is trivial to extend the *Proposition* and its *Corollary* to also include the case in which one or more of the coefficients $c_m(t)$ in (A1) vanishes; then the corresponding points (m,ρ) must simply be ignored in the construction leading to the identification of the *upper curve*, as well as in the definition of ρ_+ (see A14), of m_+ and so on.

Another easy extension of the above *Proposition* and of its *Corollary* treats the other limit, $t \to -\infty$. Then the role of the *upper curve* is taken over by the, analogously defined, *lower curve*, while all the formulas stand unchanged. In this case the quantities $p^{(s)}$, as defined by (A8), are of course, in the generic case, all *negative* (rather than *positive*), and the zeros associated with segments of the *lower curve* having *negative* slope go to infinity as $t \to -\infty$, while those associated with segments of the *lower curve* having *positive* slope tend to zero. As for the results of the *Corollary*, of course the key role, to determine the behavior of the n zeros $z_j(t)$ as $t \to -\infty$, is played by the value of the quantity

$$\rho_- = \inf_{m=1,..,n} [\rho_m]; \tag{A26}$$

and the formulation of the *Corollary* relevant to the $t \to -\infty$ limit coincides essentially with that detailed above for the $t \to +\infty$ case, with ρ_+ replaced by ρ_- and a reversal of some of the inequality signs, as obviously appropriate.

Finally let us look, as an explicit example, to the instance illustrated in Fig. 1. In this (generic) case, as $t \to +\infty$ the 7 zeros $z_j(t)$ belong to 3 distinct families, one $(s=1, m_1^{(-)}=0, m_1^{(+)}=2)$ containing 2 members and spiraling to infinity, a second one $(s=2, m_2^{(-)}=2, m_2^{(+)}=5)$ containing 3 members and also spiraling to infinity (albeit less fast), and a third one $(s=3, m_3^{(-)}=5, m_3^{(+)}=7=n)$ of 2 members spiraling to zero; while there are only 2 families in the $t \to -\infty$ limit, one containing 4 members which spiral to infinity, and one with 3 members which spiral to zero.

In conclusion, let us emphasize that, while these results provide an easy technique to predict the asymptotic behavior as $t \to \pm\infty$ of the zeros $z_j(t)$ of the polynomial (A1) with (A2), there is no easy way to identify *which* zero behaves *how*, nor to connect the behavior of any particular zero as $t \to -\infty$ with its behavior as $t \to +\infty$.

APPENDIX B: TWO-DIMENSIONALIZATION VIA COMPLEXIFICATION: PRESERVING A HAMILTONIAN STRUCTURE

Suppose one is given a Hamiltonian function, $H(\mathbf{q},\mathbf{p})$, hence the corresponding standard evolution equations,

$$\dot{q}_j = \partial H/\partial p_j, \quad \dot{p}_j = -\partial H/\partial q_j, \quad j=1,\ldots,n, \tag{B1}$$

implying of course

$$\ddot{q}_j = \sum_{k=1}^{n} [(\partial^2 H/\partial p_j\, \partial q_k)(\partial H/\partial p_k) - (\partial^2 H/\partial p_j\, \partial p_k)(\partial H/\partial q_k)], \quad j=1,\ldots,n. \tag{B2}$$

From these equations for the n ''canonical coordinates'' q_j and the n ''canonical momenta'' p_j one can obtain evolution equations for $2n+2n=4n$ quantities *by complexification*, namely by setting

$$q_j = x_j + \mathrm{i}y_j, \quad j=1,\ldots,n, \tag{B3a}$$

$$p_j = \xi_j - \mathrm{i}\eta_j, \quad j=1,\ldots,n, \tag{B3b}$$

of course with x_j, y_j, ξ_j, η_j real. Note the (convenient, see below) choice of the minus sign in the right-hand-side of the second of these equations.

The evolution equations for the $4n$ real quantities x_j, y_j, ξ_j, η_j are, of course, easily obtained by taking the real and imaginary parts of (B1) or (B2): and the capability to solve (B1) or (B2) in

the *complex* domain entails the solvability of these evolution equations, which can of course also be interpreted as evolution equations for the $2n$ two-dimensional vectors

$$\vec{r}_j \equiv (x_j, y_j), \quad \vec{\rho}_j \equiv (\xi_j, \eta_j). \tag{B4}$$

The question that is addressed in this appendix is whether these (real, two-vector) equations are themselves Hamiltonian, namely whether there exist a (real) function $\mathscr{H}$ of the $2n$ two-vectors $\vec{r}_j, \vec{\rho}_j$ such that these evolution equations read

$$\dot{\vec{r}}_j = \partial \mathscr{H} / \partial \vec{\rho}_j, \quad \dot{\vec{\rho}}_j = -\partial \mathscr{H} / \partial \vec{r}_j, \tag{B5}$$

consistently with the interpretation of $\vec{r}_j$ as (two-vector) canonical variables and $\vec{\rho}_j$ as (two-vector) canonical momenta.

The (presumably well-known) answer to this question is positive, if the original Hamiltonian, considered as a function of the complex variables q_j, p_j, is *analytic*, namely if, by setting [via (B3)]

$$H(\mathbf{q},\mathbf{p}) = F(\{x_j, y_j, \xi_j, \eta_j; j = 1,..,n\}) + \mathrm{i}G(\{x_j, y_j, \xi_j, \eta_j; j = 1,..,n\}), \tag{B6}$$

of course with F and G real, there hold the equations [see (A3a)]

$$\partial F / \partial x_j = \partial G / \partial y_j, \quad \partial G / \partial x_j = -\partial F / \partial y_j, \tag{B7a}$$

and [see (A3b)]

$$\partial F / \partial \xi_j = -\partial G / \partial \eta_j, \quad \partial G / \partial \xi_j = \partial F / \partial \eta_j. \tag{B7b}$$

Indeed, using these equations, it is easily seen that (B1) coincides with (B5), provided one sets [via (B3), (B4), and (B6)]

$$\mathscr{H}(\{\vec{r}_j, \vec{\rho}_j; j = 1,..,n\}) = F(\{x_j, y_j, \xi_j, \eta_j; j = 1,...n\}). \tag{B8}$$

It is also easily seen that a second Hamiltonian structure is also automatically entailed by this approach, with the new Hamiltonian function yielded by G [see (B6)], and with an appropriate redefinition of the canonical variables; hence all two-dimensional models obtained by complexification from an analytic Hamiltonian are (at least) bi-Hamiltonian.

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On Abelianization of first class constraints

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A systematic method for the conversion of first class constraints to an equivalent set of the Abelian constraints based on the Dirac equivalence transformation is developed. A representation for the corresponding matrix of this transformation is proposed. This representation allows one to reduce the problem of Abelianization to the solution of a certain system of first order linear differential equations for matrix elements. © *1996 American Institute of Physics.* [S0022-2488(96)01003-4]

I. INTRODUCTION

It is the purpose of this note to describe a practical method for the conversion of non-Abelian constraints into the Abelian form in the theories with first class constraints. To explain the practical importance of this procedure, let us briefly recall the general principles of the description of the standard Dirac theory of Hamiltonian systems with constraints.[1–5]

For the sake of simplicity we will, as usual, discuss the main ideas using a mechanical system, i.e., a system with a finite number of degrees of freedom, having in mind that the direct extension of the results to a field theory is in general possible only in the local sense.

Suppose that the system with $2n$-dimensional phase space Γ acquires the following set of irreducible first class constraints $\varphi_\alpha(p,q)$ $(\alpha=1,2,...,m)$:

$$\begin{gathered}\sigma_\alpha(p,q)=0,\\ \{\varphi_\alpha(p,q),\varphi_\beta(p,q)\}=f_{\alpha\beta\gamma}(p,q)\varphi_\gamma(p,q).\end{gathered} \tag{1}$$

This means that the dynamics of our system is constrained on a certain submanifold of the total phase space or, in other words, not all canonical coordinates are responsible for the dynamics. (Below we will symbolize by notation Γ_c this $2n-m$-dimensional submanifold of Γ, $\Gamma_c\subset\Gamma$.) The generalized Hamiltonian dynamics is described by the extended Hamiltonian that is a sum of canonical Hamiltonian $H_C(p,q)$ and a linear combination of constraints with arbitrary multipliers $u_\alpha(t)$:

$$H_E(p,q)=H_C(p,q)+u_\alpha(t)\varphi_\alpha(p,q). \tag{2}$$

The functions u_α being arbitrary reflects the presence of coordinates in the theory whose dynamics is governed in an arbitrary way. According to the principle of gauge invariance for physical quantities, these coordinates do not affect them and thus can be treated as ignorable. The main problem that arises is the identification of these coordinates. If theory contains only Abelian constraints

$$\{\varphi_\alpha(p,q),\varphi_\beta(p,q)\}=0, \tag{3}$$

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one can find these ignorable coordinates as follows. It is always possible[6–9] to define a canonical transformation to a new set of canonical coordinates

$$\begin{aligned} q_i &\mapsto Q_i = Q_i(q_i, p_i), \\ p_i &\mapsto P_i = P_i(q_i, p_i), \end{aligned} \tag{4}$$

so that m of the new P's $(\overline{P}_1, \ldots, \overline{P}_m)$ become equal to the Abelian constraints (3):

$$\overline{P}_\alpha = \varphi_\alpha(q_i, p_i). \tag{5}$$

In the new coordinates we have the following system of canonical equations

$$\begin{aligned} \dot{Q}^* &= \{Q^*, H_{Ph}\}, \quad \dot{P}^* = \{P^*, H_{Ph}\}, \\ \dot{\overline{P}} &= 0, \quad \dot{\overline{Q}} = u(t), \end{aligned} \tag{6}$$

with arbitrary functions $u(t)$ and with the physical Hamiltonian

$$H_{Ph} \equiv H_C(p,q)\big|_{\varphi_\alpha = 0} \equiv H_C(P^*, Q^*)\big|_{\overline{P}_\alpha = 0}.$$

The physical Hamiltonian H_{Ph} depends only on the remaining $(n-m)$ pairs of new canonical coordinates $(Q_1^*, P_1^*, \ldots, Q_{n-m}^*, P_{n-m}^*)$ which are gauge-invariant physical variables. This means that the coordinates $\overline{Q}_\alpha$ conjugated to the momenta $\overline{P}_\alpha$ are ignorable coordinates and the canonical system admits explicit separation of the phase space into physical and nonphysical sectors:

$$2n\left\{\begin{pmatrix} q_1 \\ p_1 \\ \vdots \\ q_n \\ p_n \end{pmatrix} \mapsto \begin{array}{ll} 2(n-m)\left\{\begin{pmatrix} Q^* \\ P^* \end{pmatrix}\right. & \text{Physical sector} \\ 2m\left\{\begin{pmatrix} \overline{Q} \\ \overline{P} \end{pmatrix}\right. & \text{Nonphysical sector.} \end{array}\right. \tag{7}$$

A straightforward generalization of this method to the non-Abelian case is unattainable; identification of momenta with constraints is forbidden due to the non-Abelian character of constraints (1). However, there exists a general proof of the possibility of a local replacement of the constraints (1) by an equivalent set of constraints forming an Abelian algebra (see, e.g., Refs. 3–5 and 9–12). This general observation, *Abelianization statement*, reads as follows:

> *For a given set of m first class constraints it is always possible to chose locally m new equivalent constraints*
>
> $$\varphi_\alpha(p,q) = 0 \Leftrightarrow \Phi_\alpha(p,q) = 0 \tag{8}$$
>
> *that define the same constraint surface* Γ_C *so that the Poisson brackets between the new constraints strongly vanish, i.e.,*
>
> $$\{\Phi_\alpha(p,q), \Phi_\beta(p,q)\} = 0. \tag{9}$$

Thus, one can deal with this equivalent set of Abelian constraints to construct the reduced phase space, the space of physical degrees of freedom. To reveal ignorable coordinates, we need an explicit form of the new Abelian constraints $\Phi_\alpha(p,q)$. We would like to emphasize that in all proofs of the Abelianization it has been assumed that the constraints form a functional group.[13] In the present paper, we shall point out two alternative schemes of realization of the Abelianization procedure: via the resolution of constraints and via ''generalized'' canonical transformation for

general non-Abelian constraints of type (1). The generalized canonical transformations[14] are those preserving the form of all constraints of the theory as well as the canonical form of the equations of motion. It will be shown that it is possible to convert constraints into the Abelian form in a constructive fashion with the help of the Dirac equivalence linear transformation

$$\boxed{\Phi_\alpha(p,q)=\mathscr{D}_{\alpha\gamma}\varphi_\gamma(p,q)} \tag{10}$$

with the nonsingular matrix $\mathscr{D}$

$$\det\|\mathscr{D}_{\alpha\gamma}\|\Big|_{\text{constraints}}\neq 0.$$

The main point of our result is that the matrix $\mathscr{D}$ can be determined by *linear* first-order differential equations.

The remaining part of this note is devoted to the proof of this statement and the application to a specific example: non-Abelian Christ–Lee model.[15]

II. ABELIANIZATION: ALTERNATIVE SCHEMES

A. Abelianization via constraint resolution

The direct way of Abelianization of constraints is as follows (see, e.g., Ref. 5). Under the assumption that $\varphi_\alpha(p,q)$ are m independent functions one can resolve the constraints (1) for m of ps,

$$p_\alpha=F_\alpha(\underline{p},q), \tag{11}$$

where $\underline{p}$ denotes the remaining ps. Let us pass to a new equivalent set of the constraints $\varphi_\alpha(p,q)$,

$$\Phi_\alpha(p,q)=p_\alpha-F_\alpha(\underline{p},q) \tag{12}$$

By explicit computing one can be convinced that the Poisson brackets of the new constraints $\{\Phi_\alpha(p,q),\Phi_\beta(p,q)\}$ are independent of p_α; however, since they again belong to the first class, a unique possibility is that their Poisson brackets with each other must vanish identically. Thus, after transformations to the new constraints $\Phi_\alpha(p,q)$ we can realize the above-mentioned canonical transformation (4) such that m of the new Ps become equal to the modified constraints Φ_α(12),

$$\overline{P}_\alpha=\Phi_\alpha(q_i,p_i), \tag{13}$$

with the corresponding conjugate ignorable coordinates $\overline{Q}_\alpha$.

B. Abelianization of constraints via the Dirac transformation

In this section, it will be demonstrated that due to the freedom in the representation of constraint surface Γ_c,

$$\begin{aligned}&\varphi_\alpha(p,q)=0,\\ &\{\varphi_\alpha(p,q),\varphi_\beta(p,q)\}=f_{\alpha\beta\gamma}(p,q)\varphi_\gamma(p,q),\end{aligned} \tag{14}$$

one can always pass, with the help of the Dirac transformation, from these first class non-Abelian constraints to the equivalent ones,

$$\Phi_\alpha(p,q)=\mathscr{D}_{\alpha\beta}(p,g)\varphi_\beta(p,q), \tag{15}$$

so that the new constraints will be Abelian:

$$\{\Phi_\alpha(p,q),\Phi_\beta(p,q)\}=0. \tag{16}$$

According to (16), the matrix $\mathscr{D}_{\alpha\beta}$ must satisfy the set of *nonlinear* differential equations

$$\{\mathscr{D}_{\alpha\gamma}(p,g)\varphi_\gamma(p,q),\mathscr{D}_{\beta\sigma}(p,g)\varphi_\sigma(p,q)\}=0. \tag{17}$$

This formulation of the Abelianization statement means a possibility of finding a particular solution for this very complicated system of *nonlinear* differential equations. Beyond the question, Eq. (17) in this form does not represent any practical value but, as it will be shown here, there is a particular solution to this equation that can be represented as

$$\mathscr{D}=\underbrace{\mathscr{D}^1(p,q)\cdots\mathscr{D}^m(p,q)}_{m}, \tag{18}$$

where each matrix $\mathscr{D}^k$ has a form of the product of ks $m\times m$ matrices:

$$\mathscr{D}^k=\mathscr{R}^{a_k+k}(p,q)\prod_{i=k-1}^{0}\mathscr{I}^{a_k+i}(p,q), \tag{19}$$

$\left(a_k\equiv\dfrac{k(k+1)}{2}\right)$

$$\mathscr{R}^{a_k+k}=\begin{pmatrix} \overbrace{\boxed{I}}^{k} & \overbrace{0}^{m-k} \\ 0 & \boxed{B^{a_k+k}} \end{pmatrix}, \tag{20}$$

$$\mathscr{I}^{a_k+i}=\begin{array}{c} \overbrace{}^{k}\ \overbrace{}^{m-k} \\ \left(\begin{array}{ccccc|ccccc} 1 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 1 & 0 & 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & \cdots & C_{k+1}^{a_k+i} & \cdots & 0 & 1 & 0 & \cdots & 0 & 0 \\ 0 & \cdots & C_{k+2}^{a_k+i} & \cdots & 0 & 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & \vdots & C_{m-1}^{a_k+i} & \cdots & 0 & 0 & 0 & \cdots & 1 & 0 \\ 0 & \cdots & C_{m}^{a_k+i} & \cdots & 0 & 0 & 0 & \cdots & 0 & 1 \end{array}\right) \\ \underbrace{}_{k-i} \end{array}, \tag{21}$$

and the corresponding matrix elements satisfy a set of first-order *linear* differential equations [see below (25)–(28)]. Just the linear character of these equations allows one to speak about a practical usage of the proposed method of Abelianization. As it will be explained below, the constraints obtained as a result of the action of k's matrices [constraints at the (a_k+k)th step],

$$\Phi_{\alpha}^{a_k+k}=(\mathscr{D}^k\cdot\mathscr{D}^{k-1}\cdots\mathscr{D}^1)_{\alpha\beta}\Phi_{\beta}^{0}, \tag{22}$$

obey the algebra where k constraints have zero Poisson brackets with any other. From the algebraic standpoint, the proposed method of Abelianization is nothing but an iterative procedure of constructing "equivalent" algebras $\mathscr{A}^{a_i}$ of constraints $\Phi_{\alpha}^{a_i}$. In a_m steps the m-dimensional non-Abelian algebra is converted into an equivalent Abelian one so that at the a_kth step the obtained algebra $\mathscr{A}^{a_k}$ possesses a center with k elements $\mathscr{Z}_k[A]=(\Phi_1^{a_k},\Phi_2^{a_k},\ldots,\Phi_k^{a_k})$:

$$\mathscr{A}^0\xrightarrow{\mathscr{S}^1}\mathscr{A}^1\xrightarrow{\mathscr{R}^2}\mathscr{A}^2\xrightarrow{\mathscr{S}^3}\mathscr{A}^3\xrightarrow{\mathscr{S}^4}\mathscr{A}^4\xrightarrow{\mathscr{R}^5}\mathscr{A}^5\cdots\xrightarrow{\mathscr{S}^{a_k}}\mathscr{A}^{a_k}\cdots\xrightarrow{\mathscr{R}^{a_k+k}}\mathscr{A}^{a_k+k}\cdots, \tag{23}$$

$$\mathscr{D}^1\qquad\mathscr{D}^2\qquad\mathscr{D}^k$$

The matrix $\mathscr{D}^k$ converts the algebra $\mathscr{A}^k$ into the algebra $\mathscr{A}^{k+1}$ in which the center contains one element more than the previous one.

The proof of the validity of the representation (19) and the equations for matrices $\mathscr{S}$ and $\mathscr{R}$ is obtained by induction. Suppose that $\Phi_{\alpha}^{a_k}$ are a set of constraints (obtained as a result of the action of $k-1$ matrices $\mathscr{D}^i$) with an algebra having the center $\mathscr{Z}_k[A]=(\Phi_1^{a_k},\Phi_2^{a_k},\ldots,\Phi_k^{a_k})$. Then, the matrix $\mathscr{D}^k$ from (18) performs the transformation to the new constraints

$$\Phi_{\alpha}^{a_{k+1}-1}=\mathscr{D}^k{}_{\alpha\beta}\Phi_{\beta}^{a_k+1}, \tag{24}$$

which form the algebra with the center $\mathscr{Z}_{k+1}[A]=(\Phi_1^{a_{k+1}},\Phi_2^{a_{k+1}},\ldots,\Phi_k^{a_{k+1}},\Phi_{k+1}^{a_{k+1}})$ if the matrices $\mathscr{S}$, $\mathscr{R}$ are solutions to the following set of linear differential equations:

$$\left.\begin{array}{r}\{\Phi_1^{a_k+i-1},S_{\alpha_k}^{a_k+i}\}=0\\ \vdots\qquad\qquad\vdots\quad\vdots\\ \{\Phi_{k-1}^{a_k+i-1},S_{\alpha_k}^{a_k+i}\}=0\end{array}\right\}\Rightarrow\{\Phi_{\overline{\alpha}_k}^{a_k+i-1},S_{\alpha_k}^{a_k+i}\}=0, \tag{25}$$

$$\{\Phi_k^{a_k+i-1},S_{\alpha_k}^{a_k+i}\}=f_{k\alpha_k\gamma_k}^{a_k+i-1}S_{\gamma_k}^{a_k+i}-f_{k\alpha_k i+1}^{a_k+i-1}, \tag{26}$$

$$\left.\begin{array}{r}\{\Phi_1^{a_k+k-1},B_{\alpha_k\beta_k}^{a_k+k}\}=0\\ \vdots\qquad\qquad\vdots\quad\vdots\\ \{\Phi_{k-1}^{a_k+k-1},B_{\alpha_k\beta_k}^{a_k+k}\}=0\end{array}\right\}\Rightarrow\{\Phi_{\overline{\alpha}_k}^{a_k+k-1},B_{\alpha_k\beta_k}^{a_k+k}\}=0, \tag{27}$$

$$\{\Phi_k^{a_k+k-1},B_{\alpha_k\beta_k}^{a_k+k}\}=-f_{k\gamma_k\beta_k}^{a_k+k-1}B_{\alpha_k\gamma_k}^{a_k+k}, \tag{28}$$

where $\alpha_k=k+1,\ldots m$, $\overline{\alpha}_k=1,2,\ldots,k-1$, and $f_{\alpha\gamma\beta}^{a_k+i}$ are structure functions of the constraint algebra A^{a_k+i} at the (a_k+i)th step.

Let us begin to construct, in a consecutive order, algebras with the center containing 1,2,...,m elements. To determine the new algebra with one central element (let φ_1), one can act in the following way:

(a) First, eliminate φ_1 from the right-hand side of Eq. (14);
(b) then realize Abelianization with all others.

To achieve the first step, we can perform the transformation with the matrix $\mathscr{S}^1$,

$$\Phi^1_\alpha = \mathscr{S}^1_{\alpha\beta}\varphi_\beta,$$

of type (21):

$$\mathscr{S}^1 = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ C_2 & 1 & 0 & \cdots & 0 \\ C_3 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ C_m & 0 & 0 & \cdots & 1 \end{pmatrix}. \tag{29}$$

In the explicit form it is

$$\Phi^1_1 = \Phi^0_1 = \varphi_1, \quad \Phi^1_{\alpha_1} = \varphi_{\alpha_1} + C^1_{\alpha_1}\varphi_1. \tag{30}$$

The algebra of new constraints remains the first class

$$\begin{aligned} \{\Phi^1_1, \Phi^1_{\alpha_1}\} &= f^1_{1\alpha_1 1}\Phi^1_1 + f^1_{1\alpha_1\gamma_1}\Phi^1_{\gamma_1}, \\ \{\Phi^1_{\alpha_1}, \Phi^1_{\beta_1}\} &= f^1_{\alpha_1\beta_1 1}\Phi^1_1 + f^1_{\alpha_1\beta_1\gamma_1}\Phi^1_{\gamma_1}. \end{aligned} \tag{31}$$

The new structure functions $f^1_{\alpha\beta\gamma}$ are determined through the old ones $f_{\alpha\beta\gamma}$ and the transformation functions $C^1_{\alpha_1}$ as follows:

$$f^1_{1\alpha_1 1} = f_{1\alpha_1 1} + f_{1\alpha_1\gamma_1}C^1_{\gamma_1} + \{\Phi^0_1, C^1_{\alpha_1}\}, \tag{32}$$

$$f^1_{\alpha_1\beta_1 1} = \tfrac{1}{2}(f_{\alpha_1\beta_1 1} - f_{\alpha_1\beta_1\gamma_1}C^1_{\gamma_1} + \{C^1_{\alpha_1}, C^1_{\beta_1}\}\Phi^0_1) - f^1_{1\alpha_1 1}C^1_{\beta_1} + \{\Phi^0_{\alpha_1}, C^1_{\beta_1}\} - (\alpha_1 \leftrightarrow \beta_1), \tag{33}$$

$$f^1_{\alpha_1\beta_1\gamma_1} = f_{\alpha_1\beta_1\gamma_1} + C^1_{\alpha_1}f_{1\beta_1\gamma_1} - C^1_{\beta_1}f_{1\alpha_1\gamma_1}, \tag{34}$$

$$f^1_{1\alpha_1\gamma_1} = f_{1\alpha_1\gamma_1}. \tag{35}$$

Now let us choose the transformation functions $C^1_{\beta_1}$ so that the Poisson bracket of the first constraint Φ^1_1 with all other modified constraints does not contain Φ^1_1:

$$\{\Phi^1_1(p,q), \Phi^1_{\alpha_1}(p,q)\} = \sum_{\gamma\neq 1} f^1_{1\alpha_1\gamma}(p,q)\Phi^1_\gamma(p,q). \tag{36}$$

These $m-1$ requirements $f^1_{1\alpha_1 1} = 0$, according to (32), mean that the transformation function $C^1_{\alpha_1}$ must satisfy the following set of linear nonhomogeneous differential equations

$$\{\Phi^0_1, C^1_{\alpha_1}\} = -f_{1\alpha_1 1} + f_{1\alpha_1\gamma_1}C^1_{\gamma_1}. \tag{37}$$

Note that the problem of existence of the solution to a set of that sort of equations has been studied very well (see, e.g., Ref. 16). Suppose we find a particular solution $C^1_{\alpha_1}$ for (37). Then, we can determine all structure functions of the modified algebra according to Eq. (32):

$$f^1_{1\alpha_1 1}=0, \tag{38}$$

$$f^1_{\alpha_1\beta_1 1}=f_{\alpha_1\beta_1 1}-f_{\alpha_1\beta_1\gamma_1}C^1_{\gamma_1}+\{C^1_{\alpha_1},C^1_{\beta_1}\}\Phi^0_1+\{\Phi^0_{\alpha_1},C^1_{\beta_1}\}+\{\Phi^0_{\beta_1},C^1_{\alpha_1}\}, \tag{39}$$

$$f^1_{\alpha_1\beta_1\gamma_1}=f_{\alpha_1\beta_1\gamma_1}+C^1_{\alpha_1}f_{1\beta_1\gamma_1}-C^1_{\beta_1}f_{1\alpha_1\gamma_1}, \tag{40}$$

$$f^1_{1\alpha_1\gamma_1}=f_{1\alpha_1\gamma_1}. \tag{41}$$

Now let us again keep the first constraint unchanged and perform the Dirac transformation for the remaining part of constraints Φ_{α_1}, $\alpha_1=2,3,...,m$,

$$\Phi^2_1=\Phi^1_1=\Phi^0_1=\varphi_1, \quad \Phi^2_{\alpha_1}=B^2_{\alpha_1\beta_1}\Phi^1_{\beta_1}, \tag{42}$$

with the requirement that the new constraints have zero Poisson brackets with the first one Φ^1_1:

$$\{\Phi^2_1,\Phi^2_{\alpha_1}\}=0. \tag{43}$$

One can verify that this requirement means that the transformation functions $B_{\alpha_1\beta_1}$ are solutions to the equation

$$\{\Phi^1_1,B^2_{\alpha_1\beta_1}\}=-f_{1\gamma_1\beta_1}B^2_{\alpha_1\gamma_1}. \tag{44}$$

In terms of a solution of Eq. (44) the modified algebra has the following structure functions:

$$f^2_{1\alpha_1 1}=0, \tag{45}$$

$$f^2_{\alpha_1\beta_1 1}=B^2_{\alpha_1\delta_1}B^2_{\beta_1\sigma_1}f^1_{\delta_1\sigma_1 1}, \tag{46}$$

$$\begin{aligned} f^2_{\alpha_1\beta_1\gamma_1}=&[\{B^2_{\alpha_1\delta_1},B^2_{\beta_1\sigma_1}\}\Phi^1_{\sigma_1}+\{B^2_{\alpha_1\delta_1},\Phi^1_{\sigma_1}\}B^2_{\beta_1\sigma_1}-\{B^2_{\beta_1\delta_1},\Phi^1_{\sigma_1}\}\\ &\times B^2_{\alpha_1\sigma_1}+B^2_{\alpha_1\kappa_1}B^2_{\beta_1\sigma_1}f^1_{\kappa_1\sigma_1\delta_1}](B^2)^{-1}_{\delta_1\rho_1}. \end{aligned} \tag{47}$$

Thus, as a result of two transformations $\mathscr{D}^1=\mathscr{S}^1\mathscr{R}^2$, we obtain the modified algebra $\mathscr{A}^2$ of constraints Φ^2_α with the central element Φ^2_1

$$\{\Phi^2_1,\Phi^2_{\alpha_1}\}=0, \tag{48}$$

$$\{\Phi^2_{\alpha_1},\Phi^2_{\beta_1}\}=f^2_{\alpha_1\beta_1 1}\Phi^2_1+f^2_{\alpha_1\beta_1\gamma_1}\Phi^2_{\gamma_1}. \tag{49}$$

The structure functions $f^2_{\alpha_1\beta_1\gamma}$ of algebra (48) and (49) possess a significant property: since Φ^2_1 is the central element, the structure functions obey the following property:

$$\{\Phi^2_1,f^2_{\alpha_1\beta_1\gamma}\}=0. \tag{50}$$

To verify this, it is sufficient to calculate the Poisson bracket of Φ^2_1 with (49) and use the Jacobi identity.

To extend the center of the new algebra $\mathscr{A}^2$ by Φ_2^2, we will act by analogy with the previous case.

(a) Eliminate Φ_1^2 and Φ_2^2 from the right-hand side of Eq. (49).
(b) Then, perform the Abelianization with all others.

To carry out the first point of this program, we will deal with two consecutive transformations $\mathscr{S}^3$ and $\mathscr{S}^4$. Let us require that the first transformation $\mathscr{S}^3$ of type (21),

$$\begin{aligned} &\Phi_1^3=\Phi_1^2, \quad \Phi_2^3=\Phi_2^2 \\ &\Phi_{\alpha_2}^2=\Phi_{\alpha_2}^2+C_{\alpha_2}^3\Phi_1^2, \quad \alpha_2=3,\ldots,m, \end{aligned} \tag{51}$$

leads to the new algebra of constraints so that Φ_1^3 is again the central element,

$$\{\Phi_1^3,\Phi_{\alpha_1}^2\}=0, \tag{52}$$

and the Poisson brackets of the second constraint Φ_2^3 with all other modified constraints does not contain Φ_1^3:

$$\{\Phi_2^3,\Phi_{\alpha_2}^2\}=\sum_{\gamma\neq 1} f_{2\alpha_2\gamma}^3\Phi_\gamma^3. \tag{53}$$

This requirement leads to the following equations:

$$\{\Phi_1^3,C_{\alpha_2}^3\}=0, \quad \{\Phi_2^2,C_{\alpha_2}^3\}=f_{2\alpha_2\gamma_2}^2C_{\gamma_2}^3-f_{2\alpha_21}^2. \tag{54}$$

As for the existence of solutions to these equations, one can verify that the integrability condition for the system of differential equations (54) is nothing else but (50). In full analogy with the previous case one can express the new structure functions $f_{\alpha,\beta\gamma}^3$ through $f_{\alpha,\beta\gamma}^2$ and verify that they obey the following property:

$$\{\Phi_1^3,f_{2\alpha_2\gamma}^3\}=0. \tag{55}$$

Now one can realize the transformation $\mathscr{S}^4$ of type (21),

$$\begin{aligned} &\Phi_1^4=\Phi_1^3, \quad \Phi_2^4=\Phi_2^3, \\ &\Phi_{\alpha_2}^4=\Phi_{\alpha_2}^3+C_{\alpha_2}^4\Phi_2^2, \end{aligned} \tag{56}$$

so that Φ_1^4 is again the central element,

$$\{\Phi_1^4,\Phi_{\alpha_1}^2\}=0, \tag{57}$$

and the Poisson brackets of the second constraint Φ_4^2 with all other modified constraints do not contain Φ_1^4 and Φ_2^4:

$$\{\Phi_2^4,\Phi_{\alpha_2}^4\}=\sum_{\gamma\neq 1,2} f_{2\alpha_2\gamma}\Phi_\gamma^3. \tag{58}$$

This requirement leads to the following equations:

$$\{\Phi_1^4,C_{\alpha_2}^4\}=0, \quad \{\Phi_2^3,C_{\alpha_2}^4\}=f_{2\alpha_2\gamma_2}^3C_{\gamma_2}^4-f_{2\alpha_22}^3. \tag{59}$$

TABLE I. Abelianization stages for the algebra with two central elements.

	Constraints	Algebra	Conditions
Φ^0_α	$\Phi^0_\alpha=\varphi_\alpha$	$\{\Phi^0_\alpha,\Phi^0_\beta\}=f^0_{\alpha\beta\gamma}\Phi^0_\gamma$	
Φ^1_α	$\Phi^1_1=\Phi^0_1$ $\Phi^1_{\alpha_1}=\Phi^0_{\alpha_1}+C^1_{\alpha_1}\Phi^0_1$	$\{\Phi^1_1,\Phi^1_\alpha\}=f^1_{1\alpha\gamma_1}\Phi^1_{\gamma_1}$	$\{\Phi^0_1,C^1_{\alpha_1}\}=f_{1\alpha_1\gamma_1}C^1_{\gamma_1}-f_{1\alpha_1 1}$
Φ^2_α	$\Phi^2_1=\Phi^1_1=\Phi^0_1$ $\Phi^2_{\alpha_1}=B^2_{\alpha_1\beta_1}\Phi^1_{\beta_1}$	$\{\Phi^2_1,\Phi^1_\alpha\}=0$	$\{\Phi^1_1,B^2_{\alpha_1\beta_1}\}=-f^1_{1\gamma_1\beta}B^2_{\alpha_1\gamma_1}$
1	$\{\Phi^2_1,\Phi^2_\alpha\}=0$		
Φ^3_α	$\Phi^3_1=\Phi^2_1=\Phi^1_1$ $\Phi^3_2=\Phi^2_2$ $\Phi^3_{\alpha_2}=\Phi^2_{\alpha_2}+C^3_{\alpha_2}\Phi^1_1$	$\{\Phi^3_1,\Phi^3_\alpha\}=0$ $\{\Phi^3_2,\Phi^3_\alpha\}=f^3_{1\alpha\gamma_1}\Phi^2_{\gamma_1}$	$\{\Phi^3_1,C^3_{\alpha_2}\}=0$ $\{\Phi^2_2,C^3_{\alpha_2}\}=f^2_{2\alpha_2\gamma_2}C^2_{\gamma_2}-f^2_{2\alpha_2 1}$
Φ^4_α	$\Phi^4_1=\Phi^3_1\cdots=\Phi^1_1$ $\Phi^4_2=\Phi^3_2=\Phi^2_2$ $\Phi^4_{\alpha_2}=\Phi^3_{\alpha_2}+C^4_{\alpha_2}\Phi^3_2$	$\{\Phi^4_1,\Phi^4_\alpha\}=0$ $\{\Phi^4_2,\Phi^4_\alpha\}=f^4_{2\alpha\gamma_2}\Phi^4_{\gamma_2}$	$\{\Phi^4_1,C^4_{\alpha_2}\}=0$ $\{\Phi^3_2,C^{4^2}_{\alpha_2}\}=f^3_{2\alpha_2\gamma_2}C^4_{\gamma_2}-f^3_{2\alpha_2 2}$
Φ^5_α	$\Phi^5_1=\Phi^4_1\cdots\Phi^1_1$ $\Phi^5_2=\Phi^4_2\cdots\Phi^2_2$ $\Phi^5_{\alpha_2}=B^5_{\alpha_2\beta_2}\Phi^4_{\beta_2}$	$\{\Phi^5_1,\Phi^5_\alpha\}=0$ $\{\Phi^5_2,\Phi^5_\alpha\}=0$	$\{\Phi^4_1,B^5_{\alpha_2\beta_2}\}=0$ $\{\Phi^4_2,B^{5^2}_{\alpha_2\beta_2}\}=-f^4_{2\gamma_2\beta_2}B^5_{\alpha_2\gamma_2}$
2	$\{\Phi^5_1,\Phi^5_\alpha\}=\{\Phi^5_2,\Phi^5_\alpha\}=0$		

This system is consistent by virtue of Eqs. (55). For the new structure function one can again verify that

$$\{\Phi^4_1,f^4_{2\alpha_2\gamma}\}=0 \tag{60}$$

as for the previous step [see Eqs. (55)]. Now for Abelianization of two constraints Φ^4_1 and Φ^5_2, it is enough to perform the last transformation with a matrix $\mathscr{R}$ of type (20) if its elements are solutions to the equations

$$\{\Phi^4_1,B^5_{\alpha_2\beta_2}\}=0,\quad \{\Phi^4_2,B^5_{\alpha_2\beta_2}\}=-f^4_{2\gamma_2\beta_2}B^5_{\alpha_2\gamma_2}. \tag{61}$$

As a result,

$$\{\Phi^5_1,\Phi^5_\alpha\}=\{\Phi^5_2,\Phi^5_\alpha\}=0.$$

Note that (60) provides a solution to Eqs. (61) to exist. As a result, one can easily verify that the new structure functions possess the property

$$\{\Phi^{\,5}_{\overline{\alpha}_2},f^5_{\alpha_2\beta_2\gamma}\}=0,\quad \overline{\alpha}_2=1,2. \tag{62}$$

Thus, in five steps (for summary, see Table I) we obtained algebra $\mathscr{A}^5$, an equivalent to the initial one with two central elements $\Phi^{\,5}_{\overline{\alpha}_2}$.

Now let us suppose that by acting in this way we obtain the algebra $\mathscr{A}^{k-1}$ (see Table II),

$$\{\Phi^{a_k-1}_\alpha,\Phi^{a_k-1}_\beta\}=f^{a_k-1}_{\alpha\beta\gamma}\Phi^{a_k-1}_\gamma, \tag{63}$$

with the center composed of $(k-1)$ elements

TABLE II. Abelianization stages for the algebra with k central elements.

	Constraints	Algebra	Conditions
$k-1$	$\{\Phi_1^{a_k-1},\Phi_\alpha^{a_k-1}\}=\{\Phi_2^{a_k-1},\Phi_\alpha^{a_k-1}\}=\cdots=\{\Phi_{k-1}^{a_k-1},\Phi_\alpha^{a_k-1}\}=0$		
	$\Phi_1^{a_k}=\Phi_1^{a_k-1}\cdots=\Phi_1^1$	$\{\Phi_1^{a_k},\Phi_\alpha^{a_k}\}=0$	$\{\Phi_1^{a_k},C_{\alpha_k}^{a_k}\}=0$
	$\Phi_2^{a_k}=\Phi_2^{a_k-1}\cdots=\Phi_2^2$	$\{\Phi_2^{a_k},\Phi_\alpha^{a_k}\}=0$	$\{\Phi_2^{a_k},C_{\alpha_k}^{a_k}\}=0$
	$\vdots$		
	$\Phi_k^{a_k}=\Phi_k^{a_k-1}$ $\Phi_{\alpha_k}^{a_k}=\Phi_\alpha^{a_k-1}+C_{\alpha_k}^{a_k}\Phi_1^1$	$\{\Phi_k^{a_k},\Phi_\alpha^{a_k}\}=f_{k\alpha\gamma_1}^{a_k}\Phi_{\gamma_1}^{a_k}$	$\{\Phi_k^{a_k-1},C_{\alpha_k}^{a_k}\}=f_{k\alpha_k\gamma_k}^{a_k-1}C_{\gamma k}^{a_k}-f_{k\alpha_k 1}^{a_k-1}$
	$\vdots$	$\vdots$	$\vdots$
	$\vdots$	$\vdots$	$\vdots$
	$\Phi_1^{a_k+k}=\cdots=\Phi_1^1$	$\{\Phi_1^{a_k+k},\Phi_\alpha^{a_k+k}\}=0$	$\{\Phi_1^{a_k+k},B_{\alpha_k\beta_k}^{a_k+k}\}=0$
	$\Phi_2^{a_k+k}=\cdots=\Phi_2^2$	$\{\Phi_2^{a_k+k},\Phi_\alpha^{a_k+k}\}=0$	
	$\vdots$	$\vdots$	$\vdots$
	$\Phi_k^{a_k+k}=\Phi_k^{a_k-1}$ $\Phi_{\alpha_k}^{a_k}=B_{\alpha_k\beta_k}^{a_k+k}\Phi_{\beta_k}^{a_k+k-1}$	$\{\Phi_k^{a_k+k},\Phi_\alpha^{a_k+k}\}=0$	$\{B_{\alpha_k\beta_k}^{a_k+k},\Phi_k^{a_k+k}\}=f_{k\gamma_k\beta_k}^{a_k+k-1}B_{\alpha_k\gamma_k}^{a_k+k}$
k	$\{\Phi_1^{a_{k+1}-1},\Phi_\alpha^{a_{k+1}-1}\}=\{\Phi_2^{a_{k+1}-1},\Phi_\alpha^{a_{k+1}-1}\}=\cdots=\{\Phi_k^{a_{k+1}-1},\Phi_\alpha^{a_{k+1}-1}\}=0$		

$$\mathscr{Z}_{k-1}=(\Phi_1^{a_k-1},\Phi_2^{a_k-1},\ldots\Phi_{k-1}^{a_k-1}),$$

$$\{\mathscr{Z}_{k-1},\Phi_\alpha^{a_k-1}\}=0,$$

and the structure functions of this algebra have the property

$$\{\Phi_{\underline{\alpha}_k}^{a_k-1},f_{\alpha_k\beta_k\gamma}^{a_k-1}\}=0,\quad \overline{\alpha}_k=k-1,\ldots,m. \tag{64}$$

Now by direct calculations it is easy to verify that via the transformation of the matrix $\mathscr{D}^k$ with elements, the solutions to Eqs. (25) and (28), we obtain the algebra $\mathscr{A}^k$ with the center composed of k elements

$$\begin{aligned}\mathscr{Z}_{k-1}&=(\Phi_1^{a_k-1},\Phi_2^{a_k-1},\ldots,\Phi_{k-1}^{a_k-1}),\\ \{\mathscr{Z}_{k-1},\Phi_\alpha^{a_k-1}\}&=0.\end{aligned} \tag{65}$$

The conditions (64) represent the integrability conditions for the system of Eqs. (25) and (28).

For completion we should only prove the following property of structure functions:

$$\{\Phi_{\underline{\alpha}_{k+1}}^{a_k+k},f_{\alpha_{k+1}\beta_{k+1}\gamma}^{a_k+k}\}=0. \tag{66}$$

To verify this, we can consider the algebra of constraints

$$\{\Phi_{\alpha_{k+1}}^{a_k+k},\Phi_{\beta_{k+1}}^{a_k+k}\}=f_{\alpha_{k+1}\beta_{k+1}\overline{\gamma}_{k+1}}^{a_k+k}\Phi_{\underline{\gamma}_{k+1}}^{a_k+k}+f_{\alpha_{k+1}\beta_{k+1}\gamma_{k+1}}^{a_k+k}\Phi_{\gamma_{k+1}}^{a_k+k} \tag{67}$$

and compose the Poisson bracket of (67) with $\Phi_{\underline{\alpha}_{k+1}}^{\alpha_k+k}$. Taking into account that $\Phi_{\underline{\alpha}_{k+1}}^{a_k+k}$ are central elements of the algebra $\mathscr{A}^k$, we immediately obtain the desired result (66) with the help of the Jacobi identity.

III. CHRIST–LEE MODEL

In this section we will apply the above-described procedure to the well-known example, the non-Abelian Christ–Lee model described by the Lagrangian

$$\mathscr{L}(\mathbf{x},\dot{\mathbf{x}},\mathbf{y})=\tfrac{1}{2}(\dot{\mathbf{x}}-[\mathbf{y},\mathbf{x}])^2-V(\mathbf{x}^2),$$

where $\mathbf{x}$ and $\mathbf{y}$ are three-dimensional vectors, (x_1,x_2,x_3) and (y_1,y_2,y_3).

It is easy to verify that except for three primary constraints

$$\pi=\frac{\partial\mathscr{L}}{\partial\dot{\mathbf{y}}}=0,$$

there are two independent constraints

$$\Phi_1^0=x_2p_3-x_3p_2, \quad \Phi_2^0=x_3p_1-x_1p_3, \tag{68}$$

with the algebra

$$\{\Phi_1^0,\Phi_2^0\}=-\frac{x_1}{x_3}\,\Phi_1^0-\frac{x_2}{x_3}\,\Phi_2^0. \tag{69}$$

The Abelianization procedure for this simple case consists of two stages. At the first step, the transformation $\mathscr{S}^1$ is reduced to

$$\Phi_1^1=\Phi_1^0, \quad \Phi_2^1=\Phi_2^0+C\Phi_1^0, \tag{70}$$

and Eq. (25) looks like

$$\{\Phi_1^0,C\}=\frac{x_2}{x_3}\,C+\frac{x_1}{x_3}. \tag{71}$$

We can write down a particular solution to this equation:

$$C(x)=\frac{x_1}{x_3}\arctan\left(\frac{x_2}{x_3}\right). \tag{72}$$

So, as a result of first step, we obtain a new algebra

$$\{\Phi_1^1,\Phi_2^1\}=-\frac{x_2}{x_3}\,\Phi_2^1. \tag{73}$$

Now let us perform the second transformation $\mathscr{R}^2$,

$$\Phi_1^2=\Phi_1^1,$$

$$\Phi_2^1=B\Phi_2^1, \tag{74}$$

with the function B satisfying an equation such as (28)

$$\{\Phi_1^1,B\}=\frac{x_2}{x_3}. \tag{75}$$

A particular solution to this equation reads

$$B(x)=\ln\left(\frac{\sqrt{x_2^2+x_3^2}}{x_3}\right). \tag{76}$$

Thus, the constraints equivalent to the initial Abelian constraints are of the form

$$\begin{aligned}\Phi_1^2&=x_2p_3-x_3p_2,\\ \Phi_2^2&=\ln\left(\frac{\sqrt{x_2^2+x_3^2}}{x_3}\right)\left[(x_3p_1-x_1p_3)+\frac{x_1}{x_3}\arctan\left(\frac{x_2}{x_3}\right)(x_2p_3-x_3p_2)\right].\end{aligned} \tag{77}$$

IV. CONCLUDING REMARKS

We have discussed the iterative procedure of converting first class constraints in an arbitrary singular theory to the Abelian form of constraints. Our final goal is to apply the Abelianization procedure to construct a reduced phase space in the gauge non-Abelian theory and gravity. To extend the proposed method to field theory, it is necessary to clear up some points. For field models, where the Poisson brackets of constraints contain derivatives of constraints such as reparametrization-invariant theories, a direct application of our scheme is impossible. However, for a wide class of gauge-invariant field models, e.g., the non-Abelian Yang–Mills theory, the algebra of constraints is similar to the considered algebra, and we expect that the presented method of Abelianization will be useful in this case. The Abelianization procedure will be applied to the SU(2) Yang–Mills theory in a separate forthcoming publication.

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The complete Kepler group can be derived by Lie group analysis

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It is shown that the complete symmetry group for the Kepler problem, as introduced by Krause, can be derived by Lie group analysis. The same result is true for any autonomous system. © *1996 American Institute of Physics.*
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I. INTRODUCTION

In Ref. 1, a new concept of symmetry group for ordinary differential equations, which have $x_k = x_k(t)$, $(k=1,2,\ldots,N)$ as unknown functions, was introduced. Krause defined a complete symmetry group by adding two properties to the definition of Lie symmetry group:

(i) the manifold of solutions is a homogeneous space of the group;
(ii) the group is specific to the system (no other system admits it).

This definition of the complete symmetry group needed a new type of symmetry to be introduced. For example, neither Lie point symmetries nor contact symmetries give rise to a complete symmetry group for the Kepler problem. The generator of the new symmetry was defined to be

$$Y=\left[\int \xi(t,x_1,\ldots,x_N)dt\right]\partial_t+\sum_{k=1}^{N}\eta_k(t,x_1,\ldots,x_N)\partial_{x_k}, \tag{1}$$

which is different from the generator of a Lie point symmetry group[2–11] because of the appearance of the integral of ξ.

Here, we show that if the system under study is autonomous then the complete symmetry group can be recovered by Lie group analysis. In particular, the extra symmetries that Krause claimed not to be found by Lie group analysis for the Kepler problem can be so determined. This is explained by the following observation. If the system is autonomous, then one of the unknown functions can be taken to be the new independent variable and the system consequently can be rewritten. Thus, Lie group analysis applied to the transformed system leads to different results, and in particular the extra symmetries which were found by applying Krause's method can be retrieved.

II. OUTLINE OF THE METHOD

Let us consider the following autonomous system of N second-order ordinary differential equations

$$\ddot{x}_k=F_k(x_1,x_2,\ldots,x_N,\dot{x}_1,\ldots,\dot{x}_N) \quad (k=1,2,\ldots,N). \tag{2}$$

A generator of a Lie point symmetry group for this system has the form

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$$X=\tau(t,x_1,\ldots,x_N)\partial_t+\sum_{k=1}^{N}\eta_k(t,x_1,\ldots,x_N)\partial_{x_k}. \tag{3}$$

System (2) can be converted into the following autonomous system of $2N$ first-order ordinary differential equations[10]

$$\dot{u}_k=u_{N+k}, \tag{4}$$

$$\dot{u}_{N+k}=F_k(u_1,u_2,\ldots,u_N,u_{N+1},\ldots,u_{2N}). \tag{5}$$

Now, we can choose one of the dependent variables to be the new independent variable y. For example, let us take $u_N=y$. Then, system (4)–(5) becomes the following nonautonomous system of $2N-1$ first-order ordinary differential equations with independent variable y

$$\frac{du_j}{dy}=\frac{u_{N+j}}{u_{2N}}, \tag{6}$$

$$\frac{du_{N+j}}{dy}=\frac{F_j(u_1,u_2,\ldots,u_{N-1},y,u_{N+1},\ldots,u_{2N})}{u_{2N}}, \tag{7}$$

$$\frac{du_{2N}}{dy}=\frac{F_N(u_1,u_2,\ldots,u_{N-1},y,u_{N+1},\ldots,u_{2N})}{u_{2N}}, \tag{8}$$

where $(j=1,2,\ldots,N-1)$. From Eqs. (6) we can deduce that

$$u_{N+j}=u_{2N}\frac{du_j}{d_y},$$

which when substituted into Eqs. (7) and (8) yields the following system of $N-1$ second-order ordinary differential equations and one first-order equation for the unknowns $u_j=u_j(y)$, and $u_{2N}=u_{2N}(y)$

$$u_j''=\frac{1}{u_{2N}^2}[F_j(u_1,u_2,\ldots,u_{N-1},y,u_1',\ldots,u_{N-1}',u_{2N}) - F_N(u_1,u_2,\ldots,u_{N-1},y,u_1',\ldots,u_{N-1}',u_{2N})u_j'], \tag{9}$$

$$u_{2N}'=\frac{F_N(u_1,u_2,\ldots,u_{N-1},y,u_1',\ldots,u_{N-1}',u_{2N})}{2_{2N}}, \tag{10}$$

where $'$ denotes differentiation by y. A generator of a Lie point symmetry group for this system is of the form:

$$Z=V(y,u_1,\ldots,u_{N-1},u_{2N})\partial_y+\sum_{j=1}^{N-1}G_j(y,u_1,\ldots,u_{N-1},u_{2N})\partial_{u_j}+G_{2N}(y,u_1,\ldots,u_{N-1},u_{2N})\partial_{u_{2N}}, \tag{11}$$

which can be transformed into the operator Y in (1) by substituting u_j,y,u_{2N} with $x_j,x_N,\dot{x}_N$, respectively, and solving the following system for ξ and η_k

$$Y(x_j)\equiv\eta_j=G_j, \tag{12}$$

$$Y(x_N) \equiv \eta_N = V, \tag{13}$$

$$Y^{(1)}(\dot{x}_N) \equiv \frac{d\eta_N}{dt} - \xi \dot{x}_N = G_{2N}, \tag{14}$$

where $Y^{(1)}$ denotes the first prolongation of Y. Therefore, Krause's symmetries can be recovered by means of Lie group analysis applied to system (9), or other nonautonomous systems which can be deduced from (4)–(5) by choosing $u_j = y$. Vice versa, Y in (1) can be transformed into Z in (11) by means of (12)–(14).

However, it should be noticed that Z in (11) could lead to a more general operator than Y in (1) because of the appearance of $\dot{x}_N$. In this case, a sort of contact symmetry generalization of Y would be needed.

Finally, Z can be transformed into a generator of a Lie point symmetry group X in (3), with $\tau = \int \xi\, dt$, if (12)–(14) yield that η_k do not depend on $\dot{x}_N$, and either ξ is constant or $\xi = f(x_N)\dot{x}_N$, with f arbitrary function of x_N.

III. KEPLER PROBLEM

The Kepler problem provides a good example of the method outlined in the previous paragraph. The original Kepler problem is given by the following system:

$$\ddot{x}_1 = \frac{-Kx_1}{(x_1^2+x_2^2+x_3^2)^{3/2}}, \quad \ddot{x}_2 = \frac{-Kx_2}{(x_1^2+x_2^2+x_3^2)^{3/2}}, \quad \ddot{x}_3 = \frac{-Kx_3}{(x_1^2+x_2^2+x_3^2)^{3/2}}. \tag{15}$$

It is well known[7] that Lie group analysis applied to (15) yields a five-dimensional Lie symmetry algebra generated by

$$\begin{gathered} X_1 = \partial_t, \quad X_2 = 3t\partial_t + 2x_1\partial_{x_1} + 2x_2\partial_{x_2} + 2x_3\partial_{x_3}, \\ X_3 = x_2\partial_{x_1} - x_1\partial_{x_2}, \quad X_4 = x_3\partial_{x_1} - x_1\partial_{x_3}, \quad X_5 = x_3\partial_{x_2} - x_2\partial_{x_3}. \end{gathered} \tag{16}$$

Instead, the eight-dimensional complete symmetry group of (15) is generated by X_1, X_2, X_3, X_4, X_5, and

$$\begin{aligned} Y_1 &= 2\left(\int x_1\, dt\right)\partial_t + x_1^2\partial_{x_1} + x_1x_2\partial_{x_2} + x_1x_3\partial_{x_3}, \\ Y_2 &= 2\left(\int x_2\, dt\right)\partial_t + x_1x_2\partial_{x_1} + x_2^2\partial_{x_2} + x_2x_3\partial_{x_3}, \\ Y_3 &= 2\left(\int x_3\, dt\right)\partial_t + x_1x_3\partial_{x_1} + x_2x_3\partial_{x_2} + x_3^2\partial_{x_3}, \end{aligned} \tag{17}$$

which can be obtained by means of the new generator (1) with $N=3$.[1] Krause stated that Y_1, Y_2, and Y_3 cannot be recovered by Lie group analysis. It is true that they are not included in (16), but they can be retrieved by applying Lie group analysis to the equivalent nonautonomous systems.

Let us choose x_3 to be the new independent variable y. Then, the new system (9) becomes

$$u_1'' = \frac{-K(u_1 - yu_1')}{(u_1^2+u_2^2+y^2)^{3/2}u_6^2}, \quad u_2'' = \frac{-K(u_2 - yu_2')}{(u_1^2+u_2^2+y^2)^{3/2}u_6^2}, \quad u_6' = \frac{-Ky}{(u_1^2+u_2^2+y^2)^{3/2}u_6}, \tag{18}$$

where $'$ denotes differentiation by y. Note that, because of the symmetric form of (15), a system similar to (18) is derived, whatever dependent variable we choose as the new independent variable. Lie group analysis applied to (18) yields a three-dimensional Lie symmetry algebra generated by

$$Z_1=y^2\partial_y+yu_1\partial_{u_1}+yu_2\partial_{u_2},$$
$$Z_2=2y\partial_y+2u_1\partial_{u_1}+2u_2\partial_{u_2}-u_6\partial_{u_6},\quad Z_3=u_2\partial_{u_1}-u_1\partial_{u_2}. \tag{19}$$

If we transform these operators into the form given by Y in (1), then Z_1 becomes Y_3 in (17), and Z_2,Z_3 become X_2,X_3 in (16), respectively. In fact, transforming Z_1 into an operator of the form given by Y in (1) corresponds to solve (12)–(14), i.e.,

$$\eta_1=x_1x_3\equiv G_1, \tag{20}$$

$$\eta_2=x_2x_3\equiv G_2, \tag{21}$$

$$\eta_3=x_3^2\equiv V, \tag{22}$$

$$\frac{d\eta_3}{dt}-\xi\dot{x}_3=0\equiv G_{2N}. \tag{23}$$

Substituting (22) into Eq. (23) yields $2x_3\dot{x}_3-\xi\dot{x}_3=0$, which implies $\xi=2x_3$.

It is easy to show that Y_1 $[Y_2]$ can be obtained by applying Lie group analysis to the equivalent nonautonomous system, which has x_1 $[x_2]$ as the new independent variable.

We have used our own interactive Reduce programs[12] to perform Lie group analysis, and apply Krause's method with the generator (1).

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Standard thermal statistics with *q*-entropies

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We report results on the quantum thermal statistics *à la* Gibbs–Shannon–Szilard–Jaynes based on q-entropies $S_q[\rho]=(q-1)^{-1}(1-tr(\rho^q))$ $(0<q\neq 1)$ and the internal energy functional $U[\rho]=tr(\rho H)$ proposed by C. Tsallis [J. Stat. Phys. **52**, 479–487 (1988)]. © *1996 American Institute of Physics.*
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I. INTRODUCTION

For a discrete probability distribution $\rho=(\rho_1,\rho_2,\cdots)$, with $\rho_n\geqslant 0$, and $\Sigma_n\rho_n=1$, consider

$$S_q[\rho]=(q-1)^{-1}\left(1-\sum_n \rho_n^q\right),$$

where q is a positive real number distinct from 1. $S_q[\cdot]$ was introduced, with a different prefactor, by Z. Daróczy[1] who obtained the basic properties and gave an axiomatic characterization. One sees easily that $\lim_{q\to 1}S_q[\rho]=-\Sigma_n\rho_n\ln(\rho_n)$, the well-known Boltzmann–Shannon entropy. The quantum mechanical version

$$S_q[\rho]=(q-1)^{-1}(1-tr(\rho^q)), \tag{1}$$

of the q-entropy appears on p. 247 of Wehrl's review.[2]

The monoparametric family of entropies $S_q[\cdot]$ reappears in a paper by Tsallis,[3] who proposed a generalization of standard statistics obtained by maximizing the q-entropy at fixed internal energy given by $\Sigma_n\rho_n\epsilon_n$. This formalism has been applied to self-gravitating systems,[4] and leads to a phase-space distribution with finite associated mass in contradistinction to the results obtained using the standard statistico-mechanical formalism which lead to an infinite mass. ''Specific heat'' calculations for the harmonic oscillator using this scheme are given in Ref. 5.

In order to solve the basic problem of maximizing $S_q[\cdot]$ at fixed internal energy, Tsallis[3] introduced the function

$$S_q[\rho]+\alpha\sum_n \rho_n-\alpha t(q-1)\sum_n \epsilon_n\rho_n$$

and after a standard variation obtains the equation

$$\rho_n^{q-1}=\frac{q-1}{q}\alpha[1+t(1-q)\epsilon_n].$$

The left-hand side must be a non-negative number. If for a given t all the brackets on the right-hand side are non-zero and have the same sign we get a solution, after determining α by the normalization condition

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$$\rho_n=\left[\sum_n (1+(1-q)t\epsilon_n)^{1/(q-1)}\right]^{-1}(1+(1-q)t\epsilon_n)^{1/(q-1)}.$$

The distribution will be non-degenerate: $\rho_n>0$ for all n. When the brackets on the right-hand side do not all have the same sign or some are zero, the distribution must be degenerate; it must lie in a face of the simplex of probability distributions. One has to determine the appropriate range for t. Although t provides a convenient and explicit parametrization of the distribution with minimal free energy, it is not the reciprocal temperature associated to the problem. The reciprocal temperature is given by $\alpha t(q-1)$, which reads (H is the Hamiltonian operator with spectrum $\{\epsilon_n\}$):

$$\beta(t):=qt[tr\{(1+(1-q)tH)^{1/(q-1)}\}]^{1-q}. \tag{2}$$

The results presented here determine the range of the reciprocal pseudo-temperature t and the connection with the reciprocal temperature β; they also describe precisely the quantum mechanical state ρ_β minimizing the functional

$$\rho\mapsto\beta tr(\rho H)-S_q[\rho]. \tag{3}$$

All analogues of the familiar thermostatistical results known for the case $q=1$ are obtained. From the point of view of Boltzmann–Gibbs statistics, we find qualitative changes only for $q>1$ where ''temperatures'' inside a certain interval containing 0 are inaccessible, a fact described in Refs. 3, and 5. However, the 0^{th}-law (i.e., transitivity of thermal equilibrium) does not hold in this formalism.

We point out that Curado and Tsallis[6] subsequently proposed another formalism where the standard energy functional $U[\rho]=tr(\rho H)$ is replaced by the non-affine functional $U_q[\rho]=tr(\rho^q H)$ while keeping $S_q[\cdot]$ as the entropy. The corresponding non-standard ''thermostatistics'' is studied in Ref. 7 in the same spirit as the present paper. We include here a final section where we compare both formalisms.

The basic observation for the proofs is an application of Hölder's classic inequalities to the quantity $\Sigma_n\rho_n(\epsilon_n-\epsilon_-)$ where ϵ_- is the ground-state energy. With $\mathcal{N}=\{n:\epsilon_n>\epsilon_-\}$, one obtains

$$(1-q)^{-1}\sum_{n\in\mathcal{N}}\rho_n^q\leqslant(1-q)^{-1}\left(\sum_{n\in\mathcal{N}}\rho_n(\epsilon_n-\epsilon_-)\right)^q\left(\sum_{n\in\mathcal{N}}(\epsilon_n-\epsilon_-)^{q/(q-1)}\right)^{1-q}$$

and thus an upper bound on $S_q[\rho]$ in terms of the energy expectation value.

We record here some of the basic properties of the q-entropy. The proofs are written out in Ref. 8, and are consequences of the fact that $S_q[\cdot]$ is a member of the family of entropy functionals given by $\rho\mapsto tr(f(\rho))$ where f is a concave function defined on the unit interval.[9] Specifically

$$S_q[\rho]=tr(\eta_q(\rho)),$$

with $\eta_q(x)=(q-1)^{-1}(x-x^q)$. One has $S_q[\rho]\geqslant 0$ with equality iff ρ is pure. In the finite dimensional case (dimension d), $S_q[\cdot]$ is strictly concave and one has $S_q[\rho]\leqslant(q-1)^{-1}(1-d^{1-q})$ with equality iff ρ is the normalized trace. In the infinite dimensional case and for $q>1$, $S_q[\cdot]$ is strictly concave and one has $S_q[\rho]<(q-1)^{-1}$; moreover $S_q[\cdot]$ is Lipschitz in the trace norm. For $0<q<1$ and in infinite dimension, $S_q[\cdot]$ is generically (on a set of second category) ∞ but the set where it takes finite values is convex and $S_q[\cdot]$ is strictly concave on it.

II. GENERAL REMARKS

Assume given a selfadjoint operator H on a Hilbert space. In the infinite dimensional case, we assume that H is unbounded but its spectrum is purely discrete and consists entirely of eigenvalues

of finite multiplicity. We enumerate these as $\{\epsilon_n\}$ according to their multiplicities. We write ϵ_- (resp. ϵ_+) for the minimal (resp. maximal) energy: $\epsilon_- := \inf_n \epsilon_n$, $\epsilon_+ := \sup_n \epsilon_n$; and assume the non-trivial case $\epsilon_- < \epsilon_+$ in the finite-dimensional case. The convex set of density operators Ω is the state space. The (internal) energy functional is $U[\rho] = tr(\rho H)$. In the unbounded case, the trace is defined by taking any orthonormal basis $\{\psi_n\}$ of eigenvectors of H when the corresponding sum $\Sigma_n \epsilon_n \langle \psi_n, \rho \psi_n \rangle$ is absolutely convergent. With this definition, the set Ω_o of states ρ with finite $U[\rho]$ is convex.

For any u in the interval $\mathscr{U} = [\epsilon_-, \epsilon_+]$ (but $\pm\infty$ excluded, in the infinite dimensional case), we consider the entropy as a function of energy given by

$$S_q(u) := \sup_{\rho \in \Omega_o} \{S_q[\rho] : U[\rho] = u\}, \quad u \in \mathscr{U}. \tag{4}$$

We will distinguish the "thermodynamic" functionals, such as $S_q[\cdot]$, defined on the states from the "thermodynamic" functions, such as S_q, by using square brackets for the arguments of the former.

Since $U[\cdot]$ is affine, the set of states $\rho \in \Omega_o$ with $U[\rho] = u$ is convex. If $u = \lambda u_1 + (1-\lambda) u_2$ where $0 < \lambda < 1$ and $u_1, u_2 \in \mathscr{U}$; then

$$S_q(u) \geqslant \sup\{S_q[\lambda \rho_1 + (1-\lambda)\rho_2] : U[\rho_j] = u_j, j = 1,2\}$$

$$\geqslant \sup\{\lambda S_q[\rho_1] + (1-\lambda) S_q[\rho_2] : U[\rho_j] = u_j, j = 1,2\} = \lambda S_q(u_1) + (1-\lambda) S_q(u_2),$$

so the entropy function S_q is concave. If ω is a maximizing state, i.e., $S_q(u) = S_q[\omega] < \infty$; then it is unique because $S_q[\cdot]$ is strictly concave, and we denote it by ω_u.

Consider the Legendre-Fenchel transform of S_q given by

$$\phi_q(\beta) := \inf_{u \in \mathscr{U}} \{\beta u - S_q(u)\}, \quad \beta \in \mathbf{R}. \tag{5}$$

The function $\beta \mapsto \beta^{-1} \phi_q(\beta)$ is — in appropriate dimensionless variables — the analogue of the Helmholtz free-energy of the system. We first remark that ϕ_q is equal to the **infimum over states** of the corresponding free-energy functional (3):

$$\phi_q(\beta) = \inf_{\rho \in \Omega_o} \{\beta U[\rho] - S_q[\rho]\}. \tag{6}$$

Because the functional (3) is strictly convex where it is finite we conclude that if ρ is a minimizer of (6) — i.e., $\phi_q(\beta) = \beta U[\rho] - S_q[\rho]$, for some β — then it is unique and we denote it by ρ_β.

From (5) it is clear that ϕ_q is a concave function. From (6) and the positivity of $S_q[\cdot]$ one concludes that the "free-energy" function $\beta \mapsto \beta^{-1} \phi_q(\beta)$ is non-decreasing in the intervals $(-\infty, 0)$ and $(0, \infty)$. The inequality $\beta \epsilon_\pm + \phi_q(0) \leqslant \phi_q(\beta) \leqslant \beta \epsilon_\pm$, where the $+$ sign (resp. $-$ sign) applies for negative (resp. positive) β, is obtained directly from (6), for $\epsilon_\pm$ finite respectively.

If, in the infinite dimensional case, H is unbounded above (resp. below) we have $\phi_q(\beta) = -\infty$ for all negative (resp. positive) β. Thus, if H is unbounded both above and below then $\phi_q \equiv -\infty$ except at $\beta = 0$ when $q > 1$; the "thermostatistics" is empty.

The next question is if the unique minimizer ρ_β (resp. maximizer ω_u) is diagonal in an orthonormal basis diagonalizing H. Let $\{\psi_n\}$ be such a basis; and define

$$\hat{\rho} = \sum_n \langle \psi_n, \rho \psi_n \rangle |\psi_n\rangle\langle\psi_n|.$$

Then $\hat{\rho}$ is a state and $U[\rho] = U[\hat{\rho}]$. Moreover, one concludes that $S_q[\hat{\rho}] \geqslant S_q[\rho]$, since for any unit vector ψ in the Hilbert space one has $\langle \psi, \rho^q \psi \rangle \geqslant \langle \psi, \rho \psi \rangle^q$ if $q > 1$; and $\langle \psi, \rho^q \psi \rangle \leqslant \langle \psi, \rho \psi \rangle^q$ if

$0<q<1$. This then implies that the minimizer (resp. maximizer) is indeed diagonal. The reader will notice that all the above results are quite general since they depend exclusively on the strict concavity property of the entropy functional.[10] The problem is now to find ρ_β and ω_u explicitly for the specific entropy $S_q[\,\cdot\,]$. This problem will be solved completely in the following two sections.

III. THE FINITE DIMENSIONAL CASE

We distinguish the two cases depending on whether q is below or above 1.

A. $0<q<1$

Let $t_o=(q-1)^{-1}(\epsilon_+-\epsilon_-)^{-1}$. For t in the interval (t_o,∞), let $\beta(t)$ be defined by [compare with (2)]

$$\beta(t):=qt[tr\{(1+(1-q)t(H-\epsilon_-))^{1/(q-1)}\}]^{1-q}. \tag{7}$$

Then, $\beta(\cdot)$ is a strictly increasing and continuous function, with $\lim_{t\to t_o}\beta(t)=-\infty$ and $\lim_{t\to\infty}\beta(t)=\infty$. Thus $\beta(\cdot)$ maps the interval (t_o,∞) one-to-one and onto $\mathbf{R}$. Tsallis's **reciprocal pseudo-temperature** is given by the map $\tau:\mathbf{R}\to(t_o,\infty)$ inverse to $\beta(\cdot)$.

Proposition 1: For $0<q<1$, with $H\neq c\cdot 1$ and in finite dimension one has:

1. *The maps $\mathscr{U}\ni u\mapsto S_q(u)$ and $\mathbf{R}\ni\beta\mapsto\phi_q(\beta)$ are strictly concave, differentiable and each other's Legendre transforms. One has*

$$S_q(\epsilon_\pm)=\frac{1}{q-1}(1-g_\pm^{1-q}), \tag{8}$$

where $g_\pm$ is the degeneracy of the eigenvalue $\epsilon_\pm$.

The derivative $\mathbf{R}\ni\beta\mapsto(d\phi_q)/(d\beta)(\beta)=:U(\beta)$ of ϕ_q is strictly decreasing and the inverse of the derivative of S_q. One has $\lim_{\beta\to\pm\infty}U(\beta)=\epsilon_\mp$; and $\lim_{u\to\epsilon_\pm}(dS_q)/(du)(u)=\mp\infty$.

2. *For each $u\in\mathscr{U}$ there exists a unique maximizer ω_u with $S_q(u)=S_q[\omega_u]$. For each $\beta\in\mathbf{R}$ there exists a unique equilibrium state ρ_β minimizing ϕ_q. One has*

$$\omega_{U(\beta)}=\rho_\beta,\quad \omega_u=\rho_{\beta(u)} \tag{9}$$

where $\beta(u)$ is determined uniquely by $U(\beta(u))=u$. One has

$$U(\beta)=U[\rho_\beta]. \tag{10}$$

3. *For each $\beta\in\mathbf{R}$, the unique equilibrium state ρ_β is given by*

$$\rho_\beta=\frac{(1+(1-q)\tau(\beta)(H-\epsilon_-))^{1/(q-1)}}{tr[(1+(1-q)\tau(\beta)(H-\epsilon_-))^{1/(q-1)}]}. \tag{11}$$

From the point of view of Boltzmann–Gibbs thermodynamics there are no qualitative changes whatsoever; these will appear in the other following case.

B. $q>1$

For $q>1$, we define critical q-dependent reciprocal "temperatures" by

$$\beta_c^+=\frac{qg_-^{1-q}}{(q-1)(\epsilon_-^*-\epsilon_-)}>0;\quad \beta_c^-=\frac{qg_+^{1-q}}{(1-q)(\epsilon_+-\epsilon_+^*)}<0; \tag{12}$$

where ϵ_+^* is the first energy below the ceiling energy, and ϵ_-^* is the first excited state energy. Let

$$t_1=\frac{1}{(1-q)(\epsilon_+-\epsilon_+^*)}<0, \quad t_2=\frac{1}{(q-1)(\epsilon_-^*-\epsilon_-)}>0.$$

An index $\oplus$ denotes the positive part of the indexed operator. Define

$$\beta(t)=qt\cdot\begin{cases}[tr\{(1+(1-q)t(H-\epsilon_+))_\oplus^{1/(q-1)}\}]^{1-q}, & \text{for } t_1<t\leqslant 0\\ [tr\{(1+(1-q)t(H-\epsilon_-))_\oplus^{1/(q-1)}\}]^{1-q}, & \text{for } 0\leqslant t<t_2\end{cases}. \tag{13}$$

Then, $\beta(\cdot)$ is a strictly increasing and continuous function with $\lim_{t\to t_1}\beta(t)=\beta_c^-$ and $\lim_{t\to t_2}\beta(t)=\beta_c^+$. Thus $\beta(\cdot)$ maps the interval (t_1,t_2) one-to-one and onto $\mathscr{T}\equiv(\beta_c^-,\beta_c^+)$. Tsallis's **reciprocal pseudo-temperature** is given by the map $\tau:\mathscr{T}\to(t_1,t_2)$ inverse to $\beta(\cdot)$.

Proposition 2: For $q>1$, with $H\neq c\cdot 1$ and in finite dimension one has:

1. *The map $\mathscr{U}\ni u\mapsto S_q(u)$ is strictly concave and differentiable; (8) is satisfied. The map* **R** $\ni\beta\mapsto\phi_q(\beta)$ *is concave, and differentiable. Moreover*

$$\phi_q(\beta)=\begin{cases}\beta\epsilon_-+\dfrac{1}{1-q}(1-g_-^{1-q}), & \text{if } \beta\geqslant\beta_c^+\\ \beta\epsilon_++\dfrac{1}{1-q}(1-g_+^{1-q}), & \text{if } \beta\leqslant\beta_c^-\end{cases};$$

and ϕ_q is strictly concave on $\mathscr{T}\equiv(\beta_c^-,\beta_c^+)$. S_q and *ϕ_q are each others Legendre transforms, but $S_q(u)=\inf_{\beta\in\mathscr{T}}\{\beta u-\phi_q(\beta)\}$. The derivative $U(\cdot)$ of ϕ_q is continuous; it satisfies*

$$U(\beta)=\begin{cases}\epsilon_-, & \text{if } \beta\geqslant\beta_c^+\\ \epsilon_+, & \text{if } \beta\leqslant\beta_c^-\end{cases};$$

and is strictly decreasing on $\mathscr{T}$ with inverse given by the derivative of S_q. One has $\lim_{u\to\epsilon_\pm}(dS_q)/(du)\,(u)=\beta_c^\pm$.

2. *For each $u\in\mathscr{U}$ there exists a unique maximizer ω_u with $S_q(u)=S_q[\omega_u]$. For each $\beta\in$* **R** *there exists a unique equilibrium state ρ_β minimizing ϕ_q. One has*

$$\rho_\beta=\begin{cases}g_-^{-1}P^-, & \text{if } \beta\geqslant\beta_c^+\\ g_+^{-1}P^+, & \text{if } \beta\leqslant\beta_c^-\end{cases},$$

where $P^\pm$ is the orthogonal projection onto the eigenspace to the eigenvalue $\epsilon_\pm$. Moreover (9) is satisfied with $\beta(u)$ in the closure of $\mathscr{T}$ determined uniquely by $U(\beta(u))=u$. (10) is satisfied.

3. *For each $\beta\in\mathscr{T}$, the unique equilibrium state ρ_β is given by*

$$\rho_\beta=\begin{cases}\dfrac{(1+(1-q)\tau(\beta)(H-\epsilon_+))_\oplus^{1/(q-1)}}{tr[(1+(1-q)\tau(\beta)(H-\epsilon_+))_\oplus^{1/(q-1)}]}, & \text{for } \beta_c^-<\beta\leqslant 0\\ \dfrac{(+(1-q)\tau(\beta)(H-\epsilon_-))_\oplus^{1/(q-1)}}{tr[(1+(1-q)\tau(\beta)(H-\epsilon_-))_\oplus^{1/(q-1)}]}, & \text{for } 0\leqslant\beta<\beta_c^+\end{cases}. \tag{14}$$

Since $U(\beta)$ is constant outside the closure of the interval $\mathscr{T}$, we have that the analogue of the specific heat is zero for all ''temperatures'' T with $[1-q)g_+^{q-1}/q]\,(\epsilon_+-\epsilon_+^*)<T<[(q-1)g_-^{q-1}/q]\,(\epsilon_-^*-\epsilon_-)$. These ''temperatures'' are thus inaccessible. Notice also that the equilibrium state ρ_β will be degenerate as soon as the corresponding operator on the right-hand side of (14) has a non-zero negative part. At $\beta=0$ the equilibrium state is the normalized trace. As we increase β away from zero (decrease positive ''temperature'') we reach a β_1 where

$1+(1-q)\tau(\beta_1)(\epsilon_+-\epsilon_-)=0$; at this β_1 the ceiling state is depopulated and remains so if we increase β further. Proceeding, we reach a β_2 such that $1+(1-q)\tau(\beta_2)(\epsilon_+^*-\epsilon_-)=0$ and the first de-excited state energy ϵ_+^* is depopulated. Continuing, one depopulates successively from above the energies ϵ_n until β_c^+ is reached where only the ground-state energy level ϵ_- is populated. Decreasing β away from 0 (increasing negative ''temperatures'') the energy levels are depopulated successively from below until the ceiling energy level ϵ_+ is reached at β_c^-.

We mention here that for $q\geqslant 2$ the ''specific heat'' C_q connected to the second derivative of ϕ_q by $C_q=-\beta^2[(d^2\phi_q)/(d\beta^2)](\beta)$ has discontinuities at each β where a depopulation occurs. This does not happen when $1<q<2$.

C. Peierls–Bogoljubov Inequality

In both cases, the equilibrium state ρ_β depends continuously on β and on the Hamiltonian H specifying $U[\cdot]$. From this and the concavity of the map $\lambda\mapsto\phi_q^{(\lambda H_1+(1-\lambda)H_2)}(\beta)$ on the unit interval for each β, one obtains the inequality

$$\phi_q^{(H_1)}(\beta)\leqslant\phi_q^{(H_2)}(\beta)+\beta tr(\rho_\beta^{(H_2)}(H_1-H_2));$$

which in terms of the free-energy $f_q^{(H)}(\beta)=\beta^{-1}\phi_q^{(H)}(\beta)$ is the familiar Peierls–Bogoljubov inequality

$$f_q^{(H_1)}(\beta)\leqslant f_q^{(H_2)}(\beta)+tr(\rho_\beta^{(H_2)}(H_1-H_2)),\quad \beta>0;$$

$$f_q^{(H_1)}(\beta)\geqslant f_q^{(H_2)}(\beta)+tr(\rho_\beta^{(H_2)}(H_1-H_2)),\quad \beta<0.$$

D. Equilibrium ?

We have referred to the unique minimizer ρ_β of the variational problem (6) as the equilibrium state. This is pushing the analogy with statistical mechanics too far because the analogue of the 0^{th}-Law of Thermodynamics is not satisfied at all! Indeed, if one considers two non-interacting systems with Hamiltonians H_1 and H_2 respectively, then the composite is described by the Hamiltonian $H=H_1\otimes\mathbf{I}+\mathbf{I}\otimes H_2$ on the Hilbert space $\mathscr{H}_1\otimes\mathscr{H}_2$. It is clear from Propositions 1 and 2, that the unique minimizer $\rho_\beta^{(H)}$ associated with H is not a product-state, i.e.,

$$\rho_\beta^{(H)}\neq(\rho_\beta^{(H)})_1\otimes(\rho_\beta^{(H)})_2,$$

where $(\cdots)_j$ denotes the restriction of the state to the j-th subsystem ($j=1,2$) obtained by taking the partial trace over the other subsystem. Moreover, $(\rho_\beta^{(H)})_j\neq\rho_{\beta'}^{(H_j)}$ for all possible β'. Thus it is impossible to assign a ''temperature'' to the subsystems; and it follows that ''equilibrium'' defined via β is not transitive.

The reason behind this feature is the fact that although the internal energy functional is additive

$$U^{(H)}[\rho\otimes\varphi]=U^{(H_1)}[\rho]+U^{(H_2)}[\varphi];$$

the q-entropy is not

$$S_q[\rho\otimes\varphi]=S_q[\rho]+S_q[\varphi]+(1-q)S_q[\rho]S_q[\varphi].$$

The variational problem (6) for the composite non-interacting system does not ''factorize.''

IV. THE INFINITE DIMENSIONAL CASE

We have already commented on the unbounded case. The relation $\phi_q^{(H)}(-\beta)=\phi_q^{(-H)}(\beta)$, obtained directly from (6), shows that it suffices to study the case where H is bounded below but not above. We assume this, and recall our standing assumption that the spectrum of H is purely discrete — that is it consists entirely of eigenvalues of finite multiplicities. Then ϵ_- is an eigenvalue, and $\mathscr{U}=[\epsilon_-,\infty)$. We have remarked before that $\phi_q(\beta)=-\infty$ for all $\beta<0$.

A. $0<q<1$

Looking at the corresponding finite dimensional case, the parameter t_o which gives us the minimal reciprocal pseudo-temperature is 0. The transformation

$$\beta(t):=qt[tr\{(1+(1-q)t(H-\epsilon_-))^{1/(q-1)}\}]^{1-q},\quad t>0 \tag{15}$$

is well defined if the trace

$$\sum_n\ (1+(1-q)t(\epsilon_n-\epsilon_-))^{1/(q-1)} \tag{16}$$

is finite. This imposes a condition on the spectrum (notice that $1/(q-1)<0$). An illustrative example is the spectrum $\epsilon_n=n^r$. If $r\geqslant 1$, then (16) is finite for all $q\in(0,1)$; if $0<r<1$, then (16) is infinite for all $q\in(0,1-r]$ and finite for all $q\in(1-r,1)$.

The following result isolates the pertinent spectral conditions and describes their interrelations.

Lemma: Let $0<q<1$, *and* H *be bounded below with purely discrete spectrum.*

One has

$$\sum_{\{n:\epsilon_n\neq\epsilon_-\}}(\epsilon_n-\epsilon_-)^{1/(q-1)}<\infty \tag{17}$$

if and only if (16) is finite for some $t>0$; *in which case it is finite and continuous for all* $t>0$, *the sum converging uniformly in* t *for any compact subset of* $(0,\infty)$.

One has

$$\sum_{\{n:\epsilon_n\neq\epsilon_-\}}(\epsilon_n-\epsilon_-)^{q/(q-1)}<\infty \tag{18}$$

if and only if

$$\sum_n\ (1+(1-q)t(\epsilon_n-\epsilon_-))^{q/(q-1)} \tag{19}$$

is finite for some $t>0$; *in which case it is finite and continuous for all* $t>0$, *the sum converging uniformly in* t *for any compact subset of* $(0,\infty)$.

Moreover, (18) implies (17).

Remark that when $\epsilon_n=n$, (17) is true, but (18) is true if and only if $\frac{1}{2}<q<1$.

Proposition 3: Let $0<q<1$, *and* H *be bounded below with purely discrete spectrum. If (18) holds then* $\beta(\cdot)$ *is well defined by (15), is strictly increasing and continuous, and maps* $(0,\infty)$ *one-to-one and onto itself. One has*

1. *The maps* S_q *and* ϕ_q *on* $\mathscr{U}=[\epsilon_-,\infty)$ *and* $(0,\infty)$, *respectively, are strictly concave, differentiable and each other's Legendre transforms. One has* $S_q(\epsilon_-)=[1/(q-1)](1-g_-^{1-q})$.

The derivative $U(\cdot)$ of ϕ_q is continuous, strictly decreasing and the inverse of the derivative of S_q. One has $\lim_{\beta\to\infty}U(\beta)=\epsilon_-$, and $\lim_{u\to\epsilon_-}(dS_q/du)(u)=\infty$.

2. *For each $u\in\mathcal{U}$ there exists a unique maximizer ω_u with $S_q(u)=S_q[\omega_u]$. For each $\beta\in(0,\infty)$ there exists a unique equilibrium state ρ_β minimizing ϕ_q. One has $\omega_{U(\beta)}=\rho_\beta$, and $\omega_u=\rho_{\beta(u)}$, where $\beta(u)$ is determined uniquely by $U(\beta(u))=u$. One has $U(\beta)=U[\rho_\beta]$.*
3. *For each $\beta\in(0,\infty)$, the unique equilibrium state ρ_β is given by (11) where τ is the inverse of the map (15).*

If (18) fails to hold, then $\phi_q(\beta)=-\infty$ for all $\beta\geqslant 0$; and

$$S_q(u)=\begin{cases}(q-1)^{-1}(1-g_-^{1-q}), & \text{if } u=\epsilon_-\\ \infty, & \text{if } u>\epsilon_-\end{cases}.$$

One has $\omega_{\epsilon_-}=g_-^{-1}P^-$.

B. $q>1$

Looking at the corresponding finite dimensional case, we need only the positive branch (i.e., $t\geqslant 0$) of the map $t\mapsto\beta(t)$. The relevant maximal reciprocal pseudo-temperature is $t_2=(q-1)^{-1}(\epsilon_-^*-\epsilon_-)^{-1}$, and the critical reciprocal "temperature" is $\beta_c^+=qg_-^{1-q}t_2$. The transformation

$$\beta(t):=qt[tr\{(1+(1-q)t(H-\epsilon_-))_\oplus^{1/(q-1)}\}]^{1-q},\quad 0<t\leqslant t_2 \tag{20}$$

is always well defined because the operator

$$(1+(1-q)t(H-\epsilon_-))_\oplus \tag{21}$$

has finite rank for every $t\in(0,t_2]$. The trace in (20) is always a finite sum. One has $\lim_{t\to 0}\beta(t)=0=:\beta(0)$, and $\beta(t_2)=\beta_c^+$. Here, the **reciprocal pseudo-temperature** τ is given by the map on $[0,\beta_c^+]$ inverse to the strictly increasing continuous map $\beta(\cdot)$.

Proposition 4: For $q>1$, and H bounded below with purely discrete spectrum, the operator (21) has finite rank for each $t\in(0,t_2]$. One has

1. *The map S_q on $\mathcal{U}=[\epsilon_-,\infty)$ is strictly concave and differentiable; $S_q(\epsilon_-)=[1/(q-1)](1-g_-^{1-q})$. The map ϕ_q on $(0,\infty)$ is concave, and differentiable. Moreover $\phi_q(\beta)=\beta\epsilon_-+[1/(1-q)](1-g_-^{1-q})$ for all $\beta\geqslant\beta_c^+$ and ϕ_q is strictly concave on $(0,\beta_c^+)$. S_q and ϕ_q are each other's Legendre transforms, with $S_q(u)=\inf_{\beta\in(0,\beta_c^+)}\times\{\beta u-\phi_q(\beta)\}$. The derivative $U(\cdot)$ of ϕ_q is continuous and given by $U(\beta)=\epsilon_-$ for all $\beta\geqslant\beta_c^+$; it is strictly decreasing on $(0,\beta_c^+]$ with inverse given by the derivative of S_q. One has $\lim_{u\to\epsilon_-}(dS_q/du)(u)=\beta_c^+$.*
2. *For each $u\in\mathcal{U}$ there exists a unique maximizer ω_u with $S_q(u)=S_q[\omega_u]$. For each $\beta\in(0,\infty)$ there exists a unique equilibrium state ρ_β minimizing ϕ_q. One has $\rho_\beta=g_-^{-1}P^-$ for all $\beta\geqslant\beta_c^+$. Moreover $\omega_u=\rho_{\beta(u)}$, where $\beta(u)$ is determined uniquely in $(0,\beta_c^+]$ by $U(\beta(u))=u$. One has $U[\rho_\beta]=U(\beta)$.*
3. *For each $\beta\in(0,\beta_c^+)$, the unique equilibrium state ρ_β is given by*

$$\rho_\beta=\frac{(1+(1-q)\tau(\beta)(H-\epsilon_-))_\oplus^{1/(q-1)}}{tr[(1+(1-q)\tau(\beta)(H-\epsilon_-))_\oplus^{1/(q-1)}]} \tag{22}$$

where τ is the inverse of the map (20).

V. PROOFS

Proof of the Lemma: Let $a_n(t)=1+(1-q)t(\epsilon_n-\epsilon_-)$ for $t>0$. One has $a_n(t)>(1-q)t(\epsilon_n-\epsilon_-)\geqslant 0$. For n sufficiently large, $a_n(t)\leqslant 2(1-q)t(\epsilon_n-\epsilon_-)$. These two facts are used to prove everything except the uniform convergence and continuity statements. By computing second derivatives, it is seen that the functions $t\mapsto a_n(t)^{1/(q-1)}$ and $t\mapsto a_n(t)^{q/(q-1)}$ are convex. If either of the sums (16) or (19) converge, they are convex and thus continuous in $t>0$ as limits of convex functions; moreover, again by convexity, the convergence is uniform on compact subsets of $(0,\infty)$. This implies the continuity. □

The four results are minor variations on a single theme. We first give the proof of the claim made in point 3. of each result. The key ingredient for this is Hölder's classic inequality.

Consider the case $0<q<1$ of Propositions 1 and 3. For each $t\in(t_o,\infty)$, the operator

$$A(t)=1+(1-q)t(H-\epsilon_-) \tag{23}$$

is strictly positive; we write $a_n(t)=1+(1-q)t(\epsilon_n-\epsilon_-)$. Due to the Lemma, in the infinite dimensional case condition (18) implies (17), which implies that $tr(A(t)^{1/(q-1)})$ given by (16) is finite. Thus (15) is well defined, strictly increasing and continuous. Moreover $\lim_{t\to 0}\beta(t)=0$, and $\lim_{t\to\infty}\beta(t)=\infty$.

As commented in the introduction, consideration of the "diagonal" state $\hat{\rho}$ reduces the variation in (6) to states which are diagonal. We have

$$\phi_q(\beta)=\beta\epsilon_- -(q-1)^{-1}+\inf_{\rho=\hat{\rho}}\Lambda[\rho] \quad \text{where } \Lambda[\rho]:=\beta tr(\rho(H-\epsilon_-))+(q-1)^{-1}tr(\rho^q).$$

Let us rewrite the functional Λ in terms of the reciprocal pseudo-temperature via (7) or (15):

$$\begin{aligned}\Lambda[\rho]&=qt[tr(A(t)^{1/(q-1)})]^{1-q}tr(\rho(H-\epsilon_-))-(1-q)^{-1}tr(\rho^q)\\&=q(1-q)^{-1}[tr(A(t)^{1/(q-1)})]^{1-q}[tr(\rho A(t))-1]-(1-q)^{-1}tr(\rho^q).\end{aligned}$$

Restricting to diagonal $\rho=\hat{\rho}$ states and applying Hölder's classic inequality we have

$$\begin{aligned}tr(\rho A(t))=\sum_n \rho_n a_n(t)&\geqslant\left(\sum_n \rho_n^q\right)^{1/q}\left(\sum_n a_n(t)^{q/(q-1)}\right)^{(q-1)/q}\\&=tr(\rho^q)^{1/q}tr(A(t)^{q/(q-1)})^{(q-1)/q}.\end{aligned}$$

When the right-hand side of the inequality is finite, there is equality here if and only if $\rho_n^q=ca_n(t)^{q/(q-1)}$ for all n with a positive constant c. But $tr(A(t)^{q/((q-1)})$ is precisely the sum (19), which by the Lemma is finite when (18) holds. Thus, under the latter condition, and with the same condition for equality,

$$\begin{aligned}\Lambda[\rho]&\geqslant q(1-q)^{-1}[tr(A(t)^{1/(q-1)})]^{1-q}[tr(\rho^q)^{1/q}tr(A(t)^{q/(q-1)})^{(q-1)/q}-1]\\&\quad-(1-q)^{-1}tr(\rho^q).\end{aligned}$$

With $\eta:=tr(A(t)^{1/(q-1)})tr(\rho^q)^{1/q}$, and $\xi:=tr(A(t)^{q/(q-1)})^{1/q}$ we rewrite this as

$$\begin{aligned}\Lambda[\rho]&\geqslant(1-q)^{-1}tr(A(t)^{1/(q-1)})^{-q}\\&\quad\times[(\eta-\xi)q\xi^{q-1}+\xi^q-\eta^q-(1-q)\xi^q-qtr(A(t)^{1/(q-1)})].\end{aligned}$$

The map $x \mapsto g(x) = x^q$ is strictly concave for $0 < q < 1$ on the positive reals, and has derivative $g'(x) = qx^{q-1}$. Thus,

$$(\eta - \xi) q \xi^{q-1} = (\eta - \xi) g'(\xi) \geqslant g(\eta) - g(\xi) = \eta^q - \xi^q$$

with equality if and only if $\eta = \xi$. From this we conclude that

$$\Lambda[\rho] \geqslant -(1-q)^{-1} tr(A(t)^{1/(q-1)})^{-q} [(1-q) tr(A(t)^{q/(q-1)}) + q tr(A(t)^{1/(q-1)})].$$

Going through the conditions for equality, we conclude that this bound is attained precisely when $\rho = tr(A(t)^{1/(q-1)})^{-1} A(t)^{1/(q-1)}$.

In the case $q > 1$ corresponding to Propositions 2 and 4, we proceed analogously. The reciprocal "temperature" $\beta(\cdot)$ as a function of Tsallis's reciprocal pseudo-temperature t is given by (13) and (20). Again, we deal with positive operators. It is clear that in the infinite dimensional case, our spectral assumption implies that the operator (23) can have only a finite number of strictly positive eigenvalues for t in the interval $(0,\infty)$; in fact it has exactly one strictly positive eigenvalue (namely 1) for each $t \geqslant t_2$.

We consider first positive t's, and rewrite the variational problem in terms of $\beta(t)$ in the finite and infinite dimensional cases. With

$$\Lambda[\rho] = \beta tr(\rho(H - \epsilon_-)) + (q-1)^{-1} tr(\rho^q),$$

we have $\phi_q(\beta) = \beta \epsilon_- - (q-1)^{-1} + \inf_{\rho = \hat{\rho}} \Lambda[\rho]$. Using (13) or (20) also beyond t_2 for all positive t, we get

$$\Lambda[\rho] = q(1-q)^{-1} [tr(A(t)_\oplus^{1/(q-1)})]^{1-q} [tr(\rho A(t)) - 1] - (1-q)^{-1} tr(\rho^q).$$

Let $R_\pm$ be the orthogonal projections onto the subspaces of non-zero eigenvalues of $A(t)_\oplus$ and $A(t)_\ominus$, respectively; these operators being the positive, respectively negative parts of $A(t) = A(t)_\oplus - A(t)_\ominus$. Put $R = 1 - R_+ - R_-$. For $\rho = \hat{\rho}$ we have $\rho = \rho_+ + \rho_- + R\rho R$, where $\rho_\pm = R_\pm \rho R_\pm$. Moreover $\rho^q = \rho_+^q + \rho_-^q + (R\rho R)^q$, and $tr(\rho A(t)) = tr(\rho_+ A(t)_\oplus) - tr(\rho_- A(t)_\ominus)$. We can now write

$$\Lambda[\rho] = \Lambda^+[\rho_+] + \Lambda^-[\rho_-] + (q-1)^{-1} tr((R\rho R)^q),$$

with

$$\Lambda^+[\rho_+] = q(q-1)^{-1} tr(A(t)_\oplus^{1/(q-1)})^{1-q} [1 - tr(\rho_+ A(t)_\oplus)] + (q-1)^{-1} tr(\rho_+^q);$$

$$\Lambda^-[\rho_-] = q(q-1)^{-1} tr(A(t)_\oplus^{1/(q-1)})^{1-q} tr(\rho_- A(t)_\ominus) + (q-1)^{-1} tr(\rho_-^q).$$

Now, $\Lambda^-[\rho_-] \geqslant 0$ with equality if and only if $\rho_- = 0$; and also $tr((R\rho R)^q) \geqslant 0$ with equality if and only if $R\rho = \rho R = R\rho R = 0$. Thus,

$$\inf_{\rho = \hat{\rho}} \Lambda[\rho] = \inf_{\{\rho = \hat{\rho} : \rho = \rho_+\}} \Lambda^+[\rho].$$

Letting $K = \{n : a_n(t) > 0\}$, and applying Hölder's inequality with $\rho = \hat{\rho}$, we get

$$tr(\rho A(t)_\oplus) = \sum_{n \in K} \rho_n a_n(t) \leqslant \left(\sum_{n \in K} \rho_n^q \right)^{1/q} \left(\sum_{n \in K} a_n(t)^{q/(q-1)} \right)^{(q-1)/q}$$

$$= tr(\rho^q)^{1/q} tr(A(t)_\oplus^{q/(q-1)})^{(q-1)/q};$$

there being equality if and only if $\rho_n^q = c a_n(t)^{q/(q-1)}$ for all $n \in K$ with a positive constant c. With the same condition for equality, we then have for $\rho = \rho_+$

$$\Lambda[\rho] = \Lambda^+[\rho] \geqslant (q-1)^{-1} tr(\rho^q) + q(q-1)^{-1}[tr(A(t)_\oplus^{1/(q-1)})]^{1-q} \times [1 - tr(\rho^q)^{1/q} tr(A(t)_\oplus^{q/(q-1)})^{(q-1)/q}].$$

With $\eta := tr(A(t)_\oplus^{1/(q-1)}) tr(\rho^q)^{1/q}$, and $\xi := tr(A(t)^{q/(q-1)})^{1/q}$ we rewrite this as

$$\Lambda[\rho] = \Lambda^+[\rho] \geqslant (q-1)^{-1} tr(A(t)_\oplus^{1/(q-1)})^{-q} \times [(\xi - \eta) q \xi^{q-1} - \xi^q + \eta^q + (1-q)\xi^q + q tr(A(t)_\oplus^{1/(q-1)})].$$

The map $x \mapsto h(x) = x^q$ is strictly convex for $q > 1$ on the positive reals, and has derivative $h'(x) = q x^{q-1}$. Thus,

$$(\eta - \xi) q \xi^{q-1} = (\eta - \xi) h'(\xi) \leqslant h(\eta) - h(\xi) = \eta^q - \xi^q$$

with equality if and only if $\eta = \xi$. From this we conclude that

$$\Lambda[\rho] = \Lambda^+[\rho] \geqslant (q-1)^{-1} tr(A(t)_\oplus^{1/(q-1)})^{-q} [(1-q) tr(A(t)_\oplus^{q/(q-1)}) + q tr(A(t)_\oplus^{1/(q-1)})].$$

Going through the conditions for equality, we conclude that this bound is attained precisely when $\rho = tr(A(t)_\oplus^{1/(q-1)})^{-1} A(t)_\oplus^{1/(q-1)}$. We notice that for $t \geqslant t_2$, we get $A(t)_\oplus = P^-$ where P^- is the spectral projection of H onto the eigensubspace to the ground state energy ϵ_-. Thus, for $t \geqslant t_2$ or equivalently $\beta \geqslant \beta_c^+$, we have $\rho_\beta = g_-^{-1} P^-$ where $g_- = tr(P^-)$ is the multiplicity of ϵ_-.

We now consider the case of negative t's in the finite dimensional case when $q > 1$ (Proposition 2). With

$$\Lambda[\rho] = \beta tr(\rho(H - \epsilon_+)) + (q-1)^{-1} tr(\rho^q),$$

we have $\phi_q(\beta) = \beta \epsilon_+ - (q-1)^{-1} + \inf_{\rho = \hat{\rho}} \Lambda[\rho]$. Using (13) also beyond t_1 for all negative t, we get

$$\Lambda[\rho] = q(1-q)^{-1}[tr(B(t)_\oplus^{1/(q-1)})]^{1-q}[tr(\rho B(t)) - 1] - (1-q)^{-1} tr(\rho^q),$$

where $B(t) = 1 + (1-q)t(H - \epsilon_+)$. We can now repeat the argument of the previous case replacing $A(t)$ by $B(t)$ to get that the infimum is attained precisely when $\rho = tr(B(t)_\oplus^{1/(q-1)})^{-1} B(t)_\oplus^{1/(q-1)}$. Again, for $t \leqslant t_1$, we have $B(t)_\oplus = P^+$ where P^+ is the projection onto the eigenspace to the ceiling energy ϵ_+ etc.

The reader may have noticed that by invoking the non-commutative versions of Hölder's inequalities, one can avoid the introduction of the diagonal state $\hat{\rho}$.

This completes the proof of the claims made in point 3 of each result. For each $t = \tau(\beta)$ in the appropriate case-dependent domain, we have found the unique minimizer $\rho_\beta = \rho_{\beta(t)}$.

We now turn to the differentiability and strict concavity of ϕ_q. We first remark that if $U[\rho_{\beta_o}]$ is finite, then it is a subdifferential for ϕ_q at β_o. Indeed,

$$\phi_q(\beta_o) + (\beta - \beta_o) U[\rho_{\beta_o}] = \beta_o U[\rho_{\beta_o}] - S_q[\rho_{\beta_o}] + (\beta - \beta_o) U[\rho_{\beta_o}]$$

$$= \beta U_q[\rho_{\beta_o}] - S_q[\rho_{\beta_o}] \geqslant \phi_q(\beta).$$

It follows that if $\beta_2 \geqslant \beta_1$, then

$$(\beta_2-\beta_1)U[\rho_{\beta_1}]\geqslant\phi_q(\beta_2)-\phi_q(\beta_1)\geqslant(\beta_2-\beta_1)U[\rho_{\beta_2}] \tag{24}$$

so the map $\beta\mapsto U[\rho_\beta]$ is non-increasing.

In the finite dimensional case $U[\rho_\beta]$ is clearly finite. When $q>1$ in the infinite dimensional case, ρ_β is degenerate and has a finite number of non-zero eigenvalues, so again $U[\rho_\beta]$ is finite. When $0<q<1$ and in infinite dimension, condition (18) implies that

$$tr(A(t)^{1/(q-1)}H)=\sum_n \epsilon_n a_n(t)^{1/(q-1)} \tag{25}$$

is also finite and a continuous function of $t>0$. To see this, notice first that $tr(A(t)^{1/(q-1)}H)=tr(A(t)^{1/(q-1)}(H-\epsilon_-))+\epsilon_- tr(A(t)^{1/(q-1)})$. Now

$$tr(A(t)^{1/(q-1)}(H-\epsilon_-))=\sum_n (\epsilon_n-\epsilon_-)a_n(t)^{1/(q-1)}; \tag{26}$$

but $a_n(t)>(1-q)t(\epsilon_n-\epsilon_-)$, so that $(\epsilon_n-\epsilon_-)a_n(t)^{1/(q-1)}\leqslant((1-q)t)^{1/(q-1)}(\epsilon_n-\epsilon_-)^{q/(q-1)}$ and (18) implies that (26) is convergent, and as a limit of sums of convex functions it is convex and thus continuous.

One can now verify that the map $\beta\mapsto U[\rho_\beta]\equiv U(\beta)$ is continuous since $\beta(\cdot)$ is continuous. This is immediate in the finite dimensional case or in the infinite dimensional case when $q>1$ since U is a finite sum of continuous functions. For $0<q<1$ we have just established the continuity of $t\mapsto tr(A(t)^{1/(q-1)}H)$.

From the continuity of U and (24), one concludes that ϕ_q is differentiable and its derivative is U.

Suppose that $\beta_1>\beta_o$ and $U[\rho_{\beta_1}]=U[\rho_{\beta_o}]$, so that U is not strictly decreasing. It follows from the non-increasing property of U that $U(\beta)=U[\rho_\beta]=U[\rho_{\beta_o}]$, and from (24), that $\phi_q(\beta)=\phi_q(\beta_o)+(\beta-\beta_o)U[\rho_{\beta_o}]$, for all $\beta\in[\beta_o,\beta_1]$. But then $\beta U[\rho_\beta]-S_q[\rho_\beta]=\phi_q(\beta)=\phi_q(\beta_o)+(\beta-\beta_o)U[\rho_{\beta_o}]=\beta_o U[\rho_{\beta_o}]-S_q[\rho_{\beta_o}]+(\beta-\beta_o)U[\rho_{\beta_o}]=\beta U[\rho_{\beta_o}]-S_q[\rho_{\beta_o}]$, and uniqueness of the minimizer implies $\rho_\beta=\rho_{\beta_o}$. This provides us with a criterion for the strict decrease of U or equivalently the strict concavity of ϕ_q, which can be thus checked in terms of the minimizers. This we use to prove the corresponding claims of point 1 in each result.

For each u in the interior of $\mathscr{U}$ there is a unique $\beta\in(\beta^-,\beta^+)$ such that $U(\beta)=u$. When $\epsilon_\pm$ is finite, it can be checked that $U(\beta^\pm)=\epsilon_\mp$. Thus for each possible finite energy value u there is a unique $\beta=\beta(u)$ with $U(\beta)=u$.

Consider the Legendre–Fenchel transform $\phi_q^*(u)=\inf_{\beta\in\mathbf{R}}\{\beta u-\phi_q(\beta)\}$ of ϕ_q; for $u\in\mathscr{U}$ this definition implies that $S_q(u)\leqslant\phi_q^*(u)$. But for given finite $u\in\mathscr{U}$ there is a unique $\beta(u)$ such that $\rho_{\beta(u)}$ is a minimizer of (3) and $U[\rho_{\beta(u)}]=u$; thus $S_q[\rho_{\beta(u)}]\leqslant S_q(u)\leqslant\phi_q^*(u)\leqslant\beta(u)u-\phi_q(\beta(u))=\beta(u)u-\beta(u)U[\rho_{\beta(u)}]+S_q[\rho_{\beta(u)}]=S_q[\rho_{\beta(u)}]$. It follows that $\phi_q^*(u)=S_q(u)=S_q[\beta(u)]$, and $\rho_{\beta(u)}=\omega_u$.

Once we know that ϕ_q is differentiable and strictly concave on (β^-,β^+) — with the appropriate $\beta^\pm$ — we get the rest of the claims of points 1 and 2 from general results on the theory of convex/concave functions as developed in sections 12, 25 and 26 of Ref. 11; or from straightforward computations.

What remains, is the proof of the claims of the second part of Proposition 3. Assuming that (18) fails, that is $\Sigma_{\{n:\epsilon_n>\epsilon_-\}}(\epsilon_n-\epsilon_-)^{q/(q-1)}=\infty$, we first show that if $\epsilon_-<u<\epsilon_-^*$ then $S_q(u)=\infty$. To do this we construct for a given arbitrary positive real R, a diagonal state ρ such that $tr(\rho H)=u$ and $S_q[\rho]\geqslant R$. Let $g=g_-$ be the multiplicity of the ground-state energy ϵ_- and enumerate the ϵ_n's such that $\epsilon_j=\epsilon_-$ for $j=1,2,\cdots,g$. For any integer $N\geqslant g+1$, let $B(N)=\Sigma_{n=g+1}^N(\epsilon_n-\epsilon_-)^{q/(q-1)}$; and

$$\lambda_n(N)=\begin{cases}(1-\Lambda(N))/g, & \text{if } 1\leqslant n\leqslant g\\ (u-\epsilon_-)B(N)^{-1}(\epsilon_n-\epsilon_-)^{1/(q-1)}, & \text{if } g+1\leqslant n\leqslant N\end{cases},$$

where $\Lambda(N)=(u-\epsilon_-)B(N)^{-1}\Sigma_{n=g+1}^{N}(\epsilon_n-\epsilon_-)^{1/(q-1)}$. From the inequality $u-\epsilon_-<(\epsilon_n-\epsilon_-)$ for each $n\geqslant g+1$, we conclude that $\Lambda(N)<1$. Thus $\lambda_n(N)$ lies in (0,1), and $\Sigma_{n=1}^{N}\lambda_n(N)=1$. Moreover, $\Sigma_{n=1}^{N}\lambda_n(N)(\epsilon_n-\epsilon_-)=u-\epsilon_-$. Thus the degenerate diagonal state $\rho(N)$ with non-zero eigenvalues $\lambda_n(N)$, satisfies $tr(\rho(N)H)=u$. But

$$S_q[\rho(N)]=(q-1)^{-1}+(1-q)^{-1}\left(\sum_{n=1}^{g}\lambda_n(N)^q+\sum_{n=g+1}^{N}\lambda_n(N)^q\right)$$

$$\geqslant(q-1)^{-1}+(1-q)^{-1}\sum_{n=g+1}^{N}\lambda_n(N)^q$$

$$=(q-1)^{-1}+(1-q)^{-1}(u-\epsilon_-)^qB(N)^{1-q}.$$

Since $\lim_{N\to\infty}B(N)=\infty$ we can choose N sufficiently large so that $S_q[\rho(N)]$ is as large as we want, proving the claim. If now $u\geqslant\epsilon_-^*$ then there exists $u_1\in(\epsilon_-,\epsilon_-^*)$ and $t\in(0,1)$ such that $u=tu_1+(1-t)u_2$. By concavity of S_q we then have $S_q(u)\geqslant tS_q(u_1)+(1-t)S_q(u_2)$ so that $S_q(u)=\infty$ since $S_q(u_1)=\infty$. It then follows directly from (5) that $\phi_q(\beta)=-\infty$ for all $\beta\in\mathbf{R}$. Finally, by the variational principle, $U[\rho]=\epsilon_-$ if and only if $\rho P^-=\rho$ where P^- is the projection onto the eigenspace of the ground-state energy. It is then clear that the state ρ with $\rho P^-=\rho$ and maximal entropy is the equipartition $g_-^{-1}P^-$ of pure ground states with q-entropy $(q-1)^{-1}(1-g_-^{1-q})$.

VI. COMPARISON WITH THE NON-STANDARD FORMALISM

If the reader allows us to refer to the formalism studied here as the standard one, by the non-standard formalism we mean the one based on the energy-functional

$$U_q[\rho]=tr(\rho^qH)$$

and the entropy $S_q[\cdot]$, as proposed in Ref. 6. Notice that $U_q[\cdot]$ is not affine. Moreover, adding a constant c to the Hamiltonian $U_q^{H+c}(\rho)=U_q^H(\rho)+ctr(\rho^q)$. The thermostatistics obtained will depend on the choice of the zero of energy. Despite these unusual features, the entropy function S_q — defined by (4) with $U[\cdot]$ replaced by $U_q[\cdot]$ — is concave in u, and one can recover a complete ''thermostatistics'' (without 0^{th}-law). The detailed analysis is given in Ref. 7. In the standard formalism the parametrization of ρ_β in terms of β is not explicit since one has to invert the map $t\to\beta(t)$ to find the reciprocal pseudo-temperature τ as a function of β. In the non-standard version, the ''equilibrium'' state is parametrized directly and explicitly by β: The formula for the non-standard ρ_β is obtained (formally) by replacing $(1-q)\tau(\beta)$ by $(q-1)\beta$ in the standard formula. The basic features of the non-standard thermostatics are qualitatively the same as those described here, after interchanging ''$q>1$'' with ''$q<1$''. For $q<1$, there are inaccessible temperatures and the depopulation mechanism operates to produce a degenerate ρ_β.

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Non-standard thermal statistics with *q*-entropies

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We consider the quantum thermal statistics *à la* Gibbs–Shannon–Szilard–Jaynes based on q-entropies $S_q[\rho]=(q-1)^{-1}(1-tr(\rho^q))$ $(0<q\neq 1)$ and the non-standard ''internal energy'' functionals $U_q[\rho]=tr(\rho^q H)$ proposed by C. Tsallis [J. Stat. Phys. **52**, 479–487 (1988)]. © *1996 American Institute of Physics.* [S0022-2488(96)01403-1]

I. INTRODUCTION

For a discrete probability distribution $\rho=(\rho_1,\rho_2,\cdots)$, with $\rho_n\geqslant 0$, and $\Sigma_n\rho_n=1$, consider the monoparametric family of entropies (the q-entropies):

$$S_q[\rho]=(q-1)^{-1}\left(1-\sum_n \rho_n^q\right),$$

where q is a real number distinct from 0 and from 1. One sees easily that S_q is a concave function on the convex set of probability distributions when $q>0$; and that $\lim_{q\to 1}S_q[\rho]=-\Sigma_n\rho_n \ln(\rho_n)$, the well-known Boltzmann–Shannon entropy.

Tsallis[1] proposed to build up a ''thermostatistics'' by maximizing the q-entropies at given fixed internal energy given by $\Sigma_n\rho_n\epsilon_n$. To this end he introduces the function $S_q[\rho]+\alpha\Sigma_n\rho_n-\alpha\beta(q-1)\Sigma_n\epsilon_n\rho_n$ and after a standard variation obtains the distribution $\rho_n \propto (1-\beta(q-1)\epsilon_n)^{1/(q-1)}$. Although β provides a convenient and explicit parametrization of the distribution with maximal q-entropy, it is not the reciprocal temperature associated to the problem. This reciprocal temperature is given by $\alpha\beta(q-1)$. Nevertheless, it is possible to perform the analysis with the correct reciprocal temperature and obtain a ''thermal'' statistics using $S_q[\cdot]$ instead of the Boltzmann–Shannon entropy.[2] In subsequent papers, Tsallis and coworkers[3,4] proposed to build up a ''thermostatistics'' using the q-entropies but replacing the standard expression for the internal energy by the functional $U_q[\rho]=\Sigma_n\epsilon_n\rho_n^q$ with the same q used for the entropy. This functional is not affine for $q\neq 1$, i.e., $U_q[\lambda\rho_1+(1-\lambda)\rho_2]\neq\lambda U_q[\rho_1]+(1-\lambda)U_q[\rho_2]$ for the mixture of distributions ρ_1, ρ_2 in proportions λ and $(1-\lambda)$ respectively. The variational calculation involving classical distributions only and using Lagrange multipliers was carried out in Ref. 3, but the analysis is incomplete since the multiplier ranges are not determined or determined ad hoc. In the last few years, a lot of researchers have explored the features of the formalism proposed by Tsallis, and have developed applications to physics, astrophysics, biology, economics, statistical inference problems, etc. For a review see Ref. 4.

In this paper, we consider the ''thermostatistics'' associated with the q-entropies for $0<q\neq 1$ and the non-standard constraint $U_q[\cdot]=$ constant. We determine by a direct method (using Hölder's inequality as the key ingredient) the quantum mechanical state(s) ρ_β minimizing the functional:

$$\rho\mapsto\beta U_q[\rho]-S_q[\rho]. \tag{1}$$

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We then proceed to establish all ''thermostatistical'' results analogous to those known for the case $q=1$ of Boltzmann–Gibbs statistics. We thus complete the program proposed in Ref. 3 as follows: For each possible ''internal energy'' u there is a unique state ω_u among those states ρ with $U_q[\rho]=u$ which maximizes $S_q[\cdot]$; the q-entropy as a function of the ''internal energy'' is a concave differentiable function; for each β in a certain explicitly determined interval, the minimizer ρ_β is unique and it is equal to ω_u where $u=U_q[\rho_\beta]$, moreover β is the value of the derivative of S_q with respect to u evaluated at u; the minimal value of the functional (1) is equal to the Legendre transform (with respect to u) of S_q as a function of u. However, despite all these results we warn the reader that the parameter β, which we call ''reciprocal temperature,'' does not satisfy the analogue of the 0^{th}-law of Thermodynamics (See Sec. IV C).

$S_q[\cdot]$ for discrete probability distributions was introduced, with a different prefactor, by Z. Daróczy[5] who obtained the basic properties and gave an axiomatic characterization. The quantum mechanical version

$$S_q[\rho]=(q-1)^{-1}(1-tr(\rho^q)),$$

appears on page 247 of Wehrl's review.[6] These entropies are intimately related to the Renyi entropies.[6] We record here some of the basic properties of the q-entropies; the proofs are given in Ref. 7. $S_q[\rho]\geqslant 0$ with equality iff ρ is pure. In the finite dimensional case (dimension d), $S_q[\cdot]$ is strictly concave and one has $S_q[\rho]\leqslant(q-1)^{-1}(1-d^{1-q})$ with equality iff ρ is the normalized trace. In the infinite dimensional case, if $q>1$ $S_q[\cdot]$ is strictly concave and one has $S_q[\rho]<(q-1)^{-1}$; moreover $S_q[\cdot]$ is Lipschitz in the trace norm. If $0<q<1$, in infinite dimension, $S_q[\cdot]$ is generically (on a set of second category) infinity but the set where it takes finite values is convex and $S_q[\cdot]$ is strictly concave on it.

We do not consider the case $q<0$. In this case, the expressions for S_q make sense in finite dimensions when the distribution is not degenerate, or when zero is not an eigenvalue of the state. In infinite dimension however, S_q is identically equal to infinity.

In Sec. II, we study the ''internal energy'' functionals $U_q[\cdot]$. In Sec. III, we develop the basic facts about the ''thermostatistics'' based on the pair $U_q[\cdot]$, $S_q[\cdot]$. The variational problem associated with the minimization of the functional (1) is worked out in Sec. IV; where some of the main features of the formalism are established as direct consequences of the results. In Sec. V, we consider as an illustration the non-standard ''thermostatistics'' for the harmonic oscillator. The extension of the results to the multidimensional case, corresponding to fixing the values of N functionals U_q based on N Hamiltonians, is considered in Sec. VI. Section VII contains our final comments. The general results about all the variational problems discussed in this paper are proved in the Appendix.

In this paper we work with the extended real numbers and use the usual conventions for addition; the equalities and inequalities appearing here are to be understood in this sense. By $\Re$ we denote the usual real numbers without $\pm\infty$.

II. THE FUNCTIONAL $U_q[\cdot]$

Assume given a selfadjoint operator H whose spectrum consists entirely of eigenvalues $\{\epsilon_n\}$ which are enumerated according to their multiplicities. Accordingly, in the classical case, $\{\epsilon_n\}$ is a (possibly finite) sequence of real numbers. We write ϵ^+ (resp. ϵ^-) for the maximal (resp. minimal) energy:

$$\epsilon^+:=\sup_n \epsilon_n; \quad \epsilon^-:=\inf_n \epsilon_n.$$

We assume the non-trivial case $\epsilon_-<\epsilon_+$. For $q>0$, define the ''internal energy'' functionals

$$U_q[\rho]=\begin{cases}\sum_n \epsilon_n \rho_n^q, & \text{in the discrete classical case}\\ tr(\rho^q H), & \text{in the quantum case.}\end{cases} \tag{2}$$

In the infinite dimensional case and when H is unbounded, we have to specify what the trace of the operator $\rho^q H$ means. We will make the following assumption: **the spectrum of H is purely discrete;** that is to say it consists entirely of isolated eigenvalues with finite multiplicity, alternatively $\{\epsilon_n\}$ has no accumulation points. $U_q[\cdot]$ can be defined under milder assumptions, but the above condition will be necessary to insure existence of the minimizers ρ_β of the functional (1). This spectral assumption insures that we have a sequence $\{P_m\}$ of pairwise orthogonal finite-rank projections P_m such that $H=\Sigma_m \hat{\epsilon}_m P_m$ ($\hat{\epsilon}_m$ are the distinct eigenvalues of H). Now, $tr(\rho^q P_m)$ is finite, even when ρ^q is not trace-class as can happen for $0<q<1$. If the series $\Sigma_m \hat{\epsilon}_m tr(\rho^q P_m)$ is absolutely convergent, we define it as $tr(\rho^q H)$; otherwise, the trace remains undefined. If the trace is defined then, for any complete orthonormal basis $\{\psi_n\}$ of eigenvectors ψ_n of H to the eigenvalue ϵ_n, one has

$$tr(\rho^q H)=\sum_n \epsilon_n \langle \psi_n, \rho^q \psi_n\rangle.$$

We denote the set of all states ρ (i.e., density operators in the quantum case or probability distributions in the classical case) by Ω. It is immediate in finite dimensions that for $q \neq 1$, $U_q[\cdot]$ is not affine on Ω. But if ρ is pure (i.e., an extremal point of Ω), then $U_q[\rho]=U_1[\rho]=tr(\rho H)$. In infinite dimension, the set Ω_q where $U_q[\cdot]$ is defined contains the convex set of ρ's whose matrix in an eigenbasis of H has the block form

$$\begin{pmatrix} D & 0 & \cdots \\ 0 & 0 & \cdots \\ \vdots & \vdots & \end{pmatrix}$$

with D an arbitrary finite density matrix.

We write

$$U_q^+ := \sup_{\rho\in\Omega_q} U_q[\rho], \quad U_q^- := \inf_{\rho\in\Omega_q} U_q[\rho].$$

The variational problems posed by $U_q^\pm$ are solved in the Propositions A.1 and A.2 of the Appendix. If we denote by H_+ (H_-) the positive, (resp. negative) part of the operator H; applying Proposition A.1, we directly determine $U_q^\pm$ for $q>1$. And from Proposition A.2 we immediately obtain $U_q^\pm$ for $0<q<1$:

$$U_q^+=\begin{cases}\begin{cases}\epsilon^+, & \text{if } \epsilon^+\geqslant 0\\ -\{tr((H_-)^{1/(1-q)})\}^{1-q}, & \text{if } \epsilon^+<0\end{cases} & \text{for } q>1\\ \begin{cases}\{tr((H_+)^{1/(1-q)})\}^{1-q}, & \text{if } \epsilon^+>0\\ \epsilon^+, & \text{if } \epsilon^+\leqslant 0\end{cases} & \text{for } 0<q<1\end{cases}, \tag{3}$$

$$U_q^- = \begin{cases} \begin{cases} \epsilon^-, & \text{if } \epsilon^- \leqslant 0 \\ \{tr((H_+)^{1/(1-q)})\}^{1-q}, & \text{if } \epsilon^- > 0 \end{cases} & \text{for } q>1 \\ \begin{cases} -\{tr((H_-)^{1/(1-q)})\}^{1-q}, & \text{if } \epsilon^- < 0 \\ \epsilon^-, & \text{if } \epsilon^- \geqslant 0 \end{cases} & \text{for } 0<q<1 \end{cases} . \tag{4}$$

In this context, the traces in the infinite dimensional case are understood with respect to any orthonormal basis of eigenvectors of H, i.e., $tr(H_\pm^{1/(1-q)}) = \Sigma_n' |\epsilon_n|^{1/(1-q)}$ where the sum runs over the positive (negative) eigenvalues of H for H_+ (H_-).

The lack of affinity of the functional $U_q[\cdot]$ manifests itself again since we can have $U_q^+ > \epsilon^+$ or $U_q^- < \epsilon^-$. As we show in the Appendix, when $U_q^\pm = \epsilon^\pm$ and finite, the extremizers are eigenstates of H to the eigenvalue $\epsilon^\pm$ (pure eigenstates if $\epsilon^\pm \neq 0$). If $U_q^\pm \neq \epsilon^\pm$ and $tr((H_\pm)^{1/(1-q)})$ is finite, the extremizer is unique and given by the Hölder state:

$$\rho_\pm = \frac{(H_\pm)^{1/(1-q)}}{tr((H_\pm)^{1/(1-q)})} \tag{5}$$

where ρ_+ (ρ_-) is associated with H_+ (H_-) in the expressions for $U_q^\pm$.

III. BASIC THERMAL STATISTICS

In this section we resume the general program of the thermal statistics. The results quoted below are independent of the specification of the ''internal energy'' and entropy functionals.

For any u in the interval $[U_q^-, U_q^+]$, we write $\mathscr{K}_q(u)$ for the set of ρ's with $U_q[\rho] = u$ $(\mathscr{K}_q(u) \subset \Omega_q)$. We can now define entropy as a function of ''internal energy'' by

$$S_q(u) := \sup_{\rho \in \mathscr{K}_q(u)} \{S_q[\rho]\}, \quad u \in [U_q^-, U_q^+]. \tag{6}$$

We are distinguishing the ''thermodynamic'' functionals, such as $S_q[\cdot]$, defined on the states from the ''thermodynamic'' functions, such as S_q, by using square brackets for the arguments of the former.

We consider the Legendre–Fenchel transform of S_q given by

$$\phi_q(\beta) := \inf_{u \in (U_q^-, U_q^+)} \{\beta u - S_q(u)\}, \quad \beta \in \mathfrak{R}. \tag{7}$$

The function $\beta \mapsto \beta^{-1}\phi_q(\beta)$ is—in appropriate dimensionless variables—the ''Helmholtz free-energy'' of the system whose ''internal energy'' functional is $U_q[\cdot]$. We first show that ϕ_q is equal to the *infimum over states* of the corresponding ''free-energy'' functional (1), and remark that the Legendre–Fenchel transform of ϕ_q w.r.t. β (the Legendre-Fenchel transform of the Legendre–Fenchel transform of S_q) is the concave, uppersemicontinuous regularization of S_q:

Lemma 1:

$$\phi_q(\beta) = \inf_{\rho \in \Omega_q} \{\beta U_q[\rho] - S_q[\rho]\}, \tag{8}$$

$$S_q(u) \leqslant \inf_{\beta \in \mathfrak{R}} \{\beta u - \phi_q(\beta)\} =: (\phi_q)^*(u). \tag{9}$$

Proof : Both statements are general consequences of the definition (7): (9) is a general fact in the theory of Legendre–Fenchel transforms (see e.g., Ref. 8); moreover

$$\phi_q(\beta) = \inf_u\{\beta u - \sup_{\rho\in\mathscr{K}(u)} S_q[\rho]\} = \inf_u \inf_{\rho\in\mathscr{K}(u)}\{\beta u - S_q[\rho]\}$$
$$= \inf_u \inf_{\rho\in\mathscr{K}(u)}\{\beta U[\rho] - S_q[\rho]\} = \inf_{\rho\in\Omega_q}\{\beta U[\rho] - S_q[\rho]\}.$$

The restriction to Ω_q guarantees that the functional $U_q[\,\cdot\,]$ is defined in infinite dimension. □

The problem of ''equivalence of ensembles,'' at this level, is the proof that one has equality in (9). One has then that S_q is indeed concave (and upper semicontinuous) and a reasonable entropy function.[9] If, however, S_q is not concave, then the appropriate entropy function is in fact $(\phi_q)^*$. The following simple result will be important here.

Lemma 2: If u is such that there exists $\beta_0 \in \mathfrak{R}$ and $\rho_o \in \Omega_q$ satisfying $U_q[\rho_o] = u$, and $\phi_q(\beta_o) = \beta_o U_q[\rho_o] - S_q[\rho_o]$, then $S_q(u) = S_q[\rho_o] = (\phi_q)^*(u)$, and $U_q[\rho]$ is a subdifferential (see Ref. 8) of ϕ_q at β_o: $\phi_q(\beta) \leqslant \phi_q(\beta_o) + (\beta - \beta_o)U_q[\rho_o]$ for all β.

Proof: By the definitions of $(\phi_q)^*$ [l.h.s. of (9)], and of S_q, the assumptions give: $(\phi_q)^*(u) \leqslant \beta_o u - \phi_q(\beta_o) = \beta_o u - \beta_o U_q[\rho_o] + S_q[\rho_o] \leqslant S_q(u)$. The first claim follows from (9). Also $\phi_q(\beta_o) + (\beta - \beta_o)U_q[\rho_o] = \beta_o U_q[\rho_o] - S_q[\rho_o] + (\beta - \beta_o)U_q[\rho_o] = \beta U_q[\rho_o] - S_q[\rho_o] \geqslant \phi_q(\beta)$. □

Lemma 2 tells us when the minimizer of the variational problem (8) is the maximizer of the variational problem (6). We will deal with the problem posed by (8), since it is a variational problem without constraints on ρ and thus easier to solve. Once this problem is solved we must verify that for each possible value $u \in (U_q^-, U_q^+)$ there is β satisfying the hypothesis of Lemma 2 to get the solution of the original problem (6). The next question for any thermal statistics is to know if one has a unique extremizer, or not. If so, the unique extremizer ρ_β is the equilibrium state at reciprocal temperature β. Another natural question arises in connection with the variational problems. Suppose that ρ is a maximizer in (6) or a minimizer in (8) both in the quantum case; is it true that ρ is *diagonal* ?, that is to say, it is diagonalized by some orthonormal basis which also diagonalizes H.

We now record some general properties of the function ϕ_q:

Lemma 3: $\mathfrak{R} \ni \beta \mapsto \phi_q(\beta)$ is a concave, upper-semicontinuous function, which is continuous on the interior of the convex (hence connected) subset $dom(\phi_q)$ of $\mathfrak{R}$ where it takes finite values.

One has $\phi_q(0) = -\sup_{\rho\in\Omega} S_q[\rho] (< 0)$, and $\beta U_q^{-(+)} + \phi_q(0) \leqslant \phi_q(\beta) \leqslant \beta U_q^{-(+)}$ if $\beta > 0$ (resp. $\beta < 0$). *Thus, if $U_q^+ = \infty$* (resp. $U_q^- = -\infty$), *then $\phi_q(\beta) = -\infty$ for all $\beta < 0$* (resp. all $\beta > 0$).

$\mathfrak{R} \ni \beta \mapsto \beta^{-1}\phi_q(\beta)$ is non-decreasing on $(-\infty, 0)$ and on $(0, \infty)$. In the finite dimensional case, or in general for $q > 1$, $\lim_{\beta\to+(-)\infty} \beta^{-1}\phi_q(\beta) = U_q^{-(+)}$.

If for some $\beta_o > 0$ (resp. $\beta_o < 0$), *one has $\phi_q(\beta_o) = \beta_o U_q^{-(+)}$, then $\phi_q(\beta) = \beta U_q^{-(+)}$ for every $\beta \geqslant \beta_o$* (resp. $\beta \leqslant \beta_o$).

Proof: The basic properties (concavity, upper semicontinuity, etc.) are well known consequences (see e.g., Ref. 8) of the definition (7). Since Ω_q contains all density operators whose matrix in an eigenbasis of H has finite rank, the supremum over Ω_q of $S_q[\,\cdot\,]$ is equal to the supremum over the whole state space Ω. The inequality for ϕ_q is obtained from (8) using the inequality $0 \leqslant S_q[\rho] \leqslant \sup_\rho S_q[\rho]$. The increasing property of $\beta^{-1}\phi_q(\beta)$ follows from (8) using the positivity of $S_q[\,\cdot\,]$ and the fact that $\beta \mapsto -\beta^{-1}$ is increasing on the intervals $(-\infty, 0)$ and $(0, \infty)$. Using that $S_q[\,\cdot\,]$ is finite in finite dimension or when $q > 1$, one can show the assertion of the limit for $\beta \to \pm\infty$. The last claim, concerning attainment of the bounds, follows from the increasing property of $\beta^{-1}\phi_q(\beta)$ and the inequality. □

The largest entropy can be computed easily, and from what was said in the Introduction, it follows that:

$$\phi_q(0)=\begin{cases}(1-q)^{-1}(1-d^{1-q}), & \forall q \text{ in finite dimension } d\\ \begin{cases}(1-q)^{-1} & \text{if } q>1,\\ -\infty & \text{if } 0<q<1,\end{cases} & \text{in infinite dimension}\end{cases}.$$

The following symmetry property is immediate from (8): $\phi_q^{(H)}(-\beta)=\phi_q^{(-H)}(\beta)$, where the superscript indicates the Hamiltonian used in $U_q[\cdot]$.

If, in the infinite dimensional case, H is unbounded both above and below then $\phi_q\equiv-\infty$ except at $\beta=0$ when $q>1$. The ''thermostatistics'' is empty; and we rule out this case from further consideration. We assume then that in the infinite dimensional case H is semibounded. Under this condition, ϕ_q is a proper concave function, that is to say: it does not take the value ∞ and it is not identically $-\infty$.

The inequality of the above lemma implies a familiar fact in Boltzmann–Gibbs thermodynamics: if $U_q^{\pm}=\pm\infty$ — as happens when $\epsilon^{\pm}=\pm\infty$, that is H is not bounded above (resp. below) — then $\phi_q(\beta)=-\infty$ for all negative (resp. positive) β. We will see in what follows that in the present context the bound $\beta U_q^{-(+)}$ can be attained at a finite positive (resp. negative) β; this does not occur in Boltzmann–Gibbs statistics. Thus, the present formalism presents the feature that temperatures below (above) a certain positive (negative) value are unattainable. This unfamiliar feature persists if the constraint $U_q[\cdot]$ is replaced by the physical constraint $U_1[\cdot]$.[2]

IV. DETERMINATION OF ϕ_q AND THE MINIMIZERS

We now compute ϕ_q by solving the variational problem (8); this will also give us the corresponding minimizers. Notice that $\beta U_q[\rho]-S_q[\rho]=(1-q)^{-1}+tr\{\rho^q(\beta H+(q-1)^{-1}I)\}$, so that

$$\phi_q(\beta)=(1-q)^{-1}+\inf_{\rho}\, tr\{\rho^q A(\beta,q)\}, \tag{10}$$

where we have introduced the selfadjoint operator $A(\beta,q):=\beta H+(q-1)^{-1}I$. Thus, the problem is solved by the results of the Appendix as soon as the lower bound $\alpha^-(\beta,q)=\inf_n\{\beta\epsilon_n+(q-1)^{-1}\}$ of the spectrum of $A(\beta,q)$ is known. But

$$\alpha^-(\beta,q)=(q-1)^{-1}+\beta\cdot\begin{cases}\epsilon^-, & \text{if } \beta\geqslant 0\\ \epsilon^+, & \text{if } \beta\leqslant 0\end{cases}; \tag{11}$$

with the usual convention $0(\pm\infty)=0$. Since the solution of (10) is governed — via Propositions A.1 and A.2 of the Appendix — by whether $\alpha^-(\beta,q)$ is negative or not, there are two ''critical'' values of β, the solutions of the equation $\alpha^-(\beta,q)=0$. These numbers can be finite or $\pm\infty$.

We distinguish the two cases $0<q<1$ and $q>1$. As before, all traces in the infinite dimensional case are to be understood with respect to an arbitrary orthonormal basis diagonalizing H.

A. Case $q>1$

We define positive and negative critical reciprocal temperatures $\beta_c^+(q)$ and $\beta_c^-(q)$ respectively by

$$\beta_c^+(q)=\begin{cases}\infty, & \text{if } \epsilon^-\geqslant 0\\ \dfrac{1}{(1-q)\epsilon^-}, & \text{if } \epsilon^-<0\end{cases};\quad \beta_c^-(q)=\begin{cases}-\infty, & \text{if } \epsilon^+\leqslant 0\\ \dfrac{1}{(1-q)\epsilon^+}, & \text{if } \epsilon^+>0\end{cases}. \tag{12}$$

Notice that if H is not bounded above (resp. below) then $\beta_c^-=0$ (resp. $\beta_c^+=0$); at least one of these critical reciprocal temperatures is finite; and if the spectrum has both negative and positive elements, then both critical β's are finite.

It is immediately verified that

$$\alpha^-(\beta,q)\begin{cases} \leqslant 0 & \text{if} \quad \beta \leqslant \beta_c^-(q) < 0 \qquad \text{with equality iff } \beta = \beta_c^-(q) \\ > 0 & \text{if} \quad \beta_c^-(q) < \beta \leqslant 0 \\ > 0 & \text{if} \quad 0 \leqslant \beta < \beta_c^+(q) \\ \leqslant 0 & \text{if} \quad 0 < \beta_c^+(q) \leqslant \beta \qquad \text{with equality iff } \beta = \beta_c^+(q) \end{cases}.$$

Furthermore, $\alpha^-(\beta,q) = -\infty$ if $\beta < \beta_c^- = 0$ or $\beta > \beta_c^+ = 0$. With this, Proposition A.1 of the Appendix leads us to the solution of (10) as follows:

Theorem 1: Let $q > 1$, and let positive and negative critical reciprocal temperatures be defined by (12), then

$$\phi_q(\beta) = (q-1)^{-1}\{[tr[(\beta(q-1)H+I)^{1/(1-q)}]]^{1-q} - 1\}, \qquad \text{if } \beta_c^-(q) < \beta < \beta_c^+(q), \quad (13)$$

$$\phi_q(\beta) = \begin{cases} \beta\epsilon^+, & \text{if } \beta \leqslant \beta_c^-(q) < 0 \quad \text{or } \beta < \beta_c^-(q) = 0 \\ \beta\epsilon^-, & \text{if } \beta \geqslant \beta_c^+(q) > 0 \quad \text{or } \beta > \beta_c^+(q) = 0 \end{cases}. \quad (14)$$

Moreover

1. For $\beta_c^-(q) < \beta < \beta_c^+(q)$ there is a unique minimizer ρ_β given by the Tsallis–Hölder state:

$$\rho_\beta = \frac{(\beta(q-1)H+I)^{1/(1-q)}}{tr[(\beta(q-1)H+I)^{1/(1-q)}]} \quad (15)$$

when $tr[(\beta(q-1)H+I)^{1/(1-q)}] < \infty$; and no minimizer if this trace is ∞ in which case $\phi_q(\beta) = (1-q)^{-1}$ (infinite dimensional case).

*2. For $0 < \epsilon^+ < \infty$ and $\beta = \beta_c^-(q)$ [*resp. *$\beta < \beta_c^-(q)$] the minimizers are the eigenstates (resp. pure eigenstates) of H to the eigenvalue ϵ^+.*

3. *For $-\infty < \epsilon^- < 0$ and $\beta = \beta_c^+(q)$ [resp. $\beta > \beta_c^+(q)$] the minimizers are the eigenstates (resp. pure eigenstates) of H to the eigenvalue ϵ^-.*

The unique equilibrium state ρ_β given by (15) when $\beta \in \mathscr{T} \equiv (\beta_c^-(q), \beta_c^+(q))$ will be referred to as Tsallis–Hölder (TH) state. As their name intends to convey, these states were introduced by C. Tsallis (in a remark at the bottom of page 483 of Ref. 1, and then in Ref. 3 and subsequent papers), and they saturate Hölder's inequality on the mathematical side. The first important observation to be made is that, whenever the TH state exists, it is the *unique* minimizer of the ''free-energy'' functional, and thus *the* equilibrium state.

Now, before clarifying further features, we give a sketchy description in words of the content of Theorem 1. For $\beta \in \mathscr{T}$, the operator $\beta(q-1)H+I$ is strictly positive. Let

$$a_n(\beta) := (\beta(q-1)\epsilon_n + 1)^{1/(1-q)}.$$

The TH state has eigenvalues $(\rho_\beta)_n = (\Sigma_n a_n(\beta))^{-1} a_n(\beta)$ with eigenfunction ψ_n, where $H\psi_n = \epsilon_n \psi_n$. In particular, the state is non-degenerate: every eigenstate of H is populated. Consider the case when H is bounded below but not above; there being an analogous argument for the opposite case. Recall that $\beta_c^-(q) = 0$ here. As one increases β away from 0, $(\rho_\beta)_n$ decreases for all n with $\epsilon_n \neq \epsilon^-$, and increases for n with $\epsilon_n = \epsilon^-$. When $\beta_c^+(q)$ is reached, assuming it is finite, i.e., $-\infty < \epsilon^- < 0$, $\rho_\beta = (tr(P^-))^{-1} P^-$ where P^- is the orthogonal projection onto the eigenspace to the eigenvalue ϵ^-, and $tr(P^-)$ gives the multiplicity of this eigenvalue. At $\beta_c^+(q)$, our result says that any eigenstate to the eigenvalue ϵ^- minimizes $\phi_q(\beta_c^+(q)) = \beta_c^+(q)\epsilon^- = (1-q)^{-1}$. Above $\beta_c^+(q)$, only pure eigenstates to ϵ^- are minimizers. Thus, there is a discontinuity here if ϵ^- is degenerate. However, this is of no relevance since β's above $\beta_c^+(q)$ are not accessible: ϕ_q is linear, and its second derivative related to the ''specific heat'' is zero. If $\epsilon^- > 0$, we have $\beta_c^+(q) = \infty$ and $0 \leqslant U_q^- < \epsilon^-$. Here, we get another unusual feature which, for want of a better

name, we refer to as *strong* violation of the third law. Indeed, as $\beta\to\infty$, i.e., $T\to 0$, the TH equilibrium state ρ_β tends to the Hölder state ρ_+ of (5) (recall that $H_+=H$ here) with ''internal energy'' U_q^-. This state is non-degenerate, i.e., all eigenstates are populated, and has non-zero entropy (independently of the degeneracy of the ground-state energy). The situation for $\beta<0$ in the case where H is bounded above is totally analogous.

In what follows we will consider the questions relating to the differentiability of the ''thermodynamical'' functions. Consider the function U_q (''internal energy'' as a function of reciprocal temperature) given by $U_q(\beta):=U_q[\rho_\beta]$, whenever the minimizer ρ_β exists and $U_q[\rho_\beta]$ is finite. In the finite dimensional case, where everything is finite, it can be verified that U_q is continuous and the derivative of ϕ_q by direct differentiation in (13) and (14). The concavity of ϕ_q implies then that $\beta\mapsto U_q(\beta)$ is decreasing (recall the assumption $\epsilon^-<\epsilon^+$) and strictly so for $\beta\in\mathscr{T}$. One can also verify directly that

$$\lim_{\beta\to\beta_c^{\pm}(q)} U_q(\beta)=U_q^{\mp}.$$

This guarantees that for each $u\in(U_q^-,U_q^+)$ there exists a unique $\beta\in\mathscr{T}$ such that $U_q(\beta)=u$. This, via Lemma 2 insures that $S_q=(\phi_q)^*$. As a consequence,[8] S_q is strictly concave and differentiable with derivative $\beta(u)$ determined by the inverse of the map $\beta\mapsto U_q(\beta)$. One can also verify the differentiability of U_q connected to the ''specific heat'' C_q by

$$C_q(\beta)=-\beta^2\frac{dU_q}{d\beta}(\beta). \tag{16}$$

Always in the finite dimensional case, C_q is finite and positive for all $\beta\in\mathscr{T}$.

The existence of ρ_β in the infinite dimensional case imposes conditions on the eigenvalue set. For the harmonic oscillator spectrum, $\Sigma_n a_n(\beta)=\infty$ for all $q\geqslant 2$. It is perhaps remarkable that under our assumption on the spectrum of H (purely discrete), the existence of ρ_β guarantees differentiability of ϕ_q. ϕ_q is given, up to trivial summands and a power, by the ''trace'' $\Sigma_n a_n(\beta)$ of the positive operator $(\beta(q-1)H+1)^{1/(1-q)}$. If this ''trace'' converges for some β_o, then ρ_{β_o} exists and assuming $U_q(\beta_o)$ is defined, we know from Lemma 2 that it is a subdifferential of ϕ_q at β_o.

The following two Lemmas summarize our results about differentiability in the infinite dimensional case:

Lemma 4: Let $\mathscr{D}$ be the interior of the domain of ϕ_q. The following conditions

1. ϕ_q is differentiable in $\mathscr{D}$,

2. U_q is continuous in $\mathscr{D}$, are equivalent,

and they imply that U_q is the derivative of ϕ_q.

Proof: We have remarked, in Lemma 2, that U is a subgradient for ϕ (we omit the index q). If the latter function is differentiable, the subgradient is unique and equal to the derivative.

Consider the left- and right-derivatives ϕ'_- and ϕ'_+ respectively of ϕ which exist by concavity and satisfy:

$$\frac{\phi(\beta_1)-\phi(\beta_2)}{\beta_1-\beta_2}\geqslant\phi'_-(\beta_2)\geqslant\phi'_+(\beta_2)\geqslant\frac{\phi(\beta_3)-\phi(\beta_2)}{\beta_3-\beta_2}$$

whenever $\beta_1<\beta_2<\beta_3$. Using the definition of ϕ and the minimizing property of ρ_β we estimate

$$\frac{\phi(\beta_2)-\phi(\beta_1)}{\beta_2-\beta_1}\leqslant\frac{\beta_2U(\beta_1)-S[\rho_{\beta_1}]-\phi(\beta_1)}{\beta_2-\beta_1}=U(\beta_1);$$

$$\frac{\phi(\beta_3)-\phi(\beta_2)}{\beta_3-\beta_2}\geqslant\frac{\phi(\beta_3)-\beta_2U(\beta_3)+S[\rho_{\beta_3}]}{\beta_3-\beta_2}=U(\beta_3).$$

Thus, $U(\beta_1)\geqslant\phi'_-(\beta_2)\geqslant\phi'_+(\beta_2)\geqslant U(\beta_3)$ under the same condition for the β's. Thus, if U is continuous, ϕ is differentiable and U its derivative. □

Lemma 5: Suppose H is bounded below but not above [implying $\beta_c^-(q)=0$]. If $\mathrm{tr}[(\beta(q-1)H+1)^{1/(1-q)}]$ *is finite for some $\beta\in\mathscr{T}$, then it is finite for all $\beta\in\mathscr{T}$. In this case, ρ_β exists for all $\beta\in\mathscr{T}$ and ϕ_q is twice differentiable with derivative U_q and second derivative $-\beta^{-2}C_q(\beta)$ on $\mathscr{T}$.*

Proof: We first notice that (the prime denotes derivation with respect to β)

$$a_n'(\beta)=-\epsilon_n(\beta(q-1)\epsilon_n+1)^{q/(1-q)},\quad a_n''(\beta)=q\epsilon_n^2(\beta(q-1)\epsilon_n+1)^{(2q-1)/(1-q)};$$

so that a_n is convex on $\mathscr{T}$. Let us number the eigenvalues of H as $\epsilon^-=\epsilon_o\leqslant\epsilon_1\leqslant\epsilon_2\leqslant\cdots$. It follows that $s_n(\beta):=\Sigma_{k=0}^n a_k(\beta)$ is convex on $\mathscr{T}$, and thus if the sequence converges on some bounded subinterval of $\mathscr{T}$, the convergence is uniform. Suppose now that the sequence converges for some $\beta_o\in\mathscr{T}$; then, due to our assumption $\epsilon^+=\infty$, for all n sufficiently large $\beta_o(q-1)\epsilon_n\geqslant 1$ so that

$$a_n(\beta_o)\geqslant(2\beta_o(q-1))^{1/(1-q)}\epsilon_n^{1/(1-q)}.$$

It follows from this and the assumption that the spectrum of H is purely discrete, that the infinite series $\Sigma_n\epsilon_n^{1/(1-q)}$ is absolutely convergent. But since, for every $\beta\in\mathscr{T}$ we have

$$a_n(\beta)<(\beta(q-1)\epsilon_n)^{1/(1-q)}$$

as soon as n is sufficiently large (i.e., as soon as $\epsilon_n\geqslant 0$), we conclude that s_n converges uniformly on any compact subset of $\mathscr{T}$. We also notice that as soon as $\epsilon_n\geqslant 0$, we have

$$|a_n'(\beta)|<(\beta(q-1))^{-1}a_n(\beta),\quad a_n''(\beta)<\left(\beta\frac{q-1}{q}\right)^{-1}|a_n'(\beta)|.$$

This implies that both sequences $s_n'(\beta)$ and $s_n''(\beta)$ converge absolutely for all $\beta\in\mathscr{T}$. From this one can deduce the existence of U_q and C_q, and then the continuity and differentiability of U_q, which leads to the differentiability of ϕ_q in $\mathscr{T}$. The argument continued proves that ϕ_q is C^∞. □

B. Case $0<q<1$

The path to be followed is as in the former case, but the results are more involved. There are two sets of critical temperatures. The supercritical reciprocal temperatures are given by:

$$\beta_c^+(q)=\begin{cases}0, & \text{if } \epsilon^-=-\infty\\ \infty, & \text{if } -\infty<\epsilon^-\leqslant 0\\ \dfrac{1}{(1-q)\epsilon^-}, & \text{if } \epsilon^->0\end{cases}\qquad \beta_c^-(q)=\begin{cases}0, & \text{if } \epsilon^+=\infty\\ -\infty, & \text{if } 0\leqslant\epsilon^+<\infty\\ \dfrac{1}{(1-q)\epsilon^+}, & \text{if } \epsilon^+<0\end{cases}.\tag{17}$$

The other set involves the first excited-state energy above ϵ^-, and the first de-excited-state energy below ϵ^+. We define:

$$\epsilon_*^-:=\inf\{\epsilon_n:\epsilon_n>\epsilon^-\};\quad \epsilon_*^+:=\sup\{\epsilon_n:\epsilon_n<\epsilon^+\}.$$

TABLE I. Critical and supercritical reciprocal temperatures when H is semibounded in the $0<q<1$ case.

ϵ^-	ϵ_*^-	$\beta_c^+(q)$	$\beta_*^+(q)$
$-\infty$	$-\infty$	0	0
finite, <0	finite, $\leqslant 0$	∞	∞
finite, $\leqslant 0$	finite, >0	∞	$((1-q)\epsilon_*^-)^{-1}$
finite, >0	finite, >0	$((1-q)\epsilon^-)^{-1}$	$((1-q)\epsilon_*^-)^{-1}$
ϵ^+	ϵ_*^+	$\beta_c^-(q)$	$\beta_*^-(q)$
∞	∞	0	0
finite, >0	finite, $\geqslant 0$	$-\infty$	$-\infty$
finite, $\geqslant 0$	finite, <0	$-\infty$	$((1-q)\epsilon_*^+)^{-1}$
finite, <0	finite, <0	$((1-q)\epsilon^+)^{-1}$	$((1-q)\epsilon_*^+)^{-1}$

Notice that in the finite dimensional case $\epsilon_*^+<\epsilon^+$ and $\epsilon_*^->\epsilon^-$; and also that if H is unbounded above (resp. below) $\epsilon_*^+=\epsilon^+=\infty$ (resp. $\epsilon_*^-=\epsilon^-=-\infty$). The critical reciprocal temperatures are given by

$$\beta_*^+(q)=\begin{cases}0, & \text{if } \epsilon_*^-=-\infty\\ \infty, & \text{if } -\infty<\epsilon_*^-\leqslant 0\\ \dfrac{1}{(1-q)\epsilon_*^-}, & \text{if } \epsilon_*^->0\end{cases}\qquad \beta_*^-(q)=\begin{cases}0, & \text{if } \epsilon_*^+=\infty\\ -\infty, & \text{if } 0\leqslant\epsilon_*^+<\infty\\ \dfrac{1}{(1-q)\epsilon_*^+}, & \text{if } \epsilon_*^+<0\end{cases}. \tag{18}$$

One always has $\beta_c^+(q)\geqslant\beta_*^+(q)\geqslant 0$ and $\beta_c^-(q)\leqslant\beta_*^-(q)\leqslant 0$. In Table I we show all possibilities for the critical and supercritical reciprocal temperatures in the semibounded case. We can again determine $\alpha^-(\beta,q)$ as a function of β:

$$\alpha^-(\beta,q)\begin{cases}\geqslant 0 & \text{if } \beta\leqslant\beta_c^-(q)<0 \quad \text{with equality iff } \beta=\beta_c^-(q)\\ <0 & \text{if } \beta_c^-(q)<\beta\leqslant 0\\ <0 & \text{if } 0\leqslant\beta<\beta_c^+(q)\\ \geqslant 0 & \text{if } 0<\beta_c^+(q)\leqslant\beta \quad \text{with equality iff } \beta=\beta_c^+(q)\end{cases}.$$

Furthermore, $\alpha^-(\beta,q)=-\infty$ if $\beta<\beta_c^-=0$ or $\beta>\beta_c^+=0$.

For β's inside the interval $(\beta_c^-(q),\beta_c^+(q))$, the minimizer is unique and given by the negative part of the operator $A(\beta,q)$. But, in this interval, $A(\beta,q)_-$ has finite rank. Moreover, for β in the interval $(\beta_c^-(q),\beta_*^-(q)]$ (resp. $[\beta_*^+(q),\beta_c^+(q))$), $A(\beta,q)_-$ has exactly one non-zero eigenvalue, and the minimizer is the equidistribution of ceiling states (resp. ground states). This, and Proposition A.2 of the Appendix leads to

Theorem 2: Let $0<q<1$, *and let positive and negative supercritical and critical reciprocal temperatures be defined by (17) and (18) respectively, then*

1. If $\beta<\beta_c^-(q)<0$ $(-\infty<\epsilon^+<0)$ *then*

$$\phi_q(\beta)=\beta\epsilon^+$$

and the minimizers are the pure eigenstates to the eigenvalue ϵ^+.

$$\phi_q(\beta_c^-(q))=\begin{cases}(1-q)^{-1}, & \text{if } -\infty<\beta_c^-(q)<0\\ -\infty, & \text{if } \beta_c^-(q)=0, \textit{ which occurs only in infinite dimension.}\end{cases}$$

2. When $\beta_c^-(q)=0$ the minimizers are not unique. In the other case, the minimizers are all the eigenstates to the eigenvalue ϵ^+.

3. If $\beta_c^-(q)\leqslant\beta\leqslant\beta_*^-(q)<0$ then

$$\phi_q(\beta)=\beta g_+^{1-q}\epsilon^+-\frac{g_+^{1-q}-1}{1-q}$$

and there is a unique minimizer given by the equidistribution of ceiling states $g_+^{-1}P^+$, where P^+ is the orthogonal projection onto the eigenspace to the eigenvalue ϵ^+, and $g_+=tr(P^+)$ is the multiplicity of this eigenvalue.

4. If $\beta_*^-(q)<\beta<\beta_*^+(q)$ then the operator $(\beta(q-1)H+I)_+$, the positive part of the operator $\beta(q-1)H+I$ (see Sec. II), has finite rank,

$$\phi_q(\beta)=(1-q)^{-1}\{1-[tr[(\beta(q-1)H+I)_+^{1/(1-q)}]]^{1-q}\},$$

and there is a unique minimizer given by

$$\rho_\beta=\frac{(\beta(q-1)H+I)_+^{1/(1-q)}}{tr[(\beta(q-1)H+I)_+^{1/(1-q)}]}. \tag{19}$$

5. If $0<\beta_*^+(q)\leqslant\beta\leqslant\beta_c^+(q)$ then

$$\phi_q(\beta)=\beta g_-^{1-q}\epsilon^--\frac{g_-^{1-q}-1}{1-q}$$

and there is a unique minimizer given by the equidistribution of ground states $g_-^{-1}P^-$, where P^- is the orthogonal projection onto the eigenspace to the eigenvalue ϵ^-, and $g_-=tr(P^-)$ is the multiplicity of this eigenvalue.

$$\phi_q(\beta_c^+(q))=\begin{cases}(1-q)^{-1}, & \text{if } 0<\beta_c^+(q)<\infty\\ -\infty, & \text{if } \beta_c^+(q)=0 \text{ which occurs only in infinite dimension.}\end{cases}$$

6. When $\beta_c^+(q)=0$ the minimizers are not unique. In the other case, the minimizers are all the eigenstates to the eigenvalue ϵ^-.

7. If $0<\beta_c^+(q)\leqslant\beta$ $(0<\epsilon^-<\infty)$ then

$$\phi_q(\beta)=\beta\epsilon^-$$

and the minimizers are the pure eigenstates to the eigenvalue ϵ^-.

The TH state is based on the positive part of the operator $\beta(q-1)H+I$ which has finite rank. Using the notation $\Delta_n(\beta)=1-\beta(1-q)\epsilon_n$ the eigenvalues are given by

$$(\rho_\beta)_n=\begin{cases}\left(\sum_k \Delta_k(\beta)^{1/(1-q)}\right)^{-1}\Delta_n(\beta)^{1/(1-q)}, & n \text{ such that } \Delta_n(\beta)>0\\ 0, & n \text{ such that } \Delta_n(\beta)\leqslant 0\end{cases},$$

where the sum runs over k such that $\Delta_k(\beta)>0$. Not every eigenstate of H is populated as soon as $\beta(q-1)H+I$ has non-zero negative part. This is impossible in the exponential Gibbs–Boltzmann distribution. Now, we discuss the typical features.

In the finite dimensional case, if the spectrum has more than one positive eigenvalue and more than one negative eigenvalue, both critical β's are not finite. At $\beta=0$ the TH state is the normal-

ized trace. As we increase β away from 0, all energy eigenstates are populated until we reach $\beta=((1-q)\epsilon^{+})^{-1}$. At this point, all eigenstates to this highest eigenvalue are depopulated and all other eigenstates remain populated. As we continue increasing β nothing interesting happens until we reach $\beta=((1-q)\epsilon_{*}^{+})^{-1}$, recall $\epsilon_{*}^{+}>0$ here. At this point, the eigenstates corresponding to ϵ_{*}^{+} are also depopulated. As we continue increasing β we depopulate successively downwards the positive energy eigenstates until there are none left. From then onwards, only the non-positive eigenstates are populated. As we continue increasing β we approach asymptotically the Hölder state ρ_{-} of (5). For $\beta<0$ we have the same features, but now the negative energy eigenstates are depopulated successively upwards until only the non-negative energy eigenstates remain populated, and the Hölder state ρ_{+} of (5) is approached asymptotically as $\beta\to-\infty$. There is thus strong violation of the third law at $T=0^{\pm}$.

If the spectrum is strictly positive, $\beta_{*}^{+}(q)$ is finite and $\beta_{*}^{-}(q)=-\infty$. As we increase β away from 0 the eigenstates are successively depopulated downwards, until there is just ground-states left; this happens precisely at $\beta_{*}^{+}(q)$; we then have $g_{-}^{-1}P^{-}$, the equidistribution of ground states. As we further increase β nothing changes until we reach $\beta_{c}^{+}(q)$. Our result claims that any ground-state is a minimizer at $\beta_{c}^{+}(q)$; and any pure ground-state is a minimizer above $\beta_{c}^{+}(q)$. But, as before, the β's above $\beta_{*}^{+}(q)$ are inaccessible. Decreasing β away from 0, all eigenstates are always populated [since $\beta(q-1)\epsilon_{n}+1>0$] and the Hölder state ρ_{+} of (5) is reached asymptotically for $\beta\to-\infty$. The features of the strictly negative spectrum case, are analogous to those of the strictly positive spectrum case reversing signs and directions, and replacing ground- by ceiling-states and so on.

When H is bounded below but not above, we have $\phi_{q}(\beta)=-\infty$ for every $\beta\leqslant 0$. The features for $\beta>0$ are exactly the same as those of the corresponding finite-dimensional case.

The successive depopulation of eigenstates has a drastic effect which cannot be seen at first glance in ϕ_{q} which is a nice concave (in fact differentiable) function. This feature is detected, as we will discuss below, in the function $U_{q}(\beta):=U_{q}[\rho_{\beta}]$ whose graph is a staircase: the derivative of U_{q} w.r.t. β, does not exist for each β (negative or positive) where a depopulation occurs. More precisely, the derivative has different limits as we approach these β's from left or right. Since tr is always a finite sum, we can analyze the differentiability of ϕ_{q} term by term. One checks that $U_{q}(\beta)$ is the derivative of ϕ_{q} for all $\beta\in(\beta_{*}^{-},\beta_{*}^{+})\equiv\mathscr{T}_{*}$.

The general expression for the ''specific heat'' C_{q} can be derived from (16):

$$C_{q}(\beta)=q\beta^{2}Z(\beta)^{-(1+q)}(Z(\beta)A_{2}(\beta)-A_{1}(\beta)^{2}),$$

where

$$Z(\beta)=\sum_{n}\Delta_{n}(\beta)^{1/(1-q)},\quad A_{1}(\beta)=\sum_{n}\Delta_{n}(\beta)^{q/(1-q)}\epsilon_{n},\quad A_{2}(\beta)=\sum_{n}\Delta_{n}(\beta)^{(2q-1)/(1-q)}\epsilon_{n}^{2}.$$

The summations run over n such that $\Delta_{n}>0$. From this we can see also that $C_{q}\geqslant 0$. The differentiability of U_{q} is guaranteed except at all points $\beta_{n}=1/(1-q)\epsilon_{n}$ lying inside $\mathscr{T}_{*}$. Taking $\beta=\beta_{n}\mp\delta$ (according to whether $\beta_{n}\gtrless 0$) and if we denote:

$$F^{+}(\beta_{n}):=\lim_{\delta\to 0+}F(\beta_{n}\mp\delta);\quad F^{-}(\beta_{n}):=\lim_{\delta\to 0-}F(\beta_{n}\mp\delta),$$

and $\gamma=(1-q)|\epsilon_{n}|\delta$ we can prove that:

$$Z^{+}(\beta_{n})=Z^{-}(\beta_{n})+\lim_{\delta\to 0+}\gamma^{1/(1-q)},$$

$$A_{1}^{+}(\beta_{n})=A_{1}^{-}(\beta_{n})+\epsilon_{n}\lim_{\delta\to 0+}\gamma^{q/(1-q)},$$

$$A_2^+(\beta_n)=A_2^-(\beta_n)+\epsilon_n^2 \lim_{\delta\to 0+} \gamma^{(2q-1)/(1-q)},$$

where $Z^-(\beta_n)$, $A_1^-(\beta_n)$, and $A_2^-(\beta_n)$ are finite quantities. For $\frac{1}{2}<q<1$, Z, A_1, and A_2 are continuous at β_n, hence C_q is continuous for all $\beta \in \mathscr{T}_*$. For $q=\frac{1}{2}$, Z and A_1 are continuous but $A_2^+=A_2^-+\epsilon_n^2$, therefore the ''specific heat'' presents finite discontinuities at β_n. For $0<q<\frac{1}{2}$, A_2^+ diverges (Z and A_1 are still continuous) and in consequence C_q^+ diverges:

$$C_q(\beta)\to\begin{cases}\infty & \text{if } \beta\uparrow\beta_n>0 \quad \text{or } \beta\downarrow\beta_n<0\\ finite & \text{if } \beta\downarrow\beta_n>0 \quad \text{or } \beta\uparrow\beta_n<0\end{cases}.$$

In the $q\to 0$ limit, C_q vanishes everywhere except at β_n where the lateral divergences survive.

Let us look closely at the case $0<\epsilon^-<\epsilon_*^-$. ϕ_q is a straight line in the interval $[\beta_*^+(q),\beta_c^+(q))$ with slope $g_-^{1-q}\epsilon^-$ and $C_q(\beta)=0$. At $\beta_c^+(q)$ this line connects to the straight line $\beta\epsilon^-$ which gives the value of ϕ_q for $\beta\geqslant\beta_c^+(q)$. When the ground state is degenerate, i.e., $g_-\geqslant 2$, these lines have different slope and ϕ_q is not differentiable at $\beta_c^+(q)$. There is a discontinuity in U_q at $\beta_c^+(q)$:

$$\lim_{\beta\uparrow\beta_c^+(q)} U_q(\beta)=g_-^{1-q}\epsilon^->U_q^-=\epsilon^-=\lim_{\beta\downarrow\beta_c^+(q)} U_q(\beta).$$

This happens also at $\beta_c^-(q)$ when the ceiling state is degenerate, i.e., $g_+\geqslant 2$, and $\epsilon_*^+<\epsilon^+<0$. The range of the function $\beta\mapsto U_q(\beta)$ is not $[U_q^-,U_q^+]$ when there are degeneracies in the ground or ceiling states and these states have non-zero finite energy. There are then energies u for which there is no reciprocal temperature.

When $g_->1$, we can compute ϕ_q^*, defined in (9), as follows. To each $u\geqslant g_-^{1-q}\epsilon^-$, there corresponds a unique $\beta(u)\in(-\infty,\beta_*^+(q)]$ and the corresponding minimizers lead us, using Lemma 2, to $S_q(u)=\phi_q^*(u)=S_q[\rho_{\beta(u)}]$. For u in the non-thermal interval $(\epsilon^-,g_-^{1-q}\epsilon^-)$ there is no β such that $U_q[\rho_\beta]=u$. But we can compute the Legendre–Fenchel transform of ϕ_q directly for this interval. The result is:

$$\phi_q^*(u)=\beta_c^+(u-\epsilon^-)=\frac{1}{(1-q)\epsilon^-}u+\frac{1}{q-1}, \quad \text{for } u\in[\epsilon^-,g_-^{1-q}\epsilon^-].$$

Thus ϕ_q^* is a straight line on the non-thermal u-interval. We know by Lemma 1, that $S_q(u)\leqslant\phi_q^*(u)$. We also know that $S_q(g_-^{1-q}\epsilon^-)=\phi_q^*(g_-^{1-q}\epsilon^-)$ because at this point there is a minimizer $\rho_{\beta_*^+(q)}$. We can compute the value of S_q at ϵ^- directly from the definition (6). Indeed, the only states ρ such that $U_q[\rho]=\epsilon^-$ are the pure eigenstates to that eigenvalue; thus $S_q(\epsilon^-)=0=\phi_q(\epsilon^-)$. Since in the non-thermal interval S_q lies below ϕ_q^* and coincides with ϕ_q^* at the end-points we conclude that if $S_q(u)<\phi_q^*(u)$ for some u inside this interval, then S_q is not concave, and the correct entropy function is (the straight line) ϕ_q^* on this interval. This strange effect of degeneracy is rather drastic. In the finite dimensional case, when g_- is so large that $g_-^{1-q}\epsilon^->\epsilon^+$, the whole spectrum $\{\epsilon_n\}$ lies inside the non-thermal interval. The non-thermal interval disappears as soon as $\epsilon^-\leqslant 0$ even when $\epsilon_*^->0$ and $g_-\geqslant 2$. Indeed, here $\beta_c^+(q)=\infty$ and the least energy $U_q^-=g_-^{1-q}\epsilon^-$ is reached at $\beta_*^+(q)$ where the minimizer is $g_-^{-1}P^-$ and coincides with the Hölder state ρ_- of (5).

C. A remark about equilibrium

We have been referring to the TH state ρ_β, which is the unique minimizer of the variational problem (8), as the equilibrium state at reciprocal temperature β. In fact, this is a gross abuse of the analogy with the connection between Boltzmann–Gibbs statistical mechanics and Thermody-

namics. We should first analyze if this notion of equilibrium entails its transitivity; that is, if the familiar 0^{th}-law of thermodynamics holds in this formalism. *It does not*. Suppose one has two systems with Hamiltonians H_j described on the Hilbert spaces $\mathscr{H}_j$ such that H_j is not a multiple of the identity ($j=1,2$). The composite noninteracting system is described by the Hamiltonian $H=H_1\otimes I+I\otimes H_2$ on the Hilbert space $\mathscr{H}=\mathscr{H}_1\otimes\mathscr{H}_2$. The TH state ρ_β at reciprocal temperature β in $\mathscr{T}$, which is the unique minimizer of (8) with $U_q^{(H)}[\rho]=tr_{\mathscr{H}}(\rho^q H)$, is not a product-state:

$$\rho_\beta \neq (\rho_\beta)_1\otimes(\rho_\beta)_2,$$

where $(\rho_\beta)_j$ is the restriction of ρ_β to a state of the j-th subsystem. Moreover, $(\rho_\beta)_j$ is not a TH state of the system j in the sense that it does not minimize (8) with $U_q^{(H_j)}[\omega]=tr_{\mathscr{H}_j}(\omega^q H_j)$ for any β. Thus, it is impossible to assign a reciprocal temperature to the subsystems when the composite non-interacting system is in the state ρ_β. It follows that this notion of equilibrium is not transitive and the analogue of the 0^{th}-law is not true. Thus, a possible connection between this ''thermostatistics'' and some thermometrical notion cannot be established with the parameter β.

The reason behind this unwanted feature is to be seen in the non-additivity property of the q-entropy

$$S_q[\rho\otimes\omega]=S_q[\rho]+S_q[\omega]+(1-q)S_q[\rho]S_q[\omega];$$

and of the functional $U_q[\cdot]$

$$U_q^{(H)}[\rho\otimes\omega]=U_q^{(H_1)}[\rho]+U_q^{(H_2)}[\omega]+(1-q)(U_q^{(H_1)}[\rho]S_q[\omega]+U_q^{(H_2)}[\omega]S_q[\rho]).$$

These properties can be easily checked.

For $0<q<1$, Tsallis[4] introduced the notion ''thermally forbidden region'' for the intervals $\beta\leqslant\beta_c^-$ and $\beta\geqslant\beta_c^+$, and ''thermally frozen region'' for the intervals $\beta_c^-<\beta\leqslant\beta_*^-$ and $\beta_*^+\leqslant\beta<\beta_c^+$. For the $q>1$ case, the intervals $\beta\leqslant\beta_c^-$ and $\beta\geqslant\beta_c^+$ were called ''thermally frozen region.'' For us, all these regions are thermally inaccessible, without further discrimination, because the ''free-energy'' function ϕ_q, which is well defined, is linear therein. In consequence the ''specific heat'' in these regions is identically zero. It is worthwhile to stress that the variational problem posed by (8) only gives a *unique* minimizer state, the TH equilibrium state, for $\beta_c^-<\beta<\beta_c^+$.

V. ILLUSTRATION

At present, ''specific heat'' calculations for non-standard thermal statistics based on q-entropies (as was worked out in Ref. 3), are available for the two-level system, a free particle,[10] and the Ising chain.[11]

In this Section we present as an application of the non-standard formalism developed above, the ''free-energy'' function ϕ_q and the ''specific heat'' of the harmonic oscillator characterized by the spectrum:

$$\epsilon_n=n-\alpha,\quad n=0,1,2,\cdots,$$

where $\alpha\in\Re$. Immediately we have $\epsilon^+=\epsilon_*^+=\infty$ and $\epsilon^-=-\alpha$, $\epsilon_*^-=1-\alpha$. The influence of α is relevant for $q\neq 1$. For conventional use, we will present the results of this section as functions of the temperature T instead of $\beta=1/T$. The ''Helmholtz free-energy'' is $T\phi_q(T)$. Here, H is bounded below but not above, in consequence $T_c^-=T_*^-=-\infty$ and the thermally relevant region is $T>T_c^+$ for $q>1$ and $T>T_*^+$ for $0<q<1$.

Case q>1:

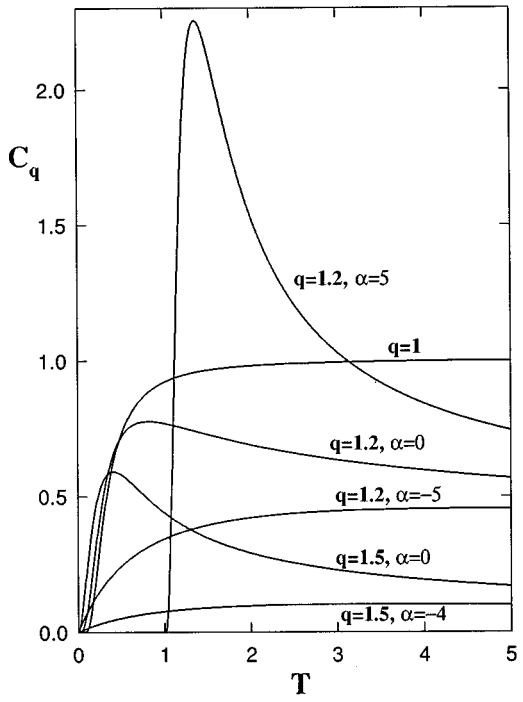

FIG. 1. Thermal dependence of C_q in the harmonic oscillator for typical values of $q>1$. For $\alpha\leqslant 0$, $T_c=0$. In the case $q=1.2$, for $\alpha=5$, $T_c^+=1$. The case $q=1$ is also shown for a comparison with the Boltzmann–Gibbs curve.

$$T_c^+=\begin{cases}0, & \alpha\leqslant 0\\ (q-1)\alpha, & \alpha>0\end{cases},$$

$$\phi_q(T)=\begin{cases}-\infty, & T\leqslant 0\\ -\dfrac{\alpha}{T}, & 0<T\leqslant T_c^+\\ \dfrac{1}{1-q}\left\{\left[\displaystyle\sum_{n\geqslant 0}\left(\frac{(q-1)(n-\alpha)}{T}+1\right)^{1/(1-q)}\right]^{1-q}-1\right\}, & T>T_c^+\end{cases}.$$

The convergence of the series is obtained only for $q<2$. For $q\geqslant 2$, formally we obtain $\phi(T)=(1/1-q)$ for $T>T_c^+$, then $C_q(T)=0$.

Figure 1 illustrates the thermal dependence of the ''specific heat'' for typical values of $q>1$ and α. For $T\to\infty$ the contribution to the series are from the terms with $n>>\alpha$. Then for a given $q>1$, the ''specific heat'' curves for different values of α coalesce asymptotically.

Case $0<q<1$*:*

$$T_c^+=\begin{cases}0, & \alpha\geqslant 0\\ -(1-q)\alpha, & \alpha<0\end{cases};T_*^+=\begin{cases}0, & \alpha\geqslant 1\\ (1-q)(1-\alpha), & \alpha<1\end{cases}$$

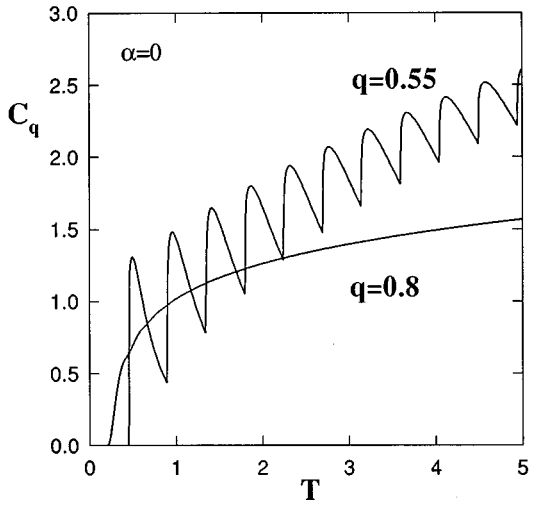

FIG. 2. Thermal dependence of C_q in the harmonic oscillator for two values of q in the region $\frac{1}{2}<q<1$ and $\alpha=0$.

$$\phi_q(T)=\begin{cases} -\infty, & T\leqslant 0 \\ -\dfrac{\alpha}{T}, & 0<T\leqslant T_*^+ \\ \dfrac{1}{1-q}\left\{\left(\sum_n{}' \left(1-\dfrac{(1-q)(n-\alpha)}{T}\right)^{1/(1-q)}\right)^{1-q}-1\right\}, & T>T_*^+, \end{cases}$$

where Σ' runs over $n<T/(1-q)+\alpha$.

Figure 2 shows the thermal dependence of C_q for typical values of q in the interval $(\frac{1}{2},1)$. We observe strong oscillations in the ''specific heat'' but it is continuous everywhere. For $q\leqslant\frac{1}{2}$ the function $U_q(T)$ is not differentiable in the points $T_n=(1-q)(n-\alpha)>0$. These points are equally spaced for the harmonic oscillator. The case $q=\frac{1}{2}$ is presented in Figure 3, where we can observe the finite discontinuities in C_q at T_n. The lateral divergences in C_q at T_n for a typical $q<\frac{1}{2}$ are shown in Figure 4. The ''specific heat'' was numerically evaluated in all presented pictures.

VI. RESULTS ON THE MULTIDIMENSIONAL CASE

The results of the Appendix apply immediately to the case where one imposes N constraints via N Hamiltonians $H_1,H_2,\cdots,H_N$.[12] Let

$$S_q(u_1,u_2,\cdots,u_N)=\sup_\rho\{S_q[\rho]:U_q^{(j)}[\rho]:=tr(\rho^q H_j)=u_j,j=1,2,\cdots,N\};$$

then one has

$$\phi_q(\vec{\beta}):=\inf_{\vec{u}}\{\vec{\beta}\cdot\vec{u}-S_q(\vec{u})\}=\inf_\rho\left\{\sum_{j=1}^N \beta_j U_q^{(j)}[\rho]-S_q[\rho]\right\}$$

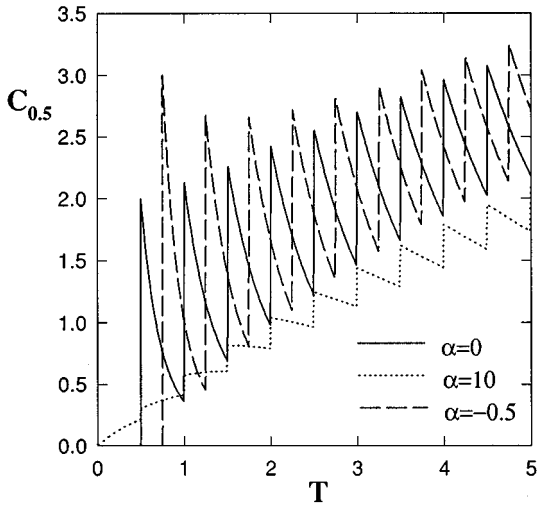

FIG. 3. Thermal dependence of C_q in the harmonic oscillator for $q=\frac{1}{2}$ and typical values of α, showing discontinuities.

for the Legendre–Fenchel transform of S_q at the point $\vec{\beta}=(\beta_1,\beta_2,\cdots,\beta_N)\in\Re^N$. The solution of this variational problem is controlled, via Propositions A.1 and A.2 of the Appendix, by the sign of the least eigenvalue of the operator $A(\vec{\beta},q):=\Sigma_{j=1}^{N}\beta_j H_j+(q-1)^{-1}I$.

In the infinite dimensional case there are domain problems to be taken into account and one has to establish conditions such that the operator has purely discrete spectrum. To avoid all this we consider in what follows only the finite dimensional case.

For $q>1$, let $\mathcal{I}_q:=\{\vec{\beta}:\alpha^-(\vec{\beta},q)>0\}$. Since the function $\Re^N \ni \vec{\beta}\mapsto\alpha^-(\vec{\beta},q):=\inf\{spec(A(\vec{\beta},q))\}$ is concave, $\mathcal{I}_q$ is a convex subset of $\Re^N$. The boundary of $\mathcal{I}_q$ defines the

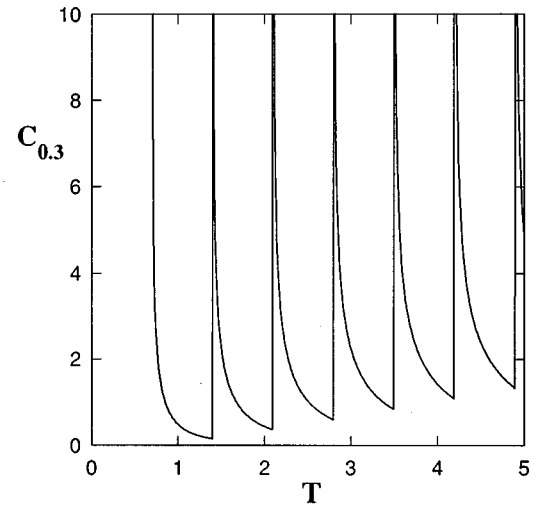

FIG. 4. Thermal dependence of C_q in the harmonic oscillator for $q=0.3$ and $\alpha=0$.

hypersurface of critical $\vec{\beta}$'s; this hypersurface is difficult to describe explicitly and globally when the Hamiltonians do not commute with each other. There is a unique minimizer when $\vec{\beta} \in \mathscr{T}_q$ given by the Tsallis–Hölder state

$$\rho_{\vec{\beta}} = tr(A(\vec{\beta},q)^{1/(1-q)})^{-1} A(\vec{\beta},q)^{1/(1-q)}.$$

On the critical hypersurface, the minimizers are ground- or ceiling-states of $A(\vec{\beta},q)$. Outside the closure of $\mathscr{T}_q$, the minimizers are pure ground- or ceiling- states of $A(\vec{\beta},q)$.

For $0<q<1$, the relevant regions are $\mathscr{T}_q := \{\vec{\beta}: \alpha^-(\vec{\beta},q)<0\}$, and a second region $\mathscr{T}_q^*$ defined as the complement in $\mathfrak{R}^N$ of the $\vec{\beta}$'s with either $\alpha^-(\vec{\beta},q) \geqslant 0$ or such that the operator $A(\vec{\beta},q)_-$ has exactly one non-zero eigenvalue; alternatively $\mathscr{T}_q^* := \{\vec{\beta}: \alpha^-(\vec{\beta},q)<0$, and $A(\vec{\beta},q)_-$ has more than one non-zero eigenvalue$\}$. Neither of these sets is convex in general. For $\vec{\beta} \in \mathscr{T}_q^*$, the minimizer is unique and given by the Tsallis–Hölder state

$$\rho_{\vec{\beta}} = tr(A(\vec{\beta},q)_-^{1/(1-q)})^{-1} A(\vec{\beta},q)_-^{1/(1-q)}.$$

For $\vec{\beta} \in \mathscr{T}_q / \mathscr{T}_q^*$, the minimizer is the equidistribution of ground- or ceiling-states of $A(\vec{\beta},q)$. On the boundary or outside of $\mathscr{T}_q$ the situation is as in the case $q>1$.

Clearly, the multidimensional case reduces to the case of only one constraint. Taking an arbitrary unit vector (i.e., direction) $\vec{e}$ in $\mathfrak{R}^N$, and letting $H(\vec{e}) = \Sigma_{j=1}^N e_j H_j$, the problem is reduced to that which we have solved explicitly:

$$\phi_q^{(\vec{e})}(\beta) := \phi_q(\beta \vec{e}) = \inf_\rho \{\beta U_q^{(H(\vec{e}))}[\rho] - S_q[\rho]\}.$$

Thus the intersections of the sets $\mathscr{T}_q$ and $\mathscr{T}_q^*$ with the rays in $\mathfrak{R}^N$ are described explicitly in terms of direction dependent $\beta_c^{\pm}(\vec{e},q)$'s and, for $0<q<1$, $\beta_*^{\pm}(\vec{e},q)$'s.

VII. CONCLUDING REMARKS

We have solved rigorously the variational problem associated with the q-entropies under the non-affine constraint $U_q[\cdot] =$ constant. We have determined by use of the Hölder inequality the corresponding quantum states minimizing the functional $\beta U_q[\cdot] - S_q[\cdot]$. Then we have established all the ''thermostatistical'' consequences. In particular, the analogue of the 0^{th}-law of Thermodynamics does not hold in terms of β.

For $q>1$ the bizarre feature as perceived from familiar Boltzmann–Gibbs statistics, apart from the manifest dependence on the energy-zero, is the unattainability of temperatures in the interval $[1/(\beta_c^-(q)), 1/(\beta_c^+(q))]$, and what we have called strong violation of the third law.

The case $0<q<1$ is much richer. Generally speaking the case $0<q<1$, presents the same features as the case $q>1$: strong violation of the third law, and unattainability of low temperatures (but not always). But the depopulation phenomenon of levels, has a drastic effect in the ''specific heat,'' which may present oscillations, discontinuities and lateral divergences.

Note added in proof: We complete a point left open in the case $0<q<1$, and show that S_q is concave. In the last two paragraphs of part B in Sec. IV, we had seen that if the ground-state energy is degenerate, i.e., $g_- \geqslant 2$ (alternatively the ceiling-state is degenerate, $g_+ \geqslant 2$), then there are energies u for which there are no reciprocal temperatures when $\epsilon^- > 0$. The corresponding energy interval $(\epsilon^-, g_-^{1-q}\epsilon^-)$ was referred to as the non-thermal interval. We computed the Legendre–Fenchel transform ϕ_q^* of ϕ_q for this interval obtaining $\phi_q^*(u) = \beta_c^+(u-\epsilon^-) = (q-1)^{-1}(1-u/\epsilon^-)$. We then said that, due to the general inequality $S_q \leqslant \phi_q^*$, and the fact that $S_q = \phi_q^*$ at the end-points of the non-thermal interval, we could conclude that S_q is not concave if for some non-thermal u we had $S_q(u) < \phi_q^*(u)$. Here we show that $S_q = \phi_q^*$ on the whole non-

thermal interval, so that S_q is indeed always concave. Take a state ρ such that $\rho P_- = \rho$ [recall that $\epsilon^- > 0$ is degenerate, i.e., $g_- = tr(P_-) \geq 2$]. Then $tr(\rho^q H) = \epsilon_- tr(\rho^q)$, so that $S_q[\rho] = (q-1)^{-1}(1 - U_q[\rho]/\epsilon^-)$. Since $1 \leq tr(\rho^q) = tr(\rho^q P_-) \leq g_-^{1-q}$, given u in the non-thermal interval, we can choose a ρ satisfying the conditions with $U_q[\rho] = u$ and thus $S_q[\rho] = \phi_q^*(u)$. On the other hand, for any state ρ with $U_q[\rho] = u$, we have $S_q[\rho] \leq S_q(u) \leq \phi_q^*(u)$. We conclude that $S_q(u) = \phi_q^*(u)$ on the non-thermal interval. The same argument applies to the case of degenerate ceiling-energy.

ACKNOWLEDGMENTS

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APPENDIX: THE BASIC VARIATIONAL PROBLEM

Here we solve the two variational problems $\inf_\rho tr(\rho^q A)$ and $\sup_\rho tr(\rho^q A)$ for $0 < q \neq 1$, where A is selfadjoint and its spectrum consists entirely of isolated eigenvalues of finite multiplicity. These we number as $\{a_n\}$ according to their multiplicities:

$$A = \sum_n a_n |\psi_n\rangle\langle\psi_n|,$$

where $\{\psi_n\}$ is a complete orthonormal basis of eigenvectors for A. We let $\alpha^+ := \sup_n a_n$, $\alpha^- := \inf_n a_n$, and remark that if either of these two numbers is finite, then it is an eigenvalue of A. The traces in question are always understood as

$$tr(\rho^q A) = \sum_n a_n \langle \psi_n, \rho^q \psi_n \rangle \tag{A.1}$$

when the series on the right-hand side is absolutely convergent.

The solution requires use of the classic Hölder inequality which we quote from Ref. 13 for the readers convenience:

Hölder Inequalities: *Let k be a real number distinct from* 0 *and from* 1, *and put $k' = k/(k-1)$. Let $\{a_n\}$ and $\{b_n\}$ be sequences of non-negative real numbers, then:*

$$\sum_n a_n b_n \leq \left(\sum_n a_n^k \right)^{1/k} \left(\sum_n b_n^{k'} \right)^{1/k'} \quad \text{for } k > 1, \tag{A.2}$$

with equality iff either $a_n^k = c b_n^{k'}$ or $c a_n^k = b_n^{k'}$ for every n with a non-negative real c;

$$\sum_n a_n b_n \geq \left(\sum_n a_n^k \right)^{1/k} \left(\sum_n b_n^{k'} \right)^{1/k'} \quad \text{for } k < 1, \tag{A.3}$$

with equality iff either $a_n b_n = 0$, or $a_n^k = c b_n^{k'}$ for every n, with a positive real c.

We will also use the following well known result:

Lemma A.1: For any unit vector ψ,

$$\begin{aligned} \langle \psi, \rho^q \psi \rangle &\geq \langle \psi, \rho \psi \rangle^q, && \text{for } q > 1 \\ \langle \psi, \rho^q \psi \rangle &\leq \langle \psi, \rho \psi \rangle^q, && \text{for } 0 < q < 1 \end{aligned}.$$

In both inequalities there is equality if and only if $\rho\psi=\langle\psi,\rho\psi\rangle\psi$*, i.e., if* ψ *is an eigenvector of* ρ.

Proof: Let $\{P_m\}$ be a family of orthogonal projections with $\Sigma_m P_m=I$, and $\rho P_m=\rho_m P_m$, where $\{\rho_m\}$ are the distinct eigenvalues of ρ. Then, $tr(P_m)$ is the multiplicity of the eigenvalue ρ_m, and $\Sigma_m\langle\psi,P_m\psi\rangle=1$. The map $x\mapsto x^q$ is strictly convex (resp. strictly concave) on the unit interval for $q>1$ (resp. $0<q<1$); thus

$$\langle\psi,\rho^q\psi\rangle=\sum_m \rho_m^q\langle\psi,P_m\psi\rangle \underset{(\leqslant)}{\geqslant}\left(\sum_m \rho_m\langle\psi,P_m\psi\rangle\right)^q=\langle\psi,\rho\psi\rangle^q.$$

In both cases we have equality if and only if either all ρ_m are equal (as happens if ρ is the normalized trace in finite dimensions) or else $\langle\psi,P_m\psi\rangle=\delta_{m,m_o}$ for some m_o. In both cases, it follows that $\rho\psi=\rho_{m_o}\psi=\langle\psi,\rho\psi\rangle\psi$. □

A useful and immediate consequence of the equality condition of this result is that, since the eigenvalues of ρ lie in $[0,1]$: $tr(\rho^q)\leqslant(\text{ resp. }\geqslant)tr(\rho)=1$ for $q>1$ (resp. $0<q<1$); with equality iff ρ is a pure state ($\Leftrightarrow\rho^q=\rho$).

Lemma A.2: Suppose $\alpha^-\geqslant 0$. For every state ρ, one has:

1. For $q>1$,

$$\alpha^+\geqslant tr(\rho^q A)\geqslant\begin{cases}\{tr(A^{1/(1-q)})\}^{1-q}, & \text{if } \alpha^->0\\ 0, & \text{if } \alpha^-=0\end{cases}. \tag{A.4}$$

When $0<\alpha^+<\infty$*, there is equality on the l.h.s. iff* ρ *is a pure eigenstate of* A *to the eigenvalue* α^+*. When* $\alpha^->0$*, and* $tr(A^{1/(1-q)})$ *is finite, there is equality in the r.h.s. iff*

$$\rho=\frac{A^{1/(1-q)}}{tr(A^{1/(1-q)})}. \tag{A.5}$$

When $\alpha^-=0$*, there is equality on the r.h.s. iff* ρ *is an eigenstate of* A *to the eigenvalue* 0.

2. If $0<q<1$,

$$\alpha^-\leqslant tr(\rho^q A)\leqslant\{tr(A^{1/(1-q)})\}^{1-q}. \tag{A.6}$$

When $\mathrm{tr}(A^{1/(1-q)})$ *is finite, there is equality in the r.h.s. iff* ρ *is given by (A.5). When* $\alpha^-=0$ (resp. $\alpha^->0$) *there is equality on the l.h.s. iff* ρ *is an eigenstate (resp. pure eigenstate) to the eigenvalue* α^-.

We call the states such as (A.5) Hölder states because they saturate Hölder's inequality.

Proof:

1. Case $q>1$. Suppose that $\alpha^+<\infty$. We have $tr(\rho^q A)\leqslant\alpha^+ tr(\rho^q)\leqslant\alpha^+$. If $\alpha^+>0$, there is equality in the second inequality iff ρ is a pure state. But then there is also equality in the first inequality if ρ is a pure eigenstate to the eigenvalue α^+. If $\alpha^+=\infty$ there is nothing to prove.

Suppose $\alpha^-=0$; then, since $a_n\geqslant 0$, obviously $tr(\rho^q A)\geqslant 0$ with equality iff $\langle\psi_n,\rho^q\psi_n\rangle=0$ for every n with $a_n>0$. The latter condition is equivalent to $\langle\psi_n,\rho\psi_n\rangle=0$ for every n with $a_n>0$. This is equivalent to $tr(\rho A)=0$ which, with the variational characterization of the bottom of the spectrum, is equivalent to ρ being an eigenstate of A to the eigenvalue 0.

Suppose $\alpha^->0$; then Lemma A.1 and Hölder's inequality (A.3) with $k=1/q$ together with $a_n>0$, produces

$$tr(\rho^q A)\geqslant\sum_n a_n\langle\psi_n,\rho\psi_n\rangle^q\geqslant\left(\sum_n\langle\psi_n,\rho\psi_n\rangle\right)^q\left(\sum_n a_n^{1/(1-q)}\right)^{1-q}.$$

There is equality in the last inequality iff $\langle\psi_n,\rho\psi_n\rangle=ca_n^{1/(1-q)}$ for every n with $c>0$. But then, there is equality in the first inequality iff ρ is diagonal in the $\{\psi_n\}$ basis, that is $\langle\psi_n,\rho\psi_n\rangle=\rho_n=ca_n^{1/(1-q)}$.

If $\Sigma_n a_n^{1/(1-q)}$ is finite, then one can determine c by normalization to be $(\Sigma_n a_n^{1/(1-q)})^{-1}$ and obtain the assertions. If the sum is ∞, the r.h.s. of (A.4) which is 0 is not attained.

2. Case $0<q<1$. We have $tr(\rho^q A)\geqslant\alpha^- tr(\rho^q)\geqslant\alpha^-$. When $\alpha^->0$, there is equality in the last inequality iff ρ is a pure state; and also in the first inequality iff ρ is a pure eigenstate of A to the eigenvalue α^-. When $\alpha^-=0$, there is equality in the first inequality iff ρ is an eigenstate of A to the eigenvalue 0.

Applying Lemma A.1, and Hölder's inequality (A.2) with $k=1/q>1$, together with the assumption that $a_n\geqslant 0$, we get

$$tr(\rho^q A)\leqslant\sum_n a_n\langle\psi_n,\rho\psi_n\rangle^q\leqslant\left(\sum_n\langle\psi_n,\rho\psi_n\rangle\right)^q\left(\sum_n a_n^{1/(1-q)}\right)^{1-q}.$$

The rest of the claim can be got as in the case $q>1$. If $\Sigma_n a_n^{1/(1-q)}$ is ∞, then the r.h.s. of (A.6) which is ∞ is not attained. □

It is instructive to consider the case where A is the Hamiltonian of the harmonic oscillator with eigenvalues $a_n\propto n$. Here $\Sigma_n a_n^{1/(1-q)}=\infty$ if $0<q<1$ or $q\geqslant 2$; so the r.h.s. of (A.4) which is 0, and the r.h.s of (A.6) which is ∞, are not attained in these cases.

Having solved the case of a strictly positive A it is now easy to solve the general case as follows.

Proposition A.1: For $q>1$

$$\inf_\rho tr(\rho^q A)=\begin{cases}\{tr(A^{1/(1-q)})\}^{1-q}, & \text{if } \alpha^->0\\ \alpha^-, & \text{if } \alpha^-\leqslant 0\end{cases}.$$

If $\alpha^->0$ and $\mathrm{tr}(A^{1/(1-q)})$ is finite there is a unique minimizer, the Hölder state given by (A.5). If $\alpha^-=0$ (resp. $-\infty<\alpha^-<0$), then the minimizers are the eigenstates (resp. pure eigenstates) of A to the eigenvalue α^-.

$$\sup_\rho tr(\rho^q A)=\begin{cases}-\{tr((-A)^{1/(1-q)})\}^{1-q}, & \text{if } \alpha^+<0\\ \alpha^+, & \text{if } \alpha^+\geqslant 0\end{cases}.$$

If $\alpha^+<0$ and $\mathrm{tr}((-A)^{1/(1-q)})$ is finite, there is a unique maximizer, the Hölder state given by (A.5) with the positive operator $-A$. If $\alpha^+=0$ (resp. $0<\alpha^+<\infty$), then the maximizers are the eigenstates (resp. pure eigenstates) of A to the eigenvalue α^+.

We recall the definitions of the positive A_+ and negative A_- parts of the operator A: $A_\pm=\Sigma_n[(|a_n|\pm a_n)/2]|\psi_n\rangle\langle\psi_n|$. One has that both A_+ and A_- are non-negative, and $A=A_+-A_-$.

Proposition A.2: For $0<q<1$,

$$\inf_\rho tr\rho^q A)=\begin{cases}-\{tr((A_-)^{1/(1-q)})\}^{1-q}, & \text{if } \alpha^-<0\\ \alpha^-, & \text{if } \alpha^-\geqslant 0\end{cases}.$$

If $\alpha^-<0$ and $\mathrm{tr}((A_-)^{1/(1-q)})$ is finite, then there is a unique minimizer, the Hölder state given by (A.5) with A_-. If $\alpha^-=0$ (resp. $\alpha^->0$), the minimizers are the eigenstates (resp. pure eigenstates) of A to the eigenvalue α^-.

$$\sup_{\rho} tr(\rho^q A)=\begin{cases}\{tr((A_+)^{1/(1-q)})\}^{1-q}, & \text{if } \alpha^+>0\\ \alpha^+, & \text{if } \alpha^+\leqslant 0\end{cases}.$$

If $\alpha^+>0$ *and* $\mathrm{tr}((A_+)^{1/(1-q)})$ *is finite, then there is a unique maximizer, the Hölder state given by (A.5) with* A_+. *If* $\alpha^+=0$ (resp. $\alpha^+<0$) *the maximizers are the eigenstates (resp. pure eigenstates) of A to the eigenvalue* α^+.

Proof of the Propositions: Since $\sup_\rho tr(\rho^q A)=-\inf_\rho tr(\rho^q(-A))$, it suffices to prove the assertions for the infimum. In view of Lemma A.2, it remains only to consider the case $\alpha^-<0$. But then, letting A_- (resp. A_+) be the negative (resp. positive) part of the operator A, we have

$$\inf_{\rho} tr(\rho^q A)=\inf_{\{\rho:tr(\rho^q A_+)=0\}} tr(\rho^q(-A_-))=-\inf_{\{\rho:tr(\rho^q A_+)=0\}} tr(\rho^q A_-),$$

so that Lemma A.2, proves the statements after a careful and detailed analysis of the condition $tr(\rho^q A_+)=0$. □

We want to remark that in this variational problem we can have $\sup_\rho tr(\rho^q A)>\epsilon^+$ or $\inf_\rho tr(\rho^q A)<\epsilon^-$ because of the lack of affinity of the functional $tr(\rho^q A)$.

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Covariant quantum Markovian evolutions

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Quantum Markovian master equations with generally unbounded generators, having physically relevant symmetries, such as Weyl, Galilean or boost covariance, are characterized. It is proven in particular that a fully Galilean covariant zero spin Markovian evolution reduces to the free motion perturbed by a covariant stochastic process with independent stationary increments in the classical phase space. A general form of the boost covariant Markovian master equation is discussed and a formal dilation to the Langevin equation driven by quantum Boson noises is described. © *1996 American Institute of Physics.* [S0022-2488(96)01503-X]

I. INTRODUCTION

The classification of Galilean or Poincare covariant elementary systems is a cornerstone in the mathematical foundations of quantum mechanics.[1,2] The question of covariant irreversible evolutions (such as unstable particles) was also raised some time ago. However, in that case the answer remained far from being complete; essentially quasi-free dynamical semigroups, corresponding to Gaussian reservoirs were studied in detail (see Refs. 3 and 4 and the references therein).

In this paper we fill this gap by giving a complete characterization of Galilean covariant quantum Markovian evolutions (with zero spin). We prove in particular that in the case of the full Galilean covariance (Sec. III) these reduce to the free motion perturbed by a covariant stochastic process with stationary independent increments in the classical phase space. The reservoir of a Galilean covariant zero spin system is thus a classical noise, but not necessarily Gaussian: the variety of possible noises is described by the Levy–Khinchin formula. This result is based on the characterization of Weyl covariant dynamical semigroups given in Sec. II.

In the second part of this paper (Secs. IV and V) we consider much a broader class of evolutions, covariant only with respect to the Galilean boosts. The boost covariance is of fundamental importance as this is essentially the symmetry of particle motion in arbitrary potential field. In Sec. IV the general boost covariant Markovian master equation is discussed, based on a noncommutative generalization of the Levy–Khinchin formula obtained in Ref. 5, which is presented here in a more accessible form. Then in Sec. V the quantum Langevin equations are given, dilating this master equation with Boson quantum noise.

Being covariant with respect to noncompact symmetry groups, the generators of evolutions under consideration are, as a rule, unbounded operators. Existence and uniqueness of a dynamical semigroup with the generator given by a densely defined operator expression become nontrivial problems in this case. A recently developed framework for these problems, briefly outlined below (see also Appendix A), shifts the accent from the semigroup to the Markovian master equation it satisfies.

Let $\mathscr{B}(\mathscr{H})$ be the algebra of all bounded operators in a Hilbert space $\mathscr{H}$. By a *dynamical semigroup* in $\mathscr{B}(\mathscr{H})$ we shall call a semigroup Φ_t, $t\geqslant 0$, of normal completely positive maps in $\mathscr{B}(\mathscr{H})$, weak*-continuous, satisfying $\Phi_0=\mathrm{Id}$ [the identity map of $\mathscr{B}(\mathscr{H})$], and $\Phi_t[I]\leqslant I$ (the unit operator in $\mathscr{H}$). Here Φ_t is called *unital* if $\Phi_t[I]=I$. Let $\mathscr{T}(\mathscr{H})$ be the Banach space of trace-class operators in $\mathscr{H}$, so that $\mathscr{T}(\mathscr{H})^*=\mathscr{B}(\mathscr{H})$. There is a unique strongly continuous preadjoint semi-

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group $\Psi_t=(\Phi_t)_*$ in $\mathcal{T}(\mathcal{H})$, such that $\Psi_t{}^*=\Phi_t$. Denoting its generator $\mathcal{L}_*$ one has the differential equation

$$\frac{d}{dt}\,\mathrm{Tr}\,\rho\Phi_t[X]=\mathrm{Tr}\,\mathcal{L}_*[\rho]\Phi_t[X],\quad X\in\mathcal{B}(\mathcal{H}). \tag{1.1}$$

If ρ runs through $\mathrm{dom}\,\mathcal{L}_*\subset\mathcal{T}(\mathcal{H})$, then this equation determines Φ_t uniquely. However, in applications $\mathcal{L}_*$ is usually given only on a dense subspace D. Typically a dense domain $\mathcal{D}\subset\mathcal{H}$ is given and

$$\mathsf{D}=\mathrm{lin}\{\rho:\rho=|\phi\rangle\langle\psi|,\quad \phi,\psi\in\mathcal{D}\}, \tag{1.2}$$

while $\mathcal{L}_*$ is defined by an expression of the *standard form*:

$$\mathcal{L}_*[\rho]=\sum_i |L_j\phi\rangle\langle L_j\psi|-|K\phi\rangle\langle\psi|-|\phi\rangle\langle K\psi|,\quad \rho=|\phi\rangle\langle\psi|, \tag{1.3}$$

where L_j, K are operators defined on $\mathcal{D}$ (or by similar expression with the sum replaced by an integral). The *dissipativity condition*

$$\sum_j \|L_j\psi\|^2\leqslant 2\,\mathrm{Re}\langle\psi|K\psi\rangle,\quad \psi\in\mathcal{D}, \tag{1.4}$$

is assumed (implying in particular that K is accretive: $\mathrm{Re}\langle\psi|K\psi\rangle\geqslant 0$, $\psi\in\mathcal{D}$). Equation (1.1) then reduces to the equation for the matrix elements of $\Phi_t[X]$:

$$\frac{d}{dt}\,\langle\psi|\Phi_t[X]\phi\rangle=\mathcal{L}(\psi;\Phi_t[X],\phi);\quad \phi,\psi\in\mathcal{D}, \tag{1.5}$$

where

$$\mathcal{L}(\psi;X;\phi)=\mathrm{Tr}\,\mathcal{L}_*[|\phi\rangle\langle\psi|]X=\sum_j \langle L_j\psi|XL_j\phi\rangle-\langle K\psi|X\phi\rangle-\langle\psi|XK\phi\rangle \tag{1.6}$$

is the *form-generator*.[6,7] We call (1.5) the *(backward) Markovian master equation*.

If D is a core for $\mathcal{L}_*$, then this equation determines Φ_t uniquely, otherwise it may have a nonunique solution. Of special interest is the case of a *unital* generator, satisfying $\mathrm{Tr}\,\mathcal{L}_*[\psi\rangle\langle\phi|]\equiv 0$ or

$$\sum_j \|L_j\psi\|^2=2\,\mathrm{Re}\langle\psi|K\psi\rangle,\quad \psi\in\mathcal{D}. \tag{1.7}$$

Then under the condition that K is maximal accretive and $\mathcal{D}$ is an invariant domain for e^{-Kt}, $t\geqslant 0$, there exists a dynamical semigroup $\Phi_t{}^\infty$ giving the *minimal solution* of Eq. (1.5) in the sense that for any other solution Φ_t the difference $\Phi_t-\Phi_t{}^\infty$ is completely positive (see Appendix A). In general $\Phi_t{}^\infty$ may not be unital; however, if it is, then $\Phi_t{}^\infty$ is the unique solution of (1.5).[8–10]

Under the additional assumption that operators L_j^*, K^* are defined on a dense domain $\mathcal{D}^*$, and

$$\sum_j \|L_j^*\psi\|^2<\infty,\quad \psi\in\mathcal{D}^*, \tag{1.8}$$

one can write also the *forward* Markovian master equation for the preadjoint semigroup Ψ_t:

$$\frac{d}{dt}\langle\phi|\Psi_t[\rho]\psi\rangle=\mathscr{L}_*(\phi;\Psi_t[\rho];\psi),\quad \phi,\psi\in\mathscr{D}^*, \tag{1.9}$$

where

$$\mathscr{L}_*(\phi;\rho;\psi)=\mathrm{Tr}\ \rho\mathscr{L}[|\psi\rangle\langle\phi|]=\sum_j\langle L_j^*\phi|\rho L_j^*\psi\rangle-\langle K^*\phi|\rho\psi\rangle-\langle\phi|\rho K^*\psi\rangle. \tag{1.10}$$

Here $\mathscr{L}$ denotes the generator of the semigroup Φ_t. Assuming K^* to be maximal accretive and $\mathscr{D}^*$ to be an invariant domain for e^{-K^*t}, $t\geqslant 0$, we can prove that $\Psi_t^\infty=(\Phi_t^{\ \infty})_*$ is the minimal solution of the forward equation (see Appendix A). Thus the situation is similar to that for the Kolmogorov–Feller differential equations in the theory of Markov processes.[11] If Φ_t^∞ is not unital, then there is a positive probability of ''explosion,'' i.e., exit from the phase space for the corresponding Markov process. Additional ''boundary conditions'' are required to specify the solution, which amounts to a certain maximal extension of $\mathscr{L}_*$ from D.

From the results in Secs. II and III it follows in particular that an explosion can never occur for the fully Galilean covariant Markovian evolutions. However, this is possible for the boost covariant evolutions potentially interesting for applications. The mathematical study of these is far from being complete; the presentation in Secs. IV and V is thus on a formal level, and we only outline a few rigorous results and a number of problems waiting for their mathematical solutions.

II. WEYL COVARIANT DYNAMICAL SEMIGROUPS

Let Z be a finite-dimensional symplectic space with a nondegenerate symplectic form $\Delta(z,z')$ and let $z\to W(z)$ be an irreducible representation of the Weyl–Segal CCR:

$$W(z)W(z')=\exp\ i\Delta(z,z')W(z')W(z) \tag{2.1}$$

in a Hilbert space $\mathscr{H}$.

Proposition 1: A dynamical semigroup Φ_t in $\mathscr{B}(\mathscr{H})$ is Weyl covariant,

$$\Phi_t[W(z)^*XW(z)]=W(z)^*\Phi_t[X]W(z),\quad z\in Z, \tag{2.2}$$

if and only if

$$\Phi_t[W(z)]=W(z)e^{tl(z)}, \tag{2.3}$$

where $l(z)$ is a continuous conditionally positive definite function satisfying $l(0)\leqslant 0$.

Proof: By weak*-continuity the semigroup Φ_t is uniquely defined by the values of $\Phi_t[W(z)]$, $z\in Z$. From (2.2) and (2.1) $\Phi_t[W(z')]$ satisfies the same relation (2.1) as $W(z')$, hence $\Phi_t[W(z')]W(z')^*$ commutes with $W(z)$, $z\in Z$. Since the representation $z\to W(z)$ is irreducible,

$$\Phi_t[W(z)]=W(z)\phi_t(z),$$

where $\phi_t(z)$ is a complex function. From the definition of dynamical semigroup, it is continuous in t, z and satisfies $\phi_{t+s}(z)=\phi_t(z)\phi_s(z)$, $\phi_0(z)=1$, $\phi_t(0)\leqslant 1$. Hence $\phi_t(z)=\exp tl(z)$, with $l(z)$ continuous and $l(0)\leqslant 0$. From complete positivity of Φ_t it follows[12,13] that $\phi_t(z)$ is positive definite in z for all $t\geqslant 0$. Indeed for any finite collections $\{z_j\}\subset Z$, $\{c_j\}\subset\mathbf{C}$,

$$\sum_{j,k}\overline{c}_j c_k\phi_t(z_j-z_k)=\sum_{j,k}\overline{c}_j c_k\langle W(z_j)\psi|\Phi_t[W(z_j)W(z_k)^*]W(z_k)\psi\rangle\geqslant 0,$$

where $\psi\in\mathscr{H}$ is arbitrary unit vector. Then by a theorem of Schoenberg $l(z)$ is conditionally positive definite.

Conversely, let the operator $\Phi_t[W(z)]$ be defined by (2.3). There exists a stochastic process ζ_t, $t\geqslant 0$, with stationary independent increments in Z, having the characteristic function

$$\mathbf{M}e^{i\Delta(z,\zeta_t)}=e^{t(l(z)-l(0))} \tag{2.4}$$

(see, e.g., Refs. 11 and 14). Then for all $X\in\mathscr{B}(\mathscr{H})$

$$\Phi_t[X]=\mathbf{M}W(\zeta_t)^*XW(\zeta_t)e^{tl(0)}, \tag{2.5}$$

since for $X=W(z)$ this follows from (2.1) and (2.4), and then can be extended by weak*-continuity. One easily sees that the right-hand side defines Weyl-covariant dynamical semigroup; in particular the semigroup property follows from the fact that ζ_t has stationary independent increments. □

Obviously Φ_t is unital if and only if $l(0)=0$. In this case the relation (2.5) gives a dilation of the Markovian evolution Φ_t to the unitary stochastic evolution

$$X\to X(t)=W(\zeta_t)^*XW(\zeta_t). \tag{2.6}$$

Defining the canonical observables $R(z)$ as self-adjoint operators, linearly depending on z, and satisfying $W(z)=\exp iR(z)$, one has from (2.6) $R(z;t)=R(z)+\Delta(z,\zeta_t)I$. This is equivalent to the Langevin–Heisenberg equation

$$dR(z;t)=\Delta(z,d\zeta_t)I,\quad R(z;0)=R(z), \tag{2.7}$$

which due to (2.1) can be viewed as an infinitesimal canonical transformation implemented by the interaction Hamiltonian $dH_{int}=-R(d\zeta_t)$.

Let us describe the general master and Langevin equations for the evolution (2.5). By the multidimensional Levy–Khinchin formula[11,14]

$$l(z)-l(0)=i\beta(z)-\frac{1}{2}\,\alpha(z)+\int_{z'\neq 0}[e^{i\Delta(z,z')}-1-i\Delta(z,z')1_\epsilon(z')]\nu(dz'), \tag{2.8}$$

where $\beta(z)$ is real linear, $\alpha(z)$ is non-negative quadratic function on Z, and $\nu(dz)$ is positive Levy measure on $Z\backslash\{0\}$ satisfying

$$\int_{z\neq 0}[1_\epsilon(z)|z|^2+(1-1_\epsilon(z))]\nu(dz)<\infty. \tag{2.9}$$

Here $1_\epsilon(z)$ is the indicator of the set $|z|<\epsilon$ for some fixed norm $|\cdot|$ in Z, and $\epsilon>0$. One has

$$\beta(z)=\Delta(z,z_0),\quad \alpha(z)=\sum_{j=1}^{r}\Delta(z,z_j)^2, \tag{2.10}$$

where $z_0\in Z$, $\{z_j\}$ is a linearly independent system in Z, $r\leqslant\dim Z$. The process ζ_t has the Ito representation[14]

$$d\zeta_t=d\zeta_t^c+\int_{z\neq 0}z1_\epsilon(z)\tilde{\Pi}(dzdt)+\int z[1-1_\epsilon(z)]\Pi(dzdt), \tag{2.11}$$

where ζ_t^c is the Wiener process in Z with the moments

$$\mathbf{M}\Delta(z,\zeta_t^c)=\beta(z)dt, \quad \mathbf{D}\Delta(z,\zeta_t^c)=\alpha(z)dt,$$

$\Pi(dzdt)$ is the Poisson random measure such that

$$\mathbf{M}\Pi(dzdt)=\nu(dz)dt,$$

and $\widetilde{\Pi}(dzdt)=\Pi(dzdt)-\nu(dz)dt$ is the compensated Poisson random measure. Formula (2.11) gives the decomposition of ζ_t into the continuous, "small-jumps" and "big-jumps" components, the stochastic integral for small jumps (of magnitudes $|z|<\epsilon$) converging in the mean-square sense, while for big jumps converges pathwise, via the condition (2.9).

Consider the domain

$$\mathscr{D}=\bigcap_{z\in Z}\ \mathrm{dom}\ R(z)^2.$$

Then $\mathscr{D}$ is a dense domain in $\mathscr{H}$, invariant under $W(z)$. Let D be defined by (1.2) with this domain $\mathscr{D}$.

Proposition 2: The dynamical semigroup (2.5) is the unique solution of the Markovian master equation (1.5) with

$$\mathscr{L}_*[\rho]=l(0)\rho+i[R(z_0),\rho]-\frac{1}{2}\sum_{j=1}^{r}[R(z_j),[R(z_j),\rho]]$$
$$+\int_{z'\neq 0}(W(z')\rho W(z')^*-\rho-i[R(z'),\rho]1_\epsilon(z'))\,\nu(dz') \tag{2.12}$$

for $\rho\in\mathsf{D}$. The domain D is a core for $\mathscr{L}_*$, and Φ_t is unital if and only if $\mathscr{L}_*$ is such.

The random density operator

$$\rho(t)=W(\zeta_t)\rho W(\zeta_t)^*e^{tl(0)}, \quad \rho\in\mathsf{D}, \tag{2.13}$$

satisfies the Langevin–Schroedinger equation

$$d\rho(t)=i[R(d\zeta_t^c),\rho(t)]+\int_{z'\neq 0}(W(z')\rho(t)W(z')^*-\rho(t))\widetilde{\Pi}(dz'dt)+\mathscr{L}_*[\rho(t)]dt, \tag{2.14}$$

understood as stochastic equation in the weak operator topology.

Proof: From (2.3)

$$\frac{d}{dt}\,\mathrm{Tr}\ \rho\Phi_t[W(z)]=l(z)\mathrm{Tr}\ \rho\Phi_t[W(z)], \quad \rho\in\mathrm{dom}\ \mathscr{L}_*,$$

where

$$\mathrm{Tr}\ \mathscr{L}_*[\rho]W(z)=l(z)\mathrm{Tr}\ \rho W(z).$$

For $\rho\in\mathsf{D}$

$$\Delta(z,z')\mathrm{Tr}\ \rho W(z)=\mathrm{Tr}[R(z'),\rho]W(z) \tag{2.15}$$

(see Ref. 15), hence also

$$\Delta(z,z')^2\ \mathrm{Tr}\ \rho W(z)=\mathrm{Tr}[R(z'),[R(z'),\rho]]W(z'). \tag{2.16}$$

By using (2.8), (2.9), and (2.1) we obtain (2.12).

To show that D is a core for $\mathscr{L}_*$, we remark that $\rho\in\mathsf{D}$ implies $\rho(t)\in\mathsf{D}$, since D is invariant under the Weyl automorphisms $\rho\to W(z)\rho W(z)^*$. Assuming that D is not a core for $\mathscr{L}_*$, we can find $\lambda_0>0$ such that $(\lambda_0\,\mathrm{Id}-\mathscr{L}_*)(\mathsf{D})$ is not dense in $\mathscr{T}(\mathscr{H})$ (see Ref. 16, theorem X.49). Then there exists $X_0\in\mathscr{B}(\mathscr{H})$, $X_0\neq 0$, such that $\mathrm{Tr}(\lambda_0\rho(t)-\mathscr{L}_*[\rho(t)])X_0=0$. From (2.5) and (1.1)

$$\frac{d}{dt}\,\mathrm{Tr}\,\rho\Phi_t[X]=\mathrm{Tr}\,\rho\Phi_t[\mathscr{L}[X]]=\mathbf{M}\,\mathrm{Tr}\,\rho W(\zeta_t)^*\mathscr{L}[X]W(\zeta_t)e^{tl(0)}$$

$$=\mathbf{M}\,\mathrm{Tr}\,\rho(t)\mathscr{L}[X]=\mathbf{M}\,\mathrm{Tr}\,\mathscr{L}_*[\rho(t)]X$$

for $X\in\mathrm{dom}\,\mathscr{L}$ and $\rho\in\mathsf{D}$. Integrating,

$$\mathrm{Tr}\,\rho\Phi_t[X]-\mathrm{Tr}\,\rho X=\int_0^t\mathbf{M}\,\mathrm{Tr}\,\mathscr{L}_*[\rho(s)]X\,ds$$

for $X\in\mathsf{D}$ and hence for all $X\in\mathscr{B}(\mathscr{H})$ by weak*-continuity. Taking $X=X_0$, we obtain

$$\mathrm{Tr}\,\rho\Phi_t[X_0]=e^{\lambda_0 t}\,\mathrm{Tr}\,\rho X_0,\quad \rho\in\mathsf{D},$$

which contradicts the contraction property of Φ_t. Thus D is a core for $\mathscr{L}_*$.

It is sufficient to establish the relation (2.14) for $\rho=|\psi\rangle\langle\psi|$, $\psi\in\mathscr{D}$. Then $\rho_t=|\psi_t\rangle\langle\psi_t|$, where $\psi_t=\exp\frac{1}{2}[tl(0)+i\int_0^t\Delta(\zeta_s,d\zeta_s)]W(\zeta_t)\psi$. The vector ψ_t satisfies the following exponential stochastic differential equation

$$d\psi_t=\left\{iR(d\zeta_t^c)+\int_{z\neq 0}(W(z)-I)\tilde{\Pi}(dz\,dt)\right.$$

$$\left.+\left[\frac{1}{2}\left(l(0)I-\sum_{j=1}^r R(z_j)^2\right)+\int_{z\neq 0}(W(z)-I-iR(z)1_\epsilon(z))\nu(dz)\right]dt\right\}\psi_t. \qquad (2.17)$$

To prove this formula we can use a concrete form of the CCR, e.g., the so-called regular representation in the space $L^2(Z)$:

$$W(z')\psi(z)=\psi(z+z')\exp\frac{i}{2}\,\Delta(z,z'),$$

$$R(z')\psi(z)=[-i\nabla(z')+\tfrac{1}{2}\Delta(z,z')]\psi(z).$$

Then

$$\psi_t(z)=\psi(z+\zeta_t)\exp\frac{1}{2}\left[tl(0)+i\int_0^t\Delta(z+\zeta_s,d\zeta_s)\right].$$

By using the Ito formula[14] one arrives at (2.17). Then the stochastic equation (2.14) for the matrix elements $\langle\psi|\rho(t)\phi\rangle=\langle\psi|\psi_t\rangle\langle\psi_t|\phi\rangle$ follows from (2.17) by application of the Ito product rule.

Apparently unitality of the generator (2.12) implies unitality of Φ_t, since both are equivalent to $l(0)=0$. □

The Langevin equation (2.14) gives the dilation of the dynamical semigroup Φ_t with the classical Wiener process and Poisson random measure as the driving noises. The structure of the generator (2.12) is in formal agreement with a result of Ref. 17, in which finite-dimensional

dynamical semigroups admitting dilation with a classical noise were described. It was shown there that the generator of such semigroup is a sum of ''Gaussian'' and ''Poissonian'' terms

$$[L,\,[L,\,X]],\quad V^*XV-X,$$

where L is Hermitean and V is unitary operator. In our case we have unbounded self-adjoint operators in the ''Gaussian'' part and the sum of ''Poissonian'' terms is replaced by integral over all possible magnitudes of jumps. Also the ''small-jumps'' correction [the commutator term under the integral in (2.12)] is peculiar to the infinite-dimensional case.

The generator (2.12) has the standard form since it can be represented as

$$\mathscr{L}_*[\rho]=l(0)\rho+\sum_{j=1}^{r} R(z_j)\rho R(z_j)+\int_{z\neq 0}[W(z)-1_\epsilon(z)I]\rho[W(z)-1_\epsilon(z)I]^*\nu(dz)-K\rho-\rho K^*,$$

where

$$K=\frac{1}{2}\sum_{j=1}^{r} R(z_j)^2+\int_{z\neq 0}\left\{1_\epsilon(z)[I-W(z)+iR(z)]+[1-1_\epsilon(z)]\,\frac{I}{2}\right\}\nu(dz).$$

From these formulas one sees that the analog of condition (1.8) holds with $\mathscr{D}^*=\mathscr{D}$. Thus $\Psi_t=(\Phi_t)_*$ is the unique solution of the forward Markovian master equation (1.9) with

$$\mathscr{L}[X]=l(0)X+i[X,R(z_0)]-\frac{1}{2}\sum_{j=1}^{r}[[X,\,R(z_j)],R(z_j)]$$

$$+\int_{z\neq 0}\{W(z)^*XW(z)-X-i[X,\,R(z)]1_\epsilon(z)\}\nu(dz).$$

III. GALILEAN COVARIANT EVOLUTIONS

Let (ξ,τ), $\xi\in\mathbf{R}^3$, $\tau\in\mathbf{R}$, be a point in the four-dimensional nonrelativistic space–time, and let $(x,v,R,t):(\xi,\tau)\to(\xi',\tau')$ be the Galilei transformation

$$\xi'=R\xi+x+v\tau,\quad \tau'=\tau+t, \tag{3.1}$$

where $x\in\mathbf{R}^3$ is the space shift of the reference system, $v\in\mathbf{R}^3$ is the Galilean boost, R is the matrix of rotation in $\mathbf{R}^3$, and $t\in\mathbf{R}$ is the time shift. The Galilean covariant elementary quantum system is given by an irreducible projective unitary representation $(x,v,R,t)\to U(x,v,R,t)$ of the group of transformations (3.1), satisfying

$$U(x_1,v_1,R_1,t_1)U(x_2,v_2,R_2,t_2)=\exp\frac{im}{2}\,(v_1\cdot R_1x_2-x_1\cdot R_1v_2-t_2v_1\cdot R_1v_2)$$

$$\times U(R_1x_2+x_1+t_2v_1,R_1v_2+v_1,R_1R_2,t_1+t_2), \tag{3.2}$$

where m is the mass constant.[1,2] In particular, the kinematics is described by the unitary representations

$$(x,v)\to W_{x,v}=U(x,v,E,0),\quad R\to U_R=U(0,0,R,0),$$

where E is the unit matrix, $W_{x,v}$ is projective representation of $\mathbf{R}^3\times\mathbf{R}^3$, satisfying the Weyl commutation relation

$$W_{x_1,v_1}W_{x_2,v_2}=\exp\, im(v_1\cdot x_2-x_1\cdot v_2)W_{x_2,v_2}W_{x_1,v_1}, \tag{3.3}$$

and U_R is a unitary representation of the rotation group, satisfying

$$U_R W_{x,v}=W_{Rx,Rv}U_R\,. \tag{3.4}$$

The reversible dynamics is given by the one-parameter unitary group $t\to U_t=U(0,0,E,-t)$, satisfying

$$W_{x,v}U_t=U_t W_{x-vt,v}\,, \tag{3.5}$$

$$U_R U_t=U_t U_R\,. \tag{3.6}$$

Restricting to the case of zero-spin elementary system, we assume that the representation $W_{x,v}$ is irreducible. The well-known solution of (3.3)–(3.6) is

$$W_{x,v}=\exp\, i(mv\cdot Q-x\cdot P), \tag{3.7}$$

$$U_t=\exp\left(-it\,\frac{|P|^2}{2m}\right), \tag{3.8}$$

where $Q=(Q_1,Q_2,Q_3)$, $P=(P_1,P_2,P_3)$ are canonical position and momentum observables.

Turning to the Markovian dynamics, we assume, following Ref. 3, that it is described by a dynamical semigroup Φ_t, $t\geqslant 0$ in $\mathscr{B}(\mathscr{H})$. Then the covariance conditions (3.5) and (3.6) are replaced by

$$\Phi_t[W_{x,v}^* X W_{x,v}]=W_{x-vt,v}^*\Phi_t[X]W_{x-vt,v}\,, \tag{3.9}$$

$$\Phi_t[U_R^* X U_R]=U_R^*\Phi_t[X]U_R\,. \tag{3.10}$$

Let $\mathscr{L}_*$ be the generator of the preadjoint semigroup $(\Phi_t)_*$. Let $\mathscr{D}\subset\mathscr{H}$ be the dense domain

$$\mathscr{D}=\bigcap_{x,v\in\mathbf{R}^3}\mathrm{dom}(mv\cdot Q-x\cdot P)^2, \tag{3.11}$$

and let $\mathsf{D}\subset\mathscr{B}(\mathscr{H})$ be the domain defined by the relation (1.2).

Theorem: Let Φ_t be a dynamical semigroup satisfying the covariance conditions (3.9) and (3.10), and assume $\mathsf{D}\subset\mathrm{dom}\,\mathscr{L}_*$. Then

$$\Phi_t[W_{x,v}]=W_{x-vt,v}\,\exp\int_0^t l(x-vs,v)\,ds, \tag{3.12}$$

where

$$l(x,v)=l_0-\frac{1}{2}\,(\alpha_{PP}|x|^2+2\alpha_{PQ}mx\cdot v+\alpha_{QQ}m^2|v|^2)$$
$$+\int\int_{|x|^2+|y|^2>0}[e^{im(x\cdot v'-v\cdot x')}-1]\nu(dx'dv')\}. \tag{3.13}$$

Here $l_0\leqslant 0$, the real 2×2 matrix $[\begin{smallmatrix}\alpha_{PP} & \alpha_{PQ}\\ \alpha_{PQ} & \alpha_{QQ}\end{smallmatrix}]$ is positive definite and ν is a positive measure on $\mathbf{R}^3\times\mathbf{R}^3\backslash\{0\}$, satisfying the Levy condition

$$\int \int_{0<|x|^2+|v|^2<\epsilon} (|x|^2+|v|^2)\,\nu(dxdv)+\int \int_{\epsilon\leqslant|x|^2+|v|^2} \nu(dxdv)<\infty, \tag{3.14}$$

and invariant in the sense $\nu((Rdx)(Rdy))=\nu(dxdy)$ for all rotations R. [The integration in (3.13) should be taken first over the spheres $|x|=r_1$, $|v|=r_2$, and then with respect to r_1,r_2.]

This semigroup is the unique solution of the Markovian master equation (1.5) with

$$\mathscr{L}_*[\rho]=l_0\rho-i\left[\frac{|P|^2}{2m},\rho\right]-\frac{1}{2}\sum_{j=1}^{3}\{\alpha_{PP}[P_j,[P_j,\rho]]+2\alpha_{PQ}[P_j,[Q_j,\rho]]+\alpha_{QQ}[Q_j,[Q_j,\rho]]\}$$

$$+\int \int_{|x|^2+|v|^2>0}\{W_{x,v}\rho W_{x,v}^*-\rho\}\,\nu(dxdv), \tag{3.15}$$

Moreover D is a core for $\mathscr{L}_*$, and Φ_t is unital if and only if $\mathscr{L}_*$ is such.

Proof: From the covariance relation (3.9) and irreducibility of $W_{x,v}$ it follows as in the proof of Proposition 1

$$\Phi_t[W_{x,v}]=W_{x-vt,v}\,\phi_t(x,v),$$

where $\phi_t(x,v)$ is a continuous function. The semigroup property implies (cf. Ref. 13)

$$\phi_{t+s}(x,v)=\phi_s(x-vt,v)\,\phi_t(x,v). \tag{3.16}$$

From the assumption $\mathsf{D}\subset\mathrm{dom}\,\mathscr{L}_*$ it follows that

$$\phi_t(x,v)=\langle\phi|\Phi_t[W_{x,v}]\psi\rangle\langle\phi|W_{x-vt,v}\psi\rangle^{-1},\quad \phi,\psi\in\mathscr{D},$$

is differentiable with respect to t; the relation (3.16) then implies

$$\frac{d}{dt}\,\phi_t(x,v)=l(x-vt,v)\,\phi_t(x,v),$$

where $l(x,v)=(d/dt)\,\phi_t(x,v)|_{t=0}$, whence (3.12) follows.

On the other hand, differentiating (3.9) at $t=0$, we have for $\rho\in\mathsf{D}$

$$W_{x,v}^*\mathscr{L}_*[W_{x,v}\rho W_{x,v}^*]W_{x,v}=\mathscr{L}_*[\rho]+i[v\cdot P,\rho]. \tag{3.17}$$

This is an inhomogeneous linear equation with respect to $\mathscr{L}_*$, thus we can write

$$\mathscr{L}_*[\rho]=\mathscr{L}_*^0[\rho]-i\left[\frac{|P|^2}{2m},\,\rho\right], \tag{3.18}$$

where the second term is the generator of the free particle motion, giving a particular solution of (3.17), and $\mathscr{L}_*^0$ is the general solution of the homogeneous equation

$$W_{x,v}^*\mathscr{L}_*^0[W_{x,v}\rho W_{x,v}^*]W_{x,v}=\mathscr{L}_*^0[\rho], \tag{3.19}$$

expressing Weyl covariance of $\mathscr{L}_*^0$. Applying proposition 2 [relation (2.12) for a Weyl covariant generator] and using rotational covariance (3.10) results in the expression (3.13), where $l_0=l(0,0)$ (single commutator terms disappear due to rotational covariance, provided the order of integration is as stated in the theorem). From (3.12) and (3.17),

$$\mathrm{Tr}\;\mathscr{L}_*^0[\rho]W_{x,v}=l(x,v)\mathrm{Tr}\;\rho,$$

where (3.15) follows, taking into account (3.3) and (2.16).

We now describe a stochastic dilation of the semigroup Φ_t. Let $\binom{\xi_t}{\eta_t}$ be a classical stochastic process with stationary independent increments in $\mathbf{R}^3\times\mathbf{R}^3$, defined by the characteristic function

$$\mathbf{M}\ \exp\, i(mv\cdot\xi_t - x\cdot\eta_t) = \exp\, t(l(x,v)-l_0).$$

Consider the stochastic differential equations

$$dQ_t = \frac{P_t}{m}\,dt + d\xi_t, \quad dP_t = d\eta_t, \tag{3.20}$$

with initial conditions $Q_0 = Q$ and $P_0 = P$. The solution of these equations

$$Q_t = Q + \frac{Pt}{m} + \xi_t + \frac{1}{m}\int_0^t \eta_s\,ds, \quad P_t = P + \eta_t. \tag{3.21}$$

We define stochastic unitary operators

$$U_t(\xi,\eta) = W_{(\xi_t+(1/m)\int_0^t \eta_s ds),\,\eta t/m} U_t = U\left(\xi_t + \frac{1}{m}\int_0^t (\eta_s-\eta_t)ds,\ \frac{\eta_t}{m}, E, -t\right),$$

so that $U_t(\xi,\eta)^*\binom{Q}{P}U_t(\xi_t,\eta) = \binom{Q_t}{P_t}$, and prove that

$$\Phi_t[X] = \mathbf{M}U_t(\xi,\eta)^* X U_t(\xi,\eta)e^{tl_0}. \tag{3.22}$$

It is sufficient to establish this for $X = W_{x,v}$. Then

$$U_t(\xi,\eta)^* W_{x,v} U_t(\xi,\eta) = \exp\, i(mv\cdot Q_t - x\cdot P_t) = W_{x-vt,v}\ \exp\, i\left[mv\cdot\left(\xi_t + \frac{1}{m}\int_0^t \eta_s\,ds\right) - x\cdot\eta_t\right].$$

However,

$$\mathbf{M}\ \exp\, i\left[mv\cdot\left(\xi_t + \frac{1}{m}\int_0^t \eta_s\,ds\right) - x\cdot\eta_t\right]e^{tl_0} = \mathbf{M}\ \exp\, i\int_0^t [mv\cdot d\xi_s - (x-(v(t-s))\cdot d\eta_s)]e^{tl_0}$$

$$= \exp\int_0^t l(x-v(t-s),v)ds = \phi_t(x,v),$$

and the relation (3.22) follows from (3.12).

To prove that D is a core for $\mathscr{L}_*$, we observe that $\mathscr{D}$ is invariant under $U(x,v,R,t)$ and hence under $U_t(\xi,\eta)$. Then the rest can be proved as in proposition 2. □

The equations (3.20) are the Langevin–Heisenberg equations for the canonical observables P,Q. They can be interpreted as infinitesimal canonical transformation implemented by the Hamiltonian

$$dH_t = \frac{|P|^2}{2m}\,dt + P\cdot d\xi_t - Q\cdot d\eta_t.$$

The random density operator

$$\rho(t) = U_t(\xi,\eta)\rho U_t(\xi,\eta)^* e^{tl_0}$$

satisfies the Langevin–Schroedinger equation similar to (2.14).

IV. BOOST COVARIANT MARKOVIAN MASTER EQUATIONS

If we abandon covariance with respect to space shifts and rotations, we are left with the *boost covariance*, the condition obtained from (3.9) by putting $x=0$:

$$\Phi_t[V_v^* X V_v] = V_v^* U_{-vt}^* \Phi_t[X] U_{-vt} V_v , \tag{4.1}$$

where

$$v \to V_v = \exp(imv\cdot Q), \quad x \to U_x = \exp(-ix\cdot P) \tag{4.2}$$

are the unitary representations of the shifts in velocity and position, respectively. The generator $\mathscr{L}$ of the semigroup Φ_t satisfies the equation [the following formal calculation can be made precise by using the form-generator (1.6) with the appropriate domain $\mathscr{D}$]

$$V_v \mathscr{L}[V_v^* X V_v] V_v^* = \mathscr{L}[X] + i[v\cdot P, X]. \tag{4.3}$$

The general solution of this equation

$$\mathscr{L}[X] = \mathscr{L}^0[X] + i[H, X], \tag{4.4}$$

where $H = |P|^2/2m + \beta\cdot P + \tilde{\mathscr{U}}(Q)$, $\tilde{\mathscr{U}}(Q)$ being a real function, and $\mathscr{L}^0$ is a solution of the homogeneous equation

$$V_v \mathscr{L}^0[V_v^* X V_v] V_v^* = \mathscr{L}^0[X]. \tag{4.5}$$

By making a gauge transformation we replace $P + m\beta$ with P, so that

$$H = \frac{|P|^2}{2m} + \mathscr{U}(Q), \tag{4.6}$$

where $\mathscr{U}(\cdot)$ is again a real function.

The mathematical study of Eq. (4.5), under the regularity assumption that an analog of the conditions (1.7) and (1.8) holds with $\mathscr{D}^* = \mathscr{D} = C_0^2(\mathbf{R}^3)$ in the Schroedinger representation, is presented in Ref. 5. The main tool of this study is harmonic analysis of operator-valued cocycles of the symmetry group. The general solution has the Levy–Khinchin structure similar to (2.12):

$$\mathscr{L}^0[X] = K_0(Q)\circ X + \mathscr{L}^1[X] + \mathscr{L}^2[X] + \mathscr{L}^3[X], \tag{4.7a}$$

where $K_0(\cdot)$ is a nonpositive function (vanishing for a unital generator), $\circ$ means the Jordan product, and $\mathscr{L}^1$, $\mathscr{L}^2$, $\mathscr{L}^3$ are ''continuous,'' ''big-jumps,'' and ''small-jumps'' components, respectively. The continuous component is

$$\mathscr{L}^1[X] = \sum_{k=1}^{r} (\tilde{P}_k + L_k(Q))^* X (\tilde{P}_k + L_k(Q)) - K_1^* X - X K_1 , \tag{4.7b}$$

where $r \leqslant 3$, $\tilde{P}_k = \Sigma_{j=1}^3 \beta_{kj} P_j$ ($\beta_{kj} \in \mathbf{R}$), $L_k(\cdot)$ are complex functions, and

$$K_1 = \frac{1}{2} \sum_{k=1}^{r} (\tilde{P}_k^2 + 2\tilde{P}_k L_k(Q) + |L_k(Q)|^2). \tag{4.8a}$$

The essential ingredient of the discontinuous components are a positive Levy measure $\mu(dx)$ on $\mathbf{R}^3$, and a family of complex functions $L_{jx}(\cdot)$; $j=1,2,...$; $x\in\mathbf{R}^3$, satisfying

$$\int_{\mathbf{R}^3}\sum_j |L_{jx}(\cdot)|^2\mu(dx)<\infty. \tag{4.9}$$

The simpler big-jumps component has the form

$$\mathscr{L}^2[X]=\int_{\epsilon\leqslant|x|}\sum_j L_{jx}(Q)^*U_x^*XU_xL_{jx}(Q)-K_2\circ X, \tag{4.7c}$$

where

$$K_2=\frac{1}{2}\int_{\epsilon\leqslant|x|}\sum_j |L_{jx}(Q)|^2\mu(dx), \tag{4.8b}$$

while the small-jumps component is

$$\mathscr{L}^3[X]=\int_{|x|<\epsilon}\sum_j (U_xL_{jx}(Q)+(U_x-I)\omega_j(x))^*X(U_xL_{jx}(Q) +(U_x-I)\omega_j(x))\mu(dx)-K_3^*X-XK_3, \tag{4.7d}$$

where

$$K_3=\int_{|x|<\epsilon}\sum_j \left\{(I-U_x-ix\cdot P)|\omega_j(x)|^2+(I-U_x)L_{jx}(Q)\overline{\omega_j}(x)+\frac{1}{2}|L_{jx}(Q)|^2\right\}\mu(dx), \tag{4.8c}$$

and $\omega_j(x)$ are complex functions satisfying

$$\int_{|x|<\epsilon}|x|^2\sum_j |\omega_j(x)|^2\mu(dx)<\infty. \tag{4.10}$$

Several remarks are in order.

(1) The shift covariance (4.5) of the expressions (4.7b)–(4.7d) can be checked by using the Weyl CCR

$$U_xV_v=e^{-imx\cdot v}V_vU_x \tag{4.11}$$

and its consequence

$$V_v^*PV_v=P+mv. \tag{4.12}$$

The regularity assumption on $\mathscr{L}$ implies certain local properties of the functions $K_0(\cdot),\mathscr{U}(\cdot),L_j(\cdot),L_{jx}(\cdot)$ (see Ref. 5), which are omitted here.

(2) In concrete problems $\mathscr{L}$ usually reduces to one of its components. Particular generators of the form $\mathscr{L}^1$ or $\mathscr{L}^2$ appeared in Refs. 18 and 19 as a result of taking special (weak-coupling or low-density) Markovian limit for an open quantum system. To our knowledge the general form of $\mathscr{L}^1$ and $\mathscr{L}^3$ was not observed before. Some insight into the physical meaning of the functions $L_j(\cdot)$ and $L_{jx}(\cdot)$ can be obtained from the Langevin equations to be described in Sec. V.

The term $i[\beta\cdot P+\widetilde{\mathscr{U}}(Q),\ X]$, incorporated into the Hamiltonian component in (4.4), may be also included in any of $\mathscr{L}^j$. The point $x=0$ is not excluded from the integral in the small-jumps component. Therefore, if $\mu(dx)$ has positive mass μ_0 at $x=0$, it contributes the ''zero-jump'' term

$$\mu_0 \sum_j \left[L_{j0}(Q)^* X L_{j0}(Q) - |L_{j0}(Q)|^2 \circ X\right]$$

to $\mathscr{L}^3$. Inclusion of this term into $\mathscr{L}^3$ is a convention and it may appear in $\mathscr{L}^1$ or $\mathscr{L}^2$ as well.

(3) By defining $\omega_j(x)=0$ for $|x|\geqslant\epsilon$, one can write the discontinuous part $\mathscr{L}^{2,3}=\mathscr{L}^2+\mathscr{L}^3$ in the form (4.7d) with the integral extended to the whole $\mathbf{R}^3$. On the other hand, if the functions $\omega_j(x)$ are such that

$$\int_{|x|<\epsilon} \sum_j |\omega_j(x)|^2 \mu(dx) < \infty, \tag{4.13}$$

then by replacing $L_{jx}(\cdot)+\omega_j(x)$ with $L_{jx}(\cdot)$ and by redefining the Hamiltonian term it is possible to write the discontinuous part in the form (4.7c) with the integral extended to $\mathbf{R}^3$.

(4) Previous remarks show that the decomposition (4.7a) is not unique, the nonuniqueness being essentially related to the fact that the operators $L_j(Q)$ and $L_{jx}(Q)$ are defined up to scalar additive terms. The transformation $L_j(Q)\to L_j(Q)+c_j$, $L_{jx}(Q)\to L_{jx}(Q)+\omega_j(x)$ [with $\omega_j(x)$ satisfying (4.13)] does not change the form of the components, provided the proper compensation in the Hamiltonian term is made.[8]

(5) The shift-covariance (4.5) implies that the maximal Abelian algebra of operators $X=f(Q)$ is invariant under the corresponding evolution. Let $f\in C^2(\mathbf{R}^3)$. Using formulas

$$i[P_k,\, f(Q)] = \frac{\partial f(Q)}{\partial Q_k}, \quad U_x^* f(Q) U_x = f(Q+x), \tag{4.14}$$

one obtains

$$\begin{aligned}\mathscr{L}^0[f(Q)] = K_0(Q) f(Q) &+ \sum_{k=1}^3 \beta_k(Q) \frac{\partial f(Q)}{\partial Q_k} + \frac{1}{2} \sum_{l,k=1}^3 \sigma_{lk} \frac{\partial^2 f(Q)}{\partial Q_l \partial Q_k} \\ &+ \int \left[f(Q+x) - f(Q) - 1_\epsilon(x) \sum_{k=1}^3 x_k \frac{\partial f(Q)}{\partial Q_k} \right] \mu(dx|Q),\end{aligned} \tag{4.15}$$

where

$$\begin{aligned}\beta_k(Q) &= 2\sum_{j=1}^r \beta_{kj} \operatorname{Im} L_j(Q) + \int_{|x|<\epsilon} x_k \sum_j \left[|L_{jx}(Q)+\omega_j(x)|^2 - |\omega_j(x)|^2\right] \mu(dx), \\ \sigma_{lk} &= \sum_{j=1}^r \beta_{jl}\beta_{jk}, \quad \mu(dx|Q) = \sum_j |L_{jx}(Q)+\omega_j(x)|^2 \mu(dx).\end{aligned} \tag{4.16}$$

This is the generator of a classical (sub-)Markov process in the position space $\mathbf{R}^3$ (called process with locally independent increments[20]). It comprises diffusion with the drift $\beta_j(Q)$ and the constant diffusion matrix σ_{lk}, and jump process with intensities $\mu(dx|Q)$ for jumps of magnitudes x from a point Q.

(6) We shall finally briefly comment on the existence and uniqunes of the solution of the boost covariant Markovian master equation (1.5). According to theorem A1 (see Appendix A), to establish existence of the minimal solution one has to prove that the operator of the form

$$K = iH + K_0 + K_1 + K_2 + K_3,$$

where H is given by (4.6), and K_1, K_2, K_3 by (4.8a)–(4.8c), is maximal accretive with a core $\mathscr{D}$. Although this problem resembles the well-studied problem of essential self-adjointness for quantum mechanical Hamiltonians (see, e.g., Ref. 16), there are only few specific results on it (see Ref. 8 for the case $K=K_1$ in one dimension).

Assuming $K_0(Q)=0$, uniqueness reduces to the unitality of the minimal solution. There is a general criterion for covariant dynamical semigroups,[7] which implies that for $\mathscr{L}=\mathscr{L}^0$ unitality is equivalent to nonexplosion of the classical Markov process with the generator (4.15). Application of this result to the boost covariant Markovian master equation will be considered elsewhere.

V. THE QUANTUM LANGEVIN EQUATIONS

We start with a formal description of the quantum noise, which will give driving terms in the Langevin equation, corresponding to the boost covariant generator (4.4) and (4.7a). For the continuous component $\mathscr{L}^1$ it arises from the the representation of CCR

$$[a_j(t),a_l^\dagger(s)]=\delta_{jl}\delta(t-s), \quad j,l=1,\ldots,r, \quad t,s\in\mathbf{R}_+, \tag{5.1}$$

in the Fock space $\mathsf{H}_1=\Gamma(\mathscr{H}_1\otimes L^2(\mathbf{R}_+))$, where $\mathscr{H}_1=\mathbf{C}^r$ (see Appendix B). The Ito stochastic differentials

$$dA_j(t)=\int_t^{t+dt} a_j(s)ds, \quad dA_j^\dagger(t)=\int_t^{t+dt} a_j^\dagger(s)ds, \tag{5.2}$$

with $dt>0$, obey the quantum Ito rule [cf. (B2)], to be described below.

The driving noises for the discontinuous part $\mathscr{L}^{2,3}$ live in the Fock space $\mathsf{H}_{2,3}=\Gamma(\mathscr{H}_{2,3}\otimes L^2(\mathbf{R}_+))$, where $\mathscr{H}_{2,3}=L^2(\mathbf{R}^3,\mu)\otimes l^2$, and arise from the CCR:

$$[a_{jx}(t),\ a_{ly}^\dagger(s)]=\delta_{jl}\delta_\mu(x-y)\,\delta(t-s), \quad j,l=1,2,\ldots, \quad x,y\in\mathbf{R}^3; t,s\in\mathbf{R}_+, \tag{5.3}$$

where δ_μ is the delta-function in $L^2(\mathbf{R}^3,\mu)$. The stochastic differentials

$$\begin{gathered} dA_{j,dx}(t)=\int_t^{t+dt} a_{jx}(s)ds\mu(dx), \quad dA_{j,dx}^\dagger(t)=\int_t^{t+dt} a_{jx}^\dagger(s)ds\mu(dx), \\ d\Lambda_{j,dx}(t)=\int_t^{t+dt} a_{jx}^\dagger(s)a_{jx}(s)ds\mu(dx) \end{gathered} \tag{5.4}$$

obey the corresponding Ito rule; to express it we shall use more spectacular formal notation for all stochastic differentials:

$$\begin{gathered} dA_j(t)=a_j(t+)dt,\ldots,dA_{j,dx}=a_{jx}(t+)\mu(dx)dt,\ldots, \\ d\Lambda_{jx}(t)=a_{jx}^\dagger(t+)a_{jx}(t+)dt\mu(dx), \end{gathered} \tag{5.5}$$

having in mind that the symbols $a_j(t+)$,..., have meaning only in combination with dt. Then the Ito rule takes the form

$$a_j(t+)a_j^\dagger(t+)(dt)^2=dt, \tag{5.6a}$$

$$a_{jx}(t+)a_{jx}^\dagger(t+)(dt)^2\mu(dx)=dt, \tag{5.6b}$$

with all other products containing $(dt)^2$ vanishing. Due to the CCR (5.1), (5.3) and the definition of the Ito stochastic differentials (5.2) and (5.4) the symbols $a_j(t+),...$ must be considered as commuting with any operator depending on system observables in the Hilbert space $\mathscr{H}$ and on the values of all noises $a_j(s),...,$ at times $s\leqslant t$.

To describe interaction of the system with the noise, we introduce the family of operators U_t; $t\in\mathbf{R}_+$, in the Hilbert space $\mathscr{H}\otimes\Gamma$, where $\Gamma=\Gamma((\mathscr{H}_1\oplus\mathscr{H}_{2,3})\otimes L^2(\mathbf{R}_+))$ is the full Fock space, satisfying the left quantum stochastic differential equation of the type (B4):

$$dU_t=dZ_tU_t, \tag{5.7}$$

where

$$dZ_t=Hdt+dZ_t^1+dZ_t^{2,3}, \tag{5.8a}$$

with

$$dZ_t^1=\sum_{k=1}^{r}[a_k^\dagger(t+)(\widetilde{P}_k+L_k(Q))-\text{h.c.}]dt-K_1dt, \tag{5.8b}$$

$$dZ_t^{2,3}=\int\sum_j\{(U_x-I)a_{jx}^\dagger(t+)a_{jx}(t+)+a_{jx}^\dagger(t+)[U_xL_{jx}(Q)+(U_x-I)\omega_j(x)]$$
$$-[L_{jx}(Q)+\omega_j(x)(I-U_x^*)]^*a_{jx}(t+)\}\mu(dx)dt-(K_2+K_3)dt, \tag{5.8c}$$

where from now on we systematically use the convention that $\omega_j(x)=0$ for $|x|\geqslant\epsilon$ (see Remark 3 in Sec. IV).

These equations are written by analogy with Eq. (B5), where the coefficients W,L,K are taken from the generators $\mathscr{L}^1,\mathscr{L}^2,\mathscr{L}^3$ [see (4.7b)–(4.7d)]. These coefficients satisfy the formal conditions for the unitarity of U_t. In fact, by applying the exponential formula (B6), we get the representation

$$U_t=\overleftarrow{\exp}\left(-i\int_0^t dH_s\right), \tag{5.9}$$

where

$$dH_t=Hdt+dH_t^1+dH_t^{2,3} \tag{5.10a}$$

is formally self-adjoint with

$$dH_t^1=\sum_{k=1}^{r}\{i[(a_k(t+)+L_k(Q))^\dagger(\widetilde{P}_k+L_k(Q))-\text{h.c.}]\}dt, \tag{5.10b}$$

$$dH_t^{2,3}=\int\sum_j\left\{[\text{h.c.}](x\cdot P)[a_{jx}(t+)+((I-e^{ix\cdot P})^{-1}+(ix\cdot P)^{-1})[L_{jx}(Q)+\omega_j(x)]]\right.$$
$$\left.+L_{jx}(Q)^*\left(x\cdot P-\frac{1}{2}\operatorname{ctg}\frac{x\cdot P}{2}\right)L_{jx}(Q)-(x\cdot P)|\omega_j(x)|^2\right\}\mu(dx)dt, \tag{5.10c}$$

where one should keep in mind that $e^{-ix\cdot P}=U_x$ and [h.c.] means Hermitean conjugate of the expression in squared brackets.

Assuming U_t unitary, the time evolution of a system observable X is

$$X(t)=U_t^*(X\otimes I_\Gamma)U_t,$$

where I_Γ is the unit operator in the noise Fock space. From (5.7a) and (B.9), we have the quantum stochastic differential equation

$$dX(t)=dZ(t)^*X(t)Z(t)+Z(t)^*X(t)dZ(t)+dZ(t)^*X(t)dZ(t), \tag{5.11}$$

where $dZ(t)=U_t^*dZ_tU_t$. Since

$$U_t^*a_j(t+)U_t=a_j(t+),\quad U_t^*a_{jx}^\dagger(t+)U_t=a_{jx}^\dagger(t+),$$

$dZ(t)$ is given by the same expression as dZ_t with P,Q replaced with $P(t)$, $Q(t)$. Due to the fact that

$$dZ^j(t)^*X(t)dZ^k(t)=0\quad\text{for } j\neq k$$

[the driving noises in $dZ^j(t)=U_t^*dZ_t^jU_t$ involve different modes], we obtain the Langevin–Heisenberg equation in the form

$$dX(t)=i[H(t),\,X(t)]dt+dX^1(t)+dX^{2,3}(t), \tag{5.12a}$$

where $H(t)=|P(t)|^2/2m+\mathscr{U}(Q(t))$, and $dX^j(t)$ are calculated from (5.11) with $dZ(t)$ replaced with $dZ^j(t)$. By analogy with (B8) we obtain

$$\begin{aligned}dX^1=\sum_{k=1}^r\{&[\tilde{P}+\mathrm{Re}\,L_k(Q),\,X](a_k(+)-a_k^\dagger(+))\\&-i[\mathrm{Im}\,L_k(Q),\,X](a_k(+)+a_k^\dagger(+))+\hat{\mathscr{L}}^1[X]\}dt,\end{aligned} \tag{5.12b}$$

$$\begin{aligned}dX^{2,3}=\int\sum_j\{&(U_x^*XU_x-X)a_{jx}^\dagger(+)a_{jx}(+)+[(L_{jx}(Q)+\omega_j(x))^*U_x^*,\,X]U_xa_{jx}(+)\\&-U_x^*[U_x(L_{jx}(Q)+\omega_j(x)),X]a_{jx}^\dagger(+)\}\mu(dx)dt+(\hat{\mathscr{L}}^2[X]+\hat{\mathscr{L}}^3[X])dt,\end{aligned} \tag{5.12c}$$

where $\hat{\mathscr{L}}^j[X]=U_t^*\mathscr{L}^j[X]U_t$, and the argument t is omitted from all observables to simplify notations. The Langevin–Heisenberg equation (5.12a) is a dilation of the forward Markovian master equation (1.9), corresponding to the unital generator $\mathscr{L}$, given by (4.4) and (4.7a) with $K_0(Q)=0$, in the sense that averaging Eq. (5.12a) with respect to the vacuum state of the noises gives this Markovian master equation.

Taking $X=f(Q)$ in (5.12a) gives

$$df(Q)=i\left[\frac{|P|^2}{2m},f(Q)\right]dt+df^1(Q)+df^{2,3}(Q), \tag{5.13a}$$

where

$$df^1(Q)=\sum_{k=1}^r\sum_{j=1}^3\beta_{kj}\frac{\partial f(Q)}{\partial Q_j}\{i(a_k^\dagger(+)-a_k(+))+2\,\mathrm{Im}\,L_k(Q)\}dt+\frac{1}{2}\sum_{j,l=1}^3\sigma_{jl}\frac{\partial^2f(Q)}{\partial Q_j\partial Q_l}\,dt, \tag{5.13b}$$

$$df^{2,3}(Q)=\int \sum_j \Big\{[f(Q+x)-f(Q)]\cdot(a_{jx}(+)+L_{jx}(Q)+\omega_j(x))^\dagger(a_{jx}(+)$$
$$+L_{jx}(Q)+\omega_j(x))-|\omega_j(x)|^2\sum_{k=1}^{3}\frac{\partial f(Q)}{\partial Q_k}x_k\Big\}\mu(dx)dt. \tag{5.13c}$$

Thus $df^1(Q)$ describes the diffusion component driven by the classical Wiener process [cf. (B12)]

$$dW_k(t)=i(a_k^\dagger(t+)-a_k(t+))dt,\quad 1\leqslant k\leqslant r,$$

while $df^{2,3}(Q)$ describes the jump component driven by the classical martingale measure

$$\Pi(dxdt)=\sum_j (a_{jx}(t+)+L_{jx}(Q)+\omega_j(x))^\dagger(a_{jx}(t+)+L_{jx}(Q)+\omega_j(x))\mu(dx)dt$$

with the compensator[14] $\mu(dx|Q)$ [see (4.16)].

On the other hand, by taking $X=P_l$, we obtain

$$dP_l=\frac{\partial\mathscr{U}(Q)}{\partial Q_l}dt+dP_l^1+dP_l^{2,3}, \tag{5.14a}$$

where

$$dP_l^1=-i\sum_{k=1}^{r}\Big\{\Big(a_k(+)+\frac{1}{2}L_k(Q)\Big)^\dagger\frac{\partial L_k(Q)}{\partial Q_l}-\text{h.c.}\Big\}dt, \tag{5.14b}$$

$$dP_l^{2,3}=-i\int\sum_j\Big\{\Big(a_{jx}(+)+\frac{1}{2}L_{jx}(Q)\Big)^\dagger\frac{\partial L_{jx}(Q)}{\partial Q_l}-\text{h.c.}\Big\}\mu(dx)dt. \tag{5.14c}$$

Thus the momentum P is subject to a force represented by a quantum diffusion with coefficients depending on Q.

The problems of existence, uniqueness, and unitarity of solution of the quantum stochastic differential equation (5.7) and (5.8a) with sufficiently general functions $L_j(\cdot)$ and $L_{jx}(\cdot)$ will be treated elsewhere. Some results on abstract quantum stochastic differential equations with unbounded operator coefficients were obtained in Refs. 21–23, where mainly right equations were considered. In particular, it was proved in Ref. 22 that the solution of the right equation $\widetilde{U}_t$ is isometric if and only if the related dynamical semigroup Φ_t^∞ is unital, and a similar condition for the co-isometry of $\widetilde{U}_t$ holds. Contrary to the case of bounded operators (see Appendix B) the approaches via right and left equations become inequivalent in general, as they lead, correspondingly, to the backward and forward Markovian master equations. Other questions to be investigated are the rigorous treatment of quantum stochastic integrals and equations with ''big jumps'' (that are treated pathwise in the classical case) and extension of the time-ordered exponential representation (B6) to the case of unbounded operator coefficients.

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APPENDIX A: THE BACKWARD AND FORWARD QUANTUM MARKOVIAN MASTER EQUATIONS

We assume the following regularity properties for a solution of the backward equation (1.5): this should be a family $\Phi_t, t\geqslant 0$, of normal completely positive maps in $\mathscr{B}(\mathscr{H})$, uniformly bounded in norm, satisfying $\Phi_0=\mathrm{Id}$, and such that all functions $t\to \mathrm{Tr}\,\rho\Phi_t[X]$, $\rho\in\mathscr{T}(\mathscr{H})$, $X\in\mathscr{B}(\mathscr{H})$ are continuous.

Theorem A1: Let K be maximal accretive and $\mathscr{D}$ be an invariant domain of the semigroup $\exp(-Kt)t, \geqslant 0$. Then there exists the minimal solution Φ_t^∞ of Eq. (1.5), which is a dynamical semigroup.

Proof (Sketch): Introducing the dynamical semigroup $\check{\Psi}_t[\rho]=e^{-Kt}\rho e^{-K^*t}$, we see that D, defined by (1.2), is an invariant domain for $\check{\Psi}_t$. Defining $\Lambda[\rho]=\Sigma_j|L_j\phi\rangle\langle L_j\psi|$ for $\rho=|\phi\rangle\langle\psi|\in\mathsf{D}$, one can show[7] that (1.5) is equivalent to the integral equation

$$\mathrm{Tr}\,\rho\Phi_t[X]=\mathrm{Tr}\,\Psi_t[\rho]X+\int_0^t \mathrm{Tr}\,\Lambda[\check{\Psi}_s[\rho]]\Phi_{t-s}[X]ds,\quad \rho\in\mathsf{D}, X\in\mathscr{B}(\mathscr{H}). \tag{A1}$$

Indeed, under the assumptions of the theorem both equations are equivalent to

$$\frac{d}{ds}\,\mathrm{Tr}\,\check{\Psi}_s[\rho]\Phi_{t-s}[X]=-\mathrm{Tr}\,\Lambda[\check{\Psi}_s[\rho]]\Phi_{t-s}[X],\quad 0\leqslant s\leqslant t.$$

Note that in (A1) $\mathscr{B}(\mathscr{H})$ may be replaced by any weak*-dense subspace.

The existence of the minimal solution of (A1) is proved by considering iterations[10,22]

$$\mathrm{Tr}\,\rho\Phi_t^{n+1}[X]=\mathrm{Tr}\,\check{\Psi}_t[\rho]X+\int_0^t \mathrm{Tr}\,\Lambda[\check{\Psi}_s[\rho]]\Phi_{t-s}^n[X]ds \tag{A2}$$

with $\Phi_t^1[X]=\check{\Phi}_t[X]=e^{-K^*t}Xe^{-Kt}$. Complete positivity of Λ implies that $\Phi_t^{n+1}-\Phi_t^n$ is completely positive, and (1.4) implies $\Phi_t^n[I]\leqslant I$, by induction. By bounded monotone convergence there exists $\lim_{n\to\infty}\Phi_t^n=\Phi_t^\infty$, satisfying (A1). Since for any other solution Φ_t the difference $\Phi_t-\Phi_t^n$ is completely positive by induction, Φ_t^∞ is the minimal solution. For detailed proof of properties of Φ_t^∞ see Refs. 10, 8, and 22. □

Assuming (1.8), let us consider the forward equation (1.9). For a solution $\Psi_t; t\geqslant 0$, of (1.9) we demand that Ψ_t^* should satisfy the regularity properties of solution of the backward equation. Defining

$$\mathsf{D}^*=\mathrm{lin}\{X=|\psi\rangle\langle\phi|;\phi,\psi\in\mathscr{D}^*\}$$

and $\Lambda^*[X]=\Sigma_j|L_j^*\psi\rangle\langle L_j^*\phi|$ for $X=|\psi\rangle\langle\phi|\in\mathsf{D}^*$, we have

$$\mathrm{Tr}\,\Lambda[\rho]X=\mathrm{Tr}\,\rho\Lambda^*[X],\quad \rho\in\mathsf{D}, X\in\mathsf{D}^*. \tag{A3}$$

Theorem A2: Let K (hence K^*) be maximal accretive and $\mathscr{D}^*$ an invariant domain of the semigroup $\exp(-K^*t); t\geqslant 0$. Then $\Psi_t^\infty=(\Phi_t^\infty)_*$ is the minimal solution of the forward equation (1.9).

Proof (Sketch): As in the previous theorem, one can prove that (1.9) is equivalent to

$$\mathrm{Tr}\,\Psi_t[\rho]X=\mathrm{Tr}\,\rho\check{\Phi}_t[X]+\int_0^t \mathrm{Tr}\,\Psi_{t-s}[\rho]\Lambda^*[\check{\Phi}_s[X]]ds,\quad \rho\in\mathscr{T}(\mathscr{H}), X\in\mathsf{D}^*,$$

where $\mathscr{T}(\mathscr{H})$ can be replaced by any norm-dense subspace. Consider the iterations

$$\mathrm{Tr}\ \Psi_t^{n+1}[\rho]X=\mathrm{Tr}\ \rho\check{\Phi}_t[X]+\int_0^t \mathrm{Tr}\ \Psi_{t-s}^n[\rho]\Lambda^*[\check{\Phi}_s[X]]ds, \tag{A4}$$

with $\Psi_t^1[\rho]=\check{\Psi}_t[\rho]$. If these iterations converge, then the limit is the minimal solution, by the same argument as in previous theorem. We shall prove by induction that $\Psi_t^n=(\Phi_t^n)_*$; then the convergence will follow from the proof of theorem A1.

We can write (A2) and (A4) shortly as

$$\Phi_{(\cdot)}^{n+1}=\check{\Phi}_{(\cdot)}+A[\Phi_{(\cdot)}^n],$$

$$\Psi_{(\cdot)}^{n+1}=\check{\Psi}_{(\cdot)}+B[\Psi_{(\cdot)}^n],$$

where A and B are the corresponding integral operators. Following argument of Refs. 11 and 24, one can see that

$$A[\check{\Phi}_{(\cdot)}]=B[\check{\Psi}_{(\cdot)}]^*$$

and

$$A[B[\Phi_{(\cdot)*}]^*]=B[A[\Phi_{(\cdot)}]_*]^*.$$

It follows that $\Psi_{(\cdot)}^n=(\Phi_{(\cdot)}^n)_*$. □

APPENDIX B: QUANTUM STOCHASTIC CALCULUS

There is a profound connection between the symmetric Fock space and the Levy–Khinchin formula for infinitely divisible representations of Lie groups,[25] which underlies quantum processes with independent increments. We give here a brief informal account of quantum stochastic calculus with one-mode Boson noise in the Fock space. See Ref. 26 for the mathematical presentation of the general case and Refs. 27 and 28 for physical motivation and applications.

The role of the one-particle space is played by the Hilbert space $L^2(\mathbf{R}_+)$ of complex square-integrable functions of $t\in\mathbf{R}_+$ [in the case of many modes one takes $\mathscr{K}\otimes L^2(\mathbf{R}_+)$, where $\mathscr{K}$ is the Hilbert space representing modes]. Let $\Gamma(L^2(\mathbf{R}_+))$ be the Boson Fock space over $L^2(\mathbf{R}_+)$ (see, e.g., Ref. 16) with the irreducible representation of the CCR

$$[a(t),\ a^\dagger(s)]=\delta(t-s),\quad t,s\geqslant 0,$$

satisfying $a(t)|0\rangle=0$, where $|0\rangle$ is the vacuum state vector. The basic operator processes

$$A(t)=\int_0^t a(s)ds,\quad A^\dagger(t)=\int_0^t a^\dagger(s)ds,\quad \Lambda(t)=\int_0^t a^\dagger(s)a(s)ds \tag{B1}$$

obey the quantum Ito rule

$$dA(t)dA^\dagger(t)=dt,\quad d\Lambda(t)^2=d\Lambda(t),$$

$$dA(t)d\Lambda(t)=dA(t),\quad d\Lambda(t)dA^\dagger(t)=dA^\dagger(t), \tag{B2}$$

with all other products, including those comprising dt, vanishing. Moreover, the quantum stochastic differentials should be regarded as commuting with any *adapted* process, i.e., a family of bounded operators depending for each t on $a(s)$, $a^\dagger(s)$ with $s\leqslant t$, and possibly on operators in some fixed *initial* space $\mathscr{K}$. Quantum stochastic integral

$$Y(t)=\int_0^t [X_1(s)d\Lambda(s)+X_2(s)dA^\dagger(s)+X_3(s)dA(s)+X_4(s)ds]$$

can be defined for sufficiently regular adapted processes $X_j(t)$, and the Ito product formula

$$d(Y_1\cdot Y_2)=dY_1\cdot Y_2+Y_1\cdot dY_2+dY_1\cdot dY_2 \tag{B3}$$

can be established, where the products are to be calculated by using the quantum Ito table.

Let W be unitary and L and K bounded operators in the initial Hilbert space $\mathscr{H}$, satisfying

$$L^*L=K+K^*,$$

so that $K=\frac{1}{2}L^*L+iH$, where H is bounded Hermitean operator. The left and right quantum stochastic differential equations

$$dU_t=dZ_t\,U_t, \quad d\widetilde{U}_t=\widetilde{U}_t\,dZ_t, \tag{B4}$$

where

$$dZ_t=(W-I)d\Lambda(t)+LdA^\dagger(t)-L^*WdA(t)-Kdt, \tag{B5}$$

have unique unitary solutions $U_t,\widetilde{U}_t,t\geqslant 0$, satisfying $U_0=\widetilde{U}_0=I$ (see Ref. 26). These solutions can be represented in the form of time-ordered exponentials

$$\left.\begin{matrix}U_t\\ \widetilde{U}_t\end{matrix}\right\}=\left\{\begin{matrix}\overleftarrow{\exp}\\ \overrightarrow{\exp}\end{matrix}\right\} i\int_0^t\left\{\Phi d\Lambda(s)-\frac{\Phi}{e^{i\Phi}-I}\,LdA^\dagger(s)-\text{h.c.}-\left[H+L^*\,\frac{\sin\Phi-\Phi}{(2\sin\Phi/2)^2}\,L\right]ds\right\}, \tag{B6}$$

where Φ is a bounded Hermitean operator such that $W=e^{i\Phi}$ and $\Phi/(e^{i\Phi}-I)$,..., are the corresponding meromorphic functions of this operator.[28]

Let

$$X(t)=U_t^*(X\otimes I_\Gamma)U_t, \quad \widetilde{X}(t)=\widetilde{U}_t^*(X\otimes I_\Gamma)\widetilde{U}_t, \tag{B7}$$

where X is a bounded operator in $\mathscr{H}$. From (B2) and (B3) one derives the following equation for the family $X(t)$

$$dX=(W^*XW-X)d\Lambda-W^*[L,X]dA^\dagger+[L^*,X]WdA+\hat{\mathscr{L}}[X]dt, \tag{B8}$$

where

$$\hat{\mathscr{L}}[X]=\mathscr{L}[X](t)=U_t^*\mathscr{L}[X]U_t, \quad \mathscr{L}[X]=L^*XL-K^*X-XK, \tag{B9}$$

and the argument (t) is omitted from all operators in (B8) to simplify notations. The family $\widetilde{X}(t)$ satisfies similar equation, in which, however, W, L, and $\mathscr{L}$ are time independent and the argument (t) is omitted only from $\widetilde{X}$ and the noises.

Consider the vacuum expectations

$$\Phi_t[X]=\langle 0|X(t)|0\rangle, \quad \widetilde{\Phi}_t[X]=\langle 0|\widetilde{X}(t)|0\rangle, \quad t\geqslant 0. \tag{B10}$$

Averaging (B8) and the similar equation for $\widetilde{X}(t)$, and taking into account that the vacuum expectation of all noises vanish, one obtains the forward and the backward equations

$$d\Phi_t[X]=\Phi_t[\mathscr{L}[X]]dt, \quad d\widetilde{\Phi}_t[X]=\mathscr{L}[\widetilde{\Phi}_t[X]]dt, \tag{B11}$$

where $\Phi_t=\widetilde{\Phi}_t=\exp t\mathscr{L}$ is a unital quantum dynamical semigroup with the generator $\mathscr{L}$.

The relations to the classical stochastic processes are as follows. Each of the operator families

$$Q(t)=A(t)+A^\dagger(t), \quad P(t)=i(A^\dagger(t)-A(t)),$$
$$\Pi(t)=\Lambda(t)+\mu A^\dagger(t)+\overline{\mu}A(t)+|\mu|^2 t=\int_0^t (a(s)+\mu)^\dagger(a(s)+\mu)ds \tag{B12}$$

is a family of commuting self-adjoint operators in the Fock space $\Gamma(L^2(\mathbf{R}_+))$, thus unitary equivalent to a classical stochastic process in the corresponding L^2 space with 1 as the vacuum vector. The processes $Q(t)$ and $P(t)$ are unitary equivalent to the standard Wiener process (via Segal's ''duality maps''), while $\Pi(t)$ is unitary equivalent to the Poisson process of intensity $|\mu|^2$ (see Ref. 26). However $Q(t)$, $P(t)$, and $\Pi(t)$ do not commute and hence cannot be diagonalized simultaneously.

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On realizations of solutions of the KdV equation by determinants on operator ideals

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Using new developments in the theory of traces, determinants, and elementary operators on quasi-Banach operator ideals we clarify and extend Marchenko's method for realizing solutions of the KdV equation. Moreover, we point out why abstract traces and determinants on quasi-Banach operator ideals are appropriate tools for obtaining solutions of the KdV equation. The method we present can also be applied to other nonlinear equations in soliton physics. © *1996 American Institute of Physics.* [S0022-2488(96)01903-6]

I. INTRODUCTION

Within the frame of bounded linear operators and trace ideals on the class of Banach spaces we give an approach for the realization of solutions of the Korteweg–de Vries equation (KdV)

$$u_t = u_{xxx} + 6uu_x .$$

As an application we obtain solutions of the KdV equation with finitely as well as infinitely many parameters among the N-soliton solutions.

Given a bounded operator $A \in \mathscr{L}(E)$ and a nuclear operator $B \in \mathscr{N}(E)$ on a Banach space E with the approximation property such that $\operatorname{rank}(AB+BA)=1$, then

$$u(t,x) = 2\frac{\partial^2}{\partial x^2} \ln \det(I + e^{Ax+A^3t}B)$$

is a solution of the KdV equation.

We will provide conditions on A such that for $a \in E'$ and $c \in E$ we may find a nuclear operator B with $AB+BA = a \otimes c$. In connection with this we refer to A as a generating operator for the realization of solutions of the KdV equation. In the case where the generating operator is a diagonal operator D on certain Banach sequence spaces we may even realize these solutions of the KdV equation by a corresponding diagonal operator on l_1. Hence, in a sense, the l_1 space is universal for realizations of the KdV equation generated by diagonal operators.

The summability behavior of the eigenvalues of the operator B with $DB+BD = a \otimes c$ will be the key for defining a determinant on an appropriate operator ideal admitting a spectral trace.

Since solutions of the integrated KdV equation

$$v_t = v_{xxx} + 3v_x^2$$

yield solutions of the KdV equation ($u = v_x$), we will refer to this as KdV equation, too, if no confusion is possible.

In this paper a more or less abstract model for gaining new solutions of the KdV equation from a so-called "germ" solution may be described by the following steps:

(1) Let v be a solution of the KdV equation $v_t = v_{xxx} + 3v_x^2$.

(2) By trial and error we give, if possible, an appropriate interpretation of $v=v(t,x)$ as an operator family $V=V(t,x):E\to E$ acting on a Banach space E and check for this family a corresponding operator KdV equation

$$V_t=V_{xxx}+3V_x^2.$$

(3) The main problem is to find appropriate (continuous, linear) functionals τ on quasi-Banach operator ideals transforming the operator family $V(t,x)$ into the new solution $v=\tau(V)$ of the (scalar) KdV equation $v_t=v_{xxx}+3v_x^2$.

Because of the nonlinear expression V_x^2 in the operator KdV equation the functional τ has to satisfy a multiplicativity property

$$\tau(S^2)=\tau(S)^2,$$

at least for certain operators S. It turns out that a nonvanishing linear functional τ on the smallest ideal $\mathscr{F}$ of finite rank operators with the multiplicativity property at least for rank 1 operators necessarily has to be the trace on $\mathscr{F}$. Consequently, traces will be the appropriate functionals for gaining new solutions of the KdV equation from a solution of the corresponding operator KdV equation. Finally, the new solutions can be described by continuous determinants on appropriate quasi-Banach operator ideals. They allow a more convenient calculation of the solution. Several examples are given.

This method is also applicable to other nonlinear equations in soliton physics such as Sine–Gordon equation, mKdV equation, Toda lattice, etc.[1]

II. BASIC NOTIONS, TRACES, AND DETERMINANTS

For the convenience of the reader we recall some notions from the theory of (bounded linear) operators in Banach spaces, traces, and determinants on operator ideals. More about notions and recent results concerning traces on operator ideals can be found in the Appendix of this paper. For this area the monographs by König[2] and Pietsch[3] are a general reference.

In the following E and F denote real or complex Banach spaces. When dealing with eigenvalues, the considerations are restricted to the complex case only. The value of the functional $a\in E'$ (dual Banach space) at the element $x\in E$ is denoted by $\langle x,a\rangle$. Moreover, $\mathscr{L}(E,F)$ stands for the Banach space of all (bounded linear) operators $T:E\to F$ acting from E into F. The usual norm is given by $\|T\|:=\sup\{\|Tx\|:\|x\|\leqslant 1\}$. We write $\mathscr{L}(E)$ instead of $\mathscr{L}(E,E)$. Given $a\in E'$ and $y\in F$, then $a\otimes y:x\mapsto\langle x,a\rangle y$ yields an operator from E into F with $\|a\otimes y\|=\|a\|\cdot\|y\|$. An operator $T\in\mathscr{L}(E,F)$ is said to be a finite rank operator if there exists a so-called finite representation

$$T=\sum_{i=1}^{n} a_i\otimes y_i\,.$$

The collection of all finite rank operators from E into F is denoted by $\mathscr{F}(E,F)$. We again write $\mathscr{F}(E)$ instead of $\mathscr{F}(E,E)$. Finally, l_∞ and l_p, $0<p<\infty$, stand for the classical sequence spaces of all bounded sequences and p-bounded sequences, respectively. With respect to the norm

$$\|(\xi_i)\|_p:=\begin{cases}\left(\sum_{i=1}^{\infty}|\xi_i|^p\right)^{1/p} & \text{for } 1\leqslant p<\infty,\\ \sup|\xi_i| & \text{for } p=\infty,\end{cases}$$

the l_p-spaces are Banach spaces for $1\leqslant p\leqslant\infty$.

A. Operator ideals

The general notion of an operator ideal or of a quasi-Banach operator ideal, respectively, was introduced by Pietsch.[4] For a recent treatise to this subject we refer to Defant and Floret.[5] Suppose that for every pair of Banach spaces E and F, we are given a subset $\mathscr{A}(E,F)$ of $\mathscr{L}(E,F)$. The class

$$\mathscr{A} := \bigcup_{E,F} \mathscr{A}(E,F)$$

is called an *operator ideal* if the following conditions are satisfied:

(i) $a \otimes y \in \mathscr{A}(E,F)$ for $a \in E'$ and $y \in F$,
(ii) $S+T \in \mathscr{A}(E,F)$ for $S,T \in \mathscr{A}(E,F)$,
(iii) $YTX \in \mathscr{A}(E_0,F_0)$ for $X \in \mathscr{L}(E_0,E)$, $T \in \mathscr{A}(E,F)$, $Y \in \mathscr{L}(F,F_0)$.

In particular, we have $\lambda T \in \mathscr{A}(E,F)$ for $T \in \mathscr{A}(E,F)$, $\lambda \in \mathbb{K}$, where $\mathbb{K}$ stands either for the field $\mathbb{R}$ of real numbers or $\mathbb{C}$ of complex numbers.

Hence every component $\mathscr{A}(E,F)$ is a linear subset of $\mathscr{L}(E,F)$. We write $\mathscr{A}(E)$ instead of $\mathscr{A}(E,E)$. The class $\mathscr{L}$ of all operators is the largest operator ideal and the class $\mathscr{F}$ of finite rank operators is the smallest operator ideal.

A function $\|\cdot|\mathscr{A}\|$ which assigns to every operator $T \in \mathscr{A}$ a non-negative number $\|T|\mathscr{A}\|$ is called a *quasi-norm* on the operator ideal $\mathscr{A}$ if it has the following properties:

(i) $\|a \otimes y|\mathscr{A}\| = \|a\| \cdot \|y\|$ for $a \in E'$ and $y \in F$,
(ii) $\|S+T|\mathscr{A}\| \leq c_{\mathscr{A}}(\|S|\mathscr{A}\| + \|T|\mathscr{A}\|)$ for $S,T \in \mathscr{A}(E,F)$,
(iii) $\|YTX|\mathscr{A}\| \leq \|Y\| \cdot \|T|\mathscr{A}\| \cdot \|X\|$ for $X \in \mathscr{L}(E_0,E)$, $T \in \mathscr{A}(E,F)$, $Y \in \mathscr{L}(F,F_0)$. In particular, $\|\lambda T|\mathscr{A}\| = |\lambda| \cdot \|T|\mathscr{A}\|$ for $T \in \mathscr{A}(E,F)$, $\lambda \in \mathbb{K}$.

Obviously, $\|T\| \leq \|T|\mathscr{A}\|$. In the case $c_{\mathscr{A}}=1$ we simply speak of a norm.

An operator ideal $\mathscr{A}$ is called a *quasi-Banach operator ideal* if all components $\mathscr{A}(E,F)$ are complete with respect to the quasi-norm $\|\cdot|\mathscr{A}\|$ given on $\mathscr{A}$. In particular, if $\|\cdot|\mathscr{A}\|$ is a norm, then $\mathscr{A}$ is called a *Banach operator ideal*.

Remark: The concept of an operator ideal $\mathscr{A}=\cup_{E,F}\mathscr{A}(E,F)$ also makes sense if E and F range only over a certain subclass of Banach spaces. Of particular interest is the case $\mathscr{A} := \cup_{H,K}\mathscr{A}(H,K)$, where H and K are arbitrary Hilbert spaces.

An important example of an operator ideal are the so-called nuclear operators in the sense of Grothendieck. Let us recall that an operator $T \in \mathscr{L}(E,F)$ is *nuclear* if it admits a representation

$$Tx = \sum_{i=1}^{\infty} \langle x, a_i \rangle y_i ,$$

where $a_i \in E'$, $y_i \in F$ and $\Sigma_{i=1}^{\infty} \|a_i\| \cdot \|y_i\| < \infty$. By $\mathscr{N}$ we denote the class of all nuclear operators. Regarding all possible representations of $T \in \mathscr{N}(E,F)$ and taking the infimum

$$\|T|\mathscr{N}\| := \inf\left\{ \sum_{i=1}^{\infty} \|a_i\| \cdot \|y_i\| \right\},$$

one obtains the Banach operator ideal $\mathscr{N}$ of all nuclear operators. The Hilbert space components $\mathscr{N}(H)$, H being a Hilbert space, are the well-known trace classes of Schatten.

B. Traces

An approach to traces and determinants which live on certain operator ideals is due to König[2] and Pietsch.[3] For the following axiomatic concept we refer to Pietsch:[3] A complex-valued function $\tau : \cup_E \mathscr{A}(E) \to \mathbb{C}$ on an operator ideal $\mathscr{A}$ is called a *trace* if for all Banach spaces E and F the following properties are satisfied:

(i) τ is linear on each component $\mathscr{A}(E)$.
(ii) $\tau(a \otimes x) = \langle x, a \rangle$ for all $a \in E'$, $x \in E$.
(iii) $\tau(XT) = \tau(TX)$ for $T \in \mathscr{A}(E,F)$, $X \in \mathscr{L}(F,E)$.

It is well known that on the smallest operator ideal $\mathscr{F}$ of finite rank operators there is a unique trace which is given by

$$\mathrm{tr}(T) := \sum_{i=1}^{n} \langle x_i, a_i \rangle,$$

where $T = \Sigma_{i=1}^{n} a_i \otimes x_i$ is any finite representation of $T \in \mathscr{F}$.

A trace τ defined on a quasi-Banach operator ideal $\mathscr{A}$ is said to be *continuous* if the function $T \mapsto \tau(T)$ has this property on all components $\mathscr{A}(E)$. This is equivalent with the property that there is a universal constant $c \geqslant 1$ such that

(iv) $|\tau(T)| \leqslant c \|T|\mathscr{A}\|$ for all $T \in \mathscr{A}(E)$ and all Banach spaces E.

C. Determinants

A complex-valued function $\delta : \cup_E \mathscr{A}(E) \to \mathbb{C}$ on an operator ideal $\mathscr{A}$ is called a determinant if for all Banach spaces E,F the following conditions are satisfied:[3]

(i) $\delta((I+S)(I+T)) = \delta(I+S)\,\delta(I+T)$ for all $S,T \in \mathscr{A}(E)$.
(ii) $\delta(I + a \otimes x) = 1 + \langle x, a \rangle$ for all $a \in E'$, $x \in E$.
(iii) $\delta(I_E + XT) = \delta(I_F + TX)$ for all $T \in \mathscr{A}(E,F)$ and all $X \in \mathscr{L}(F,E)$.
(iv) $\delta(I + zT)$ is an entire function in z for every $T \in \mathscr{A}(E)$.

Here I stands for the identity operator on E.

A determinant δ defined on a quasi-Banach operator ideal $\mathscr{A}$ is said to be *continuous* if the function $T \mapsto \delta(I+T)$ has this property on all components $\mathscr{A}(E)$. Moreover, $I+T$ is invertible if and only if $\delta(I+T) \neq 0$. The link between traces and determinants in general is governed by the so-called

Trace-determinant theorem:[3] There exists a one-to-one correspondence between continuous traces and continuous determinants for every quasi-Banach operator ideal.

Furthermore, let δ be a continuous determinant on a quasi-Banach operator ideal $\mathscr{A}$. Suppose that the $\mathscr{A}(E)$-valued function $T(z)$ is defined on a domain of the complex plane. If $T(z)$ is differentiable with respect to the quasi-ideal norm at a point z_0, then so is the complex-valued function $\delta(I+T(z))$. In the particular case when $I+T(z_0)$ is invertible, the derivative is given by[3]

(v) $(\delta(I+T(z_0))) = \dot{\delta}((I+T(z_0))^{-1}\dot{T}(z_0))\delta(I+T(z_0))$, where $\dot{\delta}$ is the corresponding trace defined by

$$\dot{\delta}(S) := \lim_{z \to 0} \frac{\delta(I+zS)-1}{z} \quad \text{for } S \in \mathscr{A}(E).$$

We now establish a counterpart to the trace formula of finite rank operators $\mathscr{F}$.

There exists a unique determinant on the operator ideal $\mathscr{F}$

$$\det(I+T) := \det(\delta_{ij}+\langle x_i, a_j\rangle)_{i,j=1}^{n} \quad \text{for } T=\sum_{i=1}^{n} a_i \otimes x_i, \quad a_i \in E', \quad x_i \in E.$$

Finally, for illustrating the previous abstract results we consider the Banach operator ideal $\mathcal{N}$ of nuclear operators introduced in Sec. II A. It was an important example for developing a trace and determinant theory of operators in Banach spaces. If $T \in \mathcal{N}(E)$, E being a Banach space, is a nuclear operator and

$$T=\sum_{i=1}^{\infty} a_i \otimes x_i, \quad a_i \in E', \quad x_i \in E,$$

a representation of T, then we may define

$$\tau(T)=\sum_{i=1}^{\infty} \langle x_i, a_i\rangle.$$

The long outstanding problem was to prove that this expression does not depend on the underlying representation. Unfortunately, it does! This was shown by Enflo[6] when he constructed a Banach space without the so-called approximation property. However, in most of the classical Banach spaces, in particular in the l_p-spaces, everything goes well. A Banach space has the *approximation property* (a.p.) if, given any precompact subset M of E and any $\epsilon>0$, there exists a finite rank operator $L \in \mathcal{F}(E)$ such that $\|z-Lz\| \leqslant \epsilon$ for all $z \in M$.

The unique extension of the determinant formula of finite operators to the ideal of nuclear operators $\mathcal{N}$ over the class of Banach spaces with the a.p. may be described by

$$\det_{\mathcal{N}}(I+T)=1+\sum_{n=1}^{\infty} \alpha_n \quad \text{for } T=\sum_{i=1}^{\infty} a_i \otimes x_i \in \mathcal{N}(E),$$

where

$$\alpha_n(T) := \frac{1}{n!} \sum_{i_1=1}^{\infty} \cdots \sum_{i_n=1}^{\infty} \det \begin{pmatrix} \langle x_{i_1}, a_{i_1}\rangle & \cdots & \langle x_{i_1}, a_{i_n}\rangle \\ \vdots & & \vdots \\ \langle x_{i_n}, a_{i_1}\rangle & \cdots & \langle x_{i_n}, a_{i_n}\rangle \end{pmatrix}.$$

In subsequent sections we consider several examples of quasi-Banach operator ideals admitting continuous determinants.

III. TRACES, DETERMINANTS AND SOLUTIONS OF THE KdV EQUATION

In this section we stress the role of traces and determinants for realizations of solutions of the KdV equation.

A. Why use traces?

Let $V=V(x,t): E \to E$ $(t,\ x \in \mathbb{R})$ be a smooth family of operators acting on a Banach space E satisfying the "operator" KdV equation

$$V_t = V_{xxx} + 3V_x^2.$$

The problem arises of how to transform V into a scalar-valued solution of the KdV equation. In other words we are going to look for a functional τ: $V \mapsto v$ that guarantees a transformation of a

solution of the operator KdV equation into a solution of the KdV equation. Indeed, we analyze the properties of such a functional by applying it to the operator KdV equation. We recognize that we need the equation

$$(\tau(V))_t=(\tau(V))_{xxx}+3[(\tau(V))_x]^2,$$

which can be achieved if the functional τ is linear, multiplicative $\tau(V_x^2)=\tau(V_x)^2$, and continuous. Unfortunately, a nonvanishing linear functional τ even on the smallest operator ideal of finite rank operators $\mathscr{F}(E)$, E being an arbitrary Banach space, with the multiplicativity property $\tau(S^2)=\tau(S)^2$, does not exist at all! However, if we confine ourselves to the multiplicativity property for rank 1 operators only, then we shall see that a functional τ necessarily has to be the trace on $\mathscr{F}$. This observation shows that, in a sense, traces on operator ideals will be appropriate tools for realizations of solutions of the KdV equation from solutions of the operator KdV equation. In fact we state a basic lemma.

Lemma III A 1: Let E be a Banach space and $\tau: \mathscr{F}(E)\to\mathbb{C}$ a nonvanishing linear functional on the finite rank operators. Then the following assertions are equivalent:

(i) $\tau(S^2)=\tau(S)^2$ for all $S\in\mathscr{F}(E)$ with rank $(S)=1$.
(ii) $\tau(P)=1$ for all projections $P\in\mathscr{F}(E)$ with rank $(P)=1$.
(iii) $\tau(a\otimes x)=\langle x,a\rangle$ for all $a\in E'$, $x\in E$.

Proof: Step 1. First we show that (i) implies (ii). Given a rank 1 projection P, by (i) we obtain

$$(\tau(P))^2=\tau(P^2)=\tau(P),$$

yielding $\tau(P)=0$ or $\tau(P)=1$. We claim that $\tau(P)=0$ is impossible. For doing this we suppose $(\tau(S))^2=\tau(S^2)$ for all $S\in\mathscr{L}(E)$ with rank $(S)=1$ and there is a rank 1 projection $P_0\in\mathscr{F}(E)$ with $\tau(P_0)=0$. We are going to show that $\tau(a\otimes c)=0$ for all rank 1 operators, which immediately implies that τ is identically zero on the finite rank operators $\mathscr{F}(E)$.

First of all we assume that $a\otimes c$ is nilpotent, i.e., $\langle c,a\rangle=0$. Because

$$(a\otimes c)^2=\langle c,a\rangle a\otimes c=0$$

we have by the multiplicativity property of τ,

$$(\tau(a\otimes c))^2=\tau((a\otimes c)^2)=\tau(0)=0.$$

Hence, $\tau(a\otimes c)=0$. Now let $\langle c,a\rangle\neq 0$. Then

$$P=\frac{1}{\langle c,a\rangle}\,a\otimes c$$

is a rank 1 projection. Consequently, it remains for us to show that

$$\tau(a\otimes x)=0 \quad \text{for all } a\in E' \quad \text{and } x\in E \text{ with } \langle x,a\rangle=1.$$

By our assumption there exists a rank 1 projection

$$P_0=a_0\otimes x_0 \quad \text{with } \tau(a_0\otimes x_0)=0.$$

In a first case we prove $\tau(b\otimes x_0)=0$ for all $b\in E'$ with $\langle x_0,b\rangle=1$. Indeed, for the nilpotent operator $(b-a_0)\otimes x_0$ we have already $\tau((b-a_0)\otimes x_0)=0$. Therefore,

$$\tau(b\otimes x_0)=\tau(a_0\otimes x_0)+\tau((b-a_0)\otimes x_0)=0.$$

Now we treat the general case. For this purpose let $a \in E'$ and $x \in E$ be arbitrary with $\langle x,a\rangle = 1$. If $x \in \mathrm{span}\{x_0\}$, then $\tau(a \otimes x) = 0$ by the previous case. So we assume $x \notin \mathrm{span}\{x_0\}$, which means $x_0 \notin \mathrm{span}\{x - x_0\}$. By the Hahn–Banach theorem there exists an element $b \in E'$ such that $\langle x - x_0, b\rangle = 0$ and $\langle x_0, b\rangle = 1$. Thus, $\langle x, b\rangle = 1$. From the already proved relations,

$$\tau(b \otimes x_0) = 0 \quad \text{and} \quad \tau(b \otimes (x - x_0)) = 0,$$

we obtain

$$\tau(b \otimes x) = \tau(b \otimes x_0) + \tau(b \otimes (x - x_0)) = 0.$$

Next, put $Q := (b + a) \otimes x$. Then rank $(Q) = 1$ and

$$\tau(Q) = \tau(b \otimes x) + \tau(a \otimes x) = \tau(a \otimes x).$$

Moreover,

$$Q^2 = \langle x, b + a\rangle Q = 2Q$$

and

$$(\tau(Q))^2 = \tau(Q^2) = \tau(2Q) = 2\tau(Q)$$

by the multiplicativity property of τ for rank 1 operators. Taking into account these relations and using again the multiplicativity property for rank 1 operators we infer

$$\tau(a \otimes x) = \tau((a \otimes x)^2) = (\tau(a \otimes x))^2 = (\tau(Q))^2 = \tau(Q^2) = 2\tau(Q) = 2\tau(a \otimes x),$$

implying

$$\tau(a \otimes x) = 0 \quad \text{for all} \quad a \in E' \quad \text{and} \quad x \in E \quad \text{with} \quad \langle x,a\rangle = 1.$$

Finally, since each rank 1 operator $a \otimes x$ is either nilpotent or a multiple of a rank 1 projection, we conclude

$$\tau(a \otimes x) = 0 \quad \text{for all} \quad a \in E' \quad \text{and} \quad x \in E,$$

yielding the desired conclusion.

Step 2: For showing (ii) implies (iii) let $S := a \otimes x$ with $a \in E'$ and $x \in E$. Without loss of generality, we assume $x \neq 0$. If $\langle x,a\rangle \neq 0$, then $P := (1/\langle x,a\rangle) a \otimes x$ is a rank 1 projection. From (ii) we conclude

$$1 = \tau(P) = \frac{1}{\langle x,a\rangle}\, \tau(a \otimes x) \quad \text{or} \quad \tau(a \otimes x) = \langle x,a\rangle$$

as desired. In the case where $\langle x,a\rangle = 0$ we choose an element $b \in E'$ such that $\langle x,b\rangle = 1$. Then $P := b \otimes x$ is again a rank 1 projection. From $\mathrm{rank}(S + P) = \mathrm{rank}((a + b) \otimes x) = 1$ and

$$(S + P)^2 = ((a + b) \otimes x)^2 = \langle x, a + b\rangle (S + P) = S + P$$

we obtain, again by (ii), that

$$1 = \tau(S + P) = \tau(S) + \tau(P) = \tau(S) + 1,$$

yielding

$$\tau(S)=\tau(a\otimes x)=0=\langle x,a\rangle.$$

Combining both cases we conclude (iii).

Step 3: It remains for us to show that (iii) implies (i). To this end, let $S=a\otimes x$. From $S^2=\langle a,x\rangle S$ and (iii) we check the multiplicativity formula (i),

$$\tau(S^2)=\langle x,a\rangle\tau(S)=\langle x,a\rangle\langle x,a\rangle=(\tau(S))^2,$$

which completes the proof. □

The discussion at the very beginning of this section can be summarized in the following.

Proposition III A 2: (i) Let E be a Banach space and $\tau:\mathscr{F}(E)\to\mathbb{C}$ a nonvanishing linear functional with the multiplicativity property

$$\tau((a\otimes c)^2)=(\tau(a\otimes c))^2$$

for rank 1 operators. Then τ has necessarily to be the trace on the finite rank operators $\mathscr{F}(E)$, $\tau=\mathrm{tr}$.

(ii) Let $\mathscr{A}$ be a quasi-Banach operator ideal such that the finite rank operators $\mathscr{F}(E)$ are $\|\cdot|\mathscr{A}\|$-dense in $\mathscr{A}(E)$. If $\tau:\mathscr{A}(E)\to\mathbb{C}$ is a nonvanishing continuous linear functional on each ideal component $\mathscr{A}(E)$ with the above multiplicativity property for rank 1 operators, then τ is the unique continuous trace $\mathrm{tr}_{\mathscr{A}}$ on $\mathscr{A}(E)$.

Proof: The assertion (i) follows from the previous lemma while (ii) is a consequence of (i) and the trace extension theorem (cf. the Appendix). □

Remarks: (i) A surprising and important fact has been discovered by Kalton.[7] Namely, there exists a quasi-Banach operator ideal $\mathscr{A}$ with different continuous traces. If $\tau_1\neq\tau_2$ are such traces, then $\tau=\tau_1-\tau_2$ is a continuous linear functional vanishing on the finite rank operators $\mathscr{F}$. Hence the multiplicativity property $\tau((a\otimes c)^2)=((a\otimes c))^2=0$ is automatically satisfied. But τ is not a trace. This example shows that there are functionals with the multiplicativity property $\tau((a\otimes c)^2)=(\tau(a\otimes c))^2$ for rank 1 operators and which behave rather strangely if the operator ideal $\mathscr{F}$ is not $\|\cdot|\mathscr{A}\|$-dense in the considered quasi-Banach operator ideal $\mathscr{A}$.

(ii) Let us mention that the property (ii) of the previous lemma clarifies the fact that Marchenko[8] used rank 1 projections for realizing certain solutions within the frame of operator algebras.

B. Realizations of solutions of the KdV equation

In what follows we use the background knowledge of the previous section to describe solutions of the KdV equation by traces and determinants of operators. A rather general result is stated in the following proposition.

Proposition III B 1: Let $\mathscr{A}$ be a quasi-Banach operator ideal admitting a continuous trace τ. If $V=V(x,t)$ is an $\mathscr{A}(E)$-valued solution of the operator KdV equation

$$V_t=V_{xxx}+3V_x^2\quad(x,t\in\mathbb{R})$$

such that $\mathrm{rank}(V_x)=1$, then $v=\tau(V)$ is a solution of the KdV equation

$$v_t=v_{xxx}+3v_x^2.$$

Proof: Applying the trace τ to the operator KdV equation and using the multiplicativity property of τ for the rank 1 operators V_x we check

$$\tau(V_t)=\tau(V_{xxx})+3\tau(V_x^2)=\tau(V_{xxx})+3(\tau(V_x))^2.$$

Finally, the continuity of τ yields the desired assertion

$$(\tau(V))_t=(\tau(V))_{xxx}+3[(\tau(V))x]^2.$$

□

An important conclusion for future references is stated in the following theorem.

Theorem III B 2: (i) Let E be a Banach space, A, $B\in\mathscr{L}(E)$, and $L(x,t):=e^{Ax+A^3t}B$ $(x,t\in\mathbb{R})$. Then the operator family

$$V=V(x,t)=(I+L)^{-1}(AL+LA)=(I+L)^{-1}e^{Ax+A^3t}(AB+BA),$$

provided that $(I+L)^{-1}$ exists, is a solution of the operator KdV equation

$$V_t=V_{xxx}+3V_x^2.$$

Moreover, if $\operatorname{rank}(AB+BA)=1$, then

$$v=\operatorname{tr}((I+L)^{-1}(AL+LA))$$

is a solution of the KdV equation

$$v_t=v_{xxx}+3v_x^2.$$

(ii) Let $\mathscr{A}$ be any quasi-Banach operator ideal admitting a continuous determinant δ. If $A\in\mathscr{L}(E)$ and $B\in\mathscr{A}(E)$ such that $\operatorname{rank}(AB+BA)=1$, then the solution of (i) may be realized by the determinant δ as

$$v=\operatorname{tr}((I+L)^{-1}(AL+LA))=2\frac{(\delta(I+L))_x}{\delta(I+L)}.$$

Proof: Using the equations

$$L_x=AL \quad \text{and} \quad L_t=A^3L,$$

we may show by a tedious calculation that $V=(I+L)^{-1}(AL+LA)$ solves the operator KdV equation. The proof is straightforward and left to the reader.

The ''moreover'' part of (i) follows from Proposition III B 1 by taking, for instance, the operator ideal $\mathscr{N}_{2/3}$ of $\frac{2}{3}$-nuclear operators which admits a continuous trace (cf. the Appendix). Indeed, because $\operatorname{rank}(AB+BA)=1$, we have that $V=(I+L)^{-1}e^{Ax+A^3t}(AB+BA)$, V_x, V_{xxx}, and V_t are rank 1 operators. Therefore,

$$v=\operatorname{tr}_{\mathscr{N}_{2/3}}(V)=\operatorname{tr}(V)$$

is a solution of the KdV equation.

Since the operator V is a rank 1 operator we may also give an alternative proof similar to Ref. 8. Indeed, we have

$$AB+BA=a\otimes c \quad \text{with some } a\in E' \text{ and } c\in E.$$

Hence, V may be written as

$$V=a\otimes c(x,t)$$

with $c(x,t)=(I+L)^{-1}e^{Ax+A^3t}c$. Furthermore, $V_t=a\otimes c_t$, $V_x=a\otimes c_x$, $V_{xxx}=a\otimes c_{xxx}$. Inserting this equation into the operator KdV equation we obtain

$$a\otimes c_t = a\otimes c_{xxx} + 3(a\otimes c_x)^2 = a\otimes c_{xxx} + 3\langle c_x, a\rangle a\otimes c_x .$$

Because of $a\neq 0$ there is an element $z\in E$ with $\langle z,a\rangle = 1$. Consequently, the previous equation applied to z yields

$$\langle z,a\rangle c_t = \langle z,a\rangle c_{xxx} + 3\langle c_x, a\rangle\langle z,a\rangle c_x$$

or

$$c_t = c_{xxx} + 3\langle c_x, a\rangle c_x .$$

Now, applying the functional a to this equation we obtain

$$\langle c_t, a\rangle = \langle c_{xxx}, a\rangle + 3(\langle c_x, a\rangle)^2.$$

Finally, the continuity of the functional a implies

$$(\langle c,a\rangle)_t = (\langle c,a\rangle)_{xxx} + 3((\langle c,a\rangle)_x)^2,$$

which states that

$$v = \langle c(x,t), a\rangle = \mathrm{tr}(a\otimes c(x,t)) = \mathrm{tr}(V)$$

is a solution of the KdV equation.

Finally, we turn to (ii). Because $B\in\mathscr{A}(E)$ we have $L = e^{Ax+A^3t}B \in \mathscr{A}(E)$ and $L_x = AL \in \mathscr{A}(E)$. Since $V=(I+L)^{-1}(AL+LA)$ has rank 1 it follows

$$\mathrm{tr}(V) = \mathrm{tr}((I+L)^{-1}(AL+LA)) = \dot{\delta}((I+L)^{-1}(AL+LA)),$$

where the continuous trace $\dot{\delta}$ is related by the trace-determinant theorem (cf. Sec. II C) via the formula

$$(\delta(I+L))_x = \dot{\delta}((I+L)^{-1}L_x)\delta(I+L).$$

Using the properties of a trace we obtain

$$\dot{\delta}((I+L)^{-1}(AL+LA)) = \dot{\delta}((I+L)^{-1}AL) + \dot{\delta}((I+L)^{-1}LA)$$

and

$$\dot{\delta}((I+L)^{-1}LA) = \dot{\delta}(L(I+L)^{-1}A) = \dot{\delta}((I+L)^{-1}AL).$$

Hence,

$$\dot{\delta}((I+L)^{-1}(AL+LA)) = 2\,\dot{\delta}((I+L)^{-1}AL) = 2\,\dot{\delta}((I+L)^{-1}L_x).$$

Combining the previous formulas and using (i) we check

$$v = \mathrm{tr}((I+L)^{-1}(AL+LA)) = 2\,\dot{\delta}((I+L)^{-1}L_x) = 2\,\frac{(\delta(I+L))_x}{\delta(I+L)}.$$

This completes the proof. □

Remark: The previous theorem stresses the fact that the solution

$$v=\mathrm{tr}((I+L)^{-1}(AL+LA))=2\,\frac{(\delta(I+L))_x}{\delta(I+L)}$$

of the KdV equation may be realized by any continuous determinant $\delta(I+L)$ provided that the operator B appearing in $L = e^{Ax+A^3t}B$ belongs to an operator ideal $\mathscr{A}$ admitting a continuous determinant and satisfies the rank 1 condition $\mathrm{rank}(AB+BA)=1$. The advantage of expressing the solution of the KdV equation by determinants is that one may avoid the inverse operator $(I+L)^{-1}$. This provides us the flexibility to study solutions in concrete cases as we will see in subsequent sections.

IV. REALIZATIONS OF SOLUTIONS BY DETERMINANTS

This section is devoted to several important examples of realizations of solutions of the KdV equation by determinants. We mainly illustrate the abstract theory of traces and determinants by applying this machinery to matrix operators on sequence spaces.

A. The equation $XA+BX=C$

Because of the rank 1 condition, $\mathrm{rank}(AX+XA)=1$, of the foregoing Theorem III B 2, the following problem arises: Let $A\in\mathscr{L}(E)$ and $B\in\mathscr{L}(F)$ be bounded operators on the Banach spaces E and F, respectively. We are interested in the operator equation

$$XA+BX=C,$$

where $C\in\mathscr{A}(E,F)$ is a given operator of a Banach operator ideal $\mathscr{A}$ and $X\in\mathscr{A}(E,F)$ is the solution. This equation has been studied extensively for the operator ideal $\mathscr{L}$ of bounded operators. For our purpose, we consider the operator

$$\Phi:\mathscr{A}(E,F)\to\mathscr{A}(E,F),\quad \text{given by } \Phi(X)=XA+BX.$$

The existence and uniqueness of the above problem is equivalent to saying that Φ is invertible on $\mathscr{A}$. Thus, it is natural to ask for the spectrum $\mathrm{spec}(\Phi)$ of this operator. Recall the spectrum $\mathrm{spec}(T)$ of a bounded operator $T\in\mathscr{L}(E)$ on a Banach space E,

$$\mathrm{spec}(T)=\{\lambda\in\mathbb{C}\,|\,\lambda I-T \text{ is not invertible in } \mathscr{L}(E)\}.$$

A result of Eschmeier[9] states that

$$\mathrm{spec}(\Phi)=\mathrm{spec}(A)+\mathrm{spec}(B),$$

where the right-hand side of this equation refers to the Minkowski sum of two sets,

$$\mathrm{spec}(A)+\mathrm{spec}(B):=\{\lambda+\mu\in\mathbb{C}\,|\,\lambda\in\mathrm{spec}(A),\mu\in\mathrm{spec}(B)\}.$$

Consequently, $\Phi^{-1}:\mathscr{A}(E,F)\to\mathscr{A}(E,F)$ exists if and only if $0\notin\mathrm{spec}(A)+\mathrm{spec}(B)$.

Remark: Recently, the first-named author found a different approach to this result which extends to all p-Banach operator ideals. We will not use this in the sequel.

We note the following lemma, of which use will be made in later arguments.

Lemma IV A 1: Let E,F be Banach spaces, and let $A\in\mathscr{L}(E)$, $B\in\mathscr{L}(F)$ be bounded operators. Then the following assertions are true:

(i) If $0\notin\mathrm{spec}(A)+\mathrm{spec}(B)$, then for any Banach operator ideal $\mathscr{A}$ and any $C\in\mathscr{A}(E,F)$ there exists a unique operator $X\in\mathscr{A}(E,F)$ satisfying the equation

$$XA+BX=C.$$

(ii) If

$$\int_0^\infty \|e^{Bs}Ce^{As}|\mathscr{A}\|\, ds<\infty$$

for a Banach operator ideal $\mathscr{A}$, then the operator X defined by the improper integral

$$X=-\int_0^\infty e^{Bs}Ce^{As}\, ds$$

in $\mathscr{A}(E,F)$ satisfies the equation

$$XA+BX=C.$$

Proof: The assertion (i) follows directly from Eschmeier's result mentioned above. So we turn to the proof of (ii). Observe that the map $f:[0,\infty)\to\mathscr{A}(E,F)$ defined by $f(s)=e^{Bs}Ce^{As}$ is continuously differentiable in $\mathscr{A}$ and

$$\frac{df}{ds}(s)=f(s)A+Bf(s).$$

Moreover, for every $R>0$ we have

$$\int_0^R f(s)ds\in\mathscr{A}(E,F).$$

Because of our assumption, $\int_0^\infty\|e^{Bs}Ce^{As}|\mathscr{A}\|ds<\infty$, we find that the operators $\int_0^R f(s)ds$ form a Cauchy-net in $\mathscr{A}(E,F)$. The completeness of $\mathscr{A}$ implies that $X=-\int_0^\infty f(s)ds$ $=-\lim_{R\to\infty}\int_0^R f(t)dt\in\mathscr{A}(E,F)$.

Since $\Phi:\mathscr{A}(E,F)\to\mathscr{A}(E,F)$, again defined by $\Phi(Z)=ZA+BZ$, is bounded, we check $\Phi(X)=(-\lim_{R\to\infty}\int_0^R f(s)ds)A+B(-\lim_{R\to\infty}\int_0^R f(s)ds)=-\lim_{R\to\infty}(\int_0^R f(s)A+Bf(s)ds)$ $=-\lim_{R\to\infty}\int_0^R(df/ds)(s)ds=-\lim_{R\to\infty}[f(R)-f(0)]=C-\lim_{R\to\infty}f(R)$. Consequently,

$$\lim_{R\to\infty}\|f(R)|\mathscr{A}\|=\|\Phi(X)-C|\mathscr{A}\|.$$

Using this and the assumption $\int_0^\infty\|f(s)|\mathscr{A}\|ds<\infty$, we infer

$$\|\Phi(X)-C|\mathscr{A}\|=0,$$

implying that $\Phi(X)=C$ as desired. □

B. Realizations of solutions by determinants of nuclear operators

Under certain restrictions on the operator $A\in\mathscr{L}(E)$ appearing in Theorem III B 2 we can formulate the following version of this theorem.

Theorem IV B 1: Let E be a Banach space with the approximation property and $A\in\mathscr{L}(E)$. Then the following assertions are true:

(i) If $0\notin\mathrm{spec}(A)+\mathrm{spec}(A)$, then for any $a\in E'$ and $c\in E$ there exists a unique operator $B\in\mathscr{N}(E)$ satisfying the equation $AB+BA=a\otimes c$, and

$$v=\mathrm{tr}((I+L)^{-1}(AL+LA))=2\,\frac{(\det_{\mathscr{N}}(I+L))_x}{\det_{\mathscr{N}}(I+L)},$$

where $L := e^{Ax+A^3t}B$, is a solution of the KdV equation

$$v_t = v_{xxx} + 3v_x^2,$$

provided that $(I+L)^{-1}$ exists.

(ii) If

$$\int_0^\infty \|e^{A's}a\| \cdot \|e^{As}c\| ds < \infty \quad \text{for } a \in E' \quad \text{and } c \in E,$$

then the nuclear operator

$$B = -\int_0^\infty e^{A's}a \otimes e^{As}c \; ds$$

is a solution of the operator equation

$$AB + BA = a \otimes c,$$

and

$$v = \operatorname{tr}((I+L)^{-1}(AL+LA)) = 2\frac{(\det_{\mathscr{N}}(I+L))_x}{\det_{\mathscr{N}}(I+L)},$$

where $L := e^{Ax+A^3t}B$, is a solution of the KdV equation $v_t = v_{xxx} + 3v_x^2$, provided that $(I+L)^{-1}$ exists.

Proof: Put $\mathscr{A} := \mathscr{N}$ on the class of Banach spaces with the a.p. and $\delta := \det_{\mathscr{N}}$ in Theorem III B 2 and set $C := a \otimes c$ in Lemma IV A 1.

Combining Theorem III B 2 and Lemma IV A 1 we immediately check the assertions (i) and (ii) of the theorem. □

Remark: Since the right-hand side $a \otimes c$ of the operator equation

$$AB + BA = a \otimes c$$

is always nuclear, it follows that the solution B also has to be nuclear, provided that A satisfies the conditions of the previous theorem. However, for special A we even obtain solutions B belonging to quasi-Banach operator ideals admitting a spectral trace and spectral determinant, respectively.

For illustrating our theorem we give an example in the finite-dimensional case.

Example: Let $A: \mathbb{C}^N \to \mathbb{C}^N$ be an $N \times N$ matrix such that $0 \notin \operatorname{spec}(A) + \operatorname{spec}(A)$. Let J be the Jordan form of $A = T^{-1}JT$ with Jordan blocks

$$J_i = \begin{pmatrix} k_i & 1 & & & \\ & \ddots & 0 & & \\ & & \ddots & & \\ & & & \ddots & 1 \\ 0 & & & & k_i \end{pmatrix}, \quad k_i \in \operatorname{spec}(A).$$

If $a, c \in \mathbb{C}^N$, then $B: \mathbb{C}^N \to \mathbb{C}^N$ is a solution of the equation $AB + BA = a \otimes c$ if and only if $\widetilde{B} = TBT^{-1}$ is a solution of the equation $J\widetilde{B} + \widetilde{B}J = (T^{-1})' a \otimes Tc$.

Hence, $L(t,x) = e^{Ax+A^3t}B = T^{-1}e^{Jx+J^3t}\widetilde{B}\,T$ is related to $e^{Jx+J^3t}\widetilde{B}$.

Thus, we may confine ourselves to a matrix A having Jordan form. Moreover, one may show that $\det(I+L_N(t,x))$ has the shape

$$\det(\delta_{ij}+p_{ij}(t,x)e^{k_i x+k_i^3 t})_{i,j=1}^N,$$

where the p_{ij} are polynomials in t and x generated by the Jordan blocks of A, and

$$v=2\frac{(\det(\delta_{ij}+p_{ij}(t,x)e^{k_i x+k_i^3 t}))_x}{\det(\delta_{ij}+p_{ij}(t,x)e^{k_i x+k_i^3 t})},$$

is a solution of the KdV equation $v_t=v_{xxx}+3v_x^2$.

C. Diagonal operators and realizations of solutions by spectral determinants

In this section we continue the investigations of the previous section. We realize solutions

$$v=2\frac{(\det_\lambda(I+L))_x}{(\det_\lambda(I+L))}$$

of the KdV equation by spectral determinants, where $L:=e^{Dx+D^3t}B$ is defined by a diagonal operator D on a Banach sequence space E and an operator B satisfying the equation

$$DB+BD=a\otimes c,\quad a\in E',\quad c\in E.$$

It turns out that under certain conditions on D the operator B belongs to a quasi-Banach operator ideal $\mathscr{A}$ possessing a spectral determinant $\det_\lambda$. Moreover, we are going to show that such solutions, in a universal way, may also be represented by the determinant of a corresponding operator L of the ideal component $\mathscr{N}(l_1)$. The results complement results of Gesteczy *et al.*[10]

For our purpose we need the following quasi-Banach operator ideal which is of eigenvalue type l_1 and, hence, possesses a spectral trace (cf. the Appendix). Let E,F be arbitrary Banach spaces. An operator $T\in\mathscr{L}(E,F)$ belongs to the product operator ideal $\mathscr{L}_\infty\circ\mathscr{H}\circ\mathscr{L}_1$ if there exists a Hilbert space H, an L_1-space, and an L_∞-space, and there are operators $X\in\mathscr{L}(E,L_1)$, $R\in\mathscr{L}(L_1,H)$, $S\in\mathscr{L}(H,L_\infty)$, and $Y\in\mathscr{L}(L_\infty,F)$ such that T may be written as a product operator $T=YSRX$. Put

$$\|T|\mathscr{L}_\infty\circ\mathscr{H}\circ\mathscr{L}_1\|:=\inf\{\|Y\|\cdot\|S\|\cdot\|R\|\cdot\|X\|:\quad T=YSRX\},$$

where the infimum is taken over all such representations of T. Then, $\mathscr{L}_\infty\circ\mathscr{H}\circ\mathscr{L}_1$ becomes a quasi-Banach operator ideal in the sense of Pietsch.[4] For our purpose we need two lemmas. The first one is well known for specialists in Banach space theory. However, for the convenience of the reader we give a proof of it.

Lemma IV C 1: Each operator of the operator ideal $\mathscr{L}_\infty\circ\mathscr{H}\circ\mathscr{L}_1$ possesses absolutely summable eigenvalues.

Proof: Given $T\in\mathscr{L}_\infty\circ\mathscr{H}\circ\mathscr{L}_1(E)$, then T admits the following factorization:

$$\begin{array}{ccccc} E & & \xrightarrow{\quad T\quad} & & E \\ X\downarrow & & & & \uparrow Y \\ L_1 & \xrightarrow{R} & H & \xrightarrow{S} & L_\infty \end{array}.$$

Now we consider the related operator U defined by the factorization diagram

$$\begin{array}{ccccc} \mathrm{H} & & \xrightarrow{\quad U \quad} & & \mathrm{H} \\ S \downarrow & & & & \uparrow R \\ L_\infty & \xrightarrow{Y} & E & \xrightarrow{X} & L_1 \end{array} .$$

By Grothendieck's theorem[2,11] we know that each operator from L_∞ into L_1 factors through a Hilbert space K. Hence, we may factorize U according to the following diagram:

$$\begin{array}{ccccc} \mathrm{H} & & \xrightarrow{\quad U \quad} & & \mathrm{H} \\ S \downarrow & & & & \uparrow R \\ L_\infty & \xrightarrow{V} & K & \xrightarrow{W} & L_1 \end{array} .$$

Using again Grothendieck's theorem we infer that the operators VS and RW are Hilbert–Schmidt operators.[2,11] Furthermore, the product of Hilbert–Schmidt operators is a nuclear operator. Hence, $U \in \mathcal{N}(H)$. Because nuclear operators on Hilbert spaces possess one-summing sequences of eigenvalues we infer, by the principle of related operators (cf. the Appendix), that T is a Riesz operator having the same nonzero eigenvalues with the same algebraic multiplicities as the eigenvalues of the operator U. Hence, the sequence of eigenvalues of T belongs to l_1, which means that $\mathcal{L}_\infty \circ \mathcal{H} \circ \mathcal{L}_1$ is of eigenvalue type l_1. □

Lemma IV C 2: (i) Let $(k_i) \in l_\infty$ such that $\inf|k_i + k_j| > 0$. Then

$$T := \left(\frac{1}{k_i + k_j} \right)_{i,j=1}^{\infty} \in \mathcal{N}(l_1, l_\infty).$$

(ii) Let $(k_i) \in l_\infty$ and $k_i > 0$, $i = 1,2,3,\ldots$. Then

$$T = \left(\frac{k_i^{1/2} k_j^{1/2}}{k_i + k_j} \right)_{i,j=1}^{\infty} : l_1 \to l_\infty$$

factors through the Hilbert space $L_2[0,\infty)$ according to the following diagram:

$$\begin{array}{ccc} l_1 & \xrightarrow{\quad T \quad} & l_\infty \\ & R \searrow \quad \nearrow R' & \\ & L_2 & \end{array}$$

where R is defined on the canonical basis $\{e_i\}$ of l_1 by $Re_i = f_i$ with $f_i(s) = k_i^{1/2} e^{-k_i s}$. Moreover, $\|R\| = \sqrt{\frac{1}{2}}$ and $\|T\| = \|R\|^2 = \frac{1}{2}$.

Proof: For the proof of (i) we consider the diagonal operator $D: (\xi_i) \mapsto (k_i \xi_i)$ which defines diagonal operators D_1 on l_1 and D_∞ on l_∞, respectively. Since $\inf|k_i + k_j| > 0$, it follows by Lemma IV A 1 (i) that the equation

$$D_\infty X + X D_1 = e_0 \otimes e_0 ,$$

where $e_0 = (1,1,\ldots) \in l_\infty$, has the unique nuclear solution $X = T = (1/(k_i + k_j))_{i,j=1}^{\infty} \in \mathcal{N}(l_1, l_\infty)$.

Now let us turn to (ii). For the entries of T we easily check

$$\langle Te_j, e_i\rangle = \langle R' Re_j, e_i\rangle = \langle Re_j, Re_i\rangle = \int_0^\infty f_j(s)\overline{f_i(s)}ds = k_i^{1/2}k_j^{1/2}\int_0^\infty e^{-(k_i+k_j)s}\,ds = \frac{k_i^{1/2}k_j^{1/2}}{k_i+k_j}.$$

Because $\|f_i\| = \sqrt{\frac{1}{2}}$, $i=1,2,...$, we have $\|R\| = \|R'\| = \sqrt{\frac{1}{2}}$. Moreover,

$$\|T: l_1 \to l_\infty\| = \sup_{i,j=1,2,\ldots}\left|\frac{k_i^{1/2}k_j^{1/2}}{k_i+k_j}\right| = \frac{1}{2},$$

which completes the proof. □

Now we are prepared to prove the following proposition.

Proposition IV C 3: Let E be one of the classical sequence spaces c_0, $l_p(1\leqslant p<\infty)$ or weighted l_p-spaces and let $k=(k_i)\in l_\infty$. If one of the following conditions is satisfied,

(i) $\inf|k_i+k_j|>0$, $a=(a_i)\in E'$, $c=(c_i)\in E$, or

(ii) $k_i>0$, $i=1,2,...$, $(a_i/\sqrt{k_i})\in E'$, $(c_i/\sqrt{k_i})\in E$, then

$$L := \left(\frac{a_j c_i}{k_i+k_j}\, e^{-(k_i x + k_i^3 t)}\right)_{i,j=1}^{\infty}$$

defines an operator on E belonging to a quasi-Banach operator ideal admitting a spectral determinant

$$\det_\lambda(I+L) = \prod_{i=1}^{\infty}(1+\lambda_i(L)).$$

Moreover,

$$v = 2\frac{(\det_\lambda(I+L))_x}{\det_\lambda(I+L)},$$

provided that $\det_\lambda(I+L)\neq 0$, is a solution of the KdV equation $v_t = v_{xxx} + 3v_x^2$.

Proof: First we treat the case (i). To this end define diagonal operators

$$D: E\to E, \quad (\xi_i)\mapsto(k_i\xi_i),$$

$$D_a: E\to l_1, \quad (\xi_i)\mapsto(a_i\xi_i), \quad (a_i)\in E',$$

$$D_c: l_\infty\to E, \quad (\xi_i)\mapsto(c_i\xi_i), \quad (c_i)\in E,$$

and an operator

$$T = \left(\frac{1}{k_i+k_j}\right)_{i,j=1}^{\infty} : l_1\to l_\infty.$$

By Lemma IV C 2 (i) we have that T is nuclear. Consequently, T factors through the Hilbert space l_2, and the operator

$$B = D_c T D_a = \left(\frac{a_j c_i}{k_i+k_j}\right)_{i,j=1}^{\infty} : E\to E$$

belongs to the ideal $\mathscr{L}_\infty\circ\mathscr{H}\circ\mathscr{L}_1$. Moreover,

$$DB+BD=a\otimes c.$$

Now we turn to the case (ii) and show a corresponding result. In analogy to the previous case we define diagonal operators,

$$D:E\to E,\quad (\xi_i)\mapsto(k_i\xi_i),$$

$$D_{a/\sqrt{k}}:E\to l_1,\quad (\xi_i)\mapsto(a_i/\sqrt{k_i}\xi_i),\quad (a_i/\sqrt{k_i})\in E',$$

$$D_{c/\sqrt{k}}:l_\infty\to E,\quad (\xi_i)\mapsto(c_i/\sqrt{k_i}\xi_i),\quad (c_i/\sqrt{k_i})\in E,$$

and an operator

$$T=\left(\frac{k_i^{1/2}k_j^{1/2}}{k_i+k_j}\right)_{i,j=1}^{\infty}:l_1\to l_\infty.$$

Using Lemma IV C 2 (ii) we check that the operator T factors through a Hilbert space. Hence, the operator

$$B=D_{c/\sqrt{k}}TD_{a/\sqrt{k}}=\left(\frac{a_jc_i}{k_i+k_j}\right)_{i,j=1}^{\infty}:E\to E$$

again belongs to the ideal $\mathscr{L}_\infty\circ\mathscr{H}\circ\mathscr{L}_1$ and satisfies the equation

$$DB+BD=a\otimes c.$$

Finally, applying Theorem III B 2 to the operator

$$L:=\left(\frac{a_jc_i}{k_i+k_j}\,e^{-(k_ix+k_i^3t)}\right)_{i,j=1}^{\infty}:E\to E,$$

we find that in both cases (i) and (ii),

$$v=\operatorname{tr}((I+L)^{-1}(DL+LD))=2\,\frac{(\det_\lambda(I+L))_x}{\det_\lambda(I+L)}$$

satisfies the KdV equation $v_t=v_{xxx}+3v_x^2$, where $\det_\lambda$ is the spectral determinant on $\mathscr{L}_\infty\circ\mathscr{H}\circ\mathscr{L}_1$.

□

The following theorem is the main result of this section. It stresses the fact that there is, in a sense, a universal realization of solutions given in the previous proposition by determinants of nuclear operators on l_1. To this end, we note that a nuclear operator $T\in\mathscr{N}(l_1)$ may be expressed by a matrix $T=(\tau_{ij})$ such that

$$\|T|\mathscr{N}\|=\sum_{i=1}^{\infty}\sup_j|\tau_{ij}|<\infty.$$

Moreover, the quantities $\alpha_n(T)$ in Sec. II C may be described by the formula

$$\alpha_n(T) := \frac{1}{n!} \sum_{i_1}^{\infty} \cdots \sum_{i_n}^{\infty} \det \begin{pmatrix} \tau_{i_1 i_1} & \cdots & \tau_{i_1 i_n} \\ \vdots & & \vdots \\ \tau_{i_n i_1} & \cdots & \tau_{i_n i_n} \end{pmatrix},$$

and for the determinant $\det_{\mathcal{N}}(I+T)$ we have the expansion

$$\det_{\mathcal{N}}(I+T) = 1 + \sum_{n=1}^{\infty} \alpha_n(T).$$

Furthermore, a preliminary lemma is required.

Lemma IV C 4: Let $\mathcal{A}$ and $\mathcal{B}$ be quasi-Banach operator ideals admitting continuous traces. If $\mathcal{A}(E) \subset \mathcal{B}(E)$ and the finite rank operator $\mathcal{F}(E)$ are $\|\cdot|\mathcal{A}\|$-dense in $\mathcal{A}(E)$, then

$$\mathrm{tr}_{\mathcal{A}}(T) = \tau(T) \quad \text{for all } T \in \mathcal{A}(E),$$

where $\mathrm{tr}_{\mathcal{A}}$ is the unique continuous trace on $\mathcal{A}(E)$ and τ is any continuous trace on $\mathcal{B}(E)$.

Proof: Since $\mathcal{A}(E) \subset \mathcal{B}(E)$, we find by the closed graph theorem that $\mathcal{A}(E)$ is continuously embedded in $\mathcal{B}(E)$. Hence, τ is a continuous trace on $\mathcal{A}(E)$ which is unique by the trace extension theorem (cf. the Appendix). □

Theorem IV C 5: Let $k=(k_i) \in l_\infty$ and let one of the following conditions be satisfied:

(i) $\inf|k_i + k_j| > 0$, $c=(c_i) \in l_1$, or

(ii) $k_i > 0$, $i=1,2,\cdots$, $(c_i/k_i) \in l_1$.

Then the operator

$$L = \left(\frac{c_i}{k_i + k_j} e^{-(k_i x + k_i^3 t)} \right)_{i,j=1}^{\infty}$$

belongs to the nuclear component $\mathcal{N}(l_1)$, and

$$v = 2 \frac{(\det_{\mathcal{N}}(I+L))_x}{\det_{\mathcal{N}}(I+L)}$$

solves the KdV equation $v_t = v_{xxx} + 3v_x^2$, provided that $(I+L)^{-1}$ exists. Moreover, each of the solutions of Proposition IV C 3 may be expressed in this way.

Proof: The first part of the theorem is an immediate consequence of Theorem IV B 1. Indeed, let $D: l_1 \to l_1$ be the diagonal operator defined by

$$D(\xi_i) = (k_i \xi_i), \quad (k_i) \in l_\infty.$$

Then, because of our assumptions (i) and (ii), Lemma IV A 1 guarantees that

$$L := e^{-Dx - D^3 t} B = \left(\frac{c_i}{k_i + k_j} e^{-(k_i x + k_i^3 t)} \right) : l_1 \to l_1$$

is a nuclear operator, where the nuclear operator

$$B = \left(\frac{c_i}{k_i + k_j} \right) : l_1 \to l_1$$

satisfies the equation

$$DB + BD = e_0 \otimes c$$

with $e_0=(1,1,\ldots)\in l_\infty$ and $c=(c_i)\in l_1$ in the case of (i), and $(c_i/k_i)\in l_1$ in the case of (ii), respectively. Now Theorem IV B 1 implies that

$$v=2\frac{(\det_{\mathscr{N}}(I+L))_x}{\det_{\mathscr{N}}(I+L)}$$

is a solution of the KdV equation $v_t=v_{xxx}+3v_x^2$. This proves the first part of the theorem.

Finally, it remains for us to show that each solution of the KdV equation given in Proposition IV C 3 may be expressed in this form. We first treat the more involved case (ii) of the previous proposition. It is readily seen that the operator L appearing in Proposition IV C 3,

$$L=\left(\frac{a_jc_i}{k_i+k_j}\,e^{-(k_ix+k_i^3t)}\right)_{i,j=1}^{\infty}:E\to E,$$

where $(a_i/\sqrt{k_i})\in E'$ and $(c_i/\sqrt{k_i})\in E$, is related to

$$\tilde{L}=\left(\frac{k_i^{1/2}k_j^{1/2}}{k_i+k_j}\frac{a_ic_i}{k_i}\,e^{-(k_ix+k_i^3t)}\right)_{i,j=1}^{\infty}:l_1\to l_1.$$

Hence, for the spectral determinants we have

$$\det_\lambda(I+L)=\det_\lambda(I+\tilde{L})$$

by the principle of related operators (cf. the Appendix). According to Lemma IV C 4 it follows

$$\det_\lambda(I+\tilde{L})=\det_{\mathscr{N}}(I+\tilde{L}).$$

This is due to the fact[2,4,11] that $\mathscr{L}_\infty\circ\mathscr{H}\circ\mathscr{L}_1(l_1)\subset\mathscr{N}(l_1)$ and that the finite rank operators $\mathscr{F}(l_1)$ are $\|\cdot|\mathscr{L}_\infty\circ\mathscr{H}\circ\mathscr{L}_1\|$-dense in $\mathscr{L}_\infty\circ\mathscr{H}\circ\mathscr{L}_1(l_1)$.

Furthermore, because of the assumption $(a_i/\sqrt{k_i})\in E'$ and $(c_i/\sqrt{k_i})\in E$, we have that $(a_ic_i/k_i)\in l_1$. Thus, by the first part of the theorem,

$$\tilde{\tilde{L}}=\left(\frac{a_ic_i}{k_i+k_j}\,e^{-(k_ix+k_i^3t)}\right)_{i,j=1}^{\infty}:l_1\to l_1$$

defines a nuclear operator from l_1 into l_1. Comparing the determinants of $I+\tilde{L}$ and $I+\tilde{\tilde{L}}$,

$$\det_{\mathscr{N}}(I+\tilde{L})=1+\sum_{n=1}^{\infty}\alpha_n(\tilde{L})$$

and

$$\det_{\mathscr{N}}(1+\tilde{\tilde{L}})=1+\sum_{n=1}^{\infty}\alpha_n(\tilde{\tilde{L}}),$$

respectively, we recognize, again by the principle of related operators, that

$$\alpha_n(\tilde{L})=\alpha_n(\tilde{\tilde{L}}),\quad n=1,2,\ldots\ .$$

Hence,

$$\det_{\mathscr{N}}(I+\tilde{L})=\det_{\mathscr{N}}(I+\tilde{\tilde{L}}).$$

Obviously, $\tilde{\tilde{L}}$ has the desired shape of our theorem and this completes the proof in the case (ii). In the case (i) we immediately find that L is related to $\tilde{\tilde{L}}$. This follows from the fact that, by Lemma IV C 2, $(1/(k_i+k_j))$ defines a nuclear operator from l_1 into l_∞. Thus the principle of related operators implies

$$\det_\lambda(I+\tilde{L})=\det_\lambda(I+\tilde{\tilde{L}}),$$

where $\det_\lambda(I+\tilde{\tilde{L}})$ is the spectral determinant on $(\mathcal{N}\circ\mathcal{N})(l_1)$. Finally, again by Lemma IV C 4,

$$\det_\lambda(I+\tilde{L})=\det_{\mathcal{N}}(I+\tilde{\tilde{L}}).$$

This completes the proof. □

Finally, we will give the first conservation law for solutions of the KdV equation generated by diagonal operators with positive entries. Taking the assumptions of Theorem IV C 5 and using the expansion formula for the determinant of nuclear matrices in $t=0$, $\det_{\mathcal{N}}(I+L)$ has the shape

$$\det_{\mathcal{N}}(I+L(x,0))=1+\sum_I d_I e^{-b_I x},$$

where I runs through all nonempty finite subsets of $\mathbb{N}$ and where

$$b_I=\sum_I k_{i_r} \quad \text{and} \quad d_I=\det\left(\frac{c_{i_r}}{k_{i_r}+k_{i_s}}\right)=\left(\prod_{r=1}^{n} c_{i_r}\right)\left(\frac{\Pi_{r>s}(k_{i_r}-k_{i_s})^2}{\Pi_{r,s}(k_{i_r}+k_{i_s})}\right),$$

$I=\{i_1,\ldots,i_n\}$, $i_1<i_2<\cdots<i_n$ (see Ref. 12, p. 92 for the last equality).

If $k_i>0$ and $c_i>0$, then $\det(I+L)\neq 0$ for all $(x,t)\in\mathbb{R}^2$. Hence, $I+L$ is invertible and $(I+L)^{-1}L_x$ is infinitely times continuously differentiable. This implies $\mathrm{tr}((I+L)^{-1}L_x)\in C^\infty(\mathbb{R}^2)$.

Theorem IV C 6: Take the assumptions of Theorem IV C 5 (i) or (ii) with $k_i>0$, $c_i>0$, $i=1,2\ldots$ and $k_i\neq k_j$ for $i\neq j$. Let

$$u=2\frac{\partial}{\partial x}\,\mathrm{tr}((I+L)^{-1}L_x)=2\frac{\partial}{\partial x}\,\frac{(\det(I+L))_x}{\det(I+L)}.$$

Then, $u\in C^\infty(\mathbb{R}^2)$ solves the KdV equation

$$u_t=u_{xxx}+6uu_x$$

and

$$\int_{-\infty}^{\infty}u(x,0)dx=2\sum k_i\in(0,\infty)\cup\{\infty\}.$$

Proof: The proof of the trace relation is a slight modification of the proof in Ref. 10.

Let

$$v=2\frac{(\det(I+L))_x}{\det(I+L)}=2\,\mathrm{tr}((I+L)^{-1}L_x),$$

then

$$\int_{-\infty}^{\infty}u(x,0)dx=\lim_{r\to\infty}v(r,0)-\lim_{r\to-\infty}v(r,0).$$

Since

$$\|L(r,0)|\mathcal{N}\| = \sum_i \sup_j \left| e^{-k_i r} \frac{c_i}{k_i + k_j} \right| \leqslant \sum_i e^{-k_i r} \left| \frac{c_i}{k_i} \right| \to 0 \quad \text{as } r \to \infty,$$

we obtain $\lim_{r\to\infty} v(r,0) = 0$.

Using the preceding remark we find

$$-v(r,0) = 2 \frac{\Sigma_i d_i b_i e^{-b_i r}}{1 + \Sigma_i d_i e^{-b_i r}} \quad \text{with } d_i b_i > 0 \quad \text{and } (d_i) \in l_1.$$

As

$$\frac{\Sigma_i d_i b_i e^{-b_i r}}{1 + \Sigma_i d_i e^{-b_i r}} \leqslant \sup b_i,$$

we only have to prove that

$$\frac{\Sigma_i d_i b_i e^{-b_i r}}{1 + \Sigma_i d_i e^{-b_i r}} \geqslant b \quad \text{for all } 0 < b < \sup b_i \text{ and sufficiently large} - r.$$

Let $A_1 = \{j \in \mathbb{N} : b - b_j < 0\} \neq \emptyset$ and $A_2 = \mathbb{N} \setminus A_1$, then

$$\sum_{A_1} d_j (b_j - b) e^{-(b_j - b)r} \to \infty \quad \text{as } r \to -\infty$$

and

$$\sum_{A_2} d_j (b - b_j) e^{-(b_j - b)r} \quad \text{is bounded by } b \sum_{A_2} d_j \text{ for all } r \leqslant 0.$$

Hence, there is an $M > 0$ such that for all $r < -M$

$$\sum_{A_1} d_j (b_j - b) e^{-(b_j - b)r} \geqslant \sum_{A_2} d_j (b - b_j) e^{-(b_j - b)r} + b e^{br}.$$

This yields

$$\frac{\Sigma_i d_i b_i e^{-b_i r}}{1 + \Sigma_i d_i e^{-b_i r}} \geqslant b \quad \text{for all } r < -M.$$

□

V. CONCLUDING REMARKS

As already mentioned the first-named author recently proved the following theorem.[13]

Theorem V.1: Let E, F be Banach spaces and $A \in \mathcal{L}(E)$, $B \in \mathcal{L}(F)$, such that $0 \notin \operatorname{spec}(A) + \operatorname{spec}(B)$. Then the equation

$$BX + XA = a \otimes c, \quad a \in E', c \in F,$$

has a unique solution X belonging to any p-Banach operator ideal, in particular, to the operator ideal $\mathcal{N}_p$ of p-nuclear operators for any $0 < p \leqslant 1$.

This theorem guarantees that we may drop the assumption that E has the approximation property in the case of Theorem IV B 1 (i). As a further consequence we find that the operator in IV C 2 (i) is even p-nuclear for any p with $0<p\leqslant 1$. Moreover, the above theorem implies directly that the operator L in Proposition IV C 3 (i) possesses a spectral determinant for any sequence space E.

Lemma IV A 1 (ii) cannot be extended to p-Banach operator ideals ($p<1$). This was shown to us by Thomas Kühn,[14] who gave an example of a nuclear matrix $(c_i c_j/(k_i+k_j))\in\mathcal{N}(l_2)$ which is not p-nuclear for any $p<1$.

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APPENDIX

We collect some recent results concerning the existence and uniqueness of traces on operator ideals.

A quasi-Banach operator ideal $\mathcal{A}$ with a continuous trace is contained in the Banach operator ideal of so-called integral operators.[3] Therefore, the component $\mathcal{A}(E)$ consists entirely of Riesz operators. Since the elements $\lambda\neq 0$ of the spectrum of a Riesz operator are isolated eigenvalues with finite algebraic multiplicity having no point of accumulation except possibly for $\lambda=0$ we may assign to every Riesz operator $T\in\mathcal{L}(E)$ an eigenvalue sequence $(\lambda_n(T))$ by the following rule:

Every eigenvalue $\lambda\neq 0$ is counted consecutively according to its multiplicity and the eigenvalues are arranged in order of nonincreasing absolute values. If T possesses less than n eigenvalues $\lambda\neq 0$, then $\lambda_n(T)=\lambda_{n+1}(T)=\cdots=0$. By this rule we always have an infinite sequence of eigenvalues. A useful tool for investigating the behavior of eigenvalues of operators in Banach spaces is Pietsch's principle of related operators.[3]

Principle of related operators. The operators $S\in\mathcal{L}(E)$ and $T\in\mathcal{L}(F)$ are said to be *related* if there exists $A\in\mathcal{L}(F,E)$ and $B\in\mathcal{L}(E,F)$ such that $S=AB$ and $T=BA$. Let $S\in\mathcal{L}(E)$ and $T\in\mathcal{L}(F)$ be related. If S is a Riesz operator, then so is T. Moreover, both operators have the same nonzero eigenvalues with the same multiplicities.

We say that a quasi-Banach operator ideal $\mathcal{A}$ has *eigenvalue type* l_p if, for arbitrary Banach spaces E, all operators $T\in\mathcal{A}(E)$ are Riesz operators and $(\lambda_n(T))\in l_p$. Moreover, we mention an important tool of the theory of eigenvalue distributions.

Principle of uniform boundedness.[3] Let $\mathcal{A}$ be a quasi-Banach operator ideal which is of eigenvalue type l_p. Then there exists a universal constant $c\geqslant 1$ such that $\|(\lambda_n(T))\|_p\leqslant c\|T|\mathcal{A}\|$ for all $T\in\mathcal{A}(E)$ and all Banach spaces E.

The following striking result about spectral traces has been recently obtained by Ransford, Taylor, and White.[15]

Spectral trace. Let $\mathcal{A}$ be a quasi-Banach operator ideal of eigenvalue type l_1. For arbitrary Banach spaces E and every $T\in\mathcal{A}(E)$ we define

$$\mathrm{tr}_\lambda(T):=\sum_{n=1}^{\infty}\lambda_n(T).$$

Then the function $\mathrm{tr}_\lambda:\cup_E\mathcal{A}(E)\to\mathbb{C}$ is a continuous trace and is called the *spectral trace*.

As already mentioned in Sec. III A, Kalton[7] showed the existence of a quasi-Banach operator ideal $\mathcal{A}$ admitting different continuous traces.[3] In contrast to this result we give an elementary but useful statement concerning the uniqueness of traces.

Trace extension theorem.[3] Let $\mathcal{A}$ be a quasi-Banach operator ideal such that for all Banach spaces E and F the finite rank operators $\mathcal{F}(E,F)$ are $\|\cdot|\mathcal{A}\|$-dense in $\mathcal{A}(E,F)$ and such that there exists a constant $c \geqslant 1$ with $|\tau(T)| \leqslant c\|T|\mathcal{A}\|$ for all $T \in \mathcal{F}(E)$ and all Banach spaces E.
Then $\mathcal{A}$ admits a unique continuous trace denoted by $\mathrm{tr}_{\mathcal{A}}$.

The unique trace $\mathrm{tr}_{\mathcal{A}}: \mathcal{A}(E) \to \mathbb{C}$ can be defined for all $T \in \mathcal{A}(E)$ by the $\|\cdot|\mathcal{A}\|$-continuous extension of $\mathrm{tr}: \mathcal{F}(E) \to \mathbb{C}$.

There are many useful quasi-Banach operator ideals admitting spectral traces.[2,3] Combining the trace extension theorem with the spectral trace we obtain the so-called spectral trace theorem.

Spectral trace theorem. Let $\mathcal{A}$ be a quasi-Banach operator ideal of eigenvalue type l_1. If for all Banach spaces E and F the finite rank operators $\mathcal{F}(E,F)$ are $\|\cdot|\mathcal{A}\|$-dense in $\mathcal{A}(E,F)$, then there is an unique continuous trace on $\mathcal{A}$ which is a spectral trace, i.e.,

$$\mathrm{tr}_{\mathcal{A}}(T) := \sum_{n=1}^{\infty} \lambda_n(T) = \mathrm{tr}_{\lambda}(T) \quad \text{for all } T \in \mathcal{A}(E) \quad \text{and all Banach spaces } E.$$

The trace-determinant theorem (cf. Sec. II C) states that there is a one-to-one correspondence between continuous traces and continuous determinants. Moreover, a quasi-Banach operator ideal admits a *spectral determinant* $\det_{\lambda}$ if and only if it admits a spectral trace, where $\det_{\lambda}$ is defined by

$$\det_{\lambda}(I+T) := \prod_{n=1}^{\infty} (1+\lambda_n(T)) \quad \text{for } T \in \mathcal{A}(E) \quad \text{and all } E.$$

For the spectral determinant one has the formula (cf. Sec. II C)

$$(\det_{\lambda}(I+T(z)))^{\cdot} = \mathrm{tr}_{\lambda}((I+T(z))^{-1}\dot{T}(z))\det_{\lambda}(I+T(z)).$$

Finally, for illustrating the previous abstract results we consider again the Banach operator ideal $\mathcal{N}$ of nuclear operators.

The approximation property of a Banach space E (cf. Sec. II C) is equivalent to the estimate

$$\mathrm{tr}_{\mathcal{N}}(T) \leqslant \|T|\mathcal{A}\| \quad \text{for } T \in \mathcal{F}(E),$$

which already appeared in the trace extension theorem.[2,3] Hence, by this theorem there exists a unique continuous trace $\mathrm{tr}_{\mathcal{N}}: \mathcal{N}(E) \to \mathbb{C}$ on the class of Banach spaces with the a.p. given by the formula

$$\mathrm{tr}_{\mathcal{N}}(T) = \sum_{i=1}^{\infty} \langle x_i, a_i \rangle$$

for any representation $T = \Sigma_{i=1}^{\infty} a_i \otimes x_i$ of $T \in \mathcal{N}(E)$.

Since the operator ideal $\mathcal{N}$ is of eigenvalue type l_2 only, we cannot expect that $\mathrm{tr}_{\mathcal{N}}$ is a spectral trace. For instance,[2] the ideal components $\mathcal{N}(l_p)$, $1 \leqslant p \leqslant \infty$, possess the optimal eigenvalue type l_r with $1/r = 1 - |\frac{1}{2} - 1/p|$. Consequently, for $p = 1$ or ∞ we have the worst eigenvalue type l_2 and for the Hilbert space component $\mathcal{N}(l_2)$ the best eigenvalue type l_1. In the case of $\mathcal{N}(l_2)$ we obtain by the spectral trace theorem in this way Lidskij's well-known spectral trace formula

$$\mathrm{tr}_{\mathcal{N}}(T) = \sum_{n=1}^{\infty} \lambda_n(T) \quad \text{for } T \in \mathcal{N}(l_2).$$

However, in contrast to that, the ideal component $\mathcal{N}(l_1)$ behaves rather strangely. Indeed, by Enflo[6] there exists an operator $S \in \mathcal{N}(l_1)$ such that

$$\mathrm{tr}_{\mathcal{N}}(S)=1 \quad \text{and} \quad S^2=0.$$

Hence the nilpotent operator S cannot possess any eigenvalue $\lambda_0\neq 0$. Thus it is impossible to compute the trace $\mathrm{tr}_{\mathcal{N}}(S)=1$ from the trivial eigenvalue sequence (0,0,...).

The previous facts indicate that even for the smallest Banach operator ideal $\mathcal{N}$ of nuclear operators, a well-defined trace cannot exist for nuclear operators between arbitrary Banach spaces as they were originally defined. In view of these difficulties one was interested in smaller operator ideals admitting traces with all the desired properties. This automatically leads to the notion of a quasi-Banach operator ideal. Hence, Grothendieck reduced the ideal of nuclear operators to that of r-nuclear operators, $0<r\leqslant 1$. Let us recall that an operator $T\in\mathcal{L}(E,F)$ is *r-nuclear* if it admits a representation

$$Tx=\sum_{i=1}^{\infty}\langle x,a_i\rangle y_i, \quad a_i\in E',y_i\in F,$$

such that $\Sigma_{i=1}^{\infty}\|a_i\|^r\|y_i\|^r<\infty$. By $\mathcal{N}_r$ we denote the collection of all r-nuclear operators. Regarding all possible representations of $T\in\mathcal{N}_r(E,F)$ and taking the infimum

$$\|T|\mathcal{N}_r\|:=\inf\left\{\left(\sum_{i=1}^{\infty}\|a_i\|^r\|y_i\|^r\right)^{1/r}\right\},$$

we obtain the quasi-Banach operator ideal $\mathcal{N}_r$ of all r-nuclear operators with $\mathcal{N}_1=\mathcal{N}$.

It is well known[3] that the ideal $\mathcal{N}_r$ is of eigenvalue type l_q with $1/q=1/r-\frac{1}{2}$. Since $\mathcal{N}_{2/3}$ is of eigenvalue type l_1 and $\mathcal{N}_r\subset\mathcal{N}_{2/3}$ for $0<r\leqslant\frac{2}{3}$ we find that there exists a spectral trace on $\mathcal{N}_r$ for $0<r\leqslant\frac{2}{3}$. Moreover, in this case we know that by

$$\mathrm{tr}_{\mathcal{N}_r}(T)=\sum_{i=1}^{\infty}\langle x_i,a_i\rangle \quad \text{for } T=\sum_{i=1}^{\infty}a_i\otimes x_i\in\mathcal{N}_r,$$

a trace on $\mathcal{N}_r(E)$ for all Banach spaces E is defined. Since the finite rank operators are $\|\cdot|\mathcal{N}_r\|$-dense in $\mathcal{N}_r$, we conclude by the spectral trace theorem that, for $0<r\leqslant\frac{2}{3}$,

$$\mathrm{tr}_{\mathcal{N}_r}(T)=\sum_{n=1}^{\infty}\lambda_n(T)=\mathrm{tr}_{\lambda}(T) \quad \text{for } T\in\mathcal{N}_r(E) \quad \text{and all } E.$$

Finally, we mention[3] that on the components $\mathcal{N}_r(l_1)$ there exists no spectral trace in the case $\frac{2}{3}<r\leqslant 1$.

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Singular and unstable solutions of the Korteweg–de Vries hierarchy

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The Korteweg–de Vries (KdV) equation is solved using an inverse scattering transform approach using the continuous part of the spectrum of the Schrödinger equation. It is assumed that the reflection coefficient that corresponds to the initial condition of the KdV equation is a rational function of the wave number. It is shown that the Lyapunov exponent of the associated nonlinear evolution equation can be larger than zero if the reflection coefficient has poles that are close to zero. A positive Lyapunov exponent suggests that corresponding solutions of the KdV equation are unstable. This approach is generalized to the KdV hierarchy. © *1996 American Institute of Physics.* [S0022-2488(96)01304-2]

I. INTRODUCTION

Many papers have been published concerning the Korteweg–de Vries (KdV) hierarchy, a topic that is related to a wide variety of physical phenomena, varying from the propagation of water waves to subjects in quantum field theories. The most common method that is used to find solutions of the KdV equation is the inverse scattering transformation (IST) that was developed by Gardner, Greene, Kruskal, and Miura (GGKM).[1,2] It was shown by these authors that the KdV equation can be solved using the inverse problem of the Schrödinger equation assuming that the time-dependent potential function is a solution of the KdV equation. In the papers by GGKM a method is presented to formulate the time-dependence of the scattering data of the potential function that acts as the initial condition of the KdV equation.[1,2] It was also shown by GGKM that soliton solutions could be constructed using the discrete part of the spectrum of the Schrödinger equation.[1,2]

Meanwhile, it was shown by Lax[3] that the IST approach could be applied on a wide variety of differential equations as long as they form a so called ''Lax-pair.'' Lax formulated a general method to compute the time-dependence of the scattering data, followed by investigations of a great number of nonlinear differential equations using the IST.[4,5] It was observed that using the discrete part of the spectrum leads to soliton solutions of these differential equations.

Solitons are understood to be nondispersive because dispersion effects and effects due to the nonlinearity cancel each other out. Furthermore, from the observation that solitons maintain their shape over long time scales indicates that solitons are stable. This is in contradiction with the fact that the KdV equation is a nonlinear differential equation that can be expected to have unstable solutions.

It is remarkable that after nearly thirty years of studying the IST, only the discrete part of the spectrum of the Schrödinger equation is taken into account. Recently, from studies of the stability of the inverse problem of the Schrödinger equation,[6–10] it was observed that the inverse problem of the Schrödinger equation is very sensitive to small errors in the low energy content of the spectrum of the reflection coefficient. From this, the idea has risen that using the continuous part of the spectrum might lead to unstable solutions of the KdV equation. In this paper singular solutions of the KdV equation are constructed using the continuous part of the spectrum, and it is shown that these solutions correspond to a positive Lyapunov coefficient.

This paper has the following structure. In Sec. II, solutions of the KdV equation are constructed using the continuous part of the spectrum of the Schrödinger equation. In Sec. III, it is

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shown that these solutions correspond to positive Lyapunov coefficients. In Sec. IV, singular solutions for the complete KdV hierarchy are derived. The results are discussed in Sec. V. Technical issues concerning to the Gelfand–Levitan–Marchenko equation are added in two appendices.

II. SINGULAR SOLUTIONS OF THE KdV EQUATION

Consider the KdV equation:

$$\begin{aligned} &u_{xxx}-6u_x u+u_t=0,\\ &u(x,t=0)=u^{(0)}(x). \end{aligned} \tag{1}$$

In Eq. (1), $u^{(0)}(x)$ represents the initial condition of the KdV equation at $t=0$. The most commonly used strategy to generate solutions of the KdV equation is using the inverse scattering transformation.[11] Following this approach, the KdV equation can be solved by using the following Lax pair:[4,12]

$$\psi_{xx}-u\psi=-k^2\psi, \tag{2}$$

$$(C-u_x)\psi+2(u+2k^2)\psi_x=\psi_t. \tag{3}$$

The physical asymptotic behavior of the Schrödinger equation (2) is given by

$$\psi_1(k,x)\sim\begin{cases} e^{ikx}+R_+(k)e^{-ikx}, & x<0,\\ T(k)e^{ikx}, & x\to+\infty. \end{cases} \tag{4}$$

In the limit $x\to\infty$, the potential function u and its derivative u_x tend to zero, so Eq. (3) reduces to

$$\psi_t\approx 4k^2\psi_x+C\psi. \tag{5}$$

Substitution of the asymptotic behavior (4) of the function ψ in Eq. (3), leads to the following result:

$$\frac{d}{dt}R_+(k,t)e^{ikx}=(4ik^3+C)R_+(k,t)e^{ikx}+(-4ik^3+C)e^{-ikx}. \tag{6}$$

Hence, for $C=4ik^3$,

$$\frac{d}{dt}R_+(k,t)=8ik^3R_+(k,t). \tag{7}$$

Solving this differential equation one finds that:

$$R_+(k,t)=R_+(k,t=0)e^{8ik^3t}. \tag{8}$$

In Eq. (8), the reflection coefficient $R_+(k,t=0)$ belongs to the initial condition $u(x,t=0)$. In a similar fashion it can be derived that the discrete part of the spectrum evolves as

$$c_n(k,t)=c_n(k_n,t=0)e^{4k_n^3t}. \tag{9}$$

In Eq. (9) the bound states $c_n(k_n,t=0)$ are the residues that correspond to the poles of the transmission coefficient of the initial condition $u(x,t=0)$ that are positioned at the positive imaginary axis. The numbers k_n are the discrete eigenvalues of the Schrödinger equation.

In most applications of the inverse scattering method, the discrete part of the spectrum of the Schrödinger equation is used. In this way, soliton solutions can be constructed.[4] In contrast to this,

in this paper the continuous part of the spectrum of the Schrödinger equation is used. Furthermore, it is assumed that the reflection coefficient of this potential function is a rational function of the wave number. This implies that Sabatiers method,[13] which is described briefly in Appendix A, can be used to solve the inverse problem of the Schrödinger equation. Let p_i be a pole of the rational reflection coefficient $R_+(k)$ in equation (A10) that corresponds to the initial condition $u(x,t=0)$. It follows that the pole position p_i remains invariant under the transformation (8). The residue however undergoes the transformation $R_i \rightarrow R_i e^{8ip_i^3 t}$. Using this information, the time-dependence of the kernel $K_+(x,x,t)$ can be formulated:

$$K_+(x,x) \rightarrow K_+(x,x,t) = \frac{\mathscr{D}'_+(x,t)}{\mathscr{D}_+(x,t)}, \tag{10}$$

where

$$\mathscr{D}_+(x,t) = \det\{\delta_{ij} - (p_i + p_j)^{-1} R_j \exp[2i(p_j x + 4p_j^3 t)]\}. \tag{11}$$

The solution $u(x,t)$ of the KdV equation is then equal to

$$u(x,t) = -2\frac{d}{dx} K_+(x,x,t). \tag{12}$$

In two papers by Dorren[7,8] the stability of the Marchenko equation is investigated is the case of a reflection coefficient that is a rational function of the wave number. One of the major results of these studies is that the inverse problem of the Schrödinger equation is unstable for values of x for which the the determinant $\mathscr{D}_+(x,t=0)$ is close to zero. Similarly, it can be concluded that if the space coordinate x is fixed, the kernel $K_+(x,x,t)$ is unstable for those values of t, for which the numerical value of the determinant $\mathscr{D}_+(x=\text{const},t)$ is close to zero. Due to the fact that the time-dependence of the spectral reflection coefficient $R_+(k,t)$ manifests itself only in the exponent of Eq. (11), it can be concluded that if the determinant $\mathscr{D}_+(x,t=0)$ is zero for large values of x, the determinant $\mathscr{D}_+(x=\text{const},t)$ will also be zero at large time t. If the determinant (11) is equal to zero for certain values of x or t, the solution $u(x,t)$ of the KdV equation is singular.

As an example, the simplest case in which $u(x,t=0)$ is represented by one pole in $\mathbb{C}^+$ whose position is given by $p_i = i\beta$ is considered. Causality of the solution requires that $\beta > 0$. Furthermore, one residue positioned on the imaginary axis $R_i(t=0) = \text{id}$ $(d \in \mathbb{R})$ is chosen. From Eqs. (10)–(12), it follows that the corresponding solution of the KdV equation is equal to

$$u(x,t) = \frac{8d\beta e^{-2(\beta x - 4\beta^3 t)}}{(1 - (d/\beta)e^{-2(\beta x - 4\beta^3 t)})^2}. \tag{13}$$

It follows from substitution of Eq. (13) in Eq. (1), that Eq. (13) is a solution of the KdV equation for any choice of d and β. Furthermore, it follows that the solution (13) is unstable with respect to the ratio d/β, if the denominator of Eq. (13) is close to zero. This implies that if d/β is larger than zero, for certain values of x and t singularities in the solution (13) exist.

If d is chosen negative, a causal solution can never have a vanishing denominator. In this situation the solution (13) is always stable. The solution (13) can then be reformulated as

$$u(x,t) = \frac{-8\beta^2}{\left(\exp\left\{\beta x - 4\beta^3 t - \frac{1}{2}\log\left(-\frac{d}{\beta}\right)\right\} + \exp-\left\{\beta x - 4\beta^3 t - \frac{1}{2}\log\left(-\frac{d}{\beta}\right)\right\}\right)^2}. \tag{14}$$

Using the fact that $\operatorname{sech}^2(z) = 4/(e^z + e^{-z})^2$ and $\beta = \frac{1}{2}\sqrt{c}$, the equation takes the following form:

$$u(x,t)=-\frac{c}{2}\,\mathrm{sech}^2\left\{\frac{1}{2}\sqrt{c}(x-ct+x_0)\right\} \tag{15}$$

in which

$$x_0=-\frac{1}{\sqrt{c}}\log\left(-\frac{d}{\beta}\right). \tag{16}$$

For the special choice of a positive β and a negative d, the logarithm (16) exists and the solution (13) reduces to the well-known soliton solution.

If d is chosen positive, a new result is obtained. In this case the solution (13) is no longer a soliton solution. If d/β is larger than zero, the solution (13) has singularities for certain values of x and t. In the most simple case if only one pole and one residue are present, the solution (13) has a singularity that evolves nondispersively in time. If the initial condition of the KdV equation $u^{(0)}(x)$ is represented by more poles and residues, then it can be shown that the time evolution of this initial condition can be decomposed in an infinite series of nondispersive waves. However their total sum shows dispersive behavior. It can be concluded that if the reflection coefficient $R_+(k,t)$ is used to generate solutions of the KdV equation, a larger class of solutions is obtained than only the soliton solutions. That the soliton solutions are also present if the continuous part of the spectrum of the Schrödinger equation is used is not surprising since it has been shown that isolated poles of the reflection $R_+(k,t)$ on the positive imaginary axis are equal to the poles of transmission coefficient, and that they form the bound states of the potential function.[14] In contrast to this, the reflection coefficient $R_+(k,t)$ has poles that are not limited to the positive imaginary axis. It is concluded that solutions of the KdV equation that can be associated with the reflection coefficient $R_+(k,t)$ form a class of solutions that contains soliton solutions but also singular solutions.

The solution of the KdV equation which is given by Eqs. (10)–(12) is generated from the time-evolution of the reflection coefficient $R_+(k,t)$ that corresponds to the initial condition $u(x,t=0)$. This transformation is given by Eq. (8). If the reflection coefficient is given by Eq. (A10) in Appendix A, it follows that the poles remain invariant under the transformation (8). However the residues undergo the following transformation:

$$R_i\rightarrow R_i e^{8ip_i^3 t}. \tag{17}$$

In Appendix B, it is shown that a solution of the Marchenko equation can be decomposed in an infinite series of exponential functions. By applying the transformation (17) on Eq. (B9) in Appendix B, a series solution of the KdV equation that corresponds to the continuous part of the spectrum of the Schrödinger equation can be constructed. This result can be formulated in the following theorem:

Theorem II.1: *The function*,

$$\begin{aligned}u(x,t)=&4\sum_{i=1}^{N} R_i p_i e^{2i(p_i x+4p_i^3 t)}+4\sum_{i,j=1}^{N} R_i R_j e^{2i\{(p_i+p_j)x+4(p_i^3+p_j^3)t\}}\\&+4\sum_{ijl}^{N}\frac{(R_iR_jR_l)(p_i+p_j+p_l)}{(p_i+p_j)(p_j+p_l)}\,e^{2i\{(p_i+p_j+p_l)x+4(p_i^3+p_j^3+p_l^3)t\}}+\cdots,\end{aligned} \tag{18}$$

is a solution of the KdV-equation. If the position of the poles p_i and the residues R_j of the reflection coefficient are chosen as in Appendix A, the solution (18) is real.

A proof of Theorem II.1 is given in Appendix B. It follows from Theorem II.1 that a solution of the KdV equation can be decomposed in an infinite sum of nondispersive basis functions. Their

total sum $u(x,t)$ exhibits dispersive behavior. The IST can therefore be regarded as a nonlinear generalization of the Fourier transform that can be applied on nonlinear differential equations like the KdV equation. It depends on the structure of the kernel $K_+(x,x,t)$ whether the series expansion (18) converges or not. If the determinant $\mathscr{D}_+(x,x,t)$ is close to zero for certain values of x or t, the series expansion (18) will not converge. The convergence of $K_+(x,x,t=0)$ is related to the convergence of (18):

$$K_+(x,x,t=0)=i\sum_{i=1}^{N} R_i e^{2ip_i x}\left\{1+\sum_{j=1}^{N}\frac{R_j}{p_i+p_j}e^{2ip_j x}+\frac{R_j R_l}{(p_i+p_j)(p_j+p_l)}e^{2i(p_j+p_l)x}+\cdots\right\}. \tag{19}$$

The convergence of the kernel $K_+(x,x,t=0)$ is achieved for every x when

$$\left|\sum_{i,j=1}^{N}\frac{R_i}{(p_i+p_j)}e^{2ip_i x}\right|\leqslant\left|\sum_{i,j=1}^{N}\frac{R_i}{(p_i+p_j)}\right|\leqslant 1. \tag{20}$$

This result can be summarized in the following lemma:

Lemma II.1: The kernel $K_+(x,x,t)$ diverges if

$$\left|\sum_{i,j}^{N}\frac{R_i}{(p_i+p_j)}\right|\geqslant 1. \tag{21}$$

If the kernel $K_+(x,x,t)$ diverges, the corresponding solution $u(x,t)$ of the KdV equation can be arbitrarily large. This can be achieved by moving the positions of the poles close to the origin of the complex plane.

In this section it is argued that singular solutions of the KdV equation exist. Furthermore, it is shown in Theorem II.1 that they can be decomposed in an infinite sum of nondispersive basis functions. Their total sum however, exhibits dispersive behavior. The fundamental reason for this phenomena lays in the structure of Eq. (17). From this equation it follows that the time-dependence of the residue R_i can be obtained by multiplication with an exponential function in which only the poles p_i and the time t are present. Singular solutions of the KdV equation exists if the determinant $\mathscr{D}_+(x,t)$ is zero. If the discrete part of the spectrum of the Schrödinger equation is used, singular solutions do not exist since the determinant $\mathscr{D}_+(x,t)$ can not be zero. The singular solutions are not in the Faddeev class of physical potential functions (Appendix A), however it follows from substitution that these singular solutions satisfy the KdV equation. The main result of this section is that the instability of the Marchenko equation corresponds to the existence of singular solutions of the KdV equation. This suggests that Theorem II.1 can be generalized to all other hierarchies of differential equations that can be solved using the IST. In Sec. III, it is shown that solutions of the KdV equation which are constructed using the continuous part of the spectrum can be sensitive to small perturbations in the initial condition.

III. STABILITY ESTIMATES FOR THE KdV EQUATION

In this section it is shown that the time-evolution of the solution of the KdV equation is sensitive to small errors in the initial condition. This result is obtained using a discrete representation of the time evolution of the KdV equation (1):

$$u^{(n+1)}(x)=u^{(n)}(x)+\Delta t[6u_x^{(n)}(x)u^{(n)}(x)-u_{xxx}^{(n)}(x)]. \tag{22}$$

In Eq. (22) $u^{(n)}(x)=u(x,t=t_n)$. The derivatives $u_x^{(n)}(x)$ and $u_{xxx}^{(n)}(x)$ are defined by $u_x(x,t=t_n)$ and $u_{xxx}(x,t=t_n)$, respectively. The discrete time step is given by Δt. It follows from Eq. (22) that a solution $u^{(n+1)}(x)$ of the KdV equation can be computed, if at time $t=t_n$ the solution $u^{(n)}(x)$

and its derivatives $u_x^{(n)}(x)$ and $u_{xxx}^{(n)}(x)$ are known. Suppose that the solution $u^{(n)}(x)$ at time $t=t_n$ is contaminated with a small perturbation $\Delta u^{(n)}(x)$. This implies that the derivatives $u_x^{(n)}(x)$ and $u_{xxx}^{(n)}(x)$ are contaminated, respectively, with errors $\Delta u_x^{(n)}(x)$ and $\Delta u_{xxx}^{(n)}(x)$. Then, an error $\Delta u^{(n+1)}(x)$ in $u^{(n+1)}(x)$ is generated according to

$$\Delta u^{(n+1)}(x)=\Delta u^{(n)}(x)+6\Delta t\{u_x^{(n)}(x)[\Delta u^{(n)}(x)]+[\Delta u_x^{(n)}(x)]u^{(n)}(x)\}-\Delta t\Delta u_{xxx}^{(n)}(x). \quad (23)$$

From Eq. (23), the derivatives $\Delta u_x^{(n+1)}(x)$ and $\Delta u_{xxx}^{(n+1)}(x)$ can be computed. Hence by continuing the process of iteration the error $\Delta u^{(i)}(x)$ can be computed at arbitrary time $t=t_i$.

If the initial condition $u^{(0)}(x)$ is contaminated with an error $\Delta u^{(0)}(x)$, after n iterations an error $\Delta u^{(n)}(x)$ in $u^{(n)}(x)$ is generated according to

$$\Delta u^{(n)}(x)=\prod_{k=1}^{n} A^{(k-1)}[\Delta u^{(0)}(x)]. \quad (24)$$

The operator $A^{(n)}$, in Eq. (24), is defined by

$$A^{(n)}[\Delta u^{(n)}(x)]=\{1+6\Delta t[u_x^{(n)}(x)+u^{(n)}(x)\partial_x]-\Delta t\partial_{xxx}\}[\Delta u^{(n)}(x)]. \quad (25)$$

Equation (24) describes the error $\Delta u^{(n)}(x)$ in $u^{(n)}(x)$ as a result of an error $\Delta u^{(0)}(x)$ in $u^{(0)}(x)$. If a large number of iterations is performed, Eq. (24) can be approximated by

$$\Delta u^{(n)}(x)=\langle t^{(n)}(x)\rangle_{\text{av}}^{n}\Delta u^{(0)}(x). \quad (26)$$

In Eq. (26), $\langle t^{(n)}(x)\rangle_{\text{av}}$, is the average growth of the error $\Delta u^{(n)}(x)$ per iteration:

$$\langle t^{(n)}(x)\rangle_{\text{av}}=\frac{\Sigma_{k=1}^{n}|\Delta u^{(k)}(x)|}{n}. \quad (27)$$

Equation (26) can be reformulated as

$$\Delta u^{(n)}(x)=e^{n\log\langle t^{(n)}(x)\rangle_{\text{av}}}\Delta u^{(0)}(x)=e^{n\lambda_n(x)}\Delta u^{(0)}(x). \quad (28)$$

From Eq. (28), it follows that the corresponding Lyapunov exponent $\lambda_n(x)$ is given by

$$\lambda_n(x)=\frac{1}{n}\log\left\{\frac{\Sigma_{k=1}^{n}|\Delta u^{(k)}(x)|}{n}\right\}. \quad (29)$$

Equation (29) presents a nonstandard representation of the Lyapunov exponent $\lambda_n(x)$. However, it still describes the average growth of errors. If the Lyapunov exponent $\lambda_n(x)$ is positive, the error $\Delta u^{(n)}(x)$ in the discrete time-series $u^{(n)}(x)$ grow. This implies that the solution $u^{(n)}(x)$ is sensitive to small errors in its initial condition. Conversely, if the Lyapunov exponent $\lambda_n(x)$ is negative, the error in the discrete time-series $\lambda_n(x)$ is damped out. This implies that the solution $u^{(n)}(x)$ is not sensitive to small errors in the initial condition $u^{(0)}(x)$.

Usually, the error propagation in discrete systems is examined as a function of the free parameters in the associated difference equation. An illustrative example is given by quadratic mapping:[15,16]

$$y_{n+1}=a(1+y_n)y_n, \quad (30)$$

where the error Δy_n in y_n is examined as a function of the parameter a. If the difference equation (23) is investigated, it appears that in this case the free parameters of the iterative solution of the KdV equation (22) are the poles p_i and the residues R_i in the solution of the KdV equation (18).

It follows from Lemma II.1 that the error in the iteration series $u^{(0)}(x),u^{(1)}(x),u^{(2)}(x),...$ grows for those values of x for which the solution of the KdV equation is nearly singular. This situation can be obtained by tuning the ratio $\Sigma_{i,j}\ R_i/(p_i+p_j)$ in such a way, that the error $\Delta u^{(n)}(x)$ in Eq. (23) is so large at every time $t=t_n$, that the corresponding Lyapunov exponent $\lambda_n(x)$ is positive. If the error $\Delta u^{(n)}(x)$ is so large that the Lyapunov exponent $\lambda_n(x)$ is positive, the error in the iteration series $u^n(x)$ grows for that value of x. This implies that the time-evolution of these solutions of the KdV equation is sensitive to small perturbations in their initial condition. A positive Lyapunov exponent is often associated with unstable behavior.[15,16] As a result of this it can be concluded that singular, or nearly singular solutions of the KdV equation have an unstable time-evolution.

IV. EXTENSION TO THE KdV HIERARCHY

In this section, it is shown that conclusions that are drawn for the KdV equation can be extended to the whole KdV hierarchy. It was shown by Lax,[3] that the inverse scattering approach as developed by GGKM[1,2] can be extended to a much wider class of equations, the so-called KdV hierarchy. Let L be the Schrödinger operator, then Lax showed that a one parameter family of operators B_n satisfying the relation

$$\frac{\partial L}{\partial t}=[B_n,L], \tag{31}$$

where $[B_n,L]=B_nL-LB_n$ can also be solved using an inverse scattering approach. The one parameter family of operators B_n is given by

$$B_n=\frac{\partial^{2n+1}}{\partial x^{2n+1}}+\sum_{j=1}^{n}\left\{b_j\ \frac{\partial^{2j-1}}{\partial x^{2j-1}}+\frac{\partial^{2j-1}}{\partial x^{2j-1}}\ b_j\right\}. \tag{32}$$

In Eq. (32), the coefficients b_j depend on the solution $u(x,t)$ of the KdV hierarchy. Their specific form follows as a constraint on Eq. (31). The coefficients b_j consist modulo a constant of multiplications of the specific solution u of the KdV hierarchy and their derivatives u_n. Furthermore, it was shown by Lax[3] that the discrete eigenvalues of L are constant in time, and that the corresponding eigenfunctions satisfy the following time-dependence:

$$\frac{\partial \psi}{\partial t}=(B_n+C)\psi, \tag{33}$$

where C is an arbitrary function of t.

This result of Lax is used to find a general time-evolution for the continuous part of the spectrum of the Schrödinger equation. This result is used to show that for the whole KdV hierarchy, the positions of the poles are constant in time, and the time evolution of the residues is similar to that of Eq. (17). In order to find the time-dependence of the reflection coefficient, Eq. (32) is substituted into Eq. (33). This leads to the following expression:

$$\psi_t=\partial_{2n+1}\psi+\sum_{j=1}^{n}\{b_j\partial_{2j-1}\psi+(\partial_{2j-1}b_j)\psi\}+C\psi. \tag{34}$$

By letting the operator ∂_{2n-1} act on both sides of the Schrödinger equation it can be shown that

$$\partial_{2n+1}\psi-\sum_{m=1}^{n-1}\binom{n-1}{m}u_m\psi_{n-1-m}=-k^2\psi_{2n-1}, \tag{35}$$

if Eq. (35) is substituted into Eq. (34) it is shown that

$$\psi_t = -k^2\psi_{2n-1} + \sum_{m=1}^{n-1} \binom{n-1}{m} u_m \psi_{n-1-m} + \sum_{j=1}^{n} \{b_j \partial_{2j-1}\psi + (\partial_{2j-1} b_j)\psi\} + C\psi. \tag{36}$$

If $x \to \pm\infty$, then $u \to 0$ and $u_m \to 0$ $(m>0)$. Hence, $\partial_{2j-1} b_j \to 0$, and $b_j \to \gamma_j$, where the coefficients γ_j are constant. Equation (36) then reduces to

$$\psi_t = -k^2\psi_{2n-1} + C\psi + \sum_{j=1}^{n} \gamma_j (ik)^{2j-1}\psi. \tag{37}$$

The physical boundary conditions of Eq. (4) are given by

$$\psi = e^{-ikx} + R_+(k,t)e^{ikx}, \tag{38}$$

$$\psi_t = \frac{\partial R_+(k,t)}{\partial t}\, e^{ikx}, \tag{39}$$

$$\psi_{2j-1} = (ik)^{2j-1}\{R_+(k,t)e^{ikx} - e^{-ikx}\}. \tag{40}$$

From substitution of Eqs. (38)–(40) into Eq. (37), it follows that

$$C = -k^2(ik)^{2n-1} + \sum_{j=1}^{n} \gamma_j (ik)^{2j-1}. \tag{41}$$

From substitution of Eq. (41) into Eq. (37) it follows that

$$\frac{\partial R_+(k,t)}{\partial t} = 2k^2(-ik)^{2n-1}R_+(k,t) + \sum_{j=1}^{n} 2R_+(k,t)\gamma_j (ik)^{2j-1}. \tag{42}$$

Hence, the time-evolution of the reflection coefficient is given by

$$R_+(k,t) = R_+(k,t=0)\exp\left(-2k^2(ik)^{2n-1} + \sum_{j=1}^{n} 2\gamma_j (ik)^{2j-1} \right) t. \tag{43}$$

If we choose $n=1$ and $\gamma_1 = -3k^2$ we find the time-evolution of the reflection coefficient of the KdV equation. The general time-evolution of the solutions of the KdV hierarchy is given by Eq. (43). It is clear that this transformation does not change the position of the poles of the reflection coefficient $R_+(k,t=0)$, and it affects only the residues. From this it can be concluded that the general transformation rule for the residues is given by

$$R_i \to R_i e^{\phi(p_i)t}, \tag{44}$$

where the function $\phi(p_i)$ is given by

$$\phi(p_i) = -2p_i^2(ip_i)^{2n-1} + \sum_{j=1}^{n} 2\gamma_j (ip_i)^{2j-1}. \tag{45}$$

From this it can be concluded that all the members of the KdV hierarchy have solutions similar to Eq. (18). The transformation of the residues is given by Eq. (44). As a result of this it could be expected that all the solutions of the KdV hierarchy have solutions that are generalizations of Eq. (18) and can be expected to have an unstable time-evolution.

V. DISCUSSION

In the literature, solutions of the KdV equation are usually associated with solitons (an overview is given in the book by Ablowitz and Clarkson[4]). This result is obtained by solving the KdV equation using an IST in which the discrete part of the spectrum is used. In this article the KdV equation is solved using the continuous part of the spectrum. In Sec. II two new results are derived: the first is that singular solutions of the KdV equation exist and have a nondispersive time-evolution. Second, it is shown that a solution of the KdV equation, having an initial condition that is associated with the continuous part of the spectrum can be decomposed into an infinite series of basis functions as given by Eq. (18). All of the basis functions exhibit nondispersive behavior.

These singular solutions do not exist if only the discrete part of the spectrum of the Schrödinger equation is used because in this case the corresponding determinant $\mathscr{D}_+(x,t)$ in Eq. (11) can not be zero. It is shown explicitly in Sec. III, that by making the ratio $\Sigma_{i,j} R_i/(p_i+p_j)$ in Lemma II.1 large enough, the Lyapunov exponent $\lambda_n(x)$ that corresponds to the series $u^{(0)}(x),u^{(1)}(x),u^{(2)}(x),...$ can be made positive. From this it can be concluded that the time-evolution of solutions of the KdV equation associated with the continuous part of the spectrum is sensitive to small errors in the initial condition. In fact, a positive Lyapunov exponent $\lambda_n(x)$ is often associated with a chaotic time-evolution.

The mathematical reason for the singular behavior of the solutions of the KdV equation is related to the unstable behavior of the inverse scattering problem. In previous studies,[6–10] it is shown that the Marchenko equation is unstable in the low energy part of the reflection coefficient (poles close to the origin in the upper half-plane). This is also the reason that in Sec. IV the results of the KdV equation could be extended to the KdV hierarchy. This suggests that all other hierarchies of differential equations that can be solved using an IST approach have singular solutions that are unstable.

In the real physical world singular solutions of the KdV equations do not exist. However, from the results of this paper it can be concluded that if the initial condition of the KdV equation has a large amplitude the corresponding time-evolution is unstable. It is shown that similar behavior exists for all the other members of the KdV hierarchy, and it is indicated that these results can be generalized to all the other hierarchies that can be solved using an IST.

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APPENDIX A: THE INVERSE PROBLEM FOR RATIONAL REFLECTION COEFFICIENTS

In this appendix a brief formulation of the inverse problem for rational reflection coefficients based upon the formulation of Sabatier[13] is given. For a detailed treatment of the mathematics we refer to the book of Chadan and Sabatier.[14] Our starting-point is the following equation:

$$F_{\pm}(k,x)-1=\frac{1}{2\pi i}\lim_{\epsilon\to 0^+}\int_{-\infty}^{\infty}\frac{1-T(k')F_{\mp}(k',x)}{k'+k+i\epsilon}\,dk' + \frac{1}{2\pi i}\lim_{\epsilon\to 0^+}\int_{-\infty}^{\infty}\frac{R_{\pm}(k')F_{\pm}(k',x)\,\exp[\pm 2ik'x]}{k'+k+i\epsilon}\,dk'. \tag{A1}$$

In Eq. (A1) $F_+(k,x)$ is defined for $x>0$, and $F_-(k,x)$ for $x<0$, $k\in\mathbb{C}$. The function $F_\pm(k,x)$ is defined by

$$F_\pm(k,x)=\exp[\mp ikx]f_\pm(k,x). \tag{A2}$$

The Jost solutions $f_\pm(k,x)$ are those solutions of the Schrödinger equation satisfying the following boundary conditions:

$$f_+(k,x):\ \lim_{x\to\infty} e^{-ikx}f_+(k,x)=1, \tag{A3}$$

$$f_-(k,x):\ \lim_{x\to-\infty} e^{ikx}f_-(k,x)=1. \tag{A4}$$

They satisfy the following integral equations:

$$f_+(k,x)=e^{ikx}-\int_x^\infty \frac{\sin k(x-t)}{k}\,V(t)f_+(k,t)dt, \tag{A5}$$

$$f_-(k,x)=e^{-ikx}-\int_{-\infty}^x \frac{\sin k(x-t)}{k}\,V(t)f_-(k,t)dt. \tag{A6}$$

It is quite well-known[14] that the functions $f_\pm(k,x)$ and therefore also the functions $F_\pm(k,x)$ are holomorphic in $\mathbb{C}^+$. The potential $V(x)$ has to be in the Faddeev class L_1^1:

$$\int_{-\infty}^{\infty}(1+|x|)|V(x)|<\infty. \tag{A7}$$

The scattering coefficients $R_+(k),R_-(k),T(k)$ are defined by the asymptotic behavior of the physical solution of the Schrödinger equation:

$$\psi_1(k,x)\sim\begin{cases} e^{ikx}+R_+(k)e^{-ikx}, & x<0,\\ T(k)e^{ikx}, & x\to+\infty,\end{cases} \tag{A8}$$

$$\psi_2(k,x)\sim\begin{cases} T(k)e^{-ikx}, & x<0,\\ e^{-ikx}+R_-(k)e^{ikx}, & x\to+\infty.\end{cases} \tag{A9}$$

In the case of rational reflection coefficients they take the following form:[13]

$$R_+(k)=\frac{P(-k)}{\Pi_{j=1}^q(\lambda_j-k)}\prod_{\mu_i\in M^+}\frac{\mu_i+k}{\mu_i-k}\prod_{\lambda_l\in L^+}\frac{\lambda_i+k}{\lambda_i-k}, \tag{A10}$$

$$T(k)=\frac{\Pi_{i=1}^q(\mu_i+k)}{\Pi_{j=1}^q(\lambda_i+k)}, \tag{A11}$$

$$R_-(k)=\frac{P(k)}{\Pi_{j=1}^q(\lambda_j-k)}\prod_{\mu_i\in M^-}\frac{\mu_i-k}{\mu_i+k}\prod_{\lambda_l\in L^-}\frac{\lambda_i-k}{\lambda_i+k}. \tag{A12}$$

Following Sabatier,[13] the degree of the polynomial $P(k)$ has to be smaller than q. Further, Im $\mu_i>0$ except if $\mu_i=0$, Im $\lambda_l<0$. The transmission coefficient $T(k)$ is supposed to be an irreducible fraction, and the sets M^+,M^-,L^+,L^- contain numbers $\neq 0$. If the potential is real then μ_k,λ_k are pure imaginary. If μ_k,λ_k are not pure imaginary then there exists $-\mu_k^*$, $-\lambda_k^*$. It can be shown[14] that $T(k)$ is meromorphic in $\mathbb{C}^+$ and if there are poles they are in Im k. If there are no

bound states $T(k)F_{\mp}(k,x)$ is holomorphic in $\mathbb{C}^+$ and the first integral of (A1) is zero. If $T(k)F_{\mp}(k,x)$ is holomorphic in $\mathbb{C}^+$ and all the poles p_i of $R_+(k)$ are simple, the integral (A1) can be solved by contour integration in the upper-half plane. The result is

$$F_+(k,x)-1=\sum_{p_j\in\mathscr{P}}\frac{R_jF_+(p_j,x)\exp[2ip_jx]}{p_j+k}. \tag{A13}$$

Solving (A13), by letting k run through the set of poles $\mathscr{P}$ we obtain a linear set of algebraic equations that determine $F_+(p_j)$ for all values of j. Solving this set making use of Cramer's rule we obtain after putting $y=x$:

$$K_+(x,x)=\frac{\mathscr{D}'_+(x)}{\mathscr{D}_+(x)}, \tag{A14}$$

where

$$\mathscr{D}_+(x)=\det\{\delta_{ij}-(p_i+p_j)^{-1}R_j\ \exp[2ip_jx]\}, \tag{A15}$$

and $\mathscr{D}'_+(x)$ is the derivative of $\mathscr{D}_+(x)$ with respect to x.

APPENDIX B: PROOF OF THEOREM II.1

Our starting point is the Marchenko equation without bound states in the wavenumber domain:[14]

$$F_+(k,x)=1+\frac{1}{2\pi i}\lim_{\epsilon\to 0+}\int_{-\infty}^{\infty}dk'\ \frac{R_+(k')F_+(k',x)\exp[2ik'x]}{k'+k+i\epsilon}=1+\int_{-\infty}^{\infty}C(k,k')F(k',k,x)dk'. \tag{B1}$$

The function $F_+(k,x)$ is related to kernel $K_+(x,y)$ by the following Fourier transform:

$$K_+(x,y)=(2\pi)^{-1}\int_{-\infty}^{\infty}dk\ e^{-ik(y-x)}(F_+(k,x)-1). \tag{B2}$$

The kernel $C(k',k)$ in Eq. (B1) is given by

$$C(k,k')=\lim_{\epsilon\to 0+}\frac{1}{2i\pi}\frac{R_+(k')\exp[2ik'x]}{k'+k+i\epsilon}. \tag{B3}$$

We can expand Eq. (B1) in a series:

$$F_+(k,x)=1+\int_{-\infty}^{\infty}C(k',k)dk'+\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}C(k,k')C(k',k'')dk'\ dk''+\cdots \tag{B4}$$

or alternatively

$$F_+(k,x)-1=\lim_{\epsilon\to 0}\frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{R_+(k')e^{2ik'x}}{k+k'+i\epsilon}dk'$$
$$+\lim_{\epsilon\to 0}\frac{1}{(2\pi i)^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}dk'\ dk''\ \frac{R_+(k')e^{2ik'x}}{k+k'+i\epsilon}\frac{R_+(k'')e^{2ik''x}}{k'+k''+i\epsilon}+\cdots. \tag{B5}$$

If the reflection coefficients $R_+(k)$ in Eq. (B3) are rational functions of the wave number the integrals in Eq. (B4) can be solved analytically by performing a contour integration in $\mathbb{C}^+$. This is justified by the fact that the reflection coefficient $R_+(k)\rightarrow\mathcal{O}(1/k)$ if $k\rightarrow\infty$. The poles of the denominator of Eq. (B5) are all situated in $\mathbb{C}^-$ so the only contribution to the integrals of Eq. (B5) comes from the poles of $R_+(k)$ which are situated in $\mathbb{C}^+$. The following expression is obtained:

$$F_+(k,x)-1=\sum_{i=1}^{N}\frac{R_i}{k+p_i}e^{2ip_ix}+\sum_{i,j=1}^{N}\frac{R_iR_j}{(k+p_j)(p_i+p_j)}e^{2i(p_i+p_j)x}+\sum_{i,j,l=1}^{N}\frac{R_iR_jR_l}{(k+p_l)(p_j+p_l)(p_i+p_j)}e^{2i(p_i+p_j+p_l)x}+\cdots . \tag{B6}$$

The Fourier transform (B2) can now be performed to obtain the kernel $K_+(x,y)$:

$$K_+(x,y)=i\sum_{i=1}^{N}R_ie^{ip_i(x+y)}+i\sum_{i,j=1}^{N}\frac{R_iR_j}{p_i+p_j}e^{ip_j(x+y)}e^{2ip_ix}+i\sum_{i,j,l=1}^{N}\frac{R_iR_jR_l}{(p_j+p_l)(p_i+p_j)}e^{ip_l(x+y)}e^{2i(p_i+p_j)x}+\cdots . \tag{B7}$$

After setting $y=x$ and taking the derivative

$$V(x)=-2\frac{d}{dx}K_+(x,x), \tag{B8}$$

the following expression for the recovered potential is obtained.

$$V(x)=4\sum_{i=1}^{N}R_ip_ie^{2ip_ix}+4\sum_{i,j=1}^{N}R_iR_je^{2i(p_i+p_j)x}+4\sum_{ijl}^{N}\frac{(R_iR_jR_l)(p_i+p_j+p_l)}{(p_i+p_j)(p_j+p_l)}e^{2i(p_i+p_j+p_l)x}+\cdots . \tag{B9}$$

Application of the transformation (17) on Eq. (B9) leads to the series solution of the KdV equation (18):

$$u(x,t)=4\sum_{i=1}^{N}R_ip_ie^{2i(p_ix+4p_i^3t)}+4\sum_{i,j=1}^{N}R_iR_je^{2i\{(p_i+p_j)x+4(p_i^3+p_j^3)t\}}+4\sum_{ijl}^{N}\frac{(R_iR_jR_l)(p_i+p_j+p_l)}{(p_i+p_j)(p_j+p_l)}e^{2i\{(p_i+p_j+p_l)x+4(p_i^3+p_j^3+p_l^3)t\}}+\cdots . \tag{B10}$$

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Integrability, partial integrability, and nonintegrability for systems of ordinary differential equations

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The integrability of systems of ordinary differential equations with polynomial vector fields is investigated by using the singularity analysis methods. Three types of results are obtained. First, a general relationship between the degrees of first integrals and the so-called Kowalevskaya exponents is derived. Second, it is shown that all solutions of algebraically integrable systems can be expanded in Puiseux series. Third, a new method to study partially integrable systems is studied. These different aspects allow us to study algorithmically the integrability, partial integrability, and nonintegrability of differential systems. © *1996 American Institute of Physics.* [S0022-2488(96)01103-3]

I. INTRODUCTION

In recent years many works have focused on the definition of integrability for dynamical systems. However, it is well known that ''integrability'' in a general sense is ill defined. This is mainly due to a confusion between Hamilton theory, dynamical systems approach, and singularity analysis. Each field has a different definition for ''integrability'' which makes sense within the theory. The difficulty arises when one tries to establish possible relationships between different fields. The main problem treated here is to find a connection, if any, between the Painlevé property and another notion of integrability which could be used to effectively build the solutions or gain some global knowledge on the dynamics in phase space. While it is widely believed that the Painlevé property is incompatible with chaotic motions, there is to date no rigorous proof of this simple statement. From the other point of view, it is known that Liouville integrability is not directly related to the Painlevé property. Therefore, if we want to draw arrows between these different fields it is necessary to introduce some rigorous notions of integrability which could be explicitly related to the Painlevé property, or, at least, to the Painlevé test. More generally, one needs a simple test for the existence or nonexistence of first integrals in a given function space (polynomial, rational, algebraic,...) and it is the purpose of this paper to show that singularity analysis provides it.

The algebraic integrability for an n-dimensional systems of ODEs with rational vector fields is defined as the existence of $(n-1)$ algebraic first integrals. This notion of integrability is very strong. Indeed, Liouville integrability for an n degrees of freedoms Hamiltonian only requires the existence of n single-valued first integrals; the remaining $(n-1)$ angle variables expressed as closed one-form are not, in general, algebraic or even single-valued first integrals. Liouville integrability is therefore a much weaker statement on the singularities than algebraic integrability. This explains why it has not been possible so far to decide from the singularity analysis the Liouville integrability for general Hamiltonians. From the other point of view, the notion of algebraic integrability constrains the solutions of the systems in such a way that general statements on the meromorphicity of the solutions are possible.

Another problem relates to partial integrability, that is the existence of a certain number of

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first integrals less than the number required for the complete integration. The singularity analysis has been a successful tool for finding integrable systems. Many new systems, Hamiltonian and non-Hamiltonian, have been built.[1] However, most of the Hamiltonian systems although Liouville integrable cannot be detected by the singularity analysis. In the same way, most of the dynamical systems admit a few invariants related to physical conservation laws, but only a handful of them will admit enough constants of motion to effectively build the complete analytical global solution. More generally, there is no decision procedure to test the simple question: Is there a polynomial first integral for a given systems of ODEs? Or, alternatively: Is there a bound for the degree of polynomial first integrals?

The explicit computation of first integrals is not an easy task. The different techniques depend on the space of functions considered for the first integrals. If we are interested in polynomial or rational first integral, then all methods of explicit construction rely on the same idea. Consider a system $S:\dot{x}=f(x)$ where f is a given polynomial vector field and let us look for a first integral of *given* degree d. We insert a polynomial or rational ansatz in the system and look for the coefficients. If no first integral is found, then one has to increase the value of d and, with good luck and prayer, hope to obtain a first integral.[2–5] Some of these methods are based on the Carleman procedure for finding first integrals.[6–10]

The main problem of all these methods is to set the degree d. We show here that the degree of a first integral is related to the Kowalevskaya exponents. This relation gives a first choice for the possible values of the degree d.

From the other point of view, it is sometimes possible to prove nonintegrability, that is, the nonexistence of constants of motion. For Hamiltonian systems, there is the Ziglin theory for the n degrees of freedom systems. This theory has been proved to be useful for the following systems: the motion of rigid body around a fixed point,[11,12] homogeneous potentials,[13,14] the Toda lattices,[15,16] a perturbed Kepler potential,[17] nonhomogeneous potentials,[18] and a reduced Yang–Mills potential.[19]

Ziglin's theory is based on the monodromy properties around particular solutions (straight line notions). However, it is quite difficult to apply in general and is limited to low degrees of freedom and, mostly, homogeneous potentials.

For non-Hamiltonian systems, only a few results on nonintegrability are available. Let us mention a recent work for homogeneous vector fields due to Moulin-Ollagnier *et al.*,[20] where some new results on the nonexistence of polynomial first integrals of motion based on algebraic considerations are given.

Both theories, integrability and nonintegrability, are dichotomous in the sense that, if integrability is not proved by the singularity analysis, then nothing can be said about the existence of first integrals. Nonintegrability, in the same way, is a statement on the nonexistence of at least one first integral.

However, most of the systems encountered in physics do not fall in the set of completely integrable or completely nonintegrable systems. Indeed, if a system admits one or two first integrals, then nonintegrability cannot be proved in general. In Sec. V, we show that singularity analysis can be effectively used to find partially integrable cases. Therefore, it can be applied to n degrees of freedom Hamiltonian systems where only $(n-1)$ first integrals have to be built to complete the Liouville integrability. These necessary conditions provide a direct and algorithmic proof of the nonintegrability of these systems.

This paper is divided as follows. In Sec. II, I review the definitions and the relevant works concerning algebraic integrability for systems of ODEs. In Sec. III, I present a new and general result relating the degrees of first integrals for homogeneous vector fields with the Kowalevskaya exponents. In Sec. IV, the main theorems of this paper are presented. It is proved that algebraic integrability implies that the solutions can be expanded in Puiseux series. Finally, in Sec. V, I present a new method for finding necessary conditions for partial integrability for nonhomogeneous vector fields whose homogeneous part is partially integrable.

II. ALGEBRAIC INTEGRABILITY

I briefly recall the main general results concerning the existence of first integrals.

A. Definitions and preparations

Consider a system of n first-order ODEs:

$$S(f;x,t):\dot{x}=f(x), \tag{2.1}$$

where $x\in\mathbb{R}^n$ and $f_i(x)$ are polynomial functions of x.

A *first integral* $I=I(x,t)$ of $S(f;x,t)$ is a nonconstant function of (x,t) with the property

$$\nabla I.f+\frac{\partial I}{\partial t}=0. \tag{2.2}$$

This relation holds if and only if $I(x,t)$ is constant along all particular solutions $x=x(t)$ of S.

Definition 2.1: An algebraic function $I(x)=C$ is a solution of

$$q_0+q_1C+q_2C^2+\cdots+q_{s-1}C^{s-1}+C^s=0, \tag{2.3}$$

where $q_i(x)$ are rational functions of x, and s is the smallest positive integer for which such a relation holds. The relation (2.3) is referred to as the minimal polynomial of I.

Let us recall that two first integrals are *independent* if there is at least one point $x_0\in\mathbb{R}^n$ such that their gradients are linearly independent. In the same way, l first integrals are *independent* if there is a point $x_0\in\mathbb{R}^n$ such that

$$\operatorname{rank}(\nabla I_1(x_0),\nabla I_2(x_0),\ldots,\nabla I_l(x_0))=l. \tag{2.4}$$

Let us note that if $x_0=x(t_0)$ is the initial condition, the first integrals remain independent for all $x(t)$ $(t\in\mathbb{R})$ solutions of S with initial conditions x_0. Indeed, the gradients of the first integrals are solutions of a system of linear differential equations, the *adjoint variational equations*. This results from a general property of linear differential equations that linearly independent solutions remain independent under the flow.[21]

Two different notions of algebraic integrability were alternatively used in the literature. The weaker definition is an extension of the Hamilton–Jacobi theorem to more general vector fields:

Definition 2.2: The system S is algebraically integrable in the weak sense if there exist k independent algebraic first integrals $I_i(x)=K_i$ $(i=1,\ldots,k)$. These k first integrals define an $(n-k)$-dimensional algebraic variety. In addition, there must exist other $(n-1-k)$ independent first integrals given by the integral of a total differential defined on the algebraic variety:

$$J_i=\sum_{j=1}^{n-k}\int^{x_j}\phi_{ij}(x)dx_j, \quad i=1,\ldots,n-1-k, \tag{2.5}$$

where $\phi_{ij}(x)$ are algebraic functions of x.

This definition seems to be useless for non-Hamiltonian systems where the existence of a total differential is not *a priori* known. However, in some cases such a situation may occur.[22] A classical example is given by the six-dimensional Euler equations for the rigid body motion around a fixed point where only four first integrals are required to complete the integration, the fifth one being given by the integral of a total differential (Ref. 23, p. 108). However, it is understood that this definition is, in most cases, likely to be applicable to Hamiltonian systems.

The stronger definition of algebraic integrability is equivalent to the weak definition with the condition $k=n-1$.

Definition 2.3: The system S is algebraically integrable if there exist $(n-1)$ *independent algebraic first integrals* I_i $(i=1,\ldots,n)$.

Still, there exist other definitions of algebraic integrability for Hamiltonian systems: the so-called *algebraic complete integrability* introduced by Adler and van Moerbeke[24] and the *hyperelliptically separable systems* by Ercolani and Siggia.[25] Their definitions cover systems which can be integrated in terms of Abelian functions. Whereas their approaches are mainly geometric, our approach is algebraic in the sense that we are mainly interested in showing the existence of algebraic functions as constants of the motion rather than proving some particular structure for the complexified phase space.

B. Reduction of algebraic first integrals

The algebraic first integrals can be reduced to rational first integrals. Indeed, we prove that any algebraic integral is algebraically compounded from weight-homogeneous rational first integrals. This can be summarized by the following result:

Lemma 2.4: If the system $S:\dot{x}=f(x)$ *has* $l(1\leqslant l\leqslant n-1)$ *independent algebraic first integrals, then there exist* l *independent rational first integrals.*

We now give a short proof of this result:

Proof 2.4: Let $I(x)=C$ be a nontrivial algebraic first integral and $P(C)=q_0+q_1C+\cdots+q_{s-1}C^{s-1}+C^s$ its minimal polynomial. We apply the operator $f.\nabla$ on the polynomial:

$$f.\nabla(P(C))=0=(f.\nabla q_0+Cf.\nabla q_1+\cdots+C^{s-1}f.\nabla q_{s-1}) + (f.\nabla C)(q_1+\cdots+(s-1)q_{s-1}C^{s-2}+sC^{s-1}). \tag{2.6}$$

Using the fact that $I(x)=C$ is a first integral $(f.\nabla C=0)$, one finds

$$(f.\nabla q_0+Cf.\nabla q_1+\cdots+C^{s-1}f.\nabla q_{s-1})=0. \tag{2.7}$$

This is a polynomial of degree smaller than the minimal polynomial $P(C)=0$, so that we have $f.\nabla q_i=0$, $i=1,\ldots,s-1$. The first integral $C=I(x)$ is nontrivial (different from a constant), so that at least one of the $q_i(x)$ is nontrivial [if all q_i are trivial, so is $I(x)$]. This q_i is a nontrivial rational first integral of the system S.

Now, consider another independent algebraic first integral $I'(x)=C'$. Its minimum polynomial reads $P(C')=q_0'+q_1'C+\cdots+q_{s'-1}'C^{s'-1}+C^{s'}$. We know from the previous paragraph that each q_i' is a first integral. It follows from the independence of I with I' that there exist (i,j) $(i<s-1,j<s'-1)$ so that the two rational functions q_i and q_j' are nontrivial and independent (if all rational functions q_i and q_i' are dependent, so are the first integrals). Therefore, these two rational functions are independent nontrivial rational first integrals. Proceeding so, we can build l independent rational first integrals from the l algebraic first integrals. □

Let us note that this result was already contained in a paper by Bruns (1887), in a different setting (see Ref. 26).

We conclude that the study of algebraic first integrals reduces to the study of rational first integrals.

C. Elementary first integrals

Is there a special place for algebraic first integrals among other types of first integrals? Why not study the existence of more complex or peculiar forms of first integrals? The answers to these questions lie in a result of Prelle and Singer[27] (see also Refs. 28 and 29). They show that if there exists an *elementary first integral* (that is, a first integral built up from rational functions using exponentiation, integration, and algebraic functions) for a system of first-order ODEs with polynomial vector fields, then it is of the form

$$I_0(x)+\sum c_i \log I_i(x), \tag{2.8}$$

where $I_i(x)$ are algebraic functions.

Therefore, algebraic functions play a special role in the class of elementary functions since all elementary first integrals can be built out of them. Our interest is to find the relationship between the existence of first integrals and the local single-valuedness of the solution. It has been shown by Ishii[30] that the appearance of a logarithmic dependence in the first integrals implies, in general, that the solutions are multivalued in a neighborhood of their singularities. The solutions lie then on a Riemann surface. The consequence is that the system has no Puiseux expansion with $(n-1)$ arbitrary coefficients around the movable singularities. In other words, infinitely many-valuedness of a first integral brings infinitely many-valuedness of the solutions. We will therefore focus on the existence of algebraic first integrals as the first building blocks of elementary first integrals. The next step is to show that the single-valuedness of first integrals implies the single-valuedness of the solutions.

D. Scale invariant systems

The construction of a first integral relies on a decomposition of the vector field S in homogeneous and nonhomogeneous components. In order to build explicitly a first integral we start from a truncation of the vector field retaining the higher nonlinear terms and then we consider lower-order corrections. As a consequence, we first focus our study on a particular class of systems S which exhibits some particular scaling properties:

Definition 2.5: The system $S:\dot{x}=f(x)$ is similarity invariant if there exists $g\in\mathbb{Q}^n$ such that S is invariant under the transformation

$$x\to\alpha^g x, \quad t\to\alpha^{-1}t \tag{2.9}$$

for all $\alpha\in\mathbb{R}_0$.

We shall refer to g as the *weight* of S. More generally, a function $F(x,t)$ is *weight-homogeneous* with respect to g of *weighted degree* d if

$$F(\alpha^{-1}t,\alpha^g x)=\alpha^d F(t,x). \tag{2.10}$$

As a consequence, a system $S:\dot{x}=f(x)$ is similarity invariant if each component f_i of the vector field is weight-homogeneous of weight g_i+1 with respect to the weight g. Weight-homogeneous functions are the natural generalization of homogeneous functions and most of the properties of homogeneous functions can be readily translated in terms of weights.

III. ALGEBRAIC INTEGRABILITY FOR HOMOGENEOUS SYSTEMS

A. Yoshida's analysis

One of the pioneering works in the domain is due to Yoshida.[31,32] Using a singularity-analysis-type method, he was able to derive necessary conditions for algebraic integrability.

Consider a similarity-invariant system (w.r.t. a weight g) $S:\dot{x}=f(x)$. The interest of similarity-invariant systems lies in the existence of particular scale-invariant solutions of the form

$$x=ct^{-g}, \tag{3.1}$$

where the coefficients $c\in\mathbb{C}^n$ are given by the algebraic equation

$$f(c)+cg=0. \tag{3.2}$$

For a given g, there may exist different sets of values c which will be referred to as different *balances*. We now consider one of these solutions and we introduce the matrix K:

$$K = Df(c) + \mathrm{diag}(g), \tag{3.3}$$

where $(Df(c))_{ij} = (\partial f_i/\partial x_j)(c)$ is the Jacobian evaluated on $x = c$.

Here again, the eigensystem of matrix K can be used to build particular solutions to the variational equations. Let the *Kowalevskaya exponents* be the eigenvalues of K. (Sophia Kowalevskaya was the first to introduce the determinant of K to compute the Laurent series solutions of the rigid body motion: ''Afin que les séries... contiennent le nombre suffisant de constantes arbitraires, il faut que le déterminant de ces équations linéaires ...s'évanouisse pour cinq valeurs différentes de m égales à des nombres entiers positifs.''[33])

It can be shown that there always exists a Kowalevskaya exponent $\rho = -1$ related to the arbitrariness of t_0.

Yoshida's results are twofold. First, he proves that, under certain conditions, the weighted degree of a first integral is a Kowalevskaya exponent. Second, he shows that if one of the Kowalevskaya exponents is not rational, then the system cannot be algebraically integrable.

Theorem 3.1 (Yoshida): *Let $I(x)$ be a weight-homogeneous first integral of weighted degree d for the similarity invariant system S. Assume that $\nabla I(c)$ is not identically zero for at least one choice of c. Then, d is a Kowalevskaya exponent.*

1. Example: A Hamiltonian system

As an example, we study the following three degrees of freedom Hamiltonian system:[34]

$$H = \tfrac{1}{2}(p_1^2 + p_2^2 + p_3^2) + (x_1^4 + 16x_2^4 + \mu x_3^4 + 12x_1^2x_2^2). \tag{3.4}$$

This Hamiltonian system is weight-homogeneous with respect to the weights $g = (1,1,1,2,2,2)$ [where $(x_1,x_2,x_3,x_4,x_5,x_6) = (x_1,x_2,x_3,p_1,p_2,p_3)$]. Moreover, it is integrable with second and third constants of motion given by

$$C_1 = p_3^2 + 2\mu x_3^4, \tag{3.5}$$

$$C_2 = x_2p_1^2 - x_1p_1p_2 - 8x_1^2x_2^3 - 4x_1^3x_2^2. \tag{3.6}$$

The weights of H, C_1, C_2 w.r.t. g are, respectively, $d_h = 4$, $d_1 = 4$, $d_2 = 5$. The first step of Yoshida's analysis consists of finding all the possible dominant balances, that is, the scale-invariant solutions $x_i = c_i t^{-g_i}$. We found 24 different solutions for c_i. For each dominant balance, we can compute the Kowalevskaya exponents ρ using relation (3.3) and the gradients of the first integrals estimated on the scale invariant solutions $x = ct^{-g}$. As an example, we give three different dominant balances in order to illustrate Yoshida's theorem:

$$\begin{aligned}
&c = \left(\frac{i}{\sqrt{2}}, 0, \frac{i}{\sqrt{2\mu}}, \frac{-i}{\sqrt{2}}, 0, \frac{-i}{\sqrt{2\mu}}\right), \quad \rho = \{-2,-1,-1,4,4,5\},\\
&\nabla H(c) \neq (0), \quad \nabla C_1(c) \neq (0), \quad \nabla C_2(c) \neq (0);\\
&c = \left(\frac{1}{2}, \frac{i}{2\sqrt{2}}, \frac{i}{\sqrt{2\mu}}, -\frac{1}{2}, \frac{-i}{2\sqrt{2}}, \frac{-i}{\sqrt{2\mu}}\right), \quad \rho = \{-2,-1,-1,2,4,5\},\\
&\nabla H(c) \neq (0), \quad \nabla C_1(c) = (0), \quad \nabla C_2(c) \neq (0);
\end{aligned} \tag{3.7}$$

$$c=\left(-\frac{1}{2},\frac{-i}{2\sqrt{2}},0,-\frac{1}{2},\frac{i}{2\sqrt{2}},0\right),\quad \rho=\{-2,-1,1,2,4,5\},$$

$$\nabla H(c)\neq(0),\quad \nabla C_1(c)=(0),\quad \nabla C_2(c)=(0).$$

In the first case, the gradients of the first integrals do not vanish on the scale-invariant solution. As a consequence, d_h, d_1, and d_2 are Kowalevskaya's exponents. In the second case, ∇C_1 vanishes identically and d_1 is not a Kowalevskaya exponent, while in the third case only $\nabla H(c)$ does not vanish.

Although this result was the first bridge between the degrees of first integrals and the singularity analysis, it is not of great predictive power. Indeed, while the Kowalevskaya exponents can be computed in a finite procedure, the functional form of the first integral is not known *a priori*. Therefore, the first integrals may not satisfy the assumptions. In particular, it does not forbid the existence of a first integral of higher degree for which $\nabla I(c)$ could vanish identically. We will come back to this problem in the following sections.

Let us note that the converse statement holds. Indeed, it will be proved in the next section that $\nabla I(c)\neq(0)$ if and only if d (the degree of I w.r.t. to g) is a Kowalevskaya exponent for the balance under consideration (where d is considered here with the proper algebraic multiplicity).

Another interesting point is that this result seems to be valid outside the class of algebraic first integrals. Indeed, Yoshida's argument does not rely on the fact that I is an algebraic function but only on the weight-homogeneity of the vector field and the first integral.

For Hamiltonian systems there is an interesting relation between the Kowalevskaya exponent which was first pointed out by Yoshida and given in its final form by Lochak:[35]

Proposition 3.2 (Lochak, 1985): Let S be a system whose Hamiltonian is H. If ρ is a Kowalevskaya exponent for the system S, then so is $h-1-\rho$ (where h is the weighted degree of the Hamiltonian H).

In other words, the Kowalevskaya exponents always come by pairs for Hamiltonian systems. This is analogous to the linearized eigenvalues at a fixed point (this analogy is more than formal and can be made rigorous).

The next statement is the main result of Yoshida, it connects the occurrence of irrational Kowalevskaya exponents with nonintegrability:

If the system S is algebraically integrable in the weak sense, then all Kowalevskaya exponents are rational.

However, despite the fact that this result has been widely applied and frequently verified, this last statement is not correct as illustrated in the next example due to Kummer *et al.*:[36]

$$H=p_1(p_1^2+x_1^2)+\omega x_1(p_2^2+x_2^2). \tag{3.8}$$

It can be easily verified that this system has Kowalevskaya's exponents: $\{-1,3,1\pm 2i\omega\}$ for the similarity invariant solution $(x_1,x_2,p_1,p_2)=(-1,0,0,0)t^{-1}$. However, there exists a second polynomial first integral:

$$I=p_2^2+x_2^2. \tag{3.9}$$

The correct statement of Yoshida's theorem is only related to the stronger definition of algebraic integrability:

Theorem 3.3: *If the system S is algebraically integrable, then all Kowalevskaya exponents are rational.*

To the best of my knowledge, there is not published proof of this basic result. Therefore, a proof will be given in Sec. III D as a corollary of a more general result (see Proposition 3.5).

Although Yoshida's statement was not correct in full generality, Yoshida managed to prove it in a particular case using Ziglin's theory of nonintegrability.[11,12] He studied the case of n degrees of freedom Hamiltonian systems with diagonal kinetic contribution and homogeneous potential:

$$H=\tfrac{1}{2}(p_1^2+\cdots+p_n^2)+V(q_1,\ldots,q_n), \tag{3.10}$$

where $V(x)$ is homogeneous of degree k but $k\neq 0,\pm 2$. The Kowalevskaya exponents always come by pairs $\rho_i+\rho_{i+n}=(k+2)/(k-2)$, so that we can define the difference between two exponents of each pair $\Delta\rho_i=\rho_{i+n}-\rho_i$.

Theorem 3.4 (Ref. 14): *If the n numbers $\Delta\rho_i$ are $\mathbb{Q}$-independent, then the Hamiltonian system has no additional first integral beside the Hamiltonian itself.*

As a corollary, for the case of planar Hamiltonian systems with homogeneous potential, we obtain the following: If the Hamiltonian $H=\frac{1}{2}(p_1^2+p_2^2)+V(x_1,x_2)$ possesses a second invariant, then the Kowalevskaya exponents are rational.[14]

B. The generalized Kowalevskaya exponents

Consider a system $S(f;x,t)$, and assume for the time being that f is weight-homogeneous. Beside the Kowalevskaya exponent there is yet another set of indices that can be defined, the so-called *resonances* of the Painlevé test.[1] The Painlevé test is an algorithmic procedure which provides necessary conditions for the Painlevé property. Essentially, the Painlevé test checks the formal existence of Laurent series as a solution. Let us recall the main ingredients of the Painlevé test:

The first step consists in finding all the truncations of $\hat{f}$ of the vector field

$$\dot{x}=f(x)=\hat{f}(x)+\check{f}(x) \tag{3.11}$$

such that the *leading behavior* $x=\alpha(t-t_*)^p$, $\alpha\in\mathbb{C}_0^n$, is an exact scale-invariant solution of the homogeneous system

$$\dot{x}=\hat{f}(x), \tag{3.12}$$

where $p\in\mathbb{Q}^n$ with at least one negative component.

It is also required that $\check{f}(x)=\Sigma_i f^{(i)}(x)$ is *not dominant*, that is, at the singularity,

$$\check{f}^{(i)}(x)(\alpha(t-t_*)^p)=\gamma^{(i)}(t-t_*)^{p+q^{(i)}-1} \tag{3.13}$$

with $q^{(i)}\in\mathbb{N}_0^n$.

Each *balance* (α,p) defines a different expansion.

The second step is the computation of the *resonances*. Each balance defines a new set of resonances. These resonances are the indices j of the coefficients a_j in the Laurent series at which arbitrary constants first appear. It is a standard matter to show that these resonances are given by the eigenvalues of the matrix R:

$$R=D\hat{f}(\alpha)-\mathrm{diag}(p) \tag{3.14}$$

where again $D\hat{f}(\alpha)$ is the Jacobian matrix evaluated in α.

The resonances are labeled r_i, $i=1,\ldots,n$, with $r_1=-1$. The necessary condition for the existence of the Laurent series, in this set of variables, is that all resonances are integer ($r_i\in\mathbb{Z}$).

The third and last step of the Painlevé test consists of checking that the arbitrariness of the coefficient a_r for the full system (3.11) does not introduce incompatible constraints on the coefficients $a_j(j<r)$. This is achieved by computing all coefficients in the Laurent expansions up to the highest resonances.

We have introduced two set of indices for a given vector field f: the resonances of the Painlevé test and the Kowalevskaya exponents. The main difference is not in the definition of the exponents (they are both obtained as the eigenvalues of a matrix built on the Jacobian matrix of a particular solution), but rather on the choice of the particular solution. Indeed, in the Painlevé test, one looks for a particular solution of $S(f^{(0)})$ under the form $x=\alpha(t-t_*)^p$ where $\alpha\in\mathbb{C}_0^n$ while in Yoshida's analysis the particular solution of $S(f)$ is $x=c(t-t_*)^{-g}$ with $c\in\mathbb{C}^n$ (not in $\mathbb{C}_0^n$!). This rather subtle difference introduces a shift in the exponents that we now make explicit. Let us stress before proceeding that both sets of exponents have their own interest and they correspond to different types of analysis. Yoshida's analysis stresses that the weight of polynomial functions and the existence of series involving logarithmic terms is not a relevant feature since only the rationality of the Kowalevskaya exponents comes into play. From the other point of view, the Painlevé test is designed to test the existence of Laurent series as formal solution. It is common to mistake both sets. This is why we explained in length these differences.

Consider the system $S(f;x,t)$ (where f is weight-homogeneous of weight $g\in\mathbb{Q}^n$). We build a particular solution of this system using the singularity analysis, that is, a balance (α,p) of order l. Therefore, there is a truncation of the vector field $f=f^{(0)}+f^{(1)}+\cdots+f^{(l')}$ $(1\leqslant l'\leqslant n-l)$ and a particular solution of $S(f^{(0)})$:

$$x=\alpha(t-t_*)^p, \tag{3.15}$$

where, without loss of generality (i.e., up to a permutation of indices), we have α_i arbitrary for $i=l+1,\ldots,n$.

For each balance (α,p), there corresponds a particular solution of $S(f)$ as defined in the previous section:

$$x=c(t-t_*)^{-g} \tag{3.16}$$

where $c_i=\alpha_i$, $i=1,\ldots,l$, and $c_i=0$, $i=l+1,\ldots,n$.

Therefore, to a balance of order l, there corresponds a particular solution with $n-l$ vanishing entries. Moreover, from the homogeneity of the vector field, we can deduce the relation $f(c)=f^{(0)}(\alpha)$ and the shift between the dominant exponents p and the weights g. Let n_i be the number of nonvanishing components of $f^{(i)}$, then we have

$$p_j=-g_j+q^{(i)},\quad j=n_{i-1}+1,\ldots,n_{i-1}+n_i,\quad i=0,\ldots,l', \tag{3.17}$$

with $n_{-1}=0$ and $q_0=0$

In the same way it is possible to build the eigenvalues of the Kowalevskaya matrix (3.3) from the resonances:

$$\rho_i=r_i \quad \text{for all } i \text{ such that } r_i\neq 0, \tag{3.18}$$

$$\rho_i=q_i \quad \text{with multiplicity } n_i. \tag{3.19}$$

Now, the correspondence (3.18) can be used as a new definition for the Kowalevskaya exponents for nonhomogeneous vector fields $S(f;x,t)$. Let us note that the number of these *generalized Kowalevskaya exponents* can exceed the number of variables n. Only n of these m exponents corresponds to independent arbitrary constants. However, all exponents may be used to test the existence of homogeneous first integrals.

C. Necessary conditions for algebraic integrability

Yoshida's result only concerns complete integrability. However, following the same arguments, his result can be generalized to study partial or nonintegrability. In this section I establish a fundamental equality between the Kowalevskaya exponents for nonhomogeneous systems and the existence of first integrals.

Proposition 3.5: If there is l independent algebraic first integrals $I_1,...,I_l$ *of weighted degrees* $d_1,\dots,d_l$ *for a system* $\dot{x}=f(x)$, *then there is l independent linear relations*:

$$\sum_{j=1} N_{ij}\rho_j = d_i, \quad i=1,\dots,l, \tag{3.20}$$

with $N_{ij}\in\mathbb{Z}$.

Proof 3.5: According to Lemma 2.4, we consider l independent rational weight-homogeneous first integrals. The proof is divided into two parts. First, we show that the existence of a commensurate relation between the degrees of the first integrals and the Kowalevskaya exponents. Second, we show that these relations are linearly independent as a consequence of the independence of the l first integrals.

The similarity invariant solution $x=ct^{-g}$ is the first term of a formal solution around a singularity t_*:

$$x=(t-t_*)^{-g}\sum_{i_j}^{\infty} a_{i_1\dots i_m}\prod_{j=1}^{m}\xi_j^{i_j}, \tag{3.21}$$

where $\xi_j=\lambda_j(t-t_*)^{\rho_j}$, the λ_js are independent arbitrary constants, and $\rho_1,...,\rho_m$ are the positive Kowalevskaya exponents. The coefficients $a_{i_1\dots i_m}$ are polynomial in $\log(t-t_*)$ and the sum Σ_{i_j} is taken over all positive i_j.

Now, consider the weight-homogeneous rational first integral I:

$$I=\frac{\Sigma c_i x^{E_i}}{\Sigma d_j x^{F_j}} \tag{3.22}$$

with $(E_i-F_j).g=d\forall i,\ j$.

This first integral I can be evaluated on $x=x(t-t_*)$ as a function of $(t-t_*)$ by inserting (3.21) in (3.22):

$$I=(t-t_*)^{-d}\sum_{i_j} K_{i_1\dots i_m}\prod_{j=1}^{m}\xi_j^{i_j}, \tag{3.23}$$

where $i_j\in\mathbb{Z}\forall j$.

On the lhs of (3.23), I is an arbitrary constant, therefore, there exists on the rhs of (3.23), a combination of the arbitrary constants λ_i to order $(t-t_*)^0$, that is, there exists at least one set of integers $\{i_1,\dots,i_j\}$ such that $K_{i_1,\dots,i_m}\neq 0$ and $i_1\rho_1+\cdots+i_m\rho_m=d$ with $i_j\in\mathbb{Z}\forall j$.

We digress at this point to notice that, had we considered a *polynomial* first integral, rather than a *rational* first integral, we would have obtained the relation $i_1\rho_1+\cdots+i_m\rho_m=d$ with $i_j\in\mathbb{N}\forall j$.

We now have to prove the independence of the linear relations. To do so, we consider two first integrals I and I' and show that at least two independent linear relation $i_1\rho_1+\cdots+i_m\rho_m=d$ can be obtained. The result for the independence of l linear relations naturally follows.

Let us introduce the variables $\{\xi_1=\lambda_1(t-t_*)^{\rho_1},\dots,\ \xi_m=\lambda_m(t-t_*)^{\rho_m},\ \xi_{m+1}=\lambda_{m+1}(t-t_*)^{\rho_{m+1}},\dots,\ \xi_{n-1}=\lambda_{n-1}(t-t_*)^{\rho_{n-1}},\ \xi_n=(t-t_*)^{-1}\}$. The constants $\{\lambda_1,\dots,\lambda_{n-1},t_*\}$ are arbitrary independent constants. Locally around t_*, the gradient of I can be written in terms of ξ_i:

$$\nabla I = J.\left(\frac{\partial I}{\partial \xi_1},\ldots,\frac{\partial I}{\partial \xi_n}\right) \tag{3.24}$$

with $J^{-1}=(\partial \xi_i/\partial x_j)$ is the Jacobian matrix. In terms of the variables ξ_i, the first integrals I, I' read

$$I=\sum_{i_j} K_{i_1,\ldots,i_n}\prod_{j=1}^{n} \xi_j^{i_j}, \tag{3.25}$$

$$I'=\sum_{i'_j} K'_{i'_1,\ldots,i'_n}\prod_{j=1}^{n} \xi_j^{i'_j}, \tag{3.26}$$

where the sum in the first (resp. second) integral is over all $\{i_j\}$ such that $i_1\rho_1+\cdots+i_{n-1}\rho_{n-1}+d\rho_n=0$ (resp. d') and the coefficients $K_{i_1,\ldots,i_n}\in\mathbb{C}$.

Using the relation (3.24) and the explicit form of ξ_i in terms of $(t-t_*)$, we obtain the gradients of I, I':

$$\nabla I = J.\sum_{i_j} L_{i_1,\ldots,i_n}(i_1(t-t_*)^{-\rho_1},\ldots,i_n(t-t_*)^{-\rho_n}), \tag{3.27}$$

$$\nabla I' = J.\sum_{i'_j} L'_{i'_1,\ldots,i'_n}(i'_1(t-t_*)^{-\rho_1},\ldots,i'_n(t-t_*)^{-\rho_n}). \tag{3.28}$$

Now, the relation $\alpha\nabla I+\alpha'\nabla I'=0$ implies $\alpha=\alpha'=0$. Therefore, written in terms of i_j, i'_j, there exists at least one pair of vector-integers $\{(i_1,\ldots,i_n),\ (i'_1,\ldots,i'_n)\}$ such that $\alpha(i_1,\ldots,i_n)+\alpha'(i'_1,\ldots,i'_n)=0\Rightarrow\alpha=\alpha'=0$. The proposition follows. □

As a corollary of our general result we obtain Yoshida's theorem:[32]

Corollary 3.6: If there exists at least one irrational or imaginary Kowalevskaya exponent, the system is not algebraically integrable.

Proof 3.6: From the previous proposition, we know that the existence of $(n-1)$ first integrals implies that there exists $(n-1)$ relations $N_i.\rho=d_i$, $i=1,\ldots,n-1$. Therefore, there exists a matrix $N\in\mathrm{GL}\ (n-1,\ \mathbb{Z})$, such that $N.\rho=d$ (ρ the vector of Kowalevskaya exponents, d the vector of degrees). We find $\rho=N^{-1}.d$ which implies $\rho\in\mathbb{Q}^{n-1}$. □

Yoshida's theorem gives necessary conditions for complete integrability. Conversely, we now find sufficient conditions for complete nonintegrability, that is, the nonexistence of at least one first integral:

Corollary 3.7: If all Kowalevskaya exponents are $\mathbb{Z}$-independent, then there is no rational first integral.

Proof 3.7: If $\rho_1,\ldots,\rho_n$ are $\mathbb{Z}$-independent, there is no relation $i_1\rho_1+\cdots+i_{n-1}\rho_{n-1}=d$ where $d\in\mathbb{Q}$. □

Corollary 3.8: If all Kowalevskaya exponents are $\mathbb{N}$-independent, then there is no polynomial first integral.

Proof 3.8: In the demonstration of the proposition we noticed that in the case of polynomial first integrals, the fundamental relation between the Kowalevskaya exponents and the degrees of first integrals reads $i_1\rho_1+\cdots+i_{n-1}\rho_{n-1}=d$, but with $i_j\in\mathbb{N}\forall j$. The result follows. □

These two last corollaries are equivalent to a recent result given in Ref. 20. Their results are obtained in a completely different setting and illustrated on many examples.

IV. ALGEBRAIC INTEGRABILITY FOR NONHOMOGENEOUS SYSTEMS

We found necessary conditions for a homogeneous system to be integrable. The conditions are simply given in terms of the Kowalevskaya exponents. More precisely, the maximum number of independent algebraic first integrals is given by the dimension of the vector space spanned by Kowalevskaya's exponents over the integers (the positive integers for polynomial first integrals). We can go one step further in our analysis. First, we focus on nonhomogeneous systems and we show that algebraic integrability brings only finite sheeting of the solution. That is, all solutions can be expanded in Puiseux series. In the first part, we show the absence of the logarithmic terms in the series expansions if the degrees of the first integrals are related to the Kowalevskaya exponents. This is reminiscent of the work of Ishii[37] for nth-order differential equations. Then, we show that the hypothesis on the Kowalevskaya exponents can be dropped and obtain the fundamental result that algebraic integrability always brings single-valuedness of the expansions.

A. Algebraic integrability and logarithmic branch points: Part I

We consider a system $S(f;x,t)$. We have seen in the previous sections that a necessary condition for algebraic integrability is that the set of all Kowalevskaya exponents $K_\alpha=\cup_{i=1}^n\{\rho_i\}$ is such that

$$K_\alpha\in\mathbb{Q}^n, \tag{4.1}$$

for all possible balances (α,p).

Therefore, we assume that S follows this assumption. Another assumption is required. We assume that the system S is completely integrable with $(n-1)$ polynomial first integrals. For each balance (α,p), the first integral I_i has a weighted degree d_i. Let the set of weighted degree $D_\alpha=\cup_{i=1}^n\{d_i\}$ be such that

$$D_\alpha=K_\alpha \tag{4.2}$$

for all balances (α,p).

That is, we assume that the degrees of the first integrals can be identified with the Kowalevskaya exponents. This assumption also implies that each balance (α,p) is a *principal balance*. That is, all the Kowalevskaya exponents but one are positive, and all solutions can be expanded in Puiseux series with exactly $(n-1)$ arbitrary constants. This assumption is fundamental for the rest of the analysis since it allows us to identify the arbitrary constants in the series expansion with the arbitrary constants of the first integrals:

Theorem 4.1: *Let the system* $S:\dot{x}=f(x)\in QM(n)$ *be algebraically integrable with* $D_\alpha=K_\alpha\forall$ *balances* (α,p). *Then, all solutions can be expanded in Puiseux series.*

In particular, if $K_\alpha\in\mathbb{Z}^n$, then the Painlevé test is satisfied in the variables $\{x,t\}$. The situation for which $K_\alpha\in\mathbb{Q}^n$ corresponds to the weak Painlevé case.[1] Let us already note that the converse statement is not true in general. They are, indeed, many systems with the Painlevé property which are not algebraically integrable (the Painlevé equations, for instance). It would be of much interest to find which extra conditions are required beside the Painlevé test for algebraic integrability to hold.

Proof 4.1: Consider the system $S(f(x);x,t)$ for given dominant balances (α,p) and assume first that matrix K is diagonalizable with a set of distinct eigenvalues $K_\alpha\in\mathbb{Q}^n$. We have to show that the series expansions built on the dominant balance do not exhibit logarithmic branching. In other words, the compatibility conditions are satisfied for all Kowalevskaya's exponents. For all positive Kowalevskaya's exponents, we define $h_i=s\rho_i$ where $h_i\in\mathbb{N}$ and s is the smallest natural number for which such a relation holds for all i.

We want to show by recurrence that if the compatibility conditions are satisfied up to the Kowalevskaya exponent ρ', then they will be satisfied for the next Kowalevskaya exponent $\rho>\rho'$.

For the dominant balance (α,p), there exists a formal series expansion, solutions of $S(f(x);x,t)$:

$$x=(t-t_*)^g\sum_{i=1}^{\infty} a_i(t-t_*)^{i/s}, \tag{4.3}$$

where $a_i=a_i(\log(t-t_*))=\Sigma_j a_{ij}(\log(t-t_*))^j$ is a polynomial in $\log(t-t_*)$ of degree less than or equal to i.

If the compatibility conditions are satisfied up to $\rho'=h'/s$, then the coefficients a_i are independent of $\log(t-t_*)$:

$$a_i=a_{i0} \quad \forall i<h, \tag{4.4}$$

where $h=\rho s$. We have to prove that the existence of a first integral I of degree $d=\rho$ implies that a_h is also independent of $\log(t-t_*)$.

The most general form of a_h is $a_h=a_{h0}+a_{h1}\log(t-t_*)$. The recursion relation for the coefficient a_i $(i=1,\ldots, h-1)$ reads

$$K.a_{i0}=\frac{i}{s}a_{i0}+P_{i0}(a_{10},\ldots,a_{i-1,0}), \quad i=1,\ldots,h-1, \tag{4.5}$$

where P_{i0} is polynomial in its arguments and can be obtained by the recursion relation for the coefficients a_{ij}.

Taking into account the possibility of a logarithmic contribution for a_h, the recursion relation gives rise to a linear system for a_{hj}, $j=0$, 1:

$$K.a_{h0}=\frac{h}{s}a_{h0}+P_h(a_1,\ldots,a_{h-1})+a_{h1}, \tag{4.6}$$

$$K.a_{h1}=\frac{h}{s}a_{h1}. \tag{4.7}$$

The general solution of this system is

$$a_{h1}=\mu\beta_\rho, \tag{4.8}$$

$$a_{h0}=\lambda\beta_\rho+\delta_\rho, \tag{4.9}$$

where $\beta_\rho\in\mathbb{C}^n$ is the eigenvector of K of eigenvalue ρ, $\lambda\in\mathbb{C}$ is an arbitrary constant, and $\delta_\rho\in\mathbb{C}^n$ is a constant vector.

The constant μ is fixed by the compatibility condition:

$$\mu=\overline{\beta_\rho}.P_h, \tag{4.10}$$

where $\overline{\beta_\rho}$ is the eigenvector of K^T.

If the compatibility conditions at Kowalevskaya's exponent ρ are satisfied, then $\mu=0$.

Now, we consider the first integral $I(x)=C$, where C is an arbitrary constant and $I(x)$ is a function in many variables. This first integral is, by definition, constant along all solutions. Therefore, it is constant on the formal solution (4.3). We then expand the first integral in powers of $(t-t_*)$:

$$I\left[(t-t_*)^g\sum a_i(t-t_*)^{i/s}\right]=(t-t_*)^{-d}\sum b_i(t-t_*)^{i/s}, \tag{4.11}$$

where a_i and b_i are polynomial functions of $\log(t-t_*)$. Now, the integral is constant on any solution curve. Therefore, one has $b_i=0 \forall i \neq h$. To order $O((t-t_*)^0)$, the coefficient b_h can be estimated:

$$b_h = \nabla I(a_0).a_{h0} + \log(t-t_*)\nabla I(a_0).a_{h1} + O(\log(t-t_*)^2). \tag{4.12}$$

The general form of the coefficients a_{h0} and a_{h1} are known from (4.8). Therefore, a new arbitrary constant λ enters at order $O((t-t_*)^0)$. This constant has to match the arbitrary constant of the first integral:

$$\lambda \nabla I(a_0).\beta_\rho = C. \tag{4.13}$$

Now, consider the first logarithmic contribution to the integral $I=I(x)$, that is, the order $O(\log(t-t_*))$ of $I(x(t-t_*))$:

$$\mu \nabla I(a_0).\beta_\rho = 0. \tag{4.14}$$

The constant C is arbitrary, therefore one has $\nabla I(a_0).\beta_\rho \neq 0$, and we conclude that $\mu=0$ and that the compatibility conditions for the Kowalevskaya exponent ρ is satisfied if the compatibility conditions up to Kowalevskaya's exponent ρ are satisfied. Iterating this process up to the last positive Kowalevskaya exponent, we see that there is no logarithmic contribution, that is, all solution can be expanded in Puiseux series. □

1. Problems and limitation

We have seen in this section that algebraic integrability is closely related to the absence of logarithmic points in the complex plane. This is a first step to a general relationship between integrability and singularity analysis. There is, however, a limitation in this method in the assumption on the degrees of first integrals, they should be related to the resonances of the system. If the degree d is not an eigenvalue of K, then from relation (4.13) with $C=0$, we have

$$\nabla I(a_0) = (0), \tag{4.15}$$

that is, the gradient of the first integral whose degree is not a Kowalevskaya exponent vanishes identically, and nothing can be said about the existence of logarithmic singularities in the complex plane.

This is the main difficulty of the method. For instance, suppose that there exists an irreducible first integral of degree $d > \rho_{\max}$, what can be said about the series expansions? Our proof relies heavily on the fact that $\nabla I(a_0) \neq (0)$, therefore in the case the gradient vanishes identically, no information can be found. Can we prove that such integrals do not exist, that is, if $K_\alpha \in \mathbb{Q}^n$, then one always has $D_\alpha = K_\alpha$?

We now overcome this difficulty by deriving necessary conditions for integrability of nonhomogeneous vector fields independently of the degree of the first integrals.

B. Algebraic integrability and logarithmic branch points: Part II

In the last section we proved that if the degrees of the first integrals are identical to the Kowalevskaya exponents, then algebraic integrability brings the single-valuedness of the solution. We now show that this result can be generalized in the sense that the assumption on the resonances can be dropped. Indeed, the key of the former proof is that the first logarithmic contribution to the first integral is given in terms of the gradient of the first integral around the particular solution $x=a_0 t^{-g}$. Therefore, the first integrals whose gradient vanishes on this particular solution cannot be used to prove single-valuedness.

We now extend the former result by considering variations around the general solution. We only retain from the previous assumptions that all balances are principal, that is, for each balance there exists $(n-1)$ positive Kowalevskaya exponents: Let $K_\alpha=\{\rho_1,...,\ \rho_{n-1},\ -1\}$ be the set of Kowalevskaya's exponents for the balance (α,g). Then, for all balances (α,g),

$$\rho_i>0 \quad \forall \rho_i \in K_\alpha, \quad i=1,\ldots,n-1. \tag{4.16}$$

Theorem 4.2: *Assume that the system* $S:\dot{x}=f(x)$ *has only principal balances and is algebraic integrable with* $(n-1)$ *first integrals* $I_1,\ldots,I_{n-1}$. *Then, all solutions can be expanded in Puiseux series*.

Proof 4.2: Under the assumptions, there exists a formal expansion of the solution around a movable singularity t_* of the form:

$$x=\sum_{i=1}^{\infty} x_i Z^i, \tag{4.17}$$

$$Z=\log(t-t_*), \tag{4.18}$$

$$x_i=(t-t_*)^p\sum_{j=1}^{\infty} a_{ij}(t-t_*)^{j/s}\equiv(t-t_*)^p\Psi_i, \tag{4.19}$$

where $p\in\mathbb{Q}^n$ and $s\in\mathbb{N}$.

We consider a first integral I. It is constant on all solutions. Therefore, one has

$$I(x(t-t_*))=C=(t-t_*)^{-d}[I(\Psi_0)+Z\nabla I(\Psi_0).\Psi_1+O(Z^2)]. \tag{4.20}$$

Since I is constant, we obtain to orders $O(Z^0)$, $O(Z^1)$:

$$(t-t_*)^{-d}I(\Psi_0)=C, \tag{4.21}$$

$$\nabla I(\Psi_0).\Psi_1=0. \tag{4.22}$$

These relations hold for all first integrals I_i:

$$(t-t_*)^{-d_i}I_i(\Psi_0)=C_i, \quad i=1,\ldots,n-1, \tag{4.23}$$

$$\nabla_i(\Psi_0).\Psi_1=0, \quad i=1,\ldots,n-1. \tag{4.24}$$

We conclude from the first expression that the arbitrary constants $C_i=C_i(\lambda_1,\ldots,\lambda_{n-1})$ are polynomial in the arbitrary constants $(\lambda_1,...,\lambda_{n-1})$ appearing in the series Ψ_0. The second expression implies that Ψ_1 is proportional to Ψ_0:

$$\Psi_1=K(t)\Psi_0, \tag{4.25}$$

where $K(t)$ is analytic in t.

The series Ψ_1 can be locally expanded around t_*:

$$\Psi_1=\mu p(t-t_*)^q+O((t-t_*)^{q+1}), \tag{4.26}$$

where $q\in\mathbb{N}$ and $\mu\in\mathbb{C}$ is an arbitrary constant and p is the leading exponent of $x_0=c(t-t_*)^p(1+O((t-t_*)))$.

From the other point of view, we know from the local analysis [see Eq. (4.8)] that

$$\Psi_1=\mu\beta_\rho(t-t_*)^\rho+O((t-t_*)^{\rho+1}), \tag{4.27}$$

where ρ is the first Kowalevskaya exponent at which the compatibility conditions are not identically satisfied and μ is a constant fixed by the compatibility conditions; β_ρ is the eigenvector of K of eigenvalue ρ.

Therefore, we have that either $\mu=0$ or $p=\beta_\rho$, which is not possible since we know that $p.\beta_\rho=0$ for all positive Kowalevskaya exponents. We conclude that $\mu=0$ and $\Psi_1=0$.

Now, if $\Psi_1=0$, we obtain to order $O(Z^2)$

$$\nabla I(\Psi_0).\Psi_2=0, \tag{4.28}$$

and the same conclusions apply to Ψ_2.

Iterating this process, we conclude that $\Psi_i=0 \forall i>0$, that is, the solution can be expanded in Puiseux series. □

1. Example: The Lorenz system

As an example, we consider the famous Lorenz system[38] which has been thoroughly investigated as a dynamical system[39] and eventually became a paradigmatic system for integrability theories.[2,3,5,7,9,40,41] From the singularity analysis point of view, it was first studied by Segur[42] and more recently in Ref. 43. The system reads

$$\dot{x}=\sigma(y-x), \tag{4.29}$$

$$\dot{y}=\rho x-y-xz, \tag{4.30}$$

$$\dot{z}=xy-\beta z, \tag{4.31}$$

$$\tag{4.32}$$

where $x,y,z,\ \sigma,\ \beta,\ \rho\in\mathbb{R}$.

The Lorenz system has only principal balances with $c=(2i,-2i/\sigma,-2/\sigma)$ and $g=(1,1,2)$. The resonance set is $K_1=\{-1,2,4\}$.

There is one set of parameters values for which the system has two first integrals, namely $\{\beta,\sigma,\rho\}=\{1,\frac{1}{2},0\}$ with first integrals

$$I_1=(x^2-2\sigma z)e^t, \tag{4.33}$$

$$I_2=(y^2+z^2)e^{2t}, \tag{4.34}$$

and the solutions can be expressed in terms of Jacobi elliptic functions.

In addition, there exist two set of values for which the system satisfies the Painlevé test: $\{\beta,\sigma,\rho\}=\{1,2,\frac{1}{9}\}$ with one time-dependent integral

$$I_3=(x^2-2\sigma z)e^{2\sigma t}, \tag{4.35}$$

and $\{\beta,\sigma,\rho\}=\{0,\frac{1}{3},\rho\}$ with the time-dependent integral

$$I_4=(-\rho x^2+\tfrac{1}{3}y^2+\tfrac{2}{3}xy+x^2z-\tfrac{3}{4}x^4)e^{(4/3)t}. \tag{4.36}$$

For all other values of the parameters the system does not satisfy the Painlevé test and we conclude, using Theorem 3.2:

Proposition 4.3: If $\{\beta,\sigma,\rho\}\neq\{1,\frac{1}{2},0\}$, *the Lorenz system is not algebraically integrable (with two first integrals).*

2. A conjecture

We have seen that the existence of a complete set of first integrals and only principal balances constrains the system so that it must have the weak Painlevé property. Two questions are in order: Can we relax the conditions on the balances? Are these conditions also sufficient? In Ref. 25 it was suggested that it is indeed the case. Our conjecture reads then

If a system of ODEs with polynomial vector fields is algebraically integrable, then it enjoys the weak Painlevé property.

To date, among all known examples and to the best of my knowledge, there is no counterexample to this conjecture.

V. PARTIAL INTEGRABILITY

A. A natural arbitrary small parameter

We consider a nonhomogeneous system

$$S: \dot{x} = f(x), \quad x \in \mathbb{K}^n, \tag{5.1}$$

where f_i are rational functions of x over $\mathbb{K}$, a field of constants (typically $\mathbb{K}=\mathbb{C}$ or $\mathbb{K}=\mathbb{R}$).

The problem is to find necessary conditions for the existence of first integrals. The theory we developed in the previous sections is only applicable for complete algebraic integrability. As a consequence, it cannot be directly applied to Hamiltonian systems, since for most of the Liouville integrable systems only half of the constants of motion are algebraic.

From the other point of view, the integrability conditions related to the Kowaleskaya exponents are based on similarity-invariant systems. However, most of the systems do not exhibit such a scaling property. Indeed, as soon as dissipation or damping is included under the form of linear terms, the system will lose the scale invariance. Nevertheless, similarity-invariant systems are the first-order systems in a perturbation expansion based on the scale invariance. With this idea in mind we can decompose the problem of finding necessary conditions for the existence of l first integrals ($l<n-1$) into two parts.

The first part of the analysis consists of finding conditions for the existence of l first integrals of all weight-homogeneous parts of the vector field. According to the weight g, the vector field can be truncated so that

$$f(x) = f^{(0)}(x) + \cdots + f^{(m)}(x), \tag{5.2}$$

$$f^{(i)}(\alpha^{-g}x) = \alpha^{-g-1+i} f^{(i)}(x). \tag{5.3}$$

The leading weight-homogeneous system $\dot{x} = f^{(0)}(x)$ is scale invariant under the symmetry ($x \to \alpha^g x$, $t \to \alpha^{-1} t$). According to this scaling symmetry, any first integral can be decomposed into a finite sum of weight-homogeneous components:

$$I(x,t) = I^{(0)}(x) + \epsilon I^{(1)}(x,t) + \cdots, \tag{5.4}$$

$$I^{(i)}(\alpha^g x) = \alpha^{d+i} I^{(i)}(x), \tag{5.5}$$

where $\epsilon = 1/\alpha$.

The following lemma shows that a necessary condition for the existence of a first integral for a vector field is given by the existence of a first integral for its similarity invariant part.

Lemma 5.1: Let $I(x,t)$ be a first integral of $\dot{x} = f(x,t)$. Then, $I^{(0)}(x)$ is a first integral of $\dot{x} = f^{(0)}(x)$.

Proof 5.1: The condition for $I(x,t)$ to be a first integral reads

$$0 = \nabla I . f + \partial_t I = \nabla I^{(0)} . f^{(0)} + \epsilon (\nabla I^{(0)} . f^{(1)} + \nabla I^{(1)} . f^{(0)} + \partial_t I^{(1)}) + O(\epsilon^2). \tag{5.6}$$

This expansion is valid for arbitrary ϵ, indeed ϵ is an arbitrary parameter and can assume any value. Therefore, in the limit $\epsilon \to 0$, one finds $0 = \nabla I^{(0)} . f^{(0)}$. □

Let us stress again that ϵ is an arbitrary parameter that can assume any value and does not have to be small. Therefore, our method does not rely on the smallness of ϵ. If there is a small parameter in the system a perturbation expansion can be performed (see, for instance, Ref. 44).

The second part of the analysis is based on the existence of first integrals for the similarity invariant part. Assuming that such first integrals exist, we derive necessary conditions for the existence of first integrals for the nonhomogeneous contributions.

Our strategy is the following:

(1) Find necessary conditions for the existence of l $(0 < l < n)$ first integrals of the weight-homogeneous vector field $\dot{x} = f^{(0)}$.

(2) Build the l first integrals, $I_i^{(0)}$ $(i = 1,\ldots,l)$.

(3) Find necessary conditions for the existence of l' $(l' \leqslant l)$ first integrals for the nonhomogeneous systems.

(4) Build the l' first integrals F_i $(i = 1,\ldots,l')$. Each F_i is of the form

$$F = F^{(0)}(x) + \epsilon F^{(1)}(x,t) + \cdots , \tag{5.7}$$

$$F^{(0)} = P(I_1^{(0)},\ldots,I_l^{(0)}), \tag{5.8}$$

where P is a rational, weight-homogeneous function.

The scaling symmetry is interesting in many respects. By contrast to the linear perturbation theory, starting from the lower linear terms of the systems and building higher-order corrections valid in the neighborhood of the fixed point, our nonlinear perturbation theory starts from the highest nonlinear terms and consider lower-orders perturbation. It allows us to build integrable corrections valid everywhere and for all values of the parameters.

B. Necessary conditions for partial integrability

Here we assume that the analysis has already been performed on the weight-homogeneous components of the vector fields and the explicit form of the first integrals are known. Therefore, we study the persistence of the first integrals, or homogeneous combinations of first integrals, when lower nonlinearities are added to the system.

We consider again the nonhomogeneous system

$$S: \dot{x} = f(x). \tag{5.9}$$

For this system, there may exist different truncations, that is, different weights g decomposing the vector field, according to the scaling $(x \to \alpha^g x,\ t \to \alpha^{-1} t)$, in dominant and nondominant parts. We consider all such vectors g and assume that each weight-homogeneous component admits the maximum number of possible first integrals. For a given vector g, we have a truncation of the vector field (5.2), so that $I_i = I_i(x)$ $(i = 1,\ldots,l)$ is a set of independent first integrals for the system $\dot{x} = f^{(0)}(x)$. Each first integral has a given weighted degree h_i w.r.t. the weight g:

$$I_i(\alpha^g x) = \alpha^{h_i} I_i(x). \tag{5.10}$$

We are interested in the existence of first integrals for the complete system. The most general form the first integrals can assume is given by

$$F(x,t) = F^{(0)}(x) + \epsilon F^{(1)}(x,t) + \epsilon^2 F^{(2)}(x,t) + \cdots , \tag{5.11}$$

where by construction $F^{(0)}$ is built on the first integrals I_i:

$$F^{(0)}=P(I_1,\ldots,I_l), \tag{5.12}$$

where P is weight-homogeneous w.r.t. the scaling $(I_i\to\epsilon^{h_i}I_i)$.

Let us recall that two different first integrals F_1 and F_2 are independent iff $\nabla F_1^{(0)}$ and $\nabla F_2^{(0)}$ are linearly independent. Now, we derive necessary conditions for the existence of F.

First, we note that there is a series expansion involving l free constants (corresponding to the l free arbitrary constants) and we compute the following $\psi-\epsilon$ expansion:[44]

$$x=x_0+\epsilon x_1+\epsilon^2 x_2+\cdots, \tag{5.13}$$

$$x_i=\sum_{j=0}^{i-k+1} s_{ij}[\log(t-t_*)]^j, \tag{5.14}$$

where $s_{ij}\in\mathbb{C}((t-t_*))$ are convergent Laurent series with finite principal parts and k is the first order in ϵ where logarithmic corrections are required, so that x reads

$$x=s_{00}+\epsilon s_{10}+\epsilon^2 s_{20}+\cdots+\epsilon^k(s_{k0}+s_{k1}\log(t-t_*))+O(\epsilon^{k+1}). \tag{5.15}$$

Second, assuming there exists a first integral, we expand $F(x)$ around x_0:

$$\begin{aligned}F(x,t)=F(x_0)+\epsilon(\nabla F^{(0)}(x_0).x_1+F^{(1)}(x_0,t))+\epsilon^2(\nabla F^{(0)}(x_0).x_2\\ +\nabla F^{(1)}(x_0,t).x_1+\nabla^2 F^{(0)}(x_0):x_1x_1+F^{(2)}(x_0,t))+O(\epsilon^3).\end{aligned} \tag{5.16}$$

Note that $F(x,t)$ is constant along all solution curves and the parameter ϵ is a scaling parameter which assume arbitrary values. As a consequence, each order in ϵ is constant in time. In particular, there is no logarithmic dependence and we obtain the following.

Lemma 5.2: Assume there exists a first integral $F(x,t)=F^{(0)}(x)+\epsilon F^{(1)}(x,t)+\cdots$ *for the system S. Then the following identity holds*:

$$\nabla F^{(0)}.s_{k1}=0. \tag{5.17}$$

Proof 5.2: Inserting the expansion of x in terms of s_{ij} in (5.16), we obtain

$$\begin{aligned}F(x,t)=F^{(0)}(s_{00})+\epsilon(\nabla F^{(0)}(s_{00}).s_{10}+F^{(1)}(s_{00},t))+\cdots\\ +\epsilon^k(\nabla F^{(0)}(s_{00}).(s_{k0}+\log(t-t_*)s_{k1}+\ldots))+O(\epsilon^{k+1}).\end{aligned} \tag{5.18}$$

The coefficients of ϵ are constant at each order and the first logarithmic correction enters to order $O(e^k)$. Hence, we obtain

$$\nabla F^{(0)}.s_{k1}=0. \tag{5.19}$$

□

There is yet another instructive way to complete this result. To do so, we consider a system $S:\dot{x}=f(x)$ and assume it has a first integral $I(x,t)$. Let $\hat{x}=\hat{x}(t)$ be a solution of S and introduce the *variational equation,*

$$\dot{v}=Df(\hat{x}).v, \tag{5.20}$$

where $Df(\hat{x})$ is the Jacobian matrix estimated on the solution $\hat{x}$.

Lemma 5.3 (Poincaré): Let $I=I(x)$ *be a first integral of S and let v be any solution of the variational equation. Then,*

$$\nabla I(\hat{x}).v=C, \tag{5.21}$$

where C is a constant.

Now, consider $F^{(0)}$, a first integral of $\dot{x}=f^{(0)}(x)$. The solution s_{00} is a local convergent Laurent series around the singularity t_*, and s_{k1} is, by construction, a solution of

$$\dot{v}=Df(s_{00}).v. \tag{5.22}$$

Therefore, using Poincaré's lemma, we obtain $\nabla F^{(0)}.s_{k1}=C$. Inserting this result in (5.18) and asking the log contribution to vanish identically at each order in ϵ, we obtain Lemma 5.2.

The point of this lemma is to provide a necessary condition for $F^{(0)}$ to be the homogeneous part of the nonhomogeneous first integral $F(x,t)$. However, the functional form of $F^{(0)}$ is not known except for the fact that it is built out of the first integrals I_i $(i=1,\ldots,l)$.

Now, consider the l first integrals $I_i=I_i(x)$ $(i=1,\ldots,l)$. For each first integral, we define the conditions

$$c_i=\nabla I_i^{(0)}(s_{00}).s_{k1}. \tag{5.23}$$

If there exist l first integrals for the system S, they are built on the first integrals I_i, and the existence condition for these first integrals depends on the conditions c_i:

Proposition 5.4: Assume there exist l independent analytic first integrals $I_i=I_i(x)$ for the similarity invariant system $S_0:\dot{x}=f^{(0)}(x)$. Then, a necessary condition for the existence of l independent analytic first integrals for $\dot{x}=f(x)$ is $c_1=c_2=\cdots=c_l=0$.

Proof 5.4: Suppose that there exist l independent first integrals F_i for S. Let F be any of such integral. According to Lemma 5.3, for each integral we have

$$\nabla F^{(0)}(s_{00}).s_{k1}=0. \tag{5.24}$$

As already explained, $F^{(0)}$ is weight-homogeneous in I_j so that

$$\nabla F^{(0)}(s_{00})=\sum_{j=1}^{l} A_{ij}\nabla I_j^{(0)}(s_{00}) \tag{5.25}$$

with $A\in \mathrm{GL}(l,\mathbb{C})$, owing to the independence of the first integrals and the fact that the series s_{00} depends on l free parameters.

Therefore the integrability condition reads

$$\sum_{j=1}^{l} A_{ij}\nabla I_j^{(0)}(s_{00}).s_{k1}=\sum_{j=1}^{l} A_{ij}c_j=0. \tag{5.26}$$

Since $A\in \mathrm{GL}(l,\mathbb{C})$, we have $c_i=0\,\forall i=1,\ldots,l$. □

1. A first example

As a first example, we consider the following three degrees of freedom Hamiltonian:[45]

$$H=\tfrac{1}{2}(p_1^2+p_2^2+p_3^2)+\tfrac{1}{4}(x_1^4+x_2^4+x_3^4)+\epsilon(\mu_1x_2x_3+\mu_2x_3x_1+\mu_3x_1x_2), \tag{5.27}$$

where $\mu_i\neq 0$, $i=1,2,3$

For $\epsilon=0$, the system is integrable with three obvious constants of motion, the Hamiltonians of the decoupled systems

$$I_i^{(0)}=2p_i^2+x_i^4, \quad i=1,2,3, \tag{5.28}$$

and the solutions can be expanded in Laurent series $s=(x_1,x_2,x_3,p_1,p_2,p_3)$:

$$s_{00}=(t-t_*)^p\sum_{i=0}^{\infty} a_i(t-t_*)^i, \tag{5.29}$$

where $p=(-1,-1,-1,-2,-2,-2)$, $a_i\in\mathbb{C}^6$, and a_4 is arbitrary (resonance $r\in K_1=\{-1,-1,-1,4,4,4\}$).

The series expansion for the perturbed problem can be readily computed:

$$x=s_{00}+\epsilon s_{10}+\epsilon^2(s_{20}+s_{21}\log(t-t_*))+O(e^3), \tag{5.30}$$

where $s_{ij}\in\mathbb{C}^6((t-t_*))$.

The first logarithmic contribution enters to order $O(\epsilon^2)$. The integrability conditions read

$$c_i=\nabla I_i^{(0)}.s_{21}, \quad i=1,2,3. \tag{5.31}$$

The conditions $c_1=c_2=c_3=0$ gives then

$$2\mu_2\mu_3-\mu_1\mu_3-\mu_1\mu_2=0, \tag{5.32}$$

$$-\mu_2\mu_3+2\mu_1\mu_3-\mu_1\mu_2=0, \tag{5.33}$$

$$-\mu_2\mu_3-\mu_1\mu_3+2\mu_1\mu_2=0. \tag{5.34}$$

As a consequence, if $\mu_i\neq\mu_j$, $i\neq j$, the Hamiltonian is not Liouville integrable, that is there exists at most another constant of motion beside the Hamiltonian. In Ref. 45, it was shown that the Hamiltonian (5.27) for $\mu_1=0$, $\mu_2=\mu_3=1$, does not possess a second constant of motion.

2. Another example

The second example is also a three degrees of freedom Hamiltonian:[34]

$$H=\tfrac{1}{2}(p_1^2+p_2^2+p_3^2)+(x_1x_3^2+x_2x_3^2)+\epsilon(\mu_1x_1^2+\mu_2x_2^2+\mu_3x_3^2), \tag{5.35}$$

where $\mu_i\neq 0$, $i=1,2,3$.

We first consider the unperturbed system ($\epsilon=0$). Is the system Liouville integrable? By inspection or using direct methods, a second constant of motion is easily found:

$$I=p_1-p_2. \tag{5.36}$$

A third constant of motion is lacking to complete the integration:

Lemma 5.5: The Hamiltonian system $H=\tfrac{1}{2}(p_1^2+p_2^2+p_3^2)+(x_1x_3^2+x_2x_3^2)$ *is not Liouville integrable.*

Proof 5.5: We compute the Kowalevskaya exponents for the scale-invariant solution $(x_1,x_2,x_3,p_1,p_2,p_3)=-3t^{-3}(t/2,t/2,-t,-1,-1,-2)$: $\rho\in\{-1,2,3,6,(5\pm i\sqrt{23})/2\}$. The occurrence of irrational Kowalevskaya exponents are incompatible with Liouville integrability for potential with diagonal kinetic part (see Theorem 3.4). □

Now, we consider the full system (5.35), and build the ψ–ϵ expansion up to order $O(\epsilon)$:

$$x=s_{00}+\epsilon(s_{10}+s_{11}\log(t-t_*))+O(\epsilon^2), \tag{5.37}$$

where $x=(x_1,x_2,x_3,p_1,p_2,p_3)$ and s_{00},s_{10} are Laurent series. The series s_{11} reads

$$s_{11}=-\tfrac{3}{4}(\mu_1-\mu_2)(1,-1,0,0,0,0)+O((t-t_*)^2). \tag{5.38}$$

The conditions $0=\nabla H.s_{11}$ and $0=\nabla I.s_{11}$ lead to $\mu_1=\mu_2$. In this case the second constant of motion is found to be

$$I=(p_1^2+\mu_1 x_1^2)+(p_2^2+\mu_1 x_2^2)-2(p_1p_2+\mu_1 x_1 x_2). \tag{5.39}$$

We have proved the following.

Proposition 5.6: The Hamiltonian system (5.35) does not have a second constant of motion unless $\mu_1=\mu_2$.

VI. CONCLUSIONS

This paper studies the relationship between the singularity analysis and the algebraic integrability. We first considered weight-homogeneous systems and showed that there exists a fundamental relationship between the Kowalevskaya exponents and the degrees of the first integrals. We concluded from this relation that the number of first integrals is equal or less than the dimension of the vector space spanned by the Kowalevskaya exponents over the integers. I believe that this relationship, although restricted, is the most complete information one can hope to obtain by using only the Kowalevskaya exponents. In order to obtain more information on the integrability, or lack thereof, of a system, one has to take into account the specific structure of logarithmic or algebraic branch points. As a corollary, we proved the well-known Yoshida's statement: a necessary condition for complete algebraic integrability is that all Kowalevskaya exponents be rational. A second important result concerns completely algebraically integrable system. We proved that if all balances are principal [i.e., $(n-1)$ positive resonances], then algebraic integrability implies that all solutions can be expanded in Puiseux series. Moreover, I believe that the assumption that all balances are principal can actually be removed. The third main result of this paper concerns partial integrability. Partial integrability seems the most common feature of dynamical systems emerging from physical model; indeed often by symmetry or conservation laws, a few constants of the motion exist. Assuming that the weight-homogeneous part of the vector field is algebraically integrable, we derived necessary conditions for the existence of first integrals based on the nonexistence of logarithmic branch points. This result can be used, for instance, to show that first integrals disappear in the presence of linear dissipative terms.

I hope that these three aspects put together will give a general picture of the type of information concerning integrability one can hope to obtain using singularity analysis. It also provides direct algorithmic methods to answer such questions.

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The singular manifold method revisited

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For many completely integrable partial differential equations (PDEs) the singular manifold method of Weiss allows the recovery of the Lax pair and Darboux transformation (DT), and so also the Bäcklund transformation, from a truncated Painlevé expansion. Recently the so-called ''two-singular manifold method'' has been proposed in order to handle PDEs such as the modified Korteweg–de Vries (MKdV) equation. Here we present a more natural extension of the Weiss singular manifold method which makes use of only one singular manifold but is capable of dealing with such PDEs. In this approach we allow the possibility that the DT might in fact correspond to an infinite Painlevé expansion, for a certain choice of the arbitrary coefficients. This then leads us to a new and more consistent definition of ''singular manifold equation'' (SME); this can give SMEs different from those usually presented. The summation of infinite Painlevé expansions is effected by seeking a truncation in a new Riccati variable Z. The use of this variable greatly simplifies the recovery of Lax pairs from Painlevé analysis. Practical and theoretical aspects of our approach are illustrated using MKdV as an example. The results of this analysis are confirmed by the consideration of fifth-order MKdV. We then make a further extension of this method which allows it to be applied to a PDE in $2+1$ dimensions, and so simultaneously to reductions of the latter to PDEs in $1+1$ dimensions. A corollary of our analysis is a direct proof of the convergence of infinite WTC expansions for a certain choice of the arbitrary coefficients therein. In addition, the approach developed here allows us to place within the context of Painlevé analysis a larger class of exact solutions than was possible hitherto. Again, our analysis greatly simplifies the recovery of such solutions. [S0022-2488(96)01404-9]

I. INTRODUCTION: PAINLEVÉ ANALYSIS AND TRUNCATION

A. The Painlevé test

The now well-known connection between complete integrability and the Painlevé property was first remarked upon by Ablowitz and Segur,[1] who observed that similarity reductions of nonlinear partial differential equations (PDEs) solvable by an Inverse Scattering Transform give rise to nonlinear ordinary differential equations (ODEs) whose only movable singularities are poles. Here ''movable'' means that the location of the singularity depends upon constants of integration. Having only poles as movable singularities is a special case of the property required of an ODE by Painlevé[2,3]—i.e., that the general solution of the ODE should have no movable branched singularities—in his search for ODEs defining new functions. The precise nature of this connection between complete integrability and the Painlevé property continues to be the subject of much intensive research.

Ablowitz, Ramani, and Segur[4,5] developed an algorithm, based on the work of Kowalevskaya,[6,7] to give necessary conditions for an ODE to have the Painlevé property. This was later extended by Weiss, Tabor, and Carnevale (WTC)[8] so as to be applicable directly to PDEs.

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The WTC test involves seeking a solution of the PDE, for example an equation in $U(x,t)$,

$$E[U]=0, \tag{1}$$

as an expansion of the form

$$U=\varphi^p\sum_{j=0}^{\infty} U_j^{\varphi}\varphi^j, \tag{2}$$

where each U_j^{φ} is a function of x and t, and $\varphi(x,t)=0$ defines an arbitrary noncharacteristic[9] movable singular manifold. Here the superscript φ on the coefficient U_j^{φ} denotes the expansion variable.

This analysis requires first a choice of expansion family, i.e., a choice of leading order exponent p (here assumed negative), leading order coefficient U_0^{φ}, and dominant terms $\hat{E}[U]$. For each family there is a set of indices $\{j_1,\ldots,j_N\}$ which give the values of j for which arbitrary data should be introduced in (2). Bearing in mind also more recent extensions of the Painlevé test,[10,11] we have the following necessary conditions for the PDE (1) to have the Painlevé property: for any family which represents either the general or a particular solution p must be integer; the indices must be distinct integers; and all compatibility conditions corresponding to each index must be satisfied. This test has proved to be an extremely effective tool in testing PDEs for complete integrability.

However, the WTC approach has also been of use in providing a constructive proof of integrability. It was shown[8,12] that from a truncated expansion U_T,

$$U_T=\varphi^p\sum_{j=0}^{-p} U_j^{\varphi}\varphi^j, \tag{3}$$

it is possible to obtain the Lax pairs of many integrable PDEs. The singular manifold method of Weiss,[12] later phrased algorithmically by Musette and Conte,[13] can also give the Darboux transformation (DT)—and so together with the Lax pair the Bäcklund transformation (BT)—for the PDE. This singular manifold method involves seeking a constraint on φ, the so-called ''singular manifold equation'' (SME), for the truncation of the WTC expansion at constant level (3) to exist.

We later give a new definition of ''singular manifold equation.'' For now we simply remark that (3) represents the trivial (because finite) summation of (2) for certain choices of the arbitrary coefficients, and with φ subject to the SME. In particular, all arbitrary coefficients of positive powers of φ in (2) have been set equal to zero.

B. The invariant Painlevé analysis

Conte[14] introduced an expansion variable χ given in terms of the singular manifold φ by

$$\chi=\left(\frac{\varphi_x}{\varphi}-\frac{\varphi_{xx}}{2\varphi_x}\right)^{-1}, \tag{4}$$

such that the coefficients U_j^{χ} of the resulting expansion

$$U=\chi^p\sum_{j=0}^{\infty} U_j^{\chi}\chi^j \tag{5}$$

are invariant under arbitrary homographic transformations on φ. This function χ satisfies the Riccati system

$$\chi_x = 1 + \tfrac{1}{2} S \chi^2, \tag{6}$$

$$\chi_t = -C + C_x \chi - \tfrac{1}{2}(C_{xx} + CS)\chi^2, \tag{7}$$

where S, the Schwarzian derivative of φ, and C are given by

$$S = \{\varphi; x\} = \left(\frac{\varphi_{xx}}{\varphi_x}\right)_x - \frac{1}{2}\left(\frac{\varphi_{xx}}{\varphi_x}\right)^2, \quad C = -\frac{\varphi_t}{\varphi_x}. \tag{8}$$

The cross-derivative condition on (6), (7) is

$$S_t + C_{xxx} + 2SC_x + S_x C = 0 \tag{9}$$

which is identically satisfied in terms of φ.

The Painlevé expansion (5) is a resummation the WTC expansion (2); transformation formulae between the coefficients U_j^{φ} and U_j^{χ} are given in Ref. 14. The advantage of the invariant analysis is that the expressions for the coefficients of the expansion are greatly shortened.

The truncated WTC expansion (3) can then be rewritten as

$$U_T = \chi^p \sum_{j=0}^{-p} U_j^{\chi} \chi^j. \tag{10}$$

Musette and Conte[13] showed that (second- and third-order) Lax pairs can be recovered algorithmically when (10) corresponds to a DT of the form

$$U_T = \mathscr{D} \log \psi + u, \tag{11}$$

where $\mathscr{D}$ is the singular part operator[15] and u is a second solution of the PDE.

This is done by expressing $\chi^{-1} - \psi_x/\psi$, S and C in terms of three functions Y_1, Y_2, Y_3:

$$\chi^{-1} - \frac{\psi_x}{\psi} = -\tfrac{1}{2} Y_1, \quad S = Y_{1,x} - \tfrac{1}{2} Y_1^2 + 2Y_2, \quad C = -Y_3. \tag{12}$$

In the case of a second-order Lax pair $Y_1 = 0$, and the Lax pair is obtained simply as the linearization of the Riccati system (6), (7) via $\chi^{-1} = \psi_x/\psi$:

$$\psi_{xx} = -\tfrac{1}{2} S \psi, \tag{13}$$

$$\psi_t = -C\psi_x + \tfrac{1}{2} C_x \psi. \tag{14}$$

In the case of a third-order Lax pair Y_3 is defined in terms of Y_1, and the Lax pair is obtained by identifying it with the resulting projective Riccati system in Y_1, Y_2. Details may be found in Ref. 13.

C. Higher order truncation and a new expansion variable

It was noticed in Ref. 16 that a further advantage of using an expansion variable satisfying a system of Riccati equations is that it allows the possibility of truncating at a positive power. This was used to extend the class of exact solutions that it is possible to obtain from a truncated Painlevé expansion, as follows. When S and C are constant,

$$S = -\tfrac{1}{2} k^2, \quad C = c, \tag{15}$$

the general solution of the Riccati system (6), (7) is

$$\chi^{-1}=\frac{k}{2}\tanh\left(\frac{1}{2}k(x-ct+\alpha)\right), \tag{16}$$

α being an arbitrary constant.

In the case of a higher order truncation with S and C constant, simple trigonometric identities allow us to identify negative and positive powers of χ as[16]

$$\chi^{-1}=\frac{k}{2}(\tau_0-\sigma_0), \tag{17}$$

$$\chi=\frac{2}{k}(\tau_0+\sigma_0), \tag{18}$$

where

$$\tau_0\equiv\tanh(k(x-ct+\beta)),\quad \sigma_0\equiv i\ \mathrm{sech}(k(x-ct+\beta)),\quad \beta=\alpha+\frac{i\pi}{2k}. \tag{19}$$

Clearly,

$$\tau_0^2=\sigma_0^2+1. \tag{20}$$

We recall that such higher order truncations correspond to the summation of infinite WTC expansions for certain choices of arbitrary data.[16]

Using this higher order truncation we can recover the one-soliton solution of the modified Korteweg–de Vries (MKdV) equation.[16] The recovery of this soliton solution is important for the following reason:

> *If a (truncated) Painlevé expansion is to lead to the Lax pair and Darboux transformation for a given PDE then a necessary condition is that it can be made to yield the one-soliton solution.*

However in order to obtain the Lax pair for MKdV using this higher order truncation a further extension needs to be made: a more general Riccati system than (6), (7) has to be used. In Refs. 17 and 18 the Riccati system

$$Y_x=R_0+R_1Y+R_2Y^2, \tag{21}$$

$$Y_t=S_0+S_1Y+S_2Y^2, \tag{22}$$

having three cross-derivative conditions, was introduced. This is the so-called ''two-singular manifold method,'' and it allowed the recovery of the BTs for the MKdV and sine-Gordon (s-G) equations (in fact the BT for s-G can be recovered using the standard singular manifold method—see the Appendix). In Ref. 19 these results were extended to the scalar Broer–Kaup (BK) equation.[20–22] We noted in Ref. 19 that this approach has the advantages over other approaches[23,24] that a single expansion variable Y is used, coefficients of Y in the resulting expansion of the PDE are set to zero independently, and the spectral parameter is introduced by the process of solving the resulting determining equations. These points remain true for the new Riccati variable introduced in Sec. II.

D. Questions and remarks

We now make the following remarks on the Riccati system (21), (22), when compared to (6), (7):

- No relationship is given between Y and the WTC singular manifold φ. Is there a corresponding WTC expansion? If so, what is its relationship to the DT obtained? Is there a corresponding singular manifold equation?
- When solving the system of determining equations we are left with some gauge freedom in the Riccati variable Y which means that a new Riccati variable—e.g., $\lambda Y/R_0$ for MKdV[18]—has to be introduced in order to remove this freedom. Similar remarks hold for BK[19] (s-G is discussed in the Appendix). Can we introduce a Riccati variable for which this gauge freedom is absent?
- Is it necessary to obtain the DT in advance?
- In Ref. 25 the recovery of solutions polynomial in two functions σ, τ was considered. These functions depend on a parameter μ such that when $\mu=0$, $\sigma=\sigma_0$, and $\tau=\tau_0$ given by (19). Thus far only this subclass of solutions polynomial in σ_0 and τ_0 has been placed within the context of Painlevé analysis; is it possible to remove this restriction $\mu=0$ and obtain the full class of solutions polynomial in σ and τ from Painlevé analysis, i.e., from a Painlevé expansion in a *single* variable?

It is these questions that we address in the following sections. This we do by introducing a much simpler Riccati system, one which arises in quite a natural way. We explore the practical and theoretical implications of our analysis using MKdV as an example. The results obtained for MKdV are then corroborated by an application of this analysis to the fifth order modified Korteweg–de Vries (MKdV5) equation. The techniques developed here are then further extended and applied to a PDE in $2+1$ dimensions. We will also see how our approach allows us to place the full class of solutions polynomial in σ and τ within the context of Painlevé analysis.

II. A NEW RICCATI VARIABLE

A. A new Riccati variable: motivation

The Riccati system (6), (7) linearizes onto the system (13), (14) via $\chi^{-1}=\psi_x/\psi$. A natural way therefore to construct a more general Riccati system is to consider the nonlinearization of the most general second-order scalar linear system given by

$$\eta_{xx}=A\eta_x+B\eta, \tag{23}$$

$$\eta_t=-C\eta_x+\left(\int^x D\ dx'\right)\eta. \tag{24}$$

We note that Lax pairs having a spatial part of the form (23) have been discussed for example in Ref. 26. The sign of C and integration of D in (24) are chosen for convenience.

The corresponding Riccati system, obtained via $Z^{-1}=\eta_x/\eta$, is

$$Z_x=1-AZ-BZ^2, \tag{25}$$

$$Z_t=-C+(AC+C_x)Z-(D-BC)Z^2, \tag{26}$$

which has as cross-derivative condition

$$(Z_x)_t-(Z_t)_x\equiv x_1Z+x_2Z^2=0, \tag{27}$$

where

$$-x_1 \equiv A_t + (AC)_x + C_{xx} - 2D = 0, \tag{28}$$

$$-x_2 \equiv B_t - D_x + 2BC_x + B_x C + AD = 0. \tag{29}$$

The integration of D is performed in (24) since the coefficient of η in (24) appears in Eqs. (25)–(29) by its x-derivative only, and it is only these equations that we will use in seeking a truncated expansion in Z.

Remarks:

We could, by solving (28) for D, consider a Riccati system with coefficients depending on three functions A,B,C instead of four, and having one cross-derivative condition instead of two. However in practice it is easier to use the above system together with the two cross-derivative conditions (28), (29).

For $A=0$ this system reduces to that previously considered, with the identification $B=-S/2$, $C=C$.

An objection that might be raised immediately to the above approach is that it is possible to set $A=0$ in (25), (26) by a simple gauge transformation, and so this system is in fact equivalent to the system (6), (7). We shall see that whereas it is true that such a gauge transformation exists, truncations in Z can give more information than truncations in χ.

This gauge transformation is

$$Z^{-1} = \chi^{-1} + \tfrac{1}{2}A, \tag{30}$$

and leads to a system of the form (6), (7), with $C=C$ and S being given by

$$-\tfrac{1}{2}S = B + \tfrac{1}{4}A^2 - \tfrac{1}{2}A_x, \tag{31}$$

where we have used (28) to solve for D. The corresponding transformation between (23), (24) and (13), (14) is of course

$$\eta = (e^{(1/2)\int^x A\, dx'})\psi. \tag{32}$$

However the equivalence of these two Riccati systems does not mean that consideration of the Riccati system (25), (26) is useless. Consider a truncated expansion of the form[16]

$$U_T = U^Z_{0,1} \log Z + Z^p \sum_{j=0}^{-(p+p')} U^Z_j Z^j, \quad U^Z_{0,1} \text{ constant} \tag{33}$$

such that the PDE (1) has the resulting expansion

$$E[U_T] = Z^q \sum_{j=0}^{-(q+q')} E^Z_j Z^j, \tag{34}$$

where q is the singularity order of E, and p', q' correspond to a possible second family (for a higher order truncation we often have $p'=p$, $q'=q$).

We note that if we choose to set $p'=0$ and $U^Z_{0,1}=0$, so that $q'=0$ and (33) corresponds to a standard truncation at constant level, then the transformation (30) gives rise to a corresponding truncation in χ of the form (10), and so does indeed correspond to the removal of an arbitrary gauge. However when the truncation is such that (34) includes positive powers of Z, i.e., $p'<0$ or

$U^Z_{0,1} \neq 0$, then for $A \neq 0$ there is for each of (33) and (34) no corresponding *finite* series in χ. In fact the truncation (33) then corresponds to the summation of an infinite series in χ, or ϕ, for certain choices of arbitrary data (see examples below).

The above discussion allows us to answer immediately one of the questions raised above, i.e., that of relating the expansion variable to the original singular manifold φ. We see from (30), (31) that we may define this new expansion variable Z in terms of the singular manifold φ, together with an auxiliary function A, as

$$Z = \left(\frac{\varphi_x}{\varphi} - \frac{\varphi_{xx}}{2\varphi_x} + \frac{1}{2} A \right)^{-1}, \tag{35}$$

where this variable satisfies the Riccati system (25), (26), B and C being also defined in terms of φ and A as

$$B = -\frac{1}{2} \left[\left(\frac{\varphi_{xx}}{\varphi_x} \right)_x - \frac{1}{2} \left(\frac{\varphi_{xx}}{\varphi_x} \right)^2 \right] + \frac{1}{2} A_x - \frac{1}{4} A^2, \tag{36}$$

$$C = -\frac{\varphi_t}{\varphi_x}, \tag{37}$$

and D being obtained from (28).

An immediate consequence of the equivalence of the system (25), (26) with (6), (7) is that there is no possibility of a discrepancy when performing the Painlevé test; it is sufficient to perform this test using the variable χ introduced by Conte.[14]

Finally we give, for future reference, four equivalent linearizations of the Riccati system (25), (26). The first is via $Z^{-1} = \eta_x / \eta$ onto (23), (24).

The second is via $Z^{-1} = \psi_2 / \psi_1$ onto

$$\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}_x = \begin{pmatrix} -\frac{1}{2}A & 1 \\ B & \frac{1}{2}A \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}, \tag{38}$$

$$\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}_t = \begin{pmatrix} \frac{1}{2}(AC + C_x) & -C \\ (D - BC) & -\frac{1}{2}(AC + C_x) \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}. \tag{39}$$

This system has of course the same cross-derivative conditions (28), (29) as the system (23), (24).

The third is via $Z^{-1} = (\xi_2 / \xi_1) + (A/2)$ onto (note the combination of A and B)

$$\begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix}_x = \begin{pmatrix} 0 & 1 \\ B + \frac{1}{4}A^2 - \frac{1}{2}A_x & 0 \end{pmatrix} \begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix}, \tag{40}$$

$$\begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix}_t = \begin{pmatrix} \frac{1}{2}C_x & -C \\ \frac{1}{2}C_{xx} - (B + \frac{1}{4}A^2 - \frac{1}{2}A_x)C & -\frac{1}{2}C_x \end{pmatrix} \begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix}. \tag{41}$$

These last two linearizations are related via the gauge transformation

$$\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ \frac{1}{2}A & 1 \end{pmatrix} \begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix}. \tag{42}$$

Since $\psi_2=\psi_{1,x}+\frac{1}{2}A\psi_1$ and $\xi_2=\xi_{1,x}$ we see that

$$Z^{-1}=\frac{\psi_{1,x}}{\psi_1}+\frac{1}{2}A=\frac{\xi_{1,x}}{\xi_1}+\frac{1}{2}A, \tag{43}$$

which corresponds to Eq. (30), and so ψ_1 and ξ_1 both satisfy the same linear system (13), (14) as ψ with S being given by (31). This is our fourth linearization; the corresponding cross-derivative condition is of course (9) for this choice of S. This means that when linearization onto a scalar Lax pair (13), (14) is inappropriate for a particular PDE—for example because the cross-derivative condition evaluates to an operator acting on that PDE rather than just the PDE itself—an appropriate linearization onto a matrix spectral problem (38), (39) may still be available.

For S given by (31), one should recognize immediately here that the second-order linear equation (13) can be written as

$$[(\partial_x-\tfrac{1}{2}A)(\partial_x+\tfrac{1}{2}A)-B]\psi=0, \tag{44}$$

which of course underlies the gauge transformation (42). In the case where B is the spectral parameter this is the well-known factorization of the Schrödinger operator, and the corresponding gauge transformation (42), or for the Riccati pseudopotential (30), is by now standard (it can be found for example in Ref. 27). The most famous example of such a factorization is of course for MKdV.

We now use MKdV as an example in order to consider both the practical and theoretical aspects of our analysis. Of course the question of recovering the spectral problem for MKdV from Painlevé analysis has been tackled before;[18,24] we use MKdV here simply as an example which allows us to demonstrate the power and simplicity of our new method. It will also provide the framework within which to give the correct interpretation of this method as a natural extension of the Weiss singular manifold method. We will see that while there is clearly a close connection between the singularity structure and the DT[18] (or the Hirota form[23]) of the equations considered—this connection lying behind the ''two-singular manifold method''—the DT can in fact be identified with a Painlevé expansion involving only one singular manifold.

B. Practical considerations: example of MKdV

We now consider once again the recovery of the Lax pair and DT (and so the BT) for the MKdV equation,

$$-U_t+\left(U_{xx}-\frac{2}{\kappa^2}U^3\right)_x=0, \tag{45}$$

from a truncated expansion as performed in Ref. 18. We will see how the use of the Riccati system (25), (26) greatly simplifies this process, and also that it is not necessary to obtain the DT in advance. In the next section we discuss the theoretical implications of our results.

For simplicity we consider the potential MKdV (PMKdV) equation,

$$E[V]\equiv -V_t+V_{xxx}-\frac{2}{\kappa^2}V_x^3=0, \quad U=V_x. \tag{46}$$

Equation (46) has two families, both principal, with indices $\{-1,0,4\}$. The truncated expansion for either of these families (here κ may take either sign) is

$$V_T=\kappa\log Z+v, \tag{47}$$

where for the full expansion v is the arbitrary coefficient corresponding to the index at 0. Substitution of this expression into (46) gives

$$E[V_T] \equiv Z^{-3} \sum_{j=0}^{6} E_j^Z Z^j = 0, \tag{48}$$

where $E_0^Z \equiv 0$ and $E_6^Z \equiv 0$ since we have already set the leading order coefficient in (47), and

$$E_1^Z \equiv 3(\kappa A - 2v_x) = 0, \tag{49}$$

$$E_2^Z \equiv \left(\kappa C + 4\kappa B + \kappa A_x - \frac{2}{\kappa} v_x^2 \right) - \frac{1}{\kappa} (5\kappa A - 2v_x)(\kappa A - 2v_x) = 0, \tag{50}$$

$$\begin{aligned} E_3^Z \equiv & \left(-v_t + v_{xxx} - \frac{2}{\kappa^2} v_x^3 \right) + \frac{1}{\kappa} (\kappa^2 A A_x - 4 v_x v_{xx}) - 6B(\kappa A - 2v_x) \\ & - A \left(\kappa C + 4\kappa B + \kappa A_x - \frac{2}{\kappa} v_x^2 \right) - \left(\kappa C + 4\kappa B + \kappa A_x - \frac{2}{\kappa} v_x^2 \right)_x \\ & + \frac{2}{\kappa} A(\kappa A - v_x)(\kappa A - 2v_x) + 3\kappa B_x = 0, \end{aligned} \tag{51}$$

$$\begin{aligned} E_4^Z \equiv & \kappa D + 2\kappa B A_x - B \left(\kappa C + 4\kappa B + \kappa A_x - \frac{2}{\kappa} v_x^2 \right) + 2\kappa A B_x - \kappa B_{xx} \\ & + \frac{1}{\kappa} B(5\kappa A - 2v_x)(\kappa A - 2v_x) = 0, \end{aligned} \tag{52}$$

$$E_5^Z \equiv 3\kappa B B_x + 3B^2(\kappa A - 2v_x) = 0. \tag{53}$$

The solution of these equations is easily obtained as

$$A = \frac{2}{\kappa} v_x, \tag{54}$$

$$B = \lambda^2, \tag{55}$$

$$C = -\frac{1}{\kappa^2} (4\kappa^2 \lambda^2 - 2v_x^2 + 2\kappa v_{xx}), \tag{56}$$

$$D = -\frac{4}{\kappa} \lambda^2 v_{xx}, \tag{57}$$

where $\lambda = \lambda(t)$ is an arbitrary function of integration, and E_3^Z becomes

$$E_3^Z \equiv -v_t + v_{xxx} - \frac{2}{\kappa^2} v_x^3 = 0, \tag{58}$$

which tells us that v is a second solution of (46). Substitution of (54)–(57) into the cross-derivative conditions (28), (29) then gives

$$-x_1 \equiv -\frac{2}{\kappa}\left(-v_t + v_{xxx} - \frac{2}{\kappa^2} v_x^3\right)_x = 0, \tag{59}$$

$$-x_2 \equiv (\lambda^2)_t = 0, \tag{60}$$

which tell us that λ is a constant (the spectral parameter), and that (25), (26) form a Riccati pseudopotential for MKdV in $u = v_x$.

Thus (38), (39) give the matrix spectral problem for MKdV. The corresponding DT is obtained from (47) by setting $U_T = V_{T,x}$, $u = v_x$:

$$U_T = \kappa(\log Z)_x + u = \kappa(\log(\psi_1/\psi_2))_x + u. \tag{61}$$

A simple gauge transformation yields the AKNS spectral problem for MKdV,[28] and the DT (61) is then equivalent to that given in Refs. 29 and 30.

These results are equivalent to those obtained in Ref. 18. However here the solution of the determining equations (49)–(53) is much simpler. The reason for this is that the solution obtained is exact, i.e., we have removed the gauge freedom encountered in Ref. 18. Similar remarks hold for BK[31] (s-G is discussed in the Appendix). We have thus answered the second of our questions about the Riccati variable Y.

The above derivation is also much simpler than the approach adopted in Ref. 24, where a Lax pair for MKdV of the form (23), (24) was obtained. This method relies on manipulations involving two singular manifolds, as opposed to seeking an expansion in a single variable Z satisfying a system of Riccati equations. As we shall see in the next section, the DT for MKdV can be represented as a Painlevé expansion using only one singular manifold; this representation forms a natural extension of the usual Weiss singular manifold method.

Finally, we note that it is not necessary to obtain the DT in advance; the identification of the second solution of MKdV results from our analysis. In particular, no use need be made of a second equation (as KdV was used in Ref. 18). Similar remarks hold for BK[31] and the other examples discussed herein. This then answers the third of our questions.

In fact, the derivation of the DT for MKdV (and s-G) given in Ref. 18 relies on the fact that the two functions ψ_1, ψ_2 appearing in the quotient $Z^{-1} = \psi_2/\psi_1$ each satisfy a pair of linear equations such that the pair for ψ_2 is obtained from the pair for ψ_1 via $\{\psi_1, u\} \to \{\psi_2, -u\}$. This places in advance some restrictions on the coefficients of our Riccati system: see Ref. 31 for details. Of course, it remains the case that the *assumption* of the form of the DT may simplify the process of obtaining the Lax pair.[13]

C. Theoretical considerations: example of MKdV

We now consider the theoretical implications of the above analysis. We begin, however, by insisting on the correct definition of ''singular manifold,'' i.e. that originally given by WTC.[8] The singular manifold defines the location of the singularity about which our Painlevé expansion is made. This Painlevé expansion involves only one singular manifold. The question we now ask is: what is the connection between this Painlevé expansion for MKdV and the DT (61)?

We have already discussed the relationship of the new Riccati variable Z to the original WTC singular manifold φ. We now see that the DT (61) corresponds to the summation of an infinite Painlevé expansion, of course about a *single* singular manifold, for certain choices of arbitrary data. Using (30) we rewrite the DT for MKdV in terms of χ (which is equivalent to the WTC φ) as

$$U_T = \kappa(\log Z)_x + u = \kappa Z^{-1} - u - \kappa\lambda^2 Z$$

$$= \kappa\chi^{-1} - \kappa\lambda^2\chi\left(1 + \frac{1}{\kappa}u\chi\right)^{-1}$$

$$= \kappa\chi^{-1} - \kappa\lambda^2\chi + u\lambda^2\chi^2 - \frac{1}{\kappa}u^2\lambda^2\chi^3 + \cdots, \tag{62}$$

where for this χ the coefficients S and C are obtained from (31) and (54)–(56) as

$$S = -2\lambda^2 - \frac{2}{\kappa^2}u^2 + \frac{2}{\kappa}u_x, \tag{63}$$

$$C = -4\lambda^2 + \frac{2}{\kappa^2}u^2 - \frac{2}{\kappa}u_x. \tag{64}$$

The Painlevé indices of the MKdV equation (45) are $\{-1,3,4\}$, and so we see that we have an infinite expansion in χ of the form (5), where S and C are given by (63), (64), and the arbitrary coefficients at 3 and 4 have been chosen as

$$U_3^{\chi} = u\lambda^2, \quad U_4^{\chi} = -\frac{1}{\kappa}u^2\lambda^2. \tag{65}$$

Corresponding to (62) we have an infinite WTC expansion of the form (2), where φ is subject to the constraints given by (63) and (64), and we have again a certain choice of arbitrary coefficients U_3^{φ} and U_4^{φ}.

We now note that (63), (64) are a parametrization of the relation

$$S + C + 6\lambda^2 = 0, \tag{66}$$

which is just the SME of the KdV equation.[12] However this SME has now been shown to hold for the infinite expansion (62). This prompts us to introduce the following more consistent definition of ''singular manifold equation:''

The singular manifold equation of a PDE is the constraint on the WTC expansion variable φ such that, for a certain choice of arbitrary coefficients, the Painlevé expansion corresponds to the Darboux transformation of the PDE.

Thus we see that the correct SME for MKdV is in fact (66), which we give here for the first time within the context of a Painlevé expansion involving only one singular manifold. In the standard singular manifold method it is insisted that the Painlevé expansion truncate at χ^0 (or equivalently φ^0): as is easily seen from (62), this forces $\lambda = 0$ in (66), which explains the absence of the spectral parameter from the SME given by Weiss.[12]

We note that in Ref. 24 Eq. (66) has been shown to hold for each of the two singular manifolds used therein, together with a further constraint involving these two singular manifolds and the spectral parameter. What we have shown here is that by extending the usual singular manifold method so as to allow the identification of the DT with an *infinite* Painlevé expansion, and with a corresponding modification of the definition of singular manifold equation, we can obtain the SME complete with spectral parameter using only one singular manifold. This SME—a constraint on the single singular manifold in the expansion—can be obtained from the Painlevé expansion corresponding to *either* one of the two families of MKdV: we do not need to try to use these two families in conjunction. This is then in contrast to the approach used in Ref. 24.

Within the context of our new definition of SME, the only difference between the DT of KdV and MKdV is that, whereas for the former the corresponding Painlevé expansion truncates, for the latter it does not: for both we sum the Painlevé expansion subject to a choice of arbitrary coeffi-

cients and a constraint (66) on φ. Our approach therefore forms a natural extension of the usual Weiss singular manifold method. The BK equation is another example where, in order to obtain the correct SME, we have to take into account the fact that it is an infinite Painlevé expansion which corresponds to the DT.[31] Other examples are presented in Sec. III.

It is not surprising that the SME of MKdV is the same as that of KdV: when seeking a Lax pair and DT from Painlevé analysis we expect the SME to yield the Lax pair, and the Painlevé expansion to yield the DT. Since it is well-known that the KdV and MKdV spectral problems are related via the gauge transformation (42), or equivalently[27]

$$Z^{-1}=\chi^{-1}+\frac{1}{2}A=\chi^{-1}+\frac{1}{\kappa}u, \tag{67}$$

it is only natural that these two equations should have the same SME.

Indeed, if we consider the solution $W=W_T$ of the KdV equation,

$$-W_t+(W_{xx}+3W^2)_x=0, \tag{68}$$

obtained via the Miura map,

$$W_T=\left(\frac{U_T}{\kappa}\right)_x-\left(\frac{U_T}{\kappa}\right)^2, \tag{69}$$

where U_T is as in (61), then we obtain, using (67) to rewrite the resulting expression in terms of χ,

$$W_T=-2\chi^{-2}-w+2\lambda^2, \tag{70}$$

where

$$w=\left(\frac{u}{\kappa}\right)_x-\left(\frac{u}{\kappa}\right)^2. \tag{71}$$

The action of the Miura map on the infinite expansion U_T has produced a constant-level truncation W_T. This is of course the truncated Painlevé expansion corresponding to the DT of KdV, and for which the SME (66) holds.[12]

We can mirror iterations of the DT for MKdV using the Painlevé expansion (62): setting $u=0$ gives

$$U_T=\kappa(\chi^{-1}-\lambda^2\chi), \quad \text{with} \quad S=-2\lambda^2, \quad C=-4\lambda^2. \tag{72}$$

This corresponds to Eq. (3.1.9) in Ref. 16, and gives the one-soliton solution. This expression (72), although now finite in χ, still corresponds to an infinite WTC expansion in φ; the significance of summing such infinite expansions was argued in Ref. 16. The expansion (62) is therefore a generalization of our previous work, extending the infinite WTC expansion representing the one-soliton solution to one representing the DT.

We also remark that, since our analysis gives by construction the summation of an infinite WTC expansion, we obtain in this way a direct proof of the convergence of the MKdV Painlevé expansion for

$$0<|\chi|<|\kappa u^{-1}|, \tag{73}$$

provided that Eqs. (63), (64) hold and the arbitrary coefficients U_3^χ and U_4^χ are chosen as in (65).

III. FURTHER EXAMPLES

A. MKdV5

We now briefly consider the application of our analysis to the fifth-order MKdV equation (MKdV5),

$$-U_t+\left(U_{xxxx}-\frac{10}{\kappa^2}U^2U_{xx}-\frac{10}{\kappa^2}UU_x^2+\frac{6}{\kappa^4}U^5\right)_x=0. \tag{74}$$

We should expect our results for this equation to be analogous to those already obtained for MKdV. In particular, we should expect that the SME for MKdV5 is identical to that for fifth-order KdV (KdV5): we will see that this is indeed the case.

We consider the potential form (PMKdV5) of (74):

$$E[V]\equiv -V_t+V_{xxxxx}-\frac{10}{\kappa^2}V_x^2V_{xxx}-\frac{10}{\kappa^2}V_xV_{xx}^2+\frac{6}{\kappa^4}V_x^5=0,\quad U=V_x. \tag{75}$$

This equation has the four (κ may take either sign) families $V=\kappa\log\chi+\cdots$ and $V=2\kappa\log\chi+\cdots$, with indices $\{-1,0,2,3,6\}$ and $\{-3,-1,0,6,8\}$, respectively. Here we consider the truncated expansion corresponding to either of the two principal families:

$$V_T=\kappa\log Z+v, \tag{76}$$

where once again for the full expansion v is the arbitrary coefficient corresponding to the index at 0. Substitution of (76) into (75) gives

$$E[V_T]\equiv Z^{-5}\sum_{j=0}^{10}E_j^ZZ^j=0, \tag{77}$$

where $E_0^Z\equiv 0$ and $E_{10}^Z\equiv 0$ since the leading order coefficient is already set in (76). We then find

$$E_1^Z\equiv 10(\kappa A-2v_x)=0, \tag{78}$$

$$E_9^Z\equiv 10B^4(\kappa A-2v_x)+10\kappa B^3B_x=0, \tag{79}$$

which then gives

$$A=\frac{2}{\kappa}v_x, \tag{80}$$

$$B=\lambda^2, \tag{81}$$

where $\lambda=\lambda(t)$ is an arbitrary function of integration. For this choice of A and B we find

$$E_2^Z\equiv 0,\quad E_3^Z\equiv 0,\quad E_7^Z\equiv 0,\quad E_8^Z\equiv 0. \tag{82}$$

This then leaves us with the three equations:

$$E_4^Z\equiv\kappa C+16\kappa\lambda^4-\frac{8}{\kappa}\lambda^2v_x^2+\frac{6}{\kappa^3}v_x^4+8\lambda^2v_{xx}-\frac{12}{\kappa^2}v_x^2v_{xx}+\frac{2}{\kappa}v_{xx}^2-\frac{4}{\kappa}v_xv_{xxx}+2v_{xxxx}=0, \tag{83}$$

$$E_5^Z \equiv \left(-v_t + v_{xxxxx} - \frac{10}{\kappa^2} v_x^2 v_{xxx} - \frac{10}{\kappa^2} v_x v_{xx}^2 + \frac{6}{\kappa^4} v_x^5 \right) - (E_4^Z)_x - \frac{2}{\kappa} v_x E_4^Z = 0, \tag{84}$$

$$E_6^Z \equiv \left(\kappa D + 16\lambda^4 v_{xx} - \frac{24}{\kappa^2} \lambda^2 v_x^2 v_{xx} + 4\lambda^2 v_{xxxx} \right) - \lambda^2 E_4^Z = 0. \tag{85}$$

From these we easily obtain C and D,

$$C = -16\lambda^4 - 8\lambda^2 \left(\frac{v_{xx}}{\kappa} - \frac{v_x^2}{\kappa^2} \right) - 6\left(\frac{v_{xx}}{\kappa} - \frac{v_x^2}{\kappa^2} \right)^2 - 2\left(\frac{v_{xx}}{\kappa} - \frac{v_x^2}{\kappa^2} \right)_{xx}, \tag{86}$$

$$D = -\frac{16}{\kappa} \lambda^4 v_{xx} + \frac{24}{\kappa^3} \lambda^2 v_x^2 v_{xx} - \frac{4}{\kappa} \lambda^2 v_{xxxx}, \tag{87}$$

and also the information from (84) that v is a second solution of PMKdV5. Substitution of these values of A,B,C,D into the cross-derivative conditions (28), (29) gives

$$-x_1 = -\frac{2}{\kappa} \left(-v_t + v_{xxxxx} - \frac{10}{\kappa^2} v_x^2 v_{xxx} - \frac{10}{\kappa^2} v_x v_{xx}^2 + \frac{6}{\kappa^4} v_x^5 \right)_x = 0, \tag{88}$$

$$-x_2 = (\lambda^2)_t = 0, \tag{89}$$

which tell us that λ is a constant, and that (25), (26) form a Riccati pseudopotential for MKdV5 in $u = v_x$. Thus (38), (39) give the matrix spectral problem for MKdV5; the corresponding DT is obtained from (76) by setting $U_T = V_{T,x}$, $u = v_x$:

$$U_T = \kappa(\log Z)_x + u = \kappa(\log(\psi_1/\psi_2))_x + u. \tag{90}$$

The BT now follows just as it does for MKdV.

We note that this calculation is very straightforward, and certainly much less difficult than it would have been had we used the Riccati system (21), (22). Also, the DT is once again obtained from the analysis, so no attempt need be made to derive it beforehand.

Our main interest in this example, however, is in the representation of the DT as a Painlevé expansion and the corresponding SME. Rewriting the DT in terms of χ using (30) we obtain as for MKdV

$$\begin{aligned} U_T &= \kappa\chi^{-1} - \kappa\lambda^2\chi\left(1 + \frac{1}{\kappa} u\chi \right)^{-1} \\ &= \kappa\chi^{-1} - \kappa\lambda^2\chi + u\lambda^2\chi^2 - \frac{1}{\kappa} u^2\lambda^2\chi^3 + \frac{1}{\kappa^2} u^3\lambda^2\chi^4 - \frac{1}{\kappa^3} u^4\lambda^2\chi^5 + \cdots, \end{aligned} \tag{91}$$

where for this χ the coefficients S and C are now obtained from (31) and (80), (81), (86) as

$$S = -2\lambda^2 + 2\left(\frac{u_x}{\kappa} - \frac{u^2}{\kappa^2} \right), \tag{92}$$

$$C = -16\lambda^4 - 8\lambda^2 \left(\frac{u_x}{\kappa} - \frac{u^2}{\kappa^2} \right) - 6\left(\frac{u_x}{\kappa} - \frac{u^2}{\kappa^2} \right)^2 - 2\left(\frac{u_x}{\kappa} - \frac{u^2}{\kappa^2} \right)_{xx}. \tag{93}$$

The Painlevé indices for this family of MKdV5 (74) are $\{-1,2,3,5,6\}$ and so we see that the DT corresponds to an infinite expansion in χ of the form (5), with S and C as above and the arbitrary coefficients at 2, 3, 5 and 6 chosen as

$$U_2^\chi = -\kappa\lambda^2, \quad U_3^\chi = u\lambda^2, \quad U_5^\chi = \frac{1}{\kappa^2}\,u^3\lambda^2, \quad U_6^\chi = -\frac{1}{\kappa^3}\,u^4\lambda^2. \tag{94}$$

Corresponding to this expansion we have an infinite WTC expansion of the form (2), where φ is subject to the constraints given by (92) and (93), and we have again a certain choice of arbitrary coefficients U_2^φ, U_3^φ, U_5^φ and U_6^φ.

The values of S and C (92), (93) are a parametrization of the relation

$$C + S_{xx} + \tfrac{3}{2}S^2 + 10\lambda^2 S + 30\lambda^4 = 0, \tag{95}$$

which is the SME for KdV5.[12] From (91) we see that constant level truncation in χ will only give the SME for a zero value of the spectral parameter,

$$C + S_{xx} + \tfrac{3}{2}S^2 = 0. \tag{96}$$

It is easy to verify that the constant level truncation in χ for a principal branch of MKdV5 is $U_T = \kappa\chi^{-1}$ together with the constraint (96).

Once again we see that it is an infinite Painlevé expansion which corresponds to the DT. The correct SME—the constraint such that the Painlevé expansion, for a certain choice of arbitrary coefficients, corresponds to the DT—is (95): this differs again from the constraint (96) that would be obtained using the usual singular manifold method. We note that this SME, a constraint on a single singular manifold, can be obtained from the Painlevé expansion corresponding to either one of the two principal families: we do not need to try to use these two families in conjunction.

A corollary of our analysis is a direct proof of the convergence of the Painlevé expansion for a principal family of MKdV5 for

$$0 < |\chi| < |\kappa u^{-1}|, \tag{97}$$

provided that Eqs. (92) and (93) hold and the arbitrary coefficients U_2^χ, U_3^χ, U_5^χ and U_6^χ are chosen as in (94).

B. A system in 2+1 dimensions

1. Preliminaries: extension of the Riccati system

We now consider the extension of the method developed above so as to make it applicable to systems in 2+1 dimensions. We do this by augmenting the system of Riccati equations (25), (26) as follows:

$$Z_x = 1 - AZ - BZ^2, \tag{98}$$

$$Z_t = -C + (AC + C_x)Z - (D - BC)Z^2, \tag{99}$$

$$Z_y = -E + (AE + E_x)Z - (F - BE)Z^2. \tag{100}$$

This system has the cross-derivative conditions

$$(Z_x)_t - (Z_t)_x \equiv x_1 Z + x_2 Z^2 = 0, \tag{101}$$

$$(Z_x)_y - (Z_y)_x \equiv y_1 Z + y_2 Z^2 = 0, \tag{102}$$

$$(Z_t)_y-(Z_y)_t\equiv z_0+z_1Z+z_2Z^2=0, \tag{103}$$

where

$$-x_1\equiv A_t+(AC)_x+C_{xx}-2D=0, \tag{104}$$

$$-x_2\equiv B_t-D_x+2BC_x+B_xC+AD=0, \tag{105}$$

$$-y_1\equiv A_y+(AE)_x+E_{xx}-2F=0, \tag{106}$$

$$-y_2\equiv B_y-F_x+2BE_x+B_xE+AF=0, \tag{107}$$

$$-z_0\equiv C_y-E_t+EC_x-CE_x=0, \tag{108}$$

and z_1,z_2 are zero modulo x_1, x_2, y_1, y_2, and z_0. We note that the system (98)–(100) is much simpler than the natural generalization of (21), (22), which would involve nine undetermined coefficients.

Under the gauge transformation (30) this system of three Riccati equations is easily seen to be equivalent to the system of three Riccati equations in χ given in Ref. 32:

$$\chi_x=1+\tfrac{1}{2}S\chi^2, \tag{109}$$

$$\chi_t=-C+C_x\chi-\tfrac{1}{2}(C_{xx}+CS)\chi^2, \tag{110}$$

$$\chi_y=-E+E_x\chi-\tfrac{1}{2}(E_{xx}+ES)\chi^2. \tag{111}$$

Here E is defined as $E=-\varphi_y/\varphi_x$. This system has the cross-derivative conditions

$$S_t+C_{xxx}+2SC_x+S_xC=0, \tag{112}$$

$$S_y+E_{xxx}+2SE_x+S_xE=0, \tag{113}$$

$$C_y-E_t+EC_x-CE_x=0. \tag{114}$$

The remarks made earlier for the system (25), (26) remain true for our augmented system (98)–(100): since the systems in Z and χ are equivalent it is sufficient to perform the Painlevé test using χ, but it may be possible to obtain more information from a higher order truncation in Z than one in χ. The coefficients of the Riccati system, and Z itself, can be given in terms of φ and the auxiliary function A.

We now consider for future reference a special case of the system (98)–(100). Let

$$C=\Gamma E+\widetilde{C},\quad D=\Gamma F+\widetilde{D},\quad \Gamma_x=0. \tag{115}$$

In this case our Riccati system becomes

$$Z_x=1-AZ-BZ^2, \tag{116}$$

$$Z_t=\Gamma Z_y-\widetilde{C}+(A\widetilde{C}+\widetilde{C}_x)Z-(\widetilde{D}-B\widetilde{C})Z^2, \tag{117}$$

and the cross-derivative condition now reads

$$(Z_x)_t-(Z_t)_x\equiv\widetilde{x}_1Z+\widetilde{x}_2Z^2=0, \tag{118}$$

where

$$-\tilde{x}_1 \equiv A_t + (A\tilde{C})_x + \tilde{C}_{xx} - 2\tilde{D} - \Gamma A_y = 0, \tag{119}$$

$$-\tilde{x}_2 \equiv B_t - \tilde{D}_x + 2B\tilde{C}_x + B_x\tilde{C} + A\tilde{D} - \Gamma B_y = 0. \tag{120}$$

The corresponding system in χ obtained by the gauge transformation (30) is

$$\chi_x = 1 + \tfrac{1}{2}S\chi^2, \tag{121}$$

$$\chi_t = \Gamma\chi_y - \tilde{C} + \tilde{C}_x\chi - \tfrac{1}{2}(\tilde{C}_{xx} + \tilde{C}S)\chi^2, \tag{122}$$

where S is given by (31). The corresponding cross-derivative condition is

$$S_t + \tilde{C}_{xxx} + 2S\tilde{C}_x + S_x\tilde{C} - \Gamma S_y = 0. \tag{123}$$

Clearly, linearization of the Riccati system (116), (117) leads to a time evolution for the eigenfunctions different from that given previously. For $Z^{-1} = \eta_x/\eta$ we obtain the linear system given by (23) together with

$$\eta_t = \Gamma\eta_y - \tilde{C}\eta_x + \left(\int^x \tilde{D}\, dx'\right)\eta, \tag{124}$$

and for $Z^{-1} = \psi_2/\psi_1$ we obtain (38) together with

$$\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}_t = \begin{pmatrix} \Gamma & 0 \\ 0 & \Gamma \end{pmatrix}\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}_y + \begin{pmatrix} \tfrac{1}{2}(A\tilde{C} + \tilde{C}_x) & -\tilde{C} \\ (\tilde{D} - B\tilde{C}) & -\tfrac{1}{2}(A\tilde{C} + \tilde{C}_x) \end{pmatrix}\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}. \tag{125}$$

Both of these linearizations have as cross-derivative conditions (119), (120). For the linearization $Z^{-1} = (\xi_2/\xi_1) + (A/2)$ we obtain (40) together with

$$\begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix}_t = \begin{pmatrix} \Gamma & 0 \\ 0 & \Gamma \end{pmatrix}\begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix}_y + \begin{pmatrix} \tfrac{1}{2}\tilde{C}_x & -\tilde{C} \\ \tfrac{1}{2}\tilde{C}_{xx} - (B + \tfrac{1}{4}A^2 - \tfrac{1}{2}A_x)\tilde{C} & -\tfrac{1}{2}\tilde{C}_x \end{pmatrix}\begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix}. \tag{126}$$

As before the eigenfunctions ψ_1 and ξ_1 both satisfy the same scalar linear system, in this case (13) and

$$\psi_t = \Gamma\psi_y - \tilde{C}\psi_x + \tfrac{1}{2}\tilde{C}_x\psi, \tag{127}$$

S being given by (31): the cross-derivative condition is (123) for this choice of S. We also have the same gauge transformations as before: (32) between (23), (124) and (13), (127); and (42) between (38), (125) and (40), (126).

From the above we see that for a Riccati system of the form (116), (117) we may have a choice of several linearizations (some of which may be better than others).

2. Application to a system in 2+1 dimensions

We now consider the application of the analysis developed above to the following system in 2+1 dimensions:

$$E_1[U,V] \equiv U_{xt} + V_y + \tfrac{1}{2}(U_xU_y)_x = 0, \tag{128}$$

$$E_2[U,V] \equiv V_t + \kappa^2 U_{xxxy} + U_{xy}V + \tfrac{1}{2}(U_xV_y + U_yV_x) = 0. \tag{129}$$

In order to apply the Painlevé test to this system we take χ as expansion variable, with gradient given by (109)–(111). We find two (κ may take either sign) families, both principal, given by $U=2\kappa\log\chi+\cdots$, $V=-2\kappa^2\chi^{-2}+\cdots$ with indices $\{-1,0,2,3,4\}$. All compatibility conditions are identically satisfied.

We therefore seek a truncated expansion of the form

$$U_T=U^Z_{0,1}\log Z+u,\quad U^Z_{0,1}\ \text{constant},\tag{130}$$

$$V_T=Z^{-2}\sum_{j=0}^{4}V^Z_jZ^j,\tag{131}$$

where the gradient of Z is given by (98)–(100), and where for the full expansion u is the arbitrary coefficient corresponding to the index at 0. Substitution of (130), (131) into (128), (129) gives

$$E_1[U_T,V_T]\equiv Z^{-3}\sum_{j=0}^{6}E^Z_{1,j}Z^j=0,\tag{132}$$

$$E_2[U_T,V_T]\equiv Z^{-4}\sum_{j=0}^{8}E^Z_{2,j}Z^j=0.\tag{133}$$

We find

$$E^Z_{1,0}\equiv E[(U^Z_{0,1})^2+2V^Z_0]=0,\tag{134}$$

$$E^Z_{2,0}\equiv 3E[2\kappa^2+V^Z_0]U^Z_{0,1}=0,\tag{135}$$

$$E^Z_{1,6}\equiv-(F-BE)[(U^Z_{0,1})^2B^2+2V^Z_4]=0,\tag{136}$$

$$E^Z_{2,8}\equiv 3B(F-BE)[2\kappa^2B^2+V^Z_4]U^Z_{0,1}=0.\tag{137}$$

We take

$$U^Z_{0,1}=2\kappa,\quad V^Z_0=-2\kappa^2,\quad V^Z_4=-2\kappa^2B^2,\tag{138}$$

where once again κ may take either sign.

We then find

$$\frac{1}{3\kappa}\left(E^Z_{1,1}-\frac{1}{4\kappa}E^Z_{2,1}\right)\equiv C-\left(\kappa A-\frac{1}{2}u_x\right)E-\frac{1}{2}u_y=0,\tag{139}$$

which gives

$$C=(\kappa A-\tfrac{1}{2}u_x)E+\tfrac{1}{2}u_y.\tag{140}$$

For this value of C,

$$E^Z_{1,1}\equiv\frac{1}{4\kappa}E^Z_{2,1}\equiv E(V^Z_1-2\kappa^2A)=0,\tag{141}$$

and so

$$V^Z_1=2\kappa^2A.\tag{142}$$

Using the above value of C, we find

$$\frac{1}{3\kappa B}\left(E^Z_{1,5}+\frac{1}{4\kappa B}\,E^Z_{2,7}\right)\equiv D-\left(\kappa A-\frac{1}{2}\,u_x\right)F-\kappa B_y=0, \tag{143}$$

which gives

$$D=(\kappa A-\tfrac{1}{2}u_x)F+\kappa B_y\,. \tag{144}$$

For this value of D,

$$E^Z_{1,5}\equiv-\frac{1}{4\kappa B}\,E^Z_{2,7}\equiv-(F-BE)(V^Z_3+2\kappa^2AB-2\kappa^2B_x)=0, \tag{145}$$

and so

$$V^Z_3=-2\kappa^2AB+2\kappa^2B_x\,. \tag{146}$$

Then for C and D as above, and modulo the cross-derivative conditions (105), (107), we obtain

$$E^Z_{1,2}\equiv 0,\quad E^Z_{2,2}\equiv 2\kappa E(V^Z_2+2\kappa^2A_x-\kappa u_{xx})=0, \tag{147}$$

$$E^Z_{1,4}\equiv 0,\quad E^Z_{2,6}\equiv 2\kappa B(F-BE)(V^Z_2-2\kappa^2A_x+\kappa u_{xx})=0. \tag{148}$$

Thus

$$V^Z_2=0, \tag{149}$$

and

$$A=\frac{1}{2\kappa}\,u_x-\frac{\lambda}{\kappa}, \tag{150}$$

where $\lambda=\lambda(y,t)$ is an arbitrary function of integration. Using this value of A in the above expressions for C and D we get

$$C=-\lambda E+\tfrac{1}{2}u_y\,,\quad D=-\lambda F+\kappa B_y\,. \tag{151}$$

For these values of A, C and D, our remaining determining equation obtained from the expansion of E_1 becomes

$$E^Z_{1,3}\equiv 2(\lambda_t+\lambda\lambda_y)=0, \tag{152}$$

which gives us the constraint

$$\lambda_t+\lambda\lambda_y=0 \tag{153}$$

on the arbitrary function λ.

The values of C and D in (151) are of the form (115) with

$$\Gamma=-\lambda,\quad \widetilde{C}=\tfrac{1}{2}u_y\,,\quad \widetilde{D}=\kappa B_y\,, \tag{154}$$

and so we now switch to the Riccati system (116), (117). For A, $\widetilde{C}$ and $\widetilde{D}$ given by (150), (154) the cross-derivative conditions (119), (120) read

$$-\widetilde{x}_1 \equiv \frac{1}{2\kappa}\left(u_{xt}+(\kappa u_{xx}-4\kappa^2 B)_y+\frac{1}{2}(u_x u_y)_x-2(\lambda_t+\lambda\lambda_y)\right)=0, \tag{155}$$

$$-\widetilde{x}_2 \equiv B_t-\kappa B_{xy}+u_{xy}B+\tfrac{1}{2}(u_x B_y+u_y B_x)=0. \tag{156}$$

Setting—as is suggested by (155)—

$$\kappa u_{xx}-4\kappa^2 B=v \tag{157}$$

these equations become

$$-\widetilde{x}_1 \equiv \frac{1}{2\kappa}(E_1[u,v]-2(\lambda_t+\lambda\lambda_y))=0, \tag{158}$$

$$-\widetilde{x}_2 \equiv \frac{1}{4\kappa}(E_1[u,v])_x-\frac{1}{4\kappa^2}E_2[u,v]=0, \tag{159}$$

which, recalling the constraint (153), tell us that u and v are a second solution of the system (128), (129).

For B given by (157), we find that D becomes

$$D=-\lambda F-\frac{1}{4\kappa}(v-\kappa u_{xx})_y. \tag{160}$$

For the values of A, B, C and D obtained here we then find that the remaining three determining equations obtained from the expansion of E_2 ($E^Z_{2,3}$, $E^Z_{2,4}$, and $E^Z_{2,5}$) are identically satisfied modulo $E_1[u,v]=0$, $E_2[u,v]=0$ and the constraint (153).

Remark: If instead we had begun by considering the system obtained by adding functions $p(x,y,t)$ and $q(x,y,t)$ to $E_1[U,V]$ and $E_2[U,V]$, respectively, the results of the Painlevé test would have been $p=g(y,t)$, $q=0$. Performing the truncation for the system $F_1\equiv E_1+g=0$, $F_2\equiv E_2=0$ would then have resulted at the stage of (152) in the equation $g+2(\lambda_t+\lambda\lambda_y)=0$, which fixes the form of g in F_1. Equations (158), (159) then tell us that for this g, u, and v are a second solution of $F_1=0$, $F_2=0$. The remaining determining equations from the expansion of F_2 are then identically satisfied modulo $F_1[u,v]=0$ and $F_2[u,v]=0$, again for $g=-2(\lambda_t+\lambda\lambda_y)$.

Let us now briefly summarize the results of our truncation for the system (128), (129). Noting the form of the coefficients V^Z_j we see that this truncation can be written in the form

$$U_T=2\kappa\ \log Z+u, \quad V_T=2\kappa^2(Z^{-1}+BZ)_x-4\kappa^2 B, \tag{161}$$

where the coefficients of the Riccati system (98)—(100) are given by

$$A=-\frac{\lambda}{\kappa}+\frac{1}{2\kappa}u_x, \tag{162}$$

$$B=-\frac{1}{4\kappa^2}(v-\kappa u_{xx}), \tag{163}$$

$$C=-\lambda E+\frac{1}{2}u_y, \tag{164}$$

$$D=-\lambda F-\frac{1}{4\kappa}(v-\kappa u_{xx})_y, \tag{165}$$

and the arbitrary function λ of y and t is subject to the constraint

$$\lambda_t+\lambda\lambda_y=0. \tag{166}$$

The corresponding coefficients of the Riccati system (116), (117) are

$$\Gamma=-\lambda, \quad \widetilde{C}=\frac{1}{2}u_y, \quad \widetilde{D}=-\frac{1}{4\kappa}(v-\kappa u_{xx})_y. \tag{167}$$

Equations (158) and (159) tell us that (116) and (117) form a Riccati pseudopotential for the system (128), (129). The linearization $Z^{-1}=\psi_2/\psi_1$ then gives a matrix spectral problem of the form (38), (125):

$$\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}_x=-\frac{1}{4\kappa^2}\begin{pmatrix}-\kappa(2\lambda-u_x) & -4\kappa^2\\ (v-\kappa u_{xx}) & \kappa(2\lambda-u_x)\end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}, \tag{168}$$

$$\begin{aligned}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}_t=&\begin{pmatrix}-\lambda & 0\\ 0 & -\lambda\end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}_y\\ &+\frac{1}{8\kappa^2}\begin{pmatrix}\kappa(2\kappa u_{xy}+u_xu_y-2\lambda u_y) & -4\kappa^2u_y\\ (2\kappa^2u_{xxy}-\kappa u_{xx}u_y-2\kappa v_y+vu_y) & -\kappa(2\kappa u_{xy}+u_xu_y-2\lambda u_y)\end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}.\end{aligned} \tag{169}$$

The corresponding Darboux transformation is obtained from (161) as

$$U_T=2\kappa\log(\psi_1/\psi_2)+u, \quad V_T=2\kappa^2(\log(\psi_1\psi_2))_{xx}+v-\kappa u_{xx}, \tag{170}$$

where we have used the fact that for ψ_1 and ψ_2 satisfying (38),

$$Z^{-1}+BZ=\frac{\psi_{1,x}}{\psi_1}+\frac{\psi_{2,x}}{\psi_2}. \tag{171}$$

The form of the above DT is interesting, since it maps to a new solution U_T,V_T from the combinations u and $v-\kappa u_{xx}$ of an old solution u,v. We note once again that we did not need to derive the DT in advance (which for this example might prove to be difficult).

We may also of course linearize our Riccati pseudopotential onto either of the scalar Lax pairs (23), (124), or (13) (127) [we do not consider here (40), (126)]. The former gives

$$\eta_{xx}=-\frac{1}{\kappa}\left(\lambda-\frac{1}{2}u_x\right)\eta_x-\frac{1}{4\kappa^2}(v-\kappa u_{xx})\eta, \tag{172}$$

$$\eta_t=-\lambda\eta_y-\frac{1}{2}u_y\eta_x-\frac{1}{4\kappa}\left(\int^x(v-\kappa u_{xx})_y dx'\right)\eta, \tag{173}$$

which has the same cross-derivative conditions (158), (159) as the above matrix spectral problem. The latter, with S obtained from (31), gives

$$\psi_{xx}=-\frac{1}{4\kappa^2}[v-(\lambda-\tfrac{1}{2}u_x)^2]\psi, \tag{174}$$

$$\psi_t=-\lambda\psi_y-\tfrac{1}{2}u_y\psi_x+\tfrac{1}{4}u_{xy}\psi \tag{175}$$

which has the cross-derivative condition

$$S_t+\widetilde{C}_{xxx}+2S\widetilde{C}_x+S_x\widetilde{C}-\Gamma S_y=\frac{1}{2\kappa^2}E_2[u,v]+\frac{1}{2\kappa^2}\left(\lambda-\frac{1}{2}u_x\right)(E_1[u,v]-2(\lambda_t+\lambda\lambda_y))=0. \tag{176}$$

We note that similar nonisospectral scattering problems in $2+1$ dimensions, with $\lambda=\lambda(y,t)$ subject to constraints of the form (166), have been discussed in Ref. 33 for ''breaking soliton'' equations.

If we now use (30) to rewrite (161) in terms of χ, we find that this DT corresponds, once again, to an infinite Painlevé expansion in χ for a certain choice of the arbitrary coefficients [here A and B are given in terms of u and v via (162), (163)]:

$$U_T=2\kappa\log\chi+u-\kappa A\chi+\tfrac{1}{4}\kappa A^2\chi^2-\tfrac{1}{12}\kappa A^3\chi^3+\cdots, \tag{177}$$

$$V_T=-2\kappa^2\chi^{-2}+\tfrac{1}{2}\kappa^2A^2+2\kappa^2(B_x-AB)\chi+\cdots, \tag{178}$$

where for this χ, S, C, and E are related via

$$S=\frac{1}{2\kappa^2}\left[v-\left(\lambda-\frac{1}{2}u_x\right)^2\right],\quad C=-\lambda E+\frac{1}{2}u_y. \tag{179}$$

For this example obtaining the SME is not as simple as for our previous examples since it is not a question of eliminating a single field between two expressions. However the two expressions in (179) can be solved for u and v:

$$v=2\kappa^2S+(\lambda-\tfrac{1}{2}u_x)^2,\quad \tfrac{1}{2}u_y=C+\lambda E, \tag{180}$$

and we can now use the fact that u and v satisfy (128) to get

$$\tfrac{1}{2}E_1[u,v]=\omega_{xt}+\kappa^2S_y+(\lambda-\omega_x)(\lambda-\omega_x)_y+(\omega_x\omega_y)_x=0, \tag{181}$$

where $\omega=u/2$ is given by

$$\omega=\int^y(C+\lambda E)dy'. \tag{182}$$

Equation (176) tells us that the expression resulting from substitution of u and v into (129) instead of (128) is dependent on that obtained above together with the cross-derivative condition (123).

Substitution of ω from (182) into (181) provides a single constraint on S, C, E, and λ, which we claim should be understood as the SME for the system (128), (129). This claim is supported by the fact that if we consider the reduction of (128), (129) to BK, this SME reduces to that of BK, and the latter is obtained from the elimination of a single field between expressions for S and C: details can be found in Ref. 31. We note again that this SME—a constraint which, in accordance with our new definition, holds when the Painlevé expansion, for a certain choice of arbitrary coefficients, corresponds to the DT—can be obtained from the Painlevé expansion corresponding to *either* one of the two families (both of which are principal).

Finally we remark that our method gives a direct proof of the convergence of the Painlevé expansion for the system (128), (129), for a certain choice of the arbitrary coefficients and with S, C, and E satisfying (179), for χ in the cut plane with

$$|\chi|<2|\kappa(\tfrac{1}{2}u_x-\lambda)^{-1}|. \tag{183}$$

3. Reductions to systems in 1+1 dimensions

We have for the system (128), (129) the Riccati pseudopotential (116), (117) together with the DT (161); for the linearization $Z^{-1}=\psi_2/\psi_1$ this DT takes the form (170). We now consider the three reductions of the system (128), (129) to PDEs in 1+1 dimensions given by

$$(\partial_x,\partial_y,\partial_t)\to(\partial_x,\partial_x,\partial_t), \tag{184}$$

$$(\partial_x,\partial_y,\partial_t)\to(\partial_x,\partial_t,\partial_x), \tag{185}$$

$$(\partial_x,\partial_y,\partial_t)\to(\partial_x,\partial_t,\partial_t), \tag{186}$$

where in (185) the relabeling of y as t is simply for convenience.

Case One: $(\partial_x,\partial_y,\partial_t)\to(\partial_x,\partial_x,\partial_t)$.

In this case our system becomes

$$E_1[U,V]\equiv U_{xt}+(V+\tfrac{1}{2}U_x^2)_x=0, \tag{187}$$

$$E_2[U,V]\equiv V_t+(\kappa^2U_{xxx}+U_xV)_x=0, \tag{188}$$

which is just the classical Boussinesq system[20–22] in U_x and V. From the point of view of seeking a truncated expansion, making this reduction $\partial_y=\partial_x$ means forcing $E=-1$ and $F=0$ in (98), (99), (100), so only (98) and (99) remain. Also the Riccati system (116), (117) becomes just another copy of (98), (99) with cross-derivative conditions $\tilde{x}_1\equiv x_1=0$, $\tilde{x}_2\equiv x_2=0$; this is easily seen by replacing Z_y in (117) by Z_x from (116) and identifying, from (115),

$$C=-\Gamma+\tilde{C},\quad D=\tilde{D},\quad \Gamma_x=0. \tag{189}$$

In the course of solving the determining equations resulting from the truncation we now obtain at the stage of equation (150) that our function of integration is a function of t only, i.e., $\lambda=\lambda(t)$. The constraint (153) then tells us that $\lambda_t=0$, i.e., λ is constant.

Using Eqs. (162)–(165) we thus obtain for the classical Boussinesq system in U_x and V the Riccati pseudopotential (98), (99) with

$$A=-\frac{\lambda}{\kappa}+\frac{1}{2\kappa}u_x, \tag{190}$$

$$B=-\frac{1}{4\kappa^2}(v-\kappa(u_x)_x), \tag{191}$$

$$C=\lambda+\tfrac{1}{2}u_x, \tag{192}$$

$$D=-\frac{1}{4\kappa}(v-\kappa(u_x)_x)_x. \tag{193}$$

The corresponding DT under $Z^{-1}=\psi_2/\psi_1$ is given by (170):

$$(U_x)_T=2\kappa(\log(\psi_1/\psi_2))_x+(u_x),\quad V_T=2\kappa^2(\log(\psi_1\psi_2))_{xx}+v-\kappa(u_x)_x. \tag{194}$$

This maps one solution u_x,v of the classical Boussinesq system to another solution $(U_x)_T,V_T$. We have available of course the other possible linearizations, as discussed above for the system in 2+1 dimensions.

We thus obtain the Riccati pseudopotential presented in Ref. 19 for the scalar BK equation, an equation obtained by the elimination of V from the classical Boussinesq system. However here the

use of the Riccati system (98), (99) simplifies the solution of the determining equations, again because of the removal of a gauge freedom. Furthermore, we have here obtained the DT for the field V of the classical Boussinesq system as well as that for U; in Ref. 19 the former is left defined implicitly by a nonlinear relation. We also note that the extra $-\kappa(u_x)_x$ term in (194) distinguishes this DT from the auto-Bäcklund transformation involving two singular manifolds presented in Ref. 23.

In addition, our analysis provides us with the correct SME for the classical Boussinesq system: when $\partial_y=\partial_x$, (181) and (182) yield

$$C_t+3CC_x-4\lambda C_x+\kappa^2 S_x=0. \tag{195}$$

This SME is given in accordance with our new definition. Once again the constraint for a constant-level truncation to exist—i.e., the SME usually given for the classical Boussinesq system—differs from the SME presented here. This point is discussed in more detail in Ref. 31.

Remarks made earlier for the system in $2+1$ dimensions of course go through for this reduction: the DT corresponds to the summation of an infinite Painlevé expansion for a certain choice of arbitrary coefficients and with S and C given by

$$S=\frac{1}{2\kappa^2}\left[v-\left(\lambda-\frac{1}{2}\,u_x\right)^2\right],\quad C=\lambda+\frac{1}{2}\,u_x; \tag{196}$$

the SME can be obtained from the Painlevé expansion for either of the two families; and we have an immediate proof of the convergence, within the same domain as the system in $2+1$ dimensions, of the Painlevé expansion for the classical Boussinesq system for this special choice of arbitrary coefficients and S and C as above.

Case Two: $(\partial_x,\partial_y,\partial_t)\rightarrow(\partial_x,\partial_t,\partial_x)$.

In this case our system becomes

$$E_1[U,V]\equiv U_{xx}+V_t+\tfrac{1}{2}(U_xU_t)_x=0, \tag{197}$$

$$E_2[U,V]\equiv V_x+\kappa^2U_{xxxt}+U_{xt}V+\tfrac{1}{2}(U_xV_t+U_tV_x)=0, \tag{198}$$

which is in fact the first negative flow of the classical Boussinesq hierarchy. In following through the truncation for this reduction we see that we must force $C=-1$ and $D=0$, and relabel E as C and F as D. We then get the Riccati system (98), (99). The Riccati system (116), (117) is then equivalent to (98), (99), with the same cross-derivative conditions $\tilde{x}_1\equiv x_1=0$, $\tilde{x}_2\equiv x_2=0$. This is easily seen by replacing Z_t and Z_y in (117) by Z_x from (116) and Z_t respectively, and identifying, using (115),

$$-\Gamma C=1+\tilde{C},\quad -\Gamma D=\tilde{D},\quad \Gamma_x=0. \tag{199}$$

In this case at the stage of Eq. (150), when solving the determining equations for the truncation, we have that the arbitrary function of integration is a function of t only, i.e., $\lambda=\lambda(t)$. The constraint (153) then becomes $\lambda\lambda_t=0$ which tells us that λ is constant.

Using Eqs. (162)–(165) we thus obtain for the above system the Riccati pseudopotential (98), (99) with

$$A=-\frac{\lambda}{\kappa}+\frac{1}{2\kappa}\,u_x, \tag{200}$$

$$B=-\frac{1}{4\kappa^2}\,(v-\kappa u_{xx}), \tag{201}$$

$$C=\frac{1}{\lambda}\left(1+\frac{1}{2}u_t\right), \tag{202}$$

$$D=-\frac{1}{4\kappa\lambda}(v-\kappa u_{xx})_t, \tag{203}$$

and the same DT (170) under the linearization $Z^{-1}=\psi_2/\psi_1$.

We have available of course the same linearizations as for our original system in 2+1 dimensions. Thus for example the Lax pair for the first negative flow of the classical Boussinesq system having as spatial part an energy-dependent Schrödinger operator is

$$\psi_{xx}=-\frac{1}{4\kappa^2}\left[v-\left(\lambda-\frac{1}{2}u_x\right)^2\right]\psi, \tag{204}$$

$$\psi_t=-\frac{1}{\lambda}\left(1+\frac{1}{2}u_t\right)\psi_x+\frac{1}{4\lambda}u_{xt}\psi. \tag{205}$$

We do not write down here the other linear problems for the system (197), (198); this is a trivial exercise.

The expansion in χ corresponding to the DT is convergent within the same domain as that for the system (128), (129), has the same value of S, but has C as in (202). The SME is given by the substitution of

$$\omega=\int^t(\lambda C-1)dt' \tag{206}$$

into

$$\omega_{xx}+\kappa^2 S_t+(\lambda-\omega_x)(\lambda-\omega_x)_t+(\omega_x\omega_t)_x=0. \tag{207}$$

This SME can be obtained from the Painlevé expansion for either of the two families.

Case Three: $(\partial_x,\partial_y,\partial_t)\to(\partial_x,\partial_t,\partial_t)$.

In this case our system becomes

$$E_1[U,V]\equiv U_{xt}+V_t+\tfrac{1}{2}(U_xU_t)_x=0, \tag{208}$$

$$E_2[U,V]\equiv V_t+\kappa^2U_{xxxt}+U_{xt}V+\tfrac{1}{2}(U_xV_t+U_tV_x)=0, \tag{209}$$

which under the transformation

$$U\to U-2x+2t \tag{210}$$

becomes (197), (198). We do not therefore consider this example further here beyond remarking that the values of A, B, C, and D obtained from (162)–(165) by setting $C=E$ and $D=F$ are mapped into (200)–(203) above by the transformation (210) together with $\lambda\to(\lambda-1)$ [and (153) tells us that λ is constant].

4. Reduction to a linearizable subequation

Setting $V=\kappa U_{xx}$ in (128), (129) we find $E_2[U,\kappa U_{xx}]=\kappa(E_1[U,\kappa U_{xx}])_x$, and so we have a reduction to

$$E[U]\equiv E_1[U,\kappa U_{xx}]\equiv U_{xt}+\kappa U_{xxy}+\tfrac{1}{2}(U_xU_y)_x=0 \tag{211}$$

(we choose not to integrate this with respect to x). This equation is presented in Ref. 33 as a $2+1$ extension of Burgers equation, linearizable under $U=2\kappa \log \varphi$ onto

$$\varphi_t+\kappa\varphi_{xy}=0. \tag{212}$$

Indeed, (211) has reductions both to Burgers equation in U_x and the first negative flow of Burgers hierarchy. Trivial solutions of (212)

$$\varphi=\sum_{j=1}^{N+1} e^{(k_jx+l_jy+\omega_jt+\delta_j)}, \quad \omega_j+\kappa k_jl_j=0, \tag{213}$$

lead to solutions of (128), (129) which are $2+1$ analogs of those solutions of the classical Boussinesq system which exhibit fission and fusion.[34,35] These latter are obtained under the reduction $\partial_y\to\partial_x$, i.e. in seeking solutions of (212) of the form (213) with $k_j=l_j$.

The above reduction can be consistently made in our truncation for (128), (129). Setting $v=\kappa u_{xx}$ in (162)–(165) we find

$$A=-\frac{\lambda}{\kappa}+\frac{1}{2\kappa}u_x, \tag{214}$$

$$B=0, \tag{215}$$

$$C=-\lambda E+\frac{1}{2}u_y, \tag{216}$$

$$D=-\lambda F. \tag{217}$$

Since $B=0$ we have $\kappa(U_T)_{xx}=2\kappa^2(Z^{-1}-A)_x+\kappa u_{xx}=2\kappa^2(Z^{-1})_x=V_T$ and so the reduction is indeed consistent.

So we have for (211) the truncation

$$U_T=2\kappa \log Z+u. \tag{218}$$

The coefficients of the Riccati system (116), (117) are given by A and B above and

$$\Gamma=-\lambda, \quad \widetilde{C}=\tfrac{1}{2}u_y, \quad \widetilde{D}=0, \tag{219}$$

and so this Riccati system takes the form

$$Z_x=1-AZ, \tag{220}$$

$$Z_t=\Gamma Z_y-\widetilde{C}+(A\widetilde{C}+\widetilde{C}_x)Z, \tag{221}$$

with single cross-derivative condition

$$-\widetilde{x}_1\equiv A_t+(A\widetilde{C}+\widetilde{C}_x)_x-\Gamma A_y=0. \tag{222}$$

This case having $B=\widetilde{D}=0$ is worthy of more careful consideration. The first point to be made is that the truncation for the field $W=U_x$ of the nonlocal equation[33] associated to (211) truncates at constant-level in Z, and so also in χ, since

$$(U_T)_x=2\kappa(Z^{-1}-A)+u_x=2\kappa Z^{-1}+2\lambda=2\kappa\chi^{-1}+(\lambda+\tfrac{1}{2}u_x). \tag{223}$$

The second point is that when $B=\widetilde{D}=0$, the linearization onto a second-order Lax pair (13), (127) would appear to be misleading since this is related by a gauge transformation to (23), (124), and thus under $\eta_x=\zeta$ to the pair of linear equations

$$\zeta_x=A\zeta, \quad \zeta_t=\Gamma\zeta_y-(A\widetilde{C}+\widetilde{C}_x)\zeta, \tag{224}$$

i.e. a first-order system. The cross-derivative condition for this system is (222), which evaluates to

$$-\widetilde{x}_1\equiv\frac{1}{2\kappa}\,(E[u]-2(\lambda_t+\lambda\lambda_y))=0, \tag{225}$$

and we know of course that λ satisfies the constraint (166). The system (220), (221) is of course already a first-order linear system, although inhomogeneous.

This remark that the apparent second-order linear system obtained by linearization of our Riccati system can be transformed onto a first-order linear system is of course true also of the reductions (184), (185), (186) of (211) to systems in $1+1$ dimensions, respectively to Burgers equation in U_x, the first negative flow of Burgers hierarchy, and a PDE which under (210) is mapped onto the first negative flow of Burgers hierarchy.

Thus if, by way of example, we consider the reduction (184)—remembering that this means $E=-1$ and $F=0$—we find from (223) the truncation for Burgers equation[12] in $W=U_x$:

$$W_T=2\kappa\chi^{-1}+(\lambda+\tfrac{1}{2}w)=2\kappa\chi^{-1}+C, \tag{226}$$

where $w=u_x$, λ is a constant (from our previous considerations), and where for this χ,

$$S=\frac{1}{2\kappa^2}\left[\kappa w_x-\left(\lambda-\frac{1}{2}\,w\right)^2\right], \quad C=\lambda+\frac{1}{2}\,w. \tag{227}$$

Elimination of w in (227) gives the relation

$$\kappa^2S-\kappa C_x+\tfrac{1}{2}(2\lambda-C)^2=0. \tag{228}$$

This latter is *not* the constraint on S and C found by seeking a constant-level truncation for Burgers equation; seeking such a truncation gives (226) together with the constraint[12]

$$C_t+CC_x+2\kappa C_{xx}-\kappa^2S_x=0. \tag{229}$$

Equation (228) is, however, the relation *imposed* by Weiss[12] to make (229) consistent with the cross-derivative condition (9), since when (228) holds,

$$S_t+C_{xxx}+2SC_x+S_xC=\frac{1}{\kappa^2}\,(2\lambda-C+\kappa\partial_x)(C_t+CC_x+2\kappa C_{xx}-\kappa^2S_x). \tag{230}$$

The advantage of looking at the truncation for Burgers equation as a reduction of that for the classical Boussinesq system is that the constraint (228) falls out naturally. We also note the further advantage of our approach that we have built in to our analysis the linearization to the linear system in η. This means that we are able to recognize immediately that the second-order linear system in ψ is related by a gauge transformation to that in η, and thus in turn to the the first-order linear system in ζ. For Burgers equation this last—using (224) with $\partial_y=\partial_x$—gives

$$\zeta_x=\frac{1}{\kappa}\left(\frac{1}{2}\,w-\lambda\right)\zeta, \quad \zeta_t=\frac{1}{\kappa}\left[\lambda^2-\frac{1}{2}\left(\kappa w_x+\frac{1}{2}\,w^2\right)\right]\zeta. \tag{231}$$

Thus it is this first-order linear system that is the result of the truncation for Burgers equation. That such first-order linear systems result from the truncation for Burgers hierarchy has already been noted in Ref. 36, using a different approach.

Similar arguments to the above follow also for the reduction of (211) to the first negative flow of Burgers hierarchy. In this case the relation between S and C, obtained by elimination of the field between $S=-(A^2/2)+A_x$ and C, is—as it is for the $2+1$ equation (211)—nonlocal. The first-order linear system (224) gives

$$\zeta_x=\frac{1}{\kappa}\left(\frac{1}{2}\,u_x-\lambda\right)\zeta,\quad \zeta_t=\frac{1}{\kappa}\left[1+\frac{1}{2}\,u_t-\frac{1}{2\lambda}\left(u_x+\kappa u_{xt}+\frac{1}{2}\,u_x u_t\right)\right]\zeta, \tag{232}$$

where λ is now constant (from our previous considerations). Again, it is this first order system—whose compatibility condition is trivially the first negative flow of Burgers hierarchy—which is the result of the truncation for this reduction.

Finally we remark that we can extend the truncation in the WTC singular manifold φ, as done in Ref. 8 for Burgers equation and extended in Ref. 36 to the entire hierarchy, to the $2+1$ equation (211). Seeking a solution of (211) as

$$U=2\kappa\,\log\,\varphi+u \tag{233}$$

we easily find that we must have

$$E[U]\equiv E[u]+2\kappa\left[\frac{1}{\varphi}\left(\varphi_t+\kappa\varphi_{xy}+\frac{1}{2}\,(u_y\varphi_x+u_x\varphi_y)\right)\right]_x=0 \tag{234}$$

and so identifying different powers of φ we see that (233) provides a Bäcklund transformation from one solution u of (211) to a second solution U, where φ must satisfy

$$\varphi_t+\kappa\varphi_{xy}+\tfrac{1}{2}(u_y\varphi_x+u_x\varphi_y)=0. \tag{235}$$

This truncation corresponds to those presented in Refs. 8 and 36 for Burgers equation and its hierarchy respectively. As for members of Burgers hierarchy we can recognize two special cases: $u=0$ leading to the linearization onto (212) as given in Ref. 33; and $\varphi=u_x$ for which (235) becomes another copy of $E[u]=0$. It is a simple matter to write down the corresponding truncation and two special cases for the associated nonlocal equation in $W=U_x$.

IV. EXACT SOLUTIONS

Now, as done previously for the system (6), (7), we consider the recovery of exact solutions from our Riccati system (25), (26) by setting the coefficients to be constant. In order to satisfy the cross-derivative conditions (28), (29) we take $A=a$, $B=b$, $C=c$, where a, b, and c are constant, and $D=0$. The general solution of the Riccati system (25), (26) is then given by

$$Z^{-1}=\tfrac{1}{2}[a+k\,\tanh(\tfrac{1}{2}k(x-ct+\alpha))],\quad b+\tfrac{1}{4}a^2=\tfrac{1}{4}k^2. \tag{236}$$

We now consider, for this case of constant coefficients, the power series in Z corresponding to the sum and difference of the logarithmic derivatives of ψ_1 and ψ_2 satisfying (38), (39). Again using simple trigonometric identities—and deliberately keeping our notation close to that used in Refs. 25 and 37—we obtain

$$\left.\begin{aligned}(\log Z)_x = Z^{-1} - a - bZ = \frac{\psi_{1,x}}{\psi_1} - \frac{\psi_{2,x}}{\psi_2} = -k\sigma,\\ Z^{-1} + bZ = \frac{\psi_{1,x}}{\psi_1} + \frac{\psi_{2,x}}{\psi_2} = k\tau,\end{aligned}\right\}, \tag{237}$$

where

$$\sigma = \frac{\sqrt{\mu^2-1}}{\cosh(k(x-ct+\gamma))+\mu}, \quad \tau = \frac{\sinh(k(x-ct+\gamma))}{\cosh(k(x-ct+\gamma))+\mu}, \tag{238}$$

and

$$\gamma = \alpha + \frac{1}{k}\left[\frac{i\pi}{2} + \tanh^{-1}\left(\frac{a}{k}\right)\right] = \beta + \frac{1}{k}\tanh^{-1}\left(\frac{a}{k}\right), \quad \mu = \frac{ia}{\sqrt{k^2-a^2}}. \tag{239}$$

The functions σ and τ defined above are as given in Ref. 25; thus we have succeeded in extending the work in Ref. 16 so as to place this entire class of solutions within the context of Painlevé analysis. This means that we are now able to recover this class of solutions by making an expansion in a *single* variable; compare with the methods outlined in Refs. 25 and 37.

For a higher order truncation the relations (237) allow us to identify negative and positive powers of Z as

$$Z^{-1} = \frac{k}{2}\left(\tau - \sigma + \frac{a}{k}\right), \tag{240}$$

$$Z = \frac{k}{2b}\left(\tau + \sigma - \frac{a}{k}\right). \tag{241}$$

The relations (237) also imply that $(k\tau)^2 - (a - k\sigma)^2 = 4b = k^2 - a^2$, and so

$$\tau^2 = \sigma^2 - 2\frac{a}{k}\sigma + 1 = \sigma^2 - 2\frac{\mu}{\sqrt{\mu^2-1}}\sigma + 1. \tag{242}$$

Differentiation of the relations (237) with respect to x, and using the Riccati equation (25) and the above identity leads to

$$\sigma' = -\sigma\tau, \quad \tau' = -\tau^2 - \frac{\mu}{\sqrt{\mu^2-1}}\sigma + 1, \tag{243}$$

where $'$ denotes differentiation of σ and τ with respect to their argument. This coupled system of projective Riccati equations and the identity (242), here easily derived, are of course precisely as given in Ref. 25.

Finally, we remark that in the case $a=0$ ($\mu=0$), for which $Z=\chi$, we have $\sigma=\sigma_0$, $\tau=\tau_0$, and the expressions (240), (241) and (242) reduce to (17), (18) and (20), respectively. The results of this section answer the last of the four questions raised in Sec. I D.

A. First negative classical Boussinesq flow

As a first example of the recovery of an exact solution we consider obtaining a solution of (197), (198) by assuming constant values for the coefficients of the Riccati system as described above. From (200)–(203) we see that such values must satisfy

$$a=-\frac{\lambda}{\kappa}+\frac{1}{2\kappa}u_x, \tag{244}$$

$$b=-\frac{1}{4\kappa^2}(v-\kappa u_{xx}), \tag{245}$$

$$c=\frac{1}{\lambda}\left(1+\frac{1}{2}u_t\right), \tag{246}$$

$$0=-\frac{1}{4\kappa\lambda}(v-\kappa u_{xx})_t, \tag{247}$$

and so we have

$$u=\delta+2(\kappa a+\lambda)x+2(\lambda c-1)t, \tag{248}$$

$$v=-\kappa^2(k^2-a^2), \tag{249}$$

where δ is an arbitrary constant (trivial since only derivatives of U appear in our system), and where in (249) we have used the relation $b=(k^2-a^2)/4$. Thus we obtain the exact solution given by

$$U_T=2\kappa\ \log\ Z+\delta+2(\kappa a+\lambda)x+2(\lambda c-1)t, \tag{250}$$

$$V_T=2\kappa^2(k\tau)_x-\kappa^2(k^2-a^2), \tag{251}$$

where of course $(\log Z)_x=-k\sigma$ and $(\log Z)_t=ck\sigma$, σ and τ being given by (238). Ignoring δ, we see that this is a four-parameter (a,c,k,λ) solution. Asking that $U_{T,x}$ and $U_{T,t}$ be finite for large x and t requires $\kappa a+\lambda=0$ and $\lambda c-1=0$; this then gives the one-soliton solution of (197), (198).

The advantage of our approach, which identifies the solution (250), (251) with a WTC expansion and thus places it firmly within the framework of Painlevé analysis, is that we can now recover such solutions using an expansion in a single variable Z.

B. Kaup–Kupershmidt equation

In this section we consider the representation of the one-soliton solution of the Kaup–Kupershmidt (KK) equation[38,39]

$$E[U]\equiv-U_t+(U_{xxxx}+5UU_{xx}+\tfrac{15}{4}U_x^2+\tfrac{5}{3}U^3)_x=0. \tag{252}$$

Assuming that the coefficients of our Riccati system are constant, as above, we find that (252) admits the truncated expansion in Z

$$U_T=-3Z^{-2}+3aZ^{-1}+(2b-\tfrac{1}{4}a^2)-3abZ-3b^2Z^2 \tag{253}$$

provided that

$$c=-\tfrac{1}{16}(a^4-112a^2b+256b^2). \tag{254}$$

Using (240), (241), and (242), and writing $b=(k^2-a^2)/4$ these expressions may be rewritten as

$$U_T=\left(\frac{3}{4}a^2-k^2\right)+3k^2\left(\frac{a}{k}\sigma-\sigma^2\right),\quad c=-\tfrac{15}{4}a^2(\tfrac{3}{4}a^2-k^2)-k^4. \tag{255}$$

In the case $a^2=4k^2/3$, for which $\mu=2$, this gives the one-soliton of KK,

$$U_T=3k^2\,\frac{1+2\cosh(k(x+k^4t+\gamma))}{[2+\cosh(k(x+k^4t+\gamma))]^2}, \tag{256}$$

again obtained from an expansion in a single variable Z. This soliton solution corresponds to the summation of an infinite Painlevé expansion (in both χ and φ). We note that the representation (253) is related to the scalar second-order linear system (23), (24).

The expansion (253) can be written

$$U_T=3(Z^{-1}+bZ)_x+(\tfrac{3}{4}a^2-k^2), \tag{257}$$

and so using (237) we see easily the representation of the one-soliton solution as the second logarithmic derivative of the product of two entire functions, as remarked in Ref. 37.

V. CONCLUSIONS

We have introduced a new and more consistent definition of SME, as the constraint on φ such that for certain choices of arbitrary data the Painlevé expansion corresponds to the DT. This approach, whereby we no longer expect the DT to correspond to a WTC expansion truncated at constant level, provides a natural extension of the Weiss singular manifold method. The summation of infinite WTC expansions has been effected by construction using the higher order truncation allowed when the expansion variable satisfies a system of Riccati equations. For the examples considered, this new SME can be obtained from the Painlevé expansion for *either* of the two principal families, i.e. we make use of only one singular manifold. The approach developed here is algorithmic, although of course other PDEs may require still further extensions of the singular manifold method.

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APPENDIX: SINE-GORDON EQUATION

We give here for completeness the results of our analysis for s-G,

$$E[U]\equiv U_{xt}-\sin U=0. \tag{A1}$$

These results turn out to be equivalent to those given by Weiss[40] for the equation

$$F[V]\equiv 2(VV_{xt}-V_xV_t)-V^3+V=0,\quad V=e^{iU}, \tag{A2}$$

and thus we show that s-G can in fact be dealt with using the usual singular manifold method.

Equation (A2) has a Painlevé expansion with indices $\{-1,2\}$ given by[8,14]

$$V=\chi^{-2}\sum_{j=0}^{\infty}V_j^{\chi}\chi^j, \tag{A3}$$

where $V_0^{\chi}=-4C$, $V_1^{\chi}=4C_x$ and V_2^{χ} is arbitrary. The Painlevé expansion for the field U of s-G is then

$$U=-i\ \log\ V=2i\ \log\ \chi-i\ \log(-4C)+i\ \frac{C_x}{C}\ \chi+U_2^{\chi}\chi^2+\cdots\ , \tag{A4}$$

where

$$U_2^{\chi}=\frac{i}{4}\left(\frac{V_2^{\chi}}{C}+2\left(\frac{C_x}{C}\right)^2\right) \tag{A5}$$

is an arbitrary coefficient which enters at χ^2. We note that the leading order logarithm in the field U of s-G has previously been remarked upon in Refs. 41 and 42.

From (A4) it is clear that the natural truncation for s-G is

$$U_T=2i\ \log\ Z+w. \tag{A6}$$

Substitution of (A6) into (A1) gives

$$E[U_T]\equiv Z^{-2}\sum_{j=0}^{4}\ E_j^Z Z^j=0, \tag{A7}$$

and the solution of the equations $E_j^Z=0$, together with the cross-derivative conditions (28), (29), is easily obtained as

$$A=-iu_x,\quad B=\lambda^2,\quad C=-\frac{1}{4\lambda^2}\ e^{iu},\quad D=-\tfrac{1}{2}iu_{xt}, \tag{A8}$$

where λ is a constant of integration, $u=w-2i\ \log\lambda$, and E_4^Z becomes

$$E_4^Z\equiv\lambda^2E[u]=0, \tag{A9}$$

which tells us that u is a second solution of s-G. Rewriting $D=(-i/2)\sin u$ we find that (28) becomes $-x_1=-iE[u]$, and so we have the Riccati pseudopotential

$$Z_x=1+iu_xZ-\lambda^2Z,\quad Z_t=\frac{1}{4\lambda^2}\ e^{iu}-\frac{1}{4}\ e^{-iu}Z^2, \tag{A10}$$

together with the DT, which again it is not necessary to obtain in advance,

$$U_T=2i\ \log(\lambda Z)+u. \tag{A11}$$

These results are equivalent to those given in Ref. 18 under $Z=Y/\lambda$. We note that in this case no gauge freedom arose in the solution obtained in Ref. 18; this is because, although the Riccati system used does allow such a freedom, the DT taken was too restrictive for this to be incorporated into the solution. The fact that this freedom is still allowed in the Riccati system in Y means that the recovery of the spectral problem and DT is still much easier using our Riccati variable Z. The derivation of the DT for s-G in Ref. 18 is subject to the same remarks as is that for MKdV (see Sec. II B).

Rewriting the DT in terms of χ using (30) gives for U_T the infinite expansion

$$\begin{aligned}U_T&=2i\ \log(\lambda Z)+u=2i\ \log\ \chi+(u+2i\ \log\ \lambda)-2i\ \log(1+\tfrac{1}{2}A\chi)\\&=2i\ \log\ \chi+(u+2i\ \log\ \lambda)-iA\chi+\frac{i}{4}\ A^2\chi^2+\cdots\ ,\end{aligned} \tag{A12}$$

with corresponding S and C for this χ obtained from (31) and (A8) as

$$S=-iu_{xx}+\frac{1}{2}u_x^2-2\lambda^2, \quad C=-\frac{1}{4\lambda^2}e^{iu}. \tag{A13}$$

These values are a parametrization of the equation

$$S+\frac{C_{xx}}{C}-\frac{1}{2}\left(\frac{C_x}{C}\right)^2+2\lambda^2=0, \tag{A14}$$

which is therefore the SME for s-G. The Painlevé expansion corresponding to the DT—having the previously arbitrary $U_2^\chi=(i/4)(C_x/C)^2$ and subject to (A14)—is convergent for χ in the cut plane such that

$$|\chi|<2|u_x^{-1}|. \tag{A15}$$

The SME (A14) is the same as that given previously for s-G,[40,14] obtained from the constant level truncation for (A2). If we now consider this equation, we obtain from U_T—writing $v=e^{iu}$, and using the identities $A=-C_x/C$, $v=-4\lambda^2C$—a corresponding V_T:

$$V_T=e^{iU_T}=\frac{v}{\lambda^2}Z^{-2}=-4C\left(\chi^{-1}-\frac{1}{2}\left(\frac{C_x}{C}\right)\right)^2=-4C\chi^{-2}+4C_x\chi^{-1}-\frac{C_x^2}{C}. \tag{A16}$$

This is just the standard truncation for (A2) with SME (A14).[40,14] We have thus shown that this truncation corresponds to the DT for s-G. The matrix spectral problem for s-G is obtained from (6), (7) by[27]

$$\chi^{-1}=Z^{-1}-\frac{1}{2}A=\frac{\psi_2}{\psi_1}+\frac{1}{2}iu_x. \tag{A17}$$

So it is possible to obtain the DT and Lax pair (and hence the BT) for s-G using the standard truncation for the equation in the form (A2). The Lax pair given by Weiss[40]—(13), (14) with S, C given by (A13)—is seen to be related to the matrix spectral problem by a simple gauge transformation.

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Zero curvature formulations of dual hierarchies

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Zero curvature formulations are given for the ''dual hierarchies'' of standard soliton equation hierarchies, recently introduced by Olver and Rosenau, including the physically interesting Fuchssteiner–Fokas–Camassa–Holm hierarchy. © *1996 American Institute of Physics.* [S0022-2488(96)02702-X]

Through the years since the discovery of the notion of ''integrability'' in PDEs, quite a number of integrable PDEs have been discovered, most of which remain obscure for lack of any physical significance. For nearly 15 years now, the equation

$$u_t+2\kappa u_x-u_{xxt}+3uu_x=2u_xu_{xx}+uu_{xxx}, \tag{1}$$

derived by Fuchssteiner and Fokas,[1] has enjoyed such obscurity; but in a recent paper of Camassa and Holm,[2] this equation was rediscovered, and looks likely to be of some importance. Like Fuchssteiner and Fokas, Camassa and Holm showed that, for $\kappa=0$, Eq. (1) has *bi-Hamiltonian structure*: if we write $m=u-u_{xx}$, then Eq. (1) takes the form

$$m_t=-J_1\frac{\delta H_2}{\delta m}=-J_2\frac{\delta H_1}{\delta m}, \tag{2}$$

where

$$J_1=\partial-\partial^3, \quad J_2=\partial m+m\partial \tag{3}$$

are two compatible Hamiltonian operators, and

$$H_2=\frac{1}{2}\int_{-\infty}^{\infty}(u^3+uu_x^2)dx, \quad H_1=\frac{1}{2}\int_{-\infty}^{\infty}(u^2+u_x^2)dx. \tag{4}$$

The novelty of Camassa and Holm's work was that they gave a *physical derivation* of Eq. (1). Furthermore, for $\kappa=0$, they found solutions to Eq. (1) which they named ''peakons'' (traveling wave solutions with a corner at their peak); these take the simple form

$$u=c\ \exp(-|x-ct|). \tag{5}$$

More generally they showed that

$$u=\sum_{i=1}^{N}p_i(t)\exp(-|x-q_i(t)|) \tag{6}$$

gives an N-peakon solution, provided $\{p_i(t),q_i(t)\}$ solves Hamilton's equations for the Hamiltonian

$$H_A=\frac{1}{2}\sum_{i,j=1}^{N}p_ip_j\ \exp(-|q_i-q_j|). \tag{7}$$

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Camassa and Holm proved this Hamiltonian system is integrable, and gave its solution for $N=2$. For $\kappa\neq 0$, solutions of Eq. (1) have been investigated numerically in Ref. 3.

Prior to Camassa and Holm's work, Rosenau and Hyman[4] made the remarkable observation that a large class of nonlinear PDEs with nonlinear dispersion terms exhibited ''compacton'' solutions, viz. solitons with compact spatial support. Rosenau[5] further showed that this phenomenon can also occur in integrable PDEs; in particular, if we replace (x,t) in the Fuchssteiner–Fokas–Camassa–Holm equation (1) by (ix,it), we find the equation

$$u_t+2\kappa u_x+u_{xxt}+3uu_x+2u_xu_{xx}+uu_{xxx}=0 \tag{8}$$

and this admits, for $\kappa=0$, the compacton solution

$$u=c\ \cos(x-ct), \quad |x-ct|\leqslant\frac{\pi}{2}. \tag{9}$$

(The compacton solutions of Eq. (8) are actually unstable; but it serves to illustrate that compactons can occur in the framework of integrability; in addition it seems further equations in its hierarchy have acceptable properties. I thank Philip Rosenau for information on this point.)

In the wake of this work, two apparently widely applicable constructions of integrable PDEs with nonlinear dispersion terms have been given. The first, due to Rosenau,[6] consists of applying Lagrange transformations to soliton-bearing integrable PDEs, such as the KdV and MKdV equations. The philosophy here is that the standard solitons in such equations, despite being of infinite spatial extent, carry finite mass and/or momentum, and hence must be of compact support when measured in mass and/or momentum units. The second construction, due to Olver and Rosenau[7] (again a rediscovery of Fuchssteiner and Fokas' earlier work;[1] the reader should also see the modern work[8] of Fokas), starts from the observation that the two Hamiltonian operators J_1,J_2 given in Eq. (3) look like recombinations of terms from the two standard Hamiltonian operators of the KdV equation (see, e.g., Ref. 9). In fact it turns out that if a bi-Hamiltonian integrable hierarchy has one Hamiltonian operator which is a constant coefficient differential operator, and another Hamiltonian operator which is a linear combination of a constant coefficient differential operator and another operator which scales homogeneously with nonzero degree when the fields are rescaled, then by recombining terms from these Hamiltonian operators one can construct a new hierarchy. In Ref. 7 this procedure is followed to construct dual hierarchies of the KdV, MKdV, Broer–Kaup–Kupershmidt, and Ito hierarchies (the NLS hierarchy is also dualized by a variant of the general procedure). The aim of this article is to provide yet another method of constructing dual hierarchies, reproducing the results of Ref. 7. This time the initial observation is the similarity of the linear system associated with the Camassa–Holm equation (the linear system is given in Eq. (6) of Ref. 2), and the linear system associated with the KdV equation. We will see that *zero curvature formulations* of dual hierarchies can be obtained by a simple modification of the well-known zero curvature formulations of the standard soliton equation hierarchies.

The original purpose of this work was twofold. First, for standard soliton equation hierarchies, the zero curvature formulation is a springboard for revealing many other properties of the hierarchies. In particular, in the zero curvature formulation one sees a natural group action on the space of solutions (the group of ''dressing transformations''), which, when it can be made explicit, gives rise to a host of solutions of the hierarchies (for a compact overview of how the group of dressing transformations gives rise to the tau-function formalism for the MKdV equation, see Ref. 10). Alas, while the zero curvature formulations of dual hierarchies are only slight variations of those for standard hierarchies, this slight variation complicates the explicit realization of dressing transformations, and we have been unable, as of yet, to compute explicit dressing transformations and generate solutions this way. The second hope in undertaking this work was that, while Olver and Rosenau's construction[7] *cannot* be extended to, for example, the Boussinesq (SL(3) KdV) equation (one Hamiltonian operator is a constant coefficient differential operator, as required, but the

other is the sum of a constant coefficient differential operator and another term that does not scale homogeneously under any rescaling of the fields), it was hoped that the zero curvature formulations would suggest an extension. Extensive experiments in this direction—which will not be reported here—have so far yielded only negative results. It seems quite possible that dual hierarchies can only be constructed for a handful of soliton equation hierarchies, and not for all the various infinite chains of hierarchies, like the SL(N) KdV hierarchies,[11] that exist.

The content of this article is therefore limited to presenting zero curvature formulations of the existing dual hierarchies. It is to be hoped that these will be of use in further studies of these hierarchies, and in finding solutions. We will see some minor immediate benefits of our labor; in particular, we will see that the dual Broer–Kaup–Kupershmidt hierarchy and the dual Ito hierarchy are equivalent, and we clarify a little further the structure of the dual NLS hierarchy. Also, of course, the zero curvature forms we will present can be used to derive ''standard'' Lax pairs for the dual hierarchies, via a simple procedure we will illustrate.

(1) Zero curvature formulations. The notion of a zero curvature formulation for a soliton equation dates back to the work of Ref. 12 (and other works in Soviet literature). In Ref. 12 it was observed that several equations of physical interest could be written in the form

$$\partial_t A = \partial_x B + [B,\, A], \tag{10}$$

where A,B are functions of x,t valued in the Lie algebra of the SL(2) loop group, that is, A,B are traceless, 2×2 matrix valued functions of x, t, and λ. Equation (10) reduces to the desired soliton equation by specifying a very particular dependence on the ''spectral parameter'' λ. In greater generality, the majority of (if not all) soliton equation hierarchies can be written in the form

$$\partial_{t_r} A = \partial_x B_r + [B_r\,,\, A], \tag{11}$$

where $A,\{B_r\}$ (r runs over an appropriate index set) are functions of x, $\{t_r\}$, and λ valued in some matrix Lie algebra, with a certain specified λ dependence. The classic example is the KdV hierarchy, for which $r \in \{1,3,5,...\}$ and

$$A = \begin{pmatrix} 0 & 1 \\ u(x,t)+\lambda & 0 \end{pmatrix}, \quad B_r = \begin{pmatrix} 0 & 0 \\ \lambda^{(r+1)/2} & 0 \end{pmatrix} + \begin{pmatrix} \text{polynomial of} \\ \text{degree } \dfrac{r-1}{2} \text{ in } \lambda \end{pmatrix}. \tag{12}$$

(Note that requiring consistency of Eqs. (11) almost fully determines the matrices B_r from the information in Eq. (12). To precisely determine the B_r's one should add on (1) the conditions $\partial_{t_r} B_s = \partial_{t_s} B_r + [B_r, B_s]$, and (2) certain homogeneity conditions. For brevity, we shall overlook these details in this article.) The utility of this formulation of the hierarchy is that Eqs. (11) are invariant under *gauge transformations*:

$$A \to \xi A \xi^{-1} + \partial_x \xi \xi^{-1}, \quad B_r \to \xi B_r \xi^{-1} + \partial_{t_r} \xi \xi^{-1}, \tag{13}$$

where ξ is a function of x, $\{t_r\}$, λ, valued in the appropriate Lie group. The group of such gauge transformations that leave the specified λ dependence of $A,\{B_r\}$ unchanged is the group of dressing transformations[13] referred to above.

Other gauge transformations that are of interest are those that map one hierarchy to another, known as Miura maps. To illustrate, the MKdV hierarchy is given by Eqs. (11), with $r \in \{1,3,5,...\}$ again, and

$$A = \begin{pmatrix} j(x,t) & 1 \\ \lambda & -j(x,t) \end{pmatrix}, \quad B_r = \begin{pmatrix} 0 & 0 \\ \lambda^{(r+1)/2} & 0 \end{pmatrix} + \begin{pmatrix} \text{polynomial of} \\ \text{degree } \dfrac{r-1}{2} \text{ in } \lambda \end{pmatrix}. \tag{14}$$

Choosing

$$\xi=\begin{pmatrix} 1 & 0 \\ j(x,t) & 1 \end{pmatrix}, \tag{15}$$

the MKdV choice of $A,\{B_r\}$ [Eq. (14)] is mapped to the KdV choice (12), with $u=j_x+j^2$. (Note that in Ref. 10, Wilson works with an apparently different zero curvature formulation of MKdV; he is simply using a different matrix representation of the SL(2) loop group.)

As for all the hierarchies we will consider in this article, the $r=1$ equations for KdV and MKdV are trivial. In each case $B_1=A$, and the flow equations are $u_{t_1}=u_x$ and $j_{t_1}=j_x$, respectively. From these equations we see t_1 can be identified with x. The first nontrivial equations are obtained from $r=3$: for KdV,

$$B_3=\begin{pmatrix} \frac{1}{4}u_x & \lambda-\frac{1}{2}u \\ \lambda^2+\frac{1}{2}\lambda u+\frac{1}{4}u_{xx}-\frac{1}{2}u^2 & -\frac{1}{4}u_x \end{pmatrix} \text{ yielding } u_{t_3}=\tfrac{1}{4}u_{xxx}-\tfrac{3}{2}uu_x, \tag{16}$$

and for MKdV,

$$B_3=\begin{pmatrix} \lambda_j+\frac{1}{4}(j_{xx}-2j^3) & \lambda-\frac{1}{2}(j_x+j^2) \\ \lambda^2+\frac{1}{2}\lambda(j_x-j^2) & -\lambda j-\frac{1}{4}(j_{xx}-2j^3) \end{pmatrix} \text{ yielding } j_{t_3}=\tfrac{1}{4}j_{xxx}-\tfrac{3}{2}j^2j_x. \tag{17}$$

The procedure for extracting standard Lax pairs from zero curvature formulations is as follows. Equations (11) are consistency conditions for the equations

$$\partial_x\psi=A\psi, \quad \partial_{t_r}\psi=B_r\psi. \tag{18}$$

(Here $\psi(x,t)$ is a vector in an appropriate representation of the appropriate Lie algebra.) For KdV and $r=3$, we eliminate ψ_2 from Eq. (18) to arrive at the KdV Lax pair:

$$\psi_{1xx}=(u+\lambda)\psi_1, \quad \psi_{1t_3}=\tfrac{1}{4}u_x\psi_1+(\lambda-\tfrac{1}{2}u)\psi_{1x}. \tag{19}$$

The zero curvature formulations of the other standard hierarchies relevant to this article follow; all are associated with the SL(2) loop algebra.

(1) The Broer–Kaup–Kupershmidt (BKK) hierarchy. (This hierarchy was brought to prominence by Kupershmidt in Ref. 14, where it was attributed to Broer and Kaup. It seems, however, that it should also be attributed to Whitham. It is frequently just referred to as a ''Boussinesq-type'' hierarchy.)

$$\begin{gathered} A=\begin{pmatrix} \lambda+v(x,t) & 1 \\ u(x,t) & -\lambda-v(x,t) \end{pmatrix}, \\ B_r=\begin{pmatrix} \lambda^r & 0 \\ 0 & -\lambda^r \end{pmatrix}+\begin{pmatrix} \text{polynomial of} \\ \text{degree } r-1 \text{ in } \lambda \end{pmatrix}, \quad r=1,2,3,\ldots . \end{gathered} \tag{20}$$

Taking

$$B_2=\begin{pmatrix} \lambda^2+\frac{1}{2}v_x-v^2 & \lambda-v \\ \lambda u-\frac{1}{2}u_x-uv & -\lambda^2-\frac{1}{2}v_x+v^2 \end{pmatrix} \tag{21}$$

yields the lowest nontrivial equation:

$$v_{t_2}=(\tfrac{1}{2}v_x-v^2+\tfrac{1}{2}u)_x,\qquad u_{t_2}=(-\tfrac{1}{2}u_x-2uv)_x. \tag{22}$$

(2) The NLS hierarchy.

$$A=\begin{pmatrix}\lambda & \psi(x,t)\\ \overline{\psi}(x,t) & -\lambda\end{pmatrix},\quad B_r=\begin{pmatrix}\lambda^r & 0\\ 0 & -\lambda^r\end{pmatrix}+\begin{pmatrix}\text{polynomial of}\\ \text{degree } r-1 \text{ in } \lambda\end{pmatrix},\quad r=1,2,3,\ldots . \tag{23}$$

Taking

$$B_2=\begin{pmatrix}\lambda^2-\frac{1}{2}\psi\overline{\psi} & \lambda\psi+\frac{1}{2}\psi_x\\ \lambda\overline{\psi}-\frac{1}{2}\overline{\psi_x} & -\lambda^2+\frac{1}{2}\psi\overline{\psi}\end{pmatrix} \tag{24}$$

yields the lowest nontrivial equation

$$\psi_{t_2}=\tfrac{1}{2}\psi_{xx}-\psi^2\overline{\psi},\quad \overline{\psi}_{t_2}=-\tfrac{1}{2}\overline{\psi}_{xx}+\psi\overline{\psi^2}. \tag{25}$$

Miura map to the BKK hierarchy:

$$\xi=\begin{pmatrix}\dfrac{1}{\sqrt{\psi}} & 0\\ 0 & \sqrt{\psi}\end{pmatrix} \tag{26}$$

giving $v=-\psi_x/2\psi$, $u=\psi\overline{\psi}$. (The relationship of NLS to the BKK hierarchy, and many other ''NLS-type'' equations, was given in Ref. 15.)

(3) The Ito hierarchy.[16]

$$\begin{gathered}A=\begin{pmatrix}0 & 1\\ \dfrac{p(x,t)}{\lambda}+q(x,t)+\lambda & 0\end{pmatrix},\\ B_r=\begin{pmatrix}0 & 0\\ \lambda^{(r+1)/2} & 0\end{pmatrix}+\begin{pmatrix}\text{polynomial of}\\ \text{degree } \dfrac{r-1}{2} \text{ in } \lambda\end{pmatrix}+f(x,t)A,\quad r=1,3,5,\ldots .\end{gathered} \tag{27}$$

Taking

$$B_3=\begin{pmatrix}\frac{1}{4}q_x & \lambda-\frac{1}{2}q\\ \lambda^2+\frac{1}{2}\lambda q+(\frac{1}{4}q_{xx}-\frac{1}{2}q^2+p)-(1/2\lambda)pq & -\frac{1}{4}q_x\end{pmatrix} \tag{28}$$

yields the lowest nontrivial equation

$$q_{t_3}=\tfrac{1}{4}q_{xxx}-\tfrac{3}{2}qq_x+p_x,\quad p_{t_3}=-pq_x-\tfrac{1}{2}qp_x \tag{29}$$

(the substitution $p=r^2$ returns the standard form of the Ito equation). The Ito hierarchy is just one of what we shall call the *generalized Ito hierarchies* (which in turn are just a subset of the hierarchies discussed in Ref. 17). For any non-negative integer M there exists a hierarchy with

$$A=\begin{pmatrix}0 & 1\\ \lambda+S & 0\end{pmatrix},\quad S=\sum_{n=0}^{M}s_n(x,t)\lambda^{-n}, \tag{30}$$

and B_r ($r=1,3,5,...$) specified by the requirement that its upper right-hand entry is a polynomial of degree $(r-1)/2$ in λ with leading order coefficient 1. For $M=0$ this is the KdV hierarchy, for $M=1$ the usual Ito hierarchy, and for $M=2$ it is a simple exercise to show the lowest nontrivial equation in the hierarchy takes the form

$$s_{0t_3}=\tfrac{1}{4}s_{0xxx}-\tfrac{3}{2}s_0s_{0x}+s_{1x}, \quad s_{1t_3}=s_{2x}-s_1s_{0x}-\tfrac{1}{2}s_0s_{1x}, \quad s_{2t_3}=-s_2s_{0x}-\tfrac{1}{2}s_0s_{2x}. \tag{31}$$

For the KdV and MKdV hierarchies, and for the three hierarchies just listed, *the zero curvature formulations of the dual hierarchies are obtained by rescaling entries in the matrices A by appropriate powers of* λ, and adjusting the matrices $\{B_r\}$ to maintain consistency. For example, for the Fuchssteiner–Fokas–Camassa–Holm hierarchy (the dual of KdV), we take

$$A=\begin{pmatrix} 0 & 1 \\ u(x,t)/\lambda+1 & 0 \end{pmatrix}, \tag{32}$$

that is A has the same form as for the KdV hierarchy, but with its (2,1) entry rescaled by a factor λ^{-1}. Choosing B_r of the form ''polynomial of degree $(r-1)/2$ in λ plus a multiple of A,'' it is straightforward to obtain the flows

$$u_{t_r}=[(\partial_x u+u\partial_x)(\tfrac{1}{2}\partial_x^3-2\partial_x)^{-1}]^{r-1/2}u_x. \tag{33}$$

These are the flows of the Fuchssteiner–Fokas–Camassa–Holm hierarchy; in particular, setting $r=1$, and defining v via $u=\frac{1}{2}v_{xx}-2v$, we obtain

$$2v_{t_3}-\tfrac{1}{2}v_{xxt_3}=6vv_x-v_xv_{xx}-\tfrac{1}{2}vv_{xxx}, \tag{34}$$

a simple rescaling of Eq. (1). Note the form of B_r is also obtained from that of the KdV hierarchy, by rescaling its (2,1) entry by a factor λ^{-1}.

For the dual of MKdV we take

$$A=\begin{pmatrix} j(x,t)/\sqrt{\lambda} & 1 \\ 1 & -j(x,t)/\sqrt{\lambda} \end{pmatrix}. \tag{35}$$

This is of the same as for MKdV [Eq. (14)], after a rescaling of the (1,1) and (2,2) entries by $\lambda^{-1/2}$, and of the (2,1) entry by λ^{-1}. The appropriate choice for B_r this time cannot be found from a rescaling of the MKdV form: in particular, powers of $\sqrt{\lambda}$ appear in the off-diagonal terms of B_r. However, B_r can be completely specified (up to an unimportant overall factor) by the requirement that the sum of its off-diagonal elements be a polynomial in λ of degree $(r-1)/2$. For $r=1$ we have $B_1=A$, as usual, and for $r=2$ we find

$$B_3=\begin{pmatrix} \sqrt{\lambda}(j-\frac{1}{4}m_{xx})+(1/\sqrt{\lambda})js & \lambda+s+\frac{1}{2}\sqrt{\lambda}m_x \\ \lambda+s-\frac{1}{2}\sqrt{\lambda}m_x & -\sqrt{\lambda}(j-\frac{1}{4}m_{xx})-(1/\sqrt{\lambda})js \end{pmatrix}, \tag{36}$$

where m is related to j by $j=\frac{1}{4}m_{xx}-m$, and $s=\frac{1}{2}(\frac{1}{4}m_x^2-m^2)$. This gives the flow equation

$$j_{t_3}=\left[\frac{j}{2}\left(\frac{m_x^2}{4}-m^2\right)\right]_x, \quad j=\tfrac{1}{4}m_{xx}-m \tag{37}$$

(cf. Ref. 7). The general flow is

$$j_{t_r}=[\partial_x j\partial_x^{-1}j(\tfrac{1}{4}\partial_x^2-1)^{-1}]^{r-1/2}j_x. \tag{38}$$

Note that there is no obvious Miura map from the dual of MKdV to the dual of KdV. The small modifications we have made to the matrices A in each case have been sufficient to destroy this, and in general Miura maps do not survive the dualization procedure. We will see that it is also the case that new Miura maps can emerge. It remains an interesting open question as to whether there exists a modification of the Fuchssteiner–Fokas–Camassa–Holm equation.

We now list the zero curvature forms for the duals of the other hierarchies listed above.

(1) The dual BKK hierarchy. We take

$$A=\begin{pmatrix} 1+v(x,t)/\lambda & 1/\sqrt{\lambda} \\ u(x,t)/\sqrt{\lambda} & -1-v(x,t)/\lambda \end{pmatrix},$$
$$B_r=\begin{pmatrix} \beta(1+v(x,t)/\lambda)-\frac{1}{2}\beta_x & \beta/\sqrt{\lambda} \\ \sqrt{\lambda}\gamma+u\beta/\sqrt{\lambda} & -\beta(1+v(x,t)/\lambda)+\frac{1}{2}\beta_x \end{pmatrix}, \quad r=1,2,3,\ldots, \tag{39}$$

where

$$\beta=\lambda^{r-1}+\sum_{n=0}^{r-2}\beta_n(x,t)\lambda^n, \qquad \gamma=\sum_{n=0}^{r-2}\gamma_n(x,t)\lambda^n. \tag{40}$$

It is straightforward to check this gives the flow

$$\partial_{t_r}\begin{pmatrix} v \\ u \end{pmatrix}=[\mathscr{S}\mathscr{R}^{-1}]^{r-1}\begin{pmatrix} v_x \\ u_x \end{pmatrix}, \tag{41}$$

where

$$\mathscr{S}=\begin{pmatrix} 0 & \partial_x v \\ 2v & \partial_x u+u\partial_x \end{pmatrix}, \quad \mathscr{R}=\begin{pmatrix} 1 & \frac{1}{2}\partial_x^2-\partial_x \\ -\partial_x-2 & 0 \end{pmatrix}. \tag{42}$$

$\mathscr{S}\mathscr{R}^{-1}$ is (up to simple rescalings) the recursion operator found in Ref. 7, but in Ref. 7 it is factored as $\tilde{\mathscr{S}}\tilde{\mathscr{R}}^{-1}$, where

$$\tilde{\mathscr{S}}=\mathscr{S}\begin{pmatrix} \partial_x & 0 \\ 0 & 2 \end{pmatrix}=\begin{pmatrix} 0 & 2\partial_x v \\ 2v\partial_x & 2(\partial_x u+u\partial_x) \end{pmatrix},$$
$$\tilde{\mathscr{R}}=\mathscr{R}\begin{pmatrix} \partial_x & 0 \\ 0 & 2 \end{pmatrix}=\begin{pmatrix} \partial_x & \partial_x^2-2\partial_x \\ -\partial_x^2-2\partial_x & 0 \end{pmatrix}. \tag{43}$$

To write the $r=2$ flow in local form, in Ref. 7 the substitution

$$\begin{pmatrix} v \\ u \end{pmatrix}=\tilde{\mathscr{R}}\partial_x^{-1}\begin{pmatrix} V \\ U \end{pmatrix}=\begin{pmatrix} V-2U+U_x \\ -2V-V_x \end{pmatrix} \tag{44}$$

is introduced, giving the flow

$$\partial_{t_2}\begin{pmatrix} V-2U+U_x \\ -2V-V_x \end{pmatrix}=\begin{pmatrix} 2(UV-2U^2+UU_x)_x \\ (-8UV+V^2-2UV_x)_x \end{pmatrix}. \tag{45}$$

From the zero curvature approach it is rather more natural to perform the substitution

$$\begin{pmatrix} v \\ u \end{pmatrix} = \begin{pmatrix} \widetilde{V} \\ \frac{1}{2}\widetilde{U}_{xx} - 2\widetilde{U} - 2\widetilde{V} - \widetilde{V}_x \end{pmatrix} \tag{46}$$

giving the flow

$$\partial_{t_2}\begin{pmatrix} \widetilde{V} \\ \frac{1}{2}\widetilde{U}_{xx} - 2\widetilde{U} - 2\widetilde{V} - \widetilde{V}_x \end{pmatrix} = \begin{pmatrix} (\widetilde{U}\widetilde{V})_x \\ (\frac{1}{2}\widetilde{U}\widetilde{U}_{xx} + \frac{1}{4}\widetilde{U}_x^2 - (\widetilde{U}\widetilde{V})_x + \widetilde{V}^2 - 2\widetilde{U}\widetilde{V} - 3\widetilde{U}^2)_x \end{pmatrix}, \tag{47}$$

or, equivalently,

$$\partial_{t_2}\begin{pmatrix} \widetilde{V} \\ \frac{1}{2}\widetilde{U}_{xx} - 2\widetilde{U} \end{pmatrix} = \begin{pmatrix} (\widetilde{U}\widetilde{V})_x \\ (\frac{1}{2}\widetilde{U}\widetilde{U}_{xx} + \frac{1}{4}\widetilde{U}_x^2 + \widetilde{V}^2 - 3\widetilde{U}^2)_x \end{pmatrix}, \tag{48}$$

an equation that will appear again later. Note that the relationship of U, V and $\widetilde{U}, \widetilde{V}$ is given by

$$V = \widetilde{V} - \tfrac{1}{2}\widetilde{U}_x + \widetilde{U}, \quad U = \tfrac{1}{2}\widetilde{U}. \tag{49}$$

(The origin of this variable $\widetilde{U}$ is that β introduced in Eqs. (41) and (42) takes the form $\lambda + \widetilde{U}$ for $r = 2$.)

(2) The dual NLS hierarchy. To obtain the dual NLS hierarchy of Ref. 7, take

$$A = \begin{pmatrix} 1 & \psi(x,t)/\sqrt{\lambda} \\ \psi(x,t)/\sqrt{\lambda} & -1 \end{pmatrix}, \quad B_r = \begin{pmatrix} \alpha & \sqrt{\lambda}\beta \\ \sqrt{\lambda}\gamma & -\alpha \end{pmatrix}, \quad r = 1,2,3,\ldots, \tag{50}$$

where

$$\alpha = \lambda^{r-1} + \sum_{n=0}^{r-2} \alpha_n(x,t)\lambda^n, \quad \beta = \sum_{n=0}^{r-2} \beta_n(x,t)\lambda^n, \quad \gamma = \sum_{n=0}^{r-2} \gamma_n(x,t)\lambda^n \tag{51}$$

to get the flows

$$\partial_{t_r}\begin{pmatrix} \psi \\ \overline{\psi} \end{pmatrix} = \left[\begin{pmatrix} \psi\partial_x^{-1}\overline{\psi} & -\psi\partial_x^{-1}\psi \\ -\overline{\psi}\partial_x^{-1}\overline{\psi} & \overline{\psi}\partial_x^{-1}\psi \end{pmatrix} \begin{pmatrix} \frac{1}{2}\partial_x - 1 & 0 \\ 0 & \frac{1}{2}\partial_x + 1 \end{pmatrix}^{-1} \right]^{r-1} \begin{pmatrix} 2\psi \\ -2\overline{\psi} \end{pmatrix}. \tag{52}$$

Note the unusual form of the $r = 1$ flow. For $r = 2$ we set $\psi = \frac{1}{2}v_x e^{2x}$, $\overline{\psi} = \frac{1}{2}w_x e^{-2x}$, to get the flow

$$\partial_{t_2}\partial_x\begin{pmatrix} v \\ w \end{pmatrix} = vw\begin{pmatrix} v_x \\ -w_x \end{pmatrix}, \tag{53}$$

with conserved quantity $v_x w_x$ as noted in Ref. 7.

The forms (50) and (51) are not the most natural guess for the zero curvature formulation in this case; for example, we note that the ansatz does not permit choosing $B_1 = A$, which is why the $r = 1$ equation obtained above is nonstandard. We therefore consider the more general ansatz

$$A = \begin{pmatrix} 1 & \psi(x,t)/\sqrt{\lambda} \\ \overline{\psi}(x,t)/\sqrt{\lambda} & -1 \end{pmatrix}, \quad B_r = \begin{pmatrix} \alpha & \beta/\sqrt{\lambda} \\ \gamma/\sqrt{\lambda} & -\alpha \end{pmatrix}, \quad r = 1,2,3,\ldots, \tag{54}$$

where

$$\alpha=\lambda^{r-1}+\sum_{n=0}^{r-2}\alpha_n(x,t)\lambda^n,\quad \beta=\sum_{n=0}^{r-1}\beta_n(x,t)\lambda^n,\quad \gamma=\sum_{n=0}^{r-1}\gamma_n(x,t)\lambda^n. \tag{55}$$

Equations (50) and (51) are just this with the restriction $\beta_0=\gamma_0=0$. It turns out that the ansatz (54) and (55) is consistent provided $\beta_0=\psi\mathscr{M}(x,t)$, $\gamma_0=\bar{\psi}\mathscr{M}(x,t)$ for some function $\mathscr{M}(x,t)$ (there is a small further freedom; consistency only determines the α_n's up to a constant, which can be fixed by a homogeneity condition). In particular, we can now choose $B_1=A$ (for this $\beta_0=\psi$, $\gamma_0=\bar{\psi}$) to recover a standard $r=1$ flow equation. For the choice $\beta_0=\psi$, $\gamma_0=\bar{\psi}$ it is straightforward to find the $r=2$ flow equation:

$$\partial_{t_2}\begin{pmatrix} v \\ w \end{pmatrix}=\begin{pmatrix} v_{xx}+wvv_x \\ w_{xx}-wvw_x \end{pmatrix}. \tag{56}$$

Defining new coordinates x',t_2', via $\partial_{x'}=\partial_x$, $\partial_{t_2'}=\partial_{t_2}-\partial_x$, we see Eq. (56) is equivalent to Eq. (53). This reflects a simple general symmetry of the system (11): adding cA (c constant) to each B_r can be exactly cancelled by a change of coordinates from x,t_r to x',t_r' defined by

$$\partial_{x'}=\partial_x,\quad \partial_{t_r'}=\partial_{t_r}-c\partial_x. \tag{57}$$

Taking $\beta_0=\psi$, $\gamma_0=\overline{\psi}$ in the ansatz (54) and (55) is, taking into account the freedom to add a constant to α_0, equivalent to adding A to each of the B_r's of the ansatz (50) and (51), thus explaining the relationship of Eqs. (53) and (56). (Note this freedom we have just mentioned does not exist in B_1, so the two $r=1$ equations we have obtained above are *not* related by a change of coordinates of the form (57)!)

At this stage it may be appropriate to mention another general symmetry of Eq. (11), for the case where A,B_r are traceless 2×2 matrices. Writing

$$A=A_+E^++A_-E^-+A_0E^0,\quad B_r=B_{r+}E^++B_{r-}E^-+B_{r0}E^0, \tag{58}$$

where

$$E^+=\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix},\quad E^-=\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix},\quad E^0=\frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{59}$$

Eq. (11) is symmetric under

$$\begin{gathered} A_+\to\lambda^{\alpha}A_+,\quad A_-\to\lambda^{-\alpha}A_-,\quad A_0\to A_0, \\ B_{r+}\to\lambda^{\alpha}B_{r+},\quad B_{r-}\to\lambda^{-\alpha}B_{r-},\quad B_{r0}\to B_{r0}, \end{gathered} \tag{60}$$

for any constant α. In both the dual BKK and dual NLS hierarchies, the form of A has been obtained by scaling the (1,1) and (2,2) entries of A in the standard hierarchy by λ^{-1}, and the (1,2) and (2,1) entries by $\lambda^{-1/2}$. The symmetry (60) allows one to express the rescaling of the components of A necessary to pass from the standard to the dual hierarchies in a variety of equivalent ways. We will exploit this shortly.

(3) The dual Ito and generalized Ito hierarchies. For the dual of the Ito hierarchy we take

$$A=\begin{pmatrix} 0 & 1 \\ 1+q(x,t)/\lambda+p(x,t)/\lambda^2 & 0 \end{pmatrix},$$
$$B=\begin{pmatrix} -\frac{1}{2}\beta_x & \beta \\ \beta(1+p/\lambda+q/\lambda^2)-\frac{1}{2}\beta_{xx} & \frac{1}{2}\beta_x \end{pmatrix}, \quad r=1,3,5,\ldots, \tag{61}$$

with

$$\beta=\lambda^{(r-1)/2}+\sum_{n=0}^{(r-3)/2}\beta_n(x,t)\lambda^n. \tag{62}$$

The matrix A has been obtained from that of the standard Ito hierarchy by the same scaling used to obtain Fuchssteiner–Fokas–Camassa–Holm from KdV, that is, the (2,1) entry of A has been multiplied by λ^{-1}. For $r=3$ we have $\beta=\lambda+b(x,t)$, and we find that we can take $p=\frac{1}{2}b_{xx}-2b$, to obtain the flow

$$(\tfrac{1}{2}b_{xx}-2b)_{t_3}=q_x+b_{xx}b_x+\tfrac{1}{2}bb_{xxx}-6bb_x, \quad q_{t_3}=2qb_x+bq_x. \tag{63}$$

On substituting $q=w^2$ this becomes

$$(\tfrac{1}{2}b_{xx}-2b)_{t_3}=(w^2+\tfrac{1}{4}b_x^2+\tfrac{1}{2}bb_{xx}-3b^2)_x, \quad w_{t_3}=(wb)_x, \tag{64}$$

that is, we have recovered the lowest nontrivial flow in the dual BKK hierarchy, Eq. (48).

The relationship between the dual BKK hierarchy and the dual Ito hierarchy we have just seen is an instance of a Miura map ''born'' after dualization. Exploiting the symmetry (60) of Eq. (11), with $\alpha=\frac{1}{2}$, we observe that the BKK hierarchy has a zero curvature formulation with

$$A=\begin{pmatrix} 1+v(x,t)/\lambda & 1 \\ u(x,t)/\lambda & -1-v(x,t)/\lambda \end{pmatrix}. \tag{65}$$

Via gauge transformation with

$$\xi=\begin{pmatrix} 1 & 0 \\ 1+v(x,t)/\lambda & 1 \end{pmatrix} \tag{66}$$

this is brought to the form

$$A=\begin{pmatrix} 0 & 1 \\ 1+(u+2v+v_x)/\lambda+v^2/\lambda^2 & 0 \end{pmatrix}, \tag{67}$$

which is of the form used in Eq. (61), and therefore defines a Miura map from the dual BKK hierarchy to the dual Ito hierarchy. When written out in the variables we have used to write the lowest nontrivial flows of the dual BKK and dual Ito hierarchies, the Miura map becomes an equivalence.

Finally, we note that the generalized Ito hierarchies can be dualized in the same way as the KdV and Ito hierarchies, that is, we take

$$A=\begin{pmatrix} 0 & 1 \\ 1+S & 0 \end{pmatrix}, \quad S=\sum_{n=0}^{M} s_n(x,t)\lambda^{-n-1}, \tag{68}$$

with B_r $(r=1,3,5,...)$ specified by the requirement that its upper right-hand entry is a polynomial of degree $(r-1)/2$ in λ with leading order coefficient 1. Thus we have at least one infinite family of integrable hierarchies that affords dualization.

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Killing vectors in asymptotically flat space–times. I. Asymptotically translational Killing vectors and the rigid positive energy theorem

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We study Killing vector fields in asymptotically flat space–times. We prove the following result, implicitly assumed in the uniqueness theory of stationary black holes. If the conditions of the rigidity part of the positive energy theorem are met, then in such space–times there are no asymptotically null Killing vector fields, except if the initial data set can be embedded in Minkowski space–time. We also give a proof of the nonexistence of nonsingular (in an appropriate sense) asymptotically flat space–times that satisfy an energy condition and that have a null ADM four-momentum, under conditions weaker than previously considered. © *1996 American Institute of Physics.* [S0022-2488(96)01604-1]

I. INTRODUCTION

A prerequisite for an analysis of stationary black holes is the understanding of properties of Killing vector fields in asymptotically flat space–times. There exist various papers analyzing properties of Killing vector fields in asymptotically flat space–times.[1–4] These papers do not, however, seem to give answers to the questions asked here. Moreover, the asymptotic conditions here are considerably weaker than considered in those references. Consider an asymptotically flat partial Cauchy surface Σ in a space–time $(M,g_{\mu\nu})$ with a Killing vector field X^μ. In the case of a stationary black hole one is interested in situations where X^μ is time-like in the asymptotic regions. [Here we say that an asymptotically flat space–time $(M,g_{\mu\nu})$ with a Killing vector field X^μ is stationary if X^μ is time-like in the asymptotic regions of M.] A natural question to ask is, how does X^μ behave in the asymptotic regions? Now it is easily seen from the equations

$$\nabla_\mu \nabla_\nu X_\alpha = R^\lambda{}_{\mu\nu\alpha} X_\lambda \tag{1.1}$$

(which are a well-known consequence of the Killing equations) and from the asymptotic flatness conditions (cf. Propositions 2.1, Sec. II, for a precise description of the asymptotic conditions needed here) that there exist constants A^μ such that every Killing vector field X^μ that is time-like for $r \geqslant R$ for some R satisfies

$$\begin{aligned} X^\mu - A^\mu &\to_{r\to\infty} 0, \\ \eta_{\alpha\beta} A^\alpha A^\beta &\leqslant 0. \end{aligned} \tag{1.2}$$

Here $\eta_{\alpha\beta}$ is the Minkowski metric, and we use the signature $(-,+,+,+)$. It should be emphasized that the requirement of time-likeness of X^μ for large r does *not* exclude the possibility that $\eta_{\alpha\beta}A^\alpha A^\beta$ vanishes. Indeed, an explicit example of a metric (not satisfying any reasonable field

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equations) with an everywhere time-like Killing vector that is asymptotically null can be found in Ref. 5 (cf. the Remark preceding Theorem A.1, Appendix A of Ref. 5. (Let us point out that by a null vector we mean a nonzero vector of zero Lorentzian length.) Now in the uniqueness theory of black holes it is customary to assume that $A^\mu = \delta^\mu_0$ in an asymptotically flat coordinate system in which Σ is given by an equation $x^0 = 0$. If the orbits of the Killing vector field X^μ are complete (at least in the asymptotic region) and if A^μ is time-like, then Σ can be deformed (''boosted'') to a new partial Cauchy surface for which $A^\mu = \delta^\mu_0$ (in an appropriately redefined asymptotically flat coordinate system). If, however, X^μ is asymptotically null [by which we mean that the vector A^μ appearing in (1.2) is null], then no such deformation is possible and we are faced with the intriguing possibility of existence of stationary space–times in which the Killing vector cannot be reduced to a standard form, where the flat background metric is diagonal and the vector A^μ of (1.2) equals δ^μ_0. As has been argued in Ref. 6, the existence of such Killing vector fields does not seem to be compatible with the rigidity part of the positive energy theorems. Here we make the arguments of Ref. 6 precise and show the following (the reader is referred to Theorem 3.4 for a more precise formulation).

Theorem 1.1: *Let $(M,g_{\mu\nu})$ be a space–time with a Killing vector field that is asymptotically null along an (appropriately regular) asymptotically flat space-like hypersurface Σ. Then the ADM energy-momentum vector of Σ vanishes.*

To say more about space–times considered in Theorem 1.1, one can use the positive energy theorem. In Sec. IV below we prove the following.

Theorem 1.2 (''Time-like future-pointing four-momentum theorem''): *Under the conditions of Theorems 4.1 and 4.2 below, suppose that the initial data (Σ,g_{ij},K_{ij}) are not initial data for Minkowski space–time. Then the ADM energy-momentum vector p^μ of Σ satisfies*

$$p^0 > \sqrt{\sum_{i=1}^{3} (p^i)^2}.$$

(*Various variants of Theorem 1.2 are, of course, well known; cf. Sec. IV for a detailed discussion.*)

Theorem 1.1 can be used together with Theorem 1.2 to obtain the following.

Theorem 1.3: *Let $(M,g_{\mu\nu})$ be a maximal globally hyperbolic space–time with a Cauchy surface satisfying the requirements of Theorems 4.1 and 4.2. Let X^μ be a Killing vector field on M that is asymptotically null along an asymptotically flat Cauchy surface. Then X^μ is everywhere null and $(M,g_{\mu\nu})$ is the Minkowski space–time.*

Theorem 1.3 and the results of Ref. 7 [cf. also Ref. 6 (Theorem 1.7)] show that there is no loss of generality in assuming that $A^\mu = \delta^\mu_0$ in, say electrovacuum, maximal globally hyperbolic space-times with an appropriately regular asymptotically flat Cauchy surface. Let us mention that the results here settle in the positive Conjecture 1.8 of Ref. 6.

This paper is organized as follows. In Sec. II we discuss some general properties of Killing vector fields in asymptotically flat space–times. In order to minimize the number of assumptions, we adopt a $3+1$-dimensional point of view; the various advantages for doing that are explained at the beginning of Sec. II. The main result there is Proposition 2.1, which establishes the asymptotic behavior of Killing vectors along asymptotically flat space-like surfaces. In that section we also introduce the notion of *Killing development*, which turns out to be very useful in our analysis. In Sec. III we study the relationship between the ADM four-momentum and the asymptotic behavior of the Killing vector. The results there can be summarized as follows: If $X^\mu \to_{r\to\infty} A^\mu$ along an asymptotically flat space-like surface Σ, then the ADM four-momentum is proportional to A^μ. The proportionality constant is zero when A^μ is not time-like. Let us point out that some similar results can be found in Ref. 1. However, in that reference the possibility of asymptotically null Killing vector fields is not taken into consideration. Also, in Ref. 1, rather strong asymptotic conditions are imposed. In a sense most of the work here consists in showing that the asymptotic conditions needed to be able to obtain the desired conclusions can actually be derived from the decay

conditions on the matter sources and from the hypothesis of existence of Killing vector fields. In Sec. IV we prove a positive energy theorem with hypotheses and asymptotic conditions appropriate for our purposes. In Theorems 4.1 and 4.2 there are improvements of known results; cf. the beginning of Sec. IV for a more detailed discussion.

II. KILLING VECTORS AND SPACE-LIKE HYPERSURFACES

Consider a space–time $(M,g_{\mu\nu})$ with a Killing vector field X^μ,

$$\nabla_\mu X_\nu + \nabla_\nu X_\mu = 0, \tag{2.1}$$

where ∇_μ is the covariant derivative operator of the metric $g_{\mu\nu}$. Let Σ be a space-like hypersurface in M and suppose that on Σ the field of unit normals n^μ can be defined; this will be the case, e.g., if $(M,g_{\mu\nu})$ is time orientable. On Σ define a scalar field N and a vector field Y^i by the equations

$$N = -n_\mu X^\mu, \tag{2.2}$$

$$g_{ij} Y^i \, dx^j = i^*(g_{\mu\nu} X^\mu \, dx^\nu), \tag{2.3}$$

where i denotes the embedding of Σ into M. We use the symbol g_{ij} to denote the pull-back metric $i^* g_{\mu\nu}$. Equation (2.1) with $\mu = i$ and $\nu = j$ reads as

$$2NK_{ij} + \mathscr{L}_Y g_{ij} = 0, \tag{2.4}$$

where $\mathscr{L}$ denotes the Lie derivative and K_{ij} is the extrinsic curvature tensor of $i(\Sigma)$ in $(M,g_{\mu\nu})$, defined as the pull-back to Σ of $\nabla_\mu n_\nu$. (K_{ij} as defined here is $-K_{ij}$ as in Ref. 8; however, J^i as defined here coincides with J^i as defined there.) Set

$$\Sigma_{N>0} = \{p \in \Sigma : N \neq 0\}.$$

In a neighborhood of $\Sigma_{N>0}$ we can introduce a coordinate system (u,x^i) in which $X^\mu \partial_\mu = \partial_u$ and in which $\Sigma_{N>0}$ is given by the equation $u = 0$. The metric on this neighborhood takes the form

$$g_{\mu\nu} \, dx^\mu \, dx^\nu = -N^2 \, du^2 + g_{ij}(dx^i + Y^i \, du)(dx^j + Y^j \, du), \tag{2.5}$$

with some functions that do not depend upon u. Let $G_{\mu\nu}$ be the Einstein tensor of $g_{\mu\nu}$, that is, $G_{\mu\nu} = R_{\mu\nu} - (g^{\alpha\beta} R_{\alpha\beta}/2) g_{\mu\nu}$, where $R_{\mu\nu}$ is the Ricci tensor of $g_{\mu\nu}$. We have the 3+1 decomposition formulas (cf. e.g., Ref. 8),

$$2G_{\mu\nu} n^\mu n^\nu = {}^3R + K^2 - K^{ij} K_{ij}, \tag{2.6}$$

$$G_{i\mu} n^\mu = D_j(K^{ij} - g^{kl} K_{kl} g^{ij}), \tag{2.7}$$

$$\begin{aligned} G_{ij} - \tfrac{1}{2} g^{kl} G_{kl} g_{ij} = {}& {}^3R_{ij} + K K_{ij} - 2K_{ik} K^k, \\ & - N^{-1}(\mathscr{L}_Y K_{ij} + D_i \, D_j N) - \tfrac{1}{2} G_{\mu\nu} n^\mu n^\nu g_{ij}. \end{aligned} \tag{2.8}$$

Here g^{ij} is the tensor inverse to g_{ij}, $K = g^{kl} K_{kl}$, ${}^3R_{ij}$ is the Ricci tensor of the metric g_{ij}, and ${}^3R = g^{ij} \, {}^3R_{ij}$. All the above is, of course, well known; we have written it down in detail to fix the notation and to spell out the conditions needed for the definition of the fields N and Y^i. In particular, we wish to emphasize that we did not need to assume completeness of the orbits of X^μ, we did not need to assume that the orbits of X^μ intersect Σ only once, etc. It is, however, the case that those last properties are needed for several arguments, e.g., in the uniqueness theory of black holes (cf., e.g., Ref. 6). By way of example, consider a maximal globally hyperbolic space–time

$(M,g_{\mu\nu})$ with an asymptotically flat Cauchy surface with compact interior, with a metric satisfying the Einstein–Yang–Mills–Higgs equations, and with a Killing vector field X^μ. While one expects the orbits of X^μ to be complete (cf., e.g., Ref. 7 for an analysis in the vacuum case), no proof of such a result has been established so far. It is therefore of interest to establish various properties of space–times $(M,g_{\mu\nu})$ with Killing vectors with a minimal amount of global assumptions on M. As one is often interested in globally hyperbolic space–times it does not seem to be overly restrictive to assume the existence in M of a space-like hypersurface Σ satisfying the hypotheses spelled out at the beginning of this section. The construction above yields then a scalar field N and a vector field Y^i defined on Σ, such that Eqs. (2.4)–(2.8) hold. Consider then a set $(\Sigma,g_{ij},K_{ij},N,Y^i)$. We shall call the *Killing development of* $(\Sigma,g_{ij},K_{ij},N,Y^i)$ the space–time $(\hat{M},\hat{g}_{\mu\nu})$, where

$$\hat{M}=\mathbf{R}\times\Sigma_{N>0},$$

and where $\hat{g}_{\mu\nu}$ is given by the equation

$$\begin{aligned}&\hat{g}_{\mu\nu}\,dx^\mu\,dx^\nu=-\hat{N}^2\,du^2+\hat{g}_{ij}(dx^i+\hat{Y}^i\,du)(dx^j+\hat{Y}^j\,du),\\&\hat{N}(u,x^i)=N(x^i),\quad \hat{g}_{ij}(u,x^i)=g_{ij}(x^i),\quad \hat{Y}^i(u,x^i)=Y^i(x^i).\end{aligned}\tag{2.9}$$

Here the u coordinate runs over the $\mathbf{R}$ factor in $\mathbf{R}\times\Sigma_{N>0}$. Clearly the vector field $X^\mu\partial_\mu=\partial_u$ is a Killing vector, so that

$$\hat{\mathbf{\nabla}}_\mu X_\nu+\hat{\mathbf{\nabla}}_\nu X_\mu=0,\tag{2.10}$$

where $\hat{\mathbf{\nabla}}_\mu$ is the covariant derivative operator of the metric $\hat{g}_{\mu\nu}$. Note that

$$X_i|_{u=0}=Y_i,\quad \hat{N}|_{u=0}=N.\tag{2.11}$$

Consider the extrinsic curvature tensor $\hat{K}_{ij}$ of the slices $u=$const. In general, $\hat{K}_{ij}$ will have nothing to do with the tensor field K_{ij}. Suppose, however, that (2.4) holds. Equation (2.10), with $i=\mu$ and $\nu=j$; Eqs. (2.11) and (2.4) give, then, at $u=0$,

$$\hat{K}_{ij}=K_{ij}.\tag{2.12}$$

Since $\hat{K}_{ij}$ is u independent, it follows that this last relation holds throughout $\hat{M}$. One also notices that (2.12) will hold if and only if (2.4) holds.

Consider, next, the Einstein tensor $\hat{G}_{\mu\nu}$ of the metric $\hat{g}_{\mu\nu}$. It is given by the hatted equivalent of Eqs. (2.6)–(2.8). Given the set $(\Sigma,g_{ij},K_{ij},N,Y^i)$, one can define on $\Sigma_{N>0}$ a scalar field ρ, a vector field J^i, and a tensor field τ_{ij} via the equations

$$2\rho={}^3R+K^2-K^{ij}K_{ij},\tag{2.13}$$

$$J^i=D_j(-K^{ij}+Kg^{ij}),\tag{2.14}$$

$$\begin{aligned}\tau_{ij}-\tfrac{1}{2}g^{kl}\tau_{kl}g_{ij}={}&{}^3R_{ij}+KK_{ij}-2K_{ik}K^k{}_j\\&-N^{-1}(\mathscr{L}_Y K_{ij}+D_i\,D_jN)-(\rho/2)g_{ij}.\end{aligned}\tag{2.15}$$

If Eq. (2.4) holds, it follows from (2.11)–(2.12) that we will have

$$\hat{G}_{\mu\nu}\hat{n}^\mu\hat{n}^\nu(u,x^l)=\rho(x^l),\quad \hat{G}_{i\nu}\hat{n}^\nu(u,x^l)=-J_i(x^l),\quad G_{ij}(u,x^l)=\tau_{ij}(x^l),\tag{2.16}$$

where $\hat{n}_\mu$ is the unit normal to the slices $u=$const.

It is of interest to consider the case of covariantly constant Killing vector fields. In that case on a hypersurface Σ as at the beginning of this section, we will have

$$NK_{ij}+D_iY_j=0, \tag{2.17}$$

$$K_{ij}Y^j+D_iN=0. \tag{2.18}$$

Let us show that if (2.17)–(2.18) hold, then the vector field $X^\mu\partial_\mu=\partial_\mu$ on the Killing development $(\hat{M},\hat{g}_{\mu\nu})$ of $(\Sigma,g_{ij},K_{ij},N,Y^i)$ will be covariantly constant. To see that, note that Eqs. (2.17), (2.11), and (2.12) imply

$$\hat{\nabla}_iX_j=0,$$

at $u=0$, hence, throughout $\hat{M}$. Equation (2.18) similarly gives

$$\hat{\nabla}_iX_0=0.$$

As X^μ satisfies (2.10), the equations $\hat{\nabla}_\mu X_\nu=0$ readily follow.

When considering space–times with symmetries, it is essential to have precise information on the behavior of Killing vector fields in the asymptotic regions. The following is a straightforward consequence of Eqs. (2.13) and (2.15) (cf. also Ref. 9, Theorem 3.3 and Proposition 3.2). The notation O_k is defined in Appendix A. An outline of the proof is given in Appendix C.

Proposition 2.1: Let $R>0$ and let (g_{ij},K_{ij}) be initial data on $\Sigma_R\equiv\mathbf{R}^3\backslash B(R)$, satisfying

$$g_{ij}-\delta_{ij}=O_k(r^{-\alpha}),\quad K_{ij}=O_{k-1}(r^{-1-\alpha}), \tag{2.19}$$

with some $k>1$ and some $0<\alpha<1$. Let N be a C^2 scalar field and Y^i a C^2 vector field on Σ_R, such that Eqs. (2.4), (2.13), and the equation

$$N(\tau_{ij}-\tfrac{1}{2}g^{kl}\tau_{kl}g_{ij})=N({}^3R_{ij}+KK_{ij}-2K_{ik}K^k{}_j)-\mathcal{L}_YK_{ij}-D_i\,D_jN-N(\rho/2)g_{ij},$$

hold, with some ρ and τ_{ij} satisfying

$$|\rho|+|\tau_{ij}|\leqslant C(1+r)^{-2-\alpha}. \tag{2.20}$$

Then there exists numbers $\Lambda_{\mu\nu}=\Lambda_{[\mu\nu]}$, such that we have

$$Y^i-\Lambda_{ij}x^j=O_k(r^{1-\alpha}),\quad N+\Lambda_{0i}x^i=O_k(r^{1-\alpha}). \tag{2.21}$$

If $\Lambda_{\mu\nu}=0$, then there exist numbers A^μ, such that we have

$$Y^i-A^i=O_k(r^{-\alpha}),\quad N-A^0=O_k(r^{-\alpha}). \tag{2.22}$$

If $\Lambda_{\mu\nu}=A^\mu=0$, then $Y^i\equiv N\equiv 0$.

Let us remark that if $\alpha=1$, then Proposition 2.1 holds with the function $r^{1-\alpha}$ in the right-hand side of Eq. (2.21) replaced by $1+|\log r|$; similarly in (2.22), $r^{-\alpha}$ has to be replaced by $r^{-1}(1+|\log r|)$.

A Killing vector field for which $\Lambda_{\mu\nu}=0$ will be called *asymptotically translational*.

For further use let us mention the following: Consider (g_{ij},K_{ij}), such that (2.19) holds, and suppose that (N,Y^i) satisfy (2.22) with some $A^0\neq 0$. Suppose finally that (2.4) is weakened to

$$2NK_{ij}+\mathcal{L}_Yg_{ij}=O_{k-1}(r^{-\beta}), \tag{2.23}$$

with some $\beta\geqslant 1$. In that case (2.16) will be replaced by

$$\hat{G}_{\mu\nu}\hat{n}^{\mu}\hat{n}^{\nu}-\rho=O_{k-1}(r^{-\min(1+\alpha,\beta)-\beta}),\quad \hat{G}_{i\nu}\hat{n}^{\nu}+J_i=O_{k-2}(r^{-\beta-1}),$$
$$\hat{G}_{ij}-\tau_{ij}=O_{k-2}(r^{-\beta-1}). \tag{2.24}$$

III. ADM FOUR-MOMENTUM IN SPACE–TIMES WITH ASYMPTOTICALLY TRANSLATIONAL KILLING VECTORS

In this section we address the following question: Consider a space–time with an asymptotically flat space-like surface Σ, and with a translational Killing vector field X^{μ}, that is, there exist constants A^{μ} such that $X^{\mu}\to_{r\to\infty}A^{\mu}$ along Σ. Then, is it true that

(1) If $A^{\mu}A_{\mu}\geqslant 0$, then the ADM four-momentum p^{μ} vanishes.

(2) If $A^{\mu}A_{\mu}<0$, then p^{μ} is proportional to A^{μ}.

We shall show that this is indeed the case, using the three-dimensional framework discussed in Sec. II. Proposition 2.1 in that section justifies our fall-off conditions on the fields N and Y^i. The results here are actually slightly more general than stated above, in that we allow for fields that satisfy the relevant Killing equations up to terms that decay at an appropriate rate; cf. below for the precise conditions.

Proposition 3.1: Let $R>0$ and let (g_{ij},K_{ij}) be initial data on $\Sigma_R\equiv\mathbf{R}^3\backslash B(R)$, satisfying

$$g_{ij}-\delta_{ij}=O_2(r^{-\alpha}),\quad K_{ij}=O_1(r^{-1-\alpha}),\quad \alpha>\tfrac{1}{2}, \tag{3.1}$$

$$J^i=O(r^{-3-\epsilon}),\quad \rho=O(r^{-3-\epsilon}),\quad \epsilon>0. \tag{3.2}$$

Let N be a C^1 scalar field and Y^i a C^1 vector field on Σ_R, such that

$$N-A^0=O_1(r^{-\alpha}),\quad Y^i\to_{r\to\infty}A^i, \tag{3.3}$$

for some set of constants $(A^{\mu})\not\equiv 0$. Suppose further that

$$2NK_{ij}+\mathscr{L}_Y g_{ij}=O_1(r^{-2-\epsilon}). \tag{3.4}$$

Let p^{μ} be the ADM four-momentum of Σ_R. Then

(1) If $A^0=0$, then $p^0=0$.

(2) If $A^0\neq 0$, then p^{μ} is proportional to A^{μ}.

Remark: The pointwise decay estimates assumed above can be weakened to weighted Sobolev spaces conditions. To avoid a tedious discussion of technicalities we shall, however, not consider such fields here.

Proof: Without loss of generality we may assume that both α and ϵ are strictly smaller than 1. Equation (3.3) and a simple analysis of Eq. (3.4) (cf., e.g., the proof of Proposition 2.1, Appendix C) show that

$$Y^i-A^i=O_2(r^{-\alpha}). \tag{3.5}$$

By our asymptotic conditions, Eq. (3.4) can be rewritten as

$$g_{ij,k}A^k+Y^i{}_{,j}+Y^j{}_{,i}=-2A^0K_{ij}+O_1(r^{-2-\epsilon}), \tag{3.6}$$

and we have redefined ϵ to be $\min(\epsilon,2\alpha-1)>0$. The momentum-constraint equation reads as

$$\partial_i K_{ij}=\partial_j K+O(r^{-3-\epsilon}), \tag{3.7}$$

where $K=g^{ij}K_{ij}$. Taking the divergence of (3.6) and using (3.7) gives

$$g_{ij,kj}A^k+\Delta_{\delta}Y^i+\partial_i(Y^j{}_{,j})=-2A^0K_{,i}+O(r^{-3-\epsilon}). \tag{3.8}$$

Here $\Delta_\delta = \Sigma_i \partial_i \partial_i$. Contracting i with j in (3.6) allows us to eliminate $\partial_j Y^j$ in (3.8) in terms of $K_{,i}$, so that (3.8) leads to

$$\Delta_\delta Y^i = -A^0 K_{,i} - (g_{ij,j} - \tfrac{1}{2} g_{jj,i})_{,k} A^{,k} + O(r^{-3-\epsilon}).$$

In what follows we shall freely make use of properties of harmonic functions on Σ_R that were established in, e.g., (Refs. 10–12). Increasing R if necessary we may choose harmonic coordinates on Σ_R,

$$\partial_i (g^{ij} \sqrt{\det g}) = 0,$$

with

$$g_{ij} - \delta_{ij} = O_1(r^{-\alpha}).$$

[There arises a slight difficulty here, related to the fact that the metric might not satisfy the conditions (3.1) in harmonic coordinates due to a loss of classical differentiability. All the details of the proof as written here can be justified if a Hölder differentiability index λ is added in Eqs. (3.1)–(3.2). We wish to stress that the statement of our result is correct as stated. This can be verified by keeping track of weighted Sobolev differentiability of various error terms that arise in our equations, making use of the estimates of Ref. 11. In order to make the argument more transparent we have chosen to present our proof without the introduction of weighted Sobolev spaces.]

If $A^0 = 0$, define φ to be identically zero; otherwise let $\varphi = O_1(r^{1-\alpha})$ be a solution of

$$\Delta_\delta \varphi = -A^0 K. \tag{3.9}$$

Setting $Z^i = Y^i - A^i - \varphi^{,i}$, one is led to

$$\Delta_\delta Z^i = O(r^{-3-\epsilon}),$$

so that there exist numbers $\alpha^i \in \mathbf{R}$ such that

$$Z^i = \frac{\alpha^i}{r} + O_1(r^{-1-\epsilon}).$$

A contraction over i and j in (3.6) gives

$$Z^i{}_{,i} = -\frac{\alpha^i x^i}{r^3} + O(r^{-2-\epsilon}) = -\frac{1}{2} g_{ii,k} A^k + O(r^{-2-\epsilon}). \tag{3.10}$$

The scalar constraint equation in harmonic coordinates gives

$$\Delta_\delta g_{ii} = O(r^{-3-\epsilon}) \Rightarrow g_{ii} = 3 + \frac{\beta}{r} + O_1(r^{-1-\epsilon}), \tag{3.11}$$

for some constant β. Equation (3.11) inserted in the formula for the ADM mass yields

$$m = \frac{1}{16\pi} \int_{S_\infty} (g_{ij,j} - g_{jj,i})\, dS_i = -\frac{1}{32\pi} \int g_{jj,i}\, dS_i = \frac{\beta}{8}. \tag{3.12}$$

Inserting this in (3.10), one is led to

$$\alpha^i = -4mA^i,$$

so that one finally obtains

$$Y^i = A^i\left(1-\frac{4m}{r}\right)+\varphi_{,i}+O_1(r^{-1-\epsilon}). \tag{3.13}$$

Suppose first that $A^0=0$. In this case we necessarily have $A^i\not\equiv 0$, and rescaling $X^\mu\partial_\mu$ if necessary, we can choose coordinates so that $A^i=\delta^i_z$. Equation (3.6) now reads as

$$g_{AB,z}=O(r^{-2-\epsilon}), \tag{3.14}$$

$$(g_{zz}+2Y^z)_{,z}=O(r^{-2-\epsilon}), \tag{3.15}$$

$$g_{zA,z}=\left(\frac{4m}{r}\right)_{,A}+O(r^{-2-\epsilon}). \tag{3.16}$$

Let $\rho^2=x^2+y^2$. For $\rho\geqslant R$, Eq. (3.16) gives

$$0=x^A\int_{-\infty}^{\infty} g_{zA,z}\,dz=-4m\int_{-\infty}^{\infty}\frac{dz}{(1+z^2)^{3/2}}+\int_{-\infty}^{\infty}O(r^{-2-\epsilon})dz.$$

To estimate the second integral, it is convenient to consider separately the integrals $\int_{-\infty}^{-\rho}$, $\int_{-\rho}^{\rho}$, and $\int_{\rho}^{\infty}$. Elementary estimates then show that this integral is $O(\rho^{-\epsilon})$; passing to the limit $\rho\to\infty$, one subsequently obtains $m=0$, which establishes point 1. To establish point 2, suppose that $A^0\neq 0$. After a rescaling of X^μ if necessary, we can, without loss of generality, assume that $A^0=1$. Eq. (3.6) thus gives

$$K_{ij}=-\tfrac{1}{2}\{Y^i{}_{,j}+Y^j{}_{,i}+g_{ij,k}A^k\}+O_1(r^{-1-2\alpha})=-\tfrac{1}{2}\{Z^i{}_{,j}+Z^j{}_{,i}+2\varphi_{,ij}+g_{ij,k}A^k\}+O_1(r^{-1-2\alpha}). \tag{3.17}$$

Consider the ADM momentum p_i [the unusual sign in Eq. (3.18) is due to our convention on K_{ij}; cf. the remark in parentheses after Eq. (2.4)]:

$$p_i=-\frac{1}{8\pi}\int_{S_\infty}(K_i{}^j-K\delta_i{}^j)dS_j. \tag{3.18}$$

After insertion of (3.17) in (3.18), one finds

$$p_i=\frac{1}{16\pi}\int_{S_\infty}(Z^i{}_{,j}+Z^j{}_{,i}+A_j g_{ik,k})dS_j. \tag{3.19}$$

Here the φ contribution drops out because of the following calculation:

$$\int_{S_\infty}(\Delta_\delta\varphi\,\delta_{ij}-\partial_i\,\partial_j\varphi)dS_j=\int_{S_\infty}(\partial_k\varphi\;\delta_{ij}-\partial_j\varphi\;\delta_{ki})_{,k}\,dS_j=0. \tag{3.20}$$

We have also used the identities

$$g_{ij,k}A^k=(g_{ij}A^k-g_{ik}A^j)_k+g_{ik,k}A^j,$$

and integration by parts to rearrange the $g_{ij,k}A^k$ terms. Inserting (3.13) in (3.19) and using the harmonic coordinates condition, one obtains

$$p_i=mA_i,$$

which had to be established. □

Point 1 of Proposition 3.1 suggests strongly that the ADM four-momentum must vanish when A^μ is space-like. We can show that if we assume some further asymptotic conditions on the fields under consideration. A similar result has been established previously in Ref. 1 under rather stronger asymptotic and global conditions.

Proposition 3.2: Under the hypotheses of Proposition 3.1, suppose further that N is C^2 and that

$$N\tau_{ij}=O(r^{-3-\epsilon}). \tag{3.21}$$

If

$$(A^0)^2<\sum_i A^iA^i, \tag{3.22}$$

then p^μ vanishes.

Proof: It follows from Eqs. (3.3), (3.4), and (3.21) that

$$Y^i-A^i=O_2(r^{-\alpha}),\quad N-A^0=O_2(r^{-\alpha}). \tag{3.23}$$

Consider first the case $A^0=0$; by Proposition 3.1 we have $p^0=0$. Let ψ be any function on Σ_R such that $\psi_{,z}=N$. Equation (3.21) gives

$$(K_{ij}-\partial_i\,\partial_j\psi)_{,z}=O(r^{-3-\epsilon}),$$

so that by z integration one obtains

$$K_{ij}-\partial_i\,\partial_j\psi=O(r^{-2-\epsilon}).$$

Inserting this in Eq. (3.18), one obtains

$$\begin{aligned} p_i&=-\frac{1}{8\pi}\int_{S_\infty}(\Delta_\delta\psi\delta_{ij}-\partial_i\,\partial_j\psi)dS_j\\ &=-\frac{1}{8\pi}\int_{S_\infty}(\partial_k\psi\delta_{ij}-\partial_j\psi\,\delta_{ki})_{,k}\,dS_j\\ &=0. \end{aligned} \tag{3.24}$$

Consider, next, the case $A^0\neq 0$; let $(\hat{M},\hat{g}_{\mu\nu})$ be the Killing development of $(\Sigma_R,g_{ij},K_{ij},N,Y^i)$ as constructed in Sec. II. As discussed in the paragraph preceding Eq. (2.24), Eqs. (3.2) and (3.21) imply that the Einstein tensor $\hat{G}_{\mu\nu}$ of $\hat{g}_{\mu\nu}$ will satisfy the fall-off condition

$$\hat{G}_{\mu\nu}=O(r^{-3-\epsilon}). \tag{3.25}$$

Let $\Lambda^\mu{}_\nu$ be the matrix of a Lorentz transformation such that $\Lambda^0{}_\nu A^\nu=0$. Further, let $\Lambda\Sigma$ be the image under $\Lambda^\mu{}_\nu$ of $\Sigma_R\cap\hat{M}$ in $\hat{M}$. On $\Lambda\Sigma$ the Killing vector X^μ satisfies $X^0\to_{r\to\infty}0$. Equation (3.25) shows that we can apply the previous analysis to conclude that the ADM four-momentum of $\Lambda\Sigma$ vanishes. Moreover, the decay condition (3.25) ensures (cf. e.g., Ref. 13) that p^μ transforms as a Lorentz vector under Lorentz transformations of hypersurfaces, so that the ADM four-momentum of Σ_R vanishes as well.

It is of interest to consider Killing vector fields that are covariantly constant. As discussed in Sec. II, in such a case Eqs. (3.26)–(3.27) below will hold (with 0 on the right-hand sides). We have the following result, which does not cover asymptotically null Killing vectors.

Proposition 3.3: Under the hypotheses of Proposition 3.1, assume, moreover, that N is C^2; that Eq. (3.21) holds and that

$$NK_{ij}+D_iY_j=O_1(r^{-2-\epsilon}), \tag{3.26}$$

$$K_{ij}Y^j+D_iN=O_1(r^{-2-\epsilon}), \quad A^\mu A_\mu\neq 0. \tag{3.27}$$

Then the ADM four-momentum p^μ vanishes.

Proof: Let $(\hat{M},\hat{g}_{\mu\nu})$ be the Killing development of $(\Sigma_R,g_{ij},K_{ij},N,Y^i)$, as constructed in Sec. II. From what is said in that section [cf. the discussion following Eqs. (2.17)–(2.18)], it follows that $X^\mu\partial_\mu=\partial_u$ will satisfy

$$\hat{\nabla}_\mu X_\nu=O_1(r^{-2-\epsilon}). \tag{3.28}$$

As is well known,[14,1] we have

$$p_\mu A^\mu=\lim_{r\to\infty}\frac{1}{8\pi}\int \hat{\nabla}^{[\mu}X^{\nu]}\,dS_{\mu\nu} \tag{3.29}$$

(cf., e.g., Ref. 13 for a proof under the present asymptotic conditions). By (3.28) we have $p_\mu A^\mu=0$. Now, by Proposition 3.1, p_μ is proportional to A_μ, so if $A^\mu A_\mu\neq 0$ the result follows.□

The main result of this section addresses the case of asymptotically null Killing vectors. Unfortunately the proof below requires more asymptotic regularity than one would wish to have. It would be of some interest to find out whether or not the result below is sharp, in the sense that decay conditions on three derivatives of the metric and two derivatives of the extrinsic curvature are necessary.

Theorem 3.4: *Let $R>0$ and let (g_{ij},K_{ij}) be initial data on $\Sigma_R=\mathbf{R}^3\backslash B(R)$, satisfying*

$$g_{ij}-\delta_{ij}=O_{3+\lambda}(r^{-\alpha}), \quad K_{ij}=O_{2+\lambda}(r^{-1-\alpha}), \tag{3.30}$$

$$J^i=O_{1+\lambda}(r^{-3-\epsilon}), \quad \rho=O_{1+\lambda}(r^{-3-\epsilon}),$$
$$\alpha>\tfrac{1}{2}, \quad \epsilon>0, \quad 0<\lambda<1. \tag{3.31}$$

Let N be a scalar field and Y^i a vector field on Σ_R such that

$$N\to_{r\to\infty}A^0, \quad Y^i\to_{r\to\infty}A^i, \quad A^\mu A_\mu=0,$$

for some constants $A^\mu\not\equiv 0$. Suppose further that

$$2NK_{ij}+\mathscr{L}_Y g_{ij}=O_{3+\lambda}(r^{-2-\epsilon}), \tag{3.32}$$

$$\tau_{ij}=O_{1+\lambda}(r^{-3-\epsilon}), \tag{3.33}$$

where τ_{ij} is defined by the equation

$$N(\tau_{ij}-\tfrac{1}{2}g^{kl}\tau_{kl}g_{ij})=N({}^3R_{ij}+KK_{ij}-2K_{ik}K^k{}_j)-\mathscr{L}_Y K_{ij}+D_iD_jN-(\rho/2)Ng_{ij}. \tag{3.34}$$

Then the ADM four-momentum of Σ_R vanishes.

Remark: There is little doubt that the result is still true with $\lambda=0$. To prove that one would however, need to extend the weighted-Sobolev estimates of Ref. 11 to the case dim $M=2$, a task that lies beyond the scope of this paper.

Proof: Arguments similar to the proof of Proposition 2.1, Appendix C, show that

$$N-A^0=O_{3+\lambda}(r^{-\alpha}),\quad Y^i-A^i=O_{3+\lambda}(r^{-\alpha}).$$

Rescaling A^μ if necessary, we can choose the coordinate system so that $A^0=1$, $A^i=\delta^i_z$. Replacing ϵ by any number smaller than one if necessary, we can assume that $\epsilon<1$ and $\epsilon\leqslant 2\alpha-1$. Taking the trace of Eq. (3.33) and using the scalar constraint equation, we find

$$\Delta_\delta N+K_{,z}=O_{1+\lambda}(r^{-3-\epsilon}).$$

Here, as before, $\Delta_\delta=\partial_x^2+\partial_y^2+\partial_z^2$. Let φ be as in Eq. (3.9), we obtain

$$\Delta_\delta(N-\varphi_{,z})=O_{1+\lambda}(r^{-3-\epsilon});$$

hence there exists a constant D such that

$$N-\varphi_{,z}=1+\frac{D}{r}+O_{3+\lambda}(r^{-1-\epsilon}). \tag{3.35}$$

In harmonic coordinates, Eqs. (3.4), (3.13), (3.33), and (3.35) give

$$-\tfrac{1}{2}\Delta_2 g_{ij}=\chi_{ij}+\Psi_{ij}, \tag{3.36}$$

$$\chi_{ij}=-2m\partial_z\left[\delta^j_z\partial_i\frac{1}{r}+\delta^i_z\partial_j\frac{1}{r}\right]+\partial_i\partial_j\frac{D}{r}, \tag{3.37}$$

$$\Psi_{ij}=O_{1+\lambda}(r^{-3-\epsilon}). \tag{3.38}$$

Here $\Delta_2=\partial_x^2+\partial_y^2$. In what follows the indices A, B, etc. take values in the set $\{1,2\}$. Consider the equation (3.36) with $i=z$, $j=A$. We have

$$\Delta_2 g_{zA}=(8m-2D)\partial_A\partial_z\frac{1}{r}+O(r^{-3-\epsilon}). \tag{3.39}$$

It follows from Refs. 12 and 10 that for every fixed value of z the functions g_{zA} have the asymptotic expansion,

$$g_{zA}=C_{AB}(z)\partial_B\ln\rho+O_{(1)}(\rho^{-1-\epsilon}\ln\rho). \tag{3.40}$$

Here $\rho^2=x^2+y^2$, the functions $C_{AB}(z)$ are functions of z only, and we write

$$f=O_{(1)}(\rho^{-\alpha}\ln^\beta\rho),\quad \text{if } |f|+\rho|\partial_A f|\leqslant C(1+\rho)^{-\alpha}[1+\ln(1+\rho)]^\beta, \tag{3.41}$$

for some constant C that may depend upon z. Let us define $S(\rho,a)$ to be a circle of radius ρ centered at $x=y=0$ lying in the plane $z=a$. Equation (3.40) shows that for any fixed value of z the limits

$$\lim_{\rho\to\infty}\int_{S(\rho,z)} g_{zB}\,dx^C,\quad \lim_{\rho\to\infty}\int_{S(\rho,z)} x^D\,\partial_A g_{zB}\,dx^C,$$

exist. It also follows from our asymptotic conditions on g_{ij}, Eq. (3.30), that these limits are z independent. Set

$$\Omega=\lim_{\rho\to\infty}\int_{S(\rho,z)}(x^A\,\partial_C g_{zA}-g_{zC})dx^C. \tag{3.42}$$

For $|z|>R$ by the Stokes theorem we have

$$\Omega=\int_{\mathbf{R}^2} x^A\ \Delta_2 g_{Az}=(1)+(2),$$

$$(1)=(8m-2D)\int_{\mathbf{R}^2} x^A\ \partial_z\partial_A\ \frac{1}{r},$$

$$(2)=\int_{\mathbf{R}^2} x^A\Psi_{Az}$$

with Ψ_{Az} as in (3.36). The first integral is easily calculated and equals

$$8\pi(4m-D)\operatorname{sgn} z, \tag{3.43}$$

where $\operatorname{sgn} z$ denotes the sign of z. To estimate the second integral, it is convenient to split the region of integration into the sets $\rho\leqslant|z|$ and $\rho\geqslant|z|$. One then finds

$$|(2)|\leqslant C|z|^{-\epsilon}, \quad \text{for } |z|>R, \tag{3.44}$$

with a constant C that does *not* depend upon z. Equations (3.43)–(3.44) are consistent with $\partial\Omega/\partial z=0$ if and only if

$$4m=D. \tag{3.45}$$

Consider now Eq. (3.36) with $i=A$, $j=B$. Differentiating this equation with respect to z, one obtains

$$\Delta_2\ \frac{\partial g_{AB}}{\partial z}=-2D\partial_A\ \partial_B\partial_Z\ \frac{1}{r}+O(r^{-4-\epsilon}). \tag{3.46}$$

By hypothesis we have $\partial g_{ij}/\partial z=O(r^{-1-\epsilon})$, and the estimates of Refs. 12 or 10 show that there exist functions $D_{ABCD}(z)$ such that for any fixed value of z, we have

$$\frac{\partial g_{AB}}{\partial z}=D_{ABCD}\ \partial_C\partial_D\ \ln\rho+O_{(1)}(\rho^{-2-\epsilon}\ \ln\rho). \tag{3.47}$$

Let us set

$$\Omega'=\lim_{\rho\to\infty}\int_{S(\rho,z)}(2x^Ax^B\partial_C\ \partial_z g_{AB}-x^Ax^A\partial_C\ \partial_z g_{BB}+2x_C\ \partial_z g_{AB}-4x^B\ \partial_z g_{CB})dx^C.$$

(3.47) shows that Ω' is well defined, while (3.30) implies that Ω' is z independent. For $|z|>R$ we again use the Stokes theorem to obtain

$$\Omega'=\int_{\mathbf{R}^2}(2x^Ax^B\Delta_2\ \partial_z g_{AB}-x^Ax^A\Delta_2\ \partial_z g_{BB}).$$

A calculation as above leads to

$$\Omega'=16\pi D\ \operatorname{sgn} z+O(|z|^{-\epsilon}), \quad |z|>R.$$

Hence $D=m=0$ [cf. Eq. (3.45)], which together with Proposition 3.1, establishes our claims. □

IV. A POSITIVE ENERGY THEOREM

In this section we shall prove a ''future-pointing-time-like-or-vanishing-energy-momentum theorem,'' under conditions weaker than previously considered. The main two issues we wish to address are (1) the impossibility of a null ADM four-momentum and (2) a result that invokes hypotheses concerning only the fields g_{ij} and K_{ij}.

Let us start with an example of a metric with ''null ADM four-momentum.'' Recall that in Ref. 15, Aichelburg and Sexl consider a sequence of Schwarzschild space–times with energy-momentum vector $(m,0,0,0)$. After applying a ''boost'' transformation to the Schwarzschild space–time, one obtains an energy-momentum vector $(\gamma m,\gamma v m,0,0)$. Then one takes the limit $v\to 1$, keeping γm equal to a fixed constant p. The resulting space–time has a distributional metric, and it is not clear if it is asymptotically flat. Nevertheless, it seems reasonable to assign to the Aichelburg–Sexl solutions a null energy-momentum vector $(p,p,0,0)$. So, in this sense, there exist space–times with a null energy-momentum vector.

The Aichelburg–Sexl metrics are plane-fronted waves, and it is of interest to inquire whether any asymptotically flat plane-fronted wave metrics exist. Recall that the usual approach in defining asymptotic flatness is to introduce coordinate systems on $(\mathbf{R}^3\backslash B(R))$. Thus, consider a plane-fronted wave metric on $\mathbf{R}\times(\mathbf{R}^3\backslash B(R))$,

$$ds^2=-2\,du\,dz+\alpha\,dz^2+dx^2+dy^2. \tag{4.1}$$

As is well known (cf., e.g., Refs. 16, 17), the metric (4.1) is vacuum if and only if $\alpha=\alpha(x,y,z)$, with

$$(\partial_x^2+\partial_y^2)\alpha=0. \tag{4.2}$$

Then, let α be any solution of (4.2) such that $\alpha=1$ for $|z|\geqslant R$, but $\alpha\not\equiv 1$. Such solutions are easily found, and for any finite l we can choose α to satisfy

$$0\leqslant k\leqslant l,\quad |\partial_{A_1}\cdots\partial_{A_k}(\alpha-1)|\leqslant Cr^{-k-1}.$$

An example is given by the function

$$\alpha=1+\phi(z)C^{A_1\cdots A_l}\partial_{A_1}\cdots\partial_{A_l}\ln\rho, \tag{4.3}$$

where $\phi(z)$ is a smooth compactly supported function and $C^{A_1\cdots A_l}$ is a totally symmetric tensor with constant coefficients. We have the following.

(1) If $l=1$, the metric (4.1) with α given by (4.3) will not satisfy the fall-off requirements of the positive energy theorem; cf. Theorem 4.1 below, because the z derivatives of the metric do not vanish fast enough as r tends to infinity. This fall-off of the metric is not known to be sufficient for a well-defined notion of ADM mass (compare Refs. 11, 13, and 18). However, one can calculate the ADM integral (3.12) in the coordinate system (x,y,z) as above and find that this integral vanishes.

(2) For all $l\geqslant 2$ the hypersurfaces $u=$const will have a well-defined vanishing ADM mass. This does, however, not follow from Theorem 3.4 unless $l\geqslant 3$. (Strictly speaking, we would need to have $l\geqslant 4$ to be able to apply Theorem 3.4 as is; cf., however, the remark following that theorem. When we know *a priori* that the metric is a plane-fronted wave, we can use independent arguments to get rid of the Hölder differentiability index λ in Theorem 3.4; no details will be given.)

Nevertheless, this example shows that nontrivial, vacuum, asymptotically flat plane-fronted waves exist (with $p^\mu=0$), as long as no further global conditions are imposed.

With those examples in mind, let us briefly recall what is known about the nonexistence of appropriately regular space–times with null energy momentum. In Ref. 19 an argument was given

to support the expectation that the ADM momentum cannot be null for vacuum or electrovacuum space–times, the general case being left open. In Ref. 20 this case has been excluded under rather strong global hypotheses on the space–time and under stringent asymptotic conditions. In Ref. 21 a proof was given, assuming only hypotheses on the initial data. However, the proof there is rather more complicated than ours. Moreover, the asymptotic conditions of Ref. 21 are more restrictive than ours.

We wish next to emphasize the following issue: The statement that the ADM mass m is non-negative requires only the inequality $\rho \geqslant \sqrt{J_i J^i}$, where ρ and J^i are quantities that can be purely defined in terms of the fields g_{ij} and K_{ij}; cf. Eqs. (4.5)–(4.6) below. Now the published Witten-type proofs that the vanishing of m implies, loosely speaking, flatness of the resulting space–time, involve the full dominant energy condition ($T_{\mu\nu}X^\mu Y^\nu \geqslant 0$ for all time-like consistently time-oriented vectors X^μ and Y^ν) (cf., e.g., Ref. 22). Recall that the corresponding statement of Schoen and Yau[23] does not involve any supplementary field $T_{\mu\nu}$. (Their proof, however, requires rather strong asymptotic conditions on the fields. Moreover, Schoen and Yau require the trace of the extrinsic curvature to fall-off at least as r^{-3}. In general, this can be justified by applying a ''logarithmic supertranslation'' in time to the initial data surface, and requires the supplementary hypothesis that the associated space–time is large enough. Finally, to guarantee that all the required hypotheses hold on the deformed hypersurface, one needs again the full dominant energy condition.) Similarly, both the proof in Ref. 20 and the proof in Ref. 21 that exclude a null ADM energy momentum assume the full dominant energy condition. A result involving only conditions on g_{ij} and K_{ij} seems to be much more satisfactory from a conceptual point of view, and it seems reasonable to expect that the desired conclusion could be obtained in the Witten-type setting without imposing conditions on fields other than g_{ij} and K_{ij}. We show below that this is indeed the case.

Before passing to the statement of our results, in addition to the papers already quoted, let us mention the papers,[11,24–35] where proofs or arguments relevant to the positive energy theorem have been given. The review paper[36] contains some further references.

We have the following.

Theorem 4.1 [(Rigid) positive energy theorem]: *Consider a data set* (Σ, g_{ij}, K_{ij}), *with* Σ *of the form* $\Sigma = \Sigma_{int} \cup_{i=1}^{I} \Sigma_i$, *for some* $I < \infty$. *Here we assume that* Σ_{int} *is compact, and that each of the ends* Σ_i *is diffeomorphic to* $\mathbf{R}^3 \backslash B(R_i)$ *for some* $R_i > 0$, *with* $B(R_i)$*—coordinate ball of radius* R_i. *In each of the ends* Σ_i *the fields* (g,K) *are assumed to satisfy the following inequalities*:

$$|g_{ij} - \delta_{ij}| + |r\ \partial_k g_{ij}| + |rK_{ij}| \leqslant Cr^{-\alpha}, \tag{4.4}$$

for some constants $C > 0$ *and* $\alpha > \frac{1}{2}$, *with* $r = \sqrt{\Sigma (x^i)^2}$. *Suppose, moreover, that the quantities* ρ *and* J,

$$2\rho := {}^3R + K^2 - K^{ij}K_{ij}, \tag{4.5}$$

$$J^k := D_l(-K^{kl} + Kg^{kl}), \tag{4.6}$$

are well defined (perhaps in a distributional sense), and satisfy

$$\sqrt{g_{ij}J^iJ^j} \leqslant \rho \leqslant C(1+r)^{-3-\epsilon}, \quad \epsilon > 0. \tag{4.7}$$

Then the ADM four-momentum (m,p^i) *of any of the asymptotic ends of* Σ *satisfies* $m \geqslant \sqrt{p_j p^i}$. *If* $m = 0$, *then* $\rho \equiv J^i \equiv 0$, *and there exists an isometric embedding* i *of* Σ *into Minkowski space–time* $(\mathbf{R}^4, \eta_{\mu\nu})$ *such that* K_{ij} *represents the extrinsic curvature of* $i(\Sigma)$ *in* $(\mathbf{R}^4, \eta_{\mu\nu})$. *Moreover,* $i(\Sigma)$ *is an asymptotically flat Cauchy surface in* $(\mathbf{R}^4, \eta_{\mu\nu})$.

Proof: Under the conditions here the ADM four-momentum of each of the asymptotic regions of Σ is finite and well defined.[18,11] As discussed, e.g., in Ref. 13, under the present boundary

conditions the Witten boundary integral reproduces correctly the ADM four-momentum. The arguments of any of the references[11,31,13] show that one can find solutions to the Witten equation that asymptote to a constant nonzero spinor in one of the asymptotic ends, and to zero in all the other ones. Witten's identity subsequently implies that the ADM momentum of each of the ends is non-space-like.

Suppose that in one of the ends m vanishes. Then for each $\vec{n}\in\mathbf{R}^3$ there exists a spinor field $\lambda_M(\vec{n})$ defined on Σ satisfying Eq. (B7), such that the corresponding vector field $Y^j(\vec{n})$ defined via Eq. (B8), and the scalar field $N(\vec{n})$ defined by Eq. (B9), satisfy

$$Y^j(\vec{n})\to_{r\to\infty}\vec{n}^j,\quad N(\vec{n})\to_{r\mathring{a}\to\infty}|\vec{n}|_\delta.$$

Here $|\vec{n}|_\delta$ is the norm of $\vec{n}$ in the flat metric on $\mathbf{R}^3$. As shown in Appendix B, the fields $N(\vec{n})$ and $Y^i(\vec{n})$ satisfy the linear system of equations [cf. Eqs. (B11) and (B.12)],

$$D_iY_j+NK_{ij}=0, \tag{4.8}$$

$$D_iN+K_{ij}Y^j=0. \tag{4.9}$$

Consider the fields

$$Y_j=Y_j((\tfrac{1}{2},\tfrac{1}{2},0))-Y_j((-\tfrac{1}{2},\tfrac{1}{2},0))-Y_j((1,0,0)), \tag{4.10}$$

$$N=N((\tfrac{1}{2},\tfrac{1}{2},0))-N((-\tfrac{1}{2},\tfrac{1}{2},0))-N((1,0,0)). \tag{4.11}$$

The fields Y_j and N satisfy Eqs. (4.8)–(4.9) by linearity of those equations. Moreover, we have

$$Y^j\to_{r\to\infty}0,\quad N\to_{r\to\infty}1. \tag{4.12}$$

Let $(\hat{M},\hat{g}_{\mu\nu})$ be the Killing development of $(\Sigma,g_{ij},K_{ij},N,Y_i)$. As discussed in Sec. II, it follows from Eqs. (4.8)–(4.9) that the vector field $X^\mu\partial_\mu=\partial_u$ is covariantly constant on $\hat{M}$; (4.12) implies then

$$\hat{g}_{\mu\nu}X^\mu X^\nu=-1\Rightarrow N^2-g_{ij}Y^iY^j=1. \tag{4.13}$$

By Proposition 3.1 of Ref. 5, Σ is a Cauchy surface for $(\hat{M},\hat{g}_{\mu\nu})$. We wish to show that $(\hat{M},\hat{g}_{\mu\nu})$ is geodesically complete. Consider, then, an affinely parametrized geodesic $x^\mu(s)$, and let p denote the constant of motion associated with the Killing vector X^μ:

$$p=\hat{g}_{\mu\nu}\dot{x}^\mu X^\nu=-\dot{u}+Y_i\dot{x}^i. \tag{4.14}$$

Here Eqs. (2.9) and (4.13) have been taken into account; a dot over a quantity means differentiation with respect to s. Since s is an affine parameter we have, with $\epsilon=0,\pm1$,

$$-\dot{u}^2+2Y_i\dot{x}^i\dot{u}+g_{ij}\dot{x}^i\dot{x}^j=\epsilon. \tag{4.15}$$

Equations (4.14) and (4.15) give

$$(g_{ij}+Y_iY_j)\dot{x}^i\dot{x}^j=\epsilon+p^2. \tag{4.16}$$

(4.16) and (4.15) imply that there exists a function $C(p)$, such that

$$|\dot{x}|_g+|\dot{u}|\leqslant C(p). \tag{4.17}$$

Choose $p \in \mathbf{R}$ and consider the set Ω_p of maximally extended affinely parametrized geodesics with that value of p, with $x^\mu(0) \in \Sigma$. We can, without loss of generality, assume that $\alpha<1$; an analysis of Eqs. (4.8)–(4.9) along the lines of Appendix C shows that $\hat{g}_{\mu\nu} - \eta_{\mu\nu} = O_1(r^{-\alpha})$. By asymptotic flatness of $\hat{g}_{\mu\nu}$ (cf. Proposition 2.1) and the interior compactness condition on Σ, there exists $\delta>0$ such that all geodesics in Ω_p are defined for $s \in (-\delta, \delta)$. Equation (4.17) shows that in that affine time the value of $|u|$ can change at most by $C(p)\delta$, similarly for the value of $r(s) \equiv (x^2(s)+y^2(s)+z^2(s))^{1/2}$ in the asymptotic regions. One can now invoke the fact that the u translations are isometries to conclude that all geodesics in Ω_p are complete, and the result follows.

Let us show now that $(\hat{M}, \hat{g})$ is flat. Let $Y^i_k = Y^i(\vec{e}_k)$, where $Y^i(\vec{n})$ is as at the beginning of this proof and where the $\vec{e}_k$'s, $k=1,2,3$, form an orthonormal basis of $\mathbf{R}^3$. Let $N_{(k)} = N(\vec{e}_k)$ be the corresponding lapse functions. On $\hat{M}$ define the fields $X^\mu_{(k)}$ by the equation

$$
\begin{aligned}
&X^\mu_{(k)}\partial_\mu = \hat{N}_{(k)} n^\mu \partial_\mu + \hat{Y}^i_{(k)}\partial_i, \\
&\hat{Y}^i_{(k)}(u,x^i) = Y^i_{(k)}(x^i), \quad \hat{N}_{(k)}(u,x^i) = N_{(k)}(x^i).
\end{aligned}
\tag{4.18}
$$

Here n^μ is the field of unit normals to the slices $\{u=\text{const}\}$. By Eqs. (B11) and (B12), we have

$$
\hat{\mathbf{\nabla}}_j X^\mu_{(k)} = 0. \tag{4.19}
$$

By construction of $(\hat{M}, \hat{g}_{\mu\nu})$, it also holds that

$$
\hat{\mathbf{\nabla}}_\mu X^\nu = \hat{\Gamma}^\nu_{\mu\lambda} X^\lambda = \hat{\Gamma}^\nu_{\mu u} = 0. \tag{4.20}
$$

As the components of $X^\mu_{(i)}$ are u independent by (4.18), Eq. (4.20) gives

$$
\hat{\mathbf{\nabla}}_u X^\mu_{(k)} = \partial_u X^\mu_{(k)} + \hat{\Gamma}^\mu_{\lambda u} X^\lambda_{(k)} = 0. \tag{4.21}
$$

Consequently,

$$
\hat{\mathbf{\nabla}}_\mu X^\nu_{(k)} = 0. \tag{4.22}
$$

Differentiating (4.22), one obtains

$$
\hat{R}_{\mu\nu\rho\sigma} X^\sigma_{(i)} = 0. \tag{4.23}
$$

As the vector fields $X^\sigma_{(i)}$ are everywhere null and linearly independent, standard algebra gives

$$
\hat{R}_{\mu\nu\rho\sigma} \equiv 0. \tag{4.24}
$$

Consider, next, the universal covering space $\widetilde{\Sigma}$ of Σ with fields $(\widetilde{g}_{ij}, \widetilde{K}_{ij}, \widetilde{Y}_i, \widetilde{N})$ obtained by pull-back. Let $(\overline{M}, \overline{g_{\mu\nu}})$ be the Killing development of $\widetilde{\Sigma}, \widetilde{g}_{ij}, \widetilde{K}_{ij}, \widetilde{Y}_j, \widetilde{N}$. Clearly, $\overline{M}$ is the universal covering space of $\hat{M}$ with $\overline{g_{\mu\nu}}$ being the pull-back of $\hat{g}_{\mu\nu}$. It is easily seen that $(\overline{M}, \overline{g})$ inherits from $(\hat{M}, \hat{g})$ the following properties:

(1) $(\overline{M}, \overline{g_{\mu\nu}})$ is globally hyperbolic with Cauchy surface $\widetilde{\Sigma}$;

(2) $(\overline{M}, \overline{g_{\mu\nu}})$ is geodesically complete; and

(3) $(\overline{M}, \overline{g_{\mu\nu}})$ is flat.

As $\overline{M}$ is simply connected, it follows, e.g., from Ref. 37. Theorem 2.4.9 that $(\overline{M},\overline{g_{\mu\nu}})$ is the Minkowski space–time $(\mathbf{R}^4,\eta_{\mu\nu})$. As $\widetilde{\Sigma}$ is a Cauchy surface for $\overline{M}$, it is necessarily a graph over a space-like plane $t=0$ in $(\mathbf{R}^4,\eta_{\mu\nu})$. In particular, $\widetilde{\Sigma}$ has only one asymptotically flat end (compare also [Ref. 38, Lemma 2]). If Σ had been nonsimply connected, then $\widetilde{\Sigma}$ would have had more than one asymptotic end. It follows that $\Sigma = \widetilde{\Sigma}$, $\hat{M}=\mathbf{R}^4$, and our claims follow. □

To exclude the case of a null ADM four-momentum, we need to assume some further asymptotic regularity conditions.

Theorem 4.2: *Under the hypotheses of Theorem 4.1, suppose, moreover, that in some of the asymptotic ends it holds that*

$$g_{ij}-\delta_{ij}=O_{3+\lambda}(r^{-\alpha}),\quad K_{ij}=O_{2+\lambda}(r^{-1-\alpha}), \tag{4.25}$$

$$\rho=O_{1+\lambda}(r^{-3-\epsilon}), \tag{4.26}$$

with some $0<\lambda<1$. *Then the ADM four-momentum of that end cannot be null.*

Remark: It can be shown by rather different techniques that the result is still true with $\lambda=0$; we shall, however, not discuss that here.

Proof: Consider an asymptotic end Σ_1 in which Eqs. (4.25)–(4.26) hold and that has a null ADM four-momentum p^μ. As discussed in the proof of Theorem 4.1 and in Appendix B, the hypotheses of Proposition B.1 and Corollary B.2 are satisfied. We can thus apply Theorem 3.4 to conclude that the ADM four-momentum of the end under consideration vanishes, and the result follows from Theorem 4.1. □

Let us close this section by proving Theorem 1.3: By the arguments given above, ρ and J^i vanish on Σ. It follows from a result of Hawking and Ellis (Ref. 39, Chap. 4, Sec. 4.3) that $(M,g_{\mu\nu})$ must be a vacuum. By uniqueness of the maximal globally hyperbolic vacuum developments, it follows that the Killing development constructed in the proof of Theorem 4.2 (cf. Appendix B) coincides with the maximal globally hyperbolic development of (Σ,g_{ij},K_{ij}), and Theorem 1.3 follows.

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APPENDIX A: DEFINITIONS AND CONVENTIONS

We say that $(M,g_{\mu\nu})$ is a C^k space–time if M is a paracompact, connected, Hausdorff, orientable manifold of C^k differentiability class, with a C^{k-1} Lorentzian metric. We use the signature $(-,+,+,+)$.

Consider a function f defined on $\Sigma_R\equiv\mathbf{R}^3\backslash B(R)$, where $B(R)$ is a closed ball of radius $R>0$. We shall write $f=O_k(r^\beta)$ if there exists a constant C, such that we have

$$0\leqslant i\leqslant k,\quad |\partial^i f|\leqslant Cr^{\beta-i}.$$

For $\sigma\in(0,1)$ we shall write $f=O_{k+\sigma}(r^\beta)$ if $f=O_k(r^\beta)$ and if there exists a constant C, such that we have

$$|y-x| \leqslant r(x)/2 \Rightarrow |\partial^k f(x) - \partial^k f(y)| \leqslant C|x-y|^{\sigma} r^{\beta-k-\sigma}.$$

Let us note that $f = O_{k+1}(r^{\beta})$ implies $f = O_{k+\sigma}(r^{\beta})$ for all $\sigma \in (0,1)$, so that the reader unfamiliar with Hölder-type spaces might wish to simply replace, in the hypotheses of our theorems, the $k+\sigma$ by $k+1$ wherever convenient.

APPENDIX B: COVARIANTLY CONSTANT SPINORS

In this appendix we prove a differential geometric proposition on initial data sets (Σ, g_{ij}, K_{ij}) having a nowhere vanishing spinor field that is covariantly constant on Σ with respect to the ''Sen-connection''[40] [cf. Eq. (B7) below]. This result forms the local input of the rigidity part of the positive-mass theorem. Similar results in the literature we are aware of implicitly or explicitly use Cauchy developments $(M, g_{\mu\nu}, \phi^A)$ of $(\Sigma, g_{ij}, K_{ij}, \psi^A)$ for some fields ϕ^A with Cauchy data ψ^A, with energy-momentum tensor $T_{\mu\nu}$ satisfying the *full* dominant energy condition (cf. the discussion at the beginning of Sec. IV). For our results below, neither the existence of such a Cauchy evolution nor, in fact, the DEC for the given triple (Σ, g_{ij}, K_{ij}) (i.e., $\sqrt{g_{ij}J^iJ^j} \leqslant \rho$) is required.

In the case of a ''bad'' matter model—such as, e.g., dust as a source for the Einstein equations—an evolution is not known to exist. Similarly, even for ''good'' models, such as vacuum Einstein equations, the differentiability hypotheses on the initial data in Theorems 4.1 and 4.2 are not known to guarantee existence of a Cauchy development.

To motivate our three-dimensional discussion, we shall, as before, start with the four-dimensional picture. Consider thus a space–time $(M, g_{\mu\nu})$ with $g_{\mu\nu}$ in C^2 and a nowhere zero C^2 spinor field λ_M on M, satisfying

$$\nabla_{\mu}\lambda_N = 0 \Leftrightarrow \nabla_{MM'}\lambda_N = 0, \tag{B1}$$

i.e., λ_M is covariantly constant. We use capital letters in the second half of the alphabet to denote spinor indices. Since the considerations in this appendix are purely local, there is no question of the existence of a spinor structure. The spinorial Ricci identities (cf. Ref. 41, Vol. 1, pp. 242–244) immediately imply that the Ricci scalar $R_{\mu}{}^{\mu}$ of $g_{\mu\nu}$ is zero, and that the spinor equivalent of $S_{\mu\nu} := R_{\mu\nu} - \frac{1}{4} g_{\mu\nu} R_{\lambda}{}^{\lambda}$, namely the Hermitian spinor $\phi_{MNM'N'}$ satisfies

$$\lambda^M \phi_{MNM'N'} = 0$$

$$\Rightarrow \epsilon_{MN} \lambda^P \phi_{PRR'(M'} \overline{\lambda}_{N')} + \lambda_{(M} \phi_{N)RP'R'} \overline{\lambda}^{P'} \epsilon_{M'N'} = 0. \tag{B2}$$

This last equation, in tensor terms, says that

$$X_{[\mu} S_{\nu]\lambda} = 0, \tag{B3}$$

where X^{μ} is the null vector corresponding to $\lambda_M \overline{\lambda}_{M'}$. Consequently,

$$R_{\mu\nu} = \sigma X_{\mu} X_{\nu}, \tag{B4}$$

for some function σ on M. By Eq. (B1), X^{μ} is covariantly constant, i.e.,

$$\nabla_{\mu} X_{\nu} = 0, \quad \text{with } g_{\mu\nu} X^{\mu} X^{\nu} = 0. \tag{B5}$$

According to one of several equivalent definitions (cf., e.g., Ref. 17), Eqs. (B4)–(B5) imply that $(M, g_{\mu\nu})$ is a pp space–time. We have recovered the well-known fact (cf., e.g., Refs. 42, 43, 17) that a space–time admitting a covariantly constant spinor describes a pp wave.

Next, let Σ be a space-like hypersurface of $(M,g_{\mu\nu})$ with unit-normal n_μ. With $n_{MM'}$ being the spinor equivalent of n_μ, Eq. (B1) implies that

$$n_{(M}{}^{M'}\nabla_{N)M'}\lambda_P=0\Leftrightarrow n_{[\mu}\nabla_{\nu]}\lambda_P=0. \tag{B6}$$

Equation (B6) contains only derivatives tangential to Σ. When λ_M is interpreted as a SU(2)-spinor on (Σ,g_{ij},K_{ij}), (B6) can be written as (we use the conventions of Appendix A of Ref. 44),

$$D_{MN}\lambda_P+\frac{i}{\sqrt{2}}K_{MNPQ}\lambda^Q=0, \tag{B7}$$

where K_{MNPQ} is the $SU(2)$-spinor version of K_{ij} and D_{MN} the covariant derivative on Σ associated with g_{ij}.

Let us turn to the three-dimensional formulation of the problem. Suppose that we are given (Σ,g_{ij},K_{ij}) with g_{ij} in C^k, for some $k\geqslant 1$, K_{ij} in C^{k-1}, and a C^k-spinor λ_M satisfying Eq. (B7). We want to embed Σ into some Lorentz manifold $(M,g_{\mu\nu})$ in which λ_M extends to a spinor field obeying Eq. (B1).

Denote by M_i the complex-valued null vector field on Σ associated with $\lambda_M\lambda_N$ and define a real vector Y_i by

$$Y_i=\frac{i}{\sqrt{g_{jk}M^j\overline{M^k}}}\epsilon_i{}^{jk}M_j\overline{M_k}, \tag{B8}$$

and a real positive scalar N by

$$N=\sqrt{g_{ij}M^i\overline{M^j}}=\sqrt{g_{ij}Y^iY^j}. \tag{B9}$$

By, e.g., Ref. 22, Lemma 4.3, λ_N is nowhere zero; hence N is nowhere vanishing. From (B7), M_i satisfies

$$D_iM_j=-i\epsilon^{lm}{}_jK_{il}M_m, \tag{B10}$$

which, after some calculation, implies

$$D_iY_j+NK_{ij}=0. \tag{B11}$$

We also note, for use in the body of the paper, the equation

$$D_iN+K_{ij}Y^j=0, \tag{B12}$$

which follows from (B9) and (B11). Now define $(\hat{M},\hat{g}_{\mu\nu})$ to be the Killing development $(\mathbf{R}\times\Sigma,\hat{g}_{\mu\nu})$ of (Σ,g_{ij},K_{ij}) based on (N,Y^i), i.e.,

$$\hat{g}_{\mu\nu}\,dx^\mu\,dx^\nu=-N^2(x^l)du^2+g_{ij}(x^l)[dx^i+Y^i(x^l)du][dx^j+Y^j(x^l)du]. \tag{B13}$$

This, as shown in Sec. II, has $X=\partial/\partial u$ as a covariantly constant null vector, the induced metric on $u=0$ coincides with g_{ij}, and the extrinsic curvature is K_{ij}. The field of unit normals n_μ to the hypersurfaces $\{u=\text{const}\}$ is Lie derived by this Killing, vector field,

$$\mathscr{L}_Xn_\mu=0, \tag{B14}$$

which can be seen as follows: By construction $X(u)=1$. Since Lie derivation and exterior differentiation commute, we have that $\mathscr{L}_X\, du=0$. By the Killing property of X, $\mathscr{L}_X(du,du)$ is also zero, and Eq. (B14) follows. But, by the covariant constancy of X, i.e.,

$$\hat{\nabla}_\mu X_\nu=0, \tag{B15}$$

this implies that

$$X^\nu\ \hat{\nabla}_\nu n_\mu=0. \tag{B16}$$

Now extend λ_M off $u=0$ to a spinor field $\hat{\lambda}_{\mathrm{M}}$ on $(M,\hat{g}_{\mu\nu})$ by requiring

$$X^\mu\ \hat{\nabla}_\mu \hat{\lambda}_M=0. \tag{B17}$$

Consider the expression

$$U_{MNP}=n_{(M}{}^{M'}\hat{\nabla}_{N)M'}\hat{\lambda}_P\,. \tag{B18}$$

By Eqs. (B6)–(B7), U_{MNP} vanishes for $u=0$. Now compute

$$X^\mu\ \hat{\nabla}_\mu U_{MNP}=n_{(M}{}^{M'}X^\mu\hat{\nabla}_{|\mu|}\hat{\nabla}_{N)M'}\hat{\lambda}_P\,, \tag{B19}$$

where we have used (B16). Since X is covariantly constant, $X^\mu\hat{\nabla}_\mu$ commutes with covariant differentiation. Applying this on the right-hand side of (B19) and using (B16), we infer

$$X^\mu\ \hat{\nabla}_\mu U_{MNP}=0. \tag{B20}$$

Thus

$$n_{(M}{}^{M'}\ \hat{\nabla}_{N)M'}\hat{\lambda}_P=0\Leftrightarrow n_{[\mu}\ \hat{\nabla}_{\nu]}\hat{\lambda}_P=0. \tag{B21}$$

By (B17) we also have that

$$(Nn^\mu\hat{\nabla}_\mu+Y^i\hat{\nabla}_i)\hat{\lambda}_M=0. \tag{B22}$$

Due to (B21) the second term in (B22) is zero. As N is nowhere vanishing, we obtain

$$n^\mu\ \hat{\nabla}_\mu\hat{\lambda}_P=0. \tag{B23}$$

Since n^μ is time-like and again using (B21) we get

$$\hat{\nabla}_\mu\hat{\lambda}_P=0, \tag{B24}$$

as promised. (Strictly speaking, the above calculations require $k\geqslant 2$. One can use a slightly different argument to show that Proposition B.1 is correct as stated.) Combining the above calculation with Eq. (B4), we obtain the following.

Proposition B.1: Let $k\geqslant 1$ and let (Σ,g_{ij},K_{ij}), $g_{ij}\in C^k$, $K_{ij}\in C^{k-1}$ be such that there exists a C^k spinor field satisfying Eq. (B7). Then there exists a nowhere zero vector field Y_i in C^k, such that

$$D_iY_j+NK_{ij}=0, \tag{B25}$$

where $N:=\sqrt{g_{ij}Y^iY^j}$. If, moreover, $k\geqslant 2$, then the fields (ρ,J_i,τ_{kl}) defined in Eqs. (2.13)–(2.15) satisfy

$$NJ_i=\rho Y_i\,,\quad N^2\tau_{ij}=\rho Y_iY_j\,. \tag{B26}$$

In the case where the ADM four-momentum p^μ is null, the Witten argument gives rise to a spinor field on Σ obeying Eq. (B7) (cf. the discussion and the references in the proof of Theorem 4.1). Proposition B.1 and an analysis of Eqs. (B11)–(B12) similar to that of Appendix C lead to the following.

Corollary B.2: Let (Σ, g_{ij}, K_{ij}) *satisfy the hypotheses of Theorem 4.1 and let* p^μ *be null. Then there exists a nowhere zero* C^1 *field* Y_i *with* $Y^i - A^i = O_1(r^{-\alpha})$ *for some constants* A^i*, so that Eq. (B25) holds. If, moreover, the hypotheses of Theorem 4.2 are satisfied, then* $Y^i - A^i = O_3(r^{-\alpha})$*, and (B26) holds.*

APPENDIX C: PROOF OF PROPOSITION 2.1

Equation (2.4) gives the equation

$$D_i\, D_j Y_k = R_{mijk} Y^m + D_k(NK_{ij}) - D_i(NK_{jk}) - D_j(NK_{ki}). \tag{C1}$$

Here R_{mijk} is the curvature tensor of the metric g_{ij}. Consider the system of equations,

$$\frac{\partial N}{\partial r} = \frac{x^i}{r}\, \partial_i N, \tag{C2}$$

$$\partial_r Y_i = \frac{x^j}{r}\, (D_j Y_i + \Gamma^k_{ij} Y_k), \tag{C3}$$

$$\partial_r D_i N = \frac{x^k}{r}\, (D_k\, D_i N + \Gamma^j_{ki}\, D_j N), \tag{C4}$$

$$\partial_r D_i Y_j = \frac{x^k}{r}\, (D_k\, D_i Y_j + \Gamma^l_{ki} D_l Y_j + \Gamma^l_{kj}\, D_i Y_l). \tag{C5}$$

Here we are implicitly assuming that, in (C4) and (C5), the terms $D_k\, D_i N$ and $D_k\, D_i Y_j$ have been eliminated using (2.15) and (C1). Set $f = (f^A) = (N, r\, D_i N, Y_j, r\, D_i Y_j)$, $g = \Sigma_A f^A f^A$. We have

$$\left|\frac{\partial g}{\partial r}\right| \leqslant \frac{Cg}{r}, \tag{C6}$$

and by r integration one finds

$$|f| \leqslant C(1 + r^\beta), \tag{C7}$$

for some constants C, β. Suppose that $\beta > 2$, using (C7) and (C2)–(C5), one finds by r integration $|f| \leqslant C(1 + r^{\beta - \alpha})$, so that (C7) has been improved by α. Iterating this process, one obtains (2.21) and (2.22); cf. also Ref. 38. Appendix A, Lemma. Suppose finally that $A^\mu = \Lambda_{\mu\nu} = 0$. Iterating further, one finds

$$|f| \leqslant C r^{-\sigma}, \quad \text{for any } \sigma > 0. \tag{C8}$$

Note that if $g(r_0) = 0$, at some r_0, then by (C6) we will have $g \equiv 0$. Suppose thus that for all r there holds $g(r) \neq 0$. For $r_1 \geqslant r_0$ we then have, by (C6),

$$\frac{\partial g}{\partial r} \geqslant -\frac{Cg}{r} \Rightarrow \ln(g(r_1) r_1^C) \geqslant \ln(g(r_0) r_0^C).$$

Passing with r_1 to infinity from (C8), we obtain $g(r_0)=0$, which gives a contradiction, and the result follows. □

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Similarity solutions for the type D fluid plates in 5-D flat space

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All the similarity solutions, describing the Petrov-type D, plane symmetric perfect fluid distributions of imbedding class one, have been derived by using the Lie continuous point group similarity transformation method. © *1996 American Institute of Physics.* [S0022-2488(96)02303-7]

I. INTRODUCTION

The perfect fluid distributions expressed by a five-dimensional (5-D) flat metric (metric of imbedding class one) are either of Petrov-type O or Petrov-type D[1]. All the solutions of type O are known,[1] but type D solutions are yet to be exhausted. The type D solutions available so for include (i) all the perfect fluid distributions with geodesic flow,[2] (ii) all the stiff self-gravitating fluids admitting a three-parameters group of isometries with the trajectories $r=$constant, $t=$constant,[3] (iii) the most general static solution with nongeodesic flow by Kohler and Chao[4] and some of its nonstatic analogues due to Gupta *et al.*[5] In the present article, the authors have considered a plane symmetric metric in 5-D flat form and derived all possible similarity solutions of type D by using the Lie continuous point group similarity transformation method (STM). The solutions so obtained do not belong to a class of solutions with geodesic flow. The basic idea of similarity transformation method of solving PDE and ODE is mentioned in Appendices A and B, respectively.

II. BASIC EQUATIONS OF THE PROBLEMS

A five flat metric can be expressed as

$$ds^2=-(dz^1)^2-(dz^2)^2-(dz^3)^2+(dz^4)^2\pm(dz^5)^2. \tag{2.1}$$

Let us introduce plane symmetry by introducing

$$z^1=(t-r)\theta\cos\phi,\quad z^2=(t-r)\theta\sin\phi,\quad z^3=\frac{\theta^2}{2}(t-r)+r,$$

$$z^4=\frac{\theta^2}{2}(t-r)+t,\quad z^5=u(r,t), \tag{2.2}$$

and consequently (2.1) turns out to be

$$ds^2=-dr^2-(t-r)^2(d\theta^2+\theta^2\,d\phi^2)+dt^2\pm du^2. \tag{2.3}$$

However, (2.3) can be transformed to the following metrics depending upon the $+ve$ or $-ve$ sign before du^2:

$$ds^2=-dr^2-r^2(d\theta^2+\theta^2 d\phi^2)+2\,dr\,dt+du^2 \tag{2.4}$$

and

$$ds^2=-t^2(d\theta^2+\theta^2\,d\phi^2)+dt^2+2\,dr\,dt-du^2. \tag{2.5}$$

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The Einstein's field equations, so that the metric (2.5) may describe perfect fluid distribution, can be furnished as below:

$$8\pi T_1^1=\frac{2u_r}{tm^2}\,[u_r^2u_{tt}+u_{rt}-u_ru_tu_{rt}]+\frac{u_r^2}{t^2m}=8\pi[(\rho+p)v_1v^1-p], \tag{2.6}$$

$$8\pi T_2^2=8\pi T_3^3=8\pi\epsilon-\frac{2(u_{tt}u_{rr}-u_{rt}^2)}{m^2}+\frac{u_r^2}{t^2m}=-8\pi p, \tag{2.7}$$

$$8\pi T_4^4=\frac{2u_r}{tm^2}\,[-u_{rr}+u_t^2u_{rr}+u_{rt}-u_ru_tu_{rt}]+\frac{u_r^2}{t^2m}=8\pi[(\rho+p)v_4v^4-p], \tag{2.8}$$

$$8\pi T_1^4=\frac{2u_r}{tm^2}\,(u_ru_tu_{rr}-u_{rr}-u_r^2u_{rt})=8\pi(\rho+p)v_1v^4, \tag{2.9}$$

$$8\pi T_4^1=\frac{2u_r}{tm^2}\,(u_ru_tu_{tt}+u_{rt}-u_{tt}-u_t^2u_{rt})=8\pi(\rho+p)v_4v^1, \tag{2.10}$$

$$m=1+u_r^2-2u_ru_t,\quad v^1v_1+v^4v_4=1,\quad v^2=v_2=v^3=v_3=0, \tag{2.11}$$

where ρ, p, and v^i are energy-density, pressure, and flow-vector, respectively.

The consistency of (2.6)–(2.11) demands the condition

$$\epsilon(\epsilon+R)=0, \tag{2.12}$$

where ϵ is the eigenvalue of conformal tensor and is given by

$$8\pi\epsilon=\frac{-u_{rr}u_{tt}+u_{rt}^2}{m^2}-\frac{u_r}{tm^2}\,[-u_{rr}(1-u_t^2)+u_r^2u_{tt}+2u_{rt}(1-u_ru_t)]+\frac{u_r^2}{t^2m}\,[1+u_r^2-2u_ru_t]. \tag{2.13}$$

It has been verified that the vanishing of the first factor implies the vanishing of the conformal curvature tensor and the corresponding fluid distribution will be conformally flat and hence of the type O. However, the vanishing of the second factor corresponds to a fluid distribution with nonvanishing conformal tensor and hence of the type D in the present case. In the later case, we come across a partial differential equation to be satisfied by $u(r,t)$ as

$$-u_{rr}u_{tt}+u_{rt}^2+\frac{u_r}{t}\,[-u_{rr}(1-u_t^2)+u_r^2u_{tt}+2u_{rt}(1-u_ru_t)]+\frac{u_r^2}{t^2}\,(1+u_r^2-2u_ru_t)=0. \tag{2.14}$$

Associated expressions for pressure and density are given by

$$8\pi p=\frac{u_r^2}{mt^2}, \tag{2.15}$$

$$8\pi\rho=\frac{u_r^2}{mt^2}+\frac{2(u_{rr}u_{tt}-u_{rt}^2)}{m^2}. \tag{2.16}$$

A similar discussion in the case of the metric (2.4) yields a negative pressure; therefore, the study of the metric (2.4) is being dropped out in the present article.

III. SIMILARITY SOLUTIONS OF THE EQUATIONS

The Lie symmetries of Eq. (2.14) are

$$T=\alpha t, \tag{3.1}$$

$$R=\alpha r+\beta t^3+\gamma, \tag{3.2}$$

$$U=\alpha u+\delta, \tag{3.3}$$

where α, β, γ, and δ are constants.

Now, we are going to find all similarity solutions (see Appendix A). The following subcases occur: (i) $\alpha=0$, (ii) $\alpha\neq 0$.

Case (i). $\alpha=0$:

$$\frac{dt}{0}=\frac{dr}{\beta t^3+\gamma}=\frac{du}{\delta} \tag{3.4}$$

which immediately yields

$$u=\frac{r}{at^3+b}+f(t), \tag{3.5}$$

where

$$a=\frac{\beta}{\delta}, \quad b=\frac{\gamma}{\delta}$$

when inserted in (2.14) requires

$$\dot{f}=\frac{df}{dt}=-\frac{1}{14(at^3+b)^2}\,[8a^3t^9-42ab^2t^3+14at^3-7b^3-7b+14ct^2], \tag{3.6}$$

where c is an arbitrary constant.

Consequently, the metric (2.5) takes the form

$$\begin{aligned} ds^2=&-(at^3+b)^{-2}dr^2-t^2(d\theta^2+\theta^2 d\phi^2)+\left[1-\left\{\dot{f}-\frac{3art^2}{(at^3+b)^2}\right\}^2\right]dt^2\\ &+2\left[1-\frac{1}{at^3+b}\left\{\dot{f}-\frac{3art^2}{(at^3+b)^2}\right\}\right]dr\,dt. \end{aligned} \tag{3.7}$$

The corresponding expressions for pressure and density can be furnished as

$$\begin{aligned} 8\pi p&=\frac{7(at^3+b)}{t^2[-14ct^2+42art^2+15a^3t^9+21at^3(abt^3-b^2+1)]},\\ 8\pi(\rho-p)&=\frac{-18a^2t^4(at^3+b)^2}{[(at^3+b)^3+at^3+b+6art^2-2\,\dot{f}(at^3+b)^2]^2}; \end{aligned} \tag{3.8}$$

clearly $\rho\leqslant p$ in the above case.

Case (ii). $\alpha\neq 0$:

$$\frac{dt}{\alpha t}=\frac{dr}{\alpha r+\beta t^3+\gamma}=\frac{du}{\alpha u+\delta} \tag{3.9}$$

which immediately suggests the form of ''u'' as

$$u=\frac{ty(\eta)-\delta}{\alpha} \quad \text{with} \quad \eta=\frac{2\alpha r-\beta t^3+2\gamma}{t}. \tag{3.10}$$

On inserting (3.10) into the original Eq. (2.14) we get

$$y''(y^2-\alpha x)+2xy'^3-2yy'^2+\frac{\alpha}{2}y'=0, \tag{3.11}$$

where $y'=dy/dx$ and $x=\alpha+\eta$.

Now, in order to solve Eq. (3.11), the procedure can be divided into two parts.

A. When $y^2-\alpha x=0$

Equation (3.11) is satisfied and the corresponding metric and expressions for pressure and density are furnished as below:

$$\begin{aligned} ds^2=&-\left[1+\frac{1}{\alpha t}(2\alpha r-\beta t^3+2\gamma)\right]^{-1}dr^2-t^2(d\theta^2+\theta^2 d\phi^2)\\ &+\left[1-\frac{\{\alpha+(1/t)(\alpha r-2\beta t^3+\gamma)\}^2}{\alpha\{\alpha+(1/t)(2\alpha r-\beta t^3+2\gamma)\}}\right]dt^2+\frac{2}{t}\left[\frac{\alpha r+\beta t^3+\gamma}{\alpha+(1/t)(2\alpha r-\beta t^3+2\gamma)}\right]dr\,dt, \end{aligned} \tag{3.12}$$

$$8\pi\rho=3(8\pi p)=\frac{\alpha}{\beta t^4}. \tag{3.13}$$

It is worth pointing out that the obtained solution is of Petrov type O.

B. When $y^2\neq\alpha x$

The similarity method (see Appendix B) provides the infinitesimals ξ and η as

$$\xi=\alpha_0 y \quad \text{and} \quad \eta=\frac{\alpha\alpha_0}{2}. \tag{3.14}$$

Now Eq. (3.11) can be reduced to the first-order equation by means of two invariants u and v as follows:

$$\frac{dx}{\alpha_0 y}=\frac{dy}{\alpha\alpha_0/2}=\frac{d(y')}{-\alpha_0 y'^2}. \tag{3.15}$$

Consequently, two solutions of (3.15) provide u and v as

$$u(x,y)=\frac{y^2-\alpha x}{\alpha} \tag{3.16}$$

and

$$v(x,y,y')=\frac{\alpha-2yy'}{\alpha y'}. \tag{3.17}$$

Equations (3.16) and (3.17), using (3.11), give

$$v\,\frac{dv}{du}+\frac{v^2}{2u}=-\frac{4}{\alpha} \tag{3.18}$$

which, on integration, provides

$$v^2=\frac{4u}{\alpha}+\frac{\beta_0}{u}, \tag{3.19}$$

where β_0 is constant. Equation (3.19), together with (3.16) and (3.17), give

$$y'\left[2y+\sqrt{4(y^2-\alpha x)+\frac{\alpha^3\beta_0}{y^2-\alpha x}}\right]=\alpha. \tag{3.20}$$

Ordinary differential equations can further be integrated as follows. Let

$$y^2-\alpha x=W$$

and x and W be functions of y. Then Eq. (3.20) assumes the shape

$$\frac{dW}{dy}=-\sqrt{\frac{4W^2+\alpha^3\beta_0}{W}}. \tag{3.21}$$

On integration, we get

$$y=-\int\sqrt{\frac{W}{4W^2+\alpha^3\beta_0}}\,dW+\gamma_0 \tag{3.22}$$

which is hyperbolic or elliptic integral.[6]

Equation (3.22) relates W and y (and hence y and x) implicitly. However, the metric and expressions for density and pressure can be furnished in terms of y and x as follows:

$$\begin{aligned}ds^2=&-4\alpha^2\left[2y+\sqrt{4(y^2-\alpha x)+\frac{\alpha^3\beta_0}{y^2-\alpha x}}\right]^{-2}dr^2-t^2(d\theta^2+\theta^2d\phi^2)\\&+\left[1-\frac{1}{\alpha^2}\left\{y-\frac{2\alpha(\alpha r+\gamma+\beta t^3)}{t(2y+\sqrt{4(y^2-\alpha x)+(\alpha^3\beta_0/(y^2-\alpha x))})}\right\}^2\right]dt^2\\&+2\left[1-\left\{\frac{2}{(2y+\sqrt{4(y^2-\alpha x)+(\alpha^3\beta_0/(y^2-\alpha x))})}\right\}\right.\\&\left.\times\left\{y-\frac{2\alpha(\alpha r+\gamma+\beta t^3)}{t(2y+\sqrt{4(y^2-\alpha x)+(\alpha^3\beta_0/(y^2-\alpha x))})}\right\}\right]dr\,dt,\end{aligned} \tag{3.23}$$

$$8\pi\rho=\frac{4\alpha^2[\beta_0\alpha^2(y^2-\alpha x)+12\beta t^2(y^2-\alpha x)^2+6\beta\beta_0\alpha^2t^2]}{t^2[\beta_0\alpha^2+12\beta t^2(y^2-\alpha x)^2]}, \tag{3.24}$$

and

$$8\pi p=\frac{4\alpha^2(y^2-\alpha x)}{t^2[\beta_0\alpha^2+12\beta t^2(y^2-\alpha x)]}. \tag{3.25}$$

IV. DISCUSSIONS AND CONCLUSIONS

In the foregoing section, three metrics, e.g., (3.7), (3.12), and (3.23), have been obtained. Out of these (3.12) is not new, as it is conformally flat and all the conformally flat (type O) solutions are known. As far as (3.7) and (3.23) are concerned, it will be demonstrated that both of these possess nonvanishing acceleration and do not belong to the class of solutions, due to Barnes[2] and hence are new. Workers in the field have not indicated the solutions with nongeodesic flow through the metric (2.5) so far. Quite possible (but the authors are not aware) that some of the workers in the field might have obtained the above solutions in different context other than the imbedding class one.

(a) Metric (3.7). The metric can be transformed to the following normal form:

$$ds^2=-dR^2+(14at^3+14b)^{-1}[Q+84at^2(at^3+b)(R-f\ )]dt^2-t^2(d\theta^2+\theta^2d\phi^2) \tag{4.1}$$

through the transformation

$$r=\left[R+\left(\frac{at^4}{4}+bt-f\ \right)\right](at^3+b), \tag{4.2}$$

where

$$Q=42at^3+51a^3t^9+42ab^2t^3+147a^2bt^6+28ct^2. \tag{4.3}$$

The metric (4.1) in no way belongs to the most general metric due to Barnes[2] for geodesic flow, i.e.,

$$ds^2=-[h(r)t+\alpha t^2+g(r)]^2dr^2-t^2(d\theta^2+\theta^2d\phi^2)+t^2\ dt^2$$

except in one case when $a=0$ in (4.1) which corresponds to a Zeldovich fluid with acceleration zero. The flow vector for (4.1) reads as follows:

$$v^1=-\left[\frac{18a^2t^2M}{7(at^3+b)P^2-18a^2t^2M}\right]^{1/2},$$

$$v^2=v^3=0,$$

$$v^4=\frac{14(at^3+b)}{M}\left[-\frac{36a^2t^2}{p^2}+\frac{14(at^3+b)}{M}\right]^{-1/2},$$

where

$$P=12a(R-f\ )+\{14t^2(at^3+b)^2\}^{-1}\{84a^2t^6+102a^4t^{12}+378a^2b^2t^6$$
$$+396a^2bt^9+56act^5+84abt^3+84ab^3t^3+56bct^2\},$$

$$M=84at^2(at^3+b)(R-f\ )+42at^3+51a^3t^9+42ab^2t^3+147a^2bt^6+28ct^2.$$

(b) Metric (3.23). In this case, metric potentials are available in implicit form and therefore its transformation into the normal form is not possible explicitly. However, associated acceleration

vector reveals that the metric and, hence, the corresponding fluid distribution is with nongeodesic flow. Following are the expressions for flow vector and acceleration vector:

$$v^1=\frac{1}{\alpha^2}\left[\frac{1}{K}\left(\frac{\alpha^3\beta_0}{y^2-\alpha x}+12\alpha\beta t^2\right)\right]^{1/2}\left[\left(2y+\sqrt{4(y^2-\alpha x)+\frac{\alpha^3\beta_0}{y^2-\alpha x}}\right)(y^2-\alpha x)^2\right.$$
$$\left.+\frac{\alpha}{t}\sqrt{y^2-\alpha x}\left(4(y^2-\alpha x)+\frac{\alpha^3\beta_0}{y^2-\alpha x}\right)^{1/2}(\alpha r+\beta t^3+\gamma)\right],$$

$$v^2=v^3=0,$$

$$v^4=[y^2-\alpha x]\left[\frac{1}{K}\left\{12\alpha\beta t^2+\frac{\alpha^3\beta_0}{y^2-\alpha x}\right\}\left\{4(y^2-\alpha x)+\frac{\alpha^3\beta_0}{y^2-\alpha x}\right\}\right]^{1/2},$$

and acceleration vector $(\dot{v}_1,0,0,\dot{v}_4)$ is

$$\dot{v}_1=\frac{-\alpha^4\beta_0}{Jt}\left[\frac{\sqrt{4(y^2-\alpha x)+(\alpha^3\beta_0/y^2-\alpha x)}}{2y+\sqrt{4(y^2-\alpha x)+(\alpha^3\beta_0/(y^2-\alpha x))}}\right]$$
$$\times\left[1-\frac{2(y^2-\alpha x)}{K}\{\alpha^4\beta_0^2+24\alpha^2\beta\beta_0t^2(y^2-\alpha x)+144\beta^2t^4(y^2-\alpha x)^2\}\right]$$

and

$$\dot{v}_4=-\frac{\dot{v}_1}{\alpha^2}\left[\frac{\alpha}{t}(\alpha r+\beta t^3+\gamma)+(y^2-\alpha x)^{3/2}\left\{\frac{\sqrt{4(y^2-\alpha x)+(\alpha^3\beta_0/y^2-\alpha x)}}{2y+\sqrt{4(y^2-\alpha x)+(\alpha^3\beta_0/(y^2-\alpha x))}}\right\}^{-1}\right],$$

where

$$J=\beta_0\alpha^2(y^2-\alpha x)+12\beta t^2(y^2-\alpha x)^2+3\beta\beta_0\alpha^2t^2,$$

$$K=\alpha^4\beta_0^2(y^2-\alpha x)+3\alpha^5\beta\beta_0^2t^2+24\alpha^2\beta\beta_0t^2(y^2-\alpha x)^2$$
$$+36\alpha^3\beta^2\beta_0t^4(y^2-\alpha x)^2+144\beta^2t^4(y^2-\alpha x)^3.$$

It is clear that the acceleration is zero only when y is constant or equal to αx, or $\beta_0=0$.

It is worth pointing out here that all the spherically symmetric and hyperbolic symmetric similarity solutions are found to satisfy the barotropic equation of state pressure equal to energy density.

APPENDIX A: STM FOR SECOND-ORDER PDE

The Lie continuous point group similarity transformation method[7] involves the invariance of the partial differential equation

$$H(r,t,u,u_r,u_t,u_{rr},u_{rt},u_{tt})=0 \tag{A1}$$

under a family of one-parameter infinitesimal continuous point group transformation such as

$$u=u+\epsilon U(r,t,u)+O(\epsilon^2), \tag{A2}$$

$$r=r+\epsilon R(r,t,u)+O(\epsilon^2), \tag{A3}$$

$$t=t+\epsilon T(r,t,u)+O(\epsilon^2), \tag{A4}$$

where U, R and T are the infinitesimals of the variables u, r, and t, respectively, and ϵ is an infinitesimal parameter. Similarly derivatives of u are transformed, according to

$$u_r=u_r+\epsilon[U_r]+O(\epsilon^2), \tag{A5}$$

$$u_t=u_t+\epsilon[U_t]+O(\epsilon^2), \tag{A6}$$

$$u_{rr}=u_{rr}+\epsilon[U_{rr}]+O(\epsilon^2), \tag{A7}$$

and so on, where $[U_r]$, $[U_t]$, $[U_{rr}]$, etc. are the infinitesimals of the transformations of derivatives u_r, u_t, u_{rr}, etc., respectively, and are given by

$$[U_r]=U_r+(U_u-R_r)u_r-T_ru_t-R_uu_r^2-T_uu_ru_t, \tag{A8}$$

$$[U_t]=U_t+(U_u-T_t)u_t-R_tu_r-T_uu_t^2-R_uu_ru_t, \tag{A9}$$

$$\begin{aligned}[U_{rr}]=&U_{rr}+(2U_{ru}-R_{rr})u_r-T_{rr}u_t+(U_{uu}-2R_{ru})u_r^2-2T_{ru}u_ru_t-R_{uu}u_r^3\\&-T_{uu}u_r^2u_t+(U_u-2R_r)u_{rr}-2T_ru_{rt}-3R_uu_{rr}u_r-T_uu_{rr}u_t-2T_uu_{rt}u_r,\end{aligned} \tag{A10}$$

$$\begin{aligned}[U_{tt}]=&U_{tt}+(2U_{tu}-T_{tt})u_t-R_{tt}u_r+(U_{uu}-2T_{tu})u_t^2-2R_{tu}u_ru_t-T_{uu}u_t^3\\&-R_{uu}u_t^2u_r+(U_u-2T_t)u_{tt}-2R_tu_{rt}-3T_uu_{tt}u_t-R_uu_{tt}u_r-2R_uu_{rt}u_t,\end{aligned} \tag{A11}$$

$$\begin{aligned}[U_{rt}]=&U_{rt}+(U_{ru}-T_{tr})u_t+(U_{tu}-R_{tr})u_r-T_{ru}u_t^2+(U_{uu}-R_{ru}-T_{ut})u_ru_t-R_{tu}u_r^2-T_{uu}u_ru_t^2\\&-R_{uu}u_tu_r^2-T_ru_{tt}+(U_u-R_r-T_t)u_{rt}-R_tu_{rr}-2T_uu_tu_{rt}-2R_uu_ru_{rt}-T_uu_ru_{tt}-R_uu_tu_{rr}.\end{aligned} \tag{A12}$$

The invariance requirement of (A1) under the set of transformations (A2) to (A12) leads to the invariant surface condition:

$$R\frac{\partial H}{\partial r}+T\frac{\partial H}{\partial t}+U\frac{\partial H}{\partial u}+[U_r]\frac{\partial H}{\partial u_r}+[U_t]\frac{\partial H}{\partial u_t}+[U_{rr}]\frac{\partial H}{\partial u_{rr}}+[U_{rt}]\frac{\partial H}{\partial u_{rt}}+[U_{tt}]\frac{\partial H}{\partial u_{tt}}=0. \tag{A13}$$

On solving the (A13), the infinitesimals R, T, and U can be uniquely determined, which give the similarity group under which the system (A1) is invariant.

By the infinitesimal transformations (A2)–(A4), we have

$$u(r+\epsilon R+O(\epsilon^2),t+\epsilon T+O(\epsilon^2))=u+\epsilon U+O(\epsilon^2). \tag{A14}$$

By comparing the coefficient of $O(\epsilon)$ on either side of (A14) gives

$$R\frac{du}{dr}+T\frac{du}{dt}-U=0, \tag{A15}$$

which is a quasilinear equation of first order and admits a solution by Lagrange method as

$$u=f(\sigma), \quad \text{where} \quad \sigma=\sigma(r,t). \tag{A16}$$

On substituting (A16) into Eq. (A1) the latter turns out to be an ordinary differential equation involving only the derivatives with respect to the variable σ (called similarity variable).

APPENDIX B: STM FOR SECOND-ORDER ODE

Now we shall provide the necessary details of the similarity transformation method[7] for reducing a second-order ordinary differential equation into a first-order equation.

A second-order equation

$$F(x,\ y,\ y',\ y'')=y''-\omega(x,\ y,\ y')=0 \tag{B1}$$

admits all the transformations of one-parameter infinitesimal group

$$x=x+\xi(x,y)\,\tau, \tag{B2}$$

$$y=y+\eta(x,y)\,\tau, \tag{B3}$$

where ξ and η are the infinitesimals and τ is an infinitesimal parameter.

The general condition for group invariance is

$$\xi\,\frac{\partial F}{\partial x}+\eta\,\frac{\partial F}{\partial y}+\eta'\,\frac{\partial F}{\partial y'}+\eta''\,\frac{\partial F}{\partial y''}=0, \tag{B4}$$

where

$$\eta'=\eta_x+(\eta_y-\xi_x)y'-\xi_y y'^2 \tag{B5}$$

and

$$\eta''=\eta_{xx}+(2\eta_{xy}-\xi_{xx})y'+(\eta_{yy}-2\xi_{xy})y'^2-\xi_{yy}y'^3+(\eta_y-2\xi_x)y''-3\xi_y y'y''. \tag{B6}$$

The condition (B4) with reference to (B1) reads as

$$\begin{aligned}&-\xi\,\frac{\partial\omega}{\partial x}-\eta\,\frac{\partial\omega}{\partial y}-[\eta_x+(\eta_y-\xi_x)y'-\xi_y y'^2]\,\frac{\partial\omega}{\partial(y')}+\eta_{xx}+2(\eta_{xy}-\xi_{xx})y'\\&+(\eta_{yy}-2\xi_{xy})y'^2-\xi_{yy}y'^3+[\eta_y-2\xi_x-3\xi_y y']\omega=0.\end{aligned} \tag{B7}$$

Equation (B1) can be reduced to a first-order equation by finding out two invariants of the group (u,v) which, in turn, are found from solving the characteristic differential equations

$$\frac{dx}{\xi(x,y)}=\frac{dy}{\eta(x,y)}=\frac{d(y')}{\eta'(x,y,y')} \tag{B8}$$

as

$$u(x,y)=a\ \text{ and }\ v(x,y,y')=b. \tag{B9}$$

Then, the second-order differential equation can be expressed as

$$\frac{dv}{du}=\phi(u,v)=\frac{v_x+v_y y'+v_{y'}y''}{u_x+u_y y'}. \tag{B10}$$

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The twisting connection of space–time

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The compatibility between general relativity and the property that space–times are embedded manifolds is examined. It is shown that the signature of the embedding space is uniquely determined when its dimension is the smallest possible. In this case, the twisting vector transforms as a Yang–Mills potential under the signature preserving symmetry group, whose curvature is described by Ricci's equation. The use of complex embeddings is also discussed in association with signature and topology changes. © *1996 American Institute of Physics.*
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I. INTRODUCTION

It has been known for a long time that Riemannian manifolds can be seen as a submanifold of some higher dimensional space. This embedding corresponds to the inverse of Riemann's problem: To find the extrinsic geometry for a given intrinsic (metric) one. The existence of the embedding is the object of the fundamental theorem of submanifolds (as an extension of the fundamental theorem of curves and surfaces).[1] The adaptation of the embedding program to the case of a pseudo-Riemannian manifold offers little difficulty,[1,2] and there is a long list of references on applications to space–times of general relativity.[3–9]

It is clear that if we embed a space–time but insist on using only its intrinsic properties (that is, those derived from the metric only), then there is nothing to gain except the mathematical exercise.[10] However, the embedding equations state that the metric (the gravitational field) of the embedded space–time is induced by that of the embedding space via the embedding parametrization. Thus, as in a vielbein formalism, the embedding functions transfer some of the physical properties of the space–time either to the metric or to the parametrization of the embedding space. Furthermore, since the space–time acts as an arena for all physical phenomena, we cannot avoid considerations on the physics at the interface between the two manifolds. Conceivably a extremely high energy process in space–time (possibly above 1 TeV!), such as a collision of particles could eject some particles outside space–time, or else we should be able to explain why it does not happen.[11] If particles are ejected, then the conservation laws and particle structure should be adapted to this new condition. The possible contribution of the embedding space to particle kinematics, including internal structure has been conjectured long ago.[5,6]

Thus, in this embedding picture of space–time there are some unavoidable questions such as: What is the meaning of the extrinsic objects of a space–time and in particular of its extrinsic curvature? Why should the space–time remain as a stable four dimensional submanifold instead of being ''diluted'' or ''evaporated'' in the ambient space, as a consequence of the above conjecture? Is the metric of the space–time the only physically meaningful quantity among all embedding functions?

There are at least two basic problems which must be considered before we should answer

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some of these questions. The first problem (the signature problem), described in section II refers to the existence of different signatures for a given space–time and the same embedding dimension. We show that this may be solved with a natural condition to be imposed on the embedding dimension. The other problem described in section III refers to the physical meaning of one of the fundamental forms the space–time called the twisting vector. (Also known as the torsion vector, frequently mistaken by the torsion tensor.) We show that this is a well defined connection in space–time whose curvature is described by Ricci's equation.

We start with some comments and review briefly the main properties of space–time embeddings. The dimension D of the embedding space depends on the differentiable character of the embedding functions. If we agree with Janet and Cartan that those functions are analytic, then the embedding space has dimension $D \leqslant d(d+1)/2$.[12] However, analytic functions may be too special as compared to differentiable functions to describe high energy processes. If we use a differentiable embedding, then the number of dimensions increases to $D \leqslant d(d+3)/2$.[13] Of course, in most known situations we need less than those limits and in the case of physics it makes sense to adopt a principle of economy of dimensions: If a given space–time has been proven to be embeddable in D dimensions, then we will not use more than D dimensions. We will see that this principle is also relevant for the uniqueness of the signature.

The choice of the geometry of the embedding space presents a second problem for, if the embedding space has anything to do with physics, then its curvature will be a dynamical object. Therefore, unlike the purely mathematical embedding problem, physics may imply a dynamical embedding model, where the geometry and topology of the embedding space changes continuously with time. Comparing with Kaluza–Klein theory it would be natural to assume that such geometry could be derived from the Einstein–Hilbert action. On the other hand, following another trend, the space–times could also be regarded as four-membranes in the embedding space whose dynamics follows from the Nambu action.[7] In any of these situations, the four-dimensional intrinsic geometry of the embedded space–time would emerge only at the low energy limits of the theories. Nonetheless, known results for Euclidean metrics say that it is always possible to determine a flat embedding space for a given manifold. Therefore, we may also assume at least as an initial step, that at the end there will be a flat space embedding for any space–time (which could be taken to be to some kind of ground state).

Consider a space–time V_4 with metric g_{ij}, solution of Einstein's equations and its local isometric embedding in a flat D-dimensional manifold $\mathscr{M}_D$. That is, a 1:1 map $\mathscr{Y}: V_4 \to \mathscr{M}_D$ such that[1]

$$g_{ij} = \mathscr{Y}^{\mu}{}_{,i}\mathscr{Y}^{\nu}{}_{,j}\mathscr{G}_{\mu\nu}, \quad \mathscr{N}^{\mu}_{A}\mathscr{Y}^{\nu}{}_{,i}\mathscr{G}_{\mu\nu} = 0, \quad \mathscr{N}^{\mu}_{A}\mathscr{N}^{\nu}_{B}\mathscr{G}_{\mu\nu} = g_{AB} = \epsilon_A \delta_{AB}, \tag{1}$$

where x^i are coordinates in space–time and $\mathscr{N}_A$ are $D-4$ vector fields orthogonal to the embedded space–time. (Lower case Latin indices run from 1 to 4 and capital Latin indices run from 5 to D. All Greek indices run from 1 to D. The indicated antisymetrization applies only to indices of the same kind closer to the brackets.) Here $\epsilon_A = \pm 1$ and $\mathscr{G}_{\mu\nu}$ denote the components of the metric of $\mathscr{M}_D$ in the embedding coordinates $\mathscr{Y}^{\mu}$. Since $\mathscr{M}_D$ is flat we may use Cartesian coordinates with metric components $\eta_{\mu\nu}$.

The embedding coordinates $\mathscr{Y}^{\mu}(x^i)$ can be obtained by integrating the Gauss and Weingarten equations:

$$\mathscr{Y}^{\mu}_{;ij} = g^{MN} b_{ijM} \mathscr{N}^{\mu}{}_{N}, \tag{2}$$

$$\mathscr{N}^{\mu}_{A;j} = -g^{mn} b_{jmA} \mathscr{Y}^{\mu}{}_{,n} + g^{MN} A_{jAM} \mathscr{N}^{\mu}{}_{N}, \tag{3}$$

where b_{ijA} are the components of the second fundamental form and A_{iAB} are the components of the twisting vector. Since $\mathscr{M}_D$ is flat we may always choose $\mathscr{Y}^{\mu}$ as Cartesian coordinates. In this case, we obtain explicitly

$$b_{ijA} = -\mathscr{Y}^{\mu}{}_{,i}\mathscr{N}^{\nu}{}_{A,j}\eta_{\mu\nu} = \mathscr{Y}^{\mu}{}_{,ij}\mathscr{N}^{\nu}_{A}\eta_{\mu\nu}. \tag{4}$$

It follows that b_{ijA} is symmetric in the first two indices. Likewise, the expression of the twisting vector is:

$$A_{iAB} = \mathscr{N}^{\mu}{}_{A}\mathscr{N}^{\nu}{}_{B,i}\eta_{\mu\nu}, \tag{5}$$

so that $A_{iAB} = -A_{iBA}$. These two quantities, determine completely the extrinsic geometry of the space–time, giving a measure of the local shape of the space–time as compared to the tangent space.

Obviously, if the embedding of the space–time is given by the embedding coordinates (as for example in Ref. 14) then all we have to do is calculate $\mathscr{N}^{\mu}{}_{A}$, b_{ijA} and A_{iAB}.[15] However, if we do so we learn very little over what we already know from the intrinsic geometry. As mentioned before, the situation may be different if we assume that the embedding is not known, but that it results from the space–time dynamics. Since in general b_{ijA} and A_{iAB} are independent of the metric, we may express this dynamics in terms of those variables instead of the embedding coordinates $\mathscr{Y}^{\mu}$. The integrability conditions for (2) and (3) are the well known Gauss, Codazzi and Ricci equations for submanifolds which may be written respectively as

$$\begin{aligned} R_{ijkl} &= 2g^{MN}b_{i[kM}b_{jlN}, \\ b_{i[jA;k]} &= g^{MN}A_{[kAM}b_{jiN}, \\ A_{[jAB;k]} + g^{MN}A_{[jMA}A_{k]NB} &= -g^{mn}b_{m[jA}b_{k]nB}. \end{aligned} \tag{6}$$

There are some specific procedures for integrating these equations, as for example in Refs. 4 and 8. However, their physical implications are often neglected. We will come back to them in section III.

II. THE UNIQUENESS PROBLEM

Assuming that the space–time has a Lorentz signature, then the embedding space has necessarily a pseudo-Euclidean signature, possibly with several time-like directions, one of them necessarily lying on the tangent plane. For a give space–time, it is possible to find different embedding signatures with the same dimension. If the embedding space has physical significance, then such ambiguity is not acceptable. In particular, a given gravitational field would produce different trajectories in higher dimensions. The above mentioned principle of economy of dimensions has the following consequence:

Theorem 1: *If D is the smallest dimension in which we can isometrically embed a non-flat space–time V_4 in a real space $\mathscr{M}_D$, then the signature of the embedding space is unique.*

Suppose that we have two embeddings of the same space–time $\mathscr{Y}: V_4 \to \mathscr{M}_D$ and $\mathscr{Y}': \mathscr{V}_4 \to \mathscr{M}'_D$ which differ only in signature: (p,q) in the first case and (p',q') in the second. Since the tangent spaces to V_4 have the same Minkowski signature, without loss of generality they may be identified. That is, we may define a map $T: \mathscr{M}_D \to \mathscr{M}'_D$ such that its derivative T^* restricted to the tangent space TV_4 is the identity: $T^*\rfloor_{TV_4} = T_1^* = Id$. On the other hand, the restriction T_2^* to the subspaces $V_4^{\perp}$ of $\mathscr{M}_D$ orthogonal to the space–time, is a general linear transformation (Fig. 1). In terms of the embedding coordinates and normal vectors this is equivalent to

$$\mathscr{Y}'^{\mu}{}_{,i} = \mathscr{Y}^{\mu}{}_{,i}, \quad \mathscr{N}'_{B} = T^{A}{}_{B}\mathscr{N}_{A}. \tag{7}$$

And from its definition (4), the second fundamental form transforms as $b'_{ijB} = T^{A}{}_{B}b_{ijA}$. The Gauss equation for $\mathscr{Y}'$ is

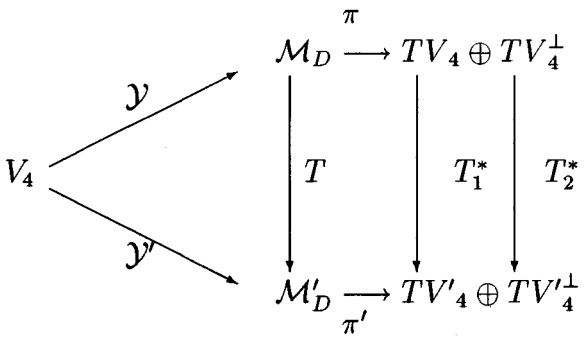

FIG. 1. Two embeddings of V_4.

$$R_{ijkl}=2g'^{MN}b'_{i[kM}b'_{l]jN}, \tag{8}$$

Comparing with Gauss' equation for $\mathscr{Y}$, we obtain

$$2\sum_{A=5}^{D} g''^{AB}b_{i[kA}b_{l]jB}=0, \tag{9}$$

where we have denoted

$$g''^{AB}=g^{AB}-g'^{MN}T^{A}{}_{M}T^{B}{}_{N}. \tag{10}$$

It remains to be seen if (9) admits a non-trivial solution g''^{AB} of the form $\epsilon''_A\delta_{AB}$, with $\epsilon''^{A}=\pm 1$. We have the following possibilities:

(a) All g''^{AB} coincide with g^{AB}: $g''^{AB}=g^{AB}$ $\forall A,B=5,\ldots,D$. In this case we have $g'^{MN}T^{A}_{M}T^{B}_{N}=0$ which is not possible since the left hand side of equation (8) becomes identically zero, contradicting the hypothesis of a non-flat V_4.

(b) Only some values of g''^{AB} coincide with g^{AB}. For example, suppose that $g''^{AB}\neq g^{AB}$ for $A,B=5,\ldots,D_1$ and $g''^{AB}=g^{AB}$ for $A,B=D_1+1,\ldots,D$, where $5<D_1<D$. From (9), it follows that

$$2\sum_{A,B=5}^{D_1} g''^{AB}b_{i[kA}b_{l]jB}+2\sum_{A,B=D_1+1}^{D} g^{AB}b_{i[kA}b_{l]jB}=0.$$

Therefore, replacing the last term in the Gauss equation of (6), we get

$$R_{ijkl}=2\sum_{A,B=5}^{D_1} g^{AB}b_{i[kA}b_{l]jB}+2\sum_{A,B=D_1+1}^{D} g^{AB}b_{i[kA}b_{l]jB}=2\sum_{A,B=5}^{D_1}(g^{AB}-g''^{AB})b_{i[kA}b_{l]jB}.$$

Since, the quadratic form $g^{AB}-g''^{AB}$ can always be diagonalized, we may write $g^{AB}-g''^{AB}=g'''^{AB}=\epsilon'''_A\delta^{AB}$. Therefore the last equation corresponds to Gauss' equation for a third embedding of V_4 in a space with D_1 dimensions, contradicting the hypothesis.

(c) The remaining possibility corresponds to a trivial solution $g''^{AB}=0$, for all $A,B=5,..,D$. In other words,

$$g^{AB}=T^{A}{}_{M}g'^{MN}T^{B}_{N}. \tag{11}$$

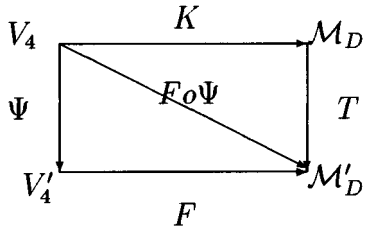

FIG. 2. The embeddings of Schwarzschild's space–time.

In matrix notation, $g = Tg'T^t$, so that $(\det T)^2 = \det g / \det g'$. Therefore, we have $\det(T) = \pm 1$, or $\det(T) = \pm i$. In the cases $\det(T) = \pm 1$ the signature of the embedding space remains unchanged. In particular when $\det(T) = 1$, T belongs to the group of pseudo rotations of the normal vectors $\mathcal{N}^{\mu}{}_A$. Since the tangent space to V_4 has a Minkowski signature and $\mathcal{M}_D$ has signature (p,q), this group is $SO(p-3,q-1)$.

On the other hand if $\det(T) = \pm i$ we have different signatures corresponding to a complex T, producing a complexification of $\mathcal{M}_D$ defined by a pair of maps $(+,*)$ from $\mathcal{M}_D \times \mathcal{M}_D$ to $\mathcal{M}_D \times \mathcal{M}_D$ such that[16]:

$$(u,v)+(w,x) = (u+w, v+x) \quad \text{and} \quad (u,v)*(w,t) = (uw - vt, vw + ux).$$

A complex embedding may result from a complexification of $\mathcal{M}_D$. In our case, the complexification of $\mathcal{M}_D$ induced by T occurs only on the subspace of $\mathcal{M}_D$ orthogonal to the space–time V_4 which remains real and preserves its light cone structure. The resulting complex manifold $\mathcal{M}_D/\mathbb{C}$, defines a ''complex embedding'' of a real space–time.

As an example of the signature change problem consider two well known embeddings of the Schwarzschild space–time in six dimensional pseudo Euclidean flat spaces: Kasner[14] $K: V_4 \to \mathcal{M}_6$ $ds^2 = d\mathcal{Y}_1^2 + d\mathcal{Y}_2^2 - d\mathcal{Y}_3^2 - d\mathcal{Y}_4^2 - d\mathcal{Y}_5^2 - d\mathcal{Y}_6^2$, Fronsdal[9] $F: \mathcal{V}_4 \to \mathcal{M}_6'$ $-ds^2 = d\mathcal{Y}'^2_1 - d\mathcal{Y}'^2_2 - d\mathcal{Y}'^2_3 - d\mathcal{Y}'^2_4 - d\mathcal{Y}'^2_5 - d\mathcal{Y}'^2_6$, given by (here we assume mass units such that $2m = 1$):

$$K \begin{cases} \mathcal{Y}_1 = \left(1 - \dfrac{1}{r}\right)^{1/2} \cos t, \\ \mathcal{Y}_2 = \left(1 - \dfrac{1}{r}\right)^{1/2} \sin t, \\ \mathcal{Y}_3 = f(r), \ \left(\dfrac{df}{dr}\right)^2 = \dfrac{1 + 4r^3}{4R^3(r-1)}, \\ \mathcal{Y}_4 = r \ \text{sen}\theta \sin\phi, \\ \mathcal{Y}_5 = r \sin\theta \cos\phi, \\ \mathcal{Y}_6 = r \cos\theta, \end{cases} \quad \text{and} \quad F \begin{cases} \mathcal{Y}_1' = 2\left(1 - \dfrac{1}{r}\right)^{1/2} \sinh\left(\dfrac{t}{2}\right), \\ \mathcal{Y}_2' = 2\left(1 - \dfrac{1}{r}\right)^{1/2} \cosh\left(\dfrac{t}{2}\right), \\ \mathcal{Y}_3' = g(r), \ \left(\dfrac{dg}{dr}\right)^2 = \dfrac{(r^2 + r + 1)}{r^3}, \\ \mathcal{Y}_4' = r\text{sen}\theta \sin\phi, \\ \mathcal{Y}_5' = r \sin\theta \cos\phi, \\ \mathcal{Y}_6' = r \cos\theta. \end{cases}$$

In the first case we have two time-like dimensions while in the second case we have only one (we are using $-ds^2$ instead of ds^2). Both correspond to the same space–time, except for a difference in topology: In K, the space–time extends only to $r = 1$, while in F it extends to $r = 0$. The second embedding corresponds in fact to the maximal analytic extension of the Schwarzschild space–time also known as Kruskal's space–time. Since the Schwarzschild space–time can be seen as a subset embedded in Kruskal's space–time defined by an extension map Ψ.[17] Then there is a third embedding of Schwarzschild's space–time, given by composite map $Fo\Psi$ (Fig. 2), consistent

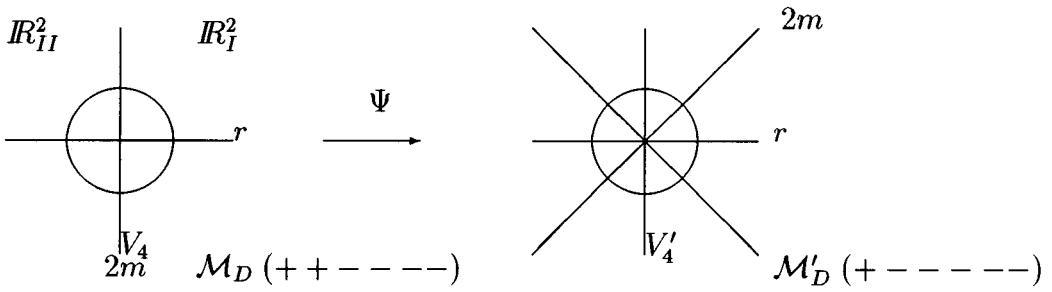

FIG. 3. Topology and signature changes.

with the one defined by Fronsdal and it has the appropriate signature.

It has been noted that the embedding defined by Kasner is not causal.[9] Indeed, any curve in the plane $(\mathscr{Y}_1, \mathscr{Y}_2)$ with a parameter range greater than 2π is closed in that embedding. Since we are required to perform genuine non-local experiments in space–time to apply the equivalence principle and to distinguish causal and non causal propagation, we cannot rely on the implicit function theorem alone to characterize an embedding properly. Unless he remains strictly local, an observer in the space–time would be able to detect if his space–time is embedded or not simply by observing a classical breaking of causality. Consequently, the Kasner embedding is not physical.

Now, consider the linear transformation T between the two above embeddings. The matrix representing T is

$$(T^A{}_B) = \begin{pmatrix} a & b \\ c & d \end{pmatrix}.$$

Replacing in (11) with $g_{55}=1,\ g_{66}=-1$ and $g'_{55}=1,\ g'_{66}=1$, we obtain

$$a^2+b^2=1,\ c^2+d^2=-1,\ ac+bd=0,\ (ad-bc)^2=-1.$$

One possible solution producing a complex T is $a=d=0,\ c=i,\ b=1$.

The change of signature of $\mathscr{M}_D$ may have some topological consequences.[18] This can be seen by taking the embedding diagrams for Schwarzschild (Kasner) and Kruskal (Fronsdal) space–times. In Figure 3, the circle in the left represent an open sphere S^2 which intersects regions $\mathbb{R}^2_I$ and $\mathbb{R}^2_{II}$ excluding the plane $r=2m=1$. The corresponding topology is then $(\mathbb{R}^2_I \cup \mathbb{R}^2_{II}) \times S^2$. On the other hand, in the right hand side the resulting topology is $\mathbb{R}^2 \times S^2$.[19]

The above result shows that by use of complex embeddings it is possible to preserve the space–time signature while altering only the signature of the embedding space. For example, we may use complex transformations to make $\mathscr{M}_D$ truly Minkowskian (with just one time-like dimension) and use it as a fixed background in a possible canonical quantization procedure, while keeping intact the classical space–time signature. In this case the group of rotations of the normal vectors would be $SO(D-4)$. This Minkowskian signature may be relevant for the recent debate on the need or not of changing the space–time signature to apply path integrals in quantum cosmology.[20]

The change of signature of the embedding space may also be a consequence of the space–time dynamics. Considering the embedding equations as part of the dynamical equations, together with Einstein's equations, any 4-surface of discontinuity of the second fundamental form b_{ij} may induce a classical change of signature of $\mathscr{M}_D$. This would be analogous to the process of classical

change of signature described in Ref. 21, but now extended to four-dimensional hypersurfaces. In turn, this change of signature of the embedding space may promote eventual topological changes.[22]

III. THE TWISTING CONNECTION

In the following we consider the embeddings of a given space–time in a real space with the same signature (we consider as equivalent signatures which differ only by a factor -1, or by a mere relabelling of the embedding coordinates) (p,q). Therefore the signature preserving symmetry is $T=SO(p-3,q-1)$.

The fundamental theorem of submanifolds says that given the symmetric tensor g_{ij}, $D-4$ tensors b_{ijA} and $(D-4)(D-5)/2$ vectors A_{iAB} satisfying (6) then there is a four-dimensional submanifold of a flat space $\mathscr{M}_D$ which has g_{ij} as its metric, b_{ijA} as its second fundamental form and A_{iAB} as its twisting vector.

Actually that theorem gives a $D-4$ parameter family or foliation of embedded manifolds with parametrization

$$\mathscr{Z}^{\mu}(x^i,x^A)=\mathscr{Y}^{\mu}(x^i)+x^A N^{\mu}_A.$$

The metric of $\mathscr{M}_D$ in the Gaussian coordinate system (x^i,x^A) is

$$\mathscr{G}'_{\alpha\beta}=\mathscr{Z}^{\mu}{}_{,\alpha}\mathscr{Z}^{\nu}{}_{,\beta}\mathscr{G}_{\mu\nu}=\begin{pmatrix}\tilde{g}_{ij}+x^A x^B g^{MN}A_{iMA}A_{jNB} & g_{iA}\\ g_{jB} & g_{AB}\end{pmatrix}, \tag{12}$$

where we have denoted

$$\tilde{g_{ij}}=g_{ij}-2x^A b_{ijA}+x^A x^B g^{mn}b_{imA}b_{jnB}, \quad \text{and} \quad g_{iA}=x^M A_{iMA}.$$

Now let us recall a remarkable property of the twisting vector:

Theorem 2: *Under an infinitesimal pseudo rotation of the normal vectors N, the twisting vector transforms as*:

$$A'_{iAB}=A_{iAB}-f^{EF}_{ABMN}A_{iEF}\Theta^{MN}-\Theta_{AB,i}, \tag{13}$$

where f^{EF}_{ABMN} denote the structure constants and Θ^{MN} denote the parameters of the group $SO(p-3,q-1)$.

From (12) we may express the torsion vector as $A_{iAB}=\partial\mathscr{G}_{iA}/\partial x^B$. Therefore under an infinitesimal transformation of $SO(p-3,q-1)$:

$$x'^i=x^i, \quad x'^A=x^A+\xi^A.$$

Keeping only the linear terms in ξ, the infinitesimal transformation of A_{iAB} is:

$$A'_{iAB}=\frac{\partial\mathscr{G}'_{iA}}{\partial x^{B'}}=(\delta^M_A-\xi^M_A)\frac{\partial}{\partial x'^M}((\delta^{\mu}_i-\xi^{\mu}_{,i})(\delta^{\nu}_A-\xi^{\nu}_{,A})\mathscr{G}_{\mu\nu}).$$

Since $\xi^k=0$ and $\xi^A=\Theta^A_M(x^i)x^M$ we end up with

$$A'_{iAB}=A_{iAB}-2g^{MN}A_{iM[A}\Theta_{NB]}-\Theta^M{}_{A,i}g_{MB}. \tag{14}$$

The Lie algebra of $SO(p-3,q-1)$ with generators L^{AB} is given by

$$[L^{MN},L^{PQ}]=f^{MNPQ}_{AB}L^{AB},$$

where

$$f_{AB}^{MNPQ}=4\alpha\delta_A^{[N}g^{M][P}\delta_B^{Q]} \quad \text{and} \quad f_{ABMN}^{PQ}=4\alpha\delta_{[A}^{P}g_{B][M}\delta_{N]}^{Q}, \tag{15}$$

where α is a normalization constant. Therefore,

$$A'_{iAB}=A_{iAB}-2A_{iEF}\frac{1}{4\alpha}f_{ABMN}^{EF}\Theta^{MN}-\Theta^{M}{}_{A}g_{MB}.$$

Hence, for $\alpha=1/2$ we obtain (13), which is the same as the transformation of a gauge potential in Yang-Mills theory, with respect to the gauge group $SO(p-3,q-1)$.

The Lie-algebra valued ''twisting'' vector field is defined as

$$A_i=A_{iAB}L^{AB}.$$

The transformation (13) suggests that A_i induce a gauge-like connection in V_4, the twisting connection, with the corresponding ''gauge'' covariant derivative operator given by

$$D_i=\nabla_i+\beta A_i,$$

where β is another constant to be appropriately chosen, not necessarily meaning a coupling constant. This covariant derivative acts on Lie algebra valued functions $\mathbf{f}$ as $D_i\mathbf{f}=\nabla_i\mathbf{f}+\beta[A_i,\mathbf{f}]$. In particular, for scalar functions f, $D_if=\nabla_if$, so that $D_ig_{jk}=0$. Using the fact that $\nabla_iL^{AB}=0$, we obtain the commutator

$$[D_i,D_j]=\beta(\nabla_iA_j-\nabla_jA_i+\beta[A_i,A_j]). \tag{16}$$

Next we consider the Clifford algebra associated with the metric g^{AB} defined by

$$E^AE^B+E^BE^A=2g^{AB}E^0,$$

where E^0 is the identity element $E^AE^0=E^0E^A=E^A$. This algebra is closely related with the isometry group of g^{AB}. In fact, if the Lie algebra of this group is generated by L^{AB}, then[23]

$$L^{AB}=\frac{1}{\gamma}[E^A,E^B], \tag{17}$$

where again γ is another scale constant to be chosen. The indices A, B,... are raised and lowered with g_{AB} and g^{AB} such that $E^A=g^{AB}E_B$. Therefore, given the coefficients of the second fundamental form b_{ijA} we, may define the Clifford algebra valued tensors $b_{ij}=b_{ijA}E^A$.

Theorem 3: *If F_{ij} is the curvature associated with the twisting connection, then Codazzi's and Ricci's equations are respectively equivalent to*

$$D_{[k}b_{ij]}=0, \tag{18}$$

$$F_{ij}=-2g^{mn}b_{m[i}b_{j]n}. \tag{19}$$

In fact, since D_i and $[D_i,D_j]$ are Lie-algebra valued functions, we may write $[D_i,D_j]=[D_i,D_j]_{AB}L^{AB}$, where we have denoted [from (16)]

$$[D_i,D_j]_{AB}=\beta(\nabla_iA_{jAB}-\nabla_jA_{iAB}+\beta A_{iMN}A_{jPQ}f_{AB}^{MNPQ}). \tag{20}$$

From the definition of structure constants it follows that

$$f_{AB}^{MNPQ}L^{AB}=[L^{MN},L^{PQ}]_{AB}L^{AB}.$$

Therefore, (20) may be written as

$$[D_i,D_j]_{AB}=2\beta(\nabla_{[i}A_{j]AB}+\beta g^{MN}A_{[iMA}A_{j]NB}). \tag{21}$$

Comparing the right hand side of this expression to the left hand side of Ricci's equation in (6) we obtain with $\beta=-1$, $D_i=\nabla_i-A_i$ and

$$[D_i,D_j]=g^{mn}b_{m[jA}b_{i]nB}\frac{1}{\gamma}[E^A,E^B]=\frac{4}{\gamma}g^{mn}b_{[jm}b_{i]n}. \tag{22}$$

To complete the demonstration, introduce the notation

$$D_{kA}^N=\delta_A^N\nabla_k b_{jiN}-g^{MN}A_{kAM}.$$

Then the second equation (6) can be written as

$$D_{[kA}^N b_{j]iN}=0. \tag{23}$$

On the other hand, using the definition of D_i, the gauge covariant derivative of b_{ij} is given by

$$D_k b_{ij}=\nabla_k b_{ij}-[A_k,b_{ij}]. \tag{24}$$

However, we can easily see that

$$[A_k,b_{ij}]=A_k b_{ij}-b_{ij}A_k=\frac{8}{\gamma}g^{AB}A_{kCB}b_{ijA}E^C.$$

Consequently,

$$D_k b_{ji}=\left(\delta_A^M\nabla_k-\frac{8}{\gamma}g^{MN}A_{kAN}\right)b_{ijM}E^A.$$

Comparing with (23) it follows that for $\gamma=8$ we obtain Codazzi's equation (18):

$$D_{[k}b_{ij]}=D_{[kA}^M b_{ij]}ME^A=0.$$

Finally, the curvature associated with A_i is $F_{ij}=[D_i,D_j]$, so that from (22) we obtain (19).

As we see, Gauss and Ricci's equations are equivalent in the sense that the curvature tensors of the Levi-Civita and twisting connections are expressed in terms of the variable b_{ij}, which act as a source field subjected to Codazzi's equation.

For completeness we may also write the Gauss equation in the same algebraic form. This is easily accomplished using the definition of the Clifford algebra $\{E^A\}$ in the first equation of (6), obtaining

$$R_{ijkl}E^0=b_{i[k}b_{l]j}-b_{j[k}b_{l]i}. \tag{25}$$

In conclusion, the conditions for the embedding of a space–time may be compatible with the physics of the space–time, provided the integrability conditions are included as part of the dynamics and with the adoption of the principle of economy of dimensions.

The hidden internal indices $A,B,..$ in the algebraic form of the equations (18),(19) and (23), merely reflect the degrees of freedom for the embedding which is defined up to a transformation of the normal vectors. As such they do not affect the number of independent equations. To

understand the space–time as a four-dimensional submanifold and why it stays like that, depends on further understanding of b_{ij} and A_i as physical fields in addition to the metric (the gravitational field). This requires further considerations on the fundamental theorem of submanifolds as adapted to the case of space–times, which will be presented in a subsequent paper.

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Geodesic motion and confinement in van Stockum space–time

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Geodesic motion of test particles in van Stockum space–time, which represents the internal gravitational field produced by a rigidly rotating dust cylinder, is studied. In particular, it is found that confinement occurs quite generally in the radial direction, while the motion in the axial direction is free. The possible relevance of the confinement to the extragalactic jet formation is pointed out. © *1996 American Institute of Physics.* [S0022-2488(96)00503-6]

I. INTRODUCTION

After the pioneering work of Levi-Civita (LC),[1] Lanczos,[2] van Stockum,[3] and Marder,[4] space–times with cylindrical symmetry have been studied intensively, because of both their mathematical simplicity and (more important) their physical relevance to our realistic world.[5,6] However, due to the particular difficulties that they possess, our understanding on such space–times is still by far from mature. For example, even in the simplest case of the LC solution,[1] its physical interpretation is not completely understood, yet. In general, it contains two independent parameters, in contrast to the spherical case, in which there is only one mass parameter. It was not clear until quite recently that one of them corresponds to topological defects.[4,7] The second parameter, σ, is still unclear, although most believe that it is connected with the mass per unit length. It is this belief that gives rise to a serious problem: In which form it is related to such a mass, since the two values, $\sigma=0$, $\frac{1}{2}$, all correspond to a flat space–time.[8] This problem has been further studied quite recently.[7,9]

On the other hand, partially motivated by the inflationary Universe scenario,[10] a large class of exact solutions to the Einstein vacuum equations with a nonvanishing cosmological constant was recently found by Santos,[11] which represents the gravitational field outside a cylindrically distributed matter source, and studied in detail by Bonnor, MacCallum, and Santos.[12]

To get some insight into those space–times, another alternative is to study the geodesic motion of test particles in the space–times. As a matter of fact, in this paper, as well as in the forthcoming ones, we shall engage ourselves on this problem. In particular, in the present paper we shall study the geodesic motion in the van Stockum space–time,[3] which represents the gravitational field produced by a rigidly rotating dust cylinder with a finite thickness. The matching of this space–time to the vacuum Lewis space–time[13] was also completed in Ref. 3, and studied in detail by Bonnor.[14] Since here we are mainly interested in the geodesic motion of test particles inside the dust cylinder, we shall restrict ourselves only to the internal solution of the rigidly rotating dust cylinder, i.e., the van Stockum space–time.

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II. GEODESIC MOTION IN VAN STOCKUM SPACE–TIME

The van Stockum dust cylinder is given by[3]

$$ds^2=g_{\alpha\beta}\,dx^\alpha\,dx^\beta=-f\,dt^2+2k\,dt\,d\phi+e^\mu(dr^2+dz^2)+l\,d\phi^2, \tag{1}$$

where f, k, μ, and l are given by

$$f=1,\quad k=ar^2,\quad \mu=-a^2r^2,\quad l=r^2(1-a^2r^2), \tag{2}$$

with a being an arbitrary positive constant. The coordinates are numbered

$$x^0=t,\quad x^1=r,\quad x^2=z,\quad x^3=\phi, \tag{3}$$

ranging

$$-\infty<t<\infty,\quad -\infty<z<\infty,\quad 0<\phi<2\pi, \tag{4}$$

and the hypersurfaces $\phi=0$ and $\phi=2\pi$ being identified. The energy density and the four velocity of the dust are

$$\kappa\rho=4a^2e^{a^2r^2},\quad u^\mu=\delta^\mu_0, \tag{5}$$

where κ is the gravitational coupling constant. The angular velocity of the fluid with respect to a locally nonrotating frame[14] is $\omega=a(1-a^2r^2)^{-1}$. Since near the axis, $\omega\to a$, we can interpret a as the angular velocity of the fluid on the axis.

Now we calculate the geodesics,

$$\frac{d^2x^\alpha}{d\lambda^2}+\Gamma^\alpha_{\beta\gamma}\frac{dx^\beta}{d\lambda}\frac{dx^\gamma}{d\lambda}=0, \tag{6}$$

of a test particle in the space–time (1), where λ is an affine parameter along the geodesics. Substituting Eqs. (1) and (2) into Eq. (6), we obtain

$$\ddot{t}+2a^2r\dot{r}\dot{t}-2a^3r^3\dot{r}\dot{\phi}=0, \tag{7}$$

$$\ddot{r}-a^2r(\dot{r}^2-\dot{z}^2)-r(1-2a^2r^2)e^{a^2r^2}\dot{\phi}^2-2are^{a^2r^2}\dot{t}\dot{\phi}=0, \tag{8}$$

$$\ddot{z}-2a^2r\dot{r}\dot{z}=0, \tag{9}$$

$$\ddot{\phi}+\frac{2}{r}(1-a^2r^2)\dot{r}\dot{\phi}+2\frac{a}{r}\dot{t}\dot{r}=0, \tag{10}$$

where the overdot stands for differentiation with respect to the affine parameter. For time-like geodesics, it is the proper time τ. Integrating Eqs. (7), (9), and (10), we obtain

$$\dot{t}=E(1-a^2r^2)+aP_\phi, \tag{11}$$

$$\dot{z}=P_ze^{a^2r^2}, \tag{12}$$

$$\dot{\phi}=P_\phi\frac{1}{r^2}-aE, \tag{13}$$

where E, P_z and P_ϕ are integration constants. Instead of integrating Eq. (8) we can use the line element (1) and obtain

$$-\epsilon=-\dot{t}^2+2ar^2\dot{t}\dot{\phi}+e^{-a^2r^2}(\dot{r}^2+\dot{z}^2)+(1-a^2r^2)r^2\dot{\phi}^2, \tag{14}$$

where $\epsilon=0$, 1, or -1 if the geodesics are null, time-like, or space-like. In the following, we shall be concerned only with the null and time-like geodesics.

Introducing the momenta of the test particle defined by

$$p_\alpha=g_{\alpha\beta}\dot{x}^\beta, \tag{15}$$

we obtain from Eqs. (2) and (11)–(13),

$$p_0=-E, \quad p_1=e^{-a^2r^2}\dot{r}, \quad p_2=P_z, \quad p_3=P_\phi. \tag{16}$$

Hence E can be interpreted as the total energy of the particle, and will be always taken non-negative. P_z can be interpreted as its momentum along z and P_ϕ its angular momentum. We restrict the study of geodesic motion of test particles to $0\leqslant ar\leqslant 1$, since at $ar=1$ the circle of this radius about the axis is a closed null curve. At greater values of $ar>1$ it defines closed time-like curves about the axis.[14]

Introducing the quantity

$$x\equiv ar, \tag{17}$$

we can rewrite Eq. (8) as

$$\ddot{x}=a^2xe^{x^2}\left(2aEP_\phi-\epsilon-E^2x^2-2P_z^2e^{x^2}+a^2P_\phi^2\,\frac{1-x^2}{x^4}\right). \tag{18}$$

From the above equation we have

$$\ddot{x}'=a^2e^{x^2}\left[-\epsilon(1+2x^2)-2P_z^2e^{x^2}(1+4x^2)+2E^2\,\frac{g(x)}{x^4}\right], \tag{19}$$

where the prime stands for differentiation with respect to x and

$$g(x)=C^2(-x^4+\tfrac{3}{2}x^2-\tfrac{3}{2})+C(2x^6+x^4)-x^8-\tfrac{3}{2}x^6, \tag{20}$$

with

$$C=\frac{aP_\phi}{E}. \tag{21}$$

If $P_\phi\leqslant 0$, or $C\leqslant 0$, we have from Eq. (20), $g<0$, which means from Eq. (19) that $\ddot{x}'<0$. But if $P_\phi>0$, since from Eq. (20),

$$g(0)=-\tfrac{3}{2}C^2<0, \quad g(1)=-\tfrac{5}{2}+3C-C^2<0, \tag{22}$$

and there are no real C roots for $g(x)=0$ in the interval $0\leqslant x\leqslant 1$, we also have $g(x)<0$. Hence $\ddot{x}'<0$ for $P_\phi>0$. Therefore $\ddot{x}(x)$ is steadily decreasing for increasing values of x for $P_\phi\leqslant 0$ as well as for $P_\phi>0$.

On the other hand, setting

$$V_0 \equiv E^2 + 2aEP_\phi - \epsilon, \quad V(x) \equiv E^2 x^2 + P_z^2 e^{x^2} + \frac{a^2 P_\phi^2}{x^2}, \tag{23}$$

Eq. (14) can be written as

$$\dot{x}^2 = a^2 e^{x^2}[V_0 - V(x)]. \tag{24}$$

Note that $V(x)$ is non-negative. Thus, in order to have Eq. (24) meaningful for real x, we must have $V_0 > 0$, which is equivalent to

$$E > (a^2 P_\phi^2 + \epsilon)^{1/2} - aP_\phi. \tag{25}$$

To further study the motion of test particles, we consider the cases where $P_\phi = 0$ and $P_\phi \neq 0$ separately.

Case A: $P_\phi = 0$. For this case Eqs. (18) and (24) become

$$\ddot{x} = -a^2 x e^{x^2}(\epsilon + E^2 x^2 + 2P_z^2 e^{x^2}), \tag{26}$$

$$\dot{x}^2 = a^2 e^{x^2}[E^2(1 - x^2) - (\epsilon + P_z^2 e^{x^2})]. \tag{27}$$

From Eq. (27) we can see that for the radially moving photons, $\epsilon = 0$ and $P_z = 0$, the maximum radius that the photons can reach is $x = 1$. The acceleration of these photons is zero at the symmetry axis, and is increasing exponentially with its direction being always inward as x increases. As a result, all of them will be drawn backward when they reach the maximum radius $x = 1$, where their velocity becomes zero. As they move inward from thereon, they reach at the axis with nonzero velocity, and are reflected by it, and then move outward. This procedure will be repeated endlessly.

For photons with $P_z \neq 0$ and, or, time-like particles, the motion is similar along x, and the difference is that the maximum radius that they can reach is less than 1. But meanwhile they have motion too in the axial direction with velocity given by Eq. (12),

$$\dot{z} = P_z e^{x^2}, \tag{28}$$

which means that the particles increase their speed along z when distancing radially from the axis, while diminish their axial speed when moving radially toward the axis.

Therefore, for this class of photons and time-like particles, they are always confined inside the cylinder $x = 1$. We observe that, in spite of $P_\phi = 0$, the particles have angular velocity different from zero since (13) gives

$$\dot{\phi} = -aE, \tag{29}$$

because of the dragging of space–time.

Case B: $P_\phi \neq 0$. From (23) we find

$$V'(x) = 2x\left(E^2 + P_z^2 e^{x^2} - \frac{a^2 P_\phi^2}{x^4}\right). \tag{30}$$

Thus, the equation $V'(x) = 0$ has only one solution, say, $x = x_c$, which satisfies

$$E^2 + P_z^2 e^{x_c^2} = \frac{a^2 P_\phi^2}{x_c^4}. \tag{31}$$

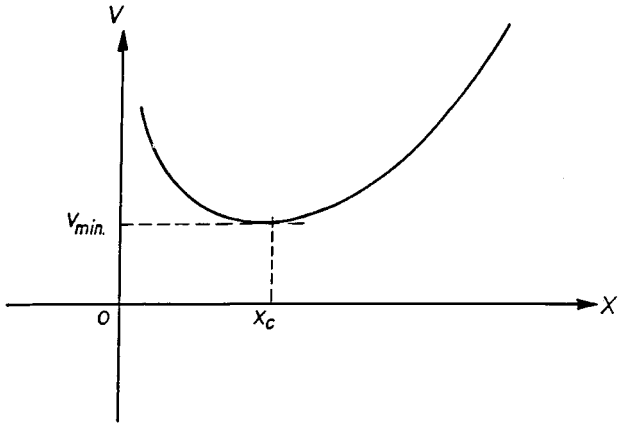

FIG. 1. The generic behavior of the function $V(x)$, defined by Eq. (3.7) in the text. It has only one minimum at $x=x_c$.

On the other hand, from Eq. (23) we find that when $x\to 0$ or ∞, $V(x)\to\infty$. Therefore it is concluded that $x=x_c$ is the point where $V(x)$ has its minimum (cf. Fig. 1).

From Eq. (24) and Fig. 1 we can see that if the equation

$$V_0-V(x)=0, \tag{32}$$

has two real roots, say, $x_{\min}$ and $x_{\max}$, with $0<x_{\min}<x_{\max}\leqslant 1$, then motion of the test particles will be confined inside the shell $x_{\min}\leqslant x\leqslant x_{\max}$. If Eq. (32) has only one real root, say, $x=x_0$, with $0<x_0\leqslant 1$, then the motion will be confined outside the cylinder $x=x_0$. Note that the test particles with $P_\phi\neq 0$ can never reach the axis $x=0$, since in this case the accelerations at the axis are infinitely large and directed outward [cf. Eq. (18)]. So, any particle, both time-like and null, moving inward initially, will be pulled out before they reach the axis by a huge force proportional to x^{-3}. This indicates that the gravitational collapse of a cylinder with rotation can never develop singularities at the axis, and instead, after it collapses along the radius, it will be bounced out.[15,16] If Eq. (32) has no real solution in the interval $0<x\leqslant 1$, it means that motion of test particles is forbidden. Thus, to study the motion of test particles now reduces to study the roots of Eq. (32) for $0<x\leqslant 1$. From Fig. 1, we can see that the number of the roots crucially depends on the fact of whether $x_c\leqslant 1$. Clearly, if $x_c\geqslant 1$, the number of roots of Eq. (32) is one or zero, depending on if

$$\Delta V\equiv V_0-V(1)=2aEP_\phi-(\epsilon+a^2P_\phi^2+eP_z^2), \tag{33}$$

is greater than or equal to zero, or less than zero, respectively.

When $x_c<1$, Eq. (32) will have two, one, or zero roots, depending on if

$$\delta V\equiv V_0-V_{\min}, \tag{34}$$

is greater than, equal to, or less than zero, respectively. To see whether the minimum of $V(x)$ occurs inside the cylinder $x=1$ or not, it is sufficient to consider $V'(x)$ given by Eq. (30) at $x=1$ is greater than, equal to, or less than zero. When $V'(1)>0$, we must have $x_c<1$; when $V'(1)=0$, we have $x_c=1$; and when $V'(1)<0$ we must have $x_c>1$ (see Fig. 2).

From Eq. (30) we find that

$$V'(x=1)=2[E^2-(a^2P_\phi^2-eP_z^2)]. \tag{35}$$

Thus, we have the following three distinguishable subcases:

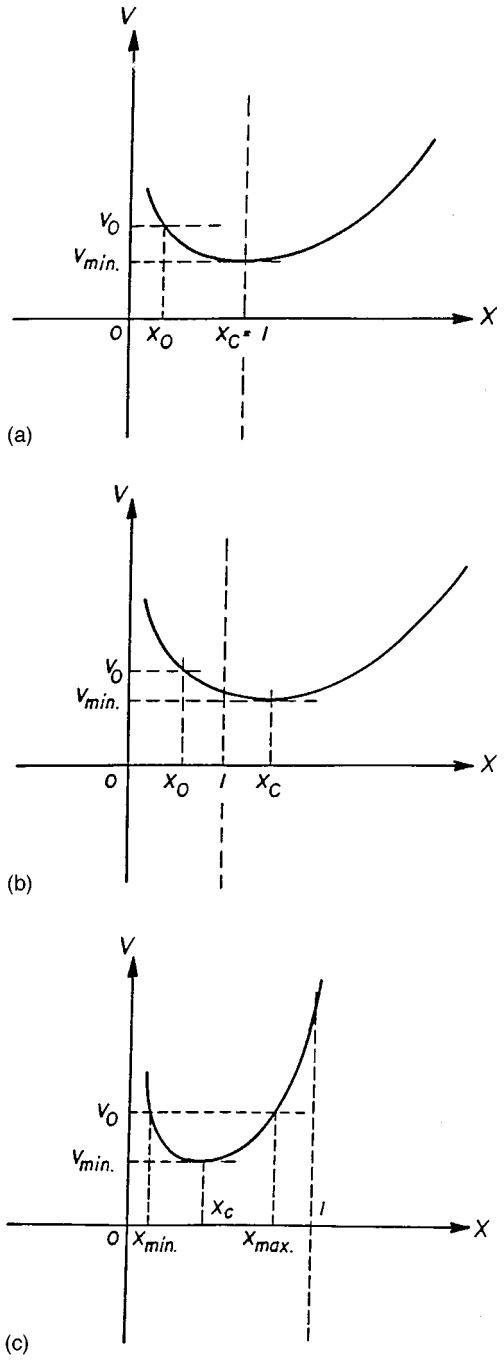

FIG. 2. Three distinguishing cases for the function $V(x)$: (a) $V'(x=1)=0$; (b) $V'(x=1)<0$; and (c) $V'(x=1)>0$.

$$\text{(i)} \quad \left|\frac{P_\phi}{P_z}\right| > \frac{\sqrt{e}}{a}, \quad E^2 = a^2 P_\phi^2 - e P_z^2 \quad [V'(1)=0]; \tag{36}$$

$$\text{(ii)} \quad \left|\frac{P_\phi}{P_z}\right| > \frac{\sqrt{e}}{a}, \quad E^2 < a^2 P_\phi^2 - e P_z^2 \quad [V'(1)<0]; \tag{37}$$

$$\text{(iii)} \quad E^2 > a^2 P_\phi^2 - e P_z^2 \quad [V'(1) > 0]. \tag{38}$$

Let us consider them case by case.

Case B(i). From Eqs. (25) and (33), we find that when any of the two conditions,

$$\text{(a)} \quad P_\phi < 0;$$

or

$$\text{(b)} \quad P_\phi > 0, \quad E < \frac{1}{2aP_\phi}(\epsilon + a^2 P_\phi^2 + e P_z^2), \tag{39}$$

holds, we will have $\Delta V < 0$. Since in the present case we have $V'(x=1)=0$ [cf. Eq. (36)], then we have $\Delta V = V_0 - V(1) = V_0 - V_{\min} < 0$. Thus, for any x, we always have $\dot{x}^2 = a^2 x^2 e^{-x^2}[V_0 - V(x)] < 0$. In other words, in these two subcases the motion of test particles is forbidden. When $\Delta V \geqslant 0$, which is equivalent to

$$P_\phi > 0, \quad E \geqslant \frac{1}{2aP_\phi}(\epsilon + a^2 P_\phi^2 + e P_z^2), \tag{40}$$

and when Eq. (25) is fulfilled, Eq. (32) has a solution, $x = x_0$, in which the motion is confined outside the cylinder $x = x_0$ [cf. Fig. 2(a)].

Case B(ii). From Eq. (33), we find that when Eq. (39) is satisfied, Eq. (32) has no real solution for $0 < x \leqslant 1$. Therefore, the motion in this case is forbidden. When Eqs. (25) and (40) are fulfilled, Eq. (32) has a real solution $x = x_0$ for $0 < x \leqslant 1$. In this case the motion is confined outside the cylinder $x = x_0$ [see Fig. 2(ii)].

Case B(iii). From Fig. 2(c), we can see that when $\Delta V \geqslant 0$ and Eq. (25) holds, Eq. (32) has one real solution, $x = x_0$. Thus, in this case, the motion is confined outside the cylinder $x = x_0$. When $\Delta V \leqslant 0$, the nature of the roots of Eq. (32) depends on the signs of δV defined by (34). In particular, when $\delta V > 0$, Eq. (32) has two real solutions, $x = x_{\min}$ and $x = x_{\max}$, and the motion is confined inside the shell $x_{\min} \leqslant x \leqslant x_{\max}$. The bigger δV is, the thicker the shell. As $\delta V \to 0^+$, the shell becomes infinitely thin. When $\delta V < 0$, Eq. (32) has no solution and the motion is forbidden.

III. DISCUSSION AND CONCLUSION

Interesting features arise from the geodesic motion of test particles in a cylinder filled with dust rigidly rotating. The space–time generated by van Stockum solution produces the property of confinement for test particles in the radial direction, while the motion in the axial and azimuthal directions is free. It means that the particles are constrained to move endlessly inside a shell of the cylinder. This property was noticed in Gödel space–time[17] independently by Kundt[18] and by Chandrasekhar and Wright.[19]

We show that null particles can reach the maximum radius $x = 1$, which is the causal limit of van Stockum's space–time, when $P_z = P_\phi = 0$. In this case, the null particles move radially between the axis, $x = 0$, and $x = 1$ where they attain null velocities. In spite of $P_\phi = 0$, these particles have angular velocity different from zero because of the dragging of space–time. If $P_z \neq 0$ and, or, the particles are massive, the radial motion is similar but do not reach up to $x = 1$. Meanwhile, they have a motion along the axis, increasing their axial speed when distancing radially from the axis, and diminishing their axial speed when moving toward the axis.

If the test particles have $P_\phi \neq 0$, they can never reach $x = 0$, since in this case the accelerations at the axis are infinitely large and directed outward. So any particle, massless or massive, initially moving in the radial direction will be pulled out before reaching the axis of the cylinder. This fact

indicates that the gravitational collapse of a rotating cylinder filled with matter can never develop singularities at the axis.[15,16] For this case test particles can leave or be confined inside the cylinder $x=1$, depending on the values of its initial parameters E, P_z, and P_ϕ.

We mention that the particles that consist the dust cylinder also move along geodesic lines. This can be seen by simply calculating their four accelerations from Eq. (5), which is given by

$$a^\mu \equiv u^\mu{}_{;\nu} u^\nu = 0. \tag{41}$$

In analogy to Eq. (15), we can also define the four momenta for the particles by

$$P_\alpha \equiv E g_{\alpha\beta} u^\beta = E(-\delta^t_\alpha + a r^2 \delta^\phi_\alpha), \tag{42}$$

where $E \equiv mc$, and m denotes the rest mass of the particles, c is the speed of light. Then, its square is

$$P_\alpha P^\alpha = -c^2 m^2. \tag{43}$$

From Eq. (42), we can see that these particles have no motion in the radial and axial directions, but they do have in the angular direction. Moreover, P_ϕ now depends on the radial coordinate r, in contrast to that of test particles. This is because the dust cylinder is rigidly rotating, and, as a result, the particles that consist the dust cylinder are also rigidly rotating. Consequently, particles at different radii will move with different velocities. Moreover, since the space–time is cylindrically symmetric and stationary, we expect that these particles have no motion in the radial and axial directions.

Ubiquitous extragalactic jets appear in active galaxies and various models have been suggested for their origin. A classic model is that of Blandford and Rees.[20] In their model a hot plasma is assumed to be steadily generated at the center of the galaxy. The central object is surrounded by a gravitationally confined rotating gas cloud. The thermal pressure of this gas cloud constrains the outflowing relativistic plasma within two oppositely directed channels. An equilibrium flow is possible only if the channel shape adjusts so that a nozzle forms where the external pressure has dropped to one-half its central value. The shape of the channel is assumed to adjust itself to a de Laval nozzle. This configuration, with a light fluid supporting a heavier fluid in a gravitational field, is well known to be unstable. Recently, Goncalves, Jatenco-Pereira, and Opher[21] suggested that Alfvén waves, created above the steep density gradient near galactic nuclei, are the origin of extragalactic jets. The differential rotation and turbulent motion in galactic nuclei create a bipolar magnetic field by dynamo action and the twisting and the reconnection of the magnetic field lines produce Alfvén waves. Various Alfvén wave damping mechanisms were investigated.

Here we point out that the confinement of the test particles in the radial direction might provide another source for the extragalactic jet formation. Our arguments go as follows: The gravitational field produced by jets usually is negligible compared with the one produced by the matter at the center of the galaxy. Thus, to the first-order approximation, it is sufficient to model those jets as made of test particles. Also, almost all the galaxies are rotating, as a first step, we can model the center of a galaxy by a rotating cylinder. This approximation seems reasonable as long as the gravitational field in the middle of the rotating galaxy is concerned, though we admit that it is indeed highly simplified. Assuming that the above simplified model can capture some essence of physics, we can see that the confinement can be related to the jets. Certainly, to have this idea really work, more realistic models should be built. For example, a rotating dust cloud with axial symmetry and being asymptotically flat in all the three spatial directions as that considered in Ref. 22. Work in this direction is in progress.

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Overall rotation of a many-body system in Dixon's theory

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Using Dixon's theory, an expression for the angular momentum of an N-body system, whose constituent bodies are monopoles that do not interact gravitationally, is obtained. In this expression the contributions to the angular momentum due to the rotational and internal motions of the material system are separated. It is also shown how the existence of a frame with respect to which the total angular momentum of an N-body system is reduced to an expression formally similar to that corresponding to a rigid body instantaneously equivalent to the material system considered. Finally, in space–times of small curvature, a separation of the energy into a part due to the rotational motion and other due to the internal motion, is investigated. © *1996 American Institute of Physics.* [S0022-2488(96)00909-8]

I. INTRODUCTION

Dixon's theory[1] gives an exact framework to describe the motion of extended material systems in a relativistic spacetime endowed with a prefixed metric structure. In this theory one uses a countably set of multipolar moments covariantly defined satisfying a finite set of ordinary differential equations which generalize the laws of motion obtained in the pole–dipole approximation by Mathisson[2] and Papapetrou.[3] Dixon's laws of motion have been confirmed by Künzle[4] using a presymplectic approach, and by Bailey and Israel[5] using the Lagrangian formalism.

In this article we consider a material system constituted by an ensemble of N bodies which are monopoles that do not interact gravitationally, and we analyze the motion referred to a rotating frame whose origin is on the center of the mass line. Firstly, we study the separability of the angular momentum into a part due to the overall rotation and a part due to both the internal motions and the choice of the temporal vector in the reference frame. Secondly, we analyze the existence of a frame with respect to which the total angular momentum of the material system is reduced to an expression formally analogous to that corresponding to a rigid body with the same instantaneous configuration (in a sense which will be precise). And, finally, we study the vanishing of the coupling terms in the expression of the energy.

In Newtonian mechanics the problems of separation in N-body systems were solved a long time ago by Tisserand.[6] He proved that for a system of particles in nonrigid motion satisfying the Liouville equations there exist frames—Tisserand axes—with their origin on the center of mass with respect to which the angular momentum is the same as that of a rigid body instantaneously equivalent to the N-particle system. Using a Tisserand frame one obtains a separation of the kinetic energy into a part due to the internal motion and another due to the overall rotation of the material system. In such a frame the Coriolis energy vanishes. The Tisserand axes can also be defined by the condition of the kinetic energy being minimum relative to such frames.

A similar energy separation has been obtained by Jellinek and Li[7] in the polyatomic molecule theory using an Eckart frame. They have shown that for a fixed total angular momentum in the center of mass frame, the configuration of the N-body system for which the total kinetic energy is minimum corresponds to that of an instantaneous rigid body. Marsden *et al.*[8] have obtained similar results for general rotating structures using a generalization of the block diagonalization theorem (see, e.g., Ref. 9).

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The remainder of this article is as follows: in Sec. II we establish basic definitions, assumptions and notation. In Sec. III we obtain one expression for the total angular momentum as a sum of three quantities associated with the motion of the center of mass, the motion of the bodies relative to the center of mass frame, and the overall rotation motion. This last contribution is written in a way analogous to that of a rigid body. In Sec. IV we show that in some cases, it is possible to define a frame (Tisserand frame) relative to which the total angular momentum is given only by a term associated to the overall rotation motion. Finally, in Sec. V we study the coupling terms which appear in the energy expression, noting that, even in a Tisserand frame, such terms do not vanish. We have verified that if the Riemannian curvature is small enough and constant, one can choose a frame with angular velocity equal to the mean angular velocity, such that in the first order of approximation with respect to the curvature the coupling terms vanish.

II. DEFINITIONS AND BASIC ASSUMPTIONS

A. Geometric model

Let $\mathscr{R}$ be a region in the space–time (M,g) of the general relativity, such that topologically it is diffeomorphic to a product manifold $\Sigma\times\mathscr{T}$ where Σ is a three-dimensional manifold and $\mathscr{T}$ is an interval in $\mathbb{R}$. We assume that in $\mathscr{R}$ there exists a differentiable function t globally defined on $\mathscr{R}$ whose gradient Dt is timelike everywhere and, also, that on $\mathscr{R}$ a foliation is defined such that its leaves are spacelike hypersurfaces Σ_t given by the level surfaces of the function t.

Now, let $l:z(t)$ be an arbitrary timelike curve of class C^1 contained in the region $\mathscr{R}$. On the curve l a field of unitary timelike vectors $n(t)$ orthogonal to Σ_t, for each $t\in\mathscr{T}$, is defined. In Dixon's theory the parametrization of l is chosen so that

$$\langle n(t),u(t)\rangle=1, \tag{1}$$

where $u(t):=dz/dt$ is tangent to the curve l at the point $z(t)$. Here we assume that for each $t\in\mathscr{T}$ and each $x\in\Sigma_t$ there exists a unique spacelike curve $\Upsilon:x(\zeta)$, $\zeta\in[0,1]\subset\mathbb{R}$, joining the points $z(t)=x(0)$ and $x=x(1)$, being its support contained in Σ_t. Then one can define the distance function[10] by

$$\sigma(z,x)=\frac{1}{2}\int_0^1\left\langle\frac{dx(\zeta)}{d\zeta},\frac{dx(\zeta)}{d\zeta}\right\rangle d\zeta. \tag{2}$$

If the exponential map $\exp_z:T_z\Sigma_t\to\Sigma_t$ is bijective, for all t, then the vector $X:=-\partial\sigma(z,x)/\partial z\in T_zM$ is equal to $X=\exp_z^{-1}x$, and X can be interpreted as the position vector of the point x relative to z.

Given a geodesic variation of Υ

$$\alpha:[0,1]\times[-\delta,\delta]\to M,\quad(\zeta,t)\mapsto\alpha(\zeta,t), \tag{3}$$

with $\alpha(\zeta,0)=\Upsilon$ and $\delta>0$, we denote by $u(x)$ the Jacobi field defined on the geodesic Υ in the form

$$u(x):=\frac{\partial\alpha}{\partial t}(\zeta,0). \tag{4}$$

In particular, if $\zeta=0$, we denote by $u(z)$ the corresponding vector. Under a variation of Υ with end points z,x moving on the curves $z(t)=\alpha(0,t)$, $x(t)=\alpha(1,t)$, respectively, the derivative of the position vector X with respect to t is given by

$$\dot{X}=DX\cdot u(x)+\mathbb{D}X\cdot u(z), \tag{5}$$

where we have used the the following notation: (1) D and $\mathbb{D}$ (see Ref. 11) denote the covariant derivatives with respect to the variables x and z, respectively; (2) $\dot{Z} := dZ/dt$, for all vector Z; (3) $A \cdot B$ denote the contracted product of two tensors A and B. Then covariant derivatives can be interpreted as linear maps DX and $\mathbb{D}X$

$$DX: T_x M \to T_z M, \quad \mathbb{D}X: T_z M \to T_z M. \tag{6}$$

Since one has assumed that for each $x \in \Sigma_t$ there is no point conjugate to x on Σ_t then there exist the inverse maps $(DX)^{-1}$ and $(\mathbb{D}X)^{-1}$, so that using the vectors X, $\dot{X} \in T_z M$ one can define on Σ_t the vector field $u(x)$ by

$$u(x) = K(z,x)u(z) + H(z,x)\dot{X}, \tag{7}$$

where the propagators $H(z,x)$ and $K(z,x)$ are the two-point tensors of type $\binom{10}{01}$ defined by

$$H(z,x) := (DX)^{-1}, \quad K(z,x) := -(\mathbb{D}X)(DX)^{-1}. \tag{8}$$

B. Description of the material system

We now consider a material system consisting of N-bodies of masses m_A $(A = 1,2,\ldots,N)$ modeled in space–time as a set of timelike curves $x_A(s_A)$ contained in the region $\mathscr{R}$ and parametrized by the arclength $s_A \in \mathscr{I}_A \subset \mathbb{R}$. At each point $x \in M$ the matter distribution is described by the symmetric tensor given by the sum of the energy tensors associated with the bodies

$$T(x) = |\det g|^{-1} \sum_{A=1}^{N} \int_{\mathscr{I}} m_A^* v_A(x) \otimes v_A(x)\, \delta(x - x_A)\, dt, \tag{9}$$

where $v_A := dx_A/ds_A$ is the normalized four-velocity of the body A, $\delta(x - x_A)$ is the Dirac distribution, and m_A^* is defined by

$$m_A^* := m_A \frac{ds_A}{dt}. \tag{10}$$

Let $n(x)$ be the unit normal vector field on an arbitrary leaf Σ_t of the foliation of $\mathscr{R}$. The metric tensor g on M induces on Σ_t a Riemann metric

$$\gamma(x) := g(x) - n^\flat(x) \otimes n^\flat(x), \tag{11}$$

where $\flat$ denotes the index lowering operator. Let $d\Sigma$ denote the volume element on Σ_t defined by the metric γ. In Dixon's theory, given an energy-momentum distribution $T(x)$ one defines[1] the linear momentum vector $p(z,\Sigma) \in T_z M$ and the angular momentum bivector $S(z,\Sigma) \in \Lambda^2(T_z M)$ relative to a reference curve l and a leaf Σ_t as

$$p(z,\Sigma) := \int_{\Sigma_t} K(z,x)(T(x) \cdot n(x))\, d\Sigma \tag{12}$$

and

$$\mathsf{S}(z,\Sigma) := \int_{\Sigma_t} X \wedge [H(z,x)(T(x) \cdot n(x))]\, d\Sigma, \tag{13}$$

respectively. Thus, for the energy-momentum (9) one obtains

$$p(z,\Sigma)=\sum_{A=1}^{N} m_A^* K(z,x)v_A(x), \tag{14}$$

$$\mathsf{S}(z,\Sigma)=\sum_{A=1}^{N} m_A^* X_A \wedge (H(z,x)v_A(x)). \tag{15}$$

Now, from the second expression in Eq. (8) one can define, for each body, a vector $\mathsf{p}_A(x)$ by

$$\mathsf{p}_A(z):=-(\mathbb{D}X_A)^{-1}(p_A(z)). \tag{16}$$

Using the vectors $\mathsf{p}_A(x)$ one can write Eq. (15) in the equivalent form

$$\mathsf{S}(z,\Sigma)=\sum_{A=1}^{N} X_A \wedge \mathsf{p}_A(z) \tag{17}$$

formally analogous to the classical expression of the angular momentum.

From now on we assume that the energy-momentum distribution and the curvature of the space–time satisfy the conditions stated by Schattner,[12] to assure the existence and uniqueness of the center of mass line defined by

$$\mathsf{S}(z,\Sigma)\lrcorner n^\flat(z)=0. \tag{18}$$

The reference curve l will be taken to be the center of the mass line. The angular momentum (vector) relative to the curve l and the foliation Σ_t is the vector field S defined on the reference line by

$$S=\star(\mathsf{S}\wedge n), \tag{19}$$

where $\star$ denotes the Hodge star operator. Due to Eq. (18) the vectors S and n satisfy the orthogonality conditions

$$S\lrcorner n^\flat=0. \tag{20}$$

III. ANGULAR MOMENTUM RELATIVE TO A ROTATING FRAME

Let $\{e_\kappa(t)\}$ and $\{e_{\kappa'}(t)\}$ $(\kappa,\kappa'=0,1,2,3)$ be orthonormal frame fields on the line l satisfying $e_0(t)=e_{0'}(t)=n(t)$, for all $t\in\mathscr{I}$, and such that the frame $\{e_\kappa(t)\}$ satisfies the Dixon transport law without rotation

$$\dot{e}_\kappa=(n\wedge n)\lrcorner e_\kappa^\flat, \tag{21}$$

while $\{e_{\kappa'}(s)\}$ satisfies the Dixon transport law with rotation

$$\dot{e}_{\kappa'}=(n\wedge\dot{n}+\Omega')\lrcorner e_\kappa^\flat, \tag{22}$$

where Ω' is the angular velocity bivector of the frame $\{e_{\kappa'}\}$ relative to $\{e_\kappa\}$. For this bivector the orthogonality condition

$$\Omega'\lrcorner n^\flat=0 \tag{23}$$

holds. From Ω' one can define the angular velocity (vector) ω' as

$$\omega':=\star(\Omega'\wedge n'). \tag{24}$$

The frames $\{e_\kappa(t)\}$ and $\{e_{\kappa'}(t)\}$ are related by a pure spacelike rotation $R(t)$. We use the following notation: $Z(t)$ refers to an arbitrary vector in T_zM expressed in the frame $\{e_\kappa(t)\}$ while $Z'(t)$ refers to the same vector expressed in the frame $\{e_{\kappa'}\}$. So, if Z' is a spacelike vector then Z is given by

$$Z(t)=R(t)Z'(t). \tag{25}$$

Differentiating Eq. (25) with respect to t one obtains

$$\dot{Z}=R(\dot{Z}'+\Omega'\lrcorner Z'). \tag{26}$$

The components of the vector $X=\exp_z^{-1}x$ with respect to the bases $\{e_\kappa(t)\}$ and $\{e_{\kappa'}(t)\}$ define, respectively, on the submanifold Σ_t normal coordinate systems $\{X^a\}$ and $\{X^a\}$ with a pole at z. Moreover, choosing $X^0=X'^0=t$ one obtains in the region $\mathscr{R}$ normal coordinate systems $\{X^\mu\}$ and $\{X'^\mu\}$ with base line l. Following Dixon, we treat a two-point tensor $t(z,x)$ of type $\binom{s0}{r0}$ as a tensor dependent on of the variables z and X. Since $dx=H(z,x)dX$, we have that the Jacobian of the coordinate transformation of (z,x) into (z,X) is given by $H(z,x)$. Therefore, if $\{X^\mu\}$ is chosen to be a normal coordinate system then the Jacobian is reduced to the unit matrix. Henceforth we will use only normal coordinates.

From Eqs. (16) and (26) one obtains for the vector field $\mathsf{p}(z)$ relative to the frame $\{e'_\kappa\}$ the expression

$$\mathsf{p}'_A(z)=m_A^*(U'_A+\dot{X}'_A+\Omega'\lrcorner X'_A), \tag{27}$$

where

$$U'_A:=-R^{-1}(\mathbb{D}X_A\cdot u(z)) \tag{28}$$

has been defined. Then, from Eqs. (19), (17), and (27) we obtain for the total angular momentum $S'(z)$ relative to the center of mass line l and the foliation Σ_t the expression

$$S'(z)=S'^{\mathrm{REL}}+S'^{\mathrm{DEF}}+S'^{\mathrm{ROT}} \tag{29}$$

where

$$S'^{\mathrm{REL}}:=\sum_{A=1}^{N}\star(X'_A\wedge U'_A\wedge n'_A)m_A^*, \tag{30}$$

$$S'^{\mathrm{DEF}}:=\sum_{A=1}^{N}\star(X'_A\wedge \dot{X}'_A\wedge n'_A)m_A^*, \tag{31}$$

$$S'^{\mathrm{ROT}}:=\sum_{A=1}^{N}\star(X'_A\wedge\Omega'\cdot X'_A\wedge n'_A)m_A^*. \tag{32}$$

If the space–time is flat then, in suitable coordinates, $\mathbb{D}X$ is given by the unit matrix and one gets $U'_A(z)=R^{-1}u(z)$. Furthermore, if $u(z)$ is parallel to $n(z)$, then S'^{REL} vanishes.

On the other hand, if the position vectors of each body relative to the frame $\{e'_\kappa\}$ are independent of the parameter t then S'^{DEF} vanishes. So, S'^{DEF} may be regarded as the angular momentum due to the deformation of the material system.

Finally, S'^{ROT} may be interpreted as the angular momentum due to the overall rotation of the material system. In fact, if we define the inertia momentum map

$$\mathbb{I}':T_zM \to T_zM, \quad \omega' \mapsto \sum_{A=1}^{N} \star(X'_A \wedge (\Omega' \lrcorner X'_A) \wedge n')m_A^*, \tag{33}$$

where Ω' and ω' are related by Eq. (24), then Eq. (32) can be written as

$$S'^{\mathrm{ROT}} = \mathbb{I}' \cdot \omega' \tag{34}$$

or in the equivalent form

$$S'^{\mathrm{ROT}} = \sum_{A=1}^{N} [m_A^*(X'_A \cdot X'_A)\mathbb{1} - X'_A \otimes X'_A] \cdot \omega'. \tag{35}$$

Expressions (34) and (35) for S^{ROT} are similar to those in classical rigid body dynamics. Note, however, that the evolution of the inertia tensor $\mathbb{I}(t)$, does not correspond to that associated with a rigid body (see Ref. 13). For motions of the material system satisfying $S'^{\mathrm{REL}} + S'^{\mathrm{DEF}} = 0$ at a fixed time t, S^{ROT} coincides with the total angular momentum of an ensemble of N bodies of masses m_A^* whose instantaneous configuration is the same as the configuration of the material system considered (at that instant t). Next, we verify that at each time there exists a rotating frame with angular velocity ϖ' such that the total angular momentum relative to this frame is Eq. (34).

IV. EXISTENCE OF TISSERAND'S AXES IN GENERAL RELATIVITY

Assuming that no external moments act on an arbitrary material system whose multipolar structure is of the type pole–dipole, the total angular momentum $S(z)$ relative to a frame $\{e_\mu(z)\}$ defined by Eq. (21) satisfies[1]

$$\dot{S} = p \wedge v. \tag{36}$$

Using the angular momentum vector $S \in \langle n \rangle^{\perp}$, defined by Eq. (19), Eq. (36) can also be written as

$$\Pi(\dot{S}) = 0, \tag{37}$$

where Π is the projector onto $\langle n \rangle^{\perp}$ associated to (11).

From Eqs. (26) and (37) it follows that the equation for the angular momentum relative to the frame $\{e'_\mu(z)\}$ defined by Eq. (22) is given by

$$\Pi(\Omega' \lrcorner S' + \dot{S}) = 0. \tag{38}$$

Furthermore, since the orthogonality condition $S' \cdot n'^{\flat} = 0$ is equivalent to Eq. (20), Eq. (38) can be expressed as

$$\dot{S}' = -(\dot{n}'^{\flat} \cdot S')n' - \Pi(\star(\omega' \wedge n') \lrcorner S'). \tag{39}$$

Then, for an N-body system with angular momentum $S'(z)$ given by Eq. (29), Eq. (39) is the relativistic analog to the Liouville equation (see Ref. 6).

We now suppose that $\{e'_\mu(z)\}$ is rotating relative to $\{e_\mu(z)\}$ with angular velocity ϖ', and that the angular momentum S' is given by Eq. (34). Then the angular velocity ϖ' satisfies the linear differential equation

$$\mathbb{I}'\dot{\varpi}' = -(\dot{n}'^{\flat} \lrcorner (\mathbb{I}' \cdot \varpi'))n' - \Pi[\star(\varpi' \wedge n') \lrcorner (\mathbb{I}' \cdot \varpi')^{\flat}] - \dot{\mathbb{I}}' \cdot \varpi'. \tag{40}$$

Here the inertia tensor $\mathbb{I}'(t)$ is taken to be a known function of $t \in \mathscr{I}$. Fix an initial value $\varpi'(0)$ for the angular velocity, Eq. (40) determines a unique vector field $\varpi'(z)$ on the reference curve l. On

the other hand, given an initial frame $\{e'_\mu(0)\}$, Eq. (22) (with Ω' replaced by ϖ') defines a unique orthonormal frame field $\{\tilde{e}'_\mu(t)\}$ with respect to which the angular momentum satisfies $S'=\mathbb{I}'\cdot\varpi'$. So, this frame field corresponds precisely with the Tisserand axes.[14]

V. SEPARATION OF THE ENERGY

Let us consider the linear momentum written in the form

$$p'_A(z)=\mathbb{D}X'_A\cdot(\mathsf{p}'^{\,\mathrm{INT}}_A+\mathsf{p}'^{\,\mathrm{ROT}}_A), \tag{41}$$

where $\mathsf{p}'^{\,\mathrm{INT}}_A$ and $\mathsf{p}'^{\,\mathrm{ROT}}_A$ are defined by

$$\mathsf{p}'^{\,\mathrm{ROT}}_A:=m^*_A\Omega'\lrcorner X'^{\,\flat}_A,\quad \mathsf{p}'^{\,\mathrm{INT}}_A:=m^*_A(U'_A+\dot{X}'_A), \tag{42}$$

which represent the parts of p'_A associated to the overall rotation of the material system and the rest of motions, respectively.

Let ξ'_A be one-form fields defined on each curve $x_A(t)$ as

$$\xi'_A:=m_A^{-1}p'_A.$$

At each time the energy of the material system is defined by

$$\mathscr{E}=\sum_{A=1}^{N}\langle p'_A,\xi'_A\rangle. \tag{43}$$

In a neighborhood of the curve l the derivative $\mathbb{D}X'_A$ can be represented as a power series whose summands depend on the Riemann tensor, Riem. Thus, if the curvature is small, $\mathbb{D}X$ can be approximated retaining in the series the summands of first order in Riem given explicitly in Synge.[10] We write

$$\mathbb{D}X_A(z,x)=g(z)+\mathscr{G}_A(z,x)+O(|\mathrm{Riem}|^2), \tag{44}$$

where $g(z)$ is the metric tensor at the point z, and $\mathscr{G}_A$ is the summand of first order in Riem. Therefore Eq. (43) is equivalent to

$$\mathscr{E}=\sum_{A=1}^{N} m_A^{-1}\langle\mathsf{p}'_A,\mathsf{p}'_A\rangle+m_A^{-1}\langle\mathsf{p}'_A,\mathscr{G}_A\cdot\mathsf{p}'_A\rangle+m_A^{-1}\langle\mathscr{G}_A\cdot\mathsf{p}'_A,\mathscr{G}_A\cdot\mathsf{p}'_A\rangle. \tag{45}$$

In first approximation with respect to the curvature one gets from Eqs. (45) and (41), the expression

$$\mathscr{E}=\sum_{A=1}^{N} m_A^{-1}\langle\mathsf{p}'^{\,\mathrm{INT}}_A,\mathsf{p}'^{\,\mathrm{INT}}_A\rangle+m_A^{-1}\langle\mathsf{p}'^{\,\mathrm{ROT}}_A,\mathsf{p}'^{\,\mathrm{ROT}}_A\rangle+2m_A^{-1}\langle\mathsf{p}'^{\,\mathrm{INT}}_A,\mathsf{p}'^{\,\mathrm{ROT}}_A\rangle$$
$$+2m_A^{-1}\langle\mathsf{p}'_A,\mathscr{G}_A\cdot\mathsf{p}'_A\rangle+O(|\mathrm{Riem}|^2). \tag{46}$$

Let us first consider the zero order of approximation to Eq. (45). In this case the only coupling term is $\Sigma_{A=1}^{N}\langle\mathsf{p}'^{\,\mathrm{INT}}_A,\mathsf{p}'^{\,\mathrm{ROT}}_A\rangle$. From Eq. (42) this term can be written as

$$\sum_{A=1}^{N} m_A^{-1}\langle\mathsf{p}'^{\,\mathrm{INT}}_A,\mathsf{p}'^{\,\mathrm{ROT}}_A\rangle=\sum_{A=1}^{N}\mathsf{p}'^{\,\mathrm{INT}}_A\cdot(\star(\omega'\wedge n')\lrcorner X^{\flat}_A)m^*_Am_A^{-1}. \tag{47}$$

But, given the unitary orthogonal vectors $V,W\in T_zM$ the equation

$$Y\cdot(\star(V\wedge W)\lrcorner Z^{\flat})=W\cdot(\star(V\wedge Z\wedge Y)) \tag{48}$$

is satisfied for all $Y,Z\in T_zM$. Thus Eq. (47) takes the form

$$\sum_{A=1}^{N} m_A^{-1}\langle \mathsf{p}_A'^{\mathrm{INT}},\mathsf{p}_A'^{\mathrm{ROT}}\rangle=\omega'\cdot\sum_{A=1}^{N}\star(\mathsf{p}_A'^{\mathrm{INT}}\wedge X_A'\wedge n')\,\frac{ds_A}{dt}, \tag{49}$$

where we have used definition (10).

We now choose a frame which rotates with an angular velocity ϖ such that the angular momentum (29) is reduced to

$$\tilde{S}(z)=\mathbb{I}\cdot\varpi \tag{50}$$

so that the sum of Eqs. (30) and (31) vanishes

$$\sum_{A=1}^{N}\star(X_A'\wedge\mathsf{p}_A'^{\mathrm{INT}}\wedge n')m_A^{*}=0. \tag{51}$$

Note that in general relativity the above choice of the frame is not sufficient to establish the vanishing of the expression (49). However, if the coefficients ds_A/dt in Eq. (49) coincide, one gets a separation of $\mathscr{E}$ into a part associated with the overall rotation and other due to internal motions.

Let us return to the expression of first order (46). In this order of approximation the following coupling terms are also present:

$$2\sum_{A=1}^{N}(m_A^{-1}\langle \mathsf{p}_A'^{\mathrm{INT}},\mathscr{G}_A\cdot\mathsf{p}_A'^{\mathrm{ROT}}\rangle+m_A^{-1}\langle \mathsf{p}_A'^{\mathrm{ROT}},\mathscr{G}_A\cdot\mathsf{p}_A'^{\mathrm{INT}}\rangle). \tag{52}$$

Now, given arbitrary vectors $Y(0),Z(0)\in T_zM$, let $Y(\zeta),Z(\zeta)\in T_xM$ be the images of $Y(0),Z(0)$, respectively, obtained by parallel transport from z to the point $x(\zeta)$ on the geodesic $x_A(\zeta)$; we have

$$\langle Y(0),\mathscr{G}_A\cdot Z(0)\rangle=\frac{3}{2}\int_0^1\mathscr{S}(Y(\zeta),V(\zeta))V(\zeta)\cdot Z(\zeta)(1-\zeta)^2\,d\zeta, \tag{53}$$

where $V(\zeta)$ is the tangent vector to $x_A(\zeta)$, and $\mathscr{S}(A,B)C$ is the symmetrized Riemann tensor[10] defined by

$$\mathscr{S}(A,B)C=-\tfrac{1}{3}(R(A,C)B+R(A,B)C) \tag{54}$$

for all $A,B,C\in T_xM$, satisfying the properties

$$\mathscr{S}(A,B)=\mathscr{S}(B,A), \tag{55}$$

$$\mathscr{S}(A,B)C\cdot D=\mathscr{S}(A,B)D\cdot C, \tag{56}$$

$$\mathscr{S}(A,B)C\cdot D=\mathscr{S}(C,D)A\cdot B. \tag{57}$$

So, from Eqs. (53) and (55)–(57) one obtains for Eq. (52) an equivalent expression of the form

$$4\sum_{A=1}^{N} m_A^{-1}\langle \mathsf{p}_A'^{\mathrm{INT}},\mathscr{G}_A\cdot\mathsf{p}_A'^{\mathrm{ROT}}\rangle. \tag{58}$$

In arbitrary space–times this expression is nonvanishing. However, one exception occurs when the space–time is of constant curvature. Indeed, if the curvature is constant, then

$$\mathscr{R}(Y,V)V\cdot Z=\tfrac{2}{3}K[(Y\cdot Z)(V\cdot V)-(Y\cdot V)V\cdot Z)], \tag{59}$$

where K is the Riemannian curvature. Consequently Eq. (58), in this special case, is equivalent to

$$4K\sum_{A=1}^{N} m_A^{-1}\int_0^1[(\mathsf{p}_A'^{\mathrm{INT}}\cdot\mathsf{p}_A'^{\mathrm{ROT}})(V\cdot V)-(\mathsf{p}_A'^{\mathrm{INT}}\cdot V)(V\cdot\mathsf{p}_A'^{\mathrm{ROT}})](1-\zeta)^2\,d\zeta \tag{60}$$

and, since $x_A(\zeta)$ is a geodesic, the term in square brackets in Eq. (60) is independent of ζ. Therefore Eq. (60) becomes

$$\frac{4}{3}K\sum_{A=1}^{N} m_A^{-1}(\mathsf{p}_A'^{\mathrm{INT}}\cdot\mathsf{p}_A'^{\mathrm{ROT}})(V\cdot V)-\frac{4}{3}K\sum_{A=1}^{N} m_A^{-1}(\mathsf{p}_A'^{\mathrm{INT}}\cdot V)(V\cdot\mathsf{p}_A'^{\mathrm{ROT}}). \tag{61}$$

If the coupling term (47) vanishes, then the first sum in (61) also vanishes. Finally, using Eq. (48) we obtain

$$V\cdot\mathsf{p}_A'^{\mathrm{ROT}}=V\cdot(\star(\omega'\wedge n')\lrcorner X_A'^{\,b})m_A^*=\omega'\cdot(\star(V\wedge X_A'\wedge n'))m_A^*, \tag{62}$$

which vanishes since V and X_A' are parallel.

VI. CONCLUSION

We have shown in Eq. (29) that the total angular momentum of an ensemble of N-bodies, relative to a frame satisfying the Dixon transport law along the center of mass line, admits a separation in three terms. Apart from two summands depending, respectively, on the deformation and overall rotation motions (analogous to those which appear in Newtonian mechanics) in this separation a summand which depends on the choice of the unit vector field n on the center of mass line is also present.

On the other hand, we have verified that one can choose a Tisserand-type frame relative to which the total angular momentum is, for each $t\in\mathscr{T}$, similar to that corresponding to a rigid solid. In the associated inertia tensor the mass of the bodies has been substituted by m_A^* defined in Eq. (10). So, the inertia tensor depends both on the geometric configuration and the parametrization of the timelike curve associated to each particle.

Finally, in Eq. (46) an approximate expression for the energy of an N-body system has been obtained in the case of small Riemannian curvature. The choice of a Tisserand-type frame does not imply, in general, that the coupling terms (47) and (52) presented in Eq. (46) vanish. We have studied a case in which such coupling terms vanish. For this we have assumed (1) that the world lines in the material system all have the same parametrization and (2) that the curvature is constant.

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Obstructions to pin structures on Kleinian manifolds

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We develop various topological notions on four-manifolds of Kleinian signature $(--++)$. In particular, we extend the concept of ''Kleinian metric homotopy'' to nonorientable manifolds. We then derive the topological obstructions to pin-Klein cobordism for all of the pin groups. Finally, we discuss various examples and applications which arise from this work. © *1996 American Institute of Physics.* [S0022-2488(96)03101-3]

I. INTRODUCTION

Let M be any smooth four-manifold, then we say that a metric g on M is of *Kleinian signature* if it has signature $(--++)$. In recent work,[1] we derived the topological obstruction to spin-Klein cobordism, and in this paper, we treat the interesting and nontrivial problem of extending this work to nonorientable manifolds.

An orientable Kleinian manifold (M,g) has orthonormal frame bundle $\tau(M)$ with structure group SO(2,2). We say that M admits a *spin structure* if and only if there exists a $2-1$ covering, $\bar{\tau}(M)\rightarrow\tau(M)$, such that the following diagram commutes:

$$\begin{array}{ccccc} \mathrm{Spin}(2,2) & \longrightarrow & \bar{\tau}(M) & \longrightarrow & M \\ \downarrow 2-1 & & \downarrow 2-1 & & \downarrow \ \text{identity} \\ SO(2,2) & \longrightarrow & \tau(M) & \longrightarrow & M \end{array}$$

where Spin(2,2) is the double cover of SO(2,2).

When M is nonorientable, one cannot reduce the tangent bundle $\tau(M)$ to a bundle with structure group SO(2,2); indeed, $\tau(M)$ can only be reduced to a bundle with structure group O(2,2). In analogy with the above construction, we then seek all groups $\overline{\mathrm{O}}(2,2)$ which are double covers of O(2,2); that is, we seek all groups $\overline{\mathrm{O}}(2,2)$ so that the following sequence is exact:

$$1\rightarrow\mathbb{Z}_2\rightarrow\overline{\mathrm{O}}(2,2)\rightarrow\mathrm{O}(2,2)\rightarrow 1.$$

In fact (see, e.g., Refs. 2 and 3), there are eight distinct such groups which are double covers of O(2,2). Following Dabrowski,[2] we will call these covers the *pin groups* for Kleinian signature and write them as

$$h^{a,b,c}:\mathrm{Pin}^{a,b,c}(2,2)\rightarrow\mathrm{O}(2,2)$$

with $a,b,c\in\{+,-\}$.

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In order to interpret the signs a, b, and c, it is convenient to keep some of the terminology from Lorentzian geometry. Thus we will say that a vector $v \in T_p(M)$ is *spacelike* if $g(v,v)>0$, *timelike if* $g(v,v)<0$, and *null* if $g(v,v)=0$.

Now we recall that O(2,2) is not path-connected; there are four components, given by the identity connected component $\mathrm{O}_0(2,2)$ and the three components corresponding to ''space'' inversion S, ''time'' inversion T, and the combination of these two, ST (i.e., O(2,2) decomposes into a semidirect product, $\mathrm{O}(2,2)\simeq \mathrm{O}_0(2,2)\odot(\mathbb{Z}_2\times\mathbb{Z}_2)$) (i.e., O(2,2) is the disjoint union $\mathrm{O}(2,2)\simeq \mathrm{O}_0(2,2)\cup S(\mathrm{O}_0(2,2))\cup T(\mathrm{O}_0(2,2))\cup ST(\mathrm{O}_0(2,2))$). By space inversion, we mean reflection about a plane, $v^{\perp}$, perpendicular to some spacelike vector v; likewise, time inversion is reflection about a plane perpendicular to a timelike vector. The signs of a, b, and c then correspond to the signs of the squares of the elements in $\mathrm{pin}^{a,b,c}(2,2)$ which cover space inversion, time inversion, and a combination of the two, respectively.

Indeed, with these conventions we can write out the explicit form of the groups $\mathrm{Pin}^{a,b,c}(2,2)$; they are given by the semidirect product[2]

$$\mathrm{Pin}^{a,b,c}(2,2)\simeq \frac{(\mathrm{Spin}_0(2,2)\odot C^{a,b,c})}{\mathbb{Z}_2},$$

where $C^{a,b,c}$ are the double coverings of $\mathbb{Z}_2\times\mathbb{Z}_2$, as outlined in Refs. 2 and 3.

On surveying the above constructions, one might wonder why we are concerned with developing the obstruction theory for $\mathrm{Pin}^{a,b,c}(2,2)$ fiber bundles, since with $\pi_1(\mathrm{O}(2,2))\simeq\mathbb{Z}\times\mathbb{Z}$, and so there is no way that the pin bundles will allow us to represent all of the information contained in the tangent bundle in a simply connected manner.[3] Indeed, if we wished to represent the information in $\tau(M)$ in a simply connected manner, we would seek a bundle $\xi(M)$, with structure group $\hat{\mathrm{O}}$ given by the exact sequence

$$1\rightarrow \pi_1(\mathrm{O}(2,2))\simeq\mathbb{Z}\times\mathbb{Z}\rightarrow\hat{\mathrm{O}}\rightarrow\mathrm{O}(2,2)\rightarrow 1,$$

whereas the pin groups are given by the short exact sequence

$$1\rightarrow\mathbb{Z}_2\rightarrow\mathrm{Pin}^{a,b,c}(2,2)\rightarrow\mathrm{O}(2,2)\rightarrow 1.$$

It follows that any pin bundle $P(M)$ (i.e., any bundle with fiber $\mathrm{Pin}^{a,b,c}(2,2)$) will not represent information in a simply connected way. This means that at a point $p\in M$ there exist paths ρ_1, $\rho_2\in\mathrm{Pin}^{a,b,c}(2,2)$ which might act on the fiber $P(M)|_p$ equivalently (in the sense that, for $x\in P(M)|_p$, $\rho_1(x)=\rho_2(x)$), but with the property that ρ_1 and ρ_2 (viewed as curves in $\mathrm{Pin}^{a,b,c}(2,2)$) are not homotopic. Indeed, one sees that the ''particles'' corresponding to such a simply connected representation could have arbitrary fractional statistics and would be ''anyons.''[4] The point is that for both Riemannian and Lorentzian signature (in four dimensions) one obtains a simply connected representation of tangent bundle information by passing to a fermionic (or pin) bundle; it is only for Kleinian signature that this does not work and one needs to introduce some anyonic structure.

At any rate, these mathematical considerations aside, the primary reason why we wish to understand the obstructions to pin bundles comes from physics. In particular, recent work on signature change (see, e.g., Refs. 5–8) has suggested that we should allow for regions of non-Lorentzian signature in our description of nature. The idea is that we should consider manifolds of the form $M\cong M_L\cup M_R$ and $M'\cong M'_L\cup M'_K$, where (for example) M_R is some Riemannian manifold, M_L and M'_L are some Lorentzian manifolds, and M'_K is some Kleinian manifold (where $\emptyset\neq\partial M_L=\Sigma=\partial M_R$ and $\partial M'_L=\Sigma'=\partial M'_K\neq\emptyset$, so that the signature is said to ''change'' across the three-surfaces Σ and Σ', which are generically taken to be stationary with respect to the ambient

four-metrics). If one is going to assert that there are ''regions'' of Kleinian signature, then one should try to make sense of field theory[8] in signature $(---+)$. In particular, one must make sense of the Dirac equation:

$$i\gamma^a\partial_a\psi=0, \tag{1}$$

where $\{\gamma^a,\gamma^b\}=2g^{ab}$. Solutions of Eq. (1) will generically take values in some pin bundle, and so this is one reason the cobordism problem is so interesting. There are other physical applications for Kleinian signature manifolds, including the $N=2$ superstring theory.[9] In this theory, the Weyl anomaly cancels provided the string propagates in a four-dimensional target space, and if the worldsheet has Lorentzian signature then the target space must have Kleinian signature.

II. KLEIN METRIC HOMOTOPY

We wish to understand the topology of Klein metrics on four-manifolds which are not necessarily orientable. The fundamental result we begin with is the following lemma of Steenrod:[10]

Lemma 1: Let M be a smooth four-manifold without boundary. Then M admits a globally defined (nonsingular) Klein metric if and only if there exists a globally defined (nonsingular) field of 2-planes on M.

In Ref. 1, we restricted our consideration to fields of oriented 2-planes; i.e., since we were only considering orientable four-manifolds M, we assumed that there were no closed loops γ in M around which we could propagate a 2-plane, P, and end up with the opposite orientation (of the plane P). Technically, this meant that we assumed our plane fields to be sections of the fiber bundle over M with fiber $G_{2,4}\cong S^2\times S^2$, where $G_{2,4}$ is (by definition) the set of oriented 2-planes in $\mathbb{R}^4$.

If, however, M is nonorientable then there will exist loops in M such that, when we propagate plane fields around them, the orientation of the planes will be reversed. In this case, we must now define a *plane field* to be a section of the bundle of unoriented planes. That is, let $\widetilde{G}_{2,4}$ denote the set of unoriented plane fields in $\mathbb{R}^4$. Then a field of 2-planes is a section of the fiber bundle with fiber $\widetilde{G}_{2,4}$.

This situation is reminiscent of what happens in Lorentzian geometry when one passes from the study of time-orientable geometries to non-time-orientable geometries[3,11]; there, one passes from a vector field to a ''line'' field (i.e., an undirected or unoriented vector field). However, the analogy should not be taken too far. In Lorentzian geometry, non-time-orientability is a serious matter since it implies that we have no local notion of an ''arrow of time,'' and thus many of our thermodynamical notions become tenuous.

For Kleinian geometry, there is no ''arrow of time,'' since at a point there is a ''2-plane's'' worth of timelike directions. In other words, when we identify a Kleinian metric g with a 2-plane field P, we can essentially take P to be the plane spanned by the set of timelike directions (at each point). Indeed, in this paper we will always take P to be a ''timelike'' plane field. It follows that there is no sensible notion of causal structure, or of causality, in a Kleinian manifold. In fact, there are ''closed timelike curves'' through every point. One can always just ''rotate'' into one's own past. Indeed, time itself has a chirality (i.e., the orientation of the plane field P). These considerations, if anything, make it clear that orientability is less relevant in Kleinian geometry than it is in Lorentzian geometry.

Now that we have made sense of what we mean by a ''field of unoriented 2-planes,'' we need to consider the obstruction to constructing such a 2-plane field which is globally nonsingular. To do this, we first examine the details of Hirzebruch and Hopf's[12] original treatment of the subject.

Let M be an oriented smooth manifold, and P some field of oriented 2-planes on M. Generically, P will be singular on a finite set of points, $\{p_1,p_2,\ldots,p_n\}$ in M. Each singularity p_i of P will have associated to it an index. The index of the singularity p_i is the homotopy type of the map (defined by the plane field P) from a little three-sphere, $S^3(p_i)$, surrounding p_i to $G_{2,4}$. Such

homotopy classes are in one-to-one correspondence with elements of $\pi_3(G_{2,4}) \simeq \mathbb{Z}\oplus\mathbb{Z}$. Thus, the index of P at p_i is classified by a pair of integers (intuitively, this index measures the ''winding'' of P as one moves around $S^3(p_i)$). We denote the index of P at p_i by the symbol $\mathrm{ind}(P,p_i)$. Since there are generically finitely many singular points p_i, one can form the *index* of P on M:

$$\text{index of } P \text{ on } M = \sum_{i=1}^{n} \mathrm{ind}(P,p_i).$$

In Ref. 12, Hirzebruch and Hopf developed a result which gives the exact form of the index for orientable manifolds without boundary. The statement of their result is as follows:

Let M be an oriented compact four-manifold without boundary. Let H denote the free Abelian group $H^2(M,\mathbb{Z})$/torsion subgroup, and let S denote the intersection pairing on H defined by the cup-product (i.e., S defines a map from $H\otimes H$ to $\mathbb{Z}$ by taking the cup-product of elements in H and evaluating them on the fundamental orientation class of M). Define the coset $W\subseteq H/2H$ by $w\in W$ if $S(w,x)=S(x,x) \bmod 2$ for all $x\in H$. Finally, let Ω denote the set of integers $\{S(w,w)|w\in W\}$, then we have (Refs. 12 and 13)

Theorem 1: Let M be an oriented compact four-manifold without boundary. Then M has a field of 2-planes with finite singularities. The total index of such a field is given by a pair of integers (a,b). The following integers, and only these, occur as the index for some plane field on M:

$$a=\tfrac{1}{4}(\alpha-3\sigma-2\chi), \quad b=\tfrac{1}{4}(\beta-3\sigma+2\chi),$$

where $\alpha,\beta\in\Omega$, $\chi=\chi(M)$ denotes the Euler number of M, and $\sigma=\sigma(M)$ denotes the Hirzebruch signature of M.

We wish to be able to calculate the index of a plane field on a nonorientable manifold, and thus it is instructive to examine the proof of this theorem to see exactly which steps are invalid when one passes to the nonorientable case.

To begin with, recall that the *Stiefel manifold* $V_{2,4}$ is defined to be the set of oriented dyads[14] $\{v_1,v_2\}$ in $\mathbb{R}^4$. It is clear that any dyad $\{v_1,v_2\}$ induces a plane P (i.e., P is spanned by v_1 and v_2) and so we have the inclusion

$$\varphi: V_{2,4}\rightarrow G_{2,4}.$$

Likewise, we can consider the Stiefel manifold $\widetilde{V}_{2,4}$ of unoriented dyads in $\mathbb{R}^4$; then we have the inclusion

$$\widetilde{\varphi}: \widetilde{V}_{2,4}\rightarrow \widetilde{G}_{2,4}.$$

Now, in Ref. 12, the construction begins by considering the *skeleton*[15] of M. Let M^1 denote the 1-skeleton, M^2 the 2-skeleton, etc., then we always can put a dyad field $\{v_1,v_2\}$ (a section of the fiber bundle with fiber $V_{2,4}$ or $\widetilde{V}_{2,4}$) on the 2-skeleton. If M is oriented, we can take this dyad field to be oriented; if M is not oriented, we will generically have to take the dyad field to be unoriented. We then want to extend the dyad field on M^2 to a dyad field on M^3. In the oriented case, the obstruction to doing this is $w_3(M)$[14], the third Stiefel–Whitney class of M. Of course, for a compact oriented M, $w_3(M)=0$, and so one is able to conclude[12] that the obstruction to extending a plane field to all of M must be an element of $H^4(M;\pi_3(G_{2,4}))\simeq H^4(M;\mathbb{Z}\oplus\mathbb{Z})$ $\simeq H^4(M;\mathbb{Z})\oplus H^4(M;\mathbb{Z})\simeq\mathbb{Z}\oplus\mathbb{Z}$.

When M is not oriented, it might be thought that there is some other obstruction to extending a dyad field (and thus a plane field) from M^2 to M^3. However, this is not the case. Although Wu's formula[14] shows that $w_3(M)$ can be nonvanishing for M nonoriented, $w_3(M)$ will no longer be the obstruction to extending the field P to M^3 since we are now allowing the plane field to be

unoriented. Indeed, the obstruction to this extension vanishes as long as P is a section of a $\widetilde{G}_{2,4}$ bundle. It follows that the obstruction to extending an unoriented plane field P over an unoriented four-manifold M is an element of $H^4(M;\pi_3(\widetilde{G}_{2,4}))$. But $G_{2,4}$ is the $2-1$ cover of $\widetilde{G}_{2,4}$ and so

$$\pi_3(G_{2,4})\simeq\pi_3(\widetilde{G}_{2,4})\simeq\mathbb{Z}\oplus\mathbb{Z}.$$

Thus, in both the oriented and nonoriented cases, the obstruction to extending P over M is an element of $H^4(M;\mathbb{Z}\oplus\mathbb{Z})$.

At first, this may seem strange, since for a nonorientable manifold M, $H^4(M;\mathbb{Z})\simeq\mathbb{Z}_2$, and so the total index would seem to be an element of

$$H^4(M;\mathbb{Z}\oplus\mathbb{Z})\simeq H^4(M;\mathbb{Z})\oplus H^4(M;\mathbb{Z})\simeq\mathbb{Z}_2\oplus\mathbb{Z}_2,$$

and so the index is only defined ''up to parity.'' However, as we shall see, the parity of the index is the only thing relevant in the construction of our obstructions.

Before continuing with the derivation of the form of the index, it is necessary to recall some elementary topological objects which we will make use of later. To begin with, we have that a manifold M admits a globally defined metric of Kleinian signature if and only if the tangent bundle of M ($\tau(M)$) can be globally decomposed into the Whitney sum

$$\tau(M)\simeq\tau^+\oplus\tau^-,$$

where τ^+ is the subbundle of $\tau(M)$ generated by spacelike vectors and τ^- is the subbundle generated by timelike vectors. Let $w_1(M)=w_1(\tau(M))$ denote the *first Stiefel–Whitney class* of M. As is well known,[14] $w_1(M)=0$ if and only if M is orientable. Since w_1 is a 1-cochain, this means that M is orientable if and only if there are no closed loops, $\gamma\in M$, such that $w_1[\gamma]\neq 0$. Under the Whitney sum, $w_1(\tau(M))$ can be decomposed as

$$w_1(\tau(M))=w_1(\tau^+)+w_1(\tau^-). \tag{2}$$

We shall adopt the notation $w_1^+=w_1(\tau^+)$ and $w_1(\tau^-)=w_1^-$. Thus, M is *space-orientable* if and only if $w_1^+=0$, and *time-orientable* if and only if $w_1^-=0$. Note that if there exists some loop, $\gamma\in M$, such that M is neither space nor time-orientable, then M is orientable since $w_1(\tau(M))=w_1^++w_1^-=1+1=0 \mod 2$. (We always count mod 2 since these cochains always take values in $\mathbb{Z}_2^3$.) As we shall see, w_1^+ and w_1^- are critical components of the obstructions to all of the pin structures.

Let us denote the *second Stiefel–Whitney class*, $w_2(M)=w_2(\tau(M))$. Recall that this class vanishes if and only if M admits a spin structure.

Now as in Theorem 3, we can apply Wu's formula and obtain the identity

$$(w_2(M)+w_1(M)\smile w_1(M))\smile x_2=x_2\smile x_2 \quad \text{for any } x_2\in H^2(M;\mathbb{Z}_2), \tag{3}$$

where ''$\smile$'' is the cup product.[14] Since we are allowing M to be nonorientable, we work in $\mathbb{Z}_2$ coefficients and write the intersection pairing

$$h:H_2(M;\mathbb{Z}_2)\times H_2(M;\mathbb{Z}_2)\to\mathbb{Z}_2. \tag{4}$$

This is defined by $h(x,y)=x\cdot y=(x_2\smile y_2)\frown w_1$, where $x_2, y_2\in H^2(M;\mathbb{Z}_2)$ satisfy $x_2\frown w=x$ and $y_2\frown w=y$, $w\in H^4(M;\mathbb{Z}_2)$ is the fundamental homology class and ''$\frown$'' denotes cap product. Taking the dual of Eq. (4) yields the intersection pairing on $H^2(M;\mathbb{Z}_2)$.

As we saw in Ref. 3, the following result of Kervaire and Milnor[16] holds even for nonorientable M:

Lemma 2: Let M be a smooth four-dimensional manifold. Let $u(\partial M)$ (the mod 2 Kervaire semicharacteristic) be given by

$$u(\partial M)=\dim_{\mathbb{Z}_2}(H_0(\partial M;\mathbb{Z}_2)\oplus H_1(\partial M;\mathbb{Z}_2))\bmod 2.$$

Then the rank of the intersection pairing h satisfies

$$\operatorname{rank}(h)=(u(\partial M)+e(M))\bmod 2,$$

where $e(M)$ is the Euler number of M.

It is now easy to check[3] that $\operatorname{rank}(h)=0$ if and only if

$$w_2+w_1\smile w_1=0 \mod 2.$$

Combining this observation with Lemma 2 then yields

Lemma 3: Let M be a smooth four-dimensional manifold with tangent bundle $\tau(M)$. Then

$$w_2(\tau(M))+w_1(\tau(M))\smile w_1(\tau(M))=0\Leftrightarrow(u(\partial M)+e(M))\bmod 2=0.$$

We have now developed enough mathematical machinery to calculate the index of a nonorientable plane field on a general (not necessarily oriented) four-dimensional manifold M. Our basic strategy is the following: If M is oriented, we are done (we just apply the Hirzebruch–Hopf result, Theorem 1). If M is not orientable, we pass to the *oriented double cover* $\widetilde{M}$ of M and apply Theorem 1 on $\widetilde{M}$. We then "push down" the plane field $\widetilde{P}$ on $\widetilde{M}$, under the projection π: $\widetilde{M}\to M$, and deduce the form of the index of $P=\pi^*(\widetilde{P})$ on M. Since any plane field P on M can be so obtained, we thus derive the general form of the index on M.

Suppose then we are given some smooth four-dimensional manifold M without boundary, with Klein metric "g_K" defined on M. As we have seen, the metric corresponds to some two-plane field P on M. The singularities of the metric g_K therefore correspond to the singularities of the plane field P. Construct the (oriented) $2-1$ cover over M, denoted $\widetilde{M}$, with projection π: $\widetilde{M}\to M$. Now lift the plane field P (which will generally be a section of a $\widetilde{G}_{2,4}$ bundle, B, over M) to a plane field $\widetilde{P}$ over $\widetilde{M}$ (where $\widetilde{P}$ will now be a section of a $G_{2,4}$ bundle, $\widetilde{B}$, over $\widetilde{M}$). Since $\widetilde{M}$ is oriented, we know the form of the total index of $\widetilde{P}$ on $\widetilde{M}$ is, by Theorem 1,

$$\operatorname{ind}(\widetilde{P},\widetilde{M})=\tfrac{1}{4}(\alpha-3\sigma-2\chi,\beta-3\sigma+2\chi), \tag{5}$$

where $\sigma=\sigma(\widetilde{M})$, $\chi=\chi(\widetilde{M})$. As in Theorem 1, we find that

$$\alpha=\sigma(\widetilde{M})\bmod 8,\quad \beta=\sigma(\widetilde{M})\bmod 8, \tag{6}$$

hence

$$\alpha-\sigma=8n,\quad n\in\mathbb{Z},\quad \beta-\sigma=8m,\quad m\in\mathbb{Z}, \tag{7}$$

so the index becomes

$$\operatorname{ind}(\widetilde{P},\widetilde{M})=\tfrac{1}{4}(8n-2(\sigma(\widetilde{M})+\chi(\widetilde{M})),\quad 8m-2(\sigma(\widetilde{M})-\chi(\widetilde{M}))), \tag{8}$$

where m and n are some integers. It follows that we must have

$$\sigma(\widetilde{M})=\chi(\widetilde{M})\bmod 2. \tag{9}$$

We must now determine how the parity of $\chi(\widetilde{M})$ is related to the parity of $\chi(M)$. To do this we introduce a new invariant.

Definition: Let M be a smooth four-dimensional manifold with boundary $\partial M\cong\Sigma_1\cup\Sigma_2\cup\cdots\cup\Sigma_n$ the disjoint union of finitely many (not necessarily orientable) closed three-

manifolds. Let $\partial\widetilde{M} \cong \widetilde{\Sigma}_1 \cup \widetilde{\Sigma}_2 \cup \cdots \cup \widetilde{\Sigma}_n$ denote the oriented double cover of ∂M (that is, $\widetilde{\Sigma}_i$ is the oriented double cover of Σ_i for each i, and $\partial\widetilde{M}$ is the disjoint union of the $\widetilde{\Sigma}_i$.) Then we define the element $U(\partial M) \in \mathbb{Z}_2$ by the formula

$$U(\partial M) = (u(\partial M) - u(\partial\widetilde{M})) \bmod 2.$$

Thus, $U(\partial M)$ measures (modulo 2) the total number of torsion generators of $H_1(\partial M)$ which are "destroyed" when we pass to the double cover.

For example, suppose that $\partial M \cong S^1 \times \mathbb{RP}^2$, then $u(\partial M) = 1$ since $\mathbb{RP}^2$ has a torsion generator; and $\partial\widetilde{M} \cong S^1 \times S^2$ so $u(\partial\widetilde{M}) = 0$, hence $U(\partial M) = 1$. Similarly all the torsion generators are destroyed if we take $\partial M \cong \mathbb{RP}^3$.

On the other hand, there are torsion generators which do not completely "unwrap." For example, take $\partial M \cong S^1 \times K$, where K denotes the Klein bottle. We then find that $u(\partial M) = 0$, where one of the $H_1(\partial M)$ factors is torsion, and that $\partial\widetilde{M} \cong S^1 \times T^2$ has $u(\partial\widetilde{M}) = 0$. Hence $U(\partial M) = 0$, which makes sense since the torsion generator in K lifts to a nontrivial loop in T^2.

We must also introduce another new invariant, which we define as follows:

Definition: Let M be a smooth four-manifold, with or without boundary. Then we define the element $\delta(M) \in \mathbb{Z}_2$ as follows:

$$\delta(M) = \begin{cases} 0 & \text{iff there do not exist distinct} \\ & \text{two-cycles } c, c' \in H^2(M) \text{ such that} \\ & w_2[c] \neq 0 \quad \text{and } w_1 \smile w_1[c] = 0, \quad \text{but} \\ & w_2[c'] \neq 0 \quad \text{and } w_1 \smile w_1[c'] \neq 0 \\ 1 & \text{iff there do exist such two-cycles} \\ & c, c' \in H^2(M) \end{cases}.$$

Now suppose we are given a manifold M with boundary ∂M. Let $\widetilde{M}$ and $\partial\widetilde{M}$ denote the respective double covers. Then by Lemma 3, we have

$$\begin{aligned} u(\partial M) + \chi(M) &= w_2(M) + w_1 \smile w_1(M) \bmod 2, \\ u(\partial\widetilde{M}) + \chi(\widetilde{M}) &= w_2(\widetilde{M}) \bmod 2. \end{aligned} \tag{10}$$

Thus, we see that $\chi(M) + U(\partial M) = \chi(\widetilde{M}) \bmod 2$ if and only if

$$w_2(M) + w_1(M) \smile w_1(M) = w_2(\widetilde{M}) \bmod 2.$$

We therefore obtain

Lemma 4: Let M be a smooth nonorientable four-dimensional manifold with boundary. Let $\widetilde{M}$ denote the oriented double cover of M, as above. Then

$$U(\partial M) + \chi(M) = \chi(\widetilde{M}) \bmod 2$$

if and only if $\delta(M) = 0$.

Proof: ($\Rightarrow$) Suppose $U(\partial M) + \chi(M) = \chi(\widetilde{M}) \bmod 2$, then $w_2(M) + w_1(M) \smile w_1(M) = w_2(\widetilde{M}) \bmod 2$. There are three cases to consider:

(i) $w_2(M) = w_2(\widetilde{M}) = 0$,

(ii) $w_2(M) = 1$ and $w_2(\widetilde{M}) = 0$,

(iii) $w_2(M) = 1 = w_2(\widetilde{M})$.

If (i) holds, then M and $\widetilde{M}$ are both spin, and so we trivially have $\delta(M) = 0$.

If (ii) holds, then $\widetilde{M}$ is spin, but M is not. It follows that there exists some two-cycle $c \in H^2(M)$ such that $w_2[c] \neq 0$, and that this two-cycle lifts (under π: $\widetilde{M} \overset{2-1}{\rightarrow} M$) to a two-cycle $\widetilde{c} \in H^2(\widetilde{M})$ such that $w_2[\widetilde{c}] = 0$. Since $w_2[c] + w_1 \smile w_1[c] = w_2[\widetilde{c}]$ for any such two-cycle we must have $w_1 \smile w_1[c] = 1$ for all two-cycles $c \in H^2(M)$ such that $w_2[c] = 1$. Thus we must have $\delta(M) = 0$.

If (iii) holds, then neither M nor $\widetilde{M}$ is spin. Since $U(\partial M) + \chi(M) = \chi(\widetilde{M}) \bmod 2$, it follows that for all two-cycles $c \in H^2(M)$ such that $w_2[c] \neq 0$, we must have $w_1 \smile w_1[c] = 0$, and so $\delta(M) = 0$.

($\Leftarrow$) Conversely, suppose that $\delta(M) = 0$. Then case (i) gives $\chi(M) + U(\partial M) = \chi(\widetilde{M}) \bmod 2$ trivially.

Likewise, if (ii) holds, then on any of the two-cycles c, for which $w_2[c] = 1$, we must have $w_1 \smile w_1[c] = 1$, thus $\chi(M) + U(\partial M) = \chi(\widetilde{M}) \bmod 2$.

Finally, case (iii) again implies that neither M nor $\widetilde{M}$ is spin. However, $\delta(M) = 0$ again implies $w_2(\widetilde{M}) = w_2(M) + w_1(M) \smile w_1(M) \bmod 2$ and thus $\chi(M) + U(\partial M) = \chi(\widetilde{M}) \bmod 2$. □

Thus, $U(\partial M) + \delta(M) \in \mathbb{Z}_2$ is an invariant which tells us whether the Euler number of a manifold M has the same parity as the Euler number of the double cover $\widetilde{M}$ of M. For convenience, we will henceforth write

$$I(M, \partial M) = U(\partial M) + \delta(M).$$

Suppose we are given some four-dimensional manifold M with boundary ∂M and its double cover $\widetilde{M}$. Next form the double[1] of each manifold, i.e., we double M to get $2M$, and $\widetilde{M}$ to get $2\widetilde{M}$. $2\widetilde{M}$ is then the oriented cover of $2M$. As in Lemma 1, we have that

$$\sigma(2\widetilde{M}) = 0, \tag{11}$$

and so the index of any plane field $\widetilde{P}$ on $2\widetilde{M}$ becomes

$$\mathrm{ind}(\widetilde{P}, 2\widetilde{M}) = \tfrac{1}{4}(8n - 2\chi(2\widetilde{M}), 8m + 2\chi(2\widetilde{M})), \tag{12}$$

where $m, n \in \mathbb{Z}$. We also know that

$$\chi(2\widetilde{M}) = 2\chi(\widetilde{M}), \tag{13}$$

and so we obtain

$$\mathrm{ind}(\widetilde{P}, 2\widetilde{M}) = (2n - \chi(\widetilde{M}), 2m + \chi(\widetilde{M})). \tag{14}$$

We can assume that there are an equal number of singularities in each ''half'' of the double $2M$. As in 1, we then push all of the singularities over ∂M into one of the halves. Then by construction, one of the halves of $2M$ is free of singularities, and taking this half we have constructed a nonsingular plane field on M. The degree of the map from ∂M to $\widetilde{G}_{2,4}$ (defined by the plane field) must be, combining Eq. (14) with Lemma 4,

$$(2n - \chi(M) + I(M, \partial M), 2m + \chi(M) + I(M, \partial M)) \bmod 2. \tag{15}$$

As in Lemma 1, we shall call this degree the *Klein kink* of the metric g_K (determining the plane field) with respect to ∂M and we denote it

$$\mathrm{kink}(\partial M; g_K).$$

Combining the above, we obtain

Theorem 2: Let M be any smooth four-dimensional manifold with the boundary $\partial M \cong \Sigma_1 \cup \Sigma_2 \cup \cdots \cup \Sigma_n \neq \emptyset$, where $\{\Sigma_i | i=1,\ldots,n\}$ is some collection of closed three-manifolds. Then there always exist globally defined nonsingular metrics g_K of Kleinian signature on M. Furthermore every such metric must satisfy $\text{kink}(\partial M; g_K) = (k_1, k_2)$ where

$$k_i = \chi(M) + I(M, \partial M) \bmod 2, \quad i = 1,2.$$

Thus for an arbitrary nonsingular Klein metric g_K on M, the parity of the kink number of g_K on ∂M is completely determined.

III. OBSTRUCTIONS TO PIN STRUCTURES

As detailed in the Introduction, there are eight double covers of O(2,2), which we denote

$$h^{a,b,c}: \text{Pin}^{a,b,c}(2,2) \to \text{O}(2,2),$$

where a is the sign of the square of space inversion, b is the sign of the square of time inversion, and c is the sign of the square of the two combined. The obstructions to constructing a globally well-defined bundle, with fiber $\text{Pin}^{a,b,c}(2,2)$, can be deduced using the constructions in Theorem 3. Indeed, we obtain the following:

Theorem 3: Let M be a Kleinian four-manifold (with tangent bundle $\tau(M)$ an O(2,2) bundle). Then M admits either $\text{Pin}^{+,+,+}(2,2)$ or $\text{Pin}^{+,+,-}(2,2)$ structure if and only if

$$w_2(M) = 0.$$

Theorem 4: Let M be a Kleinian four-manifold (with tangent bundle $\tau(M)$ an O(2,2) bundle). Then M admits either $\text{Pin}^{-,+,+}(2,2)$ or $\text{Pin}^{-,+,-}(2,2)$ structure if and only if

$$w_2(M) + w_1^+ \smile w_1^+ = 0.$$

Theorem 5: Let M be a Kleinian four-manifold (with tangent bundle $\tau(M)$ an O(2,2) bundle). Then M admits either $\text{Pin}^{+,-,+}(2,2)$ or $\text{Pin}^{+,-,-}(2,2)$ structure if and only if

$$w_2(M) + w_1^- \smile w_1^- = 0.$$

Theorem 6: Let M be a Kleinian four-manifold (with tangent bundle $\tau(M)$ an O(2,2) bundle). Then M admits either $\text{Pin}^{-,-,+}(2,2)$ or $\text{Pin}^{-,-,-}(2,2)$ structure if and only if

$$w_2(M) + w_1^+ \smile w_2^+ + w_1^- \smile w_1^- = 0.$$

With these results, we can now investigate the obstructions to pin-Klein cobordism.

IV. OBSTRUCTIONS TO PIN-KLEIN COBORDISM

In this section $\{\Sigma_i | i=1,\ldots,n\}$ will always denote some collection of closed three-manifolds.

Definition: We will say that there exists a $\text{Pin}^{a,b,c}(2,2)$ cobordism for $\{\Sigma_i | i=1,\ldots,n\}$ if and only if there exists a Kleinian four-manifold M (with a globally nonsingular Kleinian metric g_K) admitting $\text{Pin}^{a,b,c}(2,2)$ structure and satisfying

$$\partial M \cong \Sigma_1 \cup \Sigma_2 \cup \cdots \cup \Sigma_n .$$

Corollary 1: There exists either a $\text{Pin}^{+,+,+}(2,2)$ or a $\text{Pin}^{+,+,-}(2,2)$ cobordism M for $\{\Sigma_i | i=1,\ldots,n\}$ if and only if

$$(u(\partial M) + k_i + I(M, \partial M)) = (w_1^+ \smile w_1^+ + w_1^- \smile w_1^-) \bmod 2,$$

where k_i is either of the integers in $\text{kink}(\partial M; g_K) = (k_1, k_2)$.

Proof: ($\Rightarrow$) Suppose such a pin-Klein cobordism, M, exists. Then by Theorem 2, we know that

$$k_i = (\chi(M) + I(M, \partial M)) \bmod 2 \tag{16}$$

(since the Kleinian metric g_K is nonsingular). Furthermore, by Theorem 3, we must have

$$w_2(M) = 0, \tag{17}$$

and by Lemma 3, we know that

$$w_2(M) + w_1^+ \smile w_1^+ + w_1^- \smile w_1^- = (u(\partial M) + \chi(M)) \bmod 2. \tag{18}$$

Thus, combining Eqs. (16), (17), and (18), we obtain

$$(u(\partial M) + k_i + I(M, \partial M)) = (w_1^+ \smile w_1^+ + w_1^- \smile w_1^-) \bmod 2. \tag{19}$$

($\Leftarrow$) Conversely, suppose Eq. (19) holds. Take any globally defined Klein metric g_K on M, then we must have

$$k_i = (\chi(M) + I(M, \partial M)) \bmod 2.$$

Hence $w_2 = 0$, and so M is pin-Klein with the pin bundle fiber being $\text{Pin}^{+,+,\pm}(2,2)$. □

Using the above proof as a model, we also obtain:

Corollary 2: There exists either a $\text{Pin}^{-,+,+}(2,2)$ or a $\text{Pin}^{-,+,-}(2,2)$ cobordism M for $\{\Sigma_i | i = 1, \ldots, n\}$ if and only if

$$(u(\partial M) + k_i + I(M, \partial M)) = w_1^- \smile w_1^- \mod 2,$$

where k_i is either of the integers in $\text{kink}(\partial M; g_K) = (k_1, k_2)$.

Corollary 3: There exists either a $\text{Pin}^{+,-,+}(2,2)$ or a $\text{Pin}^{+,-,-}(2,2)$ cobordism M for $\{\Sigma_i | i = 1, \ldots, n\}$ if and only if

$$(u(\partial M) + k_i + I(M, \partial M)) = w_1^+ \smile w_1^+ \mod 2,$$

where k_i is either of the integers in $\text{kink}(\partial M; g_K) = (k_1, k_2)$.

Corollary 4: There exists either a $\text{Pin}^{-,-,+}(2,2)$ or a $\text{Pin}^{-,-,-}(2,2)$ cobordism M for $\{\Sigma_i | i = 1, \ldots, n\}$ if and only if

$$(u(\partial M) + k_i + I(M, \partial M)) = 0 \mod 2,$$

where k_i is either of the integers in $\text{kink}(\partial M; g_K) = (k_1, k_2)$.

Thus we see that the obstructions to $\text{Pin}^{a,b,c}(2,2)$ cobordism depend only on boundary data (i.e., $u(\partial M)$ and $\text{kink}(\partial M; g_K) = (k_1, k_2)$), the values of $a, b \in \{\pm\}$, the choice of orientation (i.e., $w_1^+ \smile w_1^+$ and $w_1^- \smile w_1^-$) and the invariant $I(M, \partial M)$.

Finally, we note that in all the above corollaries, the expression $u(\partial M) + k_i + I(M, \partial M)$ may be replaced by the expression $u(\partial \widetilde{M}) + k_i + \delta(M)$, since $I(M, \partial M) = U(\partial M) + \delta(M) = (u(\partial M) + u(\partial \widetilde{M})) \bmod 2 + \delta(M)$.

V. EXAMPLES AND APPLICATIONS

The constructions introduced in this paper have many applications to theoretical physics. We now give some examples and applications.

Example 1: Let K denote the Klein bottle and $T \cong S^1 \times S^1$ the Torus. Then form a Kleinian metric on $M \cong K \times T$ by taking the product metric formed by using the natural negative definite metric on K and the natural positive definite metric on T. Although M is nontime orientable (since traversing the orientation-reversing loop in K inverts the timelike subbundle), M is still spin since $w_2(K) = 0$, and so all $\mathrm{Pin}^{a,b,c}(2,2)$ structures are allowed on M.

Now suppose that we take M to be the product space $M \cong \mathbb{RP}^2 \times T$ where, as above, we endow M with the natural product metric such that $\mathbb{RP}^2$ is timelike. Then we clearly have $w_1^- \smile w_1^-(\mathbb{RP}^2) = 1$ and $w_2(M) = 1 \bmod 2$. Thus not all pin structures will be allowed. Indeed, one easily calculates that $\mathrm{Pin}^{+,+,\pm}(2,2)$ and $\mathrm{Pin}^{-,+,\pm}(2,2)$ structures will not be allowed, while $\mathrm{Pin}^{+,-,\pm}(2,2)$ and $\mathrm{Pin}^{-,-,\pm}(2,2)$ are allowed.

Example 2: An interesting application is to Kaluza–Klein-type theories in which some of the internal dimensions are allowed to be timelike. We could take the ground state of such a theory to be a manifold of the form $M \times S^1$ where M is a Lorentzian three-manifold, and the internal space S^1 is timelike. Then the total metric on $M \times S^1$ would have signature $--++$, and the obstruction to this metric being nonsingular would again be the condition that there exists a plane field. We could even allow the Kleinian metric to spin around, so that the internal space fluctuates from being timelike to being spacelike (so that the signature of the space-time M would change from $-++$ to $+--$). That is, in terms of the effective three-dimensional theory, this would correspond to signature change.

In general, in order to produce a nonsingular theory, we may wish to consider manifolds M with Kleinian, or even more exotic, signatures. For example, if $M \cong S^2 \times S^2$ then M does not admit a nonsingular Lorentz metric, but does admit a nonsingular Klein metric. Such choices will generically change the types of pin structures which are admitted in the Kaluza–Klein (or other) type theory.

Example 3: There has been considerable interest recently in the study of signature changing space-times.[5–8] In an extension to the example given in Example 1 we note that we can have the nucleation of a single Kleinian region across a single zero-kink surface homeomorphic to S^3. As an example, let M be the Kleinian manifold formed by removing a four-ball from $\mathbb{RP}^2 \times S^2$ such that the S^2 factor is timelike. We have $\partial M \cong S^3$, and so $I(M, \partial M) = 0$. In order to produce signature change we require that the kink on ∂M is zero. Then since $u(S^3) = 1$, we see that such a signature change scenario is possible since M admits a $\mathrm{Pin}^{-,+,\pm}(2,2)$ structure.

Example 4: Finally, we note that our results would be potentially useful in generalizing the Penrose flag-plane construction[17] to nonorientable manifolds.

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A relation between the Kauffman and the HOMFLY polynomials for torus knots

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Polynomial invariants corresponding to the fundamental representation of the gauge group SO(N) are computed for arbitrary torus knots in the framework of Chern–Simons gauge theory making use of knot operators. As a result, a formula that relates the Kauffman and the HOMFLY polynomials for torus knots is presented. © *1996 American Institute of Physics.* [S0022-2488(96)03103-4]

I. INTRODUCTION

Knot operators[1,2] have shown to be a powerful tool in Chern–Simons gauge theory[3] to obtain general expressions for knot invariants related to torus knots and links. Computations by other methods[4–10] have been successful for specific knots but not to obtain general expressions for knot sequences as torus knots. Knot operators have been used in Ref. 11, where a formula for the invariants for torus knots and links carrying arbitrary representations of the gauge group SU(2) has been presented. For the fundamental representation it covers the case of the Jones polynomial,[12,13] while for higher-dimensional representations it covers the case of the Akutsu–Wadati polynomials.[14] They have also been used in Ref. 15, where a formula for the HOMFLY polynomial[16,13] for arbitrary torus knots and links has been presented. For the case of torus knots the formula obtained in Ref. 15 for the HOMFLY polynomial coincides with the one presented by Jones in Ref. 13 and later reobtained using quantum groups by Rosso and Jones in Ref. 17.

Knot operators were constructed in Refs. 1 and 2 for the gauge group SU(N). In this paper we will present the form of these operators for arbitrary simple compact groups. Then, we will use them to compute knot invariants for arbitrary torus knots carrying the fundamental representation of SO(N). As a consequence, a formula for the Kauffman polynomial[18] for this type of knots is obtained. This formula turns out to be equivalent to the one obtained in Ref. 19 using a different method. Comparing this formula for the Kauffman polynomial to the one obtained in Refs. 13, 17, and 15 for the HOMFLY polynomial, we obtain a rather simple relation between them. Denoting the HOMFLY polynomial for a torus knot $\{n,m\}$ [n and m are coprime integers, $(n,m)=1$] in terms of its standard variables a and z by $P_{n,m}(a,z)$, and the Kauffman polynomial (Dubrovnik version) by $Y_{n,m}(a,z)$, we find

$$P_{n,m}(a,z)=\frac{1}{2}\,(Y_{n,m}(a,z)+Y_{n,m}(a,-z))+\frac{z}{2(a-a^{-1})}\,(Y_{n,m}(a,z)-Y_{n,m}(a,-z)). \quad (1.1)$$

This is the main new result presented in this paper. The existence of a formula like (1.1) is rather remarkable. In general, the Kauffman polynomial contains very many more terms than the HOMFLY polynomial. This means that an important cancellation of terms occur in (1.1). Notice also that this formula indicates that at least for torus knots the Kauffman polynomial distinguishes more knots than the HOMFLY polynomial. Two torus knots that have the same Kauffman polynomial also have the same HOMFLY polynomial, but it might occur that two torus knots have the

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same HOMFLY polynomial but different Kauffman polynomials. At least for torus knots one can state that the Kauffman polynomial is more fundamental than the HOMFLY polynomial.

As a byproduct of formula (1.1), it will be obtained in Sec. IV a formula for the Alexander–Conway polynomial in terms of the first derivative at $a=1$ of the corresponding Kauffman polynomial.

The paper is organized as follows. In Sec. II we present the generalization of the construction of knot operators based on Chern–Simons gauge theory for an arbitrary simple compact gauge group. In Sec. III we calculate the Kauffman polynomial for torus knots, obtaining a result in full agreement with a previous calculation. In Sec. IV we prove formula (1.1) and derive a formula for the Alexander–Conway polynomial for torus knots in terms of the corresponding Kauffman polynomial. In Sec. V we add final comments and remark on our results. The conventions used in this paper are conveniently compiled in an Appendix.

II. KNOT OPERATORS FOR ARBITRARY SIMPLE GAUGE GROUP

In this section we present the generalization of the operator formalism developed in Refs. 1 and 2 for an arbitrary simple compact gauge group and the construction of the corresponding knot operators. We begin introducing Chern–Simons gauge theory. Let M be a boundary-less three-dimensional manifold and let A be a connection associated to a principal G-bundle for some simple Lie group G. The action that defines Chern–Simons gauge theory has the form

$$S_k(A)=\frac{k}{4\pi}\int_M \mathrm{Tr}\left(A\wedge dA+\frac{2}{3}A\wedge A\wedge A\right), \tag{2.1}$$

where Tr is the trace over the fundamental representation of the simple gauge group G, and, for the moment, k is an arbitrary real number. Under a gauge transformation,

$$A\to g^{-1}\,dg+g^{-1}Ag, \tag{2.2}$$

the action (2.1) transforms as

$$S_k(A)\to S_k(A)-\frac{k}{12\pi}\int_M \mathrm{Tr}(g^{-1}\,dg\wedge g^{-1}\,dg\wedge g^{-1}\,dg). \tag{2.3}$$

The last quantity is closely related to the winding number of the map $g:M\to G$, which is defined as

$$\Upsilon(g)=\frac{1}{48\pi}\int_M \epsilon^{\mu\nu\rho}f^{abc}\psi^2 C^a_\mu C^b_\nu C^c_\rho, \tag{2.4}$$

where C^a_μ is given by

$$g^{-1}\,\partial_\mu g=C^a_\mu T^a, \tag{2.5}$$

being T^a, $a=1,\ldots,\dim(G)$, the generators of the simple group G. In (2.4), f^{abc} are the structure constants corresponding to this group, and ψ^2 the squared length of the longest simple root of G. The quantity $\Upsilon(g)$ in (2.4) is always 2π times an integer.[20] To study its relation to the second term on the right-hand side of (2.3) we must take into account that the generators can be chosen in such a way that

$$\mathrm{Tr}(T^aT^b)=-y\,\psi^2\delta^{ab}, \tag{2.6}$$

where y is the Dynkin index of the fundamental representation of the simple group G. It is clear from (2.6) that this index is independent of the scale chosen for the gauge group generators. From (2.4) and (2.6), it follows that (2.3) can be written as

$$S_k(A)\rightarrow S_k(A)-2yk\Upsilon(g). \tag{2.7}$$

The values of y for SU(N) and SO(N) are 1/2 and 1, respectively. For other groups y is a half-integer or an integer (see the Appendix). Therefore, if k is an integer the action (2.1) changes into 2π times an integer and the exponential $\exp(iS_k(M))$ is gauge invariant. Furthermore, for the case of SO(N), it is enough to require k to be a half-integer. Defining

$$x=2yk, \tag{2.8}$$

one has, in general, the following quantization condition:

$$x=2yk\in\mathbf{Z}. \tag{2.9}$$

For values of k satisfying the quantization condition (2.9), the partition function of the theory is defined as

$$Z_k(M)=\int [\mathscr{D}A]_M \exp(iS_k(A)), \tag{2.10}$$

where the functional integration is over gauge nonequivalent connections. This partition function is a topological invariant because the action $S_k(A)$ does not depend on the metric on M. Other topological-invariant quantities are constructed, introducing operators in the integrand of the functional integral present in (2.10). These operators must be gauge invariant and metric independent to lead to topological-invariant quantities. Wilson lines constitute an important class of these operators. Let γ be a close curve in M and let R be an irreducible representation of the gauge group. The Wilson line operator associated to γ and R is

$$W_R^{\gamma}(A)=\mathrm{Tr}_R\left(P\ \exp\int_{\gamma} A\right), \tag{2.11}$$

where P denotes a path-ordered product along γ. We will be interested in computing the vacuum expectation values of products of these operators, i.e., functional integrations of the form

$$\int [\mathscr{D}A]_M\left(\prod_{i=1}^{n} W_{R_i}^{\gamma^i}\right)\exp(iS_k(A)). \tag{2.12}$$

In order to generalize the operator formalism developed in Refs. 1 and 2, let us assume that there are some Wilson lines L_i on the manifold M. We will perform a Heegaard splitting on M in such a way that no Wilson line is cut. The case in which this does not happen has been studied in Ref. 21. In this formalism, the vacuum expectation values are expressed as an inner product of states in a Hilbert space. These states are defined as functional integrals over configurations on each of the g-handlebodies M_1 and M_2, which result from the Heegaard splitting. In order to construct these states let us introduce complex local coordinates on the Riemann surface Σ, which corresponds to the common boundary of M_1 and M_2,

$$z=\sigma_1+i\sigma_2, \quad \overline{z}=\sigma_1-i\sigma_2, \tag{2.13}$$

and let us use complex components for the part of the gauge connection parallel to the surface Σ:

$$A_z=\tfrac{1}{2}\,(A_1-iA_2),\quad A_{\bar z}=\tfrac{1}{2}\,(A_1+iA_2). \tag{2.14}$$

Our aim is to define wave functionals that will be functional integrals over field configurations in the g-handlebodies, resulting after the splitting with the value of $A_{\bar z}$ fixed at the boundary. The inner product will be implemented as an integration over the components A_z and $A_{\bar z}$ on the common boundary.

Following Refs. 1 and 2, we will use the formalism of the holomorphic quantization. Wave functionals associated to the g-handlebody M_1 enclosing p Wilson lines are defined as

$$\Psi_1[A_{\bar z}]=\int [\mathscr{D}A]_{M_1}\left(\prod_{i=1}^{p} W_{R_i}^{\gamma^i}\right)\exp\left(iS_k(A)-\frac{k}{2\pi}\int_\Sigma \mathrm{Tr}(A_zA_{\bar z})\right), \tag{2.15}$$

where $[\mathscr{D}A]_{M_1}$ represents the functional integration measure over gauge orbits such that $A_{\bar z}$ is fixed at the boundary Σ. A similar expression defines the wave functional $\Psi_2[A_z]$ for the g-handlebody M_2. The vacuum expectation value (2.12) is given by the following inner product:

$$(\Psi_2|\Psi_1)=\int [\mathscr{D}A_z\ \mathscr{D}A_{\bar z}]_\Sigma\ \exp\left(\frac{k}{\pi}\int_\Sigma \mathrm{Tr}(A_zA_{\bar z})\right)\overline{\Psi_2[A_{\bar z}]}\Psi_1[A_{\bar z}]. \tag{2.16}$$

Let us recall a few important facts related to this formalism. Boundary terms like the one in (2.15) are introduced to make the wave functional well defined, i.e., depending on $A_{\bar z}$ on the boundary Σ. Also, such a term is the one responsible for having a functional integral in (2.15), which is extremal for gauge configurations, such that the field strength of A vanishes in the interior of M_1.

The commutation relations of the canonically conjugate fields A_z and $A_{\bar z}$ on Σ can be read from the exponent of the exponential inserted in (2.16). They take the form

$$[A_z^a(\sigma),A_z^b(\sigma')]=\frac{\pi}{2y\psi^2k}\,\delta^{ab}\delta^{(2)}(\sigma-\sigma'). \tag{2.17}$$

Our next step is to compute explicitly the wave functionals (2.15) in order to obtain a description of the Hilbert space of the theory. To carry this out we will use standard parametrizations of the gauge fields A_z and $A_{\bar z}$ on the Riemann surface Σ. We will address the situations corresponding to genus zero and one.

A. Genus-zero handlebody

Let M_1 be a solid ball and $\Sigma=S^2$ its boundary. On S^2 the fields A_z and $A_{\bar z}$ can be parametrized as

$$A_{\bar z}=u^{-1}\,\partial_{\bar z}u,\quad A_z=\overline{u}^{-1}\,\partial_z\overline{u}, \tag{2.18}$$

where u is a single-valued map $u:S^2\to G^c$, G^c being the complexification of G. Since $A_{\bar z}^\dagger=-A_z$, one has that $u^\dagger=\overline{u}^{-1}$. The gauge transformations (2.2) take the following form for fields on the surface S^2:

$$A_{\bar z}\to g^{-1}\,\partial_{\bar z}g+g^{-1}A_{\bar z}g,\quad A_z\to g^{-1}\,\partial_z g+g^{-1}A_z g, \tag{2.19}$$

where g is a map $g:S^2\to G$. In the parametrization (2.18) these gauge transformations take the simple form $u\to ug$.

The next step is to express the measure $[\mathscr{D}A_z\ \mathscr{D}A_{\bar z}]_{S^2}$ in (2.16) in terms of an infinite product of de Haar measures of G^c. This involves the computation of a Jacobian, which takes the form[22,23]

$$[\mathscr{D}A_z\ \mathscr{D}A_{\bar{z}}]_{S^2}=\exp\left(\frac{g^\vee}{2y}\,\Gamma(u\overline{u}^{-1})\right)|\det\,\partial_z\partial_{\bar{z}}|du\ d\overline{u}, \tag{2.20}$$

where $g^\vee$ is the dual Coxeter number of G and $\Gamma(\alpha)$ is the Wess–Zumino–Witten action:[20]

$$\Gamma(u)=\frac{1}{2\pi}\int_{S^2}\mathrm{Tr}(\alpha^{-1}\,\partial_z\alpha\ \alpha^{-1}\,\partial_{\bar{z}}\alpha)+\frac{i}{12\pi}\int_{M_1}\epsilon^{\mu\nu\rho}\,\mathrm{Tr}(\widetilde{\alpha}^{-1}\,\partial_\mu\widetilde{\alpha}\,\widetilde{\alpha}^{-1}\,\partial_\nu\widetilde{\alpha}\,\widetilde{\alpha}^{-1}\,\partial_\rho\widetilde{\alpha}). \tag{2.21}$$

In (2.21) α is a map $\alpha: S^2\to G$, and $\widetilde{\alpha}$ is one of the extensions of this map to the interior of the solid ball M_1. The measure (2.21) does not depend on the choice of extension of the map α. For different choices, the resulting Wess–Zumino–Witten actions differ by $2iy$ times an integral of the form (2.4), where $M=S^2$. Therefore, since $g^\vee$ is always an integer, the measure (2.20) is well defined. It is also important to remark that this measure is gauge invariant.

In order to write wave functionals in terms of u and $\overline{u}$, one would like to factor the measure (2.20) appropriately. This is, however, not obvious due to the Polyakov–Wiegmann condition[22] satisfied by the Wess–Zumino–Witten action:

$$\Gamma(\alpha\beta)=\Gamma(\alpha)+\Gamma(\beta)+\langle\alpha,\beta\rangle, \tag{2.22}$$

where we have introduced

$$\langle\alpha,\beta\rangle=\frac{1}{\pi}\,\mathrm{Tr}(\alpha^{-1}\,\partial_{\bar{z}}\alpha\ \partial_z\beta\ \beta^{-1}). \tag{2.23}$$

As in Refs. 1 and 2, we will solve this problem making the following choice of measure on the boundaries of M_1 and M_2: take the measure (2.20) without those factors that only depend on the gauge variables that are not being integrated over in the path integral representation of the wave functional. Working in a gauge where the radial component of A on S^2 vanishes, this amounts to the choice

$$\exp\left(\frac{g^\vee}{2y}\,(\Gamma(\overline{u}^{-1})+\langle u,\overline{u}^{-1}\rangle)\right)d\overline{u},\quad\text{for }\Psi_1, \tag{2.24}$$

and

$$\exp\left(\frac{g^\vee}{2y}\,(\Gamma(u)+\langle u,\overline{u}^{-1}\rangle)\right)du,\quad\text{for }\Psi_2. \tag{2.25}$$

In doing this, an extra factor $\exp(\langle u,\overline{u}^{-1}\rangle)$ has been introduced. One must account for it in (2.16). This implies that the exponential factor in (2.16) has to be redefined to

$$\exp\left(\frac{1}{\pi}\left(k+\frac{g^\vee}{2y}\right)\int_\Sigma\mathrm{Tr}(A_{\bar{z}}A_z)\right), \tag{2.26}$$

so that the inner product (2.16) becomes

$$(\Psi_2|\Psi_1)=\int du\ d\overline{u}|\det\,\partial_z\partial_{\bar{z}}|\exp\left(\frac{1}{\pi}\left(k+\frac{g^\vee}{2y}\right)\int_\Sigma\mathrm{Tr}(A_{\bar{z}}A_z)\right)\overline{\Psi_2[A_{\bar{z}}]}\Psi_1[A_{\bar{z}}], \tag{2.27}$$

where A_z and $A_{\bar{z}}$ are given by (2.18).

As shown in Refs. 1 and 2, the form of the wave functional is determined using gauge invariance. Under the gauge transformations (2.19), the wave functional (2.15) transforms as

$$\Psi[A_{\bar z}]\to\Psi[g^{-1}A_{\bar z}g+g^{-1}\,\partial_{\bar z}g]=\exp\left(-\left(k+\frac{g^\vee}{2y}\right)\left(\Gamma(g)+\frac{1}{\pi}\int_\Sigma \mathrm{Tr}(A_{\bar z}\partial_z g\; g^{-1})\right)\right)\Psi[A_{\bar z}], \tag{2.28}$$

where the variation of the factor (2.24) introduced in the measure has been taken into account. Notice that in doing the gauge transformation (2.28), an extension to the interior of M_1 of the map g on the boundary Σ has been done. The result (2.28) is independent of the choice of extension when k satisfies the quantization condition (2.9). The solution to (2.28) has the form

$$\Psi[A_{\bar z}]=\xi\,\exp\left(-\left(k+\frac{g^\vee}{2y}\right)\Gamma(u)\right). \tag{2.29}$$

It is known[3] that the Hilbert space for the case of the solid ball is one dimensional. Independently of the form of the Wilson lines contained in the solid ball, the corresponding wave functional must be proportional to (2.29). The wave functional (2.29) satisfies the Gauss law emanating from the Chern–Simons action (2.1):

$$F^a_{\bar z z}\Psi[A_{\bar z}]=0, \tag{2.30}$$

where $F^a_{\bar z z}$ are the components of the gauge field strength. To verify (2.30) one must use the commutation relations for the gauge fields A_z and $A_{\bar z}$ resulting from (2.27).

B. Genus-one handlebody

In this section we describe the construction of the operator formalism for the case of genus one: $\Sigma=T^2$. The strategy is similar to the one in the previous section. The nontrivial homology structure of the torus T^2 will provide a richer framework. Let us first introduce some data to characterize the torus.

We will denote the holomorphic abelian differential of a torus T^2 with modular parameter τ by $\omega(z)$. Labeling the homology cycle on T^2, which is contractible in the handlebody by α, and the one that is not by β, the holomorphic form $\omega(z)$ satisfies

$$\int_\alpha \omega=1,\quad \int_\beta \omega=\tau,\quad \int_{T^2}\omega\wedge\overline{\omega}=\mathrm{Im}\;\tau. \tag{2.31}$$

The gauge fields A_z and $A_{\bar z}$ on T^2 can be parametrized in the following way:[23]

$$A_{\bar z}=(u_a u)^{-1}\partial_{\bar z}(u_a u),\quad A_z=(u_a\overline{u})^{-1}\partial_z(u_a\overline{u}), \tag{2.32}$$

where u is a single-valued map, $u:T^2\to G^c$, and u_a a non-single-valued map, $u_a:T^2\to G$, which takes the form

$$u_a=\exp\left(\frac{i\pi}{\mathrm{Im}\;\tau}\int^{\bar z}\overline{\omega}(z')a\cdot H-\frac{i\pi}{\mathrm{Im}\;\tau}\int^z\omega(z')\overline{a\cdot H}\right), \tag{2.33}$$

where

$$a=\sum_{i=1}^{l}a_i\lambda^{(i)},\quad H=\sum_{i=1}^{l}H_i\lambda^{(i)}, \tag{2.34}$$

$\lambda^{(i)}$, $i=1,\ldots,l$, being the fundamental weights of a simple group G of rank l. A summary of the group-theoretical conventions used in this paper is contained in the Appendix. Notice that u_a is in the maximal torus of G and that $u_a^+ = u_a^{-1}$. As before, $u^\dagger = \overline{u}^{-1}$, so that $A_z^\dagger = -A_z$.

The generalization of the measure (2.20) for the case of the torus has the form[23]

$$[\mathscr{D}A_z\ \mathscr{D}A_{\bar{z}}]_{T^2} = \exp\left(\frac{g^\vee}{2y}\,\Gamma(u\overline{u}^{-1},C)\right)|\Pi(a,\tau)|^4(\mathrm{Im}\ \tau)^l\ \exp\left(-\frac{g^\vee}{y}\,\langle u_a,u_a^{-1}\rangle\right) \tag{2.35}$$

$$|\det \partial_z\partial_{\bar{z}}|\,du\ d\overline{u}\ du_a\ du_a^\dagger,$$

where $\Gamma(g,B)$ is the gauged Wess–Zumino–Witten action,[24]

$$\Gamma(g,B) = \Gamma(g) - \frac{1}{\pi}\int_\Sigma \mathrm{Tr}(g^{-1}B_{\bar{z}}gB_z - B_{\bar{z}}\partial_z g\ g^{-1} + g^{-1}\ \partial_{\bar{z}}g\ B_z - B_zB_{\bar{z}}) \tag{2.36}$$

and

$$\Pi(a,\tau) = \exp\left(\frac{g^\vee\psi^2\pi}{4\ \mathrm{Im}\ \tau}\,a^2\right)\Theta^A_{g^\vee,\rho}(a,\tau), \tag{2.37}$$

$\Theta^A_{g^\vee,\rho}(a,\tau)$ being the Weyl antisymmetrized theta function of level $g^\vee$ (see the Appendix), and

$$\rho = \sum_{i=1}^{l}\lambda^{(i)}. \tag{2.38}$$

The field C in the measure (2.35) is

$$C_{\bar{z}} = u_a^{-1}\ \partial_{\bar{z}}u_a, \quad C_z = u_a^{-1}\ \partial_z u_a, \tag{2.39}$$

while the measure $du_a\ du_a^\dagger$ takes the form

$$du_a\ du_a^\dagger = \frac{d^la\ d^l\overline{a}}{(\mathrm{Im}\ \tau)^l}. \tag{2.40}$$

The measure (2.35) is invariant under the gauge transformations (2.19), which now take the form

$$u \to ug, \tag{2.41}$$

which will be called of type (i); under transformations that leave the fields A_z and $A_{\bar{z}}$ invariant,

$$u \to \hat{g}^{-1}u, \quad u_a \to u_a\hat{g}, \tag{2.42}$$

where $\hat{g}$ is a map from T^2 into the Cartan torus of G; and under modular transformations. This last set of transformations is described in the Appendix. The transformations (2.42), which will be denoted as type (ii), involve maps $\hat{g}$ that are labeled in the following way:

$$\hat{g}_{m,n} = \exp\left(\frac{2\pi i}{\psi^2\ \mathrm{Im}\ \tau}\left((n+m\tau)\cdot H\int^{\bar{z}}\overline{\omega(z)} - (n+m\overline{\tau})\cdot H\int^z\omega(z)\right)\right), \tag{2.43}$$

n and m being elements of the lattice generated by the long roots of G, which will be denoted by $\mathscr{L}_R$, i.e., $n,m\in\mathscr{L}_R$. Notice that the maps (2.43) are not connected to the identity map.

The analog of the Polyakov–Wiegmann condition (2.22) for the case of the Wess–Zumino–Witten action[20] takes the form

$$\Gamma(u\overline{u^{-1}},C)=\Gamma(u)+\langle u_a,u\rangle+\Gamma(\overline{u^{-1}})+\langle\overline{u^{-1}},\overline{u_a^{-1}}\rangle-\langle u_a,u_a^{-1}\rangle-\frac{1}{\pi}\int_\Sigma \mathrm{Tr}(C_z C_{\bar z}). \quad (2.44)$$

This expression leads to similar factorization problems as the ones found from (2.22). Following Refs. 1 and 2 we take

$$\exp\left(\frac{g^\vee}{2y}\left(\Gamma(u\overline{u^{-1}},C)-\Gamma(u)-\langle u_a,u\rangle\right)\right)d\overline{u}\,d u_a^\dagger, \quad \text{for } \Psi(A_{\bar z}), \quad (2.45)$$

and

$$\exp\left(\frac{g^\vee}{2y}\left(\Gamma(u\overline{u^{-1}},C)-\Gamma(\overline{u^{-1}})-\langle\overline{u^{-1}},u_a^{-1}\rangle\right)\right)du\;du_a, \quad \text{for } \Psi(A_z). \quad (2.46)$$

After comparing the products of these two factors to the one in (2.35), one finds that the inner product (2.16) now takes the form

$$(\Psi_2|\Psi_1)=\int du\;d\overline{u}\,du_a\;d\overline{u_a}|\Pi(a,\tau)|^4(\mathrm{Im}\;\tau)^l\exp\left(-\frac{g^\vee}{2y}\langle u_a,u_a^{-1}\rangle\right)$$
$$\times\exp\left(\frac{1}{\pi}\left(k+\frac{g^\vee}{2y}\right)\int_\Sigma \mathrm{Tr}(A_z A_{\bar z})\right)\overline{\psi_2[A_{\bar z}]}\psi_1[A_{\bar z}]. \quad (2.47)$$

As in the genus-zero case, the general form of the wave functional is obtained using arguments based on its properties under symmetry transformations. Performing a gauge transformation of type (i) (2.41), one finds

$$\Psi[A_{\bar z}]\to\exp\left(-\left(k+\frac{g^\vee}{2y}\right)(\Gamma(g)+\langle u_a u,g\rangle)\right)\Psi[A_{\bar z}]. \quad (2.48)$$

Using the Polyakov–Wiegmann condition (2.22) one finds that the solution to (2.48) can be written as

$$\Psi[A_{\bar z}]=\xi\psi_{2yk+g^\vee}(u_a u)\Lambda(u_a), \quad (2.49)$$

where ξ is a constant, $\Lambda(u_a)$ is arbitrary, and $\psi_{2yk+g^\vee}(u_a u)$ is a functional that satisfies

$$\psi_{2yr}(u_a v)=\psi_{2yr}(u_a)\exp(-r(\Gamma(v)+\langle u_a,v\rangle)), \quad (2.50)$$

for any single-valued map $v:T^2\to G$.

To search for solutions to (2.50), let us perform a symmetry transformation of type (ii) (2.42). One finds

$$\Psi[A_{\bar z}]\to\exp\left(\frac{g^\vee}{2y}\left(\Gamma(\hat g)+\langle u_a,\hat g\rangle\right)\right)\Psi[A_{\bar z}], \quad (2.51)$$

which implies the following property for $\Lambda(u_a)$ in (2.49):

$$\Lambda(u_a\hat g)=\exp\left(\frac{g^\vee}{2y}\left(\Gamma(\hat g)+\langle u_a,\hat g\rangle\right)\right)\Lambda(u_a). \quad (2.52)$$

Comparing to (2.50), it turns out that $\Lambda(u_a)$ and $\psi_{2yr}(u_a)$ are related in the following way:

$$\Lambda(u_a)=[\psi_{g^\vee}(u_a)]^{-1}. \tag{2.53}$$

We need now to solve for (2.50). Let us consider the situation in which the map v is a map as in (2.43) of the form $\hat{g}_{n_{[i]},0}$ with $n_{[i]}=\Sigma_{j=1}^{l} n_{[i]}^j \alpha_{(j)}$ and $n_{[i]}^j=\delta_i^j$, $\alpha_{(j)}$ being the simple roots of the group G. Equation (2.50) takes the form

$$\psi_{2yr}(u_{a+n_{[i]}})=\exp\left(2yr\left(\frac{\pi}{\psi^2\ \mathrm{Im}\ \tau}\, n_{[i]}\cdot n_{[i]}+\frac{\pi}{\mathrm{Im}\ \tau}\, a\cdot n_{[i]}\right)\right)\psi_{2yr}(u_a). \tag{2.54}$$

For maps of the form $g_{0,m_{[i]}}$ with $m_{[i]}=\Sigma_{j=1}^{l} m_{[i]}^j \alpha_{(j)}$ and $m_{[i]}^j=\delta_i^j$, one finds

$$\psi_{2yr}(u_{a+m_{[i]}r})=\exp\left(2yr\left(\frac{\pi\tau\overline{\tau}}{\psi^2\ \mathrm{Im}\ \tau}\, m_{[i]}\cdot m_{[i]}+\frac{\pi}{\mathrm{Im}\ \tau}\, a\cdot m_{[i]}\overline{\tau}\right)\right)\psi_{2yr}(u_a). \tag{2.55}$$

The two types of maps under consideration generate the maps (2.43), as described in Ref. 2. The general solution to Eqs. (2.54) and (2.55) can be expressed in terms of theta functions of level r:

$$\psi_{2yr,p}(a,\tau)=\exp\left(\frac{yr\pi\psi^2 a^2}{2\ \mathrm{Im}\ \tau}\right)\Theta_{2yr,p}(a,\tau), \tag{2.56}$$

where p is an element of the weight lattice modulo $2yr$ times the root lattice, i.e., $p\in\Lambda_W/2yr\Lambda_R$. The properties of the theta functions $\Theta_{2yr,p}(a,\tau)$ are briefly summarized in the Appendix.

Our analysis leads to the following form for the wave functional:

$$\Psi[A_{\bar{z}}]=\xi\ \exp\left(-\left(k+\frac{g^\vee}{2y}\right)(\Gamma(u)+\langle u_a,u\rangle)\right)\ \frac{\psi_{2yk+g^\vee}(u_a)}{\psi_{g^\vee}(u_a)}, \tag{2.57}$$

where ξ is a constant and $\psi_{2yk+g^\vee}(u_a)$ and $\psi_{g^\vee}(u_a)$ represent certain linear combinations of the solutions (2.56). As shown in Refs. 1 and 2, the u dependence of the wave functional can be integrated out, obtaining an effective theory. Using (2.57), the inner product (2.47) becomes

$$\begin{aligned}(\Psi'|\Psi)=&\int du_a\ du_a^\dagger |\Pi(a,\tau)|^4(\mathrm{Im}\ \tau)^l\ \exp\left(-\left(k+\frac{g^\vee}{y}\right)\langle u_a,u_a^{-1}\rangle\right)\\ &\times\overline{\xi'}\xi\left[\frac{\psi'_{2yk+g^\vee}(u_a)}{\psi'_{g^\vee}(u_a)}\right]\frac{\psi_{2yk+g^\vee}(u_a)}{\psi_{g^\vee}(u_a)}\int du\ d\overline{u}\\ &\times\exp\left(-\left(k+\frac{g^\vee}{2y}\right)\Gamma(u\overline{u}^{-1},C)\right),\end{aligned} \tag{2.58}$$

which, after using the result[23]

$$\int du\ d\overline{u}\exp\left(-\left(k+\frac{g^\vee}{2y}\right)\Gamma(u\overline{u}^{-1},C)\right)=(\mathrm{Im}\ \tau)^{-l/2}|\Pi(a,\tau)|^{-2}\ \exp\left(\frac{g^\vee}{2y}\langle u_a,u_a^{-1}\rangle\right), \tag{2.59}$$

becomes

$$(\Psi'|\Psi)=\int du_a\, du_a^{\dagger}|\Pi(a,\tau)|^2(\mathrm{Im}\ \tau)^{l/2}\exp\left(-\left(k+\frac{g^{\vee}}{y}\right)\langle u_a,u_a^{-1}\rangle\right)$$
$$\times\overline{\xi'}\xi\left[\frac{\psi'_{2yk+g^{\vee}}(u_a)}{\psi'_{g^{\vee}}(u_a)}\right]\frac{\psi_{2yk+g^{\vee}}(u_a)}{\psi_{g^{\vee}}(u_a)}. \tag{2.60}$$

Weyl invariance forces us to choose antisymmetric combinations of the solutions (2.56). Defining

$$\lambda_{2yr,p}(a,\tau)=\sum_{w\in W}\epsilon(w)\psi_{2yr,w(p)}(a,\tau), \tag{2.61}$$

where W is the Weyl group and $\epsilon(w)$ is the signature of the element $w\in W$, the effective inner product (2.60) becomes

$$(\lambda_{2yk+g^{\vee},q}|\lambda_{2yk+g^{\vee},p})=|\xi|^2\int d^la\, d^l\bar{a}\,(\mathrm{Im}\ \tau)^{-l/2}\exp\left(-(2yk+g^{\vee})\frac{\pi\psi^2}{2\,\mathrm{Im}\ \tau}a\cdot\bar{a}\right)$$
$$\times\overline{\lambda_{2yk+g^{\vee},q}(a,\tau)}\lambda_{2yk+g^{\vee},p}(a,\tau). \tag{2.62}$$

From this inner product for the effective theory one can read the commutation relations of its basic operators:

$$[\bar{a}^{\dagger},a_j]=\frac{2\,\mathrm{Im}\ \tau}{\pi(2yk+g^{\vee})\psi^2}\delta^i_j. \tag{2.63}$$

The states $\lambda_{2yr,p}$ of the form (2.61), which are independent in $\Lambda_W/2yr\Lambda_R$, constitute the physical states or Hilbert space of the theory. The set of weights labeling those states constitute the fundamental chamber $\mathscr{F}_{2yr}$.

Knot operators are associated to Wilson lines. They correspond to the form of these operators when represented in the framework of the Hilbert space that has been constructed. Let us consider a torus knot labeled by two coprime integers n and m, and their corresponding Wilson line:

$$W_{\Lambda}^{(n,m)}=\mathrm{Tr}_{\Lambda}\left(P\ \exp\int_{n,m}A\right). \tag{2.64}$$

We use the convention in which $n(m)$ denotes the number of times that the Wilson line winds along the β-cycle (α-cycle) on the torus.

We are interested in the form of this operator when the single valued map u in (2.32) has been integrated out. In other words, we need the expression for the Wilson line (2.64) when $u=1$. Using (2.33) it turns out to be

$$W_{\Lambda}^{(n,m)}=\mathrm{Tr}_{\Lambda}\left(\exp\left(\frac{i\pi}{\mathrm{Im}\ \tau}((n\bar{\tau}+m)a\cdot H-(n\tau+m)\bar{a}\cdot H)\right)\right)$$
$$=\sum_{\mu\in M_{\Lambda}}\exp\left(-\frac{\pi}{\mathrm{Im}\ \tau}(n\bar{\tau}+m)a\cdot\mu+\frac{2(n\tau+m)}{(2yk+g^{\vee})\psi^2}\mu\cdot\frac{\partial}{\partial a}\right), \tag{2.65}$$

where in the last step we have used (2.63), and the fact that H is made out of diagonal matrices whose entries are related to the components of the set of weights $\mu\in M_{\Lambda}$, M_{Λ} being the set of weights corresponding to an irreducible representation of highest weight Λ. Using the standard properties of the theta functions that are compiled in the Appendix, one finds

$$W_\Lambda{}^{(n,m)}\lambda_{2yk+g^\vee,p}=\sum_{\mu\in M_\Lambda}\exp\left(\frac{2i\pi\mu^2nm}{\psi^2(2yk+g^\vee)}+\frac{4i\pi mp\cdot\mu}{\psi^2(2yk+g^\vee)}\right)\lambda_{2yk+g^\vee,p+n\mu}. \tag{2.66}$$

These operators are called knot operators. They satisfy the following important relation:

$$W_\Lambda{}^{(1,0)}|\rho\rangle=|\rho+\Lambda\rangle, \tag{2.67}$$

where $|\rho\rangle$ is the state corresponding to the weight (2.38). As discussed in Refs. 1 and 2, this relation allows us to think of the operators $W_\Lambda{}^{(1,0)}$ as creation operators since they create the state corresponding to the highest weight Λ when acting on the vacuum state $|\rho\rangle$.

One important ingredient in the computation of knot invariants for torus knots is the knowledge of the corresponding representation on the set of homeomorphisms on T^2. These homeomorphisms are generated by modular transformations S and T on T^2, which possess the following representation:[25]

$$T_{p,p'}=\delta_{p,p'}e^{2\pi i(h_p-c/24)},$$

$$S_{p,p'}=\frac{i^{|\Delta_+|}}{(2yk+g^\vee)^{1/2}}\left(\frac{\text{Vol }\mathscr{L}_R^*}{\text{Vol }\mathscr{L}_R}\right)\sum_{w\in W}\epsilon(w)e^{-[4\pi ip\cdot w(p')]/\psi^2(2yk+g^\vee)}, \tag{2.68}$$

where $|\Delta_+|$ is the number of positive roots, $\mathscr{L}_R$ is the lattice of long roots, and $\mathscr{L}_R^*$ is its dual. In (2.68), h_p and c represent the conformal weight and central charge of the corresponding two-dimensional conformal field theory:

$$h_p=\frac{p^2-\rho^2}{\psi^2(2yk+g^\vee)},\quad c=\frac{2yk\ \dim(G)}{2yk+g^\vee}. \tag{2.69}$$

Knot operators provide a very useful tool to compute knot invariants in lens spaces. These spaces are boundary-less three-dimensional manifolds that can be built by joint of two tori. The gluing is carried out by a homeomorphism whose representation in the Hilbert space that we have constructed is written in terms of the generators (2.68). If we denote this representation by F, the vacuum expectation value for a Wilson line corresponding to a torus knot carrying an irreducible representation of highest weight Λ of a simple group G is

$$V_\Lambda{}^{(n,m)}|_F=\frac{\langle\rho|FW_\Lambda{}^{(n,m)}|\rho\rangle}{\langle\rho|F|\rho\rangle}. \tag{2.70}$$

To connect with the standard form in which polynomial invariants are written, we need to correct (2.70) in three aspects. First of all in (2.70), a choice of frame for the knot and the manifold has been done. Invariants are usually expressed in the standard frames and we must correct (2.70) so that the contribution from the knot framing factor is cancelled, and that the appropriate choice of F is made. Taking the three-sphere as our choice of lens space, which will be the case of interest in this paper, the standard frame is accomplished considering $F=S$, S being one of the two generators of modular transformations. As shown in Ref. 2, the correction relative to the frame of the knot is easily accomplished, multiplying by

$$e^{-2\pi inmh_{\rho+\Lambda}}, \tag{2.71}$$

where $h_{\rho+\Lambda}$ is the conformal weight given in (2.69). The second aspect leading to an additional correction for (2.70) is the fact that the orientation chosen for the torus T^2 is opposite to the standard one. We must therefore do the following change $m\to -m$. Finally, the third aspect is that

usually knot invariants are normalized in such a way that their value for the unknot is one. We must therefore normalize (2.70) by its value for the unknot. These three aspects lead to the following proposition.

Proposition 2.1: The normalized knot invariant for a torus knot $\{n,m\}$ in the standard framing, carrying a G irreducible representation of highest weight Λ on S^3 in the standard framing, is

$$X_\Lambda{}^{(n,m)}=e^{2\pi i n m h_{\rho+\Lambda}}\,\frac{V_\Lambda{}^{(n,-m)}|_{S^3}}{V_\Lambda{}^{(1,0)}|_{S^3}}=e^{2\pi i n m h_{\rho+\Lambda}}\,\frac{\langle\rho|SW_\Lambda{}^{(n,-m)}|\rho\rangle}{\langle\rho|SW_\Lambda{}^{(1,0)}|\rho\rangle}. \tag{2.72}$$

The structures of the knot operators (2.66) and the matrix $S_{p,p'}$ in (2.68) allow to express this invariant in terms of the variable

$$t=e^{2\pi i/(2yk+g^\vee)}, \tag{2.73}$$

which encloses all the dependence on k. The main purpose of this paper is to compute (2.72) for the fundamental representation of the group SO(N). This will lead to the Kauffman polynomial[18] for torus knots. The resulting formula agrees with the one given in Ref. 19. The comparison of this formula to the corresponding known expression for the HOMFLY polynomial[13,15,17] will allow to prove (1.1).

III. KAUFFMAN POLYNOMIAL FOR TORUS KNOTS

In this section we will make use of Proposition 2.1 to compute the Kauffman polynomial for torus knots. We must evaluate (2.72) for the fundamental representation of SO(N), i.e., we must make $\Lambda=\lambda^{(1)}$. The result is stated in the following theorem.

Theorem 3.1: The Kauffman polynomial for a torus knot $\{n,m\}$ is given by

$$X^{(n,m)}_{\lambda^{(1)}}=\frac{[1]\lambda^{nm}}{[1]+[0;1]}\left(\sum_{\substack{\gamma+\beta+1=n\\ \beta,\gamma\geqslant 0}} t^{-(m/2)(\beta-\gamma)}\lambda^{-m}(-1)^\gamma\left(\frac{1}{[n]}+\frac{1}{[\beta-\gamma;1]}\right)\right.$$
$$\left.\times\frac{1}{[\beta]![\gamma]!}\prod_{j=-\gamma}^{\beta}[j;1]+\begin{cases}0, & n \text{ odd}\\ 1, & n \text{ even}\end{cases}\right), \tag{3.1}$$

where

$$[p]=t^{p/2}-t^{-p/2},\quad [p;y]=t^{p/2}\lambda^y-t^{-p/2}\lambda^{-y},\quad \lambda=t^{(N-1)/2},\quad t=e^{2\pi i/(2k+g^\vee)}, \tag{3.2}$$

with $g^\vee=N-2$.

Proof: The rest of this section deals with the proof of this theorem. As SO(N) has two different algebras, depending on whether N is odd or even, we will have to study both cases separately. We will begin with SO($2l+1$), B_l being the corresponding algebra. The main feature of this case is that the simple roots of B_l are not all of the same length. Notice that since an $\{n,m\}$ torus knot is isotopically equivalent to the $\{-n,-m\}$ torus knot, we can restrict ourselves to torus knots with $n>0$. Also, we will consider the case in which $l>n$. Our results, however, as in the case of the HOMFLY polynomial computed in Ref. 5, are valid for arbitrary l. In this proof we make the following choice of normalization for the long roots:

$$\psi^2=2. \tag{3.3}$$

Notice also that for SO(N) the Dynkin index for the fundamental representation is $y=1$ and therefore (2.73) becomes

$$t=e^{2\pi i/(2k+g^\vee)}. \tag{3.4}$$

A. SO(2*l*+1)

Let us begin working out the action of the knot operator $W^{(n,m)}_{\lambda^{(1)}}$ on the vacuum state. Using (2.66), (3.3), and the form of t in (3.4), we have

$$W^{(n,-m)}_{\lambda^{(1)}}|\rho\rangle=\sum_{i=1}^{2l+1} t^{-(1/2)\mu_i^2 nm-m\mu_i\cdot\rho}|\rho+n\mu_i\rangle, \tag{3.5}$$

where μ_i, $i=1,\ldots,2l+1$, are the weights in $M_{\lambda^{(1)}}$ whose explicit expression is given in (A20). Following the framework described in the previous section, we must find the canonical representatives in the fundamental chamber $\mathscr{F}_{2k+g^\vee}$ (notice that $2yr=2yk+g^\vee$ and $y=1$) of the weights appearing in the sum. The weights present in (3.5) have the following structure:

$$\begin{gathered}
\rho+n\mu_1=(n+1,1,\ldots,1),\\
\vdots,\\
\rho+n\mu_j=(1,\ldots,1,\overset{j}{1-n},1+n,1,\ldots,1),\\
\vdots,\\
\rho+n\mu_l=(1,\ldots,1,1-n,1+2n),\\
\rho+n\mu_{l+1}=\rho,\\
\rho+n\mu_{l+2}=(1,\ldots,1,1+n,1-2n),\\
\vdots,\\
\rho+n\mu_{l+1+j}=(1,\ldots,1,\overset{l-j+1}{1+n,1-n},l,\ldots,1),\\
\vdots,\\
\rho+n\mu_{2l+1}=(1-n,1,\ldots,1).
\end{gathered} \tag{3.6}$$

Every weight in the weight lattice can be written as $w(\mu)+(2k+g^\vee)\alpha$, where w is an element of the Weyl group, α is a long root, and μ is a weight whose components are non-negative. In the Hilbert space constructed in the previous section the weights that possess one or more components that vanish are represented by null vectors. Since $2l+1>n$ there is no need to add terms of the form $(2k+g^\vee)\alpha$ to the weights in (3.6) to bring them to a form in which their components are non-negative. A series of Weyl reflections will be sufficient. If $n=1$ all the weights in (3.6) except the first one and $\rho+n\mu_{l+1}$ have one vanishing component, and therefore there are only these two contributions in the sum present in (3.5). If $n>1$, notice first that the weights $\rho+n\mu_1$ and $\rho+n\mu_{l+1}$ in (3.6) are already in $\mathscr{F}_{2k+g^\vee}$. For the rest we have the following cases:

1. Case $i=2,\ldots,l$

(a) $2\leqslant i\leqslant n$. We perform the chain of Weyl reflections:

$$\begin{aligned}\rho+n\mu_i &\overset{\sigma_1}{\longrightarrow}\cdots\overset{\sigma_{i-2}}{\longrightarrow}\overset{\sigma_{i-1}}{\longrightarrow}\nu_i=(n+1-i,1,\ldots,\overset{i}{2},\ldots,1),\quad i=2,\ldots,l-1,\\ \rho+n\mu_l &\overset{\sigma_1}{\longrightarrow}\cdots\overset{\sigma_{l-2}}{\longrightarrow}\overset{\sigma_{l-1}}{\longrightarrow}\nu_l=(n+1-l,1,\ldots,1,3).\end{aligned}\tag{3.7}$$

The weight $i=l$ will not be considered, as we restrict ourselves to $n<l$.

(b) $i>n$. The chain of Weyl reflections is like the one in (3.7):

$$\begin{aligned}\rho+n\mu_i &\overset{\sigma_{i+1-n}}{\longrightarrow}\cdots\overset{\sigma_{i-1}}{\longrightarrow}=(1,\ldots,1,\overset{i-n}{0},1,\ldots,\overset{i}{2},\ldots,1),\quad i=1,\ldots,l-1,\\ \rho+n\mu_l &\overset{\sigma_{l+1-n}}{\longrightarrow}\cdots\overset{\sigma_{l-1}}{\longrightarrow}=(1,\ldots,1,\overset{l-n}{0},\ldots,1,3).\end{aligned}\tag{3.8}$$

After $n+1$, reflections the weights get a vanishing component and therefore all these weights correspond to null vectors and do not contribute to the sum in (3.5). This fact is very important in this calculation because it implies that the sum (3.5) is truncated. Its upper limit turns out to be n instead of $2l+1$.

2. Case $i=l+2,\ldots,2l+1$

As $i>n$ for the weights in this case, we would expect that all of them would achieve a vanishing component after a chain of Weyl reflections. What actually happens is that for n odd an extra weight will contribute:

$$\rho+n\mu_{l+2}\overset{\sigma_l}{\longrightarrow}=(1,\ldots,1,2-n,2n-1)=\rho,\quad \text{for } n=1.$$

For $j=2,\ldots,l$, one has the following situations:

$n\leqslant j$,

$$\rho+n\mu_{l+1+j}\overset{\sigma_{l-j+n-1}}{\longrightarrow}\cdots\overset{\sigma_{l-j+1}}{\longrightarrow}=(1,\ldots,1,\overset{l-j}{2},\ldots,1,\ldots,\overset{l-j+n}{0},\ldots,1);$$

$j<n<2j-1$,

$$\rho+n\mu_{l+1+j}\overset{\sigma_{l+j-n}}{\longrightarrow}\cdots\overset{\sigma_l}{\longrightarrow}\overset{\sigma_{l-1}}{\longrightarrow}\cdots\overset{\sigma_{l-j+1}}{\longrightarrow}=(1,\ldots,1,\overset{l-j}{2},\ldots,1\cdots\overset{l+j-1-n}{0},\ldots,1);\tag{3.9}$$

$n=2j-1$,

$$\rho+n\mu_{l+1+j}\overset{\sigma_{l-j+1}}{\longrightarrow}\cdots\overset{\sigma_l}{\longrightarrow}\overset{\sigma_{l-1}}{\longrightarrow}\cdots\overset{\sigma_{l-j+1}}{\longrightarrow}=(1,\ldots,1,2j-n,n-(2j-2)\ldots,1)=\rho;$$

$2j-1<n<l$,

$$\rho+n\mu_{l+1+j}\overset{\sigma_{l+j-n+1}}{\longrightarrow}\cdots\overset{\sigma_l}{\longrightarrow}\overset{\sigma_{l-1}}{\longrightarrow}\cdots\overset{\sigma_{l-j+1}}{\longrightarrow}=(1,\ldots,1,\overset{l+j-n}{0},\ldots,1\cdots\overset{l-j+1}{2},\ldots,1).$$

We see that all the vectors have a vanishing component, except when $n=2j-1$, where the weight $\nu_{l+1+j}=\rho$ belongs to $\mathscr{T}_{2k+g^\vee}$. Taking into account these considerations, we find that the weights contributing to the sum in (3.5) are

$$\begin{aligned}
&\nu_i=\epsilon(\omega_i)\cdot(n+1-i,1\cdots\overset{i}{2}\cdots 1), \quad i=1,\ldots,n,\\
&\nu_{l+1}=\epsilon(\omega_{l+1})\cdot\rho,\\
&\nu_{l+1+i}=\epsilon(\omega_{l+1+i})\cdot\rho, \qquad\qquad n=2i-1,
\end{aligned} \tag{3.10}$$

where $\epsilon(\omega)$ is the signature of the Weyl chain, given by the number of Weyl reflections we have made to bring the weights to this form:

$$\begin{aligned}
&\omega_i=\sigma_1\cdots\sigma_{i-1}, && \Rightarrow\epsilon(\omega_i)=(-1)^{i-1},\\
&\omega_{l+1}=I, && \Rightarrow\epsilon(\omega_{l+1})=(-1)^0=1,\\
&\omega_{l+1+i}=\sigma_{l+1-i}\cdots\sigma_{l-1}\sigma_l\sigma_{l-1}\cdots\sigma_{l-i+1}, && \Rightarrow\epsilon(\omega_{l+1+i})=(-1)^{2i-1}=-1.
\end{aligned}$$

Using these results and the scalar products in (A22), the sum in (3.5) becomes

$$W_\Lambda{}^{(n,-m)}|\rho\rangle=\sum_{i=1}^{n} t^{-(nm/2)-m(2l+1-2i)}(-1)^{i-1}|\nu_i\rangle+\begin{cases}0, & n \text{ odd};\\ |\rho\rangle, & n \text{ even}.\end{cases} \tag{3.11}$$

This equation is valid for any $n\geqslant 1$ as long as $l>n$. The vacuum expectation value (2.70) that enters (2.72) takes the form

$$V^{(n,-m)}_{\lambda^{(1)}}=\frac{\langle\rho|SW^{(n,-m)}_{\lambda_1}|\rho\rangle}{\langle\rho|S|\rho\rangle}=\sum_{i=1}^{n} t^{-(nm/2)-m(2l+1-2i)}(-1)^{i-1}\frac{S_{\rho,\nu_i}}{S_{\rho,\rho}}+\begin{cases}0, & n \text{ odd};\\ 1, & n \text{ even}.\end{cases} \tag{3.12}$$

The weights ν_i have the general expression $\nu_i=\rho+(n-i,0\cdots\overset{i}{1}\cdots 0)=\rho+\Lambda$. If Λ is a highest weight, the ratio $S_{\rho,\rho+\Lambda}/S_{\rho,\rho}$ can be written in terms of the character associated to Λ with the help of the Weyl formula,

$$\frac{S_{\rho,\rho+\Lambda}}{S_{\rho,\rho}}=\frac{\Sigma_{w\in W}\epsilon(w)t^{\rho\cdot w(\rho+\Lambda)}}{\Sigma_{w\in W}\epsilon(w)t^{\rho\cdot w(\rho)}}=\mathrm{ch}_\Lambda\left[-\frac{2\pi i}{2k+g^\vee}\rho\right]. \tag{3.13}$$

All the weights entering (3.12) can be thought of as highest weights, and therefore we can express $V^{(n,-m)}_{\lambda^{(1)}}$ in terms of characters:

$$V^{(n,-m)}_{\lambda^{(1)}}=\sum_{i=1}^{n} t^{-(nm/2)-m(2l+1-2i)}(-1)^{i-1}\,\mathrm{ch}_{(n-i)\lambda^{(1)}+\lambda^{(i)}}\left[-\frac{2\pi i}{2k+g^\vee}\rho\right]+\begin{cases}0, & n \text{ odd};\\ 1, & n \text{ even}.\end{cases} \tag{3.14}$$

Let us compute first $V^{(1,0)}_{\lambda^{(1)}}$, which is the quantity entering the denominator in (2.72). From (3.12) and (3.13) it follows that one needs to compute the character for the fundamental representation. This calculation is done very simply just summing over the weights of the representation:

$$\mathrm{ch}_{\lambda^{(1)}}\left[-\frac{2\pi i}{2k+g^\vee}\rho\right]=\sum_{\mu\in M_{\lambda^{(1)}}} t^{-\mu\cdot\rho}=1+\sum_{j=1}^{l} t^{-\mu_j\cdot\rho}+\sum_{k=1}^{l} t^{-\mu_{l+1+k}\cdot\rho}=1+\frac{t^l-t^{-l}}{t^{1/2}-t^{-1/2}}. \tag{3.15}$$

Using this result, it turns out that

$$V^{(1,0)}_{\lambda^{(1)}}=1+\frac{\lambda-\lambda^{-1}}{t^{1/2}-t^{-1/2}}, \tag{3.16}$$

which has been written entirely in terms of the variables λ and t in (3.2) (notice that in this case $N=2l+1$). This result agrees with previous calculations for the unknot.[7,10]

For representations different from the fundamental one, however, it is more useful to compute the character using its expression in terms of a product over positive roots:

$$\mathrm{ch}_\Lambda\left[-\frac{2\pi i}{2k+g^\vee}\rho\right]=\sum_{\mu\in M_\Lambda} t^{-\mu\cdot\rho}=\prod_{\alpha>0}\frac{t^{(1/2)\alpha\cdot(\rho+\Lambda)}-t^{-(1/2)\alpha\cdot(\rho+\Lambda)}}{t^{(1/2)\alpha\cdot\rho}-t^{-(1/2)\alpha\cdot\rho}}. \tag{3.17}$$

In this equation, the symbol $\alpha>0$ indicates that the product has to be performed over all the positive roots. For B_l, these are given in the Appendix. Our next task is to compute the characters appearing in (3.14) with the help of this formula.

In order to simplify our notation, from now on we will denote $\mathrm{ch}_\Lambda[-2\pi i\rho/(2k+g^\vee)]$ simply by ch_Λ. Also, we introduce the following notation regarding q numbers and q factorials:

$$\begin{gathered}[p]=t^{p/2}-t^{-p/2},\\ [p]!=[p][p-1]\cdots[1],\quad [0]!=1.\end{gathered} \tag{3.18}$$

This allows us to write the character formula in the form

$$\mathrm{ch}_\Lambda=\prod_{\alpha>0}\frac{[\alpha\cdot(\rho+\Lambda)]}{[\alpha\cdot\rho]}. \tag{3.19}$$

In order to compute (3.14) we must perform the products in (3.19) for weights of the form $(n-i)\lambda^{(1)}+\lambda^{(i)}$. Taking into account the form of the positive roots listed in (A6), this suggests the organization of the product in (3.19) splitting the set of positive roots in two groups, I and II, depending on whether the positive root contains the simple root $\alpha_{(1)}$ or not. Another thing we have to take into account is that the metric between fundamental weights and simple roots of this algebra, for the normalization chosen for the long roots, is the following:

$$\alpha_{(i)}\cdot\lambda^{(j)}=\mathrm{diag}(1\cdots1,\tfrac{1}{2}), \tag{3.20}$$

due to the fact that the simple root $\alpha_{(l)}$ is shorter than the others. Let us carry out the computation of the character.

The products of the positive roots with the Weyl vector are

$$\beta_{(j)}\cdot\rho=l-j+\tfrac{1}{2},\quad \gamma_{(j,k)}\cdot\rho=1+k,\quad \delta_{(j,k)}\cdot\rho=2l-2j-k, \tag{3.21}$$

and with the weights $\nu_i=\rho+(n-i,0\cdots\overset{i}{1}\cdots0)$, $i=1,\ldots,l-1$:

(a) group I, positive roots with $\alpha_{(1)}$

$$\beta_{(1)}\cdot\nu_i = l-1+\tfrac{1}{2}+n-i+1,$$

$$\gamma_{(1,k)}\cdot\nu_i = 1+k+n-i+\begin{cases}1, & i\leqslant k+1;\\ 0, & k\leqslant i-2;\end{cases} \tag{3.22}$$

$$\delta_{(1,k)}\cdot\nu_i = 2l-2-k+n-i+\begin{cases}1, & i\leqslant k+1;\\ 2, & k\leqslant i-2;\end{cases}$$

(b) group II, positive roots without $\alpha_{(1)}$

$$\beta_{(j)}\cdot\nu_i = \begin{cases} l-j+\tfrac{1}{2}+1, & j\leqslant i;\\ l-j+\tfrac{1}{2}, & j>i;\end{cases}$$

$$\gamma_{(j,k)}\cdot\nu_i = \begin{cases} 1+k, & j>i, \text{ or } i\geqslant j+k+1;\\ 2+k, & j\leqslant i\leqslant j+k;\end{cases} \tag{3.23}$$

$$\delta_{(j,k)}\cdot\nu_i = \begin{cases} 2l-2j-k, & j>i;\\ 2l-2j-k+1, & i\leqslant j\leqslant j+k;\\ 2l-2j-k+2, & i\geqslant j+k+1.\end{cases}$$

We have these two contributions to the characters:

$$\begin{aligned}\prod_{\alpha\in 1}\frac{[\alpha\cdot\nu_i]}{[\alpha\cdot\rho]} &= \frac{[l+\frac{1}{2}+n-i]}{[l-\frac{1}{2}]}\prod_{k=0}^{i-2}\frac{[1+k+n-i]}{[1+k]}\prod_{k=i-1}^{l-2}\frac{[2+k+n-i]}{[1+k]}\prod_{k=0}^{i-2}\frac{[2l+n-i-k]}{[2l-2-k]}\\ &\quad\times\prod_{k=i-1}^{l-2}\frac{[2l-1-k+n-i]}{[2l-2-k]}\\ &= \frac{1}{[n][2l+n-2i+1]}\frac{[n-i+l+\frac{1}{2}]}{[l-\frac{1}{2}]}\frac{[2l+n-i]!}{[n-i]![2l-2]!}\end{aligned} \tag{3.24}$$

and

$$\prod_{\alpha\in \mathrm{II}} \frac{[\alpha\cdot\nu_i]}{[\alpha\cdot\rho]} = \prod_{j=2}^{i} \frac{[l-j+1+\frac{1}{2}]}{[l-j+\frac{1}{2}]} \prod_{j=2}^{i-1} \prod_{k=0}^{i-j-1} \frac{[2l-2j-k+2]}{[2l-2j-k]} \prod_{j=2}^{i} \prod_{k=i-j}^{l-j-1} \frac{[2l-2j-k+1]}{[2l-2j-k]}$$
$$\times \prod_{j=2}^{i} \prod_{k=i-j}^{i-j-1} \frac{[2+k]}{[1+k]}$$
$$= \frac{[l-\frac{1}{2}]}{[l-i+\frac{1}{2}]} \frac{[2l-2i+1]}{[i-1]!} \frac{[2l-2]!}{[2l-i]!}. \tag{3.25}$$

Taking into account (3.24) and (3.25) we finally obtain a formula for the character in terms of q numbers:

$$\mathrm{ch}_{(n-i)\lambda^{(1)}+\lambda^{(i)}} = \prod_{\alpha>0} \frac{[\alpha\cdot\nu_i]}{[\alpha\cdot\rho]} = \left(\frac{1}{[n]} + \frac{1}{[n+2l-2i+1]}\right) \frac{1}{[n-i]![i-1]!} \prod_{j=-(i-1)}^{n-i} [2l+j]. \tag{3.26}$$

From this it is straightforward to write an expression for (3.14) involving only the variables t and λ. First we introduce the notation

$$[p;y] = t^{p/2}\lambda^{y} - t^{-p/2}\lambda^{-y}, \quad \beta = n-i, \quad \gamma = i-1. \tag{3.27}$$

Recall that λ is defined as $\lambda = t^{(N-1)/2} = t^{l}$. One finds

$$V^{(n,-m)}_{\lambda^{(1)}} = \sum_{\substack{\gamma+\beta+1=n \\ \gamma,\beta\geq 0}} t^{-(m/2)(\beta-\gamma)} \lambda^{-m} (-1)^{\gamma} \left(\frac{1}{[n]} + \frac{1}{[\beta-\gamma;1]}\right)$$
$$\times \frac{1}{[\beta]![\gamma]!} \prod_{j=-\gamma}^{\beta} [j;1] + \begin{cases} 0, & n \text{ odd;} \\ 1, & n \text{ even.} \end{cases} \tag{3.28}$$

It remains only to obtain the deframing phase factor. The conformal weight for the fundamental representation of SO($2l+1$) is given by (2.69):

$$h_{\rho+\lambda^{(1)}} = \frac{(\rho+\lambda^{(1)})^2 - \rho^2}{2(2k+g^{\vee})} = \frac{l}{(2k+g^{\vee})}, \tag{3.29}$$

which gives the deframing factor

$$e^{2\pi i n m h_{\rho+\lambda^{(1)}}} = t^{lmn} = \lambda^{nm}. \tag{3.30}$$

From (3.28), (3.30), and (3.16), one obtains the final expression for the knot invariant (2.72), which equals the one stated in Theorem 3.1. This ends the proof for the case SO($2l+1$).

B. SO(2*l*)

As the calculation procedure is the same as in the previous case, we will simply give the main results at each step. The Lie algebra is now D_l and its main features are summarized in the Appendix.

The action of the knot operator on the vacuum state is given by

$$W_{\lambda^{(1)}}^{(n,-m)}|\rho\rangle=\sum_{i=1}^{2l} t^{-(1/2)\mu_i^2 nm-m\mu_i\cdot\rho}|\rho+n\mu_i\rangle, \tag{3.31}$$

where $\mu_i=1,\ldots,2l$ are the weights in $M_{\lambda^{(1)}}$ whose expression is in (A25). The vectors $\rho+n\mu_i$ have the structure

$$\begin{gathered}
\rho+n\mu_1=(n+1,1,\ldots,1),\\
\vdots\\
\rho+n\mu_j=(1,\ldots,1,\overset{j}{1-n},1+n,1,\ldots,1),\\
\vdots\\
\rho+n\mu_{l-1}=(1,\ldots,1,1-n,1+n,1+n),\\
\rho+n\mu_l=(1,\ldots,1,1-n,1+n),\\
\rho+n\mu_{l+1}=(1,\ldots,1,1+n,1-n),\\
\rho+n\mu_{l+2}=(1,\ldots,1,1+n,1-n,1-n),\\
\vdots\\
\rho+n\mu_{l+j}=(1,\ldots,1,\overset{l-j}{1+n},1-n,1,\ldots,1),\\
\vdots\\
\rho+n\mu_{2l-1}=(1+n,1-n,1,\ldots,1),\\
\rho+n\mu_{2l}=(1-n,1,\ldots,1),
\end{gathered} \tag{3.32}$$

and those who contribute to the sum in (3.31), for the case $n<l$, after taking the suitable chain of Weyl reflections, and the corresponding signature, are

$$\begin{gathered}
\nu_i=(-1)^{(i-1)}\cdot(n+1-i,1,\ldots,\overset{i}{2},\ldots,1),\quad i=1,\ldots,n,\\
\nu_{l+1+i}=\rho,\quad n=2i.
\end{gathered} \tag{3.33}$$

We see that, very similarly to the SO($2l+1$) case, the number of weigths we have to take into account is bounded by n and that there is an extra one in the case of n even. So the expression (3.31) becomes, after using the scalar products in (A27),

$$W_{\lambda^{(1)}}^{(n,-m)}|\rho\rangle=\sum_{i=1}^{n} t^{-(nm/2)-m(l-i)}(-1)^{i-1}|\nu_i\rangle+\begin{cases}0, & n \text{ odd};\\ |\rho\rangle, & n \text{ even}.\end{cases} \tag{3.34}$$

The quantity $V_{\lambda^{(1)}}^{(1,0)}$ is obtained from the character of the fundamental representation:

$$V^{(1,0)}_{\lambda^{(1)}}=\sum_{\mu\in M_{\lambda^{(1)}}} t^{-\mu\cdot\rho}=1+\frac{\lambda-\lambda^{-1}}{t^{1/2}-t^{-1/2}}=\frac{[1]+[0;1]}{[1]}, \tag{3.35}$$

where for the last equality we have use the definitions (3.18) and (3.27). To calculate $V^{(n,-m)}_{\lambda^{(1)}}$ we again need the characterization of the positive roots that is contained in (A7). Then one computes the products of these roots with the Weyl vector and the weigths ν_i. From these we obtain the following formula for the characters:

$$\prod_{\alpha>0}\frac{[\alpha\cdot\nu_i]}{[\alpha\cdot\rho]}=\left(\frac{1}{[n]}+\frac{1}{[n+2l-2i]}\right)\frac{1}{[n-i]![i-1]!}\prod_{j=-(i-1)}^{n-i}[2l+j-1]. \tag{3.36}$$

Using again (3.27), one gets

$$V^{(n,-m)}_{\lambda^{(1)}}=\sum_{\substack{\gamma+\beta+1=n\\ \gamma,\beta\geqslant 0}} t^{-(m/2)(\beta-\gamma)}\lambda^{-m}(-1)^{\gamma}\left(\frac{1}{[n]}+\frac{1}{[\beta-\gamma;1]}\right)$$
$$\times\frac{1}{[\beta]![\gamma]!}\prod_{j=-\gamma}^{\beta}[j;1]+\begin{cases}0, & n \text{ odd};\\ 1, & n \text{ even}\end{cases} \tag{3.37}$$

The framing factor for this case is given by

$$e^{2\pi i n m h_{\rho+\lambda^{(1)}}}=t^{(nm/2)(2l-1)}=\lambda^{nm}. \tag{3.38}$$

It is easy to see that taking into account (3.38), (3.35), and (3.37) we obtain the expression (3.1) for the knot invariant associated to the fundamental representation of SO($2l$). Notice also that although λ is defined in a different way with respect to the rank of the algebra, l, its definition is the same for both cases in terms of the variable N of SO(N). This completes the proof of Theorem 3.1.

C. Natural variables of the Kauffman polynomial and Yokota's formula

The Dubrovnik version of the Kauffman polynomial, as described on p. 215 of Ref. 26, depends on two variables, a (which is called α in Ref. 26) and z. We will refer to these variables as the natural ones. In those variables the skein rules have the simple form shown in Ref. 26. We will denote the Dubrovnik version of the Kauffman polynomial, normalized in such a way that for the unknot its value is unity, by $Y_K(a,z)$, and will try to identify these variables in terms of ours. This can be done comparing the skein rules in Ref. 26 to the skein rules obtained from Chern–Simons theory in Refs. 5, 7 and 8. It turns out that

$$a=\lambda=e^{2\pi i h_{\rho+\lambda^{(1)}}},\quad z=[1]=t^{1/2}-t^{-1/2}. \tag{3.39}$$

The formula in Theorem 3.1 can therefore be stated as

$$Y_{n,m}(\lambda,t^{1/2}-t^{-1/2})=X^{(n,m)}_{\lambda^{(1)}}, \tag{3.40}$$

where $X^{(n,m)}_{\lambda^{(1)}}$ is given in (3.1).

To compare our formula (3.40) to the one obtained by Yokota in Ref. 19 we will use (3.39) and the identification done in Ref. 19 between its variables, q and α, and the natural ones. Proceeding in this way one concludes that the relation between our variables and Yokota's is

$$q=t^{-1/2},\quad a^2=-(q\lambda)^{-1}. \tag{3.41}$$

Taking into account that Yokota uses an orientation opposite to ours, and therefore we must compare (3.40) to its formula for $Y_{n,m}(a^{-1},-z)$, one finds complete agreement after substituting (3.41) in the formula given in Ref. 19.

IV. RELATION BETWEEN THE HOMFLY AND KAUFFMAN POLYNOMIALS FOR TORUS KNOTS

The HOMFLY[16] and Kauffman polynomials[18] have the common characteristic of being functions of two variables defined for oriented links, although their behavior under change of orientation of some of the link components is quite different. On the other hand, the skein rules that define them are also different: in the first one the relation is established among three diagrams and in the second one among four. Both are able to differentiate in many cases one knot from its mirror image, although Kauffman's is more powerful in this sense. These two polynomials are considered as independent, in the sense that there is not a subtle change of variables taking one into the other. In Ref. 27 there are examples of knots with the same Kauffman and different HOMFLY, and *vice versa*. We will prove that for the particular case of torus knots there is a relation between these two polynomials. Let us begin recalling the expression of the HOMFLY polynomial for torus knots. It was first obtained in Ref. 13, reobtained in Ref. 17 using quantum groups, and in Ref. 15 from the Chern–Simons theory with gauge group SU(N). The corresponding invariant has the form[15]

$$\begin{aligned} P_{n,m}(a,z) &= P_{n,m}((\lambda t)^{1/2}, t^{1/2}-t^{-1/2}) \\ &= \left(\frac{1-t}{1-t^n}\right)\frac{\lambda^{(1/2)(m-1)(n-1)}}{\lambda t-1}\sum_{\substack{p+i+1=n\\ p,i\geqslant 0}}(-1)^i t^{mi+(1/2)p(p+1)}\frac{\Pi_{j=-p}^{i}(\lambda t-t^j)}{\Pi_{j=1}^{i}(t^j-1)\Pi_{j=1}^{p}(t^j-1)} \\ &= \frac{[1](\lambda t)^{1/2m(n-1)}}{[-1;-\frac{1}{2}]}\sum_{\substack{\beta+\gamma+1=n\\ \beta,\gamma\geqslant 0}}(-1)^{\gamma}t^{(m/2)(\beta-\gamma)}\frac{1}{[n][\beta]![\gamma]!}\times\prod_{j=-\gamma}^{\beta}[j-1;-\tfrac{1}{2}], \end{aligned} \tag{4.1}$$

where

$$\lambda = t^{N-1}, \quad t = e^{2\pi i/k+g^{\vee}}. \tag{4.2}$$

If one performs one of these two changes of variables,

$$t^{1/2}\to t^{-1/2} \quad \text{or} \quad t^{1/2}\to -t^{1/2}, \tag{4.3}$$

one finds that (3.1) transforms into

$$\begin{aligned} Y_{n,m}(a,-z) &= Y_{n,m}(\lambda, t^{-1/2}-t^{1/2}) \\ &= -\frac{[1]\lambda^{nm}}{[1]-[0;1]}\times\Bigg(\sum_{\substack{\gamma+\beta+1=n\\ \gamma,\beta\geqslant 0}} t^{-(m/2)(\beta-\gamma)}\lambda^{-m}(-1)^{\gamma} \\ &\quad\times\left(\frac{1}{[n]}-\frac{1}{[\beta-\gamma;1]}\right)\frac{1}{[\beta]![\gamma]!}\times\prod_{j=-\gamma}^{\beta}[j;1]+\begin{cases}0, & n \text{ odd}\\ -1 & n \text{ even}\end{cases}\Bigg) \end{aligned} \tag{4.4}$$

It is worthwhile to remark that this is exactly the formula obtained when one calculates the polynomial for torus knots associated to the fundamental representation of Sp(N) from Chern–Simons theory. This can be shown explicitly using the methods developed in the previous section,

or from the form of the skein rules for the fundamental of Sp(N) obtained in Refs. 7 and 8 from Chern–Simons gauge theory. Let us compare (3.1), (4.1), and (4.4). The crucial point is that, using the auxiliary variable q, these three expressions can be written as follows:

$$Y_{n,m}(a,q-q^{-1})=\frac{a^{nm}[1]_q}{[1]_q+a-a^{-1}}\Bigg(\sum_{\substack{\gamma+\beta+1=n\\ \gamma,\beta\geqslant 0}} q^{-m(\beta-\gamma)}a^{-m}(-1)^{\gamma} \times\left(\frac{1}{[n]_q}+\frac{1}{q^{\beta-\gamma}a-q^{\gamma-\beta}a^{-1}}\right)\frac{1}{[\beta]_q![\gamma]_q!} \times\prod_{j=-\gamma}^{\beta}(q^{j}a-q^{-j}a^{-1})+\begin{cases}0, & n \text{ odd}\\ 1, & n \text{ even}\end{cases}\Bigg), \tag{4.5}$$

$$Y_{n,m}(a,-(q^{-1}-q))=-\frac{a^{nm}[1]_q}{[1]_q-a+a^{-1}}\Bigg(\sum_{\substack{\gamma+\beta+1=n\\ \gamma,\beta\geqslant 0}} q^{-m(\beta-\gamma)}a^{-m}(-1)^{\gamma} \times\left(\frac{1}{[n]_q}-\frac{1}{q^{\beta-\gamma}a-q^{\gamma-\beta}a^{-1}}\right)\frac{1}{[\beta]_q![\gamma]_q!} \times\prod_{j=-\gamma}^{\beta}(q^{j}a-q^{-j}a^{-1})+\begin{cases}0, & n \text{ odd}\\ -1, & n \text{ even}\end{cases}\Bigg), \tag{4.6}$$

and

$$P_{n,m}(a,q^{-1}-q)=\frac{a^{m(n-1)}[1]_q}{a-a^{-1}}\sum_{\substack{\gamma+\beta+1=n\\ \gamma,\beta\geqslant 0}} q^{-m(\beta-\gamma)}(-1)^{\gamma}\frac{1}{[n]_q[\beta]_q![\gamma]_q!} \times\prod_{j=-\gamma}^{\beta}(q^{j}a-q^{-j}a^{-1}), \tag{4.7}$$

where

$$[n]_q=q^{n}-q^{-n}. \tag{4.8}$$

The structure on the right-hand side of (4.7) shows that the HOMFLY polynomial, $P_{n,m}(a,z)$, can be expressed in terms of a linear combination of the polynomials $Y_{n,m}(a,z)$ and $Y_{n,m}(a,-z)$. In fact, after performing some algebra from (4.5), (4.6), and (4.7), one obtains

$$P_{n,m}(a,z)=\frac{1}{2}\,(Y_{n,m}(a,z)+Y_{n,m}(a,-z))+\frac{z}{2(a-a^{-1})}\,(Y_{n,m}(a,z)-Y_{n,m}(a,-z)). \tag{4.9}$$

This ends the proof of the relation (1.1) between the HOMFLY and Kauffman polynomials, which was presented in the Introduction.

For $a=1$, the ordinary version of the Kauffman polynomial, $F_{\mathrm{K}}(a,z)$, becomes the unoriented polynomial invariant of ambient isotopy discovered in Refs. 28 and 29 which is usually denoted by $Q_{\mathrm{K}}(z)=F_{\mathrm{K}}(1,z)$. Similarly, we define

$$\widetilde{Q}_{\mathrm{K}}(z)=Y_{\mathrm{K}}(1,z). \tag{4.10}$$

It turns out that for torus knots, after performing the limit $N\to 1$ in (3.1), which is equivalent to $a\to 1$, one finds

$$\widetilde{Q}_{n,m}(z)=1. \tag{4.11}$$

In the case of the HOMFLY polynomial, the limit $a\to 1$ leads to the Alexander–Conway polynomial, $\Delta_{\rm K}(z)=P_{\rm K}(1,z)$. From (4.9) and (4.11), one finds

$$\Delta_{n,m}(z)=1+\frac{z}{4}\frac{\partial}{\partial a}\left(Y_{n,m}(a,z)-Y_{n,m}(a,-z)\right)\Big|_{a=1}. \tag{4.12}$$

Notice that this expression is consistent with the fact that $\Delta_{n,m}(z)$ must be 1 plus a polynomial containing only even powers of z.

V. CONCLUSIONS AND PROSPECTS

In this paper we have presented the construction of the operator formalism, originally discussed in Ref. 1 and Ref. 2 for the groups SU(2) and SU(N), respectively, for an arbitrary simple group. The main result in this respect is the general form for knot operators presented in (2.66).

Knot operators are utilized to compute the knot invariant corresponding to the fundamental representation of the gauge group SO(N). The resulting formula is presented in (3.40) and (3.1), and shown to agree with a previous expression for the Kauffman polynomial. This formula is compared to known expressions for the HOMFLY polynomial and the relation (1.1) between the Kauffman and the HOMFLY polynomials for torus knots is proved.

Our result (1.1) confirms that the Kauffman polynomial is more fundamental than the HOMFLY polynomial. The simplicity of the relation obtained suggests that it could be obtained by other methods. In this respect it would very interesting if it could be reobtained using skein rules.

It would be also worthwhile to study how our results fit in Jaeger's expansions for the Kauffman polynomial in terms of HOMFLY polynomials (see, for example, p. 219 of Ref. 26). Finally, one should also study if there exist similar formulas for other sets of knots. In this respect one would like to start studying the situation in sets characterized by a generalization of the notion of a torus knot. A torus knot is a knot that can be placed on the surface of a standardly embedded torus in S^3 without self-intersection. There are knots that can be placed on a standardly embedded genus two surface without self-intersection, but not on a genus one surface. One could analyze, for example, if there is a relation of the type (1.1) for these knots. In general, one could study the problem for knots placed on a genus g surface. Work in this direction will be presented elsewhere.

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APPENDIX: GROUP THEORY AND THETA FUNCTIONS

1. Group-theoretical conventions

In this section of the Appendix we will summarize our group-theoretical conventions. Let G be a compact simple group of rank l, with generators T^a, $a=1,\ldots,\dim(G)$, which are chosen to be anti-Hermitian. For the fundamental representation of G they are normalized as follows:

$$\mathrm{Tr}(T^aT^b)=-y\psi^2\delta^{ab}, \tag{A1}$$

where y is the Dynkin index of the fundamental representation and ψ^2 is the squared length of the longest simple root of G. The value of y for the groups SU(N), SO(N), Sp(N), E_6, E_7, E_8, F_4, and G_2 are 1/2, 1, 1/2, 9, 12, 30, 6, and 3, respectively.

We will denote the l fundamental roots of G by α_i, $i=1,\ldots,l$. In the explicit calculations carried out in Sec. III they have been chosen in such a way that the long roots have length $\sqrt{2}$, i.e., $\psi^2=2$. The Cartan matrix g_{ij},

$$g_{ij}=2\frac{\alpha_{(i)}\cdot\alpha_{(j)}}{\alpha_{(i)}\cdot\alpha_{(i)}}, \tag{A2}$$

takes the following forms for the two Lie algebras B_l [$l=(N-1)/2$, N odd] and D_l [$l=N/2$, N even] associated to the simple group SO(N), which is the one that has been considered in this paper:

$$g_{ij}(B_l)=\begin{pmatrix} 2 & -1 & 0 & 0 & \cdot & \cdot & \cdot & \cdot & 0 \\ -1 & 2 & -1 & 0 & \cdot & \cdot & \cdot & \cdot & 0 \\ 0 & -1 & 2 & -1 & \cdot & \cdot & \cdot & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & \cdot & \cdot & 2 & -1 & 0 \\ 0 & 0 & 0 & 0 & \cdot & \cdot & -1 & 2 & -1 \\ 0 & 0 & 0 & 0 & \cdot & \cdot & 0 & -2 & 2 \end{pmatrix}, \tag{A3}$$

and

$$g_{ij}(D_l)=\begin{pmatrix} 2 & -1 & 0 & 0 & \cdot & \cdot & \cdot & \cdot & \cdot & 0 \\ -1 & 2 & -1 & 0 & \cdot & \cdot & \cdot & \cdot & \cdot & 0 \\ 0 & -1 & 2 & -1 & \cdot & \cdot & \cdot & \cdot & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & \cdot & \cdot & \cdot & \cdot & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdot & \cdot & -1 & 2 & -1 & -1 \\ 0 & 0 & 0 & 0 & \cdot & \cdot & 0 & -1 & 2 & 0 \\ 0 & 0 & 0 & 0 & \cdot & \cdot & 0 & -1 & 0 & 2 \end{pmatrix}. \tag{A4}$$

We will denote the root lattice by Λ_R. This l-dimensional space is generated by the fundamental roots $\alpha_{(i)}$, which can be taken as a basis, the root basis. Any vector x in this basis has components x^i given by

$$x=\sum_{i=1}^{l} x^i\alpha_{(i)}. \tag{A5}$$

Among all the roots in Λ_R there is a subset that plays an important role in the calculation performed in the paper. These are the positive roots. For SO(N) they take the following form:[30] algebra B_l,

$$\beta_{(j)}=\alpha_{(j)}+\cdots+\alpha_{(l)}, \quad j=1,\ldots,l,$$

$$\gamma_{(j,k)}=\alpha_{(j)}+\cdots+\alpha_{(j+k)}, \quad i=1,\ldots,l-1, \quad k=1,\ldots,l-j-1, \tag{A6}$$

$$\delta_{(j,k)}=\alpha_{(j)}+\cdots+\alpha_{(j+k)}+2(\alpha_{(j+k+1)}+\cdots+\alpha_{(l)}), \quad j=1,\ldots,l-1, \quad k=0,\ldots,l-j-1;$$

algebra D_l,

$$\alpha_{(j)}, \quad j=1,\ldots,l,$$

$$\beta_{(j)}=\alpha_{(j)}+\cdots+\alpha_{(l-2)}+\alpha_{(l)}, \quad j=1,\ldots,l-2,$$

$$\gamma_{(j,k)}=\alpha_{(j)}+\cdots+\alpha_{(j+k)}, \quad j=1,\ldots,l-2, \quad k=1,\ldots,l-j, \tag{A7}$$

$$\delta_{(j,k)}=\alpha_{(j)}+\cdots+\alpha_{(j+k)}+2(\alpha_{(j+k+1)}+\cdots+\alpha_{(l-2)})+\alpha_{(l-1)}+\alpha_{(l)},$$

$$j=1,\ldots,l-3, \quad k=0,\ldots,l-3-j.$$

The fundamental weights $\lambda^{(i)}$, $i=1,\ldots,l$, satisfy

$$2\frac{\alpha_{(i)}\cdot\lambda^{(j)}}{\alpha_{(i)}\cdot\alpha_{(i)}}=\delta_i^j. \tag{A8}$$

The fundamental weights generate over $\mathbf{Z}$ an l-dimensional lattice called the weight lattice, which will be denoted by Λ_W. The lattices Λ_R and Λ_W are dual to each other and $\Lambda_R\in\Lambda_W$. The l-dimensional basis expanded by the fundamental weights is called the Dynkin basis. Any vector x has in this basis components x_i given by

$$x=\sum_{i=1}^{l} x_i\lambda^{(i)}. \tag{A9}$$

The matrix $G^{ij}=\lambda^{(i)}\cdot\lambda^{(j)}$ gives the metric in weight space, so it allows us to rise indices. Its expression for the algebras D_l and B_l is

$$G^{ij}(D_l)=\frac{1}{2}\begin{pmatrix} 2 & 2 & 2 & \cdot & \cdot & \cdot & 2 & 1 & 1 \\ 2 & 4 & 4 & \cdot & \cdot & \cdot & 4 & 2 & 2 \\ 2 & 4 & 6 & \cdot & \cdot & \cdot & 6 & 3 & 3 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 2 & 4 & 6 & \cdot & \cdot & \cdot & 2(l-2) & l-2 & l-2 \\ 1 & 2 & 3 & \cdot & \cdot & \cdot & l-2 & l/2 & (l-2)/2 \\ 1 & 2 & 3 & \cdot & \cdot & \cdot & l-2 & (l-2)/2 & l/2 \end{pmatrix}, \tag{A10}$$

and

$$G^{ij}(B_l)=\frac{1}{2}\begin{pmatrix} 2 & 2 & 2 & \cdot & \cdot & \cdot & 2 & 1 \\ 2 & 4 & 4 & \cdot & \cdot & \cdot & 4 & 2 \\ 2 & 4 & 6 & \cdot & \cdot & \cdot & 6 & 3 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 2 & 4 & 6 & \cdot & \cdot & \cdot & 2(l-1) & l-1 \\ 1 & 2 & 3 & \cdot & \cdot & \cdot & l-1 & l/2 \end{pmatrix}. \tag{A11}$$

Among the weights in Λ_W there is one that plays an important role in Chern–Simons theory because it can be regarded as the vacuum. This weight is denoted by ρ and all its components are one:

$$\rho=\sum_{i=1}^{l}\lambda^{(i)}. \tag{A12}$$

The irreducible representations of G are characterized by highest weights Λ. Highest weights can be written uniquely as a linear combination of fundamental weights with non-negative integer coefficients h_i,

$$\Lambda=\sum_{i=1}^{l}h_i\lambda^{(i)}. \tag{A13}$$

The set of weights of an irreducible representation of highest weight Λ will be denoted as M_Λ. To build this set one may use the following rule: if a weight $\mu\in M_\Lambda$ has the kth Dynkin component greater than zero (i.e., $\mu_k>0$), then the vectors obtained by subtracting $t\alpha_k$ ($t=1,\ldots,\mu_k$) from μ are also elements of M_Λ. One can start applying this rule to Λ and then to the successive weights obtained to build the different elements of M_Λ. The multiplicities of each weight can be obtained using Freudenthal's formula.[31]

The Weyl group is generated by r reflections α_i, $i=1,\ldots,l$, on weight space,

$$x\in\Lambda_W,\quad \alpha_i(x)=x-\frac{2}{\alpha_{(i)}\cdot\alpha_{(i)}}\alpha_{(i)}(\alpha_{(i)}\cdot x). \tag{A14}$$

It divides the weight lattice Λ_W into domains. The fundamental domain or Weyl chamber is chosen to be the one containing all the weights $x\in\Lambda_W$, such that

$$\alpha_{(i)}\cdot x\geqslant 0. \tag{A15}$$

The Weyl character for an irreducible representation of highest weight Λ is defined as

$$\mathrm{ch}_\Lambda(a)=\sum_{\mu\in M_\Lambda}e^{a\cdot\mu}, \tag{A16}$$

where $a=a_i\lambda^{(i)}$. The Weyl character satisfies the equation[31]

$$\mathrm{ch}_\Lambda(a)=\frac{\Sigma_{w\in W}\epsilon(w)e^{w(\Lambda+\rho)\cdot a}}{\Sigma_{w\in W}\epsilon(w)e^{w(\rho)\cdot a}}, \tag{A17}$$

known as the Weyl character formula. When $a=-\rho$, we have an expression for the character[25] that is particularly useful:

$$\sum_{\mu \in M_\Lambda} e^{-\mu\cdot\rho} = \prod_{\alpha>0} \frac{e^{(1/2)\alpha\cdot(\rho+\Lambda)} - e^{-(1/2)\alpha\cdot(\rho+\Lambda)}}{e^{(1/2)\alpha\cdot\rho} - e^{-(1/2)\alpha\cdot\rho}}, \tag{A18}$$

where $\alpha>0$ denotes a sum over all positive roots.

An important set of weights used in this work is the one made by Weyl-antisymmetric combinations of weights in $\Lambda_W/s\Lambda_R$, where s is an arbitrary non-negative integer. This set of weights builds the fundamental chamber $\mathscr{F}_s$.

2. Fundamental representation of SO(2*l*+1)

The fundamental representation of B_l is associated to the highest weight $\Lambda=\lambda^{(1)}=(1,0,...,0)$, and the corresponding weight space is

$$M_{\lambda^{(1)}}=\{\mu_i : 1\leqslant i\leqslant 2l+1\}, \tag{A19}$$

where

$$\begin{gathered}
\mu_1=\lambda^{(1)}=(1,0,\ldots,0),\\
\mu_j=\mu_{j-1}-\alpha_{(j-1)}=(0,\ldots,\overset{j}{-1},1,0,\ldots,0), \quad j=1\ldots l-1,\\
\mu_l=\mu_{l-1}-\alpha_{(l-1)}=(0,\ldots,0,-1,2),\\
\mu_{l+1}=\mu_l-\alpha_{(l)}=0,\\
\mu_{l+1+i}=-\mu_{l+1-i}, \quad i=1,\ldots,l.
\end{gathered} \tag{A20}$$

We can write these weights as follows:

$$\begin{gathered}
\mu_j=[-\delta_{j-1,i}+\delta_{j,i}]\lambda^{(i)}, \quad j=1,\ldots,l-1,\\
\mu_l=[-\delta_{l-1,i}+2\,\delta_{l,i}]\lambda^{(i)},\\
\mu_{l+1+i}=-\mu_{l+1-i}, \quad i=1,\ldots,l.
\end{gathered} \tag{A21}$$

We also need the scalar products $\rho\cdot\mu_i$ and $\mu_i\cdot\mu_i$. Using the form (A20) and (A11), we can easily find

$$\begin{gathered}
\mu_i^2=1, \quad i=1,\ldots,2l+1, \quad i\neq l+1,\\
\mu_{l+1}^2=0,\\
\rho\cdot\mu_i=\tfrac{1}{2}\,[2l-(2i-1)], \quad i=1,\ldots,l,\\
\rho\cdot\mu_{l+1}=0,\\
\rho\cdot\mu_{l+1+i}=-\tfrac{1}{2}\,(2i-1), \quad i=1,\ldots,l.
\end{gathered} \tag{A22}$$

The action of the Weyl reflections on the fundamental weights $\lambda^{(i)}$ follows from (A14):

$$\begin{aligned}
&\sigma_1(x)=(-x_1,x_2+x_1,x_3,\ldots,x_l),\\
&\sigma_i(x)=(x_1,\ldots,x_{i-1}+x_i,-x_i,x_i+x_{i+1},\ldots,x_l),\quad i=1,\ldots,l-2,\\
&\sigma_{l-1}(x)=(x_1,\ldots,x_{l-3},x_{l-2}+x_{l-1},-x_{l-1},x_l+2x_{l-1}),\\
&\sigma_l(x)=(x_1,\ldots,x_{l-2},x_{l-1}+x_l,-x_l).
\end{aligned}\tag{A23}$$

3. Fundamental representation of SO(2*l*)

In this section we present the results concerning the fundamental representation of D_l. It is associated to the highest weight $\Lambda=\lambda^{(1)}=(1,0,...,0)$, and the corresponding weight space is

$$M_{\lambda^{(1)}}=\{\mu_i;1\leqslant i\leqslant 2l\},\tag{A24}$$

where

$$\begin{aligned}
&\mu_1=\lambda^{(1)}=(1,0,\ldots,0),\\
&\mu_j=\mu_{j-1}-\alpha_{(j-1)}=(0,\ldots,\overset{j}{-1},1,0,\ldots,0),\quad j=1,\ldots,l-2,\\
&\mu_{l-1}=\mu_{l-2}-\alpha_{(l-2)}=(0,\ldots,0,-1,1,1),\\
&\mu_l=\mu_{l-1}-\alpha_{(l-1)}=(0,\ldots,0,-1,1),\\
&\mu_{l+i}=-\mu_{l+1-i},\quad i=1,\ldots,l.
\end{aligned}\tag{A25}$$

We can write these weights as follows:

$$\begin{aligned}
&\mu_j=\sum_{i=1}^{l}[-\delta_{j-1,i}+\delta_{j,i}]\lambda^{(i)},\quad j=1,\ldots,l\quad j\neq l-1,\\
&\mu_{l-1}=[-\delta_{l-2,i}+\delta_{l-1,i}+\delta_{l,i}]\lambda^{(i)},\\
&\mu_{l+i}=-\mu_{l+1-i},\quad i=1,\ldots,l.
\end{aligned}\tag{A26}$$

We also need the scalar products $\rho\cdot\mu_i$ and $\mu_i\cdot\mu_i$. Using the form (A26) and (A10), we easily find

$$\begin{aligned}
&\mu_i^2=1,\quad i=1,\ldots,2l,\\
&\rho\cdot\mu_i=l-i,\quad i=1,\ldots,l,\\
&\rho\cdot\mu_{l+i}=-(i-1),\quad i=1,\ldots,l.
\end{aligned}\tag{A27}$$

The action of the Weyl reflections on the fundamental weights λ_i follows from (A14):

$$\begin{aligned}
&\sigma_1(x)=(-x_1,x_2+x_1,x_3,\ldots,x_l),\\
&\sigma_i(x)=(x_1,\ldots,x_{i-1}+x_i,-x_i,x_i+x_{i+1},\ldots,x_l),\quad i=1,\ldots,l-3,\\
&\sigma_{l-2}(x)=(x_1,\ldots,x_{l-4},x_{l-3}+x_{l-2},-x_{l-2},x_{l-1}+x_{l-2},x_l+x_{l-2}),
\end{aligned}\tag{A28}$$

$$\sigma_{l-1}(x)=(x_1,\ldots,x_{l-3},x_{l-2}+x_{l-1},-x_{l-1},x_l),$$

$$\sigma_l(x)=(x_1,\ldots,x_{l-3},x_{l-2}+x_l,x_{l-1},-x_l).$$

4. Theta functions of level *s*

The theta functions of level s (s being an arbitrary positive integer) play a fundamental role in the construction of the Hilbert space presented in Sec. II. They are defined as follows:[25]

$$\Theta_{s,p}(a,\tau)=\sum_{\nu\in\mathscr{L}_R}\exp\left\{\frac{2\pi i\tau s}{\psi^2}\left(\nu+\frac{p}{s}\right)^2+2\pi i s\left(\nu+\frac{p}{s}\right)\cdot a\right\},\tag{A29}$$

where $\mathscr{L}_R$ stands for the long root lattice. These functions are well defined for Im $\tau>0$, which makes the sum convergent. We will consider the case where p belongs to the weight lattice Λ_W.

The Theta functions in (A29) satisfy some important properties.[32] The first one, which follows trivially from its definition (A29) is the following: a displacement of p by a vector in $s\mathscr{L}_R$ does not change (A29),

$$\Theta_{s,p+s\alpha}(a,\tau)=\Theta_{s,p}(a,\tau),\quad \alpha\in\mathscr{L}_R.\tag{A30}$$

This shows that p in $\Theta_{s,p}(a,\tau)$ lives in the domain $p\in\Lambda_W/s\mathscr{L}_R$. Another important property is the following. Consider m and n two vectors in $\mathscr{L}_R$, $m,n\in\mathscr{L}_R$. Then

$$\Theta_{s,p}\left(a+\frac{2(m+n\tau)^{i^\tau}}{\psi^2}\right)=e^{2\pi i s\tau[(n\cdot n)/\psi^2]-2\pi i s n\cdot a}\Theta_{s,p}(a,\tau).\tag{A31}$$

Of particular interest in our analysis are the Weyl antisymmetric combinations of Theta functions of level s. Let us define them as

$$\Theta^A_{s,p}(a,\tau)=\sum_{w\in W}\epsilon(w)\Theta_{s,w(p)}(a,\tau),\tag{A32}$$

where $\epsilon(w)$ is the signature of the permutation corresponding the Weyl group element w. These functions satisfy

$$\Theta^A_{s,p}(a,\tau)=\epsilon(w)\Theta^A_{s,w(p)}(a,\tau),\tag{A33}$$

so they are Weyl antisymmetric. This property implies some relations between the antisymmetrized theta functions of level s. Finally, we recall the behavior of the theta functions under modular transformations. The modular group is generated by the transformation S,

$$\tau\to-\frac{1}{\tau},\quad a\to\frac{a}{\tau},\tag{A34}$$

and the transformation T,

$$\tau\to\tau+1,\quad a\to a.\tag{A35}$$

The theta functions of level s transform under them as

$$\Theta_{s,p}\left(\frac{a}{\tau},\frac{-1}{\tau}\right)=\left(\frac{\mathrm{Vol}\ \mathscr{L}_R^*}{\mathrm{Vol}\ \mathscr{L}_R}\right)^{1/2}\left(\frac{\tau}{is}\right)^{l/2}e^{(i\pi s/\tau)a^2\psi^2}\sum_{q\in\Lambda_W/s\mathscr{L}_R}e^{-4\pi i[(p\cdot q)/s\psi^2]}\Theta_{s,q}(a,\tau),\tag{A36}$$

and

$$\Theta_{s,p}(a,\tau+1)=e^{2\pi i(p^2/s\psi^2)}\Theta_{s,p}(a,\tau). \tag{A37}$$

In (A36), Vol $\mathscr{L}_R$ is the volume of the fundamental cell of the long root lattice $\mathscr{L}_R$, and Vol $\mathscr{L}_R^*$ that of its dual lattice, $\mathscr{L}_R^*$. The values of their quotient are

$$\left(\frac{\text{Vol }\mathscr{L}_R^*}{\text{Vol }\mathscr{L}_R}\right)^{1/2}=\begin{cases} N^{-1/2}, & \text{SU}(N), \\ \frac{1}{2}, & \text{SO}(N), \\ 2^{-N/4}, & Sp(N). \end{cases} \tag{A38}$$

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Analytical results for a class of sums involving Bessel functions and square arrays

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We consider a class of sums involving Bessel functions summed over the square array. The sums involve the length (ξ) of an arbitrary vector lying within the central unit cell. We establish conditions under which the sums reduce to polynomial forms in ξ (possibly with a single logarithmic term in addition), and show how these polynomials may be conveniently evaluated. © *1996 American Institute of Physics.* [S0022-2488(96)00403-X]

I. INTRODUCTION

In solving the problem of wave propagation through two-dimensional periodic media by the extended Rayleigh method, one needs to evaluate lattice sums of the form

$$S_l^Y(k,\mathbf{k}_0)=\sum_{p\neq 0} Y_l(kR_p)e^{il\varphi_p}e^{i\mathbf{k}_0\cdot\mathbf{R}_p}, \tag{1}$$

with $l\in\mathbb{Z}$, extending over nonzero array vectors $\mathbf{R}_p=p_1\mathbf{e}_1+p_2\mathbf{e}_2$, $p=(p_1,p_2)\in\mathbb{Z}^2$. Here, $\mathbf{e}_1$ and $\mathbf{e}_2$ are fundamental translation vectors of the array and, in polar coordinates, $\mathbf{R}_p=(R_p,\varphi_p)$. Also, Y_l are Bessel functions of the second kind, $\mathbf{k}_0$ is the Bloch momentum, and k is the wave number of the propagating wave. The series in (1) are conditionally convergent, but, by means of Poisson summation formula, we can derive a representation in terms of absolutely converging series over the reciprocal array:[1]

$$S_l^Y(k,\mathbf{k}_0)J_l(k\xi)=-Y_0(k\xi)\delta_{l,0}-i^l\frac{4}{A}\sum_h \frac{J_l(Q_h\xi)}{Q_h^2-k^2}e^{il\theta_h}, \tag{2}$$

where $\boldsymbol{\xi}$ is a vector in the central unit cell, $\mathbf{Q}_h=\mathbf{K}_h+\mathbf{k}_0$ [in polar coordinates $\mathbf{Q}_h=(Q_h,\theta_h)$] and $\mathbf{K}_h$, $h\in\mathbb{Z}^2$, are the reciprocal array vectors. Also, A is the area of the unit cell in the direct array, $\delta_{l,0}$ is the Kronecker symbol, and J_l represents Bessel functions of the first kind. The series in (2) converge as $1/Q_h^{2.5}$ but, for numerical evaluations, we may accelerate the convergence by integrating with respect to ξ.[1]

A specific set of lattice sums is involved in the study of the behavior of the physical system in the quasistatic limit, when $k=\alpha k_0+\beta k_0^2$ and $k_0\to 0$. The constant α defines the dynamic refractive index of the periodic media,[2,3] while β represents the second-order correction. Such calculations involve lattice sums (Schlömilch double series) having the form

$$\mathscr{S}_{l,m,n}(\xi)=\sum_{h\neq 0}\frac{J_l(K_h\xi)}{K_h^n}e^{im\psi_h}, \tag{3}$$

with $l,m=0,\pm 1,\pm 2,\ldots$, $n=2,3,\ldots$, and, in polar coordinates, $\mathbf{K}_h=(K_h,\psi_h)$. Note that, for negative indices, the lattice sums (3) satisfy the relations

$$\mathscr{S}_{-l,m,n}(\xi)=(-1)^l\mathscr{S}_{l,m,n}(\xi), \tag{4}$$

$$\mathscr{S}_{l,-m,n}(\xi)=\mathscr{S}^{*}_{l,m,n}(\xi), \tag{5}$$

where the asterisk denotes complex conjugation.

The purpose of this paper is to present the cases when exact analytic expressions can be obtained for the lattice sums (3). Note that we will restrict our attention to vectors $\boldsymbol{\xi}$ lying in the central unit cell, with $0<\xi<d$ [with $d=\min(|\mathbf{e}_1|,|\mathbf{e}_2|)$].

It is remarkable that polynomial formulas can be established for a wide class of double sums of the form (3), which appear not to have been considered previously. Indeed, standard tabulations of integrals and sums[4–8] have remarkably few results concerning double series. We hope the results we derive here will be of use to some, and the methods used may be generalized by others to deal with other classes of functions. We suspect similar results will be able to be found for double sums of bases of functions involved in the solution of the Helmholtz equation (e.g., for Mathieu functions).

II. THE SQUARE ARRAY

For simplicity, we will consider a square array but the results can be easily extended to a rectangular array. Thus, the array vectors have the form

$$\mathbf{R}_p=d(p_1,p_2), \quad p=(p_1,p_2)\in\mathbb{Z}^2, \tag{6}$$

with d being the array constant, and the vector $\boldsymbol{\xi}$, which is restricted to the central unit cell, being represented as

$$\boldsymbol{\xi}=d(x,y), \quad 0\leqslant x,y<1. \tag{7}$$

Also, the vectors of the reciprocal array are

$$\mathbf{K}_h=\frac{2\pi}{d}(h_1,h_2), \quad h=(h_1,h_2)\in\mathbb{Z}^2. \tag{8}$$

The symmetry of the square array implies that the lattice sums (3) vanish, unless m is zero or a multiple of four, so that we have to evaluate lattice sums of the form

$$S_{l,4m,n}(\xi)=\frac{1}{d^n}\sum_{h\neq 0}\frac{J_l(K_h\xi)}{K_h^n}e^{i4m\psi_h}, \tag{9}$$

with $l,m=0,1,2,\ldots$, $n=2,3,\ldots$. Here, we have introduced the factor $1/d^n$ to compensate the dimension of K_h, making the lattice sums (9) pure numbers. For $n=0$ or 1, the series in (9) has a meaning only in the context of the theory of generalized functions, and distributive behavior can occur whenever ξ coincides with an array point $\mathbf{R}_p$. Also, for $m=0$ and $n=2$, *all* the series in (9) are nonanalytic functions of ξ, at $\xi=0$.

III. THE CASE $m=0$

A. Recurrence relations

Now, we make use of the integrals:[9,6]

$$\int_0^a x^{l+1}J_l(bx)dx=a^{l+1}\frac{J_{l+1}(ba)}{b}, \tag{10}$$

$$\int_0^a x^{-l+1}J_l(bx)dx=\frac{b^{l-2}}{2^{l-1}\Gamma(l)}-a^{-l+1}\frac{J_{l-1}(ba)}{b}, \tag{11}$$

to obtain the lattice sums of types $(l+1,0,n+1)$ and $(l-1,0,n+1)$, from the lattice sums of type $(l,0,n)$. Thus, we have

$$\int_0^{\xi} \eta^{l+1} S_{l,0,n}(\eta)\, d\eta = d\,\xi^{l+1}\, S_{l+1,0,n+1}(\xi), \tag{12}$$

$$\int_0^{\xi} \eta^{-l+1} S_{l,0,n}(\eta)\, d\eta = \frac{d^{-l+2}}{2^{l-1}\Gamma(l)} \sum_{h\neq 0} \frac{1}{(K_h d)^{n-l+2}} - d\,\xi^{-l+1}\, S_{l-1,0,n+1}(\xi), \quad n-l>0. \tag{13}$$

For a square array, the first series on the right-hand side of (13) takes the form[10,11]

$$\sum_{h\neq 0} \frac{1}{(K_h d)^s} = \frac{4}{(2\pi)^s}\left[\sum_{h_1,h_2=1}^{\infty} \frac{1}{(h_1^2+h_2^2)^{s/2}} + \sum_{p=1}^{\infty} \frac{1}{p^s}\right] = \frac{4}{(2\pi)^s}\,\zeta\left(\frac{s}{2}\right)\beta\left(\frac{s}{2}\right), \tag{14}$$

where $\zeta(s)$ is the Riemann zeta function and

$$\beta(s) = \sum_{n=0}^{\infty} (-1)^n (2n+1)^{-s}. \tag{15}$$

Actually, (12) and (13) act as raising and lowering operators with respect to l, respectively, at the same time increasing n. The inverse of these operators, decreasing n, may be obtained on the basis of the formulas[9]

$$\left[\frac{1}{b}\, x^{l+1} J_{l+1}(bx)\right]' = x^{l+1} J_l(bx), \tag{16}$$

$$\left[\frac{1}{b}\, x^{-l+1} J_{l-1}(bx)\right]' = -x^{-l+1} J_l(bx), \tag{17}$$

where the prime denotes a differentiation with respect to x. Consequently, with the definition (9) we have

$$S_{l-1,0,n-1}(\xi) = d\,\xi^{-l}[\xi^l S_{l,0,n}(\xi)]', \tag{18}$$

$$S_{l+1,0,n-1}(\xi) = -d\,\xi^{l}[\xi^{-l} S_{l,0,n}(\xi)]'. \tag{19}$$

Another recurrence relation between the lattice sums may be derived by using the recurrence relations satisfied by the Bessel functions:[6]

$$\frac{2l}{z}\, J_l(z) = J_{l-1}(z) + J_{l+1}(z). \tag{20}$$

Consequently, we obtain

$$S_{l+2,0,n}(\xi) = (l+1)\left(\frac{2d}{\xi}\right) S_{l+1,0,n+1}(\xi) - S_{l,0,n}(\xi). \tag{21}$$

B. $l+n$=even

First, we will consider the lowest-order lattice sum in the set

$$S_{0,0,2}(\xi)=\frac{1}{d^2}\sum_{h\neq 0}\frac{J_0(K_h\xi)}{K_h^2}. \tag{22}$$

To evaluate the lattice sum (22) we use the formula[12]

$$\frac{1}{d^2}\sum_{h\neq 0}\frac{e^{i\mathbf{K}_h\cdot\boldsymbol{\xi}}}{K_h^2}=\left(\frac{\xi}{2d}\right)^2[1+\cos(2\varphi)]-\frac{1}{6\pi}\ln 2-\frac{1}{2\pi}\ln\left|\frac{\theta_1(\pi\alpha,q)}{[\theta_1'(0,q)]^{1/3}}\right|, \tag{23}$$

where $\boldsymbol{\xi}=d(x,y)=(\xi,\varphi)$, $\alpha=y+ix$, $q=\exp(-\pi)$. Also, $\theta_1(z,q)$ and $\theta_1'(z,q)$ represent the theta function and its first derivative with respect to z.[13] On the left-hand side of (23) we expand the exponential in terms of Bessel functions:[6]

$$e^{i\mathbf{K}_h\cdot\boldsymbol{\xi}}=\sum_{l=-\infty}^{\infty}i^lJ_l(K_h\xi)e^{il(\varphi-\psi_h)}. \tag{24}$$

Then, we expand in Taylor series the logarithm of the theta function:

$$\ln|\theta_1(\pi\alpha,q)|=\ln\left(\frac{\xi}{2d}\right)+\ln[2\pi\theta_1'(0,q)]+\pi\frac{\theta_1''(0,q)}{\theta_1'(0,q)}\left(\frac{\xi}{2d}\right)\sin\varphi+\cdots. \tag{25}$$

By substituting the series expansions (24) and (25) in (23), and equating the terms independent of φ, we obtain

$$S_{0,0,2}(\xi)=-\frac{1}{2\pi}\ln\left(\frac{\xi}{2d}\right)+\omega_0+\left(\frac{\xi}{2d}\right)^2, \tag{26}$$

where

$$\omega_0=-\frac{1}{6\pi}[3\ln\pi+4\ln 2+2\ln\theta_1'(0,q)]=-0.318\,895\,593\,319\,827. \tag{27}$$

The recurrence relations (12), (13), (18), (19), and (21) allow us to obtain any lattice sums of the type $(l,0,n)$, with $l+n$=even, from the lattice sum of the type (0,0,2). For example, starting with (26) and using (12), we obtain

$$S_{1,0,3}(\xi)=-\frac{1}{2\pi}\left(\frac{\xi}{2d}\right)\ln\left(\frac{\xi}{2d}\right)+\left(\omega_0+\frac{1}{4\pi}\right)\left(\frac{\xi}{2d}\right)+\frac{1}{2}\left(\frac{\xi}{2d}\right)^3. \tag{28}$$

By applying a second time (12), we have

$$S_{2,0,4}(\xi)=-\frac{1}{4\pi}\left(\frac{\xi}{2d}\right)^2\ln\left(\frac{\xi}{2d}\right)+\frac{1}{2}\left(\omega_0+\frac{3}{8\pi}\right)\left(\frac{\xi}{2d}\right)^2+\frac{1}{6}\left(\frac{\xi}{2d}\right)^4. \tag{29}$$

Now, by applying (13) on (28), we obtain the equation

$$S_{0,0,4}(\xi)=\frac{1}{2\pi}\left(\frac{\xi}{2d}\right)^2\ln\left(\frac{\xi}{2d}\right)+\frac{\lambda}{24\pi^2}-\left(\omega_0+\frac{1}{2\pi}\right)\left(\frac{\xi}{2d}\right)^2-\frac{1}{4}\left(\frac{\xi}{2d}\right)^4, \tag{30}$$

where we have used the formulas[6]

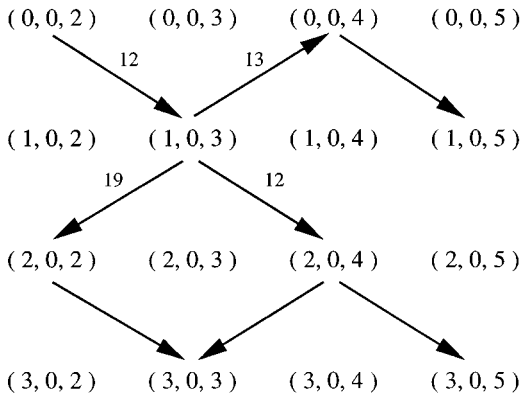

FIG. 1. The recurrence relations between lattice sums of the type $(l,0,n)$ with $l+n=$even. The equation numbers on the first four arrows identify the relevant recurrence relation. The same set of recurrence relations apply to the lattice sums with $l+n=$odd.

$$\zeta(2)=\pi^2/6, \quad \beta(2)=\lambda, \tag{31}$$

with $\lambda=0.915\ 965\ 594\ 177\ 219$ denoting the Catalan constant. Also, with (26) and (28), by means of the recurrence relation (21), we are led to the formula

$$S_{2,0,2}(\xi)=\frac{1}{4\pi}-\frac{1}{2}\left(\frac{\xi}{2d}\right)^2. \tag{32}$$

[Note that we obtain the same result by acting with (19) on (28).] From (32), by using (12), we have

$$S_{3,0,3}(\xi)=\frac{1}{8\pi}\left(\frac{\xi}{2d}\right)-\frac{1}{6}\left(\frac{\xi}{2d}\right)^3. \tag{33}$$

Note that we may continue indefinitely this procedure (see Fig. 1).

As a numerical verification of the formulas (26) and (28)–(33), we have compared their results with numerically evaluated partial sums of high orders in the corresponding definition (9), and have obtained a relative error less than 10^{-5}. In the numerical evaluations, we used a square array of 1001 by 1001 points in the reciprocal array, so that the relative errors are, in fact truncation errors. Also, Fig. 2 compares the result of (32) with direct summation. Note the nonzero value for $\xi=0$: the sum, as defined by (9), is actually a nonanalytic function of ξ at the point $\xi=0$.

C. $l+n=$odd

For $l>n$ we may include the term for $h=0$ in the series (9) without changing its value, and we may apply the Poisson summation formula:

$$\sum_h f(\mathbf{K}_h)=\left(\frac{d}{2\pi}\right)^2\sum_p F(\mathbf{R}_p), \tag{34}$$

where

$$F(\mathbf{R}_p)=\int f(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{R}_p}\,d\mathbf{k}. \tag{35}$$

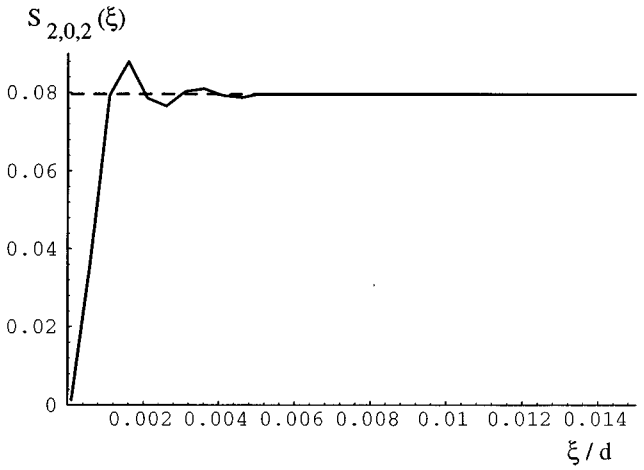

FIG. 2. The lattice sum $S_{2,0,2}(\xi)$ obtained by direct summation (—) over the reciprocal array with 1001 by 1001 points, and from the analytic formula (32) (---), for small values of ξ/d. Note that, as the direct summation region is enlarged, the region of numerical instability (here $0<\xi<0.005d$) contracts.

From (9) and (35) we are led to a particular form of the Weber–Schafheitlin integral,[6]

$$F(\mathbf{R}_p)=\frac{2\pi}{d^n}\int_0^\infty \frac{J_l(k\xi)J_0(kR_p)}{k^{n-1}}\,dk. \tag{36}$$

The integral converges for $l-n>-2$, $n>0$, and $0<\xi<R_p$, and may be expressed as a hypergeometric function:[6]

$$F(\mathbf{R}_p)=\frac{\xi^l\pi\Gamma[(l-n+2)/2]}{2^{n-2}R_p^{l-n+2}\,d^n\Gamma(l+1)\Gamma[(n-l)/2]}\,{}_2F_1\left(\frac{l-n+2}{2},\frac{l-n+2}{2};l+1;\left(\frac{\xi}{R_p}\right)^2\right). \tag{37}$$

In our case we have $l>n\geqslant 2$ and $0<\xi<R_p$, $\forall p\neq 0$, so that the conditions of convergence are satisfied. For $p=0$ we have $R_0=0$, $\xi>0$, and the integral in (36) becomes

$$F(0)=\frac{2\pi}{d^n}\int_0^\infty \frac{J_l(k\xi)}{k^{n-1}}\,dk, \tag{38}$$

with $n\geqslant 2$ and $l>n$, so that[6]

$$F(0)=\frac{2\pi}{d^n}\,\xi^{n-2}\,\frac{2^{-n+1}\Gamma[(l-n+2)/2]}{\Gamma[(l+n)/2]}. \tag{39}$$

Consequently, from (34) we have

$$S_{l,0,n}(\xi)=\frac{2^{-n}}{\pi}\frac{\Gamma[(l-n+2)/2]}{\Gamma[(l+n)/2]}\left(\frac{\xi}{d}\right)^{n-2} + \frac{2^{-n}}{\pi}\sum_{p\neq 0}\frac{\xi^l d^{-n+2}\Gamma[(l-n+2)/2]}{R_p^{l-n+2}\,l!\,\Gamma[(n-l)/2]}\,{}_2F_1\left(\frac{l-n+2}{2},\frac{l-n+2}{2};l+1;\frac{\xi^2}{R_p^2}\right). \tag{40}$$

The hypergeometric function has a series expansion of the form[6]

$$ {}_2F_1(a,b;c;z)=\frac{\Gamma(c)}{\Gamma(a)\Gamma(b)}\sum_{k=0}^{\infty}\frac{\Gamma(a+k)\Gamma(b+k)}{\Gamma(c+k)}\frac{z^k}{k!}. \tag{41} $$

In our case $a+b-c=-n+1<0$, so that the hypergeometric series in (40) is absolutely convergent. The series over p contains terms of the form $1/R_p^{2k+l-n+2}$, with exponents $2k+l-n+2\geqslant 3$, so that these series are also absolutely convergent, and we may change the order of summation in (40). Thus, we have[10,11]

$$ \sum_{p\neq 0}\frac{1}{R_p^s}=\frac{4}{d^s}\left[\sum_{p_1,p_2=1}^{\infty}\frac{1}{(p_1^2+p_2^2)^{s/2}}+\sum_{k=1}^{\infty}\frac{1}{k^s}\right]=\frac{4}{d^s}\,\zeta\left(\frac{s}{2}\right)\beta\left(\frac{s}{2}\right), \tag{42} $$

and

$$ S_{l,0,n}(\xi)=\frac{2^{-n}\Gamma(q)}{\pi\Gamma(q+n-1)}\left(\frac{\xi}{d}\right)^{n-2}+\frac{2^{-n+2}(-1)^{l-n}}{\pi^2}\sum_{k=0}^{\infty}\frac{[\Gamma(k+q)]^2}{k!(k+l)!}\,\zeta(k+q)\beta(k+q)\left(\frac{\xi}{d}\right)^{2k+l}, \tag{43} $$

where $q=(l-n)/2+1$. Therefore, in the case $l+n=$odd, the lattice sums (9) become power series in ξ.

For example, with $l=3$ and $n=2$, the lattice sum may be expressed in the form

$$ S_{3,0,2}(\xi)=\frac{1}{6\pi}-\frac{1}{\pi^2}\sum_{k=0}^{\infty}\frac{[\Gamma(k+\frac{3}{2})]^2}{k!(k+3)!}\,\zeta\left(k+\frac{3}{2}\right)\beta\left(k+\frac{3}{2}\right)\left(\frac{\xi}{d}\right)^{2k+3}. \tag{44} $$

A direct comparison of the formula (44) with numerically evaluated partial sums of high orders (square array of 2001 by 2001 points in the reciprocal array) from the corresponding definition (9) shows a relative error less than 10^{-5}, for $0<\xi<d$.

The equation (43) is valid for $l>n$ but, starting with (44), by means of the recurrence relations (12), (13), (18), (19), and (21), we may obtain any lattice sum with $l+n=$odd.

IV. THE CASE $m\neq 0$

In this case, the recurrence relations (12), (18), (19), and (21) are still valid. Due to the dependence of the lattice sums on ψ_h, the recurrence relation (13) takes the form

$$ \int_0^{\xi}\eta^{-l+1}S_{l,m,n}(\eta)\,d\eta=\frac{d^{-l+2}}{2^{l-1}\Gamma(l)}\sum_{h\neq 0}\frac{e^{im\psi_h}}{(K_h d)^{n-l+2}}-d\xi^{-l+1}\,S_{l-1,m,n+1}(\xi),\quad n-l\geqslant 0. \tag{45} $$

For a square array, the series in (45) may be written as[14]

$$ \sum_{h\neq 0}\frac{e^{im\psi_h}}{(K_h d)^s}=\frac{1}{(2\pi)^s}\sum_{h_1,h_2\neq 0,0}\frac{e^{im\psi_h}}{(h_1^2+h_2^2)^{s/2}}=\frac{1}{(2\pi)^s}\left[\sigma_s^{(m)}-\frac{\pi}{2}\,\delta_{s,2}\right], \tag{46} $$

where $\psi_h=\arctan(h_2/h_1)$. Actually, in our case, the lattice sums (46) are identical with the lattice sums over the direct array. They are nonzero if m is a multiple of four, except for $s=2$, when the corresponding lattice sums are conditionally convergent. Highly accurate numerical values of $\sigma_m^{(m)}$ have been given by many authors.[14–19] Also, the lattice sums $\sigma_{m-2}^{(m)}$ have been evaluated in connection with problems of elastostatics.[14,17–19] With these notations, from (45) we obtain the recurrence relation,

$$\int_0^{\xi} \eta^{-l+1} S_{l,m,n}(\eta)\, d\eta = \frac{d^{-l+2}}{2^{l-1}\Gamma(l)(2\pi)^{n-l+2}} \left[\sigma^{(m)}_{n-l+2} - \frac{\pi}{2}\, \delta_{l,n} \right] - d\xi^{-l+1}\, S_{l-1,m,n+1}(\xi),$$
$$n-l \geqslant 0. \tag{47}$$

Now, for $l \geqslant n \geqslant 2$ and $m > 0$, we may obtain an explicit dependence on ξ of the lattice sums (9) by means of the Poisson summation formula (34). Thus, we have

$$S_{l,4m,n}(\xi) = \sum_h \frac{J_l(K_h \xi)}{(K_h d)^n}\, e^{i4m\psi_h} - \frac{1}{l!}\left(\frac{\xi}{2d}\right)^l \delta_{l,n} = \left(\frac{d}{2\pi}\right)^2 \sum_p F(\mathbf{R}_p) - \frac{1}{l!}\left(\frac{\xi}{2d}\right)^l \delta_{l,n}, \tag{48}$$

where we have considered that the argument of $\mathbf{K}_0 = 0$ is $\psi_0 = 0$. Also, $F(\mathbf{R}_p)$ is given by (35):

$$F(\mathbf{R}_p) = \frac{2\pi}{d^n}\, e^{i4m\varphi_p} \int_0^{\infty} \frac{J_l(k\xi) J_{4m}(kR_p)}{k^{n-1}}\, dk. \tag{49}$$

Here, we have used the polar coordinates for the vectors in the direct array, $\mathbf{R}_p = (R_p, \varphi_p)$. The Weber–Schafheitlin integral in (49) converges for $l + 4m - n + 2 > 0$ and $n > 0$. It vanishes for $R_p = 0$ and may be expressed as an absolutely converging hypergeometric series:[6]

$$\frac{\xi^l \Gamma[(l-n+4m+2)/2]}{2^{n-1} R_p^{l-n+2} l! \Gamma[(4m-l+n)/2]}\, {}_2F_1\left(\frac{l-n+4m+2}{2}, \frac{l-n-4m+2}{2}; l+1; \frac{\xi^2}{R_p^2} \right), \tag{50}$$

for $0 < \xi < R_p$. Consequently, (48) becomes

$$S_{l,4m,n}(\xi) = -\frac{1}{l!}\left(\frac{\xi}{2d}\right)^l \delta_{l,n} + \sum_{p \neq 0} \frac{\xi^l d^{-n+2} e^{i4m\varphi_p} \Gamma[(l-n+4m+2)/2]}{2^n \pi R_p^{l-n+2} l! \Gamma[(4m-l+n)/2]}$$
$$\times {}_2F_1\left(\frac{l-n+4m+2}{2}, \frac{l-n-4m+2}{2}; l+1; \frac{\xi^2}{R_p^2} \right). \tag{51}$$

The hypergeometric series reduces to a polynomial of degree q if $l - 4m - n + 2 = -2q$, with $q = 0,1,2,3,\ldots$. This condition also implies $l - n =$ even. In these cases the lattice sum may be represented as a polynomial of degree $2q + l$ in ξ:

$$S_{l,4m,n}(\xi) = \frac{2^{-n}\Gamma(4m-q)}{\pi\Gamma(1+q)} \sum_{s=0}^{q} \frac{(4m-q)_s (-q)_s}{s!(s+l)!}\, \sigma^{(4m)}_{2s+l-n+2} \left(\frac{\xi}{d}\right)^{2s+l} - \frac{1}{l!}\left(\frac{\xi}{2d}\right)^l \delta_{l,n}, \tag{52}$$

where $(a)_0 = 1$, $(a)_s = a(a+1)\cdots(a+s-1)$ represents Pochhammer's symbol. Otherwise, we obtain a power series in ξ:

$$S_{l,4m,n}(\xi) = \frac{2^{-n}}{\pi\Gamma(1-w+4m)\Gamma(w-4m)} \sum_{s=0}^{\infty} \frac{\Gamma(w+s)\Gamma(w-4m+s)}{s!(s+l)!}$$
$$\times \sigma^{(4m)}_{2s+l-n+2} \left(\frac{\xi}{d}\right)^{2s+l} - \frac{1}{l!}\left(\frac{\xi}{2d}\right)^l \delta_{l,n}, \tag{53}$$

with $w = (l-n)/2 + 2m + 1$.

The simplest analytic form of the lattice sums, for $m \neq 0$, appears in the case $l = 4m$ and $n = 2$, when $q = 0$ and, from (52), we have

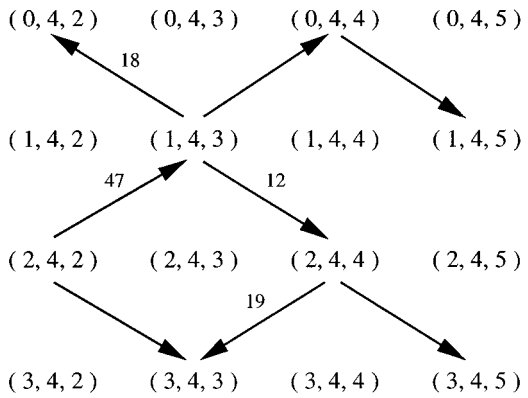

FIG. 3. The recurrence relations between lattice sums of the type $(l,4m,n)$ with $m=1$ and $l+n=$even. The equation numbers on the arrows identify the relevant recurrence relation. The same set of recurrence relations apply to the lattice sums $l+n=$odd.

$$S_{4m,4m,2}(\xi)=\frac{\sigma_{4m}^{(4m)}}{16\pi m}\left(\frac{\xi}{d}\right)^{4m}. \tag{54}$$

A characteristic lattice sum is obtained for $l=n=2$ and $m>0$:

$$S_{2,4m,2}(\xi)=\frac{m}{2\pi}\sum_{s=0}^{2m-1}\frac{(2m+1)_s(-2m+1)_s}{s!(s+2)!}\,\sigma_{2s+2}^{(4m)}\left(\frac{\xi}{d}\right)^{2s+2}-\frac{1}{8}\left(\frac{\xi}{d}\right)^{2}. \tag{55}$$

The importance of this lattice sum resides in the fact that, for every $m>0$, we have a table of the form displayed in Fig. 3 and, starting with (55), by means of the recurrence relations (12), (18), (19), (21), and (47), we may obtain any lattice sum in the set.

For example, if $m=1$, we have

$$S_{2,4,2}(\xi)=\frac{1}{\pi}\left[\sigma_2^{(4)}-\frac{\pi}{2}\right]\left(\frac{\xi}{2d}\right)^{2}-\frac{4}{\pi}\,\sigma_4^{(4)}\left(\frac{\xi}{2d}\right)^{4}, \tag{56}$$

where[14,18,19]

$$\sigma_2^{(4)}=4.078\,451\,161\,1614,\qquad \sigma_4^{(4)}=3.151\,212\,002\,153\,9. \tag{57}$$

From (56), by means of recurrence relations (47) and (12) we obtain, respectively,

$$S_{1,4,3}(\xi)=\frac{1}{(2\pi)^2}\,\widetilde{\sigma_2^{(4)}}\left(\frac{\xi}{2d}\right)-\frac{1}{\pi}\,\widetilde{\sigma_2^{(4)}}\left(\frac{\xi}{2d}\right)^{3}+\frac{2}{\pi}\,\sigma_4^{(4)}\left(\frac{\xi}{2d}\right)^{5}, \tag{58}$$

$$S_{3,4,3}(\xi)=\frac{1}{3\pi}\,\widetilde{\sigma_2^{(4)}}\left(\frac{\xi}{2d}\right)^{3}-\frac{1}{\pi}\,\sigma_4^{(4)}\left(\frac{\xi}{2d}\right)^{5}, \tag{59}$$

with $\widetilde{\sigma_2^{(4)}}=\sigma_2^{(4)}-\pi/2$. Then, by applying (12), (18), and (47) to (58), we are led to expressions for other lattice sums:

$$S_{2,4,4}(\xi)=\frac{1}{8\pi^2}\,\widetilde{\sigma_2^{(4)}}\left(\frac{\xi}{2d}\right)^{2}-\frac{1}{3\pi}\,\widetilde{\sigma_2^{(4)}}\left(\frac{\xi}{2d}\right)^{4}+\frac{1}{2\pi}\,\sigma_4^{(4)}\left(\frac{\xi}{2d}\right)^{6}, \tag{60}$$

$$S_{0,4,2}(\xi)=\frac{1}{(2\pi)^2}\,\widetilde{\sigma_2^{(4)}}-\frac{2}{\pi}\,\widetilde{\sigma_2^{(4)}}\left(\frac{\xi}{2d}\right)^2+\frac{6}{\pi}\,\sigma_4^{(4)}\left(\frac{\xi}{2d}\right)^4, \tag{61}$$

$$S_{0,4,4}(\xi)=\frac{1}{(2\pi)^4}\,\sigma_4^{(4)}-\frac{1}{(2\pi)^2}\,\widetilde{\sigma_2^{(4)}}\left(\frac{\xi}{2d}\right)^2+\frac{1}{2\pi}\,\widetilde{\sigma_2^{(4)}}\left(\frac{\xi}{2d}\right)^4-\frac{2}{3\pi}\,\sigma_4^{(4)}\left(\frac{\xi}{2d}\right)^6. \tag{62}$$

Also, from (62) by using (12), we have

$$S_{1,4,5}(\xi)=\frac{1}{(2\pi)^4}\,\sigma_4^{(4)}\left(\frac{\xi}{2d}\right)-\frac{1}{8\pi^2}\,\widetilde{\sigma_2^{(4)}}\left(\frac{\xi}{2d}\right)^3+\frac{1}{6\pi}\,\widetilde{\sigma_2^{(4)}}\left(\frac{\xi}{2d}\right)^5-\frac{1}{6\pi}\,\sigma_4^{(4)}\left(\frac{\xi}{2d}\right)^7. \tag{63}$$

The series over the reciprocal array in (63) is rapidly convergent. By evaluating it at some different values of ξ, we may obtain, if we need them, numerical values for the lattice sums $\widetilde{\sigma_2^{(4)}}$ and $\sigma_4^{(4)}$.

V. CONCLUSIONS

We have been unable to find any references in the standard compilations of sums to the results presented here. Given the simplicity of the expressions we have derived, there is motivation for further work on similar sums over arrays and lattices. It would also be of interest to study in more detail the distributive nature of these sums, in order to remove the restriction $0<\xi<d$ on the value of this length parameter.

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Lie–Poisson deformation of the Poincaré algebra

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We find a one-parameter family of quadratic Poisson structures on $\mathbf{R}^4\times \mathrm{SL}(2,C)$ which satisfies the properties: (a) that it reduces to the standard Poincaré algebra for a particular limiting value of the parameter (which we associate with the ''canonical limit''), as well as, (b) that it is preserved under the Lie–Poisson action of the Lorentz group (and the Lie–Poisson transformations reduce to canonical ones in the canonical limit). As with the Poincaré algebra, our deformed Poincaré algebra has two Casimir functions which correspond to ''mass'' and ''spin.'' The constant mass and spin surfaces in $\mathbf{R}^4\times \mathrm{SL}(2,C)$ define symplectic leaves which we parametrize with space–time coordinates, momenta, and spin. We thereby obtain realizations of the deformed Poincaré algebra for both spinning and spinless particles. The formalism can be applied for finding a one-parameter family of canonically inequivalent descriptions of the photon. © *1996 American Institute of Physics.* [S0022-2488(96)00604-X]

I. INTRODUCTION

A number of authors have examined deformations of the Poincaré algebra in quantum theory, in addition to investigating the effects of deforming the usual symmetries of space–time.[1–7] Of course, there exists no unique procedure for carrying out such deformations and certainly one cannot apply physical insight since effects of such deformations are not expected to be relevant away from the Planck scale. The proposals which have been made so far are generally within the mathematical framework of Hopf algebras, and they often rely upon making a contraction of the quantum de Sitter algebra.

Another approach, which is the one that we shall follow here, is to deform the Poincaré algebra already at the classical level.[8] Then the deformed algebra is to be realized in terms of Poisson brackets rather than commutation relations, and the construction should be made within the framework of Poisson–Lie groups in order to later make connection with Hopf algebras in the quantum theory.

The classical analysis is considerably simpler than its quantum counterpart for a number of reasons. One advantage, of course, is that the elements of the algebra, i.e., the classical observables, are commuting variables. In addition to this, to check the consistency of the algebra we essentially only need to verify the Jacobi identity (although this may not always be so easy). Furthermore, in the classical theory symmetries are associated with ordinary Lie groups, and not quantum groups.

With regard to the group of classical symmetries, which we shall denote by $\mathscr{S}$, we shall here only be concerned with the Lorentz group [or actually, $\mathrm{SL}(2,C)$]. To it we attach a Poisson structure which is consistent with left or right group multiplication, thereby making $\mathscr{S}$ a Poisson–Lie group. Such Poisson structures are well known. Our choice of Poisson brackets $\{\,,\}_{\mathscr{S}}$ is such that it corresponds to the classical limit of the defining relations for $\mathrm{SL}_q(2,C)$.[9]

With regard to the space of classical observables, which we denote by $\mathscr{O}$, we shall examine a

one-parameter family of algebras defined on the Poincaré group, or more precisely on $\mathbf{R}^4\times\mathrm{SL}(2,C)$. These algebras are chosen to be preserved under the Lie–Poisson action of $\mathscr{S}$. Furthermore, they reduce to the Poincaré algebra for a particular limiting value of the parameter. We associate the limiting value with the ''canonical limit.'' This is because $\mathscr{S}$ has trivial Poisson brackets in the limit, i.e., $\{\,,\}_{\mathscr{S}}\to 0$, and hence the Lie–Poisson action of $\mathscr{S}$ on $\mathscr{O}$ reduces to the canonical one.

For all values of the deformation parameter, $\mathscr{S}$ will act on $\mathscr{O}$ in the standard way. That is, in $\mathscr{O}$ we can identify ''momentum'' and ''angular momentum'' variables; the momentum transforms as a Lorentz vector, while angular momentum transforms according to the adjoint representation of $\mathrm{SL}(2,C)$. This defines a map, $\sigma:\mathscr{S}\times\mathscr{O}\to\mathscr{O}$. For us, σ must be a Poisson map, which means that if f_1 and f_2 are functions on $\mathscr{O}$, then

$$\{f_1,f_2\}_{\mathscr{O}}\circ\sigma=\{f_1\circ\sigma,f_2\circ\sigma\}_{\mathscr{O}\times\mathscr{S}}, \tag{1}$$

where the product Poisson structure is assumed on $\mathscr{O}\times\mathscr{S}$. (Simply put, this means that the symmetry variables have zero Poisson brackets with the classical observables.)

Our deformed Poincaré algebra on $\mathscr{O}$ can be completely specified by four quadratic Poisson bracket relations $\{\,,\}_{\mathscr{O}}$ which we give below. The brackets are evaluated between variables, i.e., ''momenta'' and ''angular momenta,'' spanning $\mathbf{R}^4\times\mathrm{SL}(2,C)$. The momenta will be expressed in terms of a 2×2 Hermitean matrix $\tilde{p}$, while the angular momenta are contained in a 2×2 complex unimodular matrix γ. The four Poisson bracket relations can be written in terms of a classical r-matrix (and its Hermitean conjugate $r^\dagger$). Here r is assumed to satisfy the modified classical Yang–Baxter equations. Using tensor product notation, the four relations are as follows:

$$\{\underset{1}{\tilde{p}},\underset{2}{\tilde{p}}\}=r\,\underset{1}{\tilde{p}}\,\underset{2}{\tilde{p}}+\underset{1}{\tilde{p}}\,\underset{2}{\tilde{p}}\,r^\dagger-\underset{2}{\tilde{p}}\,r^\dagger\,\underset{1}{\tilde{p}}-\underset{1}{\tilde{p}}\,r\,\underset{2}{\tilde{p}}, \tag{2}$$

$$\{\underset{1}{\gamma},\underset{2}{\gamma}\}=r^\dagger\,\underset{1}{\gamma}\,\underset{2}{\gamma}+\underset{1}{\gamma}\,\underset{2}{\gamma}\,r-\underset{2}{\gamma}\,r\,\underset{1}{\gamma}-\underset{1}{\gamma}\,r^\dagger\,\underset{2}{\gamma}, \tag{3}$$

$$\{\underset{1}{\gamma},\underset{2}{\overline{\gamma}}\}=r\,\underset{1}{\gamma}\,\underset{2}{\overline{\gamma}}+\underset{1}{\gamma}\,\underset{2}{\overline{\gamma}}\,r-\underset{2}{\overline{\gamma}}\,r\,\underset{1}{\gamma}-\underset{1}{\gamma}\,r\,\underset{2}{\overline{\gamma}}, \tag{4}$$

$$\{\underset{1}{\tilde{p}},\underset{2}{\gamma}\}=r^\dagger\,\underset{1}{\tilde{p}}\,\underset{2}{\gamma}+\underset{1}{\tilde{p}}\,\underset{2}{\gamma}\,r-\underset{2}{\gamma}\,r^\dagger\,\underset{1}{\tilde{p}}-\underset{1}{\tilde{p}}\,r^\dagger\,\underset{2}{\gamma}, \tag{5}$$

where $\overline{\gamma}=\gamma^{\dagger-1}$. The 1 and 2 labels refer to two separate vector spaces, with $\underset{1}{\tilde{p}}=\tilde{p}\otimes\mathbb{1}$, $\underset{2}{\tilde{p}}=\mathbb{1}\otimes\tilde{p}$, $\underset{1}{\gamma}=\gamma\otimes\mathbb{1}$, and $\underset{2}{\gamma}=\mathbb{1}\otimes\gamma$, $\mathbb{1}$ being the unit operator acting on the vector spaces. Here r acts nontrivially on both vector spaces. We shall utilize the following 4×4 matrix realization for r:

$$r=\frac{i\lambda}{2}\begin{pmatrix}1&&&\\&-1&&\\&4&-1&\\&&&1\end{pmatrix}, \tag{6}$$

λ being a real parameter.

Equations (2)–(5) thus give a one-parameter family of quadratic Poisson structures on $\mathscr{O}$. We outline some of their properties. Equations (2) and (3) can be shown to define skew symmetric brackets, the former being invariant under Hermitean conjugation. Jacobi identities involving $\tilde{p}$, γ, and $\overline{\gamma}$ are satisfied in part due to the r-matrix satisfying the modified classical Yang–Baxter

equations. (We, however, found it more convenient to use algebraic manipulation packages to check them.) It can be verified that $\det(\gamma)$ has vanishing brackets with all observables and hence Eqs. (2)–(5) are consistent with the unimodularity condition.

$\mathcal{O}$, unlike $\mathcal{S}$, does not define a Poisson–Lie group. In Sec. II, we shall show, however, that the quadratic algebra on $\mathcal{O}$ defined by Eqs. (2)–(5) is preserved under the Lie–Poisson action of $\mathcal{S}$. There we shall also show that the algebra is a deformation of the standard Poincaré algebra, the latter being recovered when $\lambda \to 0$. In that limit (the canonical limit), the Lie–Poisson transformations reduce to canonical transformations. Like with the Poincaré algebra, the algebra described by Eqs. (2)–(5) has two Casimir invariants. One of the Casimirs is the square of the momenta, while the other is the square of a vector corresponding to the Pauli–Lubanski vector. We can therefore associate the two classical Casimir functions with ''mass'' and ''spin.''

In Secs. III and IV, we parametrize the symplectic leaves of $\mathcal{O}$ with variables which we associate with space–time coordinates x, momenta $\tilde{p}$, and spin γ_s. We give a realization of the algebra defined by (2)–(5) in terms of x and $\tilde{p}$ in Sec. III. The Poisson structure for x and $\tilde{p}$ was already written down in Ref. 10, and it too was shown to be preserved under the Lie–Poisson action of $\mathcal{S}$. These Poisson brackets for x and $\tilde{p}$ were also shown to be a deformation of the canonical Poisson brackets for a relativistic particle, i.e., $\{x_\mu, p_\nu\} = \eta_{\mu\nu}$, $\eta = \mathrm{diag}\,(-1,1,1,1)$. In Sec. III (and in the Appendix), we shall realize the algebra for γ in terms of space–time coordinates x and momenta $\tilde{p}$. The resulting expression for γ is a deformation of the usual expression for the orbital angular momentum of a relativistic particle $j_{\mu\nu} = x_\mu p_\nu - x_\nu p_\mu$. Only here γ is an infinite series in x and $\tilde{p}$ (and λ). We shall show that the deformed Pauli–Lubanski vector is zero for this realization (for any value of λ), and hence we conclude that we have a description of a spinless particle. We also remark that if the classical Hamiltonian for the system is taken to be the momentum squared (i.e., $\det \tilde{p}$) times a Lagrange multiplier, then the resulting dynamics is identical to that of a free massless particle (for any value of λ). We thus arrive at a one-parameter family of canonically inequivalent descriptions for the photon. Upon quantization, the resulting photon states are expected to transform under the action of the quantum Lorentz group $\mathrm{SL}_q(2,C)$.

In Sec. IV, we show how the algebra (2)–(5) can be realized for a spinning particle. Thus here the Pauli–Lubanski vector is not zero. Unlike in the standard Hamiltonian description, we find that the spin associated with a particle must have nonvanishing Poisson brackets with both the space–time coordinates and the momenta. This is a consequence of the result that $\mathcal{O}$, unlike $\mathcal{S}$, is not a Poisson–Lie group. When the mass shell constraint is taken for the Hamiltonian, the classical spin is found to have a trivial dynamics, i.e., there is no spin precession, and this is just as in the standard theory.[11]

In Sec. V, we give a preliminary discussion of the quantization of the Poisson bracket algebra (2)–(5), while concluding remarks are made in Sec. VI. The issue of quantization will be discussed more fully in a later article.

II. THE DEFORMED POINCARÉ ALGEBRA

Here we will examine the two distinct Poisson manifolds $\mathcal{S}$ and $\mathcal{O}$, which are associated respectively with the space of symmetries and the space of classical observables. As stated in the Introduction, we shall identify $\mathcal{S}$ with the six-dimensional Lorentz group [or more precisely, its covering group $\mathrm{SL}(2,C)$], having Poisson brackets $\{\,,\}_{\mathcal{S}}$ corresponding to that of a Poisson–Lie group.[9,10] $\mathcal{O}$ will be assumed to be $\mathbf{R}^4 \times \mathrm{SL}(2,C)$ with Poisson brackets $\{\,,\}_{\mathcal{O}}$, which are essentially given by Eqs. (2)–(5).

In Sec. II A, we review the Poisson structure on $\mathcal{S}$ (Refs. 9 and 10), while we elaborate on the Poisson brackets (2)–(5) in Sec. II B. (For simplicity of notation we shall drop the subscripts $\mathcal{S}$ and $\mathcal{O}$ on the Poisson brackets.) Finally, in Sec. II C we write down the classical Casimir functions on $\mathcal{O}$.

A. Symmetries

Let g be a 2×2 complex unimodular matrix which we use to parametrize the space of symmetries $\mathscr{S}$. For $\mathscr{S}$ to be a Poisson–Lie group its Poisson brackets must be compatible with left and right group multiplication. The requirement of compatibility is satisfied for the set of brackets,

$$\{\underset{1}{g},\underset{2}{g}\}=[r,\ \underset{1}{g}\ \underset{2}{g}], \tag{7}$$

where we again utilize tensor product notation, with $\underset{1}{g} = g\otimes \mathbb{1}$, $\underset{2}{g} = \mathbb{1}\otimes g$ and the r-matrix defined in Eq. (6). Since the r-matrix is proportional to λ, the group elements have zero Poisson brackets in the canonical limit. The Jacobi identity holds due to the r-matrix satisfying the modified classical Yang–Baxter equation. It can also be checked from Eq. (7) that $\det(g)$ has zero Poisson brackets with all components of g and hence we may consistently set $\det(g)=1$. (The Leibniz identity for the Poisson brackets is assumed to be valid here and throughout this article.)

The transformations of the observables involve g as well as its Hermitean conjugate. Therefore in addition to Eq. (7) we will need to know the Poisson brackets for $g^\dagger$ or $\overline{g}=(g^\dagger)^{-1}$. For this we demand that the Poisson structure for g and $g^\dagger$ is consistent with complex conjugation, antisymmetry, and the Jacobi identity. All three of these conditions are met for the following set of relations:[10]

$$\{\underset{1}{g},\underset{2}{\overline{g}}\}=[r,\ \underset{1}{g}\ \underset{2}{\overline{g}}], \tag{8}$$

$$\{\underset{1}{\overline{g}},\underset{2}{g}\}=[r^\dagger,\ \underset{1}{\overline{g}}\ \underset{2}{g}], \tag{9}$$

$$\{\underset{1}{\overline{g}},\underset{2}{\overline{g}}\}=[r,\ \underset{1}{\overline{g}}\ \underset{2}{\overline{g}}], \tag{10}$$

in addition to (7). The Poisson brackets (7) and (8)–(10) coincide with the classical limit of the $SL_q(2,C)$ commutation relations given in Refs. 7 and 9.

We note that Eqs. (7) and (10) can be rewritten with r replaced by $r^\dagger$. This is because $r-r^\dagger$ serves as an adjoint invariant for $SL(2,C)$. More specifically, using the matrix representation (6) for r we have the identity

$$r-r^\dagger=i\lambda(2\Pi-\mathbb{1}), \tag{11}$$

where $\mathbb{1}$ is the unit operator (now acting on the entire tensor product space) and Π is the permutation operator, i.e., Π switches the two vector spaces. Thus, for example, $\underset{1}{g}\Pi = \Pi\underset{2}{g}$ and $\underset{2}{g}\Pi = \Pi\underset{1}{g}$.

B. Observables

Here we discuss the Poisson structure on $\mathscr{O}$. Following Eqs. (2)–(5) it is expressed in terms of the ten observables contained in $\tilde{p}$ and γ. The former corresponds to the momenta and it transforms as a Lorentz vector, i.e., it is associated with the $(\frac{1}{2},\frac{1}{2})$ representation of the Lorentz group. The latter corresponds to the angular momenta and it transforms as the (1,0) and (0,1) representations. We shall show that the Poisson structure (2)–(5) is a deformation of the standard Poincaré algebra and that it is preserved under the Lie–Poisson action of the Lorentz group.

We first discuss the Poisson brackets (2) for the momenta $\tilde{p}$. Actually, these brackets were already given in Ref. 10. There we wrote $\tilde{p}$ as a 2×2 Hermitean matrix

$$\tilde{p}=\begin{pmatrix} -p_0+p_3 & p_1-ip_2 \\ p_1+ip_2 & -p_0-p_3 \end{pmatrix}, \tag{12}$$

p_μ being the space–time components. Under a Lorentz transformation

$$\tilde{p}\to\tilde{p}'=\overline{g}\tilde{p}g^{-1}. \tag{13}$$

The Poisson structure for $\tilde{p}$ is required to be compatible with such transformations, i.e., the Poisson brackets for $\tilde{p}$ should be preserved upon assuming the Poisson brackets (7) and (8)–(10) for g and $\overline{g}$. (As stated earlier, we assume the product Poisson structure on $\mathcal{O}\times\mathcal{S}$, meaning that g and $\overline{g}$ have zero Poisson brackets with all observables.) The Poisson brackets are also required to be skewsymmetric, invariant under Hermitean conjugation and satisfy the Jacobi identity.

A solution to all of the above requirements is Eq. (2). It is easy to check that Eq. (2) is compatible with Lorentz transformations,

$$\{\underset{1}{\tilde{p}},\underset{2}{\tilde{p}}\}\to\{\underset{1}{\tilde{p}}',\underset{2}{\tilde{p}}'\}=\{\underset{1}{\overline{g}}\,\underset{1}{\tilde{p}}\,\underset{1}{g^{-1}},\underset{2}{\overline{g}}\,\underset{2}{\tilde{p}}\,\underset{2}{g^{-1}}\}=r\,\underset{1}{\tilde{p}}'\,\underset{2}{\tilde{p}}'+\underset{1}{\tilde{p}}'\,\underset{2}{\tilde{p}}'\,r^{\dagger}-\underset{2}{\tilde{p}}'\,r^{\dagger}\,\underset{1}{\tilde{p}}'-\underset{1}{\tilde{p}}'\,r\,\underset{2}{\tilde{p}}'. \tag{14}$$

Since the r-matrix is proportional to λ, all of the brackets between the momentum components vanish in the limit $\lambda\to 0$ and we recover the canonical result. The skewsymmetry of the bracket and invariance under Hermitean conjugation is also easily checked.

In terms of the space–time components of $\tilde{p}$, Eq. (2) can be written as

$$\begin{aligned} &\{p_i,p_j\}=2\lambda\epsilon_{ijk}p_k(p_0+p_3), \\ &\{p_i,p_0\}=0, \quad i,j,k=1,2,3. \end{aligned} \tag{15}$$

Thus the time component p_0 is in the center of the algebra. Also in the center is the magnitude of spatial components $\sqrt{p_ip_i}$ and consequently the invariant mass-squared, i.e., $p^\mu p_\mu=\det(\tilde{p})$. We expect that analogous central elements appear in the quantum theory, indicating that simultaneous measurements of the ''energy,'' the magnitude of the ''momentum'' and one of the spatial components p_i of the momentum are possible.[4]

We next take up the Poisson structure of the angular momenta. The angular momenta j can be represented by a 2×2 complex traceless matrix. Actually, however, we find it more convenient to deal with an exponentiation of j which we denote by $\gamma=e^{i\lambda j}$. Like g, γ is unimodular, i.e., $\det(\gamma)=1$, and hence it is an SL(2,C) matrix. (Unlike g, γ will not span a Poisson–Lie group.) Our space of classical observables is spanned by $\tilde{p}$ and γ. It is thus $\mathbf{R}^4\times\mathrm{SL}(2,C)$.

Under Lorentz transformations,

$$\gamma\to\gamma'=g\gamma g^{-1}. \tag{16}$$

The Poisson structure for γ is required to be compatible with this transformation. It is also required to be antisymmetric, consistent with the constraint $\det(\gamma)=1$ and satisfy the Jacobi identity. A solution to these requirements is Eq. (3). Under a Lorentz transformation,

$$\{\underset{1}{\gamma},\underset{2}{\gamma}\}\to\{\underset{1}{\gamma}',\underset{2}{\gamma}'\}=\{\underset{1}{g}\,\underset{1}{\gamma}\,\underset{1}{g^{-1}},\underset{2}{g}\,\underset{2}{\gamma}\,\underset{2}{g^{-1}}\}=r^{\dagger}\,\underset{1}{\gamma}'\,\underset{2}{\gamma}'+\underset{1}{\gamma}'\,\underset{2}{\gamma}'\,r-\underset{2}{\gamma}'\,r\,\underset{1}{\gamma}'-\underset{1}{\gamma}'\,r^{\dagger}\,\underset{2}{\gamma}', \tag{17}$$

and hence Eq. (3) is preserved. From Eq. (3) it can be checked that $\det(\gamma)$ has zero Poisson brackets with all components of γ and hence we may consistently set $\det(\gamma)=1$.

In addition to Eq. (3), we need to specify the Poisson brackets of $\gamma^\dagger$ or $\overline{\gamma}=(\gamma^\dagger)^{-1}$. For this we again demand that they be preserved under Lorentz transformations and that they are consistent with the Jacobi identity. These conditions are met for Eq. (4). By applying complex conjugation to (3) and (4) we obtain additional relations. They are

$$\{\underset{1}{\overline{\gamma}},\underset{2}{\overline{\gamma}}\}=r\,\underset{1}{\overline{\gamma}}\,\underset{2}{\overline{\gamma}}+\underset{1}{\overline{\gamma}}\,\underset{2}{\overline{\gamma}}r^\dagger-\underset{2}{\overline{\gamma}}r^\dagger\underset{1}{\overline{\gamma}}-\underset{1}{\overline{\gamma}}r\,\underset{2}{\overline{\gamma}}, \tag{18}$$

$$\{\underset{1}{\overline{\gamma}},\underset{2}{\gamma}\}=r^\dagger\underset{1}{\overline{\gamma}}\,\underset{2}{\gamma}+\underset{1}{\overline{\gamma}}\,\underset{2}{\gamma}r^\dagger-\underset{2}{\gamma}r^\dagger\underset{1}{\overline{\gamma}}-\underset{1}{\overline{\gamma}}r^\dagger\underset{2}{\gamma}. \tag{19}$$

The remaining Poisson brackets of the observables are between the momenta $\tilde{p}$ and the variables γ and $\overline{\gamma}$. For these mixed brackets we find Eq. (5) along with its complex conjugate

$$\{\underset{1}{\tilde{p}},\underset{2}{\overline{\gamma}}\}=r\,\underset{1}{\tilde{p}}\,\underset{2}{\overline{\gamma}}+\underset{1}{\tilde{p}}\,\underset{2}{\overline{\gamma}}r-\underset{2}{\overline{\gamma}}r^\dagger\underset{1}{\tilde{p}}-\underset{1}{\tilde{p}}r\,\underset{2}{\overline{\gamma}}. \tag{20}$$

Using Eqs. (4) and (20), we have checked that $\{\det(\gamma),\tilde{p}\}=\{\det(\gamma),\overline{\gamma}\}=0$ and therefore that these Poisson brackets are consistent with the condition of unimodularity.

The Poisson structure of all ten observables is given by Eqs. (2)–(5) and (19) and (20). [Actually, we only need to specify Eqs. (2)–(5) as the remaining relations are obtained by conjugation.] We have used algebraic manipulation packages to verify that the Jacobi identity for $\tilde{p}$, γ, and $\overline{\gamma}$ is satisfied.

We next show that the algebra generated by $\tilde{p}$, γ, and $\overline{\gamma}$ is a deformation of the standard Poincaré algebra, the latter being recovered in the limit $\lambda\to 0$. For this we substitute $\gamma=e^{i\lambda j}$ and $\overline{\gamma}=e^{i\lambda j^\dagger}$ into the Poisson bracket relations and expand around $\lambda=0$, keeping only the lowest order contributions. As stated earlier, Eq. (2) gives

$$\{\underset{1}{\tilde{p}},\underset{2}{\tilde{p}}\}\to 0. \tag{21}$$

The lowest-order contributions to Eqs. (3) and (4) are quadratic in λ, yielding

$$\{\underset{1}{j},\underset{2}{j}\}\to 2\Pi(\underset{2}{j}-\underset{1}{j}),\quad \{\underset{1}{j},\underset{2}{j^\dagger}\}\to 0, \tag{22}$$

where we used Eq. (11). Lastly, from Eq. (5) we obtain

$$\{\underset{1}{\tilde{p}},\underset{2}{j}\}\to\underset{1}{\tilde{p}}(2\Pi-\mathbb{1}). \tag{23}$$

The limiting algebra in Eqs. (21)–(23) is the Poincaré algebra. It can be expressed in a more familiar form, i.e.,

$$\{p_\mu,p_\nu\}=0, \tag{24}$$

$$\{j_{\mu\nu},j_{\rho\sigma}\}=\eta_{\mu\rho}j_{\nu\sigma}+\eta_{\nu\sigma}j_{\mu\rho}+\eta_{\mu\sigma}j_{\rho\nu}+\eta_{\nu\rho}j_{\sigma\mu}, \tag{25}$$

$$\{p_\mu,j_{\nu\rho}\}=\eta_{\mu\rho}p_\nu-\eta_{\mu\nu}p_\rho, \tag{26}$$

$$\eta=\mathrm{diag}(-1,1,1,1), \tag{27}$$

upon applying the matrix representation [cf. Eq. (12)] for $\tilde{p}$, along with the following representation for the 2×2 complex traceless matrix j:

$$j=\begin{pmatrix} -ij_{12}+j_{30} & -ij_{23}-ij_{20}-j_{31}+j_{10} \\ -ij_{23}+ij_{20}+j_{31}+j_{10} & ij_{12}-j_{30} \end{pmatrix}. \tag{28}$$

C. Casimirs

Like the Poincaré algebra, the algebra generated by $\tilde{p}$, γ, and $\overline{\gamma}$ has two central elements, which we will associate with ''mass'' and ''spin.''

With regard to the mass, this classical Casimir function is identical in form to that of the Poincaré algebra. [This, however, is not the case at the quantum level.[4] To define the latter, one introduces a deformed determinant.] That is, $p^\mu p_\mu=\det(\tilde{p})$ is the Casimir function. From Eqs. (2), (5), and (20), we have that

$$\{\det(\tilde{p}),\tilde{p}\}=\{\det(\tilde{p}),\gamma\}=\{\det(\tilde{p}),\overline{\gamma}\}=0, \tag{29}$$

and therefore that it is in the center of the algebra.

With regard to the spin, the second Casimir function can be defined as the square of a new vector w_μ. For this we define

$$\tilde{w}=\frac{1}{2\lambda}\,(\overline{\gamma}^{-1}\tilde{p}\gamma-\tilde{p}); \tag{30}$$

$\tilde{w}$ is a 2×2 Hermitean matrix, so we can write

$$\tilde{w}=\begin{pmatrix} -w_0+w_3 & w_1-iw_2 \\ w_1+iw_2 & -w_0-w_3 \end{pmatrix}. \tag{31}$$

It is a deformation of the standard Pauli–Lubanski vector. To see this, we substitute $\gamma=e^{i\lambda j}$ and $\overline{\gamma}=e^{i\lambda j^\dagger}$ in Eq. (30) and expand around $\lambda=0$, yielding

$$\tilde{w}=\frac{i}{2}\,(\tilde{p}j-j^\dagger\tilde{p})+\mathcal{O}(\lambda). \tag{32}$$

The zeroth-order term in λ is the Pauli–Lubanski vector.

Under Lorentz transformations, $\tilde{w}$ transforms as $\tilde{p}$ does, i.e., $\tilde{w}\to\tilde{w}'=\overline{g}\tilde{w}g^{-1}$. In addition, we find that its Poisson brackets with the observables γ and $\overline{\gamma}$ are identical in form to those of $\tilde{p}$, i.e.,

$$\{\underset{1}{\tilde{w}},\underset{2}{\gamma}\}=r^\dagger\underset{1}{\tilde{w}}\ \underset{2}{\gamma}+\underset{1}{\tilde{w}}\ \underset{2}{\gamma r}-\underset{2}{\gamma r^\dagger}\underset{1}{\tilde{w}}-\underset{1}{\tilde{w}}\underset{2}{r^\dagger\gamma}, \tag{33}$$

$$\{\underset{1}{\tilde{w}},\underset{2}{\overline{\gamma}}\}=r\underset{1}{\tilde{w}}\ \underset{2}{\overline{\gamma}}+\underset{1}{\tilde{w}}\ \underset{2}{\overline{\gamma r}}-\underset{2}{\overline{\gamma r}^\dagger}\underset{1}{\tilde{w}}-\underset{1}{\tilde{w}}\underset{2}{r\overline{\gamma}}. \tag{34}$$

These equations are to be compared with (5) and (20). The Poisson brackets for $\tilde{w}$ with $\tilde{p}$ are given by

$$\{\underset{1}{\tilde{w}},\underset{2}{\tilde{p}}\}=r\underset{1}{\tilde{w}}\ \underset{2}{\tilde{p}}+\underset{1}{\tilde{w}}\ \underset{2}{\tilde{p}r^\dagger}-\underset{2}{\tilde{p}r^\dagger}\underset{1}{\tilde{w}}-\underset{1}{\tilde{w}}\underset{2}{r\tilde{p}}, \tag{35}$$

which in terms of space–time components can be expressed as follows:

$$\begin{aligned} &\{w_i,p_j\}=2\lambda(\epsilon_{ijn}(p_0+p_3)-\delta_{j3}\epsilon_{ikn}p_k)w_n, \\ &\{w_i,p_0\}=2\lambda\,\epsilon_{ijk}p_jw_k, \quad i,j,k=1,2,3, \quad \{w_0,p_\mu\}=0. \end{aligned} \tag{36}$$

We then find that, in analogy to Eq. (29),

$$\{\det(\tilde{w}),\tilde{p}\}=\{\det(\tilde{w}),\gamma\}=\{\det(\tilde{w}),\overline{\gamma}\}=0, \tag{37}$$

and hence that $w_\mu w^\mu=\det(\tilde{w})$ is a classical Casimir function.

We expect that there are no additional independent Casimir functions and therefore that the symplectic leaves in $\mathcal{O}$ are eight-dimensional, just as is the case with the Poincaré algebra. In the two sections which follow, we shall show how to parametrize the symplectic leaves with variables which one can naturally associate with position, momenta, and spin.

For completeness we compute the Poisson brackets for $\tilde{w}$ with itself. From Eqs. (33)–(35), we find

$$\underset{1}{\{}\tilde{w},\underset{2}{\tilde{w}}\}=r\underset{1}{\tilde{w}}\ \underset{2}{\tilde{w}}+\underset{1}{\tilde{w}}\ \underset{2}{\tilde{w}}r^\dagger-\underset{2}{\tilde{w}}r^\dagger\underset{1}{\tilde{w}}-\underset{1}{\tilde{w}}r\underset{2}{\tilde{w}}-i\Pi(\underset{1}{\tilde{w}}\ \underset{2}{\tilde{p}}-\underset{2}{\tilde{w}}\ \underset{1}{\tilde{p}}), \tag{38}$$

or, in terms of the space–time components of $\tilde{w}$,

$$\begin{aligned}\{w_i,w_j\}&=\epsilon_{ijk}(w_0p_k-p_0w_k+2\lambda(w_0+w_3)w_k),\\ \{w_0,w_i\}&=\epsilon_{ijk}p_jw_k,\quad i,j,k=1,2,3.\end{aligned} \tag{39}$$

From Eqs. (36) and (39), we deduce that the set of commuting operators in the quantum theory can be enlarged to those associated with

$$p_0,\quad p_3,\quad \text{and } w_0,$$

in addition to the two Casimirs $p_\mu p^\mu$ and $w_\mu w^\mu$.

[We note that in Ref. 4, a set of commuting operators for the spinless particle was found in an analogous quantum system. The set contained operators associated with p_0, p_3, and the third component of angular momentum. All of these operators were shown to have a discrete quantum spectrum for the case of a particle with nonzero mass. (From Ref. 10, we surmise that such a particle is not free, but instead has a nontrivial interaction with the space–time.) With regard to p_0 and p_3, we expect that a similar spectrum will occur for us. We do not know what the third component of angular momentum corresponds to in our formalism, nor do we know if an analog of w_0 can be included in the set of commuting operators of Ref. 4.]

III. SPIN ZERO REALIZATION

Here we discuss a realization of our deformed Poincaré algebra defined by Eqs. (2)–(5) in terms of space–time coordinates x_μ and the momenta p_μ. The realization is based on the system described in Ref. 10, where we deformed the standard symplectic structure for a relativistic particle. As we shall see, this realization has the Casimir $\det(\tilde{w})$ equal to zero, and we therefore associate it with the description of a (deformed) spinless relativistic particle. Actually, here we get the even stronger constraint that $\tilde{w}=0$, or, from (30),

$$\tilde{p}\,\gamma=\overline{\gamma\tilde{p}}. \tag{40}$$

This result is analogous to what is obtained in the standard Hamiltonian description of spinless particles, where all of the components of the Pauli–Lubanski vector vanish.

From Eq. (12) the four components of momentum p_μ are contained in the momentum matrix $\tilde{p}$. With regard to the space–time coordinates x_μ, we find it convenient to introduce the following 2×2 Hermitean matrix

$$x=\begin{pmatrix}-x_0-x_3 & -x_1+ix_2\\ -x_1-ix_2 & -x_0+x_3\end{pmatrix}. \tag{41}$$

In contrast to $\tilde{p}$, x transforms according to

$$x \to x' = g x \overline{g^{-1}}. \tag{42}$$

As stated previously, the Poisson structure for x and $\tilde{p}$ is a deformation of the canonical Poisson brackets for a relativistic particle. In addition, it should be preserved under the Lie–Poisson action of the Lorentz group, satisfy the Jacobi identity, and be Hermitean. The following Poisson brackets are consistent with all of the above conditions:

$$\{x,x\} = r_{12} x_1 x_2 + x_1 x_2 r^{\dagger}_{12} - x_2 r_{21} x_1 - x_1 r^{\dagger}_{12} x_2, \tag{43}$$

$$\{x,\tilde{p}\} = r_{12} x_1 \tilde{p}_2 + x_1 \tilde{p}_2 r^{\dagger}_{12} - \tilde{p}_2 r_{21} x_1 - x_1 r^{\dagger}_{12} \tilde{p}_2 - \Pi(f^{\dagger}_1 + f_2), \tag{44}$$

along with Eq. (2). Here f is a 2×2 complex matrix. For Eq. (44) to be preserved under Lorentz transformations, it must transform like γ, i.e.,

$$f \to g f g^{-1}. \tag{45}$$

Here f must be a nontrivial function of λ. This is since in order to recover the canonical Poisson bracket relations, we need that f tends to the unit matrix $\mathbb{1}$ when $\lambda \to 0$, while it cannot be $\mathbb{1}$ for all λ because, as some work shows, it would then violate the Jacobi identity. In this regard, the issue of whether the Jacobi identity is satisfied was only partially addressed in Ref. 10. Here we find (with the aid of algebraic manipulation packages) that the Jacobi identity involving the position and momentum variables holds provided that f satisfies the following Poisson brackets with x and $\tilde{p}$:

$$\{\tilde{p},f\} = r^{\dagger}_{12} \tilde{p}_1 f_2 + \tilde{p}_1 f_2 r_{12} - f_2 r^{\dagger}_{21} \tilde{p}_1 - \tilde{p}_1 r^{\dagger}_{12} f_2 + i\lambda \tilde{p}_1 f_2, \tag{46}$$

$$\{x,f\} = r^{\dagger}_{12} x_1 f_2 + x_1 f_2 r^{\dagger}_{12} - f_2 r_{21} x_1 - x_1 r^{\dagger}_{12} f_2 - i\lambda x_1 f_2. \tag{47}$$

In the above, it appears that we have enlarged the phase space spanned by x and $\tilde{p}$ to also include the variables f. However, it is not necessary to regard f as independent variables. Rather, it is possible to express f in terms of x and $\tilde{p}$, and still satisfy the Poisson brackets (46) and (47), as well as recover the correct canonical limit $f \to \mathbb{1}$. This was done in Ref. 10, where we wrote f according to

$$f = \exp\{i\lambda J\}, \quad \text{where } \sin \lambda J = \lambda x \tilde{p}. \tag{48}$$

By this we meant the following Taylor expansion:

$$f = \mathbb{1} + i\lambda x\tilde{p} - \frac{1}{2}(\lambda x\tilde{p})^2 - \frac{1}{8}(\lambda x\tilde{p})^4 \cdots - \frac{1\cdot 3\cdot 5\cdot \cdots \cdot(2n-3)}{2\cdot 4\cdot 6\cdot \cdots \cdot 2n}(\lambda x\tilde{p})^{2n} \cdots . \tag{49}$$

It is easily seen that this expression Lorentz transforms as in Eq. (45) and that it tends to the unit matrix $\mathbb{1}$ when $\lambda \to 0$. It can also be shown that it is in agreement with the Poisson brackets (46). We do this in the Appendix. In a similar manner, it can be shown to be in agreement with the Poisson brackets (47). Also in a similar manner, we can use Eq. (48) to obtain the brackets for f with itself and with $f^{\dagger}$. We find

$$\{f,f\} = r^{\dagger}_{12} f_1 f_2 + f_1 f_2 r_{12} - f_2 r_{21} f_1 - f_1 r^{\dagger}_{12} f_2, \tag{50}$$

$$\{f,f^\dagger\}=r\underset{1}{f}\underset{2}{f^\dagger}+\underset{1}{f}\underset{2}{f^\dagger}r-\underset{2}{f^\dagger}r\underset{1}{f}-\underset{1}{f}r\underset{2}{f^\dagger}. \tag{51}$$

We have checked that these relations are consistent with the Jacobi identity.

We next would like to express γ is terms of x and $\tilde{p}$. We note that the Poisson bracket for f with itself is identical in form to the Poisson bracket (3) for γ with itself, the only difference between them being that while γ appearing in Eq. (3) is unimodular, f is not. In this regard, we note that we are not allowed to set $\det(f)$ equal to one, because although $\det(f)$ has zero brackets with f and $f^\dagger$ [which follows from Eqs. (50) and (51)], it does not have zero brackets with the coordinates or the momenta. Instead, from Eq. (46), we find that

$$\begin{aligned}\{x,\det(f)\}&=-2i\lambda x\ \det(f),\\ \{\tilde{p},\det(f)\}&=2i\lambda\tilde{p}\ \det(f).\end{aligned} \tag{52}$$

Alternatively, we can easily define a unimodular matrix from f by simply dividing by $\sqrt{\det(f)}$. This is in fact how we make the identification with γ. That is, we set

$$\gamma=\frac{f}{\sqrt{\det(f)}}, \tag{53}$$

and thereby have an expression for γ in terms of x and $\tilde{p}$. It then follows that if we again write $\gamma=e^{i\lambda j}$ and use Eq. (48), then j corresponds to the traceless part of $J=(1/\lambda)\sin^{-1}(\lambda x\tilde{p})$,

$$j=J-\tfrac{1}{2}\mathbb{1}\ \mathrm{Tr}\ J. \tag{54}$$

Upon keeping terms linear in λ, in the expression (49) we see that j reduces to the usual expression for orbital angular momentum in the canonical limit $\lambda\to 0$, i.e.,

$$j\to x\tilde{p}-\tfrac{1}{2}\mathbb{1}\ \mathrm{Tr}\ x\tilde{p}.$$

The identification (53) of γ in terms of x and $\tilde{p}$ is valid because from it we can recover the full set of Poisson brackets (3)–(5) starting from the brackets for f [specifically, (46), (50), and (51)]. Since we also have Eq. (2), we obtain a realization of the entire deformed Poincaré algebra. Using Eqs. (47) and (52), we can further obtain the brackets between the space–time coordinates x and γ:

$$\{x,\gamma\}=r^\dagger\underset{1}{x}\underset{2}{\gamma}+\underset{1}{x}\underset{2}{\gamma r^\dagger}-\gamma\underset{2}{r}\underset{1}{x}-\underset{1}{x}\underset{2}{r^\dagger}\gamma. \tag{55}$$

It now only remains to show that the condition (40) is satisfied or, equivalently, that the deformed Pauli–Lubanski vector is zero. This follows using results from the Appendix, specifically Eqs. (A3) and (A5), which lead to

$$\tilde{p}e^{i\lambda J}=e^{i\lambda J^\dagger}\tilde{p}, \tag{56}$$

If we now divide both sides of this equation by $\sqrt{\det(f)}$ and use (53), we obtain Eq. (40). Hence we have the description of a (deformed) spinless particle. We can then associate the expression for γ in terms of x and $\tilde{p}$ with the ''orbital angular momentum'' of the particle.

In Ref. 10, we made some remarks concerning dynamics on a Poisson manifold spanned by x and $\tilde{p}$. We showed that if the standard mass shell constraint is chosen for the Hamiltonian function, i.e.,

$$H=\alpha(\det(\tilde{p})-m^2), \tag{57}$$

then it, along with the Poisson brackets (2), (43), and (44), yields a nontrivial interaction of the particle with the space–time when λ and m are different from zero (α denotes a Lagrange multiplier). In Ref. 10 we solved for the particle trajectory and found that it originates and terminates at singular points. The particle has a lifetime equal to

$$\left|\frac{\mathrm{Tr}(\gamma p)}{\lambda\ \det(\tilde{p})}\right|, \tag{58}$$

where $p=\sigma_2\tilde{p}^T\sigma_2$, T denoting transpose and σ_2 being the second Pauli matrix. Thus when λ and m are different from zero, it appears that the dynamics corresponds to a kind of ''virtual'' particle which is off its ''physical'' mass shell. [In this regard, $\det(\tilde{p})=m^2$ does not define the ''physical'' mass shell since we identify the conserved quantity $\tilde{p}$ with the deformed momentum and not the ''physical'' momentum.]

We note that the expression (58) is singular for the case of a massless particle, i.e., $m=0$, indicating that such a particle has an infinite lifetime. Actually, we can show that the Hamiltonian (57) with $m=0$ [along with the Poisson brackets (2), (43), and (44)] describes a free photon (or any massless particle) for arbitrary values of λ. For this we compute the Hamiltonian equations of motion:

$$\dot{x}=\frac{d}{d\tau}x=\alpha\{x,\det(\tilde{p})\}=-\alpha(fp+pf^{\dagger}), \tag{59}$$

$$\dot{\tilde{p}}=\frac{d}{d\tau}\tilde{p}=\alpha\{\tilde{p},\det(\tilde{p})\}=0. \tag{60}$$

It then follows that for $m=0$,

$$\dot{x}\tilde{p}=-\alpha(fp+pf^{\dagger})\tilde{p}=0, \tag{61}$$

where we have used the mass shell constraint $\tilde{p}p=p\tilde{p}=\det(\tilde{p})1=0$, in addition to the series expansion Eq. (49) for f. The traceless part of Eq. (61) is equivalent to $\dot{x}_\mu p_\nu-\dot{x}_\nu p_\mu=0$ and hence

$$\dot{x}_\mu=\kappa p_\nu. \tag{62}$$

The trace of Eq. (61) implies that $\dot{x}^\mu p_\mu=0$, and thus gives no constraint on the proportionality constant κ. We therefore arrive at a *free* lightlike trajectory. Furthermore, since λ is arbitrary, we get an entire family of canonically inequivalent Hamiltonian descriptions of a photon trajectory. Upon quantization, the resulting states are expected to transform covariantly under the action of the quantum Lorentz group $\mathrm{SL}_q(2,C)$.

Actually, to truly describe a photon, we should introduce a spin and check that its equation of motion is the usual one. That is, there should be no classical spin precession. Spin will be introduced in Sec. IV. There we indeed find that there is no precession of the classical spin (even for the case $m\neq 0$).

IV. INCLUSION OF SPIN

In the standard description of a relativistic particle,[11] spin is introduced as an additional term in the angular momentum. This term is defined to have zero Poisson brackets with coordinates and momenta, and it, unlike the orbital angular momentum, gives a nonvanishing contribution to the Pauli–Lubanski vector. We shall look for an analogous prescription for including spin in our deformed Poincaré algebra.

There is, of course, no unique procedure for including spin in the deformed Poincaré algebra. We should require that it reduce to the standard prescription in the limit $\lambda\to 0$. In what follows, our

choice shall be to multiply the SL(2,C) matrix γ obtained in the previous section on the right by another SL(2,C) matrix which we denote by γ_s. The former matrix is once again to be regarded as the orbital angular momentum, while γ_s plays the role of ''spin.'' Thus we replace

$$\gamma \to \gamma\gamma_s = \frac{f\gamma_s}{\sqrt{\det(f)}}. \tag{63}$$

To get back the standard prescription, i.e., $j \to j+s$, when $\lambda \to 0$, we can take $\gamma_s = e^{i\lambda s}$, s being a traceless complex matrix. Furthermore, using Eq. (63) we get that the ''spin'' γ_s, and not the ''orbital angular momentum'' $f/\sqrt{\det(f)}$, contributes to the deformed Pauli–Lubanski vector equation (30), analogous to what happens in the standard description. [This would not have been the case if instead of Eq. (63), we had multiplied γ on the left by γ_s.] Thus we now get

$$\tilde{w} = \frac{1}{2\lambda}(\overline{\gamma_s}^{1}\tilde{p}\gamma_s - \tilde{p}) \neq 0,$$

and furthermore $\det(\tilde{w}) \neq 0$. We next show that *unlike* in the usual theory, the spin has nonzero Poisson brackets with momentum and position, and that this is a consequence of the fact that the space spanned by the matrices γ does not form a Poisson–Lie group (unlike the space spanned by matrices g).

Because $\mathscr{S}$ is a Poisson–Lie group, the Poisson structure for the SL(2,C) matrices g is preserved under left or right group multiplication, i.e., the Poisson brackets (7) are compatible with the group product.[12–15] As we show below, the analogous statement does not, however, apply to the Poisson structure for the SL(2,C) matrices γ. That is, the Poisson brackets (3) are not compatible with group multiplication and hence the space spanned by γ is not a Poisson–Lie group.

To see that the Poisson structure for symmetries is preserved under group multiplication, one defines a variable $g' \in \mathrm{SL}(2,C)$ which satisfies the same relations as g,

$$\{\underset{1}{g'},\underset{2}{g'}\} = [r, \underset{1}{g'}\underset{2}{g'}], \tag{64}$$

in addition to $\{\underset{1}{g'},\underset{2}{g}\} = 0$. Then under right multiplication $g \to gg'$, we obtain

$$\{\underset{1}{g},\underset{2}{g}\} \to \{\underset{1}{g}\,\underset{1}{g'},\underset{2}{g}\,\underset{2}{g'}\} = [r, \underset{1}{g}\,\underset{2}{g}]\underset{1}{g'}\underset{2}{g'} + \underset{1}{g}\,\underset{2}{g}[r, \underset{1}{g'}\underset{2}{g'}] = [r, (\underset{1}{g}\,\underset{1}{g'})(\underset{2}{g}\,\underset{2}{g'})], \tag{65}$$

and hence that the Poisson structure given by (7) is preserved.

Let us now try the same thing for the observables γ. We define $\gamma_s \in \mathrm{SL}(2,C)$ to satisfy the same relations as γ,

$$\{\underset{1}{\gamma_s},\underset{2}{\gamma_s}\} = r^{\dagger}\underset{1}{\gamma_s}\underset{2}{\gamma_s} + \underset{1}{\gamma_s}\underset{2}{\gamma_s}r - \underset{2}{\gamma_s}r\underset{1}{\gamma_s} - \underset{1}{\gamma_s}r^{\dagger}\underset{2}{\gamma_s}, \tag{66}$$

in addition to $\{\underset{1}{\gamma_s},\underset{2}{\gamma}\} = 0$. However, it is easily checked that this Poisson structure is not preserved under right (or left) multiplication $\gamma \to \gamma\gamma_s$. Therefore that γ expressed as $f\gamma_s/\sqrt{\det(f)}$ does not give a realization of the relations (3).

To proceed further we shall drop the assumption that the product space spanned by γ and γ_s has a product Poisson structure, i.e., we drop the assumption that the spin γ_s has zero Poisson brackets with the orbital angular momentum γ (and hence also with the coordinates and momenta) in the deformed theory, i.e., $\{\underset{1}{\gamma_s},\underset{2}{\gamma}\} \neq 0$. Instead we take

$$\{\underset{1}{\gamma_s},\underset{2}{\gamma}\} = r^{\dagger}\underset{1}{\gamma_s}\underset{2}{\gamma} + \underset{1}{\gamma_s}\underset{2}{\gamma}r^{\dagger} - \underset{2}{\gamma}r^{\dagger}\underset{1}{\gamma_s} - \underset{1}{\gamma_s}r^{\dagger}\underset{2}{\gamma}, \tag{67}$$

or, equivalently,

$$\{\underset{1}{\gamma},\underset{2}{\gamma_s}\}=r\,\underset{1}{\gamma}\,\underset{2}{\gamma_s}+\underset{1}{\gamma}\,\underset{2}{\gamma_s}r-\underset{2}{\gamma_s}r\,\underset{1}{\gamma}-\underset{1}{\gamma}r\,\underset{2}{\gamma_s}. \tag{68}$$

It then can be checked that the product $\gamma\gamma_s$ carries the same Poisson structure as γ [i.e. Eq. (3)],

$$\{\underset{1}{\gamma}\,\underset{1}{\gamma_s},\underset{2}{\gamma}\,\underset{2}{\gamma_s}\}=r^{\dagger}(\underset{1}{\gamma}\,\underset{1}{\gamma_s})(\underset{2}{\gamma}\,\underset{2}{\gamma_s})+(\underset{1}{\gamma}\,\underset{1}{\gamma_s})(\underset{2}{\gamma}\,\underset{2}{\gamma_s})r-(\underset{2}{\gamma}\,\underset{2}{\gamma_s})r(\underset{1}{\gamma}\,\underset{1}{\gamma_s})-(\underset{1}{\gamma}\,\underset{1}{\gamma_s})r^{\dagger}(\underset{2}{\gamma}\,\underset{2}{\gamma_s}). \tag{69}$$

Thus, in this sense we can preserve the Poisson structure for the observables. We note that the Poisson bracket relations for γ and γ_s are identical in form to those of γ and $\gamma^{\dagger}$. Then since the Jacobi identity holds for the latter variables, it must also hold for γ and γ_s. In addition, we have that $\{\det(\gamma),\gamma_s\}=\{\det(\gamma_s),\gamma\}=0$, and therefore the Poisson brackets (67) are consistent with the unimodularity of both γ and γ_s. We note that Eq. (67) is also consistent with the canonical limit, because if we write $\gamma=e^{i\lambda j}$ and $\gamma_s=e^{i\lambda s}$, then, to lowest order in λ, we obtain that s has zero Poisson brackets with j.

As stated before, in the standard theory for a relativistic particle the spin has zero Poisson brackets with the momenta. Here, however, if the Poisson bracket (5) is to be preserved under Eq. (63), we need that $\{\underset{1}{\gamma_s},\underset{2}{\tilde{p}}\}\neq 0$. Specifically, we need

$$\{\underset{1}{\tilde{p}},\underset{2}{\gamma_s}\}=r^{\dagger}\,\underset{1}{\tilde{p}}\,\underset{2}{\gamma_s}+\underset{1}{\tilde{p}}\,\underset{2}{\gamma_s}r-\underset{2}{\gamma_s}r^{\dagger}\,\underset{1}{\tilde{p}}-\underset{1}{\tilde{p}}r\,\underset{2}{\gamma_s}. \tag{70}$$

For then

$$\{\underset{1}{\tilde{p}},\underset{2}{\gamma}\,\underset{2}{\gamma_s}\}=r^{\dagger}\,\underset{1}{\tilde{p}}(\underset{2}{\gamma}\,\underset{2}{\gamma_s})+\underset{1}{\tilde{p}}(\underset{2}{\gamma}\,\underset{2}{\gamma_s})r-(\underset{2}{\gamma}\,\underset{2}{\gamma_s})r^{\dagger}\,\underset{1}{\tilde{p}}-\underset{1}{\tilde{p}}r^{\dagger}(\underset{2}{\gamma}\,\underset{2}{\gamma_s}), \tag{71}$$

which is identical in form to the relation (5).

We have checked that Poisson brackets (67) and (70) are consistent with the Jacobi identity for γ, $\tilde{p}$, and γ_s. We also verified that $\{\det(\gamma_s),\tilde{p}\}=0$ and that $\tilde{p}$ has zero brackets with s in the limit $\lambda\to 0$.

Just as γ_s does not have zero Poisson brackets with the momenta, it also does not have zero Poisson brackets with the position. That $\{\underset{1}{\gamma_s},\underset{2}{x}\}\neq 0$ is easily seen because, if it were not so, we would not then be able to recover the correct brackets (67) for γ_s with the orbital angular momenta γ [given as a function of $x\tilde{p}$ in Eqs. (49) and (53)]. What works instead is

$$\{\underset{1}{x},\underset{2}{\gamma_s}\}=r\underset{1}{x}\,\underset{2}{\gamma_s}+\underset{1}{x}\,\underset{2}{\gamma_s}r^{\dagger}-\underset{2}{\gamma_s}r\underset{1}{x}-\underset{1}{x}r^{\dagger}\underset{2}{\gamma_s}. \tag{72}$$

From it and Eq. (70) we find that

$$\{(\underset{1}{x}\,\underset{1}{\tilde{p}})^n,\underset{2}{\gamma_s}\}=r(\underset{1}{x}\,\underset{1}{\tilde{p}})^n\underset{2}{\gamma_s}+(\underset{1}{x}\,\underset{1}{\tilde{p}})^n\underset{2}{\gamma_s}r-\underset{2}{\gamma_s}r(\underset{1}{x}\,\underset{1}{\tilde{p}})^n-(\underset{1}{x}\,\underset{1}{\tilde{p}})^n r\,\underset{2}{\gamma_s}. \tag{73}$$

Hence the Poisson brackets between γ_s and *any* polynomial function of $x\tilde{p}$ has precisely the same form as the Poisson brackets between γ_s and γ given in Eq. (67). Thus

$$\{\underset{1}{f},\underset{2}{\gamma_s}\}=rf\,\underset{1}{\gamma_s}+\underset{1}{f}\,\underset{2}{\gamma_s}r-\underset{2}{\gamma_s}rf-fr\,\underset{2}{\gamma_s}. \tag{74}$$

From previous arguments we then also know that $\{\det(f),\gamma_s\}=0$. The Poisson brackets (67) between γ and γ_s are realized for $\gamma=f/\sqrt{\det(f)}$ by dividing both sides of Eq. (74) by $\sqrt{\det(f)}$. Now γ expressed as $f\gamma_s/\sqrt{\det(f)}$ realizes the Poisson bracket relations (3). From Eq. (72) it also follows that $\{\underset{1}{x},\underset{2}{s}\}\to 0$ when $\lambda\to 0$ and hence we recover the usual canonical limit.

To summarize, we have obtained a realization of the deformed Poincaré algebra defined by Eqs. (2)–(5) with $\det(\tilde{w})\neq 0$. (Actually for this we also need to have the Poisson brackets between

γ_s and $\overline{\gamma}$. We shall assume that a consistent set of such brackets exist.) Thus unlike in the previous section, we now have a description of a particle with spin. We have shown that we get back the standard description of a spinning particle when $\lambda \to 0$. Under Lorentz transformations, γ_s must transform as does γ, i.e., $\gamma_s \to g \gamma_s g^{-1}$. It is easy to check that all Poisson brackets with γ_s are compatible with such transformations and once again that the Lorentz group induces a Lie–Poisson action on the observables. (Here we assume, as usual, that the classical observables, including γ_s, have zero Poisson brackets with the classical symmetry variables g and $\overline{g}$.)

Finally, we remark about the spin dynamics. For this purpose we want again to utilize the Hamiltonian function (57). We then need to compute the Poisson bracket of γ_s with $\det(\tilde{p})$. From Eq. (70), we find that this Poisson bracket vanishes. This means that for the Hamiltonian function (57), the classical spin has a trivial dynamics (i.e., there is no precession). This is just as in the standard formulation of a classical spinning particle.[11]

V. TOWARDS QUANTIZATION

Here we make some preliminary remarks concerning quantization. We plan to address this issue more fully in a subsequent publication.

There exists a standard quantization scheme (called deformation quantization) which can be applied in this case. It is known to deform the space of symmetries $\mathcal{S}$ to a Hopf algebra, specifically, $\mathrm{SL}_q(2,C)$.[9] We remark on this first. We then comment on a possible quantization of the classical observables. The system which results appears to be different from q-Poincaré algebras discussed previously in the literature.[3–7]

With regard to the symmetries, one standardly replaces g by an $\mathrm{SL}_q(2,C)$ matrix, which we denote by T, and the Poisson brackets (7) by the corresponding quantum commutation relations. The matrix elements in T are constrained by the condition that the ''deformed'' determinant is equal to one, and this is the analogue of the unimodularity condition on g. The commutation relations are given in terms of a quantum R matrix, satisfying the quantum Yang–Baxter equations, and can be written according to

$$\underset{12}{R}\ \underset{1}{T}\ \underset{2}{T} = \underset{2}{T}\ \underset{1}{T}\ \underset{12}{R}. \tag{75}$$

This algebra can presumably be realized on the space $\mathcal{S}$ of classical symmetries with the use of a star product. In order to recover the correct classical limit one only requires that $\underset{12}{R} \to 1 - i\hbar r + \mathcal{O}(\hbar^2)$ when $\hbar \to 0$.

In addition to Eq. (75), one needs the quantum analogues of the Poisson brackets (8) and (10). For this we introduce another $\mathrm{SL}_q(2,C)$ matrix T which in analogy to the classical observable $\overline{g}$ is related to T by: $\overline{T} = T^{\dagger -1}$. Then along with Eq. (75), we write

$$\underset{12}{R}\ \underset{1}{T}\ \underset{2}{\overline{T}} = \underset{2}{\overline{T}}\ \underset{1}{T}\ \underset{12}{R}, \tag{76}$$

$$\underset{12}{R}\ \underset{1}{\overline{T}}\ \underset{2}{\overline{T}} = \underset{2}{\overline{T}}\ \underset{1}{\overline{T}}\ \underset{12}{R}, \tag{77}$$

which corresponds to Eqs. (8) and (10) when $\hbar \to 0$. By switching vector space indices 1 and 2, we see that we can replace R in Eqs. (75) and (77) by R^{-1}. Thus $\underset{12}{R}\ \underset{21}{R}$ must commute with $\underset{2}{T}\ \underset{1}{T}$ and $\underset{2}{\overline{T}}\ \underset{1}{\overline{T}}$. This is analogous to the statement that $r - r^{\dagger}$ is an adjoint invariant in the classical theory.

Concerning the quantum observables, we shall require that their algebra is preserved under the action of the quantum symmetries, in analogy to what happens in the classical theory. We also want that this algebra is consistent with the classical Poisson bracket algebra in the limit $\hbar \to 0$.

A quantum algebra for the momenta was already given in Ref. 7 that is consistent with these properties, so we will adopt it here. There one replaces the classical variable $\tilde{p}$ by a 2×2 matrix P whose elements are operator valued. The Poisson brackets (2) are replaced by what were referred to as reflection equations,

$$\underset{12}{R}\ \underset{1}{P}\ \underset{12}{R^{-1}}\underset{2}{P}=\underset{2}{P}\ \underset{21}{R^{-1}}\underset{1}{P}\ \underset{21}{R}. \tag{78}$$

With this choice, one can easily obtain the correct classical limit. For this one notes that, using the matrix expression (6) for r, one obtains that $\underset{21}{R}\to\mathbb{1}+i\hbar r\dagger+\mathcal{O}(\hbar 2)$ when $\hbar\to 0$. Furthermore, as desired, the commutation relations (78) are preserved under $\mathrm{SL}_q(2,C)$ transformations. Here in analogy to Eq. (13), one assumes that P transforms as a vector under the action of the quantum Lorentz group, i.e.,

$$P\to P'=\overline{T}PT^{-1}, \tag{79}$$

and that the matrix elements of T and $\overline{T}$ commute with those of P. Then using the relations (75)–(77), one obtains that the left-hand side of (78) transforms according to

$$\begin{aligned}\underset{12}{R}\ \underset{1}{P}\ \underset{12}{R^{-1}}\underset{2}{P}\to\underset{12}{R}\ \underset{1}{P'}\underset{12}{R^{-1}}\underset{2}{P'}&=\underset{2}{\overline{T}}\ \underset{1}{\overline{T}}\ \underset{12}{R}\ \underset{1}{P}\ \underset{12}{R^{-1}}\underset{2}{P}\ \underset{1}{T^{-1}}\underset{2}{T^{-1}}\\&=\underset{2}{\overline{T}}\ \underset{1}{\overline{T}}\ \underset{2}{P}\ \underset{21}{R^{-1}}\underset{1}{P}\ \underset{21}{R}\ \underset{1}{T^{-1}}\underset{2}{T^{-1}}=\underset{2}{P'}\underset{21}{R^{-1}}\underset{1}{P'}\underset{21}{R},\end{aligned} \tag{80}$$

and hence that Eq. (78) is preserved.

We may assume that the quantum matrix P is Hermitean, analogous to the fact that the classical matrix $\tilde{p}$ is Hermitean. It is easy to check that this property is consistent with the transformation property (79). It is also consistent with the commutation relation (78), provided that we have the following condition on the quantum R-matrix:

$$\underset{12}{R^{\dagger}}=\underset{21}{R}. \tag{81}$$

An R-matrix which satisfies this requirement, as well as the Yang–Baxter equations, and has the correct classical limit is

$$\underset{12}{R}=q^{-1/2}\begin{pmatrix} q & & & \\ & 1 & & \\ & q-q^{-1} & 1 & \\ & & & q\end{pmatrix},\quad q=e^{\hbar\lambda}. \tag{82}$$

It remains to specify the quantum analogues of Poisson brackets (3)–(5). For this we associate the classical observables γ and $\overline{\gamma}$ with operator-valued 2×2 matrices Γ and $\overline{\Gamma}$, which in analogy to (16) transform as

$$\Gamma\to\Gamma'=T\Gamma T^{-1},\quad \overline{\Gamma}\to\overline{\Gamma}'=\overline{T\Gamma T^{-1}}, \tag{83}$$

under the action of $\mathrm{SL}_q(2,C)$. As with T, we can assume that matrix elements of Γ are constrained by the condition that the ''deformed'' determinant is equal to one, in analogy to the unimodularity condition on γ. We propose that the Γs satisfy the following commutation relations amongst themselves and with P:

$$R^{-1}_{21}\Gamma_1 R_{21}\Gamma_2 = \Gamma_2 R_{12}\Gamma_1 R^{-1}_{12}, \tag{84}$$

$$R_{12}\Gamma_1 R^{-1}_{12}\overline{\Gamma}_2 = \overline{\Gamma}_2 R_{12}\Gamma_1 R^{-1}_{12}, \tag{85}$$

$$R^{-1}_{21}P_1 R_{21}\Gamma_2 = \Gamma_2 R^{-1}_{21}P_1 R^{-1}_{12}. \tag{86}$$

It can be checked that from these relations one recovers the correct quadratic algebra, i.e., Eqs. (3)–(5), as $\hbar\to 0$. Also, using Eqs. (75)–(77) and the assumption that the matrix elements of T and $\overline{T}$ commute with those of Γ and $\overline{\Gamma}$, it can be checked that the commutation relations (84)–(86) are preserved under $\mathrm{SL}_q(2,C)$ transformations (79) and (83). The procedure is analogous to that used in Eq. (80).

If we define $\overline{\Gamma}=\Gamma^{\dagger -1}$ in analogy to what was done in the classical theory, then by taking the Hermitean conjugates of Eqs. (84)–(86) we get the quantum analogs of the Poisson brackets (18)–(20). Using (81), we obtain

$$R_{12}\overline{\Gamma}_1 R^{-1}_{12}\overline{\Gamma}_2 = \overline{\Gamma}_2 R^{-1}_{21}\overline{\Gamma}_1 R_{21}, \tag{87}$$

$$R^{-1}_{21}\overline{\Gamma}_1 R_{21}\Gamma_2 = \Gamma_2 R^{-1}_{21}\overline{\Gamma}_1 R_{21}, \tag{88}$$

$$R_{12}P_1 R^{-1}_{12}\overline{\Gamma}_2 = \overline{\Gamma}_2 R^{-1}_{21}P_1 R^{-1}_{12}, \tag{89}$$

which correspond to Eqs. (18)–(20) when $\lambda\to 0$.

Although the set of symmetry operators $\{T\}$ defines a Hopf algebra, the same does not seem to be the case for the set of quantum operators $\{\Gamma\}$. In this regard we do not know how to define a coproduct for the latter. This is not too surprising since the set of classical variables $\{\gamma\}$ did not define a Poisson–Lie group. For this reason it appears that our quantum algebra defined in Eqs. (78) and (84)–(86) differs from those given previously.[3–7] Equations (78) and (84)–(86) define a set of the quadratic commutation relations between the quantum mechanical observables P, Γ, and $\overline{\Gamma}$, which nevertheless are preserved under the action of a Hopf algebra. Whether or not it is necessary to impose higher-order relations on the observables remains to be checked.

From the observables p, Γ, and $\overline{\Gamma}$, it is possible to construct the quantum mechanical deformed Pauli–Lubanski vector, and also Casimir operators corresponding to mass and spin. It should then be possible to look for eigenvectors of these operators along with the quantum analogues of p_0, p_3, and w_0. This will be addressed in a forthcoming article. We can also hope to obtain realizations of the quantum algebra for the cases of a spinless and spinning relativistic particle in a manner similar to what was done in Secs. III and IV.

VI. CONCLUDING REMARKS

Here we outline additional future avenues of research.

We have obtained a deformation of the Poincaré algebra which is covariant with respect to the Lie–Poisson action of the Lorentz group. It is of interest to know whether or not this algebra can also be made to be covariant under the Lie–Poisson action of the translation group, and hence under the action of the full Poincaré group. It is also of interest to know whether or not the angular momenta γ can somehow play the role of generators of Lorentz transformations, as in the canonical theory, and also whether or not the momenta $\tilde{p}$ can somehow play the role of generators of translations. One thing which is clear is that infinitesimal Lorentz transformations are not obtained (as in the canonical theory) by simply taking Poisson brackets with γ. Similarly, translations are

not obtained by simply taking Poisson brackets with $\tilde{p}$. (Generators of Lie–Poisson symmetries have been found previously in physical systems. In Ref. 16 we examined the system of a isotropic rigid rotator. That system was invariant under the Lie–Poisson action of the chiral symmetry group. There we were able to find the generators of the chiral symmetry, and they took values in a group which was dual to the symmetry group. Similar novel features are anticipated for the Lie–Poisson generators of the space–time symmetries of a relativistic particle.)

In Secs. III and IV, realizations for the deformed Poincaré algebra were found which were associated with a single relativistic particle. It is of interest to know how one constructs representations for two or more particles. This is not straightforward because as we found in Sec. IV, the Poisson structure for the observables γ is not compatible with the group product, i.e., the space spanned by γ is not a Poisson–Lie group. Also, it can be checked that the Poisson structure for the observables $\tilde{p}$ is not compatible with addition of the momenta. Just as we found in Sec. IV that the spin does not commute with the orbital angular momentum, we can already conclude the angular momenta for different particles does not commute, and we also suspect that the momenta of different particles does not commute.

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APPENDIX: VERIFICATION OF EQ. (46)

Here we show that the Poisson brackets (46) for $\tilde{p}$ with f can be deduced using the realization for f in terms of x and $\tilde{p}$ given in Eq. (48). For this we will assume the Poisson brackets (2) and (44).

We start by computing the brackets for $\tilde{p}$ with $\sin\lambda J=\lambda x\tilde{p}$. From Eqs. (2) and (44) we obtain

$$\{\underset{1}{\tilde{p}},\ \sin(\lambda \underset{2}{J})\}=r^{\dagger}\tilde{p}_1\sin(\lambda J)_2+\tilde{p}_1\sin(\lambda J)_2 r^{\dagger}-\sin(\lambda J)_2 r^{\dagger}\tilde{p}_1-\tilde{p}_1 r^{\dagger}\sin(\lambda J)_2+\lambda(f^{\dagger}+f)_1\tilde{p}_1\Pi. \tag{A1}$$

To determine the brackets of $\tilde{p}$ with f, we also need $\{\underset{1}{\tilde{p}},\ \cos(\lambda \underset{2}{J})\}$. We can deduce it by knowing the brackets for $\tilde{p}$ with $\cos^2\lambda J=1-\sin^2\lambda J$, which are easily obtained from Eq. (A1),

$$\{\underset{1}{\tilde{p}},\ \cos^2(\lambda \underset{2}{J})\}=r^{\dagger}\tilde{p}_1\cos^2(\lambda J)_2+\tilde{p}_1\cos^2(\lambda J)_2 r^{\dagger}-\cos^2(\lambda J)_2 r^{\dagger}\tilde{p}_1-\tilde{p}_1 r^{\dagger}\cos^2(\lambda J)_2$$
$$-\lambda\left(\sin(\lambda \underset{2}{J})(f^{\dagger}+f)_2+(f^{\dagger}+f)_2\sin(\lambda J^{\dagger})_1\right)\tilde{p}_1\Pi, \tag{A2}$$

where we have used

$$\tilde{p}\,\sin(\lambda J)=\sin(\lambda J^{\dagger})\tilde{p}. \tag{A3}$$

Then a solution is

$$\{\underset{1}{\tilde{p}},\ \cos(\lambda \underset{2}{J})\}=r^{\dagger}\tilde{p}_1\cos(\lambda J)_2+\tilde{p}_1\cos(\lambda J)_2 r^{\dagger}-\cos(\lambda J)_2 r^{\dagger}\tilde{p}_1-\tilde{p}_1 r^{\dagger}\cos(\lambda J)_2-i\lambda(f^{\dagger}-f)_1\tilde{p}_1\Pi. \tag{A4}$$

To check that Eq. (A2) follows from Eq. (A4), we can apply the identities

$$\tilde{p}\,\cos(\lambda J)=\cos(\lambda J^{\dagger})\tilde{p}, \tag{A5}$$

and

$$\sin(\lambda J)(f^\dagger + f) + (f^\dagger + f)\sin(\lambda J^\dagger) = i\,\cos(\lambda J)(f^\dagger - f) + i(f^\dagger - f)\cos(\lambda J^\dagger). \tag{A6}$$

The former identity follows after writing J as an infinite series in $x\tilde{p}$, while the latter follows after writing $f=\cos(\lambda J)+i\,\sin(\lambda J)$. Finally, from Eqs. (A1) and (A4), and using a third identity, i.e., Eq. (11), we then obtain the desired result Eq. (46).

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On tractability of path integration

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Many applications require approximate values of path integrals. A typical approach is to approximate the path integral by a high dimensional integral and apply a Monte Carlo (randomized) algorithm. However, Monte Carlo algorithm requires roughly ϵ^{-2} integrand evaluations to provide an ϵ approximation. Moreover, the error bound of ϵ is guaranteed only in a stochastic sense. Do we really need to use randomized algorithms for path integrals? Perhaps, we can find a *deterministic* algorithm that is more effective even in the worst case setting. To answer this question, we study the *worst case complexity* of path integration, which, roughly speaking, is defined as the minimal number of the integrand evaluations needed to compute an approximation with error at most ϵ. We consider path integration with respect to a Gaussian measure, and for various classes of integrands. Tractability of path integration means that the complexity depends polynomially on $1/\epsilon$. We show that for the class of r times Frechet differentiable integrands, tractability of path integration holds iff the covariance operator of the Gaussian measure has finite rank. Hence, if the Gaussian measure is supported on an infinite dimensional space then path integration is intractable. In this case, there exists no effective deterministic algorithm, and the use of randomized algorithms is justified. In fact, for this class of integrands, the classical Monte Carlo algorithm is (almost) optimal and the complexity in the randomized setting is proportional to ϵ^{-2}. On the other hand, for a particular class of entire integrands, the worst case complexity of path integration is at most of order ϵ^{-p} with p depending on the Gaussian measure. Hence, path integration is now tractable. Furthermore, for any Gaussian measure, the exponent p is less than or equal to 2. For the Wiener measure, $p=2/3$. For this class, we provide effective deterministic algorithms which solve the path integration problem with (worst case) cost that is usually much less than the (randomized) cost of the classical Monte Carlo algorithm. © *1996 American Institute of Physics.* [S0022-2488(96)01204-6]

I. INTRODUCTION

Approximate computation of integrals is undoubtedly one of the most important problems of computational mathematics. In many cases, integrals involve functions of finitely many variables d. Not surprisingly, the univariate case $d=1$ is best understood and has a rich and well-developed theory. Elements of the classical theory of univariate integration can be found in almost all numerical analysis textbooks. The study of the complexity of continuous problems has started from the pioneering work of Sard and Nikolskij on univariate integration; see Refs. 1 and 2.

The multivariate case, with d finite and greater than one, is much harder and is a subject of very active research. For large d, a typical approach is to use Monte Carlo (randomized) algorithms. However, for some classes of integrands, deterministic algorithms can be also very effec-

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tive. An example is provided by integrands with bounded mixed derivatives, for which algorithms based on low discrepancy points can be used. The state of the art can be found in Ref. 3. Complexity of multivariate integration in various settings is also an active research area. An account of recent progress can be found in Refs. 4–11.

In this paper, we consider the case $d=+\infty$. That is, we deal with integrals of functions of infinitely many variables. This is usually called the *path integration* problem. The name is derived from the most typical case, in which we integrate over continuous functions (paths) with respect to the Wiener measure, see Ref. 12. Sometimes, instead of path integration, the name *functional* integration is used; see Refs. 13 and 14. The latter stresses that we integrate over a class of functions.

One may suspect that the path integration problem is merely of theoretical interest. However, the opposite is true. Path integrals occur in many applied fields, including quantum physics and chemistry, differential equations, and financial mathematics, as well as average case complexity. Here are a few examples. In the forties, R. P. Feynman introduced path integration in quantum physics; see Ref. 12. The work of Feynman initiated a very fruitful stream of research in quantum physics and chemistry which continues to be active; see, e.g., Refs. 13 and 15–23. A rigorous mathematical foundation for Feynman path integration can be found in Ref. 24. In the fifties, M. Kac observed that the approach of Feynman can be used for the solution of parabolic differential equations, and established what today is called the Feynman-Kac formula; see Ref. 25. In fact, solutions of many differential and operator equations can be expressed as path integrals; see Ref. 14. Also many problems in financial mathematics are expressed as generalized Feynman-Kac formulas, and hence their solution may be reduced to computing path integrals; see Ref. 26–28. Finally, in average case complexity, we need to estimate the average error of an algorithm; this error is, once more, given as a path integral. A more complete list of applications is given in the introduction of Ref. 14.

A typical approach to computing path integrals is to switch to a multivariate integral and apply a Monte Carlo (randomized) algorithm. That is, the infinite dimensional integral is approximated by a d dimensional integral, where d may be large (or even huge). Then the classical Monte Carlo algorithm can be used since its speed of convergence, although not great, does not depend on d. This approach usually requires on the order of ε^{-2} integrand evaluations to obtain the expected error at most ε, see Sec. II for more details.

Due to this relatively high cost of Monte Carlo and only stochastic error assurance, one would like to know weather there is an effective *deterministic* algorithm which approximates path integrals with a small (deterministic) error. Obviously, the existence of such a deterministic algorithm depends on the probability measure μ occurring in the path integral as well as on the class F of integrands. Hence, for a given measure μ and a given class F, we wish to find the *worst case complexity* of path integration. Roughly speaking, the worst case complexity is proportional to the minimal number of integrand evaluations needed to compute an approximation with worst case error at most ε.

We are mainly interested in how the complexity depends on ε. If the complexity is of order ε^{-p} with $p<2$ then we beat the bound ε^{-2} of the classical Monte Carlo algorithm. For $p=2$, the bounds are of the same order. However, even for $p>2$, we may prefer to use a deterministic algorithm since its error is guaranteed to be at most ε, whereas for the classical Monte Carlo algorithm we only know that its expected error is at most ε. Moreover, with deterministic algorithms, we do not have to cope with the problem of generating random numbers or functions.

This discussion motivates the concept of tractability of path integration. Namely, we say that the path integration problem is *tractable* if the worst case complexity depends polynomially on $1/\varepsilon$. In other settings such as the randomized or average case settings, tractability of path integration is obvious in classes for which the L_2 norms of integrands are uniformly bounded. However, for problems that are not path integration, the study of tractability in other settings is an interesting subject; see Refs. 29 and 30.

Tractability of path integration depends on the probability measure μ and the class F of integrands. We now comment on the assumptions regarding μ and F.

We begin with the measure μ. In most applications of path integration, the classical Wiener measure (Brownian motion) is used. The Wiener measure is an example of a Gaussian measure which is appropriate for many applications. Its role can be hardly overestimated. It would be tempting to study path integration only for the Wiener measure. However, we prefer to be more general and to study path integration for arbitrary Gaussian measures, and to illustrate the results for the Wiener measure as a primary example. In this way we will better understand the influence of the Gaussian measure on the complexity of path integration. Of course, it would also be interesting to study path integration for a non-Gaussian measure, although no such application is known to us.

We now turn to the class F of integrands. Here, the situation is far more complex since there is no class of integrands which plays a dominant role corresponding to the Wiener measure. Even for the multivariate case, there is no class which is singled out. On contrary, many different classes seem to be relevant and their choice depends on the particular application. Usually these classes are characterized by some global smoothness properties of the integrands.

For path integration, we follow the multivariate approach and we analyze classes defined by global smoothness. First, we consider the class of integrands that are r times continuously Frechet differentiable. We prove that in this case, tractability of path integration holds iff the covariance operator of the Gaussian measure has finite rank. Hence, the problem of path integration is *intractable* if the Gaussian measure is supported on an infinite dimensional space. Then it is reasonable to switch to the randomized setting. It turns out that the classical Monte Carlo algorithm is (almost) optimal and the complexity in the randomized setting is proportional to ϵ^{-2}.

Next we analyze a specific class of entire functions. For this class, the path integration problem is tractable, and the worst case complexity is of order ϵ^{-p} with p depending, in particular, on the Gaussian measure used. For the Wiener measure, we have $p=2/3$, which means that we need substantially fewer integrand evaluations than for the classical Monte Carlo algorithm even though we guarantee that the worst case error is at most ϵ. We stress, however, that to get this result we assume that integrands are entire functions and that we can use derivatives as permissible information. It is well known that the classical Monte Carlo algorithm requires no smoothness of the integrands; it is enough to assume that they are square integrable.

The classes of integrands studied in this paper are characterized by global smoothness properties. In a forthcoming paper, see Ref. 31, we consider a different class of integrands. This class is related to the Feynman–Kac formula. More precisely, this is the class of potential and initial conditions functions which define the heat equation. Although these functions do not need to be very smooth, we prove tractability of path integration, and in many cases, the worst case complexity is substantially smaller than ϵ^{-2}.

II. FORMULATION OF THE PROBLEM

In this section we formulate the path integration problem and explain a typical computational approach to approximating path integrals. We also define the worst case complexity and tractability of path integration.

Let X be a separable Banach space. The norm in X is denoted by $\|\cdot\|_X$. An example of X is provided by the space $X=C([0,1])$ of continuous scalar functions defined on $[0,1]$ with the sup norm, $\|x\|_X=\sup_{t\in[0,1]}|x(t)|$.

We assume that X is equipped with a zero mean Gaussian measure μ; see, e.g., Ref. 32. An example of μ is provided by the Wiener measure $\mu=w$ for which $X=C([0,1])$ and

$$\int_{C[0,1]} x(t_1)x(t_2)w(dx)=\min\{t_1,t_2\}.$$

It is known that X can be embedded in the Hilbert space $L_2([0,1])$. It is an obvious corollary of the Banach (sometimes called the Banach–Mazur or Banach–Alaoglu) theorem which states that X is isometrically isomorphic to a subspace of $C([0,1])$ which, in turn, can be treated as a subspace of $L_2([0,1])$. This means that there exists a one-to-one linear continuous mapping $\mathrm{Im}: X \to L_2([0,1])$. We denote the inner product of $L_2([0,1])$ by $\langle \cdot,\cdot \rangle$. Then the measure $\nu = \mu\,\mathrm{Im}^{-1}$ is also a zero mean Gaussian measure on $L_2([0,1])$. Let $C_\nu : L_2([0,1]) \to L_2([0,1])$ be the covariance operator of ν. The operator C_ν is self-adjoint, non-negative definite, and has finite trace. That is, there exists an orthonormal system $\{\eta_i\}_i$ of $L_2([0,1])$, $\langle \eta_i, \eta_j \rangle = \delta_{i,j}$, for which

$$C_\nu \eta_i = \lambda_i \eta_i, \quad \lambda_1 \geq \lambda_2 \geq \cdots \geq 0 \quad \text{and} \quad \sum_{i=1}^{\infty} \lambda_i < +\infty. \tag{1}$$

Observe that if all $\lambda_1 = 0$, then the path integration problem becomes trivial. Indeed, μ is then an atomic measure at zero and $S(f) = f(0)$. This, of course, can be solved exactly by using one function value. To omit this trivial case, we assume that at least one eigenvalue is positive,

$$\lambda_1 > 0.$$

Without loss of generality, we may assume that $\eta_i \in \mathrm{Im}(X)$. Indeed, the measure ν is concentrated on $\mathrm{Im}(X)$, $\nu[\mathrm{Im}(X)] = 1$, and $\eta_i \in \mathrm{Im}(X)$, where the closure of $\mathrm{Im}(X)$ is taken in the norm of $L_2([0,1])$. Hence, we can approximate η_i with an arbitrarily small error by elements of $\mathrm{Im}(X)$. To avoid this cumbersome approximation of η_i, we assume, for simplicity, that η_i belong to $\mathrm{Im}(X)$.

For the Wiener measure $\mu = w$, we have

$$\mathrm{Im}(x) = x, \quad \eta_i = \sqrt{2}\,\sin\left(\frac{2i-1}{2}\,\pi x\right), \quad \lambda_i = \frac{4}{\pi^2 (2i-1)^2}.$$

Let F be a class of (Borel) measurable real functions defined on X. An example of such F studied in this paper is the class $F = F^r$ of r times Frechet differentiable functions for which $\|f^{(i)}\| = \sup_{x \in X} \|f^{(i)}(x)\| \leq 1$ for $i = 0,1,\ldots,r$. Here, $f^{(i)}(x)$ is an i-linear form from X^i to $\mathbb{R}$, and its norm is defined as $\|f^{(i)}(x)\| = \sup_{\|x_j\|_X \leq 1} |f^{(i)}(x) x_1 x_2 \ldots x_i|$.

The *path integration* problem is defined as approximating integrals of f from F. That is, we want to approximate the expectation of f with respect to the Gaussian measure μ,

$$S(f) = \int_X f(x)\,\mu(dx), \quad \forall f \in F. \tag{2}$$

Since X is usually infinite dimensional, the integrand f in (2) depends on infinitely many variables. That is why the path integration problem can be viewed as an integration of functions of infinitely many variables.

We now illustrate the path integrals problem for finite and infinite dimensional spaces X. Assume first that $X = \mathbb{R}^d$ for some finite d, and let μ be the standard Gaussian measure with λ_i as the eigenvalues of its covariance operator. Then (2) becomes

$$S(f) = \frac{1}{(2\pi)^{d/2}} \frac{1}{\sqrt{\lambda_1 \lambda_2 \cdots \lambda_d}} \int_{\mathbb{R}^d} f(t_1, t_2, \cdots, t_d) \exp[-t_1^2/(2\lambda_1) - \cdots - t_d^2/(2\lambda_d)]\, d\mathbf{t},$$

where $\mathbf{t} = [t_1, t_2, \ldots, t_d] \in \mathbb{R}^d$.

Hence, for finite dimensional spaces X, the path integration problem reduces to finite dimensional integration with respect to a Gaussian measure.

Assume now that X is of infinite dimension. We now show how $S(f)$ can be approximated by finite dimensional integrals. Let $x=\mathrm{Im}^{-1}(\mathrm{Im}\,x)$. Note that Im^{-1} is well defined on the set $\mathrm{Im}(X)$ which is of a full ν measure. Hence, $\mathrm{Im}^{-1}(\mathrm{Im}\,x)$ is defined almost everywhere. By changing variables $y=\mathrm{Im}(x)$ we may rewrite (2) as

$$S(f)=\int_{L_2([0,1])} f[\mathrm{Im}^{-1}(y)]\,\nu(dy).$$

The elements y from $L_2([0,1])$ can be approximated by

$$P_d y=\sum_{i=1}^{d}\langle y,\eta_i\rangle\,\eta_i.$$

Then the integral $S(f)$ is approximated by $S_d(f_d)$, where $f_d:\mathbb{R}^d\to\mathbb{R}$ is defined by

$$f_d(\mathbf{t})=f[\mathrm{Im}^{-1}(t_1\eta_1+t_2\eta_2+\cdots+t_d\eta_d)],$$

for $\mathbf{t}=[t_1,t_2,\ldots,t_d]\in\mathbb{R}^d$, and

$$S_d(f_d)=\frac{1}{(2\pi)^{d/2}}\,\frac{1}{\sqrt{\lambda_1\lambda_2\cdots\lambda_d}}\int_{\mathbb{R}^d} f_d(\mathbf{t})\exp\left(\frac{-t_1^2}{(2\lambda_1)}-\cdots-\frac{t_d^2}{(2\lambda_d)}\right)d\mathbf{t}. \tag{3}$$

Observe that S_d is a finite dimensional integral, as for the case of a finite dimensional space X. However, unlike the latter case, the eigenvalues λ_i tend to zero, and $\lambda_i\leq a/i$ with $a=\Sigma_{i=1}^{\infty}\lambda_i<+\infty$. Hence, there is a decreasing dependence on the successive variables t_i in (3).

For a function f that satisfies the Banach–Lebesgue theorem (it is enough to assume that f is continuous and $|f[\mathrm{Im}^{-1}(P_d y)]|\leq g[\mathrm{Im}^{-1}(y)]$, $\forall d$, for some function g for which $S(g)$ is finite), we have

$$S(f)=\lim_{d\to\infty} S_d(f_d).$$

This suggests that to approximate $S(f)$ it is enough to choose a sufficiently large d and approximate a finite dimensional integral $S_d(f_d)$. The choice of d depends on the smoothness of the elements of F. For example, assume that $F=F_{\mathrm{Lip}}$ is the class of Lipschitz functions,

$$F_{\mathrm{Lip}}=\{f:X\to\mathbb{R},\quad |f(x_1)-f(x_2)|\leq K\|\mathrm{Im}(x_1)-\mathrm{Im}(x_2)\|_{L_2([0,1])},\quad \forall x_1,x_2\in X\},$$

for some positive constant K. Then for $f\in F_{\mathrm{Lip}}$ we have

$$|S(f)=S_d(f_d)|\leq K\left(\int_{L_2([0,1])}\sum_{i=d+1}^{\infty}\langle y,\eta_i\rangle^2\,\nu(dy)\right)^{1/2}=K\left(\sum_{i=d+1}^{\infty}\lambda_i\right)^{1/2}.$$

Hence, to guarantee that the error $|S(f)-S_d(f_d)|\leq\epsilon$, $\forall f\in F_{\mathrm{Lip}}$, it is enough to define d as the smallest integer for which

$$\sum_{i=d+1}^{\infty}\lambda_i\leq\epsilon^2/K^2.$$

For $\lambda_i=\Theta(i^{-k})$ with $k>1$, we get

$$d=\Theta[(K/\epsilon)^{2/(k-1)}]\quad\text{as}\quad\epsilon\to 0^+.$$

For the Wiener measure we have $k=2$ and

$$d=\frac{1}{\pi^2}\left(\frac{K}{\epsilon}\right)^2[1+o(1)] \quad \text{as} \quad \epsilon\to 0^+.$$

Hence, for infinite dimensional spaces X, we can approximate path integration by d dimensional integrals with respect to a Gaussian measure, where $d=d(\epsilon)$ goes to infinity as the error tolerance ϵ goes to zero. How fast $d(\epsilon)$ goes to infinity depends on the decay of the eigenvalues of λ_i.

In either case of X, we see that path integrals may be approximated by d dimensional integrals, where d is typically (very) large. For $f\in L_2(X,\mu)$, the high-dimensional integration is usually done by the classical Monte Carlo algorithm applied to the function f_d,

$$S_d(f_d)\sim \mathrm{MC}_n(f_d;\mathbf{u})=\frac{1}{n}\sum_{i=1}^{n} f_d(u_i),$$

where $\mathbf{u}=[u_1,u_2,\ldots,u_n]\in\mathbb{R}^{nd}$ and u_i are independent random points of $\mathbb{R}^d$ which are distributed according to the Gaussian measure of zero mean and variances $\lambda_1,\lambda_2,\ldots,\lambda_d$. It is well known that

$$E[S_d(f_d)-\mathrm{MC}_n(f_d;\mathbf{u})]^2=\frac{1}{n}\left[\int_{L_2([0,1])} h^2(P_d y)\,\nu(dy)-\left(\int_{L_2([0,1])} h(P_d y)\,\nu(dy)\right)^2\right],$$

where $h=f\circ \mathrm{Im}^{-1}$ and E stands for the expectation with respect to the random selection of the points u_i.

Note that

$$E[S(f)-\mathrm{MC}_n(f_d;\mathbf{u})]^2=|S(f)-S_d(f_d)|^2+E[S_d(f_d)-\mathrm{MC}_n(f_d;\mathbf{u})]^2$$

and

$$\begin{aligned}\int_{L_2([0,1])} h^2(P_d y)\,\nu(dy)&=\int_{L_2([0,1])}[h(P_d y)-h(y)+h(y)]^2\,\nu(dy)\\ &\le 2\int_{L_2([0,1])}[h(y)-h(P_d y)]^2\,\nu(dy)\\ &\quad+2\int_{L_2([0,1])} h^2(y)\,\nu(dy).\end{aligned}$$

Obviously, $\int_{L_2([0,1])} h^2(y)\,\nu(dy)=\int_X f^2(x)\,\mu(dx)$. Hence, for the class F_{Lip} of Lipschitz functions we have

$$E[S(f)-\mathrm{MC}_n(f_d;\mathbf{u})]^2\le K^2(1+2n^{-1})\sum_{i=d+1}^{\infty}\lambda_i+\frac{2}{n}\int_X f^2(x)\,\mu(dx).$$

To guarantee that the randomized error of the classical Monte Carlo algorithm is at most ϵ, we choose n of order ϵ^{-2} and d, such that $\Sigma_{i=d+1}^{\infty}\lambda_i$ is of order $(\epsilon/K)^2$. For $\lambda_i=\Theta(i^{-k})$, the cost of the classical Monte Carlo algorithm with randomized error at most ϵ is proportional to the cost of computing ϵ^{-2} values of functions of $d=\Theta[(K/\epsilon)^{2/(k-1)}]$ variables.

The goal of this paper is to investigate whether path integration can be solved by *deterministic* algorithms in the *worst case* setting. More precisely, we are interested in the *worst case complexity* $\mathrm{comp}(\epsilon,F)$ of path integration. This is defined as the minimal cost among all deterministic algo-

rithms which compute an approximation whose error is at most ϵ for all $f \in F$. In what follows, we assume that the cost of one integrand evaluation is $\mathbf{c}$, and the cost of one arithmetic operation or comparison of real numbers is unity. Of course, $\mathbf{c} \geq 1$, and in many cases $\mathbf{c}$ is much larger than unity. The precise definition of $\mathrm{comp}(\epsilon,F)$ can be found, e.g., in Ref. 8. Here we only mention that in our case $\mathrm{comp}(\epsilon,F)$ can be (roughly) defined as the minimal number of integrand evaluations needed to compute an approximation whose error is at most ϵ for all $f \in F$.

It is usually difficult to find $\mathrm{comp}(\epsilon,F)$. That is why we settle for some characteristics of $\mathrm{comp}(\epsilon,F)$. We say that the path integration problem is *tractable* in the worst case setting iff there exist two non-negative numbers K and p such that

$$\mathrm{comp}(\epsilon,F) \leq K \mathbf{c} \epsilon^{-p}, \quad \forall \epsilon \in (0,1). \tag{4}$$

The smallest (or rather infimum of) p for which (4) holds is called the *exponent* of the path integration problem,

$$p(F) = \inf\{p \ : \ \limsup_{\epsilon \to 0^+} \epsilon^p \ \mathrm{comp}(\epsilon,F) < +\infty\}.$$

III. FINITE REGULARITY

In this section, we study tractability of path integration for the class $F = F^r$ of r times continuously Frechet differentiable functions, where r is a non-negative integer,

$$F^r = \{f: X \to \mathbb{R} \ : \ f^{(r)} \ \text{is continuous and} \ \|f^{(k)}(x)\| \leq 1, \quad \forall x \in X, \quad k = 0,1,\ldots,r\}.$$

As we shall see, tractability of path integration depends on the eigenvalues λ_i of the correlation operator C_ν in (1).

Theorem 1: (i) *If $r = 0$ or all the eigenvalues λ_i are positive, i.e., $\lambda_i > 0$, $\forall i \geq 1$, then the path integration problem is intractable.* (ii) *If $r \geq 1$ and only k eigenvalues λ_i are positive, i.e., $\lambda_k > 0$ and $\lambda_{k+1} = 0$, then the path integration problem is tractable with exponent k/r, i.e.,*

$$\mathrm{comp}(\epsilon,F^r) = \Theta(\mathbf{c}\epsilon^{-k/r}).$$

The assumption that all eigenvalues λ_i are positive is natural since, otherwise, the measure μ is concentrated on a finite dimensional subspace of X which contradicts the essence of the path integration problem. Hence, Theorem 1 provides a negative result about tractability of path integration. It indicates that the class F^r of finite smoothness is too large to permit tractability of path integration in the worst case setting. To get tractability in the worst case setting, we need to shrink the class F^r. This can be done in different ways. One of them is to consider a class of entire functions, i.e., functions with infinite smoothness $r = +\infty$, and this is the subject of Sec. IV. Another one will be reported in a forthcoming paper.[31]

For completeness, we also consider the case where only k eigenvalues are positive. Then, as we shall see, the path integration problem becomes a k dimensional weighted integration problem and is tractable with exponent k/r. Note, however, that if k is large relative to r then the exponent is large.

Remark 1 Intractability of path integration in the worst case setting can be broken by switching to the randomized setting. Indeed, for the class F^r, the Monte Carlo algorithm applied to $S_d(f_d)$, as discussed in Introduction, yields an approximation whose expected error is at most ϵ and cost equals $(\mathbf{c}+1)\epsilon^{-2}$. The Monte Carlo algorithm is almost optimal. Indeed, it can be proven that the complexity of the path integration problem for the class F^r in the randomized setting is

$$\mathrm{comp}^{\mathrm{ran}}(\epsilon,F^r) = \Theta(\mathbf{c}\epsilon^{-2}), \quad \forall r \geq 0,$$

assuming that the eigenvalues λ_i of (1) do not go to zero too fast, i.e., $\lambda_i = \Omega(i^{-k})$ for some $k > 1$.

Without any assumption on the eigenvalues λ_i, one can prove that the complexity $\mathrm{comp}^{\mathrm{ran}}(\epsilon,F^r)$ goes to infinity faster than $\epsilon^{-2+\delta}$ for any positive δ.

For the definition of the randomized setting see, e.g., Ref. 8. The proof of the lower bound on the complexity uses results of Refs. 33 and 4 for the finite dimensional case, and the proof of Theorem 1.

Proof of Theorem 1: We first prove (i). Suppose on the contrary that we have tractability, i.e.,

$$\mathrm{comp}(\epsilon,F^r)\leq K\mathbf{c}\epsilon^{-p} \tag{5}$$

for some nonnegative K and p.

For $r=0$ let $d=1$, and for $r\geq 1$ let d be an integer such that $d>rp$. For $D=[0,1]^d$ define the class $C^{r,d}(D)$ of functions $g:\mathbb{R}^d\to\mathbb{R}$ which are r times continuously differentiable, whose support is contained in the set D, and for which $\|g^{(i)}(\mathbf{t})\|\leq 1$ for all $\mathbf{t}\in\mathbb{R}^d$ and $i=0,1,\ldots,r$. Here, the norm $\|g^{(i)}(\mathbf{t})\|$ is defined as in Sec. II with the 2-norm of $\mathbf{t}$, i.e., $\|\mathbf{t}\|^2=\sum_{j=1}^d t_j^2$.

For $g\in C^{r,d}(D)$, $\mathrm{Ry}=[\langle y,\eta_1\rangle,\langle y,\eta_2\rangle,\ldots,\langle y,\eta_d\rangle]$ for $y\in L_2([0,1])$, and $P=R\circ\mathrm{Im}: X\to\mathbb{R}^d$ define

$$f(x)=g(Px),\quad \forall x\in X.$$

It is easy to check that

$$f^{(i)}(x)x_1x_2\cdots x_i=g^{(i)}(Px)(Px_1)^T(Px_2)^T\cdots(Px_i)^T,\quad \forall x_1,x_2,\ldots x_i\in X.$$

This yields

$$|f^{(i)}(x)x_1\cdots x_i|\leq\|Px_1\|\cdots\|Px_i\|\leq\|\mathrm{Im}(x_1)\|\cdots\|\mathrm{Im}(x_i)\|\leq\beta^i\|x_1\|_X\cdots\|x_i\|_X,$$

where $\beta=\|\mathrm{Im}\|$. Hence

$$\|f^{(i)}(x)\|\leq\beta^r,\quad \forall x\in X,\quad \forall i\leq r.$$

This means that $\beta^{-r}f$ belongs to F^r. Since $\eta_i\in\mathrm{Im}(X)$, we have $P(X)=\mathbb{R}^d$, and it is easy to check that

$$S(f)=\int_D g(\mathbf{t})\rho_d(\mathbf{t})d\mathbf{t}, \tag{6}$$

where the weight ρ_d is given by

$$\rho_d(\mathbf{t})=\frac{1}{(2\pi)^{d/2}\sqrt{\lambda_1\lambda_2\cdots\lambda_d}}\exp[-t_1^2/(2\lambda_1)-t_2^2/(2\lambda_2)-\cdots-t_d^2/(2\lambda_d)].$$

Observe that ρ_d is well defined since the λ_i are positive for $1\leq i\leq d$. Indeed, if $r=0$ then $d=1$ and $\lambda_1>0$, and if $r\geq 1$ then all eigenvalues λ_i are positive.

The essence of (6) is that the (ϵ/β^r) complexity of path integration cannot be smaller than the ϵ complexity of d dimensional weighted integration in the class $C^{r,d}(D)$. Since (5) holds, this implies that the latter complexity is also $O(\mathbf{c}\epsilon^{-p})$. We now show that this is not true.

Let $m_n=m_n[C^{r,d}(D)]$ denote the minimal error of algorithms using n function values for the weighted integration problem (6) in the class $C^{r,d}(D)$. It is known, see, e.g., p. 58 of Ref. 8, that

$$m_n=\inf_{\mathbf{t}_1,\mathbf{t}_2,\ldots,\mathbf{t}_n\in D}\ \sup_{g\in C^{r,d}(D),g(\mathbf{t}_i)=0}\int_D g(\mathbf{t})\rho_d(\mathbf{t})d\mathbf{t}.$$

Clearly, the above supremum will not increase if we additionally constrain g by adding $g \geqslant 0$. There exists a positive number $\alpha = \alpha(d, \lambda_i)$ such that $\rho_d(\mathbf{t}) \geqslant \alpha > 0$, $\forall \mathbf{t} \in [0,1]^d$. Hence

$$m_n \geqslant \alpha \inf_{\mathbf{t}_1, \mathbf{t}_2, \ldots, \mathbf{t}_n \in D} \sup_{g \in C^{r,d}(D), g \geqslant 0, g(\mathbf{t}_i) = 0} \int_D g(\mathbf{t}) d\mathbf{t}.$$

The right-hand side is known to be $\Theta(n^{-r/d})$; see Ref. 4. Hence, $m_n = \Omega(n^{-r/d})$.

If $r = 0$, then m_n is bounded uniformly from below in n by a positive number. This means that for small ϵ, the complexity is infinite, and we have intractability of path integration.

If $r \geqslant 1$, then to guarantee $m_n \leqslant \epsilon$ we have to take $n = \Omega(\epsilon^{-d/r})$. This also means that the complexity is $\Omega(\mathbf{c}\epsilon^{-d/r})$. Since $d/r > p$, this is a contradiction, which completes the proof of (i).

We now prove (ii). We will be using the notation and results from the proof of part (i). Since we have only k positive eigenvalues,

$$S(f) = \int_{\mathbb{R}^k} g(\mathbf{t}) \rho_k(t) d\mathbf{t},$$

where

$$g(\mathbf{t}) = f[\mathrm{Im}^{-1}(t_1 \eta_1 + t_2 \eta_2 + \cdots + t_k \eta_k)].$$

As in the proof of (i), we conclude that there exists a positive number $\gamma = \gamma(k)$ such that $\gamma g \in C^{r,k}(\mathbb{R}^k)$.

From (i) we also conclude that

$$\mathrm{comp}(\epsilon, F^r) = \Omega(\mathbf{c}\epsilon^{-k/r}).$$

Thus, we need a matching upper bound. First, we change variables $u_i = t_i / \sqrt{\lambda_i}$ to get

$$S(f) = \int_{\mathbb{R}^k} h(\mathbf{u}) w_k(\mathbf{u}) d\mathbf{u},$$

where $h(\mathbf{u}) = g(\sqrt{\lambda_1} u_1, \ldots, \sqrt{\lambda_k} u_k)$ and

$$w_k(\mathbf{u}) = (2\pi)^{-k/2} \exp(-\|\mathbf{u}\|^2/2), \quad \|\mathbf{u}\|^2 = \sum_{i=1}^{k} u_i^2.$$

There exists a positive number $M = M(k, r, \{\lambda_i\})$ depending on k, r, and the eigenvalues, such that $M^{-1} h \in C^{r,k}(\mathbb{R}^k)$.

Note that our problem can be expressed as

$$S(f) = \int_{\|\mathbf{u}\| \leqslant 2} h(\mathbf{u}) w_k(\mathbf{u}) d\mathbf{u} + \sum_{i=1}^{\infty} \int_{2^i \leqslant \|\mathbf{u}\| \leqslant 2^{i+1}} h(\mathbf{u}) w_k(\mathbf{u}) d\mathbf{u}. \tag{7}$$

Without loss of generality assume that n is a power of two. We will approximate the successive terms in (7), $i = 0, 1, \ldots, -1 + \log_2 n$, using $n/2^{i+1}$ points. We choose these points $\mathbf{t}_{i,j}$ to minimize the error of approximating the function h in the L_2 sense over the domain

$$D_i = \{\mathbf{t} \in \mathbb{R}^k \ : \ \|\mathbf{t}\| \leqslant 2^{i+1}\}.$$

Let $m_j(D_i)$ denote the error of such an approximation when j function values are used. It is easy to check that

$$m_j(D_i) = O[2^{i(r+k/2)} m_j(D_0)], \quad \forall i.$$

Here and below the factors in the O notation may depend on k and r. It is known, see, e.g., Ref. 4, that

$$m_j(D_0) = \Theta(j^{-r/k}).$$

There is a linear algorithm, $A_i(h) = \Sigma_{j=1}^{n/2^i} h(\mathbf{t}_{i,j}) h_{i,j}^*$ for some functions $h_{i,j}^*$, whose error is $m_j(D_0)$. We approximate the ith term of (7) by

$$\int_{D_i \setminus D_{i-1}} A_i(h)(\mathbf{u}) w_k(\mathbf{u}) d\mathbf{u},$$

where

$$D_{-1} = \emptyset.$$

Clearly, its error is bounded by

$$\|h - A_i(h)\|_{L_2(D_i)} \|w_k\|_{L_2(D_i \setminus D_{i-1})}.$$

Observe that

$$\|w_k\|_{L_2(D_i \setminus D_{i-1})} = O[\exp(-2^{2i-1})].$$

Hence, the total error e_n of this approximation is bounded by

$$e_n = O\left(m_{n/2}(D_0) + \sum_{i=1}^{-1+\log_2 n} \exp(-2^{2i-1}) m_{n/2^{i+1}}(D_i) + \int_{\|\mathbf{u}\| \geq n} \exp(-\|\mathbf{u}\|^2/2) d\mathbf{u} \right).$$

Since the last term is $O[\exp(-n)]$ we finally have

$$e_n = O\left[n^{-r/k} \left(1 + \sum_{i=1}^{-1+\log_2 n} \exp(-2^{2i-1}) 2^{i(r+k/2+r/k)} \right) \right].$$

Since the series $\Sigma_{i=1}^{\infty} \exp(-2^{2i-1}) 2^{i(r+k/2+r/k)}$ is convergent, we conclude that $e_n = O(n^{-r/k})$. Setting $n = O(\epsilon^{-k/r})$, and keeping in mind that our algorithm is linear (so that its cost is proportional to $\mathbf{c}n$), we conclude that the complexity is bounded by $O(c\epsilon^{k/r})$. This completes the proof of (ii). □

IV. ENTIRE *F*

In this section, we demonstrate tractability of path integration for a certain class F of entire functions defined on an infinite dimensional space X. We do this assuming additionally that we can compute the derivatives of integrands at zero.

First, we need to analyze the case of entire functions defined on the finite dimensional space $\mathbb{R}^d$, and then we extend the analysis to the space X. In what follows, the spaces of entire functions will depend on a sequence of positive numbers β_k such that

$$\max_k \lambda_k \beta_k < 1 \quad \text{and} \quad \max_k \beta_k < \infty. \tag{8}$$

Without loss of generality, we assume that

$$\lambda_k\beta_k \geqslant \lambda_{k+1}\beta_{k+1}, \quad \forall k.$$

Since λ_k are summable, so are $\lambda_k\beta_k$, and, in particular, they converge to zero. As we shall see, the complexity of the problem depends on how fast they decay. More precisely, it depends on the *sum-exponent* $p_{\lambda\beta}$ of the sequence $\{\lambda_k\beta_k\}_k$ defined as follows:

$$p_{\lambda\beta} = \inf\left\{ p \ : \ \sum_{k=1}^{\infty} (\lambda_k\beta_k)^p < \infty \right\}. \tag{9}$$

Of course, we always have $p_{\lambda\beta} \leqslant 1$.

A. Finite dimensional case

In this subsection, we consider d dimensional integration for a class of entire functions defined on $\mathbb{R}^d$.

Let $\mathbb{N}_+^d$ denote the set of multi-indices $\mathbf{i}=[i_1,i_2,\ldots,i_d]$ with non-negative integers i_k. By $|\mathbf{i}|$ we mean $\Sigma_{k=1}^d i_k$. Consider the Hilbert space H_d of entire functions $f : \mathbb{R}^d \to \mathbb{R}$ with the inner product

$$\langle f,g\rangle_{H_d} = \sum_{\mathbf{i}\in\mathbb{N}_+^d} \frac{f^{(\mathbf{i})}(0)g^{(\mathbf{i})}(0)}{\Pi_{k=I}^d i_k!\beta_k^{i_k}},$$

where

$$f^{(\mathbf{i})}(0) = \frac{\partial^{|\mathbf{i}|} f(0)}{\partial x_1^{i_1}\ldots\partial x_d^{i_d}}.$$

Define the function

$$R_d(x,t) = \exp\left(\sum_{k=1}^{d} x_k t_k \beta_k \right), \quad x,t\in\mathbb{R}^d.$$

Note that

$$R_d^{(\mathbf{i})}(\cdot,t)|_{x=0} = \prod_{k=1}^{d} t_k^{i_k}\beta_k^{i_k},$$

and therefore,

$$\langle f,R_d(\cdot,t)\rangle_{H_d} = \sum_{\mathbf{i}\in\mathbb{N}_+^d} f^{(\mathbf{i})}(0)\prod_{k=1}^{d} \frac{t_k^{i_k}}{i_k!} = f(t).$$

Note that the last series is absolutely convergent, since it is bounded by

$$\left(\sum_{\mathbf{i}\in\mathbb{N}_+^d} \frac{f^{(\mathbf{i})}(0)^2}{\Pi_{k=1}^d i_k!\beta_k^{i_k}} \right)^{1/2} \left(\sum_{\mathbf{i}\in\mathbb{N}_+^d} \prod_{k=1}^{\infty} \frac{t_k^{2i_k}\beta_k^{i_k}}{i_k!} \right)^{1/2} = \|f\|_{H_d} \exp\left(\sum_{k=1}^{d} t_k^2\beta_k/2 \right).$$

This verifies that H_d is a space of entire functions and that R_d is its reproducing kernel. (Basic information on reproducing kernel Hilbert spaces can be found, e.g., in Ref. 34.) Let F_d be the unit ball of H_d,

$$F_d=\{f\in H_d\ :\ \|f\|_{H_d}\leq 1\}.$$

As in the previous section, let S_d be the following linear functional from H_d to $\mathbb{R}$:

$$S_d(f)=\frac{1}{\prod_{k=1}^d\sqrt{2\pi\lambda_k}}\int_{\mathbb{R}^d}\exp\left(-\sum_{k=1}^d t_k^2/(2\lambda_k)\right)f(t)dt.$$

We approximate S_d by algorithms that use $f^{(\mathbf{j})}(0)$ as information about f. For a given finite subset $M\subset\mathbb{N}_+^d$, we compute $f^{(2\mathbf{i})}(0)$ for $\mathbf{i}\in M$ and define the algorithm

$$A_{d,M}(f)=\sum_{\mathbf{i}\in M}f^{(2\mathbf{i})}(0)\prod_{k=1}^d\frac{\lambda_k^{i_k}(2i_k-1)!!}{(2i_k)!}. \tag{10}$$

We prove that $A_{d,M}$ is *optimal* in the class of algorithms that use information $f^{(2\mathbf{i})}(0)$ for $\mathbf{i}\in M$. Here, optimality is understood in the sense of minimizing the worst case error. The worst case error of the algorithm $\phi(f)=\phi[f^{(2\mathbf{i})}(0):\mathbf{i}\in M]$ in the unit ball F_d of H_d is defined as

$$e(\phi)=\sup_{f\in F_d}|S_d(f)-\phi(f)|.$$

Theorem 2. *The algorithm $A_{d,M}$ is optimal and we have*

$$e^2(A_{d,M})=\sum_{\mathbf{i}\notin M}\prod_{k=1}^d\frac{(\lambda_k\beta_k)^{2i_k}((2i_k-1)!!)^2}{(2i_k)!}. \tag{11}$$

For any $\alpha\in(0,2)$,

$$e^2(A_{d,M})\leq C_{d,\alpha}\max_{\mathbf{i}\notin M}\prod_{k=1}^d(\lambda_k\beta_k)^{i_k\alpha} \tag{12}$$

with

$$C_{d,\alpha}=\prod_{k=1}^d(1-(\lambda_k\beta_k)^{2-\alpha})^{-1/2}.$$

Proof: Take an arbitrary algorithm ϕ that uses information $f^{(2\mathbf{i})}(0)$ for $\mathbf{i}\in M$. Due to Smolyak's theorem (see, e.g., p. 76 of Ref. 8), we know that the worst case error is minimized by a linear algorithm. Therefore, we may assume that ϕ is linear, $\phi(f)=\Sigma_{\mathbf{i}\in M}a_{\mathbf{i}}f^{(2\mathbf{i})}(0)$ for some weights $a_{\mathbf{i}}$. Observe that for $a_{\mathbf{i}}=a_{\mathbf{i}}^*$ with $a_{\mathbf{i}}^*=\Pi_{k=1}^d\lambda_k^{i_k}(2i_k-1)!!/(2i_k)!$ we have $\phi=A_{d,M}$.

Since H_d is a reproducing kernel Hilbert space and both S_d and ϕ are continuous linear functionals, the worst case error of ϕ is equal to the average case error of ϕ for a certain space and a certain measure (see, e.g., p. 304 of Ref. 8 and Ref. 35). More precisely, there exists a separable Banach space B_d of functions defined on $\mathbb{R}^d$ such that H_d is a dense subset of B_d. The space B_d is equipped with a zero mean Gaussian measure ν_d whose covariance function is the reproducing kernel R_d,

$$R_d(x,t)=\int_{B_d}f(x)f(t)\nu_d(df).$$

Then

$$e^2(\phi)=\int_{B_d}|S_d(f)-\phi(f)|^2\nu_d(df).$$

Since for every $x=[x_1,\ldots,x_d]\in\mathbb{R}^d$ and every $f\in H_d$,

$$f(x)=\sum_{\mathbf{i}\in\mathbb{N}_+^d} f^{(\mathbf{i})}(0)\prod_{k=1}^{d}\frac{x_k^{i_k}}{i_k!},$$

we have

$$S_d(f)=\sum_{\mathbf{i}\in\mathbb{N}_+^d} f^{(2\mathbf{i})}(0)\prod_{k=1}^{d}\frac{\lambda_k^{i_k}(2i_k-1)!!}{(2i_k)!}.$$

It is easy to check that

$$\int_{B_d} f^{(\mathbf{i})}(0)f^{(\mathbf{j})}(0)\,\nu_d(df)=R_d^{(\mathbf{i},\mathbf{j})}(0,0)=\delta_{\mathbf{i},\mathbf{j}}\prod_{k=1}^{d} i_k!\beta_k^{i_k},$$

where $\delta_{\mathbf{i},\mathbf{j}}$ is the Kronecker delta. From this, we conclude that

$$e^2(\phi)=\sum_{\mathbf{i}\in M}(a_{\mathbf{i}}-a_{\mathbf{i}}^*)^2\prod_{k=1}^{d}(2i_k)!\beta_k^{2i_k}+\sum_{\mathbf{i}\notin M}\prod_{k=1}^{d}\frac{(\lambda_k\beta_k)^{2i_k}[(2i_k-1)!!]^2}{(2i_k)!}.$$

Hence, the worst case error is minimized iff $a_{\mathbf{i}}=a_{\mathbf{i}}^*$. That is, $\phi=A_{d,M}$ and the error of $A_{d,M}$ is given by (11).

We now estimate $e^2(A_{d,M})$ as follows:

$$e^2(A_{d,M})\leq\left(\max_{\mathbf{i}\notin M}\prod_{k=1}^{d}(\lambda_k\beta_k)^{i_k\alpha}\right)\left(\sum_{\mathbf{i}\in\mathbb{N}_+^d}\prod_{k=1}^{d}\frac{(\lambda_k\beta_k)^{i_k(2-\alpha)}((2i_k-1)!!)^2}{(2i_k)!}\right).$$

We now compute the last sum. Note that it has the same form as (11) for $M=\emptyset$ and $\widetilde{\lambda}_k=\lambda_k^{1-\alpha/2}$, $\widetilde{\beta}_k=\beta_k^{1-\alpha/2}$. This corresponds to the square of the error of the zero algorithm for approximating

$$\widetilde{S}_d(f)=\frac{1}{\Pi_{k=1}^{d}\sqrt{2\pi\widetilde{\lambda}_k}}\int_{\mathbb{R}^d} e^{-\Sigma_{k=1}^{d}t_k^2/(2\widetilde{\lambda}_k)}f(t)dt,$$

where the functions f are now from a reproducing kernel Hilbert space with kernel $\widetilde{R}_d(x,t)=\exp(\Sigma_{k=1}^{d}x_kt_k\widetilde{\beta}_k)$. That is, denoting this sum by γ, we have

$$\gamma=\int_{\widetilde{B}_d}|\widetilde{S}_d(f)|^2\widetilde{\nu}_d(df)=\int_{\mathbb{R}^d}\frac{\exp[-\Sigma_{k=1}^{d}x_k^2/(2\widetilde{\lambda}_k)]}{\Pi_{k=1}^{d}\sqrt{2\pi\widetilde{\lambda}_k}}\int_{\mathbb{R}^d}\frac{\exp[-\Sigma_{k=1}^{d}t_k^2/(2\widetilde{\lambda}_k)]}{\Pi_{k=1}^{d}\sqrt{2\pi\widetilde{\lambda}_k}}\widetilde{R}_d(x,t)dt\,dx.$$

It is easy to verify that the right-hand side equals $\Pi_{k=1}^{d}[1-(\lambda_k\beta_k)^{2-\alpha}]^{-1/2}$. This completes the proof. □

We now choose a subset M such that the error of the algorithm $A_{d,M}$ is at most ϵ. For $\alpha\in(0,2-p_{\lambda\beta})$, let

$$M_{d,\alpha}(\epsilon)=\left\{\mathbf{i}\in\mathbb{N}_+^d \ : \ \prod_{k=1}^{d}(\lambda_k\beta_k)^{i_k}>(\epsilon^2/C_{d,\alpha})^{1/\alpha}\right\}. \tag{13}$$

Note that the sequence $\{C_{d,\alpha}\}_d$ is increasing and

$$C_\alpha=\lim_{d\to\infty} C_{d,\alpha}=\prod_{k=1}^{\infty}[1-(\lambda_k\beta_k)^{2-\alpha}]^{-1/2} \tag{14}$$

exists. It is finite since $\alpha<2-p_{\lambda\beta}$ implies that $\Sigma_{k=1}^{\infty}(\lambda_k\beta_k)^{(2-\alpha)}<+\infty$. Denote

$$A_{d,\alpha}(\epsilon)=A_{d,M_{d,\alpha}(\epsilon)}. \tag{15}$$

The next theorem presents the error and cost bounds of the algorithm $A_{d,\alpha}(\epsilon)$.

Theorem 3: *For every d, $\epsilon>0$, and $\alpha\in(0,2-p_{\lambda\beta})$, the algorithm $A_{d,\alpha}(\epsilon)$ has error at most ϵ, and its cost is at most $(\mathbf{c}+2)n_{d,\alpha}(\epsilon)$. Here, $n_{d,\alpha}(\epsilon)$ is the cardinality of the set $M_{d,\alpha}(\epsilon)$ and denotes how many derivative evaluations of f are used, and*

$$n_{d,\alpha}(\epsilon)\leq K_\alpha\epsilon^{-2(2-\alpha)/\alpha}, \tag{16}$$

where

$$K_\alpha=\prod_{i=1}^{\infty}[1-(\lambda_i\beta_i)^{2-\alpha}]^{-1}\sup_{\epsilon\in(0,1)}\epsilon^{2(2-\alpha)/\alpha}\left(2+\frac{\ln C_\alpha/\epsilon^2}{\alpha\ \ln 1/(\lambda_1\beta_1)}\right)<+\infty.$$

Proof: The bound ϵ on the error of the algorithm follows directly from (12) of Theorem 2.

We now prove the bound on $n_{d,\alpha}(\epsilon)$. Note that $\alpha<2-p_{\lambda\beta}$ implies that K_α is finite. Let $p=2(2-\alpha)/\alpha$.

For $d=1$, we have

$$n_{1,\alpha}(\epsilon)\leq 1+\{(\ln C_\alpha/\epsilon^2)/[\alpha\ \ln 1/(\lambda_1\beta_1)]\}\leq K_{1,\alpha}\epsilon^{-p},$$

where

$$K_{1,\alpha}=\sup_{\epsilon\in(0,1)}\epsilon^p\left(2+\frac{\ln C_\alpha/\epsilon^2}{\alpha\ \ln 1/(\lambda_1\beta_1)}\right).$$

Hence (16) holds for $d=1$ since $K_{1,\alpha}\leq K_\alpha$.

By induction, suppose that $n_{d-1,\alpha}(\epsilon)\leq K_{d-1,\alpha}\epsilon^{-p}$. Then,

$$n_{d,\alpha}(\epsilon)\leq\sum_{i=1}^{\infty} n_{d-1,\alpha}[\epsilon/(\lambda_d\beta_d)^{\alpha i/2}]\leq K_{d-1,\alpha}\epsilon^{-p}\sum_{i=0}^{\infty}(\lambda_d\beta_d)^{\alpha ip/2}=K_{d,\alpha}\epsilon^{-p},$$

where

$$\begin{aligned}K_{d,\alpha}=K_{d-1,\alpha}[1-(\lambda_d\beta_d)^{2-\alpha}]^{-1}&=K_{1,\alpha}\prod_{i=1}^{d}[1-(\lambda_i\beta_i)^{2-\alpha}]^{-1}\\&\leq K_{1,\alpha}\prod_{i=1}^{\infty}[1-(\lambda_i\beta_i)^{2-\alpha}]^{-1}=K_\alpha.\end{aligned}$$

This proves (16). The algorithm $A_{d,M}$ is linear and its weights $a_{\mathbf{i}}^*$ can be precomputed. Hence, its cost is equal to $n_{d,\alpha}(\epsilon)$ derivative evaluations, $n_{d,\alpha}(\epsilon)$ multiplications, and $n_{d,\alpha}(\epsilon)-1$ additions. Hence, it is bounded by $(\mathbf{c}+2)n_{d,\alpha}(\epsilon)$, as claimed. This completes the proof. □

Theorem 3 presents an upper bound on the worst case complexity of multivariate integration S_d in the unit ball F_d. Namely

$$\mathrm{comp}(\epsilon)\leqslant(\mathbf{c}+2)K_\alpha\epsilon^{-p^*},$$

where $p^*=2(2-\alpha)/\alpha$. Since α can be arbitrarily close to $\alpha^*=2-p_{\lambda\beta}$, we may have

$$p^*\simeq\frac{2p_{\lambda\beta}}{2-p_{\lambda\beta}}.$$

Since $p_{\lambda\beta}\leqslant 1$, the exponent p^* of the multivariate problem S_d is always bounded by two. Hence, it is no larger than the exponent of $1/\epsilon$ in the cost function of the classical Monte Carlo method. It can be even smaller than 2. For instance, for $\lambda_k\beta_k=\Theta(k^{-r})$ with $r>1$, we have

$$p^*\simeq\frac{2}{2r-1}. \tag{17}$$

Observe that $\lambda_k\beta_k=\Theta(k^{-r})$ holds for $\beta_k\simeq 1$ and for the $(r-2)$-fold Wiener measure μ. For the classical Wiener measure μ, we have $r=2$ and $p^*\simeq 2/3$.

B. Infinite dimensional case

We now consider the infinite dimensional case, $d=+\infty$. To that end, let $\mathbb{N}_+^\infty$ denote the set of infinite multi-indices $\mathbf{i}=[i_1,i_2,\ldots]$ with non-negative integers i_k for which $|\mathbf{i}|=\Sigma_{k=1}^\infty i_k$ is finite. This means that any $\mathbf{i}\in\mathbb{N}_+^\infty$ has almost all coefficients equal zero.

We define the Hilbert space H_∞ of entire functions as a limiting case of spaces H_d. That is, H_∞ is a space of entire functions $f: X\to\mathbb{R}$ with inner product

$$\langle f,g\rangle_{H_\infty}=\sum_{\mathbf{i}\in\mathbb{N}_+^\infty}\frac{(f^{(\mathbf{i})}(0)\Pi_{k=1}^\infty(\mathrm{Im}^{-1}\ \eta_k)^{i_k})(g^{(\mathbf{i})}(0)\Pi_{k=1}^\infty(\mathrm{Im}^{-1}\ \eta_k)^{i_k})}{\Pi_{k=1}^\infty\ i_k!\beta_k^{i_k}},$$

where, as before, η_k are the eigenelements of the covariance operator C_ν.

This is a reproducing kernel Hilbert space whose reproducing kernel is

$$R_\infty(x,t)=\exp\left(\sum_{k=1}^\infty\langle\mathrm{Im}(x),\eta_k\rangle\langle\mathrm{Im}(t),\eta_k\rangle\beta_k\right),\quad x,t\in X.$$

Consider the class F as the unit ball of H_∞, i.e.,

$$F=\{f\in H_\infty\ :\ \|f\|_{H_\infty}\leqslant 1\}.$$

This class is a limiting case of the unit balls F_d in the spaces H_d, and all the results from the previous section apply. More precisely, for a given finite subset M of $\mathbb{N}_+^\infty$, let

$$A_M(f)=\sum_{\mathbf{i}\in M}\left(f^{(2\mathbf{i})}(0)\prod_{k=1}^\infty(\mathrm{Im}^{-1}\ \eta_k)^{2i_k}\right)\prod_{k=1}^\infty\frac{\lambda_k^{i_k}(2i_k-1)!!}{(2i_k)!}. \tag{18}$$

For $\alpha\in(0,2-p_{\lambda\beta})$ and

$$C_\alpha = \prod_{k=1}^{\infty} [1-(\lambda_k \beta_k)^{2-\alpha}]^{-1/2},$$

see (14), let

$$M_\alpha(\epsilon) = \left\{ \mathbf{i} \in \mathbb{N}_+^\infty \ : \ \prod_{k=1}^{\infty} (\lambda_k \beta_k)^{i_k} > (\epsilon^2 / C_\alpha)^{1/\alpha} \right\}. \tag{19}$$

We have the following theorem.

Theorem 4: *(i) The algorithm A_M is optimal in the class of algorithms that use the same information, and its worst case error is given by*

$$e^2(A_M) = \sum_{\mathbf{i} \in \mathbb{N}_+^\infty \setminus M} \prod_{k=1}^{\infty} \frac{(\lambda_k \beta_k)^{2 i_k} [(2 i_k - 1)!!]^2}{(2 i_k)!}.$$

(ii) For every ϵ and $\alpha \in (0, 2-p_{\lambda\beta})$, the algorithm $A_{M_\alpha(\epsilon)}$ has error at most ϵ, and its cost is bounded by

$$(\mathbf{c}+2) K_\alpha \epsilon^{-2(2-\alpha)/\alpha}.$$

(iii) The path integration problem is tractable and its exponent $p(F)$ is bounded by

$$p(F) \leqslant \frac{2 p_{\lambda\beta}}{2 - p_{\lambda\beta}}.$$

For $\lambda_i \beta_i = \Theta(i^{-r})$ with some $r > 1$, we have

$$p(F) = \frac{2 p_{\lambda\beta}}{2 - p_{\lambda\beta}} = \frac{2}{2r-1},$$

if the information is restricted to function and derivative values at zero.

Proof: The proof of (i) and (ii) follows from the results of the previous section. Indeed, given d and $f \in F$, let

$$f_d(\mathbf{t}) = f[\mathrm{Im}^{-1}(t_1 \eta_1 + \cdots + t_d \eta_d)], \quad \text{with } \mathbf{t} = [t_1, \ldots, t_d] \in \mathbb{R}^d.$$

Then $f_d^{(\mathbf{i})}(0) = f^{(|\mathbf{i}|)}(0)(\mathrm{Im}^{-1}\, \eta_1)^{i_1} \cdots (\mathrm{Im}^{-1} \eta_d)^{i_d}$, and $\|f_d\|_{H_d} \leqslant \|f\|_{H_\infty}$. Hence, f_d belongs to the unit ball of the space H_d.

For a given M, let $d_M = \max\{k : i_k \neq 0 \text{ for some } \mathbf{i} \in M\}$. Then, for every $f \in F$, we have

$$A_M(f) = A_{d,M}(f_d), \quad \forall d \geqslant d_M.$$

Since $S(f) = \lim_{d \to \infty} S_d(f_d)$, the first part of Theorem 4 follows from Theorem 2.

Let $n_\alpha(\epsilon)$ be the cardinality of the set $M_\alpha(\epsilon)$. Since $n_{d,\alpha}(\epsilon) \leqslant n_{d+1,\alpha}(\epsilon)$ for every d, and $n_{d,\alpha}(\epsilon) = n_\alpha(\epsilon)$ for $d \geqslant d_{M_\alpha(\epsilon)}$, the second part follows from Theorem 3.

We now prove (iii). Obviously, it is enough to show that $2/(2r-1)$ is a lower bound on $p(F)$ in the class of information restricted to function and derivative values at zero. Consider arbitrary information consisting of n function and derivative values at 0. This corresponds to a subset M of $\mathbb{N}_+^\infty$ having cardinality n. The minimal worst case error is given by $e^2(A_M)$, where the algorithm A_M is given by (18). We have

$$e^2(A_M)=\sum_{\mathbf{i}\in\mathbb{N}_+^\infty}\prod_{k=1}^{\infty}\frac{(\lambda_k\beta_k)^{2i_k}[(2i_k-1)!!]^2}{(2i_k)!}-\sum_{\mathbf{i}\in M}\prod_{k=1}^{\infty}\frac{(\lambda_k\beta_k)^{2i_k}[(2i_k-1)!!]^2}{(2i_k)!}.$$

Observe that the first sum is greater than $1+\Sigma_{k=1}^{\infty}(\lambda_k\beta_k)^2/2$. Since the second sum has only n elements, we have

$$e^2(A_M)\geq\frac{1}{2}\sum_{k=n}^{\infty}(\lambda_k\beta_k)^2=\Theta(n^{-(2r-1)}).$$

To guarantee that the error is at most ϵ we have to take $n=\Omega(\epsilon^{-2/(2r-1)})$. This completes the proof of Theorem 4. □

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Addendum: Debye potentials and Hamiltonians for magnetic field line flow [J. Math. Phys. 36, 3413–3418 (1995)]

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After the publication of this paper it was brought to the author's attention that its content overlaps a part of an earlier article by I. Mezić and S. Wiggins,[1] which contains many other results on the geometry of three-dimensional, divergence-free vector fields.

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Why the Thirring model cannot fulfill canonical anticommutation relations

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Perturbative and constructive arguments show that the Gross–Neveu model with $N \geqslant 2$ flavor degrees is asymptotically free. Assuming canonical anticommutation relations (CAR), which are quite plausible, and some technicalities, we show for the Thirring model, i.e., the case of $N=1$ flavor, that the fields are necessarily free. This explains from an axiomatic point of view the different behavior depending on the number of flavors. © *1996 American Institute of Physics.* [S0022-2488(96)01504-5]

I. INTRODUCTION AND RESULTS

The Thirring[1] model is a soluble relativistic field theory of interacting Fermi fields in $1+1$ space time dimensions. The Gross–Neveu[2] model is a generalization thereof to $N \geqslant 2$ flavor degrees of freedom, i.e., there are N complex spinor fields ψ_i and the bare interaction is given by

$$-g\left(\sum_{i=1}^{N} \overline{\psi_i}\gamma^{\mu}\psi_i\right)\left(\sum_{j=1}^{N} \overline{\psi_j}\gamma_{\mu}\psi_j\right). \tag{1.1}$$

From perturbation theory[3] and from the constructive approach[4,5] it is known that for $N \geqslant 2$ the massive Gross–Neveu model is asymptotically free. It may even be that the fields fulfill canonical anticommutation relations (CAR). This is quite satisfactory because in an earlier paper[6] we have shown that in $1+1$ dimensions only 4-Fermi interaction may be compatible with CAR. On the other hand, all explicitely known solutions of the massless Thirring model[7] (i.e., $N=1$) have noncanonical field dimensions except for the noninteracting case. To shed some light on this strikingly different behavior depending on the number N of flavors we shall use an axiomatic approach. Assuming CAR, irreducibility of the fields, and some technicalities we shall show that for $N=1$ free fields are the only solutions.

Let us outline how the paper will be organized:

At the end of this section we shall give the precise assumptions, state our results, and make some comments. In Sec. II we derive estimates on l-fold commutators based on L_2-bounds for the fields inherent in CAR. In Sec. III we use these estimates to characterize the structure of multiple commutators, where also first and second time derivatives are involved. The methods used in these two sections are closely related to those used by Powers[8] to prove his famous ICAR-theorem. In Sec. IV we derive a second order field equation. Using the Jost–Lehmann–Dyson representation we shall show that free fields are the only solutions. This closes the proof of our theorem. Finally, in Appendices A and B we give some mathematical background which in our opinion is necessary for a complete and thorough treatment of the problem.

General assumptions: Within the Wightman framework of quantum field theory we consider a complex Fermi field $\psi=(\psi_1,...,\psi_{2N})$ with $2N$ components and its adjoint field $\psi^{\dagger}=(\psi_1^{\dagger},\ldots,\psi_{2N}^{\dagger})$ in $1+1$ space-time dimensions. For convenience of notation we put $\psi_{2N+1}:=\psi_1^{\dagger},\ldots,\psi_{4N}:=\psi_{2N}^{\dagger}$.

We assume

(i) canonical anticommutation relations (CAR)

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$$\{\psi_k(t,x),\psi_l(t,y)\}=\delta_{k+2N,l}\delta(y-x). \tag{1.2}$$

(ii) Irreducibility of the smeared time zero fields $\psi_k(0,f)$ with $f\in L_2(\mathbf{R})$ and $k=1,\ldots,4N$, i.e., the only bounded operators commuting with all $\psi_k(f)$ are c-numbers.

(iii) Technical assumption: (a) On the dense domain $\mathscr{D}_1=\{\mathscr{P}(\psi(0,f))\Omega, f\in\mathscr{S}(\mathbf{R})\}$ (polynomials in the smeared time zero fields acting on the vacuum) there exist the operators $\dot{\psi}_k(0,f)$. (b) The following limits shall exist in the strong sense on $\mathscr{D}_1$

$$\lim_{t\to 0}\frac{1}{t}[\psi(t,f)-\psi(0,f)]=\dot{\psi}(0,f) \tag{1.3}$$

for all $f\in\mathscr{S}(\mathbf{R})$.

Remark: Concerning the domain $\mathscr{D}_1$ these technical assumptions can be weakened, but we cannot assume $\dot{\psi}(t,f)$ to be a *bounded* operator, because this implies immediately that ψ is a free field (see Lemma 5).

Main theorem: Under the above general assumptions with $N=1$ and the additional technical assumption (iii) (c) On the domain $\mathscr{D}_1$ there exist the operators $\ddot{\psi}_k(0,f)$ for all $f\in\mathscr{S}(\mathbf{R})$. (d) The following limits shall exist in the strong sense on $\mathscr{D}_1$

$$\lim_{t\to 0}\frac{1}{t^2}[\psi(t,f)-2\psi(0,f)+\psi(-t,f)]=\ddot{\psi}(0,f) \tag{1.4}$$

for all $f\in\mathscr{S}(\mathbf{R})$.

We shall show that ψ is necessarily a free field.

Remark: Similar to CAR the technical assumptions (iii) impose restrictions on the high energy behavior of the theory. Free Dirac fields do fulfill all these assumptions of course.

Crucial for this proof is the fact that there are at most four independent fields available! This result demonstrates that $N=1$, i.e., just one flavor degree of freedom, is a very special case. Nontrivial solutions of the Thirring model (regardless of mass) will always behave in a noncanonical way and never fulfill CAR. Neither the special form of the bare interaction nor Lorentz covariance do play any role.

II. ESTIMATES OF *l*-FOLD COMMUTATORS

Let $C[\psi_0(t,f_0),\psi_1(f_1),\ldots,\psi_l(f_l)]$ denote an l-fold commutator, i.e.,

$$C[\psi_0(t,f_0),\ldots,\psi_l(f_l)]=\begin{cases}\{[\ldots[\{\psi_0(t,f_0),\psi_1(f_1)\}\psi_2(f_2)]\cdots\psi_l(f_l)\}, & l \text{ odd},\\ [\{\ldots[\{\psi_0(t,f_0),\psi_1(f_1)\}\psi_2(f_2)]\cdots\psi_l(f_l)], & l \text{ even},\end{cases} \tag{2.1}$$

where the fields $\psi_1,\ldots,\psi_1$ are fields at time zero (whenever we write ψ without a time argument we mean ψ at $t=0$). All test functions $f_0,\ldots,f_l$ are elements of $\mathscr{S}(\mathbf{R})$ and in addition f_0 shall have compact support contained in an interval of length L.

Lemma 2.1: In the limit $t\to 0$ we have the estimate

$$\|C[\psi_0(t,f_0),\ldots,\psi_l(f_l)]\|\propto|t|^{(l-1)/2}. \tag{2.2}$$

Remark: To prove this lemma only CAR and locality are needed. So this lemma and its corollaries are true for an arbitrary number of independent Fermi fields too.

Corollary 2.2: If two of the Fermi fields $\psi_1,\ldots,\psi_l$ are equal then the estimate is improved by a factor $|t|$, i.e.,

$$\|C[\psi_0(t,f_0),\ldots,\psi_l(f_l)]\|\propto|t|^{(l+1)/2}. \tag{2.3}$$

Corollary 2.3: If we replace the distribution $C[\psi_0(t,x_0),\ldots,\psi_l(x_l)]$ by $C[\psi_0(t,x_0),\ldots,\psi_l(x_l)]\Pi_{m=1}^{M}(x_{k_m}-x_{l_m})$ with $k_m,l_m\in\{0,1,\ldots,l\}$ then the estimate is improved by a factor $|t|^M$, i.e.,

$$\left\| \int dx\ f(x_0)\cdots f(x_l)C[\psi_0(t,x_0),\ldots,\psi_l(x_l)]\prod_{m=1}^{M}(x_{k_m}-x_{l_m}) \right\| \propto |t|^{(l-1+2M)/2}. \tag{2.4}$$

Corollary 2.4: If we interchange two of the test functions $f_1,\ldots,f_l$ then we get for the difference of the two corresponding multiple commutators the estimate

$$\|C[\psi_0(t,f_0),\ldots,\psi_k(f_k)\cdots\psi_m(f_m)\cdots]-C[\psi_0(t,f_0),\ldots,\psi_k(f_m)\cdots\psi_m(f_k)\cdots]\|\propto|t|^{(l+1)/2}. \tag{2.5}$$

Proof: (i) From CAR it follows

$$\|\psi(t,f\ )\|\leqslant\|f\|_2 \quad (L_2-\text{norm of } f\ ). \tag{2.6}$$

With the help of a partition of unity (in L_2-sense) consisting of characteristic functions χ_m^t of length $|t|$ and centered around $m|t|$ we have

$$f=\sum_m f\chi_m^t. \tag{2.7}$$

Because of locality and because of the Jacobi identities

$$[A\{B,C\}]+[B\{C,A\}]+[C\{A,B\}]=0, \tag{2.8}$$

$$\{A[B,C]\}+\{B[A,C]\}+[C\{A,B\}]=0, \tag{2.9}$$

we get

$$C[\psi_0(t,f_0),\ldots,\psi_l(f_l)]=\sum_{\substack{m_0,m_1,\ldots,m_l\\ |m_k-m_0|\leqslant 1}} C[\psi_0(t,f_0\chi_{m_0}^t),\ldots,\psi_l(f_l\chi_{m_l}^t)]. \tag{2.10}$$

The sum over m_0 has at most $(L/|t|)+2$ terms because supp f_0 is contained in an interval of length L. Now

$$\|\psi(t,f\chi_m^t)\|=\|\psi(0,f\chi_m^t)\|=\|f\chi_m^t\|_2\leqslant\|f\|_\infty|t|^{1/2} \tag{2.11}$$

and therefore

$$\|C[\psi_0(t,f_0),\ldots,\psi_l(f_l)]\|\leqslant\left(\frac{L}{|t|}+2\right)2^l3^l\|f_0\|_\infty\cdots\|f_l\|_\infty|t|^{(l+1)/2}\propto|t|^{(l-1)/2}. \tag{2.12}$$

This proves Lemma 2.1.

Remark: For even l we can improve Lemma 2.1 by a factor $|t|^{1/2}$ using the same methods but by estimating $\|\{C^\dagger,C\}\|$ instead of $\|C\|$!

(ii) For our convenience we consider only the case l odd. Assume that ψ_{k_1} and ψ_{k_2} are the same fields. We can use the Jacobi identities to rearrange the fields in the multiple commutator under consideration such that ψ_{k_1} and ψ_{k_2} are at the last two positions. We have to estimate $\{[C_{l-2},\psi(f_{l-1}]\psi(f_l)\}$ where C_{l-2} is some $l-2$-fold commutator. Now ψ is a Fermi field and therefore the Jacobi identity implies

$$\{[C_{l-2},\psi(f_{l-1})]\psi(f_l)\}=\tfrac{1}{2}(\{[C_{l-2},\psi(f_{l-1})]\psi(f_l)\}-\{[C_{l-2},\psi(f_l)]\psi(f_{l-1})\})$$
$$=\frac{1}{2}\sum_{\substack{m_0,m_1,\ldots,m_l\\ |m_k-m_0|\leqslant 1}}(\{[C_{l-2},\psi(f_{l-1}\chi^t_{m_{l-1}})]\psi(f_l\chi^t_{m_l})\}$$
$$-\{[C_{l-2},\psi(f_l\chi^t_{m_{l-1}})]\psi(f_{l-1}\chi^t_{m_l})\}), \tag{2.13}$$

where in the last line C_{l-2} is a short hand notation of $C[\psi_0(t,f_0\chi^t_{m_0}),\ldots,\psi_{l-2}(f_{l-2}\chi^t_{m_{l-2}})]$. Now

$$(f\chi^t_m)(x)=f(x^t_m)\chi^t_m(x)+(f(x)-f(x^t_m))\chi^t_m(x), \tag{2.14}$$

where the point x^t_m is defined to be the center of the characteristic function χ^t_m and by linearity we get

$$\psi(f\chi^t_m)=f(x^t_m)\psi(\chi^t_m)+\psi((f-f(x^t_m))\chi^t_m). \tag{2.15}$$

But

$$\|\psi((f-f(x^t_m))\chi^t_m)\|\leqslant\left[\int_{-t/2}^{t/2}|f(x^t_m+x)-f(x^t_m)|^2dx\right]^{1/2}$$
$$\leqslant\|f'\|_\infty\left[\int_{-t/2}^{t/2}x^2\,dx\right]^{1/2}$$
$$=\|f'\|_\infty(\tfrac{1}{12})^{1/2}|t|^{3/2}, \tag{2.16}$$

whereas $\|\psi(f(x^t_m)\chi^t_m)\|\leqslant\|f\|_\infty|t|^{1/2}$. So to prove Corollary 2.2 we have to control only products of terms like $f(x^t_m)\psi(\chi^t_m)$. All other contributions behave already like $|t|(l+1)/2$.

$$\{[C_{l-2},\psi(f_{l-1}]\psi(f_l)\}=\sum_{\substack{m_0,m_1,\ldots,m_l\\ |m_k-m_0|\leqslant 1}}\{[C_{l-2},\psi(\chi^t_{m_{l-1}}]\psi(\chi^t_{m_l})\}\,\frac{1}{2}\,(f_{l-1}(x^t_{m_{l-1}})f_l(x^t_{m_l})$$
$$-f_l(x^t_{m_{l-1}})f_{l-1}(x^t_{m_l}))+O(|t|^{(l+1)/2}). \tag{2.17}$$

The distance between the points $x^t_{m_l}$ and $x^t_{m_{l-1}}$ is less or equal to $3|t|$ because the indices m_l and m_{l-1} differ at most by 2. This implies the bound

$$|f_{l-1}(x^t_{m_{l-1}})f_l(x^t_{m_l})-f_l(x^t_{m_{l-1}})f_{l-1}(x^t_{m_l}|$$
$$\leqslant|f_{l-1}(x^t_{m_{l-1}})||f_l(x^t_{m_l})-f_l(x^t_{m_{l-1}})|+|f_l(x^t_{m_l})||f_{l-1}(x^t_{m_{l-1}})-f_{l-1}(x^t_{m_l})|$$
$$\leqslant 3|t|[\|f_{l-1}\|_\infty\|f'_l\|_\infty+\|f_l\|_\infty\|f'_{l-1}\|_\infty]. \tag{2.18}$$

This additional factor $|t|$ in front proves Corollary 2.2.

(iii) Corollary 2.3 is obvious because by locality we may assume without loss of generality

$$|x_{k_m}-x_{l_m}|\leqslant 3|t|. \tag{2.19}$$

(iv) The proof of Corollary 2.4 uses the same ideas as are used in the proof of corollary 2.2. As in (ii) we consider only the case l odd and we use the Jacobi identities to rearrange the fields such that ψ_k and ψ_m are at the last two positions. We have to estimate

$$\|\{[C_{l-2},\psi_{l-1}(f_{l-1})]\psi_l(f_l)\}-\{[C_{l-2},\psi_{l-1}(f_l)]\psi_l(f_{l-1})\}\|. \tag{2.20}$$

Except for a factor of 2 this equals the right hand side in the first line of Eq. (2.13) with the only difference that the Fermi fields in the positions $l-1$ and l are not necessarily the same but this does not hamper the following argumentation.

III. MULTIPLE COMMUTATORS INVOLVING $\dot{\psi}$ RESP. $\ddot{\psi}$

Now we have the technical tools to get some structural results on multiple commutators at time 0 but involving $\dot{\psi}$ and $\ddot{\psi}$.

Theorem 3:

(1) Under the above assumptions we have

$$\{[\{\dot{\psi}_{k_0}(x_0),\psi_{k_1}(x_1)\}\psi_{k_2}(x_2)]\psi_{k_3}(x_3)\}=\lambda_{k_0k_1k_2k_3}\prod_{i=1}^{3}\delta(x_i-x_0), \tag{3.1}$$

with $\lambda_{k_0k_1k_2k_3}\in\mathbf{C}$ bounded by $24\sqrt{3}$ and $\lambda_{k_0k_1k_2k_3}$ antisymmetric under the exchange of two neighboring indices k_0,k_1,k_2,k_3.

(2) If in addition $\ddot{\psi}_{k_0}(f)$ exists then

$$\{[\{\ddot{\psi}_{k_0}(x_0),\psi_{k_1}(x_1)\}\psi_{k_2}(x_2)]\cdots\psi_{k_5}(x_5)\}=\lambda_{k_0;k_1\cdots k_5}\prod_{i=1}^{5}\delta(x_i-x_0), \tag{3.2}$$

with $\lambda_{k_0;k_1\cdots k_5}$ bounded and antisymmetric with respect to $k_1,\ldots,k_5$.

(3) If furthermore the model is built up from just four independent Fermi fields $\psi_1,\psi_2,\psi_3=\psi_1^\dagger,\psi_4=\psi_2^\dagger$ then

$$\{[\{\ddot{\psi}_{k_0}(x_0),\psi_{k_1}(x_1)\}\psi_{k_2}(x_2)]\psi_{k_3}(x_3)\}=[A_{k_0;k_1k_2k_3}+B_{k_0;k_1k_2k_3}\cdot\partial_0]\prod_{i=1}^{3}\delta(x_i-x_0) \tag{3.3}$$

with A and B antisymmetric w.r.t. k_1,k_2,k_3.

Proof: (i) Statement (1) has already been proven in Ref. 6 and for statement (2) we use the same line of argumentation. To keep the paper self-contained let me sketch the proof:

From Lemma 2.1 it follows that

$$\lim_{t\to0}\left\|\left[\left\{\left[\left\{\frac{\psi_{k_0}(t,f_0)-\psi_{k_0}(f_0)}{t},\psi_{k_1}(f_1)\right\}\psi_{k_2}(f_2)\right]\psi_{k_3}(f_3)\right\}\psi_{k_4}(f_4)\right]\right\|=0, \tag{3.4}$$

because for finite t it behaves $\propto(1/|t|)|t|^{3/2}$ and furthermore

$$\lim_{t\to0}\left\|\left\{\left[\left\{\frac{\psi_{k_0}(t,f_0)-\psi_{k_0}(f_0)}{t},\psi_{k_1}(f_1)\right\}\psi_{k_2}(f_2)\right]\psi_{k_3}(f_3)\right\}\right\|<\infty. \tag{3.5}$$

By irreducibility of the time zero fields we get

$$\{[\{\dot{\psi}_{k_0}(f_0),\psi_{k_1}(f_1)\}\psi_{k_2}(f_2)]\psi_{k_3}(f_3)\}=(\Omega,\{[\{\dot{\psi}_{k_0}(f_0),\psi_{k_1}(f_1)\}\psi_{k_2}(f_2)]\psi_{k_3}(f_3)\}\Omega). \tag{3.6}$$

By locality it is obvious that $\{[\{\dot{\psi}_{k_0}(x_0),\psi_{k_1}(x_1)\}\psi_{k_2}(x_2)]\psi_{k_3}(x_3)\}$ has its support on the manifold $x_0=x_1=x_2=x_3$ only and from Corollary 2.3 we conclude that

$$\{[\{\dot{\psi}_{k_0}(x_0),\psi_{k_1}(x_1)\}\psi_{k_2}(x_2)]\psi_{k_3}(x_3)\}(x_{k_j}-x_{k_i})\equiv 0. \tag{3.7}$$

This gives immediately

$$\{[\{\dot{\psi}_{k_0}(x_0),\psi_{k_1}(x_1)\}\psi_{k_2}(x_2)]\psi_{k_3}(x_3)\}=\lambda\,\delta(x_1-x_0)\,\delta(x_2-x_0)\,\delta(x_3-x_0). \tag{3.8}$$

If we want to interchange two neighboring fields we have to use either the Jacobi identities (2.8/9) or the relation

$$\{\dot{\psi}_k(x_0),\psi_l(x_1)\}+\{\psi_k(x_0),\dot{\psi}_l(x_1)\}=0, \tag{3.9}$$

which follows from CAR via differentiation with respect to time. This proves statement (1) and also—by small modifications—statement (2).

(ii) To prove statement (3) we start from (2) and we observe that at least two of the fields $\psi_{k_1},\ldots,\psi_{k_5}$ must be equal because there are only four different fields by assumption. Under these circumstances it follows from Corollary 2.2 that

$$\{[\{[\{\ddot{\psi}_{k_0}(f_0),\psi_{k_1}(f_1)\}\psi_{k_2}(f_2)]\cdots\psi_{k_5}(f_5)\}\equiv 0 \tag{3.10}$$

for all possible fields ψ_{k_5} and all test functions f_5. Furthermore

$$C_4:=[\{[\{\ddot{\psi}_{k_0}(f_0),\psi_{k_1}(f_1)\}\cdots\psi_{k_4}(f_4)] \tag{3.11}$$

is a bounded operator for any choice of test functions (this can be seen by estimating $\{C_4^\dagger,C_4\}$ using the methods of Lemma 2.1). Because all odd n-point functions vanish, there exists a unitary and Hermitean operator U_I (see Ref. 9) such that

$$U_I\Omega=\Omega,\quad U_I\psi_k(t,f\,)U_I^{-1}=-\psi_k(t,f\,). \tag{3.12}$$

With the help of U_I we can reformulate (3.10) as follows

$$[U_IC_4,\psi_{k_5}(f_5)]=U_I\{C_4,\psi_{k_5}(f_5)\}=0 \tag{3.13}$$

and by irreducibility we conclude

$$U_IC_4=(\Omega,U_IC_4\Omega)=(\Omega,C_4\Omega)=0 \tag{3.14}$$

because C_4 is an odd monomial in the Fermi fields. But U_I is unitary and therefore

$$\underbrace{C_4=[\{[\{\ddot{\psi}_{k_0}(f_0),\psi_{k_1}(f_1)\}\psi_{k_2}(f_2)]\psi_{k_3}(f_3)\}\psi_{k_4}(f_4)]}_{C_3:=}\equiv 0. \tag{3.15}$$

In contrast to C_4 the operator C_3 is not *a priori* a bounded operator, so it is not allowed to conclude naively from irreducibility that C_3 is a c-number too. We have to proceed more carefully.

First of all C_3 can be uniquely extended to a closed operator $\overline{C_3}$, because the adjoint operator $C_3^\dagger$ is densely defined. From (3.15) it follows that C_3 commutes with all $\psi_k(f)$ for $f \in \mathscr{S}(\mathbf{R})$. Due to the facts that

(i) $\mathscr{S}(\mathbf{R})$ is dense in $L_2(\mathbf{R})$,
(ii) $\underline{\psi_k}(f)$ are bounded by $\|f\|_2$, and
(iii) C_3 is a closed operator

it follows that $\overline{C_3}$ commutes with all $\psi_k(f)$ for $f \in L_2(\mathbf{R})$. Since the fields act irreducibly on the Hilbert space $\mathscr{H}$, it follows from the generalized Schur lemma that C_3 is a c-number (see Appendix B for details). Therefore

$$\{[\{\ddot{\psi}_{k_0}(f_0), \psi_{k_1}(f_1)\}\psi_{k_2}(f_2)]\psi_{k_3}(f_3)\} = (\Omega, \{[\{\ddot{\psi}_{k_0}(f_0), \psi_{k_1}(f_1)\}\psi_{k_2}(f_2)]\psi_{k_3}(f_3)\}\Omega). \tag{3.16}$$

From Corollary 2.3 with $M=2$ we see

$$\{[\{\ddot{\psi}_{k_0}(x_0), \psi_{k_1}(x_1)\}\psi_{k_2}(x_2)]\psi_{k_3}(x_3)\}(x_{l_1}-x_{m_1})(x_{l_2}-x_{m_2}) \equiv 0. \tag{3.17}$$

So we end up with the representation

$$\{[\{\ddot{\psi}_{k_0}(x_0), \psi_{k_1}(x_1)\}\psi_{k_2}(x_2)]\psi_{k_3}(x_3)\} = (A - B_1\partial_1 - B_2\partial_2 - B_3\partial_3)_{k_0;k_1k_2k_3} \prod_{i=1}^{3} \delta(x_i - x_0), \tag{3.18}$$

with 4×4 matrices A, B_i.

Finally we have to show $B_1 = B_2 = B_3 =: B$. If so, we can write

$$(A - B_1\partial_1 - B_2\partial_2 - B_3\partial_3)\prod_{i=1}^{3} \delta(x_i - x_0) = (A + B\partial_0)\prod_{i=1}^{3} \delta(x_i - x_0). \tag{3.19}$$

To prove $B_1 = B_2 = B_3 =: B$ we combine Corollary 2.4 with Corollary 2.3. As a result we get

$$\begin{aligned}\int_{\mathbf{R}^4} &\{[\{\ddot{\psi}_{k_0}(x_0), \psi_{k_1}(x_1)\}\psi_{k_2}(x_2)]\psi_{k_3}(x_3)\}(x_l - x_m)\cdot f_0(x_0)f_1(x_1)[f_2(x_2)f_3(x_3) \\ &- f_3(x_2)f_2(x_3)]dx_0\, dx_1\, dx_2\, dx_3 = 0,\end{aligned} \tag{3.20}$$

and consequently we get for the difference

$$\begin{aligned}\Delta :=& \{[\{\ddot{\psi}_{k_0}(f_0), \psi_{k_1}(f_1)\}\psi_{k_2}(f_2)]\psi_{k_3}(f_3)\} - \{[\{\ddot{\psi}_{k_0}(f_0), \psi_{k_1}(f_1)\}\psi_{k_2}(f_3)]\psi_{k_3}(f_2)\} \\ &= \delta \int_{\mathbf{R}} (f_0 f_1 f_2 f_3)(x)dx, \quad \text{for some } \delta.\end{aligned} \tag{3.21}$$

On the other hand a direct calculation of Δ using relation (3.18) gives

$$\Delta = (B_3 - B_2)\left\{ \int_{\mathbf{R}} (f_0 f_1 f_2' f_3)(x)dx - \int_{\mathbf{R}} (f_0 f_1 f_2 f_3')(x)dx \right\}, \tag{3.22}$$

for all $f_k \in \mathscr{S}(\mathbf{R})$. This can only be true if $B_2 = B_3$ and $\delta = 0$. In a similar way we show $B_1 = B_2$.

From the Jacobi identities we get the antisymmetry with respect to k_1, k_2, k_3 of the coefficients $A_{k_0;k_1k_2k_3}$ and $B_{k_0;k_1k_2k_3}$ under the exchange of two neighboring indices.

IV. A FIELD EQUATION FOR ψ

Theorem 4: Under the above assumptions the field $\underline{\psi}$ with the four components $\psi_1,...,\psi_4$ fulfills the second order differential equation

$$\ddot{\underline{\psi}}(t,x)-[A^{(0)}+A^{(1)}\partial_x]\dot{\underline{\psi}}(t,x)-[B^{(0)}+B^{(1)}\partial_x+B^{(2)}\partial_x^2]\underline{\psi}(t,x)=0, \tag{4.1}$$

with constant 4×4 matrices $A^{(i)}$ and $B^{(j)}$.

Proof: It suffices to prove (4.1) at $t=0$ because time translations are implemented by unitary operators.

(i) The starting point is the representation formulas (3.3) resp. (3.1) for the three-fold commutators

$$\{[\{\ddot{\psi}_{k_0}(x),\psi_{k_1}(x_1)\}\psi_{k_2}(x_2)]\psi_{k_3}(x_3)\}=[A_{k_0;k_1k_2k_3}+B_{k_0;k_1k_2k_3}\cdot\partial_x]\prod_{i=1}^{3}\delta(x_i-x), \tag{4.2}$$

respectively,

$$\{[\{\dot{\psi}_{k_0}(x),\psi_{k_1}(x_1)\}\psi_{k_2}(x_2)]\psi_{k_3}(x_3)\}=\lambda\cdot\epsilon_{k_0k_1k_2k_3}\prod_{i=1}^{3}\delta(x_i-x). \tag{4.3}$$

We assume $\lambda\neq0$, because otherwise $\underline{\psi}$ is a free field from the very beginning as has been shown in Ref. 6.

For fixed index k_0 it should be possible to subtract a suitable linear combination of $\dot{\psi}_l$ and $\partial_x\dot{\psi}_l$, $l=1,2,3,4$ from $\ddot{\psi}_{k_0}$ such that

$$\left\{\left[\left\{\ddot{\psi}_{k_0}(x)-\sum_{l=1}^{4}(A^{(0)}_{k_0l}\dot{\psi}_l(x)+A^{(1)}_{k_0l}\partial_x\dot{\psi}_l(x)),\psi_{k_1}(x_1)\right\}\psi_{k_2}(x_2)\right]\psi_{k_3}(x_3)\right\}\equiv0 \tag{4.4}$$

for all indices k_1, k_2, and k_3. The coefficients $A^{(1)}_{k_0l}$ and $A^{(2)}_{k_0l}$ are determined by the equations

$$A_{k_0;k_1k_2k_3}=\lambda\sum_{l=1}^{4}A^{(0)}_{k_0l}\cdot\epsilon_{lk_1k_2k_3},\quad B_{k_0;k_1k_2k_3}=\lambda\sum_{l=1}^{4}A^{(1)}_{k_0l}\cdot\epsilon_{lk_1k_2k_3}. \tag{4.5}$$

If two of the three indices k_1, k_2, and k_3 agree then $A_{k_0;k_1k_2k_3}=0=B_{k_0;k_1k_2k_3}$. Therefore there are only four different sets of indices such that $A_{k_0;k_1k_2k_3}$ and $B_{k_0;k_1k_2k_3}$ do not vanish identically, namely {1,2,3}, {2,3,4}, {1,3,4,}, {1,2,4,}.

As a result we get (remember $\epsilon_{1234}=1$)

$$A^{(0)}_{k_01}=\frac{1}{\lambda}A_{k_0;234},\quad A^{(0)}_{k_02}=-\frac{1}{\lambda}A_{k_0;134},\quad A^{(0)}_{k_03}=\frac{1}{\lambda}A_{k_0;124},\quad A^{(0)}_{k_04}=-\frac{1}{\lambda}A_{k_0;123} \tag{4.6}$$

and similar expressions for $A^{(1)}_{k_0l}$.

(ii) Now we want to apply irreducibility to Eq. (4.4) smeared with test functions

$$\left\{\left[\left\{\ddot{\psi}_{k_0}(f)-\sum_{l=1}^{4}(A^{(0)}_{k_0l}\dot{\psi}_l(f)+A^{(1)}_{k_0l}(\partial_x\dot{\psi}_l)(f)),\psi_{k_1}(f_1)\right\}\psi_{k_2}(f_2)\right]\psi_{k_3}(f_3)\right\}\equiv0. \tag{4.7}$$

The operator $[\{\ddot{\psi}_{k_0}(f) - \Sigma_{l=1}^{4}(A_{k_0 l}^{(0)}\dot{\psi}_l(f) + A_{k_0 l}^{(1)}(\partial_x\dot{\psi}_l)(f)), \psi_{k_1}(f_1)\}\psi_{k_2}(f_2)]$ is unbounded, it contains the operator C_3 of Eq. (3.15), but we can proceed as we did in Sec. III with C_3 and conclude that

$$\left[\left\{\ddot{\psi}_{k_0}(f) - \sum_{l=1}^{4}(A_{k_0 l}^{(0)}\dot{\psi}_l(f) + A_{k_0 l}^{(1)}(\partial_x\dot{\psi}_l)(f)), \psi_{k_1}(f_1)\right\}\psi_{k_2}(f_2)\right]$$
$$= \left(\Omega, \left[\left\{\ddot{\psi}_{k_0}(f) - \sum_{l=1}^{4}(A_{k_0 l}^{(0)}\dot{\psi}_l(f) + A_{k_0 l}^{(1)}(\partial_x\dot{\psi}_l)(f)), \psi_{k_1}(f_1)\right\}\psi_{k_2}(f_2)\right]\Omega\right) = 0 \tag{4.8}$$

because the vacuum expectation value of three Fermi fields vanishes.

Following the same line of argumentation we can even go a step further and use irreducibility again to obtain

$$\left\{\ddot{\psi}_{k_0}(f) - \sum_{l=1}^{4}(A_{k_0 l}^{(0)}\dot{\psi}_l(f) + A_{k_0 l}^{(1)}(\partial_x\dot{\psi}_l)(f)), \psi_{k_1}(f_1)\right\}$$
$$= \left(\Omega, \left\{\ddot{\psi}_{k_0}(f) - \sum_{l=1}^{4}(A_{k_0 l}^{(0)}\dot{\psi}_l(f) + A_{k_0 l}^{(1)}(\partial_x\dot{\psi}_l)(f)), \psi_{k_1}(f_1)\right\}\Omega\right). \tag{4.9}$$

(iii) We want to determine the singularity structure of the two-point function (4.9). By locality the corresponding commutator function at equal times consists of a δ-distribution and finitely many derivatives thereof. From Corollary 2.3 we get

$$\left\| \int_{\mathbf{R}^2} \{\psi_k(t,x), \psi_l(y)\}(y-x)^M f(x)g(y)dx\, dy \right\| \propto |t|^M \tag{4.10}$$

but this implies

$$(\Omega, \{\dot{\psi}_k(x), \psi_l(y)\}\Omega)(y-x)^2 \equiv 0, \quad \text{resp.}(\Omega, \{\ddot{\psi}_k(x), \psi_l(y)\}\Omega)(y-x)^3 \equiv 0. \tag{4.11}$$

Therefore

$$\left(\Omega, \left\{\ddot{\psi}_{k_0}(x) - \sum_{l=1}^{4}(A_{k_0 l}^{(0)} + A_{k_0 l}^{(1)}\partial_x)\dot{\psi}_l(x), \psi_{k_1}(y)\right\}\Omega\right)$$
$$= C_{k_0 k_1}^{(0)}\delta(y-x) + C_{k_0 k_1}^{(1)}\delta'(y-x) + C_{k_0 k_1}^{(2)}\delta''(y-x). \tag{4.12}$$

But because of CAR we have

$$\delta(y-x) = \{\psi_{k_1}^{\dagger}(x), \psi_{k_1}(y)\} \quad \text{and} \quad \psi_{k_1}^{\dagger} = \psi_{k_1 + 2 \bmod 4}. \tag{4.13}$$

So there exist matrices $B^{(0)}$, $B^{(1)}$, and $B^{(2)}$ such that

$$\left\{\ddot{\psi}_{k_0}(x) - \sum_l [A_{k_0 l}^{(0)} + A_{k_0 l}^{(1)}\partial_x]\dot{\psi}_{k_0}(x) - \sum_l [B_{k_0 l}^{(0)} + B_{k_0 l}^{(1)}\partial_x + B_{k_0 l}^{(2)}\partial_x^2]\psi_{k_0}(x), \psi_{k_1}(y)\right\} \equiv 0, \tag{4.14}$$

for all $k_0, k_1 \in \{1,2,3,4\}$. Or written with test functions

$$\left\{ \ddot{\psi}_{k_0}(f) - \sum_l \left[A^{(0)}_{k_0 l} \dot{\psi}_{k_0}(f) + A^{(1)}_{k_0 l} (\partial_x \dot{\psi})_{k_0}(f) + B^{(0)}_{k_0 l} \psi_{k_0}(f) + B^{(1)}_{k_0 l} (\partial_x \psi)_{k_0}(f) + B^{(2)}_{k_0 l} \right.\right.$$
$$\left.\left. \times (\partial_x^2 \psi)_{k_0}(f) \right], \ \psi_{k_1}(g) \right\} \equiv 0, \tag{4.15}$$

for all $g \in \mathscr{S}(\mathbf{R})$ and all $k_1 = 1,2,3,4$. Irreducibility proves the theorem notwithstanding the fact that the operator under consideration is unbounded.

V. PROOF OF THE MAIN THEOREM

(i) Theorem 4 is valid under the assumptions of the main theorem. In Fourier space the second order differential equation (4.1) looks as follows:

$$\{-p_0^2 - i p_0 A^{(0)} - p_0 p_1 A^{(1)} - B^{(0)} + i p_1 B^{(1)} + p_1^2 B^{(2)}\} \underline{\tilde{\psi}}(p_0, p_1) = 0. \tag{5.1}$$

For $|p_1| < C$, $C > 0$ arbitrary, and sufficiently large $|p_0|$ the operator

$$\left\{ -\mathbf{1} - \frac{1}{p_0} (i A^{(0)} + p_1 A^{(1)}) - \frac{1}{p_0^2} (B^{(0)} - i p_1 B^{(1)} - p_1^2 B^{(2)}) \right\} \tag{5.2}$$

is invertible. Therefore $\tilde{\psi}_k(p_0, p_1) = 0$ if $|p_1| < C$ and if $p_0^2 > M^2 - C^2$ for some $M^2 > 0$. But by the Jost–Lehmann–Dyson representation it follows that

$$\tilde{\psi}_k(\underline{p}) \Omega = 0 \quad \text{if } \underline{p}^2 > M^2. \tag{5.3}$$

In a former paper[10] we have shown that under these circumstances $\underline{\psi}$ can be decomposed into $\underline{\psi}(x_0, x_1) = \underline{\psi}^{(0)}(x_0, x_1) + \underline{\psi}^{(1)}(x_0, x_1)$, where $\underline{\psi}^{(0)}$ is a generalized free field, i.e.,

$$\{\underline{\psi}^{(0)}(x_0, x_1), \underline{\psi}^{(0)}(y_0, y_1)\} = (\Omega, \{\underline{\psi}^{(0)}(x_0, x_1), \underline{\psi}^{(0)}(y_0, y_1)\} \Omega), \tag{5.4}$$

and $\underline{\psi}^{(1)}$ fulfills the wave equation $\Box \underline{\psi}^{(1)}(x_0, x_1) = 0$. Both fields are local and

$$\{\underline{\psi}^{(0)}(x_0, x_1), \underline{\psi}^{(1)}(y_0, y_1)\} = (\Omega, \{\underline{\psi}^{(0)}(x_0, x_1), \underline{\psi}^{(1)}(y_0, y_1)\} \Omega). \tag{5.5}$$

(ii) Our aim is to show that the operators $\dot{\psi}_k(x_0, f)$ are bounded for all $k = 1,...,4$ and all $f \in \mathscr{S}(\mathbf{R})$.

From CAR we see that at equal times $x_0 = y_0$ we have

$$\{\underline{\psi}^{(1)}(x_0, x_1), \underline{\psi}^{(1)}(x_0, y_1)\} = (\Omega, \{\underline{\psi}^{(1)}(x_0, x_1), \underline{\psi}^{(1)}(x_0, y_1)\} \Omega). \tag{5.6}$$

The general solution of $\Box \underline{\psi}^{(1)}(x_0, x_1) = 0$ is of the form

$$\underline{\psi}^{(1)}(x_0, x_1) = \underline{\psi}^{(+)}(x_0 + x_1) + \underline{\psi}^{(-)}(x_0 - x_1) \tag{5.7}$$

and from locality we get $\{\underline{\psi}^{(+)}(x_0 + x_1), \underline{\psi}^{(-)}(y_0 - y_1)\} \equiv 0$. Because of

$$\partial_0 \underline{\psi}^{(+)}(x_0 + x_1) = \partial_1 \underline{\psi}^{(+)}(x_0 + x_1), \quad \partial_0 \underline{\psi}^{(-)}(x_0 - x_1) = -\partial_1 \underline{\psi}^{(-)}(x_0 - x_1) \tag{5.8}$$

and by differentiating (5.6) with respect to x_1 and y_1 we have

$$\{\dot{\underline{\psi}}^{(1)}(x_0,x_1),\dot{\underline{\psi}}^{(1)}(x_0,y_1)\}=\{\dot{\underline{\psi}}^{(+)}(x_0+x_1),\dot{\underline{\psi}}^{(+)}(x_0+y_1)\}+\{\dot{\underline{\psi}}^{(-)}(x_0-x_1),\dot{\underline{\psi}}^{(-)}(x_0-y_1)\}$$
$$=(\Omega,\{\dot{\underline{\psi}}^{(1)}(x_0,x_1),\dot{\underline{\psi}}^{(1)}(x_0,y_1)\}\Omega). \tag{5.9}$$

Therefore $\dot{\underline{\psi}}^{(1)}(x_0,f)$ is bounded. Obviously $\dot{\underline{\psi}}^{(0)}(x_0,f)$ is bounded too because $\underline{\psi}^{(0)}$ is a generalized free field.

(iii) Finally we want to prove the following.

Lemma 5: If in addition to CAR and irreducibility we require $\dot{\psi}_k(t,f)$ for all k and all $f\in\mathscr{S}(\mathbf{R})$ to be bounded operators then ψ_k are free fields.

Proof: For $\varepsilon>0$ let $\{h_l^\varepsilon,\ l\in\mathbf{Z}\}$ be a smooth partition of unity such that

(i) $h_l^\varepsilon\in\mathscr{D}([(l-\frac{3}{4})\varepsilon,(l+\frac{3}{4})\varepsilon])$,
(ii) $0\leqslant h_l^\varepsilon(x)\leqslant 1$,
(iii) $\Sigma_{l\in\mathbf{Z}}h_l^\varepsilon(x)\equiv 1$,

Take $f\in\mathscr{D}([-L,L])$ and $g_1,g_2,g_3\in\mathscr{S}(\mathbf{R})$ and put $t=0$. For any $\varepsilon>0$ we have

$$\{[\{\dot{\psi}_{k_0}(f\ ),\psi_{k_1}(g_1)\}\psi_{k_2}(g_2)]\psi_{k_3}(g_3)\}=\sum_{l_0,l_1,l_2,l_3}\{[\{\dot{\psi}_{k_0}(fh_{l_0}^\varepsilon),\psi_{k_1}(g_1\chi_{l_1}^\varepsilon)\}$$
$$\times\psi_{k_2}(g_2\chi_{l_2}^\varepsilon)]\psi_{k_3}(g_3\chi_{l_3}^\varepsilon)\}, \tag{5.10}$$

where the indices of summation are restricted to $|l_0-l_1|\leqslant 1$, $|l_2-l_1|\leqslant 2$, and $|l_3-l_1|\leqslant 3$ because of locality. l_1 has about $(2|L|+2)/\varepsilon$ values and we have

$$\{\dot{\psi}_{k_0}(f[h_{l_1-1}^\varepsilon+h_{l_1}^\varepsilon+h_{l_1+1}^\varepsilon]),\psi_{k_1}(g_1\chi_{l_1}^\varepsilon)\}=\{\dot{\psi}_{k_0}(f\ ),\psi_{k_1}(g_1\chi_{l_1}^\varepsilon)\}. \tag{5.11}$$

Therefore

$$\|\{[\{\dot{\psi}_{k_0}(f\ ),\psi_{k_1}(g_1)\}\psi_{k_2}(g_2)]\psi_{k_3}(g_3)\}\|\leqslant\frac{2|L|+2}{\varepsilon}\|\dot{\psi}_{k_0}(f\ )\|\|g_1\|_\infty\|g_2\|_\infty\|g_3\|_\infty 2^3 5\cdot 7\varepsilon^{3/2}$$
$$\to 0\ \text{ as }\ \varepsilon\ \text{ goes to }\ 0. \tag{5.12}$$

All operators under consideration are bounded, so we can apply irreducibility twice and we get

$$\{\dot{\psi}_{k_0}(f\ ),\psi_{k_1}(g_1)\}=(\Omega,\{\dot{\psi}_{k_0}(f\ ),\psi_{k_1}(g_1)\}\Omega). \tag{5.13}$$

Finally using Corollary 3.3 to determine the singularity structure of the 2-point function (5.13) and irreducibility again we see that $\underline{\psi}$ must obey a first order differential equation

$$\dot{\underline{\psi}}(t,x)+[A+B\partial_x]\underline{\psi}(t,x)=0. \tag{5.14}$$

APPENDIX A: AN UPPER BOUND FOR λ

From Theorem 3 we know

$$\{[\{\dot{\psi}_{k_0}(f_0),\psi_{k_1}(f_1)\}\psi_{k_2}(f_2)]\psi_{k_3}(f_3)\}=\lambda_{k_0k_1k_2k_3}\int_{\mathbf{R}}(f_0f_1f_2f_3)(x)dx. \tag{A1}$$

If we take $f_0,\ldots,f_3$ equal to the characteristic function of the interval $[0,1]$ the integral on the rhs is just 1. For this choice we get

$$\|\{[\{\dot{\psi}_{k_0}(f_0),\psi_{k_1}(f_1)\}\psi_{k_2}(f_2)]\psi_{k_3}(f_3)\}\| = |\lambda_{k_0k_1k_2k_3}|. \tag{A2}$$

We approximate $\dot{\psi}_{k_0}(f_0)$ by $(1/t)(\psi_{k_0}(t,f_0) - \psi_{k_0}(f_0))$ and have to estimate

$$\begin{aligned}\frac{1}{|t|}&\|\{[\{\psi_{k_0}(t,f_0),\psi_{k_1}(f_1)\}\psi_{k_2}(f_2)]\psi_{k_3}(f_3)\}\| \\ &= \frac{1}{|t|}\sum_m \{[\{\psi_{k_0}(t,f_0\chi_m^t),\psi_{k_1}(f_1(\chi_{m-1}^t+\chi_m^t+\chi_{m+1}^t))\}\psi_{k_2}(f_2(\chi_{m-1}^t+\chi_m^t \\ &\quad +\chi_{m+1}^t))]\psi_{k_3}(f_3(\chi_{m-1}^t+\chi_m^t+\chi_{m+1}^t))\}\|. \end{aligned}\tag{A3}$$

The sum has at most $(1/|t|)+2$ terms. From the bounds

$$\|\psi_{k_0}(t,f_0\chi_m^t)\| \leqslant \|\chi_m^t\|_2 = |t|^{1/2}, \quad \|\psi_k(f)(\chi_{m-1}^t+\chi_m^t+\chi_{m+1}^t)\| \leqslant |3t|^{1/2} \tag{A4}$$

we get immediately the following estimate for the rhs of (A3)

$$\leqslant 8\frac{1}{|t|}\left(\frac{1}{|t|}+2\right)|t|^{1/2}|3t|^{3/2} \to 24\sqrt{3} \approx 41.57. \tag{A5}$$

APPENDIX B: IRREDUCIBILITY FOR UNBOUNDED OPERATORS

Whereas the fields $\psi(t,f)$ are bounded operators because of CAR, this is no longer true *a priori* for the time derivatives $\dot{\psi}(t,f)$, $\ddot{\psi}(t,f)$,... . Nevertheless we want to use irreducibility arguments for these fields too. So we have to explain why this is correct. We do this in some detail even if most of the material collected here can be found in rudimentary form already in the article by Powers.[8]

Lemma B1: For $f \in L_2(\mathbf{R})$ let $\psi_k(f)$, $k=1,\ldots,2K$ be an irreducible representation of the CAR algebra in the Hilbert space $\mathscr{H}$ and let T be a closed operator on $\mathscr{H}$ satisfying $\psi_k(f)T \subset T\psi_k(f)$ for all $k=1,\ldots,2K$ and $f \in L_2(\mathbf{R})$.
Then $T=\lambda\mathbf{1}$ with $\lambda \in \mathbf{C}$.

Proof: We refer to the book *Normed Algebras* by M. A. Naimark.[11] From Sec. 21.2 we cite the following.

''*Corollary 1:* Suppose $x \to A_x$, $x \to B_x$ are irreducible representations in $\mathscr{H}$ resp. $\mathscr{H}'$ (of a fixed symmetric algebra) and that T is a closed linear operator from $\mathscr{H}$ into $\mathscr{H}'$ satisfying $B_xT \subset TA_x$.

Then either $T=0$, or the representations are equivalent and $T=\rho U$, where ρ is a positive number.''

U is an isometry from $\mathscr{H}$ to $\mathscr{H}'$. Specializing to the case $\mathscr{H}=\mathscr{H}'$ we get U unitary. If $A_x=B_x$ then $A_xU=UA_x$ and therefore $U=u\mathbf{1}$ with $u \in \mathbf{C}$, $|u|=1$. As a consequence we have $T=\rho u\mathbf{1}$ with $\rho u=\lambda \in \mathbf{C}$. If we take as A_x the irreducible algebra generated by $\mathbf{1}$, $\psi_k(f)$, $f \in L_2(\mathbf{R})$ we get Lemma B1.

In our framework the operators T show up as limits of bounded operators in $\mathscr{B}(\mathscr{H})$. The following lemma gives a criterion whether T is closable.

Lemma B2: For $t \in \mathbf{R}\{0\}$ let $A(t) \in \mathscr{B}(\mathscr{H})$. On a dense domain $\mathscr{D}_1 \subset \mathscr{H}$ we assume that $s-\lim_{t\to 0}A(t)\Phi = A\Phi$ exists and also $s-\lim_{t\to 0}A(t)^\dagger\Phi = \hat{A}\Phi$.
Then A is closable and can be uniquely extended to the closed operator $\overline{A}$.

Proof: A and $\hat{A}$ are densely defined. For all Φ_1, $\Phi_2 \in \mathscr{D}_1$ we have $(\Phi_1, A\Phi_2) = (\hat{A}\Phi_1, \Phi_2)$. This implies $A^\dagger \supset \hat{A}$ and $A^\dagger$ is densely defined. Therefore A is closable.

Corollary B3: Let $\mathscr{D}_1 = \{\mathscr{P}(\psi(f))\Omega,\ f \in \mathscr{S}(\mathbf{R})\}$ and $\mathscr{H}=\mathscr{D}_1$. Let $A(t)$ be either

$$\frac{1}{t}[\psi_k(t,f)-\psi_k(0,f)]f\in\mathscr{D}(\mathbf{R}) \quad \text{or} \tag{B1}$$

$$\frac{1}{t^2}[\psi_k(t,f)-2\psi_k(0,f)+\psi_k(-t,f)] \tag{B2}$$

and assume the existence of $s-\lim_{t\to 0}A(t)=A$ on $\mathscr{D}_1$ in the strong sense. Then A is closable. The same is true for the multiple commutators $C(t)$ like $\{A(t),\psi_{k_1}(f_1)\}$,$[\{A(t),\psi_{k_1}(f_1)\}\psi_{k_2}(f_2)]$,$\{[\{A(t),\psi_{k_1}(f_1)\}\psi_{k_2}(f_2)]\psi_{k_3}(f_3)\}$ and so on, i.e., $s-\lim_{t\to 0}C(t)=C$ exists on $\mathscr{D}_1$ and C is closable.

For $f\in\mathscr{S}(\mathbf{R})$ obviously we have $\psi_k(f)\mathscr{D}_1\subset\mathscr{D}_1$ and $\|\psi_k\|\leqslant\|f\|_2$ because of CAR.

Lemma B4: For $f\in\mathscr{S}(\mathbf{R})$ and all k assume

$$\|[A(t),\psi_k(f)]\|\leqslant c|t|^{\alpha},\alpha>0 \tag{B3}$$

then on $\mathscr{D}_{\overline{A}}$ we have for all $f\in L_2(\mathbf{R})$

$$[\overline{A},\psi_k(f)]=0. \tag{B4}$$

We prove the lemma in three steps:

(i) On $\mathscr{D}_1$ we have for $f\in\mathscr{S}(\mathbf{R})$

$$[A,\psi_k(f)]=0. \tag{B5}$$

Proof: Let $\Phi\in\mathscr{D}_1$

$$\|A(t)\psi_k(f)\Phi-\psi_k(f)A(t)\Phi\|\leqslant\|[A(t),\psi_k(f)]\|\|\Phi\|\to 0 \text{ as } t \text{ goes to } 0$$

$$s-\lim_{t\to 0}A(t)\psi_k(f)\Phi=A\psi_k(f)\Phi \text{ exists because } \psi_k(f)\mathscr{D}_1\subset\mathscr{D}_1,$$

$$s-\lim_{t\to 0}\psi_k(f)A(t)\Phi=\psi_k(f)A\Phi \text{ exists because } \psi_k(f) \text{ is bounded.} \tag{B6}$$

(ii) On $\mathscr{D}_{\overline{A}}$ we have for $f\in\mathscr{S}(\mathbf{R})$

$$[\overline{A},\psi_k(f)]=0. \tag{B7}$$

Proof: On $\mathscr{D}_1$ the operators A and $\overline{A}$ agree. To each $\Phi\in\mathscr{D}_{\overline{A}}$ there exists a sequence $(\Phi_n\in\mathscr{D}_1|n\in\mathbf{N})$ such that

$$\lim_{n\to\infty}(\|\Phi-\Phi_n\|+\|\overline{A}\Phi-\overline{A}\Phi_n\|)=0. \tag{B8}$$

By (i) we have $\overline{A}\psi_k(f)\Phi_n=\psi_k(f)\overline{A}\Phi_n$. Now $\psi_k(f)$ is bounded and therefore

$$\lim_n\psi_k(f)\overline{A}\Phi_n=\psi_k(f)\overline{A}\Phi \text{ resp. } \lim_n\psi_k(f)\Phi_n=\psi_k(f)\Phi \tag{B9}$$

exist. But $\overline{A}$ is closed and therefore $\overline{A}\psi_k(f)\Phi=\omega_k(f)\overline{A}\Phi$.

(iii) On $\mathscr{D}_{\overline{A}}$ we have for $f\in L_2(\mathbf{R})$

$$[\overline{A},\psi_k(f)]=0. \tag{B10}$$

Proof: We have $\|\psi_k(f)\| \leqslant \|f\|_2$. To each $f \in L_2(\mathbf{R})$ there is a sequence $(f_n \in \mathscr{S}(\mathbf{R}) | n \in \mathbf{N})$ such that $\lim_n \|f - f_n\|_2 = 0$. For $\Phi \in \mathscr{D}_{\overline{A}}$ we get by (ii) the relation $A\psi_k(f_n)\Phi = \psi_k(f_n)A\Phi$ and trivially $\lim_n \psi_k(f_n)\Phi = \psi_k(f)\Phi$, respectively, $\lim_n \psi_k(f_n)A\Phi = \psi_k(f)A\Phi$. Therefore $\lim_n A\psi_k(f_n)\Phi = \psi_k(f)A\Phi$ exists and because A is closed we get $A\psi_k(f)\Phi = \psi_k(f)A\Phi$ for $\Phi \in \mathscr{D}_{\overline{A}}$.

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The doublet representation of non-Hilbert eigenstates of the Hamiltonian

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We find the minimal mathematical structure to represent quantum eigenstates with complex eigenvalues with no need of analytic continuation. These eigenvectors build doublets in non-Hilbert spaces. We construct exact solutions for the Friedrichs model that continuously join the ones of the free Hamiltonian. We extend the Wigner operator to these non-Hilbert spaces and enlarge the concept of normalized vectors via the definition of the doublets. Making use of these doublets, we describe systems whose states have initial conditions out of Hilbert space. © *1996 American Institute of Physics.* [S0022-2488(96)00204-4]

I. INTRODUCTION

As it is generally known, unstable quantum states can be rigorously represented by (Gamow) vectors of rigged Hilbert spaces defined using Hardy class functions.[1–4] Then a natural question arises: is this the most general rigorous mathematical model for unstable quantum states?

The aim of this paper is to find the minimal mathematical structure to represent quantum states in non-Hilbert spaces and to conjecture a provisional definition of probability for them. In this approach we describe the states in an eigenbasis of the free Hamiltonian $\{|1\rangle,|\omega\rangle\}$, where ω $(0\leqslant\omega<\infty)$ is the frequency which represents the energy of the system and $|1\rangle$ is a discrete eigenstate of eigenvalue $\omega_0>0$.

We know that the eigenvalue problem for unbounded self-adjoint operators is not solvable in Hilbert space.[5] The Gelfand–Maurin theorem[6–8] deals with this problem and allows the appearance of eigenvalues that belong eventually to the complex plane. This is the case, for example, of the Hamiltonian of a discrete harmonic oscillator coupled to a bath described by the Fredrichs model which is usually solved by analytic continuation (and, in this case, there are unstable quantum states that belong to the above mentioned rigged Hilbert space[9–14]) or by perturbation methods.[15]

In this work we construct exact solutions for the Friedrichs model that are continuous in the coupling constant. This is a desirable property of the solutions we are looking for. In other words, we would like to bypass the Poincaré cathastrophe[16] generalized to the quantum domain. Then, all the solutions emerge in a natural way, with no need of analytic continuations[17] or perturbative methods[15] and they belong to a vector space that contains Hilbert space $\mathscr{H}$. This extended space is defined by the construction itself. Rigged Hilbert space will be a particular case of this construction and we believe that it encompasses other mathematical structures where unstable quantum states can be rigorously defined (nuclear spaces or convex algebras of operators[18]).

Furthermore, as the extended wave functions do not belong to Hilbert space any more, they lose their usual role in the probabilistic interpretation. Making use of the Friedrichs example, we

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introduce a doublet, namely the wave function plus a partner wave function, both belonging to convenient extended spaces, which seems to yield a criterion for extending the definition of probability.

The paper is organized as follows: in Sec. II we show that the requirement of continuity in the coupling parameter implies the appearance of complex eigenvalues. In Sec. III we define an operation (the star operation) which assigns a real number to the components of the doublet in generalized spaces. Section IV is devoted to well posing the Hamilton equations in the new space and in Sec. V we find the spectrum of the Hamiltonian. In Sec. VI we discuss the relation between the star operation and an extension of the time reversal Wigner operator. In Sec. VII we discuss the problem of defining probabilities and finding mean values in non-Hilbert spaces. In Sec. VIII we give a brief resume of the results. In Appendix A we show that our treatment allows us to recover the non-pure-exponential decay in Hilbert space. In Appendix B we study the statistics of a non-Hilbert eigenvector and its corresponding energy.

II. COMPLEX EIGENVALUES AND ANALYTICITY IN THE COUPLING PARAMETER

In this section we study the consequences of demanding a well-behaved $\lambda \to 0$ limit for the eigenvectors and eigenvalues of the Friedrichs Hamiltonian H. This Hamiltonian reads

$$H = H_0 + H_{\text{int}}, \tag{1}$$

where

$$H_0 = \omega_0 |1\rangle\langle 1| + \int_0^\infty \omega |\omega\rangle\langle\omega| d\omega$$

is the free Hamiltonian,

$$H_{\text{int}} = \lambda \int_0^\infty g(\omega)[|\omega\rangle\langle 1| + |1\rangle\langle\omega|] d\omega,$$

ω_0 is the discrete eigenvalue, $\omega \in \Re^+$ is the continuous spectrum, and the eigenvectors of the free Hamiltonian satisfy

$$\langle 1|1\rangle = 1, \quad \langle 1|\omega\rangle = \langle\omega|1\rangle = 0, \quad \langle\omega|\omega'\rangle = \delta(\omega - \omega'),$$

$\lambda \in \Re$ and the interaction $\lambda g(\omega)$ causes transitions between the discrete and continuous states. Let $|\psi\rangle$ be a vector belonging to the vector space Ξ spanned by the eigenvectors of H_0, the space where H_0 and H are defined,

$$|\psi\rangle = \varphi_1 |1\rangle + \int_0^\infty \varphi(\omega) |\omega\rangle, \quad |\psi\rangle \in \Xi, \tag{2}$$

where

$$\varphi_1 = \langle 1|\psi\rangle \quad \text{and} \quad \varphi(\omega) = \langle\omega|\psi\rangle.$$

In Hilbert space $\mathscr{H}$, where quantum mechanics of stable states is formulated, the coefficients satisfy

$$\varphi_1 \varphi_1^* + \int_0^\infty \varphi(\omega)\varphi^*(\omega) d\omega < \infty \tag{3}$$

(∗ indicates complex conjugation). With this condition, $\mathscr{H}$ and its conjugated space have the topology of the norm. Nevertheless, as H_0 and H are unbounded continuous operators, we can relax condition (3) to work in the less restrictive vector space $\Xi \supset \mathscr{H}$.

In terms of wave functions, we have the evolution equations

$$\langle 1|H|\psi\rangle = \omega_0 \varphi_1 + \lambda \int g(\omega)\varphi(\omega)d\omega = i\,\frac{\partial}{\partial t}\,\varphi_1, \tag{4}$$

$$\langle \omega|H|\psi\rangle = \omega\varphi(\omega) + \lambda g(\omega)\varphi_1 = i\,\frac{\partial}{\partial t}\,\varphi(\omega). \tag{5}$$

As (4) and (5) are true for any $|\psi\rangle$, we have

$$\langle 1|H = \omega_0\langle 1| + \lambda \int_0^\infty g(\omega)\langle \omega|d\omega = \langle 1|i\,\frac{\partial}{\partial t}, \tag{6}$$

$$\langle \omega|H = \omega\langle \omega| + \lambda g(\omega)\langle 1| = \langle \omega|i\,\frac{\partial}{\partial t}. \tag{7}$$

If we call $\langle \tilde{1}|$ and $\langle \tilde{\omega}|$ the left eigenstates of H, we have

$$\langle \tilde{1}|H = \tilde{\omega}_0\langle \tilde{1}| = \langle \tilde{1}|i\,\frac{\partial}{\partial t}, \tag{8}$$

$$\langle \tilde{\omega}|H = \tilde{\omega}\langle \tilde{\omega}| = \langle \tilde{\omega}|i\,\frac{\partial}{\partial t}, \tag{9}$$

H being a self-adjoint operator acting on $\mathscr{H}$ and $\tilde{\omega}_0$, $\tilde{\omega} \in \Re$.

To obtain the vectors that diagonalize the Hamiltonian, let $\langle 1|$, $\langle \omega|$ and $\langle \tilde{1}|$, $\langle \tilde{\omega}|$ be linked by the ansatz

$$\langle \tilde{1}| = \xi\langle 1| + \int_0^\infty \phi(\omega)\langle \omega|d\omega, \tag{10}$$

$$\langle \tilde{\omega}| = \xi_{\tilde{\omega}}\langle 1| + \int_0^\infty \phi_{\tilde{\omega}}(\omega)\langle \omega|d\omega. \tag{11}$$

Taking into account that we have not defined a topology in Ξ, all we can demand of the vectors with respect to the continuous parameter λ is that

$$\lim_{\lambda\to 0}\langle \tilde{1}|\psi\rangle = \langle 1|\psi\rangle, \tag{12}$$

$$\lim_{\lambda\to 0}\langle \tilde{\omega}|\psi\rangle = \langle \omega|\psi\rangle, \tag{13}$$

$\forall|\psi\rangle \epsilon \Xi$ and

$$\lim_{\lambda\to 0}\tilde{\omega}_0 = \omega_0. \tag{14}$$

For short we will write (12) and (13) as

$$\lim_{\lambda\to 0}\langle\widetilde{1}|=\langle 1|, \tag{15}$$

$$\lim_{\lambda\to 0}\langle\widetilde{\omega}|=\langle|\omega, \tag{16}$$

and refer to them as ''the weak limits.''

The ansatz (10) and (11) plus the dynamical evolution lead to the following equations for the coefficients ξ, $\phi(\omega)$:

$$(\widetilde{\omega}_0-\omega_0)=\lambda\int_0^\infty \phi(\omega)g(\omega)d\omega, \tag{17}$$

$$(\widetilde{\omega}_0-\omega)\phi(\omega)=\xi\lambda g(\omega). \tag{18}$$

If $\widetilde{\omega}_0\in\Re^+$, the solution to (17) and (18) is

$$\phi(\omega)=\delta(\widetilde{\omega}_0-\omega)+\frac{\lambda g(\omega)}{(\widetilde{\omega}_0-\omega\pm i\epsilon)}. \tag{19}$$

This solution should be rejected because when replacing (19) in (10) the δ-function causes the undesired behavior

$$\lambda=0\Rightarrow\langle\widetilde{1}|=\xi\langle 1|+\langle\omega_0|\neq\langle 1|. \tag{20}$$

Therefore to guarantee that the δ-function disappears from $\phi(\omega)$, $\widetilde{\omega}_0$ must not belong to $\Re^+$. In this case we have

$$\phi(\omega)=\frac{\lambda g(\omega)}{(\widetilde{\omega}_0-\omega)}. \tag{21}$$

Replacing (21) in (17) we have the condition

$$\alpha(\widetilde{\omega}_0)\cdot\xi=0 \quad \text{with} \quad \alpha_\pm(\omega)=\omega_0-\omega-\lambda^2\int_0^\infty\frac{g^2(\omega')d\omega'}{\omega\pm i\epsilon-\omega'}, \tag{22}$$

where

$$\alpha_+(\omega)-\alpha_-(\omega)=-2\pi i\lambda^2 g^2(\omega). \tag{23}$$

If α were different from zero, ξ had to be zero, and we would have again, in Eq. (10), the undesired behavior

$$\lambda=0\Rightarrow\langle\widetilde{1}|\neq\langle 1|.$$

So we need $\alpha(\widetilde{\omega}_0)=0$.

In this section we have considered only real eigenvalues. Therefore, reminding the reader that the eigenvalue $\widetilde{\omega}_0$ does not belong to $\Re^+$, if $\widetilde{\omega}_0$ is real, it must belong to $\Re^-$. However, as $\omega_0>0$, when λ approaches continuously 0, $\widetilde{\omega}_0$ goes through the forbidden zone $\widetilde{\omega}_0>0$. So we conclude that there is no acceptable $\widetilde{\omega}_0$ real solution. Then the root $\widetilde{\omega}_0$ of $\alpha(\omega)=0$ must be complex and it cannot be an eigenvalue of a self-adjoint Hamiltonian operator over $\mathscr{H}$.

III. THE STAR OPERATION

In order to diagonalize the Hamiltonian preserving continuity in λ, we reformulate the problem from the very beginning, namely, from the field equations (6)–(9). Let us define the space Ξ' of the linear functionals over Ξ

$$F(\varphi_1,\varphi(\omega))=n\epsilon\mathscr{C}$$

where $(\varphi_1,\varphi(\omega))$ are the components of vector $|\psi\rangle\epsilon\Xi$. In space Ξ, in spite of the fact that we have lost the notion of normalizability, a physical meaningful concept of probability can be defined all the same as we shall see. To do this, let us define a mapping $\star$ on vectors of Ξ:

$$\star:\Xi\rightarrow\Xi'$$

$$\star:(\varphi_1,\varphi(\omega))\rightarrow(\varphi_1,\varphi(\omega))^\star\equiv(\varphi_1^\star,\varphi^\star(\omega)),$$

$$F_{(\varphi_1,\varphi(\omega))}((\varphi_1,\varphi(\omega)))=\varphi_1\varphi_1^\star+\int_0^\infty\varphi(\omega)\varphi^\star(\omega)=\langle\psi^\star|\psi\rangle,$$

satisfying

(a) $F_{(\varphi_1,\varphi(\omega))}((\varphi_1,\varphi(\omega)))$ is a (finite) number constant in time and

(b) $[(\varphi_1,\varphi(\omega))^\star]^\star=(\varphi_1,\varphi(\omega))$. Then vector

$$|\psi\rangle=\varphi_1|1\rangle+\varphi(\omega)|\omega\rangle$$

and its partner

$$\langle\psi^\star|=\varphi_1^\star\langle1|+\varphi^\star(\omega)\langle\omega|=F_{(\varphi_1,\varphi(\omega))}(\cdot),$$

whose coefficients obey conditions (a) and (b), are said to belong to the spaces Φ and $\Phi^\star$. These spaces satisfy $\mathscr{H}\subset\Phi\subset\Xi$ and $\mathscr{H}'\subset\Phi^\star\subset\Xi'$. (We will show in Appendix B that there is at least one vector in Φ which does not belong to $\mathscr{H}$.) Properties (a) and (b) make bra $\langle\psi^\star|$ a convenient partner of ket $|\psi\rangle$ in order to define probabilities.

Of course, if $|\psi\rangle\in\mathscr{H}$ we have that

$$\langle\psi^\star|=\langle\psi|,\quad \varphi_1^\star=\varphi_1^*,\quad \text{and}\quad \varphi^\star(\omega)=\varphi^*(\omega),$$

and the usual state of affairs is reproduced.

As we shall see in Sec. IV, the time evolution of $\varphi_1^\star$ and $\varphi^\star(\omega)$ is completely determined by the action of the Hamiltonian over φ_1 and $\varphi(\omega)$ and conditions (a) and (b).

IV. FIELD EQUATIONS IN THE EXTENDED SPACE $\Phi\oplus\Phi^\star$

We demand the action of the ''partner'' of the Hamiltonian, namely $H^\star$, which determines the temporal evolution of $F_{(\varphi_1,\varphi(\omega))}$ to satisfy

$$H^\star F_{(\varphi_1,\varphi(\omega))}(\varphi_1,\varphi(\omega))=F_{(\varphi_1,\varphi(\omega))}(H(\varphi_1,\varphi(\omega))).\tag{24}$$

In order to find it explicitly, we use the fact that the temporal evolution of $(\varphi_1,\varphi(\omega))$ is given by (4) and (5) and the independence of time requested by condition (a) of Sec. III. Then, in components, Eq. (24) reads

$$\omega_0\varphi_1\varphi_1^\star+\lambda\int_0^\infty g(\omega)\varphi(\omega)\varphi_1^\star(\omega)d\omega+\int_0^\infty\omega\varphi(\omega)\varphi^\star(\omega)d\omega+\lambda\int_0^\infty g(\omega)\varphi_1\varphi^\star(\omega)d\omega$$

$$=-i\varphi_1\partial_t\varphi_1^\star-i\int_0^\infty\varphi(\omega)\partial_t\varphi^\star(\omega)d\omega,\tag{25}$$

which splits into

$$\omega_0|1\rangle+\lambda\int_0^\infty g(\omega)|\omega\rangle d\omega=(-i)\,\overline{\frac{\partial}{\partial t}}\,|1\rangle, \tag{26}$$

$$\omega|\omega\rangle+\lambda g(\omega)|1\rangle=(-i)\,\overline{\frac{\partial}{\partial t}}\,|\omega\rangle, \tag{27}$$

which are nothing but the ket version of (6) and (7) ($\overline{\partial}$ indicates left derivative).

Now we want to obtain the diagonal form of the complete set of equations in the $\Phi\oplus\Phi^\star$ extended space of doublets $\{|\psi\rangle,\langle\psi^\star|\}$. The set of equations for the bras has the same form as (8) and (9) but, in order to indicate that the Hamiltonian eigenvalues may be complex, we call them $\widetilde{z_0}$, $\widetilde{z}$ instead of $\widetilde{\omega}_0$, $\widetilde{\omega}$:

$$\langle\widetilde{1}|H=\widetilde{z}_0\langle\widetilde{1}|=\langle\widetilde{1}|i\,\frac{\partial}{\partial t}, \tag{28}$$

$$\langle\widetilde{z}|H=\widetilde{z}\langle\widetilde{z}\,|=\langle\widetilde{z}\,|i\,\frac{\partial}{\partial t}. \tag{29}$$

The ket set of the diagonal equations is obtained from Eq. (24) using (28) and (29). They are

$$H^\star|\widetilde{1}\rangle=\widetilde{z}_0|\widetilde{1}\rangle=(-i)\,\overline{\frac{\partial}{\partial t}}\,|\widetilde{1}\rangle, \tag{30}$$

$$H^\star|\widetilde{z}\rangle=\widetilde{z}|\,\widetilde{z}\,\rangle=(-i)\,\overline{\frac{\partial}{\partial t}}\,|\widetilde{z}\rangle. \tag{31}$$

Kets $|\,\widetilde{1}\,\rangle$, $|\widetilde{z}\rangle$ are the right eigenvectors of $H^\star$.

We want to emphasize that, in general, $\langle\,\widetilde{1}\,|\neq(|\,\widetilde{1}\,\rangle)^\star$ and $\langle\widetilde{z}|\neq(|\widetilde{z}\rangle)^\star$, i.e., $\langle\,\widetilde{1}\,|$ and $\langle\widetilde{z}\,|$ are not necessarily the partners of $|\,\widetilde{1}\rangle$, $|\widetilde{z}\rangle$. Indeed, the star operation is not always well defined among the right and left eigenvectors of H.

V. THE SPECTRUM OF THE HAMILTONIAN

The Friedrichs model has been long treated in the literature. Recently, in Ref. 15, it was found a basis that diagonalized the Hamiltonian preserving continuity in the coupling parameter λ using a perturbative method. On the other hand, in Ref. 17 an exact solution was obtained regardless of the continuity in λ.

Here we find a diagonal basis for the same problem that it is not only an exact solution but also preserves the desired continuity in λ. In order to diagonalize the Hamiltonian we will use an ansatz to relate the diagonal and nondiagonal basis, namely,

$$\langle\,\widetilde{1}\,|=\xi\langle 1|+\int_0^\infty\phi(\omega)\langle\omega|d\omega, \tag{32}$$

$$|\widetilde{1}\rangle=\xi^\star|1\rangle+\int_0^\infty\phi^\star(\omega)|\omega\rangle d\omega, \tag{33}$$

$$\langle\widetilde{z}\,|=\xi_{\widetilde{z}}\langle 1|+\int_0^\infty\phi_{\widetilde{z}}(\omega)\langle\omega|d\omega, \tag{34}$$

$$|\tilde{z}\rangle = \xi^{\star}_{\tilde{z}}|1\rangle + \int_0^{\infty} \phi^{\star}_{\tilde{z}}(\omega)|\omega\rangle d\omega. \tag{35}$$

Applying the Hamiltonian to the ansatz (32)–(35) we obtain

$$\phi(\omega) = \xi \frac{\lambda g(\omega)}{\tilde{z}_0 - \omega}, \quad \phi^{\star}(\omega) = \xi^{\star} \frac{\lambda g(\omega)}{\tilde{z}_0 - \omega},$$

$$\xi\left(\omega_0 - \tilde{z}_0 - \lambda^2 \int_0^{\infty} \frac{g^2(\omega)}{\tilde{z}_0 - \omega}\, d\omega \right) = 0 \Rightarrow \alpha(\tilde{z}_0) = 0.$$

Requiring the good behavior with respect to λ, the coefficient $\phi_{\tilde{z}}(\omega)$ results:

$$\phi_{\tilde{z}}(\omega) = \delta(\tilde{z} - \omega) + \xi_{\tilde{z}} \frac{\lambda g(\omega)}{\tilde{z} - \omega}. \tag{36}$$

Here $\delta(\tilde{z} - \omega)$ is the δ-function generalized to complex numbers. This extension of Dirac's δ-function as mentioned by Gelfand and Shilov[19] goes beyond the tempered distributions and was used by Nakanishi[20] in the discussion of the Friedrichs model. In order to preserve the good limit, $\delta(\tilde{z} - \omega)$ must be different from zero for every $\tilde{z}$, i.e., $\{\tilde{z}\}$ must coincide with $\Re^+$. So we call $\tilde{\omega}$ this real variable:

$$\phi_{\tilde{\omega}}(\omega) = \delta(\tilde{\omega} - \omega) + \xi_{\tilde{\omega}} \frac{\lambda g(\omega)}{\tilde{\omega} - \omega}, \tag{37}$$

$$\xi_{\tilde{\omega}}(\tilde{\omega} - \omega_0) = \lambda g(\tilde{\omega}) + \xi_{\tilde{\omega}} \lambda^2 \int_0^{\infty} \frac{g^2(\omega)}{\tilde{\omega} - \omega}\, d\omega, \tag{38}$$

i.e.,

$$\xi_{\tilde{\omega}} = \frac{\lambda g(\tilde{\omega})}{\alpha(\tilde{\omega})} \quad \text{and} \quad \phi_{\tilde{\omega}}(\omega) = \delta(\tilde{\omega} - \omega) + \frac{\lambda^2 g(\omega) g(\tilde{\omega})}{(\tilde{\omega} - \omega)\alpha(\tilde{\omega})}.$$

The singularities in $\alpha(\tilde{\omega})$ and $(\tilde{\omega} - \omega)^{-1}$ must be avoided making the shift $\pm i\epsilon$. We do not write it explicitly so as not to embarrass the notation. The equivalent star equations to (37) and (38) yield

$$\xi^{\star}_{\tilde{\omega}} = \frac{\lambda g(\tilde{\omega})}{\alpha(\tilde{\omega})}$$

and

$$\phi^{\star}_{\tilde{\omega}}(\omega) = \delta(\tilde{\omega} - \omega) + \frac{\lambda^2 g(\omega) g(\tilde{\omega})}{(\tilde{\omega} - \omega)\alpha(\tilde{\omega})}.$$

Putting it all together, the change of basis that diagonalizes the Hamiltonian results in

$$\langle \tilde{1} | = \xi \langle 1| + \xi \int_0^{\infty} \frac{\lambda g(\omega)}{\tilde{z}_0 - \omega} \langle \omega | d\omega, \tag{39}$$

$$|\tilde{1}\rangle = \xi^\star |1\rangle + \xi^\star \int_0^\infty \frac{\lambda g(\omega)}{\tilde{z}_0 - \omega} |\omega\rangle d\omega, \tag{40}$$

$$\langle \tilde{\omega}| = \frac{\lambda g(\tilde{\omega})}{\alpha(\tilde{\omega})} \langle 1| + \int_0^\infty \left[\delta(\tilde{\omega} - \omega) + \frac{\lambda^2 g(\omega) g(\tilde{\omega})}{(\tilde{\omega} - \omega)\alpha(\tilde{\omega})} \right] \langle \omega| d\omega, \tag{41}$$

$$|\tilde{\omega}\rangle = \frac{\lambda g(\tilde{\omega})}{\alpha(\tilde{\omega})} |1\rangle + \int_0^\infty \left[\delta(\tilde{\omega} - \omega) + \frac{\lambda^2 g(\omega) g(\tilde{\omega})}{(\tilde{\omega} - \omega)\alpha(\tilde{\omega})} \right] |\omega\rangle d\omega, \tag{42}$$

where

$$[\xi \xi^\star]^{-1} = \left. \frac{\partial \alpha(z)}{\partial z} \right|_{z = \tilde{z}_0} \equiv \alpha'.$$

When the initial conditions belong to $\mathscr{H}$, solutions (39)–(42) are such that temporal evolution keeps the state into $\mathscr{H}$. As we have already said, $\langle \tilde{\omega}|$ of Eq. (41) must be understood as $\langle \tilde{\omega} \pm |$ and the same for $|\tilde{\omega}\rangle$ of Eq. (42). Taking this into account, a straightforward computation proves that they are nothing but the retarded and advanced Lippman–Schwinger solutions, which are exact solutions of the Friedrichs model.[21]

We will also need the inverse of the ansatz. To obtain it, we posed the inverse problem and, after some calculation, we obtained

$$\langle 1| = \eta \langle \tilde{1}| + \int_0^\infty \frac{\lambda g(\tilde{\omega})}{\alpha(\tilde{\omega})} \langle \tilde{\omega}| d\tilde{\omega}, \tag{43}$$

$$|1\rangle = \eta^\star |\tilde{1}\rangle + \int_0^\infty \frac{\lambda g(\tilde{\omega})}{\alpha(\tilde{\omega})} |\tilde{\omega}\rangle d\tilde{\omega}, \tag{44}$$

$$\langle \omega| = \frac{\lambda g(\omega)}{\tilde{z}_0 - \omega} \eta \langle \tilde{1}| + \int_0^\infty \left[\delta(\omega - \tilde{\omega}) + \frac{\lambda^2 g(\omega) g(\tilde{\omega})}{(\tilde{\omega} - \omega)\alpha(\tilde{\omega})} \right] \langle \tilde{\omega}| d\tilde{\omega}, \tag{45}$$

$$|\omega\rangle = \frac{\lambda g(\omega)}{\tilde{z}_0 - \omega} \eta^\star |\tilde{1}\rangle + \int_0^\infty \left[\delta(\omega - \tilde{\omega}) + \frac{\lambda^2 g(\omega) g(\tilde{\omega})}{(\tilde{\omega} - \omega)\alpha(\tilde{\omega})} \right] |\tilde{\omega}\rangle d\tilde{\omega}. \tag{46}$$

The composition of the transformations (39)–(42) and (43)–(46) gives the identity transformation, so one is the inverse of the other. Having found a regular transformation which has a regular inverse, we conclude that we have found a new basis for the space $\Phi \oplus \Phi^\star$ and also the spectrum of the Hamiltonian.

VI. THE STAR OPERATION AND TIME REVERSAL

In order to avoid the difficulties of the bra–ket notation when dealing with antilinear operators,[22] we will use the wave function formalism to generalize the time reversal operator and to compare it with the star operation.

We know that in $\mathscr{H}$ the action of the time reversal operator T, in the wave function formalism, comes from the conjugation of the Schrödinger equation, i.e., we have

$$T: \mathscr{H} \to \mathscr{H},$$

$$\varphi \to \varphi^* \quad \text{and} \quad t \to -t.$$

In Φ, Schrödinger equations (28)–(31) (with $\tilde{z}=\tilde{\omega}$) in the wave function formalism read

$$H\tilde{\varphi}_1=\tilde{z}_0\tilde{\varphi}_1=i\,\frac{\partial}{\partial t}\,\tilde{\varphi}_1, \tag{47}$$

$$H\tilde{\varphi}(\tilde{\omega})=\tilde{\omega}\tilde{\varphi}(\tilde{\omega})=i\,\frac{\partial}{\partial t}\,\tilde{\varphi}(\tilde{\omega}), \tag{48}$$

$$H^\star\tilde{\varphi}_1^\star=\tilde{z}_0\tilde{\varphi}_1^\star=-i\,\frac{\partial}{\partial t}\,\tilde{\varphi}_1^\star, \tag{49}$$

$$H^\star\tilde{\varphi}^\star(\tilde{\omega})=\tilde{\omega}\tilde{\varphi}^\star(\tilde{\omega})=-i\,\frac{\partial}{\partial t}\,\tilde{\varphi}^\star(\tilde{\omega}). \tag{50}$$

As we can immediately see, in the extended space the appearance of complex eigenvalues forces the time reversal to be related to the star operation which is not a simple complex conjugation. In the extended space we can define an extension of T,

$$\tilde{T}:\Phi\rightarrow\Phi^\star,\quad \tilde{T}^{-1}:\Phi^\star\rightarrow\Phi,$$

whose action can be represented by

$$\varphi\rightarrow\varphi^\star\quad\text{when}\quad t\rightarrow -t.$$

On the other hand, as $\tilde{z}_0=\tilde{\omega}_0-i\gamma/2$ with $\gamma\in\Re^+$ (conventionally), solution to Eq. (47),

$$\tilde{\varphi}_1(t)=\tilde{\varphi}_1(0)\exp(-i\tilde{z}_0t)=\tilde{\varphi}_1(0)\exp(-i\tilde{\omega}_0t)\exp(\gamma t/2),$$

is not defined when $t\rightarrow\infty$. Analogously, solution to Eq. (49),

$$\tilde{\varphi}_1^\star(t)=\tilde{\varphi}_1^\star(0)\exp(i\tilde{z}_0t)=\tilde{\varphi}_1^\star(0)\exp(i\tilde{\omega}_0t)\exp(-\gamma t/2),$$

is not defined when $t\rightarrow-\infty$. So, temporal evolution described by Eqs. (47)–(50) is not defined in the whole interval $[-\infty,\infty]$ but in $[-\infty,\infty)$ for solutions which evolve with H and in $(-\infty,\infty]$ for those which evolve with H^*. This fact could be related to the splitting of the system evolution group into two semigroups[15] for the case of non-pure states and will be studied elsewhere.

VII. DISCUSSION ABOUT PROBABILITY AND MEAN VALUE OF OBSERVABLES IN EXTENDED SPACES

In this section we will sketch a discussion about a possible probabilistic interpretation for our extended formalism. Consider that the system is initially free and that the self-interaction begins at $t=0$ and finishes at an arbitrary time t, when the system becomes free again. During the interaction, eigenvalues of the operator H may be complex and states represented by $|\psi\rangle$ and $\langle\psi\star|$ may also belong to the extended space. In order to define probability in this space we consider again the scalar quantity

$$\langle\psi^\star|\psi\rangle=\varphi_1\varphi_1^\star+\int_0^\infty\varphi(\omega)\varphi^\star(\omega)d\omega=\langle\tilde{\psi}^\star|\tilde{\psi}\rangle=\tilde{\varphi}_1\tilde{\varphi}_1^\star+\int_0^\infty\tilde{\varphi}(\tilde{\omega})\tilde{\varphi}^\star(\tilde{\omega})d\tilde{\omega} \tag{51}$$

that we have introduced in Sec. III to construct the space $\Phi^\star$ and we normalize it to 1. Here $\langle\psi^\star|\psi\rangle$ is a scalar conserved under the change of basis and constant in time and reduces to the standard norm when $|\psi\rangle$ belongs to $\mathscr{H}$. However, we cannot be assured that each term of Eq. (51) is a real

number. Nevertheless, if it is so, we are able to interpret each term of the sum (51) as a probability itself, i.e., $\varphi_1(t)\varphi_1^\star(t)$ represents the probability of finding the system in the discrete eigenstate of the free Hamiltonian and

$$\int_{\omega}^{\omega+\Delta\omega} \varphi(\omega,t)\varphi^\star(\omega,t)d\omega$$

represents the probability of finding the system in the continuous spectrum with frequencies into $[\omega, \omega+\Delta\omega]$ after the interaction. In this case, we have a natural extension of the definition of probability from $\mathscr{H}$ to the extended space $\Phi\oplus\Phi^\star$.

Notice that, even in cases in which the $\star$ operation is well defined in the extended space and is conserved in time and under changes of basis, these facts are not enough to guarantee that the first term and any partial integral in the sum (51) belong to the interval [0, 1]. As it was pointed out,[23] we can interpretate this fact as being related with initial conditions not possible to be realized or representing a situation for which probability cannot be verified directly or a combination of both. These situations would be impossible, not in the sense that the chance for their occurrence is zero, but in the sense that the conditions of preparation or verification of those states are unattainable. The problem of an adequate interpretation of negative probabilities has been long studied. See, for example, Refs. 23 and 24.

With our definition of probability the mean value of a constant of motion A is defined as

$$\overline{A}=\Sigma_i a_i P(\varphi_i)+\int a\mathscr{P}(\varphi(a))da=\Sigma_i a_i\varphi_i\varphi_i^\star+\int a\varphi(a)\varphi^\star(a)da,$$

where a_i and a belong to the discrete and continuous spectra of A, respectively. $\overline{A}$ is in general a complex number and reduces to a real one when A is a self-adjoint operator on $\mathscr{H}$. Notice that when the eigenvalues a_i are positive real numbers, the mean value A is a positive real number if probability also is. This allows us to have states with positive defined unperturbed energy out of $\mathscr{H}$. Namely, even in the extended space, when the initial conditions are so that their corresponding probabilities belong to [0, 1], we can guarantee the positivity of the mean value of the unperturbed energy H_0:

$$\overline{H_0}=\omega_0|1\rangle\langle 1|+\int_0^\infty \omega|\omega\rangle\langle\omega|d\omega.$$

So we can relate reality and positivity of probability with positivity of this energy. It is in this sense that we have said that negative probabilities correspond to impossible initial conditions.

Regardless our interpretation is merely a conjecture we will use to see how it works in two cases: in Appendix A the conjecture applied to a Hilbert space vector lets us reproduce the non-pure exponential decay. In Appendix B we use the conjecture to compute probabilities and mean values of energy for a system whose initial conditions are out of $\mathscr{H}$.

VIII. CONCLUSIONS

We have found an exact solution of the Friedrichs model which for the continuous spectrum coincides with the Lippman–Schwinger solutions. To find the right and left eigenvectors of the Hamiltonian with interaction, we have neither made use of analytic continuations nor perturbative methods. As we have preserved continuity in the coupling parameter λ, our approach is also applicable to systems that must be treated in a perturbative way. We also found the minimal mathematical structure to represent quantum states. To generalize the notion of probability from $\mathscr{H}$, we defined the star operation in Sec. III and constructed the doublets of wave functions. The star operation is also related to the time reversal operation in the extended space. The main tool

that we have is the scalar magnitude defined by Eq. (51). This scalar magnitude, built up with a doublet of wave functions, plays in the extended space an analogous role to the norm in $\mathscr{H}$ and reduces to it when the star operation reduces to the conjugation. Then we have a probabilistic interpretation of this extension of the norm. Further restrictions conducing to the choice of a particular topology will be imposed when they appear necessary because of physical reasons. In a forthcoming work we will try to apply our formalism to more realistic models like those of Refs. 25–29.

Finally we show in Appendix A that our approach gives the correct non-purely exponential decay amplitude and, in Appendix B, our formalism is applied to describe quantum states out of $\mathscr{H}$.

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APPENDIX A: THE NON-PURE EXPONENTIAL DECAY

Here we apply our formalism to study the decay of a state whose initial condition belongs to $\mathscr{H}$ and that represents, at $t=0$, a particle with energy ω_0:

$$\langle 1| = \begin{pmatrix} \varphi_1 = 1 \\ \varphi(\omega) = 0 \end{pmatrix}.$$

Then, as $\langle 1|$ belongs to $\mathscr{H}$, we have

$$(\langle 1|)^\star \equiv |1^\star\rangle = |1\rangle = \begin{pmatrix} \varphi_1^\star = 1 \\ \varphi^\star(\omega) = 0 \end{pmatrix}.$$

Temporal evolution in the diagonal basis is

$$\tilde{\varphi}_1(t) = \frac{1}{\sqrt{\alpha'}}\, e^{-i\tilde{z}_0 t}, \quad \tilde{\varphi}_1^\star(t) = \frac{1}{\sqrt{\alpha'}}\, e^{i\tilde{z}_0 t},$$

$$\tilde{\varphi}(\tilde{\omega},t) = \frac{\lambda g(\tilde{\omega})}{\alpha(\tilde{\omega})}\, e^{-i\tilde{\omega}t}, \quad \tilde{\varphi}^\star(\tilde{\omega},t) = \frac{\lambda g(\tilde{\omega})}{\alpha(\tilde{\omega})}\, e^{i\tilde{\omega}t}.$$

So, in the nondiagonal basis, the wave functions are

$$\langle 1|1(t)\rangle = \varphi_1(t) = \frac{e^{-i\tilde{z}_0 t}}{\alpha'} + \int_0^\infty \frac{\lambda^2 g^2(\tilde{\omega})}{\alpha^2(\tilde{\omega})}\, e^{-i\tilde{\omega}t}\, d\tilde{\omega},$$

$$\langle 1^\star(t)|1\rangle = \varphi_1^\star(t) = \frac{e^{i\tilde{z}_0 t}}{\alpha'} + \int_0^\infty \frac{\lambda^2 g^2(\tilde{\omega})}{\alpha^2(\tilde{\omega})}\, e^{i\tilde{\omega}t}\, d\tilde{\omega}.$$

Changing the contours of integration appropriately (see Appendix A of Ref. 17) and Eq. (23), $\varphi_1(t)$ results in

$$\varphi_1(t) = -\frac{i}{2\pi} \int_\Gamma \frac{e^{-izt}}{\alpha(z)}\, dz.$$

With our definition, the probability of having the system in the discrete state is $\varphi_1\varphi_1^\star$. By direct computation it can be seen that

$$\varphi_1^\star(t)=\varphi_1^*(t)$$

as corresponds to a vector belonging to $\mathscr{H}$. So

$$\varphi_1\varphi_1^\star=\varphi_1\varphi_1^*=|\varphi_1|^2$$

predicts the correct non-pure exponential decay amplitude with the Zeno[30,31] and Khalfin effects.[32,33]

APPENDIX B: PROBABILITY AND UNPERTURBED ENERGY OF A NON-HILBERT EIGENSTATE

We consider now a system whose initial state is the discrete eigenstate of H with eigenvalue $\tilde{z}_0$:

$$\langle\tilde{1}|=\begin{pmatrix}1\\0\end{pmatrix}. \tag{B1}$$

Given (B1), its partner satisfying Eq. (51) is

$$(\langle\tilde{1}|)^\star\equiv|\tilde{1}^\star\rangle=|\tilde{1}\rangle=\begin{pmatrix}1\\0\end{pmatrix}.$$

Temporal evolution gives

$$\left[\begin{pmatrix}e^{-i\tilde{z}_0t}\\0\end{pmatrix},\begin{pmatrix}e^{i\tilde{z}_0t}\\0\end{pmatrix}\right].$$

In terms of the eigenfunctions of the free Hamiltonian, the doublet reads

$$\varphi_1(t)=\frac{1}{\sqrt{\alpha'}}\,e^{-i\tilde{z}_0t},\quad \varphi_1^\star(t)=\frac{1}{\sqrt{\alpha'}}\,e^{i\tilde{z}_0t}, \tag{B2}$$

$$\varphi(\omega)=\frac{\lambda g(\omega)}{\tilde{z}_0-\omega}\,\frac{1}{\sqrt{\alpha'}}\,e^{-i\tilde{z}_0t},\quad \varphi^\star(\omega)=\frac{\lambda g(\omega)}{\tilde{z}_0-\omega}\,\frac{1}{\sqrt{\alpha'}}\,e^{i\tilde{z}_0t}. \tag{B3}$$

As (B2) and (B3) are solutions of the Schrödinger equations that do not belong to Hilbert space, they need to be given a physical interpretation.

First we check the conservation of probability:

$$\tilde{\varphi}_1\tilde{\varphi}_1^\star+\int_0^\infty\tilde{\varphi}(\tilde{\omega})\tilde{\varphi}^\star(\tilde{\omega})d\tilde{\omega}=1$$

and

$$\varphi_1\varphi_1^\star+\int_0^\infty\varphi(\omega)\varphi^\star(\omega)d\omega=\frac{1}{\alpha'}+\int_0^\infty\frac{1}{\alpha'}\,\frac{\lambda^2g^2(\omega)}{(\tilde{z}_0-\omega)^2}\,d\omega=\frac{1}{\alpha'}+\frac{\alpha'-1}{\alpha'}=1$$

because

$$\alpha = z - \omega_0 - \lambda^2 \int_0^\infty \frac{g^2(\omega)}{(z-\omega)}\, d\omega \Rightarrow \left.\frac{\partial \alpha(z)}{\partial z}\right|_{z=\tilde{z}_0} = \alpha' = 1 + \lambda^2 \int_0^\infty \frac{g^2(\omega)}{(\tilde{z}_0-\omega)^2}\, d\omega.$$

With this procedure we have a way to identify a pure state corresponding to a complex eigenvalue in terms of the eigenfunctions of the free Hamiltonian: it is a state with probability $1/\alpha'$ of being in the discrete level with energy ω_0 and probability $(\alpha'-1)/\alpha'$ of being in any level ω of the continuum, respectively. These probabilities are constant in time as it corresponds to an eigenstate of $\mathscr{H}$.

We now compute the mean value of the energy when the interaction finishes:

$$\overline{H}_{0(\tilde{\varphi}_1,\tilde{\varphi}_1^\star)} = \omega_0 \varphi_1 \varphi_1^\star + \int_0^\infty \omega \varphi(\omega) \varphi^\star(\omega) d\omega. \tag{B4}$$

Using (B2) and (B3) we have

$$\overline{H}_{0(\tilde{\varphi}_1,\tilde{\varphi}_1^\star)} = \frac{1}{\alpha'(\tilde{z}_0)} \left(\omega_0 + \int_0^\infty \omega\, \frac{\lambda^2 g^2(\omega)}{(\tilde{z}_0-\omega)^2}\, d\omega \right). \tag{B5}$$

Some comments are in order:

(1) $\overline{H_0}$ is a real number if probability is.
(2) If the interaction $g(\omega)$ is such that $(\tilde{\varphi}_1, \tilde{\varphi}_1^\star)$ is a possible initial condition, the unperturbed energy of the state is a positive number.
(3) When $\lambda \to 0$, we have the correct limit $\lim_{\lambda\to 0} \overline{H_0} = \omega_0$.
(4) The mean value of the evolution operator during the interaction that corresponds to $(\tilde{\varphi}_1, \tilde{\varphi}_1^\star)$ state is the complex number $\overline{H}_{(\tilde{\varphi}_1,\tilde{\varphi}_1^\star)} = \tilde{z}_0$. This is not surprising because it is only the evolution operator and the energy is not defined during the interaction.

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Maximal localization in the presence of minimal uncertainties in positions and in momenta

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Small corrections to the uncertainty relations, with effects in the ultraviolet and/or infrared, have been discussed in the context of string theory and quantum gravity. Such corrections lead to small but finite minimal uncertainties in position and/or momentum measurements. It has been shown that these effects could indeed provide natural cutoffs in quantum field theory. The corresponding underlying quantum theoretical framework includes small ''noncommutative geometric'' corrections to the canonical commutation relations. In order to study the full implications on the concept of locality, it is crucial to find the physical states of then maximal localization. These states and their properties have been calculated for the case with minimal uncertainties in positions only. Here we extend this treatment, though still in one dimension, to the general situation with minimal uncertainties both in positions and in momenta. © *1996 American Institute of Physics.*
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I. INTRODUCTION

The short distance structure of conventional geometry can be considered experimentally confirmed up to the order of 1 TeV (see, e.g., Ref. 1). In string theory and quantum gravity certain corrections to the short distance structure and the uncertainty relations have been suggested to appear at smaller scales (the latest at the Planck scale) (see, e.g., Refs. 2–7 and, for a recent review, Ref. 8).

Here we continue a series of articles[9–15] in which are studied the quantum theoretical consequences of small corrections to the canonical commutation relations

$$[\mathbf{x}_i\,,\ \mathbf{p}_j]=i\hbar(\,\delta_{ij}+\alpha_{ijkl}\mathbf{x}_k\mathbf{x}_l+\beta_{ijkl}\mathbf{p}_k\mathbf{p}_l+\cdots), \tag{1}$$

including the possibility that also $[\mathbf{x}_i\,,\,\mathbf{x}_j]\neq 0$, $[\mathbf{p}_i\,,\,\mathbf{p}_j]\neq 0$. A crucial feature of this ''noncommutative geometric'' ansatz, which was first studied in Ref. 11, is that for appropriate matrices α and β, Eq. (1) implies the existence of finite lower bounds to the determination of positions and momenta. These bounds take the form of finite minimal uncertainties Δx_0 and Δp_0, obeyed by all physical states. In fact, the approach covers the case of those corrections to the uncertainty relations which we mentioned above (see Ref. 12).

A framework with a finite minimal uncertainty Δx_0 can as well be understood to describe effectively nonpointlike particles than as describing a fuzzy space. As discussed in Refs. 12–15, the approach, with appropriately adjusted scales, could have therefore more generally a potential for an effective description of nonpointlike particles, such as, e.g., nucleons or quasi-particles in solids.

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Analogously, on large scales a minimal uncertainty Δp_0 may offer new possibilities to describe situations where momentum cannot be precisely determined, in particular on curved space.[13]

Using the path integral formulation it has been shown in Ref. 13 that such noncommutative background geometries can ultraviolet and infrared regularize quantum field theories in arbitrary dimensions through minimal uncertainties $\Delta x_0, \Delta p_0$. However, a complete analysis of the modified short distance structure, and, in particular, the calculation of the states of maximal localization, has so far only been carried out for the special case of the commutation relations $[\mathbf{x}, \mathbf{p}]=i\hbar(1+\beta\mathbf{p}^2)$, in Ref. 15. The reason is that those cases are representation theoretically much easier to handle in which either α or β vanish, i.e., with minimal uncertainties in either position or in momenta only. We now solve the more general, though still one-dimensional, problem involving both minimal uncertainties in positions and in momenta.

We define the associative Heisenberg algebra $\mathscr{A}$ with corrections parametrized by small constants $\alpha,\beta \geqslant 0$,

$$[\mathbf{x},\ \mathbf{p}]=i\hbar(1+\alpha\mathbf{x}^2+\beta\mathbf{p}^2), \tag{2}$$

or, in a notation which will prove more convenient ($q \geqslant 1$),

$$[\mathbf{x},\ \mathbf{p}]=i\hbar\left[1+(q^2-1)\left(\frac{x^2}{4L^2}+\frac{\mathbf{p}^2}{4K^2}\right)\right], \tag{3}$$

where the constants L,K carry units of length and momentum and are related by

$$4KL=\hbar(1+q^2). \tag{4}$$

While the first correction term contributes for large $\langle\mathbf{x}^2\rangle=\langle\mathbf{x}\rangle^2+(\Delta x)^2$, which is the definition of the infrared, the second correction term contributes for large $\langle\mathbf{p}^2\rangle=\langle\mathbf{p}\rangle^2+(\Delta p)^2$, i.e., in the ultraviolet.

The corresponding uncertainty relation

$$\Delta x\Delta p \geqslant \frac{\hbar}{2}\{1+\alpha((\Delta x)^2+\langle\mathbf{x}\rangle^2)+\beta((\Delta p)^2+\langle\mathbf{p}\rangle^2)\} \tag{5}$$

holds in all $*$-representations of the commutation relations and reveals these infrared and ultraviolet modifications as minimal uncertainties in positions and momenta:[12]

$$(\Delta x_{\min})^2=L^2\,\frac{q^2-1}{q^2}\left[1+(q^2-1)\left(\frac{\langle\mathbf{x}\rangle^2}{4L^2}+\frac{\langle\mathbf{p}\rangle^2}{4K^2}\right)\right], \tag{6}$$

$$(\Delta p_{\min})^2=K^2\,\frac{q^2-1}{q^2}\left[1+(q^2-1)\left(\frac{\langle\mathbf{x}\rangle^2}{4L^2}+\frac{\langle\mathbf{p}\rangle^2}{4K^2}\right)\right]. \tag{7}$$

In particular, for all physical states, i.e., for all $|\psi\rangle \in D$ with $D \subset H$ being any $*$-representation of the commutation relations of $\mathscr{A}$ in a Hilbert space H, there are finite absolutely smallest uncertainties (all $|\psi\rangle$ normalized):

$$(\Delta x_{|\psi\rangle})=\langle\psi|(\mathbf{x}-\langle\mathbf{x}\rangle)^2|\psi\rangle^{1/2} \geqslant L\sqrt{1-q^{-2}} \quad \forall|\psi\rangle \in D, \tag{8}$$

$$(\Delta p_{|\psi\rangle})=\langle\psi|(\mathbf{p}-\langle\mathbf{p}\rangle)^2|\psi\rangle^{1/2} \geqslant K\sqrt{1-q^{-2}} \quad \forall|\psi\rangle \in D. \tag{9}$$

We will here only deal with the kinematical consequences of possible corrections to the commutation relations. Arbitrary systems can be considered and studies on dynamical systems, including

the calculation of the spectra of Hamiltonians and integral kernels such as Green's functions, have been carried out for example systems in Refs. 9 and 10. Comparison can also be made with the features of the discretized quantum mechanics studied, e.g., in Refs. 16–18. An interesting canonical field theoretical approach with a similar motivation is focusing on generalizing the uncertainty relations among the coordinates.[19]

II. HILBERT SPACE REPRESENTATION

A crucial consequence of Eqs. (8) and (9) is that there are no eigenvectors to **x** nor to **p** in any space of physical states, i.e., in any $*$-representation D of the generalized commutation relations. As is clear from the definition of uncertainties, e.g., $(\Delta x)^2_{|\psi\rangle}=\langle\psi|(\mathbf{x}-\langle\psi|\mathbf{x}|\psi\rangle)^2|\psi\rangle$, eigenvectors to **x** or **p** could only have vanishing uncertainty in position or momentum. In particular, the commutation relations of A no longer find spectral representations of **x** nor of **p**.

In the situation of $\alpha=0$ (or $\beta=0$), i.e., with $\Delta p_0=0$ (or $\Delta x_0=0$), there is still the momentum (or position) representation of $\mathscr{A}$ available, in which case the maximal localization states have been calculated in Ref. 15. Let us now perform the analogous studies for the general case with $\alpha,\beta>0$, where position and momentum space representations are both ruled out.

To this end we use a Hilbert space representation of $\mathscr{A}$ on a generalized Fock space. The position and momentum operators can be represented as

$$\mathbf{x}=L(a^\dagger+a), \quad \mathbf{p}=iK(a^\dagger-a), \tag{10}$$

where the a and $a^\dagger$ obey generalized commutation relations

$$aa^\dagger-q^2a^\dagger a=1 \tag{11}$$

and act on the domain D of physical states $D:=\{|\psi\rangle=\text{polynomial}(a^\dagger)|0\rangle\}$ as

$$\begin{aligned} a|0\rangle&=0,\\ a^\dagger|n\rangle&=\sqrt{[n+1]}|n+1\rangle,\\ a|n\rangle&=\sqrt{[n]}|n-1\rangle, \end{aligned} \tag{12}$$

where $[n]$ denotes the partial geometric sum or "q"-number

$$[n]=\frac{q^{2n}-1}{q^2-1}, \tag{13}$$

and where the $|n\rangle:=([n]!)^{-1/2}(a^\dagger)^n|0\rangle$, $n=1,...,\infty$, are orthonormalized,

$$\langle n_1|n_2\rangle=\delta_{n_1,n_2}, \tag{14}$$

and D is analytic and dense in the Hilbert space $H=l^2$.

While **x** and **p** ordinarily are essentially self-adjoint, they are now merely symmetric, which is sufficient to insure that all expectation values are real. The deficiency indices of **x** and **p** are (1,1), implying the existence of one-parameter families of self-adjoint extensions. While ordinarily self-adjoint extensions, e.g., for a particle in a box, need to and can be fixed, there is now the subtle effect of the self-adjoint extensions not being on common domains, which prevents the diagonalization of **x** or **p** on physical states, as can also be understood through the uncertainty relations. For the full functional analytical details see Ref. 12, where these structures have first been found. We will come back to these functional analytical studies in Sec. VI where we will explicitly calculate the diagonalizations in H. They are of use for the calculation of inverses of **x**

and **p**, which are not only needed to describe certain quantum mechanical potentials, but ultimately also to invert kinetic terms, e.g., of the form $\mathbf{p}^2-m^2$ to obtain propagators from the field theoretical path integral (see Ref. 13).

III. MAXIMAL LOCALIZATION STATES

The absence of eigenvectors of **x** or **p** in all $*$-representations D of the commutation relations physically implies the absence of absolute localizability in position or momentum, i.e., there are no physical states that would have $\Delta x=0$ or $\Delta p=0$. More precisely, the uncertainty relation, holding in all D, implies a ''minimal uncertainty gap:''

$$\nexists|\psi\rangle\in D:\Delta x_{|\psi\rangle}<\Delta x_0 \quad \text{and} \quad \nexists|\psi\rangle\in D:\Delta p_{|\psi\rangle}<\Delta p_0. \tag{15}$$

The state of maximal localization in position $|\psi_x^{ml}\rangle$ with given position expectation x and vanishing momentum expectation is defined through

$$\langle\psi_x^{ml}|\mathbf{x}|\psi_x^{ml}\rangle=x, \quad \langle\psi_x^{ml}|\mathbf{p}|\psi_x^{ml}\rangle=0, \quad (\Delta x)_{|\psi_x^{ml}\rangle}=\Delta x_{\min}. \tag{16}$$

Explicitly the minimal uncertainty in position then reads

$$(\Delta x)^2_{|\psi_x^{ml}\rangle}=L^2\,\frac{q^2-1}{q^2}\left(1+(q^2-1)\,\frac{\langle\mathbf{x}\rangle^2}{4L^2}\right) \tag{17}$$

with the corresponding (now not infinite) uncertainty in momentum:

$$(\Delta p)^2_{|\psi_x^{ml}\rangle}=K^2\,\frac{(q^2+1)^2}{q^2(q^2-1)}\left(1+(q^2-1)\,\frac{\langle\mathbf{x}\rangle^2}{4L^2}\right). \tag{18}$$

We focus on maximal localization in **x**; the case of maximal localization in **p** is fully analogous.

As shown in Ref. 15, a state of maximal localization is determined by the equation

$$((\mathbf{x}-\langle\mathbf{x}\rangle)+i\alpha(\mathbf{p}-\langle\mathbf{p}\rangle))|\psi_x^{ml}\rangle=0, \tag{19}$$

where $\alpha=\Delta x/\Delta p$. Inserting Eqs. (17) and (18) we obtain

$$\alpha=\frac{L(q^2-1)}{K(q^2+1)}, \tag{20}$$

so that the condition reads

$$\left(\frac{q^2+1}{L}\,(\mathbf{x}-\langle\mathbf{x}\rangle)+i\,\frac{q^2-1}{K}\,\mathbf{p}\right)|\psi_x^{ml}\rangle=0. \tag{21}$$

A. Maximal localization states in the Fock basis

In order to explicitly calculate those states that realize the now maximally possible localization we expand the $|\psi_x^{ml}\rangle$ in the Fock basis,

$$|\psi_x^{ml}\rangle:=\frac{1}{\mathcal{N}(x)}\sum_{n=0}^{\infty}q^{-3n/2}c_n(x)|n\rangle, \tag{22}$$

where the $c_n(x)$ are real coefficients and

$$\mathcal{N}(x) := \sum_{n=0}^{\infty} q^{-3n} c_n^2(x) \tag{23}$$

is a normalization factor (the inserted factors $q^{-3n/2}$ will be convenient later).

The condition for maximal localization Eq. (21) reads in the Fock representation:

$$\left[(q^2+1)\left(a^\dagger + a - \frac{x}{L} \right) - (q^2-1)(a^\dagger - a) \right] |\psi_x^{ml}\rangle = 0. \tag{24}$$

Inserting the ansatz equation (22) we are led to the recursion relation

$$\frac{q+q^{-1}}{2L}\, x c_n(x) = \sqrt{q^{-1}[n+1]}\, c_{n+1}(x) + \sqrt{q[n]}\, c_{n-1}(x). \tag{25}$$

Together with

$$c_{-1}(x) = 0 \quad \text{and} \quad c_0(x) = 1, \tag{26}$$

the coefficients $c_n(x)$ are therefore determined as polynomials of degree n in x.

B. Relation to continuous *q*-Hermite polynomials

The coefficients $c_n(x)$ are related to the so-called continuous q-Hermite polynomials. An excellent review on these and other q-orthogonal polynomials is Ref. 20.

We use the notation of shifted q-factorials[20]

$$(a;q^2)_n := \prod_{k=0}^{n-1} (1 - a q^{2k}), \tag{27}$$

which obey the identity

$$(a;q^2)_n = (-a)^n q^{n(n-1)} (a^{-1};q^{-2})_n. \tag{28}$$

Furthermore, we define for later convenience

$$j(x) := \frac{\operatorname{arcsinh}(\omega x)}{\ln q}, \quad x(j) = \frac{q^j - q^{-j}}{2\omega}, \tag{29}$$

where

$$\omega := \frac{1}{4L} (q+q^{-1}) \sqrt{q^2-1}. \tag{30}$$

The continuous q-Hermite polynomials $H_n(z|q^2)$ are defined through

$$H_{-1}(z|q^2) = 0, \quad H_0(z|q^2) = 1, \tag{31}$$

and the recurrence relation (see Ref. 20)

$$2z H_n(z|q^2) = H_{n+1}(z|q^2) + (1-q^{2n}) H_{n-1}(z|q^2). \tag{32}$$

It is not difficult to check that this recursion relation can be brought into the form of the recursion relation equation (25) for the coefficients $c_n(x)$, by expressing them in terms of the $H_n(z|q^2)$ as

$$c_n(x)=\sqrt{\frac{q^n}{[n]!(q^2-1)^n}}\,i^{-n}H_n(i\omega x|q^2). \tag{33}$$

As shown in Ref. 20 the continuous q-Hermite polynomials $H_n(z|q^2)$ can be written as

$$H_n(z|q^2)=\sum_{k=0}^{n}\begin{pmatrix} n \\ k \end{pmatrix}_{q^2} e^{i(n-2k)\theta}, \quad z=\cos\,\theta, \tag{34}$$

with the q-binomial coefficients

$$\begin{pmatrix} n \\ k \end{pmatrix}_{q^2}=\frac{(q^2;q^2)_n}{(q^2;q^2)_k(q^2;q^2)_{n-k}}. \tag{35}$$

Inserting Eq. (34) into Eq. (33) and replacing $[n]!$ by

$$[n]!=\frac{(-)^n(q^2;q^2)_n}{(q^2-1)^n}=\frac{q^{n^2}(q^{-2};q^{-2})_n}{(q-q^{-1})^n} \tag{36}$$

yields

$$c_n(x)=\frac{1}{\sqrt{q^{n^2}(q^{-2};q^{-2})_n}}\,i^{-n}\sum_{k=0}^{n}\begin{pmatrix} n \\ k \end{pmatrix}_{q^2} e^{i(n-2k)\theta}, \quad i\omega x=\cos\,\theta. \tag{37}$$

Because of $i\omega x=\frac{1}{2}(q^{j(x)}-q^{-j(x)})$, we may also write $e^{i\theta}=iq^{j(x)}$ and therefore obtain the following exact expression for the coefficients $c_n(x)$:

$$c_n(x)=\frac{1}{\sqrt{q^{n^2}(q^{-2};q^{-2})_n}}\sum_{k=0}^{n}\begin{pmatrix} n \\ k \end{pmatrix}_{q^2}(-)^k q^{(n-2k)j(x)}. \tag{38}$$

We derive further useful properties of the $c_n(x)$.

Classical limit: For $q\to 1$ the recursion relation equation (25) reduces to

$$\frac{x}{L}\,c_n(x)=\sqrt{n+1}\,c_{n+1}(x)+\sqrt{n}\,c_{n-1}(x). \tag{39}$$

By substituting $x=L\sqrt{2}z$ and $H_n(z)=\sqrt{n!2^n}c_n(x)$ we obtain $H_0(z)=1$ and

$$2zH_n(z)=H_{n+1}(z)+2nH_{n-1}(z), \tag{40}$$

which is the defining recursion relation for classical Hermite polynomials $H_n(z)$. Thus the classical limit of the polynomials $c_n(x)$ is given by

$$\lim_{q\to 1}\,c_n(x)=\frac{1}{\sqrt{n!2^n}}\,H_n\left(\frac{x}{L\sqrt{2}}\right). \tag{41}$$

Representation by the formula of Rodriguez: As a short notation we write $x(j)$ as x_j. Then, introducing the q-difference operator

$$Df(x_j)=\frac{f(x_{j+1})-f(x_{j-1})}{x_{j+1}-x_{j-1}}, \tag{42}$$

the polynomials $c_n(x_j)$ can be expressed as

$$c_n(x_j)=\frac{(-)^n}{\kappa_n}\,q^{j^2}D^n q^{-j^2}, \tag{43}$$

where

$$\kappa_n=\sqrt{q^{-n^2}[n]!}\left(\frac{q+q^{-1}}{2L}\right)^n. \tag{44}$$

Equation (43) generalizes the formula of Rodriguez, $H_n(x)=(-)^n e^{x^2}(d^n/dx^n)e^{-x^2}$, for classical Hermite polynomials. A proof for Eq. (43) is outlined in Appendix A.

q-difference equation: The generalized formula of Rodriguez equation (43) implies that

$$c_n(x_{j+1})-c_n(x_{j-1})=\sqrt{q(1-q^{-2n})}(q^j+q^{-j})c_{n-1}(x_j), \tag{45}$$

which generalizes the differentiation rule $(d/dx)H_n(x)=nH_{n-1}(x)$ for classical Hermite polynomials. In order to prove this equation, we rewrite its lhs using Eqs. (42) and (43):

$$c_n(x_{j+1})-c_n(x_{j-1})=(x_{j+1}-x_{j-1})Dc_n(x_j)=(x_{j+1}-x_{j-1})D\,\frac{(-)^n}{\kappa_n}\,q^{j^2}D^n q^{-j^2}. \tag{46}$$

Carrying out the first differentiation on the rhs of this formula [c.f. Eq. (A1)], one obtains a linear combination of the polynomials $c_n(x_j)$ and $c_{n+1}(x_j)$, which in turn can be expressed through the recurrence relation equation (25) in terms of $c_{n-1}(x_j)$.

It can also be shown by induction that Eq. (45) implies the following q-difference equation for the polynomials $c_n(x)$;

$$q^j c_n(x_{j-1})+q^{-j}c_n(x_{j+1})=q^{-n}(q^j+q^{-j})c_n(x_j), \tag{47}$$

which corresponds to the differential equation $2xH_n'(x)-H_n''(x)=2nH_n(x)$ for classical Hermite polynomials.

Orthogonality: The polynomials $c_n(x)$ obey the orthogonality relation

$$\sum_{j=-\infty}^{\infty}(x_{2j+\kappa+1}-x_{2j+\kappa-1})q^{-(2j+\kappa)^2}c_m(x_{2j+\kappa})c_n(x_{2j+\kappa})=N_\kappa q^n\delta_{m,n}, \tag{48}$$

where

$$N_\kappa=\sum_{j=-\infty}^{\infty}(x_{2j+\kappa+1}-x_{2j+\kappa-1})q^{-(2j+\kappa)^2}. \tag{49}$$

The parameter $0\leqslant\kappa\leqslant 2$ can be choosen arbitrarily and fixes a family of positions occurring in the sum.

Equation (48) can be proved as follows. The case $m=n=0$ is trivial. For $n=0$ and $m>0$ one can show that the lhs of Eq. (48) is equal to

$$\sum_{j=-\infty}^{\infty}(x_{2j+\kappa+1}-x_{2j+k-1})D^m q^{-(2j+\kappa)^2}=D^{m-1}q^{-j^2}\Big|_{j=-\infty}^{j=+\infty}=0. \tag{50}$$

Keeping m fixed, a further induction for $n>0$ completes the proof.

Generating function: A generating function of the polynomials $c_n(x)$ is

$$(tq^{-j(x)};q^{-2})_\infty(-tq^{j(x)};q^{-2})_\infty=\sum_{n=0}^{\infty}\frac{c_n(x)}{\sqrt{q^{n(n-2)}(q^{-2};q^{-2})_n}}\,t^n. \tag{51}$$

In order to verify this expression, we use the q-difference equation Eq. (47) and obtain

$$\begin{aligned}&q^j(tq^{-j+1};q^{-2})_\infty(-tq^{j-1};q^{-2})_\infty+q^{-j}(tq^{-j-1};q^{-2})_\infty(-tq^{j+1};q^{-2})_\infty\\&\quad=(q^j+q^{-j})(tq^{-j-1};q^{-2})_\infty(-tq^{j-1};q^{-2})_\infty,\end{aligned} \tag{52}$$

which in turn can be proved by inserting the definition of the q-factorials [c.f. Eq. (27)].

IV. QUASI-POSITION AND MOMENTUM WAVE FUNCTIONS

Generally, all information on position and momentum is contained in the matrix elements of the position and momentum operators, and matrix elements can, of course, be calculated in arbitrary bases, such as the Fock basis. Ordinarily, the position and the momentum information content of a state $|\phi\rangle$ of the particle is easily obtained by writing the state as a position or momentum space wave function $\phi(x)=\langle x|\phi\rangle$ or $\phi(p)=\langle p|\phi\rangle$, which is to project onto position or momentum eigenstates, i.e., to project onto states of maximal localization in **x** or **p**.

In the new setting we can now project arbitrary states $|\phi\rangle$ onto the states which realize the maximally possible localization in position (or in momentum), which are given by Eqs. (16), (22), and (38). We call the collection of these projections the quasi-position wave function $\phi(x)$ of $|\phi\rangle$:

$$\phi(x):=\langle\psi_x^{ml}|\phi\rangle. \tag{53}$$

Here $\phi(x)$ yields the probability amplitude for finding the particle in a state of maximal localization around the position x with vanishing momentum expectation. As is easily seen from Eqs. (16), (21), and (24) the generalization to arbitrary momentum expectations is straightforward. The framework for quasi-momentum wave functions

$$\phi(p):=\langle\psi_p^{ml}|\phi\rangle \tag{54}$$

is analogous with $\phi(p)$ being the probability amplitude for finding the particle in a state of maximal localization in its momentum, with the momentum expectation p and vanishing position expectation (again the definition may easily be generalized to include arbitrary position expectations).

Aiming at the calculation of examples of quasi-wave functions, we need to complete our studies on the maximal localization states by calculating their norm and scalar product. To this end an important technical tool will be the Christoffel–Darboux theorem, for the application of which we will need the limiting cases of the coefficients $c_n(x)$ of the maximal localization states.

A. Limits of $(-1)^n c_{2n}(x)$ and $(-1)^n c_{2n+1}(x)$ for $n\to\infty$

As we prove in Appendix B, the polynomials $c_n(x)$, for all odd and for all even n have the nontrivial property that their limit for $n\to\infty$ exists. Denoting again $x_j:=x(j)$ these limits are

$$c^+(x_j)=\lim_{m\to\infty}(-)^m c_{2m}(x_j)=Aq^{j^2/2}\theta_2\left(\frac{\pi j}{2},\lambda\right), \tag{55}$$

$$c^-(x_j)=\lim_{m\to\infty}(-)^m c_{2m+1}(x_j)=Aq^{j^2/2}\theta_1\left(\frac{\pi j}{2},\lambda\right), \tag{56}$$

where $\theta_i(z,\lambda)$ are the Jacobi-, or elliptic θ-functions defined as

$$\theta_1(z,\lambda) := 2\lambda^{1/4}\sum_{n=0}^{\infty}(-)^n\lambda^{n(n+1)}\sin((2n+1)z), \tag{57}$$

$$\theta_2(z,\lambda) := 2\lambda^{1/4}\sum_{n=0}^{\infty}\lambda^{n(n+1)}\cos((2n+1)z), \tag{58}$$

and where in Eqs. (55) and (56) the constants λ and A are defined as

$$\lambda := e^{-\pi^2/(2\ln q)} \tag{59}$$

and

$$A^2 := \frac{\pi}{2(q^{-2};q^{-2})_\infty^3 \ln q} = \frac{2}{q^{1/4}\theta_2(0,q^{-1})\theta_2^2(0,\lambda)}. \tag{60}$$

B. Normalization and scalar product of maximal localization states

In order to evaluate the scalar product of two maximally localized states

$$\langle \psi_x^{ml} | \psi_{x'}^{ml} \rangle = \frac{1}{\sqrt{\mathcal{N}(x)\mathcal{N}(x')}} \sum_{n=0}^{\infty} q^{-3n} c_n(x) c_n(x') \tag{61}$$

the q-difference equation (47) can be used to rewrite this expression as

$$\langle \psi_x^{ml} | \psi_{x'}^{ml} \rangle = \frac{q^{j+j'} f_{j-1,j'-1} + q^{j-j'} f_{j-1,j'+1} + q^{j'-j} f_{j+1,j'-1} + q^{-j-j'} f_{j+1,j'+1}}{(q^j+q^{-j})(q^{j'}+q^{-j'})\sqrt{\mathcal{N}(x)\mathcal{N}(x')}}, \tag{62}$$

where we defined

$$f_{j,j'} := \sum_{n=0}^{\infty} q^{-n} c_n(x) c_n(x') \tag{63}$$

and where we abbreviated $j := j(x)$ and $j' := j(x')$. We can compute $f_{j,j'}$ by applying the Christoffel–Darboux[21] theorem,

$$\sum_{n=0}^{m} q^{-n} c_n(x) c_n(x') = \frac{2L\sqrt{[m+1]}}{q^{m+1/2}(q+q^{-1})} \frac{c_{m+1}(x)c_m(x') - c_m(x)c_{m+1}(x')}{x-x'}, \tag{64}$$

which can be proved as follows. For $m>0$ (the case $m=0$ is trivial), we use the recursion relation [c.f. Eq. (25)]

$$c_{m+1}(x) = \sqrt{\frac{q}{[m+1]}}\left(\frac{q+q^{-1}}{2L} x c_m(x) - \sqrt{q[m]}\, c_{m-1}(x)\right) \tag{65}$$

in order to replace $c_{m+1}(x)$ and $c_{m+1}(x')$ on the rhs of Eq. (64), which then takes the form

$$\text{rhs} = q^{-m} c_m(x) c_m(x') - \frac{2L\sqrt{[m]}}{q^{m-1/2}(q+q^{-1})} \frac{c_{m-1}(x)c_m(x') - c_m(x)c_{m-1}(x')}{x-x'} \tag{66}$$

so that Eq. (64) follows by induction.

Since the polynomials $c_m(x)$ have well-defined limits as m goes to infinity, the Christoffel–Darboux theorem implies that the expression $f_{j,j'}$ is given by

$$f_{j,j'}=\sum_{n=0}^{\infty} q^{-n}c_n(x)c_n(x')=\frac{\sqrt{q}}{2\omega}\,\frac{c^-(x)c^+(x')-c^+(x)c^-(x')}{x-x'}. \tag{67}$$

Inserting Eqs. (55) and (56) yields

$$f_{j,j'}=\frac{2A^2q^{1/2(j^2+j'^2+1)}}{q^j-q^{-j}-q^{j'}+q^{-j'}}\;\theta_1\left(\frac{\pi}{2}(j-j'),\lambda^2\right)\theta_4\left(\frac{\pi}{2}(j+j'),\lambda^2\right) \tag{68}$$

with the definition of θ_4 being

$$\theta_4(z,\lambda^2):=1+2\sum_{n=1}^{\infty}(-)^n\lambda^{2n^2}\cos(2nz). \tag{69}$$

In the limit $x\to x'$, Eq. (68) reduces to

$$f_{j,j}=\sum_{n=0}^{\infty} q^{-n}c_n^2(x)=\frac{q^{j^2+1/4}\theta_2(0,q^{-1})}{(q^j+q^{-j})\,\theta_4(0,\lambda^2)}\;\theta_4(\pi j,\lambda^2). \tag{70}$$

Inserting Eq. (67) into Eq. (62) we eventually obtain an exact expression for the scalar product of two quasi-position states:

$$\langle\psi_x^{ml}|\psi_{x'}^{ml}\rangle=\frac{2A^2q^{(1/2)(j^2+j'^2+1)}(q^2-1)^2(1+q^{-2})}{\sqrt{\mathcal{N}(x)\mathcal{N}(x')}G^0_{j,j'}G^1_{j,j'}G^{-1}_{j,j'}}\;\theta_1\left(\frac{\pi}{2}(j'-j),\lambda^2\right)\theta_4\left(\frac{\pi}{2}(j+j'),\lambda^2\right), \tag{71}$$

where

$$G^s_{j,j'}=(q^{(1/2)(j-j')+s}-q^{-(1/2)(j-j')-s})(q^{(1/2)(j+j')+s}+q^{-(1/2)(j+j')-s}). \tag{72}$$

Note that the poles in the denominator of Eq. (71) are cancelled by the zeros of the θ_1-function. The limit $x\to x'$ yields the norm [Eq. (23)]

$$\mathcal{N}(x)=\frac{2q^{j^2}(q^2+1)\,\theta_4(\pi j,\lambda^2)}{A^2(q^j+q^{-j})(q^{j+1}+q^{-j-1})(q^{j-1}+q^{-j+1})\,\theta_2^2(0,\lambda)\lambda_4(0,\lambda^2)}. \tag{73}$$

C. Example: The quasi-position wave function of $|\psi_0^{ml}\rangle$

As an example we draw in Fig. 1 the graph of the quasi-position wave function $\phi(x)$ for the state $|\phi\rangle$ that describes maximal localization around $x=0$, i.e., for $|\phi\rangle:=|\psi_x^{ml}\rangle$, i.e., with

$$\phi(x)=\langle\psi_x^{ml}|\psi_0^{ml}\rangle. \tag{74}$$

The analytic form of the wave function is given in Eq. (71). For the width of the main peak note that the graph shows the overlap of pairs of localization states, each with its finite position uncertainty.

We have thus generalized the treatment of Ref. 15 where the corresponding graph was calculated and drawn for the special case without a minimal momentum uncertainty ($\alpha=0,\beta>0$).

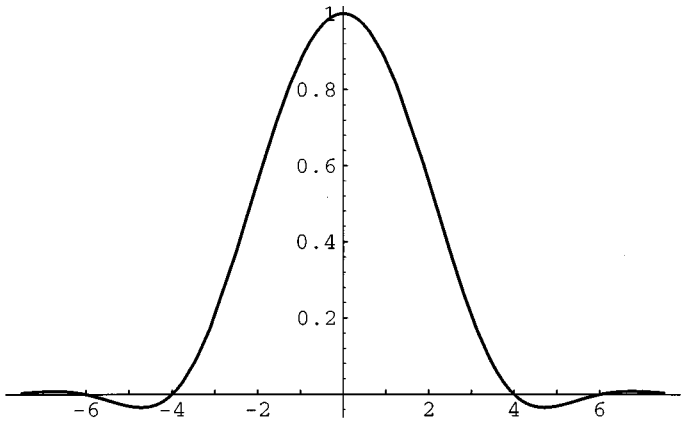

FIG. 1. Quasi-position wave function $\phi(x)$ for $|\phi\rangle := |\psi_0^{ml}\rangle$, drawn over $j(x)$ for $q=1.5$.

V. APPROXIMATIONS

For potential applications of the formalism the parameters α and β in Eq. (2) can be assumed small, in which case useful simplifications hold.

In the notation of Eq. (3) this is the case when $q\to 1$. Then $\lambda\to 0$ and the θ-functions in Eqs. (55) and (56) can be approximated by $\theta_1(\pi j/2,\lambda)\approx 2\lambda^{1/4}\sin \pi j/2$ and $\theta_2(\pi j/2,\lambda)\approx 2\lambda^{1/4}\cos \pi j/2$. This implies that

$$c^+(x_j)\approx \tilde{c}^+(x_j) := Bq^{j^2/2}\cos\frac{\pi j}{2},$$
$$c^-(x_j)\approx \tilde{c}^-(x_j) := Bq^{j^2/2}\sin\frac{\pi j}{2}, \tag{75}$$

where

$$B^4=\frac{4\ln q}{\pi\sqrt{q}}. \tag{76}$$

The relative error of this approximation is illustrated in Table I. Using Eq. (75) we can give approximations for the scalar product for q close to 1:

$$\langle \psi_x^{ml}|\psi_{x'}^{ml}\rangle \approx \frac{B^2 q^{(1/2)(j^2+j'^2+1)}(q^2-1)^2(1+q^{-2})}{\sqrt{\tilde{\mathcal{N}}(x)\tilde{\mathcal{N}}(x')}G^0_{j,j'}G^1_{j,j'}G^{-1}_{j,j'}}\sin\frac{\pi}{2}(j'-j), \tag{77}$$

where

TABLE I. Relative error of the approximation of the $c^{\pm}$.

q	1.2	1.5	2	5
$\left\lvert 1-\frac{\tilde{c}^{\pm}(x)}{c^{\pm}(x)}\right\rvert$	$<5\times10^{-15}$	$<1\times10^{-10}$	$<2\times10^{-6}$	$<7\times10^{-3}$

$$\mathcal{N}(x)\approx\tilde{\mathcal{N}}(x):=\frac{2q^{j^2}(q^2+1)}{B^2(q^j+q^{-j})(q^{j+1}+q^{-j-1})(q^{j-1}+q^{-j+1})}. \tag{78}$$

For example, for $1<q<1.2$, the relative error of this approximation is less than 10^{-14}.

It is interesting to consider also the limiting case where

$$q\to 1, \quad K(q):=\sqrt{\frac{q^2-1}{4\beta}}, \quad L(q)=\hbar\,\frac{q^2+1}{2}\,\sqrt{\frac{\beta}{q^2-1}}. \tag{79}$$

In this limit the commutation relations equation (3) turn into the relations equation (2) with β finite but $\alpha=0$, which is the special case considered in Ref. 15. There is then only a minimal uncertainty in position and no minimal uncertainty in momentum. As can be shown easily, the limit $q\to 1$ of the scalar product equations (77) and (78) is given by

$$\lim_{q\to 1}\langle\psi^{ml}_{x'}|\psi^{ml}_{x}\rangle=\frac{\sin\dfrac{\pi}{2}(j'-j)}{\pi\left(\dfrac{j-j'}{2}\right)\left(\dfrac{j-j'}{2}+1\right)\left(\dfrac{j-j'}{2}-1\right)}. \tag{80}$$

In the limit given by Eqs. (79), x and j are related linearly through $x_j=x(j)=\hbar\sqrt{\beta}j$. We thus obtain the limiting expression for the scalar product:

$$\langle\psi^{ml}_{x'}|\psi^{ml}_{x}\rangle=\frac{1}{\pi}\left[\frac{x-x'}{2\hbar\sqrt{\beta}}-\left(\frac{x-x'}{2\hbar\sqrt{\beta}}\right)^3\right]^{-1}\sin\left(\frac{x-x'}{2\hbar\sqrt{\beta}}\,\pi\right). \tag{81}$$

This result coincides with the expression found in Ref. 15, thus providing a nontrivial consistency check: We calculated the scalar product using q-analysis on a discrete q-Fock space representation. However, the calculation[15] of this scalar product in the special case $\alpha=0$, which we here recover in the limit, had been performed with entirely different analytic methods in a continuous representation.

VI. SELF-ADJOINT EXTENSIONS OF x AND p

In this section we continue formal considerations of Ref. 12 where it was proved that the operators **x** and **p** separately do have one-parameter families of self-adjoint extensions in H. To be precise, **x** on D is symmetric, while its adjoint $\mathbf{x}^*$ is closed but nonsymmetric; $\mathbf{x}^{**}$ is closed and symmetric and has deficiency indices (1,1). There are families of diagonalizations of **x** in H, though of course not in D. The same holds for **p**. The corresponding eigenvectors are unphysical states, separated from the physical domain by the minimal uncertainty gap [see Eq. (15)].

While in Ref. 12 the existence only of self-adjoint extensions had been proven, we can now explicitly solve the eigenvalue problem

$$\mathbf{x}\cdot|v_x\rangle=x|v_x\rangle. \tag{82}$$

For the solution we make the ansatz

$$|v_x\rangle=N^{-1}(x)\sum_{n=0}^{\infty}q^{-n/2}d_n(x)|n\rangle \tag{83}$$

yielding the recurrence relation

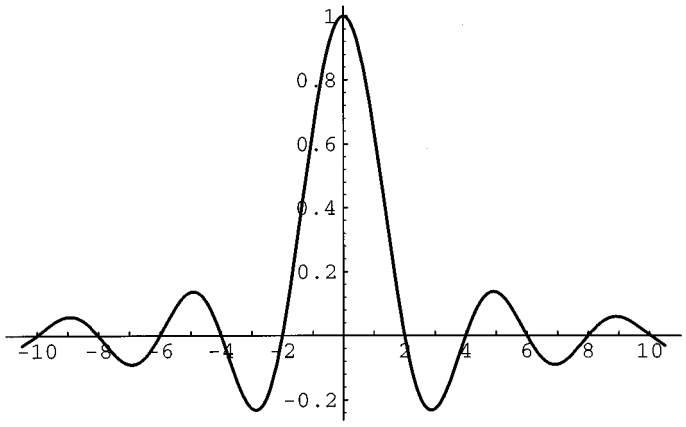

FIG. 2. Scalar product $\langle v_x|v_0\rangle$ of formal eigenvectors, drawn over $j(x)$.

$$\frac{x}{L}\, d_n(x) = \sqrt{[n+1]q^{-1}}\, d_{n+1}(x) + \sqrt{q[n]}\, d_{n-1}(x) \tag{84}$$

with $d_{-1}=0$ and $d_0=1$. In fact, Eq. (84) can be transformed into the recurrence relation equation (25), i.e., the d_n can be transformed into our previously considered coefficients c_n:

$$d_n(x) = c_n(2x(q+q^{-1})^{-1}). \tag{85}$$

In the expansion of $|v_x\rangle$, the factor $q^{-n/2}$ is different from the corresponding factor $q^{-3n/2}$ in the expansion of the $|\psi_x^{ml}\rangle$, implying that the scalar product and normalization constant of the formal eigenvectors are different from those of the maximal localization states which we had calculated earlier:

$$N(x) = = \frac{q^{j^2+1/4}\theta_4(\pi j,\lambda^2)\,\theta_2(0,q^{-1})}{(q^j+q^{-j})\,\theta_4(0,\lambda^2)}, \tag{86}$$

$$\langle v_x|v_{x'}\rangle = \frac{A^2 q^{1/2(j^2+j'^2+1)}\theta_1\left(\frac{\pi}{2}(j-j')\lambda^2\right)\theta_4\left(\frac{\pi}{2}(j+j'),\lambda^2\right)}{(x-x')\,\overline{\omega}\sqrt{N(x)N(x')}}, \tag{87}$$

where now

$$x(j) := \frac{q^j - q^{-j}}{2\overline{\omega}} \quad \text{with} \quad \overline{\omega} = \frac{\sqrt{q^2-1}}{2L} \tag{88}$$

and where we abbreviated again $j' := j(x')$.

In Fig. 2 we draw the graph of the scalar product over j for $j'=0$. From the zeroes of θ_1 we read off that the $|v_x\rangle$ are mutually othogonal for $j-j' \in 2\mathbb{N}$. Using j' as a parameter in the range $j' \in [0, 2[$ we identify for each value of j' a diagonalization of **x**. Thus, j' labels the self-adjoint extensions with the corresponding eigenvalues $(x_n)_{n\in\mathbb{N}}$ being

$$x_n = \frac{q^{2n+j'} - q^{-2n-j'}}{2\sqrt{q^2-1}}\, L = \frac{\sinh((2n+j')\ln q)}{\sqrt{q^2-1}}\, L \quad (n \in \mathbb{N}). \tag{89}$$

Compare this also with the graph of the scalar product which had been calculated only numerically in Ref. 12. Having found the analytic form of the scalar product in terms of θ-functions, we were able to determine the one-parameter family of diagonalizations of **x**, of which we had so far only known its existence. As is not difficult to see, we recover for vanishing minimal uncertainty in momentum, i.e., for $\alpha \to 0$, the linear spectrum found in Ref. 15 for that special case.

Analogously to above we obtain the eigenvalues of **p** in its self-adjoint extensions ($j'' \in [0, 2[$):

$$p_n = \frac{q^{2n+j''} - q^{-2n-j''}}{2\sqrt{q^2-1}} K = \frac{\sinh((2n+j'')\ln q)}{\sqrt{q^2-1}} K \quad (n \in \mathbb{N}). \tag{90}$$

We stress that the parameters j', j'' of Eqs. (89) and (90) label *different* extensions of the domain D of **x** and **p**. Recall that the uncertainty relation implies that the formal **x**- or **p**- eigenvectors which we here calculated do not lie in any *common* extension of the domain D of **x** and **p**. They are not physical states and are separated from the physical domain by the uncertainty gap [see Eq. (15)].

However, these families of diagonalizations of **x** or **p** in H- can still be of use, e.g., for the calculation of inverses of **x** and **p**, which would have been difficult to invert as nondiagonal operators in the Fock basis $\mathbf{x} = L(a + a^\dagger)$ and $\mathbf{p} = iK(a - a^\dagger)$.

VII. OUTLOOK

In quantum field theory, interaction terms, which on ordinary geometry would be ultraviolet regular but nonlocal, can in fact be regular and strictly local on a geometry with a minimal position uncertainty. The reason is that an interaction is to be considered strictly local if no nonlocality could be observed. Intuitively this is the case if a small apparent nonlocality of the interaction term is unobservable due to a comparatively larger minimal uncertainty in the underlying space. We already mentioned that, as has been shown in Ref. 13, quantum field theories can be naturally regularized when working on a generalized geometry with intrinsic minimal uncertainties. Generally, in order to explicitly compare the size of nonlocality of an arbitrary interaction term with the size of the intrinsic uncertainty of the generalized geometry it is crucial to have available the states of maximal localization on this geometry. Similarly, maximal localization in a momentum space with minimal uncertainty Δp_0 is of interest in the context of infrared regularization.

So far, we have studied the properties of the maximal localization states in one dimension only. The generalized Fourier transformations which map between the (quasi-) position and the (quasi-) momentum representations have only been studied in the special case $\alpha = 0$. For the general case techniques should be useful which have been developed for the Fourier theory[22] on quantum planes.[23] Also, the unitary equivalence of *all* Hilbert space representations, in the sense in which it holds for the ordinary commutation relations, has not yet been proven. Most interesting further physical insight into the nature of these generalized geometries can be expected from studies on maximal localization in n dimensions where $[\mathbf{x}_i, \mathbf{x}_j] \neq 0$ and $[\mathbf{p}_i, \mathbf{p}_j] \neq 0$ lead also to $\Delta x_i \Delta x_j \neq 0$ and $\Delta p_i \Delta p_j \neq 0$. Work in this direction is in progress.

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APPENDIX A: GENERALIZED FORMULA OF RODRIGUEZ

In the following we outline a proof for the equivalence of the formula of Rodriguez Eq. (43) and the recurrence relation Eq. (25). We use the notation $Af(x_j) := \frac{1}{2}(f(x_{j-1}) + f(x_{j+1}))$, which allows the differentiation of products to be written in the form

$$D(fg) = (Df)(Ag) + (Af)(Dg). \tag{A1}$$

We first prove the identity

$$D^{n+1} q^{-j^2} = -\left(\frac{q+q^{-1}}{2L}\right)^2 (q^{-2n+1}[n] D^{n-1} + x q^{-n} D^n) q^{-j^2}. \tag{A2}$$

The case $n=0$ can be verified easily by hand. Induction from n to $n+1$ implies that

$$D^{n+1} q^{-j^2} = D(D^n q^{-j^2}) = -D\left(\frac{q+q^{-1}}{2L}\right)^2 (q^{-2n+3}[n-1] D^{n-2} + x q^{-n+1} D^{n-1}) q^{-j^2}. \tag{A3}$$

Comparing the rhs of Eqs. (A2) and (A3) and using Eq. (A1), one is led to the condition

$$(A D^{n+1} + \tfrac{1}{2}(q - q^{-1}) x D^n - q^{-n} D^{n-1}) q^{-j^2} = 0, \tag{A4}$$

which can be proved by a further induction where the identities

$$Dx = 1, \quad Ax = \tfrac{1}{2}(q+q^{-1})x, \quad DA - \tfrac{1}{2}(q+q^{-1})AD = \tfrac{1}{4}(q-q^{-1})^2 x D^2$$

turn out to be very useful. Once Eq. (A2) is proved, one obtains the recursion relation Eq. (25) by inserting the formula of Rodriguez which completes the proof.

APPENDIX B: THE LIMITS $c^{\pm}(x)$

We prove the limits $c^{\pm}(x)$, i.e., we prove Eqs. (55) and (60):

$$c^{+}(x_j) = \lim_{m \to \infty} (-)^m c_{2m}(x_j) = \sqrt{\frac{\pi}{2(q^{-2};q^{-2})_\infty^3 \ln q}}\, q^{j^2/2} \theta_2\left(\frac{\pi j}{2}, \lambda\right). \tag{B1}$$

Let us first rewrite expression Eq. (38) by

$$c_{2m}(x_j) = \frac{1}{q^{2m^2}\sqrt{(q^{-2};q^{-2})_{2m}}} \sum_{k=-m}^{m} \begin{pmatrix} 2m \\ m+k \end{pmatrix}_{q^2} (-)^{m+k} q^{2kj}. \tag{B2}$$

Choosing an integer $0 < r < m$, we split up this sum into two parts:

$$(-)^m c_{2m}(x_j) = S^{(1)}_{m,r} + S^{(2)}_{m,r}, \tag{B3}$$

where

$$S^{(1)}_{m,r} = \frac{1}{q^{2m^2}\sqrt{(q^{-2};q^{-2})_{2m}}} \sum_{k=-r}^{r} \begin{pmatrix} 2m \\ m+k \end{pmatrix}_{q^2} (-)^k q^{2kj}, \tag{B4}$$

$$S^{(2)}_{m,r} = \frac{1}{q^{2m^2}\sqrt{(q^{-2};q^{-2})_{2m}}} \sum_{k=r+1}^{m} \begin{pmatrix} 2m \\ m+k \end{pmatrix}_{q^2} (-)^k (q^{2kj} + q^{-2kj}). \tag{B5}$$

Now let m go to infinity and keep r fixed. From $q^2>1$ and Eq. (28) we have the identity

$$\left(\begin{matrix}2m\\ m+k\end{matrix}\right)_{q^2}=q^{2(m^2-k^2)}\left(\begin{matrix}2m\\ m+k\end{matrix}\right)_{q^{-2}}. \tag{B6}$$

Because of

$$\lim_{m\to\infty}\left(\begin{matrix}2m\\ m+k\end{matrix}\right)_{q^{-2}}=\frac{1}{(q^{-2};q^{-2})_\infty}, \tag{B7}$$

the first part converges to

$$S_r^{(1)}=\lim_{m\to\infty}S_{m,r}^{(1)}=\frac{1}{(q^{-2};q^{-2})_\infty^{3/2}}\sum_{k=-r}^{r}(-)^k q^{2kj-2k^2}. \tag{B8}$$

The second part, $S_{m,r}^2$, can be estimated as follows. As can be seen from Eq. (B6) the inequality

$$\left(\begin{matrix}2m\\ m+k\end{matrix}\right)_{q^{-2}}=\frac{\Pi_{i=m+k+1}^{2m}(1-q^{-2i})}{\Pi_{i=1}^{m-k}(1-q^{-2i})}\leqslant\frac{1}{\Pi_{i=1}^{2m}(1-q^{-2i})}=\frac{1}{(q^{-2};q^{-2})_{2m}} \tag{B9}$$

implies that

$$\left(\begin{matrix}2m\\ m+k\end{matrix}\right)_{q^2}\leqslant\frac{q^{2(m^2-k^2)}}{(q^{-2};q^{-2})_\infty}. \tag{B10}$$

Therefore,

$$|S_{m,r}^{(2)}|\leqslant\frac{2}{q^{2m^2}\sqrt{(q^{-2};q^{-2})_{2m}}}\sum_{k=r+1}^{m}\left(\begin{matrix}2m\\ m+k\end{matrix}\right)_{q^2}q^{2kj}\leqslant\frac{2}{(q^{-2};q^{-2})_{2m}^{3/2}}\sum_{k=r+1}^{m}q^{2(kj-k^2)}, \tag{B11}$$

so that

$$|S_r^{(2)}|=|\lim_{m\to\infty}S_{m,r}^{(2)}|\leqslant\frac{2q^{2rj-2r^2}}{(q^{-2};q^{-2})_\infty^{3/2}}\sum_{k=1}^{\infty}q^{2(kj-k^2)}. \tag{B12}$$

Since the sum on the rhs is finite, this expression tends to zero as r goes to infinity. Thus we conclude that

$$c^+(x_j)=\lim_{r\to\infty}S_r^{(1)}=\frac{1}{(q^{-2};q^{-2})_\infty^{3/2}}\sum_{k=-\infty}^{\infty}(-)^k q^{2kj-2k^2}. \tag{B13}$$

The sum on the rhs of this expression is essentially a Jacobi θ_2-function. In order to see this, notice that its definition Equation (58) can also be written as

$$\theta_2(z,e^{-\tau})=\sqrt{\frac{\pi}{\tau}}\sum_{k=0}^{\infty}(-)^k e^{-(1/\tau)(z-\pi k)^2}. \tag{B14}$$

Inserting $\tau=-\ln\lambda=\pi^2/(2\ln q)$ and $z=\pi j/2$ we can express the sum in Eq. (B13) by

$$\sum_{k=-\infty}^{\infty} (-)^k q^{-2k^2+2kj} = \sqrt{\frac{\pi}{2\ln q}}\, q^{j^2/2}\theta_2(z,\lambda), \tag{B15}$$

which completes the proof for $c^+(x_j)$. The proof for $c^-(x_j)$ follows the same lines.

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Discrete decay and continuous measurement

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In this paper measurement is defined via an observation operator with simple, purely discrete spectrum. When the quantum Zeno effect holds, a continuously measured quantum process with fixed initial state ''freezes'' in that state. Such states are called ''regular'' states. If the final state is also fixed, then movement from the initial state to the final state is forced to occur, whether or not the initial state is regular. This forced movement is studied here in the context of a discrete state model which contains a distinguished nonregular state which mediates all transitions. In this model the forced movement between any two states satisfies a ''least action'' principle, wherein action is identified with change of state transitions. For completeness, the model is also studied when only the initial state is fixed under continuous measurement. In that case the distinguished state exhibits exact exponential decay at all times. The model is of interest independently of issues related to continuous measurement inasmuch as it is a ''discrete'' approximation to a ''continuous'' decay model. More precisely, the distinguished state exhibits exact exponential decay on a finite time interval which expands without bound as the discrete decay products densely approach the continuum. This unexpected result provides a striking confirmation of Fermi's ''golden rule.'' © *1996 American Institute of Physics.* [S0022-2488(96)00405-X]

I. OVERVIEW OF THE PAPER

A. Introduction

When the quantum Zeno effect holds,[1] a continuously observed quantum process with fixed initial state ''freezes'' in that state. Such states are called ''regular'' states. In nonregular cases the quantum Zeno effect fails and decay is observed.[2] Recently the study of continuously observed quantum processes where both the initial and final states are fixed was undertaken in Kanter.[3] Under hypotheses which imply that all states are regular, it was shown that fixing the final state forces the process to perform a well-behaved stochastic motion from initial to final state. This motion satisfies a ''least action'' principle, wherein action is identified with change of state transitions. In this paper we will show that this result continues to hold in the nonregular case for a particularly simple quantum model with decay. For completeness we will also study the effect of continuous measurement in this model when only the initial state is fixed. The model is of interest independently of issues related to continuous measurement inasmuch as it is a ''discrete'' approximation to a ''continuous'' decay model. More precisely a distinguished state exists which exhibits exact exponential decay on a finite time interval which expands without bound as the discrete decay products densely approach the continuum. This unexpected result provides a striking confirmation of Fermi's ''golden rule.''

For our purposes a quantum process is characterized by a strongly continuous group $(U(t):t\in R)$ of unitary operators acting on a given Hilbert space L, where R stands for the real line. We shall assume that L is separable and single out a particular basis $\{\phi_j:j\in J\}$ for L, consisting of the normalized eigenvectors of a quantum observable with simple, purely discrete spectrum. We shall call $\{\phi_j:j\in J\}$ a *discrete measurement basis.* If the quantum process is in the

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pure state ϕ before measurement, then $|\langle\phi|\phi_j\rangle|^2$ is the probability that the process is in the pure state ϕ_j just after measurement. We shall say that the element j in J is observed when the process is in state ϕ_j after a measurement. In between measurements the pure state ϕ evolves according to the equation $\phi(t)=U(t)\phi$. The infinitesimal generator of the group $U(t)$, called the Hamiltonian of the quantum process, is written as the self-adjoint operator H. [Thus $U(t)=e^{itH}$.]

The rate of decay of a state ϕ_j in the measurement basis is defined as the right-hand derivative at zero of the function $-|\langle\phi_j|\phi_j(t)\rangle|^2$. We say $\{\phi_j : j\in J\}$ is a *discrete decay model* if there is a distinguished state d in J such that ϕ_d is not regular. The other states $\{\phi_j : j\neq d\}$ in the basis may be viewed as decay products from the state ϕ_d. [Note that a discrete decay model is specified by the entire collection $\langle\phi_j|\phi_k(t)\rangle$ of functions for $j,k\in J$, rather than just the function $\langle\phi_d|\phi_d(t)\rangle$.]

In this paper we shall study quantum measurements which are ''nonselective,'' other than the selection at initial or final times. Specifically, let $a,b\in J$ and let $0=t_0<N^{-1}=t_1<\cdots<t_{N-1}=(N-1)N^{-1}<t_N=1$ denote the instants at which the quantum process is measured via the observable corresponding to $\{\phi_j : j\in J\}$. We consider an ensemble of independent replications of the $N+1$ sequential measurements above and then restrict our attention to the subensemble of replications for which $j_0=a$ is observed at time 0. The observed values $(j_n : 0\leqslant n\leqslant N)$ will have a well-defined statistical distribution P_N^a, given this subensemble. This distribution has physical meaning as a summary of the statistical results to be expected in such an experiment, i.e., what fraction of measurements do we find the process in state ϕ_j at time N^{-1} and in state ϕ_k at time $2N^{-1}$, given that it was in state ϕ_0 at time 0. Similarly, if we restrict our attention to the subensemble of replications for which $j_0=a$ is observed at time 0 and $j_N=b$ is observed at time 1, then the observed values will have a well-defined distribution P_N^{ab}, given this subensemble. We note that the measures P_N^a and P_N^{ab} are not consistent as N varies. The distribution of the observed value at $t=\frac{1}{2}$ (for instance) depends on N, because measurement affects the evolution of a quantum process.

As $N\to\infty$ the limit of P_N^a will yield the distribution of a continuously measured quantum process with initial state ϕ_a, whereas the limit of P_N^{ab} will yield the distribution of a continuously measured quantum process with initial state ϕ_a and final state ϕ_b. The study of the limit as $N\to\infty$ for the measures P_N^{ab} is both more difficult and more novel than for the measures P_N^a. The primary purpose of this paper is to study the limit behavior of the measures P_N^{ab} in the context of our discrete decay model. For completeness we will also study the measures P_N^a as well. (We note that we can trivially construct a discrete decay model by letting the distinguished state $\phi_d=(\pi(1+x^2))^{-1/2}$, where H is multiplication by x. Then $\langle\phi_d|U(t)\phi_d\rangle=\exp(-|t|)$. If we let $\{\phi_j : j\in J\}$ stand for any orthonormal basis of $L^2(R)$ containing ϕ_d, then we get a discrete decay model. Unfortunately we do not know how to further specify the decay products ϕ_j so as to be able to characterize the limit behavior of the measures P_N^{ab} for such a model.)

B. Relation to previous work

In Sec. IV we will establish a result (Theorem A) for our discrete decay model, wherein the measures P_N^d approach a distribution with exponential waiting time to leave ϕ_d as $N\to\infty$. A similar result was previously proven for a large class of quantum processes in Kanter,[4] however, it is not evident that our discrete decay model is a member of this class.

The measures P_N^{ab} were first considered in Kanter,[5] whose results we paraphrase in the context of our discrete decay model as Theorem B in Sec. IV. This theorem establishes the least action principle associated with our discrete decay model under continuous measurement. Whereas the original version of Theorem B was proved for quantum processes whose Hamiltonian was a Hilbert–Schmidt operator, such a strong hypothesis is not necessary here. On the other hand, the model considered in this paper is special in that the measurement basis contains a distinguished state ϕ_d with the property that no change of state transitions occur unless one of the states involved is ϕ_d.

Many decay models with a distinguished state ϕ_d as above have been postulated, such as the famous Friedrichs–Lee model.[6] These models involve nonseparable Hilbert spaces, and the decay products $\{\phi_j : j \neq d\}$ contain a continuum of generalized Dirac delta functions. Thus, these models may be called ''continuous'' decay models. (Note that our simplistic approach to measurement relies on J being countable.)

Discrete decay models have been previously considered by Davis[7] and Cohen-Tannoudji *et al.*[8] In these models the set J is decomposed as

$$J = \{d\} \cup J_0, \tag{1.1}$$

where J_0 is a subset of the integers. Given a positive number Δ and a complex number c, these authors consider a Hamiltonian $H = H(\Delta, c)$ satisfying

$$H\phi_j = c\Delta^{1/2}\phi_d + j\Delta\phi_j \quad (\text{for } j \neq d). \tag{1.2}$$

With various levels of precision they show that

$$\lim_{\Delta \to 0} \langle \phi_d | e^{itH} \phi_d \rangle = \exp(-\pi\alpha|t|) \quad (\text{for } t \in R), \tag{1.3}$$

where $\alpha = |c|^2$. [Davies does not state (1.3) precisely and defines $J_0 = J_0(\Delta)$ to be the set of integers with absolute value bounded by $K\Delta^{-1}$ for some constant K. Thus, Davies' model is only an ''approximate'' discrete decay model, since ϕ_d is regular and only becomes nonregular in the limit as $\Delta \to 0$. Cohen-Tannoudji *et al.* let $J_0 = Z$ and state (1.3) precisely, indicating its connection with Fermi's ''golden rule.'' However, their treatment of the model is not mathematically rigorous.] The parameter Δ is the energy gap between the decay products ϕ_j. Thus, as $\Delta \to 0$, the decay products ϕ_j densely approach the continuum of Dirac delta functions.

In this paper we shall treat the model (1.2) with $J_0 = Z$ in a mathematically rigorous fashion to obtain the new and striking result

$$\langle \phi_d | e^{itH} \phi_d \rangle = \exp(-\pi\alpha|t|) \quad (\text{for } |t| \leqslant 2\pi\Delta^{-1}). \tag{1.4}$$

[We derive a recursive expression for $\langle \phi_d | e^{itH} \phi_d \rangle$ outside the interval $|t| \leqslant 2\pi\Delta^{-1}$.] We note that (1.3) is a direct consequence of (1.4). We shall see that $\phi_d \notin D(H)$, the domain of H, and that under continuous observation the model exhibits exact exponential decay at all times if ϕ_d is the initial state.

C. Summary of other sections

The rest of this paper is divided into five sections. In Sec. II we shall present the main features of our discrete decay model, but will delay the proofs of some of our results until Secs. V and VI. In Sec. III we will determine decay rates and bounds for all the states ϕ_j in the measurement basis for our model. In Sec. IV we will use the results of Sec. III in order to study the limiting behavior of P_N^a and P_N^{ab} for our model. In particular we will state and prove Theorems A and B. In Secs. V and VI we will put our model on a mathematically rigorous footing. In particular, Sec. VI contains a derivation of the key equation (1.4).

II. THE MODEL

In this section we will present the main features of our discrete decay model, though we will delay the nontrivial proofs of our first two theorems until Secs. V and VI. We start by gathering some definitions.

Definition 2.1: We let C stand for the set of all complex numbers c and write $\overline{c} = u - iv$ if $c = u + iv$ for $u, v \in R$. We let Z stand for the set of all integers and Z' for the set of nonzero

integers. We let $R-Z$ stand for the set of real numbers not in Z. We let $L_2(Z')$ represent the set of all square summable C-valued sequences indexed by Z'. We let $\langle\cdot|\cdot\rangle$ stand for the usual inner product on $L_2(Z')$, i.e.,

$$\langle x|y\rangle=\sum_{n\in Z'}\overline{x_n}y_n \quad [\text{for } x,y\in L_2(Z')]. \tag{2.1}$$

From now on all measurement bases will be indexed by the set

$$Z_d=\{d\}\cup Z, \tag{2.2}$$

this being a special case of (1.1). In Sec. V we shall show that each positive real number Δ and nonzero c in C specify a discrete decay model with measurement basis $\{\phi_j:j\in Z_d\}$. (We shall set $\Delta=1$ for notational simplicity throughout the paper and comment on the general case at the end of Sec. VI.) Although the models are distinct, they have essentially the same properties, hence no confusion need arise when we refer to *the* model. To briefly summarize, let $\alpha=|c|^2$. We will construct two sequences $(p_n:n\in Z')$ and $(\lambda_n:n\in Z')$ depending only on α such that $p_n\geqslant 0$, $p_n=p_{-n}$, $\lambda_n\in R-Z$, and $\lambda_n=-\lambda_{-n}$ for all n in Z'. Furthermore the following theorems hold:

Theorem 2.1: (To be proved in Sec. V.) For j in Z_d, define

$$\phi_j=\begin{cases}((p_n)^{1/2}:n\in Z') & \text{if } j=d,\\ (c(p_n)^{1/2}(\lambda_n-j)^{-1}:n\in Z') & \text{if } j\in Z.\end{cases} \tag{2.3}$$

Then $\{\phi_j:j\in Z_d\}$ is an orthonormal collection of vectors in $L_2(Z')$.

We define the unitary group $(U(t):t\in R)$ on $L_2(Z')$ via

$$(U(t)x)_n=(e^{it\lambda_n})x_n \quad (\text{for } n\in Z'), \tag{2.4}$$

where $x=(x_n:n\in Z')\in L_2(Z')$. It is clear that $U(t)$ is strongly continuous on $L_2(Z')$, and that the infinitesimal generator H of $U(t)$ is simply the multiplication operator

$$(Hx)_n=\lambda_n x_n \quad (\text{for } n\in Z'). \tag{2.5}$$

Of course Hx is defined only for $x\in D(H)$, i.e., if

$$\langle x|H^2|x\rangle=\sum_{n\in Z'}\lambda_n^2|x_n|^2<\infty. \tag{2.6}$$

We let L stand for the closed subspace of $L_2(Z')$ spanned by $\{\phi_j:j\in Z_d\}$.

Theorem 2.2: (To be proved in Sec. VI.) For all t in R, the inclusion $U(t)L\subset L$ holds.

We shall show in Sec. V that $\phi_d\notin D(H)$, hence $\langle\phi_d|H|\phi_d\rangle$ is not defined. Since $H^*=H$, all the remaining numbers $\langle\phi_j|H|\phi_k\rangle$ are formally defined by

$$\langle\phi_j|H|\phi_k\rangle=\begin{cases}\alpha\displaystyle\sum_{n\in Z'}p_n\lambda_n(\lambda_n-j)^{-1}(\lambda_n-k)^{-1} & \text{for } j,k\in Z,\\ c\displaystyle\sum_{n\in Z'}p_n\lambda_n(\lambda_n-k)^{-1} & \text{for } j=d,k\in Z.\end{cases} \tag{2.7}$$

Theorem 2.3: Given ϕ_j as defined in (2.3) and H as in (2.5), the infinite sums in (2.7) are absolutely convergent. Furthermore we can write

$$\langle \phi_j|H|\phi_k\rangle=\begin{cases} j\delta_{jk} & \text{for } j,k \text{ in } Z, \\ c & \text{for } j=d \text{ and } k \text{ in } Z, \end{cases} \tag{2.8}$$

where $\delta_{jk}=1$ if $j=k$ and 0 otherwise.

Proof: We note the identity

$$\lambda_n(\lambda_n-k)^{-1}=1+k(\lambda_n-k)^{-1} \quad (\text{for } n\in Z' \text{ and } k\in Z), \tag{2.9}$$

where we remember that $\lambda_n\notin Z$, hence both sides of (2.9) are always finite. Since Theorem 2.1 guarantees, among other things, that $\langle \phi_j|\phi_j\rangle<\infty$ for all j in Z_d, we can use the Cauchy–Schwartz inequality to conclude that the infinite sums in (2.7) are absolutely convergent. The relation (2.8) now follows from (2.9) and the orthonormality of $\{\phi_j : j\in Z_d\}$. □

Theorem 2.4: Given ϕ_j and H as in Theorem 2.3, it follows that

$$\langle \phi_j|H^2|\phi_j\rangle-(\langle \phi_j|H|\phi_j\rangle)^2=\alpha \quad (\text{for } j\in Z). \tag{2.10}$$

Proof: We can write

$$\langle \phi_j|H^2|\phi_j\rangle=\sum_{n\in Z'} \alpha p_n\lambda_n^2(\lambda_n-j)^{-2} \quad (\text{for } j\in Z) \tag{2.11}$$

as a consequence of (2.3) and (2.5). We note the identity

$$\lambda_n^2=(\lambda_n-j)^2+2\lambda_n j-j^2 \quad (\text{for } j\in Z) \tag{2.12}$$

and apply Theorem 2.1 to conclude that

$$\langle \phi_j|H^2|\phi_j\rangle=\alpha+2j\langle \phi_j|H|\phi_j\rangle-j^2 \quad (\text{for } j\in Z). \tag{2.13}$$

We recall (2.8) with $j=k$ to get (2.10). □

Remark 2.1: The expression on the left-hand side of (2.10) is called the ''energy variance'' in state ϕ_j. We conclude that all states in the measurement basis except ϕ_d have the same finite energy variance. We note also that $\phi_j\in D(H)$ if and only if ϕ_j has finite energy variance, as can easily be verified. Furthermore, we can write

$$H\phi_j=c\phi_d+j\phi_j \quad (\text{for } j\in Z), \tag{2.14}$$

as follows from (2.8). [No rigorous expression for $H\phi_d$ is possible since $\phi_d\notin D(H)$, as will be directly demonstrated in Remark 5.2.]

In the next two sections we shall see that the distinction between ϕ_d and the other states in the measurement basis has significant consequences when the quantum process is continuously measured.

III. DECAY RATES AND BOUNDS

In this section we will provide exact results and bounds for the decay out of an initial state when our model is *not* continuously observed.

Definition 3.1: For t in R, let

$$Q_{jk}(t)=|\langle \phi_j|\phi_k(t)\rangle|^2 \quad (\text{for } j,k\in Z_d), \tag{3.1}$$

where $\phi_k(t)=U(t)\phi_k$ and $U(t)=\exp(itH)$.

Remark 3.1: The normalization $\|\phi_j\|=1$ for j in Z_d ensures that the matrix $Q(t)=(Q_{jk}(t): j,k\in Z_d)$ is a doubly stochastic matrix. (All rows and columns sum to 1.)

Definition 3.2: We say ϕ_j has decay rate $\beta \in [0, \infty)$ if

$$\lim_{t \downarrow 0} t^{-1}(1 - Q_{jj}(t)) = \beta. \tag{3.2}$$

We define ϕ_j to be regular if $\beta = 0$ in (3.2).

Remark 3.2: Since $Q_{jj}(t)$ is symmetric around 0, it is clear that $\beta = 0$ in (3.2) if and only if $Q_{jj}(t)$ is differentiable at 0. It is also clear that the Zeno effect holds for a continuously observed quantum process with initial state ϕ_j if and only if ϕ_j is regular, since $\lim_{N \to \infty}(Q_{jj}(t/N))^N = 1$ for all $t > 0$ if and only if the limit in (3.2) is 0. It is obvious that the condition $\phi_j \in D(H)$ is sufficient for ϕ_j to be regular.

For j in Z_d we define the amplitude functions

$$\Phi_j(t) = \langle \phi_j | \phi_j(t) \rangle \quad (\text{for } t \in R). \tag{3.3}$$

We conclude from (2.3) and (2.4) that

$$\Phi_d(t) = \sum_{n \in Z'} p_n e^{i\lambda_n t} = 2 \sum_{n > 0} p_n \cos(\lambda_n t), \tag{3.4}$$

where the last equality follows because $p_n = p_{-n}$ and $\lambda_n = -\lambda_{-n}$ for $n \in Z'$. We shall show in Sec. VI that

$$\Phi_d(t) = \exp(-\pi\alpha|t|) \quad (\text{for } |t| \leqslant 2\pi). \tag{3.5}$$

It follows directly that

$$\lim_{t \downarrow 0} t^{-1}(1 - Q_{dd}(t)) = 2\alpha\pi, \tag{3.6}$$

i.e., ϕ_d has nonzero decay rate $2\alpha\pi$ and thus is not regular. In particular $\phi_d \notin D(H)$ as will be directly demonstrated in Remark 5.2.

Definition 3.3: For $j \in Z_d, k \in Z$, we define

$$\Psi_{jk}(t) = \langle \phi_j | \phi_k(t) \rangle e^{-ikt} \quad (\text{for } t \in R). \tag{3.7}$$

Using (2.14) or computing directly, we can differentiate (3.7) to obtain

$$\Psi'_{dk}(t) = ic\Phi_d(t)e^{-ikt} \quad (\text{for } k \in Z). \tag{3.8}$$

It follows that

$$\Psi_{dk}(s) = ic \int_0^s \Phi_d(r) e^{-ikr}\, dr \tag{3.9}$$

since $\Psi_{dk}(0) = 0$ for $k \in Z$. We conclude

$$\lim_{t \to 0} t^{-2} Q_{dk}(t) = \alpha \quad (\text{for } k \in Z). \tag{3.10}$$

We can also use (2.14) to write

$$\Psi'_{jk}(t) = ic\langle \phi_j | \phi_d(t) \rangle e^{-ikt} \quad (\text{for } j, k \in Z). \tag{3.11}$$

Since $U(t)$ is unitary we know that $\langle \phi_j | \phi_d(t) \rangle$ is the complex conjugate of $\langle \phi_d | \phi_j(-t) \rangle$. A little calculation then yields

$$\Psi'_{jk}(t) = ic\overline{\Psi}_{dj}(-t)e^{i(j-k)t} = i\overline{c\Psi}_{dj}(t)e^{i(j-k)t}, \tag{3.12}$$

where the last equality follows from (3.9).

Lemma 3.1: For $j \in Z$, ϕ_j has decay rate 0.

Proof: It follows from (3.9) and (3.12) that

$$\Psi_{jk}(t) = \delta_{jk} - \alpha \int_0^t \int_0^s \Phi_d(r) e^{-ijr} e^{-i(k-j)s}\, dr ds \tag{3.13}$$

for $j,k \in Z$. Letting $j=k$, we interchange order of integration to obtain

$$\Psi_{jj}(t) = 1 - \alpha \int_0^t (t-r)\Phi_d(r) e^{-ijr}\, dr. \tag{3.14}$$

Since $|\Phi_d| \leqslant 1$ we conclude that

$$1 - |\Psi_{jj}(t)| \leqslant (1/2)\alpha t^2 \quad (\text{for } j \in Z). \tag{3.15}$$

We also have $|\Psi_{jj}| \leqslant 1$, hence

$$1 - Q_{jj}(t) \leqslant \alpha t^2 \quad (\text{for } j \in Z). \tag{3.16}$$

The lemma now follows. □

Remark 3.3: It follows from (3.16) and Remark 3.1 that for all t in R

$$Q_{jk}(t) \leqslant \alpha t^2 \quad (\text{for } j,k \in Z_d, j \neq k). \tag{3.17}$$

Furthermore, it follows from (3.13) that

$$\lim_{t \to 0} t^{-4} Q_{jk}(t) = (\tfrac{1}{4})\alpha^2 \quad (\text{for } j,k \in Z, j \neq k). \tag{3.18}$$

IV. APPLICATIONS TO CONTINUOUS MEASUREMENT

In this section we will define the measures P_N^a and P_N^{ab} in more detail, and we will summarize their limit behavior as $N \to \infty$ via Theorems A and B.

Definition 4.1: Given $n>0$ and $t \in (0,\infty)$, let $Q^{(n)}(t)$ stand for the n-fold matrix product of $Q(t)$ with itself. For short we let Q stand for $Q(N^{-1})$ and $Q^{(n)}$ stand for $Q^{(n)}(N^{-1})$. We define the non-negative measure P_N on $(Z_d)^{N+1}$ by

$$P_N(x_0,\ldots,x_N) = \prod_{n=1}^{N} Q_{x_{n-1}x_n} \quad [\text{for } (x_0,\ldots,x_N) \in (Z_d)^{N+1}]. \tag{4.1}$$

We let Ω_a stand for the set of all sequences $(x_0,\ldots,x_N)$ in $(Z_d)^{N+1}$ such that $x_0 = a$, and we define Ω_{ab} similarly, with the additional restriction that $x_N = b$. We note that

$$P_N(\Omega_{ab}) = Q_{ab}^{(N)} = Q_{ab}^{(N)}(N^{-1}). \tag{4.2}$$

We define the conditional probability measures P_N^a and P_N^{ab} by conditioning P_N on the sets Ω_a and Ω_{ab}, respectively. [For example,

$$P_N^{ab}(G)=P_N(G\Omega_{ab})/P_N(\Omega_{ab}) \tag{4.3}$$

for $G\subset(Z_d)^{N+1}$.] Clearly P_N^a is the distribution of the Markov chain $X_0,\ldots,X_N$ with transition kernel Q, constrained so that $X_0=a$; while P_N^{ab} is similarly characterized with the additional constraint that $X_N=b$.

We can now state Theorems A and B.

Theorem A: Given a,b in Z_d and $t>0$,

$$\lim_{N\to\infty} Q_{ab}^{(N)}(t/N)=\delta_{ab}\exp(-2\alpha\delta_{ad}\pi t). \tag{4.4}$$

This result establishes exponential decay valid for all t, which is characteristic of our model in the context of continuous measurement.

Theorem B: As $N\to\infty$, the measures P_N^{ab} assign all but a vanishingly small fraction of their mass to observed state sequences with exactly $\rho(a,b)$ change of state transitions, none of which returns to a previously observed state. Here $\rho(a,b)$ is defined by

$$\rho(a,b)=\inf\left\{r:\prod_{s=1}^{r}\langle\phi_{j_{s-1}}|H|\phi_{j_s}\rangle\neq 0\right\}, \tag{4.5}$$

where the infimum is taken over all sequences $j_0,\ldots,j_r$ in Z_d satisfying

$$a=j_0\neq j_1\neq\cdots\neq j_{r-1}\neq j_r=b. \tag{4.6}$$

This result establishes the least action principle for our discrete decay model subject to continuous measurement and constraints at the initial and final states.

The rest of this section is devoted to establishing a sequence of results leading up to Theorems A and B. We note first that $\rho(a,b)$ in (4.5) is well defined for our discrete decay model, because $\langle\phi_j|H|\phi_k\rangle$ is well defined if $j\neq k$. We note also that $\rho(a,b)=0$ if and only if $a=b$. We now present a definition which will clarify the content of Theorem B.

Definition 4.2: Given any integer $r\geqslant 0$, we let $\Omega_{ab}^{(r)}$ stand for the set of all sequences $(x_0,\ldots,x_N)$ in Ω_{ab} such that for some sequence $j_0,\ldots,j_r$ in Z_d satisfying (4.6) and some sequence $n_0,\ldots,n_r$ of non-negative integers satisfying

$$r+\sum_{s=0}^{r} n_s=N \tag{4.7}$$

we have

$$x_n=j_s \qquad \left(\text{for } s+\sum_{t=0}^{s-1} n_t\leqslant n\leqslant s+\sum_{t=0}^{s} n_t\right). \tag{4.8}$$

[Thus $\Omega_{ab}^{(r)}$ consists of those sequences $(a,x_1,\ldots,x_{N-1},b)$ in Ω_{ab} which make exactly r change of state transitions.]

Remark 4.1: The set of non-negative integers $n_0,\ldots,n_s,\ldots,n_r$ satisfying (4.7) has cardinality $\binom{N}{r}$, as is obvious by interpreting the integers n_s as the number of spaces between r objects placed in N slots.

Theorem 4.1: For a in Z_d

$$\lim_{N\to\infty} P_N^{aa}(\Omega_{aa}^{(0)})=1. \tag{4.9}$$

Proof: Since $P_N(\Omega_{aa}^{(0)})=(Q_{aa})^N$, we can write

$$P_N(\Omega_{aa}) = (Q_{aa})^N + \sum (Q_{aa})^{n_0} Q_{aj} Q_{jk}^{(n_1)} Q_{ka} (Q_{aa})^{n_2}, \tag{4.10}$$

where the sum is taken over all non-negative integers n_0, n_1, n_2 satisfying (4.7) with $r=2$ and over all j,k in Z_d such that $a \neq j$ and $k \neq a$. Using (3.17) and Remark 4.1, we conclude that

$$|P_N(\Omega_{aa}) - (Q_{aa})^N| \leqslant \binom{N}{2} N^{-4} \alpha^2. \tag{4.11}$$

Furthermore, we know from (3.6) and (3.16) that

$$\lim_{N\to\infty} (Q_{aa})^N = \exp(-2\alpha \delta_{ad} \pi) \quad (\text{for } \alpha \in Z_d). \tag{4.12}$$

We obtain (4.9) from (4.11) and (4.12). □

Theorem 4.2: For b in Z

$$\lim_{N\to\infty} P_N^{db}(\Omega_{db}^{(1)}) = 1. \tag{4.13}$$

Proof: Given a,b in Z_d with $a \neq b$, write

$$P_N(\Omega_{ab}) = P_N(\Omega_{ab}^{(1)}) + \sum (Q_{aa})^{n_0} Q_{aj} Q_{jk}^{(n_1)} Q_{kb} (Q_{bb})^{n_2}, \tag{4.14}$$

where the sum is taken over all non-negative integers n_0, n_1, n_2 satisfying (4.7) with $r=2$ and all j,k in Z_d with $a \neq j$ and $k \neq b$. We can also write

$$P_N(\Omega_{ab}^{(1)}) = \sum (Q_{aa})^{n_0} Q_{ab} (Q_{bb})^{n_1}, \tag{4.15}$$

where the sum is taken over all non-negative integers n_0, n_1 satisfying (4.7) with $r=1$. It follows that

$$P_N(\Omega_{ab}^{(1)}) \geqslant N (Q_{aa})^N (Q_{bb})^N Q_{ab}. \tag{4.16}$$

We now use (3.10) and (4.12) to conclude that

$$\liminf_{N\to\infty} N P_N(\Omega_{ab}^{(1)}) \geqslant \alpha \exp(-2\alpha\pi). \tag{4.17}$$

On the other hand

$$|P_N(\Omega_{ab}) - P_N(\Omega_{ab}^{(1)})| \leqslant \binom{N}{2} N^{-4} \alpha^2, \tag{4.18}$$

using Remark 4.1, (3.17), and (4.14). We conclude (4.13) from (4.17) and (4.18) by setting $a=d$ and letting $b \in Z$. □

Theorem 4.3: Let a,b in Z with $a \neq b$. Then

$$\lim_{N\to\infty} P_N^{ab}(\Omega_{ab}^{(2)}) = 1. \tag{4.19}$$

Proof: We can write

$$P_N(\Omega_{ab}) = P_N(\Omega_{ab}^{(1)}) + P_N(\Omega_{ab}^{(2)}) + P_N\left(\bigcup_{r=3}^{N} \Omega_{ab}^{(r)}\right). \tag{4.20}$$

We use (4.15) to write

$$P_N(\Omega_{ab}^{(1)}) \leqslant N Q_{ab}, \tag{4.21}$$

and we conclude from (3.18) that

$$\limsup_{N\to\infty} N^{-3} P_N(\Omega_{ab}^{(1)}) \leqslant (\tfrac{1}{4})\alpha^2. \tag{4.22}$$

We now note that

$$P_N(\Omega_{ab}^{(2)}) \leqslant \sum (Q_{aa})^{n_0} Q_{ad} (Q_{dd})^{n_1} Q_{db} (Q_{bb})^{n_2}, \tag{4.23}$$

where the sum is taken over all non-negative integers n_0, n_1, and n_2 satisfying (4.7) with $r=2$. Using Remark 4.1, it follows that

$$P_N(\Omega_{ab}^{(2)}) \geqslant \binom{N}{2} (Q_{aa} Q_{dd} Q_{bb})^N Q_{ad} Q_{db}. \tag{4.24}$$

We conclude from (3.6) and (3.10) that

$$\liminf_{N\to\infty} N^2 P_N(\Omega_{ab}^{(2)}) \geqslant (\tfrac{1}{2})\alpha^2 \exp(-2\alpha\pi). \tag{4.25}$$

Let $p = \sup(Q_{jk})$, where the supremum is taken over all j,k in Z_d with $j \neq k$. We have

$$P_N\left(\bigcup_{r=3}^{N} \Omega_{ab}^{(r)}\right) \leqslant \binom{N}{3} p^3 \tag{4.26}$$

by virtue of Lemma 3.2 in Kanter.[9] It follows from (3.17) that

$$P_N\left(\bigcup_{r=3}^{N} \Omega_{ab}^{(r)}\right) \leqslant (\tfrac{1}{6})\alpha^3 N^{-3}. \tag{4.27}$$

Clearly (4.19) follows from (4.20), (4.22), (4.25), and (4.27). □

We conclude the section by supplying proofs for Theorems A and B.

Proof of Theorem A: We shall prove (4.4) for $t=1$. For other $t>0$ the same proof will work by redefining P_N in terms of $Q(t)$ instead of Q and making other obvious changes of scale in our argument (e.g., α is replaced by αt^2 throughout). Thus we conclude from (4.2), (4.11), (4.12), and (4.18) that (4.4) holds if $t=1$ and $a=b$. Furthermore, for a,b in Z_d with $a \neq b$ we have

$$P_N(\Omega_{ab}^{(1)}) \leqslant N Q_{ab} \leqslant \alpha N^{-1}, \tag{4.28}$$

using (3.17) and (4.15). It follows from (4.2) and (4.18) that (4.4) holds if $t=1$ and $a \neq b$. □

Remark 4.2: If $a=d$, we can interpret (4.4) as stating that under continuous observation ϕ_d decays exponentially with rate $2\alpha\pi$. Furthermore, when decay occurs, the process ''explodes'' in the sense that the distribution characterizing where it goes becomes infinitely diffuse. This result is in accordance with Theorem 2.2 in Kanter,[10] although we have not verified that our discrete

decay model satisfies the Approximation Hypothesis used there. If $a \in Z$, then (4.4) asserts that ϕ_a decays at rate zero under continuous observation, in accordance with the Zeno paradox.

Proof of Theorem B: It follows from (2.8) that

$$\rho(a,b)=\begin{cases} 0 & \text{if } a=b, \\ 1 & \text{if } a\neq b \quad \text{and } d\in\{a,b\}, \\ 2 & \text{otherwise.} \end{cases} \tag{4.29}$$

Furthermore, we can readily confirm that no returns to a previously visited state can take place in a sequence (a,b) or (a,j,b) with $a\neq b$ and $a\neq j\neq b$. Thus Theorem B follows from (4.29) and from Theorems 4.1–4.3. □

Remark 4.3: The equation (4.29) expresses the distinguished nature of the state ϕ_d, in allowing only those change of state transitions which involve ϕ_d.

V. ORTHONORMALITY OF THE MEASUREMENT BASIS

In this section we shall prove Theorem 2.1 by obtaining the Mitteg–Leffler expansion of the Laplace transform of the amplitude Φ_d in (3.4). We start with a definition.

Definition 5.1: An infinite series $\Sigma_{n\in Z'} f_n$ of meromorphic functions defined on the complex plane C is said to be *normally convergent on C* if the series is uniformly convergent on any compact set disjoint from any of the poles of the functions f_n.

Remark 5.1: If $\Sigma_{n\in Z'} f_n$ is normally convergent to f, then $\Sigma_{n\in Z'} f_n^{(p)}$ is normally convergent to $f^{(p)}$, where $g^{(p)}$ stands for the pth derivative of the meromorphic function g. (See Palka.[11])

Proof of Theorem 2.1: We start our arguments by defining the meromorphic function

$$K_\alpha(z)=(z+\alpha\pi\ \coth(\pi z))^{-1} \tag{5.1}$$

on the complex plane C. [Here $\alpha>0$ is a parameter which will be identified with $|c|^2$ in (2.3).] We shall show that

$$K_\alpha(z)=\sum_{n\in Z'} p_n(z-i\lambda_n)^{-1} \tag{5.2}$$

is normally convergent on C, where p_n and λ_n satisfy the conditions given before Theorem 2.1.

We now need the known fact that $(K_\alpha(z))^{-1}$ has only imaginary roots. (See Hille.[12]) Letting $z_n=i\lambda_n$ stand for the roots, we solve for λ_n via the equation

$$\lambda_n=\alpha\pi\ \cot(\lambda_n\pi). \tag{5.3}$$

Graphical inspection shows that the solutions of (5.3) can be indexed by n in Z' so that $\lambda_n=-\lambda_{-n}$ for n in Z' and

$$\lambda_n\in(n-1,n-2^{-1}) \quad (\text{for } n>0). \tag{5.4}$$

Since $\{i\lambda_n : n\in Z'\}$ comprises the set of all poles of K_α, we conclude that K_α has no poles of the form ij for $j\in Z$.

As a first step in demonstrating (5.2) we shall show that

$$K_\alpha(z)=\sum_{n\in Z'} p_n((z-i\lambda_n)^{-1}-i\lambda_n^{-1}) \tag{5.5}$$

is a normally convergent sum on C, where p_n is the residue of $K_\alpha(z)$ at $z=i\lambda_n$ for n in Z'. Let $G(z)=(K_\alpha(z))^{-1}$. We compute

$$p_n=\left(\frac{d}{dz}\,G(z)\bigg|_{z=i\lambda_n}\right)^{-1}=(1+\alpha\pi^2\,\sin^{-2}(\pi\lambda_n))^{-1}. \tag{5.6}$$

We note $p_n>0$ for n in Z', hence all the poles of K_α are simple.

Let M stand for a positive integer and let C_M stand for the boundary of the square with vertices at $(M+2^{-1})(\pm 1\pm i)$ in the complex plane. It is shown in Palka[13] that

$$|\coth(\pi z)|\leqslant(1+e^{-3\pi})(1-e^{-3\pi})^{-1}\quad(\text{for } z\in C_M), \tag{5.7}$$

hence it follows that

$$|K_\alpha(z)|\leqslant 2M^{-1}\quad(\text{for } z\in C_M) \tag{5.8}$$

if M is sufficiently large. (Note $|z|\geqslant|M|$ for z in C_M.) In particular, K_α is bounded on the system of contours $(C_M: M\geqslant 1)$ taken as a whole. The validity of (5.5) as a normally convergent sum now follows from the general criteria for such expansions in Titchmarsh.[14]

We can use Remark 5.1 to differentiate both sides of (5.5). We obtain

$$(K_\alpha(z))^2(1-\alpha\pi^2(\sinh(\pi z))^{-2})=\sum_{n\in Z'}p_n(z-i\lambda_n)^{-2} \tag{5.9}$$

as a normally convergent sum on C. Now for j in Z the point $z=ij$ is not a pole in the expansion (5.9), hence we conclude that

$$\lim_{x\to j}(x-\alpha\pi\,\cot(\pi x))^{-2}(1+\alpha\pi^2(\sin(\pi x))^{-2})=\sum_{n\in Z'}p_n(j-\lambda_n)^{-2}, \tag{5.10}$$

where the variable x is real. In particular the right-hand side of (5.10) is finite and

$$\alpha^{-1}=\sum_{n\in Z'}p_n(j-\lambda_n)^{-2}\quad(\text{for } j\in Z). \tag{5.11}$$

This shows that the vectors $(\phi_j: j\in Z)$ all have norm 1.

We now examine the norm of ϕ_d. We combine (5.3) and (5.6) to write

$$p_n=(1+\alpha\pi^2+\alpha^{-1}\lambda_n^2)^{-1}. \tag{5.12}$$

Remembering (5.4), we conclude that $\|\phi_d\|<\infty$. It follows that

$$\sum_{n\in Z'}p_n|c(j-\lambda_n)^{-1}|\leqslant\|\phi_d\|\|\phi_j\|<\infty\quad(\text{for } j\in Z), \tag{5.13}$$

by virtue of the Cauchy–Schwartz inequality. We conclude that

$$\sum_{n\in Z'}p_n(j-\lambda_n)^{-1}=0\quad(\text{for } j\in Z) \tag{5.14}$$

using $p_n=p_{-n}$ and $\lambda_n=-\lambda_n$ for $n\in Z'$. Letting $j=0$, this proves (5.2) as a consequence of (5.5). We define the Laplace transform of Φ_d in (3.4) via

$$\hat{\Phi}_d(z)=\int_0^\infty e^{-zt}\Phi_d(t)dt\quad[\text{for } z\in C \text{ with } \mathrm{Re}(z)>0]. \tag{5.15}$$

It follows from (5.2) that

$$\hat{\Phi}_d(z)=(z+\alpha\pi\ \coth(\pi z))^{-1} \quad [\text{for } \mathrm{Re}(z)>0]. \tag{5.16}$$

We now use the well-known relation

$$\lim_{x\to\infty} x\hat{\Phi}_d(x)=\lim_{t\downarrow 0}\Phi_d(t) \quad [\text{where } x\in(0,\infty)] \tag{5.17}$$

to conclude $\|\phi_d\|=1$, since $\lim_{x\to+\infty} x(x+\alpha\pi\coth(\pi x))^{-1}=1$.

In order to verify that $\{\phi_j: j\in Z_d\}$ are orthonormal, it remains to show that ϕ_j and ϕ_k are orthogonal if $j\neq k$, for j,k in Z. [Note that ϕ_d is orthogonal to ϕ_j for all j in Z on account of (5.14).] However, we can write

$$\sum_{n\in Z'} p_n(\lambda_n-j)^{-1}(\lambda_n-k)^{-1}=(k-j)\sum_{n\in Z'} p_n((\lambda_n-k)^{-1}-(\lambda_n-j)^{-1}) \tag{5.18}$$

for j,k in Z with $j\neq k$, where absolute convergence is assured by (5.13). Applying (5.14), we obtain

$$\sum_{n\in Z'} p_n(\lambda_n-j)^{-1}(\lambda_n-k)^{-1}=\langle\phi_j|\phi_k\rangle=0 \tag{5.19}$$

for j,k in Z with $j\neq k$. This completes the proof of Theorem 2.1. □

Remark 5.2: We note that $\phi_d\notin D(H)$. In fact, $\lambda_n^2\geqslant(|n|-1)^2$ for $n\in Z'$ by (5.4), hence $p_n\geqslant 2^{-1}\alpha\lambda_n^{-2}$ for $|n|$ sufficiently large by (5.12). It immediately follows that

$$\langle\phi_d|H^2|\phi_d\rangle=\sum_{n\in Z'}\lambda_n^2 p_n=\infty, \tag{5.20}$$

whence $\phi_d\notin D(H)$.

Remark 5.3: Not only is $\phi_d\notin D(H)$, but in fact ϕ_d is not regular by virtue of (3.6). It is therefore of interest to write down a spectral condition for regularity to facilitate comparison with (5.20). Using results in Feller,[15] such a condition is given by

$$\lim_{M\to\infty} MP[|X|\geqslant M]=0, \tag{5.21}$$

where X is a random variable with $E(\exp(itX))=\Phi_d(t)$. [Thus X has distribution p_n as in (3.4).] Arguing as for (5.20) it is easy to see that (5.21) is violated as a consequence of (5.4) and (5.12).

Remark 5.4: A set of sufficient conditions for the Zeno effect is given in Misra and Sudarshan.[16] (That paper considers projections more general than the single state projections $\phi><\phi$ in defining the quantum Zeno effect.) It can be shown that the conditions in Misra and Sudarshan are all satisfied for ϕ_d except the condition that H be semi-bounded.[17] (Similar considerations are given in Kanter[18] with respect to the trivial decay model cited at the end of Section I A.)

VI. SOLVING THE MODEL

In this section we will use classical Fourier series arguments to prove Theorem 2.2. Along the way we will give an explicit representation for the transition amplitude function Φ_d in (3.4). In particular we will show that (1.4) holds.

Lemma 6.1: Let p_n and λ_n be given as in (5.2) for n in Z'. We then have

$$[\lambda_n] \leqslant 1/2(1+(n-1)^2(\alpha\pi)^{-2})^{-1/2} \quad (\text{for } n \geqslant 1), \tag{6.1}$$

where $[\lambda_n]$ stands for λ_n minus the greatest integer less than or equal to λ_n. It is also true that $\lambda_n p_n$ is a decreasing function of n for $n \geqslant (\alpha+\alpha^2\pi^2)^{1/2}+1$ and

$$\lim_{n\to\infty} np_n|\lambda_n| = \alpha. \tag{6.2}$$

Proof: It follows from (5.3) that

$$\sin^2(\pi\lambda_n) = (1+\lambda_n^2(\alpha\pi)^{-2})^{-1}. \tag{6.3}$$

We now use the well-known inequality

$$(2/\pi)x \leqslant \sin x \quad (\text{for } 0 \leqslant x \leqslant \pi/2) \tag{6.4}$$

to conclude that

$$4[\lambda_n]^2 \leqslant (1+(n-1)^2(\alpha\pi)^{-2})^{-1} \quad (\text{for } n \geqslant 1), \tag{6.5}$$

since $\sin^2(\pi\lambda_n) = \sin^2(\pi[\lambda_n])$ and

$$0 \leqslant \lambda_n - n + 1 = [\lambda_n] \leqslant \tfrac{1}{2} \quad (\text{for } n \leqslant 1) \tag{6.6}$$

by (5.4). This proves (6.1).

We let $A = \alpha+\alpha^2\pi^2$ and use (5.12) to write

$$\lambda_n p_n = \alpha\lambda_n(A+\lambda_n^2)^{-1}. \tag{6.7}$$

Letting $f(\lambda) = \lambda(A+\lambda^2)^{-1}$, we note that $f'(\lambda) = (A-\lambda^2)(A+\lambda^2)^{-2}$. It follows that $f(\lambda)$ is decreasing for $\lambda \geqslant A^{1/2}$. Using (6.6), we conclude that $\lambda_n p_n$ is a decreasing function of n for $n \geqslant A^{1/2}+1$. Finally, (6.2) follows from (5.4) and (5.12). □

Definition 6.1: We let $2\pi Z$ stand for the set $\{2\pi j : j \in Z\}$.

Lemma 6.2: The function $\Phi_d(t)$ is differentiable at any point $t \notin 2\pi Z$. The derivative Φ_d' is bounded on any bounded set disjoint from $2\pi Z$ and continuous on any closed interval disjoint from $2\pi Z$.

Proof: Define

$$\Psi(m,t) = -2\sum_{n=1}^{m} \lambda_n p_n \sin((n-1)t). \tag{6.8}$$

It follows from Lemma 6.1 and the results of Hardy and Rogosinski[19] regarding Fourier series with decreasing coefficients that the series $\Psi(\infty,t)$ is boundedly convergent on R and is uniformly convergent on any finite closed interval disjoint from $2\pi Z$.

We now define

$$\Phi_d(m,t) = 2\sum_{n=1}^{m} p_n \cos(\lambda_n t), \tag{6.9}$$

and we let $D(m,t) = \Phi_d'(m,t) - \Psi(m,t)$. For any integers $0 < m < M$

$$|D(M,t) - D(m,t)| \leqslant 4\sum_{n=m+1}^{M} \lambda_n p_n |\sin([\lambda_n]t/2)| \tag{6.10}$$

by virtue of the trigonometric relation

$$\sin(\lambda_n t)-\sin((n-1)t)=2\sin([\lambda_n]t/2)\cos(\lambda_n^* t), \tag{6.11}$$

where $\lambda_n^* = 1/2(\lambda_n + n - 1)$. It follows from (6.1) that

$$|D(M,t)-D(M,t)|\leqslant \sum_{n=m+1}^{M} \lambda_n p_n(1+(n-1)^2(\alpha\pi)^{-2})^{-1}|t|. \tag{6.12}$$

We now use (5.4) and (5.12) to write

$$|D(M,t)-D(m,t)|\leqslant \sum_{n=m+1}^{M} \pi^2\alpha^3(n-1)^{-3}|t|. \tag{6.13}$$

Given $T>0$ it follows that

$$\lim_{m\to\infty}\left(\sup \sum_{n=m+1}^{M} |D(M,t)-D(m,t)|\right)=0, \tag{6.14}$$

where the supremum is taken over t and M such that $|t|\leqslant T$ and $M>m$. We now write

$$\Phi_d(m,t)-2\sum_{n=1}^{m} p_n=\int_0^t \Phi_d'(m,s)ds \quad (\text{for } |t|\leqslant T). \tag{6.15}$$

Since $\Phi_d'(m,t)$ converges boundedly to a limit $\Phi^*(t)$ on $[-T,T]$ by virtue of (6.14) and the bounded convergence of $\Psi(m,t)$, we can let $m\to\infty$ in (6.15) to obtain

$$\Phi_d(t)-1=\int_0^t \Phi^*(s)ds \quad (\text{for } |t|\leqslant T). \tag{6.16}$$

We also know that Φ^* is continuous on any subinterval of $[-T,T]$ disjoint from $2\pi Z$ by virtue of (6.14) and the uniform convergence of $\Psi(m,t)$ on such an interval. It follows by elementary calculus that $\Phi^* = \Phi_d'$ on $[-T,T]$ and the lemma is proved by letting $T\to\infty$. □

Lemma 6.3: We can write

$$\Phi_d'(t)=\sum_{2\pi|n|\leqslant t} -\pi\alpha\Phi_d(t-2\pi|n|) \quad (\text{for } t>0), \tag{6.17}$$

where we adopt the convention that both sides of (6.17) satisfy

$$f(t)=(\tfrac{1}{2}(\lim_{s\uparrow t} f(s)+\lim_{s\downarrow t} f(s)) \quad (\text{for } t>0). \tag{6.18}$$

Proof: Given z in C with $\mathrm{Re}(z)>0$, we define

$$B(z)=\int_0^\infty \sum_{0\leqslant 2\pi|n|\leqslant t} \Phi_d(t-2\pi|n|)e^{-zt}\,dt. \tag{6.19}$$

We can write

$$B(z)=\sum_{n\in Z}\int_{2\pi|n|}^\infty \Phi_d(t-2\pi|n|)e^{-zt}\,dt, \tag{6.20}$$

where the justification for the interchange of summation and integration is made apparent when we change variables in (6.20) to obtain

$$B(z)=\sum_{n\in Z}\int_0^\infty \Phi_d(s)e^{-zs}e^{-2\pi z|n|}\,ds \quad [\text{for } \mathrm{Re}(z)>0]. \tag{6.21}$$

[Just note that if we take the absolute value of the integrand in (6.21), then the resulting sum will be finite and then use Fubini's theorem, as given by Halmos.[20]] It follows that

$$B(z)=\hat{\Phi}_d(z)\coth(\pi z) \quad [\text{for } \mathrm{Re}(z)>0], \tag{6.22}$$

where the Laplace transform $\hat{\Phi}_d(z)$ is given as in (5.15).

If we now let $\hat{\Phi}_d'(z)$ be defined via

$$\hat{\Phi}_d'(z)=\lim_{T\to\infty}\int_0^T e^{-zt}\Phi_d'(t)dt, \tag{6.23}$$

then it is standard to verify that

$$\hat{\Phi}_d'(z)=z\hat{\Phi}_d(z)-1. \tag{6.24}$$

Combining (5.16), (6.22), and (6.24), we conclude that both sides of (6.17) have the same Laplace transform for z with $\mathrm{Re}(z)>0$. Also both sides of (6.17) are absolutely integrable on any finite interval. [We use, in particular, the boundedness of Φ_d' on bounded sets proved in Lemma 6.2. The values of Φ_d' on $2\pi Z$ are, of course, immaterial in the integral defining $\hat{\Phi}_d'$ in (6.23).] It now follows from the uniqueness result in Widder[21] that both sides of (6.17) are equal almost everywhere with respect to Lebesgue measure on the positive real numbers. Since the right-hand side of (6.17) can be modified on $2\pi Z$ so as to satisfy (6.18), it follows the same is true for the left-hand side of (6.17). □

We can now set forth a very interesting explicit determination of the amplitude function $\Phi_d(t)$.

Theorem 6.1: Let $h(t)=\exp(\pi\alpha t)\Phi_d(t)$ for $t\geqslant 0$. Then $h(t)=1$ for $0\leqslant t\leqslant 2\pi$ and

$$h(t)=h(2\pi n)-2\pi\alpha\int_{2n\pi}^{t}\sum_{m=1}^{n}\tau_m h(s-2\pi m)ds \tag{6.25}$$

for $2n\pi\leqslant t\leqslant 2(n+1)\pi$, where $\tau_m=\exp(\pi\alpha(2\pi)^m)$.

Proof: It is clear from Lemma 6.3 that $h(t)=1$ for $0\leqslant t\leqslant 2\pi$. We shall prove (6.25) by induction on n. We note that

$$h'(t)=\exp(\pi\alpha t)(\pi\alpha\Phi_d(t)+\Phi_d'(t)) \tag{6.26}$$

for $2n\pi<t<2(n+1)\pi$. Using (6.17), it follows that

$$h'(t)=-2\pi\alpha\sum_{m=1}^{n}\tau_m h(s-2\pi m). \tag{6.27}$$

for $2n\pi<t<2(n+1)\pi$. □

Remark 6.1: We note that $\Phi_d(t)$ is an even function of t, hence (6.25) gives complete information about $\Phi_d(t)$ for all t. In particular we conclude that the exact exponential decay law (3.5) holds for $|t|\leqslant 2\pi$.

Theorem 6.2: For any t in R, we have

$$\sum_{j\in Z_d} Q_{dj}(t)=1. \tag{6.28}$$

Proof: We can assume $t>0$ without loss of generality. Using (3.9) we can rewrite (6.28) as

$$1-\Phi_d(t)^2=\alpha\sum_{k\in Z}\int_0^t\int_0^t \Phi_d(r)\Phi_d(s)e^{ik(s-r)}\,dr ds. \tag{6.29}$$

Changing variables in (6.29), we obtain

$$1-\Phi_d(t)^2=\alpha\sum_{k\in Z}\int_{-t}^{t} g_t(w)e^{ikw}\,dw, \tag{6.30}$$

where

$$g_t(w)=\int_{-w^-}^{t-w^+}\Phi_d(r+w)\Phi_d(r)dr, \tag{6.31}$$

$w^+=2^{-1}(w+|w|)$ and $w^-=2^{-1}(w-|w|)$. We note that $g_t(w)=0$ if $-w^-\geqslant t-w^+$, i.e., if $|w|\geqslant t$. It follows we can write

$$g_t(w)=\int_{-\infty}^{+\infty} h_t(r+w)h_t(r)dr, \tag{6.32}$$

where $h_t(r)=\Phi_d(r)I_{[0,t]}(r)$ and $I_{[0,t]}$ is the indicator function of $[0,t]$.

We claim that the sum

$$\sum_n g_t(w+2\pi n)=\sum_{|w+2\pi n|\leqslant t} g_t(w+2\pi n) \tag{6.33}$$

is a continuous function of w. In fact, we can write

$$\sum_n g_t(w+2\pi n)=\sum_{2\pi|n|\leqslant t+2\pi} g_t(w+2\pi n) \tag{6.34}$$

for $|w|\leqslant 2\pi$, since $|w+2\pi n|\geqslant 2\pi|n|-|w|$. This proves the claim, since each summand $g_t(w+2\pi n)$ in (6.34) is a continuous function of w and the sum is periodic with period 2π.

The validity of the claim in conjunction with the fact that g_t is non-negative definite [as follows from (6.32)] shows that the conditions given by Feller[22] for the application of the Poisson summation formula to g_t are met. We conclude in particular that

$$2\pi\sum_{n\in Z} g_t(2\pi n)=\sum_{k\in Z}\int g_t(w)e^{ikw}\,dw. \tag{6.35}$$

Thus (6.30) is equivalent to the relation

$$1-\Phi_d(t)^2=2\pi\alpha\sum_{2\pi|n|\leqslant t}\int_{-(2\pi n)^-}^{t-(2\pi n)^+}\Phi_d(r+2\pi n)\Phi_d(r)dr. \tag{6.36}$$

In order to establish (6.36) it suffices to show that the derivative of both sides are equal, i.e., we need to show that

$$2\Phi_d(t)\Phi_d'(t) = -2\pi\alpha \sum_{2\pi|n|\leqslant t} \Phi_d(t)\Phi_d(t-2\pi|n|) \tag{6.37}$$

for $t \notin 2\pi Z$. However, (6.37) follows immediately from (6.17) for $t>0$. □

Proof of Theorem 2.2: We note the identity

$$\left\| \phi_d(t) - \sum_{j\in Z_d} \langle \phi_d(t)|\phi_j\rangle \phi_j \right\|^2 = 1 - \sum_{j\in Z_a} Q_{dj}(t), \tag{6.38}$$

where $\phi_j(t) = U(t)\phi_j$ for $j \in Z_d$. In combination with Theorem 6.2 this identity implies that $\phi_d(t) \in L$ for all t in R. It remains to prove that $\phi_j(t) \in L$ for $j \in Z$, where we may assume that $t>0$ without loss of generality.

We claim that for all n and j in Z with $n \geqslant 1$ we can write

$$\phi_j(t) = ijS_n(t,\phi_j) + d_n(t,j)\phi_j + (ic)\sum_{m=1}^{n} S_m(t,\phi_d), \tag{6.39}$$

where

$$S_m(t,\phi_k) = (ik)^{m-1}\int_0^t \int_0^{t_{m-1}} \cdots \int_0^{t_1} \phi_k(t_0)dt_0\cdots dt_{m-1} \tag{6.40}$$

for k in Z_d and

$$d_n(t,j) = \sum_{m=0}^{n-1} (ijt)^m/m!. \tag{6.41}$$

To show that (6.39) holds when $n=1$, we note $\phi_j \in D(H)$, hence

$$\phi_j(t) = i\int_0^t U(s)H\phi_j ds + \phi_j. \tag{6.42}$$

We now use (2.14) to obtain (6.39) with $n=1$. We will finish the proof of the claim by induction on n. Given the representation (6.39), we use (2.14) and (6.42) to conclude that (6.39) is valid when n is advanced by one.

We now note that $S_m(t,\phi_d) \in L$ for all m by virtue of the fact that $\phi_d(t) \in L$ for all t in R, which has already been demonstrated. Thus we can establish that $\phi_j(t) \in L$ by showing that

$$\lim_{n\to\infty} \|S_n(t,\phi_j)\| = 0 \quad (\text{for } t>0). \tag{6.43}$$

In fact, we have

$$\|S_n(t,\phi_j)\| \leqslant (jt)^n/n! \tag{6.44}$$

since $\|\phi_j\|=1$. The right-hand side of (6.44) tends to 0 as $n\to\infty$, hence the theorem is proved. □

Remark 6.2: For completeness we give some indications of the proof for (1.4) when $\Delta \neq 1$. We start by replacing $K_\alpha(z)$ in (5.1) by

$$K_{\Delta,\alpha}(z) = (z + \alpha\pi \coth(\pi\Delta^{-1}z))^{-1}. \tag{6.45}$$

It is then easy to show that p_n in (5.6) becomes

$$p_n=(1+\alpha\pi^2\Delta^{-1}\sin^{-2}(\pi\Delta^{-1}\lambda_n))^{-1}. \tag{6.46}$$

The arguments for (5.10) and (5.11) lead us to conclude that the basis ϕ_j is now of the form

$$\phi_j=c(\Delta p_n)^{1/2}(\lambda_n-\Delta j)^{-1}. \tag{6.47}$$

We replace $\Psi(m,t)$ in (6.8) by

$$\Psi(m,t)=-2\sum_{n=1}^{m}\lambda_n p_n\sin((n-1)\Delta t) \tag{6.48}$$

and conclude that $\Phi_d(t)$ is differentiable for any $t\notin 2\pi\Delta Z$. The argument for (1.4) is then straightforward.

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Quantum Riemann surfaces for arbitrary Planck's constant

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We continue our study of quantum Riemann surfaces initiated in Refs. 1–3 [S. Klimek and A. Lesniewski, Commun. Math. Phys. **146**, 103–122 (1992); Lett. Math. Phys. **24**, 125–139 (1992); **32**, 45–61 (1994)]. We construct a one parameter family of deformations of compact Riemann surfaces of genus $g \geqslant 2$. Our construction does not require any discreteness condition on the value of Planck's constant. It coincides with the construction of Ref. 2 [Lett. Math. Phys. **24**, 125–139 (1992)] in the case when Planck's constant assumes the discrete set of values dictated by geometric quantization. © *1996 American Institute of Physics.*
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I. INTRODUCTION

In a series of papers,[1–3] we studied nonperturbative deformation quantization of Riemann surfaces. Our approach is based on the ideas of Ref. 4 (for related developments, see also Refs. 5–7, and references therein). A satisfactory picture of uniformization of exceptional quantum Riemann surfaces emerged from these investigations. In the case of higher genus ($g \geqslant 2$) Riemann surfaces, the uniformization on the quantum level is a more complex issue. In fact, if M is a Riemann surface and N is a covering of M, then the quantization of N is a covering of the quantization of M in the sense of Ref. 3 only if the fundamental group of the covering $N \to M$ is Abelian. Part of the problem is the presence of topological sectors (similar to the θ-vacua in gauge theory) in the quantum theory, which is related to the nonsimple connectedness of the classical phase space. These sectors are classified by the characters of the fundamental group of the phase space. This does not reflect the noncommutativity of that group. On the other hand, whether the fundamental group is commutative or not seems to be important for the quantum uniformization in the sense of Ref. 3. A similar phenomenon was discussed previously in Ref. 8.

Quantization of Riemann surfaces in the framework of geometric quantization (see, e.g., Ref. 9) requires a restriction on the allowed values of the deformation parameter r (''the quantization condition''). However, it is desirable to have a definition of quantum Riemann surfaces for all values of r. A definition consistent with geometric quantization was given in Ref. 2, for $r = n(2g-2)^{-1}$, where $n \in \mathbb{N}$. In principle, quantum uniformization allows for a construction of quantum Riemann surfaces for all values of r, using the universal covering, the Poincaré disk, as the point of departure. Since the fundamental groups of higher genus Riemann surfaces are non-Abelian, it is likely, however, that the so defined algebra of quantized functions does not reduce to the algebra of Ref. 2, when $r = n(2g-2)^{-1}$.

In this paper, we construct quantization of compact Riemann surfaces for arbitrary values of $r > 0$ in a manner consistent with Ref. 2. Our starting point is a noncompact covering space $\hat{M}$ such that the group of cover transformation is the Abelian group $\mathbb{Z}$. Since $\hat{M}$ is a noncompact Riemann surface, all holomorphic line bundles are holomorphically trivial,[10] and geometric quantization does not impose any restrictions on Planck's constant. It was explained in Ref. 2 that geometric quantization of Riemann surfaces leads to certain operator algebras on Hilbert spaces of automorphic forms. We define the quantization of M in terms of Toeplitz operators with invariant

symbols on a space of automorphic forms on $\hat{M}$, and prove deformation estimates. The proof of the estimates is based on the methods developed in Ref. 2 (see Ref. 11 for a different approach).

The paper is organized as follows. In Sec. II, we study the fundamental groups of M and $\hat{M}$. We define and study suitable spaces of automorphic forms on M and $\hat{M}$ in Sec. III. Section IV contains proofs of deformation estimates.

II. THE FUNDAMENTAL GROUPS

In this section, we fix our notation and describe certain group theoretic properties of the fundamental groups of Riemann surfaces which will be useful in later sections. Let M be a compact Riemann surface of genus $g \geqslant 2$. We pick a basis $\{a_i, b_i\}$, $i=1,..,g$, of one-cycles on M. The fundamental group Γ of M is a finitely generated group with generators $\{a_i, b_i\}$, $i=1,\ldots,g$, obeying the relation (see e.g., Ref. 12)

$$\prod_{i=1}^{g} a_i b_i a_i^{-1} b_i^{-1} = 1.$$

We denote $a := a_g$ and $b := b_g$. An element $\gamma \in \Gamma$ can be represented as

$$\gamma = \prod_{j=1}^{\infty} \prod_{i=1}^{g} a_i^{n_{i,j}} b_i^{m_{i,j}},$$

where almost all integers $n_{i,j}, m_{i,j}$ are equal to zero. Consider now the homomorphism

$$\gamma \to \sum_j m_{g,j} \in \mathbb{Z}.$$

One can easily verify that the above map is well defined, i.e., it does not depend on the way we represent γ, and is indeed a homomorphism of groups. We denote the kernel of this homomorphism by Γ_0. The group Γ_0 is no longer finitely generated. In fact, it is not difficult to see that the following elements are its generators:

$$a, b^n a_i b^{-n}, b^n b_i b^{-n}, \quad \text{where} \quad n \in \mathbb{N}, \quad i = 0,1,\ldots,g-1,$$

and there are no relations among them, i.e., Γ_0 is the free product of infinite cyclic groups generated by the above generators.

Let $\hat{M}$ be a covering of M with no branching points and such that $\pi_1(\hat{M}) = \Gamma_0$. The group of cover transformations of the covering $\hat{M} \to M$ is then equal to $\mathbb{Z}$. Intuitively, $\hat{M}$ is obtained from M by cutting along the a cycle and then continuing M across the cut along the b cycle. One can visualize $\hat{M}$ as an infinite cylinder with infinite number of handle bodies attached, each handle body having $g-1$ handles. $\hat{M}$ is a noncompact Riemann surface.

The universal covering space of both M and $\hat{M}$ is the unit disk $\mathscr{U}$. The groups Γ and Γ_0 can be thought of as Fuchsian groups on $\mathscr{U}$. For

$$\gamma = \begin{bmatrix} a & b \\ \overline{a} & \overline{b} \end{bmatrix} \in \Gamma,$$

we denote

$$\gamma(z) = \frac{az+b}{\overline{bx+a}} \quad z \in \mathscr{U}. \tag{2.1}$$

Since the derivative of (2.1) is $\gamma'(z)=(\overline{bz}+\overline{a})^{-2}$, we can set:

$$\gamma'(z)^{1/2}:=(\overline{bz}+\overline{a})^{-1}.$$

Let G be either Γ or Γ_0, and let $r>0$. A multiplier of weight r for the group G is a map $v:G\to\mathbb{C}$ such that[12]

$$|v(\gamma)|=1,$$

and

$$\gamma_1'(\gamma_2(z))^{-r/2}\gamma_2'(z)^{-r/2}v(\gamma_1)v(\gamma_2)=(\gamma_1\gamma_2)'(z)^{-r/2}v(\gamma_1\gamma_2). \tag{2.2}$$

In (2.2), the standard branch of the logarithm is taken to define the rth power. The existence of multipliers is a cohomological question, see Ref. 13 for the modern treatment. Equation (2.2) can be interpreted as the triviality of a 2-cocycle in the group cohomology of G. A multiplier is essentially a 1-cochain whose coboundary is that 2-cocycle. It is well-known that multipliers exist for Γ if and only if $r=n(2g-2)^{-1}$, $n=1, 2,\ldots$. The situation is different for Γ_0.

Proposition 2.1: The second cohomology group $H^2(\Gamma_0,\mathbb{Z})$ of Γ_0 is trivial.

Proof: Since $\Gamma_0=\pi_1(\hat{M})$, and the universal covering space of $\hat{M}$ is contractible, it follows from Eilenberg–MacLane's theorem[14] that

$$H^*(\Gamma_0,\mathbb{Z})\cong H^*(\hat{M},\mathbb{Z}).$$

By Poincaré duality,[15] $H^2(\hat{M},\mathbb{Z})$ is isomorphic to the compactly supported cohomology group of $\hat{M}$ in dimension zero. The latter is trivial, as $\hat{M}$ is noncompact. □

Consequently, multipliers for Γ_0 exist for arbitrary r. Let us also remark that the ratio of two multipliers is a character of the group.

III. AUTOMORPHIC FORMS

As before, let G be either Γ or Γ_0, and let v be a multiplier for the group G. Recall that a holomorphic function $\phi:\mathcal{U}\to\mathbb{C}$ is called an automorphic form for G of weight $r>0$ with multiplier v, if:[12]

$$\phi(\gamma(z))=v(\gamma)\gamma'(z)^{-r/2}\phi(z), \tag{3.1}$$

for each $\gamma\in G$. Automorphic forms for infinitely generated Fuchsian groups like Γ_0 have been studied less extensively than those for finitely generated groups, but there is a fair amount of information available, see Refs. 16 and 17, and references therein.

Let R be a fundamental polygon for Γ. Then $R_0:=\cup_{n\in\mathbb{Z}}b^nR$ is a fundamental polygon for Γ_0. It has infinitely many sides. Here we use the same symbol b to denote the group element of Γ corresponding to the cycle $b=b_g$. For $r=n(2g-2)^{-1}$, we define $\mathcal{H}^r(\Gamma,v)$ to be the Hilbert space of automorphic forms for Γ equipped with the following scalar product:

$$(\phi,\psi):=\int_R\overline{\phi(z)}\psi(z)d\mu^r(z), \tag{3.2}$$

where the measure $d\mu^r(z)$ is

$$d\mu^r(z):=\frac{r-1}{\pi}(1-|z|^2)^{r-2}d^2z.$$

For arbitrary $r>0$, let $\mathscr{H}^r(\Gamma_0,v)$ be the space of automorphic forms for Γ_0 with the scalar product as in (3.2) but R_0 replacing R.

If v is a multiplier for Γ and $e^{i\theta}\in S^1$, we let v_θ denote a new multiplier for Γ defined by:

$$v_\theta(b)=v(b)e^{i\theta},$$

and $v_\theta=v$ on all other generators. In particular $v_0=v$. All of the multipliers v_θ are equal when restricted to the subgroup Γ_0. The restricted multiplier will be again denoted by v.

Theorem 3.1: *With the above definitions, there is a canonical isomorphism*

$$\mathscr{H}^r(\Gamma_0,v)\simeq\int_{S^1}^{\oplus}\mathscr{H}^r(\Gamma,v_\theta)d\theta,\quad r=n(2g-2)^{-1},\quad n=1,2,\ldots .$$

Proof: For an automorphic form ϕ for Γ_0, define

$$U\phi(z)=b'(z)^{r/2}\phi(bz). \tag{3.3}$$

We claim that (3.3) is again an automorphic form, and in fact U is a unitary operator on $\mathscr{H}^r(\Gamma_0,v)$. Let us first verify (3.1):

$$U\phi(\gamma z)=b'(\gamma z)^{r/2}\phi(b\gamma b^{-1}bz)=v(b\gamma b^{-1})b'(\gamma z)^{r/2}(b\gamma b^{-1})'(bz)^{-r/2}\phi(bz).$$

Using the chain rule and (2.2), we obtain (3.1). Unitary of U is a consequence of the following calculation:

$$(U\phi,U\psi)=\int_{R_0}\overline{b'(z)^{r/2}\phi(bz)}b'(z)^{r/2}\psi(bz)d\mu^r(z)=\int_{R_0}\overline{\phi(bz)}\psi(bz)d\mu^r(bz)=(\phi,\psi),$$

where we have used the transformation properties of $d\mu^r(z)$ and the fact that R_0 is invariant under b.

The isomorphism of Hilbert spaces that we want to establish is in essence the spectral decomposition of U. Explicitly, we define

$$P:\mathscr{H}^r(\Gamma_0,v)\to\int_{S^1}^{\oplus}\mathscr{H}^r(\Gamma,v_\theta)d\theta$$

by the following formula:

$$P\phi(\zeta,\theta)=\sum_{n\in\mathbb{Z}}v_\theta(b^{-n})U^n\phi(z). \tag{3.4}$$

We need to verify that the right-hand side of (3.4) is in $\mathscr{H}^r(\Gamma,v_\theta)$. If $\gamma\in\Gamma_0$, this follows from the fact that $U^n\phi(z)$ are automorphic forms for Γ_0, and the fact that $v_\theta|_{\Gamma_0}=v|_{\Gamma_0}$. If $\gamma=b$, we have

$$U\left(\sum_{n\in\mathbb{Z}}v_\theta(b^{-n})U^n\phi(z)\right)=v_\theta(b)\left(\sum_{n\in\mathbb{Z}}v_\theta(b^{-n})U^n\phi(z)\right).$$

The general case follows easily.

We verify that P is an isometry:

$$\begin{aligned}\|P\phi\|^2 &= \int_{-\pi}^{\pi}\left(\int_R |P\phi(z,\theta)|^2 d\mu^r(z)\right)\frac{d\theta}{2\pi}\\ &= \int_{-\pi}^{\pi}\left(\int_R \sum_{n,m} \overline{U^n\phi(z)}U^m\phi(z)v_\theta(b)^{n-m}d\mu^r(z)\right)\frac{d\theta}{2\pi}\\ &= \int_R \sum_n |U^n\phi(z)|^2 d\mu^r(z)\\ &= \sum_n \int_{b^n R} |\phi(z)|^2 d\mu^r(z)\\ &= \int_{R_0} |\phi(z)|^2 d\mu^r(z).\end{aligned}$$

Similar calculations show that the inverse of P is given by

$$P^{-1}\psi(z) = \int_{-\pi}^{\pi} \psi(z,\theta)d\theta.$$

□

This result implies that the quantization of Riemann surfaces proposed in this paper reduces, when $r = n(2g-2)^{-1}$, to the definition of Ref. 2.

IV. TOEPLITZ QUANTIZATION

In this section, we construct a quantization of the Riemann surface M in terms of Toeplitz operators on $\mathscr{H}^r(\Gamma, v_\theta)$. We first recall the relevant definitions. The reproducing kernel $K^r_{\Gamma_0,v}(z,w)$ for $\mathscr{H}^r(\Gamma_0,v)$ is given by the following Poincaré series:

$$K^r_{\Gamma_0,v}(z,w) = \sum_{\gamma\in\Gamma_0} v(\gamma)^{-1}\gamma'(z)^{r/2}K^r(\gamma(z),w), \tag{4.1}$$

where

$$K^r(z,w) = (1-z\overline{w})^{-1}.$$

Let $C_\Gamma(\mathscr{U})$ be the $\mathbb{C}^*$-algebra of bounded continuous functions on $\mathscr{U}$ which are invariant under Γ, so that $C_\Gamma(\mathscr{U}) \cong C(M)$. For $f \in C_\Gamma(\mathscr{U})$, we define the Toeplitz operator $T^r_{\Gamma_0,v}(f)$ on $\mathscr{H}^r(\Gamma_0,v)$ with symbol f by:

$$(T^r_{\Gamma_0,v}(f)\phi)(z) = \int_{\Gamma_0} K^r_{\Gamma_0,v}(z,w)f(w)\phi(w)d\mu^r(w). \tag{4.2}$$

The goal of this section is to prove that the correspondence $f \mapsto T^r_{G_0,v}(f)$ is a quantization of M. This means that for $f \in C_\Gamma(\mathscr{U})$ we have the norm limit

$$\lim_{r\to\infty} \|T^r_{\Gamma_0,v}(f)\| = \|f\|_\infty, \tag{4.3}$$

where $\|\cdot\|$ denotes the operator norm, and where $\|\cdot\|_\infty$ denotes the sup-norm. If, moreover, f,g are smooth, then

$$\lim_{r\to\infty}\|r[T^r_{\Gamma_0,v}(f\ ),T^r_{\Gamma_0,v}(g)]+T^r_{\Gamma_0,v}(i\{f,g\})\|=0, \tag{4.4}$$

where $\{f,g\}$ is the usual Poisson bracket,

$$\{f,g\}(z)=i(1-|z|^2)^2[\partial f(z)\overline{\partial g}(z)-\partial g(z)\overline{\partial f}(z)]. \tag{4.5}$$

Theorem 4.1: *With the above definitions, the correspondence*

$$f\mapsto T^r_{\Gamma_0,v}(f\ )$$

is a quantization of M.

Proof: The details of analogous estimates were explained in Refs. 1 and 2. Here we follow Ref. 2, where the estimates were proved for the quantization based on automorphic forms of Γ. However, the compactness of the fundamental domain of Γ was used in an essential way in several places, so that the results cannot be applied to the case of Γ_0 (as R_0 is not compact in $\mathscr{U}$). The main difference is that ''transfer of regularity'' argument has to be done more carefully in the present case.

To prove (4.3), we consider the vectors

$$\phi_w(z):=K^r_{\Gamma_0,v}(w,w)^{-1/2}K^r_{\Gamma_0,v}(z,w)$$

in $\mathscr{H}^r(\Gamma_0,v)$, and verify that:

$$\sup_{x\in R}|f(w)-(\phi_w,T^r_{\Gamma_0,v}(f\ )\phi_w)|\to 0,\quad \text{as}\ \ r\to\infty, \tag{4.6}$$

in a way analogous to Ref. 2. The proof there was based on Lemmas 4.1 and 4.2 which are also valid for $\Gamma_0\subset\Gamma$. Since f is invariant under Γ, and not just Γ_0, and since the supremum in (4.6) is taken over a compact set, (4.6) follows exactly as in Ref. 2.

The estimate (4.4) is a consequence of

$$\|r(T^r_{\Gamma_0,v}(f\ )T^r_{\Gamma_0,v}(g)-T^r_{\Gamma_0,v}(fg))+T^r_{\Gamma_0,v}((1-|z|)^2\partial f\overline{\partial g})\|\to 0,\quad \text{as}\ \ r\to\infty, \tag{4.7}$$

for $f,g\in C^\infty_\Gamma$. To prove (4.7), one expands $(\phi,T^r_{\Gamma_0,v}(f\ )T^r_{\Gamma_0,v}(g)\psi)$ in a Taylor series as in Ref. 2 formula (5.6). The first three terms in that formula combine to give the second and third terms in (4.7). The analog of the fourth term of Ref. 2, formula (5.6), is $O(r^{-2})$ as in Ref. 1. It remains to estimate the remainder.

The technique developed in Ref. 1 for estimating the remainder terms can be applied to our case with one modification. The integral $\int_{\mathscr{U}}|\psi(w)|^2d\mu^r(w)$ is infinite if $\psi\in\mathscr{H}^r(\Gamma_0,v)$, and one needs to transfer a power of $1-|w|^2$ to make it convergent. This ''transfer of regularity'' trick was explained in detail on the last two pages of Ref. 2 for Γ-automorphic forms. However, the compactness of the fundamental domain of Γ was used in an essential way. We show below that a modification of the argument used in Ref. 2 can be used in our case.

Lemma 4.2: Let $\psi\in\mathscr{H}^r(\Gamma_0,v)$ and $s>1$. Then we have:

$$\int_{\mathscr{U}}|\psi(w)|^2(1-|w|^2)^s d\mu^r(w)=O(1)\|\psi\|^2.$$

Lemma 4.3: Let $b\in SU(1,1)$ be hyperbolic, let K be a compact set in $\mathscr{U}$, and let $t>0$. Then we have:

$$\sup_{z\in K}\sum_{n\in\mathbb{Z}}|(b^n)'(z)|^t=O(1).$$

We will prove these lemmas after we have completed the main line of the argument.

We now use the above lemmas to estimate the term in formula (5.16) of Ref. 2. This will conclude the proof of Theorem 4.1. That term reads:

$$\int_{R_0\times\mathscr{U}}|\phi(z)|(1-|z|^2)^{1-r/2}|\psi(\gamma_z(w))\|\gamma_z'(w)|^{r/2}\frac{|w|^2}{(1-|w|^2)^{11}}\,d\mu^r(z)d\mu^r(w), \tag{4.8}$$

where $\gamma_z(w)=(w+z)/(\overline{z}w+1)$. Let $0<\epsilon<1/2$. We multiply and divide the integrand by $(1-|\gamma_z(w)|^2)^{1-\epsilon}$, and use the following elementary bound:

$$\frac{1}{(1-|\gamma_z(w)|^2)^{1-\epsilon}}\leqslant\frac{O(1)}{(1-|z|^2)^{1-\epsilon}(1-|w|^2)}.$$

The integral in (4.8) is consequently less then

$$O(1)\int_{R_0\times\mathscr{U}}|\phi(z)|(1-|z|^2)^{\epsilon-r/2}|\psi(\gamma_z(w))|(1-|\gamma_z(w)|^2)^{1-\epsilon}|\gamma_z'(w)|^{r/2}$$
$$\times\frac{|w|^2}{(1-|w|^2)^{12}}\,d\mu^r(z)d\mu^r(z). \tag{4.9}$$

Using the Schwarz inequality and changing variables in the ψ term, we get the following bound:

$$O(1)\|\phi\|\left(\int_{R_0}(1-|z|^2)^{2\epsilon-r}d\mu^r(z)\right)^{1/2}\left(\int_{\mathscr{U}}|\psi(w)|^2(1-|w|^2)^{2-2\epsilon}d\mu^r(w)\right)^{1/2}$$
$$\times\left(\int_{\mathscr{U}}\frac{|w|^4}{(1-|w|^2)^{24}}\,d\mu^r(w)\right)^{1/2}. \tag{4.10}$$

With our choice $0<\epsilon<1/2$, the exponent $2-2\epsilon$ in the third factor is greater than 1, and so we can apply Lemma 4.2 to it, and conclude that it is $O(1)\|\psi\|^2$. The fourth factor is $O(r^{-1})$ by Ref. 2, formula (5.18). One can analyze the second factor in (4.10) as follows:

$$\begin{aligned}\int_{R_0}(1-|z|^2)^{2\epsilon-r}d\mu^r(z)&=O(r)\int_{R_0}(1-|z|^2)^{2\epsilon}d\mu_P(z)\\&=O(r)\sum_{n\in\mathbb{Z}}\int_{b^{-n}R}(1-|z|^2)^{2\epsilon}d\mu_P(z)\\&=O(r)\sum_{n\in\mathbb{Z}}\int_R(1-|b^nz|^2)^{2\epsilon}d\mu_P(z)\\&=O(r)\int_R\sum_{n\in\mathbb{Z}}|(b^n)'(z)|^{2\epsilon}(1-|z|^2)^{2\epsilon}d\mu_P(z)\\&\leqslant O(r)\sup_{z\in R}\sum_{n\in\mathbb{Z}}|(b^n)'(z)|^{2\epsilon}.\end{aligned} \tag{4.11}$$

In (4.11), $d\mu_P(z)$ is the Poincaré measure on $\mathscr{U}$, and we have used the fact that R is compact. Since $2\epsilon>0$ it follows from Lemma 4.3 that (4.11) is $O(r)$. This concludes the transfer of regularity argument.

Proof of Lemma 4.2: We decompose $\mathscr{U}$ into the translates of R_0:

$$\begin{aligned}\int_{\mathscr{U}}|\psi(w)|^2(1-|w|^2)^s d\mu^r(w) &= \sum_{\gamma\in\Gamma_0}\int_{\gamma^{-1}R_0}|\psi(w)|^2(1-|w|^2)^s d\mu^r(w)\\ &= \sum_{\gamma\in\Gamma_0}\int_{R_0}|\psi(w)|^2(1-|\gamma(w)|^2)^s d\mu^r(w)\\ &\leqslant\left(\sup_{w\in\mathscr{U}}\sum_{\gamma\in\Gamma_0}(1-|\gamma(w)|^2)^s\right)\|\psi\|^2.\end{aligned}$$

To estimate the supremum factor, we proceed as in the proof of Ref. 2 lemma 4.2:

$$\begin{aligned}1&=(1-|w|^2)^s\int_{\mathscr{U}}|K^s(w,z)|^2 d\mu^s(z)\\ &=(1-|w|^2)^s\sum_{\gamma\in\Gamma_0}\int_{\gamma^{-1}R_0}|K^s(w,z)|^2 d\mu^s(z)\\ &=(1-|w|^2)^s\sum_{\gamma\in\Gamma_0}|\gamma'(w)|^s\int_{R_0}|K^s(\gamma(w),z)|^2 d\mu^s(z)\\ &=\sum_{\gamma\in\Gamma_0}(1-|\gamma(w)|^2)^s\int_{R_0}|K^s(\gamma(w),z)|^2 d\mu^s(z)\\ &\geqslant\sum_{\gamma\in\Gamma_0}(1-|\gamma(w)|^2)^s\frac{1}{2^{2s}}\int_{R_0}d\mu^s(z).\end{aligned}$$

Hence, $\sup_{w\in\mathscr{U}}\Sigma_{\gamma\in\Gamma_0}(1-|\gamma(w)|^2)^s = O(1)$, if $s>1$. This concludes the proof of Lemma 4.2.

Proof of Lemma 4.3: Since b is a hyperbolic element of SU(1,1), it has two real eigenvalues λ, $1/\lambda$ with $|\lambda|>1$. Letting

$$b^n=\begin{bmatrix}\alpha_n & \beta_n\\ \overline{\beta_n} & \overline{\alpha_n}\end{bmatrix},$$

we have $\alpha_n=O(|\lambda|^{|n|})$. Furthermore, we have the following bound:

$$|(b^n)'(z)|=|\overline{\beta_n}z+\overline{\alpha_n}|^{-2}=|\alpha_n|^{-2}\left|1+\frac{\overline{\beta_n}}{\overline{\alpha_N}}z\right|^{-2}\leqslant|\alpha_n|^{-2}(1-|z|)^{-2}.$$

Since z varies over a compact set and $t>0$, it follows that the series $\Sigma_{n\in\mathbb{Z}}|(b^n)'(z)|^t$ is bounded, uniformly in z, by a convergent geometric series. This concludes the proof of Lemma 4.3 and Theorem 4.1. □

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Radial Coulomb and oscillator systems in arbitrary dimensions

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A mapping is obtained relating analytical radial Coulomb systems in any dimension greater than one to analytical radial oscillators in any dimension. This mapping, involving supersymmetry-based quantum-defect theory, is possible for dimensions unavailable to conventional mappings. Among the special cases is an injection from bound states of the three-dimensional radial Coulomb system into a three-dimensional radial isotropic oscillator where one of the two systems has an analytical quantum defect. The issue of mapping the continuum states is briefly considered. © *1996 American Institute of Physics.* [S0022-2488(96)03105-X]

I. INTRODUCTION

Various types of correspondence between the Kepler–Coulomb and the isotropic-oscillator systems have been extensively investigated since the influential work of Levi-Civita early this century.[1] Among the correspondences of interest are mappings that can be constructed between the radial equations of the quantum systems. This subject was initiated over 50 years ago in a paper by Schrödinger[2] addressing the solution of eigenvalue problems by factorization. Schrödinger discovered a connection between the radial equation of the three-dimensional quantum Coulomb problem and the radial equation of a D-dimensional quantum harmonic oscillator. Using a quadratic transformation in the radial coordinate, he showed that the mapping images all the states in the three-dimensional discrete Coulomb spectrum only for oscillators with $D=2$ or 4.

Schrödinger's idea was subsequently rediscovered or investigated by a number of authors.[3–7] An extension relating the radial equations of the d-dimensional Coulomb system and the D-dimensional oscillator for the special case of even dimensions $d=D$ was given in Ref. 8. A more general mapping for arbitrary d and even D that involves a free parameter was presented in Ref. 9, along with the corresponding mappings to the supersymmetric partners of these systems. All these correspondences involve oscillators in even dimensions, and they incorporate constraints on the allowed range of angular momenta. It is possible in general to map all the states of the d-dimensional Coulomb system into half the states of a D-dimensional oscillator, where d is greater than one and D must be even.

Recently, it has been proposed that some restrictions on the dimensions or angular momenta can be removed with the introduction of suitable analytical deformations called quantum defects in one or both systems.[10] The motivation for this derives from the use of supersymmetric quantum mechanics[11,12] in the context of atomic physics,[13] where supersymmetry-based quantum-defect theory (SQDT)[14] provides an explicit example with direct physical relevance.

One goal of the present paper is to investigate the issue of relaxing the dimensional constraints on the radial correspondences via the introduction of analytical quantum defects. The treatment incorporates not only the Coulomb and oscillator systems but also their supersymmetric partners. We show that with a suitable choice of defect it is indeed possible to remove restrictions on the mappings. For instance, among the examples discussed below is a generalized mapping taking any state in the three-dimensional radial Coulomb problem into a state in an analytically modified three-dimensional radial oscillator. We also briefly consider the continuum states of the two radial systems.

The focus of this work is the set of radial correspondences as summarized above. We do not

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address here the different issue of obtaining surjective mappings between the full D-dimensional oscillator and the full d-dimensional Coulomb systems. This interesting question has been addressed by a number of authors, originating with the parabolic-coordinate transformation of Levi-Civita[1] that relates $D=2$ to $d=2$ and with the mapping of Kustaanheimo and Stiefel[15] in their work on celestial mechanics that relates $D=4$ to $d=3$. The latter transformation in particular has been much investigated in the quantum context,[16–19] and in recent years extensions connecting $D=8$ and $d=5$ have been studied.[20,21] While more complete than the purely radial mappings, all these surjective correspondences are restricted to a narrow range of dimensions.

The organization of this paper is as follows. Section II consists primarily of background on the supersymmetric radial Coulomb and oscillator systems in arbitrary dimensions and the known correspondences between them. It contains key equations needed in the subsequent sections and provides a perspective useful for our purposes. In section III, we introduce SQDT for the radial Coulomb and oscillator systems in arbitrary dimensions, and we define mappings relating these systems to the supersymmetric sectors of the associated zero-defect cases. The general correspondence between different SQDT for the Coulomb and oscillator systems in arbitrary dimensions is established in section IV. This permits, for instance, the entire set of Coulomb radial states to be injected into a subset of the oscillator radial states for any dimensions, including odd oscillator dimensions. Section V provides a short discussion of some results arising for the continuum Coulomb states. We summarize in section VI.

To distinguish comparable quantities in the two systems, we adopt the convention that lowercase letters are used for Coulomb-system variables while upper-case letters are used for oscillator-system variables. An exception is made in denoting energies, for which the symbol E with various sub- and superscripts is used in the Coulomb system while F is used in the oscillator system.

II. PRELIMINARIES

In this section, we establish our conventions and present some preliminary material and results. Section II A begins with definitions and solutions for the radial Coulomb problem in arbitrary dimensions, while in section II B we similarly treat the harmonic-oscillator radial problem. A one-parameter mapping between these systems is presented in section II C. Key equations for supersymmetric quantum mechanics are given in section II D. The supersymmetric counterpart of the results in section II A is discussed in section II E, while that of sections II B and II C is covered in section II F.

A. Coulomb bound states in *d* dimensions

The quantum Kepler–Coulomb system in d dimensions is governed by the Hamiltonian

$$h=-\frac{\hbar^2}{2\mu}\nabla^2-\frac{\kappa}{r}, \tag{1}$$

where μ is the reduced mass, κ is the force constant, and r is the usual radial variable. To avoid normalization issues, we assume $d>1$. The associated radial equation is obtained from the Schrödinger equation $h\psi=E\psi$ by separating the wave function ψ in generalized polar coordinates, $\psi(r,\theta_1,\ldots,\theta_{d-1})=s(r)\,\theta(\theta_1,\ldots,\theta_{d-1})$. Normalizable solutions to the ensuing radial equation are found for discrete eigenenergies given by

$$E_{n,\gamma}=\frac{-E_0}{4(n+\gamma)^2}, \tag{2}$$

where $E_0=2\mu\kappa^2/\hbar^2$, $\gamma=\frac{1}{2}(d-3)$, and n is the principal quantum number taking values $n=l+1, l+2, \ldots$, with l the angular-momentum quantum number arising from the separation of

variables. For $d \geqslant 3$, $l = 0, 1, 2, \ldots$ as usual. When $d = 2$, the angular-momentum quantum number takes the values $0, \pm 1, \pm 2, \ldots$. In this case, we define the symbol l to represent the modulus of the angular momentum. Note that E_0 is the magnitude of the ground-state energy in the lowest dimension considered, $d = 2$.

To simplify the equations that follow, we introduce a dimensionless radial variable $y = r/r_0$, where $r_0 = \hbar^2/2\kappa\mu$. It is also convenient for later considerations involving supersymmetry to work with a scaled radial function $w(y) = y^{\gamma+1} s(r \equiv r_0 y)$, which effectively removes the first-order derivative appearing in the radial equation for s. The radial equation becomes

$$\left\{ -\frac{d^2}{dy^2} + \frac{(l+\gamma)(l+\gamma+1)}{y^2} - \frac{1}{y} - \frac{E}{E_0} \right\} w_{d,n,l}(y) = 0. \tag{3}$$

The eigensolutions involve Sonine-Laguerre polynomials and are given by

$$w_{d,n,l}(y) = c_{dnl} y^{l+\gamma+1} \exp\left(\frac{-y}{2(n+\gamma)} \right) L_{n-l-1}^{(2l+2\gamma+1)}\left(\frac{y}{n+\gamma} \right), \tag{4}$$

with normalization

$$c_{dnl} = \left[\frac{\Gamma(n-l)}{2 r_0^d (n+\gamma)^{2l+d+1} \Gamma(n+l+d-2)} \right]^{1/2}. \tag{5}$$

B. Oscillator bound states in *D* dimensions

The quantum Hamiltonian for the isotropic harmonic oscillator in D dimensions, $D \geqslant 1$, is

$$H = -\frac{\hbar^2}{2M} \nabla^2 + \frac{1}{2} M \Omega^2 R^2, \tag{6}$$

where M is the oscillator mass, Ω is the frequency, and R is the usual radial variable. Separating variables in generalized polar coordinates as before produces a radial equation that has normalizable solutions for energy eigenvalues given by

$$F_{N,\Gamma} = F_0 (2N + 2\Gamma + 3), \tag{7}$$

where $\Gamma = \frac{1}{2}(D-3)$, $F_0 = \frac{1}{2}\hbar\Omega$ is the ground-state energy for the lowest dimension $D = 1$, and N is the principal quantum number taking values $N = L, L+2, L+4, \ldots$, with L the quantized angular momentum arising from the separation of variables. For $D \geqslant 3$, $L = 0, 1, 2, \ldots$ as usual. For $D = 2$, the angular momentum ranges over $0, \pm 1, \pm 2, \ldots$, and we define L to be its modulus. For $D = 1$, the only possibilities are $L = 0$ and 1. The corresponding angular variable has two discrete values, distinguishing the two orientations of the radial vector. These two cases represent distinct *radial* systems for the one-dimensional oscillator, as opposed to the full one-dimensional oscillator with configuration space including both positive and negative coordinate values. For convenience in what follows, we define the parity of the radial wave functions as even if $L = 0$ and odd if $L = 1$.

Defining the dimensionless variable $Y = R/R_0$ with $R_0 = (\hbar/M\Omega)^{1/2}$ and introducing for later convenience the scaled radial function $W(Y) = Y^{\Gamma+1} S(R \equiv R_0 Y)$, the radial equation becomes

$$\left\{ -\frac{d^2}{dY^2} + \frac{(L+\Gamma)(L+\Gamma+1)}{Y^2} + Y^2 - \frac{F}{F_0} \right\} W(Y) = 0. \tag{8}$$

The eigenfunctions are

$$W_{D,N,L}(Y)=C_{DNL}Y^{L+\Gamma+1}\exp(-\tfrac{1}{2}Y^2)L_{N/2-L/2}^{(L+\Gamma+1/2)}(Y^2), \tag{9}$$

with normalization

$$C_{DNL}=\left[\frac{2\Gamma(N/2-L/2+1)}{R_0^D\Gamma(N/2+L/2+D/2)}\right]^{1/2}. \tag{10}$$

With our definitions for L above, these expressions hold for all integral $D\geqslant 1$. Note that the $D=1$ normalization coefficients differ from the canonical ones by a factor of $\sqrt{2}$ because the above construction produces a normalization on the half line only.

C. Mappings between the Coulomb and oscillator problems

The wave function (4) can be mapped to the wave function (9) through the quadratic transformation

$$Y^2=\frac{y}{(n+\gamma)}. \tag{11}$$

This correspondence also interconnects the differential equations (3) and (8). The explicit relation between eigensolutions is

$$W_{D,N,L}(Y)=K_{dn\lambda}Y^{-1/2}w_{d,n,l}((n+\gamma)Y^2), \tag{12}$$

where the quantity $K_{dn\lambda}$ maintains the normalization of the wave functions and is given by

$$K_{d,n,\lambda}=\frac{(2n+d-3)r_0^{d/2}}{R_0^{d-1-\lambda}}. \tag{13}$$

The quantity λ provides an extra degree of freedom in the mapping.

The ensuing relationships among the dimensionalities and the quantum numbers of the two systems are[9]

$$D=2d-2-2\lambda, \quad N=2n-2+\lambda, \quad L=2l+\lambda. \tag{14}$$

The last of these equations constrains λ to be integral. It then follows from the first equation that this mapping has image only in the oscillators of even dimension D.

For given angular momenta l and L, the relation (14) between the principal quantum numbers ensures that the stack $n\geqslant l+1$ of Coulomb states is in one-to-one correspondence with the stack $N\geqslant L$ of oscillator states, with ground states coinciding. This relation between N and n determines a condition relating the energies E and F of the two systems:

$$\frac{F_{N,\Gamma}}{F_0}=2\sqrt{\frac{E_0}{-E_{n,\gamma}}}. \tag{15}$$

The factor of two can be viewed as originating from the scaling of N relative to n in the second equation in (14). Absorbing it in the definitions of E_0 or F_0 would change equations (3) or (8).

Condition (14) shows that successive Coulomb angular momenta l map to every second oscillator angular momentum L. The *entire* set of radial states $|n,l\rangle$ of the d-dimensional Coulomb system can be mapped into a subset of the states $|N,L\rangle$ of the D-dimensional oscillator provided D satisfies $2\leqslant D\leqslant 2d-2$. For even or odd λ, the mapping is then an isomorphism to even or odd L, respectively. For given d, the allowed values of the pair (D,λ) characterizing this mapping are distinct: $(2,d-2)$, $(4,d-3)$, ..., $(2d-4,1)$, $(2d-2,0)$. We recover in this way

Schrödinger's result that all states of the three-dimensional Coulomb system can be mapped only into oscillators of dimension two or four. Note that if instead l is taken to be fixed, so that only a subset of states is imaged, then the allowed range of D is[4] $2 \leqslant D \leqslant 2d-2+4l$.

D. Supersymmetric quantum mechanics

For the purposes of the present paper, only a few of the basic results of supersymmetric quantum mechanics are needed. We restrict our attention to systems with a quantum-mechanical Hamiltonian H_S and two supersymmetry charges Q and $Q^\dagger$, obeying the defining relations of the superalgebra sqm(2):

$$\{Q,Q^\dagger\}=H_S, \quad [Q,H_S]=[Q^\dagger,H_S]=0. \tag{16}$$

The representation of this algebra relevant here is two dimensional and may be parametrized as[11,12]

$$Q=\begin{pmatrix} 0 & 0 \\ A & 0 \end{pmatrix}, \quad Q^\dagger=\begin{pmatrix} 0 & A^\dagger \\ 0 & 0 \end{pmatrix}, \quad H_S=\begin{pmatrix} H^+ & 0 \\ 0 & H^- \end{pmatrix}. \tag{17}$$

There are two component Hamiltonians in this system and two associated Hilbert spaces. If the bosonic Hamiltonian H^+ acts on wave functions ψ^+, while the fermionic Hamiltonian H^- acts on ψ^-, then the corresponding Schrödinger equations can be written as

$$H^\pm\psi^\pm=\left[-\frac{d^2}{dy^2}+V^\pm(y)\right]\psi^\pm=E^\pm\psi^\pm, \tag{18}$$

where A is the operator $A=-i\partial_y-iU'$ and where the supersymmetric partner potentials are defined by $V^\pm(y)=U'^2\mp U''$, with $U'=\partial_y U(y)$ a specified function called the superpotential.

The ground state of a supersymmetric system lies in the bosonic sector and has zero energy. Every state in the bosonic sector other than the ground state is degenerate with a distinct state in the fermionic sector, and the operators Q, $Q^\dagger$ map between these paired states.

E. Supersymmetric Coulomb system

To construct the supersymmetric Coulomb system, the bosonic-sector combination H^+-E^+ from Eq. (18) is identified with the radial equation (3). In the latter, a suitable constant must be added to the energy eigenvalues and incorporated in the potential to ensure that the ground-state energy is zero. Thus, the eigenvalues are

$$E^+_{nl}=\frac{1}{4(l+1+\gamma)^2}-\frac{1}{4(n+\gamma)^2}, \tag{19}$$

and the bosonic potential function is

$$v^+(y)=\frac{(l+\gamma)(l+\gamma+1)}{y^2}-\frac{1}{y}+\frac{1}{4(l+1+\gamma)^2}. \tag{20}$$

The last term in Eq. (20) is the energy shift ensuring a zero ground-state energy. Since it must be constant, l must be fixed to define a supersymmetric partner.

The superpotential is specified by the function[13]

$$u(y)=\frac{y}{2(l+\gamma+1)}-(l+\gamma+1)\ln y. \tag{21}$$

The fermionic Hamiltonian and hence the associated fermionic radial equation can then be calculated as

$$\left\{-\frac{d^2}{dy^2}+\frac{(l'+\gamma)(l'+\gamma+1)}{y^2}-\frac{1}{y}+\frac{1}{4(l'+\gamma)^2}\right\}w^-(y)=E^-_{n'l'}w^-(y), \tag{22}$$

where $l'=l+1$ and n' takes on all values of n except the lowest one, $l+1$. The fermionic wave functions $w^-(y)$ have the same functional form as the bosonic wave functions $w^+(y)\equiv w(y)$ given in Eq. (4), but with n and l replaced by n' and l':

$$w^-_{d,n',l'}(y)=w_{d,n',l'}(y). \tag{23}$$

The two sets of eigenvalues are degenerate for $n'=n$: $E^-_{n'=n,l'}=E^+_{nl}$.

With fixed l, the bosonic stack of eigenstates in order of increasing energy consists of the series of kets $|n=l+1,\ l\rangle$, $|n=l+2,\ l\rangle$, ... , with lowest energy zero. The associated fermionic stack has angular momentum greater by one unit and starts with lowest energy corresponding to the second state of the bosonic sector: $|n'=l+2,\ l+1\rangle$, $|n'=l+3,\ l+1\rangle$, ... The use of n' here is consistent with spectroscopic notation. For example, when the s orbitals of lithium are interpreted as the supersymmetric partner of the hydrogen atom, $n'=2$ corresponds to the ground state, as expected.

A useful one-to-one correspondence between these two stacks identifies the lowest states with each other, and successively higher states of the bosonic sector with successively higher states of the fermionic sector. It is defined by the following replacements in the bosonic wave function:

$$n\mapsto n'=n+1, \quad l\mapsto l'=l+1. \tag{24}$$

This stack correspondence relates eigenstates with different eigenvalues. Along with similar stack correspondences defined below, it plays a useful role in the analyses to follow.

F. Supersymmetric oscillator and composition mapping

The bosonic component of the supersymmetric oscillator can be obtained from the radial equation (8) under a suitable energy shift. The eigenvalues are

$$F^+_{NL}=2(N-L). \tag{25}$$

The superpotential is specified via the function

$$U(Y)=\tfrac{1}{2}Y^2-(L+\Gamma+1)\ln Y, \tag{26}$$

which generates the fermionic equation

$$\left\{-\frac{d^2}{dY^2}+\frac{(L'+\Gamma)(L'+\Gamma+1)}{Y^2}+Y^2-(2L'+2\Gamma-1)\right\}W^-(Y)=F^-_{N'L'}W^-(Y), \tag{27}$$

where L' is defined by $L'=L+1$. The principal quantum number N' takes the values $N'=L'$, $L'+2, L'+4$, ... The fermionic wave functions $W^-(y)$ have the same functional form as the bosonic wave functions $W^+(Y)\equiv W(Y)$ of Eq. (9), with N, L replaced by N', L', respectively:

$$W^-_{D,N',L'}(Y)=W_{D,N',L'}(Y). \tag{28}$$

The fermionic energies $F^-_{N'L'}=2(N'-L'+2)$ are degenerate with the bosonic energies for $N'+1=N$, $F^-_{N'L'}=F^+_{N=N'+1,L}$.

In order of increasing energy, the bosonic stack with fixed L consists of the kets $|N=L,\ L\rangle$, $|N=L+2,\ L\rangle$, $|N=L+4,\ L\rangle$, ..., with lowest energy zero. The associated fermionic stack has angular momentum one unit greater and contains the kets $|N'=L'=L+1,\ L+1\rangle$, $|N'=L+3,\ L+1\rangle$, ...

The $D=1$ case is unusual and warrants special attention. As mentioned above, the ''angular momentum'' L for the one-dimensional oscillator takes the values zero and one, corresponding to even and odd parity. The system resembles a single stack, but is composed of two interlocking substacks. As a result, the spacing between neighboring eigenvalues is half its value in higher dimensions. Also, in constructing the supersymmetric partner, the energy shift is L dependent. Consequently, distinct shifts appear for each substack. The formalism thus establishes *two* independent supersymmetries, each of which respects the parity and only one of which may be considered at a time. These supersymmetries for the one-dimensional radial oscillator differ from the usual one for the full one-dimensional oscillator, where a single energy shift is effected and states of opposite parity are degenerate under the supersymmetry.

In later sections, for reasons that emerge from the construction of the generalized mapping, it is more natural to focus on the supersymmetric partner of the fermionic oscillator rather than the fermionic oscillator itself. This system, which we call ''second fermionic,'' has wave functions $W^{=}_{DN''L''}$ given by

$$W^{=}_{DN''L''}(Y)=W_{D,N'',L''}(Y). \tag{29}$$

Here, L'' is defined by $L''=L'+1$, and N'' takes values L'', $L''+2$, $L''+4$, ... The differential equation for this system has the same functional form as the fermionic equation (27), except for the replacement of N and L with N'' and L'', respectively.

The oscillator bosonic sector may be put into one-to-one correspondence with the second-fermionic sector by making the following replacements in the bosonic wave function:

$$N\mapsto N''=N+2, \quad L\mapsto L''=L+2. \tag{30}$$

By composition of this mapping and the ones given in sections II C and II E, a correspondence may be established between the fermionic sector of the Coulomb system and the second-fermionic sector of the oscillator. It is given by

$$W^{=}_{D,N'',L''}(Y)=K_{d,n',\lambda}Y^{-1/2}w^{-}_{dn'l'}((n'+\gamma)Y^2), \tag{31}$$

$$Y^2=\frac{y}{(n'+\gamma)}, \tag{32}$$

$$N''=2n'-2+\lambda, \tag{33}$$

$$L''=2l'+\lambda. \tag{34}$$

The dimensions are still related as in Eq. (14). See Figure 1. We emphasize that this commutative diagram involves mappings different from those presented in Ref. 9, where the second-fermionic sector is not considered.

III. GENERALIZED SUPERSYMMETRY-BASED QUANTUM-DEFECT THEORY

In this section, we introduce analytical SQDT for the Coulomb and oscillator systems in arbitrary dimensions. From the present perspective, the goal is to obtain effective radial equations

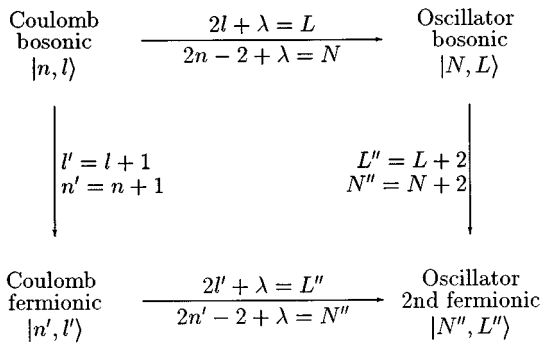

FIG. 1. Supersymmetric mappings. Relationships are shown interconnecting the bosonic and fermionic partners of the Coulomb and oscillator systems. The diagram is commutative.

that offer sufficient flexibility to obviate the dimension and angular-momentum constraints of the usual mappings, while maintaining eigensolutions with analytical structure comparable in simplicity to those of the Coulomb and oscillator systems.

The existence of suitable deformations of the Coulomb and oscillator systems satisfying these criteria is by no means apparent *a priori*. In what follows, we take as a guide the SQDT that is known to provide a useful analytical description of the valence structure of physical atoms in terms of an effective one-particle radial equation.[14] This model determines an effective radial potential modifying the three-dimensional radial Coulomb equation. It generates solutions with physical eigenvalues given by the Rydberg expression

$$E_{n^*} = -E_0/4n^{*2}. \tag{35}$$

Here, n^* is the principal quantum number modified by subtracting the quantum defect δ, which in general depends on the angular momentum and the principal quantum number. In section III A, we generalize this model to the d-dimensional situation. For simplicity, we take δ and its generalization in arbitrary dimensions to be independent of the principal quantum number. This approximation is excellent in, for example, real alkali-metal atoms.[22]

Similar ideas can be implemented for the radial equation of the D-dimensional oscillator. The resulting oscillator SQDT are presented in section III B. A possible physical application of these oscillator models is to the description of a valence particle in geonium atoms formed by a group of charged particles bound in a Penning trap.[10]

A. Generalized SQDT for the Coulomb system

Given the d-dimensional Coulomb radial equation (3) with fixed angular momentum l, we seek to implement two modifications via an effective potential $v_{\text{eff}}(y)$ added to the left-hand side. The first desired modification is a shift in dimension, from d to $d^*=d+j$, where j is an integer that in principle could depend on l. We require $d^*>1$, so j must satisfy $j>1-d$. The second desired modification is a shift in energy eigenvalues from $E_{n,\gamma}$ in Eq. (2) to the d^*-dimensional extension of the Rydberg series [see Eq. (41) below]. We want both these changes to be implemented while maintaining analytical eigenfunctions with form similar to those in Eq. (4).

Remarkably, these goals can be accomplished with a relatively simple effective potential, given by

$$v_{\text{eff}}(y) = \frac{(n+\gamma)^2-(n^*+\gamma^*)^2}{4(n+\gamma)^2(n^*+\gamma^*)^2} + \frac{(l^*+\gamma^*)(l^*+\gamma^*+1)-(l+\gamma)(l+\gamma+1)}{y^2}. \tag{36}$$

Here, the quantity γ^* is defined by $\gamma^* = (d^* - 3)/2$. The quantities n^* and l^* are defined as

$$n^* \equiv n_s - \delta = n + i - \delta, \tag{37}$$

$$l^* = l + i - \delta, \tag{38}$$

where δ is the quantum defect determining the energy shifts for the generalized Rydberg series and where $i = i(l)$ is an integral-valued function of the angular momentum. In the supersymmetric interpretation for the valence electron of physical atoms, $i(l)$ is the number of filled lower levels with angular momentum l. The introduction of n_s is motivated by the three-dimensional case, where it is equal to the principal quantum number and takes conventional values in the standard spectroscopic notation. It satisfies $n_s = n + i$, where n takes the usual values characteristic of the exact Coulomb system. As an example, the s states of the supersymmetric sodium atom in three dimensions have $i(0) = 2$, giving $n_s = 3$, $n_s = 4$, $n_s = 5$ for the first three levels.[13] The corresponding values of n are $n = 1$, $n = 2$, $n = 3$. For the supersymmetric partner of the exact Coulomb system, $i = 1$ and so $n_s = n + 1 = n'$, consistent with our previous notation for the supersymmetric case.

The first term of Eq. (36) has the effect of shifting the energy levels, while the second term performs a corresponding shift in the angular-momentum barrier. The combined effect of both terms incorporates the desired dimensional shift. With a nonzero quantum defect $\delta(l)$, the effective potential $v_{\text{eff}}(y)$ plays the role of a supersymmetry-breaking potential. The resulting radial equation has analytical solutions given in terms of the usual Coulomb solutions $w_{d,n,l}(y)$ by $w_{d^*,n^*,l^*}(y)$. These solutions exist for $n \geqslant l + 1$, or $n_s \geqslant l + i + 1$. Requiring the existence and orthonormalizability of the wave functions restricts $\delta - i$ according to

$$\delta - i < l + \gamma + 1 + \tfrac{1}{2} j. \tag{39}$$

It is convenient to define a dimensionless quantity $a(l)$ by

$$a(l) = i - \delta + \tfrac{1}{2} j. \tag{40}$$

The eigenvalues of the differential equation can then be expressed as

$$\frac{E_{n^*,\gamma^*}}{E_0} = \frac{-1}{4(n^* + \gamma^*)^2} = \frac{-1}{4(n + \gamma + a)^2}. \tag{41}$$

In this equation, we have chosen the eigenenergies so that the limiting case with $d = 3$ and $i = j = 0$ reproduces the Rydberg series (35). For i, δ, and j chosen so that $a = 0$, we obtain the bosonic equation of the Coulomb system discussed in section II E, up to an energy shift. If $a = 1$, the fermionic sector of the Coulomb problem is generated instead. Moreover, the supersymmetric partner of the fermionic sector is generated by setting $a = 2$, and each successive iteration of the supersymmetry increments a by one unit.

A useful stack correspondence can be established between the spectrum of the bosonic sector of the supersymmetric Coulomb system and the SQDT Coulomb spectrum. The map is given by making the following replacements in $w^+_{d,n,l}$:

$$\begin{aligned} d &\mapsto d^* = d + j, \\ n &\mapsto n^* = n + i - \delta = n_s - \delta, \\ l &\mapsto l^* = l + i - \delta. \end{aligned} \tag{42}$$

B. Generalized SQDT for the oscillator system

The techniques of section III A can also be applied to the radial oscillator system in D dimensions. For fixed angular momentum L, we can obtain an effective potential $V_{\rm eff}(Y)$ to be added to Eq. (8) that maintains analytical eigenfunctions while inducing an integral shift to a new dimension $D^* \equiv D+J \geq 1$ and simultaneously modifying the oscillator energy eigenvalues via a shift to a new principal quantum number N^*. We refer to the resulting theory as the oscillator SQDT.

The appropriate choice of effective potential is

$$V_{\rm eff}(Y) = 2(N-N^*+\Gamma-\Gamma^*) + \frac{(L^*+\Gamma^*)(L^*+\Gamma^*+1)-(L+\Gamma)(L+\Gamma+1)}{Y^2}, \tag{43}$$

where $\Gamma^* = (D^*-3)/2$ and the shifted quantum numbers are given by

$$N^* \equiv N_s - I - \Delta \equiv N + I - \Delta, \tag{44}$$

$$L^* = L + I - \Delta. \tag{45}$$

Here, $I = I(L)$ is an integral-valued function, analogous to $i(l)$ in the Coulomb case, that can be interpreted as the number of inaccessible lower levels. The quantity $\Delta(N,L)$ is the oscillator equivalent of the Rydberg quantum defect $\delta(n,l)$, modifying the radial-repulsion term in the differential equation. For simplicity in what follows, we take Δ to depend only on L, thereby paralleling the case of alkali-metal atoms for which δ depends only on l. We have also defined a quantity N_s playing the role of the principal quantum number in the spectroscopic notation, given by $N_s = N + 2I$. If the dimension is unmodified and $\Delta = 0$, the choice $I = 1$ yields the fermionic sector of the supersymmetry discussed in section II F. In this limit $N' = N^* = N+1 \neq N_s$, which differs from the supersymmetric limit of the Coulomb SQDT where $n' = n^* = n_s$. With our definitions, degenerate levels in the bosonic and fermionic sectors have values of N differing by $2I$ units, but have the same value of N_s.

The first term in Eq. (43) implements the eigenenergy shift to the oscillator analogue of the Rydberg series, while the second term is the corresponding anharmonic modification to the potential that maintains analytical eigensolutions. The eigenfunctions solving the resulting effective radial equation are given in terms of the oscillator wave functions $W_{D,N,L}(Y)$ of Eq. (9) by $W_{D^*,N^*,L^*}(Y)$. The existence of these solutions requires that the principal quantum number takes the values $N_s = L+2I,\ L+2I+2,\ L+2I+4,\ \ldots$, or $N = L,\ L+2,\ L+4,\ \ldots$. Requiring orthonormalizability of the wave functions restricts the range of $\Delta - I$ to

$$\Delta - I < L + \Gamma + \tfrac{3}{2} + \tfrac{1}{2}J. \tag{46}$$

We can again introduce a useful dimensionless quantity $A(L)$ by

$$A(L) = I - \Delta + \tfrac{1}{2}J. \tag{47}$$

The eigenvalues of the differential equation can be expressed as

$$\frac{F_{N^*,\Gamma^*}}{F_0} = 2N^* + 2\Gamma^* + 2A + 3 = 2N + 2\Gamma + 4A + 3. \tag{48}$$

We have chosen the ground-state eigenenergy in analogy with the Coulomb case (41). The extra factor of $2A$ appears to ensure that the bosonic and fermionic spectra of the limiting supersymmetric case with $\Delta = 0$, $J = 0$ have the characteristic degenerate pairing. If I, Δ, and J are selected so that $A = 0$, then this SQDT system reduces to the bosonic oscillator discussed in section II F, up

to an energy shift. If $A=1$, it reduces instead to the fermionic partner. If $A=2$, the second-fermionic sector of the supersymmetric oscillator is produced. Each further iteration of supersymmetry produces an additional unit increment of A. Note that for fixed L the spacing between successive eigenvalues is always four units, regardless of the value of A.

A correspondence can be established between the oscillator SQDT and the bosonic sector of the supersymmetric oscillator. The images of the wave functions are obtained by making the replacements

$$D\mapsto D^*=D+J, \quad N\mapsto N^*=N+I-\Delta, \quad L\mapsto L^*=L+I-\Delta. \tag{49}$$

IV. MAPPINGS BETWEEN BOUND STATES OF THE COULOMB AND OSCILLATOR SQDT

Composition of the mappings in sections II C, III A, and III B allows us to establish a correspondence between the d^*-dimensional Coulomb SQDT and the D^*-dimensional oscillator SQDT. This mapping is described in section IV A. One of its striking features is that the odd-dimensional oscillator can be imaged. In section IV B, we illustrate the mapping with examples involving the three-dimensional Coulomb and oscillator systems.

A. The general case

The general mapping is given by

$$W_{D^*,N^*,L^*}(Y)=K_{d^*,n^*,\lambda-J/2+j}Y^{-1/2}w_{d^*,n^*,l^*}((n^*+\gamma^*)Y^2), \tag{50}$$

$$Y^2=y/(n^*+\gamma^*), \tag{51}$$

$$D^*=2d^*-2-2\lambda+J-2j, \tag{52}$$

$$N^*=2n^*-2+\lambda-\tfrac{1}{2}J+j, \tag{53}$$

$$L^*=2l^*+\lambda-\tfrac{1}{2}J+j, \tag{54}$$

$$A=2a. \tag{55}$$

This mapping, like the Coulomb-oscillator case discussed in section II C, is based on a quadratic relationship between the radial variables of the two systems. The constant K can be chosen to preserve the normalization of the wave functions, in which case it has the functional form given in Eq. (13). Note that Eq. (53) is equivalent to a generalization of Eq. (15), given by

$$\frac{F_{N^*,\Gamma^*}}{F_0}=2\sqrt{\frac{E_0}{-E_{n^*,\gamma^*}}}+4a. \tag{56}$$

Note also that the allowed ranges of the quantum defects given in Eq. (39) and Eq. (46) are compatible with Eq. (55), which guarantees that the image of any orthonormalizable Coulomb radial system is an orthonormalizable oscillator.

To gain insight about the flexibility of this mapping, consider the choice $j=0$. Then, D^* lies in the range $1+J\leqslant D^*\leqslant 2d-2+J$ with allowed values separated by two units. Since we require $J\geqslant 1-D$, any $D^*\geqslant 1$ is possible. Moreover, d may take any value greater than one. The above general mapping therefore relates any Coulomb dimension $d>1$ to any oscillator dimension $D^*\geqslant 1$. In particular, Eq. (52) shows that D^* is odd if J is chosen to be an odd integer. This is in striking contrast to the usual restriction of D to even values only, as given by Eq. (14).

The Coulomb-oscillator mappings defined earlier are special cases of our general mapping. The correspondence of section II C is recovered by setting $i=\delta=j=0$ in the Coulomb system and

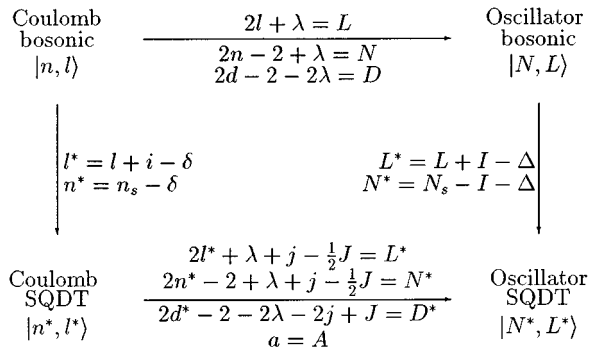

FIG. 2. SQDT mappings. Relationships are shown interconnecting the bosonic and SQDT sectors of the Coulomb and oscillator systems. The diagram is commutative.

$I=\Delta=J=0$ in the oscillator system, so that $A=2a=0$. Figure 2 is a commutative diagram showing the relationship between this simpler mapping and the general mapping. Similarly, the mapping of section II F between the fermionic sector of the supersymmetric Coulomb system and the second-fermionic sector of the supersymmetric oscillator is reproduced with the choices $i=1$, $\delta=0$, $j=0$ and $I=2$, $\Delta=0$, $J=0$, so that $A=2a=2$.

For the case of constant nonnegative integral A and a, Eq. (55) controls the relationship between the supersymmetric sectors of the two systems. While any iteration of the supersymmetry for the Coulomb system can be taken, only *even* iterations of the oscillator supersymmetry appear. This is why we introduced the second-fermionic sector of the supersymmetric oscillator in section II F. It is therefore possible to combine Figures 1 and 2 in a single commutative diagram. Moreover, the general mapping shows that Figure 1 can be extended downward to incorporate higher iterations of the supersymmetry. The result is an infinite series of mappings relating Coulomb systems with $a=2, 3, 4, \ldots$ to oscillator systems with $A=4, 6, 8, \ldots$, respectively.

B. Three-dimensional Coulomb and oscillator systems

To obtain further insight about the content of the general mapping of section IV A, we next restrict attention to the special case where both systems are three-dimensional. Since this choice can be implemented with $j=0$, we assume this in what follows.

The general mapping becomes

$$W_{3,N^*,L^*}(Y)=K_{3,n^*,1/2}Y^{-1/2}w_{3,n^*,l^*}(n^*Y^2), \tag{57}$$

$$N^*=2n^*-\tfrac{3}{2}, \tag{58}$$

$$L^*=2l^*+\tfrac{1}{2}, \tag{59}$$

$$\Delta-I=2(\delta-i)+\lambda-\tfrac{1}{2}. \tag{60}$$

The values of λ allowed by Eq. (54) are $\lambda=0,1$. The orthonormality requirements Eq. (39) and Eq. (46) become

$$\delta-i<l+1, \tag{61}$$

$$\Delta-I<L+\tfrac{3}{2}. \tag{62}$$

We can regard Eq. (61) and Eq. (62) as conditions limiting the choice of quantum defects in the two systems to a semi-infinite region of the $(\Delta - I)$ versus $(\delta - i)$ plane. The condition (60) then further restricts the choice to a straight line in this region.

One interesting special case is obtained by requiring that the oscillator be exact in the sense that $\Delta - I = 0$. Then, Eq. (60) becomes

$$\delta - i = -a = \tfrac{1}{2}(\tfrac{1}{2} - \lambda), \tag{63}$$

showing that a nonzero defect in the Coulomb system is necessary. The eigenvalues of the equations are

$$E_{n^*,\gamma^*} = \frac{-E_0}{(2n + \lambda - \frac{1}{2})^2}, \tag{64}$$

$$F_{N,\Gamma} = F_0(2N + 2\lambda + 2), \tag{65}$$

and the relationships among the principal quantum numbers and the angular momenta become

$$L = 2l^* + \tfrac{1}{2}, \tag{66}$$

$$N = 2n^* - \tfrac{3}{2}. \tag{67}$$

Selecting $\lambda = 1$ for definiteness, we see that Eq. (66) maps each successive Coulomb angular momentum $l^* = \frac{1}{4}$, $l^* = \frac{5}{4}$, $l^* = \frac{9}{4}$, ... to every second oscillator angular momentum starting at $L = \lambda$: $L = 1$, $L = 3$, $L = 5$, ... The mapping therefore preserves the degeneracy of states. For instance, the kets $|n^* = \frac{9}{4}, l^* = \frac{1}{4}\rangle$ and $|n^* = \frac{9}{4}, l^* = \frac{5}{4}\rangle$, which are degenerate in the Coulomb system, are mapped to the degenerate states $|N = 3, L = 1\rangle$ and $|N = 3, L = 3\rangle$ in the oscillator system. This feature is also a characteristic of the original mapping of section II C. The main differences here are that the Coulomb effective angular momenta l^* are nonintegral and, more importantly, that both systems are three dimensional.

A second case of interest is obtained when the Coulomb system is exact, i.e., $\delta - i = 0$. The condition $j = 0$ implies that $a = 0$ too. Then, Eq. (55) becomes $\Delta - I = \lambda - \frac{1}{2}$, showing that a nonzero defect is again needed, this time in the oscillator system. The eigenvalues are

$$E_{n,\gamma} = \frac{-E_0}{4n^2}, \tag{68}$$

$$F_{N^*,\Gamma^*} = F_0(2N - 2\lambda + 4), \tag{69}$$

and the mapping gives

$$L^* = 2l + \tfrac{1}{2}, \tag{70}$$

$$N^* = 2n - \tfrac{3}{2}. \tag{71}$$

The first of these equations shows every second oscillator angular momentum is imaged, which again preserves the degeneracy of states. If, for example, we choose $\lambda = 0$, then the degenerate Coulomb states $|n = 3, l = 1\rangle$ and $|n = 3, l = 2\rangle$ map to the degenerate oscillator states $|N^* = \frac{9}{2}, L^* = \frac{5}{2}\rangle$ and $|N^* = \frac{9}{2}, L^* = \frac{9}{2}\rangle$.

In the above examples, the quantities $\Delta - I$ and $\delta - i$ are constant. In physical systems such as alkali-metal atoms, $\delta - i$ depends on l and tends towards zero as l increases. This feature can also

TABLE I. Possible parameters for a mapping between the radial Coulomb and oscillator systems in three dimensions. For the choices $j=0$ and $\lambda=1$, values of l, i, n, n_s, and δ are tabulated for sodium along with the corresponding values of L, I, N, N_s, and Δ under the mapping (60). The quantities $I(L)$ have been selected to fill all levels below $N_s=5$.

Coulomb system (sodium)					Oscillator system				
l	i	n	n_s	δ	L	I	N	N_s	Δ
0	2	$\geqslant 1$	$\geqslant 3$	1.35	1	2	$\geqslant 1$	$\geqslant 5$	1.20
1	1	$\geqslant 2$	$\geqslant 3$	0.859	3	1	$\geqslant 3$	$\geqslant 5$	1.218
2	0	$\geqslant 3$	$\geqslant 3$	0.01	5	0	$\geqslant 5$	$\geqslant 5$	0.52
3	0	$\geqslant 4$	$\geqslant 4$	0	7	0	$\geqslant 7$	$\geqslant 7$	0.50
$\geqslant 4$	0	$\geqslant l+1$	$\geqslant l+1$	0	$\geqslant 9$	0	$\geqslant L$	$\geqslant L$	0.5

be incorporated in our general mapping. It implies a dependence of $\Delta - I$ on L, which might reflect a realistic feature of a physical oscillator such as a cloud of particles caught in a Penning trap.

As an example, we map the SQDT radial equation for the physical sodium atom into a three-dimensional SQDT oscillator. In sodium, the inaccessibility of the levels occupied by the ten inner electrons is implemented by the choices $i(0)=2$, $i(1)=1$, and $i(l\geqslant 2)=0$. The quantum defects $\delta(l)$ in this case are known.[22] Choosing for definiteness $\lambda=1$ and selecting $I(0)=2$, $I(1)=1$, $I(L\geqslant 2)=0$, the values of Δ can be found from Eq. (60). Table I lists the results. As expected, the values of Δ tend towards $\frac{1}{2}$ as L increases.

V. MAPPINGS FOR CONTINUUM STATES

In previous sections, we have explored mappings between the bound states of the Coulomb and oscillator systems. It is natural to consider whether similar mappings exist taking the unbound Coulomb states into an appropriate oscillator. This question is of lesser physical interest at present, so we restrict ourselves here to a brief outline of a possible approach to this issue.

The Coulomb problem with energies $E>0$ can be viewed as a scattering problem. Following the general procedure of section II A again yields the differential equation (3), but with $E>0$. In terms of the confluent hypergeometric function ${}_1F_1$, the solutions are

$$w_{d,E,l}(y)\propto y^{l+\gamma+1}\exp\left(\pm iy\sqrt{\frac{E}{E_0}}\right){}_1F_1\left(l+\gamma+1\pm\frac{1}{2i}\sqrt{\frac{E_0}{E}},2(l+\gamma+1),\mp 2iy\sqrt{\frac{E}{E_0}}\right). \tag{72}$$

The upper and lower signs correspond to outgoing and incoming waves, respectively. The results of section II A can be recovered by taking E to be negative and choosing the upper sign.

It turns out that the appropriate image oscillator system[23] is the *inverted* oscillator, with potential $U(R)=-\frac{1}{2}M\Omega R^2$. This system is unbound. The procedure of section II B gives a differential equation identical to Eq. (8) except that the sign of the potential Y^2 is reversed. The solutions $W_{D,F,L}(Y)$ are

$$W_{D,F,L}(Y)\propto Y^{L+\Gamma+1}\exp\left(\pm\frac{1}{2}iY^2\right){}_1F_1\left(\frac{1}{2}\left(L+\Gamma+\frac{3}{2}\right)\mp\frac{iF}{4F_0},L+\Gamma+\frac{3}{2},\mp iY^2\right). \tag{73}$$

These functions may not be physically permissible, but are relevant for the purposes of establishing a mapping. With the choice of the upper sign, the wave functions for the usual oscillator may be obtained up to a constant by the analytic continuation $Y^2\to iY^2$ and $F\to -iF$.

A correspondence analogous to the mapping of section II C exists between the continuum Coulomb states and the inverted-oscillator functions. It is

$$W_{D,F,L}(Y) \propto Y^{-1/2} w_{d,E,l}\left(\frac{Y^2}{2\sqrt{E/E_0}}\right), \tag{74}$$

$$Y^2 = 2y\sqrt{E/E_0}, \tag{75}$$

$$D = 2d - 2 - 2\lambda, \tag{76}$$

$$L = 2l + \lambda, \tag{77}$$

$$\frac{F}{F_0} = 2\sqrt{\frac{E_0}{E}}\,. \tag{78}$$

There are many similarities between this mapping and the one discussed in section II C. Again, λ must be integral, so only even-dimensional oscillators are available as images. Also, the angular momenta L are restricted to being either all odd or all even, thus eliminating half the oscillator states. However, the energy relation (78), unlike (15), involves continuous values of E and F. It also reveals that negative energies F are excluded from the mapping. As one energy tends to zero the other tends to infinity.

As an aside, we remark that the negative energies F do appear when considering the *repulsive* Coulomb problem. The differential equation of this problem is mapped into the inverted-oscillator differential equation[24] by a map with (74) through (77) unchanged but with a negative sign taken for the square root in Eq. (78).

Although this lies outside the scope of the present work, it seems feasible that supersymmetry could be introduced into these systems along with the corresponding SQDT. We conjecture that this allows for odd dimensions D. Since parabolic coordinates have some advantages for scattering problems, it would also be interesting to perform an analysis in terms of the dual parabolic-coordinate supersymmetries of Ref. 25 instead of the spherical-coordinate supersymmetry used here.

VI. SUMMARY

In this paper, we generalized the radial mappings first identified by Schrödinger that relate the Coulomb and oscillator systems. Our principal result is a mapping between the supersymmetry-based quantum-defect theories for the Coulomb and oscillator systems in arbitrary dimensions. In particular, odd oscillator dimensions can be accessed as well as the usual even ones. The mapping and some of its limits are illustrated in Figures 1 and 2.

In deriving this result, we have extended to arbitrary dimensions the analytical SQDT in three dimensions used to describe physical alkali-metal atoms. An analogous SQDT for the harmonic oscillator in arbitrary dimensions has also been presented. In suitable limits, these theories reproduce the bosonic and fermionic sectors of the corresponding supersymmetric quantum-mechanical systems. We have elucidated a basic relationship between the supersymmetric radial Coulomb and oscillator systems: the qth iteration of supersymmetry for the Coulomb system corresponds naturally to the $2q$th iteration of supersymmetry for the oscillator. For the special case of the one-dimensional radial oscillator, we uncovered a quantum-mechanical supersymmetry in which the parity is restricted to be either odd or even. We have also briefly considered mappings relating the continuum-spectrum states of the Coulomb and oscillator systems.

The issue of the physical relevance of our results has also been addressed in part. The three-dimensional Coulomb SQDT is known to provide a good analytical description of the behavior of Rydberg atoms. Our mapping provides a means of obtaining an equivalent analytical oscillator SQDT. An explicit example mapping the sodium atom to an oscillator SQDT is given in Table I. It is also possible that an oscillator SQDT could be used to describe a suitable physical

system, perhaps the Penning trap. If this can be realized in practice, the generalized mapping presented here could provide a connection between two apparently disparate physical systems.

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Long-time approximation to the evolution of resonant and nonresonant anharmonic oscillators in quantum mechanics

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A simple normal-form approach is used to obtain uniform long-time approximations to the evolution of a resonant or nonresonant anharmonic oscillator system governed by a Hamiltonian H_ε which is a self-adjoint operator acting in the Hilbert space $\mathscr{H}=L^2(\mathbf{R}^\nu)$ $(\nu\geqslant 2)$ and is given formally by $H_0+\varepsilon V$. Here H_0 denotes the Hamiltonian of ν one-dimensional harmonic oscillators whose coupling is represented by εV, where V is an operator of multiplication by a smooth function of at most polynomial growth at infinity and $\varepsilon\geqslant 0$ is a small parameter. We consider the general situation in which $\rho\geqslant 1$ of the frequencies of these oscillators are rationally independent, imposing a standard diophantine condition on the independent frequencies if $\rho\geqslant 2$. Under these assumptions, which are stated in a mathematically precise way in the paper, an Nth-order approximant $\psi_N(t,\varepsilon)$ to the exact solution $\psi(t,\varepsilon)$ of the Schrödinger equation id $\psi(t,\varepsilon)/dt=H_\varepsilon\psi(t,\varepsilon)$ satisfying the initial condition $\psi(0,\varepsilon)=\psi_0$ is constructed inductively, ψ_0 being an arbitrary ε-independent member of a suitable family of smooth functions dense in $\mathscr{H}$. Our main result is that $\psi_N(t,\varepsilon)$ differs from $\psi(t,\varepsilon)$ in $\mathscr{H}$-norm by $\leqslant$const $\varepsilon^{N+1}(|t|+1)$ for all $t\in\mathbf{R}$ and all ε in an arbitrary compact interval $[0,\varepsilon_0]$. © *1996 American Institute of Physics.* [S0022-2488(96)00704-1]

I. INTRODUCTION

Since the earliest days of quantum mechanics, physicists have been interested in developing approximate methods for calculating the long-time evolution of quantum mechanical systems. Such methods avoid the troublesome secular terms arising when this evolution is computed via the usual time-dependent perturbation procedures. Indeed, if such a calculation is carried out by a method which leads to secular terms, it should be expected to be accurate at most over relatively small time intervals.

Shortly after the discovery of quantum mechanics, Wigner[1] gave a brief but incisive discussion of a way to obtain long-time approximate solutions of the Schrödinger equation id $\psi(t)/dt=H\psi(t)$ for time-independent Hamiltonians H. More recently, two closely related systematic approaches have been developed for deriving Nth-order approximants, free from secular terms, to the exact evolution of a variety of quantum mechanical systems: the normal-form approach and quantum averaging. Wigner's pioneering remarks are best regarded as anticipating quantum averaging in a special case. The earliest systematic treatments of quantum averaging were independently given by Lochak[2,3] and Case,[4] respectively, and the latter's ideas were elaborated by his student Lee.[5] Such averaging can be viewed as an extension of the Bogoliubov–Mitropolski averaging method for classical nonlinear systems[6] to quantum mechanics. Ellison and his student Ben Lemlih[7,8] were the first to use modern functional analysis methods to develop quantum-averaging approximations to the long-time evolution of the quartic anharmonic oscillator and other physically important systems, as well as to derive rigorous error bounds for these approximate solutions. On the other hand, Kummer[9] was the first to discuss systematically a normal-form approach to quantum evolution over long times. His work was strongly influenced by that of

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Moser's in classical mechanics.[10] The approach in Ref. 9 was rigorized and extended in various ways by Kummer and his students Antoniou[11] and Gompa.[12–14] In Refs. 12 and 13, two normal-form methods were applied to obtain an Nth normal-form approximation to the evolution of nonresonant quantum anharmonic oscillator systems whose Hamiltonian operators were time-independent polynomials in coordinates and momenta. In the first method, this was done in the setting of Bargmann's Hilbert space of analytic functions[15] by using graded Lie algebra procedures analogous to those applied in normal-form studies of vector fields and classical Hamiltonian systems.[16,17] In Refs. 12 and 14, this method was also applied to time-dependent quantum Hamiltonians of the latter polynomial type. The second, somewhat simpler normal-form approach is closely related to the perturbation theory discussed by Born and Jordan.[18] For further bibliographical information on normal forms in quantum mechanics, the reader is referred to Refs. 9, 13, and 19.

The principal goal of this paper is to construct in a mathematically rigorous way a long-time, uniform approximation to the solution of the initial-value problem (IVP) defined by[20]

$$i\,\frac{d\psi(t,\varepsilon)}{dt}=H_\varepsilon\psi(t,\varepsilon), \tag{1.1a}$$

$$\psi(0,\varepsilon)=\psi_0. \tag{1.1b}$$

Here H_ε denotes a self-adjoint operator acting in the Hilbert space $\mathscr{H}=L^2(\mathbf{R}^\nu)$ ($\nu\geqslant 2$) and defined formally by

$$H_\varepsilon=H_0+\varepsilon V \tag{1.2}$$

and d/dt the strong t-derivative in $\mathscr{H}$. In (1.2), H_0 is the Hamiltonian of ν uncoupled simple harmonic oscillators or, more precisely, the unique self-adjoint operator in $\mathscr{H}$ such that

$$H_0=\sum_{j=1}^{\nu}\left(-\frac{\partial^2}{\partial x_j^2}+\omega_j^2x_j^2\right) \tag{1.3}$$

when acting on functions in $C_0^\infty(\mathbf{R}^\nu)$. Moreover, $\varepsilon\geqslant 0$ is a small parameter and V denotes an operator of multiplication by a $C^\infty(\mathbf{R}^\nu)$ function which together with its derivatives has at most polynomial growth at infinity. We assume that the frequencies $\omega_1,\ldots,\omega_\nu$ are positive and that an arbitrary number ρ of them ($1\leqslant\rho\leqslant\nu$) are rationally independent. If $\rho\geqslant 2$, the rationally independent ω_is are assumed to obey a standard diophantine inequality. No other conditions are imposed on these frequencies.

Using a rigorous version of the second normal-form method in Ref. 13, we will construct for each $N\geqslant 1$ an Nth-order approximant $\psi_N(t,\varepsilon)$ to the exact solution $\psi(t,\varepsilon)$ of the IVP (1.1) satisfying the uniform error estimate

$$\|\psi(t,\varepsilon)-\psi_N(t,\varepsilon)\|\leqslant\text{const }\varepsilon^{N+1}(|t|+1) \tag{1.4}$$

for $t\in\mathbf{R}$, $0\leqslant\varepsilon\leqslant\varepsilon_0$, where ε_0 is an arbitrary positive constant and $\|.\|$ the usual $L^2(\mathbf{R}^\nu)$-norm. This error estimate is our main result. Although its rigorous proof is lengthy (Sec. IV), the basic ideas underlying it are quite simple, as will be clear from its heuristic proof given in the next section.

This paper is the first to carry out this construction for systems of resonant and nonresonant harmonic oscillators coupled by a local potential V, which is not necessarily a polynomial, under very general conditions on the frequencies ω_i. Outside of using a version of the last-mentioned normal-form method and certain other ideas in Refs. 7–9 and 13, our treatment is quite different from theirs. In particular, the fact that we allow the eigenvalues of H_0 to be degenerate and consider nonpolynomial coupling introduces nontrivial complications in the rigorous definitions of

the relevant operators, as well as self-adjointness and convergence complications not encountered in the works of these authors. Moreover, the elegant algebraic and analytic approaches used in Refs. 12–14 are inappropriate for dealing with the class of potentials considered here.

The organization of this paper is as follows. In Sec. II, we construct the above Nth-order approximant heuristically. In Sec. III, we state our assumptions on V and the frequencies ω_i precisely, and define the dense domain $C^\infty(H_0)$ in which our initial state lies. This domain is invariant under the action of the operators entering the theory, whose exact definitions are given in that section. Therein we also state Theorem 1, which asserts that the error bound (1.4) holds at the above-stated t,ε-values. This theorem is proven in Sec. IV on the basis of a series of lemmas. Results needed to establish some of these lemmas are collected in the Appendix.

Some of the conclusions of the present paper were announced without detailed proofs in an earlier publication,[21] whose main purpose was to construct uniform approximations to the long-time quantum evolution of one-dimensional anharmonic oscillators.

II. FORMAL CONSTRUCTION OF THE *N*TH-ORDER APPROXIMANT

In this section, we will review the second normal-form approach of Refs. 12 and 13 in a heuristic way which will prove convenient for the purposes of Secs. III and IV, where the procedure will be reformulated rigorously.[22] We fix $\nu \geqslant 2$ in this section.

A central role in the construction of the Nth-order approximant ($N \geqslant 1$) is played by the ''normalizing'' operator $S_N(\varepsilon)$, which reduces H_ε to normal form to order N. By this we mean that $S_N(\varepsilon)$ is such that

$$H_\varepsilon S_N(\varepsilon) = S_N(\varepsilon) K_N(\varepsilon) + \varepsilon^{N+1} R_N(\varepsilon), \tag{2.1}$$

where $K_N(\varepsilon)$, the normal form of H_ε to order N, is a self-adjoint operator commuting formally with H_ε, and $\varepsilon^{N+1} R_N(\varepsilon)$ is a ''remainder,'' with $R_N(\varepsilon) = O(1)$ in ε, again in a formal sense.[23] Here

$$S_N(\varepsilon) = I + \sum_{i=1}^{N} \varepsilon^i S^{(i)}, \tag{2.2a}$$

$$K_N(\varepsilon) = H_0 + \sum_{i=1}^{N} \varepsilon^i K^{(i)}, \tag{2.2b}$$

where the $S^{(i)}$s and $K^{(i)}$s are independent of ε and each $K^{(i)}$ commutes with H_0 formally. One obtains the following recursive formulas for the $S^{(i)}$s and $K^{(i)}$s by inserting the expressions (2.2a) and (2.2b) into (2.1) and equating coefficients of powers of ε:

$$[H_0,\, S^{(i)}] = K^{(i)} - V^{(i)} \quad (i \geqslant 1), \tag{2.3a}$$

$$R_N(\varepsilon) = V^{(1)} S^{(N)} - \sum_{j=0}^{N-1} \varepsilon^j \sum_{k=j+1}^{N} S^{(k)} K^{(N+j-k+1)}. \tag{2.3b}$$

Here the $V^{(i)}$s are determined recursively by

$$V^{(1)} = V, \tag{2.4a}$$

$$V^{(i)} = V^{(1)} S^{(i-1)} - \sum_{j=1}^{i-1} S^{(j)} K^{(i-j)} \quad (i \geqslant 2). \tag{2.4b}$$

The matrix representation of relevant operator equations such as (2.3) and (2.4) in a basis which diagonalizes H_0 is an indispensable ingredient in our analysis. Denote by $\mathbf{Z}_+^p$ ($p \in \mathbf{N}$=the positive integers) the set of all vectors $r=(r_1,\ldots,r_p)$ whose components r_i are non-negative integers. We will use the familiar basis $\Phi=\{\Phi_m\}(m \in \mathbf{Z}_+^\nu)$ consisting of the complete orthonormal set of eigenfunctions of H_0 of the form

$$\Phi_m(x_1,\ldots,x_\nu)=\prod_{i=1}^{\nu} \varphi_{m_i}^{(i)}(x_i), \tag{2.5a}$$

where $\varphi_{m_i}^{(i)}(x_i)$ is the usual (real) eigenfunction of $-d^2/dx_i^2+\omega_i^2 x_i^2$ $(i=1,\ldots,\nu)$ having unit $L^2(\mathbf{R})$-norm. Hence for all $m \in \mathbf{Z}_+^\nu$,

$$H_0\Phi_m=\lambda_m\Phi_m, \tag{2.5b}$$

with

$$\lambda_m=\sum_{i=1}^{\nu} \omega_i(m_i+\tfrac{1}{2}). \tag{2.5c}$$

Since some of the frequencies $\omega_1,\ldots,\omega_\nu$ may be rationally dependent, the eigenvalues λ_m are generally degenerate, a fact which will complicate our analysis in Sec. IV.

The scalar product in $\mathscr{H}=L^2(\mathbf{R}^\nu)$ will be denoted by $\langle .,. \rangle$, and in accordance with the usual practice in quantum mechanics it will be supposed to be *antilinear* in the first entry and *linear* in the second. Assuming for the present that they exist,[24] we will denote the quantities $\langle \Phi_m, S^{(i)}\Phi_n\rangle, \langle \Phi_m, K^{(i)}\Phi_n\rangle, \langle \Phi_m, V^{(i)}\Phi_n\rangle$ by $S_{mn}^{(i)}, K_{mn}^{(i)}, V_{mn}^{(i)}$, respectively, and will define the infinite matrices $\mathscr{S}^{(i)}=(S_{mn}^{(i)})$, $\mathscr{K}^{(i)}=(K_{mn}^{(i)})$, $\mathscr{V}^{(i)}=(V_{mn}^{(i)})$ $(m,n \in \mathbf{Z}_+^\nu)$. In general, given an operator A in $\mathscr{H}$, its matrix elements $\langle \Phi_m, A\Phi_n\rangle$ will be denoted by A_{mn}.[25]

By (2.3a) and (2.5b),

$$(\lambda_m-\lambda_n)S_{mn}^{(i)}=K_{mn}^{(i)}-V_{mn}^{(i)} \quad (i \geqslant 1). \tag{2.6}$$

Since $K^{(i)}$ has been assumed to commute with H_0, $K_{mn}^{(i)}=0$ if $\lambda_m \neq \lambda_n$. From this and (2.6) it follows that

$$S_{mn}^{(i)}=-V_{mn}^{(i)}/(\lambda_m-\lambda_n) \quad (i \geqslant 1, \lambda_m \neq \lambda_n), \tag{2.7}$$

$$K_{mn}^{(i)}=V_{mn}^{(i)}\delta_{\lambda_m,\lambda_n} \quad (i \geqslant 1). \tag{2.8}$$

Since Eq. (2.3a) leaves the matrix elements $S_{mn}^{(i)}$ with $\lambda_m=\lambda_n$ undetermined for $i \geqslant 1$, one can choose them in any manner consistent with the formal self-adjointness of the $K^{(i)}$s.[26] When all the $\omega_1,\ldots,\omega_\nu$ are rationally independent, the eigenvalues of H_0 are nondegenerate and thus the $K^{(i)}$s are formally self-adjoint, since then each $\mathscr{K}^{(i)}$ is a real diagonal matrix. Hence, in this case the above matrix elements can be chosen arbitrarily. However, if the ω_ks are not all rationally independent, such a choice is generally incompatible with the formal self-adjointness of the $K^{(i)}$s, and this would lead to a breakdown of our analysis. We will select these matrix elements in such a way that it will not be necessary to distinguish between the nondegenerate (nonresonant) and degenerate (resonant) cases. Thus, henceforth our remarks will apply to either of these two situations.

Before defining the $S_{mn}^{(i)}$s for $\lambda_m=\lambda_n$, we introduce some notation. Given an operator A in $\mathscr{H}$, we split it uniquely as follows:

$$A=\hat{A}+\tilde{A}, \tag{2.9a}$$

where

$$\hat{A}_{mn}=\delta_{\lambda_m,\lambda_n}A_{mn}, \quad \tilde{A}_{mn}=(1-\delta_{\lambda_m,\lambda_n})A_{mn}. \tag{2.9b}$$

We write $\hat{S}^{(i)}\equiv(S^{(i)})\hat{}$, $\tilde{S}^{(i)}\equiv(S^{(i)})\tilde{}$ and $\hat{S}^{(i)}_{mn}\equiv(\hat{S}^{(i)})_{mn}$, $\tilde{S}^{(i)}_{mn}\equiv(\tilde{S}^{(i)})_{mn}$. We define the operators $\hat{S}^{(i)}$ recursively by

$$\hat{S}^{(1)}=0, \tag{2.10a}$$

$$\hat{S}^{(i)}=\hat{S}^{(i)*}=-\frac{1}{2}\sum_{j=1}^{i-1}(S^{(j)}S^{(i-j)*})\hat{} \quad (i\geqslant 2). \tag{2.10b}$$

Here the notation A^* designates the adjoint of an operator A in $\mathscr{H}$, so that $(A^*)_{mn}=\overline{A_{mn}}$, the bar denoting complex conjugation. Naturally, at the moment Eq. (2.10b) is completely formal. The choice (2.10) of the $\hat{S}^{(i)}$s has two important consequences, which follow by using a simple and ingenious inductive argument presented in Ref. 13. The first is that $S_N(\varepsilon)^*$ is an approximate right-inverse of $S_N(\varepsilon)$:

$$S_N(\varepsilon)S_N(\varepsilon)^*=I+\varepsilon^{N+1}U_N(\varepsilon), \tag{2.11a}$$

where $U_N(\varepsilon)$ is a polynomial in ε defined by

$$U_N(\varepsilon)=\sum_{j=0}^{N-1}\varepsilon^j\sum_{k=j+1}^{N}S^{(k)}S^{(N+j-k+1)*}. \tag{2.11b}$$

The second consequence is that the $K^{(i)}$s are formally self-adjoint. A rigorous version of this inductive argument will be presented in Sec. IV.

In terms of matrix elements, Eqs. (2.10) can be expressed as follows by using (2.9b):

$$\hat{S}^{(1)}_{mn}=0, \tag{2.12a}$$

$$\hat{S}^{(i)}_{mn}=\overline{\hat{S}^{(i)}_{nm}}=-\frac{1}{2}\sum_{j=1}^{i-1}\sum_{r\in\mathbf{Z}_+^\nu}(\tilde{S}^{(j)}_{mr}\overline{\tilde{S}^{(i-j)}_{nr}}+\hat{S}^{(j)}_{mr}\overline{\hat{S}^{(i-j)}_{nr}})\delta_{\lambda_m,\lambda_n} \quad (i\geqslant 2). \tag{2.12b}$$

Similarly, we arrive heuristically at the following matrix form of (2.4) by invoking (2.8), in particular,

$$V^{(1)}_{mn}=V_{mn}, \tag{2.13a}$$

$$V^{(i)}_{mn}=\sum_{r\in\mathbf{Z}_+^\nu}V^{(1)}_{mr}S^{(i-1)}_{rn}-\sum_{j=1}^{i-1}\sum_{r\in\mathbf{Z}_+^\nu}S^{(j)}_{mr}K^{(i-j)}_{rn} \quad (i\geqslant 2). \tag{2.13b}$$

Equations (2.7), (2.8), (2.13), and (2.12) allow us to calculate $\mathscr{S}^{(i)}$, $\mathscr{K}^{(i)}$ for $i\geqslant 1$ and $\mathscr{V}^{(i)}$ for $i\geqslant 2$ systematically in terms of $\mathscr{V}^{(1)}=(V_{mn})$.

Assuming that the sums in (2.12b) and (2.13b) converge,[24] it follows trivially from (2.7), (2.8), (2.12), and (2.13) that all the matrix elements $S^{(i)}_{mn}, K^{(i)}_{mn}, V^{(i)}_{mn}$ $(i\geqslant 1)$ are real, making the bars in the sum over r in (2.12b) superfluous. However, the reality of these matrix elements does not play a significant role in this paper, and hence it will usually be ignored.

We define an Nth-order approximant to the exact solution of the IVP (1.1) by[20]

$$\psi_N(t,\varepsilon)=S_N(\varepsilon)\exp(-itK_N(\varepsilon))S_N(\varepsilon)^*\psi_0. \tag{2.14}$$

We conclude this section by giving the promised heuristic derivation of the basic error estimate (1.4) for $\psi_N(t,\varepsilon)$. Differentiating (2.14) formally with respect to t and using (2.1), we obtain

$$i\,\frac{d\psi_N(t,\varepsilon)}{dt}=H_\varepsilon\psi_N(t,\varepsilon)+\varepsilon^{N+1}g_N(t,\varepsilon), \tag{2.15}$$

where $\|g_N(t,\varepsilon)\|=O(1)$ in ε formally. Integrating (2.15) by the method of variation of constants and using (2.11a), we find

$$\psi_N(t,\varepsilon)=\exp(-itH_\varepsilon)[I+\varepsilon^{N+1}U_N(\varepsilon)]\psi_0-i\varepsilon^{N+1}\int_0^t \exp[-i(t-s)H_\varepsilon]g_N(s,\varepsilon)ds. \tag{2.16}$$

By (2.16), $\psi(t,\varepsilon)=\exp(-itH_\varepsilon)\psi_0$, the unitarity of $\exp(-itH_\varepsilon)$, and the boundedness of $\|g_N(t,\varepsilon)\|$ and $\|U_N(\varepsilon)\psi_0\|$ for $t\in\mathbf{R}$, $0\leqslant\varepsilon\leqslant\varepsilon_0<\infty$ [see (4.42)], because of our hypotheses on V and the ω_is in Sec. III, we infer that

$$\begin{aligned}\|\psi(t,\varepsilon)-\psi_N(t,\varepsilon)\|&=\varepsilon^{N+1}\left\|U_N(\varepsilon)\psi_0+\int_0^t \exp(isH_\varepsilon)g_N(s,\varepsilon)ds\right\|\\&\leqslant\varepsilon^{N+1}\left(\|U_N\psi_0\|+\int_0^{|t|}\|g_N(s,\varepsilon)\|ds\right)\\&\leqslant\text{const }\varepsilon^{N+1}(|t|+1)\end{aligned}$$

at these t,ε-values.

III. ASSUMPTIONS AND MAIN RESULT

The considerations of the previous section were mostly heuristic. In the present section, we will state precise definitions and assumptions under which the results of this paper hold rigorously.

Until further notice, we fix $\nu\geqslant 2$ and assume that the potential V in (1.2) has the following properties:

(I) V is a maximal operator of multiplication in $\mathscr{H}=L^2(\mathbf{R}^\nu)$ by a real-valued function in $C^\infty(\mathbf{R}^\nu)$ which will also be denoted by V.

(II) For each $r=(r_1,\ldots,r_\nu)\in\mathbf{Z}_+^\nu$, there exist non-negative constants Γ_r,μ_r such that

$$\left|\frac{\partial^{|r|}V(x)}{\partial x_1^{r_1}\cdots\partial x_\nu^{r_\nu}}\right|\leqslant\Gamma_r(|x|+1)^{\mu_r}$$

at each $x=(x_1,\ldots,x_\nu)\in\mathbf{R}^\nu$, where $|r|=r_1+\cdots+r_\nu$ and $|x|=\Sigma_{i=1}^\nu|x_i|$.

(III) The differential operator

$$\frac{1}{2}\sum_{j=1}^{\nu}\left(-\frac{\partial^2}{\partial x_j^2}+\omega_j^2x_j^2\right)+\varepsilon V(x_1,\ldots,x_\nu)$$

on $C_0^\infty(\mathbf{R}^\nu)$ is essentially self-adjoint in $\mathscr{H}$ for each $\varepsilon\geqslant 0$, its unique self-adjoint extension in $\mathscr{H}$ being denoted by H_ε at each such ε. The frequencies ω_j are fixed positive numbers.

Remark: Property (III) is implied by (I) and (II) if $\frac{1}{2}\Sigma_{i=1}^\nu\omega_i^2x_i^2+\varepsilon V(x)$ is bounded below on $\mathbf{R}^\nu$.[27]

Given the set $\{\omega_1,...,\omega_\nu\}$ of ν positive numbers, there exists a maximum number $1\leqslant\rho\leqslant\nu$ of rationally independent ω_is, which by suitable labeling can (and will) be chosen to be $\{\omega_1,...,\omega_\rho\}$. Writing $|j|_\rho=\Sigma_{i=1}^{\rho}|j_i|$ for the norm of vectors $j\in\mathbf{R}^\rho$, we suppose that the following diophantine condition is satisfied:

(IV) If $\rho\geqslant 2$, there exist positive constants $\gamma,\ \eta$ such that for all $0\neq k=(k_1,\ldots,k_\rho)\in\mathbf{Z}^\rho$,

$$\left|\sum_{i=1}^{\rho}\omega_i k_i\right|\geqslant\gamma|k|_\rho^{-\eta},\tag{3.1}$$

where $\mathbf{Z}^r$ is the set of all vectors $(j_1,\ldots,j_r)$ whose components are integers.

Remarks: (1) Note that (IV) holds trivially if $\rho=1$. For in that case, (3.1) is satisfied for $0\neq k\in\mathbf{Z}$ if $\gamma\leqslant\omega_1,\ \eta>0$.

(2) If $\rho\geqslant 2$, then for each $m\in\mathbf{Z}_+^\nu$ one has $\inf\{|\lambda_m-\lambda_n|:n\in\mathbf{Z}_+^\nu,\lambda_m\neq\lambda_n\}=0$. This can cause convergence difficulties in sums [such as the first sum in (2.13b)] which involve differences of this type as factors in denominators. Condition (IV) is introduced to help control these small denominators. These difficulties are analogous to ones occurring in perturbation problems in classical mechanics.[28]

(3) It is well known that if $\rho\geqslant 2$ and $\eta\geqslant\nu$, then the set of vectors $(\omega_1,...,\omega_\rho)$ with positive components for which there exists no $\gamma>0$ such that the condition (3.1) holds for all $0\neq k\in\mathbf{Z}^\rho$ has Lebesgue measure zero.[29]

In order for our main theorem to have a precise meaning, we need to define the Nth-order approximant $\psi_N(t,\varepsilon)$ more carefully than in Sec. II. The following definitions and remarks are made for this purpose, as well as to set the stage for the developments of Sec. IV.

Definition 1: If A is an operator in a complex, separable Hilbert space $\mathscr{X}$, then we let[30]

$$C^\infty(A)=\bigcap_{j=1}^{\infty}D(A^j).$$

Remarks: (1) If A is self-adjoint, then $C^\infty(A)$ is dense in $\mathscr{X}$.[31] In particular, $C^\infty(H_0)$ is dense in $\mathscr{H}$ and contains the Schwartz space $S(\mathbf{R}^\nu)$ of functions of fast decrease.

(2) $C^\infty(H_0)$ is invariant under H_0, V, and the other key operators in this paper.

Our last assumption, which is motivated by these properties of $C^\infty(H_0)$ and by the desire to avoid unessential complications which would ensue by admitting ε-dependent initial states, is as follows:

(V) The initial state $\psi_0=\psi(0,\varepsilon)$ has the following properties:

$$\psi_0=\psi(0,\varepsilon)\in C^\infty(H_0),\tag{3.2a}$$

$$\psi_0\ \text{ is }\ \varepsilon\text{-independent.}\tag{3.2b}$$

Remark: Fix $\varepsilon\geqslant 0$. A simple but important fact is that our assumptions on V and ψ_0 entail the relation $\psi_0\in D(H_\varepsilon)$, and thus that the IVP (1.1) has the unique solution $\psi(t,\varepsilon)=\exp(-itH_\varepsilon)\psi_0$ for all $t\in\mathbf{R}$. To prove this relation, we use the fact that the operator $(H_0+\varepsilon V)|C^\infty(H_0)$ is a symmetric extension of the essentially self-adjoint operator $(H_0+\varepsilon V)|C_0^\infty(\mathbf{R}^\nu)$, as follows by (III) and $C_0^\infty(\mathbf{R}^\nu)\subset C^\infty(H_0)$. Since H_ε is defined as the unique self-adjoint extension of $(H_0+\varepsilon V)|C_0^\infty(\mathbf{R}^\nu)$, it follows that $D(H_\varepsilon)\supset C^\infty(H_0)$. By this and (3.2a), $\psi_0\in D(H_\varepsilon)$.

Infinite sums were used heuristically in Sec. II. The next definition states the sense in which such sums will be understood henceforth.

Definition 2: Fixing $p \in \mathbf{N}$, let $\Gamma = \mathbf{Z}_+^p$; let $\{\Psi_\alpha\}$ $(\alpha \in \Gamma)$ be an orthonormal set in a Hilbert space $\mathscr{X}$; and $\{\Delta_n\}$ be a sequence of finite subsets $\Delta_n \subset \Gamma$ such that Δ_n eventually contains any given finite subset of Γ. A sum of the form $\Sigma_{\alpha\in\Gamma} g_\alpha$ with each $g_\alpha \in \mathbf{C}$ is defined as $\lim_{n\to\infty} \Sigma_{\alpha\in\Delta_n} g_\alpha$ in the $\mathbf{C}$-topology if the limit exists. Analogously, a sum of the form $\Sigma_{\alpha\in\Gamma} g_\alpha \Psi_\alpha$ is defined as s $-$ $\lim_{n\to\infty} \Sigma_{\alpha\in\Delta_n} g_\alpha \Psi_\alpha$ in the strong operator topology in $\mathscr{X}$ if the limit exists.

Definition 3: Let $\Psi = \{\Psi_\alpha\}$ $(\alpha \in \Gamma)$ be a complete orthonormal set in a complex Hilbert space $\mathscr{X}$ with inner product $\langle .,. \rangle$, which we agree is antilinear in the first argument and linear in the second. Here Γ is as above. Let $\mathscr{A} = (A_{\alpha\beta})(\alpha,\beta \in \Gamma)$ be a matrix of complex numbers which is square-summable by rows and columns, i.e., $\Sigma_{\alpha\in\Gamma} |A_{\alpha\beta}|^2 < \infty$ $(\beta \in \Gamma)$ and $\Sigma_{\beta\in\Gamma} |A_{\alpha\beta}|^2 < \infty$ $(\alpha \in \Gamma)$, respectively. Then the linear operator A with domain

$$D(A) = \left\{ f \in \mathscr{X} : \sum_{\alpha\in\Gamma} \left| \sum_{\beta\in\Gamma} A_{\alpha\beta} \langle \Psi_\beta, f \rangle \right|^2 < \infty \right\} \tag{3.3a}$$

and action

$$Af = \sum_{\alpha\in\Gamma} \left(\sum_{\beta\in\Gamma} A_{\alpha\beta} \langle \Psi_\beta, f \rangle \right) \Psi_\alpha \quad (f \in D(A)) \tag{3.3b}$$

will be said to be *associated* with $\mathscr{A}$ wrt Ψ, or $A \leftrightarrow \mathscr{A}$ wrt Ψ.

Remarks: (1) Stone[32] has considered linear operators associated with infinite matrices in the sense of Definition 3.

(2) Note that the sums over β in (3.3a) and (3.3b) converge absolutely, because of the square-summability of $\mathscr{A}$ by columns, together with Schwarz's inequality in $\ell^2(\Gamma)$ and Parseval's identity.

(3) Note also that the condition $A \leftrightarrow \mathscr{A}$ wrt Ψ implies: (i) A^* exists, (ii) $\Psi \subset D(A) \cap D(A^*)$, and (iii) $A_{\alpha\beta} = \langle \Psi_\alpha, A\Psi_\beta \rangle$ $(\alpha,\beta \in \Gamma)$. Properties (i)–(iii) follow by the square-summability properties of $\mathscr{A}$ and the orthonormality and completeness of the Ψ_αs.

(4) The product $\mathscr{A}.\mathscr{B}$ of two infinite matrices $\mathscr{A},\mathscr{B}$ with which linear operators A,B in $\mathscr{X}$ are associated wrt Ψ exists. Indeed, the square-summability of $\mathscr{A}$ by columns and of $\mathscr{B}$ by rows entails that $(\mathscr{A}.\mathscr{B})_{\alpha\beta} = \Sigma_{\sigma\in\Gamma} A_{\alpha\sigma} B_{\sigma\beta}$ converges absolutely by Schwarz's inequality in $\ell^2(\Gamma)$. However, even if the product AB of two such operators exists, it is not necessarily associated with $\mathscr{A}.\mathscr{B}$ wrt Ψ. These and other pathologies of infinite matrices generally severely limit their usefulness for investigating the properties of linear operators.[33] However, the infinite matrices associated with the linear operators considered in this paper are sufficiently well behaved to be effective tools for the task of deriving its conclusions.

Definition 4: The set of linear operators in $\mathscr{H}$ whose domains contain the dense set $C^\infty(H_0)$ and leave it invariant is denoted by $\mathscr{M}$.

In this section and Sec. IV we will proceed in a manner which is partly the reverse of that in Sec. II. This means that certain definitions in the previous section, when stated precisely, will now be consequences of Definitions 5(a)–5(c) below.

Definition 5(a): The infinite matrices $\tilde{\mathscr{S}}^{(i)} = (\tilde{S}^{(i)}_{mn})$, $\hat{\mathscr{S}}^{(i)} = (\hat{S}^{(i)}_{mn})$, $\mathscr{V}^{(i)} = (V^{(i)}_{mn})$, $\mathscr{K}^{(i)} = (K^{(i)}_{mn})$ $(i \geqslant 1)$ are defined recursively as follows:

(1) One defines

$$\tilde{S}^{(i)}_{mn} = \begin{cases} -V^{(i)}_{mn}/(\lambda_m - \lambda_n) & \lambda_m \neq \lambda_n, \\ 0, & \lambda_m = \lambda_n, \end{cases} \tag{3.4}$$

for $i \geqslant 1$ and defines $\hat{S}^{(i)}_{mn}$ by (2.12a) [resp., (2.12b)] for $i = 1$ (resp., $i \geqslant 2$).

(2) The $K^{(i)}_{mn}$s are given by (2.8) for $i \geqslant 1$. Each $V^{(1)}_{mn}$ is defined by (2.13a), with

$$V_{mn} = \langle \Phi_{mn}, V\Phi_n \rangle, \tag{3.5}$$

as before, and the $V_{mn}^{(i)}$s by (2.13b) for $i \geqslant 2$.

Remarks: (1) Note that $D(V) \supset S(\mathbf{R}^\nu) \supset \Phi$ by (I) and (II) in particular, where again $S(\mathbf{R}^\nu)$ denotes the Schwartz space of functions of fast decrease on $\mathbf{R}^\nu$ and Φ the harmonic oscillator basis defined in Sec. II. Thus definition (2.13a) makes sense.

(2) Estimates (4.13) (Sec. IV) play a central role in showing that the infinite sums over r in (2.12b) and (2.13b) converge absolutely. Thus (2.12b) and (2.13b) make sense as recursive definitions.

Definition 5(b): (1) For $i \geqslant 1$, the operators $\widetilde{S}^{(i)}, \hat{S}^{(i)}, K^{(i)}, V^{(i)}$ are those associated with the respective matrices $\widetilde{\mathscr{S}}^{(i)}, \hat{\mathscr{S}}^{(i)}, \mathscr{K}^{(i)}, \mathscr{V}^{(i)}$ wrt Φ,[34] and $S^{(i)}$ is defined as the operator sum $\widetilde{S}^{(i)} + \hat{S}^{(i)}$.

(2) For $\varepsilon \geqslant 0$, $N \geqslant 1$, the operators $S_N(\varepsilon), K_N(\varepsilon), R_N(\varepsilon)$ are defined by the rhs of (2.2a), (2.2b), (2.3b), respectively, viewed as operator sums.

Remarks: (1) Since all the matrices in part (1) of Definition 5(b) are square-summable by rows and columns, as follows by using, in particular, estimates (4.13), the definitions of $\widetilde{S}^{(i)}, \hat{S}^{(i)}, K^{(i)}, V^{(i)}$ make sense for all $i \geqslant 1$.

(2) By Lemma 4(1),[35] $\widetilde{S}^{(i)}, \hat{S}^{(i)}, K^{(i)}, V^{(i)}$ $(i \geqslant 1)$ are in $\mathscr{M}$, and therefore they and $S^{(i)}$ $(i \geqslant 1)$, $S_N(\varepsilon), K_N(\varepsilon), R_N(\varepsilon)$ are densely defined in $\mathscr{H}$. Hence the adjoints of all these operators exist, and by Lemma 4(2) they also are in $\mathscr{M}$.

Definition 5(c): The Nth-order approximant $\psi_N(t,\varepsilon)$ is defined for all $N \geqslant 1$, $t \in \mathbf{R}$, $\varepsilon \geqslant 0$ by

$$\psi_N(t,\varepsilon) = S_N(\varepsilon) \exp(-it\overline{K_N}(\varepsilon)) S_N(\varepsilon)^* \psi_0, \tag{3.6}$$

where $\overline{K_N}(\varepsilon)$ is the unique self-adjoint extension (closure) of $K_N(\varepsilon)$ in Definition 5(b), $S_N(\varepsilon)$ is as in the latter definition, and ψ_0 is an initial state satisfying conditions (3.2).

Remarks: (1) The existence of $K_N(\varepsilon)$ is guaranteed by Lemma 6.

(2) Definition 5(c) makes sense in view of (3.2a) and of the facts that $S_N(\varepsilon), S_N(\varepsilon)^* \in \mathscr{M}$ and that $\exp(-itK_N(\varepsilon))$ is a well-defined unitary operator in $\mathscr{M}$ [see step (4) of the proof of Lemma 6]. The self-adjointness of $K_N(\varepsilon)$ ensures that this exponential makes sense.

(3) The operator $K_N(\varepsilon)$ just defined is nothing more than a precise version of the operator denoted by $K_N(\varepsilon)$ is Sec. II. Indeed, all operator equations in that section involving $K_N(\varepsilon)$ hold rigorously on appropriate dense domains with $K_N(\varepsilon)$ replaced by $\overline{K_N}(\varepsilon)$, provided that the remaining operators in these equations are understood in the sense of the present section. This readily follows from the relevant definitions, together with results proved in Sec. IV.

We are now ready to state our main result.

Theorem 1: Let H_0 and V obey conditions (I)–(III), let (IV) hold if $\rho \geqslant 2$, and let the initial state satisfy condition (V). Then for each $N \geqslant 1$, $0 \leqslant \varepsilon_0 < \infty$ we have the uniform estimate

$$\|\psi(t,\varepsilon) - \psi_N(t,\varepsilon)\| \leqslant C_N \varepsilon^{N+1}(|t|+1) \tag{3.7}$$

if $t \in \mathbf{R}$, $0 \leqslant \varepsilon \leqslant \varepsilon_0$, where $\|.\|$ is the $\mathscr{H}$-norm and $C_N = C_N(\psi_0, \varepsilon_0)$ is a positive constant.

Remarks: (1) This theorem is the first rigorous result of this degree of generality applying to cases in which V is not a polynomial and/or H_0 has degenerate eigenvalues. Its conclusions hold for $\nu = 1$ under the assumption that (I)–(III) hold. The proof of this statement which is sketched in Ref. 21 is much simpler than that of Theorem 1.

(2) Lochak[3] (resp., Case[4]) arrived at an Nth-order quantum-averaging error estimate of type (3.7) [resp., stronger than (3.7)] under an assumption of operator boundedness which does not hold in the present context. Besides being partially heuristic, the corresponding proof in Ref. 4 is incomplete [there is an obvious misprint in Eq. (124) of that reference]. Rigorous estimates of type (3.7) for various quantum mechanical systems with unbounded Hamiltonian operators were first derived by Ben Lemlih and Ellison.[7,8] Estimates of this kind were proved in Refs. 12 and 13 for multi-dimensional nonresonant oscillator systems coupled by potentials which are polynomials in the coordinates and momenta.

(3) An obvious but important consequence of Theorem 1, noted in Refs. 3 and 4, is that, under the conditions in Theorem 1, $\psi_N(t,\varepsilon)$ approximates $\psi(t,\varepsilon)$ uniformly in norm over $O(\varepsilon^{-\delta})$ t-intervals for each $\delta\in(0,N+1]$. More precisely, for each such δ and each pair of positive numbers T,ε_0,

$$\|\psi(t,\varepsilon)-\psi_N(t,\varepsilon)\|\leqslant C'_{N,\delta}\varepsilon^{N+1-\delta} \tag{3.8}$$

for $0\leqslant t\leqslant T\varepsilon^{-\delta}$, where $C'_{N,\delta}=C'_{N,\delta}(\psi_0,\varepsilon_0,T)$ is a positive constant. This is a very unusual result in averaging theory, where generally the analogous approximations have only been expected (and proved) to be valid over $O(\varepsilon^{-1})$ time intervals. Key properties leading to (3.7), and hence to (3.8), are the linearity of the IVP (1.1), together with the facts that $\psi(t,\varepsilon)$ and $\psi_N(t,\varepsilon)$ exist for $t\in\mathbf{R}$, $\varepsilon\geqslant 0$, that H_ε is self-adjoint at each such ε, and that the uniform boundedness properties (4.41) hold.

IV. AUXILIARY RESULTS AND PROOF OF THEOREM 1

Lemmas 1–7 below will be used to prove our main result—Theorem 1. In this section, we fix $N\geqslant 1$, $\nu\geqslant 2$, and the number $\rho\in\{1,...,\nu\}$ of rationally independent frequencies ω_i. We will denote the positive integers by $\mathbf{N}$ and the non-negative integers by $\mathbf{Z}_+$, and, as usual, $\mathbf{Z}^\nu$ will signify the set of all vectors $(n_1,\ldots,n_\nu)$ with integer components (positive, negative, or zero). Recall that for $j=(j_1,\ldots,j_\rho)\in\mathbf{R}^\rho$ we defined $|j|_\rho=\Sigma_{i=1}^{\rho}|j_i|$. However, when $j=(j_1,\ldots j_\nu)\in\mathbf{R}^\nu$, we will write $|j|=\Sigma_{i=1}^{\nu}|j_i|$ and $(\omega,j)=\Sigma_{i=1}^{\nu}\omega_i j_i$.

The following simple lemma is relevant to the proofs of Lemmas 3 and 7.

Lemma 1: (1) For any $m,n\in\mathbf{Z}_+^\nu$ such that $\lambda_m\neq\lambda_n$, the eigenvalues of H_0 satisfy the inequality

$$|\lambda_m-\lambda_n|\geqslant\text{const}|m-n|^{-\eta}, \tag{4.1a}$$

where η is the positive constant in Condition (IV) and const is independent of m,n.[36]

(2) The following estimate holds for the multiplicity g_m of λ_m:

$$g_m\leqslant(|m|+1)^{\nu-\rho}. \tag{4.1b}$$

Proof: (1) Fix $k=(k_1,\ldots,k_\nu)\in\mathbf{Z}^\nu$ such that $(\omega,k)\neq 0$. Since $\{\omega_1,...,\omega_\rho\}$ is a maximal rationally independent subset of $\{\omega_1,...,\omega_\nu\}$,

$$(\omega,k)=\frac{1}{M}\sum_{i=1}^{\rho}\omega_i\left(\sum_{j=1}^{\nu}t_{ij}k_j\right), \tag{4.2}$$

where each $t_{ij}=t_{ij}(\rho)$ is an integer and $M=M(\rho)$ is a positive integer. Moreover, since $(\omega,k)\neq 0$, it follows trivially that $k\neq 0$ and that at least one of the integers $\Sigma_{j=1}^{\nu}t_{ij}k_j$ $(i=1,...,\rho)$ is nonvanishing. Therefore, one has for the fixed $\rho\geqslant 1$ of interest, by (4.2), (IV), and Remark (1) to (IV),

$$|(\omega,k)|\geqslant\frac{\gamma}{M}\left(\sum_{i=1}^{\rho}\left|\sum_{j=1}^{\nu}t_{ij}k_j\right|\right)^{-\eta}\geqslant\text{const}|k|^{-\eta}. \tag{4.3}$$

But (2.5c) implies that

$$\lambda_m-\lambda_n=(\omega,m-n). \tag{4.4}$$

Statement (4.1a) follows immediately for $\lambda_m\neq\lambda_n$ from (4.3) and (4.4).

(2) Estimate (4.1b) follows by the rational independence of $(\omega_1,...,\omega_\rho)$ and a simple combinatorial argument. □

The next lemma provides an estimate which is needed in the proof of Lemma 3, and in turn that lemma is a basic logical underpinning of the remainder of this section.

Lemma 2: For all $m,n\in\mathbf{Z}_+^\nu$,

$$|V_{mn}|\leqslant \text{const}\ \lambda_m^{\alpha(1,p)}\lambda_n^{-p}\quad (p\in\mathbf{N}), \tag{4.5}$$

where const and $\alpha(1,p)$ are independent of m,n, but may depend on p.

Proof: Since the spectrum of H_0 is in $(0,\infty)$, H_0^{-1} exists. Combining this fact with (3.5), the self-adjointness of V and H_0 [by (I) and (III)], and $V\Phi_n\in C^\infty(H_0)$ [by (I) and $\Phi_n\in S(\mathbf{R}^\nu)$], we may write

$$\begin{aligned}|V_{mn}|=|\langle\Phi_m,V\Phi_n\rangle|=|\langle\Phi_n,V\Phi_m\rangle|=|\langle H_0^{-p}\Phi_n,H_0^pV\Phi_m\rangle|=\lambda_n^{-p}|\langle\Phi_n,H_0^pV\Phi_m\rangle|\\ \leqslant\lambda_n^{-p}\|H_0^pV\Phi_m\|\end{aligned} \tag{4.6}$$

at each of the stated m,n,p values.

To complete the proof of the lemma, we will estimate $\|H_0^pV\Phi_m\|$ in steps (1)–(3).

(1) The first step is to prove that

$$H_0^pV\Phi_m=\sum_{k=0}^{p}E_{k,p}\lambda_m^{p-k}[\Delta,\ V]_k\Phi_m\quad (p\in\mathbf{N}), \tag{4.7}$$

where $\Delta=\Sigma_{j=1}^{\nu}\partial^2/\partial x_j^2$, the $E_{k,p}$s are constants independent of m, and the multiple commutator $[A,\ B]_k$ $(k\geqslant 0)$ of two operators A and B in a Hilbert space is defined as usual by

$$[A,\ B]_0=B,\ \ [A,\ B]_1=AB-BA,$$

$$[A,\ B]_k=[A,[A,\ B]_{k-1}]\quad (k\geqslant 2),$$

on elements in this space where these definitions make sense.

Equation (4.7) follows easily by induction, noting in particular that it holds for $p=1$, in view of

$$H_0V\Phi_m=VH_0\Phi_m+[H_0,\ V]\Phi_m=\lambda_mV\Phi_m-\tfrac{1}{2}[\Delta,\ V]\Phi_m,$$

where we have used, in particular, the fact that (1.3) holds on $S(\mathbf{R}^\nu)\supset\Phi$.

(2) Note that

$$[\Delta,\ V]_jg=\sum_{|r|+|s|=2j}F_{rs}^{(j)}D^{|r|}V.D^{|s|}g\quad [j\geqslant 1,g\in S(\mathbf{R}^\nu)], \tag{4.8}$$

where the $F_{rs}^{(j)}$s are constants and $D^{|r|}=\partial^r/\partial x_1^{r_1}\cdots\partial x_\nu^{r_\nu}$, with $r=(r_1,\ldots,r_\nu),s\in\mathbf{Z}_+^\nu$. For each such g, Eq. (4.8) holds trivially for $j=1$ and is easily proved by induction for $j\geqslant 1$.

By (4.7) and (4.8),

$$\|H_0^pV\Phi_m\|\leqslant\text{const}\sum_{k=0}^{p}\lambda^{p-k}\sum_{|r|+|s|=2k}\|D^{|r|}V.D^{|s|}\Phi_m\|\quad (p\in\mathbf{N}), \tag{4.9}$$

where the constant is independent of m.

(3) In this step, we estimate $\|D^{|r|}V.D^{|s|}\Phi_m\|$ in (4.9) for fixed $r,s\in\mathbf{Z}_+^\nu$. In doing this, we will assume wlg that μ_r in condition (II) is a *non-negative integer*.

By considering the regions $|x|<1$, $|x|>1$ in $\mathbf{R}^\nu$ and using (II), we arrive at the inequality

$$\|D^{|r|}V.D^{|s|}\Phi_m\| \leqslant \text{const}\left[\|D^{|s|}\Phi_m\| + \left\|\left(\sum_{i=1}^{\nu} x_i^2\right)^{\mu_r/2} D^{|s|}\Phi_m\right\|\right]. \tag{4.10}$$

The rhs of (4.10) may be estimated by using the inequality

$$\left\|\left(\sum_{i=1}^{\nu} x_i^2\right)^{\mu_r/2} D^{|s|}\Phi_m\right\| \leqslant \text{const } \lambda_m^{(k+|s|)/2} \quad (k \in \mathbf{Z}_+). \tag{4.11}$$

This inequality can be proved by expressing each $x_j, \partial/\partial x_j$ $(j=1,...,\nu)$ inside the norm in terms of creation and annihilation operators $a_j, a_j^{\dagger}$:

$$a_j = 2^{-1/2}\left(x_j + i\,\frac{\partial}{\partial x_j}\right), \quad a_j^{\dagger} = 2^{-1/2}\left(x_j - i\,\frac{\partial}{\partial x_j}\right),$$

and using an estimate analogous to one which holds in the case $\nu=1$.[37]

By (4.10), (4.11), and the fact that $\lambda_m^{-\mu}$ is bounded as a function of m for fixed $\mu \geqslant 0$,

$$\|D^{|r|}V.D^{|s|}\Phi_m\| \leqslant \text{const } \lambda_m^{(\mu_r+|s|)/2}. \tag{4.12}$$

The desired inequality (4.5) follows immediately from (4.6), (4.9), and (4.12). □

Lemma 3: The inductive definitions (2.12b) and (2.13b) make sense for $i \geqslant 2$ and $m,n \in \mathbf{Z}_+^{\nu}$, and the following estimates hold for all $i,p \in \mathbf{N}$ and all such m,n:

$$|V_{mn}^{(i)}| \leqslant \text{const } \lambda_m^{\alpha(i,p)}\lambda_n^{-p}, \tag{4.13a}$$

$$|V_{mn}^{(i)}| \leqslant \text{const } \lambda_n^{\alpha(i,p)}\lambda_m^{-p}, \tag{4.13b}$$

$$|\tilde{S}_{mn}^{(i)}| \leqslant \text{const } \lambda_m^{\beta(i,p)}\lambda_n^{-p} \quad (\lambda_m \neq \lambda_n), \tag{4.13c}$$

$$|\tilde{S}_{mn}^{(i)}| \leqslant \text{const } \lambda_n^{\beta(i,p)}\lambda_m^{-p} \quad (\lambda_m \neq \lambda_n), \tag{4.13d}$$

$$|\hat{S}_{mn}^{(i)}| \leqslant \text{const } \lambda_m^{\gamma(i)} \quad (\lambda_m = \lambda_n), \tag{4.13e}$$

where the real constants $\alpha(i,p), \beta(i,p), \gamma(i)$ and the other constants in these estimates are independent of m,n.

Proof: It will be inductive. Fixing $i \in \mathbf{N}$ until further notice, we remark that the assumption that (4.13a) obtains at each $p \in \mathbf{N}$, together with (2.7) and (4.1a), entails for $\lambda_m \neq \lambda_n$:

$$|\tilde{S}_{mn}^{(i)}| \leqslant \text{const } \lambda_m^{\alpha(i,q)}\lambda_n^{-q}|m-n|^{\eta} \leqslant \text{const } \lambda_m^{\alpha(i,q)+\eta}\lambda_n^{-q+\eta} \leqslant \text{const } \lambda_m^{\alpha(i,q)+\eta}\lambda_n^{-q+\eta[\eta]+1} \quad (q \in \mathbf{N}), \tag{4.14}$$

where $[y]$ denotes the greatest integer $\leqslant y \in \mathbf{R}$. In arriving at (4.14) we have also used the crude inequality $|m-n| \leqslant \text{const } \lambda_m\lambda_n$, holding for $m \neq n$, and the fact that $\lambda_n^{\eta}/\lambda_n^{[\eta]+1}$ is bounded for $|n| \to \infty$. Because of (4.14), (4.13c) holds for all $p \in \mathbf{N}$, as one sees by setting $p = q - [\eta] - 1$ and $\beta(i,p) = \alpha(i,q) + \eta$. Similar arguments entail that (4.13d) holds for all such p if (4.13b) does. We have thus reduced the task of establishing that Eqs. (4.13) obtain for each $i,p \in \mathbf{N}$ to proving that (4.13a), (4.13b), and (4.13e) do.

Note that estimates (4.13a)–(4.13e) hold for $i=1$, $p \in \mathbf{N}$, by $V_{mn}^{(1)} = V_{mn} = V_{nm}$, (4.5), (2.12a), and the results of the last paragraph. In steps (1)–(3) below, we will show that if these five estimates obtain for all $1 \leqslant i \leqslant k$ for some $k \geqslant 1$, they also obtain for $i = k+1$, and thus for all $i \geqslant 1$.[38]

(1) In order to prove that (4.13a) holds for $i=k+1$, we will use the inequality

$$|V_{mn}^{(k+1)}| \leqslant \sum_r |V_{mr}^{(1)}|(|\tilde{S}_{rn}^{(k)}|+|\hat{S}_{rn}^{(k)}|)+\sum_{j=1}^{k}\sum_r (|\tilde{S}_{mr}^{(j)}|+|\hat{S}_{mr}^{(j)}|)|K_{rn}^{(k-j+1)}|\ , \tag{4.15}$$

which is an obvious formal consequence of definition (2.13b) for $i=k+1$.[39] Our inductive approach will show that the first sum over r in (4.15) converges (the second such sum contains only a finite series of nonvanishing terms by (2.8) and $g_m<\infty$), thereby entailing that the latter definition makes sense for $i=k+1$, and hence for $i\geqslant 2$.

We claim that

$$\sum_r |V_{mr}^{(1)}|\cdot|\tilde{S}_{rn}^{(k)}| \leqslant \text{const}\ \lambda_m^{a(k,p)}\lambda_n^{-p}, \tag{4.16a}$$

$$\sum_r |V_{mr}^{(1)}|\cdot|\hat{S}_{rn}^{(k)}| \leqslant \text{const}\ \lambda_m^{b(k,p)}\lambda_n^{-p}, \tag{4.16b}$$

$$\sum_r |\tilde{S}_{mr}^{(j)}|\cdot|K_{rn}^{(k-j+1)}| \leqslant \text{const}\ \lambda_m^{c(k,p)}\lambda_n^{-p}, \tag{4.16c}$$

$$\sum_r |\hat{S}_{mr}^{(j)}|\cdot|K_{rn}^{(k-j+1)}| \leqslant \text{const}\ \lambda_m^{d(k,p)}\lambda_n^{-p}\delta_{\lambda_m,\lambda_n} \tag{4.16d}$$

for all $p\in\mathbf{N}$ and all $j=1,\ldots,k$, where const and $a(k,p),\ldots,d(k,p)$ denote constants independent of m,n. Choosing $a(k+1,p)\geqslant\max\{a(k,p),\ldots,d(k,p)\}$, (4.13a) follows for $i=k+1$ by (4.15) and (4.16). We will only prove (4.16a) and (4.16c) in detail; (4.16b) and (4.16d) can be established similarly to (4.16c).

To prove (4.16a), we need the estimate

$$\sum_{r\in\mathbf{Z}_+^\nu} \lambda_r^{-\mu}<\infty \quad (\mu>\nu), \tag{4.17}$$

which follows by (2.5c), the positivity of the ω_is, and a well-known result.[40] Using (4.5), (4.13a) for $i=1,\ldots,k$, and (4.17), we obtain

$$\sum_r |V_{mr}^{(1)}|\cdot|\tilde{S}_{rn}^{(k)}| \leqslant \text{const}\ \lambda_m^{\alpha(1,q)}\lambda_n^{-p}\sum_r \lambda_r^{\beta(k,p)}\lambda_r^{-q}<\infty$$

at each $p\in\mathbf{N}$ if $q=q(k,p)$ is a positive integer $>\beta(k,p)+\nu$. Thus (4.16a) holds with $a(k,p)=\alpha(1,q(k,p))$.

To prove (4.16c), we use (4.13a) and (4.13d) for $i=1,\ldots,k$, together with (2.8) and the inequality

$$g_n \leqslant \text{const}\ \lambda_n^{\nu-\rho} \tag{4.18}$$

[which follows from (4.1b) and (2.5c)] to infer that

$$\begin{aligned}\sum_r |\tilde{S}_{mr}^{(j)}|\cdot|K_{rn}^{(k-j+1)}| &\leqslant \text{const}\sum_r \lambda_m^{\beta(j,s)}\lambda_r^{-s}\cdot\lambda_r^{\alpha(k-j+1,1)}\lambda_n^{-1}\delta_{\lambda_r,\lambda_n}\\ &= \text{const}\ \lambda_m^{\beta(j,s)}\lambda_n^{-s+\alpha(k-j+1,1)-1}g_n \leqslant \text{const}\ \lambda_m^{\beta(j,s)}\lambda_n^{-s+\alpha(k-j+1,1)-1+\nu-\rho}\end{aligned}$$

if $s\in\mathbf{N}$. Choosing a positive integer $s=s(k,p)>p+|\alpha(k-j+1,1)|+\nu-p-1$ for every $p\in\mathbf{N}$, and since $\lambda_n^{-\mu}$ is bounded for $|n|\to\infty$ for fixed $\mu>0$, we conclude that

$$\sum_r |\tilde{S}^{(j)}_{mr}| \cdot |K^{(k-j+1)}_{rn}| \leqslant \text{const } \lambda_m^{\beta(j,s(k,p))} \lambda_n^{-p}$$

at each such p. Thus (4.16c) holds for all $p \in \mathbf{N}$ and all $j=1,\ldots,k$ if we set $c(k,p) = \max_{1\leqslant\sigma\leqslant k} \beta(\sigma,s(k,p))$.

(2) To show that (4.13b) is true for $i=k+1$, we first note that estimates (4.16a)–(4.16c) hold with m and n interchanged if $a(k,p),b(k,p),c(k,p)$ are replaced by suitable constants $\tilde{a}(k,p),\tilde{b}(k,p),\tilde{c}(k,p)$ in the respective rhs of these estimates. This remark and the fact that the rhs of (4.16d) is symmetric with respect to this interchange obviously imply that (4.13b) holds for $i=k+1$ if we choose $\alpha(k+1,p) \geqslant$ than the largest of the seven constants $a(k,p),\ldots,d(k,p)$, $\tilde{a}(k,p),\ldots,\tilde{c}(k,p)$. That estimates (4.16a)–(4.16c) hold in the modified form mentioned in the penultimate sentence follows by arguments similar to, but somewhat simpler than, those used to prove them in their original form.

(3) Recall that in step (1) we demonstrated inductively that the first sum over r in (2.13b) converges absolutely for $i \geqslant 2$, and hence that (2.13b) makes sense. We will now complete the proof of the present lemma by showing that definition (2.12b) also makes sense for $i \geqslant 2$ and that (4.13e) is true at each such i.

By (2.12b), we find formally

$$|\hat{S}^{(i)}_{mn}| \leqslant \frac{1}{2} \sum_{j=1}^{i-1} \sum_r (|\tilde{S}^{(j)}_{mr}||\tilde{S}^{(i-j)}_{nr}| + |\hat{S}^{(j)}_{mr}| \cdot |\hat{S}^{(i-j)}_{nr}|)\, \delta_{\lambda_m,\lambda_n} \quad (i \geqslant 2). \tag{4.19}$$

Because of our inductive hypothesis, the sum over r in (4.19) converges for $1 \leqslant j \leqslant i-1, 2 \leqslant i \leqslant k+1$. This assertion and the fact that (4.13e) holds for $i=k+1$ follow from the assumption that (4.13d) and (4.13e) obtain for $i=1,\ldots,k$, together with arguments similar to those adduced to derive (4.16a) and (4.16c). We have thus proved (4.13e) for arbitrary $i \geqslant 1$. Hence our proof that the sum over r in (4.19) converges for $i=k+1$ extends to all $i \geqslant 2$ and implies that the recursive definition (2.12b) makes sense for all such i. □

Lemma 4: (1) At each $i \geqslant 1$, $V^{(i)},K^{(i)},\tilde{S}^{(i)},\hat{S}^{(i)}$ are well-defined operators in $\mathscr{M}$, and hence so are $S^{(i)},S_N(\varepsilon),K_N(\varepsilon),R_N(\varepsilon)$ [Definition 5(b)].

(2) At each $i \geqslant 1$, the adjoints $V^{(i)*},K^{(i)*},\tilde{S}^{(i)*},\hat{S}^{(i)*}$ exist and are in $\mathscr{M}$, and hence so are $S^{(i)*},S_N(\varepsilon)^*,K_N(\varepsilon)^*,R_N(\varepsilon)^*$.

Proof: (1) We fix $i \geqslant 1$ in the proof. In order to show that $V^{(i)},K^{(i)},\tilde{S}^{(i)},\hat{S}^{(i)}$ are well defined, it suffices to show that the respective matrices with which they are associated are square-summable by rows and columns. This is trivially true for $\mathscr{K}^{(i)}$ and $\hat{\mathscr{S}}^{(i)}$. Indeed, by (2.8), (2.12a), and (2.12b) the $K^{(i)}_{mn}$s and $\hat{S}^{(i)}_{mn}$s are nonzero only if $\lambda_m \neq \lambda_n$, and therefore at most for a finite number of n-values for each m, and vice versa. We proceed to show that these two square-summability properties are possessed by $\mathscr{V}^{(i)}$, $\tilde{\mathscr{S}}^{(i)}$.

As to $\mathscr{V}^{(i)}$, we note that (4.13b) and (4.17) entail

$$\sum_m |V^{(i)}_{mn}|^2 \leqslant \text{const } \lambda_n^{2\alpha(i,p)} \sum_m \lambda_m^{-2p} < \infty \quad (n \in \mathbf{Z}_+^\nu) \tag{4.20a}$$

for‘ each positive integer $p > \nu/2$. The fact that

$$\sum_n |V^{(i)}_{mn}|^2 < \infty \quad (m \in \mathbf{Z}_+^\nu) \tag{4.20b}$$

follows similarly from (4.13a) and (4.17). As to $\tilde{\mathscr{S}}^{(i)}$, its square-summability by rows (resp., by columns) follows from (4.13d) [resp., (4.13c)] via considerations of the type invoked to prove (4.20a) [resp., (4.20b)].

We show next that $V^{(i)} \in \mathscr{M}$, i.e., that $H_0^p V^{(i)} f \in \mathscr{H}$ for all $p \in \mathbf{Z}_+$, $f \in C^\infty(H_0)$. This is the case iff

$$\sum_m \lambda_m^{2p} \Big| \sum_n V_{mn}^{(i)} \langle \Phi_n, f \rangle \Big|^2 < \infty \quad [p \in \mathbf{Z}_+, f \in C^\infty(H_0)], \tag{4.21}$$

as follows from $V^{(i)} \leftrightarrow \mathscr{V}^{(i)}$, the orthonormality and completeness of Φ, and the spectral theorem for H_0^p. By the positivity of the λ_ms and Schwarz's inequality in $\ell^2(\mathbf{Z}_+^\nu)$, (4.21) holds if

$$\sum_{m,n} \lambda_m^p |V_{mn}^{(i)}| \cdot |\langle \Phi_n, f \rangle| < \infty \quad [p \in \mathbf{Z}_+, f \in C^\infty(H_0)]. \tag{4.22}$$

To prove that condition (4.22) is satisfied, we invoke (4.13b), (4.17), and the inequality

$$|\langle \Phi_n, g \rangle| \leqslant \lambda_n^{-r} \| H_0^r g \| \quad [r \in \mathbf{N}, g \in C^\infty(H_0)], \tag{4.23}$$

whose derivation is similar to that of (4.6). We thus see that at each p, f in (4.22)

$$\begin{aligned} \sum_{m,n} \lambda_m^p |V_{mn}^{(i)}| \cdot |\langle \Phi_n, f \rangle| &\leqslant \text{const} \sum_{m,n} \lambda_m^p \cdot \lambda_n^{\alpha(i,q)} \lambda_m^{-q} \cdot \lambda_n^{-r} \| H_0^r f \| \\ &\leqslant \text{const} \Big(\sum_m \lambda_m^{p-q} \Big) \Big(\sum_n \lambda_n^{\alpha(i,q)-r} \Big) \| H_0^r f \| < \infty \end{aligned}$$

at every $q, r \in \mathbf{N}$, such that $q > p + \nu, r > \alpha(i,q) + \nu$.

In view of (2.8), (4.22) holds with $V_{mn}^{(i)}$ replaced by $K_{mn}^{(i)}$. This fact and $K^{(i)} \leftrightarrow \mathscr{K}^{(i)}$ entail $K^{(i)} \in \mathscr{M}$ by considerations analogous to those adduced to prove $V^{(i)} \in \mathscr{M}$. Considerations of the same type based on (4.13d) and (4.13e), in particular, show that $\tilde{S}^{(i)}, \hat{S}^{(i)} \in \mathscr{M}$. Recalling the definition $S^{(i)} = \tilde{S}^{(i)} + \hat{S}^{(i)}$, we thus conclude that $S^{(i)} \in \mathscr{M}$. Similarly, $S_N(\varepsilon), K_N(\varepsilon), R_N(\varepsilon) \in \mathscr{M}$ because the operators on the rhs of (2.2a), (2.2b), (2.3b) are in $\mathscr{M}$.

(2) We proceed to prove assertion (2) of the lemma. Since $V^{(i)}, K^{(i)}, \tilde{S}^{(i)}, \hat{S}^{(i)}$ are defined on the dense set $C^\infty(H_0)$, their adjoints exist. The following considerations show that they are all in $\mathscr{M}$. We begin by proving that $V^{(i)*}$ has this property.

Since $\mathscr{V}^{(i)}$ is quadratically-summable by rows and columns, so is $\mathscr{V}^{(i)*}$, and thus it is legitimate to define $\check{V}^{(i)}$ as the operator associated with $\mathscr{V}^{(i)*}$. To prove that $V^{(i)*}$ is in $\mathscr{M}$, we will show that $\check{V}^{(i)}$ is and that

$$\check{V}^{(i)} | C^\infty(H_0) \subset V^{(i)*}. \tag{4.24}$$

Note that $\check{V}^{(i)} \in \mathscr{M}$ if (4.22), modified by replacing $V_{mn}^{(i)}$ by $\overline{V_{nm}^{(i)}}$, holds, as one sees by arguments similar to those adduced to prove that $V^{(i)} \in \mathscr{M}$ is implied by the original equation (4.22). The modified form of (4.22) can be proved similarly to the way (4.22) itself was. Next, we note that

$$\sum_{m,n} |V_{mn}^{(i)}| \cdot |\langle \Phi_m, f \rangle| \cdot |\langle \Phi_n, g \rangle| < \infty \quad [f, g \in C^\infty(H_0)], \tag{4.25}$$

as follows by considerations of the same type as those leading to (4.22). By $V^{(i)} \leftrightarrow \mathscr{V}^{(i)}$, $\check{V}^{(i)} \leftrightarrow \mathscr{V}^{(i)*}$, $C^\infty(H_0) \subset D(V^{(i)}) \cap D(\check{V}^{(i)})$, and (4.25), we may apply Lemma A3 of the Appendix [with $\mathscr{N} = C^\infty(H_0)$] to conclude that (4.24) holds.

The property $K^{(i)*} \in \mathscr{M}$ is entailed by the fact that (4.22) [resp., (4.25)] obviously holds with $V_{mn}^{(i)}$ replaced by $\overline{K_{nm}^{(i)}}$ (resp., $K_{mn}^{(i)}$) and arguments analogous to ones invoked to prove $V^{(i)*} \in \mathscr{M}$.

The relations $\tilde{S}^{(i)*},\hat{S}^{(i)*}\in\mathscr{M}$ follow for similar reasons, and $S^{(i)*}\in\mathscr{M}$ is immediately implied by them and $S^{(i)*}\supset\tilde{S}^{(i)*}+\hat{S}^{(i)*}$, which is entailed by the definition $S^{(i)}=\tilde{S}^{(i)}+\hat{S}^{(i)}$.[41]

The relations $S_N(\varepsilon)^*,K_N(\varepsilon)^*,R_N(\varepsilon)^*\in\mathscr{M}$ follow because the adjoints of the operators on the rhs of (2.2a), (2.2b), (2.3b) are in $\mathscr{M}$, and because of familiar relations of the adjoints of operator sums and products.[41] □

The next lemma provides information on the connection between V and $V^{(1)}$ which is needed in the proof of Lemma 6.

Lemma 5: The following statements hold:

$$V^{(1)}\supset V, \tag{4.26a}$$

$$V^{(1)}=V \text{ on } C^\infty(H_0). \tag{4.26b}$$

Proof: (1) Since $\Phi\subset D(V)$, $V=V^*$ [by (I) and (II)], and $V^{(1)}\leftrightarrow\mathscr{V}^{(1)}=(V_{mn})$, Lemma A1 of the Appendix immediately implies (4.26a).

(2) The first step in proving (4.26b) is to show that

$$D(V)\supset C^\infty(H_0). \tag{4.27}$$

To this end, we fix $f\in C^\infty(H_0)$ and define

$$f_M=\sum_{|n|\leqslant M}\langle\Phi_n,f\rangle\Phi_n \quad (M\in\mathbf{Z}_+). \tag{4.28}$$

Since the sum (4.28) has only a finite number of terms and $\Phi\subset D(V)$, it follows that $f_M\in D(V)$. Since, in addition, Φ is an orthonormal basis,

$$Vf_M=\sum_{|n|\leqslant M}\langle\Phi_n,f\rangle\sum_m V_{mn}\Phi_m. \tag{4.29}$$

By (4.28) and $f\in\mathscr{H}$,

$$f=s-\lim_{M\to\infty} f_M. \tag{4.30a}$$

The second step in the proof of (4.26b) is to show that the limit

$$g=\mathrm{s}-\lim_{M\to\infty} Vf_M \tag{4.30b}$$

exists, as we will do shortly. From its existence and the fact that V is closed, Eqs. (4.30) entail that $g=Vf$, and hence that (4.27) holds. In turn, (4.26a) and (4.27) imply (4.26b).

The strong limit in (4.30b) exists because

$$\begin{aligned}\left\|\sum_{|n|\geqslant M+1}\sum_m V_{mn}\langle\Phi_n,f\rangle\Phi_m\right\| &\leqslant \sum_{|n|\geqslant M+1}\sum_m |V_{mn}|\cdot|\langle\Phi_n,f\rangle| \\ &\leqslant \text{const}\sum_{|n|\geqslant M+1}\sum_m \lambda_n^{\alpha(1,p)}\lambda_m^{-p}.\lambda_n^{-q}\|H_0^q f\| \\ &\leqslant \text{const}\left(\sum_m \lambda_m^{-p}\right)\left(\sum_{|n|\geqslant M+1}\lambda_n^{-[q-\alpha(1,p)]}\right)\to 0 \quad (M\to\infty)\end{aligned} \tag{4.31}$$

for all $p,q \in \mathbf{N}$ such that $p > \nu$ and $q > \nu + \alpha(1,p)$. To obtain the second line of (4.31), one uses (4.5), $V_{mn} = V_{nm}$, and (4.23). As to the third line of (4.31), note that the sums $\Sigma_m \lambda_m^{-p}$ and $\Sigma_n \lambda_n^{-[q-\alpha(1,p)]}$ are convergent at the stated p,q values by (4.17). □

Lemma 6: For each $\varepsilon \geqslant 0$, $K_N(\varepsilon)$ is essentially self-adjoint. Its unique self-adjoint extension $\overline{K_N(\varepsilon)}$ is the operator associated with the Hermitian matrix

$$\mathscr{K}_N(\varepsilon) = \sum_{j=0}^{N} \varepsilon^j \mathscr{K}^{(j)}(\varepsilon), \tag{4.32}$$

where $\mathscr{K}^{(0)} = (\lambda_m \delta_{\lambda_m,\lambda_n})$.

Remark: The essential self-adjointness of $K_N(\varepsilon)$ will not be used in the sequel.

Proof of Lemma 6: It is given in steps (1)–(4) below, in which $\varepsilon \geqslant 0$ should be considered fixed in the absence of an explicit statement to the contrary, and in which the dependence of the relevant operators on this parameter will usually be omitted.

(1) In this step, we show that (2.1) holds rigorously on $C^\infty(H_0)$. We *define*

$$S_{mn}^{(i)} = \langle \Phi_m, S^{(i)} \Phi_n \rangle \quad (i \geqslant 1), \tag{4.33a}$$

which together with the definitions of $S^{(i)}, \tilde{S}^{(i)}, \hat{S}^{(i)}$, and because these operators are in $\mathscr{M}$, entails

$$S_{mn}^{(i)} = \tilde{S}_{mn}^{(i)} + \hat{S}_{mn}^{(i)} \quad (i \geqslant 1). \tag{4.33b}$$

Equation (2.7) holds by (2.12), (3.4), and (4.33b). By (2.7) and definition (2.8), (2.6) follows. Fixing $i \geqslant 1$ for the moment, we now prove that (2.3a) holds on $C^\infty(H_0)$. To this end, we first calculate the action of the rhs of (2.3a) on an arbitrary element $f \in C^\infty(H_0)$ using Lemma A2 [with $r=2$; $A^{(1)}, A^{(2)} = H_0, S^{(i)}$ and $A^{(1)}, A^{(2)} = S^{(i)}, H_0$; $\mathscr{N} = C^\infty(H_0)$; etc.], whose application is justified since $H_0, S^{(i)}$ and their adjoints are in $\mathscr{M}$, and since $C^\infty(H_0) \supset \Phi$. Second, we compute the action of the lhs of (2.3a) on f by using $K^{(i)} \leftrightarrow \mathscr{K}^{(i)}$, $V^{(i)} \leftrightarrow \mathscr{V}^{(i)}$, and (2.8). Since the results of these two calculations agree, (2.3a) obtains in the stated sense. A similar approach using (2.3a), definitions (2.2b), (2.3b), and (4.27b), and the facts that (1.2) holds on $C^\infty(H_0)$ and that all the relevant operators are in $\mathscr{M}$, shows that (2.1) obtains on $C^\infty(H_0)$.

(2) Let us postmultiply (2.1) by $S_N(\varepsilon)^*$ and premultiply the equation ''adjoint'' to (2.1) by $S_N(\varepsilon)$. Subtracting the second equation from the first, we obtain formally

$$[H_0,\ S_N S_N^*] = S_N(K_N - K_N^*)S_N^* - \varepsilon[V,\ S_N S_N^*] + \varepsilon^{N+1}(R_N S_N^* - S_N R_N^*). \tag{4.34}$$

We claim that (4.34) obtains rigorously on $C^\infty(H_0)$.[42] One can prove this by using the facts that (2.1) holds on this dense subset, that the operators in (2.1) and their adjoints are in $\mathscr{M}$, and that the elementary properties of adjoints invoked above hold.[41]

(3) In this step, we show that each matrix $\mathscr{K}^{(i)}$ $(i \geqslant 1)$ is Hermitian:

$$K_{mn}^{(i)} = \overline{K_{nm}^{(i)}} \quad (i \geqslant 1), \tag{4.35}$$

and hence that the matrix $\mathscr{K}_N(\varepsilon)$ in (4.32) has this property, which is essential in proving the self-adjointness of $\mathscr{K}_N(\varepsilon)$. We will prove (4.35) by using a rigorous version of the argument in Ref. 13 alluded to in Sec. II.

Define $(S_N S_N^*)^{(i)}$ as the coefficient of ε^i in $S_N S_N^* = (\Sigma_{j=0}^N \varepsilon^j S_N^{(j)})(\Sigma_{k=1}^N \varepsilon^k S_N^{(k)*})$. We claim that

$$(S_N S_N^*)_{mn}^{(i)} \equiv \langle \Phi_m, (S_N S_N^*)^{(i)} \Phi_n \rangle = 0 \quad (1 \leqslant i \leqslant N) \tag{4.36}$$

holds for $N \geqslant 1$. We will establish this claim, and at the same time prove (4.35), in two steps. First, we note that (4.35) and (4.36) obtain for each such N if $i=1$. Indeed, $K^{(1)}_{mn} = \overline{K^{(1)}_{mn}}$ by (2.8) and $V^{(1)}_{mn} = V_{mn} = \overline{V_{nm}} = \overline{V^{(1)}_{nm}}$; and $(S_N S_N{}^*)^{(1)}_{mn}=0$ for $N \geqslant 1$ by (2.7), (2.12a), the latter property of $V^{(1)}_{mn}$, and

$$(S_N S_N{}^*)^{(1)} = S^{(1)} + S^{(1)*}.$$

Second, fixing $N \geqslant 2$ until further notice, we make the inductive hypothesis that (4.35) and (4.36) obtain for $1 \leqslant i \leqslant k$, for some positive integer $k \in \{1,\ldots,N-1\}$, and proceed to show that this implies that they obtain for $i=k+1$.

Because (4.34) holds on the dense set $C^\infty(H_0)$ for each $\varepsilon \geqslant 0$ and both sides of this equation can be expressed as polynomials in ε whose coefficients are operators defined on this set, the coefficients of equal powers of ε on the rhs and lhs are equal on $C^\infty(H_0)$. Equating the coefficients of ε^{k+1} and using our inductive hypothesis, we arrive at a relation which can be expressed in the form

$$\begin{aligned}([H_0, (S_N S_N{}^*)^{(k+1)}])_{mn} &\equiv \langle \Phi_m, [H_0, (S_N S_N{}^*)^{(k+1)}]\Phi_n\rangle \\ &= (\lambda_m - \lambda_n)(S_N S_N{}^*)^{(k+1)}_{mn} = K^{(k+1)}_{mn} - \overline{K^{(k+1)}_{nm}},\end{aligned}$$

in terms of the relevant matrix elements. Whence

$$K^{(k+1)}_{mn} = \overline{K^{(k+1)}_{nm}}, \tag{4.37a}$$

$$(S_N S_N{}^*)^{(k+1)}_{mn} = 0 \quad (\lambda_m \neq \lambda_n). \tag{4.37b}$$

We proceed to show that (4.37b) also holds for $\lambda_m = \lambda_n$, thereby completing the proof that (4.35) and (4.36) obtain for $i=k+1$.

Expressing

$$(S_N S_N{}^*)^{(k+1)} = S^{(k+1)} + S^{(k+1)*} + \sum_{k=1}^{k} S^{(j)} S^{(k+1-j)*}$$

in terms of matrix elements, one finds

$$[(S_N S_N{}^*)^{(k+1)}]_{mn} = S^{(k+1)}_{mn} + \overline{S^{(k+1)}_{nm}} + \sum_{j=1}^{k} \sum_{r} (\tilde{S}^{(j)}_{mr}\overline{\tilde{S}^{(k+1-j)}_{nr}} + \hat{S}^{(j)}_{mr}\overline{\hat{S}^{(k+1-j)}_{nr}}) \quad (\lambda_m = \lambda_n). \tag{4.38}$$

The formally obvious occurrence of the sum over r in the rhs of (4.38) can be justified by applying Lemma A2 of the Appendix [with $r=2$, $A^{(1)}=S^{(j)}$, $A^{(2)}=S^{(k+1-j)*}$, $\mathscr{N}=C^\infty(H_0)$], whose use is legitimate since each $S^{(i)}, S^{(i)*}$ is in $\mathscr{M}$. Equations (2.12b) and (4.38) immediately imply that (4.37b) obtains for $\lambda_m = \lambda_n$.

(4) Fixing $N \geqslant 1$ henceforth, we will complete the proof of the lemma by showing: (i) $K_N \subset K_N$, (ii) K_N is essentially self-adjoint, and (iii) $\overline{K_N} = K_N{}^*$. Property (i) follows directly from the relevant definitions and the Schwarz inequality in $\mathscr{C}^2(\mathbf{Z}^\nu_+)$. Property (ii) follows from (i),

$D(K_N)\supset C^\infty(H_0)$, (iii) (which we will prove shortly), and the essential self-adjointness of $K_N|C^\infty(H_0)$. This essential self-adjointness property is entailed by (iii), $D(K_N)\supset C^\infty(H_0)$, and $\exp(-itK_N)\in\mathscr{M}$.[43] The last relation follows from

$$\langle\Phi_m,\exp(-it\overline{K_N})\Phi_n\rangle=0 \quad (\lambda_m\neq\lambda_n), \tag{4.39}$$

the unitarity of $\exp(-it\overline{K_N})$, and arguments similar to those adduced to prove $V^{(i)}\in\mathscr{M}$ [step (1) of the proof of Lemma 4]. The statement (4.39) is a consequence of the fact that $\langle\Phi_m,K_N\Phi_n\rangle=\langle\Phi_m,K_N\Phi_n\rangle=0$ for $\lambda_m\neq\lambda_n$ [by $K_N\leftrightarrow\mathscr{K}_N$ and (i)], which implies that H_0 and K_N commute in the usual technical sense.[44] In turn, this commutativity entails that $\exp(-itK_N)H_0\subset H_0\exp(-itK_N)$, from which (4.39) follows immediately.

Finally, we will prove (iii). The last-mentioned property of the matrix elements $\langle\Phi_m,\overline{K_N}\Phi_n\rangle$ and the finite degeneracy of the eigenvalues λ_m play key roles in the proof. Namely, letting $\{\Lambda_\sigma\}$ ($\sigma\in\mathbf{N}$) be the set of distinct eigenvalues λ_m of H_0 (say with $\Lambda_\sigma<\Lambda_\tau$ for $\sigma<\tau$), they entail that each finite set $\mathscr{J}_\sigma=\{m\in\mathbf{Z}_+^\nu:\lambda_m\in\Lambda_\sigma\}(\sigma\in\mathbf{N})$ has the properties attributed to J_σ in the Corollary to Lemma A4. Applying this corollary (with $A=K_N$, $\mathscr{A}=\mathscr{K}_N$, $J_\sigma=\mathscr{J}_\sigma$, $\Psi=\Phi$), the self-adjointness of K_N follows. This completes the proof of the lemma. □

We recall that the Nth-approximant $\psi_N(t,\varepsilon)$ is defined by (3.6) and that this definition makes sense in view of (3.2a) and the fact that $S_N(\varepsilon),S_N(\varepsilon)^*,\exp(-itK_N(\varepsilon))\in\mathscr{M}$.

Lemma 7: The following statements hold:

(1) For all $t\in\mathbf{R}$, $\varepsilon\geqslant 0$, $\psi_N(t,\varepsilon)$ satisfies the differential equation

$$i\,\frac{d\psi_N(t,\varepsilon)}{dt}=H_\varepsilon\psi_N(t,\varepsilon)+\varepsilon^{N+1}g_N(t,\varepsilon) \tag{4.40a}$$

and the initial condition

$$\psi_N(0,\varepsilon)=[I+\varepsilon^{N+1}U_N(\varepsilon)]\psi_0, \tag{4.40b}$$

where d/dt denotes the strong derivative in $\mathscr{H}$, the operator $U_N(\varepsilon)$ is defined on $C^\infty(H_0)$ by (2.11b), and

$$g_N(t,\varepsilon)=-R_N(\varepsilon)\exp(-it\overline{K_N}(\varepsilon))S_N{}^*\psi_0. \tag{4.41}$$

(2) At each such ε, $g_N(t,\varepsilon)$ is strongly continuous in t on $\mathbf{R}$, and the following uniform boundedness properties hold:

$$\sup_{(t,\varepsilon)\in\mathbf{R}\times[0,\,\varepsilon_0]}\|g_N(t,\varepsilon)\|<0, \tag{4.42a}$$

$$\sup_{\varepsilon\in[0,\,\varepsilon_0]}\|U_N(\varepsilon)\psi_0\|<\infty, \tag{4.42b}$$

where $0\leqslant\varepsilon_0<\infty$.

Proof: (1) We proceed to prove assertion (1) of the lemma, fixing $\varepsilon\geqslant 0$ until further notice and again suppressing the ε-dependence of the pertinent vectors and operators. Our first task is to justify the equation[20]

$$i\,\frac{d\psi_N(t)}{dt}=S_N\overline{K_N}\,\exp(-it\overline{K_N})S_N{}^*\psi_0, \tag{4.43}$$

which is obtained by formally differentiating (3.6). Note that the rhs of (4.43) makes sense for reasons similar to those for which (3.6) does. If S_N were a bounded operator (which it is generally

not), then it could be interchanged with d/dt (strong derivative) without further ado, and in view of the facts that the relevant operators are in $\mathscr{M}$ and that (3.2a) holds, (4.43) would emerge immediately. We will prove (4.43) by a uniform-convergence argument which justifies this interchange.

Write

$$\psi_N(t)=\sum_m F_m(t)\Phi_m, \tag{4.44}$$

where

$$F_m(t)=\langle \Phi_m, S_N \exp(-it\overline{K_N})S_N^*\psi_0\rangle=\langle S_N^*\Phi_m, \exp(-it\overline{K_N})S_N^*\psi_0\rangle. \tag{4.45}$$

By (4.45) and because $S_N^*\Psi_0\in C^\infty(H_0)\subset D(\overline{K_N})$, it follows that $F_m\in C^1(\mathbf{R})$, with

$$\frac{dF_m(t)}{dt}=-i\langle S_N^*\Phi_m, \overline{K_N}\exp(-it\overline{K_N})S_N^*\psi_0\rangle=-i\langle \Phi_m, S_N\exp(-it\overline{K_N})\overline{K_N}S_N^*\psi_0\rangle. \tag{4.46}$$

We claim that the series

$$\sum_m \frac{dF_m(t)}{dt}\Phi_m \tag{4.47}$$

obtained from (4.44) by term-by-term strong differentiation converges uniformly wrt t on $\mathbf{R}$ in the strong $L^2(\mathbf{R}^\nu)$ sense. This entails that $d\psi_N(t)/dt$ is given by the series (4.47) at each $t\in\mathbf{R}$, and hence that (4.43) holds at all such t.

We will now show that

$$\sum_m \sup_{t\in\mathbf{R}}\left|\frac{dF_m(t)}{dt}\right|<\infty, \tag{4.48}$$

thus proving that the series (4.47) has the claimed uniform-convergence property.

Now, (4.48) holds if it does when $F_m(t)$ is replaced by each of the quantities $\tilde{F}_m^{(j)}(t)(j\geqslant 1)$ and $\hat{F}_m^{(j)}(t)$ $(j\geqslant 0)$, where $\tilde{F}_m^{(j)}(t)$ [resp., $\hat{F}_m^{(j)}(t)$] is given by the expression after the first equality in (4.45), but with the operator S_N replaced by $\tilde{S}^{(j)}$ (resp., $\hat{S}^{(j)}$), where $\hat{S}^{(0)}=I$. [Recall (2.2a) and (4.33).] Fixing $j\geqslant 1$, we will prove that

$$\sum_m \sup_{t\in\mathbf{R}}\left|\frac{d\tilde{F}_m^{(j)}(t)}{dt}\right|<\infty, \tag{4.49}$$

the proof of the analogous estimates involving $\hat{F}_m^{(k)}$ $(k\geqslant 0)$ being even simpler. Setting $w_N=\overline{K_N}S_N^*\psi_0\in C^\infty(H_0)$, we have for each $p\in\mathbf{N}$

$$\begin{aligned}\left|\frac{d\tilde{F}_m^{(j)}(t)}{dt}\right| &= |\langle \Phi_m, \tilde{S}^{(j)}\exp(-it\overline{K_N})w_N\rangle| \\ &\leqslant \sum_{r,s}|\tilde{S}_{mr}^{(j)}|\cdot|\langle \Phi_r, \exp(-it\overline{K_N})\Phi_s\rangle|\cdot|\langle \Phi_s, w_N\rangle| \\ &\leqslant \sum_r |\tilde{S}_{mr}^{(j)}|\cdot g_r\lambda_r^{-q(p,r)}\|H_0^{q(p,r)}w_N\| \\ &\leqslant \text{const}\ \lambda_m^{-p}\sum_r \lambda_r^{\alpha(r,p)}\lambda_r^{\nu-\rho}\lambda_r^{-q(p,r)}\|H_0^{q(p,r)}w_N\|\leqslant \text{const}\ \lambda_m^{-p},\end{aligned} \tag{4.50}$$

if $q(p,r)>2\nu-\rho+\alpha(r,p)$ for each such p and all $r\in\mathbf{Z}_+^\nu$. Here const is independent of m. To arrive at the second line of (4.50), we have used Lemma A2 [with $r=2$, $A^{(1)}=\tilde{S}^{(j)}$, $A^{(2)}=\exp(-itK_N)$, etc.], as we may because $\exp(-itK_N)$ and the other relevant operators are in $\mathscr{M}$. The third line of (4.50) follows from (4.39), the unitarity of $\exp(-itK_N)$, and (4.23); and the fourth line from (4.18), (4.13d), (4.23), and (4.17). The desired result (4.49) now follows from (4.50) and (4.17) by choosing $p>\nu$.

In order to complete the proof of part (1) of the lemma, we still need to show that $\psi_N(t,\varepsilon)$ satisfies (4.40a) and (4.40b) at the stated t,ε-values. The former equation follows by using (4.43) and (4.41), as well as the facts that (1.2) and (2.1), with K_N replaced by K_N, hold on $C^\infty(H_0)$, and that the pertinent operators are in $\mathscr{M}$. Equation (4.40b) is an immediate implication of (3.6) and (2.11a). Note that U_N is well defined on $C^\infty(H_0)$ by (2.11b), since all the $S^{(i)}$s and $S^{(i)}$*s are in $\mathscr{M}$. Note also that Eqs. (2.11) hold on $C^\infty(H_0)$ by (2.2a), a repeatedly used relation for the adjoint of an operator sum, the last-mentioned property of the $S^{(i)}$ s and $S^{(i)}$*s, and the fact that $(S_N S_N^*)^{(i)}=0$ on $C^\infty(H_0)$ for $1\leqslant i\leqslant N$. This fact follows from (4.36) and Lemma A1, which is applicable because the operator $S_N S_N^*$ is symmetric and in $\mathscr{M}$.

(2) The strong continuity of $g_N(t,\varepsilon)$ in t on $\mathbf{R}$ for fixed $\varepsilon\geqslant 0$ can be shown by arguments analogous to those invoked to prove (4.49). The boundedness statements (4.42a) and (4.42b) also follow from arguments of the latter type. The proof of the lemma is therefore complete. □

With the results of Lemma 7 in hand, we proceed to give a short rigorous proof of our main result.

Proof of Theorem 1: We fix $\varepsilon\geqslant 0$ in this paragraph. Since $\psi(t,\varepsilon)$ is a solution of the IVP (1.1) for $t\in\mathbf{R}$ and since $\psi_N(t,\varepsilon)$ solves the IVP (4.40) at all such t by Lemma 7(1), it follows that $f_N(t,\varepsilon)=\psi(t,\varepsilon)-\psi_N(t,\varepsilon)$ is a solution of the IVP

$$i\,\frac{df_N(t,\varepsilon)}{dt}=H_\varepsilon f_N(t,\varepsilon)-\varepsilon^{N+1}g_N(t,\varepsilon), \tag{4.51a}$$

$$f_N(0,\varepsilon)=-U_N(\varepsilon)\psi_0. \tag{4.51b}$$

By (4.51), together with the self-adjointness of H_ε and the strong continuity of $g_N(t,\varepsilon)$ stated in Lemma 7(2), it follows rigorously[45] that

$$\|f_N(t,\varepsilon)\|\leqslant\|f_N(0,\varepsilon)\|+\varepsilon^{N+1}\int_0^{|t|}\|g_N(s,\varepsilon)\|ds \tag{4.52}$$

for $t\in\mathbf{R}$.

By (4.51b), (4.52), and the boundedness properties (4.42) of $g_N(t,\varepsilon)$ and $U_N(\varepsilon)\psi_0$, we infer that

$$\|f_N(t,\varepsilon)\|\leqslant\text{const }\varepsilon^{N+1}(|t|+1)$$

for $t\in\mathbf{R}$, $\varepsilon\in[0,\varepsilon_0]$, where the constant is independent of ε. This completes the proof of Theorem 1. □

APPENDIX: SIMPLE LEMMAS ON OPERATORS IN HILBERT SPACE

In this appendix, we state Lemmas A1–A4 and a corollary to Lemma A4. Except for Lemma A4, this material is applied in Sec. IV in the proofs of Lemmas 4–7. We will use the following notation: $\mathscr{X}$ denotes a Hilbert space spanned by the orthonormal set $\Psi=\{\Psi_\alpha\}$, $A_{\alpha\beta}=0(\alpha\in\Gamma)(\alpha\in\Gamma)$, with $\Gamma=\mathbf{Z}_+^p$ for some $p\in\mathbf{N}$, and $\langle .,.\rangle$ denotes the inner product in $\mathscr{X}$ (anti-linear in the first argument and linear in the second). When the matrix element of an operator A in $\mathscr{X}$ exists, we denote it by $A_{\alpha\beta}$. The adjoint of an operator A is written as A^*, as usual, and $\mathscr{A}^*$ denotes the Hermitian adjoint of a matrix $\mathscr{A}=(A_{\alpha\beta})$. In this Appendix, all operators have domains dense in $\mathscr{X}$ and when any operator is assumed to be associated with an infinite matrix, this association is always wrt Ψ. Hence we will omit explicit references to these two properties.

We proceed to state three elementary lemmas, the proofs of the first two being based on the well-known argument in (A1) below.

Lemma A1: Let A be an operator such that $\Psi\subset D(A)\cap D(A^*)$ and let A_1 be the linear operator associated with $(A_{\alpha\beta})(\alpha,\beta\in\Gamma)$. Then $A\subset A_1$. In particular, if $A_{\alpha\beta}=0$ $(\alpha,\beta\in\Gamma)$, then A is a restriction of the zero operator.

Proof: By our assumptions on A,

$$\langle\Psi_\alpha,Ag\rangle=\langle A^*\Psi_\alpha,g\rangle=\sum_{\beta\in\Gamma}\langle\Psi_\alpha,A\Psi_\beta\rangle\langle\Psi_\beta,g\rangle=\sum_{\beta\in\Gamma}A_{\alpha\beta}\langle\Psi_\beta,g\rangle\quad(\alpha\in\Gamma),\tag{A1}$$

from which the lemma immediately follows. □

Lemma A2: Let $A^{(1)},\ldots,A^{(r)}$ $(2\leqslant r<\infty)$ be operators such that each $A^{(i)}$ has the properties:

(i) $A^{(i)}\mathscr{N}\subset\mathscr{N}$, where $\mathscr{N}$ is a subset in $\mathscr{X}$ such that $\Psi\subset\mathscr{N}\subset D(A^{(i)})$;

(ii) $D(A^{(i)}*)\supset\Psi$.

Then

$$\langle\Psi_\alpha,A^{(1)}\cdots A^{(r)}f\rangle=\sum_{\beta_1\in\Gamma}A^{(1)}_{\alpha\beta_1}\sum_{\beta_2\in\Gamma}A^{(2)}_{\beta_1\beta_2}\cdots\sum_{\beta_{r-1},\beta_r\in\Gamma}A^{(r)}_{\beta_{r-1}\beta_r}\langle\Psi_{\beta_r},f\rangle\quad(f\in\mathscr{M},\alpha\in\Gamma),$$

where the sums over $\beta_1,\ldots,\beta_r$ converge absolutely.

Lemma A3: Let A and $\check{A}$ be operators associated with the respective matrices $\mathscr{A}=(A_{\alpha\beta})(\alpha,\beta\in\Gamma)$ and $\mathscr{A}^*$, and let $\mathscr{N}$ be a dense subset in $\mathscr{X}$ contained in $D(A)\cap D(\check{A})$. In addition, let

$$\sum_{(\alpha,\beta)\in\Gamma\times\Gamma}|A_{\alpha\beta}||\langle\Phi_\alpha,g\rangle|\cdot|\langle\Phi_\beta,f\rangle|<\infty\quad(f,g\in\mathscr{N}).\tag{A2}$$

Then

$$\check{A}|\mathscr{N}\subset A^*.$$

Proof: It follows directly from the definitions and the use of (A2) to interchange the order of summation in the relevant absolutely convergent iterated sums. □

The final lemma is a version of a result of Stone, stated in Theorem 3.4, pp. 91, 92, Ref. 32.[46]

Lemma A4: Let A be an operator associated with a Hermitian matrix $\mathscr{A}=(A_{\alpha\beta})(\alpha,\beta\in\Gamma)$. Moreover, assume that for all $f,g\in D(A)$ the necessarily convergent series

$$\sum_\alpha\left(\sum_\beta A_{\alpha\beta}\langle\Psi_\beta,g\rangle\right)\overline{\langle\Psi_\alpha,f\rangle},\tag{A3a}$$

$$\sum_\beta\left(\sum_\alpha A_{\alpha\beta}\overline{\langle\Psi_\alpha,f\rangle}\right)\langle\Psi_\beta,g\rangle,\tag{A3b}$$

have the same sum.[47] Then A is self-adjoint.

Corollary to Lemma A4: Let A be an operator associated with a Hermitian matrix $\mathscr{A}=(A_{\alpha\beta})(\alpha,\beta\in\Gamma)$. In addition, assume that there exists a collection of finite subsets J_σ $(\sigma\in\mathbf{N})$ such that

$$\bigcup_{\sigma\in\mathbf{N}}J_\sigma=\Gamma,\quad J_\sigma\cap J_\tau=\varnothing\ \ (\sigma\neq\tau),\tag{A4}$$

and that $A_{\alpha\beta}\neq0$ only if $\alpha,\beta\in J_\sigma$ for some $\sigma\in\mathbf{N}$. Then A is self-adjoint.

Proof: Let $f,g\in D(A)$. Since $A\leftrightarrow\mathscr{A}=\mathscr{A}^*$, one concludes that

$$\sum_{\alpha}\left|\sum_{\beta}A_{\alpha\beta}\langle\Psi_{\beta},g\rangle\right|\cdot|\langle\Psi_{\alpha},f\rangle|<\infty,$$

$$\sum_{\beta}\left|\sum_{\alpha}A_{\alpha\beta}\overline{\langle\Psi_{\alpha},f\rangle}\right|\cdot|\langle\Psi_{\beta},g\rangle|<\infty,$$

i.e., that the sum over α (resp., over β) in (A3a) [resp., (A3b)] converges absolutely. By this conclusion, together with (A4), the finiteness of each set J_{σ}, and the assumption that $A_{\alpha\beta}\neq 0$ only if $\alpha,\beta\in J_{\sigma}$ for some $\sigma\in\mathbf{N}$, the convergent sums (A3a) and (A3b) are both equal to

$$\sum_{\sigma\in N}\sum_{\alpha,\beta\in J_0}A_{\alpha\beta}\overline{\langle\Psi_{\alpha},f\rangle}\langle\Psi_{\beta},g\rangle.$$

The self-adjointness of A now follows from Lemma A4. □

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[20] In what follows, all equations involving t (resp., ε) hold for $t\in\mathbf{R}$ (resp., $\varepsilon\geqslant 0$), in the absence of an explicit statement to the contrary.
[21] A. W. Sáenz, in Ref. 19, p. 163.
[22] In this reformulation, it will turn out that all the operators defined heuristically in the present section have domains containing a common dense set in $L^2(\mathbf{R}^{\nu})$ which they leave invariant. The operator equations in this section hold on this set.
[23] If convergence questions are ignored, one can express (2.1) as $S_{\varepsilon}^{-1}H_{\varepsilon}S_{\varepsilon}=K_{\varepsilon}$, where, in a heuristic sense, S_{ε} and K_{ε} are self-adjoint and unitary operators, respectively, given by formal power series in ε. Such a heuristic equation was used by Born and Jordan[18] to create early versions of nondegenerate and degenerate perturbation theory in matrix mechanics. As mentioned in the text, our approach is very close in spirit to theirs. For a rigorous discussion of this equation for a special type of H_{ε}s with compact resolvents and simple spectra, see Ref. 11.
[24] This will be proved in Sec. IV on the basis of the assumptions on V in Sec. III.
[25] Henceforth, all equations involving free subscripts m,n labeling matrix elements of linear operators in the Φ-basis should be understood to hold for all $m,n\in\mathbf{Z}_{+}^{\nu}$. Similarly, summations over subscripts labeling such elements range over $\mathbf{Z}_{+}^{\nu}$.
[26] This merely means that the matrices $\mathscr{K}^{(i)}$ are Hermitian.
[27] M. Reed and B. Simon, *Methods of Modern Mathematical Physics* (Academic, New York, 1975), Vol. II, Example 3, p. 266.
[28] See, e.g., V. I. Arnold, Russ. Math. Surv. **18**, 85 (1963) and G. Gallavotti, *The Elements of Mechanics* (Springer-Verlag, New York, 1983), § 5.12.

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[33] See, e.g., J. von Neumann, Math. Ann. **102**, 49 (1929); J. Math. **161**, 208 (1929).
[34] In the main text, all operators associated with matrices have this property wrt Φ. Hence the last qualifier will be usually omitted.
[35] The notations Lemma 3(1), Lemma 4(2), etc., denote assertion (1) of Lemma 3, assertion (2) of Lemma 4, etc.
[36] Henceforth, all constants in equations involving the free indices m,n should be understood to be independent of m,n even if this is not stated explicitly.
[37] See the above volume by Reed and Simon, Ref. 27, Eq. (X.28), p. 175.
[38] When any of the estimates (4.13) or (4.16) is mentioned henceforth in the text, it should be understood to hold for all $p \in \mathbf{N}$, even if this is not stated explicitly.
[39] Henceforth, we use the symbols $\Sigma_m, \Sigma_n, \Sigma_r, \ldots$, involving indices $m,n,r,\ldots$, which label eigenfunctions or matrix elements, as abbreviations for $\Sigma_{m\in\mathbf{Z}_+^\nu}$, $\Sigma_{n\in\mathbf{Z}_+^\nu}$, $\Sigma_{r\in\mathbf{Z}_+^\nu},\ldots$, and $\Sigma_{m,n}$ denotes $\Sigma_{(m,n)\in\mathbf{Z}_+^\nu\times\mathbf{Z}_+^\nu}$, naturally with $\mathbf{Z}_+^\nu\times\mathbf{Z}_+^\nu$ identified with $\mathbf{Z}_+^{2\nu}$.
[40] See the theorem on p. 121 of J. Dixmier, *General Topology* (Springer-Verlag, New York, 1984).
[41] Recall the relations

$$(\Sigma_{j=1}^r A^{(j)})^* \supset \Sigma_{j=1}^r A^{(j)*}, \quad (B^{(1)}B^{(2)}\cdots B^{(s)})^* \supset B^{(s)*}\cdots B^{(2)*}B^{(1)*},$$

the first (resp., second) of which holds for operators $A^{(j)}(1\leqslant j\leqslant r,\ 2\leqslant r\leqslant\infty)$ [resp., $B^{(k)}(1\leqslant k\leqslant r,\ 2\leqslant s\leqslant\infty)$] in a Hilbert space whose sum $\Sigma_{j=1}^r A^{(j)}$ (resp., product $B^{(1)}B^{(2)}\cdots B^{(s)}$) is densely defined.
[42] In the remainder of this step of the proof, operator equations are intended to hold on $C^\infty(H_0)$, even if this is not stated explicitly.
[43] See M. Reed and B. Simon, *Methods of Modern Mathematical Physics*, Vol. I (Academic, New York, 1972), Theorem VIII.11, p. 269.
[44] See, e.g., the last cited volume of Reed and Simon, Ref. 43, pp. 270, 271.
[45] See, e.g., V. P. Maslov and M. V. Fedoriuk, *Semi-Classical Approximation in Quantum Mechanics* (Reidel, Dordrecht, the Netherlands, 1981), Proposition 10.6, p. 186.
[46] Unfortunately, the crucial third sentence of this theorem is confusing. But what it was meant to state is readily reconstructed from the proof of the theorem (Ref. 32, especially p. 92), whose arguments imply a result stronger than our Lemma A4.
[47] Here and henceforth, summations over α,β range over Γ unless otherwise stated.

An equivalence proof of the background gauge field quantization and the conventional one

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The background gauge field quantization is a convenient tool for studying weakly interacting gauge and matter fields or analyzing anomalous current conservation in fermionic structures. This method is from the mid 1970's, but it is only today that it received renewed interest for investigating nonperturbative evolution equations in Yang–Mills theory, as well as gauge field effective action formulations. We reviewed, to start with, the general formulation and assumptions about this method, and we pointed out some critical observations concerning it. In particular, we focus on some of the most common equivalence proofs presently known in the literature. We attempted to give a most convincing demonstration of this equivalence as it stands between the background gauge field scattering operator and the conventional one. The result shown here clearly indicates these methods are indeed physically equivalent. In proving that, we neglected all the infrared problems afflicting the pure Yang–Mills gauge theory; as a matter of fact, they appear to be a parallel, but nonintersecting problem with respect to the present one, i.e., to prove the equivalence. © *1996 American Institute of Physics.* [S0022-2488(96)01904-0]

I. INTRODUCTION

The theory of the background field quantization method is a convenient tool in order to study the interplay between classical and quantum interacting fields or to compute, for instance, the generation of quantum anomalies in fermion-scalar systems as well as to analyze the evolution equations of a non-Abelian quantum gauge field in four dimensions. Very recently, it has resulted in a convincing tool in the study of interacting quantum Yang–Mills fields, in effective Lagrangian theories and in beta function computations.[1] Also, in the generalization of the Nambu–Jona Lasinio model of QCD with a background gluon field,[2] it seemed to be quite appropriate. Nevertheless, the physical equivalence of such a quantization method with respect to the more conventional one, has never been proved in a full satisfactory way, at least to our knowledge. On the contrary, it ever seemed to be a bit fragile. We tried, hence, to prove this equivalence in a, possibly, more exhaustive way.

In Sec. II we recall some of the most popular concepts from the conventional functional quantization approach to gauge and non-gauge field theories, by introducing the formal scattering $\hat{S}$ operator of the LSZ reduction prescription.[3] Then, in Sec. III we deal with the proper definition of the background gauge field quantization method for a pure Yang–Mills theory, thus opening the discussion of Sec. IV, where the expression of the gauge invariant effective action is formulated and analyzed in some detail. But the original contribution to this subject stems from Sec. V, where an equivalence proof between the ordinary Yang–Mills $\hat{S}$ scattering matrix operator and the background gauge $\hat{S}_\varphi$ one is exhibited. This is obtained after a lengthy and accurate algebraic computation, which avoids any diagrammatic expansions. Quite general and conclusive remarks have thus been collected together in Sec. VI. In an appendix we explain our reasons for not making use throughout the present equivalence demonstration, of the validity of global BRS symmetry.

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II. THE QUANTIZED YANG–MILLS FIELD

We will begin by reviewing some of the basic ingredients in gauge quantum field theory.[4] As is known, in the functional integral approach to gauge, Yang–Mills field theory, the classical Lagrangian density merely writes

$$L_0 = \tfrac{1}{2} F^{\mu\nu a} F^a_{\mu\nu}, \tag{2.1}$$

where the repeated indices are summed up and

$$F^a_{\mu\nu}(x) \equiv \partial_\mu A^a_\nu(x) - \partial_\nu A^a_\mu(x) + f^a_{bc} A^b_\mu(x) A^c_\nu(x). \tag{2.2}$$

In order to quantize it, one has merely to complete L_0 with two known local functionals that depend on the gauge and auxiliary fields, and to perform then a formal functional integration over the entire set of resulting *effective quantum fields*. For pure Yang–Mills gauge theory, such a quantum Lagrangian density translates into the so-called ''Faddeev–Popov Lagrangian,'' viz.

$$L_{\mathrm{FP}} = L_0 + L_{\mathrm{gf}} + L_{fpg}. \tag{2.3}$$

Here, beside the classical L_0 term of the $A^a_\mu(x)$ gauge potential, one recognizes the L_{gf} gauge fixing term used to break classical gauge invariance, written as

$$L_{\mathrm{gf}} = -\frac{1}{2\alpha} [F(A_\mu)]^2, \tag{2.4}$$

and the L_{fpg} term, which is the functional Jacobian determinant expressing the admissibility condition for the chosen gauge function. In terms of auxiliary ghost fields, $c, \overline{c}$, one has

$$L_{fpg} = \overline{c^a}(x) M^{ab}(x,y) c^b(y) = \mathrm{tr}[\partial_\mu \mathbf{c}^{\dagger a}(x) \cdot D_\mu \mathbf{c}^a(x)]. \tag{2.5}$$

But the physically most important object of this quantization method is the renormalized functional integral of connected Green's functions, $W(J,\eta) = -\ln Z[J,\eta]$, whose arguments are the ''sources'' $J^a(x)$, for the set of effective quantum fields present, and the ''external fields'', $\eta^a(x)$, coupling to the composite operators of the theory. By expressing auxiliary quantum fields in the form of a scalar field $\varphi^a(x)$, all that is written as

$$Z[J,\eta] = \int \mathscr{D}\varphi \, \mathscr{D}A_\mu \, \exp \int d^4x \{L_0 + L_{\mathrm{gf}} + L_{fpg}\}(x). \tag{2.6}$$

To each functional variation $\delta Z(J,\eta)$ induced by the external fields, it is possible, moreover, to correspond the action of a formal operator, to be contracted with $Z[J,\eta]$, namely

$$\frac{\delta Z(J,\eta)}{\delta \eta(x)} \equiv (\Delta_{\eta(x)} \cdot Z)(J,\eta). \tag{2.7}$$

This is a linear operator ''$\Delta_{\eta\cdot}$,'' consisting of insertions into the renormalized time-ordered product, which defines $Z(J,\eta)$. Sometimes one writes it as ''$[\delta/\delta\eta(x)] \int dy L(y)$,'' where the quotation marks indicate that actually we are neglecting the quantum corrections induced by the renormalization procedure.

In particular we aim to formally express the scattering $\hat{S}$ operator as the action of a local operator contracted with $Z[J,\eta]$. Such an operator would act by isolating each of the connected Green's functions obtained by $Z[J,\eta]$, would then amputate the propagators present in the external lines of the Feynman diagrams, and will set the external momenta on their physical values, the *mass shell* values. An operator expression of $\hat{S}$ satisfying that is[5]

$$\hat{S}=:\exp\int d^4x\ d^4y\ \psi^{\mathrm{in}}(x)K(x,y)\zeta\frac{\delta}{\delta J(y)}:Z(J,\eta)\Big|_{J=\eta=0}\equiv(\Sigma_J\cdot Z_{J,\eta}),\tag{2.8}$$

with $\psi\equiv(\varphi,A)$. In so doing, one introduces the *in*coming *asymptotic fields*, $\varphi^{\mathrm{in}}(x)$, the corresponding classical wave operators $K(x,y)$, the sources $J^a(x)$ for the interacting fields, and the function ζ, i.e. the residue at the pole of the propagator, which generates the Fourier transform of the two point functions on the mass shell. The subsequent choice of a gauge condition,

$$F(\varphi,A_\mu)=0,\tag{2.9}$$

makes such a procedure definitely non-gauge invariant, except for very peculiar choices of the field surface F. Note that this surface, implicitly defined by Eq. (2.9), is properly defined in the space $\Phi\times\mathbf{R}^4$, which is the quotient space

$$\Phi\times\mathbf{R}^4\approx(\Phi\times G/\text{action of } G \text{ on } \Phi)\times\mathbf{R}^4.\tag{2.10}$$

Here Φ is the representation space $\Phi\equiv V\oplus\mathscr{G}\times\mathbf{R}^4$, where V is a vector representation of the gauge group G and $\mathscr{G}$ its Lie algebra. The ''coordinates'' on $\Phi\times G$ are thus the sets $(\varphi, A_\mu, \mathbf{e}\equiv\text{identity of } G)$. To vary the φ field *on the fibers*, that is in the G space, will correspond to introduce a covariant connection 1-form, defined on G and with values in $\mathscr{G}$. This is the canonical, ''left invariant'' connection of Maureer and Cartan, $\omega(x)$, satisfying

$$\delta\omega=-[\omega,\omega],\tag{2.11}$$

with the external derivative δ acting on G. The particular value $\omega|_e\equiv\overline{c}$, is of the greatest importance for gauge theories, since it is one of the two Faddeev–Popov ghost fields. The invariance of the gauge condition on the fibers thus becomes

$$\delta F=\left(\overline{c},\frac{\delta_\omega F}{\delta\omega}\right)\equiv M\overline{c}=0.\tag{2.12}$$

We conclude by recalling a remarkable general invariance property satisfied by this theory under a particular nonlocal field transformation. This is the so-called Slavnov–Taylor identity, whose corresponding quantum analog is the *Becchi–Rouet–Stora (BRS) global symmetry transformation*,[6] which is a very general field transformation involving the fermion and boson fields together.

III. BACKGROUND GAUGE FIELD QUANTIZATION

The early formulation of such an alternative quantization method traces back on the middle of the 1970's,[7] when attempts were made to define the gauge covariance of some particular quantum field models, or, at least, of some subsectors of them. One of the most important efforts on it was done by De Witt.[8]

After some alternating issues, a clear formulation has then been consistently developed; in principle, only at one loop level,[9] soon after in the multiloop expansion.[10] At present, it is supported with a detailed proof of its renormalizability,[11] obviously only when the corresponding conventional formulation does possess it.

Initially the background field formulation provided its usefulness in computations with auto-interacting quantum gauge fields; but after a while it was also applied to many quantum and classical fields interacting together. The most typical situations occur in the interaction of a fermion field with a classical gauge potential, giving the form of the chiral anomalies and of asymmetries in the vacuum state; however, it is also used in the perturbative evaluation of the

fermion beta function,[12] as well as to generate other fermion currents. Even the propagation of quantum particles in a curved space–time,[13] or the evaluation of complex diagrams in quantum gravity models sometimes looks for it as a useful approximation.

The essence of the argument simply relies on a separation of the classical functional integration variable (viz. the quantum dynamical field) into two parts; i.e., a classical component, defined as the ''*background field*,'' and the corresponding quantum fluctuation, called the ''*fluctuation field*.'' This procedure reproduces the separation of the solution in conformal field theories, where one usually defines a classical soliton solution with the addition of a quantum correction.

The Green's functions in this method, that is, the functional derivatives of the effective action with respect to the background field, result now in gauge covariant expressions, which become independent of the gauge condition when the background fields are set on the mass-shell values. The possible existence of quantum anomalies, indeed, can only be done after defining the ''background field effective Lagrangian.''

A. Non-gauge formulation

Let $S_0[a(x)]$ be the classical action for a singlet scalar field $a(x)$,

$$S_0[a]=\int d^4x\ L_0(a(x),\partial_\mu a(x)), \tag{3.1}$$

with the usual meaning of the symbols used. The corresponding quantum generating functional is then

$$Z[J]\equiv\exp(-W[J])=N\int \mathscr{D}a\ e^{-\{S_0[a]+(J,a)\}}, \tag{3.2}$$

where (J,a) is the scalar product. This functional is trivially invariant under a shift of the integrand function of the kind

$$a(x)\rightarrow a(x)+f(x), \tag{3.3}$$

as it can be easily proved. One introduces the classical component or *background field*, $\varphi(x)$, together with its quantum fluctuation, $\phi(x)$, by means of the analogous position

$$a(x)=\phi(x)+\varphi(x), \tag{3.4}$$

and one sets

$$\exp(-\widetilde{W}[\varphi,J])\equiv N'\int \mathscr{D}\phi\ e^{-\{S_0[\phi+\varphi]+(J,\phi)\}}, \tag{3.5}$$

with the condition that $\varphi(x)$ is completely stationary in applying the variational principle to $a(x)$, i.e.

$$\int \mathscr{D}a(x)\equiv\int \mathscr{D}\phi(x). \tag{3.6}$$

As it is important to note, this definition is well posed, in the sense that the function $\widetilde{W}[J,\varphi]$ cannot be obtained by the $W[J]$ function by the shift $a(x)\rightarrow a(x)+\varphi(x)$. $\widetilde{W}[J,\varphi]$ do effectively depend on $\varphi(x)$, since the only field coupled to an external source is the quantum piece $\phi(x)$. In gauge field theory, this difference will result in the gauge fixing term too, since the corresponding field operator will now be parametrized by the φ field.

In complete analogy with the conventional formulation, one defines the *classical field* in the presence of a background field,

$$\hat{\phi}(x) \equiv \frac{\delta \widetilde{W}[\varphi, J]}{\delta J(x)}, \tag{3.7}$$

and the effective action with a background field is

$$\widetilde{\Gamma}[\hat{\phi}, \varphi] \equiv \widetilde{W}[\varphi, J] - (J, \hat{\phi}), \tag{3.8a}$$

$$\frac{\delta \widetilde{\Gamma}[\hat{\phi}, \varphi]}{\delta \hat{\phi}(x)} = -J(x). \tag{3.8b}$$

Hereafter we will indicate scalar products, such as $(J, \hat{\phi})$, with the notation

$$J \cdot \hat{\phi} \equiv \int d^4x \; J^{\mu a}(x) \hat{\phi}^a_\mu(x). \tag{3.9}$$

The relationship between $\widetilde{W}$ and W is simply

$$\widetilde{W}[\varphi, J] = W[J] - J \cdot \varphi, \tag{3.10}$$

by which

$$\widetilde{\Gamma}[\hat{\phi}, \varphi] = \Gamma[\hat{\phi} + \varphi] \equiv \Gamma[\overline{\varphi(x)}], \tag{3.11}$$

where the ''effective field'' $\overline{\varphi(x)}$ is the field resuming all the dynamical status of the theory.

An important consequence of the relationship $\Gamma[\overline{\varphi}] = \widetilde{\Gamma}[\overline{\varphi}, 0]$, is that one can get the effective action of the $\overline{\varphi}$ field by summing up the 1P*I* one-particle irreducible diagrams of the physical vacuum in the presence of the effective field only. Proper vertices and *S* matrix elements will then turn out this way, and we will perturbatively construct the effective action by merely summing up these vacuum Feynman diagrams.

B. Gauge field formulation

In the ordinary Lagrangian formulation, hereafter called the *conventional* one, the classical gauge invariant action for the potentials $A_\mu \equiv A_\mu{}^a T^a$, is customarily written as

$$S_0 = S_0[A] \equiv \int d^4x \; L_0(A_\mu, \partial_\nu A_\mu, \ldots), \tag{3.12}$$

with the dots for higher-order terms, if any. Infinitesimal gauge transformations, parametrized by the parameters $\delta\xi_a(x)$ act on it through

$$A^a_\mu \to A'^a_\mu = A^a_\mu + D^{ab}_\mu[A] \delta\xi_b, \tag{3.13}$$

and the covariant derivatives $D^{ab}_\mu[A]$ constitute the so-called gauge group $\mathcal{G}$, such that

$$\left(\frac{\delta}{\delta A^c_\nu} D^{ad}_\mu \right) D^{bc}_\nu - \left(\frac{\delta}{\delta A^c_\nu} D^{bd}_\mu \right) D^{ac}_\nu = D^{cd}_\mu f_c{}^{ab}. \tag{3.14}$$

The Green's functions generating functional of customary bare Yang–Mills theory includes, as we saw, the classical action for the integration variable $A_\mu(x)$, a Jacobian determinant for the integration measure, a source term $J^\mu(x) \equiv J^\mu_a T^a$ coupled to the gauge potential, and a gauge-fixing

functional, $(F^{\mu}A_{\mu})^2$, with the $1/\alpha$ real parameter of it actually included in the definition of F^{μ}. Frequently, in the following, we will also make use of the shortand notation A^iB_i to mean the double contraction $A^a_{\mu}B^{\mu}_a$ between Lorentz indices and internal symmetry indices, as already shown in Eq. (3.9). We then obtain

$$Z[J]=\exp(-W[J])=N\int \mathscr{D}A\ \det(F^i_aD^b_i[A])$$
$$\times\exp-\left\{S_0[A]+\frac{1}{2}\int d^4x\ \eta^{ab}\eta^{cd}F^{\mu}_{ac}F^{\nu}_{bd}A_{\mu c}A_{\nu d}+J\cdot A\right\}. \quad (3.15)$$

An easy and common assumption about F^{μ}_{ab} is

$$F^{\mu}_{ab}\equiv\frac{1}{\alpha}\,\delta_{ab}\partial^{\mu}, \quad (3.16)$$

with δ^{ab} the Kronecker symbol. In Eq. (3.15), in addition, N is a normalization constant, given by $\langle 0^{\text{in}}|0^{\text{out}}\rangle$, and η^{ab} is the metric tensor of the internal symmetry space. Just as shown in the non-gauge theory, we make now a change of variable, by setting

$$A_{\mu}=a_{\mu}+\varphi_{\mu}. \quad (3.17)$$

The integral functional that turns out is a formally well-defined quantity since we have now subtracted out the infinite factor of the orbit volume in the gauge group space; analogously to the former case, we can write

$$\overline{Z_F}[J,\varphi]=\exp(-\overline{W_F}[J,\varphi])$$
$$=N\int \mathscr{D}a\exp-\left\{S_0[a+\varphi]+\frac{1}{2}\int d^4x\ \eta^{ab}F^i_a[\varphi]F^j_b[\varphi]a_ia_j+J\cdot a\right\}$$
$$\times\det(F^i_a[\varphi]D^b_i[a+\varphi]), \quad (3.18)$$

which is in complete analogy with the treatment of Ref. 14. In this formulation the effective action $\overline{\Gamma}[\hat{\phi},\varphi]$ is deduced from $W_F[J,\varphi]$ by means of the customary Légendre transform,

$$\hat{a}(x)\equiv\frac{\delta\overline{W_F}}{\delta J(x)}[J,\varphi], \quad (3.19a)$$

$$\overline{\Gamma}[\hat{a},F[\varphi],\varphi]=\overline{W_F}[J[\hat{a}],F[\varphi],\varphi]-J^{\mu}\cdot\hat{a}_{\mu}. \quad (3.19b)$$

Remarkably, all the Green's functions out of the mass shell as well as all the counterterms needed to renormalize the physical parameters result gauge covariant, while the entangled Slavnov–Taylor identities of the original theory take now a very simple form. More explicitly, one writes

$$e^{-\overline{\Gamma}[\hat{a},\varphi]}=N''\int \mathscr{D}a\ \det[F^i_a[\varphi]D^b_i[a+\varphi]]$$
$$\times\exp-\left\{S_0[a+\varphi]+\frac{1}{2}\int d^4x\ F^{\mu a}_b[\varphi]a_{\mu a}F^b_{\nu c}[\varphi]a^{\nu c}-\frac{\delta\overline{\Gamma}[\hat{a},\varphi]}{\delta\hat{a}_i}(a_i-\hat{a}_i)\right\}, \quad (3.20)$$

corresponding to

$$e^{-\tilde{\Gamma}[\hat{A},\varphi]}=N''\int \mathscr{D}A\ \det(F^i_a[\varphi]D^b_i[A])$$
$$\times\exp-\left\{S_0[A]+\frac{1}{2}\int d^4x\ F^{\mu a}_b[\varphi](A-\varphi)_{\mu a}\right.$$
$$\left.\times F^b_{\nu c}[\varphi](A-\varphi)^{\nu c}-\frac{\delta\tilde{\Gamma}[\hat{A},\varphi]}{\delta\hat{A}_i}(A_i-\hat{A}_i)\right\}. \tag{3.21}$$

Some of the most striking aspects of the background field method are listed below.

The expectation value of the quantum a field, called $\hat{a}$, in the limit of $J_\mu\to 0$, satisfies in the quantum version the same gauge condition originally introduced to break classical gauge invariance, viz.

$$\lim_{J\to 0}\langle F^i_a\hat{a}_i\rangle=0. \tag{3.22}$$

The generating functional $\overline{W_F}[J,\varphi]\equiv\overline{W}[J,F[\varphi],\varphi]$ is invariant, inasmuch as one acts on it with a background field-induced gauge transformation $\varphi\to\varphi'$ and, simultaneously, one rotates the source field $J(x)$, i.e.

$$\frac{\delta\overline{W_F}[J,\varphi]}{\delta\varphi_i}D^a_i[\varphi]+\frac{\delta\overline{W_F}[J,\varphi]}{\delta J^i}J^jD^a_{j,i}\equiv 0. \tag{3.23}$$

In a similar fashion, one proves the relationship

$$\lim_{J\to 0}\frac{\delta\overline{\Gamma}}{\delta\hat{a}_\mu}\langle D^a_\mu[\hat{a}+\varphi]\Pi^b_a[\hat{a},\varphi]\rangle=0, \tag{3.24}$$

where, in addition, there appears the ghost field propagator in the background field gauge $\Pi^b_a[\hat{a},\varphi]$. This last is defined as the negative inverse of the $\mathscr{F}^a_b$ operator, that is

$$\mathscr{F}^a{}_b\equiv F^i{}_bD^a_i[\hat{a}+\varphi], \tag{3.25a}$$

$$\mathscr{F}^a{}_c[\hat{a},\varphi]\Pi^c{}_b[\hat{a},\varphi]=-\delta^a_b. \tag{3.25b}$$

Observe that the derivative of this operator, $V_\mu{}^a{}_b\equiv\mathscr{F}_\nu{}^aD^\nu{}_{b,\mu}$, turns out to be the usual ghost–ghost–quantum field vertex operator.

The most interesting property of this method, however, is a very peculiar gauge invariance, valid for the appropriately defined effective action, as we will show in the next section. Such a property is written as

$$\left\langle\frac{\delta\overline{\Gamma}}{\delta\varphi_i}F^a{}_i[\varphi]+\frac{\delta\overline{\Gamma}}{\delta\hat{a}_j}\frac{\delta D[\varphi]^a{}_j}{\delta\varphi_i}\hat{a}_i\right\rangle=0, \tag{3.26}$$

for some peculiar $\overline{\Gamma}[\hat{a},\varphi]$. As formerly said, in the present formulation the effective action of the effective field can be perturbatively constructed by summing only vacuum diagrams with respect to the $\hat{a}$ field.

IV. GAUGE INVARIANT EFFECTIVE ACTION

In the context of the background field method, it is possible to generate a very peculiar *gauge invariant effective action* $\tilde{\Gamma}[\varphi]$. In order to do that, let us be precise in the sense in which such an invariance holds. As we have seen, in the conventional Yang–Mills generating functional,

$$Z[J]=N\int DA'\ e^{i(S_{\rm eff}[A']+J\cdot A')}, \tag{4.1}$$

one is mainly concerned with the effective action $S_{\rm eff}$, given by

$$S_{\rm eff}\equiv S_0[A']+\frac{1}{2\alpha}\int d^4x[(\partial\cdot A')^2]+S_{fpg}[A'], \tag{4.2}$$

plus, in addition, with the so-called source term. Choosing now an arbitrary gauge function, $\theta(x)$, the classical action $S_0[A']$ results invariant under the transformation

$$\delta_\theta A'_\mu(x)=\partial_\mu\theta(x)+[A'_\mu(x),\theta(x)], \tag{4.3}$$

i.e.

$$\delta_\theta S_0[A']\equiv 0. \tag{4.4}$$

As a matter of fact, by dividing the gauge potential into a *quantum* piece, (q), and a *background* component, (b), $A'_\mu = A_\mu{}^{(q)} + A_\mu{}^{(b)}$, the classical action $S_0[A']$ is indeed invariant under a wider class of gauge transformations; these are subdivided into two classes, namely

$$\delta_\theta^{(q)}A_\mu^{(q)}=\partial_\mu\theta+[A_\mu^{(q)}+A_\mu^{(b)},\theta],\quad \delta_\theta^{(q)}A_\mu^{(b)}=0, \tag{4.5a}$$

and

$$\delta_\theta{}^{(b)}A_\mu{}^{(q)}=[A_\mu{}^{(q)},\theta],\quad \delta_\theta^{(b)}A_\mu{}^{(b)}=\partial_\mu\theta+[A_\mu{}^{(b)},\theta]. \tag{4.5b}$$

In each case it results

$$\delta_\theta{}^{(q)}S_0[A']\equiv 0,\quad \delta_\theta^{(b)}S_0[A']\equiv 0. \tag{4.6}$$

In the framework of the background field method, one can choose such a peculiar effective action $S_{\rm eff}$ (namely our $\tilde{\Gamma}[\varphi]$), such that

$$\delta_\theta{}^{(b)}S_{\rm eff}[\varphi]\equiv 0. \tag{4.7}$$

In this case the effective action $\tilde{\Gamma}[\varphi]$ is said to be the ''gauge (b) invariant effective action.'' To get this result let us begin with introducing the *background gauge* generating functional $\tilde{Z}[J,\varphi]$ in the form of

$$\begin{aligned}\tilde{Z}[J,F[\varphi],\varphi]\equiv\tilde{Z}_F[J,\varphi]&=\exp\{-\tilde{W}_F[J,\varphi]\}\\ &=N'\int\mathscr{D}\tilde{A}\ \exp-\Big\{S_0[A]+\frac{1}{2}\int d^4x\ \eta^{ab}F_a^i[\varphi]F_b^j[\varphi]\\ &\quad\times(A_i-\varphi_i)(A_j-\varphi_j)+J\cdot A\Big\}\det(F[\varphi]_a^{c\mu}D_{\mu c}^b[A]).\end{aligned} \tag{4.8}$$

In this formulation it is necessary to assume $J=J[\varphi]$. The gauge potential A_μ is evidently related to a_μ via Eq. (3.17), namely $\hat{A}_\mu=\hat{a}_\mu+\varphi_\mu$, since it results that

$$\widetilde{W}_F[J,\varphi]=\overline{W_F}[J,\varphi]+J\cdot\varphi. \tag{4.9}$$

Similarly, the effective action turns out to be

$$\begin{aligned}\overline{\Gamma}[\overline{a},F[\overline{a}],\varphi]&=\overline{W_F}[J,\varphi]-J\cdot\hat{a}=\widetilde{W}_F[J,\varphi]-J\cdot\varphi-J\cdot\hat{a}\\&=\widetilde{W}_F[J,\varphi]-J^\mu\cdot\hat{A}_\mu\equiv\widetilde{\Gamma}_F[\hat{A},\varphi].\end{aligned} \tag{4.10}$$

Observe that, in so doing, we introduced into S_{eff} two ''external sources,'' $J(x)$ and $\varphi(x)$, which are quite arbitrary and uncorrelated. We are so free to impose another, very useful constraint on the theory; we are setting $J=J[\varphi]$, or $\varphi=\varphi[J]$, such that it is

$$\varphi=\hat{A}, \quad \text{or} \quad \hat{a}=0. \tag{4.11}$$

The resulting effective action, that is $\widetilde{\Gamma}_F[\hat{A}(J[\varphi]),\varphi]\equiv\Gamma_F[\varphi]$, turns out to be our claimed gauge (b) invariant effective action, satisfying

$$\frac{\delta\widetilde{\Gamma}_F[\varphi,\varphi]}{\delta\varphi_i}F_i^a[\varphi]\equiv\left\{\frac{\delta\widetilde{\Gamma}_F[\hat{A},\varphi]}{\delta\hat{A}_i}+\frac{\delta\widetilde{\Gamma}_F[\hat{A},\varphi]}{\delta\varphi_i}\right\}\Bigg|_{\varphi=\hat{A}}\cdot F_i^a[\varphi]=0. \tag{4.12}$$

In explicit form, it becomes

$$\begin{aligned}e^{-\widetilde{\Gamma}[\hat{A},\hat{A}]}=N''\int\mathscr{D}A\ \det[F_a^i[\hat{A}]D_i^b[A]]\exp-\Bigg\{S_0[A]+\frac{1}{2}\int d^4x[F_c^{\mu a}[\hat{A}](A_{\mu a}-\hat{A}_{\mu a})\\\times F_c^{\nu b}[\hat{A}](A_{\nu b}-\hat{A}_{\nu b})]+\frac{\delta\Gamma[\hat{A}]}{\delta\hat{A}_\mu^a}(A_\mu^a-\hat{A}_\mu^a)\Bigg\},\end{aligned} \tag{4.13}$$

with

$$\frac{\delta\Gamma[\hat{A}]}{\delta\hat{A}_\mu^a}\equiv\left\{\frac{\delta\widetilde{\Gamma}[\hat{A},\varphi]}{\delta\hat{A}_\mu^a}+\frac{\delta\widetilde{\Gamma}[\hat{A},\varphi]}{\delta\varphi_\mu^a}\right\}\Bigg|_{\varphi=\hat{A}}. \tag{4.14}$$

It is important to note that to introduce the background component into the customary Yang–Mills theory can be seen as the development of the ordinary Lagrangian formulation in the presence of a *nonconventional* gauge-fixing term.[12] By generalizing the idea of Abbott *et al.*, we will assume

$$F[\varphi]_{ab}^\mu A_\mu^b\equiv\partial^\mu A_\mu^a-gf_{abc}\varphi_\mu{}^b A_\mu{}^c=B_\varphi{}^a(x), \tag{4.15a}$$

where the functions $B_\varphi^a(x)$ are independent of $a_\mu(x)$ and such that

$$\lim_{\varphi\to0}B_\varphi{}^a(x)\equiv0. \tag{4.15b}$$

The adoption of the Feynman rules into $\widetilde{\Gamma}[\hat{A},\varphi]$ will result in the usual diagrammatic expansion. All the well-known Feynman diagrams of the customary formulation will, in fact, emerge but, in addition to these, some new diagrams, will now result as vertices given by the functional derivatives of $\widetilde{\Gamma}[\hat{A},\varphi]$ with respect to φ. These new vertices require a bit more attention in the diagrammatic treatment of the theory than the conventional ones. Indeed, in order to derive the physical consequences by applying the rules of the LSZ reduction prescription to the S matrix, one should

examine all of the tree diagrams present in the background field, then to combining these together with all possible external lines, with the propagators ''amputated.'' As a matter of fact, the 1P*I* Green's functions are obtained by differentiating $\widetilde{\Gamma}[\hat{A},\varphi]$ with respect to the quantum $\hat{a}$ field, leaving φ constant. In the gauge invariant version of the background field method, however, it corresponds to functionally differentiate $\widetilde{\Gamma}[\hat{A},\varphi]$ with respect to each of the two arguments $\hat{A}$ and φ, and, after it, to set $\varphi=\hat{A}$. This is why we generate the new vertices in the background theory and, consequently, why we need to prove that the conventional S matrix operator coincides with that of the background field method, or, in other words, that all the new vertices are physically influent. Up to date such a question as well as the renormalization itself of this method have been treated in the physical condition of mass—shell with a perturbation expansion in the background field, at least to our knowledge. Frequently, moreover, one has used the global symmetries of the conventional theory, such as the BRS symmetry, to prove things, without any preliminary checks on it. A careful analysis of these basic assumptions in the background gauge (b) invariant formulation and its S matrix operator seems now to be necessary. The results of it are the following.

Let us first recall, (a), that in spite of the fact that the background gauge invariant model contains many additional (b) vertices, many remarkable shortcomings for the computation of the renormalization constants[15] are valid for it.[13] This happens because in the $\varphi\to\hat{A}$ limit the N-point vertex functions, radiatively corrected, become interrelated by the simple Ward–Lee identities, such as

$$\widetilde{\Gamma}_{,\mu\nu}=-\widetilde{\Gamma}_{,j}D^{j}{}_{a,\mu}\hat{a}^{a}{}_{\nu}. \tag{4.16}$$

Contrary to this, in the conventional Yang–Mills theory one is ever dealing with the more entangled Slavnov–Taylor identities. Hence, if the theory under consideration is more complex than bare Yang–Mills, but renormalizable, it will be sufficient to search for the little number of counterterms allowed, constructed from the most simple, admissible integral invariant terms of it, gauge (b) invariant and of the correct dimension.

Second, (b) note that the coincidence limit $\varphi\to\hat{A}$ inside $\widetilde{\Gamma}[\hat{\phi},\varphi]$ leads one to consider the background gauge φ field as a second, effective dynamical variable. As such, it also requires an additional $J'^{\mu}(x)$ source term to couple with, as well as an additional gauge fixing operator, $F'^{\mu}{}_{ab}$, needed to break gauge symmetry with respect to φ.[13] Concerning the need of such a term, let us observe that the condition

$$\varphi=\hat{A}, \quad \text{equivalent to } 0=\hat{a}=\frac{\delta\overline{W_F}}{\delta J}, \tag{4.17}$$

shows that the Légendre transform from $\overline{W_F}$ to $\overline{\Gamma_F}$ *is singular* in this value. Actually it will follow that $\Gamma[\varphi]$ is no more the Légendre transform of $\widetilde{W}[J[\varphi],\varphi]$.

As a third observation, (c) we point out that the Slavnov–Taylor identities and related BRS gauge symmetry are expressed, in their original form, acting on the generating functional $\widetilde{Z}_F[J,\varphi]$; it is only *after a Légendre transform* from $\widetilde{W}_F$ that they become a property of the $\widetilde{\Gamma}[\hat{a},\varphi]$ functional. This means, hence, that this symmetry could also be invalidated in the critical value $\hat{a}=0$, and it must be explicitly checked. Such a check, however, is a difficult task to do, because the effective action is normally expressed only in a perturbative sense. In the Appendix we give a computation showing that global BRS invariance of the effective action in this quite simple model does not seems to hold anymore.

Going on, (d) if, nevertheless, we were to analyze the bare Yang–Mills effective action and its BRS symmetry in order to ''graphically demonstrate'' that all the diagrams containing at least one functional derivative of $\widetilde{Z}_F$ with respect to φ sum up to zero, then, it would be necessary to apply these symmetries to the fully corrected functional; we mean a functional that contains the gauge fixing term $F'_{ab}{}^{\mu}$ for the background field *from the very beginning*, i.e. no more by introducing it only ''when it is required.'' Let us observe also that, following the simplest formu-

lation of the BRS invariance, one is led to hypothesize that *the same cutoff* needed to get the physical subsector of the quantum A_μ field states, which spoils these states of their null modes, *must also hold* for the auxiliary φ field. Only with this assumption one can introduce *one and the same* Faddeev–Popov's pair of ghost fields for the two subspaces considered.

To end up, (e), as previously noted,[15] to each order in the loop expansion of $\tilde{\Gamma}[\hat{a},\varphi]$, one encounters subdiagrams of the vertex functions $\tilde{\Gamma}_{,i_1,\ldots,i_n}$, or renormalization parts, which are not mere insertions of lower-order vertices and propagators. As a consequence, the renormalization program in this method will include parts that do not depend on the functional derivatives of $\tilde{\Gamma}$. The commonly used results of an iterative way to exhibit the renormalizability of a conventional theory are now insufficient. The final expression of $\tilde{\Gamma}$ will include, at least, one counterterm for each of the gauge fixing parameters. Nevertheless, the renormalization of $\tilde{\Gamma}[\hat{A},\varphi]$ can be achieved in an indirect way,[11] i.e., by proving that all the divergencies of $\tilde{W}_F[J,\varphi]$ can be subtracted with a finite number of local counterterms. This implies that the whole $\tilde{\Gamma}[\hat{A},\varphi]$ will be subtracted and regularized and, in particular, that $\tilde{\Gamma}[\varphi,\varphi]$ is also finite.

We considered this last question very briefly, by merely assuming that we can add the appropriate counterterms to the naive $\tilde{Z}_F[J,\varphi]$ generating functional, such that the renormalized expression of this model formally coincides with the naive one, namely with the expression given above [see Eqs. (3.20) and (3.21)]. Hereafter, all the involved fields shall then be considered as the renormalized versions of their naive counterpart, as assumed up to now. Since in the current literature of the background gauge field method there seems not to be any, fully satisfactory proof on the equivalence between the $\hat{S}$ matrix operators, namely a demonstration respecting all items, from (a) to (e), listed above, we proceeded as follows.

V. AN EQUIVALENCE PROOF OF THE *S* MATRIX

To start with, let us assume, in each closed and bounded domain $\mathbf{O}_L$ of an assigned space-time manifold $\mathcal{O}$, the presence of a local algebra $\mathcal{A}(\mathbf{O}_L)$ of the physical observables of a given theory or, better, a set of operations acting on the physical observables defined and with support in $\mathbf{O}_L$. We will limit ourselves to consider the presence in $\mathcal{O}$ of a self-interacting Yang–Mills field $A_\mu(x)$; we will neglect, moreover, the presence of gravity into the field dynamics. Then, let us introduce the particular functional operator $\hat{S}$, which, while acting on the local physical observables, generates the scattering matrix elements for assigned asymptotic conditions. Such a functional, as known, satisfies the algebra of the gauge transformations in $\mathbf{O}_L$, namely

$$\underline{A}_\mu \to \underline{A}^{\epsilon}_\mu = [T^a \underline{A}^a_\mu]^{\epsilon} = \underline{U}(\epsilon)\left[T^a \underline{A}^a_\mu - \frac{i}{g}\,\underline{U}(\epsilon)^{-1}\,\partial_\mu \underline{U}(\epsilon)\right]\underline{U}(\epsilon)^{-1}, \tag{5.1}$$

$$\underline{A}^a_\mu \to \underline{A}^a_\mu + \delta\underline{A}^a_\mu = \underline{A}^a_\mu - \frac{1}{g}\,\partial_\mu \epsilon^a + f^{abc}\epsilon^b \underline{A}^c_\mu, \tag{5.2}$$

where the underline means the local restriction to $\mathbf{O}_L$. These last create an *endomorphism G* into the space of the $\hat{S}$ generated physical observables, that is

$$\mathcal{G}_L : \langle \hat{S}(\mathbf{O}_L)\rangle \to \langle \hat{S}(\mathbf{O}_L)\rangle. \tag{5.3}$$

In the background gauge quantization method, the $\hat{S}$ scattering operator contracted between asymptotic states, $\langle \hat{S}\rangle$, is parametrized by the same background field, namely $\hat{S}=\hat{S}[\varphi]$. In a quite general formulation, this parametrization is reflected in the aforementioned *nonconventional* gauge fixing operator $F[\varphi]$ and in the dependence on φ of the source current $J=J[\varphi]$, in such a way as

$$\hat{S}_\varphi \equiv \hat{S}[F_\varphi] \equiv \hat{S}[F[\varphi], J[\varphi], \varphi], \tag{5.4}$$

[see Eqs. (2.11) and (3.18)]. Now it turns out that, besides the usual algebraic operations defined in the vector space of the physical states, one can introduce another *composition law* in $\mathscr{G}_L$, interesting the $\hat{S}_\varphi$ group elements. With this we mean the combined action of two or more successive scattering processes, each one parametrized by an independent, arbitrary background gauge condition, viz.

$$\hat{S}_\eta \circ \hat{S}_\zeta \equiv \hat{S}[F_\eta] \circ \hat{S}[G_\zeta] = \langle \Omega, \hat{S}_\eta \hat{S}_\zeta^{-1} \Omega \rangle. \tag{5.5}$$

Here the *in*coming fields of the second $\hat{S}_\eta$ operator are defined as the *out*going fields of the inverse $\hat{S}_\zeta$ operator, where η and ζ are two arbitrary background field configurations. Since the choice of the gauge fixing operators, F and G, for any parametrized $\hat{S}_\varphi$ scattering operator is arbitrary and physically influent, we can reduce the previous definition to

$$\hat{S}_\eta \circ \hat{S}_\zeta \equiv \hat{S}[F_\eta] \circ \hat{S}[F_\zeta], \tag{5.6}$$

and to assume $F[\varphi]$ as in Eqs. (4.15). It is then easy to derive the composition law [see Eq. (2.8)],

$$\hat{S}_\eta \circ \hat{S}_\zeta = (\Sigma_\eta \cdot ((\Sigma_\zeta \cdot Z_\zeta)^{-1} Z_\eta)), \tag{5.7}$$

in such a way as, with our choice of $F[\varphi]$, it is

$$\hat{S}_\eta \circ \hat{S}_\zeta = \hat{S}[F_\eta - F_\zeta, J_\eta - J_\zeta, \eta - \zeta] \tag{5.8a}$$

$$= \hat{S}[F_{\eta-\zeta}, J_{\eta-\zeta}, \eta - \zeta] \equiv \hat{S}_{\eta-\zeta}. \tag{5.8b}$$

In physical terms, Eqs. (5.7) and (5.8) are as follows. A gauge, self-interacting A_μ field is divided into a classical background component ζ_μ and a quantum fluctuation field a_μ, whence one derives the associated scattering operator $\hat{S}_\zeta$. After defining the inverse scattering of these fields, one similarly separates the a_μ field into another classical background component η_μ and a remaining second quantum fluctuation a'_μ. The matrix elements for the scattering of a'_μ in the presence of the classical η_μ field, will thus result the same as those for the scattering of the a_μ field in the presence of the $\zeta_\mu - \eta_\mu$ background.

With our composition law the ordinary group properties then read as

$$\begin{gathered}
\hat{S}_\varphi^{-1} \equiv \hat{S}_{-\varphi} = \hat{S}[-F_\varphi, -J_\varphi, -\varphi]; \\
\hat{S}[F_\varphi] \circ \hat{S}[F_\varphi]^{-1} = \hat{S}[0] \equiv \mathrm{Id}; \\
\hat{S}[F_\varphi] \circ \mathrm{Id} = \mathrm{Id} \circ \hat{S}[F_\varphi] = \hat{S}[F_\varphi]; \\
(\hat{S}[F_\eta] \circ \hat{S}[F_\theta]) \circ \hat{S}[F_\zeta] = \hat{S}[F_\eta] \circ (\hat{S}[F_\theta] \circ \hat{S}[F_\zeta]).
\end{gathered} \tag{5.9}$$

The key point, now, is to realize that the transition from the generic background gauge field effective action $\Gamma_F[\hat{a}, \varphi]$ to the manifestly gauge (b) invariant expression $\tilde{\Gamma}_F[\hat{A}, \varphi]|_{\varphi = A}$, can be provided by a one parameter *automorphism* acting in the quoted subalgebra of parametrized S matrix operators, $\hat{S}[F_\varphi]$.

We will begin, hence, by substituting the pair of fields $(a, \varphi) = (A - \varphi, \varphi)$ with the pair of ''interpolating fields,'' $(A^\tau, \tau\varphi)$, where

$$A^\tau{}_\mu \equiv (1 - \tau) a_\mu + \tau \varphi_\mu, \tag{5.10}$$

$0 \leqslant \tau \leqslant 1$, in such a way as to create a τ-dependent $\tilde{\Gamma}_F[\hat{A}^\tau, \tau\varphi]$ functional. Going on this way, we will arrive at a τ parametrization of the same $\hat{S}$ operator, or, in other words, to a family of S matrix operators, $\hat{S}^\tau_\varphi = \hat{S}^\tau[F_\varphi]$.

To gain our final goal, i.e., the equivalence between $\hat{S}$ matrices, two preliminary results are thus in order. If we can prove, indeed, that the transformation $\hat{S}_\varphi \to \hat{S}^\tau_\varphi$ is an automorphism in the group of the local operators $\hat{S}_\varphi$, while showing, at the same time, that the relationship

$$(\Omega, \hat{S}[F_\varphi]\Omega) = (\Omega, \hat{S}^\tau[F_\varphi]\Omega), \quad \forall \tau \in [0,1] \tag{5.11}$$

also holds, it will follow that the given transformation can be unitarily implemented, i.e.

$$\hat{S}^\tau_\varphi = U(\tau)\hat{S}_\varphi U(\tau)^{-1}. \tag{5.12}$$

This will imply that the physical predictions stemming from the model with $\tau = 1$, which is the background gauge (b) invariant one, are the same of those stemming from the $\tau = 0$ model, viz. the conventional gauge theory. From the continuity of this transformation, the result will then be true with each τ value.

We begin, thus, by showing that there is a condition of relative locality between the (a, φ) and $(A^\tau, \tau\varphi)$ pairs of fields. This corresponds to the realistic assumption that the asymptotic Hilbert spaces of this theory, $\mathscr{H}^{\text{in}}$ and $\mathscr{H}^{\text{out}}$, are unaffected by the previous transformation of field variables. In fact, to perform a translation of an integration field variable $a(x)$ by a classical component $\varphi(x)$, and to follow this with a multiplication by a real number τ, *would not affect* the asymptotic properties of the theory.

From the canonical quantization viewpoint, these conclusions can be easily supported. Let us recall, indeed, that a pair of quantum field operators $\Psi_a(x)$ and $\Psi_b(y)$ are said to be relatively local (antilocal) iff the commutation (anticommutation) relation,

$$[\Psi_a(x), \Psi_b(y)]_{-(+)} = 0, \quad \forall (x-y)^2 < 0, \tag{5.13}$$

holds, at least in a weak sense. This property verifies the transitive rule, so that if Ψ_a and Ψ_b are relatively local with respect to Ψ_c, they are also relatively local. Since a classical field, like $\varphi(x)$, defines a set of cyclic states with respect to the vacuum state, it turns out that

$$[\varphi(x), a(y)]_- = 0 = [\varphi(x), A(y)]_-, \tag{5.14}$$

and, by the transitive property,

$$[a(x), A^\tau(y)]_- = 0, \tag{5.15}$$

all that is customary in local relativistic causal quantum field theory.

The local operations obtained by acting with $\hat{S}^\tau$ on the vacuum then have support in the same space-time region $\mathbf{O}_L$ in which are supported the $\hat{S}$ generated ones. This means the transformation $\hat{S} \to \hat{S}^\tau$ lies inside the same subalgebra $\underline{\mathscr{S}}(\mathbf{O}_L)$ in which we defined $\hat{S}$.

We are now in the position to write down our interpolating transformation, as it emerges by the former functional integral expression of $\tilde{W}_F[J, \varphi]$. Taking into account the previous remarks, items from (a) to (e), the right starting point just becomes

$$\overline{Z_F}[J, J', \varphi] = N \int \mathscr{D}a \, \exp - \Big\{ S_0[a] + \frac{1}{2}\, \eta^{ab} \int d^4x [F^i_a[\varphi] F^j_b[\varphi] a_i a_j + F'^i_a + F'^j_b \varphi_i \varphi_j] + J^i \cdot a_i$$
$$+ J'^j \cdot \varphi_j \delta(\hat{a}) \Big\} \det(F^i_a[\varphi] D_{bi}[a]) \det(F'^j_a D_{jb}[\varphi]), \tag{5.16}$$

where $\delta(x)$ is Dirac's delta function. An implicit definition of $\overline{\Gamma}_F$ will then follow, namely

$$e^{-\overline{\Gamma}_F[\hat{a},\varphi]}=N''\int \mathscr{D}a\ \det(F_a^i[\varphi]D_{ib}[a+\varphi])\det(F_a'^jD_{jb}[\varphi])\exp-\Bigg\{S_0[a+\varphi]$$
$$+\frac{1}{2}\int d^4x[(F_a^i[\varphi]a_i)^2+(F_a'^i\varphi_i)^2]+\frac{\delta\overline{\Gamma}_F[\hat{a},\varphi]}{\delta\hat{a}_\mu^a}(a_\mu^a-\hat{a}_\mu^a)-\frac{\delta\overline{\Gamma}[\hat{a},\varphi]}{\delta\varphi_\mu^a}\varphi_\mu^a\delta(\hat{a})\Bigg\}. \tag{5.17}$$

This is also equivalent to

$$e^{-\widetilde{\Gamma}_F[\hat{A},\varphi]}=N''\int \mathscr{D}A\ \det(F_a^i[\varphi]D_{ib}[A])\det(F_a'^iD_{ib}[\varphi])$$
$$\times\exp-\Bigg\{S_0[A]+\frac{1}{2}\int d^4x[F_b^{\mu a}[\varphi](\hat{A}-\varphi)_\mu^aF_c^{\nu b}[\varphi](\hat{A}-\varphi)_\nu^c+F_b'^{\mu a}\varphi_{\mu a}F_b'^{\nu c}\varphi_{\nu c}]$$
$$\times\frac{\delta\widetilde{\Gamma}[\hat{A},\varphi]}{\delta\hat{A}_\mu^a}(A_\mu^a-\hat{A}_\mu^a)-\frac{\delta\widetilde{\Gamma}}{\delta\varphi_\mu^a}\varphi_\mu^a\delta(\hat{A}-\varphi)\Bigg\}. \tag{5.18}$$

With the freedom of redefining the normalization parameter N inside $\widetilde{Z}_F$, we can now neglect the last term of Eq. (5.18), since it does not depend on a_μ, so as to obtain the corresponding $\widetilde{Z}_F[J,\varphi]$ functional. With that we can introduce our *interpolating effective action* $\Gamma_\tau[\hat{A}^\tau,\tau\varphi]$, which takes the form

$$e^{-\Gamma_\tau}\equiv e^{-\widetilde{\Gamma}_F[\hat{A}^\tau,\tau\varphi]}\equiv N''\int \mathscr{D}a\ \exp-\Bigg\{S_0[A^\tau]+\frac{1}{2}\int d^4x[\{F_a^i[\tau\varphi](A_i^\tau-\tau\varphi_i)\}^2+\{F_a'^i\tau\varphi_i\}^2]$$
$$+J_\tau[\hat{A}^\tau]\cdot(A^\tau-\hat{A}^\tau)\Bigg\}\times\det(F_a^i[\tau\varphi]D_{ib}[A])\det(F_a'^iD_{ib}[\tau\varphi]), \tag{5.19}$$

$0\leqslant\tau\leqslant1$, where we defined the current

$$J_\tau^{\mu a}(x)\equiv\frac{\delta\Gamma_\tau[\hat{A}^\tau]}{\delta\hat{A}^\tau{}_{\mu a}(x)}-\frac{\delta\widetilde{\Gamma}[\hat{A}^\tau,\psi]}{\delta\psi_{\mu a}}\Bigg|_{\psi=\tau\varphi}. \tag{5.20}$$

After a customary Légendre transformation of Eq. (5.19), corresponding to get the interpolating transformation

$$\widetilde{W}_F[J,\varphi]\to W^\tau[J^\tau]\equiv\widetilde{\Gamma}_\tau[\hat{A}^\tau,\tau\varphi]+J_\tau\cdot\hat{A}^\tau, \tag{5.21}$$

we also obtain

$$Z^\tau[J_\tau,\tau\varphi]=e^{-W^\tau}\equiv N'\int \mathscr{D}a\ \exp-\Bigg\{S_0[A^\tau]+\frac{1}{2}\int d^4x\ \eta^{ab}(F_a^i[\tau\varphi]F_b^j[\tau\varphi]$$
$$\times(A_i^\tau-\tau\varphi_i)(A_j^\tau-\tau\varphi_j)+F_a'^iF_b'^j\tau^2\varphi_i\varphi_j)+J_\tau\cdot A^\tau\Bigg\}$$
$$\times\det(F_a^i[\tau\varphi]D_{ib}[A^\tau])\det(F_a'^iD_{ib}[\tau\varphi]). \tag{5.22}$$

The limits $\tau\to0$ and $\tau\to1$, of the $Z^\tau[J_\tau,\tau\varphi]$ functional, reproduce, respectively, the normally defined Yang–Mills theory generating functional and the background field (b) gauge invariant one

of Abbott *et al.* As a matter of fact, the constant term $\exp-\frac{1}{2}(F'\hat{A})^2\times\det(F'D[\hat{A}])$, which results as an additional term in Eq. (5.22), can be easily reabsorbed into the renormalization procedure of W_τ, or, in other words, into the N' normalization constant.

Hence, as an effect of the LSZ reduction prescription, we assert that the operator

$$\Sigma_\tau \equiv :\exp\int d^4x\ d^4y\left[A^\tau{}_\mu{}^{(\mathrm{in})}(x)K^{\mu\nu}(x,y)\ \frac{\delta}{\delta J^\nu{}_\tau(y)}\right]: \tag{5.23a}$$

$$=:\exp\int d^4x\ d^4y\left[(1-\tau)a_\mu{}^{(\mathrm{in})}(x)K^{\mu\nu}(x,y)\frac{\delta}{\delta J_\tau{}^\nu(y)}\right]:, \tag{5.23b}$$

while acting on $Z^\tau[J_\tau,\tau\varphi]$, for fixed τ, defines the interpolating scattering matrix elements of the $A^\tau{}_\mu$ and $\tau\varphi_\mu$ fields, namely the $\hat{S}^\tau{}_\varphi[F,F']$ operator.

The first preliminary step, that the translation $\hat{S}\to\hat{S}^\tau$ is an automorphism $\hat{\alpha}_\tau$ in the subset of local scattering operators defined in $\mathbf{O}_L$, will soon emerge by showing that $\hat{\alpha}_\tau$ is a map conserving the group and commutator operations,

$$\hat{\alpha}_\tau(aX\circ bY)=a\hat{\alpha}_\tau(X)\circ b\hat{\alpha}_\tau(Y), \tag{5.24}$$

$$\hat{\alpha}_\tau([X,Y])=[\hat{\alpha}_\tau(X),\hat{\alpha}_\tau(Y)]. \tag{5.25}$$

This corresponds to prove that the action

$$\hat{\alpha}_\tau(a\hat{S}_\eta\circ b\hat{S}_\zeta)=ab\hat{\alpha}_\tau(\hat{S}_\eta\circ\hat{S}_\zeta)=ab\hat{\alpha}_\tau(\hat{S}_{\eta-\zeta}), \tag{5.26a}$$

is exactly equivalent to the composition

$$a\hat{\alpha}_\tau(\hat{S}_\eta)\circ b\hat{\alpha}_\tau(\hat{S}_\zeta)=ab\hat{\alpha}_\tau(\hat{S}_{\eta-\zeta}). \tag{5.26b}$$

In the same time it must also be that

$$\hat{\alpha}_\tau(\hat{S}_\eta\circ\hat{S}_\zeta\circ\hat{S}_\eta^{-1}\circ\hat{S}_\zeta^{-1})=\hat{\alpha}_\tau(\hat{S}_0)=\hat{\alpha}_\tau(\hat{S}_\eta)\circ\hat{\alpha}_\tau(\hat{S}_\zeta)\circ\hat{\alpha}_\tau(\hat{S}_\eta^{-1})\circ\hat{\alpha}_\tau(\hat{S}_\zeta^{-1}). \tag{5.27}$$

Both of these relations are fulfilled if it results that

$$\hat{S}^\tau[F_\eta-F_\zeta]=\hat{S}^\tau[F_\eta]\circ\hat{S}^\tau[F_\zeta]. \tag{5.28}$$

This is nothing but our formerly defined group operation of the φ-parametrized family of $\hat{S}$ matrix operators, now extended to the arbitrary τ values. It is conceivably true that this assumption holds, since it is said that the self-interaction of the $a_\mu+\tau\eta_\mu$ field, followed by the scattering with the $a_\mu+\tau\zeta_\mu$ field, is the same as the self-interaction of the $a_\mu+\tau(\eta_\mu-\zeta_\mu)$ field. To see this, let us consider the following two transformations:

$$[\eta^{ab}(F_\eta-F_\zeta)^i_a(F_\eta-F_\zeta)^j_b a_i a_j]\to[\eta^{ab}(1-\tau)^2(F_{\tau\eta}-F_{\tau\zeta})^i_a(F_{\tau\eta}-F_{\tau\zeta})^j_b a_i a_j], \tag{5.29a}$$

$$\begin{aligned}&\{\eta^{ab}(1-\tau)^2[(F_{\tau\eta})^i_a(F_{\tau\eta})^j_b a_i a_j\circ(F_{\tau\zeta})^i_a(F_{\tau\zeta})^j_b a_i a_j]\}\\&\quad\to\{\eta^{ab}(1-\tau)^2[(F_{\tau\eta})^i_a(F_{\tau\eta})^j_b-(F_{\tau\zeta})^i_a(F_{\tau\zeta})^j_b]a_i a_j\}],\end{aligned} \tag{5.29b}$$

and the analogous ones for the $(F'_\eta)^i_a$ operators. By the symmetry in the μ, ν indices, as well as that in the η^{ab} tensor, the difference between the two transformed right-hand sides reduces to

$$\langle\Omega,[(F_\eta)^i{}_a,(F_\zeta)^j{}_b]a_i{}^a a_j{}^b\Omega\rangle. \tag{5.30}$$

This is indeed zero since the gauge fixing operators F_η and F_ζ were assumed as independent. Quite similarly, the determinantal shift,

$$\det[(F_\eta - F_\zeta)^a{}_i D^{ib}(a)] \to \det[(F_{\tau\eta} - F_{\tau\zeta})_i{}^a D^{ib}(A^\tau)], \tag{5.31a}$$

can be shown to be equivalent to

$$\det[(F_{\tau\eta})_i{}^a D^{ib}(A^\tau)] \circ \det[(F_{\tau\zeta})_i{}^a D^{ib}(A^\tau)] \to \det[(F_{\tau\eta} - F_{\tau\zeta})_i{}^a D^{ib}(A^\tau)]. \tag{5.31b}$$

By this we conclude that $\hat{\alpha}_\tau$ operates on the $\hat{S}_\varphi(F_\varphi, J_\varphi)$ family as an automorphism. What it remains to prove, then, is the validity of the relationship

$$(\Omega, \hat{S}[F_\varphi]\Omega) = (\Omega, \hat{S}^\tau[F_\varphi]\Omega), \quad \forall \tau \in [0,1]. \tag{5.32}$$

To this aim let us write it as

$$\frac{d}{d\sigma}(\Omega, \hat{S}^\sigma[F_\varphi]\Omega)\bigg|_{\sigma=\tau} = 0, \quad \forall \tau, \sigma \in [0,1], \tag{5.33a}$$

namely

$$\frac{d}{d\sigma}(\Omega, \hat{S}^\sigma \Omega)\bigg|_{\sigma=\tau} = \frac{d}{d\sigma}(\Omega, \hat{S}^{\sigma+\tau}\Omega)\bigg|_{\sigma=0} = \frac{d}{d\sigma}(\Omega, (\hat{S}^\tau)^\sigma \Omega)\bigg|_{\sigma=0} = 0. \tag{5.33b}$$

In our formulation this translates to

$$\frac{d}{d\sigma}[(\Sigma_\tau \cdot Z^\tau)^\sigma]\bigg|_{\sigma=J=0} = 0. \tag{5.34}$$

As we previously said, the $\hat{\alpha}_\tau$ interpolation is active only when the quantum field to be integrated over, $\underline{A}$, has been divided into a classical component plus a novel quantum piece, i.e. $\underline{A} \to \underline{a} + \underline{\varphi}$. In order to get the action of $\hat{\alpha}_\sigma$ after the action of $\hat{\alpha}_\tau$, it is then necessary to introduce a second decomposition, quite similar to the former one, which separates the quantum $\underline{a}$ field into a second classical component and a third quantum fluctuation, i.e.

$$\underline{a} \to \underline{a}' + \varphi'. \tag{5.35}$$

This defines a functional integral $\tilde{Z}_{F,G}[J, \varphi, \varphi']$ that depends on two background field components, as well as on two gauge fixing operators. Hence, we have to interpolate the first interpolating functional integral $Z^\tau[J^\tau, \tau\varphi]$ between the values $\varphi' = 0$ and $\varphi' = \underline{a}'$, with the condition to reproduce the known expression of the gauge invariant effective action $\tilde{\Gamma}[\varphi, \underline{\varphi}]$ in the limit $\varphi' \to \underline{a}'$, $\tau = 1$. We introduce such a ''doubly interpolating effective action,'' $\Gamma_{\tau,\sigma}[\hat{A}^{\tau,\sigma}, \tau\varphi + \sigma\varphi']$ with the positions

$$\hat{A}^{\tau,\sigma} = (1-\tau)(1-\sigma)\hat{a}' + \tau\varphi + \sigma\varphi' \tag{5.36a}$$

and

$$\Phi \equiv \varphi + \varphi'. \tag{5.36b}$$

It is to be

$$e^{-\Gamma_{0,0}} \equiv e^{-\Gamma_{\tau,\sigma}}\big|_{\tau=\sigma=0} = e^{-\overline{\Gamma}[\hat{a}]} \quad (conventional), \tag{5.37a}$$

$$e^{-\Gamma_{1,1}}=e^{-\tilde{\Gamma}[\Phi,\Phi]} \quad (gauge\ \ invariant), \tag{5.37b}$$

$$\begin{aligned} e^{-\Gamma_{\tau,0}}&=e^{-\Gamma_{\tau}[\hat{A}^{\tau}]} \\ e^{-\Gamma_{0,\sigma}}&=e^{-\Gamma_{\sigma}[A^{\sigma}]} \quad (interpolating), \end{aligned} \tag{5.37c}$$

$$\begin{aligned} e^{-\Gamma_{\tau,1}}&=C_{\tau}e^{-\tilde{\Gamma}[\Phi,\Phi]}, \\ e^{-\Gamma_{1,\sigma}}&=C_{\sigma}e^{-\tilde{\Gamma}[\Phi,\Phi]}, \end{aligned} \tag{5.37d}$$

with C a real numerical parameter. Analogously, the associated interpolating source current will be

$$J^{\mu a}_{\tau,\sigma}=\frac{\delta\Gamma_{\tau,\sigma}[\hat{A}^{\tau,\sigma}]}{\delta\hat{A}^{\tau,\sigma}{}_{\mu a}}-\left.\frac{\delta\tilde{\Gamma}[\hat{A}^{\tau,\sigma},\psi]}{\delta\psi_{\mu a}}\right|_{\psi=\tau\varphi+\sigma\varphi'}. \tag{5.38}$$

Except for very special assumptions, it is also possible to rearrange the incoming field asymptotic conditions of φ and φ', such that

$$\tau\varphi_{\mu}{}^{(\mathrm{in})}+\sigma\varphi'{}_{\mu}{}^{(\mathrm{in})}=(\tau+\sigma-\tau\sigma)a'{}_{\mu}{}^{(\mathrm{in})}, \tag{5.39}$$

for arbitrary values of τ and σ, so as to have

$$A^{\tau,\sigma}{}_{\mu}{}^{(\mathrm{in})}=a'^{(\mathrm{in})}_{\mu}, \quad \forall\,\tau,\sigma\in[0,1]. \tag{5.40}$$

After introducing the gauge fixing operators $G[\varphi']$ and G' for the a'_{μ} and φ'_{μ} fields, quite analogous to the $F[\varphi]$ and F' ones, the *doubly interpolating* $\hat{S}^{\tau,\sigma}$ *operator* will turn to be completed. By the usual group properties of the $\hat{\alpha}_{\tau,\sigma}$ endomorphism we write it as $\hat{S}^{\tau,\sigma}=(\Sigma_{\tau,\sigma}\cdot Z^{\tau,\sigma})$, with

$$\Sigma_{\tau,\sigma}\equiv:\exp\int d^4x\ d^4y\left[a'{}_{\mu}{}^{(\mathrm{in})}(x)K'^{\mu\nu}(x,y)\ \frac{\delta}{\delta J^{\nu}{}_{\tau,\sigma}(y)}\right]: \tag{5.41}$$

and

$$\begin{aligned} Z^{\tau,\sigma}=\mathcal{N}\int \mathscr{D}a'\ \exp-\Bigg\{ & S_0[A^{\tau,\sigma}]+\frac{1}{2}\int d^4x\ \eta^{ab}[\{G[\sigma\varphi']^i_a G[\sigma\varphi']^j_b+F[\tau\varphi]^i_a F[\tau\varphi]^j_b\} \\ & \times(A^{\tau,\sigma}_i-\tau\varphi_i-\sigma\varphi'_i)(A^{\tau,\sigma}_j-\tau\varphi_j-\sigma\varphi'_j)+(\sigma^2 G'^{\,i}_a G'^{\,j}_b\varphi'_i\varphi'_j+\tau^2 F'^{\,i}_a F'^{\,j}_b\varphi_i\varphi_j)]+J_{\tau,\sigma}\cdot A^{\tau,\sigma}\Bigg\} \\ & \times\det[F[\tau\varphi]^i{}_a D[A^{\tau,\sigma}]^b{}_i]\det[G[\sigma\varphi']^j{}_a D[A^{\tau,\sigma}]^b{}_j]\det[F'^{\,i}_a D[\tau\varphi]^b{}_i]\times\det[G'^{\,j}_a D[\sigma\varphi']^b_j]. \end{aligned} \tag{5.42}$$

In this way one is led to consider the equation

$$0=\left[\frac{d}{d\sigma}(\Omega,(\hat{S}^{\tau})^{\sigma}\Omega)\right]\Bigg|_{\sigma=J=0}=\lim_{\sigma\to 0}\left\{\lim_{J_{\tau,\sigma}\to 0}\left[\frac{d}{d\sigma}(\Sigma_{\tau,\sigma}\cdot Z^{\tau,\sigma}[J_{\tau,\sigma}])\right]\right\}$$

$$=\lim_{\sigma\to 0}\lim_{J_{\tau,\sigma}\to 0}\left\{\left(\Sigma_{\tau,\sigma}:\exp\int d^4x\ d^4y\left[a'^{(\mathrm{in})}_{\mu}(x)K^{\mu\nu}(x,y)\left[\frac{d}{d\sigma}\frac{\delta}{\delta J^{\nu}_{\tau,\sigma}(y)}\right]\right]:\cdot Z^{\tau,\sigma}\right)\right.$$

$$-\left(\Sigma_{\tau,\sigma}\cdot\left[\frac{\delta S_0}{\delta A^{\tau,\sigma}_i}[(\tau-1)a'_i+\varphi'_i]+\eta^{ab}(G[\sigma\varphi']^{i,k}_a G[\sigma\varphi']^{j}_b(1-\tau)^2(1-\sigma)^2 a'_i a'_j\varphi'_k\right.\right.$$

$$-\{F[\tau\varphi]^i_a F[\tau\varphi]^j_b+G[\sigma\varphi']^i_a G[\sigma\varphi']^j_b\}(1-\tau)^2(1-\sigma)a'_i a'_j+\sigma G'^{i}_a G'^{j}_b\varphi'_i\varphi'_j)$$

$$+J_{\tau,\sigma}\cdot\frac{dA^{\tau,\sigma}}{d\sigma}+A^{\tau,\sigma}_i\left[\frac{\delta^2\tilde{\Gamma}[\hat{A}^{\tau\sigma},\psi]}{\delta\hat{A}^{\tau,\sigma}_i\delta\hat{A}^{\tau,\sigma}_j}[(\tau-1)a'_j+\varphi'_j]+\frac{\delta^2\tilde{\Gamma}[\hat{A}^{\tau\sigma},\psi]}{\delta\hat{A}^{\tau,\sigma}_i\delta\psi'_j}\varphi'_j\right]\Bigg|_{\psi=\tau\varphi+\sigma\varphi'}$$

$$+\det(F[\tau\varphi]D[A])\det(F'D[\tau\varphi])(\det(G'^{i,j}_a[\sigma\varphi']D_{ib}[A]\varphi'_j)\det(G'^{i}_a D_{ib}[\sigma\varphi'])$$

$$\left.\left.+\det(G^j_a[\sigma\varphi]D_{jb}[A])\det(G'^{a}_i Di_{jb}[\sigma\varphi']\varphi_j))\right]\cdot Z^{\tau,\sigma}\right)\right\},\tag{5.43}$$

where we put (and analogously for the $D^i_a[\psi']$ operator)

$$G^{i,j}_a[\sigma\varphi']\equiv\frac{\delta G^i_a[\psi']}{\delta\psi'_j}\Bigg|_{\psi'=\sigma\varphi'}.\tag{5.44}$$

The first line of Eq. (5.43), namely $([(d/d\sigma)\Sigma_{\tau,\sigma}]\cdot Z^{\tau,\sigma})$, is zero by formally writing it as

$$\left[\frac{d}{d\sigma}\frac{\delta}{\delta J_{\tau,\sigma}}\right]\cdot Z^{\tau,\sigma}=\lim_{\sigma'\to\sigma}\frac{1}{\sigma'-\sigma}\left(\frac{\delta Z^{\tau,\sigma'}}{\delta J_{\tau,\sigma'}}-\frac{\delta Z^{\tau,\sigma}}{\delta J_{\tau,\sigma}}\right).\tag{5.45}$$

Indeed, from the linearity of the $J_{\tau,\sigma}\cdot A^{\tau,\sigma}$ coupling, and by interchanging the limits $\sigma\to 0$ and $\sigma'\to\sigma$, two identical and σ-independent expressions will result in the functional derivatives. In physical terms, that means the Σ scattering operator for the LSZ reduction prescription to the physical states is invariant under a gauge field reparametrization. We have to show, thus, that the last ten terms in Eq. (5.43), those enclosed between the external square brackets, compensate reciprocally to zero. This will conclude the present equivalence proof. Note that in Eq. (5.43) these ten terms have been written by regrouping as two by two into each line, except for the last two, which are lonely. We note first that the fifth and sixth terms of it are straightforwardly zero, 5th+6th$\equiv$0, in the prescribed limits, as well as the second and fourth term also do, after a functional integration by parts, by observing that in the limit $J_{\tau,\sigma}\to 0$ the gauge fixing functions $B^a_{\varphi}(x)$, $B^b_{\varphi'}(x)$ tend to zero, that is

$$\lim_{J_{\tau,\sigma}\to 0}\ 2\mathrm{nd}+4\mathrm{th}=0.\tag{5.46}$$

Concerning the seventh and eighth terms of it, namely those enclosed inside internal square brackets, let us write them as

$$7\mathrm{th}+8\mathrm{th}=\lim_{J_{\tau,\sigma}\to 0}\frac{\delta}{\delta\hat{A}^{\tau,\sigma}_i}\left[\frac{\delta\tilde{\Gamma}}{\delta\hat{A}^{\tau,\sigma}_j}(\tau-1)a'_j+J^k_{\tau,\sigma}\varphi'_k\right]=\frac{\delta}{\delta\hat{A}^{\tau,\sigma}_i}\left[\frac{\delta\tilde{\Gamma}}{\delta\hat{A}^{\tau,\sigma}_j}(\tau-1)a'_j\right].\tag{5.47}$$

By collecting together this resulting term with the first and third ones of Eq. (5.43), we thus obtain

$$1\text{st}+3\text{rd}+7\text{th}+8\text{th}=\frac{\delta S_0}{\delta A^{\tau,\sigma}}[(\tau-1)a'+\varphi']-\frac{1}{2}\int d^4x((F[\tau\varphi]^i(\tau-1)a_i')^2)$$
$$+A_i{}^{\tau,\sigma}\left[\frac{\delta^2\tilde{\Gamma}_{\tau,\sigma}}{\delta\hat{A}_i^{\tau,\sigma}\,\delta\hat{A}_j^{\tau,\sigma}}[(\tau-1)a_j'+\varphi_j']+\frac{\delta^2\tilde{\Gamma}_{\tau,\sigma}}{\delta\hat{A}_i^{\tau,\sigma}\delta\varphi_j'}\,\varphi_j'\right]. \tag{5.48}$$

The term

$$\lim_{\sigma\to 0}\frac{\delta S_0[A^{\tau,\sigma}]}{\delta A_k^{\tau,\sigma}}\,\varphi_k'\equiv\delta_\theta^{(q)}S_0[A^\tau], \tag{5.49}$$

annihilates in this limit because the *classical action* $S_0[A^{\tau,\sigma}]$ is a gauge (b) and (q) invariant action, whence satisfying Eqs. (4.6) with $\theta(x)\equiv\sigma\varphi'(x)$. Restricting now on a compact manifold, with the space-time boundary conditions imposing a null gauge field $A(x)$, and by performing an integration by parts on the third and seventh terms, we are then led to formally write Eq. (5.48) as

$$\lim_{J_{\tau,\sigma}\to 0}\frac{\delta}{\delta\hat{A}^{\tau,\sigma}{}_j}\left\{S_0[A^\tau]+\frac{1}{2}\int d^4x\;F^2[\tau\varphi]-\tilde{\Gamma}[\hat{A}^\tau]\right\}(\tau-1)a_j'\equiv 0. \tag{5.50}$$

Still, considering the ninth and tenth terms of Eq. (5.43), namely the variations in the determinantal factors, we proceed as follows. Let us set

$$D_i{}^a[\sigma\varphi']=D_i{}^a[0]+D_i{}^{a,j}[\sigma\varphi']\varphi_j', \tag{5.51}$$

so as to have

$$\det(G_a'{}^iD_i^b[\sigma\varphi])=\det(G_a'{}^iD_i^b[0])+\det(G_a'{}^iD_i{}^{b,j}[\sigma\varphi]\varphi_j). \tag{5.52}$$

By decomposing in such a way the ninth and tenth terms, we find

$$9\text{th}+10\text{th}=\det(G_a'{}^iD_i{}^{b,j}[\sigma\varphi']\varphi_j')\times[\det(G_a^{i,j}[\sigma\varphi']D_i{}^b[A^{\tau,\sigma}]\varphi_j')+\det(G_a^i[\sigma\varphi']D_i^b[A^{\tau,\sigma}])]$$
$$+\text{e.t.}=\det(G_a'{}^iD_i{}^{b,j}[\sigma\varphi']\varphi_j')\det\{D_i{}^b[A^{\tau,\sigma}][G_a^{i,j}[\sigma\varphi']\varphi_j'+G_a^i[A^{\tau,\sigma}]]\}+\text{e.t.}, \tag{5.53}$$

where the e.t.≡"*ending term*" of the above string will be defined in a moment. Using the linearity of the $D_\mu[\psi]$ operator, it is then easy to show that

$$\lim_{\sigma\to 0}D_i{}^{a,j}[\sigma\varphi]=\lim_{\sigma\to 0}\sigma D_i{}^{a,j}[\varphi]=0. \tag{5.54}$$

A quite similar reasoning applied to the ending term, namely to

$$\text{e.t.}=\det(G_a^{i,j}[\sigma\varphi']D_b^i[A^{\tau,\sigma}]\varphi_j')\det(G_a'{}^iD_b^i[0]), \tag{5.55}$$

then leads one to conclude that Eq. (5.53) annihilates in the $\sigma\to 0$ limit. We recall, indeed, that our gauge fixing operator $G_a^i[\varphi']$ is linear with respect to $\varphi'(x)$ [see Eq. (4.15(a)].

This would terminate the present demonstration on the unitarity of the transformation $\hat{S}_\varphi\to\hat{S}_\sigma{}^\tau$ giving also, as a consequence, a confirmation of the equivalence between the scattering matrix $\hat{S}_\varphi$ operator of the background gauge field method and the $\hat{S}$ of the conventional one.

VI. CONCLUSION

Even though it is largely known that the scattering theory of the background field method should be physically equivalent to the conventional one, at least for renormalizable scalar and one-dimensional gauge field theories, as suggested by many conformal field theory computations, we succeeded to show it for the case of a non-Abelian, pure Yang–Mills theory. We tried to get such a proof very explicitly and our treatment was done with much care concerning all the possible troubling matters, such as those collected at the end of Sec. IV. In the present proof, indeed, there was no use of any doubtful assumptions, such as the adoption of *one and the same* pair of Faddeev–Popov's ghost fields for all the involved fields, or the hypothesized full *BRS invariance* of the background parametrized Lagrangian, or, also, the naive computation of the cancellations occurring in *customary* Feynman's diagrammatic expansion in the effective Lagrangian. In the present proof, on the contrary, we assumed to prove the equivalence of the scattering matrix from the very beginning definition of it, namely as a formal functional operator. Concerning the general, classical BRS invariance of the model theory considered here, we raised our perplexities on its supposed validity by computing it in the Appendix. The bare Yang–Mills gauge theory is also plagued, as is well known, by the most important renormalization problem of the infrared divergencies. This problem would limit the present scattering matrix definition to a mere formal, mathematical construct. On the other hand, such a problem does not seems to afflict the present equivalence proof more heavily than it does for the others, preexisting, equivalence demonstrations. This means, hence, that one will have to consider the true physical theory, that underlying the mathematical model dealt with here, simply as the infrared cutoff regularized version of this last. On a compact manifold, moreover, these problems frequently disappear. In general, however, we think that the need to cut off the intrinsic divergencies and the physical equivalence of the scattering theory could likely be considered as two separate and noninteracting problems. This will hold, at least in our effective action approximate formulation, but we are planning to investigate this problem further, as well as to check on the other, existing equivalence proofs.

APPENDIX: BRS TRANSFORMATION OF THE EFFECTIVE ACTION

We point out that in the proof presented here we have never used the global BRS symmetry of the background gauge field effective action, supposedly for it to be valid, for the gauge (b) invariant version of it. The reason for our choice lies in a trivial computation, as we show here, which, however, suggested us to avoid to apply BRS symmetry to S_{eff}, unless it shall be proved more carefully.

It is seen, in fact, that the exact Yang–Mills effective action of the background field method *does not result BRS invariant*, but, rather, such a property will hold only under very particular assumptions. By postulating, indeed, some ''ad hoc'' transformation properties for the source current $J^i[\varphi(x)]$, BRS invariance could, nevertheless, be recovered.

The functional to be varied, in accordance with the BRS transformation rules, is written as

$$\exp-\widetilde{W}[J,\varphi]=(\det\ \hat{\eta})^{-1/2}\int\ [DA\ Dc\ D\overline{c}]\exp\Bigg\{-\Bigg(S_0[A]+\frac{1}{2\alpha}\int d^4x\ \eta^{ab}[F^i_a[\varphi](A_i-\varphi_i)$$

$$\times F^j_b[\varphi](A_j-\varphi_j)+F'^{\,i}_a\varphi_i F'^{\,j}_b\varphi_j]+\int d^4x\ \eta^{ad}[\overline{c}_a F^i_d[\varphi]D_{ib}[A]c^b$$

$$+\overline{c}_a F'^{\,i}_d D_{ib}[\varphi]c^b]+\mathscr{S}..\mathscr{T}.\Bigg)\Bigg\}, \tag{A1}$$

where, in observation to the customary assumptions, the source terms of it, named the $\mathscr{S}..\mathscr{T}.$ term, will not intervene in the computation of the BRS variation of $\widetilde{W}$. Then we write such a variation,

$$\delta_{\mathrm{BRS}}\exp-\widetilde{W}[J,\varphi]=(\det\ \hat{\eta})^{-1/2}\int[\delta_{\mathrm{BRS}}(DA\ Dc\ D\overline{c})]e^{-(S_{\mathrm{eff}}+\mathscr{J}\cdot\mathscr{F}\cdot)}$$
$$-(\det\ \hat{\eta})^{-1/2}\int[DA\ Dc\ D\overline{c}](\delta_{\mathrm{BRS}}S_{\mathrm{eff}})e^{-(S_{\mathrm{eff}}+\mathscr{J}\cdot\mathscr{F}\cdot)}$$
$$=-(\det\ \hat{\eta})^{-1/2}\int[DA\ Dc\ D\overline{c}](\delta_{\mathrm{BRS}}S_{\mathrm{eff}})e^{-(S_{\mathrm{eff}}+\mathscr{J}\cdot\mathscr{F}\cdot)},\tag{A2}$$

due to the invariance of the integration measure. In order to calculate $(\delta_{\mathrm{BRS}}S_{\mathrm{eff}})$ we recall the transformations

$$\delta A^a_\mu\equiv-D^{ab}_\mu[A]c^b\ \delta\lambda=-(\partial_\mu\delta^{ab}-gf^{acb}A_{\mu c})c_b\delta\lambda,\tag{A3}$$

$$\delta c^a\equiv-\tfrac{1}{2}\,gf^{abc}c_bc_c\ \delta\lambda,\tag{A4}$$

$$\delta\overline{c^a}\equiv-\frac{1}{\alpha}\,F^{ab}_\mu[\varphi](A-\varphi)_{\mu b}\ \delta\lambda;\tag{A5}$$

and, in addition to these, we have the positions

$$\delta S_0[A]\equiv0,\tag{A6}$$

$$\delta F'_{\ \mu}{}^{dc}\equiv0,\tag{A7}$$

$$\delta F_{\mu}{}^{ac}[\varphi]\equiv\xi_{\mu}{}^{ac}\ \delta\lambda.\tag{A8}$$

Note that one must assume that $F[\varphi]$ itself, being an operator depending on the background field φ, will undergo some kind of transformation in passing through the critical value $\varphi=\hat{A}$, when the φ field is itself a dynamical variable. If the gauge fixing operator is linear in the φ and A variables, as is generally the case, the BRS variation of $F[\varphi]$ will be proportional to the BRS variation of this field, hence to $D^{ab}_\mu c^b$. In this way the result of the action of ξ^{ac}_μ on the $A_{\mu c}$ field shall be intended, then, as the writing $\sim D^{ac}_\mu c_c\ \delta\lambda$.

The BRS transformation of our effective action thus gives

$$\delta_{\mathrm{BRS}}S_{\mathrm{eff}}=\frac{1}{2\alpha}\ \eta^{ab}2(\delta F^{ac}_\mu)(A-\varphi)^c_\mu F^{bd}_\nu(A-\varphi)^d_\nu+\frac{1}{2\alpha}\ \eta^{ab}2F^{ac}_\mu(\delta A^c_\mu)F^{bd}_\nu(A-\varphi)^d_\nu+\eta^{ad}(\delta\overline{c^a})$$
$$\times(FD)_{db}c^b+\eta^{ad}\overline{c^a}(\delta F^{dc}_\mu)D^{cb}_\mu c_b+\eta^{ad}\overline{c^a}F^{dc}_\mu(\delta D^{cb}_\mu)c_b+\eta^{ad}\overline{c^a}(FD)_{db}(\delta c^b)$$
$$+\eta^{ad}(\delta\overline{c^a})(FD)_{db}c^b+\eta^{ad}\overline{c^a}(\delta F')^{dc}_\mu D^{cb}_\mu c_b+\eta^{ad}\overline{c^a}(F'D)_{db}(\delta c^b)$$
$$=\frac{1}{\alpha}\ \eta^{ab}(\xi^{ac}_\mu(A-\varphi)^c_\mu\ \delta\lambda\ F^{bd}_\nu(A-\varphi)^d_\nu+F^{ac}_\mu(-D^{cb}_\mu[A]c^b\ \delta\lambda)F^{bd}_\nu(A-\varphi)^d_\nu)$$
$$+\eta^{ad}\Big\{-\frac{1}{\alpha}\,F^{ae}_\mu(A-\varphi)^e_\mu\ \delta\lambda(FD)_{db}c^b+\overline{c^a}(\xi^{dc}_\mu\ \delta\lambda\ D_\mu[A]^{cb})c_b$$
$$+\overline{c^a}F^{dc}_\mu(-gf^{ceb}(\delta A^e_\mu))c_b+\overline{c^a}(FD)_{db}\Big[-\frac{1}{2}\,gf^{bef}c_ec_f\ \delta\lambda\Big]+\Big(-\frac{1}{\alpha}\,F^{ae}_\mu(A-\varphi)^e_\mu\ \delta\lambda\Big)$$
$$\times(F'D)_{db}c^b+\overline{c^a}(F'D)_{db}(-\tfrac{1}{2}\,gf^{bef}c_ec_f\ \delta\lambda)$$

$$= \eta^{ad}\Bigg\{ \frac{1}{\alpha}\,(\xi_\mu^{ac}(A-\varphi)_\mu^c)(F_\nu^{db}(A-\varphi)_\nu^b)\,\delta\lambda - \frac{1}{\alpha}\,(F_\mu^{ac}D_\mu^{ce}[A]c_e)(F_\nu^{db}(A-\varphi)_\nu^b)$$

$$+ \frac{1}{\alpha}\,(F_\mu^{ac}(A-\varphi)_\mu^c)(F_\nu^{db}D_\nu^{eb}[A]c_b)\,\delta\lambda + \overline{c^a}\xi_\mu^{dc}D_\mu^{cb}[A]\delta\lambda\ c_b - \overline{c^a}gf^{ceb}(F_\mu^{dc}D_\mu^{eg}[A]c_g)$$

$$\cdot\,\delta\lambda - \frac{1}{2}\,g\overline{c^a}(FD)_{db}f^{bef}c_ec_f\ \delta\lambda + \frac{1}{\alpha}\,(F_\mu^{ae}(A-\varphi)_\mu^e)(F'D[\varphi])_{db}c^b\ \delta\lambda$$

$$- \frac{1}{2}\,g\overline{c^a}(F'D[\varphi])_{db}f^{bef}c_ec_f\ \delta\lambda\Bigg\}$$

(after interchanging the μ and ν indices in the third term)

$$= \eta^{ad}\Bigg\{ \frac{1}{\alpha}\,[F_\nu^{db}(A-\varphi)_\nu^b\xi_\mu^{ac}(A-\varphi)_\mu^c + F_\nu^{de}(A-\varphi)_\nu^e(F'D[\varphi])_{ab}c^b]$$

$$- \frac{1}{\alpha}\,[F_\nu^{db}(A-\varphi)_\nu^bF_\mu^{ac}D_\mu^{ce}[A]c_e - F_\nu^{dc}(A-\varphi)_\nu^cF_\mu^{ae}D_\mu^{eb}[A]c_b] - \overline{c^a}[\xi_\mu^{dc}D_\mu^{cb}[A]c_b$$

$$+ gf^{ceb}F_\mu^{dc}D_\mu^{ef}c_fc_b + \tfrac{1}{2}\,g(FD)_{db}f^{bef}c_ec_f + \tfrac{1}{2}\,g(F'D[\varphi])_{db}f^{bef}c_ec_f]\Bigg\}\,\delta\lambda$$

$$= \eta^{ad}\Bigg\{ \frac{1}{\alpha}\,F_\nu^{db}(A-\varphi)_\nu^b[\xi_\mu^{ae}(A-\varphi)_\mu^c + F'^{ae}_\mu D_{\mu eb}[A]c^b] - \overline{c^a}[\xi_\mu^{dc}D_\mu^{cb}[A]c_b + gf^{ceb}F_\mu^{dc}D_\mu^{ef}[A]c_fc_b$$

$$+ \tfrac{1}{2}\,gf^{ceb}(FD)_{dc}c_ec_b + \tfrac{1}{2}\,gf^{ceb}(F'D[\varphi])_{dc}c_ec_b]\Bigg\}\,\delta\lambda$$

$$= \eta^{ad}\Bigg\{ \frac{1}{\alpha}\,F_\nu^{db}(A-\varphi)_\nu^b[\xi_\mu^{ac}(A-\varphi)_\mu^c + F'^{ac}_\mu(D_\mu^{ce}[A]c_e)] - \overline{c^a}(\xi_\mu^{dc}D_\mu^{cb}[A])c_b$$

$$- gF_\mu^{*df}\overline{c_a}[f^{feb}D_\mu^{ec}c_cc_b + \tfrac{1}{2}\,f^{ceb}D_\mu^{fc}c_ec_b] - \tfrac{1}{2}\,gF'^{*df}_\mu\overline{c^a}f^{ceb}D_\mu^{fc}c_ec_b\Bigg\}\,\delta\lambda$$

(by the properties of the f^{ceb} tensor, the fourth and fifth term mutually annihilate)

$$= \eta^{ad}\Bigg\{ \frac{1}{\alpha}\,F_\nu^{db}(A-\varphi)_\nu^b[\xi_\mu^{ac}(A-\varphi)_\mu^c + F'^{ac}_\mu D_\mu^{ce}c_e] - \overline{c^a}\xi_\mu^{dc}D_\mu^{cb}c_b$$

$$- \frac{1}{2}\,gF'^{*dc}_\mu\overline{c^a}f^{feb}D_\mu^{fc}c_ec_b\Bigg\}\,\delta\lambda, \tag{A9}$$

where F'^{*}_μ is the operator Hermitian conjugate to F'_μ. Finally, by writing explicitly the formal ξ_μ operator as

$$\xi_\mu^{dc} \sim gf^{dce}D_\mu^{ef}c_f\ \delta\lambda, \tag{A10}$$

which is undetermined only by a multiplicative constant, we see that the second term vanishes,

$$\xi_\mu^{dc}D_\mu^{cb}[A]c_b \sim gf^{dce}D_\mu^{ef}c_f\ \delta\lambda\ D_\mu^{cb}c_b = 0, \tag{A11}$$

as a consequence of the antisymmetry of f^{dce}. The final conclusion will thus be resumed as

$$\left\{\frac{\delta_{\mathrm{BRS}}S_{\mathrm{eff}}}{\delta\lambda}\right\}=\eta^{ad}\left\{F'^{*dc}_{\mu}\cdot\left[\overline{c^a}f^{feb}D^{fc}_{\mu}c_e c_b+\frac{1}{\alpha}F^{ab}_{\nu}(A-\varphi)^{h}_{\nu}D^{ce}_{\mu}c_e\right]\right.$$
$$\left.+\frac{1}{\alpha}\xi^{*dc}_{\mu}F^{ab}_{\nu}(A-\varphi)^{b}_{\nu}(A-\varphi)^{c}_{\mu}]\right\}. \tag{A12}$$

This result, as we previously announced, clearly indicates that the presence of the background field φ, unless other peculiar assumptions concerning $\mathscr{S}\ldots\mathscr{T}$., induces a non-complete invariance of the effective action $\widetilde{W}[J,\varphi]$ introduced above.

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Transient waves in nonstationary media

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This paper treats propagation of transient waves in nonstationary media, which has many applications in, for example, electromagnetics and acoustics. The underlying hyperbolic equation is a general, homogeneous, linear, first-order 2×2 system of equations. The coefficients in this system depend on one spatial coordinate and time. Furthermore, memory effects are modeled by integral kernels, which, in addition to the spatial dependence, are functions of two different time coordinates. These integrals generalize the convolution integrals, frequently used as a model for memory effects in the medium. Specifically, the scattering problem for this system of equations is addressed. This problem is solved by a generalization of the wave splitting concept, originally developed for wave propagation in media which are invariant under time translations, and by an imbedding or a Green's functions technique. More explicitly, the imbedding equation for the reflection kernel and the Green's functions (propagator kernels) equations are derived. Special attention is paid to the problem of nonstationary characteristics. A few numerical examples illustrate this problem. © *1996 American Institute of Physics.* [S0022-2488(96)00104-8]

I. INTRODUCTION AND BASIC SYSTEM OF EQUATIONS

In a recent paper,[1] a new method of analyzing wave propagation in nonstationary or time-varying media was suggested. This method is an extension of the well-established methods of wave splitting, invariant imbedding, and Green's functions techniques (see Refs. 2–8). Wave propagation in nonstationary media has also been investigated with other methods (see, e.g., Refs. 9–11).

Nonstationary media are characterized by material parameters that are changing with time. Relevant examples are found in, e.g., telecommunication problems, such as fading and modulation problems, and in problems concerning moving media. The analysis of the wave propagation phenomena in linear, nonstationary media also serves as an indispensable tool for analyzing wave propagation in nonlinear media by means of linearization.

The investigation of wave propagation problems in nonstationary media leads to hyperbolic partial differential equations (PDE) with coefficients varying both in time and space. The purpose of this paper is to systematically investigate the wave propagation problem in a general nonstationary medium. This paper presents the theory of the techniques; subsequent papers will develop numerical solutions to pertinent problems.

Investigations of wave propagation, some of which are mentioned in Sec. II, suggest a generalized form of the dynamics of the wave fields. In the present work, the parameters of the medium are assumed to vary in one spatial direction, here taken to the z-direction, and time t. The basic equation is the following first-order 2×2 system of equations:

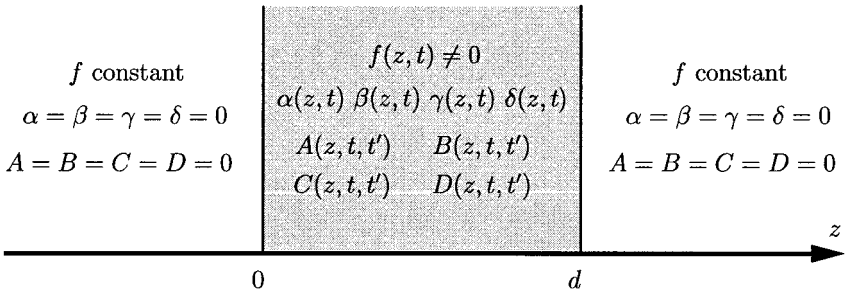

FIG. 1. Geometry of the problem.

$$\frac{\partial}{\partial z}\begin{pmatrix} u^+(z,t) \\ u^-(z,t)\end{pmatrix} = f(z,t)\begin{pmatrix} -1 & 0 \\ 0 & 1\end{pmatrix}\frac{\partial}{\partial t}\begin{pmatrix} u^+(z,t) \\ u^-(z,t)\end{pmatrix} + \begin{pmatrix} \alpha(z,t) & \beta(z,t) \\ \gamma(z,t) & \delta(z,t)\end{pmatrix}\begin{pmatrix} u^+(z,t) \\ u^-(z,t)\end{pmatrix} + \int_{-\infty}^{t}\begin{pmatrix} A(z,t,t') & B(z,t,t') \\ C(z,t,t') & D(z,t,t')\end{pmatrix}\begin{pmatrix} u^+(z,t') \\ u^-(z,t')\end{pmatrix} dt'. \tag{1}$$

The reason for the $\pm$ superscript is described in the subsequent sections. The slowness function $f(z,t)$ is a notation for

$$f(z,t) = \frac{1}{c(z,t)} > 0,$$

where $c(z,t)$ is the wave (phase) velocity. In order to model also nonstationary memory effects, integral terms have been included in the equation. These memory effects are nonlocal in time. In the integrals, the variable t describes the current time, whereas the variable t' is an integral measure, relating to the starting time of the excitation (see also Appendix B). The system (1) is a strictly hyperbolic system.

The positive function $f(z,t)$ is a continuous, bounded function of the variables z and t everywhere. Furthermore, it is assumed to be constant outside the slab $(0,d)$

$$f(z,t) = 1/c_0, \quad z<0, \quad f(z,t) = 1/c_d, \quad z>d, \tag{2}$$

and continuously differentiable, with bounded derivatives, in z and t everywhere inside the slab, i.e., $(z,t) \in (0,d)\times(-\infty,\infty)$ (see also Fig. 1). This implies that $f(0,t) = 1/c_0$ and $f(d,t) = 1/c_d$ for all times t.

The functions $\alpha(z,t)$, $\beta(z,t)$, $\gamma(z,t)$, and $\delta(z,t)$ are equal to zero outside the slab and they are continuous, bounded functions inside the slab (not necessarily continuous at the edges of the slab).

The functions $A(z,t,t')$, $B(z,t,t')$, $C(z,t,t')$, and $D(z,t,t')$ are always zero outside of the slab $(0,d)$. Due to causality, they vanish identically inside the slab provided $t<t'$. For simplicity, the functions $A(z,t,t')$, $B(z,t,t')$, $C(z,t,t')$, and $D(z,t,t')$ are assumed continuous and bounded as functions of the variables z, t, and t' in the region $t>t'$, $0<z<d$.

The assumptions described above can, of course, be relaxed, and the results presented in this paper then hold for a larger class of parameters. However, the purpose of this paper is not to formulate the results for the weakest set of assumptions possible, but to exploit the potential of the method for a set of physically reasonable assumptions.

In the scattering application addressed in this paper, the incident wave is assumed to impinge normally on a slab. Two different scattering problems can be identified. In the direct scattering

problem, the material parameters are known and the goal is to calculate the response of a known incoming field. On the other hand, the inverse problem assumes knowledge of the incident and the scattered field (data collected exterior to the medium) and the problem is to infer information about the material parameters. Both these problems can be investigated by the methods presented in this paper. However, the main pertinence of the method is in connection with applications to the direct scattering problem. Some aspects of the nonstationary inverse scattering problem were analyzed in Ref. 1.

After this introductory section, a few explicit examples of applications are given in Sec. II. The analysis of the nonstationary characteristic curves is found in Sec. III. The imbedding equation for the reflection kernel is derived in Sec. IV, and the Green's functions (propagator kernels) equations are derived in Sec. V. Some explicit simplifications and concluding remarks are given in Secs. VI and VII, respectively. Three appendices contain some technical mathematical details and some numerical illustrations of characteristic traces.

II. EXAMPLES

This section contains a few examples of general interest to the formulation presented in this paper. The underlying equations of the fields in all these examples are the Maxwell equations:

$$\nabla\times\mathbf{E}(\mathbf{r},t)=-\frac{\partial\mathbf{B}}{\partial t}(\mathbf{r},t),\quad \nabla\times\mathbf{H}(\mathbf{r},t)=\frac{\partial\mathbf{D}}{\partial t}(\mathbf{r},t).$$

Here, $\mathbf{E}(\mathbf{r},t)$ and $\mathbf{H}(\mathbf{r},t)$ are the electric and the magnetic fields, respectively, $\mathbf{B}(\mathbf{r},t)$ is the magnetic induction, and $\mathbf{D}(\mathbf{r},t)$ is the electric displacement field. All fields are assumed to be quiescent before a fixed time. This property guarantees that all fields vanish at $t\to-\infty$.

A. Electromagnetic waves in inhomogeneous and dispersive media

To model wave propagation in a nonstationary, inhomogeneous, and dispersive medium, the following constitutive relations are relevant:[1]

$$\mathbf{D}(\mathbf{r},t)=\epsilon_0\left(\epsilon(z)\mathbf{E}(\mathbf{r},t)+\int_{-\infty}^{t}\chi_e(z,t,t')\mathbf{E}(\mathbf{r},t')dt'\right),$$

$$\mathbf{B}(\mathbf{r},t)=\mu_0\mathbf{H}(\mathbf{r},t).$$

Here $\epsilon_0\epsilon(z)>0$ is the permittivity of the medium, and μ_0 is the permeability of vacuum. The nonstationary dispersive effects are modeled by the susceptibility kernel $\chi_e(z,t,t')$.

The vector wave propagation problem is reduced to a scalar problem by assuming that the electric field is transverse to the stratification of the medium, and, furthermore, depends only on the coordinates (z,t). The dynamics of the fields is cast into the form of (1) by the following nonunique wave splitting:[4]

$$\begin{pmatrix}u^+(z,t)\\ u^-(z,t)\end{pmatrix}=\frac{1}{2}\begin{pmatrix}1 & -\dfrac{c_0}{\sqrt{\epsilon(z)}}\,\partial_t^{-1}\\ 1 & \dfrac{c_0}{\sqrt{\epsilon(z)}}\,\partial_t^{-1}\end{pmatrix}\begin{pmatrix}E(z,t)\\ \partial_z E(z,t)\end{pmatrix},$$

where the antiderivative ∂_t^{-1} is defined as

$$\partial_t^{-1}g(t)=\int_{-\infty}^{t}g(t')dt'.$$

The coefficients of the dynamics, (1), in this example are

$$f(z,t)=\sqrt{\epsilon(z)}/c_0,$$

$$\alpha(z,t)=-\gamma(z,t)=-\frac{1}{4}\frac{d}{dz}\ln\epsilon(z)-\frac{1}{2c_0\sqrt{\epsilon(z)}}\chi_e(z,t,t')\Big|_{t'=t},$$

$$\beta(z,t)=-\delta(z,t)=\frac{1}{4}\frac{d}{dz}\ln\epsilon(z)-\frac{1}{2c_0\sqrt{\epsilon(z)}}\chi_e(z,t,t')\Big|_{t'=t},$$

$$A(z,t,t')=B(z,t,t')=-C(z,t,t')=-D(z,t,t')=-\frac{1}{2c_0\sqrt{\epsilon(z)}}\frac{\partial\chi_e}{\partial t}(z,t,t').$$

Note that the regularity assumptions made on the susceptibility kernel $\chi_e(z,t,t')$ in Ref. 1 [continuously differentiable in $z\in(0,L)$ and t', and twice continuously differentiable in t, $t\geqslant t'$] are stronger than needed to meet the assumptions made on the functions $A(z,t,t')$, $B(z,t,t')$, $C(z,t,t')$, and $D(z,t,t')$ in Sec. I, and are not needed if the splitting is made from Maxwell's equations directly (see Sec. II C).

B. A generalized wave equation

An obvious extension of the results presented in Ref. 1 concerning propagation of electromagnetic waves in inhomogeneous and time-varying media is to allow the permittivity $\epsilon_0\epsilon$ to vary in time as well as in space. The relevant constitutive relations in this example are

$$\mathbf{D}(\mathbf{r},t)=\epsilon_0\epsilon(z,t)\mathbf{E}(\mathbf{r},t),\quad \mathbf{B}(\mathbf{r},t)=\mu_0\mathbf{H}(\mathbf{r},t),$$

where the relative permittivity $\epsilon(z,t)>0$. This is a model of an inhomogeneous, nondispersive, nonstationary medium. For the sake of simplicity, the dispersive memory terms in Sec. II A are omitted. However, the more complex model, where these memory terms are included, is straightforward to analyze.

With the usual assumption of an electric field **E** that is transverse to the z-axis and that depends on z and t only, the wave equation is

$$\frac{\partial^2 E}{\partial z^2}(z,t)-\frac{\partial^2(f^2E)}{\partial t^2}(z,t)=0, \tag{3}$$

where

$$f(z,t)=\sqrt{\mu_0\epsilon_0\epsilon(z,t)}.$$

This equation is a special case of a more generalized wave equation

$$\frac{\partial^2 u}{\partial z^2}(z,t)-\frac{\partial^2(f^2u)}{\partial t^2}(z,t)+\mathscr{A}(z,t)\frac{\partial u}{\partial z}(z,t)+\mathscr{B}(z,t)\frac{\partial u}{\partial t}(z,t)+\mathscr{C}(z,t)u(z,t)=0, \tag{4}$$

which also has applications in, e.g., linear acoustics in media where the propagation conditions change rapidly with time.

In order to see how Eq. (4) is related to the general hyperbolic wave equation (1), the concept of wave splitting is introduced. The wave splitting can be defined in several different ways. The

definition adopted here renders a very simple $u^{\pm}$-dynamics for the wave equation in (3). Thus, proceeding formally, the wave splitting is defined by the following transformation of the dependent variables:

$$\begin{pmatrix} u^{+}(z,t) \\ u^{-}(z,t) \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & -\dfrac{1}{f(z,t)}\,\partial_t^{-1} \\ 1 & \dfrac{1}{f(z,t)}\,\partial_t^{-1} \end{pmatrix} \begin{pmatrix} u(z,t) \\ u_z(z,t) \end{pmatrix},$$

which generalizes the wave splitting introduced in Ref. 4. The new fields $u^{\pm}(z,t)$ satisfy a first-order 2×2 system of hyperbolic partial differential equations, which is identical to the generalized $u^{\pm}$-dynamics in (1). The explicit expressions of the coefficients are

$$\alpha(z,t) = -\frac{1}{2}\frac{\partial}{\partial z}\ln f(z,t) - \frac{3}{2}\frac{\partial f}{\partial t}(z,t) - \frac{1}{2}\mathscr{A}(z,t) + \frac{1}{2}\frac{\mathscr{B}(z,t)}{f(z,t)},$$

$$\beta(z,t) = +\frac{1}{2}\frac{\partial}{\partial z}\ln f(z,t) - \frac{1}{2}\frac{\partial f}{\partial t}(z,t) + \frac{1}{2}\mathscr{A}(z,t) + \frac{1}{2}\frac{\mathscr{B}(z,t)}{f(z,t)},$$

$$\gamma(z,t) = +\frac{1}{2}\frac{\partial}{\partial z}\ln f(z,t) + \frac{1}{2}\frac{\partial f}{\partial t}(z,t) + \frac{1}{2}\mathscr{A}(z,t) - \frac{1}{2}\frac{\mathscr{B}(z,t)}{f(z,t)},$$

$$\delta(z,t) = -\frac{1}{2}\frac{\partial}{\partial z}\ln f(z,t) + \frac{3}{2}\frac{\partial f}{\partial t}(z,t) - \frac{1}{2}\mathscr{A}(z,t) - \frac{1}{2}\frac{\mathscr{B}(z,t)}{f(z,t)},$$

and

$$A(z,t,t') = \frac{1}{2}\frac{1}{f(z,t)}\left[f(z,t')\frac{\partial \mathscr{A}}{\partial t'}(z,t') - \frac{\partial \mathscr{B}}{\partial t'}(z,t') + \mathscr{C}(z,t') \right],$$

$$B(z,t,t') = \frac{1}{2}\frac{1}{f(z,t)}\left[-f(z,t')\frac{\partial \mathscr{A}}{\partial t'}(z,t') - \frac{\partial \mathscr{B}}{\partial t'}(z,t') + \mathscr{C}(z,t') \right],$$

$$C(z,t,t') = -A(z,t,t'),$$

$$D(z,t,t') = -B(z,t,t').$$

C. Wave propagation on the transmission line

In this example, propagation of current-voltage waves on a transmission line is considered. The material of the transmission line, i.e., the conductors together with the insulation, may vary in time as well as in space. In this model, memory effects are permitted.

The equivalent circuit segment model of Fig. 2 provides the basis of the derivation of the general transmission line equations. Here, $R(z,t)$ and $G(z,t)$ are the series resistance and the shunt conductance per unit length of the transmission line, respectively. The series inductance and the shunt capacitance per unit length, which are denoted $L(z,t)$ and $C(z,t)$, respectively, are both assumed positive and finite. The voltage $v(z,t)$ and the current $i(z,t)$ are related, respectively, to the magnetic flux $\Phi(z,t)$ and the charge $q(z,t)$ through

$$\Phi(z,t) = L(z,t)i(z,t) + \int_{-\infty}^{t} \chi_m(z,t,t')i(z,t')dt',$$

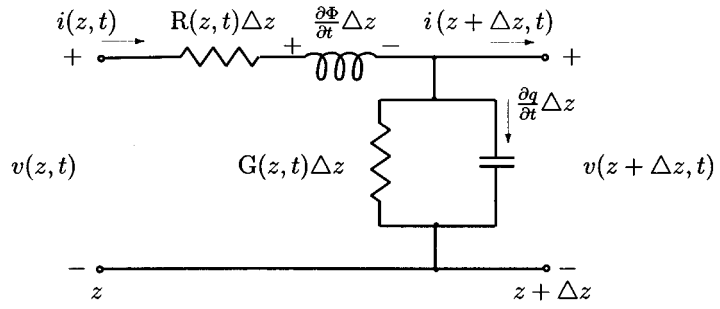

FIG. 2. Transmission line model.

$$q(z,t)=C(z,t)v(z,t)+\int_{-\infty}^{t}\chi_e(z,t,t')v(z,t')dt'.$$

The magnetic flux, $\Phi(z,t)$, and the electric charge, $q(z,t)$, depend on the current $i(z,t)$ and the voltage $v(z,t)$ at time t, respectively. In addition to these multiplicative terms, Φ and q are connected to the previous values of the currents and voltages of the transmission line. The memory functions are modeled by the two integral terms with the kernel functions $\chi_m(z,t,t')$ describing the inductive susceptibility and $\chi_e(z,t,t')$ modeling the capacitive susceptibility. Simplifications occur in a material that is invariant under time translations. In this case, the susceptibility kernels are functions of the difference argument $t-t'$ rather than of t and t'. A comparison between the pertinent parameter symbols used in this transmission line application and the material properties of Sec. II A is found in Table I.

The Kirchhoff current and voltage relations are now applied to the circuit mesh of Fig. 2. In the limit $\Delta z\to 0$, the two general transmission line equations are obtained. They are represented in the following matrix form:

$$\begin{pmatrix} 0 & C(z,t) \\ L(z,t) & 0 \end{pmatrix}\frac{\partial}{\partial t}\begin{pmatrix} i(z,t) \\ v(z,t) \end{pmatrix}+\frac{\partial}{\partial z}\begin{pmatrix} i(z,t) \\ v(z,t) \end{pmatrix}=B\begin{pmatrix} i(z,t) \\ v(z,t) \end{pmatrix}, \tag{5}$$

TABLE I. Correspondence between the parameter symbols used and the material properties relevant in the two main applicable problems.

Transmission line		Maxwell's equations	
Parameter	Symbol	Parameter	Symbol
Inductance	$L(z,t)$	Magnetic permeability	$\mu(z,t)$
Capacitance	$C(z,t)$	Electric permittivity	$\epsilon(z,t)$
Series resistance	$R(z,t)$	Magnetic conductivity	$\sigma_m(z,t)$
Shunt resistance	$G(z,t)$	Electric conductivity	$\sigma_e(z,t)$
Inductive susceptibility	$\chi_m(z,t,t')$	Magnetic susceptibility	$\chi_m(z,t,t')$
Capacitive susceptibility	$\chi_e(z,t,t')$	Electric susceptibility	$\chi_e(z,t,t')$

where the operator matrix B is given by

$$B=\begin{pmatrix} 0 & -G(z,t)-\dfrac{\partial C}{\partial t}(z,t)-\dfrac{\partial}{\partial t}\displaystyle\int_{-\infty}^{t}\chi_e(z,t,t')\bullet\, dt' \\ -R(z,t)-\dfrac{\partial L}{\partial t}(z,t)-\dfrac{\partial}{\partial t}\displaystyle\int_{-\infty}^{t}\chi_m(z,t,t')\bullet\, dt' & 0 \end{pmatrix},$$

where the symbol $\bullet$ denotes the place holder for the operand.

This system of equations is easily transformed into the general first-order 2×2 system of hyperbolic equations, (1). The following wave splitting diagonalizes the system (5):

$$\begin{pmatrix} u^+(z,t) \\ u^-(z,t) \end{pmatrix}=\frac{1}{2}\begin{pmatrix} 1 & \sqrt{\dfrac{C(z,t)}{L(z,t)}} \\ 1 & -\sqrt{\dfrac{C(z,t)}{L(z,t)}} \end{pmatrix}\begin{pmatrix} i(z,t) \\ v(z,t) \end{pmatrix}. \tag{6}$$

The explicit expressions of the coefficients are

$$\begin{aligned} f(z,t)&=\sqrt{L(z,t)C(z,t)}, \\ \alpha(z,t)&=\tfrac{1}{2}[+h_1(z,t)+h_2(z,t)-h_3(z,t)-h_4(z,t)], \\ \beta(z,t)&=\tfrac{1}{2}[-h_1(z,t)-h_2(z,t)+h_3(z,t)-h_4(z,t)], \\ \gamma(z,t)&=\tfrac{1}{2}[+h_1(z,t)-h_2(z,t)-h_3(z,t)+h_4(z,t)], \\ \delta(z,t)&=\tfrac{1}{2}[-h_1(z,t)+h_2(z,t)+h_3(z,t)+h_4(z,t)], \end{aligned} \tag{7}$$

and

$$\begin{aligned} A(z,t,t')&=-\frac{1}{2}\left[\frac{\partial\chi_e}{\partial t}(z,t,t')\sqrt{\frac{\mathrm{L}(z,t')}{\mathrm{C}(z,t')}}+\sqrt{\frac{\mathrm{C}(z,t)}{\mathrm{L}(z,t)}}\frac{\partial\chi_m}{\partial t}(z,t,t')\right], \\ B(z,t,t')&=\frac{1}{2}\left[\frac{\partial\chi_e}{\partial t}(z,t,t')\sqrt{\frac{\mathrm{L}(z,t')}{\mathrm{C}(z,t')}}-\sqrt{\frac{\mathrm{C}(z,t)}{\mathrm{L}(z,t)}}\frac{\partial\chi_m}{\partial t}(z,t,t')\right], \\ C(z,t,t')&=-B(z,t,t'),\quad D(z,t,t')=-A(z,t,t'), \end{aligned} \tag{8}$$

where the functions $h_1(z,t)$, $h_2(z,t)$, $h_3(z,t)$, and $h_4(z,t)$ are given by

$$h_1(z,t)=\frac{1}{2}\sqrt{\mathrm{L}(z,t)\mathrm{C}(z,t)}\,\frac{\partial}{\partial t}\ln\frac{\mathrm{C}(z,t)}{\mathrm{L}(z,t)},$$

$$h_2(z,t)=\frac{1}{2}\frac{\partial}{\partial z}\ln\frac{\mathrm{C}(z,t)}{\mathrm{L}(z,t)},$$

$$h_3(z,t)=\sqrt{\frac{\mathrm{L}(z,t)}{\mathrm{C}(z,t)}}\left[\mathrm{G}(z,t)+\frac{\partial\mathrm{C}}{\partial t}(z,t)+\chi_e(z,t,t')\big|_{t'=t}\right],$$

$$h_4(z,t)=\sqrt{\frac{\mathrm{C}(z,t)}{\mathrm{L}(z,t)}}\left[\mathrm{R}(z,t)+\frac{\partial L}{\partial t}(z,t)+\chi_m(z,t,t')\big|_{t'=t}\right].$$

The regularity requirements of the coefficients stated in Sec. I are met if $R(z,t)$ and $G(z,t)$ are continuous functions, and $C(z,t)$ and $L(z,t)$ continuously differentiable in both z and t. Moreover, the functions $\chi_e(z,t,t')$ and $\chi_m(z,t,t')$ are assumed continuous in z and t' and continuously differentiable in t.

The next two sections contain the main equations for the solution of the scattering problem in inhomogeneous, nonstationary, dispersive media. Specifically, the imbedding equation and the Green's functions equations are derived.

III. CHARACTERISTIC CURVES

One of the major differences between the treatment of the problems in this paper and earlier work is that the characteristics of Eq. (1) are nonstationary in time. This complicates many of the formulas when compared to those applicable to media which admit time translation symmetries. When the slowness is independent of time but the dynamics is nonstationary, there is still a lack of invariance under time translation due to lower-order terms. In this case some simplifications can be made. This is evidenced by comparing the imbedding equation (15) of Sec. IV, the Green's functions equations (21) and (22) of Sec. V, and equations (4.3), (5.2), and (5.3) of Ref. 1.

In Ref. 1, as the slowness was *not* a function of time, it was quite easy to make a transformation into travel time coordinates to straighten the characteristic curves. In the more general situation considered here, such a transformation is more difficult to perform and implies that a problem of almost the same complexity as the original problem has to be solved. No transformation to straighten the characteristic curves is therefore made in this paper. Thus, the examination of the properties of the characteristic traces of (1) is appropriate. In Appendix A some of the properties of the transformation to straighten the characteristic curves are outlined.

The characteristic traces for the u^+-equation satisfy

$$\frac{d\tau^+}{d\zeta} = f(\zeta, \tau^+(\zeta)), \tag{9}$$

with an initial condition [the curve passes through the point (z,t)]

$$\tau^+(z) = t. \tag{10}$$

The superscript plus has been used on the characteristic with positive slope; traces with negative slope appear in later sections and will have superscript minus.

The existence of a unique, locally defined, solution of the initial value problem in (9) and (10) is guaranteed by the assumption of f in Sec. I.[12,13] To emphasize the dependence of the initial conditions, the solution is written in the form

$$\tau^+ = \tau^+(\zeta; z, t), \tag{11}$$

where $(\zeta, \tau^+(\zeta;z,t))$ describes a curve in $\mathbb{R}^2$ passing through (z,t) and ζ is a parameter.

Figure 3 shows the system of coordinates (ζ,τ^+). The position of the physical slab coincides with the interval $(0,d)$ of the ζ-axis. The assumptions of the slowness f ensure that a locally defined flow has been defined.[14] Maximal extension of this flow up to any point, at which it becomes undefined, is ensured. This is a property that depends purely on the slowness f. This flow forms a group with respect to the parameter ζ and as such it has a unique inverse and unit element. For the purposes of this paper, the form of the solution formally represented by Eq. (11) suffices. The inverse elements are

$$\tau^+(\zeta; z, \tau^+(z;\zeta,t)) = t, \quad \tau^+(z;\zeta,\tau^+(\zeta;z,t)) = t,$$

and the unit element can be written as

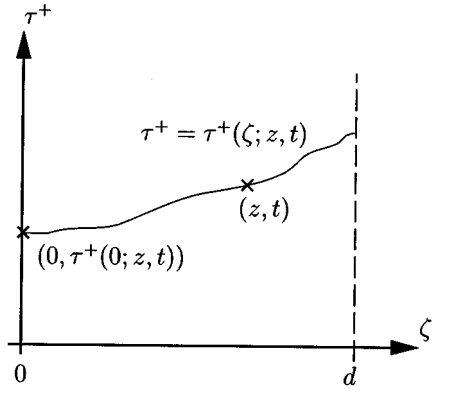

FIG. 3. The characteristic of the u^+-equation.

$$\tau^+(z;z,t)=t.$$

One other formula obtained from elementary calculus that is needed in the sequel is

$$\frac{\partial\tau^+}{\partial t}(\zeta;z,t)\bigg|_{t=\tau^+(z;\zeta,t)}=\left(\frac{\partial\tau^+}{\partial t}(z;\zeta,t)\right)^{-1}$$

or its dual

$$\frac{\partial\tau^+}{\partial t}(z;\zeta,t)\bigg|_{t=\tau^+(\zeta;z,t)}=\left(\frac{\partial\tau^+}{\partial t}(\zeta;z,t)\right)^{-1}.$$

In this paper, of particular importance is the case of $\zeta=0$.

From the presumptions of the function $f(z,t)$ given in Sec. I and from Eq. (9), it is clear that the derivative $d\tau^+/d\zeta$ is a continuous function in ζ. Furthermore, these presumptions also guarantee that the partial derivatives $\partial\tau^+/\partial z$ and $\partial\tau^+/\partial t$ exist.[13]

Also note that if (z,t) is a point on the characteristic curve, so is $(\zeta',\tau^+(\zeta';z,t))$. Thus $\tau^+=\tau^+(\zeta;z,t)$ and $\tau^+=\tau^+(\zeta;\zeta',\tau^+(\zeta',z,t))$ are two equivalent representations of the same characteristic curve.

Integration of Eq. (9) along the characteristic yields an expression for the function τ^+:

$$\tau^+(\zeta_2;z,t)-\tau^+(\zeta_1;z,t)=\int_{\zeta_1}^{\zeta_2}f(\zeta',\tau^+(\zeta';z,t))d\zeta', \tag{12}$$

which specifies the time needed for the u^+-wave to move from position ζ_1 to position ζ_2 along the characteristic passing through (z,t).

An additional relation for the u^+-characteristics, needed for the derivations in Sec. V, is now derived. In (12), let $\zeta_2=\zeta$ and $\zeta_1=z$, and differentiate the equation with respect to z and t. This shows that the function

$$\phi(\zeta;z,t)=\frac{\partial\tau^+}{\partial z}(\zeta;z,t)+f(z,t)\,\frac{\partial\tau^+}{\partial t}(\zeta;z,t)$$

is a solution to the uniquely solvable homogeneous Volterra equation of the second kind,

$$\phi(\zeta;z,t)+\int_{\zeta}^{z}\frac{\partial f}{\partial\tau^{+}}(\zeta',\tau^{+}(\zeta';z,t))\phi(\zeta';z,t)d\zeta'=0,$$

which therefore must only have the trivial solution. Thus, the following identity holds:

$$\frac{\partial\tau^{+}}{\partial z}(\zeta;z,t)+f(z,t)\frac{\partial\tau^{+}}{\partial t}(\zeta;z,t)=0. \tag{13}$$

The interpretation of this conservation equation states the obvious result that as (z,t) varies along one particular characteristic trace, for fixed ζ, τ^{+} is invariant. Another more simple proof of (13) is to use the fact that $\tau^{+}=\tau^{+}(\zeta;z,t)$ and $\tau^{+}=\tau^{+}(\zeta;\zeta',\tau^{+}(\zeta';z,t))$ are two equivalent representations of the same characteristic curve. Differentiation wrt ζ' then gives the identity (13).

Some explicit examples of characteristic curves are found in Appendix C.

IV. IMBEDDING EQUATION

The two split fields, $u^{\pm}(z,t)$, introduced in a previous section, are interrelated. This is because when the wave propagates through a medium in which the properties are changing, the $u^{\pm}$-waves are related through a scattering operator. This operator is represented by a time integral, which can be derived from Duhamel's integral (see Appendix B). The result is

$$u^{-}(z,t)=\int_{-\infty}^{t}R(z,t,t')u^{+}(z,t')dt'. \tag{14}$$

Here, the kernel $R(z,t,t')$, which is the reflection kernel of a subsection (z,d) of the total slab $(0,d)$, is identical to the one used in Ref. 1. By causality, $R(z,t,t')=0$, $t<t'$.

The reflection kernel, $R(z,t,t')$, satisfies a partial differential equation, which describes the variation in $R(z,t,t')$ as the coordinates z, t, and t' vary. This equation, the imbedding equation, is derived by differentiating (14) and using the dynamics (1). This operation yields the imbedding equation for the reflection kernel $R(z,t,t')$, valid in the domain $0<z<d$, $t>t'$:

$$\begin{aligned}
&\frac{\partial R}{\partial z}(z,t,t')-f(z,t)\frac{\partial R}{\partial t}(z,t,t')+\frac{\partial R}{\partial t'}(z,t,t')f(z,t')\\
&\quad=C(z,t,t')+\delta(z,t)R(z,t,t')+R(z,t,t')\left[-\frac{\partial f(z,t')}{\partial t'}-\alpha(z,t')\right]\\
&\qquad-\int_{t'}^{t}R(z,t,t'')\beta(z,t'')R(z,t'',t')dt''-\int_{t'}^{t}R(z,t,t'')A(z,t'',t')dt''\\
&\qquad+\int_{t'}^{t}D(z,t,t'')R(z,t'',t')dt''-\int_{t'}^{t}\left\{\int_{t'}^{t''}R(z,t,t'')B(z,t'',t''')R(z,t''',t')dt'''\right\}dt''.
\end{aligned} \tag{15}$$

The initial condition of the reflection kernel $R(z,t,t')$ is

$$R(z,t,t')|_{t'=t}=-\frac{1}{2}\frac{\gamma(z,t)}{f(z,t)} \tag{16}$$

and the boundary condition at $z=d$, $t>t'$, is

$$R(d,t,t')=0.$$

The Cauchy problem of the imbedding equation, (15), with data specified on the plane parametrized by $\mathbf{r}=(z,t,t)$ [see (16)], is well posed. This is a consequence of the nonvanishing functional determinant (Ref. 15, p. 26)

$$J=\begin{vmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 1 & -f(z,t) & f(z,t) \end{vmatrix} = 2f(z,t)\neq 0.$$

The functional differential equation for the reflection kernel $R(z,t,t')$ can be solved numerically given the material parameters. This implies that the solution to the direct scattering problem, i.e., the determination of the reflected fields, can be computed through (14). The inverse problem, i.e., the determination of the material parameters, given the reflection kernel $R(z,t,t')$, can also be approached through (15). This problem will be addressed in another paper.

A. Discontinuity of the reflection kernel

The solution of the imbedding equation, $R(z,t,t')$, is continuous everywhere except across the surface $t'=h(z,t)$, where $R(z,t,t')$ has a possible jump discontinuity. This finite jump discontinuity is introduced by the possible jump discontinuity in $\gamma(z,t)$ at $z=d$, i.e., if $\gamma(d^-,t)=\lim_{z\to d-0}\gamma(z,t)\neq 0$ [see (16)]. The normal to the surface $t'=h(z,t)$, i.e., $(h_z,h_t,-1)$, satisfies the characteristic equation

$$\frac{\partial h}{\partial z}(z,t)-f(z,t)\frac{\partial h}{\partial t}(z,t)=f(z,h(z,t))$$

and, due to (16), the surface contains the line $\mathbf{r}=(d,t,t)$, i.e., $t=h(d,t)$.

The vector field describing the characteristic traces is $(1,-f(z,t),f(z,t'))$ and it lies on a hyper-surface. The projection of this vector field onto the (z,t)-plane is described by

$$\frac{d\tau^-}{d\zeta}=-f(\zeta,\tau^-(\zeta)) \tag{17}$$

so that this curve, on planes $t'=$constant, has representation $(\zeta,\tau^-(\zeta;z,t),t')$. To emphasize the dependence of the initial conditions, the solution to (17) has been written in the form

$$\tau^-=\tau^-(\zeta;z,t).$$

Similarly, the projection of the vector field onto the (z,t')-plane is described by Eq. (9) and this curve on planes $t=$constant has representation $(\zeta,t,\tau^+(\zeta;z,t'))$. All curves of interest here will originate from the line $\mathbf{r}=(d,t,t)$, so that a characteristic trace, Γ, emanating from this line has parametric form

$$\Gamma:\mathbf{r}(z,t)=(z,\tau^-(z;d,t),\tau^+(z;d,t)).$$

As mentioned previously, the R kernel has a possible initial jump discontinuity on the (d,t,t)-line, in the direction of increasing t, of size

$$[R]_{\Gamma(z=d)}=\frac{1}{2}\frac{\gamma(d,t)}{f(d,t)}. \tag{18}$$

The bracket notation used here denotes the finite jump discontinuity of the reflection kernel R, with respect to positive t-direction. This discontinuity propagates along the characteristic as

$$\left.\frac{d[R]}{dz}\right|_{\Gamma}=\left(\delta(z,\tau^{-}(z;d,t))-\left.\frac{\partial f}{\partial t'}(z,t')\right|_{t'=\tau^{+}(z;d,t)}-\alpha(z,\tau^{+}(z;d,t))\right)[R]_{\Gamma},$$

which upon integrating from d to z, and with use of (18), yields

$$[R]_{\Gamma}=\frac{1}{2}\frac{\gamma(d,t)}{f(d,t)}\exp\left\{\int_{d}^{z}\left(\delta(z',\tau^{-}(z';d,t))-\left.\frac{\partial f}{\partial t'}(z',t')\right|_{t'=\tau^{+}(z';d,t)}-\alpha(z',\tau^{+}(z';d,t))\right)dz'\right\}.$$

V. GREEN'S FUNCTIONS

The relationship between the split fields $u^{\pm}$ in Sec. IV was evaluated at a specific z-value and the reflection kernel $R(z,t,t')$ was interpreted as the reflection kernel for a subslab (z,d) of the physical slab $(0,d)$. This interpretation was performed by the use of an imbedding argument.

In contrast to the analysis presented in the previous section, this section contains an analysis of the relationship between the exterior excitation $u^{+}(0,t)$ and the internal fields $u^{\pm}(z,t)$ of the physical slab $(0,d)$. The operator that maps the excitation $u^{+}(0,d)$ to the internal fields $u^{\pm}(z,t)$ has an integral representation. This representation leads to the definition of the Green's functions $G^{\pm}(z,t,t')$ of the propagation problem.

From Duhamel's integral (see Appendix B), an explicit mapping of the excitation $u^{+}(0,t)$ to the internal fields $u^{\pm}(z,t)$ can be obtained. For convenience this mapping is evaluated at two different times. The basic difference between the two definitions in Eqs. (19) and (20) is that, in (19), the time coordinate t is evaluated at the field position z while, in (20), it is evaluated at the left endpoint of the slab, $z=0$. Both of them are needed to derive the equations in this section. The expressions $\tau^{+}(0;z,t)$ and $\tau^{+}(z;0,t)$ denote specific points along the relevant characteristics of the wave front (see Sec. III). The expressions are

$$\begin{aligned}u^{+}(z,t)&=u^{+}(0,\tau^{+}(0;z,t))p(z,\tau^{+}(0;z,t))+\int_{-\infty}^{\tau^{+}(0;z,t)}G^{+}(z,\tau^{+}(0;z,t),t')p(z,t')u^{+}(0,t')dt',\\ u^{-}(z,t)&=\int_{-\infty}^{\tau^{+}(0;z,t)}G^{-}(z,\tau^{+}(0;z,t),t')p(z,t')u^{+}(0,t')dt',\end{aligned}\tag{19}$$

or evaluated at time $\tau^{+}(z;0,t)$ [use the fact that $\tau^{+}(0;z,\tau^{+}(z;0,t))=t$]

$$\begin{aligned}u^{+}(z,\tau^{+}(z;0,t))&=u^{+}(0,t)p(z,t)+\int_{-\infty}^{t}G^{+}(z,t,t')p(z,t')u^{+}(0,t')dt',\\ u^{-}(z,\tau^{+}(z;0,t))&=\int_{-\infty}^{t}G^{-}(z,t,t')p(z,t')u^{+}(0,t')dt',\end{aligned}\tag{20}$$

where the attenuation factor is defined as

$$p(z,t)=\exp\left\{\int_{0}^{z}\alpha(\zeta,\tau^{+}(\zeta;0,t))d\zeta\right\}.$$

In this formula, the integration of the function α is performed along the characteristics of the first equation in (1) (see Sec. III for more details on characteristic curves in nonstationary media and Appendix B for details on the propagation of finite jump discontinuities along characteristic curves). By causality, the Green's functions $G^{\pm}(z,t,t')=0$ for $t'>t$.

The Green's functions equations are derived by performing the calculation of

$$\frac{\partial}{\partial z}\begin{pmatrix} u^+ \\ u^- \end{pmatrix}$$

in two different ways. The first way is obtained through explicit differentiation of the definition of the Green's functions in (20), and the second way is obtained by using the general dynamics, (1). In both cases repeated use of the definition of the Green's functions, (20), and the general dynamics, (1), is necessary. The comparison between these two expressions leads to the following Green's functions equations, $0<z<d$, $t>t'$:

$$\begin{aligned}
&\frac{\partial G^+}{\partial z}(z,t,t') - \alpha(z,\tau^+(z;0,t))G^+(z,t,t') + G^+(z,t,t')\alpha(z,\tau^+(z;0,t')) \\
&\quad - \beta(z,\tau^+(z;0,t))G^-(z,t,t') - A(z,\tau^+(z;0,t),\tau^+(z;0,t'))\frac{\partial \tau^+}{\partial t'}(z;0,t') \\
&\quad - \int_{t'}^{t} A(z,\tau^+(z;0,t),\tau^+(z;0,t''))\frac{\partial \tau^+}{\partial t''}(z;0,t'')G^+(z,t'',t')dt'' \\
&\quad - \int_{t'}^{t} B(z,\tau^+(z;0,t),\tau^+(z;0,t''))\frac{\partial \tau^+}{\partial t''}(z;0,t'')G^-(z,t'',t')dt'' = 0,
\end{aligned} \tag{21}$$

and

$$\begin{aligned}
&\frac{\partial G^-}{\partial z}(z,t,t') - 2f(z,\tau^+(z;0,t))\left(\frac{\partial \tau^+}{\partial t}(z;0,t)\right)^{-1}\frac{\partial G^-}{\partial t}(z,t,t') - \delta(z,\tau^+(z;0,t))G^-(z,t,t') \\
&\quad + G^-(z,t,t')\alpha(z,\tau^+(z;0,t')) - \gamma(z,\tau^+(z;0,t))G^+(z,t,t') \\
&\quad - C(z,\tau^+(z;0,t),\tau^+(z;0,t'))\frac{\partial \tau^+}{\partial t'}(z;0,t') \\
&\quad - \int_{t'}^{t} C(z,\tau^+(z;0,t),\tau^+(z;0,t''))\frac{\partial \tau^+}{\partial t''}(z;0,t'')G^+(z,t'',t')dt'' \\
&\quad - \int_{t'}^{t} D(z,\tau^+(z;0,t),\tau^+(z;0,t''))\frac{\partial \tau^+}{\partial t''}(z;0,t'')G^-(z,t'',t')dt'' = 0,
\end{aligned} \tag{22}$$

with the initial condition

$$G^-(z,t,t')|_{t'=t} = -\frac{1}{2}\frac{\gamma(z,\tau^+(z;0,t))}{f(z,\tau^+(z;0,t))}\frac{\partial \tau^+}{\partial t}(z;0,t). \tag{23}$$

The initial condition on $G^+(z,t,t')|_{t'=t}$ is obtained by integrating (21), i.e.,

$$\begin{aligned}
G^+(z,t,t')|_{t'=t} = -\frac{1}{2}\int_0^z \Bigg[&\frac{\beta(z',\tau^+(z';0,t))\gamma(z',\tau^+(z';0,t))}{f(z',\tau^+(z';0,t))} \\
&- 2A(z',\tau^+(z';0,t),\tau^+(z';0,t))\Bigg]\frac{\partial \tau^+}{\partial t}(z';0,t)dz'
\end{aligned} \tag{24}$$

These differential equations for the Green's functions generalize those given in, e.g., Refs. 1, 5, and 16. Note that the Green's functions $G^{\pm}(z,t,t')=0$ for $t'>t$.

From the definition of the Green's functions $G^{\pm}(z,t,t')$, (20), and the definition of the reflection kernel $R(z,t,t')$, (14), at $z=0$, the following boundary conditions of $G^{\pm}$ at $z=0$ and $z=d$ are obtained for all times:

$$G^{+}(0,t,t')=0, \quad G^{-}(d,t,t')=0, \quad G^{-}(0,t,t')=R(0,t,t').$$

The last boundary condition is a special case of a more general interrelationship between the Green's functions $G^{\pm}(z,t,t')$ and the reflection kernel $R(z,t,t')$. Specifically, from the definition of the Green's functions $G^{\pm}(z,t,t')$, (20), and the reflection kernel $R(z,t,t')$, (14), it is straightforward to obtain for $0\leqslant z\leqslant d$, $t>t'$,

$$G^{-}(z,t,t')=R(z,\tau^{+}(z;0,t),\tau^{+}(z;0,t'))\,\frac{\partial\tau^{+}}{\partial t'}\,(z;0,t') + \int_{t'}^{t} R(z,\tau^{+}(z;0,t),\tau^{+}(z;0,t''))\,\frac{\partial\tau^{+}}{\partial t''}\,(z;0,t'')G^{+}(z,t'',t')\,dt''.$$

Notice, that

$$\frac{\partial\tau^{+}}{\partial t}\,(\zeta;z,t)\bigg|_{\zeta=z}=1.$$

This identity is easily obtained by letting $\zeta_2=\zeta$ and $\zeta_1=z$ in (12) and differentiating with respect to t and finally letting $\zeta=z$.

For completeness, an alternative definition of the Green's function equations is given:

$$u^{+}(z,t)=u^{+}(0,\tau^{+}(0;z,t))p(z,\tau^{+}(0;z,t))+\int_{-\infty}^{\tau^{+}(0;z,t)} g^{+}(z,t,t')p(z,t')u^{+}(0,t')\,dt',$$
$$u^{-}(z,t)=\int_{-\infty}^{\tau^{+}(0;z,t)} g^{-}(z,t,t')p(z,t')u^{+}(0,t')\,dt'. \tag{25}$$

These Green's functions may be more suitable for numerical computation, and the use of the transformation

$$G^{\pm}(z,t,t')=g^{\pm}(z,\tau^{+}(z;0,t),t') \tag{26}$$

enables Eqs. (21) and (22) to be transformed into

$$\frac{\partial g^{+}}{\partial z}\,(z,t,t')+f(z,t)\,\frac{\partial g^{+}}{\partial t}\,(z,t,t')-\alpha(z,t)g^{+}(z,t,t')+g^{+}(z,t,t')\alpha(z,\tau^{+}(z;0,t')) - \beta(z,t)g^{-}(z,t,t')-A(z,t,\tau^{+}(z;0,t'))\,\frac{\partial\tau^{+}}{\partial t'}\,(z;0,t') - \int_{\tau^{+}(z;0,t')}^{t} A(z,t,t'')g^{+}(z,t'',t')\,dt''-\int_{\tau^{+}(z;0,t')}^{t} B(z,t,t'')g^{-}(z,t'',t')\,dt''=0$$

and

$$\frac{\partial g^{-}}{\partial z}\,(z,t,t')-f(z,t)\,\frac{\partial g^{-}}{\partial t}\,(z,t,t')-\delta(z,t)g^{-}(z,t,t')+g^{-}(z,t,t')\alpha(z,\tau^{+}(z;0,t'))$$

$$-\gamma(z,t)g^+(z,t,t')-C(z,t,\tau^+(z;0,t'))\,\frac{\partial\tau^+}{\partial t'}\,(z;0,t')$$

$$-\int_{\tau^+(z;0,t')}^{t} C(z,t,t'')g^+(z,t'',t')dt''-\int_{\tau^+(z;0,t')}^{t} D(z,t,t'')g^-(z,t'',t')dt''=0$$

with the initial condition

$$g^-(z,t,t')|_{t'=\tau^+(0;z,t)}=-\frac{1}{2}\,\frac{\gamma(z,t)}{f(z,t)}\left(\frac{\partial\tau^+}{\partial t}\,(0;z,t)\right)^{-1}.$$

The initial condition on $g^+(z,t,t')|_{t'=\tau^+(0;z,t)}$ is obtained from the transformation (26) and the initial condition for $G^+(z,t,t')|_{t'=t}$ in (24).

The relation between the reflection kernel and this alternative definition of the Green's functions reads

$$g^-(z,t,t')=R(z,t,\tau^+(z;0,t'))\,\frac{\partial\tau^+}{\partial t'}\,(z;0,t')+\int_{\tau^+(z;0,t')}^{t} R(z,t,t'')g^+(z,t'',t')dt''.$$

A. Propagation of discontinuities

The solutions of the first-order system of PDEs (21) and (22) are continuous along the characteristic curves associated with the system, but may be discontinuous across these curves.

From (21) it is seen that the characteristic traces are $t=$constant for G^+ and as $G^+(0,t,t')$ is continuous for all t and t', it follows G^+ is continuous throughout its domain of definition. However, examination of the initial condition (23) shows that any discontinuity in the functions γ and f will be propagated along the characteristic curves described by (22). The conditions imposed on these functions in Sec. I ensure $G^-(z,t,t)$ is continuous except possibly at $z=d$. The initial value for G^- has the jump discontinuity in the direction of increasing t:

$$[G^-](d,t,t)=\frac{1}{2}\,\frac{\gamma(d,\tau^+(d;0,t))}{f(d,\tau^+(d;0,t))}\,\frac{\partial\tau^+}{\partial t}\,(d;0,t).$$

This jump in G^- will propagate along the characteristic curves of G^-.

The characteristic traces for $G^-(z,t,t')$ are independent of the third parameter t' and can be described by an equation $\eta=\eta(\zeta;z,t)$. The notation used here is similar to that used in Eq. (11). The function η satisfies the equation

$$\frac{d\eta}{d\zeta}\,(\zeta;z,t)=-2f(\zeta,\tau^+(\zeta;0,\eta(\zeta;z,t)))\,\frac{\partial\tau^+}{\partial t}\,(0;\zeta,t)|_{t=\tau^+(\zeta;0,\eta(\zeta;z,t))}.$$

The discontinuity propagates along the curve Υ emanating from the line (d,t,t) and where Υ has parametric form

$$\Upsilon:\mathbf{r}(z,t)=(z,\eta(z;d,t),t).$$

It follows that the equation describing the propagation of the discontinuity in G^- is

$$\left.\frac{d[G^-]}{dz}\right|_{\Upsilon}=(\delta(z,\tau^+(z;0,\eta(\zeta;d,t)))-\alpha(z,\tau^+(z;0,t)))[G^-]_{\Upsilon}.$$

Integrating this equation from d to z yields

$$[G^-]_Y=[G^-]_{Y(z=d)}\exp\left\{\int_d^z(\delta(z',\tau^+(z';0,\eta(z';d,t)))-\alpha(z',\tau^+(z';0,t)))dz'\right\}.$$

The discontinuous behavior of g^- can be found from the relationship between g^- and G^- [see (26)], namely

$$g^-(z,\tau^+(z;0,t),t')=G^-(z,t,t')$$

with the substitution $t\to\eta(z;d,t)$, and with use of the identity $(z=d)$

$$\tau^+(\zeta;0,\eta(\zeta;z,t))=\tau^-(\zeta;z,\tau^+(z;0,t))$$

the appropriate expression for $[g^-]$ is found.

VI. EXPLICIT EXPRESSIONS

In this section, the theory presented in the previous sections is illustrated by the examples from Sec. II.

In Sec. II A, propagation of electromagnetic waves in nonstationary, inhomogeneous, dispersive media was considered. A detailed analysis of the imbedding equation and the Green's function equations for this example was presented in Ref. 1, and the reader is referred to this paper for more details.

The generalized wave equation, (4), in Sec. II B and the transmission line equations, (5), in Sec. II C imply no significant simplifications of the results in Secs. IV and V. However, the less complex wave equation, (3), offers some simplifications. Accordingly, the wave equation (3) has an imbedding equation

$$\begin{aligned}&\frac{\partial R}{\partial z}(z,t,t')-f(z,t)\frac{\partial R}{\partial t}(z,t,t')+\frac{\partial R}{\partial t'}(z,t,t')f(z,t')\\&\quad=+\delta(z,t)R(z,t,t')+R(z,t,t')\left[-\frac{\partial f}{\partial t'}(z,t')-\alpha(z,t')\right]\\&\qquad-\int_{t'}^{t}R(z,t,t'')\beta(z,t'')R(z,t'',t')dt''\end{aligned}$$

and Green's functions equations

$$\begin{aligned}&\frac{\partial G^+}{\partial z}(z,t,t')-\alpha(z,\tau^+(z;0,t))G^+(z,t,t')+G^+(z,t,t')\alpha(z,\tau^+(z;0,t'))\\&\qquad-\beta(z,\tau^+(z;0,t))G^-(z,t,t')=0\end{aligned}$$

and

$$\begin{aligned}&\frac{\partial G^-}{\partial z}(z,t,t')-2f(z,\tau^+(z;0,t))\left(\frac{\partial\tau^+}{\partial t}(z;0,t)\right)^{-1}\frac{\partial G^-}{\partial t}(z,t,t')\\&\qquad-\delta(z,\tau^+(z;0,t))G^-(z,t,t')+G^-(z,t,t')\alpha(z,\tau^+(z;0,t'))\\&\qquad-\gamma(z,\tau^+(z;0,t))G^+(z,t,t')=0\end{aligned}$$

with

$$\alpha(z,t) = -\frac{1}{2}\frac{\partial}{\partial z}\ln f(z,t) - \frac{3}{2}\frac{\partial f}{\partial t}(z,t),$$

$$\beta(z,t) = +\frac{1}{2}\frac{\partial}{\partial z}\ln f(z,t) - \frac{1}{2}\frac{\partial f}{\partial t}(z,t),$$

$$\gamma(z,t) = +\frac{1}{2}\frac{\partial}{\partial z}\ln f(z,t) + \frac{1}{2}\frac{\partial f}{\partial t}(z,t),$$

$$\delta(z,t) = -\frac{1}{2}\frac{\partial}{\partial z}\ln f(z,t) + \frac{3}{2}\frac{\partial f}{\partial t}(z,t).$$

VII. CONCLUSIONS

This paper contains a detailed analysis of wave propagation of transient waves in media whose properties are changing in space and time—nonstationary media. The underlying dynamics of the wave propagation problem is a general, linear, homogeneous, nonstationary, first-order 2×2 system of hyperbolic equations. A new wave splitting is introduced, which is a generalization of the well-established wave splitting in media that have time translation symmetries. The scattering problem is solved by an imbedding or a Green's functions technique. Specifically, the imbedding equation for the reflection kernel is derived. This equation is a nonlinear, hyperbolic equation in one space and two time variables. Furthermore, the Green's functions equations are derived. They constitute a system of linear, hyperbolic equations in one space and two time variables. The characteristic curves of the dynamics are discussed in some detail, and a few numerical illustrations give the typical behavior of the nonstationary properties of these characteristic curves.

ACKNOWLEDGMENTS

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APPENDIX A: STRAIGHTENING THE CHARACTERISTICS

To illustrate how the characteristic of (1) may be straightened, consider

$$\frac{\partial u^{\pm}}{\partial z}(z,t) \pm f(z,t)\frac{\partial u^{\pm}}{\partial t}(z,t) = F^{\pm}(z,t,u^{+},u^{-}), \tag{A1}$$

where $f(z,t)>0$ in the domain of interest.

Introduce the diffeomorphic transformation of the independent variables

$$z = z(x,s), \quad t = t(x,s),$$

with the associated inverse functions

$$x = x(z,t), \quad s = s(z,t).$$

The PDE (A1) can then be written in terms of the new independent variables as

$$\left(\frac{\partial x}{\partial z} \pm f\frac{\partial x}{\partial t}\right)\frac{\partial u^{\pm}}{\partial x} + \left(\frac{\partial s}{\partial z} \pm f\frac{\partial s}{\partial t}\right)\frac{\partial u^{\pm}}{\partial s} = G^{\pm}(x,s,u^{+},u^{-}).$$

It is easily seen, to straighten the characteristics of the transformed equation, a necessary condition is

$$\frac{\partial x}{\partial z}+f\,\frac{\partial x}{\partial t}=a\left(\frac{\partial s}{\partial z}+f\,\frac{\partial s}{\partial t}\right),\quad \frac{\partial x}{\partial z}-f\,\frac{\partial x}{\partial t}=b\left(\frac{\partial s}{\partial z}-f\,\frac{\partial s}{\partial t}\right), \tag{A2}$$

provided

$$f^2\left(\frac{\partial s}{\partial t}\right)^2-\left(\frac{\partial s}{\partial z}\right)^2\neq 0. \tag{A3}$$

In this expression a and b are nonzero constants. The only way to violate this condition is if either $x-as=$constant or $x-bs=$constant.

The constants a and b cannot be equal if the transformation is to be diffeomorphic. For convenience, choose $a=1$, $b=-1$, so converting the system (A2) to

$$\frac{\partial}{\partial z}\begin{pmatrix}x\\ s\end{pmatrix}=\begin{pmatrix}0 & f\\ f & 0\end{pmatrix}\frac{\partial}{\partial t}\begin{pmatrix}x\\ s\end{pmatrix},$$

which can be converted by diagonalization to the uncoupled system

$$\frac{\partial}{\partial z}\begin{pmatrix}v_1\\ v_2\end{pmatrix}=\begin{pmatrix}-f & 0\\ 0 & f\end{pmatrix}\frac{\partial}{\partial t}\begin{pmatrix}v_1\\ v_2\end{pmatrix},$$

where

$$\begin{pmatrix}v_1\\ v_2\end{pmatrix}=\frac{1}{2}\begin{pmatrix}-1 & 1\\ 1 & 1\end{pmatrix}\begin{pmatrix}x\\ s\end{pmatrix},\quad \begin{pmatrix}x\\ s\end{pmatrix}=\begin{pmatrix}-1 & 1\\ 1 & 1\end{pmatrix}\begin{pmatrix}v_1\\ v_2\end{pmatrix}.$$

A convenient set of initial conditions for x and s is

$$x(z,0)=\int_0^z f(z',0)\,dz',\quad s(z,0)=0.$$

This initial value problem for the hyperbolic system has a unique solution, which means that the characteristics can always be straightened. In fact, these initial conditions imply that (A3) is always satisfied, since $f(z,t)>0$.

In the special case that $f=f(z)$, then the solution of these systems yields

$$x(z,t)=\int_0^z f(z')\,dz',\quad s(z,t)=t.$$

This is the well-known travel time transformation.

APPENDIX B: DUHAMEL'S INTEGRAL

The derivation of the imbedding equation in Sec. IV and the Green's functions equations in Sec. V relies on a result that is obtained from Duhamel's integral.[17] Since the basic first-order 2×2 system of equations, (1), has coefficients varying both in space and time, a slight modification of the standard result is needed. Therefore, it is of interest here to give a few of the intermediate steps leading to the relation (14), which defines the reflection kernel $R(z,t,t')$, and to equation (20) defining the Green's functions $G^{\pm}(z,t,t')$.

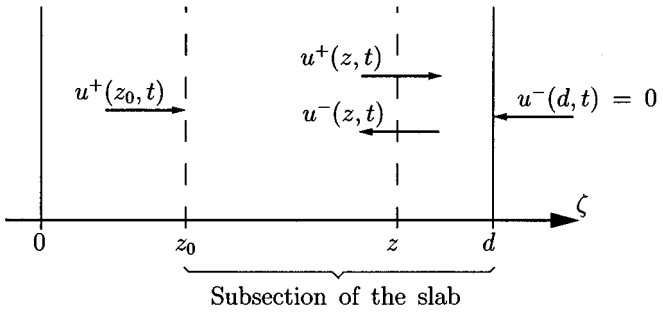

FIG. 4. The geometry used in Appendix B.

In order to cover both the definition of the reflection kernel and the definition of the Green's functions, a subsection (z_0,d) of the physical slab $(0,d)$ is considered. The full slab $(0,d)$ is therefore imbedded in a one-parameter family of sub-slabs (z_0,d), where the left end of the slab z_0 varies between 0 and d (see Fig. 4).

The basic dynamics of the problem is given by (1):

$$\frac{\partial}{\partial z}\begin{pmatrix} u^+(z,t) \\ u^-(z,t) \end{pmatrix} = f(z,t)\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}\frac{\partial}{\partial t}\begin{pmatrix} u^+(z,t) \\ u^-(z,t) \end{pmatrix} + \begin{pmatrix} \alpha(z,t) & \beta(z,t) \\ \gamma(z,t) & \delta(z,t) \end{pmatrix}\begin{pmatrix} u^+(z,t) \\ u^-(z,t) \end{pmatrix} + \int_{-\infty}^{t}\begin{pmatrix} A(z,t,t') & B(z,t,t') \\ C(z,t,t') & D(z,t,t') \end{pmatrix}\begin{pmatrix} u^+(z,t') \\ u^-(z,t') \end{pmatrix} dt'. \tag{B1}$$

The domain of interest in this appendix is $z_0<z<d$, $t>0$.

Problem 1: A specific solution to Eq. (B1) is now considered. This solution satisfies the following mixed initial-boundary value $(t'>0)$:

$$u^{\pm}(z,0)=0, \quad z_0<z<d,$$

$$u^{+}(z_0,t)=H(t-t'), \quad t>0,$$

$$u^{-}(d,t)=0, \quad t>0.$$

The boundary condition at $z=d$ shows that there are no sources in the region to the right of the slab, $z>d$.

The solution to this problem, which is assumed to be unique, depends on the parameters $z_0\in(0,d)$ and $t'>0$, and the solution is denoted $U^{\pm}(z,t;z_0,t')$, i.e.,

$$u^{\pm}(z,t)=U^{\pm}(z,t;z_0,t').$$

Causality implies that $U^{\pm}(z,t;z_0,t')=0$ for $t'>\tau^+(z_0;z,t)$ or, stated equivalently, $t<\tau^+(z;z_0,t')$. The variable t' denotes the starting time of the excitation at the left boundary z_0 of the sub-slab (z_0,d). If the medium is invariant under time translations, the solution is only a function of z and z_0, and the difference $t-t'$.

The solutions $U^{\pm}(z,t;z_0,t')$ are continuously differentiable everywhere, except along the characteristics of the u^+-equation (see Sec. III). With the method of characteristics, it is straightforward to show that U^- is continuous at the leading edge, while U^+ has a finite jump disconti-

nuity there. The leading edge is defined as the characteristic curve in the (z,t)-plane passing through the point (z_0,t'), i.e., $t=\tau^+(z;z_0,t')$, $z_0<z<d$. The explicit values at the leading edge are

$$U^+(z,t;z_0,\tau^+(z_0;z,t))=\exp\left\{\int_{z_0}^{z}\alpha(\zeta,\tau^+(\zeta;z,t))d\zeta\right\},$$

$$U^-(z,t;z_0,\tau^+(z_0;z,t))=0.$$

Problem 2: Consider now the solution of Eq. (B1) subject to the mixed initial-boundary value $(t'>0)$

$$\begin{aligned} &u^{\pm}(z,0)=0, \quad z_0<z<d,\\ &u^+(z_0,t)=g(t), \quad t>0,\\ &u^-(d,t)=0, \quad t>0. \end{aligned} \tag{B2}$$

Again, the boundary condition at $z=d$ shows that there are no sources in the region to the right of the slab, $z>d$. Here, $g(t)$ is an arbitrary continuously differentiable function, which for $t>0$ can be approximated from below by the piecewise constant function

$$g_1(t)=g(0)H(t)+\sum_{k=1}^{\infty}[g(k\Delta t')-g((k-1)\Delta t')]H(t-k\Delta t').$$

Due to the linearity of the equation (B1), superposition is used to find the solution of the approximate boundary value $g_1(t)$. In the limit, $\Delta t'\to 0$, the result is

$$u^{\pm}(z,t)=u^+(z_0,0)U^{\pm}(z,t;z_0,0)+\int_0^{\tau^+(z_0;z,t)}\frac{\partial u^+}{\partial t'}(z_0,t')U^{\pm}(z,t;z_0,t')dt',$$

where the causality of the solutions $U^{\pm}(z,t;z_0,t')$ has been used to truncate the infinite integration range and, furthermore, the substitution $g(t)=u^+(z_0,t)$ for $t>0$ has been made. It is easy to verify that the expressions $u^{\pm}(z,t)$ satisfy the given mixed initial-boundary value problem, with the use of (13) and the fact that $U^-(z,t;z_0,\tau^+(z_0;z,t))=0$. Integration by parts now shows that the unique solution of the mixed boundary value problem (B1) and (B2) is

$$\begin{aligned} u^+(z,t)&=u^+(z_0,\tau^+(z_0;z,t))U^+(z,t;z_0,\tau^+(z_0;z,t))-\int_0^{\tau^+(z_0;z,t)}u^+(z_0,t')\frac{\partial U^+}{\partial t'}(z,t;z_0,t')dt',\\ u^-(z,t)&=-\int_0^{\tau^+(z_0;z,t)}u^+(z_0,t')\frac{\partial U^-}{\partial t'}(z,t;z_0,t')dt'. \end{aligned} \tag{B3}$$

These equations now offer two possibilities, namely to define the reflection kernel $R(z_0,t,t')$ of the sub-slab (z_0,d) and the Green's functions $G^{\pm}(z,t,t')$ of the full slab $(0,d)$.

For the definition of the reflection kernel use the second equation in (B3) and let $z=z_0$. Define the reflection kernel

$$R(z_0,t,t')=-\frac{\partial U^-}{\partial t'}(z_0,t;z_0,t').$$

The relation between the $u^{\pm}$-waves at the left endpoint of the sub-slab is (the subscript on z_0 is dropped)

$$u^-(z,t)=\int_{-\infty}^{t} R(z,t,t')u^+(z,t')dt',$$

which is identical to (14).

In the definition of the Green's functions $G^{\pm}(z,t,t')$, let $z_0=0$ in (B3). The result is

$$u^+(z,t)=u^+(0,\tau^+(0;z,t))p(z,\tau^+(0;z,t))-\int_0^{\tau^+(0;z,t)} u^+(0,t')\,\frac{\partial U^+}{\partial t'}\,(z,t;0,t')dt',$$

$$u^-(z,t)=-\int_0^{\tau^+(0;z,t)} u^+(0,t')\,\frac{\partial U^-}{\partial t'}\,(z,t;0,t')dt',$$

where

$$p(z,t)=\exp\left\{\int_0^z \alpha(\zeta,\tau^+(\zeta;0,t))d\zeta\right\}.$$

It is convenient to introduce an extra factor $p(z,t')$ in the definition of the Green's functions. Therefore, the definition of $G^{\pm}(z,t,t')$ is

$$-\frac{\partial}{\partial t'}\,U^+(z,t;0,t')=p(z,t')G^+(z,\tau^+(0;z,t),t'),$$

$$-\frac{\partial}{\partial t'}\,U^-(z,t;0,t')=p(z,t')G^-(z,\tau^+(0;z,t),t').$$

APPENDIX C: EXAMPLES ON CHARACTERISTICS OF THE u^+-EQUATION

The explicit form of the function f determines whether a closed form expression can be found for the characteristics in (9) or not. In most cases this is not possible. In this section, the theory of the characteristics is illustrated with an analytic and a numerical example.

Analytic example: The function $f(z,t)$ has to be consistent with the boundary conditions, (2), given in Sec. I, and simple enough to permit closed form solutions of (9). Thus, for $\tau^+\geqslant 0$ and $0\leqslant\zeta\leqslant d$, let

$$f(\zeta,\tau^+)=\frac{1}{v_0}\,[1+a\zeta(d-\zeta)\tau^+].$$

Here d is the thickness of the slab, v_0 is a constant, and a is a parameter. Outside the slab, i.e., for $\zeta<0$ or $\zeta>d$, and everywhere for $\tau^+<0$, let

$$f(\zeta,\tau^+)=\frac{1}{v_0}.$$

Figure 5 shows the velocity profile $c(z,t)$ inside the slab ($d=2$), surrounded by a medium with the constant wave velocity $v_0=1$, and $a=1$. A set of characteristics for this case is illustrated in Fig. 6.

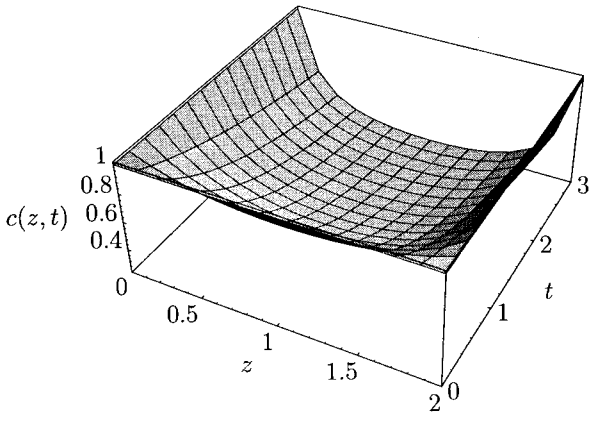

FIG. 5. The velocity profile $c(z,t)=1/(1+z(d-z)t)$, where $d=2$.

If f is inserted into Eq. (9), a linear first-order ordinary differential equation in $\tau^+(\zeta)$ is obtained. This equation is easily solvable after multiplication with the integrating factor $e^{g(\zeta)}$ where

$$g(\zeta)=\frac{1}{v_0}\,a\left(-\frac{1}{2}\,d\zeta^2+\frac{1}{3}\,\zeta^3\right).$$

The explicit form of the characteristic curve passing through the point (z,t) is

$$\tau^+(\zeta;z,t)=te^{g(z)}e^{-g(\zeta)}+\frac{1}{v_0}\,e^{-g(\zeta)}\int_z^\zeta e^{g(\zeta')}d\zeta'.$$

Specifically, the solution at $\zeta=0$ is

$$\tau^+(0;z,t)=te^{g(z)}-\frac{1}{v_0}\int_0^z e^{g(\zeta')}\,d\zeta'$$

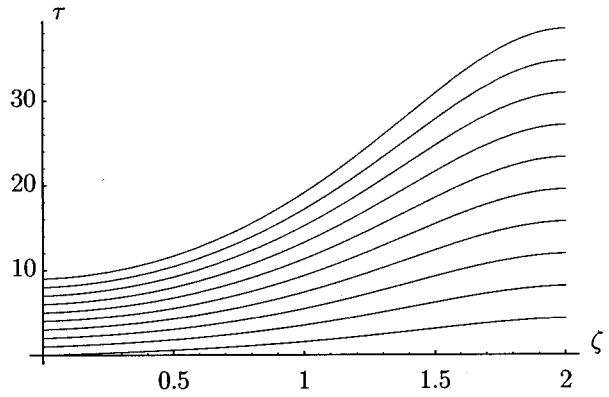

FIG. 6. A set of characteristics for the case, $f(z,t)=1+z(d-z)t$, where $d=2$.

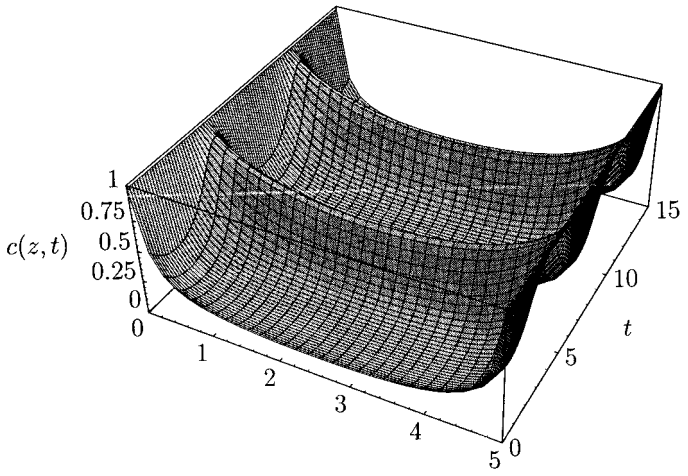

FIG. 7. The velocity profile $c(z,t)$ for the example in (C1) for $d=5$.

and the solution at z starting at $(0,t)$ is

$$\tau^+(z;0,t)=te^{-g(z)}+\frac{1}{v_0}\,e^{-g(z)}\int_0^z e^{g(\zeta')}\,d\zeta'.$$

Differentiation with respect to t and z gives

$$\frac{\partial\tau^+(\zeta;z,t)}{\partial t}=e^{g(z)}e^{-g(\zeta)}$$

and

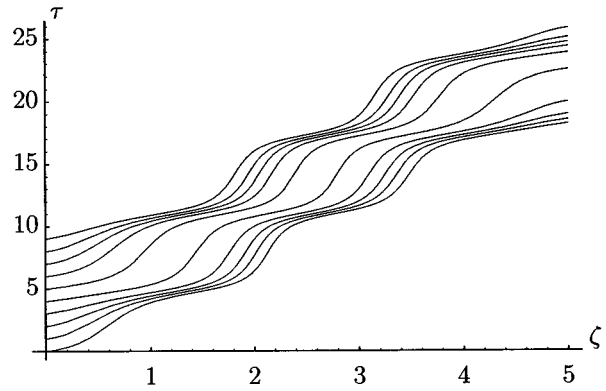

FIG. 8. A set of characteristics for the example in (C1) for $d=5$.

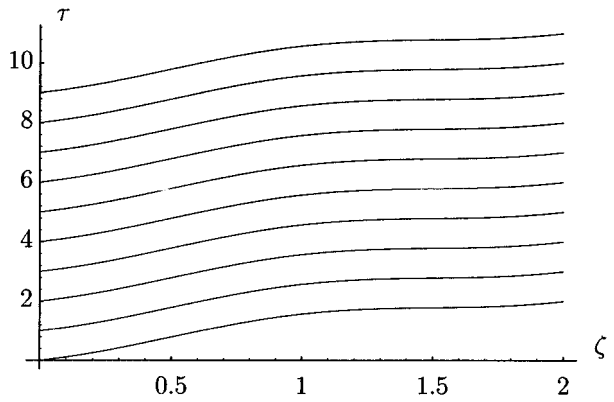

FIG. 9. A set of characteristics for the stationary case, $f(z)=1+0.9\sin 2\pi z/d$, where $d=2$.

$$\frac{\partial\tau^{+}(\zeta;z,t)}{\partial z}=tg'(z)e^{g(z)}e^{-g(\zeta)}-\frac{1}{v_0}e^{g(z)}e^{-g(\zeta)}=-f(z,t)e^{g(z)}e^{-g(\zeta)}$$

and (13) is satisfied.

Numerical example: In Figs. 7 and 8, the phase velocity and a set of characteristics, respectively, for a nonlinear case are depicted. The phase velocity of the nonstationary medium in this example is

$$f(z,t)=\begin{cases}1, & z<0;\\ 1+z(d-z)(1.1+\sin t), & 0<z<d;\\ 1, & z>d.\end{cases}\tag{C1}$$

These curves have been obtained by numerical integration.

Note that the flow depicted by Figs. 6 and 8 illustrates a flow field that is non-area preserving, i.e., the flow field has nonzero divergence (compressible). Compare this with Fig. 9 for which $f(z,t)=f(z)$ and so the flow field is area preserving.

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An ongoing big bang model in the special relativistic Maxwell–Dirac equations

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An exact, analytical solution of the combined Maxwell–Dirac equation is presented. The solution is regular inside a wedgelike domain of the flat space–time. On the boundary of that domain, the solution exhibits singular behavior. © *1996 American Institute of Physics.* [S0022-2488(96)01505-2]

I. INTRODUCTION

Exact, analytical solutions of interacting second-quantized fields are not available yet. However, classical interacting fields are more tractable for analysis. The coupled Maxwell–Klein–Gordon equations have yielded some exact solutions.[1] The coupled Eistein–Maxwell equations have produced scores of exact solutions.[2] Exact analytical solutions have been found within the complicated system of the coupled Einstein–Maxwell–Klein–Gordon equations.[3] The coupled Maxwell–Dirac equations are predecessors of the quantum electro-dynamics. These equations also provide some valuable insights for the standard theory.[4] The initial-value problem of the coupled Maxwell–Dirac equation has been probed by Flato, Simon, and Taflin.[5] The class of exact plane wave solutions of the type $\psi(x)=\alpha(p)\exp[ip_\mu x^\mu]$, within the framework of the Maxwell–Dirac equations, has been thoroughly explored.[6] It was discovered that, for $m\neq 0$, not a single nontrivial solution exists! However, infinitely many solutions exist for $m=0$. The coupled Maxwell–Dirac equations in the $1+1$-dimensional space–time is known as the classical Schwinger theory.[7] In the case of $m=0$, the most general solutions of the classical Schwinger theory have been discovered recently.[8] The massive Schwinger theory is much more complicated to solve. However, a particular solution of the massive theory was found in the same paper. Our present exact solution in this paper is based on that solution.

None of the exact solutions of the quasilinear, coupled field equations discussed so far uses the perturbation methods or Fourier integrals. These are the usual tools people use to explore the quantum theory of interacting fields. Unfortunately, the Fourier integral techniques discard more solutions than they generate. For example, consider the one-dimensional wave equation $[(\partial_x)^2-(\partial_t)^2]\psi(x,t)=0$. Denumerably infinite number of solutions of this equation, given by $\psi_n(x,t)=(x-t)^{2n}+(x+t)^{2n}$, $n\in\mathbb{Z}^+$, cannot be obtained by use of Fourier integrals. So, we are not surprised to find that our present solution of the Maxwell–Dirac equations cannot be captured by the Fourier integrals. However, we have managed to obtain a sequence of *approximate* solutions which can be expressed as Fourier cosine integrals. In the limit $n\to\infty$, the sequence of approximate solutions goes over into the present exact solution, which itself is not amenable to the Fourier cosine integrals.

Our exact solution can be defined only in a proper subset of flat space–time. This domain looks like a wedge (see Fig. 1) and solutions become singular on its boundary. That is why it is an ongoing big bang model in the framework of the special theory of relativity.

II. NOTATIONS AND FIELD EQUATIONS

The flat space–time manifold is denoted by M_4. A global Minkowski coordinate chart is used. A space–time event, which is an element of M_4, is coordinatized by $x:=(x^0,x^1,x^2,x^3)$. Here, x^0

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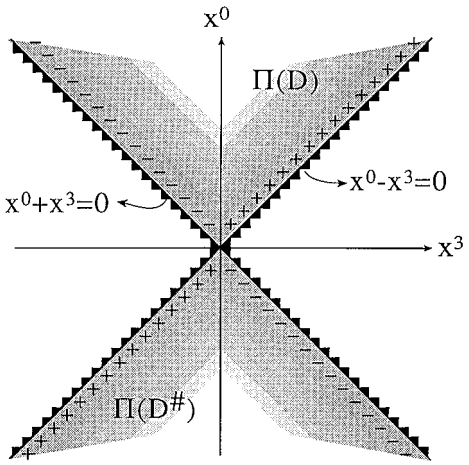

FIG. 1. Space–time diagram depicting ongoing big bang crunch followed by ongoing big bang.

denotes the time coordinate. A Greek index takes values from {0,1,2,3} and a Roman index takes from {1,2,3}. The signature of the metric tensor $\eta_{\mu\nu}$ is -2. Einstein's summation convention is followed.

The electromagnetic four-potential is denoted by $A^{\mu}(x)$. The four-component (Dirac) bispinor field and its Hermitian conjugate are indicated by $\psi(x)$ and $\psi^{\dagger}(x)$, respectively. The four Dirac matrices are denoted by γ^{μ} and we shall adopt Weyl's representation of these matrices. In an open, convex domain $D\subset\mathbb{R}^4$ corresponding to such a domain in M_4, we assume that the potential functions A^{μ} are of the differentiability class $C^3(D\subset\mathbb{R}^4;\mathbb{R})$ and the bispinor components $\psi_1,\psi_2,\psi_3,\psi_4$ are of the class $C^2(D\subset\mathbb{R}^4;\mathbb{C})$. In such a setting, the coupled Maxwell–Dirac equations (in the units $\hbar=c=1$) can be written as

$$M^{\mu}(x):=\partial^{\nu}\partial_{\nu}A^{\mu}(x)-j^{\mu}(x)=0, \tag{2.1a}$$

$$j^{\mu}(x):=e\,\psi^{\dagger}(x)\,\gamma^0\gamma^{\mu}\psi(x), \tag{2.1b}$$

$$L(x):=\partial_{\mu}A^{\mu}(x)=0, \tag{2.1c}$$

$$D(x):=\{i\gamma^{\mu}[\partial_{\mu}+ieA_{\mu}(x)]-mI_{(4)}\}\psi(x)=0, \tag{2.1d}$$

$$\gamma^0:=\begin{bmatrix}0 & I_{(2)}\\ I_{(2)} & 0\end{bmatrix},\quad \gamma^k:=\begin{bmatrix}0 & -\sigma^k\\ \sigma^k & 0\end{bmatrix}. \tag{2.1e}$$

Here, e and m are the charge and the mass parameters, respectively. Moreover, $I_{(4)},I_{(2)}$ are identity matrices and σ^ks are Pauli matrices.

Now we shall make some general observations about the system of equations (2.1a)–(2.1e). There exists one differential identity among the equations and it is given by

$$\partial_{\mu}M^{\mu}-\partial_{\mu}\partial^{\mu}L-ie[\psi^{\dagger}(x)\psi^0D(x)-D^{\dagger}(x)\gamma^0\psi(x)]\equiv 0. \tag{2.2}$$

The gauge-invariant, symmetric energy-momentum-stress tensor density is given by

$$\theta_{ab}(x):=(i/2)\{\psi^{\dagger}(x)\gamma^0\gamma_b[(\partial_a+ieA_a)\psi]-[(\partial_a-ieA_a)\psi^{\dagger}(x)]\gamma^0\gamma_b\psi(x)\}$$
$$-F^{c}{}_{a}(x)F_{bc}(x)+\tfrac{1}{4}\eta_{ab}F_{cd}(x)F^{cd}(x), \tag{2.3a}$$

$$F_{ab}(x) := \partial_b A_a - \partial_a A_b\,, \tag{2.3b}$$

$$\partial_b \theta^{ab}(x) = 0. \tag{2.3c}$$

By a straightforward computation we obtain

$$j_\mu(x) j^\mu(x) = 4e^2 |\psi_1^*(x)\psi_3(x) + \psi_2^*(x)\psi_4(x)|^2 \geqslant 0. \tag{2.4}$$

Therefore, the four-current vector $j^\mu(x)$ is always nonspacelike, irrespective of the real (or complex) values of m. Preliminary analysis of the system of equations (2.1a)–(2.1e) with $m \neq 0$ reveals that solutions of the type $|\psi_1|^2 + |\psi_2|^2 > 0$, $\psi_3 = \psi_4 \equiv 0$ or else $\psi_1 = \psi_2 \equiv 0$, $|\psi_3|^2 + |\psi_4|^2 > 0$, do *not* exist. Therefore, in every nontrivial solution of the system both particles as well as antiparticles must be present.

The Maxwell's equations (2.1a) are linear, second-order partial differential equations. In the absence of the external electromagnetic fields, these equations can be integrated to obtain

$$A_\mu(x) = e \int G_{inh}(x - x')\, \psi^\dagger(x')\, \gamma^0 \gamma_\mu \psi(x')\, d^4x', \tag{2.5}$$

where G_{inh} is a nonhomogeneous Green's function suitable for a prescribed initial-boundary-value problem. Substituting (2.5) into (2.1d) we obtain

$$[i\gamma^\mu \partial_\mu - mI_4]\psi(x) + ie^2 \left[\int G_{inh}(x - x')\, \gamma^\mu \psi^\dagger(x')\, \gamma^0 \gamma_\mu \psi(x')\, d^4x' \right] \psi(x) = 0. \tag{2.6}$$

The above is a nonlinear, integro-differential equation[9] for ψ which automatically incorporates the electro magnetic self-interactions of the Dirac particle–antiparticle system. The equation (2.6) implies that the time evolution of the system $\partial_0 \psi$ depends on the local property of the wave function $\gamma^k \partial_k \psi$ and also on the past history of the system inherent in the integral involving Green's function.

III. A PARTICULAR EXACT SOLUTION

We furnish a special, exact solution of the system (2.1a)–(2.1e) by the following:

$$A^1(x) = A^2(x) \equiv 0, \tag{3.1a}$$

$$A^0(x) = \left(\frac{m}{4e}\right) \left\{ \ln|(x^0)^2 - (x^3)^2| - 2\left[\frac{(x^0)^2 + (x^3)^2}{(x^0)^2 - (x^3)^2}\right] \right\}, \tag{3.1b}$$

$$A^3(x) = -\left(\frac{m}{4e}\right) \left\{ \ln\left|\frac{x^0 - x^3}{x^0 + x^3}\right| + \frac{4x^0 x^3}{[(x^0)^2 - (x^3)^2]} \right\}, \tag{3.1c}$$

$$\psi_2(x) = \psi_4(x) \equiv 0, \tag{3.1d}$$

$$\psi_1(x) = \left[\frac{\sqrt{m}}{e(x^0 - x^3)}\right] \exp\left\{ -i\left(\frac{m}{4}\right)[(x^0 - x^3)\ln|x^0 + x^3| + (x^0 + x^3)\ln|x^0 - x^3|] \right\}, \tag{3.1e}$$

$$\psi_3(x) = \left[\frac{\sqrt{m}}{e(x^0 + x^3)}\right] \exp\left\{ -i\left(\frac{m}{4}\right)[(x^0 - x^3)\ln|x^0 + x^3| + (x^0 + x^3)\ln|x^0 - x^3|] \right\}, \tag{3.1f}$$

$$j^1(x) = j^2(x) \equiv 0, \tag{3.1g}$$

$$j^0(x)=\left(\frac{m}{e}\right)\left[\frac{1}{(x^0-x^3)^2}+\frac{1}{(x^0+x^3)^2}\right], \tag{3.1h}$$

$$j^3(x)=\left(\frac{m}{e}\right)\left[\frac{1}{(x^0-x^3)^2}-\frac{1}{(x^0+x^3)^2}\right], \tag{3.1i}$$

$$F_{01}(x)=F_{02}(x)=F_{12}(x)=F_{23}(x)=F_{31}(x)\equiv 0, \tag{3.1j}$$

$$F_{03}(x):=\partial_3 A_0-\partial_0 A_3=\left(\frac{m}{e}\right)\left[\frac{1}{(x^0+x^3)}-\frac{1}{(x^0-x^3)}\right], \tag{3.1k}$$

$$A_\mu(x)j^\mu(x)=\left(\frac{m}{2e}\right)^2\left\{\left[\frac{1}{(x^0-x^3)^2}+\frac{1}{(x^0+x^3)^2}\right]\left[\ln|(x^0)^2-(x^3)^2|-2\left(\frac{(x^0)^2+(x^3)^2}{(x^0)^2-(x^3)^2}\right)\right]\right.$$
$$\left.+\left[\frac{1}{(x^0-x^3)^2}-\frac{1}{(x^0+x^3)^2}\right]\left[\ln\left|\frac{x^0-x^3}{x^0+x^3}\right|+\frac{4x^0x^3}{((x^0)^2-(x^3)^2)}\right]\right\}. \tag{3.1l}$$

In the above solution there are no external electromagnetic fields. The self-electric field is in the direction of the x^3 axis. There is no self-magnetic field. The current vector density is along x^3 axis. The self-energy density is given by the equation (3.1l). The particle wave function is given by $\psi_1(x)$ and the antiparticle wave function is given by $\psi_3(x)$. The corresponding phase functions satisfy $\arg\psi_1(x)=\arg\psi_3(x)+2N\pi$, where N is an integer. The solutions (2a)–(2f) are valid in the open, unbounded, convex domain D of the flat space–time characterized by

$$D:=\{(x^0,x^1,x^2,x^3):x^0>0,(x^0)^2-(x^3)^2>0,x^1\in\mathbb{R},x^2\in\mathbb{R}\}. \tag{3.2}$$

(A similar wedge-shaped domain has been considered[10] in general relativity.) The boundary of this domain is given by the three-dimensional hypersurface:

$$\partial D:=\{(x^0,x^1,x^2,x^3):x^0\geqslant 0,(x^0)^2-(x^3)^2=0,x^1\in\mathbb{R},x^2\in\mathbb{R}\}. \tag{3.3}$$

These three-dimensional edges satisfy $\phi(x):=(x^0)^2-(x^3)^2=0$, and thus imply that $\eta^{\mu\nu}(\partial_\mu\phi)(\partial_\nu\phi)=0$. Therefore, the boundary ∂D constitutes a three-dimensional null hyper-surface of two-content.[11] Precisely on this null boundary, the solutions (2a)–(2f) are undefined or singular. The particle wave function $\psi_1(x)$ is singular on $x^0-x^3=0$ and the antiparticle wave function $\psi_3(x)$ is singular on $x^0+x^3=0$. That is why these solutions constitute an ongoing big bang model.

It is understandable that the usual Fourier integral techniques of the relativistic field theory fail to capture these solutions. However, a sequence of approximate solutions, expressible by Fourier cosine integrals, exist such that the limit of the sequence yields the present solutions. The key to this construction of the approximate solutions is the Fourier cosine integral:[12]

$$\frac{1}{(u)^{(1-1/n)}}=\frac{\Gamma(1/n)}{\pi}\int_{0^+}^{\infty}\frac{\cos[pu-(\pi/2n)]dp}{p^{1/n}},\quad u>0;n\in\{2,3,4,\ldots\}. \tag{3.4}$$

Here, Γ is the usual gamma function. Note that in the limit $n\to\infty$, the left-hand side tends to u^{-1}, but the right-hand side limit does not exist. The sequence of the approximate solutions are given by

$$A^1_{(n)}(x)=A^2_{(n)}(x)\equiv 0, \tag{3.5a}$$

$$A^0_{(n)}(x)=\left[\frac{m}{4e(1-2/n)}\right]\Big\{(n/2)[(x^0+x^3)^{2/n}+(x^0-x^3)^{2/n}-2]$$
$$-\frac{(x^0+x^3)}{(x^0-x^3)^{(1-2/n)}}-\frac{(x^0-x^3)}{(x^0+x^3)^{(1-2/n)}}\Big\}, \tag{3.5b}$$

$$A^3_{(n)}(x)=-\left[\frac{m}{4e(1-2/n)}\right]\Big\{(n/2)[(x^0-x^3)^{2/n}-(x^0+x^3)^{2/n}]$$
$$+\frac{(x^0+x^3)}{(x^0-x^3)^{(1-2/n)}}-\frac{(x^0-x^3)}{(x^0+x^3)^{(1-2/n)}}\Big\}, \tag{3.5c}$$

$$\psi_{2(n)}(x)=\psi_{4(n)}(x)\equiv 0, \tag{3.5d}$$

$$\psi_{1(n)}(x)=\frac{\sqrt{m}}{e(x^0-x^3)^{(1-1/n)}}\exp\Big\{-i\left(\frac{mn}{8}\right)[(x^0+x^3)((x^0-x^3)^{2/n}-1)$$
$$+(x^0-x^3)((x^0+x^3)^{2/n}-1)]\Big\}$$
$$=\left[\frac{\sqrt{m}\Gamma(1/n)}{\pi e}\right]\cdot\exp\Big\{-i\left(\frac{mn}{8}\right)[(x^0+x^3)((x^0-x^3)^{2/n}-1)$$
$$+(x^0-x^3)((x^0+x^3)^{2/n}-1)]\Big\}\int_{0^+}^{\infty}(p)^{-1/n}\cos\left[p(x^0-x^3)-\left(\frac{\pi}{2n}\right)\right]dp, \tag{3.5e}$$

$$\psi_{3(n)}(x)=\frac{\sqrt{m}}{e(x^0+x^3)^{(1-1/n)}}\exp\Big\{-i\left(\frac{mn}{8}\right)[(x^0+x^3)((x^0+x^3)^{2/n}-1)$$
$$+(x^0-x^3)((x^0+x^3)^{2/n}-1)]\Big\}$$
$$=\left[\frac{\sqrt{m}\Gamma(1/n)}{\pi e}\right]$$
$$\cdot\exp\Big\{-i\left(\frac{mn}{8}\right)[(x^0+x^3)((x^0-x^3)^{2/n}-1)+(x^0-x^3)((x^0+x^3)^{2/n}-1)]\Big\}$$
$$\times\int_{0^+}^{\infty}(p)^{-1/n}\cos\left[p(x^0+x^3)-\left(\frac{\pi}{2n}\right)\right]dp, \tag{3.5f}$$

$$\partial^\nu\partial_\nu A^\mu_{(n)}(x)-j^\mu_{(n)}(x)=0, \tag{3.5g}$$

$$\partial_\mu A^\mu_{(n)}(x)=0, \tag{3.5h}$$

$$\{i\gamma^\mu[\partial_\mu+ieA_{\mu(n)}(x)]-mI_{(4)}\}\psi_{(n)}(x)=0(1/n). \tag{3.5i}$$

It can be proved that if the terms involving Fourier cosine integrals are not considered, then the limits $n\to\infty$ of the sequence of approximate solutions in (3.5) are precisely the solutions in (3.1).

The solutions (3b), (3c), (3e), (3f), (3h), (3i), and (3k) exhibit unphysical features in having simple poles at $e=0$ in the complex e-plane. (Such singular behaviors were predicted in Ref. 13.) However, in case the mass parameter m is not independent of the charge parameter e, and the

relation $m=e^2/r_0$ holds for some length parameter r_0, these spurious singularities at $e=0$ disappear. Making this assumption $m=e^2/r_0$, we can express the solutions in (3.1) as the following power series of e:

$$A^1(x)=A^2(x)\equiv 0, \tag{3.6a}$$

$$A^0(x)=\left(\frac{e}{4r_0}\right)\left\{\ln|(x^0)^2-(x^3)^2|-2\left[\frac{(x^0)^2+(x^3)^2}{(x^0)^2-(x^3)^2}\right]\right\}, \tag{3.6b}$$

$$A^3(x)=-\left(\frac{e}{4r_0}\right)\left\{\ln\left|\frac{x^0-x^3}{x^0+x^3}\right|+\frac{4x^0x^3}{[(x^0)^2-(x^3)^2]}\right\}, \tag{3.6c}$$

$$\psi_2(x)=\psi_4(x)\equiv 0, \tag{3.6d}$$

$$\psi_1(x)=\left[\frac{1}{\sqrt{r_0}(x^0-x^3)}\right]\sum_{k=0}^{\infty}\frac{1}{k!}\left\{\left(\frac{-ie^2}{4r_0}\right)[(x^0-x^3)\ln|x^0+x^3|+(x^0+x^3)\ln|x^0-x^3|]\right\}^k, \tag{3.6e}$$

$$\psi_2(x)=\left[\frac{1}{\sqrt{r_0}(x^0+x^3)}\right]\sum_{k=0}^{\infty}\frac{1}{k!}\left\{\left(\frac{-ie^2}{4r_0}\right)[(x^0-x^3)\ln|x^0+x^3|+(x^0+x^3)\ln|x^0-x^3|]\right\}^k, \tag{3.6f}$$

$$|\psi_1(x)|=\frac{1}{\sqrt{r_0}|x^0-x^3|}, \tag{3.6g}$$

$$|\psi_2(x)|=\frac{1}{\sqrt{r_0}|x^0+x^3|}, \tag{3.6h}$$

$$j^1(x)=j^2(x)\equiv 0, \tag{3.6i}$$

$$j^0(x)=\left(\frac{e}{r_0}\right)\left[\frac{1}{(x^0-x^3)^2}+\frac{1}{(x^0+x^3)^2}\right], \tag{3.6j}$$

$$j^3(x)=\left(\frac{e}{r_0}\right)\left[\frac{1}{(x^0-x^3)^2}-\frac{1}{(x^0+x^3)^2}\right], \tag{3.6k}$$

$$F_{12}(x)=F_{23}(x)=F_{31}(x)=F_{01}(x)=F_{02}(x)\equiv 0, \tag{3.6l}$$

$$F_{03}(x)=\left(\frac{e}{r_0}\right)\left[\frac{1}{(x^0+x^3)}-\frac{1}{(x^0-x^3)}\right], \tag{3.6m}$$

$$A_\mu(x)j^\mu(x)=\left(\frac{e^2}{4r_0^2}\right)\left\{\left[\frac{1}{(x^0-x^3)^2}+\frac{1}{(x^0+x^3)}\right]\left[\ln|(x^0)^2-(x^3)^2|-2\left(\frac{(x^0)^2+(x^3)^2}{(x^0)^2-(x^3)^2}\right)\right]+\left[\frac{1}{(x^0-x^3)^2}-\frac{1}{(x^0+x^3)^2}\right]\left[\ln\left|\frac{x^0-x^3}{x^0+x^3}\right|+\frac{4x^0x^3}{(x^0)^2-(x^3)^2}\right]\right\}. \tag{3.6n}$$

In the limit $e\to 0$, the mass $m=(e^2/r_0)$ and all solutions in (3.6), *except* (3.6e)–(3.6h) vanish. In that limit, Dirac field components go over into

$$\psi_1(x)=\frac{1}{\sqrt{r_0}(x^0-x^3)},\quad \psi_3(x)=\frac{1}{\sqrt{r_0}(x^0+x^3)},\quad \psi_2(x)=\psi_4(x)\equiv 0. \tag{3.7}$$

These are exact solutions of the *massless, free* Dirac equations. Therefore, in this model, the self-electric field and the mass vanish in case the coupling constant e goes to zero.

The solutions $(7a-n)$ of the Maxwell–Dirac equations are also valid in the alternate domain

$$D^{\#}:=\{(x^0,x^1,x^2,x^3):x^0<0,(x^0)^2-(x^3)^2>0,x^1\in\mathbb{R},x^2\in\mathbb{R}\}. \tag{3.8}$$

The solutions (3.6a)–(3.6n) in the combined domain $D^{\#}\cup D$ can be regarded as a model of an ongoing big crunch immediately followed by an ongoing big bang in the arena of the special relativistic Maxwell–Dirac equations.

To picture these domains, it will be convenient to introduce a projection function $\pi:\mathbb{R}^4\to\mathbb{R}$ such that

$$\pi(x^0,x^1,x^2,x^3):=(x^0,x^3).$$

The corresponding projections of domains are given by

$$\pi(D)=\{(x^0,x^3):x^0>0,(x^2)^2-(x^3)^2>0\},$$

$$\pi(D^{\#})=\{(x^0,x^3):x^0<0,(x^0)^2-(x^3)^2>0\}.$$

The pictures of these domains in $\mathbb{R}^2$, corresponding to two-flats[11] in M_4, are exhibited in Fig. 1.

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Quantum random walk for $U_q(su(2))$ and a new example of quantum noise

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We derive the quantum version of the central limit theorem for sample sums of q-independent q-identically distributed quantum variables for $q \in \mathbf{R}^+ - \{1\}$. In particular, we consider $U_q(su(2))$, for which we obtain in the limit a state Ψ on the algebra generated by q-commuting q-oscillators indexed by pairs of real numbers (r,s), where $0 \leqslant r < s$, giving a new example of non-additive quantum noise. © *1996 American Institute of Physics.* [S0022-2488(96)00303-3]

I. INTRODUCTION

The aim of this paper is to prove the central limit theorem for sample sums of q-independent variables of the Hopf algebra $U_q(su(2))$ type, and thus is a contribution to the area of non-commutative theory of processes[1] with independent ''increments.'' More precisely, we prove convergence of finite joint correlations for sample sums of q-independent, q-identically distributed random variables indexed by pairs of positive real numbers (r,s). In particular, we take the sums of quantum variables of $U_q(su(2))$ and for that case we find a realization of the limit in terms of creation and annihilation operators satisfying certain q-commutation relations, which gives rise to a new example of non-additive quantum noise, defined on a non-separable Hilbert space. However, it should be pointed out that in this paper we do not prove the functional limit theorem (or Donsker's invariance principle[2]), but only its simplest case for sample sums and thus it can be viewed only as the central limit theorem or a quantum random walk for certain quantum q-variables, in particular those of the ''generic'' $U_q(su(2))$.

Processes with independent and stationary increments are usually called white noise. They are used to model a quantum-mechanical heat bath. It is known that functional limit theorems are the source of both classical and quantum noises. The first quantum version of the functional central limit theorem was shown by Cockroft, Gudder and Hudson,[3] who proved in 1977 a quantum mechanical analog of the functional central limit theorem and obtained a canonical Wiener process[4] in the limit. Later, the stochastic calculi for the CCR and CAR algebras were developed by Hudson and Parthasarathy[5] and Applebaum and Hudson,[6] respectively. Connected with the concept of free independence of Voiculescu[7] was the free white noise studied by Speicher[8] with the stochastic calculus developed in Ref. 9.

The framework for the general theory of quantum white noise on graded $*$-bialgebras was proposed by Accardi, Schürmann and von Waldenfels.[10] In their approach, a white noise on a $*$-bialgebra $\mathscr{B}$ is a family $(j_{rs})_{0 \leqslant r \leqslant t}$ of quantum random variables on $\mathscr{B}$, i.e., homomorphisms from $\mathscr{B}$ into a $*$-algebra $\mathscr{A}$ with a state $\hat{\phi}$ with the following properties:
(WN0) increment property: $j_{rs} * j_{st} = j_{rt}$ for $0 \leqslant r < s < t$, and $j_{rr} = \delta 1$, where δ is the co-unit and $*$ is the convolution product;
(WN1) independence, i.e., for time-ordered products the following factorization holds:

$$\hat{\phi}(j_{r_1 s_1}(b_1) \ldots j_{r_n s_n}(b_n)) = \hat{\phi}(j_{r_1 s_1}(b_1)) \ldots \hat{\phi}(j_{r_n s_n}(b_n))$$

for all $n \in \mathbf{N}$, $0 \leqslant r_1 < s_1 < \ldots < r_n < s_n$, where $b_1, \ldots, b_n \in \mathscr{B}$, and

$$j_{rs}(b) j_{r's'}(b') = j_{r's'}(b') j_{rs}(b)$$

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for all disjoint semi-closed time-intervals $[r,s),[r',s')$ and any $b,b' \in \mathscr{B}$;
(WN2) stationarity, i.e., $\hat{\phi} \circ j_{rs} = \hat{\phi} \circ j_{0,s-r}$ for $r<s$;
(WN3) continuity, i.e., $\lim_{r \downarrow 0} \hat{\phi} \circ j_{0,r}(b) = \delta(b)$ for all $b \in \mathscr{B}$, where δ is the co-unit.

Generalized white noises were studied by many authors.[11–18] Also, certain deformed (or, q-) white noises were considered. For instance, two examples of q-white noises were considered by Schürmann,[17,18] where q is a deformation parameter. Namely, it was shown that the normalized sample sums converge to the two-dimensional Azema noise and to an interpolation of the two-dimensional quantum Brownian motion in the case of q-right- and q-left bialgebras, respectively.

Another approach to construct q-deformed white noises was proposed by Bożejko and Speicher.[11,12] They define certain deformed creation and annihilation operators living in a generalized Fock space $\Gamma_q(\mathscr{H})$, where $\mathscr{H}=L^2(\mathbf{R})$, subject to deformed commutation relations. In the simplest case[11] they read

$$c(f)c^*(g)-qc^*(g)c(f)=\langle f,g\rangle 1$$

where $f,g \in \mathscr{H}$ and $c(f),c^*(f)$ stand for the annihilation and creation operators, respectively. Then they show that one can define a deformed scalar product on $\Gamma_q(\mathscr{H})$ which makes them mutually adjoint. This approach essentially boils down to some non-trivial positivity proofs that ensure the existence of a scalar product on a subspace of the full Fock space.

In Refs. 19 and 20 it was shown that functional limit theorems for quantum Bernoulli processes lead to the Boson and Fermion Brownian motions. Viewing quantum two-level systems as fundamental in our understanding of quantum central limit theorems (qclt), we studied first[21] the central limit in the discrete case for the q-analog of $su(2)$, namely $U_q(su(2))$, the q-deformed enveloping algebra of $su(2)$, and obtained the q-oscillator in the limit, corresponding to the q-Gaussian distribution. The result produced a commutative diagram, in which the qclt of $U_q(su(2))$ gives the q-oscillator, in addition to the qclt of Ref. 19, where the qclt of $su(2)$ gives the harmonic oscillator. Thus, in search for interesting examples of quantum noises, we study in this work the quantum random walk for $U_q(su(2))$, which we view as a fundamental structure in the q-deformed symmetries.

In our approach we obtain a quantum noise from the central limit theorem for sums of random-walk type. The object we start with is a unital $*$-algebra $\mathscr{C}_q$ over $\mathbf{C}$ generated (as a $*$-algebra) by the set $\mathscr{V}_+ \cup \{t,t^{-1}\}$, where t,t^{-1} are hermitian, subject to $t^\sigma t^{-\sigma}=1$ and $t^\sigma w = \epsilon(t^\sigma,w)wt^\sigma$, where $w \in \mathscr{V}=\mathscr{V}_+ \cup \mathscr{V}_-$, $\mathscr{V}_-=\mathscr{V}_+^*$ and $\epsilon(t^\sigma,v)=q^{-2\sigma}$, $\epsilon(t^\sigma,v^*)=q^{2\sigma}$, for $q \in \mathbf{R}^+$, $v \in \mathscr{V}_+$. We equip $\mathscr{C}_q$ with the bialgebra structure and refer to it as a q-$*$-bialgebra. Later, in Sec. VI, by adding

$$[v^*,v]=\frac{t^2-t^{-2}}{q^2-q^{-2}}$$

we consider the Hopf algebra $U_q(su(2))$, which leads to the simplest quantum noise covered by our theory.

Our approach is different from the one presented in Refs. 17 and 18 due to the fact that our collective variables are in fact not only q-independent, but also q-identically distributed. This is achieved by assuming that $\phi(t) \neq 1$, where t can be viewed as a twisted identity. This assumption is justified by the fact that $\phi(t) \neq 1$ if ϕ is the vacuum state of the representations of $U_q(su(2))$, and has its origins in Ref. 21, where we took ϕ to be the vacuum state of its fundamental representation (see also Refs. 22–24). Therefore, the qclt on coalgebras[17,18] cannot be applied here.

As we mentioned earlier, the results of Secs. II–V can be applied to q-$*$-bialgebras. However, for simplicity, in the outline of the results given below we restrict our attention to the case of

$U_q(su(2))$. Thus we consider sums of q-independent, q-identically distributed variables indexed by semi-closed time intervals, i.e., for a state ϕ on $\mathscr{C}_q$ with $\phi(t)=q$, and $w \in \mathscr{V}$ we put

$$S_{rs}^N(w)=\sqrt{\frac{q_{rs}}{N_{rs}}}\Delta_{rs}^N(w)$$

where

$$\Delta_{rs}^N(w)=\sum_{i=N_r+1}^{N_s} j_i^{N_rN_s}(w)$$

and $j_i^{N_rN_s}:\mathscr{C}_q\to\mathscr{C}_q^{\otimes\infty}$ are given by

$$j_i^{N_rN_s}(w)=1^{\otimes N_r}\otimes(t^{-1})^{\otimes(i-N_r-1)}\otimes w\otimes t^{\otimes(N_s-i)}\otimes 1^{\otimes\infty},$$

where $N_{rs}=[N_s-N_r]$, $q_{rs}=[s-r]$ and $[x]=(q^{2x}-q^{-2x})/(q^2-q^{-2})$ is the q-analog of x. In other words, $S_{rs}^N(w)$ are normalized collective variables associated with w. Note that the normalization is different from $1/\sqrt{N}$, appearing in both the classical probability and the quantum central limit theorems considered by other authors. However, in the case of Hopf algebras $U_q(g)$ deformed normalization has to be used when the vacuum state is considered. Note that q_{rs}/N_{rs} is the q-analog of $(s-r)/(N_s-N_r)$, the latter being $1/\sqrt{N}$, and in the limit, when q approaches 1, it coincides with it.

Further, we can define normalized ''increments''

$$S_{rs}^N(t^\sigma)=q^{\sigma(N_r-N_s)}\Delta_{rs}^N(t^\sigma)=q^{\sigma(N_r-N_s)}(1^{N_r}\otimes(t^\sigma)^{\otimes(N_s-N_r)}\otimes 1^{\otimes\infty})$$

where $\sigma\in\{1,-1\}$. It can be shown that in the case of $U_q(su(2))$, for all $r<s$ and $N\in\mathbf{N}$, Δ_{rs}^N are Hopf algebra homomorphisms and, viewed as functions of r and s, satisfy (WN1–WN4). However, the normalized ''increments'' fail to do so. It is due to the fact that the normalization comes from a type of group contraction which loses the Hopf algebra structure.

The central limit theorem, understood in our paper in the sense of convergence of correlations, can be written as

$$\lim_{N\to\infty}\hat{\phi}(S_{r_1s_1}^N(v_1)\ldots S_{r_ns_n}^N(v_n))=\Psi(B_{r_1s_1}(v_1)\ldots B_{r_ns_n}(v_n))$$

where $v_1,\ldots,v_n\in\{v,v^*,t,t^{-1}\}$ and $\hat{\phi}=\phi^{\otimes\infty}$. The correlations of the limiting functional Ψ can be expressed solely in terms of q_{rs}, the variance of the limiting process B_{rs}. We show that the following conditions are satisfied by the limiting correlations for $a<1$ (the case of $a>1$ is similar):

(QN0) q_{rs} is a continuous deformation of the Brownian variance, i.e.,

$$\lim_{q\to 1} q_{rs}=s-r;$$

(QN1) independence, i.e.,

$$\Psi(B_{r_1s_1}(c_1)\ldots B_{r_ns_n}(c_n))=\Psi\left(\prod_{i\in I_1}B_{r_is_i}(v_i)\right)\times\ldots\times\Psi\left(\prod_{i\in I_n}B_{r_is_i}(v_i)\right)$$

where $s_1=\ldots=s_{j_1}<\ldots<s_{j_{n-1}+1}=\ldots=s_{j_n}=s_p$ defines the partition $\{I_1,\ldots,I_n\}$ of $\{1,\ldots,p\}$ into subsets corresponding to equal upper end-points of the time intervals, with commutations for disjoint time intervals $[r,s),[r',s')$:

$$B_{rs}(w)B_{r's'}(w')=B_{r's'}(w')B_{rs}(w)$$

for $w,w' \in \mathscr{V}$, and q-commutations for non-disjoint intervals with $s'>s$:

$$B_{rs}(w)B_{r's'}(w')=q^{2d(w')}B_{r's'}(w')B_{rs}(w);$$

(QN2) stationarity, i.e., q_{rs} depends only on $s-r$,
(QN3) continuity, i.e. $\lim_{s\downarrow r}q_{rs}=0$.

In addition, our example of quantum noise satisfies the following commutation relations for (non-disjoint) time intervals with equal upper end points:
(QN4) for any $r<s$, $r'<s$ the operators $B_{rs}(v)$, $B_{r's}(v^*)$ satisfy the following relations

$$[B_{rs}(v^*),B_{r's}(v)]=\sqrt{q_{rs}q_{r's}}q^{2\hat{N}_{(r,s)}+2\hat{N}_{(r',s)}+4\hat{N}_s}$$

where $\hat{N}_{(rs)}$, $\hat{N}_s$ are the number operators that count the numbers of creation operators with the upper end-points falling into (r,s) and $\{s\}$, respectively.

This gives a new example of non-additive quantum noise, in which lengths of time intervals enter in a multiplicative fashion and the scalar product governs the behavior at the upper end-points.

In Sec. II we give basic definitions and an outline of the combinatorics involved. In Sec. III we state the qclt on q-bialgebras for fixed time-interval. In Sec. IV we derive two important lemmas, the Factorization Lemma, and the Clustering Lemma, which provide the rules for calculating arbitrary limiting correlations. Using those lemmas, in Sec. V, we state and prove the general version of the functional qclt on q-bialgebras. Finally, in Sec. VI, we give the GNS construction for the limiting functional in the case of $U_q(su(2))$. Thus, we define creation and annihilation operators acting on some generalized Fock space $\Gamma_q(\mathscr{H})$, where $\mathscr{H}=\mathscr{H}_0\otimes\mathscr{H}_1$, $\mathscr{H}_0$ comes from the GNS triple $(\mathscr{H}_0,\pi,\omega)$ for the vacuum state ϕ for the two-dimensional representation of $\mathscr{C}_q$, and the time-domain Hilbert space is $\mathscr{H}_1=l^2[0,\infty)$. Note that this example of noise is given on a non-separable Hilbert space.

II. PRELIMINARIES

Let us start with an outline of the combinatorics used in the sequel. By an *ordered partition* S of an index set I we understand an r-tuple $S=(S_1,\ldots,S_r)$, where $S_1\cup\ldots\cup S_r=I$ and $S_1,\ldots,S_r$ are mutually disjoint. The set of such partitions for fixed r will be denoted by $\mathscr{P}_r^{ord}(I)$, or $\mathscr{P}_r^{ord}\{1,\ldots,p\}$ for $I=\{1,\ldots,p\}$. In turn, $\mathscr{P}_r(I)$ will stand for the set of all (non-ordered) partitions of I consisting of r sets, i.e., $\{S_1,\ldots,S_r\}$. Thus, for each partition $S \in \mathscr{P}_r$, there exist $r!$ ordered partitions naturally associated with it. By the *signature* γ_S of an ordered partition S we understand the r-tuple

$$(\gamma_{S_1},\ldots,\gamma_{S_r})=(\#(S_1),\ldots,\#(S_r))$$

where $\#(S_j)$ denotes the number of elements in S_j. Partitions for which $\#(S_j)$ is even for all $j=1,\ldots,r$ are called *even* and the set of all ordered even partitions of $\{1,\ldots,p\}$ will be denoted by $\mathscr{P}_e^{ord}\{1,\ldots,p\}$. Further, for given $v_1,\ldots,v_p \in \mathscr{V}_+\cup\mathscr{V}_-$ and an ordered partition S of $\{1,\ldots,p\}$ associated with it, let

$$S_j^+=\{k\in S_j|v_k\in\mathscr{V}_+\},\quad S_j^-=\{k\in S_j|v_k\in\mathscr{V}_-\},$$

and, $\gamma_{S_j^+}=\#(S_j^+)$, $\gamma_{S_j^-}=\#(S_j^-)$. We also put

$$|\gamma_{S^+}|=\sum_{j=1}^{r}\gamma_{S_j^+}, \quad |\gamma_{S^-}|=\sum_{j=1}^{r}\gamma_{S_j^-}.$$

By the set of inversions of an ordered partition S we will understand the set

$$W_S=\{(i,j)|i\in S_k, j\in S_n, i<j, k>n\}.$$

Also, for a given ordered partition $S=(S_1,\ldots,S_r)$ let ${}^rS=(S_r,\ldots,S_1)$, i.e., with sets taken in the reverse order.

Let now I be a partition of $\{1,\ldots,p\}$ into r disjoint subsets $S_1,\ldots,S_r$. By an *ordered subpartition of* $\{1,\ldots,p\}$ *associated with* I we shall understand any set of ordered partitions of $\{I_1,\ldots,I_r\}$, i.e., any set of the form:

$$\mathbf{I}=\{(I_1^1,\ldots,I_1^{i_1}),\ldots,(I_r^1,\ldots,I_r^{i_r})\}$$

where $(I_k^1,\ldots,I_k^{i_k})$ is an ordered partition of I_k. In turn, such a partition will be called *even* if all its ordered partitions are even. For instance, let $\{1,\ldots,8\}$ be the index set and let $I=\{I_1,I_2\}$, where $I_1=\{1,2,4,5\}$, $I_2=\{3,6,7,8\}$. Then $\{(\{1,2\},\{4,5\}),(\{3,6\},\{7,8\})\}$ is an ordered subpartition of $\{1,\ldots,8\}$ associated with I, and is different from $\{(\{1,2\},\{4,5\}),(\{7,8\},\{3,6\})\}$. Note that the number of subpartitions associated with I is equal to the product of the numbers of ordered partitions of $I_1,\ldots,I_k$, respectively. The set of ordered subpartitions (even ordered subpartitions) of the index set $\{1,\ldots,p\}$ associated with I will be denoted by $\mathscr{P}^I\{1,\ldots,p\}$ ($\mathscr{P}_e^I\{1,\ldots,p\}$).

Since all results except the GNS construction given in Sec. V remain valid for $\mathscr{C}_q$ being a bialgebra, we start with a more general setting than the specific example of q-noise given in Sec. VI. Thus assume $\mathscr{C}$ to be a free $*$-algebra over $\mathbf{C}$ generated (as a $*$-algebra) by the set $\mathscr{V}_+$ and let $\mathscr{V}=\mathscr{V}_+\cup\mathscr{V}_-$, where $\mathscr{V}_-=\{v^*|v\in\mathscr{V}_+\}$. On $\mathscr{C}$ we define a $\mathbf{Z}$-gradation by $d(v)=1$, $d(v^*)=-1$, $d(\mathscr{C})=0$. The corresponding direct sum decomposition will be denoted by

$$\mathscr{C}=\ldots\oplus\mathscr{C}_{(-1)}\oplus\mathscr{C}_{(0)}\oplus\mathscr{C}_{(1)}\oplus\ldots.$$

We also define an $\mathbf{N}$-gradation by $d_1(v)=1$, $v\in\mathscr{V}$, $d_1(\mathbf{C})=0$, extended to all free products in the only possible way. We denote the direct sum decomposition resulting from this $\mathbf{N}$-gradation with superscripts:

$$\mathscr{C}=\mathscr{C}^{(0)}\oplus\mathscr{C}^{(1)}\oplus\ldots.$$

The algebra $\mathscr{C}$ can be twisted by adding hermitian generators t^σ, $\sigma\in\{1,-1\}$ subject to $t^\sigma t^{-\sigma}=1$ and $t^\sigma w=\epsilon(t^\sigma,w)wt^\sigma$, where $w\in\mathscr{V}$ and $\epsilon(t^\sigma,v)=q^{2\sigma}$, $\epsilon(t^\sigma,v^*)=q^{-2\sigma}$, where $q\in\mathbf{R}^+$, $v\in\mathscr{V}_+$. For details, see Ref. 24. The twisted $*$-algebra thus obtained will be denoted by $\mathscr{C}_q$. Both gradations are extended to $\mathscr{C}_q$ in the trivial way, i.e., $d(t^\sigma)=0$, $d_1(t^\sigma)=0$.

We consider the following coproduct on $\mathscr{C}_q$:

$$\Delta:\mathscr{C}_q\to\mathscr{C}_q\otimes\mathscr{C}_q$$

as the homomorphic extension of

$$\Delta(1)=1\otimes1, \quad \Delta(t^\sigma)=t^\sigma\otimes t^\sigma, \quad \Delta(v)=t^{-1}\otimes v+v\otimes t$$

where $v\in\mathscr{V}$. Further, let δ be the counit defined by $\delta(1)=\delta(t)=\delta(t^{-1})=1$, $\delta(v)=0$, $v\in\mathscr{V}$.

III. CENTRAL LIMIT THEOREM FOR FIXED INTERVAL

In this section we first introduce the increments Δ_{rs}^N. Then we calculate the variance $\hat{\phi}(\Delta_{rs}^N(v^*)\Delta_{rs}^N(v))$ for $v \in \mathscr{V}_+$ in order to find a suitable normalization. Then we define the normalized increments S_{rs}^N and state the qclt for fixed $r \leqslant s$.

Let $\mathscr{C}_q^{\otimes\infty}$ be the infinite tensor product of the $*$-algebra $\mathscr{C}_q$. Let ϕ be a state on $\mathscr{C}_q$ such that $\phi(t^\sigma)=a^\sigma$. We define injections $j_i^{N_rN_s}:\mathscr{C}_q \to \mathscr{C}_q^{\otimes\infty}$ by

$$j_i^{N_rN_s}(w)=1^{\otimes N_r}\otimes(t^{-1})^{\otimes(i-N_r-1)}\otimes w\otimes t^{\otimes(N_s-i)}\otimes 1^{\otimes\infty}.$$

Further, let

$$\Delta_{rs}^N(w)=\sum_{i=N_r+1}^{N_s} j_i^{N_rN_s}(w)$$

and $\Delta_{rr}^N(w)=0$ for $w \in \mathscr{V}$ and

$$\Delta_{rs}^N(t^\sigma)=1^{N_r}\otimes(t^\sigma)^{\otimes(N_s-N_r)}\otimes 1^{\otimes\infty}.$$

Note that if $r=0$, $s=1$, then $N_r=0$, $N_s=N$, and the projection of Δ_{rs}^N onto $\mathscr{C}_q^{\otimes N}$ becomes the $N-1$-th iteration of the coproduct. In the case of $U_q(su(2))$ it can be seen that Δ_{rs}^N is a Hopf algebra homomorphism for any pair $r<s$ and $N \in \mathbf{N}$.

We also assume that $\phi \in \mathscr{C}_q^*$ is *left and right* $\mathbf{C}[t,t^{-1}]=\mathscr{C}_q^{(0)}$*- independent*, i.e.,

$$\phi(acb)=\phi(a)\phi(c)\phi(b)$$

for any $a,b \in \mathscr{C}^{(0)}$. It should be noted that the Cauchy–Schwartz inequality implies that if ϕ is a state and a homomorphism on $\mathscr{C}_q^{(0)}$, then it is $\mathscr{C}_q^{(0)}$-independent. Also, we shall assume that ϕ is *even*, i.e., vanishes outside of $(\mathscr{C}_q)_{(0)}$. In particular, this implies that the first moments of $w \in \mathscr{V}$ vanish.

Proposition 3.1. *Let* $v \in \mathscr{V}_+$ *and let* ϕ *be an even functional and let* $\phi(t^\sigma)=a^\sigma \in \mathbf{R}^+-\{1\}$. *Then*

$$\hat{\phi}(\Delta_{rs}^N(v^*)\Delta_{rs}^N(v))=N_{rs}\phi(v^*v)$$

where $N_{rs}=[N_s-N_r]$ *and* $[x]=(a^{2x}-a^{-2x})/(a^2-a^{-2})$.

Proof. Since ϕ is even, we obtain

$$\begin{aligned}
\hat{\phi}(\Delta_{rs}^N(v^*)\Delta_{rs}^N(v)) &= \hat{\phi}\left(\sum_{i=N_r+1}^{N_s} j_i^{N_rN_s}(v^*)j_i^{N_rN_s}(v)\right)\\
&= \hat{\phi}\left(\sum_{i=N_r+1}^{N_s} 1^{\otimes N_r}\otimes(t^{-2})^{\otimes(i-N_r-1)}\otimes v^*v\otimes(t^2)^{\otimes(N_s-i)}\otimes 1^{\otimes\infty}\right)\\
&= \phi(v^*v)\sum_{i=N_r+1}^{N_s} a^{-2(i-N_r-1)+2(N_s-i)}\\
&= \phi(v^*v)a^{2N_s+2N_r+2}\sum_{i=N_r+1}^{N_s} a^{-4i}\\
&= \phi(v^*v)\frac{a^{2N_s-2N_r}-a^{-2N_s+2N_r}}{a^2-a^{-2}}=\phi(v^*v)N_{rs}. \qquad \square
\end{aligned}$$

Besides, it is clear that

$$\hat{\phi}(\Delta_{rs}^N(t^\sigma)\Delta_{rs}^N(t^\sigma))=a^{2\sigma(N_s-N_r)}.$$

This allows us to take normalized increments of the form

$$S_{rs}^N(w)=\sqrt{\frac{a_{rs}}{N_{rs}}}\Delta_{rs}^N(w)$$

for $w\in\mathscr{V}$, where $a_{rs}=[s-r]$. Then the normalization constants $\sqrt{a_{rs}/N_{rs}}=\sqrt{[s-r]/[N_s-N_r]}$ are the analogs of $\sqrt{(s-r)/(N_s-N_r)}$. Later, when considering the quantum noise obtained from $U_q(su(2))$, we will put $a=q$, which appears in the commutation factor, obtaining the simplest example of a one-parameter q-noise. Then q_{rs} will stand for the variance of that q-noise. Clearly, we also have

$$S_{rs}^N(t^\sigma)=a^{\sigma(N_r-N_s)}\Delta_{rs}^N(t^\sigma).$$

Moreover, we put $S_{rs}^N(c_1c_2)=S_{rs}^N(c_1)S_{rs}^N(c_2)$. It can be shown that with the canonical product on $\mathscr{C}^{\otimes\infty}$, the increments Δ_{rs}^N, viewed as functions of r,s, satisfy (WN1–WN4). However, it is not the case for the normalized non-additive increments.

Let us now define a two-parameter functional $\Psi_{a,q}\equiv\Psi$ on the free algebra with unity generated by $\mathscr{V}$, obtained in the qclt studied in Refs. 20–22. Let $v_1,\ldots,v_p\in\mathscr{V}$. For an ordered partition $S=(S_1,\ldots,S_r)$ of $I=\{1,\ldots,p\}$ we denote by

$$v_{S_j}=\prod_{i\in S_j} v_i$$

where the product is taken in the ascending order of indices. Then, let

$$\Psi(v_1\ldots v_p)=\sum_{r=1}^{p}\sum_{S=(S_1,\ldots,S_r)\in\mathscr{P}_e^{ord}(I)} Q(S)D(S|a)\prod_{j=1}^{r}\phi(v_{S_j})$$

where

$$D(S|a)=D_{k,r}(\gamma_{S_1},\ldots,\gamma_{S_r}|a)=\frac{(a^{-4}-1)^{p/2}}{(a^{-2\gamma_{S_1}}-1)(a^{-2\gamma_{S_1}-2\gamma_{S_2}}-1)\ldots(a^{-2\gamma_{S_1}-\cdots-2\gamma_{S_r}}-1)}$$

for $0<a<1$, and $D(S|a)=D({}^rS|a^{-1})$ for $1<a<\infty$. Here, $Q(S)$ denotes the combinatorial q-dependent commutation factor:

$$Q(S)=\prod_{(i,j)\in W_S}\epsilon(v_i,v_j)$$

where $\epsilon(v_i,v_j)=\epsilon(t,v_i)\epsilon(t,v_j)$. In particular, when $a=q$ we obtain the limit functional considered in Ref. 21, to which we will restrict our attention when constructing the q-noise.

For fixed $r\leqslant s$, the following q-analog of the qclt is merely the theorem proved in Ref. 23, restated in the new context.

Theorem 3.2. *Let $v_1,\ldots,v_p\in\mathscr{V}$. Let $\phi\in\mathscr{C}_q^*$ be an even functional that is left and right $\mathscr{C}_q^{(0)}$-independent with $\phi(t)=a\in\mathbf{R}^+-\{1\}$. Then, if $p=2k$,*

$$\lim_{N\to\infty}\hat{\phi}(S_{rs}^N(v_1)\ldots S_{rs}^N(v_p))=\Psi(B_{rs}(v_1)\ldots B_{rs}(v_p))$$

where $\Psi(B_{rs}(v_1)\ldots B_{rs}(v_p))\equiv a_{rs}^k\Psi(v_1\ldots v_p)$. *If p is odd, then the above limit vanishes.*

In the sequel we will generalize this theorem to correlations indexed by arbitrary (in general, different) time intervals.

IV. CLUSTERING AND FACTORIZATION LEMMAS

Two main features of the limiting functional we are going to obtain are factorization and ''clustering.'' Factorization of the correlations for disjoint time-intervals taken in the increasing order may be considered as standard and it can be easily proven to hold also in our case. However, we will show that for $a<1$ $(a>1)$ the limiting correlations also factorize if the upper (lower) end-points of time intervals are different. On the other hand, increments that have the same upper (lower) end points cluster together for $a<1$ $(a>1)$, thus giving rise to the property we call clustering. This allows us to express the limiting correlations as linear combinations of products of clustered correlations. It can also be noticed that the case $a>1$ is analogous to the case $a<1$ and therefore we will provide proofs only for the former and merely state the corresponding results for the latter. In the sequel the symbol $\times$ will always denote multiplication of numbers and is used for notational clarity.

Lemma 4.1 (Clustering Lemma). *Let* $v_1,\ldots,v_p\in\mathscr{V}$. *Suppose that* $\phi\in\mathscr{C}_q^*$ *is left and right* $\mathscr{C}_q^{(0)}$*- independent and even. Let* $\phi(t)=a<1$. *If* $s_1=s_2=\ldots=s_p$ *and* $r_i\leqslant s_i$, *then*

$$\lim_{N\to\infty}\hat{\phi}(S^N_{r_1s_1}(v_1)\ldots S^N_{r_ps_p}(v_p))=\Psi(B_{r_1s_1}(v_1)\ldots B_{r_ps_p}(v_p))$$

where $\Psi(B_{r_1s}(v_1)\ldots B_{r_ps}(v_p))\equiv\sqrt{\Pi_{i=1}^p a_{r_is}}\Psi(v_1\ldots v_p)$. *In particular, when p is odd, then the above limit vanishes.*

Proof. We prove only the non-trivial case, when $r_i<s_i$ for all $i=1,\ldots,p$. First we consider the special case of ordered lower end-points, which we choose to prove by induction with respect to the number of blocks for which the lower end-points of time intervals coincide. A sketch of the proof of the general case will be given below.

Thus, let n be the number of blocks with different lower end-points and let $I_1,\ldots,I_n$ be the index sets associated with those blocks. We put

$$v_{I_i}=\prod_{j\in I_i}v_j.$$

First we will calculate the limit of

$$\hat{\phi}(S^N_{r_1s_1}(v_{I_1})\ldots S^N_{r_ns_n}(v_{I_n}))$$

with $s_1=s_2=\ldots=s_p>r_1>r_2>\ldots>r_p$, i.e., in the case of ordered lower end-points. The case $n=1$ follows from Theorem 3.1. Suppose the statement holds for $n=k$. For notational convenience we put $r_{k+1}=r$, $s_{k+1}=s$, $r_k=t$. We also put $I_{k+1}=I$. Then we have

$$S^N_{rs}(v_j)=\alpha_{rts}S^N_{rt}(v_j)\Delta^N_{ts}(t)+\beta_{rts}\Delta^N_{rt}(t^{-1})S^N_{ts}(v_j)$$

for any $j\in I$, where $\alpha_{rts}=\sqrt{(a_{rs}N_{rt})/(a_{rt}N_{rs})}$ and $\beta_{rts}=\sqrt{(a_{rs}N_{ts})/(a_{ts}N_{rs})}$. Now,

$$\begin{aligned}M_N&\equiv\hat{\phi}(S^N_{r_1s_1}(v_{I_1})\ldots S^N_{r_ks_k}(v_{I_k})S^N_{rs}(v_I))\\&=\sum_{\{J,K\}\in\mathscr{P}(I)}c_{JK}\alpha_{rts}^{|J|}\beta_{rts}^{|K|}\hat{\phi}(S^N_{r_1s_1}(v_{I_1})\ldots S^N_{r_ks_k}(v_{I_k})S^N_{rt}(v_K)\Delta_{rt}(t^{|J|}))\\&\quad\times\hat{\phi}(\Delta_{ts}(t^{-|K|})S^N_{ts}(v_J))\end{aligned}$$

where $|J|$, $|K|$ denote cardinalities of the sets J and K, respectively, and c_{JK} are constants obtained from commutations. Using left and right $\mathscr{C}^{(0)}$-independence of ϕ, we obtain

$$M_N=\sum_{\{J,K\}\in\mathscr{P}(I)} c_{JK}\alpha_{rts}^{|J|}\beta_{rts}^{|K|}a^{(N_s-N_t)|J|-(N_t-N_r)|K|} \times\hat{\phi}(S^N_{r_1s_1}(v_{I_1})\ldots S^N_{r_ks_k}(v_{I_k})S^N_{rt}(v_K))\hat{\phi}(S^N_{ts}(v_J)).$$

The N-dependent parts of the coefficients are of the form:

$$\left(\frac{N_{rt}}{N_{rs}}\right)^{|J|/2}\left(\frac{N_{ts}}{N_{rs}}\right)^{|K|/2}a^{(N_s-N_t)|J|-(N_t-N_r)|K|}$$

and, if $0<a<1$, behave for large N as

$$\frac{a^{(N_r-N_t)|J|+(N_t-N_s)|K|}}{a^{(N_r-N_s)(|J|+|K|)}}a^{(N_s-N_t)|J|-(N_t-N_r)|K|}=a^{2(N_s-N_t)|J|}\to 0$$

unless $|J|=0$. Notice that for $J=\emptyset$ we have $c_{JK}=1$ and the above expression is equal to 1. Collecting the N-independent part of the coefficients α_{rts}, β_{rts} and using the induction hypothesis we obtain

$$\begin{aligned}\lim_{N\to\infty}M_N&=\left(\frac{a_{rs}}{a_{ts}}\right)^{|I|/2}\lim_{N\to\infty}\hat{\phi}(S^N_{r_1s_1}(v_{I_1})\ldots S^N_{r_ks_k}(v_{I_k})S^N_{r_ks_k}(v_{I_{k+1}}))\\&=\left(\frac{a_{rs}}{a_{ts}}\right)^{|I|/2}a_{ts}^{|I|/2}\left(\prod_{i=1}^{k}a_{r_is_i}^{|I_i|/2}\right)\Psi(v_1\ldots v_p)\\&=\left(\prod_{i=1}^{k+1}a_{r_is_i}^{|I_i|/2}\right)\Psi(v_1\ldots v_p)\end{aligned}$$

which finishes the proof in the case of ordered lower end-points. The general case is proved along the same lines. Namely, we put $R=\max\{r_1,\ldots,r_p\}$ and we decompose each $S_{r_is}(v_i)$ for all $r_i<R$ as above, i.e.:

$$S^N_{r_is}(v_i)=\alpha_{r_iRs}S^N_{r_iR}(v_i)\Delta^N_{Rs}(t)+\beta_{r_iRs}\Delta^N_{r_iR}(t^{-1})S^N_{Rs}(v_i).$$

Then the proof boils down to showing that any non-zero power of α_{r_iRs} makes the term disappear in the limit. The argument is similar to the one presented above. Namely, each α_{r_iRs} produces the N-dependent factor of the form $a^{2(N_s-N_R)}$, which goes to zero as $N\to\infty$. Thus, the only surviving terms are those involving $S^N_{Rs}(v_i)$ only. This finishes the proof. □

Lemma 4.2 (Factorization Lemma). *Let $v_1,\ldots,v_p\in\mathscr{V}$. Suppose that $\phi\in\mathscr{C}_q^*$ is left and right $\mathscr{C}_q^{(0)}$ -independent and even. Let $\phi(t)=a<1$. If $s_1\leqslant s_2\leqslant\ldots\leqslant s_p$, then*

$$\lim_{N\to\infty}\hat{\phi}(S^N_{r_1s_1}(v_1)\ldots S^N_{r_ps_p}(v_p))=\Psi\left(\prod_{i\in I_1}B_{r_is_i}(v_i)\right)\times\ldots\times\Psi\left(\prod_{i\in I_n}B_{r_is_i}(v_i)\right)$$

where $s_1=\ldots=s_{j_1}<\ldots<s_{j_{n-1}+1}=\ldots=s_{j_n}=s_p$ defines the partition $\{I_1,\ldots,I_n\}$ of $\{1,\ldots,p\}$ into subsets corresponding to equal upper end-points of the time intervals. In particular, if any of $v_{I_1},\ldots,v_{I_n}$, where $v_{I_i}=\prod_{i\in I_i}v_i$, is odd with respect to either of the gradations, then the limit vanishes.

Proof. The case $n=1$ is just the statement of the Clustering Lemma. Assume now that this lemma holds for $n=k$ blocks. Add block $I_{k+1}=I$ and let $I'=\{i \in I | r_i<s_k\}$, i.e., the subset of those indices i in I, for which time intervals $[r_i,s_i)$ are non-disjoint from all intervals associated with I_k. For any v_i, $i \in I'$, we use the decomposition familiar from the proof of the Clustering Lemma:

$$S^N_{r_i s}(v_i)=\alpha_{r_i ts}S^N_{r_i t}(v_i)\Delta^N_{ts}(t)+\beta_{r_i ts}\Delta^N_{r_i t}(t^{-1})S^N_{ts}(v_i)$$

where we denoted $s_i=s$ for any $i \in I'$. Then, supposing that the last block consists of l elements, we obtain

$$\begin{aligned}
M_N &\equiv \hat{\phi}(S^N_{r_1 s_1}(v_1)\ldots S^N_{r_p s_p}(v_p)S^N_{r_{p+1},s}(v_{p+1})\ldots S^N_{r_{p+l},s}(v_{p+l}))\\
&= \sum_{\{J,K\}\in\mathscr{P}(I')} c_{JK}\left(\prod_{j\in J}\alpha_{r_j ts}\right)\left(\prod_{k\in K}\beta_{r_k ts}\right)\\
&\quad\times\hat{\phi}\left(S^N_{r_1 s_1}(v_1)\ldots S^N_{r_p s_p}(v_p)\prod_{j\in J}S^N_{r_j t}(v_j)\prod_{k\in K}\Delta_{r_k t}(t^{-1})\right)\hat{\phi}\left(\Delta_{ts}(t^{|J|})\prod_{k\in K}S^N_{ts}(v_k)\right)\\
&= \sum_{\{J,K\}\in\mathscr{P}(I')} c_{JK}\left(\prod_{j\in J}\alpha_{r_j ts}\right)\left(\prod_{k\in K}\beta_{r_k ts}\right)\left(\prod_{k\in K}a^{-(N_t-N_{r_k})}\right)a^{(N_s-N_t)|J|}\\
&\quad\times\hat{\phi}\left(S^N_{r_1 s_1}(v_1)\ldots S^N_{r_p s_p}(v_p)\prod_{j\in J}S^N_{r_j t}(v_j)\right)\hat{\phi}\left(\prod_{k\in K}S^N_{ts}(v_k)\right)
\end{aligned}$$

where c_{JK} are constants resulting from commutations. As in the proof of the Clustering Lemma, consider the N-dependent part of each numerical coefficient appearing in the sum. It is of the following form:

$$a^{(N_s-N_t)|J|}\left(\prod_{j\in J}\left(\frac{N_{r_j t}}{N_{r_j s}}\right)^{1/2}\right)\left(\prod_{k\in K}\left(\frac{N_{ts}}{N_{r_k s}}\right)^{1/2}a^{N_{r_k}-N_t}\right)$$

which, for $0<a<1$ and large N, behaves like

$$\prod_{j\in J}\left(\frac{a^{N_{r_j}-N_t}}{a^{N_{r_j}-N_s}}a^{N_s-N_t}\right)\prod_{j\in J}\left(\frac{a^{N_t-N_s}}{a^{N_{r_k}-N_s}}a^{N_{r_k}-N_t}\right)=\prod_{j\in J}a^{2(N_s-N_t)}=a^{2|J|(N_s-N_t)}$$

and thus tends to zero when N tends to infinity unless $|J|=0$, when it goes to one. Thus the only term that survives in the limit is the one corresponding to $|J|=0$. Hence,

$$\lim_{N\to\infty}M_N=\prod_{i\in I'}\left(\frac{a_{r_i s}}{a_{ts}}\right)\lim_{N\to\infty}\hat{\phi}(S^N_{r_1 s_1}(v_1)\ldots S^N_{r_p s_p}(v_p))\lim_{N\to\infty}\hat{\phi}(S^N_{R_1,s}(v_{p+1})\ldots S^N_{R_l,s}(v_{p+l}))$$

where $R_i=\max\{r_{p+i},s_p\}$, $i=1,\ldots,l$. But the last expression is equal to

$$\left(\prod_{i=1}^{p+l}a^{1/2}_{r_i s_i}\right)\Psi(v_{I_1})\ldots\Psi(v_{I_k})\Psi(v_I)=\Psi\left(\prod_{i\in I_1}B_{r_i s_i}(v_i)\right)\times\ldots\times\Psi\left(\prod_{i\in I_{k+1}}B_{r_i s_i}(v_i)\right).$$

□

Thus, the Factorization Lemma says that correlations factorize when they have different upper end-points.

The situation for $a>1$ is similar. We obtain the following.

Lemma 4.1.* *Let $v_1,\ldots,v_p \in \mathscr{V}$. Suppose that $\phi \in \mathscr{C}_q^*$ is left and right $\mathscr{C}_q^{(0)}$- independent and even. Let $\phi(t)=a>1$. If $r_1=r_2=\ldots=r_p$ and $r_i \leqslant s_i$, then*

$$\lim_{N\to\infty} \hat{\phi}(S^N_{r_1s_1}(v_1)\ldots S^N_{r_ps_p}(v_p))=\Psi(\widetilde{B}_{r_1s_1}(v_1)\ldots\widetilde{B}_{r_ps_p}(v_p))$$

where $\Psi(\widetilde{B}_{r_1s_1}(v_1)\ldots\widetilde{B}_{r_ps_p}(v_p))=\sqrt{\prod_{i=1}^p a_{r_is_i}}\Psi(v_1\ldots v_p)$. In particular, when p is odd, then the above limit vanishes.

Lemma 4.2.* Let $v_1,\ldots,v_p \in \mathscr{V}$. Suppose that $\phi \in \mathscr{C}_q^*$ is left and right $\mathscr{C}_q^{(0)}$ -independent and even. Let $\phi(t)=a>1$. If $r_1 \geqslant r_2 \geqslant \ldots \geqslant r_p$, then

$$\lim_{N\to\infty} \hat{\phi}(S^N_{r_1s_1}(v_1)\ldots S^N_{r_ps_p}(v_p))=\Psi\left(\prod_{i\in I_1}\widetilde{B}_{r_is_i}(v_i)\right)\times\ldots\times\Psi\left(\prod_{i\in I_n}\widetilde{B}_{r_is_i}(v_i)\right)$$

where $r_1=\ldots=r_{j_1}>\ldots>r_{j_{n-1}+1}=\ldots=r_{j_n}=r_p$ defines the partition $\{I_1,\ldots,I_n\}$ of $\{1,\ldots,p\}$ into subsets associated with equal lower end-points of the time intervals. In particular, if any of $v_{I_1},\ldots,v_{I_n}$, where $v_{I_i}=\Pi_{i\in I_i}v_i$, is odd with respect to either of the gradations, then the limit vanishes.

It should be remembered that the dependence of Ψ on q and a is suppressed in the formulas given above.

V. CENTRAL LIMIT THEOREM FOR SAMPLE SUMS

We are ready to state the qclt for sample sums, of which Theorem 3.2 as well as the Clustering and Factorization Lemmas are special cases. In fact, the general case looks similar to the Factorization Lemma, except that we don't assume any ordering of the end-points, the only restriction being $r_i \leqslant s_i$ for all $i=1,\ldots,p$. Without loss of generality we assume that $r_i<s_i$, since if $r_i=s_i$ for any i, then the limit trivially vanishes.

For a given set of time intervals $T=\{[r_i,s_i)|i=1,\ldots,p\}$ let $\{I_1,\ldots,I_n\}$ be the partition of $\{1,\ldots,p\}$ into subsets for which upper (lower) end-points are equal for $a<1(a>1)$. Let us concentrate on the case $a<1$. Thus, for any $j,k \in I_i$ we have $s_j=s_k$ and for any $j \in I_i$, $k \in I_m$, $i \neq m$, we have $s_j \neq s_k$. Further, fix the order on $\{I_1\ldots,I_n\}$ according to increasing upper end-points, i.e., if $j \in I_i, k \in I_m$, then $s_j<s_k$.

We are going to express the limiting correlations

$$\lim_{N\to\infty} \hat{\phi}(S^N_{r_1s_1}(v_1)\ldots S^N_{r_ps_p}(v_p))=\begin{cases}\Psi(B_{r_1s_1}(v_1)\ldots B_{r_ps_p}(v_p)) & \text{if} \quad a<1,\\ \Psi(\widetilde{B}_{r_1s_1}(v_1)\ldots\widetilde{B}_{r_ps_p}(v_p)) & \text{if} \quad a>1\end{cases}$$

in terms of the products appearing in Lemmas 4.2., 4.2.*, except for certain commutation factors.

We concentrate on the case of $a<1$. To bring the above correlation into the product form we need to commute certain operators. That is why we associate with the set T the set of inversions of the upper end-points of time intervals, i.e.,

$$I_T=\{(s_i,s_j)|i<j, s_i>s_j, [r_i,s_i)\cap[r_j,s_j)\neq\emptyset\}.$$

Clearly, if $[r_i,s_i)\cap[r_j,s_j)=\emptyset$, then the variables commute, therefore there is no need to consider such inversions. On the other hand, each inversion $(s_i,s_j) \in I_T$ contributes a non-trivial commutation factor. Further, for given $v_1\ldots,v_p \in \mathscr{V}$, let

$$I_{T^+}=\{(s_i,s_j)\in I_T|v_j\in V_+\}, \quad I_{T^-}=\{(s_i,s_j)\in I_T|v_j\in V_-\}.$$

Our aim now is to determine the commutation factors resulting from the commutations that need to be performed in order to bring the products into their ordered forms as in the Factorization Lemma. It is also perhaps interesting to note that no simple commutation relations can be derived for $S^N_{rs}(w)$'s for non-disjoint (but not equal) time intervals. However, in the limit the (weak) commutation relations are much simpler.

Proposition 5.1. *Let* $w,w' \in \mathscr{V}$. *If* $[r,s)\cap[r',s')=\emptyset$, *then* $B_{rs}(w)$ *and* $B_{r's'}(w')$ *commute. If* $[r,s)\cap[r',s') \neq \emptyset$, $s>s'$, *then*

$$B_{rs}(w)B_{r's'}(w')=q^{2d(w')}B_{r's'}(w')B_{rs}(w).$$

Proof. Consider two cases: Case A: $r\geqslant r'$, and Case B: $r<r'$.

Case A. Let

$$S^N_{rs}(w)=\alpha_{rs's}S^N_{rs'}(w)\Delta^N_{s's}(t)+\beta_{rs's}\Delta^N_{rs'}(t^{-1})S^N_{s's}(w).$$

We showed in the proofs of the Lemmas that each $a^{N_s-N_{s'}}\alpha_{rs's}$ goes to zero when $N\to\infty$, hence only the second summand gives a non-zero contribution to the limit. Hence, when commuting $S^N_{rs}(w)$ through $S^N_{r's'}(w)$, we only need to commute $\Delta^N_{rs'}(t^{-1})S^N_{s's}(w)$ through $S^N_{r's'}(w')$. Using

$$[S^N_{s's}(w),S^N_{r's'}(w')]=0$$

and

$$[\Delta^N_{rs'}(t^{-1}),S^N_{r's'}(w')]=\epsilon(t^{-1},w')=q^{2d(w')},$$

we obtain the result.

Case B. Let $r_1>r_2$. We decompose both $S^N_{rs}(w)$ and $S^N_{r's'}(w')$, the first one in the same manner as in Case A, and the second one as

$$S^N_{r's'}(w')=\alpha_{r'rs'}S^N_{r'r}(w')\Delta^N_{rs'}(t)+\beta_{r'rs'}\Delta^N_{r'r}(t^{-1})S^N_{rs'}(w').$$

In the (weak) limit only the second terms survive in both decompositions. Hence, the commutation factor obtained in the limit comes from commuting $\Delta^N_{rs'}(t^{-1})S^N_{s's}(w)$ through $\Delta^N_{r'r}(t^{-1})S^N_{rs'}(w')$, thus it is equal to the commutator

$$[\Delta^N_{rs'}(t^{-1}),S^N_{rs'}(w')]=\epsilon(t^{-1},w').$$

This finishes the proof. □

Theorem 5.2. *Let* $v_1,\ldots,v_p \in \mathscr{V}$. *Let* $\phi \in \mathscr{C}_q^*$ *be left and right* $\mathscr{C}^{(0)}$*-independent and even and let* $q \in \mathbf{R}^+$. *Further, if* $\phi(t)=a<1$, *suppose that* $r_j\leqslant s_j$, $j=1,\ldots,p$, *and denote by* $\{I_1,\ldots,I_n\}$ *the partition of* $\{1,\ldots,p\}$ *into subsets corresponding to equal upper end-points of the time intervals. Then*

$$\lim_{N\to\infty}\hat{\phi}(S^N_{r_1,s_1}(v_1)\ldots S^N_{r_p,s_p}(v_p))=Q_T\Psi\left(\prod_{i\in I_1}B_{r_is_i}(v_i)\right)\times\ldots\times\Psi\left(\prod_{i\in I_n}B_{r_is_i}(v_i)\right)$$

where

$$Q_T=q^{2|I_{T^+}|-2|I_{T^-}|}$$

denotes the commutation factor resulting from commuting variables associated with time intervals with different upper end-points.

Proof. Immediate from the Factorization Lemma, Proposition 5.1 and the relations: $\epsilon(t^{-1},v)=q^2$, $\epsilon(t^{-1},v^*)=q^{-2}$, for $v \in \mathscr{V}_+$.

Thus, we can characterize our limiting process using the following notion of independence:
(F) the factorization principle:

$$\Psi(B_{r_1s_1}(v_1)\ldots B_{r_ps_p}(v_p))=\Psi\left(\prod_{i\in I_1} B_{r_is_i}(v_i)\right)\times\ldots\times\Psi\left(\prod_{i\in I_n} B_{r_is_i}(v_i)\right)$$

where $I_1,\ldots,I_n$ are as in Theorem 5.2;
(C) commutations for disjoint intervals:

$$B_{rs}(w)B_{r's'}(w')=B_{r's'}(w')B_{rs}(w);$$

(qC) q-commutations for non-disjoint intervals with $s'>s$:

$$B_{rs}(w)B_{r's'}(w')=q^{2d(w')}B_{r's'}(w')B_{rs}(w).$$

Thus, (F) together with (C) and (qC) give (QN1), which can be viewed as the definition of independence.

The following Corollary gives the limiting correlations in a more explicit form.

Corollary 5.3. *Under the assumptions of Theorem 5.2 we obtain*

$$\Psi(B_{r_1s_1}(v_1)\ldots B_{r_ps_p}(v_p))=\sum_{\mathbf{I}\in\mathscr{P}_e^I\{1,\ldots,p\}} Q(\mathbf{I})D(\mathbf{I})\prod_{i=1}^{n}\prod_{j=1}^{r_i}\phi(v_{S_j^i})$$

where

$$Q(\mathbf{I})=Q(I_1)\ldots Q(I_n)Q_T,\quad D(\mathbf{I})=D(I_1|a)\ldots D(I_n|a)$$

and I is the partition $\{I_1,\ldots,I_n\}$ and the summation runs over all even ordered subpartitions **I** *associated with I.*

Note that for a given ordered subpartition **I** associated with the partition I, the commutation factor $Q(\mathbf{I})$ is the product of commutation factors associated with ordered partitions of $I_1,\ldots,I_n$, respectively, resulting from the commutations with t,t^{-1} within blocks that have the same upper (lower) end-points, and Q_T resulting from the commutations bringing the product into the ordered form.

The case $a>1$ is completely analogous. As a result we obtain the analogs of Proposition 5.1, Theorem 5.2 and Corollary 5.2 with

$$\widetilde{Q}_T=q^{2|I_{T^-}|-2|I_{T^+}|}$$

and $\widetilde{D}(\mathbf{I})=D({}^rI_1|a^{-1})\ldots D({}^rI_n|a^{-1})$. They lead to
(F*) the factorization principle:

$$\Psi(\widetilde{B}_{r_1s_1}(v_1)\ldots\widetilde{B}_{r_ps_p}(v_p))=\Psi\left(\prod_{i\in I_1}\widetilde{B}_{r_is_i}(v_i)\right)\times\ldots\times\Psi\left(\prod_{i\in I_n}\widetilde{B}_{r_is_i}(v_i)\right)$$

where $I_1,\ldots,I_n$ denotes the partition of $\{1,\ldots,p\}$ into subsets corresponding to equal lower end-points of the time intervals,
(C*) commutations for disjoint intervals;

$$B\tilde{}_{rs}(w)\tilde{B}_{r's'}(w')=\tilde{B}_{r's'}(w')\tilde{B}_{rs}(w);$$

(qC^*) q-commutations for non-disjoint intervals with $r<r'$:

$$B\tilde{}_{rs}(w)\tilde{B}_{r's'}(w')=q^{-2d(w')}\tilde{B}_{r's'}(w')\tilde{B}_{rs}(w).$$

The results obtained thus far can be easily generalized to include $S^N_{rs}(t)$, $S^N_{rs}(t^{-1})$, but the limits obtained then can be expressed in terms of correlations without t,t^{-1}, as in Theorem 5.2, except that a different commutation factor replaces Q_T.

VI. AN EXAMPLE OF QUANTUM NOISE

In this section we apply our results to $\mathscr{C}_q=U_q(su(2))$, for which we give the realization of the limiting quantum stochastic processes $B_{rs}(v)$, $B_{rs}(v^*)$ ($\tilde{B}_{rs}(v)$, $\tilde{B}_{rs}(v^*)$) as creation and annihilation operators, respectively, living in a Hilbert space of Fock type. More specifically, they will be defined on a subspace of the full Fock space

$$\Gamma_f(\mathscr{H})=\bigoplus_{n\geq 0}\mathscr{H}^{\otimes n}$$

where $\mathscr{H}^{\otimes 0}=\mathbf{C}$, $\mathscr{H}=\mathscr{H}_0\otimes\mathscr{H}_1$, where $\mathscr{H}_0=\mathbf{C}^2$ and $\mathscr{H}_1=l^2[0,\infty)$. Let ω be the vacuum vector of the two-dimensional representation π of $U_q(su(2))$ and ϕ the corresponding vacuum state. Thus, we have $\phi(v^*v)=1$, $\phi(vv)=\phi(v^*v^*)=\phi(vv^*)=0$. Further, let $\phi(t)=q$, $\phi(t^{-1})=q^{-1}$.

In $\mathscr{H}_1$ we distinguish functions

$$\delta_p(x)=\begin{cases}1 & \text{if } x=p\\ 0 & \text{otherwise}\end{cases},$$

and the scalar product on $\mathscr{H}_0$ is given by $\langle\delta_p,\delta_r\rangle=\delta_{pr}$. Now, let D be the linear span of vectors

$$f_1\otimes\ldots\otimes f_p \quad \text{and} \quad \Omega=1,$$

where $f_i=\pi(v)\omega\otimes\delta_{s_i}$ and $s_1\leq s_2\leq\ldots\leq s_p$. For a given $f=\pi(v)\omega\otimes\delta_s$ we will refer to s as the support of f. The ordering of supports defines the partition $\{I_1,\ldots,I_n\}$ of $\{1,\ldots,p\}$ and we can write

$$f_1\otimes\ldots\otimes f_p=\bigotimes_{j=1}^{n}F_j$$

where $F_j=\bigotimes_{i\in I_j}f_i$. Moreover, we introduce the following notation

$$F_{s)}=\bigotimes_{s_j<s}f_j,\quad F_s=\bigotimes_{s_j=s}f_j,\quad F_{(s}=\bigotimes_{s_j>s}f_j.$$

Thus, we can also write

$$f_1\otimes\ldots\otimes f_p=F_{s)}\otimes F_s\otimes F_{(s}$$

for any $s\in\{s_1,\ldots,s_p\}$.

We also introduce the number operator

$$\hat{N}_s(f_1\otimes\ldots\otimes f_p)=N_s(f_1\otimes\ldots\otimes f_p)$$

where $N_s=\#\{s_i|s_i=s\}$. Thus, it counts functions with support s. Similarly we define other number operators, such as $\hat{N}_{(r,s)}$, $\hat{N}_{s)}$, $\hat{N}_{s]}$, with eigenvalues $N_{(r,s)}=\#\{s_i|s_i\in(r,s)\}$, $N_{s)}=\#\{s_i|s_i<s\}$, $N_{s]}=\#\{s_i|s_i\leqslant s\}$, respectively. In other words, those operators count functions whose time support falls into appropriate intervals. We will also need number operators that give us information on the supports of functions with indices smaller than or equal to k. Thus, we define $\hat{N}_s^k$ and $\hat{N}_{(r,s)}^k$ with eigenvalues $N_s^k=\#\{s_i|s_i=s,i\leqslant k\}$ and $N_{(r,s)}^k=\#\{s_i|s_i\in(r,s),i\leqslant k\}$, respectively.

We first define creation operators $B_{rs}(v)$ and annihilation operators $B_{rs}(v^*)$ (by abuse of notation we use the same notation as in the weak case) on the subspace D_s of D spanned by the vacuum vector and tensor products of functions with support equal to s. Thus, let

$$B_{rs}(v)\Omega=\sqrt{q_{rs}}\,f,$$

$$B_{rs}(v)(f_1\otimes\ldots\otimes f_p)=\sqrt{q_{rs}}\,f\otimes f_1\otimes\ldots\otimes f_p$$

be the creation operators, where $f=\pi(v)\omega\otimes\delta_s$, and let

$$B_{rs}(v^*)\Omega=0,$$

$$B_{rs}(v^*)(f_1\otimes\ldots\otimes f_p)=\sqrt{q_{rs}}\sum_{k=1}^{p}q^{4(p-k)}f_1\otimes\ldots f_{k-1}\otimes f_{k+1}\otimes\ldots\otimes f_p$$

be the annihilation operators. In fact, we could write the action of $B_{rs}(v)$, $B_{rs}(v^*)$ on vectors of the form $f^{\otimes p}$, but we choose the above definition, which is open for generalizations and bears resemblance to the one-particle case of the Fock space considered in Ref. 11 (note that here $\langle f,f\rangle=1$).

Proposition 6.1. *On the subspace D_s of D spanned by the vacuum vector and tensor products of functions with support s, the following commutation relations hold:*

$$[B_{rs}(v^*),B_{r's}(v)]=\sqrt{q_{rs}q_{r's}}q^{4\hat{N}_s}.$$

Proof.

$$\begin{aligned}
&[B_{rs}(v^*),B_{r's}(v)]\,f_1\otimes\ldots\otimes f_p\\
&\quad=\sqrt{q_{rs}q_{r's}}\left(\sum_{k=1}^{p}q^{4(p-k)}f\otimes f_1\otimes\ldots\otimes f_{k-1}\otimes f_{k+1}\otimes\ldots\otimes f_p+q^{4p}f_1\otimes\ldots\otimes f_p\right)\\
&\qquad-\sqrt{q_{rs}q_{r's}}\sum_{k=1}^{p}q^{4(p-k)}f\otimes f_1\otimes\ldots\otimes f_{k-1}\otimes f_{k+1}\otimes\ldots\otimes f_p\\
&\quad=\sqrt{q_{rs}q_{r's}}q^{4p}f_1\otimes\ldots\otimes f_p.
\end{aligned}$$

□

We are now ready to consider the general case and define $B_{rs}(v)$ and $B_{rs}(v^*)$ on all of D. Of course, the action on the vacuum is the same as above. For other vectors with ordered support we define the creation operator as follows:

$$B_{rs}(v)(f_1\otimes\ldots\otimes f_p)=q^{2N_{(r,s)}F_{s)}}\otimes(B_{rs}(v)F_s)\otimes F_{(s}=\sqrt{q_{rs}}q^{2N_{(r,s)}F_{s)}},\otimes f\otimes F_s\otimes F_{(s}.$$

Thus we can say that the operator $B_{rs}(v)$ creates function $f=\pi(v)\omega\otimes\delta_s$ at the beginning of the block with the same time support s. If such a block does not exist in the string of functions, it

creates such a block at the right place. When passing through blocks with support smaller than s, it produces q^2 whenever that support falls into the interval (r,s); otherwise, it does not produce any non-trivial commutation factor.

In turn, the annihilation operators will be defined by

$$B_{rs}(v^*)(f_1\otimes\ldots\otimes f_p)=q^{2N_{(r,s)}}F_{s)}\otimes(B_{rs}(v^*)F_s)\otimes F_{(s}$$
$$=\sqrt{q_{rs}}q^{2N_{(r,s)}}\sum_{k=N_{s)}+1}^{N_{s]}}q^{4(N_s-N_s^k)}F_{s)}\otimes\Big(\bigotimes_{s_j=s,j\neq k}f_j\Big)\otimes F_{(s}.$$

If in the tensor product $f_1\otimes\ldots\otimes f_p$ there are no functions with support equal to s, then we put

$$B_{rs}(v^*)f_1\otimes\ldots\otimes f_p=0.$$

The action of the annihilation operators can of course be written using the scalar product on $\mathscr{H}_0$ and extending the summation over all indices and not only those corresponding to functions with support equal to s, but we choose the above definition for the sake of simplicity. Thus, in other words, the annihilation operator produces the same commutation factors when passing through functions with smaller support and then acts on the block with the same support as the annihilation operator defined previously. Clearly, the previous definitions are special cases of those just given.

Proposition 6.2. *Let $s>s'$ and $w,w'\in\mathscr{V}$. If $[r,s)\cap[r',s')=\varnothing$, then $B_{rs}(w)$ and $B_{r's'}(w')$ commute. If $[r,s)\cap[r',s')\neq\emptyset$, then*

$$B_{rs}(w)B_{r's'}(w')=q^{2d(w')}B_{r's'}(w')B_{rs}(w).$$

Proof. For $s>s'$ we have

$$B_{rs}(w)B_{r's'}(w')(f_1\otimes\ldots\otimes f_p)=B_{rs}(w)(q^{2N_{(r',s')}}F_{s')}\otimes(B_{r's'}(w')F_{s'})\otimes F_{(s')}$$
$$=q^{2N_{(r',s')}+2N_{(r,s)}+2d(w')}F_{s')}\otimes(B_{r's'}(w')F_{s'})$$
$$\otimes\Big(\bigotimes_{s'<r<s}F_r\Big)\otimes(B_{rs}(w)F_s)\otimes F_{(s}.$$

On the other hand,

$$B_{r's'}(w')B_{rs}(w)(f_1\otimes\ldots\otimes f_p)=B_{r's'}(w')(q^{2N_{(r,s)}}F_{s)}\otimes(B_{rs}(w)F_s)\otimes F_{(s)}$$
$$=q^{2N_{(r',s')}+2N_{(r,s)}}F_{s')}\otimes(B_{r's'}(w')F_{s'})$$
$$\otimes\Big(\bigotimes_{s'<r<s}F_r\Big)\otimes(B_{rs}(w)F_s)\otimes F_{(s}$$

where it is understood that $N_{(r,s)}$ and $N_{(r',s')}$ refer to $f_1\otimes\ldots\otimes f_p$. □

Proposition 6.3. *Let $w\in\mathscr{V}$. The following relations hold*

$$N_{(r',s')}B_{rs}(w)=B_{rs}(w)(N_{(r',s')}+d(w)\chi_{(r',s')}(s)),$$

$$N_{s'}B_{rs}(w)=B_{rs}(w)(N_{s'}+d(w)\delta_{s's})$$

where $\chi_{(r',s')}$ is the characteristic function.

Proof. Straightforward.

Finally, we derive the commutation relation between $B_{r's}(v^*)$ and $B_{rs}(v)$. Thus we have

Proposition 6.4. *The following relations hold on D:*

$$[B_{r's}(v^*),B_{rs}(v)]=\sqrt{q_{r's}q_{rs}}q^{2\hat{N}_{(r,s)}+2\hat{N}_{(r',s)}+4\hat{N}_s}$$

Proof. Using Proposition 6.1, we obtain

$$\begin{aligned}[B_{r's}(v^*),B_{rs}(v)](\ f_1\otimes\ldots\otimes f_p)&=q^{2N_{(r,s)}+2N_{(r',s)}}(F_s)\otimes([B_{r's}(v^*),B_{rs}(v)]F_s)\otimes F_{(s}\\&=q^{2N_{(r,s)}+2N_{(r',s)}}(F_s)\otimes(q^{4\hat{N}_s}F_s)\otimes F_{(s}\\&=\sqrt{q_{r's}q_{rs}}q^{2N_{(r,s)}+2N_{(r',s)}+4N_s}(F_s)\otimes F_s\otimes F_{(s}\\&=\sqrt{q_{r's}q_{rs}}q^{2N_{(r,s)}+2N_{(r',s)}+4N_s}(\ f_1\otimes\ldots\otimes f_p),\end{aligned}$$

which ends the proof. □

Let us define a scalar product on D. Thus, writing the vectors in the block form, we put

$$\langle\Omega,\Omega\rangle_q=1,\quad \langle\Omega,F_1\otimes\ldots\otimes F_n\rangle_q=0$$

and

$$\langle F_1\otimes\ldots\otimes F_n,G_1\otimes\ldots\otimes G_m\rangle_q=\delta_{nm}\prod_{i=1}^{n}\langle F_i,G_i\rangle_q$$

where, for blocks F,G with support s,s', respectively,

$$\langle F,G\rangle_q=\langle f_1\otimes\ldots\otimes f_p,g_1\otimes\ldots\otimes g_r\rangle_q=\delta_{ss'}\delta_{rp}[[p]]!$$

where $[[p]]=(1-q^{4p})/(1-q^4)$. Let us denote the completion of D with respect to $\langle .,.\rangle_q$ by $\Gamma_q(\mathscr{H})$.

We can now state the representation theorem.

Theorem 6.5. *Let $v_1,\ldots,v_p\in\mathscr{V}$, $\phi\in\mathscr{C}_q^*$ be the vacuum state of the two-dimensional fundamental representation of $U_q(su(2))$ and let $\phi(t)=q<1$. Then, for any $r_i\leqslant s_i$, $i=1,\ldots,p$,*

$$\Psi(B_{r_1s_1}(v_1)\ldots B_{r_ps_p}(v_p))=\langle\Omega,B_{r_1s_1}(v_1)\ldots B_{r_ps_p}(v_p)\Omega\rangle_q.$$

Moreover, $B_{rs}(v)$ and $B_{rs}(v^*)$ are adjoint with respect to $\langle .,.\rangle_q$.

Proof. The commutations and q-commutations for $B_{rs}(v)$ and $B_{rs}(v^*)$ (Proposition 6.2) agree with the weak ones derived in Proposition 5.1. The factorization (F) also holds and follows directly from the definition of the action of $B_{rs}(v)$, $B_{rs}(v^*)$. In turn, relations given by Proposition 6.1 were in the weak sense derived in Ref. 21 for $\Psi(B_{01}(v_1)\ldots B_{01}(v_p))$ and that implies that they hold for $\Psi(B_{r_1s}(v_1)\ldots B_{r_ps}(v_p))$ by the Clustering Lemma. Finally, adjointness follows from the definition of the scalar product. This finishes the proof. □

The case $q>1$ is analogous and we just state the results. Thus, we introduce $\widetilde{D}$ spanned by Ω and tensor products of functions from $\mathscr{H}$ with supports ordered in the decreasing order. On $\widetilde{D}$ we define the creation operators

$$\widetilde{B}_{rs}(v)(\ f_1\otimes\ldots\otimes f_p)=q^{-2N_{(r,s)}}F_{s)}\otimes(\widetilde{B}_{rs}(v)F_s)\otimes F_{(s},$$

and the annihilation operators

$$\widetilde{B}_{rs}(v^*)(\ f_1\otimes\ldots\otimes f_p)=q^{-2N_{(r,s)}}F_{s)}\otimes(\widetilde{B}_{rs}(v^*)F_s)\otimes F_{(s}$$

where, on D_r we have

$$\widetilde{B}_{rs}(v)(\ f_1\otimes\ldots\otimes f_p)=\sqrt{q_{rs}}\ f\otimes f_1\otimes\ldots\otimes f_p$$

and

$$\widetilde{B}_{rs}(v^*)(\ f_1\otimes\ldots\otimes f_p)=\sqrt{q_{rs}}\sum_{k=1}^{p}\ q^{-4(p-k)}f_1\otimes\ldots f_{k-1}\otimes f_{k+1}\otimes\ldots\otimes f_p,$$

with the usual action on the vacuum. Similar commutation relations can be established as for $B_{rs}(v)$, $B_{rs}(v^*)$.

Proposition 6.6. *Let $w,w'\in\mathscr{V}$. Then, if $r<r'$ and $[r,s)\cap[r',s')\neq\emptyset$, then*

$$\widetilde{B}_{rs}(w)\widetilde{B}_{r's'}(w')=q^{-2d(w')}\widetilde{B}_{r's'}(w')\widetilde{B}_{rs}(w).$$

For disjoint intervals, the operators commute. In turn,

$$N_{(r',s')}\widetilde{B}_{rs}(w)=\widetilde{B}_{rs}(w)(N_{(r',s')}+d(w)\chi_{(r',s')}(s)),$$

$$N_{s'}\widetilde{B}_{rs}(w)=\widetilde{B}_{rs}(w)(N_{s'}+d(w)\delta_{s's}).$$

Finally,

$$[\widetilde{B}_{r's}(v^*),\widetilde{B}_{rs}(v)]=\sqrt{q_{r's}q_{rs}}q^{-2\hat{N}_{(r,s)}-2\hat{N}_{(r',s')}-4\hat{N}_s}.$$

Thus, it can be seen that all relations can be obtained from the previous ones by replacing q by q^{-1}.

One can also take the limit $q\to1$. However, it is interesting to note that even then we don't obtain the Brownian motion, which is illustrated by the example below. Let $B_{0s}=B_s$. Then, if $s_1=\ldots=s_4=s$, we obtain

$$\Psi(B_{s_1}(v_1)\ldots B_{s_4}(v_4))=s^2(\phi(v_1v_2)\phi(v_1v_3)+\phi(v_1v_3)\phi(v_2v_4)+\phi(v_1v_4)\phi(v_2v_3)).$$

In turn, when there are two different endpoints, for instance

$$s_{i_1}=s_{i_2}=s\neq s'=s_{i_3}=s_{i_4}$$

then we obtain

$$\Psi(B_{s_1}(v_1)\ldots B_{s_4}(v_4))=ss'\phi(v_{i_1}v_{i_2})\phi(v_{i_3}v_{i_4}).$$

This fact shows the non-interchangeability of limits in q and N. Clearly, when we take first $q\to1$ and then $N\to\infty$, we obtain the quantum Brownian motion. In turn, when we take first $N\to\infty$ and then $q\to1$, then we obtain a different noise process.

It should be possible to generalize the approach presented in this paper to other quantum groups by using the more general kind of limit theorem proved in Ref. 23.

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Universality classes for asymptotic behavior of relaxation processes in systems with dynamical disorder: Dynamical generalizations of stretched exponential

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The asymptotic behavior of multichannel parallel relaxation processes for systems with dynamical disorder is investigated in the limit of a very large number of channels. An individual channel is characterized by a state vector **x** which, due to dynamical disorder, is a random function of time. A limit of the thermodynamic type in the **x**-space is introduced for which both the volume available and the average number of channels tend to infinity, but the average volume density of channels remains constant. Scaling arguments combined with a stochastic renormalization group approach lead to the identification of two different types of universal behavior of the relaxation function corresponding to nonintermittent and intermittent fluctuations, respectively. For nonintermittent fluctuations a dynamical generalization of the static Huber's relaxation equation is derived which depends only on the average functional density of channels, $\rho[W(t')]D[W(t')]$, the channels being classified according to their different relaxation rates $W=W(t')$, which are random functions of time. For intermittent fluctuations a more complicated relaxation equation is derived which, in addition to the average density of channels, $\rho[W(t')]D[W(t')]$, depends also on a positive fractal exponent H which characterizes the fluctuations of the density of channels. The general theory is applied for constructing dynamical analogs of the stretched exponential relaxation function. For nonintermittent fluctuations the type of relaxation is determined by the regression dynamics of the fluctuations of the relaxation rate. If the regression process is fast and described by an exponential attenuation function, then after an initial stretched exponential behavior the relaxation process slows down and it is not fully completed even in the limit of very large times. For self-similar regression obeying a negative power law, the relaxation process is less sensitive to the influence of dynamical disorder. Both for small and large times the relaxation process is described by stretched exponentials with the same fractal exponent as for systems with static disorder. For large times the efficiency of the relaxation process is also slowed down by fluctuations. Similar patterns are found for intermittent fluctuations with the difference that for very large times and a slow regression process a crossover from a stretched exponential to a self-similar algebraic relaxation function occurs. Some implications of the results for the study of relaxation processes in

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condensed matter physics and im molecular biology are investigated. © *1996 American Institute of Physics.* © 1996 American Institute of Physics. [S0022-2488(96)01004-3]

I. INTRODUCTION

In the last two decades an enormous amount of experimental evidence has been accumulated showing that the decay of the average survival (relaxation) function $\langle l(t)\rangle$ in many diverse systems in condensed matter physics and in molecular biology follows the same stretched exponential law of the Kohlrausch–Williams–Watts (KWW) type

$$\langle l(t)\rangle = \exp[-(\Omega t)^{\beta}], \quad 1>\beta>0, \tag{1.1}$$

where β is a positive fractal exponent between zero and unity and Ω is a characteristic frequency. Equation (1.1) was first proposed by Kohlrausch[1] in 1864 to describe the mechanical creep and was later used by Williams and Watts[2] to describe the dielectric relaxation in polymers and by Weibull[3] for describing the failure data in reliability theory. More recently the KWW law has been used to fit the data on remanent magnetization in spin glasses,[4] the decay of luminiscence in porous glasses,[5] the relaxation processes in viscoelasticity[6] on the reaction kinetics of biopolimers,[7] and on the dynamics of recombination kinetics in radiochemistry.[8] Further applications include the description of the statistical distributions of open and closed times of ion channels in molecular biophysics[9] or even the description of the survival functions of cancer patients.[10]

The ubiquity of the stretched exponential law (1.1) has led to the idea that there should be a kind of universal mechanism generating it which is independent of the details of an individual process. An argument in favor of this opinion is the close connection between the KWW law (1.1) and the stable probability densities of the Lévy type[1,11] which emerge as a result of the occurrence of a large number of independent random events described by individual probability densities with infinite moments. Many attempts of searching for such a universal mechanism for the occurrence of the stretched exponential have been presented in the literature. A first attempt is a generalization of a mechanism of parallel relaxation initially suggested by Förster for the extinction of luminescence[12] and improved by other authors.[13] A second model assumes a complex serial relaxation on a multilevel abstract structure which emphasizes the role of hierarchically constrained dynamics.[14] A third model is a generalization of the defect-diffusion model of Shlesinger and Montroll.[15] All three of these models have been carefully examined by Klafter and Shlesinger;[16] they have shown that in spite of the different details of the three models a universal common feature exists which is the existence of a broad spectrum of relaxation rates described by a scale-invariant distribution. A complementary approach of the universal features of the stretched exponential which is mathematically oriented is based on the powerful technique of fractional calculus and its connections with the theory of Fox functions.[17]

An interesting approach has been suggested by Huber;[18] based on a careful examination of the models used for the description of the extinction of luminescence he has derived a general relaxation function

$$\langle l(t)\rangle = \exp\left\{-\int_0^{\infty}\rho(W)[1-\exp(-Wt)]dW\right\}, \tag{1.2}$$

where $\rho(W)dW$ is the number of channels involved in the relaxation process and characterized by an individual relaxation rate between W and $W+dW$. If the distribution of rates is self-similar and obeys a scaling law of the negative power law type

$$\rho(W)dW \sim \text{const}W^{-(1+\beta)}\,dW, \tag{1.3}$$

which is consistent with the general ideas of self-similarity suggested by Klafter and Shlesinger,[16] then Huber's equation (1.2) leads to the stretched exponential law (1.1). The proportionality constant in Eq. (1.3) can be easily determined in terms of the fractal exponent β and of the characteristic frequency Ω entering Eq. (1.1), resulting in

$$\rho(W)dW=[\Gamma(1-\beta)]^{-1}\beta\Omega^{\beta}W^{-(1+\beta)}\,dW, \tag{1.3$'$}$$

where $\Gamma(x)=\int_0^{\infty}t^{x-1}\exp(-t)dt,\ x>0$, is the complete gamma function. Although Huber has suggested that his equation might be generally valid for any disordered system with static disorder, the validity range of his derivation, based on the approximation of a product by an exponential, cannot be easily evaluated.

Recently two of the authors of the present paper have shown that Huber's equation (1.2) is exact for a Poissonian distribution of independent channels.[19] Moreover, it has been recently shown that Huber's equation (1.2) also holds beyond the validity range of the Poissonian distribution: it emerges as a universal scaling law for a uniform random distribution of a large number of channels characterized by nonintermittent fluctuations.[20] This result is consistent with the general idea that the Huber's equation (1.2) and the stretched exponential relaxation law (1.1) derived from it can be generated by a central limit behavior of the Lévy type which expresses the contribution of a very large number of weakly connected relaxation channels. The analysis presented in Ref. 20 also shows that Huber's equation (1.2) is not the unique universal law which emerges in the limit of a very large number of weakly coupled channels. For intermittent fluctuations of the number of channels at least one supplementary scaling law exists, which is given by

$$\langle \mathscr{C}(t)\rangle=\mathscr{J}_H\left[\int_0^{\infty}\rho(W)[1-\exp(-Wt)]dW\right], \tag{1.4}$$

where the function

$$\mathscr{J}_H(z)=H[(1+1/H)z]^{-H}\gamma(H,(1+1/H)z) \tag{1.5}$$

depends on the incomplete gamma function $\gamma(x,u)=\int_0^u t^{x-1}\exp(-t)dt$, $x>0$, $u\geqslant 0$, and H is a positive fractal exponent which characterizes the fluctuations of the number of channels. The reciprocal value of the fractal exponent, $1/H$, is a measure of the intermittency of fluctuations. In particular in the limit

$$1/H\to 0 \quad (H\to\infty), \tag{1.6}$$

the fluctuations are nonintermittent, the function $\mathscr{J}_H(z)$ becomes an exponential

$$\lim_{H\to\infty}\mathscr{J}_H(z)=\exp(-z), \tag{1.7}$$

and the scaling law (1.4) reduces to the Huber's scaling equation (1.1). The derivation of the intermittent scaling law (1.4) is based on the searching for a fixed point by means of a stochastic renormalization group approach technique.[21] Unfortunately the renormalization group technique used in Ref. 20 does not guarantee that the fixed point corresponding to Eq. (1.4) is unique, and thus other intermittent limit scaling laws corresponding to other fixed points may also exist.

By assuming that the distribution of relaxation rates is given by the scale-invariant law (1.3$'$), the intermittent generalization (1.4) of the Huber's equation leads to the relaxation law

$$\langle \mathscr{C}(t)\rangle=H(\Omega t)^{-\beta H}(1+1/H)^{-H}\gamma(H,(\Omega t)^{\beta}(1+1/H)), \tag{1.8}$$

which for small times reduces to a stretched exponential

$$\langle \mathscr{C}(t)\rangle \sim \exp[-(\Omega t)^{\beta}], \quad t \ll \Omega^{-1}, \tag{1.9}$$

and for large times it is given by a negative power law

$$\langle \mathscr{C}(t)\rangle \sim \Gamma(1+H)(\Omega t)^{-\beta H}(1+1/H)^{-H}, \quad t \gg \Omega^{-1}, \quad H = \text{finite}. \tag{1.10}$$

As the fractal exponent H increases, the intermittent nature of fluctuations becomes less and less pronounced, the stretched exponential portion of the relaxation function $\langle \mathscr{C}(t)\rangle$ given by Eq. (1.8) becomes longer and longer and the power law tail becomes shorter and shorter; eventually in the limit $H \to \infty$, corresponding to nonintermittent fluctuations, the whole relaxation function $\langle \mathscr{C}(t)\rangle$ can be represented by a stretched exponential.

All these attempts at coming up with a general derivation of the stretched exponential are based on the assumption that the disordered distribution of channels is static, i.e., that an initial fluctuation of the number of channels characterized by different relaxation rates is frozen forever; during the process of relaxation the distribution of channels remains invariant and described by the static density function $\rho(W)\, dW$. A channel initially characterized by a relaxation rate W is supposed to be characterized by the same rate W at any time in the future. Although reasonable for some problems of condensed matter physics, the validity of this assumption is questionable in molecular biology. In the case of protein–ligand interactions[7] and of ion channel kinetics[9] the distribution of relaxation channels with different rates is due to the conformational fluctuations of protein molecules which have a dynamical nature and thus the fluctuations of the numbers of channels characterized by different relaxation rates are continuously generated and destroyed by thermal agitation.

The study of rate or relaxation processes with dynamical disorder is an active field of applied statistical physics.[22–26] Although at times the possible connection between the stretched exponential relaxation and the dynamical disorder has also been considered,[27] little attention has been paid to the derivation of dynamic generalizations of the stretched exponential law which emerge in the limit of a very large number of reaction channels. The purpose of this paper is the searching for such universal scaling laws which are dynamical analogs of the general static limit laws (1.2) and (1.4). The starting point of our approach is the theory developed in Refs. 19 and 20 in which a general approach of rate processes with dynamical disorder has been suggested on the basis of the theory of random point processes.[28] In Ref. 19 in the particular case of Poissonian channels a dynamical generalization of the Huber's equation (1.2) has been suggested

$$\langle \mathscr{C}(t)\rangle = \exp\left\{ -\overline{\int\int} \rho[W(t')]D[W(t')]\left[1-\exp\left(-\int_0^t W(t')dt'\right)\right]\right\}, \tag{1.11}$$

where, due to dynamical disorder, the relaxation rate corresponding to an individual channel is a random function of time $W = W(t')$, $t \geqslant t' \geqslant 0$, $\rho[W(t')]D[W(t')]$ is an average functional density of channels characterized by different random functions $W = W(t')$, $D[W(t')]$ is a suitable integration measure over the space of functions $W(t')$, and $\overline{\int\int}$ stands for the operation of path integration. In the following we shall try to derive the dynamic analog (1.11) of Huber's law as a universal limit expression which emerges in the limit of a very large number of weakly interacting channels. We shall also try to derive a universal dynamical intermittent law which is the analog of the static scaling law (1.4):

$$\langle \mathscr{C}(t)\rangle = \mathscr{J}_H\left\{ \overline{\int\int} \rho[W(t')]D[W(t')]\left[1-\exp\left(-\int_0^t W(t')dt'\right)\right]\right\}. \tag{1.12}$$

Another objective of the article is the application of the universal laws (1.11) and (1.12) to the particular case of a self-similar dynamical distribution of channels which is the analog of the static

equation (1.3′). Carrying out this program would lead to dynamical generalizations of the stretched exponential law (1.1) and of its intermittent generalization (1.8).

The structure of the paper is as follows. In Sec. II we give a general formulation of the problem in terms of a functional generalization of the theory of random point processes. In Secs. III and IV the approach developed in Sec. II is used for the derivation of the relaxation functions (1.11) and (1.12) as universal limit laws for nonintermittent and intermittent fluctuations, respectively, valid for a very large number of weakly interacting relaxation channels. In Sec. V explicit dynamical generalizations of the stretched exponential law are derived by computing the path averages in Eqs. (1.11) and (1.12) in the particular case of a stationary self-similar dynamical distribution of relaxation channels. In Sec. VI a comparative numerical analysis of the relaxation equations for static and dynamical disorder is presented. Finally in Secs. VII and VIII some possibilities of application of our approach are analyzed and some open questions are pointed out.

II. FORMULATION OF THE PROBLEM

We consider a relaxation process in which a random (usually very large) number of relaxation modes are involved. By following the usual nomenclature in nuclear physics and molecular dynamics we shall call these modes relaxation channels. The relaxation channels are abstract entities which are characterized by different state vectors $\mathbf{x}_1(t')$, $\mathbf{x}_2(t')$,..., $t \geqslant t' \geqslant 0$, which, due to dynamical disorder, are random functions of time. The relaxation channels should not be mistaken for the actual ion channels crossing a cell membrane,[9] which are concrete objects.

The stochastic properties of the state vectors $\mathbf{x}_1(t'),..,\mathbf{x}_N(t')$ attached to the different individual relaxation channels can be described by a functional generalization of random point processes. A slightly different type of functional random point process has been suggested in Ref. 19. For describing the dynamics of the relaxation channels we introduce a set of grand canonical Janossy probability density functionals

$$Q_0, Q_N[\mathbf{x}_1(t'),\ldots,\mathbf{x}_N(t')]D[\mathbf{x}_1(t')]\cdots D[\mathbf{x}_N(t')], \tag{2.1}$$

with the normalization condition

$$Q_0+\sum_{N=1}^{\infty}\frac{1}{N!}\overline{\int\int}\cdots\overline{\int\int}Q_N[\mathbf{x}_1(t'),\ldots,\mathbf{x}_N(t')]D[\mathbf{x}_1(t')]\cdots D[\mathbf{x}_N(t')]=1. \tag{2.2}$$

Here $Q_N[\mathbf{x}_1(t'),...,\mathbf{x}_N(t')]D[\mathbf{x}_1(t')]\cdots D[\mathbf{x}_N(t')]$ is the probability that there are N relaxation channels and that these N channels are characterized by state vectors close to $\mathbf{x}_1(t'),...,\mathbf{x}_N(t')$ and $D[\mathbf{x}(t')]$ is a suitable integration measure over the space of functions $\mathbf{x}(t')$. This type of description is based on the implicit assumption that for a given realization of the process the total number N of channels is a random quantity which does not change in time. The initial number N of channels is randomly chosen and then kept constant and only the random vectors $\mathbf{x}_1(t'),...,\mathbf{x}_N(t')$ are variable in time. An alternative description of the stochastic properties of the relaxation channels is given in terms of the generating functional

$$\begin{aligned}\Lambda[f[\mathbf{x}(t')]]=Q_0+\sum_{N=1}^{\infty}\frac{1}{N!}\overline{\int\int}\cdots\overline{\int\int}Q_N[\mathbf{x}_1(t'),\ldots,\mathbf{x}_N(t')]\\ \times D[\mathbf{x}_1(t')]\cdots D[\mathbf{x}_N(t')]f[\mathbf{x}_1(t')]\cdots f[\mathbf{x}_N(t')],\end{aligned} \tag{2.3}$$

where $f[\mathbf{x}(t')]$ is a suitable test functional. The main advantage of using the generating functional $\Lambda[f[\mathbf{x}(t')]]$ is that it can be written in a form independent of the integration measure $D[\mathbf{x}(t')]$, which is generally unknown.

Considering a time interval of length t we assume that for each channel $u=1,\ldots,N$, there is a fluctuating probability of decay $p_u(t)$. This probability depends on the whole previous history of the channel, that is, $p_u(t)$ is a functional of all previous values $\mathbf{x}_u(t')$, $t\geqslant t'\geqslant 0$ of the state vector:

$$p_u(t)=p[\mathbf{x}_u(t');t]. \tag{2.4}$$

A realization of the survival (relaxation) function $\mathscr{C}(t)$, that is, the probability that the relaxation process has not occured in a time interval of length t, is simply given by the product of the complementary probabilities $1-p[\mathbf{x}_u(t');t]$ attached to all channels, which expresses the probability that none of the N channels has led to relaxation:

$$\mathscr{C}(t)=\prod_{u=1}^{N}\{1-p[\mathbf{x}_u(t');t)]\}. \tag{2.5}$$

The average relaxation function $\langle\mathscr{C}(t)\rangle$ can be computed by evaluating the average of the fluctuating function $\mathscr{C}(t)$ in terms of the grand canonical Janossy probability density functionals (2.1), which describe the random evolution of the channels:

$$\begin{aligned}\langle\mathscr{C}(t)\rangle=Q_0+\sum_{N=1}^{\infty}\frac{1}{N!}&\overline{\int\int}\cdots\overline{\int\int}\,Q_N[\mathbf{x}_1(t'),\ldots,\mathbf{x}_N(t')]D[\mathbf{x}_1(t')]\cdots D[\mathbf{x}_N(t')]\\&\times f[\mathbf{x}_1(t')]\cdots f[\mathbf{x}_N(t')]\prod_{u=1}^{N}\{1-p[\mathbf{x}_u(t');t]\}\\&=\Lambda[f[\mathbf{x}(t')]=1-p[\mathbf{x}(t');t]],\end{aligned} \tag{2.6}$$

where we have used the definition (2.3) of the generating functional $\Lambda[f[\mathbf{x}(t')]]$. It follows that the evaluation of the average relaxation function $\langle\mathscr{C}(t)\rangle$ reduces to the computation of the generating functional $\Lambda[f[\mathbf{x}(t')]]$, which describes the random couplings between the different relaxation channels, and to the computation of the probability $p[\mathbf{x}(t');t]$, which describes the individual behavior of a single channel.

For relating the generating functional, $\Lambda[f[\mathbf{x}(t')]]$, to the fluctuation dynamics of the number of channels we introduce the fluctuating functional density of channels

$$\eta[\mathbf{x}(t')]D[\mathbf{x}(t')] \quad \text{with} \quad N=\overline{\int\int}\,\eta[\mathbf{x}(t')]D[\mathbf{x}(t')], \tag{2.7}$$

characterized by a random vector near $\mathbf{x}(t')$ and the corresponding characteristic functional

$$G[K[\mathbf{x}(t')]]=\left\langle\exp\left(i\,\overline{\int\int}\,K[\mathbf{x}(t')]\,\eta[\mathbf{x}(t')]D[\mathbf{x}(t')]\right)\right\rangle, \tag{2.8}$$

where $K[\mathbf{x}(t')]$ is a suitable test functional. The fluctuations of the functional density of channels $\eta[\mathbf{x}(t')]D[\mathbf{x}(t')]$ are described in terms of the corresponding cumulants

$$\langle\langle\,\eta[\mathbf{x}_1(t')]\cdots\eta[\mathbf{x}_m(t')]\rangle\rangle, \quad m=1,2,\ldots, \tag{2.9}$$

which are assumed to exist and be finite. The characteristic functional $G[K[\mathbf{x}(t')]]$ can be expressed in terms of $\langle\langle\eta[\mathbf{x}_1(t')]\cdots\eta[\mathbf{x}_m(t')]\rangle\rangle$, $m=1,2,\ldots$, by means of the cumulant expansion

$$\ln G[K[\mathbf{x}(t')]]=\sum_{m=1}^{\infty}\frac{i^m}{m!}\overline{\int\int}\cdots\overline{\int\int}\langle\langle\eta[\mathbf{x}_1(t')]\cdots\eta[\mathbf{x}_m(t')]\rangle\rangle K[\mathbf{x}_1(t')]$$
$$\times D[\mathbf{x}_1(t')]\cdots K[\mathbf{x}_m(t')]D[\mathbf{x}_m(t')]. \tag{2.10}$$

For establishing a connection between the generating functional $\Lambda[f[\mathbf{x}(t')]]$ of the functional point process and the characteristic functional $G[K[\mathbf{x}(t')]]$ of the functional density of channels $\eta[\mathbf{x}(t')]D[\mathbf{x}(t')]$, we write a realization of the density of channels $\eta[\mathbf{x}(t')]D[\mathbf{x}(t')]$ as a sum of functional Dirac's delta symbols

$$\eta[\mathbf{x}(t')]D[\mathbf{x}(t')]=\sum_{u=1}^{N}\delta[\mathbf{x}_u(t')-\mathbf{x}(t')]D[\mathbf{x}(t')]. \tag{2.11}$$

Equation (2.11) is a functional generalization of the well-known relationship from statistical mechanics expressing the particle density fields as sums of delta functions.[29] We insert Eq. (2.11) into the definition (2.8) of the characteristic functional $G[K[\mathbf{x}(t')]]$, and compute the average in terms of the grand canonical Janossy probability density functionals (2.1). By using the definition (2.3) of the generating functional $\Lambda[f[\mathbf{x}(t')]]$ after getting rid of the functional integral in the exponent due to the filtration property of the Dirac's functional symbol and computing the resulting sum, we obtain

$$G[K[\mathbf{x}(t')]]=\Lambda[f[\mathbf{x}(t')]=\exp(iK[\mathbf{x}(t')])]. \tag{2.12}$$

It follows that the average relaxation function $\langle\mathscr{E}(t)\rangle$ can be expressed as

$$\langle\mathscr{E}(t)\rangle=G[K[\mathbf{x}(t')]=ib[\mathbf{x}(t');t]], \tag{2.13}$$

where

$$b[\mathbf{x}(t');t]=-\ln(1-p[\mathbf{x}(t');t]), \tag{2.14}$$

is the bit number[30] of the individual probability of nonrelaxation $1-p[\mathbf{x}(t');t]$ attached to an individual channel with a history characterized by the function $\mathbf{x}(t')$, $t\geqslant t'\geqslant 0$. Equation (2.13) is a dynamical generalization of a similar relationship derived in Ref. 20 for systems with static disorder by using a different method that does not make use of the theory of random point processes.

For deriving an expression for the probability of decay $p[\mathbf{x}(t');t]$ attached to an individual channel we generalize an assumption made for systems with static disorder by Huber[18] and by Vlad, Schönfisch, and Mackey.[20] We assume that a channel characterized by a state vector $\mathbf{x}$ can be either in an open state with a probability $\lambda(\mathbf{x})$ or in a closed state with a probability $1-\lambda(\mathbf{x})$. Following Ref. 20 we suppose that the state vector $\mathbf{x}$ of a channel belongs to a certain domain Σ of the state space which is simply connected and has the volume

$$V_\Sigma=\int_\Sigma d\mathbf{x}, \tag{2.15}$$

and that the probability $\lambda(\mathbf{x})$ that the channel is open is simply given by

$$\lambda(\mathbf{x})=V^*(\mathbf{x})/V_\Sigma, \tag{2.16}$$

where $V^*(\mathbf{x})$ is a characteristic volume of a neighborhood of the position $\mathbf{x}$.

We assume that an open channel characterized by a state vector $\mathbf{x}$ has a rate of relaxation $W(\mathbf{x})$ that depends only on the state vector $\mathbf{x}$. Since the state vector $\mathbf{x}$ is a random function of time, the contribution of an open state to the individual probability of survival (nonrelaxation) $1-p[\mathbf{x}(t');t]$ is given by

$$\mathcal{E}[W(\mathbf{x}(t'))]=\exp\left(-\int_0^t W(\mathbf{x}(t'))dt'\right). \tag{2.17}$$

The corresponding contribution for a closed state is simply equal to $\mathcal{E}[W(\mathbf{x}(t'))]=1$ and the individual probability of survival $1-p[\mathbf{x}(t');t]$ is given by the average of the $\mathcal{E}[W(\mathbf{x}(t'))]$-factor corresponding to the two states

$$1-p[\mathbf{x}(t');t]=\lambda(\mathbf{x}(t))\exp\left(-\int_0^t W(\mathbf{x}(t'))dt'\right)+1-\lambda(\mathbf{x}(t)), \tag{2.18}$$

from which we obtain the following expression for the individual probability of decay

$$p[\mathbf{x}(t');t]=\frac{V^*(\mathbf{x}(t))}{V_\Sigma}\left\{1-\exp\left[-\int_0^t W(\mathbf{x}(t'))dt'\right]\right\}. \tag{2.19}$$

Now the average survival function $\langle\mathcal{E}(t)\rangle$ is completely characterized by the collective stochastic properties of the fluctuations of the numbers of channels, expressed by the cumulants $\langle\langle\eta[\mathbf{x}_1(t')]\cdots\eta[\mathbf{x}_m(t')]\rangle\rangle$ given by Eqs. (2.9) or by the cumulant expansion (2.10) of the characteristic functional $G[K[\mathbf{x}(t')]]$ and by the behavior of an individual channel, characterized by the probability of decay given by Eq. (2.19). For investigating the scaling behavior emerging in the limit of a very large average number $\langle N\rangle$ of channels

$$\langle N\rangle=\overline{\int\int}\langle\langle\eta[\mathbf{x}(t')]\rangle\rangle D[\mathbf{x}(t')]\to\infty, \tag{2.20}$$

we introduce a limit of the thermodynamic type for which both the total volume V_Σ available in the $\mathbf{x}$-space and the average total number $\langle N\rangle$ of channels tend to infinity, but the average density of channels,

$$\varepsilon=\langle N\rangle/V_\Sigma, \tag{2.21}$$

remains constant

$$V_\Sigma, \quad \langle N\rangle\to\infty \quad \text{with} \quad \varepsilon=\langle N\rangle/V_\Sigma=\text{const.} \tag{2.22}$$

For evaluating the different types of asymptotic behavior emerging in the limit (2.22) we assume that the channels are weakly interacting, that is, as the total space volume increases to infinity, $V_\Sigma\to\infty$, the characteristic volumes $V^*(\mathbf{x}_1)$, $V^*(\mathbf{x}_2)$,..., of the neighborhoods of the different channels remain finite and constant; in other words, the increase of the total space volume V_Σ does not lead to an increase of the possible overlapping among the neighborhoods attached to the different channels. This assumption of locality generates the two types of asymptotic behavior investigated in Secs. III and IV.

III. LIMIT BEHAVIOR FOR NONINTERMITTENT FLUCTUATIONS

We introduce the relative fluctuations of different orders:

$$c_m[\mathbf{x}_1(t'),\ldots,\mathbf{x}_m(t')]=\frac{\langle\langle\,\eta[\mathbf{x}_1(t')]\cdots\eta[\mathbf{x}_m(t')]\rangle\rangle}{\Pi_{u=1}^{m}\{\langle\langle\,\eta[\mathbf{x}_u(t')]\rangle\rangle\}},\quad m\geqslant 2. \tag{3.1}$$

If the relative fluctuations $c_m[\mathbf{x}_1(t'),....,\mathbf{x}_m(t')]$, $m\geqslant 2$, decrease to zero in the thermodynamic limit (2.22)

$$c_m[\mathbf{x}_1(t'),\ldots,\mathbf{x}_m(t')]\to 0,\quad V_\Sigma,\langle N\rangle\to\infty,\ \text{with}\ \ \varepsilon=\text{const},m=2,3,\ldots, \tag{3.2}$$

then the fluctuations of the numbers of channels are nonintermittent. For investigating the asymptotic behavior of the survival function $\langle\not\in(t)\rangle$ for nonintermittent fluctuations in the thermodynamic limit (2.22) we introduce the average probability density functional of the state vector $\mathbf{x}(t')$ of an individual channel,

$$\xi[\mathbf{x}(t')]D[\mathbf{x}(t')]=\frac{\langle\langle\,\eta[\mathbf{x}(t')]\rangle\rangle D[\mathbf{x}(t')]}{\underline{\int\int}\langle\langle\,\eta[\mathbf{x}(t')]\rangle\rangle D[\mathbf{x}(t')]}, \tag{3.3}$$

with

$$\overline{\underline{\int\int}}\,\xi[\mathbf{x}(t')]D[\mathbf{x}(t')]=1, \tag{3.4}$$

and combine Eqs. (2.10), (2.13), (2.14), (2.19), (2.20), and (3.1). We express the cumulants of the functional density of channels in terms of the relative fluctuations $c_1[\mathbf{x}_1(t'),...,\mathbf{x}_m(t')]$ and of the average probability density functional $\xi[\mathbf{x}(t')]D[\mathbf{x}(t')]$. By inserting the resulting expression for the cumulants into the functional Taylor expansion (2.10) for the logarithm of the characteristic functional $G[K[\mathbf{x}(t')]]$ and expressing the average relaxation function $\langle\not\in(t)\rangle$ from Eqs. (2.13), (2.14), and (2.19) we obtain

$$\langle\not\in(t)\rangle=\exp\Bigg\{\sum_{m=1}^{\infty}\frac{\varepsilon^m}{m!}\overline{\underline{\int\int}}\cdots\overline{\underline{\int\int}}\,c_m[\mathbf{x}_1(t'),\ldots,\mathbf{x}_m(t')]\xi[\mathbf{x}_1(t')]D[\mathbf{x}_1(t')]\ldots\xi[\mathbf{x}_m(t')]$$
$$\times D[\mathbf{x}_m(t')]\prod_{u=1}^{m}\Bigg\{V_\Sigma\ln\Bigg\{1-\frac{V^*(\mathbf{x}_u(t))}{V_\Sigma}\Bigg[1-\exp\Bigg(-\int_0^t W(\mathbf{x}_u(t'))dt'\Bigg)\Bigg]\Bigg\}\Bigg\}\Bigg\}, \tag{3.5}$$

where

$$c_1=1. \tag{3.6}$$

From Eqs. (2.22), (3.2), (3.5), and (3.6) it follows that for nonintermittent fluctuations in the thermodynamic limit in Eq. (3.5) only the term corresponding to $m=1$ survives and the expression for the average survival function $\langle\not\in(t)\rangle$ reduces to the dynamical generalization (1.11) of Huber's equation:

$$\langle\not\in(t)\rangle\sim\exp\Bigg\{-\overline{\underline{\int\int}}\,\rho[W(t')]D[W(t')]\Bigg[1-\exp\Bigg(-\int_0^t W(t')dt'\Bigg)\Bigg]\Bigg\}\ \text{as}\ V_\Sigma,\langle N\rangle\to\infty,\varepsilon=\text{const}, \tag{3.7}$$

where

$$\rho[W(t')]D[W(t')]=\left\{\varepsilon\overline{\int\int}V^*(\mathbf{x}(t))\xi[\mathbf{x}(t')]D[\mathbf{x}(t')]\delta[W(t')-W(\mathbf{x}(t'))]\right\}D[W(t')] \tag{3.8}$$

is the average density of channels involved in the relaxation process, the channels being classified according to their relaxation rates $W(t')$, $t\geqslant t'\geqslant 0$.

IV. LIMIT BEHAVIOR FOR INTERMITTENT FLUCTUATIONS

For the study of the asymptotic scaling behavior of the average survival function for intermittent fluctuations a renormalization group technique should be used. In the following we apply a probabilistic version[21] of the Shlesinger–Hughes stochastic renormalization procedure[31] which has been recently applied to the study of space-dependent epidemic processes with high migration.[32] The method consists of starting out from an initial characteristic functional $G[K[\mathbf{x}(t')]]$ of the functional density of states for which the fluctuations are nonintermittent and constructing, by means of a succession of decimation processes, a renormalized characteristic functional $\tilde{G}[K[\mathbf{x}(t')]]$ for which the fluctuations of the density of states are intermittent. The main steps of such an approach are presented in another context in Ref. 21 and a simplified derivation is also presented in Ref. 32. Here we give only the final expression for the renormalized characteristic functional $\tilde{G}[K[\mathbf{x}(t')]]$:

$$\tilde{G}[K[\mathbf{x}(t')]]=H\int_0^1 z^{H-1}G[-i\ln[1-z[1-\exp(iK[\mathbf{x}(t')])]]]\,dz;H>0, \tag{4.1}$$

where H is a positive fractal exponent similar to the one entering the static equations (1.4)–(1.10).

For evaluating the limit scaling law for the average relaxation function $\langle\mathscr{N}(t)\rangle$ corresponding to the renormalized expression (4.1) we expand in Eq. (4.1) the nonrenormalized characteristic functional $G[K[\mathbf{x}(t')]]$ in the cumulant expansion (2.10) and express the corresponding cumulants in terms of the nonrenormalized relative fluctuations $c_m[\mathbf{x}_1(t');...;\mathbf{x}_m(t')]$ and in terms of the average renormalized density of channels

$$\varepsilon=\frac{\langle\tilde{N}\rangle}{V_\Sigma}=\frac{H}{H+1}\cdot\frac{\langle N\rangle}{V_\Sigma}. \tag{4.2}$$

Here we have used the relationship between the nonrenormalized average number of channels $\langle N\rangle$ and the corresponding renormalized average $\langle\tilde{N}\rangle$:

$$\langle\tilde{N}\rangle=\langle N\rangle H/(H+1). \tag{4.3}$$

The relationship (4.3) can be derived from the renormalization group equation (4.1) by means of functional differentiation followed by the application of the relationships

$$\langle N\rangle=\overline{\int\int}\langle\langle\eta[\mathbf{x}(t')]\rangle\rangle D[\mathbf{x}(t')]=\overline{\int\int}\frac{\delta\ln G[K=0]}{\delta K[\mathbf{x}(t')]}D[\mathbf{x}(t')], \tag{4.4}$$

$$\langle\tilde{N}\rangle=\overline{\int\int}\langle\langle\tilde{\eta}[\mathbf{x}(t')]\rangle\rangle D[\mathbf{x}(t')]=\overline{\int\int}\frac{\delta\ln\tilde{G}[K=0]}{\delta K[\mathbf{x}(t')]}D[\mathbf{x}(t')], \tag{4.5}$$

which can be derived by expanding the characteristic functionals $G[K[\mathbf{x}(t')]]$ and $\tilde{G}[K[\mathbf{x}(t')]]$ in cumulant series of the type (2.10).

By using Eqs. (2.10), (2.13), and (2.14) applied for the renormalized characteristic functional $\tilde{G}[K[\mathbf{x}(t')]]$ combined with Eqs. (4.1) and (4.2) and using the same steps as in Sec. III we obtain the following expression for the average relaxation function $\langle \mathscr{l}(t) \rangle$:

$$\langle \mathscr{l}(t) \rangle = H \int_0^1 z^{H-1}\, dz\, \exp\left\{ \sum_{m=1}^{\infty} \frac{1}{m!} \left[\varepsilon \left(1 + \frac{1}{H} \right) \right]^m \overline{\int\int} \cdots \overline{\int\int} c_m[\mathbf{x}_1(t'),\ldots,\mathbf{x}_m(t')] \xi[\mathbf{x}_1(t')] \right.$$
$$\times D[\mathbf{x}_1(t')] \cdots \xi[\mathbf{x}_m(t')] D[\mathbf{x}_m(t')] \prod_{u=1}^{m} \left\{ V_\Sigma \ln \left[1 - zV^*(\mathbf{x}_u(t))(V_\Sigma)^{-1} \right.\right.$$
$$\left.\left. \left. \times \left(1 - \exp\left(- \int_0^t W(\mathbf{x}_u(t'))dt' \right) \right) \right] \right\} \Bigg\}, \tag{4.6}$$

from which, by taking into account the nonintermittency conditions (3.2) for the nonrenormalized relative fluctuations of the density of channels we obtain the following scaling law in the thermodynamic limit (2.22):

$$\langle \mathscr{l}(t) \rangle \sim \mathscr{J}_H \left\{ \overline{\int\int} \rho[W(t')] D[W(t')] \left[1 - \exp\left(- \int_0^t W(t')dt' \right) \right] \right\},$$
$$\text{as} \quad V_\Sigma, \langle \tilde{N} \rangle \to \infty \quad \text{with} \quad \varepsilon = \langle \tilde{N} \rangle / V_\Sigma = \text{const}, \tag{4.7}$$

where the function $\mathscr{J}_H(z)$ and the functional density of channels involved in the relaxation process, $\rho[W(t')]D[W(t')]$, are given by Eqs. (1.5) and (3.8), respectively.

Equation (4.7) justifies the conjecture (1.12) made without proof in Sec. I. This equation is the dynamical analog of the intermittent scaling law (1.4) derived for systems with static disorder in Ref. 20. Just like in the static case the reciprocal value of the fractal exponent H, $1/H$, is a measure of the degree of intermittency of the fluctuations of the number of channels. In particular in the limit $H \to \infty$ the fluctuations become nonintermittent and Eq. (4.7) reduces to the dynamical analogue (1.2) of Huber's equation. The renormalization group approach for dynamical disorder used in this paper has the same drawback as the similar static approach developed in Ref. 20: it does not guarantee that the limit scaling relationship (4.7) is the unique asymptotic law which emerges in the thermodynamic limit for intermittent fluctuations. The renormalization group procedure introduced in Ref. 21 does not provide a hint that the fixed point corresponding to Eq. (4.1) is the unique fixed point of the problem. It is possible that further research may lead to other scaling laws characteristic for intermittent fluctuations.

V. DYNAMICAL GENERALIZATIONS OF STRETCHED EXPONENTIAL

The main difficulty related to the application of the dynamical scaling laws (3.7) and (4.7) is connected to the evaluation of the path integral:

$$I(t) = \overline{\int\int} \rho[W(t')] D[W(t')] \left[1 - \exp\left(- \int_0^t W(t')dt' \right) \right]. \tag{5.1}$$

The evaluation of such path integrals would be trivial provided that the functional density of states $\rho[W(t')]D[W(t')]$ would have a Gaussian behavior. Unfortunately a Gaussian form for $\rho[W(t')]D[t')]$ must be ruled out because it does not include the static power law distribution (1.3′) as a particular case.

A formal solution of the problem can be given by introducing an average probability density functional of the relaxation rates $W(t')$, $t \geqslant t' \geqslant 0$:

$$\varphi[W(t')]D[W(t')]=\rho[W(t')]D[W(t')]/\langle N^*\rangle, \tag{5.2}$$

with the normalization condition

$$\overline{\int\int}\,\varphi[W(t')]D[W(t')]=1, \tag{5.3}$$

and where

$$\langle N^*\rangle=\overline{\int\int}\,\rho[W(t')]D[W(t')]=\varepsilon\overline{\int\int}\,V^*(\mathbf{x}(t))\xi[\mathbf{x}(t')]D[\mathbf{x}(t')] \tag{5.4}$$

is the average effective number of channels involved in the relaxation process. Generally the average effective number of channels involved in relaxation, $\langle N^*\rangle$, is at most equal to the total average number of channels, $\langle N\rangle$. By using the expression (5.2) for the average probability density functional $\varphi[W(t')]D[W(t')]$, the factor $I(t)$ can be expressed in terms of a dynamical average of the random function

$$\mathcal{A}[W(t')]=\exp\left(-\int_0^t W(t')dt'\right) \tag{5.5}$$

[see also Eq. (2.17)]. We have

$$I(t)=\langle N^*\rangle\{1-\langle\mathcal{A}[W(t')]\rangle\}, \tag{5.6}$$

where the dynamical average $\langle\mathcal{A}[W(t')]\rangle$ is given by

$$\langle\mathcal{A}[W(t')]\rangle=\overline{\int\int}\,\varphi[W(t')]D[W(t')]\mathcal{A}[W(t')]. \tag{5.7}$$

In this paper we limit ourselves to the simplest case of dynamical disorder for which the random process corresponding to the average probability density functional $\varphi[W(t')]D[W(t')]$ is Markovian. Moreover we consider that the average effective number of channels involved in the relaxation process, $\langle N^*\rangle$, is time independent:

$$\langle N^*\rangle=\text{const.} \tag{5.8}$$

Under these circumstances the probability density functional $\varphi[W(t')]D[W(t')]$ can be represented as

$$\begin{aligned}\varphi[W(t')]D[W(t')]=\lim_{\substack{m\to\infty\\(\Delta t\to 0)}}\,[&\varphi(W_m;m\Delta t|W_{m-1};(m-1)\Delta t)dW_m\cdots\varphi(W_2;2\Delta t|W_1;\Delta t)dW_2\\&\times\varphi(W_1;\Delta t|W_0;0)dW_1\varphi_{st}(W_0)dW_0],\quad t\geqslant t'\geqslant 0,\end{aligned} \tag{5.9}$$

where

$$m=t/\Delta t; \tag{5.10}$$

$$\varphi_{st}(W)dW\quad\text{with}\quad\int\varphi_{st}(W)dW=1, \tag{5.11}$$

is an average one-time stationary probability density of an individual relaxation rate attached to a given channel corresponding to static disorder and

$$\varphi(W;t|W';t')dW \quad \text{with} \quad \int \varphi(W;t|W';t')dW=1 \tag{5.12}$$

is the average conditional probability density of the relaxation rate W at time t provided that at time t' the relaxation rate was W'. For a Markov process both $\varphi_{st}(W)$ and $\varphi(W;t|W';t')$ are the solutions of an evolution equation of the type

$$\partial_t\varphi=\mathbb{L}\varphi, \tag{5.13}$$

where $\mathbb{L}$ is a linear Markovian evolution operator of the Liouville, Fokker–Planck, or the master type. In this case the probability $\varphi_{st}(W)$ is the stationary solution of Eq. (5.13), whereas the conditional probability density $\varphi(W;t|W';t')$ is the Green's function of the equation (5.13) corresponding to the initial condition

$$\varphi(W;t=t'|W';t')=\delta(W-W'). \tag{5.14}$$

For the above-mentioned Markovian systems there is a general method for computing dynamical path averages of the type (5.7) without the explicit evaluation of a path integral. The method was suggested by Lax in the sixties[33] in connection with certain problems of quantum optics and rediscovered independently by Van Kampen.[34,35] For a recent application of this technique to the study of a rate process with dynamical disorder, the passage over a fluctuating activation energy barrier, see Ref. 26. The idea is based on the observation that a realization of the function $\mathscr{E}(t)=\mathscr{E}[W(t')]$ given by Eq. (5.5) obeys a stochastic differential equation with a random coefficient:

$$\frac{d\mathscr{E}(t)}{dt}=-W(t)\mathscr{E}(t) \quad \text{with} \quad \mathscr{E}(0)=1. \tag{5.15}$$

Since Eq. (5.15) is local in time and the coefficient $W(t)$ is Markovian it follows that the pair of random variables $(W(t),\mathscr{E}(t))$ is also Markovian and the one-time joint probability density,

$$P(W,\mathscr{E};t)dWd\mathscr{E} \quad \text{with} \quad \int\int P(W,\mathscr{E};t)dWd\mathscr{E}=1, \tag{5.16}$$

obeys a compound stochastic Liouville equation,[33–35]

$$\partial_t P(W,\mathscr{E};t)=\partial_{\mathscr{E}}\{W\mathscr{E}P(W,\mathscr{E};t)\}+\mathbb{L}P(W,\mathscr{E};t), \tag{5.17}$$

with the initial condition

$$P(W,\mathscr{E};t=0)=\delta(\mathscr{E}-1)\varphi_{st}(W). \tag{5.18}$$

The dynamical average $\langle\mathscr{E}[W(t')]\rangle$ can be expressed as an average value corresponding to the joint probability density $P(W,\mathscr{E};t)$:

$$\langle\mathscr{E}[W(t')]\rangle=\int\int \mathscr{E}P(W,\mathscr{E};t)dWd\mathscr{E}=\int F(W,t)dW, \tag{5.19}$$

where

$$F(W,t)=\int \mathscr{C}P(W,\mathscr{C};t)d\mathscr{C} \tag{5.20}$$

is a marginal average. By multiplying Eqs. (5.17) and (5.18) by $\mathscr{C}$ and integrating over $\mathscr{C}$ after a partial integration we obtain a closed equation for the marginal average $F(W;t)$:

$$\partial_t F(W;t)+WF(W;t)=\mathbb{L}F(W;t), \tag{5.21}$$

with the initial condition

$$F(W;t=0)=\varphi_{st}(W). \tag{5.22}$$

From the above considerations it turns out that for a stationary Markovian average random process the evaluation of the average survival function $\langle \mathscr{C}(t)\rangle$ reduces to the evaluation of the marginal average $F(W,t)$ by solving the evolution equation (5.21) with the initial condition (5.22) followed by the application of Eqs. (3.7), (4.7), (5.1), (5.6), and (5.19).

For applying the suggested Markovian approach we should come up with a suitable definition of the Markovian evolution operator $\mathbb{L}$. The simplest possible choice would be a Liouville operator of the type suggested in Ref. 26 determined by starting out from the stationary probability density $\varphi_{st}(W)$ corresponding to the static density of states (1.3′) attached to a stretched exponential of the type (1.1) and by assuming that the regression of the fluctuations of the relaxation rate is described by a generally time-dependent regression rate $\omega(t)$. Now we notice a minor difficulty related to the self-similar form (1.3′) of the static density of states $\rho(W)dW$: due to the infrared divergence of $\rho(W)$ given by Eq. (1.3′) at $W=0$, the average effective number $\langle N^*\rangle$ of channels involved in the relaxation process is infinite:

$$\langle N^*\rangle=\int_0^\infty \rho(W)dW=\int_0^\infty [\Gamma(1-\beta)]^{-1}\beta\Omega^\beta W^{-(1+\beta)}dW=\infty. \tag{5.23}$$

Due to the time independence condition (5.8) for $\langle N^*\rangle$, the divergent behavior carries over for systems with dynamical disorder. This divergence is, however, spurious because the corresponding integral expressions for the average survival function $\langle \mathscr{C}(t)\rangle$ are well behaved. The problem can be solved by introducing an infrared cutoff $W^*\neq 0$ and by passing to the limit $W^*\to 0$ after performing the computations.

For a cutoff value $W^*\neq 0$, the total effective average number of channels $\langle N^*\rangle$ is finite:

$$\langle N^*\rangle=\int_{W^*}^\infty \rho(W)dW=[\Gamma(1-\beta)]^{-1}\left(\frac{\Omega}{W^*}\right)^\beta, \tag{5.24}$$

and the stationary probability density $\varphi_{st}(W)\ dW$ is given by

$$\varphi_{st}(W)dW=\rho(W)dW/\langle N^*\rangle=\beta(W^*)^\beta W^{-(1+\beta)}dW, \tag{5.25}$$

which obviously fulfills the normalization condition

$$\int_{W^*}^\infty \varphi_{st}(W)dW=1. \tag{5.26}$$

By following the approach suggested in Ref. 26 we express $\varphi_{st}(W)$ as the normalized solution of a Bloch-like equation

$$\beta\left(\beta\varphi_{st}(W)+\frac{\partial}{\partial W}[W\varphi_{st}(W)]\right)=0, \tag{5.27}$$

and suggest a dynamical generalization of Eq. (5.27) depending on the regression frequency $\omega(t)$:

$$\frac{\partial\varphi}{\partial t}=-\beta\omega(t)\left[\beta\varphi+\frac{\partial}{\partial W}(W\varphi)\right]=\mathbb{L}\varphi, \tag{5.28}$$

where the Liouville operator $\mathbb{L}$ is given by

$$\mathbb{L}\ldots=-\beta\omega(t)\left[\beta\ldots+\frac{\partial}{\partial W}(W\ldots)\right]. \tag{5.29}$$

All solutions of the Liouville equation (5.28) should be properly defined, that is, they should be non-negative and conserve the normalization to unity at any time

$$\varphi\geqslant 0;\ \int_{W^*}^{\infty}\varphi\ dW=1. \tag{5.30}$$

By integrating Eq. (5.28) term by term it is easy to check that it conserves the normalization of φ to unity provided that the following boundary condition is fulfilled:

$$\varphi(W=W^*;t)=\beta/W^*;\quad t\geqslant 0. \tag{5.31}$$

Concerning the non-negativity of φ we express any solution of Eq. (5.28) in terms of the Green's function $\varphi(W;tW';t')$, which is the solution of Eq. (5.28) with the initial condition (5.14), and of the initial condition $\varphi(W;t=0)$:

$$\varphi(W;t)=\int_{W^*}^{\infty}\varphi(W;t|W';0)\varphi(W';t=0)dW'. \tag{5.32}$$

The Green's function $\varphi(W;t|W';0)$ can be easily evaluated by integrating Eq. (5.28) along the characteristics with the initial condition (5.14) applied for $t'=0$ and with the boundary condition (5.31), resulting in

$$\begin{aligned}\varphi(W;t|W';0)=&h\left[W^*\exp\left(\beta\int_0^t\omega(t')dt'\right)-W\right]\left(\frac{\beta}{W^*}\right)\left(\frac{W^*}{W}\right)^{1+\beta}\\&+h\left[W-W^*\exp\left(\beta\int_0^t\omega(t')dt'\right)\right]\exp\left(-\beta^2\int_0^t\omega(t')dt'\right)\\&\times\delta\left[W-W'\exp\left(\beta\int_0^t\omega(t')dt'\right)\right],\end{aligned} \tag{5.33}$$

where $h(x)$ is the Heaviside's step function. From Eqs. (5.32) and (5.33) we obtain

$$\begin{aligned}\varphi(W;t)=&h\left[W^*\exp\left(\beta\int_0^t\omega(t')dt'\right)-W\right]\left(\frac{\beta}{W^*}\right)\left(\frac{W^*}{W}\right)^{1+\beta}+h\left[W-W^*\left(\beta\int_0^t\omega(t')dt'\right)\right]\\&\times\exp\left(-\beta^2\int_0^t\omega(t')dt'\right)\varphi\left(W\exp\left(-\beta\int_0^t\omega(t')dt'\right);t=0\right).\end{aligned} \tag{5.34}$$

Both Eqs. (5.33) and (5.34) conserve the non-negativity and normalization conditions (5.30) provided that the initial probability density $\varphi(W;t=0)$ is non-negative and normalized to unity and is equal to zero for any rate smaller than the cutoff value $W=W^*$:

$$\varphi(W;t=0)\geqslant 0; \quad \int_{W^*}^{\infty}\varphi(W;t=0)dW=1; \quad \varphi(W<W^*;t=0)=0. \tag{5.35}$$

By applying the above-mentioned Markovian approach it follows that the marginal average $F(W,t)$ is the solution of the partial differential equation

$$\partial_t F(W,t)+WF(W,t)=-\beta\omega(t)[\beta F(W,t)+\partial_W[WF(W,t)]], \tag{5.36}$$

with the initial condition

$$F(W,t=0)=\beta(W^*)^{-1}(W^*/W)^{1+\beta}. \tag{5.37}$$

By integrating Eq. (5.36) by means of the method of characteristics we can express the marginal average $F(W,t)$ in terms of an arbitrary function. By determining this arbitrary function from the initial condition (5.37) we obtain

$$F(W,t)=\beta(W^*)^{-1}\left(\frac{W^*}{W}\right)^{1+\beta}\exp\left\{-Wg^{\beta}(t)\int_0^t g^{-\beta}(t')dt'\right\}, \tag{5.38}$$

where $g(t)$, the attenuation factor of the regression of fluctuations of the relaxation rate attached to a given channel, is given by

$$\frac{dg(t)}{dt}=-\omega(t)g(t), \quad g(0)=1, \tag{5.39}$$

that is,

$$g(t)=\exp\left(-\int_0^t\omega(t')dt'\right). \tag{5.40}$$

From Eqs. (5.1), (5.6), (5.19), and (5.38) if follows that the exponent $I(t)$ is equal to

$$I(t)=\frac{\beta\Omega^{\beta}}{\Gamma(1-\beta)}\int_{W^*}^{\infty}\frac{1-\exp[-Wg^{\beta}(t)\int_0^t g^{-\beta}(t')dt']}{W^{1+\beta}}\,dW. \tag{5.41}$$

As expected in the limit $W^*\to 0$, the exponent $I(t)$ is well behaved and in this limit the integral over W in Eq. (5.41) can be explicitly computed, resulting in

$$I(t)=\left[\Omega g^{\beta}(t)\int_0^t g^{-\beta}(t')dt'\right]^{\beta}. \tag{5.42}$$

From the above computations it turns out that for the model considered in this section the universal scaling laws (3.7) and (4.7) for dynamical nonintermittent and intermittent fluctuations become

$$\langle\ell(t)\rangle=\exp\left\{-\left[\Omega g^{\beta}(t)\int_0^t g^{-\beta}(t')dt'\right]^{\beta}\right\} \tag{5.43}$$

and

$$\langle\ell(t)\rangle=\mathcal{J}_H\left\{\left[\Omega g^{\beta}(t)\int_0^t g^{-\beta}(t')dt'\right]\right\}, \tag{5.44}$$

respectively. Equations (5.43) and (5.44) are dynamical analogs of the stretched exponential law (1.1) and of its static intermittent generalization (1.8). The concrete form of these two equations depends on the dynamics of the regression of the fluctuations of the relaxation rate expressed by the attenuation function $g(t)$. A comparison between the relaxation behavior corresponding to some important types of dynamical disorder and the relaxation behavior of the similar systems with static disorder is presented in the following section.

VI. STATIC VERSUS DYNAMICAL DISORDER

The dynamical relaxation equations (5.43) and (5.44) include the stretched exponential (1.1) and its static intermittent analogue (1.8) as particular cases corresponding to a regression rate $\omega(t)$ equal to zero for which there is no attenuation of the fluctuations

$$\omega(t)=0, \quad g(t)=1, \tag{6.1}$$

and an initial fluctuation of the relaxation rate is frozen forever.

In this paper we limit ourselves to the study of only two types of dynamical disorder. The first case corresponds to a fast regression of the fluctuations for which the frequency $\omega(t)$ is constant and the attenuation function $g(t)$ is exponentially decreasing in time:

$$\omega(t)=\omega_0=\text{const} \quad \text{and} \quad g(t)=\exp(-\omega_0 t). \tag{6.2}$$

The second case corresponds to a self-similar regression process described by slowly decaying functions $\omega(t)$ and $g(t)$ which obey negative power laws of time as $t \gg t_0$:

$$\omega(t)=\alpha/(t+t_0)\sim \alpha/t \quad \text{as} \quad t \gg t_0, \tag{6.3}$$

$$g(t)=[t_0/(t+t_0)]^{\alpha}\sim (t_0/t)^{\alpha} \quad \text{as} \quad t \gg t_0, \tag{6.4}$$

where $t_0>0$ is a possibly very small but, however, different from zero time constant which has been introduced in order to avoid the divergence of the frequency $\omega(t)$ in the limit $t\to 0$. The relationships between these two cases can be clarified by requiring that as $t\to 0$ the regression rates $\omega(t)$ have the same values, resulting in

$$\omega(0)=\alpha/t_0=\omega_0. \tag{6.5}$$

By using Eq. (6.5) the relationship (6.4) for the attenuation function $g(t)$ becomes

$$g(t)=[\alpha/(\omega_0 t+\alpha)]^{\alpha}. \tag{6.6}$$

For small values of α the function $g(t)$ given by Eq. (6.6) has a long tail of the negative power law type. As the fractal exponent α increases the tail of the attenuation function $g(t)$ is getting shorter and shorter and in the limit $\alpha\to\infty$ we recover the exponential decay law (6.2).

In order to outline the analogies and differences between the relaxation processes in systems with static and dynamical disorder we compare the static relaxation equations (1.1) and (1.8) for nonintermittent and intermittent fluctuations, respectively, with the dynamical relaxation equations (5.43) and (5.44) applied in the case of the attenuation functions $g(t)$ given by Eqs. (6.2) and (6.4). It is also of interest to compare the probability densities of the relaxation time

$$\psi(t)dt=-\left[\frac{\partial\langle \mathscr{C}(t)\rangle}{\partial t}\right]dt, \tag{6.7}$$

the corresponding moments

$$\langle t^m\rangle=\int_0^\infty t^m\psi(t)dt=\lim_{t\to\infty} t^m\langle\chi(t)\rangle+m\int_0^\infty t^{m-1}\langle\chi(t)\rangle dt, \tag{6.8}$$

and the effective rates of relaxation

$$W_{\text{eff}}(t)=\psi(t)/\langle\chi(t)\rangle=-\partial_t \ln\langle\chi(t)\rangle. \tag{6.9}$$

For computing these functions we express the average relaxation functions for nonintermittent and intermittent fluctuations in terms of the exponent $I(t)$ given by Eq. (5.42):

$$\langle\chi(t)\rangle=\exp[-I(t)], \tag{6.10}$$

$$\langle\chi(t)\rangle=\mathcal{J}_H[I(t)]. \tag{6.11}$$

The application of Eqs. (1.5), (5.42), and (6.7)–(6.11) leads to the following relationships for the functions $\psi(t)$ and $W_{\text{eff}}(t)$:

$$\psi(t)=q(t)I(t)\exp[-I(t)], \tag{6.12}$$

$$W_{\text{eff}}(t)=q(t)I(t), \tag{6.13}$$

for nonintermittent fluctuations and

$$\psi(t)=q(t)\mathcal{F}_H[I(t)]\mathcal{J}_H[I(t)], \tag{6.14}$$

$$W_{\text{eff}}(t)=q(t)\mathcal{F}_H[I(t)], \tag{6.15}$$

for intermittent fluctuations. Here the functions $q(t)$ and $\mathcal{F}_H(z)$ are given by

$$q(t)=\frac{d[\ln I(t)]}{dt}=\beta\left\{g^{-\beta}(t)\left[\int_0^t g^{-\beta}(t')dt'\right]^{-1}-\beta\omega(t)\right\}, \tag{6.16}$$

$$\mathcal{F}_H(z)=(H+1)\left\{1+\left[\left(1+\frac{1}{H}\right)^H z^H\right]\frac{\exp[-z(1+1/H)]}{\gamma[H+1;z(1+1/H)]}\right\}^{-1}. \tag{6.17}$$

For applying these equations for systems with nonintermittent or intermittent static disorder and for systems with nonintermittent or intermittent dynamical disorder with exponential or self-similar regression we should evaluate the functions $I(t)$ and $q(t)$ corresponding to all these particular cases. After some computations we come to

$$I(t)=(\Omega t)^\beta, \quad q(t)=\beta/t, \tag{6.18}$$

for static disorder;

$$I(t)=\left\{\frac{\Omega[1-\exp(-\omega_0\beta t)]}{[\omega_0\beta]}\right\}^\beta, \tag{6.19}$$

$$q(t)=\beta^2\omega_0\exp(-\omega_0\beta t)[1-\exp(-\omega_0\beta t)]^{-1}, \tag{6.20}$$

for nonintermittent and intermittent dynamical disorder with exponential attenuation; and

$$I(t)=\{\Omega^*[t+t_0-t_0[t_0/(t+t_0)]^{\alpha\beta}]\}^\beta, \tag{6.21}$$

$$q(t)=\beta^2\alpha(t_0)^{-1}[t_0/(t+t_0)]^{\alpha\beta+2}\{1-[t_0/(t+t_0)]^{\alpha\beta+1}\}^{-1}, \tag{6.22}$$

TABLE I. Limit behavior of the average relaxation function $\langle l(t)\rangle$ for different types of static and dynamical disorder for small and large times.

Case	$\langle l(t)\rangle$ for small times	$\langle l(t)\rangle$ for large times
(1) Nonintermittent static disorder	$\exp[-(\Omega t)^{\beta}]$	$\exp[-(\Omega t)^{\beta}]$
(2) Nonintermittent dynamical disorder with exponential regression	$\exp[-(\Omega t)^{\beta}]$; $\Omega t \ll \Omega/\omega_0$	$\exp[-(\Omega/\beta\omega_0)^{\beta}]=$const; $\Omega t \gg \Omega/\omega_0$
(3) Nonintermittent dynamical disorder with self-similar regression	$\exp[-(\Omega t)^{\beta}]$; $\Omega t \ll \Omega t_0$	$\exp[-(\Omega^* t)^{\beta}]$; $\Omega t \gg \Omega t_0$
(4) Intermittent static disorder	$\exp[-(\Omega t)^{\beta}]$; $\Omega t \ll 1$	$(\Omega t)^{-\beta H}(1+1/H)^{-H}\Gamma(1+H)$; $\Omega t \gg 1$
(5) Intermittent dynamical disorder with exponential regression	$\exp[-(\Omega t)^{\beta}]$; $\Omega t \ll \Omega/\omega_0$; $\Omega t \ll 1$	(a) $(\Omega t)^{-\beta H}(1+1/H)^{-H}\Gamma(1+H)$; $\Omega/\omega_0 \gg \Omega t \gg 1$ (b) $(\Omega/\beta\omega_0)^{-\beta H}(1+1/H)^{-H}\Gamma(1+H)$; $\Omega t \gg \Omega/\omega_0 \gg 1$
(6) Intermittent dynamical disorder with self-similar regression	$\exp[-(\Omega t)^{\beta}]$; $\Omega t \ll 1$; $\Omega t \ll \Omega t_0$	(a) $(\Omega t)^{-\beta H}(1+1/H)^{-H}\Gamma(1+H)$; $\Omega t_0 \gg \Omega t \gg 1$ (b) $(\Omega^* t)^{-\beta H}(1+1/H)^{-H}\Gamma(1+H)$; $\Omega t \gg \Omega t_0 \gg 1$

for nonintermittent and intermittent dynamical disorder with self-similar attenuation. Here

$$\Omega^* = \Omega/(1+\alpha\beta). \tag{6.23}$$

By combining Eqs. (6.7)–(6.22) we can derive six sets of functions $\langle \chi(t)\rangle$, $\psi(t)$, and $W_{\text{eff}}(t)$ corresponding to nonintermittent and intermittent static disorder, to the two types of nonintermittent dynamical disorder, and to the two types of intermittent dynamical disorder considered in this article. The resulting equations are rather complicated and to save space they are not given here. We present only two tables with the different types of limit behavior of these functions for short and large times, respectively.

Table 1 shows the asymptotic behavior of the average survival function $\langle l(t)\rangle$ in the six cases considered. For nonintermittent fluctuations the dynamical disorder decreases the efficiency of relaxation both for exponential and self-similar attenuation. The effect is much more pronounced for exponential attenuation for which the relaxation function tends towards a positive value different from zero as $t\to\infty$ and thus the relaxation process is never complete, not even after an infinitely large period of time. For self-similar attenuation this decrease in efficiency is less pronounced. An interesting effect in this case is that both for small and large times the relaxation process is described by stretched exponentials with the same exponent β and different characteristic frequencies, Ω and $\Omega^*=\Omega/(1+\alpha\beta)<\Omega$, respectively. For large times the decrease of efficiency due to dynamical disorder is displayed by the decrease of the characteristic frequency from Ω to Ω^*. Similar patterns occur in the intermittent cases for which the dynamical disorder also slows down the relaxation process. For exponential attenuation after an initial stretched exponential behavior for large times a self-similar region exists for which the relaxation function is described by a negative power law of time. The self-similar region is eventually followed by a horizontal asymptote of the relaxation function which has a positive residual value even in the limit $t\to\infty$, a situation which corresponds to incomplete relaxation. Just as in the nonintermittent

TABLE II. Limit behavior for small and large times of the effective relaxation rate $W_{\text{eff}}(t)$ and the values of the positive moments $\langle t^m \rangle$, $m \geqslant 1$, of the relaxation time for different types of static and dynamical disorder.

Case	$W_{\text{eff}}(t)$ for small times	$W_{\text{eff}}(t)$ for large times	$\langle t^m \rangle, m \geqslant 1$
(1) Nonintermittent static disorder	$\beta \Omega^{\beta} t^{\beta-1}$	$\beta \Omega^{\beta} t^{\beta-1}$	$\Omega^{-m} \Gamma(1+m/\beta) = \text{finite}$
(2) Nonintermittent dynamical disorder with exponential regression	$\beta \Omega^{\beta} t^{\beta-1}$; $\Omega t \ll \Omega/\omega_0$	~ 0; $\Omega t \gg \Omega/\omega_0$	∞
(3) Nonintermittent dynamical disorder with self-similar regression	$\beta \Omega^{\beta} t^{\beta-1}$; $\Omega t \ll \Omega t_0$	$\beta (\Omega^*)^{\beta} t^{\beta-1}$; $\Omega t \gg \Omega t_0$	finite
(4) Intermittent static disorder	$\beta \Omega^{\beta} t^{\beta-1}$; $\Omega t \ll 1$	H/t; $\Omega t \gg 1$	∞
(5) Intermittent dynmical disorder with exponential regression	$\beta \Omega^{\beta} t^{\beta-1}$; $\Omega t \ll \Omega/\omega_0$; $\Omega t \ll 1$	(a) H/t; $\Omega/\omega_0 \gg \Omega t \gg 1$ (b) ~ 0; $\Omega t \gg \Omega/\omega_0 \gg 1$	∞
(6) Intermittent dynamical disorder with self-similar regression	$\beta \Omega^{\beta} t^{\beta-1}$; $\Omega t \ll 1$; $\Omega t \ll \Omega t_0$	(a) H/t; $\Omega t_0 \gg \Omega t \gg 1$ (b) H/t; $\Omega t \gg \Omega t_0 \gg 1$	∞

case for self-similar attenuation, the decrease in efficiency of the relaxation process is less pronounced in comparison with the case of exponential attenuation. For small times a stretched exponential behavior exists with a characteristic frequency

$$\Omega^{**} = \Omega. \tag{6.24}$$

For large times both the intermittent behavior and the regression of fluctuations lead to the slowing down of the relaxation process. The intermittent behavior is dominant leading to a long time tail of the average survival function.

Table II displays the asymptotic values of the effective relaxation rate $W_{\text{eff}}(t)$ for small and large times as well as the values of the positive moments of the relaxation time. The expressions for the effective relaxation rate are consistent with the data presented in Table I for the average survival function. A survival function of the stretched exponential type corresponds to a negative power law function of time for the effective relaxation rate of the type

$$W_{\text{eff}} \sim 1/t^{1-\beta}. \tag{6.25}$$

Similarly a power law tail of the survival function corresponds to an asymptotic hyperbolic time dependence of the effective relaxation rate

$$W_{\text{eff}} \sim 1/t \quad \text{as} \quad t \to \infty, \tag{6.26}$$

whereas a positive residual value of the relaxation function for large times, $\langle l(\infty) \rangle > 0$, corresponds to an asymptotic value of the effective relaxation rate equal to zero:

$$W_{\text{eff}} \sim 0 \quad \text{as} \quad t \to \infty. \tag{6.27}$$

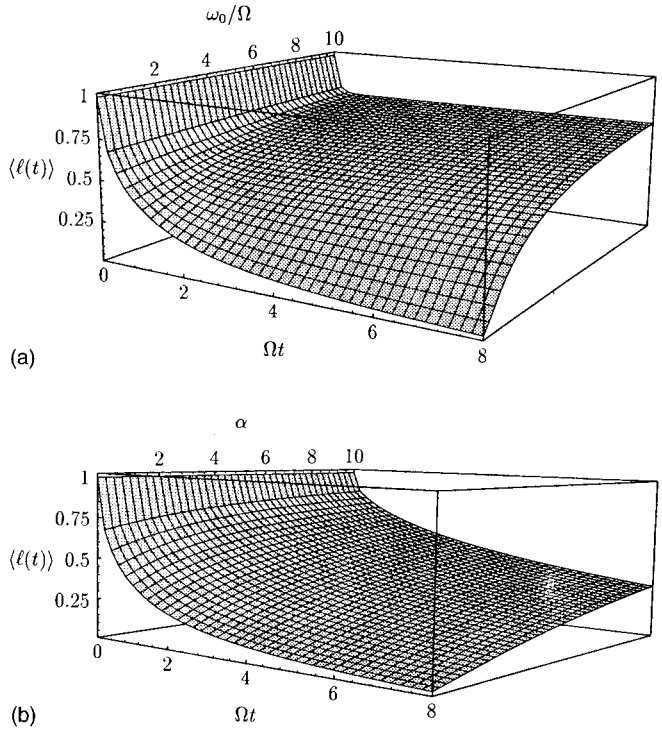

FIG. 1. (a) The dependence of the average survival function $\langle l(t) \rangle$ on the dimensionless time Ωt and on the relative frequency of regression ω_0/Ω for nonintermittent dynamical fluctuations with exponential attenuation, $\beta=0.6$. (b) The dependence of the average survival function $\langle l(t) \rangle$ on the dimensionless time Ωt and on the attenuation exponent α for nonintermittent dynamical fluctuations with self-similar regression, $\beta=0.6$ and $\Omega t_0=0.1$.

The analysis of the values of the moments of the relaxation time, $\langle t^m \rangle$, is of interest because their divergence may be related to the possible statistical fractal behavior of the probability density $\psi(t)$ of the relaxation time. To save space the asymptotic values of $\psi(t)$ are not given in Tables I and II; however, the asymptotic expressions for $\psi(t)$ can be easily evaluated from these tables by noticing that from Eq. (6.9) we have

$$\psi(t)=\langle l(t) \rangle W_{\text{eff}}(t). \tag{6.28}$$

Special attention is deserved by the investigation of the asymptotic behavior of the probability density $\psi(t)dt$ of the relaxation time in the case when a residual value different from zero exists for the average survival function, a situation which corresponds to incomplete relaxation. In this case the probability density $\psi(t)dt$ of the relaxation time is apparently not normalized to unity because we have

$$\int_0^\infty \psi(t)dt=-\int_0^\infty \partial_t \langle l(t) \rangle dt=\langle l(0) \rangle-\langle l(\infty) \rangle=1-\langle l(\infty) \rangle<1. \tag{6.29}$$

The physical explanation of this result is the following: the factor $\langle l(\infty) \rangle$ expresses the proportion of systems (particles) which never relax. Notice, however, that the violation of normalization of the probability density $\psi(t)dt$ is only apparent because the expression (6.7) for $\psi(t)dt$ does not

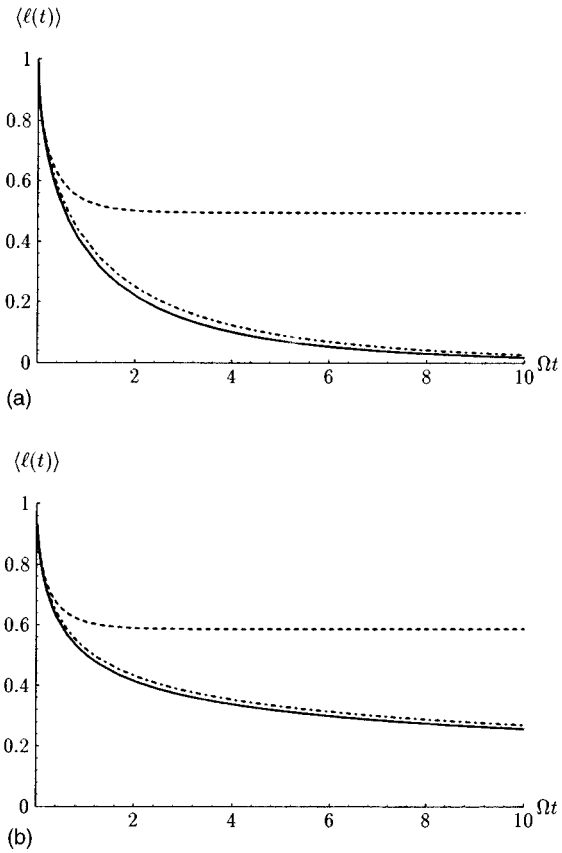

FIG. 2. (a) The dependence of the average relaxation function $\langle l(t)\rangle$ on the dimensionless time Ωt for nonintermittent fluctuations corresponding to a static process (full line), to a dynamical process with exponential attenuation (dashed line), and to a dynamical process with self-similar attenuation (dash-pointed), $\beta=0.6$, $\omega_0/\Omega=3$, $\alpha=0.3$, $\Omega t_0=0.1$. (b) The dependence of the average relaxation function $\langle l(t)\rangle$ on the dimensionless time Ωt for intermittent fluctuations corresponding to a static process (full line), to a dynamical process with exponential attenuation (dashed line), and to a dynamical process with self-similar attenuation (dash-pointed), $\beta=0.6$, $\omega_0/\Omega=3$, $\Omega t_0=0.1$, and $H=0.5$.

take into account the contribution of systems (particles) which survive up to infinity. These particles give rise to a contribution to the expression for $\psi(t)dt$ having the form of a delta function displaced to infinity. Equation (6.7) should be rewritten

$$\psi(t)=-\partial\langle l(t)\rangle/\partial t+\langle l(\infty)\rangle\delta(t-t^*) \quad \text{with} \quad t^*\to\infty. \tag{6.30}$$

This definition of the probability density $\psi(t)dt$ leads to a normalized expression even if $\langle l(\infty)\rangle\neq 0$.

The significance of the values of the moments of the relaxation time displayed in Table II is clear. A stretched exponential relaxation function is relatively fast decreasing and the resulting shape of the tail of $\psi(t)$ ensures the convergence of the moments, a situation which corresponds to static nonintermittent disorder and to dynamical nonintermittent disorder with self-similar regression. In the other four cases presented in Table II the moments are divergent. There are two different causes for this divergence. For nonintermittent and intermittent dynamical disorder with exponential regression it is due to the existence of a finite proportion of particles which never relax. For intermittent static disorder and for intermittent dynamical disorder with self-similar regression the infinite moments are generated by the self-similar features of the tails of the

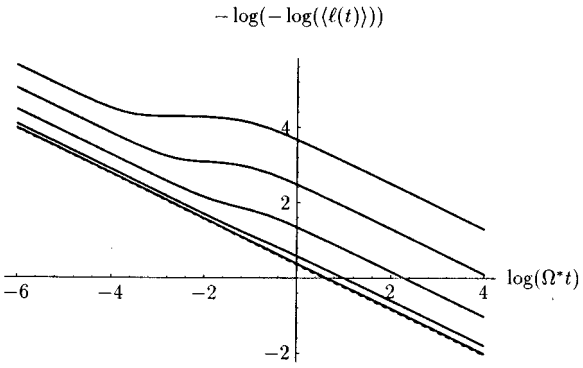

FIG. 3. The average relaxation function $\langle l(t)\rangle$ for nonintermittent, self-similar fluctuations (full line) in comparison to the static average relaxation function (dashed line). In the logarithmic coordinates used the stretched exponential portions of the relaxation functions appear as straight lines: $\beta=0.6$, $\Omega^*\equiv\Omega/(1+\alpha\beta)=1s^{-1}$, and $\Omega^* t_0=0.1$ for $\alpha=0.1$, 1, 10, 100, 1000 (from bottom to top).

probability density $\psi(t)dt$. By using Eq. (6.28) and the data displayed in Tables I and II it is easy to see that in both of these cases the large time behavior of the probability density of the relaxation time is described by

$$\psi(t)\sim t^{-(1+\beta H)} \quad \text{as} \quad t\to\infty, \tag{6.31}$$

that is, $\psi(t)$ has a power law tail with a fractal exponent $1+\beta H$. It is interesting that this fractal exponent is independent of the exponent α of attenuation; the proportionality coefficient in Eq. (6.31) is, however, generally α-dependent.

For a better understanding of the behavior of the average relaxation function $\langle l(t)\rangle$ in the different cases investigated in this paper we present some graphs of this function. As expected these graphs are consistent with the results of asymptotic analysis presented in Tables I and II. By examining Fig. 1(a) corresponding to nonintermittent dynamical fluctuations with exponential regression we notice that the fraction of particles which never relax increases with the increase of the frequency of regression ω_0, a result which is consistent with the asymptotic expression of

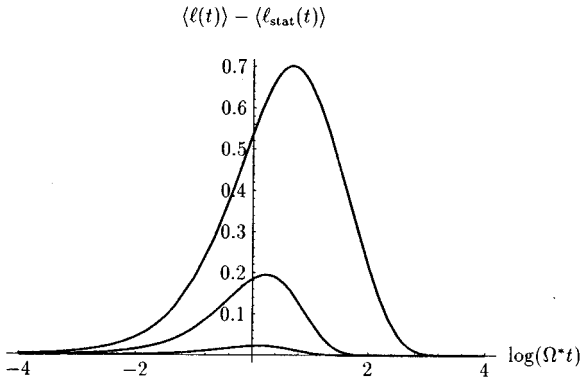

FIG. 4. The dependence of the difference $\langle l(t)\rangle - \langle l_{\text{stat}}(t)\rangle$ between the relaxation function for dynamical nonintermittent fluctuations with self-similar attenuation and the relaxation function for static systems in terms of the logarithm of dimensionless time $\ln(\Omega^* t)$, $\beta=0.6$, $\Omega^*\equiv\Omega/(1+\alpha\beta)=1s^{-1}$, and $\Omega^* t_0=0.1$ for $\alpha=0.1$, 1, 10 (from bottom to top).

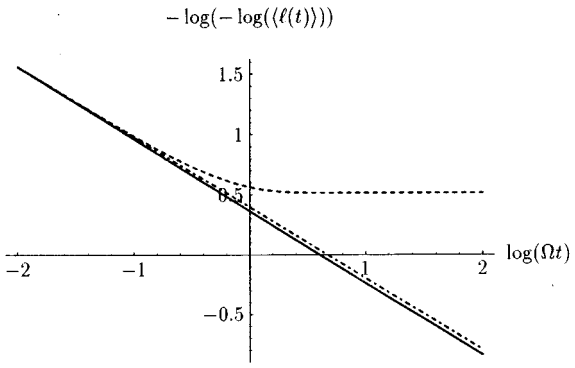

FIG. 5. Average relaxation functions for nonintermittent dynamical fluctuations with exponential attenuation (dashed) and self-similar attenuation (dash-pointed) in comparison with the static stretched exponential law (full line). In the logarithmic coordinates used, the stretched exponential portions of the relaxation functions appear as straight lines: $\beta=0.6$, $\omega_0/\Omega=3$, $\alpha=0.3$, and $\Omega t_0=0.1$.

$\langle l(t)\rangle$ for large time corresponding to this case and presented in Table I. A similar effect can be noticed in Fig. 1(b) corresponding to nonintermittent dynamical disorder with self-similar attenuation. Although in this case the decrease of efficiency of relaxation due to dynamical disorder is less pronounced and eventually as $t\to\infty$ all particles relax, the graph clearly shows that an increase of the attenuation exponent α slows down the relaxation process. Figures 2(a) and 2(b) show some graphs of the average relaxation function for static disorder, dynamical disorder with exponential and self-similar regression for nonintermittent and intermittent fluctuations, respectively. For the consistency of comparison the parameters ω_0, α, and t_0 fulfill the relationship (6.5) so that for dynamical disorder the initial frequency of regression is the same in all cases. In Fig. 2 the same pattern is observed in both cases, that is, the exponential regression leads to incomplete relaxation and, for relatively low values of the attenuation exponent, $1>\alpha\geqslant 0$, the self-similar attenuation leads to relaxation functions which are very close to the functions corresponding to the static case. Significant differences occur only if the attenuation exponent α is bigger than the unity.

The relative insensitivity with respect to the variations of the attenuation exponent α of the average relaxation function for dynamical disorder with self-similar regression is consistent with

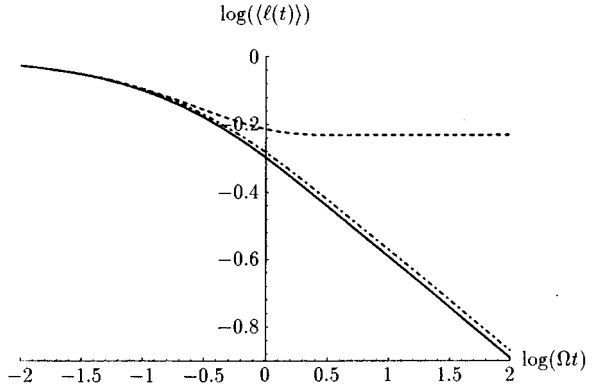

FIG. 6. Average relaxation functions for intermittent dynamical fluctuations with exponential attenuation (dashed) and self-similar attenuation (dash-pointed) in comparison with the intermittent static average relaxation function (full line). In the logarithmic coordinates used, the power law portions of the relaxation functions appear as straight lines: $\beta=0.6$, $\omega_0/\Omega=3$, $\alpha=0.3$, $\Omega t_0=0.1$, and $H=0.5$.

the ubiquity in nature of the stretched exponential. The occurrence of the stretched exponential relaxation for these types of systems is not limited to small values of the exponent α. From Table I it follows that for nonintermittent self-similar dynamical fluctuations a stretched exponential emerges for large times for any values of the exponent α, small or large. In this case the passage from small to large times corresponds to a crossover from a stretched exponential with characteristic frequency Ω to another stretched exponential with a smaller characteristic frequency $\Omega^*=\Omega/(1+\alpha\beta)<\Omega$. Figure 3 displays this crossover phenomenon for different values of the exponent α from very small to very large. For this graph multiple logarithmic coordinates have been used for which the stretched exponential portions of the average relaxation functions appear as straight lines. Stretched exponential portions of the average relaxation functions exist both for small and large times for any values of the exponent α, small or large and all these stretched exponentials have the same exponent β. We emphasize that, even though all these stretched exponentials have the same exponent β, they may actually look very different because their characteristic frequencies may vary very much. This fact is clearly illustrated in Fig. 4.

Figure 5 displays the departure of the different relaxation functions from a stretched exponential in the nonintermittent case. Even for small values of the attenuation rates the exponential regression leads to a large time saturation behavior which is very different from the one described by a stretched exponential. In contrast the self-similar regression leads to a behavior close to the one corresponding to a stretched exponential. Similarly in Fig. 6 the departure from the power law relaxation is investigated for intermittent fluctuations. In this case, too, even for small regression rates the exponential regression leads to incomplete relaxation whereas the self-similar attenuation generates an average relaxation function with a long tail which is close to the one corresponding to the static intermittent case.

The comparative analysis presented in this section shows that for the approach developed in Sec. V the dynamical disorder decreases the efficiency of relaxation. For small regression rates the self-similar attenuation of fluctuations leads to relaxation patterns similar to the ones corresponding to the static processes. For exponential attenuation, however, even the slowest regression rate leads to a different behavior corresponding to incomplete relaxation. For self-similar nonintermittent dynamical disorder the stretched exponential relaxation behavior emerges for large times even if the attenuation exponent α is very large; the corresponding stretched exponentials, although characterized by the same fractal exponent β as in the static case, may be very different from the static stretched exponential, because their characteristic frequencies may vary very much.

VII. DISCUSSION

In this section we discuss some physical implications of the approach suggested in Sec. V. The physical interpretation of the method of computing path averages based on Eqs. (5.6)–(5.17) is related to an apparently obscure mathematical problem, the choice of the initial and boundary conditions for the evolution equations (5.21) or (5.36) for the marginal average $F(W,t)$. In order to ensure the normalization to unity of the average probability density $\varphi(W)dW$ of an individual relaxation rate, for solving the evolution equation (5.28) we have used the boundary condition (5.31). This boundary condition expresses the generation of new fluctuations which are then destroyed by the regression process. In contrast, for solving the partial differential evolution equations (5.21) or (5.36) for the marginal average $F(W,t)$ no such similar boundary conditions have been used. This omission of a boundary condition is required by the main characteristics of the type of dynamical disorder investigated in Sec. V. The main assumption of our approach is that the fluctuations are generated at the beginning of the relaxation process and then they regress as the relaxation process is going on. We start out by considering an initial fluctuation with statistical properties described by the probability density $\varphi_{st}(W)dW$ given by Eq. (5.25), and then we follow its regression during the relaxation process. As time increases, due to the regression process, the channels with high relaxation rates lose their reactivity and their rates become smaller and smaller.

During the relaxation process the size of a set of channels with high relaxation rates is shrinking; of the average number $\langle N^* \rangle$ of channels involved in the process, more and more have low relaxation rates, resulting in the decrease of efficiency described by the model. No mechanism of transition of a channel from a state characterized by a small relaxation rate to a state with a high relaxation rate is supposed to exist for $t>0$. Such a mechanism acts only at the beginning of the process, for $t=0$, when the fluctuations are generated and thus we should impose a boundary condition only for this moment:

$$F(W=W^*,t=0)=\beta/W^*. \tag{7.1}$$

Such a condition, however, does not need to be taken explicitly into account in the computation because it is contained in the initial condition (5.37).

The above considerations are closely related to the physical interpretation of Eq. (5.28) for the time evolution of the probability density $\varphi(W)dW$. From the physical point of view Eq. (5.28) is a stochastic Liouville equation which describes the regression of fluctuations only and it would lead to a probability loss $\int \varphi(W)dW<1$ if the generation of new fluctuations is not taken into account. The introduction of the boundary condition (5.31) compensates the ''probability loss'' due to the regression process by an ''influx of probability fluid'' into the system. In contrast, the compound stochastic Liouville equation (5.17), which describes the relaxation process and Eq. (5.36) derived from it, cannot accomodate a boundary condition of the type (5.31). This limitation is due to the Markovian approximation introduced in Sec. V. Within its framework a given feature of the regression process can be modeled only by assuming that the regression frequency $\omega(t)$ is generally time dependent, resulting in a time-inhomogeneous evolution equation for the overall relaxation process for which a boundary condition of the type (5.31) cannot be formulated in a simple way.

We emphasize that this type of pure regression mechanism without generation of new fluctuations for $t>0$ is the only one which includes the case of the static disorder as a particular case, corresponding to the situation when the rate of regression is equal to zero. If the fluctuations are generated for $t>0$, the system is characterized by dynamical disorder, even if the regression process is missing. Although, at least in principle, this type of dynamical disorder can also be described by the dynamical Huber law (3.7) or by its intermittent analog (4.7), it is different from the type of dynamical disorder considered in Sec. V. Some preliminary research concerning the generation of fluctuations for $t>0$ is presented in Ref. 19; it has been shown that, as expected, this type of dynamical disorder leads to an increase in the efficiency of relaxation, because it generates an increase in the number of channels with high relaxation rates. In particular, if the regression process is missing, this type of dynamical disorder leads to a compressed exponential relaxation described by the average survival function

$$\langle l(t) \rangle \sim \exp(-\text{const } t^{1+\beta}); \quad 1>\beta>0. \tag{7.2}$$

Our analysis has shown that the self-similar regression has the remarkable feature that for small regression rates it does not affect the shape of the average relaxation function, generating only small corrections. Moreover, even for very large regression rates, for large times the process is described by a stretched exponential with the same fractal exponent β as in the static case. These results, which might provide an explanation for the universality of the stretched exponential relaxation law, are consistent with the ideas developed by West[36,37] concerning the insensitivity of the statistical fractal systems to random perturbations. From the mathematical point of view for the model developed in Sec. V, this insensitivity is due to the slow decrease of the relaxation rates in the case of self-similar regression, especially for large times.

At the end of this section we point out an apparent contradiction between the results reported here and the results presented in Ref. 26. In Ref. 26 an analysis of the passage over a fluctuating

activation energy barrier has been suggested based on a path average technique similar to the one used in Sec. V. Although both models assume the existence of a pure regression mechanism for $t>0$, the analysis from Ref. 26 shows that the dynamical disorder leads to an increase of the transparency factor of the barrier which apparently contradicts the results reported here. The explanation of this apparent paradox is simple. In Ref. 26 the regression of fluctuations leads to a decrease in the height of the activation energy barrier, that is, to an increase of the speed of relaxation, whereas for our model the regression of fluctuations leads to small rates.

VIII. CONCLUSIONS

In this paper an attempt has been made to construct dynamical analogs of the stretched exponential relaxation. The main idea of the suggested approach is to search for the asymptotic relaxation laws which emerge in the limit of a very large number of relaxation modes. The mathematical structure of the theory is based on a formal functional generalization of the theory of random point processes for which to each random point a random function is attached. In the limit of very large numbers of relaxation modes two universal relaxation laws have been identified corresponding to nonintermittent and intermittent dynamical fluctuations, respectively. An attempt to evaluate the path averages entering the asymptotic relaxation laws has been made for Markovian systems with pure regression. It has been shown that the regression of fluctuations leads to a decrease of the efficiency of the relaxation process. For nonintermittent fluctuations the process is relatively insensitive to the effect of self-similar attenuation of fluctuations, even for high regression rates. This effect might provide an explanation for the wide applicability of stretched exponential law for describing various relaxation processes with dynamical disorder.

Further research should focus on the evaluation of the path averages for the more general case when there is a competition between the generation and the extinction of fluctuations and on the study of suitable applications. Ideal candidates for the application of the theory are the systems in which a large number of degrees of freedom are involved in the relaxation process, for instance, the protein–ligand interactions,[7] or the ion channel kinetics,[9] where the relaxation modes correspond to a large number of molecular conformations.

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Bi-Hamiltonian structures of the coupled AKNS hierarchy and the coupled Yajima–Oikawa hierarchy

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The Hamiltonian theory for the two-component AKNS hierarchy and Yajima–Oikawa hierarchy is considered from the viewpoint of reduction. We show that the second Hamiltonian structures of the former is a Dirac reduction of the sl(3) current algebra, while the latter is related to the classical $W_4^{(3)}$ algebra. © *1996 American Institute of Physics.* [S0022-2488(96)01905-8]

I. INTRODUCTION

The KP hierarchy is universal in the sense that various integrable systems are just special reductions of it. The best known one is the so-called n-reduction, which turns out to be the Gelfand–Dickey hierarchy. Recently, another reduction, known as constrained KP hierarchy, is proposed and studied considerably.[1–4] This hierarchy is the result of generalizing Cao's nonlinearization[5] to the 2+1-dimensional case. Interestingly, as the famous Gelfand–Dickey hierarchy,[6] the constrained KP hierarchy is not only mathematically important, but also has physical relevance. On the one hand, it contains physically applicable models, such as Yajima–Oikawa model[7] and Melnikov model.[8] On the other hand, the constrained KP hierarchy is Bi-Hamiltonian,[4] has Darboux transformation,[9] can be modified,[10] and is relevant to the W algebra theory.[11] We also point out that the constrained KP is shown to be just a special case of a more general restriction of the KP hierarchy.[12]

A generalization of the constrained KP hierarchy is considered.[13] This may be termed as multi-component constrained KP hierarchy, since it is the hierarchy associated with the following Lax operator:

$$L_n=\partial^n+u_{n-2}\partial^{n-2}+\cdots+u_0+\sum_{i=1}^{m} q_i\partial^{-1}r_i\,. \tag{1.1}$$

The corresponding flows may be constructed by means of Fractional Power Method (FPM).[6] In the case $n=1$, one has multi-component AKNS hierarchy, which includes the important coupled nonlinear Schrödinger equation[14] as a special case. For the cases $n=2$ and $n=3$, one has the multi-component generalizations of the Yajima–Oikawa hierarchy and Melnikov hierarchy, respectively. Sidorenko and Strampp[13] further constructed recursion operators for the cases $n=2$ and $n=3$ by means of variational calculus or residue calculus.[15] They claimed that the factorization of their recursion operators leads to bi-Hamiltonian structures for the related hierarchies (see Ref. 16). We remark that while the residue calculus is very effective in constructing Hamiltonian operators, this does not means that each operator calculated this way is Hamiltonian automatically.[15,17] Since these operators are rather complicated, direct proof would be too tedious to do by hand.

This paper is complemental to Sidorenko and Strampp's results.[13] The aim of the paper is twofold: correcting an error of Sidorenko and Strampp and providing a proof for the Hamiltonian

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nature of their operators. For simplicity, we will consider the simplest nontrivial cases: two-component cases. We will show that the second Hamiltonian operator of the coupled Yajima–Oikawa hierarchy is the Dirac reduction of the classical $W_4^{(3)}$ algebra. This algebra is calculated by Depireux and Mathieu.[18] Thus, as a by-product, the coupled Yajima–Oikawa hierarchy is shown to be related to this W algebra. This is interesting in its own right. The generalization to the multi-component case will be commented on in due course.

The paper is arranged as follows. The next section is on the two-component AKNS systems. We show that the well-known recursion operator leads to a bi-Hamiltonian structure for this hierarchy. The Hamiltonian nature of the second operator is proved by showing that it is the Dirac reduction of the sl(3) current algebra. In Sec. III we present our main results: giving Sidorenko–Strampp's operator in its correct form and proving its Hamiltonian nature. That is, we prove rigorously that the two-component Yajima–Oikawa hierarchy is bi-Hamiltonian. Section IV contains some comments on generalizations of the results of Secs. II and III.

II. THE COUPLED AKNS HIERARCHY

We consider the two-component AKNS system next. This hierarchy has been known for a long time. In fact, the very important coupled nonlinear Schrödinger equation[14] is a reduction of it. Its recursion operator is already calculated out.[19] However, to the best of my knowledge, a proof of the bi-Hamiltonian for the hierarchy is still not available. Even the hereditary property of the recursion operator is not proved.

We start with the Lax operator

$$L_1=\partial-q_1\partial^{-1}r_1-q_2\partial^{-1}r_2. \tag{2.1}$$

The corresponding flows are

$$L_{1_{t_k}}=[((L_1)^k)_+, L_1], \tag{2.2}$$

where subscript + means the projection to the differential part.

The recursion operator for the hierarchy (2.2)[19] is

$$\mathbf{R}=\begin{bmatrix} R_1 & -q_1\partial^{-1}r_2 & -2q_1\partial^{-1}q_1 & -q_1\partial^{-1}q_2-q_2\partial^{-1}q_1 \\ -q_2\partial^{-1}r_1 & R_2 & -q_1\partial^{-1}q_2-q_2\partial^{-1}q_1 & -2q_2\partial^{-1}q_2 \\ 2r_1\partial^{-1}r_1 & r_1\partial^{-1}r_2+r_2\partial^{-1}r_1 & (R_1)^* & r_1\partial^{-1}q_2 \\ r_1\partial^{-1}r_2+r_2\partial^{-1}r_1 & 2r_2\partial^{-1}r_2 & r_2\partial^{-1}q_1 & (R_2)^* \end{bmatrix}, \tag{2.3}$$

where R_1 and R_2 are defined by

$$R_1=\partial-2q_1\partial^{-1}r_1-q_2\partial^{-1}r_2, \quad R_2=\partial-q_1\partial^{-1}r_1-2q_2\partial^{-1}r_2. \tag{2.4}$$

The recursion operator (2.3) has the following factorization: $\mathbf{R}=\mathbf{B}_1(\mathbf{B}_0)^{-1}$ with

$$\mathbf{B}_0=\begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix}, \tag{2.5}$$

and

$$\mathbf{B}_1=\begin{bmatrix} 2q_1\partial^{-1}q_1 & q_1\partial^{-1}q_2+q_2\partial^{-1}q_1 & R_1 & -q_1\partial^{-1}r_2 \\ q_1\partial^{-1}q_2+q_2\partial^{-1}q_1 & 2q_2\partial^{-1}q_2 & -q_2\partial^{-1}r_1 & R_2 \\ -(R_1)^* & -r_1\partial^{-1}q_2 & 2r_1\partial^{-1}r_1 & r_1\partial^{-1}r_2+r_2\partial^{-1}r_1 \\ -r_2\partial^{-1}q_1 & -(R_2)^* & r_1\partial^{-1}r_2+r_2\partial^{-1}r_1 & 2r_2\partial^{-1}r_2 \end{bmatrix}, \tag{2.6}$$

where $\mathbf{R}_i$ $(i=1,2)$ are given by (2.4).

Thus, the hierarchy has the following representation:

$$\mathbf{q}_{t_k}=\mathbf{B}_0\,\frac{\delta H_{k+1}}{\delta \mathbf{q}}=\mathbf{B}_1\,\frac{\delta H_k}{\delta \mathbf{q}}, \tag{2.7}$$

where $\mathbf{q}=(q_1,q_2,r_1,r_2)^T$ and H_k is defined by

$$H_k=\frac{1}{k}\,(\mathrm{Res}(L_1)^k).$$

The explicit form of the first three Hamiltonians is

$$H_1=-(q_1r_1+q_2r_2),\quad H_2=\tfrac{1}{2}(q_1r_{1_x}-r_1q_{1_x}+q_2r_{2_x}-r_2q_{2_x}),\quad H_3=\tfrac{1}{3}(-r_1q_{1_{xx}}-r_2q_{2_{xx}}+q_{1_x}r_{1_x}$$
$$+q_{2_x}r_{2_x}+3q_1^2r_1^2+3q_2^2r_2^2+6q_1q_2r_1r_2-q_1r_{1_{xx}}-q_2r_{2_{xx}}).$$

The first two flows are

$$\begin{aligned} q_{1_{t1}}&=-q_{1_x},\quad q_{2_{t1}}=-q_{2_x}, \\ r_{1_{t1}}&=-r_{1_x},\quad r_{2_{t1}}=-r_{2_x}, \end{aligned} \tag{2.8}$$

and

$$\begin{aligned} q_{1_{t2}}&=-q_{1_{xx}}+2q_1^2r_1+2q_1q_2r_2, \\ q_{2_{t2}}&=-q_{2_{xx}}+2q_2^2r_2+2q_1q_2r_1, \\ r_{1_{t2}}&=r_{1_{xx}}-2r_1^2q_1-2r_1r_2q_2, \\ r_{2_{t2}}&=r_{2^{xx}}-2r_2^2q_2-2q_1r_1r_2. \end{aligned} \tag{2.9}$$

Our next task is to prove the Hamiltonian nature of the operator (2.6). Since this operator is obviously skew-symmetric and compatible with the operator (2.5), the Hamiltonian property of the operator $\mathbf{B}_1$ will lead us to the conclusion: the coupled AKNS hierarchy (2.2) is a well-defined bi-Hamiltonian system.

Remarks:

(1) Two compatible Hamiltonian operators ensure that the resulting recursion operator is hereditary. We should stress that the hereditary property is an important property for a recursion operator since such an operator makes the related flows commute.[16]

(2) We notice that Asano and Kato[20] considered the $N\times N$ AKNS system and one may try to construct the recursion operator of the coupled AKNS hierarchy by some reduction of their

general formula. However, reduction often destroys the hereditary property, so one has to check this property for the reduced operator by hand. This will be a much more involved calculation. To prove our claim, we consider the general sl(3) spectral problem

$$\begin{bmatrix} \phi \\ \phi_1 \\ \phi_2 \end{bmatrix}_x = \begin{bmatrix} \lambda - u_1 & q_1 & q_2 \\ r_1 & u_1+u_2 & v \\ r_2 & w & -\lambda - u_2 \end{bmatrix} \begin{bmatrix} \phi \\ \phi_1 \\ \phi_2 \end{bmatrix} \equiv (\lambda A + U)\Phi, \tag{2.10}$$

now choosing the time evolution of the wave function Φ as $\Phi_t = V\Phi$. Then the zero-curvature representation leads to

$$U_t = \mathbf{P}_U(V) - \lambda \mathbf{Q}_U(V),$$

where the Poisson tensors defined by

$$\mathbf{P}_U = \partial + [\cdot, U], \quad \mathbf{Q}_U = [A, \cdot]$$

introduce a bi-Hamiltonian structure, which is referred as the Zakharov–Shabat bi-Hamiltonian structure (see Ref. 21 and the references there, for example). Our main interest is the second one and a straightforward calculation shows that the explicit form of the $\mathbf{P}_U$, which is denoted by $\mathbf{P}_{(\mathbf{q},\mathbf{u})}$ for convenience, reads as

$$\mathbf{P}_{(\mathbf{q},\mathbf{u})} = \begin{bmatrix} 0 & 0 & \partial + u_2 + 2u_1 & w & -q_1 & 0 & -q_2 & 0 \\ 0 & 0 & v & \partial - u_2 + u_1 & -q_2 & q_2 & 0 & -q_1 \\ \partial - u_2 - 2u_1 & -v & 0 & 0 & r_1 & 0 & 0 & r_2 \\ -w & \partial - u_1 + u_2 & 0 & 0 & r_2 & -r_2 & r_1 & 0 \\ q_1 & q_2 & -r_1 & -r_2 & \frac{2}{3}\partial & -\frac{1}{3}\partial & 0 & 0 \\ 0 & -q_2 & 0 & r_2 & -\frac{1}{3}\partial & \frac{2}{3}\partial & -v & w \\ q_2 & 0 & 0 & -r_1 & 0 & v & 0 & \partial - 2u_2 - u_1 \\ 0 & q_1 & -r_2 & 0 & 0 & -w & \partial + u_1 + 2u_2 & 0 \end{bmatrix}, \tag{2.11}$$

where $\mathbf{q} = (q_1, q_2, r_1, r_2)^T$ and $\mathbf{u} = (u_1, u_2, v, w)^T$.

We remark that this operator leads to so-called sl(3) current algebra.

In order to recover our candidate for the second Hamiltonian structure $\mathbf{B}_1$(2.6) from the Hamiltonian operator $\mathbf{P}_{(\mathbf{q},\mathbf{u})}$, we have to do a reduction by imposing the constraint $\mathbf{u} = 0$. Indeed, the reduction involved here is the so-called Dirac reduction which is discussed by Oevel and Ragnisco.[22] Basically, suppose we are given a space with the coordinates $\mathbf{q}$, $\mathbf{u}$ and a Poisson tensor

$$\mathbf{P}_{(\mathbf{q},\mathbf{u})} = \begin{bmatrix} P_{qq} & P_{qu} \\ P_{uq} & P_{uu} \end{bmatrix}$$

on this space; then the Dirac reduction of $\mathbf{P}_{(\mathbf{q},\mathbf{u})}$ to the subspace spanned by $\mathbf{q}$ is provided by the reduced Hamiltonian operator

$$\mathbf{P}_{\mathbf{q}}^{(\mathrm{red})} = P_{qq}(q,0) - P_{qu}(q,0)(\mathbf{P}_{uu}(q,0))^{-1} P_{uq}(q,0),$$

where the existence of the operator $(P_{uu}(q,0))^{-1}$ is assumed.

In the present case, we have

$$P_{qq}=\begin{bmatrix} 0 & 0 & \partial+u_2+2u_1 & w \\ 0 & 0 & v & \partial-u_2+u_1 \\ \partial-u_2-2u_1 & -v & 0 & 0 \\ -w & \partial-u_1+u_2 & 0 & 0 \end{bmatrix},$$

$$P_{qu}=\begin{bmatrix} -q_1 & 0 & -q_2 & 0 \\ -q_2 & q_2 & 0 & -q_1 \\ r_1 & 0 & 0 & r_2 \\ r_2 & -r_2 & r_1 & 0 \end{bmatrix}, \quad P_{uq}=\begin{bmatrix} q_1 & q_2 & -r_1 & -r_2 \\ 0 & -q_2 & 0 & r_2 \\ q_2 & 0 & 0 & -r_1 \\ 0 & q_1 & -r_2 & 0 \end{bmatrix},$$

$$P_{uu}=\begin{bmatrix} \frac{2}{3}\partial & -\frac{1}{3}\partial & 0 & 0 \\ -\frac{1}{3}\partial & \frac{2}{3}\partial & -v & w \\ 0 & v & 0 & \partial-2u_2-u_1 \\ 0 & -w & \partial+2u_2+u_1 & 0 \end{bmatrix}.$$

Now the elementary calculation shows that the reduced Hamiltonian operator $\mathbf{P}_{\mathbf{q}}^{(\mathrm{red})}$ is nothing but our operator $\mathbf{B}_1$. Thus, we complete our proof.

Remark: The first two flows (2.8) and (2.9) have the following alternative representation:

$$\mathbf{q}_{t_k}=\hat{\mathbf{B}}_0\frac{\delta H_{k+1}}{\delta \mathbf{q}}=\hat{\mathbf{B}}_1\frac{\delta H_k}{\delta \mathbf{q}}, \quad (k=1,2),$$

where $\mathbf{q}=(q_1,q_2,r_1,r_2)^T$, and

$$\hat{\mathbf{B}}_0=\mathbf{B}_0$$

and

$$\hat{\mathbf{B}}_1=\begin{bmatrix} 2q_1\partial^{-1}q_1 & 2q_1\partial^{-1}q_2 & \partial-2q_1\partial^{-1}r_1 & -2q_1\partial^{-1}r_2 \\ 2q_2\partial^{-1}q_1 & 2q_2\partial^{-1}q_2 & -2q_2\partial^{-1}r_1 & \partial-2q_2\partial^{-1}r_2 \\ \partial-2r_1\partial^{-1}q_1 & -2r_1\partial^{-1}q_2 & 2r_1\partial^{-1}r_1 & 2r_1\partial^{-1}r_2 \\ -2r_2\partial^{-1}q_1 & \partial-2r_2\partial^{-1}q_2 & 2r_2\partial^{-1}r_1 & 2r_2\partial^{-1}r_2 \end{bmatrix}.$$

However, it can be shown that this is NOT a bi-Hamiltonian representation for the flows. In fact, it can be proved that the resulting operator $\hat{\mathbf{R}}=\hat{\mathbf{B}}_1(\hat{\mathbf{B}}_0)^{-1}$ is not even hereditary.

III. THE COUPLED YAJIMA–OIKAWA HIERARCHY

The hierarchy we are interested in is associated to the following Lax operator:

$$L_2=\partial^2-u-q_1\partial^{-1}r_1-q_2\partial^{-1}r_2. \tag{3.1}$$

The flows, which may be calculated by means of fractional power method, have the following representation:

$$\mathbf{u}_{t_k}=\mathbf{B}_0\frac{\delta H_{k+1}}{\delta \mathbf{u}}=\mathbf{B}_1\frac{\delta H_k}{\delta \mathbf{u}}, \tag{3.2}$$

where $\mathbf{u}=(u,q_1,q_2,r_1,r_2)^T$ and

$$H_k=\frac{2}{k}\,(\mathrm{Res}(L_2)^{k/2}) \tag{3.3}$$

and

$$\mathbf{B}_0=\begin{bmatrix} -2\partial & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 0 & 1\\ 0 & -1 & 0 & 0 & 0\\ 0 & 0 & -1 & 0 & 0 \end{bmatrix} \tag{3.4}$$

and

$$\mathbf{B}_1=\begin{bmatrix} -\frac{1}{2}\partial^3+u\partial+\partial u & q_1\partial+\frac{1}{2}\partial q_1 & q_2\partial+\frac{1}{2}\partial q_2 & r_1\partial+\frac{1}{2}\partial r_1 & r_2\partial+\frac{1}{2}\partial r_2\\ \partial q_1+\frac{1}{2}q_1\partial & \frac{3}{2}q_1\partial^{-1}q_1 & I(q_1,q_2) & I_1 & -\frac{1}{2}q_1\partial^{-1}r_2\\ \partial q_2+\frac{1}{2}q_2\partial & I(q_2,q_1) & \frac{3}{2}q_2\partial^{-1}q_2 & -\frac{1}{2}q_2\partial^{-1}r_1 & I_2\\ \partial r_1+\frac{1}{2}r_1\partial & -I_1^* & -\frac{1}{2}r_1\partial^{-1}q_2 & \frac{3}{2}r_1\partial^{-1}r_1 & I(r_1,r_2)\\ \partial r_2+\frac{1}{2}r_2\partial & -\frac{1}{2}r_2\partial^{-1}q_1 & -I_2^* & I(r_2,r_1) & \frac{3}{2}r_2\partial^{-1}r_2 \end{bmatrix}, \tag{3.5}$$

where $I(v_1,v_2)\equiv\frac{1}{2}v_1\partial^{-1}v_2+v_2\partial^{-1}v_1$, $I_1\equiv\partial^2-u-\frac{3}{2}q_1\partial^{-1}r_1-q_2\partial^{-1}r_2$, and $I_2\equiv\partial^2-u-\frac{3}{2}q_2\partial^{-1}r_2-q_1\partial^{-1}r_1$

Remark: We see that the first operator $\mathbf{B}_0$ is the same as the one presented in Ref. 13. However, the second one, $\mathbf{B}_1$, is not their operator. In fact, we may easily show that their operator, which is mistakenly presented, does not qualify as a Hamiltonian operator.

Our next task is to prove that the hierarchy (3.2) is a bi-Hamiltonian system. That is to say, we shall prove $\mathbf{B}_i(i=0,1)$ are compatible Hamiltonian operators. The Hamiltonian property of $\mathbf{B}_0$ and the compatibility condition are obvious. Thus, we need only to prove the Hamiltonian nature of the operator $\mathbf{B}_1$.

Our strategy is the same as before, and we consider the following more general spectral problem:

$$\phi_x=\begin{bmatrix} 0 & 0 & 0 & 1\\ r_2 & w_1 & v_1 & 0\\ r_1 & v_2 & w_2 & 0\\ u+\lambda & q_2 & q_1 & -w_1-w_2 \end{bmatrix}\phi. \tag{3.6}$$

We see that the above form is the one presented in Ref. 18 for the classical $W_4^{(3)}$ algebra from the Hamiltonian reduction approach. To construct the related Hamiltonian structures, we may calculate the Zakharov–Shabat bi-Hamiltonian structure[21] as we did in Sec. II. Since the argument is standard, we just give the results here. Two Hamiltonian operators are defined conveniently by the following Poisson brackets:

$$\{u(x),u(y)\}_0=-2\partial\delta(x-y),\quad \{q_1(x),r_1(y)\}_0=\delta(x-y),\quad \{q_2(x),r_2(y)\}_0=\delta(x-y), \tag{3.7}$$

and

$$\{u(x),u(y)\}_1=(\tfrac{3}{4}(-\partial^3+\partial^2(w_1+w_2)-(w_1+w_2)\partial^2+(w_1+w_2)\partial(w_1+w_2))+u\partial+\partial u)\,\delta(x-y),$$

$$\{u(x),q_1(y)\}_1=(q_1\partial-q_1(w_1+2w_2)-q_2v_1)\delta(x-y),$$

$$\{u(x),q_2(y)\}_1=(q_2\partial-q_2(2w_1+w_2)-q_1v_2)\delta(x-y),$$

$$\{u(x),r_1(y)\}_1=(\partial r_1+r_1\partial+r_1(w_1+2w_2)+r_2v_2)\delta(x-y),$$

$$\{u(x),r_2(y)\}_1=(\partial r_2+r_2\partial+r_2(w_2+2w_1)+r_1v_1)\delta(x-y),$$

$$\{u(x),w_i(y)\}_1=-\tfrac{1}{4}(\partial+w_1+w_2)\partial\delta(x-y),$$

$$\{q_1(x),r_1(y)\}_1=(\partial^2+\partial w_2-u+(w_1+2w_2)(\partial-w_2)+v_1v_2)\delta(x-y),$$

$$\{q_1(x),r_2(y)\}_1=(\partial v_1+v_1\partial+2(w_1+w_2)v_1)\delta(x-y), \tag{3.8}$$

$$\{q_1(x),v_2(y)\}_1=-q_2\delta(x-y),$$

$$\{q_1(x),w_2(y)\}_1=-q_1\delta(x-y),\quad \{q_2(x),r_1(y)\}_1=(\partial v_2+v_2\partial+2(w_1+w_2)v_2)\delta(x-y),$$

$$\{q_2(x),r_2(y)\}_1=(\partial^2+\partial w_1-u+(2w_1+w_2)(\partial+w_1)+v_1v_2)\delta(x-y),$$

$$\{r_1(x),v_1(y)\}_1=r_2\delta(x-y),\quad \{r_1(x),w_2(y)\}_1=r_1\delta(x-y),$$

$$\{r_2(x),v_2(y)\}_1=r_1\delta(x-y),\quad \{r_2(x),w_1(y)\}_1=r_2\delta(x-y),$$

$$\{v_1(x),v_2(y)\}_1=(\partial-w_1+w_2)\delta(x-y),\quad \{v_1(x),w_i(y)\}_1=\mp v_1\delta(x-y),$$

$$\{v_2(x),w_i(y)\}_1=\pm v_2\delta(x-y),\quad \{w_i(x),w_j(y)\}_1=(\delta_{ij}-\tfrac{1}{4})\partial\delta(x-y),$$

where $i,j=1,2$, and all other brackets vanish.

This Poisson bracket algebra (3.8) is equivalent to the classical $W_4^{(3)}$ algebra.[18] We also notice that the spectral problem (3.6) is a special case of the more general problem considered recently by Feher and Marshall.[23] In their notation, our case corresponds to the partition: $n=4=2+1+1(r=2,s=2,p=1)$. Thus, our brackets (3.7) and (3.8) also follow from their general structures.

We see that the first Hamiltonian bracket (3.7) is degenerate in this general case. That means the general flows are not a well-defined bi-Hamiltonian system since we are not able to form the important recursion operator. Therefore, we have to do reduction. Indeed, by Dirac reduction described in the above section, we find that the Poisson bracket (3.8) is reduced to the bracket introduced by the operator $\mathbf{B}_1$. Thus, we recover the second structure $\mathbf{B}_1$ by the Dirac reduction and we complete our proof.

Here we remark that we have a by-product: we find that the coupled Yajima–Oikawa hierarchy (3.2) is the hierarchy related to the classical $W_4^{(3)}$ algebra *directly* in the sense of Ref. 18.

IV. SUMMARY

In this paper, we studied the coupled AKNS hierarchy and coupled Yajima–Oikawa hierarchy from the bi-Hamiltonian viewpoint. We prove rigorously that both hierarchies are well-defined bi-Hamiltonian systems. For the coupled Yajima–Oikawa hierarchy, we corrected an error of Ref. 13. Also, we showed that this hierarchy is just the one related to the classical $W_4^{(3)}$ algebra directly.[18] The present consideration may be generalized to the generic multi-component case although the calculation will be extremely tedious.

It is interesting and important to construct the modified hierarchies of the hierarchies of Secs. II and III. We notice that for the nonreduced hierarchies, this problem is considered in Ref. 23. In general, doing reduction often destroys the related Miura maps, and it is necessary to consider the reduced hierarchies separately.

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The $W_{1+\infty}(gl_s)$-symmetries of the s-component KP hierarchy

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Adler, Shiota, and van Moerbeke obtained for the KP and Toda lattice hierarchies a formula which translates the action of the vertex operator on tau-functions to an action of a vertex operator of pseudodifferential operators on wave functions. This relates the additional symmetries of the KP and Toda lattice hierarchy to the $W_{1+\infty-}$, respectively, $W_{1+\infty} \times W_{1+\infty-}$ algebra symmetries. In this paper we generalize the results to the s-component KP hierarchy. The vertex operators generate the algebra $W_{1+\infty}(gl_s)$, the matrix version of $W_{1+\infty}$. Since the Toda lattice hierarchy is formally equivalent to the 2-component KP hierarchy, the results of this article uncover in that particular case a much richer structure than the one obtained by Adler, Shiota, and van Moerbeke. © *1996 American Institute of Physics.* [S0022-2488(96)02004-X]

I. INTRODUCTION

The KP hierarchy is the set of deformation equations

$$\frac{\partial L}{\partial t_k} = [(L^k)_+, L],$$

for the first-order pseudodifferential operator

$$L \equiv L(x,t) = \partial + u_1(x,t)\partial^{-1} + u_2(x,t)\partial^{-2} + \cdots,$$

here $\partial = \partial/\partial x$ and $t = (t_1, t_2, \ldots)$. It is well-known that L dresses as $L = P\partial P^{-1}$ with

$$P \equiv P(\tau,x,t) = 1 + a_1(x,t)\partial^{-1} + a_2(x,t)\partial^{-2} + \cdots = \frac{\tau(x,t-[\partial^{-1}])}{\tau(x,t)},$$

where τ is the famous τ-function, introduced by the Kyoto group[1–3] and $[z] = (z, z^2/2, z^3/3, \ldots)$.

The wave or Baker–Akhiezer function

$$\Psi \equiv \Psi(\tau,x,t,z) = W(\tau,x,t,\partial)e^{zx},$$

where

$$W \equiv W(\tau,x,t,z) = P(\tau,x,t)e^{\xi(t)} \quad \text{with} \quad \xi(t) = \sum_{k=1}^{\infty} t_k \partial^k$$

is an eigenfunction of L, viz.,

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$$L\Psi = z\Psi \quad \text{and} \quad \frac{\partial \Psi}{\partial t_k} = (L^k)_+ \Psi .$$

From this point of view, the introduction by Orlov and Schulman[4] of another pseudodifferential operator $M \equiv M(x,t) = WxW^{-1}$ which action on Ψ amounts to

$$M\Psi = \frac{\partial \Psi}{\partial z}$$

is rather natural.

Recently, Adler, Shiota, and van Moerbeke[5,6] proved a conjecture of Orlov and Schulman, viz., that there exists a relation between $(M^l L^{k+l})_-$ acting on Ψ and the generators $W_k^{(l+1)} \sim -t^{k+l}(\partial/\partial t)^l$ of the $W_{1+\infty}$-algebra acting on the τ-function. More explicitly, let

$$Y(\tau,y,w) = \sum_{l=0}^{\infty} \frac{(y-w)^l}{l!} \sum_{k\in\mathbb{Z}} M^l L^{k+l} w^{-k-l-1}$$

be the generating series of the $M^l L^{k+l}$ and let

$$\begin{aligned} W(y,w) &= \sum_{l=0}^{\infty} \frac{(y-w)^l}{l!} \sum_{k\in\mathbb{Z}} W_k^{(l+1)} w^{-k-l-1} \\ &= \frac{1}{y-w} \exp\left(x(y-w) + \sum_{k=1}^{\infty} t_k (y^k - w^k) \right) \exp\left(-\sum_{k=1}^{\infty} \frac{\partial}{\partial t_k} \frac{y^{-k} - w^{-k}}{k} \right) \end{aligned} \tag{1.1}$$

be the vertex operator of the KP hierarchy, then one has the following formula:[5]

$$-Y(\tau,y,w)_-\Psi(\tau,x,t,z) = \Psi(\tau,x,t,z)\left(\exp -\sum_{k=1}^{\infty} \frac{\partial}{\partial t_k} \frac{z^{-k}}{k} - 1 \right)\left(\frac{W(y,w)\tau(x,t)}{\tau(x,t)} \right). \tag{1.2}$$

Dickey gave another proof of this formula.[7] The ''geometric interpretation'' of this Adler–Shiota–van Moerbeke formula is as follows. The transformation $e^{\lambda W(y,w)} = 1 + \lambda W(y,w)$ is a symmetry transformation or a kind of auto-Bäcklund transformation of the KP hierarchy. If one rewrites (1.2) as

$$-\lambda Y(\tau,y,w)_-\Psi(\tau,x,t,z) = \Psi(\tau,x,t,z)\left(\exp -\sum_{k=1}^{\infty} \frac{\partial}{\partial t_k} \frac{z^{-k}}{k} - 1 \right)\left(\frac{e^{\lambda W(y,w)}\tau(x,t)}{\tau(x,t)} \right), \tag{1.3}$$

then one easily sees that (1.2) is in fact a formula that relates this Bäcklund transformation to the so-called additional symmetries of the KP hierarchy. To be more precise, let σ be the new solution of the KP hierarchy which one obtains from τ by this Bäcklund transformation, i.e., $\sigma = e^{\lambda W(y,w)}\tau$, then

$$\begin{aligned} \Psi(\sigma,x,t,z) &= \sigma(x,t)^{-1} \exp -\sum_{k=1}^{\infty} \frac{\partial}{\partial t_k} \frac{z^{-k}}{k} \sigma(x,t) e^{\xi(t)} e^{zx} \\ &= \frac{\tau(x,t)}{\sigma(x,t)} \exp -\sum_{k=1}^{\infty} \frac{\partial}{\partial t_k} \frac{z^{-k}}{k} \left(\frac{e^{\lambda W(y,w)}\tau(x,t)}{\tau(x,t)} \right) \Psi(\tau,x,t,z) \\ &= \Psi(\tau,x,t,z) + \frac{\tau(x,t)}{\sigma(x,t)} \left(\exp -\sum_{k=1}^{\infty} \frac{\partial}{\partial t_k} \frac{z^{-k}}{k} - 1 \right)\left(\frac{e^{\lambda W(y,w)}\tau(x,t)}{\tau(x,t)} \right) \Psi(\tau,x,t,z). \end{aligned}$$

Now using (1.3) one obtains

$$\Psi(\sigma,x,t,z)=\left(1-\lambda\,\frac{\tau(x,t)}{\sigma(x,t)}\,Y(\tau,y,w)_-\right)\Psi(\tau,x,t,z).$$

Hence $Y(\tau,y,w)_-$ produces, as a consequence of formula (1.2), the Bäcklund transformation of the wave function corresponding to τ.

Adler, Shiota, and van Moerbeke also treated in Ref. 6 the Toda lattice hierarchy of Ueno and Takasaki[8] and showed that an analogous formula also holds. In their treatment they considered two vertex operators, each depending on a different time flow $t^{(j)}=(t_1^{(j)},t_2^{(j)},\ldots)$, $j=1,2$, of a form similar to that of (1.1). Hence The $W_{1+\infty}$-algebra of the KP hierarchy is replaced by two copies of this algebra.

Using 2×2-matrix pseudodifferential operators instead of infinite shift operators, one can show that the Toda lattice hierarchy is formally equivalent to the 2-component KP hierarchy as treated by Kac and the author in Ref. 9. In that case there are however more vertex operators than only the ones of the form (1.1), viz., one also has

$$W^{(ab)}(y,w)=\frac{C^{(ab)}(y,w)}{(y-w)^{\delta_{ab}}}\exp\left(x(y-w)+\sum_{k=1}^{\infty}(t_k^{(a)}y^k-t_k^{(b)}w^k)\right)$$
$$\times\exp-\sum_{k=1}^{\infty}\frac{1}{k}\left(\frac{\partial}{\partial t_k^{(a)}}\,y^{-k}-\frac{\partial}{\partial t_k^{(b)}}\,w^{-k}\right),$$

here $C^{(ab)}(y,w)$ are operators that act on the twisted group algebra of the root lattice of sl_2. A natural question now is: Are there also matrix pseudodifferential operators such that a formula as (1.2) hold for these $W^{(ab)}(y,w)$? In this article we show that a similar result holds, not only for the 2-component KP hierarchy, but in general for the s-component KP hierarchy. One finds that the natural generalization of $W_{1+\infty}$ is not $(W_{1+\infty})^s$ but $W_{1+\infty}(gl_s)$, the central extension of the algebra of differential operators on $(\mathbb{C}[t,t^{-1}])^s$. Hence one can conclude, at least formally as we will show in Sec. VII, that the results of Ref. 6 for the Toda lattice hierarchy are not complete, but that the structure is richer.

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II. a_∞ AND THE KP HIERARCHY IN THE FERMIONIC PICTURE (REF. 9)

Consider the infinite dimensional complex Lie algebra $a_\infty := \overline{gl_\infty}\oplus\mathbb{C}c$, where

$$\overline{gl_\infty}=\{a=(a_{ij})_{i,j\in\mathbb{Z}+1/2}\,|\,a_{ij}=0 \quad \text{if} \quad |i-j|\gg 0\},$$

with Lie bracket defined by

$$[a+\alpha c,b+\beta c]=ab-ba+\mu(a,b)c, \tag{2.1}$$

for $a,b\in\overline{gl_\infty}$ and $\alpha,\beta\in\mathbb{C}$. Here μ is the following 2-cocycle:

$$\mu(E_{ij},E_{kl})=\delta_{il}\delta_{jk}(\theta(i)-\theta(j)) \tag{2.2}$$

with E_{ij} the matrix that has a 1 on the (i,j)-th entry and zeros elsewhere and θ: $\mathbb{R}\to\mathbb{C}$ the function defined by

$$\theta(i):=\begin{cases}0 & \text{if } i>0,\\ 1 & \text{if } i\leqslant 0.\end{cases} \tag{2.3}$$

Let $\mathbb{C}^\infty = \oplus_{j\in\mathbb{Z}+1/2}\mathbb{C}v_j$ be the infinite dimensional complex vector space with fixed basis $\{v_j\}_{j\in\mathbb{Z}+1/2}$. The Lie algebra a_∞ acts linearly on $\mathbb{C}^\infty$ via the usual formula:

$$E_{ij}(v_k)=\delta_{jk}v_i\,.$$

We introduce, following Ref. 10, the corresponding semi-infinite wedge space $F=\Lambda^{1/2\infty}\mathbb{C}^\infty$, this is the vector space with a basis consisting of all semi-infinite monomials of the form $v_{i_1}\wedge v_{i_2}\wedge v_{i_3}\cdots$, where $i_1>i_2>i_3>\cdots$ and $i_{l+1}=i_l-1$ for $l\gg 0$. In order to describe representations of the Lie algebra on this space, we find it convenient to define wedging and contracting operators ψ_j^- and ψ_j^+ $(j\in\mathbb{Z}+\frac{1}{2})$ on F by

$$\psi_j^-(v_{i_1}\wedge v_{i_2}\wedge\cdots)=\begin{cases}0, & \text{if} \quad j=-i_s \ \text{ for some } \ s\\ (-1)^s v_{i_1}\wedge v_{i_2}\cdots\wedge v_{i_s}\wedge v_{-j}\wedge v_{i_{s+1}}\wedge\cdots\,, & \text{if} \quad i_s>-j>i_{s+1},\end{cases}$$

$$\psi_j^+(v_{i_1}\wedge v_{i_2}\wedge\cdots)=\begin{cases}0, & \text{if} \quad j\neq i_s \ \text{ for some } \ s\\ (-1)^{s+1} v_{i_1}\wedge v_{i_2}\cdots\wedge v_{i_{s-1}}\wedge v_{i_{s+1}}\wedge\cdots\,, & \text{if} \quad j=i_s\,.\end{cases}$$

These wedging and contracting operators satisfy the following relations $(i,j\in\mathbb{Z}+\frac{1}{2},\lambda,\mu=+,-)$:

$$\psi_i^\lambda\psi_j^\mu+\psi_j^\mu\psi_i^\lambda=\delta_{\lambda,-\mu}\delta_{i,-j}\,, \tag{2.4}$$

hence they generate a Clifford algebra, which we denote by $\mathcal{C}l$.

Introduce the following elements of $F(m\in\mathbb{Z})$:

$$|-m\rangle=v_{m-1/2}\wedge v_{m-3/2}\wedge v_{m-5/2}\wedge\cdots\,.$$

It is clear that F is an irreducible $\mathcal{C}l$-module such that $\psi_j^\pm|0\rangle=0$ for $j>0$. Define a representation $\hat{r}$ of a_∞ on F by

$$\hat{r}(E_{ij})=:\psi_{-i}^-\psi_j^+:, \quad \hat{r}(c)=I, \tag{2.5}$$

where : : stands for the *normal ordered product* defined in the usual way $(\lambda,\mu=+ \text{ or } -)$:

$$:\psi_k^\lambda\psi_l^\mu:=\begin{cases}\psi_k^\lambda\psi_l^\mu, & \text{if} \quad l\geqslant k\\ -\psi_l^\mu\psi_k^\lambda, & \text{if} \quad l<k.\end{cases} \tag{2.6}$$

Define the *charge decomposition*

$$F=\bigoplus_{m\in\mathbb{Z}}F^{(m)} \tag{2.7}$$

by letting

$$\text{charge}(|0\rangle)=0 \quad \text{and} \quad \text{charge}(\psi_j^\pm)=\pm 1. \tag{2.8}$$

It is easy to see that each $F^{(m)}$ is an irreducible a_∞-highest weight module with highest weight vector $|m\rangle$.

We are now able to define the *KP hierarchy in the fermionic picture*, it is the equation

$$\sum_{k\in\mathbb{Z}+\frac{1}{2}}\psi_k^+\tau\otimes\psi_{-k}^-\tau=0, \tag{2.9}$$

for $\tau \in F^{(0)}$. One can prove (see, e.g., Ref. 10 or 11) that this equation characterizes the group orbit of the vacuum vector $|0\rangle$ for the the group GL_∞. Since the group does not play an important role in this article, we will not introduce it here.

III. $W_{1+\infty}(gl_s)$ AS SUBALGEBRA OF a_∞

Let e_i, $1 \leqslant i \leqslant s$ be a basis of $\mathbb{C}^s$. By identifying $(\mathbb{C}[t,t^{-1}])^s$ with $\mathbb{C}^\infty$, we can embed $W_{1+\infty}(gl_s)$ into a_∞. This, however, can be done in many different ways, the simplest one is the following. We put $(1 \leqslant a \leqslant s,\ j \in \mathbb{Z}+\frac{1}{2})$:

$$v_j^{(a)} = v_{sj+(1/2)(s-2a+1)} = t^{-j-1/2} e_a, \quad \psi_j^{\pm(a)} = \psi^{\pm}_{sj\pm(1/2)(s-2a+1)}. \tag{3.1}$$

Notice that with this relabeling we have: $\psi_k^{\pm(a)}|0\rangle = 0$ for $k > 0$. We introduce the generating series of the fermions, the so-called fermionic fields $(z \in \mathbb{C}^\times)$:

$$\psi^{\pm(a)}(z) \overset{\text{def}}{=} \sum_{k \in \mathbb{Z}+\frac{1}{2}} \psi_k^{\pm(a)} z^{-k-1/2}. \tag{3.2}$$

We also rewrite the E_{jk}'s:

$$E_{j,k}^{(ab)} = E_{sj+(1/2)(s-sa+1),sk+(1/2)(s-2b+1)}, \tag{3.3}$$

then $\hat{r}(E_{jk}^{(ab)}) = :\psi_{-j}^{-(a)} \psi_k^{+(b)}:$.

We can associate to $(\mathbb{C}[t,t^{-1}])^s$ the Lie algebra of differential operators on this space, it has as basis the operators:

$$-t^{k+l}\left(\frac{\partial}{\partial t}\right)^l e_{ij}, \quad \text{for} \quad k \in \mathbb{Z}, \quad l \in \mathbb{Z}_+, \quad 1 \leqslant i,j \leqslant s.$$

We will denote this Lie algebra by $D(gl_s)$. We can embed this algebra via (3.1) into $\overline{gl_\infty}$ and also into a_∞, one finds

$$-t^{k+l}\left(\frac{\partial}{\partial t}\right)^l e_{ij} \mapsto \sum_{m \in \mathbb{Z}} -m(m-1)\cdots(m-l+1) E^{(ij)}_{-m-k-1/2,-m-1/2}. \tag{3.4}$$

It is straightforward, but rather tedious, to calculate the corresponding 2-cocycle, the result is as follows (see also Refs. 12–14). Let $f(t), g(t) \in \mathbb{C}[t,t^{-1}]$ and $a,b \in gl_s$ then

$$\mu\left(f(t)\left(\frac{\partial}{\partial t}\right)^l a, g(t)\left(\frac{\partial}{\partial t}\right)^m b\right) = \frac{l!m!}{(l+m+1)!} \operatorname{Res}_{t=0} dt\ f^{(m+1)}(t) g^{(l)}(t) \operatorname{trace}(ab).$$

Hence in this way we get a central extension $W_{1+\infty}(gl_s) = D(gl_s) \oplus \mathbb{C}c$ of $D(gl_s)$ with Lie bracket

$$\begin{aligned}\left[f(t)\left(\frac{\partial}{\partial t}\right)^l a + \alpha c, g(t)\left(\frac{\partial}{\partial t}\right)^m b + \beta c\right] &= f(t)\left(\frac{\partial}{\partial t}\right)^l g(t)\left(\frac{\partial}{\partial t}\right)^m ab - g(t)\left(\frac{\partial}{\partial t}\right)^m f(t)\left(\frac{\partial}{\partial t}\right)^l ba \\ &\quad + \mu\left(f(t)\left(\frac{\partial}{\partial t}\right)^l a, g(t)\left(\frac{\partial}{\partial t}\right)^m b\right) c.\end{aligned} \tag{3.5}$$

Since we have the representation $\hat{r}$ of a_∞, we find that

$$\hat{r}\left(-t^{k+l}\left(\frac{\partial}{\partial t}\right)^l e_{ba}\right) = \sum_{m \in \mathbb{Z}} m(m-1)\cdots(m-l+1) :\psi^{+(a)}_{-m-1/2} \psi^{-(b)}_{m+k+1/2}:.$$

In terms of the fermionic fields (3.2), we find

$$\sum_{k\in\mathbb{Z}} \hat{r}\left(-t^{k+l}\left(\frac{\partial}{\partial t}\right)^l e_{ba}\right) z^{-k-l-1} =: \frac{\partial^l \psi^{+(a)}(z)}{\partial z^l}\, \psi^{-(b)}(z):. \tag{3.6}$$

Now define

$$W_k^{(ab,l+1)} := \hat{r}\left(-t^{k+l}\left(\frac{\partial}{\partial t}\right)^l e_{ba}\right), \quad W^{(ab,l+1)}(z) := \sum_{k\in\mathbb{Z}} W_k^{(ab,l+1)} z^{-k-l-1}, \tag{3.7}$$

then

$$\begin{aligned} W^{(ab)}(y,z) :=: \psi^{+(a)}(y)\psi^{-(b)}(z): &= \sum_{l=0}^{\infty} \frac{(y-z)^l}{l!}\, W^{(ab,l+1)}(z) \\ &= \sum_{l=0}^{\infty} \frac{(y-z)^l}{l!} \sum_{k\in\mathbb{Z}} W_k^{(ab,l+1)} z^{-k-l-1}. \end{aligned} \tag{3.8}$$

IV. THE *s*-COMPONENT BOSON FERMION CORRESPONDENCE

Using a bosonization one can rewrite (2.9) as a system of partial differential equations and express the basis elements of $W_{1+\infty}(gl_s)$ in terms of vertex operators. We begin by introduce bosonic fields ($1\leqslant i\leqslant s$):

$$\alpha^{(i)}(z) \equiv \sum_{k\in\mathbb{Z}} \alpha_k^{(i)} z^{-k-1} \overset{\text{def}}{=} :\psi^{-(i)}(z)\psi^{+(i)}(z):. \tag{4.1}$$

Since $\alpha^{(i)}(z) = -W^{(ii,1)}(z)$, one easily checks that the operators $\alpha_k^{(i)}$ satisfy the canonical commutation relation of the associative oscillator algebra, which we denote by $\mathfrak{a}$:

$$[\alpha_k^{(i)}, \alpha_l^{(j)}] = k\,\delta_{ij}\delta_{k,-l}, \tag{4.2}$$

and one has

$$\alpha_k^{(i)}|m\rangle = 0 \quad \text{for} \quad k>0. \tag{4.3}$$

It is easy to see that restricted to $\hat{gl}_s$, which is the subalgebra generated by the elements $W_k^{(ij,1)}$, $F^{(0)}$ is its basic highest weight representation (see Ref. 15, Chap. 12).

We will now describe the s-component boson–fermion correspondence (see Ref. 9). Let L be a lattice with a basis $\delta_1,\ldots,\delta_s$ over $\mathbb{Z}$ and the symmetric bilinear form $(\delta_i|\delta_j) = \delta_{ij}$, where δ_{ij} is the Kronecker symbol. Let

$$\epsilon_{ij} = \begin{cases} -1, & \text{if} \quad i>j \\ 1, & \text{if} \quad i\leqslant j \end{cases}. \tag{4.4}$$

Define a bimultiplicative function ϵ: $L\times L\to\{\pm 1\}$ by letting

$$\epsilon(\delta_i,\delta_j) = \epsilon_{ij}. \tag{4.5}$$

Let $\delta = \delta_1+\cdots+\delta_s$, $Q = \{\gamma\in L|(\delta|\gamma)=0\}$, $\Delta = \{\alpha_{ij} := \delta_i-\delta_j | i,j=1,\ldots,s, i\neq j\}$. Of course Q is the root lattice of $sl_s(\mathbb{C})$, the set Δ being the root system.

Consider the vector space $\mathbb{C}[L]$ with basis e^{γ}, $\gamma\in L$, and the following twisted group algebra product:

$$e^{\alpha}e^{\beta}=\epsilon(\alpha,\beta)e^{\alpha+\beta}. \tag{4.6}$$

Let $\mathbb{C}[t]$ be the space of polynomials in indeterminates $t=\{t_k^{(i)}\}$, $k=1,2,...$, $i=1,2,\ldots,s$ and denote by $B=\mathbb{C}[t]\otimes_c\mathbb{C}[L]$ be the tensor product of these algebras. Then the s-component boson–fermion correspondence is the vector space isomorphism

$$\sigma: F \xrightarrow{\sim} B, \tag{4.7}$$

given by $\sigma(|0\rangle)=1$ and

$$\sigma\psi^{\pm(a)}(z)\sigma^{-1}=e^{\pm\delta_a z^{\pm\delta_a}}\exp\left(\pm\sum_{k=1}^{\infty}t_k^{(a)}z^k\right)\exp\left(\mp\sum_{k=1}^{\infty}\frac{\partial}{\partial t_k^{(a)}}\frac{z^{-k}}{k}\right), \tag{4.8}$$

where

$$\delta_a(p(t)\otimes e^{\gamma})=(\delta_a|\gamma)p(t)\otimes e^{\gamma}. \tag{4.9}$$

The transported charge then is as follows:

$$\text{charge}(p(t)\otimes e^{\gamma})=(\delta|\gamma).$$

We denote the transported charge decomposition by $B=\oplus_{m\in\mathbb{Z}}B^{(m)}$, then the transported action of the operators $\alpha_m^{(i)}$ is given by

$$\begin{cases}\sigma\alpha_{-m}^{(j)}\sigma^{-1}(p(t)\otimes e^{\gamma})=mt_m^{(j)}p(t)\otimes e^{\gamma}, & \text{if} \quad m>0,\\ \sigma\alpha_m^{(j)}\sigma^{-1}(p(t)\otimes e^{\gamma})=\dfrac{\partial p(t)}{\partial t_m}\otimes e^{\gamma}, & \text{if} \quad m>0,\\ \sigma\alpha_0^{(j)}\sigma^{-1}(p(t)\otimes e^{\gamma})=(\delta_j|\gamma)p(t)\otimes e^{\gamma}.\end{cases} \tag{4.10}$$

If one substitutes (4.8) into (3.8), one obtains the following vertex operator expression for the generating series of the fields $W^{(ab,l+1)}(z)$:

$$W^{(ab)}(y,z)=\frac{1}{(y-z)^{\delta_{ab}}}(X^{(ab)}(y,z)-\delta_{ab}),$$

where

$$X^{(ab)}(y,z)=\epsilon(\delta_a,\delta_b)e^{\delta_a-\delta_b}y^{\delta_a}z^{-\delta_b}\widetilde{X}^{(ab)}(y,z), \tag{4.11}$$

and

$$\widetilde{X}^{(ab)}(y,z)=\exp\left(\sum_{k=1}^{\infty}(t_k^{(a)}y^k-t_k^{(b)}z^k)\right)\exp\left(-\sum_{k=1}^{\infty}\left(\frac{\partial}{\partial t_k^{(a)}}\frac{y^{-k}}{k}-\frac{\partial}{\partial t_k^{(b)}}\frac{z^{-k}}{k}\right)\right).$$

The fields for which $l=0$, give the vertex operator realization of the homogeneous realization of $\hat{gl}_s$, which was first found by Frenkel and Kac[16] and independently by Segal[17] (see also Ref. 18 for more details).

Using the isomorphism σ we can reformulate the KP hierarchy (2.9) in the bosonic picture. We start by observing that (2.9) can be rewritten as follows:

$$\mathrm{Res}_{z=0}\, dz\left(\sum_{j=1}^{s}\psi^{+(j)}(z)\tau\otimes\psi^{-(j)}(z)\tau\right)=0,\quad \tau\in F^{(0)}. \tag{4.12}$$

Notice that for $\tau\in F^{(0)}$, $\sigma(\tau)=\Sigma_{\gamma\in Q}\,\tau_\gamma(t)e^\gamma$. Here and further we write $\tau_\gamma(t)e^\gamma$ for $\tau_\gamma(t)\otimes e^\gamma$. Using (4.8), Eq. (4.12) turns under $\sigma\otimes\sigma: F\otimes F\xrightarrow{\sim}\mathbb{C}[t,t']\otimes(\mathbb{C}[L]\otimes\mathbb{C}[L'])$ into the following set of equations; for all $\alpha,\beta\in L$ such that $(\alpha|\delta)=-(\beta|\delta)=1$ we have:

$$\mathrm{Res}_{z=0}\left(dz\sum_{j=1}^{s}\epsilon(\delta_j,\alpha-\beta)z^{(\delta_j|\alpha-\beta-2\delta_j)}\exp\left(\sum_{k=1}^{\infty}(t_k^{(j)}-t_k^{(j)'})z^k\right)\right.$$
$$\left.\times\exp\left(-\sum_{k=1}^{\infty}\left(\frac{\partial}{\partial t_k^{(j)}}-\frac{\partial}{\partial t_k^{(j)'}}\right)\frac{z^{-k}}{k}\right)\tau_{\alpha-\delta_j}(t)(e^\alpha)\tau_{\beta+\delta_j}(t')(e^\beta)'\right)=0. \tag{4.13}$$

Notice that if $s=2$, the set of equations (4.13) are formally equivalent (for more general τ) to the Toda lattice hierarchy of Ueno and Takasaki.[8] For this reason, *we assume from now on that* $\tau=\Sigma\tau_\alpha e^\alpha$ *is any solution of* (4.13). Hence formally the results of this article also hold for the Toda lattice hierarchy, as we will show explicitly in Sec. VII.

In order to define the equations (4.13) in terms of formal pseudodifferential operators it will be convenient to replace $t_k^{(j)}$ by $t_k^{(j)}+\delta_{k,1}x$ and to introduce the notations

$$\xi^{(j)}(t,z)=\sum_{i=1}^{\infty}t_i^{(j)}z^i,\quad \xi^{(j)}(x,t,z)=zx+\xi^{(j)}(t,z)$$

and

$$\eta^{(j)}(t,z)=\sum_{i=1}^{\infty}\frac{\partial}{\partial t_i^{(j)}}\frac{z^{-i}}{i}.$$

Next we replace α resp. β by $\alpha+\delta_i$ and $\beta-\delta_k$ then for all $\alpha,\beta\in Q$ and $1\leqslant i,k\leqslant s$ (4.13) turns into

$$\mathrm{Res}_{z=0}\, dz\left(\sum_{j=1}^{s}\epsilon(\delta_j,\alpha+\delta_i-\beta+\delta_k)z^{(\delta_j|\alpha-\beta+\delta_i+\delta_k-2\delta_j)}\right.$$
$$\times e^{\xi^{(j)}(x,t,z)-\xi^{(j)}(x',t',z)}e^{-\eta^{(j)}(t,z)+\eta^{(j)}(t',z)}\tau_{\alpha+\delta_i-\delta_j}(x,t)$$
$$\left.\times(e^{\alpha+\delta_j})\tau_{\beta+\delta_j-\delta_k}(x',t')(e^{\beta-\delta_k})'\right)=0. \tag{4.14}$$

V. THE ALGEBRA OF FORMAL PSEUDODIFFERENTIAL OPERATORS AND THE *s*-COMPONENT KP HIERARCHY AS A DYNAMICAL SYSTEM

We proceed now to rewrite the formulation (4.14) of the s-component KP hierarchy in terms of formal pseudodifferential operators, generalizing the results of Refs. 1–3. For more details see Ref. 9. For each $\alpha\in\mathrm{supp}\,\tau:=\{\alpha\in Q\,|\,\tau=\Sigma_{\alpha\in Q}\,\tau_\alpha e^\alpha,\tau_\alpha\neq 0\}$ we define the (matrix valued) functions

$$\Psi^{\pm}(\alpha,z)\equiv\Psi^{\pm}(\tau_\alpha,x,t,z)=(\Psi^{+}_{ij}(\tau_\alpha,x,t,z))_{i,j=1}^{s} \tag{5.1}$$

as follows:

$$\Psi_{ij}^{\pm}(\tau_\alpha,x,t,z)\overset{\text{def}}{=}\epsilon(\delta_j,\alpha+\delta_i)z^{(\delta_j|\pm\alpha+\delta_i-\delta_j)}e^{\pm\xi^{(j)}(x,t,z)}e^{\mp\eta^{(j)}(t,z)}\tau_{\alpha\pm(\delta_i-\delta_j)}(x,t)/\tau_\alpha(x,t)$$
$$=\epsilon(\delta_j,\alpha+\delta_i)z^{(\delta_j|\pm\alpha+\delta_i-\delta_j)}\tau_{\alpha\pm(\delta_i-\delta_j)}(x,t^{(k)}\mp\delta_{jk}[z^{-1}])/$$
$$\tau_\alpha(x,t)e^{\pm\xi^{(j)}(x,t,z)},\tag{5.2}$$

where $[w]=(w,w^2/2,w^3/3,\ldots)$. It is easy to see that Eq. (4.14) is equivalent to the following bilinear identity:

$$\mathrm{Res}_{z=0}\ \Psi^+(\tau_\alpha,x,t,z)^t\Psi^-(\tau_\beta,x',t',z)dz=0\quad\text{for all}\quad\alpha,\beta\in Q.\tag{5.3}$$

Define $s\times s$ matrices $S^{\pm(m)}(\tau_\alpha,x,t)$ by the following generating series [cf. (5.2)]:

$$\sum_{m=0}^{\infty}S_{ij}^{\pm(m)}(\tau_\alpha,x,t)(\pm z)^{-m}=\epsilon_{ji}z^{\delta_{ij}-1}e^{\mp\eta(t,z)}\tau_{\alpha\pm(\delta_i-\delta_j)}(x,t)/\tau_\alpha(x,t)$$
$$=\epsilon_{ji}z^{\delta_{ij}-1}\tau_{\alpha\pm(\delta_i-\delta_j)}(x,t^{(k)}\mp\delta_{jk}[z^{-1}])/\tau_\alpha(x,t).\tag{5.4}$$

We see from (5.2) that $\Psi^{\pm}(\tau_\alpha,x,t,z)$ can be written in the following form:

$$\Psi^{\pm}(\tau_\alpha,x,t,z)=\left(\sum_{m=0}^{\infty}S^{\pm(m)}(\tau_\alpha,x,t)R^{\pm}(\alpha,\pm z)(\pm z)^{-m}\right)e^{\pm\xi(x,t,z)},\tag{5.5}$$

where

$$R^{\pm}(\alpha,z)=\sum_{i=1}^{s}\epsilon(\delta_i,\alpha)e_{ii}(\pm z)^{\pm(\delta_i|\alpha)}.\tag{5.6}$$

As before e_{ij} stands for the $s\times s$ matrix whose (i,j) entry is 1 and all other entries are zero. Let

$$\partial=\frac{\partial}{\partial x},$$

we can now rewrite $\Psi^{\pm}(\tau_\alpha,x,t,z)$ in terms of formal pseudodifferential operators, define

$$e^{\pm\xi(t,\pm\partial)}=\sum_{j=1}^{s}e^{\pm\xi^{(j)}(t,\pm\partial)}e_{jj},$$

$$P^{\pm}(\alpha)\equiv P^{\pm}(\tau_\alpha,x,t,\partial)=I_s+\sum_{m=1}^{\infty}S^{\pm(m)}(\tau_\alpha,x,t)\partial^{-m},\tag{5.7}$$

$$R^{\pm}(\alpha)\equiv R^{\pm}(\alpha,\partial)\quad\text{and}\quad W^{\pm}(\alpha)\equiv W^{\pm}(\tau_\alpha,x,t,z)=P^{\pm}(\alpha)R^{\pm}(\alpha)e^{\pm\xi(t,\pm\partial)}$$

then

$$\Psi^{\pm}(\tau_\alpha,x,t,z)=W^{\pm}(\alpha)e^{\pm zx}=P^{\pm}(\alpha)R^{\pm}(\alpha)e^{\pm\xi(t,\pm\partial)}e^{\pm zx}.\tag{5.8}$$

As usual one denotes the differential part of $P(x,t,\partial)$ by $P_+(x,t,\partial)=\Sigma_{j\geqslant 0}\ P_j(x,t)\partial^j$, and writes $P_-=P-P_+$. The linear anti-involution $*$ is defined by the following formula:

$$\left(\sum_j P_j\partial^j\right)^* = \sum_j (-\partial)^j \circ {}^tP_j. \tag{5.9}$$

Here and further ${}^tP$ stands for the transpose of the matrix P. Then one has the following fundamental lemma:

Lemma 5.1: Let P,Q be two formal pseudodifferential operators, then

$$(PQ^*) = \sum_{i<0} R_i\partial^i$$

if and only if

$$\mathrm{Res}_{z=0}\, dz(P(x,\partial)e^{zx})^t(Q(x',\partial')e^{-zx'}) = \sum_{i<0} R_i(x)\,\frac{(x-x')^{-i-1}}{(-i-1)!}.$$

Proof: Let $y=x-x'$, $P(x,z)=\Sigma P_i(x)z^i$ and $Q(x,z)=\Sigma Q_i(x)(-z)^i$, then

$$\begin{aligned}
\mathrm{Res}_{z=0}\, dz(P(x,\partial)e^{zx})^t(Q(x',\partial')e^{-zx'}) &= \mathrm{Res}_{z=0}\, dz\; P(x,z)\sum_{k\geqslant 0}\frac{(-1)^k}{k!}\frac{\partial^k\,{}^tQ(x,-z)}{\partial x^k}y^k e^{zy}\\
&= \mathrm{Res}_{z=0}\, dz \sum_{k,l\geqslant 0,i,j}\frac{(-1)^k}{k!}P_i(x)\frac{\partial^k\,{}^tQ_j(x)}{\partial x^k}\frac{y^{k+l}}{l!}z^{i+j+l}\\
&= \sum_{k\geqslant 0,i+j\leqslant -1}\frac{(-1)^k}{k!(-i-j-1)!}P_i(x)\frac{\partial^k\,{}^tQ_j(x)}{\partial x^k}y^{k-i-j-1}\\
&= \sum_{k\geqslant 0,i+j\leqslant -1}\binom{i+j}{k}P_i(x)\frac{\partial^k\,{}^tQ_j(x)}{\partial x^k}\frac{y^{k-i-j-1}}{(k-i-j-1)!}.
\end{aligned} \tag{5.10}$$

Next we calculate

$$\begin{aligned}
(P(x,\partial)Q^*(x,\partial))_- &= \left(\sum_{i,j} P_i(x)\partial^{i+j}\,{}^tQ_j(x)\right)_-\\
&= \left(\sum_{k\geqslant 0,i,j}\binom{i+j}{k}P_i(x)\frac{\partial^k\,{}^tQ_j(x)}{\partial x^k}\partial^{i+j-k}\right)_-\\
&= \left(\sum_{k\geqslant 0,i+j-k<0}\binom{i+j}{k}P_i(x)\frac{\partial^k\,{}^tQ_j(x)}{\partial x^k}\partial^{i+j-k}\right)_-\\
&= \sum_{k\geqslant 0,i+j\leqslant -1}\binom{i+j}{k}P_i(x)\frac{\partial^k\,{}^tQ_j(x)}{\partial x^k}\partial^{i+j-k},
\end{aligned} \tag{5.11}$$

here we have used the fact that $\binom{i+j}{k}=0$ if $i+j>0$ and $i+j-k<0$. Now comparing (5.10) and (5.11) gives the desired result. □

Using this lemma one deduces the following

$$(W^+(\tau_\alpha,x,t,\partial)W^-(\tau_\beta,x,t',\partial)^*)_- = 0. \tag{5.12}$$

By putting $t=t'$, one proves in a similar way as in Ref. 9 that given $\beta\in\text{supp }\tau$, all the pseudo-differential operators $P^{\pm}(\alpha)$, $\alpha\in\text{supp }\tau$, are completely determined by $P^{+}(\beta)$ from the following equations

$$R^{-}(\alpha)^{-1}=R^{+}(\alpha)^{*}, \tag{5.13}$$

$$P^{-}(\alpha)=(P^{+}(\alpha)^{*})^{-1}, \tag{5.14}$$

$$(P^{+}(\alpha)R^{+}(\alpha-\beta)P^{+}(\beta)^{-1})_{-}=0 \quad \text{for all} \quad \alpha,\beta\in\text{supp }\tau. \tag{5.15}$$

This and the above lemma can be used to prove the following proposition which will be crucial later on. Adler, Shiota, and van Moerbeke stated this proposition in the 1-component case.[6]

Proposition 5.2: Let $\Psi^{\pm}(\alpha,x,t,z)$ satisfy the bilinear identity (5.3) for $\beta=\alpha$ and let $Q(x,t,\partial)$ be an arbitrary pseudodifferential operator. Then Q is a differential operator if and only if

$$\text{Res}_{z=0}\ dz\ Q(x,t,\partial)\Psi^{+}(\tau_{\alpha},x,t,z)^{t}\Psi^{-}(\tau_{\alpha},x',t',z)=0. \tag{5.16}$$

Proof: Suppose that Q is a differential operator, then since by Lemma 5.1 $W^{+}(\tau_{\alpha},x,t,\partial)W^{-}(\tau_{\alpha},x,t',\partial)$ is a differential operator

$$(Q(x,t,\partial)W^{+}(\tau_{\alpha},x,t,\partial)W^{-}(\tau_{\alpha},x,t',\partial)^{*})_{-}=0. \tag{5.17}$$

Conversely, suppose (5.16) holds, then again by Lemma 5.1 (5.17) holds. Now put $t=t'$, and use (5.13)–(5.14), then one deduces that $Q(x,t,\partial)_{-}=0$. □

In Ref. 9 Victor Kac and the author also showed the following.

Proposition 5.3: Consider $\Psi^{+}(\tau_{\alpha},x,t,z)$ and $\Psi^{-}(\tau_{\alpha},x,t,z)$, $\alpha\in Q$, of the form (5.8), then the bilinear identity (5.3) for all $\alpha,\beta\in\text{supp }\tau$ is equivalent to the Sato equation:

$$\frac{\partial P^{+}(\alpha)}{\partial t_{k}^{(j)}}=-(P^{+}(\alpha)e_{jj}\partial^{k}P^{+}(\alpha)^{-1})_{-}P^{+}(\alpha), \tag{5.18}$$

for each $\alpha\in\text{supp }\tau$ and the matching conditions (5.13)–(5.15) for all $\alpha,\beta\in\text{supp }\tau$.

As a consequence of (5.18) one obtains for each $W^{+}(\alpha)$:

$$\frac{\partial W^{+}(\alpha)}{\partial t_{k}^{(j)}}=(P^{+}(\alpha)e_{jj}\partial^{k}P^{+}(\alpha)^{-1})_{+}W^{+}(\alpha)=(W^{+}(\alpha)e_{jj}\partial^{k}W^{+}(\alpha)^{-1})_{+}W^{+}(\alpha). \tag{5.19}$$

Fix τ and $\alpha,\beta\in Q$, introduce the following formal pseudodifferential operators $L(\alpha)$, Γ, $M(\alpha)$, $N(\alpha,\beta)$, $\Delta^{(ij)}$, $C^{(ij)}(\alpha)$ and differential operators $B_{m}^{(ij)}(\alpha)$:

$$L(\alpha)=W^+(\alpha)\partial W^+(\alpha)^{-1}=P^+(\alpha)\partial P^+(\alpha)^{-1},$$

$$\Gamma=x+\sum_{a=0}^{s}\sum_{k=0}^{\infty} kt_k^{(a)}\partial^{k-1}e_{aa},$$

$$M(\alpha)=W^+(\alpha)xW^+(\alpha)^{-1}=P^+(\alpha)R^+(\alpha)\Gamma R^+(\alpha)^{-1}P^+(\alpha)^{-1},$$

$$N(\alpha,\beta)=W^+(\alpha)W^+(\beta)^{-1}=P^+(\alpha)R^+(\alpha-\beta)P^+(\beta)^{-1}, \tag{5.20}$$

$$\Delta^{(ij)}=\epsilon^{\xi(t,\partial)}e_{ij}e^{-\xi(t,\partial)},$$

$$C^{(ij)}(\alpha)=W^+(\alpha)e_{ij}W^+(\alpha)^{-1}=P^+(\alpha)R^+(\alpha)\Delta^{(ij)}R^+(\alpha)^{-1}P^+(\alpha)^{-1},$$

$$B_m^{(i)}(\alpha)=(W^+(\alpha)e_{ii}\partial^m W^+(\alpha)^{-1})_+.$$

Notice that $M(\alpha)$ and $C^{(ij)}(\alpha)$ are not well-defined pseudodifferential operators. One should regard them as a product of operators on $\Psi^+(\alpha,z)$.

Here we write x for xI_s. Denote by $C^{(i)}(\alpha)=C^{(ii)}(\alpha)$. Then

$$[L(\alpha),M(\alpha)]=I_s,\quad \sum_{i=1}^{s}C^{(i)}(\alpha)=I_s,\quad C^{(ij)}(\alpha)L(\alpha)=L(\alpha)C^{(ij)}(\alpha),$$

$$C^{(ij)}(\alpha)C^{(kl)}(\alpha)=\delta_{jk}C^{(il)}(\alpha),\quad L(\alpha)N(\alpha,\beta)=N(\alpha,\beta)L(\beta),$$
$$M(\alpha)N(\alpha,\beta)=N(\alpha,\beta)M(\beta),\quad C^{(ij)}(\alpha)N(\alpha,\beta)=N(\alpha,\beta)C^{(ij)}(\beta), \tag{5.21}$$

$$N(\alpha,\beta)N(\beta,\gamma)=N(\alpha,\gamma).$$

Remark 5.4: (i) It is our purpose to describe the general operators

$$Y_k^{(ab,l+1)}(\alpha,\beta)=W^+(\alpha)x^l\partial^{k+l}e_{ab}W^+(\beta)^{-1}.$$

One can express them in the operators defined in (5.20), viz.,

$$Y_k^{(ab,l+1)}(\alpha,\beta)=M(\alpha)^lL(\alpha)^{k+l}C^{(ab)}(\alpha)N(\alpha,\beta).$$

(ii) Notice that (5.14) is equivalent to $N(\alpha,\beta)_-=0$, so from now on we will assume that $N(\alpha,\beta)$ is a differential operator.

Proposition 5.5: If for every $\alpha,\beta\in Q$ the formal pseudodifferential operators $L(\alpha)$, $M(\alpha)$, $C^{(ij)}(\alpha)$ and the differential operators $N(\alpha,\beta)$ satisfy conditions (5.21) and if the equations

$$\begin{cases} L(\alpha)P^+(\alpha)R^+(\alpha)=P^+(\alpha)R^+(\alpha)\partial \quad [\text{or equivalently } L(\alpha)P^+(\alpha)=P^+(\alpha)\partial],\\ M(\alpha)P^+(\alpha)R^+(\alpha)=P^+(\alpha)R^+(\alpha)\Gamma,\\ N(\alpha,\beta)P^+(\beta)R^+(\beta)=P^+(\alpha)R^+(\alpha),\\ C^{(ij)}(\alpha)P^+(\alpha)R^+(\alpha)=P^+(\alpha)R^+(\alpha)\Delta^{(ij)},\\ \dfrac{\partial P^+(\alpha)}{\partial t_k^{(j)}}=-(C^{(j)}(\alpha)L(\alpha)^k)_-P^+(\alpha) \end{cases} \tag{5.22}$$

have a solution $P^+(\alpha)$ of the form (5.7), then the differential operators $B_k^{(j)}(\alpha)$ satisfies the following conditions:

$$\begin{cases} \dfrac{\partial L(\alpha)}{\partial t_k^{(j)}} = [B_k^{(j)}(\alpha), L(\alpha)], \\ \dfrac{\partial M(\alpha)}{\partial t_k^{(j)}} = [B_k^{(j)}(\alpha), M(\alpha)], \\ \dfrac{\partial N(\alpha,\beta)}{\partial t_k^{(j)}} = B_k^{(j)}(\alpha)N(\alpha,\beta) - N(\alpha,\beta)B_k^{(j)}(\beta), \\ \dfrac{\partial C^{(il)}(\alpha)}{\partial t_k^{(j)}} = [B_k^{(j)}(\alpha), C^{(il)}(\alpha)]. \end{cases} \tag{5.23}$$

Now (5.23) implies that

$$\frac{\partial Y_m^{(ab,l+1)}(\alpha,\beta)}{\partial t_k^{(j)}} = B_k^{(j)}(\alpha)Y_m^{(ab,l+1)}(\alpha,\beta) - Y_m^{(ab,l+1)}(\alpha,\beta)B_k^{(j)}(\beta).$$

Notice that the conditions (5.22) are equivalent to one of the following conditions:

$$\begin{cases} L(\alpha)W^+(\alpha) = W^+(\alpha)\partial, \\ M(\alpha)W^+(\alpha) = W^+(\alpha)x, \\ N(\alpha,\beta)W^+(\beta) = W^+(\alpha), \\ C^{(ij)}(\alpha)W^+(\alpha) = W^+(\alpha)e_{ij}, \\ \dfrac{\partial W^+(\alpha)}{\partial t_k^{(j)}} = B_k^{(j)}(\alpha)W^+(\alpha), \end{cases} \qquad \begin{cases} L(\alpha)\Psi^+(\alpha,z) = z\Psi^+(\alpha,z), \\ M(\alpha)\Psi^+(\alpha,z) = \dfrac{\partial \Psi^+(\alpha,z)}{\partial z}, \\ N(\alpha,\beta)\Psi^+(\beta,z) = \Psi^+(\alpha,z), \\ C^{(ij)}(\alpha)\Psi^+(\alpha,z) = \Psi^+(\alpha,z)e_{ij}, \\ \dfrac{\partial \Psi^+(\alpha,z)}{\partial t_k^{(j)}} = B_k^{(j)}(\alpha)\Psi^+(\alpha,z). \end{cases} \tag{5.24}$$

VI. THE ADLER–SHIOTA–VAN MOERBEKE FORMULA

Fix $\alpha,\beta \in Q$ and recall

$$Y_k^{(ab,l+1)}(\alpha,\beta) \equiv Y_k^{(ab,l+1)}(\tau_\alpha,\tau_\beta) = W^+(\alpha)x^l\partial^{k+l}e_{ab}W^+(\beta)^{-1}, \tag{6.1}$$

then define

$$\begin{aligned} Y^{(ab)}(\alpha,\beta,y,w) &\equiv Y^{(ab)}(\tau_\alpha,\tau_\beta,y,w) \\ &= \sum_{l=0}^{\infty} \frac{(y-w)^l}{l!} \sum_{k\in\mathbb{Z}} w^{-k-l-1} Y_k^{(ab,l+1)}(\alpha,\beta) \\ &= \sum_{l=0}^{\infty} \frac{(y-w)^l}{l!} \sum_{k\in\mathbb{Z}} w^{-k-l-1} M(\alpha)^l L(\alpha)^{k+l} C^{(ab)}(\alpha)N(\alpha,\beta). \end{aligned} \tag{6.2}$$

We write $Y_k^{(ab,l+1)}(\alpha)$ and $Y^{(ab)}(\alpha,y,w) \equiv Y^{(ab)}(\tau_\alpha,y,w)$ for, respectively, $Y_k^{(ab,l+1)}(\alpha,\alpha)$, $Y^{(ab)}(\alpha,\alpha,y,w)$, then

$$Y^{(ab)}(\alpha,y,w) = \sum_{l=0}^{\infty} \frac{(y-w)^l}{l!} \sum_{k\in\mathbb{Z}} w^{-k-l-1} M(\alpha)^l L(\alpha)^{k+l} C^{(ab)}(\alpha).$$

One deduces the following:

Proposition 6.1:

$$Y^{(ab)}(\alpha,\beta,y,w)_- = \Psi^+(\alpha,y)e_{ab}\partial^{-1t}\Psi^-(\beta,w). \tag{6.3}$$

Proof: First, notice that

$$\begin{aligned}(W^+(\alpha)x^l\partial^{k+l}e_{ab}W^+(\beta)^{-1})_- &= \sum_{j=1}^{\infty}\partial^{-j}\,\mathrm{Res}_\partial\,\partial^{j-1}W^+(\alpha)x^l\partial^{k+l}e_{ab}W^+(\beta)^{-1}\\ &= \sum_{j=1}^{\infty}\partial^{-j}\,\mathrm{Res}_{z=0}\,dz(\partial^{j-1}W^+(\alpha)x^l\partial^{k+l}e^{zx})e_{ab}{}^t(W^-(\beta)e^{-zx})\\ &= \mathrm{Res}_{z=0}\,dz\sum_{j=1}^{\infty}\partial^{-j}\left[\left(\frac{\partial}{\partial x}\right)^{j-1}\left(z^{k+l}\,\frac{\partial^l\Psi^+(\alpha,z)}{\partial z^l}\right)\right]e_{ab}{}^t\Psi^-(\beta,z)\\ &= \mathrm{Res}_{z=0}\,dz z^{k+l}\,\frac{\partial^l\Psi^+(\alpha,z)}{\partial z^l}\,e_{ab}\partial^{-1t}\Psi^-(\beta,z).\end{aligned}$$

Hence

$$\begin{aligned}Y^{(ab)}(\alpha,\beta,y,w)_- &= \sum_{l=0}^{\infty}\frac{(y-w)^l}{l!}\sum_{k\in\mathbb{Z}}w^{-k-l-1}\,\mathrm{Res}_{z=0}\,dz\,z^{k+l}\,\frac{\partial^l\Psi^+(\alpha,z)}{\partial z^l}\,e_{ab}\partial^{-1t}\Psi^-(\beta,z)\\ &= \sum_{l=0}^{\infty}\frac{(y-w)^l}{l!}\,\frac{\partial^l\Psi^+(\alpha,w)}{\partial w^l}\,e_{ab}\partial^{-1t}\Psi^-(\beta,w)=\Psi^+(\alpha,y)e_{ab}\partial^{-1t}\Psi^-(\beta,w).\end{aligned}$$

□

Proposition 6.1 was obtained in the 1-component case by Dickey.[7]

Next we calculate

$$\begin{aligned}Y^{(ab)}(\alpha,\beta,y,w)\Psi^+(\beta,z) &= \sum_{l=0}^{\infty}\frac{(y-w)^l}{l!}\sum_{k\in\mathbb{Z}}w^{-k-l-1}W^+(\alpha)x^l\partial^{k+l}e_{ab}e^{zx}\\ &= W^+(\alpha)\,\delta(w,z)e^{(y-w)(\partial/\partial z)}e^{zx}e_{ab}=W^+(\alpha)\,\delta(w,z)e^{(z+y-w)x}e_{ab}\\ &= W^+(\alpha)\,\delta(w,z)e^{yx}e_{ab}=\delta(w,z)\Psi^+(\alpha,y)e_{ab},\end{aligned}\tag{6.4}$$

where $\delta(w,z)=\Sigma_{n\in\mathbb{Z}}\,w^{-n}z^{n-1}$.

Define

$$\begin{aligned}\mathbb{X}^{(ab)}(y,w) &= X^{(ab)}(y,w)e^{(y-w)x},\\ \mathbb{W}^{(ab)}(y,w) &= \sum_{l=0}^{\infty}\frac{(y-w)^l}{l!}\sum_{k\in\mathbb{Z}}\mathbb{W}_k^{(ab,l+1)}w^{-k-l-1}=(y-w)^{-\delta_{ab}}(\mathbb{X}^{(ab)}(y,w)-\delta_{ab}),\end{aligned}\tag{6.5}$$

then

$$\mathbb{W}^{(ab)}(y,w)=:\psi^{+(a)}(y)\psi^{-(b)}(w):e^{(y-w)x}.$$

It is straightforward that the $\mathbb{W}_k^{(ab,l+1)}$ have the same commutation relations as the $W_k^{(ab,l+1)}$, since we have only replaced all $t_1^{(j)}$ by $t_1^{(j)}+x$ and kept $\partial/\partial t_1^{(j)}$ unchanged in the vertex operator (4.11) of $W^{(ab)}(y,w)$ ($\partial/\partial x$ does not appear in this expression).

One has the following:

Lemma 6.2:

$$\mathbb{X}^{(ab)}(y,w)\psi^{+(j)}(z)e^{zx}=\delta_{bj}(y-w)^{\delta_{ab}}\delta(w,z)\psi^{+(a)}(y)e^{yx}+\psi^{+(j)}(z)e^{zx}\mathbb{X}^{(ab)}(y,w).$$

Proof: Let $\gamma\in Q$, we calculate

$$\begin{aligned}\mathbb{X}^{(ab)}(y,w)\psi^{+(j)}(z)e^{zx}\tau_\gamma(x,t)e^{\gamma}=&\epsilon(\delta_a,\delta_b)\epsilon(\delta_a-\delta_b,\gamma+\delta_j)\epsilon(\delta_j,\gamma)y^{(\delta_a|\gamma+\delta_j)}w^{-(\delta_b|\gamma+\delta_j)}z^{(\delta_j|\gamma)}\\&\times(1-z/y)^{\delta_{aj}}(1-z/w)^{-\delta_{bj}}e^{\xi^{(a)}(x,t,y)-\xi^{(b)}(x,t,w)+\xi^{(j)}(x,t,z)}\\&\times e^{-\eta^{(a)}(t,y)+\eta^{(b)}(t,w)-\eta^{(j)}(t,z)}\tau_\gamma e^{\gamma+\delta_j+\delta_a-\delta_b}.\end{aligned}$$

Now use the fact that $(1-z/w)^{-1}=w\delta(w,z)-(w/z)(1-w/z)^{-1}$, $1-z/y=-(z/y)(1-y/z)$ and that $\epsilon(\delta_m,\delta_n)\epsilon(\delta_n,\delta_m)=-(-1)^{\delta_{mn}}$, then

$$\begin{aligned}&\mathbb{X}^{(ab)}(y,w)\psi^{+(j)}(z)e^{zx}\tau_\gamma(x,t)e^{\gamma}\\&\quad=\delta_{bj}\epsilon(\delta_a,\delta_b)\epsilon(\delta_a-\delta_b,\gamma+\delta_b)\epsilon(\delta_b,\gamma)(y-z)^{\delta_{ab}}\delta(w,z)y^{(\delta_a|\gamma)}w^{-(\delta_b|\gamma)}z^{(\delta_b|\gamma)}\\&\qquad\times e^{\xi^{(a)}(x,t,y)-\xi^{(b)}(x,t,w)+\xi^{(b)}(x,t,z)}e^{-\eta^{(a)}(t,y)+\eta^{(b)}(t,w)-\eta^{(b)}(t,z)}\tau_\gamma e^{\gamma+\delta_a}\\&\qquad+\epsilon(\delta_a,\delta_b)\epsilon(\delta_a-\delta_b,\gamma+\delta_j)\epsilon(\delta_j,\gamma)(-)^{\delta_{aj}}(-)^{\delta_{bj}}y^{(\delta_a|\gamma)}w^{-(\delta_b|\gamma)}z^{(\delta_j|\gamma+\delta_a-\delta_b)}\\&\qquad\times e^{\xi^{(j)}(x,t,z)}e^{\eta^{(j)}(t,z)}e^{\xi^{(a)}(x,t,y)-\xi^{(b)}(x,t,w)}e^{-\eta^{(a)}(t,y)+\eta^{(b)}(t,w)}\tau_\gamma e^{\gamma+\delta_j+\delta_a-\delta_b}\\&\quad=\{\delta_{bj}(y-w)^{\delta_{ab}}\delta(w,z)\psi^{+(a)}(y)e^{yx}+\psi^{+(j)}(z)e^{zx}\mathbb{X}^{(ab)}(y,w)\}\tau_\gamma e^{\gamma}.\end{aligned}$$

□

Recall the bilinear identity (4.14) with α replaced by $\alpha+\delta_b-\delta_a$ in a slightly different version, viz.,

$$\begin{aligned}&\mathrm{Res}_{z=0}\,dz\sum_{j=1}^{s}\psi^{+(j)}(z)e^{zx}\tau_{\alpha+\delta_i+\delta_b-\delta_j-\delta_a}(x,t)e^{\alpha+\delta_i+\delta_b-\delta_j-\delta_a}\\&\qquad\times\psi^{-(j)'}(z)e^{-zx'}\tau_{\beta+\delta_j-\delta_k}(x',t')(e^{\beta+\delta_j-\delta_k})'=0.\end{aligned}$$

Let $\mathbb{X}^{(ab)}(y,w)$ act on this identity, then using Lemma 6.2 one obtains:

$$\begin{aligned}&\mathrm{Res}_{z=0}\,dz\Big\{\{(y-w)^{\delta_{ab}}\delta(w,z)\psi^{+(a)}(y)e^{zx}\tau_{\alpha+\delta_i-\delta_a}(x,t)e^{\alpha+\delta_i-\delta_a}\psi^{-(a)'}(z)\\&\quad+\sum_{j=1}^{s}\psi^{+(j)}(z)e^{zx}\mathbb{X}^{(ab)}(y,w)\tau_{\alpha+\delta_i+\delta_b-\delta_j-\delta_a}(x,t)e^{\alpha+\delta_i+\delta_b-\delta_j-\delta_a}\psi^{-(j)'}(z)\Big\}\\&\quad\times e^{-zx'}\tau_{\beta+\delta_j-\delta_k}(x',t')(e^{\beta+\delta_j-\delta_k})'=0.\end{aligned}\tag{6.6}$$

Now divide by $\tau_\alpha(x,t)\tau_\beta(x',t')$ and remove the factors $e^{\alpha+\delta_i}$ and $(e^{\beta-\delta_k})'$. Notice that by doing this, the action of $\mathbb{X}^{(ab)}(y,w)$ is no longer well-defined, for that reason we introduce $\hat{X}^{(ab)}(y,w)$ by

$$\begin{aligned}\hat{X}^{(ab)}(y,w)\tau_\gamma(x,t)=&\epsilon(\delta_a,\delta_b)\epsilon(\delta_a-\delta_b,\gamma)y^{(\delta_a|\gamma)}w^{-(\delta_b|\gamma)}\\&\times e^{\xi^{(a)}(x,t,y)-\xi^{(b)}(x,t,w)}e^{\eta^{(a)}(t,y)+\eta^{(b)}(t,w)}\tau_\gamma(x,t)\end{aligned}$$

and

$$\hat{W}^{(ab)}(y,w)=\sum_{l=0}^{\infty}\frac{(y-w)^l}{l!}\sum_{k\in\mathbb{Z}}\hat{W}_k^{(ab,l+1)}w^{-k-l-1}=(y-w)^{-\delta_{ab}}(\hat{X}^{(ab)}(y,w)-\delta_{ab}). \quad (6.7)$$

Then (6.6) turns into

$$\begin{aligned}\mathrm{Res}_{z=0}\,dz\Bigg\{&(y-w)^{\delta_{ab}}\delta(w,z)\Psi_{ia}^{+}(\alpha,y)\Psi_{kb}^{-}(\beta,z)'+\sum_{j=1}^{s}e^{-\eta^{(j)}(t,z)}\\&\times\left(\frac{\hat{X}^{(ab)}(y,w)\tau_{\alpha+\delta_i+\delta_b-\delta_j-\delta_a}(x,t)}{\tau_{\alpha+\delta_i-\delta_j}(x,t)}\right)\Psi_{ij}^{+}(\alpha,z)\Psi_{kj}^{-}(\beta,z)'\Bigg\}=0. \quad (6.8)\end{aligned}$$

Using (6.4) one obtains

$$\begin{aligned}\mathrm{Res}_{z=0}\,dz\Bigg\{e_{ii}\Bigg(&(y-w)^{\delta_{ab}}Y^{(ab)}(\alpha,y,w)\Psi^{+}(\alpha,z)+\sum_{j=1}^{s}e^{-\eta^{(j)}(t,z)}\\&\times\left(\frac{\hat{X}^{(ab)}(y,w)\tau_{\alpha+\delta_i+\delta_b-\delta_j-\delta_a}(x,t)}{\tau_{\alpha+\delta_i-\delta_j}(x,t)}\right)\Bigg)\Psi^{+}(\alpha,z)e_{jj}\Bigg\}\ {}^{t}\Psi^{-}(\beta,z)'=0.\end{aligned}$$

Now notice that

$$\begin{aligned}&e^{-\eta^{(j)}(t,z)}\left(\frac{\hat{X}^{(ab)}(y,w)\tau_{\alpha+\delta_i+\delta_b-\delta_j-\delta_a}(x,t)}{\tau_{\alpha+\delta_i-\delta_j}(x,t)}\right)\Psi^{+}(\alpha,z)e_{jj}\\&=\sum_{k=0}^{\infty}c_{jk}L(\alpha)^{-k}C^{(j)}(\alpha)\Psi^{+}(\alpha,z)\\&=\left\{\left(\sum_{k=1}^{\infty}c_{jk}L(\alpha)^{-k}C^{(j)}(\alpha)\right)_{-}+\frac{\hat{X}^{(ab)}(y,w)\tau_{\alpha+\delta_i+\delta_b-\delta_j-\delta_a}(x,t)}{\tau_{\alpha+\delta_i-\delta_j}(x,t)}e_{jj}\right\}\Psi^{+}(\alpha,z),\end{aligned}$$

hence

$$\mathrm{Res}_{z=0}\,dz\;e_{ii}\left((y-w)^{\delta_{ab}}Y^{(ab)}(\alpha,y,w)+\sum_{j=1}^{s}\sum_{k=0}^{\infty}c_{jk}L(\alpha)^{-k}C^{(j)}(\alpha)\right)\Psi^{+}(\alpha,z)^{t}\Psi^{-}(\beta,z)'=0.$$

Now using Proposition 5.2 for $\beta=\alpha$, one obtains

$$e_{ii}\left((y-w)^{\delta_{ab}}Y^{(ab)}(\alpha,y,w)_{-}+\sum_{j=1}^{s}\left(\sum_{k=0}^{\infty}c_{jk}L(\alpha)^{-k}C^{(j)}(\alpha)\right)_{-}\right)=0.$$

Hence

$$
\begin{aligned}
&-e_{ii}(y-w)^{\delta_{ab}}Y^{(ab)}(\alpha,y,w)_-\Psi^+(\alpha,z)\\
&\quad=e_{ii}\sum_{j=1}^{s}e^{-\eta^{(j)}(t,z)}\left(\frac{\hat{X}^{(ab)}(y,w)\tau_{\alpha+\delta_i+\delta_b-\delta_j-\delta_a}(x,t)}{\tau_{\alpha+\delta_i-\delta_j}(x,t)}\right)\Psi^+(\alpha,z)e_{jj}\\
&\qquad-\frac{\hat{X}^{(ab)}(y,w)\tau_{\alpha+\delta_b-\delta_a}(x,t)}{\tau_\alpha(x,t)}e_{ii}\Psi^+(\alpha,z).
\end{aligned}
$$

So we obtain the following generalization of the Adler–Shiota–van Moerbeke formula

Theorem 6.3:

$$
\begin{aligned}
(y-w)^{\delta_{ab}}(-Y^{(ab)}(\alpha,y,w)_-\Psi^+(\alpha,z))_{ij}=&\left\{e^{-\eta^{(j)}(t,z)}\left(\frac{\hat{X}^{(ab)}(y,w)\tau_{\alpha+\delta_i+\delta_b-\delta_j-\delta_a}(x,t)}{\tau_{\alpha+\delta_i-\delta_j}(x,t)}\right)\right.\\
&\left.-\frac{\hat{X}^{(ab)}(y,w)\tau_{\alpha+\delta_b-\delta_a}(x,t)}{\tau_\alpha(x,t)}\right\}\Psi^+_{ij}(\alpha,z). \qquad (6.9)
\end{aligned}
$$

In a similar way as in the introduction the operator $e^{\lambda\mathbb{X}^{(ab)}(y,w)}=1+\lambda\mathbb{X}^{(ab)}(y,w)$ is an auto-Bäcklund transformation of the s-component KP hierarchy (see also Ref. 9). Now let

$$
\sigma(x,t)=\sum_{\gamma\in Q}\sigma_\gamma(x,t)e^\gamma=e^{\lambda\mathbb{X}^{(ab)}(y,w)}\sum_{\gamma\in Q}\tau_\gamma(x,t)e^\gamma=\sum_{\gamma\in Q}(\tau_\gamma(x,t)+\lambda\hat{X}^{(ab)}(y,w)\tau_{\gamma+\delta_b-\delta_a})e^\gamma,
$$

then (6.9) is equal to

$$
\begin{aligned}
&-\lambda(y-w)^{\delta_{ab}}(Y^{(ab)}(\tau_\alpha,y,w)_-\Psi^+(\tau_\alpha,x,t,z))_{ij}\\
&\quad=\left\{e^{-\eta^{(j)}(t,z)}\left(\frac{\sigma_{\alpha+\delta_i-\delta_j}(x,t)}{\tau_{\alpha+\delta_i-\delta_j}(x,t)}\right)-\frac{\sigma_\alpha(x,t)}{\tau_\alpha(x,t)}\right\}\Psi^+_{ij}(\tau_\alpha,x,t,z).
\end{aligned}
$$

So

$$
\begin{aligned}
\Psi^+_{ij}(\sigma_\alpha,x,t,z)&=\frac{e^{-\eta^{(j)}(t,z)}\sigma_{\alpha+\delta_i-\delta_j}(x,t)}{\sigma_\alpha(x,t)}e^{\xi^{(j)}(x,t,z)}\\
&=\frac{\tau_\alpha(x,t)}{\sigma_\alpha(x,t)}e^{-\eta^{(j)}(t,z)}\left(\frac{\sigma_{\alpha+\delta_i-\delta_j}(x,t)}{\tau_{\alpha+\delta_i-\delta_j}(x,t)}\right)\Psi^+_{ij}(\tau_\alpha,x,t,z)\\
&=\left(\left(1-\lambda\frac{\tau_\alpha(x,t)}{\sigma_\alpha(x,t)}(y-w)^{\delta_{ab}}Y^{(ab)}(\tau_\alpha,y,w)_-\right)\Psi^+(\tau_\alpha,x,t,z)\right)_{ij}
\end{aligned}
$$

and we obtain the following consequence of Theorem 6.3:

Corollary 6.4: Let $\tau(x,t)$ be a solution of the s-component KP hierarchy, then $\sigma(x,t)=e^{\lambda\mathbb{X}^{(ab)}(y,w)}\tau(x,t)$ is a new solution of this hierarchy and the wave functions are related by

$$
\Psi^+_{ij}(\sigma_\alpha,x,t,z)=\left(\left(1-\lambda\frac{\tau_\alpha(x,t)}{\sigma_\alpha(x,t)}(y-w)^{\delta_{ab}}Y^{(ab)}(\tau_\alpha,y,w)_-\right)\Psi^+(\tau_\alpha,x,t,z)\right)_{ij}.
$$

Hence (6.9) relates this Bäcklund transformation of the s-component KP hierarchy acting on the τ-function to a ''Bäcklund transformation'' on the wave function.

Since the left-hand-side of (6.9) is also equal to

$$\left\{ e^{-\eta^{(j)}(t,z)} \left(\frac{(\hat{X}^{(ab)}(y,w)-\delta_{ab})\tau_{\alpha+\delta_i+\delta_b-\delta_j-\delta_a}(x,t)}{\tau_{\alpha+\delta_i-\delta_j}(x,t)} \right) - \frac{(\hat{X}^{(ab)}(y,w)-\delta_{ab})\tau_{\alpha+\delta_b-\delta_a}(x,t)}{\tau_\alpha(x,t)} \right\} \Psi^+_{ij}(\alpha,z),$$

we have the following:

Corollary 6.5:

$$(-(M(\alpha)^l L(\alpha)^{k+l} C^{(ab)}(\alpha))_- \Psi^+(\alpha,z))_{ij} = \left\{ e^{-\eta^{(j)}(t,z)} \left(\frac{\hat{W}_k^{(ab,l+1)}\tau_{\alpha+\delta_i+\delta_b-\delta_j-\delta_a}(x,t)}{\tau_{\alpha+\delta_i-\delta_j}(x,t)} \right) - \frac{\hat{W}_k^{(ab,l+1)}\tau_{\alpha+\delta_b-\delta_a}(x,t)}{\tau_\alpha(x,t)} \right\} \Psi^+_{ij}(\alpha,z).$$

Proof: Compare in (6.9) the expansions for the vertex operators $Y^{(ab)}(\alpha,y,w)$ as in (6.2) and for $\hat{W}^{(ab)}(y,w)$ as in (6.7). □

As an application of Corollary 6.5 we see that if

$$\sum_{a=1}^{s}\sum_{l=0}^{\infty}\sum_{k\in\mathbb{Z}} c_{alk}(M(\alpha)^l L(\alpha)^{k+l} C^{(a)}(\alpha))_- = 0,$$

one finds that that for any $1 \leqslant j \leqslant s$

$$(e^{-\eta^{(j)}(t,z)}-1)\left(\frac{\sum_{a=1}^{s}\sum_{l=0}^{\infty}\sum_{k\in\mathbb{Z}} c_{alk}\hat{W}_k^{(a,l+1)}\tau_\alpha(x,t)}{\tau_\alpha(x,t)} \right) = 0,$$

hence

$$\sum_{a=1}^{s}\sum_{l=0}^{\infty}\sum_{k\in\mathbb{Z}} c_{alk}\mathbb{W}_k^{(a,l+1)}\tau_\alpha(x,t)e^\alpha = \text{constant } \tau_\alpha(x,t)e^\alpha.$$

Thus Corollary 6.5 provides an alternative proof of Theorem 6.5 of Ref. 19.

VII. THE ADLER–SHIOTA–VAN MOERBEKE FORMULA FOR THE 2-DIMENSIONAL TODA LATTICE HIERARCHY

To convince the reader that a generalized Adler–Shiota–van Moerbeke formula also exists for the 2-dimensional Toda lattice hierarchy of Ueno and Takasaki,[8] we reformulate the results of Sec. VI in the case that $s=2$. We will use most of the notations of the Adler–Shiota–van Moerbeke paper.[6]

From now on we assume that $s=2$ and denote by $\tau_n(t) = (-)^{n(n-1)/2}\tau_{n(\delta_1-\delta_2)}(0,t)$ (so put $x=0$). Following Ref. 6 we write $\tau \in F^{(0)}$ as an infinite column vector, viz., $\tau = (\tau_n)_{n\in\mathbb{Z}}$ and introduce the wave or Baker–Akhiezer vectors $\Psi_a^{\pm}(t,z) = (\widetilde{\Psi}_{an}^{\pm}(t,z))_{n\in\mathbb{Z}}$ for $a=1,2$, where

$$\begin{aligned}\widetilde{\Psi}^{\pm}_{1n}(t,z)&=z^{1/2\mp 1/2}\Psi^{\pm}_{11}((n+\tfrac{1}{2}\mp\tfrac{1}{2})(\delta_1-\delta_2),0,t,z)=\frac{e^{\mp\eta^{(1)}(t,z)}\tau_{n+1/2\mp 1/2}(t)}{\tau_{n+1/2\mp 1/2}(t)}\,e^{\pm\xi^{(1)}(t,z)}z^{\pm n},\\ \widetilde{\Psi}^{\pm}_{2n}(t,z)&=\mp z^{-1/2\mp 1/2}\Psi^{\pm}_{12}((n+\tfrac{1}{2}\mp\tfrac{1}{2})(\delta_1-\delta_2),0,t,z^{-1})\\ &=\frac{e^{\mp\eta^{(2)}(t,z^{-1})}\tau_{n+1/2\pm 1/2}(t)}{\tau_{n+1/2\mp 1/2}(t)}\,e^{\pm\xi^{(2)}(t,z^{-1})}z^{\pm n}.\end{aligned}\tag{7.1}$$

Then (4.13) and (5.3) is equivalent to

$$\mathrm{Res}_{z=0}\,\frac{dz}{z}\,\Psi^{+}_{1}(t,z)^{t}\Psi^{-}_{1}(t',z)-\Psi^{+}_{2}(t,z^{-1})^{t}\Psi^{-}_{2}(t',z^{-1})=0.\tag{7.2}$$

We want to write these wave vectors as the action of infinite matrices acting on the vectors $\chi(z)=\chi^{+}(z)=(z^{n})_{n\in\mathbb{Z}}$ and $\chi^{-}(z)=(z^{-n})_{n\in\mathbb{Z}}$. Let $\Lambda=\Sigma_{i\in\mathbb{Z}}\,E_{ii}$, then

$$\begin{aligned}\Psi^{\pm}_{1}(t,z)&=W^{\pm}_{1}(t,\Lambda)\chi^{\pm}(z)=S^{\pm}_{1}(t,\Lambda)e^{\pm\xi^{(1)}(t,\Lambda^{\pm 1})}\chi^{\pm}(z),\\ \Psi^{\pm}_{2}(t,z)&=W^{\pm}_{2}(t,\Lambda)\chi^{\pm}(z)=S^{\pm}_{2}(t,\Lambda)e^{\pm\xi^{(2)}(t,\Lambda^{\mp 1})}\chi^{\pm}(z),\end{aligned}\tag{7.3}$$

where

$$S^{\pm}_{1}(t,\Lambda)=\sum_{i=0}^{\infty}\,\mathrm{diag}(p^{\pm}_{ni}(t))_{n\in\mathbb{Z}}\Lambda^{\mp i},\quad S^{\pm}_{2}(t,\Lambda)=\sum_{i=0}^{\infty}\,\mathrm{diag}(q^{\pm}_{ni}(t))_{n\in\mathbb{Z}}\Lambda^{\pm i},\tag{7.4}$$

with the $p^{\pm}_{ni}$ and $q^{\pm}_{ni}$ defined by

$$\frac{e^{\mp\eta^{(1)}(t,z)}\tau_{n+1/2\mp 1/2}(t)}{\tau_{n+1/2\mp 1/2}(t)}=\sum_{i=0}^{\infty}\,p^{\pm}_{ni}(t)z^{-i},\quad \frac{e^{\mp\eta^{(2)}(t,z^{-1})}\tau_{n+1/2\pm 1/2}(t)}{\tau_{n+1/2\mp 1/2}(t)}=\sum_{i=0}^{\infty}\,q^{\pm}_{ni}(t)z^{i}.\tag{7.5}$$

As in Ref. 6 it will be convenient to take pairs of matrices, so let D be the algebra of pairs of infinite $(\mathbb{Z}\times\mathbb{Z})$ matrices (P_1,P_2) such that $(P_1)_{ij}=0$ for $j-i\gg 0$ and $(P_2)_{ij}=0$ for $i-j\gg 0$. Then

$$D_{+}=\{(P_1,P_2)\in D\,|\,P_1=P_2\},$$

$$D_{-}=\{(P_1,P_2)\in D\,|\,(P_1)_{ij}=0\quad\text{if}\quad j\geqslant i,\quad (P_2)_{ij}=0\quad\text{if}\quad i>j\},$$

so that $(P_1,P_2)=(P_1,P_2)_{+}+(P_1,P_2)_{-}$ is given by

$$\begin{aligned}(P_1,P_2)_{+}&=(P_{1u}+P_{2l},P_{1u}+P_{2l}),\\ (P_1,P_2)_{-}&=(P_{1l}-P_{2l},P_{2u}-P_{1u}),\end{aligned}\tag{7.6}$$

where P_u and P_l denote the upper (including the diagonal) and strictly lower triangular parts of the matrix P, respectively. It is straightforward to prove the following fundamental lemma (see, e.g., Ref. 6):

Lemma 7.1: Let $U=(U_1,U_2)$, $V=(V_1,V_2)\in D$ whose coefficients depend on t, then (i) the following identities hold

$$\mathrm{Res}_{z=0}\,\frac{dz}{z}\,U_i\chi^{+}(z^{-(-1)^{i}})^{t}({}^{t}V_i\chi^{-}(z^{-(-1)^{i}}))=U_iV_i,$$

(ii) we have $(UV)_-=0$ *if and only if*

$$\mathrm{Res}_{z=0}\frac{dz}{z}\{U_1\chi^+(z)^t({}^tV_1\chi^-(z))-U_2\chi^+(z^{-1})^t({}^tV_2\chi^-(z^{-1}))\}.$$

Now applying this Lemma to (7.2), using (7.3), one obtains for $W^\pm(t,\Lambda)=(W_1^\pm(t,\Lambda),W_2^\pm(t,\Lambda))$ that

$$(W^+(t,\Lambda)^tW^-(t',\Lambda))_-=(W_1^+(t,\Lambda)^tW_1^-(t',\Lambda),W_2^+(t,\Lambda)^tW_2^-(t',\Lambda))_-=0. \tag{7.7}$$

Now put $t=t'$, then one deduces that $(S^+(t,\Lambda)^tS^-(t,\Lambda))_-=(S_1^+(t,\Lambda)^tS_1^-(t,\Lambda),\ S_2^+(t,\Lambda)^tS_2^-(t,\Lambda))_-=0$, hence for $a=1,2$ one finds

$$S_a^+(t,\Lambda)=({}^tS_a^-(t,\Lambda))^{-1}. \tag{7.8}$$

Differentiate (7.2) to $\partial/\partial t_i^{(a)}$ and use (7.8) and Lemma 7.1, then it is straightforward to deduce the following Sato equations for $S^+=(S_1^+,S_2^+)$ [cf. (5.18)]

$$\frac{\partial S^+}{\partial t_i^{(1)}}=-(S_1^+\Lambda^iS_1^{+-1},0)_-S^+,\quad \frac{\partial S^+}{\partial t_i^{(2)}}=-(0,S_2^+\Lambda^{-i}S_2^{+-1})_-S^+. \tag{7.9}$$

From now on let $\Psi=(\Psi_1,\Psi_2)=(\Psi_1^+,\Psi_2^+)$, $W=(W_1,W_2)=(W_1^+,W_2^+)$, $S=(S_1,S_2)=(S_1^+,S_2^+)$ and define

$$L=(L_1,L_2)=(W_1\Lambda W_1^{-1},W_2\Lambda^{-1}W_2^{-1})=(S_1\Lambda S_1^{-1},S_2\Lambda^{-1}S_2^{-1}),$$

then (7.9) is equivalent to one of the following statements [cf. (4.24)]:

$$\begin{aligned}
&\frac{\partial S}{\partial t_i^{(1)}}=-(L_1^i,0)_-S,\quad \frac{\partial S}{\partial t_i^{(2)}}=-(0,L_2^i)_-S,\\
&\frac{\partial W}{\partial t_i^{(1)}}=(L_1^i,0)_+W,\quad \frac{\partial W}{\partial t_i^{(2)}}=(0,L_2^i)_+W,\\
&\frac{\partial \Psi}{\partial t_i^{(1)}}=(L_1^i,0)_+\Psi,\quad \frac{\partial \Psi}{\partial t_i^{(2)}}=(0,L_2^i)_+\Psi.
\end{aligned} \tag{7.10}$$

Next define

$$M=(M_1,M_2)=(W_1\epsilon_1W_1^{-1},W_2\epsilon_2W_2^{-1}),$$

where

$$\epsilon_1=\sum_{n\in\mathbb{Z}}nE_{n,n-1}\quad\text{and}\quad \epsilon_2=\sum_{n\in\mathbb{Z}}nE_{-n,1-n},$$

then $[L_a,M_a]=1$ and

$$L\Psi=(z,z^{-1})\Psi,\quad M\Psi=\left(\frac{\partial}{\partial z},\frac{\partial}{\partial z^{-1}}\right)\Psi. \tag{7.11}$$

More generally one has

$$M^k L^{k+l}\Psi = \left(z^{k+l}\left(\frac{\partial}{\partial z}\right)^k, (z^{-1})^{k+l}\left(\frac{\partial}{\partial z^{-1}}\right)^k \right)\Psi. \tag{7.12}$$

Using (7.10) or (7.11) one easily deduces the following Lax equations for the Toda lattice hierarchy [cf. (5.23)]. Let $X=M$ or L, then

$$\frac{\partial X}{\partial t_i^{(1)}} = [(L_1^i,0)_+, X], \quad \frac{\partial X}{\partial t_i^{(2)}} = [(0,L_2^i)_+, X]. \tag{7.13}$$

In a similar way as in Sec. VI we derive the generalized Adler–Shiota–van Moerbeke formula. Define [cf. (6.1)]

$$Y^{(ab)}(y,w) = \sum_{l=0}^{\infty} \frac{(y-w)^l}{l!} \sum_{k\in\mathbb{Z}} W_a(t,\Lambda)\epsilon_b^l \Lambda^{-(-1)^b(k+l)} W_b(t,\Lambda)^{-1} w^{-k-l-1}. \tag{7.14}$$

Notice that the left-hand side of (7.14) for $a\neq b$ is not well-defined. One should see this as product of operators on $\Psi_b(t,z)$.

It is easy to show that [cf. (6.4)]

$$Y^{(ab)}(y,w)\Psi_b(t,z) = \delta(w,z^{-(-1)^b})\Psi_a(t,y^{-(-1)^b}). \tag{7.15}$$

Now rewrite (6.8) for $i=k=1$, $\alpha=n(\delta_1-\delta_2)$ and $\beta=(m+1)(\delta_1-\delta_2)$ in the new notations:

$$\begin{aligned}
&\mathrm{Res}_{z=0}\frac{dz}{z}\Bigg(-(-)^b\left(\frac{w}{y^{\delta_{a2}}}\right)^{\delta_{b2}} (y-w)^{\delta_{ab}}\delta(w,z)\widetilde{\Psi}^+_{an}(t,y^{-(-1)^a})\widetilde{\Psi}^-_{bm}(t',z^{-(-1)^b}) \\
&\quad +(-)^{a+b}\Bigg\{ e^{-\eta^{(1)}(t,z)}\left(\frac{(w^{(-1)^b}/y^{(-)^a})^{n+a-b}\widetilde{X}^{(ab)}(y,w)\tau_{n+a-b}(t)}{\tau_n(t)}\right)\widetilde{\Psi}^+_{1n}(t,z)\widetilde{\Psi}^-_{1m}(t',z) \\
&\quad -e^{-\eta^{(2)}(t,z)}\left(\frac{(w^{(-1)^b}/y^{(-1)^a})^{n+a-b+1}\widetilde{X}^{(ab)}(y,w)\tau_{n+a-b+1}(t)}{\tau_{n+1}(t)}\right) \\
&\quad \times\widetilde{\Psi}^+_{2n}(t,z^{-1})\widetilde{\Psi}^-_{2m}(t,z^{-1})\Bigg\}\Bigg) = 0.
\end{aligned}$$

Next sum over all n and m and use (7.15), then this turns into

$$\begin{aligned}
&\mathrm{Res}_{z=0}\frac{dz}{z}\Bigg(-(-)^b\left(\frac{w}{y^{\delta_{a2}}}\right)^{\delta_{b2}} (y-w)^{\delta_{ab}}Y^{(ab)}(y^{(-1)^{a+b}},w)\Psi^+_b(t,z^{-(-1)^b})^t\Psi^-_b(t',z^{-(-1)^b}) \\
&\quad +(-)^{a+b}\sum_{n\in\mathbb{Z}}\Bigg\{ e^{-\eta^{(1)}(t,z)}\left(\frac{(w^{(-1)^b}/y^{(-1)^a})^{n+a-b}\widetilde{X}^{(ab)}(y,w)\tau_{n+a-b}(t)}{\tau_n(t)}\right)E_{nn} \\
&\quad \times\Psi^+_1(t,z)^t\Psi^-_1(t',z) - e^{-\eta^{(2)}(t,z)}\left(\frac{(w^{(-1)^b}/y^{(-1)^a})^{n+a-b+1}\widetilde{X}^{(ab)}(y,w)\tau_{n+a-b+1}(t)}{\tau_{n+1}(t)}\right) \\
&\quad \times E_{nn}\Psi^+_2(t,z^{-1})^t\widetilde{\Psi}^-_2(t,z^{-1})\Bigg\}\Bigg) = 0.
\end{aligned} \tag{7.16}$$

Let

$$\sum_{k=0}^{\infty} c_{kn}^{(i)} z^{-k} = e^{-\eta^{(i)}(t,z)} \left(\frac{(w^{(-1)^b}/y^{(-1)^a})^{n+a-b} \widetilde{X}^{(ab)}(y,w)\tau_{n+a-b}(t)}{\tau_n(t)} \right)$$
$$= \frac{(w^{(-1)^b}/y^{(-1)^a})^{n+a-b} \widetilde{X}^{(ab)}(y,w)\tau_{n+a-b}(t)}{\tau_n(t)} + \sum_{k=1}^{\infty} c_{kn}^{(i)} z^{-k},$$

then (7.16) is equivalent to

$$\mathrm{Res}_{z=0} \frac{dz}{z} \left(-(-)^b \left(\frac{w}{y^{\delta_{a2}}} \right)^{\delta_{b2}} (y-w)^{\delta_{ab}} Y^{(ab)}(y^{(-1)^{a+b}}, w) \Psi_b^+(t, z^{-(-1)^b}) {}^t\Psi_b^-(t', z^{-(-1)^b}) \right.$$
$$+ (-)^{a+b} \sum_{n\in\mathbb{Z}} \left\{ \sum_{k=0}^{\infty} c_{kn}^{(1)} E_{nn} L_1^{-k} \Psi_1^+(t,z) {}^t\Psi_1^-(t',z) \right.$$
$$\left. \left. - \sum_{k=0}^{\infty} c_{k+1,n}^{(2)} E_{nn} L_2^{-k} \Psi_2^+(t,z^{-1}) {}^t\Psi_2^-(t,z^{-1}) \right\} \right) = 0. \tag{7.17}$$

Using the Lemma 7.1 and (7.8) one deduces

$$\left((-)^{a+b} \sum_{n\in\mathbb{Z}} \sum_{k=0}^{\infty} c_{kn}^{(1)} E_{nn} L_1^{-k} + \delta_{b1} (y-w)^{\delta_{ab}} Y^{(a,1)}(y^{-(-1)^a}, w), (-)^{a+b} \sum_{n\in\mathbb{Z}} \sum_{k=0}^{\infty} c_{k+1,n}^{(2)} E_{nn} L_2^{-k} \right.$$
$$\left. + \delta_{b2} \frac{w}{y^{\delta_{a2}}} (y-w)^{\delta_{ab}} Y^{(a,2)}(y^{(-1)^a}, w) \right)_- = 0.$$

Hence

$$-(y-w)^{\delta_{ab}} \left(\frac{w}{y^{\delta_{a2}}} \right)^{\delta_{b2}} Y^{(ab)}(y^{(-1)^{a+b}}, w)_-$$
$$= (-)^{a+b} \left(\sum_{n\in\mathbb{Z}} \sum_{k=1}^{\infty} c_{kn}^{(1)} E_{nn} L_1^{-k}, \sum_{n\in\mathbb{Z}} \left\{ \sum_{k=0}^{\infty} c_{k+1,n}^{(2)} E_{nn} L_2^{-k} - c_{0n}^{(1)} E_{nn} \right\} \right).$$

Hence we have the following generalization of the Adler–Shiota–van Moerbeke formula for the Toda lattice hierarchy

Theorem 7.2:

$$-(y-w)^{\delta_{ab}} Y^{(ab)}(y^{a+b}, w)_- \Psi(t,z)$$
$$= (-)^{a+b} \left(\frac{y^{\delta_{a2}}}{w} \right)^{\delta_{b2}} \left(\sum_{n\in\mathbb{Z}} \{ e^{-\eta^{(1)}(t,z)} - 1 \} \left(\frac{(w^{(-1)^b}/y^{(-1)^a})^{n+a-b} \widetilde{X}^{(ab)}(y,w)\tau_{n+a-b}(t)}{\tau_n(t)} \right) E_{nn}, \right.$$
$$\sum_{n\in\mathbb{Z}} \left\{ e^{-\eta^{(2)}(t,z^{-1})} \left(\frac{(w^{(-1)^b}/y^{(-1)^a})^{n+a-b+1} \widetilde{X}^{(ab)}(y,w)\tau_{n+a-b+1}(t)}{\tau_{n+1}(t)} \right) \right.$$
$$\left. \left. - \frac{(w^{(-1)^b}/y^{(-1)^a})^{n+a-b} \widetilde{X}^{(ab)}(y,w)\tau_{n+a-b}(t)}{\tau_n(t)} \right\} E_{nn} \right) \Psi(t,z).$$

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A new integrable symplectic map associated with lattice soliton equations

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A method is developed that extends the nonlinearization technique to the hierarchy of lattice soliton equations associated with a discrete 3×3 matrix spectral problem. A new integrable symplectic map and its involutive system of conserved integrals are obtained by the nonlinearization of spatial parts and the time parts of Lax pairs and their adjoint Lax pairs of the hierarchy. Moreover, the solutions of the typical system of lattice equations in the hierarchy are reduced to the solutions of a system of ordinary differential equations and a simple iterative process of the symplectic map. © *1996 American Institute of Physics.* [S0022-2488(96)00504-3]

I. INTRODUCTION

The study of constructing finite-dimensional integrable systems from soliton hierarchies has received considerable attention in recent years. At least two systematic approaches, the nonlinearization technique[1,2] and the stationary flow technique,[3] have been developed through that quite a few new finite-dimensional integrable systems have been obtained in the Liouville sense.[1–5] Very recently, the two techniques have been generalized to lattice soliton hierarchies associated with discrete 2×2 matrix spectral problems,[6–8] and thus some integrable symplectic maps,[9] i.e., discrete version of classical integrable systems, have been presented.

In this paper, we are going to develop further the nonlinearization technique to treat the lattice soliton hierarchy associated with a discrete 3×3 matrix spectral problem. We give a Bargmann constraint between the eigenfunctions, the adjoint eigenfunctions, and potentials. The discrete 3×3 matrix spectral problem and its adjoint problem are nonlinearized to be a new integrable symplectic map. The nonlinearization of the time parts of the Lax pairs and their adjoint Lax pairs for the lattice soliton hierarchy leads to the involutive system of conserved integrals of the symplectic map. The solutions of the typical system of lattice equations in the hierarchy are reduced to the solutions of a system of ordinary differential equations and a simple iterative process of the symplectic map. We first construct the lattice soliton hierarchy associated with the discrete 3×3 matrix spectral problem and their Hamiltonian structures. Then we discuss the nonlinearization of Lax pairs and their adjoint ones of the lattice soliton hierarchy in detail.

II. THE LATTICE SOLITON HIERARCHY AND THE HAMILTONIAN STRUCTURES

Let us define the shift operator and difference operators by

$$Ef(n)=f(n+1),\quad \Delta f(n)=(E-1)f(n),\quad \Delta^{+}f(n)=(E^{-1}-1)f(n),\quad n\in\mathbf{Z}.$$

We usually write $f(n)=f$, $f(n+k)=E^{k}f$, $k\in\mathbf{Z}$, for the sake of convenience. Consider the discrete 3×3 matrix spectral problem:[10]

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$$E\psi(\lambda)=U\psi(\lambda),\quad U=\begin{pmatrix}0 & 1 & 0\\ b-\lambda & a & 1\\ c & 0 & 0\end{pmatrix},\quad \psi=\begin{pmatrix}\psi^1(\lambda)\\ \psi^2(\lambda)\\ \psi^3(\lambda)\end{pmatrix},\tag{1}$$

where a,b,c are three potentials and λ is a constant spectral parameter. The adjoint representation equation of (1) reads

$$(EV)U-UV=0,\quad V=(V_{ij})_{3\times 3},\tag{2}$$

where each entry $V_{ij}=V_{ij}(A(\lambda),B(\lambda),D(\lambda))$ of the 3×3 matrix V is a Laurent expansion of λ:

$$V_{11}=D(\lambda),\quad V_{12}=E^{-1}A(\lambda),\quad V_{13}=B(\lambda),$$

$$V_{21}=cEB(\lambda)+(b-\lambda)A(\lambda),\quad V_{22}=ED(\lambda)+aA(\lambda),\quad V_{23}=A(\lambda),$$

$$V_{31}=E^{-1}cE^{-1}A(\lambda)-E^{-1}acB(\lambda),\quad V_{32}=E^{-1}cB(\lambda),$$

$$V_{33}=E^2D(\lambda)+\Delta aA(\lambda)-(b-\lambda)B(\lambda),$$

$$A(\lambda)=\sum_{j\geqslant -1}A_j\lambda^{-j},\quad B(\lambda)=\sum_{j\geqslant -1}B_j\lambda^{-j},\quad D(\lambda)=\sum_{j\geqslant -1}D_j\lambda^{-j}.$$

Then adjoint representation equation (2) is equivalent to the recursion relations:

$$\begin{gathered}(E-E^{-1})A_{-1}=0,\quad (E^2-1)D_{-1}+\Delta aA_{-1}=0,\quad \Delta B_{-1}=0,\\ a\Delta(aA_{j-1}+ED_{j-1})+(Eb-bE^{-1})A_{j-1}+(EcE-E^{-1}c)B_{j-1}=(E-E^{-1})A_j,\\ (cE-E^{-1}cE^{-1}+b\Delta a)A_{j-1}+(E^{-1}ac-acE)B_{j-1}+b(E^2-1)D_{j-1}=(E^2-1)D_j+\Delta aA_j,\\ \Delta EaA_{j-1}+(E^3-1)D_{j-1}-\Delta bB_{j-1}=-\Delta B_j.\end{gathered}\tag{3}$$

The above recursion equations can be solved successively to deduce the following results:

$$\begin{gathered}A_{-1}=0,\quad B_{-1}=1,\quad D_{-1}=0,\\ A_0=c,\quad B_0=b,\quad D_0=-E^{-1}ac,\\ A_1=c(Eb+b),\quad B_1=ac+E^{-1}ac+b^2,\quad D_1=E^{-1}cE^{-1}c-E^{-1}ac(Eb+b).\end{gathered}\tag{4}$$

We define $\{F_j\}$ by the following relation:

$$cF_j=-EaA_j-E^2D_j-ED_j.\tag{5}$$

It is easy to see that

$$\begin{gathered}(\Delta-\Delta^+)D_j=\Delta^+aA_j+\Delta^+E^{-1}cF_j,\\ \Delta aA_j+(E^2-1)D_j=\Delta^+cF_j,\\ ED_j+aA_j=(\Delta-\Delta^+)^{-1}\Delta^+cF_j-(\Delta-\Delta^+)^{-1}\Delta^+aA_j,\\ \Delta EaA_j+(E^3-1)D_j=\Delta(\Delta-\Delta^+)^{-1}\Delta^+aA_j-(\Delta c-\Delta^+c)F_j-\Delta(\Delta-\Delta^+)^{-1}\Delta^+cF_j.\end{gathered}\tag{6}$$

Substituting the above expressions into (3), we obtain

$$KG_{j-1}=JG_j, \quad G_j=(A_j,B_j,F_j)^T, \quad j\geqslant 0, \tag{7}$$

where K and J, the so-called Lenard's operator pair, are two skew-symmetric operators:

$$K=\begin{pmatrix} Eb-bE^{-1}-a\Delta(\Delta-\Delta^+)^{-1}\Delta^+a & EcE-E^{-1}c & a\Delta(\Delta-\Delta^+)^{-1}\Delta^+c \\ cE-E^{-1}cE^{-1} & E^{-1}ac-acE & b\Delta^+c \\ c\Delta(\Delta-\Delta^+)^{-1}\Delta^+a & -c\Delta b & c[\Delta^+-\Delta-\Delta(\Delta-\Delta^+)^{-1}\Delta^+]c \end{pmatrix},$$

$$J=\begin{pmatrix} E-E^{-1} & 0 & 0 \\ 0 & 0 & \Delta^+c \\ 0 & -c\Delta & 0 \end{pmatrix}.$$

From (4) and (7), we have

$$G_{-1}=\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad G_0=\begin{pmatrix} c \\ b \\ a \end{pmatrix}, \quad G_1=\begin{pmatrix} c(Eb+b) \\ b^2+ac+E^{-1}ac \\ a(Eb+b)-Ec-E^{-1}c \end{pmatrix}.$$

Let $\psi(\lambda)$ satisfy the spectral problem (1) and its auxiliary problem

$$\frac{\partial}{\partial t}\psi(\lambda)=V^{(m)}\psi(\lambda), \tag{8}$$

where

$$V^{(m)}=(V_{ij}^{(m)})_{3\times 3}, \quad V_{ij}^{(m)}=V_{ij}(A^{(m)}(\lambda),B^{(m)}(\lambda),D^{(m)}(\lambda)),$$

$$A^{(m)}(\lambda)=\sum_{j=-1}^{m}A_j\lambda^{m-j}, \quad B^{(m)}(\lambda)=\sum_{j=-1}^{m}B_j\lambda^{m-j}, \quad D^{(m)}(\lambda)=\sum_{j=-1}^{m}D_j\lambda^{m-j}.$$

Then the compatibility condition $(\partial/\partial t)E\psi(\lambda)=E(\partial/\partial t)\psi(\lambda)$ between (1) and (8) yields the discrete zero-curvature equation

$$\frac{\partial}{\partial t}U=(EV^{(m)})U-UV^{(m)},$$

which implies the lattice solition equations

$$\frac{\partial}{\partial t}u=X_{m+1}, \quad u=(a,b,c)^T, \quad m\geqslant -1, \tag{9}$$

where $X_j=JG_j=KG_{j-1}$, $j\geqslant 0$. When $m=-1$, (9) is reduced to

$$\frac{\partial}{\partial t}\begin{pmatrix} a(n) \\ b(n) \\ c(n) \end{pmatrix}=\begin{pmatrix} c(n+1)-c(n-1) \\ a(n-1)c(n-1)-c(n)a(n) \\ c(n)(b(n)-b(n+1)) \end{pmatrix}. \tag{10}$$

The Hamiltonian structures of lattice soliton equations (9) can be established by the trace identity.[11] We need the following quantities, which are easy to calculate:

$$\mathrm{tr}\left(\hat{V}\frac{\partial U}{\partial \lambda}\right)=-B(\lambda),\quad \mathrm{tr}\left(\hat{V}\frac{\partial U}{\partial a}\right)=A(\lambda),\quad \mathrm{tr}\left(\hat{V}\frac{\partial U}{\partial b}\right)=B(\lambda),$$

$$\mathrm{tr}\left(\hat{V}\frac{\partial V}{\partial c}\right)=c^{-1}[D(\lambda)+(\lambda-b)B(\lambda)], \tag{11}$$

where $\hat{V}=VU^{-1}$. By means of the trace identity, we have

$$\left(\frac{\delta}{\delta a},\frac{\delta}{\delta b},\frac{\delta}{\delta c}\right)(-B(\lambda))=\left[\lambda^{-\varepsilon}\left(\frac{\partial}{\partial \lambda}\right)\lambda^{\varepsilon}\right]\left(A(\lambda),B(\lambda),\frac{D(\lambda)+(\lambda-b)B(\lambda)}{c}\right), \tag{12}$$

where ε is a constant to be fixed. Equating the coefficients of λ^{-j-1} on both sides of (12), we arrive at

$$(\delta/\delta a,\delta/\delta b,\delta/\delta c)B_{j+1}=(j-\varepsilon)(A_j,B_j,c^{-1}(D_j-bB_j+B_{j+1})), \tag{13}$$

and $(\varepsilon+2)c^{-1}=0$ which implies $\varepsilon=-2$. Notice the third expression of (3), which together with (5) leads to

$$D_j-bB_j+B_{j+1}=cF_j. \tag{14}$$

By (13) and (14), we have

$$(\delta/\delta a,\delta/\delta b,\delta/\delta c)H_j=G_j^T,H_j=\frac{B_{j+1}}{j+2},\quad j\geqslant -1. \tag{15}$$

Hence we deduce that the desired Hamiltonian form of (9)

$$\frac{\partial}{\partial t}u=X_{m+1}=J(\delta/\delta a,\delta/\delta b,\delta/\delta c)^T H_{m+1},\quad m\geqslant -1. \tag{16}$$

III. A SYMPLECTIC MAP

Let us consider another discrete 3×3 matrix spectral problem

$$E\varphi(\lambda)=(U^{-1})^T\varphi(\lambda),\varphi(\lambda)=(\varphi^1(\lambda),\varphi^2(\lambda),\varphi^3(\lambda))^T, \tag{17}$$

which is usually called the adjoint spectral problem of (1). For N mutual distinct eigenvalues $\lambda_1,\ldots,\lambda_N$, the systems associated with (1) and (17) can be written in the form

$$\begin{aligned}E(q_j^1,q_j^2,q_j^3)&=(q_j^1,q_j^2,q_j^3)U(u,\lambda_j)^T,\\ E(p_j^1,p_j^2,p_j^3)&=(p_j^1,p_j^2,p_j^3)U(u,\lambda_j)^{-1},\end{aligned} \tag{18}$$

where $q_j^i=\psi^i(\lambda_j)$, $p_j^i=\varphi^i(\lambda_j)$, $1\leqslant i\leqslant 3$, $1\leqslant j\leqslant N$. It is easy to calculate that the functional gradient of the eigenvalue λ_j with regard to the potentials (a,b,c) is

$$\nabla\lambda_j=\begin{pmatrix}\delta\lambda_j/\delta a\\ \delta\lambda_j/\delta b\\ \delta\lambda_j/\delta c\end{pmatrix}=\begin{pmatrix}q_j^2p_j^3\\ q_j^1p_j^3\\ c^{-1}(q_j^1p_j^1+\lambda_j q_j^1p_j^3-bq_j^1p_j^3)\end{pmatrix}. \tag{19}$$

Such a gradient satisfies the following equation

$$K\nabla\lambda_j=\lambda_j J\nabla\lambda_j, \tag{20}$$

which can be verified by a straightforward computation.

Consider the Bargmann constraint

$$G_0=\sum_{j=1}^{N}\nabla\lambda_j, \tag{21}$$

which implies

$$\begin{gathered}a=\langle q^2,p^3\rangle^{-1}(\langle q^1,p^1\rangle+\langle \Lambda q^1,p^3\rangle-\langle q^1,p^3\rangle^2),\\ b=\langle q^1,p^3\rangle,\quad c=\langle q^2,p^3\rangle,\end{gathered} \tag{22}$$

where $\langle\cdot,\cdot\rangle$ is the standard inner-product in R^N, $\Lambda=\mathrm{diag}\ (\lambda_1,\ldots,\lambda_N)$, $q^i=(q_1^i,\ldots,q_N^i)^T$, $p^i=(p_1^i,\ldots,p_N^i)^T$, $1\leqslant i\leqslant 3$. Substituting (22) into (18) yields the discrete Bargmann system

$$\begin{gathered}Eq^1=q^2,\\ Eq^2=-\Lambda q^1+\langle q^1,p^3\rangle q^1+\langle q^2,p^3\rangle^{-1}(\langle q^1,p^1\rangle+\langle \Lambda q^1,p^3\rangle-\langle q^1,p^3\rangle^2)q^2+q^3,\\ Eq^3=\langle q^2,p^3\rangle q^1,\\ Ep^1=p^2-\langle q^2,p^3\rangle^{-1}(\langle q^1,p^1\rangle+\langle \Lambda q^1,p^3\rangle-\langle q^1,p^3\rangle^2)p^3,\\ Ep^2=p^3,\\ Ep^3=\langle q^2,p^3\rangle^{-1}[p^1+(\Lambda-\langle q^1,p^3\rangle)p^3].\end{gathered} \tag{23}$$

Equations (23) determine a symplectic map H,

$$E(q^1,q^2,q^3,p^1,p^2,p^3)=H(q^1,q^2,q^3,p^1,p^2,p^3), \tag{24}$$

because by direct calculations

$$\sum_{j=1}^{N}\sum_{i=1}^{3}d(Eq_j^i)\wedge d(Ep_j^i)=\sum_{j=1}^{N}\sum_{i=1}^{3}dq_j^i\wedge dp_j^i.$$

IV. THE INTEGRABILITY OF THE SYMPLECTIC MAP

In this section, we want to search for the conserved integrals of the symplectic map H. Let us consider the adjoint equation of (8),

$$\frac{\partial}{\partial t}\varphi(\lambda)=-V^{(m)T}\varphi(\lambda), \tag{25}$$

which together with (17) composes another kind of zero curvature representation for the lattice soliton equations (9). As a matter of fact, we can directly deduce that $(\partial/\partial t)U=(EV^{(m)})U-UV^{(m)}$ if and only if $(\partial/\partial t)(U^{-1})^T=-(EV^{(m)})^T(U^{-1})^T+(U^{-1})^TV^{(m)T}$. In what follows we discuss the nonlinearization of (8) and (25). Resorting to (7), (20), and the constraint (21), we take the following restriction:

$$G_j=\sum_{k=1}^{N}\lambda_k^j\nabla 6\lambda_k, \tag{26}$$

which is a special solution of (7). Equation (26) is equivalent to

$$A_j=\langle\Lambda^j q^2,p^3\rangle,\quad B_j=\langle\Lambda^j q^1,p^3\rangle,$$
$$F_j=c^{-1}(\langle\Lambda^j q^1,p^1\rangle+\langle\Lambda^{j+1}q^1,p^3\rangle-b\langle\Lambda^j q^1,p^3\rangle),\quad j\geqslant 0. \tag{27}$$

Substituting (27) into the first expression of (6), we obtain a solution of D_j, that is

$$D_j=\langle\Lambda^j q^1,p^1\rangle,\quad j\geqslant 0. \tag{28}$$

By using (27), (28), (23), and (22), we have

$$E^{-1}A_j=\langle\Lambda^j q^1,p^2\rangle,\quad E^{-1}cB_j=\langle\Lambda^j q^3,p^2\rangle,$$
$$cEB_j+bA_j=\langle\Lambda^j q^2,p^1\rangle+\langle\Lambda^{j+1}q^2,p^3\rangle,$$
$$E^{-1}cE^{-1}A_j-E^{-1}acB_j=\langle\Lambda^j q^3,p^1\rangle,$$
$$E^2D_j+EaA_j-aA_j-bB_j=\langle\Lambda^j q^3,p^3\rangle-\langle\Lambda^{j+1}q^1,p^3\rangle,$$
$$ED_j+aA_j=\langle\Lambda^j q^2,p^2\rangle,\quad E^{-1}c=\langle q^1,p^2\rangle,\quad Eac=\langle q^3,p^3\rangle.$$

Substituting the above expressions, (27), and (28) into N replicas of (8) and (17) associated with $\lambda_1,\ldots,\lambda_N$,

$$\frac{\partial}{\partial t}(q^1,q^2,q^3)=(q^1,q^2,q^3)V^{(m)}(u,\Lambda_j)^T,$$
$$\frac{\partial}{\partial t}(p^1,p^2,p^3)=-(p^1,p^2,p^3)V^{(m)}(u,\Lambda_j), \tag{29}$$

we arrive at the finite-dimensional Hamiltonian systems

$$\frac{\partial}{\partial t}q^i=\frac{\partial F_m}{\partial p^i},\ \frac{\partial}{\partial t}p^i=-\frac{\partial F_m}{\partial q^i},\quad m\geqslant -1,\quad 1\leqslant i\leqslant 3 \tag{30}$$

with the Hamiltonian functions

$$F_{-1}=\langle\Lambda q^3,p^3\rangle+\langle q^3,p^1\rangle+\langle q^1,p^2\rangle\langle q^2,p^3\rangle-\langle q^3,p^3\rangle\langle q^1,p^3\rangle.$$
$$F_m=\langle\Lambda^{m+2}q^3,p^3\rangle+\langle\Lambda^{m+1}q^3,p^1\rangle+\langle q^1,p^2\rangle\langle\Lambda^{m+1}q^2,p^3\rangle-\langle q^3,p^3\rangle\langle\Lambda^{m+1}q^1,p^3\rangle$$
$$+\frac{1}{2}\sum_{j=0}^{m}\sum_{i=1}^{3}\langle\Lambda^j q^i,p^i\rangle\langle\Lambda^{m-j}q^i,p^i\rangle+\sum_{j=0}^{m}\sum_{1\leqslant i<k\leqslant 3}\langle\Lambda^j q^i,p^k\rangle\langle\Lambda^{m-j}q^k,p^i\rangle. \tag{31}$$

To prove the above Hamiltonian functions are in involution in pairs, $\{F_k,F_m\}=0$, with respect to the Poisson bracket by

$$\{f,g\}=\sum_{i=1}^{3}\sum_{j=1}^{N}\left(\frac{\partial f}{\partial q_j^i}\frac{\partial g}{\partial p_j^i}-\frac{\partial f}{\partial p_j^i}\frac{\partial g}{\partial q_j^i}\right),$$

we consider a bilinear function $\overset{ik}{Q}_\lambda$ on R^N and its partial-fraction expansion and Laurent expansion:

$$\overset{ik}{Q}_\lambda=\langle(\lambda-\Lambda)^{-1}q^i,p^k\rangle=\sum_{j=1}^{N}\frac{q_j^ip_j^k}{\lambda-\lambda_j}=\sum_{m\geqslant -1}\lambda^{-m-2}\langle\Lambda^{m+1}q^i,p^k\rangle.$$

Let

$$\begin{aligned}I_\lambda&=\overset{33}{Q}_\lambda(\Lambda)+\overset{31}{Q}_\lambda+\langle q^1,p^2\rangle\overset{23}{Q}_\lambda-\langle q^3,p^3\rangle\overset{13}{Q}_\lambda,\\ T_\lambda&=\frac{1}{2}\sum_{i=1}^{3}\overset{ii}{Q}_\lambda\overset{ii}{Q}_\lambda+\sum_{1\leqslant i<k\leqslant 3}\overset{ik}{Q}_\lambda\overset{ki}{Q}_\lambda,\end{aligned}\tag{32}$$

where $\overset{ik}{Q}_\lambda(\Lambda^l)=\langle(\lambda-\Lambda)^{-1}\Lambda^lq^i,p^k\rangle$. Noticing the formulas

$$\overset{ik}{Q}_\lambda(\Lambda)=\lambda\overset{ik}{Q}_\lambda-\langle q^i,p^k\rangle,$$

$$\langle(\lambda-\Lambda)^{-1}(\mu-\Lambda)^{-1}q^i,p^k\rangle=(\mu-\lambda)^{-1}(\overset{ik}{Q}_\lambda-\overset{ik}{Q}_\mu),$$

we can verify by a direct calculation that

$$\begin{aligned}\{I_\lambda,I_\mu\}&=(\mu-\lambda)^{-1}(\overset{23}{Q}_\lambda\overset{32}{Q}_\mu-\overset{23}{Q}_\mu\overset{32}{Q}_\lambda+\overset{13}{Q}_\lambda\overset{31}{Q}_\mu-\overset{13}{Q}_\mu\overset{31}{Q}_\lambda),\\ \{I_\lambda,T_\mu\}+\{T_\lambda,I_\mu\}&=(\mu-\lambda)^{-1}(\overset{23}{Q}_\mu\overset{32}{Q}_\lambda-\overset{23}{Q}_\lambda\overset{32}{Q}_\mu+\overset{31}{Q}_\lambda\overset{13}{Q}_\mu-\overset{13}{Q}_\lambda\overset{31}{Q}_\mu),\\ \{T_\lambda,T_\mu\}&=0,\quad\forall\lambda,\mu\in\mathbf{C}.\end{aligned}\tag{33}$$

Using the bilinear property of the Poisson bracket, we have

$$\{\mathscr{F}_\lambda,\mathscr{F}_\mu\}=0,\quad\forall\lambda,\mu\in\mathbf{C},\tag{34}$$

with $\mathscr{F}_\lambda=I_\lambda+T_\lambda$. Substituting the Laurent expansion of $\overset{ik}{Q}_\lambda$ into (32), we obtain

$$\mathscr{F}_\lambda=\sum_{m\geqslant -1}\lambda^{-m-2}F_m,\tag{35}$$

which together with (34) implies $\{F_m,F_l\}=0$ for any l,m. Hence we have immediately the following fact.

Theorem 1: The symplectic map H defined by (24) is completely integrable with the involutive system of conserved integrals $\{F_m\}$.

Theorem 2: Let $(q^1(t),q^2(t),q^3(t),p^1(t),p^2(t),p^3(t))$ be a solution of the initial value problem for the system of ordinary differential equations

$$\begin{aligned}&\frac{\partial}{\partial t}q^i=\frac{\partial F_{-1}}{\partial p^i},\quad\frac{\partial}{\partial t}p^i=-\frac{\partial F_{-1}}{\partial q^i},\quad 1\leqslant i\leqslant 3,\\ &(q^i,p^i)|_{t=0}=(q^i(0),p^i(0)),\end{aligned}\tag{36}$$

and

$$(q^1(n,t),\ldots,q^3(n,t),p^1(n,t),\ldots,p^3(n,t))=H^n(q^1(t),\ldots,q^3(t),p^1(t),\ldots,p^3(t)). \tag{37}$$

Then

$$a(n,t)=\langle q^2(n,t),p^3(n,t)\rangle^{-1}(\langle q^1(n,t),p^1(n,t)\rangle+\langle \Lambda q^1(n,t),p^3(n,t)\rangle-\langle q^1(n,t),p^3(n,t)\rangle^2),$$
$$b(n,t)=\langle q^1(n,t),p^3(n,t)\rangle, c(n,t)=\langle q^2(n,t),p^3(n,t)\rangle \tag{38}$$

solve the system of lattice soliton equations (10).

Proof: Equations (37) and (36) are equivalent to (24) and the system

$$\frac{\partial}{\partial t}q^i(n)=\frac{\partial}{\partial p^i(n)}F_{-1}(q^1(n),\ldots,q^3(n),p^1(n),\ldots,p^3(n)),$$
$$\frac{\partial}{\partial t}p^i(n)=\frac{\partial}{\partial q^i(n)}F_{-1}(q^1(n),\ldots,q^3(n),p^1(n),\ldots,p^3(n)). \tag{39}$$

By using (38), (39), and (21), we obtain

$$\frac{\partial}{\partial t}u(n,t)=J\sum_{j=1}^{N}\nabla\lambda_j=JG_0(n)=X_0(n,t),$$

which is the system (10). The proof is completed.

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New no-scalar-hair theorem for black holes

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A new no-hair theorem is formulated which rules out a very large class of nonminimally coupled finite scalar dressing of an asymptotically flat, static, and spherically symmetric black hole. The proof is very simple and based on a covariant method for generating solutions for nonminimally coupled scalar fields starting from the minimally coupled case. Such a method generalizes the Bekenstein method for conformal coupling and other recent ones. We also discuss the role of the finiteness assumption for the scalar field. © *1996 American Institute of Physics.* [S0022-2488(96)00905-1]

I. INTRODUCTION

Black-hole solutions are very rigid in gravitational physics. We know that the Schwarzschild solution is the only asymptotically flat and spherically symmetric solution of the vacuum Einstein equations. The no-hair conjecture[1] states that the exterior region of a black hole admits only fields for which there is a geometrical Gauss-like law, as electromagnetic fields for example. Early no-hair theorems excluding for the exterior region of a black hole minimally coupled Klein–Gordon,[2] massive vectors,[3] and spinor[4] fields have stressed the conjecture.

The problem of the existence of scalar hairs for black holes has received some attention recently. Although we know that scalar fields are not elementary fields in nature, they commonly arise in effective actions. In fact, some scalar actions have been considered recently in astrophysical contexts (see, for instance Ref. 5). However, with the conformally coupled case as the only exception,[6–8] only minimally coupled scalar fields have been examined. In Ref. 9 a new theorem is presented that rules out a multicomponent scalar hair with nonquadratic Lagrangian, but with minimal coupling to gravity. As it is stressed in Ref. 9, scalar fields effective actions are obtained by integrating the functional integral of the elementary fields in nature over some of the fields, and more complicated actions involving nonminimally coupling should arise.

The purpose of the present work is to point toward the filling of this gap by presenting a theorem that excludes finite scalar hairs of any asymptotically flat, static, and spherically symmetric black hole solution of the system described by the action

$$S[g,\phi]=\int d^4x\sqrt{-g}\{f(\phi)R-h(\phi)g^{\mu\nu}\partial_\mu\phi\partial_\nu\phi\}, \tag{1}$$

with $f(\phi)$ and $h(\phi)>0$. We adopt all the conventions of Ref. 10. Many physically relevant theories belong to the class described by (1). Maybe the most popular nonminimal coupling for the scalars fields corresponds to the choice $f(\phi)=1-\xi\phi^2$ and $h(\phi)=1$. The case $\xi=\frac{1}{6}$ corresponds to the conformal coupling case, and the Bekenstein method[11] allows us to construct its exact solutions from the solutions of the minimally coupled case ($\xi=0$). A method for generating solutions for arbitrary ξ is presented in Ref. 12. The extension of Bekenstein method for n dimensions ($n>3$) was obtained recently in Ref. 6, and used to study conformal scalar hairs[6,7] and gravitational waves.[13] Dilaton-like gravity is given by $f(\phi)=\frac{1}{4}h(\phi)=e^{-2\phi}$. The general model of Bergman, Wagoner, and Nordtved discussed in Ref. 10 corresponds to the choice $f(\phi)=\phi$ and $h(\phi)=\omega(\phi)/\phi$, from which Brans–Dicke theory is obtained from the limit ω constant.

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The paper is organized as follows. In Section II we present a covariant method for generating solutions for the system described by (1). This method will be the central point for the formulation of the theorem, which is presented in the same section. In Section III, we analyze as particular cases the Brans–Dicke theory and one of its generalizations in order to shed light on the role of the finiteness assumption for the scalar field and its relation to naked singularities. The last section is devoted to some concluding remarks, in particular a comparison between our results and recent ones.

II. THE THEOREM

The proof of our theorem centers on a covariant method for generating solutions for the Euler–Lagrange equations of (1) starting from the well-known solutions for the minimally coupled case,

$$\overline{S[g,\phi]}=\int d^4x\sqrt{-\overline{g}}\,\{\overline{R}-\overline{g}^{\mu\nu}\partial_\mu\overline{\phi}\partial_\nu\overline{\phi}\}. \tag{2}$$

The method uses a conformal transformation, and generalizes the Bekenstein one[11] and the one proposed in Ref. 12. Such a method has a long history, and Ref. 14, for instance, presents a good set of references on the subject. A method of this type was also used in Ref. 15 to show that the action given by $\int d^4x\sqrt{-g}\{F(\phi,R)-g^{\mu\nu}\partial_\mu\phi\partial_\nu\phi\}$ is equivalent to an Einstein–Hilbert action plus minimally coupled self-interacting scalar fields, equivalent in the sense that there is a conformal transformation and ϕ-redefinition connecting them.

The Euler–Lagrange equations obtained from (1) are

$$\begin{aligned} f(\phi)R_{\mu\nu}-h(\phi)\partial_\mu\phi\partial_\nu\phi-D_\mu D_\nu f(\phi)-\tfrac{1}{2}g_{\mu\nu}\Box f(\phi)=0,\\ 2h(\phi)\Box\phi+h'(\phi)g^{\alpha\beta}\partial_\alpha\phi\partial_\beta\phi+f'(\phi)R=0, \end{aligned} \tag{3}$$

where the prime denotes derivation with respect to ϕ. Equations (3) are clearly much more complicated than the Euler–Lagrange equations derived from (2), namely

$$\begin{aligned} \overline{R}_{\mu\nu}-\partial_\mu\overline{\phi}\partial_\nu\overline{\phi}=0,\\ \overline{\Box}\ \overline{\phi}=0. \end{aligned} \tag{4}$$

In order to realize how the solutions of (3) and (4) are related, consider the conformal transformation $g_{\mu\nu}=\Omega^2\overline{g}_{\mu\nu}$. Under a conformal transformation, the scalar of curvature transforms as $R(\Omega^2\overline{g}_{\mu\nu})=\Omega^{-2}R-6\Omega^{-3}\overline{\Box}\Omega$, and with the choice

$$f(\phi)=\Omega^{-2}, \tag{5}$$

one gets from (1)

$$S[\Omega^2\overline{g},\phi]=\int d^4x\sqrt{-\overline{g}}\left\{\overline{R}-\left(\frac{3}{2}\left(\frac{d}{d\phi}\ln f(\phi)\right)^2+\frac{h(\phi)}{f(\phi)}\right)\overline{g}^{\mu\nu}\partial_\mu\phi\partial_\nu\phi\right\}. \tag{6}$$

Now, defining $\overline{\phi}(\phi)$ as

$$\overline{\phi}(\phi)=\int_a^\phi d\xi\sqrt{\frac{3}{2}\left(\frac{d}{d\xi}\ln f(\xi)\right)^2+\frac{h(\xi)}{f(\xi)}}, \tag{7}$$

with arbitrary a, we get the desired result, $S[\Omega^2\overline{g},\phi(\overline{\phi})]=\overline{S[\overline{g},\overline{\phi}]}$. Due to the assumption of f and h positive, the right-hand side of (7) is a monotonically increasing function of ϕ, which guarantees the existence of the inverse $\phi(\overline{\phi})$. The constant a is determined by the boundary conditions of ϕ and $\overline{\phi}$. Also, we have that $\lim_{\overline{\phi}\to\infty}\phi(\overline{\phi})=\infty$.

The transformation given by Eqs. (5) and (7), therefore, maps a solution $(g_{\mu\nu},\phi)$ of (3) to a solution $(\overline{g_{\mu\nu}},\phi)$ of (4). The transformation is independent of any assumption of symmetries, and in this sense is covariant. We can easily infer that the transformation is one-to-one in general, in the sense that any solution of (3) is mapped in a unique solution of (4). Also, the transformation preserves symmetries, which means that if $\overline{g_{\mu\nu}}$ admits a Killing vector ξ such that $\pounds_\xi\overline{\phi}=0$, then ξ is also a Killing vector of $g_{\mu\nu}$ and $\pounds_\xi\phi=0$. From this, one concludes if we know all solutions $(\overline{g_{\mu\nu}},\phi)$ with a given symmetry we automatically know all $(g_{\mu\nu},\phi)$ with the same symmetry. This is the base of the proof.

The general asymptotically flat, static, and spherically symmetric solution $(\overline{g_{\mu\nu}},\overline{\phi})$ of (4) is known. (See Ref. 16 for some properties of the solution and references.) It is given by a two-parameter (λ,r_0) family of solutions

$$\overline{\phi}=\sqrt{2(1-\lambda^2)}\ln\mathscr{R},$$

$$ds^2=\overline{g_{\mu\nu}}dx^\mu dx^\nu=-\mathscr{R}^{2\lambda}dt^2+\left(1-\frac{r_0^2}{r^2}\right)^2\mathscr{R}^{-2\lambda}(dr^2+r^2d\Omega^2), \tag{8}$$

where $\mathscr{R}=(r-r_0)/(r+r_0)$. The parameter λ can take values in $[-1,1]$ in principle, but we neglect the negative range because the solution will have a negative ADM mass.[16] For $\lambda=1$, the solution is the usual exterior vacuum Schwarzschild solution with the horizon at $r_0'=4r_0$, as one can check by using the coordinate transformation $r'=r(1+r_0/r)^2$. For $0\leqslant\lambda<1$, (8) does not represent a black hole due to the fact that the surface $r=r_0$ is not a horizon, i.e., a regular null surface, but it is instead a naked singularity, as we can check, for instance, by calculating the scalar of curvature

$$\overline{R}=\frac{8r_0^2r^4}{(r+r_0)^{2(2+\lambda)}}\times\frac{1-\lambda^2}{(r-r_0)^{2(2-\lambda)}}. \tag{9}$$

In total accordance with the original scalar no-hair theorem,[2] we see the only black hole solution of (8) is that one for which $\lambda=1$ and consequently $\phi=0$, i.e., the usual Schwarzschild solution.

Any asymptotically flat, static, and spherically symmetric solution of (3) can be obtained from (8) by means of the transformations (5) and (7). This provides us with a two-parameter family of $(g_{\mu\nu},\phi)$ solutions. The discussed properties of the transformation (7) and the expression for $\phi(r)$ in (8) lead to the conclusion that the only solution with ϕ finite in the surface $r=r_0$ is that one for which ϕ is constant for $r>r_0$. In this case, (5) is only a rigid scale transformation, and the solution $(g_{\mu\nu},\phi=a)$ is the usual Schwarzschild solution. This is the desired result, which we formulate for clearness as follows.

Theorem: The only asymptotically flat, static, and spherically symmetric exterior solution of the system governed by the action

$$S=\int d^4x\sqrt{-g}\{f(\phi)R-h(\phi)g^{\mu\nu}\partial_\mu\phi\partial_\nu\phi\},\quad f(\phi),h(\phi)>0,$$

with ϕ everywhere finite is the Schwarzschild solution.

It is important to note that the used conformal transformation forbids that $f(\phi)\to\infty$ for any $r\neq r_0$.

Our approach can be extended in a straightforward way to other dimensions. The transformations (5) and (7) can be defined for any dimension $n>2$. They shall be replaced by

$$f=\Omega^{2-n},$$
$$\overline{\phi}(\phi)=\int_a^{\phi} d\xi \sqrt{\frac{n-1}{n-2}\left(\frac{d}{d\xi}\ln f(\xi)\right)^2+\frac{h(\xi)}{f(\xi)}}. \tag{10}$$

The general asymptotically flat, static, and spherically symmetric solution for any space–time dimension $n>3$ of (4) is known.[16] Its expression in isotropic coordinates is given by

$$\overline{\phi}=\sqrt{\frac{n-2}{n-3}(1-\lambda^2)}\ln \mathscr{R}_n,$$
$$ds^2=\overline{g}_{\mu\nu}dx^\mu dx^\nu=-\mathscr{R}_n^{2\lambda}dt^2+\left(1-\frac{r_0^{2n-6}}{r^{2n-6}}\right)^{2/(n-3)}\mathscr{R}_n^{-2\lambda/(n-3)}(dr^2+r^2d\Omega^2), \tag{11}$$

where $\mathscr{R}_n=(r^{n-3}-r_0^{n-3})/(r^{n-3}+r_0^{n-3})$ and $d\Omega$ denotes the metric of the unitary $(n-2)$ sphere. The behavior of the solution (11) is similar to the four-dimensional case. The only true black hole solution is the usual one ($\lambda=1$), due to the fact that the hypersurface $r=r_0$ is not a regular one if $\lambda \neq 1$, as one can see from the expression for the scalar of curvature

$$\overline{R}=\frac{4(n-2)(n-3)r_0^{2(n-3)}r^{2(n-4)}}{(r^{n-3}+r_0^{n-3})^{2(n-2+\lambda)/(n-3)}}\times\frac{1-\lambda^2}{(r^{n-3}-r_0^{n-3})^{2(n-2-\lambda)/(n-3)}}. \tag{12}$$

By applying (10) and the same arguments used in the four-dimensional case we can extend our theorem for any space–time dimension $n>3$.

III. AN EXPLICIT EXAMPLE

A closer look at an explicit example will help us to understand the role of the assumption of finiteness of the scalar field. We see from (8) and (9) that for the minimal coupling, the finiteness of $\overline{\phi}$ is related to the regularity of the horizon. The scalar field diverges in the surface $r=r_0$ for $\lambda \neq 1$; in this case the scalar of curvature has a nonremovable singularity, which confirms that such surface is not a regular one, but it corresponds to a naked singularity. We will see that this is the case for some non-minimal couplings also. To this end, let us consider the Brans–Dicke theory, for which $f(\phi)=\phi$ and $h(\phi)=\omega/\phi$. Using the transformations (5) and (7) we can construct its general asymptotically flat, static, and spherical symmetric solution starting from the minimally coupled solution $(\overline{g}_{\mu\nu},\overline{\phi})$,

$$g_{\mu\nu}=\phi^{-1}\overline{g}_{\mu\nu} \qquad \overline{\phi}=\sqrt{\frac{3}{2}+\omega}\int_a^{\phi}\frac{d\xi}{|\xi|}. \tag{13}$$

The expression for $\overline{\phi}$ is divergent for $a=0$. Also, if we choose $a>0$, then ϕ must be positive too to avoid the singularity. Let us take the solution $(\overline{g}_{\mu\nu},-\overline{\phi})$ of (4), and consider $\phi \in [a,\infty)$, $a>0$. In this case we have

$$\left(\frac{\phi}{a}\right)^{\sqrt{3/2+\omega}}=\left(\frac{r+r_0}{r-r_0}\right)^{\sqrt{2(1-\lambda^2)}}. \tag{14}$$

The expression (14) hides a subtleness in the limit of large ω, maybe the most important limit in Brans–Dicke theory; recent solar system experiments have established $\omega > 600$.[10] In the limit $\omega \to \infty$, the left-hand side of (14) can be 1 or ∞, according to if $\phi = a$ or $\phi > a$. Due to the fact that the right-hand side is bounded for any λ and for $r > r_0$, the consistency of the equation implies that λ must be 1 and $\phi = a$ in the limit $\omega \to \infty$. This would guarantee that one gets the General Relativity in the limit $\omega \to \infty$. Taking this into account we have from (13)

$$\begin{aligned} \phi &= a.\mathscr{R}^{-k}, \\ ads^2 &= -\mathscr{R}^{2\lambda+k}dt^2 + \left(1 - \frac{r_0^2}{r^2}\right)^2 \mathscr{R}^{-2\lambda+k}(dr^2 + r^2 d\Omega^2), \end{aligned} \tag{15}$$

where $k = \sqrt{4(1-\lambda^2)/(3+2\omega)}$. The two-parameter (λ, r_0) family of solutions (15) corresponds to the general asymptotically flat, static, and spherically symmetrical solution of the Brans–Dicke theory.

Our theorem states that the only black hole solution of (15) with finite ϕ is the Schwarzschild one, but, at first sight, we can think that the null-surface $r = r_0$ might be a horizon for some λ or ω. We can check that such a surface is not a regular null-surface, but instead it is a naked singularity for any solution with nonconstant ϕ. To this end, consider the scalar of curvature obtained from (3),

$$R = \frac{\omega}{\phi^2} g^{\mu\nu} \partial_\mu \phi \partial_\nu \phi = \frac{4 r_0^2 r^4}{(r+r_0)^{4+2\lambda-k}} \times \frac{\omega k^2}{(r-r_0)^{4-2\lambda+k}}. \tag{16}$$

One has that $4 - 2\lambda + k > 0$ for $\lambda \in [0,1]$ and for $\omega \in [0,\infty)$, and thus (15) has a nonremovable singularity for any $\lambda \neq 1$ and $\omega \neq 0$. We see that the only true black hole solution is that one for which $\lambda = 1$, i.e., again the Schwarzschild solution with $\phi = a$, as it was predicted by the theorem. The case $\omega = 0$ can be ruled out by analyzing the singularities of quadratic invariants, as for example $R_{\mu\nu}R^{\mu\nu}$, that can be written through (3) by means of ϕ. We notice that the first no-hair theorem for Brans–Dicke theory is due to Hawking,[17] and that Bekenstein also proved recently the absence of scalar hairs in Brans–Dicke theory by using his novel no-hair theorem for minimally coupled scalar fields with non-quadratic Lagrangian.[9]

We can extend this result for theories such that $\omega(\phi)$ is a C^1 function and $\lim_{\phi\to\infty}\omega(\phi) = \omega_c$. For such a case, we can evaluate an asymptotic expression for the scalar of curvature valid for the vicinity of the horizon, and it will lead us to the conclusion that the only black hole solution also for this case is the Schwarzschild one. From (7) one can see that for $\lim_{\phi\to\infty}\omega(\phi) = \omega_c$ and $r \to r_0$ we have

$$\phi(r) \approx a.\mathscr{R}^{-\sqrt{4(1-\lambda^2)/(3-2\omega_c)}}. \tag{17}$$

From (17) we have that the expression for R valid for $r \to r_0$ is the same one of (16), from which we conclude that there is no scalar hair in the model of Bergman, Wagoner, and Nordtved with $\lim_{\phi\to\infty}\omega(\phi) = \omega_c$. The result is valid for any space–time dimension $n > 3$.

We can easily apply analogous arguments to prove the absence of scalar hair in dilaton gravity for any space-time dimension $n > 3$.

IV. FINAL REMARKS

In spite of the theorem's broad assumptions, there are situations that it does not cover. In situations where the divergence of the scalar field is not related to a naked singularity it is possible, in principle, for a scalar hair to exist. This is the case of the Bekenstein conformal scalar hair,[11] which obviously escapes from the theorem's assumptions due to the divergence of the scalar field

in the horizon. Such divergence is not related to any space–time singularity, and for an observer that does not interact directly with the scalar field the divergence is physically harmless.

A recent result due to Zannias[8] also stresses the relevant role of the divergence of the scalar field in the existence of hairs. In our approach, the finiteness of ϕ guarantees that the only null-surface of $g_{\mu\nu}$ corresponds to $r=r_0$. If ϕ diverges for some point of the space–time, say r_1, the conformal factor $\Omega(r_1)$ in (5) vanishes and consequently $g_{00}(r_1)=0$, which would induce another null-surface for $r=r_1$. This is precisely what happens with the Bekenstein conformal hair. However, in principle one can find out case by case asymptotic expressions for the geometrical quantities, as we did in Sec. III, and to control the regions very close to the horizons.

We finish noting that two recent works are devoted to problems similar to the ones discussed here. In Ref. 18 Heusler studies with great detail the case of self-gravitating nonlinear sigma models, for which the action would be given in our notation by

$$S[g,\phi^i]=\int d^4x\sqrt{-g}\{R-h_{jk}(\phi^i)g^{\mu\nu}\partial_\mu\phi^j\partial_\nu\phi^k+W(\phi^i)\}, \tag{18}$$

where $i\in(1,\ldots,N)$. He proved that the only asymptotically flat, static, and spherically symmetric black-hole solution of (18) is the Schwarzschild one. Sudarsky[19] considered the case where $h_{jk}(\phi^i)=\delta_{jk}$, getting the same result in a simpler way. These results are in agreement with our theorem since the case $N=1$ and $W(\phi)=0$ corresponds to our $f=1$ case. However, we believe that our proof is much more simple.

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Projective group representations in quaternionic Hilbert space

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We extend the discussion of projective group representations in quaternionic Hilbert space that was given in our recent book. The associativity condition for quaternionic projective representations is formulated in terms of unitary operators and then analyzed in terms of their generator structure. The multi-centrality and centrality assumptions are also analyzed in generator terms, and implications of this analysis are discussed. © *1996 American Institute of Physics.*
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I. ASSOCIATIVITY CONDITION FOR QUATERNIONIC PROJECTIVE GROUP REPRESENTATIONS

In quaternionic quantum mechanics, all symmetries of the transition probabilities are generated by unitary transformations acting on the states of Hilbert space.[1–3] In the simplest case, the unitary transformations $U_a, U_b, \ldots$ form a representation (or vector representation) of the symmetry group with elements $a, b, \ldots$,

$$U_b U_a = U_{ba}. \tag{1}$$

A more general possibility is that the group multiplication table is represented over the *rays* corresponding to a complete set of physical states, but not over individual state vectors chosen as ray representatives. This more general composition rule defines a quaternionic *projective representation* (or ray representation), and takes the form (Ref. 4, Sec. 4.3)

$$U_b U_a |f\rangle = U_{ba} |f\rangle \omega(f;b,a), \quad |\omega(f;b,a)| = 1, \tag{2}$$

for one particular complete set of states $|f\rangle$ and a set of quaternionic phases $\omega(f;b,a)$. When we change ray representative from $|f\rangle$ to $|f_\phi\rangle \equiv |f\rangle\phi$, with $|\phi| = 1$, the phase defining the projective representation is easily seen to transform as

$$\omega(f_\phi;b,a) = \overline{\phi}\omega(f;b,a)\phi, \tag{3}$$

with the bar denoting quaternion conjugation. Equation (3) shows clearly that the projective phase ω must depend on the state label f as well as on the group elements a, b; failure to take this into account can lead[4] to erroneous conclusions (as in Ref. 5) concerning quaternionic projective representations.

The defining relation for quaternionic projective representations given in Eq. (2) can be rewritten in operator form by defining a left-acting operator $\Omega(b,a)$,

$$\Omega(b,a) = \sum_f |f\rangle \omega(f;b,a) \langle f|, \tag{4a}$$

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which, using Eq. (3), is seen to be independent of the ray representative chosen for the states $|f\rangle$. Multiplying Eq. (2) from the right by $\langle f|$ and summing over the complete set of states $|f\rangle$, we obtain the operator form of the projective representation,

$$U_b U_a = U_{ba}\Omega(b,a). \tag{4b}$$

It is also immediate from the definition of Eq. (4a), and the fact that $|\omega|=1$, that the operator $\Omega(b,a)$ is quaternion unitary,

$$\Omega(b,a)^\dagger \Omega(b,a) = \Omega(b,a)\Omega(b,a)^\dagger = 1. \tag{5}$$

Note that if we were to make the definition of a quaternionic projective representation more restrictive by requiring that Eq. (2) hold for *all* states in Hilbert space, rather than for one particular complete set of states, then we would require $\Omega(b,a)=1$, since the unit operator is the only unitary operator which is simultaneously diagonal on all complete bases in quaternionic Hilbert space. Hence this more restrictive definition excludes quaternionic embeddings of complex projective representations, whereas these are admitted as quaternionic projective representations by the definition of Eq. (2).

A nontrivial condition on the projective representation structure is obtained from the associativity of multiplication in quaternionic Hilbert space, which implies

$$(U_c U_b)U_a = U_c(U_b U_a). \tag{6}$$

Applying Eq. (4b) twice to the left-hand side of Eq. (6), we obtain

$$(U_c U_b)U_a = U_{cb}\Omega(c,b)U_a = U_{cb}U_a U_a^{-1}\Omega(c,b)U_a = U_{cba}\Omega(cb,a)U_a^{-1}\Omega(c,b)U_a, \tag{7a}$$

while applying Eq. (4b) twice to the right-hand side of Eq. (6) gives

$$U_c(U_b U_a) = U_c U_{ba}\Omega(b,a) = U_{cba}\Omega(c,ba)\Omega(b,a). \tag{7b}$$

Upon multiplying from the left by U_{cba}^{-1}, Eqs. (7a) and (7b) give the operator form of the *associativity condition*:

$$\Omega(c,ba)\Omega(b,a) = \Omega(cb,a)U_a^{-1}\Omega(c,b)U_a. \tag{8}$$

We can also express the associativity condition as a condition on the quaternionic phase $\omega(f;b,a)$ introduced in Eq. (2), by applying the spectral representation of Eq. (4a) to the operator form of the associativity condition given in Eq. (8). From Eq. (4a) we obtain

$$\Omega(c,ba) = \sum_f |f\rangle\omega(f;c,ba)\langle f|, \tag{9a}$$

which when multiplied from the right by Eq. (4a) gives

$$\Omega(c,ba)\Omega(b,a) = \sum_f |f\rangle\omega(f;c,ba)\omega(f;b,a)\langle f|. \tag{9b}$$

Equation (4a) and the unitarity of $\Omega(cb,a)$ also imply that

$$\Omega(cb,a)^{-1} = \sum_f |f\rangle\overline{\omega(f;cb,a)}\langle f|, \tag{9c}$$

and so the associativity condition of Eq. (8) can be rewritten as

$$U_a^{-1}\Omega(c,b)U_a=\Omega(cb,a)^{-1}\Omega(c,ba)\Omega(b,a)=\sum_f |f\rangle\overline{\omega(f;cb,a)}\omega(f;c,ba)\omega(f;b,a)\langle f|. \tag{10}$$

Hence $U_a^{-1}\Omega(c,b)U_a$ is diagonal in the basis spanned by the states $|f\rangle$. Taking matrix elements of Eq. (10), and using the unitarity of U_a, the associativity condition gives the two relations

$$\overline{\omega(f;cb,a)}\omega(f;c,ba)\omega(f;b,a)=\sum_{f''} \overline{\langle f''|U_a|f\rangle}\omega(f'';c,b)\langle f''|U_a|f\rangle, \tag{11}$$

and, when $\langle f'|f\rangle=0$,

$$0=\sum_{f''} \overline{\langle f''|U_a|f\rangle}\omega(f'';c,b)\langle f''|U_a|f'\rangle. \tag{12}$$

We conclude this section by comparing the quaternionic Hilbert space form of the associativity condition with the simpler form which is familiar from complex Hilbert space.[6,7] In a complex Hilbert space, the phase $\omega(f;b,a)$ introduced in Eq. (2) is a complex number, and commutes with the phase ϕ, also now complex, which we introduced in Eq. (3) to describe a change of ray representative. Hence Eq. (3) implies, in the complex case, that $\omega(f;b,a)$ is independent of the ray representative chosen for the state $|f\rangle$, and it is then consistent to assume that $\omega(f;b,a)$ is independent of the state label f, so that

$$\omega(f;b,a)=\omega(b,a) \quad \text{complex Hilbert space.} \tag{13a}$$

Substituting Eq. (13a) into Eq. (4a), we now obtain

$$\Omega(b,a)=\sum_f |f\rangle\omega(b,a)\langle f|=\omega(b,a)\sum_f |f\rangle\langle f|=\omega(b,a)1, \tag{13b}$$

where 1 denotes the unit operator in complex Hilbert space. Since the complex phase $\omega(b,a)$ is a c-number in complex Hilbert space, on substituting Eq. (13b) into Eq. (4b) we learn that

$$U_bU_a=U_{ba}\omega(b,a)=\omega(b,a)U_{ba}, \tag{14a}$$

which is the standard definition of a projective representation in complex Hilbert space. Moreover, since Eq. (13b) implies that $\Omega(b,a)$ commutes with the unitary operator U_a, the associativity condition of Eqs. (8) and (11) reduces to the familiar complex Hilbert space form

$$\omega(c,ba)\omega(b,a)=\omega(cb,a)\omega(c,b). \tag{14b}$$

II. THE ASSOCIATIVITY CONDITION IN GENERATOR FORM

Let us now assume that the symmetry group with which we are dealing is a Lie group, so that in the neighborhood of the identity e the unitary transformations $U_a, U_b, U_{ba}, \ldots$ can be written in terms of a set of anti-self-adjoint generators $\tilde{G}_A$ as

$$U_a=\exp\left(\sum_A \theta_A^a\tilde{G}_A\right), \quad U_b=\exp\left(\sum_A \theta_A^b\tilde{G}_A\right), \quad U_{ba}=\exp\left(\sum_A \theta_A^{ba}\tilde{G}_A\right),\ldots, \tag{15a}$$

with $\theta_A^e=0$ and $U_e=1$. Then Eq. (4b) implies that $\Omega(b,a)$ must be unity when either a or b is the identity, and thus the generator form for this operator is

$$\Omega(b,a)=\exp\left(\frac{1}{2}\sum_{BA}\left[\theta_B^b\theta_A^a\widetilde{I}_{BA}+\sum_C\ \theta_B^b\theta_C^b\theta_A^a\widetilde{J}^{(1)}_{(BC)A}+\sum_C\ \theta_B^b\theta_A^a\theta_C^a\widetilde{J}^{(2)}_{B(AC)}+O(\theta^4)\right]\right), \quad (15b)$$

where the parentheses ( ) around a set of indices indicate that the tensor in question is symmetric in those indices, and where we use the tilde to indicate operators which are anti-self-adjoint. The parameters θ_C^{ba} must be functions of the parameters θ_A^a and θ_B^b,

$$\theta_C^{ba}=\psi_C^{ba}(\{\theta_B^b\},\{\theta_A^a\})=\theta_C^b+\theta_C^a+\frac{1}{2}\sum_{BA}\ C_{BAC}\theta_B^b\theta_A^a+O(\theta^3), \quad (15c)$$

where in making the Taylor expansion we have used the fact that $U_{be}=U_b$ and $U_{ea}=U_a$, which fixes the linear terms in the expansion and requires the quadratic term to be bilinear.

We proceed now to derive a number of relations by combining the generator expansions of Eqs. (15a)–(15c) with the formulas of Sec. I. We begin by substituting Eqs. (15a)–(15c) into Eq. (4b) using the Baker–Campbell–Hausdorff formula,

$$\exp X\ \exp Y=\exp(X+Y+\tfrac{1}{2}[X,\ Y]+\cdots), \quad (16a)$$

to combine exponents arising from the factors on the left and right. From the left-hand side of Eq. (4b) we obtain,

$$U_bU_a=\exp\left(\sum_B\ \theta_B^b\widetilde{G}_B+\sum_A\ \theta_A^a\widetilde{G}_A+\frac{1}{2}\sum_{BA}\ \theta_B^b\theta_A^a[\widetilde{G}_B,\ \widetilde{G}_A]+O(\theta^3)\right), \quad (16b)$$

while from the right-hand side of Eq. (4b) we obtain

$$U_{ba}\Omega(b,a)=\exp\left(\sum_C\ (\theta_C^b+\theta_C^a)\widetilde{G}_C+\frac{1}{2}\sum_{CBA}\ C_{BAC}\theta_B^b\theta_A^a\widetilde{G}_C+\frac{1}{2}\sum_{BA}\ \theta_B^b\theta_A^a\widetilde{I}_{BA}+O(\theta^3)\right). \quad (16c)$$

Equating Eqs. (16b) and (16c) thus gives the relations

$$[\widetilde{G}_B,\ \widetilde{G}_A]=\sum_C\ C_{[BA]C}\widetilde{G}_C+\widetilde{I}_{[BA]} \quad (17a)$$

and

$$0=\sum_C\ C_{(BA)C}\widetilde{G}_C+\widetilde{I}_{(BA)}, \quad (17b)$$

where the square brackets [ ] around a set of indices indicates that the tensor in question is antisymmetric in these indices. We shall restrict ourselves henceforth to the case in which $C_{(BA)C}=0$, which by Eq. (17b) implies that $\widetilde{I}_{(BA)}=0$; making this assumption then implies that $C_{BAC}=C_{[BA]C}$ and $\widetilde{I}_{BA}=\widetilde{I}_{[BA]}$. In other words, we are assuming that the structure constants C_{BAC} for a projective representation have the same antisymmetric form as holds for a vector representation. Changing the summation index C to D in Eq. (17a), and then taking the commutator of Eq. (17a) with $\widetilde{G}_C$, we find

$$[\widetilde{G}_C,[\widetilde{G}_B,\ \widetilde{G}_A]]=\sum_D\ C_{[BA]D}[\widetilde{G}_C,\ \widetilde{G}_D]+[\widetilde{G}_C,\ \widetilde{I}_{[BA]}]; \quad (18a)$$

adding to this identity the two related identities obtained by cyclically permuting A,B,C, using the fact that the left-hand side of the sum vanishes by the Jacobi identity for the commutator, and substituting Eq. (17a) for the commutators appearing on the right-hand side of the sum, we obtain the identity

$$\sum_{DE}\ (C_{[BA]D}C_{[CD]E}+C_{[CB]D}C_{[AD]E}+C_{[AC]D}C_{[BD]E})\widetilde{G}_E$$
$$+\sum_{D}\ (C_{[BA]D}\widetilde{I}_{[CD]}+C_{[CB]D}\widetilde{I}_{[AD]}+C_{[AC]D}\widetilde{I}_{[BD]})$$
$$+[\widetilde{G}_C\,,\,\widetilde{I}_{[BA]}]+[\widetilde{G}_A\,,\,\widetilde{I}_{[CB]}]+[\widetilde{G}_B\,,\,\widetilde{I}_{[AC]}]=0. \tag{18b}$$

We next substitute Eqs. (15a)–(15c) into the associativity condition of Eq. (8), now keeping cubic terms in the exponent of the form $\theta_A^a\theta_B^b\theta_C^c$, but dropping cubic terms, such as $\theta_A^a\theta_B^a\theta_C^c$, that do not contain all three of the upper indices a,b,c. For the first factor on the left-hand side of Eq. (8), we find from Eqs. (15b) and (15c) that

$$\Omega(c,ba)=\exp\left(\frac{1}{2}\sum_{BA}\ \left(\ \theta_B^c\theta_A^{ba}\widetilde{I}_{[BA]}+\sum_{C}\ \theta_B^c\theta_A^{ba}\theta_C^{ba}\widetilde{J}^{(2)}_{B(AC)}\right)\right)$$
$$=\exp\left(\frac{1}{2}\sum_{BA}\ \left[\ \theta_B^c\left(\ \theta_A^b+\theta_A^a+\frac{1}{2}\sum_{DE}\ C_{[DE]A}\theta_D^b\theta_E^a\right)\widetilde{I}_{[BA]}\right.\right.$$
$$\left.\left.+2\sum_{C}\ \theta_B^c\theta_A^b\theta_C^a\widetilde{J}^{(2)}_{B(AC)}\right]\right), \tag{19a}$$

while for the second factor on the left-hand side of Eq. (8) we have

$$\Omega(b,a)=\exp\left(\frac{1}{2}\sum_{BA}\ \theta_B^b\theta_A^a\widetilde{I}_{[BA]}\right). \tag{19b}$$

Since the exponents in Eqs. (19a) and (19b) both begin at order θ^2, through order θ^3 we can simply add exponents to get the product on the left-hand side of Eq. (8). Proceeding similarly for the first factor on the right-hand side of Eq. (8), we obtain

$$\Omega(cb,a)=\exp\left(\frac{1}{2}\sum_{BA}\ \left(\ \theta_B^{cb}\theta_A^a\widetilde{I}_{[BA]}+\sum_{C}\ \theta_B^{cb}\theta_C^{cb}\theta_A^a\widetilde{J}^{(1)}_{(BC)A}\right)\right)$$
$$=\exp\left(\frac{1}{2}\sum_{BA}\ \left[\left(\ \theta_B^c+\theta_B^b+\frac{1}{2}\sum_{DE}\ C_{[DE]B}\theta_D^c\theta_E^b\right)\theta_A^a\widetilde{I}_{[BA]}\right.\right.$$
$$\left.\left.+2\sum_{C}\ \theta_B^c\theta_C^b\theta_A^a\widetilde{J}^{(1)}_{(BC)A}\right]\right), \tag{20a}$$

while for the second factor on the right-hand side of Eq. (8), use of the Baker–Campbell–Hausdorff formula gives

$$U_a^{-1}\Omega(c,b)U_a=\exp\left(-\sum_{A}\ \theta_A^a\widetilde{G}_A\right)\exp\left(\frac{1}{2}\sum_{CB}\ \theta_C^c\theta_B^b\widetilde{I}_{[CB]}\right)\exp\left(\sum_{A}\ \theta_A^a\widetilde{G}_A\right)$$

$$=\exp\left(\frac{1}{2}\sum_{CB}\ \theta_C^c\theta_B^b\widetilde{I}_{[CB]}-\frac{1}{2}\sum_{A}\ \sum_{CB}\ \theta_A^a\theta_C^c\theta_B^b[\widetilde{G}_A\,,\ \widetilde{I}_{[CB]}]\right). \tag{20b}$$

Since the exponents in Eqs. (20a) and (20b) begin at order θ^2, it again suffices to simply add the exponents to form the product appearing on the right-hand side of Eq. (8). Thus, to the requisite order, the content of Eq. (8) is obtained by equating the sum of the exponents in Eqs. (19a) and (19b) to the corresponding sum of exponents in Eqs. (20a) and (20b). The quadratic terms in θ are immediately seen to be identical on left and right, while the cubic term proportional to $\theta_A^a\theta_B^b\theta_C^c$ gives (after some relabeling of dummy summation indices) the nontrivial identity

$$\widetilde{J}^{(2)}_{C(BA)}+\frac{1}{4}\sum_{D}\ C_{[BA]D}\widetilde{I}_{[CD]}=\widetilde{J}^{(1)}_{(CB)A}+\frac{1}{4}\sum_{D}\ C_{[CB]D}\widetilde{I}_{[DA]}-\frac{1}{2}\,[\widetilde{G}_A\,,\ \widetilde{I}_{[CB]}]. \tag{21}$$

On totally antisymmetrizing with respect to the indices A,B,C, the terms in Eq. (21) involving $\widetilde{J}^{(1,2)}$ drop out, and we are left with the identity

$$\sum_{D}\ (C_{[BA]D}\widetilde{I}_{[CD]}+C_{[CB]D}\widetilde{I}_{[AD]}+C_{[AC]D}\widetilde{I}_{[BD]})+[\widetilde{G}_C\,,\ \widetilde{I}_{[BA]}]+[\widetilde{G}_A\,,\widetilde{I}_{[CB]}]+[\widetilde{G}_B\,,\widetilde{I}_{[AC]}]=0. \tag{22a}$$

In other words, associativity implies that the sum of the second and third lines of Eq. (18b) vanishes separately; hence the first line of Eq. (18b) must also vanish, and since the generators $\widetilde{G}_E$ are linearly independent this gives the Jacobi identity for the structure constants,

$$\sum_{DE}\ (C_{[BA]D}C_{[CD]E}+C_{[CB]D}C_{[AD]E}+C_{[AC]D}C_{[BD]E})=0. \tag{22b}$$

In the complex case, in which $\Omega(a,b)=\omega(a,b)1$ is a c-number, the tensor $\widetilde{I}_{[AB]}$ is a c-number ''central charge'' and the commutator terms in Eqs. (18b) and (22a) vanish identically. Therefore, in the complex case, Eq. (18b) implies both Eq. (22b) and the identity

$$\sum_{D}\ (C_{[BA]D}\widetilde{I}_{[CD]}+C_{[CB]D}\widetilde{I}_{[AD]}+C_{[AC]D}\widetilde{I}_{[BD]})=0\quad\text{complex case,} \tag{23}$$

and so one obtains the entire content of the associativity condition from the simpler analysis leading to Eq. (18b), without having to perform the third-order expansion needed to obtain Eq. (22a).

III. GENERAL, MULTI-CENTRAL, AND CENTRAL QUATERNIONIC PROJECTIVE REPRESENTATIONS

The analysis of Sec. II applies to the general case (apart from the restriction $C_{(BA)C}=0$) of a quaternionic projective representation; in order to obtain more detailed results it is necessary to introduce further structural assumptions. In Ref. 4 two special classes of quaternionic projective representations are defined. A quaternionic projective representation is defined to be *multi-central* if

$$[\Omega(b,a),\ U_a]=[\Omega(b,a),\ U_b]=0,\quad\text{all}\ \ a,b, \tag{24a}$$

while it is defined to be *central* if

$$[\Omega(b,a),\ U_c]=0,\quad\text{all}\ \ a,b,c. \tag{24b}$$

Expressed in terms of the generators introduced in Eqs. (15a)–(15b), the multi-centrality condition takes the form

$$\sum_{ABC} \theta_A^a \theta_B^b \theta_C^a [\tilde{G}_C, \tilde{I}_{[BA]}] = \sum_{ABC} \theta_A^a \theta_B^b \theta_C^b [\tilde{G}_C, \tilde{I}_{[BA]}] = 0, \quad \text{all } a,b, \tag{25a}$$

while the centrality condition becomes

$$\sum_{ABC} \theta_A^a \theta_B^b \theta_C^c [\tilde{G}_C, \tilde{I}_{[BA]}] = 0, \quad \text{all } a,b,c. \tag{25b}$$

Making the definition

$$\Delta_{[AB]C} = [\tilde{G}_C, \tilde{I}_{[BA]}], \tag{25c}$$

we see from Eq. (25a) that multi-centrality requires that $\Delta_{[AB]C}$ be antisymmetric in A,C and in B,C as well as in A,B; thus in the multi-central case Δ is totally antisymmetric, which we will indicate by writing it as $\Delta_{[ABC]}$. From Eq. (25b), we see that centrality requires that $\Delta_{[AB]C}$ must vanish.

Using the generator formulation, we proceed now to discuss successively the general, multi-central, and central cases in the light of the associativity analysis of Sec. II.

(1) *The general case.* An example given in Eqs. (13.54g) and (14.23a) of Ref. 4 shows that one can have a quaternionic projective representation which is neither central nor multi-central. The example is constructed from n independent fermion creation and annihilation operators $b_\ell^\dagger$, b_ℓ, $\ell = 1,\ldots,n$, which commute with a left algebra quaternion basis $E_0 = 1, E_1 = I, E_2 = J, E_3 = K$. Consider the set of three generators $\tilde{G}_A$ defined by

$$\tilde{G}_A = -\tfrac{1}{2} E_A N, \quad A = 1,2,3, \tag{26a}$$

with N the number operator

$$N = \sum_{\ell=1}^{n} b_\ell^\dagger b_\ell. \tag{26b}$$

The commutator algebra of these generators has the form of a projective representation of SU(2),

$$\begin{aligned} [\tilde{G}_B, \tilde{G}_A] &= -\sum_{C=1}^{3} \epsilon_{[BAC]} \tilde{G}_C + \tilde{I}_{[BA]}, \\ \tilde{I}_{[BA]} &= \sum_{C=1}^{3} \epsilon_{[BAC]} \frac{1}{2} E_C N(N-1), \end{aligned} \tag{26c}$$

with ϵ the usual three-index antisymmetric tensor. A simple calculation now shows that

$$[\tilde{G}_A, \tilde{I}_{[BC]}] = -N(N-1)(\delta_{AB}\tilde{G}_C - \delta_{AC}\tilde{G}_B), \tag{27a}$$

which is not antisymmetric in either the index pair A,C or the pair A,B, and so the multi-centrality condition is not satisfied. Another simple calculation shows that

$$\sum_D (\epsilon_{[BAD]}\tilde{I}_{[CD]} + \epsilon_{[CBD]}\tilde{I}_{[AD]} + \epsilon_{[ACD]}\tilde{I}_{[BD]}) = 0, \tag{27b}$$

by virtue of the Jacobi identity for the structure constant ϵ, and also

$$[\tilde{G}_C,\tilde{I}_{[BA]}]+[\tilde{G}_A,\tilde{I}_{[CB]}]+[\tilde{G}_B,\tilde{I}_{[AC]}]=0. \tag{27c}$$

Hence the associativity condition of Eq. (22a) is satisfied, with the first and second lines each vanishing separately.

(2) *The multi-central case*. Let us now consider the multi-central case, in which $\Delta_{[AB]C}$ defined in Eq. (25c) is totally antisymmetric in A,B,C, as indicated by the notation $\Delta_{[ABC]}$. The associativity condition of Eq. (22a) then simplifies to

$$\sum_D (C_{[BA]D}\tilde{I}_{[CD]}+C_{[CB]D}\tilde{I}_{[AD]}+C_{[AC]D}\tilde{I}_{[BD]})+3\Delta_{[ABC]}=0. \tag{28a}$$

A further equation involving Δ is obtained from the Jacobi identity

$$[\tilde{G}_D,[\tilde{G}_C,\tilde{I}_{[BA]}]]-[\tilde{G}_C,[\tilde{G}_D,\tilde{I}_{[BA]}]]=[\tilde{I}_{[BA]},[\tilde{G}_C,\tilde{G}_D]], \tag{28b}$$

which on substituting Eqs. (17a) and (25c) becomes

$$[\tilde{G}_D,\Delta_{[AB]C}]-[\tilde{G}_C,\Delta_{[AB]D}]=-\sum_E C_{[CD]E}\Delta_{[AB]E}+[\tilde{I}_{[BA]},\tilde{I}_{[CD]}], \tag{28c}$$

an equation which holds even in the general case in which Δ is not totally antisymmetric. Specializing Eq. (28c) to the multi-central case and contracting it with $\delta_{AC}\delta_{BD}$, the left-hand side vanishes because of the antisymmetry of Δ, while the commutator term on the right-hand side becomes $\Sigma_{AB}[\tilde{I}_{[BA]},\tilde{I}_{[AB]}]=0$, leaving the identity (after relabeling the dummy index E as C)

$$\sum_{ABC} C_{[AB]C}\Delta_{[ABC]}=0. \tag{29}$$

Thus in order for a multi-central projective representation to exist which has $\Delta\neq 0$ and so is not also central, there must be a three-index antisymmetric tensor $\Delta_{[ABC]}$ which vanishes when all three indices are contracted with the structure constant $C_{[AB]C}$. This condition is not easy to satisfy and so we pose the question, which we have not been able to answer: Can one construct an example of a multi-central quaternionic projective representation which is not central, or can one prove (in general, or with a restriction, e.g., to simple or semi-simple groups) that a multi-central quaternionic projective representation must always be central? The application of multi-centrality in Ref. 4 sheds no light on this issue; multi-centrality was used there (e.g., in Sec. 12.3) to show that quaternionic Poincaré group projective representations outside the zero energy sector can always be transformed to complex Poincaré group projective representations, which in the sector continuously connected to the identity are known[8] to be transformable to vector representations.

(3) *The central case*. Let us finally consider the central case in which $\Delta=0$, which by Eqs. (25c) and (28c) implies that $\tilde{I}_{[BA]}$ commutes with both $\tilde{G}_C$ and $\tilde{I}_{[CD]}$ for arbitrary values of the indices. Thus $\tilde{I}_{[BA]}$ behaves as a central charge, justifying the name ''central'' for this case. The various results obtained in Bargmann[6] can be immediately generalized to the quaternionic central case; for example, the analysis of Ref. 6 can be easily extended to show that the central charges associated with a quaternionic central projective representation of a semi-simple Lie group can always be removed by redefinition of the generators; and again, the nontrivial illustration[6] of a complex projective representation, constructed in terms of the phase space translation generators in nonrelativistic quantum mechanics, can be embedded[4] in quaternionic quantum mechanics as a central projective representation.

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Derivation of conservation laws from nonlocal symmetries of differential equations

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An identity is derived which yields a correspondence between symmetries and conservation laws for self-adjoint differential equations. This identity does not rely on use of a Lagrangian as needed to obtain conservation laws by Noether's theorem. Moreover, unlike Noether's theorem, which can only generate conservation laws from local symmetries, the derived identity generates conservation laws from *nonlocal* as well as local symmetries. It is explicitly shown how Noether's theorem is extended by the identity. Conservation laws arising from nonlocal symmetries are obtained for a class of scalar wave equations with variable wave speeds. The constants of motion resulting from these nonlocal conservation laws are shown to be linearly independent of all constants of motion resulting from local conservation laws. © *1996 American Institute of Physics.* [S0022-2488(96)02405-2]

I. INTRODUCTION

Conservation laws can be found for self-adjoint systems of differential equations by Noether's theorem.[1–3] If a local symmetry admitted by a given system leaves invariant the variational principle of the system, Noether's theorem yields a corresponding conservation law of local type. Conversely, all conservation laws of local type for a given system arise from the local symmetries admitted by the system. A limitation of Noether's theorem, however, is that it can only directly deal with local symmetries and hence conservation laws of local type. This poses a significant incompleteness in the study of differential equations since conservation laws of nonlocal type are equally as useful as those of local type. In particular, as will be shown in this article, conservation laws of nonlocal type yield additional constants of motion and thus expand the utility of methods of analysis which depend on conservation laws.

In this article we introduce an expression that yields conservation laws from nonlocal symmetries as well as local symmetries admitted by an arbitrary self-adjoint system of differential equations. Significantly, in contrast to the formulation of Noether's theorem, the expression is derived from a bilinear identity that makes no use of a Lagrangian. As preliminaries to the derivation and main results, we now give definitions of local and nonlocal symmetries and conservation laws of local and nonlocal type for self-adjoint systems of differential equations.

Consider a system of differential equations (DEs) given by

$$G_\sigma(x,u,\underset{1}{u},\ldots,\underset{K}{u})=0, \quad \sigma=1,\ldots,M \tag{1.1}$$

for $M\geqslant 1$ dependent variables $u=(u^1,\ldots,u^M)$ which are functions of $N\geqslant 1$ independent variables $x=(x^1,\ldots,x^N)$, with $\underset{J}{u}$ denoting all Jth order derivatives of u with respect to x. For the sequel, we let D_i denote total differentiation with respect to x^i, where $i=1,\ldots,N$, and we use the index notation $u^\gamma_{i_1\cdots i_J} = D_{i_1}\cdots D_{i_J}u^\gamma$ for differentiations of u, where $\gamma=1,...,M$, $i_J=1,\ldots,N$, and

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$J=1,2,\ldots$. Hereafter, unless otherwise stated, we use the index conventions that all Greek indices range from 1 to M, all Latin indices (lower case) range from 1 to N, while summation is assumed over any repeated indices in all expressions.

Definition 1.1: The Fréchet derivative associated with system (1.1) is the matrix linear operator

$$\mathscr{T}_{\sigma\rho}=\frac{\partial G_\sigma}{\partial u^\rho}+\frac{\partial G_\sigma}{\partial u^\rho_i}D_i+\cdots+\frac{\partial G_\sigma}{\partial u^\rho_{i_1\cdots i_K}}D_{i_1}\cdots D_{i_K}. \tag{1.2}$$

Definition 1.2: A symmetry admitted by system (1.1) is characterized by an infinitesimal generator

$$\mathbf{X}=\eta^\mu\partial/\partial u^\mu, \tag{1.3}$$

where η^μ *satisfies*

$$\mathscr{T}_{\sigma\rho}\eta^\rho=0 \tag{1.4}$$

for every solution $u(x)$ *of system (1.1).*

Definition 1.3: A local symmetry admitted by system (1.1) is a symmetry with an infinitesimal generator of the form

$$\mathbf{X}=\eta^\mu(x,u,\underset{1}{u},\ldots,\underset{P}{u})\partial/\partial u^\mu \tag{1.5}$$

such that, for all values of x, η^μ *depends on* $u,\underset{1}{u},\ldots,\underset{P}{u}$ *only through* $u(x),\underset{1}{u}(x),\ldots,\underset{P}{u}(x)$ *evaluated at* x.

Definition 1.4: A nonlocal symmetry admitted by system (1.1) is a symmetry with an infinitesimal generator $\mathbf{X}=\eta^\mu\partial/\partial u^\mu$ *not of the form (1.5), such that* η^μ *has other than just a local dependence on* $u(x)$ *and derivatives of* $u(x)$ *to some finite order.*

All local symmetries of system (1.1) can be determined by Lie's algorithm.[2,3] No corresponding procedure exists to find *all* nonlocal symmetries of system (1.1).

There is an algorithm[3–6] to determine special nonlocal symmetries, called *potential symmetries*, if one DE of system (1.1) is a divergence expression. These potential symmetries arise as local symmetries admitted by auxiliary systems associated to system (1.1). In the case of two independent variables ($N=2$), suppose system (1.1) has a DE of the form

$$G_\sigma(x,u,\underset{1}{u},\ldots,\underset{K}{u})=D_1f^1(x,u,\underset{1}{u},\ldots,\underset{K-1}{u})+D_2f^{\,2}(x,u,\underset{1}{u},\ldots,\underset{K-1}{u})=0,\quad \sigma=M. \tag{1.6}$$

Through Eq. (1.6) one can introduce an auxiliary potential variable v and form a potential system given by

$$G_\sigma=0,\quad \sigma=1,\ldots,M-1, \tag{1.7}$$

$$D_2v=f^1,\quad D_1v=-f^{\,2}. \tag{1.8}$$

If $(u(x),v(x))$ satisfies system (1.7)–(1.8), then $u(x)$ satisfies system (1.1); if $u(x)$ satisfies system (1.1), then there exists some $v(x)$ (unique up to the addition of an arbitrary constant) such that $(u(x),v(x))$ satisfies system (1.7)–(1.8). Since $v(x)$ is determined in terms of integrals of $u(x)$, a local symmetry of system (1.7)–(1.8) may yield a nonlocal symmetry of system (1.1). In particular, such a nonlocal symmetry arises if and only if an infinitesimal generator of a local

symmetry of system (1.7)–(1.8) does not project onto an infinitesimal generator of a local symmetry admitted by system (1.1). Similar considerations hold for the case of more than two independent variables.

Definition 1.5: A conservation law of system (1.1) is a divergence free expression $D_i\Psi^i=0$ *which holds for every solution of system (1.1) and its differential consequences. The conservation law is local (conservation law of local type) if and only if it has the form* $D_i\Psi^i(x,u,\underset{1}{u},\ldots,\underset{L}{u})=0$ *where, for all values of* x, Ψ^i *depends on* $u,\underset{1}{u},\ldots,\underset{L}{u}$ *only through* $u(x),\underset{1}{u}(x),\ldots,\underset{L}{u}(x)$ *evaluated at* x. *Otherwise the conservation law is nonlocal (conservation law of nonlocal type).*

Definition 1.6: The adjoint of the Fréchet derivative (1.2) is the matrix linear operator $\mathscr{T}^*_{\sigma\rho}$ *satisfying*

$$V^\sigma \mathscr{T}_{\sigma\rho} W^\rho - W^\sigma \mathscr{T}^*_{\sigma\rho} V^\rho = D_i P^i \tag{1.9}$$

for all K times differential functions $V^\gamma(x)$ *and* $W^\gamma(x)$, *for some* P^i *which depends on* x^i, u^γ, V^γ, W^γ *and the derivatives of* u^γ, V^γ, W^γ *to some finite order.*

Definition 1.7: The system (1.1) is self-adjoint if and only if

$$\mathscr{T}_{\sigma\rho} = \mathscr{T}^*_{\sigma\rho} \quad . \tag{1.10}$$

In Sec. II, we derive the bilinear identity giving a correspondence between symmetries and conservation laws for self-adjoint systems of DEs (1.1). From this identity we obtain an expression that yields a conservation law for each pair of symmetries, *local* or *nonlocal*, admitted by any such system (linear or nonlinear). Furthermore, as each such linear system admits a trivial scaling symmetry, we obtain a conservation law for all nontrivial symmetries of any self-adjoint linear system of DEs (1.1). In particular, each nonlocal symmetry admitted by such a linear system thereby leads to a corresponding nonlocal conservation law.

From the known connection between local conservation laws and local symmetries[2,7] for self-adjoint systems of DEs it follows that all local conservation laws obtained through the bilinear identity derived in Sec. II are also obtainable from Noether's theorem. In the case when such a system is linear, we show in Sec. III that each local symmetry leaving invariant a corresponding variational principle yields the same conservation law through our bilinear identity as through Noether's theorem.

In Sec. IV, as an example of a self-adjoint linear DE, we consider the two-dimensional scalar wave equation with a variable wave speed. For a large class of wave speeds this equation admits nonlocal symmetries realized as potential symmetries.[3–5] The nonlocal character of these symmetries means that we cannot obtain corresponding conservation laws by applying Noether's theorem to the variational principle of the scalar wave equation. Moreover, we show that the potential system for this equation does not have a variational principle, and hence Noether's theorem cannot be applied to the potential system to obtain any conservation laws. By using our conservation law expression derived in Sec. II, we obtain nonlocal conservation laws for the admitted nonlocal symmetries. In Sec. V, we obtain corresponding constants of motion for the scalar wave equation. We show that these constants of motion are linearly independent of each other as well as linearly independent of all constants of motion arising from local symmetries of the scalar wave equation.

In Sec. VI, we expand on some of the ideas and results presented in earlier sections.

II. DERIVATION OF THE CONSERVATION LAW EXPRESSION

We consider a system (1.1) that is self-adjoint. Then the DEs in system (1.1) must satisfy the following Helmholtz identities:[7]

$$\frac{\partial G_\sigma}{\partial u^\rho} = \frac{\partial G_\rho}{\partial u^\sigma} - D_i\left(\frac{\partial G_\rho}{\partial u^\sigma_i}\right) + \cdots + (-1)^K D_{i_1}\cdots D_{i_K}\left(\frac{\partial G_\rho}{\partial u^\sigma_{i_1\cdots i_K}}\right), \tag{2.1}$$

$$\frac{\partial G_\sigma}{\partial u^\rho_{i_1\cdots i_j}}=(-1)^J\frac{\partial G_\rho}{\partial u^\sigma_{i_1\cdots i_J}}+(-1)^{J+1}C_J^{J+1}D_{i_{J+1}}\left(\frac{\partial G_\rho}{\partial u^\sigma_{i_1\cdots i_{J+1}}}\right)$$
$$+\cdots+(-1)^K C_J^K D_{i_{J+1}}\cdots D_{i_K}\left(\frac{\partial G_\rho}{\partial u^\sigma_{i_1\cdots i_K}}\right),\quad J=1,\ldots,K-1, \tag{2.2}$$

$$\frac{\partial G_\sigma}{\partial u^\rho_{i_1\cdots i_K}}=(-1)^K\frac{\partial G_\rho}{\partial u^\sigma_{i_1\cdots i_K}}, \tag{2.3}$$

where $C_J^L=L!/J!(L-J)!$ for positive integers $L\geqslant J$. As a consequence of these identities, one can verify by direct calculation that the Fréchet derivative (1.2) leads to the identity

$$\mathscr{F}_{\sigma\rho}\omega^\rho=\omega^\rho\frac{\partial G_\rho}{\partial u^\sigma}-D_i\left(\omega^\rho\frac{\partial G_\rho}{\partial u^\sigma_i}\right)+\cdots+(-1)^K D_{i_1}\cdots D_{i_K}\left(\omega^\rho\frac{\partial G_\rho}{\partial u^\sigma_{i_1\cdots i_K}}\right) \tag{2.4}$$

for arbitrary functions ω^ρ.

Using Eq. (2.4) and the Leibnitz rule for differentiation, one finds that the following bilinear skew-symmetric identity holds for arbitrary functions ω^ρ and ν^ρ:

$$\nu^\sigma\mathscr{F}_{\sigma\rho}\omega^\rho-\omega^\sigma\mathscr{F}_{\sigma\rho}\nu^\rho=D_i\Phi^i[\nu,\omega], \tag{2.5}$$

where

$$\Phi^i[\nu,\omega]=-\frac{1}{2}\left\{\nu^\sigma\frac{\partial G_\rho}{\partial u^\sigma_i}\omega^\rho+(D_j\nu^\sigma-\nu^\sigma D_j)\left(\frac{\partial G_\rho}{\partial u^\sigma_{ji}}\omega^\rho\right)+\cdots+(D_{i_1}\cdots D_{i_{K-1}}\nu^\sigma\right.$$
$$\left.+\cdots+(-1)^K\nu^\sigma D_{i_1}\cdots D_{i_{K-1}})\left(\frac{\partial G_\rho}{\partial u^\sigma_{i_1\cdots i_{K-1}i}}\omega^\rho\right)\right\}$$
$$+\frac{1}{2}\left\{\omega^\sigma\frac{\partial G_\rho}{\partial u^\sigma_i}\nu^\rho+(D_j\omega^\sigma-\omega^\sigma D_j)\left(\frac{\partial G_\rho}{\partial u^\sigma_{ji}}\nu^\rho\right)+\cdots+(D_{i_1}\cdots D_{i_{K-1}}\omega^\sigma\right.$$
$$\left.+\cdots+(-1)^K\omega^\sigma D_{i_1}\cdots D_{i_{K-1}})\left(\frac{\partial G_\rho}{\partial u^\sigma_{i_1\cdots i_{K-1}i}}\nu^\rho\right)\right\}. \tag{2.6}$$

The functions ω^ρ and ν^ρ here can have arbitrary (local or nonlocal) dependence on u and derivatives of u.

This bilinear identity leads to a connection between symmetries and conservation laws:

Theorem 2.1: *Suppose* $\mathbf{X}_1=\eta_1^\mu\partial/\partial u^\mu$ *and* $\mathbf{X}_2=\eta_2^\mu\partial/\partial u^\mu$ *are infinitesimal generators of symmetries (local or nonlocal) of a self-adjoint system (1.1). The bilinear identity (2.5) then yields the conservation law*

$$D_i\Phi^i[\eta_1,\eta_2]=0 \tag{2.7}$$

with $\Phi^i[\eta_1,\eta_2]$ *defined by Eq. (2.6).*

We now specialize to the case when system (1.1) is a linear homogeneous system

$$G_\sigma(x,u,\underset{1}{u},\ldots,\underset{K}{u})=G_{\sigma\rho}(x)u^\rho+G^i_{\sigma\rho}(x)u^\rho_i+\cdots+G^{i_1\cdots i_K}_{\sigma\rho}(x)u^\rho_{i_1\cdots i_K}=0 \tag{2.8}$$

with coefficients $G_{\sigma\rho}(x), G^i_{\sigma\rho}(x), \ldots, G^{i_1\cdots i_K}_{\sigma\rho}(x)$. Every such system admits the trivial scaling symmetry

$$\mathbf{X}_s = u^\mu \partial/\partial u^\mu. \tag{2.9}$$

Using this symmetry as one of the symmetries in Theorem 2.1 now leads to the following correspondence:

Theorem 2.2: *Suppose a self-adjoint linear system (2.8) admits a nontrivial symmetry (local or nonlocal) with infinitesimal generator* $\mathbf{X} = \eta^\mu \partial/\partial u^\mu$. *Then Eq. (2.7) yields the conservation law*

$$D_i \Phi^i[u, \eta] = 0, \tag{2.10}$$

where

$$\begin{aligned}\Phi^i[u,\eta] = &-\tfrac{1}{2}\Big\{u^\sigma G^i_{\rho\sigma}(x)\,\eta^\rho + (u^\sigma_j - u^\sigma D_j)(G^{ji}_{\rho\sigma}(x)\,\eta^\rho) \\ &+ \cdots + (u^\sigma_{i_1\cdots i_{K-1}} + \cdots + (-1)^K u^\sigma D_{i_1}\cdots D_{i_{K-1}})(G^{i_1\cdots i_{K-1}i}_{\rho\sigma}(x)\,\eta^\rho)\Big\} \\ &+ \tfrac{1}{2}\Big\{\eta^\sigma G^i_{\rho\sigma}(x) u^\rho + (D_j\eta^\sigma - \eta^\sigma D_j)(G^{ji}_{\rho\sigma}(x) u^\rho) + \cdots + (D_{i_1}\cdots D_{i_{K-1}}\eta^\sigma \\ &+ \cdots + (-1)^K \eta^\sigma D_{i_1}\cdots D_{i_{K-1}})(G^{i_1\cdots i_{K-1}i}_{\rho\sigma}(x) u^\rho)\Big\}.\end{aligned} \tag{2.11}$$

III. RELATIONSHIP TO NOETHER'S THEOREM

Noether's theorem only relates local symmetries to conservation laws (of local type) for self-adjoint systems. The variational principle for a (linear or nonlinear) self-adjoint system (1.1) has Lagrangian L given by[2,7]

$$L(x, u, \underset{1}{u}, \ldots, \underset{K}{u}) = \int_0^1 u^\sigma G_\sigma(x, \lambda u, \lambda \underset{1}{u}, \ldots, \lambda \underset{K}{u})\, d\lambda. \tag{3.1}$$

Definition 3.1: An infinitesimal generator $\mathbf{X} = \eta^\mu(x, u, \underset{1}{u}, \ldots, \underset{P}{u})\partial/\partial u^\mu$ *is a variational symmetry of a self-adjoint system (1.1) if and only if*

$$\mathbf{X}^{(K)} L(x, u, \underset{1}{u}, \ldots, \underset{K}{u}) = D_i A^i \tag{3.2}$$

for some $A^i(x, u, \underset{1}{u}, \ldots, \underset{L}{u})$, *where* $\mathbf{X}^{(K)}$ *is the Kth prolongation generator given by*

$$\mathbf{X}^{(K)} = \eta^\mu \partial/\partial u^\mu + (D_i \eta^\mu)\partial/\partial u^\mu_i + \cdots + (D_{i_1}\cdots D_{i_K}\eta^\mu)\partial/\partial u^\mu_{i_1\cdots i_K}. \tag{3.3}$$

Noether's theorem yields a local conservation law for each variational symmetry admitted by system (1.1). Specifically, one can show that

$$\mathbf{X}^{(K)} L = G_\sigma \eta^\sigma + D_i S^i = D_i A^i, \tag{3.4}$$

where $S^i = \eta^\sigma \partial L/\partial u^\sigma_i + (D_j\eta^\sigma - \eta^\sigma D_j)(\partial L/\partial u^\sigma_{ji}) + \cdots + (D_{j_1}\cdots D_{j_{K-1}}\eta^\sigma + \cdots + (-1)^{K-1}\eta^\sigma D_{j_1}\cdots D_{j_{K-1}})(\partial L/\partial u^\sigma_{j_1\cdots j_{K-1}i})$.[2,3,7] Then Eq. (3.4) yields Noether's identity

$$D_i N^i[\eta] = -G_\sigma \eta^\sigma \tag{3.5}$$

with $N^i[\eta] = S^i - A^i$. Consequently, for any solution of system (1.1) we obtain the Noether conservation law

$$D_i N^i[\eta]=0. \tag{3.6}$$

Using the Helmholtz identities (2.1) to (2.3), along with Noether's identity (3.5) and the fact that the Euler–Lagrange operator annihilates divergences, one can show that any variational symmetry $\mathbf{X}=\eta^\mu\partial/\partial u^\mu$ satisfies the identity

$$\mathscr{T}_{\sigma\rho}\eta^\rho=-G_\rho\frac{\partial\eta^\rho}{\partial u^\sigma}+D_i\left(G_\rho\frac{\partial\eta^\rho}{\partial u_i^\sigma}\right)+\cdots+(-1)^{P+1}D_{i_1}\cdots D_{i_P}\left(G_\rho\frac{\partial\eta^\rho}{\partial u_{i_1\cdots i_P}^\sigma}\right). \tag{3.7}$$

From Eq. (3.7) it immediately follows that all variational symmetries are local symmetries of system (1.1). [The converse does not always hold, as seen from the fact that scaling symmetries (2.9) generally do not satisfy Eq. (3.7).]

For the rest of this section we restrict the self-adjoint system (1.1) to be a linear homogeneous system (2.8). Before relating conservation laws from Noether's theorem to conservation laws arising from the bilinear identity (2.5), we establish the following result:

Lemma 3.2: Suppose $\eta^\mu(x,u,\underset{1}{u},\ldots,\underset{P}{u})$ *is analytic in* u *and derivatives of* u. *Then any local symmetry generator of the form* $\mathbf{X}=\eta^\mu(x,u,\underset{1}{u},\ldots,\underset{P}{u})\partial/\partial u^\mu$ *admitted by a linear homogeneous system* (2.8) *can be expressed as a superposition of homogeneous local symmetry generators*:

$$\eta^\mu(x,u,\underset{1}{u},\ldots,\underset{P}{u})=\sum_{n=0}^{\infty}\overset{(n)}{\eta}{}^\mu(x,u,\underset{1}{u},\ldots,\underset{P}{u}), \tag{3.8}$$

where

$$\overset{(n)}{\eta}{}^\mu(x,u,\underset{1}{u},\ldots,\underset{P}{u})=\lambda^{-n}\overset{(n)}{\eta}{}^\mu(x,\lambda u,\lambda\underset{1}{u},\ldots,\lambda\underset{P}{u}) \tag{3.9}$$

for all positive constants λ.

Proof: Since system (2.8) admits the scaling symmetry (2.9), it must also admit the symmetry $\eta^\mu(x,\lambda u,\lambda\underset{1}{u},\ldots,\lambda\underset{P}{u})\partial/\partial u^\mu$ for all constants λ. Then the analyticity property of η^μ leads to

$$\eta^\mu(x,\lambda u,\lambda\underset{1}{u},\ldots,\lambda\underset{P}{u})=\sum_{n=0}^{\infty}\lambda^n\overset{(n)}{\eta}{}^\mu(x,u,\underset{1}{u},\ldots,\underset{P}{u}), \tag{3.10}$$

where $\overset{(n)}{\eta}{}^\mu(x,u,\underset{1}{u},\ldots,\underset{P}{u})=\partial^n\eta^\mu(x,\lambda u,\lambda\underset{1}{u},\ldots,\lambda\underset{P}{u})/\partial\lambda^n|_{\lambda=0}$ and $\overset{(n)}{\eta}{}^\mu(x,u,\underset{1}{u},\ldots,\underset{P}{u})=\eta^\mu(x,\lambda,u,\lambda\underset{1}{u},\ldots,\lambda\underset{P}{u})|_{\lambda=0}$. It then follows that each $\overset{(n)}{\eta}{}^\mu(x,u,\underset{1}{u},\ldots,\underset{P}{u})\partial/\partial u^\mu$, for $n=0,1,2,\ldots$, is a local symmetry of system (2.8). Setting $\lambda=1$ in the superposition (3.10) then yields Eq. (3.8).□

As an aside we remark that every infinitesimal generator of a point symmetry $\mathbf{X}=\eta^\mu(x,u,\underset{1}{u})\partial/\partial u^\mu$ has $\overset{(n)}{\eta}{}^\mu(x,u,\underset{1}{u})=0$ for $n\neq1$ when system (2.8) is a scalar PDE of order $K\geqslant2$ (with $N\geqslant2$).[8]

Without loss of generality we assume that each infinitesimal generator of a symmetry admitted by system (2.8) satisfies the homogeneity property (3.9). We then have the following identity

$$u^\sigma\frac{\partial\eta^\rho}{\partial u^\sigma}+u_i^\sigma\frac{\partial\eta^\rho}{\partial u_i^\sigma}+\cdots+u_{i_1\cdots i_P}^\sigma\frac{\partial\eta^\rho}{\partial u_{i_1\cdots i_P}^\sigma}=n\eta^\rho \tag{3.11}$$

for some integer $n\geqslant0$.

We now establish the relationship between Noether's conservation law expression (3.6) and our conservation law expression (2.10):

Theorem 3.3: *Suppose a variational symmetry of a self-adjoint linear system (2.8) has an infinitesimal generator* $\mathbf{X}=\eta^{\mu}\partial/\partial u^{\mu}$ *satisfying Eq. (3.11). Then up to the addition of a divergence free expression, one has*

$$\Phi^i[u,\eta]=(1+n)N^i[\eta], \tag{3.12}$$

for every solution of the system (2.8).

Proof. From the bilinear identity (2.5) we have

$$D_i\Phi^i[u,\eta]=u^{\sigma}\mathscr{F}_{\sigma\rho}\eta^{\rho}-\eta^{\sigma}\mathscr{F}_{\sigma\rho}u^{\rho}. \tag{3.13}$$

Since system (2.8) is linear, it satisfies the identity

$$\mathscr{F}_{\sigma\rho}u^{\rho}=G_{\sigma}. \tag{3.14}$$

Using the Leibnitz rule for differentiation to manipulate Eq. (3.7), we get

$$u^{\sigma}\mathscr{F}_{\sigma\rho}\eta^{\rho}=-G_{\rho}\left(u^{\sigma}\frac{\partial\eta^{\rho}}{\partial u^{\sigma}}+u_i^{\sigma}\frac{\partial\eta^{\rho}}{\partial u_i^{\sigma}}+\cdots+u^{\sigma}_{i_1\cdots i_P}\frac{\partial\eta^{\rho}}{\partial u^{\sigma}_{i_1\cdots i_P}}\right)+D_iB^i, \tag{3.15}$$

where

$$\begin{aligned}B^i=&u^{\sigma}G_{\rho}\frac{\partial\eta^{\rho}}{\partial u_i^{\sigma}}+(u_j^{\sigma}-u^{\sigma}D_j)\left(G_{\rho}\frac{\partial\eta^{\rho}}{\partial u_{ji}^{\sigma}}\right)+\cdots\\&+(u^{\sigma}_{i_1\cdots i_{P-1}}+\cdots+(-1)^{P-1}u^{\sigma}D_{i_1}\cdots D_{i_{P-1}})\left(G_{\rho}\frac{\partial\eta^{\rho}}{\partial u^{\sigma}_{i_1\cdots i_{K-1}i}}\right).\end{aligned} \tag{3.16}$$

Consequently, after substituting Eqs. (3.14) and (3.15) into Eq. (3.13) and then using Eq. (3.11), we obtain

$$D_i\Phi^i[u,\eta]=-(1+n)\,\eta^{\sigma}G_{\sigma}-D_iB^i. \tag{3.17}$$

Then Noether's identity (3.5) yields

$$D_i\Phi^i[u,\eta]=(1+n)D_iN^i[\eta]-D_iB^i. \tag{3.18}$$

Now observe that $B^i=0$ when $G_p=0$, and hence $B^i=0$ for every solution of system (2.8). Thus we arrive at Eq. (3.12). □

IV. NONLOCAL CONSERVATION LAWS FOR SCALAR WAVE EQUATIONS

Throughout the sequel, we set $x^1=x$, $x^2=t$, and we use a subscript notation for total differentiation with respect to x and t.

Consider the scalar wave equation

$$u_{xx}-c^{-2}u_{tt}=0 \tag{4.1}$$

with a variable wave speed $c(x)$. From Eq. (1.8) we introduce the corresponding potential system

$$v_t=u_x,\quad v_x=c^{-2}u_t. \tag{4.2}$$

The wave equation (4.1) has nonlocal symmetries which are realized as potential symmetries resulting from local point symmetries of potential system (4.2) if and only if the wave speed satisfies the fourth order DE[3,4]

$$(cc'(c/c')'')'=0. \tag{4.3}$$

Such wave speeds are bounded away from zero for $-\infty<x<\infty$ when $c(x)$ satisfies the first order DE

$$c'=\nu^{-1}\sin(\nu\log c),\quad \nu=\text{const}, \tag{4.4}$$

up to arbitrary scalings of c and x.[9]

Classification of the point symmetries of system (4.2) yielding nonlocal (potential) symmetries of the wave equation (4.1) leads to two cases[3–5] with, respectively, one and two admitted infinitesimal generators $\mathbf{X}=\eta\partial/\partial u$ of the form

$$\eta=f(x,t)u+g(x,t)v-\xi(x,t)u_x-\tau(x,t)u_t, \tag{4.5}$$

where $g(x,t)$ is not identically zero.

Case I (one nonlocal symmetry): The wave speed $c(x)$ satisfies

$$(c/c')'=\gamma=\text{const}. \tag{4.6}$$

Here we have

$$\begin{aligned} &f(x,t)=a'(t)(1-\tfrac{1}{2}\gamma),\quad g(x,t)=-\tfrac{1}{2}a''(t)c(x)/c'(x),\\ &\xi(x,t)=a'(t)c(x)/c'(x),\quad \tau(x,t)=a(t)(\gamma-1)+a''(t)d(x), \end{aligned} \tag{4.7}$$

where $d(x)$ is a definite integral of $1/(c(x)c'(x))$, and $a(t)$ satisfies the first order ODE $(a/t^2)'=0$, which thus leads to the existence of one generator $\mathbf{X}=\eta\partial/\partial u$.

Case II (two nonlocal symmetries): The wave speed $c(x)$ satisfies

$$cc'(c/c')''=\mu=\text{const}\neq 0. \tag{4.8}$$

Here we have

$$\begin{aligned} &f(x,t)=b'(t)(2-(c(x)/c'(x))'),\\ &g(x,t)=-\mu b(t)c(x)/c'(x),\\ &\xi(x,t)=2b'(t)c(x)/c'(x),\\ &\tau(x,t)=2b(t)((c(x)/c'(x))'-1), \end{aligned} \tag{4.9}$$

where $b(t)$ satisfies the second order ODE $b''-\mu b=0$, which thus leads to the existence of two generators $\mathbf{X}=\eta\partial/\partial u$.

Conservation laws for all symmetries admitted by the wave equation (4.1) are obtainable from Theorem 2.2 since the wave equation is linear and self-adjoint. Hence, each nonlocal symmetry $\mathbf{X}=\eta\partial/\partial u$ admitted in Cases I and II gives rise to a corresponding nonlocal conservation law. From Eqs. (2.11) and (4.5), these conservation laws are given by

$$(\Phi^1[u,\eta])_x+(\Phi^2[u,\eta])_t=0 \tag{4.10}$$

with

$$\Phi^1[u,\eta]=u\eta_x-\eta u_x+(\tau uu_x+c^{-2}\xi uu_t)_t$$
$$=g_xuv-gu_xv+f_xu^2+c^{-2}guu_t-c'c^{-1}\xi uu_x+c^{-2}\xi u_t^2+\xi u_x^2+2\tau u_xu_t, \quad (4.11)$$

$$\Phi^2[u,\eta]=c^{-2}(\eta u_t-u\eta_t)-(\tau uu_x+c^{-2}\xi uu_t)_x$$
$$=c^{-2}(-g_tuv+gu_tv-f_tu^2-guu_x+c'c^{-1}\xi uu_t-\tau u_t^2-c^2\tau u_x^2-2\xi u_xu_t), \quad (4.12)$$

where f,g,ξ,τ satisfy Eq. (4.7) in Case I and Eq. (4.9) in Case II. The identically divergence free terms in Φ^1 and Φ^2 have been added to eliminate all terms involving second order derivatives u_{xx}, u_{tt}, and u_{xt}.

These nonlocal conservation laws arising from the nonlocal symmetries $\mathbf{X}=\eta\partial/\partial u$ cannot be obtained through Noether's theorem for the scalar wave equation (4.1) since Noether's theorem is applicable only to local symmetries that leave invariant a variational principle for Eq. (4.1). Moreover, even though the symmetries $\mathbf{X}=\eta\partial/\partial u$ are realized as local symmetries of the potential system (4.2), Noether's theorem still cannot be applied since, as will now be demonstrated, the potential system is not self-adjoint and hence has no variational principle. Let

$$\begin{bmatrix}u^1\\u^2\end{bmatrix}=\begin{bmatrix}u\\v\end{bmatrix}$$

define a column vector. Then the Fréchet derivative (1.2) associated to system (4.2) is given by the matrix operator

$$\mathscr{T}=\begin{bmatrix}-\partial/\partial x & \partial/\partial t\\ -c^{-2}\partial/\partial t & \partial/\partial x\end{bmatrix}. \quad (4.13)$$

By direct calculation, using Eq. (1.9), the adjoint of the Fréchet derivative is

$$\mathscr{T}^*=-\mathscr{T}, \quad (4.14)$$

and thus the potential system is not self-adjoint.

V. NEW CONSTANTS OF MOTION FOR SCALAR WAVE EQUATIONS

Given a conservation law $(\Phi^1[u,\eta])_x+(\Phi^2[u,\eta])_t=0$ arising from Theorem 2.2 for a symmetry $\mathbf{X}=\eta\partial/\partial u$ of the scalar wave equation (4.1), we let

$$C[\eta]=\int_{-\infty}^{\infty}\Phi^2[u,\eta]dx. \quad (5.1)$$

If $u(x,t)$ has appropriate asymptotic properties as $x\to\pm\infty$, then

$$\frac{dC[\eta]}{dt}=-\Phi^1[u,\eta]|_{x=-\infty}^{x=\infty}=0, \quad (5.2)$$

from which it follows that $C[\eta]$ defines a constant of motion for Eq. (4.1).

Now consider compact support initial data

$$u(x,t_0)=\varphi(x), \quad u_t(x,t_0)=\psi(x), \quad (5.3)$$

for the scalar wave equation (4.1). This determines corresponding data for the potential system (4.2), with

$$v(x,t_0)=\theta(x)=\int_{-\infty}^{x} c(\tilde{x})^{-2}\psi(\tilde{x})d\tilde{x} \tag{5.4}$$

(up to the addition of an arbitrary constant). Evaluating the nonlocal conservation laws given by Eqs. (4.10) to (4.12) with this initial data we find

$$\lim_{x\to\pm\infty} \Phi^1[u,\eta]=0 \tag{5.5}$$

and hence Eq. (5.1) yields constants of motion for the scalar wave equation (4.1). In terms of the initial data (5.3) and (5.4) we obtain

$$C[\eta]=\int_{-\infty}^{\infty} c(x)^{-2}\{(g(x,t_0)\psi(x)-g_t(x,t_0)\varphi(x))\theta(x)-g(x,t_0)\varphi(x)\varphi'(x)-f_t(x,t_0)\varphi(x)^2$$
$$+\xi(x,t_0)(c(x)^{-1}c'(x)\varphi(x)-2\varphi'(x))\psi(x)-\tau(x,t_0)(\psi(x)^2+c(x)^2\varphi'(x)^2)\}dx. \tag{5.6}$$

For each wave speed $c(x)$ satisfying Eq. (4.6), the expression $C[\eta]$ yields one constant of motion, with f,g,ξ,τ satisfying Eq. (4.7); for each wave speed $c(x)$ satisfying Eq. (4.8), the expression $C[\eta]$ yields two constants of motion, with f,g,ξ,τ satisfying Eq. (4.9).

A. Linear independence of constants of motion

Let $C[\eta_1],C[\eta_2],\ldots,C[\eta_k]$ define $k>1$ constants of motion arising for the scalar wave equation (4.1) from symmetries $\mathbf{X}_1=\eta_1\partial/\partial u$, $\mathbf{X}_2=\eta_2\partial/\partial u,\ldots$, $\mathbf{X}_k=\eta_k\partial/\partial u$, respectively.

Definition 5.1: Suppose $c_1,\ldots,c_k$ are constants such that $c_1C[\eta_1]+\cdots+c_kC[\eta_k]$ vanishes for arbitrary initial data (5.3). Then $C[\eta_1],\ldots,C[\eta_k]$ are linearly independent constants of motion if and only if $c_1=\cdots=c_k=0$.

The following theorem now establishes that each constant of motion (5.6) arising from the admitted nonlocal symmetries (4.5) of Eq. (4.1) in Cases I and II is linearly independent of the constants of motion arising from all admitted point symmetries of Eq. (4.1). A subsequent theorem then establishes further that the two constants of motion (5.6) in Case II are linearly independent of each other modulo all point symmetry constants of motion.

Theorem 5.2: *For the scalar wave equation (4.1), the constants of motion (5.6) obtained from the admitted nonlocal symmetries (4.5) are each linearly independent of the constants of motion obtained from all admitted point symmetries.*

Proof: Every point symmetry admitted by a scalar linear PDE is characterized by an infinitesimal generator $\eta\partial/\partial u$ either with η linear in u and first order derivatives of u (in which case the symmetry is called *nontrivial*) or with η independent of u and derivatives of u (in which case the symmetry is called *trivial*).[8] Thus, for the scalar wave equation (4.1), every nontrivial point symmetry as well as every nonlocal symmetry (4.5) has an infinitesimal generator that is linear in u and first order derivatives of u. The constants of motion obtained from these symmetries through Theorem 2.2 are thereby quadratic expressions in terms of initial data $u(x,t_0)$ and $u_t(x,t_0)$, while the constants of motion obtained from trivial symmetries are only linear expressions in terms of this data.

These properties imply that the constants of motion obtained from nontrivial point symmetries and nonlocal symmetries (4.5) are linearly independent of all constants of motion obtained from trivial point symmetries, since these constants of motions have a different scaling dimension under scalings of initial data. Consequently, to complete the proof of the theorem, we need only establish that each constant of motion obtained from the nonlocal symmetries (4.5) is linearly independent of all constants of motion obtained from nontrivial point symmetries.

Let $\tilde{\eta}\partial/\partial u$ correspond to the generator of a nonlocal symmetry (4.5) admitted by Eq. (4.1), and let $\eta_1\partial/\partial u, \ldots, \eta_k\partial/\partial u$ correspond to the generators of all distinct nontrivial point symmetries admitted by Eq. (4.1). Let $C[\tilde{\eta}]$, $C[\eta_1],\ldots,C[\eta_k]$ denote the resulting constants of motion obtained through Theorem 2.2.

Consider the one-parameter family of nonnegative initial data:

$$u(x,t_0;\lambda)=\varphi(x;\lambda)\geqslant 0, \quad u_t(x,t_0;\lambda)=\psi(x;\lambda)\geqslant 0, \tag{5.7}$$

with

$$v(x,t_0;\lambda)=\theta(x;\lambda)=\int_{-\infty}^{x} c(\tilde{x})^{-2}\psi(\tilde{x};\lambda)d\tilde{x}\geqslant 0, \tag{5.8}$$

such that the supports of

$$\begin{aligned}
&\varphi_1(x)=\varphi(x;0), \quad \varphi_2(x)=\frac{\partial\varphi}{\partial\lambda}(x;0),\\
&\psi_1(x)=\psi(x;0), \quad \psi_2(x)=\frac{\partial\psi}{\partial\lambda}(x;0),
\end{aligned} \tag{5.9}$$

are compact and mutually disjoint. Now define

$$\begin{aligned}
&\theta_1(x)=\theta(x;0)=\int_{-\infty}^{x} c(\tilde{x})^{-2}\psi_1(\tilde{x})d\tilde{x},\\
&\theta_2(x)=\frac{\partial\theta}{\partial\lambda}(x;0)=\int_{-\infty}^{x} c(\tilde{x})^{-2}\psi_2(\tilde{x})d\tilde{x}.
\end{aligned} \tag{5.10}$$

If $\tilde{c},c_1,\ldots,c_k$ are constants such that

$$\tilde{c}C[\tilde{\eta}]+c_1C[\eta_1]+\cdots+c_kC[\eta_k]=0 \tag{5.11}$$

for arbitrary initial data, then

$$\tilde{c}C[\tilde{\eta};\lambda]+c_1C[\eta_1;\lambda]+\cdots c_kC[\eta_k;\lambda]=0, \tag{5.12}$$

where $C[\eta_1;\lambda],\ldots,C[\eta_k;\lambda]$ are the constants of motion evaluated for the one-parameter family of initial data (5.9) and (5.10). Hence we must have

$$\left(\tilde{c}\,\frac{\partial C[\tilde{\eta};\lambda]}{\partial\lambda}+c_1\,\frac{\partial C[\eta_1;\lambda]}{\partial\lambda}+\cdots+c_k\,\frac{\partial C[\eta_k;\lambda]}{\partial\lambda}\right)\Bigg|_{\lambda=0}=0. \tag{5.13}$$

Using the earlier remarks about the quadratic properties of $C[\eta]$ for nontrivial point symmetries, and taking account of the disjoint supports of $\varphi_1(x)$, $\varphi_2(x)$, $\psi_1(x)$, $\psi_2(x)$, we have

$$\frac{\partial C[\eta;\lambda]}{\partial\lambda}\Bigg|_{\lambda=0}=0 \tag{5.14}$$

for $\eta=\eta_1,\ldots,\eta=\eta_k$. Hence, from Eq. (5.13), we get

$$\tilde{c}\left.\frac{\partial C[\tilde{\eta};\lambda]}{\partial\lambda}\right|_{\lambda=0}=0, \tag{5.15}$$

where

$$\left.\frac{\partial C[\tilde{\eta};\lambda]}{\partial\lambda}\right|_{\lambda=0}=\int_{-\infty}^{\infty}c(x)^{-2}\{g(x,t_0)(\psi_2(x)\theta_1(x)+\psi_1(x)\theta_2(x))$$
$$-g_t(x,t_0)(\varphi_2(x)\theta_1(x)+\varphi_1(x)\theta_2(x))\}dx, \tag{5.16}$$

using Eq. (5.6).

Now we further restrict the initial data so that the supports of $\varphi_1(x),\varphi_2(x),\psi_1(x),\psi_2(x)$ are to the left of each other, respectively. Then Eq. (5.16) reduces to

$$\left.\frac{\partial C[\tilde{\eta};\lambda]}{\partial\lambda}\right|_{\lambda=0}=\int_{-\infty}^{\infty}c(x)^{-2}g(x,t_0)\psi_2(x)\theta_1(x)dx\neq 0. \tag{5.17}$$

Hence Eq. (5.15) leads to $\tilde{c}=0$ in Eq. (5.11), which implies that the constant of motion arising from the nonlocal symmetry $\tilde{\eta}\partial/\partial u$ is linearly independent of the constants of motion arising from the nontrivial point symmetries $\eta_1\partial/\partial u,\ldots,\eta_k\partial/\partial u$. □

Theorem 5.3: *The two constants of motion (5.6) obtained for the scalar wave equation (4.1) from the nonlocal symmetries (4.5) in Case II are linearly independent modulo all constants of motion obtained from point symmetries.*

Proof: We proceed by the same argument used in proving Theorem 5.2. Let $\tilde{\eta}_1\partial/\partial u$ and $\tilde{\eta}_2\partial/\partial u$ correspond to the generators of the two nonlocal symmetries (4.5) of Eq. (4.1), and let $\eta_1\partial/\partial u,\ldots,\eta_k\partial/\partial u$ correspond to the generators of all distinct nontrivial point symmetries. Let $C[\tilde{\eta}_1],C[\tilde{\eta}_2],C[\eta_1],\ldots,C[\eta_k]$ denote the resulting constants of motion. Consider the same one-parameter initial data used in the previous proof, with the supports of $\varphi_1(x),\varphi_2(x),\psi_1(x),\psi_2(x)$ lying to the left of each other.

If $\tilde{c}_1,\tilde{c}_2,c_1,\ldots,c_k$ are constants such that

$$\tilde{c}_1C[\tilde{\eta}_1]+\tilde{c}_2C[\tilde{\eta}_2]+c_1C[\eta_1]+\cdots+c_kC[\eta_k]=0 \tag{5.18}$$

for arbitrary initial data, then we have

$$\left(\tilde{c}_1\frac{\partial C[\tilde{\eta}_1;\lambda]}{\partial\lambda}+\tilde{c}_2\frac{\partial C[\tilde{\eta}_2;\lambda]}{\partial\lambda}\right)\Bigg|_{\lambda=0}=0, \tag{5.19}$$

where $C[\tilde{\eta}_1;\lambda]$ and $C[\tilde{\eta}_2;\lambda]$ are the constants of motion evaluated for the one-parameter family of initial data. From Eq. (5.16) we find that Eq. (5.19) simplifies to

$$\int_{-\infty}^{\infty}c(x)^{-2}(\tilde{c}_1g_1(x,t_0)+\tilde{c}_2g_2(x,t_0))\psi_2(x)\theta_1(x)dx=0, \tag{5.20}$$

where, by use of Eq. (4.9), we have

$$\tilde{c}_1g_1(x,t_0)+\tilde{c}_2g_2(x,t_0)=-\mu(\tilde{c}_1b_1(t_0)+\tilde{c}_2b_2(t_0))c(x)/c'(x). \tag{5.21}$$

Then Eq. (5.20) reduces to

$$-(\tilde{c}_1b_1(t_0)+\tilde{c}_2b_2(t_0))\mu\int_{-\infty}^{\infty}c(x)^{-1}c'(x)^{-1}\psi_2(x)\theta_1(x)dx=0 \tag{5.22}$$

with $\int_{-\infty}^{\infty} c(x)^{-1}c'(x)^{-1}\psi_2(x)\theta_1(x)dx \neq 0$. It then follows that $\tilde{c}_1 b_1(t_0)+\tilde{c}_2 b_2(t_0)=0$, and since we can choose the value of t_0 freely, we then must have $\tilde{c}_1 b_1(t)+\tilde{c}_2 b_2(t)=0$ for all t. However, from Eq. (4.9) we note that $b=b_1(t)$ and $b=b_2(t)$ are linearly independent functions satisfying $b''-\mu b=0$. Thus $\tilde{c}_1=0=\tilde{c}_2$. The linear independence of the constants of motion $C[\tilde{\eta}_1]$ and $C[\tilde{\eta}_2]$ modulo the constants of motion $C[\eta_1],\ldots,C[\eta_k]$ then follows from Eq. (5.18). □

B. Analytical example of new constants of motion

Theorems 5.2 and 5.3 establish new constants of motion for the scalar wave equation (4.1) for wave speeds given by Eq. (4.6) in Case I and Eq. (4.8) in Case II. The wave speeds in Case II satisfying the ODE (4.4) have the most physical interest since they are bounded (above and below) away from zero. These wave speeds $c(x)$ are implicitly given by the integral

$$\int_{c(x_0)}^{c(x)} \frac{\nu\, dc}{\sin(\nu \log c)} = x - x_0, \tag{5.23}$$

where ν and x_0 are arbitrary constant parameters. From Eq. (5.23), $c(x)$ can be shown to increase monotonically from the asymptotic value $c\to 1$ for $x\to-\infty$ to the asymptotic value $c\to e^{\pi/\nu}$ for $x\to+\infty$. In physical terms, this describes a medium of two layers, with wave speeds $c\approx 1$ and $c\approx e^{\pi/\nu}$, separated by a smoothly varying transition layer having width $\Delta x\approx \nu(e^{\pi/\nu}-1)$, controlled by the value of ν.[9]

The scalar wave equation (4.1) with wave speeds (5.23) has no constants of motion arising from nontrivial point symmetries other than time translation symmetries generated by $\mathbf{X}=u_t\partial/\partial u$. These symmetries give rise through Theorem 2.2 to an energy constant of motion

$$E=\int_{-\infty}^{\infty} c(x)^{-2}(\psi(x)^2+c(x)^2\varphi'(x)^2)dx, \tag{5.24}$$

where $\varphi(x)$ and $\psi(x)$ are initial data (5.3).

Two additional constants of motion arise from the nonlocal symmetries (4.5) admitted by the scalar wave equation (4.1) with these wave speeds. In terms of the potential v introduced through Eq. (4.2), the nonlocal symmetry generators $\mathbf{X}=\eta\partial/\partial u$ have the explicit form (4.5) with

$$\begin{aligned} f(x,t)&=\pm(1+B(x))e^{\pm t}, \quad g(x,t)=-A(x)e^{\pm t},\\ \xi(x,t)&=\pm 2A(x)e^{\pm t}, \quad \tau(x,t)=-2B(x)e^{\pm t}, \end{aligned} \tag{5.25}$$

where

$$A(x)=\nu c(x)\csc(\nu \log c(x)), \quad B(x)=\nu\cot(\nu \log c(x)). \tag{5.26}$$

The corresponding constants of motion given by Eq. (5.6) are

$$\begin{aligned} C_\pm=\int_{-\infty}^{\infty} c(x)^{-2}&(-A(x)(\psi(x)\pm\varphi(x))\theta(x)\pm(\varphi(x)-2A(x)\varphi'(x))\psi(x)\\ &-\tfrac{1}{2}(1+B(x))\varphi(x)^2+2B(x)(\psi(x)^2+c(x)^2\varphi'(x)^2))dx, \end{aligned} \tag{5.27}$$

where $\varphi(x)$ and $\psi(x)$ are initial data (5.3), and $\theta(x)$ is determined nonlocally from $\psi(x)$ by Eq. (5.4). $C_\pm$ and E comprise a linearly independent set of constants of motion as shown by Theorems 5.2 and 5.3.

The new constants of motion $C_\pm$ may have utility in the mathematical analysis of wave propagation for two layered media described by wave speeds (5.23). In particular, $C_\pm$ may supple-

ment the use of the energy constant of motion E in addressing certain problems, such as the time evolution analysis for dispersal of waves initially localized across the transition boundary between the layers, and the scattering theory analysis of traveling waves incident on the transition boundary.

VI. CONCLUDING REMARKS

(1) In Sec. II we presented an explicit conservation law arising from any pair of symmetries, local or nonlocal, admitted by an arbitrary self-adjoint system of (linear or nonlinear) DEs (1.1). This conservation law expression does not require use of a variational principle for the system. Specializing to self-adjoint systems of linear DEs, we obtained a conservation law from any admitted local or nonlocal symmetry, by using a scaling symmetry as a second symmetry. A similar conservation law also can be obtained for any nonlinear system which admits a scaling symmetry (e.g., the Einstein equations in General Relativity theory). For variational symmetries (which are always local symmetries) admitted in the case of self-adjoint linear systems, we showed in Sec. III that the resulting local conservation laws are the same as those obtained from Noether's theorem. (The proof can be generalized straightforwardly to the conservation laws arising in the case of nonlinear systems with a scaling symmetry.)

The following theorem shows how our conservation law for a pair of symmetries is connected to Noether's theorem.

Theorem 6.1: *Suppose* $\mathbf{X}_1=\eta_1^\mu(x,u,\underset{1}{u},\ldots,\underset{P_1}{u})\partial/\partial u^\mu$ *and* $\mathbf{X}_2=\eta_2^\mu(x,u,\underset{1}{u},\ldots,\underset{P_2}{u})\partial/\partial u^\mu$ *are variational symmetries of a self-adjoint (linear or nonlinear) system (1.1). Then the resulting conservation law (2.7) is the same as the conservation law obtained through Noether's theorem for the commutator symmetry*

$$[\mathbf{X}_1,\mathbf{X}_2]=\eta^\mu(x,u,\underset{1}{u},\ldots,\underset{P}{u})\partial/\partial u^\mu \tag{6.1}$$

with $P\leqslant P_1+P_2$.

Proof: The commutator $[\mathbf{X}_1,\mathbf{X}_2]=\eta^\rho\partial/\partial u^\rho$ is given by

$$\begin{aligned}\eta^\rho=&\left(\frac{\partial\eta_2^\rho}{\partial u^\sigma}\,\eta_1^\sigma+\frac{\partial\eta_2^\rho}{\partial u_i^\sigma}\,D_i\eta_1^\sigma+\cdots+\frac{\partial\eta_2^\rho}{\partial u^\sigma_{i_1\cdots i_{P_2}}}\,D_{i_1}\cdots D_{i_{P_2}}\eta_1^\sigma\right)\\&-\left(\frac{\partial\eta_1^\rho}{\partial u^\sigma}\,\eta_2^\sigma+\frac{\partial\eta_1^\rho}{\partial u_i^\sigma}\,D_i\eta_2^\sigma+\cdots+\frac{\partial\eta_1^\rho}{\partial u^\sigma_{i_1\cdots i_{P_1}}}\,D_{i_1}\cdots\,D_{i_{P_1}}\eta_2^\sigma\right).\end{aligned} \tag{6.2}$$

From Eq. (2.5) we see that

$$\eta_1^\sigma\mathscr{F}_{\sigma\rho}\eta_2^\rho-\eta_2^\sigma\mathscr{F}_{\sigma\rho}\eta_1^\sigma=D_i\Phi^i[\,\eta_1,\eta_2]. \tag{6.3}$$

Then similarly to the derivation of Eq. (3.15), the identity (3.7) now leads to

$$\eta_1^\sigma\mathscr{F}_{\sigma\rho}\eta_2^\rho=-G_\rho\left(\frac{\partial\eta_2^\rho}{\partial u^\sigma}\,\eta_1^\sigma+\frac{\partial\eta_2^\rho}{\partial u_i^\sigma}\,D_i\eta_1^\sigma+\cdots+\frac{\partial\eta_2^\rho}{\partial u^\sigma_{i_1\cdots i_{P_2}}}\,D_{i_1}\cdots D_{i_{P_2}}\eta_1^\sigma\right)+D_iH^i[\,\eta_1,\eta_2] \tag{6.4}$$

for a certain $H^i[\,\eta_1,\eta_2]$. Hence, using Eqs. (6.2) to (6.4), we have

$$G_\rho\eta^\rho=D_i\Omega^i, \tag{6.5}$$

where $\Omega^i = -\Phi^i[\eta_1, \eta_2] + H^i[\eta_1, \eta_2] - H^i[\eta_2, \eta_1]$. As the commutator of any two variational symmetries is itself a variational symmetry, we see from Eq. (3.4) that Eq. (6.5) is a conservation law obtainable from Noether's theorem. □

The set of all variational symmetries for a given self-adjoint system (1.1) forms a Lie algebra $\mathscr{A}$. If all Lie algebra generators can be realized as commutators, in which case we say $\mathscr{A}$ is ''perfect,'' then Theorem 6.1 yields all local conservation laws for the system. We remark that all semisimple Lie algebras, as well as the Poincaré algebra (which is not semisimple), are perfect.

(2) The questions of how to find and how to characterize useful potential systems in order to find nonlocal symmetries admitted by a system of DEs is considered in Ref. 6.

Potential systems of a given system (1.1) rely on the existence of at least one divergence free equation in the system. However, if an appropriate divergence free equation cannot be found, one may still be able to embed system (1.1) as a subsystem of a related potential system.[10] This may allow one to find nonlocal symmetries which are generalizations of potential symmetries.

(3) The conservation laws derived in Sec. II for a system of DEs (1.1) require that the system is self-adjoint. If a given system (1.1) is not self-adjoint, one may still be able to find a related potential system that is self-adjoint. Through the embedding into the potential system, any symmetry (local or nonlocal) admitted by the given system will induce a symmetry of the potential system. (An induced symmetry will be a nonlocal symmetry unless its generator has strictly local dependence on the dependent variables in the potential system.) As a result, conservation laws for the given system can then be obtained as conservation laws arising from the induced symmetries (local and nonlocal) of each self-adjoint potential system. If a system (1.1) is itself self-adjoint, conservation laws from *any* admitted symmetry will correspondingly arise through each self-adjoint potential system found for system (1.1) as well as through system (1.1) itself.

For the wave equation (4.1), the first order potential system (4.2) considered in Sec. IV is not self-adjoint. There are several different ways, nevertheless, to introduce potential variables for system (4.2) leading to potential systems that are self-adjoint. As we will discuss in a forthcoming article, the conservation law expressions arising through each such potential system are different from the conservation law expressions obtained through the wave equation (4.1) itself. In particular, the nonlocal symmetries admitted by Eq. (4.1) as point symmetries of system (4.2) induce nonlocal symmetries of these potential systems, leading to corresponding nonlocal conservation laws different than the ones derived in Sec. IV. These additional conservation laws for the wave equation (4.1) are not obtainable by Noether's theorem applied to any of the self-adjoint potential systems, since Noether's theorem only deals with local symmetries.

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Projective representations of the 1+1-dimensional Poincaré group

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The unitary irreducible representations of the central extension of the Poincaré group in 1+1 dimensions are constructed by an application of the Kirillov theory. These are then lifted to projective unitary irreducible representations of the Poincaré group. The 1+1 Galilean group is treated separately in an appendix. © *1996 American Institute of Physics.* [S0022-2488(96)01305-X]

I. INTRODUCTION

We continue a program initiated some time ago to study the properties of symmetry groups of $d+1$-dimensional space–times with $d<3$. In earlier publications the Galilean group for the case $d=2$ was considered, its central extension carried out,[1] and the system of unitary irreducible representations, both faithful and projective, constructed.[2] The representations of the Galilean group have been constructed independently by Grigore[3] via considerations of a certain group, which is the central extension of the universal covering group of the Galilean group. The conclusions of Ref. 3 are in agreement with those of Refs. 1 and 2. In this paper we consider the Poincaré group for $d=1$ and construct its projective representations. As for the faithful representations of this group, these are well understood and are discussed, for instance, by Barut and Raczka.[4] The Galilean group for $d=1$ is discussed separately in the Appendix.

As is well understood, the projective representations of a group can be obtained from the ordinary representations of its universal central extension.[5,6] The 1+1-dimensional Poincaré group $P(1,1)$ has a one parameter family of central extensions, as shown by Bargmann.[5] This is true of central extension either by the circle group T or by the additive group R of reals. The latter choice has certain technical advantages since the corresponding centrally extended group is simply connected. Here we focus attention on $\hat{P}(1,1)$, which is the central extension of $P(1,1)$ by R.

The group $\hat{P}(1,1)$ is a (non-nilpotent) solvable group (recall that a nilpotent group is solvable but a solvable group is not necessarily nilpotent). The representations of $\hat{P}(1,1)$ may be constructed by an application of the method of Kirillov,[7] wherein the group representations are induced from one-dimensional representations of certain subgroups associated with the co-adjoint orbits of the group. An important question for a general (non-nilpotent) solvable group is if the Kirillov construction yields *all* the irreducible representations of the group. A broad criterion for this to happen is given by the Auslander–Kostant theorem.[8] The latter states that for a connected and simply connected solvable Lie group of type 1 (a Lie group whose representations generate type 1 Von Neumann algebras), the Kirillov method, or possibly a generalization of the original method involving passage from real to complex extension groups, will yield all the irreducible representations. A less general result was given earlier by Bernat,[9] which states that for a solvable Lie group which is exponential (an exponential group is one for which the canonical map from the Lie algebra to the group is surjective), the Kirillov method will give all the irreducible representations. While it is true that $\hat{P}(1,1)$ is exponential and of type 1, as will be shown below, it is actually not necessary to appeal to results of such generality.[8,9] A more restrictive result due to Kirillov,[7] which states that for a *completely solvable* group his method will yield all the representations, is sufficient for our purpose. A completely solvable group, as defined in Ref. 7, is a solvable Lie group G that contains an increasing chain of normal subgroups

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$\{e\}=G_0\subset G_1\subset\cdots\subset G_n=G$ whose dimensions increase by one at each step so that dim $G_k=k$. Our $\hat{P}(1,1)$ is completely solvable by this definition (see below).

This paper is organized as follows. In the next section, we study the groups $P(1,1)$ and $\hat{P}(1,1)$ and establish some of their properties. The co-adjoint orbits of $\hat{P}(1,1)$ are obtained in Secs. III and IV. The unitary irreducible linear representations of $\hat{P}(1,1)$ are obtained in Sec. V and the corresponding projective ones of $P(1,1)$ in Sec. VI. Concluding remarks are made in Sec. VII.

The 1+1 Galilean group is treated separately (from the main body of the paper) in the Appendix. Here the only contribution that we claim as original is in the construction of the central extension of the group. Once this is done, the centrally extended group is recognized to be isomorphic with a certain group whose representations are already known in the mathematical literature.

II. THE POINCARÉ GROUP AND ITS CENTRAL EXTENSION

We denote by $P(1,1)$ the 1+1-dimensional Poincaré group. Let x and t be the coordinates of space–time. The set of transformations $(x,t)\rightarrow(x',t')$, where

$$t'=t\ \cosh z+x\ \sinh z+\eta,\quad x'=t\ \sinh z+x\ \cosh z+u \tag{2.1}$$

constitute $P(1,1)$ under composition. Here z, η, and u are real parameters and $\tanh z$ is the relative velocity connecting the two inertial frames. Thus the typical group element can be displayed in the fashion $(z,\mathbf{u})$, when $\mathbf{u}$ is a 1+1 vector and the group multiplication law is

$$(z,\mathbf{u})(z',\mathbf{u}')=(z+z',\mathbf{u}+\delta(z)\mathbf{u}'), \tag{2.2}$$

where

$$\mathbf{u}=\begin{pmatrix}\eta\\ u\end{pmatrix}\quad\text{and}\quad \delta(z)=\begin{pmatrix}\cosh z & \sinh z\\ \sinh z & \cosh z\end{pmatrix}. \tag{2.3}$$

$P(1,1)$ has two distinguished subgroups. Elements of the form $(z,0)$ generate the subgroup of homogeneous Lorentz transformations, isomorphic with the additive group R of reals. The normal subgroup of translations consists of elements $(0,\mathbf{u})$ and is a two-dimensional vector group R^2. The group $P(1,1)$ is a semi-direct product of these two subgroups. The group $P(1,1)$ as defined above is connected and simply connected and is a solvable (non-nilpotent) group of rank 2, as is easy to verify.

The central extension of $P(1,1)$ is given by Bargmann.[5] For any pair $\mathbf{u},\mathbf{u}'$ of 1+1 vectors let $\mathbf{u}\wedge\mathbf{u}'=\eta u'-u\,\eta'$. Let $r=(z,\mathbf{u})$, $r'=(z',\mathbf{u}')$; $r,r'\in P(1,1)$. Then an R-valued representative (of an equivalence class with respect to coboundaries) two-cocycle on $P(1,1)$ is[5]

$$m(r,r')=\mathbf{u}\wedge\delta(z)\mathbf{u}'. \tag{2.4}$$

The above two-cocycle gives the desired central extensions. We have the central extension of $P(1,1)$ by T (circle group) given by $\{(r,\xi)\}$, $r\in P(1,1)$, $\xi\in T$, with the composition law

$$(r,\xi)(r'\xi')=(rr',\xi\xi'\ \exp(i\lambda/2)m(r,r')). \tag{2.5}$$

On the other hand, the central extension of $P(1,1)$ by R—the group $\hat{P}(1,1)$—consists of elements (r,ω), $r\in P(1,1)$, $\omega\in R$, with the multiplication rule

$$(r,\omega)(r'\omega')=(rr',\omega+\omega'+\tfrac{1}{2}m(r,r')), \tag{2.6}$$

where rr' is given by Eq. (2.2) and $m(r,r')$ by Eq. (2.4). We proceed to analyze the structure of $\hat{P}(1,1)$.

Elements of $\hat{P}(1,1)$ of the form $(r,0)$ with $r \in P(1,1)$ restricted to be of the form $r=(z,0)$ constitute a subgroup isomorphic with the homogeneous Lorentz group. We call this subgroup L. Elements (r,ω) with r having the form $r \in P(1,1)=(0,\mathbf{u}) \equiv (0,\eta,u)$ generate a subgroup isomorphic with the Heisenberg–Weyl group (the group of 3×3 triangular matrices under matrix multiplication); the required isomorphy is given by

$$(\eta,u,\omega) \equiv (0,\eta,u,\omega) \leftrightarrow \begin{pmatrix} 1 & \eta & \omega+\frac{1}{2}\eta u \\ 0 & 1 & u \\ 0 & 0 & 1 \end{pmatrix}. \tag{2.7}$$

Call the above subgroup N. First, it is easy to check using Eq. (2.6) that the first derived group (commutator subgroup) of $\hat{P}(1,1)$ is N, the second derived group is $R=\{(0,0,\omega)\}$, and the third derived group is trivial; thus $\hat{P}(1,1)$ is a solvable group of rank 3. It is also easy to verify that $\hat{P}(1,1)$ is not nilpontent. Further, $\hat{P}(1,1)$ has the structure of a semi-direct product. This follows from the existence of a unique decomposition for every element $(r,\omega) \equiv (z,\eta,u,\omega) \in \hat{P}(1,1)$ given by

$$(z,\eta,u,\omega)=(0,\eta,u,\omega)(z,0,0,0), \tag{2.8}$$

where $(0,\eta,u,\omega) \in N$ and $(z,0,0,0) \in L$, plus the fact that the only element that N and L share in common is the identity of $\hat{P}(1,1)$. Thus $\hat{P}(1,1)=NL$ with N normal. The group $\hat{P}(1,1)$ is connected and simply connected; in fact, the group manifold is just R^4 topologically. We note next that the semi-direct product is *regular*, in the sense of Mackey. This may be seen as follows. Let N^* denote the dual space of N (the space of equivalence classes of unitary, irreducible representations of N). The unitary irreducible representations of N are of two types:[7] (i) those labeled by a nonzero real number λ, which is essentially the eigenvalue of the central charge of the Lie algebra of N, and (ii) those labeled by a pair (p_0,p) of real numbers, which is the case when the central charge has eigenvalue zero, the group effectively Abelian ($\approx R^2$), and (p_0,p) label the characters of R^2. Thus the space N^* may be visualized as a plane with a line perpendicular to it. Under the action of L the points of N^* respond as follows: the points on the line, labeled by λ, do not move, since the central charge of Lie (N) commutes with the L-action, and the points on the plane $\{(p_0,p)\}$ behave as $1+1$ vectors. We thus see that the L-orbits in N^* are as follows: (i) one-point orbits for each value of λ, (ii) the one-point orbit given by (0,0) on the plane, and (iii) the sets $\{(p_0,p)\}$ with $p_0^2-p^2=\pm m^2$, $m \geqslant 0$, the corresponding orbits being hyperbolas and ''light-cones.'' Now, the semi-direct product $\hat{P}(1,1)=NL$ will be regular if there exists in N^* a set (a Borel set) that meets each L-orbit in N^* at exactly one point.[10] The desired set is simply the union of the λ-line with S, where S is a Borel set that meets each planar orbit at one point. The set S may be constructed without difficulty. Thus the semi-direct product is regular. Consider now the stability groups (little groups) of the L-orbits in N^*. It is clear from the foregoing discussion that the stability group of each one-point orbit is L, and the stability group of each non-one-point orbit is trivial (one element group). In every case, the stability group is of type 1. From the last conclusion and using the regularity of the semi-direct product, it now follows from a theorem of Mackey[10] that $\hat{P}(1,1)$ is a group of type 1. The same conclusion may also be reached from an analysis of the co-adjoint orbits (see below).

We shall now show that the group $\hat{P}(1,1)$ is completely solvable, in the sense of Kirillov.[7] For this purpose, the coordinate system on the group that we have used thus far is not convenient. Another set of (global) coordinates on $\hat{P}(1,1)$ will be introduced in Sec. IV [see Eq. (4.2)]. Using the latter, and the corresponding group multiplication law given by Eq. (4.3), we may verify the existence of the following sequence of normal subgroups [normal in $\hat{P}(1,1)$]:

$$\{e\}=G_0 \subset G_1 \subset G_2 \subset G_3=N \subset G_4=\hat{P}(1,1), \tag{2.9}$$

where $\dim(G_k)=k$. Here $G_2=\{(0,x,0,\omega)\}=R^2$ and $G_1=\{(0,0,0,\omega)\}=R$, in the notation of Eq. (4.2). This proves that $\hat{P}(1,1)$ is completely solvable.

The sequence (2.9) gives rise to a corresponding sequence at the level of Lie algebras in which every entry G_k is replaced by its Lie algebra Lie (G_k), every Lie (G_k) is an ideal in Lie $(\hat{P}(1,1))$, and dim Lie $(G_k)=k$. Since $\hat{P}(1,1)$ is connected, simply connected, and solvable, the existence of such a sequence of ideals in its *real* Lie algebra implies, via a result due to Dixmier[11] (corollary to his theorem 3), that $\hat{P}(1,1)$ is an exponential group.

We pass on to compute the co-adjoint orbits of $\hat{P}(1,1)$.

III. COADJOINT ORBITS

The Lie algebra of $\hat{P}(1,1)$ is a four-dimensional real vector space. We may choose basis vectors N, H, P, and E that obey the commutation relations

$$[N,\ H]=P,\quad [N,\ P]=H,\quad [H,\ P]=E; \tag{3.1}$$

N,P,H are the infinitesimal generators of Lorentz transformation, space translations, and time translation, respectively, E is the central generator. The operators H, P, and E generate the Heisenberg algebra, which is an ideal.

The typical element (z,η,u,ω) of the group $\hat{P}(1,1)$ is

$$(z,\eta,u,\omega)=\exp(\omega E+\eta H+uP)\exp(zN). \tag{3.2}$$

Several comments are in order. First, in writing Eq. (3.2), we utilized the semi-direct product structure of $\hat{P}(1,1)$ plus the fact that the Heisenberg–Weyl group is nilpotent and hence exponential; here η, u and ω are the exponential coordinates. Thus (3.2) gives a globally valid coordinate system. The group multiplication law can be derived from Eqs. (3.1) and (3.2) together with the use of the Baker–Hausdorff formula; one thus obtains Eq. (2.6). An alternative route to the same conclusion will employ a faithful matrix representation of Eq. (3.1). Such a representation is

$$N=\begin{pmatrix}0&0&0&0\\0&0&1&0\\0&1&0&0\\0&0&0&0\end{pmatrix},\quad H=\begin{pmatrix}0&0&1&0\\0&0&0&1\\0&0&0&0\\0&0&0&0\end{pmatrix},$$
$$P=\begin{pmatrix}0&-1&0&0\\0&0&0&0\\0&0&0&1\\0&0&0&0\end{pmatrix},\quad E=\begin{pmatrix}0&0&0&2\\0&0&0&0\\0&0&0&0\\0&0&0&0\end{pmatrix}. \tag{3.3}$$

It is useful to note $H^2=P^2=E^2=0$ and $N^3=N$ and further that

$$N^2=\begin{pmatrix}0&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&0\end{pmatrix}. \tag{3.4}$$

A group acts on its Lie algebra with the aid of the adjoint representation. Precisely, this action is $\mathrm{Ad}\ (g)W=gWg^{-1}$ for $g\in G$, $W\in\mathrm{Lie}(G)$. Use of the above matrix realization together with Eq. (3.2) thus allows us to explicitly compute the adjoint action. Let us write the generic element

W of the Lie algebra as $W=aE+bH+cP+dN$, where a,b,c,d are real numbers. Then the adjoint action of g^{-1} [it will turn out more useful for us to consider the action of the inverse element; here, g is given by Eq. (3.2)] is Ad $(g^{-1})W=W'=a'E+b'H+c'P+d'N$, where

$$\begin{aligned} a' &= a-c\,\eta+bu+(d/2)(u^2-\eta^2), \\ b' &= (b+du)\cosh z-(c+d\,\eta)\sinh z, \\ c' &= (c+d\,\eta)\cosh z-(b+du)\sinh z, \quad d'=d, \end{aligned} \tag{3.5}$$

as a straightforward calculation shows.

A group acts on a vector space which is dual to its Lie algebra with the aid of the co-adjoint representation. Let E^*, H^*, P^*, and N^* be a basis in the dual vector space to Lie $\hat{P}(1,1)$. This means

$$\begin{aligned} &(E^*,E)=1, \quad (E^*,X)=0 \quad \text{for } X=H,P,N, \\ &(H^*,H)=1, \quad (H^*,X)=0 \quad \text{for } X=E,P,N, \\ &(P^*,P)=1, \quad (P^*,X)=0 \quad \text{for } X=E,H,N, \\ &(N^*,N)=1, \quad (N^*,X)=0 \quad \text{for } X=E,H,P, \end{aligned} \tag{3.6}$$

where (,) denotes a scalar product. Let us consider the typical element ℓ of the dual space

$$\ell=\delta E^*+\beta H^*+\gamma P^*+\alpha N^*, \tag{3.7}$$

and let W be, as before,

$$W=aE+bH+cP+dN. \tag{3.8}$$

Then

$$(\ell,W)=a\,\delta+b\,\beta+c\,\gamma+d\,\alpha. \tag{3.9}$$

Let us write $\ell(W)=(\ell,W)$. Let K denote the co-adjoint action and $K(g)\ell$ denote that of g on ℓ. Then precisely

$$(K(g)\ell)(W)=\ell(\mathrm{Ad}(g^{-1})W) \tag{3.10}$$

defines the co-adjoint action. Let $K(g)\ell=\ell'=\delta' E^*+\beta' H^*+\gamma' P^*+\alpha' N^*$. Then we compute from Eqs. (3.5) and (3.10) that

$$\begin{aligned} \delta' &= \delta, \quad \beta'=u\,\delta+\beta\,\cosh z-\gamma\,\sinh z, \\ \gamma' &= -\,\eta\delta-\beta\,\sinh z+\gamma\,\cosh z, \\ \alpha' &= \alpha+(\delta/2)(u^2-\eta^2)+\beta(u\,\cosh z-\eta\,\sinh z)+\gamma(\eta\,\cosh z-u\,\sinh z), \end{aligned} \tag{3.11}$$

where g is given by Eq. (3.2). It follows, from the above, that $\beta^2-\gamma^2-2\delta\alpha$ remain invariant under the co-adjoint action. The co-adjoint orbits (K-orbits) are now easy to enumerate. Each K-orbit is two-dimensional, since $\{(\alpha,\beta,\gamma)\}$ generate an orbit and there is a constraint connecting these three (real) variables. Each K-orbit is characterized by two numbers: the value of δ and that of the invariant $\beta^2-\gamma^2-2\delta\alpha$. The K-orbits are of two broad types.

The K-orbits of $\hat{P}(1,1)$ for the case $\delta=0$ plainly coincide with the K-orbits of P (1,1). A complete listing of the latter may be found in a recent contribution of Ali and Mueller.[12] The representations constructed from these orbits coincide with the known[4] faithful representations of $P(1,1)$. We do not discuss these orbits any further.

Consider now the K-orbits corresponding to $\delta\neq 0$. An orbit is characterized by δ and the constant $c=\beta^2-\gamma^2-2\delta\alpha$. The point $(\alpha_0=-c/2\delta,0,0,\delta)\equiv\delta E^*+\alpha_0 N^*$ belongs to the orbit. Indeed, we can reach the typical point $(\alpha=-(c+\gamma^2-\beta^2)/2\delta,\beta,\gamma,\delta)$ on the orbit from the point $(\alpha_0,0,0,\delta)$ under the action (3.11) of the group element $(0,\eta,u,0)$ with $\eta=-\gamma/\delta$ and $u=\beta/\delta$. Thus the constant c plays no essential role and we may simply characterize an orbit by the point $(\alpha,0,0,\delta)$ belonging to it. Consider now the stability group H of the orbit, i.e., of the representative point $(\alpha,0,0,\delta)$. From Eq. (3.11) we obtain $H=\{(z,0,0,\omega)\}\equiv R\otimes R$. From the group multiplication law (2.6), it follows that every element of $\hat{P}(1,1)$ admits the decomposition

$$(z,\eta,u,\omega)=(z,0,0,\omega)(0,\eta',u',0), \tag{3.12}$$

where $\eta'=\eta\cosh z-u\sinh z$ and $u'=u\cosh z-\eta\sinh z$. Thus η and u may be chosen to (globally) parametrize the homogeneous space of right cosets of H in $\hat{P}(1,1)$. Plainly, the coset space is R^2. The K-orbit is homeomorphic to the coset space since $\hat{P}(1,1)$ is locally compact. Thus the K-orbit has trivial de Rham cohomology. In particular, the Kostant–Kirillov symplectic two-form on the K-orbit is *exact* (the conclusion remains valid for $\delta=0$ orbits).[12]

From the above it would follow, via an application of the Auslander–Kostant theorem, that $\hat{P}(1,1)$ is a group of type 1, provided the *space of orbits* can be shown to possess the T_0 separability property. As for the latter requirement, we note that each K-orbit is parametrized by the pair (α,δ) of real numbers [or equivalently by the pair (c,δ) of real numbers] and hence the space of orbits is the plane R^2 which has T_0 separability property. The conclusion, once again, is that $\hat{P}(1,1)$ belongs to type 1.

In the Kirillov method, a vital role is played by the admissible subalgebras corresponding to an orbit. We proceed to construct these. Let G be a Lie group, Lie (G) its Lie algebra, Ω a K-orbit of G, and $\tilde{\ell}$ a point belong to Ω. A sub-Lie algebra A of Lie (G) is said to be *admissible* (or *polarizing*) if the following conditions are satisfied:[13]

(1) $\tilde{\ell}([X,Y])=0$ for arbitrary X and Y belonging to A; here, as before, $\tilde{\ell}(X)\equiv(\tilde{\ell},X)$. The algebra A is said to be subordinate to the point $\tilde{\ell}$.
(2) The codimension of A in Lie(G) [that is the difference dim Lie$(G)-\dim A$] is one-half the dimension of Ω.
(3) $\tilde{\ell}+A^{\perp}\subset\Omega$; here $A^{\perp}$ is the set of all points F belonging to the dual space of Lie(G) for which $F(X)=0$ for all $X\in A$; this is Pukanszky's condition.

We select the point $\tilde{\ell}=(\alpha,0,0,\delta)$ on the orbit. Then we have two admissible subalgebras A_+ and A_-; A_+ is generated by N, P_+, and E while A_- is generated by N, P_-, and E; here $P_\pm=H\pm P$. First, these are subalgebras since $[N,P_\pm]=\pm P_\pm$. The condition (1) above is checked easily. Thus for A_+, let $X=x_1N+x_2P_++x_3E$ and $Y=y_1N+y_2P_++y_3E$. Then $[X,Y]=(x_1y_2-x_2y_1)P_+$ and $\tilde{\ell}([X,Y])=0$ follows from Eq. (3.9). Now $\dim A_\pm=3$ and dim Lie $(\hat{P}(1,1))=4$; thus codim $A_\pm=1$; moreover dim $\Omega=2$ (proved before). Thus condition (2) is satisfied. That condition (3) is fulfilled will be shown in the next section using a different set of group coordinates better suited for this purpose.

IV. LIGHT-CONE COORDINATES

As we saw above, the basis in our Lie algebra given by the basis vectors N, P_+, P_-, and E will be more convenient for the discussion to follow. Here $P_\pm=H\pm P$ and we may note

$$[N,P_\pm]=\pm P_\pm,\quad [P_-,P_+]=2E. \tag{4.1}$$

Note the existence of a sequence of ideals generated by E, (E,P_+), and (E,P_+,P_-) as stated in the penultimate paragraph of Sec. II. Corresponding to the present choice of the basis in the Lie algebra, there is a coordinate system for the group manifold. Let us write the typical group element (z,x,y,ω) in the fashion

$$(z,x,y,\omega)=e^{\omega E}e^{xP_+}e^{yP_-}e^{zN}. \tag{4.2}$$

The new coordinates are related to the old by $x+y=\eta$, $x-y=u$; the parametrization of ω above is simply related to that in Eq. (3.2), via the Baker–Hausdorff formula (see below). The group multiplication law in these coordinates is given by

$$(z,x,y,\omega)(z',x',y',\omega')=(z+z',x+e^z x',y+e^{-z}y',\omega+\omega'+2e^z yx'). \tag{4.3}$$

Note the expression for the inverse

$$(z,x,y,\omega)^{-1}=(-z,-e^{-z}x,-e^z y,2xy-\omega). \tag{4.4}$$

The co-adjoint action in the present coordinate system may be computed exactly as before. Let the typical point ℓ on the dual space be

$$\ell=\delta E^*+\tilde{\beta}P_+^*+\tilde{\gamma}P_-^*+\alpha N^*. \tag{4.5}$$

Then under the action of (z,x,y,ω), $(\delta,\tilde{\beta},\tilde{\gamma},\alpha)$ go over to $(\delta',\tilde{\beta}',\tilde{\gamma}',\alpha')$, where

$$\delta'=\delta,\quad \tilde{\beta}'=e^{-z}\tilde{\beta}-2\delta y,\quad \tilde{\gamma}'=e^z\tilde{\gamma}+2\delta x,\quad \alpha'=\alpha+xe^{-z}\tilde{\beta}-ye^z\tilde{\gamma}-2\delta xy, \tag{4.6}$$

and $\tilde{\beta}\tilde{\gamma}-2\delta\alpha$ is an invariant of the orbit. Indeed, a comparison of Eq. (4.5) with Eq. (3.7) shows $\tilde{\beta}=\beta+\gamma$, $\tilde{\gamma}=\beta-\gamma$. Further, let us call the parameter ω in Eq. (3.2) as $\overline{\omega}$ and ω be as in Eq. (4.2); then $\overline{\omega}=\omega-xy$. From these observations and the fact that $\overline{\omega}$ does not appear in Eq. (3.11), Eq. (4.6) now follows easily from Eq. (3.11). As before, the point $(\alpha,0,0,\delta)\equiv\alpha N^*+\delta E^*$ belongs to the K-orbit, and the subalgebras $A_\pm$ with codimension one are subordinate to this point. We may now verify Pukanszky's condition. The annihilators are $A_+^\perp=\{\xi P_-^*\}$, ξ real; $A_-^\perp=\{\rho P_+^*\}$, ρ real. Consider the case A_-. Then $(\alpha,0,0,\delta)+A_-^\perp$ is the set $\{(\alpha,\rho,0,\delta)\}$ as ρ ranges over reals. The question is do these points belong to the K-orbit? The answer is yes, since a point $(\alpha,\rho,0,\delta)$ may be reached from the point $(\alpha,0,0,\delta)$ on the orbit, under the action (4.6) of the group element (z,x,y,ω) with $z=x=\omega=0$ and $y=-\rho/2\delta$. One similarly verifies the condition for the subalgebra A_+. Thus, Pukansky's condition stands satisfied and the proof of the fact that $A_\pm$ are *admissible* subalgebras is now complete.

V. REPRESENTATIONS

In the Kirillov theory, the group representations are constructed as follows. One selects a point $\tilde{\ell}$ on the co-adjoint orbit and an accompanying admissible subalgebra A. Let K denote the subgroup corresponding to A. The point $\tilde{\ell}$ allows one to construct *one-dimensional* representations of K (since A is subordinate to $\tilde{\ell}$, it is *effectively* Abelian on $\tilde{\ell}$). The group representations are the induced representations; induced from the one-dimensional representations of subgroup K.

We may note the following general features of the Kirillov theory. First, the precise choice of $\tilde{\ell}$ plays no role; one can select any point on the orbit depending on one's convenience. Second, one may work with any one of the admissible subalgebras, in case there are more than one such, corresponding to a chosen $\tilde{\ell}$. Thus there is a one-to-one correspondence between representations and co-adjoint orbits. *The representation constructed as above will be irreducible*. The representations can be made unitary with respect to a suitable inner product in a Hilbert space.

Let us select the admissible subalgebra A_+ for the chosen point $\tilde{\ell}=(\alpha,0,0,\delta)$. Let K denote the subgroup corresponding to A_+. As before, A_+ is spanned by generators N, P_+, and E and is a real

subalgebra; the subgroup K is the set $\{(z,x,0,\omega)\}$ in the notation of Eq. (4.2). Notice K is *not* a normal subgroup, and A_+ *not* an ideal. Let $k=(z,x,0,\omega)$, $k\in K$, and we set

$$\chi(k)=e^{i\delta\omega}e^{i\alpha z}. \tag{5.1}$$

Then it follows that χ satisfies the character equation $\chi(k)\chi(k')=\chi(kk')$. Thus χ is a one-dimensional representation of K. We have to carry out the inducing construction from this representation χ.

At this stage, let us recall the basic idea behind the construction of induced representations. Let G be a (Lie) group, K a closed subgroup of G, and L_k a (finite dimensional) unitary representation of K in a Hilbert space L. Consider measurable L-valued functions f on G (functions of group parameters) that satisfy the condition

$$f(gk)=L_k^{-1}f(g), \quad g\in G,k\in K, \tag{5.2}$$

and let

$$(U^L(g_0)f\ )(g)=\rho_{g_0}(g)f(g_0^{-1}g), \tag{5.3}$$

where $\rho_{g_0}(g)$ is a certain positive function (see below). Then the map $g\to U^L(g)$ is a representation of G induced by the representation L_k of K. The condition (5.2) is the covariance condition on left cosets and because of it we shall be able to identify the functions f with certain functions (L-valued) defined on the left coset space $X=G/K$. The $\rho_{g_0}(g)$ appearing in (5.3) is precisely the square root of the Radon–Nikodym derivative $d\mu(g_0^{-1}x)/d\mu(x)$, where $x=\pi(g)$ and $\pi{:}G\to X$ is the natural projection. Here μ is a measure on X that is *quasi-invariant* under the action of G. Further restrictions on the functions f will be spelled out as the need arises. In our case L_k is given by χ [see (5.1)] and f are ordinary functions.

We make a remark. The above construction actually gives the group representation on the left coset space. We may similarly construct representations on the right coset space $X_R=K\backslash G$. Now Eq. (5.2) will modify to $f(kg)=L_kf(g)$ and Eq. (5.3) to $(U^L(g_0)f\ )(g)=\rho_{g_0}(g)f(gg_0)$. Here $\rho_{g_0}(g)$ is the square root of $d\mu(xg_0)/d\mu(x)$, where x belongs to the right coset and xg_0 is the right action of g_0 on x.

We proceed to construct the group representations. The covariance condition (5.2) becomes

$$f(gk)=\chi^{-1}(k)f(g). \tag{5.4}$$

Let $g=(z',x',y',\omega')$ and $k=(z,x,0,\omega)$; then using the multiplication law equation (4.3) we have

$$gk=(z'+z,x'+e^{z'}x,y',\omega'+\omega+2e^{z'}y'x), \tag{5.5}$$

and Eq. (5.4) acquires the form

$$f(z'+z,x'+e^{z'}x,y',\omega'+\omega+2e^{z'}y'x)=e^{-i\delta\omega}e^{-i\alpha z}f(z',x',y',\omega'). \tag{5.6}$$

The solution of (5.6) is shown without difficulty to be given by

$$f(z,x,y,\omega)=e^{-i\alpha z}e^{-i\delta(\omega-2xy)}F(y), \tag{5.7}$$

where $F(y)$ is a function of y alone. One may check that Eq. (5.7) solves Eq. (5.6). Because of Eq. (5.7) the group representations defined on functions f will factor into those defined on functions F; that is, on the left coset space whose point y is.

The next problem is to figure out the form of the Radon–Nikodym derivative. First, we note that every group element g admits the decomposition $g=sk$ with $k\in K$ and $s\in G$. This is given by

$$(z,x,y,\omega)=(0,0,y,0)(z,x,0,\omega-2xy) \tag{5.8}$$

and thus the left coset space may be parametrized by y [the element $(0,0,y,0)\in G$ goes over to y under natural projection]. The left action of the group on the coset space is computed as follows. With g as above we have

$$(z,x,y,\omega)(0,0,y_0,0)=(z,x,y+e^{-z}y_0,\omega)=(0,0,y+e^{-z}y_0,0)(z,x,0,\omega-2x(y+e^{-z}y_0)) \tag{5.9}$$

and thus $y_0\to e^{-z}y_0+y$ under the left action of (z,x,y,ω). Similarly, $y_0\to e^{z}(y_0-y)$ under the left action of the inverse $(z,x,y,\omega)^{-1}$. Thus the Lebesgue measure dy on the left coset space is not invariant under the group action; it is actually an example of the so-called quasi-invariant measure that behaves under group action as $dy\to e^{-z}\,dy$, and dy and its transform share the same null set. Here we choose the quasi-invariant Lebesgue measure dy and then the Radon–Nikodym derivative $d\mu(g_0^{-1}y)/d\mu(y)$ is just e^{z}. Thus $\rho_{g_0}(g)$ is $e^{z/2}$. We are now in a position to write down the explicit form of the group representation. From Eq. (5.3) we have

$$\begin{aligned}&(U(z,x,y,\omega)f\,)(z',x',y',\omega')\\&\quad=e^{z/2}f((z,x,y,\omega)^{-1}(z',x',y',\omega'))\\&\quad=e^{z/2}f(z'-z,e^{-z}(x'-x),e^{z}(y'-y),\omega'-\omega+2y(x-x')),\end{aligned} \tag{5.10}$$

where Eqs. (4.3) and (4.4) have been utilized in the second step. Equation (5.10) gives the desired representation; here the functions f satisfy the condition given by Eq. (5.7). We proceed to analyze the content of the representation obtained. First, we note

$$\begin{aligned}(U(e^{\omega E})f\,)(z',x',y'\omega')&\equiv(U(0,0,0,\omega)f\,)(z',x',y',\omega')\\&=f(z',x',y',\omega'-\omega)\\&=e^{i\delta\omega}f(z',x',y',\omega'),\end{aligned} \tag{5.11}$$

where Eq. (5.7) was used at the last step. It follows from the above that

$$E=i\delta. \tag{5.12}$$

Next we have from Eq. (5.10)

$$(U(e^{xP_+})f\,)(z',x',y',\omega')\equiv(U(0,x,0,0)f\,)(z',x',y',\omega')=f(z',x'-x,y',\omega'). \tag{5.13}$$

Differentiating the above with respect to x and then setting $x=0$, we obtain

$$(U(P_+)f\,)(z',x',y',\omega')=-\frac{\partial}{\partial x'}f(z',x',y',\omega')=-2i\delta y'f(z',x',y',\omega'), \tag{5.14}$$

where Eq. (5.7) was used at the last step. Thus acting on $f(z,x,y,\omega)$, P_+ is the operator of multiplication by $-2i\delta y$. The remaining operators of interest are similarly found. We obtain

$$(U(P_-)f\,)(z,x,y,\omega)=\left(2i\delta x-\frac{\partial}{\partial y}\right)f(z,x,y,\omega), \tag{5.15}$$

$$(U(N)f\,)(z,x,y,\omega)=\left(\frac{1}{2}-\frac{\partial}{\partial z}+y\,\frac{\partial}{\partial y}-x\,\frac{\partial}{\partial x}\right)f(z,x,y,\omega). \tag{5.16}$$

With the aid of Eq. (5.7) the above action of the operators on f may be translated into action on the functions F. The result is

$$(U(P_-)F)(y) = -\frac{d}{dy}F(y), \tag{5.17}$$

$$(U(N)F)(y) = \left(\frac{1}{2} + y\frac{d}{dy} + i\alpha\right)F(y). \tag{5.18}$$

The above expressions satisfy the correct commutation relations of operators N, P_+, P_-, and E, as may be verified.

We should finally consider the restrictions on the function F. From (5.17) we see that for *finite* translation by y to be defined, the function F must be infinitely differentiable; that is, F is an analytic function of the real variable y. Next, we shall restrict F to be square integrable with respect to the Lebesgue measure dy on the left coset space. The set of all such functions, which may be taken to be real valued, then constitute a separable Hilbert space H with respect to the inner product

$$(F_1, F_2) = \int F_1(y)F_2(y)dy. \tag{5.19}$$

Our representation is then unitary in H and is strongly continuous (continuous in the strong topology of H); it is irreducible because of reasons explained before. This concludes our discussion of the representations of $\hat{P}(1,1)$.

VI. PROJECTIVE REPRESENTATIONS OF THE 1+1 POINCARÉ GROUP

The nontrivial projective unitary irreducible representations of the Poincaré group $P(1,1)$ may now be obtained from the representations of the centrally extended group $\hat{P}(1,1)$ constructed in Sec. V.

In the light-come coordinates the typical element of the Poincaré group $P(1,1)$ is written in the fashion (z,x,y) and the multiplication law is

$$(z,x,y)(z',x',y') = (z+z', x+e^z x', y+e^{-z}y') \tag{6.1}$$

as follows from Eq. (2.2). The desired representations of $P(1,1)$ follow from Eqs. (5.10) and (5.7) upon setting $\omega=\omega'=0$. Defining $f(z,x,y)\equiv f(z,x,y,0)$ we thus have

$$(U(z,xy)f)(z',x',y') = e^{z/2}e^{2i\delta(x'-x)y}f(z'-z, e^{-z}(x'-x), e^z(y'-y)). \tag{6.2}$$

The expressions for the generators N, P_+, P_- of the Lie algebra are exactly the same as those in Sec. V. The above is a projective representation of $P(1,1)$. Indeed, from (6.2) we compute

$$(U(0,0,y)U(0,x,0)f)(z',x',y') = e^{2i\delta x'y}f(z',x'-x,y'-y). \tag{6.3}$$

On the other hand, from (6.1) and (6.2), it follows

$$(U((0,0,y)(0,x,0))f)(z',x',y') = (U(0,x,y)f)(z',x',y') = e^{2i\delta(x'-x)y}f(z',x'-x,y'-y), \tag{6.4}$$

and thus

$$U(0,0,y)U(0,x,0) = e^{2i\delta xy}U((0,0,y)(0,x,0)), \tag{6.5}$$

which shows that our representation is projective.

VII. CONCLUDING REMARKS

The faithful representations of $P(1,1)$ corresponding to timelike and lightlike representations describe the states of a massive or massless particle in one spatial dimension. The projective representations of $P(1,1)$ clearly do not admit a free-particle interpretation; the intriguing question is if they possess any physical application. Unfortunately, we have not found an answer to this question, thus far. On the other hand, the group $\hat{P}(1,1)$ does seem to possess physical utility. A *gauge* theory built upon $\hat{P}(1,1)$ was shown by Cangemi and Jackiw[14] to be efficacious in analyzing the structure of 1+1-dimensional ''black-hole'' models.

The group $\hat{P}(1,1)$ is closely related to two other groups of interest in physics and it may not be out of place to make a few remarks concerning these relationships. The group $P(1,1)$ is related to $E(2)$—the Euclidean group on the plane. Indeed, by replacing the 1+1 Lorentz transformation by a planar rotation we pass from $P(1,1)$ to $E(2)$. The central extension of these two groups are similarly related. The central extension $\hat{E}(2)$ of $E(2)$ by R is locally isomorphic with (shares an isomorphic Lie algebra with) the quantum harmonic oscillator group; the difference between the two at the global level resides entirely on the range of one of the group parameters. The parameter of rotation in $\hat{E}(2)$ is an angle that ranges from 0 to 2π; while the corresponding parameter for the oscillator group—the time parameter conjugate to the Hamiltonian—ranges over the real line. The representations of the oscillator group were constructed by Streater[15] a long time ago, using the Kirillov (actually a generalization of the original Kirillov method involving complex Lie algebras) as well as the Mackey method. The close parallelism between Streater's treatment and that of the present paper should be noted. It also follows that the projective representations of $E(2)$ can be obtained very simply from the results of Streater.[15] Actually, the projective representations of $E(2)$ are useful in the problem of electrons in a uniform magnetic field. An elegant treatment of this problem has been given by Divakaran and Rajagopal.[16]

Note added in proof. Projective representations of the 2+1 and 1+1 Galilean group are constructed independently in H. D. Doebner and H. J. Mann, J. Math. Phys. **36**, 3210 (1995). Many properties of the centrally extended 1+1 Poincaré group are discussed in D. Cangemi and R. Jackiw, Ann. Phys. (NY) **225**, 229 (1993) and Phys. Rev. D **50**, 3913 (1994). In particular, the exactness of the symplectic two-form on the co-adjoint orbit is proved by explicit construction in the latter. It is a pleasure to thank R. Jackiw for correspondence regarding these and related matters.

APPENDIX: THE 1+1 GALILEAN GROUP

The 1+1 Galilean group is the group under composition of the set of space–time transformations

$$x' = x - vt + u, \quad t' = t + \eta. \tag{A1}$$

The typical group element is (v, η, u) with the multiplication law

$$(v, \eta, u)(v', \eta', u') = (v + v', \eta + \eta', u + u' - \eta' v). \tag{A2}$$

The group is isomorphic with the Heisenberg–Weyl group, the isomorphism being explicitly

$$(v, \eta, u) \leftrightarrow \begin{pmatrix} 1 & -v & u \\ 0 & 1 & \eta \\ 0 & 0 & 1 \end{pmatrix}. \tag{A3}$$

The corresponding Lie algebra is a three-dimensional real vector space in which one can choose basis vectors N, P, H that satisfy the commutation relations

$$[N, H]=P, \quad [N, P]=0, \quad [H, P]=0. \tag{A4}$$

We consider the problem of central extension of the Galilean group. It has two equivalence classes of two-cocycles. We can choose the representative two-cocycles (one from each equivalence class) to be

$$m_1(r,r')=\tfrac{1}{2}v^2\eta'-v u', \quad m_2(r,r')=\tfrac{1}{2}v\,\eta'^2-\eta u'+v\,\eta\eta', \tag{A5}$$

where $r\equiv(v,\eta,u)$ and $r'=(v',\eta',u')$. That the above expressions satisfy the cocycle identities and are nontrivial (not coboundaries) may be checked along the same lines as in Ref. 1. We may thus construct the universal centrally extended group as follows. The typical group element is $(r,\theta_1,\theta_2)\equiv(v,\eta,u;\theta_1,\theta_2)$ with the multiplication law

$$(r,\theta_1,\theta_2)(r',\theta_1',\theta_2')=(rr',\theta_1+\theta_1'+m_1(r,r'),\theta_2+\theta_2'+m_2(r,r')). \tag{A6}$$

where θ_1 and θ_2 are a pair of real variables. It is useful to note the corresponding Lie algebra central extension, which is given by

$$[N, H]=P, \quad [N, P]=A, \quad [H, P]=B, \tag{A7}$$

where A and B are central charges (commute with every generator). Note P is no longer central.

The centrally extended group, as defined above, is connected and simply connected. Furthermore, it is a *nilpotent* Lie group (of dimension five), as is easy to check from Eq. (A6) or from Eq. (A7). At this stage we recall the fact that all nilpotent Lie groups of dimension less than 6 were classified by Dixmier[17] in 1959. Thus our centrally extended group must be one in his classification. In fact, *our group is the group* $\Gamma_{5,4}$ *in the Dixmier classification*. The complete system of unitary, irreducible representation of $\Gamma_{5,4}$ has been given in Ref. 17. Lifting the latter to projective representations of the Galilean group is trivial (be setting $\theta_1=\theta 2=0$), and there remains nothing more to discuss.

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Quantum homogeneous spaces as quantum quotient spaces

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It is shown that certain embeddable homogeneous spaces of a quantum group that do not correspond to a quantum subgroup still have the structure of quantum quotient spaces. A construction of quantum fibre bundles on such spaces is proposed. The quantum plane and the general quantum two-spheres are discussed in detail. [S0022-2488(96)02705-1]

I. INTRODUCTION

A homogeneous space X of a Lie group G may be always identified with the quotient space G/G_0, where G_0 is a Lie subgroup of G. When the notion of a homogeneous space is generalized to the case of quantum groups or noncommutative Hopf algebras the situation becomes much more complicated. A general quantum homogeneous space of a quantum group H need not be a quotient space of H by its quantum subgroup. By a quantum subgroup of H we mean a Hopf algebra H_0 such that there is a Hopf algebra epimorphism $\pi{:}H\to H_0$. The quotient space is then understood as a subalgebra of H of all points that are fixed under the coaction of H_0 on H induced by π. A quantum homogeneous space B of H might be such a quotient space but it is not in general. There is, however, a certain class of quantum homogeneous spaces, of which the quantum two sphere of Podleś[1] is the most prominent example, that not being quotient spaces by a quantum subgroup of H, may be embedded in H. One terms such homogeneous spaces *embeddable*.[2] The general quantum two sphere $S^2_q(\mu,\nu)$ is such an embeddable homogeneous space of the quantum group $\mathrm{SU}_q(2)$, and it is a quantum quotient space in the above sense when $\nu=0$. In the latter case the corresponding subgroup of $\mathrm{SU}_q(2)$ may be identified with the algebra of functions on $U(1)$. In this article it is shown that certain embeddable quantum homogeneous spaces, and the general quantum two-sphere $S^2_q(\mu,\nu)$ among them, can still be understood as quotient spaces or fixed point subalgebras. It is shown that there is a coalgebra C and a coalgebra epimorphism $\pi{:}H\to C$ such that the fixed point subspace of H under the coaction of C on H induced from the coproduct in H by a pushout by π is a subalgebra of H isomorphic to B.

The interpretation of embeddable quantum homogeneous spaces as quantum quotient spaces allows one to develop the quantum group gauge theory of such spaces following the lines of Ref. 3. The study of such a gauge theory becomes even more important once the appearance of the quantum homogeneous spaces in the A. Connes geometric description of the standard model was announced.[4] For this purpose, however, one needs to generalize the notion of a quantum principal bundle of Ref. 3 so that a Hopf algebra playing the role of a quantum structure group there may be replaced by a coalgebra. Such a generalization is proposed (see Ref. 5 for further details). Since the theory of quantum principal bundles is strictly related to the theory of Hopf–Galois extensions (cf. Ref. 6), a generalization of such extensions is proposed.

The article is organized as follows. In Sec. II the notation used in the sequel is described. Section III shows a fixed point subalgebra structure of embeddable quantum homogeneous spaces. A suitable generalization of the notion of a quantum principal bundle in Sec. IV is proposed. Sections V and VI are devoted to careful study of two examples of quantum embeddable spaces,

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namely the quantum plane $\mathbf{C}_q^2$ (Ref. 7) and the quantum sphere $S_q^2(\mu,\nu)$.[1]

II. PRELIMINARIES

In the sequel all the vector spaces are over the field k of characteristic not 2. C denotes a coalgebra with the coproduct $\Delta: C\to C\otimes C$ and the counit $\epsilon: C\to k$ which satisfy the standard axioms, cf. Ref. 8. For the coproduct the Sweedler sigma notation is used:

$$\Delta c = c_{(1)}\otimes c_{(2)} \quad (\Delta\otimes id)\circ\Delta c = c_{(1)}\otimes c_{(2)}\otimes c_{(3)}, \text{ etc.},$$

where $c\in C$, and the summation sign and the indices are suppressed. A vector space A is a left C-comodule if there exists a map $\Delta_L: A\to C\otimes A$, such that $(\Delta\otimes id)\circ\Delta_L = (id\otimes\Delta_L)\circ\Delta_L$, and $(\epsilon\otimes id)\circ\Delta_L = id$. For Δ_L we use the explicit notation

$$\Delta_L a = a_{(1)}\otimes a_{(\infty)},$$

where $a\in A$ and all $a_{(1)}\in C$ and all $a_{(\infty)}\in A$.

Similarly a vector space A is a right C-comodule if there exists a map $\Delta_R: A\to A\otimes C$, such that $(\Delta_R\otimes id)\circ\Delta_R = (id\otimes\Delta)\circ\Delta_R$, and $(id\otimes\epsilon)\circ\Delta_R = id$. For Δ_R the explicit notation is used:

$$\Delta_R a = a_{(0)}\otimes a_{(1)},$$

where $a\in A$ and all $a_{(1)}\in C$ and all $a_{(0)}\in A$.

H denotes a Hopf algebra with product $m: H\otimes H\to H$, unit 1, coproduct $\Delta: H\to H\otimes H$, counit $\epsilon: H\to k$ and antipode $S: H\to H$. Sweedler's sigma notation is used as before. Similarly as for a coalgebra right and left H-comodules are defined. For a right H-comodule A we denote by $A^{\mathrm{co}H}$ a vector subspace of A of all elements $a\in A$ such that $\Delta_R a = a\otimes 1$. A right (respectively, left) H-comodule A is a right (respectively, left) H-comodule algebra if A is an algebra and Δ_R (respectively, Δ_L) is an algebra map.

A vector subspace J of H such that $\epsilon(J)=0$ and $\Delta J\subset J\otimes H\oplus H\otimes J$ is called a *coideal* in H. If J is a coideal in H then $C=H/J$ is a coalgebra with a coproduct Δ given by $\Delta=(\pi\otimes\pi)\circ\Delta$, where $\pi: H\to C$ is a canonical surjection. The counit ϵ in C is defined by the commutative diagram

$$\begin{array}{ccc} H & \xrightarrow{\epsilon} & k \\ {\scriptstyle\pi}\downarrow & & \downarrow{\scriptstyle id} \\ C & \xrightarrow{\epsilon} & k \end{array} .$$

III. QUANTUM HOMOGENEOUS SPACES

In this section it is shown that if an embeddable quantum homogeneous space satisfies certain additional assumption it may be identified with a quantum quotient space.

Definition 3.1:[2] Let H be a Hopf algebra and B be a left H-comodule algebra with the coaction $\Delta_L: B\to H\otimes B$. B is an *embeddable quantum homogeneous space* or simply an *embeddable* H-space if there exists an algebra inclusion $i: B\hookrightarrow H$ such that $\Delta\circ i = (id\otimes i)\circ\Delta_L$, i.e., i is an intertwiner.

Proposition 3.2: (1) *A left H comodule algebra B is an embeddable H-space if and only if there exists an algebra character $\kappa: B\to k$ such that the linear map $i_\kappa: B\to H$, $i_\kappa: b\mapsto b_{(1)}\kappa(b_{(\infty)})$ is injective.* (2) *If B is an embeddable H-space then the linear map $\chi_L: B\otimes B\to H\otimes B$, $\chi_L: b\otimes b'\mapsto b_{(1)}\otimes b_{(\infty)}b'$ is injective.*

Proof: (1) If B is an embeddable quantum homogeneous space then $\kappa=\epsilon\circ i$ is a character of B. Since i is an intertwiner, for any $b\in B$, compute

$$i_\kappa(b)=b_{(1)}\epsilon(i(b_{(\infty)}))=i(b)_{(1)}\epsilon(i(b)_{(2)})=i(b),$$

thus i_κ is an inclusion.

Conversely assume that there is a character $\kappa:B\to k$ such that i_κ is injective. Then clearly i_κ is an algebra inclusion. Furthermore,

$$\Delta(i_\kappa(b))=b_{(1)}\otimes b_{(2)}\kappa(b_{(\infty)})=b_{(1)}\otimes i_\kappa(b_{(\infty)})=(id\otimes i_\kappa)\circ\Delta_L(b).$$

Therefore i_κ is an intertwiner as required.

(2) The canonical map *can:* $H\otimes H\to H\otimes H$, *can:* $u\otimes v\mapsto u_{(1)}\otimes u_{(2)}v$ is a linear isomorphism. Consider the diagram

$$\begin{array}{ccccc} & & 0 & & 0 \\ & & \downarrow & & \downarrow \\ & & B\otimes B & \xrightarrow{\chi_L} & H\otimes B \\ & & {\scriptstyle i\otimes i}\downarrow & & \downarrow{\scriptstyle id\otimes i} \\ 0 & \longrightarrow & H\otimes H & \xrightarrow{can} & H\otimes H \end{array} \quad . \tag{3.1}$$

Clearly, both the rows and the columns of diagram (3.1) are exact. Moreover for any $b,b'\in B$:

$$\begin{aligned}(id\otimes i)\circ\chi_L(b\otimes b')&=b_{(1)}\otimes i(b_{(\infty)}b')=b_{(1)}\otimes i(b_{(\infty)})i(b')=i(b)_{(1)}\otimes i(b)_{(2)}i(b')\\&=can(i(b)\otimes i(b')),\end{aligned}$$

and hence diagram (3.1) is also commutative. Therefore the sequence $0\to B\otimes B\xrightarrow{\chi_L}H\otimes B$ is exact, i.e., the map χ_L is injective. □

Remark 3.3: The second assertion of Proposition 3.2, i.e., the injectiveness of χ_L, is a dual version of the statement that the action of a group on its homogeneous space is transitive.

Proposition 3.4: *Let B be an embeddable H space corresponding to the character $\kappa:B\to k$. Define a right ideal $J_\kappa\subset H$ by $J_\kappa=\{\Sigma_j(i_\kappa(b_j)-\kappa(b_j))u_j;\forall b_j\in B,\forall u_j\in H\}$. Then J_κ is a coideal in H.*

Proof: Clearly

$$\epsilon(i_\kappa(b)-\kappa(b))=\epsilon(b_{(1)})\kappa(b_{(\infty)})-\kappa(b)=\kappa(b)-\kappa(b)=0.$$

Furthermore,

$$\begin{aligned}\Delta(i_\kappa(b)-\kappa(b))&=i_\kappa(b)_{(1)}\otimes i_\kappa(b)_{(2)}-\kappa(b)1\otimes 1=b_{(1)}\otimes(i_\kappa(b_{(\infty)})-\kappa(b_{(\infty)}))+b_{(1)}\kappa(b_{(\infty)})\otimes 1\\&\quad-\kappa(b)1\otimes 1=b_{(1)}\otimes(i_\kappa(b_{(\infty)})-\kappa(b_{(\infty)}))+(i_\kappa(b)-\kappa(b))\otimes 1.\end{aligned}$$

Therefore for any $b\in B$,

$$\Delta(i_\kappa(b)-\kappa(b))\in H\otimes J_\kappa\oplus J_\kappa\otimes H,$$

so that J_κ is a coideal as stated. □

Since J_κ is a coideal of H, the vector space $C=H/J_\kappa$ is a coalgebra and the canonical subjection $\pi:H\to C$ is a coalgebra map. This in turn implies that H is a right C-comodule with the coaction $\Delta_R=(id\otimes\pi)\circ\Delta:H\to H\otimes C$. Let $H^{coC}=\{u\in H;\Delta_R u=u\otimes\pi(1)\}$.

Proposition 3.5: *Let B be an embeddable H-space corresponding to the character $\kappa: B \to k$, J_κ be as in Proposition 3.4 and $C = H/J_\kappa$. Then: (1) H^{coC} is a subalgebra of H; (2) B is a subalgebra of H^{coC}.*

Proof: (1) Since $\ker \pi = J_\kappa$ is a right ideal in H there is a natural right action $\rho_0: C \otimes H \to C$ of H on C given by the commutative diagram

$$\begin{array}{ccc} H \otimes H & \xrightarrow{m} & H \\ {\scriptstyle \pi \otimes id}\downarrow & & \downarrow{\scriptstyle \pi} \\ C \otimes H & \xrightarrow{\rho_0} & C \end{array} .$$

In other words for any $a \in C$ and $u \in H$, $\rho_0(a,u) = \pi(vu)$, where $v \in \pi^{-1}(a)$. For any $u,v \in H^{coC}$ we compute

$$\begin{aligned} \Delta_R(uv) &= u_{(1)}v_{(1)} \otimes \pi(u_{(2)}v_{(2)}) = u_{(1)}v_{(1)} \otimes \rho_0(\pi(u_{(2)}), v_{(2)}) = uv_{(1)} \otimes \rho_0(\pi(1), v_{(2)}) \\ &= uv_{(1)} \otimes \pi(v_{(2)}) = uv \otimes \pi(1). \end{aligned}$$

Therefore $uv \in H^{coC}$ and H^{coC} is a subalgebra of H as required.

(2) For any $b \in B$ we compute

$$\Delta_R(i_\kappa(b)) = i_\kappa(b)_{(1)} \otimes \pi(i_\kappa(b)_{(2)}) = b_{(1)} \otimes \pi(i_\kappa(b_{(\infty)})) = b_{(1)} \otimes \kappa(b_{(\infty)})\pi(1) = i_\kappa(b) \otimes \pi(1).$$

Hence $i_\kappa: B \hookrightarrow H^{coC}$ is the required algebra inclusion. □

Proposition 3.5 shows therefore that if $H^{coC} \subset i_\kappa(B)$ then the embeddable H-space B may be identified with the quantum quotient space H^{coC}. For example, exploiting the argument of the proof of Proposition 1.2.4 of Ref. 9, one can conjecture that the above inclusion holds if H is a faithfully flat B-module.

IV. A POSSIBLE GENERALIZATION OF QUANTUM PRINCIPAL BUNDLES

Once an H-embeddable space B is identified with a quotient space H^{coC}, it is natural to view H as a total space of a principal bundle over B. Therefore one would like to apply the general theory of quantum principal bundles of Ref. 3 to this case too. In general, however, neither C is a Hopf algebra nor, if it happens to be a Hopf algebra, C is a quantum subgroup of H. Hence the induced coaction of C on H is not an algebra map. Therefore, to develop a gauge theory on embeddable homogeneous spaces one needs to generalize the theory of quantum principal bundles. In this section such a generalization is proposed. It is based on a simple observation that the structure of quantum principal bundles is mainly determined by the coalgebra structure of the quantum group. The notions studied in this section are developed to great extent in Ref. 5.

Let C be a coalgebra and let P be an algebra and a right C-comodule. Assume that there is an action $\rho: P \otimes C \otimes P \to P \otimes C$ of P on $P \otimes C$ and an element $1 \in C$ such that

(1) For any $u,v \in P$, $\rho(u \otimes 1, v) = uv_{(0)} \otimes v_{(1)}$;

(2) the following diagram:

$$\begin{array}{ccc} P \otimes P & \xrightarrow{m} & P \\ {\scriptstyle (\Delta_R \otimes id)}\downarrow & & \downarrow{\scriptstyle \Delta_R} \\ P \otimes C \otimes P & \xrightarrow{\rho} & P \otimes C \end{array} ,$$

where m is a product in P, is commutative.

Define $B=P^{\mathrm{co}C}=\{u\in P;\Delta_R u=u\otimes 1\}$.

Lemma 4.1: *B is a subalgebra of P.*

Proof: Take any $u,v\in B$. Then

$$\Delta_R(uv)=\rho(u_{(0)}\otimes u_{(1)},v)=\rho(u\otimes 1,v)=uv_{(0)}\otimes v_{(1)}=uv\otimes 1. \qquad \square$$

Definition 4.2: Let P, C, ρ, and B be as before. It is said that $P(B,C,\rho)$ is a *C-Galois extension or a quantum ρ-principal bundle (with universal differential structure)* if the canonical map $\chi:P\otimes_B P\to P\otimes C$, $\chi:u\otimes_B v\mapsto uv_{(0)}\otimes v_{(1)}$ is a bijection.

Example 4.3: A quantum principal bundle $P(B,H)$ as defined in Ref. 3 is a ρ-principal bundle with the action $\rho:P\otimes H\otimes P\to P\otimes H$ given by $\rho(u\otimes a,v)=uv_{(0)}\otimes av_{(1)}$.

Example 4.4: Let H be a Hopf algebra, C a coalgebra, and $\pi:H\to C$ a coalgebra surjection. Then H is a right C-comodule with a coaction $\Delta_R=(id\otimes\pi)\circ\Delta$. Denote $1=\pi(1)\in C$ and define $B=H^{\mathrm{co}C}$ as before. Assume that $\ker\pi$ is a minimal right ideal in H such that $\{u-\epsilon(u);u\in B\}\subset\ker\pi$ (compare Sec. III). Then a canonical right action $\rho_0:C\otimes H\to C$ as in the proof of Proposition 3.5 can be defined. Furthermore,

$$\rho(u\otimes a,v)=uv_{(1)}\otimes\rho_0(a,v_{(2)})$$

for any u, $v\in H$, $a\in C$. With these definitions $H(B,C,\rho)$ is a quantum ρ-principal bundle.

Proof: First we show that $\rho:H\otimes C\otimes H\to H\otimes C$ is a right action and it has the properties (1) and (2). Since ρ_0 is a right action, for any u, v, $w\in H$, $a\in C$, compute

$$\begin{aligned}\rho(u\otimes a,vw)&=uv_{(1)}w_{(1)}\otimes\rho_0(a,v_{(2)}w_{(2)})=uv_{(1)}w_{(1)}\otimes\rho_0(\rho_0(a,v_{(2)}),w_{(2)})\\&=\rho(uv_{(1)}\otimes\rho_0(a,v_{(2)}),w)=\rho(\rho(u\otimes a,v),w),\end{aligned}$$

and thus ρ is an action as required. Furthermore,

$$\rho(u\otimes 1,v)=uv_{(1)}\otimes\rho_0(1,v_{(2)})=uv_{(1)}\otimes\pi(v_{(2)})=uv_{(0)}\otimes v_{(1)}$$

and

$$\rho(u_{(0)}\otimes u_{(1)},v)=u_{(1)}v_{(1)}\otimes\rho_0(\pi(u_{(2)}),v_{(2)})=u_{(1)}v_{(1)}\otimes\pi(u_{(2)}v_{(2)})=\Delta_R(uv).$$

Therefore ρ has all the required properties.

To prove that the canonical map χ is bijective we first note that, by assumption, $\ker\pi\subset m\circ(\ker\pi|_B\otimes H)$ and then use a suitably modified argument of the proof of Lemma 5.2 of Ref. 3 to deduce that χ is a bijection. It is clear that χ is a surjection since for any $\Sigma_k u_k\otimes a_k\in H\otimes C$ we can choose $\Sigma_k u_k Sv_{k(1)}\otimes_B v_{k(2)}\in H\otimes_B H$, where $\forall k,v_k\in\pi^{-1}(a_k)$, and compute

$$\chi\left(\sum_k u_k Sv_{k(1)}\otimes_B v_{k(2)}\right)=\sum_k u_k(Sv_{k(1)})v_{k(2)}\otimes\pi(v_{k(3)})=\sum_k u_k\otimes\pi(v_k)=\sum_k u_k\otimes a_k.$$

Next we compute $\ker\chi\subset H\otimes_B H$. Take any $\Sigma_k u_k\otimes_B v_k\in\ker\chi$. Then $\Sigma_k u_k v_{k(1)}\otimes\pi(v_{k(2)})=0$. Applying $id\otimes\epsilon$ to the last equality, we find that $\Sigma_k u_k v_k=0$, i.e., $\Sigma_k u_k\otimes v_k\in\ker m$. Any $\Sigma_i w_i'\otimes w_i''\in\ker m$ can be written as $\Sigma_k u_k Sv_{k(1)}\otimes v_{k(2)}\in H\otimes H$, where $\forall k$, $v_k\in\ker\epsilon$ and u_k are linearly independent. Thus

$$\chi\left(\sum_i w_i'\otimes_B w_i''\right)=\chi\left(\sum_k u_k Sv_{k(1)}\otimes_B v_{k(2)}\right)=\sum_k u_k\otimes\pi(v_k).$$

If $\Sigma_i w_i'\otimes_B w_i''\in\ker\chi$ then $\Sigma_k u_k\otimes\pi(v_k)=0$, thus for all k, $\pi(v_k)=0$. By assumption $v_k=\Sigma_j b_k^j v_k^j$, where $b_k^j\in\ker\epsilon|_B=\ker\pi|_B$. Therefore,

$$\sum_i w_i' \otimes_B w_i'' = \sum_k u_k S v_{k(1)} \otimes_B v_{k(2)} = \sum_{j,k} u_k (S v^j_{k(1)}) S b^j_{k(1)} \otimes_B b^j_{k(2)} v^j_{k(2)}$$

$$= \sum_{j,k} \epsilon(b^j_k) u_k S v^j_{k(1)} \otimes_B v^j_{k(2)} = 0.$$

So $\ker \chi = 0$, and χ is a bijection as required. □

Therefore it is shown that an embeddable H space which is a quotient space $B = H^{\mathrm{co}C}$ as described in Sec. III may be identified with a base manifold of the generalized quantum principal bundle, or equivalently that H is a C-Galois extension of B.

V. MANIN'S PLANE AS A QUANTUM QUOTIENT SPACE

In this section we show that Manin's plane is a quotient space of the quantum general linear group $\mathrm{GL}_q(2,\mathbf{C})$. Recall that Manin's plane $\mathbf{C}^2_q$ is defined for any nonzero $q \in \mathbf{C}$ as an associative polynomial algebra over $\mathbf{C}$ generated by $1, x, y$ subject to the relations $xy = qyx$. It is a quantum homogeneous space of the quantum linear group $\mathrm{GL}_q(2,\mathbf{C})$. $\mathrm{GL}_q(2,\mathbf{C})$ is defined as follows. First consider an algebra generated by the matrix $\mathbf{t} = \left(\begin{smallmatrix} \alpha & \beta \\ \gamma & \delta \end{smallmatrix}\right)$ and the relations

$$\alpha\beta = q\beta\alpha, \quad \alpha\gamma = q\gamma\alpha, \quad \alpha\delta = \delta\alpha + (q - q^{-1})\beta\gamma, \tag{5.1a}$$

$$\beta\gamma = \gamma\beta, \quad \beta\delta = q\delta\beta, \quad \gamma\delta = q\delta\gamma. \tag{5.1b}$$

The quantum determinant $c = \alpha\delta - q\beta\gamma$ is central in the algebra (5.1); thus it can be enlarged with c^{-1}. The resulting algebra is called $\mathrm{GL}_q(2,\mathbf{C})$. The quantum linear group $\mathrm{GL}_q(2,\mathbf{C})$ is a Hopf algebra of a matrix group type, i.e.,

$$\Delta\mathbf{t} = \mathbf{t} \otimes \mathbf{t}, \quad \epsilon\mathbf{t} = 1, \quad S\mathbf{t} = c^{-1} \begin{pmatrix} \delta & -q^{-1}\beta \\ -q\gamma & \alpha \end{pmatrix}.$$

The left coaction of $\mathrm{GL}_q(2,\mathbf{C})$ on $\mathbf{C}^2_q$ is given by

$$\Delta_L \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \otimes \begin{pmatrix} x \\ y \end{pmatrix}.$$

$\mathbf{C}^2_q$ is not only a homogeneous space of $\mathrm{GL}_q(2,\mathbf{C})$ but also an embeddable $\mathrm{GL}_q(2,\mathbf{C})$ space. The linear map $\kappa: \mathbf{C}^2_q \to \mathbf{C}$, $\kappa(x^n y^m) = \delta_{m0}$, $m, n \in \mathbf{Z}_{\geqslant 0}$ is a character of $\mathbf{C}^2_q$. By Proposition 3.2 it induces an algebra map $i_\kappa: \mathbf{C}^2_q \to \mathrm{GL}_q(2,\mathbf{C})$, which is explicitly given by $i_\kappa(x) = \alpha$, $i_\kappa(y) = \gamma$. The map i_κ is clearly an inclusion. Thus the right ideal J_κ is generated by $\alpha - 1$ and γ. The coalgebra $C = \mathrm{GL}_q(2,\mathbf{C})/J_\kappa$ may be easily computed. It is spanned by $a_{m,n} = \pi(\beta^m c^n)$, $m \in \mathbf{Z}_{>0}$, $n \in \mathbf{Z}$ and $a_{0,0} = 1 = \pi(1)$, where $\pi: \mathrm{GL}_q(2,\mathbf{C}) \to C$ is a canonical surjection. To see that the $a_{m,n}$ really span C, note that since J_κ is generated by $\alpha - 1$ and γ as a right ideal in $\mathrm{GL}_q(2,\mathbf{C})$, every α which multiplies any element of $\mathrm{GL}_q(2,\mathbf{C})$ from the left is replaced by 1 and similarly any γ is replaced by 0 when the resulting element of $\mathrm{GL}_q(2,\mathbf{C})$ is acted upon by π. Then we compute

$$\pi(\alpha^k\beta^l\gamma^m\delta^n c^r) = \pi(\beta^l\gamma^m\delta^n c^r) = \delta_{m0}\pi(\beta^l\delta^n c^r) = \delta_{m0} q^{ln} \pi(\delta^n\beta^l c^r) = \delta_{m0} q^{ln} (\pi(\alpha\delta\delta^{n-1}\beta^l c^r)$$
$$- q^{-1}\pi(\gamma\beta\delta^{n-1}\beta^l c^r)) = \delta_{m0} q^{ln} \pi(\delta^{n-1}\beta^l c^{r+1}) = \cdots = \delta_{m0} q^{ln} a_{l,r+n}.$$

Therefore any element of $C = \pi(\mathrm{GL}_q(2,\mathbf{C}))$ may be expressed as a linear combination of $a_{m,n}$.

The coalgebra structure of C is found from the coalgebra structure of $\mathrm{GL}_q(2,\mathbf{C})$, since $\Delta_C = (\pi \otimes \pi) \circ \Delta_{\mathrm{GL}_q(2,\mathbf{C})}$. Explicitly

$$\Delta a_{m,n}=\sum_{k=0}^{m}\begin{pmatrix}m\\k\end{pmatrix}_q a_{k,n}\otimes a_{m-k,n+k},\quad \epsilon(a_{m,n})=\delta_{m0}, \tag{5.2}$$

where the quantum binomial coefficients are defined by

$$\begin{pmatrix}m\\k\end{pmatrix}_q=\frac{[m]_q!}{[m-k]_q![k]_q!},\quad [m]_q=\frac{q^m-q^{-m}}{q-q^{-1}},\quad [m]_q!=\prod_{k=1}^{m}[k]_q,\quad [0]_q!=1.$$

The next step in the identification of $\mathbf{C}_q^2$ as a quantum quotient space consists of computing the fixed point subalgebra $B=\mathrm{GL}_q(2,\mathbf{C})^{\mathrm{co}C}$. For a general monomial $\alpha^k\gamma^l\beta^m\delta^n c^r\in\mathrm{GL}_q(2,\mathbf{C})$, $k,l,m,n\in\mathbf{Z}_{\geqslant 0}$, $r\in\mathbf{Z}$, we find

$$\Delta_R(\alpha^k\gamma^l\beta^m\delta^n c^r)=\alpha^k\gamma^l c^r\sum_{i=0}^{m}\sum_{j=0}^{n}q^{j(m-i)}\begin{pmatrix}m\\i\end{pmatrix}_q\begin{pmatrix}n\\j\end{pmatrix}_q\alpha^{m-i}\beta^i\gamma^{n-j}\delta^j\otimes a_{m+n-(i+j),i+j+r}. \tag{5.3}$$

The right-hand side of Eq. (5.3) has the form $u\otimes 1$ for some $u\in\mathrm{GL}_q(2,\mathbf{C})$ if and only if $m=n=r=0$. Thus B is spanned by all $\alpha^k\gamma^l$. Therefore $B\subset i_\kappa(\mathbf{C}_q^2)$ and since $i_\kappa(\mathbf{C}_q^2)\subset B$ by Proposition 3.5 we conclude that $\mathbf{C}_q^2\cong\mathrm{GL}_q(2,\mathbf{C})^{\mathrm{co}C}$. By Example 4.4 $\mathrm{GL}_q(2,\mathbf{C})(\mathbf{C}_q^2,C,\rho)$ is a quantum principal ρ-bundle. The action $\rho_0: C\otimes\mathrm{GL}_q(2,\mathbf{C})\to C$ is given explicitly by

$$\rho_0(a_{i,j},\alpha^k\beta^l\gamma^m\delta^n c^r)=\delta_{m0}q^{i(n-k)+ln}a_{i+l,j+n+r}.$$

One can now proceed to define an algebra structure on C so that it becomes a Hopf algebra. Define the product in C by

$$a_{k,l}a_{m,n}=q^{lm-kn}a_{k+m,l+n}.$$

First we notice that $a_{0,0}=1$ is the unit element with respect to this product. Next we show that this product is compatible with the coalgebra structure of C. Compute

$$\begin{aligned}\Delta(a_{k,l})\Delta(a_{m,n})&=\sum_{i=0}^{k}\sum_{j=0}^{m}\begin{pmatrix}k\\i\end{pmatrix}_q\begin{pmatrix}m\\j\end{pmatrix}_q a_{i,l}a_{j,n}\otimes a_{k-i,l+i}a_{m-j,n+j}\\&=q^{lm-nk}\sum_{i=0}^{k}\sum_{j=0}^{m}q^{im-kj}\begin{pmatrix}k\\i\end{pmatrix}_q\begin{pmatrix}m\\j\end{pmatrix}_q a_{i+j,l+n}\otimes a_{k+m-(i+j),l+n+i+j}\\&=q^{lm-nk}\sum_{r=0}^{k+m}\begin{pmatrix}k+m\\r\end{pmatrix}_q a_{r,l+n}\otimes a_{k+m-r,l+n+r}=q^{lm-kn}\Delta(a_{k+m,l+n})=\Delta(a_{k,l}a_{m,n}).\end{aligned}$$

The third equality is a consequence of the following property of the q-deformed binomial coefficients

$$\forall r\in[0,k+m],\quad \sum_{i=0}^{k}\sum_{j=0}^{m}\delta_{i+j,r}q^{im-kj}\begin{pmatrix}k\\i\end{pmatrix}_q\begin{pmatrix}m\\j\end{pmatrix}_q=\begin{pmatrix}k+m\\r\end{pmatrix}_q.$$

Clearly the counit of C is an algebra homomorphism. Before defining an antipode, we show that C is a polynomial algebra. Let $a=a_{0,1}$, $a^{-1}=a_{0,-1}$, $b=a_{1,0}$. Then for any $m\in\mathbf{Z}_{>0}$, $n\in\mathbf{Z}$,

$$a_{m,n}=q^{-mn}a^n b^m,\quad ab=q^2ba,\quad aa^{-1}=a^{-1}a=1.$$

Therefore C is a polynomial algebra indeed, and it is isomorphic to $\mathbf{C}^2_{q^2}[x^{-1}]$. The coalgebra structure of C written in terms of a and b reads

$$\Delta a^{\pm 1}=a^{\pm 1}\otimes a^{\pm 1},\quad \Delta b=1\otimes b+b\otimes a,\quad \epsilon(a^{\pm 1})=1,\quad \epsilon(b)=0$$

and hence the antipode is defined as $Sa^{\pm 1}=a^{\mp 1}$, $Sb=-ba^{-1}$.

We have just shown that C may be equipped with an algebra structure of $\mathbf{C}^2_{q^2}[x^{-1}]$, and then the coalgebra structure of C becomes a standard coalgebra structure of the latter. Therefore we have proven

Theorem 5.1:

$$\mathbf{C}^2_q=\mathrm{GL}_q(2,\mathbf{C})^{\mathrm{co}\mathbf{C}^2_{q^2}[x^{-1}]}.$$

Notice that clearly neither $\pi:\mathrm{GL}_q(2,\mathbf{C})\to\mathbf{C}^2_{q^2}[x^{-1}]$ nor $\Delta_R=(id\otimes\pi)\circ\Delta:\mathrm{GL}_q(2,\mathbf{C})\to\mathrm{GL}_q(2,\mathbf{C})\otimes\mathbf{C}^2_{q^2}[x^{-1}]$ are algebra maps. Still, following the proposal of Sec. IV the generalized principal bundle $\mathrm{GL}_q(2,\mathbf{C})(\mathbf{C}^2_q,\mathbf{C}^2_{q^2}[x^{-1}],\rho,\pi)$ can be defined and analyzed. In particular one can truly develop a gauge theory, define connections and their curvature, closely following the quantum group gauge theory introduced in Ref. 3.

VI. PODLEŚ' SPHERE AS A QUANTUM QUOTIENT SPACE

In this section we prove that the quantum two-sphere is a quantum quotient space in the sense explained in Sec. III. In the presentation of the quantum sphere the conventions of Ref. 10 are followed.

The general quantum two-sphere $S^2_q(\mu,\nu)$ is a polynomial algebra generated by the unit and x,y,z, and the relations

$$xz=q^2zx,\quad xy=-q(\mu-z)(\nu+z),$$

$$yz=q^{-2}zy,\quad yx=-q(\mu-q^{-2}z)(\nu+q^{-2}z),$$

where μ, ν, and $q\neq 0$ are real parameters, $\mu\nu\geqslant 0$, $(\mu,\nu)\neq(0,0)$. The quantum sphere is a $*$ algebra with the $*$ structure $x^*=-qy$, $z^*=z$.

The quantum sphere $S^2_q(\mu,\nu)$ is an $\mathrm{SU}_q(2)$ homogeneous quantum space. $\mathrm{SU}_q(2)$ is defined as a quotient of $\mathrm{GL}_q(2,\mathbf{C})$ by the relation $c=1$, and has a $*$-structure given by $\delta=\alpha^*$, $\gamma=-q^{-1}\beta^*$. The coaction of $\mathrm{SU}_q(2)$ on $S^2_q(\mu,\nu)$ is defined as follows. Let $\phi_-=x$, $\phi_0=(1+q^{-2})^{-1/2}(\mu-\nu-(1+q^{-2})z)$, $\phi_+=y$. Then

$$\Delta_L\begin{pmatrix}\phi_-\\ \phi_0\\ \phi_+\end{pmatrix}=\begin{pmatrix}\alpha^2 & (1+q^{-2})^{1/2}\alpha\beta & \beta^2\\ (1+q^{-2})^{1/2}\alpha\gamma & 1+(q+q^{-1})\beta\gamma & (1+q^{-2})^{1/2}\beta\delta\\ \gamma^2 & (1+q^{-2})^{1/2}\gamma\delta & \delta^2\end{pmatrix}\otimes\begin{pmatrix}\phi_-\\ \phi_0\\ \phi_+\end{pmatrix}.$$

The quantum sphere $S^2_q(\mu,\nu)$ is not only a quantum homogeneous space but also an embeddable $\mathrm{SU}_q(2)$ space. There is a $*$ character $\kappa:S^2_q(\mu,\nu)\to\mathbf{C}$ given by

$$\kappa(x)=q\sqrt{\mu\nu},\quad \kappa(y)=-\sqrt{\mu\nu},\quad \kappa(z)=0.$$

Therefore there is also a $*$-algebra homomorphism $i_\kappa:S^2_q(\mu,\nu)\to\mathrm{SU}_q(2)$, which reads explicitly

$$i_\kappa(x)=\sqrt{\mu\nu}(q\alpha^2-\beta^2)+(\mu-\nu)\alpha\beta,$$

$$i_\kappa(y)=\sqrt{\mu\nu}(q\gamma^2-\delta^2)+(\mu-\nu)\gamma\delta,$$

$$i_\kappa(z) = -\sqrt{\mu\nu}(q\alpha\gamma - \beta\delta) - (\mu - \nu)\beta\gamma,$$

and is clearly an inclusion. From now on we assume that $\mu \neq \nu$ (but also see Remark 6.5). In this case $S_q^2(\mu,\nu)$ depends on two real parameters only, namely q and $p = \sqrt{\mu\nu}/(\mu - \nu)$. By Proposition 3.4 the inclusion i_κ induces a coideal $J_\kappa \subset \mathrm{SU}_q(2)$, generated as a right ideal in $\mathrm{SU}_q(2)$ by the following three elements:

$$p(q\alpha^2 - \beta^2) + \alpha\beta - pq, \quad p(q\gamma^2 - \delta^2) + \gamma\delta + p, \quad p(q\alpha\gamma - \beta\delta) + q\beta\gamma.$$

Therefore we can construct the coalgebra $C(p) = \mathrm{SU}_q(2)/J_\kappa$, and the corresponding quotient space $B(p) = \mathrm{SU}_q(2)^{\mathrm{co}C(p)}$ as described in Sec. III. At the end of this procedure we identify $B(p)$ with $S_q^2(\mu,\nu)$, $\mu \neq \nu$. We start with the coalgebra $C(p)$.

Proposition 6.1: *$C(p)$ is a vector space spanned by $1 = \pi(1)$, $x_n = \pi(\alpha^n)$ and $y_n = \pi(\delta^n)$, where $\pi: \mathrm{SU}_q(2) \to C(p)$ is a canonical surjection and $n \in \mathbf{Z}_{>0}$.*

Proof: For any $u \in \mathrm{SU}_q(2)$ we use the explicit form of the generators of J_κ and the relations in $\mathrm{SU}_q(2)$ to find that

$$\begin{aligned}\pi(\beta u) &= \pi(\beta\alpha\delta u) - q\,\pi(\beta\gamma\beta u) = q^{-1}\pi(\alpha\beta\delta u) - q\,\pi(\beta\gamma\beta u) = -p\,\pi(\alpha^2\delta u) + pq^{-1}\pi(\beta^2\delta u) \\ &\quad + p\,\pi(\delta u) + pq\,\pi(\alpha\gamma\beta u) - p\,\pi(\beta\delta\beta u) = p\,\pi(\delta u) - p\,\pi(\alpha u), \end{aligned} \tag{6.1a}$$

and similarly

$$\pi(\gamma u) = p\,\pi(\delta u) - p\,\pi(\alpha u). \tag{6.1b}$$

From Eq. (6.1) it follows that for any $u \in \mathrm{SU}_q(2)$, $\pi(u\beta^m\gamma^n) = \pi(u\beta^{m+n})$. Since $\mathrm{SU}_q(2)$ is spanned by the monomials $\alpha^m\beta^k\gamma^l, \delta^m\beta^k\gamma^l$ (cf. Lemma 7.1.2 of Ref. 11) it suffices to prove that the following elements of $C(p)$,

$$a_{k-}^{(n)} = \pi(\delta^k\beta^{n-k}), \quad a_{k+}^{(n)} = \pi(\alpha^k\beta^{n-k}), \tag{6.2}$$

where $n \in \mathbf{Z}_{>0}$, $k = 0,1,\ldots,n$ can be expressed as linear combinations of 1, x_m, y_m. Clearly $a_{0-}^{(n)} = a_{0+}^{(n)}$. Thus we simply write $a_0^{(n)}$. Also, $a_{n+}^{(n)} = x_n$ and $a_{n-}^{(n)} = y_n$. For $n = 1$, $a_0^{(1)} = \pi(\beta) = p(y_1 - x_1)$. For a general n we apply the rules (6.1) to $a_{k\pm}^{(n)}$ and express the latter in terms of $a_{l\pm}^{(m)}$, $m < n$, and x_n, y_n. We make the inductive assumption that for all $m < n$, $a_{l\pm}^{(m)}$ can be written as linear combinations of 1, x_r, y_r. Therefore, for $n \geqslant 2$ we arrive at the system of equations:

$$\begin{aligned} &a_{k\pm}^{(n)} \pm pq^{\pm k}a_{k+1\pm}^{(n)} \mp pq^{\mp(k-1)}a_{k-1\pm}^{(n)} = \pm pq^{\pm k}a_{k-1\pm}^{(n-2)}, \\ &a_0^{(n)} - pa_{1-}^{(n)} + pa_{1+}^{(n)} = 0, \end{aligned} \tag{6.3}$$

where $k = 1,2,\ldots,n-1$. This is a system of $2n-1$ equations with $2n-1$ unknowns provided that the right-hand sides and x_n, y_n are treated as known parameters. Obviously it has a solution if its determinant is nonzero. The determinant D_n of the system (6.3) may be easily computed. It does not depend on q and it can be reduced to the determinant of the following $2n-1 \times 2n-1$ matrix:

$$\begin{pmatrix} 1 & -p & p & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 \\ p & 1 & 0 & -p & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 \\ -p & 0 & 1 & 0 & p & 0 & \dots & 0 & 0 & 0 & 0 & 0 \\ 0 & p & 0 & 1 & 0 & -p & \dots & 0 & 0 & 0 & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 1 & 0 & -p & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \dots & -p & 0 & 1 & 0 & p \\ 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & p & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & -p & 0 & 1 \end{pmatrix}. \tag{6.4}$$

By the Laplace theorem D_n can be further developed to give

$$D_n = A_{2n-2} + p^2(A_{2n-3} + A_{2n-4}) + p^4 A_{2n-5},$$

where A_m is zero for negative m, $A_0 = 1$ and for any $m < 2n-1$, A_m is the determinant of the matrix obtained from Eq. (6.4) by removing the first $2n-1-m$ rows and columns. The determinants A_m are the standard ones and we finally obtain the determinant of the system (6.3) as a polynomial

$$D_n = P_{n-1}(p^2) \equiv \sum_{k=0}^{n-1} \binom{2n-1-k}{k} p^{2k}.$$

For any $x \in \mathbf{R}_{\geqslant 0}$, $P_n(x) \geqslant 1$, and hence $D_n \neq 0$ for any real p. Therefore the system (6.3) always has a solution and the coalgebra $C(p)$ is spanned by x_n, y_n, $n \in \mathbf{Z}_{>0}$, and 1 as required. □

The vector space $C(p)$ has a coalgebra structure induced by π from the coalgebra structure of $\mathrm{SU}_q(2)$. The coproduct reads explicitly

$$\Delta x_n = \sum_{k=0}^{n} q^{-(n-k)k} \binom{n}{k}_q a_{k+}^{(n)} \otimes a_{k+}^{(n)}, \quad \Delta y_n = \sum_{k=0}^{n} q^{(n-k)k} \binom{n}{k}_q a_{k-}^{(n)} \otimes a_{k-}^{(n)},$$

where $a_{k\pm}^{(n)}$ are given by Eq. (6.2). Therefore the coalgebra $C(p)$ is cocommutative.

Remark 6.2: It is an interesting problem, whether it is possible to define a Hopf algebra structure on $C(p)$. For example, for $n=1$ we have

$$\Delta x_1 = (1+p^2) x_1 \otimes x_1 - p^2 (x_1 \otimes y_1 + y_1 \otimes x_1 - y_1 \otimes y_1),$$

$$\Delta y_1 = (1+p^2) y_1 \otimes y_1 - p^2 (x_1 \otimes y_1 + y_1 \otimes x_1 - x_1 \otimes x_1).$$

If one defines

$$x_1' = \frac{1}{\mu - \nu} (\mu x_1 - \nu y_1), \quad y_1' = \frac{1}{\mu - \nu} (\mu y_1 - \nu x_1)$$

then x_1' and y_1' are grouplike, i.e., $\Delta x_1' = x_1' \otimes x_1'$ and $\Delta y_1' = y_1' \otimes y_1'$. If it were possible to define a new basis of $C(p)$ consisting only of grouplike elements then clearly one would be able to solve the above problem and make $C(p)$ into a Hopf algebra of functions on $U(1)$.

Remark 6.3: According to Ref. 1 quantum spheres can also be defined for a discrete series of complex numbers p given by $p^2 = -(q^k + q^{-k})^{-2}$, $k = 1,2,\dots$. It is shown in Ref. 2 that such quantum spheres are $*$-embeddable in $\mathrm{SU}_q(2)$ for $k=1$.

One easily finds that $P_n(x - 1/4) = \sum_{k=0}^{n} c_k^n x^k$, where

$$c_k^n=\sum_{l=k}^{n}(-1/4)^{l-k}\binom{2n+1-l}{l}\binom{l}{k}.$$

For any n and any $0\leqslant k\leqslant n$, $c_k^n\geqslant c_0^n=(n+1)/4^n$ and thus all the coefficients c_k^n are positive. Therefore $P_n(x-1/4)\neq 0$ for all real $x\geqslant 0$. This implies that the determinants D_n of the proof of Proposition 6.1 are nonzero provided that $p^2\geqslant -1/4$. Since for any q, $q+q^{-1}\geqslant 2$ one sees that the assertion of Proposition 6.1 holds for the exceptional quantum spheres too.

In a different context, polynomials $P_n(x)$ appeared in Ref. 12. It was shown there that all the zeros of P_n are real and equal to $x_k=-\frac{1}{4}\sec^2(\pi k/2n+2)$, $k=1,2,\ldots,n$. The numbers $-1/x_k$ are the discrete values of the index for subfactors of type II_1 von Neumann algebras.

Proposition 6.4: *Let $C(p)$ be a coalgebra described in Proposition 6.1 and let $B(p)=\mathrm{SU}_q(2)^{\mathrm{co}C(p)}$. Then $i_\kappa(S_q^2(\mu,\nu))=B(p)$ for all $\mu\neq\nu$ such that $p=\sqrt{\mu\nu}/(\mu-\nu)$.*

Proof: By Proposition 3.5, $i_\kappa(S_q^2(\mu,\nu))\subset B(p)$, therefore one needs to show that $B(p)\subset i_\kappa(S_q^2(\mu,\nu))$. Introduce the grading $d:\mathrm{SU}_q(2)\to\mathbf{Z}$ by

$$d(\alpha)=d(\beta)=1,\quad d(1)=0,\quad d(\gamma)=d(\delta)=-1,\quad d(uv)=d(u)+d(v) \tag{6.5}$$

for any monomials $u,v\in\mathrm{SU}_q(2)$. A set of all elements of $\mathrm{SU}_q(2)$ of degree $k\in\mathbf{Z}$ forms a vector subspace of $\mathrm{SU}_q(2)$, which is denoted by $\mathrm{SU}_q(2)^{(k)}$, and $\mathrm{SU}_q(2)=\oplus_{k\in\mathbf{Z}}\mathrm{SU}_q(2)^{(k)}$. Moreover if $\Delta u=\Sigma_i u_i'\otimes u_i''$ for any $u\in\mathrm{SU}_q(2)^{(k)}$, then for all i, $d(u_i')=k$. To see that the last statement is true one can explicitly verify it for α, β, γ, δ and then use definition (6.5) of d to prove it for any $\mathrm{SU}_q(2)$. Therefore d induces a grading of $B(p)$ and $B(p)=\oplus_{k\in\mathbf{Z}}B(p)^{(k)}$.

Next, notice that $B(p)$ is contained in the subalgebra of $\mathrm{SU}_q(2)$ spanned by monomials of even degree. Therefore for any $k\in\mathbf{Z}$, $B(p)^{(2k+1)}=0$.

To prove the required inclusion observe that due to the form of π and $C(p)$, $B(p)$ is a deformation of $B(0)$, i.e., $B(0)=\lim_{p\to 0}B(p)$. Denote by $B(p)_{2n}^{(2k)}$ the vector space of homogeneous polynomials $u\in B(p)$ of degree $2n$ such that $d(u)=2k$, $|k|\leqslant n$. Notice that $B(p)_{2n}^{(2k)}$ and $B(p)_{2l}^{(2k)}$ need not be distinct for $l\neq n$. $B(0)_{2n}^{(2k)}$ is spanned by $\alpha^m\beta^{n+k-m}\gamma^{n-m}\delta^{m-k}$, where $m=k,k+1,\ldots,n$ for $k\geqslant 0$ and $m=0,1,\ldots,n+k$ for $k<0$, and hence is $n-|k|+1$-dimensional. This is exactly the dimension of $i_\kappa(S_q^2(\mu,\nu))_{2n}^{(2k)}$. Suppose that $B(p)_{2n}^{(2k)}$ is at least $n-|k|+2$-dimensional. Then one can find $u\in B(p)_{2n}^{(2k)}$ that does not contain any of the monomials spanning $B(0)_{2n}^{(2k)}$. If $\lim_{p\to 0}u\neq 0$, then one would obtain that $B(0)_{2n}^{(2k)}$ is at least $n-|k|+2$-dimensional, hence contradiction. $\lim_{p\to 0}u$ is meant as the polynomial obtained from u by replacing its coefficients with their $p=0$ limits. Assume that $\lim_{p\to 0}u=0$. The polynomial u may be written as a linear combination of monomials of degree $2n$ with coefficients that vanish as polynomials when p tends to 0. Therefore there exists a positive integer m such that $\lim_{p\to 0}p^{-m}u$ exists, is finite and nonzero, and is an element of $B(0)_{2n}^{(2k)}$. Thus we have a contradiction again. Since the above argument does not depend on n and k, and $i_\kappa(S_q^2(\mu,\nu))\subset B(p)$ we conclude that $i_\kappa(S_q^2(\mu,\nu))=B(p)$. □

Therefore we have shown that for $\mu\neq\nu$ the quantum sphere $S_q^2(\mu,\nu)$ is a quantum quotient space. By Example 4.4 one has a principal ρ-bundle, $\mathrm{SU}_q(2)(S_q^2(\mu,\nu),C(p),\rho,\pi)$.

Remark 6.5: When $\mu=\nu\neq 0$ the coideal J_κ is generated as a right ideal in $\mathrm{SU}_q(2)$ by the following elements:

$$q\alpha^2-\beta^2-q,\quad q\gamma^2-\delta^2+1,\quad q\alpha\gamma-\beta\delta.$$

Therefore for any $u\in\mathrm{SU}_q(2)$,

$$\pi(\delta u)=\pi(\alpha u),\quad \pi(\beta u)=\pi(\gamma u),\quad \pi(\gamma^2 u)=q^{-1}\pi(\alpha^2 u)-q^{-1}\pi(u),$$

and hence the coalgebra $C=\mathrm{SU}_q(2)/J_\kappa$ is spanned by $1=\pi(1)$, $x_n=\pi(\alpha^n)$, $y_n=\pi(\alpha^{n-1}\gamma)$, $n\in\mathbf{Z}_{\geqslant 1}$. We conjecture that also for this case $S_q^2(\mu,\mu)\cong\mathrm{SU}_q(2)^{\mathrm{co}C}$.

VII. CONCLUSIONS

In this article we have shown that certain embeddable quantum homogeneous spaces may be viewed as quantum quotient spaces. The examples of such quantum embeddable spaces include the general quantum two-sphere $S_q^2(\mu,\nu)$ and the quantum plane $\mathbf{C}_q^2$. The interpretation of quantum embeddable spaces presented in this article seems specially interesting from the point of view of quantum group gauge theory, the suitable generalization of which has also been proposed. We think that it would be interesting and indeed desirable to further develop this generalization of quantum group gauge theory, and in particular, to construct connections on the quantum spaces described in this article. For example this would allow for extending the construction of the Dirac q monopole of Ref. 3 to general quantum spheres. This program of studying coalgebra gauge theories, which will also incorporate braided group gauge theories, is currently being carried out and the first results may be found in Ref. 5 (cf. Ref. 13).

Note added in proof. After completing this article I have learned that the results similar to those of Sec. III were also obtained in M. S. Dijkhuizen and T. H. Koornwinder, Geom. Dedicata. **52**, 291 (1994).

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Point-group symmetrized boson representation. Algebraic solution for symmetry-adapted bases of O_h

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A point group symmetrized boson representation (SBR) is introduced that is particularly convenient for describing molecular vibrations. In this paper the SBR is elucidated using the example of the molecule SF_6 with O_h symmetry. The advantages of the SBR are that its basis vectors have a clear physical picture, their number is very small (equal to one-eighth of the dimension of the reducible representation for O_h), and the irreducible bases for any concrete cases can be obtained trivially from those for the general case without any projection. All the irreducible bases for the group chains $O_h \supset D_4 \supset C_4$ or $O_h \supset D_4 \supset D_2$ are tabulated once and for all. As an application, the Hamiltonian in the algebraic model of Iachello and Oss for stretching vibrations of the molecule SF_6 is diagonalized in the symmetry adapted bases. © *1996 American Institute of Physics.* [S0022-2488(96)02905-4]

I. INTRODUCTION

The theory of point symmetry groups has long played a fundamental role in atomic and molecular physics.[1] In recent times, increasing attention has been devoted to the point groups with higher symmetry, an interest intensified by the discovery of the fullerene molecule, C_{60}.[2] Perhaps the most important contribution of this theory is to provide symmetry-adapted bases to simplify the solution of the Schrödinger equation. Despite the spectacular growth in computing power, it will continue to be important to use such bases, not only to keep the dimensionality of Hamiltonian matrices under control, but also to understand the physical significance of the results found.

As a simple example consider a molecule with v vibrational excitation quanta[3] (or vibrons[4]) distributed among n equivalent bonds, and restrict the Hamiltonian to one for which v is conserved.[3,4] Thus each value of v defines an invariant subspace, L_v, in which the Hamiltonian is to be diagonalized. For this case the dimension of L_v is equal to the dimension $d_{n,v}$ of the totally symmetric representation $[v]$ of the unitary group $U(n)$,[5]

$$d_{n,v}=\begin{pmatrix} n+v-1 \\ v \end{pmatrix},$$

where

$$\begin{pmatrix} a \\ b \end{pmatrix}$$

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is the binomial coefficient. For Fullerene, $d_{60,1}=60$ (one-vibron space), $d_{60,2}=1830$ (two-vibron space), $d_{60,3}=37{,}820$ (three-vibron space). Clearly, the dimension of L_v increases drastically with the number of vibrons. Without using the symmetry adapted basis, it is impossible to deal with the case with $v\geqslant 2$.

Basically, in molecular physics we encounter two kinds of symmetry adaptation problems:

(i) Point group symmetry adaptation of a system of v vibrational quanta[3] or vibrons[4] distributed over n bonds. We use

$$\varphi_0\equiv|a_1a_2\cdots a_n)\equiv|1^{a_1}2^{a_2}\cdots n^{a_n}\rangle,\qquad v=\sum_{i=1}^{n}a_i, \tag{1}$$

to denote a basis state which has a_i vibrons in the bond i, and call a_i the occupation number for the bond i.

(ii) Permutation group symmetry (or spin symmetry) adaptation of n-electron wave functions. Suppose that there are n electrons occupying n orbits $a_1,a_2,\cdots,a_n$. The vector

$$\varphi_0\equiv|a_1a_2\cdots a_n)\equiv|\psi_{a_1}(1)\psi_{a_2}(2)\cdots\psi_{a_n}(n)\rangle, \tag{2}$$

denotes an n-electron state with electron i occupying the i-th orbits a_i. The state (1) or (2) will be referred to as the normal order state.

Since any point group is isomorphic to a subgroup of the permutation group, S_n, these two problems are closely related to one another with the following dictionary for translating terminologies:

bond index$\leftrightarrow$coordinate index;

number of vibrons$\leftrightarrow$single-particle-state index.

Therefore we can borrow the techniques of the theory of the permutation groups[6] for the symmetry adaptation of Eq. (1).

Since they are simple in comparison with the permutation groups, it is somewhat surprising that up to the present the representation problem for point groups has evaded any algebraic solution. The known solutions have all been obtained by numerical procedures as by the projection operator method,[1,7] eigenfunction method (EFM),[6,8,9] or other methods.[3]

Besides the fact that it needs repetitive work, another great disadvantage of the numerical solution is that the explicit expression of an irreducible basis vector does not give a physical picture and usually involves so many terms that it looks chaotic. For example, the basis vector for the one-dimensional irrep A_{2u} of O_h in the subspace $L_{v=4}$ (to be derived in Sec. V) is

$$\begin{aligned}A_{2u}=&|1^225-2^235+3^245-4^215\rangle-|1^226-2^236+3^246-4^216\rangle\\&+|12^25-23^25+34^25-41^25\rangle-|12^26-23^26+34^26-41^26\rangle\\&+|125^2-235^2+345^2-415^2\rangle-|126^2-236^2+346^2-416^2\rangle,\end{aligned} \tag{3}$$

where $|A+B+\cdots\rangle\equiv|A\rangle+|B\rangle+\cdots$. Although this may not look too formidable in today's terms, it is considerably more complicated than the concise expression to be introduced below, and the contrast becomes really extreme for more complicated groups, such as the icosahedral group.

In this paper we will introduce a point-group symmetrized boson representation, or SBR for short, to solve the problem. As is well known, boson representation is always totally symmetric. Here the symmetrization refers to the bond indices. In the C_{4h}-SBR to be described in Sec. III, the above irreducible basis vector can be written as

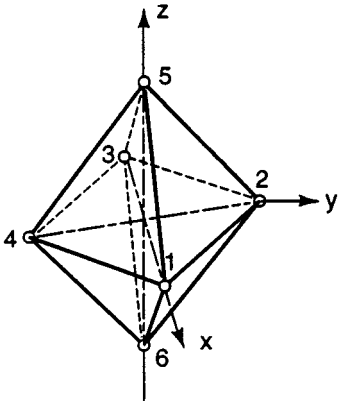
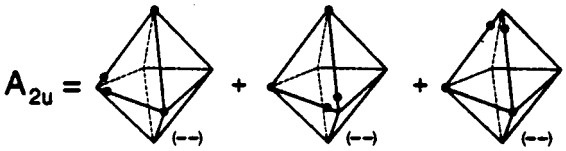


FIG. 1. Octahedron with O_h symmetry. The bonds 1,2,3,4 and 5,6 are called the horizontal and vertical bonds, respectively.

$$A_{2u}=|21;1\rangle_{--}+|12;1\rangle_{--}+|11;2\rangle_{--}, \tag{4}$$

where $|21;1\rangle_{--}$, $|12;1\rangle_{--}$ and $|11;2\rangle_{--}$ just represent the first, second and third lines in Eq. (3). For example, $|21;1\rangle_{--}$ represents a state which has three vibrons distributed over the four horizontal bonds (see Fig. 1) with one bond having two vibrons and the other having one, and one vibron distributed over the vertical bonds, with the cycle symmetry ρ (the quantum number of C_{4z})$=-1$ and the inversion symmetry $i_0=-1$. Equation (4) can be represented by the graphs,



.

In SBR we disregard the irrelevant thing—the indexing of the bonds, and focus on the essential thing—the distribution of the vibrons over the bonds, thereby greatly simplifying not only the finding but also the presentation of the irreducible bases. *The simplification can be compared to the one brought about by the second quantization over the first quantization.*

In the SBR, the reduction of the regular representation of the group O_h for the group chain $O_h\supset D_4\supset C_4$ or $O_h\supset D_4\supset D_2$ is reduced to a trivial problem, finding the eigenvectors of a 3×3 matrix

$$\begin{pmatrix} 0 & 2 & 2 \\ 2 & 0 & 2 \\ 2 & 2 & 4 \end{pmatrix}.$$

Succinct algebraic expressions for the irreducible bases of O_h in the most general cases are obtained in this way without any use of the characters or irreducible matrix elements, while the irreducible bases for any specific cases can be obtained from the general case easily by a procedure called assimilation (to be introduced below) without any projection, as in the projection operator method,[1,7] or eigenequation-solution, as in the eigenfunction method.[6] All the specific cases have been worked out and presented in tables; therefore the irreducible basis vectors for the

above two group chains have been obtained once and for all. To show the convenience of the SBR, the Hamiltonian in the algebraic model of Iachello and Oss for stretching vibrations of SF_6, which has been solved in a non-symmetrized basis, is resolved in the symmetry adapted basis. Not only is the dimension of the eigenequation reduced by one order of magnitude, but also the structure of the eigenstates are obtained. For the icosahedral group, the reduction of the dimensionality will be more drastic.

Since we are dealing with a venerable subject, and different methods may appear similar under superficial examination, we have taken great pain in the last section to compare the method developed in this paper with the prior work in order to establish unambiguously that we are not repeating a known technology.

The outline of the paper is as follows: We begin with a brief review of the EFM in Sec. II. The construction of the symmetrized boson representation for O_h and the properties of the symmetrical bases are addressed in Sec. III. The algebraic expressions of the irreducible basis of O_h is derived in Sec. IV for the most general case and in Sec. V, using the assimilation procedure, for any specified cases. The Hamiltonian of Iachello and Oss is rediagonalized in Sec. VI. The final section is a summary of various methods for symmetry adaptation.

II. BRIEF REVIEW OF THE EFM

Since the derivation of algebraic expressions for the symmetry adapted bases utilizes the EFM, it is appropriate to initiate the exposition with a summary. For details, readers are referred to Refs. 6 and 8. The essence of the EFM is best illustrated by the three-dimensional rotation group SO_3. According to the terminology in Ref. 6, the Casimir operator $\mathbf{J}^2$ is called the first kind of complete set of commuting operators (CSCO-I) of SO_3, which is a CSCO in the class parameter space. The operator set $(\mathbf{J}^2, J_z)$ is called the second kind of CSCO (CSCO-II) of SO_3, which is a CSCO in the configuration space of the unit sphere, the (θ, φ) space, while $(\mathbf{J}^2, J_z, J_z)$ is called the third kind of CSCO (CSCO-III), which is a CSCO in the group parameter space. The operator J_z is the third component of the angular momentum in the intrinsic coordinate system. The set of operators (J_x, J_y, J_z) are the generators of the intrinsic group SO_3, which commutes with and is anti-isomorphic to the rotation group SO_3, and describes the rotation of a system (such as a molecule) around its intrinsic (or body-fixed) axes.[6,1] The eigenfunctions of the CSCO-I, -II and -III in the class parameter space, ordinary configuration space, and group parameter space, respectively, give the complex conjugate of the primitive characters, the irreducible basis, and the complex conjugates of the irreducible matrices of SO_3 in the $SO_3 \supset SO_2$ classification.

It was shown that the above approach can be extended to any compact group. For a finite group G, the Casimir operator $\mathbf{J}^2$ of SO_3 is replaced by the CSCO-I of the finite group G, denoted by C, which is a linear combination of a few class operators of G, and the Casimir operator J_z of SO_2 is replaced by the CSCO-I, denoted by C', of a canonical subgroup G' of G. Similarly J_z is replaced by the operator C' of the corresponding subgroup G' of the intrinsic group G, which commutes with and is anti-isomorphic to G. The intrinsic group G is a generalization of the intrinsic rotation group SO_3.

The eigenvectors of the CSCO-I, -II and -III again give the complex conjugate of primitive characters, the irreducible basis and the complex conjugate of irreducible matrix elements of G in the $G \supset G'$ classification. The CSCO-I of G is also called the CSCO of G for simplicity. The CSCO of finite groups are easily found and those for the commonly used point groups are listed in Table I.

Finding the irreducible basis in the regular representation is equivalent to finding the simultaneous eigenvectors of the CSCO-III. For the SO_3 and a finite group G, these equations read, respectively,

TABLE I. The CSCO of point groups.

D_2	D_{2d}	D_3	D_4	D_{4d}	D_5	D_6
(C_{2x},C_{2y})	$(2C_2,2\sigma_d)$	$(3C_2)$	$(2C_2,2C_2')$	$(2S_8,4\sigma_d)$	$(2C_5,5C_2)$	$(2C_6,3C_2\prime)$
C_{2v}	C_{3v}	C_{4v}	C_{5v}	C_{6v}	$C_{\infty v}$	D_{6d}
(C_{2z},σ_y)	$(3\sigma_v)$	$(2C_4,2\sigma_d)$	$(2C_5,5\sigma_v)$	$(2C_6,3\sigma_v)$	$(2C_z(\varphi),\sigma_y)$	$(2S_{12},6\sigma_d)$
$D_{\infty v}$	T	T_d	O	O_h	I	I_h
$(2C_z(\varphi),\sigma_y,\hat{I})$	$(4C_3)$	$(6\sigma_d)$	$(6C_2)$	$(6\sigma,\hat{I})$	$(12C_5)$	$(12C_5,\hat{I})$

$$\begin{pmatrix} \mathbf{J}^2 \\ J_z \\ \overline{J_z} \end{pmatrix} \psi_m^{(j)\overline{m}} = \begin{pmatrix} j(j+1) \\ m \\ \overline{m} \end{pmatrix} \psi_m^{(j)\overline{m}}, \tag{5}$$

$$\begin{pmatrix} C \\ C' \\ \overline{C'} \end{pmatrix} \psi_\rho^{(\nu)\overline{\rho}} = \begin{pmatrix} \nu \\ \rho \\ \overline{\rho} \end{pmatrix} \psi_\rho^{(\nu)\overline{\rho}}. \tag{6}$$

The eigenvector $\psi_\rho^{(\nu)\overline{\rho}}$ gives the component ρ associated with the point group G with $\overline{\rho}$ as the multiplicity label of the irrep ν, but at the same time it gives the component $\overline{\rho}$ associated with the intrinsic point group G with ρ as the multiplicity label of the irrep ν. Notice that $\overline{\rho}$ and ρ have the same set of quantum numbers, just as $m,\overline{m}=j,j-1,\cdots,-j$ for the SO_3 group.

In the group space, the irreducible basis $\psi_\rho^{(\nu)\rho}$ becomes the normalized generalized projection operator $\mathbf{P}_\rho^{(\nu)\rho}$ (the usual form for the generalized projection operator is denoted as $\mathbf{P}_{\rho\rho}^{(\nu)}=\sqrt{h_\nu/g}\mathbf{P}_\rho^{(\nu)\overline{\rho}}$)

$$\mathbf{P}_\rho^{(\nu)\overline{\rho}} = \sqrt{\frac{h_\nu}{g}} \sum_{a=1}^{g} D_{\rho\overline{\rho}}^{(\nu)}(R_a)^* R_a, \tag{7}$$

where h_ν is the dimension of the irrep ν, g the order of G, R_a the a-th group element, and $D_{\rho\overline{\rho}}^{(\nu)}(R_a)$ is $(\rho,\overline{\rho})$-th entry of the irreducible matrix. For a one-dimensional irreducible basis, $\rho=\overline{\rho}$, and the quantum numbers ρ and $\overline{\rho}$ are redundant. Therefore, for this case we write $\psi_\rho^{(\nu)\rho}\equiv\psi^{(\nu)}$.

A program packet is written[9] based on the EFM which can compute *ab initio* subgroup-symmetry adapted (both single- and double-valued) irreps and Clebsch-Gordan coefficients of point groups and space groups. These are numerical solutions. Our aim in this paper is to find algebraic solutions for the irreducible bases of point groups. We still use the EFM; however, instead of solving the eigenequation of the CSCO-III in the g-dimensional group space, we solve the eigenequation of the CSCO-I in the double SBR with dimensions much lower (3 for O_h and 4 for I_h) than the group order g. Before introducing the SBR, we review some of the concepts that will be utilized in its development.

As is well known, each point group is isomorphic to a subgroup of a permutation group. However, there are two kinds of permutation groups for either of the bases represented by Eqs. (1) and (2).

(i) The coordinate permutation group S_n, whose element p permutes the bond indices or the coordinate indices. For example, the permutation $p_{123}\equiv(123)$ is defined as

$$(123)|a_2a_3a_1\rangle=(123)|\psi_{a_2}(1)\psi_{a_3}(2)\psi_{a_1}(3)\rangle$$

$$=|\psi_{a_2}(2)\psi_{a_3}(3)\psi_{a_1}(1)\rangle$$

$$\equiv|a_1a_2a_3\rangle. \tag{8}$$

(ii) The state permutation group $\mathscr{S}_n$ whose element $\wp$ permutes the state indices a_i.[10] For example, the action of $\wp_{123}\equiv(a_1a_2a_3)$ is

$$\wp_{123}|a_2a_3a_1\rangle=|a_3a_1a_2\rangle. \tag{9}$$

The operators p and $\wp$ commute and are independent, and only when acting on the normal order state φ_0 do we have $p=\wp^{-1}$,

$$p\varphi_0=\wp^{-1}\varphi_0. \tag{10}$$

Obviously, the groups S_n and $\mathscr{S}_n$ are isomorphic. S_n and $\mathscr{S}_n$ are called the permutation group on particle labels and state labels, respectively, in Ref. 11.

Returning to the consideration of the point groups, any such group has the following three kinds of realization:

(i) A point group G is isomorphic to a subgroup of the coordinate permutation group S_n, which is again denoted by G.

(ii) G is also isomorphic to a subgroup of the state-permutation group $\mathscr{S}_n$. This subgroup is called the state-point group and denoted by $\mathscr{G}$. G and $\mathscr{G}$ commute and are isomorphic. Corresponding operators, R_a and $\mathscr{R}_a$, are two different operators, but because of Eq. (10) R_a and $\mathscr{R}_a^{-1}$ are equal when acting on the normal order state,

$$R_a\varphi_0=\mathscr{R}_a^{-1}\varphi_0. \tag{11}$$

(iii) The intrinsic point group $\overline{G}$, which is defined as follows: For each element of a group G we can associate a corresponding operator R in the group space L_g through the following equation:

$$\overline{R}S=SR, \qquad \text{for all } S\in L_g. \tag{12}$$

It is important to emphasize that Eq. (12) is not an identity, but rather a definition of the operator $\overline{R}$. (For further discussion of this fundamental distinction, the reader should consult Refs. 6 and 8.) The group formed by the totality of operators $\overline{R}$ is called the intrinsic point group, denoted as $\overline{G}$, which is a generalization of the intrinsic rotation group SO_3. $\overline{G}$ commutes with and is anti-isomorphic to G.

The state-point group $\mathscr{G}$ can be regarded as a realization of the intrinsic point group $\overline{G}$ on the product space (1) or (2). The relation between the two is

$$\overline{R}=\mathscr{R}^{-1}. \tag{13}$$

From Eqs. (11) and (13) we have

$$R\varphi_0=\overline{R}\varphi_0. \tag{14}$$

An important fact is that the CSCO-I of the groups $G,\mathscr{G}$ and $\overline{G}$ are equal (cf. $\mathbf{J}^2=\overline{\mathbf{J}^2}$),

$$C=\mathscr{C}=\overline{C}. \tag{15}$$

Therefore, the irreps of G and $\overline{G}$ are labeled by the same quantum number, just as the irreps of SO_3 and SO_3 are labeled by the same quantum number j. As will be seen, our approach relies heavily on the interplay of these three groups $G, \mathscr{G}$ and G. The group $\mathscr{G}$ or G will provide the multiplicity operator for distinguishing equivalent irreps of G. In the group space, we need to use the intrinsic group G, while in the product space (1) or (2), it is more convenient to use $\mathscr{G}$.

As examples, consider the molecule XY_6. The numbering of its 6 vertices is shown in Fig. 1. For convenience, the bonds 1–4 and 5 and 6 will be referred to as the horizontal and vertical bonds, respectively. From Table I it is known that the CSCO-I of O_h is $(6\sigma,\hat{I})$. Here and in the following we will change our notation slightly by using C to denote the class operator 6σ which consists of the six reflection planes instead of denoting the CSCO-I of O_h. The CSCO-I of the cyclic group C_4 is C_{4z}. According to Fig. 1, we have

$$\begin{gathered} C=(12)(34)+(14)(23)+(15)(36)+(16)(35)+(25)(46)+(26)(45), \\ \hat{I}=(13)(24)(56), \quad C_{4z}=(1234). \end{gathered} \tag{16}$$

Now turn to the state-point group. Let us consider the most general case when the bonds 1–6 all have different non-zero number of vibrons. Suppose the bonds 1–6 have $a-f$ vibrons, respectively. If we identify $a-f$ with a_1-a_6, respectively, then the following state will be our normal order state

$$\varphi_0=|abcdef). \tag{17}$$

The counterpart of Eq. (16) for the state-point groups can be obtained from (16) by the index replacements: $1\rightarrow a, 2\rightarrow b, \cdots 6\rightarrow f$,

$$\begin{gathered} \mathscr{C}=(ab)(cd)+(ad)(bc)+(ae)(cf)+(af)(ce)+(be)(df)+(bf)(de), \\ \mathscr{I}=(ac)(bd)(ef), \quad \mathscr{C}_{4z}=\overline{C_{4z}^{-1}}=(abcd). \end{gathered} \tag{18}$$

Notice that $C=\mathscr{C}, \hat{I}=\mathscr{I}$, but $C_{4z}\neq\mathscr{C}_{4z}$.

III. THE C_4-SYMMETRIZED BOSON REPRESENTATION FOR O_h

The standard irreducible basis[12] for the group O_h is the $O_h\supset D_4\supset D_2$ basis. The components of the standard irreps E, F_1 and F_2 are labeled by $(\theta,\epsilon),(x,y,z)$ and (ξ,η,ζ), respectively, as given by Griffith.[12]

Another commonly used group chain is $O_h\supset D_4\supset C_4$. Since C_4 is a canonical subgroup of O_h (each irrep of C_4 occurs at most once in any irrep of O_h), the intermediate group D_4 is redundant for classifying the basis. Therefore we will refer the second basis as the $O_h\supset C_4$ basis. The components of the irreps F_1 and F_2 in the $O_h\supset C_4$ group chain will be labeled by (x',y',z) and (ξ',η',ζ), respectively. The relation between the two bases is

$$x'=-\sqrt{\tfrac{1}{2}}(x+iy), y'=\sqrt{\tfrac{1}{2}}(x-iy), \quad \xi'=-\sqrt{\tfrac{1}{2}}(\xi+i\eta), \eta'=\sqrt{\tfrac{1}{2}}(\xi-i\eta). \tag{19}$$

Therefore the basis vectors for the irreps A and E, as well as the third components of the irreps F are the same for the two group chains. It is known that for each irrep we only have to calculate one component, called the principal component, since owing to the existence of the Wigner-Eckart theorem, that is all we need for calculating the matrix element of any tensor operator and, consequently, any observable. We choose the second component of the irrep E and the third component of the irreps F as the principal components. Therefore, by using the $O_h\supset C_4$ group chain we can get the principal components for both the group chains. The CSCO-II for the $O_h\supset C_4$ group chain

TABLE II. The eigenvalues of the CSCO-II, $(6\sigma,\hat{I},C_{4z})$, of O_h.

	A_{1g}	A_{2g}	$E_{g,(\theta,\epsilon)}$	$F_{1g,(x',y',z)}$	$F_{2g,(\xi',\eta',\zeta)}$	A_{1u}	A_{2u}	$E_{u,(\theta,\epsilon)}$	$F_{1u,(x',y',z)}$	$F_{2u,(\xi',\eta',\zeta)}$
6σ	6	-6	0	-2	2	-6	6	0	2	-2
$\hat{I}$	1	1	1	1	1	-1	-1	-1	-1	-1
C_{4z}	1	-1	$(1,-1)$	$(-i,i,1)$	$(-i,i,-1)$	1	-1	$(1,-1)$	$(-i,i,1)$	$(-i,i,-1)$

$x'=-\sqrt{\frac{1}{2}}(x+iy)$, $y'=\sqrt{\frac{1}{2}}(x-iy)$; $\xi'=-\sqrt{\frac{1}{2}}(\xi+i\eta)$, $\eta'=\sqrt{\frac{1}{2}}(\xi-i\eta)$.

is $(6\sigma,\hat{I},C_{4z})$. The correspondence between its eigenvalues and the standard labels are listed in Table II. From the table it is seen that we only need to find the basis vectors corresponding to the real eigenvalues, $\rho=\pm 1$, of C_{4z}.

In the numerical approach to the EFM, we generate the regular representation space from $|abcdef)$ and then diagonalize the CSCO-III, $(6\sigma,\hat{I},C_{4z},C_{4z})$, in this 48-dimensional space. To obtain the algebraic solution, our strategy is first to construct the eigenspace $L^{i_0}_{\rho,\overline{\rho}}$—of the operators $(\hat{I},C_{4z}.\overline{C_{4z}})$, and then diagonalize 6σ in $L^{i_0}_{\rho,\overline{\rho}}$—with the eigenvalues $\rho,\overline{\rho}$ and i_0 as parameters. In this way we obtain a unified expression of the irreducible bases $\psi^{(\nu,i_0)\overline{\rho}}_{\rho}$ for all possible values of $\rho,\overline{\rho}$ and i_0, which is what we mean by an algebraic solution.

Since $(C_{4z},\hat{I})$ is the CSCO of C_{4h}, to finding the eigenvectors of $(C_{4z},\hat{I})$ is equivalent to find the irreducible basis of C_{4h}, which is most easily done by using the projection operators,

$$\sqrt{8}\varphi^1\equiv\sqrt{8}\varphi^1_{\rho i_0}=|abcd;ef\rangle_{\rho i_0}\equiv|abcd;ef\rangle=P^{\rho}P^{i_0}|abcdef), \tag{20}$$

where P^{ρ} and P^{i_0} are un-normalized projection operators

$$P^{\rho}=\sum_{j=0}^{3}(C_{4z})^j\rho^{*j},\qquad P^{i_0}=1+i_0\hat{I}. \tag{21}$$

Notice that φ^1 is a normalized, symmetrized vector, where the quantum numbers (ρ,i_0) are implied in the notation $|abcd;ef\rangle$, and the semicolon means symmetrization with respect to the subgroup C_{4h}. φ^1 satisfies the following equations:

$$C_{4z}\varphi^1=\rho\varphi^1,\qquad \hat{I}\varphi^1=\mathscr{I}\varphi^1=i_0\varphi^1,\quad \mathscr{C}_{4z}\varphi^1=\rho^*\varphi^1. \tag{22}$$

The eigenvalues ρ and i_0 of C_{4z} and $\hat{I}$ are referred to as the quantum numbers for cyclic and inversion symmetries, respectively. In case we need to specify (ρ,i_0) explicitly, we attach the subscripts(ρ,i_0) to the ket symbol. The four bases with $(\rho,i_0)=(1,1),(-1,1),(1,-1),(-1,-1)$ are denoted as

$$|abcd;ef\rangle_{++},\qquad |abcd;ef\rangle_{-+},\quad |abcd;ef\rangle_{+-},|abcd;ef\rangle_{--}. \tag{23}$$

The basis $|abcd;ef\rangle$ has the symmetries

$$|abcd;ef\rangle=\rho|bcda;ef\rangle=\rho^*|dabc;ef\rangle=\rho^2|cdab;ef\rangle=\cdots=i_0\rho^2|abcd;fe\rangle. \tag{24}$$

For the cases with real ρ, from (20) and (24) it is seen that the basis vector $|abcd;ef\rangle_{\rho i_0}$ can be factorized into two parts, $|abcd;\rangle_{\rho}$ and $|;ef\rangle_{i_0}$. The first one is related to the horizontal bonds carrying the quantum number ρ, while the second one is related to the vertical bonds carrying the quantum number i_0, i.e.,

TABLE III. The action of six reflections on $\varphi^1=|abcd;ef\rangle$.

$(ad)(bc)$	$(ab)(cd)$	$(ae)(cf)$	$(af)(ce)$	$(be)(df)$	$(bf)(de)$
$\|dcba;ef\rangle$	$\|badc;ef\rangle$	$\|ebfd;ac\rangle$	$\|fbed;ca\rangle$	$\|aecf;bd\rangle$	$\|afce;db\rangle$

$$|abcd;ef\rangle_{\rho i_0}=|abcd;\rangle_\rho|;ef\rangle_{i_0}, \qquad \text{for } \rho=\pm 1, \tag{25}$$

where

$$\begin{aligned}|abcd;\rangle_\rho\equiv|abcd;\rangle=P^\rho|abcd)&=|(1234+\rho^*2341+\rho^{*2}3412+\rho^{*3}4123)^{abcd}\rangle,\\ &=|abcd)+\rho|bcda)+\rho^2|cdab)+\rho^3|dabc),\end{aligned} \tag{26}$$

$$|;ef\rangle_{i_0}\equiv|;ef\rangle=P^{i_0}|5^e6^f\rangle=|(56+i_065)^{ef}\rangle\equiv|5^e6^f+i_06^e5^f\rangle, \tag{27}$$

where we used the notation

$$|(3412)^{abcd}\rangle\equiv|3^a4^b1^c2^d\rangle=|1^c2^d3^a4^b\rangle. \tag{28}$$

Notice that the bond indices are symmetrized and hidden in $|abcd;ef\rangle$. Instead of specifying how many vibrons are in each bond, we only need to specify that there are a,b,c,d vibrons distributed over the four horizontal bonds and e,f vibrons distributed over the vertical bonds with the cyclic symmetry ρ and inversion symmetry i_0. $|abcd;ef\rangle$ is a basis vector in what is called the C_{4h}-symmetrized boson representation. In analogy with the second quantization formalism which makes the particle labels meaningless, here the SBR makes the bond indices within the horizontal or vertical set meaningless, resulting in great simplification.

A usual way to construct a representation of a large group from the irreps of its subgroup is by using induction[13]; i.e., by applying the six coset representatives of O_h to φ^1, we can get six basis vectors that carry the induced representation. However, the new vectors formed in this way are no longer eigenvectors of C_{4z}, since the coset representatives do not commute with C_{4z}. But to keep within the eigenspace, L_ρ of C_{4z} is the key point to getting algebraic expressions of the irreducible bases as a function of ρ. Therefore, we have to find another way to generate the representation of O_h from the irreps of its subgroup C_{4h}.

Since the state permutation operators commutes with C_{4z} and $\hat{I}$, we may applying some state permutation operators on φ^1 to generate an eigenspace space of C_{4z}. How to find these operators? Due to the fact that $\mathscr{C}=C$, the diagonalization of C can be replaced by that of $\mathscr{C}$. Since in $|abcd;ef\rangle$ the bond indices are symmetrized and hidden, and $|abcd;ef\rangle$ is a linear combination of 10 product states, it would be rather difficult to find the action of the reflections (12), (34), etc. on $|abcd;ef\rangle$, but it is trivial to find the operation of the state permutation on it. For example $(ab)(cd)|abcd;ef\rangle=|badc;ef\rangle$. Applying the six reflections $(ab)(cd),(ad)(bc),(ae)\times(cf),(af)(ce),(be)(df)$ and $(bf)(de)$ in $\mathscr{C}$ to $|abcd;ef\rangle$, yields five additional symmetrized vectors, as shown in Table III. All these vectors are eigenvectors of C_{4z} with the same eigenvalues ρ. We might choose them as the basis vectors; however it is more convenient to choose the following six vectors as our basis,

$$\begin{aligned}&\varphi^1=\frac{1}{\sqrt{8}}|abcd;ef\rangle, \qquad \varphi^2=\frac{1}{\sqrt{8}}|adcb;fe\rangle, \quad \varphi^3=\frac{1}{\sqrt{8}}|bedf;ac\rangle,\\ &\varphi^4=\frac{1}{\sqrt{8}}|ecfa;db\rangle, \quad \varphi^5=\frac{1}{\sqrt{8}}|bfde;ca\rangle, \qquad \varphi^6=\frac{1}{\sqrt{8}}|fcea;bd\rangle.\end{aligned} \tag{29}$$

TABLE IV. The action of $\overline{C_{4z}}=(adcb)$ on $\varphi^3-\varphi^6$.

	φ^3	φ^4	φ^5	φ^6
$\overline{C_{4z}}\varphi^i$	$\rho\varphi^4$	$\rho\varphi^5$	$\rho\varphi^6$	$\rho\varphi^3$

Though different choices have no effect on the final results, a proper choice will make the intermediate steps simpler. The eigenspace $L_\rho^{i_0}=\{\varphi^i: i=1,\ldots,6\}$ is a representation space of the operator $\mathscr{C}$, called the C_{4h}-symmetrized boson representation (SBR). Notice that $L_\rho^{i_0}$ is invariant only under $\mathscr{C}$, but not under O_h, and thus is not a representation space of O_h. Only if one allows ρ to take all possible values, do they carry a representation of O_h. It should be emphasized again that SBR is not the induced representation.

IV. IRREDUCIBLE BASES OF O_h IN THE REGULAR REPRESENTATION

The original 48-dimensional group space has been reduced to six-dimensional eigenspace $L_{\underline{\rho}}^{i_0}$. To get the expression for irreducible basis of O_h which is ''analytic'' in the quantum number $\underline{\rho}$, and to further reduce the space, we construct the common eigenspace $L_{\underline{\rho\rho}}^{i_0}$ of $(\hat{I},C_{4z},\overline{C_{4z}})$, i.e., to combine $\varphi^1,\cdots,\varphi^6$ into eigenvectors $\varphi_{\underline{\rho\rho}}^i$ of $\overline{C_{4z}}=(adcb)$. φ^1 and φ^2 are already eigenvectors of $\overline{C_{4z}}$ with eigenvalue $\overline{\rho}=\rho$, ρ^*, respectively,

$$\overline{C_{4z}}\varphi^1=\frac{1}{\sqrt{8}}|dabc;ef\rangle=\rho\varphi^1=\overline{\rho\varphi}^1,\quad \overline{C_{4z}}\varphi^2=\frac{1}{\sqrt{8}}|dcba,fe\rangle=\rho^*\varphi^2=\overline{\rho\varphi}^2. \tag{30}$$

From Eq. (30) we have

$$\varphi_{\underline{\rho\rho}}^1=\varphi^1\delta_{\underline{\rho\rho}},\qquad \varphi_{\underline{\rho\rho}}^2=\varphi^2\delta_{\underline{\rho\rho}^*}. \tag{31}$$

Therefore we only need to combine $\varphi^3-\varphi^6$ into eigenvectors of $\overline{C_{4z}}$. Applying $\overline{C_{4z}}=(adcb)$ [see Eq. (18)] to $\varphi^3-\varphi^6$, we get Table IV. Using Table IV, it is easy to obtain the third eigenvector of (C_{4z},C_{4z}),

$$\varphi_{\underline{\rho\rho}}^3=\tfrac{1}{2}\overline{P^\rho}\varphi^3=\tfrac{1}{2}\sum_{j=0}^{3}(\overline{C_{4z}})^j\overline{\rho^*}^j\varphi^3=\tfrac{1}{2}[\varphi^3+\overline{\rho^*}\rho\varphi^4+(\overline{\rho\rho})^2\varphi^5+\overline{\rho\rho}^*\varphi^6]_\rho. \tag{32}$$

The basis $\varphi_{\underline{\rho\rho}}^1$ - $\varphi_{\underline{\rho\rho}}^3$ is the $C_{4h}\times\overline{C_{4h}}$- symmetrized basis, and the representation it carries may be called the double SBR. The diagonalization of the CSCO-III in the 48-dimensional space is now reduced to diagonalize the operator $\mathscr{C}$ in the three-dimensional space $L_{\underline{\rho\rho}}^{i_0}=\{\varphi_{\underline{\rho\rho}}^i: i=1,2,3\}$.

The eigenvalues of the class operator 6σ in the eigenspace of $(C_{4z},\hat{I})$ are shown in Table V. The group O_h has ten inequivalent irreps, $A_{1g},A_{2g},E_g,F_{1g},F_{2g},A_{1u},A_{2u},E_u,F_{1u}$, F_{2u}. The subscripts in the Mulliken notation are related to the eigenvalues (ρ,i_0) of the operator set $(C_{4z},\hat{I})$, as shown in Table VI. Using Table VI, Table V is reduced to Table VII.

TABLE V. The eigenvalues of 6σ in the eigenspace of $(C_{4z},\hat{I})$.

$(\rho,i_0)=(1,1)$:	A_{1g}	$E_{g,\theta}$	$F_{1g,z}$	$(1,-1)$:	A_{1u}	$E_{u,\theta}$	$F_{1u,z}$
6σ	6	0	-2		-6	0	2
$(\rho,i_0)=(-1,1)$:	A_{2g}	$E_{g,\epsilon}$	$F_{2g,\zeta}$	$(-1,-1)$:	A_{2u}	$E_{u,\epsilon}$	$F_{2u,\zeta}$
6σ	-6	0	2		6	0	-2

TABLE VI. Notation switchboard.

ρi_0	$++$	$-+$	$+-$	$--$	ρi_0	$-+$	$--$
$A_{\rho i_0}$	A_{1g}	A_{2g}	A_{1u}	A_{2u}	$E_{i_0,\rho}$	$E_{g,\epsilon}$	$E_{u,\epsilon}$
$F_{\rho i_0,\rho}$	$F_{1g,z}$	$F_{2g,\zeta}$	$F_{1u,z}$	$F_{2u,\zeta}$			

To construct the representation matrix of $\mathscr{C}$ in $L^{i_0}_{\rho\overline{\rho}}$, we need first find its representation matrix in the space $L^{i_0}_{\rho}$.

By using the symmetries (24), the basis vectors in the second row of Table III can be expressed in terms of φ^1-φ^6, and from it we get the action of $\mathscr{C}$ on φ^1, as shown in the second row of Table VIII. By index replacements, from $\mathscr{C}\varphi^1$ we can get the action of $\mathscr{C}$ on φ^2-φ^6, as shown in Table VIII.

From Table VIII and (31)–(32), we can compose the representative matrix of $\mathscr{C}$ in the basis $\{\varphi^i_{\rho\overline{\rho}}: i=1,2,3\}$. Its transpose has the following form:

$$\widetilde{M}=i_0\begin{pmatrix} 0 & (\rho+\rho^*)\delta_{\overline{\rho}\rho} & 2\rho^*\delta_{\overline{\rho}\rho} \\ (\rho+\rho^*)\delta_{\overline{\rho}\rho} & 0 & 2\rho\delta_{\overline{\rho}\rho^*} \\ 2\rho\delta_{\overline{\rho}\rho} & 2\rho^*\delta_{\overline{\rho}\rho^*} & \rho^2(\overline{\rho}+\overline{\rho^*})+\overline{\rho}^2(\rho+\rho^*) \end{pmatrix}. \tag{33}$$

It is seen that when $\rho \neq \overline{\rho}, \overline{\rho^*}$, the matrix M becomes one dimensional and its solution is simply the basis vector $\varphi^3_{\rho\overline{\rho}}$,

$$\psi^{(\nu)\overline{\rho}}_{\rho}=\varphi^3_{\rho\overline{\rho}}, \qquad \rho\neq\overline{\rho,\rho^*}. \tag{34}$$

The $\rho \neq \overline{\rho,\rho^*}$ case can be subdivided into the sub-cases:

(i) Both ρ and $\overline{\rho}$ are real, $\rho,\overline{\rho}=\pm 1$. According to the possible eigenvalues of $\overline{\rho}$ and ρ in each irrep given in Table II, we know that the eigenvectors with $\overline{\rho}=\pm 1$ must belong to the irreps E,

$$\psi^{(E_{i_0})-\rho}_{\rho}=\tfrac{1}{2}(\varphi^3-\varphi^4+\varphi^5-\varphi^6)_{\rho}, \quad \rho=\pm 1. \tag{35}$$

(ii) $\overline{\rho}$ is imaginary and $\rho=\pm 1$. For the same reason we know that this case must belong to the irreps $F_{\rho i_0}$, namely

$$\psi^{(F_{\rho i_0})\overline{\rho}}_{\rho}=\tfrac{1}{2}[\varphi^3+\overline{\rho^*}\rho\varphi^4+(\overline{\rho}\rho)^2\varphi^5+\overline{\rho}\rho^*\varphi^6]_{\rho}, \quad \overline{\rho}=\pm i, \rho=\pm 1. \tag{36}$$

Since we are free to choose the multiplicity separation, the two eigenvectors $\psi^{(F_{\rho i_0})\overline{\rho}=\pm i}_{\rho}$ with imaginary quantum number $\overline{\rho}$ can be recombined into two other vectors, labeled by the multiplicity label $\tau=1,2$,

$$\psi^{(F_{\rho i_0})\tau=1}_{\rho}=\frac{1}{\sqrt{2}}[\psi^{(F_{\rho i_0})-i}_{\rho}+\psi^{(F_{\rho i_0})i}_{\rho}]=\frac{1}{\sqrt{2}}(\varphi^3_{\rho}-\varphi^5_{\rho}), \quad \rho=\pm 1, \tag{37}$$

TABLE VII. The eigenvalues of 6σ in the eigenspace $L_{\rho,\overline{\rho}=\rho}$ of $(C_{4z},\overline{C_{4z}})$.

	$A_{\rho i_0}$	$E_{i_0,\rho}$	$F_{\rho i_0}$
6σ	$6\rho i_0$	0	$-2\rho i_0$

TABLE VIII. The action of 6σ on φ^i.

	φ^1	φ^2	φ^3	φ^4	φ^5	φ^6
$(6\sigma)\varphi^1$		$(\rho+\rho^*)i_0$	$\rho^* i_0$	$\rho^* i_0$	$\rho^* i_0$	$\rho^* i_0$
$(6\sigma)\varphi^2$	$(\rho+\rho^*)i_0$		ρi_0	$\rho^* i_0$	ρi_0	$\rho^* i_0$
$(6\sigma)\varphi^3$	ρi_0	$\rho^* i_0$		$\rho^* i_0$	$(\rho+\rho^*)i_0$	ρi_0
$(6\sigma)\varphi^4$	ρi_0	ρi_0	ρi_0		$\rho^* i_0$	$(\rho+\rho^*)i_0$
$(6\sigma)\varphi^5$	ρi_0	$\rho^* i_0$	$(\rho+\rho^*)i_0$	ρi_0		$\rho^* i_0$
$(6\sigma)\varphi^6$	ρi_0	ρi_0	$\rho^* i_0$	$(\rho+\rho^*)i_0$	ρi_0	

$$\psi_\rho^{(F_{\rho i_0})\tau=2}=\frac{1}{\sqrt{2}}\rho i_0[\psi_\rho^{(F_{\rho i_0})-i}-\psi_\rho^{(F_{\rho i_0})i}]=\frac{1}{\sqrt{2}}(\varphi_\rho^4-\varphi_\rho^6),\quad \rho=\pm 1.$$

The above transformation corresponds to the basis transformation shown in Eq. (19) for the irreps F_1, F_2 of the intrinsic point group G.

For the case with $\rho=\overline{\rho}=\pm 1$ we have three linearly independent vectors,

$$\varphi^1,\quad \varphi^2,\quad \varphi^3_{\rho\rho}=\tfrac{1}{2}(\varphi^3+\varphi^4+\varphi^5+\varphi^6). \tag{38}$$

This is the only case where the operator $\mathscr{C}=6\sigma$ has to be diagonalized. Using (33) we get the eigenvalue equation for the coefficients A_i in the expansion of $\psi_\rho^{(\nu)\rho}=A_1\varphi^1+A_2\varphi^2+A_3\varphi^3_{\rho\rho}$,

$$\rho i_0\begin{pmatrix}0&2&2\\2&0&2\\2&2&4\end{pmatrix}\begin{pmatrix}A_1\\A_2\\A_3\end{pmatrix}=\nu\begin{pmatrix}A_1\\A_2\\A_3\end{pmatrix}. \tag{39}$$

The corresponding eigenvectors of $\mathscr{C}=6\sigma$ are

$$\psi^{(A_{\rho i_0})}=\psi_\rho^{(6\rho i_0)\rho}=\frac{1}{\sqrt{6}}(\varphi^1+\varphi^2+2\varphi^3_{\rho\rho}),$$

$$\psi_\rho^{(E_{i_0})\rho}=\psi_\rho^{(0)\rho}=\frac{1}{\sqrt{3}}(\varphi^1+\varphi^2-\varphi^3_{\rho\rho}), \tag{40}$$

$$\psi_\rho^{(F_{\rho i_0})\tau=3}=\psi_\rho^{(-2\rho i_0)\rho}=\frac{1}{\sqrt{2}}(\varphi^1-\varphi^2).$$

Equations (35), (37) and (40), are the algebraic expression for the standard basis of O_h, and its compactness in the double SBR is impressive. However, the basis vectors in the double SBR do not have a clear physical picture and it is preferable to express the irreducible basis in terms of the SBR, as shown in Table IX. The results are spelled out in more detail in Table X, which covers all cases.

V. IRREDUCIBLE BASIS OF O_h IN THE NON-REGULAR REPRESENTATIONS

Starting from the most general case with all the integers a-f being non-zero and different, by letting some equal to zero or equal to one another, we can cover all possible cases for stretching or bending vibrations of the molecule XY_6. This procedure is called assimilation.

TABLE IX. Analytic expressions for standard basis of O_h.

	τ	$\sqrt{8}N$	φ^1	φ^2	φ^3	φ^4	φ^5	φ^6
$A_{\rho i_0}$	1	$\sqrt{\frac{1}{6}}$	1	1	1	1	1	1
$E^{\rho}_{i_0,\rho}$	1	$\sqrt{\frac{1}{12}}$	2	2	-1	-1	-1	-1
$E^{-\rho}_{i_0,\rho}$	2	$\frac{1}{2}$			1	-1	1	-1
$F_{\rho i_0,\rho}$	1	$\sqrt{\frac{1}{2}}$			1		-1	
	2	$\sqrt{\frac{1}{2}}$				1		-1
	3	$\sqrt{\frac{1}{2}}$	1	-1				

To specify the different cases it is convenient to introduce the concept ''configuration,'' $\langle f\rangle$, for multi-vibron systems, which is defined as a given distribution pattern of v vibrons among the n bonds. The subspace $L_{\langle f\rangle}$ characterized by configuration $\langle f\rangle=\langle abcdef\rangle$ is the one generated from the basis vector $|abcdef)$ by the operators of O_h, which carries a reducible representation of O_h. The space with given number of vibrons is a direct sum of $L_{\langle f\rangle}$,

$$L_v=\sum_{\langle f\rangle}\oplus L_{\langle f\rangle}. \tag{41}$$

The following shorthand notation for configuration is also used

$$\langle abcde\rangle=\langle abcde0\rangle,$$

$$\langle abcd\rangle=\langle abcd00\rangle\cdots,$$

$$\langle ab;cd\rangle\equiv\langle ab00cd\rangle=\langle ac0db\rangle.$$

The last equation shows that the subspace $L_{\langle ab;cd\rangle}$ can be generated either from the basis vector $|ab00cd\rangle$ or $|ac0db\rangle$. Notice that $\langle f\rangle$ is similar to the ''set'' defined by Halonen *et al.* in their Table I.[3] For example, for $v=2$, we have $\langle f\rangle=\langle 2\rangle$ (two vibrons in a bond), $\langle f\rangle=\langle 11\rangle$ (two adjacent bonds each has a vibron), and $\langle f\rangle=\langle 101\rangle$ (two opposite bonds each has a vibron). It is convenient to use diagrams to denote configurations. For example, the configurations $\langle 11\rangle,\langle 101\rangle,\langle 21\rangle,\langle 201\rangle,\langle 111\rangle\langle 11;1\rangle,\langle 211\rangle$ and $\langle 21;1\rangle$ are represented by the diagrams in Fig. 2.

One of the merits of the SBR is that the assimilation is trivial as is shown by the following:

TABLE X. Standard basis of O_h in reg. rep.

	ρi_0		ρi_0	τ	φ^1	φ^2	φ^3	φ^4	φ^5	φ^6
A_{1g}	$++$	A_{1u}	$+-$		1	1	1	1	1	1
A_{2g}	$-+$	A_{2u}	$--$		1	1	1	1	1	1
$E_{g,\epsilon}$	$-+$	$E_{u,\epsilon}$	$--$	1	2	2	-1	-1	-1	-1
	$-+$		$--$	2			1	-1	1	-1
$F_{1g,z}$	$++$	$F_{1u,z}$	$+-$	1			1		-1	
	$++$		$+-$	2				1		-1
	$++$		$+-$	3	1	-1				
$F_{2g,\zeta}$	$-+$	$F_{2u,\zeta}$	$--$	1			1		-1	
	$-+$		$--$	2				1		-1
	$-+$		$--$	3	1	-1				

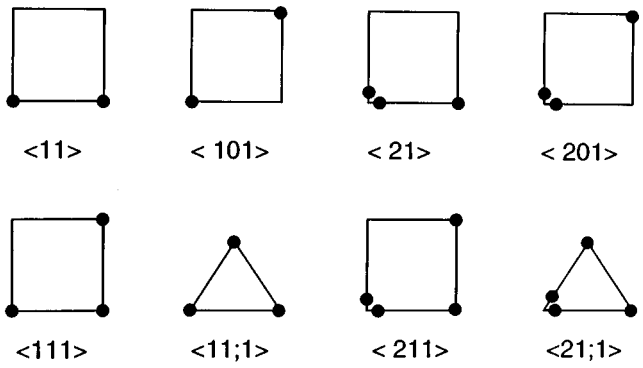


FIG. 2. Diagramatical representations of some simple configurations $\langle f\rangle$ for O_h.

$$
\begin{aligned}
|abcd;00\rangle &\equiv |abcd;0\rangle = (1+i_0)|abcd;\rangle,\\
|0000;ef\rangle &\equiv |0;ef\rangle = 4\delta_{\rho,1}|;ef\rangle,\\
|abc;\rangle &\equiv |abc0;\rangle = |(123+\rho^*234+\rho^2341+\rho412)^{abc}\rangle,\\
|ab;\rangle &\equiv |ab0;\rangle = |(12+\rho^*23+\rho^234+\rho41)^{ab}\rangle,\\
|\underline{ab};\rangle &\equiv |a0b;\rangle = |(13+\rho^*24+\rho^231+\rho42)^{ab}\rangle,\\
|a;\rangle &\equiv |a0;\rangle = |(1+\rho^*2+\rho^23+\rho4)^{a}\rangle,\\
|;a\rangle &\equiv |;a0\rangle = |5^a+i_06^a\rangle,
\end{aligned}
\tag{42}
$$

$$
\tag{43}
$$

where $|ab;\rangle(|\underline{ab};\rangle)$ indicates a state with two adjacent (opposite) bonds occupied by a and b vibrons.

Symmetries of the basis vectors are given by the equations,

$$
\begin{aligned}
&|abcd;\rangle = \rho|bcda;\rangle = \rho^2|cdab;\rangle = \rho^*|dabc;\rangle,\\
&|abc;\rangle = \rho|bc0a;\rangle = \rho^2|c0ab;\rangle = \rho^*|0abc;\rangle,\\
&|ab;\rangle = \rho^*|0ab;\rangle, \qquad |a;\rangle = \rho^*|0a;\rangle, \qquad |\underline{ab};\rangle = \rho^2|\underline{ba};\rangle,\\
&|;ef\rangle = i_0|;fe\rangle, \qquad |;e\rangle \equiv |;e0\rangle = i_0|;0e\rangle,
\end{aligned}
\tag{44}
$$

with some special cases to be noted as follows:

$$
\begin{aligned}
&|a;bb\rangle = (1+i_0)|a;\rangle|5^b6^b\rangle, \quad |;bb\rangle = (1+i_0)|5^b6^b\rangle, \qquad |aaaa;\rangle = 4\delta_{\rho,1}|1^a2^a3^a4^a\rangle,\\
&|\underline{aa};\rangle = 2|(13+\rho24)^{aa}\rangle, \qquad \rho = \pm 1.
\end{aligned}
\tag{45}
$$

It is essential to not confuse the basis $|12\rangle = |21\rangle$, a two-vibron unsymmetrized state, with $|12;\rangle = |(12+\rho23+34+\rho41)^{12}\rangle \neq |\ 21;\rangle$, a symmetrized three-vibron state.

In the process of assimilation, we find many different cases, some belonging to the regular representation and some to non-regular representations. The assimilation for the symmetrized basis is shown in Table XI.

TABLE XI. Assimilation of the symmetrized basis of O_h.[a]

$\langle f\rangle$	dim	T	φ^1	φ^2	φ^3	φ^4	φ^5	φ^6
$\langle abcdef\rangle$	48	10	$\lvert adcd;ef\rangle$	$\lvert adcb;fe\rangle$	$\lvert bedf;ac\rangle$	$\lvert ecfa;db\rangle$	$\lvert bfde;ca\rangle$	$\lvert fcea;bd\rangle$
$\langle abcde\rangle$			$\lvert abcd;e\rangle$	$i_0\lvert adcb;e\rangle$	$\lvert bed;ac\rangle$	$\rho\lvert aec;db\rangle$	$\lvert$deb;ca$\rangle$	$\rho\lvert$cea;bd$\rangle$
$\langle ab;cd\rangle$			$\rho\lvert dac;b\rangle$	$\rho i_0\lvert cad;b\rangle$	$\lvert cbd;a\rangle$	$\rho\lvert ab;dc\rangle$	$i_0\lvert dbc;a\rangle$	$\lvert$ba;cd$\rangle$
$\langle ab;bc\rangle$			$\rho\lvert$cab;b$\rangle$	$\rho i_0 bac;b\rangle$	$\lvert bbc;a\rangle$	$\rho\lvert$ab;cb$\rangle$	$i_0\lvert cbb;a\rangle$	$\lvert ba;bc\rangle$
$\langle ab;ab\rangle$			$\rho\lvert baa;b\rangle$	$\rho i_0\lvert aab;b\rangle$	$\lvert abb;a\rangle$	$\rho\lvert ab;ba\rangle$	$i_0\lvert bba;a\rangle$	$\lvert ba;ab\rangle$
$\langle ab;c\rangle$			$\lvert ac;b\rangle$	$\rho i_0\lvert ca;b\rangle$	$\lvert cb;a\rangle$	$\rho i_0\lvert ab;c\rangle$	$\rho i_0\lvert bc;a\rangle$	$\lvert ba;c\rangle$
$\langle abcd\rangle$	24	13	$\lvert abcd;0\rangle$	$\lvert adcb;0\rangle$	$\lvert \underline{bd};ac\rangle$	$\rho\lvert \underline{ac};db\rangle$	$i_0\varphi^3$	$i_0\varphi^4$
$\langle abbc\rangle$			$\lvert abbc;0\rangle$	$\lvert acbb;0\rangle$	$\lvert \underline{bc};ab\rangle$	$\rho\lvert \underline{ac};cb\rangle$	$i_0\varphi^3$	$i_0\varphi^4$
$\langle abc\rangle$			$\lvert abc;0\rangle$	$\lvert cba;0\rangle$	$\lvert b;ac\rangle$	$\rho i_0\lvert \underline{ac};b\rangle$	$i_0\varphi^3$	$i_0\varphi^4$
$\langle abb\rangle$			$\lvert abb;0\rangle$	$\lvert bba;0\rangle$	$\lvert b;ab\rangle$	$\rho i_0\lvert \underline{ab};b\rangle$	$i_0\varphi^3$	$i_0\varphi^4$
$\langle ab\rangle$			$\lvert ab;0\rangle$	$\rho\lvert ba;0\rangle$	$\lvert b;a\rangle$	$\rho i_0\lvert a;b\rangle$	$i_0\varphi^3$	$i_0\varphi^4$
$\langle ab;bb\rangle$	24	14	$\rho\lvert bab;b\rangle$	$i_0\varphi^1$	$\lvert bbb;a\rangle$	$\rho\lvert ab;bb\rangle$	$i_0\varphi^3$	$\lvert ba;bb\rangle$
$\langle ac;bb\rangle$			$\rho\lvert bab;c\rangle$	$i_0\varphi^1$	$\lvert bcb;a\rangle$	$\rho\lvert ac;bb\rangle$	$i_o\varphi^3$	$\lvert ca;bb\rangle$
$\langle abbbb\rangle$			$\lvert abbb;b\rangle$	$i_0\varphi^1$	$\lvert bbb;ab\rangle$	$\rho\lvert abb;bb\rangle$	$i_0\varphi^3$	$\rho\lvert bba;bb\rangle$
$\langle ab0bb\rangle$			$\rho\lvert bab;b\rangle$	$i_0\varphi^1$	$\lvert bbb;a\rangle$	$\rho\lvert ab;bb\rangle$	$i_0\varphi^3$	$\lvert ba;bb\rangle$
$\langle aaa0b\rangle$	24	24	$\lvert aaa;b\rangle$	$i_0\varphi^1$	$\lvert ab;aa\rangle$	$\rho i_0\lvert aba;a\rangle$	$\rho\lvert ba;paa\rangle$	$i_0\varphi^4$
$\langle aa;bc\rangle$	24	15	$\rho\lvert cab;a\rangle$	$\rho i_0\lvert bac;a\rangle$	$\rho i_0\varphi^2$	$\rho\lvert aa;cb\rangle$	$\rho i_0\varphi^1$	$\rho i_0\varphi^4$
$\langle ab;b\rangle$	24	15	$\lvert ab;b\rangle$	$\rho i_0\lvert ba;b\rangle$	$\lvert bb;a\rangle$	$\rho i_0\varphi^1$	$\rho i_0\varphi^3$	$\rho i_0\varphi^2$
$\langle abb0b\rangle$			$\lvert abb;b\rangle$	$i_0\lvert bba;b\rangle$	$\lvert bb;ab\rangle$	$i_0\varphi^1$	$\rho i_0\varphi^3$	$\rho i_0\varphi^2$
$\langle abbac\rangle$	24	16	$\lvert abba;c\rangle$	$\rho i_0\varphi^1$	$\lvert bca;ab\rangle$	$\rho\lvert acb;ab\rangle$	$\rho i_0\varphi^4$	$\rho i_0\varphi^3$
$\langle abac\rangle$	12	17	$\lvert abac;0\rangle$	σ^1	$\lvert \underline{bc};aa\rangle$	$\rho\lvert \underline{aa};cb\rangle$	$i_0\varphi^3$	$i_0\varphi^4$
$\langle abbb\rangle$			$\lvert abbb;0\rangle$	φ^1	$\lvert \underline{bb};ab\rangle$	$\rho\lvert \underline{ab};bb\rangle$	$i_0\varphi^3$	$i_0\varphi^4$
$\langle aba\rangle$			$\lvert aba;0\rangle$	φ^1	$\lvert b;aa\rangle$	$\rho i_0\lvert \underline{aa};n\rangle$	$i_0\varphi^3$	$i_0\varphi^4$
$\langle aaa\rangle$			$\lvert aaa;0\rangle$	φ^1	$\lvert a;aa\rangle$	$\rho i_0\lvert \underline{aa};a\rangle$	$i_0\varphi^3$	$i_0\varphi^4$
$\langle aaab\rangle$			$\lvert aaab;0\rangle$	φ^1	$\lvert \underline{ab};aa\rangle$	$\rho\lvert \underline{aa};ba\rangle$	$i_0\varphi^3$	$i_0\varphi^4$
$\langle ababc\rangle$	12	18	$\lvert abab;c\rangle$	$i_0\varphi^1$	$\lvert bcb;aa\rangle$	$\rho\lvert aca;bb\rangle$	φ^3	φ^4
$\langle aabb\rangle$	12	19	$\lvert aabb;0\rangle$	$\rho\varphi^1$	$\lvert ab;ab\rangle$	$\rho i_0\varphi^3$	$i_0\varphi^3$	$\rho\varphi^3$
$\langle aa\rangle$			$\lvert aa;0\rangle$	$\rho\varphi^1$	$\lvert a;a\rangle$	$\rho i_0\varphi^3$	$i_0\varphi^3$	$\rho\varphi^3$
$\langle aa;a\rangle$	8	20	$\lvert aa;a\rangle$	$\rho i_0\varphi^1$	φ^1	$\rho i_0\varphi^1$	$\rho i_0\varphi^1$	φ^1
$\langle aaaab\rangle$	6	21	$\lvert aaaa;b\rangle$	$i_0\varphi^1$	$\lvert aba;aa\rangle$	$\rho\varphi^3$	$i_0\varphi^3$	$\rho\varphi^3$
$\langle a0b\rangle$	6	22	$\lvert \underline{ab};0\rangle$	φ^1	$\lvert 0;ab\rangle$	$\rho\varphi^1$	$i_0\varphi^3$	$\rho\varphi^1$
$\langle a\rangle$			$\lvert a;0\rangle$	φ^1	$\lvert 0;a\rangle$	$\rho\varphi^1$	$i_0\varphi^3$	$\rho\varphi^1$
$\langle abab\rangle$	6	23	$\lvert abab;0\rangle$	φ^1	$\lvert bb;aa\rangle$	$\rho\lvert aa;bb\rangle$	φ^3	φ^4
$\langle a0a\rangle$	3	24	$\lvert \underline{aa};0\rangle$	φ^1	$\lvert 0;aa\rangle$	$\rho\varphi^1$	φ^3	$\rho\varphi^1$

[a]This table is valid only for real ρ. The third column gives the index of the table listing the irreducible basis for the configuration $\langle f\rangle$.

For non-regular representations, the vectors $\varphi^1 \ldots \varphi^6$ are no longer linearly independent. However, Table IX or X remains valid with φ^i replaced by the corresponding term in Table XI. The irreducible bases are no longer normalized and some may become zero or linearly dependent. We only take the linearly independent ones. Since for vibrational modes, $\lvert 1^a \cdots 6^a\rangle$ carries the

TABLE XII. $\langle abcd\rangle$; $\varphi^1_{\rho,-}=\varphi^2_{\rho,-}=0$.

	τ	φ^1	φ^2	φ^3	φ^4
$A_{\rho i_0}$		1	1	$1+i_0$	$1+i_0$
$E_{i_0,\rho}$	1	2	2	$-1-i_0$	$-1-i_0$
	2			$1+i_0$	$-1-i_0$
$F_{\rho i_0,\rho}$	1			$1-i_0$	
	2				$1-i_0$
	3	1	-1		

identity representation, the configuration $\langle a'b'c'd'e'f'\rangle$ is equivalent to $\langle abcde\rangle$ with $a=a'$-$f',b=b'$-$f',\cdots,e=e'$-f'. The irreducible basis for $\langle abcde\rangle$ can be obtained from the configuration $\langle abcdef\rangle$ by letting $f=0$. By setting $abcde$ equal to $ac0db$, respectively, we get the configuration $\langle ab;cd\rangle$, and by letting $abcd$ equal to some special values, we get other special configurations, for example $\langle ab;bc\rangle$,$\langle ab;ab\rangle$ and $\langle ab;c\rangle$. As an example, consider the configuration $\langle abcd\rangle$, which has dimension 24. From Table IX and XI, we derive the algebraic expression of the irreducible basis of O_h for the configuration $\langle abcd\rangle$ listed in Table XII. From the latter we can obtain the explicit form shown in Table XIII. Similarly, we can obtain Tables XIV–XXIV.

The multiplicity of a given irrep in the configuration $\langle f\rangle$ can be calculated from character theory. The result is given in Table XXV (part of it were given previously by Halonen[3]). These results provide a useful check for the correctness of Tables XII–XXIV.

If a given irrep occurs only once in the representation space L_v, then it is said to be a unique state. It can be shown that a unique state is necessarily an irreducible basis of the permutation group S_6,[14] which means that these states have a symmetry higher than the geometric symmetry. The implication of the existence of a higher symmetry in molecules will be discussed in a forthcoming paper.[14]

As an application of Tables XII–XXIV, the un-normalized irreducible basis of O_h for $v=1$-3 are given below with bold-face symbols denoting the unique states. The steps for finding them are: (1) According to $\langle f\rangle$, find the corresponding table from Tables XII–XXIV. (2) according to $\langle f\rangle$ from Table XI find the expression of φ^i in the SBR, and thus yields a concise expression for the irreducible basis vectors. If one needs more explicit (but, unfortunately, more cumbersome) expressions, one can use Eq. (43) to write out the vectors in the SBR in terms of the unsymmetrized basis vectors. The results are the following:

$v=a,\langle f\rangle=\langle a\rangle$, dim= 6. From Table XXII:

TABLE XIII. $\langle abcd\rangle$, dim=24.

	τ	ρi_0	φ^1	φ^2	φ^3	φ^4
A_{1g}		$++$	1	1	2	2
A_{2g}		$-+$	1	1	2	2
$E_{g,\epsilon}$	1	$-+$	1	1	-1	-1
	2	$-+$			1	-1
$F_{1g,z}$	3	$++$	1	-1		
$F_{2g,\zeta}$	3	$-+$	1	-1		
$F_{1u,z}$	1	$+-$			1	
	2	$+-$				1
$F_{2u,\zeta}$	1	$--$			1	
	2	$--$				1

TABLE XIV. $\langle ab;bb\rangle$ and $\langle aaa0b\rangle$, dim=24.

$\langle ab;bb\rangle$	τ	ρi_0	φ^1	φ^3	φ^4	φ^6
$\langle aaa0b\rangle$	τ	ρi_0	φ^1	φ^4	φ^5	φ^3
A_{1g}		$++$	2	2	1	1
A_{2g}		$-+$	2	2	1	1
$E_{g,\epsilon}$	1	$-+$	4	-2	-1	-1
	2	$-+$		2	-1	-1
$F_{1g,z}$		$++$			-1	1
$F_{2g,\zeta}$		$-+$			-1	1
$F_{1u,z}$	1	$+-$		1		
	2	$+-$	1			
$F_{2u,\zeta}$	1	$--$		1		
	2	$--$	1			

$$\mathbf{A}_{1g}=|a;\rangle_{++}+|;a\rangle_{++}=\sum_{i=1}^{6}|i^a\rangle,$$

$$\mathbf{E}_{g,\epsilon}=|a;\rangle_{-+}=|1^a-2^a+3^a-4^a\rangle, \tag{46}$$

$$\mathbf{F}_{1u,z}=|;a\rangle_{+-}=|5^a-6^a\rangle.$$

It is to be noted that only for $v=1$ are the above states unique.

$v=2,\langle f\rangle=\langle 11\rangle$, dim=12. From Table XIX:

$$A_{1g}=(|11;\rangle+|1;1\rangle)_{++}=\sum_{i\rangle j}{}'\ |ij\rangle,$$

$$E_{g,\epsilon}=|1;1\rangle_{-+}=|(1-2+3-4)(5+6)\rangle,$$

$$\mathbf{F}_{2g,\zeta}=|11;\rangle_{-+}=|(1-3)(2-4)\rangle, \tag{47}$$

$$F_{1u,z}=|1;1\rangle_{+-}=|(1+2+3+4)(5-6)\rangle,$$

$$\mathbf{F}_{2u,\zeta}=|1;1\rangle_{--}=|(1-2+3-4)(5-6)\rangle,$$

where a prime in the summation symbol means the exclusion of the opposite bonds $ij=13,\ 24,$ and 56.

TABLE XV. $\langle aa;bc\rangle$ and $\langle ab;b\rangle$, dim=24.

$\langle aa;bc\rangle$	τ	ρi_0	φ^1	φ^2	φ^4
$\langle ab;b\rangle$	τ	ρi_0	φ^1	φ^2	φ^3
A_{1g}		$++$	1	1	1
A_{2u}		$--$	1	1	1
$E_{g,\epsilon}$		$-+$	1	1	
$F_{1g,z}$		$++$	1	-1	
$F_{2g,\zeta}$	1	$-+$			1
	2	$-+$	1	-1	
$E_{u,\epsilon}$		$--$	1	1	-2
$F_{1u,z}$	1	$+-$			1
	2	$+-$	1	-1	
$F_{2u,\zeta}$		$--$	1	-1	

TABLE XVI. $\langle abbac\rangle$, dim=24.

	τ	ρi_0	φ^1	φ^3	φ^4
A_{1g}		$++$	1	1	1
A_{2u}		$--$	1	1	1
$E_{g,\epsilon}$		$-+$		1	-1
$F_{1g,z}$		$++$		1	-1
$F_{2g,\zeta}$	1	$-+$		1	1
	2	$-+$	1		
$E_{u,\epsilon}$		$--$	2	-1	-1
$F_{1u,z}$	1	$+-$		1	1
	2	$+-$	1		
$F_{2u,\zeta}$		$--$		1	-1

$v=2,\langle f\rangle=\langle 101\rangle$, dim=3. From Table XXIV:

$$A_{1g}=(|\underline{11};\rangle+|;11\rangle)_{++}=|13+24+56\rangle,\quad E_{g,\epsilon}=|\underline{11};\rangle_{-+}=|13-24\rangle. \tag{48}$$

$v=3,\langle f\rangle=\langle 21\rangle$, dim=24. From Table XIII:

$$A_{1g}=(|21;\rangle+|12;\rangle+|1;2\rangle+|2;1\rangle)_{++}=\sum_{i\rangle j}^{6'}|i^2j+ij^2\rangle,$$

$$A_{2g}=(|21;\rangle-|12;\rangle+|1;2\rangle-|2;1\rangle)_{-+},$$

$$E_{g,\epsilon}^{\tau=1}=(2|21;\rangle-2|12;\rangle-|1;2\rangle+|2;1\rangle)_{-+},$$

$$E_{g,\epsilon}^{\tau=2}=(|1;2\rangle+|2;1\rangle)_{-+},\quad \mathbf{F}_{1g,z}=(|21;\rangle-|12;\rangle)_{++},\quad F_{2g,\zeta}=(|21;\rangle+|12;\rangle)_{-+}, \tag{49}$$

$$F_{1u,z}^{\tau=1}=|1;2\rangle_{+-},\quad F_{1u,z}^{\tau=2}=|2;1\rangle_{+-},\quad F_{2u,\zeta}^{\tau=1}=|1;2\rangle_{--},\quad F_{2u,\zeta}^{\tau=2}=|2;1\rangle_{--}.$$

$v=3,\langle f\rangle=\langle 201\rangle$, dim=6. From Table XXII:

$$A_{1g}=(|\underline{21};\rangle+|;21\rangle)_{++}=\sum_{i\rangle j}^{6}{}''\,|i^2j+ij^2\rangle,$$

$$E_{g,\epsilon}=|\underline{21};\rangle_{-+}=|1^23+13^2-2^24-24^2\rangle, \tag{50}$$

$$F_{1u,z}=|;21\rangle_{+-}=|5^26-56^2\rangle.$$

TABLE XVII. $\langle abac\rangle$, dim=12.

	τ	ρi_0	φ^1	φ^3	φ^4
A_{1g}		$++$	1	1	1
A_{2g}		$-+$	1	1	1
$E_{g,\epsilon}$	1	$-+$	2	-1	-1
	2	$-+$		1	-1
$F_{1u,z}$		$+-$			1
$F_{2u,\zeta}$		$--$			1

TABLE XVIII. $\langle ababc\rangle$, dim=12.

	τ	ρi_0	φ^1	φ^3	φ^4
A_{1g}		$++$	1	1	1
A_{2g}		$-+$	1	1	1
$E_{g,\epsilon}$	1	$-+$	2	-1	-1
	2	$-+$		1	-1
$F_{1u,z}$		$+-$	1		
$F_{2u,\zeta}$		$--$	1		

where the double prime in the summation symbol means ij are restricted to the opposite bonds, $ij=13,\ 24$, and 56.

$v=3, \langle f'\rangle=\langle 11;1\rangle$, dim=8. From Table XX:

$$\begin{aligned} A_{1g}&=|11;1\rangle_{++}=|(1+3)(2+4)(5+6)\rangle,\\ F_{2g,\zeta}&=|11;1\rangle_{-+}=|(1-3)(2-4)(5+6)\rangle,\\ F_{1u,z}&=|11;1\rangle_{+-}=|(1+3)(2+4)(5-6)\rangle,\\ \mathbf{A}_{2u}&=|11;1\rangle_{--}=|(1-3)(2-4)(5-6)\rangle. \end{aligned} \tag{51}$$

$v=3, \langle f'\rangle=\langle 111\rangle$ (three adjacent bonds), dim=12. From Table XVII:

$$\begin{aligned} A_{1g}&=\tfrac{1}{2}(2|111;\rangle+|1;11\rangle+|\underline{11};1\rangle)_{++}=\sum_{i\rangle j\rangle k}^{6}|ijk\rangle-A_{1g}^{\langle 11;1\rangle},\\ A_{2g}&=\tfrac{1}{2}(2|111;\rangle+|1;11\rangle-|\underline{11};1\rangle)_{-+}\\ E_{g,\epsilon}^{\tau=1}&=(4|111;\rangle-|1;11\rangle+|\underline{11};1\rangle)_{-+},\\ E_{g,\epsilon}^{\tau=2}&=(|1;11\rangle+|\underline{11};1\rangle)_{-+},\\ F_{1u,z}&=|\underline{11};1\rangle)_{+-}=|(13+24)(5-6)\rangle,\\ F_{2u,\zeta}&=|\underline{11};1\rangle)_{--}=|(13-24)(5-6)\rangle. \end{aligned} \tag{52}$$

For $v=4$, from Table XV we obtain the two unique states:

TABLE XIX. $\langle aa\rangle$ and $\langle aabb\rangle$, dim=12.

	ρi_0	φ^1	φ^3
A_{1g}	$++$	1	2
$E_{g,\epsilon}$	$-+$		1
$F_{2g,\zeta}$	$-+$	1	
$F_{1u,z}$	$+-$		1
$F_{2u,\zeta}$	$--$		1

TABLE XX. $\langle aa;a\rangle$ dim=8.

	ρi_0	$\varphi^1=\|aa;a\rangle$
A_{1g}	$++$	1
A_{2u}	$--$	1
$F_{2g,\zeta}$	$-+$	1
$F_{1u,z}$	$+-$	1

$$\begin{aligned}\mathbf{A}_{2u}^{\langle 21;1\rangle}&=|21;1\rangle_{--}+|12;1\rangle_{--}+|11;2\rangle_{--}\\&=|(1-3)(2-4)(1+2+3+4)(5-6)\rangle+|(12-14-23+34)\\&\quad\times(5^2-6^2)\rangle,\end{aligned}\tag{53}$$

$$\begin{aligned}\mathbf{E}_{u,\epsilon}^{\langle 21;1\rangle}&=|21;1\rangle_{--}+|12;1\rangle_{--}-2|11;2\rangle_{--}\\&=|(1-3)(2-4)(1+2+3+4)(5-6)\rangle-2|(12-14-23+34)\\&\quad\times(5^2-6^2)\rangle.\end{aligned}$$

The physical picture of the state $\mathbf{A}_{2u}^{\langle 21;1\rangle}$ is given in the Introduction.

VI. DIAGONALIZATION OF THE HAMILTONIAN IN SYMMETRY ADAPTED BASES

In the algebraic model of Iachello and Oss for stretching or bending vibration of molecules,[4,15] each bond is associated with a $U^{(i)}(2)$ algebra realized in terms of the bosons $a_i^\dagger$ and $b_i^\dagger$ and they interact with each other through diagonal and nondiagonal interactions B_{ij} (denoted as C_{ij} in Ref. 4) and M_{ij}, respectively. From the matrix elements of B_{ij} and M_{ij} given in Ref. 4 we can infer that explicit form of these operators are as follows:

$$B_{ij}=4[(J_{iz}+J_{jz})^2-(J_i+J_j)^2],\qquad M_{ij}=-2(\mathbf{J}_i\cdot\mathbf{J}_j-J_iJ_j),\tag{54}$$

with $J_i=J_j=N_i/2$, $N_i=a_i^\dagger a_i+b_i^\dagger b_i$ and $[N_i/2]$ is the total number of bound states in a Morse potential, where B_{ij} and M_{ij} are invariants of $O_{ij}(2)$ and $U_{ij}(2)$, respectively. Specified for the XY_6 molecule, the Hamiltonian they utilized has the form

$$H=aB+a'B'+\lambda M+\lambda' M',\tag{55}$$

$$B=\sum_i^6 B_i,\quad B'=\sum_{i>j}^6 B_{ij},\qquad M=\sum_{i>j}^6 M_{ij},\qquad M'=\sum_{i>j}^{6\,\prime} M_{ij},\tag{56}$$

where the prime in the summation symbol indicates exclusion of the opposite bonds $ij=13$, 24 and 56, and

$$B_i=4[(J_{iz})^2-(J_i)^2]\tag{57}$$

TABLE XXI. $\langle aaaab\rangle$, dim=6.

	ρi_0	φ^1	φ^3
A_{1g}	$++$	1	2
$E_{g,\epsilon}$	$-+$		1
$F_{1u,z}$	$+-$	1	

TABLE XXII. $\langle a\rangle$ and $\langle a0b\rangle$, dim=6.

$\langle a\rangle$	ρi_0	$\|a;\rangle$	$\|;a\rangle$
$\langle a0b\rangle$	ρi_0	$\|ab;\rangle$	$\|;ab\rangle$
A_{1g}	$++$	$\overline{1}$	1
$E_{g,\epsilon}$	$-+$	1	
$F_{1u,z}$	$+-$		1

is the Hamiltonian for the Morse potential of the bond i.[16]

Notice that the parameters λ and λ' listed in Table I of Ref. 4 are not consistent with Iachello and Oss' definition as given in (12), but are the parameters λ_T and λ'_T shown below:

$$H=aB+a'B'+\lambda_T M'+\lambda'_T(M-M').$$

In Ref. 4 the Hamiltonian (55) was diagonalized in the product basis, and it is referred to as a pure numerical solution. It will be much nicer to diagonalize the Hamiltonian in the symmetry-adapted basis. The advantages of using symmetry adapted basis are:

(1) The dimension for the expectation equation of H can be reduced by one order of magnitude for O_h.

(2) Using symmetry adapted basis we can obtain the structure of the eigenstates of H, while no physical pictures of the eigenstates are emerged in a pure numerical solution.

(3) The identification of the eigenstates with irrep labels, a necessary procedure in numerical solution, is avoided.

We diagonalized the H for the molecules SF_6, WF_6 and UF_6 in the the $O_h\supset C_4$ basis $\psi_\rho^{(\nu)\langle f\rangle\tau}$. The parameters are listed in Table XXVI. The mean square deviations from the experimental values are 14.34, 4.78, and 3.76 for the molecules SF_6, WF_6, and UF_6, respectively. The fit is a little better than in Ref. 4 where the corresponding mean square deviations are 15.71, 6.60 and 3.79, respectively.

The eigen-energies and wave functions for SF_6 are listed in Tables XXVII–XXIX. The coefficients listed there are $a_{\mathscr{E},f\tau}$ in the following expansion of the eigenstate

$$\Psi_\rho^\nu(\mathscr{E})=\sum_{f\tau} a_{\mathscr{E},f\tau}\psi_\rho^{(\nu)\langle f\rangle\tau}. \tag{58}$$

From Tables XXVII–XXIX we can see clearly the distribution pattern of the vibrons in the eigenstates.

VII. DISCUSSION

In the past, several methods have been available for obtaining the subgroup-symmetry adapted bases of point groups. A separate discussion for the regular and non-regular representations is adequate.

TABLE XXIII. $\langle abab\rangle$, dim=6.

	τ	ρi_0	φ^1	φ^3	φ^4
A_{1g}		$++$	1	1	1
A_{2g}		$-+$	1	1	1
$E_{g,\epsilon}$	1	$-+$	2	-1	-1
	2	$-+$		1	-1

TABLE XXIV. $\langle a0a\rangle$, dim=3.

	ρi_0	$\underline{\underline{\vert aa;\rangle}}$	$\vert;aa\rangle$
A_{1g}	$++$	1	1
$E_{g,\epsilon}$	$-+$	1	

A. Regular representation

1. The recursive or factorization method

The generalized projection operator $P^{\nu}_{\rho\rho}$ for the group chain $G \supset H$ can be factored as a product of the projection operators P^{ν} and P^{ρ} of the group G and its subgroup H, respectively by the following formula (see p. 73 in Ref. 6):

$$P^{\nu}_{\rho} \equiv P^{\nu}_{\rho\rho} = \text{const } P^{\nu} P^{\rho}, \qquad P^{\nu}_{\rho\overline{\rho}} = \text{const } P^{\nu}_{\rho} R_a P^{\overline{\rho}}, \tag{59}$$

where R_a is a properly chosen operator of G so that $P^{\rho} R_a P^{\overline{\rho}} \neq 0$.

Recently, Harter[1] gave a slightly different form for the non-diagonal part,

$$P^{\nu}_{\rho\overline{\rho}} = \text{const } P^{\nu}_{\rho} R_a P^{\nu}_{\overline{\rho}}. \tag{60}$$

It is to be noted that Eq. (59) is simpler than Eq. (60). This method depends heavily on hand calculation.

2. The eigenfunction method

With a computer code, it is much easier to obtain the generalized projection operator by the EFM. A versatile program package is available.[9]

B. Non-regular representation

1. Projection operator method in its primitive form (Refs. 1, 7, and 17)

The main shortcomings of this method are that we have to know all the irreducible matrix elements and the effects of all the g operators. For a high symmetry group it is a daunting task to

TABLE XXV. The multiplicity of an irrep in the configuration $\langle f\rangle$.

dim	$\langle f\rangle$	A_{1g}	A_{2g}	E_g	F_{1g}	F_{2g}	A_{1u}	A_{2u}	E_u	F_{1u}	F_{2u}
48	$\langle abcde\rangle,\langle ab;cd\rangle,\langle ab;bc\rangle$ $\langle ab;ab\rangle,\langle ab;c\rangle$	1	1	2	3	3	1	1	2	3	3
24	$\langle abcd\rangle,\langle abbc\rangle,\langle abc\rangle$ $\langle abb\rangle,\langle ab\rangle,\langle ab;bb\rangle$ $\langle ac;bb\rangle,\langle ab^4\rangle,\langle ab0bb\rangle$ $\langle a^3 0b\rangle$	1	1	2	1	1				2	2
24	$\langle aa;bc\rangle,\langle ab;b\rangle,\langle abb0b\rangle$ $\langle abbac\rangle$	1		1	1	2		1	1	2	1
12	$\langle abac\rangle,\langle ab^3\rangle,\langle aba\rangle$ $\langle aaa\rangle,\langle a^3 b\rangle,\langle ababc\rangle$	1	1	2						1	1
12	$\langle aabb\rangle,\langle aa\rangle$	1		1		1				1	1
8	$\langle aa;a\rangle$	1				1		1		1	
6	$\langle a^4 b\rangle,\langle a0b\rangle,\langle a\rangle$	1		1						1	
6	$\langle abab\rangle$	1	1	2							
3	$\langle a0a\rangle$	1		1							
1	$\langle a^6\rangle,\langle 0\rangle$	1									

TABLE XXVI. The parameters in H (all values except N are in cm^{-1}).

	N	a	a'	λ	λ'
SF_6	180	$-.9273$	-1.530×10^{-2}	.7219	$-.8407$
WF_6	200	$-.2889$	-6.796×10^{-2}	7.300×10^{-3}	-8.600×10^{-2}
UF_6	250	$-.1931$	-5.289×10^{-2}	9.573×10^{-2}	$-.1842$

generate symmetry adapted bases in view of the mental dexterity required to envisage the effects of the g operators on a reducible basis vector.[3] A further problem is the multiple occurence of a given symmetry.

2. Coset factored projection operator

Suppose that H is an Abelian subgroup of G. The left coset decomposition of G with respect to H is denoted by $G=\Sigma_i a_i H$, a_i are the so called coset representatives, or coset leaders. The projection operator can be factored as[1]

$$P^{\nu}_{\rho\rho}=\frac{h_\nu}{g}\sum_i D^{\nu}_{\rho\rho}(a_i)^* a_i P^{\rho}, \tag{61}$$

where P^ρ is defined as in (21). The coset factorization allows one to tabulate many fewer $D(R)$ matrices and cuts the arithmetical labor down by a factor of g/h (h being the order of the subgroup H) if the dimension of the reducible representation is g/h and one induces the representation from a basis vector which belongs to the identity representation of H.

3. Double coset factored projection operator

A group G can also be decomposed in the following way:

$$G=\sum_i Ha_i+\sum_j Hb_jH, \tag{62}$$

where $Ha_i=a_iH$, i.e., the left and right coset are identical, and Hb_jH is a double coset. The generalized projection operator $P^{\nu}_{\rho\rho}$ can be factored as[18]

$$P^{\nu}_{\rho\rho}=\frac{h_\nu}{g}\left[\sum_i D^{\nu}_{\rho\rho}(a_i)^* P^{\rho} a_i+\sum_j D^{\nu}_{\rho\rho}(b_j)^* P^{\rho} b_j P^{\rho}\right]. \tag{63}$$

The methods (ii) and (iii) cannot yield algebraic expressions for the irreducible basis; therefore, tedious work cannot be avoided for each case.

TABLE XXVII. The eigen-energies and eigen-functions of H for SF_6, $v=1$.

$\mathbf{E_g}$	E_{exp} (cm^{-1})	$\langle 1\rangle$
645.44	643.35	1.0000
$\mathbf{A_{1g}}$		$\langle 1\rangle$
773.80	774.54	1.0000
$\mathbf{F_{1u}}$		$\langle 1\rangle$
948.09	948.10	1.0000

TABLE XXVIII. Same as the Table XXVII with $v=2$.

A_{1g}	E_{exp} (cm^{-1})	$\langle 2\rangle$	$\langle 11\rangle$	$\langle 101\rangle$
1288.34		−.5836	.5709	−.5776
1546.17		.4077	.8210	.3996
1890.69	1889.05	.7023	−.0023	−.7119
E_g		$\langle 2\rangle$	$\langle 11\rangle$	$\langle 101\rangle$
1289.65		−.4193	.8075	−.4149
1416.50		.5749	.5899	.5670
1890.69	1889.05	−.7026	.0008	.7116
$\mathbf{F_{2g}}$		$\langle 11\rangle$		
1896.30	1896.53	1.0000		
F_{1u}		$\langle 2\rangle$	$\langle 11\rangle$	
1588.27	1588.10	.8333	−.5528	
1719.25	1719.59	.5528	.8333	
$\mathbf{F_{2u}}$		$\langle 11\rangle$		
1593.65		1.0000		

4. Use of the CG coefficients of point groups

Starting from the irreducible basis for the basic configuration $\langle 1\rangle$, using the CG coefficients stepwise, we can construct the irreducible basis for other configurations.[3] The trouble is that in coupling two irreducible basis by means of CG coefficients one obtains the following linear combination:

$$\Psi_\rho^{(\nu)}=\sum_{f\tau} a_{\rho,f\tau}^{(\nu)}\psi_\rho^{(\nu)\langle f\rangle\tau}, \tag{64}$$

where $a_{\rho,f\tau}^{(\nu)}$ are coefficients, τ is the multiplicity label for the irrep ν in a given configuration $\langle f\rangle$, and the sum runs over τ and all possible $\langle f\rangle$ in the space L_v with a given vibron number v. Notice that in the above equation both $\langle f\rangle$ and τ serve as multiplicity labels for the irrep ν in L_v. The dimension of L_v can be very large for large v, and it is nontrivial to extract the irreducible basis $\psi_\rho^{(\nu)\langle f\rangle\tau}$ from the sum in Eq. (64). A code has been used in Ref. 3 to calculate the irreducible basis of O_h for $v=1-8$.

5. The eigenfunction method (Ref. 6)

The irreducible bases are obtained by solving the eigenvalue equation of the CSCO-II of G in the reducible representation space.

All the above methods are numerical. In the present work we have added a new method which gives algebraic solutions, and has a number of attractive features:

C. Regular representation

One only needs to solve an eigenequation of a 3×3 matrix to get a compact algebraic solution for irreducible basis of O_h as a function of i_0,ρ and $\overline{\rho}$,

$$\psi_\rho^{(\nu_{i_0})\overline{\rho}}=F_\rho^{(\nu_{i_0})\overline{\rho}}(\varphi^1,\cdots,\varphi^6), \tag{65}$$

which involves only 6 terms instead of 48 terms in numerical solutions.

D. Non-regular representation

(i) For non-regular representation, irreducible basis vectors are easily obtained from the above by assimilation,

TABLE XXIX. Same as the Table XXVII with $v=3$.

$\mathbf{A_{2u}}$	E_{exp} (cm^{-1})	$\langle 11;1\rangle$					
2844.63	2845.28	1.0000					
A_{1g}		$\langle 3\rangle$	$\langle 21\rangle$	$\langle 201\rangle$	$\langle 11;1\rangle$	$\langle 111\rangle$	
1932.52		.2553	−.4099	.4330	.6441	−.4056	
2056.75		.4088	.0229	.6901	−.5962	.0243	
2317.09		−.1662	−.5829	−.2761	−.4793	−.5714	
2525.39		−.7301	.3724	.4326	−.0010	−.3756	
2659.45		−.4549	−.5941	.2699	.0024	.6060	
A_{2g}			$\langle 21\rangle$		$\langle 111\rangle$		
1932.71			.7107		.7035		
2536.36			−.7035		.7107		
E_g		$\langle 3\rangle$	$\langle 21\rangle_{\tau=1}$	$\langle 21\rangle_{\tau=2}$	$\langle 201\rangle$	$\langle 111\rangle_{\tau=1}$	$\langle 111\rangle_{\tau=2}$
1929.97		−.3029	.5705	.0052	−.5138	.5646	.0051
2057.94		−.2938	−.3090	.4929	−.4960	−.3058	.4855
2186.14		−.2861	−.2899	−.5145	−.4796	−.2877	−.5065
2525.39		.7300	−.3234	−.1864	−.4328	.3246	.1875
2536.37		.0002	.3519	−.6075	.0002	−.3552	.6172
2659.44		−.4551	−.5164	−.2975	.2696	.5229	.3026
$\mathbf{F_{1g}}$			$\langle 21\rangle$				
2534.07			1.0000				
F_{2g}			$\langle 21\rangle$	$\langle 11;1\rangle$			
2539.22			.7982	−.6024			
2664.71			.6024	.7982			
F_{1u}		$\langle 3\rangle$	$\langle 21\rangle_{\tau=1}$	$\langle 21\rangle_{\tau=2}$	$\langle 201\rangle$	$\langle 11;1\rangle$	$\langle 111\rangle$
2226.37	2227.50	−.6112	.6426	−.1791	−.3456	−.1750	−.1773
2237.35		.0381	−.0344	−.4993	.0215	.7095	−.4942
2356.79		−.5609	−.3958	.3242	−.3148	.4715	.3198
2488.96	2488.40	.2646	.6552	.3465	.1465	.4937	.3398
2827.78	2827.55	.4903	−.0026	−.0003	−.8715	−.0004	−.0002
2839.02	2839.04	.0001	.0012	−.7024	.0002	.0015	.7118
F_{2u}		$\langle 21\rangle_{\tau=1}$	$\langle 21\rangle_{\tau=2}$	$\langle 111\rangle$			
2232.70		−.8251	.4016	.3975			
2361.95		.5650	.5874	.5794			
2839.01	2840.35	.0008	−.7026	.7116			

$$\psi_{\rho}^{(\nu_{i_0})\tau}=F_{\rho}^{(\nu_{i_0})\tau}(\varphi^{j_1},\cdots,\varphi^{j_d}), \tag{66}$$

where d is equal to one eighth of the dimension of the reducible representation, verses $8d$ terms in a numerical solution.

(ii) The states $|abcd;ef\rangle$ in the SBR have a clear physical picture about the distribution pattern of the vibrons over the two sets of equivalent bonds, as illustrated in the Introduction.

(iii) The results are independent of the labeling of bonds. For a molecule with many bonds, such as fullerene, C_{60}, this independence is of special value.

(iv) The multiplicity separation is automatic: the configuration $\langle f\rangle$ naturally provides one of the multiplicity labels, while the intrinsic operator $\overline{C_{4z}}$ provides the other.

(v) Facilitate the programming of diagonalization of a Hamiltonian in the symmetry adapted bases.

It is remarkable that to carry out this process, we utilize only the CSCO's of a group G and its subgroup, with no knowledge required either of the primitive characters or of the irreducible matrices, and even without using the group table!

As a first application of this new method, we have derived algebraic expressions for the irreducible bases of the group O_h for all cases of current practical interest and much more. The application to other groups is straightforward. For example, the algebraic expression of the irre-

ducible bases and irreducible matrices for the icosahedral group will be discussed in the sequent paper.[19] The combination of the algebraic model[4] and this new technique provides a powerful tool for the solution of many problems in physics and chemistry. One is now in a position to compute in a simple way, even in an algebraic way for the unique states,[14] the spectra and infrared or Raman transition rates of many molecules, including mid-size and large molecules.[3]

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General eigenvalue formula for Casimir invariants of type I quantum superalgebras

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Induced invariant forms and the multiplicity labeling problem are investigated for typical summands of the tensor product of an arbitrary finite dimensional irreducible representation and a typical one, for the type I quantum superalgebras. The results are applied to obtain a general eigenvalue formula for Casimir invariants, corresponding to an arbitrary finite dimensional irreducible reference representation. © *1996 American Institute of Physics.* [S0022-2488(96)01704-8]

I. INTRODUCTION

Quantum algebras are well known for their role in solving the Yang–Baxter equation[1] which, in turn, give rise to new exactly solvable models[2,3] and link polynomials. Similarly, their $\mathbb{Z}_2$-graded counterparts, quantum superalgebras, play an equally important role in knot theory[4] and supersymmetric integrable models.[5–7] For applications in this general area, it is thus desirable to have a well developed *representation* (rep) theory for the quantum (super)algebras.

This article is concerned with an important aspect of the rep theory for the type I quantum superalgebras; namely the determination of a general eigenvalue formula for Casimir invariants. The type I quantum superalgebras, consisting of $U_q[gl(m|n)]$ and $U_q[osp(2|2n)]$, are particularly interesting for the following reasons. First, of all the quantum superalgebras (except the trivially graded case of quantum algebras), only those of type I admit finite dimensional unitary reps which will thus be of importance to physical theories where unitarity is a basic requirement. Second, they admit one parameter families of inequivalent *irreducible representations* (irreps) which have interesting applications such as providing solutions to the Yang–Baxter equation, and corresponding exactly solvable models, with extra (nonadditive) parameters. An example of the latter is the generalized Hubbard model proposed in Ref. 7 where the parameter labeling the irreps is directly related to the Hubbard interaction parameter. Another application is to the construction of two variable link polynomials[8] and their multivariable extensions.[9]

A general method for constructing Casimir invariants, corresponding to an arbitrary reference irrep, has been previously developed for both quantum algebras[10,11] and quantum superalgebras,[12,13] utilizing the universal R matrix. In the case of quantum algebras their eigenvalues have been explicitly determined,[11] based on techniques previously developed for simple Lie algebras.[14,15] However, this problem has not been solved for quantum superalgebras, or their classical counterparts, mainly due to the zero (q) supertrace problem over typical irreps. In this article we present a solution to this problem and obtain a general eigenvalue formula for Casimir invariants, valid for an arbitrary reference irrep. Our results are new, even in the classical limit $q\rightarrow 1$, and generalize, to arbitrary reference irreps, the results of Refs. 16 and 17.

Aside from their intrinsic interest to representation theory, particularly in connection with superdimensions and infinitesimal characters, our results are of importance for obtaining two variable link polynomials, in fully explicit form, corresponding to any unitary irrep for these algebras. This gives rise to infinite families of inequivalent two variable link polynomials which will be studied elsewhere.[18] As part of our approach we will also determine a useful method for obtaining the multiplicities of typical summands occurring in the tensor product of an arbitrary irrep with a typical one, and investigate the Clebsch–Gordan multiplicity problem for such cases. Moreover we obtain a symmetry relation for the corresponding Clebsch–Gordan coefficients,

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which are defined below with respect to the naturally induced form on the tensor product space.

The article is set up as follows. Section II summarizes previously known results on quantum superalgebras and their reps. In Sec. III we investigate invariant sesquilinear forms induced on irreps and their tensor products, and their behavior under duality. Section IV is concerned with an orthogonal labeling scheme for typical irreps occurring in the tensor product of two irreps and these results are applied in Sec. V to obtain a new supertrace formula. In Sec. VI we investigate the $1-1$ correspondence between the imbeddings $V(\nu)\subseteq V(\Lambda)\otimes V(\mu)$, $V(\mu)\subseteq V(\Lambda)^*\otimes V(\nu)$ (for μ, ν typical but Λ arbitrary) and symmetries of Clebsch–Gordan coefficients. A general eigenvalue formula for Casimir invariants is then developed in Secs. VII and VIII and we conclude in Sec. IX with a brief discussion of our main results.

II. PRELIMINARIES

Throughout, L denotes a type I basic classical Lie superalgebra of rank $l+1$, with Cartan subalgebra H. We let α_i, $0\leqslant i\leqslant l$ be a distinguished[19] system of simple roots of L with α_0 the unique odd simple root; then $\alpha_1,\ldots,\alpha_l$ constitute the simple roots of the (reductive) even Lie subalgebra L_0 of L. $\Phi^+=\Phi_0^+\cup\Phi_1^+$ denotes the set of positive roots of L with Φ_0^+ (resp. Φ_1^+) the set of even (resp. odd) positive roots. As usual we define

$$\rho_0=\frac{1}{2}\sum_{\alpha\in\Phi_0^+}\alpha,\quad \rho_1=\frac{1}{2}\sum_{\beta\in\Phi_1^+}\beta$$

and set $\rho=\rho_0-\rho_1$. We let $(\ ,\ )$ be a fixed bilinear form on H^*, the dual of the Cartan subalgebra, induced by a given nondegenerate invariant bilinear form on L; note that $(\ ,\ )$ is invariant under the Weyl group of L_0. Associated with any weight $\lambda\in H^*$, we have $h_\lambda\in H$ defined by $\mu(h_\lambda)=(\mu,\lambda)$, $\forall\mu\in H^*$. In particular we may define the Cartan elements h_{ρ_0}, h_{ρ_1}, $h_\rho=h_{\rho_0}-h_{\rho_1}$, $h_i\equiv h_{\alpha_i}$ $(0\leqslant i\leqslant l)$, which play an important role below. We let $\geqslant$ be the usual partial ordering induced on H^* by the positive roots.

Associated with L we have the quantum superalgebra $U_q(L)$ with simple generators:

$$q^{\pm(1/2)h_i},e_i,f_i,\quad 0\leqslant i\leqslant l.$$

The defining relations for $U_q(L)$ will not be given here and we refer to Refs. 20–23 for details. We merely note that $U_q(L)$ has the structure of a $\mathbb{Z}_2$-graded quasitriangular Hopf algebra with co-product defined by

$$\Delta(q^{\pm(1/2)h_i})=q^{\pm(1/2)h_i}\otimes q^{\pm(1/2)h_i},\quad \Delta(x)=x\otimes q^{-(1/2)h_i}+q^{(1/2)h_i}\otimes x;\quad x=e_i,f_i$$

which extends to an algebra homomorphism $\Delta:U_q(L)\to U_q(L)\otimes U_q(L)$ in an obvious way. We emphasize that the multiplication rule on the latter is defined for homogeneous elements $a,b,c,d\in U_q(L)$ by

$$(a\otimes b)(c\otimes d)=(-1)^{[b][c]}(ac\otimes bd) \tag{1}$$

and extended to all of $U_q(L)\otimes U_q(L)$ by linearity; here and below $[a]\in\mathbb{Z}_2$ denotes the degree[19,20] of homogeneous $a\in U_q(L)$. Throughout we adopt the sigma notation of Sweedler[24] and write

$$\Delta(a)=\sum_{(a)}a_{(1)}\otimes a_{(2)},\quad a\in U_q(L). \tag{2}$$

The antipode S is given by

$$S(a)=q^{-h_\rho}\gamma(a)q^{h_\rho},\quad a\in U_q(L), \tag{3}$$

where γ is the *principal antiautomorphism* defined on $U_q(L)$ by[25]

$$\gamma(1)=1, \quad \gamma(x)=-x; \quad x=e_i,f_i,h_i$$

and extended to a $\mathbb{Z}_2$-graded antihomorphism in the obvious way so that for homogeneous $a,b\in U_q(L)$:

$$\gamma(ab)=(-1)^{[a][b]}\gamma(b)\gamma(a).$$

We omit the formula for the co-unit ϵ: $U_q(L)\to\mathbb{C}$, since it is not required below.

It is worth noting that $U_q(L)$ also constitutes a $\mathbb{Z}_2$-graded quasitriangular Hopf algebra, with a co-unit ϵ and antipode S^{-1} under the opposite coproduct $\Delta'=T\cdot\Delta$, where $T:U_q(L)\otimes U_q(L)\to U_q(L)\otimes U_q(L)$ is the twist map defined for homogeneous $a,b,\in U_q(L)$ by

$$T(a\otimes b)=(-1)^{[a][b]}(b\otimes a).$$

This is referred to as the *opposite Hopf algebra structure* on $U_q(L)$. Δ and Δ' are related via the universal R matrix $R\in U_q(L)\otimes U_q(L)$ which satisfies the well known relations

$$R\Delta(a)=\Delta'(a)R, \quad \forall a\in U_q(L), \tag{4a}$$

$$(1\otimes\Delta)R=R_{13}R_{12}, \quad (\Delta\otimes 1)R=R_{13}R_{23}. \tag{4b}$$

A direct consequence of these relations is that R satisfies the graded Yang–Baxter equation[6,7,20]: here we again emphasize that all tensor products are to be interpreted in light of Eq. (1). Then $R^T\equiv T(R)$ also gives rise to a universal R matrix under the opposite Hopf algebra structure on $U_q(L)$.

We note that the quantum algebra $U_q(L_0)$, with generators $q^{\pm(1/2)h_i}$, e_i, f_i $(1\leqslant i\leqslant l)$, gives rise to an even Hopf subalgebra of $U_q(L)$. We let $U_q(B)$ [resp. $U_q(N)$] be the $\mathbb{Z}_2$-graded sub-Hopf algebra of $U_q(L)$ with generators $q^{\pm(1/2)h_i}$, e_i (resp. $q^{\pm(1/2)h_i}$, f_i), $0\leqslant i\leqslant l$. Following Kac,[19] we define a $\mathbb{Z}_2$-consistent $\mathbb{Z}$ gradation on $U_q(L)$ by

$$\deg(e_i)=\deg(f_i)=0, \quad 1\leqslant i\leqslant l, \quad \deg(h_i)=0, \quad 0\leqslant i\leqslant l,$$

$$\deg(e_0)=-\deg(f_0)=1.$$

This gives rise to the $\mathbb{Z}$ gradation

$$U_q(L)=\bigoplus_n U_q^{(n)}(L),$$

where $U_q^{(n)}(L)=\{a\in U_q(L)|\deg(a)=n\}$.

Below an important role is played by the operators

$$T_+=\prod_{\beta\in\Phi_1^+}E_\beta, \quad T_-=\prod_{\beta\in\Phi_1^+}F_\beta. \tag{5}$$

Here E_β,F_β are (odd) Cartan–Weyl elements of $U_q(L)$; for details we refer to Ref. 26 for the case $L=gl(m|n)$ and Ref. 27 for the case of $L=osp(2|2n)$. We set

$$\Gamma=T_+T_- \tag{6}$$

which commutes with the elements of $U_q(L_0)$. Following the Poincare–Birkhoff–Witt (PBW) theorem we may write

$$\Gamma=\Gamma_0+\Gamma_+, \tag{7}$$

where Γ_0 is a central element of $U_q(L_0)$ and $\Gamma_+\in U_q^{(-1)}(L)U_q(L)U_q^{(1)}(L)$. $T_\pm$ possess the following important properties:[26,27]

$$\begin{aligned} aT_+&=T_+a=0, \quad \forall a\in U_q^{(1)}(L),\\ aT_-&=T_-a=0, \quad \forall a\in U_q^{(-1)}(L), \end{aligned} \tag{8}$$

so that from Eq. (7),

$$T_+T_-T_+=\Gamma T_+=\Gamma_0T_+. \tag{9a}$$

Moreover, it is easily verified that

$$(1\otimes T_+)\Delta(T_-)(1\otimes T_+)=q^{h_{\rho_1}}\otimes(T_+T_-T_+)=q^{h_{\rho_1}}\otimes(\Gamma_0T_+). \tag{9b}$$

We now say something about the representation theory of $U_q(L)$. The finite dimensional irreducible $U_q(L)$ modules are uniquely labeled by their highest weights Λ and have the same dimensions and weight spectrum as the corresponding L modules of the same highest weight. We denote the set of dominant weights of L [and hence $U_q(L)$] by D^+. For $\Lambda\in D^+$, we let $V(\Lambda)$ denote the irreducible $U_q(L)$ module with highest weight Λ and we let π_Λ be the representation afforded by $V(\Lambda)$. Throughout $V_0(\Lambda)$ denotes the finite dimensional irreducible $U_q(L_0)$ module with highest weight $\Lambda\in D^+$, and we let[28,29]

$$D_q^0[\Lambda]\equiv\prod_{\alpha\in\Phi_0^+}\frac{[(\Lambda+\rho,\alpha)]_q}{[(\rho,\alpha)]_q} \tag{10}$$

be the *q dimension* of $V_0(\Lambda)$, where we have adopted the convention, maintained throughout,

$$[x]_q\equiv(q^x-q^{-x})/(q-q^{-1}).$$

We recall[26,27] that on $V_0(\Lambda)$ the $U_q(L_0)$ central element Γ_0 of Eq. (7), takes the eigenvalue

$$\chi_\Lambda(\Gamma_0)=c\prod_{\beta\in\Phi_1^+}[(\Lambda+\rho,\beta)]_q, \tag{11}$$

where $c\neq0$ is a representation-independent constant. Following Kac,[19] we say that $\Lambda\in D^+$ and the corresponding irreducible $U_q(L)$ module $V(\Lambda)$ are *typical* if this eigenvalue is nonzero, or equivalently,

$$(\Lambda+\rho,\beta)\neq0, \quad \forall\beta\in\Phi_1^+;$$

otherwise, Λ and $V(\Lambda)$ are called *atypical*. Note, from definition [cf. Eqs. (6) and (7)], Γ must vanish on all irreducible atypical modules.

Every finite dimensional irreducible $U_q(L)$ module admits a natural $\mathbb{Z}$ gradation[19,25]:

$$V(\Lambda)=\bigoplus_{k=0}^{d}V_k(\Lambda), \tag{12}$$

compatible with the $\mathbb{Z}$ gradation on $U_q(L)$, in which case we say that $V(\Lambda)$ *admits* $d+1$ *levels* ($V_d(\Lambda)\neq(0)$ assumed). Here $V_k(\Lambda)$ is the $\mathbb{Z}$-homogeneous subspace consisting of vectors of degree $-k$. In view of the PBW theorem we have

$$V(\Lambda)=U_q(L)v_+^\Lambda=U_q(N)v_+^\Lambda \tag{13}$$

with $v_+^\Lambda\in V_0(\Lambda)$ the maximal weight vector of $V(\Lambda)$. Throughout the article we assume, unless otherwise stated, that the maximal $\mathbb{Z}$-graded component $V_0(\Lambda)$ has parity $+1$ (i.e., belongs to the even subspace of $V(\Lambda)$).

If V, W are finite dimensional $U_q(L)$ modules then $\mathrm{Hom}(V,W)$, the space of linear maps from V to W, becomes a $U_q(L)$ module with the definition

$$(a\circ w)(v)=\sum_{(a)}(-1)^{[w][a_{(2)}]}a_{(1)}w(\gamma(a_{(2)})v)$$

for all homogeneous $a\in U_q(L)$, $w\in\mathrm{Hom}(V,W)$, $v\in V$, with $\Delta(a)$ as in Eq. (2). Note that this definition differs from the usual one which here would have γ replaced by the antipode S. However, in view of Eq. (3), these definitions give rise to equivalent representations.

In particular $V^*=\mathrm{Hom}(V,\mathbb{C})$ becomes a $U_q(L)$ module with the definition

$$(aw^*)(v)=(-1)^{[w^*][a]}w^*(\gamma(a))$$

for all homogeneous $a\in U_q(L)$, $w^*\in V^*$, $v\in V$. In rep theoretic terms, let $\{w_i\}$ be a homogeneous basis for V with $[i]\in\mathbb{Z}_2$ the degree of basis vector w_i. We then have the matrix representation π defined by

$$aw_i=\pi(a)_{ji}w_j,\quad \forall a\in U_q(L)$$

(summation on j assumed here and below). If $\{w_i^*\}$ denotes the corresponding dual basis for V^* so that

$$w_i^*(w_j)=\delta_{ij},$$

then the dual representation π^* is given by

$$aw_i^*=\pi^*(a)_{ji}w_j^*,\quad \forall a\in U_q(L),$$

where

$$\pi^*(a)_{ij}=(-1)^{[a][j]}\pi(\gamma(a))_{ji} \tag{14}$$

for homogeneous $a\in U_q(L)$. Equivalently

$$\pi^*(a)=\pi^T(\gamma(a)),\quad \forall a\in U_q(L),$$

where T denotes supertranspose.[30]

With these constructions, we have[11,30]

Lemma 2.1: The mapping ξ: $V^*\otimes W\to\mathrm{Hom}(V,W)$, *defined by*

$$\xi(u^*\otimes w)(v)=(-1)^{[w][v]}u^*(v)w$$

for all homogeneous $u^*\in V^*$, $v\in V$, $w\in W$, *determines a* $U_q(L)$ *module isomorphism.* □

In particular given a finite dimensional irreducible $U_q(L)$ module $V(\Lambda)$, we have the canonical isomorphism

$$V(\Lambda)^*\otimes V(\Lambda)\cong\mathrm{Hom}(V(\Lambda),V(\Lambda)). \tag{15}$$

If $\{w_i\}$ denotes a homogeneous basis for $V(\Lambda)$ with corresponding dual basis $\{w_i^*\}$ for $V(\Lambda)^*$, we obtain

Lemma 2.2: The identity module occurs exactly once in $V(\Lambda)^*\otimes V(\Lambda)$ and is spanned by the vector

$$w_\Lambda=\sum_i\ (-1)^{[i]}(q^{-h_\rho}w_i^*)\otimes w_i\,,$$

where $(-1)^{[i]}$ is the parity of basis vector w_i.

Proof: In view of Eq. (15) and Schur's lemma, the identity module must occur exactly once in the tensor product space. For homogeneous $a\in U_q(L)$ we have, in the notation of Eq. (2):

$$\Delta(a)w_\Lambda=\sum_{i,(a)}\ (-1)^{[i]+[i][a_{(2)}]}(a_{(1)}q^{-h_\rho}w_i^*)\otimes a_{(2)}w_i\,.$$

From Eq. (14) we have (summation on j)

$$\begin{aligned}a_{(1)}q^{-h_\rho}w_i^*&=q^{-h_\rho}\pi_\Lambda^*(q^{h_\rho}a_{(1)}q^{-h_\rho})_{ji}w_j^*\\&=(-1)^{[i][a_{(1)}]}q^{-h_\rho}\pi_\Lambda(\gamma[q^{h_\rho}a_{(1)}q^{-h_\rho}])_{ij}w_j^*\\&=(-1)^{[i][a_{(1)}]}q^{-h_\rho}\pi_\Lambda(S^{-1}[a_{(1)}])_{ij}w_j^*\,,\end{aligned}$$

where the last equality follows from Eq. (3). We thus arrive at

$$\begin{aligned}\Delta(a)w_\Lambda&=\sum_{i,j(a)}\ (-1)^{[i](1+[a])}(q^{-h_\rho}w_j^*)\otimes a_{(2)}\pi_\Lambda(S^{-1}[a_{(1)}])_{ij}w_i\\&=\sum_{j,(a)}\ (-1)^{([j]+[a_{(1)}])(1+[a])}(q^{-h_\rho}w_j^*)\otimes a_{(2)}S^{-1}(a_{(1)})w_j\\&=\sum_j\ (-1)^{[j](1+[a])}(q^{-h_\rho}w_j^*)\otimes\sum_{(a)}\ (-1)^{[a_{(1)}][a_{(2)}]}a_{(2)}S^{-1}(a_{(1)})w_j\\&=\sum_j\ (-1)^{[j](1+[a])}(q^{-h_\rho}w_j^*)\otimes\epsilon(a)w_j\\&=\epsilon(a)w_\Lambda\end{aligned}$$

since, for a nonzero contribution, a must be even. This is sufficient to prove the result. □

Now let Z denote the center of $U_q(L)$. A fundamental role in the construction of central elements is played by[12]

Proposition 2.1: If $c\in\mathrm{End}V(\Lambda)\otimes U_q(L)$ *satisfies* $\Delta_\Lambda(a)c=c\Delta_\Lambda(a)$, $\forall a\in U_q(L)$, *where* $\Delta_\Lambda=(\pi_\Lambda\otimes 1)\Delta$, *then*

$$C^\Lambda=(\mathrm{str}_q\otimes 1)c\in Z.$$

Here str_q *denotes the q supertrace defined by*

$$\mathrm{str}_q\pi_\Lambda(a)=\mathrm{str}\ \pi_\Lambda(q^{2h_\rho}a),\quad \forall a\in U_q(L)$$

with str *the usual supertrace.*[30] □

An important example is afforded by[12]

$$c=(I\otimes 1-R_\Lambda^TR_\Lambda)/(q-q^{-1})$$

and its powers, where $R_\Lambda=(\pi_\Lambda\otimes 1)R$. It is one of our aims in this article to derive a universal formula for the eigenvalues of the corresponding Casimir invariants

$$C_k^\Lambda=(\mathrm{str}_q\otimes 1)(c^k) \tag{16}$$

on any finite dimensional irrep, thus solving an outstanding problem in the rep theory of the type I quantum superalgebras. In particular the eigenvalue formula allows an explicit determination of link polynomials[18] associated with any finite dimensional irreducible $U_q(L)$ module $V(\Lambda)$.

Throughout the article we assume $q>0$ is a positive real parameter (although our final results will hold for complex q by analytic continuation). With this assumption we have a conjugation operation † defined on $U_q(L)$ by[25]

$$e_i^\dagger=f_i,\quad f_i^\dagger=e_i,\quad (q^{\pm(1/2)h_i})^\dagger=q^{\pm(1/2)h_i},\quad 0\leqslant i\leqslant l$$

which we extend to an (even) algebra antihomomorphism on all of $U_q(L)$ so that

$$\alpha^\dagger=\overline{\alpha},\quad \alpha\in\mathbb{C};\quad (ab)^\dagger=b^\dagger a^\dagger,\quad \forall a,b\in U_a(L),$$

where the overbar denotes normal complex conjugation in $\mathbb{C}$. We note that † so defined is indeed consistent with the $U_q(L)$ defining relations as well as the coproduct, i.e.,

$$\Delta(a)^\dagger=\Delta(a^\dagger),\quad \forall a\in U_q(L),$$

where

$$(a\otimes b)^\dagger\equiv(-1)^{[a][b]}a^\dagger\otimes b^\dagger$$

for all homogeneous $a,b\in U_q(L)$. (We stress that this rule defines a conjugation operation on $U_q(L)\otimes U_q(L)$ whereas the usual prescription $(a\otimes b)^\dagger=a^\dagger\otimes b^\dagger$ does not.) Moreover, if γ denotes the principal antiautomorphism on $U_q(L)$, we have[25]

$$\gamma(a^\dagger)=\gamma(a)^\dagger,\quad \forall a\in U_q(L)$$

so that, from Eq. (3),

$$S(a^\dagger)=[S^{-1}(a)]^\dagger,\quad \forall a\in U_q(L).$$

We conclude this section by noting that the operators $T_\pm$ of Eq. (5) satisfy the conjugation rule (up to a scalar)

$$T_+^\dagger=T_-,\quad T_-^\dagger=T_+. \tag{17}$$

Below we assume $T_\pm$ normalized so that Eq. (17) applies. With this convention $\Gamma=T_+T_-$ is a self-adjoint operator with respect to † as is the operator $\Gamma_0\in U_q(L_0)$ of Eq. (7). Taking the conjugate of Eq. (9a) we arrive at

$$T_-T_+T_-=T_-\Gamma=T_-\Gamma_0. \tag{18}$$

Finally we observe that

$$U_q(B)^\dagger=U_q(N),\quad U_q(N)^\dagger=U_q(B),\quad U_q(L)^\dagger=U_q(L).$$

III. TYPICAL COMPONENTS AND INDUCED FORMS

A sesquilinear form $\langle\ ,\ \rangle : V\otimes V\to\mathbb{C}$ on a finite dimensional $U_q(L)$ module V is called *symmetric* if

$$\langle v,w\rangle=\overline{\langle w,v\rangle},\quad \forall v,w\in V$$

and *invariant* if

$$\langle av,v\rangle=\langle v,a^{\dagger}w\rangle,\quad \forall a\in U_q(L);\quad v,w,\in V$$

with † the conjugation operation on $U_q(L)$. If moreover $\langle\ ,\ \rangle$ is nondegenerate then it has all the properties of an inner product except that it is not generally positive definite. When it is, V gives rise to a type I unitary module[25] (and thus is completely reducible) but we do not make this assumption here.

Lemma 3.1: Let V be a finite dimensional $U_q(L)$ module equipped with a symmetric invariant sesquilinear form $\langle\ ,\ \rangle$. If $V(\nu)$, $V(\nu')$ are two irreducible submodules of V with different highest weights, then they are orthogonal under the form.

Proof: Let $v_+^{\nu}, v_+^{\nu'}$ *be the maximal weight vectors of* $V(\nu)$, $V(\nu')$ resp., $\nu\neq\nu'$. Then, since the Cartan elements are self-adjoint under the form, we have

$$\begin{aligned}0&=\langle v_+^{\nu'},v_+^{\nu}\rangle=\langle v_+^{\nu'},U_q(B)v_+^{\nu}\rangle=\langle U_q(N)v_+^{\nu'},v_+^{\nu}\rangle=\langle V(\nu'),v_+^{\nu}\rangle=\langle U_q(L)V(\nu'),v_+^{\nu}\rangle\\&=\langle V(\nu'),U_q(L)v_+^{\nu}\rangle=\langle V(\nu'),V(\nu)\rangle.\end{aligned}$$

□

Note that if $V(\nu)\subseteq V$ is typical then it must split in V. We let

$$\overline{V(\nu)}=V(\nu)\oplus V(\nu)\oplus\cdots\oplus V(\nu)\subseteq V\quad (m\ \text{ copies})$$

(m the multiplicity of $V(\nu)\subseteq V$) be the corresponding isotypic component. If $\langle\ ,\ \rangle$ on V is nondegenerate, our aim here is to show that its restriction to $V(\nu)$ is also nondegenerate, so that an orthogonal labeling scheme can be found which diagonalizes the form on $V(\nu)$. This result is obvious, in view of Lemma 3.1, if V is completely reducible. The problem, however, is that in general V contains indecomposables.[19]

Following Sec. II we set

$$\Gamma=T_+T_-=\Gamma_0+\Gamma_+$$

and recall that $\Gamma_0\in U_q(L_0)$, Γ commute with the elements of $U_q(L_0)$ and are self-adjoint with respect to †. From Eq. (8) we have

$$\Gamma^2=(\Gamma_0+\Gamma_+)\Gamma=\Gamma_0\Gamma=\Gamma\Gamma_0$$

and more generally we obtain

$$\Gamma^{m+1}=\Gamma\Gamma_0^m.$$

Definition 3.1: We say a finite dimensional $U_q(L)$ module V is of *atypical type* if its irreducible composition factors are all atypical. Note that all (nonirreducible) indecomposable modules are of atypical type as are direct sums of irreducible atypical modules.

Proposition 3.1: Let V be a finite dimensional $U_q(L)$ module of atypical type. Then

$$T_-\Gamma_0V=\Gamma\Gamma_0V=(0).$$

Proof: First V decomposes into a direct sum of irreducible $U_q(L_0)$ modules:

$$V=\bigoplus_{\nu} m_\nu V_0(\nu).$$

Next Γ vanishes on all irreducible atypical modules so that Γ must be nilpotent on V; hence we may set $\Gamma^{m+1}=0$, $m\in\mathbb{Z}_+$. Then for each $V_0(\nu)$ we have

$$(0)=\Gamma^{m+1}V_0(\nu)=\Gamma\Gamma_0^m V_0(\nu)=\chi_\nu(\Gamma_0)^m T_+T_-V_0(\nu).$$

Applying T_- to the left we obtain, from Eq. (18),

$$(0)=\chi_\nu(\Gamma_0)^m T_-T_+T_-V_0(\nu)=\chi_\nu(\Gamma_0)^{m+1}T_-V_0(\nu).$$

Thus either $\chi_\nu(\Gamma_0)=0$ or else $T_-V_0(\nu)=(0)$. In either case,

$$T_-\Gamma_0V_0(\nu)=(0),\quad \forall\nu\Rightarrow T_-\Gamma_0V=(0)\Rightarrow T_+T_-\Gamma_0V=\Gamma\Gamma_0V=(0).$$

□

Clearly every finite dimensional $U_q(L)$ module V admits a $U_q(L)$ module decomposition

$$V=V_T\oplus V_A,$$

where V_T is the direct sum of the typical irreducible submodules of V (which split in V), called its *typical component*, and V_A is necessarily of atypical type. From the result above, $\Gamma\Gamma_0V_A=(0)$, so that

$$V_T=U_q(L)\Gamma\Gamma_0V.$$

Proposition 3.2: Let V be a finite dimensional $U_q(L)$ module equipped with a symmetric, invariant nondegenerate sesquilinear form $\langle\ ,\ \rangle$. Then the restriction of $\langle\ ,\ \rangle$ to V_T (or V_A) is nondegenerate.

Proof: Since $\Gamma\Gamma_0=\Gamma_0\Gamma$ is self-adjoint under the form, V_T and V_A must be orthogonal under $\langle\ ,\ \rangle$: indeed

$$\langle V_T,V_A\rangle=\langle U_q(L)\Gamma\Gamma_0V,V_A\rangle=\langle\Gamma\Gamma_0V,U_q(L)V_A\rangle=\langle\Gamma\Gamma_0V,V_A\rangle=\langle V,\Gamma\Gamma_0V_A\rangle=0,$$

where the last equality follows from Proposition 3.1. Thus the restriction of $\langle\ ,\ \rangle$ to V_T (or V_A) is nondegenerate. □

It now follows from Lemma 3.1 and Proposition 3.2 that if $V(\nu)$ is a typical irreducible submodule of V with isotypic component $V(\nu)=mV(\nu)\subseteq V$, then

Corollary (notation as above): The restriction of $\langle\ ,\ \rangle$ to $V(\nu)$ is nondegenerate. □

We recall[31] that every finite dimensional irreducible $U_q(L_0)$ module $V_0(\Lambda)$ with a real highest weight $\Lambda\in D^+$ is equivalent to a unitary module and thus may be equipped with an invariant inner product $\langle\ ,\ \rangle$ so that

$$\langle av,w\rangle=\langle v,a^\dagger w\rangle,\quad \forall a\in U_q(L_0);\quad v,w\in V_0(\Lambda).$$

We may then extend this form to the entire $U_q(L)$ module $V(\Lambda)$ with the definition[25] [notation as in Eq. (12)]

$$\langle V_0(\Lambda),V_k(\Lambda)\rangle=0,\quad 0<k\leqslant d,$$

$$\langle a^\dagger v,w\rangle=\langle v,aw\rangle,\quad \forall a\in U_q^{(1)}(L),$$

$$\langle av_1+\beta v_2,w\rangle=\overline{\alpha}\langle v_1,w\rangle+\overline{\beta}\langle v_2,w\rangle,\quad \forall\alpha,\beta\in\mathbb{C}.$$

Then it can be shown[25,32] that $\langle\ ,\ \rangle$ so defined gives rise to a symmetric, invariant nondegenerate sesquilinear form on $V(\Lambda)$. Moreover,[25,32]

Lemma 3.2: The above form $\langle\ ,\ \rangle$ induced on $V(\Lambda)$ is the unique (up to scalar multiples) symmetric, invariant nondegenerate sesquilinear form on $V(\Lambda)$. □

Throughout we let $\langle\ ,\ \rangle$ denote the above induced form on $V(\Lambda)$ so that its restriction to the maximal $\mathbb{Z}$-graded component $V_0(\Lambda)$ is positive definite (and thus gives rise to an inner product). It is worth noting (by an argument similar to that of Lemma 3.1) that $U_q(L_0)$ modules with different highest weights are orthogonal under this form. In particular the decomposition (12) is orthogonal with respect to $\langle\ ,\ \rangle$.

Given two irreducible finite dimensional $U_q(L)$ modules $V(\Lambda)$, $V(\mu)$ equipped with the natural induced forms, we have a corresponding sesquilinear form induced on $V(\Lambda)\otimes V(\mu)$ in a natural way; viz.

$$\langle w'\otimes v',w\otimes v\rangle=\langle w',w\rangle\langle v',v\rangle,\quad \forall w,w'\in V(\Lambda);\quad v,v'\in V(\mu).$$

Proposition 3.3: The sesquilinear form $\langle\ ,\ \rangle$ on $V(\Lambda)\otimes V(\mu)$ is symmetric, invariant, and nondegenerate.

Proof: It is easily seen that the form is symmetric. As to invariance we have, in the notation of Eq. (2), for all homogeneous $a\in U_q(L)$,

$$\langle\Delta(a)(w'\otimes v'),w\otimes v\rangle=\sum_{(a)}(-1)^{[a_{(2)}][w']}\langle a_{(1)}w'\otimes a_{(2)}v',w\otimes v\rangle.$$

Using

$$\begin{aligned}\langle a_{(1)}w'\otimes a_{(2)}v',w\otimes v\rangle&=\langle a_{(1)}w',w\rangle\langle a_{(2)}v',v\rangle\\&=\langle w',a_{(1)}^{\dagger}w\rangle\langle v',a_{(2)}^{\dagger}v\rangle\\&=(-1)^{[a_{(2)}][w]}\langle w'\otimes v',(a_{(1)}^{\dagger}\otimes a_{(2)}^{\dagger})(w\otimes v)\rangle\end{aligned}$$

we obtain

$$\langle\Delta(a)(w'\otimes v'),w\otimes v\rangle=\sum_{(a)}(-1)^{[a_{(2)}][a_{(1)}]}\langle w'\otimes v',(a_{(1)}^{\dagger}\otimes a_{(2)}^{\dagger})(w\otimes v)\rangle$$

since, for a nonzero contribution, we must have $[w]+[w']=[a_{(1)}]$ (Mod 2). Moreover $(-1)^{[a_{(2)}][a_{(1)}]}(a_{(1)}^{\dagger}\otimes a_{(2)}^{\dagger})=(a_{(1)}\otimes a_{(2)})^{\dagger}$,so that

$$\langle\Delta(a)(w'\otimes v'),w\otimes v\rangle=\langle w'\otimes v',\Delta(a)^{\dagger}(w\otimes v)\rangle=\langle w'\otimes v',\Delta(a^{\dagger})(w\otimes v)\rangle$$

which establishes invariance as required. It thus remains to prove $\langle\ ,\ \rangle$ is nondegenerate. □

To this end let $\{w_i\}$ be a basis for $V(\Lambda)$ and suppose $\Sigma_i w_i\otimes v_i, v_i\in V(\mu)$ belongs to the kernel of $\langle\ ,\ \rangle$ so that

$$\left\langle w\otimes v,\sum_i w_i\otimes v_i\right\rangle=0,\quad \forall w\in V(\Lambda),\quad v\in V(\mu).$$

Then, $\forall v\in V(\mu)$, we have

$$\left\langle w,\sum_i\langle v,v_i\rangle w_i\right\rangle=0,\quad \forall w\in V(\Lambda)\Rightarrow\sum_i\langle v,v_i\rangle w_i=0$$

since the form $\langle\ ,\ \rangle$ on $V(\Lambda)$ is nondegenerate. Since the w_i constitute a basis this implies

$$\langle v,v_i\rangle=0,\quad \forall v\in V(\mu),\quad \forall i\Rightarrow v_i=0,\quad \forall i$$

by the nondegeneracy of the form on $V(\mu)$. Thus $\langle\ ,\ \rangle$ on $V(\Lambda)\otimes V(\mu)$ is nondegenerate. □

We may thus apply the results of Proposition 3.2 and its corollary to the tensor product module $X\equiv V(\Lambda)\otimes V(\mu)$. In particular if $V(\nu)$ is typical and occurs with multiplicity m_ν in X then the restriction of the form $\langle\ ,\ \rangle$ on X to the isotypic component $\overline{V(\nu)}=V(\nu)\oplus\cdots\oplus V(\nu)$ (m_ν copies) is nondegenerate. This implies that an orthogonal decomposition into irreducible submodules

$$\overline{V(\nu)}=\bigoplus_{\xi=1}^{m_\nu} V^\xi(\nu)$$

can be found which diagonalizes the form $\langle\ ,\ \rangle$ restricted to $\overline{V(\nu)}$. In Sec. IV we shall consider a convenient such multiplicity labeling.

Given $v\in V^\xi(\nu)$ we have, since $\langle\ ,\ \rangle$ is symmetric, $\langle v,v\rangle=\langle\overline{v,v}\rangle$, so that $\langle v,v\rangle$ is real. The form $\langle\ ,\ \rangle$ restricted to each $V^\xi(\nu)$ will be nondegenerate and thus, from Lemma 3.2, will coincide with the naturally induced form, up to a real scalar multiple. This leads us to

Definition 3.2 (notation as above): If this scalar multiple is positive (resp. negative) we say that $V^\xi(\nu)$ has *signature* $+1$ (resp. -1); we denote this signature by ϵ_ξ. Thus the form $\langle\ ,\ \rangle$ restricted to the maximal $\mathbb{Z}$-graded component $V_0^\xi(\nu)$ of $V^\xi(\nu)$ will be positive (resp. negative) definite if $\epsilon_\xi=\pm1$, resp. □

We conclude this section with some observations on duality and induced forms. Let $\{w_i\}$ be a $\mathbb{Z}$-graded basis for $V(\Lambda)$ with $g_{ij}=\langle w_i,w_j\rangle$ the *overlap matrix* corresponding to the natural form on $V(\Lambda)$; thus $g_{ij}=0$, unless w_i,w_j belong to the same $\mathbb{Z}$-graded level. Then g is a nonsingular Hermitian matrix and we set $g^{ij}=(g^{-1})_{ij}$. It follows that $w^i=g^{ji}w_j$ (summation on j) gives rise to a basis for $V(\Lambda)$ dual to $\{w_i\}$ under the form

$$\langle w^i,w_j\rangle=\langle w_j,w^i\rangle=\delta^i_j.$$

Moreover, $g^{ij}=\langle w^j,w^i\rangle$, and we have the expansions

$$aw_i=\sum_j\ w_j\langle w^j,aw_i\rangle,\quad aw^i=\sum_j\ w^j\langle w_j,aw^i\rangle.$$

In rep theoretic terms we have the matrix representation defined by

$$aw_i=\sum_j\ \pi_\Lambda(a)_{ji}w_j$$

so that

$$\pi_\Lambda(a)_{ji}=\langle w^j,aw_i\rangle=\langle\overline{aw_i,w^j}\rangle=\langle\overline{w_i,a^\dagger w^j}\rangle\Rightarrow aw^j=\sum_i\ \langle w_i,aw^j\rangle w^i=\sum_i\ \overline{\pi_\Lambda(a^\dagger)_{ji}}w^i. \tag{19}$$

Remarks: Since the basis $\{w_i\}$ is $\mathbb{Z}$-graded it follows that the dual basis vectors w^i,w_i must belong to the same $\mathbb{Z}$-graded component. Moreover the restriction of the natural form $\langle\ ,\ \rangle$ to the minimal $\mathbb{Z}$-graded component, which constitutes an irreducible $U_q(L_0)$ module, will be nondegenerate and thus either positive or negative definite. □

Now let $\{w_i^*\},\{(w^i)^*\}$ be corresponding dual bases for $V(\Lambda)^*$ defined by

$$w_i^*(w_j)=\delta_{ij}=(w^i)^*(w^j).$$

We then have

$$(w^i)^*=g_{ik}w_k^* \quad \text{(summation on } k\text{)}. \tag{20}$$

Proposition 3.4:

$$\langle (w^i)^*, w_j^*\rangle=(-1)^{[i]}\delta_{ij}$$

with $[i]\in\mathbb{Z}_2$ *the degree of basis vector* w_i *and thus* w_i^*, *naturally gives rise to a nondegenerate, symmetric invariant sesquilinear form which is positive definite on the minimal* $\mathbb{Z}$*-graded component of* $V(\Lambda)^*$.

Proof: In view of Eq. (20), the above result may be expressed

$$\langle w_k^*, w_i^*\rangle=(-1)^{[i]}g^{ki}=(-1)^{[i]}\langle w^i, w^k\rangle \tag{*}$$

from which it follows, with this definition, that $\langle , \rangle$ on $V(\Lambda)^*$ gives rise to a nondegenerate sesquilinear form in a natural way. Moreover if w_i, w^i belong to the *maximal* $\mathbb{Z}$-graded component of $V(\Lambda)$ we have

$$\langle w_i^*, w_i^*\rangle=(-1)^{[i]}\langle w^i, w^i\rangle=\langle w^i, w^i\rangle>0,$$

where now w_i^* belongs to the *minimal* $\mathbb{Z}$-graded component of $V(\Lambda)^*$, as required. It remains to establish invariance.

To this end we have, for homogeneous $a\in U_q(L)$ (summation over repeated indices assumed below)

$$\begin{aligned}\langle aw_k^*, w_i^*\rangle&=\langle (-1)^{[a][k]}\pi_\Lambda(\gamma(a))_{kj}w_j^*, w_i^*\rangle\\&=(-1)^{[a][k]}\overline{\pi_\Lambda(\gamma(a))_{kj}}\langle w_j^*, w_i^*\rangle\\&=(-1)^{[a][k]+[i]}\overline{\langle w^k, \gamma(a)w_j\rangle}\langle w^i, w^j\rangle,\end{aligned}$$

where the last equality follows from Eq. (*). Thus

$$\langle aw_k^*, w_i^*\rangle=(-1)^{[a][k]+[i]}\langle w^i, \langle \gamma(a)w_j, w^k\rangle w^j\rangle.$$

Now from Eq. (19) we have

$$\langle \gamma(a)w_j, w^k\rangle w^j=\langle w_j, \gamma(a)^\dagger w^k\rangle w^j=\gamma(a)^\dagger w^k=\gamma(a^\dagger)w^k$$

so that

$$\begin{aligned}\langle aw_k^*, w_i^*\rangle&=(-1)^{[a][k]+[i]}\langle w^i, \gamma(a)^\dagger w^k\rangle\\&=(-1)^{[a][k]+[i]}\langle \gamma(a)w^i, w^k\rangle\\&=(-1)^{[a][k]+[i]}\pi_\Lambda(\gamma(a)^\dagger)_{ij}\langle w^j, w^k\rangle,\end{aligned}$$

where the last step again follows from Eq. (19). Utilizing Eq. (*), we thus obtain

$$\langle aw_k^*, w_i^*\rangle=(-1)^{[a][k]+[i]+[j]}\pi_\Lambda(\gamma(a^\dagger))_{ij}\langle w_k^*, w_j^*\rangle=(-1)^{[a][k]+[a]}\langle w_k^*, \pi_\Lambda(\gamma(a^\dagger))_{ij}w_j^*\rangle$$

since, in order to obtain a nonzero contribution, we must have $[a]=[i]+[j]$ (Mod 2). Now

$$\pi_\Lambda(\gamma(a^\dagger))_{ij}w_j^* = (-1)^{[a][i]}\pi_\Lambda^T(\gamma(a^\dagger))_{ji}w_j^* = (-1)^{[a][i]}\pi_\Lambda^*(a^\dagger)_{ji}w_j^* = (-1)^{[a][i]}a^\dagger w_i^* .$$

Substituting into the above we finally arrive at

$$\langle a w_k^*, w_i^* \rangle = (-1)^{[a]([k]+[i])+[a]}\langle w_k^*, a^\dagger w_i^* \rangle = \langle w_k^*, a^\dagger w_i^* \rangle$$

since, for a nonzero contribution, we must have $[a]=[k]+[i]$ (Mod 2). This completes the proof. □

Throughout the article we may thus assume that the forms induced on $V(\Lambda)$, $V(\Lambda)^*$ are dually related as above. With this convention if $\{w_i\},\{w^i\}$ are $\mathbb{Z}$-graded dual bases under the natural form on $V(\Lambda)$, with $\{w_i^*\},\{(w^i)^*\}$ the corresponding dual bases for $V(\Lambda)^*$, then the dual vector to w_i^* under the form on $V(\Lambda)^*$ is actually $(-1)^{[i]}(w^i)^*$. The significance of the phase $(-1)^{[i]}$ will be apparent later.

Note: The dual basis vectors w_i, w_i^* have the same parity $(-1)^{[i]}$. Thus if we require the maximal $\mathbb{Z}$-graded component $V_0(\Lambda)$ of $V(\Lambda)$ have positive parity, then so too must the minimal $\mathbb{Z}$-graded component of $V(\Lambda)^*$. Hence with our convention the maximal $\mathbb{Z}$-graded component of $V(\Lambda)^*$ will then have positive parity if $V(\Lambda)$ has an odd number of levels and negative parity otherwise.

IV. ORTHOGONAL LABELING FOR $V(\nu)\subseteq V(\Lambda)\otimes V(\mu)$ (μ,ν TYPICAL)

Here we consider an irreducible typical submodule $V(\nu)$ of $X=V(\Lambda)\otimes V(\mu)$ and we assume throughout that $V(\Lambda)$ is arbitrary but $V(\mu)$ is typical. We let $\langle\ ,\ \rangle$ be the natural form on X, induced by the natural forms on $V(\Lambda)$, $V(\mu)$. If $V(\nu)$ occurs in X with multiplicity m_ν we let

$$\overline{V(\nu)} = V(\nu)\oplus V(\nu)\oplus\cdots\oplus V(\nu) \quad (m_\nu \text{ copies})$$

be its isotypic component. We recall that $\overline{V(\nu)}$ splits in X and the restriction of the form $\langle\ ,\ \rangle$ on X to $\overline{V(\nu)}$ is nondegenerate. We let $P[\nu]$ be the corresponding projection onto $\overline{V(\nu)}$ which is self-adjoint under the form.

Throughout an important role is played by the subspace

$$X_0 \equiv V(\Lambda)\otimes V_0(\mu)$$

with $V_0(\mu)$ the maximal $\mathbb{Z}$-graded component of $V(\mu)$ which thus constitutes an irreducible $U_q(L_0)$ module. Clearly X_0 give rise to a $U_q(L_0)$ module and is stable under the action of $U_q(B)$. Moreover X_0 cyclically generates the tensor product space as a $U_q(L)$ module so that, in view of the PBW theorem,

$$X = U_q(L)X_0 = U_q(N)X_0 .$$

The $\mathbb{Z}$ gradation on $V(\Lambda)$ naturally induces a $\mathbb{Z}$ gradation on X_0; given an irreducible $U_q(L_0)$ module $V_0(\nu)\subseteq X_0$, we let $[\nu]$ denote its $\mathbb{Z}$-graded level. It is worth noting that $V_0(\mu)$ is orthogonal, under the natural form, to the remaining $\mathbb{Z}$-graded levels of $V(\mu)$, so that $\langle\ ,\ \rangle$ restricted to X_0 is nondegenerate. We let P_0 denote the orthogonal projection onto X_0, induced by the $\mathbb{Z}$ gradation on $V(\mu)$, so that P_0 is self-adjoint under the form $\langle\ ,\ \rangle$, and commutes with the action of $U_q(L_0)$.

Now let $\overline{V(\nu)}$ be the isotypic component of $V(\nu)\subseteq X$ with $\nu\in D^+$ typical, as above, and let

$$\overline{V_0(\nu)} = V_0(\nu)\oplus\cdots\oplus V_0(\nu) \quad (m_\nu \text{ copies})$$

be its maximal $\mathbb{Z}$-graded component so that $V_0(\nu)$ is an irreducible $U_q(L_0)$ module. We let $X_0(\nu)\subseteq X_0$ be the isotypic component of $V_0(\nu)\subseteq X_0$ so that the form $\langle\ ,\ \rangle$ restricted to $X_0(\nu)$ is nondegenerate. We then have a $U_q(L_0)$ module homomorphism $P_0: V_0(\nu)\to X_0(\nu)$. Here we show that this in fact determines an isomorphism. We first need

Lemma 4.1: Let $V_\nu = U_q(L)V_0(\nu)$ be the $U_q(L)$ module generated by $V_0(\nu)\subseteq X_0(\nu)$. Then V_ν contains a (unique) typical irreducible $U_q(L)$ module $V(\nu)$.

Proof: With the notation of Sec. II, we first observe that $\Delta(T_-)V_0(\nu)\neq(0)$, since, in view of Eq. (9b):

$$\Delta(T_-)V_0(\nu)=(0)\Rightarrow(1\otimes T_+)\Delta(T_-)V_0(\nu)=(0)$$

$$\Rightarrow(q^{h_{\rho_1}}\otimes T_+T_-)V_0(\nu)=(0)$$

$$\Rightarrow q^{(\nu-\mu,\rho_1)}\chi_\mu(\Gamma_0)V_0(\nu)=(0)$$

which would imply, since μ is typical, that $V_0(\nu)=(0)$, a contradiction.

Thus $\Delta(T_-)V_0(\nu)\neq(0)$ must be the lowest component of a typical $U_q(L)$ module (since $\nu\in D^+$ is typical) which must therefore generate an irreducible typical module $V(\nu)\subseteq V_\nu$.

Note: Above we used the fact that for $v\in V_0(\mu)$, $T_+T_-v=\Gamma v=\Gamma_0 v=\chi_\mu(\Gamma_0)v$, which follows from Eq. (7).

Proposition 4.1: (notation as above).
$P_0: V_0(\nu)\to X_0(\nu)$ determines a $U_q(L_0)$ module isomorphism.

Proof: It suffices to show P_0 is bijective. To see it suppose $V_0(\nu)\subseteq X_0(\nu)$ is orthogonal to $P_0\overline{V_0}(\nu)$ under $\langle\ ,\ \rangle$. Then

$$0=\langle P_0\overline{V_0}(\nu),V_0(\nu)\rangle=\langle\overline{V_0}(\nu),V_0(\nu)\rangle=\langle\overline{V(\nu)},V_0(\nu)\rangle\Rightarrow P[\nu]V_0(\nu)=(0)$$

which is impossible, since by Lemma 4.1, $U_q(L)V_0(\nu)$ contains a (unique) typical irreducible submodule $V(\nu)$ so that

$$(0)\neq V(\nu)=P[\nu]U_q(L)V_0(\nu)=U_q(L)P[\nu]V_0(\nu).$$

Since the form $\langle\ ,\ \rangle$ restricted to $X_0(\nu)$ is nondegenerate, this shows that $P_0\overline{V_0}(\nu)=X_0(\nu)$.

To prove P_0 is $1-1$ suppose $V_0(\nu)\subseteq V(\nu)$ is in the kernel of P_0 (which constitutes a $U_q(L_0)$ module) so that $P_0V_0(\nu)=(0)$. Then we have

$$0=\langle X_0,V_0(\nu)\rangle=\langle U_q(B)X_0,V_0(\nu)\rangle=\langle X_0,U_q(N)V_0(\nu)\rangle$$
$$=\langle X_0,V(\nu)\rangle=\langle X_0,U_q(L)V_0(\nu)\rangle=\langle U_q(L)X_0,V_0(\nu)\rangle=\langle X,V_0(\nu)\rangle\Rightarrow V_0(\nu)=(0).$$

Thus P_0 must be $1-1$ and the result is proved. □

Corollary: m_ν=multiplicity of $V_0(\nu)\subseteq V(\Lambda)\otimes V_0(\mu)$.

Remarks: The above establishes the useful result that for typical $\nu,\mu\in D^+$, the multiplicity of $V(\nu)\subseteq V(\Lambda)\otimes V(\mu)$ is equal to the multiplicity of $V_0(\nu)\subseteq V(\Lambda)\otimes V_0(\mu)$. The latter can be obtained from the $L\downarrow L_0$ branching rules for $V(\Lambda)$ together with the known[33] characters of the finite dimensional irreducible L_0 modules.

We note that $P[\nu]: X_0(\nu)\to V_0(\nu)\subseteq V(\nu)$ also determines a $U_q(L_0)$ module homomorphism in the reverse direction. In view of Lemma 4.1, $P[\nu]$ must be $1-1$ since its kernel, which constitutes a $U_q(L_0)$ module, is trivial: indeed given $V_0(\nu)\subseteq X_0(\nu)$ we have

$$U_q(L)P[\nu]V_0(\nu)=P[\nu]U_q(L)V_0(\nu)\supseteq V(\nu)\neq(0)$$

with $V(\nu)$ the (unique) typical submodule of $V_\nu=U_q(L)V_0(\nu)$. On the other hand, from Proposition 4.1, we have $\dim X_0(\nu)=\dim V_{(0)}(\nu)$, so that $P[\nu]$ must also be onto. We thus arrive at

Proposition 4.2 (notation as above):

$$P[\nu]:X_0(\nu)\to\overline{V_0}(\nu) \text{ determines a } U_q(L_0) \text{ module isomorphism.}$$

□

Below we assume an orthogonal decomposition of $\overline{V_0}(\nu)\subseteq\overline{V(\nu)}$ into eigenspaces of the $U_q(L_0)$ invariant operator $P[\nu]P_0P[\nu]$, which is self-adjoint under the form $\langle\ ,\ \rangle$ on $X=V(\Lambda)\otimes V(\mu)$:

$$\overline{V_0}(\nu)=\bigoplus_\xi V_0^\xi(\nu) \quad \text{(orthogonal direct sum)}$$

with $V_0^\xi(\nu)$ an irreducible $U_q(L_0)$ module constituting an eigenspace of $P[\nu]P_0P[\nu]$ with eigenvalue λ_ξ, say. We allow for the possibility that some eigenvalues may be equal; i.e., $\lambda_\xi=\lambda_\xi$, $\xi\neq\xi'$, but we may still assume orthogonality of the corresponding eigenspaces. The above decomposition induces a $U_q(L)$ module decomposition

$$\overline{V(\nu)}=\bigoplus_\xi V^\xi(\nu), \tag{21}$$

where $V^\xi(\nu)=U_q(L)V_0^\xi(\nu)=U_q(N)V_0^\xi(\nu)$ is an irreducible $U_q(L)$ module.

Lemma 4.2: The decomposition (21) *is orthogonal.*

Proof: For $\xi\neq\xi'$ we have

$$0=\langle V_0^\xi(\nu),V_0^{\xi'}(\nu)\rangle=\langle U_q(B)V_0^\xi(\nu),V_0^{\xi'}(\nu)\rangle=\langle V_0^\xi(\nu),U_q(N)V_0^{\xi'}(\nu)\rangle=\langle V_0^\xi(\nu),V^{\xi'}(\nu)\rangle$$
$$=\langle V_0^\xi(\nu),U_q(L)V^{\xi'}(\nu)\rangle=\langle U_q(L)V_0^\xi(\nu),V^{\xi'}(\nu)\rangle.=\langle V^\xi(\nu),V^{\xi'}(\nu)\rangle.$$

□

Throughout the remainder of this section we adopt this orthogonal multiplicity labeling (although our final results will be independent of the labeling chosen). In view of Proposition 4.1, we have a $U_q(L_0)$ module direct sum decomposition

$$X_0(\nu)=\bigoplus_\xi V_0(\nu,\xi)\subseteq X_0, \tag{22}$$

where $V_0(\nu,\xi)\equiv P_0V_0^\xi(\nu)$ is an irreducible $U_q(L_0)$ module.

Lemma 4.3:

(i) *$V_0(\nu,\xi)$ is an eigenspace of $P_0P[\nu]P_0$ with eigenvalue λ_ξ.*

(ii) *The decomposition (22) is orthogonal.*

Proof: (i) Let $v_0^\xi=P_0v^\xi\in V_0(\nu,\xi)$, where $v^\xi\in V_0^\xi(\nu)$ so that v^ξ is an eigenvector of $P[\nu]P_0P[\nu]$ with eigenvalue λ_ξ. Then

$$P[\nu]v_0^\xi=P[\nu]P_0v^\xi=P[\nu]P_0P[\nu]v^\xi=\lambda_\xi v^\xi\Rightarrow P_0P[\nu]P_0v_0^\xi=P_0P[\nu]v_0^\xi=\lambda_\xi P_0v^\xi=\lambda_\xi v_0^\xi$$

which is sufficient to prove the result.

(ii) For $\xi\neq\xi'$ we have, since $V_0^\xi(\nu)$ are eigenspaces of $P[\nu]P_0P[\nu]$,

$$\langle V_0(\nu,\xi),V_0(\nu,\xi')\rangle=\langle P_0V_0^\xi(\nu),V_0(\nu,\xi')\rangle=\langle V_0^\xi(\nu),V_0(\nu,\xi')\rangle=\langle V_0^\xi(\nu),P_0V_0^{\xi'}(\nu)\rangle$$
$$=\langle V_0^\xi(\nu),P[\nu]P_0P[\nu]V_0^{\xi'}(\nu)\rangle=\langle V_0^\xi(\nu),V_0^{\xi'}(\nu)\rangle=0$$

as required. □

It is worth noting that the eigenvalues λ_ξ are real, since $P[\nu]P_0P[\nu]$ is self-adjoint under the form $\langle\ ,\ \rangle$, moreover

Lemma 4.4.: The eigenvalues λ_ξ are all nonzero.

Proof: Suppose $\lambda_\xi=0$ for some ξ, so that $P[\nu]P_0P[\nu]V_0^\xi(\nu)=(0)$. Then for $V_0(\nu,\xi)=P_0V_0^\xi(\nu)$ we have

$$P[\nu]V_0(\nu,\xi)=P[\nu]P_0V_0^\xi(\nu)=P[\nu]P_0P[\nu]V_0^\xi(\nu)=(0)$$

in contradiction to Proposition 4.2.

Corollary: $P[\nu]V_0(\nu,\xi)=V_0^\xi(\nu)$. In particular $V^\xi(\nu)$ is the unique irreducible submodule of highest weight ν contained in $U_q(L)V_0(\nu,\xi)$.

Proof: From above,

$$P[\nu]V_0(\nu,\xi)=P[\nu]P_0P[\nu]V_0^\xi(\nu)=V_0^\xi(\nu)$$

from which the result follows. □

Since the decompositions (21) and (22) are orthogonal, the restriction of the form $\langle\ ,\ \rangle$ on X to $V^\xi(\nu)$ is nondegenerate as is its restriction to $V_0(\nu,\xi)\subseteq X_0$. We let $P[\nu,\xi]$ be the orthogonal projection onto $V^\xi(\nu)$, which is thus self-adjoint under the form and commutes with the action of $U_q(L)$; we therefore have

$$P[\nu,\xi]X=P[\nu,\xi]\overline{V(\nu)}=V^\xi(\nu).$$

We denote the orthogonal projection onto $V_0(\nu,\xi)$, which is self-adjoint and commutes with the action of $U_q(L_0)$, by $P_0[\nu,\xi]$. We conclude this section with some technical results of importance below.

Lemma 4.5: Let $V_0(\nu')\subseteq X_0$ be an irreducible $U_q(L_0)$ module with highest weight ν'. Then

(i) *$P[\nu,\xi]V_0(\nu')=(0)$ unless $\nu'\leqslant\nu$.*

(ii) *$\Delta(T_-)P[\nu,\xi]V_0(\nu')=(0)$, $\nu\neq\nu'$. Moreover, in the case $\nu'=\nu$, we have $\Delta(T_-)P[\nu,\xi]V_0(\nu)=(0)$, if $V_0(\nu)$ is orthogonal to $V_0(\nu,\xi)$.*

Proof: (i) The $U_q(L)$ module generated by $V_0(\nu')$ will consist of a direct sum of typical irreducible modules with highest weights $\nu''\geqslant\nu'$ plus an atypical component (possibly zero). Thus

$$P[\nu,\xi]V_0(\nu')=(0)\quad\text{unless}\quad\nu\geqslant\nu',$$

where we have used the result that $\overline{V(\nu)}$ is orthogonal to the atypical component of X.

As to (ii), the last statement is obvious from the corollary to Lemma 4.4. Also from part (i),

$$\Delta(T_-)P[\nu,\xi]V_0(\nu')=(0),\quad\text{unless}\quad\nu\geqslant\nu'.$$

It thus remains to consider the case $\nu>\nu'$. Then we must have

$$\Delta(T_-)P[\nu,\xi]V_0(\nu')=(0),$$

or else the left-hand side will give a $U_q(L_0)$ submodule of $V^\xi(\nu)$ with highest weight $\nu'-2\rho_1$ which is less than the highest weight $\nu-2\rho_1$ of the minimal $\mathbb{Z}$-graded component of $V^\xi(\nu)$, which is impossible. □

Utilizing this result we arrive at

Proposition 4.3: (notation as above).

$$\Delta(T_-)P[\nu,\xi]P_0=\Delta(T_-)P_0[\nu,\xi].$$

Proof: In view of the corollary to Lemma 4.4, $(1-P[\nu,\xi])V_0(\nu,\xi)$ is contained in a direct sum of typical irreducible modules with highest weights $\nu'>\nu$ plus possibly an atypical component. Thus, from Proposition 3.1 and the Lemma above, we have

$$(0)=\Delta(T_-)\Delta(\Gamma_0)(1-P[\nu,\xi])V_0(\nu,\xi)=\chi_\nu(\Gamma_0)\Delta(T_-)(1-P[\nu,\xi])V_0(\nu,\xi).$$

Since ν is typical, $\chi_\nu(\Gamma_0)\neq 0$ so that

$$\Delta(T_-)(1-P[\nu,\xi])V_0(\nu,\xi)=(0)$$

or

$$\Delta(T_-)V_0(\nu,\xi)=\Delta(T_-)P[\nu,\xi]V_0(\nu,\xi)$$

which, in view of Lemma 4.5, is sufficient to prove the result.

V. SUPERTRACE RESULT ($\nu,\mu\in D^+$ TYPICAL)

Throughout we adopt the orthogonal labeling for $\overline{V(\nu)}\subseteq X=V(\Lambda)\otimes V(\mu)$ of Sec. IV. We let $\{e(\nu)_\alpha\}$ be a ($\mathbb{Z}$-graded) basis for $V(\nu)$ with corresponding dual basis $\{\underline{e}(\nu)^\alpha\}$ under the natural form on $V(\nu)$. We let $\{e^\xi(\nu)_\alpha\}$ be the corresponding basis for $V^\xi(\nu)\subseteq V(\nu)$ and assume the labeling normalized so that

$$\langle e^\xi(\nu)_\alpha, e^{\xi'}(\nu)_\beta\rangle=\epsilon_\xi\delta_{\xi\xi'}\langle e(\nu)_\alpha, e(\nu)_\beta\rangle$$

with $\epsilon_\xi=\pm 1$ the signature of $V^\xi(\nu)$ (cf. Definition 3.2). Then ξ gives rise to a $U_q(L)$ module homomorphism

$$\xi: V(\nu)\to V(\Lambda)\otimes V(\mu),\quad \xi(e(\nu)_\alpha)=e^\xi(\nu)_\alpha \tag{23}$$

in a natural way. It is worth noting that $e^\xi(\nu)^\alpha\equiv\epsilon_\xi\xi(e(\nu)^\alpha)$ constitutes a dual basis to $\{e^\xi(\nu)_\alpha\}$ under the form $\langle\ ,\ \rangle$ on X restricted to $V^\xi(\nu)$:

$$\langle e^\xi(\nu)^\alpha, e^{\xi'}(\nu)_\beta\rangle=\delta_{\xi\xi'}\delta^\alpha_\beta.$$

We now set

$$P[\nu]_{\xi\xi'}=\sum_\alpha |e^\xi(\nu)_\alpha\rangle\langle e^{\xi'}(\nu)^\alpha|=\epsilon_\xi\epsilon_{\xi'}\sum_\alpha |e^\xi(\nu)^\alpha\rangle\langle e^{\xi'}(\nu)_\alpha| \tag{24}$$

which commute with the action of $U_q(L)$ and satisfy the algebra

$$P[\nu]_{\xi\xi'}P[\nu]_{\eta\eta'}=\delta_{\xi'\eta}P[\nu]_{\xi\eta'},\quad P[\nu]^\dagger_{\xi\xi'}=\epsilon_\xi\epsilon_{\xi'}P[\nu]_{\xi'\xi}.$$

Note that the orthogonal projection onto $V^\xi(\nu)\subseteq\overline{V(\nu)}$ is given by $P[\nu,\xi]=P[\nu]_{\xi\xi}$. Our aim here is to prove the result

Theorem 5.1:

$$\mathrm{str}_q\otimes\mathrm{str}_q[\Delta(T_+)P[\nu]_{\xi\xi'}(1\otimes T_-)]=(-1)^{|\Phi_1^+|}q^{4(\rho,\rho_1)}\mathrm{str}_q\otimes\mathrm{str}_q[\Delta(T_-)P[\nu]_{\xi\xi'}(1\otimes T_+)]=\delta_{\xi\xi'\eta},$$

where η is a constant independent of ξ given by

$$\eta=(-1)^{[\nu]}q^{-(\mu+\nu,\rho_1)}\chi_\mu(\Gamma_0)D_q^0[\nu],$$

with $[\nu]$ the $\mathbb{Z}$-graded level of $V_0(\nu)\subseteq V(\Lambda)\otimes V_0(\mu)$.

Note. It is easily checked that the first equation above holds directly by conjugation: recall, for $A\in\mathrm{End}(X)$, that $\mathrm{str}_q(A^*)=\mathrm{str}_q(A^\dagger)$, where $A^\dagger$ is the adjoint of A with respect to the form $\langle\ ,\ \rangle$ on X. It thus suffices to prove the second formula. □

We begin with the diagonal case $\xi=\xi'$. Then utilizing Proposition 4.3 we have, since $(1\otimes T_+)X=X_0$,

$$\begin{aligned}
&\mathrm{str}_q\otimes\mathrm{str}_q[\Delta(T_-)P[\nu,\xi](1\otimes T_+)]\\
&\quad=\mathrm{str}_q\otimes\mathrm{str}_q[\Delta(T_-)P_0[\nu,\xi](1\otimes T_+)]\\
&\quad=\mathrm{str}\otimes\mathrm{str}[\Delta(q^{2h_\rho})\Delta(T_-)P_0[\nu,\xi](1\otimes T_+)]\\
&\quad=q^{-4(\rho,\rho_1)}\mathrm{str}\otimes\mathrm{str}[\Delta(T_-)\Delta(q^{2h_\rho})P_0[\nu,\xi](1\otimes T_+)]\\
&\quad=q^{-4(\rho,\rho_1)}(-1)^{|\Phi_1^+|}\mathrm{str}\otimes\mathrm{str}[(1\otimes T_+)\Delta(T_-)\Delta(q^{2h_\rho})\\
&\qquad\times P_0[\nu,\xi]],
\end{aligned}$$

where the last equality follows from the cyclic rule of supertraces. Now [cf. Eq. (9b)]

$$\begin{aligned}
(1\otimes T_+)\Delta(T_-)P_0&=(q^{h_{\rho_1}}\otimes T_+T_-)P_0=\chi_\mu(\Gamma_0)(q^{h_{\rho_1}}\otimes 1)P_0\Rightarrow(1\otimes T_+)\Delta(T_-)P_0[\nu,\xi]\\
&=q^{(\rho_1,\nu-\mu)}\chi_\mu(\Gamma_0)P_0[\nu,\xi].
\end{aligned}\tag{25}$$

Substituting into the above we arrive at

$$\begin{aligned}
\mathrm{str}_q\otimes\mathrm{str}_q[\Delta(T_-)P[\nu,\xi](1\otimes T_+)]&=(-1)^{|\Phi_1|^+}q^{-4(\rho,\rho_1)}\chi_\mu(\Gamma_0)q^{(\rho_1,\nu-\mu)}\mathrm{str}\\
&\quad\otimes\mathrm{str}[\Delta(q^{2h_\rho})P_0[\nu,\xi]]\\
&=(-1)^{|\Phi_1|^+}q^{-4(\rho,\rho_1)}\eta
\end{aligned}$$

with η as in the statement of the theorem.

For the nondiagonal case a bit more work is required. Let $\{e_0^\xi(\nu)_k\}$ be a basis for the maximal $\mathbb{Z}$-graded component $V_0^\xi(\nu)$ of $V^\xi(\nu)$ with dual basis $\{e_0^\xi(\nu)^k\}$ under the form $\langle\ ,\ \rangle$ on X and let $\{e_0(\nu,\xi)_k\}$, $\{e_0(\nu,\xi)^k\}$ be corresponding dual bases for $V_0(\nu,\xi)\subseteq X_0$. Recall that $\langle\ ,\ \rangle$ restricted to the irreducible $U_q(L_0)$ modules $V_0^\xi(\nu)$, $V_0(\nu,\xi)$ is nondegenerate and thus either positive or negative definite; we let $\epsilon=\pm1$ be the *relative* signature of the two forms (the signature of the form on $V_0^\xi(\nu)$ is ϵ_ξ, defined previously).

We may thus write

$$P_0e_0^\xi(\nu)_k=\alpha_\xi e_0(\nu,\xi)_k,\quad P_0e_0^\xi(\nu)^k=\epsilon\alpha_\xi e_0(\nu,\xi)^k,\tag{26}$$

where $\alpha_\xi\in\mathbb{C}$: note, from Proposition 4.1, that $\alpha_\xi\neq0$. Clearly (no summation)

$$\begin{aligned}
|\alpha_\xi|^2&=\epsilon\langle P_0e_0^\xi(\nu)^k,P_0e_0^\xi(\nu)_k\rangle=\epsilon\langle e_0^\xi(\nu)^k,P_0e_0^\xi(\nu)_k\rangle=\epsilon\langle e_0^\xi(\nu)^k,P[\nu]P_0P[\nu]e_0^\xi(\nu)_k\rangle\\
&=\epsilon\lambda_\xi\langle e_0^\xi(\nu)^k,e_0^\xi(\nu)_k\rangle=\epsilon\lambda_\xi>0.
\end{aligned}$$

Since $|\alpha_\xi|^2=\epsilon\lambda_\xi\neq0$ (cf. also with Lemma 4.4), Eq. (26) implies

$$\begin{aligned}
P[\nu,\xi]e_0(\nu,\xi)_k&=P[\nu]e_0(\nu,\xi)_k=\alpha_\xi^{-1}P[\nu]P_0e_0^\xi(\nu)_k=\alpha_\xi^{-1}P[\nu]P_0P[\nu]e_0^\xi(\nu)_k=\alpha_\xi^{-1}\lambda_\xi e_0^\xi(\nu)_k\\
&=\epsilon\overline{\alpha_\xi}e_0^\xi(\nu)_k.
\end{aligned}\tag{27}$$

Thus we may write

$$\Delta(T_-)P[\nu]_{\xi\xi'}P_0=\Delta(T_-)P[\nu]_{\xi\xi'}P_0[\nu,\xi']=\epsilon'\overline{\alpha}_{\xi'}\Delta(T_-)\sum_k |e_0^{\xi}(\nu)_k\rangle\langle e_0(\nu,\xi')^k|,$$

where the last equality follows from Eq. (27) together with the definition of $P[\nu]_{\xi\xi'}$. Utilizing Eq. (27) then gives

$$\epsilon\overline{\alpha}_{\xi}\Delta(T_-)P[\nu]_{\xi\xi'}P_0=\epsilon'\overline{\alpha}_{\xi'}\Delta(T_-)P[\nu,\xi]\sum_k |e_0(\nu,\xi)_k\rangle\langle e_0(\nu,\xi')^k|=\epsilon'\overline{\alpha}_{\xi'}\Delta(T_-)P_0[\nu]_{\xi\xi'},$$

where the last equality follows from Proposition 4.3 and

$$P_0[\nu]_{\xi\xi'}\equiv\sum_k |e_0(\nu,\xi)_k\rangle\langle e_0(\nu,\xi')^k|$$

determines a $U_q(L_0)$ module isomorphism from $V_0(\nu,\xi')$ to $V_0(\nu,\xi)$.

For $\xi\neq\xi'$, these latter spaces are orthogonal, so we arrive at

$$\begin{aligned}\epsilon\overline{\alpha}_{\xi}\mathrm{str}_q\otimes\mathrm{str}_q(\Delta(T_-)P[\nu]_{\xi\xi'}(1\otimes T_+))&=\epsilon'\overline{\alpha}_{\xi'}\mathrm{str}_q\otimes\mathrm{str}_q[\Delta(T_-)P_0[\nu]_{\xi\xi'}(1\otimes T_+)]\\&=\epsilon'\overline{\alpha}_{\xi'q}^{4(\rho,\rho_1)}\mathrm{str}\otimes\mathrm{str}[\Delta(T_-)\Delta(q^{2h_\rho})P_0[\nu]_{\xi\xi'}(1\otimes T_+)]\\&=\epsilon'\overline{\alpha}_{\xi'q}^{4(\rho,\rho_1)}(-1)^{|\Phi_1^+|}\mathrm{str}\otimes\mathrm{str}[(1\\&\quad\otimes T_+)\Delta(T_-)\Delta(q^{2h_\rho})P_0[\nu]_{\xi\xi'}]\\&=\epsilon'\overline{\alpha}_{\xi'q}^{4(\rho,\rho_1)}(-1)^{|\Phi_1^+|}q^{(\rho_1,\nu-\mu)}\mu_\mu(\Gamma_0)\mathrm{str}\\&\quad\otimes\mathrm{str}[\Delta(q^{2h_\rho})P_0[\nu]_{\xi\xi'}]=0,\end{aligned}$$

where we have employed Eq. (25) and the first equality follows from $(1\otimes T_+)X=X_0$.

This establishes the theorem as required. We now show that this result holds for an arbitrary multiplicity labeling for $V(\nu)\subseteq V(\Lambda)\otimes V(\mu)$, and not just the orthogonal scheme adopted above.

Extension to a general labeling

As above, let m_ν be the multiplicity of $V(\nu)\subseteq X=V(\Lambda)\otimes V(\mu)$ and let $f_{\xi\xi'}$ be the entries of an arbitrary $m_\nu\times m_\nu$ nonsingular matrix. Corresponding to a basis $\{e(\nu)_\alpha\}$ for $V(\nu)$, with dual basis $\{e(\nu)^\alpha\}$, we define a new labeling scheme:

$$e_\xi(\nu,f\ )_\alpha=f_{\xi'\xi}e^{\xi'}(\nu)_\alpha$$

(summation over repeated indices assumed here and below), giving the (not necessarily orthogonal) decomposition into $U_q(L)$ modules:

$$\overline{V(\nu)}=\bigoplus_\xi V_\xi(\nu,f\ ).$$

Note that any given labeling scheme is obtainable this way and that

$$\langle e^{\xi'}(\nu)^\alpha,e_\xi(\nu,f\ )_\beta\rangle=\delta^\alpha_\beta f_{\xi'\xi}.$$

We now introduce a *left* dual basis $e^{\xi}(\nu,f\ )^\alpha$ defined by

$$\langle e^{\xi'}(\nu,f\ )^\alpha,e_\xi(\nu,f\ )_\beta\rangle=\delta^{\xi'}_\xi\delta^\alpha_\beta$$

so that

$$e^{\xi}(\nu,f\ )^{\alpha}=\overline{f^{\xi\xi''}}e^{\xi''}(\nu)^{\alpha},$$

where $f^{\xi\xi''}\equiv(f^{-1})_{\xi\xi''}$. We set

$$P_f[\nu]_{\xi\xi'}=|e_{\xi}(\nu,f\ )_{\alpha}\rangle\langle e^{\xi'}(\nu,f\ )^{\alpha}|=f_{\xi''\xi}|e^{\xi''}(\nu)_{\alpha}\rangle\langle e^{\xi'''}(\nu)^{\alpha}|f^{\xi'\xi'''}=f_{\xi''\xi}P[\nu]_{\xi''\xi'''}f^{\xi'\xi'''}$$

with $P[\nu]_{\xi\xi'}$ as in Eq. (24). Thus $P_f[\nu,\xi]\equiv P_f[\nu]_{\xi\xi}$ is the (not necessarily orthogonal) projection onto $V_{\xi}(\nu,f\ )$. As a generalization of Theorem 5.1 we have

Theorem 5.2:

$$\begin{aligned}\mathrm{str}_q\otimes\mathrm{str}_q[\Delta(T_+)P_f[\nu]_{\xi\xi'}(1\otimes T_-)]&=(-1)^{|\Phi_1^+|}q^{4(\rho,\rho_1)}\mathrm{str}_q\otimes\mathrm{str}_q[\Delta(T_-)P_f[\nu]_{\xi\xi'}(1\otimes T_+)]\\&=\delta_{\xi\xi'}\eta\end{aligned}$$

with η as in Theorem 5.1.

Proof: Using the results above, together with Theorem 5.1, we obtain

$$\begin{aligned}\mathrm{str}_q\otimes\mathrm{str}_q[\Delta(T_+)P_f[\nu]_{\xi\xi'}(1\otimes T_-)]&=f_{\xi''\xi}\mathrm{str}_q\otimes\mathrm{str}_q[\Delta(T_+)P[\nu]_{\xi''\xi'''}(1\otimes T_-)]f^{\xi'\xi'''}\\&=f_{\xi''\xi}\eta\delta_{\xi''\xi'''}f^{\xi'\xi'''}\\&=\eta f^{\xi'\xi''}f_{\xi''\xi}=\eta\delta_{\xi'\xi}\end{aligned}$$

with η as in Theorem 5.1, as required. In a similar way we can establish the second formula. □

The advantage of this result is that it shows Theorem 5.1 in fact applies to an arbitrary multiplicity labeling, and not just the orthogonal scheme adopted in Sec. IV. We shall now apply the result of Theorem 5.2 to investigate the $1-1$ correspondence between the imbeddings $V(\nu)\subseteq V(\Lambda)\otimes V(\mu)$ and $V(\mu)\subseteq V(\Lambda)^*\otimes V(\nu)$, for $\mu,\nu\in D^+$ typical.

VI. INDUCED LABELING FOR $V(\mu)\subseteq V(\Lambda)^*\otimes V(\nu)$ ($\mu,\nu\in D^+$ TYPICAL)

Here we investigate the relationship between the imbeddings $V(\nu)\subseteq V(\Lambda)\otimes V(\mu)$ and $V(\mu)\subseteq V(\Lambda)^*\otimes V(\nu)$ for typical $\mu,\nu\in D^+$ (but $\Lambda\in D^+$ arbitrary). We denote the multiplicity of $V(\mu)\subseteq V(\Lambda)^*\otimes V(\nu)$ by $m(\mu;\Lambda^*\otimes\nu)$ and similarly for $V(\nu)\subseteq V(\Lambda)\otimes V(\mu)$.

Lemma 6.1: $m(\nu;\Lambda\otimes\mu)=m(\mu;\Lambda^*\otimes\nu)$.

Proof: From Lemma 2.1 we have

$$\begin{aligned}m(\nu;\Lambda\otimes\mu)&=\dim\ \mathrm{Hom}_{U_q(L)}(V(\nu),V(\Lambda)\otimes V(\mu))\\&=\text{multiplicity of identity irrep in } V(\nu)^*\otimes V(\Lambda)\otimes V(\mu)\\&=\text{multiplicity of identity irrep in } V(\mu)^*\otimes V(\Lambda)^*\otimes V(\nu)\\&=\dim\ \mathrm{Hom}_{U_q(L)}(V(\mu),V(\Lambda)^*\otimes V(\nu))\\&=m(\mu;\Lambda^*\otimes\nu).\end{aligned}$$

□

Here we assume the orthogonal labeling scheme $V^{\xi}(\nu)$ for $V(\nu)\subseteq V(\Lambda)\otimes V(\mu)$ considered in Sec. IV. Associated with $V^{\xi}(\nu)$ is a $U_q(L)$ module monomorphism (natural imbedding) ξ: $V(\nu)\to V(\Lambda)\otimes V(\mu)$ given by Eq. (23). We let $\xi^{\dagger}$: $V(\Lambda)\otimes V(\mu)\to V(\nu)$ be its conjugate, which thus also defines a $U_q(L)$ module homomorphism; explicity

$$\langle \xi^\dagger(w\otimes v^\mu), e^\nu\rangle = \langle w\otimes v^\mu, \xi(e^\nu)\rangle, \quad \forall w\in V(\Lambda), \quad v^\mu\in V(\mu), \quad e^\nu\in V(\nu),$$

where $\langle\ ,\ \rangle$ is the natural form on $V(\Lambda)\otimes V(\mu)$. We note that $\xi^\dagger\xi'$: $V(\nu)\to V(\nu)$ is an isomorphism and by construction of the labeling

$$\xi^\dagger\xi' = \epsilon_\xi \delta_{\xi\xi'} I,$$

where I denotes the identity operator on $V(\nu)$ and ϵ_ξ is the signature of the form $\langle\ ,\ \rangle$ restricted to $V^\xi(\nu)$ (cf. Definition 3.2).

We note, however, that if $\{e(\nu)_\alpha\}$ is a basis for $V(\nu)$ with corresponding dual basis $\{e(\nu)^\alpha\}$ under the natural form on $V(\nu)$, then

$$\xi'\xi^\dagger(w\otimes v) = \sum_\alpha\ \xi'|e(\nu)_\alpha\rangle\langle e(\nu)^\alpha, \xi^\dagger(w\otimes v)\rangle$$

$$= \epsilon_\xi \sum_\alpha\ |e^{\xi'}(\nu)_\alpha\rangle\langle e^\xi(\nu)^\alpha, w\otimes v\rangle, \quad \forall w\in V(\Lambda), \quad v\in V(\mu)$$

so that

$$\xi'\xi^\dagger = \epsilon_\xi P[\nu]_{\xi'\xi}$$

with $P[\nu]_{\xi'\xi}$ as in Eq. (24).

Now let $\{w_i\}$ be a weight basis for $V(\Lambda)$, which is thus naturally $\mathbb{Z}$-graded, with corresponding dual basis $\{w_i^*\}$ for $V(\Lambda)^*$. Following Lemma 2.2, corresponding to ξ as defined, we introduce a linear map $\hat\xi$: $V(\mu)\to V(\Lambda)^*\otimes V(\nu)$ defined by

$$\hat\xi(v) = \sum_i\ (-1)^{[i]}(q^{-h_\rho}w_i^*)\otimes\xi^\dagger(w_i\otimes v), \quad \forall v\in V(\mu). \tag{28}$$

Lemma 6.2: $\hat\xi$ determines a $U_q(L)$ module monomorphism.

Proof: $\hat\xi$ is obviously well defined and nonzero. It remains to prove it gives rise to a homomorphism. Now for $a\in U_q(L)$ we have, following Sweedler,[24]

$$\Delta(a)\hat\xi(v) = \Delta^{(2)}(a)(1\otimes\xi^\dagger)\sum_i\ (-1)^{[i]}(q^{-h_\rho}w_i^*)\otimes w_i\otimes v, \quad \forall v\in V(\mu),$$

where $\Delta^{(2)}\equiv(\Delta\otimes 1)\Delta=(1\otimes\Delta)\Delta$. Since $\xi^\dagger$ determines a $U_q(L)$ module homomorphism we thus obtain, in the notation of Eq. (2):

$$\Delta(a)\hat\xi(v) = (1\otimes\xi^\dagger)\sum_{(a)}\left[\Delta(a_{(1)})\sum_i\ (-1)^{[i]}(q^{-h_\rho}w_i^*)\otimes w_i\right]\otimes a_{(2)}v$$

$$= (1\otimes\xi^\dagger)\sum_i\ (-1)^{[i]}(q^{-h_\rho}w_i^*)\otimes w_i\otimes\sum_{(a)}\ \epsilon(a_{(1)})a_{(2)}v,$$

where we have utilized Lemma 2.2. Since $\Sigma_{(a)}\epsilon(a_{(1)})a_{(2)}=a$, we thereby arrive at

$$\Delta(a)\hat\xi(v) = \sum_i\ (-1)^{[i]}(q^{-h_\rho}w_i^*)\otimes\xi^\dagger(w_i\otimes av) = \hat\xi(av), \quad \forall a\in U_q(L), \quad v\in V(\mu)$$

as required. □

We thus set

$$V_\xi(\mu)=\hat{\xi}[V(\mu)].$$

We now show that this defines a complete labeling scheme for $V(\mu)\subseteq V(\Lambda)^*\otimes V(\nu)$ in $1-1$ correspondence with the labeling scheme for $V(\underline{\nu})\subseteq V(\Lambda)\otimes V(\mu)$.

Proposition 6.1: The isotypic component $V(\mu)$ of $V(\mu)\subseteq V(\Lambda)^*\otimes V(\nu)$ admits the $U_q(L)$ module decomposition

$$\overline{V(\mu)}=\bigoplus_\xi V_\xi(\mu).$$

Proof: Let v_+^μ be the maximal weight vector of $V(\mu)$ and $v_\xi(\mu)_+\equiv\hat{\xi}(v_+^\mu)$ the corresponding maximal weight vector of $V_\xi(\mu)$. It suffices to show, from Lemma 6.2, that these vectors are linearly independent. Suppose then that

$$\sum_\xi \alpha_\xi v_\xi(\mu)_+=0, \quad \alpha_\xi\in\mathbb{C}.$$

Then, by definition, we have

$$\sum_i (-1)^{[i]}(q^{-h_\rho}w_i^*)\otimes\sum_\xi \alpha_\xi\xi^\dagger(w_i\otimes v_+^\mu)=0 \Rightarrow\sum_\xi \alpha_\xi\xi^\dagger(w_i\otimes v_+^\mu)=0, \quad \forall i$$

$$\Rightarrow\sum_\xi \alpha_\xi\xi^\dagger(V(\Lambda)\otimes v_+^\mu)=0.$$

$\Sigma_\xi\alpha_\xi\xi^\dagger$ determines a $U_q(L)$ module homomorphism, and since $V(\Lambda)\otimes V(\mu)=U_q(L)(V(\Lambda)\otimes v_+^\mu)$, we obtain

$$\sum_\xi \alpha_\xi\xi^\dagger=0\Rightarrow\alpha_\xi=0, \quad \forall\xi$$

because the $\xi^\dagger$ are linearly independent (recall that $\xi^\dagger\xi'=\epsilon_\xi\delta_{\xi\xi'}I$, I the identity operator on $V(\nu)$). This is sufficient to prove the result.

Note: With the convention of Eq. (28), $V(\mu)\subseteq V(\Lambda)^*\otimes V(\nu)$ will have parity $+1$; i.e., its maximal $\mathbb{Z}$-graded component $V_0(\mu)$ is implicitly understood to have parity $+1$ in $V(\Lambda)^*\otimes V_0(\nu)$. □

Below we show that the decomposition of Proposition 6.1 is in fact orthogonal under the form $\langle\ ,\ \rangle$ on $V(\Lambda)^*\otimes V(\nu)$. To this end let $\{v(\mu)_k\}$ be a $\mathbb{Z}$-graded basis for $V(\mu)$ with corresponding dual basis $\{v(\mu)^k\}$ under the natural form on $V(\mu)$ and set $v_\xi=\hat{\xi}(v)$, $v\in V(\mu)$. We then have the overlap matrix $g_{\xi\xi'}$ defined by

$$\langle v_\xi(\mu)^k, v_{\xi'}(\mu)_l\rangle=g_{\xi\xi'}\delta_l^k.$$

A *left* dual basis to $\{v_\xi(\mu)_k\}\subseteq V_\xi(\mu)$ is thus given by

$$v^\xi(\mu)^k=g^{\xi\xi'}v_{\xi'}(\mu)^k$$

(summation over repeated indices assumed here and below) where $g^{\xi\xi'}\equiv(g^{-1})_{\xi\xi'}$. The (not necessarily orthogonal) projection onto $V_\xi(\mu)$ is then given by

$$P[\mu,\xi]=P[\mu]_{\xi\xi},$$

where

$$P[\mu]_{\xi\xi'}=\sum_k |v_\xi(\mu)_k\rangle\langle v^{\xi'}(\mu)^k|=\sum_k |v_\xi(\mu)^k\rangle\langle v^{\xi'}(\mu)_k|.$$

Our aim then is to show that the overlap matrix $g_{\xi\xi'}$ is diagonal. An important role in our approach is played by the operators

$$Q[\mu]_{\xi\xi'}=\sum_k |v_\xi(\mu)_k\rangle\langle v_{\xi'}(\mu)^k|=\sum_k g_{\xi'\xi''}|v_\xi(\mu)_k\rangle\langle v^{\xi''}(\mu)^k|=g_{\xi'\xi''}P[\mu]_{\xi\xi''} \tag{29}$$

with $P[\mu]_{\xi\xi''}$ as above. The $Q[\mu]_{\xi\xi'}$ satisfy the algebra

$$Q[\mu]^\dagger_{\xi\xi'}=Q[\mu]_{\xi'\xi}, \quad Q[\mu]_{\xi\xi'}Q[\mu]_{\eta\eta'}=g_{\xi'\eta}Q[\mu]_{\xi\eta'}.$$

We shall need the following result:

Proposition 6.2:

$$\mathrm{str}_q\otimes\mathrm{str}_q[\Delta(T_+)Q[\mu]_{\xi\xi'}(1\otimes T_-)]=\eta_{\xi\xi'},$$

where

$$\eta_{\xi\xi'}=g_{\xi'\xi}q^{-(\mu+\nu,\rho_1)}\chi_\nu(\Gamma_0)D^0_q[\mu].$$

Proof: Using Theorem 5.2 we obtain

$$\mathrm{str}_q\otimes\mathrm{str}_q[\Delta(T_+)Q[\mu]_{\xi\xi'}(1\otimes T_-)]=g_{\xi'\xi''}\ \mathrm{str}_q\otimes\mathrm{str}_q[\Delta(T_+)P[\mu]_{\xi\xi''}(1\otimes T_-)]=g_{\xi'\xi}\eta$$

with η as in Theorem 5.1 (but with ν and μ interchanged) so that

$$\eta=q^{-(\mu+\nu,\rho_1)}\chi_\nu(\Gamma_0)D^0_q[\mu],$$

where we have used the fact that $V_0(\mu)$ has positive parity in $V(\Lambda)^*\otimes V_0(\nu)$ (cf. note following Proposition 6.1), as required. □

Now, from definition, we have the following symmetry relation (notation as above):

$$\begin{aligned}\langle v_\xi(\mu),w_i^*\otimes e(\nu)\rangle&=\sum_j (-1)^{[j]}\langle(q^{-h_\rho}(w^j)^*)\otimes\xi^\dagger(w^j\otimes v(\mu)),w_i^*\otimes e(\nu)\rangle\\&=q^{(\lambda_i,\rho)}\langle\xi^\dagger(w^i\otimes v(\mu)),e(\nu)\rangle\\&=q^{(\lambda_i,\rho)}\langle w^i\otimes v(\mu),e^\xi(\nu)\rangle\\&=\langle(q^{h_\rho}w^i)\otimes v(\mu),e^\xi(\nu)\rangle,\quad \forall v(\mu)\in V(\mu),\quad e(\nu)\in V(\nu),\end{aligned} \tag{30}$$

where $v_\xi(\mu)\equiv\hat\xi[v(\mu)]$, $e^\xi(\nu)\equiv\xi[e(\nu)]$ and $\{w^i\}$ is the basis dual to $\{w_i\}$ under the natural form on $V(\Lambda)$: here λ_i denotes the weight of w_i and thus w^i. As before, $\{(w^i)^*\}$ is the basis for $V(\Lambda)^*$ naturally dual to $\{w^i\}$ so that $(w^i)^*(w^j)=\delta_{ij}$.

Now let $\{v(\mu)_k\}$, $\{e(\nu)_\alpha\}$ be bases for $V(\mu)$, $V(\nu)$ with corresponding dual bases $\{v(\mu)^k\}$, $\{e(\nu)^\alpha\}$ under the natural forms on $V(\mu)$, $V(\nu)$, resp. The above symmetry relation together with its conjugate, then implies the useful relation

$$\begin{aligned}&\epsilon_{\xi'}\langle(q^{h_\rho}w^i)\otimes v(\mu)^l,e^\xi(\nu)_\alpha\rangle\langle e^{\xi'}(\nu)^\beta,(q^{h_\rho}w_j)\otimes v(\mu)_k\rangle\\&\quad=\langle(w^j)^*\otimes e(\nu)^\beta,v_{\xi'}(\mu)_k\rangle\langle v_\xi(\mu)^l,w_i^*\otimes e(\nu)_\alpha\rangle,\end{aligned} \tag{31}$$

where $v_\xi = \hat{\xi}(v)$, $\forall v \in V(\mu)$ while $e^\xi(\nu)_\alpha = \xi[e(\nu)_\alpha]$, $e^\xi(\nu)^\alpha = \epsilon_\xi \xi[e(\nu)^\alpha]$. We are now in a position to prove orthogonality.

Theorem 6.1 (notation as above):

$$g_{\xi\xi'} = \epsilon_\xi \delta_{\xi\xi'} g,$$

where

$$g = (-1)^{[\nu]} \frac{\chi_\mu(\Gamma_0)}{\chi_\nu(\Gamma_0)} \frac{D_q^0[\nu]}{D_q^0[\mu]}.$$

Proof: From Eq. (31) above, we have

$$\begin{aligned}
&\epsilon_{\xi'}\langle (q^{h_\rho} w^i) \otimes v(\mu)^l, \Delta(T_-) e^\xi(\nu)_\alpha \rangle \langle e^{\xi'}(\nu)^\beta, (q^{h_\rho} w_j) \otimes T_+ v(\mu)_k \rangle \\
&\quad = \langle (w^j)^* \otimes e(\nu)^\beta, \Delta(T_+) v_{\xi'}(\mu)_k \rangle \langle v_\xi(\mu)^l, w_i^* \otimes T_- e(\nu)_\alpha \rangle \\
&\quad \Rightarrow \epsilon_{\xi'} \langle (q^{h_\rho} w^i) \otimes q^{h_\rho} v(\mu)^l, \Delta(T_-) e^\xi(\nu)_\alpha \rangle \langle e^{\xi'}(\nu)^\beta, (q^{h_\rho} w_j) \otimes q^{h_\rho} T_+ v(\mu)_k \rangle \\
&\quad = \langle (w^j)^* \otimes e(\nu)^\beta, \Delta(q^{h_\rho}) \Delta(T_+) v_{\xi'}(\mu)_k \rangle \langle \Delta(q^{h_\rho}) v_\xi(\mu)^l, w_i^* \otimes T_- e(\nu)_\alpha \rangle.
\end{aligned}$$

Setting $i=j$, $\beta=\alpha$, $k=l$ (no summation) we obtain

$$\begin{aligned}
&\langle (q^{h_\rho} w^i) \otimes q^{h_\rho} v(\mu)^k, \Delta(T_-) e^\xi(\nu)_\alpha \rangle \langle e^{\xi'}(\nu)^\alpha, q^{h_\rho} w_i \otimes q^{h_\rho} T_+ v(\mu)_k \rangle \\
&\quad = \epsilon_{\xi'} \langle (w^i)^* \otimes e(\nu)^\alpha, \Delta(q^{h_\rho}) \Delta(T_+) v_{\xi'}(\mu)_k \rangle \langle \Delta(q^{h_\rho}) v_\xi(\mu)^k, w_i^* \otimes T_- e(\nu)_\alpha \rangle.
\end{aligned}$$

Now multiply both sides by $(-1)^{[i]+[k]} = (-1)^{[\alpha]+|\Phi_1^+|}$ and sum on i, k, α to give, using the definition of Eq. (29),

$$\begin{aligned}
&\epsilon_{\xi'} \ \mathrm{str} \otimes \mathrm{str}[\Delta(q^{h_\rho}) \Delta(T_-) P[\nu]_{\xi\xi'} \Delta(q^{h_\rho})(1 \otimes T_+)] \\
&\quad = (-1)^{|\Phi_1^+|} \ \mathrm{str} \otimes \mathrm{str}[\Delta(q^{h_\rho}) \Delta(T_+) Q[\mu]_{\xi'\xi} \Delta(q^{h_\rho})(1 \otimes T_-)]
\end{aligned}$$

which may be rearranged to give

$$(-1)^{|\Phi_1^+|} q^{4(\rho,\rho_1)} \ \mathrm{str}_q \otimes \mathrm{str}_q[\Delta(T_-) P[\nu]_{\xi\xi'} (1 \otimes T_+)] = \epsilon_{\xi'} \ \mathrm{str}_q \otimes \mathrm{str}_q[\Delta(T_+) Q[\mu]_{\xi'\xi} (1 \otimes T_-)].$$

Since μ, ν are typical, we may apply Theorem 5.2 to the left-hand side and Proposition 6.2 to the right-hand side to give, noting that the factors $q^{-(\mu+\nu,\rho_1)}$ cancel from both sides:

$$(-1)^{[\nu]} \chi_\mu(\Gamma_0) D_q^0[\mu] \delta_{\xi\xi'} = \epsilon_{\xi'} g_{\xi\xi'} \chi_\nu(\Gamma_0) D_q^0[\mu]$$

from which the result follows.

Corollary: The induced labeling scheme for $V(\mu) \subseteq V(\Lambda)^* \otimes V(\nu)$ is orthogonal with respect to the induced form.

VII. SUPERTRACE FORMULA FOR TYPICAL PROJECTIONS

Throughout we adopt the notation and conventions of Sec. VI. It is worth noting that Eq. (30) is reminiscent of a well known symmetry relation satisfied by the Clebsch–Gordan coefficients of a simple Lie algebra (although in such a case one usually works with an inner product). We now come to our main result on partial q supertraces of projections onto typical irreducible submodules $V(\nu) \subseteq V(\Lambda) \otimes V(\mu)$ ($\mu \in D^+$ typical as before).

Proposition 7.1:

$$(\mathrm{str}_q \otimes 1) P[\nu]_{\xi\xi'} = \delta_{\xi'\xi} g$$

with g as in Theorem 6.1.

Proof: Using the definition of $v_\xi(\mu)_k = \hat{\xi}[v(\mu)_k] \subseteq V(\Lambda)^* \otimes V(\nu)$ [cf. Eq. (28)] we have, from Theorem 6.1,

$$\begin{aligned}
&\epsilon_\xi g\, \delta_{\xi\xi'} \langle v(\mu)_k, v(\mu)_l \rangle \\
&\quad = \langle v_\xi(\mu)_k, v_{\xi'}(\mu)_l \rangle \\
&\quad = \sum_{i,j} (-1)^{[i]+[j]} \langle q^{-h_\rho}(w^i)^* \otimes \xi^\dagger(w^i \otimes v(\mu)_k), (q^{-h_\rho} w_j^*) \otimes \xi'^\dagger(w_j \otimes v(\mu)_l) \rangle \\
&\quad = \sum_{i,j} (-1)^{[i]+[j]} q^{2(\rho,\lambda_i)} \langle (w^i)^*, w_j^* \rangle \langle \xi^\dagger(w^i \otimes v(\mu)_k), \xi'^\dagger(w_j \otimes v(\mu)_l) \rangle \\
&\quad = \sum_{i,j} (-1)^{[i]} q^{2(\rho,\lambda_i)} \langle w^i \otimes v(\mu)_k, \xi\xi'^\dagger(w_i \otimes v(\mu)_l) \rangle,
\end{aligned}$$

where w^i and w_i are assumed to have weight λ_i, and the last equality follows from Proposition 3.4. In view of the fact that $\xi\xi'^\dagger = \epsilon_{\xi'} P[\nu]_{\xi\xi'}$, with $P[\nu]_{\xi\xi'}$ as in Eq. (24); we thus arrive at

$$\begin{aligned}
\epsilon_\xi g\, \delta_{\xi\xi'} \langle v(\mu)_k, v(\mu)_l \rangle &= \epsilon_{\xi'} \sum_i (-1)^{[i]} q^{2(\rho,\lambda_i)} \langle w^i \otimes v(\mu)_k, P[\nu]_{\xi\xi'}(w_i \otimes v(\mu)_l) \rangle \\
&= \epsilon_{\xi'} \langle v(\mu)_k, [(\mathrm{str}_q \otimes 1) P[\nu]_{\xi\xi'}] v(\mu)_l \rangle.
\end{aligned}$$

Thus, in view of Proposition 2.1, $(\mathrm{str}_q \otimes 1) P[\nu]_{\xi\xi'}$ determines a $U_q(L)$ invariant on $V(\mu)$ with eigenvalue determined by

$$\epsilon_\xi g\, \delta_{\xi\xi'} \langle v(\mu)_k, v(\mu)_l \rangle = \epsilon_{\xi'} \langle v(\mu)_k, v(\mu)_l \rangle (\mathrm{str}_q \otimes 1) P[\nu]_{\xi\xi'}$$

from which the result follows.

Corollary:

$$(\mathrm{str}_q \otimes 1) P[\nu, \xi] = (-1)^{[\nu]} \frac{\chi_\mu(\Gamma_0)}{\chi_\nu(\Gamma_0)} \frac{D_q^0[\nu]}{D_q^0[\mu]}$$

with $P[\nu,\xi]$ the (orthogonal) projection onto $V^\xi(\nu) \subseteq \overline{V(\nu)}$. □

Note that the above result is independent of the multiplicity labeling ξ. Now let

$$P[\nu] = \sum_\xi P[\nu, \xi]$$

be the orthogonal projection onto the isotypic component $\overline{V(\nu)}$ of $V(\nu) \subseteq V(\Lambda) \otimes V(\mu)$. Then from the results above, we arrive at

Theorem 7.1:

$$(\mathrm{str}_q \otimes 1) P[\nu] = (-1)^{[\nu]} m_\nu \frac{\chi_\mu(\Gamma_0)}{\chi_\nu(\Gamma_0)} \frac{D_q^0[\nu]}{D_q^0[\mu]}$$

with m_ν the multiplicity of $V(\nu)\subseteq V(\Lambda)\otimes V(\mu)$ and $[\nu]$ the $\mathbb{Z}$-graded level of $V_0(\nu)\subseteq V(\Lambda)\otimes V_0(\mu)$. □

The multiplicities m_ν are given explicitly by the corollary to Proposition 4.1 while the q dimensions are given by formula (10) and the $\chi_\nu(\Gamma_0)$ by formula (11); note that the ratio $\chi_\mu(\Gamma_0)/\chi_\nu(\Gamma_0)$ is independent of the constant $c\neq 0$ of Eq. (11). We emphasize that the results above only apply to typical $\mu,\nu\in D^+$. They will be utilized below to determine the eigenvalues of the Casimir invariants (16).

VIII. EIGENVALUE FORMULA FOR CASIMIR INVARIANTS

Let $V(\mu)$ be an arbitrary (possibly infinite dimensional) irreducible $U_q(L)$ module with highest weight $\mu\in H^*$. Then on $V(\mu)$ the elements of the center Z take constant values; for $z\in Z$ we denote its eigenvalue on $V(\mu)$ by $\chi_\mu(z)$. We note that χ_μ determines an algebra homomorphism:[19]

$$\chi_\mu : Z\to\mathbb{C},\quad z\mapsto\chi_\mu(z)$$

called an *infinitesimal character*. More generally we say that a $U_q(L)$ module V admits an infinitesimal character χ_μ, $\mu\in H^*$, if the central elements $z\in Z$ take constant values $\chi_\mu(z)$ on V. Note that such a module V need not possess a maximal (or minimal) weight vector.

Throughout we let $V(\Lambda)$ be a fixed, but arbitrary, finite dimensional irreducible $U_q(L)$ module with a real highest weight $\Lambda\in D^+$. We let $\{\lambda_i\}$ denote the set of distinct weights in $V(\Lambda)$ with m_i the multiplicity of the weight λ_i. Now let $c\in(Z\otimes Z)\Delta(Z)\subseteq U_q(L)\otimes U_q(L)$; an important example is afforded by

$$c=(1\otimes 1-R^TR)/(q-q^{-1}) \tag{32}$$

with R the universal R matrix. Following Proposition 2.1, we have the family of Casimir invariants

$$C_m=(\mathrm{str}_q\otimes 1)(\pi_\Lambda\otimes 1)c^m. \tag{33}$$

To determine their eigenvalues we first need[34,35]

Definition 8.1: We say that Λ is *typically subordinate* to $\mu\in D^+$ if $\mu,\mu+\lambda_i$ are all (real) dominant and typical. We denote the set of such μ by D^+_Λ. □

From Ref. 35 we have (also cf. Refs. 15 and 34)

Lemma 8.1: The eigenvalues $\chi_\mu(C_m)$ of the invariants (33), *$\mu\in H^*$, determine functions on H^* which are uniquely defined by their restriction to D^+_Λ.* □

We thus assume $\mu\in D^+_\Lambda$ so that we have the tensor product decomposition

$$V(\Lambda)\otimes V_0(\mu)=\oplus\, m_iV_0(\mu+\lambda_i)$$

which follows from the fact that $V(\Lambda)$ is subordinate to $V_0(\mu)$, the maximal $\mathbb{Z}$-graded component of $V(\mu)$, as a $U_q(L_0)$ module. Thus all $U_q(L_0)$ modules $V_0(\mu+\lambda_i)$ occur with full multiplicity m_i in $V(\Lambda)\otimes V_0(\mu)$ (cf. Kostant[34]). Since the $\mu+\lambda_i$ are all typical we obtain, from the corollary to Proposition 4.1, the tensor product decomposition

$$V(\Lambda)\otimes V(\mu)=\bigoplus_i m_iV(\mu+\lambda_i).$$

We let $P[i]$ denote the orthogonal (central) projection of the tensor product space onto the isotypic component $V(\mu+\lambda_i)\equiv m_iV(\mu+\lambda_i)$. We then have the spectral decomposition

$$c^m=\sum_i\,\langle c\rangle^m_{\mu+\lambda_i}P[i],$$

where $\langle c\rangle_{\mu+\lambda_i}$ denotes the eigenvalue of c on $V(\mu+\lambda_i)\subseteq V(\Lambda)\otimes V(\mu)$. Since $\mu,\mu+\lambda_i$ are all dominant and typical we may apply the results of Theorem 7.1 which gives, for the eigenvalues of the invariants (33):

$$\chi_\mu(C_m)=\sum_i \langle c\rangle^m_{\mu+\lambda_i}(\mathrm{str}_q\otimes 1)P[i]=\sum_i (-1)^{[i]}m_i\langle c\rangle^m_{\mu+\lambda_i}\frac{\chi_\mu(\Gamma_0)}{\chi_{\mu+\lambda_i}(\Gamma_0)}\frac{D^0_q[\mu+\lambda_i]}{D^0_q[\mu]},\quad \mu\in D^+_\Lambda,$$

where $[i]$ denotes the degree of weight λ_i. In view of Eqs. (10) and (11) and Lemma 8.1, we thereby arrive at the following eigenvalue formula:

Theorem 8.1:

$$\chi_\mu(C_m)=\sum_i (-1)^{[i]}m_i\langle c\rangle^m_{\mu+\lambda_i}\prod_{\beta\in\Phi^+_1}\frac{[(\mu+\rho,\beta)]_q}{[(\mu+\lambda_i+\rho,\beta)]_q}\prod_{\alpha\in\Phi^+_0}\frac{[(\mu+\lambda_i+\rho,\alpha)]_q}{[(\mu+\rho,\alpha)]_q},\quad \mu\in H^*.$$

Note: The above determines a well defined function on H^*. However it will be undefined as it stands if some $\mu+\lambda_i$ is atypical or $(\mu+\rho,\alpha)=0$, for some $\alpha\in\Phi^+_0$ (this latter situation can never occur for $\mu\in D^+$). In such a case the right-hand side must first be expanded in order to avoid singularities. Note however that the set of $\mu\in H^*$ for which this occurs forms a Zariski closed subset of H^*. Thus the formula is well defined on a Zariski open, and hence dense, subset of H^*; for further details see Ref. 35. □

We now investigate the important special case where c is given by Eq. (32); the corresponding invariants (33) in this case reduced to those of Eq. (16). It is a well established result for ($\mathbb{Z}_2$-graded) quasitriangular Hopf algebras that there exists a distinguished element[12]:

$$u=\sum_t (-1)^{[t]}S(b_t)a_t,$$

where a_t and b_t are the coordinates of the universal R matrix: $R=\Sigma_t a_t\otimes b_t$. Then it can be shown that u has inverse

$$u^{-1}=\sum_t (-1)^{[t]}S^{-2}(b_t)a_t$$

and satisfies

$$\begin{aligned} S^2(a)&=uau^{-1},\quad \forall a\in U_q(L),\\ \Delta(u)&=(u\otimes u)(R^TR)^{-1}. \end{aligned}\tag{34}$$

On the other hand, from Eq. (3) we have

$$S^2(a)=q^{-2h_\rho}aq^{2h_\rho},\quad \forall a\in U_q(L)$$

which follows from the fact that the principal antiautomorphism γ satisfies $\gamma^2=I$, the identity map on $U_q(L)$. Thus $v\equiv q^{2h_\rho}u$ must be a central element which, in view of Eq. (34), satisfies

$$R^TR=(v\otimes v)\Delta(v^{-1}).$$

Moreover, it can be shown that[12]

$$\chi_\Lambda(v)=q^{-(\Lambda,\Lambda+2\rho)}.$$

Thus with c as in Eq. (32), we have for its eigenvalues on $V(\mu+\lambda_i)\subseteq V(\Lambda)\otimes V(\mu)$:

$$\langle c\rangle_{\mu+\lambda_i}\equiv a_i(\mu),\quad a_i(\mu)=\frac{1-q^{-2\alpha_i(\mu)}}{q-q^{-1}},$$

where α_i denotes the linear polynomial function on H^* given by

$$\alpha_i(\mu)=\tfrac{1}{2}(\Lambda,\Lambda+2\rho)-\tfrac{1}{2}(\lambda_i,\lambda_i+2(\mu+\rho)),\quad \forall\mu\in H^*. \tag{35}$$

It is worth noting that these are the roots of the characteristic identities[36] for the Lie superalgebra L, and in the $q\to 1$ limit, $a_i(\mu)\to\alpha_i(\mu)$ while c goes over to the characteristic matrix investigated in Refs. 16 and 36.

Hence, as a special case of Theorem 8.1, we arrive at the following formula for the eigenvalues of the Casimir invariants C_m^Λ of Eq. (16):

$$\chi_\mu(C_m^\Lambda)=\sum_i\ (-1)^{[i]}m_i a_i(\mu)^m\prod_{\beta\in\Phi_1^+}\frac{[(\mu+\rho,\beta)]_q}{[(\mu+\lambda_i+\rho,\beta)]_q}\prod_{\alpha\in\Phi_0^+}\frac{[(\mu+\lambda_i+\rho,\alpha)]_q}{[(\mu+\rho,\alpha)]_q} \tag{36}$$

for $\mu\in H^*$. This generalizes, and is in agreement with, the results of Ref. 17 obtained for the case π_Λ is the vector irrep of $U_q[gl(m|n)]$ using completely different methods. Again the above formula is well defined on a Zariski dense subset of H^*, but the right-hand side will need to be expanded if some $\mu+\lambda_i$ is atypical, or $(\mu+\rho,\alpha)=0$ for some $\alpha\in\Phi_0^+$. This can always be done, in principle, since $\chi_\mu(C_m^\Lambda)$ necessarily determines a well defined function on H^* which is given by formula (36) for generic $\mu\in H^*$. This aspect of the problem will be deferred to another article (see also Ref. 35).

In the classical limit $q\to 1$, the C_m^Λ give rise to a family of Casimir invariants for the Lie superalgebra L; they generalize those constructed by Jarvis and Green[16] to arbitrary reference irreps. From Eq. (36) their eigenvalues are given by

$$\chi_\mu(C_m^\Lambda)=\sum_i\ (-1)^{[i]}m_i\alpha_i(\mu)^m\prod_{\beta\in\Phi_1^+}\frac{(\mu+\rho,\beta)}{(\mu+\lambda_i+\rho,\beta)}\prod_{\alpha\in\Phi_0^+}\frac{(\mu+\lambda_i+\rho,\alpha)}{(\mu+\rho,\alpha)}$$

with $\alpha_i(\mu)$ as in Eq. (35). This result is also new and generalizes to arbitrary reference irreps the results of Refs. 16 and 17.

Explicit examples of the above Casimir invariants and their eigenvalues will be given in Sec. IX (see also Ref. 35). Equation (36) also plays a fundamental role in the evaluation of two variable link polynomials associated with any irrep with a real highest weight $\Lambda\in D^+$; for further details we refer to Ref. 18.

IX. EXAMPLES

In order to illustrate the application of our eigenvalue formula we will consider in this section the case of $U_q(gl(m|n))$ when the reference representation is taken to be the vector irrep (simply labeled π). We let $\{\epsilon_i\}$ denote the standard basis for H^* equipped with the invariant bilinear form

$$(\epsilon_i,\epsilon_j)=(-1)^{[i]}\delta_{ij},$$

where the $\mathbb{Z}_2$ grading on the indices is given by

$$[i]=\begin{cases}0, & i\leqslant m\\ 1, & i>m.\end{cases}$$

From Ref. 37 we have expressions for the co-product intertwiners which read

$$(\pi\otimes I)R=I\otimes I+(q-q^{-1})\sum_{i\leqslant j}(-1)^{[i]}e_i^j\otimes X_j^i,$$

$$(\pi\otimes I)R^T=I\otimes I+(q-q^{-1})\sum_{i\geqslant j}(-1)^{[i]}e_i^j\otimes X_j^i,$$

where e_j^i denote the standard elementary matrices. Above, the X_j^i are elements of $U_q(gl(m|n))$ which are given by

$$X_j^i=q^{1/2((\epsilon_i,\epsilon_i)E_i^i+(\epsilon_j,\epsilon_j)E_j^j-1)}E_j^i,\quad i\neq j,$$

$$X_i^i=(\epsilon_i,\epsilon_i)\frac{q^{(\epsilon_i,\epsilon_i)E_i^i}-1}{q-q^{-1}},$$

and the E_j^i are defined recursively as

$$E_j^i=E_k^iE_j^k-q^{-(\epsilon_k,\epsilon_k)}E_j^kE_k^i,\quad i\leqslant k\leqslant j.$$

(Note that the expressions for the X_j^i differ slightly from those in Ref. 37 due to a different choice for the co-product.)

We may write Eq. (32) in the form

$$(\pi\otimes I)c=\sum_{i,j}(-1)^{[i]}2^{\delta_{ij}}e_i^j\otimes X_j^i+(q-q^{-1})\sum_{k\geqslant i,j}(-1)^{([i]+[j])([i]+[k])}e_i^j\otimes X_j^kX_k^i$$

from which the Casimir invariants C_l of Eq. (33) can be calculated. Here we will construct the first and second order Casimir invariants only. The first order Casimir invariant reads

$$C_1=2\sum_i X_i^iq^{(2\rho,\epsilon_i)}+(q-q^{-1})\sum_{i\geqslant j}(-1)^{[j]}X_j^iX_i^jq^{(2\rho,\epsilon_j)} \tag{37}$$

while the second order invariant is given by

$$C_2=\sum_{i,j}(-1)^{[j]}4^{\delta_{ij}}X_j^iX_i^jq^{(2\rho,\epsilon_j)}+(q-q^{-1})\sum_{k\geqslant i,j}(-1)^{([i]+[j])([j]+[k])}2^{\delta_{ij}}(X_i^jX_j^kX_k^iq^{(2\rho,\epsilon_i)}$$

$$+X_j^kX_k^iX_i^jq^{(2\rho,\epsilon_j)})+(q-q^{-1})^2\sum_{k,l\geqslant i,j}(-1)^{[i][j]+[j][k]+[i][k]}X_j^kX_k^iX_i^lX_l^jq^{(2\rho,\epsilon_j)}. \tag{38}$$

The sets of even and odd positive roots are, resp, given by

$$\Phi_0^+=\{\epsilon_i-\epsilon_j|1\leqslant i<j\leqslant m+n,[i]=[j]\},$$

$$\Phi_1^+=\{\epsilon_i-\epsilon_j|1\leqslant i<j\leqslant m+n,[i]\neq[j]\},$$

in terms of which ρ is expressed as

$$\rho=\frac{1}{2}\sum_{i=1}^m(m-n-2i+1)\epsilon_i-\frac{1}{2}\sum_{j=1}^n(m+n-2j+1)\epsilon_{m+j}.$$

To determine the eigenvalues of these invariants acting on the irreducible module $V(\mu)$, $\mu=\sum_{i=1}^{m+n}\mu_i\epsilon_i$, we will apply our formula (36). The weight spectrum of the vector module is just $\{\epsilon_i\}_{i=1}^{m+n}$. In this case Eq. (36) simplifies to give

$$\chi_\mu(C_l)=\sum_{i=1}^{m+n}(-1)^{[i]}[a_i(\mu)]^l\prod_{j\neq i}\frac{q^{-(\epsilon_j,\epsilon_j)}a_i(\mu)-q^{(\epsilon_j,\epsilon_j)}a_j(\mu)+(-1)^{[j]}}{a_i(\mu)-a_j(\mu)}, \tag{39}$$

where the roots $a_i(\mu)$ are given by

$$a_i(\mu)=\frac{1-q^{(\epsilon_i,\epsilon_i+2\mu+2\rho)-m+n}}{q-q^{-1}}.$$

The above eigenvalues are all polynomial functions of the variables $q^{(\mu\epsilon_i)}$ so that Eq. (39) may be simplified for each value of l. For the case of $l=1$ it is known that the eigenvalues are given by[12]

$$\chi_\mu(C_1)=\sum_{i=1}^{m+n}(q-q^{-1})^{-1}(1-(-1)^{[i]}q^{2(\mu+\rho,\epsilon_i)}).$$

However for higher order invariants one needs to employ computing techniques to simplify these expressions. For the simple case of $U_q(gl2|1))$ we have used Mathematica to obtain the following eigenvalues for the first and second order Casimir invariants:

$$\chi_\mu(C_1)=(q-q^{-1})^{-1}(1-q^{2\mu_1}-q^{2\mu_2-2}+q^{-2\mu_3-2}),$$

$$\begin{aligned}\chi_\mu(C_2)=&(q-q^{-1})^{-2}(1+q^{2\mu_1}(q^{2\mu_1}-2)+q^{2\mu_2}(q^{2\mu_2-4}-2q^{-2})-q^{-2\mu_3}(q^{-2\mu_3-6}-2q^{-2})\\&+(q^{-2}-q^{-4})(q^{2\mu_1+2\mu_2}-q^{2\mu_1-2\mu_3}-q^{2\mu_2-2\mu_3-2})).\end{aligned}$$

These results may be checked against those obtained by explicitly evaluating the action of the invariants on the highest weight state using Eqs. (37) and (38).

X. CONCLUSIONS

We have investigated several important aspects of the rep theory of the type I quantum superalgebras. In particular it was shown in Sec. III that any finite dimensional rep for these algebras admits a natural decomposition into typical and atypical components. In the case of a tensor product of two finite dimensional irreps we have shown there is a natural, invariant, nondegenerate sesquilinear form $\langle\ ,\ \rangle$ induced on the tensor product space with respect to which its typical and atypical components are orthogonal. This implies that the restriction of the form to the isotypic component of a given typical submodule is nondegenerate, thus allowing the definition of corresponding Clebsch–Gordan coefficients with respect to the form $\langle\ ,\ \rangle$.

These results were applied in Sec. IV to construct an orthogonal multiplicity labeling for $V(\nu)\subseteq V(\Lambda)\otimes V(\mu)$ with $\mu,\nu\in D^+$ typical but $\Lambda\in D^+$ arbitrary. A useful result for the multiplicities in the tensor product module was also derived (see Proposition 4.1 and its corollary). In Sec. VI we investigated the naturally induced multiplicity labeling for $V(\mu)\subseteq V(\Lambda)^*\otimes V(\nu)$ which was also shown to be orthogonal under the form on the tensor product space and gives rise to a symmetry relation for the corresponding Clebsch–Gordan coefficients. It is worth noting that this approach is capable of further generalization, particularly for the calculation of generator matrix elements and corresponding Clebsch–Gordan coefficients for unitary irreps.

In Secs. VII and VIII we obtained a general eigenvalue formula for Casimir invariants, valid for an arbitrary reference irrep. This result is new, even in the classical limit, in which case it generalizes to arbitrary reference irreps the results of Refs. 16 and 17. Aside from solving an

outstanding problem in the rep theory of the type I quantum superalgebras, our results are particularly important for the systematic construction of new two variable link polynomials which will be investigated elsewhere.[18] Finally, the eigenvalue formula of Sec. VIII, derived for real $q>0$, can be shown to hold (analytic continuation) for (generic) complex q.

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Computation of Lie transformations from a power series: Bounds and optimum truncation

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The problem considered is the computation of an infinite product (composition) of Lie transformations generated by homogeneous polynomials of increasing order from a given asymptotic power series. Bounds are computed for the infinitesimal form of the Lie transformations and for the domain of analyticity of the first n of them. Even when the power series is convergent, the estimates exhibit a factorial-type growth, and thus do not guarantee convergence of the product. The optimum truncation is determined by minimizing the remainder after the first n Lie transformations have been applied. [S0022-2488(96)01203-2]

I. INTRODUCTION

A method based on an infinite product (composition) of Lie transformations (exponentiated vector fields) generated by homogeneous polynomials of increasing order was developed a long time ago in order to efficiently perform perturbative calculations in Hamiltonian systems when the small parameters are the dynamical variables themselves.[1,2] Subsequently, the recursion formulas for the computation of the infinite product from a single Lie transformation generated by a function analytic at the origin were derived in the nonsymplectic case.[3] It was recognized from the outset[1] that the product of Lie transformations can be computed from, or be used to compute, a power series in the dynamical variables. The relation between Lie transformations and power series, however, was established only at a formal level, that is order by order.

More recent work has provided firm bounds on the results that can be obtained using the method. In Refs. 4–6 a variant of the method is applied to the problem of bringing a Hamiltonian function or a Hamiltonian vector field to normal form. In Ref. 7, and in Ref. 6 for Hamiltonian systems, sufficient conditions are given on the coefficients of the polynomials and on the domain of the dynamical variables such that the infinite product of Lie transformations is convergent. Roughly speaking, the conditions sufficient for convergence are that the coefficients of the polynomials do not grow with order more rapidly than an exponential function, and that the transformation be restricted to a suitable domain around the origin. It can be expected that the condition on the coefficients is also necessary in general, since otherwise the norm of *each* vector field over any finite domain would grow without bound as the order of the polynomial increased.

In this paper we turn to the construction of Lie transformations from an asymptotic, that is not necessarily convergent, power series. We obtain bounds for the norms of the vector fields that are computed from such a series and determine the optimum truncation of the product of Lie transformations. Even when the power series is convergent, our results do not guarantee the convergence of the infinite product, giving instead a factorial-type growth for the estimates. The asymptotic nature of the bound is not unexpected, however, as remarked in Sec. II. As in Ref. 7, we do not require that the power series or the Lie transformations be symplectic (i.e., that they arise from Hamiltonian systems).

The organization of the paper is as follows: In Sec. II we introduce notation, which for quantities that appear in both is the same as in Ref. 7, and write down an expression for the coefficients of the polynomials in terms of the coefficients of the power series. Section III contains two lemmas which allow us to pass from the expression for the coefficients to an inequality in the

form of a recursion relation for the norms of the vector fields. In Sec. IV we then use the recursion relation to obtain a bound on the norms. The analyticity of a finite product of Lie transformations and the question of optimum truncation of the product are considered in Sec. V, and a summary of the results is given in Sec. VI.

II. PRELIMINARIES

We study the transformation $\mathscr{M}$ formally defined by

$$\mathscr{M}z = e^{L_2(z)} e^{L_3(z)} \cdots e^{L_n(z)} \cdots z, \quad z \in \mathbb{C}^d. \tag{2.1}$$

Here L_n is a vector field

$$L_n(z) = \sum_{j=1}^{d} g_j^{(n)}(z) \frac{\partial}{\partial z_j}, \tag{2.2}$$

and $g_j^{(n)}$ a homogeneous polynomial in z of order $n \geqslant 2$ with complex coefficients,

$$g_j^{(n)}(z) = \sum_{|r|=n} a_{rj}^{(n)} z^r. \tag{2.3}$$

The subscript r stands for the collection of indices $r_1,\ldots,r_d$, $|r| \overset{\text{def}}{=} r_1 + \cdots + r_d$, and z^r is defined by $z^r = z_1^{r_1} \cdots z_d^{r_d}$. The exponential of L_n is given by the usual infinite series

$$e^{L_n(z)} = \sum_{s=0}^{\infty} \frac{1}{s!} [L_n(z)]^s, \tag{2.4}$$

where $s=0$ corresponds to the identity transformation. In the definition of $\mathscr{M}$ the linear transformation has been set equal to the identity, as its computation is not germane to the problem at hand. The designation of Eq. (2.1) as formal, on the other hand, reflects the fact that we have not specified a domain in $\mathbb{C}^d$, if such one exists, on which the infinite series of Eq. (2.4) acting on z are convergent for $n=2,3,\ldots$. We also define $\mathscr{M}_n$ as the product of Lie transformations of the form (2.1) truncated at order n.

The properties of Lie transformations and their use in perturbation calculations are not discussed further in this paper. The interested reader is instead directed to Ref. 8 for a sampling of the surveys of the subject.

Suppose we are given the formal power series

$$P_k(z) = z_k + \sum_{m=2}^{\infty} \sum_{|r|=m} b_{rk}^{(m)} z^r, \tag{2.5}$$

where no restrictions are placed on the behavior of the (complex) coefficients $b_{rk}^{(m)}$ as a function of m,r,k. We are going to examine the construction of vector fields L_n chosen in such a way that $\mathscr{M}z$ and $P(z)$ agree order by order in z. For the moment we do not specify the domain over which the agreement occurs. A lower bound on this domain, $\mathscr{D}_n$, as a function of n is given in Sec. V. If the series $P(z)$ is actually convergent, we will denote its domain of analyticity by $\mathscr{D}$. ($\mathscr{D}$ evidently includes the origin.) In parallel with setting the linear transformation in $\mathscr{M}$ equal to the identity, we have assumed that, to first order in z, $P(z)=z$.

For a vector v, regardless of the vector space, we define the norm $\|v\|$ by

$$\|v\| = \max_j |v_j|, \tag{2.6}$$

where $|\cdot|$ stands for the modulus [except in the definition of index summation, as given following Eq. (2.3)]. For brevity we denote the norm of z by x, $x=\|z\|$. We also define the quantity $\alpha_j^{(n)}$ by

$$\alpha_j^{(n)}=\sum_{|r|=n}|a_{rj}^{(n)}|, \tag{2.7}$$

and α_n by $\alpha_n=\|\alpha^{(n)}\|$. The following relation holds:

$$\|L_n\|=\max_j|g_j^{(n)}(z)|=\max_j\left|\sum_{|r|=n}a_{rj}^{(n)}z^r\right|\leqslant\alpha_n x^n. \tag{2.8}$$

In the subsequent sections we will obtain a bound for α_n which will thus enable us to place a bound on $\|L_n\|$ on a given domain for x.

The first step is to write down an expression for the coefficients $a_{rj}^{(n)}$ in terms of the coefficients $b_{rj}^{(n)}$. We expand the Lie transformations into power series and match terms of the same order in z to get

$$\sum_{\mathscr{C}_n=n-1}\frac{L_2^{s_2}\cdots L_n^{s_n}}{s_2!\cdots s_n!}z_k=\sum_{|r|=n}b_{rk}^{(n)}z^r. \tag{2.9}$$

The symbol $\Sigma_{\mathscr{C}_p=q}$ is defined as a sum over $s_2,\ldots,s_p$ with a condition,

$$\sum_{\mathscr{C}_p=q}=\sum_{\substack{s_2,\cdots,s_p\geqslant 0\\ s_2+2s_3+\cdots+(p-1)s_p=q}}. \tag{2.10}$$

Note that the operators $L_i^{s_i}$ and $L_j^{s_j}$, $i\neq j$, do not commute, so the ordering is important.

In Eq. (2.9) s_n can take on only the values of 0 and 1. Together with the fact that $L_n z_k=g_k^{(n)}(z)$, this allows us to transform Eq. (2.9) into a recursion relation for $a_{rk}^{(n)}$:

$$a_{rk}^{(2)}=b_{rk}^{(2)}, \tag{2.11a}$$

$$a_{rk}^{(n)}=b_{rk}^{(n)}-\frac{\partial_z^r}{r!}\sum_{\mathscr{C}_{n-1}=n-1}\frac{L_2^{s_2}\cdots L_{n-1}^{s_{n-1}}}{s_2!\cdots s_{n-1}!}z_k;\quad n\geqslant 3, \tag{2.11b}$$

where $\partial_z^r/r!\overset{\text{def}}{=}(\partial_{z_1}^{r_1}\ldots\partial_{z_d}^{r_d})/(r_1!\ldots r_d!)$. (By the definition of coefficients a and b the condition $|r|=n$ holds.)

Before proceeding further we pause to note that even if $\mathscr{D}$ is finite [that is $P(z)$ is convergent over a finite domain], we should not expect, in general, that the coefficients $a_{rk}^{(n)}$ are bounded by an exponentially growing function of n (and hence that we will be able to ascertain the convergence of $\mathscr{M}_n z$ $n\to\infty$, as discussed in the Introduction). For simplicity we set $d=1$, in which case the indices r and k can be omitted, and note that the sums $\Sigma_{\mathscr{C}_{n-1}=n-1}$ in Eq. (2.11b) always contain the term $s_2=s_{n-1}=1$, $s_i=0$, $3\leqslant i\leqslant n-2$, for which

$$\frac{1}{n!}\frac{d^n}{dz^n}a^{(2)}z^2\frac{d}{dz}a^{(n-1)}z^{n-1}\frac{d}{dz}z=(n-1)a^{(2)}a^{(n-1)}. \tag{2.12}$$

If no other terms were present on the right side of Eq. (2.11b), this, of course, would lead to the factorial growth of $a^{(n)}$ with n. Barring a detailed cancellation of terms in the sums

$\Sigma_{\mathscr{C}_{n-1}=n-1}$, which is to be considered exceptional since none of the coefficients $a^{(2)}$ through $a^{(n-1)}$ were chosen to ensure such a cancellation, we see that one should not expect that $a^{(n)}$ as $n\to\infty$ is bounded by an exponentially growing function of n.

III. A RECURSION RELATION FOR NORMS

With the definition

$$\beta_n=\max_j\left(\sum_{|r|=n}|b_{rj}^{(n)}|\right), \tag{3.1}$$

Eq. (2.11b) yields

$$\begin{aligned}\alpha_n&=\max_k\sum_{|r|=n}\left|b_{rk}^{(n)}-\frac{\partial_z^r}{r!}\sum_{\mathscr{C}_{n-1}=n-1}\frac{L_2^{s_2}\ldots L_{n-1}^{s_{n-1}}}{s_2!\ldots s_{n-1}!}z_k\right|\\&\leqslant\beta_n+\max_k\sum_{|r|=n}\left|\sum_{\mathscr{C}_{n-1}=n-1}\frac{\partial_z^r}{r!}\frac{L_2^{s_2}\ldots L_{n-1}^{s_{n-1}}}{s_2!\ldots s_{n-1}!}\right|\\&\leqslant\beta_n+\sum_{\mathscr{C}_{n-1}=n-1}\frac{1}{s_2!\ldots s_{n-1}!}\max_k\sum_{|r|=n}\left|\frac{\partial_z^r}{r!}L_2^{s_2}\cdots L_{n-1}^{s_{n-1}}z_k\right|.\end{aligned} \tag{3.2}$$

Note that the component of the vector on the right side is determined by the component of z and is labeled here by k. Our goal is to express the right side of the last inequality in (3.2) in terms of $\alpha_2,\ldots,\alpha_{n-1}$. We accomplish this through two lemmas. (The second one will also be used in Sec. V.)

Consider a vector function F whose components are homogeneous polynomials of order $l\geqslant 0$,

$$F_k^{(l)}(z)=\sum_{|i|=l}f_{ik}^{(l)}z^i;\quad 1\leqslant k\leqslant d, \tag{3.3}$$

and for which

$$\max_k\left(\sum_{|i|=l}|f_{ik}^{(l)}|\right)\leqslant\phi_l \tag{3.4}$$

for some $\phi_l\in\mathbb{R}^+$. Define the quantities c, m, and B by

$$\sum_{|t|=m(\phi_l x^l,s_2,\ldots,s_n)}c_{tk}(F,s_2,\ldots,s_n)z^t=L_2^{s_2}\cdots L_n^{s_n}F_k^{(l)}(z), \tag{3.5a}$$

$$B(\phi_l x^l,s_2,\ldots,s_n)x^{m(\phi_l x^l,s_2,\ldots,s_n)}=\left(x^2\alpha_2\frac{d}{dx}\right)^{s_2}\cdots\left(x^n\alpha_n\frac{d}{dx}\right)^{s_n}\phi_l x^l. \tag{3.5b}$$

Here use is made of the obvious fact that the power of x in (3.5b) is the same as the power of z in (3.5a). Evidently $B(\phi_l x^l,s_2,\ldots,s_n)$ is a non-negative real quantity and $m(\phi_l x^l,s_2,\ldots,s_n)$ is a non-negative integer. The arguments of c, m, and B have been chosen to be rather explicit, so that the notation is sufficiently general for the manipulations that follow. When referring to a power of only one vector field, on the other hand, we denote the summation index by s, dropping the subscript, and replace the argument $\phi_l x^l$ of m and B by l. The following holds:

Lemma 3.1: For integers $s,l\geqslant 0$,

$$\max_k\left(\sum_{|t|=m(l,s)}|c_{tk}(F,s)|\right)\leqslant B(l,s) \tag{3.6}$$

and

$$\|L_n^s F^{(l)}(z)\|\leqslant B(l,s)x^{m(l,s)}. \tag{3.7}$$

This lemma is given in Refs. 9 and 10, though its proof is only outlined there. In the Appendix we provide a more complete proof (which extends the relations derived in Appendix A of Ref. 7).

The product of operators of the form $L_i^{s_i}$ can now be bounded by the lemma below.

Lemma 3.2: For $n\geqslant 2$ and all functions F of the form (3.3), $l\geqslant 0$,

$$\max_k\sum_{|t|=m(\phi_l x^l,s_2,\ldots,s_n)}|c_{tk}(F,s_2,\ldots,s_n)|\leqslant B(\phi_l x^l,s_2,\ldots,s_n) \tag{3.8}$$

and

$$\|L_2^{s_2}\cdots L_n^{s_n}F^{(l)}(z)\|\leqslant B(\phi_l x^l,s_2,\ldots,s_n)x^{m(\phi_l x^l,s_2,\ldots,s_n)}. \tag{3.9}$$

Proof is by induction on n and is straightforward. For $n=2$ inequalities (3.8) and (3.9) hold by Lemma 3.1, inequalities (3.6) and (3.7). Assume now (3.8) and (3.9) hold for a fixed n and all functions F of the form (3.3). Then

$$\|L_2^{s_2}\cdots L_n^{s_n}L_{n+1}^{s_{n+1}}F^{(l)}(z)\|=\|L_2^{s_2}\cdots L_n^{s_n}\tilde{F}^{(l')}(z)\|, \tag{3.10}$$

where

$$\tilde{F}_k^{(l')}(z)=\sum_{|t|=l'}c_{tk}(F,s_{n+1})z^t \tag{3.11}$$

with $l'=ns_{n+1}+l$ and, by Lemma 3.1,

$$\max_k\sum_{|t|=l'}|c_{tk}(F,s_{n+1})|\leqslant B(\phi_l x^l,s_{n+1}). \tag{3.12}$$

Use of the induction assumption yields

$$\max_k\sum_{|t|=m(B(\phi_l x^l,s_{n+1})x^{l'},s_2,\ldots,s_n)}|c_{tk}(\tilde{F},s_2,\ldots,s_n)|\leqslant B(B(\phi_l x^l,s_{n+1})x^{l'},s_2,\ldots,s_n) \tag{3.13}$$

and

$$\|L_2^{s_2}\cdots L_n^{s_n}\tilde{F}^{(l')}(z)\|\leqslant B(B(\phi_l x^l,s_{n+1})x^{l'},s_2,\ldots,s_n)x^{m(B(\phi_l x^l,s_{n+1})x^{l'},s_2,\ldots,s_n)}. \tag{3.14}$$

By unfolding the definitions of m and B we obtain

$$
\begin{aligned}
&B(B(\phi_l x^l, s_{n+1})x^{l'}, s_2, \ldots, s_n) x^{m(B(\phi_l x^l, s_{n+1})x^{l'}, s_2, \ldots, s_n)} \\
&\quad = \left(x^2 \alpha_2 \frac{d}{dx} \right)^{s_2} \cdots \left(x^n \alpha_n \frac{d}{dx} \right)^{s_n} B(\phi_l x^l, s_{n+1}) x^{l'} \\
&\quad = \left(x^2 \alpha_2 \frac{d}{dx} \right)^{s_2} \cdots \left(x^n \alpha_n \frac{d}{dx} \right)^{s_n} \left(x^{n+1} \alpha_{n+1} \frac{d}{dx} \right)^{s_{n+1}} \phi_l x^l \\
&\quad = B(\phi_l x^l, s_2, \ldots, s_n, s_{n+1}) x^{m(\phi_l x^l, s_2, \ldots, s_n, s_{n+1})}, \qquad (3.15)
\end{aligned}
$$

and so replace $B(B(\phi_l x^l, s_{n+1})x^{l'}, s_2, \ldots, s_n)$ by $B(\phi_l x^l, s_2, \ldots, s_n, s_{n+1})$ and $m(B(\phi_l x^l, s_{n+1})x^{l'}, s_2, \ldots, s_n)$ by $m(\phi_l x^l, s_2, \ldots, s_n, s_{n+1})$ in inequalities (3.13) and (3.14). With the further replacement of $c_{tk}(\tilde{F}, s_2, \ldots, s_n)$ by $c_{tk}(F, s_2, \ldots, s_n, s_{n+1})$, the proof is complete. □

We can now make progress with inequality (3.2). Since

$$
\max_k \sum_{|r|=n} \left| \frac{\partial_z^r}{r!} L_2^{s_2} \cdots L_{n-1}^{s_{n-1}} z_k \right| = \max_k \sum_{|r|=n} |c_{rk}(z, s_2, \ldots, s_{n-1})|, \qquad (3.16)
$$

use of inequality (3.8) yields

$$
\alpha_n \leqslant \beta_n + \sum_{\mathscr{C}_{n-1}=n-1} \frac{1}{s_2! \cdots s_{n-1}!} B(x, s_2, \ldots, s_{n-1}). \qquad (3.17)
$$

Note that the apparent dependence of the right side of (3.2) on z (or $\|z\|$) has disappeared, as it should.

The final step is to obtain an explicit expression for $B(x, s_2, \ldots, s_{n-1})$, which requires the evaluation of the right side of Eq. (3.5b) for $l=1$, $\phi_l=1$. First we note that

$$
\left(x^n \frac{d}{dx} \right)^s x^p = \frac{(n-1)^s \Gamma\left(\frac{s(n-1)+p}{n-1} \right)}{\Gamma\left(\frac{p}{n-1} \right)} x^{p+s(n-1)}, \qquad (3.18)
$$

where we take, as it is sufficient for our purposes, n, s, and p to be integers, with $n \geqslant 2$, $s \geqslant 0$, and $p \geqslant 1$. The relation (3.18) is easily proven by induction on s. Repeated use of (3.18) on the right side of Eq. (3.5b) then leads to

$$
\begin{aligned}
B(x, s_2, \ldots, s_{n-1}) = \alpha_2^{s_2} (2\alpha_3)^{s_3} \cdots ((n-2)\alpha_{n-1})^{s_{n-1}} \frac{\Gamma\left(\frac{1+s_{n-1}(n-2)}{n-2} \right)}{\Gamma\left(\frac{1}{n-2} \right)} \\
\times \frac{\Gamma\left(\frac{1+s_{n-1}(n-2)+s_{n-2}(n-3)}{n-3} \right)}{\Gamma\left(\frac{1+s_{n-1}(n-2)}{n-3} \right)} \cdots \frac{\Gamma\left(\frac{1+s_{n-1}(n-2)+\cdots+s_2}{1} \right)}{\Gamma\left(\frac{1+s_{n-1}(n-2)+\cdots+2s_3}{1} \right)}, \qquad (3.19)
\end{aligned}
$$

which is the desired, though admittedly cumbersome, expression for B.

With the definitions $\eta_n = n\alpha_{n+1}$, $\tau_n = n\beta_{n+1}$,

$$Q_m = 1, \quad m = n-1,$$

$$Q_m = 1 + \sum_{j=1}^{n-m-1} (n-j)s_{n-j+1}, \quad 1 \leqslant m \leqslant n-2, \tag{3.20a}$$

and

$$\mathscr{G}(s_2,\ldots,s_n) = \prod_{m=1}^{n-1} \frac{\Gamma\left(s_{m+1} + \frac{Q_m}{m}\right)}{s_{m+1}!\,\Gamma\left(\frac{Q_m}{m}\right)}, \tag{3.20b}$$

inequality (3.17) and Eq. (2.11a) become

$$\eta_1 = \tau_1, \tag{3.21a}$$

$$\eta_n \leqslant \tau_n + n \sum_{\mathscr{C}_n = n} \eta_1^{s_2} \cdots \eta_{n-1}^{s_n} \mathscr{G}(s_2,\ldots,s_n), \quad n \geqslant 2. \tag{3.21b}$$

In Sec. IV we will use these relations to get an estimate for η_n. We call attention to the interesting fact that the relations (3.21), and hence the results that follow, do not depend explicitly on d. The dimensionality of the space enters only through the definition of quantities η_n and τ_n.

IV. BOUND FOR η_n

From inequality (3.21b) we get the following bound on η_n:

Theorem 4.1: Let

$$K_n = \max_{1 \leqslant j \leqslant n} \left[\frac{\tau_j}{j^j (j-1)!} \right]^{1/j}, \quad n \geqslant 1. \tag{4.1}$$

Then

$$\eta_n \leqslant (K_n n)^n n!. \tag{4.2}$$

Proof: First we manipulate the ratios of Γ functions that appear in $\mathscr{G}$. For $1 \leqslant m \leqslant n-1$ and $s_{m+1} \geqslant 1$,

$$\frac{\Gamma\left(s_{m+1} + \frac{Q_m}{m}\right)}{\Gamma\left(\frac{Q_m}{m}\right)} = \left(s_{m+1} - 1 + \frac{Q_m}{m}\right)\left(s_{m+1} - 2 + \frac{Q_m}{m}\right) \cdots \frac{Q_m}{m} \leqslant \left(s_{m+1} - 1 + \frac{Q_m}{m}\right)^{s_{m+1}}$$

$$= \frac{1}{m^{s_{m+1}}} [m(s_{m+1}-1) + Q_m]^{s_{m+1}} \leqslant \frac{1}{m^{s_{m+1}}} (n+1-m)^{s_{m+1}}. \tag{4.3}$$

The last inequality makes use of $m s_{m+1} + Q_m \leqslant n+1$, which follows from the condition on the sums over s. The last line in Eq. (4.3) is also a valid estimate when $s_{m+1} = 0$. Hence,

$$\mathscr{G}(s_2,\ldots,s_n) \leqslant \frac{n^{s_2}(n-1)^{s_3} \cdots 2^{s_n}}{s_2! \cdots s_n!\, 1^{s_2} 2^{s_3} \cdots (n-1)^{s_n}}, \tag{4.4}$$

and inequality (3.21b) becomes

$$\eta_n \leqslant \tau_n + n \sum_{\mathscr{C}_n = n} \frac{(n\eta_1)^{s_2}[(n-1)\eta_2]^{s_3}\cdots(2\eta_{n-1})^{s_n}}{s_2!\cdots s_n! 1^{s_2}\cdots(n-1)^{s_n}}. \tag{4.5}$$

Before proceeding further we establish two inequalities. The first one is given by

$$m^m(1+n-m) \leqslant n^m, \quad n \geqslant 2, \quad 1 \leqslant m \leqslant n-1. \tag{4.6}$$

Its validity can be seen directly from the binomial expansion

$$n^m = (m+(n-m))^m \geqslant m^m + m^m(n-m) = m^m(1+n-m). \tag{4.7}$$

The other one is given by the following statement:

Propositions 4.2: When $n \geqslant 2$ and the condition $\mathscr{C}_n = n$ is satisfied,

$$1!^{s_2}2!^{s_3}\cdots(n-1)!^{s_n} \leqslant (n-1)!. \tag{4.8}$$

To prove this statement note that $\mathscr{C}_n = n$ requires that there exist at least one term $(k-1)s_k \geqslant 1$, $2 \leqslant k \leqslant n$. Then define $n_{(k)} = n-(k-1)s_k$, and consider three cases: $n_{(k)} \geqslant 2$, $n_{(k)} = 1$, and $n_{(k)} = 0$.

(i) $n_{(k)} \geqslant 2$:

$$\begin{aligned}
(n-1)! &= (n_{(k)} + (k-1)s_k - 1)! \\
&= (n_{(k)} + (k-1)s_k - 1)(n_{(k)} + (k-1)s_k - 2)\cdots((k-1)s_k + 1)!((k-1)s_k)! \\
&\geqslant n_{(k)}(n_{(k)}-1)\cdots 2((k-1)s_k)! \\
&= n_{(k)}!((k-1)s_k)! \\
&\geqslant s_2!(2s_3)!\cdots((k-2)s_{k-1})!(ks_{k+1})!\cdots((n-1)s_n)!((k-1)s_k)! \\
&\geqslant 1!^{s_2}2!^{s_3}\cdots(k-2)!^{s_{k-1}}(k-1)!^{s_k}k!^{s_{k+1}}\cdots(n-1)!^{s_n},
\end{aligned} \tag{4.9}$$

which is (4.8).

(ii) When $n_{(k)} = 1$ we must have $k = n$ and $s_2 = s_n = 1$, $s_i = 0$, $3 \leqslant i \leqslant n-1$, so the result is immediate.

(iii) $n_{(k)} = 0$ implies $(k-1)s_k = n$. As the case $k = 2$ is trivial, we consider only $(k-1) \geqslant 2$, $s_k \geqslant 2$. Then,

$$\begin{aligned}
(n-1)! &= ((k-1)s_k - 1)! \\
&= \frac{((k-1)s_k)!}{(k-1)s_k} \\
&= \frac{((k-1)(s_k-1)+(k-1))!}{(k-1)s_k} \\
&\geqslant ((k-1)(s_k-1))!(k-1)! \geqslant (k-1)!^{s_k-1}(k-1)! = (k-1)!^{s_k},
\end{aligned} \tag{4.10}$$

which is (4.8). The first inequality uses the relation $\binom{p+q}{p} \geqslant p+q$ when $p,q \geqslant 2$. This completes the proof of Proposition 4.2. □

The relation (4.2) can now be proven by induction. For $n = 1$ we have

$$\eta_1 = \tau_1 = K_1, \tag{4.11}$$

as required. Assume now that (4.2) holds through $n-1$. Starting with inequality (4.5) we then obtain

$$\begin{aligned}\eta_n &\leqslant \tau_n + n \sum_{\mathscr{C}_n=n} \prod_{m=1}^{n-1} [(n+1-m)(K_m m)^m m!]^{s_{m+1}} \frac{1}{s_2!\cdots s_n! 1^{s_2}\cdots(n-1)^{s_n}} \\ &\leqslant \tau_n + nK_n^n \sum_{\mathscr{C}_n=n} \prod_{m=1}^{n-1} [(n+1-m)m^m m!]^{s_{m+1}} \frac{1}{s_2!\cdots s_n! 1^{s_2}\cdots(n-1)^{s_n}} \\ &\leqslant \tau_n + nK_n^n \sum_{\mathscr{C}_n=n} n^{s_2+2s_3+\cdots+(n-1)s_n} \prod_{m=1}^{n-1} m!^{s_{m+1}} \frac{1}{s_2!\cdots s_n! 1^{s_2}\cdots(n-1)^{s_n}} \\ &\leqslant \tau_n + (K_n n)^n n! \sum_{\mathscr{C}_n=n} \frac{1}{s_2!\cdots s_n! 1^{s_2}\cdots(n-1)^{s_n}}. \end{aligned} \tag{4.12}$$

For the second inequality we have used $K_n \geqslant K_m$, $1 \leqslant m \leqslant n-1$, for the third one we have used inequality (4.6), and for the fourth one we have used inequality (4.8). In addition, we have repeatedly used the condition on the sum to sum the power of the summand. The remaining sums over s nicely sum to $1-1/n$, as can be demonstrated using Cauchy's identity[11]

$$\sum_{\mathscr{C}_{n+1}=n} \frac{1}{s_2!\cdots s_n! s_{n+1}! 1^{s_2}\cdots(n-1)^{s_n} n^{s_{n+1}}} = 1. \tag{4.13}$$

Substitution of this result into Eq. (4.12) leads to

$$\eta_n \leqslant \tau_n + (K_n n)^n n!(1-1/n) \leqslant (K_n n)^n n!. \tag{4.14}$$

We have used the definition of K_n given by Eq. (4.1). This completes the proof of Theorem 4.1.□

By unfolding various definitions, Theorem 4.1 can be written as

$$\|L_n\| \leqslant (n-2)!(K_{n-1}(n-1))^{n-1}\|z\|^n, \quad n \geqslant 2, \tag{4.15}$$

where K_n is given by

$$K_n = \max_{1\leqslant j\leqslant n} \left[\frac{\max_l(\Sigma_{|r|=j+1}|b_{rl}^{(j+1)}|)}{j^{j-1}(j-1)!} \right]^{1/j}, \quad n \geqslant 1. \tag{4.16}$$

Thus even when $P(z)$ is a convergent series, that is $K_n \leqslant K$ for some $K \in \mathbb{R}^+$, $n \geqslant 1$, the bound on the sequence $\{\|L_n\|\}$ exhibits a factorial-type growth with n over any finite domain containing the origin. Such behavior is typical of asymptotic sequences. Specifically, with $n^n \leqslant n!\ C^n$ for some $C \in \mathbb{R}^+$, Eq. (5.5) below, it follows that $\{\|L_n\|\}$ is a Gevrey sequence of order 2.

V. PRODUCT OF LIE TRANSFORMATIONS AND OPTIMUM TRUNCATION

Having obtained an estimate for $\|L_n\|$, we turn to the product of a *finite* number of Lie transformations. Such a product is well defined on a nonvanishing domain in $\mathbb{C}^d$ as the following result shows.

Theorem 5.1: The quantity $\mathscr{M}_n z$, $n \geqslant 2$, is an analytic function of z in the open ball

$$x < \frac{1}{K_{n-1} n^2 e^{1/4}}. \tag{5.1}$$

Proof: The function $\mathscr{M}_n z$ is given by the power series in z

$$\mathscr{M}_n z_k = \sum_{q=1}^{\infty} \sum_{\mathscr{C}_n = q-1} \frac{L_2^{s_2} \cdots L_n^{s_n}}{s_2! \cdots s_n!} z_k . \tag{5.2}$$

We determine a bound on the domain on which the sum over q is absolutely convergent. Lemma 3.2 and Eq. (3.19) yield

$$\begin{aligned} \left| \sum_{\mathscr{C}_n = q-1} \frac{L_2^{s_2} \cdots L_n^{s_n}}{s_2! \cdots s_n!} z_k \right| &\leqslant \left\| \sum_{\mathscr{C}_n = q-1} \frac{L_2^{s_2} \cdots L_n^{s_n}}{s_2! \cdots s_n!} z_k \right\| \\ &\leqslant \sum_{\mathscr{C}_n = q-1} \frac{\| L_2^{s_2} \cdots L_n^{s_n} z_k \|}{s_2! \cdots s_n!} \leqslant x^q \sum_{\mathscr{C}_n = q-1} \frac{B(x, s_2, \cdots, s_n)}{s_2! \cdots s_n!} \\ &= x^q \sum_{\mathscr{C}_n = q-1} \eta_1^{s_2} \cdots \eta_{n-1}^{s_n} \mathscr{G}(s_2, \ldots, s_n). \end{aligned} \tag{5.3}$$

Before proceeding further we derive two simple inequalities. First we replace the estimate (4.2) by

$$\eta_n \leqslant (K_n n^2)^n, \quad n \geqslant 1. \tag{5.4}$$

Justification follows from the well-known formula

$$n! = \sqrt{2\pi}\, n^{n+1/2} \exp(-n + \theta/(12n)), \quad 0 < \theta < 1. \tag{5.5}$$

Since the expression $\sqrt{2\pi n}\, \exp(-n + 1/(12n))$ is monotonically decreasing with n, and at $n=2$ takes the value 0.50 0163, we get $n! \leqslant n^n$ for $n \geqslant 1$, and the estimate (5.4) from Eq. (4.2).

Second, we establish that for $n \geqslant 2$ and $1 \leqslant m \leqslant n-1$

$$m(n-m+1)^2 \geqslant 4(n-1), \tag{5.6}$$

as can be seen directly:

$$m(n-m+1)^2 - 4(n-1) = (n-m-1)(nm+3m-4-m^2) \geqslant m(n-m-1)^2 \geqslant 0. \tag{5.7}$$

Returning to Eq. (5.3), we simplify the ratio of Γ functions occurring in $\mathscr{G}$. [It is not fruitful to use Eq. (4.3) here because the condition on the sums over s is different.] For $1 \leqslant m \leqslant n-1$ and $s_{m+1} \geqslant 1$ the following holds:

$$\begin{aligned} \frac{\Gamma\left(s_{m+1} + \frac{Q_m}{m}\right)}{\Gamma\left(\frac{Q_m}{m}\right)} &= \left(s_{m+1} - 1 + \frac{Q_m}{m}\right)\left(s_{m+1} - 2 + \frac{Q_m}{m}\right) \cdots \frac{Q_m}{m} \\ &= \frac{1}{m^{s_{m+1}}} (m s_{m+1} - m + Q_m)(m s_{m+1} - 2m + Q_m) \cdots Q_m \\ &\leqslant \frac{1}{m^{s_{m+1}}} (q-m)(q-2m) \cdots (q - s_{m+1} m) \\ &\leqslant \frac{1}{m^{s_{m+1}}} (q-1)(q-2) \cdots (q - s_{m+1}) = \frac{1}{m^{s_{m+1}}} \frac{(q-1)!}{(q-1-s_{m+1})!}. \end{aligned} \tag{5.8}$$

The first inequality relies on the relation $ms_{m+1}+Q_m \leqslant q$. Again, the last line in Eq. (5.8) is also a valid estimate when $s_{m+1}=0$. Using (5.8) and (5.4), the sums over s in Eq. (5.3) become

$$\begin{aligned}
&\sum_{\mathscr{C}_n=q-1} \eta_1^{s_2}\cdots\eta_{n-1}^{s_n}\mathscr{G}(s_2,\ldots,s_n)\\
&\quad\leqslant K_{n-1}^{q-1}\sum_{\mathscr{C}_n=q-1}\frac{(1^2n^2)^{s_2}}{n^{2s_2}}\frac{(2^4(n-1)^2)^{s_3}}{(n-1)^{2s_3}}\cdots\frac{((n-1)^{2(n-1)}2^2)^{s_n}}{2^{2s_n}}\mathscr{G}(s_2,\ldots,s_n)\\
&\quad\leqslant (K_{n-1}n^2)^{q-1}\sum_{\mathscr{C}_n=q-1}\frac{\mathscr{G}(s_2,\ldots,s_n)}{n^{2s_2}(n-1)^{2s_3}\cdots 2^{2s_n}}\\
&\quad\leqslant (K_{n-1}n^2)^{q-1}\sum_{\mathscr{C}_n=q-1}\binom{q-1}{s_2}\frac{1}{n^{2s_2}}\binom{q-1}{s_3}\frac{1}{[2(n-1)^2]^{s_3}}\cdots\binom{q-1}{s_n}\frac{1}{[(n-1)2^2]^{s_n}}\\
&\quad\leqslant (K_{n-1}n^2)^{q-1}\sum_{s_2=0}^{q-1}\cdots\sum_{s_n=0}^{q-1}\binom{q-1}{s_2}\frac{1}{n^{2s_2}}\binom{q-1}{s_3}\frac{1}{[2(n-1)^2]^{s_3}}\cdots\binom{q-1}{s_n}\frac{1}{[(n-1)2^2]^{s_n}}\\
&\quad= (K_{n-1}n^2)^{q-1}\prod_{m=1}^{n-1}\left(1+\frac{1}{m(n-m+1)^2}\right)^{q-1}\\
&\quad\leqslant (K_{n-1}n^2)^{q-1}\left(1+\frac{1}{4(n-1)}\right)^{(n-1)(q-1)} < (K_{n-1}n^2e^{1/4})^{q-1}.
\end{aligned}\tag{5.9}$$

The first inequality follows from Eq. (5.4) and the fact that K_n is nondecreasing with n, the second one from Eq. (4.6), the third one from Eq. (5.8), the fourth one is evident upon an examination of the ranges of indices s_2 through s_n subject to the condition $\mathscr{C}_n=q-1$, the fifth one from Eq. (5.6), and the last one from the relation $(1+1/(4(n-1)))^{4(n-1)}<e$. For the first two inequalities we have used the condition $\mathscr{C}_n=q-1$ to sum the power of the summand.

Use of the result (5.9) in Eq. (5.3) gives

$$\left|\sum_{\mathscr{C}_n=q-1}\frac{L_2^{s_2}\cdots L_n^{s_n}}{s_2!\cdots s_n!}z_k\right| \leqslant \frac{1}{K_{n-1}n^2e^{1/4}}(K_{n-1}xn^2e^{1/4})^q \tag{5.10}$$

and so the sum over q in Eq. (5.2) is absolutely convergent for

$$x<\frac{1}{K_{n-1}n^2e^{1/4}}. \tag{5.11}$$

□

The result stated in Theorem 5.1 is a lower bound on the domain $\mathscr{D}_n$, $n\geqslant 2$, introduced following Eq. (2.5). Even though $\mathscr{M}z$ cannot be expected to be analytic over any finite domain, inequality (5.1) shows that $\mathscr{M}_nz$ is. If $P(z)$ is convergent, $\max_{n\in\mathbb{N}}K_n$ is finite and the bound on $\mathscr{D}_n$ shrinks quadratically with n. For a general asymptotic series, on the other hand, the bound may decrease more rapidly with n, depending on K_n.

Since the estimates on $\mathscr{D}_n$ do not allow the conclusion that $\mathscr{M}_nz$ is convergent as $n\to\infty$ even when $\mathscr{D}$ is finite, we turn to the asymptotic properties of this transformation. Specifically, we examine the question of optimum truncation when $\mathscr{D}$ is finite. The most natural quantity to optimize is the difference between $P(z)$ and $\mathscr{M}_nz$, denoted here by $R(n,z)$:

$$R(n,z)\overset{\text{def}}{=}\|P(z)-e^{L_2}\cdots e^{L_n}z\|. \tag{5.12}$$

The following gives the relevant estimates on $R(n,z)$.

Proposition 5.2: If $\beta_n \leqslant c^{n-1}$ for $n \geqslant 2$ and some $c \in \mathbb{R}^+$, then the remainder $R(n,z)$ is defined in the open ball

$$x < \frac{1}{cn^2 e^{1/4}} \tag{5.13}$$

and satisfies there

$$R(n,z) < x\left[\frac{(cxn^2 C_1)^n}{1-cxn^2 e^{1/4}}\right], \tag{5.14}$$

with $C_1 = e^{1/4} + \frac{1}{4}$.

Proof follows from Theorem 5.1. Using Eqs. (5.3) and (5.9) and the condition on β we have

$$\begin{aligned} R(n,z) &= \|P(z) - e^{L_2}\cdots e^{L_n} z\| \\ &= \left\| \sum_{q=n+1}^{\infty} \sum_{|r|=q} b_{rk}^{(q)} z^r - \sum_{q=n+1}^{\infty} \sum_{\mathscr{C}_n = q-1} \frac{L_2^{s_2}\cdots L_n^{s_n}}{s_2!\cdots s_n!} z_k \right\| \\ &\leqslant \sum_{q=n+1}^{\infty} x^q \beta_q + \sum_{q=n+1}^{\infty} \left\| \sum_{\mathscr{C}_n = q-1} \frac{L_2^{s_2}\cdots L_n^{s_n}}{s_2!\cdots s_n!} z_k \right\| \\ &< \frac{1}{c} \sum_{q=n+1}^{\infty} (cx)^q + \frac{1}{cn^2 e^{1/4}} \sum_{q=n+1}^{\infty} (cxn^2 e^{1/4})^q = x\left[\frac{(cx)^n}{1-cx} + \frac{(cxn^2 e^{1/4})^n}{1-cxn^2 e^{1/4}}\right]. \end{aligned} \tag{5.15}$$

For the second inequality we have replaced K_{n-1} by c, which follows from the conditions on β_n:

$$K_{n-1} = \max_{1 \leqslant j \leqslant n-1} \left[\frac{\beta_{j+1}}{j^{j-1}(j-1)!}\right]^{1/j} \leqslant \max_{1 \leqslant j \leqslant n-1} \left[\frac{c^j}{j^{j-1}(j-1)!}\right]^{1/j} \leqslant c, \quad n \geqslant 2. \tag{5.16}$$

Evidently, the infinite sums over q in Eq. (5.15) are convergent in the open ball given by Eq. (5.13). To obtain the estimate (5.14) one more step is needed:

$$\begin{aligned} R(n,z) &< x\left[\frac{(cx)^n}{1-cx} + \frac{(cxn^2 e^{1/4})^n}{1-cxn^2 e^{1/4}}\right] \\ &< x\,\frac{(cx)^n + (cxn^2 e^{1/4})^n}{1-cxn^2 e^{1/4}} \leqslant x\,\frac{(cx(n^2 e^{1/4}+1))^n}{1-cxn^2 e^{1/4}} \leqslant x\,\frac{(cxn^2(e^{1/4}+\frac{1}{4}))^n}{1-cxn^2 e^{1/4}}. \end{aligned} \tag{5.17}$$

□

We turn to optimum truncation. Since the leading order term in $\mathscr{M}z$ is z, which is of order x, it is useful to divide R by x, so that the resulting quantity R/x can be compared to one. Note also that R/x depends on c and x only through the product cx, which we denote by $\overline{x}$. The question of optimum truncation can now be formulated as follows: given $\overline{x}$, find the value of n, denoted by n_{opt}, where the estimate for R/x reaches its minimum and find the value of the minimum.

Equation (5.14) is too complicated to carry out the required calculations analytically. We thus set

$$\frac{1}{1-\overline{x}\,n^2 e^{1/4}} < C_2 \tag{5.18}$$

for some $C_2 \in \mathbb{R}^+$. We do not yet specify the value of C_2. It should, however, satisfy the following two requirements: first, that it be as small as possible, so as to keep the value of the estimate at $n = n_{\text{opt}}$ as small as possible; and second, that it be sufficiently large so that inequality (5.18) is satisfied at $n = n_{\text{opt}}$ (and hence for all $n \leqslant n_{\text{opt}}$). We then look for the minimum of the expression $C_2(\overline{x}n^2 C_1)^n$. Considering n as real and differentiating with respect to it, the minimum is easily found at $\tilde{n} = (1/e)(1/\sqrt{\overline{x}C_1})$, so that we can take

$$n_{\text{opt}} = \text{int}\left[\frac{1}{e}\,\frac{1}{\sqrt{\overline{x}C_1}}\right], \tag{5.19}$$

where int$[\cdot]$ stands for the integer part. Note that for a given value of $\overline{x}$, n_{opt} is never larger than the value of n for which the given $\overline{x}$ could be outside of the domain of analyticity of $R(u,z)$, cf. Eq. (5.13). To obtain an explicit estimate for $R(n_{\text{opt}},z)/x$ we evaluate $C_2(\overline{x}n^2 C_1)^n$ at $n = \tilde{n} - 1$. The result is an exponentially small bound for the remainder:

$$\frac{R(n_{\text{opt}},z)}{x} < C_2 e^2 \exp\left(-\frac{2}{e\sqrt{\overline{x}C_1}}\right). \tag{5.20}$$

Since $\tilde{n} \geqslant n_{\text{opt}}$, the constant C_2 can be determined by substituting the expression for $\tilde{n}$ into Eq. (5.18), which yields

$$C_2 > \frac{C_1 e^2}{C_1 e^2 - e^{1/4}} = 1.12\ 7751\ldots\ . \tag{5.21}$$

The proximity of this limit to 1 indicates that both the value of n_{opt} and the estimate for $R(n_{\text{opt}},z)/x$ are determined primarily by the leading term in Eq. (5.14), $(\overline{x}n^2 C_1)^n$.

VI. SUMMARY

An upper bound on the norm of vector fields L_n which are computed by requiring that $\mathscr{M}z$ agrees order by order with a given asymptotic power series is given in Theorem 4.1, Eqs. (4.15) and (4.16). A lower bound on the domain of analyticity of $\mathscr{M}_n z$ is given in Theorem 5.1, Eq. (5.1).

Even when $\mathscr{D}$ is finite, the estimate for η_n grows with order more rapidly than an exponential function and the estimate for $\mathscr{D}_n$ goes to zero as $n \to \infty$. We remarked that one can expect these statements to hold true even in the exact computation of $\mathscr{M}_n z$. The estimates derived can be used to optimize the bound for the difference between $\mathscr{M}_n z$ and $P(z)$ as a function of n for a given value of $\|z\|$. The result is an exponentially small bound for the remainder, given in Eq. (5.20). It seems well worthwhile to explore next whether the procedure developed in the preceding sections can be adapted to Hamiltonian normal form calculations and used to strengthen the estimates of the type given in Ref. 6 for the norm of generating polynomials and the remainders. One can also examine the bound that the present results place on the norms of the vector fields in the transformation $\mathscr{M}$, when $\mathscr{M}$ is computed from a single Lie transformation specified by a vector field analytic at the origin (a version of the Zassenhaus formula). Good estimates for the power series derived from the action of the given Lie transformation on a point z are necessary to study this question. (Provided that the analytic vector field is multiplied by a sufficiently small parameter, such a power series is convergent, as given by standard theorems on ordinary differential equations.)

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APPENDIX: PROOF OF LEMMA 3.1

We first prove the relation (3.6) by induction on s. For $s=0$, $m(l,0)=l$, $c_{tk}(F,0)=f_{tk}^{(l)}$, and $B(l,0)=\phi_l$. Therefore (3.6) reduces to inequality (3.4). For $s=1$ we have

$$L_n F_k^{(l)}(z)=\sum_{j=1}^{d} g_j^{(n)} \frac{\partial}{\partial z_j} \sum_{|i|=l} f_{ik}^{(l)} z^i=\sum_{j=1}^{d} \sum_{|r|=n} \sum_{|i|=l} a_{rj}^{(n)} f_{ik}^{(l)} i_j z_1^{i_1+r_1}\cdots z_j^{i_j+r_j-1}\cdots z_d^{i_d+r_d}, \tag{A1}$$

which yields

$$\begin{aligned}\max_k\left(\sum_{|t|=m(l,1)} |c_{tk}(F,1)|\right) &\leq \max_k\left(\sum_{j=1}^{d} \sum_{|r|=n} \sum_{|i|=l} |a_{rj}^{(n)}||f_{ik}^{(l)}| i_j\right)\\ &\leq \alpha_n \max_k\left(\sum_{j=1}^{d} \sum_{|i|=l} |f_{ik}^{(l)}| i_j\right)=\alpha_n l \max_k\left(\sum_{|i|=l} |f_{ik}^{(l)}|\right)\leq \alpha_n l \phi_l = B(l,1),\end{aligned} \tag{A2}$$

as needed. Next, assume that (3.6) holds for a fixed s. Then

$$\begin{aligned}L_n^{s+1} F_k^{(l)}(z) &= \sum_{j=1}^{d} g_j^{(n)} \frac{\partial}{\partial z_j} \sum_{|t|=m(l,s)} c_{tk}(F,s) z^t\\ &= \sum_{j=1}^{d} \sum_{|r|=n} \sum_{|t|=m(l,s)} a_{rj}^{(n)} c_{tk}(F,s) t_j z_1^{t_1+r_1}\cdots z_j^{t_j+r_j-1}\cdots z_d^{t_d+r_d},\end{aligned} \tag{A3}$$

and we have

$$\begin{aligned}\max_k\left(\sum_{|t|=m(l,s+1)} |c_{tk}(F,s+1)|\right) &\leq \max_k\left(\sum_{j=1}^{d} \sum_{|r|=n} \sum_{|t|=m(l,s)} |a_{rj}^{(n)}||c_{tk}(F,s)| t_j\right)\\ &\leq \alpha_n \max_k\left(\sum_{j=1}^{d} \sum_{|t|=m(l,s)} |c_{tk}(F,s)| t_j\right)\\ &= \alpha_n m(l,s) \max_k\left(\sum_{|t|=m(l,s)} |c_{tk}(F,s)|\right)\\ &\leq \alpha_n m(l,s) B(l,s)=B(l,s+1).\end{aligned} \tag{A4}$$

The last inequality uses the induction assumption, whereas the last equality follows from the recursion relation satisfied by B. This completes the proof of relation (3.6).

It is now straightforward to establish (3.7). We proceed again by induction on s. For $s=0$ we use inequality (3.4) and the special values of m, c, and B given at the beginning of the Appendix to see that (3.7) holds. For the case $s=1$, on the other hand, we use relations (A1) and (A2) (second inequality) to obtain

$$\|L_n F^{(l)}(z)\| = \left\| \sum_{j=1}^{d} \sum_{|r|=n} \sum_{|i|=l} a_{rj}^{(n)} f_{ik}^{(l)} i_j z_1^{i_1+r_1} \cdots z_j^{i_j+r_j-1} \cdots z_d^{i_d+r_d} \right\|$$

$$\leqslant \max_k \left(\sum_{j=1}^{d} \sum_{|r|=n} \sum_{|i|=l} |a_{rj}^{(n)}||f_{ik}^{(l)}| i_j \right) x^{n+l-1} \leqslant B(l,1) x^{m(l,1)}. \tag{A5}$$

The first inequality is evident from the definition of the norm and for the last relation we have relied on the fact that $m(l,1)=n+l-1$. Assume now that (3.7) holds for a fixed s. With the help of relations (A3) and (A4) (second inequality) we obtain

$$\|L_n^{s+1} F^{(l)}(z)\| = \left\| \sum_{j=1}^{d} \sum_{|r|=n} \sum_{|t|=m(l,s)} a_{rj}^{(n)} c_{tk}(F,s) t_j z_1^{t_1+r_1} \cdots z_j^{t_j+r_j-1} \cdots z_d^{t_d+r_d} \right\|$$

$$\leqslant \max_k \left(\sum_{j=1}^{d} \sum_{|r|=n} \sum_{|t|=m(l,s)} |a_{rj}^{(n)}||c_{tk}(F,s)| t_j \right) x^{m(l,s)+n-1} \leqslant B(l,s+1) x^{m(l,s+1)}. \tag{A6}$$

We have made use of the recursion relation for m, $m(l,s+1)=m(l,s)+n-1$. This completes the proof of inequality (3.7).

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Geometric interpretation of fractal symmetries of a finite linear chain

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The recipe of Weyl has been applied to two crystallographically distinct realizations of a regular orbit of the cyclic group of order N: the linear chain and the n-dimensional toroidal crystal, with n being the number of different prime integers dividing N, and Sylow factors of N being the Born–von Kármán periods. It follows that some fractallike symmetries of the linear chain are isomorphic images of multidimensional inversions, which are purely geometric operators. © *1996 American Institute of Physics.* [S0022-2488(96)00505-6]

I. INTRODUCTION

The structure of a finite linear chain has been studied recently[1–3] using the method of a general recipe of Weyl.[4,5] The linear chain consisting of N nodes constitutes a regular orbit of the cyclic group C_N. This group is the translation group of the chain, and serves as the ''obvious'' symmetry group of the recipe. Then the ''hidden'' symmetry group is Aut C_N, which involves, according to the recipe, all intrinsic properties of the structure of the linear chain. It was argued in Refs. 1 and 2 that the only manifestly geometric operation enclosed within the hidden symmetry group Aut C_N is, for $N>2$, the one-dimensional inversion automorphism τ_{-1}, which reverses the cyclic order of the chain. All other automorphisms τ_r, with r mutually prime with N, are self-similar scalings such that $\tau_r(j)=rj \bmod N$ for each node j of the chain, and admit therefore an interpretation of fractallike symmetries which preserve the structure of the linear chain, but definitely destroy the geometry and ordering of nodes.

In the present paper we aim to extend this investigation of the structure of the finite linear chain by proposing another crystallographic realization of a regular orbit of the obvious symmetry group C_N. In our proposal, the set which constitutes an orbit of the free action of the cyclic group C_N can be viewed as an n-dimensional configuration which forms a toroidal crystal with periodic boundary conditions. The principal axes of this n-dimensional crystal are labelled by elements p of the socle π of N, i.e. of the set of all those prime integers which are divisors of N. The dimension $n=|\pi|$ is equal to the number of elements of the socle π, and the Born–van Kármán period in the pth direction coincides with the order N_p of the maximal Sylow subgroup $C_{N_p} \lhd C_N$.

We admit, therefore, another structural realization of a regular orbit of the cyclic group C_N. Clearly, both realizations, the linear ring and the n-dimensional toroidal crystal, exhibit completely different crystallographic meaning. For example, the coordination number (i.e., the number of nearest neighbors of a node of a crystal) for the linear ring is clearly 2, whereas for the toroidal crystal it is $2n$ [or $2(n-1)$ when $2 \in \pi$ and $N_2=2$]. Nevertheless, there are also some structural similarities between these two realizations which emerge from the hidden symmetry group. In this paper we aim to point out such similarities, by a systematic use of the recipe of Weyl. In practice, it involves an analysis of those one-to-one mappings between these two realizations, which are consistent with the hidden symmetry group Aut C_N. Some results of our analysis are, in fact, finite analogies of the theory of incommensurate phases based on projections from multidimensional crystals.[6,7] The associated mathematics is borrowed from number theory.[8]

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We point out that the multidimensional presentation of a regular orbit of the cyclic group C_N admits much more geometric interpretation for hidden symmetry operations than the case of a linear chain, since each dimension yields a one-dimensional inversion.

The paper is organized as follows. In Sec. II we formulate briefly the main definitions and results for the one-dimensional presentation of the regular orbit of the cyclic group C_N in terms of the recipe of Weyl. Section III is devoted to discussion of geometry and hidden symmetries of the toroidal crystal. In Sec. IV we present transformations between these two presentations, and in Sec. V we provide an example. The conclusions constitute Sec. VI.

II. THE LINEAR CHAIN

Let

$$\widetilde{N} =: \{j | j = 1,2,\ldots,N\} \tag{1}$$

be the set of nodes of the linear chain and

$$C_N = \{\widetilde{N}, + \bmod N\} \tag{2}$$

be the cyclic group of order N, with the additive notation. Within the terminology of the recipe of Weyl,[1–5] the set $\widetilde{N}$ exhibits the obvious symmetry, given by the group C_N. In other words, the set $\widetilde{N}$ is equipped with ordering of the group C_N, that is, with the cyclic order. This ordering is realized by a bijection $\kappa: \widetilde{N} \to C_N$, which is called a map of the group C_N on the set $\widetilde{N}$. In particular, a pramap $\kappa_0: \widetilde{N} \to C_N$ can be chosen by identifying the set $\widetilde{N}$ with the group manifold of C_N, i.e., by putting

$$\kappa_0(j) = j \in C_N, \quad j \in \widetilde{N}. \tag{3}$$

The pramap κ_0 defines canonically the action $P: C_N \times \widetilde{N} \to \widetilde{N}$ of the group C_N on the linear ring $\widetilde{N}$ by

$$P(j) = \kappa_0^{-1} \circ R^{\mathrm{reg}}(j) \circ \kappa_0, \tag{4}$$

where

$$R^{\mathrm{reg}}(j) = \begin{pmatrix} j' \\ (j + j') \bmod N \end{pmatrix}, \quad j' \in \mathbf{C}_N, \tag{5}$$

defines, for $j \in C_N$, the left regular representation $R^{\mathrm{reg}}: C_N \times C_N \to C_N$ of the group C_N acting on itself. Each permutation $P(j), j \in C_N$, realizes the obvious (translational) symmetry of the chain $\widetilde{N}$.

Clearly, the atlas of all maps $\kappa: \widetilde{N} \to C_N$ which are compatible with the action P, i.e., for which the following diagram of sets and bijections

$$\begin{array}{ccc} \widetilde{N} & \xrightarrow{P(j)} & \widetilde{N} \\ \kappa \downarrow & & \downarrow \kappa, \quad j \in \mathbf{C}_N, \\ C_N & \xrightarrow{R^{\mathrm{reg}}(j)} & C_N \end{array} \tag{6}$$

is commutative, is given by

$$\mathrm{Atl}_{\kappa_0}(\widetilde{N}, C_N) = \{\kappa = R'^{\mathrm{reg}}(j) \circ \kappa_0 | j \in C_N\}, \tag{7}$$

where

$$R'^{\mathrm{reg}}(j)=\begin{pmatrix} j' \\ (j'-j) \bmod N \end{pmatrix}, \quad j' \in C_N \tag{8}$$

defines, for $j \in C_N$, the right regular representation R'^{reg} of the group C_N on itself. The map κ differs from κ_0 in that the origin in κ is translated by the element $j \in C_N$.

The hidden symmetry of the recipe of Weyl is given by the group

$$\mathrm{Aut}\ C_N=\{\tau_r | r \in \widetilde{N}, \quad \mathrm{lcd}(r,N)=1\} \tag{9}$$

of all automorphisms

$$\tau_r=\begin{pmatrix} j \\ rj \bmod N \end{pmatrix}, \quad j \in C_N, \tag{10}$$

of the group C_N of obvious symmetry. The symbol $\mathrm{lcd}(r,N)$ in Eq. (9) denotes the largest common divisor of integers r and N. The multiplication in the group $\mathrm{Aut}\ C_N$ is specified by

$$\tau_r \tau_{r'}=\tau_{rr' \bmod N}, \quad r,r' \in \mathrm{Aut}\ C_N \tag{11}$$

(we replace τ_r by r when convenient).

The commutative diagram

$$\begin{array}{ccc} \widetilde{N} & \xrightarrow{Q(r)} & \widetilde{N} \\ \kappa_0 \downarrow & & \downarrow \kappa_0, \quad r \in \mathrm{Aut}\ C_N, \\ C_N & \xrightarrow{\tau_r} & C_N \end{array} \tag{12}$$

defines the action Q:$\mathrm{Aut}\ C_N \times \widetilde{N} \to \widetilde{N}$ of the hidden symmetry group $\mathrm{Aut}\ C_N$ on the chain $\widetilde{N}$. Each permutation $Q(r), r \in \mathrm{Aut}\ C_N$, of nodes of $\widetilde{N}$, realizes one of the ''hidden'' symmetries of the structure of the linear chain. Equations (10) and (12) imply that $Q(r), r \in \mathrm{Aut}\ C_N$, is a fractallike scaling by the factor r, centered at the node $j=N \equiv 0 \bmod N = \kappa_0(N)$.

In general, each modular scaling transformation $\tau_r, r \neq \pm 1$, yields an essential change of the initial cyclic order of the crystal $\widetilde{N}$ in a fractal manner. The only exceptions are elements of the subgroup

$$C_{1h}=\{\tau_1, \tau_{N-1}\} \lhd \mathrm{Aut}\ C_N \tag{13}$$

of all geometric symmetries of the chain. The identity τ_1 preserves the cyclic order, and the inversion $\tau_{N-1}=\tau_{-1}$ changes it into the opposite one. There are no other geometric symmetries in the case of the linear ring.

III. THE TOROIDAL CRYSTAL

We proceed to impose another crystallographic arrangement on a regular orbit of the cyclic group C_N. To this aim, we exploit the arithmetic structure of the integer N. Let

$$\pi =: \{p \in \widetilde{N} | \mathrm{lcd}(p,N)=p, p \text{ prime}\} \tag{14}$$

be the socle of N, i.e., the set of all prime divisors of $N (p>1)$. Then the arithmetic structure of N is given by the unique decomposition

$$N=\prod_{p\in\pi} N_p, \tag{15}$$

where

$$N_p=p^{\alpha_p}, \quad p\in\pi, \tag{16}$$

and α_p are arithmetic exponents. Accordingly, the Sylow decomposition of the obvious symmetry group reads

$$C_N\cong\prod_{p\in\pi}\otimes C_{N_p}=:A, \tag{17}$$

where we introduce a special symbol A for the cyclic group C_N presented in the form (17) of the direct product.

Equation (17) admits an interpretation of the direct product of cyclic groups C_{N_p} as the translation group of a new finite crystalline configuration of nodes in an n-dimensional toroid, with

$$n=|\pi| \tag{18}$$

being the number of elements in the socle π, and each $p\in\pi$ corresponding to one principal direction with the Born–van Kármán period N_p. Thus let

$$\tilde{N}_p=\{j_p=1,2,\ldots,p^{\alpha_p}\}, \quad p\in\pi, \tag{19}$$

be a regular orbit of the Sylow subgroup $C_{N_p}\lhd C_N$, and $\nu_0^p:\tilde{N}_p\to C_{N_p}$ be the pramap which identifies the set $\tilde{N}_p$ with the group C_{N_p} in the same way as in Eq. (3) for $\tilde{N}$ and C_N. Thus the pramap ν_0^p constitutes the ordering of the group C_{N_p} on the set $\tilde{N}_p$, i.e.,

$$\nu_0^p(j_p)=j_p\in C_{N_p}, \quad j_p\in\tilde{N}_p. \tag{20}$$

Moreover, let

$$\tilde{N}^{(n)}=:\prod_{p\in\pi}\times\tilde{N}_p \tag{21}$$

be the Cartesian product of sets $\tilde{N}_p, p\in\pi$, referred hereafter to as the toroidal crystal. The set $\tilde{N}^{(n)}$ is equipped with the ordering of the group A (isomorphic to the cyclic group C_N) by means of the pramap $\nu_0:\tilde{N}^{(n)}\to A$, defined by

$$\nu_0=\prod_{p\in\pi}\times\nu_0^p, \tag{22}$$

in accordance with the Cartesian product structure of $\tilde{N}^{(n)}$. This ordering defines, in fact, an n-dimensional crystallography on the set $\tilde{N}^{(n)}$. We proceed to describe it in some more detail. In the sequel, we associate the groups A and C_N with the regular orbits $\tilde{N}^{(n)}$ and $\tilde{N}$, respectively.

Elements of the Abelian group A can be uniquely presented in a form of ''vectors''

$$\mathbf{j}=(j_{p_1}\cdots j_{p_n}), \quad j_p\in\tilde{N}_p, \quad p\in\pi, \tag{23}$$

with pointwise addition

$$\mathbf{j}^{(1)}+\mathbf{j}^{(2)}=(\cdots(j_p^{(1)}+j_p^{(2)})\text{mod } N_p\cdots), \quad p\in\pi, \tag{24}$$

in the role of group multiplication in A. In particular, the vector

$$\mathbf{0}=:(\cdots N_p\cdots), \quad p\in\pi, \tag{25}$$

is the unit element of A, i.e., the null vector, and

$$-\mathbf{j}=(\cdots(N_p-j_p)\text{mod } N_p\cdots), \quad p\in\pi, \tag{26}$$

is the (additive) inverse of $\mathbf{j}\in A$. We refer herefrom to symbols $\mathbf{j}$ as vectors, and to integers $j_p\in\widetilde{N}_p, p\in\pi$, as to their components.

Let

$$\mathbf{e}_p=:(0\cdots1\cdots0), \quad p\in\pi, \tag{27}$$

be a ''unit'' vector in A, i.e., the vector with null components $(0=N_{p'} \text{ mod } N_{p'})$ for any $p'\in\pi$, $p'\neq p$, and 1 for the pth component. Then each $\mathbf{j}\in A$ can be uniquely presented as

$$\mathbf{j}=\sum_{p\in\pi} j_p\mathbf{e}_p\,. \tag{28}$$

Each set

$$\xi_p=\{\mathbf{j}=j_p\mathbf{e}_p|j_p\in\widetilde{N}_p\}\subset\widetilde{N}^{(n)}, \quad p\in\pi, \tag{29}$$

forms the pth one-dimensional coordinate ''axis,'' referred hereafter to as the pth equator on the torus. It is worthwhile to observe that the ''Cartesian coordinate system'' $\{\xi_p|p\in\pi\}$ on the toroidal crystal $\widetilde{N}^{(n)}$ can be defined globally, i.e., that it suffices to use only one map, e.g., the pramap ν_0, to cover the whole manifold $\widetilde{N}^{(n)}$ consistently with this coordinate system. As a result, the manifold resembles locally the linear structure [cf. Eq. (28)], but globally it exhibits the structure of toroid [cf. Eq. (29)].

One of characteristics of local properties of a crystalline arrangement is the coordination number q, defined as the number of nearest neighbors of a node. In the case of toroidal crystal one has

$$q=\begin{cases}2n-1, & 2\in\pi, N_2=2,\\ 2n, & \text{otherwise.}\end{cases} \tag{30}$$

The case $2\in\pi$, $N_2=2$, is distinguished since the equator ξ_2 consists of two nodes only, and thus each of them has only one neighbor.

The sequence $(\mathbf{e}_p|p\in\pi)$ of unit vectors forms an analogy of the elementary Bravais cell of the toroidal crystal $\widetilde{N}^{(n)}$. Clearly, translations of the group A of this cell reproduce the whole crystal.

The group A (as well as C_N) can be looked at as a ring, with the pointwise addition (24) and multiplication

$$\mathbf{j}^{(1)}\mathbf{j}^{(2)}=(\cdots j_p^{(1)}j_p^{(2)} \text{ mod } N_p\cdots)\in A, \quad \mathbf{j}^{(1)},\mathbf{j}^{(2)}\in A. \tag{31}$$

Accordingly, the group Aut A of hidden symmetry becomes the multiplicative group of the ring A, i.e.,

$$\text{Aut } A=A^*\subset A, \tag{32}$$

and consists of all elements of the form

$$\mathbf{r}=\sum_{p\in\pi} r_p\mathbf{e}_p,\mathrm{lcd}(r_p,N_p)=1. \tag{33}$$

The multiplicative inverse of $\mathbf{r}$ is

$$\mathbf{r}^{-1}=\sum_{p\in\pi} r_p^{(-1)}\mathbf{e}_p,\quad (r_p^{(-1)}r_p)\mathrm{mod}\ N_p=1. \tag{34}$$

In particular the neutral element of $\mathrm{Aut}\,A$ is

$$\mathbf{1}=\sum_{p\in\pi}\mathbf{e}_p. \tag{35}$$

The notation introduced for groups A and $\mathrm{Aut}\,A$ is well adapted to determination of actions $P^{(n)}:A\times\widetilde{N}^{(n)}\to\widetilde{N}^{(n)}$ and $Q^{(n)}:\mathrm{Aut}\,A\times\widetilde{N}^{(n)}\to\widetilde{N}^{(n)}$ of obvious and hidden symmetry group, respectively, on the toroidal crystal $\widetilde{N}^{(n)}$. Using the pramap $\nu_0:\widetilde{N}^{(n)}\to A$, we associate $P^{(n)}$ and $Q^{(n)}$ with the addition and multiplication in the ring A, respectively, so that

$$P^{(n)}(\mathbf{j})=\begin{pmatrix}\mathbf{j}'\\ \mathbf{j}+\mathbf{j}'\end{pmatrix},\quad \mathbf{j}'\in\widetilde{N}^{(n)},\mathbf{j}\in A, \tag{36}$$

and

$$Q^{(n)}(\mathbf{r})=\begin{pmatrix}\mathbf{j}\\ \mathbf{r}\mathbf{j}\end{pmatrix},\quad \mathbf{j}\in\widetilde{N}^{(n)},\mathbf{r}\in\mathrm{Aut}\,A. \tag{37}$$

The action $P^{(n)}$ establishes the ordering of the group A on the set $\widetilde{N}^{(n)}$. Clearly, this action is abstractly isomorphic with $P:C_N\times\widetilde{N}\to\widetilde{N}$ related to the linear chain, but the two realizations, $\widetilde{N}$ and $\widetilde{N}^{(n)}$, are crystallographically different. In particular, the ordering in each equator $\xi_p, p\in\pi$, is nowadays borrowed from the ring $\mathbb{Z}$ of integers, adapted to the value od N_p. Thus, e.g., an integer $l\in\mathbb{Z}$ can have completely different meanings, namely l mod N_p, within each equator $\xi_p, p\in\pi$. It follows that vectors $\mathbf{j}$ and $l\mathbf{j}$ in the toroidal crystal $\widetilde{N}^{(n)}$ can have, in general, different crystallographic directions. Also, the cyclic order in each equator ξ_p is only loosely related to that in the linear chain $\widetilde{N}$.

The action $Q^{(n)}$ realizes the hidden symmetry of the toroidal crystal $\widetilde{N}^{(n)}$. The actual arrangement of nodes admits much more geometric symmetry operations than in the case of the linear chain $\widetilde{N}$. Namely, each automorphism $\mathbf{i}^{(p)}\in\mathrm{Aut}\,A$, defined by its components as

$$i^{(p)}_{p'}=\begin{cases}-1 & \text{for } p'=p,\\ 1 & \text{otherwise,}\end{cases} \tag{38}$$

corresponds to the one-dimensional inversion in the pth direction. It reverses the pth component j_p of each vector $\mathbf{j}\in\widetilde{N}^{(n)}$, leaving other components unchanged, i.e.,

$$\mathbf{i}_p\mathbf{j}=\mathbf{j}-2j_p\mathbf{e}_p,\quad p\in\pi. \tag{39}$$

In the particular case when $2\in\pi$ and $N_2=2$, the automorphism $\mathbf{i}^{(2)}$ becomes identity on $\widetilde{N}^{(n)}$. In all other cases, it is a nontrivial symmetry operation.

All automorphisms $\mathbf{i}^{(p)}$ generate the group

$$E=\langle\mathbf{i}^{(p)}|p\in\pi\rangle\lhd\mathrm{Aut}\,A, \tag{40}$$

which is the group of all geometric automorphisms of the toroidal crystal $\widetilde{N}^{(n)}$. It is an Abelian elementary group

$$E=\{\mathbf{i}^{\{\sigma\}}|\sigma\subset\pi\} \tag{41}$$

with elements labeled by all subsets of the socle π, and multiplication law

$$\mathbf{i}^{\{\sigma\}}\mathbf{i}^{\{\sigma'\}}=\mathbf{i}^{\{(\sigma\cup\sigma')\setminus(\sigma\cap\sigma')\}}. \tag{42}$$

The order of this group is

$$|E|=\begin{cases}2^n & \text{for } 2\notin\pi, \text{ or } N_2>2,\\ 2^{n-1} & \text{for } N_2=2.\end{cases} \tag{43}$$

All other automorphisms $\mathbf{r}\in\mathrm{Aut}\,A$ change the ordering of the toroidal crystal in an essential, fractallike manner.

IV. PROJECTIONS FROM THE TOROIDAL CRYSTAL ONTO THE LINEAR CHAIN

In discussion of our two realizations of a regular orbit of the cyclic group C_N, we have considered, in fact, two essentially different arrangements. The main common feature is that both emerge from the same abstract group and form its regular orbits. Moreover, both realizations borrow—through the pramaps $\kappa_0:\widetilde{N}\to C_N$ and $\nu_0:\widetilde{N}^{(n)}\to A$—the natural order of the ring $\mathbb{Z}$ of integers, but they do it in definitely distinct ways! In the linear chain $\widetilde{N}$ this order is taken globally and yields a cyclic arrangement of the whole set, whereas in the toroidal crystal $\widetilde{N}^{(n)}$ the cyclic arrangement is prepared for each Sylow subgroup C_{N_p}, $p\in\pi$, separately. Thus the same group manifold is associated with two different orderings. In this section we proceed to discuss projections $\mu:\widetilde{N}^{(n)}\to\widetilde{N}$, which are consistent with the orderings imposed on the sets $\widetilde{N}^{(n)}$ and $\widetilde{N}$ by the groups A and C_N, respectively.

We start with the set $\mathrm{Iso}(A,C_N)$ of all isomorphisms $\beta:A\to C_N$ between the groups of obvious symmetry. This set can be looked at as an orbit of the right regular representation $\Xi':\mathrm{Aut}\,A\times\mathrm{Iso}(A,C_N)\to\mathrm{Iso}(A,C_N)$ of the group $\mathrm{Aut}\,A$ of hidden symmetry, in accordance with

$$\Xi(\mathbf{r})=\begin{pmatrix}\beta\\ \beta\circ\mathbf{r}^{(-1)}\end{pmatrix},\quad \beta\in\mathrm{Iso}(A,C_N),\mathbf{r}\in\mathrm{Aut}\,A. \tag{44}$$

The same set constitutes also an orbit of the left regular representation $\Theta:\mathrm{Aut}\,C_N\times\mathrm{Iso}(A,C_N)\to\mathrm{Iso}(A,C_N)$ of the other hidden symmetry group $\mathrm{Aut}\,C_N$, by virtue of

$$\Theta(r)=\begin{pmatrix}\beta\\ r\circ\beta\end{pmatrix},\quad \beta\in\mathrm{Iso}(A,C_N),r\in\mathrm{Aut}\;C_N. \tag{45}$$

Actions Ξ and Θ, together with a ''praisomorphism'' β_0 (which can be chosen arbitrarily), equip the set $\mathrm{Iso}(A,C_N)$ with group maps $\rho:\mathrm{Iso}(A,C_N)\to\mathrm{Aut}\,A$ and $\sigma:\mathrm{Iso}(A,C_N)\to\mathrm{Aut}\,C_N$, respectively, by means of formulas

$$\rho(\beta)=\mathbf{r}\quad\text{for }\beta=\beta_0\circ\mathbf{r}^{-1},\beta\in\mathrm{Iso}(A,C_N), \tag{46}$$

and

$$\sigma(\beta)=r\quad\text{for }\beta=\tau_r\circ\beta_0,\beta\in\mathrm{Iso}(A,C_N). \tag{47}$$

Mutual independence of isomorphic groups A and C_N of obvious symmetry is reflected here in arbitrariness of praisomorphism β_0. Let us choose β_0 in a way which preserves the Cartesian product structure (17) of the group A. Each Sylow subgroup

$$C_{N_p}=\{j_p\mathbf{e}_p|j_p\in\widetilde{N}_p\}\lhd A \tag{48}$$

has a natural embedding (monomorphism) $\eta_p:C_{N_p}\rightarrow C_N$ into C_N, given by

$$\eta_p(j_p\mathbf{e}_p)=j_p\overline{N_p},\quad j_p\in\widetilde{N}_p, \tag{49}$$

where

$$\widetilde{N}_p=N/N_p,\quad p\in\pi, \tag{50}$$

is the divisor of N, complementary to N_p. Clearly, each monomorphism η_p, $p\in\pi$, preserves the cyclic order of the Sylow subgroup C_{N_p}, borrowed from the ring $\mathbb{Z}$ of integers. All these monomorphisms η_p, $p\in\pi$, define uniquely the isomorphism $\beta_0:A\rightarrow C_N$, given by

$$\beta_0(\mathbf{j})=\sum_{p\in\pi} j_p\overline{N_p} \bmod N,\quad \mathbf{j}\in A. \tag{51}$$

This isomorphism preserves the Cartesian product structure of the group A, and cyclic orders for each factor C_{N_p}. It reproduces therefore the crystallography of the toroidal crystal $\widetilde{N}^{(n)}$.

Such a choice of the praisomorphism β_0 is well motivated from the point of view of the arrangement of the toroidal crystal, but, still, it is not canonical from the point of view of the more abstract ring structure of the group $A(\mathrm{End}\,A\cong A)$ and the group $C_N(\mathrm{End}\,C_N\cong C_N)$. It is a well-known fact from number theory that there is a unique ring isomorphism $\beta':A\rightarrow C_N$, which is determined by the condition of preserving the multiplicative unit of the ring, which reads

$$\beta'(\mathbf{1})=1. \tag{52}$$

Now, Eq. (44) implies that there exists such unique automorphism $\boldsymbol{\varepsilon}\in A^*$ that

$$\beta'=\beta_0\circ\boldsymbol{\varepsilon}^{(-1)}, \tag{53}$$

and

$$\sum_{p\in\pi}\varepsilon_p\overline{N_p} \bmod N=1, \tag{54}$$

where ε_p are components of the automorphism $\boldsymbol{\varepsilon}$; in particular we have

$$\mathrm{lcd}(\varepsilon_p,N_p)=1,\quad p\in\pi. \tag{55}$$

The canonical isomorphism β' is thus given explicitly by

$$\beta'(\mathbf{j})=\sum_{p\in\pi} j_p\varepsilon_p\overline{N_p} \bmod N. \tag{56}$$

The rings $\mathrm{End}\,A\cong A$ and $\mathrm{End}\,C_N\cong C_N$ are thus isomorphic, but mutually ''deformed''. The deformation is described in terms of the automorphism $\boldsymbol{\varepsilon}$. It is also worthwhile to notice that the

Bravais cell $(\mathbf{e}_p | p \in \pi)$ of the toroidal crystal $\widetilde{N}^{(n)}$ forms the unique (up to ordering) set of orthogonal idempotents of the ring A, whereas the corresponding set for the ring C_N consists of elements

$$\beta'(\mathbf{e}_p) = \varepsilon_p N_p, \quad p \in \pi. \tag{57}$$

The orthogonality of these idempotents is implied by

$$\varepsilon_p \overline{N_p} \varepsilon'_p \overline{N'_p} = \varepsilon_p \overline{N_p} \delta_{pp'}, \quad p, p' \in \pi, \tag{58}$$

since $\overline{N_p}\overline{N'_p} \bmod N = 0$ for $p \neq p'$, and the normalization is already assured by Eq. (54).

The projection $\mu: \widetilde{N}^{(n)} \to \widetilde{N}$ from the multidimensional toroid $\widetilde{N}^{(n)}$ onto the linear chain $\widetilde{N}$ which is consistent with orderings of groups A and C_N on $\widetilde{N}^{(n)}$ and $\widetilde{N}$, respectively, can now be determined as follows. Let $\nu: \widetilde{N}^{(n)} \to A$ and $\kappa: \widetilde{N} \to C_N$ be maps which impose appropriate orderings, e.g., $\nu \in Atl_{\nu_0}(\widetilde{N}^{(n)}, A)$, $\kappa \in Atl_{\kappa_0}(\widetilde{N}, C_N)$, and let $\beta \in \mathrm{Iso}(A, C_N)$. Then the projection μ, consistent with the triad (ν, κ, β), is uniquely determined by the requirement that the following diagram

$$\begin{array}{ccc} \widetilde{N}^{(n)} & \xrightarrow{\mu} & \widetilde{N} \\ \nu \downarrow & & \downarrow \kappa, \\ A & \xrightarrow{\beta} & C_N \end{array} \tag{59}$$

should be commutative, or, formally, that

$$\mu = \kappa^{-1} \circ \beta \circ \nu. \tag{60}$$

Mappings μ, given by Eq. (60), constitute a finite analogy of incommensurate phases as projections from multidimensional crystals. Let us choose, for simplicity, the natural orderings ν_0 and κ_0, and let $\beta = \beta_0$ be specified by Eq. (51). Then the regularly periodic, finite n-dimensional crystal $\widetilde{N}^{(n)}$ is projected by means of μ onto the one-dimensional crystal $\widetilde{N}$. Clearly, each dimension $p \in \pi$ yields a one-dimensional ''sublattice'' $N_p, 2N_p, \ldots, N_p N_p$ of N_p nodes, with the lattice constant N_p. It is well known ''from the beginning'' that various lattice constants are mutually commensurate, but the common unit is just 1, which can be readily seen small when comparing to $\overline{N_p}$ for N being large enough and having a rich arithmetic structure (14)–(16). Lattice constants N_p, $p \in \pi$, can be seen as ''macroscopically'' incommensurate, just as incommensurate phases really observed in laboratories, which cannot be experimentally distinguished from ''weakly commensurate'' structures, with large sizes of Bravais cells.

The projection determined by the isomorphism β_0 schuffles the sites belonging to different dimensions p, but faithfully reproduces the cyclic order corresponding to each p. The situation changes drastically after replacing β_0 by the canonical isomorphism β', given by Eqs. (56) and (57). Now, due to the modular magnification of the lattice constant N_p by the factor $\varepsilon_p > 1$ [cf. Eq. (57)], the projection μ changes the cyclic order of $\widetilde{N}_p$ in a fractallike manner. For example, nearest neighbors in the toroidal crystal $\widetilde{N}^{(n)}$ become in $\widetilde{N}$ more separated spatially than the neighbors from the ε_p-coordination sphere. Thus, the canonical isomorphism β' involves much more essential structural reconstruction of the toroidal crystal than the noncanonical but geometrically more natural isomorphism β_0.

V. AN EXAMPLE

We demonstrate behavior of hidden symmetries of a toroidal crystal in an example of $N = 36 = 2^2 \circ 3^2$. Our socle is thus $\pi = \{2,3\}$, and the toroidal crystal is two-dimensional, with $N_2 = 4$ and $N_3 = 9$ being the Born–von Kármán periods in the direction $\mathbf{e}_2$ and $\mathbf{e}_3$, respectively. The

4,8	1,8	2,8	3,8
4,7	1,7	2,7	3,7
4,6	1,6	2,6	3,6
4,5	1,5	2,5	3,5
4,4	1,4	2,4	3,4
4,3	1,3	2,3	3,3
4,2	1,2	2,2	3,2
4,1	1,1	2,1	3,1
4,9	1,9	2,9	3,9

a

3,6	4,6	1,6	2,6
3,5	4,5	1,5	2,5
3,4	4,4	1,4	2,4
3,3	4,3	1,3	2,3
3,2	4,2	1,2	2,2
3,1	4,1	1,1	2,1
3,9	4,9	1,9	2,9
3,8	4,8	1,8	2,8
3,7	4,7	1,7	2,7

b

4,8	3,8	2,8	1,8
4,7	3,7	2,7	1,7
4,6	3,6	2,6	1,6
4,5	3,5	2,5	1,5
4,4	3,4	2,4	1,4
4,3	3,3	2,3	1,3
4,2	3,2	2,2	1,2
4,1	3,1	2,1	1,1
4,9	3,9	2,9	1,9

c

4,7	1,7	2,7	3,7
4,5	1,5	2,5	3,5
4,3	1,3	2,3	3,3
4,1	1,1	2,1	3,1
4,8	1,8	2,8	3,8
4,6	1,6	2,6	3,6
4,4	1,4	2,4	3,4
4,2	1,2	2,2	3,2
4,9	1,9	2,9	3,9

d

FIG. 1. Actions $P^{(n)}:A\times\widetilde{N}^{(n)}\to\widetilde{N}^{(n)}$ and $Q^{(n)}:A\times\widetilde{N}^{(n)}\to\widetilde{N}^{(n)}$ of the group A on the toroidal crystal $\widetilde{N}^{(n)}$ for $N=36$: (a) the identity permutation $P^{(n)}(4\mathbf{e}_2+9\mathbf{e}_3)$, (b) the translation $P^{(n)}(\mathbf{e}_2+2\mathbf{e}_3)$, (c) the one-dimensional inversion along the $\mathbf{e}_2$ axis $Q^{(n)}(3\mathbf{e}_2)$, and (d) the fractallike symmetry $Q^{(n)}(2\mathbf{e}_3)$.

hidden symmetry group thus consists of $|\mathrm{Aut}\, C_{36}|=|\mathrm{Aut}\, C_4||\mathrm{Aut}\, C_9|=2\circ 6=12$ elements. Actions $P^{(n)}:A\times\widetilde{N}^{(n)}\to\widetilde{N}^{(n)}$ and $Q^{(n)}:A\times\widetilde{N}^{(n)}\to\widetilde{N}^{(n)}$ are examplified in Fig. 1 by permutations $P^{(n)}(4\mathbf{e}_2+9\mathbf{e}_3)$, $P^{(n)}(\mathbf{e}_2+2\mathbf{e}_3)$, $Q^{(n)}(3\mathbf{e}_2)$, and $Q^{(n)}(2\mathbf{e}_3)$, representing, respectively, the pramap ν_0, the translation $4\mathbf{e}_2+9\mathbf{e}_3$, the one-dimensional inversion along the axis $\mathbf{e}_2$, and the fractallike operation $\mathbf{r}=2\mathbf{e}_3$.

The subgroup E of geometric symmetry is

$$E=\{\mathbf{1},\mathbf{i}_2=3\mathbf{e}_2+\mathbf{e}_3,\mathbf{i}_3=\mathbf{e}_2+8\mathbf{e}_3,\mathbf{i}=\mathbf{i}_2\mathbf{i}_3=3\mathbf{e}_2+8\mathbf{e}_3\}. \tag{61}$$

The projection β_0, which preserves a bit of crystallography of the toroidal crystal, is given in this case by the formula

$$\beta_0(\mathbf{j})=(9j_2+4j_3)\mathrm{mod}\ 36, \tag{62}$$

and presented in Fig. 2(a). We observe that β_0 preserves the cyclic order of each equator of the toroidal crystal (i.e., the sequence 9,18,27,36 and 4,8,12,...,36 along unit vectors $\mathbf{e}_2$ and $\mathbf{e}_3$, respectively), so that the embedding of each factor C_{N_p} in C_{36} consists in rescaling its members by the factor N_p (=9 and 4 for $p=2$ and 3, respectively). However, β_0 ceases to be an isomorphism of hidden symmetry groups! We have $\beta_0(\mathbf{1})=13\neq 1$, so that already a multiplicative unit is deformed. The subgroup $E\lhd\mathrm{Aut}\, A$ of geometric symmetry is mapped under β_0 onto the set $\{\beta_0(\mathbf{1})=13, \beta_0(\mathbf{i}_2)=31, \beta_0(\mathbf{i}_3)=5, \beta_0(\mathbf{i})=23\}$, which is a subset of Aut C_{36}, but it does not form any group. The group C_{36} in its natural order is reproduced from the toroidal crystal when starting from $\mathbf{j}=\mathbf{e}_2+7\mathbf{e}_3=\beta_0^{-1}(1)$ with the step $\Delta\mathbf{j}=\mathbf{e}_2+7\mathbf{e}_3$.

The deformation vector for this case is

$$\boldsymbol{\varepsilon}=\mathbf{e}_2+7\mathbf{e}_3, \tag{63}$$

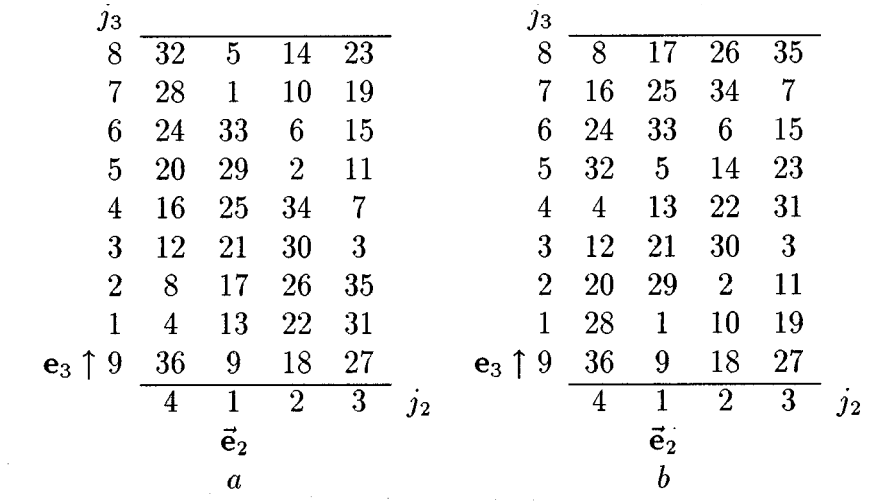

FIG. 2. Projections (a) β_0 and (b) β' of the two-dimensional toroidal crystal onto the linear chain for $N=36$. The number j in the rectangle is the value of $\beta_0(\mathbf{j})$ and $\beta'(\mathbf{j})$ for (a) and (b), respectively. The natural order of the ring Z_{36} is achieved when starting from $j=1$ along the direction $\mathbf{e}_2+7\mathbf{e}_3$ and $\mathbf{e}_2+\mathbf{e}_3$ for β_0 and β', respectively.

and the canonical isomorphism β' is given by the formula

$$\beta'(\mathbf{j})=(9j_2+28j_3)\bmod 36 \tag{64}$$

and shown in Fig. 2(b). Its restriction $\beta'|_{A^*}$ to the hidden symmetry group A^* is also an isomorphism of this group onto $\mathrm{Aut}\, C_{36}$. In particular, $\beta'(\mathbf{1})=1$, and the subgroup E of geometric symmetries of the toroidal crystal is mapped onto the subgroup

$$\{\beta'(\mathbf{1})=1,\beta'(\mathbf{i}_2)=19,\beta'(\mathbf{i}_3)=17,\beta'(\mathbf{i})=35\}\lhd \mathrm{Aut}\; C_{36}. \tag{65}$$

From the other side, however, this projection changes the crystallographic arrangement of nodes of the toroidal crystal: e.g., it preserves the cyclic order for the factor C_4, and reverses it for the factor C_9 [cf. Fig. 2(b)].

VI. FINAL REMARKS AND CONCLUSIONS

We have examined an application of the general recipe of Weyl to a special case of a regular orbit of the cyclic group C_N, by discussion of two realizations of such an orbit: the linear chain and the n-dimensional toroidal crystal, with n being the number of elements of the socle of N. These two realizations differ appreciably by their crystallographic structure, but share the obvious and hidden symmetry groups of the recipe of Weyl. It follows from our discussion that the meaning of hidden symmetry operations changes substantially from one realization to another. In particular, we have demonstrated that fractallike symmetry operations of the linear chain are isomorphic images of purely geometric symmetries of the n-dimensional toroidal crystal. Geometric origin of these n-dimensional inversions is obscured due to the fact that the two realizations are related to different orderings of the obvious symmetry group, within the same group structure. The relation between these two orderings is expressed therefore in terms of a special automorphism $\boldsymbol{\varepsilon}$ belonging to the hidden symmetry group, and describing the deformation of orthogonal idempotents of rings associated with the two crystallographic arrangements.

ACKNOWLEDGMENT

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Submanifolds and quotient manifolds in noncommutative geometry

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We define and study noncommutative generalizations of submanifolds and quotient manifolds using the derivation-based differential calculus introduced by M. Dubois-Violette and P. Michor. We give examples to illustrate these definitions.
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I. INTRODUCTION

Various noncommutative generalizations of differential forms have been proposed as well as generalizations of vector bundles and connections. What is still missing is the concept of a submanifold and of a quotient manifold, that is, how the differential structure of a given algebra must be related to the differential structure of a subalgebra (''quotient manifold'') or a quotient algebra (''submanifold''). In this paper, we propose a definition of a noncommutative submanifold and of a noncommutative quotient manifold within the context of the derivation-based differential calculus first introduced by M. Dubois-Violette,[1] and completed[2,3] with P. Michor.

In the first section, we recall various definitions related to this differential calculus. In the second section, we recall the definition of Hochschild cohomology and other cohomologies which will be used later. Submanifolds and quotient manifolds are defined respectively in Secs. IV and V.

II. NONCOMMUTATIVE DIFFERENTIAL STRUCTURES

In noncommutative geometry, the algebra of smooth functions on a manifold is replaced by a noncommutative algebra (see, for example, Refs. 4 and 5). Geometric objects are first expressed in terms of the algebra of functions and then they can be generalized to the noncommutative case. In this section, we recall the definition of differential forms, central bimodules, and connections as they are given in Refs. 1–3.

A. Noncommutative differential forms

Let $\mathscr{A}$ denote an associative algebra with unit. It is then the generalization of the algebra of smooth functions on a compact manifold. The center of the algebra will be denoted by $\mathscr{Z}(\mathscr{A})$. The differential forms we wish to introduce are based on derivations, the algebraic generalizations of vector fields on a manifold:

$$\mathrm{Der}(\mathscr{A}) = \{X : \mathscr{A} \to \mathscr{A} / X(ab) + X(a)b + aX(b)\};$$

$\mathrm{Der}(\mathscr{A})$ is naturally a $\mathscr{Z}(\mathscr{A})$-module and a Lie algebra.

The two noncommutative generalizations of the graded differential algebra of differential forms which we shall need[1,2] are constructed as follows. Let $C_{\mathscr{Z}(\mathscr{A})}(\mathrm{Der}(\mathscr{A}),\mathscr{A})$ be the graded algebra of antisymmetric $\mathscr{Z}(\mathscr{A})$-multilinear mappings from $\mathrm{Der}(\mathscr{A})$ to $\mathscr{A}$. Notice that this algebra is not graded commutative. In degree 0 we take $C^0_{\mathscr{Z}(\mathscr{A})}(\mathrm{Der}(\mathscr{A}),\mathscr{A}) = \mathscr{A}$. We introduce a differential d by the Koszul formula:

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$$d\omega(X_1,\ldots,X_{n+1})=\sum_{i=1}^{n+1}(-1)^{i+1}X_i\omega(X_1,\ldots,\overset{i}{\overset{V}{\cdot}},\ldots,X_{n+1})$$

$$+\sum_{1\leqslant i<j\leqslant n+1}(-1)^{i+j}\omega([X_i,X_j],\ldots,\overset{i}{\overset{V}{\cdot}},\ldots,\overset{j}{\overset{V}{\cdot}},\ldots,X_{n+1}),$$

for any $\omega\in C^n_{\mathcal{Z}(\mathcal{A})}(\mathrm{Der}(\mathcal{A}),\mathcal{A})$ and any set of derivations X_i.

Now, we can introduce the first generalization of differential forms over $\mathcal{A}$. We define $\Omega_{\mathrm{Der}}(\mathcal{A})$ to be the smallest differential graded subalgebra of the algebra $C_{\mathcal{Z}(\mathcal{A})}(\mathrm{Der}(\mathcal{A}),\mathcal{A})$ which contains $\mathcal{A}$. Every element $\omega\in\Omega^n_{\mathrm{Der}}(\mathcal{A})$ can be written as a finite sum of elements of the type $a_0da_1\cdots da_n$, where $da\in\Omega^1_{\mathrm{Der}}(\mathcal{A})$ is the one-form $X\mapsto Xa\in\mathcal{A}$, and where the product is that of $C_{\mathcal{Z}(\mathcal{A})}(\mathrm{Der}(\mathcal{A}),\mathcal{A})$.

The second differential graded algebra of forms we shall use is the algebra $C_{\mathcal{Z}(\mathcal{A})}(\mathrm{Der}(\mathcal{A}),\mathcal{A})$ itself, denoted by $\underline{\Omega}_{\mathrm{Der}}(\mathcal{A})$. We refer the reader to Ref. 3 for the relation between $\Omega_{\mathrm{Der}}(\mathcal{A})$, $\mathrm{Der}(\mathcal{A})$ and $\underline{\Omega}_{\mathrm{Der}}(\mathcal{A})$ from the point of view of duality.

There is a canonical Cartan operation i_X of the Lie algebra $\mathrm{Der}(\mathcal{A})$ on $\Omega_{\mathrm{Der}}(\mathcal{A})$ and $\underline{\Omega}_{\mathrm{Der}}(\mathcal{A})$.[1] For any $X\in\mathrm{Der}(\mathcal{A})$, one defines the antiderivation of degree -1

$$i_X:\Omega^n_{\mathrm{Der}}(\mathcal{A})\to\Omega^{n-1}_{\mathrm{Der}}(\mathcal{A})$$

by

$$(i_X\omega)(X_1,\ldots,X_{n-1})=\omega(X,X_1,\ldots,X_{n-1}),$$

with $i_Xa=0$ for any $a\in\mathcal{A}=\Omega^0_{\mathrm{Der}}(\mathcal{A})$. It follows that $L_X=i_Xd+di_X$ is a derivation of degree 0 on $\Omega_{\mathrm{Der}}(\mathcal{A})$.

B. Central bimodules and connections

In ordinary differential geometry, vector bundles of finite rank can be considered from an algebraic point of view through their space of sections. In fact this space is a finite projective module over the algebra of smooth functions. In noncommutative geometry, the generalization of a vector bundle will then be such a module over the algebra. However, since $\mathcal{A}$ is noncommutative this can be a right module, or a bimodule.

In Ref. 2 it was proposed that this generalization should at least have the structure of a central bimodule. We recall that a central bimodule $\mathcal{M}$ is a bimodule over $\mathcal{A}$ and which is also a module over the center $\mathcal{Z}(\mathcal{A})$ of $\mathcal{A}$ in the commutative sense. That is, for any $z\in\mathcal{Z}(\mathcal{A})$ and $m\in\mathcal{M}$, one has $zm=mz$.

It is then easy to introduce the notion of a connection on a central bimodule. A connection on $\mathcal{M}$ is a linear mapping $\boldsymbol{\nabla}$ from $\mathrm{Der}(\mathcal{A})$ into the linear endomorphisms of $\mathcal{M}$ such that

$$\boldsymbol{\nabla}_{zX}m=z\boldsymbol{\nabla}_Xm,\quad \boldsymbol{\nabla}_X(amb)=(Xa)mb+a(\boldsymbol{\nabla}_Xm)b+am(Xb)$$

for any $X\in\mathrm{Der}(\mathcal{A})$, $z\in\mathcal{Z}(\mathcal{A})$, $a,b\in\mathcal{A}$, and $m\in\mathcal{M}$.

The curvature of this connection is defined by the usual formula

$$R(X,Y)=\boldsymbol{\nabla}_X\boldsymbol{\nabla}_Y-\boldsymbol{\nabla}_Y\boldsymbol{\nabla}_X-\boldsymbol{\nabla}_{[X,\,Y]}$$

for any $X,Y\in\mathrm{Der}(\mathcal{A})$. Here $R(X,Y)$ is an $\mathcal{A}$-bimodule endomorphism of $\mathcal{M}$, antisymmetric and $\mathcal{Z}(\mathcal{A})$-linear in X,Y. We refer the reader to Ref. 3 for more properties on these connections.

III. HOCHSCHILD COHOMOLOGY AND RELATED COHOMOLOGIES

In this section we introduce a class of subcomplexes of the Hochschild complex of an associative algebra, and their cohomology. These cohomologies, in degree 1, will be useful in the next section.

A. Hochschild cohomology

We recall the definition of the ordinary Hochschild cohomology. Let $\mathscr{A}$ be an associative algebra with unit over $\mathbb{C}$, and $\mathscr{M}$ a bimodule over $\mathscr{A}$.

We define the complex $C(\mathscr{A};\mathscr{M})$ as follows: $C^n(\mathscr{A};\mathscr{M})$ is the linear space of $\mathbb{C}$-linear mappings from $\mathscr{A}^{\otimes^n}$ to $\mathscr{M}$. In degree 0, we set $C^0(\mathscr{A};\mathscr{M})=\mathscr{M}$. We set $C(\mathscr{A};\mathscr{M})=\oplus_{n\geqslant 0}C^n(\mathscr{A};\mathscr{M})$. Then we introduce the Hochschild differential δ on the space $C(\mathscr{A};\mathscr{M})$ by the formula

$$(\delta f)(a_1\otimes\cdots\otimes a_{n+1})=a_1 f(a_2\otimes\cdots\otimes a_{n+1})+\sum_{i=1}^{n}(-1)^i f(a_1\otimes\cdots\otimes a_i a_{i+1}\otimes\cdots\otimes a_{n+1})$$

$$+(-1)^{n+1}f(a_1\otimes\cdots\otimes a_n)a_{n+1}$$

for any $f\in C^n(\mathscr{A};\mathscr{M})$. Because $\mathscr{A}$ is an associative algebra, one has $\delta^2=0$. The cohomology of this differential complex is denoted by $H(\mathscr{A};\mathscr{M})$. It is the Hochschild cohomology of $\mathscr{A}$ with values in $\mathscr{M}$.

The bimodule of interest for our purpose is $\mathscr{A}$ itself. In this case, the complex $C(\mathscr{A};\mathscr{A})$ is an associative algebra (see Refs. 6 and 7 and references therein) and $H(\mathscr{A};\mathscr{A})$ inherits a structure of graded commutative algebra.

Let us consider now the previous case with $n=1$. Then $Z^1(\mathscr{A};\mathscr{A})=\mathrm{Im}\,\delta\cap C^1(\mathscr{A};\mathscr{A})$ is the Lie algebra $\mathrm{Der}(\mathscr{A})$ of derivations of $\mathscr{A}$, and $B^1(\mathscr{A};\mathscr{A})=\mathrm{Ker}\,\delta\cap C^1(\mathscr{A};\mathscr{A})$ is the Lie subalgebra $\mathrm{Int}(\mathscr{A})$ of $\mathrm{Der}(\mathscr{A})$ of inner derivations of $\mathscr{A}$. This is an ideal of $\mathrm{Der}(\mathscr{A})$, so $H^1(\mathscr{A};\mathscr{A})$ is a Lie algebra, denoted $\mathrm{Out}(\mathscr{A})$.

B. Relative Hochschild cohomology

We follow here the exposition in Ref. 6 (see also Ref. 7). Let $\mathscr{S}$ denote a subalgebra of $\mathscr{A}$, and $\mathscr{M}$ a bimodule over $\mathscr{A}$. The complex $C(\mathscr{A},\mathscr{S};\mathscr{M})$ is defined by

$$C^0(\mathscr{A},\mathscr{S};\mathscr{M})=\mathscr{M}^{\mathscr{S}}=\{m\in\mathscr{M}/sm=ms\,\forall\, s\in\mathscr{S}\}$$

and $C^n(\mathscr{A},\mathscr{S};\mathscr{M})$ is the linear space of n-linear mappings $f:\mathscr{A}\otimes\cdots\otimes\mathscr{A}\to\mathscr{M}$ such that

$$f(sa_1\otimes\cdots\otimes a_n)=sf(a_1\otimes\cdots\otimes a_n),\quad f(a_1\otimes\cdots\otimes a_n s)=f(a_1\otimes\cdots\otimes a_n)s,$$

$$f(a_1\otimes\cdots\otimes a_i s\otimes a_{i+1}\otimes\cdots\otimes a_n)=f(a_1\otimes\cdots\otimes a_i\otimes sa_{i+1}\otimes\cdots\otimes a_n)$$

for any $a_i\in\mathscr{A}$ and $s\in\mathscr{S}$. Then f is a $\mathscr{S}$-bimodule homomorphism $\mathscr{A}\otimes_{\mathscr{S}}\cdots\otimes_{\mathscr{S}}\mathscr{A}\to\mathscr{M}$.

The Hochschild differential δ maps $C^n(\mathscr{A},\mathscr{S};\mathscr{M})$ into $C^{n+1}(\mathscr{A},\mathscr{S};\mathscr{M})$, and then defines a cohomology $H(\mathscr{A},\mathscr{S};\mathscr{M})$. This is the relative Hochschild cohomology of $\mathscr{A}$ in $\mathscr{M}$ for $\mathscr{S}$. This cohomology can be calculated on a subcomplex of $C(\mathscr{A},\mathscr{S};\mathscr{M})$.[6] Let us denote by $\overline{C}(\mathscr{A},\mathscr{S};\mathscr{M})$ the linear subspace of $C(\mathscr{A},\mathscr{S};\mathscr{M})$ of elements f such that f vanishes when at least one of its arguments is in $\mathscr{S}$. This is the normalized complex of the relative Hochschild cohomology. These two complexes have the same cohomology.

Let us now consider the case where $\mathscr{S}=\mathscr{Z}(\mathscr{A})$. Then the relative Hochschild cohomology is well adapted to study central bimodules. In degree 0, one has $C^0(\mathscr{A},\mathscr{Z}(\mathscr{A});\mathscr{M})=\mathscr{M}$ for $\mathscr{M}$ a

central bimodule. In higher degrees, one can remark that $\mathcal{A} \otimes_{\mathcal{Z}(\mathcal{A})} \cdots \otimes_{\mathcal{Z}(\mathcal{A})} \mathcal{A}$ is a central bimodule, and then the normalized relative complex is a set of homomorphisms of central bimodules.

For future use, consider the case $\mathcal{S}=\mathcal{Z}(\mathcal{A})$, $\mathcal{M}=\mathcal{A}$, and $n=1$. Then $Z^1(\mathcal{A},\mathcal{Z}(\mathcal{A});\mathcal{A})$ is exactly the Lie algebra of derivations of $\mathcal{A}$ which vanish on the center $\mathcal{Z}(\mathcal{A})$. Remark that $B^1(\mathcal{A},\mathcal{Z}(\mathcal{A});\mathcal{A})$ is equal to $B^1(\mathcal{A};\mathcal{A})$. So, one has the two left exact sequences:

$$0 \to Z^1(\mathcal{A},\mathcal{Z}(\mathcal{A});\mathcal{A}) \to \mathrm{Der}(\mathcal{A}) \to \mathrm{Der}(\mathcal{Z}(\mathcal{A})),$$

$$0 \to H^1(\mathcal{A},\mathcal{Z}(\mathcal{A});\mathcal{A}) \to \mathrm{Out}(\mathcal{A}) \to \mathrm{Der}(\mathcal{Z}(\mathcal{A})),$$

which are not short exact sequences in general. The condition $H^1(\mathcal{A},\mathcal{Z}(\mathcal{A});\mathcal{A})=0$; which means that any derivation of $\mathcal{A}$ which vanishes on $\mathcal{Z}(\mathcal{A})$ is an inner derivation, gives the injectivity of the canonical homomorphism $\mathrm{Out}(\mathcal{A}) \to \mathrm{Der}(\mathcal{Z}(\mathcal{A}))$.

C. Constrained Hochschild cohomology

Let us now introduce a new subcomplex of the Hochschild complex. As before, $\mathcal{A}$ is an associative algebra with unit and $\mathcal{M}$ is a bimodule over $\mathcal{A}$. Let $\mathcal{C}$ be an ideal in $\mathcal{A}$ and $\mathcal{N}$ a sub-bimodule of $\mathcal{M}$ such that $cm, mc \in \mathcal{N}$ for any $c \in \mathcal{C}$ and $m \in \mathcal{M}$. This is equivalent to saying that $\mathcal{C}$ is included in the two side ideal

$$\mathcal{I}_{\mathcal{N}} = \{a \in \mathcal{A} / a\mathcal{M} \subset \mathcal{N} \text{ and } \mathcal{M}a \subset \mathcal{N}\}.$$

We define the subcomplex $C(\mathcal{A},\mathcal{C};\mathcal{M},\mathcal{N})$ of $C(\mathcal{A};\mathcal{M})$ of the mappings $f:\mathcal{A}\otimes\cdots\otimes\mathcal{A} \to \mathcal{M}$ such that $f(a_1\otimes\cdots\otimes a_n) \in \mathcal{N}$ if at least one of the a_i is in $\mathcal{C}$. In degree 0, $C^0(\mathcal{A},\mathcal{C};\mathcal{M},\mathcal{N})=\mathcal{M}$. It is easy to see that this subcomplex is stable by the Hochschild differential δ. So one has a cohomology $H(\mathcal{A},\mathcal{C};\mathcal{M},\mathcal{N})$. This is the constrained cohomology of $\mathcal{A}$ in $\mathcal{M}$ by $(\mathcal{C},\mathcal{N})$. One has then the following lemma:

Lemma III.1: In the above situation, one has a canonical mapping of graded vector spaces

$$H(\mathcal{A},\mathcal{C};\mathcal{M},\mathcal{N}) \to H(\mathcal{A}/\mathcal{C};\mathcal{M}/\mathcal{N}),$$

where the second cohomology is the ordinary Hochschild cohomology of the bimodule $\mathcal{M}/\mathcal{N}$ over the algebra $\mathcal{A}/\mathcal{C}$.

Proof: Let $pr:\mathcal{M} \to \mathcal{M}/\mathcal{N}$ denote the projection from the bimodule $\mathcal{M}$ over $\mathcal{A}$ on the bimodule $\mathcal{M}/\mathcal{N}$ over $\mathcal{A}/\mathcal{C}$, and $a \to [a]$ the projection $\mathcal{A} \to \mathcal{A}/\mathcal{C}$. Then one has $pr(am) = [a]pr(m)$ for any $a \in \mathcal{A}$ and $m \in \mathcal{M}$, and a similar formula for ma.

Any $f \in C(\mathcal{A},\mathcal{C};\mathcal{M},\mathcal{N})$ can be mapped into $\chi(f) \in C(\mathcal{A}/\mathcal{C};\mathcal{M}/\mathcal{N})$ by the definition

$$\chi(f)([a_1]\otimes\cdots\otimes[a_n]) = (pr\circ f)(a_1\otimes\cdots\otimes a_n).$$

Then it is easy to see that

$$pr\circ\delta = \overline{\delta}\circ pr,$$

where δ is the Hochschild differential on $C(\mathcal{A},\mathcal{C};\mathcal{M},\mathcal{N})$ and $\overline{\delta}$ the Hochschild differential on $C(\mathcal{A}/\mathcal{C};\mathcal{M}/\mathcal{N})$. □

A simpler situation occurs when one takes $\mathcal{M}=\mathcal{A}$ and $\mathcal{N}=\mathcal{C}$. Then the subcomplex is a subalgebra of $C(\mathcal{A};\mathcal{A})$, but not an ideal. We denote it by $C_{\mathcal{C}}(\mathcal{A};\mathcal{A})$, and its cohomology by $H_{\mathcal{C}}(\mathcal{A};\mathcal{A})$. In degree 1, one has obviously $B^1_{\mathcal{C}}(\mathcal{A};\mathcal{A}) = B^1(\mathcal{A};\mathcal{A})$. Here $Z^1_{\mathcal{C}}(\mathcal{A};\mathcal{A})$ is the Lie algebra of derivations of $\mathcal{A}$ which preserve $\mathcal{C}$ and $B^1_{\mathcal{C}}(\mathcal{A};\mathcal{A})$ is an ideal in this Lie algebra. Then $H^1_{\mathcal{C}}(\mathcal{A};\mathcal{A})$ is a Lie algebra.

IV. NONCOMMUTATIVE SUBMANIFOLDS

In this section, we introduce a noncommutative generalization of the notion of submanifold of a manifold.

A. The commutative case

We first recall the situation in the commutative case. Let M be a smooth compact manifold, and let $N \subset M$ be a closed submanifold. Any smooth function $f: M \to \mathbb{R}$ can be restricted to N. Thus one has a mapping

$$\mathscr{F}(M) \overset{p}{\to} \mathscr{F}(N),$$

where $\mathscr{F}(M)$ is the algebra of smooth functions on M. This mapping is in fact surjective, and there exists a short exact sequence

$$0 \to \mathscr{C} \to \mathscr{F}(M) \overset{p}{\to} \mathscr{F}(N) \to 0,$$

where $\mathscr{C}$ is the ideal of $\mathscr{F}(M)$ of functions vanishing on N.

A vector field $X \in \Gamma(M)$ on M, which satisfies $Xf \in \mathscr{C}$ for any $f \in \mathscr{C}$, can be restricted to a vector field X on N. Thus one has a homomorphism of Lie algebras

$$\Gamma_{\mathscr{C}}(M) \overset{\pi}{\to} \Gamma(N),$$

where $\Gamma_{\mathscr{C}}(M) = \{X \in \Gamma(M) / X\mathscr{C} \subset \mathscr{C}\}$. This mapping is surjective, and there exists a short exact sequence of Lie algebras:

$$0 \to \Gamma_{\mathscr{F}} \to \Gamma_{\mathscr{C}}(M) \overset{\pi}{\to} \Gamma(N) \to 0,$$

where $\Gamma_{\mathscr{F}} = \{X \in \Gamma(M) / X.\mathscr{F}(M) \subset \mathscr{C}\}$ is an ideal of the Lie algebra $\Gamma_{\mathscr{C}}(M)$.

B. The noncommutative case

Now we can generalize these notions to the framework of noncommutative geometry. Let $\mathscr{A}$ be an associative algebra over $\mathbb{C}$ with unit and let $\mathscr{C}$ be an ideal in $\mathscr{A}$. We denote by $\mathscr{Q} = \mathscr{A}/\mathscr{C}$ the quotient algebra and by $p: \mathscr{A} \to \mathscr{Q}$ the quotient mapping.

We can consider the two following Lie subalgebras of $\mathrm{Der}(\mathscr{A})$:

$$\mathscr{G}_{\mathscr{C}} = \{X \in \mathrm{Der}(\mathscr{A}) / X\mathscr{C} \subset \mathscr{C}\}$$

and

$$\mathscr{G}_{\mathscr{A}} = \{X \in \mathrm{Der}(\mathscr{A}) / X.\mathscr{A} \subset \mathscr{C}\}.$$

One sees that $\mathscr{G}_{\mathscr{A}}$ is an ideal in $\mathscr{G}_{\mathscr{C}}$. One has a mapping $\mathscr{G}_{\mathscr{C}} \overset{\pi}{\to} \mathrm{Der}(\mathscr{Q})$ defined by $\pi(X)p(a) = p(Xa)$ for any $a \in \mathscr{A}$ and $X \in \mathscr{G}_{\mathscr{C}}$. The kernel of this mapping is exactly $\mathscr{G}_{\mathscr{A}}$.

Definition IV.1: The quotient algebra $\mathscr{Q} = \mathscr{A}/\mathscr{C}$ will be called a submanifold algebra of $\mathscr{A}$ if π is surjective. The ideal $\mathscr{C}$ of $\mathscr{A}$ is called the constraint ideal for $\mathscr{Q}$.

In this situation, one has the short exact sequence of Lie algebras

$$0 \to \mathscr{G}_{\mathscr{A}} \to \mathscr{G}_{\mathscr{C}} \overset{\pi}{\to} \mathrm{Der}(\mathscr{Q}) \to 0. \tag{1}$$

The condition of the definition imposes a strong relation between the differential structure on $\mathscr{A}$ and the differential structure on $\mathscr{Q}$. This strong relation is revealed in the following proposition:

Proposition IV.1: There exists a short exact sequence of graded differential algebras

$$0 \to \Omega_{\mathrm{Der},\mathscr{C}} \to \Omega_{\mathrm{Der}}(\mathscr{A}) \xrightarrow{p} \Omega_{\mathrm{Der}}(\mathscr{Q}) \to 0. \tag{2}$$

Proof: Let $\overline{X} = \pi(X) \in \mathrm{Der}(\mathscr{Q})$ for any $X \in \mathscr{G}_{\mathscr{C}}$ and let $\overline{a} = p(a) \in \mathscr{Q}$ for any $a \in \mathscr{A}$. Then one has over $\mathscr{Q}$

$$d\overline{a}(\overline{X}) = \overline{X}\overline{a} = p(Xa) = p(da(X)).$$

One then extends p in a mapping $\Omega^n_{\mathrm{Der}}(\mathscr{A}) \to \Omega^n_{\mathrm{Der}}(\mathscr{Q})$ by the relation

$$p(a_0 da_1 \cdots da_n) = p(a_0) dp(a_1) \cdots dp(a_n),$$

and then one has

$$d \circ p = p \circ d$$

and

$$i_{\overline{X}} \circ p = p \circ i_X .$$

It is easy to see that p is surjective; so we obtain the short exact sequence (2). □

Remark 1: In the short exact sequence (2), one has

$$\Omega^n_{\mathrm{Der},\mathscr{C}} = \{\omega \in \Omega^n_{\mathrm{Der}}(\mathscr{A}) / \forall X \in \mathscr{G}_{\mathscr{C}}, i_X \omega \in \Omega^{n-1}_{\mathrm{Der},\mathscr{C}}\}$$

with $\Omega^0_{\mathrm{Der},\mathscr{C}} = \mathscr{C}$. For example, for any $a \in \mathscr{C}$, $da \in \Omega^1_{\mathrm{Der},\mathscr{C}}$.

Remark 2: In general there are no relations between $\Omega_{\mathrm{Der}}(\mathscr{A})$ and $\Omega_{\mathrm{Der}}(\mathscr{Q})$.

Let us now study the derivations of $\mathscr{Q}$. Any inner derivation of $\mathscr{A}$ is obviously in $\mathscr{G}_{\mathscr{C}}$. In the quotient homomorphism $\mathscr{G}_{\mathscr{C}} \xrightarrow{\pi} \mathrm{Der}(\mathscr{Q})$, these inner derivations are mapped on inner derivations, from the very definition of π. It is easy to see that π restricted to inner derivations is surjective on inner derivations of $\mathscr{Q}$ (even if π does not satisfy the condition of Definition IV.1, i.e., π is not surjective) and one has $\pi(ad(a)) = ad(p(a))$ for any $a \in \mathscr{A}$. So, the kernel of π contains $ad(\mathscr{C}) = \{ad(c) / c \in \mathscr{C}\} \subset \mathrm{Der}(\mathscr{A})$.

Lemma IV.1: If $\mathscr{Q} = \mathscr{A}/\mathscr{C}$ has only inner derivations, then the mapping $\mathscr{G}_{\mathscr{C}} \to \mathrm{Der}(\mathscr{Q})$ is surjective. Then $\mathscr{Q}$ is a submanifold algebra.

Proof: This is a direct consequence of the previous discussion about inner derivations. □

It is now interesting to say something about the other derivations of $\mathscr{Q}$, that is, about the first Hochschild cohomology of $\mathscr{Q}$ with values in itself. One has the following lemma:

Lemma IV.2: One has a surjective homomorphism of Lie algebras

$$H^1_{\mathscr{C}}(\mathscr{A}; \mathscr{A}) \to H^1(\mathscr{Q}; \mathscr{Q}).$$

Proof: This is a direct consequence of Lemma III.1 (with $\mathscr{M} = \mathscr{A}$ and $\mathscr{N} = \mathscr{C}$), the previous remark about inner derivations, and the surjectivity of π from Definition IV.1. □

One can say something about the kernel of this mapping, if one imposes a supplementary condition on the ideal $\mathscr{C}$.

Proposition IV.2: If the constraint ideal $\mathscr{C}$ for the submanifold algebra $\mathscr{Q}$ satisfies

$$ad(\mathscr{C}) = \{ad(a) / a \in \mathscr{A} \text{ and } [a, \mathscr{A}] \subset \mathscr{C}\}.$$

or, equivalently, if $\mathrm{Ker}\pi\cap\mathrm{Int}(\mathscr{A})=ad(\mathscr{C})$, then one has the short exact sequence of Lie algebras

$$0\to H^1(\mathscr{A};\mathscr{C})\to H^1_{\mathscr{C}}(\mathscr{A};\mathscr{A})\to H^1(\mathscr{Q};\mathscr{Q})\to 0. \tag{3}$$

In $H^1(\mathscr{A};\mathscr{C})$, $\mathscr{C}$ is considered as a bimodule over $\mathscr{A}$.

Proof: The condition on $\mathscr{C}$ means, in fact, that one has the short exact sequence of Lie algebras

$$0\to B^1(\mathscr{A};\mathscr{C})\to B^1_{\mathscr{C}}(\mathscr{A};\mathscr{A})=B^1(\mathscr{A};\mathscr{A})\to B^1(\mathscr{Q};\mathscr{Q})\to 0.$$

The new information is the exactness at $B^1_{\mathscr{C}}(\mathscr{A};\mathscr{A})$. If one associates this short exact sequence with the short exact sequence (1) written as

$$0\to Z^1(\mathscr{A};\mathscr{C})\to Z^1_{\mathscr{C}}(\mathscr{A};\mathscr{A})\to Z^1(\mathscr{Q};\mathscr{Q})\to 0,$$

then one obtains the exactness of (3). □

In algebraic geometry (Ref. 8 and references therein), one works with the commutative algebra with unit $\mathscr{A}=\mathbb{C}[X_1,\ldots,X_n]$ of complex polynomials of n variables. The geometric objects are considered as zero sets of polynomials. An ideal $\mathscr{C}$ represents the set of points $V(\mathscr{C})=\{x\in\mathbb{C}^n/P(x)=0\,\forall P\in\mathscr{C}\}$. From the point of view of the ''duality'' *set of points↔algebra of functions*, the set $V(\mathscr{C})$ is represented by the algebra $\mathscr{Q}=\mathbb{C}[X_1,\ldots,X_n]/\mathrm{Rad}(\mathscr{C})$, where $\mathrm{Rad}(\mathscr{C})=\{P\in\mathbb{C}[X_1,\ldots,X_n]/\exists k\in\mathbb{N}\ P^k\in\mathscr{C}\}$ is the radical of $\mathscr{C}$. If $\mathscr{Q}$ admits ideals, then the set $V(\mathscr{C})$ admits subsets. But if $\mathscr{Q}$ does not have any ideal, then the set $V(\mathscr{C})$ can be considered as a *point*. This is equivalent to the fact that $\mathscr{C}$ is a maximal ideal in $\mathscr{A}$. Notice that from the point of view of ordinary geometry, points are the minimal sets. The only maximal ideals of $\mathscr{A}$ are generated by n polynomials X_i-a_i where $a_i\in\mathbb{C}$. The point represented by this ideal is obviously $(a_i)\in\mathbb{C}^n$. Notice that maximal ideals are in one-to-one correspondence with the characters of $\mathscr{A}$. The quotient mapping $\mathscr{A}\to\mathscr{A}/\mathscr{C}$ is the restriction at the set of points represented by $\mathscr{C}$. If $\mathscr{C}$ is maximal, the restriction of an element $P\in\mathscr{A}$ at $\mathscr{C}$ is exactly the value of this polynomial at the point of $\mathbb{C}^n$ represented by $\mathscr{C}$.

This correspondence *points↔maximal ideals* is also used in the theory of commutative Banach algebras and commutative C^*-algebras.[9] In this context, maximal ideals are also in one-to-one correspondence with characters. If $\mathscr{C}$ is a maximal ideal in the commutative Banach algebra with unit $\mathscr{A}$, then the quotient $\mathscr{A}/\mathscr{C}$ is isomorphic to $\mathbb{C}$. (The quotient mapping $\mathscr{A}\to\mathscr{A}/\mathscr{C}$ is a character). In the theory of commutative C^*-algebras, by the Gel'fand transformation, the set of characters is exactly the set of points on which it is possible to put a canonical topology. One says that a point takes its values in the quotient $\mathscr{A}/\mathscr{C}\simeq\mathbb{C}$. So, in those two situations, points are maximal ideals, and take their values in the field $\mathbb{C}$.

In noncommutative geometry, an ideal $\mathscr{C}$ of a given complex algebra with unit $\mathscr{A}$ can also be interpreted as a ''subspace'' of the noncommutative ''space'' dually represented by $\mathscr{A}$. This subspace can be considered as a ''submanifold'' if the differential structure of $\mathscr{A}/\mathscr{C}$ is compatible with the differential structure of $\mathscr{A}$. One of the compatibility conditions one can take is Definition IV.1.

Now, if the ideal is maximal, then the quotient algebra is simple. It is then a ''point,'' in the sense that it cannot have ''proper subspaces.'' However, considering the quotient $\mathscr{Q}=\mathscr{A}/\mathscr{C}$, one sees that points take their values in (*a priori* noncommutative) simple algebras and not in fields as in the commutative case. There is then a residual structure of purely noncommutative origin. See Example 5 below for applications in physics.

To any ideal $\mathscr{C}$ in $\mathscr{A}$, one can construct $\mathscr{G}_{\mathscr{A}}\subset\mathrm{Der}(\mathscr{A})$. If $\mathscr{C}$ is a maximal ideal, the quotient of linear space $T_{\mathscr{C}}=\mathrm{Der}(\mathscr{A})/\mathscr{G}_{\mathscr{A}}$ can be considered as the ''tangent space'' at the point $\mathscr{C}$ in the ''manifold'' represented by $\mathscr{A}$. The value of a derivation X at the ''point'' $\mathscr{C}$ is the image of X by

the quotient mapping $\mathrm{Der}(\mathscr{A})\to T_{\mathscr{C}}$. One can also take the value of a one-form $\alpha\in\Omega^1(\mathscr{A})$ at $\mathscr{C}$ by the definition $\alpha_{\mathscr{C}}:T_{\mathscr{C}}\to\mathscr{Q},\alpha_{\mathscr{C}}(X_{\mathscr{C}})=p\circ\alpha(X)$ for any $X\in\mathrm{Der}(\mathscr{A})$ whose value at $\mathscr{C}$ is $X_{\mathscr{C}}$. This can be generalized for any n-form in $\Omega^n(\mathscr{A})$.

C. Examples

Example 1: The commutative case.

In the commutative case, any smooth closed submanifold of a smooth compact manifold gives a submanifold algebra: the algebra of smooth functions on this submanifold.

Example 2: The tensor algebra.

Let $\mathscr{A}$ be the free algebra with unit over $\mathbb{C}$ generated by n elements $x^1,\ldots,x^n$, with $n\geqslant 2$.

Any derivation of $\mathscr{A}$ is given by n elements $P^i(x^1,\ldots,x^n)\in\mathscr{A}$. We denote it by $D=(P^i)_{1\leqslant i\leqslant n}$. The value of this derivation on any element of $\mathscr{A}$ is obtained by the Leibniz rule and the definition $D(x^i)=P^i(x^1,\ldots,x^n)$.

If one takes $\mathscr{C}$ the ideal in $\mathscr{A}$ generated by x^1, then the algebra $\mathscr{Q}$ is the free algebra with unit over $\mathbb{C}$ generated by $x^2,\ldots,x^n$, and one has $\mathscr{A}=\mathscr{C}\oplus\mathscr{Q}$ as vector spaces.

Any derivation in $\mathscr{G}_{\mathscr{C}}$ is the sum of two kinds of derivation: $(P^i)_{1\leqslant i\leqslant n}$, with $P^i\in\mathscr{Q}$ and $P^1=0$ ($\mathscr{Q}$ is considered here as a subalgebra of $\mathscr{A}$), and $(P^i)_{1\leqslant i\leqslant n}$, with $P^i\in\mathscr{C}$. Any derivation in $\mathscr{G}_{\mathscr{A}}$ is of the second kind, and the Lie algebra of derivation of $\mathscr{Q}$ is the set of the first kind derivations in $\mathscr{G}_{\mathscr{C}}$. So the condition of the Definition IV.1 is fulfilled. Thus $\mathscr{Q}$ is a submanifold algebra of $\mathscr{A}$. In this case, one has $\mathscr{G}_{\mathscr{C}}=\mathscr{G}_{\mathscr{A}}\oplus\mathrm{Der}(\mathscr{Q})$.

As maximal ideals of $\mathscr{A}$, one has the ideals generated by the n elements x^i-a_i, where $a_i\in\mathbb{C}$. Then the point associated to such an ideal is a point in $\mathbb{C}^n$, with values in $\mathbb{C}$. This situation is analogous to the situation of the polynomial algebra generated by the n variables x^i, for which there are only those maximal ideals. It is not difficult to see that such an ideal contains the ideals generated by the expressions $x^ix^j-x^jx^i$. In the case of the tensor algebra $\mathscr{A}$, there are other interesting maximal ideals, as the following examples show.

Example 3: The Heisenberg algebra.

Let $\mathscr{A}$ be the free algebra with unit generated by two elements x,y. Consider in $\mathscr{A}$ the ideal generated by $xy-yx-i\mathbb{1}$. Then the quotient algebra is the Heisenberg algebra $\mathscr{H}$, generated by two elements p,q and the relation $pq-qp=i\mathbb{1}$. It is well known that this algebra is simple. The ideal is maximal. In the quotient, we take $x\mapsto p$ and $y\mapsto q$.

Now let us consider derivations. If we denote by $D=(X,Y)$ the derivation $D(x)=X$ and $D(y)=Y$, then one has

$$\mathscr{G}_{\mathscr{C}}=\{(X,Y)/[X,\,y]+[x,\,Y]\in\mathscr{C}\},$$

where $X,Y\in\mathscr{A}$, and

$$\mathscr{G}_{\mathscr{A}}=\{(X,Y)/X,Y\in\mathscr{C}\}.$$

On the other hand, one knows that $\mathscr{H}$ has only inner derivations (see Ref. 5, for instance), so

$$\mathrm{Der}(\mathscr{H})=\{([A,\,p],[A,\,q])/A\in\mathscr{H}\}$$

with the same notations as above. It is easy to prove that the mapping $\mathscr{G}_{\mathscr{C}}\to\mathrm{Der}(\mathscr{H})$ (the quotient by $\mathscr{G}_{\mathscr{A}}$) is surjective (one can use Lemma IV.1, but the direct calculation shows in this particular case how that works). Indeed, take $A\in\mathscr{H}$ and let $A\in\mathscr{A}$ be such that $A\mapsto A$ in the quotient mapping $\mathscr{A}\to\mathscr{H}$. Then the derivation $([A,\,x],[A,\,y])$ maps to $([A,\,p],[A,\,q])\in\mathrm{Der}(\mathscr{H})$. One must then show that this derivation is indeed in $\mathscr{G}_{\mathscr{C}}$. This is equivalent to showing $[[A,\,x],y]+[x,[A,\,y]]\in\mathscr{C}$. However, this expression equals $-[[x,\,y],\,A]$, which is obviously in the kernel of the mapping $\mathscr{A}\to\mathscr{H}$. So, it is in $\mathscr{C}$.

The Heisenberg algebra is then a submanifold algebra, which can be regarded, from the point of view of algebraic geometry, as a point in the free algebra with unit $\mathscr{A}$. Its tangent space is the linear space $\mathscr{H}\oplus\mathscr{H}$.

Example 4: The matrix algebra.

Let $\mathscr{A}$ denote as above the free algebra with unit generated by two elements x,y. Let $q\in\mathbb{C}$ be an nth unit root, $q^n=1$. Let $\mathscr{C}$ denote the ideal in $\mathscr{A}$ generated by the relations

$$xy-qyx, \quad x^n-\mathbb{1}, \quad y^n-\mathbb{1},$$

and denote by U and V the images of x and y in the quotient mapping $\mathscr{A}\to\mathscr{Q}$. Let us show that this algebra is the matrix algebra $M(n,\mathbb{C})$. Any element of $\mathscr{Q}$ can be written as

$$\sum_{0\leqslant k,l\leqslant n-1} a_{k,l}U^kV^l,$$

so $\dim\mathscr{Q}\leqslant n^2$. Now, the following two matrices in $M(n,\mathbb{C})$,

$$U=\begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & q & 0 & \cdots & 0 \\ 0 & 0 & q^2 & \cdots & 0 \\ \vdots & \vdots & & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & q^{n-1} \end{pmatrix}, \quad V=\begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 & 1 \\ 1 & 0 & \cdots & 0 & 0 \end{pmatrix}$$

satisfy the relations of the algebra $\mathscr{Q}$, and then generate a subalgebra of $M(n,\mathbb{C})$. Because the only matrices which commute with this subalgebra are the multiple of identity, this is the full matrix algebra.

It is well known that the matrix algebra has only inner derivations. By Lemma IV.1, $M(n,\mathbb{C})$ can be considered as a submanifold algebra of the tensor algebra. Notice that this algebra is simple, and so can be considered as a ''point'' in the tensor algebra.

Example 5: The matrix-valued functions.

Consider, as in Ref. 10, the algebra $\mathscr{A}=C^\infty(V)\otimes M(n,\mathbb{C})$ of matrix-valued functions on a manifold V. Let $p\in V$ any point of the manifold. Take $\mathscr{C}$ to be the ideal of functions vanishing at p. This is obviously a maximal ideal. It has been shown in Ref. 10 that $\mathrm{Der}(\mathscr{A})=[\mathrm{Der}(C^\infty(V))\otimes\mathbb{1}]\oplus[C^\infty(V)\otimes\mathrm{Der}(M(n,\mathbb{C}))]$. Then a simple calculation shows that $\mathscr{Q}=\mathscr{A}/\mathscr{C}$ is the matrix algebra $M(n,\mathbb{C})$ and is a submanifold algebra of $\mathscr{A}$. The ''tangent space'' at p is $T_pV\oplus\mathrm{Der}(M(n,\mathbb{C}))$, where T_pV is the ordinary tangent space of V at p.

The physical interpretation of this situation is the following: from the point of view of noncommutative differential geometry, each point of space–time is a matrix, instead of $\mathbb{C}$ (or $\mathbb{R}$) in ordinary differential geometry. The structure looks like a fiber bundle, the fiber being a matrix algebra, but the differential structure is different, because the purely noncommutative differential structure of the matrix algebra (which is far from being trivial) is taken into account at each point of V. This supplementary differential structure of points has important consequences for gauge fields theory, as has been shown in Ref. 10.

This situation can be modified without many changes, by taking the algebra of sections of bundle over M, with fiber $M(n,\mathbb{C})$.

V. NONCOMMUTATIVE QUOTIENT MANIFOLDS

In this section, we introduce a generalization to the noncommutative framework of the notion of quotient manifold. We then introduce the generalization of the action of a group on a manifold which gives a way to construct such quotient manifolds. We give examples and we examine the possible relations with connections on central bimodules.

A. Quotient manifold algebra

Let $\mathscr{A}$ be an associative algebra with unit. Let $\mathscr{B}$ be a subalgebra of $\mathscr{A}$. Then we define the Lie subalgebras of $\mathrm{Der}(\mathscr{A})$:

$$\mathscr{Z}_{\mathrm{Der}}(\mathscr{B})=\{X\in\mathrm{Der}(\mathscr{A})/X.\mathscr{B}=0\}$$

and

$$\mathscr{N}_{\mathrm{Der}}(\mathscr{B})=\{X\in\mathrm{Der}(\mathscr{A})/X.\mathscr{B}\subset\mathscr{B}\}.$$

Notice that $\mathscr{Z}_{\mathrm{Der}}(\mathscr{B})$ is an ideal in $\mathscr{N}_{\mathrm{Der}}(\mathscr{B})$, i.e., $[\mathscr{N}_{\mathrm{Der}}(\mathscr{B}),\mathscr{Z}_{\mathrm{Der}}(\mathscr{B})]\subset\mathscr{Z}_{\mathrm{Der}}(\mathscr{B})$. One can call $\mathscr{Z}_{\mathrm{Der}}(\mathscr{B})$ the centralizer of $\mathscr{B}$ in $\mathrm{Der}(\mathscr{A})$ and $\mathscr{N}_{\mathrm{Der}}(\mathscr{B})$ the normalizer of $\mathscr{B}$ in $\mathrm{Der}(\mathscr{A})$.

One has a natural homomorphism of Lie algebras $\rho:\mathscr{N}_{\mathrm{Der}}(\mathscr{B})\to\mathrm{Der}(\mathscr{B})$, $X\mapsto\widetilde{X}$, the restriction of X to $\mathscr{B}$. The kernel of this homomorphism is exactly $\mathscr{Z}_{\mathrm{Der}}(\mathscr{B})$.

Definition V.1: The subalgebra $\mathscr{B}$ of $\mathscr{A}$ is a quotient manifold algebra of $\mathscr{A}$ if the following three conditions are fulfilled

(i) $\mathscr{Z}(\mathscr{B})=\mathscr{B}\cap\mathscr{Z}(\mathscr{A})$,
(ii) $\mathrm{Der}(\mathscr{B})\simeq\mathscr{N}_{\mathrm{Der}}(\mathscr{B})/\mathscr{Z}_{\mathrm{Der}}(\mathscr{B})$,
(iii) $\mathscr{B}=\{a\in\mathscr{A}/Xa=0\,\forall X\in\mathscr{Z}_{\mathrm{Der}}(\mathscr{B})\}$.

Condition (i) gives to $\mathscr{N}_{\mathrm{Der}}(\mathscr{B})$ and $\mathscr{Z}_{\mathrm{Der}}(\mathscr{B})$ a structure of $\mathscr{Z}(\mathscr{B})$-module. Then $\mathscr{N}_{\mathrm{Der}}(\mathscr{B})/\mathscr{Z}_{\mathrm{Der}}(\mathscr{B})$ is naturally a $\mathscr{Z}(\mathscr{B})$-module, and condition (ii) is an isomorphism of $\mathscr{Z}(\mathscr{B})$-modules. One then has the short exact sequence of Lie algebras and $\mathscr{Z}(\mathscr{B})$-modules

$$0\to\mathscr{Z}_{\mathrm{Der}}(\mathscr{B})\to\mathscr{N}_{\mathrm{Der}}(\mathscr{B})\xrightarrow{\rho}\mathrm{Der}(\mathscr{B})\to 0. \tag{4}$$

Now, the Lie subalgebra $\mathscr{Z}_{\mathrm{Der}}(\mathscr{B})$ of $\mathrm{Der}(\mathscr{A})$ gives a Cartan operation on $\underline{\Omega}_{\mathrm{Der}}(\mathscr{A})$. Condition (iii) says that $\mathscr{B}$ is exactly the basic algebra in $\mathscr{A}$ for this operation.

Let $\omega\in\underline{\Omega}^n_{\mathrm{Der}}(\mathscr{A})$ be a basic element for the operation of $\mathscr{Z}_{\mathrm{Der}}(\mathscr{B})$, $i_X\omega=0$, and $L_X\omega=0$ for any $X\in\mathscr{Z}_{\mathrm{Der}}(\mathscr{B})$. Then $d\omega$ is also basic. One can then define $\widetilde{\omega}\in\underline{\Omega}^n_{\mathrm{Der}}(\mathscr{B})$ by the relation

$$\widetilde{\omega}(\widetilde{X}_1,\ldots,\widetilde{X}_n)=\omega(X_1,\ldots,X_n)$$

for any $\widetilde{X}_1,\ldots,\widetilde{X}_n\in\mathrm{Der}(\mathscr{B})$ and any representatives $X_1,\ldots,X_n\in\mathscr{N}_{\mathrm{Der}}(\mathscr{B})$. By the Koszul formula and condition (iii), it is easy to show that $\omega(X_1,\ldots,X_n)\in\mathscr{B}$ for $X_i\in\mathscr{N}_{\mathrm{Der}}(\mathscr{B})$. Note that condition (ii) is essential to ensure the consistency of this definition. Condition (i) shows that $\widetilde{\omega}$ is $\mathscr{Z}(\mathscr{B})$-linear. The Koszul formula shows then that $d\widetilde{\omega}=\widetilde{d\omega}$.

So one has the following lemma:

Lemma V.1: One has a mapping of graded differential algebras

$$\underline{\Omega}_{\mathrm{Der},B}(\mathscr{A})\to\underline{\Omega}_{\mathrm{Der}}(\mathscr{B}),$$

where $\underline{\Omega}_{\mathrm{Der},B}(\mathscr{A})$ *is the subalgebra of* $\underline{\Omega}_{\mathrm{Der}}(\mathscr{A})$ *of basic elements for* $\mathscr{Z}_{\mathrm{Der}}(\mathscr{B})$.

Remark 1: In degree 0, by the very definition, one has $\underline{\Omega}^0_{\mathrm{Der},B}(\mathscr{A})=\mathscr{B}=\underline{\Omega}^0_{\mathrm{Der}}(\mathscr{B})$.

Remark 2: No canonical mapping can be constructed between the basic elements of $\Omega_{\mathrm{Der}}(\mathscr{A})$ and $\Omega_{\mathrm{Der}}(\mathscr{B})$ without more information on the algebras $\mathscr{A}$ and $\mathscr{B}$.

Remark 3: Condition (ii) can be relaxed if we define $\mathrm{Der}(\mathscr{B})$ to be the Lie algebra $\mathscr{N}_{\mathrm{Der}}(\mathscr{B})/\mathscr{Z}_{\mathrm{Der}}(\mathscr{B})$, even if $\mathscr{B}$ admitted other derivations. In this situation, one has a kind of induced differential structure on $\mathscr{B}$ (see Example 1 below).

Proposition V.1: If the $\mathscr{Z}(\mathscr{A})$-module induced by $\mathscr{N}_{\mathrm{Der}}(\mathscr{B})$ in $\mathrm{Der}(\mathscr{A})$ is $\mathrm{Der}(\mathscr{A})$ itself, then we have an isomorphism of graded differential algebras

$$\underline{\Omega}_{\mathrm{Der},B}(\mathscr{A}) \simeq \underline{\Omega}_{\mathrm{Der}}(\mathscr{B}).$$

Proof: First, let us prove that the mapping $\underline{\Omega}_{\mathrm{Der},B}(\mathscr{A}) \to \underline{\Omega}_{\mathrm{Der}}(\mathscr{B})$ constructed above is injective. If $\tilde{\omega}$ is zero in $\underline{\Omega}^n_{\mathrm{Der}}(\mathscr{B})$, then for any $X_1,\ldots,X_n \in \mathscr{N}_{\mathrm{Der}}(\mathscr{B})$ we have $\omega(X_1,\ldots,X_n)=0$. Now, ω is $\mathscr{Z}(\mathscr{A})$-linear, so ω is zero on the $\mathscr{Z}(\mathscr{A})$-module induced by $\mathscr{N}_{\mathrm{Der}}(\mathscr{B})$ in $\mathrm{Der}(\mathscr{A})$. This proves injectivity.

Let $\tilde{\omega} \in \underline{\Omega}^n_{\mathrm{Der}}(\mathscr{B})$ be any n-form. Define ω as an antisymmetric n-$\mathscr{Z}(\mathscr{B})$-linear mapping from $\mathscr{N}_{\mathrm{Der}}(\mathscr{B}) \otimes_{\mathscr{Z}(\mathscr{B})} \cdots \otimes_{\mathscr{Z}(\mathscr{B})} \mathscr{N}_{\mathrm{Der}}(\mathscr{B})$ to $\mathscr{B}$ by the relation

$$\omega(X_1,\ldots,X_n) = \tilde{\omega}(\tilde{X}_1,\ldots,\tilde{X}_n) \in \mathscr{B} \subset \mathscr{A}$$

for any $X_1,\ldots,X_n \in \mathscr{N}_{\mathrm{Der}}(\mathscr{B})$. Then we extend ω on the $\mathscr{Z}(\mathscr{A})$-module induced by $\mathscr{N}_{\mathrm{Der}}(\mathscr{B})$, by $\mathscr{Z}(\mathscr{A})$ linearity. Notice that ω is already $\mathscr{Z}(\mathscr{B})$ linear. By hypothesis, ω is then an element of $\underline{\Omega}^n_{\mathrm{Der}}(\mathscr{A})$. We have $i_X\omega=0$ for any $X \in \mathscr{Z}_{\mathrm{Der}}(\mathscr{B})$, so ω is horizontal for the action of $\mathscr{Z}_{\mathrm{Der}}(\mathscr{B})$ in $\underline{\Omega}_{\mathrm{Der}}(\mathscr{A})$. Now, notice that the $(n+1)$-form in $\underline{\Omega}_{\mathrm{Der}}(\mathscr{A})$ which comes from $d\tilde{\omega}$ is exactly $d\omega$, because by the Koszul formula they coincide on $\mathscr{N}_{\mathrm{Der}}(\mathscr{B})$. So $d\omega$ is also horizontal, and then ω is basic in $\underline{\Omega}_{\mathrm{Der}}(\mathscr{A})$. This proves surjectivity. □

B. Action

Let M be a manifold and G be a Lie group. An action of G on M gives a Lie algebra homomorphism $\mathfrak{g} \to \Gamma(M)$ from the Lie algebra $\mathfrak{g}$ of G to the Lie algebra of vector fields on M. Then one has a Cartan operation of the Lie algebra $\mathfrak{g}$ on the graded commutative differential algebra $\Omega(M)$ of de Rham differential forms on M.

In the noncommutative case, we will say we have an action of the Lie algebra $\mathfrak{g}$ on an associative algebra with unit $\mathscr{A}$ if there is a homomorphism of Lie algebras $\mathfrak{g} \to \mathrm{Der}(\mathscr{A})$. In this situation one has an operation of $\mathfrak{g}$ on the graded differential algebra $\underline{\Omega}_{\mathrm{Der}}(\mathscr{A})$.

Then one can take as subalgebra of $\mathscr{A}$ the basic algebra for this operation. In this situation, if $\mathscr{B}$ is a quotient manifold algebra, then one has the noncommutative version of the quotient manifold by the ''leaves'' defined by $\mathfrak{g}$.

If the homomorphism $\mathfrak{g} \to \mathrm{Der}(\mathscr{A})$ is injective (take the image of $\mathfrak{g}$ if not), one can identify $\mathfrak{g}$ with its image. Then, one has the inclusion $\mathfrak{g} \subset \mathscr{Z}_{\mathrm{Der}}(\mathscr{B})$, but the equality is not the generic case. Between these two Lie algebras, one has a third one, the $\mathscr{Z}(\mathscr{A})$-module induced by $\mathfrak{g}$ in $\mathrm{Der}(\mathscr{A})$, denoted by $\mathfrak{g}_{\mathscr{Z}(\mathscr{A})}$. If $\mathscr{B}$ is the basic algebra in $\mathscr{A}$ for the operation of $\mathfrak{g}$, the condition (iii) of Definition V.1 is fulfilled.

C. Examples

Example 1: The inner derivations.

Let $\mathscr{A}$ be an associative algebra with unit for which there are inner derivations. Suppose one has $H^1(\mathscr{A},\mathscr{Z}(\mathscr{A});\mathscr{A})=0$. Take the operation of $\mathfrak{g}=\mathrm{Int}(\mathscr{A})$ on $\mathscr{A}$. Then one has $\mathscr{B}=\mathscr{Z}(\mathscr{A})$, $\mathscr{Z}_{\mathrm{Der}}(\mathscr{B})=\mathfrak{g}$ because the first relative cohomology group vanishes, and $\mathscr{N}_{\mathrm{Der}}(\mathscr{B})=\mathrm{Der}(\mathscr{A})$. Take then the induced differential structure on $\mathscr{B}$ by setting $\mathrm{Der}(\mathscr{B})=\mathrm{Out}(\mathscr{A})=\mathscr{N}_{\mathrm{Der}}(\mathscr{B})/\mathfrak{g}$. The algebra of differential forms associated to $\mathscr{B}$ is then, by Proposition V.1, the algebra $\underline{\Omega}_{\mathrm{Out}}(\mathscr{A})$ introduced in Ref. 3.

Example 2: The noncommutative torus.

Let T_q denote the complex associative algebra with unit of elements of the form

$$a=\sum_{k,l\in\mathbb{Z}} c_{kl}U^kV^l$$

with

$$\|a\|_m=\sup_{k,l\in\mathbb{Z}}|c_{kl}|(1+|k|+|l|)^m<\infty$$

and the relation

$$UV=qVU$$

for $q\in\mathbb{C}$ such that $q^N=1$ for $N\in\mathbb{N}$. We take N to be the minimal one for which this is true. The center of this algebra is the set of elements depending only on U^N and V^N.

The derivations of this algebra are the inner derivations and the derivations of the form

$$a(U^N,V^N)D_U+b(U^N,V^N)D_V,$$

where $D_U(U)=U$, $D_U(V)=0$, $D_V(U)=0$ and $D_V(V)=V$, and $a(U^N,V^N)$ and $b(U^N,V^N)$ belong to $\mathcal{Z}(T_q)$.

Take $\mathfrak{g}=\mathrm{Int}(T_q)$. Then $\mathcal{B}=\mathcal{Z}(T_q)$, $\mathcal{Z}_{\mathrm{Der}}(\mathcal{B})=\mathfrak{g}$, and $\mathcal{N}_{\mathrm{Der}}(\mathcal{B})=\mathrm{Der}(T_q)$. We are then in the situation of the previous example. Then the differential algebra of forms on $\mathcal{Z}(T_q)$ is the basic algebra of the differential algebra of forms on T_q. But now, remark that the center $\mathcal{Z}(T_q)$ is isomorphic to the algebra $C^\infty(S^1\times S^1)$ of smooth functions on the (ordinary) torus. This isomorphism is $U^N\mapsto e^{2\pi it}$ and $V^N\mapsto e^{2\pi is}$. Then an element $a\in\mathcal{Z}(T_q)$ is mapped on the Fourier expansion of an element of $C^\infty(S^1\times S^1)$. Thus, the algebra of forms on $\mathcal{Z}(T_q)$ is the de Rham algebra of forms on the torus.

D. Connections

Let $\mathcal{B}$ be a quotient manifold algebra of $\mathcal{A}$. Then $\mathcal{A}$ is a central bimodule over the algebra $\mathcal{B}$. Let $\psi:\mathrm{Der}(\mathcal{B})\to\mathcal{N}_{\mathrm{Der}}(\mathcal{B})$ be a splitting of the short exact sequence (4), considered as a short exact sequence of $\mathcal{Z}(\mathcal{B})$-modules (forgetting the Lie algebra structures).

Proposition V.2: For any $X\in\mathrm{Der}(\mathcal{B})$, the mapping

$$\nabla_X:\mathcal{A}\to\mathcal{A},\quad a\mapsto\psi(X)a,$$

is a connection on the central bimodule $\mathcal{A}$ over $\mathcal{B}$.

The curvature of this connection is the obstruction on ψ to be a splitting of the short exact sequence (4) of Lie algebras.

Proof: This is an immediate consequence of the fact that ψ is a $\mathcal{Z}(\mathcal{B})$-modules homomorphism, such that $\psi(X)b=Xb$ for any $b\in\mathcal{B}\subset\mathcal{A}$. The curvature of this connection is

$$R(X,Y)=[\psi(X),\ \psi(Y)]-\psi([X,\ Y]),$$

which proves the Proposition. □

Such a connection gives a projection $P:\mathcal{N}_{\mathrm{Der}}(\mathcal{B})\to\mathcal{Z}_{\mathrm{Der}}(\mathcal{B})\subset\mathcal{N}_{\mathrm{Der}}(\mathcal{B})$ of $\mathcal{Z}(\mathcal{B})$-modules defined by $P(X)=X-\psi\circ\rho(X)$. Then one has $\mathcal{N}_{\mathrm{Der}}(\mathcal{B})=\mathrm{Ker}\,P\oplus\mathcal{Z}_{\mathrm{Der}}(\mathcal{B})$.

Conversely, a projection $P:\mathcal{N}_{\mathrm{Der}}(\mathcal{B})\to\mathcal{Z}_{\mathrm{Der}}(\mathcal{B})\subset\mathcal{N}_{\mathrm{Der}}(\mathcal{B})$ of $\mathcal{Z}(\mathcal{B})$-modules defines a split, and so a connection on $\mathcal{A}$.

In Ref. 11, one can find another approach to group actions, bundles, and connections in noncommutative differential geometry.

Let $P(M,G)$ be a principal bundle, where M is the base manifold and G is the structure group, and let $\mathfrak{g}$ be its Lie algebra. Denote by $\mathcal{A}$ the (commutative) algebra of smooth functions

on P, and $\mathscr{B}$ the algebra of smooth functions on M. Then one can consider that $\mathscr{B}\subset\mathscr{A}$ because of the projection $P\to M$. The Lie algebra $\mathfrak{g}$ can be injectively mapped into $\Gamma(P)$, the vector fields on P, and, more precisely, into the vertical vector fields. Thus $\mathfrak{g}$ operates on $\mathscr{A}$. The algebra $\mathscr{B}$ is obviously the basic algebra for this operation and $\mathscr{Z}_{\mathrm{Der}}(\mathscr{B})$ is exactly the Lie algebra of vertical vector fields on P.

It is well known that a connection on P can be given as a $\mathscr{B}$-linear mapping $\Gamma(M)\to\Gamma(P), X\mapsto X^h$, the horizontal lift, with its usual properties, one of them being $[\mathfrak{g},X^h]=0$ for all $X\in\Gamma(M)$. In fact this mapping is a splitting of (4) [remember here that $\mathscr{B}=\mathscr{Z}(\mathscr{B})$].

Then one could think that the connections introduced by the construction of Proposition V.2 are generalizations of connections on principal bundles. However, this is not completely true, because a principal bundle has many more properties than a couple $(\mathscr{A},\mathscr{B})$ of an algebra and a quotient manifold algebra. For example, one can introduce associated bundles, on which connections can be transported.

In order to obtain a similar situation, one must introduce a more restrictive definition. Given a couple $(\mathscr{A},\mathscr{B})$ of an algebra and a quotient manifold algebra, suppose there exists a Lie algebra $\mathfrak{g}$ and an injective homomorphism of Lie algebras $\mathfrak{g}\to\mathrm{Der}(\mathscr{A})$ such that $\mathscr{B}$ is the basic algebra for the operation of $\mathfrak{g}$ on $\mathscr{A}$ [then $\mathfrak{g}\subset\mathscr{Z}_{\mathrm{Der}}(\mathscr{B})$]. A connection on this triple $(\mathscr{A},\mathscr{B},\mathfrak{g})$ is a splitting $\psi:\mathrm{Der}(\mathscr{B})\to\mathscr{N}_{\mathrm{Der}}(\mathscr{B})$ of $\mathscr{Z}(\mathscr{B})$-modules compatible with the operation of $\mathfrak{g}$ in the sense $[\mathfrak{g},\psi(X)]=0$ for all $X\in\mathrm{Der}(\mathscr{B})$. Such a connection is also given by a covariant projection $P:\mathscr{N}_{\mathrm{Der}}(\mathscr{B})\to\mathscr{Z}_{\mathrm{Der}}(\mathscr{B})$ where the covariance means $[Y,P(X)]=P([Y,X])$ for all $Y\in\mathfrak{g}$ and $X\in\mathscr{N}_{\mathrm{Der}}(\mathscr{B})$.

In this situation, if V is a linear space on which $\mathfrak{g}$ is represented by $\eta:\mathfrak{g}\to\mathrm{End}(V)$, then one has an associated central bimodule over $\mathscr{B}$ defined by

$$\mathscr{M}_V=\{a_i\otimes v^i\in\mathscr{A}\otimes V/(Ya_i)\otimes v^i+a_i\otimes\eta(Y)v^i=0\,\forall Y\in\mathfrak{g}\},$$

where the structure of bimodule over $\mathscr{B}$ is localized on $\mathscr{A}$.

Proposition V.3: Let $\psi:\mathrm{Der}(\mathscr{B})\to\mathscr{N}_{\mathrm{Der}}(\mathscr{B})$ be a connection on $(\mathscr{A},\mathscr{B},\mathfrak{g})$. Then, the mapping

$$\boldsymbol{\nabla}^V_X:\mathscr{M}_V\to\mathscr{M}_V,\quad a_i\otimes v^i\mapsto(\psi(X)a_i)\otimes v^i,$$

is well defined and is a connection on $\mathscr{M}_V$. This is the associated connection to ψ on $\mathscr{M}_V$.

Proof: $\nabla^V_X\mathscr{M}_V\subset\mathscr{M}_V$ because $[\mathfrak{g},\psi(X)]=0$. Other properties of ∇^V_X are immediate consequences of the definition of ψ as in Proposition V.2. □

In the case of a principal bundle, $\mathscr{M}_V$ is the module over $\mathscr{B}$ of sections of the associated vector bundle for (V,η). This module of sections is considered here as the module of equivariant mapping $P\to V$.

Let us now turn to a different problem. From the point of view of characteristic classes (even if there is not yet such a theory for the definition of connection used here), what is important in a connection is its curvature. Given a couple $(\mathscr{A},\mathscr{B})$ of an algebra and a quotient manifold algebra, suppose one has a central bimodule $\mathscr{M}$ over $\mathscr{A}$ and a connection $\boldsymbol{\nabla}$ on $\mathscr{M}$, such that its curvature is zero if one of its argument is in $\mathscr{Z}_{\mathrm{Der}}(\mathscr{B})$. Then one can transport the connection on a central bimodule over $\mathscr{B}$. Define the reduced central bimodule over $\mathscr{B}$

$$\mathscr{M}^{\mathscr{Z}_{\mathrm{Der}}(\mathscr{B})}=\{m\in\mathscr{M}/\boldsymbol{\nabla}_X m=0\,\forall X\in\mathscr{Z}_{\mathrm{Der}}(\mathscr{B})\}.$$

For any $\widetilde{X}\in\mathrm{Der}(\mathscr{B})$, take any $X\in\mathscr{N}_{\mathrm{Der}}(\mathscr{B})$ such that $\rho(X)=\widetilde{X}$. Then define, for any $m\in\mathscr{M}^{\mathscr{Z}_{\mathrm{Der}}(\mathscr{B})}$,

$$\widetilde{\boldsymbol{\nabla}}_{\widetilde{X}}m=\boldsymbol{\nabla}_X m.$$

Then, because the curvature of $\boldsymbol{\nabla}$ is zero on $\mathscr{Z}_{\mathrm{Der}}(\mathscr{B})$, this is a well-defined mapping from $\mathscr{M}^{\mathscr{Z}_{\mathrm{Der}}(\mathscr{B})}$ into itself. It is easy to verify that $\widetilde{\boldsymbol{\nabla}}$ is a connection, the curvature of which is

$$\widetilde{R}(\widetilde{X},\widetilde{Y})m = R(X,Y)m$$

for any $m \in \mathscr{M}^{\mathscr{Z}_{\mathrm{Der}}(\mathscr{B})}$.

In the case where $\mathrm{Der}(\mathscr{A}) = \mathrm{Int}(\mathscr{A})$, it has been shown in Ref. 3 that any central bimodule $\mathscr{M}$ over $\mathscr{A}$ admits the canonical connection $\nabla_{ad(a)}m = am - ma$. The curvature of this connection is zero.

Now, in the general case $[\mathrm{Der}(\mathscr{A}) \neq \mathrm{Int}(\mathscr{A})]$, if one can take this connection on $\mathrm{Int}(\mathscr{A})$ and a prolongement on $\mathrm{Der}(\mathscr{A})$, then the curvature is zero on $\mathrm{Int}(\mathscr{A})$. So one can hope to transport the connection on a reduced module over $\mathscr{B} = \mathscr{Z}(\mathscr{A})$ while keeping the same information on the curvature.

VI. CONCLUSION

In this paper we have proposed definitions of the noncommutative generalization of a submanifold and of a noncommutative quotient manifold. Various examples and related constructions seem to give them an importance for the study of derivations-based differential structures of algebras. What must be notice is the different use of the two generalizations of differential forms: $\underline{\Omega}_{\mathrm{Der}}(\mathscr{A})$ and $\Omega_{\mathrm{Der}}(\mathscr{A})$. This shows the importance of introducing various generalizations of a commutative concept adapted to different situations.

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The Racah–Wigner algebra and coherent tensors

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We present a set of tensors which are shift tensors (Wigner tensors) in accordance with the definitions of Biedenharn and Louck and satisfy the coherence conditions of Flath and Towber. Our tensors are defined for all connected compact Lie groups and for finite-dimensional representations of connected reductive Lie groups. Thus, we have a realization of the coherent tensors in a rather general setting. Moreover, this realization enables us to confirm most of the conjectures of Flath and Towber concerning the properties of coherent tensors. © *1996 American Institute of Physics.* [S0022-2488(96)03405-9]

I. INTRODUCTION

In the application of group theory in quantum mechanics, one needs to know the representations of Lie groups and their Lie algebras and the ways in which tensor products of representations decompose and recouple. The analysis of tensor coupling and recoupling has been developed to a fine art for SU(2) and is often referred to as the Racah–Wigner calculus.

Some years ago Biedenharn and his colleagues[1] initiated a program to extend the Racah–Wigner calculus to other unitary groups. They focused on the Racah–Wigner algebras of tensors on model spaces and introduced the concept of Wigner operators as the components of shift tensors (also called unit tensors). These tensors have some remarkable properties. As observed by Biedenharn *et al.*, they can be labeled by *operator patterns* in parallel with the Gel'fand patterns used to label basis vectors of an irreducible U(n) representation. Moreover, they form a basis for the Racah–Wigner algebra over the ring of scalar (invariant) operators. Shift tensors have also been used by Hughes[2] and others.

Subsequently, Flath and Towber[3] refined the definition of a shift tensor by introducing the idea of coherence. This enabled them to relate the actions of a tensor on different irreps. It also enabled them to prove a number of theorems for SU(3) and conjecture the general validity of their theorems for other connected compact Lie groups.

In this note, we give a set of tensors which are shift tensors and satisfy the coherence condition of Flath and Towber. They also have the property of being asymptotically orthonormal. Our tensors are given for connected compact Lie groups or the finite-dimensional representations of connected reductive Lie groups. The space spanned by these tensors is uniquely determined by the coherence condition. Thus, we claim to have identified the Biedenharn–Louck–Flath–Towber tensors in a rather general setting. Moreover, with explicit expressions for the coherent tensors, we find that most of Flath and Towber's conjectures concerning their properties follow automatically.

We use the following notations: G is a connected compact semisimple Lie group and $\mathfrak{g}$ is the complex extension of its Lie algebra; Λ is the set of dominant integral weights for G; V^λ is a module for an irrep R^λ of highest weight $\lambda \in \Lambda$. The direct sum $V = \Sigma_{\lambda \in \Lambda} V^\lambda$ is a model space[4] for a universal representation $R = \Sigma_{\lambda \in \Lambda} R^\lambda$, where the latter is a representation which contains every irrep of G once and once only.

If U and W are modules for representations of G, then a $U \to W$ tensor is a G-invariant set of linear $U \to W$ maps. Thus, a tensor T is a module for a representation of G. Basis elements for a tensor are referred to as components of the tensor. An irreducible tensor T^λ is characterized by a

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'highest weight $\lambda \in \Lambda$ and it has components $\{T^{\lambda}_{\alpha\nu}\}$ indexed by a weight ν, relative to a Cartan subalgebra, and a multiplicity index α. An irreducible tensor $T^{\lambda\mu}$ of highest weight λ on a model space V is called a *shift tensor* of shift μ if every component $T^{\lambda\mu}_{\alpha\nu}$ of $T^{\lambda\mu}$ maps any irreducible subspace $V^{\lambda_1} \subset V$ into the irreducible subspace $V^{\lambda_1+\mu} \subset V$.

Biedenharn *et al.*[1] sought a particular set of shift tensors $\{T^{\lambda\beta\mu}\}$ having the property that if $T^{\lambda\beta\mu}(\lambda_1)$ denotes the restriction of $T^{\lambda\beta\mu}$ to the subspace $V^{\lambda_1} \subset V$ then the set of tensors $\{T^{\lambda\beta\mu}(\lambda_1)\}$ (with μ fixed) spans the linear space of $V^1 \to V^{\lambda_1+\mu}$ tensors. We refer to such tensors as Biedenharn–Louck tensors. As Biedenharn[5] has observed, any $V \to V$ tensor can be expressed as a linear combination of Biedenharn–Louck tensors with G-invariant linear operators (tensors of highest weight $\lambda = 0$) as scalar multipliers; we say that such a set of shift tensors is complete.

We first show that a module for the universal representation is spanned, in a coherent state representation, by a subset of generalized Wigner functions. We then give a set of Biedenharn–Louck shift tensors on this space and show that they are coherent according to the definition of Flath and Towber.[3]

II. A COHERENT STATE REPRESENTATION

Let $\{|\psi^{\lambda}_{\alpha\nu}\rangle\}$ be an orthonormal basis for an irreducible subspace V^{λ} of a model space V and let $\{\langle\psi^{\lambda}_{\alpha\nu}|\}$ be the dual basis in Dirac's bra–ket notation. The inner product in this notation is then expressed

$$\langle \psi^{\lambda}_{\alpha\mu} | \psi^{\lambda'}_{\beta\nu} \rangle = \delta_{\lambda\lambda'} \delta_{\alpha\beta} \delta_{\mu\nu}. \tag{1}$$

A generalized Wigner function $\mathscr{D}^{\lambda}_{\beta\mu,\alpha\nu}$ is a $G \to \mathbb{C}$ function with

$$\mathscr{D}^{\lambda}_{\beta\mu,\alpha\nu}(g) = \langle \psi^{\lambda}_{\beta\mu} | R^{\lambda}(g) | \psi^{\lambda}_{\alpha\nu} \rangle. \tag{2}$$

From the Peter–Weyl theorem, one knows that the functions $\{\mathscr{D}^{\lambda}_{\beta\mu,\alpha\nu}\}$ span the Hilbert space $\mathscr{L}^2(G)$ and satisfy the orthogonality relation

$$d(\lambda_1) \int \mathscr{D}^{\lambda_1 *}_{\beta_1\mu_1,\alpha_1\nu_1}(g) \mathscr{D}^{\lambda_2}_{\beta_2\mu_2,\alpha_2\nu_2}(g) dv(g) = \delta_{\lambda_1\lambda_2} \delta_{\beta_1\beta_2} \delta_{\alpha_1\alpha_2} \delta_{\mu_1\mu_2} \delta_{\nu_1\nu_2}, \tag{3}$$

where dv is a suitably normalized invariant measure.

The orthornormal basis states $\{|\psi^{\lambda}_{\alpha\nu}\rangle\}$ have coherent-state wave functions $\{\psi^{\lambda}_{\alpha\nu}\}$ given by

$$\psi^{\lambda}_{\alpha\nu}(g) = \langle \psi^{\lambda}_{\lambda} | R^{\lambda}(g) | \psi^{\lambda}_{\alpha\nu} \rangle = \mathscr{D}^{\lambda}_{\lambda,\alpha\nu}(g), \tag{4}$$

where $|\psi^{\lambda}_{\lambda}\rangle$ is the (multiplicity free) highest weight state in the set $\{|\psi^{\lambda}_{\alpha\nu}\rangle\}$ (cf. Ref. 6 and references therein). Thus, the above coherent state representation is a nonisometric embedding of V in $\mathscr{L}^2(G)$

$$Q: V \to \mathscr{L}^2(G); \quad |\psi^{\lambda}_{\alpha\nu}\rangle \mapsto \psi^{\lambda}_{\alpha\nu} = \mathscr{D}^{\lambda}_{\lambda,\alpha\nu}. \tag{5}$$

It follows that the corresponding representation of the dual vector is given by

$$\langle \Psi^{\lambda}_{\alpha\nu}| \to d(\lambda) \mathscr{D}^{\lambda *}_{\lambda,\alpha\nu} \tag{6}$$

The model space V is thereby identified with a subspace of $\mathscr{L}^2(G)$. Conversely, there is a map

$$P: \mathscr{L}^2(G) \to V; \quad \mathscr{D}^{\lambda}_{\beta\mu,\alpha\nu} \mapsto \delta_{\mu\lambda} |\psi^{\lambda}_{\alpha\nu}\rangle, \tag{7}$$

which is uniquely defined by specification of the phases of the (normalized) highest weight states $|\psi^{\lambda}_{\lambda}\rangle \in V^{\lambda}$. The composition QP is seen to be a projection from $\mathscr{L}^2(G)$ to a subspace isomorphic to the model space. This subspace is invariant under the right regular representation but not under the left regular representation. This observation reflects the fact that the maps P and Q are equivariant relative to the action of the right regular representation of G on $\mathscr{L}^2(G)$ but not relative to the action of the left regular representation.

The set of coherent state wave functions $\{\psi^{\lambda}_{\alpha\nu}\}$ (i.e., the set of Wigner functions $\{\mathscr{D}^{\lambda}_{\lambda,\alpha\nu}\}$ which are of highest weight relative to the left regular representation) are a basis for the so-called *shape algebra* Λ^+G used by Flath and Towber.[3] Thus, the map $Q: V\to\Lambda^+G\subset\mathscr{L}^2(G)$ has been considered by Flath and Towber. As pointed out to us by Flath, the projection map P was also used previously by Bernstein, Gelfand, and Gelfand.[7] The coherent-state representation gives these maps a new interpretation.

The combination rule for the shape algebra (the so-called Cartan product) is simple multiplication of wave functions; i.e.,

$$[\psi^{\lambda_2}_{\alpha_2\nu_2}\cdot\psi^{\lambda_1}_{\alpha_1\nu_1}](g)=\psi^{\lambda_2}_{\alpha_2\nu_2}(g)\psi^{\lambda_1}_{\alpha_1\nu_1}(g). \tag{8}$$

Recall that Wigner functions can be combined according to the equation

$$\mathscr{D}^{\lambda}_{\beta\mu,\alpha\nu}(g)\mathscr{D}^{\lambda_1}_{\beta_1\mu_1,\alpha_1\nu_1}(g)=\sum_{\sigma\lambda_3\beta_3\alpha_3}(\lambda_1\beta_1\mu_1,\lambda\beta\mu|\sigma\lambda_3\beta_3\mu_3)\times(\lambda_1\alpha_1\nu_1,\lambda\alpha\nu|\sigma\lambda_3\alpha_3\nu_3)^*\mathscr{D}^{\lambda_3}_{\beta_3\mu_3,\alpha_3\nu_3}(g), \tag{9}$$

where $(\lambda_1\beta_1\mu_1,\lambda\beta\mu|\sigma\lambda_3\beta_3\mu_3)$ is a Clebsch–Gordan coefficient, $\mu_3=\mu_1+\mu$, $\nu_3=\nu_1+\nu$ and σ indexes the multiplicity of irreps equivalent to R^{λ_3} in the Kronecker product $R^{\lambda}\otimes R^{\lambda_1}$ (cf. Ref. 8, for example, for a derivation of this equation). It follows that the Cartan product can be expressed

$$\psi^{\lambda_2}_{\alpha_2\nu_2}\cdot\psi^{\lambda_1}_{\alpha_1\nu_1}=\sum_{\beta}\psi^{\lambda_1+\lambda_2}_{\beta\nu_1+\nu_2}(\lambda_1\lambda_1,\lambda_2\lambda_2|\lambda_1+\lambda_2,\lambda_1+\lambda_2)\times(\lambda_1\alpha_1\nu_1,\lambda_2\alpha_2\nu_2|\lambda_1+\lambda_2,\beta,\nu_1+\nu_2)^*. \tag{10}$$

Thus, if the Clebsch–Gordan coefficients are normalized such that $(\lambda_1\lambda_1,\lambda_2\lambda_2|\lambda_1+\lambda_2,\lambda_1+\lambda_2)$ is equal to 1, according to convention, the Cartan product simplifies to

$$\psi^{\lambda_2}_{\alpha_2\nu_2}\cdot\psi^{\lambda_1}_{\alpha_1\nu_1}=\sum_{\beta}\psi^{\lambda_1+\lambda_2}_{\beta\nu_1+\nu_2}(\lambda_1\alpha_1\nu_1,\lambda_2\alpha_2\nu_2|\lambda_1+\lambda_2,\beta,\nu_1+\nu_2)^*. \tag{11}$$

We shall assume in the following that Clebsch–Gordan coefficients are normalized in this way. The map $P:\mathscr{L}^2(G)\to V$ then induces a corresponding Cartan product on the model space in which

$$|\psi^{\lambda_2}_{\alpha_2\nu_2}\rangle\cdot|\psi^{\lambda_1}_{\alpha_1\nu_1}\rangle=\sum_{\beta}|\psi^{\lambda_1+\lambda_2}_{\beta\nu_1+\nu_2}\rangle(\lambda_1\alpha_1\nu_1,\lambda_2\alpha_2\nu_2|\lambda_1+\lambda_2,\beta,\nu_1+\nu_2)^*. \tag{12}$$

To simplify the notation, it will be convenient to write

$$|\psi^{\lambda_2}_{\alpha_2\nu_2}\cdot\psi^{\lambda_1}_{\alpha_1\nu_1}\rangle=|\psi^{\lambda_2}_{\alpha_2\nu_2}\rangle\cdot|\psi^{\lambda_1}_{\alpha_1\nu_1}\rangle. \tag{13}$$

We can now express Flath and Towber's definition of a coherent shift tensor in language familiar to physicists.

Definition (coherent tensor): A $V\to V$ shift tensor T^{μ} is said to be coherent if each component of T^{μ} satisfies the equation

$$\frac{1}{d(\lambda_3)}\langle\psi^{\lambda_3}_{\alpha_3\nu_3}|T^{\mu}_{\alpha\nu}|\psi^{\lambda_1}_{\alpha_1\nu_1}\rangle=\frac{1}{d(\lambda_3+\lambda_2)}\sum_{\alpha_2\nu_2}\langle\psi^{\lambda_2}_{\alpha_2\nu_2}\cdot\psi^{\lambda_3}_{\alpha_3\nu_3}|T^{\mu}_{\alpha\nu}|\psi^{\lambda_2}_{\alpha_2\nu_2}\cdot\psi^{\lambda_1}_{\alpha_1\nu_1}\rangle. \tag{14}$$

for all λ_1 and $\lambda_2\in\Lambda$, where $\lambda_3=\lambda_1+\mu$ and $d(\lambda)=\dim(V^{\lambda})$. An arbitrary coherent tensor is a finite linear combination of coherent shift tensors and a coherent linear operator is a component of a coherent tensor.

III. WIGNER TENSORS

It follows, from Eqs. (3)–(9), that the Wigner functions, with $\lambda\beta\mu$ held fixed, in the set $\{\mathscr{D}^{\lambda}_{\beta\mu,\alpha\nu}\}$ are the components of an $\mathscr{L}^2(G)\to\mathscr{L}^2(G)$ tensor with multiplicative action given by Eq. (8). Since the maps P and Q are G-equivariant [relative to the right action on $\mathscr{L}^2(G)$], it also follows that the set of operators

$$W^{\lambda\beta\mu}_{\alpha\nu}=P\mathscr{D}^{\lambda}_{\beta\mu,\alpha\nu}Q, \tag{15}$$

with $\lambda\beta\mu$ held fixed, are the components of a $V\to V$ tensor with action

$$W^{\lambda\beta\mu}_{\alpha\nu}|\psi^{\lambda_1}_{\alpha_1\nu_1}\rangle=\sum_{\sigma\alpha_3}(\lambda_1\lambda_1,\lambda\beta\mu|\sigma\lambda_3\lambda_3)(\lambda_1\alpha_1\nu_1,\lambda\alpha\nu|\sigma\lambda_3\alpha_3\nu_3)^*|\psi^{\lambda_3}_{\alpha_3\nu_3}\rangle, \tag{16}$$

where $\lambda_3=\lambda_1+\mu$ and $\nu_3=\nu_1+\nu$. We see that $W^{\lambda\beta\mu}$ is an irreducible $V\to V$ shift tensor of highest weight λ and shift μ. If we define the coupled state

$$[W^{\lambda\beta\mu}\otimes|\psi^{\lambda_1}\rangle]^{\sigma\lambda_3}_{\alpha_3\nu_3}=\sum_{\alpha_1\nu_1\alpha\nu}(\lambda_1\alpha_1\nu_1,\lambda\alpha\nu|\sigma\lambda_3\alpha_3\nu_3)^*W^{\lambda\beta\mu}_{\alpha\nu}|\psi^{\lambda_1}_{\alpha_1\nu_1}\rangle, \tag{17}$$

the action of $W^{\lambda\beta\mu}$ can be expressed in the succinct form

$$[W^{\lambda\beta\mu}\otimes|\psi^{\lambda_1}\rangle]^{\sigma\lambda_3}_{\alpha_3\nu_3}=(\lambda_1\lambda_1,\lambda\beta\mu|\sigma\lambda_3\lambda_3)|\psi^{\lambda_3}_{\alpha_3\nu_3}\rangle. \tag{18}$$

We now show that the tensors $\{W^{\lambda\beta\mu}\}$ are complete in the sense that the tensors $\{W^{\lambda\beta\mu}(\lambda_1)\}$ span the space of $V^{\lambda_1}\to V^{\lambda_1+\mu}$ tensors for all $\lambda_1\in\Lambda$, where $W^{\lambda\beta\mu}(\lambda_1)$ denotes the restriction of $W^{\lambda\beta\mu}$ to V^{λ_1}. Recall that the linear space of $V^{\lambda_1}\to V^{\lambda_3}$ tensors has a Hermitian inner product given[8] by

$$(A^{\lambda},B^{\lambda'})=\delta_{\lambda\lambda'}\sum_{\sigma}\langle\psi^{\lambda_3}||A^{\lambda}||\psi^{\lambda_1}\rangle^*_{\sigma}\langle\psi^{\lambda_3}||B^{\lambda}||\psi^{\lambda_1}\rangle_{\sigma}, \tag{19}$$

where $\langle\psi^{\lambda_3}||A^{\lambda}||\psi^{\lambda_1}\rangle_{\sigma}$ is a reduced matrix element defined by the Wigner–Eckart theorem

$$\langle\psi^{\lambda_3}_{\alpha_3\nu_3}|A^{\lambda}_{\alpha\nu}|\psi^{\lambda_1}_{\alpha_1\nu_1}\rangle=\sum_{\sigma}(\lambda_1\alpha_1\nu_1,\lambda\alpha\nu|\sigma\lambda_3\alpha_3\nu_3)^*\langle\psi^{\lambda_3}||A^{\lambda}||\psi^{\lambda_1}\rangle_{\sigma}. \tag{20}$$

It follows that the tensors $\{W^{\lambda\beta\mu}\}$ have reduced matrix elements

$$\langle\psi^{\lambda_3}||W^{\lambda\beta\mu}||\psi^{\lambda_1}\rangle_{\sigma}=(\lambda_1\lambda_1,\lambda\beta\mu|\sigma\lambda_3\lambda_3) \tag{21}$$

and that

$$(W^{\lambda\beta\mu}(\lambda_1),W^{\lambda\beta'\mu}(\lambda_1))=N^{\lambda\mu}_{\beta\beta'}(\lambda_1), \tag{22}$$

where

$$N^{\lambda\mu}_{\beta\beta'}(\lambda_1)=\sum_{\sigma}(\lambda_1\lambda_1,\lambda\beta\mu|\sigma\lambda_3\lambda_3)^*(\lambda_1\lambda_1,\lambda\beta'\mu|\sigma\lambda_3\lambda_3) \tag{23}$$

and $\lambda_3=\lambda_1+\mu$. We have shown, in Theorem 1 of Ref. 8, that the rank of the matrix $N^{\lambda\mu}(\lambda_1)$ is equal to $m(\lambda_1,\lambda;\lambda_3)$, where $m(\lambda_1,\lambda;\lambda_3)$ is the multiplicity of irreps equivalent to R^{λ_3} in the tensor product $R^{\lambda}\otimes R^{\lambda_1}$. Since this theorem is vital for the claims made in this paper, the proof is given, in more detail, in the Appendix. It follows from the theorem that the tensors $\{W^{\lambda\beta\mu}(\lambda_1)\}$ are a complete set of $V^{\lambda_1}\to V^{\lambda_1+\mu}$ tensors. We shall also show by means of the following claim that $N^{\lambda\mu}_{\beta\beta'}(\lambda_1)\to\delta_{\beta\beta'}$, for finite λ, as $\lambda_1\to\infty$. Thus, in the asymptotic limit, the tensors $\{W^{\lambda\beta\mu}(\lambda_1)\}$ become an orthonormal set. This shows that the shift tensors $\{W^{\lambda\beta\mu}\}$ are a complete, but not overcomplete, set.

Fix a highest weight λ, and consider $V^{\lambda}\otimes V^{\lambda_1}$ as $\lambda_1\to\infty$. When we write $\lambda_1\to\infty$, we will mean that λ_1 goes to ∞ ''away from the walls,'' i.e., inside a cone in the positive chamber whose only intersection with the walls is the origin. In particular, this implies that the Killing form inner product (λ_1,η) goes to infinity for any positive root η. Roughly speaking, this means that in V^{λ_1} it is possible to ''ladder down'' a large number of times from the highest weight, in the direction opposite to any positive root.

Claim: As $\lambda_1\to\infty$, any highest weight vector $|\Psi^{\sigma\lambda_3}_{\lambda_3}\rangle$ in $V^{\lambda}\otimes V^{\lambda_1}$ tends to a simple product;

$$|\Psi^{\sigma\lambda_3}_{\lambda_3}\rangle\to\left(\sum_{\alpha}(\lambda_1\lambda_1,\lambda\alpha\mu|\sigma\lambda_3\lambda_3)^*|\psi^{\lambda}_{\alpha\mu}\rangle\right)|\psi^{\lambda_1}_{\lambda_1}\rangle. \tag{24}$$

Specifically, if we fix a weight μ which occurs in V_{λ}, then any highest weight vector of weight $\lambda_3=\lambda_1+\mu$ tends to a simple product.

Proof: Note that if $V^{\lambda}\otimes V^{\lambda_1}$ contains a highest weight vector of weight λ_3, then λ_3 differs from λ_1 by a weight μ of V^{λ}. Moreover, $\lambda_3=\lambda_1+\mu\to\infty$ and (λ_3,η) goes to infinity, as $\lambda_1\to\infty$, for any positive root η.

Expand a highest weight vector as

$$|\Psi^{\sigma\lambda_3}_{\lambda_3}\rangle=\sum\epsilon_{\alpha\mu,\beta\nu}|\psi^{\lambda}_{\alpha\mu}\rangle|\psi^{\lambda_1}_{\beta\nu}\rangle. \tag{25}$$

Since $|\Psi^{\sigma\lambda_3}_{\lambda_3}\rangle$ is killed by any raising operator e_i, we find

$$\sum\epsilon_{\alpha\mu,\beta\nu}(e_i|\psi^{\lambda}_{\alpha\mu}\rangle)|\psi^{\lambda_1}_{\beta\nu}\rangle+\sum\epsilon_{\alpha'\mu',\beta'\nu'}|\psi^{\lambda}_{\alpha'\mu'}\rangle(e_i|\psi^{\lambda_1}_{\beta'\nu'}\rangle)=0, \tag{26}$$

or, taking the inner product with a fixed $\langle\psi^{\lambda}_{\alpha'\mu'}|$,

$$\sum\epsilon_{\alpha\mu,\beta\nu}\langle\psi^{\lambda}_{\alpha'\mu'}|e_i|\psi^{\lambda}_{\alpha\mu}\rangle|\psi^{\lambda_1}_{\beta\nu}\rangle+\sum\epsilon_{\alpha'\mu',\beta'\nu'}e_i|\psi^{\lambda_1}_{\beta'\nu'}\rangle=0. \tag{27}$$

If a vector $|\psi^{\lambda_1}_{\beta'\nu'}\rangle$, appearing on the r.h.s. of this equation, is not a highest weight vector, it is possible to find e_i so that $e_i|\psi^{\lambda_1}_{\beta'\nu'}\rangle\neq 0$. Moreover, as we now show, $\|e_i|\psi^{\lambda_1}_{\beta'\nu'}\rangle\|^2=\langle\psi^{\lambda_1}_{\beta'\nu'}|f_ie_i|\psi^{\lambda_1}_{\beta'\nu'}\rangle$ then tends to ∞ as $\lambda_1\to\infty$, when f_i is the Hermitian adjoint of e_i in any unitary representation. Consider the su(2) algebra spanned by e_i,f_i,h_i, with

$$[e_i,f_i]=h_i,\quad [h_i,e_i]=2e_i,\quad [h_i,f_i]=-2f_i. \tag{28}$$

Applied to $|\psi^{\lambda_1}_{\beta'\nu'}\rangle$, it generates a space which is a direct sum of su(2) irreps. The highest weights of these irreps tend to infinity with λ_1. So $\langle\psi^{\lambda_1}_{\beta'\nu'}|f_ie_i|\psi^{\lambda_1}_{\beta'\nu'}\rangle$ is a normalized sum of su(2) matrix elements

$$\langle JM|J_-J_+|JM\rangle=(J-M)(J+M+1), \tag{29}$$

with J tending to ∞ and $M\neq J$. We conclude that $\|e_i|\psi^{\lambda_1}_{\beta'\nu'}\rangle\|^2=\langle\psi^{\lambda_1}_{\beta'\nu'}|f_ie_i|\psi^{\lambda_1}_{\beta'\nu'}\rangle\to\infty$.

If $\langle\varphi(i,\lambda_1\beta'\nu')|$ is the vector dual to $e_i|\psi^{\lambda_1}_{\beta'\nu'}\rangle$, we can write

$$\epsilon_{\alpha'\mu',\beta'\nu'}=-\sum\ \epsilon_{\alpha\mu,\beta\nu}\langle\psi^{\lambda}_{\alpha'\mu'}|e_i|\psi^{\lambda}_{\alpha\mu}\rangle\langle\varphi(i,\lambda_1\beta'\nu')|\psi^{\lambda_1}_{\beta\nu}\rangle, \tag{30}$$

where the sum is over a basis $\alpha\mu$ of V^λ and the corresponding basis vectors $\beta\nu$ of V^{λ_1} with $\mu+\nu=\lambda_3$. If $\|e_i|\psi^{\lambda_1}_{\beta'\nu'}\rangle\|^2\to\infty$, then $|\varphi(i,\lambda_1\beta'\nu')\rangle\to0$. Therefore $\epsilon_{\alpha'\mu',\beta'\nu'}\to0$ as $\lambda_1\to\infty$, for all coefficients for which $e_i|\psi^{\lambda_1}_{\beta'\nu'}\rangle\neq0$. This means that the only terms in the expansion (25) that survive are the leading terms, i.e.,

$$|\Psi^{\sigma\lambda_3}_{\lambda_3}\rangle\to\sum_\alpha\ \epsilon_{\alpha\mu,\lambda_1}|\psi^{\lambda}_{\alpha\mu}\rangle|\psi^{\lambda_1}_{\lambda_1}\rangle. \tag{31}$$

This completes the proof of the claim.

Since $\{|\Psi^{\sigma\lambda_3}_{\lambda_3}\rangle\}$ and $\{|\psi^{\lambda}_{\alpha\mu}\rangle|\psi^{\lambda_1}_{\lambda_1}\rangle\}$ are orthonormal sets, it follows that the matrix O, with coefficients

$$O_{\sigma\alpha}=(\lambda_1\lambda_1,\lambda\alpha\mu|\sigma\lambda_3\lambda_3)^*, \tag{32}$$

tends to a unitary matrix as $\lambda_1\to\infty$. Therefore, it follows from the claim that

$$N^{\lambda\mu}_{\beta\beta'}(\lambda_1)=\sum_\sigma\ O_{\sigma\beta}O^*_{\sigma\beta'}\to\delta_{\beta\beta'}. \tag{33}$$

Theorem I: The tensors $\{W^{\lambda\beta\mu}\}$ are coherent.

Proof: First observe, from the definition, that the state $|\psi^{\lambda_2}_{\alpha_2\nu_2}\cdot\psi^{\lambda_1}_{\alpha_1\nu_1}\rangle$ has coherent state wave function

$$\psi^{\lambda_2}_{\alpha_2\nu_2}\cdot\psi^{\lambda_1}_{\alpha_1\nu_1}=\mathscr{D}^{\lambda_2}_{\lambda_2,\alpha_2\nu_2}\mathscr{D}^{\lambda_1}_{\lambda_1,\alpha_1\nu_1}=\sum_\beta\ (\lambda_1\alpha_1\nu_1,\lambda_2\alpha_2\nu_2|\lambda_1+\lambda_2,\beta,\nu_1+\nu_2)^*\mathscr{D}^{\lambda_1+\lambda_2}_{\lambda_1+\lambda_2,\beta\nu_1+\nu_2} \tag{34}$$

whereas, from Eq. (6), we infer that the dual state $\langle\psi^{\lambda_2}_{\alpha_2\nu_2}\cdot\psi^{\lambda_3}_{\alpha_3\nu_3}|$ has wave function

$$\begin{aligned}&d(\lambda_2+\lambda_3)\sum_\beta\ (\lambda_3\alpha_3\nu_3,\lambda_2\alpha_2\nu_2|\lambda_3+\lambda_2,\beta,\nu_3+\nu_2)\mathscr{D}^{\lambda_3+\lambda_2*}_{\lambda_1+\lambda_2,\beta\nu_1+\nu_2}\\&\quad=d(\lambda_2+\lambda_3)\mathscr{D}^{\lambda_3*}_{\lambda_3,\alpha_3\mu_3}\mathscr{D}^{\lambda_2*}_{\lambda_2,\alpha_2\nu_2}.\end{aligned} \tag{35}$$

It follows that

$$\sum_{\alpha_2\nu_2} \langle \psi^{\lambda_2}_{\alpha_2\nu_2} \cdot \psi^{\lambda_3}_{\alpha_3\nu_3} | W^{\lambda\beta\mu}_{\alpha\nu} | \psi^{\lambda_2}_{\alpha_2\nu_2} \cdot \psi^{\lambda_1}_{\alpha_1\nu_1} \rangle$$

$$= d(\lambda_2+\lambda_3) \sum_{\alpha_2\nu_2} \int \mathscr{D}^{\lambda_3 *}_{\lambda_3,\alpha_3\nu_3}(g) \mathscr{D}^{\lambda_2 *}_{\lambda_2,\alpha_2\nu_2}(g) \mathscr{D}^{\lambda}_{\beta\mu,\alpha\nu}(g) \mathscr{D}^{\lambda_2}_{\lambda_2,\alpha_2\nu_2}(g) \mathscr{D}^{\lambda_1}_{\lambda_1,\alpha_1\nu_1}(g) dv(g)$$

$$= d(\lambda_2+\lambda_3) \int \mathscr{D}^{\lambda_3 *}_{\lambda_3,\alpha_3\nu_3}(g) \mathscr{D}^{\lambda}_{\beta\mu,\alpha\nu}(g) \mathscr{D}^{\lambda_1}_{\lambda_1,\alpha_1\nu_1}(g) dv(g)$$

$$= \frac{d(\lambda_2+\lambda_3)}{d(\lambda_3)} \langle \psi^{\lambda_3}_{\alpha_3\nu_3} | W^{\lambda\beta\mu}_{\alpha\nu} | \psi^{\lambda_1}_{\alpha_1\nu_1} \rangle, \tag{36}$$

where we have used the unitarity relationship

$$\sum_{\alpha_2\nu_2} \mathscr{D}^{\lambda_2 *}_{\lambda_2,\alpha_2\nu_2}(g) \mathscr{D}^{\lambda_2}_{\lambda_2,\alpha_2\nu_2}(g) = 1. \tag{37}$$

Thus, the tensors $\{W^{\lambda\beta\mu}\}$ are coherent according to the definition.

From the way in which the tensors $\{W^{\lambda\beta\mu}\}$ are defined in terms of Wigner functions, it would appear to be manifestly appropriate to call them *Wigner tensors* in parallel with the usage of this terminology by Biedenharn *et al.* and Flath and Towber. They are shift tensors, they are irreducible, and they are coherent. The components of the Wigner tensors are also naturally called *Wigner operators*. Operators of this type were used in the paper of Bernstein *et al.*[7]

The relationship between these tensors and Wigner functions through

$$\mathscr{D}^{\lambda}_{\beta\mu,\alpha\nu} \to W^{\lambda\beta\mu}_{\alpha\nu} = P \mathscr{D}^{\lambda}_{\beta\mu,\alpha\nu} Q \tag{38}$$

gives a precise group theoretical meaning to the $\beta\mu$ labels (operator patterns). Since the $\beta\mu$ labels of the Wigner functions $\{\mathscr{D}^{\lambda}_{\beta\mu,\alpha\nu}\}$ index a basis for the left regular representation of G, it is tempting to suppose that the operators $\{W^{\lambda\beta\mu}_{\alpha\nu}\}$, with λ and $\alpha\nu$ held fixed, might span a module for a corresponding representation. However, as Biedenharn[9] has pointed out in parallel circumstances, such is not the case. The reason is that the maps P and Q are not equivariant relative to a left group action.

Theorem II: The product of two coherent tensors is a tensor which is asymptotically coherent.

Proof: First observe that the space of coherent tensors is uniquely defined by the tensors $\{W^{\lambda\beta\mu}(\lambda_1)\}$ which are an orthonormal set in the $\lambda_1 \to \infty$ asymptotic limit. Consider the product

$$(W^{\lambda_3\beta_3\mu_3}_{\alpha_3\nu_3} W^{\lambda_2\beta_2\mu_2}_{\alpha_2\nu_2} | \psi^{\lambda_1}_{\alpha_1\nu_1} \rangle)(g) = P \mathscr{D}^{\lambda_3}_{\beta_3\mu_3,\alpha_3\nu_3}(g) Q P \mathscr{D}^{\lambda_2}_{\beta_2\mu_2,\alpha_2\nu_2}(g) \mathscr{D}^{\lambda_1}_{\lambda_1,\alpha_1\nu_1}(g). \tag{39}$$

The second pair of Wigner functions on the right of this expression can be combined to give

$$\mathscr{D}^{\lambda_2}_{\beta_2\mu_2,\alpha_2\nu_2}(g) \mathscr{D}^{\lambda_1}_{\lambda_1,\alpha_1\nu_1}(g) = \sum_{\sigma\lambda\beta\alpha} (\lambda_1\lambda_1, \lambda_2\beta_2\mu_2 | \sigma\lambda\beta\mu) \times (\lambda_1\alpha_1\nu_1, \lambda_2\alpha_2\nu_2 | \sigma\lambda\alpha\nu)^* \mathscr{D}^{\lambda}_{\beta\mu,\alpha\nu}(g). \tag{40}$$

The only terms in this expression which survive, in the asymptotic limit, are those with $\lambda = \lambda_1 + \mu_2$. To show this, we first consider the highest weight state

$$|\Psi^{\sigma\lambda}_{\lambda}\rangle = \sum_{\beta_1\mu_1\beta_2\mu_2} (\lambda_1\beta_1\mu_1, \lambda_2\beta_2\mu_2 | \sigma\lambda\lambda)^* | \psi^{\lambda_2}_{\beta_2\mu_2} \rangle | \psi^{\lambda_1}_{\beta_1\mu_1} \rangle \tag{41}$$

in the tensor product space $V^{\lambda_1} \otimes V^{\lambda_2}$. We have already shown that, as $\lambda_1 \to \infty$, this state becomes

$$|\Psi_\lambda^{\sigma\lambda}\rangle \to \sum_{\beta_2} (\lambda_1\lambda_1, \lambda_2\beta_2\mu_2|\sigma\lambda\lambda)^* |\psi_{\beta_2\mu_2}^{\lambda_2}\rangle |\psi_{\lambda_1}^{\lambda_1}\rangle = \sum_{\beta_2} O_{\sigma\beta_2} |\psi_{\beta_2\mu_2}^{\lambda_2}\rangle |\psi_{\lambda_1}^{\lambda_1}\rangle \tag{42}$$

with μ_2 taking the value $\lambda - \lambda_1$. It then follows that

$$\sum_\sigma (\lambda_1\lambda_1, \lambda_2\beta_2\mu_2|\sigma\lambda\lambda)(\lambda_1\lambda_1, \lambda_2\beta_2'\mu_2|\sigma\lambda\lambda)^* = \sum_\sigma O_{\sigma\beta_2}^* O_{\sigma\beta_2'} \to \delta_{\beta_2\beta_2'}. \tag{43}$$

But, we know that

$$\sum_{\sigma\lambda'\beta} |(\lambda_1\lambda_1, \lambda_2\beta_2\mu_2|\sigma\lambda'\beta\lambda)|^2 = 1. \tag{44}$$

We conclude that

$$(\lambda_1\lambda_1, \lambda_2\beta_2\mu_2|\sigma\lambda'\beta\lambda) \to \delta_{\lambda\lambda'}(\lambda_1\lambda_1, \lambda_2\beta_2\mu_2|\sigma\lambda\lambda). \tag{45}$$

Equation (40) becomes

$$\mathscr{D}_{\beta_2\mu_2,\alpha_2\nu_2}^{\lambda_2}(g)\mathscr{D}_{\lambda_1,\alpha_1\nu_1}^{\lambda_1}(g) \to \sum_{\sigma\beta} (\lambda_1\lambda_1, \lambda_2\beta_2\mu_2|\sigma\lambda\lambda) \times (\lambda_1\alpha_1\nu_1, \lambda_2\alpha_2\nu_2|\sigma\lambda\alpha\nu)^* \mathscr{D}_{\lambda,\alpha\nu}^{\lambda}(g) \tag{46}$$

and we have shown that the intermediate projection operator QP in Eq. (39) becomes redundant, i.e.,

$$QP\mathscr{D}_{\beta_2\mu_2,\alpha_2\nu_2}^{\lambda_2}(g)\mathscr{D}_{\lambda_1,\alpha_1\nu_1}^{\lambda_1}(g) \to \mathscr{D}_{\beta_2\mu_2,\alpha_2\nu_2}^{\lambda_2}(g)\mathscr{D}_{\lambda_1,\alpha_1\nu_1}^{\lambda_1}(g). \tag{47}$$

Therefore, Eq. (39) gives

$$(W_{\alpha_3\nu_3}^{\lambda_3\beta_3\mu_3} W_{\alpha_2\nu_2}^{\lambda_2\beta_2\mu_2} |\psi_{\alpha_1\nu_1}^{\lambda_1}\rangle)(g) \to \sum_{\sigma\lambda\beta\mu\alpha\nu} (\lambda_2\beta_2\mu_2, \lambda_3\beta_3\mu_3|\sigma\lambda\beta\mu) \times (\lambda_2\alpha_2\nu_2, \lambda_3\alpha_3\nu_3|\sigma\lambda\alpha\nu)^* (W_{\alpha\nu}^{\lambda\beta\mu}|\psi_{\alpha_1\nu_1}^{\lambda_1}\rangle)(g) \tag{48}$$

as $\lambda_1 \to \infty$. If we denote the coupled product of Wigner tensors by

$$[W^{\lambda_3\beta_3\mu_3} \otimes W^{\lambda_2\beta_2\mu_2}]_{\alpha\nu}^{\sigma\lambda\beta\mu} = \sum_{\alpha_2\nu_2\alpha_3\nu_3} (\lambda_2\alpha_2\nu_2, \lambda_3\alpha_3\nu_3|\sigma\lambda\alpha\nu)^* W_{\alpha_3\nu_3}^{\lambda_3\beta_3\mu_3} W_{\alpha_2\nu_2}^{\lambda_2\beta_2\mu_2}, \tag{49}$$

this equation can be expressed in the succinct form

$$[W^{\lambda_3\beta_3\mu_3} \otimes W^{\lambda_2\beta_2\mu_2}]_{\alpha\nu}^{\sigma\lambda\beta\mu}(\lambda_1) \to (\lambda_2\beta_2\mu_2, \lambda_3\beta_3\mu_3|\sigma\lambda\beta\mu) W_{\alpha\nu}^{\lambda\beta\mu}(\lambda_1). \tag{50}$$

This completes the proof.

A corollary of Theorem II is that coherent tensors commute in the $\lambda_1 \to \infty$ asymptotic limit as Flath and Towber have conjectured. In particular, the Wigner tensors satisfy the equation

$$[W_{\alpha_3\nu_3}^{\lambda_3\beta_3\mu_3}, W_{\alpha_2\nu_2}^{\lambda_2\beta_2\mu_2}]|\psi_{\alpha_1\nu_1}^{\lambda_1}\rangle \to 0. \tag{51}$$

This follows, once the projection operator in Eq. (39) has been shown to be redundant, because Wigner functions commute.

It is interesting to note that, in specializing to SU(2), Biedenharn[9] defined a shift tensor $T^{j\mu}$ with components

$$T^{j\mu}_m = \sum |\psi^{\,j_3}_{m_3}\rangle (j_1 m_1, jm | j_3 m_3) \langle \psi^{\,j_1}_{m_1}|, \tag{52}$$

where the sum is over all j_1, m_1, j_3, and m_3 with $j_3 = j_1 + \mu$ and $m_3 = m_1 + m$. Biedenharn's tensors act on model states according to the equation

$$[T^{j\mu} \otimes |\psi^{\,j_1}\rangle]^{j_3}_{m_3} = |\psi^{\,j_3}_{m_3}\rangle \tag{53}$$

where $j_3 = j_1 + \mu$ and $m_3 = m_1 + m$. As Biedenharn observed, these tensors can be coupled according to the equation

$$[T^{j_3\mu_3} \otimes T^{j_2\mu_2}]^J_M(j_1) = \sqrt{(2J+1)(2J'+1)}\, W(j_1 j_2 j_4 j_3 : J' J) T^{J\mu}_M(j_1), \tag{54}$$

where $J' = j_1 + \mu_2$, $\mu = \mu_2 + \mu_3$, $j_4 = j_1 + \mu_2 + \mu_3$, and $W(j_1 j_2 j_4 j_3 : J' J)$ is a Racah coefficient. The $\{T^{j\mu}\}$ tensors are not coherent. However, by comparison of Eqs. (18) and (53) and noting that $(j_1 j_1, j\mu | j_3 j_3) \to 1$ as $j_1 \to \infty$, we see that Biedenharn's tensors become equal to coherent Wigner tensors in the limit; i.e.,

$$T^{j\mu}(j_1) \to W^{j\mu}(j_1), \quad \text{as} \quad j_1 \to \infty. \tag{55}$$

Thus Eq. (54) can be compared with Eq. (50) which, for SU(2), gives

$$[W^{j_3\mu_3} \otimes W^{j_2\mu_2}]^J_M(j_1) = (j_2\mu_2, j_3\mu_3 | J\mu) W^{J\mu}_M(j_1) \tag{56}$$

with $\mu = \mu_2 + \mu_3$. From the equivalence of these two expressions, it follows that

$$\sqrt{(2J+1)(2J'+1)}\, W(j_1 j_2 j_4 j_3 : J' J) \to (j_2\mu_2, j_3\mu_3 | J\mu) \tag{57}$$

as $j_1 \to \infty$, with $\mu_2 = J' - j_1$, $\mu_3 = j_4 - J'$, and $\mu = \mu_2 + \mu_3$.

IV. SUMMARY OF RESULTS

We summarize by listing some of the properties of the above-defined Wigner tensors, which generalize results of Biedenharn and Louck[1] for the unitary groups and confirm conjectures expressed by Flath and Towber[3] and proved by them in special cases.

(i) A tensor of highest weight λ is a complex vector space isomorphic to V^λ. The linear space $\mathscr{T}^{\lambda\mu}(\lambda_1)$ of all $V^{\lambda_1} \to V^{\lambda_1+\mu}$ tensors of highest weight λ (and shift μ) has dimension equal to the multiplicity, $m(\lambda_1, \lambda, \lambda_1 + \mu)$, of irreps equivalent to $R^{\lambda_1+\mu}$ in the Kronecker product $R^\lambda \otimes R^{\lambda_1}$.

(ii) The set $\mathscr{W}^{\lambda\mu}$ of all coherent tensors of highest weight λ and shift μ is a complex vector space of dimension equal to the multiplicity, $m(\mu;\lambda)$, of the weight μ in the irrep R^λ. Moreover,

$$m(\mu;\lambda) \geqslant m(\lambda_1, \lambda, \lambda_1 + \mu), \tag{58}$$

and the equality holds for sufficiently large λ_1.

(iii) For every $\lambda_1 \in \Lambda$, the map

$$\mathscr{W}^{\lambda\mu} \to \mathscr{T}^{\lambda\mu}(\lambda_1) \tag{59}$$

obtained by restricting the tensors in $\mathscr{W}^{\lambda\mu}$ from V to V^{λ_1} is subjective. Moreover, the coherent tensors $\{W^{\lambda\beta\mu}(\lambda_1)\}$ become an orthonormal set in the $\lambda_1\to\infty$ limit.

(iv) Let $\mathscr{W}$ be the linear space of all finite linear combinations of coherent linear operators on V. Equation (14) shows that the elements of $\mathscr{W}$ are associated to components of tensors on $\mathscr{L}^2(G)$ given by multiplication by Wigner functions. The Wigner functions have a dual role: (i) as components of tensors on $\mathscr{L}^2(G)$, and (ii) as elements of $\mathscr{L}^2(G)$. Thus, we obtain a map $\pi:\mathscr{W}\to\mathscr{L}^2(G)$, defined by

$$\pi(W^{\lambda\beta\mu}_{\alpha\nu})=\mathscr{D}^{\lambda}_{\beta\mu,\alpha\nu}\ . \tag{60}$$

With $\mathscr{L}^2(G)$ regarded as a module for the right regular representation, this map π is a group isomorphism from $\mathscr{W}$ onto a dense subspace of $\mathscr{L}^2(G)$. The correspondence between Wigner operators and Wigner functions, expressed by this relationship, gives a precise group theoretical meaning to the $\beta\mu$ labels (operator patterns).

(v) Let λ denote the lowest weight in the irrep R^{λ}. Then, every product of coherent tensors of the form

$$\left(\prod_i W^{\lambda_i\overline{\lambda_i}}\right)\circ\left(\prod_j W^{\lambda_j\lambda_j}\right) \tag{61}$$

is a coherent tensor. The tensors $W^{\lambda\lambda}$ (maximal-positive shift tensors) send vectors in V^{λ_1} to vectors in $V^{\lambda_1+\lambda}$. The tensors $W^{\lambda\overline{\lambda}}$ (maximal-negative shift tensors) send vectors in V^{λ_1} to vectors in $V^{\lambda_1+\overline{\lambda}}$ if $\lambda_1+\overline{\lambda}\in\Lambda$ and are zero otherwise.

(vi) The commutator of two Wigner tensors is not, in general, coherent. Because of the completeness of the Wigner tensors, a commutator can be expanded

$$[W^{\lambda_3\beta_3\mu_3}_{\alpha_3\nu_3},\ W^{\lambda_2\beta_2\mu_2}_{\alpha_2\nu_2}]=\sum\ S\left(\lambda_2{}^{\beta_2\mu_2}_{\alpha_2\nu_2},\lambda_3{}^{\beta_3\mu_3}_{\alpha_3\nu_3}\middle|\lambda_4{}^{\beta_4\mu_4}_{\alpha_4\nu_4}\right)W^{\lambda_4\beta_4\mu_4}_{\alpha_4\nu_4}, \tag{62}$$

where each $S(\lambda_2{}^{\beta_2\mu_2}_{\alpha_2\nu_2},\lambda_3{}^{\beta_3\mu_3}_{\alpha_3\nu_3}|\lambda_4{}^{\beta_4\mu_4}_{\alpha_4\nu_4})$ is a scalar, i.e., a tensor of rank $\lambda=0$. If we write $S(\lambda_2{}^{\beta_2\mu_2}_{\alpha_2\nu_2},\lambda_3{}^{\beta_3\mu_3}_{\alpha_3\nu_3}|\lambda_4{}^{\beta_4\mu_4}_{\alpha_4\nu_4})(\lambda_1)$ for the value of this scalar on the space V^{λ_1}, then as $\lambda_1\to\infty$,

$$S\left(\lambda_2{}^{\beta_2\mu_2}_{\alpha_2\nu_2},\lambda_3{}^{\beta_3\mu_3}_{\alpha_3\nu_3}\middle|\lambda_4{}^{\beta_4\mu_4}_{\alpha_4\nu_4}\right)(\lambda_1)\to 0. \tag{63}$$

Properties (i)–(iv) have been proved either above or in Ref. 8. Property (v) follows from the observation that

$$\left(\prod_i P\mathscr{D}^{\lambda_i}_{\lambda_i,\alpha_i\nu_i}Q\right)\circ\left(\prod_j P\mathscr{D}^{\lambda_j}_{\lambda_j,\alpha_j\nu_j}Q\right)=P\left(\prod_i \mathscr{D}^{\lambda_i}_{\overline{\lambda_i},\alpha_i\nu_i}\right)\circ\left(\prod_j \mathscr{D}^{\lambda_j}_{\lambda_j,\alpha_j\nu_j}\right)Q. \tag{64}$$

Property (vi) follows from the corollary to Theorem II and the asymptotic orthonormality of Wigner tensors, expressed by Eqs. (19) and (33).

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APPENDIX: THEOREM (ROWE AND REPKA, REF. 8)

The rank of the Hermitian matrix $N^{\lambda\mu}(\lambda_1)$ with entries

$$N^{\lambda\mu}_{\beta\beta'}(\lambda_1)=\sum_{\sigma}(\lambda_1\lambda_1,\lambda\beta\mu|\sigma\lambda_3\lambda_3)^*(\lambda_1\lambda_1,\lambda\beta'\mu|\sigma\lambda_3\lambda_3) \tag{A1}$$

is equal to the multiplicity of R^{λ_3} in $R^{\lambda}\otimes R^{\lambda_1}$.

Proof: The proof is given in a sequence of steps.

(i) If $\psi^{\lambda_1}_{\lambda_1}$ is a highest weight vector in the module V^{λ_1} for the irrep R^{λ_1}, then the action of the group on the subset of vectors

$$S=\{\varphi\otimes\psi^{\lambda_1}_{\lambda_1};\varphi\in V^{\lambda}\} \tag{A2}$$

generates the whole of $V^{\lambda}\otimes V^{\lambda_1}$.

(ii) Some vector in every invariant subspace $\mathscr{V}^{\alpha\lambda_3}\subset V^{\lambda}\otimes V^{\lambda_1}$ has a nonzero overlap with some vector in S. For, if this were not so, the action of the group on S must generate a space which excludes $\mathscr{V}^{\alpha\lambda_3}$ and this contradicts (i).

(iii) A highest weight vector $\Psi^{\alpha\lambda_3}_{\lambda_3}$ for the invariant subspace $\mathscr{V}^{\alpha\lambda_3}\subset V^{\lambda}\otimes V^{\lambda_1}$ has nonzero overlap with some vector in S. This is proved by showing that, if it were not so, then no vector in $\mathscr{V}^{\alpha\lambda_3}$ could have a nonzero overlap with any vector in S, which contradicts (ii). Let $\varphi\otimes\psi^{\lambda_1}_{\lambda_1}$, be a vector in S which has a nonzero overlap with some vector in $\mathscr{V}^{\alpha\lambda_3}$ and expand

$$\varphi\otimes\psi^{\lambda_1}_{\lambda_1}=C^{\alpha\lambda_3}\Psi^{\alpha\lambda_3}+\sum_{\beta\lambda_3'\neq\alpha\lambda_3}C^{\beta\lambda_3'}\Psi^{\beta\lambda_3'}, \tag{A3}$$

where $\Psi^{\beta\lambda_3'}\in\mathscr{V}^{\beta\lambda_3'}$. Let Z be a product of raising operators in $\mathfrak{g}$, the Lie algebra of G, which raises the particular vector $\Psi^{\alpha\lambda_3}$ to a highest weight vector; i.e., Z is defined such that

$$Z\Psi^{\alpha\lambda_3}=\Psi^{\alpha\lambda_3}_{\lambda_3}. \tag{A4}$$

Applying Z to both sides of Eq. (A3) gives

$$(Z\varphi)\otimes\psi^{\lambda_1}_{\lambda_1}=C^{\alpha\lambda_3}\Psi^{\alpha\lambda_3}_{\lambda_3}+\sum_{\beta\lambda_3'\neq\alpha\lambda_3}C^{\beta\lambda_3'}Z\Psi^{\beta\lambda_3'}, \tag{A5}$$

and shows that $\Psi^{\alpha\lambda_3}_{\lambda_3}$ has nonzero overlap with the nonzero vector $(Z\varphi)\otimes\psi^{\lambda_1}_{\lambda_1}\in S$.

(iv) Let $\varphi_{\alpha_1\nu_1}(\alpha\lambda_3)\in V^{\lambda}$ denote the cofactor of $\psi^{\lambda_1}_{\alpha_1\nu_1}$ in the expansion of a highest weight vector $\Psi^{\alpha\lambda_3}_{\lambda_3}$, i.e.,

$$\Psi^{\alpha\lambda_3}_{\lambda_3}=\varphi_{\lambda_1}(\alpha\lambda_3)\psi^{\lambda_1}_{\lambda_1}+\sum_{\alpha_1,\nu_1\neq\lambda_1}\varphi_{\alpha_1\nu_1}(\alpha\lambda_3)\psi^{\lambda_1}_{\alpha_1\nu_1}. \tag{A6}$$

We now claim that, if $\{\Psi^{\alpha\lambda_3}_{\lambda_3};\alpha=1,\ldots,N\}$ is a maximal set of linearly independent highest weight vectors of highest weight λ_3 in $V^{\lambda}\otimes V^{\lambda_1}$, then the corresponding vectors $\{\varphi_{\lambda_1}(\alpha\lambda_3)\}$ in V^{λ} are also linearly independent. For, if they were not, it would be possible to construct a nonzero highest weight vector $\Sigma_{\alpha}a_{\alpha}\Psi^{\alpha\lambda_3}_{\lambda_3}$ for which $\Sigma_{\alpha}a_{\alpha}\varphi_{\lambda_1}(\alpha\lambda_3)=0$ and this would contradict (iii).

(v) Let $\varphi_{\lambda_1}(\alpha\lambda_3)$ be expanded on the orthonormal basis $\{\psi^{\lambda}_{\beta\mu}\}$ for V^{λ};

$$\varphi_{\lambda_1}(\alpha\lambda_3)=\sum_{\beta\mu} C_{\beta\mu}(\alpha\lambda_3)\psi^{\lambda}_{\beta\mu}\ . \tag{A7}$$

Since the vectors $\{\varphi_{\lambda_1}(\alpha\lambda_3);\alpha = 1,\ldots,N\}$ are a linearly independent set, it follows that the N columns $\{C(\alpha\lambda_3)\}$ of the rectangular matrix $C(\lambda_3)$ are linearly independent and, hence, that the rank of the matrix M^{λ} with entries

$$M^{\lambda}_{\beta\mu,\beta'\mu'}=\sum_{\alpha} C_{\beta\mu}(\alpha\lambda_3)^* C_{\beta'\mu'}(\alpha\lambda_3) \tag{A8}$$

is equal to the number N of values the multiplicity index α can take; i.e., the multiplicity of the $\lambda\otimes\lambda_1\rightarrow\lambda_3$ coupling.

(vi) Finally, if the vectors $\{\Psi^{\alpha\lambda_3}_{\lambda_3}\}$ are an orthonormal set, the coefficients $C_{\beta\mu}(\alpha\lambda_3)$ are the Clebsch–Gordan coefficients

$$C_{\beta\mu}(\alpha\lambda_3)=(\lambda_1\lambda_1,\lambda\beta\mu|\alpha\lambda_3\lambda_3). \tag{A9}$$

Moreover, the weight μ takes the unique value $\mu=\lambda_3-\lambda_1$. It follows that the matrix $N^{\lambda\mu}(\lambda_1)$ of the theorem is given by

$$N^{\lambda\mu}_{\beta\beta'}(\lambda_1)=M^{\lambda}_{\beta\mu,\beta'\mu}\,\delta_{\mu,\lambda_3-\lambda_1} \tag{A10}$$

and that it has the same rank as M^{λ}. This complete the proof of the theorem.

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Eichler integrals and string theory

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In this article, it is shown how to obtain objects called *Eichler integrals* in the mathematical literature that can be used for calculating scattering amplitudes in string theory. These Eichler integrals are also new examples of Eichler integrals with poles. © *1996 American Institute of Physics.* [S0022-2488(96)00804-2]

I. INTRODUCTION

The concept of an Eichler integral is closely related to the concept of automorphic forms. Although automorphic forms have a large range of applications in physics and, in particular, in string theory, Eichler integrals remain relatively unknown objects to both mathematicians and physicists. One can picture Eichler integrals as a generalization of the concept of automorphic forms, and they are related to the better known *Beltrami differentials* that are used in string theory, in particular, in the calculation of multiloop scattering amplitudes of strings.

This article begins with a description of the main properties of automorphic forms with some examples that will be useful when we describe the new Eichler integrals. The definition of Eichler integrals is given next, with some examples that can be used in string theory.

II. AUTOMORPHIC FORMS

An automorphic form of weight q is a function[1] $\phi(z)$ that transforms in the following way under a projective transformation P_a:

$$\phi(P_a(z))=\left[\frac{\partial P_a(z)}{\partial z}\right]^q \phi(z).$$

Automorphic forms with just one pole will be more of our interest, since the order of the pole is limited in a simple way by the Riemann–Roch theorem.[2] We now give some examples of these functions.

A. Example 1

A simple example of an automorphic form of weight q can be given for the case where there is just one projective transformation $P(z)$, given by

$$P(z)=w(z-\alpha)+\alpha,$$

where α is the finite fixed point of the transformation (the other fixed point is at infinity) and w is the multiplier. An automorphic form $\phi(z)$ of weight q can then be given by

$$\phi(z)=(z-\alpha)^q.$$

In the case where $P(z)$ has two finite fixed points, when it can be expressed by

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$$P(z)=\frac{\alpha(z-\beta)-w\beta(z-\alpha)}{(z-\beta)-w(z-\alpha)},$$

an automorphic form of weight q is given by

$$\phi(z)=[(z-\alpha)(z-\beta)]^q.$$

B. Example 2

In the case of a single projective transformation $P(z)$ with just one finite fixed point, we may have automorphic forms with poles, given by

$$\phi_n(z)=(z-\alpha)^q\left(\frac{\partial}{\partial t}\right)^{n-1}\wp(t),\quad t=\ln(z-\alpha)-\ln(-\alpha),$$

where n is the order of the pole and $\wp(t)$ is the Weierstrass $\wp$ function[3] with periods $\ln w$ and $2\pi i$. These functions have poles of orders $\leqslant n$ at $z=0$.

In the case of $P(z)$ having two finite fixed points, we have

$$\phi_n(z)=[(z-\alpha)(z-\beta)]^q\left(\frac{\partial}{\partial t}\right)^{n-1}\wp(t),\quad t=\ln\left(\frac{z-\alpha}{z-\beta}\right)-\ln\left(\frac{\alpha}{\beta}\right)$$

instead.

C. Example 3

Still another way of obtaining an automorphic form on a genus g Riemann surface is considering the following function[1] (called a Poincaré series):

$$\phi(z,\zeta)=\sum_a\left[\frac{dT_a(z)}{dz}\right]^{-q}\frac{\zeta-k}{T_a(z)-\zeta},$$

where k is an arbitrary constant and the sum Σ_a is over all the elements $T_a(z)$ of the Schottky group, which is the group of all possible combinations of the projective transformations $P_b(z)$, $b=1,\ldots,g$.

Under a transformation $z\to T_b(z)$, one gets

$$\phi(T_b(z),\zeta)=\sum_a\left[\frac{dT_a\ T_b(z)}{dz}\right]^{-q}\frac{\zeta-k}{T_aT_b(z)-\zeta}.$$

We now perform a change of variables $T_aT_b(z)=T_c(z)$. Using the chain rule we have

$$\frac{d}{dz}\,T_c(z)=\left[\frac{d}{dz}\,T_aT_b(z)\right]\times\frac{d}{dz}\,T_b(z),$$

so that we have

$$\phi(T_b(z),\zeta)=[T_b'(z)]^q\sum_a\left[\frac{dT_c(z)}{dz}\right]^{-q}\frac{\zeta-k}{T_c(z)-\zeta}.$$

Since we are summing over all the elements of the Schottky group, the series above is equivalent to the original one, so that we have

$$\phi(T_b(z),\zeta)=[T_b'(z)]^q\phi(z,\zeta),$$

i.e. it is an automorphic form of weight q.

D. Example 4

In the multiloop case, let us consider only projective transformations P_a with finite fixed points α_a and β_a. We then consider the following series:

$$P_w(z)=\sum_b \frac{(z-\alpha_b)(z-\beta_b)}{w_b(\alpha_b-\beta_b)}\frac{\delta w_b}{\epsilon}, \tag{1}$$

where the sum is over all the elements of the Schottky group formed by these transformations and δw_b and ϵ are infinitesimals. We then have that

$$\begin{aligned}P_w(T_a(z))&=\sum_b [T_a(z)-\alpha_b][T_a(z)-\beta_b]\\&=\frac{T_a'(z)}{w_a(\alpha_a-\beta_a)^2}\times\sum_b \frac{1}{w_b(\alpha_b-\beta_b)}(\alpha_a-w_a\beta_a-\alpha_b+w_a\alpha_b)\\&\quad\times(\alpha_a-w_a\beta_a-\beta_b+w_a\beta_b)\left[z-\frac{(\alpha_a\beta_a-w_a\alpha_a\beta_a-\alpha_b\beta_a+w_a\alpha_b\alpha_a)}{(\alpha_a-w_a\beta_a-\alpha_b+w_a\alpha_b)}\right]\\&\quad\times\left[z-\frac{(\alpha_a\beta_a-w_a\alpha_a\beta_a-\beta_b\beta_a+w_a\beta_b\alpha_a)}{(\alpha_a-w_a\beta_a-\beta_b+w_a\beta_b)}\right]\frac{\delta w_b}{\epsilon}.\end{aligned}$$

Making then the following change of variables:

$$\alpha_c=\frac{(1-w_a)\alpha_a\beta_a-(\beta_a-w_a\alpha_a)\alpha_b}{\alpha_a-w_a\beta_a-(1-w_a)\alpha_b}, \tag{2}$$

$$\beta_c=\frac{(1-w_a)\alpha_a\beta_a-(\beta_a-w_a\alpha_a)\beta_b}{\alpha_a-w_a\beta_a-(1-w_a)\beta_b}, \tag{3}$$

$$w_c=w_b, \tag{4}$$

we may write

$$P_w(T_a(z))=T_a'(z)\sum_c \frac{(z-\alpha_c)(z-\beta_c)}{w_c(\alpha_c-\beta_c)}\frac{\delta w_c}{\epsilon},$$

where we have used

$$\delta w_c=\frac{\partial w_c}{\partial w_b}\delta w_b.$$

Since we are summing over all elements of the Schottky group (with the condition that the fixed points are finite), we then see that the expression on the right-hand side is equivalent to the series we started with, so that

$$P_w(T_a(z))=T_a'(z)P_w(z).$$

We may also consider the following two series:

$$P_\alpha(z)=\sum_b \frac{(1-w_b)}{w_b(\alpha_b-\beta_b)^2}(z-\beta_b)^2\frac{\delta\alpha_b}{\epsilon}, \tag{5}$$

$$P_\beta(z)=-\sum_b \frac{(1-w_b)}{(\alpha_b-\beta_b)^2}(z-\alpha_b)^2\frac{\delta\beta_b}{\epsilon}. \tag{6}$$

Using the same change of variables (2)–(4) and the fact that

$$\delta\alpha_c=\frac{\partial\alpha_c}{\partial\alpha_b}\,\delta\alpha_b=\frac{w_a(\alpha_a-\beta_a)^2}{[\alpha_a-w_a\beta_a-(1-w_a)\alpha_b]^2}\,\delta\alpha_b,$$

$$\delta\beta_c=\frac{\partial\beta_c}{\partial\beta_b}\,\delta\beta_b=\frac{w_a(\alpha_a-\beta_a)^2}{[\alpha_a-w_a\beta_a-(1-w_a)\beta_b]^2}\,\delta\beta_b,$$

we then obtain

$$P_\alpha(T_a(z))=T_a'(z)P_\alpha(z),$$

$$P_\beta(T_a(z))=T_a'(z)P_\beta(z).$$

We have then obtained three examples of automorphic forms with weight 1.

III. EICHLER INTEGRALS

An Eichler integral of order q is defined in the following way:[4,5] it is a function $f(z)$ that transforms like

$$f(T_a(z))=\left[\frac{\partial T_a(z)}{\partial z}\right]^q[f(z)+P^{q+1}(z)],$$

where $P^{q+1}(z)$ is a polynomial at most of order $q+1$. It can be pictured as a generalization of the concept of automorphic form. Eichler integrals are related with automorphic forms in the following way:[4] given an Eichler integral of order q, we then have

$$\phi(z)=\left(\frac{\partial}{\partial z}\right)^{2q+1}f(z), \tag{7}$$

where $\phi(z)$ is an automorphic form of weight $q+1$, i.e.

$$\phi(T_a(z))=\left[\frac{\partial T_a(z)}{\partial z}\right]^{q+1}\phi(z).$$

Here are some examples of Eichler integrals.

A. Example 1

A trivial example of an Eichler integral is given by any polynomial of order 2, i.e. any function of the form

$$f(z)=a+bz+cz^2,$$

where a, b, and c are constants. Such a function transforms like

$$f(T_a(z))=T_a'(z)\left[f(z)+\frac{1}{w(\alpha-\beta)^2}\,(d+ez+fz^2)\right],$$

where

$$d=(1-w)^2a+(1-w)(\alpha-w\beta)b-[w\beta^2(1-w)-2w(\alpha\beta-1)+w\alpha^2]c,$$

$$e=2(w\alpha-\beta)(1-w)a-2\alpha\beta(1-w)^2b+[2w\beta(\alpha+\beta)-2\alpha\beta(w\beta+\alpha)]c,$$

$$f=(\beta^2-w\alpha^2)(1-w)a+\alpha\beta(1-w)(\beta-w\alpha)b-w\alpha\beta^2(2-w\alpha)c.$$

Differentiating it three times, we obtain

$$\frac{d^3}{dz^3}\,f(z)=0,$$

which is a sort of automorphic form (a trivial one) so Eq. (7) holds.

B. Example 2

There are not many examples of Eichler integrals with poles in the literature. The first one was given by Ahlfors.[4] In our notation, his Eichler integral is given by

$$f(z,\zeta)=\sum_b\,[z-T_b(\zeta)]^{-1}[T_b'(\zeta)]^q,$$

where the sum is over all elements of the Schottky group.

This function transforms in the following way:

$$f(T_a(z),\zeta)=[T_a'(z)]^{q-1}\left\{f(z,\zeta)+\sum_b\,\left[\frac{T_a'T_b(\zeta)}{(T_a'(z))^{q-1/2}}-1\right]\times[z-T_b(\zeta)]^{-1}[T_b'(\zeta)]^q\right\}.$$

The second term on the right-hand side can be shown to be a polynomial of degree q. This Eichler integral has just one simple pole at $\zeta=z$.

In order to obtain Eichler integrals with poles of higher orders, one just has to form derivatives with respect to ζ:

$$f_{k+1}(z,\zeta)=\frac{\partial^k}{\partial\zeta^k}\,f(z,\zeta),$$

where $f_{k+1}(z,\zeta)$ is an Eichler integral with a pole of order $k+1$ at $\zeta=z$.

C. Example 3

As it will be shown now, not all Eichler integrals must transform in such a complicated way. It is not hard to find examples of Eichler integrals with simple and useful transformations.

As explained before, an Eichler integral can be obtained by simply integrating an automorphic form a certain number of times. It is possible to show that every automorphic form of weight q can be expressed in terms of the following Poincaré series:

$$g(z,\zeta)=\sum_b\,[T_b'(z)]^{-q}\,\frac{\zeta-k}{T_b(z)-\zeta},\tag{8}$$

where k is an arbitrary constant.

If we now take the case $q=-1$, we have simply

$$g(z,\zeta)=\sum_b\ [T_b'(z)]^{-1}\ \frac{\zeta-k}{T_b(z)-\zeta}=\sum_b\ (\zeta-k)\left[\frac{1}{z+(b_b-d_b\zeta)/(a_b-c_b\zeta)}-\frac{1}{z+d_b/c_b}\right],$$

and, by (7), we may obtain an Eichler integral of weight zero simply by integrating this expression once. Doing this we obtain the following:

$$f(z,\zeta)=\sum_b\ (\zeta-k)\ln\left(\frac{c_b}{(a_b-c_b\zeta)}\ \frac{[(a_b-c_b\zeta)z+(b_b-d_b\zeta)]}{(c_bz+d_b)}\right)+c',$$

where c' is a constant of integration that can be set to zero.

We may then make the following change of coefficients:

$$\begin{aligned} a_m&=a_b-c_b\zeta, \quad c_m=c_b,\\ b_m&=b_b-d_b\zeta, \quad d_m=d_b, \end{aligned} \tag{9}$$

and the function $f(z,\zeta)$ becomes simply

$$f(z,\zeta)=\sum_m\ (\zeta-k)\ln\left(\frac{c_m}{a_m}\ \frac{(a_mz+b_m)}{(c_mz+d_m)}\right).$$

Performing the conformal transformation,

$$T_a(z)=\frac{a_az+b_a}{c_az+d_a},$$

with $c_a\neq 0$ in the expression above, we obtain

$$f(T_a(z),\zeta)=\sum_m\ (\zeta-k)\ln\left(\frac{c_m}{a_m}\ \frac{[a_m(a_az+b_a)+b_m(c_az+d_a)]}{[c_m(a_az+b_a)+d_m(c_az+d_a)]}\right). \tag{10}$$

If we now make another change of variables,

$$\begin{aligned} a_b&=a_ma_a+b_mc_a, \quad c_b=c_ma_a+d_mc_a,\\ b_b&=a_mb_a+b_md_a, \quad d_b=c_mb_a+d_md_a, \end{aligned} \tag{11}$$

we then have

$$\begin{aligned} f(T_a(z),\zeta)&=\sum_b\ (\zeta-k)\ln\left(\frac{(c_bd_a-c_ad_b)}{(a_bd_a-c_ab_b)}\ \frac{(a_bz+b_b)}{(c_bz+d_b)}\right)\\ &=\sum_b\ (\zeta-k)\left[\ln\left(\frac{c_b}{a_b}\ \frac{(a_bz+b_b)}{(c_bz+d_b)}\right)+\ln\left(\frac{a_b(c_bd_a-c_ad_b)}{c_b(a_bd_a-c_ab_b)}\right)\right]. \end{aligned} \tag{12}$$

Since we are summing over all transformations $T_b(z)$ with $c_b\neq 0$, the first term of expression (12) is just $f(z,\zeta)$, and we then have

$$f(T_a(z),\zeta)=f(z,\zeta)+\sum_b\ (\zeta-k)\ln\left(\frac{a_b(c_bd_a-c_ad_b)}{c_b(a_bd_a-c_ab_b)}\right). \tag{13}$$

The second term of expression (13) can be readily identified as a constant, i.e. a polynomial in z of degree 0, so that it is proved that the function $f(z,\zeta)$ is an Eichler integral with weight 0.

We now consider automorphic form (8) with weight -2:

$$g(z,\zeta)=\sum_b\ [T_b'(z)]^2\ \frac{\zeta-k}{T_b(z)-\zeta},$$

where k is a constant and the sum is over all elements of the Schottky group. According to the theory of Eichler integrals, if we integrate an automorphic form of weight -2 three times, we shall obtain an Eichler integral of weight 1. If we take $T_b(z)$ to be of the form

$$T_b(z)=\frac{a_bz+b_b}{c_bz+d_b},$$

we may then write this function in the following form:

$$g(z,\zeta)=\sum_b\ \frac{\zeta-k}{(a_b-c_b\zeta)}\frac{1}{(c_bz+d_b)^3[z+(b_b-d_b\zeta)/(a_b-c_b\zeta)]}.$$

This can be easily integrated. Considering the case where $c_b\neq 0$ and performing integration three times on this automorphic form, we obtain the following function:

$$\begin{aligned}f(z,\zeta)=\sum_b\ &\frac{1}{2}(\zeta-k)[(a_b-c_b\zeta)z+(b_b-d_b\zeta)]^2\\&\times\ln\left(\frac{c_b}{(a_b-c_b\zeta)}\frac{[(a_b-c_b\zeta)z+(b_b-d_b\zeta)]}{(c_b+d_b)}\right)\\&+\frac{1}{2c_b(a_b-c_b\zeta)}z-\frac{2(a_b-c_b\zeta)d_b+1}{4c_b^2(a_b-c_b\zeta)^2}+c_1z^2+c_2z+c_3,\end{aligned}\tag{14}$$

where c_1, c_2, and c_3 are constants resulting from the integrations. Choosing these integration constants in such a way as to cancel with the polynomial part of expression (14), we then obtain

$$\begin{aligned}f(z,\zeta)=\sum_b\ &\frac{1}{2}(\zeta-k)[(a_b-c_b\zeta)z+(b_b-d_b\zeta)]^2\\&\times\ln\left(\frac{c_b}{(a_b-c_b\zeta)}\frac{[(a_b-c_b\zeta)z+(b_b-d_b\zeta)]}{(c_b+d_b)}\right).\end{aligned}\tag{15}$$

We can now make the change of coefficients (9) and the function $f(z,\zeta)$ becomes

$$f(z,\zeta)=\sum_m\ \frac{1}{2}(\zeta-k)(a_mz+b_m)^2\ \ln\left(\frac{c_m}{a_m}\frac{(a_mz+b_m)}{(c_mz+d_m)}\right).\tag{16}$$

This expression should be an Eichler integral and we are going to show it indeed is. If we perform the conformal transformation

$$T_a(z)=\frac{a_az+b_a}{c_az+d_a},\tag{17}$$

with $c_a\neq 0$ in the expression above, we obtain

$$f(T_a(z),\zeta)=\sum_m \frac{1}{2}(\zeta-k)\left[\frac{a_m(a_az+b_a)+b_m(c_az+d_a)}{c_az+d_a}\right]^2 \times\ln\left(\frac{c_m}{a_m}\frac{[a_m(a_az+b_a)+b_b(c_az+d_a)]}{[c_m(a_az+b_a)+d_m(c_az+d_a)]}\right). \tag{18}$$

If we now make another change of variables, given by (11), we then have

$$f(T_a(z),\zeta)=T_a'(z)\sum_b \frac{1}{2}(\zeta-k)(a_bz+b_b)^2\ln\left(\frac{(d_ba_a-c_bb_a)}{(b_ba_a-a_bb_a)}\frac{(a_bz+b_b)}{(c_bz+d_b)}\right)$$
$$=T_a'(z)\sum_b \frac{1}{2}(\zeta-k)(a_bz+b_b)^2\left[\ln\left(\frac{c_b}{a_b}\frac{(a_bz+b_b)}{(c_bz+d_b)}\right)+\ln\left(\frac{a_b(d_ba_a-c_bb_a)}{c_b(b_ba_a-a_bb_a)}\right)\right]. \tag{19}$$

Since we are summing over all transformations $T_b(z)$ with $c_b\neq 0$, the first term of expression (19) is just $f(z,\zeta)$, and we then have

$$f(T_a(z),\zeta)=T_a'(z)\left[f(z,\zeta)+\sum_b \frac{1}{2}(\zeta-k)(a_bz+b_b)^2\ln\left(\frac{a_b(d_ba_a-c_bb_a)}{c_b(b_ba_a-a_bb_a)}\right)\right]. \tag{20}$$

The second term of expression (20) can be readily identified with a polynomial in z of degree 2 so that it is proved that the function $f(z,\zeta)$ is an Eichler integral.

D. Example 4

We consider now the case where there is just one projective transformation,

$$T(z)=\frac{az+d}{cz+d}, \tag{21}$$

that can be written in terms of the finite fixed point α and the multiplier w as

$$T(z)=w(z-\alpha)+\alpha. \tag{22}$$

In string theory, and, in particular, in the group theoretic approach,[6] we will be interested in functions that are associated with conformal transformations that cause infinitesimal changes in the moduli of a Riemann surface with genus g. In one loop, i.e., a Riemann surface with genus 1, we have one finite fixed point α, one fixed point at infinity, and the multiplier w. In order to fix the modular invariance of the theory, we must fix three variables. Besides the one fixed point that has been already fixed at infinity, we can choose to fix the finite fixed point and one of the variables associated with the incoming strings so that the multiplier w will be the only variable associated with the loop left.

We then want a function that has the effect of changing the multiplier w infinitesimally, i.e. we want a function that transforms like

$$f(T(z))=T'(z)f(z)-\frac{\partial T(z)}{\partial w}\frac{\delta w}{\epsilon}, \tag{23}$$

i.e.

$$f(T(z))=T'(z)\left[f(z)-\frac{\delta w}{\epsilon w}(z-\alpha)\right] \tag{24}$$

and

$$f(S(z))=f(z), \tag{25}$$

where $S(z)=e^{2\pi i}z$ and where ϵ and δw are infinitesimals.

A function that transforms in this way was found in Refs. 6 and 7 in the context of string theory. It is given by

$$f(z)=\frac{\delta w}{\epsilon w}(z-\alpha)\overline{\zeta}(\ln(z-\alpha)), \tag{26}$$

where the function $\overline{\zeta}(t)$ is given by

$$\overline{\zeta}(t)=\zeta(t)-\frac{\zeta(\pi i)}{\pi i}t.$$

The function $\zeta(t)$ is Weierstrass' ζ function,

$$\zeta(t)=\frac{1}{t}+\sum_{p\neq 0}\left(\frac{1}{t-p}+\frac{1}{p}+\frac{1}{p^2}\right),$$

where p is the semi-period of the function and is given by $p=nw_1+mw_2$, $(n,m\in\mathbf{Z})$, where

$$w_1=\ln w, \quad w_2=2\pi i.$$

The Weierstrass ζ function transforms in the following way:

$$\zeta(t+w_1)=\zeta(t)+2\zeta(w_1/2),$$

$$\zeta(t+w_2)=\zeta(t)+2\zeta(w_2/2),$$

and the term $\ln(z-\alpha)$ transforms like

$$\ln(T(z)-\alpha)=\ln w+\ln(z-\alpha),$$

$$\ln(e^{2\pi i}z-e^{2\pi i}\alpha)=\ln(2\pi i)+\ln(z-\alpha),$$

so that we have

$$f(T(z))=T'(z)\left[f(z)-\frac{\delta w}{\epsilon w}(z-\alpha)\right]. \tag{27}$$

The function $\overline{\zeta}(t)$ can be related to the theta function[3] in the following way:

$$\overline{\zeta}(t)=\frac{d}{dt}\ln\theta(t,\tau),$$

where $\theta(t,\tau)$ has periods $w_1=\ln w$ and $w_2=2\pi i$.

If we take the third derivative of the function $f(z)$, we obtain

$$g(z)=f'''(z)=\frac{\delta w}{\epsilon w}\frac{1}{(z-\alpha)^2}\left[\wp(t)+\frac{\zeta(\pi i)}{\pi i}-\wp''(t)\right],$$

where $t=\ln(z-\alpha)$ and $\wp(t)$ is Weierstrass' $\wp$ function with periods $w_1=\ln w$ and $w_2=2\pi i$, given by

$$\wp(t)=-\frac{d}{dt}\zeta(t)$$

which transforms like

$$\wp(t+w_1)=\wp(t+w_2)=\wp(t),$$

i.e. it is an elliptic function.

Since $\wp(t)$ and its derivatives do not change under a transformation of $t+\ln w$ or $t+2\pi i$, we then have

$$g(T(z))=\frac{1}{w^2}g(z)=[T'(z)]^{-2}g(z),$$

i.e. $g(z)$ is an automorphic form with weight -2, as expected from the relation (7). So we have verified that $f(z)$ is an Eichler integral.

E. Example 5

We shall now search for a function with transformation properties similar to those of (23), but now for the case of many projective transformations. We want a function that transforms like

$$f_w(T_a(z))=T_a'(z)f_w(z)-\frac{\partial T_a(z)}{\partial w_a}\frac{\delta w_a}{\epsilon}, \tag{28}$$

where

$$T_a(z)=\frac{\alpha_a(z-\beta_a)-w_a\beta_a(z-\alpha_a)}{(z-\beta_a)-w_a(z-\alpha_a)},$$

for every $a=1,\ldots,g$, i.e. the action of $T_a(z)$ on this function causes infinitesimal changes in the multipliers w_a. So this function must transform like

$$f_w(T_a(z))=T_a'(z)\left[f_w(z)+\frac{(z-\alpha_a)(z-\beta_a)}{w_a(\alpha_a-\beta_a)}\frac{\delta w_a}{\epsilon}\right]. \tag{29}$$

In addition to this, we also demand that

$$f_a(S_a(z))=f_a(z), \tag{30}$$

where $z\to S_a(z)$ is the transformation that takes z once around the a_a loop for $a=1,\ldots,g$.

In order to find the Eichler integral that transforms like this, we shall make analogies between the function in one loop and the function that we must have for the multiloop case. First we notice that the series $P_w(z)$ defined in (1),

$$P_w(z)=\sum_b \frac{(z-\alpha_b)(z-\beta_b)}{w_b(\alpha_b-\beta_b)}\frac{\delta w_b}{\epsilon}$$

transforms like

$$P_w(T_a(z))=T_a'(z)P_w(z),$$

so that it is the generalization for the multiloop case of the polynomial $(z-\alpha)$ for the one loop case.

Now we must try to find an analog of the Weierstrass ζ function suitable to the multiloop case. This can be obtained by first generalizing the concept of a θ function and of the Weierstrass ζ function. This function is given by the hyperelliptic ζ function[8,9] or best, the ζ function defined in the Appendix. In our first attempt we attach a $\zeta_b(v)$ function to every element of the series $P_w(z)$, so that we have

$$f_{1w}(z)=\sum_b \frac{\delta w_b}{\epsilon}\frac{(z-\alpha_b)(z-\beta_b)}{w_b(\alpha_b-\beta_b)}\overline{\zeta_b}(v).$$

This function will not transform the way we want, since the term $(z-\alpha_b)(z-\beta_b)/(\alpha_b-\beta_b)$ and the first Abelian integrals $v_b(z)$ do not transform in the same way. We then go to the next step, which is making ζ a function not of the first Abelian integrals $v_b(z)$, but of variables $u_b(z)$ (such a change of variables can be justified, as in Baker,[8] Sec. 192), such that

$$u_b(z)=\ln\left(\frac{z-\alpha_b}{z-\beta_b}\right)-\ln\left(\frac{\alpha_a}{\beta_a}\right).$$

Under a change $z\to T_a(z)$, these variables will change like

$$u_b(T_a(z))=\frac{T_a(z)-\alpha_b}{T_a(z)-\beta_b}=\frac{(\alpha_a-w_a\beta_a-\alpha_b+w_a\alpha_b)}{(\alpha_a-w_a\beta_a-\beta_b+w_a\beta_b)}$$
$$\times\frac{[z-(\alpha_a\beta_a-w_a\alpha_a\beta_a-\alpha_b\beta_a+\alpha_bw_a\alpha_a)/(\alpha_a-w_a\beta_a-\alpha_b+w_a\alpha_b)]}{[z-(\alpha_a\beta_a-w_a\alpha_a\beta_a-\beta_b\beta_a+\beta_bw_a\alpha_a)/(\alpha_a-w_a\beta_a-\beta_b+w_a\beta_b)]}.$$

Performing the same change of variables as in (2)–(4), we then obtain

$$\frac{T_a(z)-\alpha_b}{T_a(z)-\beta_b}=w_{ca}\frac{z-\alpha_c}{z-\beta_c},$$

where the coefficient w_{ca} is given by

$$w_{ca}=\frac{(1-w_a)\beta_c-(\beta_a-w_a\alpha_a)}{(1-w_a)\alpha_c-(\beta_a-w_a\alpha_a)},$$

so that

$$u_b(T_a(z))=\ln w_{ca}+u_c(z).$$

We then redefine the generalized θ function $\theta(v)$ in the following way:

$$\theta(u)=\sum_{n=-\infty}^{\infty}\exp\left[\sum_{c,d=1}^{g}(n_c+\delta_c)\frac{1}{2}\ln w_{cd}(n_d+\delta_d)+\sum_{c=1}^{g}2\pi i\gamma_c(n_c+\delta_c)+\sum_{c=1}^{g}u_c(n_c+\delta_c)\right].$$

This function transforms like

$$\theta(u+\Omega)=\exp\left\{-\sum_{c=1}^{g}p_c\left(u_c+\frac{1}{2}\Omega_c\right)-\sum_{c=1}^{g}[\pi ip_cq_c-2\pi i(q_c\delta_c-p_c\gamma_c)]\right\}\theta(u),$$

where Ω_b is now given by

$$\Omega_b=\sum_{c=1}^{g}(2\pi i\ \delta_{bc}p_c+\ln w_{bc}q_c)=2\pi ip_b+\sum_{c=1}^{g}\ln w_{bc}q_c.$$

Defining now

$$\overline{\zeta}_b(u)=\frac{\partial}{\partial u_b}\ln\theta(u), \tag{31}$$

we have

$$\overline{\zeta}_b(u(T_a(z)))=\overline{\zeta}_b(u)-\delta_{ab}$$

and

$$\overline{\zeta}_b(u(S_a(z)))=\overline{\zeta}_b(u).$$

We then define the following function:

$$f(z)=\sum_b\frac{\delta w_b}{\epsilon}\frac{(z-\alpha_b)(z-\beta_b)}{w_b(\alpha_b-\beta_b)}\overline{\zeta}_b(u(z)). \tag{32}$$

This function transforms like

$$\begin{aligned}f_w(T_a(z))&=T_a'(z)\sum_c\frac{\delta w_c}{\epsilon}\frac{(z-\alpha_c)(z-\beta_c)}{w_c(\alpha_c-\beta_c)}[\overline{\zeta}_c(u(z))-\delta_{ac}]\\&=T_a'(z)\left[\sum_c\frac{\delta w_c}{\epsilon}\frac{(z-\alpha_c)(z-\beta_c)}{w_c(\alpha_c-\beta_c)}\overline{\zeta}_c(u(z))-\frac{\delta w_a}{\epsilon}\frac{(z-\alpha_a)(z-\beta_a)}{w_a(\alpha_a-\beta_a)}\right]\end{aligned}$$

and

$$f_w(S_a(z))=f_w(z).$$

Since we are summing over all the elements of the Schottky group, we then have

$$f_w(T_a(z))=T_a'(z)\left[f_w(z)-\frac{\delta w_a}{\epsilon}\frac{(z-\alpha_a)(z-\beta_a)}{w_a(\alpha_a-\beta_a)}\right],$$

$$f_w(S_a(z))=f_w(z),$$

which are the transformation properties we wanted. So we have obtained the Eichler integral that has the effect of changing infinitesimally the variables w_a of a Riemann surface of genus g.

One way to verify this is a true Eichler integral is to take its third derivative. The result must be an automorphic form of weight -2. Taking the third derivative of (32), we have

$$g_w(z)\equiv\frac{d^3}{dz^3}f_a(z)=\sum_b\ \frac{\delta w_b}{\epsilon w_b}\left[\frac{(\alpha_b-\beta_b)}{(z-\alpha_b)(z-\beta_b)}\right]^2[\overline{\wp}_{bc}(u(z))-\overline{\wp}''_{bc}(u(z))],\tag{33}$$

where

$$\overline{\wp}_{bc}(u)=-\frac{\partial}{\partial u_c}\overline{\zeta}_b(u)$$

is the hyperelliptic $\wp$ function and

$$\overline{\wp}''_{bc}(u)=\left(\frac{\partial}{\partial u_c}\right)\overline{\wp}_{bc}(u_b).$$

It can be easily verified that $\overline{\wp}_{bc}(u)$ and its derivatives are invariant under changes $z\to T_a(z)$ and $z\to S_a(z)$, so that the function $g(z)$ transforms like

$$g_w(T_a(z))=(T'_a(z))^{-2}g_w(z),\tag{34}$$

i.e. it is an automorphic form of weight -2. This confirms $f_w(z)$ as an Eichler integral.

F. Example 6

In the same way we found a function (Eichler integral) that changes the variables w_a of a Riemann surface infinitesimally we now want to find a function that will change the variables α_a infinitesimally. This means this function must transform like

$$f_\alpha(T_a(z))=T'_a(z)f_\alpha(z)-\frac{\partial T_a(z)}{\partial\alpha_a}\frac{\delta\alpha_a}{\epsilon},$$

for every $a=1,\ldots,g$, what implies that we want this function to transform like

$$f_\alpha(T_a(z))=T'_a(z)\left[f_\alpha(z)+\frac{(1-w_a)}{w_a(\alpha_a-\beta_a)^2}(z-\beta_a)^2\frac{\delta\alpha_a}{\epsilon}\right].\tag{35}$$

We also demand that

$$f_a(S(z))=f_a(z).\tag{36}$$

The method to obtain this function is analogous to the one used in example 5, but now we use, instead of the series $P_w(z)$, the series (5)

$$P_\alpha(z)=\sum_b\ \frac{\delta\alpha_b}{\epsilon}\frac{(1-w_b)}{w_b(\alpha_b-\beta_b)^2}(z-\beta_b)^2.$$

The function (Eichler integral) with the properties we need is then given by

$$f_\alpha(z)=\sum_b\ \frac{\delta\alpha_b}{\epsilon}\frac{(1-w_b)}{w_b(\alpha_b-\beta_b)^2}(z-\beta_b)^2\overline{\zeta}_b(u).\tag{37}$$

G. Example 7

Similarly, if we want a function that changes the variables β_a infinitesimally, we then need it to transform like

$$f_\beta(T_a(z))=T_a'(z)f_\beta(z)-\frac{\partial T_a(z)}{\partial\beta_a}\frac{\delta\beta_a}{\epsilon},$$

i.e.

$$f_\beta(T_a(z))=T_a'(z)\left[f_\beta(z)+\frac{(1-w_a)}{(\alpha_a-\beta_a)^2}(z-\alpha_a)^2\frac{\delta\beta_a}{\epsilon}\right]. \tag{38}$$

We also demand that

$$f_\beta(S(z))=f_\beta(z). \tag{39}$$

We then use the series (6)

$$P_\beta(z)=\sum_b \frac{\delta\beta_b}{\epsilon}\frac{(1-w_b)}{(\alpha_b-\beta_b)^2}(z-\beta_b)^2,$$

and build the Eichler integral,

$$f_\beta(z)=\sum_b \frac{\delta\beta_b}{\epsilon}\frac{(1-w_b)}{(\alpha_b-\beta_b)^2}(z-\alpha_b)^2\overline{\zeta_b}(u), \tag{40}$$

which has the correct transformation properties.

This concludes our series of examples. The last three examples can be used in order to calculate the measure of the scattering of N bosonic strings in any order of perturbation theory (order g) through the Group Theoretic approach to string theory. These are also new examples of Eichler integrals with poles with some nicer transformation properties.

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APPENDIX: SOME GEOMETRICAL OBJECTS DEFINED ON A GENUS g RIEMANN SURFACE

1. Generalized θ functions

The generalized ϑ function is defined in the following way:[8]

$$\vartheta(v;\gamma,\delta)=\sum_{n=-\infty}^{\infty}\exp\left\{\sum_{a,b=1}^{g}\left[\frac{1}{2\pi i}v_a\eta_{(2)ab}v_b+\pi i(n_a+\delta_a)\tau_{ab}(n_b+\delta_b)\right]\right.$$
$$\left.+\sum_{a=1}^{g}\left[v_a(n_a+\delta_a)+2\pi i\gamma_a(n_a+\delta_a)\right]\right\},$$

where the sum $\Sigma_{n=-\infty}^{\infty}$ means the sum over all n_a, $a=1,\ldots,g$. Here, v_a, v_b are the g first Abelian integrals, $\eta_{(2)ab}$ is a symmetric $g\times g$ matrix, τ_{ab} is the period matrix, n_a, n_b are integers and γ_a, δ_a are vectors with g components that are the characteristics of the function.

If all the elements in the rows p and q are integers, this function transforms like[8]

$$\vartheta(v+\Omega;\gamma,\delta)=\exp\left\{\sum_{a=1}^{g}\left[H_a\left(v_a+\frac{1}{2}\,\Omega_a\right)-\pi i p_a q_a+2\pi i(q_a\delta_a-p_a\gamma_a)\right]\right\}\vartheta(v;\gamma,\delta),$$

where

$$H_a=\sum_{b=1}^{g}\left[2\,\eta_{(1)ab}p_b+2\,\eta_{(2)ab}q_b\right],$$

$$\Omega_a=2\pi i\sum_{b=1}^{g}\tau_{ab}p_b+2\pi i q_a,$$

where $\eta_{(1)ab}$ is a symmetric $g\times g$ matrix.

We can fix $\eta_{(2)ab}=0$. This implies

$$\eta_{(1)ab}=-\tfrac{1}{2}\,\delta_{ab}.$$

We then have the following function:

$$\theta(v;\gamma,\delta)=\sum_{n=-\infty}^{\infty}\exp\left\{\sum_{a,b=1}^{g}\pi i(n_a+\delta_a)\tau_{ab}(n_b+\delta_b)+\sum_{a=1}^{g}\left[v_a(n_a+\delta_a)+2\pi i\,\gamma_a(n_a+\delta_a)\right]\right\},$$

which transforms like

$$\theta(v+\Omega;\gamma,\delta)=\exp\left\{\sum_{a=1}^{g}\left[H_a\left(v_a+\frac{1}{2}\,\Omega_a\right)-\pi i p_a q_a+2\pi i(q_a\delta_a-p_a\gamma_a)\right]\right\}\theta(v;\gamma,\delta).$$

This is the function that is generally refered to as the generalized θ function in the literature.

We may define the well-known object called the prime form in terms of the generalized θ function, which is its most general definition. It is given by

$$E(z,\zeta)=\theta(v(z)-v(\zeta))\left[\sum_{a=1}^{g}\partial_a\theta(0)w_a(z)\right]^{-1/2}\left[\sum_{b=1}^{g}\partial_b\theta(0)w_b(\zeta)\right]^{-1/2},$$

where

$$\partial_a\theta(0)\equiv\frac{\partial}{\partial v_a}\,\theta(v)\bigg|_{v=0},\quad \partial_b\theta(0)\equiv\frac{\partial}{\partial v_b}\,\theta(v)\bigg|_{v=0},$$

and $w_a(v)$, $w_b(v)$ are first Abelian differentials.

2. Hyperelliptic ζ function

We now define the *hyperelliptic ζ function*:[8,9]

$$\zeta_a(v)=\frac{\partial}{\partial v_a}\ln\,\vartheta(v;\gamma,\delta).$$

This function transforms in the following way:

$$\zeta_a(v+\Omega)=H_a+\zeta_a(v)=\sum_{b=1}^{g}(2\eta_{(1)ab}p_b+2\eta_{(2)ab}q_b)+\zeta_a(v).$$

The analogy with the one loop ζ functions is complete when we associate the matrices $\eta_{(1)}$ and $\eta_{(2)}$ with the numbers $\zeta(w_1/2)$ and $\zeta(w_2/2)$, respectively. We then have the identity

$$\sum_{c=1}^{g}2\pi i\tau_{ac}\eta_{(2)cb}-2\pi i\eta_{(1)ab}=\pi i\delta_{ab}.$$

A function that will be more useful to us is one that is invariant under a change $\Omega_a=2\pi iq_a$ so that we must fix $\eta_{(2)ab}=0$. Such a function, say $\overline{\zeta}_a$, is defined by

$$\overline{\zeta}_a(v)=\frac{\partial}{\partial v_a}\ln\,\theta(v;\gamma,\delta)$$

and transforms like

$$\overline{\zeta}_a(v+\Omega)=-p_a+\overline{\zeta}_a(v).$$

More particularly, this function shows that the function $\overline{\zeta}$ is invariant under a change $\Omega_a=2\pi i\tau_{ab}p_b$ for $b\neq a$. It only changes, and then only by a constant term, under the transformation $\Omega_a=2\pi i\tau_{aa}p_a$ for any p_a.

3. Hyperelliptic $\wp$ function

We may now define a hyperelliptic $\wp$ function in the following way:[8,9]

$$\wp_{ab}=-\frac{\partial}{\partial v_b}\zeta_a(v)=-\frac{\partial}{\partial v_b}\frac{\partial}{\partial v_a}\ln\,\theta(v).$$

This function is invariant under changes $\Omega_a=2\pi i\Sigma_{b=1}^{g}\tau_{ab}+2\pi iq_a$, i.e.

$$\wp_{ab}(v+\Omega)=\wp_{ab}.$$

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(α,β)-derivations on quantum function algebras

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(α,β)-derivations, introduced by Cohn, are defined on several noncommutative function algebras including the Hopf function algebras of the quantum groups $SL_q(n)$, $n=2,3$, where their interpretation is most apparent. In analogy with algebraic groups, left-invariant (α,β)-derivations on the Hopf function algebra of $SL_q(n)$, $n=2,3$, generate its quantum universal enveloping algebra $U_q(\mathrm{sl}(n))$. Derivations and their algebras are also found on the non-Hopf, function algebras of two noncommutative varieties, which are constructed similarly to $SL_q(2)$ and $SL_q(3)$. General (α,β) derivations (analogs of arbitrary vector fields) are found for $SL_q(2)$ and the quantum plane. The analog of the tangent bundle $TSL_q(2)$ is defined, and its relation to derivations is discussed. Some examples of (α,β) derivations on commutative algebras are also given. Generalities about (α,β) derivations and their algebras are discussed. © *1996 American Institute of Physics.*
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I. INTRODUCTION

In algebraic group theory, derivations on the commutative Hopf function algebra (FA) of a Lie group can define the Lie algebra.[1] In this article a similar role is considered for (α,β) derivations (to be called (α,β)-D) on Hopf FAs dual to quantum groups. More generally (α,β)-Ds and algebras they generate are found on various other noncommutative, deformed (quantum) FAs. (α,β)-Ds have been defined and used in the theory of noncommutative rings.[2]

This work is in the spirit of algebraic groups and fits most naturally into the approach to quantum groups given by Manin[3] in noncommutative algebraic geometry (NAG). Because of its greater complexity (compared to algebraic geometry (AG)) NAG is barely in its formative stage.[2,4] However, algebraic quantum groups occupy such a special, small corner of NAG that at least some (α,β)-Ds can be fairly easily defined there, and they seem to fit into the theory in much the same way that ordinary derivations do in algebraic groups. We explain this a little more after giving, in the following paragraph, a brief summary of those aspects of algebraic groups which have been a useful guide.[1]

The Lie algebra of a Lie group G (over k) may be defined as the Lie algebra g of left-invariant vector fields on G or as the Lie algebra T_eG of tangent vectors to G at the identity $e\in G$. On the dual Hopf FA, H, these correspond, respectively, to the Lie algebra of left-invariant derivations $D:H\to H$ denoted by $\mathrm{der}_L(H)$ and the Lie algebra of derivations $d:H\to k$ denoted by $\mathrm{der}(H,k)$. These are all isomorphic, $g\cong T_eG\cong \mathrm{der}_L(H)\cong \mathrm{der}(H,k)$. The universal enveloping algebra (UEA) of g, $U(g)$, can then be defined as $U(\mathrm{der}_L(H))$ (and similarly for $\mathrm{der}(H,k)$). In later discussions this algebra will be denoted by Der. Thus, in summary, $U(g)\cong U(\mathrm{der}_L(H))\equiv \mathrm{Der}_L(H)$.

In this article (α,β)-Ds are defined on the Hopf FAs of $SL_q(2)$, $SL_q(3)$,[5] on two FAs which will often be referred to by their noncommutative varieties we call $V_{q,p}(2)$, $V_q(3)$, on two quantum planes, and on several commutative FAs. For the quantum groups $SL_q(2)$ and $SL_q(3)$, (α,β)-Ds provide a link between FAs and quantum UEA which parallels that in algebraic groups described above, e.g., $\mathrm{Der}_L(H_q)\cong U_q(\mathrm{sl}(2))$ where H_q is the Hopf FA of $SL_q(2)$. The (α,β)-Ds on the FAs of the other noncommutative varieties, $V_{q,p}(2)$, $V_q(3)$, and the quantum planes, are found in order to show that (α,β)-Ds exist on more general FAs than those of quantum groups. Generally ''FA'' will mean a noncommutative algebra which is a deformation of a commutative FA, e.g., the ones

just mentioned. In principle, general noncommutative algebras could be considered, but the valuable guidance of nearby commutative FAs would not be available.

There is some indication that, roughly, the pattern of (α,β)-Ds found in the above cases may also be present for (α,β)-Ds on many such varieties. This motivates the definition of a q variety (q-V) such that $V_{q,p}(2)$, $V_q(3)$, $\mathrm{SL}_q(2)$, and $\mathrm{SL}_q(3)$ appear as examples of q-Vs. Here the terminology of q-V is in analogy with an algebraic group, which is a variety. However, this is mostly formal. Except in Sec. IX, where varieties are explicitly defined, we work entirely with their FAs, even when ''variety'' is mentioned. Thus ''derivations on V'' will mean ''derivations on the FA of V.''

Unfortunately our notion of a q-V is too close to quantum groups to expose much about a possible role for (α,β)-Ds more generally in NAG. A discussion of that question is beyond the scope of this work.

Here is a summary of the contents. In Sec. II (α,β)-Ds are defined in more generality than is strictly necessary for the present work. However, an example of this generality is given in Sec. V in the construction of q-Vs. In Sec. III we discuss how Hopf algebras can arise from (α,β)-Ds of an unspecified FA. Section IV is not essential, but it shows the curious possibility of antiderivations on noncommutative FAs. In Sec. V q-Vs are defined from bialgebras, and the general structure of their derivations is outlined. Two examples of q-Vs, $V_{q,p}(2)$ and $V_q(3)$, are defined in Secs. VI and VII. In Sec. VI, (α,β)-Ds are defined on $V_{q,p}(2)$ and their derivation Hopf algebra $\mathrm{Der}_0(A)$ is found. Left-invariant (α,β)-Ds on $\mathrm{SL}_q(2)$ and the Hopf algebra $\mathrm{Der}_L(H_q)\cong U_q(\mathrm{sl}(2))$ appear as a special case. The adjoint action ''$\triangleright$'' is briefly considered in the context of (α,β)-Ds. In Sec. VII an algebra $\mathrm{Der}_0(A)$ of (α,β)-Ds on $V_q(3)$ is found and compared with $U_q(\mathrm{sl}(3))$, which is realized by left-invariant (α,β)-Ds on $\mathrm{SL}_q(3)$. In Sec. VIII general (α,β)-Ds and their Hopf algebra Der are found for the quantum plane. Two subalgebras of Der are found, including a Euclidean quantum group. Another Euclidean quantum group and the Heisenberg quantum group are found from a different quantum plane. Some general non-left-invariant derivations are found on $\mathrm{SL}_q(2)$. In Sec. IX we define a noncommutative variety which is formally the q analog of the tangent bundle of SL(2). This article is primarily concerned with (α,β)-Ds on noncommutative FAs. However, in Sec. X, (α,β)-Ds on several commutative FAs are considered. For other approaches to derivations and quantum groups see Refs. 6–8.

II. (α,β)-DERIVATIONS

In this section (α,β)-derivations[2] are defined on a generally noncommutative k-algebra A, and various preliminary results and general examples of (α,β)-Ds are given for use in later sections.

An (α,β)-D has two algebra homomorphisms (Homs), α and β which go into the definition of the Leibniz rule. (The name ''(α,β)-D'' will be a generic name for any such derivation as well as for a specific one involving α and β.) The following notation will be useful. The action of α (or any Hom) on $f\in A$ will be written variously as $\alpha(f)=\alpha f=f^\alpha$, according to economy and clarity. The action of a derivation D is similarly denoted by $D(f)=Df=f^D$. Reference to k, the ground field, is usually suppressed. Thus Hom means k-Hom (k-linear map), etc.

Let A, A', and A'' be noncommutative k-algebras, and let M be a left A' module and a right A'' module. M is not necessarily a left–right A'–A'' bimodule because module multiplication may not be associative; that is, for $f'\in A'$, $g''\in A''$, and $m\in M$, it may be that $f'(mg'')\neq(f'm)g''$; an example of this occurs in Sec. V. However, algebra Homs $\alpha{:}A\to A'$ and $\beta{:}A\to A''$ may exist such that

$$f^\alpha(mg^\beta)=(f^\alpha m)g^\beta \tag{2.1}$$

for all $f,g\in A$. Then M is an Im α-Im β bimodule which we call an (α,β) bimodule. Assume M to be an (α,β) bimodule. Let $D{:}A\to M$, $\alpha{:}A\to A'$, and $\beta{:}A\to A''$ be Homs which satisfy

$$(fg)^D = f^\alpha g^D + f^D g^\beta,$$
$$(f_1 f_2)^\alpha = f_1^\alpha f_2^\alpha, \quad (g_1 g_2)^\beta = g_1^\beta g_2^\beta \tag{2.2}$$

for all $f, g, f_1, f_2, g_1, g_2 \in A$. D, α, β are linear: $D(f+g) = Df + Dg$, etc.

The first equation expresses the derivation character of D in terms of α and β. The last two equations just state that α and β are *algebra* Homs, which, together with the (α,β) bimodule structure of M in Eq. (2.1), is necessary to make D well defined on arbitrary products. For example, the two ways to apply Eq. (2.2) to $(fgh)^D$ agree if $(fg)^\alpha h^D = f^\alpha g^\alpha h^D$, $f^D(gh)^\beta = f^D f^\beta g^\beta$, and $f^\alpha(g^D h^\beta) = (f^\alpha g^D)h^\beta \equiv f^\alpha g^D g^\beta$. Equations (2.2) constitute the (α,β) Leibniz rule, and D is called an (α,β)-D, often denoted by $\{\alpha,\beta,D\}$.

Comments on the Leibniz rule.

(1) It reduces to the ordinary Leibniz rule if $M = A' = A'' = A$ and $\alpha = \beta = id_A$, the identity map on A. This is the usual situation.

(2) Algebra Homs preserve the unit ($\alpha 1_A = 1_{A'}$ and $\beta 1_A = 1_{A''}$), so $D(1_A) = 0$, which makes D a k-derivation, i.e., $D: k \to 0$. α could be interpreted as an $(\alpha,0)$-D or a $(0,\alpha)$-D, but obviously it would not be a k-derivation, i.e., $\alpha 1_A = 1_{A'} \neq 0$ (similarly for β). In this work the terms ''derivation'' and ''(α,β)-D'' will always mean that $\alpha,\beta \neq 0$.

(3) It allows the possibility of having two derivations which act identically on the generators of A but differently on products, i.e., $D = D'$ on the generators but $(\alpha,\beta) \neq (\alpha',\beta')$. It can also happen that $D \neq D'$, while D and D' are both (α,β)-Ds. Both of these situations arise. A zero (α,β)-D and a zero (α',β')-D are equivalent.

(4) The Leibniz rule (2.2) can be represented by commutative diagrams as shown in Fig. 1, which will be used to define comultiplication in Sec. III.

(5) Our approach will start with (α,β)-Ds and see what structure they generate. On hindsight, interest in (α,β)-Ds for noncommutative A may be seen by reversing the logic. A and Der(A) are contravariantly related, so noncommutativity of A corresponds to noncocommutativity of Der(A). This in turn leads via (4) above to (α,β)-Ds and the Leibniz rule. The particular form of the coproduct of the (α,β)-Ds, as in Eq. (3.6), is discussed in the *comment on [,]* near the end of Sec. III.

(6) More general objects θ^i_j, $i, j = 1,\ldots,n$ can be defined[6]:

$$(fg)^{\theta^i_j} = \sum_k f^{\theta^i_k} g^{\theta^k_j}. \tag{2.3}$$

For $n=2$, θ^1_2 is a (θ^1_1,θ^2_2)-D.

Examples: The Leibniz rule is easily checked in each case.

(1) Let $M = A \otimes A$ have the usual left–right A–A bimodule structure and α, $\beta: A \to A$ be algebra Homs. Then $D: A \to A \otimes A$ defined by

$$D(f) = 1 \otimes f^\beta - f^\alpha \otimes 1$$

is an (α,β)-D. If $\alpha = \beta = id_A$, then D is the usual universal derivation defined for noncommutative algebras.[9]

(2) Given (α,β), $m \in M$ defines an (α,β)-D $D_m: A \to M$:

$$D_m f = f^\alpha m - m f^\beta.$$

(3) A recurring special case of (2) takes $M = A' = A'' = A$ and $m = 1_A$ [usually $m = c1_A$, $c \in k$; see (5) below]. Then we write $D = \alpha - \beta$:

$$(fg)^{\alpha-\beta} = f^\alpha g^\alpha - f^\beta g^\beta = f^\alpha g^{\alpha-\beta} + f^{\alpha-\beta} g^\beta. \tag{2.4}$$

(4) Let $D:A\to A$ be an (α,β)-D and ϕ, $\psi:A\to A$ be algebra Homs, then $\varphi D\psi$ is a $(\varphi\alpha\psi,\varphi\beta\psi)$-D. (Here $\varphi D\psi\equiv\phi\circ D\circ\psi$, $\phi\alpha\psi\equiv\phi\circ\alpha\circ\psi$, etc., mean composition of maps.) In particular, if α^{-1} exists, then $\alpha^{-1}D$ and $D\alpha^{-1}$ are, respectively, $(id,\alpha^{-1}\beta)$- and $(id,\beta\alpha^{-1})$-Ds. An analogous statement holds for β if β^{-1} exists. (In the general case (2.2), ΦD is an (α,β)-D, where $\Phi:M\to M$ is an (A',A'') bimodule homomorphism.)

(5) If D is an (α,β)-D and $f\in A$, then ''$f\cdot D$'' (left ''multiplication'' of D by f) is not in general an (α,β)-D or even necessarily a derivation at all. (This is not actually module multiplication; see Sec. VIII.) However, since $D:k\to 0$, multiplication by $c\in k$ makes sense, and $cD=Dc$ is an (α,β)-D. In particular, $c(\alpha-\beta)$ is an (α,β)-D. Note that $\alpha-\beta=-(\beta-\alpha)$ is also a (β,α)-D.

III. ALGEBRA OF DERIVATIONS

In this section $M=A'=A''=A$ is an unspecified FA. The (α,β) derivations $\{\alpha,\beta,D\}$ on A generate an associative algebra $\mathscr{D}er(A)$. Multiplication $m:\mathscr{D}er(A)\otimes\mathscr{D}er(A)\to\mathscr{D}er(A)$ is given by composition and the unit $\eta:k\to\mathscr{D}er(A)$ by $\eta(1)=id_A$. In general $\mathscr{D}er(A)$ is infinitely generated. In this section we consider a Hopf subalgebra $\mathrm{Der}(A)\subset\mathscr{D}er(A)$. $\mathrm{Der}(A)$ may also be infinitely generated. For most of the FAs considered later, we are interested in some finitely generated (denoted by subscript 0) Hopf subalgebra $\mathrm{Der}_0(A)\subset\mathrm{Der}(A)$. However, this distinction is unimportant in this section. Here the purpose is to formulate relations (abbreviated Rels.) which are natural for derivations to satisfy and which make $\mathrm{Der}(A)$ a Hopf algebra. Since A is unspecified, $\mathrm{Der}(A)$ only attains a general form; the structure constants remain undetermined. This general form of $\mathrm{Der}(A)$ gives a perspective on later examples.

Consider a set of derivations on A, $\{\alpha_i,\beta_i,D_i\}_{i=1,2,\ldots}$, which generate the algebra $\mathrm{Der}(A)=k\langle\alpha_1,\beta_1,D_1,\ldots\rangle$ with as yet unspecified Rels. The Leibniz rule (2.2) does not guarantee (in contrast to the usual Leibniz rule) that the commutator $[D_i,D_j]$ of two derivations is again a derivation. For this, $\{\alpha_i,\beta_i,D_i\}$ and $\{\alpha_j,\beta_j,D_j\}$ have to satisfy certain Rels., which we now find. Consider the action of $[D_i,D_j]$ on a product $fg\in A$:

$$(fg)^{[D_i,D_j]}=f^{D_iD_j}g^{\beta_i\beta_j}-f^{D_jD_i}g^{\beta_j\beta_i}+f^{\alpha_i\alpha_j}g^{D_iD_j}-f^{\alpha_j\alpha_i}g^{D_jD_i}+f^{\alpha_iD_j}g^{D_i\beta_j}-f^{D_j\alpha_i}g^{\beta_jD_i}+f^{D_i\alpha_j}g^{\beta_iD_j}-f^{\alpha_jD_i}g^{D_j\beta_i}. \tag{3.1}$$

Here $i\neq j$ is assumed; the case $i=j$ will be discussed below. In general the first four terms on the right-hand side will make the commutator a derivation if the following Rels. are satisfied:

$$\alpha_i\alpha_j=\alpha_j\alpha_i,\quad \beta_i\beta_j=\beta_j\beta_i, \tag{3.2a}$$

$$D_i\alpha_j=t_{ij}\alpha_jD_i,\quad D_j\beta_i=t_{ij}\beta_iD_j, \tag{3.2b}$$

$$D_j\alpha_i=t_{ji}\alpha_iD_j,\quad D_i\beta_j=t_{ji}\beta_jD_i, \tag{3.2c}$$

where $t_{ij},t_{ji}\in k$. If Eqs. (3.2) hold, then $[D_i,D_j]$ is an $(\alpha_i\alpha_j,\beta_i\beta_j)$-D:

$$(fg)^{[D_iD_j]}=f^{\alpha_i\alpha_j}g^{[D_i,D_j]}+f^{[D_i,D_j]}g^{\beta_i\beta_j}.$$

Rels. (3.2) are generally satisfied. If they are not satisfied and thus do not cause a pairwise cancellation among the last four terms in Eq. (3.1), then at least one of three things happens: (1) the commutator $[D_i,D_j]$ is not a derivation, (2) $[D_i,D_j]$ may still be an $(\alpha_i\alpha_j,\beta_i\beta_j)$-D due to more complicated cancellations among these terms, (3) $[D_i,D_j]$ may ''accidentally'' be a derivation but of a different type, say an (α,β)-D where $(\alpha,\beta)\neq(\alpha_i\alpha_j,\beta_i\beta_j)$. Situation (2) occurs in the Euclidean quantum group, example (4) in Sec. VIII, and (3) occurs in Sec. X: see Eq. (10.6).

Consider one of the Rels. (3.2b) or (3.2c), say the first one. By example (4) of Sec. II, $D_i\alpha_j$ is an $(\alpha_i\alpha_j,\beta_i\alpha_j)$-D, and α_jD_i is an $(\alpha_j\alpha_i,\alpha_j\beta_i)$-D. These must represent the same derivation. This is true iff $\alpha_j\alpha_i=\alpha_i\alpha_j$ and $\alpha_j\beta_i=\beta_i\alpha_j$. Extending this to all the Rels. in Eqs. (3.2b) and (3.2c) requires two more Rels.:

$$\alpha_j\beta_i=\beta_i\alpha_j, \quad \alpha_i\beta_j=\beta_j\alpha_i. \tag{3.2d}$$

If α_i^{-1} and β_i^{-1} exist, then there may be further Rels.:

$$\alpha_i\beta_i=\beta_i\alpha_i=id_A. \tag{3.3}$$

If so, then the two Rels. in Eqs. (3.2b) and (3.2c) involving D_j become the same, which can be written as $\alpha_iD_j\beta_i=t_{ij}D_j$, where $t_{ij}=(t_{ji})^{-1}$. In addition, the Rels. in Eq. (3.2d) become a consequence of Eqs. (3.3) and (3.2a). The same comment about D_i holds if $\alpha_j\beta_j=\beta_j\alpha_j=id_A$. Then one of the Rels. (3.2a) becomes dependent. Rels. (3.3) do not always exist as $V_{q,p}(2)$ shows, but we impose them when possible.

In the diagonal case $i=j$, where $[D_i,D_j]=0$ is a trivial derivation, Eq. (3.1) reduces to $0=0$ and does not yield any Rels. of the type (3.2). Thus, the Rels. (3.2) are assumed only for $i\neq j$. Any such Rels. which exist for $i=j$, do so ''voluntarily'' as happens for $V_{q,p}(2)$.

Suppose Rels. (3.2) are satisfied, so $[D_i,D_j]$ is an $(\alpha_i\alpha_j,\beta_i\beta_j)$-D. Then there are two possibilities for further Rels. among $\{\alpha_i,\beta_i,D_i\}$ and $\{\alpha_j,\beta_j,D_j\}$. One is that $[D_i,D_j]$ is proportional to $(\alpha_i\alpha_j-\beta_i\beta_j)$, which, is also an $(\alpha_i\alpha_j,\beta_i\beta_j)$-D (see example (3) in Sec. II):

$$[D_i,D_j]=c_{ij}(\alpha_i\alpha_j-\beta_i\beta_j), \tag{3.4}$$

where $c_{ij}\in k$. The second possibility is that among the derivations $\{\alpha_i,\beta_i,D_i\}_{i=1,\ldots}$ there is one, $\{\alpha_l,\beta_l,D_l\}$, which is proportional to $\{\alpha_i\alpha_j,\beta_i\beta_j,[D_i,D_j]\}$. Then there are Rels.

$$\alpha_i\alpha_j=\alpha_l, \quad \beta_i\beta_j=\beta_l, \quad [D_i,D_j]=c_{ij}^lD_l. \tag{3.5}$$

Generally Der(A) will satisfy Rels. (3.2), and some combination of Eqs. (3.4) and (3.5). These are either verified or imposed as constraints as follows. Each side of $\alpha_j\beta_i=\beta_i\alpha_j$ is an algebra Hom, so it is sufficient to check it on the generators of A. Each side of $D_i\alpha_j=t_{ij}\alpha_jD_i$ is a derivation of the same type, so if it holds on generators then it extends to A by the Leibniz rule. Equations (3.4) and (3.5) are proved similarly. The t_{ij} in Eqs. (3.2b) and (3.2c), c_{ij} in Eq. (3.4) and c_{ij}^l in Eq. (3.5) are the structure constants of Der(A).

Der(A) as a Bialgebra. Rels. (3.2)–(3.5) give Der(A) a bialgebra structure which we now discuss. The Leibniz rule as represented in Fig. 1 suggests a comultiplication for Der(A), namely, the map which takes the bottom arrows to the top arrows. Thus we define Δ:Der(A) $\rightarrow$Der(A)$\otimes$Der(A) by

$$\Delta D_i=\alpha_i\otimes D_i+D_i\otimes\beta_i,$$

$$\Delta\alpha_i=\alpha_i\otimes\alpha_i, \quad \Delta\beta_i=\beta_i\otimes\beta_i. \tag{3.6}$$

A coproduct of this form is naturally constructed for any (α,β)-D.

Rel. (3.3) is assumed whenever possible in order to give ΔD_i the same form as the coproducts for the quantized Kac–Moody algebras given in Ref. 5. Other choices, such as $\alpha_i=id$ or $\beta_i=id$ could have been made instead of Eq. (3.3). An example of this is mentioned in connection with the algebra (6.14).

Comment. Comultiplication for the θ^i_j in Eq. (2.3) would be[6]

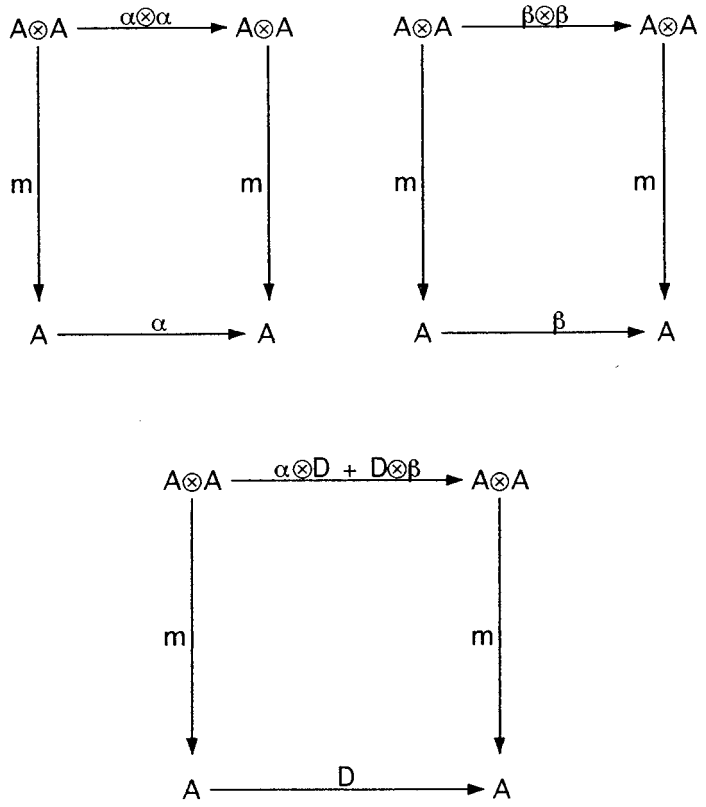

FIG. 1. Commutative diagrams expressing the Leibniz rule for an (α, β)-derivation.

$$\Delta(\theta_j^i) = \sum_k \theta_k^i \otimes \theta_j^k .$$

The counit ϵ:Der$(A) \to k$ consistent with Δ (i.e., satisfies $(\epsilon \otimes id)\Delta = id = (id \otimes \epsilon)\Delta$) is defined by

$$\epsilon(\alpha_i) = \epsilon(\beta_i) = 1, \quad \epsilon(D_i) = 0. \tag{3.7}$$

As is necessary, Δ and ϵ respect Rels. (3.2)–(3.5).

From example (4) of Sec. II, $\alpha_i D_j$ would appear in Fig. 1 as an $(\alpha_i\alpha_j, \alpha_i\beta_j)$-D and so has comultiplication

$$\Delta(\alpha_i D_j) = \alpha_i\alpha_j \otimes \alpha_i D_j + \alpha_i D_j \otimes \alpha_i\beta_j = (\alpha_i \otimes \alpha_i)(\alpha_j \otimes D_j + D_j \otimes \beta_j) = \Delta(\alpha_i)\Delta(D_j). \tag{3.8}$$

The second equality uses the definition of multiplication in Der$(A) \otimes$Der(A). Thus, Δ is an algebra Hom, which is necessary for Der(A) to form a bialgebra. Δ is coassociative, which is also necessary. Therefore the derivations $\{\alpha_i, \beta_i, D_i\}_{i=1,2,\ldots}$ generate a bialgebra $(\text{Der}(A), m, \eta, \Delta, \epsilon)$.

Der(A) as a Hopf algebra. If α_i^{-1} and β_i^{-1} exist for all i, then an antipode ι:Der$(A) \to$Der(A) can be defined by

$$\iota(\alpha_i) = \alpha_i^{-1}, \quad \iota(\beta_i) = \beta_i^{-1}, \quad \iota(D_i) = -\alpha_i^{-1} D_i \beta_i^{-1}. \tag{3.9}$$

ι preserves Rels. (3.2)–(3.5) and satisfies the compatibility conditions: $m(\iota\otimes id)\Delta = \eta\epsilon = m(id\otimes\iota)\Delta$. Then $(\mathrm{Der}(A), m, \eta, \Delta, \epsilon, \iota)$ forms a generally noncommutative and noncocommutative Hopf algebra.

Comment: $\mathrm{Der}(A)$ is defined to be a minimal algebra in the sense that it contains only those algebra Homs α_i, β_i which appear in derivations, i.e., in $\{\alpha_i, \beta_i, D_i\}_{i=1,2,\ldots}$. $\mathrm{Der}(A)$ could be enlarged by adding an unnecessary $\phi \in \mathrm{Hom}_{k\text{-}A}(A)$ to get $k\langle D_1, \alpha_1, \beta_1, \ldots, \phi\rangle$, which would contain, e.g., ϕD_i, a $(\phi\alpha_i, \phi\beta_i)$-D. Note that if D_i and D_j satisfy Eq. (3.2), then $\{\psi\alpha_i, \psi\beta_i, \psi D_i\}$ and the $\{\phi\alpha_j, \phi\beta_j, \phi D_j\}$ generally do not, even for new values of t_{ij} and t_{ji}. Thus, $[\psi D_i, \phi D_j]$ would not, in general, be an $(\psi\alpha_i\phi\alpha_j, \psi\beta_i\phi\beta_j)$-D. (See, however, the construction of the algebra (6.13)). This is true also for necessary αs and βs. Note that Eq. (3.8) also applies to a more general $(\phi\alpha\psi, \phi\beta\psi)$-D, $\phi D\psi$, where $\phi, \psi: A\to A$ are any algebra Homs and $\Delta\phi = \phi\otimes\phi$ and $\Delta\psi = \psi\otimes\psi$.

Special case: Let $i \neq j$, and suppose $\alpha_i = \alpha_j = \alpha$ and $\beta_i = \beta_j = \beta$, i.e., D_i, D_j are both (α,β)-Ds. Then the derivation Rels. reduce to

$$\alpha\beta = \beta\alpha, \quad D_i\alpha = u\alpha D_i, \quad D_j\beta = u\beta D_j,$$
$$D_j\alpha = v\alpha D_j, \quad D_i\beta = v\beta D_i, \tag{3.10a}$$

where $t_{ij} = u$, $t_{ji} = v$, and Eq. (3.4) becomes

$$[D_i, D_j] = c_{ij}(\alpha^2 - \beta^2). \tag{3.10b}$$

This is the form of $\mathrm{SL}_q(2)$ in Eq. (6.12), where α, β also satisfy Eq. (3.3).

Comment on [,]. The development of $\mathrm{Der}(A)$ starting with Eq. (3.1) has relied on the ''classical'' commutator. The coproduct (3.6) in $\mathrm{Der}(A)$ follows directly from the definition (2.2) (via the third of the diagrams in Fig. 1). The commutator and the coproduct (3.6) (or equivalently the (α,β)-Ds) are linked by Rels. (3.2b) and (3.2c). On the one hand these Rels. arise as derivation conditions on the commutator and on the other they impose conditions on the α_i, β_i, which show up in the coproducts (3.6). Instead of $[D_i, D_j]$, the adjoint action[8,10] $D_i \triangleright D_j$ could be considered in Eq. (3.1). This would alter Rels. (3.2b) and (3.2c), thereby also possibly alter the coproduct (3.6). The resulting derivation algebra $\mathrm{Der}_{\triangleright}(A)$ may, in general, be different from $\mathrm{Der}(A)$. $\mathrm{Der}_{\triangleright}(A)$ and $\mathrm{Der}(A)$ are compared for the case of $\mathrm{SL}_q(2)$ at the end of Sec. VI.

Comment on Der(H,k). For algebraic Lie groups, the Lie algebra of left-invariant derivations $D: H\to H$ is isomorphic to the Lie algebra of derivations $D': H\to k$; $\mathrm{Der}_L(H) \cong \mathrm{Der}(H,k)$.[1] They are related by $D' = \epsilon D$ and $D = (id\otimes D')\Delta$. The same result holds for (α,β)-Ds on noncommutative Hopf algebras. Thus, for the FA H_q, the algebra of left-invariant (α,β)-Ds α, β, $D: H_q\to H_q$ is isomorphic to the algebra of (α',β')-Ds $\{\alpha', \beta', D'\}: H_q\to k$, i.e., $\mathrm{Der}_L(H_q) \cong \mathrm{Der}(H_q, k)$. D and D' are related by $\epsilon: H_q\to k$: $D' = \epsilon D$, $\alpha' = \epsilon\alpha$, $\beta' = \epsilon\beta$, and $D = (id\otimes D')\Delta$, $\alpha = (id\otimes\alpha')\Delta$, $\beta = (id\otimes\beta')\Delta$. $\mathrm{Der}(H_q, k)$ will not be discussed further in this work.

IV. ANTIDERIVATIONS

In this section it is shown how a noncommutative FA, A, allows antiderivations, which are just a novelty here and are not used elsewhere in the article. An algebra antiHom is a Hom $\kappa: A\to A$ satisfying $(fg)^\kappa = g^\kappa f^\kappa$. Antiderivations stand in the same relation to algebra antiHoms as derivations do to algebra Homs.

E will be called a (π,ω) antiderivation (antiD) if $E, \pi, \omega: A\to A$ are Homs satisfying the (reversing) Leibniz rule

$$(fg)^E = g^\pi f^E + g^E f^\omega,$$
$$(g_1 g_2)^\pi = g_2^\pi g_1^\pi, \quad (f_1 f_2)^\omega = f_2^\omega f_1^\omega \tag{41}$$

for fs and gs in A.

The derivations given in the examples at the end of Sec. II have their counterparts for antiderivations which are briefly stated here. (i) Two algebra antiHoms π and ω define a (π,ω) antiD $E:A\to A\otimes A$, $Ef=1\otimes f^{\omega}-f^{\pi}\otimes 1$. (ii) $m\in M$ and the antiHoms $\chi:A\to A'$ and $\kappa:A\to A''$ define the (χ,κ) antiD $E_m:A\to M$ given by $E_m f=f^{\chi}m-mf^{\kappa}$. (iii) $D=\omega-\pi:A\to A$ is a (π,ω) antiD. (iv) If E is a (π,ω) antiD and ϕ is an algebra Hom then ϕE (recall $\phi E=\phi\circ E$) is a $(\phi\pi,\phi\omega)$ antiD. (Note that $\phi\pi$ and $\phi\omega$ are algebra antiHoms.) There is a similar statement for $E\phi$. Algebra antiHoms can be used to map derivations to antiderivations and vice versa. Thus, for example, if D is an (α,β)-D and κ is an algebra antiHom, then κD is a $(\kappa\beta,\kappa\alpha)$ antiD, and $D\kappa$ is an $(\alpha\kappa,\beta\kappa)$ antiD.

Many antiderivations can be formed from a derivation and vice versa. For example, if $\xi=\alpha^m\beta^n\kappa^{2k+1}$ and $\zeta=\alpha^{m'}\beta^{n'}\kappa^{2k'}$, then $\xi D\zeta$ is a $(\xi\beta\zeta,\xi\alpha\zeta)$ antiD. This suggests that if an antiautomorphism exists, then there are as many antiderivations as derivations.

V. DERIVATIONS AND q-VARIETIES

This section consists of three parts. The first part presents two types of derivations, L,R, to add to the examples in Sec. II. In the second part, it is shown how L,R can be used to construct FAs of the quantum groups $\mathrm{SL}_q(2)$, $\mathrm{SL}_q(3)$ and also $V_{q,p}(2)$, $V_q(3)$ (given in Secs. VI and VII). The latter are not quantum groups, but their construction is inspired by $\mathrm{SL}_q(2)$ and $\mathrm{SL}_q(3)$. We refer to an object constructed from L,R as a q-V. The third part describes, in a general way, how derivations on q-Vs are defined.

(i) *Derivations L and R.* The derivations L,R depend only on operations available in any bialgebra B. Thus, B could be taken to be an arbitrary bialgebra even though applications only use free matrix bialgebras (to yield q-Vs).

Let $(B,m,\eta,\Delta,\epsilon)$ be a bialgebra considered as a FA. $L,R:B\to B$ are defined in terms of an algebra antiHom $s:B\to B$, $(fg)^s=g^sf^s$:

$$\eta\epsilon,\quad l=m(id\otimes s)\Delta,\quad r=m(s\otimes id)\Delta, \tag{5.1}$$

$$L=l-\eta\epsilon,\quad R=r-\eta\epsilon. \tag{5.2}$$

R and L are not derivations like Eq. (2.4) because l and r are not algebra Homs like α and β (and $\eta\epsilon$) (i.e., $(fg)^l\neq f^lg^l$). Nevertheless, L and R can be interpreted as derivations in the more general context of Eq. (2.2). l and r in Eq. (5.1) are reinterpreted in terms of

$$\lambda=(id\otimes\sigma)\Delta:B\to B\otimes B^{\mathrm{op}},\quad \rho=(\sigma\otimes id)\Delta:B\to B^{\mathrm{op}}\otimes B, \tag{5.3}$$

$$\sigma:B\overset{s}{\to}B\overset{\mathrm{op}}{\to}B^{\mathrm{op}},$$

where B^{op} is the opposite algebra to B. σ is an algebra Hom (because s and op are algebra antiHoms) and thus λ and ρ are also algebra Homs. The target B of $L,R:B\to B$ will be interpreted, respectively, as $(\lambda,\eta\epsilon)$ and $(\eta\epsilon,\rho)$ bimodules. In the notation of Eq. (2.2), $A'=B\otimes B^{\mathrm{op}}$ and $A''=B$ for L ($A'=B$ and $A''=B^{\mathrm{op}}\otimes B$ for R) which uses left $B\otimes B^{\mathrm{op}}$ (right $B^{\mathrm{op}}\otimes B$) module multiplication $(f\otimes g^{\mathrm{op}})h=fhg$ ($h(f^{\mathrm{op}}\otimes g)=fhg$). Note that $(\lambda,\eta\epsilon)$ and $(\eta\epsilon,\rho)$ satisfy Eq. (2.1). With these definitions L,R satisfy the Leibniz rule:

$$(fg)^L=f^{\lambda}g^L+f^Lg^{\eta\epsilon},\quad (fg)^R=f^{\eta\epsilon}g^R+f^Rg^{\rho}, \tag{5.4}$$

which shows that L is a $(\lambda,\eta\epsilon)$-D and R is an $(\eta\epsilon,\rho)$-D.

(ii) *q-Vs from L,R.* Here, L and R in Eqs. (5.2) and (5.4) can be used to define (the FAs of) q-Vs such as $\mathrm{SL}_q(2)$, $\mathrm{SL}_q(3)$, $V_{q,p}(2)$, and $V_q(3)$. Let X_i, $i=1,2,\ldots,n$ be the generators of B. Consider the ideal $I\subset B$,

$$I=(L(X_i),R(X_i))_{i=1,2,\ldots,n}. \tag{5.5}$$

The Rels. $L(X_i),R(X_i)$ are not necessarily independent. Note that L and R are actually derivations to I, i.e., $L,R:B\to I$.

Each choice of s in $L=L_s$ and $R=R_s$ defines an ideal $I=I_s$ in Eq. (5.5). This defines the FA, $A=A_s$, dual to a q-V, $A_s\leftrightarrow V_s$:

$$A_s=B/I_s. \tag{5.6}$$

$\mathrm{SL}_q(2)$, $V_{q,p}(2)$, and $V_q(3)$ are of this form. The construction of I for $\mathrm{SL}_q(3)$ needs several derivations L,R to be defined as a q-V. Although this will not be given, the general situation is briefly discussed here.

Suppose there are many derivations, L_{lm} and R_{kn}, constructed from algebra Homs and anti-Homs $\Phi_m,S_l:B\to B$ as in Eqs. (5.1) and (5.2):

$$L_{kl}=m(\Phi_{Lk}\otimes S_{Ll})\Delta-\eta\epsilon,\quad R_{mn}=m(S_{Rm}\otimes\Phi_{Rn})\Delta-\eta\epsilon.$$

As in Eqs. (5.5) and (5.6) a collection of Rels. $\mathscr{R}$ generates an ideal, which in turn defines a FA:

$$\begin{gathered}\mathscr{R}=\{L_{kl}(X_i),R_{mn}(X_i),L_{k'l'}(X_i)-R_{m'n'}(X_i)\},\\ I_{\mathscr{R}}=(\mathscr{R}),\quad A_{\mathscr{R}}=B/I_{\mathscr{R}}.\end{gathered} \tag{5.7}$$

(iii) *Construction of Der(A).* $\mathrm{Der}(A)$ (or $\mathrm{Der}_0(A)$) is constructed from the subalgebra $\mathrm{Der}_I(B)\subset\mathscr{D}\mathscr{E}\mathscr{R}(B)$ of derivations which preserve I:

$$I^D\subset I,\quad I^\alpha\subset I,\quad I^\beta\subset I. \tag{5.8}$$

If the projection $B\to A$ is denoted by $f\to[f]$ then $D\in\mathrm{Der}_I(B)$ defines $D_A\in\mathrm{Der}(A)$ by $D_A[f]=[Df]$, $\alpha_A[f]=[\alpha f]$, etc. This gives a map $\mathrm{Der}_I(B)\to\mathrm{Der}(A)$. We will construct derivations $D\in\mathrm{Der}_I(B)$ and then not generally distinguish between $D\in\mathrm{Der}_I(B)$ and the corresponding $D_A\in\mathrm{Der}(A)$. D_A will be denoted by D. The conditions (5.8) impose Rels. on the α, β, $D\in\mathrm{Der}(A)$ which become the Rels. of $\mathrm{Der}(A)$.

The general structure of the $D\in\mathrm{Der}_0(A)$, as it exists for the examples $V_{q,p}(2)$, $\mathrm{SL}_q(2)$, and $V_q(3)$, is briefly discussed. $\mathrm{Der}_0(A)$ may be defined as generated by either or both of two types of derivations $D^l,D^r:B\to B$. Consider the decomposition

$$I=I_R+I_L,\quad I_L=(L(X_i))_{i=1,2,\ldots,n},\quad I_R=(R(X_i))_{i=1,2,\ldots,n}$$

of the ideal (5.5). Then Eq. (5.8) is satisfied by $\{\alpha^l,\beta^l,D^l\}$ and $\{\alpha^r,\beta^r,D^r\}$ each preserving I_L and I_R separately: $D^lI_L\subset I_L$, $D^lI_R\subset I_R$. $\alpha^lI_L\subset I_L$, $\alpha^lI_R\subset I_R$ etc. Actually, slightly more is true:

$$D^lL(X_i)=0,\quad D^lR(X_i)\in I_R, \tag{5.9a}$$

$$D^rR(X_i)=0,\quad D^rL(X_i)\in I_L. \tag{5.9b}$$

For purposes of example, as a matter of choice, we define $\mathrm{Der}_0(A)$ to include both D^l,D^r for $V_{q,p}(2)$ but only D^l for $V_q(3)$. When A is a Hopf algebra the $D^l(D^r)$ are actually left- (right-) invariant.

VI. (α,β) DERIVATIONS ON $V_{q,p}(2)$ AND $SL_q(2)$

In this section we define the FA, $A_{q,p}(2)=A$, of $V_{q,p}(2)$ and find a derivation algebra $\mathrm{Der}_0(A)$ with the structure (3.2) and (3.4). We get $\mathrm{Der}_L(H_q)$ of the Hopf FA, H_q, of $SL_q(2)$ as a special case.

A is constructed, as in Eq. (5.6), from the following free matrix bialgebra B and the antiHom $s:B\to B$:

$$B=k\langle T_{11},\ldots,T_{22}\rangle,$$

$$T^s_{11}=T_{22},\quad T^s_{22}=T_{11},\quad T^s_{12}=-pT_{12},\quad T^s_{21}=-q^{-1}T_{21},$$

with $q,p\in k$. Generally $p\neq q$; the case $p=q$ defining $SL_q(2)$ is discussed separately. The Rels. defined from s (as in Eq. (5.5)) are

$$l_{ij}=LT_{ij}=(TT^s-1)_{ij},\quad r_{ij}=RT_{ij}=(T^sT-1)_{ij},$$

where T is the matrix (T_{ij}). One Rel. is dependent. The ideals and algebras of interest corresponding to Eqs. (5.5) and (5.6) are

$$I_{q,p}\equiv I=(l_{ij},r_{ij})_{i,j=1,2},\quad I_q=I\big|_{p=q},$$

$$A=B/I,\quad H_q=B/I_q.$$

A is not a Hopf algebra, but H_q is the Hopf FA of $SL_q(2)$.

$\mathrm{Der}_0(A)$ is generated by derivations $\{\alpha^a_i,\beta^a_i,D^a_i\}:B\to B$ for $a=l,r$ and $i=1,2$ which satisfy

$$D^a_iI\subset I,\quad \alpha^a_iI\subset I,\quad \beta^a_iI\subset I. \tag{6.1}$$

They are defined on the generators of B by

$$\begin{gathered}D^l_{1,2}T_{ij}=T_{ij\pm1},\quad D^r_{1,2}T_{ij}=T_{i\pm1j},\\ \alpha^a_iT_{kl}=(\boldsymbol{\alpha}^a_i)_{kl}T_{kl},\quad \beta^a_iT_{kl}=(\boldsymbol{\beta}^a_i)_{kl}T_{kl},\end{gathered} \tag{6.2}$$

($T_{3j}=T_{i3}\equiv0$ by definition) and then extended to B by the Leibniz rule (2.2) (the scale factors $(\boldsymbol{\alpha}^a_i)_{kl},(\boldsymbol{\beta}^a_i)_{kl}\in k$). The Rels. defining $\mathrm{Der}_0(A)$ follow from Eqs. (6.1) and (3.2).

In the present case Rels. (3.2a)–(3.2d) have the form

$$\alpha^a_i\alpha^b_j=\alpha^b_j\alpha^a_i,\quad D^a_i\alpha^b_j=u^{ab}_{ij}\alpha^b_jD^a_i,\quad D^b_j\beta^a_i=u^{ab}_{ij}\beta^a_iD^b_j,\quad \text{etc.,} \tag{6.3}$$

which are obtained from the substitutions $\alpha_i\to\alpha^a_i$, $\alpha_j\to\alpha^b_j$, $\beta_i\to\beta^a_i$, $\beta_j\to\beta^b_j$, $D_i\to D^a_i$, $D_j\to D^b_j$, $t_{ij}\to u^{ab}_{ij}$, $t_{ji}\to u^{ba}_{ji}$. It is convenient to divide the discussion of Rels. (6.3) into three cases.

Case 1. Two subcases: $a=b=l$, $i=1$, $j=2$ *and* $a=b=r$, $i=1$, $j=2$. It turns out that all the constraints on the α^a_i, β^a_i, and u^{ab}_{ij} that come from Eq. (6.3) are supplied by these two subcases. The αs and βs in Eq. (6.2) are presented by the diagonal matrices ([...]=diag[...])

$$\begin{gathered}Q=[q^{1/2},q^{-(1/2)}],\quad P=[p^{1/2},p^{-(1/2)}],\\ X=[x,x^{-1}],\quad Y=[y,y^{-1}],\end{gathered} \tag{6.4}$$

where $x,y\in k$ are arbitrary parameters. Then α^a_i and β^a_i are expressed by their actions on the matrix T:

$$\begin{aligned} \alpha_1^l T &= TXQ^{-1}, \quad \beta_1^l T = QP^{-1}TPX, \\ \alpha_2^l T &= TX^{-1}P^{-1}, \quad \beta_2^l T = PQ^{-1}TQX^{-1}, \\ \alpha_1^r T &= YQ^{-1}TQP^{-1}, \quad \beta_1^r T = YPT, \\ \alpha_2^r T &= Y^{-1}P^{-1}TPQ^{-1}, \quad \beta_2^r T = Y^{-1}QT. \end{aligned} \tag{6.5}$$

$\alpha_1^a \neq \alpha_2^a$ and $\beta_1^a \neq \beta_2^a$ but they are related; for example, $\beta_1^r \beta_2^r T = PQT$. In the case of $\mathrm{SL}_q(2)$, $\alpha_1^a = \alpha_2^a$ and $\beta_1^a = \beta_2^a$.

The label $l(r)$ does not quite mean left (right) invariance in B because the associated $\beta_i^l(\alpha_i^r)$ is not left- (right)-invariant: $\Delta\beta_i^l \neq (id \otimes \beta_i^l)\Delta(\Delta\alpha_l^r \neq \alpha_i^r \otimes id)\Delta)$. Note, however, that the product $\beta_1^l \beta_2^l(\alpha_1^r \alpha_2^r)$ is left- (right)-invariant. Of course, since $\alpha_i^l(\beta_l^r)$ is left- (right)-invariant so is $\alpha_1^l \alpha_2^l(\beta_1^r \beta_2^r)$. This will make Eq. (6.11) left- or right-invariant. (Since A has no comultiplication, left and right invariance are not defined in A.)

Note the two Rels. evident from Eqs. (6.5):

$$\alpha_1^l \alpha_2^l \beta_1^l \beta_2^l = id_A, \quad \alpha_1^r \alpha_2^r \beta_1^r \beta_2^r = id_A. \tag{6.6}$$

The four structure constants in Eqs. (6.3) are

$$\begin{aligned} u_{12}^{ll} &= x^{-2}p^{-1}, \quad u_{21}^{ll} = x^{-2}q, \\ u_{12}^{rr} &= y^{-2}p^{-1}, \quad u_{21}^{rr} = y^{-2}q. \end{aligned} \tag{6.7}$$

Case 2. $a=b$, $i=j$. This is the diagonal case, $0=0$, mentioned in the discussion of Eq. (3.2) as not required and not assumed. Nevertheless, the following ''voluntary'' commutation Rels. exist:

$$D_i^a \alpha_i^a = u_i^a \alpha_i^a D_i^a, \quad D_i^a \beta_i^a = v_i^a \beta_i^a D_i^a; \quad a = l,r; \quad i = 1,2. \tag{6.8}$$

Note that Eq. (6.3) would have required $u_i^a = v_i^a$. However, $u_i^a \neq v_i^a$:

$$\begin{aligned} u_1^l &= v_2^l = x^2 q^{-1}, \quad u_2^l = v_1^l = x^2 p, \\ u_1^r &= v_2^r = y^2 q^{-1}, \quad u_2^r = v_1^r = y^2 p. \end{aligned} \tag{6.9}$$

Case 3. $a \neq b$. Here the conditions that make $[D_i^l, D_j^r]$ a derivation are already implied by Eq. (6.5). The structure constants are

$$\begin{aligned} u_{11}^{lr} = u_{22}^{lr} = qp^{-1}, \quad u_{12}^{lr} = u_{21}^{lr} = pq^{-1}, \\ u_{11}^{rl} = u_{12}^{rl} = u_{21}^{rl} = u_{22}^{rl} = 1. \end{aligned} \tag{6.10}$$

$[D_i^l, D_j^r]$ is a zero derivation (recorded in Eq. (6.11)). This completes the discussion of Eq. (6.3).

From the discussion of Eq. (3.2) and the above results, $[D_1^a, D_2^a]$ is an $(\alpha_1^a \alpha_2^a, \beta_1^a \beta_2^a)$-D, in fact one of the form (3.4):

$$[D_1^a, D_2^b] = \delta^{ab}(\alpha_1^a \alpha_2^b - \beta_1^a \beta_2^b)/((pq)^{1/2} - (pq)^{-(1/2)}). \tag{6.11}$$

The above results are summarized in the definition of the following derivation algebra of A and the two subalgebras;

$$\mathrm{Der}_0(A) = k\langle \alpha_i^a, \beta_i^a, D_i^a \rangle_{a=1,r,i=1,2}, \quad \mathrm{Der}_0^a(A) = k\langle \alpha_i^a, \beta_i^a, D_i^a \rangle_{i=1,2}, \quad a = l,r,$$

whose Rels. include all those of the form (3.2). Explicitly, the Rels. for $\mathrm{Der}_0(A)$ are Eq. (6.3) with structure constants (6.7) and (6.10), Rels. (6.8) with structure constants (6.9), Rels. (6.6) and (6.11) and Rels of the form (3.2a) and (3.2d). The Rels. for the subalgebras are the appropriate subsets. (Here, $x,y\in k$ are considered to have single fixed values, so $\mathrm{Der}_0(A)$ is finitely generated.) $\mathrm{Der}_0^l(A)$ and $\mathrm{Der}_0^r(A)$ do not commute (see Eq. (6.10)) because α_i^r and β_i^l act both on the right and left.

Here we note a phenomenon mentioned in Sec. II; two different derivations can act identically on generators. The first is the $(\alpha_1^l\alpha_2^l,\beta_1^l\beta_2^l)$-D in Eq. (6.11). The second is an (id,id)-D, D_3^l. Both give $T_{ij}\rightarrow(-1)^jT_{ij}$. The analogous situation holds for $a=b=r$.

The case of $SL_q(2)$. Consider the case $p=q$ when $A=H_q$, the Hopf FA of $\mathrm{SL}_q(2)$. Unlike A, comultiplication exists for H_q and left, right invariance in H_q can be considered. Then $\mathrm{Der}_0(H_q)=\mathrm{Der}_0(A)|_{p=q}$ decomposes into two commuting subalgebras:

$$\mathrm{Der}_0(H_q)=\mathrm{Der}_0^l(H_q)\cdot\mathrm{Der}_0^r(H_q).$$

Consider one of the subalgebras, say $\mathrm{Der}_0^l(H_q)$, and choose a subset of derivations with $\alpha_1^l\beta_1^l=\alpha_2^l\beta_2^l=id$. This implies that $x=1$ in Eq. (6.4) and that $\alpha_1^l=\alpha_2^l$ and $\beta_1^l=\beta_2^l$. For simplicity, the generators are renamed: $D_1^l=D_+$, $D_2^l=D_-$, $\alpha_1^l=\alpha$, and $\beta_1^l=\beta$. Then, the following algebra and relations are obtained:

$$\mathrm{Der}_L(H_q)=\mathrm{Der}_0^l(H_q)|_{x=1}=k\langle D_+,D_-,\alpha,\beta\rangle,$$

$$\alpha\beta=id,\quad \alpha\beta=\beta\alpha,\quad \alpha D_\pm\beta=q^{\pm1}D_\pm, \tag{6.12}$$

$$[D_+,D_-]=\frac{\alpha^2-\beta^2}{q-q^{-1}},$$

with the Hopf algebra operations (3.6), (3.7), and (3.9).

Connection with $U_q(\mathrm{sl}(2))$. The two rational forms of $U_q(\mathrm{sl}(2))$ (Ref. 11, p. 281) can be constructed from $\mathrm{Der}_L(H_q)$. The *simply connected form P* is the algebra generated by the two derivations, $E_+=q^{1/2}\beta D_+$ and $E_-=q^{-(1/2)}D_-\alpha$, and the (renamed) Homs $\alpha=a$ and $\beta=b$:

$$\mathrm{Der}_L^P(H_q)=k\langle E_+,E_-,a,b\rangle\cong U_q^P(\mathrm{sl}(2)). \tag{6.13}$$

The Rels. have the same form as those of $\mathrm{Der}_L(H_q)$ in Eq. (6.12). However, E_+ is an (id,b^2)-D and E_- is a (a^2,id)-D, so the Hopf algebra operations found from Eqs. (3.6), (3.7), and (3.9) are altered accordingly. The factors $q^{\pm(1/2)}$ are just to make $E_\pm$ agree with $D_\pm$ on the generators T_{ij}. The *adjoint form Q* is defined by taking $E_\pm$, $A=\alpha^2$, and $B=\beta^2$ as generators. The algebra and relations are

$$\mathrm{Der}_L^Q(H_q)=k\langle E_+,E_-,A,B\rangle\cong U_q^Q(\mathrm{sl}(2)),$$

$$AB=id,\quad AB=BA,\quad AE_\pm B=q^{\pm2}E_\pm, \tag{6.14}$$

$$[E_+,E_-]=\frac{A-B}{q-q^{-1}}.$$

E_+ is an (id,B)-D and E_- is an (A,id)-D, and the Hopf algebra operations are again determined accordingly.

Note that the adjoint form can also be obtained from $\mathrm{Der}_0^l(H_q)|_{x=p=q}\cong\mathrm{Der}_L^Q(H_q)$, i.e., $\alpha_1^l=id$, $\beta_2^l=id$ in Eq. (6.5). Note also that the simply connected form P can be considered to be the extension of the adjoint form Q by ''square-root'' generators $\sqrt{A}=a$, $\sqrt{B}=b$,[11]

$$\mathrm{Der}_L^P(H_q)=\mathrm{Der}_L^Q(H_q)\langle a,b\rangle,$$

with the appropriate change to Rels. involving a,b. This is used to obtain the simply connected form of $U_q(\mathrm{sl}(3))$ in Sec. VII.

An example of $Der_{\triangleright}(H_q)$. As a follow-up to the *comment on* [,] near the end of Sec. III, $\mathrm{Der}_{\triangleright}(H_q)$ for $\mathrm{SL}_q(2)$ is presented here and shown to have the adjoint form. Let F_i be a left-invariant (a_i,b_i)-D, $i=1,2$, where F_1,F_2 act on the generators of H_q as $D_{\pm}$ in Eq. (6.12) do. In this example it is assumed that the adjoint action

$$F_1\triangleright F_2=a_1[a_1^{-1}F_1,F_2]b_1^{-1} \tag{6.15}$$

is a derivation. Equivalently (by example (4) of Sec. II), the *deformed* commutator $[a_1^{-1}F_1,F_2]$ is a derivation. Because $a_1^{-1}F_1$ is an $(id,a_1^{-1}b_1)$-D, the derivation conditions (3.2c) are $t_{21}=1$ and $F_1b_2=b_2F_1$, which implies $b_2=id$. This determines a_2: $a_2T_{i1}=q^{-1}T_{i1}$ and $a_2T_{i2}=qT_{i2}$. a_1 is still undetermined; if $a_1=id$ is chosen (only to simplify the following isomorphism), then $b_1=a_2^{-1}$ and $\mathrm{Der}_{\triangleright}(H_q)$ has the familiar form (6.14). In fact, the map $F_1\to E_+$, $F_2\to E_-$, $a_2\to A$, $b_1\to B$ gives the isomorphism

$$\mathrm{Der}_{\triangleright}(H_q)=k\langle F_1,F_2,a_2,b_1\rangle\simeq\mathrm{Der}_L^Q(H_q).$$

Thus, the *adjoint action* gives the *adjoint form*.

Let ''$\triangleleft$'' be defined analogously to ''$\triangleright$'': $F'\triangleleft F=\iota(F_{(1)})F'F_{(2)}$, where $\Delta(F)=F_{(1)}\otimes F_{(2)}$ and ι is the antipode. Then, in contrast to Eq. (6.15), $F_1\triangleleft F_2=a_2^{-1}[F_1,F_2b_2^{-1}]b_2$. The derivation Hopf algebras resulting from the other adjoint actions, $-F_2\triangleleft F_1$, $F_1\triangleleft F_2$, and $-F_2\triangleright F_1$, all turn out to be isomorphic to $\mathrm{Der}_{\triangleright}(H_q)$, which was defined from $F_1\triangleright F_2$ in Eq. (6.15).

VII. DERIVATIONS OF $\mathrm{SL}_q(3)$ AND $V_q(3)$

The purpose of this section is to see how the picture of derivations in Sec. VI extends to higher dimensions. We find derivation algebras $\mathrm{Der}_L(H_q)$ on the Hopf FA $H_q(3)=H_q$ of $\mathrm{SL}_q(3)$ and $\mathrm{Der}_0(A)$ on a nonHopf FA $A_q(3)=A$ of $V_q(3)$. It is shown how $\mathrm{Der}_L(H_q)$ is related to $U_q(\mathrm{sl}(3))$. $V_q(3)$ is a deformation of SL(3) and, like $V_{q,p}(2)$, does not correspond to a quantum group. $\mathrm{Der}_0(A)$ is generated by a set $\{\alpha^l,\beta^l,D^l\}$ with the structure of Eq. (5.9a).

Defining H_q according to Eq. (5.7) requires a lengthy discussion which will not be given. A has the form (5.6). H_q and A are presented first; then $\mathrm{Der}_L(H_q)$ and $\mathrm{Der}_0(A)$.

The Hopf algebra H_q *of* $\mathrm{SL}_q(3)$. Although H_q is well known[5] it is stated here for convenience. H_q is a quotient of the bialgebra

$$B=k\langle T_{11},\ldots,T_{33}\rangle,\quad H_q=B/I_q, \tag{7.1}$$

where $I_q\subset B$ is the ideal generated by the Rels.:

$$\begin{aligned}
&T_{ij}T_{il}-q^{-1}T_{il}T_{ij},\quad l>j,\\
&T_{ij}T_{kj}-q^{-1}T_{kj}T_{ij},\quad i<k,\\
&T_{il}T_{kj}-T_{kj}T_{il},\quad i<k,\quad l>j,\\
&[T_{il},T_{kj}]-(q-q^{-1})T_{ij}T_{kl},\quad i>k,\quad l>j,\\
&\sum T_{1i_1}T_{2i_2}T_{3i_3}(-q^{-1})^{l(i_1i_2i_3)}-1.
\end{aligned} \tag{7.2}$$

The antipode derives from the antiautomorphism $s:B\to B$ defined by

$$T_{ij}^s=(-q^{-1})^{i-j}\det_q T(ji), \tag{7.3}$$

where $T(ij)$ is the 2×2 matrix obtained by deleting the ith row and jth column of the 3×3 matrix $T=(T_{ij})$.

The algebra A. A is defined from B in Eq. (7.1) and s in Eq. (7.3) as an example of Eqs. (5.5) and (5.6):

$$\begin{aligned} &L(T)=TT^s-1, \quad R(T)=T^sT-1, \\ &I=(L(T),R(T)), \quad A=B/I. \end{aligned} \tag{7.4}$$

Relations in (7.4) are implied by those of Eq. (7.2) giving $I\subset I_q$.

Derivations on H_q. Left-invariant derivations $\{\alpha_\mu^\pm,\beta_\mu^\pm,D_\mu^\pm\}$, $\mu=1,2$ on B are defined on the generators by

$$D_1^+T_{i1}=T_{i2}, \quad D_1^-T_{i2}=T_{i1}, \quad D_2^+T_{i2}=T_{i3}; \quad D_2^-T_{i3}=T_{i2}, \tag{7.5}$$

$$\alpha_\mu^\pm T_{ij}=(\boldsymbol{\alpha}_\mu^\pm)_jT_{ij}, \quad \beta_\mu^\pm T_{ij}=(\boldsymbol{\beta}_\mu^\pm)_jT_{ij} \tag{7.6}$$

for $i,j=1,2,3$ and extended to B by the Leibniz rule. The scale factors $(\boldsymbol{\alpha}_\mu^\pm)_j$, $(\boldsymbol{\beta}_\mu^\pm)_j\in k$ define diagonal matrices, and Eq. (7.6) can be written as $\alpha_\mu^\pm T=T\boldsymbol{\alpha}_\mu^\pm$, $\beta_\mu^\pm T=T\boldsymbol{\beta}_\mu^\pm$. These $\{\alpha_\mu^\pm,\beta_\mu^\pm,D_\mu^\pm\}$ define derivations on H_q if they satisfy the ideal conditions

$$D_\mu^\pm I_q\subset I_q, \quad \alpha_\mu^\pm I_q\subset I_q, \quad \beta_\mu^\pm I_q\subset I_q. \tag{7.7}$$

The last two conditions of Eq. (7.7) give

$$\det\,\boldsymbol{\alpha}_\mu^\pm=1, \quad \det\,\boldsymbol{\beta}_\mu^\pm=1, \tag{7.8}$$

which follow from the last Rel. of Eq. (7.2). The other Rels. of Eq. (7.2) are already preserved by the Ansatz (7.6).

The first condition of Eq. (7.7), after some calculation, implies

$$\boldsymbol{\alpha}_1^\pm=[q^{-1},q,1]\boldsymbol{\beta}_1^\pm, \quad \boldsymbol{\alpha}_2^\pm=[1,q^{-1},q]\boldsymbol{\beta}_2^\pm, \tag{7.9}$$

where [...] indicates a diagonal matrix.

From the derivations $\{\alpha_\mu^\pm,\beta_\mu^\pm,D_\mu^\pm\}$ satisfying, Eqs. (7.8) and (7.9), we choose a subset normalized by

$$\alpha_\mu^\pm\beta_\mu^\pm=id\Leftrightarrow\boldsymbol{\alpha}_\mu^\pm\boldsymbol{\beta}_\mu^\pm=\mathbb{1}, \quad \mu=1,2, \tag{7.10}$$

where $\mathbb{1}$ is the 3×3 identity matrix. These imply that $\alpha_\mu^+=\alpha_\mu^-\equiv\alpha_\mu$ and $\beta_\mu^+=\beta_\mu^-\equiv\beta_\mu$, which are then represented by the diagonal matrices

$$\begin{aligned} &\boldsymbol{\alpha}_1=[q^{-(1/2)},q^{1/2},1], \quad \boldsymbol{\beta}_1=\boldsymbol{\alpha}_1^{-1}, \\ &\boldsymbol{\alpha}_2=[1,q^{-(1/2)},q^{1/2}], \quad \boldsymbol{\beta}_2=\boldsymbol{\alpha}_2^{-1}. \end{aligned} \tag{7.11}$$

Derivations $\{\alpha_\mu,\beta_\mu,D_\mu^\pm\}$ defined by Eq. (7.11) form a ''basis'' in the following sense. A derivation $\{\alpha_\mu^\pm,\beta_\mu^\pm,D_\mu^\pm\}$ defined only by Eqs. (7.8) and (7.9) can be written in terms of a derivation $\{\alpha_\mu,\beta_\mu,D_\mu^\pm\}$ defined by Eq. (7.11) as $\{\phi_\mu^\pm\circ\alpha_\mu,\phi_\mu^\pm\circ\beta_\mu,c_\mu^\pm\phi_\mu^\pm\circ D_\mu^\pm\}$ where $\phi_\mu^\pm:H_q\to H_q$ is some left-invariant algebra automorphism of the type (7.6), and $c_\mu^\pm\in k$ is a multiplication factor. It is also possible to write $c_\mu'^\pm D_\mu^\pm\circ\phi_\mu^\pm$.

The basis derivations define the following algebra and Rels:

$$\begin{gathered}\mathrm{Der}_L(H_q)=k\langle D_\mu^{\pm},\alpha_\mu,\beta_\mu\rangle,\\ \alpha_\mu\beta_\mu=\beta_\mu\alpha_\mu=id,\quad \alpha_\mu\alpha_\nu=\alpha_\nu\alpha_\mu,\\ \alpha_\nu D_\mu^{\pm}\beta_\nu=q^{\pm A_{\mu\nu}}D_\mu^{\pm},\quad [D_\mu^{+},D_\nu^{-}]=\delta_{\mu\nu}\frac{\alpha_\mu^2-\beta_\mu^2}{q-q^{-1}},\\ D_\mu^{\pm 2}D_\nu^{\pm}-(q+q^{-1})D_\mu^{\pm}D_\nu^{\pm}D_\mu^{\pm}+D_\nu^{\pm}D_\mu^{\pm 2}=0,\quad \mu\neq\nu,\end{gathered}\tag{7.12}$$

where $A_{\mu\nu}=\frac{1}{2}a_{\mu\nu}$ and $a_{\mu\nu}$ is the Cartan matrix for the Lie algebra A_2. The last Rels. are proved by showing that the left-hand side is an $(\alpha_\mu^2\alpha_\nu,\beta_\mu^2\beta_\nu)$-D which is zero on the generators T_{ij}. $\mathrm{Der}_L(H_q)$ has the Hopf algebra operations corresponding to Eqs. (3.6), (3.7), and (3.9).

Connection with $U_q(\mathrm{sl}(3))$. Here, two *rational forms* of $U_q(\mathrm{sl}(3))$ are constructed from $\mathrm{Der}_L(H_q)$.[11] Let us define the derivations and Homs, $E_\mu^{+}=q^{1/2}\beta_\mu D_\mu^{+}$, $E_\mu^{-}=q^{-(1/2)}D_\mu^{-}\alpha_\mu$, $A_\mu=\alpha_\mu^2$, and $B_\mu=\beta_\mu^2$. Then the *adjoint rational form* Q is given by (compare Eq. (6.14))

$$\mathrm{Der}_L^{Q}(H_q)=k\langle E_\mu^{\pm},A_\mu,B_\mu\rangle_{\mu=1,2}\cong U_q^{Q}(\mathrm{sl}(3)).$$

E_μ^{+} is an (id,B_μ)-D and E_μ^{-} is an (A_μ,id)-D with the corresponding Hopf algebra operations, deduced from Eqs. (3.6), (3.7), and (3.9). The factors $q^{\pm(1/2)}$ make $E_\mu^{\pm}$ agree with $D_\mu^{\pm}$ on the generators T_{ij}. $\mathrm{Der}_L(H_q)$ is not a *rational form* [$q^{1/2}$ in Eq. (7.12)] of $U_q(\mathrm{sl}(3))$. ($\mathrm{SL}_q(2)$ is a special case; $\mathrm{Der}_L(H_q(2))$ is rational because $\frac{1}{2}a_{11}=1$.)

To obtain the *simply connected rational form* P, define the left-invariant automorphisms a_μ,b_μ, represented, as in Eq. (7.11), by

$$\boldsymbol{a}_1=[q^{-(2/3)},q^{1/3},q^{1/3}],\quad \boldsymbol{b}_1=\boldsymbol{a}_1^{-1},\quad \boldsymbol{a}_2=[q^{-(1/3)},q^{-(1/3)},q^{2/3}],\quad \boldsymbol{b}_2=\boldsymbol{a}_2^{-1}.$$

Then the form P is the extension of the form Q by a_μ,b_μ:

$$\mathrm{Der}_L^{P}(H_q)=k\langle E_\mu^{\pm},a_\mu,b_\mu\rangle_{\mu=1,2}\cong U_q^{P}(\mathrm{sl}(3)).$$

E_μ^{+} is an $(id,b_\mu^2a_\nu)$-D and E_μ^{-} is an $(a_\mu^2b_\nu,id)$-D, $\mu\neq\nu$, with the corresponding operations of Eqs. (3.6), (3.7), and (3.9). The Rels. can be obtained from those of $\mathrm{Der}_L(H_q)$ by the following replacements in Eq. (7.12): $\alpha_\mu\to a_\mu$ and $\beta_\mu\to b_\mu$ in the first three Rels.; $A_{\mu\nu}\to\delta_{\mu\nu}$; $\alpha_\mu^2\to a_\mu^2b_\kappa$ and $\beta_\mu^2\to b_\mu^2a_\kappa$, $\mu\neq\kappa$, in the next to last Rels.

We end the discussion of H_q with a comment that is relevant in comparing $\mathrm{Der}_L(H_q)$ with $\mathrm{Der}_0(A)$. Derivations on H_q of the form

$$D_3^{+}T_{i1}=T_{i3},\quad D_3^{-}T_{i3}=T_{i1}\tag{7.13}$$

do not exist. There are no algebra automorphisms $\alpha_3^{\pm}$, $\beta_3^{\pm}$ on H_q (at least of the form (7.6)) such that $D_3^{\pm}$ is an $(\alpha_3^{\pm},\beta_3^{\pm})$-D. The k-Homs $[D_2^{\pm},D_1^{\pm}]$ act like $\pm D_3^{\pm}$ on generators, but they are not derivations. (Of course, in the SL(3) limit $q\to1$, $[D_2^{\pm},D_1^{\pm}]$ and $\pm D_3^{\pm}$ both become derivations which are equal to each other.) Derivations of the type $D_3^{\pm}$ do exist on A, to which we now turn.

Derivations on A. Here $\mathrm{Der}_0(A)$ is similar to but larger than $\mathrm{Der}_L(H_q)$. Actually $\mathrm{Der}_0(A)$ has a subalgebra isomorphic to $\mathrm{Der}_L(H_q)$. Thus, we build on the results for H_q and use the same notation for this subalgebra.

Derivations (7.5) and (7.6) also exist on A because the conditions

$$D_\mu^{\pm}I\subset I,\quad \alpha_\mu^{\pm}I\subset I,\quad \beta_\mu^{\pm}I\subset I,\tag{7.14}$$

are less restrictive than those in Eq. (7.7). In fact, the same formulas (7.8) and (7.9) are implied by the conditions (7.14). Conditions (7.10) again give $\alpha_\mu^{\pm}=\alpha_\mu$ and $\beta_\mu^{\pm}=\beta_\mu$ on A which satisfy

$\alpha_\mu\beta_\mu = id$. Then we arrive at derivations on A, $\{\alpha_\mu,\beta_\mu,D_\mu^\pm\}$, which satisfy the Rels. (7.12). The new results are first stated, and then a few comments are made about how they are derived.

Derivations $D_3^\pm$ in Eq. (7.13), the new feature of A, deviate from the pattern of $D_1^\pm$ and $D_2^\pm$. After choosing a basis with

$$\alpha_3^\pm \beta_3^\pm = \beta_3^\pm \alpha_3^\pm = id_A, \tag{7.15}$$

$D_3^\pm$ is an $(\alpha_3^\pm,\beta_3^\pm)$-D, where $\alpha_3^\pm,\beta_3^\pm$ are represented by the diagonal matrices

$$\begin{aligned} \boldsymbol{\alpha}_3^+ &= [q^{-(3/2)},q,q^{1/2}], \quad \boldsymbol{\beta}_3^+ = (\boldsymbol{\alpha}_3^+)^{-1}, \\ \boldsymbol{\alpha}_3^- &= [q^{-(1/2)},q^{-1},q^{3/2}], \quad \boldsymbol{\beta}_3^- = (\boldsymbol{\alpha}_3^-)^{-1}, \end{aligned} \tag{7.16}$$

which act on T by matrix multiplication on the right as in Eq. (7.6). The Rels. satisfied by $\{\alpha_3^\pm,\beta_3^\pm,D_3^\pm\}$ are

$$\begin{gathered} \alpha_\mu\alpha_3^\pm = \alpha_3^\pm\alpha_\mu, \qquad \alpha_3^+\alpha_3^- = \alpha_3^-\alpha_3^+, \\ \alpha_3^a D_3^\pm \beta_3^a = q^{\pm 2} D_3^\pm, \qquad a = +,-, \\ \alpha_\mu D_3^\pm \beta_\mu = q^{\pm(1/2)} D_3^\pm, \qquad \mu = 1,2, \\ \alpha_3^a D_\mu^\pm \beta_3^a = q^{\pm A_{\mu a}} D_\mu^\pm, \quad A_{1+} = A_{2-} = \tfrac{5}{2}, \quad A_{1-} = A_{2+} = -\tfrac{1}{2}, \\ [D_3^+,D_3^-] = \frac{\alpha_3^+\alpha_3^- - \beta_3^+\beta_3^-}{q^2 - q^{-2}}, \\ [D_2^+,D_3^+] = 0, \quad [D_1^-,D_3^-] = 0. \end{gathered} \tag{7.17}$$

These results are summarized in the derivation algebra

$$\mathrm{Der}_0(A) = k\langle \alpha_\mu,\beta_\mu,D_\mu^\pm,\alpha_3^\pm,\beta_3^\pm,D_3^\pm\rangle_{\mu=1,2},$$

which satisfies the Rels. (7.15) and (7.17) as well as the Rels. of $\mathrm{Der}_L(H_q)$ in Eq. (7.12). $\mathrm{Der}_0(A)$ is a Hopf algebra, with operations of the form (3.6), (3.7), and (3.9).

Comment: The extra $(\alpha_3^\pm,\beta_3^\pm)$-Ds $D_3^\pm$, existing on A but not on H_q, reflect the fact that $I \subset I_q$ and $D_3^\pm$ have to satisfy fewer Rels. in I than in I_q. This is not general, but specific to this case. There could be a situation where $I_2 \subset I_1$ and $DI_1 \subset I_1$ but $DI_2 \not\subset I_2$. Then D would define a derivation on $A_1 = B/I_1$ but not on $A_2 = B/I_2$.

We now indicate how the above results leading to $\mathrm{Der}_0(A)$ were derived. As in Eq. (7.8) the last two conditions of Eq. (7.14) imply

$$\det \boldsymbol{\alpha}_\mu^\pm = 1, \quad \det \boldsymbol{\beta}_\mu^\pm = 1, \quad \mu = 1,2,3,$$

which in turn help to determine the action of α,β on T^s:

$$\alpha_\mu^\pm(T_{ij}^s) = (\boldsymbol{\alpha}_\mu^\pm)_i^{-1}(T_{ij}^s), \quad \beta_\mu^\pm(T_{ij}^s) = (\boldsymbol{\beta}_\mu^\pm)_i^{-1}(T_{ij}^s). \tag{7.18}$$

The conditions $D_\mu^\pm I \subset I$, $\mu = 1,2,3$, correspond to Eq. (5.9a). They are

$$T^\alpha T^{Ds} + T^D T^{\beta s} = 0, \quad T^{\alpha s} T^D + T^{Ds} T^\beta \in (T^s T - 1),$$

whose entries are homogeneous third degree polynomials in T_{ij}. These equations are equivalent to the following simpler ones:

$$D_1^+(T_{2j}^s)=-q^{-1}(\boldsymbol{\beta}_1^+)_3T_{1j}^s,\quad D_1^-(T_{1j}^s)=-q(\boldsymbol{\beta}_1^-)_3T_{2j}^s,$$

$$D_2^+(T_{3j}^s)=-q^{-1}(\boldsymbol{\beta}_2^+)_1T_{2j}^s,\quad D_2^-(T_{2j}^s)=-q(\boldsymbol{\beta}_2^-)_1T_{3j}^s,$$

$$D_3^+(T_{3j}^s)=-q^{-1}(\boldsymbol{\beta}_3^+)_2T_{1j}^s,\quad D_3^-(T_{1j}^s)=-q(\boldsymbol{\beta}_3^-)_2T_{3j}^s.$$

$D_\mu^\pm(T_{ij}^s)=0$ otherwise. Equations (7.18) were used in deriving these. Finally, to complete the discussion of $\mathrm{Der}_0(A)$, basis derivations satisfying $\alpha_\mu\beta_\mu=id$ and Eq. (7.15) have the solutions (7.11) and (7.16).

The results for $\mathrm{SL}_q(3)$ and $V_q(3)$ (i.e., $\mathrm{Der}_L(H_q)$ and $\mathrm{Der}_0(A)$) suggest the following conjectures.

(1) For the Hopf FA, $H_q(n)$, of $\mathrm{SL}_q(n)$, left-invariant derivations, $\{\alpha_\mu^\pm,\beta_\mu^\pm,D_\mu^\pm\}$, exist for the $\pm$ simple roots $i=1,\ldots,n-1$ of $sl(n)$. There are basis derivations, $\{\alpha_\mu,\beta_\mu,D_\mu^\pm|i=1,\ldots,n-1\}$, satisfying $\alpha_i\beta_i=id$. They generate $\mathrm{Der}_L(H_q(n))$ from which the adjoint form can be defined: $\mathrm{Der}_L^Q(H_q(n))\cong U_q^Q(sl(n))$. ''$n$th root'' Homs a_μ on $H_q(n)$ exist and give the simply connected form, $\mathrm{Der}_L^P(H_q(n))\equiv k\langle D_\mu^\pm,a_\mu,b_\mu\rangle\cong U_q^P(sl(n))$, as an extension.

(2) Let $V_q(n)$, $n>3$, be defined in analogy to $V_q(3)$ as the FA $A(n)=B(n)/I(n)$ where $I(n)=(T^sT-1,TT^s-1)$ with T the $n\times n$ matrix of generators T_{ij} of the matrix bialgebra $B(n)$ and s the antiHom of $B(n)$ generalizing Eq. (7.3). Then there are (α,β)-Ds on $A(n)$,

$$\{\alpha_i,\beta_i,D_i^\pm,\alpha_j^\pm,\beta_j^\pm,D_j^\pm|i=1,\ldots,n-1;\ \ j=n,\ldots,n(n-1)/2\},$$

where the (α_i,β_i) correspond to the simple roots of $sl(n)$, and the $(\alpha_j^\pm,\beta_j^\pm)$ to the nonsimple roots.

(3) Some form of (1) and (2) generalize to all simple Lie groups.

VIII. GENERAL DERIVATIONS: THE QUANTUM PLANE AND $\mathrm{SL}_q(2)$

In this section some general (α,β)-Ds are defined on the FA of $\mathrm{SL}_q(2)$ and the quantum plane. The usual quantum plane is

$$A=k\langle X,Y\rangle/I,\quad I=(XY-q^{-1}YX) \tag{8.1}$$

for which we give an infinitely generated Hopf algebra and two finitely generated subalgebras Der_0. Also Der_0 algebras on a different quantum plane are given in examples (4) and (5). They are isomorphic to Euclidean and Heisenberg quantum groups, respectively.

The results are presented in the following six examples.

(1) *An infinitely generated algebra of* (α,β) *derivations*. Derivations on the generators of $k\langle X,Y\rangle$ are defined by

$$E_{mn}X=q^{(1/2)n(m+1)}X^{m+1}Y^n,\quad E_{mn}Y=0,\quad m\geqslant -1,n\geqslant 0,$$

$$F_{mn}Y=q^{(1/2)m(n+1)}X^mY^{n+1},\quad F_{mn}X=0,\quad n\geqslant -1,\quad m\geqslant 0,$$

$$\alpha_{mn}X=q^{(1/2)n}X,\quad \alpha_{mn}Y=q^{-(1/2)m}Y,$$

$$\beta_{mn}X=q^{-(1/2)n}X,\quad \beta_{mn}Y=q^{(1/2)m}Y.$$

E_{mn} and F_{mn} are (α_{mn},β_{mn})-Ds on A (for which we use the same notation) because they preserve the ideal I in the sense of Eq. (5.8).

Der(A) is the associative algebra generated by the infinite set $\{\alpha_{mn},\beta_{mn},E_{mn},F_{mn}\}$. Der($A$) has the following Rels.:

$$\alpha_{00}=id_A,\quad \alpha_{mn}\beta_{mn}=\beta_{mn}\alpha_{mn}=id_A,$$

$$\alpha_{mn}\alpha_{m'n'}=\alpha_{m+m',n+n'},\quad \beta_{mn}\beta_{m'n'}=\beta_{m+m',n+n'},$$

$$\alpha_{mn}E_{m'n'}\beta_{mn}=q^{1/2(m'n-mn')}E_{m'n'},$$

$$\alpha_{mn}F_{m'n'}\beta_{mn}=q^{1/2(m'n-mn')}F_{m'n'},$$

$$[E_{mn},\ E_{m'n'}]=(m'-m)E_{m+m',n+n'},$$

$$[F_{mn},\ F_{m'n'}]=(n'-n)F_{m+m',n+n'},$$

$$[E_{mn},\ F_{m'n'}]=m'F_{m+m',n+n'}-nE_{m+m',n+n'}.$$

These Rels. are verified, according to the discussion in Sec. III, by acting on the generators X,Y. The Rels. $\alpha E\beta=qE$ equate derivations of the same type, and they guarantee that the commutators, $[E,E]$, are derivations, which can then be checked on X,Y.

(2) *A Hopf algebra* $Der_0(A)\cong U_q(sl(2))$. Let $\mathrm{Der}_0(A)$ denote the algebra generated by the following two (α,β)-Ds on A:

$$D_1X=Y,\quad D_1Y=0,\quad D_2Y=X,\quad D_2X=0,$$

$$\alpha X=q^{-(1/2)}X,\quad \alpha Y=q^{1/2}Y,\quad \beta X=q^{1/2}X,\quad \beta Y=q^{-(1/2)}Y.$$

$\mathrm{Der}_0(A)$ is isomorphic to $U_q(sl(2))$ (see $\mathrm{Der}_L(H_q)$ in Eq. (6.12)). It is not a subalgebra of Der(A) defined above.

(3) *A Euclidean quantum group.* Let $\mathrm{Der}_0^E(A)=k\langle D_1,D_2,\alpha,\beta\rangle$ be defined by its action on the quantum plane (8.1):

$$D_1X=1,\quad D_1Y=0,\quad D_2X=0,\quad D_2Y=1,$$

$$\alpha X=q^{-(1/2)}X,\quad \alpha Y=q^{1/2}Y,\quad \beta X=q^{1/2}X,\quad \beta Y=q^{-(1/2)}Y.$$

$\mathrm{Der}_0^E(A)$ is a Hopf algebra with the Rels.

$$\alpha\beta=id_A,\quad \alpha\beta=\beta\alpha,$$

$$\alpha D_1\beta=q^{1/2}D_1,\quad \alpha D_2\beta=q^{-(1/2)}D_2,$$

$$[D_1,D_2]=0.$$

The derivation conditions are satisfied, and the commutator $[D_1,D_2]$ is the zero (α,β)-D. $\mathrm{Der}_0^E(A)$ is a quantum deformation of the Euclidean group of the plane. Namely, set $\alpha=\beta^{-1}=q^K$ and take the limit $q\to1$. Then $\{K,D_1,D_2\}$ generates the Lie algebra of the Euclidean group of the two-dimensional plane.

(4) *A second Euclidean quantum group.* This example is the Euclidean quantum group, which was found as a contraction of $\mathrm{SU}_q(2)$ and was called $E(2)_q$.[12] Here $E(2)_q$ is presented as an algebra of (α,β)-Ds. For ease of comparison the notation of Ref. 12 is used here.

Define another quantum plane different from Eq. (8.1),

$$A_\xi = k\langle X,Y\rangle / I, \quad I = (XY - YX + \xi Y), \tag{8.2}$$

and two (α,β)-Ds, P_y and J, by their action on A_ξ:

$$P_y X = 0, \quad P_y Y = 1, \quad JX = iY, \quad JY = -iX,$$

$$\alpha X = X - \frac{\xi}{2}, \quad \alpha Y = Y, \quad \beta X = X + \frac{\xi}{2}, \quad \beta Y = Y.$$

These generate the algebra $\mathrm{Der}_0^E(A_\xi) = k\langle P_y, J, \alpha, \beta\rangle$ with Rels.

$$\alpha\beta = \beta\alpha = id, \quad \alpha P_y \beta = P_y, \quad \alpha J \beta = J + \frac{i\xi}{2} P_y,$$

$$[J, P_y] = \frac{i}{2\xi}(\alpha^2 - \beta^2).$$

The derivation Rels. (3.2b) and (3.2c) (compare Eq. (3.10a)) which generally have been valid in this work do not hold here for J and P_y. Nevertheless, $[J, P_y]$ is an (α^2,β^2)-D of the form (3.10b). This demonstrates the case where the last four terms in Eq. (3.1) do not cancel pairwise as a consequence of Eqs. (3.2b) and (3.2c); nevertheless, they do cancel.

The isomorphism $\mathrm{Der}_0^E(A_\xi) \cong E(2)_q$ is established by introducing an (id,id)-D P_x and expressing $\mathrm{Der}_0^E(A_\xi)$ in terms of P_x:

$$P_x X = 1, \quad P_x Y = 0, \quad \alpha = e^{-(1/2)\xi P_x}, \quad \beta = e^{(1/2)\xi P_x}.$$

(5) *Heisenberg quantum group.* The Heisenberg quantum group $H(1)_q$ has also been found as a contraction of $\mathrm{SU}_q(2)$.[12] Here $H(1)_q$ is presented as an algebra of (α,β)-Ds acting on the quantum plane (8.2). Define two (α,β)-Ds a, a^+ by

$$aX = 0, \quad aY = 1, \quad a^+ X = Y, \quad a^+ Y = 0,$$

$$\alpha X = X - \frac{\xi}{2}, \quad \alpha Y = Y, \quad \beta X = X + \frac{\xi}{2}, \quad \beta Y = Y.$$

The algebra $\mathrm{Der}_0^H(A_\xi) = k\langle a, a^+, \alpha, \beta\rangle$ has the Rels.

$$\alpha\beta = \beta\alpha, \quad \alpha\beta = id, \quad \alpha a \beta = a, \quad \alpha a^+ \beta = a^+,$$
$$[a, a^+] = \frac{-1}{2\xi}(\alpha^2 - \beta^2), \tag{8.3}$$

which are of the form (3.10). The isomorphism $\mathrm{Der}_0^H(A_\xi) \cong H(1)_q$ is found in terms of an (id,id)-D h:

$$hX = 1, \quad hY = 0, \quad \alpha = e^{-(1/2)\xi h}, \quad \beta = e^{(1/2)\xi h}.$$

This example should be contrasted with the different deformation given in example (4) of Sec. X; compare Rels. (8.3) with (10.3).

(6) *Derivations on* $\mathrm{SL}_q(2)$. General derivations on $\mathrm{SL}_q(2)$ are more complicated; only a simple class of derivations on H_q is given. We have no results on the algebra $\mathrm{Der}(H_q)$. Consider derivations whose action on generators of H_q is defined by

$$D_{c_i f} T_{i1} = c_i f T_{i2}, \quad D_{c_i f} T_{i2} = 0, \tag{8.4}$$

where $f \in H_q$ is a monomial. In particular consider

$$D_{nmk} T_{i1} = c_i T_{12}^n T_{21}^m T_{22}^k T_{i2},$$

where $c_2 = c_1^{-1} = q^{1/4(k+m+n)}$. D_{nmk} can be shown to be an (a,b)-D where $a = a_{nmk}$ and $b = b_{nmk}$ are representable as follows:

$$aT = WTV, \quad bT = W^{-1} T V^{-1}, \quad W = KMN, \quad V = K^{-1} M N Q^{-1},$$

$$K = [q^{k/4}, q^{-(k/4)}], \quad M = [q^{m/4}, q^{-(m/4)}], \quad N = [q^{n/4}, q^{-(n/4)}], \quad Q = [q^{1/2}, q^{-(1/2)}].$$

a and b have been normalized by $ab = id$. As would be expected a, b are not left- or right-invariant.

Comment on derivations. The derivation in Eq. (8.4), abbreviated $D_{c_i f} = D$ here, provides a convenient form for a general comment about derivations on noncommutative FAs. If we were to imitate the commutative theory, we would write $D = f D_+$ (D_+ is the (α,β)-D in Eq. (6.12)) and try to interpret this as module multiplication of the derivation D_+ by $f \in H_q$. That is, Eq. (8.4) would extend to $D(g) = f D_+(g)$ for any $g \in H_q$. However, in noncommutative theory, such an interpretation of D would conflict with the Leibniz rule (2.2). Thus, D is interpreted, not as a derivation D_+ multiplied by an element $f \in H_q$, but as a k-Hom $H_q \to H_q$ defined on products by the Leibniz rule for a suitable pair (α,β). At best "$f D_+$" can serve as a mnemonic for the action (8.4) of D on generators T_{ij}. Note that factors of the form $f_1 T_{ij+1} f_2$ could also have been used in Eq. (8.4).

IX. ON THE TANGENT BUNDLE OF $SL_q(2)$

The tangent bundle of an algebraic group can be defined from its Hopf FA. In this section we apply this definition to $SL_q(2)$ to obtain the deformed analog $TSL_q(2)$ of the tangent bundle TSL(2). The analogy is to the fact that a tangent bundle of a Lie group is itself a Lie group. In particular, TSL(2) is a Lie group. Here, the "tangent bundle" $TSL_q(2)$ of $SL_q(2)$ is a deformation of TSL(2). That is, the FA of $TSL_q(2)$ is a Hopf algebra, which is a q deformation of the Hopf FA of TSL(2). First, the commutative case is briefly reviewed for SL(2).

For a commutative k algebra K (e.g., $K = k$) and the commutative Hopf k algebra $H = H_{q|q=1}$ (see, Sec. VI), SL(2,K) is the set of k algebra Homs,

$$\mathrm{SL}(2,K) = \mathrm{Hom}_{k-A}(H,K), \tag{9.1}$$

called the K points (K variety) of H.

Define the K algebra (and therefore k algebra) $K[\epsilon] = K \oplus K\epsilon$ with $\epsilon^2 = 0$ called the ring of dual numbers.[1] The tangent bundle is defined as the $K[\epsilon]$ points of H:

$$\mathrm{SL}(2,K[\epsilon]) = \mathrm{Hom}_{k-A}(H,K[\epsilon]) \tag{9.2}$$

[written as TSL(2,K) below].

The tangent bundle is a Lie group over K, so it can be represented as the K points of a Hopf k algebra, called here TH, which includes generators V_{ij} for the tangent spaces:

$$TH = k[T_{11}, \ldots, T_{22}, \ V_{11}, \ldots, V_{22}]/J,$$

$$J = (T^s T - 1, \ T^s V + V^s T).$$

That is, the $K[\epsilon]$ points of H are the K points of TH, rewritten as

$$\mathrm{TSL}(2,K)=\mathrm{Hom}_{k-A}(TH,K). \tag{9.3}$$

The connection with derivations is that $\Phi=\phi+\epsilon\delta\in\mathrm{SL}(2,K[\epsilon])$ iff $\phi,\ \delta: H\to K$ and

$$(fg)^{\phi}=f^{\phi}g^{\phi},\quad (fg)^{\delta}=f^{\phi}g^{\delta}+f^{\delta}g^{\phi}. \tag{9.4}$$

Thus, $\mathrm{SL}(2,K[\epsilon])$ is the set of (ϕ,ϕ)-Ds $H\to K$, where $\phi\in\mathrm{SL}(2,K)$.

We apply the above ideas to H_q and $\mathrm{SL}_q(2)$. To get a ''rich'' set of points of H_q, K should be replaced by a noncommutative k algebra R which reflects the noncommutativity of H_q. Then the objects for $\mathrm{SL}_q(2)$ corresponding to Eqs. (9.1) and (9.2) are

$$\mathrm{SL}_q(2,R)=\mathrm{Hom}_{k-A}(H_q,R), \tag{9.5}$$

$$\mathrm{SL}_q(2,R[\epsilon])=\mathrm{Hom}_{k-A}(H_q,R[\epsilon]). \tag{9.6}$$

Denote the $R[\epsilon]$ points of H_q by $\Phi\in\mathrm{SL}_q(2,R[\epsilon])$, and let their images, $\Phi(T)=x+\epsilon y$, $x,y\in R^4$ serve as coordinates of the variety (9.6):

$$\{(x,y)\in R^8 | x^s x=1,\ xx^s=1,\ x^s y+y^s x=0,\ xy^s+yx^s=0\}. \tag{9.7}$$

$s: R\to R$ is defined from the antipode of H_q: $\Phi(T^s)=x^s+\epsilon y^s$.

The function Hopf k algebra of the variety (9.6) and (9.7) is

$$TH_q=k\langle T_{11},\ldots,T_{22},V_{11},\ldots,V_{22}\rangle/J,$$

$$J=(T^sT-1,\ TT^s-1,\ T^sV+V^sT,\ TV^s+VT^s).$$

V^s is defined from the algebra Homs Ψ: $TH_q\to R$ by $\Psi(V^s)=y^s$. [Note that J has the structure of Eq. (5.5). The coalgebra operations on V_{ij} in TH_q are $\Delta(V_{ij})=T_{ik}\otimes V_{kj}+V_{ik}\otimes T_{kj}$ and $\epsilon(V_{ij})=0$. The antipode is s.] In analogy with Eq. (9.3) the $R[\epsilon]$ points of H_q can be represented as the R points of TH_q. Writing $\mathrm{TSL}_q(2,R)$ for $\mathrm{SL}_q(2,R[\epsilon])$,

$$\mathrm{TSL}_q(2,R)=\mathrm{Hom}_{k-A}(TH_q,R).$$

How do (α,β)-Ds fit in with the above ideas? In analogy with Eq. (9.4), $\mathrm{SL}_q(2,R[\epsilon])$ would be (ϕ,ϕ)-Ds $\{\phi,\phi,\delta\}$: $H_q\to R$, where $\phi\in\mathrm{SL}_q(2,R)$. To get (ϕ,ψ)-Ds with $\phi\neq\psi$, we replace $R[\epsilon]$ by another R algebra, which is conveniently defined as an ideal I. Let $R\langle e_1,e_2,\epsilon\rangle$ be the R algebra generated by three indeterminates which satisfy

$$e_1^2=e_1,\quad e_2^2=e_2,\quad e_1e_2=e_2e_1=0,$$

$$\epsilon^2=0,\quad e_1\epsilon=\epsilon,\quad \epsilon e_1=0,\quad e_2\epsilon=0,\quad \epsilon e_2=\epsilon.$$

Define the ideal $I=(e_1,e_2,\epsilon)\subset R\langle e_1,e_2,\epsilon\rangle$. An element $r\in I$ has the form $r=x_1e_1+x_2e_2+y\epsilon$ with $x_1,x_2;y\in R$. 1_R, the zeroth power of any generator, e.g., $1_R=(e_1)^0$, $\notin I$, but $1_R(e_1+e_2)$ ''acts like'' an identity for I, and $1_R\to 1_R(e_1+e_2)$ gives the R algebra structure $R\to I$.

Now consider the I points of H_q:

$$\mathrm{SL}_q(2,I)=\mathrm{Hom}_{k-A}(H_q,I).$$

$\Phi=\phi e_1+\psi e_2+\delta\epsilon: H_q\to I$ is an I point, i.e., $(fg)^{\Phi}=f^{\Phi}g^{\Phi}$ iff the Homs $\phi,\psi,\delta: H_q\to R$ satisfy the Leibniz rule

$$(fg)^{\delta}=f^{\phi}g^{\delta}+f^{\delta}g^{\psi},\quad (fg)^{\phi}=f^{\phi}g^{\phi},\quad (fg)^{\psi}=f^{\psi}g^{\psi}.$$

$\mathrm{SL}_q(2,I)$ is the set of (α,β)-Ds $H_q \to R$. Note that $1^{\Phi}_{H_q} = 1_R(e_1 + e_2)$.

Define the ideal $I' = (e_1, e_2, \epsilon) \subset H_q\langle e_1, e_2, \epsilon\rangle$, and consider the I' points of H_q. $\mathrm{SL}_q(2,I') = \mathrm{Hom}_{k-Alg}(H_q, I')$ is the set of (α,β)-Ds $H_q \to H_q$. For example, $\Psi = \alpha e_1 + \beta e_2 + D\epsilon \in \mathrm{SL}_q(2,I')$ could correspond to one of the left-invariant derivations $\{\alpha,\beta,D^{\pm}\}$ of $\mathrm{Der}_L(H_q)$ in Eq. (6.12) or any more general $\{a,b,D\}$ in Eq. (8.4). Derivations $H_q \to R$ may be considered as the image of the map

$$\mathrm{SL}_q(2,R) \times \mathrm{SL}_q(2,I') \to \mathrm{SL}_q(2,I),$$

$$(\varphi;\alpha,\beta,D) \to \Psi = \varphi(e_1\alpha + e_2\beta + \epsilon D).$$

X. COMMUTATIVE FUNCTION ALGEBRAS

In this section several examples of (α,β)-Ds acting on commutative FAs are given. The FAs do not contain a deformation parameter q related to noncommutativity, so q in the (α,β)-Ds and their algebras is not controlled by the FA but is free to be varied independently. Some of the derivation algebras are not Hopf.

(1) *Representation of* $U_q(\mathrm{sl}(2))$ *on* $k[T]$. Consider $k[T]$, the FA of polynomials in one indeterminate T, the k line. Here (α,β)-Ds $D_{\pm}$ on $k[T]$ are defined on the generator T by

$$D_+T = T^2, \quad D_-T = -1, \quad T^{\alpha} = qT, \quad T^{\beta} = q^{-1}T, \tag{10.1}$$

which extend to T^n by the Leibniz rule (2.2):

$$(T^n)^{\alpha} = q^n T^n, \quad (T^n)^{\beta} = q^{-n}T^n, \quad D_{\pm}T^n = \pm c_n T^{n\pm 1}. \tag{10.2}$$

Here and in the following, we abbreviate $c_n = c_n(q) = (q^n - q^{-n})/(q - q^{-1})$. $\mathrm{Der}_0(k[T]) = k\langle \alpha,\beta,D_{\pm}\rangle$ is isomorphic to $U_q(\mathrm{sl}(2))$ (see Eq. (6.12)).

(2) *The ''projectivized'' representation of* sl(2).[13] Consider the following k linear maps and their action on $k[T]$:

$$J_- = D_-, \quad J_-T^n = -c_n T^{n-1}, \quad J_+ = D_+ - c_N T, \quad J_+T^n = (c_n - c_N)T^{n+1}.$$

$D_{\pm}$ are defined in Eq. (10.1), and T means multiplication by T. J_- is a derivation, but J_+ is not.

Let $P_N(T) \subset k[T]$ be the k linear subspace of polynomials spanned by 1, T, $T^2,\ldots,T^N$. J_+ is constructed so that $J_+T^N = 0$ and therefore restricts to a k-Hom on $P_N(T)$. Thus, $P_N(T)$ is closed under the actions of $\{J_{\pm},\alpha,\beta\}$. Let $k\langle J_{\pm},\alpha,\beta\rangle$ denote the algebra generated by these Homs acting on $P_N(T)$. It has the Rels.

$$\alpha\beta = \beta\alpha = id, \quad \alpha J_{\pm}\beta = q^{\pm 1}J_{\pm},$$

$$[J_+, J_-] = \frac{\alpha^2 - \beta^2}{q - q^{-1}} - c_N \frac{q^{1/2}\alpha + q^{-(1/2)}\beta}{q^{1/2} + q^{-(1/2)}}.$$

J_+ is not a derivation, so $k\langle J_{\pm},\alpha,\beta\rangle$ does not have the Hopf structure of Sec. III. Some relations in this and later examples involve Homs which are not derivations and cannot be verified by the argument ''both sides are (α,β)-Ds which agree on generators.'' The relations have to be proved by acting on a general monomial.

(3) (α,β) *Derivations on the Laurent polynomials*. In this example, we define (α,β)-Ds on the Hopf algebra $H = k[T,T^{-1}] \cong k[X,Y]/(XY-1)$ of Laurent polynomials in the indeterminate T (k=complex numbers). The set of k points of H is $\mathrm{Hom}_{k-A}(H,k) = k^*$, where $k^* = k\backslash\{0\}$ is the punctured complex plane. Two different deformations are stated. For another discussion of derivations on H see Ref. 14.

Deformation 1. The basis derivations D_n, $n=0,\pm1,\pm2,...$ are (α_n,α_n)-Ds defined on generators by

$$D_nT=T^{n+1},\quad \alpha_nT=q^nT,\quad \Rightarrow D_nT^k=kq^{n(k-1)}T^{k+n}.$$

The algebra $\mathrm{Der}_1(H)=k\langle\alpha_n,D_n\rangle_{n\in Z}$ has the Rels.

$$\alpha_0=id,\quad \alpha_n\alpha_m=\alpha_{n+m},\quad \alpha_nD_m=q^{mn}D_m\alpha_n,$$

$$[D_m,D_n]=(n-m)q^{mn}D_{m+n}.$$

Rels. (3.2) are satisfied, so $[D_m,D_n]$ is an $(\alpha_m\alpha_n,\beta_m\beta_n)$-D, as is given. $\mathrm{Der}_1(H)$ is an infinitely generated Hopf algebra of a form discussed in Sec. III. It has no subalgebra isomorphic to $U_q(sl(2))$.

Deformation 2. This is an example of a derivation algebra which is not Hopf. Here, the basis derivations are defined by

$$D_nT=-T^{n+1},\quad T^\alpha=qT,\quad T^\beta=q^{-1}T,\quad \Rightarrow D_nT^k=-c_kT^{k+n}.$$

$\mathrm{Der}(H)=k\langle\alpha,\beta,D_n\rangle_{n\in Z}$ has the Rels.

$$\alpha\beta=\beta\alpha=id,\quad \alpha D_n\beta=q^nD_n,$$

$$[D_m,D_n]=c_{1/2(m-n)}\{q^{-(1/2)(m+n)}\alpha+q^{1/2(m+n)}\beta\}D_{m+n},$$

$$D_0=-\frac{\alpha-\beta}{q-q^{-1}}.$$

The last Rel. holds because both sides are (α,β)-Ds which agree on generators. Note that in the case $m=-n$:

$$[D_n,D_{-n}]=c_n(\alpha+\beta)D_0=-c_n\frac{\alpha^2-\beta^2}{q-q^{-1}}.$$

$[D_m,D_n]$ is not, in general, a basis derivation but is the sum of an $(\alpha^2,\alpha\beta)$-D, αD_{n+m} and a $(\beta\alpha,\beta^2)$-D, βD_{n+m}. $[D_m,D_n]$ is a derivation only for $m=-n$, which is when derivation Rels. (3.2b) and (3.2c) hold. A related fact is that $\mathrm{Der}(H)$ does not have the Hopf structure of Sec. III. But it does have a Hopf subalgebra $\mathrm{Der}_2(H)=k\langle\alpha,\beta,D_{\pm1}\rangle$, which is isomorphic to $\mathrm{Der}_L(H_q)$ in Eq. (6.12) under $\{\alpha,\beta,D_{\pm1}\}\to\{\alpha,\beta,\pm D_\pm\}$.

(4) *Creation and annihilation operators*. Let $a,a^+:k[T]\to k[T]$ be k linear operators where a^+ is multiplication by T and a is an (α,β)-D given by

$$a^+f=Tf,\quad aT=1,\quad T^\alpha=xT,\quad T^\beta=x^{-1}T. \tag{10.3}$$

Then, the algebra $A=k\langle a,a^+,\alpha,\beta\rangle$ has Rels.

$$\begin{aligned}&\alpha\beta=\beta\alpha=id,\quad \alpha a^+\beta=xa^+,\quad \alpha a\beta=x^{-1}a,\\ &a^+a=\frac{\alpha-\beta}{x-x^{-1}},\quad aa^+=\frac{x\alpha-x^{-1}\beta}{x-x^{-1}}.\end{aligned} \tag{10.4}$$

$(a^+)^na$ is an (α,β)-D, and, in particular, a^+a is the indicated (α,β)-D, $(\alpha-\beta)/(x-x^{-1})$, which is the deformed ''number operator.'' This derivation (and more generally A) can be expressed in terms of the (id,id)-D, $NT^n=nT^n$, which is the undeformed number operator. Namely,

$a^+a=(x^N-x^{-N})/(x-x^{-1})$, where $\alpha=x^N$ and $\beta=x^{-N}$. (N is not actually the number operator since $k[T]$ is not Fock space.) Because α and β were introduced, the canonical commutator is a dependent Rel. Here two forms are written in terms of N:

$$[a,a^+]=\frac{x^{N+1/2}+x^{N-(1/2)}}{x^{1/2}+x^{-(1/2)}}, \quad aa^+-xa^+a=x^{-N}.$$

The second form was proposed as a q deformed oscillator algebra.[15] This is not a Hopf algebra (a^+ is not a derivation).

Two comments: (i) This picture extends to n independent sets of operators and parameters $\{a_i,a_i^+,\alpha_i,\beta_i,x_i\}$, $i=1,\ldots,n$ acting on $k[T_1,\ldots,T_n]$ with

$$\begin{gathered} a_i^+(f\,)=T_if, \quad a_i(T_j)=\delta_{ij}, \\ \alpha_i(T_j)=(x_i)^{\delta_{ij}}T_j, \quad \beta_i(T_j)=(x_i)^{-\delta_{ij}}T_j, \end{gathered} \tag{10.5}$$

and each set satisfies Eq. (10.4). (ii) The case when a is an (α,id)-D leads to an algebra corresponding to Eq. (10.4) with dependent Rels.,

$$[a,a^+]=x^N, \quad aa^+-xa^+a=1.$$

The second form is the q-mutator algebra.[16]

(5) *Deformation of an a,a^+ representation of* sl(2). In this example, a and a^+, in Eq. (10.4), are used to construct $J_+=\xi a^+a^+$ and $J_-=-\xi aa$, where $x=q^{1/2}$ and $\xi=(q^{1/2}+q^{-(1/2)})^{-1}$. Acting on $k[T]$, the Homs $J_\pm$, α, and β generate $k\langle J_\pm,\alpha,\beta\rangle$ with the Rels.

$$\alpha\beta=\beta\alpha=id, \quad \alpha J_\pm\beta=q^{\pm1}J_\pm, \quad [J_+,J_-]=\frac{q^{1/2}\alpha^2-q^{-(1/2)}\beta^2}{q-q^{-1}}.$$

$J_\pm$ are not derivations, and $k\langle J_\pm,\alpha,\beta\rangle$ does not have the usual Hopf algebra structure of Sec. III. The commutator is not an (α^2,β^2)-D of the form $c(\alpha^2-\beta^2)$ (or any derivation). Here and in the following, there are Rels. among $\{J_+J_-,\alpha,\beta\}$, and also among $\{J_-J_+,\alpha,\beta\}$, resulting from Eq. (10.4), but they are not given. Thus, $[J_+,J_-]=\ldots$ is a dependent Rel. in $k\langle J_\pm,\alpha,\beta\rangle$.

(6) *Other deformations of $U(sl(2))$ using a,a^+*. Let $\{a_i,a_i^+,\alpha_i,\beta_i,x_i\}$, $i=1,2$, be as in Eq. (10.5) and define two k-Homs $J_\pm$ on $A=k[T_1,T_2]$: $J_+=a_1^+a_2$, $J_-=a_2^+a_1$. In contrast to example (5), here J_+ is an (α_2,β_2)-D (since a_2 is), and J_- is an (α_1,β_1)-D (since a_1 is). Thus, for example, $J_+T_2=T_1$ extends to A according to

$$J_+(T_1^mT_2^n)=c_n(x_2)T_1^{m+1}T_2^{n-1}.$$

The Rels. for $\mathrm{Der}_0(A)=k\langle\alpha_i,\beta_i,J_\pm\rangle$ can be worked out keeping x_1,x_2 as two independent parameters, but we prefer to present two special cases each with a single parameter. As usual, Rels. of the type (3.2a), (3.2d), and (3.3) exist, but are not stated here.

Deformation 1. $x_1=q$, $x_2=q^{-1}$. $\mathrm{Der}_0(A)_1$ has Rels.

$$\alpha_iJ_\pm\beta_i=q^{\pm1}J_\pm, \quad [J_+,J_-]=\frac{\alpha_1\alpha_2-\beta_1\beta_2}{q-q^{-1}}.$$

$J_\pm$ satisfy Eqs. (3.2b) and (3.2c), which is related to $[J_+,J_-]$ being the $(\alpha_1\alpha_2,\beta_1\beta_2)$-D in the last Rel. $\mathrm{Der}_0(A)_1$ has the Hopf algebra structure (3.6), (3.7), and (3.9).

Deformation 2. $x_1=x_2=q$. In this case $\mathrm{Der}_0(A)_2$ has Rels.

$$\alpha_1 J_\pm \beta_1 = q^{\pm 1} J_\pm , \quad \alpha_2 J_\pm \beta_2 = q^{\mp 1} J_\pm ,$$
$$[J_+ , J_-] = \frac{\alpha_1\beta_2 - \alpha_2\beta_1}{q - q^{-1}}. \tag{10.6}$$

The derivation conditions (3.2b) and (3.2c) are not satisfied, so the commutator $[J_+ , J_-]$ does not have to be an $(\alpha_1\alpha_2, \beta_1\beta_2)$-D or any derivation. Nevertheless, it turned out to be an $(\alpha_1\beta_2, \alpha_2\beta_1)$-D as shown. $\mathrm{Der}_0(A)_2$ can be given a Hopf algebra structure if J_+ is given a coproduct Δ' which is different from the one induced by its (α_2, β_2)-D structure in Eq. (3.6): $\Delta' J_+ = \beta_2 \otimes J_+ + J_+ \otimes \alpha_2$. The antipode is $\iota J_+ = -\beta_2^{-1} J_+ \alpha_2^{-1}$. While this example makes a point, it is due to the flexibility of a commutative FA.

Comment. We end this section by noting that inconsistencies can arise in trying to define (α,β)-Ds on commutative FAs with more than one generator. For example, define an (α,β)-D, D, on $k[X,Y]$ by $DX=0$, $DY\neq 0$, $\alpha Y = \beta Y = Y$, and $\alpha X \neq \beta X$. Then $(XY)^D = X^\alpha Y^D$ but $(YX)^D = Y^D X^\beta$. This amounts to trying to define a derivation on $k[X,Y] = k\langle X,Y\rangle / I$ which fails to preserve the ideal $I = (XY - YX)$.

XI. CONCLUSION

We conclude with three comments about the results, and possible further work.

(1) Application of (α,β)-Ds on Hopf FAs corresponding to the algebraic quantum groups $\mathrm{SL}_q(2)$ and $\mathrm{SL}_q(3)$ establish an interpretation similar to that of derivations in algebraic groups. The conjectures at the end of Sec. VII suggest this role of (α,β)-Ds should extend to other algebraic quantum groups. (α,β)-Ds on slightly more general noncommutative q-Vs suggest that wider applications may be tractable.

(2) When the ideal I defining a FA, $A = k\langle X_1, \ldots, \rangle / I$, has no special structure of homogeneity and symmetry (as in quantum algebras) it becomes difficult if not impossible to determine α,β. In this case explicit (α,β)-Ds in specific examples lose importance. To be interesting here, they would probably have to be absorbed into a general theory, which would deal with arbitrary ideals.

(3) Whenever differentiation is defined on noncommutative algebras (α,β)-Ds can be considered. For example, differentiation is obviously of interest on noncommutative smooth FAs.[17] Also derivations have been used on C^* algebras.[18] Examples would be needed to help interpret (α,β)-Ds in any new context.

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On special classes of *n*-algebras

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We define n-algebras as linear spaces on which the internal composition law involves n elements: $m:V^{\otimes n}\Rightarrow V$. It is known that such algebraic structures are interesting for their applications to problems of modern mathematical physics. Using the notion of a commutant of two subalgebras of an n-algebra, we distinguish certain classes of n-algebras with reasonable properties: semisimple, Abelian, nilpotent, solvable. We also consider a few examples of n-algebras of different types, and show their properties. © *1996 American Institute of Physics.*
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I. INTRODUCTION

In 1973, Nambu[1] proposed an interesting generalization of classical Hamiltonian mechanics. It is based on a new notion of brackets, now called *the Nambu bracket*, generalizing the usual Poisson bracket, which is a binary operation on an algebra of classical observables on a phase space, to the multiple operation of higher order $n\geqslant 3$. This new operation is skew-symmetric and satisfies the Leibniz rule with respect to the usual multiplication of functions as well as the so-called *fundamental identity*, which is a natural generalization of the Jacobi identity. Takhtajan called this generalization of the Lie algebra to the multiple operation of higher order by *Nambu–Lie algebra*.[2] The homology theory and the deformation theory for Nambu–Lie gebras were considered in Ref. 3.

The canonical Nambu bracket for n classical observables on the phase space R^n with coordinates x_1, $x_2,\ldots,x_n$ is defined by $\{f_1,f_2,\ldots,f_n\}:=J(f_1,f_2,\ldots,f_n)$, where the right-hand side stands for the Jacobian of the mapping $f=\{f_1,f_2,\ldots,f_n\}:R^n\to R^n$. This formula naturally generalizes the usual canonical Poisson bracket from binary to n-ary operation on classical observables. The generalized Nambu–Hamilton equation of motion involves $n-1$ Hamiltonians H_1, $H_2,\ldots,H_{n-1}$:

$$\frac{df}{dt}=\{H_1,H_2,\ldots,H_{n-1},f\}.$$

The phase flow in the corresponding phase space is divergence-free and preserves the standard volume form $dx_1\wedge dx_2\wedge\cdots\wedge dx_n$—this is the analog of the Liouville theorem. One can find a description of the foundations of the generalized Nambu mechanics in Ref. 2 as well as a discussion of related higher-order algebraic structures. The author of Ref. 2 suspects that such structures might clarify many important problems of modern mathematical physics (Yang–Baxter equation, Poisson–Lie groups, quantum groups) for higher-dimensional cases. For the Yang–Baxter equation of higher order, it was done by Lawrence.[4,5] It should be noted that one of us emphasized in Refs. 6–9 that ternary Z_3-graded algebras are important for their applications in physics of elementary interactions.

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Ternary Nambu–Lie gebras ($n=3$) look similar to *Lie triple systems*, introduced in Ref. 10 and studied in Refs. 11 and 12. The Lie triple system is defined as a vector space V equipped with the ternary bracket which satisfies the same fundamental identity as a Nambu–Lie bracket, but instead of being skew symmetric, satisfies some other condition. The fundamental fact of the theory of Lie triple systems is the existence of standard imbedding of any such system in certain Lie algebra, sending the ternary bracket to $[[\cdot,\cdot]\cdot]$, where $[\cdot,\cdot]$ stands for the operation in the Lie algebra. Another, different generalization of Lie algebras for higher-order algebraic operations is given in Ref. 13.

There were also some attempts to find a generalization of the concept of associative algebras for higher-order algebraic operations, but only some partial results are presented in Refs. 14, 4, 5, and 3. In particular, one can introduce in a partially associative n-algebra,[14] a natural analog of Lie brackets satisfying a generalized Jacobi identity in the sense of Ref. 13.

It is well known that semisimple, Abelian, nilpotent, and solvable algebras form the most important classes of binary associative and Lie algebras. This is why our aim is to find reasonable generalizations of these notions for higher-order algebraic operations.

We define *n-algebras* as linear spaces (mainly finite dimensional) on which the internal composition law involves n elements: $m: V^{\otimes n} \Rightarrow V$. The term n-algebra has been introduced by Lawrence[4,5] to denote the objects with a richer structure, but we hope that the use of this term in our context will not lead to any confusion. The similar notion was used also in Ref. 14. Let us give an example of such a structure for the case $n=3$. An arbitrary element $a \in V \otimes V \otimes V$ can be written in the basis $\{e_k\}$ as

$$a=\sum_{k,l,m} a_{klm} e_k \otimes e_l \otimes e_m ,$$

which defines a one-to-one correspondence between the elements of $V \otimes V \otimes V$ and the three-tensors a_{klm}, which we call also *cubic matrices*.

The natural internal composition law that generalizes the multiplication of ordinary matrices is given by the following rule:

$$m(a \otimes b \otimes c)_{ijk} = (a*b*c)_{ijk} := \sum_{p,q,r} a_{ipq} b_{pjr} c_{qrk} . \tag{1}$$

In contrast with ordinary matrix multiplication it is nonassociative, neither in the strong sense, i.e.

$$(a*(b*c*d)*e) \neq (a*b*c)*d*e \neq a*b*(c*d*e),$$

nor in the sense of other generalizations of associativity presented in Refs. 14, 4, 5, and 3.

Such a ternary product has been in fact introduced by one of the authors[7,9] and independently by Lawrence.[4] It is a particular case of a more general *n-fold* multiplication defined on the n-tensors as follows:

$$m(a^{(1)} \otimes a^{(2)} \otimes \cdots \otimes a^{(n)})_{i_1 i_2 \cdots i_n} = \sum_{j_{kr}=1(k<r)}^{l} a^{(1)}_{i_1 j_{12} \cdots j_{1n}} a^{(2)}_{j_{12} i_2 j_{23} \cdots j_{2n}} \times \cdots \times a^{(k)}_{j_{1k} \cdots j_{k-1k} i_k j_{kk+1} \cdots j_{kn}} \times \cdots \times a^{(n)}_{j_{1n} \cdots j_{n-1n} i_n} , \tag{2}$$

also studied by Lawrence.[4,5]

From the mathematical point of view this structure seems to be rather complicated, so the first question is whether it is possible to distinguish the subalgebras of 3-tensors (n-tensors) with reasonable properties. We succeeded here to introduce subalgebras similar to binary Abelian, nilpotent, solvable, and semisimple algebras.

The groups S_3 and Z_3 act on cubic matrices by permuting their indices. Therefore, it is natural to distinguish subspaces of such matrices that provide the irreducible representations of these groups; e.g., there is the subspace of totally symmetric cubic matrices satisfying $a_{klm}=a_{lmk}=a_{mlk}=\ldots$, etc.

Our paper is organized as follows. In Sec. II we give basic definitions and examples related to general n-algebras (for simplicity, over the field C). Many of these definitions, such as a subalgebra, an ideal, a homomorphism are scattered in the literature, but we prefer a self-contained discussion. In Sec. III, using the important notion of a commutant of two subalgebras of an n-algebra, we distinguish several classes of n-algebras: semisimple, Abelian, nilpotent, solvable. We show that the three latter classes are invariant with respect to the operations of taking a subalgebra, a factor algebra and a homomorphic image. In Sec. IV, we consider the special case of cubic matrices and discuss a few examples of ternary algebras, which could be interesting for their applications in physics of elementary interactions.

II. BASIC DEFINITIONS AND EXAMPLES.

Definition 1: We call an n-algebra ($n\in N$) over the field C a linear space A endowed with a linear mapping (multiplication) $m:A^{\otimes n}\to A$.

One defines in an obvious way a subalgebra of an n-algebra A and the n-algebra structure in the nth tensor power $A^{\otimes n}$. The group S_n acts in $A^{\otimes n}$ in a natural way:

$$\pi(g)(a_1\otimes\cdots\otimes a_n):=a_{g(1)}\otimes\cdots\otimes a_{g(n)},$$

for arbitrary $g\in S_n$, $a_1,\ldots,a_n\in A$. In particular, the cyclic group Z_n is represented automatically (by means of the reduction of π), in the tensor product $A^{\otimes n}$.

Definition 2: An n-algebra A is called S_n commutative (Z_n commutative), if $m\circ\pi(g)=m$ for any $g\in S_n$ (resp., for any $g\in Z_n$).

Definition 3: An n-algebra A is said to be strongly associative if

$$m\circ(m\otimes id\otimes\cdots id)=m\circ(id\otimes m\otimes id\cdots\otimes id)=m\circ(id\otimes id\cdots\otimes m),$$

where all linear mappings act from $A^{\otimes(2n-1)}$ to A.

There exist other definitions of the associativity in n-algebras (see Refs. 14, 4, 5, and 3).

Example 1 (Algebra of multidimensional matrices): Consider the set A=Mat(l,n;C) of complex multidimensional matrices $a=(a_{i_1i_2\cdots i_n})$, with $i_1,i_2,\ldots,i_n=1,2,\ldots,l$ of dimension $l\times l\times\cdots\times l=l^n$. One can introduce the n-fold multiplication on this space (i.e., the product of n elements) by means of (2). Let us introduce matrix units:

$$(e_{i_1i_2\cdots i_n})_{j_1j_2\cdots j_n}:=\delta_{i_1j_1}\delta_{i_2j_2}\cdots\delta_{i_nj_n}.$$

For their product in the above-mentioned sense, we have

$$m(e_{i^{(1)}{}_1i^{(1)}{}_2\cdots i^{(1)}{}_n}\otimes\cdots\otimes e_{i^{(n)}{}_1i^{(n)}{}_2\cdots i^{(n)}{}_n})_{j_1\cdots j_n}$$
$$=\delta_{i^{(1)}{}_1j_1}\cdots\delta_{i^{(n)}{}_nj_n}\delta_{i^{(2)}{}_1i^{(1)}{}_2}\cdots\delta_{i^{(k)}{}_ri^{(r)}{}_k}\cdots\delta_{i^{(n-1)}{}_ni^{(n)}{}_{n-1}}.$$

One can easily see now that all diagonal matrix units are idempotents:

$$m(e_{i\cdots i}\otimes\cdots\otimes e_{i\cdots i})_{j_1\cdots j_n}=\delta_{ij_1}\cdots\delta_{ij_n},$$

and that all nondiagonal matrix units are nilpotents:

$$m(e_{i_1i_2\cdots i_n}\otimes\cdots\otimes e_{i_1i_2\cdots i_n})_{j_1j_2\cdots j_n}=0,$$

if at least two indices are different. If in a product of the diagonal matrix units there are at least two different indices, the product is equal to 0. The n-algebra of all the diagonal matrices gives an example of S_n-commutative n-algebra.

Obviously, for $n=2$ we get the usual matrix multiplication. For $n>2$, this operation is not associative, neither in the sense of Definition 3 nor in the sense of other generalizations of associativity presented in Refs. 3, 4, 5, and 14.

The notion of a determinant of multidimensional matrix (the so-called hyperdeterminant) has been considered in Ref. 15 (the hyperdeterminants have been considered for the first time by Cayley in the early 1840s).

Example 2: Any binary algebra A over the field C, with the multiplication p: $A\otimes A\to A$, is an n-algebra with a naturally extended multiplication by means a binary one as

$$m:=p\circ(id\otimes p)\circ(id\otimes id\otimes p)\circ(id\otimes id\otimes\cdots id\otimes p):A^{\otimes n}\to A. \tag{3}$$

If the binary multiplication p is associative, then the multiplication m defined above is obviously strongly associative, too.

Nevertheless, there exist two-dimensional ternary algebras whose multiplication cannot be expressed by means of any binary one as (3). Indeed, suppose that $m(a\otimes b\otimes c)=p(a\otimes p(b\otimes c))$ for any $a,b,c\in A$. Let us fix a basis $\{e_1,e_2\}$ in A. Then m and p can be expressed with the help of structure constants as follows:

$$m(e_i\otimes e_j\otimes e_k)=\sum_{l=1}^{2} c_{ijk}^{l}e_l,\quad p(e_i\otimes e_j)=\sum_{r=1}^{2} x_{ij}^{r}e_r,$$

for all $i,j,k\in\{1,2\}$. If the above equality is satisfied, it leads to the following system of linear equations:

$$c_{ijk}^{l}=\sum_{r=1}^{2} x_{jk}^{r}x_{ir}^{l},$$

for all values of $i,j,k,l\in\{1,2\}$. This system contains 16 equations for 8 variables. It is easy to choose c_{ijk}^{l} in such a way that this system will have no solution. Note that the ternary algebra constructed in Refs. 4 and 5 using the $6j$ symbols of the representations of quantum groups also has the multiplication that cannot be expressed via (3) with the help of a binary one.

Definition 4: An n-algebra A is called Z_k graded ($k\in N$), if $A=A_0\oplus A_1\oplus\cdots\oplus A_{k-1}$ (direct sum of linear spaces) and if there exists a mapping $g:A_i\to i\in\{0,1,\ldots,k-1\}$ having the property: $g(m(a_1\otimes a_2\otimes\cdots\otimes a_n))=g(a_1)+g(a_2)+\cdots+g(a_{n-1})(mod\ k)$ for all $a_1\in A_i$, $a_2\in A_j,\ldots,a_{n-1}\in A_l(i,j,l\in\{0,1,\ldots,k-1\})$. The elements belonging to the spaces A_i are called homogeneous of grade i, and we suppose that the product of homogeneous elements is also a homogeneous element. Evidently, A_0 is a subalgebra of A.

Definition 5: We call ideal *of an n-algebra A a linear space B, such that $m(a_1\otimes\cdots\otimes a_{n-1}\otimes b)\in B$, $m(a_1\otimes\cdots\otimes a_{n-2}\otimes b\otimes a_{n-1})\in B$, $m(b\otimes a_1\otimes\cdots\otimes a_{n-1})\in B$ for any $b\in B$, $a_1,\ldots,a_{n-1}\in A$.*

If an n-algebra A contains no other ideals except $\{0\}$ and A, it is called simple.

Remark 1: Definition 5 applied to usual binary algebras gives the definition of a two-sided ideal. Obviously, one can give an analog of the definition of a one-sided ideal extended to the n-algebras. For example, the n-algebra described in Example 1 is simple, but it has many one-sided ideals.

Example 3: Consider the following sets (the ''slices'') in Mat$(l,n;C)$*:*

$$T^s_{ip} := \{a \in \mathrm{Mat}(l,n;C) : (a_{i_1 i_2 \cdots i_n})^l_{i_1, i_2, \cdots i_n = 1} = \delta^s_{i_p} (a_{i_1 i_2 \cdots i_n})^l_{i_1, \cdots i_{p-1}, i_{p+1} \cdots, i_n = 1}\},$$

where $p,s = 1,\ldots,l$.

Every such ''slice'' $T^s_{i_p}$ defines a one-sided ideal in the n-algebra Mat$(l,n;C)$*, because applying (2), we have for all* $a^{(1)},\ldots,a^{(n)} \in Mat(l,n;C)$, $a^{(p)} \in T^s_{i_p}$*:*

$$m(a^{(1)} \otimes a^{(2)} \otimes \cdots \otimes a^{(n)})_{i_1 i_2 \cdots i_n} = \delta^s_{i_p} \sum_{j_{kr}=1 (k<r)}^{l} a^{(1)}_{i_1 j_{12} \cdots j_{1n}} a^{(2)}_{j_{12} i_2 j_{23} \cdots j_{2n}} \times \cdots \times a^{(p)}_{j_{1k} \cdots j_{p-1 p} s j_{p p+1} \cdots j_{kn}} \times \cdots \times a^{(n)}_{j_{1n} \cdots j_{n-1 n} i_n}.$$

If $a^{(q)} \in T^{s_q}_{i_p}$, then

$$m(a^{(1)},\ldots,a^{(p)},\ldots,a^{(n)})_{i_1 \cdots i_{p-1} s_p i_{p+1} \cdots i_n} = a^{(p)}_{s_1 \cdots s_n} m(a^{(1)},\ldots,a^{(p-1)},a^{(p+1)},\ldots,a^{(n)})_{i_1 \cdots i_{p-1} i_{p+1} \cdots i_n},$$

where the last of these multiplications coincides with the multiplication in $Mat(l,n-1;C)$.

Obviously, an ideal is automatically a subalgebra. The intersection of a set of ideals is also an ideal. If B and C are two ideals of n-algebra A, then the linear subspace $B+C := \{b + c | b \in B, c \in C\}$ is also the ideal of A. So we can introduce a notion of a *sum of an arbitrary set of ideals.*

Definition 6: A homomorphism of n-algebras (A_1,m_1) *and* (A_2,m_2) *is a linear mapping* $\rho: A_1 \to A_2$*, such that* $m_2 \circ (\rho \otimes \rho \otimes \cdots \otimes \rho) = \rho \circ m_1$.

The definitions of a homomorphism, a subalgebra, and an ideal have their natural extensions to the Z_k-graded n-algebras. We call the *kernel* of a homomorphism ρ the set $\mathrm{Ker}(\rho) := \{a \in A_1 : \rho(a) = 0\}$.

A representation of the n-algebra A in a linear space of dimension l is a homomorphism of A to the n-algebra $\mathrm{Mat}(l,n;C)$ (also see Ref. 4).

Theorem 1: *There exists a one-to-one correspondence between the kernels of the homomorphisms of* Z_n*-graded n-algebras* (A_1,m_1) *and* (A_2,m_2) *and the ideals of* A_1*. The images of the homomorphisms of n-algebras having the same kernels are mutually isomorphic.*

Proof: It is obvious that $\mathrm{Ker}(\rho)$ is an ideal of A_1. Let us suppose indeed that $b \in \mathrm{Ker}(\rho)$, a_1, $a_2,\ldots,a_{n-1} \in A_1$; in that case,

$$\rho \circ m_1(a_1 \otimes a_2 \otimes \cdots \otimes a_{n-1} \otimes b) = m_2(\rho(a_1) \otimes \rho(a_2) \otimes \cdots \otimes \rho(a_{n-1}) \otimes \rho(b)) = 0,$$

and one has $m(a_1 \otimes \cdots \otimes a_{n-1} \otimes b) \in \mathrm{Ker}(\rho)$. Other properties mentioned in Definition 5 can be checked in a similar way.

On the contrary, if B is an ideal in the n-algebra A, we can consider the factor space A/B of the classes of equivalency of the form $B+a$, where $(a \in A)$. It is possible to define on this space a new multiplication $\tilde{m}: (A/B)^{\otimes n} \to A/B$: $\tilde{m}((B+a_1) \otimes \cdots \otimes (B+a_n)) := B + m(a_1 \otimes \cdots \otimes a_n)$. In

this way we defined the structure of n-algebra on A/B and we showed that the linear canonical application $\pi: A \to A/B$ is the homomorphism of n-algebras. The algebra A/B is named the factor-n-algebra of A by the ideal B. Obviously, $B = \mathrm{Ker}(\pi)$.

Finally, if $\rho: A_1 \to A_2$ is a homomorphism of n-algebras, then the n-algebras $\mathrm{Im}(\rho)$ and $A/\mathrm{Ker}(\rho)$ are isomorphic. This proof is evidently valid also for Z_n-graded n-algebras. □

Now one can easily prove that if B is an ideal in the n-algebra A, then the following occurs.

(1) There exists a natural one-to-one correspondence (conserving the inclusion relation) between all subalgebras of A/B and all subalgebras of A containing B.

(2) The above correspondence also gives a one-to-one correspondence between all ideals of A/B and all ideals of A containing B, the corresponding factor algebras being isomorphic.

Remark 2: Let us define similarly the dual category of n-coalgebras. We call n-coalgebra ($n \in N$) *over the field C a linear space M endowed with a linear application (comultiplication)* $\Delta: M \to M^{\otimes n}$.

We produce a standard example of an n-coalgebra by considering the algebra M of complex-valued functions on a group with multioperators[16,17] with a unique n-ary operation ω. In this example $(\Delta f)(x_1,\ldots,x_n) := f(\omega(x_1,\ldots,x_n))$ is the homomorphism of binary algebras M and $M^{\otimes n}$.

If we introduce the structure of an n-algebra in M with the help of Definition 3 and the similar structure in $M^{\otimes n}$, it is obvious that Δ is a homomorphism of n-algebras M and $M^{\otimes n}$. This means that we have here an example of n-bialgebra in the sense of the following definition.

Definition 7: We call an n-bialgebra ($n \in N$) *over the field C a linear space A endowed with a multiplication* $m: A^{\otimes n} \to A$ *and a comultiplication* $\Delta: A \to A^{\otimes n}$, *which is the homomorphism relatively m (recall that* $A^{\otimes n}$ *has a natural structure of n-algebra generated by m).*

III. SPECIAL CLASSES OF *n*-ALGEBRAS

Definition 8: If B,C are two subalgebras of an n-algebra (A,m), *their commutant* $[B,C]_m$ *is the ideal in* (A,m), *generated by all the elements of the form*

$$[b_1,b_2,\ldots,b_n;c_1,c_2,\ldots,c_n]_m = m((b_1+c_1)\otimes(b_2+c_2)\otimes\cdots\otimes(b_n+c_n)) - m(b_1\otimes b_2\otimes\cdots\otimes b_n) - m(c_1\otimes c_2\otimes\cdots\otimes c_n), \tag{4}$$

where $b_1, b_2,\ldots,b_n \in B$, $c_1, c_2,\ldots,c_n \in C$; *in other words, the intersection of all the ideals containing all the above elements*. Obviously, $[B,C]_m = [C,B]_m$. In particular, we consider $A' := [A,A]_m$.

Lemma 1: A subalgebra B of an n-algebra (A,m) *is an ideal if and only if* $[A,B]_m \subseteq B$.

Proof: If B is an ideal, all the elements mentioned in (4), where $b_1, b_2,\ldots,b_n \in B$, $c_1, c_2,\ldots,c_n \in A$, are elements of B, and the necessary inclusion is evident. On the contrary, if this inclusion is true, then all the elements of the form (4), where $b_1, b_2,\ldots,b_n \in B$, $c_1, c_2,\ldots,c_n \in A$, are elements of B. If, in particular, all $b_i = 0$, except one, then B satisfies the definition of ideal. □

As $[A,B]_m \subseteq A' := [A,A]_m$, this lemma says that every subalgebra of the n-algebra A containing A', is an ideal in A.

Definition 9: We call an n-algebra (A,m) *Abelian, if* $[A,A]_m = \{0\}$.

Obviously, this condition is equivalent to the condition

$$m((b_1+c_1)\otimes(b_2\otimes c_2)\cdots\otimes(b_n\otimes c_n)) = m(b_1\otimes b_2\otimes\cdots\otimes b_n) + m(c_1\otimes c_2\otimes\cdots\otimes c_n),$$

where $b_1, b_2,\ldots,b_n, c_1, c_2,\ldots,c_n \in A$. If, in particular, all $b_i = 0$, except one, then $m(a\otimes b\otimes\cdots\otimes c) = 0$ for every $a, b,\ldots,c \in A$.

This means that Abelian n-algebras are exactly n-algebras with a zero multiplication. So every subalgebra, factor algebra, and homomorphic image of an Abelian n-algebra is Abelian itself.

Lemma 2: A factor algebra A/B of an n-algebra A by the ideal B is Abelian if and only if $[A,A]_m \subseteq B$.

Proof: If A/B is Abelian, then we have $[b_1+B, b_2+B,\ldots,b_n+B; c_1+B, c_2+B,\ldots,c_n+B]_m = B$ for every b_1, $b_2,\ldots,b_n$, c_1, $c_2,\ldots,c_n \in A$, from where $[b_1,b_2,\ldots,b_n;c_1,c_2,\ldots,c_n] \in B$, which means $[A,A]_m \subseteq B$. □

In particular, the factor algebra $A/[A,A]_m$ is always Abelian.

Definition 10: We call a normal series of an n-algebra (A,m) *such a finite system of subalgebras* $\{0\}=A_k \subset A_{k-1} \subset \cdots \subset A_1 \subset A_0 = A$ *that every* A_i *is a proper ideal in* A_{i-1} $(i=1,\ldots,k)$. *The natural number k is called the length of this series, and the factor algebras* A_{i-1}/A_i *are called the factors of this series.*

A normal series $\{0\}=A_k \subset A_{k-1} \subset \cdots \subset A_1 \subset A_0 = A$ *of an n-algebra* (A,m) *is called central series, if* $[A_i,A]_m \subseteq A_{i+1}$ $(i=0,1,\ldots,k-1)$.

This definition gives $[A_i,A]_m \subseteq A_i$ $(i=0,1,\ldots,k-1)$ for any central series, and Lemma 1 shows that all A_i are the ideals in A. So a central series is also an *invariant* series, i.e., a finite series of ideals of A, ordered by inclusion.

Definition 11: We call an n-algebra (A,m) nilpotent, if it has at least one central series.

In particular, every Abelian n-algebra is nilpotent because it has a central series of the form $\{0\} \subset A$.

We call a *lower central chain* of an n-algebra A the following chain of ideals: $\cdots \subseteq \hat{A}_k \subseteq \hat{A}_{k-1} \subseteq \cdots \subseteq \hat{A}_1 \subseteq \hat{A}_0 = A$, where $\hat{A}_{k+1} := [\hat{A}_k, A]_m$, $k=0,1,2,\ldots$.

Lemma 3: An n-algebra A is nilpotent if and only if in its lower central chain $\hat{A}_k=\{0\}$ *fo for some natural k.*

Proof: In fact, if $\hat{A}_k=\{0\}$, the above lower central chain becomes the central series of the n-algebra A. On the contrary, consider a central series $\{0\}=A_i \subset A_{i-1} \subset \cdots \subset A_1 \subset A_0 = A$ of the n-algebra A. Let $\hat{A}_0 = A = A_0$. Evidently, $\hat{A}_1 := [A,\hat{A}_0]_m = [A,A]_m \subseteq A_1$ and, if it has already been proved that $\hat{A}_i \subseteq A_i$, then according to the definition of the lower central chain, we have $\hat{A}_{i+1} := [\hat{A}_i, A]_m \subseteq [A_i, A]_m \subseteq A_{i+1}$, from where $\hat{A}_k \subseteq A_k = \{0\}$, i.e., $\hat{A}_k = \{0\}$.

Corollary 1: Every subalgebra B of a nilpotent n-algebra A is also nilpotent.

Proof: Let $\cdots \subseteq \hat{B}_i \subseteq \hat{B}_{i-1} \subseteq \cdots \subseteq \hat{B}_1 \subseteq \hat{B}_0 = B$ be a lower central chain for B. Then $\hat{B}_0 = B \subseteq A = \hat{A}_0$, $\hat{B}_1 = [B,\hat{B}_0]_m \subseteq [A,\hat{A}_0]_m = \hat{A}_1$, and, if it is already proved that $\hat{B}_i \subseteq \hat{A}_i$ then $\hat{B}_{i+1} := [B,\hat{B}_i]_m \subseteq [A,\hat{A}_i]_m \subseteq \hat{A}_{i+1}$. From the equality $\hat{A}_k = \{0\}$ we have now that $\hat{B}_k = \{0\}$.

Corollary 2: Every homomorphic image $H=\rho(A)$ *of a nilpotent n-algebra A is also nilpotent.*

Proof: In fact, let $\cdots \subseteq \hat{A}_i \subseteq \hat{A}_{i-1} \subseteq \cdots \subseteq \hat{A}_1 \subseteq \hat{A}_0 = A$ and $\cdots \subseteq \hat{H}_i \subseteq \hat{H}_{i-1} \subseteq \cdots \subseteq \hat{H}_1 \subseteq \hat{H}_0 = H$ be the lower central chains for A and H, respectively. Then $H = \hat{H}_0 = \rho(A) = \rho(\hat{A}_0)$. Let it be already proved that $\hat{H}_i \subseteq \rho(\hat{A}_i)$. Then $\forall a'_1,\ldots,a'_n \in \hat{H}_i$, $b'_1,\ldots,b'_n \in H \exists a_1,\ldots,a_n \in \hat{A}_i$, $b_1,\ldots,b_n \in A$, such that $a'_l = \rho(a_l)$, $b'_l = \rho(b_l) \forall l = 1,\ldots,n$; this is why $\rho([a_1,\ldots,a_n; b_1,\ldots,b_n]_m) = [a'_1,\ldots,a'_n;b'_1,\ldots,b'_n]_m$.

As the image $\rho(\hat{A}_{i+1})$ of the ideal $\hat{A}_{i+1}$ is the ideal in H (one can verify this directly), then from the above relation we have $\hat{H}_{i+1} = [\hat{H}_i, H]_m \subseteq \rho(\hat{A}_{i+1})$. From the equality $\hat{A}_k = \{0\}$ we have now that $\hat{H}_k = \{0\}$. □

Definition 12: A normal series $\{0\}=A_k \subset A_{k-1} \subset \cdots \subset A_1 \subset A_0 = A$ *of an n-algebra* (A,m) *is*

called solvable, if all factor algebras A_i/A_{i+1} $(i=0,1,\ldots,k-1)$ *of this series are Abelian, i.e., using Lemma 2, if* $[A_i,A_i]_m\subseteq A_{i+1}$ $(i=0,1,\ldots,k-1)$. *An n-algebra is called solvable if it has at least one solvable series.*

Every nilpotent *n*-algebra is solvable. In fact, let $\{0\}=A_k\subset A_{k-1}\subset\cdots\subset A_1\subset A_0=A$ be its central series; then using the relation $[A_i,A]_m\subseteq A_{i+1}$, we have $[A_i,A_i]_m\subseteq[A_i,A]_m\subseteq A_{i+1}$ $(i=0,1,\ldots,k-1)$. □

Definition 13: We call chain of commutants *of an n-algebra A a chain of its subalgebras* $\cdots\subseteq A^{(i)}\subseteq\cdots\subseteq A''\subseteq A'\subseteq A^{(0)}=A$, *such that* $A^{(i+1)}=[A^{(i)},A^{(i)}]_m$, $i=0,1,2,\ldots$.

Lemma 4: An n-algebra A is solvable if and only if in its chain of commutants $A^{(k)}=\{0\}$ *for some natural k.*

Proof: In fact, if $A^{(k)}=\{0\}$, then the above chain of commutants becomes a solvable series of the *n*-algebra *A*. On the contrary, let *A* have a solvable series $\{0\}=A_k\subset A_{k-1}\subset\cdots\subset A_1\subset A_0=A$. Put $A^{(0)}=A_0=A$. Let it be already proved that $A^{(i)}\subseteq A_i$. Then, using the Definitions 12 and 13, we have $A^{(i+1)}=[A^{(i)},A^{(i)}]_m\subseteq[A_i,A_i]_m\subseteq A_{i+1}$, from where, in particular, $A^{(k)}\subseteq A_k=\{0\}$, i.e., $A^{(k)}=\{0\}$. □

Corollary 3: Every subalgebra B of a solvable n-algebra A is also solvable.

Proof: Let $\cdots\subseteq B^{(i)}\subseteq\cdots\subseteq B''\subseteq B'\subseteq B^{(0)}=B$ be a chain of commutants for *B*. Then $B^{(0)}=B\subseteq A=A^{(0)}$. If it has already been proved that $B^{(i)}\subseteq A^{(i)}$, then $B^{(i+1)}:=[B^{(i)},B^{(i)}]_m\subseteq[A^{(i)},A^{(i)}]_m\subseteq A^{(i+1)}$. From the equality $A^{(k)}=\{0\}$ we have now that $B^{(k)}=\{0\}$. □

Lemma 5: If B and C are solvable ideals in an n-algebra A, so is $B+C$.

Proof: From Definition 8 one can easily get that

$$(B+C)'\subseteq B'+C'+B\cap C.$$

If it has already been proved that $(B+C)^{(i)}\subseteq B^{(i)}+C^{(i)}+B\cap C$, then $(B+C)^{(i+1)}:=[(B+C)^{(i)},(B+C)^{(i)}]_m\subseteq[B^{(i)}+C^{(i)}+B\cap C,\ B^{(i)}+C^{(i)}+B\cap C]_m\subseteq[B^{(i)}+C^{(i)},B^{(i)}+C^{(i)}]_m+B\cap C\subseteq B^{(i+1)}+C^{(i+1)}+B^{(i)}\cap C^{(i)}+B\cap C\subseteq B^{(i+1)}+C^{(i+1)}+B\cap C$.

Therefore, there must be an integer *k* such that $(B+C)^{(k)}\subseteq B\cap C$, which is solvable by Corollary 3. From this we deduce that $B+C$ is solvable. □

Now form $R(A):=\Sigma_\alpha B_\alpha$, where α runs over the set of all solvable ideals of *A*. Due to Lemma 5, $R(A)$ is the unique maximal solvable ideal in *A*. After this remark the following definition makes sense.

Definition 14: The radical $R(A)$ *of an n-algebra is the unique maximal solvable ideal of A. In case* $R(A)=0$, *A is called semisimple.*

Obviously, any simple *n*-algebra is automatically semisimple. Since the *n*-algebra of multidimensional matrices (Example 1) is simple, it gives automatically the example of semisimple *n*-algebra.

In order to show that every homomorphic image of the solvable *n*-algebra is also solvable, we need some general facts.

Lemma 6: Let B be an ideal and C a subalgebra of an n-algebra A. Then every element of the subalgebra $\{B,C\}$ *of A, generated by B and C, may be written as* $b+c$, *where* $b\in B$, $c\in C$, *so one can write* $\{B,C\}=B+C$.

Proof: Obviously, all elements of the form $b+c$ are contained in $\{B,C\}$. On the other hand, the set of all elements of this form is a subalgebra of *A*, containing *B* and *C*. In fact, by the definition of ideal we have for every $b_1, b_2,\ldots,b_n\in B$, $c_1, c_2,\ldots,c_n\in C$: $m((b_1+c_1)\otimes\cdots\otimes(b_n+c_n))=m(c_1\otimes\cdots\otimes c_n)+B\subseteq B+C$. □

The following theorem is often referred to as the *isomomorphism theorem.*

Theorem 2: *Let B,C be two subalgebras of an n-algebra A, and let B be ideal in the subalgebra $\{B,C\}$. Then $B\cap C$ is the ideal in C and $\{B,C\}/B$ is isomorphic to $C/(B\cap C)$.*

Proof: In fact, Lemma 6 shows that every conjugacy class of the n-algebra $\{B,C\}$ by the ideal B contains at least one element from C. Then the canonical homomorphism of $\{B,C\}$ on $\{B,C\}/B$ sends the subalgebra C onto this factor algebra. Evidently, $B\cap C$ is the kernel of this homomorphism. Theorem 1 shows that $B\cap C$ is the ideal in C. The n-algebras $\{B,C\}/B$ and $C/(B\cap C)$ consist from the conjugacy classes of the form $B+c$ and $B\cap C+c$, respectively, so one can establish an obvious one-to-one correspondence between them and verify directly that it is an isomorphism. □

A more general case is considered in the following lemma.

Lemma 7: Let B,B', C,C' be two subalgebras of an n-algebra A, let B' be an ideal in B, and let C' be an ideal in C. Then $B'+(B\cap C')$ is the ideal in $B'+(B\cap C)$, $C'+(C\cap B')$ is the ideal in $C'+(C\cap B)$, and the n-algebras $B'+(B\cap C)/B'+(B\cap C')$ and $C'+(C\cap B)/C'+(C\cap B')$ are isomorphic.

Proof: Let $D=B\cap C$. As C' is the ideal in C and $D\subseteq B$, then Theorem 2 shows that $D\cap C'=B\cap C\cap C'=B\cap C'$ is the ideal in D. The same is true for $C\cap B'$ and for the sum D' of these ideals: $D'=(B\cap C')+(C\cap B')$.

On the other hand, as B' is the ideal in B, then according to Lemma 6 $\{B',B\cap C\}=B'+(B\cap C)=B'+D$. One can represent every element from this n-algebra in the form $b'+d$, where $b'\in B'$, $d\in D$. There exists a correspondence between all elements of this form and elements of the form $D'+d$ of the algebra $E=D/D'$.

In fact, one can write the element $b'+d$ as b'_1+d_1, where $b'_1\in B'$, $d_1\in D$, so that $-b'_1+b'=d_1-d\in B'\cap D\subseteq B'\cap C\subseteq D'$; this is why $d_1=(-b'_1+b')+d\in D'+d$.

The above correspondence is a homomorphism of the n-algebra $B'+D$ into the n-algebra E: as B' is the ideal in $B'+D$, D is the subalgebra of A; then $m((b'_1+d_1)\otimes\cdots\otimes(b'_n+d_n))=b'_0+m(d_1\otimes\cdots\otimes d_n)$, where $b'_0\in B'$, $m(d_1\otimes\cdots\otimes d_n)\in D$. The kernel of this homomorphism is $B'+(B\cap C')$. In fact, this sum is contained in the kernel, because $B\cap C'\subseteq D'$.

On the other hand, if the image of the element $b'+d\in B'+D$ is contained in D', then $d\in D'=(B\cap C')+(C\cap B')$; this is why one can write $d=u+v$, where $u\in C\cap B'$, $v\in B\cap C'$. Finally, $b'+d=b'+u+v\in B'+(B\cap C')$.

One can see now that $B'+(B\cap C')$ is an ideal in $B'+D=B'+(B\cap C)$, and the n-algebras $B'+(B\cap C)/B'+(B\cap C')$ and E are isomorphic. One can similarly prove that $C'+(C\cap B')$ is an ideal in $C'+(C\cap B)$, and that the n-algebras $C'+(C\cap B)/C'+(C\cap B')$ and E are isomorphic. □

Remark 3: If $C\subseteq B,C'=\{0\}$ *Lemma 7 becomes the isomorphism theorem.*

Definition 15: We say that a normal series $\{0\}=B_l\subset B_{l-1}\subset\cdots\subset B_1\subset B_0=A$ is a condensation of a normal series $\{0\}=A_k\subset A_{k-1}\subset\cdots\subset A_1\subset A_0=A$, if every A_i $(i=1,2,\ldots,k-1)$ coincides with one from B_j (it is obvious that $k\leqslant l$). We say that two normal series are isomorphic if $k=l$, and there exists such a one-to-one correspondence between their factors, that the corresponding factors are isomorphic as n-algebras (we do not suppose that precisely the factors with the same indices are isomorphic).

Theorem 3: *Every two normal series for an n-algebra A have isomorphic condensations.*

Proof: Let $\{0\}=A_k\subset A_{k-1}\subset\cdots\subset A_1\subset A_0=A$ and $\{0\}=B_l\subset B_{l-1}\subset\cdots\subset B_1\subset B_0=A$ be two normal series for A. Put $A_{ij}=A_i+(A_{i-1}\cap B_j)$ $(i=1,\ldots,k,\ j=0,\ldots,l)$, $B_{ji}=B_j+(B_{j-1}\cap A_i)$ $(i=0,\ldots,k,\ j=1,\ldots,l)$. This makes sense according to Lemma 6: in fact, for example, A_i is an ideal and $A_{i-1}\cap B_j$ is a subalgebra in A_{i-1}. One can also remark that for $i=1,\ldots,k$, $j=1,\ldots,l$ we have $A_i=A_{il}\subseteq A_{ij}\subseteq A_{ij-1}\subseteq A_{i0}=A_{i-1}$, $B_j=B_{jk}\subseteq B_{ji}\subseteq B_{ji-1}\subseteq B_{j0}=B_{j-1}$.

According to Lemma 7, A_{ij} and B_{ji} are the ideals in A_{ij-1} and B_{ji-1}, respectively, and the

n-algebras A_{ij-1}/A_{ij} and B_{ji-1}/B_{ji} are isomorphic. If now we put all A_{ij} $(j=1,\ldots,l-1)$ between A_{i-1} and A_i $(i=1,\ldots,k)$, we get a condensation of this series, in which some members can coincide. Similarly, one can get a condensation of a second series. But using the above isomorphism, one can exclude the coinciding members. □

Now we can show that every hormomorphic image of the solvable n-algebra is also solvable. In fact, according to Theorem 1, it is sufficient to prove this statement for a factor algebra A/B. Since any condensation of a solvable series is solvable itself, then, according to Theorem 3, there exists a solvable condensation of a series $\{0\}\subset B\subset A$. According to the statements formulated just after Theorem 1, we get a solvable series in A/B. After this remark we are able to prove the following theorem about semisimple n-algebras.

Theorem 4: *If R is the radical of an n-algebra A, then A/R is semisimple, and if B is an ideal in A, such that A/B is semisimple, then* $R\subseteq B$.

Proof: (1) The ideals of A/R have the form C/R, where C is an ideal of A containing R (see the remarks following Theorem 1). Since $(C/R)^{(i)}=(C^{(i)}+R)/R$, if C/R is solvable, then, for some k, $C^{(k)}\subseteq R$. This implies that C is solvable in A, hence $C=R$, and A/R is semisimple.

(2) Suppose A/B is semisimple and consider its ideal R/B, which is solvable due to the remark preceding this theorem. Since it should be 0, then $R\subseteq B$. □

Generally, the class of solvable n-algebras is wider then the class of nilpotent ones, but they coincide if the multiplication is strongly associative. In this special case one can define a product of any $1+k(n-1)$ elements (here $k\in N\cup\{0\}$).

Lemma 8: An ideal of a strongly associative n-algebra generated by all possible products of any $1+k(n-1)$ *elements (*$k\in N\cup\{0\}$ *is fixed), coincides with the set of all linear combinations of these elements.*

Proof: In fact, multiplying any linear combination of the above products by $n-1$ arbitrary elements of A in any order, we get a linear combination of some products of $1+(k+1)(n-1)$ elements. Replacing in any such product any group of n neighboring elements by their product, we get again a linear combination of the initial form. On the other hand, the above set can be reduced to the set of all linear combinations of the elements from A. □

Corollary 4: The subalgebra $A^{(i)}$ *in a chain of commutants of a strongly associative n-algebra* $A(i\in N\cup\{0\})$ *is the ideal generated by the set of all possible products from* n^i *elements from A.*

Proof: For $n=0$ the statement is obvious; for $n=1$ it follows from the definition of a commutant. If this statement holds for some natural i, then $A^{(i+1)}=[A^{(i)},A^{(i)}]_m$ is generated by the set of all possible products from $n\circ n^i=n^{i+1}$ elements from A. □

Note that n^i can always be represented as $1+k(n-1)$ for some k.

Corollary 5: The ideal A_i in a lower central chain of a strongly associative n-algebra $A(i\in N\cup\{0\})$ is the ideal generated by the set of all possible products from $1+i(n-1)$ elements from A.

Proof: For $n=0$ the statement is obvious; for $n=1$ it follows from the definition of commutant. If this statement holds for some natural i, then $A_{i+1}=[A_i,A_i]_m$ is generated by the set of all possible products of $1+(i+1)(n-1)$ elements from A. □

Corollary 6: A strongly associative n-algebra is solvable if and only if it is nilpotent.

Proof: From the previous corollaries we have $A^{(i)}=A_{n_i}$, where $n_i=(n^i-1)/(n-1)$, so that $A^{(k)}=\{0\}$ for some natural k if and only if $A_{n_k}=\{0\}$ for this k. □

In the next section we will look more closely at the ternary algebra of complex-valued cubic matrices with $l=2$ and 3. Such a study seems to be particularly important in view of the pertinence of these matrices to a possible generalization of quantum mechanics and field theory. On the other hand, in this special case we are able to gather more information about the structure of entire algebra and its subalgebras.

IV. CUBIC MATRICES WITH *l*=2 AND 3

Consider the example 1 of multidimensional matrices for the simplest case $l=2$, $n=3$. Let us show that it is possible to obtain a decomposition of this eight-dimension alternary algebra (as a linear space) into the direct sum of its three special subalgebras. In fact, there are eight matrix units in the algebra. Three of them, e_{111}, e_{222}, e_{333}, generate a subalgebra Diag of diagonal matrices, which is obviously S_n commutative in the sense of Sec. II.

Using the formula (2) in the special case considered here, one can see that the subalgebra generated by the matrix units e_{112}, e_{121}, e_{122} has a zero multiplication, and consequently it is Abelian in the sense of Sec. IV. The same is true for the subalgebra generated by the matrix units e_{221}, e_{212}, e_{211}. Thus, we have a decomposition,

$$\mathrm{Mat}(2,3;C)=\mathrm{Diag}\oplus\{e_{112},e_{121},e_{122}\}\oplus\{e_{221},e_{212},e_{211}\},$$

in which the first summand is S_n commutative and the other two are Abelian subalgebras. This decomposition looks like a decomposition of 2×2 matrices into the diagonal and two triangular subalgebras. But it is not unique; one can get at least two similar decompositions:

$$\mathrm{Mat}(2,3;C)=\mathrm{Diag}\oplus\{e_{112},e_{212},e_{211}\}\oplus\{e_{121},e_{122},e_{221}\}$$

and

$$\mathrm{Mat}(2,3;C)=\mathrm{Diag}\oplus\{e_{121},e_{221},e_{211}\}\oplus\{e_{112},e_{122},e_{212}\}.$$

Thus, we have a few examples of Abelian ternary algebras that are automatically nilpotent and solvable. Recall that the algebra of all multidimensional matrices (Example 1) gives the example of simple *n*-algebra, which is automatically semisimple.

Since the groups S_n and Z_n act (by permutation of indices) on $\mathrm{Mat}(l,n;C)$, it is also natural to present this *n*-algebra as a direct sum of the corresponding irreducible linear subspaces. If, in particular, $n=3$ and $j=e^{2\pi i/3}$, then introduce the following subspaces:

$$M_m:=\{a\in\mathrm{Mat}(l,3;C):a_{ijk}=j^m a_{jki},\quad \text{for all } i,j,k=1,2,3\},$$

where $m=0,1,2$. For $m=1,2$ we have $\dim(M_m)=(l^3-l)/3$, and $M_0=\mathrm{Diag}\oplus M_0'$, where $\dim(M_0')=(l^3-l)/3$. Finally,

$$\mathrm{Mat}(l,3;C)=\mathrm{Diag}\oplus M_0'\oplus M_1\oplus M_2.$$

Here Diag is the S_n-commutative ternary algebra, but other summands are not ternary algebras with respect to the multiplication (4). The situation changes if we introduce a new multiplication that follows the particular symmetry of the given type of matrices. For example, in Refs. 9 and 7, the following multiplication was introduced for the two matrices $\rho^{(\alpha)}$ belonging to M_1:

$$\{\rho^{(\alpha)},\rho^{(\beta)},\rho^{(\gamma)}\}=\rho^{(\alpha)}*\rho^{(\beta)}*\rho^{(\gamma)}+j\rho^{(\beta)}*\rho^{(\gamma)}*\rho^{(\alpha)}+j^2\rho^{(\gamma)}*\rho^{(\alpha)}*\rho^{(\beta)},$$

where $\alpha,\beta,\gamma=1,2,\ldots,(l^3-l)/3$, $\rho^{(\alpha)}$, $\rho^{(\beta)}$, $\rho^{(\gamma)}\in M_1$, *and*

$$(\rho^{(\alpha)}*\rho^{(\beta)}*\rho^{(\gamma)})_{isk}:=\sum_{pqr}\rho^{(\alpha)}_{piq}\rho^{(\beta)}_{qsr}\rho^{(\gamma)}_{rkp},$$

where $i,s,k,p,q,r=1,2,\ldots,1$.

Then it is obvious that because of the symmetry of the ternary *j bracket*, one has

$$\{\rho^{(\alpha)},\rho^{(\beta)},\rho^{(\gamma)}\}_{isk}=j\{\rho^{(\alpha)},\rho^{(\beta)},\rho^{(\gamma)}\}_{ski},$$

so that it is easy to see that M_1 is a ternary algebra with respect to the *j-bracket* multiplication. Moreover, for $l=2$ we have

$$\{\rho^{(1)},\rho^{(2)},\rho^{(1)}\}=-\rho^{(2)};\quad \{\rho^{(2)},\rho^{(1)},\rho^{(2)}\}=-\rho^{(1)};$$

all other combinations being proportional to the above ones with a factor j or j^2, whereas the j brackets of three identical matrices do obviously vanish.

A natural question to ask now concerns the nature of the automorphisms of this simple ternary algebra. The most general homogeneous transformation of the cubic matrices $\rho^{(\alpha)}$ involves all their indices:

$$\tilde{\rho}^{\ (\alpha)}_{ikm}=\Lambda^{\alpha}_{\beta}U^{p}_{i}U^{r}_{k}U^{s}_{m}\rho^{(\beta)}_{prs},\quad \alpha,\beta,i,k,\ldots=1,2,$$

with (invertible) matrices Λ^{α}_{β}, U^{p}_{i} chosen in such a way that the ternary relations between the transformed cubic matrices $\tilde{\rho}^{\ (\alpha)}$ remain the same as defined above.

Let us show that even in a simplified case when we choose $U^{p}_{q}=\delta^{p}_{q}$, the condition of invariance of the ternary algebra leads to nontrivial solutions for the group of matrices Λ^{α}_{β}. As a matter of fact, we get the following system of equations for Λ^{α}_{β}:

$$\Lambda^1_1(\Lambda^2_2\Lambda^1_1-\Lambda^1_2\Lambda^2_1)=\Lambda^2_2;\quad \Lambda^1_2(\Lambda^2_1\Lambda^1_2-\Lambda^1_1\Lambda^2_2)=\Lambda^2_1,\quad \text{and}$$

$$\Lambda^2_2(\Lambda^1_1\Lambda^2_2-\Lambda^2_1\Lambda^1_2)=\Lambda^1_1;\quad \Lambda^2_1(\Lambda^1_2\Lambda^2_1-\Lambda^2_2\Lambda^1_1)=\Lambda^1_2,$$

from which it follows that $[\det(\Lambda)]^2=1$, so that either

$$\det(\Lambda)=1\quad \text{and}\ \ \Lambda^1_1=\Lambda^2_2,\quad \Lambda^1_2=-\Lambda^2_1,\quad \text{or}$$

$$\det(\Lambda)=-1\quad \text{and}\ \ \Lambda^1_1=-\Lambda^2_2,\quad \Lambda^1_2=\Lambda^2_1.$$

This group has two disjoint components; the simply connected component of unit element is a subgroup, whereas the second component can be obtained from the first one by multiplication by the matrix $\left(\begin{smallmatrix}1 & 0\\ 0 & -1\end{smallmatrix}\right)$.

The simply connected subgroup is an Abelian real two-dimensional Lie group of matrices whose general form is

$$\begin{pmatrix} a & b\\ -b & a\end{pmatrix},\quad \text{with}\ \ a,\quad b\ \ \text{complex numbers satisfying}\ \ a^2+b^2=1,$$

which can be decomposed into a product of two matrices:

$$\begin{pmatrix} \cosh\psi & i\sinh\psi\\ -i\sinh\psi & \cosh\psi\end{pmatrix}\quad (\psi\in R)\quad \text{and}\quad \begin{pmatrix} \cos\phi & \sin\phi\\ -\sin\phi & \cos\phi\end{pmatrix}\quad (\phi\in[0,2\pi)).$$

This group can be represented as the isometry group of a Minkowskian hyperboloid parametrized with two variables, ψ and ϕ, as $[0\leqslant\phi\leqslant 2\pi]\times[-\infty\leqslant\psi\leqslant\infty]$, embedded in a three-dimensional Minkowskian space as the pseudosphere $x^2+y^2-\tau^2=R^2$, so that $x=R\cosh\psi\cos\phi$, $y=R\cosh\psi\sin\phi$, $\tau=\sinh\psi$.

This invariance group reduces to $U(1)$ if we impose the reality condition on the matrices $\rho(\alpha)$, requiring that $\rho^{(\alpha)}_{ikl}=\overline{\rho}^{\ (\alpha)}_{lki}$.

A similar subspace of cubic $2\times2\times2$ matrices can be introduced, with the adjoint representation of the group Z_3 acting on them, i.e. belonging to M_2:

$$\kappa_{ikm}=j^2\kappa_{kmi}=j\kappa_{mik},$$

which is close under a j^2-skew ternary commutator composition law. Its group of automorphisms has the similar structure.

Our next aim is to find a representation of the above ternary algebra in terms of a *j-commutator* defined in an associative algebra of matrices $M_2(C)$ as follows:

$$[A,B,C]:=ABC+jBCA+j^2CAB.$$

It is easy to note that the trace of any j bracket of three matrices must vanish; therefore, the matrices that would represent the cubic matrices $\rho^{(\alpha)}$ must be traceless. Then, it is a matter of simple exercise to show that any two of the three Pauli sigma matrices divided by $\sqrt{2}$ provide us with a representation of the ternary j-skew algebra of the ρ matrices; e.g.

$$\sigma^1\sigma^2\sigma^1+j\sigma^2\sigma^1\sigma^1+j^2\sigma^1\sigma^1\sigma^2=-2\sigma^2, \quad \sigma^2\sigma^1\sigma^2+j\sigma^1\sigma^2\sigma^2+j^2\sigma^2\sigma^2\sigma^1=-2\sigma^1$$

(the same result can be obtained with the couples $\{\sigma^3,\sigma^1\}$ or $\{\sigma^2,\sigma^3\}$). Thus, it is possible to find nontrivial representations of the nonassociative j-bracket ternary algebra in the associative matrix algebra.

A similar representation can be found for cubic matrices $\kappa^{(\alpha)}$ with the j^2-skew bracket.

It is also worthwhile to note that ordinary Lie algebras with the skew-symmetric composition law can be found in the representation of the ternary j-bracket algebra in associative algebra, provided the latter is endowed with a central (unit) element. Indeed, we have

$$[A,1,C]=A1C+j1CA+j^2CA1=AC+(j+j^2)CA=AC-CA. \tag{5}$$

The ternary algebra of complex cubic matrices with $l=3$ is much more complicated. Here again, subspaces displaying a partial Z_3-symmetry can be defined, so that the whole algebra of the dimension 27 decomposes as $M=\mathrm{Diag}\oplus M_0\oplus M_1\oplus M_2$. The part Diag is three dimensional, while each of the subspaces M_a, $a=0,1,2$ contains eight independent generators. As in the previous example, M_1 becomes a ternary algebra with respect to the *j-skew* bracket $[K^{(a)},K^{(b)},K^{(c)}]=K^{(a)}*K^{(b)}*K^{(c)}+jK^{(b)}*K^{(c)}*K^{(a)}+j^2K^{(c)}*K^{(a)}*K^{(b)}$.

The group of automorphisms of this algebra is essentially richer than the two-parameter group discussed above, and we describe it in a separate paper.

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Erratum: On Wick algebras with braid relations [J. Math. Phys. 36, 2803–2812 (1995)]

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The beginning text of Theorem B is

Theorem B: *We have on the algebra following commutation relations for creation and annihilation for the representation of Wick algebra $\mathscr{W}(B,C)$ on the braid commutative algebra $\mathscr{A}$...*

The corrected version of this text should be as follows:

Theorem B: *We have the following commutation relations for creation and annihilation operators for the representation of Wick algebra $\mathscr{W}(B,C)$ on the braid commutative algebra $\mathscr{A}$...*

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Skyrme models with self-dual limits: $d=2,3$

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The most general Skyrme–Sigma models in two and three Euclidean dimensions described by $O(3)$ and $O(4)$ fields, respectively, are studied first by numerical methods, and analytic proofs of existence are subsequently given. Particular emphasis is given to the special cases of these models, where the topological inequalities can be saturated by self-duality equations. The $O(d+1)$ models in d dimensions exhibit qualitatively similar features. © *1996 American Institute of Physics.* [S0022-2488(96)00105-0]

I. INTRODUCTION

The $O(d+1)$ Sigma models in d Euclidean dimensions described in terms of scalar fields ϕ^a, $a=1,2,..,(d+1)$, subject to the condition $\phi^a\phi^a=1$ can have kinetic terms which are the squares of the n-fold antisymmetrized products of the fields $\phi_i^a=\partial_i\phi^a$, starting from $n=d$ down to $n=0$, the last one being a potential term which breaks the global $O(d+1)$ symmetry. That these kinetic terms should be the squares of antisymmetric n-forms, and not simply the squares of some arbitrary n-rank tensor field, is because we require that in any kinetic term there should be no higher power than the quadratic power of a velocity field. In the usual Skyrme model,[1] the $n=1$ and $n=2$ kinetic terms occur and the $n=3$ kinetic term as well as the $n=0$ potential term are absent. We shall refer to the class of such models as Skyrme–Sigma models after the usual Skyrme model[1] in three dimensions which features a quartic kinetic Skyrme term. In the present paper, we shall study the most general such model in any given dimension d, and will concentrate on an interesting limiting case of such models that support self-dual solutions.

While the main aim of the present work is to study the properties of the most general $O(d+1)$ Skyrme–Sigma model in d Euclidean dimensions, the particular cases of $d=2,3$ are of definite physical relevance. In $2+1$ dimensions the inclusion of a $(n=2)$ Skyrme term and a $(n=0)$ potential term in the usual $O(3)$ Sigma model renders the otherwise unstable soliton lump, stable.[2] In three dimensions, the addition of a $(n=3)$ sextic kinetic term and a $(n=0)$ potential term introduces new parameters which are exploited[3] in the phenomenological analysis of nuclear forces. Thus the mathematical problem under consideration in the present work is justified on the grounds of its physical relevance.

To make a representative study of these models, it is necessary to consider at least up to $d=3$ since $d=2$ is a very special case. One special feature of the $d=2$ case is that there exist radially symmetric solutions of arbitrary topological charge, or vorticity, all satisfying the same boundary conditions while in all higher dimensions starting with $d=3$ the spherically symmetric solution of a given topological charge satisfies a particular boundary condition specific to that topological charge. Another special feature of Sigma models in two dimensions is that they can be reparametrized in terms of the CP^1 valued fields z^α, $\alpha=1,2$, constrained by $\overline{z^\alpha}z_\alpha=1$, in which case the

additional free component in z parametrizes a local $U(1)$ invariance in the reparametrized system. This is a low-dimensional accident.

Even the $d=3$ models are in some sense special in that, due to a low-dimensional accident, it is possible to express the field ϕ^a instead as an SU(2) group element $U=\phi^a\sigma^a$, and its inverse $U^{-1}=U^\dagger=\phi^a\tilde{\sigma}^a$ in the usual way.[1] However, in this case the fields ϕ^a and U have exactly the same number of independent components and hence the question of a new local invariance resulting from the reparametrization does not arise. We shall therefore ignore this special feature of the three-dimensional models and treat them as typical examples of Sigma models in dimensions greater than 2.

We define the generic $O(d+1)$ Skyrme–Sigma model in d Euclidean dimensions by the system

$$\mathscr{L}=\kappa_d^{2d}\phi(d)^2+\kappa_{d-1}^{2(d-1)}\phi(d-1)^2+\cdots+\kappa_1^2\phi(1)^2+\lambda_0\phi(0)^2 \tag{1}$$

in terms of the d form fields defined by

$$\phi(n)=\phi^{a_1a_2\ldots a_n}_{i_1i_2\ldots i_n}=\phi^{[a_1}_{[i_1}\phi^{a_2}_{i_2}\cdots\phi^{a_n]}_{i_n]}. \tag{2}$$

where the brackets [...] imply total antisymmetrization. The notation $\phi^a_i=\partial_i\phi^a$ is used for the velocity fields, and the square of the zero-form $\phi(0)^2=V$, which is the only term in (1) that does not involve velocity fields, is an $O(d+1)$ breaking potential. We exclude all kinetic terms featuring a velocity field to a power higher than *two* in the definitions of the models (1).

The coupling constants κ_n all have the dimensions of a length, while the constant λ_0 is dimensionless. Since our study of the solutions of models (1) will be restricted to radially/spherically symmetric field configurations only, we shall find it convenient to rescale the radial variable as $r=\kappa\rho$ in terms of the constant κ with the dimensions of a length, so that the rescaled radial variable ρ is dimensionless. At that stage, the dimensional constants κ_n in (1) will be replaced by the dimensionless coupling constants λ_n defined by $\lambda_n=(\kappa_n/\kappa)^{2n}$.

The topological charge densities of these models are

$$\varrho_d=\varepsilon_{i_1i_2\cdots i_d}\varepsilon^{a_1a_2\cdots a_da_{d+1}}\phi^{a_1}_{i_1}\phi^{a_2}_{i_2}\cdots\phi^{a_d}_{i_d}\phi^{a_{d+1}}, \tag{3}$$

which provides a (topological) lower bound on the density (1). The topological charge is given by the volume integral of ϱ,

$$q_d=\int\varrho_d\,d^dx=\Omega_d\int\overline{\varrho_d}(\rho)\rho^{d-1}\,d\rho, \tag{4}$$

where Ω_d is the angular volume in d Euclidean dimensions and $\overline{\varrho_d}(\rho)$ is the density remaining in the integrand of (8) after imposing spherical symmetry on the fields $\phi^a=(\phi^\alpha,\phi^{d+1})$, $\alpha=1,2,..,d$, and integrating over the angular coordinates.

The radially/spherically symmetric Ansatz, in which n^α is the *unit* radius vector in d dimensions, is

$$\phi^\alpha=\sin f(\rho)n^\alpha,\quad \phi^{d+1}=\cos f(\rho). \tag{5}$$

Substituting (5) in (4), the topological charge reduces to a one-dimensional integral over ρ with integrand

$$\varsigma_d=\rho^{d-1}\overline{\varrho_d}=f_\rho\sin^{d-1}f, \tag{6}$$

where we have used the notation $f_\rho=\partial_\rho f$.

From (6), we can now infer a well-known property of the topological charge of the three-dimensional spherically symmetric Skyrmions,[4] namely that by choosing the asymptotic values suitably as follows,

$$\lim_{\rho\to 0} f(\rho)=m\pi, \quad \lim_{\rho\to\infty} f(\rho)=0, \tag{7}$$

one has a Skyrmion of topological charge m, where the energy of the $m=2$ Skyrmion is much larger than the energy of the unit charge Hedgehog.[4] It is easy to see by inspection of the integrals $\int \sin^{d-1} df$ between the limits (7), that for **even** d the topological charge will vanish except when m is chosen to be odd and for all odd m it equals one. For **odd** d, however, the corresponding value of the topological charge equals m, for all even and odd m. Our subsequent analyses of the $d=2$ and $d=3$ cases therefore will typify these two categories.

The main thrust of the present work is to study a particular aspect of the models (1) for $d=2,3$. It is the special subclasses of these models that support self-dual solutions.

The first such subclass of solutions is already known, namely the scale invariant hierarchy of $O(2p+1)$ Sigma models in $2p$ dimensions given in Ref. 5, the first member of which is the familiar $O(3)$ sigma model[6] in two dimensions. These are the subclass of (1) with all κ_n vanishing *except* $\kappa_{d/2}=\kappa_p$. The self-duality equations for the pth member of that hierarchy are

$$\phi(p)=*\phi(p) \tag{8}$$

with $*\phi(p)$ defined by

$$*\phi(p)=\varepsilon_{i_1\cdots i_p i_{p+1}\cdots i_{2p}}\varepsilon^{a_1\cdots a_p a_{p+1}\cdots a_{2p+1}}\phi^{a_{p+1}\cdots a_{2p}}_{i_{p+1}\cdots i_{2p}}\phi^{2p+1}. \tag{9}$$

The topologically stable and finite *energy* self-dual solutions of these scale invariant models are *power* localized to an arbitrary scale, namely to κ introduced above. With the exception of the case $p=1$, the self-duality equations (8) are overdetermined[7] and support *only* spherically symmetric solutions. The new hierarchy of models that we shall introduce here differ from the scale invariant hierarchy[5] on both those counts. As we shall see below, with a suitable choice of V in (1), they are *exponentially* localized. Furthermore, the new hierarchy of self-duality equations are not overdetermined.

The new hierarchy of $O(d+1)$ models are those obtained from (1) by setting all κ_n equal to zero with the exception of κ_d and λ_0:

$$\mathscr{L}_0=\kappa_d^{2d}\phi(d)^2+\lambda_0 V. \tag{10}$$

It is clear that the *energy* densities (10) can be absolutely minimized by a self-duality equation. In terms of the dimensionless variable $y_i=x_i/\kappa$, where κ is a constant with the dimensions of length so that $\lambda_2=(\kappa_d/\kappa)^{2d}$, this self-duality equation can be expressed as

$$\varrho_d=d!\sqrt{\frac{\lambda_0 V}{\lambda_2}}, \tag{11}$$

where ϱ_d is defined by (3).

The energy densities for fields satisfying (11) are equal to the topological charge densities, which are proportional to $\sqrt{V}\varrho_d$. The volume integral of the latter takes the same values as that of (3).

The new hierarchy of models (10) is analogous to a class of d-dimensional symmetry-breaking global $O(d)$ models introduced in Ref. 8, and further studied in Ref. 9. We shall discuss the relative properties of the $O(d+1)$ models (10) and of the $O(d)$ models of Ref. 8 in some detail. In addition to this, we shall discuss some general properties of the full models (1), but

always restricting to the radially/spherically symmetric field configurations. The cases of $d=2$ and $d=3$ are discussed respectively in Secs. II and III below, each section being subdivided into subsections dealing with the hierarchy of the full models (1) and the new hierarchy (10) supporting self-dual solutions. The self-dual solutions of the restricted models are found explicitly in Secs. II B and III B, respectively, while the solutions of the full models not admitting self-dual solutions are studied numerically in Sec. II A.

II. THE TWO-DIMENSIONAL CASE

The full model (1) in this case was studied in detail, in the context of a particular application, in Ref. 10. We shall nevertheless give a fairly complete account of it here so that the discussion of the special case (10) can be presented in a natural way. In terms of the dimensionless coordinates $y_i=x_i/\kappa$, (1) takes the form

$$\mathscr{L}=\lambda_2\phi(2)^2+\lambda_1\phi(1)^2+\lambda_0 V \tag{12}$$

in which the potential V will be specified later.

The radially symmetric field configuration of $\phi^a=(\phi^\alpha,\phi^3)$, with $\alpha=1,2$, is defined by

$$\phi^\alpha=\sin f(\rho)n^\alpha, \quad \phi^3=\cos f(\rho), \tag{13}$$

characterized by its vorticity n, defining the unit vector $n^\alpha=(\cos n\theta,\sin n\theta)$ in (13), in terms of the azimuthal angle θ. For this field configuration, the system (12) reduces to the following one-dimensional subsystem given by

$$L_2=\left(\lambda_1\rho+\lambda_2 n^2\,\frac{\sin^2 f}{\rho}\right)f_\rho^2+\lambda_2 n^2\,\frac{\sin^2 f}{\rho}+\lambda_0\rho V \tag{14}$$

defined via the *energy* integral

$$\int \mathscr{L}_2\, d^2x=2\pi\int L_2\, d\rho. \tag{15}$$

A. The full model

Here we take the full system (14) with all coupling constants λ_0, λ_1, and λ_2 nonzero, and with the choice for the potential

$$V=(1-\phi^3)^2=(1-\cos f)^2 \tag{16}$$

differing from the choice made in Ref. 10. This is done in anticipation of the considerations of the next subsection. The resulting Euler–Lagrange equations are

$$\left(\lambda_1\rho+\lambda_2 n^2\,\frac{\sin^2 f}{\rho}\right)f_{\rho\rho}+\lambda_2 n^2\,\frac{\sin f\cos f}{\rho}\,f_\rho^2+\left(\lambda_1-\lambda_2 n^2\,\frac{\sin^2 f}{\rho^2}\right)f_\rho$$
$$-\lambda_2 n^2\,\frac{\sin f\cos f}{\rho}-2\lambda_0\rho(1-\cos f)\sin f=0. \tag{17}$$

Assuming sufficiently strong decay in the $\rho\gg 1$ region, we linearize equation (17) around the asymptotic value of f given by (7)

$$\rho^2 f_{\rho\rho}+\rho f f_\rho-\frac{\lambda_2}{\lambda_1}\,n^2 f=0, \tag{18}$$

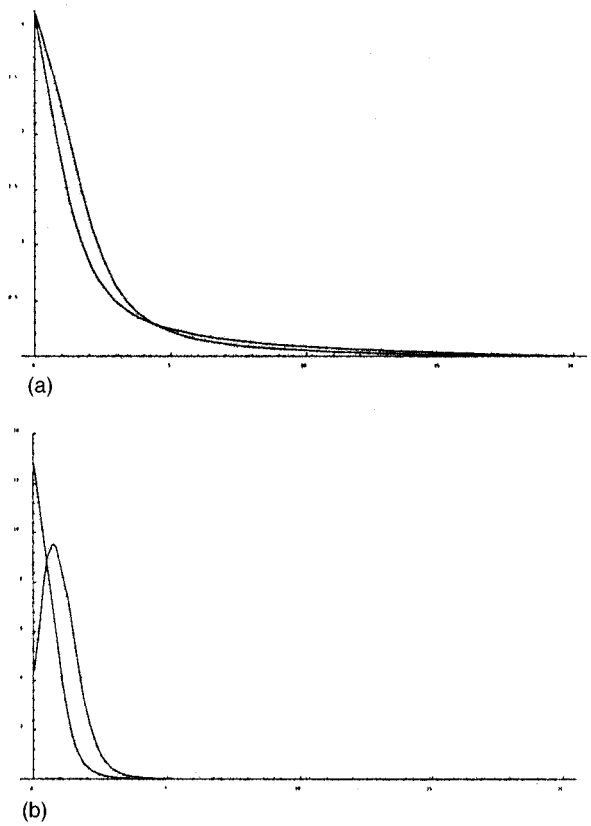

FIG. 1. (a) Profiles of f for the $d=2$ model (14) with the potential (16) and $\lambda_0=\lambda_1=\lambda_2=1$, for vorticities $n=1,2$, from left to right. (b) Profiles of the energy densities for the vortices in (a). The $n=2$ profile is ring shaped.

which yields the decaying solution

$$f \approx \frac{1}{\rho^{n\sqrt{\lambda_2/\lambda_1}}}, \tag{19}$$

justifying our linearization (18).

In the $\rho \ll 1$ region, we try a power series solution and find

$$f = \pi + A\rho^n + B\rho^{n+2} \tag{20}$$

for the two vorticities $n=1$ and $n=2$ and find

$$B = -A\,\frac{6\lambda_0 + 2\lambda_1 A^2 - \lambda_2 A^4}{24(\lambda_1 + \lambda_2 A^2)}, \quad B = -A\,\frac{\lambda_0 + 8\lambda_2 A^2}{6\lambda_1}, \tag{21}$$

respectively, with the constant A to be determined by the numerical integration. In (20), we have restricted to the value of $m=1$ given in the general case in (7). Recall that for all *even d* only *odd* values of m lead to nontrivial topological solutions and all have the same topological charge, and hence $m=1$ is essentially the unique choice.

The numerical integrations were performed for the systems with $\lambda_0=\lambda_1=\lambda_2=1$, for $n=1$ and $n=2$ with the values of $A=-1.5\,199\,879$ and $A=-12.227\,601$, respectively. The profiles of the

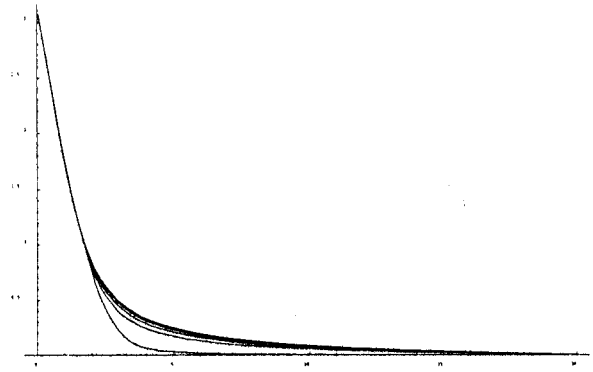

FIG. 2. Profiles of f with unit vorticity ($n=1$) for the $d=2$ model (14) with the potential (16), with $\lambda_0=\lambda_2=1$ and with λ_1 decreasing as in Table II. Lower curves correspond to lower values of λ_1.

functions f are given in Fig. 1(a), and the energy density profiles in Fig. 1(b). The total energies for these two cases were calculated to be: $E(n=1)=8.2\,259\,968$ and $E(n=2)=16.6\,605\,004$ where we find, as in Ref. 10, that $E(n=2)>2E(n=1)$, so there are no radially symmetric bound states.

Perhaps the most important lesson learnt from the work of this subsection is that the constant B in the asymptotic solution (20) for $n=1$ is nonsingular in the limit of $\lambda_1\to 0$, as seen from the first member of (21), which implies that a self-dual solution to the $p=1$ member of the hierarchy (10) exists as a limit of the $n=1$ solution found above. This is interesting in the background of the corresponding situation for the two-dimensional $O(2)$ models studied in Ref. 11. In that case the self-dual solutions to the systems introduced in Ref. 8 are not smooth limits of the solutions to the generic systems, analogous to (12) here, introduced in Ref. 11, since the expressions corresponding to (21) become infinite in this limit.

B. Restricted model: Self-dual solution

Here we ignore the well-known subsystem of (12) with $\lambda_0=\lambda_2=0$, where the self-dual solutions are known analytically[6] and which is the $p=1$ member of the hierarchy of self-duality equations (8). Rather, we consider the $p=1$, or $d=2$, member of the new hierarchy of models (10) with $\lambda_1=0$.

The $d=2$ member of the hierarchy of self-duality equations (11) with V given by (16), in the $n=1$ radially symmetric field configuration (13), reduces to an ordinary first-order equation which is immediately integrated to give the solution for f in terms of ρ^2:

$$\cos f=1-2e^{-\rho^2}, \tag{22}$$

where we have set $\lambda_0=\lambda_2=1$. It is easy to verify that (22) satisfies the asymptotic conditions (7) with $m=1$.

We have numerically integrated the equations (17) for the systems with $\lambda_0=\lambda_2=1$, and with progressively smaller values of λ_1, starting from $\lambda_1=1$ down to $\lambda_1=0.001$. The profiles of the function f for all these cases are plotted in Fig. 2. The numerical integrations were performed for each λ_1 with the values of the parameter A listed in Table I. The total energies pertaining to each of these solutions are listed in Table II, in which the lowest value is closest to the energy pertaining to the self-dual solution which in the normalization used equals 4.

It should be noted here that our ability to obtain a solution satisfying the asymptotic conditions (7) is dependent on our choice of potential. Our choice of (16), which is not unique, has led to the solution (22), which is differentiable at the origin for vorticity $n=1$ only. It is possible to

TABLE I. The parameter A for $n=1$ vortices for the two-dimensional model with potential $V(f)=(1-\cos(f))^2$.

λ_1	A
1.0	−1.5199879
0.8	−1.5042582
0.6	−1.4865913
0.4	−1.4664522
0.2	−1.4429800
0.001	−1.4143832

find well-behaved solutions for other values of the vorticity with suitable choices of V, and for each such choice the corresponding solutions for the system with nonvanishing λ_1 will be well behaved for all values of the vorticity n.

III. THE THREE-DIMENSIONAL CASE

In terms of the dimensionless coordinates $y_i=x_i/\kappa$, the full model (1) in this case reduces to

$$\mathscr{L}_3=\lambda_3\phi(3)^2+\lambda_2\phi(2)^2+\lambda_1\phi(1)^2+\lambda_0 V. \tag{23}$$

The one-dimensional subsystem L_3 defined by $\int\mathscr{L}_3\,d^3x=\int L_3\,d\rho$ is now

$$L_3=\lambda_3\,\frac{\sin^4 f}{\rho^2}\,f_\rho^2+\lambda_2\,\sin^2 f\left(2\,f_\rho^2+\frac{\sin^2 f}{\rho^2}\right)+\lambda_1(\rho^2 f_\rho^2+2\sin^2 f)+\lambda_0\rho^2 V, \tag{24}$$

leading to the Euler–Lagrange equation

$$\left(\lambda_3\,\frac{\sin^4 f}{\rho^2}+2\lambda_2\,\sin^2 f+\lambda_1\rho^2\right)f_{\rho\rho}+\left(2\lambda_3\,\frac{\sin^3 f\cos f}{\rho^2}+2\lambda_2\,\sin f\cos f\right)f_\rho^2$$
$$+2\left(-\lambda_3\,\frac{\sin^4 f}{\rho^3}+\lambda_1\rho\right)f_\rho-2\lambda_2\,\frac{\sin^3 f\cos f}{\rho^2}-2\lambda_1\,\sin f\cos f-\lambda_0\rho^2\,\frac{\partial V}{\partial f}=0, \tag{25}$$

where we have not yet specified the potential V. Unlike in the previous section dealing with the $d=2$ case, here we shall choose different potentials in the generic case where all λ_A, $A=0,1,2,3$, are nonzero, and in the case belonging to the hierarchy (10) where only λ_0 and λ_3 are nonzero. The reason for this is that in the second case our choice for V will by necessity be a highly nonlinear infinite series in the field ϕ^a like, for example, in the Sine–Gordon model, and it is probably reasonable to give the numerical demonstration of the existence of the solutions in the generic case with a simple choice of V.

TABLE II. The total energy of $n=1$ vortices for the two-dimensional model with potential $V(f)=(1-\cos(f))^2$.

λ_1	E
1.0	8.2259968
0.8	7.3986649
0.6	6.5667305
0.4	5.7280508
0.2	4.8781415
0.001	4.0046557

A. The full model

First we choose the simplest potential, used in Ref. 10,

$$V=1-\phi^4. \tag{26}$$

Assuming exponential decay in the region $\rho\gg 1$, we linearize (25) around the asymptotic value $f=0$,

$$\rho^2 f_{\rho\rho}+2\rho f_\rho-2\left(1+\frac{\lambda_0}{2\lambda_1}\rho^2\right)f=0, \tag{27}$$

which yields the exponentially decaying behavior

$$f\approx\frac{1}{\rho}\,e^{\sqrt{\lambda_0/\lambda_1}\rho}, \tag{28}$$

justifying our linearization (27).

It is appropriate to make a remark about the exponential behavior (27) here. This is a result of the presence of the $O(4)$ breaking potential (26) in (24). Setting $\lambda_0=0$ would yield the usual Skyrme model[1] supplemented by the *sextic* term $\phi(3)^2$ as in Ref. 12. In this case, as also in the usual Skyrme model,[1] the behavior of f in the $\rho\gg 1$ region is a power decay. The linear equation (27) with λ_0 in it set equal to zero in fact admits the solution $f\approx\rho^{-2}$.

In the $\rho\ll 1$ region, we try a power series solution and find

$$f=m\pi+A\rho+A\,\frac{\lambda_0+\lambda_1A^2-\frac{4}{3}\lambda_2A^4+\lambda_3A^6}{14\lambda_1+92\lambda_2A^2+30\lambda_3A^4}. \tag{29}$$

With $\lambda_0=\lambda_1=\lambda_2=\lambda_3=1$, we have integrated Eq. (25) numerically both for unit topological charge $m=1$ in (29) and for topological charge 2 corresponding to $m=2$. The profiles of the function f are plotted in Fig. 3(a), and the profiles of their energy densities are plotted in Fig. 3(b). The values of the parameter A in (29) for which the asymptotic behaviors (28) and (29) were achieved numerically are $A=-1.4\,990\,144$ for the $m=1$ solution and $A=-2.0\,554\,812$ for the $m=2$ case. The total energies corresponding to these solutions are $E(m=1)=16.0\,015\,959$ and $E(m=2)=54.3\,091\,345$. We see that $E(m=2)>E(m=1)$ for the most general $O(4)$ model as was the case[4] for the usual Skyrme model.[1]

B. Restricted model: Self-dual solution

To enable us to find a solution which is differentiable at the origin and satisfies the asymptotic conditions (7), with $m=1$, we have made a particular choice for the potential V. Unlike in the previous section, we have not found an adequate potential which is a simple function of the fields ϕ^a and, to avoid writing a cumbersome expression for it, we express this potential in terms of the function f pertaining to the spherically symmetric field configuration (5) as

$$V=\tfrac{1}{4}(\tfrac{1}{2}\sin 2f-f)^2. \tag{30}$$

With this potential, the $d=3$ member of the hierarchy of self-duality equations (11) for the spherically symmetric field configuration reduces to a first-order equation which is immediately integrated to give f as a function of ρ^3:

$$\frac{1}{2}\left(f-\frac{1}{2}\sin 2f\right)=\frac{\pi}{2}\,e^{-\rho^3}. \tag{31}$$

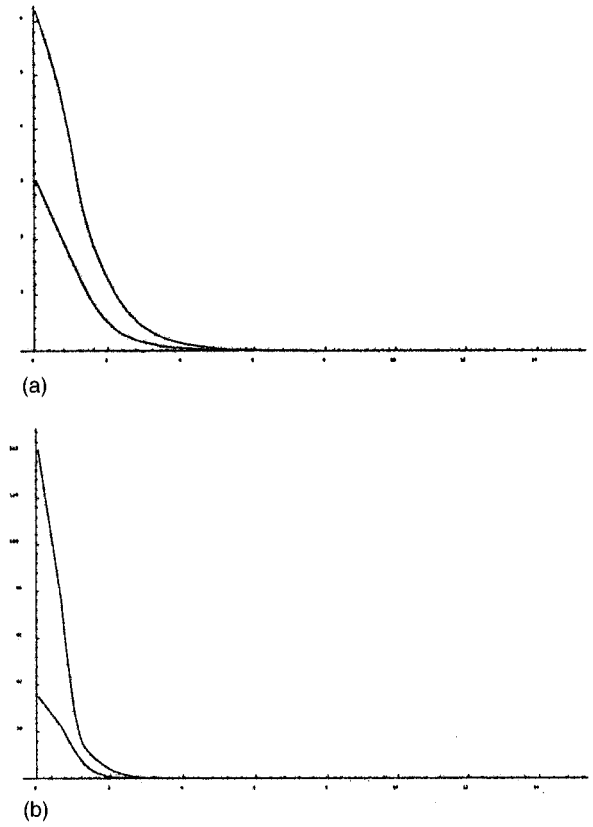

FIG. 3. (a) Profiles of f for the model (24) and $\lambda_0=\lambda_1=\lambda_2=\lambda_3=1$ with the potential (26) with topological charges $m=1,2$, from left to right. (b) Profiles of the energy densities for the hedgehogs in (a), left to right.

The function f given by (31) is easily verified to satisfy the requisite asymptotic conditions (7) with $m=1$ and to be differentiable at the origin.

In the particular normalization we are working in, the energy pertaining to this *unit* topological charge solution equals $\pi^2/4$. This absolutely minimal energy is a lower bound on the energies of the solutions of all the models defined by this potential but with nonvanishing values of the coupling constants λ_1 and λ_2.

To demonstrate this, we set out to integrate (25) with the potential (30) this time. The asymptotic behavior (28) in the region $\rho \gg 1$ is still valid in this case, but in the $\rho \ll 1$ region we compute it again and find

$$f=\pi+A\rho+A\,\frac{\lambda_0\pi^4-4\lambda_1A^2-2\lambda_2A^4+2\lambda_3A^6}{30(\lambda_1+2\lambda_2A^2+\lambda_3A^4)}\,\rho^3. \tag{32}$$

Inspecting (32), we can see that in the limit of λ_1 and λ_2 vanishing, f is well behaved near the origin. This is because the second term in (32) does not become infinite in this limit. The implication is that it should be possible to integrate (25) numerically for progressively decreasing values of λ_1 and λ_2, say with $\lambda_1=\lambda_2$, approaching the self-dual limit. To this end, Eq. (25) with the potential (30) was integrated numerically for each pair of $\lambda_1=\lambda_2$ for the values of the parameter A in (32) listed in Table III. The profiles of the function f for these solutions with $m=1,2$, are plotted in Fig. 4. The total energies pertaining to these solutions were calculated and are listed in

TABLE III. The parameter A for the $m=1$ hedgehogs for the three-dimensional model with potential $V(f)=\frac{1}{4}(\frac{1}{2}\sin(f/2)-f)^2$.

$\lambda_1=\lambda_2$	A
1.0	−1.4265617
0.8	−1.3910057
0.5	−1.3230409
0.2	−1.2257928
0.1	−1.1788389
0.05	−1.1497961
0.01	−1.1219012
0.001	−1.1146950

Table IV. Again as in the two-dimensional case, the last entry in this table is the value closest to the energy of the self-dual solution, which in this case is $\pi^2/3=2.4\,674\,011$.

IV. ANALYTIC PROOFS OF EXISTENCE

In this section, we give proofs of existence for the most general two- and three-dimensional Skyrme models studied in the previous sections. We employ the simplest choices for the potentials $V=(1-\phi^{d+1})$ with $d=2,3$, respectively, which is the choice made in Ref. 9 in the $d=2$ case, and also the choice (26) made in the $d=3$ case. One may check that our method actually covers the general situation where $V=(1-\phi^{d+1})^k$ $(k\geqslant 1)$. Note that the technically easier situation of the usual[1] hedgehog SU(2) Skyrmions in three dimensions was already considered in Ref. 13. The two- and three-dimensional cases are given respectively in the following two subsections. Again the $d=3$ case is less technical and will only be discussed briefly.

A. Two-dimensional case

The energy or mass density for radially symmetric fields is given by (14), with the choice of $V=(1-\cos f)$ for the potential. Without loss of generality, in the following we shall also use the specific values of the parameters: $\lambda_1=\lambda_2=\lambda_0=1$. The boundary conditions are stated by (7) with $m=1$.

The associated Euler–Lagrange equation of (14) governing the detailed behavior of the two-dimensional Skyrmion solitons is

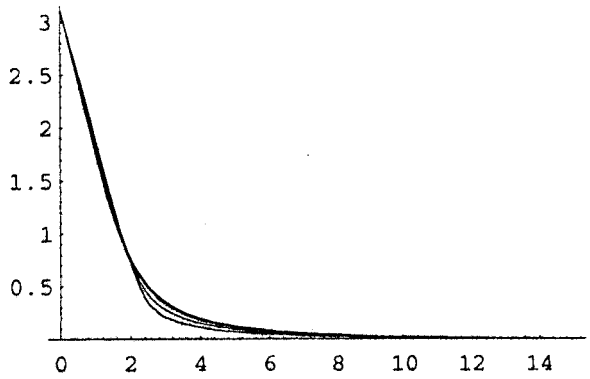

FIG. 4. Profiles of f with unit topological charge ($m=1$) hedgehogs of the $d-3$ model (24) with the potential (30), with $\lambda_0=\lambda_3=1$, and with $\lambda_1=\lambda_2$ decreasing as in Table IV.

TABLE IV. The total energy of the $m=1$ hedgehogs for the three-dimensional model with potential $V(f)=\frac{1}{4}(\frac{1}{2}\sin(f/2)-f)^2$.

$\lambda_1=\lambda_2$	E
1.0	14.6216184
0.8	12.2359948
0.5	8.6076516
0.2	4.9591982
0.1	3.7204152
0.05	3.0983267
0.01	2.5957890
0.001	2.4805067

$$\left(\rho+n^2\,\frac{\sin^2 f}{\rho}\right)\frac{\mathrm{d}^2 f}{\mathrm{d}\rho^2}+\left(n^2\,\frac{\sin f\,\cos f}{\rho}\,\frac{\mathrm{d}f}{\mathrm{d}\rho}+\left[1-n^2\,\frac{\sin^2 f}{\rho^2}\right]\right)\frac{\mathrm{d}f}{\mathrm{d}\rho}$$
$$=n^2\,\frac{\sin f\,\cos f}{\rho}+\rho\,\sin f,\quad \rho>0. \tag{33}$$

Here is the main result of this subsection, namely the existence of a radially symmetric Skyrmion in two dimensions.

Theorem 1: For any winding number n the energy (15) has a minimizer which is a smooth solution of the two-dimensional Skyrme equation (33) subject to the boundary condition

$$f(0)=\pi,\quad f(\infty)=0.$$

Moreover, this solution is strictly decreasing in $\rho>0$ and is ultimately concave up.

Note: The properties of the solution f stated above confirm precisely the numerical results obtained in Ref. 9. The rate of convergence of f at both $\rho=0$ and $\rho=\infty$ is also established.

We shall apply a variational method to prove the theorem. For this purpose, it turns out that the most natural admissible space should be defined by the prescription

$$X=\{f|f(\rho)\ \text{is continuous on}\ [0,\ \infty)\ \text{and absolutely continuous on every compact subinterval of}\ (0,\ \infty)\ \text{so that}\ f(0)=\pi, f(\infty)=0,\quad \text{and}\ E(f)<\infty\}, \tag{34}$$

where the energy $E(f)$ is defined by (14) and (15).

Our proof follows from the existence of a solution to the following optimization problem:

$$\eta\equiv\min\{E(f)|f\in X\}. \tag{35}$$

The proof splits into a few steps.

Lemma 2: Let $\{f_k\}$ be a minimizing sequence of (35). We can always modify the sequence to make it satisfy the uniform bounds

$$0\leqslant f_k\leqslant\pi,\quad k=1,2,\ldots. \tag{36}$$

Proof: We first claim that we can modify $\{f_k\}$ so that it fulfills

$$0\leqslant f_k\leqslant 2\pi,\quad k=1,2,\ldots. \tag{37}$$

In fact, if (37) is violated at some k, we can define a new function $g_k\in X$ by

$$g_k(\rho)=\begin{cases}0, & \text{if } f_k(\rho)\leqslant 0,\\ x, & \text{if } f_k(\rho)\leqslant\pi.\end{cases}$$

Then $0\leqslant g_k\leqslant\pi$, $g_k\in X$, and $E(g_k)=E(f_k)$ in view of (14). The lemma is proven.

Hence for any pair of numbers $0<\rho_1<\rho_2$ we can use Lemma 2 to assert that (35) has a $W^{1,2}(\rho_1,\rho_2)$-bounded minimizing sequence $\{f_k\}$ satisfying (36). A standard diagonal subsequence argument shows that there exists a subsequence of $\{f_k\}$ for which we still denote by the same numeration, $\{f_k\}$, so that

$$\lim_{k\to\infty} f_k=f \quad \text{weakly in } W^{1,2}(\rho_1,\rho_2) \text{ for any } 0<\rho_1<\rho_2. \tag{38}$$

The compact embedding $W^{1,2}(\rho_1,\rho_2)\to C[\rho_1,\rho_2]$ says that

$$\lim_{k\to\infty} f_k=f \quad \text{strongly in } C[\rho_1,\ \rho_2]. \tag{39}$$

It then follows from (38), (39), and (14) that

$$E(f\ )\leqslant \lim_{\rho_1\to 0,\rho_2\to\infty}\sup \lim_{k\to\infty}\inf\int_{\rho_1}^{\rho_2}\mathscr{E}(f_k)\mathrm{d}\rho\leqslant \lim_{k\to\infty}E(f_k)=\eta. \tag{40}$$

In order to show that f is a solution of (35), we still need to achieve $f\in X$. This fact is established in the following.

Lemma 3: The function f obtained above satisfies the boundary condition stated in (34).

Proof: First for the minimizing sequence $\{f_k\}$ satisfying (38) and (39) we have in view of the Schwarz inequality

$$\sin^2 f_k(\rho)=2\int_0^{\rho}\frac{\mathrm{d}f_k}{\mathrm{d}\rho'}\sin f_k\cos f_k\mathrm{d}\rho'\leqslant 2\rho\left(\int_0^{\rho}\left(\frac{\mathrm{d}f_k}{\mathrm{d}\rho'}\right)^2\frac{\sin^2 f_k'}{\rho}\,\mathrm{d}\rho'\right)^{1/2}\leqslant\frac{2\rho}{n}\sup_k E^{1/2}(f_k).$$

In particular $\sin^2 f_k(\rho)\to 0$ as $\rho\to 0$ uniformly with respect to $k=1,2,\ldots$. Therefore, $f_k(\rho)\to\pi$ as $\rho\to 0$ uniformly as well. Thus $f(0)=\pi$ as expected.

We next consider the asymptotic behavior of f as $\rho\to\infty$. We note that (36) is valid for $\{f_k\}$. Consequently,

$$\begin{aligned}1-\cos f_k&=\frac{f_k^2}{2!}\left(1-\frac{f_k^2}{3\cdot 4}\right)+\frac{f_k^6}{6!}\left(1-\frac{f_k^2}{7\cdot 8}\right)+\frac{f_k^{10}}{10!}\left(1-\frac{f_k^2}{11\cdot 12}\right)+\cdots\\&\geqslant\frac{f_k^2}{2!}\left(1-\frac{\pi^2}{3\cdot 4}\right)+\frac{f_k^6}{6!}\left(1-\frac{\pi^2}{7\cdot 8}\right)+\frac{f_k^{10}}{10!}\left(1-\frac{\pi^2}{11\cdot 12}\right)+\cdots\\&>\frac{12-\pi^2}{4!}f_k^2.\end{aligned} \tag{41}$$

Using (41) in (15) we see that f_k satisfies

$$\int_0^{\infty}\rho\left(f_k^2+\left[\frac{\mathrm{d}f_k}{\mathrm{d}\rho}\right]^2\right)\mathrm{d}\rho<C \tag{42}$$

with $C>0$ a constant independent of k. Applying the condition $f_k(\infty)=0$, we have by virtue of the Schwarz inequality again

$$f_k^2(\rho)=-2\int_{\rho}^{\infty}f_k\frac{\mathrm{d}f_k}{\mathrm{d}\rho'}\,\mathrm{d}\rho'\leqslant\frac{2}{\rho}\left(\int_0^{\infty}\rho' f_k^2(\rho')\mathrm{d}\rho'\right)^{1/2}\left(\int_0^{\infty}\rho'\left[\frac{\mathrm{d}f_k}{\mathrm{d}\rho'}\right]^2\mathrm{d}\rho'\right)^{1/2}.$$

Inserting (42) into the above we see that $f_k(\rho)\to 0$ as $\rho\to\infty$ uniformly with respect to k. Thus $f(\infty)=0$ and the lemma follows.

Since $f\in X$, we see that it indeed solves (35). The standard elliptic theory then implies that f is a smooth solution of (33). To complete the proof of Theorem 1, we have to study also the monotonicity and concavity of f.

Lemma 4: The solution f of (35) or (33) obtained above is actually positive valued.

Proof: Otherwise suppose there is a point $\rho_0>0$ so that $f(\rho_0)=0$. Since $f(\rho)\geqslant 0$, we see that ρ_0 is a minimum point of f and $(\mathrm{d}f/\mathrm{d}\rho)(\rho_0)=0$. Using these initial data in (33) and applying the uniqueness theorem of ordinary differential equations we obtain $f(\rho)\equiv 0$, which is false. Thus $f(\rho)>0$ for all $\rho>0$.

Lemma 5: Let f be the function stated in Lemma 4. Then f is strictly decreasing.

Proof: We first show that $(\mathrm{d}f/\mathrm{d}\rho)(\rho)\leqslant 0$ everywhere. Otherwise let us assume that $(\mathrm{d}f/\mathrm{d}\rho)(\rho_0)>0$ at some $\rho_0>0$. Then $f(\rho)>f(\rho_0)$ when ρ is near ρ_0 from the right: $\rho>\rho_0$. Set

$$\rho_{\min}=\max\{\rho'\in[0,\,\rho_0]\,|\,f(\rho')=\min\{f(\rho)\,|\,\rho\in[0,\,\rho_0]\}\}.$$

The property $f(\rho)\to 0$ as $\rho\to\infty$ implies that

$$S_{\min}=\{\rho\in(\rho_0,\infty)\,|\,f(\rho)=f(\rho_{\min})\}$$

is a nonempty compact subset of $(0,\infty)$. Define

$$\rho'_{\min}=\min\{\rho\,|\,\rho\in S_{\min}\}.$$

Then $\rho_{\min}<\rho'_{\min}$ of course. Let $\rho_{\max}\in(\rho_{\min},\rho'_{\min})$ be such that

$$f(\rho_{\max})=\max\{f(\rho)\,|\,\rho\in[\rho_{\min},\rho'_{\min}]\}.$$

We also have $f(\rho_{\min})=f(\rho'_{\min})<f(\rho_{\max})$.

There are two cases we need to consider separately.

(i) $f(\rho_{\max})\leqslant\frac{1}{2}\pi$.

Since both $\sin^2\theta$ and $1-\cos\theta$ are increasing functions in $0\leqslant\theta\leqslant\frac{1}{2}\pi$, we have

$$\sin^2 f(\rho_{\min})<\sin^2 f(\rho),\quad 1-\cos f(\rho_{\min})<1-\cos f(\rho),\quad \rho\in(\rho_{\min},\rho'_{\min}).$$

We can define a new function $g\in X$ by setting

$$g(\rho)=\begin{cases} f(\rho_{\min}), & \rho\in(\rho_{\min},\rho'_{\min}),\\ f(\rho), & \text{otherwise.}\end{cases}$$

Then $E(g)<E(f)$, which contradicts the property of f.

(ii) $f(\rho_{\max})>\frac{1}{2}\pi$.

In this case we introduce two numbers $0<\rho_0<\rho'_0$ by setting

$$\rho_0=\max\{\rho<\rho_{\max}\,|\,f(\rho)=\tfrac{1}{2}\pi\},$$

$$\rho'_0=\min\{\rho>\rho_{\max}\,|\,f(\rho)=\tfrac{1}{2}\pi\}.$$

Then $f(\rho)>\frac{1}{2}\pi$ for $\rho\in(\rho_0,\rho'_0)$. Define

$$g(\rho)=\begin{cases} \pi-f(\rho), & \rho\in(\rho_0,\rho'_0),\\ f(\rho), & \text{otherwise.}\end{cases}$$

Then we can check that $E(g)<E(f)$ because $\sin^2\theta$ is even about $\theta=\frac{1}{2}\pi$ and $1-\cos\theta$ is increasing for $0\leqslant\theta\leqslant\pi$. Hence we arrive at another contradiction and the proof that f is nonincreasing is complete.

We now show that f is strictly decreasing. In fact, if there are $0<\rho_1<\rho_2$ so that $f(\rho_1)=f(\rho_2)$, then $f(\rho)=f(\rho_1)$ for all $\rho\in[\rho_1,\rho_2]$. Inserting this information into Eq. (33) we obtain $\sin f(\rho_1)=0$. By Lemma 4 we must have $f(\rho_1)=\pi$. The uniqueness theorem of ordinary differential equations then implies that $f(\rho)\equiv\pi$, which is false. This proves the lemma.

Lemma 6: The solution f obtained above is ultimately concave up. More precisely, let $\rho_1>0$ be the unique point so that $f(\rho_1)=\frac{1}{2}\pi$. Then $(\mathrm{d}^2f/\mathrm{d}\rho^2)(\rho)>0$ for $\rho>\rho_0$, where $\rho_0=\max\{\rho_1,n\}$.

Proof: Lemma 5 allows us to rewrite (33) in the region $\rho\geqslant\rho_0$ as

$$\left(\rho+n^2\,\frac{\sin^2 f}{\rho}\right)\frac{\mathrm{d}^2f}{\mathrm{d}\rho^2}=\left(n^2\,\frac{\sin f|\cos f|}{\rho}\left|\frac{\mathrm{d}f}{\mathrm{d}\rho}\right|+\left[1-n^2\,\frac{\sin^2 f}{\rho^2}\right]\right)\left|\frac{\mathrm{d}f}{\mathrm{d}\rho}\right|+\left(\rho-n^2\,\frac{|\cos f|}{\rho}\right)\sin f.$$

The right-hand side of this equation is obviously positive. The lemma follows.

In summary, the proof of Theorem 1 is finished.

B. Three-dimensional case

We now consider the situation in the case $d=3$. The energy density is defined by (24) with the potential density given by (26) or

$$V(f)=1-\cos f. \tag{43}$$

Since (24) has the same monotonicity properties as the energy density (14) in the case $d=2$, the method of the previous subsection shows that an energy minimizer satisfying the boundary condition $f(0)=\pi$, $f(\infty)=0$, must be a globally decreasing function which becomes concave up outside a local region. So it remains to examine the existence of such a solution.

In fact, it suffices to see whether the boundary behavior of a field configuration can be controlled. To this end, we observe in view of (24) and the Schwarz inequality that for any ρ and function f defined on $[0,\infty)$ satisfying $f(0)=\pi$ and $f(\infty)=0$, there hold

$$\begin{aligned}\sin^2 f(\rho)&=\int_0^\rho 2\sin f(\rho')\cos f(\rho')\,\frac{\mathrm{d}f}{\mathrm{d}\rho'}\,(\rho')\mathrm{d}\rho'\\&\leqslant 2\rho^{1/2}\int_0^\rho \sin^2 f(\rho')\left(\frac{\mathrm{d}f}{\mathrm{d}\rho'}\right)^2\mathrm{d}\rho'\\&\leqslant C\rho^{1/2}E^{1/2}(f)\quad\text{for }\rho\text{ small},\end{aligned}$$

$$|f(\rho)|\leqslant\rho^{-1/2}\left(\int_0^\infty(\rho')^2\left(\frac{\mathrm{d}f}{\mathrm{d}\rho'}\right)^2(\rho')\mathrm{d}\rho'\right)^{1/2}\leqslant C\rho^{-1/2}E^{1/2}(f)\quad\text{for }\rho\text{ large}.$$

The above estimates indicate that the boundary condition is easily preserved. Consequently, the existence of an energy minimizer in the $d=3$ case is ensured as before. Thus we can state the following.

Theorem 7: In the case $d=3$, the energy $E(f)=\int L_3\,d\rho$ with L_3 being defined in (24) and the hedgehog field configuration f subject to the boundary condition $f(0)=\pi$, $f(\infty)=0$, has a minimizer. The function f is a smooth solution of the associated Euler–Lagrange equation (25). Furthermore, f is strictly decreasing in the entire region $\rho>0$ and is concave up for ρ sufficiently large.

The method employed here can be applied to obtain existence and global behavior results for many other related problems in classical field theory. For example, the SU(3) Skyrme model[14] governed by the reduced hedgehog energy functional $M(F)=\lambda_1 M_{\rm cl}(F)+\lambda_2 m_{\rm cl}(F)$, where $\lambda_1,\lambda_2>0$ and

$$M_{\rm cl}(F)=\int\left\{\frac{\rho^2}{8}\left(\frac{{\rm d}F}{{\rm d}\rho}\right)^2+\frac{\sin^2 F}{4}+\frac{\sin^4 F}{2\rho^2}+\left(\frac{{\rm d}F}{{\rm d}\rho}\right)^2\right\}{\rm d}\rho,$$

$$m_{\rm cl}(F)=\int(1-\cos F)\rho^2\,{\rm d}\rho,$$

is useful in modelling the top quark. The field F has the same boundary condition $F(0)=\pi$, $F(\infty)=0$, as before. We can show without difficulty that Theorem 7 is valid for this model.

V. SUMMARY

We have studied the radially/spherically symmetric solutions to the most general class of Skyrme models in two and three dimensions, which capture all the features that we are concerned with in all higher *even* and *odd* dimensions. Special attention is given to a subclass of these models which support self-dual solutions, which are found explicitly. In the general case, the Euler–Lagrange equations could not be explicitly integrated so their integration was performed numerically and analytic proofs for the existence of these solutions were given.

In the odd-dimensional case $d=3$ where it is possible to find finite energy topologically stable solutions of arbitrary topological charge, we have considered the charge-2 solution and found that it is heavier than two charge-1 solutions, as in the case of the usual Skyrmions.[4] In the even-dimensional case $d=2$, it is possible to find *unit* charge solutions only, but due to the low dimensionality it was possible to study solutions of arbitrary vorticity n.

One of the main purposes of this work was the study of the most general d-dimensional $O(d+1)$ Skyrme models, whose properties are typified by the $d=2$ even-, and the $d=3$ odd-, dimensional cases, respectively. These were studied both numerically and analytically. Our numerical studies lead to the conclusion that *radially and spherically symmetric static* bound states are absent in all Skyrme models with *exponentially localized* hedgehogs with $m=1$.

The other main purpose of this work was the study of a special subclass of the most general Skyrme models, defined by (10), which support self-dual solutions. This new subclass of systems differs from the previously known scale-invariant hierarchy[5,6] of scale invariant Skyrme–Sigma models in a very important respect. The latter[5] support self-dual solutions **power** localized to an arbitrary scale related to the scale invariance, while the solutions of the new system (10) by contrast can be localized **exponentially**.

Another very important difference between the self-duality equations of the two hierarchies is that, with the exception of the first[6] member of the former[5] case, they are overdetermined[7] as a result of which the only solutions these[5] support are spherically symmetric. By contrast, the hierarchy of self-duality equations (11) are underdetermined. While in this paper we have restricted ourselves to the study of radially/spherically symmetric solutions only, this last property indicates that there must exist solutions with symmetries less restrictive than radial/spherical. Indeed, the underdetermined nature of our self-duality equations results in the generation of a large class of new solutions from any given one. These aspects of the present work are deferred to a future investigation. It is expected that this would follow the lines of two intensive studies[9] of the analogous properties in a related class of d-dimensional $O(d)$ models, where multi-center solutions were found.

Perhaps the most interesting property of the systems (10) is that the self-dual solutions it supports are smoothly related to the non-self-dual solutions of the general systems (1), by letting the constants κ_p in (1) for $p=1,2,..,(d-1)$ vanish. This aspect of the $O(d)$ models was studied recently in detail in Ref. 11.

Finally, we mention a certain inflexible property of our subclass of models (10) which are essentially characterized by the potential V. The solutions of the d-dimensional self-duality equation are functions of the variable ρ^d and are differentiable at the origin **only** for suitable but nonunique choices of V. In dimensions $d>2$ the only solutions which are differentiable at the origin are the spherically symmetric solutions with unit topological charge. Only in dimension $d=2$ is it possible to find solutions of higher charge with vorticity n, where a given choice of V can lead to a well-behaved solution for a given n only.

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Correlation properties of quantum measurements

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The kind of information provided by a measurement is determined in terms of the correlation established between observables of the apparatus and the measured system. Using the framework of quantum measurement theory, necessary and sufficient conditions for a measurement interaction to produce strong correlations are given and are found to be related to properties of the final object and apparatus states. These general results are illustrated with reference to the *standard model* of the quantum theory measurement. © *1996 American Institute of Physics.* [S0022-2488(96)03506-2]

I. INTRODUCTION

Any physical measurement is carried out in order to provide information about a specified system, its state prior to or after the measurement. The procedure generally is to ascertain the values of a pointer observable, which have become correlated with some observable of the measured system. Thus the kind of information available by a given measurement depends on the statistical dependencies established by the interaction between the apparatus, or some probe system, and the object.

The minimal content of the notion of measurement in quantum mechanics is given by the *probability reproducibility* requirement; according to this condition, a particular measurement scheme qualifies as a measurement of a given observable E if for all initial states of the object system the associated probability distributions of E are reproduced in the resulting statistics of pointer readings.[1] Regarding a large ensemble of object plus apparatus systems as one individual system, this situation can be described in terms of strong correlations between the values of the frequency operators (see, e.g., Ref. 1) associated with the observable E and the pointer observable, respectively. In the present context we shall not be concerned with the ensembles regarded as individual objects but rather we shall analyze statistical dependencies between individual members of the ensembles as they show up in certain correlation quantities. The following three kinds of correlations appear naturally in the measurement context: correlations between an object observable E and the pointer observable; correlations between the values of these observables; and correlations between the conditional final states of the object system and apparatus, respectively. Our goal is to give exhaustive characterizations of the conditions under which these correlations are established. It will be found that the final component states of the object and apparatus must possess certain properties in order that such correlations may be strong.

Our investigation builds on previous work published in Ref. 2. Correcting an erroneous characterization of strong correlations used in that paper, we give here a complete account of necessary and sufficient conditions for the occurrence of strong correlations. In addition, the scope of the results is extended beyond unitary measurements and sharp observables to cover arbitrary measurements and pointer observables and general object observables. Finally, possible fields of

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applications are indicated on the basis of the standard model of measurement theory, which was recently used in various proposals for quantum and atomic optics QND measurements.[3]

II. FRAMEWORK

2.1. We follow here the Hilbert space formulation of quantum mechanics in which the description of a physical system $\mathscr{S}$ is based on a complex separable Hilbert space $\mathscr{H}$, with the inner product $\langle\cdot|\cdot\rangle$, and which builds on the dual concepts of states and observables reflecting the general structure of an experiment: preparation of the system followed by a measurement.

2.2. Let $\mathscr{L}(\mathscr{H})$ denote the set of bounded linear operators on $\mathscr{H}$ and $\mathscr{T}(\mathscr{H})$ its subset of trace class operators. A *state* of $\mathscr{S}$ is given as a positive linear operator $T:\mathscr{H}\to\mathscr{H}$ of trace one. We let $\mathscr{S}(\mathscr{H}):=\{T\in\mathscr{T}(\mathscr{H})|T\geqslant O,\ \mathrm{tr}[T]=1\}$ denote the set of states of $\mathscr{S}$, and we recall that $\mathscr{S}(\mathscr{H})$ is a (σ-)convex subset of $\mathscr{T}(\mathscr{H})$, the one-dimensional projection operators $P[\varphi]$ (generated by the unit vectors $\varphi\in\mathscr{H}$) being its extremal elements. The $P[\varphi]$ shall be called *vector states*.

2.3. Let Ω be a set and $\mathscr{F}$ a σ-algebra of subsets of Ω. An *observable* of $\mathscr{S}$ is represented as (and identified with) a normalized positive operator valued measure, a POV measure, $E:\mathscr{F}\to\mathscr{L}(\mathscr{H})$, that is, an operator valued mapping $X\mapsto E(X)$ on $\mathscr{F}$ with the properties: (i) $E(\Omega)=I$, (ii) $E(X)\geqslant O$, and $E(\cup X_i)=\Sigma E(X_i)$ for any disjoint sequence $(X_i)\subset\mathscr{F}$, with the series $\Sigma E(X_i)$ converging in the weak operator topology of $\mathscr{L}(\mathscr{H})$. We recall that the projection valued measures, the PV measures, are a particular case of the POV measures; furthermore a POV measure E is a PV measure, that is, $E(X)^2=E(X)$ for all $X\in\mathscr{F}$, if and only if E is multiplicative, that is, $E(X\cap Y)=E(X)E(Y)$ for all $X,Y\in\mathscr{F}$. Observables which are represented by PV measures are called *sharp* observables. It is by now well established that the extension of the notion of observables from PV measures to POV measures is a necessity in quantum mechanics.

2.4. The probability measure

$$p_T^E:\mathscr{F}\to[0,1],\quad X\mapsto p_T^E(X):=\mathrm{tr}[TE(X)] \tag{1}$$

defined by an observable E and a state T is related to a measurement by virtue of the minimal interpretation of quantum mechanics: *the number $p_T^E(X)$ is the probability that a measurement of the observable E performed on the system $\mathscr{S}$ in the state T leads to a result in the set X*. The intended empirical content of this statement is the following: If the same E-measurement were repeated sufficiently many times under the same conditions (characterized by T), then in the long run the relative frequency of the occurrence of the measurement results in X would approach the number $p_T^E(X)$.

III. MEASUREMENT

A. General

3.1. A *measurement scheme* for the (object) system $\mathscr{S}$ consists of a *measuring apparatus* $\mathscr{A}$ [with its Hilbert space $\mathscr{H}_\mathscr{A}$], a *pointer observable* $Z:\mathscr{F}_\mathscr{A}\to\mathscr{L}(\mathscr{H}_\mathscr{A})$ [with its ''space of values'' $(\Omega_\mathscr{A},\mathscr{F}_\mathscr{A})$], an *initial state* $T_\mathscr{A}$ of the apparatus, a *measurement coupling* V [a linear state transformation on $\mathscr{T}(\mathscr{H}\otimes\mathscr{H}_\mathscr{A})$], and a [measurable] *pointer function* $f:\Omega_\mathscr{A}\to\Omega$, with the assumption that if $T\in\mathscr{S}(\mathscr{H})$ is an initial state of $\mathscr{S}$, then $V(T\otimes T_\mathscr{A})$ is the final state of the compound object–apparatus system $\mathscr{S}+\mathscr{A}$. Taking the partial traces of $V(T\otimes T_\mathscr{A})$ over $\mathscr{H}_\mathscr{A}$ and $\mathscr{H}$, respectively, one gets the corresponding reduced states $\mathscr{R}_\mathscr{S}(V(T\otimes T_\mathscr{A}))$ and $\mathscr{R}_\mathscr{A}(V(T\otimes T_\mathscr{A}))$ of $\mathscr{S}$ and $\mathscr{A}$, respectively; then the probability measure of the pointer observable Z in the final apparatus state is completely determined as $Y\mapsto p^Z_{\mathscr{R}_\mathscr{A}(V(T\otimes T_\mathscr{A}))}(Y)=\mathrm{tr}[\mathscr{R}_\mathscr{A}(V(T\otimes T_\mathscr{A}))Z(Y)]$, $Y\in\mathscr{F}_\mathscr{A}$.

3.2. A measurement scheme $\mathscr{M}:=\langle\mathscr{H}_\mathscr{A},Z,T_\mathscr{A},V,f\rangle$ defines an observable $E^\mathscr{M}$ of $\mathscr{S}$ with the space of values $(\Omega,\mathscr{F})$ via the relation: for any $X\in\mathscr{F}$ and $T\in\mathscr{S}(\mathscr{H})$,

$$p_T^{E^\mathscr{M}}(X):=p^Z_{\mathscr{R}_\mathscr{A}(V(T\otimes T_\mathscr{A}))}(f^{-1}(X)). \tag{2}$$

This is the observable *measured* by means of the scheme $\mathscr{M}$ in the sense that the totality of the distributions $p^Z_{\mathscr{R}_{\mathscr{A}}(V(T\otimes T_{\mathscr{A}}))}$ (for all $T\in\mathscr{S}(\mathscr{H})$) of the pointer outcomes in the final apparatus states determine the POV measure $E^{\mathscr{M}}$ via Eq. (2). A measurement scheme $\mathscr{M}$ is a measurement of a given observable E if the measured observable $E^{\mathscr{M}}$ equals E.

3.3. There is an important subclass of measurement schemes for $\mathscr{S}$. They consist of a sharp pointer observable Z, a vector state preparation of $\mathscr{A}$, $T_{\mathscr{A}}=P[\phi]$, $\phi\in\mathscr{H}_{\mathscr{A}}$, $\langle\phi|\phi\rangle=1$, and a unitary measurement coupling $V(T\otimes T_{\mathscr{A}})=UT\otimes T_{\mathscr{A}}U^*$, with a unitary map U on $\mathscr{H}\otimes\mathscr{H}_{\mathscr{A}}$. Subsuming the possible pointer function in the definition of Z by identification of Ω and $\Omega_{\mathscr{A}}$, we denote such a scheme $\mathscr{M}_U:=\langle\mathscr{H}_{\mathscr{A}}, Z, P[\phi], U\rangle$ and call it a *unitary measurement scheme* (with the understanding that Z is a sharp observable). It is a basic result of the quantum theory of measurement that every observable E of $\mathscr{S}$ admits a unitary measurement, that is, there is a unitary measurement scheme $\mathscr{M}_U$ such that $E^{\mathscr{M}_U}=E$.[4] Thus the relation between measurement schemes and POV measures induced by Eq. (2) defines a map from the former onto the latter. In spite of this fundamental result, it is important to consider general measurement schemes $\mathscr{M}$, since in many applications the choices of a sharp pointer and a vector state preparation of the apparatus are not physically realizable.

3.4. Another basic condition for a measurement scheme $\langle\mathscr{H}_{\mathscr{A}}, Z, T_{\mathscr{A}}, V, f\rangle$ to qualify as a measurement is the requirement that the measurement should lead to a definite result. We take this requirement to entail, first of all, that the pointer observable Z should have assumed a definite value after the measurement. One should then be able to ''read the actual value'' of the pointer observable Z and deduce from this the value of the measured observable. As is well known, the task of explaining the occurrence of a definite pointer value at the end of a measuring process presents one of the major open problems in quantum mechanics. We do not enter this difficult question here. (For an overview of the issues involved, the reader may wish to consult Ref. 1.) There are, however, some necessary conditions for the pointer observable Z to assume a definite value in the final apparatus state $\mathscr{R}_{\mathscr{A}}(V(T\otimes T_{\mathscr{A}}))$, conditions which are tractable and which call for the study of the correlation properties of a measurement. These conditions are the subject of the present paper.

B. Reading of pointer values

3.5. The reading of measurement outcomes involves the discrimination between the elements of a finite (or, as an idealization, countable) set of alternative pointer values. In order to formulate this idea in the general context of an E-measurement $\mathscr{M}$, we introduce the notion of a *reading scale* as a countable partition of the value space of the pointer observable, $\Omega_{\mathscr{A}}=\cup f^{-1}(X_i)$, induced by a countable partition of the value space of the measured observable, $\Omega=\cup X_i$, $X_i\in\mathscr{F}$, $X_i\cap X_j=0$ for $i\neq j$. Such a reading scale will be denoted $\mathscr{R}$, and we let $\mathbf{I}$ denote its index set.

3.6. A reading scale $\mathscr{R}$ determines discrete, coarse-grained versions of the pointer observable Z and the measured observable E

$$Z^{\mathscr{R}}: i\mapsto Z_i:=Z(f^{-1}(X_i)),\quad i\in\mathbf{I}, \tag{3a}$$

$$E^{\mathscr{R}}: i\mapsto E_i:=E(X_i),\quad i\in\mathbf{I}. \tag{3b}$$

The $Z^{\mathscr{R}}$-value i refers to the pointer reading $f^{-1}(X_i)$ which, in turn, is correlated to the value set X_i of the measured observable E. If E itself is discrete there is a natural (finest) reading scale $\mathscr{R}$ such that $E=E^{\mathscr{R}}$ and $Z^f=Z^{\mathscr{R}}$. It should be noted that we have included the pointer function f in the definition of $Z^{\mathscr{R}}$ so that the two discrete observables (3) do have the same set of values.

3.7. We say that the (discrete) pointer observable $Z^{\mathscr{R}}$ *has the value* i in the state $\mathscr{R}_{\mathscr{A}}(V(T\otimes T_{\mathscr{A}}))$ if and only the measurement outcome probability for this value equals one: $\mathrm{tr}[\mathscr{R}_{\mathscr{A}}(V(T\otimes T_{\mathscr{A}}))Z_i]=1$. Since $\mathrm{tr}[TE_i]=\mathrm{tr}[\mathscr{R}_{\mathscr{A}}(V(T\otimes T_{\mathscr{A}}))Z_i]$, and, in general, $0\neq p^E_T(X_i)\neq 1$, the pointer observable does not have a value at the end of the measurement. It may, however,

occur that the state $\mathscr{R}_{\mathscr{A}}(V(T\otimes T_{\mathscr{A}}))$ is a *mixture of eigenstates of* $Z^{\mathscr{R}}$ *with the weights* $p_T^E(X_i)$. This is indeed a necessary condition for the assertion that the pointer observable Z has assumed a definite value with respect to a reading scale $\mathscr{R}$ at the end of the measurement $\mathscr{M}$. We go on to specify this case further.

3.8. We consider a measurement $\langle \mathscr{K}_{\mathscr{A}}, Z, T_{\mathscr{A}}, V, f\rangle$ of E with a fixed reading scale $\mathscr{R}$. Any X_i, $i\in\mathbf{I}$, defines a (unnormalized) *conditioned state*

$$V_i(T) := I\otimes Z_i^{1/2} V(T\otimes T_{\mathscr{A}}) I\otimes Z_i^{1/2}, \tag{4}$$

the state of $\mathscr{S}+\mathscr{A}$ on the condition that the pointer observable $Z^{\mathscr{R}}$ has value i. The (trace) norm of this state is $\mathrm{tr}[V_i(T)]=\mathrm{tr}[V(T\otimes T_{\mathscr{A}})I\otimes Z_i]=p_T^E(X_i)$, and the corresponding (normalized) reduced states, the *final component states* of $\mathscr{S}$ and $\mathscr{A}$ are

$$T_{\mathscr{S}}(i,T) := p_T^E(X_i)^{-1}.\mathscr{R}_{\mathscr{S}}(V_i(T)), \tag{5a}$$

$$T_{\mathscr{A}}(i,T) := p_T^E(X_i)^{-1}.\mathscr{R}_{\mathscr{A}}(V_i(T)). \tag{5b}$$

(If $p_T^E(X_i)=0$, we put $T_{\mathscr{S}}(i,T)=T_{\mathscr{A}}(i,T)=O$). The conditional interpretation of the states (4) and (5) presupposes, however, that the pointer observable $Z^{\mathscr{R}}$ has value i in state $T_{\mathscr{A}}(i,T)$, that is, $\mathrm{tr}[T_{\mathscr{A}}(i,T)Z_i]=1$ for all i and T whenever $p_T^E(X_i)\neq 0$.[5] This requirement is always satisfied if the pointer observable is sharp. In general this is a condition to be imposed on the measurement scheme. We call it the *pointer value-definiteness* condition and note that it may be written in either of the following equivalent forms:

$$\mathrm{tr}[T_{\mathscr{A}}(i,T)Z_i]=1 \quad (\text{whenever } p_T^E(X_i)\neq 0), \tag{6a}$$

$$Z_i T_{\mathscr{A}}(i,T) = T_{\mathscr{A}}(i,T), \tag{6b}$$

for all $i\in\mathbf{I}$ and all initial states T of $\mathscr{S}$.

3.9. For any reading scale $\mathscr{R}$ and any state $T\in\mathscr{S}(\mathscr{H})$ one has

$$\mathscr{R}_{\mathscr{S}}(V(T\otimes T_{\mathscr{A}})) = \sum\, p_T^E(X_i) T_{\mathscr{S}}(i,T); \tag{7}$$

this is to say that the final object state behaves additively with respect to the pointer conditioning: That is, the state of $\mathscr{S}$ on the plain condition that the measurement has been performed, is the same as the state of $\mathscr{S}$ after the measurement conditional on the fact that the pointer value is registered with respect to the reading scale $\mathscr{R}$.[6] Although it also holds true that for any $i\in\mathbf{I}$ and $T\in\mathscr{S}(\mathscr{H})$

$$T_{\mathscr{A}}(i,T) = p_T^E(X_i)^{-1} Z_i^{1/2}.\mathscr{R}_{\mathscr{A}}(V(T\otimes T_{\mathscr{A}}))Z_i^{1/2}, \tag{8}$$

it is not the case, in general, that the final apparatus state $\mathscr{R}_{\mathscr{A}}(V(T\otimes T_{\mathscr{A}}))$ is conditioned with respect to $\mathscr{R}$; thus, in general,

$$\mathscr{R}_{\mathscr{A}}(V(T\otimes T_{\mathscr{A}})) \neq \sum\, p_T^E(X_i) T_{\mathscr{A}}(i,T). \tag{9}$$

The requirement that $\mathscr{R}_{\mathscr{A}}(V(T\otimes T_{\mathscr{A}}))$ is a mixture of the final component states $T_{\mathscr{A}}(i,T)$ is therefore another condition on the measurement;[2] we call it the *pointer mixture condition*

$$\mathscr{R}_{\mathscr{A}}(V(T\otimes T_{\mathscr{A}})) = \sum\, p_T^E(X_i) T_{\mathscr{A}}(i,T) \tag{10}$$

for all initial states T of $\mathscr{S}$.

3.10. The pointer value-definiteness condition (6) and the pointer mixture condition (10) imply that the final apparatus state is a mixture of the pointer eigenstates $T_{\mathscr{A}}(i,T)$ with the weights $p_T^E(X_i)$; this means that the final apparatus state $\mathscr{R}_{\mathscr{A}}(V(T\otimes T_{\mathscr{A}}))$ is conditioned with respect to the reading scale $\mathscr{R}$.[2,6] One may consider the assumption that in addition to this, the state $\mathscr{R}_{\mathscr{A}}(V(T\otimes T_{\mathscr{A}}))$ admits the *ignorance interpretation* with respect to the decomposition (10): that is, the apparatus [in state $\mathscr{R}_{\mathscr{A}}(V(T\otimes T_{\mathscr{A}}))$] is actually in one of the component states $T_{\mathscr{A}}(i,T)$, and this is the case with the subjective probability $p_T^E(X_i)$. As is well known, such an interpretation of the mixed state $\mathscr{R}_{\mathscr{A}}(V(T\otimes T_{\mathscr{A}}))$ is extremely problematic and in most cases impossible; but if it were the case then the pointer could be claimed to have a definite value i (with respect to a reading scale $\mathscr{R}$) after the measurement with the subjective probability $p_T^E(X_i)$. Setting aside the difficulties with the ignorance interpretation (and thus with explaining the occurrence of definite measurement outcomes in quantum mechanics), it still is important to investigate more closely the conditions (6) and (10) and to see how these possible properties of a measurement are related to the structure of the final state of the object system.

Theorem 3.11: *Let $\mathscr{M}$ be a measurement of an observable E and $\mathscr{R}$ any reading scale. For any initial state T of the object system, the condition (a) implies the conditions (b) and (c):*

$$\text{(a)}\quad T_{\mathscr{S}}(i,T)\cdot T_{\mathscr{S}}(j,T)=O \quad \text{for } i\neq j;$$

$$\text{(b)}\quad \mathscr{R}_{\mathscr{A}}(V(T\otimes T_{\mathscr{A}}))=\Sigma p_T^E(X_i)T_{\mathscr{A}}(i,T) \quad \text{for all } i;$$

$$\text{(c)}\quad Z_i T_{\mathscr{A}}(i,T)=T_{\mathscr{A}}(i,T) \quad \text{for all } i.$$

If $\mathscr{M}$ is a unitary measurement $\mathscr{M}_U$, then (a) and (b) are equivalent conditions for any initial vector state $T=P[\varphi]$ of $\mathscr{S}$.

Proof:

(a)⇒(b)&(c): For each i, let F_i be the support projection of $T_{\mathscr{S}}(i,T)$, that is, the smallest projection of Q such that $QT_{\mathscr{S}}(i,T)=T_{\mathscr{S}}(i,T)$. Then one gets (for $i\neq j$)

$$\begin{aligned}
T_{\mathscr{S}}(i,T)\cdot T_{\mathscr{S}}(j,T)=0 &\Leftrightarrow F_i T_{\mathscr{S}}(j,T)=O\\
&\Leftrightarrow \mathrm{tr}[F_i\otimes I V_j(T)]=0\\
&\Leftrightarrow F_i\otimes Z_j^{1/2}V(T\otimes T_{\mathscr{A}})I\otimes Z_j^{1/2}=O\\
&\Leftrightarrow F_i\otimes Z_j^{1/2}V(T\otimes T_{\mathscr{A}})^{1/2}=O\\
&\Rightarrow F_i\otimes Z_j V(T\otimes T_{\mathscr{A}})^{1/2}=O. \qquad (\alpha)
\end{aligned}$$

By the definition of F_i one also has

$$\begin{aligned}
F_i T_{\mathscr{S}}(i,T)=T_{\mathscr{S}}(i,T) &\Leftrightarrow F_i\otimes Z_i^{1/2}V(T\otimes T_{\mathscr{A}})I\otimes Z_i^{1/2}=I\otimes Z_i^{1/2}V(T\otimes T_{\mathscr{A}})I\otimes Z_i^{1/2}\\
&\Rightarrow F_i\otimes Z_i V(T\otimes T_{\mathscr{A}})^{1/2}=I\otimes Z_i V(T\otimes T_{\mathscr{A}})^{1/2}. \qquad (\beta)
\end{aligned}$$

Combining (α) and (β) and using the fact that $\Sigma Z_i=I$ yields

$$F_i\otimes IV(T\otimes T_{\mathscr{A}})^{1/2}=F_i\otimes Z_i V(T\otimes T_{\mathscr{A}})^{1/2}=I\otimes Z_i V(T\otimes T_{\mathscr{A}})^{1/2}. \qquad (\gamma)$$

From this one obtains $I\otimes Z_i V(T\otimes T_{\mathscr{A}})=I\otimes Z_i^2 V(T\otimes T_{\mathscr{A}})$, which gives (c). Using (c), one shows similarly that

$$I\otimes Z_i V(T\otimes T_{\mathscr{A}})^{1/2}=I\otimes Z_i^{1/2}V(T\otimes T_{\mathscr{A}})^{1/2}.$$

Inserting this in (γ), multiplying each term with its adjoint and summing over i, one obtains

$$\sum F_i\otimes IV(T\otimes T_{\mathscr{A}})F_i\otimes I=\sum I\otimes Z_i^{1/2}V(T\otimes T_{\mathscr{A}})I\otimes Z_i^{1/2}.$$

Taking the partial trace with respect to $\mathscr{H}$ finally yields (b).

(b)⇒(a): This implication will be shown for a unitary measurement $\mathscr{M}_U$ and for vector state preparations $T=P[\varphi]$. In that case $T_{\mathscr{A}}=P[\phi]$ and $V(T\otimes T_{\mathscr{A}})=P[U(\varphi\otimes\phi)]$. Denoting the biorthogonal decomposition of this state as $U(\varphi\otimes\phi)=\Sigma_{nk}c_n\varphi_{nk}\otimes\phi_{nk}$, with $c_n>0$, we obtain $T_{\mathscr{A}}(\Omega,T)=\Sigma_{nk}|c_n|^2P[\phi_{nk}]$. Now (b) implies that all the projections Z_i commute with $T_{\mathscr{A}}(\Omega,T)$. Therefore, one can choose the orthonormal system $\{\phi_{nk}\}$ such that $Z_i\phi_{nk}=\phi_{nk}$ or $Z_i\phi_{nk}=0$. Thus there is a renumbering of this system, $\{\phi_{nk}\}=\{\phi_{il}\}$, such that $Z_i\phi_{il}=\phi_{il}$. It follows that there are corresponding renumberings $\{\varphi_{il}\}=\{\varphi_{nk}\}$ and $\{d_{il}\}=\{c_n\}$ such that $U(\varphi\otimes\phi)=\Sigma d_{il}\varphi_{il}\otimes\phi_{il}$. Then $T_{\mathscr{S}}(i,T)=\Sigma_l|d_{il}|^2P[\varphi_{il}]$. Since the subsets of vectors φ_{il} with different values of i are mutually disjoint and therefore orthogonal, one concludes that (a) holds. This completes the proof.

It can be demonstrated by means of examples that the implication (b)⇒(a) need not hold if the measurement is not unitary or if the initial pointer state is not pure.[1]

C. First kind and repeatable measurements

3.12. A measurement $\mathscr{M}$ of an observable E is of the *first kind* if the probability for a given result is the same both before and after the measurement, that is, for any $T\in\mathscr{S}(\mathscr{H})$ and for all $X\in\mathscr{F}$,

$$p_T^E(X)=p^E_{\mathscr{R}_{\mathscr{A}}(V(T\otimes T_{\mathscr{A}}))}(X). \tag{11}$$

Unitary measurement schemes with a coupling $U=e^{i\lambda A\otimes B}$, $\lambda\in\mathbf{R}$, A (on $\mathscr{H}$) and B (on $\mathscr{H}_{\mathscr{A}}$) self-adjoint, do give rise to such measurements; we refer to Sec. VIII for an analysis of this model.

3.13. A measurement $\mathscr{M}$ of an observable E is *repeatable* if its repetition does not lead to a new result. One way to express the requirement is the following: For any $T\in\mathscr{S}(\mathscr{H})$ and $X\in\mathscr{F}$, if $p_T^E(X)\neq 0$, then

$$p^E_{T_{\mathscr{S}}(X,T)}(X)=1, \tag{12}$$

(where $T_{\mathscr{S}}(X,T)$ is defined by Eqs. (3a), (4) and (5a) with $X=X_i$). Equivalently, $\mathscr{M}$ is a repeatable E-measurement if for any $T\in\mathscr{S}(\mathscr{H})$ and $X\in\mathscr{F}$, for which $p_T^E(X)\neq 0$, it holds true that

$$E(X)T_{\mathscr{S}}(X,T)=T_{\mathscr{S}}(X,T). \tag{13}$$

Another basic result of measurement theory is that an observable E which admits a repeatable measurement is discrete.[4,7]

3.14. According to Eq. (13), a repeatable measurement drives the object system into an eigenstate of the measured observable $E:i\mapsto E_i$. The orthogonality conditions of Theorem 3.11 are then satisfied and the final apparatus state $\mathscr{R}_{\mathscr{A}}(V(T\otimes T_{\mathscr{A}}))$ is the mixture of the eigenstates $T_{\mathscr{A}}(i,T)$ of $Z:i\mapsto Z_i$ with the weights $\mathrm{tr}[TE_i]$.

3.15. It is evident that repeatable measurements are also of the first kind. However, as will be demonstrated in Sec. VIII, a first kind measurement need not be repeatable, though for sharp observables the two notions coincide.[8]

IV. STATISTICAL DEPENDENCE AND CORRELATIONS

A measurement $\mathscr{M}$ of an observable E brings the compound object–apparatus system into an entangled state $V(T\otimes T_{\mathscr{M}})$. The possibility of transferring information from $\mathscr{A}$ to $\mathscr{S}$ rests on the fact that this state entails *statistical dependencies* between quantities pertaining to these systems. Accordingly, three types of *correlations* inherent in the state $V(T\otimes T_{\mathscr{M}})$ are of special interest for characterizing the measurement: (i) correlations between the measured observable and the pointer observable; (ii) correlations between the corresponding values of these observables; and (iii) correlations between the final component states of the two subsystems. For their study it is helpful to recall some basic notions and facts concerning the relation between statistical dependence and correlation.

4.1. Let μ be a probability measure on the real Borel space $(\mathbf{R}^2,\mathscr{B}(\mathbf{R}^2))$, and let μ_1 and μ_2 be the marginal measures of μ with respect to a Cartesian coordinate system: For $X,Y\in\mathscr{B}(\mathbf{R})$,

$$\mu_1(X)=\mu(X\times\mathbf{R}),\quad \mu_2(Y)=\mu(\mathbf{R}\times Y). \tag{14}$$

These marginal measures correspond to the coordinate projections (random variables) π_1: $(x,y)\mapsto x$ and π_2: $(x,y)\mapsto y$ in the sense that $\mu_i=\mu^{\pi_i}$, that is, $\mu_i(X)=\mu^{\pi_i}(X):=\mu(\pi_i^{-1}(X))$ for all $X\in\mathscr{B}(\mathbf{R})$, $i=1,2$. Assume that the expectations and the variances of μ_i are well defined and finite: $\epsilon_i=\int x\, d\mu_i(x)$, $\sigma_i^2=\int(x-\epsilon_i)^2\, d\mu_i(x)$, and let $\epsilon_{12}=\int xy\, d\mu(x,y)$. The (normalized) *correlation* of the marginal measures μ_1 and μ_2 in μ is then defined as

$$\rho(\mu_1,\mu_2;\mu):=\int \frac{(x-\epsilon_1)(y-\epsilon_2)}{\sigma_1\sigma_2}\, d\mu(x,y)=\frac{\epsilon_{12}-\epsilon_1\epsilon_2}{\sigma_1\sigma_2} \tag{15}$$

(whenever $\sigma_1\neq 0\neq\sigma_2$). The Schwarz inequality entails $|\rho(\mu_1,\mu_2;\mu)|\leqslant 1$. The marginals μ_1,μ_2 are *uncorrelated* if $\rho(\mu_1,\mu_2;\mu)=0$ (that is, $\epsilon_{12}=\epsilon_1\epsilon_2$), *strongly correlated* if $\rho(\mu_1,\mu_2;\mu)=1$ (that is, $\epsilon_{12}-\epsilon_1\epsilon_2=\sigma_1\sigma_2$), and *strongly anticorrelated* if $\rho(\mu_1,\mu_2;\mu)=-1$ (that is, $\epsilon_{12}-\epsilon_1\epsilon_2=-\sigma_1\sigma_2$). The strong correlation conditions can also be written in terms of the coordinate projections π_1 and π_2

$$\rho(\pi_1,\pi_2;\mu)=+1 \ \text{ iff } \ \pi_1=\frac{\sigma_1}{\sigma_2}(\pi_2-\epsilon_2)+\epsilon_1=:l_+\circ\pi_2 \quad (\mu\text{-a.e.}), \tag{16a}$$

$$\rho(\pi_1,\pi_2;\mu)=-1 \ \text{ iff } \ \pi_1=-\frac{\sigma_1}{\sigma_2}(\pi_2-\epsilon_2)+\epsilon_1=:l_-\circ\pi_2 \quad (\mu\text{-a.e.}). \tag{16b}$$

(Here, we have introduced the function $l_\pm: y\mapsto l_\pm(y):=\pm(\sigma_1/\sigma_2)(y-\epsilon_2)+\epsilon_1)$. A case of special interest arises when the marginals μ_1 and μ_2 have the same (finite) first and second moments so that $\epsilon_1=\epsilon_2$, $\sigma_1=\sigma_2$. Then one has

$$\rho(\mu_1,\mu_2;\mu)=+1 \ \text{ iff } \ \epsilon_{12}=\epsilon_1^2+\sigma_1^2, \quad \text{iff } \ \pi_1=\pi_2 \quad (\mu\text{-a.e.}), \tag{17a}$$

$$\rho(\mu_1,\mu_2;\mu)=-1 \ \text{ iff } \ \epsilon_{12}=\epsilon_1^2-\sigma_1^2, \quad \text{iff } \ \pi_1=-\pi_2+2\epsilon_1 \quad (\mu\text{-a.e.}). \tag{17b}$$

4.2. The notion of correlation can be applied to quantify the degree of mutual dependence of the marginal measures. In order to avoid dealing with unnecessary complications, we assume that μ_1 and μ_2 are no $\{0,1\}$-valued measures; equivalently, we let $\sigma_1\neq 0\neq\sigma_2$. μ_1 and μ_2 are *independent* if $\mu=\mu_1\times\mu_2$. Otherwise, μ_1,μ_2 are *dependent*. They are *completely dependent* if there is a (measurable) function $h:\mathbf{R}\to\mathbf{R}$ such that $\mu(X\times Y)=\mu_2(h^{-1}(X)\cap Y)$ for $X,Y\in\mathscr{B}(\mathbf{R})$. That is, the marginal measure μ_2 suffices to determine the whole measure μ. The relation of complete dependence is symmetric with respect to the two marginals only if h is bijective. This is the case of concern here.

4.3. It is evident that the statistical independence of μ_1,μ_2 implies $\rho(\mu_1,\mu_2;\mu)=0$. However, the latter condition is not sufficient to ensure their independence. (For a counter example, see, for instance, Ref. 9). On the other hand, Eqs. (16a) and (16b) show that strong (anti)correlation entails complete dependence, the dependence being given by the linear function $l_\pm$. Indeed, the condition $\pi_1=l_\pm\circ\pi_2$ (μ-a.e.) implies that $\mu(X\times Y)=0$ for all X and Y for which $l_\pm^{-1}(X)\cap Y=0$. Thus in particular, for any X and Y, and with X' denoting the complement of X one has $\mu(X'\times l_\pm^{-1}(X)\cap Y)=0=\mu(X\times l_\pm^{-1}(X')\cap Y)$. The additivity properties of μ allow one then to verify that for all $X,Y,\mu_2(l_\pm^{-1}(X)\cap Y)=\mu(X\times Y)$, that is, μ_1 and μ_2 are completely dependent with $l_\pm$. By a direct computation one can confirm that the converse implication holds true whenever the function h is linear. Therefore, we have

$$\rho(\mu_1,\mu_2;\mu)=+1 \text{ iff } \mu_1,\mu_2 \text{ are completely dependent with } h(y)=ay+b, \quad a>0, \tag{18a}$$

$$\rho(\mu_1,\mu_2;\mu)=-1 \text{ iff } \mu_1,\mu_2 \text{ are completely dependent with } h(y)=ay+b, \quad a<0. \tag{18b}$$

In both cases the constants are $a=\pm\sigma_1/\sigma_2$, $b=\epsilon_1-a\epsilon_2$, so that $h=l_\pm$.

V. STRONG CORRELATIONS BETWEEN OBSERVABLES

5.1. According to the condition (2), in an E-measurement the initial E-outcome distribution is recovered from the final Z-outcome distribution. In addition to this basic requirement, a measurement may also establish complete statistical dependence between the measured observable and the pointer observable after the measurement; that is, the observables E and Z^f may become strongly correlated in the final object–apparatus state $V(T\otimes T_{\mathscr{A}})$. In order to avoid technical complications in the formulation of this correlation, we assume that the value space of E is the real Borel space, $(\Omega,\mathscr{F})=(\mathbf{R},\mathscr{B}(\mathbf{R}))$. Then for any state $T\in\mathscr{S}(\mathscr{H})$ the map

$$\mu: X\times Y\mapsto \mathrm{tr}[V(T\otimes T_{\mathscr{A}})E(X)\otimes Z^f(Y)] \tag{19}$$

extends to a probability measure on $(\mathbf{R}^2,\mathscr{B}(\mathbf{R}^2))$.[10] The marginal distributions are

$$\mu_1: X\mapsto \mathrm{tr}[\mathscr{R}_{\mathscr{S}}(V(T\otimes T_{\mathscr{A}}))E(X)], \tag{20a}$$

$$\mu_2: Y\mapsto \mathrm{tr}[\mathscr{R}_{\mathscr{A}}(V(T\otimes T_{\mathscr{A}}))Z^f(Y)]=\mathrm{tr}[TE(Y)]. \tag{20b}$$

Denoting the correlation of μ_1 and μ_2 in μ as $\rho(E,Z^f;V(T\otimes T_{\mathscr{A}}))$, we say that the measurement $\mathscr{M}$ of E produces *strong observable-(anti)correlation* in state T if this number equals $1(-1)$. According to Eq. (18), this occurs exactly when the probability measures [(20a) and (20b)] are completely dependent, with the function $l_\pm$. In order to analyze the statistical dependence of μ_1 and μ_2 we shall make use of the concept of a state transformer (also known as an instrument) associated with a measurement.

5.2. Consider a measurement $\langle\mathscr{H}_{\mathscr{A}},Z,T_{\mathscr{A}},V,f\rangle$ of E. Any $X\in\mathscr{F}$ defines a non-normalized state

$$V_X(T):=I\otimes Z^{1/2}(f^{-1}(X))V(T\otimes T_{\mathscr{A}})I\otimes Z^{1/2}(f^{-1}(X)), \tag{21}$$

the (trace) norm of which is $\mathrm{tr}[V_X(T)]=p_T^E(X)$. Taking the partial trace of $V_X(T)$ over $\mathscr{H}_{\mathscr{A}}$ one gets the (non-normalized) reduced state of $\mathscr{S}$,

$$\mathscr{T}_X(T):=\mathscr{R}_{\mathscr{S}}(V_X(T)). \tag{22}$$

For any $X \in \mathcal{F}$ and $T \in \mathcal{S}(\mathcal{H})$, $\mathrm{tr}[\mathcal{I}_X(T)] = \mathrm{tr}[TE(X)]$, and $T \mapsto \mathcal{I}_X(T)$ is a (contractive) state transformation. The mapping $\mathcal{I}: X \mapsto \mathcal{I}_X$ has the measure property $\mathrm{tr}[\mathcal{I}_{\cup X_i}(T)] = \Sigma \mathrm{tr}[\mathcal{I}_{X_i}(T)]$ for any disjoint sequence $(X_i) \subset \mathcal{F}$ and for all $T \in \mathcal{S}(\mathcal{H})$. Moreover, $\mathrm{tr}[\mathcal{I}_\Omega(T)] = 1$ for any T. We call $\mathcal{I}$ the *state transformer* induced by the measurement $\mathcal{M}$. It describes the object system's state changes under the measurement, and it uniquely defines the measured observable via the relation $\mathrm{tr}[\mathcal{I}_X(T)] = \mathrm{tr}[TE(X)]$. We note also that $p_T^E(X) T_{\mathcal{I}}(X,T) = \mathcal{I}_X(T)$, and, in particular, $\mathcal{R}_{\mathcal{I}}(V(T \otimes T_{\mathcal{M}})) = \mathcal{I}_\Omega(T)$.

5.3. The probability measure (19) can be written as

$$\mu(X \times Y) = \mathrm{tr}[\mathcal{I}_Y(T)E(X)] = \mathrm{tr}[\mathcal{I}_X(\mathcal{I}_Y(T))], \tag{23}$$

and the second marginal is $\mu_2(Y) = \mathrm{tr}[\mathcal{I}_Y(T)]$. The strong (anti-)correlation then amounts to

$$\mathrm{tr}[\mathcal{I}_X(\mathcal{I}_Y(T))] = \mathrm{tr}[\mathcal{I}_{l_\pm^{-1}(X) \cap Y}(T)]. \tag{24}$$

A special case of complete dependence arises with l_+ being the identity function

$$\mathrm{tr}[\mathcal{I}_X(\mathcal{I}_Y(T))] = \mathrm{tr}[\mathcal{I}_{X \cap Y}(T)]. \tag{25}$$

This relation is easily seen to coincide with Eq. (12).[8] Thus if valid for all states T, Eq. (25) expresses the repeatability of the measurement, and we may conclude that any repeatable measurement leads to strong observable-correlations. The repeatability condition (25) is not necessary for the strong observable-correlation (24).

5.4. Condition (25) implies, in particular, the equality of the marginal measures μ_1, μ_2 of Eqs. (20): for all X,

$$p_T^E(X) = p^E_{\mathcal{R}_{\mathcal{I}}(V(T \otimes T_{\mathcal{M}}))}(X). \tag{26}$$

This is just the first-kind property of the measurement. It may occur that these marginal measures coincide irrespectively of whether Eq. (25) holds or not; in that case conditions (17) give the relevant characterisations of strong (anti)correlations.

Theorem 5.5: *Let $\mathcal{M}$ be a measurement of an observable E, and let $\mathcal{R}$ be any reading scale. Then (a) implies (b), where*

$$\text{(a)} \quad E(X_i) T_{\mathcal{I}}(i,T) = T_{\mathcal{I}}(i,T) \quad \text{for all} \quad T \in \mathcal{S}(\mathcal{H}), \quad X_i \in \mathcal{R};$$

$$\text{(b)} \quad \sigma(p^{E^{\mathcal{R}}}_{\mathcal{R}_{\mathcal{I}}(V(T \otimes T_{\mathcal{M}}))}) \neq 0 \ \text{ and } \ \rho(E^{\mathcal{R}}, Z^{\mathcal{R}}; V(T \otimes T_{\mathcal{M}})) = 1$$

$$\text{for all } T \in \mathcal{S}(\mathcal{H}) \text{ with } \sigma(p_T^{E^{\mathcal{R}}}) \neq 0.$$

If the reading scale $\mathcal{R}$ is finite, then (a) and (b) are equivalent.

Proof: The eigenstate condition (a) is equivalent with the repeatability condition (with respect to $\mathcal{R}$). Therefore, if (a) holds, then also (b) is true. It remains to show that (b) implies (a) whenever $\mathcal{R}$ is finite. According to Eq. (18a), the statement $\rho(E^{\mathcal{R}}, Z^{\mathcal{R}}; V(T \otimes T_{\mathcal{M}})) = 1$ is equivalent to the complete dependence, $\mu(i,j) = \mu_2(j)\delta_{i,l_+(j)}$, with a bijective linear mapping $i = l_+(j) = aj + b$, $a > 0$, between those values i,j for which $\mu_2(j) \neq 0$ (and hence $\mu_1(i) = \mu_2(\frac{1}{a}(i-b)) \neq 0$).

Case 1. Let T be such that $0 \neq \mathrm{tr}[TE_i] \neq 1$ for all $i \in \mathbf{I}$. Then $\mu(i,j)$ correlates, via $i = l_+(j) = aj + b$, *all* values $j \in \mathbf{I}$ with values $i \in \mathbf{I}$. Since l_+ is onto and monotonically increasing, $l_+(j) = j$. But the complete dependence condition, with $l_+(j) = j$, is nothing but Eq. (25) (with respect to $\mathcal{R}$), which is equivalent to (a).

Case 2. Let T be any state such that $0 \neq \mathrm{tr}[TE_k] \neq 1$ holds exactly for all $k \in \mathbf{I}_1$, a proper nonempty subset of $\mathbf{I}$. Take any T' for which $0 \neq \mathrm{tr}[T'E_l] \neq 1$ exactly for all $l \in \mathbf{I}_1'$, the complement of $\mathbf{I}_1$. Then the reasoning of Case 1 applies to $\hat{T} := \frac{1}{2}T + \frac{1}{2}T'$. Hence, $E_i \mathscr{I}_i(\hat{T}) = \mathscr{I}_i(\hat{T})$ for all $i \in \mathbf{I}$. Inserting in this equation the relation $\mathscr{I}_k(T') = O$, which holds for $k \in \mathbf{I}_1$, it follows that $E_i \mathscr{I}_i(T) = \mathscr{I}_i(T)$ for $i \in \mathbf{I}_1$. But this relation holds trivially also for $i \in \mathbf{I}_1'$ since in that case $\mathscr{I}_i(T) = O$. This completes the proof.

VI. STRONG CORRELATIONS BETWEEN VALUES

6.1. The observable $E^{\mathscr{R}}$ measured by the scheme $\mathscr{M}$ with the reading scale $\mathscr{R}$ is discrete. One may therefore ask to what degree the *values* of this observable and the pointer observable $Z^{\mathscr{R}}$ become correlated in the measurement. To answer this question requires studying the correlation $\rho(E_i, Z_i; V(T \otimes T_{\mathscr{M}}))$ of the ith values of these observables in the final object–apparatus state, that is, the correlation of quantities $E_i \otimes I$ and $I \otimes Z_i$ in the state $V(T \otimes T_{\mathscr{M}})$

$$\rho(E_i, Z_i; V(T \otimes T_{\mathscr{M}})) = \frac{\epsilon_{12} - \epsilon_1 \epsilon_2}{\sigma_1 \sigma_2}. \tag{27}$$

The respective quantities are easily determined

$$\epsilon_{12} = \mathrm{tr}[\mathscr{I}_i^2(T)], \tag{28a}$$

$$\epsilon_1 = \mathrm{tr}[\mathscr{I}(\mathbf{I})(T)E_i], \tag{28b}$$

$$\epsilon_2 = \mathrm{tr}[TE_i], \tag{28c}$$

$$\sigma_1^2 = \mathrm{tr}[\mathscr{I}(\mathbf{I})(T)E_i^2] - \mathrm{tr}[\mathscr{I}(\mathbf{I})(T)E_i]^2, \tag{28d}$$

$$\sigma_2^2 = tr[\mathscr{R}_{\mathscr{M}}(V(T \otimes T_{\mathscr{M}}))Z_i^2] - \mathrm{tr}[TE_i]^2. \tag{28e}$$

Strong correlation is then equivalent to

$$\epsilon_{12} - \epsilon_1 \epsilon_2 = \sigma_1 \sigma_2 \tag{29}$$

whenever the right-hand side is nonzero.

6.2. Assume that the final component state $T_{\mathscr{I}}(i,T)$ is a 1-eigenstate of E_i (whenever $p_T^E(X_i) \neq 0$); then one obtains $\epsilon_{12} = \epsilon_1 = \epsilon_2$ for all T. It follows that $\epsilon_{12} - \epsilon_1 \epsilon_2 = \sigma_1^2 \leqslant \sigma_1 \sigma_2$ and thus $\sigma_1 \leqslant \sigma_2$. On the other hand, the relation $\epsilon_1 = \epsilon_2 = \epsilon_{12}$ together with $\sigma_2^2 \leqslant \epsilon_2 - \epsilon_2^2 = \epsilon_{12} - \epsilon_1 \epsilon_2 = \sigma_1^2$ implies $\sigma_2 \leqslant \sigma_1$. Therefore, the correlation $\rho(E_i, Z_i; V(T \otimes T_{\mathscr{M}}))$ equals 1 whenever $0 \neq p_T^E(X_i) \neq 1$.

Another interesting implication of the eigenstate condition $\epsilon_{12} = \epsilon_2$ and the ensuing equality $\sigma_2 = \epsilon_2 - \epsilon_2^2$ is the fact that the state $T_{\mathscr{M}}(i,T)$ is a 1-eigenstate of Z_i. With these observations we have established the following result.

Theorem 6.3: *Let $\mathscr{M}$ be a measurement of an observable E and let $\mathscr{R}$ be any reading scale. Then for any state T of $\mathscr{S}$, (a) implies (b) and (c)*:

(a) $E_i T_{\mathscr{I}}(i,T) = T_{\mathscr{I}}(i,T)$ for each i;

(b) $\sigma(E_i \otimes I; V(T \otimes T_{\mathscr{M}})) \neq 0$ and $\rho(E_i, Z_i; V(T \otimes T_{\mathscr{M}})) = 1$ for each i with $0 \neq p_T^E(X_i) \neq 1$;

(c) $T_{\mathscr{M}}(i,T)$ is a 1-eigenstate of Z_i for each i with $p_T^E(X_i) \neq 0$.

This result entails that a repeatable measurement is a strong value-correlation measurement. Moreover, a necessary condition for $\mathscr{M}$ to be a repeatable measurement is that the final component state $T_{\mathscr{A}}(i,T)$ of $\mathscr{A}$ is a 1-eigenstate of the pointer observable, that is, $\mathscr{M}$ must fulfill the pointer value-definiteness condition. We recall that this last property and in addition the pointer mixture property arise already as consequences of the mutual orthogonality of the component states $T_{\mathscr{S}}(i,T)$ of $\mathscr{S}$ (Theorem 3.11). The notion of a correlation between values suggests that the observables in question do have definite values; yet it turns out that strong value-correlation does not require pointer value-definiteness, nor repeatability. Even the combination of (b) and (c) does not require the property (a) to hold, as can be demonstrated by simple examples.[1]

Theorem 6.4: *Let $\mathscr{M}$ be a measurement of a sharp observable E and $\mathscr{R}$ any reading scale. For any initial state T of $\mathscr{S}$, (a) is equivalent to (b) & (c)*:

$$\text{(a)} \quad E_i T_{\mathscr{S}}(i,T) = T_{\mathscr{S}}(i,T) \quad \text{for each } i;$$

$$\text{(b)} \quad \sigma(E_i \otimes I; V(T \otimes T_{\mathscr{A}})) \neq 0 \text{ and } \rho(E_i, Z_i; V(T \otimes T_{\mathscr{A}})) = 1 \quad \text{for each } i \text{ with } 0 \neq p_T^E(X_i) \neq 1;$$

$$\text{(c)} \quad T_{\mathscr{A}}(i,T) \text{ is a 1-eigenstate of } Z_i \text{ for each } i \text{ with } p_T^E(X_i) \neq 0.$$

Proof: In view of Theorem 6.3, we only need to show that (b) & (c) implies (a). Hence let $\epsilon_{12} - \epsilon_1 \epsilon_2 = \sigma_1 \sigma_2$ hold for each i. Condition (c) implies $\sigma_2^2 = \epsilon_2 - \epsilon_2^2$. Similarly the relation $E_i^2 = E_i$ implies $\sigma_1^2 = \epsilon_1 - \epsilon_1^2$. From Eqs. (28) we obtain $\epsilon_{12} \leqslant \epsilon_1$, $\epsilon_{12} \leqslant \epsilon_2$, and therefore

$$\sigma_1 \sigma_2 = \epsilon_{12} - \epsilon_1 \epsilon_2 \leqslant \sigma_1^2, \quad \sigma_1 \sigma_2 = \epsilon_{12} - \epsilon_1 \epsilon_2 \leqslant \sigma_2^2.$$

This implies $\sigma_1 = \sigma_2$. On the other hand,

$$\epsilon_1 \epsilon_2 + \sigma_1 \sigma_2 = \epsilon_{12} \leqslant \epsilon_1 = \sigma_1^2 + \epsilon_1^2, \quad \epsilon_1 \epsilon_2 + \sigma_1 \sigma_2 = \epsilon_{12} \leqslant \epsilon_2 = \sigma_2^2 + \epsilon_2^2.$$

Using $\sigma_1 = \sigma_2$, one concludes that $\epsilon_1 = \epsilon_2 = \epsilon_{12}$. But the last equation is equivalent to (a). This completes the proof.

VII. STRONG CORRELATIONS BETWEEN FINAL COMPONENT STATES

7.1. In the two preceding sections it was demonstrated in which way strong observable and value correlations serve as characterizations of repeatable measurements. The corresponding eigenstate condition $E_i T_{\mathscr{S}}(i,T) = T_{\mathscr{S}}(i,T)$ entails, in particular, that the final component states of the object associated with different outcomes i,j are mutually orthogonal, $T_{\mathscr{S}}(i,T) \cdot T_{\mathscr{S}}(j,T) = 0$. In some cases this orthogonality can be characterized in terms of strong correlations between the final component states of $\mathscr{S}$ and $\mathscr{A}$.

Consider a measurement scheme $\mathscr{M}$ of an observable E with respect to a reading scale $\mathscr{R}$. We say that $\mathscr{M}$, with $\mathscr{R}$, is a *strong state-(anti)correlation* measurement of E if for each initial state T of $\mathscr{S}$ it correlates strongly the final component states $T_{\mathscr{S}}(i,T)$ and $T_{\mathscr{A}}(i,T)$ of the object and the apparatus. This calls for the study of the correlation $\rho(T_{\mathscr{S}}(i,T), T_{\mathscr{A}}(i,T); V(T \otimes T_{\mathscr{A}}))$ of the probability measure defined by the self-adjoint operators $T_{\mathscr{S}}(i,T) \otimes I$ and $I \otimes T_{\mathscr{A}}(i,T)$ and the final object–apparatus state $V(T \otimes T_{\mathscr{A}})$.

Theorem 7.2: *Let $\mathscr{M}$ be a measurement of an observable E and $\mathscr{R}$ any reading scale. For any initial state T of the object system for which the component states $T_{\mathscr{S}}(i,T)$ and $T_{\mathscr{A}}(i,T)$ are vector states, (a) is equivalent to (b) & (c)*:

$$\text{(a)} \quad T_{\mathscr{S}}(i,T) \cdot T_{\mathscr{S}}(j,T) = O \quad \text{for } i \neq j;$$

$$\text{(b)}\quad \rho(T_{\mathscr{S}}(i,T),T_{\mathscr{A}}(i,T);V(T\otimes T_{\mathscr{A}}))=1 \quad \text{for each } i \text{ with } 0\neq p_T^E(X_i)\neq 1;$$

$$\text{(c)}\quad T_{\mathscr{A}}(i,T) \text{ is a 1-eigenstate of } Z_i \quad \text{for each } i \text{ with } 0\neq p_T^E(X_i)\neq 1.$$

Proof: The equivalence is shown to hold under the assumptions $T_{\mathscr{S}}(i,T)=P[\varphi_i]$ and $T_{\mathscr{A}}(i,T)=P[\phi_i]$. These two relations imply that $I\otimes Z_i^{1/2}V(T\otimes T_{\mathscr{A}})I\otimes Z_i^{1/2}$ is a vector state of the product form, that is,

$$I\otimes Z_i^{1/2}V(T\otimes T_{\mathscr{A}})I\otimes Z_i^{1/2}=p_T^E(X_i)P[\varphi_i\otimes\phi_i]. \qquad (\alpha)$$

If (a) holds, then by Theorem 3.11, $\mathscr{M}$ fulfils the pointer value-definiteness condition (c). Thus for both implications one can make use of the fact that $Z_i\phi_i=\phi_i$. Then (α) implies

$$I\otimes P[\phi_i]V(T\otimes T_{\mathscr{A}})I\otimes P[\phi_i]=p_T^E(X_i)P[\varphi_i\otimes\phi_i].$$

With this one computes

$$\epsilon_{12}=\mathrm{tr}[P[\varphi_i]\otimes P[\phi_i]V(T\otimes T_{\mathscr{A}})]=p_T^E(X_i),$$

$$\epsilon_1=\mathrm{tr}[P[\varphi_i].\mathscr{R}_{\mathscr{S}}(V(T\otimes T_{\mathscr{A}}))]=\sum_j p_T^E(X_j)\mathrm{tr}[P[\varphi_i]P[\varphi_j]],$$

$$\epsilon_2=\mathrm{tr}[I\otimes P[\phi_i]V(T\otimes T_{\mathscr{A}})]=p_T^E(X_i),$$

$$\sigma_1^2=\epsilon_1-\epsilon_1^2,\quad \sigma_2^2=\epsilon_2-\epsilon_2^2.$$

(a)⇒(b): (a) is equivalent to $\mathrm{tr}[P[\varphi_i]P[\varphi_j]]=\delta_{ij}$, one has $\epsilon_1=\epsilon_2=\epsilon_{12}$, and $\sigma_1=\sigma_2$. Thus $\epsilon_{12}-\epsilon_1\epsilon_2=\sigma_1\sigma_2$, that is, (b).

(b)&(c)⇒(a): Let $\epsilon_{12}-\epsilon_1\epsilon_2=\sigma_1\sigma_2$. Using the inequalities $\epsilon_{12}-\epsilon_1\epsilon_2\leqslant\sigma_k^2$, $k=1,2$, one concludes that $\sigma_1=\sigma_2$. Since $\epsilon_{12}=\epsilon_2$, one also has $\epsilon_{12}-\epsilon_1\epsilon_2=\sigma_2^2=\epsilon_2-\epsilon_2^2$, and therefore $\epsilon_1=\epsilon_2$. But from the definition of ϵ_1 one has $\epsilon_1\geqslant\epsilon_2$, so that the equality of these numbers implies $\mathrm{tr}[P[\varphi_i]P[\varphi_j]]=0$ whenever $i\neq j$, that is (a). This completes the proof.

7.3. One may also ask whether the requirement of strong correlation between the $\mathscr{S}$ and $\mathscr{A}$ states $\mathscr{R}_{\mathscr{S}}(V(T\otimes T_{\mathscr{A}}))$ and $\mathscr{R}_{\mathscr{A}}(V(T\otimes T_{\mathscr{A}}))$ imposes any constraint on the measurement scheme under consideration. That this cannot be expected in general can be seen in the case of a unitary measurement $\mathscr{M}_U$. Note first that the reduced states of $P[U(\varphi\otimes\phi)]$ have the same spectra, including multiplicities. The spectral decompositions can be given in terms of orthonormal systems $\{\varphi_i\}$, $\{\phi_i\}$ defined by the biorthogonal decomposition $U(\varphi\otimes\phi)=\Sigma_i c_i\varphi_i\otimes\phi_i (c_i>0)$, and a straightforward calculation shows that

$$\rho(\mathscr{R}_{\mathscr{S}}(P[U(\varphi\otimes\phi)]),\mathscr{R}_{\mathscr{A}}(P[U(\varphi\otimes\phi)]);P[U(\varphi\otimes\phi)])=1. \qquad (30)$$

Hence these states are always strongly correlated.

VIII. EXAMPLES

8.1. A particularly interesting class of measurements arises if the coupling is generated by a unitary map of the form

$$U=e^{i\lambda A\otimes B}, \qquad (31)$$

where A and B are self-adjoint operators in $\mathscr{H}$ and $\mathscr{H}_{\mathscr{A}}$, respectively, and $\lambda\in\mathbf{R}$ is a coupling constant. The operator A is usually taken to represent the (sharp) observable one aims to measure.

In order to specify the full measurement scheme and thus the actually measured observable, one needs to choose the pointer observable Z and fix the initial preparation $T_{\mathscr{A}}$ of the apparatus; the measured observable is then given by Eq. (2). Using the spectral decomposition of A, $A=\int aE^A(da)$, and denoting

$$T_{\mathscr{A}}^{\lambda a} := e^{i\lambda aB} T_{\mathscr{A}} e^{-i\lambda aB}, \tag{32}$$

the final apparatus state, for $T\in\mathscr{S}(\mathscr{H})$, assumes the form

$$\mathscr{R}_{\mathscr{A}}(UT\otimes T_{\mathscr{A}}U^*)=\int \mathrm{tr}[TE^A(da)]T_{\mathscr{A}}^{\lambda a}. \tag{33}$$

Since it is of interest to compare the measured observable E with E^A we assume from the outset that the value space of Z is $(\mathbf{R},\mathscr{B}(\mathbf{R}))$. In view of the coupling constant $\lambda(\neq 0)$ it is also convenient to introduce a pointer function $f(x)=\lambda^{-1}x$. The observable E measured by the scheme $\langle \mathscr{H}_{\mathscr{A}}, Z, T_{\mathscr{A}}, f, U\rangle$ takes then the following form: For any $X\in\mathscr{B}(\mathbf{R})$,

$$E(X)=\int_{\mathbf{R}} \mathrm{tr}[T_{\mathscr{A}}^{\lambda a} Z(\lambda X)]E^A(da). \tag{34}$$

The structure of the operators $E(X)$ show that in general the measured observable E is not the sharp observable E^A, but a smeared version of it.[11] One may ask which choices of Z and $T_{\mathscr{A}}$ would possibly yield $E=E^A$. Obviously, this is the case if and only if for (E^A-almost) all $a\in\mathbf{R}$, $\mathrm{tr}[T_{\mathscr{A}}^{\lambda a}Z(\lambda X)]=\chi_X(a)$, where χ_X is the characteristic function of the set X.

The measurement scheme thus defined is always of the first kind: The measurement outcome probabilities for E are the same both before and after the measurement; for any $T\in\mathscr{S}(\mathscr{H})$ and for all $X\in\mathscr{B}(\mathbf{R})$,

$$\mathrm{tr}[TE(X)]=\mathrm{tr}[UT\otimes T_{\mathscr{A}}U^*E(X)\otimes I]. \tag{35}$$

It may also be noticed that the measurement does neither alter the measurement outcome probabilities of E^A, though, as a rule, it is not a measurement of E^A. In fact, if the measurement were an E^A-measurement, it would also be repeatable (3.15) and A would thus have to be discrete, $A=\Sigma a_i E^A(\{a_i\})$ (3.13). In that case the measurement would also produce all the strong correlations discussed in the previous sections. In general, this is, however, not the case.

Consider next this measurement scheme with a fixed reading scale $\mathscr{R}$. The pointer observable Z as well as the measured observable E become discretized,

$$Z^{\mathscr{R}}: i\mapsto Z_i := Z(\lambda X_i), \tag{36a}$$

$$E^{\mathscr{R}}: i\mapsto E_i := E(X_i), \tag{36b}$$

and the final component states are

$$\begin{aligned} T_{\mathscr{S}}(i,T)&=p_T^E(X_i)^{-1}\mathscr{R}_{\mathscr{S}}(V_i(T))=p_T^E(X_i)^{-1}\int\int \mathscr{R}_{\mathscr{S}}(E^A(da)TE^A(da') \\ &\quad\otimes Z_i^{1/2}e^{iaB}T_{\mathscr{A}}e^{-ia'B}Z_i^{1/2}) \\ &=p_T^E(X_i)^{-1}\sum t_n\sum L_{kn}^i TL_{kn}^{i*} \qquad (37a) \\ &\quad\text{with } L_{kn}^i := \int \langle\psi_k|Z_i^{1/2}\phi_n^{\lambda a}\rangle E^A(da)\in\mathscr{L}(\mathscr{H}), \end{aligned}$$

$$T_{\mathscr{A}} = \sum\ t_n P[\phi_n] \quad \text{(spectral decomposition)}$$

$$\phi_n^{\lambda a} = e^{i\lambda a B}\phi_n\,,$$

$$\{\psi_k\} \subset \mathscr{K}_{\mathscr{A}} \text{ an orthonormal basis,}$$

$$T_{\mathscr{A}}(i,T) = p_T^E(X_i)^{-1}\mathscr{R}_{\mathscr{A}}(V_i(T)) = p_T^E(X_i)^{-1}\int \mathrm{tr}[TE^A(da)]Z_i^{1/2}T_{\mathscr{A}}^{\lambda a}Z_i^{1/2}, \tag{37b}$$

(provided that $p_T^E(X_i) \neq 0$). If $E_i^2 = E_i$ for all $i \in \mathbf{I}$, the measurement is repeatable with respect to $\mathscr{R}$, and

$$E(X_i)T_{\mathscr{A}}(i,T) = T_{\mathscr{A}}(i,T), \tag{38a}$$

$$T_{\mathscr{A}}(i,T)\cdot T_{\mathscr{A}}(j,T) = O, \quad i \neq j, \tag{38b}$$

in which case the implications of Theorems 3.11, 5.5, 6.3, 6.4, and 7.2 all hold true. We specify next two instances of the above model, one in which $E_i^2 = E_i$ and another one with $E_i^2 < E_i$.

8.2. Consider a discrete observable $A = \Sigma a_k E^A(\{a_k\})$, and assume that the set of eigenvalues of A is closed. As the apparatus (or a part of it, called probe) take a particle moving in one-dimensional space, so that $\mathscr{K}_{\mathscr{A}} = L^2(\mathbf{R})$, and couple A with its momentum $P_{\mathscr{A}}$ according to Eq. (31). Since the momentum generates translations on the position, it is natural to choose the position $Q_{\mathscr{A}}$ conjugate to $P_{\mathscr{A}}$ as the pointer observable. Assuming that the initial state of $\mathscr{A}$ is a vector state $P[\phi]$, then, in the position representation (for $\mathscr{A}$) one has $\phi^{\lambda a_k}(x) = \phi(x + \lambda a_k)$, with $\phi^{\lambda a_k} = e^{i\lambda a_k P_{\mathscr{A}}}\phi$. Assuming that the spacing between the eigenvalues a_k is greater than (δ/λ) and that ϕ is supported in $(-\frac{\delta}{2}, \frac{\delta}{2})$, then the pointer states $\phi^{\lambda a_k}$ are supported in the mutually disjoint sets λI_k, where $I_k = (a_k - (\delta/2\lambda), a_k + (\delta/2\lambda))$. Introducing yet another pointer function g such that $g(I_k) = \{a_k\}$ for each k, and $g((\cup_k I_k)') \subset \{a_k : k = 1,2,\ldots\}'$, one obtains from Eq. (34)

$$E(\{a_k\}) = \sum\ \langle \phi^{\lambda a_i} | E^{Q_{\mathscr{A}}}(\lambda I_k)\phi^{\lambda a_i}\rangle E^A(\{a_i\}) = E^A(\{a_k\}), \tag{39}$$

for each k, which shows that the observable measured by this scheme is indeed E^A. The measurement is repeatable, even a Lüders measurement with the state transformer $T \mapsto \mathscr{T}_k(T) = \mathscr{R}_{\mathscr{A}}(V_k(T)) = E^A(\{a_k\})TE^A(\{a_k\})$, and all the correlations introduced above are strong.

As an elementary quantum optical application, one may consider the measurement of the number observable $N = a^*a$ of a (single-mode) signal field by means of coupling it, via $e^{i\lambda N \otimes b^p}$, with one of the quadrature components $b^p = i/\sqrt{2}(b^* - b)$, say, of another single-mode (probe) field, and using the other quadrature component $b^q = 1/\sqrt{2}(b^* + b)$ as the readout observable. With the above choices of the initial probe state ϕ and the pointer functions one obtains a number measurement. It may be noted that neither the beam splitter coupling nor the number–number coupling leads to a sharp number measurement.[11]

8.3. The second illustration of the above model concerns the case of A being a continuous observable, such as the position of a particle or a quadrature component of a single-mode electromagnetic field. Using the quantum optical nomenclature, we take $A = a^q = 1/\sqrt{2}(a^* + a)$, the amplitude quadrature of the (single-mode) signal field with the bosonic annihilation and creation operators a, a^*. For B we take the corresponding quadrature component b^q of a (single-mode) probe field, with the annihilation and creation operators b, b^*. Using the phase quadrature

$b^p := i/\sqrt{2}(b^* - b) = \int_{\mathbf{R}} x Z(dx)$ of the probe field as the readout observable, and assuming that the probe field is prepared in a vector state $P[\phi]$ determines the measured observable (34) to be of the form

$$E(X) = \int \int |\hat{\phi}|^2(y - \lambda x)\chi_{\lambda X}(y)dy \; E^A(dx) = \int |\hat{\phi}|^2(y - \lambda a^q)\chi_{\lambda X}(y)dy$$
$$\equiv (e_\lambda * \chi_X)(a^q),$$
$$e_\lambda(y) := \lambda |\hat{\phi}|^2(-\lambda y), \tag{40}$$

where $e_\lambda * \chi_X$ denotes the convolution of the density function e_λ with the characteristic function of the set X, and $\hat{\phi}$ is the Fourier transform of ϕ.

In the present case the measured observable is the POV measure $E: X \mapsto (e_\lambda * \chi_X)(a^q)$ and not the spectral measure $X \mapsto \chi_X(a^q)$ of a^q; this is to say that the measured field observable is not the amplitude quadrature a^q but a smearing of it. In fact, if e were replaced by a delta function (concentrated at 0), then Eq. (40) would simply give the amplitude quadrature a^q. But this can never occur since the readout observable b^p has no eigenstates, that is, the initial state of the probe field cannot be so chosen that e were a delta function. We observe also that the measurement is not repeatable (since E is not discrete) though still of the first kind. Therefore, the strong correlations are not guaranteed from the outset but need to be studied separately.

Before calculating the observable-correlation produced by the measurement we compare the variance of E with that of a^q in a vector state $P[\varphi]$. Direct application of Eq. (2) yields (assuming that the involved quantities are finite)

$$\mathrm{Var}(E, \varphi) = \mathrm{Var}(a^q, \varphi) + \frac{1}{\lambda^2} \mathrm{Var}(b^p, \phi). \tag{41}$$

The initial state $P[\phi]$ of the probe field can be chosen such that $\langle \phi | b^p \phi \rangle = 0$. In this case the measured observable appears, in view of the first moments, as the amplitude quadrature a^q. However, the second moment $\langle \phi | (b^p)^2 \phi \rangle$ never equals 0, meaning that Var $(E, P[\varphi])$ is strictly greater than Var $(a^q, P[\varphi])$. However, in the limit of strong coupling, $\lambda \to \infty$, the measurement noise term $(1/\lambda^2)$Var $(b^p, P[\phi])$ tends to zero. In any case, this shows once more that the actually measured observable is not the amplitude quadrature.

The observable-correlation produced by the measurement is now found to be

$$\rho(E, Z^f; P[U(\varphi \otimes \phi)]) = \frac{\mathrm{Var}(a^q, P[\varphi])}{\mathrm{Var}(E, P[\varphi])}, \tag{42}$$

a quantity always strictly less than 1. The measurement, though of the first kind, does never lead to strong observable-correlation. Yet,

$$\lim_{\lambda \to \infty} \rho(E, Z^f; P[U(\varphi \otimes \phi)]) = 1. \tag{43}$$

In order to discuss the value- and state-correlations produced by the measurement scheme one needs to introduce a reading scale $\mathscr{R}$. The discrete observable $E^{\mathscr{R}}: i \mapsto E_i$ thus measured is

$$E_i = (e_\lambda * \chi_{X_i})(a^q), \tag{44}$$

whereas the final component states (37a) are of the form

$$T_{\mathscr{A}}(i,P[\varphi])=\langle\varphi|E_i\varphi\rangle^{-1}\int_{\lambda X_i} L_y P[\varphi]L_y^*\,dy \quad \text{with} \quad L_y:=\hat{\phi}(y-\lambda a^q). \tag{45}$$

Neither the eigenvalue condition (38a) nor the orthogonality condition (38b) can be satisfied for all initial vector states of the signal field. Therefore, the strong value and state-correlations cannot be inferred by using Theorems 6.3 and 7.2. Still the value-correlation is always strong: $\rho(E_i,Z_i;P[U(\varphi\otimes\phi)])=1$ for all i and for any $P[\varphi]$ for which $\langle\varphi|E_i\varphi\rangle\neq 0$. Indeed, due to the commutativity of the operators L_y of Eq. (45) with E_i, ϵ_{12} of Eq. (28a) equals $\langle\varphi|E_i^2\varphi\rangle$; furthermore the first kind property of the measurement and the sharp pointer yield for Eqs. (28b)–(28d): $\epsilon_1=\epsilon_2=\langle\varphi|E_i\varphi\rangle$, and $\sigma_1^2=\sigma_2^2=\mathrm{Var}(E_i,P[\varphi])$. Therefore, $\epsilon_{12}-\epsilon_1\epsilon_2=\sigma_1\sigma_2$, so that $\rho(E_i,Z_i;P[U(\varphi\otimes\phi)])=\mathrm{Var}(E_i,P[\varphi])/\mathrm{Var}(E_i,P[\varphi])=1$. Finally, a direct computation of the state-correlation $\rho(T_{\mathscr{A}}(i,P[\varphi]),T_{\mathscr{M}}(i,P[\varphi]);P[U(\varphi\otimes\phi)])$ shows that this number is not, in general, equal to one.

IX. CONCLUSION

In this paper we have investigated possible properties of the final component states of the object system and the apparatus (or probe) arrived at in a quantum measurement, properties which must be required if the occurrence of definite measurement outcomes is to be understood as the conjunction of pointer value definiteness (PVD), pointer mixture property (PM), plus the ignorance interpretation for the final reduced apparatus state. According to Theorem 3.11, the properties (PVD) and (PM) are ensured if the final component states of the object system are mutually orthogonal. Considering initial states of $\mathscr{S}$ which are vector states, this latter condition is also necessary for (PM) in the case of a unitary measurement $\mathscr{M}_U$, where (PVD) is automatically fulfilled since the pointer is a sharp observable. The orthogonality of the states $T_{\mathscr{A}}(i,T)$ is not always guaranteed.[12]

Next we have considered conditions for strong correlations between observables, their values, or between the final component states of $\mathscr{S}$ and $\mathscr{A}$. It turns out that repeatable measurements give strong observable- as well as strong value-correlations (Theorems 5.5, 6.3, 6.4). Furthermore, strong observable-correlation for finite reading scales entails repeatability and thus the orthogonality of the states $T_{\mathscr{A}}(i,T)$ and hence (PVD), via Eq. (3.11). On the other hand, strong value-correlation may occur independently of (PVD). Finally, strong state-correlation may occur under more general circumstances than the other correlations since it is independent of the repeatability property, but its implying the orthogonality of the final component states of $\mathscr{S}$ may be limited to the case where these states are vector states. However, in that case, and for a unitary measurement $\mathscr{M}_U$, strong state-correlation is equivalent to the said orthogonality and thus to the pointer mixture condition.

In conclusion, we wish to emphasize that our investigation provides an illustration of how interpretational demands entail formal constraints on measurements that may or may not be fulfilled in a concrete case. These formal features have thus to be made explicit if the consistency of an interpretation is to be demonstrated. With these findings we believe to have settled the questions left open in previous work.[2]

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Canonical quantization of spontaneously broken topologically massive gauge theory

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In this paper we investigate the canonical quantization of a non-Abelian topologically massive Chern–Simons theory in which the gauge fields are minimally coupled to a multiplet of scalar fields in such a way that the gauge symmetry is spontaneously broken. Such a model produces the Chern–Simons–Higgs mechanism in which the gauge excitations acquire mass both from the Chern–Simons term and from the Higgs–Kibble effect. The symmetry breaking is chosen to be only partially broken, in such a way that in the broken vacuum there remains a residual non-Abelian symmetry. We develop the canonical operator structure of this theory in the broken vacuum, with particular emphasis on the particle-content of the fields involved in the Chern–Simons–Higgs mechanism. We construct the Fock space and express the dynamical generators in terms of creation and annihilation operator modes. The canonical apparatus is used to obtain the propagators for this theory, and we use the Poincaré generators to demonstrate the effect of Lorentz boosts on the particle states. © *1996 American Institute of Physics.* [S0022-2488(96)03106-4]

I. INTRODUCTION

Field theories in $(2+1)$-dimensional space–time exhibit many interesting and important properties related to the masses of the particle excitations of the quantum fields. For example, gauge theories involving a Chern–Simons term support massive gauge field excitations,[1,2] which differ from the Higgs–Kibble excitations produced in conventional spontaneous symmetry breaking.[3] The combination of *both* spontaneous symmetry breaking *and* a Chern–Simons (CS) term for the gauge field leads to the Chern–Simons–Higgs (CSH) mechanism, in which the physical fields are transmuted in a process that combines the Chern–Simons and Higgs–Kibble mass-generating effects in a particularly interesting and instructive manner.

An analysis of the covariant gauge field propagator[4,5] indicates the presence of two distinct mass poles, with masses given as complicated functions of the Higgs mass scale (set by the tree-approximation minimum of the symmetry breaking potential) and the CS mass scale [coming from the CS coupling parameter which has dimensions of mass in $(2+1)$-dimensional space–time]. The two distinct mass poles may also be seen in a factorization of the Chern–Simons–Proca equations of motion.[6] A Schrödinger representation approach[7] provides a simple physical picture based on a quantum mechanical analogue which identifies the two masses precisely with the two characteristic frequencies of the planar quantum mechanical model of charged particles moving in both a uniform magnetic field and a harmonic potential well. In this present paper we investigate field theoretic aspects of the CSH mechanism more deeply, presenting a detailed analysis of the canonical quantization of spontaneously broken CS theories. In this work, we pay particular attention to the relation between the quantized fields and their particle excitation modes and to the structure of the Poincaré generators as functionals of these particle excitation operators.

We have chosen to consider a non-Abelian theory in which the non-Abelian gauge symmetry is spontaneously broken in a manner that preserves a residual non-Abelian symmetry in the broken vacuum. This choice is motivated by the question of how a spontaneously broken CS theory 'knows' to quantum-mechanically protect the residual non-Abelian gauge symmetry from topo-

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logically nontrivial gauge transformations. For non-Abelian Chern–Simons theories, quantum consistency[1] requires that the CS coupling parameter takes quantized integer values, in appropriate units. Qualitatively, this consistency condition is reminiscent of Dirac's quantum mechanical quantization condition for the magnetic monopole,[8] but since the Chern–Simons theory is a *field theory* further subtleties (such as renormalization) arise. Pisarski and Rao[9] showed that, for a Chern–Simons–Yang–Mills theory (with no matter fields or symmetry breaking), a consistent one-loop renormalization involves a finite additive renormalization of the CS mass, with the finite shift depending on the gauge group and being such that the integer quantization condition is preserved. Subsequent calculations have confirmed the conjecture[9] that there are no further radiative corrections to this result.[10] Perturbative analyses of Abelian Chern–Simons theories subject to spontaneous symmetry breaking confirm the topological basis of the integer quantization of the renormalization of the CS term.[11–13] This work has shown that, in the Abelian case, in which topological arguments do not apply, the Chern–Simons mass receives a shift, in the broken vacuum, which is not an integer, but a complicated function of the various bare mass scales. (In Ref. 14 it is suggested that this shift should not be interpreted as a finite renormalization of the Chern–Simons mass, but rather as an indication of the appearance of parity-violating terms in the effective action. This reformulation of the result extends the Coleman–Hill theorem,[15] concerning the absence of loop corrections to the Chern–Simons mass, to the case of Abelian spontaneously broken Chern–Simons theories.) In a spontaneously broken non-Abelian Chern–Simons theory, with a *completely* broken symmetry in which the invariance of the effective theory to gauge transformations is no longer supported,[13] similar behavior was found.[16] More interesting is the situation in which the non-Abelian gauge symmetry is only *partially* broken, leaving a residual *non-Abelian* symmetry in the broken phase. The presence of the non-Abelian residual symmetry suggests that the CS coupling parameter should again be quantized, and indeed a direct perturbative computation shows that the CS coupling parameter receives a quantized finite shift which preserves the quantum consistency condition in the broken vacuum.[17] An earlier calculation, by the authors who first considered this model, incorrectly reported the opposite conclusion.[18] This work confirms the validity of the effective theory that describes the quantum fluctuations of the field about the spontaneously broken vacuum; it motivates an investigation into the origins of the massive propagating particle excitations of this model, and the mechanisms by which they obtain their mass.

In this paper, we consider the canonical quantization of such a non-Abelian model, with a partially broken symmetry leaving a residual non-Abelian symmetry in the broken phase, and develop the underlying dynamical theory. We make explicit the representation of the operator-valued fields in terms of excitations that correspond to observable, propagating particles in the spontaneously broken vacuum. We formulate the model in $(2+1)$-dimensional Minkowski space–time and for definiteness we consider an octet of SU(3) gauge fields interacting with a triplet of scalar fields in the fundamental representation of SU(3). The scalar fields Φ are coupled gauge-invariantly to the gauge fields, and self-coupled through a quartic potential $V(\Phi^\dagger\Phi) = -\mu^2\Phi^\dagger\Phi + \frac{1}{2}h(\Phi^\dagger\Phi)^2$, where $\mu^2 > 0$ and $h > 0$, so that, in the tree approximation, the scalar fields have nonvanishing vacuum expectation values. The vacuum expectation values of the three constituent fields in Φ are chosen so that the residual ''effective'' fields, which represent fluctuations of these scalar fields about their tree-approximation vacuum expectation values, still maintain an unbroken SU(2) symmetry in their coupling to the gauge fields. In the canonical quantization of this model we construct time-dependent fields in an interaction picture that includes, in the ''free'' Hamiltonian that drives it, the interaction terms that become bilinear in fields when the charged scalar field Φ is expanded about its constant vacuum expectation value. We use these time-dependent interaction-picture fields to evaluate the propagators. And finally, we construct the particle states that correspond to the two different mass singularities in the propagator for this model. We express the trilinear and quartic interaction Lagrangian as a functional of these interaction-picture fields, and obtain a set of vertices that can be used to describe the theory. In

addressing these problems, we make use of technical developments that originated from separate earlier work by the authors.[7,19–23]

In Section II, we formulate the model and describe the spontaneous symmetry breaking process. In Section III, we construct the required Fock spaces, express the scalar and gauge fields as superpositions of particle and ghost excitations, and implement Gauss's law and the gauge condition. In Section IV, we construct the interaction-picture scalar and gauge fields, and evaluate their time-ordered vacuum expectation values in the spontaneously broken vacuum state to obtain the propagators for this theory. In Section V, we construct the Poincaré generators for this theory, demonstrate the validity of the Poincaré algebra, and evaluate the effect of Lorentz boosts on each of the massive gluon states. Detailed forms of the interaction Lagrangian are given in an Appendix.

II. FORMULATION OF THE MODEL

The Lagrangian for this model is given by

$$\mathcal{L}=-\frac{1}{4}\mathcal{F}^a_{\mu\nu}\mathcal{F}^{a\mu\nu}+\frac{1}{4}m\epsilon^{\mu\nu\rho}\left(\mathcal{F}^a_{\mu\nu}A^a_\rho+\frac{2}{3}ef^{abc}A^a_\mu A^b_\nu A^c_\rho\right)$$
$$+(D^\mu\Phi)^\dagger(D_\mu\Phi)+\mu^2\Phi^\dagger\Phi-\frac{1}{2}h(\Phi^\dagger\Phi)^2+\mathcal{L}_{\rm fp}+\mathcal{L}_{\rm G}, \tag{1}$$

where $\mathcal{F}^a_{\mu\nu}$ designates the SU(3) gauge field strength

$$\mathcal{F}^a_{\mu\nu}=\partial_\mu A^a_\nu-\partial_\nu A^a_\mu-2ef^{abc}A^b_\mu A^c_\nu; \tag{2}$$

we denote by $F^a_{\mu\nu}$ the ''Abelian'' part of the field strength,

$$F^a_{\mu\nu}=\partial_\mu A^a_\nu-\partial_\nu A^a_\mu, \tag{3}$$

and f^{abc} represents the SU(3) structure constants. The implied summations over repeated Latin superscripts, such as a, b, and c, are from 1 to 8 unless otherwise specified. The covariant derivative of the scalar triplet $D_\mu\Phi$ is given by

$$D_\mu\Phi=\partial_\mu\Phi+ie\lambda^a A^a_\mu\Phi, \tag{4}$$

where λ^a represents the Gell-Mann matrices which satisfy the commutation relations $[\lambda^a,\lambda^b]=2if^{abc}\lambda^c$. $\mathcal{L}_{\rm fp}$ is the part of the Lagrangian that couples the gauge fields to the Faddeev–Popov ghosts, and is given by

$$\mathcal{L}_{\rm fp}=i\partial_\mu\sigma^a_{\rm f}\partial^\mu\sigma^a_{\rm p}-2ief^{abc}A^a_\mu\sigma^b_{\rm f}\partial^\mu\sigma^c_{\rm p}+ie\sigma^a_{\rm f}\frac{\delta\mathcal{U}^a}{\delta\chi^c}\sigma^c_{\rm p}, \tag{5}$$

where $\sigma^a_{\rm f}$ and $\sigma^a_{\rm p}$ are the two self-adjoint operator-valued anticommuting scalar Faddeev–Popov fields; $\mathcal{U}^a$ is given by

$$\mathcal{U}^a=i(1-\gamma)(\langle\Phi\rangle^\dagger_0\lambda^a\Phi'-\Phi'^\dagger\lambda^a\langle\Phi\rangle_0) \tag{6}$$

and $\delta\chi^c$ is the infinitesimal gauge shift that parameterizes the first-order gauge transformation of $\mathcal{U}^a$. $\mathcal{L}_{\rm G}$ is the gauge fixing term in the Lagrangian, and is given by

$$\mathcal{L}_{\rm G}=\frac{1}{2}(1-\gamma)G^aG^a-[\partial_\mu A^{a\mu}-ie(1-\gamma)(\langle\Phi\rangle^\dagger_0\lambda^a\Phi'-\Phi'^\dagger\lambda^a\langle\Phi\rangle_0)]G^a; \tag{7}$$

G^a is the gauge-fixing field used to impose the gauge condition for the t'Hooft gauge,

$$[\partial_\mu A^{a\mu} - ie(1-\gamma)(\langle\Phi\rangle_0^\dagger \lambda^a \Phi' - \Phi'^\dagger \lambda^a \langle\Phi\rangle_0)] = 0, \tag{8}$$

which is a covariant gauge that involves both the tree-approximation vacuum expectation value (v.e.v.) of the scalar field $\langle\Phi\rangle_0$ and the fluctuation of the scalar field about that vacuum expectation value $\Phi' = \Phi - \langle\Phi\rangle_0$. The first-order variation of $\mathcal{L}$ with respect to G^a leads to an equation of motion that enables us to contain the time-evolution of the interaction-picture fields entirely within a Hilbert space in which matrix elements of G^a always vanish; that fact secures Eq. (8) as the gauge condition for this model. The technical arrangements that permit — in fact require — time evolution of the interaction-picture fields to be contained within a subspace in which matrix elements of G^a vanish will be discussed in Section III.

We choose a scheme for breaking the SU(3) symmetry that preserves an SU(2) symmetry in the effective Lagrangian. In the tree-approximation vacuum state for this effective Lagrangian, the self-interaction $V(\Phi^\dagger\Phi)$ takes on its classical minimum value for the tree-approximation v.e.v. $\langle\Phi\rangle_0$. A choice for $\langle\Phi\rangle_0$ that satisfies this requirement is

$$\langle\Phi\rangle_0 = \frac{v}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \equiv \frac{v}{\sqrt{2}} \langle\phi\rangle_0, \tag{9}$$

where $v = (2\mu^2/h)^{1/2}$. To analyze this model in the broken vacuum, we expand the scalar field Φ in terms of its fluctuations about the v.e.v. $\langle\Phi\rangle_0$,

$$\Phi' = \Phi - \langle\Phi\rangle_0, \tag{10}$$

and expand the Lagrangian as

$$\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_1 + \mathcal{L}_2. \tag{11}$$

Here $\mathcal{L}_0$ represents the ''free'' Lagrangian in which the interaction have been shut off, and $\mathcal{L}_1$ and $\mathcal{L}_2$ represent terms that are first and second order in e, respectively. Note that there are several coupling constants and mass scales to consider when making this expansion, and we need to be specific about how coupling constants are ''shut off'' in taking $\mathcal{L}$ to its noninteracting limit $\mathcal{L}_0$. The CS coupling constant m has dimensions of mass, as do e^2 (the square of the scalar-gauge coupling), v^2 (the square of the magnitude of the scalar field v.e.v.), and ev. The noninteracting limit $\mathcal{L}_0$ of the full Lagrangian $\mathcal{L}$ is defined to be the limit $e \to 0$ and $h \to 0$ with the ''Higgs'' mass scale ev kept constant, and the CS mass scale unaffected. Then the noninteracting Lagrangian is

$$\begin{aligned}
\mathcal{L}_0 = & -\frac{1}{4} F^a_{\mu\nu} F^{a\mu\nu} + \frac{m}{4} \epsilon^{\mu\nu\rho} F^a_{\mu\nu} A^a_\rho + \frac{e^2 v^2}{4} A^a_\mu A^{b\mu} \langle\phi\rangle_0^\dagger \{\lambda^a, \lambda^b\} \langle\phi\rangle_0 + |\partial_\mu \Phi'|^2 - \frac{\mu^2}{2} (\langle\phi\rangle_0^\dagger \Phi' \\
& + \Phi'^\dagger \langle\phi\rangle_0)^2 + i \frac{ev}{\sqrt{2}} A^a_\mu [(\partial^\mu \Phi')^\dagger \lambda^a \langle\phi\rangle_0 - \langle\phi\rangle_0^\dagger \lambda^a \partial^\mu \Phi'] \\
& - \left[\partial_\mu A^{a\mu} + i \frac{ev}{\sqrt{2}} (1-\gamma)(\langle\phi\rangle_0^\dagger \lambda^a \Phi' - \Phi'^\dagger \lambda^a \langle\phi\rangle_0) \right] \\
& \times G^a + \frac{1}{2}(1-\gamma) G^a G^a + i \partial_\mu \sigma^a_{\mathrm{f}} \partial^\mu \sigma^a_{\mathrm{p}}.
\end{aligned} \tag{12}$$

The $\mathcal{O}(e)$ interaction Lagrangian is[24]

$$\mathcal{L}_1 = e\Bigg\{ f^{abc}F^a_{\mu\nu}A^{b\mu}A^{c\nu} - \frac{m}{3}\epsilon^{\mu\nu\rho}f^{abc}A^a_\mu A^b_\nu A^c_\rho - 2if^{abc}A^a_\mu \sigma^b_{\rm f}\partial^\mu \sigma^c_{\rm p} + i\sigma^a_{\rm f}\frac{\delta \mathcal{U}^a}{\delta \chi^c}\sigma^c_{\rm p}$$
$$+ \frac{ev}{2\sqrt{2}}A^a_\mu A^{b\mu}(\Phi'^\dagger\{\lambda^a,\lambda^b\}\langle\phi\rangle_0 + \langle\phi\rangle_0^\dagger\{\lambda^a,\lambda^b\}\Phi')$$
$$- iA^a_\mu[\Phi'^\dagger\lambda^a\partial^\mu\Phi' - (\partial^\mu\Phi')^\dagger\lambda^a\Phi'] - \sqrt{2}\frac{\mu^2}{ev}|\Phi'|^2(\langle\phi\rangle_0^\dagger\Phi' + \Phi'^\dagger\langle\phi\rangle_0)\Bigg\}, \tag{13}$$

and the $\mathcal{O}(e^2)$ interaction Lagrangian is

$$\mathcal{L}_2 = e^2\Bigg(-f^{abc}f^{ade}A^b_\mu A^{d\mu}A^c_\nu A^{e\nu} - \frac{\mu^2}{e^2v^2}|\Phi'|^4 + \frac{1}{2}A^a_\mu A^{b\mu}\Phi'^\dagger\{\lambda^a,\lambda^b\}\Phi'\Bigg). \tag{14}$$

We note that the presence of the CS term in the original Lagrangian Eq. (11) introduces a new quadratic piece $\sim\epsilon FA$ in $\mathcal{L}_0$ and a new 3-gluon vertex piece $\sim\epsilon AAA$ in $\mathcal{L}_1$.

To identify the physical and unphysical fields in the broken vacuum, we first express Φ' in terms of *real* scalar fields

$$\Phi' = \frac{1}{\sqrt{2}}\begin{pmatrix} i\xi^4 + \xi^5 \\ i\xi^6 + \xi^7 \\ -i\xi^8 + \psi \end{pmatrix}. \tag{15}$$

Then, using the explicit form given in Eq. (9) of the v.e.v. $\langle\phi\rangle_0$, together with the Gell-Mann matrix anticommutation relations

$$\{\lambda^a,\lambda^b\} = \tfrac{4}{3}\delta^{ab}\mathbf{1} + 2d^{abc}\lambda^c, \tag{16}$$

we write the free Lagrangian $\mathcal{L}_0$ as

$$\mathcal{L}_0 = -\frac{1}{4}F^a_{\mu\nu}F^{a\mu\nu} + \frac{m}{4}\epsilon^{\mu\nu\rho}F^a_{\mu\nu}A^a_\rho + \frac{1}{2}\sum_{a=4}^{8}M^2_{(a)}A^a_\mu A^{a\mu} + \sum_{a=4}^{8}M_{(a)}A^{a\mu}\partial_\mu\xi^a$$
$$+ \frac{1}{2}\sum_{a=4}^{8}\partial_\mu\xi^a\partial^\mu\xi^a + \frac{1}{2}\partial_\mu\psi\partial^\mu\psi - \mu^2\psi^2 + \frac{1}{2}(1-\gamma)G^aG^a - \partial_\mu A^{a\mu}G^a$$
$$+ (1-\gamma)\sum_{a=4}^{8}M_{(a)}\xi^aG^a + i\partial_\mu\sigma^a_{\rm f}\partial^\mu\sigma^a_{\rm p} - i(1-\gamma)\sum_{a=4}^{8}M^2_{(a)}\sigma^a_{\rm f}\sigma^a_{\rm p}. \tag{17}$$

Here the symmetry breaking mass scales $M_{(a)}$ are given by

$$M_{(a)} = \begin{cases} 0, & a = 1,2,3, \\ M_{\rm D} = ev, & a = 4,5,6,7, \\ M_{\rm S} = \dfrac{2}{\sqrt{3}}ev, & a = 8. \end{cases} \tag{18}$$

From Eq. (17), we recognize ψ as the Higgs scalar field, with mass $\sqrt{2}|\mu|$, and ξ^a $(a = 4,\ldots,8)$ as the massless unphysical scalar fields. Furthermore, the gauge fields A^a_μ

($a=1,2,3$) have a quadratic Lagrangian of the Maxwell–Chern–Simons form, while the gauge fields A_μ^a ($a=4,\ldots,8$) have an additional Proca-like quadratic term with mass scale parameters $M_{(a)}$ as given in Eq. (18).

The interaction Lagrangians $\mathcal{L}_1$ and $\mathcal{L}_2$ can also be expanded in terms of the real fields in Eq. (15) and the symmetry breaking mass scales in Eq. (18); the resulting expansions are recorded in the Appendix. It is important to observe that (as expected) the gauge field A_μ^a ($a=1,2,3$) form an SU(2) triplet corresponding to the residual SU(2) symmetry of the broken vacuum. It proves convenient to group the real scalar fields into SU(2) ''isospinors:''

$$\Psi_1=\frac{1}{\sqrt{2}}\begin{pmatrix} i\xi^4+\xi^5 \\ i\xi^6+\xi^7 \end{pmatrix}, \tag{19}$$

$$\Psi_2=\frac{1}{\sqrt{2}}\begin{pmatrix} i\xi^4+\xi^5 \\ \psi-i\xi^8 \end{pmatrix}, \tag{20}$$

and

$$\Psi_3=\frac{1}{\sqrt{2}}\begin{pmatrix} i\xi^6+\xi^7 \\ \psi-i\xi^8 \end{pmatrix}. \tag{21}$$

With this notation, the fields A_μ^a ($a=1,2,3$) couple to Ψ_1 in an SU(2)-invariant manner, while the two gauge field doublets (A_μ^4,A_μ^5) and (A_μ^6,A_μ^7) couple to Ψ_2 and Ψ_3 so that the part of the isospin invariance that corresponds to rotation in the $i=1,2$ plane is preserved; but this latter interaction is not invariant to rotation in the entire isospin space. The remaining gauge field A_μ^8 is an SU(2) singlet.

In earlier work on Abelian theories with Chern–Simons interactions,[19–21] we implemented Gauss's law and developed a canonical formulation for the entire Lagrangian, with all interactions included. In a non-Abelian gauge theory, such a program becomes much more problematical. We will therefore implement Gauss's law only for the partial theory described by $\mathcal{L}_0$. In this case, however, because of the spontaneously broken symmetry, even the Abelian $\mathcal{L}_0$ contains part of the interaction — not only the part of the Φ^4 self-interaction implicit in the spontaneously broken vacuum state, but also the part of the gauge-invariant coupling of the gauge field to the ''charged'' scalar Φ that remains bilinear in operator-valued fields after Φ has been expressed as $\Phi=\Phi'+\langle\Phi\rangle_0$. Although this part of the interaction term is proportional to e, it does not vanish in the ''interaction-free'' limit because e combines with $h^{-1/2}$ to become one of the masses that are kept constant in the $\mathcal{L}\to\mathcal{L}_0$ limit. Implementing Gauss's law and the gauge condition, and developing the canonical formulation of the part of the theory described by $\mathcal{L}_0$, will enable us to construct the Fock space for the particle states observed in the broken vacuum. In the course of this work, we will demonstrate the process by which the masses that stem from the Higgs–Kibble effect[3] combine with the topological mass to form the masses of the propagating modes of the gauge field in this model. $\mathcal{L}_0$, defined as we have specified here, is the Lagrangian that drives the interaction-picture fields when a Higgs–Kibble effect occurs. The corresponding ''free'' Hamiltonian H_0, which is the $e\to 0$ limit of H obtained by this same limiting process, accounts for the particle spectrum of this model. Once $\mathcal{L}_0$ and H_0 have been identified, and Gauss's law and the covariant gauge condition have been imposed, the resulting apparatus can be used to develop a Fock space as well as propagators and vertices for evaluating the S-matrix elements and renormalization constants for the full theory, with $\mathcal{L}_1$ and $\mathcal{L}_2$ included.

The Euler–Lagrange equations determined by $\mathcal{L}_0$ are

$$\partial_\mu F^{a\nu\mu} - \frac{1}{2} m \epsilon^{\mu\rho\nu} F^a_{\mu\rho} - \partial^\nu G^a = M^2_{(a)} A^{a\nu} + \partial^\nu \alpha^a, \tag{22}$$

$$\partial_\mu A^{a\mu} - (1-\gamma)\alpha^a = (1-\gamma) G^a, \tag{23}$$

$$\partial_\mu \partial^\mu \psi + 2\,\mu^2 \psi = 0, \tag{24}$$

and

$$\partial_\mu \partial^\mu \xi^a + M_{(a)} \partial_\mu A^{a\mu} = (1-\gamma) M_{(a)} G^a, \tag{25}$$

where $\alpha^a = M_{(a)} \xi^a$,

$$\partial_\mu \partial^\mu \sigma^a_{\mathrm{f}} + (1-\gamma) M^2_{(a)} \sigma^a_{\mathrm{f}} = 0, \tag{26}$$

and

$$\partial_\mu \partial^\mu \sigma^a_{\mathrm{p}} + (1-\gamma) M^2_{(a)} \sigma^a_{\mathrm{p}} = 0. \tag{27}$$

From these equations, we get

$$\partial_\mu \partial^\mu G^a + (1-\gamma) M^2_{(a)} G^a = 0. \tag{28}$$

Equation (22) represents the Maxwell–Ampere law (for $\nu = 1,2$) as well as Gauss's law (for $\nu = 0$); however, as is to be expected in covariant gauges, this equation differs from the classical form of Maxwell–Ampere and Gauss's laws by the gauge-fixing term — in this case, $\partial^\nu G^a$. Implementation of the correct form of these laws will have the effect of defining a subspace for the dynamical time evolution of state vectors in which the gauge-fixing term will have vanishing matrix elements. Equation (23) will be used to impose the covariant gauge condition: $\gamma = 0$ corresponds to the Feynman, and $\gamma = 1$ to the Landau version of the covariant (t'Hooft) gauge.

To quantize this theory, we need to express the Hamiltonian in terms of the canonical momenta given by $\Pi^{a\mu} = \partial \mathcal{L}_0 / \partial(\partial_0 A^a_\mu)$. These canonical momenta are:

$$\Pi^{a\mu} = F^{a\mu 0} + \frac{1}{2} m \epsilon^{0\mu\nu} A^a_\nu - g^{0\mu} G^a, \tag{29}$$

$$\Pi_\psi = \partial_0 \psi, \tag{30}$$

$$\Pi^a_\xi = \partial_0 \xi^a + M_{(a)} A^a_0, \tag{31}$$

$$\Pi^a_{\mathrm{f}} = i \partial_0 \sigma^a_{\mathrm{p}}, \tag{32}$$

and

$$\Pi^a_{\mathrm{p}} = -i \partial_0 \sigma^a_{\mathrm{f}}; \tag{33}$$

Π^a_{f} and Π^a_{p} are the conjugate momenta to the fields σ^a_{f} and σ^a_{p}, respectively.

The only equation that does not contain any time-derivatives of fields (and therefore is a constraint) is $\Pi^{a0} = -G^a$. This constraint is manifestly consistent with canonical (Poisson) equal-time commutation rules, which we impose. The equal-time commutation rules (ETCR) are:

$$[A^q_l(\mathbf{x}), \Pi^b_n(\mathbf{y})] = i \delta_{ln} \delta^{ab} \delta(\mathbf{x} - \mathbf{y}), \tag{34}$$

$$[A_0^a(\mathbf{x}),G^b(\mathbf{y})]=-i\delta^{ab}\delta(\mathbf{x}-\mathbf{y}), \tag{35}$$

$$[\xi^a(\mathbf{x}),\Pi_\xi^b(\mathbf{y})]=i\delta^{ab}\delta(\mathbf{x}-\mathbf{y}), \tag{36}$$

$$[\psi(\mathbf{x}),\Pi_\psi(\mathbf{y})]=i\delta(\mathbf{x}-\mathbf{y}), \tag{37}$$

and all other commutators among these fields are zero. The anticommutation rules for the Faddeev–Popov ghost fields are

$$\{\sigma_{\rm f}^a(\mathbf{x}),\Pi_{\rm f}^b(\mathbf{y})\}=i\delta^{ab}\delta(\mathbf{x}-\mathbf{y}), \tag{38}$$

$$\{\sigma_{\rm p}^a(\mathbf{x}),\Pi_{\rm p}^b(\mathbf{y})\}=i\delta^{ab}\delta(\mathbf{x}-\mathbf{y}), \tag{39}$$

and all other combinations anticommute.

The Hamiltonian density $\mathcal{H}_0$, determined by $\mathcal{L}_0$ and by the canonical momenta, will be expressed as

$$\mathcal{H}_0=\sum_{a=1}^{8}\mathcal{H}^a+\mathcal{H}_\psi+\sum_{a=1}^{8}\mathcal{H}_{\rm fp}^a; \tag{40}$$

for $a=1,2,3$:

$$\mathcal{H}^a=\frac{1}{2}\Pi_l^a\Pi_l^a+\frac{1}{4}F_{ln}^aF_{ln}^a+\frac{1}{8}m^2A_n^aA_n^a+\frac{1}{2}m\epsilon_{ln}A_l^a\Pi_n^a$$
$$+A_0^a\left(\partial_l\Pi_l^a-\frac{1}{4}m\epsilon_{ln}F_{ln}^a\right)+G^a\partial_lA_l^a-\frac{1}{2}(1-\gamma)G^aG^a; \tag{41}$$

for $a=4,5,6,7,8$:

$$\mathcal{H}^a=\frac{1}{2}\Pi_l^a\Pi_l^a+\frac{1}{4}F_{ln}^aF_{ln}^a+\frac{1}{2}\left[\frac{1}{4}m^2+M_{(a)}^2\right]A_n^aA_n^a+\frac{1}{2}m\epsilon_{ln}A_l^a\Pi_n^a$$
$$+A_0^a\left[\partial_l\Pi_l^a-\frac{1}{4}m\epsilon_{ln}F_{ln}^a-M_{(a)}\Pi_\xi^a\right]+G^a[\partial_lA_l^a-(1-\gamma)M_{(a)}\xi^a]-M_{(a)}A_l^a\partial_l\xi^a$$
$$-\frac{1}{2}(1-\gamma)G^aG^a+\frac{1}{2}\Pi_\xi^a\Pi_\xi^a+\frac{1}{2}\partial_l\xi^a\partial_l\xi^a; \tag{42}$$

the other parts of $\mathcal{H}_0$ are

$$\mathcal{H}_\psi=\frac{1}{2}\Pi_\psi\Pi_\psi+\frac{1}{2}\partial_l\psi\partial_l\psi+\mu^2\psi^2; \tag{43}$$

and

$$\mathcal{H}_{\rm fp}^a=i\Pi_{\rm p}^a\Pi_{\rm f}^a+i\partial_l\sigma_{\rm f}^a\partial_l\sigma_{\rm p}^a+i(1-\gamma)M_{(a)}^2\sigma_{\rm f}^a\sigma_{\rm p}^a. \tag{44}$$

The Hamiltonian, $H_0=\int d\mathbf{x}\mathcal{H}_0(\mathbf{x})$, is the ''free'' kinetic energy limit of the entire Hamiltonian, with the proviso that in this model the free kinetic energy limit includes the part of the interaction term in which the constant tree-approximation v.e.v. of Φ combines with the charge e to form a

new constant (dimensionally a mass) whose operator-valued coefficient is bilinear in fields. This part of the interaction is not shut off in the $H \to H_0$ limit, and is absorbed into a generalized, more encompassing kinetic energy operator H_0.

III. PARTICLE STATES AND GAUSS'S LAW

Equation (22), when $\nu = 0$ and the canonical momenta replace the time derivatives of fields, has the form[25]

$$\partial_l \Pi_l^a + \frac{1}{2} m \epsilon_{ln} \partial_l A_n^a - M_{(a)} \Pi_\xi^a = \partial^0 G^a. \tag{45}$$

The right-hand side of Eq. (45) would have to vanish to express Gauss's law. But since $\partial^0 G^a = 0$ is not one of the Euler–Lagrange equations, we therefore have to take some further measures to implement Gauss's law. For later reference, we will define the ''Gauss's law operator'' $\mathcal{G}^a$ as

$$\mathcal{G}^a = \partial_l \Pi_l^a + \frac{1}{2} m \epsilon_{ln} \partial_l A_n^a - M_{(a)} \Pi_\xi^a. \tag{46}$$

In order to describe the particle states of this theory, we must construct a ''suitable'' representation for the operator-valued fields in terms of creation and annihilation operators for the observable propagating particles described by this model — and, in the case of gauge theories, generally also in terms of additional 'ghost' excitations. The first requirement for such a suitable representation is that it must be consistent with the equal-time commutation rules given in Eqs. (34)–(37). This requirement, however, though necessary, is not sufficient to provide for a consistent theory. Another requirement that a representation must satisfy in order to be suitable, is that the excitation modes for propagating, observable particles must appear in the Hamiltonian H_0 — the Hamiltonian that time-translates the interaction picture fields — in such a manner that one-particle states or noninteracting multiparticle states are eigenstates of H_0, with eigenvalues $E_k = \sqrt{m^2 + k^2}$ for one-particle states of mass m and momentum k, and with eigenvalues $\Sigma_{i=1}^n E_k(i)$ for noninteracting n-particle states. Clearly, these states must also remain invariant to the temporal evolution mediated by $\exp(-iH_0 t)$, except for time-dependent phase factors, $\exp(-iE_k t)$ for one-particle, and $\exp\{\Sigma_{i=1}^n [-iE_k(i)t]\}$ for noninteracting n-particle states. In particular, it is crucial that time-translation by $\exp(-iH_0 t)$ does not cause particle states to penetrate into the part of the Hilbert space in which probability measure is absorbed by ghost states at the expense of the observable propagating states. Once a representation in terms of particle modes — and ghosts, if required — has been constructed and demonstrated to lead to a consistent form of H_0, that fact confirms the identification of the particle modes: their existence, their masses, their stability to time-translation as noninteracting states, and ultimately through the use of the other Poincaré operators, their other kinematic properties as well. In this way, the canonical quantization procedure formally demonstrates the existence of propagating particle modes that, in the absence of explicit representations of the gauge fields as superpositions of creation and annihilation operators, can only be inferred indirectly on the basis of equations of motion and on the supposition that propagator poles are not ''spurious,'' but reflect the existence of propagating particle modes.

Although representations in terms of particle excitation operators for many familiar operator-valued fields — scalar Klein–Gordon fields or spinor Dirac fields, for example — are commonplace and easily obtained, representations for the fields that appear in this model are much less trivial to construct. The masses of the gauge field excitations in this model combine the topological mass induced by the Chern–Simons term with the effect of the v.e.v. of the scalar field, that causes parts of the cubic and quartic terms in the Lagrangian to mimic mass terms. As a result, we expect the observable particle modes of the combined scalar and gauge fields to consist of Higgs

scalars as well as gauge field excitations — massive gluons with both topological mass and mass from the spontaneously broken symmetry. The eight gauge fields in this model fall into three classes, and should give rise to particle excitations with different mass: one SU(2) triplet of gauge fields with $M_{(a)}=0$ and excitation modes that have only topological mass; two doublets of gauge fields with $M_{(a)}=M_{\mathrm{D}}$ excitations whose mass depends on both the topological mass and M_{D}; and a singlet similar to the doublet, but with M_{D} replaced by M_{S}. The pole structure of the propagator[4,5] and earlier work on related systems[6,7] suggest that the gauge fields in the doublet and singlet sectors each have two different massive gluon states. The gauge fields in the unbroken SU(2) triplet have just a single gluon excitation mode. We will make an initial *ansatz* that incorporates this set of particle states into the representation of the gauge fields. If more particle states are needed than the ones included in our *ansatz*, or if an entirely different set is required, it will be impossible to construct a suitable representation using these excitation modes. If fewer particle modes are sufficient, then it will become evident that a mode is redundant. Mistakes in the tentative choices of particle modes will therefore be self-correcting. Conversely, a consistent and suitable representation of the gauge fields will confirm that the identification of the particle excitations is correct.

It is apparent that the observable, propagating gluon modes listed above will not suffice to represent *all* the commutation rules included in Eqs. (34) and (35). Further modes, in the form of ghost excitations, are required. These ghost modes are identical to the ones that appear in Abelian Maxwell–Chern–Simons theory,[19–21] and that are also required in $(3+1)$-dimensional QED (QED_4) in covariant and axial (except for the spatial axial) gauges.[26] The excitation operators for the massive gluons are the annihilation operator $a^c(\mathbf{k})$ and its adjoint creation operator $a^{c\dagger}(\mathbf{k})$, which obey the commutation rule $[a^c(\mathbf{k}),a^{d\dagger}(\mathbf{q})]=\delta^{cd}\delta_{\mathbf{kq}}$. For the gauge fields in the doublet and singlet sectors, the second observable, propagating mode will be designated by the annihilation operator $b^c(\mathbf{k})$ and its adjoint creation operator $b^{c\dagger}(\mathbf{k})$, which obey the commutation rule $[b^c(\mathbf{k}),b^{d\dagger}(\mathbf{q})]=\delta^{cd}\delta_{\mathbf{kq}}$.

Ghost excitation operators exist in pairs. In this work, we will use the ghost annihilation operators $a_Q^c(\mathbf{k})$ and $a_R^c(\mathbf{k})$ and their respective adjoint creation operators $a_Q^{c\star}(\mathbf{k})$ and $a_R^{c\star}(\mathbf{k})$ in the representations of the gauge field. Ghost states have zero norm, but the single-particle ghost states $a_Q^{c\star}(\mathbf{k})|0\rangle$ and $a_R^{c\star}(\mathbf{k})|0\rangle$ have a nonvanishing inner product; similar nonvanishing inner products also arise for n-particle states with equal numbers of Q and R ghosts. These properties of the ghost states are implemented by the commutator algebra

$$[a_Q^c(\mathbf{k}),a_R^{d\star}(\mathbf{q})]=[a_R^c(\mathbf{k}),a_Q^{d\star}(\mathbf{q})]=\delta^{cd}\delta_{\mathbf{kq}} \tag{47}$$

and

$$[a_Q^c(\mathbf{k}),a_Q^{d\star}(\mathbf{q})]=[a_R^c(\mathbf{k}),a_R^{d\star}(\mathbf{q})]=0, \tag{48}$$

which, in turn, imply that the unit operator in the one-particle ghost (OPG) sector is

$$1_{\mathrm{OPG}}=\sum_{\mathbf{k}}\,[a_Q^{c\star}(\mathbf{k})|0\rangle\langle 0|a_R^c(\mathbf{k})+a_R^{c\star}(\mathbf{k})|0\rangle\langle 0|a_Q^c(\mathbf{k})]; \tag{49}$$

the obvious generalization of Eq. (49) applies in the n-particle sectors. The ghost excitations enable us to satisfy the equal-time commutation relations, Eqs. (34) and (35).

The requirements that Gauss's law ($\mathcal{G}^c=0$) be implemented, and that the time evolution mediated by $\exp(-iH_0t)$ keep probability measure contained within the subspace spanned by propagating, observable particle modes, have the following further consequences: The Gauss's law operator $\mathcal{G}^c(\mathbf{x})$ must be restricted to a linear combination of ghost operators for a single kind

of ghost. We will therefore express $\mathcal{G}^c(\mathbf{x})$ as a superposition of $a_Q^c(\mathbf{k})$ and $a_Q^{c\star}(\mathbf{k})$ operators only. Furthermore, the gauge-fixing field, G^c, must be expressed as a superposition of the same $a_Q^c(\mathbf{k})$ and $a_Q^{c\star}(\mathbf{k})$ ghost operators as is $\mathcal{G}^c(\mathbf{x})$.

We have found the required suitable representation of the fields by a combination of unitary transformations similar to the ones used in previous work[19–21] and of ''trial fields'' with arbitrary parameters which we then adjusted to arrive at ''suitable'' field representations. For example, we used the trial field

$$\begin{aligned}
A_l^c(\mathbf{x}) = &\sum_{\mathbf{k}} [\alpha_1(k)\epsilon_{ln}k_n + \alpha_2(k)k_l][a^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} + a^{c\dagger}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}] + \sum_{\mathbf{k}} i[\alpha_3(k)\epsilon_{ln}k_n + \alpha_4(k)k_l] \\
&\times [a^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} - a^{c\dagger}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}] + \sum_{\mathbf{k}} [\alpha_5(k)\epsilon_{ln}k_n + \alpha_6(k)k_l][b^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} + b^{c\dagger}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}] \\
&+ \sum_{\mathbf{k}} i[\alpha_7(k)\epsilon_{ln}k_n + \alpha_8(k)k_l][b^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} - b^{c\dagger}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}] + \sum_{\mathbf{k}} [\alpha_9(k)\epsilon_{ln}k_n + \alpha_{10}(k)k_l] \\
&\times [a_Q^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} + a_Q^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}] + \sum_{\mathbf{k}} i[\alpha_{11}(k)\epsilon_{ln}k_n + \alpha_{12}(k)k_l] \\
&\times [a_Q^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} - a_Q^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}] + \sum_{\mathbf{k}} [\alpha_{13}(k)\epsilon_{ln}k_n + \alpha_{14}(k)k_l][a_R^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} \\
&+ a_R^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}] + \sum_{\mathbf{k}} i[\alpha_{15}(k)\epsilon_{ln}k_n + \alpha_{16}(k)k_l][a_R^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} - a_R^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}], \qquad (50)
\end{aligned}$$

where $\alpha_1(k), \ldots, \alpha_{16}(k)$ are arbitrary real parameters. Similar substitutions were made for the other fields in the model. The previously specified requirements of ''suitability'' were then translated into a set of equations which was solved using a customized operator algebra manipulation package in MATHEMATICA.[27] The resulting gauge field representations for the SU(2)-symmetric triplet ($c=1,2,3$) that has topological mass only are

$$\begin{aligned}
A_l^c(\mathbf{x}) = &\sum_{\mathbf{k}} \frac{8ik\epsilon_{ln}k_n}{m^{5/2}}[a_Q^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} - a_Q^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}] + (1-\gamma)\sum_{\mathbf{k}} \frac{2k_l}{m^{3/2}}[a_Q^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} + a_Q^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}] \\
&- \sum_{\mathbf{k}} \frac{4k^2k_l}{m^{7/2}}[a_Q^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} + a_Q^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}] + \sum_{\mathbf{k}} \frac{m^{3/2}k_l}{16k^3}[a_R^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} + a_R^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}] \\
&- \sum_{\mathbf{k}} \frac{\sqrt{\omega(k)}k_l}{\sqrt{2}mk}[a^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} + a^{c\dagger}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}] + \sum_{\mathbf{k}} \frac{i\epsilon_{ln}k_n}{k\sqrt{2\omega(k)}}[a^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} - a^{c\dagger}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}],
\end{aligned} \qquad (51)$$

$$\begin{aligned}
\Pi_l^c(\mathbf{x}) = &-\sum_{\mathbf{k}} \frac{4ikk_l}{m^{3/2}}[a_Q^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} - a_Q^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}] + (1-\gamma)\sum_{\mathbf{k}} \frac{\epsilon_{ln}k_n}{\sqrt{m}}[a_Q^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} + a_Q^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}] \\
&+ \sum_{\mathbf{k}} \frac{6k^2\epsilon_{ln}k_n}{m^{5/2}}[a_Q^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} + a_Q^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}] + \sum_{\mathbf{k}} \frac{m^{5/2}\epsilon_{ln}k_n}{32k^3}[a_R^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} + a_R^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}] \\
&+ \sum_{\mathbf{k}} \frac{imk_l}{2^{3/2}k\sqrt{\omega(k)}}[a^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} - a^{c\dagger}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}] + \sum_{\mathbf{k}} \frac{\sqrt{\omega(k)}\epsilon_{ln}k_n}{2^{3/2}k} \\
&\times [a^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} + a^{c\dagger}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}],
\end{aligned} \qquad (52)$$

$$A_0^c(\mathbf{x}) = -\sum_{\mathbf{k}} \frac{4k^3}{m^{7/2}}[a_Q^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} + a_Q^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}] - (1-\gamma)\sum_{\mathbf{k}} \frac{2k}{m^{3/2}}[a_Q^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} + a_Q^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}]$$
$$+\sum_{\mathbf{k}} \frac{m^{3/2}}{16k^2}[a_R^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} + a_R^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}] - \sum_{\mathbf{k}} \frac{k}{m\sqrt{2\omega(k)}}[a^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} + a^{c\dagger}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}], \tag{53}$$

and

$$G^c(\mathbf{x}) = \sum_{\mathbf{k}} \frac{8ik^2}{m^{3/2}}[a_Q^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} - a_Q^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}], \tag{54}$$

where $\omega(k) = \sqrt{m^2+k^2}$; and for the doublet and singlet sectors with combined topological and ''Higgs–Kibble'' mass ($c = 4, \ldots, 8$), the fields are represented by

$$A_l^c(\mathbf{x}) = -\sum_{\mathbf{k}} \sqrt{\frac{\omega_c(k)}{2\mathrm{m}_c(\mathrm{m}_c+\bar{\mathrm{m}}_c)}}\,\frac{k_l}{k}[a^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} + a^{c\dagger}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}]$$
$$+\sum_{\mathbf{k}} \sqrt{\frac{\mathrm{m}_c}{2\omega_c(k)(\mathrm{m}_c+\bar{\mathrm{m}}_c)}}\,\frac{i\epsilon_{ln}k_n}{k}[a^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} - a^{c\dagger}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}]$$
$$+\sum_{\mathbf{k}} \sqrt{\frac{\overline{\omega_c}(k)}{2\bar{\mathrm{m}}_c(\mathrm{m}_c+\bar{\mathrm{m}}_c)}}\,\frac{ik_l}{k}[b^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} - b^{c\dagger}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}]$$
$$-\sum_{\mathbf{k}} \sqrt{\frac{\bar{\mathrm{m}}_c}{2\overline{\omega_c}(k)(\mathrm{m}_c+\bar{\mathrm{m}}_c)}}\,\frac{\epsilon_{ln}k_n}{k}[b^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} + b^{c\dagger}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}]$$
$$-\sum_{\mathbf{k}} \frac{4k^3k_l}{\kappa_c(k)\mathrm{m}_c\bar{\mathrm{m}}_c(\mathrm{m}_c-\bar{\mathrm{m}}_c)^{3/2}}[a_Q^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} + a_Q^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}]$$
$$+\sum_{\mathbf{k}} \frac{(\mathrm{m}_c-\bar{\mathrm{m}}_c)^{3/2}k_l}{16k^3}[a_R^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} + a_R^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}], \tag{55}$$

$$\Pi_l^c(\mathbf{x}) = \sum_{\mathbf{k}} \sqrt{\frac{\mathrm{m}_c(\mathrm{m}_c+\bar{\mathrm{m}}_c)}{8\omega_c(k)}}\,\frac{ik_l}{k}[a^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} - a^{c\dagger}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}]$$
$$+\sum_{\mathbf{k}} \sqrt{\frac{\omega_c(k)(\mathrm{m}_c+\bar{\mathrm{m}}_c)}{8\mathrm{m}_c}}\,\frac{\epsilon_{ln}k_n}{k}[a^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} + a^{c\dagger}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}]$$
$$+\sum_{\mathbf{k}} \sqrt{\frac{\bar{\mathrm{m}}_c(\mathrm{m}_c+\bar{\mathrm{m}}_c)}{8\overline{\omega_c}(k)}}\,\frac{k_l}{k}[b^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} + b^{c\dagger}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}]$$
$$+\sum_{\mathbf{k}} \sqrt{\frac{\overline{\omega_c}(k)(\mathrm{m}_c+\bar{\mathrm{m}}_c)}{8\bar{\mathrm{m}}_c}}\,\frac{i\epsilon_{ln}k_n}{k}[b^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} - b^{c\dagger}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}]$$
$$-\sum_{\mathbf{k}} \frac{2k^3\epsilon_{ln}k_n}{\kappa_c(k)\mathrm{m}_c\bar{\mathrm{m}}_c\sqrt{\mathrm{m}_c-\bar{\mathrm{m}}_c}}[a_Q^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} + a_Q^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}]$$
$$+\sum_{\mathbf{k}} \frac{(\mathrm{m}_c-\bar{\mathrm{m}}_c)^{5/2}\epsilon_{ln}k_n}{32k^3}[a_R^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} + a_R^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}], \tag{56}$$

$$A_0^c(\mathbf{x}) = -\sum_{\mathbf{k}} \frac{k}{\sqrt{2\omega_c(k)\mathsf{m}_c(\mathsf{m}_c+\bar{\mathsf{m}}_c)}}[a^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} + a^{c\dagger}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}]$$
$$+\sum_{\mathbf{k}} \frac{ik}{\sqrt{2\bar{\omega}_c(k)\bar{\mathsf{m}}_c(\mathsf{m}_c+\bar{\mathsf{m}}_c)}}[b^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} - b^{c\dagger}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}]$$
$$-\sum_{\mathbf{k}} \frac{4k^3}{\mathsf{m}_c\bar{\mathsf{m}}_c(\mathsf{m}_c-\bar{\mathsf{m}}_c)^{3/2}}[a_Q^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} + a_Q^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}]$$
$$+\sum_{\mathbf{k}} \frac{\kappa_c(k)(\mathsf{m}_c-\bar{\mathsf{m}}_c)^{3/2}}{16k^3}[a_R^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} + a_R^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}], \tag{57}$$

and

$$G^c(\mathbf{x}) = \sum_{\mathbf{k}} \frac{8ik^3}{\kappa_c(k)(\mathsf{m}_c-\bar{\mathsf{m}}_c)^{3/2}}[a_Q^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} - a_Q^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}]. \tag{58}$$

The unphysical scalar fields for $c=4,\ldots,8$ are

$$\xi^c(\mathbf{x}) = -\sum_{\mathbf{k}} \frac{4ik^3}{\kappa_c(k)(\mathsf{m}_c\bar{\mathsf{m}}_c)^{1/2}(\mathsf{m}_c-\bar{\mathsf{m}}_c)^{3/2}}[a_Q^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} - a_Q^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}]$$
$$-\sum_{\mathbf{k}} \frac{i(\mathsf{m}_c\bar{\mathsf{m}}_c)^{1/2}(\mathsf{m}_c-\bar{\mathsf{m}}_c)^{3/2}}{16k^3}[a_R^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} - a_R^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}] \tag{59}$$

and their canonically conjugate momenta

$$\Pi_\xi^c(\mathbf{x}) = -\sum_{\mathbf{k}} k\sqrt{\frac{\bar{\mathsf{m}}_c}{2\omega_c(k)(\mathsf{m}_c+\bar{\mathsf{m}}_c)}}\,[a^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} + a^{c\dagger}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}]$$
$$+\sum_{\mathbf{k}} ik\sqrt{\frac{\mathsf{m}_c}{2\bar{\omega}_c(k)(\mathsf{m}_c+\bar{\mathsf{m}}_c)}}[b^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} - b^{c\dagger}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}]$$
$$-\sum_{\mathbf{k}} \frac{8k^3}{(\mathsf{m}_c\bar{\mathsf{m}}_c)^{1/2}(\mathsf{m}_c-\bar{\mathsf{m}}_c)^{3/2}}[a_Q^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} + a_Q^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}], \tag{60}$$

where $\omega_c(k)=\sqrt{\mathsf{m}_c^2+k^2}$, $\bar{\omega}_c(k)=\sqrt{\bar{\mathsf{m}}_c^2+k^2}$, and

$$\kappa_c(k)=\sqrt{k^2+(1-\gamma)\mathsf{m}_c\bar{\mathsf{m}}_c}. \tag{61}$$

m_c and $\bar{\mathsf{m}}_c$ are the masses of $a^c(\mathbf{k})$ and $b^c(\mathbf{k})$ modes, respectively. They are combinations of the Chern–Simons topological mass m and of the Higgs–Kibble mass m_c; their values are

$$\mathsf{m}_c = \frac{\sqrt{4M_c^2+m^2}+m}{2} \tag{62}$$

and

$$\bar{m}_c = \frac{\sqrt{4M_c^2 + m^2} - m}{2}. \tag{63}$$

The masses M_c are given by Eq. (18). The Higgs field ψ is treated as a ''standard'' Hermitian scalar field; ψ and its canonical momentum Π_ψ and represented as

$$\psi(\mathbf{x}) = \sum_{\mathbf{k}} \frac{1}{\sqrt{2\Omega(k)}} [\alpha(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{x}} + \alpha^\dagger(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{x}}] \tag{64}$$

and

$$\Pi_\psi(\mathbf{x}) = -\sum_{\mathbf{k}} i \sqrt{\frac{\Omega(k)}{2}} [\alpha(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{x}} - \alpha^\dagger(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{x}}], \tag{65}$$

where $\Omega(k)$ is given by

$$\Omega(k) = \sqrt{2\mu^2 + k^2}. \tag{66}$$

The Faddeev–Popov ghost fields are represented as[28]

$$\sigma_{\mathrm{f}}^c(\mathbf{x}) = \sum_{\mathbf{k}} \frac{1}{\sqrt{2\kappa_c(k)}} [g_{\mathrm{f}}^c(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{x}} + g_{\mathrm{f}}^{c\,\star}(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{x}}], \tag{67}$$

$$\sigma_{\mathrm{p}}^c(\mathbf{x}) = -\sum_{\mathbf{k}} \frac{i}{\sqrt{2\kappa_c(k)}} [g_{\mathrm{p}}^c(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{x}} - g_{\mathrm{p}}^{c\,\star}(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{x}}], \tag{68}$$

$$\Pi_{\mathrm{f}}^c(\mathbf{x}) = \sum_{\mathbf{k}} i \sqrt{\frac{\kappa_c(k)}{2}} [g_{\mathrm{p}}^c(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{x}} + g_{\mathrm{p}}^{c\,\star}(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{x}}], \tag{69}$$

and

$$\Pi_{\mathrm{p}}^c(\mathbf{x}) = \sum_{\mathbf{k}} \sqrt{\frac{\kappa_c(k)}{2}} [g_{\mathrm{f}}^c(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{x}} - g_{\mathrm{f}}^{c\,\star}(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{x}}], \tag{70}$$

where $g_{\mathrm{f}}^c(\mathbf{k})$, $g_{\mathrm{p}}^c(\mathbf{k})$, $g_{\mathrm{f}}^{c\,\star}(\mathbf{k})$, and $g_{\mathrm{p}}^{c\,\star}(\mathbf{k})$ obey the anticommutation rules

$$\{g_{\mathrm{f}}^a(\mathbf{k}), g_{\mathrm{p}}^{b\,\star}(\mathbf{q})\} = \{g_{\mathrm{p}}^a(\mathbf{k}), g_{\mathrm{f}}^{b\,\star}(\mathbf{q})\} = \delta^{ab}\delta_{\mathbf{kq}} \tag{71}$$

and

$$\{g_{\mathrm{f}}^a(\mathbf{k}), g_{\mathrm{f}}^{b\,\star}(\mathbf{q})\} = \{g_{\mathrm{p}}^a(\mathbf{k}), g_{\mathrm{p}}^{b\,\star}(\mathbf{q})\} = 0. \tag{72}$$

When Eqs. (55)–(70) are substituted into the Hamiltonian H_0 given in Eq. (40), we obtain the expression

$$H_0 = \sum_{c=1}^{8} H^c + H_\psi + \sum_{c=1}^{8} H_{\mathrm{fp}}^c, \tag{73}$$

where H^c is given by

$$H^c=\sum_{\mathbf{k}}\ \omega(k)a^{c\dagger}(\mathbf{k})a^c(\mathbf{k})+\sum_{\mathbf{k}}\ k[a_R^{c\star}(\mathbf{k})a_Q^c(\mathbf{k})+a_Q^{c\star}(\mathbf{k})a_R^c(\mathbf{k})]$$

$$-(1-\gamma)\sum_{\mathbf{k}}\ \frac{64k^4}{m^3}a_Q^{c\star}(\mathbf{k})a_Q^c(\mathbf{k}) \tag{74}$$

for the $c=1,2,3$ sector of unbroken SU(2) gluon triplet, and

$$H^c=\sum_{\mathbf{k}}\ [\omega_c(k)a^{c\dagger}(\mathbf{k})a^c(\mathbf{k})+\overline{\omega_c}(k)b^{c\dagger}(\mathbf{k})b^c(\mathbf{k})]$$

$$+\sum_{\mathbf{k}}\ \kappa_c(k)[a_R^{c\star}(\mathbf{k})a_Q^c(\mathbf{k})+a_Q^{c\star}(\mathbf{k})a_R^c(\mathbf{k})], \tag{75}$$

for $c=4,\ldots,8$. For the doublet ($c=4,5,6,7$) and singlet ($c=8$) sectors, m_c and $\bar{\mathsf{m}}_c$ are given by Eqs. (62) and (63), respectively; for $c=1,2,3$ there is only a single gluon mode and the mass m is the topological mass. The Higgs Hamiltonian H_ψ is given by

$$H_\psi=\sum_{\mathbf{k}}\ \Omega(k)\alpha^\dagger(\mathbf{k})\alpha(\mathbf{k}); \tag{76}$$

and the Faddeev–Popov ghost part of the Hamiltonian H_{fp}^c, by

$$H_{\mathrm{fp}}^c=\sum_{\mathbf{k}}\ \kappa_c(k)[g_{\mathrm{f}}^{c\star}(\mathbf{k})g_{\mathrm{p}}^c(\mathbf{k})+g_{\mathrm{p}}^{c\star}(\mathbf{k})g_{\mathrm{f}}^c(\mathbf{k})]. \tag{77}$$

Inspection confirms that H_0 is diagonal in the particle number for the observable, propagating particle modes (the massive gluons and the Higgs excitations) of this model and that to this extent the representations of the gauge fields have turned out to be ''suitable.'' Explicit construction of a Fock space for this model will demonstrate that the ghost components of the Hamiltonian also satisfy the suitability requirement. We can construct a Fock space $\{|h\rangle\}$ for this model, on the foundation of the perturbative vacuum $|0\rangle$ which is annihilated by all the annihilation operators: $a^c(\mathbf{k})$, $b^c(\mathbf{k})$, $a_Q^c(\mathbf{k})$ and $a_R^c(\mathbf{k})$, as well as $\alpha(\mathbf{k})$ and the Faddeev–Popov ghosts, $g_{\mathrm{f}}^c(\mathbf{k})$ and $g_{\mathrm{p}}^c(\mathbf{k})$. In this construction, we make use of techniques developed in earlier work.[19,21,26,29] This perturbative Fock space includes all multiparticle states $|N\rangle$ consisting of observable, propagating particles (Higgs particles and massive gluons) that are created when $\alpha^\dagger(\mathbf{k})$, $a^{c\dagger}(\mathbf{k})$, and $b^{c\dagger}(\mathbf{k})$, respectively, act on $|0\rangle$. All such states $|N\rangle$ are eigenstates of H_0. States, such as $a_Q^{c\star}(\mathbf{k})|N\rangle$ or $a_Q^{c\star}(\mathbf{k})a_Q^{d\star}(\mathbf{q})|N\rangle$, in which a single variety of ghost creation operator acts on one of these multiparticle states $|N\rangle$ have zero norm; they have no probability of being observed, and have vanishing expectation values of energy, momentum, as well as all other observables. We will designate as $\{|n\rangle\}$ that subspace of $\{|h\rangle\}$ which consists of all states $|N\rangle$ and of all states in which a chain of $a_Q^{c\star}(\mathbf{k})$ operators — but *no* $a_R^{c\star}(\mathbf{k})$ operators — act on $|N\rangle$. States in which both varieties of ghosts appear simultaneously, such as $a_Q^{c\star}(\mathbf{k})a_R^{d\star}(\mathbf{q})|N\rangle$, are in the Fock space $\{|h\rangle\}$, but not in $\{|n\rangle\}$; because these states have a nonvanishing norm and contain ghosts, they are not probabilistically interpretable. Their appearance in the course of time evolution signals a defect in the theory. Since the states $|N\rangle$ constitute the set of states in $\{|n\rangle\}$ from which all zero norm states (the ones with ghost constituents) have been excised, we will sometimes speak of the set of $|N\rangle$ as a quotient space of observable propagating states. The time-evolution operator $\exp(-iH_0t)$ has the important property that, if it acts on a state vector $|n_i\rangle$ in $\{|n\rangle\}$, it can only propagate it within $\{|n\rangle\}$. We observe that the only parts of H_0 that could possibly cause a state vector to leave the subspace $\{|n\rangle\}$, are those that contain either $a_R^{c\star}(\mathbf{k})$ or $a_R^c(\mathbf{k})$ operators. The only part of H_0 that has that feature contains the combination of operators

$\Gamma^c = a_R^{c\star}(\mathbf{k})a_Q^c(\mathbf{k}) + a_Q^{c\star}(\mathbf{k})a_R^c(\mathbf{k})$. When $a_R^c(\mathbf{k})$ acts on a state vector $|n_i\rangle$, it either annihilates the vacuum or annihilates one of the $a_Q^{c\star}(\mathbf{k})$ operators in $\{|n\rangle\}$. In the latter case, Γ^c replaces the annihilated $a_Q^{c\star}(\mathbf{k})$ operator with an identical one. When $a_Q^c(\mathbf{k})$ acts on a state vector $|n_i\rangle$, it always annihilates it. It is therefore impossible for Γ^c to transform a state vector in $\{|n\rangle\}$ to one external to $\{|n\rangle\}$ in which an $a_R^{c\star}(\mathbf{k})$ operator acts on $|n_i\rangle$. The only effect of Γ^c is to translate $|n_i\rangle$ states within $\{|n\rangle\}$. These features of the Hamiltonian H_0 confirm that Eqs. (51)–(60) are suitable representations of the gauge fields. H_0 counts the number of massive gluons of momentum $\mathbf{k}$ belonging to the unbroken SU(2) sector of the original SU(3) system, and assigns an energy $\omega(k)$ to each of them. It similarly counts the two varieties of massive gluons in the doublet and singlet sectors, and assigns the energy ω_c and $\overline{\omega_c}(k)$ to the $a^c(\mathbf{k})$ and $b^c(\mathbf{k})$ varieties respectively. And lastly, H_0 counts the number of Higgs particles of mass $\sqrt{2}\mu$ and assigns the energy $\sqrt{2\mu^2+k^2}$ to each. Beyond that, the form of H_0 guarantees that any state vector initially in $\{|n\rangle\}$ is propagated by $\exp(-iH_0t)$ entirely within $\{|n\rangle\}$.

We next turn to the implementation of Gauss's law and the gauge condition. We have previously noted in Eqs. (45)–(46) that Gauss's law, $\mathcal{G}^a(\mathbf{x})=0$, is not a consequence of the Euler–Lagrange equations, and that further analysis is required to demonstrate that it is properly implemented. We further observe that, when Eqs. (51)–(70) are substituted into Eq. (46), $\mathcal{G}^a$ turns out to be a linear combination of only those ghost excitations that can live in the subspace $\{|n\rangle\}$ — $a_Q^a(\mathbf{k})$ and $a_Q^{a\star}(\mathbf{k})$. All other excitation operators — $a_R^a(\mathbf{k})$ and $a_R^{a\star}(\mathbf{k})$, and the annihilation and creation operators for both varieties of propagating particles, $a^c(\mathbf{k})$ and $b^c(\mathbf{k})$ as well as $a^{c\dagger}(\mathbf{k})$ and $b^{c\dagger}(\mathbf{k})$, respectively — cancel in $\mathcal{G}^a$. The explicit expression for $\mathcal{G}^a$ obtained from this substitution is

$$\mathcal{G}^a(\mathbf{x}) = \sum_{\mathbf{k}} \frac{8k^3}{m^{3/2}}[a_Q^a(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} + a_Q^{a\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}]. \tag{78}$$

The implementation of Gauss's law is an immediate consequence of this expression for $\mathcal{G}^a$. A state vector that describes an observable state is one of the $|N\rangle$ states in the quotient space discussed earlier. The time evolution generated by $\exp(-iH_0t)$ has previously been shown to keep any state vector that initially was an $|N\rangle$ state contained in the subspace $\{|n\rangle\}$. And the Gauss's law operator $\mathcal{G}^a$, as well as any other operator that is a linear combination of $a_Q^a(\mathbf{k})$ and $a_Q^{a\star}(\mathbf{k})$ operators, must vanish in $\{|n\rangle\}$. These facts provide for the permanent validity of Gauss's law as long as the state vector representing the system is initially one of the $|N\rangle$ states — even a state in $\{|n\rangle\}$ will suffice — and provided that $\exp(-iH_0t)$ is the time-evolution operator for the system. Similarly, G^c is also represented as a superposition of $a_Q^c(\mathbf{k})$ and $a_Q^{c\star}(\mathbf{k})$ ghost excitation operators only, so that $\langle n_b|G^c|n_a\rangle = 0$ for the same reason that $\langle n_b|\mathcal{G}^c|n_a\rangle = 0$. Equation (23) therefore shows that in the subspace $\{|n\rangle\}$, the t'Hooft gauge condition, $\partial_\mu A^{a\mu} - (1-\gamma)\alpha^a = 0$, holds. We thus have shown not only that the time-displacement operator $\exp(-iH_0t)$ keeps state vectors permanently within the subspace $\{|n\rangle\}$, but that it is also precisely in this subspace that Gauss's law and the gauge condition are permanently implemented.

It is apparent that the explicit representations of the fields we have given in Eqs. (55)–(60) are instrumental in obtaining the results we have demonstrated above. But the confirmation of the particle mode content of these fields that the self-consistency of this formulation provides is not weakened by its dependence on an explicit representation of the fields. A representation in terms of creation and annihilation operators, and the choice of a Hilbert space in which to embed the formalism — in this case the Fock spaces $\{|n\rangle\}$ and $\{|h\rangle\}$ — are inevitably important parts of the axiomatic structure of the theory. And it is a significant fact that a representation of the operator-valued fields and a Fock space have been found that permit a consistent interpretation of H_0 as a kinetic energy operator for a system of noninteracting particles in a new vacuum state, even though part of the interaction described by $\mathcal{L}$ is included in H_0. Moreover, a Fock space has been constructed within which H_0 time displaces state vectors so that unitarity, Gauss's law, and the

gauge condition are all permanently guaranteed. It should be noted that when *all* interactions are included in a *complete* Hamiltonian H, these conditions no longer apply. Under the influence of the time-evolution operator $\exp(-iHt)$, state vectors ''leak out'' of $\{|n\rangle\}$, and probabilistically uninterpretable state vectors that contain combination of ghosts, for example $a_Q^{c\star}(\mathbf{k})a_R^{d\star}(\mathbf{q})|N\rangle$, develop. Combinations of Faddeev–Popov ghosts are then necessary to compensate for such combinations of Q and R ghosts,[28] and loops of Faddeev–Popov ghost play an important role in maintaining the unitarity of the theory. One reason for the interpretability of this model is that the ''interaction-free'' limit we have described — the limit as $e\to 0$ and $h\to 0$ while e^2/h remains constant — leads to an essentially Abelian theory. The fact that $[\mathcal{G}^a(\mathbf{x}),\mathcal{G}^b(\mathbf{y})]=0$ confirms that observation. In a non-Abelian theory this commutator would not vanish, but would regenerate the Gauss's law operator $\mathcal{G}^c(\mathbf{x})$ in a pattern determined by the structure constants of the corresponding Lie group. Because of the Abelian nature of this limiting form of the theory, the Faddeev–Popov ghosts are not required in this stage of the work, and have not been included in the Fock space $\{|h\rangle\}$ or $\{|n\rangle\}$.

The more general question that pertains to the containment of the particle modes of the Heisenberg fields — i.e., the fields in the fully interacting theory — in a suitably defined subspace within which unitarity is preserved, is beyond our scope in this paper. In the simpler case of an Abelian gauge theory with a spontaneously broken gauge symmetry, the unitarity of the fully interacting theory has been resolved in earlier work.[22] In the case of non-Abelian gauge theories in axial gauges, in which Faddeev–Popov ghosts are not required, this demonstration has also been given.[30,31] The demonstration of unitarity of the S-matrix for Yang–Mills theory in covariant gauges has also been discussed elsewhere.[28] For non-Abelian theories in covariant gauges the demonstration of unitarity demands extensive algebraic manipulations, and is not pertinent to the main point of this work — the identification of the particle modes generated by the spontaneous breaking of the gauge theory of this model.

IV. THE PERTURBATIVE THEORY

The propagator for the gauge field is given by

$$D_{\mu\nu}(x_1,x_2)=\langle 0|\mathsf{T}[A_\mu(x_1),A_\nu(x_2)]|0\rangle, \tag{79}$$

where T designates time ordering, $A_\mu(x)$ is the interaction-picture field

$$A_\mu(x)=e^{iH_0t}A_\mu(\mathbf{x})e^{-iH_0t}, \tag{80}$$

$A_\mu(\mathbf{x})$ is the Schrödinger picture field, and $|0\rangle$ is the vacuum state of the $\{|n\rangle\}$ space. Similarly, the propagator for an unphysical scalar $\xi(x)$ is

$$\Delta_\xi(x_1,x_2)=\langle 0|\mathsf{T}[\xi(x_1),\xi(x_2)]|0\rangle, \tag{81}$$

and, for the Higgs field,

$$\Delta_\psi(x_1,x_2)=\langle 0|\mathsf{T}[\psi(x_1),\psi(x_2)]|0\rangle. \tag{82}$$

There are other propagators in this theory, but they vanish for $\gamma=1$ (Landau gauge) which we use in our work, and therefore are not of primary interest to us. We find that the relevant interaction-picture fields for $c=1,2,3$ are

$$A_l^c(x)=\sum_{\mathbf{k}}\frac{8ik\epsilon_{ln}k_n}{m^{5/2}}[a_Q^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}-ikt}-a_Q^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}+ikt}]$$
$$+(1-\gamma)\sum_{\mathbf{k}}\frac{2k_l}{m^{3/2}}[a_Q^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}-ikt}+a_Q^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}+ikt}]$$
$$-\sum_{\mathbf{k}}\frac{4k^2k_l}{m^{7/2}}[a_Q^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}-ikt}+a_Q^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}+ikt}]$$
$$+\sum_{\mathbf{k}}\frac{m^{3/2}k_l}{16k^3}[a_R^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}-ikt}+a_R^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}+ikt}]$$
$$-\sum_{\mathbf{k}}\frac{\sqrt{\omega(k)}k_l}{\sqrt{2}mk}[a^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}-i\omega(k)t}+a^{c\dagger}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}+i\omega(k)t}]$$
$$+\sum_{\mathbf{k}}\frac{i\epsilon_{ln}k_n}{k\sqrt{2\omega(k)}}[a^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}-i\omega(k)t}-a^{c\dagger}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}+i\omega(k)t}] \tag{83}$$

and

$$A_0^c(\mathbf{x})=-\sum_{\mathbf{k}}\frac{4k^3}{m^{7/2}}[a_Q^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}-ikt}+a_Q^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}+ikt}]$$
$$-(1-\gamma)\sum_{\mathbf{k}}\frac{2k}{m^{3/2}}[a_Q^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}-ikt}+a_Q^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}+ikt}]$$
$$+\sum_{\mathbf{k}}\frac{m^{3/2}}{16k^2}[a_R^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}-ikt}+a_R^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}+ikt}]$$
$$-\sum_{\mathbf{k}}\frac{k}{m\sqrt{2\omega(k)}}[a^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}-i\omega(k)t}+a^{c\dagger}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}+i\omega(k)t}]; \tag{84}$$

for $c=4,\ldots,8$, they are

$$A_l^c(x)=-\sum_{\mathbf{k}}\sqrt{\frac{\omega_c(k)}{2\mathrm{m}_c(\mathrm{m}_c+\bar{\mathrm{m}}_c)}}\frac{k_l}{k}[a^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}-i\omega_c(k)t}+a^{c\dagger}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}+i\omega_c(k)t}]$$
$$+\sum_{\mathbf{k}}\sqrt{\frac{\mathrm{m}_c}{2\omega_c(k)(\mathrm{m}_c+\bar{\mathrm{m}}_c)}}\frac{i\epsilon_{ln}k_n}{k}[a^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}-i\omega_c(k)t}-a^{c\dagger}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}+i\omega_c(k)t}]$$
$$+\sum_{\mathbf{k}}\sqrt{\frac{\overline{\omega_c}(k)}{2\bar{\mathrm{m}}_c(\mathrm{m}_c+\bar{\mathrm{m}}_c)}}\frac{ik_l}{k}[b^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}-i\overline{\omega_c}(k)t}-b^{c\dagger}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}+i\overline{\omega_c}(k)t}]$$
$$-\sum_{\mathbf{k}}\sqrt{\frac{\bar{\mathrm{m}}_c}{2\overline{\omega_c}(k)(\mathrm{m}_c+\bar{\mathrm{m}}_c)}}\frac{\epsilon_{ln}k_n}{k}[b^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}-i\overline{\omega_c}(k)t}+b^{c\dagger}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}+i\overline{\omega_c}(k)t}]$$
$$-\sum_{\mathbf{k}}\frac{4k^3k_l}{\kappa_c(k)\mathrm{m}_c\bar{\mathrm{m}}_c(\mathrm{m}_c-\bar{\mathrm{m}}_c)^{3/2}}[a_Q^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}-i\kappa_c(k)t}+a_Q^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}+i\kappa_c(k)t}]$$
$$+\sum_{\mathbf{k}}\frac{(\mathrm{m}_c-\bar{\mathrm{m}}_c)^{3/2}k_l}{16k^3}[a_R^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}-i\kappa_c(k)t}+a_R^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}+i\kappa_c(k)t}], \tag{85}$$

$$A_0^c(x) = -\sum_{\mathbf{k}} \frac{k}{\sqrt{2\omega_c(k)\mathrm{m}_c(\mathrm{m}_c+\bar{\mathrm{m}}_c)}}[a^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}-i\omega_c(k)t} + a^{c\dagger}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}+i\omega_c(k)t}]$$
$$+\sum_{\mathbf{k}} \frac{ik}{\sqrt{2\bar{\omega}_c(k)\bar{\mathrm{m}}_c(\mathrm{m}_c+\bar{\mathrm{m}}_c)}}[b^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}-i\bar{\omega}_c(k)t} - b^{c\dagger}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}+i\bar{\omega}_c(k)t}]$$
$$-\sum_{\mathbf{k}} \frac{4k^3}{\mathrm{m}_c\bar{\mathrm{m}}_c(\mathrm{m}_c-\bar{\mathrm{m}}_c)^{3/2}}[a_Q^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}-i\kappa_c(k)t} + a_Q^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}+i\kappa_c(k)t}]$$
$$+\sum_{\mathbf{k}} \frac{\kappa_c(k)(\mathrm{m}_c-\bar{\mathrm{m}}_c)^{3/2}}{16k^3}[a_R^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}-i\kappa_c(k)t} + a_R^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}-i\kappa_c(k)t}], \tag{86}$$

$$\xi^c(x) = -\sum_{\mathbf{k}} \frac{4ik^3}{\kappa_c(k)(\mathrm{m}_c\bar{\mathrm{m}}_c)^{1/2}(\mathrm{m}_c-\bar{\mathrm{m}}_c)^{3/2}}[a_Q^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}-i\kappa_c(k)t} - a_Q^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}+i\kappa_c(k)t}]$$
$$-\sum_{\mathbf{k}} \frac{i(\mathrm{m}_c\bar{\mathrm{m}}_c)^{1/2}(\mathrm{m}_c-\bar{\mathrm{m}}_c)^{3/2}}{16k^3}[a_R^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}-i\kappa_c(k)t} - a_R^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}+i\kappa_c(k)t}], \tag{87}$$

and

$$\psi(x) = \sum_{\mathbf{k}} \frac{1}{\sqrt{2\Omega(k)}}[\alpha(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}-i\Omega(k)t} + \alpha^{\dagger}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}+i\Omega(k)t}]. \tag{88}$$

The Faddeev–Popov ghost fields are

$$\sigma_{\mathrm{f}}^c(x) = \sum_{\mathbf{k}} \frac{1}{\sqrt{2\kappa_c(k)}}[g_{\mathrm{f}}^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}-i\kappa_c(k)t} - g_{\mathrm{f}}^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}+i\kappa_c(k)t}] \tag{89}$$

and

$$\sigma_{\mathrm{p}}^c(x) = \sum_{\mathbf{k}} \frac{i}{\sqrt{2\kappa_c(k)}}[g_{\mathrm{p}}^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}-i\kappa_c(k)t} - g_{\mathrm{p}}^{c\star}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}+i\kappa_c(k)t}]. \tag{90}$$

The propagators for the gauge fields can be expressed as

$$D_{\mu\nu}^{ab}(x_1,x_2) = -i\delta^{ab}\int \frac{d^3k}{(2\pi)^3} D_{\mu\nu}^{(a)}(k)e^{-ik^{\alpha}(x_1-x_2)_{\alpha}}; \tag{91}$$

for $a=1,2,3$:

$$D_{\mu\nu}^{(a)}(k) = (1-\gamma)\frac{k_\mu k_\nu}{(k^\alpha k_\alpha + i\epsilon)^2} - \frac{k_\mu k_\nu}{(k^\alpha k_\alpha + i\epsilon)(k^\alpha k_\alpha - m^2 + i\epsilon)}$$
$$+\frac{g_{\mu\nu}}{k^\alpha k_\alpha - m^2 + i\epsilon} + \frac{im\epsilon_{\mu\nu\lambda}k^\lambda}{(k^\alpha k_\alpha + i\epsilon)(k^\alpha k_\alpha - m^2 + i\epsilon)}; \tag{92}$$

and for $a=4,\ldots,8$:

$$D^{(a)}_{\mu\nu}(k)=\frac{(k^\alpha k_\alpha-\mathsf{m}_a\bar{\mathsf{m}}_a)g_{\mu\nu}}{(k^\alpha k_\alpha-\mathsf{m}_a^2+i\epsilon)(k^\alpha k_\alpha-\bar{\mathsf{m}}_a^2+i\epsilon)}+\frac{i(\mathsf{m}_a-\bar{\mathsf{m}}_a)\epsilon_{\mu\nu\rho}k^\rho}{(k^\alpha k_\alpha-\mathsf{m}_a^2+i\epsilon)(k^\alpha k_\alpha-\bar{\mathsf{m}}_a^2+i\epsilon)}$$
$$-\frac{\gamma(k^\alpha k_\alpha-\mathsf{m}_a\bar{\mathsf{m}}_a k_\mu k_\nu}{[k^\alpha k_\alpha-(1-\gamma)\mathsf{m}_a\bar{\mathsf{m}}_a+i\epsilon](k^\alpha k_\alpha-\mathsf{m}_a^2+i\epsilon)(k^\alpha k_\alpha-\bar{\mathsf{m}}_a^2+i\epsilon)}$$
$$-\frac{(1-\gamma)(\mathsf{m}_a-\bar{\mathsf{m}}_a{}^2k_\mu k_\nu}{[k^\alpha k_\alpha-(1-\gamma)\mathsf{m}_a\bar{\mathsf{m}}_a+i\epsilon](k^\alpha k_\alpha-\mathsf{m}_a^2+i\epsilon)(k^\alpha k_\alpha-\bar{\mathsf{m}}_a^2+i\epsilon)}. \tag{93}$$

These expressions agree with the gauge field propagators reported in Ref. 9 for $a=1,2,3$ and with Refs. 4, 5, and 18 for $a=4,\ldots,8$. These propagators were obtained by inverting the quadratic part of the gauge-fixed Lagrangian. The other propagators are given in terms of the Fourier integral

$$\Delta(x_1,x_2)=-i\int\frac{d^3k}{(2\pi)^3}\Delta(k^2)e^{-ik^\alpha(x_1-x_2)_\alpha}, \tag{94}$$

where

$$\Delta_\psi(k^2)=\frac{-1}{k^\alpha k_\alpha-2\mu^2+i\epsilon}, \tag{95}$$

$$\Delta^{(a)}_\xi(k^2)=\frac{-\delta^{ab}}{k^\alpha k_\alpha-(1-\gamma)\mathsf{m}_a\bar{\mathsf{m}}_a+i\epsilon}, \tag{96}$$

and

$$\Delta^{(a)}_{\rm fp}(k^2)=\frac{-\delta^{ab}}{k^\alpha k_\alpha-(1-\gamma)\mathsf{m}_a\bar{\mathsf{m}}_a+i\epsilon}. \tag{97}$$

In a canonical theory, the vertices are dictated by the interaction Hamiltonian $H_{\rm int}$. Since, in this model, time derivatives of operator-valued fields appear in the interaction Lagrangian as well as in $\mathcal{L}_0$, $H_{\rm int}$ will differ from $-\int d\mathbf{x}(\mathcal{L}_1+\mathcal{L}_2)$. The resulting vertices will be determined by $H_{\rm int}$, and the propagators will consist of vacuum expectation values of the time-ordered fields that appear in $H_{\rm int}$. In expanding the S-matrix for scattering from an initial state $|i\rangle$ to a final state $|f\rangle$,

$$S_{fi}=\langle f|\mathsf{T}\exp\left(-i\int dt\ e^{iH_0t}H_{\rm int}e^{-iH_0t}\right)|i\rangle, \tag{98}$$

by using the Wick theorem,[32] we will sometimes encounter time-ordered products of fields and, at other times, time-ordered products of space–time derivatives of fields. When time derivatives of fields appear as arguments of a time-ordering operation, we will replace the time-ordering operator T with the ''T-star ordering'' operator T^* which is defined so that any derivatives acting on time-ordered fields are to be taken only *after* time ordering has been carried out. In transforming T-ordered to T^*-ordered fields, additional terms are generated, which contain the $\delta(x_0-y_0)$ that is produced when time derivatives are extracted from T-ordered products of time-differentiated fields. As was pointed out by Matthews, these extra terms in which $\delta(x_0-y_0)$-functions appear just cancel the difference between $H_{\rm int}$ and $-\int d\mathbf{x}(\mathcal{L}_1+\mathcal{L}_2)$, so that the perturbative theory requires only the propagators given in Eqs. (91)–(96) and the vertices dictated by the interaction

Lagrangian.[33] Application of the Matthews rule to a model with a spontaneously broken gauge symmetry that produces massive gauge excitations also applies to this case.[22]

V. POINCARÉ STRUCTURE AND LORENTZ TRANSFORMATIONS OF MASSIVE GAUGE BOSONS

In this section we will construct the six canonical Poincaré generators in $2+1$ dimensions: the time-evolution operator, $P_0=H_0$; the two-component space-displacement operator P_l; the (scalar) rotation operator J; and the two-component Lorentz boost K_l. We will also use the Lorentz boost generators to transform the single-particle massive gauge boson states, to display their properties under Lorentz transformations as well as to obtain further confirmation of the consistency of our canonical formulation of this model.

The canonical Poincaré generators for this model are: $P_0=\int d\mathbf{x}\mathcal{P}_0(\mathbf{x})$, where $\mathcal{P}_0=\mathcal{H}_0$ with $\mathcal{H}_0$ given by Eq. (40);

$$P_l=\int d\mathbf{x}\mathcal{P}_l(\mathbf{x}), \tag{99}$$

where

$$\mathcal{P}_l=-\Pi_\xi\partial_l\xi-\Pi_n\partial_lA_n+G\partial_lA_0-\Pi_\psi\partial_l\psi-\Pi_{\mathrm{f}}\partial_l\sigma_{\mathrm{f}}-\Pi_{\mathrm{p}}\partial_l\sigma_{\mathrm{p}}; \tag{100}$$

$$J=\int d\mathbf{x}\epsilon_{ln}x_l\mathcal{P}_n(\mathbf{x})+\int d\mathbf{x}\kappa_{\mathrm{rotation}}(\mathbf{x}) \tag{101}$$

and

$$K_l=x_0P_l-\int d\mathbf{x}\; x_l\mathcal{P}_0(\mathbf{x})+\int d\mathbf{x}\;\kappa_l^{\mathrm{boost}}(\mathbf{x}) \tag{102}$$

where

$$\kappa_{\mathrm{rotation}}=\epsilon_{ln}A_l\Pi_n \tag{103}$$

and

$$\kappa_l^{\mathrm{boost}}=-A_lG+A_0\Pi_l. \tag{104}$$

The term $\kappa_{\mathrm{rotation}}$ implements the mixing of the space components of the fields during a rotation. It arises from the fact that, under an infinitesimal rotation $\delta\theta$ about an axis perpendicular to the 2-D plane, the components of A^μ transform as follows:

$$\delta A_l(\mathbf{x})=-[\epsilon_{ij}x_i\partial_jA_l(\mathbf{x})+\epsilon_{ln}A_n(\mathbf{x})]\delta\theta \tag{105}$$

and

$$\delta A_0(\mathbf{x})=-\epsilon_{ij}x_i\partial_jA_0(\mathbf{x})\,\delta\theta. \tag{106}$$

Under an infinitesimal boost $\delta\beta_l$ along the l-direction, the components of A^μ transform as follows

$$\delta A_0(\mathbf{x})=-[x_0\partial_lA_0(\mathbf{x})+x_l\partial_0A_0(\mathbf{x})-A_l(\mathbf{x})]\delta\beta_l \tag{107}$$

and

$$\delta A_i(\mathbf{x})=-[x_0\partial_lA_i(\mathbf{x})+x_l\partial_0A_i(\mathbf{x})-\delta_{il}A_0(\mathbf{x})]\delta\beta_l. \tag{108}$$

Use of the canonical commutation rules leads to the following commutation rules for the Poincaré generators:

$$[P_l,P_n]=0, \tag{109}$$

$$[H,P_l]=[H,J]=0, \tag{110}$$

$$[H,K_l]=iP_l, \tag{111}$$

$$[P_l,K_n]=i\delta_{ln}H, \tag{112}$$

$$[P_l,J]=-i\epsilon_{ln}P_n, \tag{113}$$

$$[J,K_l]=i\epsilon_{ln}K_n, \tag{114}$$

and

$$[K_l,K_n]=-i\epsilon_{ln}J. \tag{115}$$

We observe that these commutation rules form a closed Lie algebra, and that they are consistent with the transformations given in Eqs. (105)–(108).

To facilitate this investigation of the Lorentz transformation of states that are eigenstates to H_0, we shift to a description of excitation operators that have an invariant norm under Lorentz transformations. We observe, for example, that the norm of the one-particle state $a^{c\dagger}(\mathbf{k})|0\rangle$,

$$|a^{c\dagger}(\mathbf{k})|0\rangle^2=\sum_{\mathbf{q}}\langle 0|[a^c(\mathbf{q}),a^{c\dagger}(\mathbf{k})]|0\rangle=\int d\mathbf{q}\ \delta(\mathbf{k}-\mathbf{q}), \tag{116}$$

is not a Lorentz scalar because $d\mathbf{k}$ is not the Lorentz invariant measure for the phase space. The invariant measure can be established by noting that the invariant delta function

$$\delta(\mathbf{k}-\mathbf{q})\,\delta(k_0-q_0)\,\delta(q_\mu q^\mu-\mathsf{m}_c^2)\Theta(q_0)=\frac{\delta(\mathbf{k}-\mathbf{q})\,\delta[k_0-\omega_c(k)]}{2\omega_c(k)}, \tag{117}$$

so that the states $A^{c\dagger}(\mathbf{k})|0\rangle$, created by operators that obey

$$[A^c(\mathbf{k}),A^{d\dagger}(\mathbf{q})]=2\omega_c(k)(2\pi)^2\delta^{cd}\delta(\mathbf{k}-\mathbf{q}), \tag{118}$$

have unit norms in every Lorentz frame. Similarly, the normalized operators for the other modes of the gauge field obey

$$[B^c(\mathbf{k}),B^{d\dagger}(\mathbf{q})]=2\overline{\omega_c}(k)(2\pi)^2\delta^{cd}\delta(\mathbf{k}-\mathbf{q}); \tag{119}$$

and the equivalently normalized ghost operators satisfy

$$[A_Q^c(\mathbf{k}),A_R^{d\star}(\mathbf{q})]=[A_R^c(\mathbf{k}),A_Q^{d\star}(\mathbf{q})]=2\kappa_c(k)(2\pi)^2\delta^{cd}\delta(\mathbf{k}-\mathbf{q}). \tag{120}$$

The normalized operators corresponding to the mode $\alpha(\mathbf{k})$ of the Higgs field and the two Faddeev–Papov ghosts $g_{\mathrm{f}}^a(\mathbf{k})$ and $g_{\mathrm{p}}^a(\mathbf{k})$ are given by $\hat{\alpha}(\mathbf{k})$, $\hat{g}_{\mathrm{f}}^a(\mathbf{k})$, and $\hat{g}_{\mathrm{p}}^a(\mathbf{k})$, respectively. These normalized operators satisfy the following commutation and anticommutation relations:

$$[\hat{\alpha}(\mathbf{k}),\hat{\alpha}^\dagger(\mathbf{q})]=2\Omega(k)(2\pi)^2\delta(\mathbf{k}-\mathbf{q}) \tag{121}$$

and

$$\{\hat{g}^a_{\rm f}(\mathbf{k}),\hat{g}^{b\,\star}_{\rm p}(\mathbf{q})\}=\{\hat{g}^a_{\rm p}(\mathbf{k}),\hat{g}^{b\,\star}_{\rm f}(\mathbf{q})\}=2\kappa_a(k)(2\pi)^2\delta^{ab}\delta(\mathbf{k}-\mathbf{q}). \tag{122}$$

Hence, the boost operator K_l is written as

$$\begin{aligned}
K_l=&\sum_{c=1}^{8}\sum_{\mathbf{k}}\frac{\mathsf{m}_c\epsilon_{ln}k_n}{2k^2\omega_c(k)}A^{c\dagger}(\mathbf{k})A^c(\mathbf{k})-\sum_{c=4}^{8}\sum_{\mathbf{k}}\frac{\bar{\mathsf{m}}_c\epsilon_{ln}k_n}{2k^2\overline{\omega_c}(k)}B^{c\dagger}(\mathbf{k})B^c(\mathbf{k})\\
&+\sum_{c=1}^{8}\sum_{\mathbf{k}}\frac{i}{4}\left[\frac{\partial}{\partial k_l}A^{c\dagger}(\mathbf{k})A^c(\mathbf{k})-A^{c\dagger}(\mathbf{k})\frac{\partial}{\partial k_l}A^c(\mathbf{k})\right]\\
&+\sum_{c=4}^{8}\sum_{\mathbf{k}}\frac{i}{4}\left[\frac{\partial}{\partial k_l}B^{c\dagger}(\mathbf{k})B^c(\mathbf{k})-B^{c\dagger}(\mathbf{k})\frac{\partial}{\partial k_l}B^c(\mathbf{k})\right]\\
&+\sum_{c=4}^{8}\sum_{\mathbf{k}}\frac{i}{4}\left[\frac{\partial}{\partial k_l}\hat{\alpha}^{c\dagger}(\mathbf{k})\hat{\alpha}^c(\mathbf{k})-\hat{\alpha}^{c\dagger}(\mathbf{k})\frac{\partial}{\partial k_l}\hat{\alpha}^c(\mathbf{k})\right]\\
&+\sum_{c=1}^{8}\sum_{\mathbf{k}}\frac{i}{2}\left[\frac{\partial}{\partial k_l}A^{c\,\star}_Q(\mathbf{k})A^c_R(\mathbf{k})-A^{c\,\star}_R(\mathbf{k})\frac{\partial}{\partial k_l}A^c_Q(\mathbf{k})\right]\\
&+\sum_{c=1}^{8}\sum_{\mathbf{k}}\frac{i}{2}\left[\frac{\partial}{\partial k_l}\hat{g}^{c\,\star}_{\rm f}(\mathbf{k})\hat{g}^c_{\rm p}(\mathbf{k})-\hat{g}^{c\,\star}_{\rm p}(\mathbf{k})\frac{\partial}{\partial k_l}\hat{g}^c_{\rm f}(\mathbf{k})\right]\\
&+\sum_{c=1}^{8}\sum_{\mathbf{k}}\frac{5ik_l}{4k^2}[A^{c\,\star}_Q(\mathbf{k})A^c_R(\mathbf{k})-A^{c\,\star}_R(\mathbf{k})A^c_Q(\mathbf{k})]\\
&-(1-\gamma)\sum_{c=1}^{3}\sum_{\mathbf{k}}\frac{16ik^3}{m^3}\left[\frac{\partial}{\partial k_l}A^{c\,\star}_Q(\mathbf{k})A^c_Q(\mathbf{k})-A^{c\,\star}_Q(\mathbf{k})\frac{\partial}{\partial k_l}A^c_Q(\mathbf{k})\right].
\end{aligned} \tag{123}$$

Using the commutations rules given by Eqs. (118) and (119), we find that

$$\delta A^{c\dagger}(\mathbf{k})=\left[\frac{i\mathsf{m}_c\epsilon_{ln}k_n}{k^2}A^{c\dagger}(\mathbf{k})-\omega_c(k)\frac{\partial}{\partial k_l}A^{c\dagger}(\mathbf{k})\right]\delta\beta_l \tag{124}$$

and

$$\delta B^{c\dagger}(\mathbf{k})=\left[-\frac{i\bar{\mathsf{m}}_c\epsilon_{ln}k_n}{k^2}B^{c\dagger}(\mathbf{k})-\overline{\omega_c}(k)\frac{\partial}{\partial k_l}B^{c\dagger}(\mathbf{k})\right]\delta\beta_l. \tag{125}$$

Equations (124) and (125) show that all the massive gauge boson states — the single excitation mode $A^{c\dagger}(\mathbf{k})|0\rangle$ in the $(c=1,2,3)$ sectors with the residual SU(2) invariance, and the two excitation modes $A^{c\dagger}(\mathbf{k})|0\rangle$ and $B^{c\dagger}(\mathbf{k})|0\rangle$ in the $(c=4,\ldots,8)$ 'broken' doublet and singlet sectors — transform *without any mixing* with other modes. The phase factors $(\mathsf{m}_c\epsilon_{ln}k_n/k^2)\delta\beta_l$ and $-(\bar{\mathsf{m}}_c\epsilon_{ln}k_n/k^2)\delta\beta_l$ generated by the boost operator K_l, which appear in Eqs. (124) and (125), are the cocycles mentioned in Ref. 21. These phase factors have no physical implications. The physically observable consequence of Eqs. (124) and (125) is that, under a Lorentz transformation, the topologically massive gauge excitations behave like the massive excitations of a scalar field — each topologically massive gauge excitation transforms only into itself at a new space–time point.

VI. CONCLUSION

In this paper we have presented a detailed analysis of the canonical quantization of spontaneously broken topologically massive gauge theory. In $2+1$ dimensions the possibility of including a CS term in the gauge field Lagrangian leads to new forms of mass-generating effects for gauge fields. The resulting CSH mechanism differs in interesting ways from the conventional Higgs–Kibble mechanism, and in this paper we have explored the CSH mechanism by concentrating on the relation between the quantized fields and their particle excitation modes. We have found, by a series of unitary transformations, a consistent particle-mode representation of the operator-valued fields and we have constructed the corresponding Fock space which permits a consistent interpretation of the diagonalized noninteracting Hamiltonian H_0 as an energy operator for a system of noninteracting particles in a new vacuum state. Within this Fock space, H_0 acts unitarily as a time-translation generator, in such a way that Gauss's law and the gauge condition are manifestly preserved. We have computed the gauge field propagators as vacuum expectation values of time-ordered products of the gauge field operators, and formulated the corresponding perturbative expansion of the interacting theory. We have chosen to present our analysis for a non-Abelian Chern–Simons theory in which the original non-Abelian symmetry is spontaneously broken, but with a residual non-Abelian symmetry in the broken vacuum. Such a non-Abelian model clearly illustrates the interplay of the space–time and algebraic features of the CSH mechanism. This particular model is also motivated by the question of its quantum consistency. Indeed, the result reported in Ref. 17, that the bare quantum consistency condition of Deser–Jackiw–Templeton[2] is maintained at one-loop in such a broken vacuum, was in fact first obtained by us using the techniques and formalism described in this paper. An interesting further application would be to the analysis of the non-Abelian versions of the self-dual CSH systems considered in Ref. 34.

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APPENDIX: INTERACTION LAGRANGIAN

In this Appendix, we record the explicit expansions of the interaction Lagrangians $\mathcal{L}_1$ and $\mathcal{L}_2$ in terms of real fields. These interaction Lagrangians define the vertices required for perturbative computations. When the Lagrangians given in Eqs. (13) and (14) are expanded in terms of the real fields in Eq. (15) and the symmetry breaking mass scales in Eq. (18), we obtain the following: the $\mathcal{O}(e)$ interaction Lagrangian becomes

$$
\begin{aligned}
\mathcal{L}_1 = {} & e f^{abc} F^a_{\mu\nu} A^{b\mu} A^{c\nu} - \frac{1}{3} e m \epsilon^{\mu\nu\rho} f^{abc} A^a_\mu A^b_\nu A^c_\rho + \sum_{a=4}^{7} e M_{\mathrm{D}} A^{a\mu} A^a_\mu \psi + \frac{2e}{\sqrt{3}} M_{\mathrm{S}} A^{8\mu} A^8_\mu \psi \\
& + e M_{\mathrm{D}} d^{ab4} A^{a\mu} A^b_\mu \xi^5 - e M_{\mathrm{D}} d^{ab5} A^{a\mu} A^b_\mu \xi^4 + e M_{\mathrm{D}} d^{ab6} A^{a\mu} A^b_\mu \xi^7 - e M_{\mathrm{D}} d^{ab7} A^{a\mu} A^b_\mu \xi^6 \\
& - ie[\Psi_1^\dagger \mathbf{A}^\mu \cdot \boldsymbol{\tau} \partial_\mu \Psi_1 - (\partial_\mu \Psi_1)^\dagger \mathbf{A}^\mu \cdot \boldsymbol{\tau} \Psi_1] \\
& - ie[\Psi_2^\dagger (A^{4\mu}\tau^1 + A^{5\mu}\tau^2) \partial_\mu \Psi_2 - (\partial_\mu \Psi_2)^\dagger (A^{4\mu}\tau^1 + A^{5\mu}\tau^2) \Psi_2] \\
& - ie[\Psi_3^\dagger (A^{6\mu}\tau^1 + A^{7\mu}\tau^2) \partial_\mu \Psi_3 - (\partial_\mu \Psi_3)^\dagger (A^{6\mu}\tau^1 + A^{7\mu}\tau^2) \Psi_3] \\
& - ie(\Phi'^\dagger A^{8\mu} \lambda^8 \partial_\mu \Phi' - \partial_\mu \Phi'^\dagger A^{8\mu} \lambda^8 \Phi') \\
& - \frac{e\mu^2}{M_{\mathrm{D}}} \psi[(\xi^4)^2 + (\xi^5)^2 + (\xi^6)^2 + (\xi^7)^2 + (\xi^8)^2 + \psi^2]
\end{aligned}
$$

$$
\begin{aligned}
&-2ief^{abc}A^a_\mu\sigma^b_{\rm f}\partial^\mu\sigma^c_{\rm p}-ie(1-\gamma)\\
&\times M_{\rm D}\sum_{a=4}^{7}\psi\sigma^a_{\rm f}\sigma^a_{\rm p}-ie(1-\gamma)\frac{2}{\sqrt{3}}M_{\rm S}\psi\sigma^8_{\rm f}\sigma^8_{\rm p}\\
&-ie(1-\gamma)\sum_{a,b,c=4}^{8}M_{(a)}f^{abc}\xi^a\sigma^b_{\rm f}\sigma^c_{\rm p}-ie(1-\gamma)\\
&\times M_{\rm D}\sum_{a,c=4}^{7}(d^{ac5}\xi^4-d^{ac4}\xi^5+d^{ac7}\xi^6-d^{ac6}\xi^7)\sigma^a_{\rm f}\sigma^c_{\rm p} \qquad \text{(A1)}
\end{aligned}
$$

and the $\mathcal{O}(e^2)$ interaction Lagrangian becomes

$$
\begin{aligned}
\mathcal{L}_2=&-e^2f^{abc}f^{ade}A^b_\mu A^{d\mu}A^c_\nu A^{e\nu}+\frac{1}{3}e^2A^a_\mu A^{a\mu}[(\xi^4)^2+(\xi^5)^2+(\xi^6)^2+(\xi^7)^2+(\xi^8)^2+\psi^2]\\
&+e^2d^{ab1}A^{a\mu}A^b_\mu(\xi^5\xi^7+\xi^4\xi^6)+e^2d^{ab2}A^{a\mu}A^b_\mu(\xi^5\xi^6-\xi^4\xi^7)+\frac{1}{2}e^2d^{ab3}A^{a\mu}A^b_\mu[(\xi^4)^2+(\xi^5)^2\\
&-(\xi^6)^2-(\xi^7)^2]+e^2d^{ab4}A^{a\mu}A^b_\mu(\xi^5\psi-\xi^4\xi^8)-e^2d^{ab5}A^{a\mu}A^b_\mu(\xi^5\xi^8+\xi^4\psi)\\
&+e^2d^{ab6}A^{a\mu}A^b_\mu(\xi^7\psi-\xi^6\xi^8)-e^2d^{ab7}A^{a\mu}A^b_\mu(\xi^7\xi^8+\xi^6\psi)+\frac{1}{2\sqrt{3}}e^2d^{ab8}A^{a\mu}A^b_\mu[(\xi^4)^2\\
&+(\xi^5)^2+(\xi^6)^2+(\xi^7)^2-2(\xi^8)^2-2\psi^2]-\frac{e^2\mu^2}{4M_{\rm D}^2}[(\xi^4)^2+(\xi^5)^2+(\xi^6)^2+(\xi^7)^2+(\xi^8)^2+\psi^2]^2. \qquad \text{(A2)}
\end{aligned}
$$

In these expressions, $\boldsymbol{\tau}$ designates the Pauli spin matrices, and $\mathbf{A}^\mu$ denotes the gauge field triplet $A^{a\mu}$ $(a=1,2,3)$ in the unbroken SU(2) ''isospin'' subgroup. The isospinors Ψ_a $(a=1,2,3)$ are the combinations of the Higgs field ψ and the ξ^a fields given by Eqs. (19)–(21).

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The *q*-Coulomb problem

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There exist operator solutions of the *q*-Coulomb problem in both configuration and momentum space. Since the arguments of the corresponding amplitudes are noncommuting, however, there are problems of physical interpretation. Here we answer the question of physical interpretation by associating with the operator amplitude in momentum space a numerically valued amplitude lying in a Hilbert space defined by the $SU_q(2)$ algebra. This new amplitude, now depending on commuting arguments, may be interpreted by the usual rules of quantum mechanics and may also be Fourier transformed to yield the amplitude in configuration space. © *1996 American Institute of Physics.* [S0022-2488(96)01706-9]

I. INTRODUCTION

Solutions of the *q*-deformed Coulomb problem have been found in both momentum[1] and configuration[2] space. In both cases the solution amplitudes are operator wave functions lying in either the $SU_q(2)$ or $SO_q(3)$ algebra. If a direct physical interpretation of these amplitudes is attempted, it is necessary to assume that the coordinates are noncommuting in both configuration and momentum space.

One makes a less radical departure from quantum mechanics by associating numerical wave functions with the operator wave functions and basing the physical interpretation on these associated numerical amplitudes. If one follows the latter path, one is deforming not the underlying space but the wave functions lying in the usual space. In order to do this, it is necessary to introduce a Hilbert space on which the operator wave functions can operate. In the following we shall carry out this procedure for the known operator solutions in momentum space.

II. THE *q*-DEFORMED MOMENTUM STATES

Let us recall the procedure for obtaining the undeformed states of momentum in a form which makes explicit the underlying symmetry of the Coulomb problem.[3] First one transforms the Schrödinger differential equation to an integral equation on momentum space. Next momentum space is mapped onto the group space of SU(2) or SO(3) according to

$$e^{(i/2\boldsymbol{\sigma}\mathbf{w})}=\frac{p_0-i\mathbf{p}\boldsymbol{\sigma}}{p_0+i\mathbf{p}\boldsymbol{\sigma}}, \tag{2.1}$$

where $\mathbf{w}$ fixes the magnitude and axis of rotation while p_0 and $\mathbf{p}$ refer to the corresponding energy and momentum. The integral equation on momentum space then becomes an integral equation on group space,

$$\int \widetilde{K}(\mathbf{p},\mathbf{p}')\Phi(\mathbf{p}')d\tau(\mathbf{p}')=\lambda\Phi(\mathbf{p}), \tag{2.2}$$

where the momentum $\mathbf{p}$ parametrizes the group element and $d\tau(\mathbf{p})$ is the invariant volume element on group space:

$$d\tau=\sqrt{g}d\mathbf{p}, \tag{2.3}$$

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where g is the determinant of the group metric.

Here $\Phi(\mathbf{p})$ and $\widetilde{K}(\mathbf{p},\mathbf{p})$ are rescaled Fourier transforms of the wave function and the potential, respectively.

In the Coulomb case (2.2) becomes

$$\int K(\mathbf{p},\mathbf{p}')D^{j}_{mm'}(\mathbf{p}')d\tau(\mathbf{p}')=(2j+1)D^{j}_{mm'}(\mathbf{p}), \tag{2.4}$$

where the $D^{j}_{mm'}(p)$ are Wigner functions (matrix elements of irreducible representations of the rotation group). The actual wave function in momentum space is connected to $D^{j}_{mm'}(\mathbf{p})$ by a scaling function,

$$\Phi^{j}_{mm'}(\mathbf{p})=G^{2}(p)D^{j}_{mm'}(\mathbf{p}), \tag{2.5}$$

$$G=\frac{p_0^2}{p_0^2+p^2}, \tag{2.6}$$

and the energy levels are determined in terms of the eigenvalue $(2j+1)$ of the integral equation by

$$E=-\frac{m}{2}\frac{e^4}{\hbar^2}\frac{1}{(2j+1)^2} \tag{2.7}$$

so that the principal quantum number N is related to j by

$$N=2j+1. \tag{2.8}$$

The other indices, m and m', labelling $\Phi^{j}_{mm'}$, refer to the z-components of the Lenz and angular momentum vectors; but $\Phi^{j}_{mm'}$ is not an eigenfunction of the total angular momentum.

The ground state corresponds to $N=1$ or $j=0$ and the corresponding wave function is then simply

$$G^{2}D^{0}_{00}=\left(\frac{p_0^2}{p_0^2+p^2}\right)^{2} \quad 1, \tag{2.9}$$

which Fourier transforms into the usual exponential for the ground state.

In our earlier work[1] the deformation was accomplished by replacing the integral equation (2.4) by the corresponding Woronowicz integral equation on $\mathrm{SU}_q(2)$:

$$\int_W K_q(\alpha,\alpha')D^{j}_{mm'}(\alpha'|q)d_W\tau(\alpha')=\lambda^{j}_{m'}D^{j}_{mm'}(\alpha|q), \tag{2.10}$$

where W means the Woronowicz integral and where α and α' denote two distinct points in the space of the pseudogroup. The solutions of this equation are the matrix elements of the irreducible representations of $\mathrm{SU}_q(2)$, namely $D^{j}_{mm'}(\alpha|q)$, and the eigenvalues are

$$\lambda^{j}_{m'}=\frac{q^{2m'}}{[2j+1]_q^2}. \tag{2.11}$$

Assuming the same connection between energy and eigenvalues as in the $q=1$ case, one has

$$E(n,m')=-\frac{m}{2}\frac{e^4}{\hbar^2}\frac{q^{4m'}}{[n]_q^2}, \tag{2.12}$$

which approaches the Balmer formula in limit $q=1$. Here the square bracket has its usual meaning

$$[n]=\frac{q^n-q^{-n}}{q-q^{-1}}. \tag{2.13}$$

The deformed wave functions are now $G^2D^j_{mm'}(\alpha|q)$, where α stands for the set of elements defining the algebra and on which $D^j_{mm'}(\alpha|q)$ depends.

There is now the problem of interpreting these deformed wave functions since they are operator rather than c-number functions. For example, the first four excited states correspond to $N=2$ or $j=1/2$ and may be displayed as elements of the following matrix:[1]

$$D^{1/2}_{mm'}=\begin{pmatrix} a & b \\ -q_1\overline{b} & \overline{a} \end{pmatrix}, \tag{2.14}$$

where $q_1=q^{-1}$.

If $q=1$, we may parametrize $D^j_{mm'}$ by three variables such as the three components of $\mathbf{p}$ (or by other coordinate systems such as the Eulerian angles).

If the components of $\mathbf{p}$ are chosen as parameters, then in the undeformed limit we have

$$a=\frac{p_0^2-p^2}{p_0^2+p^2}+\frac{2ip_0p_3}{p_0^2+p^2}, \quad b=\frac{2ip_0(p_1-ip_2)}{p_0^2+p^2},$$

$$d=\frac{p_0^2-p^2}{p_0^2+p^2}-\frac{2ip_2p_3}{p_0^2+p^2}, \quad c=\frac{2ip_0(p_1+ip_2)}{p_0^2+p^2}, \tag{2.15}$$

$$d=\overline{a}, \quad c=-q_1\overline{b}.$$

Then the wave functions in momentum space are given by (2.5) where (a,b,c,d) are expressed as functions of the momentum. After deformation the Wigner functions become the q-Wigner functions depending on $(a,\overline{a},\overline{b},b)$, which all lie in the $SU_q(2)$ algebra and therefore obey the commutation rules of that algebra. If the connection with the components of the momentum described in (2.15) were maintained, then of course the components of momentum would also become noncommuting and momentum space would become a noncommuting space.

Instead of taking the next step of passing to a noncommuting space, however, we shall deform only the solutions of the Coulomb problem without altering the space in which they lie. This can be done by passing from the operator wave functions depending on $(abcd)$ to associated numerical wave functions obtained by evaluating the operator functions on an appropriate Hilbert space, which we shall next describe.

III. HILBERT SPACE

The natural Hilbert space is already indicated by the algebra: since b and c are commuting, we take their common eigenfunctions as reference states lying in the Hilbert space. We also pass to the notation $(a,b,b,\overline{a})$, where

$$\overline{b}=-qc, \quad \overline{a}=d. \tag{3.1}$$

Then

$$ab = qba, \quad \overline{b}\overline{a} = q\overline{a}\overline{b}, \quad a\overline{b} = q\overline{b}a, \quad b\overline{a} = q\overline{a}b. \tag{3.2}$$

Assume that $|0\rangle$ and $\langle 0|$ are common eigenfunctions of b and $\overline{b}$ such that

$$\begin{aligned} b|0\rangle &= \beta|0\rangle, \quad \langle 0|\overline{b} = \langle 0|\beta^* \\ \overline{b}|0\rangle &= \beta^*|0\rangle, \quad \langle 0|b = \langle 0|\beta, \end{aligned} \tag{3.3}$$

when β and β^* are conjugate complex numbers. Assume

$$\langle 0|0\rangle = 1. \tag{3.4a}$$

Then

$$\langle 0|b|0\rangle = \beta, \quad \langle 0|\overline{b}|0\rangle = \beta^*. \tag{3.4b}$$

One now shows that a and $\overline{a}$ behave as annihilation and creation operators since

$$ab|0\rangle = qba|0\rangle \tag{3.5}$$

or

$$b \cdot a|0\rangle = (q^{-1}\beta) \cdot a|0\rangle. \tag{3.6}$$

By iteration

$$b \cdot a^N|0\rangle = (q^{-N}\beta) \cdot a^N|0\rangle \tag{3.7}$$

and also

$$\overline{b} \cdot a^N|0\rangle = (q^{-N}\beta^*) \cdot a^N|0\rangle \tag{3.8}$$

since b and $\overline{b}$ have the same commutation relations with a. Likewise,

$$b \cdot \overline{a^N}|0\rangle = (q^N\beta) \cdot \overline{a^N}|0\rangle, \tag{3.9}$$

$$\overline{b} \cdot \overline{a^N}|0\rangle = (q^N\beta^*) \cdot \overline{a^N}|0\rangle. \tag{3.10}$$

Let

$$a^N|0\rangle = |-N\rangle, \tag{3.11}$$

$$\overline{a^N}|0\rangle = |N\rangle \tag{3.12}$$

up to a normalization. Then

$$b|-N\rangle = (q^{-N}\beta)|-N\rangle, \tag{3.13}$$

$$\overline{b}|-N\rangle = (q^{-N}\beta^*)|-N\rangle, \tag{3.14}$$

$$b|N\rangle = (q^N\beta)|N\rangle, \tag{3.15}$$

$$\overline{b}|N\rangle = (q^N\beta^*)|N\rangle. \tag{3.16}$$

By the usual argument the basis states are orthogonal since

$$\langle N|b|M\rangle=\langle N|q^M\beta|M\rangle \tag{3.17a}$$

$$=\langle N|q^N\beta|M\rangle \tag{3.17b}$$

or, by (3.13),

$$(q^M-q^N)\langle N|M\rangle=0. \tag{3.18}$$

Therefore

$$\langle N|M\rangle=0, \quad N\neq M. \tag{3.19}$$

Set

$$\overline{a}|N\rangle=\lambda_N|N+1\rangle, \quad \langle N|a=\langle N+1|\lambda_N^* \tag{3.20}$$

or

$$a|N\rangle=\mu_n|N-1\rangle, \quad \langle N|\overline{a}=\langle N-1|\mu_N^*. \tag{3.21}$$

Then

$$\langle N|a\overline{a}|N\rangle=\langle N+1|\lambda_N^*\lambda_N|N+1\rangle. \tag{3.22}$$

However,

$$a\overline{a}+b\overline{b}=1. \tag{3.23}$$

Therefore

$$\langle N|1-b\overline{b}|N\rangle=(\lambda_N)^2\langle N+1|N+1\rangle$$

and

$$(\lambda_N)^2=1-|\beta|^2q^{2N}, \tag{3.24}$$

as we assume the same normalization for all states. Likewise

$$\langle N|\overline{a}a|N\rangle=\langle N-1|\mu_N^*\mu_N|N-1\rangle. \tag{3.25}$$

However,

$$\overline{a}a+q_1^2\overline{b}b=1; \tag{3.26}$$

therefore

$$\langle N|1-q_1^2\overline{b}\overline{b}|N\rangle=(\mu_N)^2\langle N-1|N-1\rangle$$

and

$$(\mu_N)^2=1-q_1^2|\beta|^2q^{2N}. \tag{3.27}$$

Therefore to obtain the Nth state from the standard state $|0\rangle$ we form

$$\overline{a^N}|0\rangle=\overline{a}\ldots\overline{a}|0\rangle \tag{3.28}$$

$$= \prod_0^{N-1} \lambda_s |N\rangle \tag{3.29}$$

$$= \prod_0^{N-1} (1-|\beta|^2 q^{2s})^{1/2} |N\rangle \tag{3.30}$$

$$= (|\beta|^2 \| q^2)_N^{1/2} |N\rangle, \tag{3.31}$$

where $(x|q)_N$ is the shifted factorial:

$$(x|q)_N = \prod_0^{N-1} (1-xq^s). \tag{3.32}$$

The normalized eigenstates of b and $\overline{b}$ are then

$$|N\rangle = \frac{\overline{a}^N}{(|\beta|^2 \| q^2)_N^{1/2}} |0\rangle. \tag{3.33}$$

IV. EVALUATION OF $\langle N|D^j_{mm'}|N'\rangle$

After deformation, the Wigner functions $D^j_{mm'}$ become the operator functions[1]

$$D^j_{mm'} = \Delta^j_{mm'} \sum \begin{pmatrix} n_+ \\ s \end{pmatrix}_1 \begin{pmatrix} n_- \\ t \end{pmatrix}_1 q_1^{(n_+ - s+1)t} (-)^t \delta(s+t, n'_+) a^s b^{n_+ - s} \overline{b}^t \overline{a}^{n_- - t}, \tag{4.1}$$

where

$$\Delta^j_{mm'} = \left(\frac{\langle n'_+ \rangle_1 ! \langle n'_- \rangle_1 !}{\langle n_t \rangle_1 ! \langle n_- \rangle_1 !} \right)^{1/2} \quad \begin{matrix} n_\pm = j \pm m, \\ n'_\pm = j \pm m', \end{matrix} \tag{4.2}$$

and $\langle\rangle_1 = \langle\rangle_{q_1^2}$ with $q_1 = q^{-1}$. Here $(a, \overline{a}, b, \overline{b})$ lie in the $\mathrm{SU}_q(2)$ algebra. Let

$$\Pi = a^s b^{n_+ - s} \overline{b}^t \overline{a}^{n_- - t}. \tag{4.3}$$

Then we must evaluate $\langle N|\Pi|N'\rangle$.

Let us rearrange Π:

$$\Pi = (b^{n_+ - s} \overline{b}^t a^s \overline{a}^{n_- - t}) q^{n_+ + t - s}. \tag{4.4}$$

Note that

$$a^s \overline{a}^{n_- - t} = (a^s \overline{a}^s) \overline{a}^{n_- - t - s} = (b\overline{b}|q^2)_s \overline{a}^{n_- - t - s}. \tag{4.5}$$

Then

$$\Pi = q^{n_+ + t - s} b^{n_+ - s} \overline{b}^t (b\overline{b}|q^2)_s \overline{a}^{n_- - t - s} \tag{4.6}$$

$$= q^{n_+ + t - s} b^{n_+ - s - t} (b\overline{b})^t (b\overline{b}|q^2)_s \overline{a}^{n_- - t - s} \tag{4.7}$$

and

$$\langle N|\Pi|N'\rangle = q^{n_+ + t - s} (q^N \beta)^{n_+ - s - t} |\beta|^{2t} q^{2Nt} (|\beta|^2 q^{2N}|q^2)_s \langle N|\overline{a}^{n_- - t - s}|N'\rangle. \tag{4.8}$$

To evaluate this matrix element note that by (3.20)

$$\overline{a^k}|N\rangle = \prod_{N}^{N+k-1} \lambda_s |N+k\rangle \tag{4.9}$$

$$= \left[\frac{\Pi_0^{N+k-1}\lambda_s}{\Pi_0^{N-1}\lambda_s}\right]|N+k\rangle. \tag{4.10}$$

By (3.31)

$$= \left[\frac{(|\beta|^2|q^2)_{N+k}^{1/2}}{(|\beta|^2|q^2)_N^{1/2}}\right]|N+k\rangle. \tag{4.11}$$

Therefore, by (3.19),

$$\langle N|\overline{a^k}|N'\rangle = \left[\frac{(|\beta|^2|q^2)_N}{(|\beta|^2|q^2)_{N'}}\right]^{1/2}\delta(N,N'+k) \tag{4.12}$$

and

$$\langle N|\Pi|N'\rangle = q^{n_+ + t - s}q^{N(n_+ - s + t)}\beta^{n_+ - s - t}|\beta|^{2t}(|\beta|^2 q^{2N}|q^2)_s\left[\frac{(|\beta|^2|q^2)_N}{(|\beta|^2|q^2)_{N'}}\right]^{1/2}\delta(N,N'+n_- - t - s). \tag{4.13}$$

The double sum on (s,t) in (4.1) is now restricted by the following conditions;

$$n'_+ = s+t, \quad N' - N + n_- = s + t.$$

Therefore

$$N' - N = n'_+ - n_- = m' + m \tag{4.14}$$

and

$$\langle N|D^j_{mm'}|N'\rangle = \Delta^j_{mm'}\sum \left\langle \begin{matrix} n_+ \\ s \end{matrix} \right\rangle_1 \left\langle \begin{matrix} n_- \\ t \end{matrix} \right\rangle_1 (-)^t q_1^{(n_+ - s + 1)t} q^{(N+1)(n_+ + t - s)}\beta^{n_+ - s - t}|\beta|^{2t}$$
$$\times (|\beta|^2 q^{2N}|q^2)_s\left[\frac{(|\beta|^2|q^2)_N}{(|\beta|^2|q^2)_{N'}}\right]^{1/2}\delta(s+t,n'_+)\,\delta(N'-N,m+m'). \tag{4.15}$$

In particular,

$$\langle 0|D^j_{mm'}|0\rangle = \Delta^j_{mm'}\sum \left\langle \begin{matrix} n_+ \\ s \end{matrix} \right\rangle_1 \left\langle \begin{matrix} n_- \\ t \end{matrix} \right\rangle_1 q_1^{(n_+ - s)(1-t)}(-)^t\beta^{n_+ - s - t}|\beta|^{2t}$$
$$\times (|\beta|^2|q^2)_s\delta(s+t,n'_+)\,\delta(m+m',0). \tag{4.16}$$

In general, if we set $N=0$, then

$$\langle 0|D^j_{mm'}|m+m'\rangle = \Delta^j_{mm'}\sum \left\langle \begin{matrix} n_+ \\ s \end{matrix} \right\rangle_1 \left\langle \begin{matrix} n_- \\ t \end{matrix} \right\rangle_1 q^{(n_+ - s)(1-t)}(-)^t\beta^{n_+ - s - t}|\beta|^{2t}(|\beta|^2 q^2)_s$$
$$\times (|\beta|^2|q^2)^{-1/2}_{m+m'}\delta(s+t,n'_+). \tag{4.17}$$

In this way one may associate a numerically valued function $\langle 0|D^j_{mm'}|m+m'\rangle$ with the operator $D^j_{mm'}$. There is, of course, an associated degeneracy since any solution of $N'-N=m+m'$ is also acceptable.

The limit of (4.17) as $q\to 1$ is

$$\Delta^j_{mm'}\sum \binom{n_+}{s}\binom{n_-}{t}(-)^t\beta^{n_+-s-t}|\beta|^{2t}(|\beta|^2|1)_s(|\beta|^2|1)^{-1/2}_{m+m'}\delta(s+t,n'_+), \tag{4.18}$$

where

$$\beta^{n_+-s-t}|\beta|^{2t}(|\beta|^2|1)_s(|\beta|^2|1)^{-1/2}_{m+m'}=\beta^{n_+-n'_+}|\beta|^{2t}(1-|\beta|^2)^{s-(m+m')/2}. \tag{4.19}$$

Set

$$\beta=\sin\frac{\theta}{2}\,e^{i\chi}. \tag{4.20}$$

Then (4.19) becomes

$$\left(\sin\frac{\theta}{2}\right)^{m-m'+2t}\left(\cos\frac{\theta}{2}\right)^{2s-m-m'}e^{i(m-m')\chi}. \tag{4.21}$$

Then

$$\lim_{q\to 1}\langle 0|D^j_{mm'}|m+m'\rangle=\Delta^j_{mm'}\sum \binom{n_+}{s}\binom{n_-}{t}(-)^t\left(\sin\frac{\theta}{2}\right)^{2t+m-m'}\left(\cos\frac{\theta}{2}\right)^{2s-m-m'}e^{i(m-m')\chi}\delta(s+t,j+m') \tag{4.22}$$

as required.

Notice that if we let q approach unity before taking the matrix element, then $\langle 0|D^j_{m+m'}|m+m'\rangle=0$ unless $m+m'=0$. On the other hand, if we take the matrix element first, then according to (4.22) we obtain the correct $q=1$ amplitude.

V. q-DEFORMED AMPLITUDES IN MOMENTUM SPACE

The result obtained for $\langle 0|D^j_{mm'}|m+m'\rangle$ depends on q, β, and β^*. Since β and β^* are eigenvalues rather than operators, they may be parametrized by three commuting parameters (p_1,p_2,p) which we identify with two components and the magnitude of momentum

$$\beta=\frac{2ip_0(p_1-ip_2)}{p_0^2+p^2}, \tag{5.1}$$

$$\beta^*=-\frac{2i(p_1+ip_2)}{p_0^2+p^2}, \tag{5.2}$$

and we also define p_3 by

$$p_3^2=p^2-p_1^2-p_2^2. \tag{5.3}$$

Here p_0 is a constant.

Let

$$\mathscr{D}(\beta,\beta^*)\equiv\langle 0|D^j_{mm'}|m+m'\rangle. \tag{5.4}$$

Then the amplitude in momentum space is

$$\Phi(\mathbf{p})=\left(\frac{p_0}{p_0^2+p^2}\right)^2\mathscr{D}\left(\frac{2i(p_0(p_1-ip_2))}{p_0^2+p^2},\ \frac{-2ip_0(p_1+ip_2)}{p_0^2+p^2}\right). \tag{5.5}$$

This amplitude may be Fourier transformed back to configuration space by the usual rules of quantum mechanics. In this way we may obtain a q-deformed solution of the Coulomb problem in configuration space.

VI. REMARKS

The operator form of the amplitude in configuration space obtained by Feigenbaum and Freund[2] is not simply related to the operator form of the amplitude in momentum space discussed in this paper because the symmetry algebras for the two amplitudes, namely $SO_q(3)$ and $SU_q(2)$, are not the same (although the undeformed algebras are of course the same). In addition the momentum amplitude presented here is an eigenfunction of the z-components of the Lenz and angular momentum vectors while the configuration space amplitude to which it is compared is an eigenfunction of the total angular momentum and its z-component. With both of these operator amplitudes, one has the problem of physical interpretation, i.e., of relating numerical probabilities to the amplitudes.

In an earlier discussion of the harmonic oscillator a different course was followed.[4] There the amplitude in configuration space is presented as a function which both lies in the $SU_q(2)$ algebra and independently depends on the coordinates of configuration space; further, the coordinates of configuration space are required to freely commute with the $SU_q(2)$ algebra. The amplitude in momentum space has a similar structure, dependent on both the $SU_q(2)$ algebra and the coordinates of the momentum which freely commute with the algebra. The amplitudes in configuration and momentum space are related by a q-Fourier transform which is integrated over the eigenvalues of one of the conjugate operators and maps onto eigenfunctions of the other.

The numerical probability associated with either amplitude is then obtained by a Woronowicz integration over the $SU_q(2)$ algebra. This procedure differs from both conventional quantum mechanics and quaternion quantum mechanics, since in those cases the amplitude lies in either the complex plane or the SU(2) algebra, while here it lies in the $SU_q(2)$ algebra. The only natural choice for probability in the $SU_q(2)$ case is the Woronowicz measure, since it is invariant under $SU_q(2)$ transformations and still depends on x or p. The same approach can, in principle, be followed for a system with more degrees of freedom such as the q-Coulomb problem, but this has not yet been done.

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Lattice properties of quantum effects

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Sufficient conditions for the existence of the infimum $A\wedge B$ of two quantum effects A and B are given. The existence of $A\wedge B$ is characterized for commuting A and B with pure point spectrum. Properties of a generalized infimum and supremum are studied. Some previous finite dimensional, commutative results are extended to the infinite dimensional and noncommutative case. © *1996 American Institute of Physics.* [S0022-2488(96)03306-3]

I. INTRODUCTION

The basic axiomatic elements of the operational approach to quantum mechanics are the effects.[1–5] In this approach, effects represent sharp and unsharp properties of a physical system. The set of effects $\mathscr{E}$ for a physical system S carry a natural partial order, where we define $A\leqslant B$ if the expectation of the values of a measurement of A does not exceed that of B for every state of S. If H is the Hilbert space that describes the states of S, then $\mathscr{E}$ is represented by the set of self-adjoint operators on H that satisfy $0\leqslant A\leqslant I$ and $A\leqslant B$ if and only if $\langle Ax,x\rangle\leqslant\langle Bx,x\rangle$ for all $x\in H$.

Since $(\mathscr{E},\leqslant)$ is a partially ordered set, it is of interest to study the lattice properties of $\mathscr{E}$. Except in the trivial case $\dim(H)=1$, $\mathscr{E}$ is not a lattice.[6,7] This leads to the natural problem of characterizing those pairs of effects $A,B\in\mathscr{E}$ for which the greatest lower bound (infimum) $A\wedge B$ or the least upper bound (supremum) $A\vee B$ exists. Although this characterization problem has been solved for the cases $\dim(H)=2,3$,[6,8] it remains open in general. It is obvious that if A and B are comparable ($A\leqslant B$ or $B\leqslant A$) then $A\wedge B$ and $A\vee B$ exist. However, there are many examples of incomparable effects for which $A\wedge B$ (or $A\vee B$) exist.

In this paper, we give some sufficient conditions for the existence of $A\wedge B$ and solve the characterization problem for the case of commuting effects with pure point spectrum. [Note that it is not necessary to study both $A\wedge B$ and $A\vee B$ since they are related by DeMorgan's laws $(A\wedge B)'=A'\vee B'$, $(A\vee B)'=A'\wedge B'$ when one side of the equations exist, where $A'=I-A$.] We also consider the concepts of a generalized infimum $A\sqcap B$ and generalized supremum $A\sqcup B$. We show that $A\sqcap B$ and $A\sqcup B$ have many of the properties of the usual $A\wedge B$, $A\vee B$ and reduce to these when they exist. Finally, we extend some finite dimensional, commutative results in Ref. 7 to the infinite dimensional and noncommutative case.

II. A GENERALIZED INFIMUM

Let H be a complex Hilbert space and denote the set of bounded self-adjoint operators on H by $\mathscr{S}(H)$ and the set of (orthogonal) projections on H by $\mathscr{P}(H)$. We say that an element $A\in\mathscr{S}(H)$ is *positive* and write $A\geqslant 0$ if $\langle Ax,x\rangle\geqslant 0$ for all $x\in H$. For $A,B\in\mathscr{S}(H)$, we write $A\leqslant B$ if $B-A\geqslant 0$. In this way $(\mathscr{S}(H),\leqslant)$ becomes a partially ordered set. An element $A\in\mathscr{S}(H)$ that satisfies $0\leqslant A\leqslant I$ is called an *effect* and the set of effects on H is denoted $\mathscr{E}(H)$. It is well known that $(\mathscr{S}(H),\leqslant)$ and $(\mathscr{E}(H),\leqslant)$ are not lattices (unless $\dim(H)\leqslant 1$).[6,7,9] However, we shall introduce generalized infima and suprema that possess many of the properties of the usual infima and suprema and reduce to these constructs when they exist. For $A,B\in\mathscr{E}(H)$, when we write $A\wedge B$ we are always referring to the infimum (greatest lower bound) of A and B within $\mathscr{E}(H)$. The next two lemmas give useful properties of the order.

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Lemma 2.1: Let $A,B,C\in\mathscr{E}(H)$. (a) Then $BAB\in\mathscr{E}(H)$ and $0\leqslant BAB\leqslant B^2\leqslant I$. (b) If $C\leqslant A$, then $BCB\leqslant BAB$. (c) If $AB=BA$, then $0\leqslant AB\leqslant B$.

Proof: (a) That $B^2\leqslant I$ follows from the spectral theorem. The result follows because $\langle BABx,x\rangle=\langle ABx,Bx\rangle$ and

$$0\leqslant\langle ABx,Bx\rangle\leqslant\langle Bx,Bx\rangle=\langle B^2x,x\rangle.$$

(b) This follows from

$$\langle BCBx,x\rangle=\langle CBx,Bx\rangle\leqslant\langle ABx,Bx\rangle=\langle BABx,x\rangle.$$

(c) The result holds because $\langle ABx,x\rangle=\langle AB^{1/2}x,B^{1/2}x\rangle$ and

$$0\leqslant\langle AB^{1/2}x,B^{1/2}x\rangle\leqslant\langle B^{1/2}x,B^{1/2}x\rangle=\langle Bx,x\rangle.$$ □

For $A\in\mathscr{S}(H)$, let $R(A)$ be the closure of the range AH of A and $N(A)$ be the null space of A. For $A,B\in\mathscr{S}(H)$ we denote the projection onto $R(A)$ by P_A and the projection onto $R(A)\cap R(B)$ by $P_{A,B}$.

Lemma 2.2: Let $A,B,C\in\mathscr{E}(H)$. (a) If $C\leqslant A$, then $CP_A=P_AC=C$ and $C\leqslant P_A$. (b) If $C\leqslant A,B$, then $CP_{A,B}=P_{A,B}C=C$ and $C\leqslant P_{A,B}$.

Proof: (a) If $x\in N(A)$, then

$$0\leqslant\langle C^{1/2}x,C^{1/2}x\rangle=\langle Cx,x\rangle\leqslant\langle Ax,x\rangle=0.$$

Hence, $C^{1/2}x=0$ so $Cx=0$. Therefore, $N(A)\subseteq N(C)$ so

$$R(C)=N(C)^{\perp}\subseteq N(A)^{\perp}=R(A).$$

Hence, for every $y\in H$ we have $Cy=P_ACy$ so $C=P_AC$ and

$$C=C^*=(P_AC)^*=CP_A.$$

Applying Lemma 2.1(a) gives

$$C=P_ACP_A\leqslant P_A^2=P_A.$$

(b) If $C\leqslant A,B$ then from part (a) we have $R(C)\subseteq R(A),R(B)$ so $R(C)\subseteq R(A)\cap R(B)$. The result follows using the same argument as in part (a). □

For $A\in\mathscr{S}(H)$, we define $|A|=(A^2)^{1/2}$ where $(A^2)^{1/2}$ is the unique positive square root of A^2. For $A,B\in\mathscr{S}(H)$, we define the *generalized infimum* $A\sqcap B$ by

$$A\sqcap B=\tfrac{1}{2}(A+B-|A-B|).$$

The generalized infimum has been studied by various investigators.[7,9,10] Of course, $A\sqcap B$ always exists. However, for $A,B\in\mathscr{E}(H)$, it is not necessarily true that $A\sqcap B\in\mathscr{E}(H)$ because $A\sqcap B$ may not be positive.[7,10] Nevertheless, for important special cases, we do have $A\sqcap B\in\mathscr{E}(H)$. For example, if A and B are comparable or if A and B commute, then $A\sqcap B\in\mathscr{E}(H)$. It is shown in Ref. 7 that if $\dim(H)<\infty$ and A,B are commuting effects, then $A\sqcap B$ is a maximal lower bound for A,B. We shall prove a generalization of this result by showing that $\dim(H)<\infty$ can be dropped and that $AB=BA$ can be replaced by a more general condition.

Theorem 2.3: (a) If $A,B\in\mathscr{S}(H)$, then $A\sqcap B\leqslant A,B$ and

$$(A-A\sqcap B)(B-A\sqcap B)=0.$$

(b) If $A,B\in\mathscr{E}(H)$ and $A\sqcap B\geqslant 0$, then

$$(A-A\sqcap B)\wedge(B-A\sqcap B)=0.$$

Proof: (a) It follows from the spectral theorem that $A-B\leqslant|A-B|$. Hence, $A-|A-B|\leqslant B$ so $A+B-|A-B|\leqslant 2B$ and

$$A\sqcap B=\tfrac{1}{2}(A+B-|A-B|)\leqslant B.$$

Similarly, $A\sqcap B\leqslant A$. Since $A-B$ and $|A-B|$ commute, we have

$$(A-A\sqcap B)(B-A\sqcap B)=\tfrac{1}{4}(A-B+|A-B|)(B-A+|A-B|)=\tfrac{1}{4}(|A-B|^2-(A-B)^2)=0.$$

(b) Since $A\sqcap B\leqslant A,B$ and $A\sqcap B\geqslant 0$, we have $A-A\sqcap B,B-A\sqcap B\in\mathscr{E}(H)$. Suppose that $C\in\mathscr{E}(H)$ with $C\leqslant A-A\sqcap B,B-A\sqcap B$. If

$$x\in(A-A\sqcap B)H\cap(B-A\sqcap B)H,$$

then

$$x=(A-A\sqcap B)y=(B-A\sqcap B)z,$$

for some $y,z\in H$. Hence, by part (a) we have

$$\|x\|^2=\langle x,x\rangle=\langle(B-A\sqcap B)(A-A\sqcap B)y,z\rangle=0.$$

Thus, $P=P_{A-A\sqcap B,B-A\sqcap B}=0$ so by Lemma 2(b) we have $C=CP=0$. The result now follows.□

Corollary 2.4: For $A,B\in\mathscr{E}(H)$, suppose that $A\sqcap B\geqslant 0$. (a) Then $A\sqcap B$ is a maximal lower bound for A and B in $\mathscr{E}(H)$. (b) If $A\wedge B$ exists, then $A\wedge B=A\sqcap B$.

Proof: (a) From Theorem 2.3(a) we have $0\leqslant A\sqcap B\leqslant A,B$. Suppose that $A\sqcap B\leqslant C\leqslant A,B$. Then

$$0\leqslant C-A\sqcap B\leqslant A-A\sqcap B,B-A\sqcap B$$

Applying Theorem 2.3(b) gives $C-A\sqcap B=0$ so $C=A\sqcap B$. (b) Since $A\sqcap B\leqslant A\wedge B\leqslant A,B$, applying part (a) gives $A\wedge B=A\sqcap B$. □

If A and B are commuting effects, it follows from the spectral theorem that $A\sqcap B\geqslant 0$. Hence, the conclusions of Corollary 2.4 hold. This generalizes the main result in Ref. 7 to Hilbert spaces of arbitrary dimension. The next result has been proved in Ref. 10.

Lemma 2.5: For $A,B\in\mathscr{E}(H)$, $A\sqcap B=0$ if and only if $AB=0$.

In Ref. 7 it is shown that if $A,B\in\mathscr{E}(H)$ with $AB=0$ and $\dim(H)<\infty$, then $A\wedge B=0$. We now show that $\dim(H)<\infty$ is unnecessary.

Corollary 2.6: For $A,B\in\mathscr{E}(H)$, if $AB=0$, then $A\wedge B=0$.

Proof: If $AB=0$, then by Lemma 2.5 we have $A\sqcap B=0$. Since, by Corollary 2.4(a), $A\sqcap B$ is a maximal lower bound for A and B, we have $A\wedge B=0$. □

For $A\in\mathscr{E}(H)$, we define $A'\in\mathscr{E}(H)$ by $A'=I-A$.

Corollary 2.7: If $A\wedge A'$ exists, then $A\wedge A'=\tfrac{1}{2}(I-|2A-I|)$.

Proof: Since A and A' commute, if $A\wedge A'$ exists it follows from Corollary 2.4 that

$$A\wedge A'=A\sqcap A'=\tfrac{1}{2}(A+A'-|A-A'|)=\tfrac{1}{2}(I-|2A-I|).$$ □

The next corollary gives a well-known characterization of projections.[11,12]

Corollary 2.8: An effect A is a projection if and only if $A\wedge A'=0$

Proof: If $A\wedge A'=0$, then by Corollary 2.4, $A\sqcap A'=A\wedge A'=0$. Applying Lemma 2.5, we have $AA'=0$. Hence, $A-A^2=A(I-A)=0$ so A is a projection. Conversely, if A is a projection, then $AA'=0$. Applying Corollary 2.6 gives $A\wedge A'=0$. □

For $A,B\in\mathscr{S}(H)$, we defined the *generalized supremum* $A\sqcup B$ by

$$A \sqcup B = \tfrac{1}{2}(A + B + |A - B|).$$

The following theorem is analogous to Theorem 2.3 and Corollary 2.4.

Theorem 2.9: (a) If $A, B \in \mathscr{S}(H)$, then $A, B \leqslant A \sqcup B$ and

$$(A \sqcup B - A)(A \sqcup B - B) = 0.$$

Let $A, B \in \mathscr{E}(H)$ with $A \sqcup B \leqslant I$. (b) Then

$$(A \sqcup B - A) \wedge (A \sqcup B - B) = 0.$$

(c) $A \sqcup B$ is a minimal upper bound for A and B in $\mathscr{E}(H)$. (d) If $A \vee B$ exists, then $A \vee B = A \sqcup B$.

The next result gives relationships between $A \sqcap B$ and $A \sqcup B$.

Lemma 2.10: For $A, B \in \mathscr{S}(H)$ we have (a) $A \sqcap B + A \sqcup B = A + B$ and $A \sqcup B - A \sqcap B = |A - B|$; (b) $(A \sqcup B)' = A' \sqcap B'$ and $(A \sqcap B)' = A' \sqcup B'$.

Proof: (a) is clear. For (b) we have

$$A' \sqcap B' = \tfrac{1}{2}(2I - A - B - |A - B|) = I - \tfrac{1}{2}(A + B + |A - B|) = (A \sqcup B)'$$

and the last equation is similar. □

We conclude that for effects A and B that $A \sqcap B$ and $A \sqcup B$ always exist in $\mathscr{S}(H)$ and have many of the properties of an infimum and supremum, respectively. Moreover, when $A \wedge B (A \vee B)$ exists and $A \sqcap B (A \sqcup B)$ is in $\mathscr{E}(H)$, then $A \wedge B = A \sqcap B (A \vee B = A \sqcup B)$.

III. EXISTENCE OF INFIMA

An important open problem is to characterize the pairs of effects A, B for which $A \wedge B$ exists. This problem was solved for the case $\dim(H) = 2$ in Ref. 6 where it was shown that $A \wedge B$ exists if and only if A and B are comparable or $\dim P_{A,B} \leqslant 1$. This section presents some sufficient conditions for the existence of infima and the characterization problem is solved for the case of commuting effects with pure point spectrum.

Theorem 3.1: Let $A, B \in \mathscr{E}(H)$. (a) If $P \in \mathscr{P}(H)$ satisfies $AP = PA$, $BP = PB$ and if $A \wedge B$ exists, then $(PA) \wedge (PB)$ exists and equals $P(A \wedge B)P$. (b) If A and B both commute with $P_{A,B}$, then $(AP_{A,B}) \wedge (BP_{A,B})$ exists if and only if $A \wedge B$ exists and moreover, when they exist, they coincide.

Proof: (a) By Lemma 2.1(a), $PA, PB, P(A \wedge B)P \in \mathscr{E}(H)$. Since $A \wedge B \leqslant A, B$, by Lemma 2.1(b), $P(A \wedge B)P \leqslant PA, PB$. Suppose that $C \leqslant PA, PB$, where $C \in \mathscr{E}(H)$. By Lemma 2.1(c) we have $C \leqslant PA \leqslant P$ and applying Lemma 2.2(a) gives $CP = PC = C$. By Lemma 2.1(c) we have $PA \leqslant A$, $PB \leqslant B$ so $C \leqslant A, B$. Hence, $C \leqslant A \wedge B$ so applying Lemma 2.1(b) gives $C = PCP \leqslant P(A \wedge B)P$. Hence, $P(A \wedge B)P = (PA) \wedge (PB)$. (b) If $A \wedge B$ exists, it follows from part (a) that $(AP_{A,B}) \wedge (BP_{A,B})$ exists. Conversely, suppose that $(AP_{A,B}) \wedge (BP_{A,B})$ exists. As in part (a) $AP_{A,B} \leqslant A$ and $BP_{A,B} \leqslant B$ so $(AP_{A,B}) \wedge (BP_{A,B}) \leqslant A, B$. Now suppose that $C \in \mathscr{E}(H)$ with $C \leqslant A, B$. Applying Lemma 2.2(b) gives $CP_{A,B} = P_{A,B}C = C$. By Lemma 2.1(b) we have

$$C = P_{A,B}CP_{A,B} \leqslant P_{A,B}AP_{A,B} = AP_{A,B}.$$

Similarly, $C \leqslant BP_{A,B}$ so $C \leqslant (AP_{A,B}) \wedge (BP_{A,B})$ and the result follows. □

As a corollary, we obtain the following well known result.[9]

Corollary 3.2: If $A, B \in \mathscr{P}(H)$, then $A \wedge B = P_{A,B}$.

Proof: We have

$$AP_{A,B} = P_{A,B}A = BP_{A,B} = P_{A,B}B = P_{A,B}.$$

Applying Theorem 3.1(b) gives

$$P_{A,B}=P_{A,B}\wedge P_{A,B}=(AP_{A,B})\wedge(BP_{A,B})=A\wedge B. \qquad \square$$

If A and B both commute with $P_{A,B}$, then by Theorem 3.1, a sufficient condition for the existence of $A\wedge B$ is that $AP_{A,B}$ and $BP_{A,B}$ are comparable. The next theorem gives another sufficient condition.

Theorem 3.3: For $A,B\in\mathscr{E}(H)$, if $\dim(P_{A,B})\leqslant 1$, then $A\wedge B$ exists.

Proof: Suppose that $\dim(P_{A,B})\leqslant 1$ and let $C\in\mathscr{E}(H)$ satisfy $C\leqslant A,B$. By Lemma 2.2(b) $CP_{A,B}=P_{A,B}C=C$. If $P_{A,B}=0$, then $C=0$ so $A\wedge B=0$. Suppose that $P=P_{A,B}\neq 0$ so $\dim(P)=1$. Let $Px=x$ with $\|x\|=1$. Then for every $y\in H$ we have

$$Cy=CPy=C\langle y,x\rangle x=\langle y,x\rangle PCy=\langle y,x\rangle\langle Cx,x\rangle x=\langle Cx,x\rangle Px.$$

Hence, $C=\langle Cx,x\rangle P$. Let

$$t=\sup\{0\leqslant s\leqslant 1: sP\leqslant A,B\}.$$

We claim that $A\wedge B=tP$. Indeed, $tP\leqslant A$ because there exists a sequence s_i such that $0\leqslant s_i\leqslant 1$, $s_iP\leqslant A$ and $t=\lim s_i$. For $y\in H$, we have $s_i\langle Py,y\rangle\leqslant\langle Ay,y\rangle$ so

$$\langle tPy,y\rangle=t\langle Py,y\rangle=\lim(s_i\langle Py,y\rangle)\leqslant\langle Ay,y\rangle.$$

Similarly, $tP\leqslant B$. Since

$$C=\langle Cx,x\rangle P\leqslant A,B$$

we have $\langle Cx,x\rangle\leqslant t$. Hence, $C\leqslant tP$ so $A\wedge B=tP$. $\square$

The next result characterizes the existence of $A\wedge B$ for commuting effects with pure point spectrum. In this theorem we assume that H is separable.

Theorem 3.4: If A and B are commuting effects with pure point spectrum, then $A\wedge B$ exists if and only if $AP_{A,B}$ and $BP_{A,B}$ are comparable. Moreover, in this case $A\wedge B$ is the smaller of $AP_{A,B}$ and $BP_{A,B}$.

Proof: If $AP_{A,B}$ and $BP_{A,B}$ are comparable, then applying Theorem 3.1(b), we conclude that $A\wedge B$ exists and is the smaller of $AP_{A,B}$ and $BP_{A,B}$. Conversely, suppose that $A\wedge B$ exists. We can assume without loss of generality that $P_{A,B}=I$ (that is, A and B both have full rank). This is because $A\wedge B$ exists if and only if $(AP_{A,B})\wedge(BP_{A,B})$ exists [Theorem 3.1(b)] and $AP_{A,B}$ and $BP_{A,B}$ have full rank on $P_{A,B}H$. We must now show that A and B are comparable. By the spectral theorem, we can write $A=\Sigma a_iP_i$, $B=\Sigma b_iP_i$, where a_i and b_i are the eigenvalues of A and B respectively (repeated according to multiplicity) and the P_i are one-dimensional projections forming a resolution of the identity. Since A and B have full rank, we have $a_i>0$, $b_i>0$ for all i. Suppose that A and B are incomparable. Then without loss of generality, we may assume that $a_1<b_1$ and $a_2>b_2$. Letting P be the projection onto the two-dimensional subspace generated by P_1H and P_2H, we have $PA=a_1P_1+a_2P_2$ and $PB=b_1P_1+b_2P_2$. Applying Theorem 3.1 (a), we conclude that $(PA)\wedge(PB)$ exists. Since PA and PB are incomparable effects on the two-dimensional Hilbert space PH, it follows from the two-dimensional case cited previously[6] that PA or PB is a multiple of a one-dimensional projection. Hence, $a_1=0$ or $b_2=0$. But this is a contradiction so A and B are comparable. $\square$

Examples are given in Ref. 7 for which $A\wedge A'$ exists and for which $A\wedge A'$ does not exist. Such examples follow from the next result.

Corollary 3.5: If H is separable and $A\in\mathscr{E}(H)$ has pure point spectrum, then $A\wedge A'$ exists if and only if $AP_{A,A'}$ and $\frac{1}{2}P_{A,A'}$ are comparable.

Proof: Let $P=P_{A,A'}$. Applying Theorem 3.4, $A\wedge A'$ exists if and only if AP and $A'P$ are comparable. But

$$AP \leqslant A'P = P - AP$$

if and only if $AP \leqslant \frac{1}{2}P$ and $A'P \leqslant AP$ if and only if $AP \geqslant \frac{1}{2}P$. ■

Example 1: For $A = \text{diag}(1/2,1,1/3)$ we have $A' = \text{diag}(1/2,0,2/3)$. Then A and A' are incomparable, but letting $P = P_{A,A'}$ we have $P = \text{diag}(1,0,1)$ and

$$AP = \text{diag}(1/2,0,1/3) \leqslant \tfrac{1}{2}\,\text{diag}(1,0,1) = \tfrac{1}{2}P,$$

so $A \wedge A'$ exists and $A \wedge A' = \text{diag}(1/2,0,1/3)$.

Example 2: For $A = \text{diag}(1/3,2/3)$ we have $A' = \text{diag}(2/3,1/3)$. Since, $P_{A,A'} = I$ and $A, \frac{1}{2}I$ are incomparable, $A \wedge A'$ does not exist.

Example 3: If $A = \text{diag}\ (0,a)$ for $0 \leqslant a \leqslant 1$, then $A \wedge B$ exists for all $B \in \mathscr{E}(\mathbb{C}^2)$.

Example 4: Let $A = \text{diag}(1,3/8,0)$, $B = \text{diag}(1,1/3,0)$ and

$$C = \begin{bmatrix} 1/2 & 0 & 0 \\ 0 & 1/2 & 1/4 \\ 0 & 1/4 & 1/2 \end{bmatrix}.$$

Then $A \wedge C = \text{diag}(1/2,3/8,0)$ but $B \wedge C$ does not exist.

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On the diagonalization of quantum Birkhoff–Gustavson normal form

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An application to quantum mechanics of one of classical perturbation theory methods, the Birkhoff–Gustavson normal form (BGNF), is described. In the quantum case it results in the Van Vleck perturbation theory performed upon Wick normal ordered operators. Algebraic aspects of this procedure and formal construction of invariants (integrals of motion) for a perturbed system are considered. It turned out that a larger set of such operators existed in the quantum mechanics, rather than in the classical one. It is demonstrated that, according to general results of the quantum mechanical perturbation theory, the quantum BGNF may always be diagonalized, and two formal processes for such diagonalization are constructed. In the opposite case, the classical BGNF is, in general, nondiagonalizable. This reflects the fact that the classical perturbation theory cannot handle a system with two or more resonances. Possible reasons for such different behavior of two very close, in spirit, perturbation procedures are discussed. Results of the described procedure, entirely performed upon the Wick normal ordered operators, are equivalent to those of Rayleigh–Schrödinger perturbation expansion. © *1996 American Institute of Physics.* [S0022-2488(96)01803-7]

I. INTRODUCTION

Birkhoff method[1] in classical mechanics provides a procedure to transform the original nonseparable **d** dimensional oscillator Hamiltonian canonically into the normal form consisting of a power series in one-dimensional uncoupled harmonic oscillator Hamiltonians

$$H(p_1,q_1,\ldots,p_{\mathbf{d}},q_{\mathbf{d}})\rightarrow\mathscr{H}(\zeta_1^2+\eta_1^2,\ldots,\zeta_{\mathbf{d}}^2+\eta_{\mathbf{d}}^2),$$

where ζ_k and η_k are canonical coordinates and momenta, and $\mathscr{H}$ is a formal power series in $\zeta_k^2+\eta_k^2$. If the series $\mathscr{H}$ were to converge, the new equation could be easily integrated, **d** independent isolating invariants would exist, and the motion would be multiple periodic. Unfortunately it was shown that the Birkhoff normal form diverged in general because of small divisors in the coefficients.

The Birkhoff method was applied by Gustavson[2] in order to obtain power series expressions for invariants and analytically predict the Poincaré surfaces of section for the Henon-Heiles system. Doing that, Gustavson had to modify the original Birkhoff method in order to include resonances. Such calculations showed that, despite the known divergence of the power series representing the normal form, a truncated series could give accurate approximations to regular trajectories.[3]

The Birkhoff–Gustavson normal form was successfully applied to the semiclassical Einstein–Brillouin–Kemmer quantization of various systems, such as the Henon–Heiles system[4,5] and the hydrogen atom (Stark and Stark–Zeeman effects[6]) up to very high order of coupling constant.

Ali[7] and then Eckhard[8] showed that formalism of the so-called Lie-algebraic perturbation theory in classical mechanics[9,10] might be applied to the Birkhoff–Gustavson normalization and

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extended to quantum mechanical systems, either directly, resulting in the expansion which, in the classical limit, is reduced to the Birkhoff–Gustavson normal form, or within a framework of an algebraic quantization.[11] This approach culminates in Ref. 12, where the exactness of the algebraic quantization prescription was proved up to any order of $\hbar$ for the polynomially perturbed nondegenerate harmonic oscillator.

An opposite trend of investigations originates from the canonical Van Vleck perturbation theory.[13,14] This procedure is a quantum mechanical analogue of the classical Lie-algebraic perturbation method. Surprisingly it dates back about 40 years before the corresponding procedures in classical mechanics[15,16] became available. Now the Van Vleck perturbation theory is widely used in quantum chemistry both for the analytical and numerical treatment of electronic degrees of freedom and analyses of molecular vibrations (see Refs. 17 and 18 and referencies therein). Several equivalent forms of such perturbation expansions were reviewed in Ref. 19. We choose here the most conceptually simple iterative order by order reduction of the Hamiltonian.

In this paper we will review algebraic aspects of the Birkhoff–Gustavson normalization for polynomially perturbed quantum mechanical harmonic oscillator. We describe it as a procedure to construct unitary transformation of an initial Hamiltonian into an operator belonging to the algebra of invariants for an unperturbed problem. Both the transformation and the transformed Hamiltonian are obtained as a (formal) power series in the perturbation constant. Doing this, we discuss the Gustavson invariants, their validity in the quantum case and a set of new, specific to quantum mechanics, invariants. Then, we demonstrate that, unlike the classical case, we can construct a formal process of diagonalization of the quantum mechanical Birkhoff–Gustavson normal form. In fact this process is a standard block diagonalization used in the Rayleigh–Schrödinger perturbation theory, recasted in the form of Wick normal ordered operators. We also describe another diagonalization process, which is a nonlinear generalization of Bogolyubov transformations used for the diagonalization of finite dimensional bilinear operator forms.[20] After this we discuss possible origins of the different behavior of classical and quantum mechanical perturbation procedures. Thus the Birkhoff–Gustavson normalization procedure for perturbed quantum mechanical harmonic oscillator is extended to a full equivalent of the Rayleigh–Schrödinger perturbation expansion applied for such a system (under the Rayleigh–Schrödinger perturbation expansion we assume the standard quantum mechanical perturbation treatment, including the expansion of operator resolvent and the subsequent diagonalization of energy shift operator by degenerate blocks[21,22]). All steps of the described procedure are entirely made with the Wick normal ordered operators.

Note that all calculations here are only formal, in a sense that neither discussion of power series convergence nor conditions for the existence of constructed operators are present.

Let us consider a **d** dimensional system with a Hamiltonian

$$\hat{H}(\hat{p},\hat{q}) = \sum_{k=0}^{\mathbf{d}} (\hat{p}_k^2 + \omega_k^2 \hat{q}_k^2) + \alpha \hat{H}_i(\hat{p},\hat{q}), \tag{1}$$

where $\hat{H}_i(\hat{p},\hat{q})$ is some polynomial in $\hat{p}_i$, $\hat{q}_i$. These operators of momentum and coordinate satisfy the canonical commutation relations

$$[\hat{p}_i,\hat{q}_j] = -i\,\delta_{ij}.$$

We are going to simplify the Hamiltonian performing subsequent unitary transformations according to Van Vleck[13] method.

A first step in the reduction of our Hamiltonian to the Birkhoff–Gustavson normal form will be the diagonalization of the unperturbed harmonic oscillator Hamiltonian. To do this, we had to perform the canonical transformation to the representation of ladder operators

$$\hat{a}_k=\frac{1}{\sqrt{2\omega_k}}(\hat{p}_k-i\omega_k\hat{q}_k),\quad k=1,\ldots,\mathbf{d}, \tag{2}$$

$$\hat{a}_k^+=\frac{1}{\sqrt{2\omega_k}}(\hat{p}_k+i\omega_k\hat{q}_k),$$

with commutation relations

$$[\hat{a}_k,\hat{a}_l^+]=\delta_{kl},$$

and all other commutators identical to zero.

In terms of the ''number'' operators $\hat{N}_k=\hat{a}_k^+\hat{a}_k$, the initial Hamiltonian will take the form

$$\hat{H}=\sum_{k=0}^{n}\omega_k\left(\hat{N}_k+\frac{1}{2}\right)+\alpha\hat{H}_i(\hat{a}_k^+,\hat{a}_k)=\hat{H}_0+\alpha\hat{H}_i,$$

where $\hat{H}_i(\hat{a}_k^+,\hat{a}_k)$ is a polynomial in $\hat{a}_k^+$, $\hat{a}_k$.

Before describing the Birkhoff–Gustavson perturbative treatment of the above system, let us remember some facts about its zero order approximation.

II. UNPERTURBED SYSTEM—MULTIDIMENSIONAL HARMONIC OSCILLATOR

In what follows it will be very convenient for us to use a compact ''vector'' notation for multi-indices. We will write $\overline{\mathbf{n}}$ as an abbreviation for a set of $\mathbf{d}$ non-negative integer indices $(n_1,\ldots,n_{\mathbf{d}})$. We will use other related notations:

- ''scalar'' product: $(\overline{\omega}\overline{\mathbf{n}})\overset{\text{def}}{=}\sum_{i=1}^{\mathbf{d}}\omega_i n_i$,
- ''norm'': $|\overline{\mathbf{n}}|\overset{\text{def}}{=}\sum_{i=1}^{\mathbf{d}}n_i$,
- multiindex factorials and binomial coefficients:

$$\overline{\mathbf{n}}!\overset{\text{def}}{=}n_1!\ldots n_{\mathbf{d}}!,$$

$$C_{\overline{\mathbf{n}}}^{\overline{\mathbf{m}}}\overset{\text{def}}{=}\prod_{k=1}^{\mathbf{d}}C_{n_k}^{m_k},$$

- product of operators: $\hat{a}^{\overline{\mathbf{m}}}\overset{\text{def}}{=}\hat{a}_1^{m_1}\ldots\hat{a}_{\mathbf{d}}^{m_d}$,
- and as a compact form for the system of inequalities we will write:

$$\overline{\mathbf{n}}\leqslant\overline{\mathbf{m}}\overset{\text{def}}{=}\begin{cases}n_1\leqslant m_1,\\ \ldots\\ n_{\mathbf{d}}\leqslant m_{\mathbf{d}}.\end{cases}$$

Before performing any actions on operators polynomial in $\hat{a}_k^+$, $\hat{a}_k$, we must, at first, reduce these operators to some standard ordering in constituent ladder operators. We will use the Wick

normal ordering prescription, in which any raising operator must be moved, using commutation relations, to the left and any lowering operator remains on the right. The Wick normal ordered form of the operator $\hat{A}$ will look like

$$\hat{A}=\sum A^{(W)}_{\mathbf{m},\mathbf{n}}\frac{\hat{a}^{+\overline{\mathbf{m}}}}{\sqrt{\overline{\mathbf{m}!}}}\frac{\hat{a}^{\overline{\mathbf{n}}}}{\sqrt{\overline{\mathbf{n}!}}}. \tag{3}$$

Note that we explicitly write out here normalizing denominators. This will be convenient for us when discussing the Rayleigh–Schrödinger transformations. Besides, several identities in this section will take the remarkably symmetrical form with such normalization.

The reduction to the Wick normal ordering may be extremely efficiently realized with the computer algebra system, since one may take full advantage of the following identity:

$$\hat{a}^{\overline{\mathbf{n}}}\hat{a}^{+\overline{\mathbf{m}}}=\sum_{\substack{\overline{\mathbf{k}}\leqslant\overline{\mathbf{n}}\\ \overline{\mathbf{k}}\leqslant\overline{\mathbf{m}}}}\overline{\mathbf{k}!}C^{\overline{\mathbf{k}}}_{\overline{\mathbf{m}}}C^{\overline{\mathbf{k}}}_{\overline{\mathbf{n}}}\hat{a}^{+\overline{\mathbf{m}}-\overline{\mathbf{k}}}\hat{a}^{\overline{\mathbf{n}}-\overline{\mathbf{k}}}. \tag{4}$$

This identity is a direct consequence of the Wick theorem on the product of two normal ordered operators. The theorem states that the Wick normal form of this product is equal to the sum of normal operator products with *all possible couplings* between operators. For any k couplings between multipliers, one has $C^k_n C^k_m$ different choices of two sets consisting of k indices of $\hat{a}$ and $\hat{a}^+$ in multipliers and $k!$ different couplings between these sets. The generalization to many dimensional cases using the ''vector'' notation is straightforward.

Explicitly writing out the normalizing denominators, we will use this reordering identity in the form

$$\frac{\hat{a}^{\overline{\mathbf{n}}}}{\sqrt{\overline{\mathbf{n}!}}}\frac{\hat{a}^{+\overline{\mathbf{m}}}}{\sqrt{\overline{\mathbf{m}!}}}=\sum_{\substack{\overline{\mathbf{k}}\leqslant\overline{\mathbf{n}}\\ \overline{\mathbf{k}}\leqslant\overline{\mathbf{m}}}}\sqrt{C^{\overline{\mathbf{k}}}_{\overline{\mathbf{m}}}C^{\overline{\mathbf{k}}}_{\overline{\mathbf{n}}}}\frac{\hat{a}^{+\overline{\mathbf{m}}-\overline{\mathbf{k}}}}{\sqrt{(\overline{\mathbf{m}}-\overline{\mathbf{k}})!}}\frac{\hat{a}^{\overline{\mathbf{n}}-\overline{\mathbf{k}}}}{\sqrt{(\overline{\mathbf{n}}-\overline{\mathbf{k}})!}}. \tag{5}$$

Now let us more closely consider the structure of the harmonic oscillator Hilbert space (Fock space) and operators on it.[23] This space has a ground state $|\overline{\mathbf{0}}\rangle$ and a complete orthonormal basis set created by powers of the raising operator

$$|\overline{\mathbf{m}}\rangle=\frac{\hat{a}^{+\overline{\mathbf{m}}}}{\sqrt{\overline{\mathbf{m}!}}}|\overline{0}\rangle.$$

This basis naturally induces the corresponding basis for operators. Indeed, any operator on Fock space may be decomposed as

$$\hat{A}=\sum_{\mathbf{m},\mathbf{n}}A^{(M)}_{\mathbf{m},\mathbf{n}}|\overline{\mathbf{m}}\rangle\langle\overline{\mathbf{n}}|=\sum_{\mathbf{m},\mathbf{n}}A^{(M)}_{\mathbf{m},\mathbf{n}}\frac{\hat{a}^{+\overline{\mathbf{m}}}}{\sqrt{\overline{\mathbf{m}!}}}\hat{P}_{\overline{\mathbf{0}}}\frac{\hat{a}^{\overline{\mathbf{n}}}}{\sqrt{\overline{\mathbf{n}!}}}, \tag{6}$$

where $\hat{P}_{\overline{\mathbf{0}}}=|\overline{\mathbf{0}}\rangle\langle\overline{\mathbf{0}}|$ is a projector on the ground state. This decomposition is the ''matrix'' form of the operator $\hat{A}$.

For any Wick normal ordered operator one may obtain its matrix form inserting an identity expansion

$$\hat{A}=\sum_{\bar{\mathbf{m}},n}A^{(W)}_{\bar{\mathbf{m}},\bar{\mathbf{n}}}\frac{\hat{a}^{+\bar{\mathbf{m}}}}{\sqrt{\bar{\mathbf{m}}!}}\frac{\hat{a}^{\bar{\mathbf{n}}}}{\sqrt{\bar{\mathbf{n}}!}}=\sum_{\bar{\mathbf{m}},\bar{\mathbf{n}}}A^{(W)}_{\bar{\mathbf{m}},\bar{\mathbf{n}}}\frac{\hat{a}^{+\bar{\mathbf{m}}}}{\sqrt{\bar{\mathbf{m}}!}}\left\{\sum_{\bar{\mathbf{k}}}|\bar{\mathbf{k}}\rangle\langle\bar{\mathbf{k}}|\right\}\frac{\hat{a}^{\bar{\mathbf{n}}}}{\sqrt{\bar{\mathbf{n}}!}}$$

$$=\sum_{\bar{\mathbf{m}},\bar{\mathbf{n}},\bar{\mathbf{k}}}A^{(W)}_{\bar{\mathbf{m}},\bar{\mathbf{n}}}\frac{\hat{a}^{+\bar{\mathbf{m}}+\bar{\mathbf{k}}}}{\sqrt{\bar{\mathbf{m}}!\bar{\mathbf{k}}!}}\hat{P}_{\bar{\mathbf{0}}}\frac{\hat{a}^{\bar{\mathbf{n}}+\bar{\mathbf{k}}}}{\sqrt{\bar{\mathbf{n}}!\bar{\mathbf{k}}!}}.$$

Changing summation indices, we conclude matrix elements of the operator $\hat{A}$ to be

$$A^{(M)}_{\bar{\mathbf{m}},\bar{\mathbf{n}}}=\sum_{\substack{\bar{\mathbf{k}}\le\bar{\mathbf{n}}\\ \bar{\mathbf{k}}\le\bar{\mathbf{m}}}}\sqrt{C^{\bar{\mathbf{k}}}_{\bar{\mathbf{m}}}C^{\bar{\mathbf{k}}}_{\bar{\mathbf{n}}}}A^{(W)}_{\bar{\mathbf{m}}-\bar{\mathbf{k}},\bar{\mathbf{n}}-\bar{\mathbf{k}}}. \tag{7}$$

One may obtain the inverse transformation from the matrix to the Wick normal ordered form of an operator using the following formula for the normal ordered form of the ground state projector[23]

$$\hat{P}_{\bar{\mathbf{0}}}=:\exp(-\hat{a}^{+}a):=\sum_{\bar{\mathbf{n}}}(-1)^{|\bar{\mathbf{n}}|}\frac{\hat{a}^{+\bar{\mathbf{n}}}\hat{a}^{\bar{\mathbf{n}}}}{\bar{\mathbf{n}}!}. \tag{8}$$

It is easy to check that the only nonzero matrix element of the above operator will be between a ground state wavefunctions. The substitution of this ground state projector into the definition of matrix form (6) results in the following connection between coefficients of normal and matrix forms of the operator:

$$A^{(W)}_{\bar{\mathbf{m}},\bar{\mathbf{n}}}=\sum_{\substack{\bar{\mathbf{k}}\le\bar{\mathbf{m}}\\ \bar{\mathbf{k}}\le\bar{\mathbf{n}}}}(-1)^{|\bar{\mathbf{k}}|}\sqrt{C^{\bar{\mathbf{k}}}_{\bar{\mathbf{m}}}C^{\bar{\mathbf{k}}}_{\bar{\mathbf{n}}}}A^{(M)}_{\bar{\mathbf{m}}-\bar{\mathbf{k}},\bar{\mathbf{n}}-\bar{\mathbf{k}}}. \tag{9}$$

Note the similarity of coefficients in (5), (7), and (9).

Now we proceed to the discussion of dynamical features of the harmonic oscillator. It is amazing that all in the rest of this section is a consequence of the following two commutators:

$$\begin{aligned}[\hat{N}_k,\hat{a}_k^m]&=-m\hat{a}_k^m,\\ [\hat{N}_k,\hat{a}_k^{+m}]&=m\hat{a}_k^{+m}.\end{aligned} \tag{10}$$

Commutation properties and unitary transformations of operators may be treated in a convenient way with the help of the superoperator formalism.[14] Here we will only outline some basics of it. For any operator $\hat{H}$ one may introduce the quantum Liouville superoperator which acts on the operator space

$$\hat{\mathscr{L}}_{\hat{H}}=[\hat{H},.],\quad \hat{\mathscr{L}}_{\hat{H}}\hat{A}=[\hat{H},\hat{A}]$$

(we will use the *calligraphic* style letters here to denote the superoperators)

Corresponding Liouville operator in the classical mechanics acts upon any function on the phase space resulting in the Poisson bracket with H:

$$\hat{\mathscr{L}}^{cl}_{H}A=\{H,A\}=\sum_k\left(\frac{\partial H}{\partial p_k}\frac{\partial A}{\partial q_k}-\frac{\partial A}{\partial p_k}\frac{\partial H}{\partial q_k}\right).$$

An interest to study $\hat{\mathscr{L}}_{\hat{H}}$ originates from the well-known fact that the exponent of this superoperator is a unitary map in the operator space

$$\tilde{A} = e^{i\alpha\hat{\mathscr{L}}_{\hat{H}}}\hat{A} = e^{i\alpha\hat{H}}\hat{A}e^{-i\alpha\hat{H}}.$$

Some properties of the general Liouville superoperator are summarized in Appendix A.

Here, in the harmonic oscillator context, we are particularly interested in $\hat{\mathscr{L}}_{\hat{H}_0} = [\Sigma_0^n \omega_k \hat{N}_k, .]$. Using the commutation properties (10) one can verify that any Wick normal ordered monomial is an eigenoperator of $\hat{\mathscr{L}}_{\hat{H}_0}$

$$\hat{\mathscr{L}}_{\hat{H}_0}\hat{a}^{+\mathbf{m}}\hat{a}^{\mathbf{n}} = (\overline{\omega,\mathbf{m}} - \overline{\mathbf{n}})\hat{a}^{+\mathbf{m}}\hat{a}^{\mathbf{n}}. \tag{11}$$

Since it is linear, the superoperator $\hat{\mathscr{L}}_{\hat{H}_0}$ admits the decomposition of its domain $\mathscr{D}$ into the direct sum $\mathscr{D} = \mathscr{N} \oplus \mathscr{R}$, where $\mathscr{N}$ or $\mathscr{R}$ are the kernel and the range space, respectively. The decomposition of the domain $\mathscr{D}$ into the desired form means that any element of it can be written uniquely as the sum of an element in the kernel space and an element in the range space. Now it may be easily seen that the linear superoperator $\hat{\mathscr{L}}_{\hat{H}_0}$ has the above decomposition, since each term in $\mathscr{D}$ is a linear combination of monomial terms, and since each monomial belongs to the kernel (range) space of $\hat{\mathscr{L}}_{\hat{H}_0}$ if and only if $(\overline{\omega,\mathbf{m}} - \overline{\mathbf{n}})$ equals (does not equal) zero.

In other words, every polynomial operator $\hat{P}$ on the harmonic oscillator Hilbert space may be uniquely decomposed into parts commutative and noncommutative with $\hat{H}_0$

$$\begin{aligned} &\hat{P} = \langle\hat{P}\rangle + \{\hat{P}\}, \\ &\hat{\mathscr{L}}_{\hat{H}_0}\langle\hat{P}\rangle = 0, \quad \langle\hat{P}\rangle \in \mathscr{N}; \\ &\hat{\mathscr{L}}_{\hat{H}_0}\{P\} \neq 0, \quad \{\hat{P}\} \in \mathscr{R}. \end{aligned} \tag{12}$$

In the classical mechanics the above appears as the decomposition of function on the phase space into the *secular* and the *periodical* parts.

For the perturbation theory which we will discuss further, it is crucial that on the range space of $\hat{\mathscr{L}}_{\hat{H}_0}$ this superoperator may be inverted. This means that for any polynomial operator $\hat{P}$ there exists another polynomial operator $\hat{G} \in \mathscr{R}$, such that

$$\hat{\mathscr{L}}_{\hat{H}_0}\hat{G} = -\hat{\mathscr{L}}_{\hat{G}}\hat{H}_0 = \{\hat{P}\}.$$

We will denote this operator as $\hat{G} = \hat{\mathscr{L}}_{\hat{H}_0}^{-1}\hat{P}$. If we demand that $\hat{\mathscr{L}}_{\hat{H}_0}^{-1}\langle\hat{P}\rangle = 0$, then the explicit construction of $\hat{G}$ for $\hat{P}$ will be

$$\hat{\mathscr{L}}_{\hat{H}_0}^{-1}\hat{P} = \sum{}' \frac{1}{(\overline{\omega,\mathbf{m}} - \overline{\mathbf{n}})} P^{(W)}_{\mathbf{m},\mathbf{n}}\hat{a}^{+\mathbf{m}}\hat{a}^{\mathbf{n}}, \tag{13}$$

where the prime indicates that all the terms with the vanishing denominators must be omitted from the sum.

One may easily check that for any Hermitian polynomial operator $\hat{P}$, operators $\hat{\mathscr{L}}_{\hat{H}_0}\hat{P}$ and $\hat{\mathscr{L}}_{\hat{H}_0}^{-1}\hat{P}$ are anti-Hermitian. We also mention here the superoperators $\hat{\mathscr{P}}_{\mathscr{R}} = \hat{\mathscr{L}}_{\hat{H}_0}^{-1}\hat{\mathscr{L}}_{\hat{H}_0}$ and $\hat{\mathscr{P}}_{\mathscr{N}} = 1 - \hat{\mathscr{P}}_{\mathscr{R}}$, projectors on $\mathscr{R}$ and $\mathscr{N}$ spaces, respectively. Primas[14] established formal expressions for these superoperators without any explicit reference to the matrix or the Wick normal ordered forms

$$\hat{\mathscr{P}}_{\mathscr{N}} = \lim_{\alpha \to 0} \alpha \int_0^\infty dt e^{-\alpha t} e^{-it\hat{\mathscr{L}}_{\hat{H}_0}}, \tag{14}$$

$$\hat{\mathscr{L}}_{\hat{H}_0}^{-1} = i \lim_{\alpha \to 0} \int_0^\infty dt e^{-\alpha t} e^{-it\hat{\mathscr{L}}_{\hat{H}_0}} (1 - \hat{\mathscr{P}}_{\mathscr{N}}).$$

Let us describe now a null subspace $\mathscr{N}$. This is the space of operators commutative with $\hat{H}_0$—a space of invariants of the harmonic oscillator. Due to the linearity of $\hat{\mathscr{L}}_{\hat{H}_0}$ and the Liebniz property

$$\hat{\mathscr{L}}_{\hat{H}}(\hat{A}\hat{B}) = \hat{A}(\hat{\mathscr{L}}_{\hat{H}}\hat{B}) + (\hat{\mathscr{L}}_{\hat{H}}\hat{A})\hat{B},$$

this space receives an algebraic structure. In fact $\mathscr{N}$ is the representation of the algebra of invariants for the harmonic oscillator, and we are going to describe now its basis.

First of all, there are **d** invariants, commutative with each other, which corresponded to the individual dimensions

$$\hat{N}_i = \hat{a}_i^+ \hat{a}_i, \quad i,j = 1, \ldots, \mathbf{d}, \tag{15}$$

$$[\hat{N}_i, \hat{N}_j] = 0.$$

The oscillator Hamiltonian $\hat{H}_0$ is the function of these invariants. In the classical mechanics the corresponding invariants are called *actions*.

At this point we will distinguish between the degenerate (resonance in classical mechanics) and nondegenerate case. One has $\mathbf{r}^{th}$-fold degeneracy whenever the ω_i, $i = 1, \ldots, \mathbf{d}$, are connected by **r** (and only **r**) linearly independent relations of commensurability

$$\sum_{i=1}^{\mathbf{d}} D_{ki}\omega_i = 0, \quad k = 1, \ldots, \mathbf{r}, \tag{16}$$

where all D_{ki} are integers. We will use this in more convenient vector form

$$(\overline{\omega}, \vec{D}_k) = 0, \tag{17}$$

where $\vec{D}_k$ is the set of **r** independent vectors with integer coefficients. If ω_i are rationally independent, the problem is nondegenerate (nonresonance).

As is known from the classical mechanics, otherwise ergodic on the surface of constant actions (N_i), the phase space trajectory of the classical oscillator with commensurability relations between frequencies will be bounded to the lower dimensional tori. Projection of such tori on the coordinate space of a two-dimensional oscillator, for example, is the famous Lissajous figures. The quantum mechanical oscillator with commensurable frequencies will have degenerate energy levels. This particular type of the degeneracy is historically named *accidental*, in contrast with the another *intrinsical* degeneracy of quantum mechanical systems originated from the spatial symmetries. Our attention will be focused here on the accidentally degenerate systems, since this type of degeneracy is responsible for most of the resonances in the classical limit.

In the nondegenerate case operators $\hat{N}_i$ form a full system of **d** invariants for the anisotropic harmonic oscillator with incommensurable frequencies. But in the degenerate case the harmonic oscillator has some hidden symmetry (responsible for the accidental degeneracy), which reveals itself in the existence of $2\mathbf{r}$ additional noncommutative non-Hermitian invariants $\hat{K}_i$ and $\hat{K}_i^+$

$$\hat{K}_i=\prod_{k=1}^{\mathbf{d}} \hat{b}_k^{|D_{ik}|}(\mathrm{sign}D_{ik}), \quad \hat{b}_k(l)=\begin{cases}\hat{a}_k^+, & l=+1,\\ \hat{a}_k, & l=-1,\end{cases} \quad i=1,\ldots,\mathbf{r}. \tag{18}$$

In general not all of these invariants ($\hat{N}$'s, $\hat{K}$'s and $\hat{K}^+$'s) are independent. We will neither construct here a maximal set of independent Hermitian invariants, nor explicitly establish their algebraic properties. We only note that in the classical mechanics the corresponding polynomials form a Lie algebra, but the quantum mechanical case is more complicated, and nonlinear extensions or quantum deformations of this Lie algebra arise.[24]

Instead we will focus our attention on the set of operators that form the center of the above algebra—the set of invariants commutative with all other invariants of the harmonic oscillator. As was explicitly shown in Ref. 25 any operator commutative with all the above written invariants ($\hat{N}$'s, $\hat{K}$'s and $\hat{K}^+$'s) for the **d** dimensional harmonic oscillator with **r** commensurability relations between frequencies is a function of **d** independent operators. These operators are divided into two distinct subgroups

•$\mathbf{d}-\mathbf{r}$ operators (Gustavson invariants) of form:

$$\hat{I}_i=\sum_{j=1}^{\mathbf{d}} \alpha_{ij}\hat{N}_j, \quad i=1,\ldots,\mathbf{d}-\mathbf{r}. \tag{19}$$

Here $\vec{\alpha}_i$ is any set of $\mathbf{d}-\mathbf{r}$ independent vectors orthogonal to all **r** commensurability vectors $\vec{D}_k$

$$\sum_{j=1}^{\mathbf{d}} \alpha_{ij}D_{kj}=0, \quad \begin{matrix} i=1,\ldots,\mathbf{d}-\mathbf{r},\\ k=1,\ldots,\mathbf{r}.\end{matrix}$$

A classical version of these invariants appeared in Ref. 2 as ''integrals of motions for normal form.'' Since $(\overline{\omega,\vec{D}_k})=0$, it is clear that the oscillator Hamiltonian $\hat{H}_0$ is a linear function of these invariants $\hat{I}_i$. Sometimes such operators are named the ''first order Casimirs.''

•New complementary **r** periodic invariants (''generalized parities''[25]), without the classical counterpart, of the form

$$\hat{V}_i=\exp\left(2\pi i\sum_{j=0}^{\mathbf{d}} \beta_{ij}\hat{N}_j\right), \quad i=1,\ldots,\mathbf{r}. \tag{20}$$

Here $\vec{\beta}_i$ is a set of **d** vectors dual to $\vec{D}_k$. Such β_{ij} satisfy the system

$$\sum_j \beta_{ij}D_{kj}=\delta_{ik}, \quad i=1,\ldots,\mathbf{r}.$$

The existence of these invariants for the quantum mechanical oscillator is a direct consequence of the general commutation relation $\hat{F}(\hat{N})\hat{a}^{+m}\hat{a}^n=\hat{a}^{+m}\hat{a}^n\hat{F}(\hat{N}+m-n)$, which may be proven for any operator function $\hat{F}$ if one compares matrix elements in both sides of the identity.

As we will see further, these invariants ($\hat{I}_i$ and $\hat{V}_i$) will survive under the general perturbation of the harmonic oscillator. Unlike them, the invariants $\hat{N}_i$ and $\hat{K}_i$ will be destroyed under the perturbation. This means that there is no analytical extension of these invariants to the perturbed case.

Now, having described the unperturbed system we will return to the perturbed one.

III. THE BIRKHOFF–GUSTAVSON NORMALIZATION

In this section we will briefly describe the formal reduction of the general Hamiltonian

$$\hat{H}=\sum_{i=0}^{\infty}\alpha^i\hat{H}_i, \tag{21}$$

into a simpler form by unitary transformations with generators chosen from the range of $\hat{\mathscr{L}}_{\hat{H}_0}$. As we will see further, the word ''simpler'' means that the transformed Hamiltonian will have the diagonal or the block-diagonal matrix form. Since we deal now with the Wick normal ordered operators, we will use the following definition by Gustavson[2] for the Hamiltonian in the Birkhoff–Gustavson normal form (BGNF):

The Hamiltonian $\hat{H}=\Sigma_{i=0}^{\infty}\alpha^i\hat{H}_i$ *is in BGNF up to the order* α^n *if all terms in it of the order* α^i, $i<n$ *belong to the kernel subspace of* $\hat{\mathscr{L}}_{\hat{H}_0}$.

In other words, part of our Hamiltonian transformed into the BGNF will be commutative with the unperturbed Hamiltonian, and thus belongs to the algebra of invariants for the unperturbed problem. Note that by assumption our Hamiltonian is normalized (is in BGNF) at least up to the first order ($\hat{H}_0\in\ker\hat{\mathscr{L}}_{\hat{H}_0}$).

This definition of the normalized Hamiltonian was used by Gustavson in the case of the classical mechanics to describe the formal process of the reduction of the classical Hamiltonian to a simpler (integrable) form. The original version of normalization process used the formalism of *generating functions*, which in quantum mechanics leads to additional complications due to the noncommutability of operators. An example of a similar approach may be found in Ref. 26. Fortunately, the original Gustavson algorithm was modified[8] using formalism of *generators* of symplectic transformations,[9] which has the direct quantum mechanical counterpart. Let us now describe it.

Assume that quantum mechanical Hamiltonian of type (21) is in BGNF up to the order n. Our aim is to find such unitary transformation, after application of which, the original Hamiltonian will be normalized up to the order $n+1$

$$\begin{aligned}\hat{H}_{BG}=e^{i\alpha^n\hat{G}_n}\hat{H}e^{-i\alpha^n\hat{G}_n}&=e^{i\alpha^n\hat{\mathscr{L}}_{\hat{G}_n}}\left(\sum_{m=0}^{\infty}\alpha^m\hat{H}_m\right)\\&=\sum_{m=0}^{\infty}\alpha^m\left(\sum_{k=0}^{[m/n]}\frac{1}{k!}\hat{\mathscr{L}}^k_{i\hat{G}_n}\hat{H}_{m-nk}\right)\\&=\hat{H}_0+\alpha\hat{H}_1+\cdots+\alpha^{n-1}\hat{H}_{n-1}+\alpha^n(\hat{H}_n+\hat{\mathscr{L}}_{i\hat{G}_n}\hat{H}_0)+O(\alpha^{n+1})\\&=\text{(already normalized terms)}+\alpha^n(\hat{H}_n-i\hat{\mathscr{L}}_{\hat{H}_0}\hat{G}_n)+O(\alpha^{n+1});\end{aligned}$$

here $[m/n]$ denote an integer part of this quotient.

As was demonstrated in the previous section, we may always find the Hermitian operator $\hat{G}_n=-i\hat{\mathscr{L}}^{-1}_{\hat{H}_0}\{\hat{H}_n\}$ from $\mathscr{R}$ such that

$$\hat{\mathscr{L}}_{\hat{H}_0}\hat{G}_n=-i\{\hat{H}_n\}.$$

After the unitary transformation with generator $\hat{G}_n$ our Hamiltonian becomes normalized up to the order $n+1$ too,

$$\hat{H}_{BG}=\hat{H}_0+\alpha\langle\hat{H}_1\rangle+\cdots+\alpha^{n-1}\langle\hat{H}_{n-1}\rangle+\alpha^n\langle H_n\rangle+O(\alpha^{n+1}).$$

It is clear from the above that repeating the procedure for $n+1$, etc., we obtain a formal process of normalization of the original Hamiltonian to subsequently higher orders.

In summary, we describe the construction for initial Hamiltonian (21) and any number n of such unitary transformation

$$e^{i\alpha\hat{\Gamma}_{(n)}(\alpha)}=e^{i\alpha^n\hat{G}_n}\cdots e^{i\alpha^2\hat{G}_2}e^{i\alpha\hat{G}_1}, \tag{22}$$

that our Hamiltonian will be in the Birkhoff–Gustavson normal form up to the order $n+1$. Now we will demonstrate an application of the above defined procedure to two general classes of quantum mechanical systems.

A. Nondegenerate systems

In the case when no commensurability relations (16) exist, the unperturbed system has commutative symmetry algebra, and the kernel subspace of $\hat{\mathscr{L}}_{\hat{H}_0}$ consists only of polynomials of $\hat{N}_k$. In this case the Hamiltonian reduced to Birkhoff–Gustavson normal form became diagonal in representation of $\hat{N}_k$ operators.

A normalized part of the nondegenerate Hamiltonian will be a function of **d** Hermitian operators $\hat{N}_k$, each being commutative with all others (and the normalized part of Hamiltonian). These **d** operators form a Complete Set of Commutative Operators for such system. The explicit form of these operators in the initial representation is

$$\tilde{N}_k=e^{-i\alpha\hat{\mathscr{L}}_{\hat{\Gamma}_{(n)}}}\hat{N}_k=e^{-i\alpha\hat{G}_1}\cdots e^{-i\alpha^n\hat{G}_n}\hat{N}_k e^{i\alpha^n\hat{G}_n}\cdots e^{i\alpha\hat{G}_1}, \tag{23}$$

and may be easily calculated as a power series expansions up to the desired order in α.

Approximations of perturbed eigenvalues and eigenfunctions up to $o(\alpha^n)$ are classified by the complete set of **d** quantum numbers n_k and are given by

$$E_{\tilde{\mathbf{n}}}=H_{BG}(n_1,\ldots,n_{\mathbf{d}}),\quad |\tilde{\mathbf{n}}\rangle=e^{-i\alpha\hat{\Gamma}_{(n)}}|\overline{\mathbf{n}}\rangle. \tag{24}$$

Due to the uniqueness of asymptotic power series in α, the results of the above procedure coincide with the Rayleigh–Schrödinger perturbation expansion for eigenvalues and eigenfunctions of the perturbed quantum mechanical system.

Note that, if we restore powers of $\hbar$ in the above formulas, operators $\tilde{N}_k$ will naturally realize the program of the Einstein–Brillouin–Kemmer quantization for all orders of α in the quasi-classical approximation.[26] This fact leads also to the success of the so-called quasi-classical quantization of the Birkhoff normal form.[4]

1. Example 1. One-dimensional anharmonic oscillator

The system described by Hamiltonian

$$\hat{H}=\hat{p}^2+\hat{q}^2+\alpha\hat{q}^4.$$

After normalization of the Hamiltonian up to α^6

$$\begin{aligned}\hat{H}_{BG}=&2\left(\hat{N}+\frac{1}{2}\right)\\&+\alpha\left(\frac{3}{8}+\frac{3}{2}\left(\hat{N}+\frac{1}{2}\right)^2\right)\\&-\alpha^2\left(\frac{67}{32}\left(\hat{N}+\frac{1}{2}\right)+\frac{17}{8}\left(\hat{N}+\frac{1}{2}\right)^3\right)\end{aligned}$$

$$+\alpha^3\left(\frac{1539}{1024}+\frac{1707}{128}\left(\hat{N}+\frac{1}{2}\right)^2+\frac{375}{64}\left(\hat{N}+\frac{1}{2}\right)^4\right)$$
$$-\alpha^4\left(\frac{305141}{8192}\left(\hat{N}+\frac{1}{2}\right)+\frac{89165}{1024}\left(\hat{N}+\frac{1}{2}\right)^3+\frac{10689}{512}\left(\hat{N}+\frac{1}{2}\right)^5\right)$$
$$+\alpha^5\left(\frac{1456569}{32768}+\frac{9317949}{16384}\left(\hat{N}+\frac{1}{2}\right)^2+\frac{587265}{1024}\left(\hat{N}+\frac{1}{2}\right)^4+\frac{87549}{1024}\left(\hat{N}+\frac{1}{2}\right)^6\right)$$
$$+\cdots.$$

Here we see the first terms of the Rayleigh–Schrödinger perturbation expansion for the anharmonic oscillator. The growth of numerical coefficients in higher order terms reflects an asymptotic behavior of perturbative approximations. Using (24) we obtain perturbed eigenfunctions (not presented here).

The discussion of perturbation expansion for the quartic anharmonic oscillator and the reasons why coefficients in eigenvalues series are polynomials with the definite parity of $(\hat{N}+1/2)$ alone, may be found in Ref. 27.

B. Accidentally degenerate systems

Now we will consider a case of nonzero number of commensurability vectors (16). The unperturbed quantum mechanical system in such a case will have accidentally degenerate energy levels, and, as we have previously discussed, additional noncommutative invariants. Now the kernel subspace of $\hat{\mathscr{L}}_{\hat{H}_0}$ consists of not only polynomials of $\hat{N}_k$, but also includes all the Wick normal ordered monomials for which $(\omega,\overline{\mathbf{m}}-\overline{\mathbf{n}})=0$. The corresponding classical system is referred to as resonance.

Here and in what follows we will suppose that Hamiltonian is in BGNF up to sufficiently high order in α, and will usually omit the unnormalized part of it, dealing only with the normalized one.

It is clear from the previous section that the normalized Hamiltonian may be written in the form of power series in invariants of the unperturbed system. Due to noncommutativity of these invariants, some ordering for any term in this series must be imposed. Since not all of the above invariants are independent, this power series may be even nonunique. Series of such type appear as the ''standard form'' of the classical BGNF in Ref. 11 (in fact no connection was established in this paper between such series and the invariants of the unperturbed system).

Because **d** invariants $\hat{I}$ and $\hat{V}$ are commutative with all other invariants of the unperturbed problem, these operators will be commutative with the normalized Hamiltonian as well. This means that for the degenerate system we again have **d** commutative with each other and the Hamiltonian operators (compare to $\mathbf{d}-\mathbf{r}$ Gustavson invariants for the corresponding classical system). But now the reduced Hamiltonian $\hat{H}_{BG}$ is *not* a function of $\hat{I}$ and $\hat{V}$ operators only, and these **d** commutative operators *do not* form the Complete Set of Commutative Operators for the degenerate system.

Note, that any degenerate eigensubspace of the oscillator Hamiltonian is the degenerate eigensubspace for each of the **d** invariant operators $\hat{I}$ and $\hat{V}$ as well. This follows from the fact that quantum numbers $\vec{N}$ for two eigenvectors of $\hat{H}_0$ with the same eigenvalue may differ only in integer coefficient combination of $\vec{D}_i$. As a result eigenvalues of **d** operators $\hat{I}$ and $\hat{V}$ will *not* classify the degenerate eigenstates of the perturbed system. This is not surprising, since the splitting of $\hat{H}$ eigenvalues depends on the *perturbation* $\hat{H}_i$, and cannot be described by operators originating from the center of the algebra of invariants for the *unperturbed* system. One may obtain these perturbative invariants in the initial representation similar to those in (23).

1. Example 2. The Henon–Heiles system

The Henon–Heiles two-dimensional system was originally used by Gustavson[2] as the first example of BGNF. This system is described by (1:1) resonance Hamiltonian

$$\hat{H}=\tfrac{1}{2}(\hat{p}_1^2+\hat{q}_1^2+\hat{p}_2^2+\hat{q}_2^2)+\alpha(\hat{q}_2^3-\tfrac{1}{3}\hat{q}_1^2 q_2).$$

After normalization of Hamiltonian up to α^4

$$\begin{aligned}\hat{H}_{BG}=&\left(1-\frac{1}{9}\alpha^2-\frac{11}{108}\alpha^4\right)+\left(1-\frac{2}{3}\alpha^2-\frac{61}{54}\alpha^4\right)(\hat{a}_1^+\hat{a}_1+\hat{a}_2^+\hat{a}_2)\\&-\frac{1}{12}\alpha^2\left(5+\frac{47}{4}\alpha^2\right)(\hat{a}_1^{+2}\hat{a}_1^2+\hat{a}_2^{+2}\hat{a}_2^2)-\frac{7}{12}\alpha^2\left(1-\frac{1}{4}\alpha^2\right)(\hat{a}_1^{+2}\hat{a}_2^2+\hat{a}_2^{+2}\hat{a}_1^2)\\&+\frac{1}{3}\alpha^2\left(1-\frac{27}{4}\alpha^2\right)\hat{a}_1^+\hat{a}_2^+\hat{a}_1\hat{a}_2\\&+\alpha^4\left(+\frac{101}{432}\hat{a}_1^{+3}\hat{a}_1^3-\frac{161}{144}\hat{a}_1^{+3}\hat{a}_1\hat{a}_2^2-\frac{65}{16}\hat{a}_1^{+2}\hat{a}_2^+\hat{a}_1^2\hat{a}_2+\frac{175}{144}\hat{a}_1^{+2}\hat{a}_2^+\hat{a}_2^3\right.\\&\left.-\frac{235}{432}\hat{a}_2^{+3}\hat{a}_2^3-\frac{161}{144}\hat{a}_1^+\hat{a}_2^{+2}\hat{a}_1^3+\frac{47}{16}\hat{a}_1^+\hat{a}_2^{+2}\hat{a}_1\hat{a}_2^2+\frac{175}{144}\hat{a}_2^{+3}\hat{a}_1^2\hat{a}_2\right)\\&+\ldots\ .\end{aligned}\tag{25}$$

The above discussion systematizes the structure of the normalized Hamiltonian, but unfortunately has not answered the question about eigenvalues and eigenfunctions of the perturbed system. The definite solution of this may be obtained following the guidelines of the Rayleigh–Schrödinger perturbation theory for degenerate systems.

As we have already noticed, in the degenerate case the Hamiltonian reduced to the BGNF is, in general, not diagonal in the $\hat{N}_k$ representation. But, since the normalized part of the Hamiltonian $\hat{H}_{BG}$ is *commutative* with the unperturbed Hamiltonian $\hat{H}_0$, the matrix of $\hat{H}_{BG}$ must be *block-diagonal* in this representation, with blocks corresponding to degenerate eigenstates of $\hat{H}_0$. This apparently becomes evident if one converts $\hat{H}_{BG}$ into the matrix form. Doing this, it is easy to recognize that the condition $(\overline{\omega,\mathbf{n}})=(\overline{\omega,\mathbf{m}})$ means that all nonzero matrix elements of $\hat{H}_{BG}$ must connect only states corresponding to the same energy of the unperturbed system.

At this point one usually performs the standard procedure for the Rayleigh–Schrödinger perturbation theory:

With account for the matrix form of $\hat{H}_{BG}$ being block-diagonal, one needs solve secular equations for these blocks and perform a unitary diagonalizing transformation inside each block independently, obtaining eigenvalues and eigenvectors for the perturbed system.

This procedure supposes the conversion of $\hat{H}_{BG}$ into the matrix form. But it is interesting that we can perform essentially the same diagonalization in the Wick normal form of operators as well. This leads to an unusual class of unitary transformations, not infinitesimal in nature, which we will also refer to as the Rayleigh–Schrödinger transformations.

IV. RAYLEIGH–SCHRÖDINGER TRANSFORMATIONS

We will utilize now the obvious fact that due to algebraic structure, the kernel subspace of $\hat{\mathscr{L}}_{\hat{H}_0}$ is stable against unitary transformations from it. For any monomial, belonging to the kernel subspace $\mathscr{N}$ of $\hat{\mathscr{L}}_{\hat{H}_0}$ (or, equivalently, the algebra of invariants for the harmonic oscillator), we introduce the characteristic functional Λ

$$\Lambda(\hat{a}^{+\overline{\mathbf{n}}}\hat{a}^{\overline{\mathbf{m}}}) \overset{\text{def}}{=} (\overline{\omega,\mathbf{m}}) = (\overline{\omega,\mathbf{n}}). \tag{26}$$

This characteristic functional will take values of energy levels of the unperturbed system. The value of this characteristic functional for a polynomial operator will be the minimum of Λ values for individual monomials in that operator.

Now we can group the terms of the reduced Hamiltonian by Λ values

$$\hat{H}_{BG} = \sum_{\Lambda} \sum_{\substack{\overline{\mathbf{m},\mathbf{n}} \\ (\omega,\overline{\mathbf{n}})=\Lambda \\ (\omega,\overline{\mathbf{m}})=\Lambda}} H^{(W)}_{\overline{\mathbf{m},\mathbf{n}}} \frac{\hat{a}^{+\overline{\mathbf{m}}}}{\sqrt{\overline{\mathbf{m}!}}} \frac{\hat{a}^{\overline{\mathbf{n}}}}{\sqrt{\overline{\mathbf{n}!}}}. \tag{27}$$

We note here that the expansion of any operator belonging to $\mathcal{N}$ into the power series in $\hat{a}^+$ and $\hat{a}$ leads to the expansion in monomials with increasing values of characteristic functional Λ.

Whereas all presented in this section is quite clear from the matrix form point of view, it is not the case with the Wick normal ordered form of operators. Appendix B will shed some light on the underlying mathematics for products of Wick normal ordered operators belonging to $\mathcal{N}$.

In this appendix we demonstrate that:

- The value of characteristic functional Λ for the product of two operators is greater or equal to that of multipliers

$$\Lambda(\hat{A}\hat{B}) \geqslant \max(\Lambda(\hat{A}), \Lambda(\hat{B})).$$

- Terms having the minimal allowed value of $\Lambda = \Lambda_0$ in the product of two homogeneous operators: $\hat{A}, \hat{B} \in \mathcal{N}$, $\Lambda(\hat{A}) = \Lambda(\hat{B}) = \Lambda_0$, will obey the matrix multiplication law

$$\sum_{\mathbf{k}\mathbf{l}} A_{\overline{\mathbf{k}\mathbf{l}}} \frac{\hat{a}^{+\overline{\mathbf{k}}}}{\sqrt{\overline{\mathbf{k}!}}} \frac{\hat{a}^{\overline{\mathbf{l}}}}{\sqrt{\overline{\mathbf{l}!}}} \sum_{\mathbf{m}\mathbf{n}} B_{\overline{\mathbf{m}\mathbf{n}}} \frac{\hat{a}^{+\overline{\mathbf{m}}}}{\sqrt{\overline{\mathbf{m}!}}} \frac{\hat{a}^{\overline{\mathbf{n}}}}{\sqrt{\overline{\mathbf{n}!}}} = \sum_{\mathbf{k}\mathbf{n}} \left(\sum_{\mathbf{m}} A_{\overline{\mathbf{k}\mathbf{m}}} B_{\overline{\mathbf{m}\mathbf{n}}} \right) \frac{\hat{a}^{+\overline{\mathbf{k}}}}{\sqrt{\overline{\mathbf{k}!}}} \frac{\hat{a}^{\overline{\mathbf{n}}}}{\sqrt{\overline{\mathbf{n}!}}} + (\cdots).$$

We proceed now to the explicit construction of the diagonalizing transformation. Let us consider, for any possible value of $\Lambda = \Lambda_0$, a subspace of our Hilbert space spanned by eigenvectors of $\hat{H}_0$ with an eigenvalue equal to Λ_0. The orthogonal projector on this finite-dimensional subspace is

$$\hat{P} = \sum_{\substack{\overline{\mathbf{n}} \\ (\omega,\overline{\mathbf{n}})=\Lambda_0}} |\overline{\mathbf{n}}\rangle\langle\overline{\mathbf{n}}|.$$

Using (9) we convert this projector into the Wick normal ordered form

$$\hat{P} = \sum_{\Lambda \geqslant \Lambda_0} \sum_{\substack{\overline{\mathbf{n}} \\ (\omega,\overline{\mathbf{n}})=\Lambda}} \left\{ \sum_{\substack{\overline{\mathbf{k}\leqslant\mathbf{n}} \\ (\omega,\overline{\mathbf{k}})=\Lambda-\Lambda_0}} (-1)^{|\overline{\mathbf{k}}|} C^{\overline{\mathbf{k}}}_{\overline{\mathbf{n}}} \right\} \frac{\hat{a}^{+\overline{\mathbf{n}}}\hat{a}^{\overline{\mathbf{n}}}}{\overline{\mathbf{n}!}}. \tag{28}$$

For any unitary matrix $u_{\overline{\mathbf{m}\mathbf{n}}}$ with dimensions equal to those of this Λ_0 subspace we construct corresponding operator $\hat{u} = \Sigma u_{\overline{\mathbf{m}\mathbf{n}}} |\overline{\mathbf{m}}\rangle\langle\overline{\mathbf{n}}|$ with the properties

$$\hat{u}^+\hat{u} = \hat{P},$$
$$\hat{u}\hat{P} = \hat{P}\hat{u} = \hat{u},$$
$$[\hat{H}_0, \hat{u}] = 0.$$

Again we convert this ''unitary inside block'' operator into the Wick normal ordered form as

$$\hat{u}=\sum_{\Lambda\geqslant\Lambda_0}\left\{\sum_{\substack{\overline{\mathbf{m}},\overline{\mathbf{n}},\overline{\mathbf{k}}\\(\omega,\overline{\mathbf{n}})=\Lambda_0\\(\omega,\overline{\mathbf{m}})=\Lambda_0\\(\omega,\overline{\mathbf{k}})=\Lambda-\Lambda_0}}(-1)^{|\overline{\mathbf{n}}|}u_{\overline{\mathbf{m}},\overline{\mathbf{n}}}\sqrt{C^{\overline{\mathbf{k}}}_{\overline{\mathbf{m}}+\overline{\mathbf{k}}}C^{\overline{\mathbf{k}}}_{\overline{\mathbf{n}}+\overline{\mathbf{k}}}}\frac{\hat{a}^{+\overline{\mathbf{m}}+\overline{\mathbf{k}}}}{\sqrt{(\overline{\mathbf{m}}+\overline{\mathbf{k}})!}}\frac{\hat{a}^{\overline{\mathbf{n}}+\overline{\mathbf{k}}}}{\sqrt{(\overline{\mathbf{n}}+\overline{\mathbf{k}})!}}\right\}. \tag{29}$$

To finish the construction of the commutative with $\hat{H}_0$ unitary operator we must extend $\hat{u}$ to our full Hilbert space as

$$\hat{U}=1-\hat{P}+\hat{u}. \tag{30}$$

This operator is the normal form of the unitary transformation performed in the Λ_0 block of the matrix form independently. The transformation of this type is used in the Rayleigh–Schrödinger perturbation theory for the final diagonalization of the degenerate block in the Hamiltonian. We explicitly present here expressions [(28)–(30)] to outline the cumbersome structure of $\hat{U}$ in the Wick normal ordered form. The construction of the above operator makes it clear that performing the subsequent unitary transformations of type (30) we will diagonalize the Hamiltonian reduced to BGNF by blocks with increasing values of characteristic functional Λ.

Indeed, suppose that all terms in our Hamiltonian with the value of characteristic functional $\Lambda<\Lambda_0$ are already diagonalized

$$\hat{H}_{BG}=\sum_{(\omega,\mathbf{k})<\Lambda_0}H^{(\Lambda)}_{\mathbf{kk}}\frac{\hat{a}^{+\overline{\mathbf{k}}}\hat{a}^{\overline{\mathbf{k}}}}{\mathbf{k}!}+\sum_{\substack{(\omega,\overline{\mathbf{n}})=\Lambda_0\\(\omega,\overline{\mathbf{m}})=\Lambda_0}}H^{(\Lambda_0)}_{\overline{\mathbf{mn}}}\frac{\hat{a}^{+\overline{\mathbf{m}}}}{\sqrt{\overline{\mathbf{m}}!}}\frac{\hat{a}^{\overline{\mathbf{n}}}}{\sqrt{\overline{\mathbf{n}}!}}+(\cdots). \tag{31}$$

In order to construct the diagonalizing transformation $\hat{U}$ we must solve the following secular equation:

$$\det\left(H^{(\Lambda_0)}_{\overline{\mathbf{mn}}}+\sum_{(\omega,\mathbf{k})<\Lambda_0}H^{(\Lambda)}_{\mathbf{kk}}C^{\overline{\mathbf{k}}}_{\overline{\mathbf{n}}}\delta_{\overline{\mathbf{mn}}}-E_{\overline{\mathbf{nn}}}\delta_{\overline{\mathbf{mn}}}\right)=0. \tag{32}$$

Suppose that we can obtain its solution at least as a power series in some rational power of α (Puizeaux series). After this we will have the diagonalizing unitary finite-dimensional matrix $u_{\overline{\mathbf{mn}}}$ and construct its normal form (30). In the transformed operator

$$\hat{H}_D=\hat{U}\hat{H}_{BG}\hat{U}^{+},$$

all terms with the characteristic value $\Lambda=\Lambda_0$ will also be diagonal.

This process results in the expansion of the Hamiltonian in diagonal operators with increasing characteristic values of Λ, or equivalently, the increasing powers of raising and lowering operators. If we cut this expansion on some value of $\Lambda=\Lambda_0$, then analytical expressions for all exited states originating from states of the unperturbed Hamiltonian with the energy $E\leqslant\Lambda_0$ will be obtained up to the desired order of perturbation parameter α.

After such transformation the diagonalized part of $\hat{H}_D$ will be an (operator) function of **d** commutative operators $\widetilde{N}_i$. Eigenvalues of these operators will classify eigenvalues of the perturbed system with the complete set of **d** quantum numbers.

1. Example 2 (continued). Complete diagonalization of the Henon–Heiles system

As one may see from the previous example, for the reduced to the BGNF Henon–Heiles Hamiltonian (25), the first excited state, corresponding to $\Lambda=1$, is doubly degenerate. But the reduced Hamiltonian is already diagonal on the subspace spanned by kets $\hat{a}_1^+|\mathbf{0}\rangle$ and $\hat{a}_2^+|\mathbf{0}\rangle$.

On subspaces of the next exited states, corresponding to $\Lambda=2$ and 3 this Hamiltonian will be diagonalized by the unitary transformation $\hat{H}_D=\hat{U}\hat{H}_{BG}\hat{U}^+$, where

$$\begin{aligned}\hat{U}=1&+\frac{\sqrt{2}}{4}\hat{a}_2^{+2}\hat{a}_1^2-\frac{1}{2}\left(1-\frac{\sqrt{2}}{2}\right)\hat{a}_2^{+2}\hat{a}_2^2-\frac{\sqrt{2}}{4}\hat{a}_1^{+2}\hat{a}_2^2-\frac{1}{2}\left(1-\frac{\sqrt{2}}{2}\right)\hat{a}_1^{+2}\hat{a}_1^2\\&+\left(\frac{1}{3}-\frac{\sqrt{2}}{4}\right)\hat{a}_1^{+3}\hat{a}_1^3+\frac{1}{4}\hat{a}_1^{+3}\hat{a}_1^2\hat{a}_2+\frac{\sqrt{2}}{4}\hat{a}_1^{+3}\hat{a}_1\hat{a}_2^2-\frac{1}{12}\hat{a}_1^{+3}\hat{a}_2^3\\&+\frac{1}{4}\hat{a}_1^{+2}\hat{a}_2^+\hat{a}_1^3-\frac{\sqrt{2}}{4}\hat{a}_1^{+2}\hat{a}_2^+\hat{a}_1^2\hat{a}_2+\frac{1}{4}\hat{a}_1^{+2}\hat{a}_2^+\hat{a}_1\hat{a}_2^2+\frac{\sqrt{2}}{4}\hat{a}_1^{+2}\hat{a}_2^+\hat{a}_2^3\\&-\frac{\sqrt{2}}{4}\hat{a}_1^+\hat{a}_2^{+2}\hat{a}_1^3+\frac{1}{4}\hat{a}_1^+\hat{a}_2^{+2}\hat{a}_1^2\hat{a}_2-\frac{\sqrt{2}}{4}\hat{a}_1^+\hat{a}_2^{+2}\hat{a}_1\hat{a}_2^2+\frac{1}{4}\hat{a}_1^+\hat{a}_2^{+2}\hat{a}_2^3\\&+\frac{1}{12}\hat{a}_2^{+3}\hat{a}_1^3-\frac{\sqrt{2}}{4}\hat{a}_2^{+3}\hat{a}_1^2\hat{a}_2-\frac{1}{4}\hat{a}_2^{+3}\hat{a}_1\hat{a}_2^2+\left(\frac{1}{3}-\frac{\sqrt{2}}{4}\right)\hat{a}_2^{+3}\hat{a}_2^3+(\cdots).\end{aligned}\tag{33}$$

Here the first row diagonalizes $\Lambda=2$ part of $\hat{H}_{BG}$. It is easy to check the unitarity (up to $\Lambda=3$) of the above transformation. The transformed Hamiltonian will now take the following diagonal form:

$$\begin{aligned}\hat{H}_D=&\left(1-\frac{1}{9}\alpha^2-\frac{11}{108}\alpha^4\right)+\left(1-\frac{2}{3}\alpha^2-\frac{61}{54}\alpha^4\right)\hat{N}_1+\left(1-\frac{2}{3}\alpha^2-\frac{61}{54}\right)\alpha^4\hat{N}_2\\&+\alpha^2\left(\frac{1}{3}-\frac{9}{4}\alpha^2\right)\hat{N}_1\hat{N}_2\\&+\frac{1}{2}\alpha^2\left(\frac{1}{3}-\frac{9}{4}\alpha^2\right)(\hat{N}_1-1)_2-\alpha^2\left(1+\frac{5}{6}\alpha^2\right)(\hat{N}_2-1)_2\\&+\alpha^2\left(\frac{7}{6}+\frac{229}{216}\alpha^2\right)(\hat{N}_2-2)_3-\frac{95}{54}\alpha^4(\hat{N}_1-2)_3\\&-\alpha^2\left(\frac{7}{6}+\frac{1}{8}\alpha^2\right)\hat{N}_1(\hat{N}_2-1)_2-\alpha^2\left(\frac{7}{3}-\frac{1}{6}\alpha^2\right)\hat{N}_2(\hat{N}_1-1)_2+(\cdots).\end{aligned}\tag{34}$$

Notation $(x)_n$ is used here for the Pochammer polynomial

$$(x)_n=x(x+1)\cdots(x+n-1).$$

Note that (34) holds only for the values of quantum numbers n_1 and n_2 such that $n_1+n_2\leqslant 3$. This formula provides us with analytical expressions up to $o(\alpha^4)$ for the 10 lowest eigenvalues of the Henon–Heiles system.

An alternative to the above diagonalization process may be established. Since we deal with the Wick normal ordered operators, it is even more natural to diagonalize $\Lambda=\Lambda_0$ terms in (31) using the explicitly unitary operator

$$\hat{H}_D=e^{i\hat{\mathscr{Z}}_{\hat{w}}}\hat{H}_{BG}=\hat{U}\hat{H}_{BG}\hat{U}^+,$$

where

$$\hat{U}=e^{i\hat{w}}=\exp\left(i\sum_{\substack{(\omega,\mathbf{n})=\Lambda_0\\(\omega,\overline{\mathbf{m}})=\Lambda_0}} w_{\overline{\mathbf{mn}}}\frac{\hat{a}^{+\overline{\mathbf{m}}}}{\sqrt{\overline{\mathbf{m}!}}}\frac{\hat{a}^{\overline{\mathbf{n}}}}{\sqrt{\overline{\mathbf{n}!}}}\right), \tag{35}$$

and $w_{\overline{\mathbf{mn}}}$ is a finite dimensional Hermitian matrix such that the exponent of it coincides with the used above finite dimensional diagonalizing unitary matrix $u_{\overline{\mathbf{mn}}}$

$$u_{\overline{\mathbf{mn}}}=(e^{iw})_{\overline{\mathbf{mn}}}. \tag{36}$$

It immediately follows from the results of Appendix B that $\Lambda=\Lambda_0$ terms in operator (35) coincide with those of the Rayleigh–Schrödinger transformation (28)–(30), and therefore the transformed Hamiltonian will also become diagonal in Λ_0 terms. To continue the diagonalization process, we need to calculate terms with characteristic value $\Lambda>\Lambda_0$ in operator exponent (35). We can perform this exponentiation using the block-diagonality of the operator

$$\hat{w}=\sum_{\substack{(\omega,\mathbf{n})=\Lambda_0\\(\omega,\overline{\mathbf{m}})=\Lambda_0}} w_{\overline{\mathbf{mn}}}\frac{\hat{a}^{+\overline{\mathbf{m}}}}{\sqrt{\overline{\mathbf{m}!}}}\frac{\hat{a}^{\overline{\mathbf{n}}}}{\sqrt{\overline{\mathbf{n}!}}}.$$

At first we convert the operator $\hat{w}$ into the matrix form. Since it is block-diagonal, the exponent of $\hat{w}$ is reduced to exponentiation of independent finite-dimensional blocks, and may be performed by algebraic methods. The last step will be to convert the resulting operator again into the Wick normal ordered form. Unfortunately secular equations appearing during the application of this process are, in general, more complicated.

2. Example 3. Exponent of block diagonal operator

Diagonalization of $\Lambda=2$ terms in the Hamiltonian of Henon–Heiles system (25) was done in Example 2 by the first row of (33). Alternatively we may use the operator:

$$\hat{U}=\exp\frac{\pi}{8}(\hat{a}_2^{+2}\hat{a}_1^2-\hat{a}_1^{+2}\hat{a}_2^2).$$

For illustration purposes we calculate the Wick normal ordered form of this operator up to $\Lambda=3$ terms using the above procedure

$$\begin{aligned}\hat{U}=1&+\frac{\sqrt{2}}{4}\hat{a}_2^{+2}\hat{a}_1^2-\frac{1}{2}\left(1-\frac{\sqrt{2}}{2}\right)\hat{a}_2^{+2}\hat{a}_2^2-\frac{\sqrt{2}}{4}\hat{a}_1^{+2}\hat{a}_2^2-\frac{1}{2}\left(1-\frac{\sqrt{2}}{2}\right)\hat{a}_1^{+2}\hat{a}_1^2\\&+\left(\frac{1}{3}-\frac{\sqrt{2}}{4}+\frac{1}{6}\cos\left(\frac{\sqrt{3}}{4}\pi\right)\right)(\hat{a}_2^{+3}\hat{a}_2^3+\hat{a}_1^{+3}\hat{a}_1^3)\\&+\left(\frac{\sqrt{2}}{4}-\frac{\sqrt{3}}{6}\sin\left(\frac{\sqrt{3}}{4}\pi\right)\right)(\hat{a}_1^{+3}\hat{a}_1\hat{a}_2^2+\hat{a}_1^{+2}\hat{a}_2^+\hat{a}_2^3-\hat{a}_1^+\hat{a}_2^{+2}\hat{a}_1^3-\hat{a}_3^{+3}\hat{a}_1^2\hat{a}_2)\\&+\left(\frac{1}{2}\cos\left(\frac{\sqrt{3}}{4}\pi\right)-\frac{\sqrt{2}}{4}\right)(\hat{a}_1^+\hat{a}_2^{+2}\hat{a}_1\hat{a}_2^2+\hat{a}_1^{+2}\hat{a}_2^+\hat{a}_1^2\hat{a}_2)+(\cdots).\end{aligned}$$

We note that (35) is a straightforward generalization of the transformation used by Bogolyubov and Bogolyubov[20] for the diagonalization of $\Lambda=1$ bilinear operator forms.

If we restore the $\hbar$ in the above constructions, it becomes clear that these diagonalization processes are of pure quantum origin, without the classical analogue. Indeed, increasing powers of $\hbar$ will appear in the denominators of expressions corresponding to the higher energy levels. In the classical region ($N_i \to \infty$, $\hbar \to 0$, $\hbar N_i = \text{const}$), whenever the multiplicity of the degenerate energy levels tends to infinity, such diagonalizing transformations, as well as the additional perturbative invariants $\hat{V}_i$ will not have the definite limit. However more detailed studies of the intermediate quasiclassical region should be performed.

V. SUMMARY AND DISCUSSIONS

In this paper we have described the Birkhoff–Gustavson normalization as a procedure to transform the Hamiltonian of **d** dimensional harmonic oscillator with polynomial perturbation into the operator belonging to the algebra of invariants for the unperturbed problem. The transformed Hamiltonian was obtained (at least formally) as an expansion in powers of perturbation constant and generators of this algebra.

It is known[10] that in the classical perturbation theory the **d** dimensional system with the **r** resonance conditions between frequencies may be (formally) reduced to the **r** dimensional system. This reduction is made using $\mathbf{d}-\mathbf{r}$ Gustavson invariants, since each of them may be analytically continued to the invariant of perturbed system. But the classical Hamiltonian with more than one degree of freedom is, in general, nonintegrable. This means that, in general, the classical perturbation theory failed to give analytical predictions for the system with two or more resonance conditions. The perturbative description of such systems is possible only for very special classes of resonance conditions and/or perturbations.

Unlike this, the quantum mechanical perturbation theory does not have this conceptual difficulty and always results in definite (formal, but frequently asymptotic) approximations to eigenvalues and eigenvectors of the perturbed system. As has been shown in the previous section, this leads to the fact that we can always construct the process of diagonalization of the quantum mechanical Birkhoff–Gustavson normal form. Possibly, this rather different behavior of two very close in spirit procedures may be attributed to the existence of **r** additional quantum mechanical invariants.

From the other point of view, we note that the described diagonalization of the quantum mechanical BGNF is achieved using two different power series expansions. One of them was made in powers of the perturbation constant α, and the other in powers of ladder operators $\hat{a}$ and $\hat{a}^+$. Classical mechanics is more restrictive. Since all classical variables are commutative, the BGNF expansion in powers of α coincides with the expansion in powers of a and a^+. Moreover, the original definitions by Birkhoff[1] and Gustavson[2] of normalization procedure were made in terms of power series in variables, rather than the perturbation constant. Because of this, one cannot, in general, diagonalize the reduced-to-BGNF classical Hamiltonian.

It is worth mentioning that the described diagonalization process, when applied to the Wick normal ordered operators, includes the construction of very interesting, not infinitesimally close to unity, unitary transformations. These transformations may be treated as nonlinear generalizations of the finite dimensional Bogolyubov transformations.

In summary, we demonstrate that the Birkhoff–Gustavson normalization procedure for the perturbed multidimensional harmonic oscillator may be extended, in the quantum mechanics, to the full equivalent of the Rayleigh–Schrödinger perturbation expansion for such a system. All steps of this procedure are performed on Wick normal ordered operators.

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APPENDIX A: THE LIOUVILLE SUPEROPERATOR

We summarize here some of the properties of general Liouville superoperator $\hat{\mathscr{L}}_{\hat{H}}$ (α, β and ϵ constants):

1. $\hat{\mathscr{L}}_{\hat{H}}$ is linear: $\hat{\mathscr{L}}_{\hat{H}}(\alpha\hat{A}+\beta B)=\alpha\hat{\mathscr{L}}_{\hat{H}}A+\beta\hat{\mathscr{L}}_{\hat{H}}B$,
2. and antisymmetric: $\hat{\mathscr{L}}_{\hat{A}}\hat{B}=-\hat{\mathscr{L}}_{\hat{B}}\hat{A}$,
3. it obeys the Liebniz rule: $\hat{\mathscr{L}}_{\hat{H}}(\hat{A}\hat{B})=\hat{A}(\hat{\mathscr{L}}_{\hat{H}}B)+(\hat{\mathscr{L}}_{\hat{H}}A)\hat{B}$,
4. and the Jakoby identity: $\hat{\mathscr{L}}_{\hat{H}}([\hat{A},\hat{B}])=[\hat{A},\hat{\mathscr{L}}_{\hat{H}}\hat{B}]+[\hat{\mathscr{L}}_{\hat{H}}\hat{A},\hat{B}]$,
5. or equivalently: $\hat{\mathscr{L}}_{[\hat{A},\hat{B}]}=[\hat{\mathscr{L}}_{\hat{A}},\hat{\mathscr{L}}_{\hat{B}}]$,
6. $\hat{\mathscr{L}}^{n}_{\hat{H}}[\hat{A},\hat{B}]=\Sigma^{n}_{m=0}C^{m}_{n}[\hat{\mathscr{L}}^{m}_{\hat{H}}\hat{A},\hat{\mathscr{L}}^{n-m}_{\hat{H}}\hat{B}]$,

an exponent of it is the linear map which preserves the algebraic properties of operators:

7. $e^{\epsilon\hat{\mathscr{L}}_{\hat{H}}}(\alpha\hat{A}+\beta B)=\alpha e^{\epsilon\hat{\mathscr{L}}_{\hat{H}}}\hat{A}+\beta e^{\epsilon\hat{\mathscr{L}}_{\hat{H}}}\hat{B}$,
8. $e^{\epsilon\hat{\mathscr{L}}_{\hat{H}}}(\hat{A}\hat{B})=(e^{\epsilon\hat{\mathscr{L}}_{\hat{H}}}\hat{A})(e^{\epsilon\hat{\mathscr{L}}_{\hat{H}}}\hat{B})$,
9. $e^{\epsilon\hat{\mathscr{L}}_{\hat{H}}}[\hat{A},\hat{B}]=[e^{\epsilon\hat{\mathscr{L}}_{\hat{H}}}\hat{A},e^{\epsilon\hat{\mathscr{L}}_{\hat{H}}}\hat{B}]$,
10. and may be decomposed as: $e^{\epsilon\hat{\mathscr{L}}_{\hat{H}}}\hat{A}=e^{\epsilon\hat{H}}\hat{A}e^{-\epsilon\hat{H}}$.

Properties 1–9 take place both in the quantum and classical case with the corresponding change, whenever needed, of the commutator to the Poisson bracket ($[.,.]\to\{.,.\}$).

APPENDIX B: PRODUCTS OF INVARIANT POLYNOMIALS

Consider the product of two operators $\hat{A}$ and $\hat{B}$ belonging to the kernel subspace of $\hat{\mathscr{L}}_{\hat{H}_0}$. We assume that minimal values of the characteristic functional $\Lambda(\hat{a}^{+\overline{\mathbf{m}}}\hat{a}^{\overline{\mathbf{n}}})=(\overline{\omega,\mathbf{m}})=(\overline{\omega,\mathbf{n}})$ for monomials in each of the above operators are Λ_A and Λ_B, respectively. We are interested in terms with the minimal value of Λ in this product. Using (4) we may write down these terms as

$$\sum_{\overline{\mathbf{kl}}}\frac{A_{\overline{\mathbf{kl}}}}{\sqrt{\mathbf{k!l!}}}\hat{a}^{+\overline{\mathbf{k}}}\hat{a}^{\overline{\mathbf{l}}}\sum_{\overline{\mathbf{mn}}}\frac{B_{\overline{\mathbf{mn}}}}{\sqrt{\mathbf{m!n!}}}\hat{a}^{+\overline{\mathbf{m}}}\hat{a}^{\overline{\mathbf{n}}}=\sum_{\overline{\mathbf{klmn}}}D_{\overline{\mathbf{klmn}}}\hat{a}^{+\overline{\mathbf{k}}+\overline{\mathbf{m}}-\min(\overline{\mathbf{l}},\overline{\mathbf{m}})}\hat{a}^{\overline{\mathbf{n}}+\overline{\mathbf{l}}-\min(\overline{\mathbf{l}},\overline{\mathbf{m}})}+(\cdots)$$

$$=\sum_{\overline{\mathbf{klmn}}}D_{\overline{\mathbf{klmn}}}\hat{a}^{+\overline{\mathbf{k}}-\overline{\mathbf{l}}+\max(\overline{\mathbf{l}},\overline{\mathbf{m}})}\hat{a}^{\overline{\mathbf{n}}-\overline{\mathbf{m}}+\max(\overline{\mathbf{l}},\overline{\mathbf{m}})}+(\cdots), \tag{B1}$$

where terms with the greater value of characteristic functional Λ are denoted by $(\cdots)$. The notation ''$\max(\overline{\mathbf{l},\mathbf{m}})$'' is used for the vector, each component of which is the maximum of the correspondent component of $\overline{\mathbf{l}}$ and $\overline{\mathbf{m}}$. Coefficients D are

$$D_{\overline{\mathbf{klmn}}}=\frac{A_{\overline{\mathbf{kl}}}}{\sqrt{\mathbf{k!l!}}}\frac{B_{\overline{\mathbf{mn}}}}{\sqrt{\mathbf{m!n!}}}(\min(\overline{\mathbf{l},\mathbf{m}}))!C^{\overline{\mathbf{m}}-\min(\overline{\mathbf{l}},\overline{\mathbf{m}})}_{\overline{\mathbf{m}}}C^{\overline{\mathbf{l}}-\min(\overline{\mathbf{l}},\overline{\mathbf{m}})}_{\overline{\mathbf{l}}}.$$

Let us calculate characteristic values Λ for explicitly written terms in (B1)

$$\Lambda=(\overline{\omega,\mathbf{n}}-\overline{\mathbf{m}}+\max(\overline{\mathbf{l},\mathbf{m}}))=(\overline{\omega,}\max(\overline{\mathbf{l},\mathbf{m}}))\geqslant\begin{cases}(\omega,\overline{\mathbf{l}})=\Lambda_A,\\(\omega,\overline{\mathbf{m}})=\Lambda_B,\end{cases}$$

since all $\omega_i>0$.

Consider now the homogeneous case, whenever each monomial in both operators has equal characteristic value Λ_0. The minimal allowed value of Λ in product $\hat{A}\hat{B}$ will have terms with $\Lambda=\Lambda_0$, or

$$(\overline{\omega},\max(\overline{\mathbf{l}},\overline{\mathbf{m}}))=(\overline{\omega},\overline{\mathbf{l}}),$$

$$(\overline{\omega},\max(\overline{\mathbf{l}},\overline{\mathbf{m}}))=(\overline{\omega},\overline{\mathbf{m}}).$$

The above equalities may take place only for $\overline{\mathbf{l}}=\overline{\mathbf{m}}$. So, the product of homogeneous in Λ polynomials will take the form

$$\sum_{\mathbf{k}\,\mathbf{l}} A_{\overline{\mathbf{k}\,\mathbf{l}}}\frac{\hat{a}^{+\overline{\mathbf{k}}}}{\sqrt{\mathbf{k}!}}\frac{\hat{a}^{\overline{\mathbf{l}}}}{\sqrt{\mathbf{l}!}}\sum_{\mathbf{m}\,\mathbf{n}} B_{\overline{\mathbf{m}\,\mathbf{n}}}\frac{\hat{a}^{+\overline{\mathbf{m}}}}{\sqrt{\overline{\mathbf{m}!}}}\frac{\hat{a}^{\overline{\mathbf{n}}}}{\sqrt{\overline{\mathbf{n}!}}}=\sum_{\mathbf{k}\,\overline{\mathbf{n}}}\left(\sum_{\mathbf{m}} A_{\overline{\mathbf{k}\mathbf{m}}}B_{\overline{\mathbf{m}\,\mathbf{n}}}\right)\frac{\hat{a}^{+\overline{\mathbf{k}}}}{\sqrt{\mathbf{k}!}}\frac{\hat{a}^{\overline{\mathbf{n}}}}{\sqrt{\overline{\mathbf{n}!}}}+(\cdots). \tag{B2}$$

This is the standard matrix multiplication law.

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Geometries of quantum states

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The quantum analog of the Fisher information metric of a probability simplex is searched and several Riemannian metrics on the set of positive definite density matrices are studied. Some of them appeared in the literature in connection with Cramér–Rao-type inequalities or the generalization of the Berry phase to mixed states. They are shown to be stochastically monotone here. All stochastically monotone Riemannian metrics are characterized by means of operator monotone functions and it is proven that there exist a maximal and a minimal among them. A class of metrics can be extended to pure states and a constant multiple of the Fubini–Study metric appears in the extension. © *1996 American Institute of Physics.* [S0022-2488(96)00706-2]

I. INTRODUCTION

The state space of a classical system with n alternatives is the simplex of probability distributions on the n-point-space. The probability simplex is an $n-1$- dimensional manifold with boundary and its affine structure is fairly trivial. The extreme boundary consists of n discrete points. In quantum mechanics, the state space of an n level system is identified with the set of all $n\times n$ positive semidefinite complex matrices of trace 1. (They are called density matrices.) The case $n=2$ is easily visualized as the unit ball in the three-space.

$$\frac{1}{2}\begin{pmatrix} 1+x & y+iz \\ y-iz & 1-x \end{pmatrix} \leftrightarrow (x,y,z)\in\mathbb{R}^3 \quad (x^2+y^2+z^2\leqslant 1).$$

The boundary consists of noninvertible matrices and it is an infinite set. The case $n=2$ is simple but for higher n the structure of the topological boundary is rather complicated. The extreme boundary consists of the density matrices of rank one and for $n>2$ it is much smaller than the topological boundary. As far as dimensionality is concerned, the topological boundary has dimension n^2-2 and the extreme one has dimension $2n-2$. The extreme states are usually called pure and they are described in the textbooks by nonzero vectors of a complex Hilbert space of linear dimension n. The same state is described by a vector ψ as well as $\lambda\psi$, where λ is any complex number different from 0. This means that pure states are in one-to-one correspondence to rays $\{\lambda\psi: 0\neq\lambda\in\mathbb{C}\}$. The rays form a smooth manifold called complex projective space, $\mathbb{C}P^{(n-1)}$.

On the level of convex structure the difference between the classical and quantum state space is well understood. The classical one is a Choquet simplex and different axiomatizations of the quantum one are available in the literature; the reader may be referred to Ref. 1, for example. Our main concern here is the possible Riemannian structure in the quantum case. Before turning to that subject, we review briefly the classical case, that is, the Riemannian structure on the space of measures.

From the viewpoint of information geometry, the spherical representation of the probability simplex is adequate, because the squared length of the tangent vector of a curve equals the Fisher

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information. Indeed, introduce the parameters $z_i=2\sqrt{p_i}$, where $1\leqslant i\leqslant n$ and $\Sigma_i p_i=1$. Then $\Sigma_i z_i^2=4$ and the probability simplex is parametrized with a portion of the n-sphere. Let $x(t)$ be a curve on the sphere. The square of the length of the tangent is

$$\langle \partial_t x, \partial_t x\rangle=\sum_i\ (\partial_t x_i)^2=\sum_i\ p_i(t)(\partial_t\ \log\ p_i(t))^2,$$

which is the Fisher information. The geodesic distance between two probability distributions Q and R can be computed along a great circle and it is a simple transform of the Hellinger distance. Reference 2 contains further details as well as statistical applications of this geometric approach. To the best of our knowledge, Riemannian metric on quantum states was first considered by Helstrom in connection with state estimation theory.[3] Since Helstrom's work, several other metrics appeared in the literature (see, for example, Refs. 4–7) and Uhlmann approached Helstrom's metric in a different way.[8,9]

The present paper is organized as follows. In Sec. II we survey the work of Chentsov both in the probabilistic and in the quantum case. We explain how he arrived at the study of invariant metrics on the space of probability measures, motivated by decision theory, and how far he could go towards the quantum generalization after his unicity result about the Fisher information in the probabilistic context. The survey on Chentsov's work is believed to be essential. On the one hand, his papers are not easy to access and on the other hand our main result is the completion of the program he initiated. Our results are contained in Secs. III and IV. We construct monotone metrics by means of operator monotone functions and prove that all monotone metrics are obtained in this way. It turns out that the symmetric logarithmic derivative metric of Helstron (which is the same as the metric studied by Uhlmann) is monotone. Furthermore, this metric is minimal among all monotone metrics. The subject of Sec. IV is the extension of monotone metrics to pure states. We prove that if the extension exists, then it coincides with the standard metric on pure states up to a constant factor. Only the metric of the symmetric logarithmic derivative yields the Fubini–Study extension.

II. THE VIEWPOINT OF CHENTSOV

Chentsov was led by decision theory when he considered a category whose objects are probability spaces and whose morphisms are Markov kernels. Although he worked in Ref. 10 with arbitrary probability spaces, his idea can be demonstrated very well on finite ones. In this case a morphism from the probability n-simplex $\mathscr{S}_n$ to an m-simplex $\mathscr{S}_m$ is an $m\times n$ stochastic matrix. If Π is such a matrix and $P\in\mathscr{S}_n$, then $\Pi P\in\mathscr{S}_m$ is considered more random than P. Generally speaking, the parametrized family (Q_i) is more random than the parametrized family (P_i) (with the same parameter set) if there exists a stochastic matrix Π such that $\Pi P_i=Q_i$ for every value of the parameter i. Two parametric families (P_i) and (Q_i) are equivalent in the theory of statistical inferences if there are two stochastic matrices $\Pi^{(12)}$ and $\Pi^{(21)}$ such that

$$\Pi^{(12)}P_i=Q_i\quad\text{and}\quad\Pi^{(21)}Q_i=P_i \tag{2.1}$$

for every i. Chentsov said a numerical function f defined on pairs of measures to be invariant if

$$(P_1,P_2)\sim(Q_1,Q_2)\quad\text{implies}\quad f(P_1,P_2)=f(Q_1,Q_2) \tag{2.2}$$

and monotone if

$$f(P_1,P_2)\geqslant f(\Pi P_1,\Pi P_2) \tag{2.3}$$

for every stochastic matrix Π. A monotone function f is obviously invariant. Statistics and information theory know a lot of monotone functions, relative entropy, and its generalizations are so.

If a Riemannian metric is given on all probability simplexes, then this family of metrics is called invariant (respectively, monotone) if the corresponding geodesic distance is an invariant (respectively, monotone) function. Chentsov's great achievement was that up to a constant factor the Fisher information yields the only monotone family of Riemannian metrics on the class of finite probability simplexes (Ref. 10; see also Ref. 11). A decade later Chentsov turned to the quantum case, where the probability simplex is replaced by the set of density matrices. A linear mapping between two matrix spaces sends a density matrix into a density matrix if the mapping preserves trace and positivity (i.e., positive semidefiniteness). By now it is well understood that complete positivity is a natural and important requirement in the noncommutative case.[12,13] Therefore, we call a trace preserving completely positive mapping stochastic. One of the equivalent forms of the complete positivity of a map T is the following:

$$\sum_{i=1}^{n}\sum_{j=1}^{n} a_i^* T(b_i^* b_j) a_j \geqslant 0$$

for all possible choice of a_i, b_i, and n. A completely positive mapping T satisfies the Schwarz inequality: $T(a^*a) \geqslant T(a)^* T(a)$.

Chentsov recognized that stochastic mappings are the appropriate morphisms in the category of quantum state spaces. (Reference 12 contains more information about stochastic mappings; see also Ref. 13.) The above definitions of invariance and monotonicity make sense when stochastic matrices are replaced by stochastic mappings. Chentsov (with Morozova) aimed to find the invariant (or monotone) Riemannian metrics in quantum setting as well. They obtained the following result.[14] Assume that a family of Riemannian metrics is given on all spaces of density matrices, which is invariant. Then there exist a function $c(x,y)$ and a constant C such that the squared length of a tangent vector $A=(A_{ij})$ at a diagonal point $D=\mathbf{Diag}(p_1,p_2,\ldots,p_n)$ is of the form

$$C\sum_{k=1}^{n} p_k^{-1} A_{kk}^2 + 2\sum_{j<k} c(p_j,p_k)|A_{jk}|^2. \tag{2.4}$$

Furthermore, the function $c(x,y)$ is symmetric and $c(\lambda x,\lambda y)=\lambda^{-1}c(x,y)$. This result of Morozova and Chentsov was not complete. Although they had proposals for the function $c(x,y)$, they did not prove monotonicity or invariance of any of the corresponding metrics. A complete result will be given here but now a few comments on (2.4) are in order.

Both the function $c(x,y)$ and the constant are independent from the matrix size n. Restricting ourselves to diagonal matrices, which is in some sense a step back to the probability simplex, we can see that there is no ambiguity of the metric. Loosely speaking, the unicity result in the simplex case survives along the diagonal and the off-diagonal provides new possibilities for the definition of a stochastically invariant metric.

III. RIEMANNIAN METRICS ON QUANTUM STATES

The demand for Riemannian structure on the whole quantum state space or on a parametrized family of density operators appeared in mathematical physics a long time ago and in rather different contexts.

In the parametric problem of quantum statistics a family (D_θ) of states of a systems is given and one has to decide between several alternative values of the parameter by using measurements. The set of outcomes of the applied measurements is the parameter set Θ and we assume that it is a region in $\mathbb{R}^m$. So an estimator measurement M is a positive-operator-valued measure on the Borel sets of Θ and its values are observables of the given quantum system. The probability measure $B\mapsto\mu_\theta(B)=\mathrm{Tr}(D_\theta M(B))(B\subset\Theta)$ represents the result of the measurement M when the ''true'' state is D_θ. The choice of the estimators has to be made by taking into account the expected errors. The aim of an optimal decision process is to search for estimators with small

error. To an error one can attribute several sizes. For example, one can seek a measurement such that its value is ''approximately'' equal to the true parameter value. If this holds ''in the mean,'' then the estimator is free of distorsion and such an estimator is commonly called unbiased. The accuracy of an unbiased measurement is described by the total mean-square deviation which should be small on the parameter space if we want to choose an effective estimator measurement.

The quantum state estimation was initiated by Helstrom in the 1960s (Ref. 3, see also Ref. 15). He followed the Cramér–Rao pattern of mathematical statistics and introduced the concept of symmetric logarithmic derivative. Let M be a positive-operator-valued measure on $\mathbb{R}^n$. The corresponding measurement is an unbiased estimator of the parameter $\theta=(\theta_1,...,\theta_m)$ if

$$\int_{\mathbb{R}^m} \theta_i \, d\mathrm{Tr}(D_t M)(\theta) = t_i \tag{3.1}$$

for every $1 \leqslant i \leqslant m$. [The integration is taken with respect to the measure $B \mapsto \mathrm{Tr}(D_t M(B))$.] The symmetric logarithmic derivatives L_θ^i are observables defined as

$$\frac{\partial \mathrm{Tr}(D_\theta A)}{\partial \theta_i} = \frac{1}{2}\,\mathrm{Tr}((L^i(\theta)D_\theta + D_\theta L^i(\theta))A) \tag{3.2}$$

for every observable A. The measurement has two characteristic matrices, the covariance matrix $C(\theta)=(C_{ij}(\theta))$ and the information matrix $J(\theta)=(J_{ij}(\theta))$. They are determined as follows:

$$C_{ij}(\theta) = \int_{\mathbb{R}^m} (t_i-\theta_i)(t_j-\theta_j) d\mathrm{Tr}(D_\theta M)(t), \quad J_{ij}(\theta) = \mathrm{Tr}(D_\theta L^i(\theta) L^j(\theta)). \tag{3.3}$$

A quantum version of the Cramér–Rao inequality, due to Helstrom, says that

$$C(\theta) \geqslant J(\theta)^{-1} \tag{3.4}$$

for an unbiased measurement. (The inequality means that the difference is positive semidefinite.) The information matrix $J(\theta)$ may be regarded as the metric tensor on the parameter space.

From the point of view of the statistical state estimation problem, the number n of the real parameters is much smaller than the dimension of the whole state space. However, we can parametrize the whole state space as well. Assume that the parametrization is affine,

$$D_\theta = I/n + \sum_i \theta_i a_i, \tag{3.5}$$

where a_i are traceless selfadjoint matrices. Here D_θ is positive definite if θ is in a certain open subset of $\mathbb{R}^{n^2-1}$ and the mapping $D_\theta \mapsto \theta \in \mathbb{R}^{n^2-1}$ yields an atlas of a single chart. We refer to (3.5) as the affine parametrization of invertible density matrices $\mathscr{D}_n$.

The Riemannian metric of the symmetric logarithmic derivative may be written in the form (2.4) as

$$\|(A_{ij})\|_D^2 = \sum_{k=1}^n p_k^{-1} A_{kk}^2 + 2\sum_{j<k} \frac{2}{p_j+p_k} |A_{jk}|^2, \tag{3.6}$$

where $D=\mathbf{Diag}(p_1,p_2,\ldots,p_n)$ is a diagonal footpoint and A is a tangent vector at D (that is, $A=A^*$ and $\mathrm{Tr}\,A=0$). So the Morozova–Chentsov function of the metric of the symmetric logarithmic derivative is

$$c(x,y)=\frac{2}{x+y}. \tag{3.7}$$

Uhlmann obtained essentially the same Riemannian metric in a completely different approach. He wrote the density matrices D in the form

$$W^*W=D. \tag{3.8}$$

Since $\mathrm{Tr}\, W^*W=\mathrm{Tr}\, D=1$, W can be regarded as a unit vector in a larger Hilbert space, and W is often called a purification of the density matrix D. There are many choices for W when D is given. Let $D(t)$ be a smooth curve of density matrices with purification $W(t)$. If the arclength of $W(t)$ with respect to the standard Fubini–Study metric is minimal, then the so-called paralellity condition

$$W(t)^*\dot{W}(t)=\dot{W}(t)^*W(t), \quad \dot{W}(t)=\frac{dW(t)}{dt}, \tag{3.9}$$

is satisfied. The shortest purification curve leads to the Bures distance on the set of density matrices and the corresponding Riemannian metric is the metric of symmetric logarithmic derivative (see Refs. 8 and 9 for details). It is worthwhile to mention that Dittmann computed several geometric characteristics of the space of density matrices endowed with the above metric.[16] For example, this space is not locally symmetric and all sectional curvatures are greater than 1. Braunstein and Caves obtained recently the same metric by optimizing over all generalized quantum measurements that can be used to distinguish neighboring quantum states D and $D+dD$.[5]

If a distance between density matrices expresses statistical distinguishability, then this distance must decrease under coarse-graining. A good example of coarse-graining arises when a density matrix is partitioned in the form of a 2×2 block matrix, and the coarse-graining forgets about the offdiagonal:

$$\begin{pmatrix} A & B \\ B^* & C \end{pmatrix} \mapsto \begin{pmatrix} A & 0 \\ 0 & C \end{pmatrix}.$$

In the mathematical formulation, a coarse-graining is a completely positive mapping which preserves the trace and hence sends density matrix into density matrix. Such a mapping will be called stochastic below. A Riemannian metric is defined to be monotone if the differential of any stochastic mapping is a contraction. If the affine parametrization is considered, then $D_t=D+tA$ is a curve for an invertible density D and for a self-adjoint traceless A. Under a stochastic mapping $\mathbf{T}$ this curve is transformed into $\mathbf{T}(D_t)=\mathbf{T}(D)+t\mathbf{T}(A)$ provided that $\mathbf{T}(D)$ is an invertible density and the real number t is small enough. The monotonicity condition for the Riemannian metric g on $\mathscr{M}_n$ reads as

$$g_{\mathbf{T}(D)}(\mathbf{T}(A),\mathbf{T}(A))\leqslant g_D(A,A), \tag{3.10}$$

where D is an invertible density, A is traceless self-adjoint, and $\mathbf{T}$ is stochastic. Our goal is to show many examples of monotone metrics and to give their characterization in terms of operator monotone functions.

Let us recall that a function $f:\mathbb{R}^+\to\mathbb{R}$ is called operator monotone if the relation $0\leqslant K\leqslant H$ implies $0\leqslant f(K)\leqslant f(H)$ for any matrices K and H (of any order). The theory of operator monotone functions was established in the 1930s by Löwner and there are several reviews on the subject, for example, Refs. 17 and 18 are suggested.

Let us introduce some superoperators as

$$\mathbf{L}_D(A)=DA, \quad \mathbf{R}_D(A)=AD, \quad A\in M_n(\mathbb{C}). \tag{3.11}$$

Theorem 3.1: Let $f:\mathbb{R}^+\to\mathbb{R}^+$ be an operator monotone function such that $f(t)=tf(t^{-1})$ for every $t>0$ and set a superoperator

$$\mathbf{K}_D=\mathbf{R}_D^{1/2}f(\mathbf{L}_D\mathbf{R}_D^{-1})\mathbf{R}_D^{1/2} \tag{3.12}$$

acting on matrices. Then the relation

$$g_D(A,B)=\mathrm{Tr}(\mathbf{K}_D^{-1}(A)B) \tag{3.13}$$

determines a monotone Riemannian metric on $\mathscr{M}_n$.

Proof: Since an operator monotone function is analytic, the bilinear form (3.13) is smooth in D. The condition $f(t)=tf(t^{-1})$ on f makes sure that $\mathbf{K}_D^{-1}(A)$ is self-adjoint whenever A is so. Hence the bilinear form (3.13) is real. For an invertible D the superoperator $\mathbf{K}_D$ is invertible and positive definite. So (3.13) is really a nondegenerate metric and its monotonicity is to be checked.

In Ref. 19 the following inequality was obtained:

$$\mathbf{T}\mathbf{R}_F^{1/2}f(\mathbf{L}_E\mathbf{R}_F^{-1})\mathbf{R}_F^{1/2}\mathbf{T}^\star\leqslant\mathbf{R}_{\mathbf{T}(F)}^{1/2}f(\mathbf{L}_{\mathbf{T}(E)}\mathbf{R}_{\mathbf{T}(F)}^{-1})\mathbf{R}_{\mathbf{T}(F)}^{1/2}, \tag{3.14}$$

if E,F are positive definite matrices, $\mathbf{T}$ is a stochastic mapping, and $\mathbf{T}^\star$ denotes its adjoint with respect to the Hilbert–Schmidt inner product. Putting $E=F=D$, (3.14) becomes

$$\mathbf{T}\mathbf{K}_D\mathbf{T}^\star\leqslant\mathbf{K}_{\mathbf{T}(D)},$$

which is equivalent to

$$\mathbf{T}^\star\mathbf{K}_{\mathbf{T}(D)}^{-1}\mathbf{T}\leqslant\mathbf{K}_D^{-1}. \tag{3.15}$$

The latter condition is exactly the monotonicity of the metric (3.13). □

It is in order to make a comment on the relation of the function f in Theorem 3.1 and the Morozova–Chentsov function $c(x,y)$ in (2.4). Given f, we have $c(x,y)=1/yf(x/y)$ and conversely $f(t)=1/c(t,1)$. Some examples of functions f satisfying the hypothesis of Theorem 3.1 are the following:

$$\frac{2x^{\alpha+1/2}}{1+x^{2\alpha}}, \quad \frac{x-1}{\log x}, \quad \frac{x-1}{\log x}\,\frac{2\sqrt{x}}{1+x}, \quad \left(\frac{x-1}{\log x}\right)^2\frac{2}{1+x}, \quad \frac{1+x}{2}, \tag{3.16}$$

where $0\leqslant\alpha\leqslant1/2$. The lattest function f gives the Morozova–Chentsov function (3.7) and we obtain that the metric of the symmetric logarithmic derivative is monotone.

The metrics on $\mathscr{M}_2$ provided by Theorem 3.1 are rotation invariant, they depend only on $r=\sqrt{x^2+y^2+z^2}$, and split into radial and tangential components:

$$ds^2=\frac{1}{1-r^2}\,dr^2+\frac{1}{1+r}\,g\left(\frac{1-r}{1+r}\right)dn^2 \quad \text{where } g(t)=\frac{1}{f(t)}. \tag{3.17}$$

The radial component is independent of the function f. In the case of the metric of the symmetric logarithmic derivative, the tangential component is independent of r.

Theorem 3.2: Every monotone metric is provided by Theorem 3.1.

Proof: A monotone metric is invariant in the sense of Sec. II, and due to the result of Chentsov and Morozova the metric is of the form (2.4). Set a function f as $f(t)=1/c(t,1)$, where c is the function of two variables from (2.4). By means of this function the monotone metric can

be written in terms of f exactly in the form described in Theorem 3.1 [see (3.12) and (3.11)]. What we have to prove is that f is operator monotone. This will be shown following Ref. 20.

We choose a particular stochastic mapping **T**:

$$\mathbf{T}:X\equiv\begin{pmatrix} X_1 & A \\ B & X_2 \end{pmatrix}\mapsto\frac{1}{2}\begin{pmatrix} X_1+X_2 & A+B \\ A+B & X_1+X_2 \end{pmatrix}.$$

With this choice the monotonicity condition yields that

$$Y\mapsto f(\mathbf{L}_Y\mathbf{R}_Y^{-1})\mathbf{R}_Y$$

is a concave mapping, or equivalently

$$Y\mapsto f(Y\otimes(Y^{-1})^t)(I\otimes Y^t) \tag{3.18}$$

is concave for a positive definite density matrix Y. The concavity extends to all positive definite matrices obviously. We write (3.18) for a block matrix

$$Y=\begin{pmatrix} Y_1 & 0 \\ 0 & Y_2 \end{pmatrix},$$

then we observe that concavity of (3.18) implies the concavity of the mapping

$$(Y_1,Y_2)\mapsto f(Y_1\otimes(Y_2^{-1})^t)(I\otimes Y_2^t). \tag{3.19}$$

Now the choice $Y_2=I$ gives that the mapping $Y_1\mapsto f(Y_1)$ must be concave. What we have arrived at is the operator concavity of f which is known to be equivalent to the operator monotonicity of f (cf. Ref. 18). □

Let f_1 and f_2 be functions satisfying the hypothesis of Theorem 3.1 and let $\mathbf{K}^1$ and $\mathbf{K}^2$ be the corresponding superoperators defined by (3.12). If $f_1\leqslant f_2$, then $\mathbf{K}^1_D\leqslant\mathbf{K}^2_D$. The inverse changes this ordering, hence $g^1_D(A,A)\geqslant g^2_D(A,A)$ for the corresponding metrics. The relation between operator monotone functions and monotone metrics established by Theorems 3.1 and 3.2 respects ordering in the sense that bigger function gives a smaller metric. Comparison of different metrics is meaningful only under some normalization. The most natural is

$$g_D(A,A)=\mathrm{Tr}\ D^{-1}A^2 \quad \text{whenever}\ \ DA=AD, \tag{3.20}$$

which corresponds to $f(1)=1$. It is known (see Ref. 21) that among all operator monotone functions with $f(1)=1$ and $f(t)=tf(t^{-1})$ there is a minimal and a maximal. They are

$$f_{\min}(t)=\frac{2t}{1+t},\quad f_{\max}(t)=\frac{1+t}{2}. \tag{3.21}$$

So we obtain the following theorem.

Theorem 3.3: Under the normalization (3.20), the metric of the symmetric logarithmic derivative is minimal among all monotone metrics.

Proof: One has to verify that the function $f_{\max}$ yields the stated metric. From (3.12) and (3.13) we have

$$g_D(A,A)=2\langle(\mathbf{L}_D+\mathbf{R}_D)^{-1}A,A\rangle \tag{3.22}$$

and $L=2(\mathbf{L}_D+\mathbf{R}_D)^{-1}$ is exactly the solution of Eq. (3.2). Hence (3.22) matches (3.7).

We have to emphasize that the theorem states the minimality of the logarithmic derivative metric only under the essential condition that the whole state space of a spin is parametrized. If this is not the case, then no information is provided by the theorem. The largest monotone metric is the metric of the so-called left logarithmic derivative. That appeared in the literature in connection with Cramér–Rao-type inequalities. Its monotonicity was established in Ref. 7. The fact that the left logarithmic metric is larger than the symmetric one is elementary and it has been known (for example, Ref. 15, p. 282).

The metric corresponding to the Morozova–Chentsov function

$$\frac{\log x - \log y}{x-y}$$

is the Kubo (or Mori, or Bogoliubov) inner product which showed up in Ref. 7 and was studied in Ref. 22. In particular, it was proved that the Kubo product is monotone, under more general assumption than a finite spin, and a conjecture was made. Namely, the scalar curvature of the Kubo metric is monotone as well. Monotonicity of the Kubo metric is not surprising because this result is a kind of reformulation of the Lieb convexity theorem.[23] However, the monotonicity of the scalar curvature seems to be an inequality of new type (provided that the conjecture is really true). Concerning details we refer to Refs. 7 and 22.

In Ref. 6 Hasegawa introduced a family of metrics. It was proved that they can be obtained by the above construction of monotone metric.[24] The Kubo–Mori metric is an element of the family, otherwise their physical (or statistical) importance is not clear yet.

IV. EXTENSION TO PURE STATES

The objective of this section is to discuss the extension of monotone metrics of $\mathscr{M}_n$ to pure states $\mathbb{C}P^{(n-1)}$. Since pure states form a low-dimensional part of the topological boundary of $\mathscr{M}_n$, it should be well specified how the extension is understood.

Let $\mathscr{M}_n^0$ denote the set of all elements of $\mathscr{M}_n$ whose eigenvalues are distinct and define a projection $\pi:\mathscr{M}_n^0 \to \mathbb{C}P^{(n-1)}$ as follows. Let $\pi(D)$ be the one-dimensional eigenspace corresponding to the largest eigenvalue of $D \in \mathscr{M}_n^0$. This map is smooth (see Ref. 25, II.5.8) and $\mathscr{M}_n^0$ is a smooth fiber bundle over $\mathbb{C}P^{(n-1)}$ with projection π (see Ref. 26, I.5.). [The structure group of this bundle is $U(1)\times U(n-1)$, where $U(k)$ is the group of $k\times k$ unitary matrices.] The fiber space is $\pi^{-1}(e)$, where e is the ray generated by the vector $(1,0,...,0) \in \mathbb{C}^n$.

Let $T_D\pi$ be the differential of π at D and let H_D be the orthogonal complement of Ker $T_D\pi$ in $T_D\mathscr{M}_n^0$ with respect to a fixed monotone Riemannian metric $g_D(\cdot,\cdot)$. Since $T_D\pi$ is surjective, the restriction of $T_D\pi$ gives a linear isomorphism between H_D and $T_{\pi(D)}\mathbb{C}P^{(n-1)}$. If $v \in T_{\pi(D)}\mathbb{C}P^{(n-1)}$, then we can define a unique lift $\tilde{v} \in H_D$ of v such that $T_D\pi(\tilde{v}) = v$. Using this lift we can define the following inner product $k^D_{\pi(D)}(\cdot,\cdot)$ on $T_{\pi(D)}\mathbb{C}P^{n-1}$:

$$k^D_{\pi(D)}(u,v) = g_D(\tilde{u},\tilde{v}), \quad u,v \in T_{\pi(D)}\mathbb{C}P^{(n-1)}. \tag{4.1}$$

We say that a sequence $D_n \in \mathscr{M}_n^0$ is radial at $p \in \mathbb{C}P^{(n-1)}$ if $\pi(D_n) = p$ for every n and D_n is convergent to p when p is considered as a density matrix (that is, a one-dimensional projection operator). Now we can define the radial extension of $g(\cdot,\cdot)$. A smooth metric $k(\cdot,\cdot)$ on $\mathbb{C}P^{(n-1)}$ is called the radial extension of $g(\cdot,\cdot)$ if for every $p \in \mathbb{C}P^{(n-1)}, u,v \in T_p\mathbb{C}P^{(n-1)}$, and for every radial sequence D_n at p

$$\lim_{n\to\infty} g_p^{D_n}(u,v) = k_p(u,v)$$

holds. In the next theorem we give a necessary and sufficient condition for the existence of the radial extension.

Theorem 4.1: Let $g(\cdot,\cdot)$ be a monotone Riemannian metric on $\mathscr{M}_n$ and let $f:\mathbb{R}^+\to\mathbb{R}^+$ be the corresponding operator monotone function (described in Theorem 3.1). The radial extension $k(\cdot,\cdot)$ of the given metric $g(\cdot,\cdot)$ of $\mathscr{M}_n$ exists if and only if $f(0)\neq 0$. In the case of existence

$$k(\cdot,\cdot)=\frac{1}{2f(0)}\langle\cdot,\cdot\rangle,$$

where $\langle\cdot,\cdot\rangle$ is the standard Riemannian metric on $\mathbb{C}P^{(n-1)}$.

Proof: The proof is based on the direct computation of $k^D_{\pi(D)}(\cdot,\cdot)$. For any unitary matrix U and $D\in\mathscr{M}_n^0$ we have

$$\pi(UDU^{-1})=U\pi(D),$$

which implies

$$T_{UDU^{-1}}\pi(UXU^{-1})=UT_D\pi(X),\quad X\in T_D\mathscr{M}_n^0,$$

by differentiation. Since $k(\cdot,\cdot)$ is unitary invariant,

$$U(\mathrm{Ker}\ T_D\pi)U^{-1}=\mathrm{Ker}\ T_{UDU^{-1}}\pi\quad\text{and}\quad UH_DU^{-1}=H_{UDU^{-1}}.$$

Moreover, $U\widetilde{v}U^{-1}=\widetilde{U}v$ for any $v\in T_{\pi(D)}\mathbb{C}P^{(n-1)}$, hence we obtain

$$g^D_{\pi(D)}(u,v)=g^{UDU^{-1}}_{U\pi(D)}(Uu,Uv). \tag{4.2}$$

From this equality it follows that it is sufficient to compute $k^D(\cdot,\cdot)$ if D is diagonal and $\pi(D)$ is the projection onto e. Assume these and let $X\in T_D\mathscr{M}_n^0$ and let $\lambda(t)$ and $v(t)$ be the largest eigenvalue and the unit eigenvector corresponding to $\lambda(t)$ of $D+tX$ where $t\in\mathbb{R}$. For sufficiently small t, $D+tX\in\mathscr{M}_n^0$ and $\lambda(t)$ and $v(t)$ are smooth functions of t. For $D(t)=D+tX$ we have

$$(D(t)-\lambda(t))v(t)=0.$$

Differentiating this expression we obtain that $\lambda'(0)=x_{11}$ and

$$T_D\pi(X)=v'(0)=\left(0,\frac{x_{21}}{\lambda_1-\lambda_2},\ldots,\frac{x_{n1}}{\lambda_1-\lambda_n}\right), \tag{4.3}$$

where $\lambda_1,\ldots,\lambda_n$ are the eigenvalues of D, $\lambda_1=\lambda(0)$, and $X=(x_{ij})$. If $X\in\mathrm{Ker}\ T_D\pi$, then the expression of $T_D\pi(X)$

$$X=\begin{pmatrix} x_{11} & 0 & \cdots & 0\\ 0 & x_{22} & \cdots & x_{2n}\\ \vdots & \vdots & \ddots & \vdots\\ 0 & x_{n2} & \cdots & x_{nn}\end{pmatrix}.$$

Let $\mathbf{K}_D^{-1}=f(\mathbf{L}_D\mathbf{R}_D^{-1})\mathbf{R}_D$ as in (3.12). Since D is diagonal,

$$K_D(X)_{ij}=\frac{x_{ij}}{f(\lambda_i/\lambda_j)\lambda_j}, \tag{4.4}$$

hence we get $K_D(\mathrm{Ker}\ T_D\pi)=\mathrm{Ker}\ T_D\pi$. If $V\in H_D$, then the last equation gives

$$V=\begin{pmatrix} 0 & \overline{v_2} & \cdots & \overline{v_n} \\ v_2 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ v_n & 0 & \cdots & 0 \end{pmatrix}, \tag{4.5}$$

where $v_i \in \mathbb{C}$ for $i=2,\ldots,n$. If $v=(0,v_2,\ldots,v_n) \in T_{[e]}\mathbb{C}P^{(n-1)}$, then (4.3) and (4.5) give

$$\tilde{v}=\begin{pmatrix} 0 & (\lambda_1-\lambda_2)\overline{v_2} & \cdots & (\lambda_1-\lambda_n)\overline{v_n} \\ (\lambda_1-\lambda_2)v_2 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ (\lambda_1-\lambda_n)v_n & 0 & \cdots & 0 \end{pmatrix}.$$

Now we can express $g^D(\cdot,\cdot)$:

$$g^D(u,v)=\mathrm{Re}\sum_{i=2}^{n}\frac{(\lambda_1-\lambda_i)^2}{f(\lambda_i/\lambda_1)\lambda_1}\,u^i\overline{v^i}, \tag{4.6}$$

where $u,v \in T_{[e]}\mathbb{C}P^{(n-1)}$.

Let us consider now the general case. Let (D_m) be a radial sequence at p and let $u,v \in T_p\mathbb{C}P^{(n-1)}$. Let B_p^m be linear operators on $T_p\mathbb{C}P^{(n-1)}$ such that

$$g_p^{D_m}(u,v)=\langle B_p^m u,v\rangle_p,$$

where $\langle\cdot,\cdot\rangle_p$ is the inner product on $T_p\mathbb{C}P^{(n-1)}$ induced by the standard metric. Let U_m be unitary operators such that $D_m^0=U_mD_mU_m^{-1}$ is diagonal and $\pi(D_m^0)=p_0$ with $p_0=[e]$. Using (4.2) we have

$$B_p^m=U_m^{-1}\cdot B_{p_0}^m\cdot U_m. \tag{4.7}$$

Since $\lim_{m\to\infty}\lambda_1^m=1$ and $\lim_{m\to\infty}\lambda_i^m=0$ for $i=2,\ldots,n$, by (4.6)

$$\lim_{m\to\infty}\|B_{p_0}^m-cI_{p_0}\|_{p_0}=0,\quad c=1/2\ f(0), \tag{4.8}$$

where I_{p_0} is the identity map on $T_{p_0}\mathbb{C}P^{(n-1)}$ and $\|\cdot\|$ is the operator norm induced by $\langle\cdot,\cdot\rangle$. It follows from (4.7) that

$$\begin{aligned}\|B_p^m-cI_p\|&=\|U_m^{-1}\cdot B_{p_0}^m\cdot U_m-cU_m^{-1}\cdot I_{p_0}\cdot U_m\|\\&=\|U_m^{-1}\cdot(B_{p_0}^m-cI_{p_0})\cdot U_m\|\\&\leqslant\|U_m^{-1}\|\cdot\|B_{p_0}^m-cI_{p_0}\|\cdot\|U_m\|.\end{aligned}$$

Since U_m are isometries from $T_p\mathbb{C}P^{(n-1)}$ to $T_{p_0}\mathbb{C}P^{(n-1)}$, $\|U_m\|=1$ and by (4.8) we obtain

$$\lim_{m\to\infty}\|B_p^m-cI_p\|=0,\quad c=1/2\ f(0).$$

So we have proved that the radial extension exists if $f(0)\neq 0$.

The special case $n=2$ is very transparent from (3.17) and it explains the terminology ''radial extension.'' The 2×2 case shows also that the condition $f(0)\neq 0$ is necessary to speak about extension. □

V. DISCUSSION

In the classical case, decision theory provides a unique monotone metric, namely, the Fisher information. In the quantum case, there are infinitely many monotone metrics on the state space. Among them the metric of symmetric logarithmic derivative possesses several mathematically attractive properties, it is minimal among all monotone metrics, and its extension to pure state is exactly the Fubini–Study metric. In accordance with the work of Braunstein and Caves, this seems to be the canonical metric of parameter estimation theory. However, expectation values of certain relevant observables are known to lead to statistical inference theory provided by the maximum entropy principle or the minimum relative entropy principle when *a priori* information on the state is available.[27] The best prediction is a kind of generalized Gibbs state. On the manifold of those states, the differentiation of the entropy functional yields the Kubo–Mori metric, which is different from the metric of the symmetric logarithmic derivative.[4,7] Therefore, more than one privileged metric shows up in quantum mechanics. The exact clarification of this point requires and is worth further studies.

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Transformation brackets between U(ν+1)⊃U(ν)⊃SO(ν) and U(ν+1)⊃SO(ν+1)⊃SO(ν)

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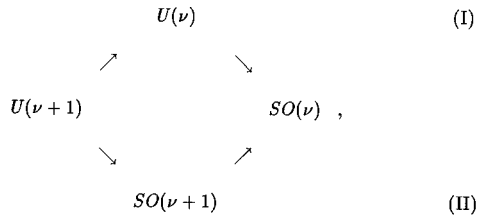
We derive a general expression for the transformation brackets between the chains U(ν+1)⊃U(ν)⊃SO(ν) and U(ν+1)⊃SO(ν+1)⊃SO(ν) for $\nu \geqslant 2$. © *1996 American Institute of Physics.* [S0022-2488(96)00703-9]

I. INTRODUCTION

The properties of bound states in a large variety of physical systems can be described by writing the Hamiltonian and other operators in terms of a spectrum generating algebra, G. In many applications the spectrum generating algebra is taken to be the unitary algebra $G=\mathrm{U}(\nu+1)$,[1] where ν denotes the dimension. Examples of this approach are the description of the five quadrupole degrees of freedom of the interacting boson model in nuclear physics in terms of the algebra U(6),[2] the description of the three dipole degrees of freedom of the vibron model in molecular physics in terms of the algebra U(4),[3] and the description of the six degrees of freedom (two dipoles) of the valence quark model of baryons in hadronic physics in terms of the algebra U(7).[4] The algebra U(ν+1) always admits (for $\nu \geqslant 2$) two subalgebra chains,



(1)

in addition, eventually, to other chains. [The special case, $\nu=1$, with U(2)⊃U(1) and U(2)⊃SO(2), in which the two subalgebras U(1) and SO(2) are isomorphic, is treated in detail in Refs. 3 and 5, and it will not be discussed further.] In the applications mentioned above, the first chain has the physical meaning of a spherical oscillator in ν dimensions, with U(ν) being the degeneracy algebra, while the second chain has the meaning of a displaced (or deformed) oscillator in ν dimensions. The best known example of the latter is the SO(6) chain of the interacting boson model,[6] which has played an important role in nuclear structure physics. In view of the fact that the algebraic method is presently being applied to a variety of problems in physics with different number of dimensions, it is of interest to derive a general expression for the transformation brackets between the two chains given in the group lattice of Eq. (1), which includes the known cases $\nu=5$ and $\nu=3$,[5] but extends the results to arbitrary $\nu(\geqslant 2)$. These transformation brackets are particularly useful if one wants to evaluate analytically certain quantities of physical interest, in

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particular matrix elements of operators, such as the electromagnetic transition operators, as discussed at length in Ref. 6. In this paper, the general result for arbitrary $\nu \geqslant 2$ will be presented.

II. SPECTRUM GENERATING ALGEBRA

As mentioned above, many applications of the method of spectrum generating algebras (SGA) for bound-state problems in ν dimensions, have made use of the unitary algebra $U(\nu+1)$. By generalizing the well-known cases of $\nu=5$[2] and $\nu=3$,[3] we introduce a realization of $U(\nu+1)$ in terms of $\nu+1$ boson operators, divided into a set of ν operators, $b_j^\dagger (j = 1,\ldots,\nu)$, which transform as the fundamental representation of $U(\nu)$ and an additional boson operator, $b_0^\dagger = s^\dagger$, which transforms as a scalar under $U(\nu)$. The $\nu+1$ boson operators, $b_j^\dagger (j = 0,\ldots,\nu)$, span the $(\nu+1)$-dimensional space of $U(\nu+1)$. The elements of $U(\nu+1)$ can be written as the bilinear products,

$$\mathcal{G} \equiv U(\nu+1); \quad G_{jk} = b_j^\dagger b_k \quad (j,k=0,1,\ldots,\nu). \tag{2}$$

The states constructed by applying the boson creation operators to a vacuum state,

$$\mathcal{B}: \quad \frac{1}{\mathcal{N}} (b_j^\dagger)^{n_j} (b_k^\dagger)^{n_k} \cdots |0\rangle \tag{3}$$

(where $\mathcal{N}$ is a normalization constant) transform as the symmetric representation $[N]$ of $U(\nu+1)$, where N is the total number of bosons,

$$\hat{N} = \sum_{j=0}^{\nu} \hat{n}_j = \sum_{j=0}^{\nu} b_j^\dagger b_j . \tag{4}$$

In the algebraic approach to bound state problems, the Hamiltonian (and other) operators are expressed as functions of the elements of $U(\nu+1)$, i.e. they are in the enveloping algebra of $U(\nu+1)$, and the basis states are the $[N]$ irreps of $U(\nu+1)$.

In this paper we discuss (i) the explicit construction of the basis states in terms of bosons operators for $U(\nu+1) \supset U(\nu) \supset SO(\nu)$ and $U(\nu+1) \supset SO(\nu+1) \supset SO(\nu)$, and (ii) the transformation brackets relating the basis states in the two chains.

A. The chain $U(\nu+1) \supset U(\nu) \supset SO(\nu)$

First we consider the chain

$$U(\nu+1) \supset U(\nu) \supset SO(\nu). \tag{5}$$

The basis states of this chain are denoted by $|[N], n, \tau\rangle$, where N is the total number of bosons with $j=0,1,\ldots,\nu$, describing the irreps $[N] \equiv [N,0,\ldots,0]$ of $U(\nu+1)$, n is the number of bosons with $j=1,\ldots,\nu$, describing the irreps $[n] \equiv [n,0,\ldots,0]$ of $U(\nu)$, and τ is the quantum number (boson seniority), describing the irreps $(\tau) \equiv (\tau,0,...,0)$ of $SO(\nu)$. The branching rules are

$$\begin{gathered} n = 0,1,\ldots,N, \\ \tau = n, n-2, \ldots, 1 \text{ or } 0 \quad (n \text{ odd or even and } \nu > 2), \\ \tau = -n, -n+2, \ldots, n \quad (\nu = 2). \end{gathered} \tag{6}$$

The branching of irreps of $SO(\nu)$ into irreps of (eventual) subalgebras of $SO(\nu)$, is of no interest for the present problem and will not be discussed.

The elements (generators) of $U(\nu)$ and $SO(\nu)$ can be written as

$$\begin{aligned} &\mathrm{U}(\nu):\ \ G_{jk}=b_j^\dagger b_k \quad (j,k=1,\ldots,\nu),\\ &\mathrm{SO}(\nu):\ \ L_{jk}=i(b_j^\dagger b_k-b_k^\dagger b_j) \quad (j<k \quad \text{and} \ \ j,k=1,\ldots,\nu). \end{aligned} \tag{7}$$

The basis states of the chain (5) can be written in a compact form as

$$\begin{aligned} |[N],n,\tau\rangle &= \frac{1}{\sqrt{(N-n)!}}\,(s^\dagger)^{N-n}|[n],n,\tau\rangle,\\ |[n],n,\tau\rangle &= B_{n\tau}(I_\nu^\dagger)^{(n-\tau)/2}|[\tau],\tau,\tau\rangle. \end{aligned} \tag{8}$$

The normalization coefficient $B_{n\tau}$ can be derived by making use of the SU(1,1) algebra, given in Eqs. (A2) and (A3) of Appendix A,

$$B_{n\tau}=(-1)^{(n-\tau)/2}\sqrt{\frac{(2\tau+\nu-2)!!}{(n+\tau+\nu-2)!!(n-\tau)!!}}. \tag{9}$$

The operator $I_\nu^\dagger$ denotes the pair creation operator in ν dimensions,

$$I_\nu^\dagger=\sum_{j=1}^{\nu} b_j^\dagger b_j^\dagger, \tag{10}$$

and commutes with the generators of SO(ν), $[I_\nu^\dagger,L_{jk}]=0$. The operator $s^\dagger(=b_0^\dagger)$ has been used in (8) to make it conform with the standard notation used in the literature.

B. The chain U(ν+1)⊃SO(ν+1)⊃SO(ν)

Next, we consider the chain

$$\mathrm{U}(\nu+1)\supset\mathrm{SO}(\nu+1)\supset\mathrm{SO}(\nu). \tag{11}$$

The basis states of this chain are denoted by $|[N],\sigma,\tau\rangle$, where $[N]$ and τ label as before the symmetric irreps of U(ν+1) and SO(ν), while $(\sigma)\equiv(\sigma,0,\ldots,0)$ labels the symmetric representation of SO(ν+1). The branching rules are

$$\begin{aligned} &\sigma=N,N-2,\ldots,1 \quad \text{or} \quad 0 \quad (N \ \text{odd or even}),\\ &\tau=0,1,\ldots,\sigma \quad (\nu>2),\\ &\tau=-\sigma,-\sigma+1,\ldots,\sigma \quad (\nu=2). \end{aligned} \tag{12}$$

The generators of SO(ν+1) and SO(ν) can be written as

$$\begin{aligned} &\mathrm{SO}(\nu+1):\ \ L_{jk}=i(b_j^\dagger b_k-b_k^\dagger b_j) \quad (j<k \quad \text{and} \ \ j,k=0,\ldots,\nu),\\ &\mathrm{SO}(\nu):\ \ L_{jk}=i(b_j^\dagger b_k-b_k^\dagger b_j) \quad (j<k \quad \text{and} \ \ j,k=1,\ldots,\nu). \end{aligned} \tag{13}$$

It is customary to separate the generators of SO(ν+1) into two pieces,

$$\begin{aligned} &L_{jk}=i(b_j^\dagger b_k-b_k^\dagger b_j) \quad (j<k \quad \text{and} \ \ j,k=1,\ldots,\nu),\\ &D_j=i(b_0^\dagger b_j-b_j^\dagger b_0)=i(s^\dagger b_j-b_j^\dagger s) \quad (j=1,\ldots,\nu). \end{aligned} \tag{14}$$

Using the same SU(1,1) algebra, as discussed in Appendix A, but with the sum in (A2) extending from $j=0$ to $j=\nu$, the basis states of the chain (11) can be written as

$$|[N],\sigma,\tau\rangle = A_{N\sigma}(I^{\dagger}_{\nu+1})^{(N-\sigma)/2}|[\sigma],\sigma,\tau\rangle. \tag{15}$$

Here $A_{N\sigma}$ is a normalization coefficient,

$$A_{N\sigma}=(-1)^{(N-\sigma)/2}\sqrt{\frac{(2\sigma+\nu-1)!!}{(N+\sigma+\nu-1)!!(N-\sigma)!!}}, \tag{16}$$

and $I^{\dagger}_{\nu+1}$ represents the pair creation operator in $\nu+1$ dimensions,

$$I^{\dagger}_{\nu+1}=\sum_{j=0}^{\nu} b^{\dagger}_j b^{\dagger}_j = s^{\dagger}s^{\dagger}+I^{\dagger}_{\nu}. \tag{17}$$

This pair creation operator commutes with the generators of SO($\nu+1$), $[I^{\dagger}_{\nu+1},L_{jk}]=[I^{\dagger}_{\nu+1},D_j]=0$. In Appendix B we show that the states $|[\sigma],\sigma,\tau\rangle$ can be written as

$$|[\sigma],\sigma,\tau\rangle = \sum_{k=0}^{[(\sigma-\tau)/2]} F_k(\sigma,\tau)(s^{\dagger})^{\sigma-\tau-2k}(I^{\dagger}_{\nu+1})^k|[\tau],\tau,\tau\rangle, \tag{18}$$

where the expansion coefficients are given by[7]

$$F_k(\sigma,\tau)=\left[\frac{(\sigma-\tau)!(2\tau+\nu-2)!!}{(2\sigma+\nu-3)!!(\sigma+\tau+\nu-2)!}\right]^{1/2}\left(-\frac{1}{2}\right)^k\frac{(2\sigma+\nu-3-2k)!!}{(\sigma-\tau-2k)!k!}. \tag{19}$$

Another realization of SO($\nu+1$) that is used frequently in physical applications, is by the generators $\overline{D}_j = s^{\dagger}b_j + b^{\dagger}_j s$ with $j=1,\ldots,\nu$ and $L_{jk}=i(b^{\dagger}_j b_k - b^{\dagger}_k b_j)$ with $j<k$ and $j,k=1,\ldots,\nu$. The corresponding pair creation operator differs from $I^{\dagger}_{\nu+1}$ in Eq. (17) by a relative sign,

$$\overline{I}^{\dagger}_{\nu+1}=s^{\dagger}s^{\dagger}-I^{\dagger}_{\nu}. \tag{20}$$

III. TRANSFORMATION BRACKETS

The transformation brackets between the two chains are obtained by taking the overlap between the two sets of basis states. Since both are written explicity in terms of the states $|[\tau],\tau,\tau\rangle$, the overlap is straightforward and yields the result

$$c^{\tau}_{n\sigma}=\langle[N],n,\tau|[N],\sigma,\tau\rangle=\sqrt{(N-n)!}\,\frac{A_{N\sigma}}{B_{n\tau}}\sum_{k=k_0}^{[(\sigma-\tau)/2]}F_k(\sigma,\tau)\begin{pmatrix} k+\dfrac{N-\sigma}{2} \\ \dfrac{n-\tau}{2}\end{pmatrix}, \tag{21}$$

with $k_0=\max(0,\frac{1}{2}(n-\tau-N+\sigma))$. For the second realization of the SO($\nu+1$) with the pair creation operator of Eq. (20), the transformation brackets have an additional sign $(-1)^{(n-\tau)/2}$. The transformation brackets of Eq. (21) can be obtained by inserting the expressions for the coefficients of Eqs. (9), (16), and (19),

$$c^{\tau}_{n\sigma}=(-1)^{(N-\sigma-n+\tau)/2}\left[\frac{(N-n)!(n+\tau+\nu-2)!!(\sigma-\tau)!(2\sigma+\nu-1)}{(N+\sigma+\nu-1)!!(N-\sigma)!!(\sigma+\tau+\nu-2)!(n-\tau)!!}\right]^{1/2}$$
$$\times\sum_{k=k_0}^{[(\sigma-\tau)/2]}(-1)^k\frac{(2\sigma+\nu-3-2k)!!(N-\sigma+2k)!!}{(\sigma-\tau-2k)!(2k)!!(N-\sigma-n+\tau+2k)!!}, \tag{22}$$

or by introducing Pochhammer's symbol, $(a)_k=\Gamma(a+k)/\Gamma(a)$, as

$$c^{\tau}_{n\sigma}=\left(-\frac{1}{2}\right)^{(N-\sigma-n+\tau)/2}(2\sigma+\nu-1)!!$$
$$\times\left[\frac{(N-n)!(N-\sigma)!!(n+\tau+\nu-2)!!}{(\sigma-\tau)!(n-\tau)!!(\sigma+\tau+\nu-2)!(N+\sigma+\nu-1)!!(2\sigma+\nu-1)}\right]^{1/2}$$
$$\times\sum_{k=k_0}^{[(\sigma-\tau)/2]}\frac{1}{k!}\frac{((N-\sigma)/2+1)_k((\tau-\sigma)/2)_k((\tau-\sigma+1)/2)_k}{((N-\sigma-n+\tau)/2+k)!(-\sigma-(\nu-3)/2)_k}. \tag{23}$$

Equations (22) and (23) reduce for $\nu=5$ and $\nu=3$ to the expressions derived in Refs. 5, 8, and 9.

For the lowest SO($\nu+1$) representation $\sigma=N$, the sum appearing in the general expression for the transformation bracket can be carried out explicitly to give

$$c^{\tau}_{nN}=\left[\frac{(N-\tau)!(N+\tau+\nu-2)!}{(N-n)!(n+\tau+\nu-2)!!(n-\tau)!!(2N+\nu-3)!!}\right]^{1/2}, \tag{24}$$

in agreement with the results obtained previously[6] for $\nu=5$ and $\nu=3$.

Equations (22) and (23) conclude the derivations of the transformation brackets for arbitrary $\nu(\geq 2)$,

$$|[N],\sigma,\tau\rangle=\sum_n c^{\tau}_{n\sigma}|[N],n,\tau\rangle. \tag{25}$$

IV. CONCLUSIONS

In this paper, we have reported a closed expression for the transformation brackets between the chains of Eq. (1) for an arbitrary number of dimensions $\nu(\geq 2)$. These transformation brackets are useful in a variety of problems that are being investigated at the present time within the framework of the algebraic method. For example, the case $\nu=2$ is of interest in the treatment of bending vibrations of linear molecules, while the case $\nu=9$ is of interest in the treatment of rotations and vibrations of nonplanar tetratomic molecules.

The transformation brackets derived here can be used to evaluate matrix elements of an operator $\hat{T}$ in the ''deformed'' chain (of great physical interest) by a two-step process, i.e. by first evaluating them in the ''spherical'' chain (which is a relatively easy calculation) and subsequently transforming the results to the ''deformed'' chain,

$$\langle[N],\sigma',\tau'|\hat{T}|[N],\sigma,\tau\rangle=\sum_{n',n}c^{\tau'}_{n'\sigma'}c^{\tau}_{n\sigma}\langle[N],n',\tau'|\hat{T}|[N],n,\tau\rangle, \tag{26}$$

where the coefficients c are the transformation brackets derived in this paper.

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APPENDIX A: THE REDUCTION U(ν)⊃SO(ν)

The normalization coefficients $B_{n\tau}$ and $A_{N\sigma}$ of Eqs. (9) and (16), can be found by making use of the properties of the SU(1,1) ''quasi-spin'' algebra for a system of bosons.[10,11] Consider a system of bosons in ν dimensions with the algebraic structure

$$\mathrm{U}(\nu)\supset\mathrm{SO}(\nu). \tag{A1}$$

The corresponding basis states are characterized by $|[n],\tau\rangle$. The operators

$$\hat{Q}_+=\frac{1}{2}\sum_{j=1}^{\nu} b_j^\dagger b_j^\dagger, \quad \hat{Q}_-=\frac{1}{2}\sum_{j=1}^{\nu} b_j b_j, \tag{A2}$$

$$\hat{Q}_0=\frac{1}{4}\sum_{j=1}^{\nu}(b_j^\dagger b_j+b_j b_j^\dagger)=\frac{1}{2}\left(\hat{n}+\frac{1}{2}\,\nu\right),$$

satisfy the commutation relations

$$[\hat{Q}_+,\hat{Q}_-]=-2\hat{Q}_0, \quad [\hat{Q}_0,\hat{Q}_\pm]=\pm\hat{Q}_\pm, \tag{A3}$$

of the SU(1,1) algebra. The basis states are labeled by $|q,q_0\rangle$. The generators of the SU(1,1) algebra defined in (A2) commute with the generators of SO(ν), L_{jk} of Eq. (7). The relation between the two sets of basis states $|q,q_0\rangle$ and $|[n],\tau\rangle$ can be found by using the generators of (A2). First, $\hat{Q}_0$ is diagonal in the basis states,

$$\begin{aligned}\hat{Q}_0|q,q_0\rangle&=q_0|q,q_0\rangle,\\ \hat{Q}_0|[n],\tau\rangle&=\tfrac{1}{2}(n+\tfrac{1}{2}\nu)|[n],\tau\rangle,\end{aligned} \tag{A4}$$

and hence $q_0=\frac{1}{2}(n+\frac{1}{2}\nu)$. Furthermore, $\hat{Q}_-$ annihilates the highest-weight state,

$$\hat{Q}_-|q=q_0,q_0\rangle=\hat{Q}_-|[n=\tau],\tau\rangle=0, \tag{A5}$$

which gives $q=\frac{1}{2}(\tau+\frac{1}{2}\nu)$. The basis states can be expanded as

$$\begin{aligned}|q,q_0\rangle&=A_{qq_0}(\hat{Q}_+)^{q_0-q}|q,q_0=q\rangle,\\ A_{qq_0}&=(-1)^{q_0-q}\sqrt{\frac{(2q-1)!}{(q_0-q)!(q_0+q-1)!}},\end{aligned} \tag{A6}$$

or alternatively as

$$\begin{aligned}|[n],\tau\rangle&=B_{n\tau}(I_\nu^\dagger)^{(n-\tau)/2}|[\tau],\tau\rangle,\\ B_{n\tau}&=(-1)^{(n-\tau)/2}\sqrt{\frac{(2\tau+\nu-2)!!}{(n+\tau+\nu-2)!!(n-\tau)!!}}.\end{aligned} \tag{A7}$$

The choice of phase in (A6) is conventional.

APPENDIX B: THE REDUCTION SO(ν+1)⊃SO(ν)

The SU(1,1) algebra of (A2) can be used for the reductions U(ν)⊃SO(ν) and U(ν+1)⊃SO(ν+1). For the chain (11) we need the further reduction SO(ν+1)⊃SO(ν). This is by far more complex. Here we use Ref. 12 and a generalization of the method discussed on pp. 152–157 of Ref. 5. The defining equations are

$$\begin{aligned}
&\hat{N}|[N],\sigma,\tau\rangle = N|[N],\sigma,\tau\rangle,\\
&\hat{C}_{\mathrm{SO}(\nu+1)}|[N],\sigma,\tau\rangle = \sigma(\sigma+\nu-1)|[N],\sigma,\tau\rangle,\\
&\hat{C}_{\mathrm{SO}(\nu)}|[N],\sigma,\tau\rangle = \tau(\tau+\nu-2)|[N],\sigma,\tau\rangle.
\end{aligned} \tag{B1}$$

The notation for the states is the same as in Sec. II A. $\hat{C}_G$ represents the quadratic Casimir invariant of G. These equations can be expressed in terms of a set of separable differential equations by introducing hyperspherical coordinates,

$$(x_1,\ldots,x_{\nu+1}) \rightarrow (r,\phi,\theta_{\nu-1},\ldots,\theta_1), \tag{B2}$$

by

$$\begin{aligned}
x_1 &= r\ \sin\ \phi\ \sin\ \theta_{\nu-1}\cdots\sin\ \theta_2\ \cos\ \theta_1,\\
x_2 &= r\ \sin\ \phi\ \sin\ \theta_{\nu-1}\cdots\sin\ \theta_2\ \sin\ \theta_1,\\
x_3 &= r\ \sin\ \phi\ \sin\ \theta_{\nu-1}\cdots\cos\ \theta_2,\\
&\vdots\\
x_\nu &= r\ \sin\ \phi\ \cos\ \theta_{\nu-1},\\
x_{\nu+1} &= r\ \cos\ \phi,
\end{aligned} \tag{B3}$$

with $0\leqslant r<\infty$ and $0\leqslant\phi,\ \theta_{\nu-1},\ldots,\theta_2<\pi$ and $0\leqslant\theta_1<2\pi$. The volume element is given by

$$dx_1\cdots dx_{\nu+1} = r^\nu(\sin\ \phi)^{\nu-1}(\sin\ \theta_{\nu-1})^{\nu-2}\cdots\sin\ \theta_2\ dr\ d\phi\ d\theta_{\nu-1}\cdots d\theta_2\ d\theta_1. \tag{B4}$$

The Casimir invariants can be obtained from the Laplacian in ν+1 dimensions and a recursion relation between the Casimir operators of the orthogonal groups (see p. 493 of Ref. 12),

$$\begin{aligned}
\nabla^2_{\nu+1} &= \frac{1}{r^\nu}\frac{\partial}{\partial r}\left(r^\nu\frac{\partial}{\partial r}\right) - \frac{1}{r^2}\hat{C}_{\nu+1}(\phi,\theta),\\
\hat{C}_{\nu+1}(\phi,\theta) &= -\frac{1}{(\sin\ \phi)^{\nu-1}}\frac{\partial}{\partial\phi}\left((\sin\ \phi)^{\nu-1}\frac{\partial}{\partial\phi}\right) + \frac{1}{(\sin\ \phi)^2}\hat{C}_\nu(\theta).
\end{aligned} \tag{B5}$$

Here $(\theta)=(\theta_{\nu-1},\ldots,\theta_1)$. The number operator expressed in hyperspherical coordinates is given by

$$\hat{N} = \frac{1}{2}\left[-\frac{1}{r^\nu}\frac{\partial}{\partial r}\left(r^\nu\frac{\partial}{\partial r}\right) + r^2 + \frac{1}{r^2}\hat{C}_{\nu+1}(\phi,\theta) - (\nu+1)\right]. \tag{B6}$$

The eigenvector equations can be solved by separation of variables and have solutions in terms of products of Laguerre and Gegenbauer polynomials,

$$\begin{aligned}\psi_{N\sigma\tau\alpha}(r,\phi,\theta) &= f_{N\sigma}(r)g_{\sigma\tau}(\phi)\Phi_{\tau\alpha}(\theta),\\ &= A_{N\sigma\tau}r^{\sigma}e^{-r^2/2}L^{(2\sigma+\nu-1)/2}_{(N-\sigma)/2}(r^2)(\sin\phi)^{\tau}C^{(2\tau+\nu-1)/2}_{\sigma-\tau}(\cos\phi)\Phi_{\tau\alpha}(\theta),\end{aligned} \tag{B7}$$

with

$$A_{N\sigma\tau}=(-1)^{(N-\sigma)/2}(2\tau+\nu-3)!!\left[\frac{2^{(2\sigma+\nu+1)/2}(2\sigma+\nu-1)(N-\sigma)!!(\sigma-\tau)!}{\pi(N+\sigma+\nu-1)!!(\sigma+\tau+\nu-2)!}\right]^{1/2}. \tag{B8}$$

Next we apply Dragt's theorem to the highest weight state with $N=\sigma$,

$$\psi_{\sigma\sigma\tau\alpha}(r,\phi,\theta)=\frac{A_{\sigma\sigma\tau}}{A_{\tau\tau\tau}}\,r^{\sigma-\tau}C^{(2\tau+\nu-1)/2}_{\sigma-\tau}(\cos\phi)\psi_{\tau\tau\tau\alpha}(r,\phi,\theta), \tag{B9}$$

by replacing

$$r\rightarrow(I^{\dagger}_{\nu+1}/2)^{1/2},\quad \cos\phi\rightarrow t^{\dagger}=s^{\dagger}/(I^{\dagger}_{\nu+1})^{1/2}, \tag{B10}$$

to obtain

$$\begin{aligned}|[\sigma],\sigma,\tau\rangle &= \frac{A_{\sigma\sigma\tau}}{A_{\tau\tau\tau}}\left(\frac{I^{\dagger}_{\nu+1}}{2}\right)^{(\sigma-\tau)/2}C^{(2\tau+\nu-1)/2}_{\sigma-\tau}(t^{\dagger})|[\tau],\tau,\tau\rangle,\\ &= \left[\frac{(\sigma-\tau)!(2\tau+\nu-2)!!}{(2\sigma+\nu-3)!!(\sigma+\tau+\nu-2)!}\right]^{1/2}\sum_{k=0}^{[(\sigma-\tau)/2]}\left(-\frac{1}{2}\right)^{k}\\ &\quad\times\frac{(2\sigma+\nu-3-2k)!!}{k!(\sigma-\tau-2k)!}\,(s^{\dagger})^{\sigma-\tau-2k}(I^{\dagger}_{\nu+1})^{k}|[\tau],\tau,\tau\rangle.\end{aligned} \tag{B11}$$

By comparing (B11) with (18), one finds the expression of Eq. (19) for the expansion coefficients $F_k(\sigma,\tau)$.

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Applications of quantum and classical Fisher information to two-level complex and quaternionic and three-level complex systems

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In the Bayesian theory of statistical inference, as first suggested by Harold Jeffreys in highly influential work, one can employ the square root of the determinant of an $n\times n$ Fisher information matrix as a reparametrization-invariant prior (generally unnormalized) measure over an n-dimensional family (Riemannian manifold) of probability distributions. Jeffreys' ansatz is adopted here to the quantum context, that is, with regard to density matrices rather than probability distributions, by computing the *quantum* Fisher information matrices (associated with Helstrom and Holevo) for the three-, five-, and eight-dimensional convex sets of two-level complex, two-level quaternionic, and three-level complex systems, respectively. In both the two-level cases, the priors have been normalized to probability distributions over the 2×2 density matrices, while, in the much more computationally demanding three-level situation, no such normalization has been accomplished. An argument is made for the general form, in terms of eigenvalues, that the (unnormalized) prior should assume over the (n^2-1)-dimensional convex set of $n\times n$ density matrices. © *1996 American Institute of Physics.* [S0022-2488(96)00506-3]

In the study of random matrices,[1] the objective is often to obtain the distribution of the eigenvalues in an ensemble of $n\times n$ Hermitian matrices as $n\to\infty$. The stochastic element is introduced by assuming that the real (complex) parts of the off-diagonal elements are identically distributed random variables. The matrices can be regarded as Hamiltonians and their eigenvalues as energy levels.

Here, a quite different—somewhat complementary—approach to ''random'' matrices is taken. Rather than viewing the matrices as Hamiltonians, they are regarded as density matrices, thus requiring in addition to Hermiticity, the nontrivial properties of non-negative definiteness and unit trace. Also, the analysis is nonasymptotic in character, focusing on the cases $n=2$ and 3, and is not—to begin with—principally concerned with the distribution of eigenvalues (two distinct density matrices can, of course, possess the same eigenvalues). The matrix ensembles under study here are the three-dimensional convex set of 2×2 (complex) density matrices, the five-dimensional convex set of 2×2 (quaternionic) density matrices, and the eight-dimensional convex set of 3×3 (complex) density matrices.

The random element is introduced by adopting an *ansatz* of Harold Jeffreys,[2,3] which has been widely applied in classical (commutative) probability,[4] to the quantum (noncommutative) domain.[5,6] In this generic approach, one computes an appropriate (classical or quantum) Fisher information matrix[4,7] and employs the square root of its determinant as a (prior) measure over a family of probability distributions (in the classical case) or density matrices (in the quantum case). The measure is invariant under reparametrizations, that is, it transforms according to the Jacobian of the transformation taking one parametrization of the probability distributions or density matrices to another.

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The Fisher information matrix defines a metric (the Jeffreys' prior serving as its volume element),[8] which, in the quantum case, is equivalent[9]—up to a proportionality factor of 4—to the Bures metric. This constitutes the extension to mixed states of the Fubini Study metric on pure states and has been widely studied.[10,11]

We now consider the three cases under examination.

(i) $n=2$ *(complex)*

The 2×2 density matrices, in quaternionic form,[12] can be parametrized as

$$\rho=\frac{1}{2}\begin{pmatrix} 1+z & x-iy-ju-kv \\ x+iy+ju+kv & 1-z \end{pmatrix}, \tag{1}$$

where $i^2=j^2=k^2=-1$, $ij=-ji=k$, $jk=-kj=i$, and $ki=-ik=j$. To begin with, let us set $u=v=0$, so that we have the usual Bloch sphere (unit ball in three-space) representation of the 2×2 density matrices.

To obtain the 3×3 quantum Fisher information matrix (J), one must first find the three symmetric logarithmic derivatives (L_x,L_y,L_z) satisfying[5,6,13]

$$\frac{\partial\rho}{\partial\alpha}=\frac{\rho L_\alpha+L_\alpha\rho}{2}, \quad \alpha=x,y,z, \tag{2}$$

and then compute entries of the form

$$J_{\beta\gamma}=\mathrm{Tr}[\rho(L_\beta L_\gamma+L_\gamma L_\beta)/2], \quad \beta,\gamma=x,y,z. \tag{3}$$

Now,

$$L_x=\frac{1}{(1-x^2-y^2-z^2)}\begin{pmatrix} x(z-1) & 1-ixy-y^2-z^2 \\ 1+ixy-y^2-z^2 & -x(z+1) \end{pmatrix},$$

$$L_y=\frac{1}{(1-x^2-y^2-z^2)}\begin{pmatrix} y(z-1) & -i(1-x^2+ixy-z^2) \\ i(1-x^2-ixy-z^2) & -y(z+1) \end{pmatrix}, \quad \text{and} \tag{4}$$

$$L_z=\frac{1}{(1-x^2-y^2-z^2)}\begin{pmatrix} 1-x^2-y^2-z & xz-iyz \\ xz+iyz & -1+x^2+y^2-z \end{pmatrix},$$

so the quantum information matrix given by (3) is

$$\frac{1}{(1-x^2-y^2-z^2)}\begin{pmatrix} 1-y^2-z^2 & xy & xz \\ xy & 1-x^2-z^2 & yz \\ xz & yz & 1-x^2-y^2 \end{pmatrix}. \tag{5}$$

Its determinant is

$$1/(1-x^2-y^2-z^2). \tag{6}$$

[The determinant of (1), with $u=v=0$, is $(1-x^2-y^2-z^2)/4$.] The square root of (6), the volume element (up to a proportionality factor) for the Bures metric,[9–11] can be normalized to form the probability distribution

$$P(x,y,z)=1/\pi^2(1-x^2-y^2-z^2)^{1/2}, \quad x^2+y^2+z^2\leqslant 1. \tag{7}$$

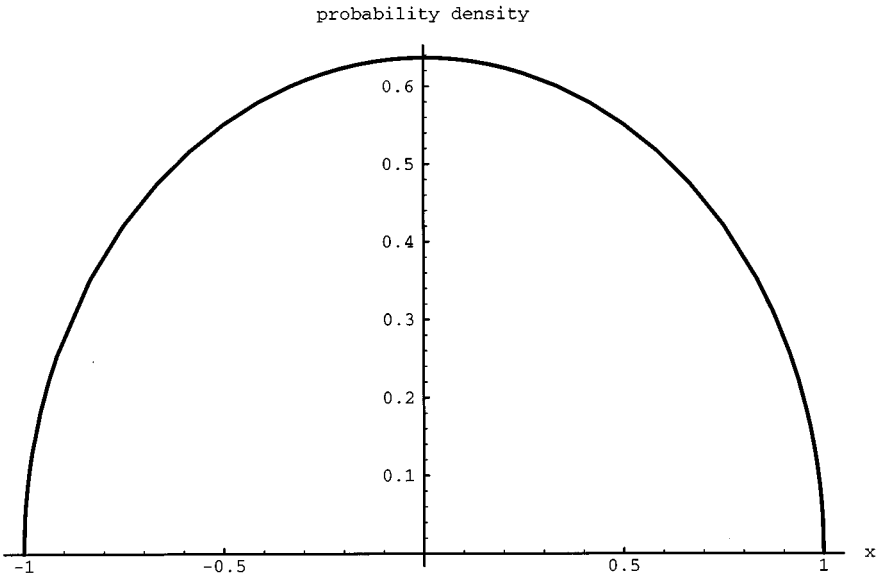

FIG. 1. Univariate marginal probability distribution, $2(1-x^2)^{1/2}/\pi$, for two-level complex quantum systems.

Our assertion is, thus, that if one chooses 2×2 complex density matrices according to this distribution, so doing will constitute a ''random'' sampling of these two-level quantum systems. If one averages the von Neumann entropy, $-\operatorname{Tr}\rho\ln\rho$, with respect to the prior (7), one obtains $2\ln 2-7/6\approx0.2196277$ for the average entropy of a 2×2 density matrix (cf. Ref. 14).

It is of interest to note that with the substitutions $x=A^{1/2}$, $y=B^{1/2}$, $z=C^{1/2}$, (7) becomes the Jeffreys' prior probability (a trivariate beta or Dirichlet distribution)

$$1/\pi^2 A^{1/2}B^{1/2}C^{1/2}(1-A-B-C)^{1/2} \tag{8}$$

for the (classical) quadrinomial distribution with probabilities A, B, C, and $1-A-B-C$.[15] Since

$$\int_{-(1-x^2-y^2)^{1/2}}^{(1-x^2-y^2)^{1/2}} P(x,y,z)\,dz=\frac{1}{\pi}, \tag{9}$$

the (three) bivariate marginal probabilities of (7) are uniform distributions over unit disks $(x^2+y^2\leqslant1,...)$. (So, Laplace's principle of insufficient reason[16] is manifested in such a form.) Then, the three univariate distributions are of the form (Fig. 1)

$$\int_{-(1-x^2)^{1/2}}^{(1-x^2)^{1/2}} \frac{1}{\pi}\,dy=\frac{2(1-x^2)^{1/2}}{\pi}. \tag{10}$$

Under the transformation, $x=2\lambda-1$, this becomes a beta distribution

$$8\lambda^{1/2}(1-\lambda)^{1/2}/\pi, \quad 0\leqslant\lambda\leqslant1 \tag{11}$$

with its two parameters equaling 1.5.

As a numerical illustration of the application of Bayes' Theorem[3,4] to the estimation of quantum systems,[17–19] let us hypothesize an experimental situation in which spin measurements are performed on each of 14 replicas of a two-level quantum system: three are taken in the X

direction: with two ''ups'' recorded, five in the Y direction with three ''ups,'' and six in the Z direction with two ''ups.'' Then the posterior (modified) probability distribution over the unit ball is proportional to the product of the prior (7) and the likelihood.

$$\left(\frac{1-x}{2}\right)\left(\frac{1+x}{2}\right)^2\left(\frac{1-y}{2}\right)^2\left(\frac{1+y}{2}\right)^3\left(\frac{1-z}{2}\right)^4\left(\frac{1+z}{2}\right)^2, \tag{12}$$

since in a two-level system with parameters x,y,z, the probability of an ''up'' in the X direction is $(1+x)/2$ and a ''down,'' $(1-x)/2$,... . This product can be normalized, through an integration over the unit ball, to comprise the posterior probability distribution

$$\frac{7168(1-x)(1+x)^2(1-y)^2(1+y)^3(1-z)^4(1+z)^2}{1903\pi^2(1-x^2-y^2-z^2)^{1/2}}. \tag{13}$$

The inverse of the information matrix (5) takes the particularly simple form

$$\begin{pmatrix} 1-x^2 & -xy & -xz \\ -xy & 1-y^2 & -yz \\ -xz & -yz & 1-z^2 \end{pmatrix}. \tag{14}$$

This serves as a (Cramér–Rao) lower bound (in the sense of positive definiteness) on the covariance matrix of unbiased estimates of the parameters of the density matrix.[5,6,13] [Each diagonal element of (14) furnishes a bound itself.]

Let us note that by transforming from Cartesian coordinates (x,y,z) to spherical ones (r,θ_1,θ_2), the Fisher information matrix (5) assumes a diagonal form

$$\begin{pmatrix} 1/(1-r^2) & 0 & 0 \\ 0 & r^2 & 0 \\ 0 & 0 & r^2 \sin\theta_1 \end{pmatrix}. \tag{15}$$

The prior probability (normalized form of the square root of its determinant) is then

$$\frac{r^2 \sin\theta_1}{\pi^2(1-r^2)^{1/2}}, \quad 0 \leqslant r \leqslant 1; 0 \leqslant \theta_1 \leqslant \pi; 0 \leqslant \theta_2 \leqslant 2\pi, \tag{16}$$

where $r^2 \sin\theta_1$ is the Jacobian of the transformation, in accordance with the principle of reparametrization invariance.[2–4]

(ii) *n=2 (quaternionic)*

The domain of the five parameters, u,v,x,y,z is the unit ball in five-space, $u^2+v^2+x^2+y^2+z^2 \leqslant 1$. Using the relations between the quaternionic elements $(1,i,j,k)$ and the Pauli matrices (Ref. 12, p. 495; Ref. 20, p. 197), the density matrix (1) can be reexpressed as the 4×4 Hermitian non-negative definite matrix of unit trace,

$$\rho = \frac{1}{4}\begin{pmatrix} 1+z & 0 & x-iy & u+iv \\ 0 & 1+z & -u+iv & x+iy \\ x+iy & -u-iv & 1-z & 0 \\ u-iv & x-iy & 0 & 1-z \end{pmatrix}. \tag{17}$$

Then, applying the formulas (2) and (3) to this matrix, we obtain the quantum Fisher information matrix

$$\frac{1}{(1-u^2-v^2-x^2-y^2-z^2)}$$

$$\times\begin{pmatrix} 1-v^2-x^2-y^2-z^2 & uv & ux & uy & uz \\ uv & 1-u^2-x^2-y^2-z^2 & vx & vy & vz \\ ux & vx & 1-u^2-v^2-y^2-z^2 & xy & xz \\ uy & vy & xy & 1-u^2-v^2-x^2-z^2 & yz \\ uz & vz & xz & yz & 1-u^2-v^2-x^2-y^2 \end{pmatrix}. \tag{18}$$

Its inverse,

$$\begin{pmatrix} 1-u^2 & -uv & -ux & -uy & -uz \\ -uv & 1-v^2 & -vx & -vy & -vz \\ -ux & -vx & 1-x^2 & -xy & -xz \\ -uy & -vy & -xy & 1-y^2 & -yz \\ -uz & -vz & -xz & -yz & 1-z^2 \end{pmatrix}, \tag{19}$$

serves as a Cramér–Rao lower bound, in the sense of non-negative definiteness, on unbiased estimates of u,v,x,y,z.[5,6,13]

The square root of the determinant of (18) can be normalized to the probability distribution

$$2/\pi^3(1-u^2-v^2-x^2-y^2-z^2)^{1/2}, \quad u^2+v^2+x^2+y^2+z^2\leqslant 1. \tag{20}$$

With the transformations, $x=A^{1/2}$, $y=B^{1/2}$, $z=C^{1/2}$, $u=D^{1/2}$, and $v=E^{1/2}$, this becomes the Jeffreys' prior

$$2/\pi^3[ABCDE(1-A-B-C-D-E)]^{1/2} \tag{21}$$

for a sextanomial distribution.[15] The marginal distribution of (20) over any of the five coordinates is a uniform distribution $(2/\pi^2)$ over a unit ball in four-space. The lower-dimensional marginals are then of the forms

$$4(1-x^2-y^2-z^2)^{1/2}/\pi^2, \quad x^2+y^2+z^2\leqslant 1, \tag{22}$$

$$2(1-x^2-y^2)/\pi, \quad x^2+y^2\leqslant 1 \tag{23}$$

(Fig. 2) and

$$8(1-x^2)^{3/2}/3\pi, \quad -1\leqslant x\leqslant 1 \tag{24}$$

[Fig. 3, cf. (10) and Fig. 1]. The conditional probability distribution of (20) with $u=v=0$ is simply (7).

In spherical coordinates $(r,\theta_1,\theta_2,\theta_3,\theta_4)$, (18) assumes the diagonal form

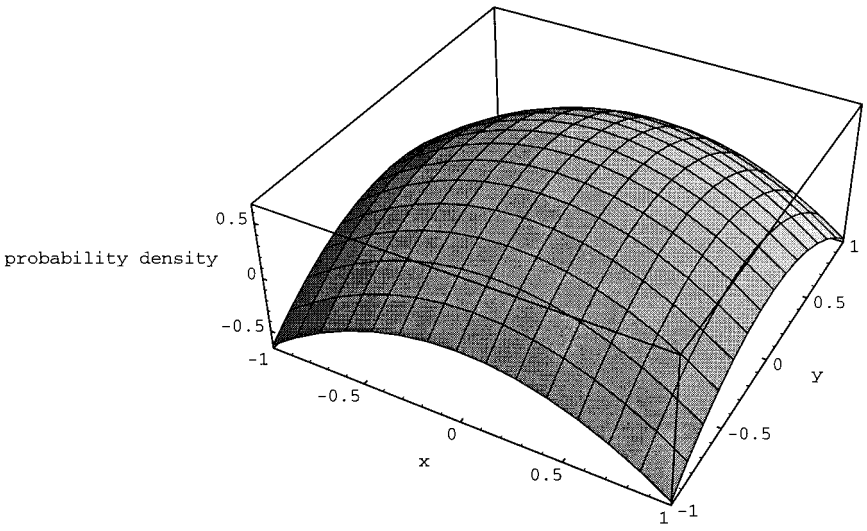

FIG. 2. Bivariate marginal probability distribution, $2(1-x^2-y^2)/\pi$, for two-level quaternionic quantum systems.

$$\begin{pmatrix} 1/(1-r^2) & 0 & 0 & 0 & 0 \\ 0 & r^2 & 0 & 0 & 0 \\ 0 & 0 & r^2 \sin^2 \theta_1 & 0 & 0 \\ 0 & 0 & 0 & r^2 \sin^2 \theta_1 \sin^2 \theta_2 & 0 \\ 0 & 0 & 0 & 0 & r^2 \sin^2 \theta_1 \sin^2 \theta_2 \sin^2 \theta_3 \end{pmatrix}. \quad (25)$$

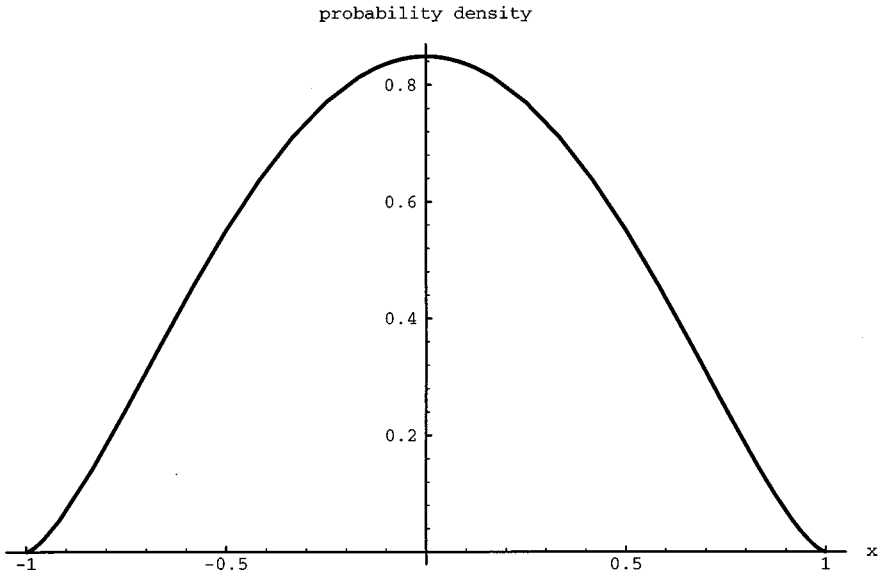

FIG. 3. Univariate marginal probability distribution, $8(1-x^2)^{3/2}/3\pi$, for two-level quaternionic quantum systems.

The normalized square root of its determinant is

$$\frac{2r^4 \sin^3 \theta_1 \sin^2 \theta_2 \sin \theta_3}{\pi^3(1-r^2)^{1/2}}, \quad 0 \leqslant r \leqslant 1; 0 \leqslant \theta_1, \theta_2, \theta_3 \leqslant \pi, 0 \leqslant \theta_4 < 2\pi, \tag{26}$$

the numerator of which is (twice) the Jacobian of the transformation from Cartesian to spherical coordinates. This reflects the property of reparametrization invariance possessed by Jeffreys' prior[2–4] [cf. (20)].

A single measurement of a two-level complex quantum system provides 0.140186 ''nats'' of information (1 nat equals 1/ln 2 bits), while a single measurement of a two-level quaternionic system furnishes less—0.090 186 2 nats. These results were obtained by computing the relative entropy (Kullback–Liebler distance or mutual information) of a posterior distribution based on one measurement [cf. (13), where 14 measurements were hypothesized] with respect to the priors (10) and (24). The relative entropy of the trivariate prior (16) with respect to the uniform distribution ($3r^2 \sin \theta_1/4\pi$) over the unit ball in three-space is 0.336099, while the relative entropy of the quintivariate prior (26) with respect to the uniform distribution ($15r^4 \sin^3 \theta_1 \sin^2 \theta_2 \sin \theta_3/8\pi^2$) over the unit ball in five-space is 0.3629558. The distribution (16), or, equivalently, (7), is thus, in this sense, smoother or less informative, closer to a uniform distribution than (26), or, equivalently, (20).

(iii) $n=3$ *(complex)*

A 3×3 density matrix is of the general form

$$\rho = \begin{pmatrix} p & r+si & t+ui \\ r-si & q & v+wi \\ t-ui & v-\omega i & 1-p-q \end{pmatrix}, \tag{27}$$

being Hermitian, non-negative definite and of trace 1.[21] Since 3 is a prime number, one can find a set of four mutually unbiased (orthonormal) bases of three-dimensional complex Hilbert space.[22–24] Following Wootters [Ref. 23, formula (3)], one such set of bases is

$$\begin{aligned} B^0 &= \left\{ \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right\}, \\ B^1 &= \left\{ \begin{pmatrix} \mathscr{S}/\sqrt{3} \\ 1/\sqrt{3} \\ \mathscr{S}/\sqrt{3} \end{pmatrix}, \begin{pmatrix} 1/\sqrt{3} \\ \mathscr{S}/\sqrt{3} \\ \mathscr{S}/\sqrt{3} \end{pmatrix}, \begin{pmatrix} \mathscr{S}/\sqrt{3} \\ \mathscr{S}/\sqrt{3} \\ 1/\sqrt{3} \end{pmatrix} \right\}, \\ B^2 &= \left\{ \begin{pmatrix} \eta/\sqrt{3} \\ 1/\sqrt{3} \\ \eta/\sqrt{3} \end{pmatrix}, \begin{pmatrix} 1/\sqrt{3} \\ \eta/\sqrt{3} \\ \eta/\sqrt{3} \end{pmatrix}, \begin{pmatrix} \eta/\sqrt{3} \\ \eta/\sqrt{3} \\ 1/\sqrt{3} \end{pmatrix} \right\}, \\ B^3 &= \left\{ \begin{pmatrix} \mathscr{S}/\sqrt{3} \\ \eta/\sqrt{3} \\ 1/\sqrt{3} \end{pmatrix}, \begin{pmatrix} \eta/\sqrt{3} \\ \mathscr{S}/\sqrt{3} \\ 1/\sqrt{3} \end{pmatrix}, \begin{pmatrix} 1/\sqrt{3} \\ 1/\sqrt{3} \\ 1/\sqrt{3} \end{pmatrix} \right\}, \end{aligned} \tag{28}$$

where $\mathscr{S}=\exp(2\pi i/3)$ and $\eta=\exp(-2\pi i/3)$. (The square of the inner product of any two vectors from different bases is $\frac{1}{3}$.) Now, by solving a set of linear equations, one can reparametrize ρ [Eq. (27)] using the relations

$$p=b_{01},\quad q=b_{02},\quad r=(2-b_{11}-b_{12}-b_{21}-b_{22}-b_{31}-b_{32})/2,$$
$$s=(b_{11}-b_{12}-b_{21}+b_{22}-b_{31}+b_{32})/2\sqrt{3},\quad t=(b_{11}+b_{21}-b_{31}-b_{32})/2,$$
$$u=(-b_{11}-2b_{12}+b_{21}+2b_{22}+b_{31}-b_{32})/2\sqrt{3},\quad v=(b_{12}+b_{22}-b_{31}-b_{32})/2,$$
$$w=(-2b_{11}-b_{12}+2b_{21}+b_{22}-b_{31}+b_{32})/2\sqrt{3}, \tag{29}$$

where b_{ij} is the expected value of ρ in the jth state of the ith base ($i=0,1,2,3$) of (28). (Alternative parametrizations of three-level quantum systems are, of course, available.[21,25–27]) It is important to note that $b_{ij}\geqslant 0$ for all i and j, and $\Sigma_{j=1}^{3} b_{ij}=1$ for all i, so four trinomial probability distributions are at hand—having a total of eight degrees of freedom. (In the two-level complex case, there are correspondingly three binomial distributions, while in the two-level quaternionic case, there are five relevant binomial distributions.)

Formula (3.8) of Ref. 11,

$$\frac{1}{4}\,\mathrm{Tr}\left\{ d\rho d\rho+\frac{3}{1-\mathrm{Tr}\,\rho^3}\,(d\rho-\rho d\rho)(d\rho-\rho d\rho)+\frac{3|\rho|}{1-\mathrm{Tr}\,\rho^3}\,(d\rho-\rho^{-1}d\rho)(d\rho-\rho^{-1}d\rho)\right\}, \tag{30}$$

gives the Bures metric over the 3×3 density matrices (ρ). This has been computed using the parametrization (29) and placed in matrix form. The result, by the analysis of Ref. 9, is proportional to the 8×8 quantum Fisher information matrix for the same parametrization.

It has not been possible to symbolically compute the determinant of this matrix since its entries are all highly involved expressions. However, several conditional results were more easily obtainable, having fixed some of the eight parameters beforehand. For example, if all the eight parameters (b_{ij}) are equated to a single one—call it b—then the square root of the Bures determinant is

$$3\cdot 3^{1/2}/256b^2(-1+2b)^2(-1+4b)^{1/2} \tag{31}$$

(Fig. 4). The range of permissible values of b is $[\frac{1}{4},\frac{1}{2}]$. If all the parameters except b_{i1} and b_{i2} (for $i=0$, 1, 2, or 3) are set equal to $\frac{1}{3}$, the conditional prior is then of the form

$$3\cdot 3^{1/2}/32(-1+b_{i1})(-1+b_{i2})(b_{i1}+b_{i2})(b_{i2}b_{i2}(1-b_{i1}-b_{i2}))^{1/2} \tag{32}$$

(Fig. 5).

Remarks: In a recent paper (Ref. 19, cf. Ref. 28), the author has presented results analogous to those given above for $n=2$ (both complex and quaternionic), but based on Fisher information matrices defined classically. These matrices were obtained by considering an $n\times n$ density matrix to represent a complex n-variate normal (Gaussian) distribution over the vectors of n-dimensional Hilbert space. For the case $n=2$ (complex), the counterpart of the information matrix (5) was [Ref. 19; Ref. 28, formula (11)]

$$\frac{1}{(1-x^2-y^2-z^2)^2}\begin{pmatrix} 2(1+x^2-y^2-z^2) & 4xy & 4xz \\ 4xy & 2(1-x^2+y^2-z^2) & 4yz \\ 4xz & 4yz & 2(1-x^2-y^2+z^2) \end{pmatrix}. \tag{33}$$

The square root of its determinant is

$$\frac{2\cdot 2^{1/2}(1+x^2+y^2+z^2)^{1/2}}{(1-x^2-y^2-z^2)^2}, \tag{34}$$

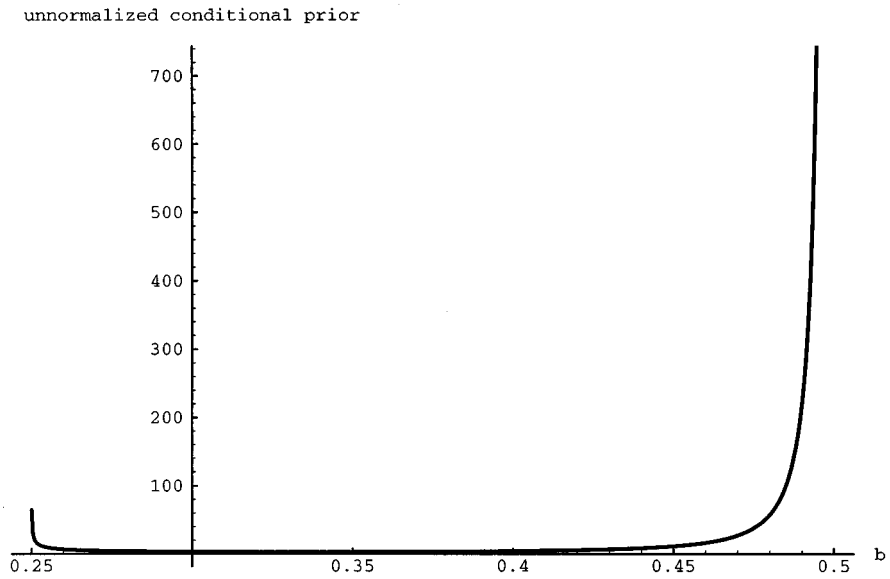

FIG. 4. Univariate unnormalized conditional prior (31) for three-level complex systems.

which *cannot* [cf. (6) and (7)] be normalized over the unit ball in three-space, though, through a limiting procedure,[19,28] one can obtain bivariate marginal probability distributions of the form

$$1/2\pi(1-x^2-y^2)^{1/2}, \quad x^2+y^2\leqslant 1. \tag{35}$$

[The quantum counterpart of this result—reported above—is the uniform distribution $(1/\pi)$.] Relatedly, one could not then obtain trivariate posterior probabilities [cf. (13)], but only bivariate ones.[19]

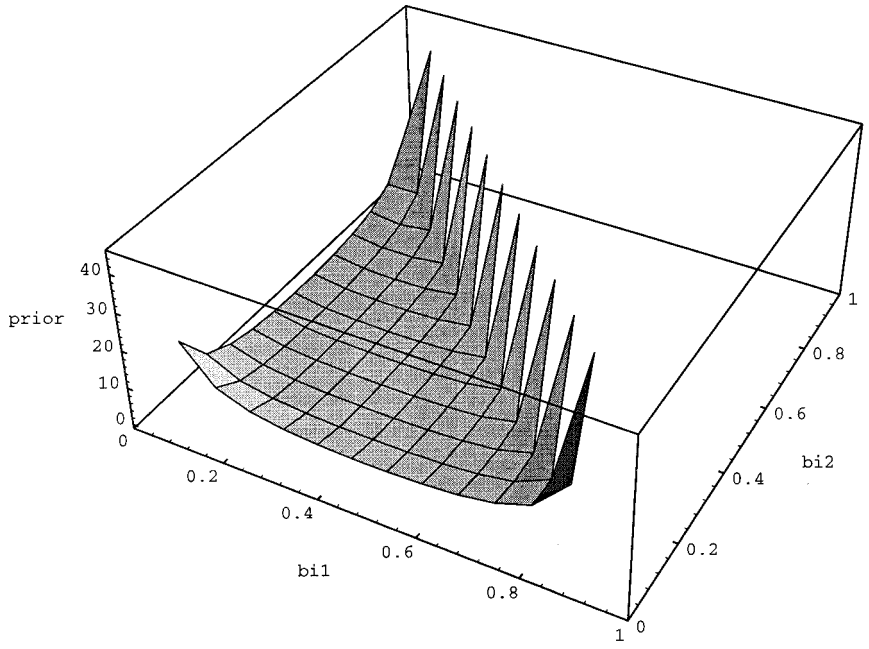

FIG. 5. Bivariate unnormalized conditional prior (32) for three-level complex systems.

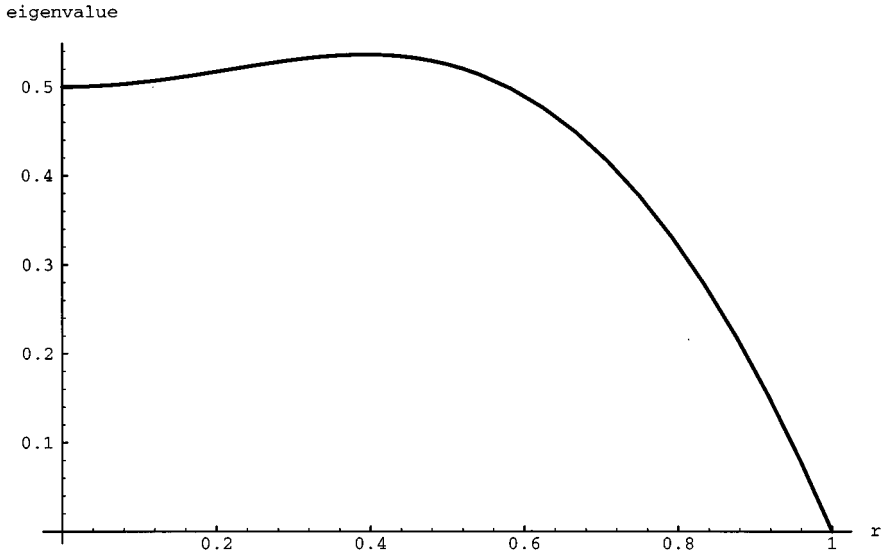

FIG. 6. Unrepeated eigenvalue of difference of inverses of 3×3 quantum and classical Fisher information matrices for two-level complex systems (spherical coordinates).

If the inverse of (33) is subtracted from the inverse of (5), that is, (14), the resulting difference has two eigenvalues both equal to $(1+x^2+y^2+z^2)/2$, which are clearly positive, and a third, which can be expressed in spherical coordinates as

$$\frac{1+2r^2-3r^4}{2(1+r^2)}. \tag{36}$$

This is positive for r, $0\leqslant r<1$ (Fig. 6). The non-negative nature of these three eigenvalues demonstrates that this difference of inverses is non-negative definite. Hence, in the sense of the Cramér–Rao lower bound,[5,6] the quantum Fisher information analysis provides a greater lower bound on the covariance matrices of unbiased estimates of x,y,z than the classical Fisher information analysis previously reported.[19,28] This result is plausible in that one can obtain only partial information concerning a quantum state through a quantum measurement.

A parallel analysis was also conducted involving the inverses of the quantum and classical quaternionic 5×5 Fisher information matrices (19). Four of the five eigenvalues of the matrix difference equalled, in spherical coordinates, $(3+r^2)/4$, where $r^2=u^2+v^2+x^2+y^2+z^2$. This value is clearly positive for r, $0\leqslant r\leqslant1$. The fifth eigenvalue (Fig. 7),

$$\frac{3+2r^2-5r^4}{4(1+r^2)} \tag{37}$$

is (cf. Fig. 6) also non-negative in the range of interest. Consequently, in the quaternionic as well as complex realms of two-level systems, the inverses of the quantum Fisher information matrices provide more stringent bounds than do the classical information matrices.[19,28] For $r=1$, that is, the pure states, since the unrepeated eigenvalues (36) and (37) are zero, there is a partial degeneracy in this regard.

For the classical Fisher information analysis of three-level systems, the counterparts of (31) and (32) have been found to be

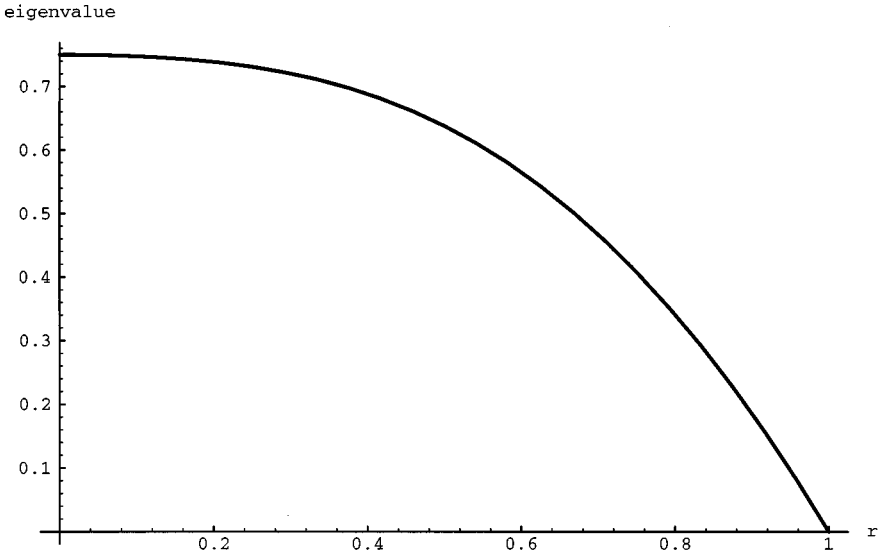

FIG. 7. Unrepeated eigenvalue of difference of inverses of 5×5 quantum and classical Fisher information matrices for two-level quaternionic systems (spherical coordinates).

$$\frac{3\cdot 3^{1/2}(3-16b+24b^2)^{1/2}}{(-1+2b)^6(-1+4b)^3} \tag{38}$$

and

$$\frac{3\cdot 3^{1/2}(1-2b_{i1}+2b_{i1}^2-2b_{i2}+2b_{i2}b_{i2}+2b_{i2}^2)^{1/2}}{(b_{i1}b_{i2}(1-b_{i1}-b_{i2}))^3}. \tag{39}$$

Dittmann [Ref. 11, formula (2.4)] has expressed the Bures metric, in general form, as

$$\tfrac{1}{2}\,\mathrm{Tr}(L_\rho+R_\rho)^{-1}(d\rho)d\rho, \tag{40}$$

where L_ρ and R_ρ are the operators of left and right multiplication of matrices by ρ. It was also observed that $L_\rho+R_\rho$ has the spectrum $\{\lambda+\mu|\ \lambda,\mu$ are eigenvalues of $\rho\}$. We have computed for the cases studied above ($n=2,3$) square roots of products of the form [that is, the square roots of the determinants of $(L_\rho+R_\rho)^{-1}$]

$$\prod_{i,j=1}^{n} 1 \Big/ (\lambda_i+\lambda_j) \tag{41}$$

and have found that this formula (conjectured to be proportional to the determinant of the quantum Fisher information matrix for all n) yields, up to proportionality, the results (6), (20), (31), and (32) reported here. [Note that, in this regard, the eigenvalues of the matrices from which (31) and (32) were generated are $(1-2b)$ (repeated) and $(-1+4b)$ and b_{i1}, b_{i2}, and $1-b_{i1}-b_{i2}$, respectively.] By the properties of the characteristic polynomial of a matrix,[29] these results would indicate that the three-level quantum prior, in general, is inversely proportional to the product of the square root of the determinant of ρ and the expression obtained by subtracting the determinant of ρ from the sum of the three principal minors of order two of the three-dimensional matrix ρ.

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Free quantum fields on the Poincaré group

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A class of free quantum fields defined on the Poincaré group is described by means of their two-point vacuum expectation values. They are not equivalent to fields defined on the Minkowski space–time and they are ''elementary'' in the sense that they describe particles that transform according to irreducible unitary representations of the symmetry group, given by the product of the Poincaré group and of the group SL(2,**C**) considered as an internal symmetry group. Some of these fields describe particles with positive mass and arbitrary spin and particles with zero mass and arbitrary helicity or with an infinite helicity spectrum. In each case the allowed SL(2,**C**) internal quantum numbers are specified. The properties of local commutativity and the limit in which one recovers the usual field theories in Minkowski space–time are discussed. By means of a superposition of elementary fields, one obtains an example of a field that presents a broken symmetry with respect to the group Sp(4,**R**) that survives in the short-distance limit. Finally, the interaction with an accelerated external source is studied and it is shown that, in some theories, the average number of particles emitted per unit of proper time diverges when the acceleration exceeds a finite critical value. © *1996 American Institute of Physics.* [S0022-2488(96)02005-7]

I. INTRODUCTION

Quantum field theories defined on the Poincaré group manifold $\mathscr{P}$ instead of the Minkowski space–time have been introduced by Lurçat[1] in 1964. A motivation of these investigations was a symmetric treatment of translations, rotations, and Lorentz boosts, namely of all the restricted Poincaré transformations. Later[2,3] it has been recognized that this point of view, in order to be really consistent, requires a symmetric treatment of velocity, angular velocity, and acceleration; since in relativistic theories there is an upper bound to the velocity of material objects, one has to introduce similar limitations to angular velocity and acceleration. The existence of an upper bound to the proper acceleration has also been suggested in Ref. 4. Brandt[5,6] has shown that a maximal acceleration of the order of $c^2 l_{\mathrm{P}}^{-1}$, where l_{P} is the Planck length, is expected as a quantum gravitational effect.

The theories studied in Ref. 1 are symmetric with respect to both the left and the right translations of the group $\mathscr{P}$. We suggest that the physical symmetry group is smaller, namely it contains all the left translations, but only the right translations generated by the homogeneous Lorentz group [or its universal covering SL(2,**C**)]. The aim of the present paper is to analyze the free fields on $\mathscr{P}$ (or on its universal covering $\tilde{\mathscr{P}}$) that satisfy this weaker symmetry requirement besides the natural positivity and spectral conditions. We begin by considering ''elementary'' fields, namely fields that describe particles that transform according to irreducible unitary representations (IURs) of the symmetry group. Other fields can be obtained by superposition of elementary fields, which could provide the building blocks for the construction of theories implementing the physical ideas indicated above.

We do not claim to have found all the fields with the assumed properties. A formal proof of this statement would require a more precise formulation of the problem, for instance, a specification of the distribution space to which the fields have to belong. We think that in a first approach

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it is more useful to find as many examples as possible and to introduce technical assumptions only when they are found to be necessary.

In order to clarify the physical meaning of our assumptions, it is convenient to consider the theories on an arbitrary group manifold as special cases of theories of a much larger class,[7–10] based on an n-dimensional differentiable manifold $\mathscr{S}$ endowed with a geometric structure defined by n vector fields A_α ($\alpha=0,...,n-1$) linearly independent at every point of $\mathscr{S}$. If $\mathscr{S}=\mathscr{G}$ is a group manifold, the vector fields A_α are the generators of the right translations (invariant under left translations)[11] and form a basis of the Lie algebra $\mathbf{l}$ of $\mathscr{G}$.

In another interesting case, $\mathscr{S}$ is the ten-dimensional principal bundle[12] of the pseudo-orthonormal frames (tetrads) of a (3+1)-dimensional pseudo-Riemannian space–time $\mathscr{M}$. The fields

$$A_4=A_{23}, \quad A_5=A_{31}, \quad A_6=A_{12}, \quad A_7=A_{10}, \quad A_8=A_{20}, \quad A_9=A_{30} \tag{1.1}$$

are the generators of the structural group of the bundle, namely of the Lorentz group acting on the tetrads. They define a basis of the ''vertical'' subspaces of the tangent spaces of $\mathscr{S}$. The fields $A_0,\ldots,A_3$ describe the infinitesimal parallel displacements along the tetrad vectors, namely they generate the ''horizontal'' subspaces which define a connection. If $\mathscr{M}$ is the flat Minkowski space–time, one can identify the bundle of frames $\mathscr{S}$ with the Poincaré group. In a similar way the de Sitter (or anti-de-Sitter) group can be identified with the bundle of frames $\mathscr{S}$ of a pseudo-Riemannian space–time $\mathscr{M}$ with constant positive (or negative) curvature.

Classical field theories including gravitation based on these ideas have been developed in Refs. 8–10, 13, and 14. If one identifies $\mathscr{S}$ with a principal bundle with a larger structural group, one can also treat Maxwell and Yang–Mills fields.[8,15] Any classical or quantum field defined on the pseudo-Riemannian space–time $\mathscr{M}$ can easily be translated into a field defined on the bundle of frames $\mathscr{S}$. We think, however, that the new formalism should be used to formulate new physical ideas.

The fields A_α define a ''teleparallelism'' in $\mathscr{S}$, namely a set of isomorphisms between all the tangent spaces of $\mathscr{S}$ and a fixed vector space $\mathscr{T}=\mathbf{R}^n$. A closed wedge $\mathscr{T}^+\subset\mathscr{T}$ defines a field of wedges in the tangent spaces of $\mathscr{S}$ which describes the causal properties of the theory and in particular the upper bounds to velocity, angular velocity, and acceleration.[2,3]

It is useful to introduce the structure coefficients $F^\gamma_{\alpha\beta}$ defined by

$$[A_\alpha, A_\beta]=F^\gamma_{\alpha\beta}A_\gamma, \tag{1.2}$$

where $[A, B]$ is the Lie bracket of two vector fields. If $\mathscr{S}$ is a group manifold, they are the structure constants of the corresponding Lie algebra. If $\mathscr{S}$ is a bundle of frames, some of the structure coefficients are the components of the curvature and torsion tensors and in a theory of gravitation they have a dynamical character, namely they depend on the distribution of matter.

In accord with the ideas indicated above, it is natural to consider theories in which all the structure coefficients $F^\gamma_{\alpha\beta}$ and all the vector fields A_α have a dynamical character. In a theory of this kind, the field equations determine both the fields A_α that describe the geometry and the fields ψ_ρ that describe matter. We assume that this theory is invariant under all the diffeomorphisms of $\mathscr{S}$ and under a symmetry group $\mathscr{F}$ acting linearly in the following way:

$$\psi_\rho\to S_\rho{}^\sigma(k)\psi_\sigma, \tag{1.3}$$

$$A_\alpha\to C_\alpha{}^\beta(k)A_\beta, \quad k\in\mathscr{F}, \tag{1.4}$$

where S and C are linear representations of $\mathscr{F}$. The representation C is real and one can consider it as acting on the vector space $\mathscr{T}$. It is natural to require that the transformations $C(k)$ leave the

wedge $\mathscr{T}^+$ invariant. It follows from the physical interpretation of the fields A_α that the element k cannot depend on the point of $\mathscr{S}$, namely $\mathscr{F}$ is a global symmetry group.

In the physically most interesting example, $\mathscr{S}$ is a ten-dimensional manifold, the group $\mathscr{F}$ contains a subgroup isomorphic to the restricted Lorentz group $SO\uparrow(3,1)$, and the representation C restricted to this subgroup is the direct sum of the vector and the antisymmetric tensor representations. Actually, in order to treat matter fields with half-integral spin, it is convenient to assume that $\mathscr{F}$ contains the universal covering of $SO^\uparrow(3,1)$, namely $SL(2,\mathbf{C})$. Under these conditions, if we assume that $\mathscr{T}^+$ is a cone (namely that $\mathscr{T}^+ \cap -\mathscr{T}^+ = \{0\}$) with interior points, this cone is determined up to a change of the units of time and length.[2,3] It has a large symmetry group given by $L(4,\mathbf{R})$ acting on $\mathscr{T}$ by means of its symmetric tensor representation.[2] In this framework, it is natural to assume that the symmetry group $\mathscr{F}$ of the theory is $L(4,\mathbf{R})$ or one of its subgroups that contain $SL(2,\mathbf{C})$. Possible choices are $SL(4,\mathbf{R})$, $Sp(4,\mathbf{R})$ or $SL(2,\mathbf{C})$.

In the present paper we consider the fields A_α as fixed classical fields and we concentrate our attention on the quantum fields that describe matter. The symmetry group of this partial theory contains only the elements of the symmetry group of the complete theory that do not affect the geometric fields A_α. For instance, the elements of $\mathscr{F}$ that do not preserve the values of the structure coefficients $F^\gamma_{\alpha\beta}$ represent broken symmetries. If we consider the values of the structure coefficients as expectation values of some fields in a vacuum state of the complete theory, this is a spontaneous symmetry breaking.

In Sec. II we discuss some general properties of quantized matter fields on an arbitrary connected Lie group. In Sec. III we begin the treatment of free quantum fields on the universal covering $\tilde{\mathscr{P}}$ of the restricted Poincaré group [namely the inhomogeneous $SL(2,\mathbf{C})$ group]. The subgroup of $\mathscr{F}$ that survives the symmetry breaking must preserve both the cone $\mathscr{T}^+$ and the structure constants of the Poincaré Lie algebra. It follows that it must coincide with $SL(2,\mathbf{C})$, as we have anticipated above. The unbroken symmetry group of the theory is the product of $\tilde{\mathscr{P}}$ and $SL(2,\mathbf{C})$, considered as an internal symmetry group. The free quantum fields are completely described by the two-point Wightman distributions [or vacuum expectation values, (VEVs)] and we give a general representation of the distributions that satisfy the appropriate symmetry, spectral, and positivity conditions. In Sec. IV we treat the commutation or anticommutation properties of the free fields and we discuss the connection between spin and statistics, which is not the usual one. For instance, a ''scalar'' field, namely a field with only one component, has to be quantized with commutators, but it can describe particles with any spin. In Sec. V we treat the positive-mass case with arbitrary spin and we write explicitly a wide class of VEVs in terms of the matrix elements of the IURs of $SL(2,\mathbf{C})$. In Sec. VI we consider the more delicate zero-mass case and find theories that describe particles with an infinite helicity spectrum (not observed in nature) and particles with an arbitrary given helicity. Scalar fields that describe particles with zero mass and given nonvanishing helicity have pathological features.

Since the nontrivial IURs of $SL(2,\mathbf{C})$ are infinite dimensional, the mass spectrum of these theories is infinitely degenerate. In order to avoid evident contradictions with the known physical phenomena, we have to require that, when the mass is within the range of presently available energies, only a finite number of internal states of the particles can be excited by the field with appreciable probability. This happens when the parameters which label the IURs of $SL(2,\mathbf{C})$ approach the limit $M=j=0$, $c\to 1$. Actually, in this limit the VEVs tend to the ones that define the usual scalar free field in Minkowski space–time. This problem is less relevant when the mass is of the order of the Planck mass. The theories with a broken higher symmetry satisfy these requirements automatically.

In Sec. VII we find the differential equations satisfied by the quantum fields defined in the preceding sections and compare them with some field equations in a flat ten-dimensional space. In Sec. VII we introduce the concept of ''spin-mass-shell'' and discuss the relation between the VEVs on $\tilde{\mathscr{P}}$ and the corresponding distributions defined on $\mathbf{R}^{10}$. We show that not all the free fields on the flat space have a corresponding field on $\tilde{\mathscr{P}}$.

In the remaining sections we give some examples, in order to illustrate the general formalism. A more complete treatment will be given elsewhere. In Sec. IX we consider a theory on the flat space symmetric with respect to the group Sp(4,**R**) and build the corresponding theory on $\tilde{\mathscr{P}}$. In this theory the higher symmetry is broken, but the VEVs maintain the higher symmetry in the short-distance limit. This is an explicit example of a new kind of broken symmetry in quantum field theory.

In Sec. X we consider an external source, represented by an accelerated disk, interacting with one of the fields defined in the present paper. We consider with more detail the field introduced in Sec. IX and we show that the number of particles emitted per unit of proper time diverges when the acceleration exceeds a finite critical value. This result shows that the formalism really contains, in some sense, the ideas that provided its motivation. Brandt[6] has suggested that, when the acceleration of a particle approaches a critical value, the energy radiated in the form of quantum black holes diverges, preventing a larger acceleration. The formalism presented here could provide a simplified model for this process, if the particles described by our fields are interpreted as quantum black holes.[16] This interpretation, however, raises several difficult problems.

II. QUANTUM FIELDS ON A GROUP MANIFOLD

As we have anticipated in the Introduction, we consider an n-dimensional manifold $\mathscr{S}$ with n vector fields A_α ($\alpha=0,...,n-1$) that, being linearly independent, define a basis in each tangent space of $\mathscr{S}$. As a consequence, we can identify all the tangent spaces with a single vector space $\mathscr{T}$. These vector fields describe the gravitational field and possibly other gauge fields, while matter is described by a set of fields ψ_ρ, on the manifold $\mathscr{S}$.[7–10] We assume that the complete field equations, including gravitation, are invariant under all the diffeomorphisms of $\mathscr{S}$ and under a group $\mathscr{F}$ which acts on the matter fields and on the geometric fields according to the linear formulas (1.3) and (1.4).

We consider the fields A_α as classical external fields and we restrict our considerations to symmetry transformations that leave them invariant. The transformations which have this property are implemented by unitary or antiunitary operators acting on the Hilbert space $\mathscr{H}$ which describes the states of matter. Since we consider only connected symmetry groups, we deal only with unitary symmetry operators.[17] Moreover, we assume that they form a continuous representation of the symmetry group.[18] The fields ψ_ρ are operator-valued distributions on $\mathscr{S}$ that act in a dense linear subspace $\mathscr{D}$ of $\mathscr{H}$. We assume that both the smeared field operators and the symmetry operators transform $\mathscr{D}$ into itself.

Field theories on an n-dimensional manifold $\mathscr{S}$ which has a symmetry group have been treated in Ref. 7. Here we consider the case in which the vector fields A_α generate a connected n-dimensional Lie group $\mathscr{G}$ of diffeomorphisms of $\mathscr{S}$. It is convenient to assume that $\mathscr{G}$ acts on the right in the space $\mathscr{S}$, namely the action of the element $g\in\mathscr{G}$ on the element $s\in\mathscr{S}$ is written as $(g,s)\to sg$. We assume also that $\mathscr{G}$ acts freely and transitively; it follows that if we choose an origin $s_0\in\mathscr{S}$, the mapping $g\to s=s_0g$ is a diffeomorphism of $\mathscr{G}$ onto $\mathscr{S}$. The action of $\mathscr{G}$ on $\mathscr{S}$ takes the form

$$s=s_0g\to s'=s_0gh=sh,\quad g,h\in\mathscr{G}, \tag{2.1}$$

namely, it corresponds to a right translation of $\mathscr{G}$. The vector fields A_α can also be considered as fields on $\mathscr{G}$, which generate the right translations. They form a basis of the Lie algebra $\mathbf{l}$ of $\mathscr{G}$, that, as a vector space, can be identified with $\mathscr{T}$.

The vector fields A_α are invariant under the left translations of $\mathscr{G}$; it follows that a transformation of the kind

$$s=s_0g\to s'=s_0hg,\quad g,h\in\mathscr{G}, \tag{2.2}$$

is a symmetry transformation that leaves the geometry of $\mathscr{S}$ invariant. It can be interpreted as a change of the origin s_0.

The diffeomorphisms of the kind (2.2) provide a first class of symmetry transformations. They act on the matter fields in the following way:

$$\psi_\rho(s_0 h^{-1} g) = U(h)^{-1} \psi_\rho(s_0 g) U(h), \quad g,h \in \mathscr{G}. \tag{2.3}$$

Note that the indices of the fields are not involved: every component behaves as a scalar field. We indicate by $U(A_\alpha)$ the generators of the continuous unitary representation U corresponding to the elements A_α of $\mathbf{l}$. The operators $iU(A_\alpha)$ are self-adjoint and are interpreted as the energy, the momentum, the relativistic angular momentum, and possibly (if $n>10$) the charges that generate some gauge transformations. Note that, as it is expected, these operators, as well as the unitary operators $U(h)$, depend on the choice of the frame s_0.

The diffeomorphisms of the kind (2.1) affect the geometric fields according to the formula

$$A_\alpha \to A_\beta B^\beta{}_\alpha(h), \tag{2.4}$$

where $B^\beta{}_\alpha(h)$ is the adjoint representation of $\mathscr{G}$. They give rise to symmetry transformations only if Eq. (2.4) can be compensated by a transformation of the kind (1.4), namely, if

$$B^\beta{}_\alpha(h) = C_\alpha{}^\beta(\hat{h}^{-1}), \quad h \in \mathscr{G}, \quad \hat{h} \in \mathscr{F}. \tag{2.5}$$

This condition defines a subgroup $\mathscr{G}_2 \subset \mathscr{G}$ and we assume that $h \to \hat{h}$ is a continuous homomorphism of $\mathscr{G}_2$ onto a subgroup $\mathscr{F}_2 \subset \mathscr{F}$. In the following we write $S(h)$ instead of $S(\hat{h})$. Then we have

$$S_\rho{}^\sigma(h) \psi_\sigma(sh) = V(h)^{-1} \psi_\rho(s) V(h), \quad h \in \mathscr{G}_2. \tag{2.6}$$

The operators $V(h)$ commute with the operators $U(g)$ and do not depend on the choice of s_0. They describe a kind of internal symmetry.

The internal automorphisms of $\mathscr{G}$, given by $g \to hgh^{-1}$, are the product of a right and a left translation and do not require a separate treatment. The external automorphisms of $\mathscr{G}$ (for instance, the space–time dilatations in the Poincaré group) give rise to a new kind of symmetry if their action on the fields A_α can be compensated by a transformation of the kind (1.4). This compensation is not possible in the cases we shall treat in the following sections.

Several general features of the quantum field theories on Minkowski space–time[19,20] can be extended to the theories on a group manifold. We assume that there is a vacuum state $\Omega \in \mathscr{D}$ invariant with respect to both the representations U and V, and we define the VEV

$$(\Omega, \psi_\rho(s_1) \psi_\sigma(s_2) \Omega) = \mathscr{W}_{\rho\sigma}(s_1, s_2). \tag{2.7}$$

It follows from Eq. (2.3) that this quantity can be considered as a distribution on $\mathscr{G}$. In fact, we have

$$\mathscr{W}_{\rho\sigma}(s_1, s_2) = \mathscr{W}_{\rho\sigma}(s_0 g_1, s_0 g_2) = W_{\rho\sigma}(g_1^{-1} g_2). \tag{2.8}$$

In the following we understand a fixed choice of s_0 and we write $\psi_\rho(g)$ instead of $\psi_\rho(s_0 g)$. The VEV of $m+1$ fields is defined in the following way as a distribution on $\mathscr{G}^m$:

$$(\Omega, \psi_{\rho_1}(g_1) \cdots \psi_{\rho_{m+1}}(g_{m+1}) \Omega) = W^{(m)}_{\rho_1 \cdots \rho_{m+1}}(g_1^{-1} g_2, \ldots, g_m^{-1} g_{m+1}). \tag{2.9}$$

If the fields $\psi_\rho(g)$ are not Hermitean, we have to consider the Hermitean conjugate as a different field and we use the notation

$$\psi^{\dagger}_{\rho}(g)=\psi_{\overline{\rho}}(g), \quad S_{\overline{\rho}}^{\ \overline{\sigma}}(h)=\overline{S_{\rho}^{\ \sigma}}(h). \tag{2.10}$$

In all the formulas any index can be replaced by a barred index and vice versa, unless it is stated otherwise. If the field is Hermitean, we have to put $\overline{\rho}=\rho$ and the representation S must be real. Then from the definition we obtain

$$\overline{W^{(m)}_{\rho_1\cdots\rho_{m+1}}}(g_1,\ldots,g_m)=W^{(m)}_{\overline{\rho}_{m+1}\cdots\overline{\rho}_1}(g_m^{-1},\ldots,g_1^{-1}) \tag{2.11}$$

and from Eq. (2.6) we obtain the symmetry property

$$S_{\rho_1}^{\ \ \sigma_1}(h)\cdots S_{\rho_{m+1}}^{\ \ \sigma_{m+1}}(h)W^{(m)}_{\sigma_1\cdots\sigma_{m+1}}(h^{-1}g_1h,\ldots,h^{-1}g_mh)=W^{(m)}_{\rho_1\cdots\rho_{m+1}}(g_1,\ldots,g_m), \quad h\in\mathscr{G}_2. \tag{2.12}$$

If we deal with free fields, all the VEVs can be obtained from the two-point distributions by means of the Wick theorem. In this case, the vectors of the kind

$$\Phi(f)=\int f^{\rho}(g)\psi^{\dagger}_{\rho}(g)dg\Omega, \tag{2.13}$$

where f is a test function and dg is an invariant measure on $\mathscr{G}$, are dense in the Hilbert space $\mathscr{H}^{(1)}$ of the ''one-particle'' states. The square of the norm of the vector (2.13) is given by

$$(\Phi(f),\Phi(f))=\int \overline{f^{\rho}}(g_1)f^{\sigma}(g_2)W_{\rho\overline{\sigma}}(g_1^{-1}g_2)dg_1dg_2\geqslant 0. \tag{2.14}$$

This is the positivity condition. For interacting field theories, we have more complicated positivity conditions that involve all the other VEVs.

The symmetry operators defined in Eqs. (2.3) and (2.6) act on the one-particle states in the following way:

$$U^{(1)}(h)\Phi(f)=\Phi(f'), \quad f'^{\rho}(g)=f^{\rho}(h^{-1}g), \tag{2.15}$$

$$V^{(1)}(h)\Phi(f)=\Phi(f'), \quad f'^{\rho}(g)=f^{\sigma}(gh)\overline{S_{\sigma}^{\ \rho}}(h^{-1}). \tag{2.16}$$

Equations (2.14)–(2.16) permit, in the usual way, the reconstruction of the one-particle Hilbert space (as the completion of a quotient) and of the operators $U^{(1)}(h)$ and $V^{(1)}(h)$. If the unitary representation $U^{(1)}\times V^{(1)}$ of $\mathscr{G}\times\mathscr{G}_2$ is irreducible, we say that the free field is ''elementary.''

III. FREE FIELDS ON THE POINCARÉ GROUP

Now we apply the general results of the preceding section to the Poincaré group. We consider the ten-dimensional manifold $\mathscr{S}$ of all the Lorentz reference frames in the Minkowski space $\mathscr{M}$ which are left-handed and future-directed. If we fix a reference frame s_0, for each reference frame s there is one and only one element of the proper orthochronous Poincaré group $\mathscr{P}$ that transforms s_0 into s. Then we can identify the space $\mathscr{S}$ with $\mathscr{P}$ and consider quantum fields defined on it. Actually, in order to treat fields with half-integral spin, it is convenient to use the universal covering $\tilde{\mathscr{P}}$ of $\mathscr{P}$, namely the semidirect product of the four-dimensional translation group $\mathbf{R}^4$ and SL(2,**C**). For the elements of this group and for their multiplication rule, we use the standard notation

$$(x,a)(y,b)=(x+\Lambda(a)y,ab), \quad x,y\in\mathbf{R}^4, \quad a,b,\in \mathrm{SL}(2,\mathbf{C}), \tag{3.1}$$

where $\Lambda(a)$ is the 4×4 Lorentz matrix corresponding to the element $a\in \mathrm{SL}(2,\mathbf{C})$. For the scalar product of two four-vectors we use the notation

$$g_{ik}x^i y^k = x\cdot y = -x^0y^0+\mathbf{x}\cdot\mathbf{y}, \quad \mathbf{x}\cdot\mathbf{y}=x^1y^1+x^2y^2+x^3y^3. \tag{3.2}$$

The one-parameter subgroups of $\mathrm{SL}(2,\mathbf{C})$ that correspond to rotations around the axes and to pure Lorentz transformations along the axes are written as

$$u_k(\theta)=\exp(-\tfrac{1}{2}i\theta\sigma_k), \quad a_k(\zeta)=\exp(\tfrac{1}{2}\zeta\sigma_k), \tag{3.3}$$

where σ_k are the Pauli matrices.

We assume that the group $\mathscr{T}$ contains $\mathrm{SL}(2,\mathbf{C})$ and that it preserves the cone $\mathscr{T}^+$ defined in Refs. 2 and 3. It is easy to see that the translations (acting on $\mathscr{T}$ by means of the adjoint representation of $\mathscr{P}$) and the space–time dilatations (which are external automorphisms of $\widetilde{\mathscr{P}}$ and of the corresponding Lie algebra) do not preserve the cone $\mathscr{T}^+$. It follows that we have to put $\mathscr{G}_2=\mathrm{SL}(2,\mathbf{C})$. Then the general equations (2.3) and (2.6) take the form

$$\psi_\rho((y,b)^{-1}(x,a))=\psi_\rho(\Lambda(b)^{-1}(x-y),b^{-1}a)=U(y,b)^{-1}\psi_\rho(x,a)U(y,b), \tag{3.4}$$

$$S_\rho{}^\sigma(b)\psi_\sigma(x,ab)=V(b)^{-1}\psi_\rho(x,a)V(b). \tag{3.5}$$

If $V(b)=1$, from Eq. (3.5) we have

$$\psi_\rho(x,a)=S_\rho{}^\sigma(a^{-1})\psi_\sigma(x,1), \tag{3.6}$$

and we are dealing with a field $\psi_\sigma(x)=\psi_\sigma(x,1)$ defined on the Minkowski space–time. From Eq. (3.4), we obtain the usual covariance property

$$S_\rho{}^\sigma(b)\psi_\sigma(\Lambda(b)^{-1}(x-y))=U(y,b)^{-1}\psi_\rho(x)U(y,b). \tag{3.7}$$

In the following we consider the case in which $V(b)$ is not trivial.

A free-field theory is completely described by the two-point VEVs

$$(\Omega,\psi_\rho(x,a)\psi_\sigma(y,b)\Omega)=W_{\rho\sigma}((x,a)^{-1}(y,b))=W_{\rho\sigma}(\Lambda(a^{-1})(y-x),a^{-1}b). \tag{3.8}$$

From the covariance property (3.5) we obtain the formula

$$W_{\rho\sigma}(\Lambda(b)x,bab^{-1})=S_\rho{}^\mu(b)S_\sigma{}^\nu(b)W_{\mu\nu}(x,a) \tag{3.9}$$

(remember our conventions about the introduction of barred indices). If the field is not Hermitean, we assume

$$W_{\rho\sigma}(x,a)=W_{\overline{\rho\sigma}}(x,a)=0 \tag{3.10}$$

(here the bars over the indices cannot be modified) and the distributions $W_{\rho\overline{\sigma}}(x,a)$ and $W_{\overline{\rho}\sigma}(x,a)$ can be treated independently unless we introduce some requirement of local commutativity (see Sec. IV).

The states of the form

$$\Phi(f)=\int f^\rho(x,a)\psi_\rho^\dagger(x,a)d^4x d^6a\,\Omega, \tag{3.11}$$

where f is an arbitrary test function with compact support and d^6a is an invariant measure on $\mathrm{SL}(2,\mathbf{C})$, form a dense set in the Hilbert subspace $\mathscr{H}^{(1)}$ of the one-particle states. Their norm is given by the formula

$$(\Phi(f),\Phi(f))=\int \overline{f^{\rho}}(x,a)f^{\sigma}(y,b)W_{\rho\sigma}(\Lambda(a^{-1})(y-x),a^{-1}b)d^4x d^6a d^4y d^6b \geqslant 0, \quad (3.12)$$

which also gives the positivity property of the two-point distribution.

We want to find the solutions of the conditions (3.9) and (3.12) that describe elementary free fields. More general solutions can be obtained by means of sums or integrals of these solutions. If we introduce the Fourier transformations

$$W_{\rho\sigma}(x,a)=\int \exp(-ik\cdot x)\widetilde{W}_{\rho\sigma}(k,a)d^4k, \quad (3.13)$$

$$\widetilde{f}^{\rho}(k,a)=\int \exp(-ik\cdot x)f^{\rho}(x,a)d^4x, \quad (3.14)$$

Eq. (3.12) takes the form

$$(\Phi(f),\Phi(f))=\int \overline{\widetilde{f}^{\rho}}(k,a)\widetilde{f}^{\sigma}(k,b)\widetilde{W}_{\rho\sigma}(\Lambda(a^{-1})k,a^{-1}b)d^6a d^6b d^4k \geqslant 0, \quad (3.15)$$

and Eq. (3.9) gives

$$\widetilde{W}_{\rho\sigma}(\Lambda(b)k,bab^{-1})=S_{\rho}{}^{\mu}(b)\overline{S_{\sigma}{}^{\nu}}(b)\widetilde{W}_{\mu\nu}(k,a). \quad (3.16)$$

We assume that the distribution $\widetilde{W}_{\rho\sigma}(k,a)$ vanishes if k does not belong to the future cone (spectral condition). Since the elementary fields have a definite mass μ, this distribution has support on the orbit defined by

$$k\cdot k=-\mu^2, \quad k^0>0, \quad (3.17)$$

and has the form

$$\widetilde{W}_{\rho\sigma}(k,a)=(2\pi)^{-3}w_{\rho\sigma}(k,a)\,\theta(k^0)\,\delta(k\cdot k+\mu^2), \quad (3.18)$$

where θ is the step function.

Following a procedure introduced by Wigner,[21] we choose a representative element on each orbit,

$$\hat{k}=(\mu,0,0,0), \quad \mu>0, \quad (3.19)$$

$$\hat{k}=(1,0,0,1), \quad \mu=0 \quad (3.20)$$

and for each value of the four-momentum k on the orbit, we choose an element $a_k\in \mathrm{SL}(2,\mathbf{C})$ with the property

$$k=\Lambda(a_k)\hat{k}. \quad (3.21)$$

Then we see from Eq. (3.16) that we can put

$$w_{\rho\sigma}(k,a)=S_{\rho}{}^{\mu}(a_k)\overline{S_{\sigma}{}^{\nu}}(a^{-1}a_k)w_{\mu\nu}(a_k{}^{-1}aa_k), \quad (3.22)$$

where

$$w_{\rho\sigma}(a)=\overline{S_{\sigma}{}^{\nu}}(a)w_{\rho\nu}(\hat{k},a). \quad (3.23)$$

In this way we obtain the integral representation

$$W_{\rho\dot{\sigma}}(x,a)=(2\pi)^{-3}\int \exp(-ik\cdot x)S_\rho{}^\mu(a_k)\overline{S_\sigma}{}^\nu(a^{-1}a_k)w_{\mu\dot{\nu}}(a_k{}^{-1}aa_k)\,\theta(k^0)\,\delta(k\cdot k+\mu^2)d^4k. \tag{3.24}$$

The positivity condition (3.15) takes the form

$$(\Phi(f),\Phi(f))=(2\pi)^{-3}\int \overline{\tilde{f}^\rho}(k,a_k a)\tilde{f}^\sigma(k,a_k b)S_\rho{}^\mu(a^{-1})\overline{S_\sigma}{}^\nu(b^{-1}) \times w_{\mu\dot{\nu}}(ba^{-1})\,\theta(k^0)\,\delta(k\cdot k+\mu^2)d^6a\,d^6b\,d^4k\geqslant 0, \tag{3.25}$$

which is equivalent to the simpler condition

$$\int \overline{f^\rho}(a)f^\sigma(b)w_{\rho\dot{\sigma}}(ba^{-1})d^6a\,d^6b\geqslant 0. \tag{3.26}$$

The little group $\mathscr{K}$ corresponding to the representative element $\hat{k}$ is defined by the condition[21]

$$\Lambda(u)\hat{k}=\hat{k},\quad u\in\mathscr{K}\subset \mathrm{SL}(2,\mathbf{C}). \tag{3.27}$$

For $\mu>0$ we have $\mathscr{K}=\mathrm{SU}(2)$, the universal covering of the rotation group SO(3). For $\mu=0$, we have $\mathscr{K}=\tilde{E}(2)$, a double covering of the Euclidean group $E(2)$. From Eq. (3.16) we get the condition

$$w_{\rho\dot{\sigma}}(uau^{-1})=S_\rho{}^\mu(u)\overline{S_\sigma}{}^\nu(u)w_{\mu\dot{\nu}}(a),\quad u\in\mathscr{K}. \tag{3.28}$$

From Eq. (2.11) we also get the property

$$\overline{W}_{\rho\dot{\sigma}}(x,a)=W_{\sigma\dot{\rho}}((x,a)^{-1}). \tag{3.29}$$

An equivalent condition is

$$\overline{w}_{\rho\dot{\sigma}}(a)=w_{\sigma\dot{\rho}}(a^{-1}), \tag{3.30}$$

which is a consequence of Eq. (3.26).

Our problem is to find solutions of the conditions (3.26) and (3.28). Then we have to verify that the product of distributions that appears in Eq. (3.24) is meaningful.

If the theory can be interpreted as a theory in Minkowski space–time, namely if $V(b)=1$, the VEVs satisfy the additional symmetry property

$$W_{\rho\dot{\sigma}}(x,ab^{-1})=\overline{S_\sigma}{}^\nu(b)W_{\rho\dot{\nu}}(x,a). \tag{3.31}$$

An equivalent condition is to require that the function $w_{\rho\dot{\sigma}}(a)$ defined by Eq. (3.23) does not depend on a.

IV. LOCAL COMMUTATIVITY

The study of the distribution $W_{\rho\dot{\sigma}}(x,a)$ can be simplified if we find an element b in such a way that

$$a=bu_3(\alpha)a_3(\beta)b^{-1},\quad -2\pi<\alpha\leqslant 2\pi,\quad \beta\geqslant 0. \tag{4.1}$$

This is possible outside the four-dimensional submanifold of SL(2,**C**) where the eigenvalues of a are equal. Since these eigenvalues are given by $\exp(\pm\frac{1}{2}(\beta - i\alpha))$, we have to avoid the ''singular'' points $\alpha = 0, 2\pi, \beta = 0$; namely, we have to impose the condition

$$\cosh\beta - \cos\alpha = 2|\sinh(\tfrac{1}{2}(\beta - i\alpha)|^2 > 0. \tag{4.2}$$

We also introduce the quantities

$$\rho^2 = (\cosh\beta - \cos\alpha)^{-1}(\cosh\beta\, x\cdot x - x\cdot\Lambda(a)x), \tag{4.3}$$

$$\sigma^2 = (\cosh\beta - \cos\alpha)^{-1}(\cos\alpha\, x\cdot x - x\cdot\Lambda(a)x), \tag{4.4}$$

which, when $a = u_3(\alpha)a_3(\beta)$, take the form

$$\rho^2 = (x^1)^2 + (x^2)^2, \quad \sigma^2 = (x^0)^2 - (x^3)^2. \tag{4.5}$$

In order to simplify the formalism, we assume that $W_{\rho\dot{\sigma}}(x,a)$ is a tempered distribution in x that depends continuously on a. This is true for the massive free fields described in Sec. V. From Eqs. (3.9) and (4.1), we see that in the open set defined by Eq. (4.2) we have

$$W_{\rho\dot{\sigma}}(x,a) = S_\rho{}^\mu(b)\overline{S_\sigma{}^\nu}(b)W_{\mu\dot{\nu}}(\Lambda(b^{-1})x, u_3(\alpha)a_3(\beta)). \tag{4.6}$$

The spectral condition implies, as in the Minkowskian field theory, that the distribution $W_{\rho\dot{\sigma}}(x,u_3(\alpha)a_3(\beta))$ for fixed values of α and β is the boundary value of an analytic function of x defined in the tube $\mathrm{Im}\, x \in V_+$, where V_+ is the open future cone. From Eq. (3.9) we also obtain

$$W_{\rho\dot{\sigma}}(\Lambda(u_3(\psi)a_3(\xi))x, u_3(\alpha)a_3(\beta))$$

$$= S_\rho{}^\mu(u_3(\psi)a_3(\xi))\overline{S_\sigma{}^\nu}(u_3(\psi)a_3(\xi))W_{\mu\dot{\nu}}(x, u_3(\alpha)a_3(\beta)). \tag{4.7}$$

If we fix the variables α,β, it is a simple application of the Bargmann Hall Wightman theorem[19,20] to find by means of Eq. (4.7) an analytic continuation of the VEV (Wightman function) which is covariant with respect to the complex two-dimensional Lorentz group acting on the coordinates x^0,x^3 and to the real rotations acting on the coordinates x^1,x^2. The real points which satisfy the condition $\sigma^2 < 0$ belong to the analyticity domain.

The universal covering of the proper complex Lorentz group is SL(2,**C**)×SL(2,**C**). We indicate its elements by the notation (a,b); the real Lorentz transformations correspond to the elements of the kind $(a,\overline{a})$. If $S(a)$ is the irreducible spinor representation $S^{(s,s')}(a) = S^{(s,0)}(a)\otimes S^{(s',0)}(\overline{a})$, its analytic continuation is given by $S^{(s,s')}(a,b) = S^{(s,0)}(a)\otimes S^{(s',0)}(b)$. $\overline{S(a)}$ is equivalent to $S^{(s',s)}(a)$ and its analytic continuations is equivalent to $S^{(s',s)}(a,b)$. We consider the following product of a complex Lorentz transformation acting on x^0,x^3 and a real rotation acting on x^1,x^2:

$$(\exp(-\tfrac{1}{2}i\pi\sigma_3), \exp(-\tfrac{1}{2}i\pi\sigma_3))(\exp(-\tfrac{1}{2}i\pi\sigma_3), \exp(\tfrac{1}{2}i\pi\sigma_3)) = (-1,1), \tag{4.8}$$

$$\Lambda(-1,1) = -1, \quad S^{(s,s')}(-1,1) = (-1)^{2s}. \tag{4.9}$$

Then, from the covariance property of the Wightman function, we obtain

$$W_{\rho\dot{\sigma}}(-x, u_3(\alpha)a_3(\beta)) = (-1)^{2(s+s')}W_{\rho\dot{\sigma}}(x, u_3(\alpha)a_3(\beta)), \tag{4.10}$$

and the same equality holds for real x if $\sigma^2<0$. The same result is valid if S is a direct sum of irreducible spinor representations all with the same value of $(-1)^{2(s+s')}$. If we use Eq. (4.6) and the general expression (4.4) for σ^2, we see that

$$W_{p\overline{\sigma}}(-x,a)=(-1)^{2(s+s')}W_{\rho\overline{\sigma}}(x,a) \tag{4.11}$$

in the open set $\mathscr{C}\subset\widetilde{\mathscr{P}}$ defined by the condition

$$\cos\ \alpha\ x\cdot x-x\cdot\Lambda(a)x<0. \tag{4.12}$$

One can show that this condition implies Eq. (4.2).

If we consider a scalar field and we introduce the variables

$$\begin{aligned} x&=(\epsilon\sigma\ \cosh\ \xi',\rho\ \cos\ \psi',\rho\ \sin\ \psi',\epsilon\sigma\ \sinh\ \xi'),\quad \sigma>0,\\ x&=(\epsilon|\sigma|\sinh\ \xi',\rho\ \cos\ \psi',\rho\ \sin\ \psi',\epsilon|\sigma|\cosh\ \xi'),\quad \sigma^2<0,\quad \epsilon=\pm 1, \end{aligned} \tag{4.13}$$

Eq. (4.7) shows that $W(x,u_3(\alpha)a_3(\beta))$ does not depend on the variables ψ' and ξ'. From Eq. (4.10) we see that if $\sigma^2<0$ it does not even depend on ϵ. In conclusion, for $\sigma^2<0$, W can be considered as a distribution in the variables $\alpha,\beta,x^1,x^2,|\sigma|$ invariant with respect to rotations acting on x^1,x^2. In particular, since a and a^{-1} have the same eigenvalues, from Eqs. (4.3) and (4.4) we obtain

$$W(x,a)=W(-x,a)=W(-x,a^{-1}),\quad (x,a)\in\mathscr{C}. \tag{4.14}$$

The commutator or the anticommutator of a free field is a numerical distribution given by

$$\begin{aligned} [\psi_\rho(x,a),\ \psi^\dagger_\sigma(y,b)]_\pm&=W_{\rho\overline{\sigma}}((x,a)^{-1}(y,b))\pm W_{\overline{\sigma}\rho}((y,b)^{-1}(x,a))\\ &=W_{\rho\overline{\sigma}}((x,a)^{-1}(y,b))\pm\overline{W}_{\overline{\rho}\sigma}((x,a)^{-1}(y,b)). \end{aligned} \tag{4.15}$$

If we consider a Hermitean scalar field, and we use Eq. (3.9), we have the simpler relation

$$[\psi(x,a),\ \psi(y,b)]_-=W(x-y,ba^{-1})-W(y-x,ab^{-1})=2i\ \mathrm{Im}\ W(x-y,ba^{-1}), \tag{4.16}$$

and from Eq. (4.14) we obtain

$$[\psi(x,a),\ \psi(y,b)]_-=0\quad \text{for}\ (x,a)^{-1}(y,b)\in\mathscr{C}. \tag{4.17}$$

We see that in the formulation of local commutativity, Eq. (4.12) is the analog of the inequality $x\cdot x>0$ in Minkowski field theory.

In the general case, if we impose a local (anti)commutativity condition of the kind

$$[\psi_\rho(x,a),\ \psi^\dagger_\sigma(y,b)]_\pm=0\quad \text{for}\ (x,a)^{-1}(y,b)\in\mathscr{C}, \tag{4.18}$$

from Eqs. (4.11) and (4.15) we obtain

$$W_{\overline{\rho\sigma}}(x,a)=\mp(-1)^{2(s+s')}\overline{W}_{\rho\overline{\sigma}}(-\overline{x,a}),\quad (x,a)\in\mathscr{C}. \tag{4.19}$$

This relation can be continued analytically in the tube $\mathrm{Im}\ x\in V_+$ and, as an equality of distributions, it holds for any real x. It is compatible with the spectral and covariance conditions, but it satisfies the positivity condition only if $\mp(-1)^{2(s+s')}=1$. In conclusion, the local (anti)commutativity relation (4.18) is satisfied if we put

$$W_{\overline{\rho\sigma}}(x,a)=\overline{W}_{\rho\overline{\sigma}}(-x,a), \tag{4.20}$$

and the statistics is determined by $(-1)^{2(s+s')}$. We shall see that $s+s'$ is not directly related to the spin of the particles described by the field and the usual relation between spin and statistics is not necessarily valid. From Eq. (3.24) we see that Eq. (4.20) is equivalent to the condition

$$w_{\overline{\rho\sigma}}(a)=\overline{w_{\rho\sigma}}(a). \tag{4.21}$$

For a Hermitean field this condition requires that $w_{\rho\sigma}(a)$ is real.

It is interesting to study the integral (3.24) in the scalar case with more detail. If $w(a)=1$, Eq. (3.24) gives the usual VEV for the Minkowskian free scalar field, namely,

$$\begin{aligned} W(x)=&i(4\pi)^{-1}\epsilon(x^0)\,\delta(s^2)+(2\pi)^{-2}\theta(-s^2)\mu|s|^{-1}K_1(\mu|s|)+(8\pi)^{-1}\\ &\times\theta(s^2)\mu s^{-1}(Y_1(\mu s)-i\epsilon(x^0)J_1(\mu s)),\quad s^2=-x\cdot x=\sigma^2-\rho^2, \end{aligned} \tag{4.22}$$

where $\epsilon(x^0)$ is the sign of x^0. The corresponding commutator vanishes for $\sigma^2<\rho^2$.

If the function $w(a_k^{-1}aa_k)$ decreases for large k, the distribution $W(x,a)$ is less singular. In order to simplify the integral (3.24), it is convenient to write the four-vector k in the following way,

$$\begin{gathered} k=(q\ \cosh\xi, p\ \cos\psi, p\ \sin\psi, q\ \sinh\xi),\quad q=(p^2+\mu^2)^{1/2},\\ 0\leqslant p<\infty,\quad -\infty<\xi<\infty,\quad 0\leqslant\psi<2\pi,\\ (2k^0)^{-1}d^3\mathbf{k}=\tfrac{1}{2}p\,dp\,d\xi\,d\psi, \end{gathered} \tag{4.23}$$

and to choose

$$a_k=u_3(\psi)a_3(\xi)a_\eta. \tag{4.24}$$

For $\mu>0$ we take

$$a_\eta=a_1(\eta),\quad p=\mu\ \sinh\ \eta,\quad q=\mu\ \cosh\ \eta,\quad 0\leqslant\eta<\infty, \tag{4.25}$$

and for $\mu=0$

$$a_\eta=a_1(\eta)u_2(\tfrac{1}{2}\pi),\quad p=q=\exp\ \eta,\quad -\infty<\eta<\infty. \tag{4.26}$$

From Eq. (4.13) we obtain

$$\begin{aligned} k\cdot x&=-\epsilon q\sigma\ \cosh(\xi-\xi')+p\rho\ \cos(\psi-\psi'),\quad \sigma^2>0,\\ k\cdot x&=\epsilon q|\sigma|\sinh(\xi-\xi')+p\rho\ \cos(\psi-\psi'),\quad \sigma^2<0. \end{aligned} \tag{4.27}$$

The integrations over the variables ξ and ψ in Eq. (3.24) can be performed in terms of Bessel functions[22] and we obtain the following formula

$$W(x,a)=(2\pi)^{-1}\int_0^\infty \Delta(q\sigma,\epsilon(x^0))\ J_0(p\rho)w(\alpha,\beta,p)p\ dp, \tag{4.28}$$

where

$$\Delta(q\sigma,\epsilon(x^0))=(2\pi)^{-1}\theta(-\sigma^2)K_0(q|\sigma|)-\tfrac{1}{4}\theta(\sigma^2)(Y_0(q\sigma)-i\epsilon(x^0)J_0(q\sigma)) \tag{4.29}$$

and

$$w(\alpha,\beta,p)=w(a_\eta^{-1}u_3(\alpha)a_3(\beta)a_\eta). \tag{4.30}$$

The commutator of a scalar Hermitean field follows from Eqs. (4.16) and (4.28) and has the form

$$2i\ \mathrm{Im}\ W(x,a)=i(4\pi)^{-1}\theta(\sigma^2)\epsilon(x^0)\int_0^\infty J_0(q\sigma)J_0(p\rho)w(\alpha,\beta,p)p\ dp. \tag{4.31}$$

We see that it vanishes for $\sigma^2<0$. Equation (4.31) can be considered as a Hankel transformation.[22] By considering the corresponding inverse transformation, one can easily see that a necessary condition to have a commutator vanishing for large ρ is that $w(\alpha,\beta,p)$ is an entire analytic function of p^2. This does not happen for the elementary fields considered in the following sections.

When $w(\alpha,\beta,p)$ is an even function of p, it is useful to rewrite Eq. (4.31) as an integral in the complex p plane,

$$2i\ \mathrm{Im}\ W(x,a)=i2^{-3}\pi^{-1}\theta(\sigma^2)\epsilon(x^0)\int_C J_0(q\sigma)H_0^{(1)}(p\rho)w(\alpha,\beta,p)p\ dp, \tag{4.32}$$

where the integration path C lies just above the real axis. For $|p|\to\infty$, $\mathrm{Im}\ p>0$, we have

$$pJ_0(q\sigma)H_0^{(1)}(p\rho)\simeq\pi^{-1}(\rho\sigma)^{-1/2}\exp(ip(\rho-\sigma)). \tag{4.33}$$

If $w=1$ and $\rho>\sigma$, we can close the integration path at infinity in the upper half-plane and the integral vanishes in accord with Eq. (4.22). Actually, the integral (4.32) is meaningful only in the sense of distribution theory; in order to deal with a convergent integral, one can multiply the integrand by $(p+i)^{-\nu}$ and take the limit $\nu\to0$ at the end. If w has singularities in the upper half-plane, one has to take into account their contributions.

V. POSITIVE-MASS FREE FIELDS

In the positive-mass case, we can find the function $w_{\rho\bar\sigma}(a)$ by exploiting the positivity properties of the matrix elements $D^{Mc}_{jmj'm'}(a)$ of the IURs of SL(2,**C**) described in Refs. 23–27. The parameter c is the same as in Ref. 23 and is called λ in Ref. 25. The parameter M is the same as in Ref. 25 and corresponds to the parameter $-\frac{1}{2}m=\pm k_0$ of Ref. 23. For the IURs of the principal series, c lies on the imaginary axis and M is an integral or half-integral number. For the IURs of the supplementary series, $M=0$ and $-1<c<1$. The representations D^{Mc} and $D^{-M,-c}$ are unitarily equivalent. The indices j,j' take the values $|M|$, $|M|+1$,..., and, if we indicate by $R^j_{mm'}(u)$ the $(2j+1)$-dimensional representation of SU(2), we have

$$D^{Mc}_{jmj'm'}(u)=\delta_{jj'}R^j_{mm'}(u),\quad u\in\mathrm{SU}(2). \tag{5.1}$$

Then we put

$$w_{\rho\bar\sigma}(a)=(2s+1)(2J+1)^{-1}\sum_{mnn'}C_{js}(J,m;n',\rho)C_{js}(J,m;n,\sigma)D^{Mc}_{jnjn'}(a), \tag{5.2}$$

where C indicates the Clebsch–Gordan coefficients. The parameters M,c,j,J,s characterize the theory; they are fixed and no sum over them is understood. After some calculation we have

$$w_{\rho\bar\sigma}(uau^{-1})=R^s_{\rho\mu}(u)\overline{R^s_{\sigma\nu}}(u)w_{\mu\bar\nu}(a), \tag{5.3}$$

and we see that Eq. (3.28) is satisfied if

$$S_\rho{}^\sigma(\mu)=R^s_{\rho\sigma}(u),\quad u\in \mathrm{SU}(2). \tag{5.4}$$

If we indicate by $S^{(s,s')}$ an irreducible spinor representation, we can put, with an appropriate choice of the basis,

$$S(a)=S^{(s,0)}(a)\quad \text{or}\quad S(a)=S^{(0,s)}(a). \tag{5.5}$$

In order to prove the positivity property, we substitute Eq. (5.2) into Eq. (3.25) and we obtain the positive expression

$$(\Phi(f),\Phi(f))=\int \sum_{mj'm'} |f_{mj'm'}(k)|^2\theta(k^0)\,\delta(k\cdot k+\mu^2)d^4k, \tag{5.6}$$

where

$$f_{mj'm'}(k)=(2\pi)^{-3/2}(2s+1)^{1/2}(2J+1)^{-1/2}C_{js}(J,m;n,\mu)\int \tilde f^\rho(k,a_k a)\overline{S_\rho}^{\mu}(a^{-1})D^{Mc}_{jnj'm'}(a)d^6a. \tag{5.7}$$

It is clear that the quantity (5.7) is the wave function in momentum space of the one-particle state $\Phi(f)$ and that its indices represent the spin and the internal quantum numbers.

Equation (2.15) takes the form

$$U^{(1)}(y,b)\Phi(f)=\Phi(f'),\quad f'^\rho(x,a)=f^\rho(\Lambda(b^{-1})(x-y),b^{-1}a). \tag{5.8}$$

The Fourier transformation (3.14) gives

$$\tilde f'^\rho(k,a)=\exp(-ik\cdot y)\tilde f^\rho(k',b^{-1}a),\quad k'=\Lambda(b^{-1})k, \tag{5.9}$$

and from Eq. (5.7) we obtain

$$f'_{mj'm'}(k)=\exp(-ik\cdot y)R^J_{mm''}(a_k^{-1}ba_{k'})f_{m''j'm'}(k'),\quad a_k^{-1}ba_{k'}\in \mathrm{SU}(2). \tag{5.10}$$

We see that the wave function transforms according to the IUR with mass $\mu>0$ and spin J defined by Wigner.[21] Equation (5.7) shows that spin has a double origin, namely the dependence of $f^\rho(x,a)$ on the index ρ and on the group element a. From Eqs. (3.24) and (5.2) we have

$$W_{\rho\sigma}(x,-a)=(-1)^{2J}W_{\rho\sigma}(x,a), \tag{5.11}$$

and a similar formula holds for the field $\psi_\rho(x,a)$, which is a one- or two-valued function on $\mathscr{P}$ if $2J$ is, respectively, even or odd.

Equation (2.16) takes the form

$$V^{(1)}(b)\Phi(f)=\Phi(f'),\quad f'^\rho(x,a)=f^\sigma(x,ab)\overline{S_\sigma}^{\rho}(b^{-1}), \tag{5.12}$$

and from Eqs. (3.14) and (5.7) we obtain

$$f'_{mj'm'}(k)=f_{mj''m''}(k)D^{Mc}_{j''m''j'm'}(b^{-1})=\overline{D}^{Mc}_{j'm'j''m''}(b)f_{mj''m''}(k). \tag{5.13}$$

We see that the wave function transforms according to the IUR $\overline{D}^{Mc}$ of the internal symmetry group SL(2,**C**). This IUR is equivalent to D^{Mc}.

The general formalism described above becomes simpler in some special cases. If $s=0$, $S(a)=1$, we have a scalar field. It is $J=j$ and Eq. (5.2) takes the form

$$w(a)=w^{Mcj}(a)=(2j+1)^{-1}\sum_m D^{Mc}_{jmjm}(a). \tag{5.14}$$

If $j=M=0$, we have $J=s$ and

$$w_{\rho\sigma}(a)=\delta_{\rho\sigma}D^{0c}_{0000}(a)=\delta_{p\sigma}w^{0c0}(a). \tag{5.15}$$

In order to give more explicit expressions for the functions $w^{Mcj}(a)$, we write the IURs of SU(2) and of SL(2,**C**) in the form

$$R^j_{mm'}(u_3(\phi)u_2(\theta)u_3(\psi))=\exp(-im\phi)r^j_{mm'}(\theta)\exp(-im'\psi), \tag{5.16}$$

$$D^{Mc}_{jmj'm'}(ua_3(\zeta)u')=\sum_{m''} R^j_{mm''}(u)d^{Mc}_{m''jj'}(\zeta)R^{j'}_{m''m'}(u'). \tag{5.17}$$

Then the function defined by Eq. (5.14) can be written as

$$w^{Mcj}(ua_3(\zeta)u')=w^{Mcj}(a_3(\zeta)u_3(\phi+\psi)u_2(\theta))=(2j+1)^{-1}\sum_m d^{Mc}_{mjj}(\zeta)r^j_{mm}(\theta)$$
$$\times\exp(-im(\phi+\psi)),\quad u'u=u_3(\phi)u_2(\theta)u_3(\psi). \tag{5.18}$$

The quantities $d^{Mc}_{mjj}(\zeta)$ are given in Refs. 24 and 25 in terms of elementary functions. It follows that the expression (5.18), too, is a combination of elementary functions. For instance, we have

$$w^{0c0}(ua_3(\zeta)u')=d^{0c}_{000}(\zeta)=(c\ \sinh(\zeta))^{-1}\ \sinh(c\zeta), \tag{5.19}$$

but the expressions become more and more complicated when the parameters M and j increase. A useful integral representation of $w^{Mcj}(a)$ is given in Appendix A, where one derives also a simple approximate expression valid for $a\to 1$.

Note that we have

$$\lim_{c\to 1} w^{0c0}(a)=\lim_{c\to 1} D^{0c}_{0000}(a)=1. \tag{5.20}$$

In this limit the distribution $w_{\rho\sigma}(a)$ given by Eq. (5.15) becomes independent of a and we have a theory which can be defined in Minkowski space–time. From the unitarity condition we also have

$$\lim_{c\to 1} D^{0c}_{00jm}(a)=\lim_{c\to 1} D^{0c}_{jm00}(a)=0,\quad j>0, \tag{5.21}$$

and if $j=M=0$ the components of the wave function (5.7) tend to zero for $j'>0$. We conclude that the theories with $M=j=0$ can possibly describe small deviations from the known physical theories. For other values of the parameters, we get theories which can only apply to the unknown physics of masses and energies beyond the Planck mass. From the mathematical point of view, Eqs. (5.20) and (5.21) show that in the limit $c\to 1$, the representation D^{0c} becomes reducible and we have[23]

$$\lim_{c\to 1} D^{0c}=1\oplus D^{1,0}. \tag{5.22}$$

We see from Eq. (3.18) that $\widetilde{W}_{\rho\bar{\sigma}}(k,a)$ can be considered as a tempered distribution in the variables k that depends continuously on the group element a and a similar statement holds for its Fourier transform $W(x,a)$. If $a=1$, Eq. (5.2) gives

$$w_{\rho\bar{\sigma}}(1)=\delta_{\rho\sigma}, \tag{5.23}$$

and from Eq. (3.24) we see that $W_{\rho\bar{\sigma}}(x,1)$ is the VEV of a field in Minkowski space, given, in the scalar case, by Eq. (4.22). If $a\neq 1$, the function $w_{\rho\bar{\sigma}}(a_k^{-1}aa_k)$ decreases for large k and the distribution $W_{\rho\bar{\sigma}}(x,a)$ is less singular.

For a scalar field we can use Eq. (4.28) and from Eq. (4.30) we obtain

$$w(\alpha,\beta,p)=w(a_3(\zeta)u_3(\phi)u_2(\theta)), \tag{5.24}$$

where

$$\cosh\,\zeta=(\cosh\,\eta)^2\,\cosh\,\beta-(\sinh\,\eta)^2\,\cos\,\alpha=\cosh\,\beta+p^2\mu^{-2}(\cosh\,\beta-\cos\,\alpha), \tag{5.25}$$

$$\cos\frac{\theta}{2}\exp\left(i\,\frac{\phi}{2}\right)=\left(\cosh\frac{\zeta}{2}\right)^{-1}\cos\frac{\alpha}{2}\cosh\frac{\beta}{2}+i\left(\sinh\frac{\zeta}{2}\right)^{-1}\sin\frac{\alpha}{2}\sinh\frac{\beta}{2}. \tag{5.26}$$

For $j=M=0$, we see that the expression (5.19) is an analytic function of $\cosh\,\zeta$ with a branch point at $\cosh\,\zeta=-1$. From Eq. (5.25) we see that it is not an entire analytic function of p^2 and the commutator function (4.31) cannot vanish for large ρ.

VI. ZERO-MASS FREE FIELDS

In order to use the method described in Sec. V in the zero-mass case, we have to write the IURs of SL(2,**C**) in a basis that evidentiates the decomposition of the representation space into spaces where IURs of $\widetilde{E}(2)$ operate. In this case, we have a direct integral decomposition and we have to introduce a ''continuous'' basis.[28]

We start from the realization of the operator $D^{Mc}(a)$ in a space of functions of a complex variable z:

$$[D^{Mc}(a)f](z)=(a_{21}z+a_{11})^{-c+M-1}(\overline{a_{21}z+a_{11}})^{-c-M-1}f((a_{22}z+a_{12})(a_{21}z+a_{11})^{-1}), \tag{6.1}$$

where

$$a=\begin{pmatrix}a_{11} & a_{12}\\ a_{21} & a_{22}\end{pmatrix}\in \mathrm{SL}(2,\mathbf{C}). \tag{6.2}$$

This representation is equivalent to the one defined in Refs. 23 and 24, which in our notation is given by $D^{-M,-c}(u_1(\pi)au_1(-\pi))$.

The elements of the little group $\widetilde{E}(2)$ have the form

$$h=\begin{pmatrix}\exp(-\frac{1}{2}i\phi) & \xi\,\exp(-\frac{1}{2}i\phi)\\ 0 & \exp(\frac{1}{2}i\phi)\end{pmatrix}\in\widetilde{E}(2), \tag{6.3}$$

with ϕ real and ξ complex. We have

$$[D^{Mc}(h)f](z)=\exp(-iM\phi)f(\exp(i\phi)z+\xi). \tag{6.4}$$

We see that $\widetilde{E}(2)$ acts on the complex z plane by means of Euclidean transformations. If we introduce the (non-normalizable) basis vectors

$$f_{\kappa m}(z)=(z|z|^{-1})^{-m}J_{-m}(\kappa|z|), \quad \kappa>0, \quad m=0,\pm 1,\pm 2,\ldots, \tag{6.5}$$

the matrix that represents an Euclidean transformation is diagonal in the index κ; namely, we have

$$f_{\kappa m}(\exp(i\phi)z+\xi)=f_{\kappa m'}(z)R^{\kappa}_{m'm}(h), \tag{6.6}$$

where the matrix

$$R^{\kappa}_{m'm}(h)=\exp(-im'\phi)(\xi|\xi|^{-1})^{m'-m}J_{m'-m}(\kappa|\xi|) \tag{6.7}$$

is unitary.[27] From Eq. (6.4), we obtain

$$[D^{Mc}(h)f_{\kappa m}](z)=\exp(-iM\phi)R^{\kappa}_{m'm}(h)f_{\kappa m'}(z). \tag{6.8}$$

We see from Eq. (6.7) that the factor $\exp(-iM\phi)$ can be eliminated by means of a ''translation'' of the indices m',m, which is irrelevant if M is an integer. If M is half-odd, we get a representation of $\widetilde{E}(2)$ that is double-valued on $E(2)$.

In analogy with Eq. (5.14) we put

$$w(a)=\sum_m (f_{\kappa m},D^{Mc}(a)f_{\kappa m}). \tag{6.9}$$

Also in this case, the conditions (3.26) and (3.28) are satisfied. In the same way as in Sec. V, we can show that the fields constructed by means of the distributions found above represent zero-mass particles with an infinite helicity spectrum[21] and with internal quantum numbers described by the IUR D^{Mc} of SL(2,**C**). Since particles of this kind are not observed in nature, we shall not discuss these fields with more detail.

The zero-mass particles present in nature have only one value m of the helicity (two if parity is taken into account) and they are described by one-dimensional IURs of the little group[21] of the kind

$$R^{m}(h)=\exp(-im\phi), \quad h\in\widetilde{E}(2), \quad m=0,\pm\tfrac{1}{2},\pm 1,\ldots, \tag{6.10}$$

where h is given by Eq. (6.3). These IURs are not contained in the IURs of SL(2,**C**) and we have to use a different method in order to find the corresponding w functions. We propose the following solutions, without explaining how they have been obtained:

$$w_0^{0c}(a)=|a_{21}|^{2c-2}, \quad 0<c<1, \tag{6.11}$$

$$w_0^{Mc}(a)=\delta^2(a_{21})a_{22}{}^{c-M}\overline{a_{22}}{}^{c+M}, \quad \text{Re } c=0. \tag{6.12}$$

It is easy to show that the symmetry condition (3.28) is satisfied. The positivity condition (3.26) follows from the formulas

$$w_0^{0c}(ba^{-1})=\int |a_{22}|^{2c}\delta^2(a_{21}-z'a_{22})|z'-z|^{2c-2}|b_{22}|^{2c}\delta^2(b_{21}-zb_{22})d^2zd^2z', \tag{6.13}$$

$$w_0^{Mc}(ba^{-1})=\int \overline{a_{22}}{}^{-c-M}a_{22}{}^{-c+M}\delta^2(a_{21}-za_{22})b_{22}{}^{c-M}\overline{b_{22}}{}^{c+M}\delta^2(b_{21}-zb_{22})d^2z. \tag{6.14}$$

Note that $|z'-z|^{2c-2}$ is a positive integral kernel, the one that defines the scalar product in the space of an IUR of the supplementary series.[23,24]

The norm (3.25) in the case (6.11) can be written as

$$(\Phi(f),\Phi(f))=\int \overline{f(k,z')}|z'-z|^{2c-2}f(k,z)\,\theta(k^0)\,\delta(k\cdot k)\,d^2z\,d^2z'\,d^4k, \tag{6.15}$$

and in the case (6.12) we obtain

$$(\Phi(f),\Phi(f))=\int |f(k,z)|^2\,\theta(k^0)\,\delta(k\cdot k)\,d^2z\,d^4k, \tag{6.16}$$

where in both cases

$$f(k,z)=(2\pi)^{-3/2}\int \tilde{f}(k,a_k a)\,a_{22}{}^{c-M}\overline{a_{22}}^{c+M}\,\delta^2(a_{21}-z a_{22})\,d^6a. \tag{6.17}$$

Of course, in the first case we have to put $M=0$.

If we consider a Poincaré transformation of the kind (5.8) and (5.9), the wave function (6.17) transforms in the following way,

$$f'(k,z)=\exp(-ik\cdot y)R^M(a_k^{-1}ba_{k'})f(k',z), \tag{6.18}$$

where k' is given by Eq. (5.9). This is the transformation property[21] of the wave function of a particle of zero mass and helicity M.

Under the ''internal'' transformation (5.12) the wave function transforms as

$$\begin{gathered} f'(k,z)=(b_{22}+zb_{12})^{-c+M-1}(\overline{b_{22}+zb_{12}})^{-c-M-1}f(k,z'),\\ z'=(b_{21}+zb_{11})(b_{22}+zb_{12})^{-1}, \end{gathered} \tag{6.19}$$

namely according to the IUR $D^{-M,-c}$ defined in Refs. 23 and 24, which is equivalent to the IUR D^{Mc}. Note that, if we fix up to equivalence the IUR D^{Mc}, we have two possible theories with helicity $\pm M$.

In order to compute the integral (3.24), we use the variables introduced in Sec. IV. If we put

$$\tilde{a}=a_\eta^{-1}u_3(\alpha)a_3(\beta)a_\eta, \tag{6.20}$$

from Eq. (4.26) we obtain

$$\tilde{a}_{21}=-p\,\sinh(\tfrac{1}{2}(\beta-i\alpha)),\quad \tilde{a}_{22}=\cosh(\tfrac{1}{2}(\beta-i\alpha)). \tag{6.21}$$

We see that the quantity $\delta^2(\tilde{a}_{21})$ that appears in Eq. (6.12) is rather badly defined when considered as a distribution in the variables k^1,k^2 for fixed values of α,β satisfying Eq. (4.2). Other difficulties arise when one tries to perform the integrals (3.24) or (4.28). We conclude that, even if the expression (6.12) satisfies the required positivity and symmetry conditions, it does not give rise to a well-behaved field theory. All the calculations based on this expression have a purely formal character.

When we substitute Eqs. (6.11) and (6.21) into Eqs. (4.28) and (4.31), the integrals can be performed in terms of Legendre functions[22,29] and we obtain

$$\begin{aligned} W_0^{0c}(x,a)=&\,2^{c-3}\pi^{-2}(\Gamma(c))^2(\cosh\beta-\cos\alpha)^{c-1}(\rho^2-\sigma^2)^{-c}\\ &\times P_{c-1}((\sigma^2+\rho^2)(\sigma^2-\rho^2)^{-1}),\quad \sigma^2<0. \end{aligned} \tag{6.22}$$

$$2i\ \mathrm{Im}\ W_0^{0c}(x,a)=i2^{c-2}\pi^{-1}\epsilon(x^0)\,\theta(\sigma^2)\Gamma(c)(\Gamma(1-c))^{-1}$$
$$\times(\cosh\,\beta-\cos\,\alpha)^{c-1}|\sigma^2-\rho^2|^{-c}P_{c-1}((\sigma^2+\rho^2)|\sigma^2-\rho^2|^{-1}). \quad (6.23)$$

The real part for $\sigma^2>0$ can be obtained by analytic continuation of Eq. (6.22). In the special case $\rho=0$, we have

$$W_0^{0c}(x,a)=2^{c-3}\pi^{-2}(\Gamma(c))^2(\cosh\,\beta-\cos\,\alpha)^{c-1}|\sigma^2|^{-c}(\,\theta(-\sigma^2)+\theta(\sigma^2)\exp(i\pi c\,\epsilon(x^0))). \quad (6.24)$$

Since we are not able to build fields starting from Eq. (6.12), in order to describe particles with a nonvanishing helicity we have to use nonscalar fields. From Eq. (6.3) we have

$$h\begin{pmatrix}1\\0\end{pmatrix}=\exp\left(-\frac{1}{2}\,i\phi\right)\begin{pmatrix}1\\0\end{pmatrix}. \quad (6.25)$$

We remark that the spinor representations $S^{(s,0)}(h)$ and $S^{(0,s)}(h)$ are equivalent to symmetrized tensor products of $2s$ matrices equal, respectively, to h or $\bar{h}$ and we adopt conventions in agreement with Eqs. (5.4) and (5.5). Then, if we put

$$S(a)=S^{(m,0)}(a),\quad m\geqslant 0,\quad S(a)=S^{(0,|m|)}(a),\quad m\leqslant 0, \quad (6.26)$$

we have

$$S_\rho{}^m(h)=\exp(-im\phi)\,\delta_\rho^m,\quad h\in\tilde{E}(2). \quad (6.27)$$

As a consequence, the expression

$$w_{\rho\bar{\sigma}}(a)=\delta_{\rho m}\delta_{\sigma m}|a_{21}|^{2c-2} \quad (6.28)$$

satisfies the symmetry condition (3.28).

Equation (6.15) is still valid if we modify Eq. (6.17) in the following way:

$$f(k,z)=(2\pi)^{-3/2}\int \tilde{f}^\rho(k,a_k a)\overline{S_\rho}{}^m(a^{-1})|a_{22}|^{2c}\delta^2(a_{21}-za_{22})d^6a. \quad (6.29)$$

Equation (6.18) holds with M replaced by m and Eq. (6.19) holds with $M=0$; this means that the theory describes zero mass particles with helicity m that transform according to the representation D^{0c} of the internal symmetry group. In the limit $c\to 1$, the expression (6.28) becomes independent of a and we get a Minkowskian theory of the kind usually adopted to describe neutrinos, photons, or gravitons.

VII. FIELD EQUATIONS

Now we find the wave equations satisfied by the scalar fields defined in the preceding sections; nonscalar fields will be treated elsewhere. We indicate by $L_{ik}=-L_{ki}$ the generators of the right translations on SL(2,**C**), considered as differential operators acting on smooth functions defined on the group. They satisfy the commutation relations

$$[L_{ik},\,L_{rs}]=g_{ir}L_{ks}-g_{kr}L_{is}-g_{is}L_{kr}+g_{ks}L_{ir} \quad (7.1)$$

of sl(2,**C**), commute with the left translations, and have the following commutation property with the finite right translation represented by the operator $T(b)$:

$$T(b^{-1})L_{ik}T(b)=\Lambda_i{}^r(b)\Lambda_k{}^s(b)L_{rs}. \quad (7.2)$$

We also need the generators L'_{ik} of the left translations, which satisfy commutation relations with the opposite sign. We have

$$L'_{ik}=\Lambda_i{}^r(a)\Lambda_k{}^s(a)L_{rs}\,, \tag{7.3}$$

and their commutation relation with a finite left translation $T'(b)$ is

$$T'(b)L'_{ik}T'(b^{-1})=\Lambda_i{}^r(b)\Lambda_k{}^s(b)L'_{rs}\,. \tag{7.4}$$

We also consider the generators A_k and A_{ik} of the right translations on the group $\tilde{\mathscr{P}}$ that satisfy the Poincaré Lie algebra. They act on functions of the kind $f(x,a)$ in the following way:

$$A_i=\Lambda^k{}_i(a)\,\frac{\partial}{\partial x^k}\,,\quad A_{ik}=L_{ik}\,. \tag{7.5}$$

For the generators of the left translations of $\tilde{\mathscr{P}}$ we have

$$A'_i=\frac{\partial}{\partial x^k}\,,\quad A'_{ik}=L'_{ik}+x_i\,\frac{\partial}{\partial x^k}-x_k\,\frac{\partial}{\partial x^i}\,. \tag{7.6}$$

From Eqs. (3.24), (7.5), and (7.6) we obtain immediately the differential equation

$$g^{ik}A_iA_kW(x,a)=g^{ik}A'_iA'_kW(x,a)=\mu^2W(x,a), \tag{7.7}$$

which is essentially the Klein–Gordon equation.

If the function $w(a)$ is a linear combination of matrix elements of the representation $D^{Mc}(a)$, as in Eqs. (5.2) and (6.9), it satisfies the differential equations[23,24]

$$\tfrac{1}{2}g^{ir}g^{ks}L_{ik}L_{rs}w(a)=\tfrac{1}{2}g^{ir}g^{ks}L'_{ik}L'_{rs}w(a)=(1-c^2-M^2)w(a), \tag{7.8}$$

$$\tfrac{1}{8}e^{ikrs}L_{ik}L_{rs}w(a)=\tfrac{1}{8}e^{ikrs}L'_{ik}L'_{rs}w(a)=-iMcw(a). \tag{7.9}$$

The functions (6.11) and (6.12) are not defined in terms of matrix elements, but it is easy to show directly that they satisfy the differential equations

$$(L'_{10}-L'_{31})w(a)=0,\quad (L'_{20}+L'_{23})w(a)=0, \tag{7.10}$$

$$L'_{12}w(a)=-iMw(a),\quad L'_{30}w(a)=(1-c)w(a). \tag{7.11}$$

By means of the formulas

$$\tfrac{1}{2}g^{ir}g^{ks}L'_{ik}L'_{rs}=-(L'_{10}+L'_{31})(L'_{10}-L'_{31})-(L'_{20}-L'_{23})(L'_{20}+L'_{23})+(L'_{12})^2-(L'_{30})^2+2L'_{30}, \tag{7.12}$$

$$\tfrac{1}{8}e^{ikrs}L'_{ik}L'_{rs}=\tfrac{1}{2}(L'_{20}-L'_{23})(L'_{10}-L'_{31})-\tfrac{1}{2}(L'_{10}+L'_{31})(L'_{20}+L'_{23})-L'_{30}L'_{12}+L'_{12}, \tag{7.13}$$

we can derive also in this case Eqs. (7.8) and (7.9).

The Casimir operators that appear in Eqs. (7.8) and (7.9) commute with the left and the right translations on SL(2,**C**) and from Eqs. (3.24) and (7.5) we obtain, for a scalar field,

$$\tfrac{1}{2}g^{ir}g^{ks}A_{ik}A_{rs}W(x,a)=(1-c^2-M^2)W(x,a), \tag{7.14}$$

$$\tfrac{1}{8}e^{ikrs}A_{ik}A_{rs}W(x,a)=-iMcW(x,a). \tag{7.15}$$

Equations (7.7), (7.14), and (7.15) identify the mass and the internal quantum numbers and hold for all the scalar fields. There are other equations that identify spin or helicity. In the positive-mass case the generators of the little group $\mathscr{K}=\mathrm{SU}(2)$ are L_{12}, L_{23}, L_{31}, and from Eqs. (5.1) and (5.2), taking into account the properties of the representations of SU(2), we obtain

$$((L'_{12})^2+(L'_{23})^2+(L'_{31})^2)w(a)=-j(j+1)w(a). \tag{7.16}$$

If $j=0$, we have the stronger result

$$L'_{12}w(a)=L'_{23}w(a)=L'_{31}w(a)=0. \tag{7.17}$$

From Eqs. (3.19) and (7.16) we obtain

$$\tfrac{1}{4}e^{jirs}\hat{k}_i L'_{rs}e_j{}^{kpq}\hat{k}_k L'_{pq}w(a)=-\mu^2 j(j+1)w(a), \tag{7.18}$$

and from Eqs. (3.21), (3.22), and (7.4)

$$\tfrac{1}{4}e^{jirs}k_i L'_{rs}e_j{}^{kpq}k_k L'_{pq}w(k,a)=-\mu^2 j(j+1)w(k,a). \tag{7.19}$$

By substitution into Eq. (3.24) we obtain the differential equation

$$g_{ik}\Sigma'^i\Sigma'^k W(x,a)=\mu^2 j(j+1)W(x,a), \tag{7.20}$$

where

$$\Sigma'^i=\tfrac{1}{2}e^{ijrs}A'_jA'_{rs}=\tfrac{1}{2}\,e^{ijrs}\frac{\partial}{\partial x^j}L'_{rs}. \tag{7.21}$$

If we also introduce the differential operators

$$\Sigma^i=\tfrac{1}{2}e^{ijrs}A_jA_{rs}=\Lambda_k{}^i(a)\Sigma'^k, \tag{7.22}$$

we have

$$g_{ik}\Sigma^i\Sigma^k W(x,a)=\mu^2 j(j+1)W(x,a). \tag{7.23}$$

If $j=0$, we have the stronger result

$$\Sigma^i W(x,a)=\Sigma'^i W(x,a)=0. \tag{7.24}$$

In the zero-mass case, the generators of the little group $\mathscr{K}=\widetilde{E}(2)$ are L_{12}, $(L_{10}-L_{31})$, $(L_{20}+L_{23})$. From Eqs. (6.8) and (6.9) we obtain the differential equation

$$((L'_{10}-L'_{31})^2+(L'_{20}+L'_{23})^2)w(a)=-\kappa^2 w(a), \tag{7.25}$$

which can be written in the form

$$\tfrac{1}{4}e^{jirs}\hat{k}_i L'_{rs}e_j{}^{kpq}\hat{k}_k L'_{pq}w(a)=-\kappa^2 w(a). \tag{7.26}$$

By means of the procedure used above, for a field with zero mass and infinite helicity spectrum we find the equation

$$g_{ik}\Sigma^i\Sigma^k W(x,a)=g_{ik}\Sigma'^i\Sigma'^k W(x,a)=\kappa^2 W(x,a). \tag{7.27}$$

If we consider a field with zero mass and given helicity M based on the functions (6.11) and (6.12), we see that Eqs. (7.10) and (7.11) can be written in the form

$$\tfrac{1}{2}e^{jirs}\hat{k}_i L'_{rs} w(a) = -iM\hat{k}^j w(a), \tag{7.28}$$

$$\hat{k}^i L'_{ik} w(a) = (c-1)\hat{k}_k w(a). \tag{7.29}$$

Proceeding as in the other cases, we obtain

$$\Sigma'_i W(x,a) = -iMA'_i W(x,a), \quad \Sigma_i W(x,a) = -iMA_i W(x,a), \tag{7.30}$$

$$A^i A_{ik} W(x,a) = (c-1)A_k W(x,a). \tag{7.31}$$

From Eqs. (3.8), (3.29), and (4.20) we obtain

$$(\Omega, \psi(x,a)\psi^\dagger(y,b)\Omega) = \overline{W}((y,b)^{-1}(x,a)), \tag{7.32}$$

$$(\Omega, \psi^\dagger(y,b)\psi(x,a)\Omega) = \overline{W}((-y,b)^{-1}(-x,a)). \tag{7.33}$$

If the function $\overline{W}(x,a)$ satisfies a differential equation invariant under left translations and under the reflection $x \to -x$, from the Wightman reconstruction theorem[19,20] we have that $\psi(x,a)$ satisfies the same equation. In this way we obtain the field equations

$$g^{ik}A_i A_k \psi(x,a) = \mu^2 \psi(x,a), \tag{7.34}$$

$$\tfrac{1}{2}g^{ir}g^{ks}A_{ik}A_{rs}\psi(x,a) = (1-c^2-M^2)\psi(x,a), \tag{7.35}$$

$$\tfrac{1}{8}e^{ikrs}A_{ik}A_{rs}\psi(x,a) = -iMc\psi(x,a). \tag{7.36}$$

For $\mu > 0$, $j > 0$, we have

$$g_{ik}\Sigma^i\Sigma^k \psi(x,a) = \mu^2 j(j+1)\psi(x,a), \tag{7.37}$$

for $\mu > 0$, $j = 0$, we have

$$\Sigma^i \psi(x,a) = 0; \tag{7.38}$$

for $\mu = 0$ and infinite helicity spectrum, we have

$$g_{ik}\Sigma^i\Sigma^k \psi(x,a) = \kappa^2 \psi(x,a); \tag{7.39}$$

and for $\mu = 0$ and helicity M, we have

$$\Sigma_i \psi(x,a) = iMA_i \psi(x,a), \tag{7.40}$$

$$A^i A_{ik}\psi(x,a) = (\overline{c} - 1)A_k \psi(x,a). \tag{7.41}$$

We have seen in Sec. VI that there is some difficulty in the definition of fields starting from the function (6.12). For these fields, the calculations given above have a purely formal character.

VIII. FLAT-SPACE THEORIES AND SPIN-MASS-SHELLS

We approximate a small region of the group manifold $\tilde{\mathscr{P}}$ by means of a tangent space with coordinates x^i and $x^{ik} = -x^{ki}$, which can be identified with the vector space $\mathscr{T}$. The operators A_i and A_{ik}, which appear in the differential equations satisfied by the fields and by their VEVs, can

be replaced by the partial derivatives with respect to these coordinates. We get in this way a field theory in the flat ten-dimensional space and the Fourier transforms of the fields and of the VEVs have their support in a Lorentz invariant manifold defined by some polynomial equations in the ten-dimensional ''spin-momentum space'' $\mathscr{T}^*$ with coordinates k_i and $k_{ik}=-k_{ki}$. These equations are obtained from the field equations by means of the substitutions $A_i \to -ik_i$, $A_{ik} \to -ik_{ik}$. To indicate the positive-energy part ($k^0=-k_0>0$) of this manifold, we use the term ''spin-mass-shell.'' The two-point VEV of the flat-space theory is the Fourier transform of a positive Lorentz invariant measure on the spin-mass-shell. As we shall see, in some cases the replacement of noncommuting operators by commuting quantities may lead to inconsistencies or ambiguities. Nevertheless, the correspondence between theories in $\tilde{\mathscr{P}}$ and in the flat space is an unavoidable heuristic instrument. Note that there is no ambiguity in the higher-degree terms of the equations defining the spin-mass-shell. If we drop all the other terms, we get a set of homogeneous equations that define an unambiguous dilatation invariant ''asymptotic'' manifold.

From Eqs. (7.7), (7.14), and (7.15) we get the following equations valid on the spin-mass-shell of all the elementary field theories.

$$g^{ik}k_ik_k=-\mu^2, \quad \tfrac{1}{2}g^{ir}g^{ks}k_{ik}k_{rs}=c^2+M^2-1, \quad \tfrac{1}{8}e^{ikrs}k_{ik}k_{rs}=iMc. \tag{8.1}$$

In a similar way from Eqs. (7.23), (7.24), (7.27), (7.30), and (7.31) we obtain other equations valid for the various specific cases.

Since the spin-mass-shell is Lorentz invariant, it is determined by its intersection with the hyperplane $k_i=\hat{k}_i$. This intersection can be considered as a manifold in the six-dimensional ''spin space'' with coordinates k_{ik} and we call it the ''spin-shell.'' Its dimension is given by the dimension of the spin-mass-shell minus three. It is convenient to introduce the three-dimensional vectors

$$\mathbf{k}=(k^1,k^2,k^3), \quad \mathbf{k}'=(k^{23},k^{31},k^{12}), \quad \mathbf{k}''=(k^{10},k^{20},k^{30}), \tag{8.2}$$

and similar notations for the coordinates x^i,x^{rs}. Then the last two conditions of Eq. (8.1) take the form

$$(\mathbf{k}')^2-(\mathbf{k}'')^2=c^2+M^2-1, \quad \mathbf{k}'\cdot\mathbf{k}''=iMc. \tag{8.3}$$

The spin-shell in the case $\mu>0$ is described by the equations

$$(\mathbf{k}')^2=j(j+1), \quad (\mathbf{k}'')^2=j(j+1)+1-c^2-M^2, \quad \mathbf{k}'\cdot\mathbf{k}''=iMc. \tag{8.4}$$

Note that the right-hand sides are real and satisfy the inequality

$$j(j+1)(j(j+1)+1-c^2-M^2)+M^2c^2=(\mathbf{k}')^2(\mathbf{k}'')^2-(\mathbf{k}'\cdot\mathbf{k}'')^2\geqslant 0. \tag{8.5}$$

If $j>0$, this manifold has dimension three, but if $j=M=0$, Eq. (8.4) takes the simpler form

$$\mathbf{k}'=0, \quad (\mathbf{k}'')^2=1-c^2, \tag{8.6}$$

and describes a two-dimensional manifold. In both cases the spin-shell is compact and the rotation group acts transitively on it; namely, the spin-shell is an orbit of the rotation group in the spin space. It follows that the spin-mass-shell is an orbit of the Lorentz group in the spin-momentum space.

The orbits of the rotation or of the Lorentz group which correspond to a field on the group $\tilde{\mathscr{P}}$ are called ''allowed orbits.'' It is useful to consider all the orbits, not necessarily allowed, which can be classified by means of the invariants $(\mathbf{k}')^2$, $(\mathbf{k}'')^2$ and $\mathbf{k}'\cdot\mathbf{k}''$ satisfying the condition (8.5). One can also use Eq. (8.4) to introduce the parameters j, c, and M, even when they do not label

any IUR. Given an orbit with $\mathbf{k}'\cdot\mathbf{k}''\neq 0$, Eq. (8.4) determines the real quantities j, M and the imaginary quantity c, up to a common change of sign of M and c. They satisfy the conditions

$$j>0, \quad c^2<0, \quad 0<M^2\leqslant j(j+1)(1+(j(j+1)+|c^2|)^{-1}). \tag{8.7}$$

Note that only some discrete values of the parameters j and M are allowed and that they are rather uniformly distributed in the set defined by Eq. (8.7). These orbits are three-dimensional in the general case, but have dimension two when the equality sign holds in Eq. (8.5) or in the last Equation (8.7), namely when the vectors $\mathbf{k}'$ and $\mathbf{k}''$ are parallel. The two-dimensional orbits correspond to values of M which are not allowed, but for large j are relatively near to the allowed values $M=\pm j$.

If $\mathbf{k}'\cdot\mathbf{k}''=0$, we have two possible choices of M and c, namely,

$$M=0, \quad 1-c^2=(\mathbf{k}'')^2-(\mathbf{k}')^2, \quad j\geqslant 0, \tag{8.8}$$

or

$$c=0, \quad M^2-1=(\mathbf{k}')^2-(\mathbf{k}'')^2, \quad j(j+1)=(\mathbf{k}')^2\geqslant M^2-1. \tag{8.9}$$

There is some ambiguity in the parametrization of the orbits, which disappears if we consider only allowed orbits and allowed values of the parameters. These orbits are three-dimensional in the general case and two-dimensional if $\mathbf{k}'=0$ or $\mathbf{k}''=0$. If both these vectors vanish, we have a zero-dimensional orbit, corresponding to $j=M=0$, $c^2=1$, namely to a Minkowskian theory.

In the case $\mu=0$, infinite helicity spectrum, the spin-shell is described by the equations (8.3) and

$$(k_{10}-k_{31})^2+(k_{20}+k_{23})^2=\kappa^2>0. \tag{8.10}$$

It has dimension three and it is an unbounded orbit of the little group $\widetilde{E}(2)$.

In the case $\mu=0$, helicity M, from Eq. (7.30) we obtain the equations

$$k_{10}=k_{31}, \quad k_{20}=-k_{23}, \quad k_{12}=M. \tag{8.11}$$

Equation (7.31) contains products of noncommuting operators and gives ambiguous results. A direct substitution gives

$$k_{30}=i(1-c), \tag{8.12}$$

but this result is not compatible with Eq. (8.3). We consider the equation

$$k_{30}=N(c), \tag{8.13}$$

without specifying the function $N(c)$, apart from the conditions $N(1)=0$ and $N(c)\simeq -ic$ for large imaginary c. If $N(c)$ is real, Eqs. (8.11) and (8.13) define a two-dimensional unbounded orbit of $\widetilde{E}(2)$, unless $M=N=0$.

In order to complete the list of the orbits of $\widetilde{E}(2)$ in the spin space, we have to consider the zero-dimensional trivial orbit, corresponding to a Minkowskian scalar field, and a set of one-dimensional bounded orbits defined by the conditions

$$k_{10}=k_{31}, \quad k_{20}=-k_{23}, \quad k_{12}=k_{30}=0, \quad (k_{31})^2+(k_{23})^2=\nu^2>0. \tag{8.14}$$

The corresponding orbits of the Lorentz group are four-dimensional and have a large symmetry group[2,7] locally isomorphic to L(4,**R**). It has been shown in Ref. 7 that they are not allowed according to our definition.

Now we study the VEVs of the flat-space theories with $\mu>0$. Given a positive-mass orbit of the Lorentz group in the spin-momentum space and positive Lorentz-invariant measure m on it, the VEV can be written in the form

$$V(x,\mathbf{x}',\mathbf{x}'')=(2\pi)^{-3}\int \exp(-ik\cdot x+i\mathbf{k}'\cdot\mathbf{x}'-i\mathbf{k}''\cdot\mathbf{x}'')\,dm$$

$$=(2\pi)^{-3}\int \exp(-ik\cdot x+i\mathbf{k}'\cdot\mathbf{x}'-i\mathbf{k}''\cdot\mathbf{x}'')\tilde{v}(\hat{\mathbf{k}}',\hat{\mathbf{k}}'')\,\theta(k^0)$$

$$\times\delta(k\cdot k+\mu^2)d^4k\,d^3\mathbf{k}'\,d^3\mathbf{k}'', \tag{8.15}$$

where

$$\hat{k}_{ik}=\Lambda^r{}_i(a_k)\Lambda^s{}_k(a_k)k_{rs}, \tag{8.16}$$

$\tilde{v}(\mathbf{k}',\mathbf{k}'')d^3\mathbf{k}'d^3\mathbf{k}''$ represents a positive rotation-invariant measure concentrated on the spin-shell, and a_k is defined by Eq. (3.21).

The integral (8.15) can be written in the form

$$V(x,\mathbf{x}',\mathbf{x}'')=(2\pi)^{-3}\int \exp(-ik\cdot x)v(\hat{\mathbf{x}}',\hat{\mathbf{x}}'')\,\theta(k^0)\,\delta(k\cdot k+\mu^2)d^4k, \tag{8.17}$$

where

$$\hat{x}^{ik}=\Lambda_r{}^i(a_k)\Lambda_s{}^k(a_k)x^{rs} \tag{8.18}$$

and

$$v(\mathbf{x}',\mathbf{x}'')=\int \exp(i\mathbf{k}'\cdot\mathbf{x}'-i\mathbf{k}''\cdot\mathbf{x}'')\tilde{v}(\mathbf{k}',\mathbf{k}'')d^3\mathbf{k}'\,d^3\mathbf{k}''. \tag{8.19}$$

If the vectors $\mathbf{k}'$, $\mathbf{k}''$ represent an arbitrary point of the spin-shell, we can put

$$v(\mathbf{x}',\mathbf{x}'')=I(\mathbf{k}',\mathbf{k}'',\mathbf{x}',\mathbf{x}'')=\int_{\mathrm{SO}(3)}\exp(iR\mathbf{k}'\cdot\mathbf{x}'-iR\mathbf{k}''\cdot\mathbf{x}'')d^3R, \tag{8.20}$$

where R is a three-dimensional rotation matrix and d^3R is the normalized invariant measure on the rotation group. In the general case, this integral cannot be expressed in terms of elementary functions, but if the vectors $\mathbf{k}'$,$\mathbf{k}''$ are parallel or antiparallel, we have

$$v(\mathbf{x}',\mathbf{x}'')=t^{-1}\sin t, \tag{8.21}$$

where

$$t^2=(\|\mathbf{k}'\|\mathbf{x}'\mp\|\mathbf{k}''\|\mathbf{x}'')^2. \tag{8.22}$$

If we consider a theory with $j=M=0$, from Eq. (8.6) we obtain

$$t^2=(1-c^2)(\mathbf{x}'')^2. \tag{8.23}$$

Equation (8.17) is similar to Eq. (3.24) and it is interesting to compare the functions $v(\mathbf{x}',\mathbf{x}'')$ and $w(a)$, where a is given by the exponential

$$a=\exp(\tfrac{1}{2}(\mathbf{x}''-i\mathbf{x}')\cdot\sigma). \tag{8.24}$$

Equation (A27) gives the power expansion of the integral (8.20) up to quadratic terms in the variables $\mathbf{x}',\mathbf{x}''$. A comparison with Eq. (A26) shows that, disregarding higher-order terms, we have

$$w(a)\simeq v(\mathbf{x}',\mathbf{x}''). \tag{8.25}$$

It follows that if $f(x)$ is a test function and a is given by Eq. (8.24), we have

$$\int f(x)W(x,a)d^4x\simeq\int f(x)V(x,\mathbf{x}',\mathbf{x}'')d^4x \tag{8.26}$$

up to terms of the second order.

In order to simplify the integral (8.17), we proceed as in Sec. IV, namely, we put

$$\mathbf{x}'=(0,0,\alpha),\quad \mathbf{x}''=(0,0,\beta), \tag{8.27}$$

and we use the definitions (4.23)–(4.25). From Eq. (8.18) we obtain

$$\begin{aligned}\hat{\mathbf{x}}'&=(0,-\beta\ \sinh\ \eta,\alpha\ \cosh\ \eta)=\mu^{-1}(0,-\beta p,\alpha q),\\ \hat{\mathbf{x}}''&=(0,\alpha\ \sinh\ \eta,\beta\ \cosh\ \eta)=\mu^{-1}(0,\alpha p,\beta q).\end{aligned} \tag{8.28}$$

The analogue of Eq. (4.28) is

$$V(x,\alpha,\beta)=(2\pi)^{-1}\int_0^\infty \Delta(q\sigma,\epsilon(x^0))J_0(p\rho)v(\mathbf{x}',\mathbf{x}'')p\ dp, \tag{8.29}$$

and in a similar way one writes the analogues of Eqs. (4.31) and (4.32), which determine the commutator.

If in Eq. (8.20) we replace the integrand by the maximum of its modulus, we obtain the inequality

$$\begin{aligned}|I(\mathbf{k}',\mathbf{k}'',\mathbf{x}'+i\mathbf{y}',\mathbf{x}''+i\mathbf{y}'')|\leqslant\exp((\mathbf{k}')^2(\mathbf{y}')^2+(\mathbf{k}'')^2(\mathbf{y}'')^2\\ +2(\mathbf{k}'\cdot\mathbf{k}'')(\mathbf{y}'\cdot\mathbf{y}'')+2\|\mathbf{k}'\times\mathbf{k}''\|\|\mathbf{y}'\times\mathbf{y}''\|)^{1/2}.\end{aligned} \tag{8.30}$$

For large $|p|$ we have $\mathrm{Im}\,q\simeq\mathrm{Im}\,p$ and, with this approximation, from Eq. (8.28) we obtain

$$|v(\hat{\mathbf{x}}',\hat{\mathbf{x}}'')|\leqslant\exp(\mu^{-1}|\mathrm{Im}\ p|(\alpha^2+\beta^2)^{1/2}((\mathbf{k}')^2+(\mathbf{k}'')^2+2\|\mathbf{k}'\times\mathbf{k}''\|)^{1/2}). \tag{8.31}$$

If we take into account Eq. (4.33), we see that in the analogue of Eq. (4.32) we can close the integration path at infinity in the upper half-plane if

$$\rho>\sigma+\mu^{-1}(\alpha^2+\beta^2)^{1/2}((\mathbf{k}')^2+(\mathbf{k}'')^2+2\|\mathbf{k}'\times\mathbf{k}''\|)^{1/2}, \tag{8.32}$$

and under this condition the commutator of the flat-space theory vanishes. We remark that the flat-space theory has stronger local commutation properties than the corresponding theory on $\tilde{\mathscr{P}}$.

For $j=M=0$, we can use Eqs. (8.21) and (8.23) and from Eq. (8.28) we have

$$t^2=(1-c^2)(\alpha^2(\sinh\ \eta)^2+\beta^2(\cosh\ \eta)^2)=(1-c^2)(\beta^2+(\alpha^2+\beta^2)\mu^{-2}p^2). \tag{8.33}$$

If we remark that, for small values of α and β, Eq. (5.25) gives

$$\zeta^2\simeq\alpha^2(\sinh\ \eta)^2+\beta^2(\cosh\ \eta)^2, \tag{8.34}$$

we can easily verify Eq. (8.26) in this special case.

IX. A THEORY WITH BROKEN Sp(4,R) SYMMETRY

Now we consider a scalar flat-space theory invariant with respect to a group $\mathscr{T}$ larger than SL(2,**C**). It is defined by a spin-mass-shell which is an orbit of $\mathscr{T}$ and can be decomposed into orbits of the Lorentz group. As a consequence, its two-point VEV is a superposition (an integral) of the Lorentz invariant VEVs $V(x,\mathbf{x}',\mathbf{x}'')$ described in Sec. VIII. If all the Lorentz orbits which appear in the decomposition are allowed (apart from a set of vanishing measure), we can consider the analogous superposition of the VEVs $W(x,a)$ and we find the VEV of a nonelementary theory on $\tilde{\mathscr{P}}$ which corresponds, in some sense, to the $\mathscr{T}$-invariant theory on the flat space. In general, the theory on $\tilde{\mathscr{P}}$ has lost the symmetry under the large group $\mathscr{T}$, but some consequence of this higher symmetry remains in the short-distance limit.

In Refs. 7 and 30 we have described several flat-space theories symmetric with respect to SL(4,**R**) or to one of its subgroups isomorphic to Sp(4,**R**), which form a one-parameter family.[2] The positivity of the energy requires that the spin-mass-shell is contained in a closed invariant cone $\mathscr{T}^{*+}$, the dual of the cone $\mathscr{T}^{+}$ that describes the causal properties of the theory. Therefore, only the allowed Lorentz orbits contained in $\mathscr{T}^{*+}$ are interesting for the purpose we are discussing. The corresponding spin-shells must be bounded, and this requirement excludes all the zero-mass allowed theories considered in Sec. VIII, but the Minkowskian zero-mass theory corresponding to the spin-shell reduced to the origin. In addition to this theory, only positive-mass elementary theories can be used in the construction of a theory on $\tilde{\mathscr{P}}$ with broken higher symmetry. If we look at the definition of the cone $\mathscr{T}^{*+}$,[7] we see that for $\mu>0$ the spin-shell must be contained in the set defined by

$$(\mathbf{k}')^2+(\mathbf{k}'')^2+2\|\mathbf{k}'\times\mathbf{k}''\|\leqslant\mu^2 \tag{9.1}$$

(see Appendix B). This inequality gives rise to a complicated constraint on the parameters j, M, and c; in particular, we obtain

$$j(j+1)+1-c^2\leqslant\mu^2. \tag{9.2}$$

The mass μ is measured in natural units of the order of the Planck mass and for the observable particles it is very small. It follows that we must have $j=M=0$ and $1-c^2\ll 1$, namely the theory must be very near to the Minkowskian limit. We also see that the particles with small μ and nonvanishing spin cannot be described by scalar fields. We have already remarked in Sec. V that spin has two different origins: in this case the spin is generated by the field indices, as in Eqs. (5.15) and (6.28). Combined with Eq. (8.32), Eq. (9.1) ensures that the commutator of the flat-space theory vanishes for

$$\rho>\sigma+(\alpha^2+\beta^2)^{1/2}. \tag{9.3}$$

We consider the spin-mass-shells described in Refs. 7 and 30 and we exclude the four-dimensional one, composed of a single zero-mass not-allowed Lorentz orbit. The decomposition of these spin-mass-shells (disregarding a set of vanishing measure) contains only positive-mass Lorentz orbits. In general, not all these orbits are allowed, but one can try to replace the integral over the continuous parameters j and M by a sum over the discrete allowed values. In this way, we may also obtain a discrete mass spectrum. This procedure will be examined elsewhere; in the following we consider a particular choice of the group $\mathscr{T}$ isomorphic to Sp(4,**R**) and a particular class of orbits in such a way that all the Lorentz orbits that appear in the decomposition are allowed.

For the description of the spin-mass-shells invariant with respect to Sp(4,**R**), locally isomorphic to the anti-de-Sitter group $SO^{\uparrow}(2,3)$, it is convenient to introduce the notation

$$k^{5i}=-k^{i5}=k^i, \quad i=0,1,2,3, \tag{9.4}$$

and to consider the quantities k^{uv} as the components of an antisymmetric tensor in a five-dimensional space with metric $g_{55}=g_{00}=-1$, $g_{11}=g_{22}=g_{33}=1$. In the following the indices u,v,w,x,y,z take the values 5,0,1,2,3.

We consider the orbit which contains the point defined by $k^0=s>0$, $\mathbf{k}=\mathbf{k}'=\mathbf{k}''=0$. Then it also contains the Lorentz orbit that corresponds to a Minkowskian theory with mass $\mu=s$. It is six-dimensional and in Ref. 30 it has been called $\mathscr{O}_{4,(1/2)s,(1/2)s}$. The following O(2,3)-invariant set of conditions is satisfied on the orbit for all the values of s:

$$e^{uvwxy}k_{vw}k_{xy}=0. \tag{9.5}$$

In the four-dimensional formalism these conditions take the form

$$e^{ikrs}k_{ik}k_{rs}=0, \quad e^{ikrs}k_k k_{rs}=0, \tag{9.6}$$

and in the three-dimensional formalism we can write

$$\mathbf{k}\cdot\mathbf{k}'=0, \quad \mathbf{k}'\cdot\mathbf{k}''=0, \tag{9.7}$$

$$\mathbf{k}'=(k^0)^{-1}\mathbf{k}''\times\mathbf{k}. \tag{9.8}$$

It is clear that Eq. (9.8) implies Eq. (9.7) and therefore the whole set of conditions (9.5). We see that these conditions are not independent and define a seven-dimensional manifold.

The O(2,3)-invariant manifold defined by Eq. (9.5) can be parametrized by means of the coordinates $\mathbf{k}$, $\mathbf{k}''$, k^0 and it is easy to control that the measure defined by

$$(k^0)^{-2}d^3\mathbf{k}d^3\mathbf{k}''dk^0 \tag{9.9}$$

is invariant under O(2,3). In order to get an orbit of $SO^{\uparrow}(2,3)$, we have to introduce the further invariant condition

$$\tfrac{1}{2}\,g^{ux}g^{vy}k_{uv}k_{xy}=(k^0)^2-(\mathbf{k})^2+(\mathbf{k}')^2-(\mathbf{k}'')^2=s^2, \tag{9.10}$$

that, together with Eq. (9.8), gives

$$k^0=\pm\left(\tfrac{1}{2}((\mathbf{k})^2+(\mathbf{k}'')^2+s^2)\pm\tfrac{1}{2}(((\mathbf{k})^2+(\mathbf{k}'')^2+s^2)^2-4\|\mathbf{k}''\times\mathbf{k}\|^2)^{1/2}\right)^{1/2}. \tag{9.11}$$

This formula describes the orbit we are considering if we choose the sign + twice.

From Eqs. (9.8) and (9.10) we see that in the decomposition of this orbit into orbits of the Lorentz group we find, besides the above-mentioned orbit with mass $\mu=s$, the allowed orbits labelled, in accord with Eq. (8.4), by the parameters

$$M=j=0, \quad \mu^2=1-c^2+s^2>s^2. \tag{9.12}$$

In order to find an invariant measure on this orbit, we have to multiply Eq. (9.9) by the appropriate invariant δ-function and integrate over dk^0. The result is

$$\begin{aligned} dm_s&=\delta((k^0)^2-(\mathbf{k})^2+(\mathbf{k}')^2-(\mathbf{k}'')^2-s^2)(k^0)^{-2}d^3\mathbf{k}d^3\mathbf{k}''dk^0\\ &=\tfrac{1}{2}(k^0)^{-1}((k^0)^2-(\mathbf{k}')^2)^{-1}d^3\mathbf{k}d^3\mathbf{k}'', \end{aligned} \tag{9.13}$$

where $\mathbf{k}'$ and k^0 are given by Eqs. (9.8) and (9.11).

The Fourier transform of this measure can be performed in two steps:

$$V_s(x,\mathbf{x}',\mathbf{x}'')=(2\pi)^{-3}\int \exp(-ik\cdot x)A(k^0,\mathbf{k},\mathbf{x}',\mathbf{x}'')d^4k, \tag{9.14}$$

$$A(k^0,\mathbf{k},\mathbf{x}',\mathbf{x}'')=(k^0)^{-2}\int \exp(i\mathbf{k}'\cdot\mathbf{x}''-i\mathbf{k}''\cdot\mathbf{x}'')\,\theta(k^0-2^{-1/2}((\mathbf{k})^2+(\mathbf{k}'')^2+s^2)^{1/2})$$
$$\times\delta((k^0)^2-(\mathbf{k})^2+(\mathbf{k}')^2-(\mathbf{k}'')^2-s^2)d^3\mathbf{k}''. \tag{9.15}$$

If $\mathbf{k}=0$, we also have $\mathbf{k}'=0$ and, therefore,

$$A(k^0,0,\mathbf{x}',\mathbf{x}'')=\theta(k^0-s)(k^0)^{-2}\int \exp(-i\mathbf{k}''\cdot\mathbf{x}'')\,\delta((\mathbf{k}'')^2-(k^0)^2+s^2)d^3\mathbf{k}''$$
$$=2\pi(k^0)^{-2}((k^0)^2-s^2)^{1/2}\theta(k^0-s)v^{0c0}(\mathbf{x}''), \tag{9.16}$$

where $v^{0c0}(\mathbf{x}'')$ is given by Eqs. (8.21) and (8.23) with $1-c^2=\mu^2-s^2$. In general, by means of the Lorentz transformation a_k we obtain

$$A(k^0,\mathbf{k},\mathbf{x}',\mathbf{x}'')=2\pi\mu^{-2}(\mu^2-s^2)^{1/2}\theta(\mu^2-s^2)\,\theta(k^0)v^{0c0}(\hat{\mathbf{x}}''), \tag{9.17}$$

where $\hat{\mathbf{x}}''$ is given by Eq. (8.18) and $\mu^2=(k^0)^2-(\mathbf{k})^2$. In conclusion, we have

$$V_s(x,\mathbf{x}',\mathbf{x}'')=(2\pi)^{-2}\int \exp(-ik\cdot x)\mu^{-2}(\mu^2-s^2)^{1/2}\theta(\mu^2-s^2)\,\theta(k^0)v^{0c0}(\hat{\mathbf{x}}'')d^4k. \tag{9.18}$$

In order to obtain the VEVs of the theory defined on $\tilde{\mathscr{P}}$, we just have to replace v^{0c0} by w^{0c0} and we obtain

$$W_s(x,a)=(2\pi)^{-2}\int \exp(-ik\cdot x)\mu^{-2}(\mu^2-s^2)^{1/2}\theta(\mu^2-s^2)\,\theta(k^0)w^{0c0}(a_k^{-1}aa_k)d^4k. \tag{9.19}$$

Also in this case we can introduce the parameters α and β, parametrize k as in Eq. (4.23), and perform the integration over the variables ξ and ψ. We obtain

$$V_s(x,\alpha,\beta)=2\int_0^\infty\int_0^\infty (q^2-p^2)^{-1}(q^2-p^2-s^2)^{1/2}$$
$$\times\theta(q^2-p^2-s^2)\Delta(q\sigma,\epsilon(x^0))J_0(p\rho)t^{-1}\sin t\; pdp\; qdq, \tag{9.20}$$

where

$$t^2=(q^2-p^2)^{-1}(q^2-p^2-s^2)(p^2\alpha^2+q^2\beta^2) \tag{9.21}$$

and

$$W_s(x,u_3(\alpha)a_3(\beta))=2\int_0^\infty\int_0^\infty (q^2-p^2)^{-1}(q^2-p^2-s^2)^{1/2}\theta(q^2-p^2-s^2)$$
$$\times\Delta(q\sigma,\epsilon(x^0))J_0(p\rho)(c\sinh\zeta)^{-1}\sinh(c\zeta)pdp\; qdq, \tag{9.22}$$

where

$$c^2=s^2-q^2+p^2+1,\quad \cosh\zeta=(q^2-p^2)^{-1}(q^2\cosh\beta-p^2\cos\alpha). \tag{9.23}$$

The field defined by W_s satisfies the equations

$$e^{uvwxy}A_{vw}A_{xy}\psi=0, \tag{9.24}$$

$$\tfrac{1}{2}g^{ux}g^{vy}A_{uv}A_{xy}\psi=-s^2\psi, \tag{9.25}$$

written in the five-dimensional formalism. In fact, it is a direct integral of fields that satisfy Eqs. (7.34)–(7.36) and (7.38) with the parameters constrained by Eq. (9.12). This field describes ''particles'' with vanishing spin and a continuous mass spectrum lying on the half-line $\mu\geqslant s$.

The function V_s has been computed in Ref. 30 and, with the conventions adopted here, is given by

$$V_s(x,\mathbf{x}',\mathbf{x}'')=\lambda_1^{-1}\lambda_2^{-1}(\lambda_1+\lambda_2)^{-1}\ \exp(-\tfrac{1}{2}s(\lambda_1+\lambda_2)), \tag{9.26}$$

where λ_1,λ_2 are given by

$$\lambda_{1,2}^2=A\pm(A^2-B)^{1/2}, \tag{9.27}$$

$$\begin{aligned} A&=-\sigma^2+\rho^2-\alpha^2+\beta^2,\\ B&=(\sigma^2-\rho^2-\alpha^2-\beta^2)^2-4\rho^2(\alpha^2+\beta^2) \end{aligned} \tag{9.28}$$

(see Appendix B for more details). The signs of λ_1,λ_2 are determined in such a way that their real parts are positive or, if one of them vanishes, it becomes positive after the addition of a small positive imaginary part to x^0.

Starting from Eqs. (9.20)–(9.23), and introducing the new integration variables $p'=\epsilon p$, $q'=\epsilon q$, it is easy to prove that

$$\lim_{\epsilon\to 0}(\epsilon^3 W_s(\epsilon x,u_3(\epsilon\alpha)a_3(\epsilon\beta)))=V_0(x,\alpha,\beta), \tag{9.29}$$

$$\lim_{\epsilon\to 0}(\epsilon^3 V_s(\epsilon x,\epsilon\alpha,\epsilon\beta))=V_0(x,\alpha,\beta). \tag{9.30}$$

This means that in the short-distance limit, namely near to the unit of the group, the VEV W_s coincides with the distribution V_0, symmetric with respect to Sp(4,**R**). In other words, the symmetry broken by the structure of the Poincaré group survives in the short-distance limit. We also see that in the short-distance limit the dependence on the parameter s disappears.

X. RADIATION FROM AN ACCELERATED SOURCE

The simplest exercise with a free quantum field is its interaction with an external source. We consider a scalar Hermitian field and we write the time integral of the interaction Hamiltonian in the form

$$F=\int H'(t)dt=\int f(x,a)\psi(x,a)d^4x\ d^6a. \tag{10.1}$$

The scattering operator is given by

$$S=\exp(-iF)=\exp(-\tfrac{1}{2}\|F\Omega\|^2):\exp(-iF): \tag{10.2}$$

(time ordering is not necessary, since it introduces only an overall phase factor). The number of emitted particles follows a Poisson distribution with average value

$$\langle n\rangle = \|F\Omega\|^2. \tag{10.3}$$

This is just the quantity given by Eq. (3.12).

In general, the function f that describes the source is not arbitrary; it may be subject to some conservation law or to some other constraint arising from the field equations. For instance, it is not clear if a point particle has to be be described by a one-dimensional trajectory in $\tilde{\mathscr{P}}$ or by a manifold with higher dimension as it is discussed in Ref. 31. The formulation of possible constraints requires a deeper understanding of the theory and we disregard this problem in the following exercise. We consider a source that is bound to an accelerated frame, obtained from an initial frame by means of the following one-parameter group of Poincaré transformations:

$$t \to ((a^{-1}\sinh(at),0,0,a^{-1}(\cosh(at)-1)),a_3(at)). \tag{10.4}$$

An infinitesimal transformation of this group is the product of a time translation by an infinitesimal amount dt and a boost along the z axis with infinitesimal velocity $a\,dt$, where a represents a constant acceleration. The parameter t is the proper time of the accelerated frame.

Since a point source is too singular, we consider a source concentrated on a disk lying in the x^1,x^2 plane of the accelerated frame; then we have

$$F = \int P(r)Q(t)\psi((a^{-1}\sinh(at),r\cos\phi,r\sin\phi,a^{-1} \times(\cosh(at)-1)),a_3(at))r\,dr\,d\phi\,dt, \tag{10.5}$$

where $P(r)$ is the ''density'' of the disk and $Q(t)$ is a function equal to one in an interval of length T and going smoothly to zero outside this interval. We expect that when T is large, $\langle n\rangle$ is proportional to T.

Then from Eq. (10.3) we obtain

$$\langle n\rangle = \int P(r_1)P(r_2)Q(t_1)Q(t_2)W(x,a_3(at_2-at_1))r_1dr_1\,d\phi_1\,r_2dr_2\,d\phi_2\,dt_1\,dt_2, \tag{10.6}$$

where

$$x^0 = a^{-1}\sinh(at),\quad x^3 = a^{-1}(\cosh(at)-1),\quad t=t_2-t_1,\quad x^1 = r_2\cos\phi_2 - r_1\cos\phi_1,$$
$$x^2 = r_2\sin\phi_2 - r_1\sin\phi_1. \tag{10.7}$$

Note that W depends on the quantities (4.5), which take the form

$$\rho^2 = r_1^2 + r_2^2 - 2r_1r_2\cos(\phi_2-\phi_1), \tag{10.8}$$

$$\sigma = 2a^{-1}\sinh(\tfrac{1}{2}at). \tag{10.9}$$

We can also write

$$\langle n\rangle = 2\pi\int \hat{P}(\rho)\hat{Q}(t)W(x,a_3(\beta))\rho d\rho\,dt, \tag{10.10}$$

where

$$x=(\sigma,\rho,0,0),\quad \beta = at, \tag{10.11}$$

$$\hat{P}(\rho)=\int P(r)P(\rho^2+r^2+2\rho r\cos\phi)r\,dr\,d\phi, \tag{10.12}$$

$$\hat{Q}(t)=\int Q(t_1)Q(t+t_1)dt_1. \tag{10.13}$$

When the proper time interval T is large, we have

$$T^{-1}\hat{Q}(t)\simeq 1-|t|T^{-1}. \tag{10.14}$$

It follows that in the same limit the average number of produced particles per unit of proper time is given by

$$T^{-1}\langle n\rangle=2\pi\int_{-\infty}^{\infty}dt\int_0^{\infty}\hat{P}(\rho)W(x,a_3(\beta))\rho d\rho, \tag{10.15}$$

if the integral converges. If we take Eq. (3.29) into account, we can write

$$T^{-1}\langle n\rangle=4\pi\int_0^{\infty}dt\int_0^{\infty}\hat{P}(\rho)\mathrm{Re}\ W(x,a_3(\beta))\rho d\rho. \tag{10.16}$$

Now we consider the theory defined in Sec. IX and we look for singularities of the integral (10.16). Since the singularities arise for small values of t and ρ, we approximate the function W by means of Eqs. (9.26)–(9.29); namely, we use the formula

$$W(x,a_3(\beta))\simeq\lambda_1^{-1}\lambda_2^{-1}(\lambda_1+\lambda_2)^{-1}=(\lambda_1^2-\lambda_2^2)^{-1}(\lambda_2^{-1}-\lambda_1^{-1})=(4\rho\beta)^{-1}$$
$$\times(((\rho-\beta)^2-\sigma^2)^{-1/2}-((\rho+\beta)^2-\sigma^2)^{-1/2}), \tag{10.17}$$

where β and σ are given as functions of t by Eqs. (10.9) and (10.11).

After some calculation, we obtain

$$\int\hat{P}(\rho)\mathrm{Re}\ W(x,a_3(\beta))\rho d\rho=(4\beta)^{-1}\int_{\sigma}^{\infty}(\hat{P}(r+\beta)-\hat{P}(|r-\beta|))(r^2-\sigma^2)^{-1/2}\,dr+\theta(\beta-\sigma)$$
$$\times(2\beta)^{-1}\int_{\sigma}^{\beta}\hat{P}(\beta-r)(r^2-\sigma^2)^{-1/2}\,dr. \tag{10.18}$$

If $\hat{P}(\rho)$ has a bounded derivative, the first integral on the right-hand side has at most a logarithmic singularity for small t. The second integral is present only if $a>1$ and for small t it behaves as

$$\hat{P}(0)(2at)^{-1}\log(a+(a^2-1)^{1/2}). \tag{10.19}$$

As a consequence, if $a>1$, the integral over t in Eq. (10.16) diverges. In other words, if the acceleration a is larger than a critical value, conventionally taken equal to 1, the number of particles and the energy radiated per unit proper time become infinite.

APPENDIX A: PROPERTIES OF THE FUNCTIONS $w^{Mcj}(a)$

The quantities defined by Eqs. (5.14) or (5.18) are elementary functions, but for large values of j they are too complicated and it is preferable to introduce some integral representations. We start from the realization[23–26] of the representation D^{Mc} by means of operators acting on the square integrable functions defined on SU(2) which have the covariance property

$$f(u_3(\phi)u)=\exp(-iM\phi)f(u). \tag{A1}$$

An orthonormal basis in this Hilbert space is given by the functions

$$f_{jm}(u)=(2j+1)^{1/2}R^j_{Mm}(u). \tag{A2}$$

The invariant measure d^3u on SU(2) is normalized in such a way that the measure of the whole group is one.

We consider the decomposition

$$a=k(a)a_0, \tag{A3}$$

where

$$a=\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \in \mathrm{SL}(2,\mathbf{C}), \tag{A4}$$

$$k(a)=\begin{pmatrix} (p(a))^{-1} & q(a) \\ 0 & p(a) \end{pmatrix}, \quad p(a)>0, \tag{A5}$$

$$a_0=\begin{pmatrix} \alpha & \beta \\ -\overline{\beta} & \overline{\alpha} \end{pmatrix} \in \mathrm{SU}(2), \quad |\alpha|^2+|\beta|^2=1. \tag{A6}$$

We see that

$$p(a)=(|a_{21}|^2+|a_{22}|^2)^{1/2}, \tag{A7}$$

$$\alpha=(p(a))^{-1}\overline{a_{22}}, \quad \beta=-(p(a))^{-1}\overline{a_{21}}. \tag{A8}$$

We shall use the properties

$$p(au)=p(a), \quad (au)_0=a_0u, \quad u\in \mathrm{SU}(2), \tag{A9}$$

$$p(u_3(\phi)a)=p(a), \quad (u_3(\phi)a)_0=u_3(\phi)a_0. \tag{A10}$$

The representation operator is defined by

$$[D^{Mc}(a)f](u)=(p(ua))^{2c-2}f((ua)_0) \tag{A11}$$

and the matrix elements we need are given by

$$D^{Mc}_{jmjm}(a)=(f_{jm},D^{Mc}(a)f_{jm})=(2j+1)\int_{\mathrm{SU}(2)}\overline{R^j_{Mm}}(u)(p(ua))^{2c-2}R^j_{Mm}((ua)_0)d^3u. \tag{A12}$$

If we sum over m and use Eq. (A9), we obtain the required formula

$$w^{Mcj}(a)=\int_{\mathrm{SU}(2)}(p(ua))^{2c-2}R^j_{MM}((uau^{-1})_0)d^3u. \tag{A13}$$

We can also use the integral representation[27]

$$R^j_{MM}(u)=(2\pi)^{-1}\int_0^{2\pi}F^{Mj}(u_3(-\phi)uu_3(\phi))d\phi, \tag{A14}$$

where

$$F^{Mj}(u)=(\alpha-\overline{\beta})^{j+M}(\overline{\alpha}+\beta)^{j-M} \tag{A15}$$

and we have used the expression (A6) for the matrix u. If we substitute Eq. (A14) into Eq. (A13) and we use the properties (A9) and (A10), we obtain

$$w^{Mcj}(a)=\int_{\mathrm{SU}(2)}(p(ua))^{2c-2}F^{Mj}((uau^{-1})_0)d^3u \tag{A16}$$

or, more explicitly,

$$w^{Mcj}(a)=\int_{\mathrm{SU}(2)}(|b_{21}|^2+|b_{22}|^2)^{c-1-j}(\overline{b_{22}}+b_{21})^{j+M}(b_{22}-\overline{b_{21}})^{j-M}\,d^3u, \tag{A17}$$

where

$$b=uau^{-1}. \tag{A18}$$

The exponential mapping can be written in the form

$$a=\exp(\tfrac{1}{2}(\mathbf{x}''-i\mathbf{x}')\cdot\sigma)=\cosh\,\chi+\tfrac{1}{2}\chi^{-1}\,\sinh\,\chi\,(\mathbf{x}''-i\mathbf{x}')\cdot\sigma, \tag{A19}$$

where

$$\chi^2=\tfrac{1}{4}(\mathbf{x}''-i\mathbf{x}')\cdot(\mathbf{x}''-i\mathbf{x}'). \tag{A20}$$

If we indicate by $R(u)$ the SO(3) rotation matrix corresponding to the element $u\in\mathrm{Su}(2)$ and we put

$$\mathbf{y}'=R(u)\mathbf{x}',\quad \mathbf{y}''=R(u)\mathbf{x}'', \tag{A21}$$

we have

$$b=uau^{-1}=\cosh\,\chi+\tfrac{1}{2}\chi^{-1}\,\sinh\,\chi\,(\mathbf{y}''-i\mathbf{y}')\cdot\sigma. \tag{A22}$$

In particular, it is

$$b_{21}=\tfrac{1}{2}(y_1''-iy_1'+iy_2''+y_2')\chi^{-1}\,\sinh\,\chi,$$

$$b_{22}=\cosh\,\chi+\tfrac{1}{2}(-y_3''+iy_3')\chi^{-1}\,\sinh\,\chi. \tag{A23}$$

If we substitute these expressions into Eq. (A17) and disregard terms of order higher than the second in the variables $\mathbf{x}'$ and $\mathbf{x}''$, we can perform the integral by means of the formulas

$$\int_{\mathrm{SU}(2)}\mathbf{y}'\,d^3u=0, \tag{A24}$$

$$\int_{\mathrm{SU}(2)}y_r'y_s''\,d^3u=\frac{1}{3}\,\delta_{rs}\mathbf{x}'\cdot\mathbf{x}'' \tag{A25}$$

and other similar consequences of Eq. (A21). The result is

$$w^{Mcj}(a)\simeq 1-\tfrac{1}{6}j(j+1)(\mathbf{x}')^2-\tfrac{1}{6}(j(j+1)+1-c^2-M^2)(\mathbf{x}'')^2+\tfrac{1}{3}iMc\mathbf{x}'\cdot\mathbf{x}''. \tag{A26}$$

Now we want to compare the integral (A17) with the integral (8.20). We can expand the exponential in Eq. (8.20), keeping terms up to the second order in the variables $\mathbf{x}'$ and $\mathbf{x}''$, and perform the integral by means of Eqs. (A24) and (A25). We obtain

$$I(\mathbf{k}',\mathbf{k}'',\mathbf{x}',\mathbf{x}'')\simeq 1-\tfrac{1}{6}(\mathbf{k}')^2(\mathbf{x}')^2-\tfrac{1}{6}(\mathbf{k}'')^2(\mathbf{x}'')^2+\tfrac{1}{3}\mathbf{k}'\cdot\mathbf{k}''\mathbf{x}'\cdot\mathbf{x}'' \tag{A27}$$

and Eq. (8.25) follows immediately.

Another interesting limit can be derived from Eqs. (A17) and (A23):

$$\begin{aligned}\lim_{n\to\infty}\ & w^{nM,nc,nj}(\exp((2n)^{-1}(\mathbf{x}''-i\mathbf{x}')\cdot\sigma))\\ &=\int_{\mathrm{SU}(2)}\exp((j-c)y_3'')\exp(\tfrac{1}{2}(j+M)(-y_3''-iy_3'+y_1''-iy_1'+iy_2''+y_2'))\\ &\quad\times\exp(\tfrac{1}{2}(j-M)(-y_3''+iy_3'-y_1''-iy_1'+iy_2''-y_2'))d^3u=I(\mathbf{k}',\mathbf{k}'',\mathbf{x}',\mathbf{x}''),\end{aligned} \tag{A28}$$

where

$$\mathbf{k}'=(-j,-iM,-M),\quad \mathbf{k}''=(iM,-j,-ic). \tag{A29}$$

The quantity $I(\mathbf{k}',\mathbf{k}'',\mathbf{x}',\mathbf{x}'')$ defined in Eq. (8.20) is an entire analytic function of its arguments and it depends on $\mathbf{k}',\mathbf{k}''$ through the invariants

$$(\mathbf{k}')^2=j^2,\quad (\mathbf{k}'')^2=j^2-c^2-M^2,\quad \mathbf{k}'\cdot\mathbf{k}''=iMc. \tag{A30}$$

If we indicate by $\mathbf{k}_n',\mathbf{k}_n''$ the coordinates of a representative point of the orbit defined by the parameters nM,nc,nj, we have

$$\begin{aligned}\lim_{n\to\infty} v^{nM,nc,nj}(n^{-1}\mathbf{x}',n^{-1}\mathbf{x}'')&=\lim_{n\to\infty} I(\mathbf{k}_n',\mathbf{k}_n'',n^{-1}\mathbf{x}',n^{-1}\mathbf{x}')\\ &=\lim_{n\to\infty} I(n^{-1}\mathbf{k}_n',n^{-1}\mathbf{k}_n'',\mathbf{x}',\mathbf{x}')=I(\mathbf{k}',\mathbf{k}'',\mathbf{x}',\mathbf{x}'),\end{aligned} \tag{A31}$$

where

$$\mathbf{k}'=\lim_{n\to\infty}(n^{-1}\mathbf{k}_n'),\quad \mathbf{k}''=\lim_{n\to\infty}(n^{-1}\mathbf{k}_n''). \tag{A32}$$

Since these limits satisfy Eq. (A30), we see that the limits (A28) and (A31) are equal. This result can be used to generalize the treatment of Sec. IX to a larger class of theories with a broken higher symmetry.

APPENDIX B: GEOMETRY OF THE VECTOR SPACES $\mathscr{T}$ AND $\mathscr{T}^*$

In this Appendix we summarize some results of Refs. 2, 3, and 7. We use the Dirac matrices with the properties

$$\gamma_i\gamma_k+\gamma_k\gamma_i=2g_{ik},\quad {\gamma_k}^T=-C^{-1}\gamma_kC,\quad C^T=-C. \tag{B1}$$

We adopt the Majorana representation in which the Dirac matrices are real and we put $C=\gamma_0$. The vectors of $\mathscr{T}$ and $\mathscr{T}^*$ can be labelled, respectively, by means of the real symmetric 4×4 matrices

$$\hat{x}=\tfrac{1}{2}x^k C^{-1}\gamma_k-\tfrac{1}{4}x^{rs}C^{-1}\gamma_r\gamma_s, \tag{B2}$$

$$\hat{k}=-\tfrac{1}{2}k_k\gamma^{\,k}C+\tfrac{1}{4}k_{rs}\gamma^{\,r}\gamma^{\,s}C. \tag{B3}$$

The closed cones $\mathscr{T}^+$ and $\mathscr{T}^{*+}$ contain the elements labelled by positive semidefinite matrices.

The following formulas are useful:

$$\mathrm{Tr}(\hat{k}\hat{x})=-k_k x^k+\tfrac{1}{2}k_{rs}x^{rs}=k^0x^0-\mathbf{k}\cdot\mathbf{x}+\mathbf{k}'\cdot\mathbf{x}'-\mathbf{k}''\cdot\mathbf{x}'', \tag{B4}$$

$$A=\mathrm{Tr}(C\hat{x})^2=x_k x^k-\tfrac{1}{2}x_{rs}x^{rs}=-(x^0)^2+(\mathbf{x})^2-(\mathbf{x}')^2+(\mathbf{x}'')^2, \tag{B5}$$

$$-s^2=\mathrm{Tr}(\hat{k}C^{-1})^2=k_k k^k-\tfrac{1}{2}k_{rs}k^{rs}=-(k^0)^2+(\mathbf{k})^2-(\mathbf{k}')^2+(\mathbf{k}'')^2, \tag{B6}$$

$$\begin{aligned}B=16\det\hat{x}=&((x^0)^2-(\mathbf{x})^2-(\mathbf{x}')^2-(\mathbf{x}'')^2)^2-4\|\mathbf{x}\times\mathbf{x}'\|^2-4\|\mathbf{x}'\times\mathbf{x}''\|^2\\&-4\|\mathbf{x}''\times\mathbf{x}\|^2-8x^0\mathbf{x}''\cdot\mathbf{x}'\times\mathbf{x},\end{aligned} \tag{B7}$$

and a similar formula for $\det\hat{k}$. Note that the parameter s which appears in Eqs. (B6) and (9.10) was indicated by $2s$ in Ref. 30.

A vector of $\mathscr{T}$ belongs to $\mathscr{T}^+$ when x^0 is larger or equal to the largest root of the equation $\det\hat{x}=0$ and a similar statement holds for $\mathscr{T}^{*+}$. For $\mathbf{k}=0$ and $k^0=\mu>0$, we have

$$16\det\hat{k}=(\mu^2-(\mathbf{k}')^2-(\mathbf{k}'')^2)^2-4\|\mathbf{k}'\times\mathbf{k}''\|^2, \tag{B8}$$

and the condition for belonging to $\mathscr{T}^{*+}$ is just Eq. (9.1).

The quantities $\pm\lambda_{1,2}$ introduced in Sec. IX are the eigenvalues of the matrix $2C\hat{x}$ (the factor 2 was not present in Ref. 30). They are given by Eq. (9.27), where A and B are given by Eqs. (B5) and (B7). If we assume Eqs. (4.5) and (8.27), we get Eq. (9.28). It has been shown in Ref. 30 that in a flat-space theory invariant under $\mathrm{Sp}(4,\mathbf{R})$ the commutator vanishes unless one of the quantities $\lambda_{1,2}^2$ is real negative. This means that the commutator vanishes if $A^2-B<0$ or if $A>0$, $B>0$. These conditions are satisfied if $\sigma^2<0$ or if Eq. (9.3) holds.

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The Stückelberg–Kibble model as an example of quantized symplectic reduction

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Recently, it has been observed that a certain class of classical theories with constraints can be quantized by a mathematical procedure known as Rieffel induction. After a short exposition of this idea, we apply the new quantization theory to the Stückelberg–Kibble model. We explicitly construct the physical state space $\mathscr{H}_{\text{phys}}$, which carries a massive representation of the Poincaré group. The longitudinal one-particle component arises from a particular Bogoliubov transformation of the five (unphysical) degrees of freedom one has started with. Our discussion exhibits the particular features of the proposed constrained quantization theory in great clarity. © *1996 American Institute of Physics.* [S0022-2488(96)02105-3]

I. INTRODUCTION

Classical gauge field theories may be defined by a set of fields $\mathscr{A}$, subject to a set of constraints $\mathscr{B}$, which, in turn, generate gauge transformations. The quantization of such theories is not a unique procedure. Indeed, already in the two best-established quantization methods very different technical setups are chosen. On the one hand, one has the canonical operator formalism, originating with Heisenberg and Pauli,[1] and now well adapted to handle non-Abelian gauge theories,[2] whereas on the other hand Feynman's path integral formalism[3] allows the quantization of such theories through the Faddeev–Popov procedure.[4] Both methods lead to identical perturbative expansions, but even at a mathematically heuristic level their possible equivalence is only known in perturbation theory.

It is certainly of general interest to have as many conceptually and mathematically different quantization schemes as possible, and to examine the particular features of each of them. The hope of obtaining some hints on how to quantize gravity may provide further motivation for investigating new quantization schemes. Especially, the modern formulation of classical mechanics in terms of symplectic manifolds and Poisson algebras (see, e.g., Ref. 5) has suggested more refined quantization procedures, such as geometric quantization[6] and strict deformation quantization.[7,8]

A particular feature of classical gauge theories that should somehow be reflected in the quantization method is that the physical (reduced) phase space may be written as a so-called Marsden–Weinstein quotient.[9,10] Given that this powerful technique can be used to construct the physical state space of the classical theory, it appears most natural to look for a quantum analogue which mimicks it. This was found by one of the authors in Ref. 11 where Rieffel induction,[12] a technique from operator algebra theory used for the construction of representations of algebras, was shown to provide a satisfactory quantum analogue of the classical Marsden–Weinstein reduction. In practice, this allows one to perform a quantization of a classical unreduced model, and to find (via Rieffel induction) the quantum-reduced phase space which coincides with a direct quantization of the reduced classical phase space.

The method advocated in Ref. 11 provides a conceptually and technically new approach to the quantization of certain gauge field theories. It has already been successfully applied to certain

finite-dimensional constrained systems,[11] as well as to free quantum electrodynamics.[13,14] These applications are mainly operator-theoretic, but a certain aspect of the path integral formalism, viz. the integration over the gauge group, will play a role as well.

The present work draws on these results. Its aim is twofold. First, we would like to present the strategy of this new quantization method in a form accessible to a wider scientific community. Therefore, in Sec. II, we briefly review the main line of argument, leading to the quantization proposal. To keep our presentation reasonably short, we refer for some of the technicalities to the aforementioned papers. Subsequently, in Sec. III we apply the new quantization scheme to the Stückelberg–Kibble model. This toy model has often been used in the investigation of the Higgs mechanism and of spontaneous symmetry breaking, see, e.g., Ref. 15. Here, we have chosen it since it already shows many of the typical complications of spontaneously broken gauge theories without the need to restrict oneself to a perturbative discussion.

As we shall demonstrate explicitly for this model, the Rieffel induction procedure provides a scheme for the construction of the physical state space of a constrained quantum theory, starting from a larger (unphysical) state space on which the unconstrained theory is defined. Our discussion will focus on the particular properties of this Rieffel-induced physical Hilbert space $\mathscr{H}_{\rm phys}$. Especially, we find that $\mathscr{H}_{\rm phys}$ carries a trivial representation of the gauge group and a massive representation of the Poincaré group. Also, the positive spectrum condition turns out to be satisfied. As an important by-product, we are able to trace back how ''would-be Goldstone bosons rearrange to a massive, longitudinal component'' in a theory exhibiting the Higgs mechanism.

The context of our work is modern symplectic geometry and reduction theory on the classical side, and algebraic quantum field theory on the quantum side. We only use the ''soft'' side of these theories. Good recent introductions are Refs. 5, 16, and 17, respectively.

II. THE QUANTIZATION OF GAUGE THEORIES WITH RIEFFEL INDUCTION

After presenting schematically the strategy which leads to Rieffel induction in the quantization of theories with constraints, in the remainder of this section we briefly specify some notational and technical prerequisites.

A. Quantization of Marsden–Weinstein reduction

The general symplectic reduction procedure, which is quantized by Rieffel induction in its full generality, is described in Ref. 11. Here we are merely concerned with a special case, viz. Marsden–Weinstein reduction at the zero level of the moment map, (cf. Refs. 5 and 18). To introduce our notation, let us consider free classical electrodynamics. For the functional-analytic and other details which are suppressed in what follows, we refer the interested reader to Ref. 13.

We start with the space M of four-component real-valued weak solutions A_μ of the wave equation whose Fourier-transformed Cauchy-data lie in $L^2(\mathbb{R}^3)\otimes\mathbb{C}^4$. That is, $M=\{A_\mu|\Box A_\mu=0\}$. The imaginary part

$$B(A,A')=2\,\mathrm{Im}(A,A')_M=-i\int \frac{d^3\mathbf{p}}{(2\pi)^3}\,[A^\mu(\mathbf{p})\overline{A'_\mu}(\mathbf{p})-\overline{A^\mu}(\mathbf{p})A'_\mu(\mathbf{p})] \tag{II.1}$$

of the indefinite covariant scalar product $(*,*)_M$ turns M into a symplectic space (M,B), which is the phase space of the unconstrained classical system. The set of constraints is given by the gauge group G, which acts on M via $A_\mu\to A_\mu+\partial_\mu g$, where

$$G=\{g\in\mathscr{S}'(\mathbb{R}^4)|\Box g=0;dg\in M\}. \tag{II.2}$$

Here, the space of distributions $\mathscr{S}'(\mathbb{R}^4)$ is the dual of the usual Schwartz space of rapidly decreasing test functions. In the present example, the reduced phase space (M_c,B_c) of the corresponding constrained system may be obtained by a so-called Marsden–Weinstein reduction.[18] This involves the moment map J from M into the dual of the Lie algebra of G. As G is a vector space, we may

identify it with its Lie algebra, so we simply write $J_g(A)$ for the value of $J(A)$ on $g \in G$. Explicitly, the moment map turns out to be $J_g(A) = \mathrm{Im}(\partial g, A)_M$ (cf. Ref. 13). The preimage of its zero level is

$$J^{-1}(0) = \{A_\mu \in M \,|\, \partial_\mu A^\mu = 0\}. \tag{II.3}$$

Then, M_c is given by the Marsden–Weinstein quotient

$$M_c = J^{-1}(0)/G, \tag{II.4}$$

and B_c inherits its structure from B. It is easy to see that (M_c, B_c) defined this way indeed describes the physical degrees of freedom of free electrodynamics: picking $J^{-1}(0)$ fixes the gauge (thus imposing the Gauss law constraint, which on elements of M becomes the Lorentz gauge condition), and quotienting by G removes the gauge degeneracy of the symplectic form B with respect to the action of G on $J^{-1}(0)$.

In principle, there are two possibilities to quantize a reduced phase space (M_c, B_c). Either, we directly quantize the Marsden–Weinstein reduced (i.e., constrained) classical system (M_c, B_c), or we quantize the unconstrained classical system (M, B) together with the set of constraints. In the latter case, a scheme has to be found which imposes constraints on the unconstrained quantized theory, thereby providing a quantum analogue of the classical Marsden–Weinstein reduction. Examples of such schemes are the Dirac or the BRST method. According to the proposal of Ref. 11, the so-called Rieffel induction procedure of operator algebra theory[12] (which we explain below) provides a rival scheme, which in all examples studied so far works as well as, or better than, the methods mentioned above.

More precisely, let us consider schematically a quantization prescription $Q_\hbar$ which relates the symplectic space (M, B) (or rather the Poisson algebra of functions on it) to some algebra of field operators on a Hilbert space $\mathscr{A}$, G to some algebra $\mathscr{B}$ generated by G, and (M_c, B_c) to some (*a priori* unknown) algebra of observables (in the sense of gauge-invariant operators) $\mathscr{A}_{\mathrm{obs}}$. Then, according to our quantization proposal, the following diagram commutes:

$$\begin{array}{ccc} & \overset{Q_\hbar}{} & \\ (M,B);G & \rightarrow & \mathscr{A};\mathscr{B} \\ \text{Marsden–Weinstein Reduction} \downarrow & & \downarrow \text{ Rieffel Induction}. \\ & \overset{Q_\hbar}{} & \\ (M_c, B_c) & \rightarrow & \mathscr{A}_{\mathrm{obs}} \end{array} \tag{II.5}$$

Our program in this paper is to specify the entries of this diagram for the Stückelberg–Kibble model. To this end, we briefly recall how, for a linear field theory, a symplectic space (M, B) can be related to a field algebra $\mathscr{A}$ of canonical commutation relations, and we explain how Rieffel induction allows one to construct new Hilbert spaces for quantum field theories, thereby eventually specifying $\mathscr{A}_{\mathrm{obs}}$.

B. Weyl algebras of canonical commutation relations

The general theory behind this subsection is explained in great detail and rigor in, e.g., Ref. 17, and the application to electromagnetism is from Ref. 19. We merely mention some of the main points.

For ϕ, $\phi' \in M$, the operators $W(\phi)$, $W(\phi')$, satisfying the Weyl form of the canonical commutation relation (CCR)

$$W(\phi)W(\phi') = W(\phi + \phi')e^{(-i/2)B(\phi,\phi')}, \tag{II.6}$$

specify a field algebra with C^*-structure which we denote by $\mathscr{A}(M,B)$. In most cases, one is primarily interested in the properties of the operator vector potential A_μ, for which we use the same notation as for its classical counterpart, as no confusion will arise. The A_μ satisfy the canonical commutation relations

$$[A_\mu(x),\, A_\nu(y)] = -ig_{\mu\nu}\, D(x-y), \tag{II.7}$$

where D denotes the commutator function satisfying $\Box D=0$, with initial conditions $D(\mathbf{x},0)=0$, $(\partial/\partial t)D(\mathbf{x},t)|_{t=0} = -\delta^{(3)}(\mathbf{x})$. To see the connection between (II.6) and (II.7), we consider the vector potential $A(f)=\int d^4x A_\mu(x) f^\mu(x)$, smeared with real test functions f. Now, (II.7) reads $[A(f),A(g)] = i\sigma(f,g)$, where $\sigma(f,g) = -\int d^4x d^4y D(x-y) f^\mu(x) g_\mu(y)$. Formally, this allows for the introduction of the operators $U(f)=e^{[iA(f)]}$, which, according to the Baker–Campbell–Haussdorff formula, satisfy the Weyl form of the canonical commutation relations $U(f)U(g) = U(f+g)e^{[-(i/2)\sigma(f,g)]}$. Here, however, $U(f)$ and $U(f')$ have the same commutation relations as long as $\int d^4x D(x-y)(f^\mu(x)-f'^\mu(x))=0$ for almost all y. To remove this degeneracy and to obtain a one-to-one correspondence between Weyl operators and test functions, one uses the map $f\to\phi$, defined by the convolution $\phi_\mu = D*f_\mu$. Then, the space M of solutions of the wave equation

$$\Box\phi_\mu = 0, \quad \phi_\mu(\mathbf{x},t) = \frac{1}{(2\pi)^3}\int \frac{d^3\mathbf{k}}{2k_0}\,[\phi_\mu(\mathbf{k})e^{-ikx} + \overline{\phi_\mu}(\mathbf{k})e^{ikx}]$$

is (our notation does not distinguish between functions ϕ and their Fourier transforms, since no confusion should arise)

$$M = \overline{\{\phi = D*f\}} = L^2(\mathbb{R}^3)\otimes\mathbb{C}^4. \tag{II.8}$$

Now, the operators $W(\phi)=U(f)$, $\phi\in M$, satisfy (II.6) with symplectic form B induced by σ and given in (II.1).

Having established the connection between Weyl operators and vector potentials, we can introduce formal annihilation and creation operators a_μ, a_μ^*, e.g., for the free electromagnetic field,

$$A_\mu(x) = \int \frac{d^3\mathbf{k}}{(2\pi)^3 2k_0}\,[e^{-ikx}a_\mu(\mathbf{k}) + e^{ikx}a_\mu^*(\mathbf{k})]|_{k_0=\mathbf{k}},$$

$$iA(f) = \int \frac{d^3\mathbf{k}}{(2\pi)^3 2k_0}\,[a_\mu(\mathbf{k})\overline{\phi_\mu}(\mathbf{k}) - a_\mu^*(\mathbf{k})\phi_\mu(\mathbf{k})] =: a_\mu(\phi^\mu) - a_\mu(\phi^\mu)^*. \tag{II.9}$$

Clearly, in terms of the annihilation and creation operators, the Weyl operators read $W(\phi^\mu)=\exp[a_\mu(\phi^\mu) - a_\mu(\phi^\mu)^*]$, where $[a_\mu(\phi^\mu), a_\nu(\phi'^\nu)^*] = (\phi',\phi)_M$, $(.,.)_M$ denoting the indefinite Minkowski inner product. Heuristically, one has

$$\frac{d}{d\lambda}\, W(\lambda\phi)\bigg|_{\lambda=0} = iA(f). \tag{II.10}$$

It is well known that this derivative does not exist in the operator norm but with respect to regular representations only, and thereby the a_μ, a_μ^* only exist in such representations, too. Nevertheless, in what follows we shall adopt the formal expressions (II.9) and (II.10), even when no explicit reference to a particular representation is made.

As a final preparatory step, we point out that subalgebras of $\mathscr{A}(M,B)$ can be specified by selecting subspaces of M. In particular, for free QED,

$$N=\{\phi_\mu\in M\,|\,k^\mu\phi_\mu(\mathbf{k})=0\}=\{\phi_\mu\in M\,|\,\partial^\mu\phi_\mu(x)=0\},$$
$$T=\{\phi_\mu\in M\,|\,\phi_\mu(\mathbf{k})=ik_\mu g(\mathbf{k})\}=\{\phi_\mu\in M\,|\,\phi_\mu(x)=\partial_\mu g(x),\Box g(x)=0\} \tag{II.11}$$

define subalgebras $\mathscr{A}(N,B)$, $\mathscr{A}(T,B)$ of $\mathscr{A}(M,B)$. Note that $T\subset N$, so that $\mathscr{A}(T,B)\subset\mathscr{A}(N,B)$. These subalgebras are Poincaré-invariant, as may be seen by recalling that the action of elements (Λ,a) of the Poincaré group $\mathscr{P}$ on $\mathscr{A}(M,B)$ is defined via the algebraic automorphism $\alpha_{(\Lambda,a)}$,

$$\alpha_{(\Lambda,a)}(W(\phi^\mu))=W(\gamma_{(\Lambda,a)}(\phi^\mu)) \quad \text{with} \quad (\gamma_{(\Lambda,a)}(\phi^\mu))(x)=\Lambda^\mu\phi'(\Lambda^{-1}(x-a)). \tag{II.12}$$

C. Rieffel induction

This subsection gives a quick ''review by example'' of some parts of the theory developed in Refs. 11 and 13.

In physics, induction methods are mainly known from Wigner's classification and construction of all irreducible unitary representations of the Poincaré group $\mathscr{P}$. In general, the method of induced representations of (locally compact) groups allows one to construct a representation of the complete group from a representation of a subgroup (cf., e.g., Ref. 20).

Also, in the theory of operator algebras (particularly C^*-algebras) a method exists for constructing a representation of an algebra, given a representation of some other algebra.[12] The latter is not necessarily a subalgebra of the former; instead, the two algebras need to be connected by a bimodule with certain additional properties. Whatever the technical details, the main idea is that the representation one induces from should be straightforward, and yet capable of producing an appropriate representation of the algebra one is really interested in. This idea will be fully realized in our context, for the second algebra will be the algebra generated by the gauge group, and the representation induced from is the trivial one. With a suitable choice of bimodule, the induced representation of the algebra of observables turns out to be the vacuum representation on a Fock space of physical photon states.

To facilitate our presentation, we proceed by example, abstracting general features afterwards. For free QED, in the diagram (II.5) we choose the field algebra $\mathscr{A}=\mathscr{A}(M,B)$ and the ''algebra of constraints'' $\mathscr{B}=\mathscr{A}(T,B)$ (cf. the previous subsection), where the choice of $\mathscr{B}$ is motivated by observing that the gauge group G equals T [cf. (II.11)]. Also, we introduce the ''algebra of weak observables'' $\mathscr{A}_c:=\mathscr{A}(N,B)$, which is the largest subalgebra of $\mathscr{A}=\mathscr{A}(M,B)$ commuting with $\mathscr{B}=\mathscr{A}(T,B)$. For simplicity, we here ignore some mathematical difficulties in defining algebras $\mathscr{B}$ for groups G which are not locally compact. This greatly simplifies our presentation. For more details, we refer to Refs. 13 and 14.

The Rieffel induction procedure will produce a representation of $\mathscr{A}_c$ induced from a representation of $\mathscr{B}$. To this end, we need a bimodule for $\mathscr{A}_c$ and $\mathscr{B}$, that is, a linear space on which $\mathscr{A}_c$ acts from the left, and $\mathscr{B}$ acts from the right (that is, in an antirepresentation), so that these two actions commute. In the case at hand, $\mathscr{A}_c$ and $\mathscr{B}$, which is Abelian, are each other's commutant in the field algebra $\mathscr{A}$, so that a representation of $\mathscr{A}$ on a Hilbert space $\mathscr{H}$ automatically defines such a bimodule. Finally, we need a representation of $\mathscr{B}$ to induce from. This is the trivial one, defined on the Hilbert space $\mathscr{H}_{\rm tr}=\mathbb{C}$. Schematically,

$$\mathscr{A}_c\rightarrow\mathscr{H}\leftarrow\mathscr{B}\rightarrow\mathscr{H}_{\rm tr}. \tag{II.13}$$

The choice of the trivial representation to Rieffel induce from is dictated by the fact that Marsden–Weinstein reduction of the classical theory is performed from the zero level of the momentum map [cf. (II.4)] (that is, the point 0 in the dual of the Lie algebra of the gauge group G corresponds to the trivial representation).[21]

The restriction of the action π on $\mathscr{H}$ of $\mathscr{A}$ to its subalgebra $\mathscr{B}$ defines a representation U of the gauge group, that is, one has $U(\phi)=\pi(W(\phi))$.

As will be discussed in more detail below, this setup allows the construction of a positive semidefinite sesquilinear form $(.,.)_0$ on $L\otimes\mathscr{H}_{\rm tr}$, where L is a suitable dense subspace of L. In the present case, this form is given by

$$(\psi\otimes v,\varphi\otimes w)_0=v\overline{w}\int_G[\mathscr{D}\phi](U(\phi)\psi,\varphi). \tag{II.14}$$

Here $[\mathscr{D}\phi]$ denotes the nonexistent ''Lebesgue'' measure on the gauge group G. The point is, however, that this flat ''measure'' combines with a factor in the integrand to define a mathematically well-defined path integral (cylindrical) measure on G.[13] Furthermore, ψ,φ are in $\mathscr{H}$, $v,w\in\mathscr{H}_{\rm tr}=\mathbb{C}$, and $(.,.)$ is the inner product on $\mathscr{H}$.

Irrespective of the explicit form of $(.,.)_0$, the induced physical Hilbert space is then defined as the completion of the quotient of $L\otimes\mathscr{H}_{\rm tr}$ by the null space of $(.,.)_0$, i.e.,

$$\mathscr{H}_{\rm phys}=\overline{(L\otimes\mathscr{H}_{\rm tr})/\mathscr{N}}, \tag{II.15}$$

where $\mathscr{N}\subset L\otimes\mathscr{H}_{\rm tr}$ is the subset of vectors with vanishing $(.,.)_0$ norm. The collection of vectors in $\mathscr{H}_{\rm phys}$ of the form $\psi\widetilde{\otimes}$v, defined as the image of $\psi\otimes v\in L\otimes\mathscr{H}_{\rm tr}$ under the quotient projection from $L\otimes\mathscr{H}_{\rm tr}$ to $\mathscr{H}_{\rm phys}$, are clearly dense in $\mathscr{H}_{\rm phys}$. The action of elements A of $\mathscr{A}_c$ on $\mathscr{H}_{\rm phys}$ is then given on this dense set by $\pi_{\rm phys}(A)\psi\widetilde{\otimes}\mathrm{v}=(\pi(A)\psi)\widetilde{\otimes}v$. Under appropriate continuity conditions[12,13] this action may be extended to all of $\mathscr{H}_{\rm tr}$.

The reader should note that $\mathscr{H}_{\rm phys}$ satisfies an essential requirement of a nondegenerate physical Hilbert space: the gauge degeneracy of elements $\mathscr{A}_c$ is removed in $\pi_{\rm phys}(\mathscr{A}_c)$. To see this, choose an arbitrary element $W(\phi)\in\mathscr{A}_c$. From equation (II.14), it is obvious that for $\phi_t\in T$ (which, we recall, coincides with the gauge group G), $\pi_{\rm phys}(W(\phi))\psi\widetilde{\otimes}v=\pi_{\rm phys}(W(\phi+\phi_t))\psi\widetilde{\otimes}v$ for all vectors $\psi\widetilde{\otimes}\mathrm{v}\in\mathscr{H}_{\rm phys}$. Hence, $\pi_{\rm phys}(W(\phi))=\pi_{\rm phys}(W(\phi+\phi_t))$. This removal of the gauge degeneracy of $\mathscr{A}_c$ is independent of the choice of $\mathscr{H}$, and hence we identify $\pi_{\rm phys}(\mathscr{A}_c)$ with the representation-independent algebra of observables $\mathscr{A}_{\rm obs}$ [cf. (II.5)].

Let us now turn to the abstract setting which has led to the $(.,.)_0$ inner product (II.14). As stated, the aim of the Rieffel induction procedure is to obtain a representation $\pi_{\rm phys}$ of $\mathscr{A}_c$ induced from a representation of $\mathscr{B}$ on some Hilbert space $\mathscr{H}_\chi$. Our example, and all similar examples involving gauge theories, have the special feature that $\mathscr{H}_\chi=\mathscr{H}_{\rm tr}=\mathbb{C}$, that is, one induces from the trivial representation of the gauge group. This will imply that the algebra of constraints $\mathscr{B}$ is represented trivially on the induced space $\mathscr{H}_{\rm phys}$. Technically, the construction of $\pi_{\rm phys}$ proceeds according to the following three-step method.

(1) Given a bimodule L for $\mathscr{A}_c$ and $\mathscr{B}$, a $\mathscr{B}$-valued scalar product $\langle.,.\rangle_{\mathscr{B}}$ has to be found on L, that is, for $\psi,\ \varphi\in L\subset\mathscr{H}$, $\langle\psi,\varphi\rangle_{\mathscr{B}}\in\mathscr{B}$.[22]

(2) Given such an operator-valued scalar product, the tensor product $L\otimes\mathscr{H}_\chi$ is equipped with a sesquilinear form $(.,.)_0$,

$$(\psi\otimes v,\varphi\otimes w)_0:=(\pi_\chi(\langle\varphi,\psi\rangle_{\mathscr{B}})v,w)_\chi. \tag{II.16}$$

Crucially, this form is positive semidefinite if the postivity condition $\pi_\chi(\langle\psi,\psi\rangle_{\mathscr{B}})\geqslant 0$ for all $\psi\in L$ is satisfied, which is the case in all our examples.

(3) The subspace $\mathscr{N}\subset L\otimes\mathscr{H}_{\rm tr}$ of vectors with vanishing $(.,.)_0$-norm is determined and the physical Hilbert space is defined as in (II.15).

The most difficult part of this procedure is to find $\langle.,.\rangle_{\mathscr{B}}$. Here, one is guided by mathematical examples.[11] One may consider, e.g., $\mathscr{B}=C^*(G)$, the C^*-group algebra of a locally compact group G (cf. Ref. 17; this is essentially the convolution algebra on the group w.r.t. the Haar measure). Then, it can be shown that a rigging map $\langle.,.\rangle_{\mathscr{B}}$ is defined as follows: $\langle\psi,\varphi\rangle_{\mathscr{B}}$ has to be some element of $C^*(G)$, i.e., a function on the group, and we prescribe that the value of this function

at $g \in G$ is given by $\langle \psi,\varphi\rangle_{\mathscr{B}}(g)=(U(g)\varphi,\psi)$, where U is a continuous unitary representation of G on $\mathscr{H}$, commuting with $\pi(\mathscr{A}_c)$, $x \in G$. Inducing from the trivial representation $\mathscr{H}_{\rm tr}=\mathbb{C}$, the general formalism leads to the prescription

$$(\psi,\varphi)_0=\int_G dx(U(x)\psi,\varphi). \tag{II.17}$$

(Here and in what follows, we use the shorthand $(\psi,\varphi)_0$ for $(\psi\otimes v,\varphi\otimes\omega)_0$, since $v,w \in \mathbb{C}$ are complex numbers which can be absorbed in the definition of ψ and φ.) At least in a heuristic sense, (II.14) is a special case of this.

So far, our presentation of the Rieffel induction procedure for quantum field theories has been slightly oversimplified with respect to one point: While the existence of a so-called ''rigged'' inner product $(.,.)_0$, defined in (II.16), is always sufficient for the quantization proposal to apply, it is not always possible to derive it from a mathematically well-defined rigging map $\langle .,.\rangle_{\mathscr{B}}$. We refer to Ref. 13 for a discussion of the technical points involved. In such cases, one cannot derive (II.17), but it still provides a well-defined starting point motivated by the general theory explained above.

In fact, in what follows, we shall base our arguments on a suitable generalization of (II.17).

To sum up: In this chapter, we have seen that Rieffel induction provides a well-defined scheme for the construction of a physical Hilbert space $\mathscr{H}_{\rm phys}$, on which gauge transformations act trivially. In the corresponding algebra of observables $\pi_{\rm phys}(\mathscr{A}_c)$, all gauge degeneracies are removed, i.e., Rieffel induction is a method to impose constraints on quantum field theories. The physical Hilbert space $\mathscr{H}_{\rm phys}$ is obtained by forming the quotient of a larger Hilbert space $L\otimes.\mathscr{H}_{\rm tr}$ with respect to a null space.

This is somewhat reminiscent of the BRST (or, in case of QED, the Gupta–Bleuler) procedure, with the major difference that with Rieffel induction no negative-norm subspace exists, obviating the need to select a physical subspace of $\mathscr{H}$. Also, certain functional-analytic problems that appear in the BRST as well as in the Dirac method are absent with our present techniques.[11,13] By definition of the inner product on the physical Hilbert space $\mathscr{H}_{\rm phys}$ calculations of correlation functions of operators in $\mathscr{A}_c$ (as represented on $\mathscr{H}_{\rm phys}$) may be performed in $L\otimes.\mathscr{H}_{\rm tr}$.[14]

Clearly, an alternative method is to construct the reduced (physical) Hilbert space using spectral analysis of the algebra of constraints. In this case, however, one has to guess the inner product on the ''improper'' subspace of the Hilbert space of the unconstrained system on which the constraints are zero. Also, the connection with the classical treatment of constraints is obscured somehow. This may be regarded as a drawback compared to the method advocated here.

III. APPLICATION TO THE STÜCKELBERG–KIBBLE MODEL

In this chapter, we specify (II.13) and (II.14) for the Stückelberg–Kibble model, thereby constructing a physical Hilbert space $\mathscr{H}_{\rm phys}$ for this model. The Stückelberg–Kibble model is an Abelian Higgs model with the modulus η of the scalar field $\phi(x)=\eta(x)e^{i\varphi(x)}$ frozen to unity, $\eta(x)=1$. It is given by the Lagrangian

$$\mathscr{L}=-\tfrac{1}{4}F_{\mu\nu}F^{\mu\nu}-\tfrac{1}{2}(\partial_\mu\varphi+eA_\mu)(\partial^\mu\varphi+eA^\mu). \tag{III.1}$$

Despite its linearity, this model has nontrivial features, and has been used as testing ground for investigations of the Higgs mechanism before.[15] Its equations of motion can be written in terms of a gauge-invariant current $j^\mu=\partial^\mu\varphi+eA^\mu$, satisfying

$$(\Box+e^2)j^\mu=0; \quad \partial_\mu j^\mu=0. \tag{III.2}$$

In fact, this is nothing but the Proca equation[23] of a massive gauge-invariant vector field. To make this model amenable to treatment by symplectic reduction and quantum induction methods, we

now make a move that is analogous to rewriting the Maxwell equation for A_μ as a massless Klein–Gordon equation plus a subsidiary Lorentz condition. Thus we pass back to the gauge-dependent fields A_μ and φ, and choose what is essentially the 't Hooft gauge as the subsidiary condition:

$$\partial_\mu A^\mu = e\varphi. \tag{III.3}$$

With this constraint, the equations of motion read

$$(\Box + e^2)A^\mu = 0, \quad (\Box + e^2)\varphi = 0, \tag{III.4}$$

and the gauge group $G = \{g | (\Box + e^2)g = 0\}$ acts on A_μ, φ via

$$A_\mu \to A_\mu + \partial_\mu g, \quad \varphi \to \varphi - eg. \tag{III.5}$$

A. Marsden–Weinstein reduction for the Stückelberg–Kibble model

A mathematically rigorous treatment of the following material, in the style of Ref. 13, is possible, but we leave the details to the interested reader; instead, readability commands us to give somewhat loose formulations.

Our investigation of the Stückelberg–Kibble model starts from the symplectic space (M_{sk}, B_{sk}), defined by

$$\begin{gathered} M_{sk} = \{(A_\mu, \varphi) | A_\mu \in L^2(\mathbb{R}^3) \otimes \mathbb{C}^4, \varphi \in L^2(\mathbb{R}^3); (\Box + e^2)A_\mu = (\Box + e^2)\varphi = 0\}, \\ B_{sk}(A_\mu, \varphi; A'_\mu, \varphi') = 2\,\mathrm{Im}(A_\mu, A'_\mu)_M - 2\,\mathrm{Im}(\varphi, \varphi'). \end{gathered} \tag{III.6}$$

The gauge group G acts on this space by the gauge transformation (III.5). This action is strongly Hamiltonian, and hence, in particular, it is symplectic. We evidently may identify the gauge group with the following subspace of M_{sk}:

$$T_{sk} = \{(A_\mu, \varphi) \in M_{sk} | A_\mu = \partial_\mu g, \varphi = -eg; g \in L^2(\mathbb{R}^3); (\Box + e^2)g = 0\}. \tag{III.7}$$

From this, the Marsden–Weinstein reduced space $(M_{c,sk}, B_{c,sk})$ is easily calculated. With similar notation as in Sec. (II. A), the moment map reads

$$J_g(A_\mu, \varphi) = 2\,\mathrm{Im}(\partial_\mu g, A_\mu)_M - 2\,\mathrm{Im}(-eg, \varphi), \tag{III.8}$$

which leads to

$$J^{-1}(0) = \{(A_\mu, \varphi) \in M_{sk} | \partial_\mu A^\mu = e\varphi\}. \tag{III.9}$$

Hence in view of (III.3) the Marsden–Weinstein quotient reads

$$M_{c,sk} = J^{-1}(0)/G = \{j_\mu \in L^2(\mathbb{R}^3) \otimes \mathbb{C}^4 | (\Box + e^2)j_\mu = 0; \partial_\mu j^\mu = 0\}. \tag{III.10}$$

The symplectic form $B_{c,sk}$ on $M_{c,sk}$ inherits its structure from B_{sk}, and is given by

$$B_{c,sk}(j, j') = \frac{2}{e^2}\,\mathrm{Im}(j_\mu, j'_\mu)_M. \tag{III.11}$$

Clearly, $(M_{c,sk}, B_{c,sk})$ is the phase space of a massive vector boson, which indeed represents the physical degrees of freedom of the Stückelberg–Kibble model. This completely specifies the left-hand side of the diagram (II.5).

B. Rieffel induction for the Stückelberg–Kibble model

1. Construction of the field algebra

Consider the canonical commutation relations of the operator fields A_μ and φ (denoted by the same symbol as their classical counterparts):

$$[\varphi(x),\ \varphi(y)]=i\Delta(x-y),$$
$$[A_\mu(x),\ A_\nu(y)]=-ig_{\mu\nu}\Delta(x-y), \tag{III.12}$$

where the commutator function Δ satisfies $(\Box+e^2)\Delta(x)=0$ with initial conditions $\Delta(\mathbf{x},0)=0$, $(\partial/\partial t)\Delta(\mathbf{x},t)|_{t=0}=-\delta^{(3)}(\mathbf{x})$. In analogy with our discussion of free QED, we specify the formal connection between the fields A_μ, φ and the corresponding Weyl operators, $W(\phi_\mu,\phi)=e^{iA_\mu(f^\mu)+i\varphi(f)}$, where $\phi_\mu=\Delta*f_\mu$, $\phi=\Delta*f$. Here, either as a consequence of (III.12) or imposed axiomatically, the operators $W(\phi_\mu,\phi)$, $W(\phi'_\mu,\phi')$ satisfy the Weyl form of the canonical commutation relations

$$W(\phi_\mu,\phi)W(\phi'_\mu,\phi')=W(\phi_\mu+\phi'_\mu,\phi+\phi')e^{-(i/2)B_{sk}(\phi_\mu,\phi;\phi'_\mu,\phi')}. \tag{III.13}$$

The field algebra of the model is then defined as the Weyl algebra $\mathcal{A}(M_{sk},B_{sk})$ generated by the Ws subject to these commutation relations (cf. Ref. 17).

Now, we want to construct the quantum counterpart of Marsden–Weinstein reduction, i.e., we want to complete the right-hand side of the diagram (II.5). Therefore, we invoke the quantization prescription for symplectic spaces as discussed in Sec. II. This leads to the field algebra $\mathcal{A}\equiv\mathcal{A}(M_{sk},B_{sk})$ defined by (III.6). Also, in analogy with our discussion in Sec. II, we choose the algebra of constraints $\mathcal{B}=\mathcal{A}(T_{sk},B_{sk})$; once again, the motivation for this is that it is the (C^*) algebra generated by the gauge group. Consequently, the algebra of weak observables, which by definition is the largest subalgebra of $\mathcal{A}(M_{sk},B_{sk})$ commuting with $\mathcal{B}(T_{sk},B_{sk})$, is given by $\mathcal{A}_c=\mathcal{A}(N_{sk},B_{sk})$, where

$$N_{sk}=\{(\phi_\mu,\phi)\,|\,\partial^\mu\phi_\mu=e\phi\}\subset M_{sk}; \tag{III.14}$$

compare this with (III.9). The subspaces N_{sk} and $T_{sk}\subset N_{sk}$ of M_{sk} are invariant under the action of symplectic transformations $\gamma_{\Lambda,a}$ associated with elements (Λ,a) of the Poincaré group $\mathcal{P}$,$(\gamma_{\Lambda,a}(\phi_\mu,\phi))(x):=(\Lambda^\nu_\mu\phi_\nu,\phi)(\Lambda^{-1}(x-a))$ [cf. (II.12)]. Consequently, the subalgebras, $\mathcal{A}_c$ and $\mathcal{B}$ are Poincaré invariant.

2. Representing the algebra of observables

Rieffel induction starts from the input data of diagram (II.13). So far, we have determined the algebra of weak observables $\mathcal{A}_c=\mathcal{A}(N_{sk},B_{sk})$ and the algebra of constraints $\mathcal{B}=\mathcal{A}(T_{sk},B_{sk})$ of the Stückelberg–Kibble model; note that $\mathcal{B}\subset\mathcal{A}_c$. What is needed is a representation of these algebras on some subspace L of a Hilbert space $\mathcal{H}$. In this subsection, we give such a representation on a bosonic Fock space (cf. the corresponding procedure for QED in Ref. 13).

For simplicity, in a first step we introduce a representation for elements $W(\phi_\mu,\phi=0)\in\mathcal{A}(M_{sk},B_{sk})$ only. This will subsequently be generalized to the whole algebra. We start from the canonical commutation relations for the smeared annihilation and creation operators $\hat{a}_\mu,\hat{a}^*_\mu$

$$\hat{a}(f)=\hat{a}_\mu(f^\mu)=\int\frac{d^3\mathbf{k}}{(2\pi)^3 2k_0}\,[\hat{a}_0(\mathbf{k})\overline{f_0}(\mathbf{k})+\hat{a}_i(\mathbf{k})\overline{f_i}(\mathbf{k})], \tag{III.15}$$

namely

$$[\hat{a}(f),\hat{a}^*(g)]=(g,f)_E:=\int \frac{d^3\mathbf{k}}{(2\pi)^3 2k_0}\, g_\mu(\mathbf{k})\,\delta^{\mu\nu}\overline{f_\nu}(\mathbf{k}). \tag{III.16}$$

For reasons to become clear soon, we have employed the so-called Fermi trick[19] which consists of defining the creation and annihilation operators of a vector field such that their commutator is a Euclidean scalar product. Introducing a vacuum state $|0\rangle$ with the property $\hat{a}(f)|0\rangle=0$ for all f, the creation and annihilation operators generate a bosonic Fock space $\mathscr{H}_1$ in the usual way. Mathematically $\mathscr{H}_1$ is, of course, the symmetric Hilbert space[24] over $L^2(\mathbb{R}^3)\otimes\mathbb{C}^4$.

We can now represent the field algebra $\mathscr{A}$, and thence its subalgebras $\mathscr{A}_c$ and $\mathscr{B}$, on $\mathscr{H}_1$ as follows:

$$\pi(W(\phi^\mu,\phi=0))=e^{[\hat{a}_\mu(\tilde{\phi}_\mu)-\hat{a}_\mu(\tilde{\phi}_\mu)^*]}, \tag{III.17}$$

where $\tilde{\phi}_\mu=(-\overline{\phi_0},\ \phi_i)$, and the symbol π for a representation has been introduced. The essential point is that the Euclidean commutation relations (III.16) are able to represent the Minkowski commutators (III.12) because of the special definition of $\tilde{\phi}_\mu$.

Now, we present a very economical notation for symmetric n-particle states by introducing ''exponential vectors.'' [24] To this aim, we represent the algebra $\mathscr{A}_c$ on the dense subset L_1 of $\mathscr{H}_1$, which is the span of all exponential vectors

$$L_1=\left\{\sum_{i=1}^{N}\lambda_i e^{\psi^{(i)}}\,\middle|\,\lambda_i\in\mathbb{C},\psi^{(i)}\in L^2(\mathbb{R}^3)\otimes\mathbb{C}^4,N<\infty\right\};$$
$$e^{\psi}:=1\oplus\psi\oplus\frac{1}{\sqrt{2}}\,\psi\otimes\psi\oplus\frac{1}{\sqrt{3!}}\,\psi\otimes\psi\otimes\psi\oplus\cdots, \tag{III.18}$$

where the tensor products are understood to be symmetrized. Note that the prefactors $1/\sqrt{n!}$ of the n-particle contributions to e^{ψ} have been chosen differently from those of a Taylor expansion of e^x. This allows for a simple form of the scalar product on L_1,

$$(e^{\psi},e^{\varphi})=e^{(\psi,\varphi)_E}. \tag{III.19}$$

A useful remark is now that symmetric n-particle states can be obtained from suitably normalized derivatives of exponential vectors,

$$\psi_1\otimes_s\cdots\otimes_s\psi_n=\frac{1}{\sqrt{n!}}\,\frac{d}{dr_1}\cdots\frac{d}{dr_n}\,e^{\Sigma_i r_i\psi_i}\bigg|_{r_i=0}. \tag{III.20}$$

The representation of $W(\phi_\mu,0)$ takes a very simple form on L_1. From (III.18) we have $e^{\hat{a}_\mu(\phi^\mu)}e^{\psi}=e^{(\psi,\phi)E}e^{\psi}$, $e^{\hat{a}_\mu(\phi^\mu)^*}e^{\psi}=e^{(\psi+\phi)}$ and hence[25]

$$\pi(W(\phi_\mu,0))e^{\psi}=e^{(-1/2)(\phi,\phi)_E+(\psi,\tilde{\phi})_E}e^{(\psi-\tilde{\phi})}. \tag{III.21}$$

The construction given above is easily generalized to the whole algebra $\mathscr{A}(M_{sk},B_{sk})$ acting on the dense subspace $L=L_1\otimes L_2$ of $\mathscr{H}=\mathscr{H}_1\otimes\mathscr{H}_2$, where $\mathscr{H}_2$ is the bosonic Fock space over $L^2(\mathbb{R}^3)$. With

$$L_2=\left\{\sum_{i}^{N}\lambda_i e^{\psi^{(i)}}\,\middle|\,\psi^{(i)}\in L^2(\mathbb{R}^3);\lambda_i\in\mathbb{C},N<\infty\right\}, \tag{III.22}$$

the scalar product of vectors in L reads

$$(e^{\psi_\mu}\otimes e^{\psi}, e^{\chi_\mu}\otimes e^{\chi}) = e^{(\psi_\mu,\chi_\mu)_E+(\psi,\chi)}, \tag{III.23}$$

and the action of $\mathscr{A}(M_{sk},B_{sk})$ (denoted by π as well, with slight abuse of notation) is

$$\pi(W(\phi_\mu,\phi))e^{\psi_\mu}\otimes e^{\psi} = e^{(-1/2)(\phi_\mu,\phi_\mu)_E+(\psi_\mu,\tilde{\phi}_\mu)_E}e^{(-1/2)(\phi,\phi)+(\psi,\phi)}e^{\psi_\mu-\tilde{\phi}_\mu}\otimes e^{\psi-\phi}. \tag{III.24}$$

It should be pointed out that L (which is the natural domain of the rigged inner product[13]) is only stable under finite linear combinations of the Ws (which span a dense subalgebra of $\mathscr{A}$), and not under all elements of $\mathscr{A}$, i.e., strictly speaking, the induction process is performed relative to the corresponding dense subalgebras of $\mathscr{A}_c$ and $\mathscr{B}$. Despite the use of bounded operators, the choice of L as a dense subspace of the Hilbert space of the unconstrained system is essential whenever the constraints have continuous spectrum. This is because in that case the rigged inner product is not defined on the whole Hilbert space. In its abstract formulation, Rieffel induction is even formulated in terms of L alone, without a Hilbert space it is embedded in.[12]

3. Constructing the physical one-particle Hilbert space

With (III.24), we have specified the bimodule L for $\mathscr{A}_c$ and $\mathscr{B}$, which in this case is a subspace of an ''unphysical'' Hilbert space $\mathscr{H}$. Our next step is to construct the corresponding physical Hilbert space, i.e., to carry out the discussion following (II.13). In this and the next subsection, we determine the null space $\mathscr{N}_{sk}$ for the Stückelberg–Kibble model, thereby eventually obtaining $\mathscr{H}_{\text{phys}}$.

We start from the inner product on elementary vectors in L

$$(e^{\psi_\mu}\otimes e^{\psi}, e^{\chi_\mu}\otimes e^{\chi})_0 = \int_{T_{sk}} [\mathscr{D}g](\pi(W(\partial_\mu g,-eg))e^{\psi_\mu}\otimes e^{\psi}, e^{\chi_\mu}\otimes e^{\chi}), \tag{III.25}$$

which is a natural generalization of (II.14) (and can, at least heuristically, be derived from an appropriate rigging map defined by a unitary representation of the gauge group on $\mathscr{H}$). As in Ref. 13, the heuristic path integral (III.25) can be turned into a well-defined integral wrt a certain cylindrical measure on $T_{sk}=G$, but here we shall proceed with the formal flat measure $\mathscr{D}g$, and certify that all manipulations below can be rigorously justified.

Using the representation (III.24) of $\mathscr{A}(N_{sk},B_{sk})$, we obtain, with $k_0=\sqrt{e^2+\mathbf{k}^2}$, and $d\tilde{k}=d\mathbf{k}^3/(2\pi)^3 2k_0$,

$$\begin{aligned}(e^{\psi_\mu}\otimes e^{\psi}, e^{\chi_\mu}\otimes e^{\chi})_0 = {} & e^{\int \tilde{d}k(-1/k_0^2)[(k_i\psi_i-ie\psi)k_0\psi_0+(k_i\overline{\chi_i}+ie\overline{\chi})k_0\overline{\chi_0}]} \\ & \times e^{\int \tilde{d}k\psi_i(\delta_{ij}-(k_ik_j/\mathbf{k}^2))\overline{\chi_j}+((e/k_0)\psi_i+i(k_i/k_0)\psi)(k_ik_j/\mathbf{k}^2)\overline{((e/k_0)\chi_j+i(k_j/k_0)\chi)}},\end{aligned} \tag{III.26}$$

where we have used $(\delta_{ij}-k_ik_j/k_0^2)=(\delta_{ij}-k_ik_j/\mathbf{k}^2)+e^2k_ik_j/k_0^2\mathbf{k}^2$ to write (III.26) in terms of projection operators.

To investigate the structure of the null space $\mathscr{N}_{sk}$, we derive the $(.,.)_0$ inner product for n-particle vectors in $\mathscr{H}$ from (III.26). For one-particle vectors in the (unphysical) space $\mathscr{H}$, we have

$$\left.\frac{d}{dr}\, e^{r\psi_\mu}\otimes e^{r\psi}\right|_{r=0} = \psi_\mu\otimes\Omega' + \Omega''\otimes\psi, \tag{III.27}$$

where $\Omega=\Omega''\otimes\Omega'$ denotes the vacuum state in $\mathscr{H}$. Since such expressions become cumbersome for higher derivatives, for notational convenience we define

$$\psi_*^{(1)}\times\cdots\times\psi_*^{(n)}:=\frac{1}{\sqrt{n!}}\frac{d}{dr_1}\cdots\frac{d}{dr_n}\,e^{\Sigma_i r_i\psi_\mu^{(i)}}\otimes e^{\Sigma_j r_j\psi^{(j)}}\Big|_{r_i=0}. \tag{III.28}$$

Then, the $(.,.)_0$ inner product on one-particle vectors in $\mathscr{H}$ reads

$$(\psi_*,\chi_*)_0=\int\tilde{d}k\,\psi_i\left(\delta_{ij}-\frac{k_ik_j}{\mathbf{k}^2}\right)\overline{\chi_j}+\left(\frac{e}{k_0}\,\psi_i+i\,\frac{k_i}{k_0}\,\psi\right)\frac{k_ik_j}{\mathbf{k}^2}\overline{\left(\frac{e}{k_0}\,\chi_j-i\,\frac{k_j}{k_0}\,\chi\right)}. \tag{III.29}$$

Clearly, the two transversal components $P_T\psi_*:=(\delta_{ij}-k_ik_j/\mathbf{k}^2)\psi_j$ and a linear combination $P_L\psi_*$ of the longitudinal component $(k_ik_j/\mathbf{k}^2)\psi_j(\mathbf{k})$ with the scalar component $\psi(\mathbf{k})$ survive, while the remaining two components lie in $\mathscr{N}_{sk}$. To be more precise, we introduce for ψ_* the *Bogoliubov-transformed components* ψ_L,ψ_N,

$$\begin{aligned}\psi_{L,i}(\mathbf{k}):&=\cos\,\theta\,\frac{k_ik_j\psi_j(\mathbf{k})}{\mathbf{k}^2}+i\,\sin\,\theta\,\frac{k_i\psi(\mathbf{k})}{|\mathbf{k}|},\\ \psi_{N,i}(\mathbf{k}):&=-\sin\,\theta\,\frac{k_ik_j\psi_j(\mathbf{k})}{\mathbf{k}^2}+i\,\cos\,\theta\,\frac{k_i\psi(\mathbf{k})}{|\mathbf{k}|},\end{aligned} \tag{III.30}$$

where $\cos\theta=e/k_0$, $\sin\theta=|\mathbf{k}|/\mathrm{k}_0$. With ψ_L, ψ_T, and ψ_N, the five-component vector $\psi_*^{(i)}$ can be specified as

$$\psi_*(\mathbf{k}):=(P_T\psi_\mu(\mathbf{k}),\psi_L(\mathbf{k}),\psi_N(\mathbf{k}),\psi_0(\mathbf{k})), \tag{III.31}$$

and the projection operator P_p onto the ''physical'' one-particle components is given by

$$(P_p\psi_*)(\mathbf{k})=(P_T\psi_\mu(\mathbf{k}),\psi_L(\mathbf{k}),0,0). \tag{III.32}$$

This is exactly what one expects: the five 'unphysical' degrees of freedom have combined into three physical ones in such a way that the longitudinal component in $\mathscr{H}$ has mixed with the scalar component.

4. The physical Hilbert space $\mathscr{H}_{phys}$

To extend (III.32) to n-particle states, we rewrite (III.26), using

$$\begin{aligned}\exp\left(\sum_i\,r_i\psi_*^{(i)}\right):&=\exp\left(\sum_i\,r_i\psi_\mu^{(i)}\right)\otimes\exp\left(\sum_i\,r_i\psi^{(i)}\right),\\ (e^{\psi_*},e^{\chi_*})_0&=(e^{\psi_*},\Omega)_0(\Omega,e^{\chi_*})_0(e^{P_p\psi_*},e^{P_p\chi_*}).\end{aligned} \tag{III.33}$$

Here we have used the remark following (III.29), which implies that

$$(\exp(P_p\psi_*),\exp(P_p\chi_*))_0=(\exp(P_p\psi_*),\exp(P_p\chi_*)).$$

From (III.33) we obtain

$$\psi_*^{(1)}\times\cdots\times\psi_*^{(n)}=\frac{d}{dr_1}\cdots\frac{d}{dr_n}\,(e^{\Sigma_i r_i\psi_*^{(i)}},\Omega)_0 e^{\Sigma_i r_i\psi_*^{(i)}}\Big|_{r_i=0}$$

$$=\sum_{q=0}^{n}\sum_{(p_i)_1^q\in\mathscr{P}_{q,n}}\lambda_{(p_i)_1^q}(P_p\psi_*^{(p_1)})\times\cdots\times(P_p\psi_*^{(p_p)})+\mathbf{n},\tag{III.34}$$

where $\mathscr{P}_{q,n}$ contains all sets of q indices $\{(p_i)_1^q\}$ out of $\{1,...,n\}$, such that $\{(p_i)_1^q\}\cup\{(\hat{p}_i)_1^{n-q}\}=\{1,\ldots,n\}$. Here,

$$\lambda_{(p_i)_1^q}=\sqrt{\frac{(q)!(n-q)!}{n!}}\,(\psi_*^{(\hat{p}_1)}\times\cdots\times\psi_*^{(\hat{p}_{n-q})}|_{p_q(I_{n,q})},\Omega)_0\tag{III.35}$$

are c-number coefficients and $\mathbf{n}$ denotes an element in $\mathscr{N}_{sk}$.

Vectors of the type (III.32) generate a Hilbert space of physical one-particle states. The bosonic Fock space over this one-particle space is evidently $\mathscr{F}_{\rm phys}:=S(L^2(\mathbb{R}^3)\otimes\mathbb{C}^3)$, the symmetric Hilbert space over $L^2(\mathbb{R}^3)\otimes\mathbb{C}^3$. It should be clear from Eq. (III.34) that the induced space $\mathscr{H}_{\rm phys}$ from the Rieffel induction procedure is naturally isomorphic to this physical Fock space.[26] To prove this, we define a map $V:L\to\mathscr{F}_{\rm phys}$ by linear extension of $V\exp(\psi_*)=(\exp(\psi_*),\Omega)_0\exp(P_p\psi_*)$. It follows from an argument similar to the one in section 3.3 of Ref. 13 that this map is well defined [which is a nontrivial property, as the basis $\{\exp(\psi_*)\}$ is overcomplete]. Equation (III.33), and the fact that the inner product in $\mathscr{F}_{\rm phys}$ is just the one in $\mathscr{H}$, restricted to the physical states, then implies the crucial property

$$(V\Psi,V\Phi)=(\Psi,\Phi)_0,\tag{III.36}$$

for all $\Psi,\Phi\in L$, where the inner product on the lhs is evidently the one in $\mathscr{F}_{\rm phys}$. Hence the null space $\mathscr{N}_{sk}$ of $(.,.)_0$ is precisely the kernel of V, and the quotient map $\tilde{V}:L/\mathscr{N}_{sk}\to\mathscr{F}_{\rm phys}$ can be extended to a unitary map (denoted by the same symbol) $\tilde{V}:\mathscr{H}_{\rm phys}\to\mathscr{F}_{\rm phys}$.

5. n-point correlation functions and gauge invariance

Having specified the physical Hilbert space $\mathscr{H}_{\rm phys}$, the next step is to determine the action of $\pi_{\rm phys}(\mathscr{A}_c)$. To this end, we consider the generating functional $\omega_{\rm vac}$ for vacuum expectation values,

$$\omega_{\rm vac}(\phi^\mu,\phi):=(\pi(W(\phi_\mu,\phi))\Omega,\Omega)_0=e^{(1/2)(\phi_\mu\phi_\mu)_M}e^{-(1/2)(\phi,\phi)}e^{-(1/k_0^2)(k_0\overline{\phi_0}(k_\mu\phi_\mu+ie\phi))},\tag{III.37}$$

where $\Omega\in\mathscr{H}$ is the (unphysical) ''vacuum'' state. By construction, only $\mathscr{A}_c=\mathscr{A}(N_{sk},B_{sk})$ acts on $\mathscr{H}$ [cf. (III.14)], and for $(\phi_\mu,\phi)\in N_{sk}$, $k_0\phi_0=k_i\phi_i-ie\phi$, we obtain

$$\omega_{\rm vac}(\phi^\mu,\phi)=e^{-(1/2)(\phi_\mu,P_T\phi_\mu)_E}e^{-(1/2)((e/k_0)\phi_i+i(k_i/k_0)\phi)(k_ik_j/\mathbf{k}^2)((e/k_0)\overline{\phi_j}-i(k_j/k_0)\overline{\phi})}$$

$$=:(\pi_{\rm phys}(\tilde{W}(P_p\phi_*))\Omega_{\rm phys},\Omega_{\rm phys})_{\rm phys}$$

$$=e^{-(1/2)\int d\tilde{k}[\overline{P_T\phi(\mathbf{k})}P_T\phi(\mathbf{k})+\overline{\phi}_{L,i}(\mathbf{k})\phi_{L,i}(\mathbf{k})]}.\tag{III.38}$$

Here, $\Omega_{\rm phys}\in\mathscr{H}_{\rm phys}$ is the physical vacuum state; it is just the projection of $\Omega\in L$ onto $L/\mathscr{N}_{sk}\subset\mathscr{H}_{\rm phys}$.

We observe that for $(\phi_\mu,\phi)\in T_{sk}$, $\pi(\mathrm{W}(\phi_\mu,\phi))$ equals the unit operator [cf. (III.7)]. This implies that the gauge group is represented trivially on $\mathscr{H}_{\rm phys}$. Moreover, one infers that $\mathscr{A}_{\rm obs}:=\pi(\mathscr{A}_c)\simeq\mathscr{A}(N_{sk}/T_{sk},B_{c,sk})$, since the image of a representation of a C^*-algebra is isomorphic to the algebra quotiented by the kernel of the representation. Now $N_{sk}/T_{sk}\simeq P_pN_{sk}$ as vector spaces (but not as carrier spaces of actions of the Poincaré group!), so that, equally well,

$\mathscr{A}_{\rm obs}\simeq\mathscr{A}(P_pN_{sk},B_{sk})$.[27] Then, it is clear from Sec. III A that $\mathscr{A}_{\rm obs}$ is precisely the Weyl algebra over the Marsden–Weinstein reduced space (i.e., the physical phase space) of the Stückelberg–Kibble model. Hence it describes three gauge-invariant, massive field components.

Thus $\widetilde{W}(P_p\phi_*)$ can be viewed as a Weyl operator in $\mathscr{A}(P_pN_{sk},B_{sk})$. In particular, the representation of $\mathscr{A}(P_pN_{sk},B_{sk})$ on exponential vectors $e^{\psi}\in\mathscr{H}_{\rm phys}=S(L^2(\mathbb{R}^3)\otimes\mathbb{C}^3)$ is given by

$$\pi_{\rm phys}(\widetilde{W}(P_p\phi_*))e^{\psi}=e^{-(1/2)(P_p\phi_*,P_p\phi_*)_p+(\psi_iP_p\phi_*)_p}e^{(\psi-P_p\phi_*)},$$
$$(\psi,P_p\phi_*)_p=\int d\tilde{k}[\overline{P_T\phi(\mathbf{k})}P_T\phi(\mathbf{k})+\overline{\phi}_{L,i}(\mathbf{k})\phi_{L,i}(\mathbf{k})]. \tag{III.39}$$

From $\omega_{\rm vac}(\phi_\mu,\phi)$, n-point correlation functions can be obtained as multiple derivatives of $\widetilde{W}(P_p\phi_*):=e^{i\widetilde{A}(f)}$, where $P_p\phi_*=\Delta*f\in\mathbb{L}^2(\mathbb{R}^3)\otimes\mathbb{C}^3$,

$$\begin{aligned}
&i^n(\pi_{\rm phys}(\widetilde{A}(f_1)\cdots\widetilde{A}(f_n))\Omega_{\rm phys},\Omega_{\rm phys})_{\rm phys}\\
&\quad=\frac{d}{dr_1}\cdots\frac{d}{dr_n}\,\omega_{\rm vac}\Big(\sum_i r_i\phi_\mu^{(i)},\sum_i r_i\phi^{(i)}\Big)\Big|_{r_i=0}\\
&\quad=\sum_{(p_i,q_i)_i^{n/2}\in\mathscr{S}_n}\prod_{i=1}^{n/2}(\pi_{\rm phys}(\widetilde{A}(f_{p_i})\widetilde{A}(f_{q_i}))\Omega_{\rm phys},\Omega_{\rm phys})_{\rm phys}\\
&\qquad\times(-1)^{n/2}
\end{aligned} \tag{III.40}$$

for n even, and zero otherwise. Here, $\mathscr{S}_n$ denotes the set of all symmetric partitions of $\{1,...,n\}$ into a set of unordered pairs (p_i,q_i). We conclude from (III.40) that the n-point correlation functions can be decomposed into products of two-point correlation functions, i.e., Wick's theorem is satisfied. The reader should note, however, that this form of Wick's theorem is satisfied for elements in $\mathscr{A}(N_{sk},B_{sk})$ only. The crucial point is that, in general, the $(.,.)_0$ inner product preserves the adjoint for test functions in N_{sk} only. This can be seen by comparing, e.g., $(d/dr_1)(d/dr_2)(\pi(W(\Sigma_i r_i\phi_\mu^{(i)},\Sigma_i r_i\phi^{(i)}))\Omega,\Omega)_0|_{r_i=0}$ with $(d/dr_1)(d/dr_2)(\pi(W(\phi_\mu^{(1)},\phi^{(1)}))\Omega,\pi(W(\phi_\mu^{(2)},\phi^{(2)}))\Omega)_0|_{r_i=0}$ [cf. III.37)].

There is an interesting parallel between this restriction of the Rieffel induced expectation values to $\mathscr{A}(N_{sk},B_{sk})$ and the general setup of the Gupta–Bleuler indefinite metric formalism as presented in Ref. 28. In the latter, one starts from an unphysical Hilbert space $\mathscr{H}_{\rm GB}$ from which the physical one is obtained as a quotient $\mathscr{H}'/\mathscr{H}''$. Without reviewing this construction, we note that $\mathscr{H}$ has to be restricted to a suitable subspace $\mathscr{H}'\subset\mathscr{H}_{\rm GB}$ before quotienting by a null space $\mathscr{H}'$. Obviously, in our setting, a similar restriction is needed on the level of the algebra, $\mathscr{A}(N_{sk},B_{sk})\subset\mathscr{A}(M_{sk},B_{sk})$. This restriction emerges in a systematic way, for as we pointed out before, the subalgebra in question is the commutant of the algebra generated by the constraints (i.e., by the gauge group).

This observation is closely related to the result of Narnhofer and Thirring[29] that covariant formulations without indefinite inner metric are possible as long as the representation on the physical Hilbert space is restricted to a certain subalgebra of weak observables. In the example of Narnhofer and Thirring, nonregular states have to be introduced. This can be avoided in the Rieffel induction setting [cf. Refs. 13 and 14 for further details].

6. Positivity of the Hamiltonian and action of the Poincaré group

On the algebra of weak observables of the Stückelberg–Kibble model $\mathscr{A}(N_{sk},B_{sk})$, the time evolution is given as an automorphism group τ,

$$\tau_t[W(\phi_\mu,\phi)]=W(e^{it\sqrt{D+e^2}}\phi_\mu,e^{it\sqrt{D+e^2}}\phi), \tag{III.41}$$

where $(D\phi)_\mu=(-\Delta\phi_0,-\Delta\phi_1,-\Delta\phi_2,-\Delta\phi_3)$. We want to construct the Hamiltonian H, corresponding to τ_t on $\mathscr{H}$. H is a representation-dependent operator, implementing the time evolution τ_t in the representation π by

$$e^{itH}\pi(W(\phi_\mu,\phi))e^{-itH}=\pi(\tau_t[W(\phi_\mu,\phi)]). \tag{III.42}$$

Comparing this with the explicit form of the representation in terms of annihilation and creation operators $\hat{a}^*_\mu,\hat{a}_\mu$ for the vector field and $\hat{b}^*,\hat{b}$ for the scalar field, we obtain

$$H=-\int d\tilde{k}\sqrt{\mathbf{k}^2+e^2}\hat{a}^*_\mu(\mathbf{k})g^{\mu\nu}\hat{a}_\nu(\mathbf{k})+\int d\tilde{k}\sqrt{\mathbf{k}^2+e^2}\hat{b}^*(\mathbf{k})\hat{b}(\mathbf{k}). \tag{III.43}$$

Regarded as an operator on $\mathscr{H}$ (with its Hilbert space inner product), this Hamiltonian clearly has the entire real axis as its spectrum. However, it is easy to see that

$$(\Psi,H\Psi)_0\geqslant 0 \tag{III.44}$$

for all $\Psi\in\mathscr{H}$. The point is that arbitrary (normalized) components of the physical one-particle state space, $(\delta_{ij}-k_ik_j/\mathbf{k}^2)\psi_j$ and $(k_i/\mathbf{k})\psi_i\cos\theta+i\psi\sin\theta$ pick up (the same) positive energy contributions. For multi-particle states, this holds true due to their decomposition into such components. The elements of $\mathscr{H}$ carrying the negative energy spectrum have ended up in the null space. Hence the induced Hamiltonian H_{phys} on $\mathscr{H}_{\text{phys}}$ is positive.

Finally, we note that $\mathscr{H}_{\text{phys}}$ carries a massive representation of the Poincaré group $\mathscr{P}$. Indeed, ω_{vac} is Poincaré invariant on N_{sk} and hence[16,17] there exists a Poincaré invariant vacuum state $\Omega_{\text{phys}}\in\mathscr{H}_{\text{phys}}$ and a representation U_p of the Poincaré group such that

$$U_p(\Lambda,a)\pi_{\text{phys}}(W(\phi_\mu,\phi))\Omega_{\text{phys}}=\pi_{\text{phys}}(W(\gamma_{\Lambda,a}(\phi_\mu,\phi)))\Omega_{\text{phys}} \tag{III.45}$$

for all $(\phi_\mu,\phi)\in N_{sk}$. It is easily shown that H_{phys} is the generator of the time-translation part of the representation thus defined. Since the spectrum of the Hamiltonian H_{phys} shows a mass gap, we are dealing with a massive representation ($m^2=e^2$) of the Poincaré group, i.e., the three components of the vector $P_p\psi^{(i)}_*$ transform as a massive one-particle state under the action of the little group SO(3).[20]

We conclude that $\mathscr{H}_{\text{phys}}$ has the main properties required by a physical Hilbert space; it transforms trivially under the gauge group, satisfies the positive spectrum condition, and carries a unitary representation of the Poincaré group.

IV. CONCLUSION

The quantization proposal employed in this paper provides a detailed scheme for imposing constraints on gauge quantum field theories. As explained in Sec. II, the main tool of this proposal is the Rieffel induction procedure, which provides a systematic scheme for the construction of representations of C^*-algebras. It may be viewed as the quantum counterpart of the symplectic reduction technique; as we have shown, this is particularly obvious for Weyl C^*-algebras. This leads to a new quantization method for gauge field theories.

In the present work, we have applied this method to the Stückelberg–Kibble model. To this end, we have defined a field algebra $\mathscr{A}$ corresponding to the field content of the Lagrangian, and an algebra of constraints $\mathscr{B}$ corresponding to the gauge group acting on $\mathscr{A}$. Also, we have specified a representation π of subalgebras of $\mathscr{A}$ on a (unphysical) Hilbert space $\mathscr{H}$. From these input data, we have constructed a representation of the physical, gauge-invariant fields on a new Hilbert space $\mathscr{H}_{\text{phys}}$.

The construction of $\mathscr{H}_{\text{phys}}$ shows some parallels to the Gupta–Bleuler indefinite metric formalism. In both settings, a degenerate inner product is defined on a (unphysical) Hilbert space $\mathscr{H}$, and $\mathscr{H}_{\text{phys}}$ is constructed by quotienting $\mathscr{H}$ by a null space with respect to this degenerate inner product. Yet, there are important differences. In contrast to the indefinite metric inner product $\langle .,. \rangle$, defined on $\mathscr{H}_{\text{GB}}$ in the Gupta–Bleuler formalism, the $(.,.)_0$ inner product is positive semidefinite. More importantly, it is a conceptual advantage of our quantization method that $(.,.)_0$ is derived from first principles (namely from the requirement to impose quantum constraints by a quantized version of the classical phase space reduction method), whereas the Gupta–Bleuler formalism takes $\langle .,. \rangle$ as starting point without further justification. A similar comment applies to the BRST technique: although a classical analogue of this procedure exists, the quantum BRST procedure is *not* in any satisfactory sense the quantization of the classical scheme.

Another remarkable difference between both formalisms is that the Gupta–Bleuler formalism restricts the unphysical Hilbert space before forming the quotient whereas the proposal of Ref. 11 restricts itself to a representation of the subalgebra $\mathscr{A}_c$ of weak observables on $\mathscr{H}$, before quotienting by the appropriate null space. As a consequence, the $(.,.)_0$ inner product preserves the adjoint for elements in $\mathscr{A}_c$ only. It remains to be seen how far this feature alters applications of usual perturbative techniques in more complicated models.

The fact that in our approach the spectral condition does not hold in the Hilbert space of the unconstrained system is of little importance, since the original inner product in this space is related to the one in the physical state space only through the rigged inner product. Also, the absence of a unitary implementation of the full Poincaré group does not lead to conceptual or technical complications. In fact, we do not exclude the existence of a Krein space with a suitable dense subspace L, on which our method is manifestly covariant in all its steps.

Most of our effort in Sec. III has gone into characterizing the particular features of the physical state space $\mathscr{H}_{\text{phys}}$. By construction, $\mathscr{H}_{\text{phys}}$ carries a trivial representation of the gauge group. Also, the states are physical in the sense that they obey a positive spectrum condition and that they carry a massive representation of the Poincaré group. Since the Stückelberg–Kibble model has been widely used in investigations of the Higgs mechanism, we emphasize again the result obtained for the one-particle subspace in $\mathscr{H}_{\text{phys}}$. The point is that in our proposal, the particular construction method of $\mathscr{H}_{\text{phys}}$ allows one to trace back how the (unphysical) components of $\mathscr{H}$ end up in the physical Hilbert space. In the present case, we have shown that the longitudinal physical one-particle component arises from a particular Bogoliubov transformation of the unphysical longitudinal and the scalar component. As expected from general considerations, two of the five components in $\mathscr{H}$ have ended up in the one-particle null space.

We conclude our discussion of the Rieffel induction procedure by pointing out that our presentation has focused on a particular way of applying Rieffel induction to gauge quantum field theories. Conceptually, the scheme is much wider. It remains to be seen how far other choices for the inner product $(.,.)_0$ and the unphysical Hilbert space $\mathscr{H}$ allow for other realizations of the physical observables of gauge field theories.

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[22] Mathematically, $\langle .,. \rangle_{\mathscr{B}}$ is a so-called rigging map which has to satisfy the following conditions for all $\psi,\varphi\in L$ (Ref. 12):

(1) $\langle \lambda\psi,\mu\varphi\rangle_{\mathscr{B}}=\overline{\lambda}\mu\langle\psi,\varphi\rangle_{\mathscr{B}}$ for all $\lambda,\mu\in\mathbb{C}$;
(2) $\langle\psi,\varphi\rangle_{\mathscr{B}}^{*}=\langle\varphi,\psi\rangle_{\mathscr{B}}$ (where the * denotes the Hermitian conjugate in $\mathscr{B}$);
(3) $\langle\psi,\varphi B\rangle_{\mathscr{B}}=\langle\psi,\varphi\rangle_{\mathscr{B}}B$ for all $B\in\mathscr{B}$ (on the left-hand side, B acts in the given right-representation on the bimodule L,
whereas on the right-hand side B acts by multiplication in the algebra $\mathscr{B}$);
(4) $\langle A\psi,\varphi\rangle_{\mathscr{B}}=\langle\psi,A^{*}\varphi\rangle_{\mathscr{B}}$ for all $A\in\mathscr{A}$;
(5) $\langle A\psi,A\psi\rangle\leqslant\|A\|^{2}\langle\psi,\psi\rangle$ for all $\psi\in L,A\in\mathscr{A}$.

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$$\pi(W(\sigma_\mu,0))\pi(W(\varphi_\mu,0))=e^{[i\ \mathrm{Im}[(\overline{\phi_0},\overline{\varphi_0})_E+(\sigma_i,\varphi_i)_E]]}\pi(W(\sigma_\mu+\varphi_\mu,0)),$$

where $\mathrm{Im}[(\overline{\phi_0},\overline{\varphi_0})_E+(\phi_i,\varphi_i)_E]=B_{sk}(\varphi_\mu,0;\phi_\mu,0)$.
[26] Of course, all Hilbert spaces of the same dimension are unitarily equivalent, but to impose such equivalence one generally has to pick a basis. We use the term ''naturally isomorphic'' to indicate that a unitary equivalence exists which does not require the choice of a basis. From the point of view of representation theory, this equivalence intertwines the actions of appropriate operator algebras, cf. the next subsection.
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The global flow of the Manev problem

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The Manev problem (a two-body problem given by a potential of the form $A/r+B/r^2$, where r is the distance between particles and A,B are positive constants) comprises several important physical models, having its roots in research done by Isaac Newton. We provide its analytic solution, then completely describe its global flow using McGehee coordinates and topological methods, and offer the physical interpretation of all solutions. We prove that if the energy constant is negative, the orbits are, generically, precessional ellipses, except for a zero-measure set of initial data, for which they are ellipses. For zero energy, the orbits are precessional parabolas, and for positive energy they are precessional hyperbolas. In all these cases, the set of initial data leading to collisions has positive measure. [S0022-2488(96)00205-7]

I. INTRODUCTION

The question we fully answer in this paper has a long history. We deal with a two-body problem given by a potential of the form $A/r+B/r^2$, where r is the distance between particles and A,B are positive constants. Newton was the first to consider it in his *Principia*. In Book I, Article IX, Proposition XLIV, Theorem XIV, Corollary 2, he claimed that such a force leads to a *precessionally elliptic* relative orbit; this means that, with respect to a fixed frame having one particle at the origin, the other particle moves on an ellipse that rotates in its plane of motion. This was the only result Newton published in connection with this gravitational model, but he tackled it for many years to follow his first edition of *Principia*. The 1888 catalogue of the Portsmouth Collection of unpublished manuscripts that are stored today in the library of Cambridge University shows Newton's interest in this model, interest which was aroused by the difficulties he encoun-

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tered in trying to explain the apsidal motion of the moon within the framework of the inverse-square-force model. After Newton, the $A/r+B/r^2$ potential was tackled by Clairaut, who finally abandoned it in favor of the classical one.

Physicists claim today that this is a well-known problem: in an equivalent formulation it appears as Problem 14 in Chapter 3 of Goldstein's *Classical Mechanics*.[1] Unfortunately Goldstein's statement is incorrect, as we will further see in the qualitative sections of this paper. Goldstein, like Newton, thought that all orbits are precessional ellipses, which is wrong. It is an error that has remained in place for a long time due to the fact that the problem has never been considered from the point of view of the qualitative theory of dynamical systems. We will see that the problem is more complex, and we will fully solve it here. For this we will use a powerful mathematical method: the McGehee transformations—well known in celestial mechanics but little known among mathematical physicists; we would like to emphasize here the importance of the McGehee transformations, because they can be applied to the study of solutions of differential equations near singularities.

Using physical principles, the Bulgarian physicist Manev[2] (or Maneff—in French and German spelling) obtained a similar potential during the third decade of our century. Assigning the mass M to the particle at the origin, the unit mass to the rotating particle and denoting $\mu=GM$, $\beta=A/\mu-1$, $\gamma=2B/\mu$, where G is the constant of gravitation, Manev's potential corresponds to the values $\beta=0$, $\gamma=3\mu/c^2$ of the constants, where c is the speed of light. This model allowed a good theoretical justification of the perihelion advance of Mercury and of the other inner planets as well as an accurate description of the moon's motion.

It is interesting to look at the physical interpretation of Manev's model. The classical point of view is that the orbit of celestial objects around the sun must be an ellipse, a parabola, or a hyperbola (depending on the initial data). However, because of the perturbation of the other objects in the system, the orbit is in fact a precessional ellipse, parabola, hyperbola, or can take a more complicated shape. Unfortunately, this classical point of view encounters difficulties: the theoretical calculations do not fit the observations, and this happens especially for celestial objects coming close to the sun. The perihelion advance of Mercury and of the other inner planets cannot be explained within the the framework of the Newtonian theory.

The study of the solar system can be maintained within the framework of classical mechanics by substituting Newton's model with the one of Manev. This is especially convenient for celestial mechanics. Of help in this sense are the results of the KAM theory. As it has been shown in a paper by Lacomba, Llibre, and Nunes,[3] if the equations of motion describing Manev's problem are slightly perturbed by some external force, which *does not have to be* Hamiltonian, ''most'' invariant cylinders and tori are (topologically) preserved under this perturbation. From the physical point of view this means that the natural (unperturbed) orbit of a celestial object around the sun is not an ellipse, parabola, or hyperbola, but a precessional ellipse, precessional parabola, or precessional hyperbola (as defined in the first paragraph), the precessional effect becoming more evident the closer the orbit is to the sun. Under the perturbation of the other celestial objects, the orbit continues to remain, in general, a precessional ellipse, precessional parabola, or precessional hyperbola, but there are exceptions. Nevertheless they are unlikely in the sense that the set of initial data for which they occur has measure zero.

Several other Manev-type models have recently been the subject of research. Mioc[4] has considered Fock's relativistic field, truncating the negligible terms and obtaining the values $\beta=2(E^2-1)$, $\gamma=6\mu E^2/c^2$ of the parameters, where $E=1+h/c^2$ and h is the total energy per unit mass of the rotating particle. Saslaw,[5] and later Mioc and Radu,[6] have considered the motion in the photogravitational field generated by a source of radiation, taking the values $\beta=-\sigma L/(4\pi\mu mc)$, $\gamma=0$ of the parameters, where σ and m are the cross-sectional area and the mass of the rotating body and L is the luminosity of the central body. The two-body problem with equivalent gravitational parameter ($\beta\neq 0$, $\gamma=0$) has been considered by Şelaru, Cucu-Dumitrescu, and Mioc.[7]

There are other directions of research where this potential occurs: Ureche[8] analyzed the

astrophysical problem of the free-fall collapse of a homogeneous sphere; Diacu[9] considered generalizations to the three-body problem in the more general mathematical context of *quasihomogeneous potentials*, showing that Manev's case represents the only bifurcation of the flow in the quasihomogeneous case. Diacu[10] also studied the gravitational isosceles three-body case, pointing out possible applications in atomic physics.

The general case of the Manev potential for any positive values of the constants A and B has been considered, in Hamiltonian formulation and for negative total energy, by Lacomba, Llibre, and Nunes (see Ref. 3), who have also applied KAM (Kolmogorov–Arnold–Moser) theory to a perturbed Manev potential, to prove the invariance of nonresonant cylinders and tori. The Melnikov integral associated with the nonhyperbolic equilibria was computed by Casasayas, Fontich, and Nunez.[11] The analytic solution and the local flow of the Manev model near collision has been obtained by Diacu, Mingarelli, Mioc, and Stoica.[12] The more complicated anisotropic Manev problem (important for understanding the connections between classical and quantum mechanics) has been recently investigated by Craig, Diacu, Lacomba, and Perez,[13] who have fully understood the flow near collision and have described some elements of the global flow, obtaining in particular the complete picture of the zero-energy case.

The goal of this paper is to provide the complete analytic, geometric, and physical description of the Manev problem. In Secs. II–IV, we compute the analytic solution, which, from the practical point of view, can be used in numerical endeavors. This has been previously done in different forms and contexts, the one we use here presenting interest mainly for astronomers. Unfortunately, the complicated closed form of the solution hides the nice properties of the model, and this is the reason why Goldstein's problem is the subject of physical misinterpretations. Therefore we continue with a qualitative analysis, which reveals the geometrical nature of the orbits. In Sec. V we use the McGehee technique[14] to blow up the collision singularity and offer new, regularized equations of motion. The main idea of this method is to paste, instead of the collision singularity, a manifold to the phase space. This manifold, though now part of the phase space, has nothing to do with the real physical orbits. Its advantage, however, is that, due to the continuity of solutions with respect to the initial data, it provides information about orbits passing close to collision. The study of the (fictitious) flow on the collision manifold is therefore important for the understanding of the local flow near collision. In this case, however, the regularized equations of motion allow us to provide a full description of the global flow. The flow on the torus is formed by periodic orbits, except the upper and lower circle, which are formed by degenerate equilibria. We observe that the global flow has a rotational symmetry, which we use to reduce the dimension of the phase space. In this reduced phase space, the collision manifold is a circle of equilibria: two of these equilibria correspond to the circles of equilibria on the torus, while all the others correspond to the periodic orbits on the torus (see Fig. 2).

In Sec. VI we treat the negative-energy case. Every energy level is a spherical cap (which is obviously topologically equivalent with a disk—see Fig. 3). There are infinitely many heteroclinic orbits connecting the equilibria of the collision circle, two homoclinic orbits, and infinitely many periodic orbits. The heteroclinic and homoclinic solutions correspond physically to orbits ejecting from a collision and also ending in a collision. The periodic orbits correspond to tori of solutions in phase space. In Sec. VII we prove that most of the tori of solutions correspond to quasiperiodic orbits (precessional ellipses), while a set of measure zero of initial data leads to elliptic orbits. In Sec. VIII we study the zero-energy and positive-energy cases. Each energy level is topologically equivalent with an annulus: in the zero-energy case it is a paraboloid with the cap removed (see Fig. 4), while in the positive-energy case, depending on the initial data, it is part of a hyperboloid of one sheet [see Fig. 5(a)], one sheet of a cone of two sheets with the cap removed [see Fig. 5(b)], or one sheet of a hyperboloid of two sheets with the cap removed [see Fig. 5(c)]. All these surfaces are bordered by the collision circle. From the physical point of view, the zero-energy case solutions correspond to precessional parabolas, whereas the positive-energy ones correspond to precessional branches of hyperbolas. In all cases, and in general, the set of initial data leading to

collisions has positive measure. Also, as we have proved in Ref. 12, the collision is not regularizable, in the sense that continuity with respect to the initial data is lost after collision.

II. THE RADIUS VECTOR—DIRECT APPROACH

The Manev problem is described by a Hamiltonian system, i.e., a system of the type

$$\dot{\mathbf{q}}=\frac{\partial H(\mathbf{p},\mathbf{q})}{\partial \mathbf{p}},\quad \dot{\mathbf{p}}=\frac{-\partial H(\mathbf{p},\mathbf{q})}{\partial \mathbf{q}},$$

where the Hamiltonian function H has the property $H(\mathbf{p},\mathbf{q})=h$ (constant), i.e., it is a first integral (called the integral of energy) of the system.

In our case, the Hamiltonian H is given by

$$H(\mathbf{p},\mathbf{q})=\frac{1}{2}\,(|\mathbf{p}_1|^2+|\mathbf{p}_2|^2)-\frac{A}{|\mathbf{q}_1-\mathbf{q}_2|}-\frac{B}{|\mathbf{q}_1-\mathbf{q}_2|^2},$$

where we have denoted by $\mathbf{q}=(\mathbf{q}_1,\mathbf{q}_2)$ the *configuration* of the system of two particles and by $\mathbf{p}=(\mathbf{p}_1,\mathbf{p}_2)$ the *momentum*, A and B being positive constants.

Since H depends only on the relative positions $\mathbf{q}_1-\mathbf{q}_2$ and not on the position vectors $\mathbf{q}_1$ and $\mathbf{q}_2$, we can reduce the Manev problem to a central force problem by introducing the relative coordinates $\mathbf{r}=\mathbf{q}_1-\mathbf{q}_2$, which transform the Hamiltonian into

$$H(\mathbf{p},\mathbf{r})=(1/2)|\mathbf{p}|^2-A/|\mathbf{r}|-B/|\mathbf{r}|^2.$$

We will use this formulation of the problem in our qualitative endeavors (Secs. V–VIII). To obtain the analytic expression of the solution (Secs. II–IV), we eliminate the momentum from the above equations and express them as a second-order system of the form

$$\ddot{\mathbf{r}}=\frac{-(1+\beta)\mu\mathbf{r}}{r^3}-\frac{\gamma\mu\mathbf{r}}{r^4},\tag{2.1}$$

where $\beta=A/\mu-1$, $\gamma=2B/\mu$, $\mu=GM$, G is the gravitational constant, $\beta=A/\mu-1$, $\gamma=2B/\mu$, $\mu=GM$, G is the gravitational constant, M is the mass of one particle, the other having mass 1, and $r=|\mathbf{r}|$.

Using polar coordinates (r,u), the equations (2.1) become

$$\ddot{r}-r\dot{u}^2=-(\mu/r^2)(1+\beta+\gamma/r),\quad r\ddot{u}+2\dot{r}\dot{u}=0.\tag{2.2}$$

Let us attach to the equations (2.2) the initial conditions

$$(r,u,\dot{r},\dot{u})(t_0)=(r_0,u_0,V_0\cos\psi,V_0\sin\psi/r_0),$$

where $V_0=V(t_0)$, $V=|\dot{\mathbf{r}}|$, and ψ is the angle between the initial radius vector and the initial velocity. Since the force field is central, the angular momentum is conserved, so the second equation in (2.2) yields the integral

$$r^2\dot{u}=C,\tag{2.3}$$

where $C=r_0V_0\sin\psi$ is the constant of the angular momentum. The integral of energy is

$$V^2=\dot{r}^2+r^2\dot{u}^2=(\mu/r)[2(1+\beta)+\gamma/r]+h,\tag{2.4}$$

where h is the energy constant.

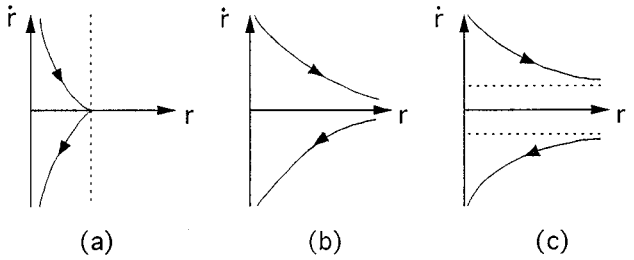

FIG. 1. (a) The case $h<0$, where $r_0 = (-A-\sqrt{A^2-2Bh})/h$. (b) The case $h=0$. (c) The case $h>0$.

The rectilinear case (which corresponds to the zero angular momentum, $C=0$) is easy to solve. The phase-space picture is given in Fig. 1. (In fact, we will recover these orbits in the qualitative analysis performed in Secs. V–VIII.) Throughout Secs. II–IV, we will assume $C\neq 0$.

Using the relation $dt=(r^2/C)du$ obtained from (2.3), the first equation in (2.1) takes the Binet-type form

$$\frac{d^2(1/r)}{du^2}+\left(1-\frac{\gamma\mu}{C^2}\right)\frac{1}{r}=\frac{(1+\beta)\mu}{C^2}, \tag{2.5}$$

with the initial conditions

$$\left(r,\frac{d(1/r)}{du}\right)(u_0)=\left(r_0,-\frac{1}{r_0\tan\psi}\right).$$

The solution of the initial value problem attached to the equations (2.5) depends on the value of the constant $\alpha=\gamma\mu/C^2$. We distinguish three cases: (a) $\alpha<1$, (b) $\alpha=1$, and (c) $\alpha>1$:

$$r=\left[\left(\frac{1}{r_0}-\frac{(1+\beta)\mu}{(1-\alpha)C^2}\right)C_\alpha(\mu)-\frac{S_\alpha(u)}{r_0\tan\psi}+\frac{(1+\beta)\mu}{(1-\alpha)C^2}\right]^{-1}, \tag{2.6a}$$

$$r=\left[\frac{(1+\beta)\mu(u-u_0)^2}{2C^2}-\frac{u-u_0}{r_0\tan\psi}+\frac{1}{r_0}\right]^{-1}, \tag{2.6b}$$

$$r=\left[\left(\frac{1}{r_0}+\frac{(1+\beta)\mu}{(\alpha-1)C^2}\right)\widetilde{C}_\alpha(u)-\frac{\widetilde{S}_\alpha(u)}{r_0\tan\psi}-\frac{(1+\beta)\mu}{(\alpha-1)C^2}\right]^{-1}, \tag{2.6c}$$

where

$$S_\alpha(u)=(1-\alpha)^{-1/2}\sin(\sqrt{1-\alpha}(u-u_0)),\quad C_\alpha(u)=\cos(\sqrt{1-\alpha}(u-u_0)),$$

$$\widetilde{S}_\alpha(u)=(1-\alpha)^{-1/2}\sinh(\sqrt{\alpha-1}(u-u_0)),\quad \widetilde{C}_\alpha(u)=\cosh(\sqrt{\alpha-1}(u-u_0)).$$

III. THE ORBITAL ELEMENTS—PERTURBATIVE APPROACH

Let us now isolate the Newtonian attraction term per unit mass, $-\mu\mathbf{r}/\mathbf{r}^3$, on the right-hand side of the equations (2.1), and treat the remaining term $-\beta\mu\mathbf{r}/r^3-\gamma\mu\mathbf{r}/r^4$ as a perturbing acceleration. In this way we can tackle the problem in the frame of the classical perturbation theory.

According to this theory, developed primarily by Lagrange and based on the variation of parameters,[15] the real (perturbed) trajectory can be regarded as the envelope of a family of oscu-

lating Keplerian orbits (conic sections) whose initial conditions change continuously. The motion will then be described by a set of relations between the Keplerian orbital elements, their time derivatives, and time; these form the so-called Newton–Euler or Gauss equations.[16] If the components of the perturbing accelerations (which appear in these equations) do not contain the time explicitly, one can choose another independent variable: one of the anomalies (as in Ref. 16, p. 157) or the argument of latitude.

We will further express the trajectory of the particle with respect to the time-dependent osculating Keplerian orbital elements: a=*the semimajor axis*, Ω=*the longitude of the ascending node*, i=*the inclination*, e=*the eccentricity*, ω=*the argument of the pericenter*, and u=*the argument of the latitude*. We will also use $p=a(1-e^2)$=*the semilatus rectum*, $v=u-\omega$=*the true anomaly*, and the parameters $q=e\cos\omega$, $k=e\sin\omega$, which are suitable for the study of small-eccentricity orbits (those close to circles), for which the pericenter is not well—or not at all—defined.[17]

Let S,T,W denote the radial, transverse, and binormal components of the perturbing acceleration, respectively. Since they do not depend explicitly on the time t, we can describe the perturbed motion by means of the Newton–Euler equations written with respect to u in the form (see, e.g., Ref. 5)

$$
\begin{aligned}
&p'=2\left(\frac{Z}{\mu}\right)r^3T, \quad \Omega'=\left(\frac{Z}{\mu}\right)r^3W\,\frac{\sin u}{p\,\sin i}, \quad i'=\left(\frac{Z}{\mu}\right)r^3W\,\frac{\cos u}{p},\\
&q'=\left(\frac{Z}{\mu}\right)\left\{r^3kW\sin u\,\frac{\cot i}{p}+r^2T\left[r\,\frac{q+\cos u}{p}+\cos u\right]+r^2S\sin u\right\},\\
&k'=\left(\frac{Z}{\mu}\right)\left\{-r^3qW\sin u\,\frac{\cot i}{p}+r^2T\left[r\,\frac{k+\sin u}{p}+\sin u\right]-r^2S\cos u\right\},\\
&t'=\frac{Zr^2}{\sqrt{\mu p}},
\end{aligned}
\tag{3.1}
$$

where $'=d/du$ and $Z=[1-r^2\dot{\Omega}(\cos i)/\sqrt{\mu p})^{-1}]$, with the initial conditions

$$(p,\Omega,i,q,k,t)(u_0)=(p_0,\Omega_0,i_0,q_0,k_0,t_0).$$

Since the perturbing force in the equations (2.1) is radial, the components of the perturbing acceleration are $S=-(\mu/r^2)(\beta+\gamma/r)$, $T=W=0$. Also notice that $Z=1$. Replacing these values into the equations (3.1), we obtain

$$p'=\Omega'=i'=0, \quad q'=-(\beta+\gamma/r)\sin u, \quad k'=(\beta+\gamma/r)\cos u, \quad t'=r^2/\sqrt{\mu p}. \tag{3.2}$$

Integrating the first three equations and using the initial data, we obtain that all along the motion $p=p_0$, $\Omega=\Omega_0$, and $i=i_0$, which means that the *semilatus rectum* is constant and the motion is planar.

According to the perturbation theory we use, we may describe the real trajectory by the equation of a conic section $r=p/(1+e\cos v)$, whose parameters are functions of u. From the definition of q and k, the relation $v=u-\omega$, and the constancy of p, this equation becomes

$$r(u)=\frac{p_0}{(1+q\cos u+k\sin u)}. \tag{3.3}$$

On the other hand, since for osculating conic sections $p=p_0=\text{const}$ (the same constant as in the Kepler problem) and C has the same value as in the Kepler problem[18] (given by $C^2/\mu=p$), we put $C^2=\mu p_0$, which, according to the previous section, leads to $\alpha=\gamma/p_0$. With this expression for α, and with (3.3), the coupled equations for q and k in (3.1) have the exact solution, for (a) $\alpha<1$, (b) $\alpha=1$, and (c) $\alpha>1$, respectively:

$$\begin{aligned} q(u)=&\{S_\alpha(u)[\sin(u-u_0)-\alpha\cos u_0\sin u]+C_\alpha(u)\cos(u-u_0)\}q_0\\ &+\{S_\alpha(u)[\cos(u-u_0)-\alpha\sin u_0\sin u]-C_\alpha(u)\sin(u-u_0)\}k_0\\ &-(\alpha+\beta)S_\alpha(u)\sin u+[(\alpha+\beta)/(1-\alpha)][1-C_\alpha(u)]\cos u,\\ k(u)=&\{-S_\alpha(u)[\cos(u-u_0)-\alpha\cos u_0\cos u]+C_\alpha(u)\sin(u-u_0)\}q_0\\ &+\{S_\alpha(u)[\sin(u-u_0)+\alpha\sin u_0\cos u]+C_\alpha(u)\cos(u-u_0)\}k_0\\ &+(\alpha+\beta)S_\alpha(u)\cos u+[(\alpha+\beta)/(1-\alpha)][1-C_\alpha(u)]\sin u, \end{aligned} \tag{3.4a}$$

$$\begin{aligned} q(u)=&[\cos(u-u_0)-(u-u_0)\sin u_0\cos u]q_0-[\sin(u-u_0)-(u-u_0)\cos u_0\cos u]\\ &\times k_0-[(1+\beta)/2](u-u_0)[2\sin u-(u-u_0)\cos u],\\ k(u)=&[\sin(u-u_0)-(u-u_0)\sin u_0\sin u]q_0+[\cos(u-u_0)+(u-u_0)\cos u_0\sin u]\\ &\times k_0+[(1+\beta)/2](u-u_0)[2\cos u+(u-u_0)\sin u], \end{aligned} \tag{3.4b}$$

$$\begin{aligned} q(u)=&\{\tilde{S}_\alpha(u)[\sin(u-u_0)-\alpha\cos u_0\sin u]+\tilde{C}_\alpha(u)\cos(u-u_0)\}q_0\\ &+\{S_\alpha(u)[\cos(u-u_0)-\alpha\sin u_0\sin u]-\tilde{C}_\alpha(u)\sin(u-u_0)\}k_0\\ &-(\alpha+\beta)\tilde{S}_\alpha(u)\sin u+[(\alpha+\beta)/(1-\alpha)][1-\tilde{C}_\alpha(u)]\cos u,\\ k(u)=&\{-\tilde{S}_\alpha(u)[\cos(u-u_0)-\alpha\cos u_0\cos u]+\tilde{C}_\alpha(u)\sin(u-u_0)\}q_0\\ &+\{S_\alpha(u)[\sin(u-u_0)+\alpha\sin u_0\cos u]+\tilde{C}_\alpha(u)\cos(u-u_0)\}k_0\\ &+(\alpha+\beta)\tilde{S}_\alpha(u)\cos u+[(\alpha+\beta)/(1-\alpha)][1-\tilde{C}_\alpha(u)]\sin u. \end{aligned} \tag{3.4c}$$

Plugging (3.4) into (3.3) we obtain the formulas of the radius vector for (a) $\alpha<1$, (b) $\alpha=1$, and (c) $\alpha>1$:

$$r=p_0\left[\frac{1+\beta}{1-\alpha}-\left(\frac{\alpha+\beta}{1-\alpha}-e_0\cos v_0\right)C_\alpha(u)-e_0\sin v_0 S_\alpha(u)\right]^{-1}, \tag{3.5a}$$

$$r=p_0\left[\frac{1+\beta}{2}(u-u_0)^2-e_0\sin v_0(u-u_0)+1+e_0\cos v_0\right]^{-1}, \tag{3.5b}$$

$$r=p_0\left[-\frac{1+\beta}{\alpha-1}+\left(\frac{\alpha+\beta}{\alpha-1}+e_0\cos v_0\right)\tilde{C}_\alpha(u)-e_0\sin v_0\tilde{S}_\alpha(u)\right]^{-1}, \tag{3.5c}$$

where $e_0=(q_0^2+k_0^2)^{1/2}$ and $v_0=u_0-\arctan(k_0/q_0)$ stay for initial conditions. These formulas are equivalent to (2.6).

IV. RELATIONSHIP BETWEEN TIME AND POLAR ANGLE

In Sec. III we have described the evolution of the radius vector as a function of the argument of latitude. To complete the integration of the equations (3.1), we will determine the function $t=t(u)$, which allows us to express the solution as a function of the time variable. For this, consider first the following notations:

$$\overline{A}=\frac{(1-\alpha)e_0\cos v_0-(\alpha+\beta)}{1+\beta},\quad \overline{B}=\frac{(1-\alpha)^{1/2}e_0\sin v_0}{1+\beta},\quad \widetilde{B}=\frac{(\alpha-1)^{1/2}e_0\sin v_0}{1+\beta},$$

$$K=2(1-\alpha)^{3/2}(1+\beta)^{-2},\quad \widetilde{K}=2(\alpha-1)^{3/2}(1+\beta)^{-2},$$

$$e^*=(\overline{A}^2+\overline{B}^2)^{1/2},\quad w=(1-e^{*2})^{1/2},\quad \widetilde{w}=(e^{*2}-1)^{1/2},$$

$$f(u)=\cot[(1/2)\sqrt{1-\alpha}(u-u_0)],\quad \widetilde{f}(u)=\coth[(1/2)\sqrt{\alpha-1}(u-u_0)],$$

$$X(u)=(\overline{A}+1)f(u)-\overline{B},\quad Y(u)=(\overline{A}+e^{*2})f(u)-\overline{B},\quad Z(u)=w^2+X^2(u),$$

$$\widetilde{X}(u)=(\overline{A}+1)\widetilde{f}(u)+\widetilde{B},\quad \widetilde{Y}(u)=(\overline{A}+e^{*2})\widetilde{f}(u)+\widetilde{B},\quad \widetilde{Z}(u)=w^2-\widetilde{X}^2(u),$$

$$x=1+e_0\cos v_0,\quad y=-e_0\sin v_0,\quad D=2(1+\beta)x-y^2,$$

$$\hat{X}(u)=\frac{2[(1+\beta)x-y^2](u-u_0)-(1+\beta)y(u-u_0)^2}{x[2x+2y(u-u_0)+(1+\beta)(u-u_0)^2]},$$

$$\hat{Y}(u)=\frac{u-u_0}{2x+y(u-u_0)},\quad \hat{Z}(u)=\frac{(1+\beta)(u-u_0)}{2y[y+(1+\beta)(u-u_0)]}.$$

Direct computations give us the following relations in each of the cases (a) $\alpha<1$, (b) $\alpha=1$, and (c) $\alpha>1$, respectively:

$$t=t_0+(Kp_0^{3/2}/w^3\sqrt{\mu})[\arctan(wX(u))-wY(u)/Z(u)],\quad \text{for } e^*<1,$$

$$t=t_0+(Kp_0^{3/2}/3\sqrt{\mu})[(2+3X(u)f(u))/X^3(u)],\quad \text{for } e^*=1, \tag{4.1a}$$

$$t=t_0+(Kp_0^{3/2}/\widetilde{w}^3\sqrt{\mu})[\widetilde{w}Y(u)/Z(u)-\operatorname{arg\,tanh}(\widetilde{w}/X(u))],\quad \text{for } e^*>1,$$

$$t=t_0-\frac{p_0^{3/2}}{D\sqrt{\mu}}[\hat{X}(u)+(2(1+\beta)/\sqrt{-D})\operatorname{arg\,tanh}(\sqrt{-D}\hat{Y}(u))],\quad \text{for } D<0,$$

$$t=t_0+4p_0^{2/3}\hat{Z}(u)/\sqrt{\mu},\quad \text{for } D=0, \tag{4.1b}$$

$$t=t_0+\frac{p_0^{3/2}}{D\sqrt{\mu}}[\hat{X}(u)+(2(1+\beta)/\sqrt{D})\arctan(\sqrt{D}\hat{Y}(u))],\quad \text{for } D>0,$$

$$t=t_0+(\widetilde{K}p_0^{3/2}/w^3\sqrt{\mu})[\operatorname{arg\,tanh}(w/\widetilde{X}(u))+w\widetilde{Y}(u)/\widetilde{Z}(u)],\quad \text{for } e^*<1,$$

$$t=t_0+(\widetilde{K}p_0^{3/2}/3\sqrt{\mu})[(3\widetilde{X}(u)\widetilde{f}(u)-2)/\widetilde{X}^3(u)],\quad \text{for } e^*=1, \tag{4.1c}$$

$$t=t_0+(\widetilde{K}p_0^{3/2}/\widetilde{w}^3\sqrt{\mu})[\widetilde{w}\widetilde{Y}(u)/\widetilde{Z}(u)+\arctan(\widetilde{w}/\widetilde{X}(u))],\quad \text{for } e^*>1.$$

Relations $p=p_0$, $\Omega=\Omega_0$, $i=i_0$, (3.4), and (4.1) give now, in closed form, the solution of the equations of motion (3.2) of the Manev problem.

V. BLOW UP AND REDUCTION

To begin our qualitative endeavors, let us write the Manev problem in Hamiltonian form, as we did at the beginning of Sec. II, with a Hamiltonian of the type

$$H(\mathbf{p},\mathbf{q})=\frac{1}{2}\,(|\mathbf{p}_1|^2+|\mathbf{p}_2|^2)-\frac{1}{|\mathbf{q}_1-\mathbf{q}_2|}-\frac{k}{|\mathbf{q}_1-\mathbf{q}_2|^2}, \tag{5.1}$$

where the units (including those of the masses) have been chosen such that the constants A and B take the values 1 and k, respectively.

Considering polar coordinates $r>0$, $\theta\in S^1$, where S^1 is the segment $[0,\ 2\pi]$ with the end points identified, the Hamiltonian takes the form

$$H(p_r,p_\theta,r)=\tfrac{1}{2}(p_r^2+p_\theta^2/r^2)-1/r-k/r^2, \tag{5.2}$$

where p_r,p_θ are the new polar variables.

To blow up the collision singularity that occurs at $r=0$, we formally multiply the energy integral by r^2 [a detailed justification of this step was given in the local study near the collision performed in a previous paper that uses McGehee transformations (see Ref. 12)]. The energy relation takes now the form

$$\tfrac{1}{2}r^2p_r^2+p_\theta^2-r-k=hr^2. \tag{5.3}$$

Introducing further the transformations $v=rp_r$ and $u=p_\theta$ and scaling the time variable by using $dt=r^2\,d\tau$, the equations given by the Hamiltonian (5.2) take the form

$$r'=rv,\quad v'=r(1+2hr),\quad \theta'=u,\quad u'=0, \tag{5.4}$$

having the energy relation (5.3) transformed into

$$v^2+u^2-2r-2hr^2=2k. \tag{5.5}$$

The prime denotes here differentiation with respect to the new, fictitious, time variable τ.

Define the *collision manifold* as the set of solutions given by relation (5.5) when $r=0$. Notice that, geometrically, the collision manifold is a cylinder in the three-dimensional space of the coordinates (u,θ,v), and, since $\theta\in[0,\ 2\pi]$, it follows that this cylinder can be identified with a torus. In fact, the two-dimensional torus representing the collision manifold is imbedded in the full four-dimensional phase space of the coordinates (r,u,θ,v). The equations (5.4) show that the flow on the collision manifold is formed almost exclusively by periodic orbits, except the upper and lower circles of the torus given by $r=0$, $u=0$, $v=\pm\sqrt{2k}$, which consist of equilibrium points [see Fig. 2(a)].

Since θ does not appear explicitly in the equations (5.4) or in the energy relation (5.5), we can further reduce the four-dimensional phase space to dimension three by factorizing the flow to S^1. Exploiting this symmetry (characteristic to this problem), we will obtain clear pictures of the global flow in phase space. In what follows we will describe the global reduced flow as well as the flow in phase space, by regarding the energy as a parameter.

Factorizing the collision manifold to S^1, the torus becomes a circle [see Fig. 2(b)]. The points M and N on this circle correspond to the circles of equilibria on the torus, while all the other points correspond to the periodic orbits on the torus.

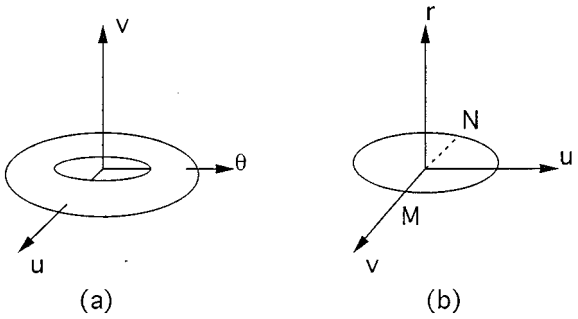

FIG. 2. (a) The collision manifold imbedded in the four-dimensional phase space. (b) The collision manifold in the reduced phase space.

VI. ORBITS OF ELLIPTIC TYPE

In this section we consider the negative-energy case, $h<0$. Let us first write the energy relation (5.5) in a convenient way as

$$v^2+u^2-2h(r+1/2h)^2=2k-1/2h, \tag{6.1}$$

which shows that, in the reduced phase space, every energy level is a two-dimensional sphere [in the three-dimensional Euclidean space (r,v,u) with $r\geqslant 0$ (see Fig. 3)]. In other words, every negative-energy level is homeomorphic with a two-dimensional disk. The boundary of this disk is $r=0$, $v^2+u^2=2k$, i.e., the circle that defines the collision manifold.

The analysis of the equations (5.4) allows us to describe the flow on the negative-energy levels. There are two equilibria outside the collision manifold, located at $r=-1/2h$, $v=0$, $u=\pm\sqrt{2k-1/2h}$. Since u is a first integral, all solutions are represented by curves lying in parallel planes, $u=$const. Therefore, depending on the constant value of u, the orbits are heteroclinic if $|u|<\sqrt{2k}$, homoclinic for $u=\pm\sqrt{2k}$, and periodic for $\sqrt{2k}<|u|<\sqrt{2k-1/2h}$. Note that in the unreduced phase space all these ''orbits'' are in fact manifolds. Each manifold consists of the product between an ''orbit'' and S.[1]

The physical interpretation in each of these cases is as follows. The heteroclinic orbit connecting M and N corresponds to rectilinear solutions starting from a collision and ending in a collision. They are homothetic orbits. All the other heteroclinic orbits connecting equilibria of the collision circle are, in full phase space, heteroclinic orbits between the periodic orbits on the collision torus. Physically they also correspond to solutions ejecting from collision and then

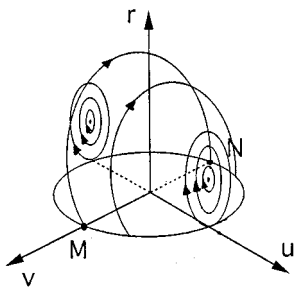

FIG. 3. The flow on each negative-energy level.

tending to collision, but the collision is not rectilinear anymore: the particle colliding with the center spirals around the center. There are, in fact, infinitely many rotations before collision, as we will prove in Sec. VII. The homoclinic orbits in Fig. 3 correspond, in full phase space, to orbits ejecting from the *big* circle of the torus and returning to it and to orbits ejecting from the *small* circle of the torus and returning to it. (The *big* and *small* circles are the ones in the ''equatorial'' plane $v=0$). Their physical interpretation is similar to that of the heteroclinic ones that spiral at ejection-collision. As we have already proved in Ref. 11, this also shows that there exists a set of positive measure of initial data that leads to collisions.

The case of periodic orbits, for $\sqrt{2k}<|u|<\sqrt{2k-1/2h}$, is the most interesting one from the mathematical point of view. In full phase space each of these orbits corresponds to a linear flow on a torus: $S^1\times S^1$. Each torus is therefore filled with either periodic or with quasiperiodic orbits (this is a well-known fact in the qualitative theory of dynamical systems[19]). It is the goal of Sec. VII to find the frequency ratio and prove that most of the tori are filled with quasiperiodic orbits and that only a negligible set of them consists of tori foliated by periodic orbits. Physically, the quasiperiodic solutions correspond to precessional ellipses that fill an annulus densely, whereas the periodic ones are either elliptic orbits or precessional orbits that close after a finite number of rotations.

The last case to discuss is that of the two equilibria outside the collision manifold at $r=-1/2h$, $v=0$, $u=\pm\sqrt{2k-1/2h}$. In full phase space they correspond to periodic orbits, and are circular orbits in physical space. This completes the description of the negative-energy case.

VII. PERIODIC AND QUASIPERIODIC ORBITS

In this section we want to determine the nature of the tori of orbits in Sec. VI. For this we will compute the frequency ratio, which will tell us whether the corresponding orbits are periodic or quasiperiodic. Periodic orbits correspond to rational ratios, whereas quasiperiodic ones correspond to irrational ratios.

Let $\rho=\sqrt{-2h}(r+1/2h)$, and observe that $\rho=1/\sqrt{-2h}=\alpha$ represents collision. From the equations of motion (5.4) we obtain

$$\rho'=(\rho+1/\sqrt{-2h})v,\quad v'=-\rho(\rho+1/\sqrt{-2h}).$$

Now observing that

$$v^2+\rho^2=2k-\frac{1}{2h}-u^2=I^2,$$

we introduce polar coordinates (I,ϕ) in the (ρ,v) plane. Notice that

$$\phi'=\frac{v\rho'-\rho v'}{\rho^2+v^2}=\rho+\alpha=I\sin\phi+\alpha.$$

Taking now $z=\tan(\phi/2)$, the equivalent equation

$$d\tau=\frac{d\phi}{I\sin\phi+\alpha}$$

takes the form

$$d\tau=\frac{2dz}{\alpha z^2+2Iz+\alpha}=\frac{2dz}{\alpha[(z+I/\alpha)^2+1-I^2/\alpha^2]}.$$

Note that $I<\alpha$ corresponds to noncollision orbits. Integrating the last equation, we obtain

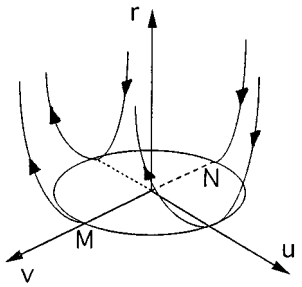

FIG. 4. The flow in the zero-energy case.

$$\tau = \frac{2}{a\alpha} \arctan \frac{z + I/\alpha}{a} + \text{const},$$

where $a = \sqrt{1 - I^2/\alpha^2}$.

The period T is given by

$$T = \tau|_0^T = \int_0^{2\pi} F(\phi) d\phi,$$

where the right-hand side is a (convergent) improper integral at $\phi = \pi$. Then

$$T = \frac{4}{a\alpha} \lim_{\phi \to \pi} \left[\arctan \frac{I/\alpha + \tan \phi/2}{a} - \arctan \frac{I}{a\alpha} \right] = \frac{2}{a\alpha} \left[\pi - 2 \arctan \frac{I}{a\alpha} \right],$$

and after replacing the values of α, a, and I we obtain

$$T = \frac{2\sqrt{-2h}}{\sqrt{2h(2k - u^2)}} \left[\pi - 2 \arctan \frac{\sqrt{1 + 2h(u^2 - 2k)}}{\sqrt{2h(2k - u^2)}} \right].$$

Notice now that if $\rho \to \alpha$, then $a \to \infty$ and $T \to \infty$. Also, if $I \to 0$, then $a \to 1$ and $T \to 2\pi/\alpha$.

Finally, the frequency ratio of the torus is

$$\frac{T}{u} = \frac{2}{u\sqrt{u^2 - 2k}} \left[\pi - 2 \arctan \frac{\sqrt{1 + 2h(u^2 - 2k)}}{\sqrt{2h(2k - u^2)}} \right].$$

It becomes clear now that, for fixed k, most of the values taken by the frequency ratio, as a continuous function of u, are irrational. This proves that, except for a set of measure zero of tori foliated by periodic orbits, most of the tori are generated by quasiperiodic orbits.

VIII. ORBITS OF PARABOLIC AND HYPERBOLIC TYPE

Let us finally consider the zero-energy, $h = 0$, and the positive-energy, $h > 0$, cases.

In the zero-energy case, the energy relation takes the form

$$v^2 + u^2 = 2r + 2k,$$

which implies that the zero-energy level is a paraboloid with the cap removed (see Fig. 4). (The cap is removed because $r \geqslant 0$.) From the topological point of view this is the complement of a disk bordered by the collision circle, i.e., an annulus. Again, the first integral, $u = \text{const}$, foliates the

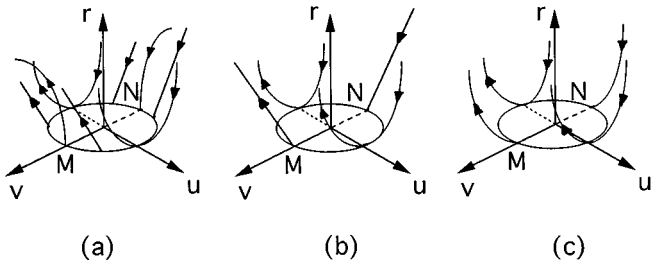

FIG. 5. The flows in the three cases of the positive-energy levels.

zero-energy level into curves lying in parallel planes. The curves are either parabolas, for $|u| \geqslant \sqrt{2k}$, or arcs of parabolas, for $|u| < \sqrt{2k}$. There are no equilibria outside the collision circle.

The physical interpretation of the orbits corresponding to the arc of parabola tending to N or ejecting from M is that of rectilinear orbits that come from (or tend to) infinity with asymptotic velocity zero. The other orbits corresponding to arcs of parabolas that tend to (or eject from) the collision circle are those of precessional parabolas that spiral at collision (ejection) and have asymptotic velocity zero at infinity. The orbits corresponding to parabolas do not encounter collisions and are precessional parabolas with asymptotic velocity zero at infinity.

In the positive-energy case, the energy relation takes the form

$$v^2+u^2-2h(r+1/2h)^2=2k-1/2h.$$

Depending on the relation between h and k, three possibilities arise: (1) $h>1/4k$, (2) $h=1/4k$, and (3) $h<1/4k$.

In case (1), the energy relation describes a hyperboloid of one sheet intersected with $r\geqslant 0$ [see Fig. 5(a)]. The first integral, $u=$const, foliates the surface in branches of hyperbolas or arcs of branches of hyperbolas and two pairs of lines. The physical interpretation is similar to that of the zero-energy case, just that parabolas are now substituted by branches of hyperbolas and the asymptotic velocity at infinity is not zero but positive.

In case (2), the energy relation is a cone intersected with $r\geqslant 0$ [see Fig. 5(b)], and the first integral, $u=$const, foliates the surface in branches of hyperbolas or arcs of branches of hyperbolas and two half-lines (those corresponding to M and N). The physical interpretation of the corresponding orbits is similar to the one of the previous case, (1).

In case (3), the energy relation is a hyperboloid of two sheets intersected with $r\geqslant 0$, i.e., one sheet with the cap removed [see Fig. 5(c)]. The first integral, $u=$const, foliates the surface in branches of hyperbolas and arcs of branches of hyperbolas. The physical interpretation of the corresponding orbits is the same as in case (1) above.

This gives the complete picture of the Manev problem.

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The time harmonic electromagnetic field in a disturbed half-space: An existence theorem and a computational method

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The scattering of time harmonic electromagnetic waves by a perfectly conducting surface that is the boundary of a ''disturbed half-space'' is considered. This problem is translated in a boundary value problem for an elliptic system of partial differential equations. Under appropriate hypotheses an existence theorem and an integral representation formula for the solution of this boundary value problem is given. Based on this integral representation formula a new method to compute the solution of the boundary value problem is proposed. This method involves only quadratures and is fully parallelizable. Finally some numerical examples of the results obtained on test problems with this computational method are shown. [S0022-2488(96)00805-5]

I. INTRODUCTION

Integral equation methods are often used to study the electromagnetic scattering by bounded obstacles (see Refs. 1 and 2). In this paper we consider the case when the scattering surface is a plane with a local disturbance. This surface as assumed to be perfectly conducting so that the electromagnetic field propagates in a ''disturbed half-space.'' This scattering problem is translated in a boundary value problem for a system of elliptic partial differential equations. Under appropriate hypotheses an existence theorem for the solution of this boundary value problem is proved. Moreover, we describe a new method to compute the electromagnetic field that is fully parallelizable. The analogous problems in the acoustic case have been studied in many papers including Refs. 3–8.

Let $\mathbf{R}^n$ be the n-dimensional real Euclidean space, $\underline{x}=(x_1,x_2,\ldots,x_n)^T\in\mathbf{R}^n$ be a generic vector, where the superscript T means transposed, and let $\mathbf{C}^n$ be the n-dimensional complex vector space, and $\underline{z}=(z_1,z_2,\ldots,z_n)^T\in\mathbf{C}^n$ be a generic vector. Let $(\cdot,\cdot)$ be the Euclidean scalar product, $\|\cdot\|$ be the Euclidean norm and $[\cdot,\cdot]$ be the Euclidean vector product. In the following, with abuse of notation, we use the notation $(\cdot,\cdot)$ and the notation $[\cdot,\cdot]$ to denote also the Euclidean scalar product and the Euclidean vector product of complex vectors. Let $\Omega\subseteq\mathbf{R}^n$ be an open set, $\mathscr{C}^k(\Omega)$, $k=0,1,2,\ldots$, be the space of real or complex-valued k-times continuously differentiable functions in Ω with the appropriate sup-norm and let $\mathscr{C}_0^k(\Omega)$, $k=0,1,2,\ldots$, be the normed space of functions belonging to $\mathscr{C}^k(\Omega)$ with compact support in Ω. Let $\mathscr{C}^\infty(\Omega)$ be the space of real- or complex-valued infinitely continuously differentiable functions defined in Ω, and $\mathscr{C}_0^\infty(\Omega)$ be the space of $\mathscr{C}^\infty(\Omega)$ functions with compact support in Ω. Let $\mathscr{S}(\mathbf{R}^n)$ be the space of fast-decreasing functions

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in $\mathbf{R}^n$ equipped with the usual Frechet structure and $\mathcal{S}'(\mathbf{R}^n)$ be the space of tempered distributions, that is the dual space of $\mathcal{S}(\mathbf{R}^n)$ (see Ref. 9, p. 219).

Let $\rho(x_1,x_2)\in\mathbf{C}_0^2(\mathbf{R}^2)$; we denote with supp $\rho\subset\mathbf{R}^2$ the support of ρ. Let

$$D=\{\underline{x}=(x_1,x_2,x_3)^T\in\mathbf{R}^3 | x_3<\rho(x_1,x_2),(x_1,x_2)^T\in\mathbf{R}^2\}. \tag{1.1}$$

It is easy to see that D is an open simply connected unbounded set. Let $\overline{D}$ be the closure of D; we have

$$D^c=\mathbf{R}^3\backslash\overline{D}=\{\underline{x}=(x_1,x_2,x_3)^T\in\mathbf{R}^3 | x_3>\rho(x_1,x_2),(x_1,x_2)^T\in\mathbf{R}^2\}. \tag{1.2}$$

We call disturbed half-space the sets of the form (1.1) and (1.2). Let ∂D be the boundary of D, that is,

$$\partial D=\{\underline{x}=(x_1,x_2,x_3)^T\in\mathbf{R}^3 | x_3=\rho(x_1,x_2),(x_1,x_2)^T\in\mathbf{R}^2\}. \tag{1.3}$$

We define

$$S_0=\{\underline{x}=(x_1,x_2,x_3)^T\in\mathbf{R}^3 | x_3=\rho(x_1,x_2),(x_1,x_2)^T\in \text{supp } \rho\}, \tag{1.4}$$

so that, since $\rho\in\mathbf{C}_0^2(\mathbf{R}^2)$, S_0 is a compact set, $S_0\subset\partial D$, and $\partial D\backslash S_0$ is an open subset of the plane $\{x_3=0\}$. Let $\underline{n}(\underline{x})$ be the outward unit normal vector to ∂D; that is,

$$\underline{n}(\underline{x})=\frac{1}{\sqrt{1+\left(\frac{\partial\rho}{\partial x_1}\right)^2+\left(\frac{\partial\rho}{\partial x_2}\right)^2}}\left(-\frac{\partial\rho}{\partial x_1},-\frac{\partial\rho}{\partial x_2},1\right)^T,\quad \underline{x}\in\partial D, \tag{1.5}$$

and let $\underline{g}(\underline{x})=(g_1(\underline{x}),g_2(\underline{x}),g_3(\underline{x}))^T$ be a continuous complex-valued vector field with compact support ''tangential'' to ∂D, that is, $(\underline{g}(\underline{x}),\underline{n}(\underline{x}))=0$, $\forall\underline{x}\in\partial D$. Let $\underline{0}=(0,0,0)^T$, let $k_0>0$ be a constant, and ι be the imaginary unit, and let $\hat{\underline{x}}=\underline{x}/\|\underline{x}\|$, for $\underline{x}\neq\underline{0}$. We consider the following boundary value problem:

$$(\Delta+k_0^2)\underline{E}(\underline{x})=0,\quad \underline{x}\in D^c, \tag{1.6}$$

$$\text{div } \underline{E}(\underline{x})=0,\quad \underline{x}\in D^c, \tag{1.7}$$

$$[\underline{n},\underline{E}](\underline{x})=\underline{g}(\underline{x}),\quad \underline{x}\in\partial D, \tag{1.8}$$

and

$$[\text{curl } \underline{E}(\underline{x}),\hat{\underline{x}}]-\iota k_0\underline{E}(\underline{x})=0\left(\frac{1}{\|\underline{x}\|}\right),\quad \|\underline{x}\|\to+\infty,\quad \underline{x}\in D^c, \tag{1.9}$$

where $\Delta(\cdot)=\Sigma_{j=1}^3\partial^2(\cdot)/\partial x_j^2$, $\text{div}(\cdot)=\Sigma_{j=1}^3\partial(\cdot)/\partial x_j$,

$$\underline{E}(\underline{x})=(E_1(\underline{x}),E_2(\underline{x}),E_3(\underline{x}))^T,\quad \Delta\underline{E}(\underline{x})=(\Delta E_1(\underline{x}),\Delta E_2(\underline{x}),\Delta E_3(\underline{x}))^T,$$

and

$$\text{curl } \underline{E}(\underline{x})=\left(\frac{\partial E_3(\underline{x})}{\partial x_2}-\frac{\partial E_2(\underline{x})}{\partial x_3},\frac{\partial E_1(\underline{x})}{\partial x_3}-\frac{\partial E_3(\underline{x})}{\partial x_1},\frac{\partial E_2(\underline{x})}{\partial x_1}-\frac{\partial E_1(\underline{x})}{\partial x_2}\right)^T.$$

It is easy to see (Ref. 1, Ch. 4) that the scattering of time harmonic electromagnetic waves by a perfectly conducting surface in a homogeneous isotropic medium that does not contain free electric charges and fills the disturbed half-space D^c reduces to the boundary value problem (1.6)–(1.9). In fact, let $\underline{E}^i$ be the incident electric field solution of (1.6) and (1.7) and let $\underline{E}^s$ be the electric field scattered by the perfectly conducting surface ∂D. We express the scattered field $\underline{E}^s$ as follows:

$$\underline{E}^s = \underline{E}^1 + \underline{E}^2, \tag{1.10}$$

where $\underline{E}^1(\underline{x}) = (-E_1^i, -E_2^i, E_3^i)^T(x_1, x_2, -x_3)$ is the electric field that would be scattered by the perfectly conducting plane $\{x_3 = 0\}$, and $\underline{E}^2$ is the contribution to the scattered field due to the presence of the perturbation S_0. It is easy to see that $\underline{E}^2$ solves the boundary value problem (1.6)–(1.9) with $\underline{g}(\underline{x}) = -[\underline{n}, \underline{E}^1 + \underline{E}^i](\underline{x})$, $\underline{x} \in \partial D$. Moreover, we have support of $\underline{g}$, supp $\underline{g} \subseteq S_0$. Finally, it is easy to see that for time harmonic waves the magnetic field is given by $\underline{H}(\underline{x}) = (1/\iota k_0)\text{curl}\, \underline{E}(\underline{x})$. In this paper we study the problem of the existence and uniqueness of the solution of the boundary value problem (1.6)–(1.9). In particular, we use the method of boundary integral equations to establish the existence of the solution. We reduce the boundary value problem (1.6)–(1.9) to an integral equation of the second kind for a vector density function $\underline{a}$ such that the vector field $\underline{E}$ solution of (1.6)–(1.9) is given by

$$\underline{E}(\underline{x}) = \int_{\partial D} \text{curl}_{\underline{x}}\{\Phi(\underline{x}, \underline{y})\underline{a}(\underline{y})\} ds(\underline{y}), \tag{1.11}$$

where $\text{curl}_{\underline{x}}$ denotes the curl operator with respect to the variable $\underline{x}$, $ds(\underline{y})$ is the surface measure on ∂D, and $\Phi(\underline{x}, \underline{y})$ is given by

$$\Phi(\underline{x}, \underline{y}) = \frac{\exp(\iota k_0 \|\underline{x} - \underline{y}\|)}{4\pi \|\underline{x} - \underline{y}\|}, \quad \underline{x} \neq \underline{y}, \quad \underline{x}, \underline{y} \in \mathbf{R}^3. \tag{1.12}$$

The uniqueness theorem is given for solutions of the boundary value problem (1.6)–(1.9), while the existence theorem is given for solutions that can be represented by (1.11) with a suitable choice of the density $\underline{a}$ in an appropriate function space. We prove an integral representation formula for $\underline{E}$ in terms of the value for $\underline{x} \in \partial D$ of $[\underline{n}, \underline{E}](\underline{x})$, $[\underline{n}, \text{curl}\, \underline{E}](\underline{x})$, and a series expansion of $\underline{E}$ when $\|\underline{x}\| \to \infty$ whose leading term contains the so-called far field. Moreover, we introduce a new numerical method to compute the function $\underline{E}(\underline{x})$ solution of (1.6)–(1.9) when ∂D is smooth, i.e., $\rho \in \mathbf{C}_0^\infty(\mathbf{R}^2)$. This method is based on the integral representation formula for $\underline{E}$ quoted above and on a new formalism that generalizes the formalism introduced in acoustics by Milder.[5] Milder[10] has also considered the electromagnetic case obtaining results similar to the ones contained in Sec. V. Let $\underline{f}(\underline{x}) = (f_1(\underline{x}), f_2(\underline{x}), f_3(\underline{x}))^T$ be a vector field defined in $\mathbf{R}^3$. We denote with $\underline{f}_{|\partial D}$ the restriction of $\underline{f}$ on ∂D, we think of $\underline{f}_{|\partial D}$ as a function of $(x_1, x_2)^T \in \mathbf{R}^2$, i.e., $\underline{f}_{|\partial D}(x_1, x_2) = (f_{1,|\partial D}, f_{2,|\partial D}, f_{3,|\partial D})^T(x_1, x_2) = \underline{f}(x_1, x_2, \rho(x_1, x_2)), (x_1, x_2)^T \in \mathbf{R}^2$.

Let $\mathcal{T} \subset S'(\mathbf{R}^2)$ and $\widetilde{\mathcal{H}}$ be the vector space given by

$$\widetilde{\mathcal{H}} = \{\underline{g}(x_1, x_2) = (g_1, g_2, g_3)^T(x_1, x_2) \in \mathbf{C}^3, \quad (x_1, x_2)^T \in \mathbf{R}^2 | \exists \underline{f}: \mathbf{R}^3 \to \mathbf{C}^3, \underline{g}(x_1, x_2) = \underline{f}_{|\partial D}(x_1, x_2), \quad (\underline{f}(\underline{x}), \underline{n}(\underline{x})) = 0, \quad \forall \underline{x} \in \partial D, \quad f_{j,|\partial D} \in \mathcal{T}, \quad j = 1,2,3\}. \tag{1.13}$$

We define (formally) a nonlocal operator $\widetilde{M}: \widetilde{\mathcal{H}} \to \widetilde{\mathcal{H}}$ such that

$$(\widetilde{M}\underline{g})(\underline{x}) = \underline{v}(\underline{x}), \quad \underline{x} \in \partial D, \tag{1.14}$$

where the vector field $\underline{v} \in \widetilde{\mathscr{H}}$ is defined as follows:

Let $\underline{E}$ be the unique solution of the boundary value problem (1.6), (1.7), (1.9) with the boundary condition

$$[\underline{n}, \underline{E}](\underline{x}) = \underline{g}(\underline{x}), \quad \underline{x} \in \partial D. \tag{1.15}$$

Then we define

$$\underline{v}(\underline{x}) = [\underline{n}, \text{ curl } \underline{E}](\underline{x}) \quad \underline{x} \in \partial D. \tag{1.16}$$

The operator $\widetilde{M}$ allows us to determine the vector field $\underline{E}$ using the integral representation formula previously announced.

In Sec. II we give some preliminary results needed to prove the main theorems. In Sec. III we give a representation theorem for $\underline{E}$, an expansion of $\underline{E}$ when $\|\underline{x}\| \to \infty$, and a uniqueness theorem for the solution of the boundary value problem (1.6)–(1.9). In Sec. IV we introduce a system of integral equations associated to the boundary value problem (1.6)–(1.9) and we prove an existence and uniqueness theorem for the solution of this system. In Sec. V we introduce a computational method that is based on a ''power'' series expansion of the operator $\widetilde{M}$. This method involves only quadratures and is fully parallelizable. In Sec. VI some numerical results obtained on test problems with the computational method of Sec. V are shown.

II. SOME PRELIMINARY RESULTS

Let R, R' be positive constants with $R' > R$, and D, D^c be given by (1.1) and (1.2). Let

$$B(\underline{0},R) = \{\underline{y} \in \mathbf{R}^3 | \|\underline{y}\| < R\}, \tag{2.1}$$

$$\Omega_R^+ = \{\underline{y} \in D^c | \|\underline{y}\| = R\}, \tag{2.2}$$

$$D_{R,R'} = \{\underline{y} \in D^c | R < \|\underline{y}\| < R'\}, \tag{2.3}$$

$$C(\underline{0},R,R') = \{\underline{y} \in \partial D | R < \|\underline{y}\| < R'\}. \tag{2.4}$$

We denote with $S_{R_0} = \overline{B(\underline{0},R_0)} \cap \partial D$ a compact subset of ∂D such that $S_0 \subseteq S_{R_0}$. We have the following lemma.

Lemma 2.1: Let $\Phi(\underline{x},\underline{y})$ be given by (1.12) and $\underline{n}$ be given by (1.5). We have

$$\frac{\partial \Phi(\underline{x},\underline{y})}{\partial \underline{n}(\underline{y})} = O\left(\frac{x_3}{\|\underline{y}\|^2}\right), \quad \text{when } \|\underline{y}\| \to +\infty, \quad \underline{y} \in \partial D \backslash S_{R_0}, \quad \underline{x} \in D^c. \tag{2.5}$$

Proof: It follows from some elementary computations and the fact that

$$(\underline{n}(\underline{y}), \underline{x} - \underline{y}) = x_3, \quad \underline{x} \in D^c, \quad \underline{y} \in \partial D \backslash S_{R_0}. \tag{2.6}$$ ■

Let $\underline{y} = (y_1, y_2, y_3)^T \in \mathbf{R}^3$, $\nabla_{\underline{y}} = (\partial/\partial y_1, \partial/y_2, \partial/\partial y_3)^T$, $R > 0$, and $B(\underline{0},R)$ be such that $S_{R_0} \subset B(\underline{0},R)$. We define the following integral kernels:

$$K_R(\underline{x},\underline{z}) = 2 \int_{\partial D \backslash B(\underline{0},R)} \Phi(\underline{x},\underline{y}) \frac{\partial \Phi(\underline{y},\underline{z})}{\partial \underline{n}(\underline{y})} \, ds(\underline{y}), \quad \underline{x},\underline{z} \in (D^c \backslash \overline{B(\underline{0},R)}) \cup S_{R_0}, \tag{2.7}$$

and

$$V_R(\underline{x},\underline{z}) = -2\int_{\partial D\setminus B(\underline{0},R)} (\underline{n}(\underline{y}),[\underline{\nabla}_{\underline{y}}\Phi(\underline{x},\underline{y}),\ \underline{\nabla}_{\underline{y}}\Phi(\underline{y},\underline{z})])ds(\underline{y}),\quad \underline{x},\underline{z}\in(D^c\setminus\overline{B(\underline{0},R)})\cup S_{R_0}. \tag{2.8}$$

We have the following Lemma.

Lemma 2.2: Let Φ be given by (1.12), $\underline{x}=(x_1,x_2,x_3)^T$, and $\underline{x}^*=(x_1,x_2,-x_3)^T$; let $\underline{\tilde{n}}$ be the outward unit normal vector to $\partial B(\underline{0},R)$, and let $G^{\pm}$ be given by

$$G^{\pm}(\underline{x},\underline{y}) = \Phi(\underline{x},\underline{y}) \pm \Phi(\underline{x}^*,\underline{y}),\quad \underline{x},\underline{y}\in\mathbf{R}^3,\quad \underline{x}\neq\underline{y}. \tag{2.9}$$

The following identities hold:

$$K_R(\underline{x},\underline{z}) - \int_{\Omega_R^+}\left\{ G^+(\underline{x},\underline{y})\,\frac{\partial\Phi}{\partial\underline{\tilde{n}}(\underline{y})}(\underline{y},\underline{z}) - \frac{\partial G^+}{\partial\underline{\tilde{n}}(\underline{y})}(\underline{x},\underline{y})\Phi(\underline{y},\underline{z})\right\}ds(\underline{y})$$
$$= \begin{cases} 0, & \underline{x},\underline{z}\in S_{R_0},\\ -\Phi(\underline{x},\underline{z}), & \underline{x}\in D^c\setminus\overline{B(\underline{0},R)},\quad \underline{z}\in S_{R_0}, \end{cases} \tag{2.10}$$

and

$$K_R(\underline{z},\underline{x}) + \int_{\Omega_R^+}\left\{ G^-(\underline{x},\underline{y})\,\frac{\partial\Phi}{\partial\underline{\tilde{n}}(\underline{y})}(\underline{y},\underline{z}) - \frac{\partial G^-}{\partial\underline{\tilde{n}}(\underline{y})}(\underline{x},\underline{y})\Phi(\underline{y},\underline{z})\right\}ds(\underline{y})$$
$$= \begin{cases} 0, & \underline{x},\underline{z}\in S_{R_0},\\ +\Phi(\underline{x},\underline{z}), & \underline{x}\in D^c\setminus\overline{B(\underline{0},R)},\quad \underline{z}\in S_{R_0}. \end{cases} \tag{2.11}$$

Proof: Given $\underline{x}\in S_{R_0}$ and $\underline{z}\in S_{R_0}$, we consider the functions $\Phi(\underline{x},\underline{y})$ and $\Phi(\underline{y},\underline{z})$, $\underline{y}\in D_{R,R'}$. Since $\partial D_{R,R'} = \Omega_R^+\cup\Omega_{R'}^+\cup\overline{C(\underline{0},R,R')}$, applying Green's formulas to $\Phi(\underline{x},\underline{y})$ and $\Phi(\underline{y},\underline{z})$, on $D_{R,R'}$ and using the Helmholtz equation we obtain

$$0 = \int_{\Omega_R^+}\left\{\Phi(\underline{x},\underline{y})\,\frac{\partial\Phi}{\partial\underline{\tilde{n}}(\underline{y})}(\underline{y},\underline{z}) - \frac{\partial\Phi}{\partial\underline{\tilde{n}}(\underline{y})}(\underline{x},\underline{y})\Phi(\underline{y},\underline{z})\right\}ds(\underline{y})$$
$$+\int_{\Omega_{R'}^+}\left\{\Phi(\underline{x},\underline{y})\,\frac{\partial\Phi}{\partial\underline{\tilde{n}}(\underline{y})}(\underline{y},\underline{z}) - \frac{\partial\Phi}{\partial\underline{\tilde{n}}(\underline{y})}(\underline{x},\underline{y})\Phi(\underline{y},\underline{z})\right\}ds(\underline{y})$$
$$+\int_{\overline{C(\underline{0},R,R')}}\left\{\Phi(\underline{x},\underline{y})\,\frac{\partial\Phi}{\partial\underline{\tilde{n}}(\underline{y})}(\underline{y},\underline{z}) - \frac{\partial\Phi}{\partial\underline{\tilde{n}}(\underline{y})}(\underline{x},\underline{y})\Phi(\underline{y},\underline{z})\right\}ds(\underline{y}),$$
$$\underline{x},\underline{z}\in S_{R_0}. \tag{2.12}$$

Since Φ satisfies the Sommerfeld radiation condition at infinity, we have

$$\lim_{R'\to\infty}\int_{\Omega_{R'}^+}\left\{\Phi(\underline{x},\underline{y})\,\frac{\partial\Phi}{\partial\underline{\tilde{n}}(\underline{y})}(\underline{y},\underline{z}) - \frac{\partial\Phi}{\partial\underline{\tilde{n}}(\underline{y})}(\underline{x},\underline{y})\Phi(\underline{y},\underline{z})\right\}ds(\underline{y}) = 0,\quad \underline{x},\underline{z}\in S_{R_0}, \tag{2.13}$$

and since $\overline{C(\underline{0},R,R')}$ coincides with $\partial D\setminus B(\underline{0},R)$ when $R'\to+\infty$, from (2.12) and (2.13) we obtain

$$0=\int_{\Omega_R^+}\left\{\Phi(\underline{x},\underline{y})\,\frac{\partial\Phi}{\partial\underline{\tilde{n}}(\underline{y})}\,(\underline{y},\underline{z})-\frac{\partial\Phi}{\partial\underline{\tilde{n}}(\underline{y})}\,(\underline{x},\underline{y})\Phi(\underline{y},\underline{z})\right\}ds(\underline{y})$$
$$-\int_{\partial D\setminus B(\underline{0},R)}\left\{\Phi(\underline{x},\underline{y})\,\frac{\partial\Phi}{\partial\underline{n}(\underline{y})}\,(\underline{y},\underline{z})-\frac{\partial\Phi}{\partial\underline{n}(\underline{y})}\,(\underline{x},\underline{y})\Phi(\underline{y},\underline{z})\right\}ds(\underline{y}),\quad \underline{x},\underline{z}\in S_{R_0}. \tag{2.14}$$

Arguing as above with $\Phi(\underline{x}^*,\underline{y})$, $\Phi(\underline{y},\underline{z})$, $\underline{y}\in D_{R,R'}$, we have

$$0=\int_{\Omega_R^+}\left\{\Phi(\underline{x}^*,\underline{y})\,\frac{\partial\Phi}{\partial\underline{\tilde{n}}(\underline{y})}\,(\underline{y},\underline{z})-\frac{\partial\Phi}{\partial\underline{\tilde{n}}(\underline{y})}\,(\underline{x}^*,\underline{y})\Phi(\underline{y},\underline{z})\right\}ds(\underline{y})$$
$$-\int_{\partial D\setminus B(\underline{0},R)}\left\{\Phi(\underline{x}^*,\underline{y})\,\frac{\partial\Phi}{\partial\underline{n}(\underline{y})}\,(\underline{y},\underline{z})-\frac{\partial\Phi}{\partial\underline{n}(\underline{y})}\,(\underline{x}^*,\underline{y})\Phi(\underline{y},\underline{z})\right\}ds(\underline{y}),\quad \underline{x},\underline{z}\in S_{R_0}. \tag{2.15}$$

It is easy to see that

$$G^+(\underline{x},\underline{y})=2\Phi(\underline{x},\underline{y}),\quad \frac{\partial G^+}{\partial\underline{n}(\underline{y})}\,(\underline{x},\underline{y})=0,\quad \underline{x}\in S_{R_0},\quad \underline{y}\in\partial D\setminus\overline{B(\underline{0},R)}, \tag{2.16}$$

$$G^-(\underline{x},\underline{y})=0,\quad \frac{\partial G^-}{\partial\underline{n}(\underline{y})}\,(\underline{x},\underline{y})=2\,\frac{\partial\Phi}{\partial\underline{n}(\underline{y})}\,(\underline{x},\underline{y}),\quad \underline{x}\in S_{R_0},\quad \underline{y}\in\partial D\setminus\overline{B(\underline{0},R)}. \tag{2.17}$$

For $\underline{x}\in S_{R_0}$ and $\underline{z}\in S_{R_0}$ from (2.14)–(2.16) we have (2.10), and from (2.14), (2.15), and (2.17) we have (2.11).

The proofs of the identities (2.10) and (2.11) for $\underline{x}\in D^c\setminus\overline{B(\underline{0},R)}$ and $\underline{z}\in S_{R_0}$ are analogous to the previous ones. This concludes the proof. ■

Lemma 2.3: Let $R>0$, $B(\underline{0},R)\supset S_{R_0}$, Ω_R^+ and $\underline{\tilde{n}}$ be as above, and let Φ and V_R be given by (1.12) and (2.8), respectively. We have

$$V_R(\underline{x},\underline{z})=2\int_{\Omega_R^+}(\underline{\tilde{n}}(\underline{y}),\mathrm{curl}_{\underline{x}}\{\Phi(\underline{x},\underline{y})\boldsymbol{\nabla}_{\underline{y}}\Phi(\underline{y},\underline{z})\})ds(\underline{y}),\quad \underline{x},\underline{z}\in(D^c\setminus\overline{B(\underline{0},R)})\cup S_{R_0}. \tag{2.18}$$

Proof: Let $R'>R>0$, let $D_{R,R'}$ be given by (2.3), and let $\underline{\hat{n}}$ be the outer normal vector to $\partial D_{R,R'}$. Applying the divergence theorem and some elementary vector identities we obtain

$$\int_{D_{R,R'}}\mathrm{div}_{\underline{y}}\,\mathrm{curl}_{\underline{x}}\{\Phi(\underline{x},\underline{y})\boldsymbol{\nabla}_{\underline{y}}\Phi(\underline{y},\underline{z})\}d\underline{y}$$
$$=-\int_{D_{R,R'}}\mathrm{div}_{\underline{y}}\{[\boldsymbol{\nabla}_{\underline{y}}\Phi(\underline{x},\underline{y}),\ \boldsymbol{\nabla}_{\underline{y}}\Phi(\underline{y},\underline{z})]\}d\underline{y}$$
$$=-\int_{\partial D_{R,R'}}(\underline{\hat{n}}(\underline{y}),[\boldsymbol{\nabla}_{\underline{y}}\Phi(\underline{x},\underline{y}),\ \boldsymbol{\nabla}_{\underline{y}}\Phi(\underline{y},\underline{z})])ds(\underline{y}),$$
$$\underline{x},\underline{z}\in(D^c\setminus\overline{B(\underline{0},R)})\cup S_{R_0}. \tag{2.19}$$

We have

$$\int_{D_{R,R'}} \operatorname{div}_{\underline{y}}\{[\nabla_{\underline{y}}\Phi(\underline{x},\underline{y}),\ \nabla_{\underline{y}}\Phi(\underline{y},\underline{z})]\}d\underline{y}=0, \quad \underline{x},\underline{z}\in(D^c\backslash\overline{B(\underline{0},R)})\cup S_{R_0}; \tag{2.20}$$

moreover, we obtain by straightforward calculation

$$\lim_{R'\to+\infty}\int_{\Omega^+_{R'}}(\hat{\underline{n}}(\underline{y}),[\nabla_{\underline{y}}\Phi(\underline{x},\underline{y}),\ \nabla_{\underline{y}}\Phi(\underline{y},\underline{z})])ds(\underline{y})=0. \tag{2.21}$$

Let $C(\underline{0},R,R')$ be given by (2.4). Since $\partial D_{R,R'}=\Omega^+_R\cup\Omega^+_{R'}\cup\overline{C(\underline{0},R,R')}$ and $\overline{C(\underline{0},R,R')}$ coincides with $\partial D\backslash B(\underline{0},R)$ when $R'\to+\infty$, from (2.19) using (2.20) and (2.21) we have the thesis.■

Lemma 2.4: Let Φ and K_R be given by (1.12) and (2.7). Let $R>0$ be such that $S_{R_0}\subset B(\underline{0},R)$, we have:

$$\int_{\partial D\backslash B(\underline{0},R)}\left\{\frac{\partial\Phi}{\partial x_j}(\underline{x},\underline{y})\,\frac{\partial\Phi}{\partial\underline{n}(\underline{y})}(\underline{y},\underline{z})\right\}ds(\underline{y})=\frac{1}{2}\,\frac{\partial K_R}{\partial x_j}(\underline{x},\underline{z}),$$

$$j=1,2, \quad \underline{x}\in(D^c\backslash\overline{B(\underline{0},R)})\cup S_{R_0}, \quad \underline{z}\in S_{R_0}. \tag{2.22}$$

Proof: For $\underline{x}\in(D^c\backslash\overline{B(\underline{0},R)})\cup S_{R_0}$ and $\underline{z}\in S_{R_0}$ we consider the following functions:

$$\frac{\partial\Phi}{\partial x_j}(\underline{x},\underline{y}), \quad \Phi(\underline{y},\underline{z}), \quad \underline{y}\in D_{R,R'}, \tag{2.23}$$

and

$$\frac{\partial\Phi}{\partial x_j}(\underline{x}^*,\underline{y}), \quad \Phi(\underline{y},\underline{z}), \quad \underline{y}\in D_{R,R'}, \tag{2.24}$$

the proof now follows as in Lemma 2.2. ■

Let $\mathscr{F}$ be the Fourier transform defined on $\mathscr{S}(\mathbf{R}^2)$, that is,

$$\hat{f}(\underline{k})=(\mathscr{F}f)(\underline{k})=\int_{\mathbf{R}^a}f(\underline{\xi})e^{-\iota(\underline{k},\underline{\xi})}d\underline{\xi}, \quad f\in\mathscr{S}(\mathbf{R}^2), \quad \underline{k}\in\mathbf{R}^2, \tag{2.25}$$

and $\mathscr{F}^{-1}$ be the inverse Fourier transform, where $\underline{k}=(k_1,k_2)^T\in\mathbf{R}^2$ is the conjugate variable of $\underline{\xi}=(\xi_1,\xi_2)^T\in\mathbf{R}^2$. We continue to denote with $\mathscr{F}$ and $\mathscr{F}^{-1}$ the extension of $\mathscr{F}$ and $\mathscr{F}^{-1}$ to $\mathscr{S}'(\mathbf{R}^2)$. Let $p:\mathbf{R}^2\to\mathbf{C}$ be the function defined by

$$p(\underline{k})=p(k_1,k_2)=\begin{cases}\sqrt{k_0^2-k_1^2-k_2^2}, & k_1^2+k_2^2\leqslant k_0^2,\\ \iota\sqrt{k_1^2+k_2^2-k_0^2}, & k_1^2+k_2^2>k_0^2,\end{cases} \tag{2.26}$$

and let $l_j:\mathbf{R}^2\to\mathbf{C}$, $j=1,2$, be the functions defined by $l_j(\underline{k})=l_j(k_1,k_2)=k_j$, $j=1,2$. From now on, with abuse of notation, we denote with f the maximal multiplication operator associated to the function $f(\underline{x})$. We define the operators $\tilde{q}$, $\tilde{q}_j$, $j=1,2$,: $\mathscr{S}'(\mathbf{R}^2)\to\mathscr{S}'(\mathbf{R}^2)$, as follows

$$\tilde{q}=\mathscr{F}^{-1}p\mathscr{F}, \tag{2.27}$$

$$\tilde{q}_j=\mathscr{F}^{-1}l_j\mathscr{F}, \quad j=1,2. \tag{2.28}$$

Let $\underline{\xi}=(\xi_1,\xi_2)^T\in\mathbf{R}^2$, $\underline{x}=(\underline{\xi}^T,x_3)^T$ be a generic vector in $\mathbf{R}^3$, let $\rho\in\mathscr{C}_0^2(\mathbf{R}^2)$ [see (1.1)–(1.3)], and D_ρ be the open set defined by

$$D_\rho=\{(\underline{\xi}^T,x_3)^T\in\mathbf{R}^3|\min\{\rho(\underline{\xi}),0\}<x_3,\underline{\xi}\in\mathbf{R}^2\}. \tag{2.29}$$

Let $z_0\in\mathbf{R}$ be a constant such that $z_0<\min_{\underline{\xi}\in\mathbf{R}^2}\{\rho(\underline{\xi})\}$. For $\tilde{u}\in\mathscr{S}'(\mathbf{R}^2)$ we define

$$F_1(\underline{k})=\frac{\iota e^{-\iota p(\underline{k})z_0}}{2p(\underline{k})}(\mathscr{F}\tilde{u})(\underline{k}),\quad \underline{k}\in\mathbf{R}^2, \tag{2.30}$$

and

$$\tilde{\mathscr{O}}=\left\{f:D_\rho\to\mathbf{C}\,\middle|\,\exists\tilde{u}\in\mathscr{S}'(\mathbf{R}^2)\right.$$
$$\text{such that } f(\underline{\xi}^T,x_3)=\int_{\mathbf{R}^2}F_1(\underline{k})e^{\iota p(\underline{k})x_3}e^{\iota(\underline{k},\underline{\xi})}\frac{d\underline{k}}{4\pi^2},$$
$$\left.\text{where } F_1(\underline{k}) \text{ is given by (2.30)},\quad (\underline{\xi}^T,x_3)^T\in D_\rho\right\}. \tag{2.31}$$

Moreover, let

$$\tilde{F}(\underline{k})=-\frac{e^{\iota p(k)z_0}}{2p(\underline{k})}[(k_1,k_2,p(\underline{k}))^T,\ ((\mathscr{F}u_1)(\underline{k}),(\mathscr{F}u_2)(\underline{k}),(\mathscr{F}u_3)(\underline{k}))^T], \tag{2.32}$$

and

$$\tilde{\mathscr{H}}=\left\{\underline{F}:D_\rho\to\mathbf{C}^3,\quad \underline{F}(\underline{x})=(F_1(\underline{x}),F_2(\underline{x}),F_3(\underline{x}))^T,\right.$$
$$|\exists\underline{u},\underline{u}(\underline{\xi})=(u_1(\underline{\xi}),u_2(\underline{\xi}),u_3(\underline{\xi}))^T,\underline{\xi}\in\mathbf{R}^2,u_j\in\mathscr{S}'(R^2),\quad j=1,2,3,$$
$$\text{such that } \underline{F}(\underline{\xi}^T,x_3)=\int_{\mathbf{R}^2}\tilde{\underline{F}}(\underline{k})e^{\iota p(\underline{k})x_3}e^{\iota(\underline{k},\underline{\xi})}d\underline{k}/4\pi^2,$$
$$\left.\text{where } \tilde{\underline{F}}(\underline{k}) \text{ is given by (2.32)},\quad (\underline{\xi}^{\mathrm{T}},\mathrm{x}_3)^{\mathrm{T}}\in\mathrm{D}_\rho\right\}. \tag{2.33}$$

We have the following.

Lemma 2.5: Let $\tilde{q},\tilde{q}_j$, $j=1,2$, be given by (2.27), (2.28), and $f\in\tilde{\mathscr{O}}$. Then f is a solution of the Helmholtz equation in D_ρ and we have

$$\frac{\partial f}{\partial x_3}(\underline{x})=\iota(\tilde{q}f\ )(\underline{x}),\quad \underline{x}\in\{x_3=0\}, \tag{2.34}$$

$$\frac{\partial f}{\partial x_j}(\underline{x})=\iota(\tilde{q}_jf\ )(\underline{x}),\quad \underline{x}\in\{x_3=0\},\quad j=1,2. \tag{2.35}$$

Moreover, let $\tilde{Z}$ be the operator defined by

$$\tilde{Z}:f(\underline{\xi}^T,0)\to f(\underline{\xi}^T,\rho(\underline{\xi})),\quad \underline{\xi}\in\mathbf{R}^2,\quad f\in\tilde{\mathscr{O}}. \tag{2.36}$$

Then the formal expansion of $\tilde{Z}$ in ''powers of ρ'' is given by

$$\tilde{Z}=\sum_{m=0}^{\infty}\frac{1}{m!}\rho^m(\iota\tilde{q})^m, \tag{2.37}$$

where we have denoted with ρ the maximal multiplication operator associated to $\rho(\underline{\xi})$, $\underline{\xi}\in\mathbf{R}^2$.

Proof (formal): An easy computation shows that any function $f\in\tilde{\mathscr{O}}$ is a solution of the Helmholtz equation in D_ρ. Formulas (2.34) and (2.35) are obtained differentiating the representation formula of $f\in\tilde{\mathscr{O}}$ [see (2.31)] and using the definition of $\tilde{q}$, $\tilde{q}_j$, $j=1,2$. The formal expansion

in ''powers of ρ'' of the operator $\tilde{Z}$ is obtained from the representation formula of $f \in \tilde{\mathcal{Q}}$ and the Taylor's expansion of $e^{\iota p(\underline{\xi})\rho(\underline{\xi})}$, with base point zero. ■

Lemma 2.6: Let $\underline{F} \in \tilde{\mathcal{A}}$. Then $F_j \in \tilde{\mathcal{Q}}$, $j=1,2,3$, and $\underline{F}(\underline{x})$, $\underline{x} \in D_\rho$ is a divergence free vector field solution of the vector Helmholtz equation on D_ρ.

Proof: In fact, we have

$$\int_{\mathbf{R}^2} \underline{\tilde{F}}(\underline{k}) e^{\iota p(\underline{k}) x_3} e^{\iota(\underline{k},\underline{\xi})} \frac{d\underline{k}}{4\pi^2} = \int_{\mathbf{R}^2} \mathrm{curl}_{\underline{x}} \{\underline{F}^*(\underline{k}) e^{\iota p(\underline{k}) x_3} e^{\iota(\underline{k},\underline{\xi})}\} \frac{d\underline{k}}{4\pi^2}, \quad (\underline{\xi}^T, x_3)^T \in D_\rho, \tag{2.38}$$

where $\underline{F}^*$ is the vector field given by

$$\underline{F}^*(\underline{k}) = \frac{\iota e^{-\iota p(\underline{k}) z_0}}{2p(\underline{k})} ((\mathcal{F}u_1)(\underline{k}), (\mathcal{F}u_2)(\underline{k}), (\mathcal{F}u_3)(\underline{k}))^T. \tag{2.39}$$

The thesis follows from the representation formula of $\underline{F} \in \tilde{\mathcal{A}}$ [see (2.33)]. ■

III. A REPRESENTATION FORMULA AND THE FAR-FIELD EXPANSION

Let $\mathcal{R}(D^c)$ be given by

$$\mathcal{R}(D^c) = \{\underline{E}: \mathbf{R}^3 \backslash D \to \mathbf{C}^3 | \underline{E} \in \mathcal{C}^2(\mathbf{R}^3 \backslash \overline{D}) \cap \mathcal{C}^0(\mathbf{R}^3 \backslash D), \quad \mathrm{div}\ \underline{E},\ \mathrm{curl}\ \underline{E} \in \mathcal{C}^0(\mathbf{R}^3 \backslash D)\},$$

and let $|\underline{E}|^2 = (\underline{E}, \overline{\underline{E}})$, where the overbar denotes the complex conjugate.

Lemma 3.1: Let $\underline{E} \in \mathcal{R}(D^c)$ be a solution of the boundary value problem (1.6)–(1.9). Then there exist two constants $c>0$, $R>0$ such that

$$\int_{\Omega_R^+} |\underline{E}(\underline{x})|^2 ds(\underline{x}) \leqslant c < \infty, \quad R > \overline{R}, \tag{3.1}$$

where Ω_R^+ is given by (2.2).

Proof: Let $D_R = D^c \cap B(\underline{0}, R)$, and let $\underline{n}_R$ be the outward unit normal vector to ∂D_R. We have

$$\partial D_R = \Omega_R^+ \cup (\partial D \cap \overline{B(\underline{0}, R)}), \tag{3.2}$$

$$\underline{n}_R(\underline{x}) = -\underline{n}(\underline{x}), \quad \underline{x} \in \partial D \cap \overline{B(\underline{0}, R)}, \tag{3.3}$$

where ∂D is given by (1.3) and $\underline{n}$ by (1.5). From the first Green's theorem and the radiation condition (1.9) we have

$$\begin{aligned} 0 &= \lim_{R \to +\infty} \int_{\Omega_R^+} |[\mathrm{curl}\ \underline{E}(\underline{y}),\ \underline{n}_R(\underline{y})]|^2 + k_0^2 |\underline{E}(\underline{y})|^2\ ds(\underline{y}) \\ &= -2\,\mathrm{Im}\left\{ k_0 \int_{\partial D} ([\underline{n}(\underline{y}),\ \underline{E}(\underline{y})], \mathrm{curl}\ \overline{\underline{E}(\underline{y})}) ds(\underline{y}) \right\}, \end{aligned} \tag{3.4}$$

where $\mathrm{Im}\{\cdot\}$ denotes the imaginary part of $\{\cdot\}$. The thesis follows from (3.4) and (1.8) noting that the last integral in (3.4) is convergent. ■

Theorem 3.2: Let $\underline{E} \in \mathcal{R}(D^c)$ be the vector field of Lemma 3.1 and let Φ be given by (1.12). Then the following representation formula holds:

$$\int_{\partial D} \mathrm{curl}_{\underline{x}}\{[\underline{n}(\underline{y}),\ \underline{E}(\underline{y})]\Phi(\underline{x},\underline{y})\}ds(\underline{y}) + \frac{1}{k_0^2}\int_{\partial D} \mathrm{curl}_{\underline{x}}\ \mathrm{curl}_{\underline{x}}\{[\underline{n}(\underline{y}),\ \mathrm{curl}\ \underline{E}(\underline{y})]\Phi(\underline{x},\underline{y})\}ds(\underline{y})$$

$$= \begin{cases} \underline{E}(\underline{x}), & \underline{x} \in D^c, \\ 0, & \underline{x} \in D. \end{cases} \tag{3.5}$$

Proof: The proof of formula (3.5) is analogous to the proof of a similar formula for the solution of the Helmholtz equation in the exterior of a bounded domain (see Ref. 1, Th. 4.5, p. 113). ■

Theorem 3.3: Let $\underline{E} \in \mathscr{R}(D^c)$ be the vector field of Lemma 3.1. There exists $R>0$ such that $\underline{E}$ can be extended to a vector field $\widetilde{\underline{E}}$ defined in $\mathbf{R}^3\backslash\overline{B(\underline{0},R)}$ and

$$\widetilde{\underline{E}}(\underline{x}) = \frac{e^{ik_0\|\underline{x}\|}}{4\pi\|\underline{x}\|}\sum_{n=0}^{\infty}\frac{\underline{F}_n(\hat{\underline{x}})}{\|\underline{x}\|^n}, \quad \hat{x} = \frac{\underline{x}}{\|\underline{x}\|}, \quad \underline{x} \neq \underline{0}, \quad \underline{x} \in \mathbf{R}^3\backslash\overline{B(\underline{0},R)}, \tag{3.6}$$

where the expansion (3.6) converges absolutely and uniformly for $\|\underline{x}\|>R$.

Moreover, we have

$$(\hat{\underline{x}}, \underline{F}_0(\hat{\underline{x}})) = 0. \tag{3.7}$$

Proof: Let $R>0$, such that $B(\underline{0},R)\supset \mathrm{supp}\ \underline{g}\cup S_0$ [see (1.4), (1.8), and (2.1)], $S_R = B(\underline{0},R)\cap\partial D$, $\underline{x} = (x_1,x_2,x_3)^T \in D^c\backslash\overline{B(\underline{0},R)}$, and $\underline{x}^* = (x_1,x_2,-x_3)^T \in D$. We define the following vector functions:

$$\underline{\eta}^{\pm} = (\eta_1^{\pm},\eta_2^{\pm},\eta_3^{\pm})^T = \mathrm{curl}_{\underline{s}}\{\Phi(\underline{s},\underline{y})[\underline{n}(\underline{y}),\ \underline{E}(\underline{y})]\}_{|_{\underline{s}=\underline{x}}} \pm \mathrm{curl}_{\underline{s}}\{\Phi(\underline{s},\underline{y})[\underline{n}(\underline{y}),\ \underline{E}(\underline{y})]\}_{|_{\underline{s}=\underline{x}^*}},$$

$$\underline{y} \in \partial D, \tag{3.8}$$

and

$$\underline{\chi}^{\pm} = (\chi_1^{\pm},\chi_2^{\pm},\chi_3^{\pm})^T = \mathrm{curl}_{\underline{s}}\ \mathrm{curl}_{\underline{s}}\{\Phi(\underline{s},\underline{y})[\underline{n}(\underline{y}),\mathrm{curl}\ \underline{E}(\underline{y})]\}_{|_{\underline{s}=\underline{x}}} \pm \mathrm{curl}_{\underline{s}}\ \mathrm{curl}_{\underline{s}}\{\Phi(\underline{s},\underline{y})$$

$$[\underline{n}(\underline{y}),\mathrm{curl}\ \underline{E}(\underline{y})]\}_{|_{\underline{s}=\underline{x}^*}}, \quad \underline{y} \in \partial D. \tag{3.9}$$

For $\underline{y} \in \partial D\backslash S_R$ we have

$$\chi_j^-(\underline{x},\underline{y}) = 0, \quad j=1,2, \quad \underline{y} \in D\backslash S_R, \quad \underline{x} \in D^c\backslash\overline{B(\underline{0},R)}, \tag{3.10}$$

and

$$\chi_3^+(\underline{x},\underline{y}) = 0, \quad \underline{y} \in \partial D\backslash S_R, \quad \underline{x} \in D^c\backslash\overline{B(\underline{0},R)}. \tag{3.11}$$

From Theorem 3.2, (3.10), (3.11), and (1.8) we obtain

$$E_j(\underline{x}) = \int_{S_R}\eta_j^-(\underline{x},\underline{y})ds(\underline{y}) + \frac{1}{k_0^2}\int_{S_R}\chi_j^-(\underline{x},\underline{y})ds(\underline{y}), \quad j=1,2, \quad \underline{x} \in D^c\backslash\overline{B(\underline{0},R)} \tag{3.12}$$

and

$$E_3(\underline{x}) = \int_{S_R}\eta_3^+(\underline{x},\underline{y})ds(\underline{y}) + \frac{1}{k_0^2}\int_{S_R}\chi_3^+(\underline{x},\underline{y})ds(\underline{y}), \quad \underline{x} \in D^c\backslash\overline{B(\underline{0},R)}. \tag{3.13}$$

Using (3.12) and (3.13), $\underline{E}$ can be extended to a vector field $\underline{\tilde{E}}$ defined in $\mathbf{R}^3\backslash\overline{B(\underline{0},R)}$, which is a divergence-free vector field satisfying the vector Helmholtz equation and the radiation condition (1.9). This field has an expansion of the form (3.6) [see Ref. 1, Th. 4.8, p. 116]. The proof of (3.7) follows from (3.6) and (1.9). ■

Corollary 3.4: Let $\hat{\underline{x}} = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)^T$. Then, the coefficients $\underline{F}_n(\hat{\underline{x}}) = \underline{F}_n(\theta,\varphi)$ in (3.6) are given by

$$2\imath k_0 n\underline{F}_n = n(n-1)\underline{F}_{n-1} + \mathscr{B}\underline{F}_{n-1}, \quad n=1,2,\ldots, \tag{3.14}$$

where

$$\mathscr{B} = \frac{1}{\sin(\theta)}\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2(\theta)}\frac{\partial^2}{\partial\varphi^2} \tag{3.15}$$

is the Beltrami operator on the sphere.

Proof: The proof follows from Theorem 3.3, since the expansion in (3.6) satisfies term-by-term the vector Helmholtz equation. ■

Corollary 3.5: Let $\underline{E} \in \mathscr{R}(D^c)$ be the vector field of Lemma 3.1. If $\underline{F}_0(\hat{\underline{x}}) \equiv 0$, $\hat{\underline{x}} = \underline{x}/\|\underline{x}\|$, $\underline{x} \neq \underline{0}$, $\underline{x} \in D^c$, then $\underline{E}(\underline{x}) \equiv \underline{0}$.

Proof: From Corollary 3.4 it is easy to see that $\underline{F}_0(\hat{\underline{x}}) \equiv 0$ implies $\underline{F}_n(\hat{\underline{x}}) \equiv 0$, $n=1,2,\ldots$. The proof follows from Theorem 3.3 using the expansion in (3.6). ■

Lemma 3.6: Let $\underline{E} \in \mathscr{R}(D^c)$ be the vector field of Lemma 3.1 and let $\underline{n}$ be given by (1.5). If

$$\mathrm{Im}\left\{k_0\int_{\partial D} ds(\underline{y})(\underline{n}(\underline{y}), [\underline{E}(\underline{y}), \mathrm{curl}\,\overline{\underline{E}(\underline{y})}])\right\} \geq 0, \tag{3.16}$$

then we have

$$\underline{E}(\underline{x}) = \underline{0}, \quad \underline{x} \in D^c. \tag{3.17}$$

Proof: The proof follows from a standard argument (see Ref. 1, Th. 4.17, p. 125), using (1.8) and (1.9). ■

Theorem 3.7: Let $\mathrm{Im}\{k_0\} \geq 0$. Then the boundary value problem (1.6)–(1.9) has at most one solution in $\mathscr{R}(D^c)$.

Proof: We assume by contradiction that $\underline{E}$ and $\underline{E}^*$ are two solutions of the boundary value problem (1.6)–(1.9). The vector field $\underline{\tilde{E}} = \underline{E} - \underline{E}^*$ is a solution of the boundary value problem (1.6)–(1.9) with homogeneous boundary condition; that is,

$$[\underline{n}(\underline{x}), \underline{\tilde{E}}(\underline{x})] = \underline{0}, \quad \underline{x} \in \partial D. \tag{3.18}$$

From condition (3.18) and the properties of the triple product $(\cdot,[\cdot,\cdot])$ we obtain

$$\mathrm{Im}\left\{k_0\int_{\partial D} (\underline{n}(\underline{y}), [\underline{\tilde{E}}(\underline{y}), \mathrm{curl}\,\overline{\underline{\tilde{E}}(\underline{y})}])\right\} = 0. \tag{3.19}$$

The thesis follows from (3.19) and Lemma 3.6. ■

IV. AN EXISTENCE AND UNIQUENESS THEOREM FOR THE SOLUTION OF THE SYSTEM OF INTEGRAL EQUATIONS

Let $S_{R_0} = \overline{B(\underline{0},R_0)} \cap \partial D$ be a compact subset of ∂D such that $S_{R_0} \supseteq S_0$. Let $\tilde{\mathscr{C}}(S_{R_0})$ be the Cartesian product of three copies of $\mathbf{C}^0(S_{R_0})$, and let $\underline{\varphi} \in \tilde{\mathscr{C}}(S_{R_0})$ be a vector continuous tangential density, that is,

$$(\underline{\varphi}(\underline{x}),\underline{n}(\underline{x}))=0, \quad \underline{x} \in S_{R_0}, \tag{4.1}$$

where $\underline{n}$ is given by (1.5).

Let $\tilde{\underline{\varphi}}$ be the vector function defined on the set $\partial D \backslash S_{R_0}$ given by

$$\tilde{\underline{\varphi}}(\underline{x}) = -2\int_{S_{R_0}} [\underline{n}(\underline{x}), \operatorname{curl}_{\underline{x}}\{\phi(\underline{x},\underline{y})\underline{\varphi}(\underline{y})\}]ds(\underline{y}), \quad \underline{x} \in \partial D \backslash S_{R_0}, \tag{4.2}$$

where the integral in (4.2) exists as a Cauchy principal value when $\underline{x} \in \partial S_{R_0}$.

Lemma 4.1: Let $\underline{\varphi}$, $\tilde{\underline{\varphi}}$ be given by (4.1) and (4.2), respectively. Then $\tilde{\underline{\varphi}}$ is a continuous tangential vector function on $\partial D \backslash S_{R_0}$, i.e., $\tilde{\underline{\varphi}} \in \tilde{\mathscr{C}}(\partial D \backslash S_{R_0})$ and we have

$$\begin{aligned}\tilde{\varphi}_1(\underline{y}) &= -2\int_{S_{R_0}} \frac{\partial \phi}{\partial y_1}(\underline{y},\underline{z})\varphi_3(\underline{z})ds(\underline{z}) + 2\int_{S_{R_0}} \frac{\partial \phi}{\partial \underline{n}(\underline{y})}(\underline{y},\underline{z})\varphi_1(\underline{z})ds(\underline{z}) \\ &= O\left(\frac{1}{\|\underline{y}\|}\right), \quad \|\underline{y}\| \to +\infty, \quad \underline{y} \in \partial D \backslash S_{R_0},\end{aligned} \tag{4.3}$$

$$\begin{aligned}\tilde{\varphi}_2(\underline{y}) &= -2\int_{S_{R_0}} \frac{\partial \phi}{\partial y_2}(\underline{y},\underline{z})\varphi_3(\underline{z})ds(\underline{z}) + 2\int_{S_{R_0}} \frac{\partial \phi}{\partial \underline{n}(\underline{y})}(\underline{y},\underline{z})\varphi_2(\underline{z})ds(\underline{z}) \\ &= O\left(\frac{1}{\|\underline{y}\|}\right), \quad \|\underline{y}\| \to +\infty, \quad \underline{y} \in \partial D \backslash S_{R_0},\end{aligned} \tag{4.4}$$

$$\tilde{\varphi}_3(\underline{y}) = 0, \quad \underline{y} \in \partial D \backslash S_{R_0}, \tag{4.5}$$

$$\tilde{\varphi}_2(\underline{y})(x_1-y_1) - \tilde{\varphi}_1(\underline{y})(x_2-y_2) = O\left(\frac{f(\underline{x})}{\|\underline{y}\|}\right), \quad \|\underline{y}\| \to +\infty, \quad \underline{y} \in \partial D \backslash S_{R_0}, \quad \underline{x} \in S_{R_0}, \tag{4.6}$$

where $f \in \mathscr{C}^0(S_{R_0})$ is a suitable function.

Proof: The proof follows by an easy computation from the definitions (1.12), (4.2), and Lemma 2.1. ■

Let K be the operator on $\tilde{\mathscr{C}}(S_{R_0})$ defined by

$$\begin{aligned}(K\underline{\varphi})(\underline{x}) &= 2\int_{S_{R_0}} [\underline{n}(\underline{x}),\ \operatorname{curl}_{\underline{x}}\{\phi(\underline{x},\underline{y})\underline{\varphi}(\underline{y})\}]ds(\underline{y}) \\ &\quad + 2\int_{\partial D \backslash S_{R_0}} [\underline{n}(\underline{x}),\ \operatorname{curl}_{\underline{x}}\{\phi(\underline{x},\underline{y})\tilde{\underline{\varphi}}(\underline{y})\}]ds(\underline{y}), \quad \underline{x} \in S_{R_0},\end{aligned} \tag{4.7}$$

where $\underline{\varphi}, \tilde{\underline{\varphi}}$ are given by (4.1) and (4.2).

Lemma 4.2: The operator K in (4.7) is a compact operator on $\tilde{\mathscr{C}}(S_{R_0})$.

Proof: Let $B(\underline{0},R)$ given by (2.1) such that $B(\underline{0},R)\supset S_{R_0}$. From the definition (4.7) we obtain

$$(K\underline{\varphi})(\underline{x})=2\int_{S_{R_0}}[\underline{n}(\underline{x}),\ \mathrm{curl}_{\underline{x}}\{\phi(\underline{x},\underline{y})\underline{\varphi}(\underline{y})\}]ds(\underline{y})$$
$$+2\int_{(\partial D\cap B(\underline{0},R))\setminus S_{R_0}}[\underline{n}(\underline{x}),\ \mathrm{curl}_{\underline{x}}\{\phi(\underline{x},\underline{y})\widetilde{\underline{\varphi}}(\underline{y})\}]ds(\underline{y})$$
$$+2\int_{\partial D\setminus B(\underline{0},R))}[\underline{n}(\underline{x}),\ \mathrm{curl}_{\underline{x}}\{\phi(\underline{x},\underline{y})\widetilde{\underline{\varphi}}(\underline{y})\}]ds(\underline{y}),\quad \underline{x}\in S_{R_0}. \tag{4.8}$$

It is easy to see that the first two integrals on the right-hand side of (4.8) have weakly singular kernels on bounded surfaces, so that they are compact operators on $\widetilde{\mathscr{C}}(S_{R_0})$ (see Ref. 1, Th.1.11, p. 6). Now we study the last integral in (4.8). From the definition (4.2) and Lemmas 2.2, 2.3, and 2.4 we have

$$\int_{\partial D\setminus B(\underline{0},R)}\mathrm{curl}_{\underline{x}}\{\phi(\underline{x},\underline{y})\widetilde{\underline{\varphi}}(\underline{y})\}ds(\underline{y})$$
$$=2\int_{S_{R_0}}ds(\underline{z})\varphi_3(\underline{z})\int_{\partial D\setminus B(\underline{0},R)}[\boldsymbol{\nabla}_{\underline{y}}\phi(\underline{x},\underline{y}),\boldsymbol{\nabla}_{\underline{y}}\phi(\underline{y},\underline{z})]ds(\underline{y})$$
$$+2\int_{S_{R_0}}ds(\underline{z})\mathrm{curl}_{\underline{x}}\left\{\underline{\varphi}(\underline{z})\int_{\partial D\setminus B(\underline{0},R)}\phi(\underline{x},\underline{y})\frac{\partial\phi}{\partial\underline{n}(\underline{y})}(\underline{y},\underline{z})ds(\underline{y})\right\},\quad \underline{x}\in S_{R_0}. \tag{4.9}$$

By an easy computation we obtain

$$\int_{\partial D\setminus B(\underline{0},R)}[\boldsymbol{\nabla}_{\underline{y}}\phi(\underline{x},\underline{y}),\ \boldsymbol{\nabla}_{\underline{y}}\phi(\underline{y},\underline{z})]ds(\underline{y})$$
$$=\frac{1}{2}\left(-\frac{\partial K_R}{\partial x_2}(\underline{x},\underline{z})+\frac{\partial K_R}{\partial z_2}(\underline{z},\underline{x}),\ \frac{\partial K_R}{\partial x_1}(\underline{x},\underline{z})-\frac{\partial K_R}{\partial z_1}(\underline{z},\underline{x}),V_R(\underline{x},\underline{z})\right)^T,$$
$$\underline{x}\in S_{R_0},\quad \underline{z}\in S_{R_0}, \tag{4.10}$$

where K_R, V_R are the kernels given by (2.7) and (2.8). The thesis follows from (4.9) and (4.10) using the representation formulas (2.10), (2.11), (2.18), and (2.22). ■

Let $\varphi,\widetilde{\varphi}$ be the functions given by (4.1) and (4.2), and let $\underline{a}$ be the following vector function:

$$\underline{a}(\underline{x})=\begin{cases}\underline{\varphi}(\underline{x}), & \underline{x}\in S_{R_0},\\ \widetilde{\underline{\varphi}}(\underline{x}), & \underline{x}\in\partial D\setminus S_{R_0}.\end{cases} \tag{4.11}$$

Theorem 4.3: Let K and $\underline{a}$ be given by (4.7) and (4.11) and let $\underline{g}$ be the vector function in (1.8) with supp $\underline{g}\subseteq S_{R_0}$. If $\varphi\in\widetilde{\mathscr{C}}(S_{R_0})$ satisfies condition (4.1) and is a solution of the integral equation

$$\underline{\varphi}(\underline{x})+(K\underline{\varphi})(\underline{x})=2\underline{g}(\underline{x}),\quad \underline{x}\in S_{R_0}, \tag{4.12}$$

then we have

$$\left| \int_{\partial D} \operatorname{curl}_{\underline{x}}\{\phi(\underline{x},\underline{y})\underline{a}(\underline{y})\}ds(\underline{y}) \right| < \infty, \quad \underline{x} \in D^c, \tag{4.13}$$

$$\underline{a} \in \widetilde{\mathscr{C}}(\partial D), \quad (\underline{a}(\underline{x}),\underline{n}(\underline{x})) = 0, \quad \underline{x} \in \partial D, \tag{4.14}$$

and the vector $\underline{E}$ given by (1.11) is a solution of the boundary value problem (1.6)–(1.9).

Proof: Formula (4.13) follows from the definition of $\underline{a}$ using Lemmas 2.1 and 4.1. Moreover, it is easy to see that $\underline{E}$ is a free divergence field, solution of the vector Helmholtz equation (1.6). Now we prove the radiation condition (1.9). Let $R>0$, $B(\underline{0},R) \supset S_{R_0}$, and $\underline{e}_3 = (0,0,1)^T \in \mathbf{R}^3$. We have

$$\begin{aligned} \underline{E}(\underline{x}) = & \int_{S_{R_0}} \operatorname{curl}_{\underline{x}}\{\phi(\underline{x},\underline{y})\varphi(\underline{y})\}ds(\underline{y}) + \int_{(\partial D \cap B(\underline{0},R))\setminus S_{R_0}} \operatorname{curl}_{\underline{x}}\{\phi(\underline{x},\underline{y})\widetilde{\varphi}(\underline{y})\}ds(\underline{y}) \\ & + \int_{\partial D \setminus B(\underline{0},R)} \operatorname{curl}_{\underline{x}}\{\phi(\underline{x},\underline{y})\widetilde{\varphi}(\underline{y})\}ds(\underline{y}), \quad \underline{x} \in D^c. \end{aligned} \tag{4.15}$$

Let K_R and V_R be the kernels defined by (2.7) and (2.8). Applying Lemma 2.5 and the Lebesgue Theorem to interchange the order of integration we obtain

$$\begin{aligned} & \int_{\partial D \setminus B(\underline{0},R)} \operatorname{curl}_{\underline{x}}\{\phi(\underline{x},\underline{y})\widetilde{\varphi}(\underline{y})\}ds(\underline{y}) \\ & \quad = \int_{S_{R_0}} \varphi_3(\underline{y}) \operatorname{curl}_{\underline{y}}\{K_R(\underline{y},\underline{x})\underline{e}_3\}ds(\underline{y}) + \int_{S_{R_0}} \operatorname{curl}_{\underline{x}}\{K_R(\underline{x},\underline{y})\varphi(\underline{y})\}ds(\underline{y}) \\ & \qquad - \int_{S_{R_0}} \operatorname{curl}_{\underline{x}}\{K_R(\underline{x},\underline{y})\varphi_3(\underline{y})\underline{e}_3\}ds(\underline{y}) + \underline{e}_3 \int_{S_{R_0}} V_R(\underline{x},\underline{y})\varphi_3(\underline{y})ds(\underline{y}), \\ & \qquad \underline{x} \in D^c \setminus \overline{B(\underline{0},R)}. \end{aligned} \tag{4.16}$$

The radiation condition (1.9) follows from (4.15) and (4.16) using Lemmas 2.2 and 2.3 and the theory of electromagnetic field generated by a magnetic dipole. We note that when $\underline{a}$ satisfies (4.14) the boundary condition (1.8) follows immediately from the jump relations. So, we must prove (4.14). From the definition of $\underline{a}$ given by (4.11), using the integral equation (4.12) and Lemma 4.2, we have

$$\varphi(\underline{x}) = -(K\varphi)(\underline{x}), \quad \underline{x} \in \partial S_{R_0}. \tag{4.17}$$

By an easy computation, from the assumption (4.1) and noting that $(\partial\phi(\underline{x},\underline{y})/\partial\underline{n}(\underline{x})) = 0$, $\underline{x},\underline{y} \in \partial D \setminus S_{R_0}$ [see (1.4)], we obtain

$$[\underline{n}(\underline{x}),\ \operatorname{curl}_{\underline{x}}\{\phi(\underline{x},\underline{y})\underline{a}(\underline{y})\}] = 0, \quad \underline{x} \in \partial S_{R_0}, \quad \underline{y} \in \partial D \setminus S_{R_0}. \tag{4.18}$$

Taking the definitions (4.2), (4.7), and (4.11) into account, from (4.17) and (4.18) we obtain $\underline{a} \in \widetilde{\mathscr{C}}(\partial D)$. Finally from the definition of $\underline{a}$ and Lemma 4.1 it follows $(\underline{a}(\underline{x}),\underline{n}(\underline{x})) = 0$, $\underline{x} \in \partial D$. This concludes the proof. ■

Theorem 4.4: The boundary integral equation (4.12) has a unique solution $\varphi \in \widetilde{\mathscr{C}}(S_{R_0})$.

Proof: The thesis follows from the Fredholm theory using Lemma 4.2, Theorems 4.3 and 3.7, and the jump relation for vector potential with continuous tangential density. ■

V. A METHOD TO COMPUTE THE ELECTRIC FIELD IN A DISTURBED HALF-SPACE

We remind the reader that the content of this section is mainly formal. Let $\mathscr{T} \subseteq \mathscr{S}'(\mathbf{R}^2)$ be a vector subspace of the space of tempered distributions such that the operator compositions used later are defined in $\mathscr{T}$.

Let $\rho_l(x_1,x_2) \in \mathbf{C}^2(\mathbf{R}^2)$, $l=1,2$, be a bounded function on R^2, Γ_l, $l=1,2$, be the following surfaces:

$$\Gamma_l = \{\underline{x} = (x_1,x_2,x_3)^T \in \mathbf{R}^3 | x_3 = \rho_l(x_1,x_2), (x_1,x_2)^T \in \mathbf{R}^2\}, \quad l=1,2, \tag{5.1}$$

and D_{Γ_l}, $l=1,2$, be the following domains:

$$D_{\Gamma_l} = \{\underline{x} = (x_1,x_2,x_3)^T \in \mathbf{R}^3 | x_3 < \rho_l(x_1,x_2), (x_1,x_2)^T \in \mathbf{R}^2\}, \quad l=1,2. \tag{5.2}$$

For $l=1,2$, let $\underline{n}_{\Gamma_l}(\underline{x})$ be the unit vector normal to Γ_l in $\underline{x} \in \Gamma_l$ pointing inside $\mathbf{R}^3 \backslash \overline{D_{\Gamma_l}}$. We denote with $\mathscr{H}_{\Gamma_l}$ the vector spaces

$$\begin{aligned}\mathscr{H}_{\Gamma_l} = \{&\underline{g}(x_1,x_2) = (g_1,g_2,g_3)^T(x_1,x_2) \in \mathbf{C}^3, (x_1,x_2)^T \in \mathbf{R}^2 | \exists \underline{f}: \mathbf{R}^3 \to \mathbf{C}^3, \underline{g}(x_1,x_2) \\ &= \underline{f}_{|\Gamma_l}(x_1,x_2), (\underline{f}(\underline{x}), \underline{n}_{\Gamma_l}(\underline{x})) = 0, \forall \underline{x} \in \Gamma_l, f_{j,|\Gamma_l} \in \mathscr{T}, j=1,2,3\}.\end{aligned} \tag{5.3}$$

We define two transformations $\widetilde{L}_{\Gamma_l}: \mathscr{H}_{\Gamma_l} \to \mathscr{H}_{\Gamma_l}$, $l=1,2$, such that

$$(\widetilde{L}_{\Gamma_l} \underline{g}_{\Gamma_l})(\underline{x}) = \underline{v}_{\Gamma_l}(\underline{x}), \quad \underline{x} \in \Gamma_l, \quad l=1,2, \tag{5.4}$$

where the vector field $\underline{v}_{\Gamma_l}$, $l=1,2$, is defined as the vector field $\underline{v}$ in (1.14), when we replace ∂D with Γ_l, $l=1,2$, in (1.15) and (1.16) and D^c with $\mathbf{R}^3 \backslash \overline{D_{\Gamma_l}}$, $l=1,2$, in (1.6), (1.7), and (1.9). We introduce the transformation $\widetilde{G}: \mathscr{H}_{\Gamma_1} \to \mathscr{H}_{\Gamma_2}$ such that

$$(\widetilde{G} \underline{g}_{\Gamma_1})(\underline{x}) = \underline{g}_{\Gamma_2}(\underline{x}), \quad \underline{x} \in \Gamma_2, \tag{5.5}$$

where $\underline{g}_{\Gamma_2}$ is defined as follows:

Let $\underline{E}_{\Gamma_1}$ be the unique solution of the boundary value problem

$$(\Delta + k_0^2) \underline{E}_{\Gamma_1}(\underline{x}) = \underline{0}, \quad \underline{x} \in \mathbf{R}^3 \backslash \overline{D_{\Gamma_1}}, \tag{5.6}$$

$$\operatorname{div} \underline{E}_{\Gamma_1}(\underline{x}) = 0, \quad \underline{x} \in \mathbf{R}^3 \backslash \overline{D_{\Gamma_1}}, \tag{5.7}$$

$$\left[\operatorname{curl} \underline{E}_{\Gamma_1}(\underline{x}), \frac{\underline{x}}{\|\underline{x}\|}\right] - \iota k_0 \underline{E}_{\Gamma_1}(\underline{x}) = o\left(\frac{1}{\|\underline{x}\|}\right), \quad \|\underline{x}\| \to +\infty, \underline{x} \in \mathbf{R}^3 \backslash \overline{D_{\Gamma_1}}, \tag{5.8}$$

$$[\underline{n}_{\Gamma_1}, \underline{E}_{\Gamma_1}](\underline{x}) = \underline{g}_{\Gamma_1}(\underline{x}), \quad \underline{x} \in \Gamma_1. \tag{5.9}$$

We assume that there exists a unique function $\underline{F}$ defined in $\mathbf{R}^3 \backslash (D_{\Gamma_1} \cap D_{\Gamma_2})$ solution of (5.6)–(5.8) in $\mathbf{R}^3 \backslash (\overline{D_{\Gamma_1} \cap D_{\Gamma_2}})$ that coincides with $\underline{E}_{\Gamma_1}$ in $\mathbf{R}^3 \backslash \overline{D_{\Gamma_1}}$, and that belongs to $\widetilde{\mathscr{H}}$ [see (2.33)] and whose components belong to $\widetilde{\mathscr{O}}$ [see (2.31)] when D_ρ is replaced by $\mathbf{R}^3 \backslash (\overline{D_{\Gamma_1} \cap D_{\Gamma_2}})$. Then we define

$$\underline{g}_{\Gamma_2}(\underline{x}) = [\underline{n}_{\Gamma_2}, \underline{F}](\underline{x}), \quad \underline{x} \in \Gamma_2. \tag{5.10}$$

In this section we choose

$$\rho_1(x_1,x_2)=0, \quad (x_1,x_2)^T\in\mathbf{R}^2, \tag{5.11}$$

$$\rho_2(x_1,x_2)=\rho(x_1,x_2), \quad (x_1,x_2)^T\in\mathbf{R}^2. \tag{5.12}$$

We have $\Gamma_1=\{x_3=0\}$, $\Gamma_2=\partial D$, $D_{\Gamma_1}=\{\underline{x}\in\mathbf{R}^3|x_3<0\}$ and $D_{\Gamma_2}=D$, $\mathscr{H}_{\Gamma_2}=\widetilde{\mathscr{H}}$, with $\widetilde{\mathscr{H}}$ given by (1.13). With this particular choice we have

$$\widetilde{M}=\widetilde{L}_{\Gamma_2}; \tag{5.13}$$

moreover,

$$\widetilde{M}=\widetilde{G}\widetilde{L}_{\Gamma_1}\widetilde{G}^{-1}. \tag{5.14}$$

It is easy to see that $\widetilde{L}_{\Gamma_l}$, $l=1,2$, are linear transformation of $\mathscr{H}_{\Gamma_l}$ into $\mathscr{H}_{\Gamma_l}$, $l=1,2$, and $\widetilde{G}$ is a linear transformation of $\mathscr{H}_{\Gamma_1}$ into $\mathscr{H}_{\Gamma_2}$ so that $\widetilde{L}_{\Gamma_l}=((\widetilde{L}_{\Gamma_l,ij}))$, $\widetilde{G}=((\widetilde{G}_{ij}))$, $i,j=1,2,3$, $l=1,2$, can be represented by three-by-three operator-valued matrices. From (5.13) we have

$$\widetilde{M}=((\widetilde{M}_{ij})), \quad \widetilde{M}_{ij}=\widetilde{L}_{\Gamma_2,ij}, \quad i,j=1,2,3. \tag{5.15}$$

The computational method proposed here is a consequence of a nonlocal expansion ''in powers of ρ'' of $\widetilde{M}$ (see Proposition 5.9). The expansion is obtained using (5.14) and expanding the elements $\widetilde{M}_{ij}$, $i,j=1,2,3$, of the operator-valued matrix $\widetilde{M}$. Different choices of the reference surface $\Gamma_1=\{x_3=0\}$ generate different expansions of the operator $\widetilde{M}$ analogous to the one derived here. We note that the procedure to construct the operators $\widetilde{G}$, $\widetilde{L}_{\Gamma_1}$ is only formal. In fact, the existence of the operator $\widetilde{G}$ is based on the assumption that there exists a unique function $\underline{F}$ solution of (5.6)–(5.8) in $\mathbf{R}^3\backslash(\overline{D_{\Gamma_1}\cap D_{\Gamma_2}})$ that coincides in $\mathbf{R}^3\backslash\overline{D_{\Gamma_1}}$ with the unique solution $\underline{E}_{\Gamma_1}$ of the boundary value problem (5.6)–(5.9). Moreover, we assume that $\underline{F}\in\widetilde{\mathscr{H}}$ with $\widetilde{\mathscr{H}}$ given by (2.33). This is not proved here and is far from obvious. Moreover, the expansion of $\widetilde{M}$ is formal, that is, its convergence is not proved.

We construct now the expansion ''in powers of ρ'' of $\widetilde{M}$. Let $\widetilde{q}$, $\widetilde{q}_j$, $j=1,2$, and $\widetilde{Z}$ be the operators given by (2.27), (2.28), and (2.37), respectively. From (2.37) we have (formally)

$$\widetilde{Z}^{-1}=\sum_{m=0}^{\infty}(-1)^m\frac{1}{m!}\rho^m(\iota\widetilde{q})^m. \tag{5.16}$$

Lemma 5.1: Let $\widetilde{\mathscr{H}}$ be given by (2.33), $\underline{E}$ be the solution of the boundary value problem (1.6)–(1.9), let $\underline{E}\in\widetilde{\mathscr{H}}$. We have

$$\widetilde{Z}:E_j(x_1,x_2,0)\rightarrow E_j(x_1,x_2,\rho(x_1,x_2)), \quad j=1,2,3,(x_1,x_2)^T\in\mathbf{R}^2, \tag{5.17}$$

$$E_3(\underline{x})=-(\widetilde{q}^{-1}\widetilde{q}_1E_1)(\underline{x})-(\widetilde{q}^{-1}\widetilde{q}_2E_2)(\underline{x}), \quad \underline{x}\in\Gamma_1, \tag{5.18}$$

$$E_3(\underline{x})=-(\widetilde{Z}\widetilde{q}^{-1}\widetilde{q}_1\widetilde{Z}^{-1}E_1)(\underline{x})-(\widetilde{Z}\widetilde{q}^{-1}\widetilde{q}_2\widetilde{Z}^{-1}E_2)(\underline{x}), \quad \underline{x}\in\Gamma_2. \tag{5.19}$$

Proof: The thesis follows immediately from Lemmas 2.5 and 2.6. ■

Lemma 5.2: Let $\widetilde{\mathscr{Q}}$ be given by (2.31) and let $\widetilde{D}:\widetilde{\mathscr{Q}}\rightarrow\widetilde{\mathscr{Q}}$, $\widetilde{D}_j:\widetilde{\mathscr{Q}}\rightarrow\widetilde{\mathscr{Q}}$, $j=1,2$, be the operators defined as follows:

$$\widetilde{D}=\widetilde{Z}(\iota\widetilde{q})\widetilde{Z}^{-1}, \tag{5.20}$$

$$\widetilde{D}_j=\widetilde{Z}(\widetilde{q}^{-1},\widetilde{q}_j)\widetilde{Z}^{-1},\quad j=1,2. \tag{5.21}$$

Then we have

$$\widetilde{D}_j\widetilde{D}=\widetilde{D}\widetilde{D}_j,\quad j=1,2,\quad \widetilde{D}_1\widetilde{D}_2=\widetilde{D}_2\widetilde{D}_1. \tag{5.22}$$

Proof: The proof follows from a simple computation based on the definitions of the operators $\widetilde{Z},\widetilde{q},\widetilde{q}_j,j=1,2$. ■

In the following, we denote with I the identity operator.

Lemma 5.3: Let $\widetilde{L}_{\Gamma_1}$ be the operator defined by (5.4) when $\Gamma_1=\{x_3=0\}$. Then we have

$$\widetilde{L}_{\Gamma_1}=\begin{pmatrix} \iota\widetilde{q}_1\widetilde{q}^{-1}\widetilde{q}_2 & -\iota(\widetilde{q}+\widetilde{q}_1\widetilde{q}^{-1}\widetilde{q}_1) & 0\\ \iota(\widetilde{q}+\widetilde{q}_2\widetilde{q}^{-1}\widetilde{q}_2) & -\iota\widetilde{q}_2\widetilde{q}^{-1}\widetilde{q}_1 & 0\\ 0 & 0 & I\end{pmatrix}. \tag{5.23}$$

Proof: Let $\underline{E}_{\Gamma_1}$ be the solution of the boundary value problem (5.6)–(5.9). The proof follows evaluating curl $\underline{E}_{\Gamma_1}(\underline{x})$ on Γ_1 through the representation formula in (2.33) and using formula (5.18), Lemmas 2.5 and 2.6, and the fact that since $\Gamma_1=\{x_3=0\}$ we have

$$\underline{g}_{\Gamma_1}(\underline{x})=[\underline{n}_{\Gamma_1},\ \underline{E}_{\Gamma_1}](\underline{x})=\begin{pmatrix} 0 & -1 & 0\\ 1 & 0 & 0\\ 0 & 0 & 1\end{pmatrix}\begin{pmatrix} E_{\Gamma_1,1}(\underline{x})\\ E_{\Gamma_1,2}(\underline{x})\\ 0\end{pmatrix},\quad \underline{x}\in\Gamma_1. \tag{5.24}$$

This concludes the proof. ■

Lemma 5.4: Let $\widetilde{Z}$, $\widetilde{G}$, and $\widetilde{D}_j$, $j=1,2$, be the operators given by (2.37), (5.5), and (5.21). Then we have

$$\widetilde{G}=\begin{pmatrix} \left(I-\dfrac{\partial\rho}{\partial x_2}\widetilde{D}_2\right)\widetilde{Z} & \dfrac{\partial\rho}{\partial x_2}\widetilde{D}_1\widetilde{Z} & 0\\ \dfrac{\partial\rho}{\partial x_1}\widetilde{D}_2\widetilde{Z} & \left(I-\dfrac{\partial\rho}{\partial x_1}\widetilde{D}_1\right)\widetilde{Z} & 0\\ \dfrac{\partial\rho}{\partial x_1}\widetilde{Z} & \dfrac{\partial\rho}{\partial x_2}\widetilde{Z} & \widetilde{Z}\end{pmatrix}. \tag{5.25}$$

Proof: We have assumed that there exists a function $\underline{F}(\underline{x})\in\widetilde{\mathscr{H}}$ [see (2.33)] solution of (5.6)–(5.8) in $\mathbf{R}^3\backslash\overline{D_{\Gamma_1}\cap D_{\Gamma_2}}$ that coincides in $\mathbf{R}^3\backslash\overline{D_{\Gamma_1}}$ with the unique solution of the boundary value problem (5.6)–(5.9). The proof follows using (5.19) and (5.24) from the fact that $\underline{n}_{\Gamma_1}(\underline{x})=(0,0,1)^T,\forall\underline{x}\in\Gamma_1$, computing the function $\underline{g}_{\Gamma_2}(\underline{x}),\underline{x}\in\Gamma_2$, given by (5.10). ■

Proposition 5.5: Let $\widetilde{Z}^{-1},\widetilde{G}^{-1}$ be the (formal) inverse of the operators $\widetilde{Z},\widetilde{G}$ respectively. We have

$$\widetilde{G}^{-1}=\begin{pmatrix} \widetilde{Z}^{-1}\left(I+\dfrac{\partial\rho}{\partial x_2}\widetilde{h}^{-1}\widetilde{D}_2\right) & -\widetilde{Z}^{-1}\dfrac{\partial\rho}{\partial x_2}\widetilde{h}^{-1}\widetilde{D}_1 & 0\\ -\widetilde{Z}^{-1}\dfrac{\partial\rho}{\partial x_1}\widetilde{h}^{-1}\widetilde{D}_2 & \widetilde{Z}^{-1}\left(I+\dfrac{\partial\rho}{\partial x_1}\widetilde{h}^{-1}\widetilde{D}_1\right) & 0\\ -\widetilde{Z}^{-1}\dfrac{\partial\rho}{\partial x_1} & -\widetilde{Z}^{-1}\dfrac{\partial\rho}{\partial x_2} & \widetilde{Z}^{-1}\end{pmatrix}, \tag{5.26}$$

where $\tilde{h}$ is the operator defined by

$$\tilde{h}=I-\tilde{D}_2\frac{\partial\rho}{\partial x_2}-\tilde{D}_1\frac{\partial\rho}{\partial x_1}, \tag{5.27}$$

and $\tilde{h}^{-1}$ is the (formal) inverse operator of $\tilde{h}$.

Proof (formal): From (5.25) we have

$$\tilde{G}\begin{pmatrix}\tilde{Z}^{-1}&0&0\\0&\tilde{Z}^{-1}&0\\0&0&\tilde{Z}^{-1}\end{pmatrix}=\begin{pmatrix}I&0&0\\0&I&0\\0&0&I\end{pmatrix}+\begin{pmatrix}\frac{\partial\rho}{\partial x_2}&0\\-\frac{\partial\rho}{\partial x_1}&0\\0&I\end{pmatrix}\begin{pmatrix}-\tilde{D}_2&\tilde{D}_1&0\\\frac{\partial\rho}{\partial x_1}&\frac{\partial\rho}{\partial x_2}&0\end{pmatrix}. \tag{5.28}$$

Now formula (5.26) follows from a simple computation. ■

Proposition 5.6: Let $\mathscr{F}$, $\tilde{L}_{\Gamma_1}$ be the operators in (2.25) and (5.23) and p, l_j, $j=1,2$, be the maximal multiplication operators defined in Sec. II. Then the inverse operator $\tilde{L}_{\Gamma_1}^{-1}$ is (formally) given by

$$\tilde{L}_{\Gamma_1}^{-1}=\begin{pmatrix}\tilde{l}_{11}&\tilde{l}_{12}&0\\\tilde{l}_{21}&\tilde{l}_{22}&0\\0&0&I\end{pmatrix}, \tag{5.29}$$

where

$$\tilde{l}_{11}=\frac{\iota}{k_0^2}\,\mathscr{F}^{-1}(l_1p^{-1}l_2)\mathscr{F}, \tag{5.30}$$

$$\tilde{l}_{12}=-\frac{\iota}{k_0^2}(\mathscr{F}^{-1}(p)\mathscr{F}+\mathscr{F}^{-1}(l_1p^{-1}l_1)\mathscr{F}), \tag{5.31}$$

$$\tilde{l}_{21}=\frac{\iota}{k_0^2}(\mathscr{F}^{-1}(p)\mathscr{F}+\mathscr{F}^{-1}(l_2p^{-1}l_2)\mathscr{F}), \tag{5.32}$$

$$\tilde{l}_{22}=-\tilde{l}_{11}. \tag{5.33}$$

Proof (formal): The proof follows from formula (5.23) and the definitions (2.27) and (2.28). ■

Let us define the following operators $\tilde{V}_j:\tilde{\mathscr{Q}}\to\tilde{\mathscr{Q}}$, $j=1,2$:

$$\tilde{V}_j=\tilde{Z}(\iota\tilde{q}_j)\tilde{Z}^{-1},\quad j=1,2. \tag{5.34}$$

We have the following lemma.

Lemma 5.7: Let $\tilde{M}$ be given by (5.14), $\tilde{M}=((\tilde{M}_{ij}))$, $i,j=1,2,3$, and let $\tilde{D},\tilde{D}_j,\tilde{h},\tilde{V}_j$, $j=1,2$, be the operators given by (5.20), (5.21), (5.27), (5.34) respectively. Then we have

$$\tilde{M}_{11}=\frac{\partial\rho}{\partial x_2}\tilde{V}_1+\tilde{V}_1\tilde{h}^{-1}\tilde{D}_2+\tilde{D}\frac{\partial\rho}{\partial x_1}\tilde{h}^{-1}\tilde{D}_2+\frac{\partial\rho}{\partial x_2}\left(\tilde{V}_1\frac{\partial\rho}{\partial x_2}-\tilde{V}_2\frac{\partial\rho}{\partial x_1}\right)\tilde{h}^{-1}\tilde{D}_2, \tag{5.35}$$

$$\widetilde{M}_{12}=-\widetilde{D}+\frac{\partial\rho}{\partial x_2}\,\widetilde{V}_2-\widetilde{V}_1\widetilde{h}^{-1}\widetilde{D}_1-\widetilde{D}\,\frac{\partial\rho}{\partial x_1}\,\widetilde{h}^{-1}\widetilde{D}_1-\frac{\partial\rho}{\partial x_2}\left(\widetilde{V}_1\,\frac{\partial\rho}{\partial x_2}-\widetilde{V}_2\,\frac{\partial\rho}{\partial x_1}\right)\widetilde{h}^{-1}\widetilde{D}_1, \quad (5.36)$$

$$\widetilde{M}_{21}=\widetilde{D}-\frac{\partial\rho}{\partial x_1}\,\widetilde{V}_1+\widetilde{V}_2\widetilde{h}^{-1}\widetilde{D}_2+\widetilde{D}\,\frac{\partial\rho}{\partial x_2}\,\widetilde{h}^{-1}\widetilde{D}_2+\frac{\partial\rho}{\partial x_1}\left(\widetilde{V}_1\,\frac{\partial\rho}{\partial x_2}-\widetilde{V}_2\,\frac{\partial\rho}{\partial x_1}\right)\widetilde{h}^{-1}\widetilde{D}_2, \quad (5.37)$$

$$\widetilde{M}_{22}=-\frac{\partial\rho}{\partial x_1}\,\widetilde{V}_2-\widetilde{V}_2\widetilde{h}^{-1}\widetilde{D}_1-\widetilde{D}\,\frac{\partial\rho}{\partial x_2}\,\widetilde{h}^{-1}\widetilde{D}_1-\frac{\partial\rho}{\partial x_1}\left(\widetilde{V}_1\,\frac{\partial\rho}{\partial x_2}-\widetilde{V}_2\,\frac{\partial\rho}{\partial x_1}\right)\widetilde{h}^{-1}\widetilde{D}_1, \quad (5.38)$$

$$\widetilde{M}_{31}=-\frac{\partial\rho}{\partial x_1}+\frac{\partial\rho}{\partial x_2}\,\widetilde{D}+\left(\frac{\partial\rho}{\partial x_1}\,\widetilde{V}_1+\frac{\partial\rho}{\partial x_2}\,\widetilde{V}_2\right)\widetilde{h}^{-1}\widetilde{D}_2+\left(\frac{\partial\rho}{\partial x_1}\,\widetilde{D}\,\frac{\partial\rho}{\partial x_1}+\frac{\partial\rho}{\partial x_2}\,\widetilde{D}\,\frac{\partial\rho}{\partial x_2}\right)\widetilde{h}^{-1}\widetilde{D}_2, \quad (5.39)$$

$$\widetilde{M}_{32}=-\frac{\partial\rho}{\partial x_2}-\frac{\partial\rho}{\partial x_1}\,\widetilde{D}-\left(\frac{\partial\rho}{\partial x_1}\,\widetilde{V}_1+\frac{\partial\rho}{\partial x_2}\,\widetilde{V}_2\right)\widetilde{h}^{-1}\widetilde{D}_1-\left(\frac{\partial\rho}{\partial x_1}\,\widetilde{D}\,\frac{\partial\rho}{\partial x_1}+\frac{\partial\rho}{\partial x_2}\,\widetilde{D}\,\frac{\partial\rho}{\partial x_2}\right)\widetilde{h}^{-1}\widetilde{D}_1, \quad (5.40)$$

$$\widetilde{M}_{13}=0, \quad \widetilde{M}_{23}=0, \quad \widetilde{M}_{33}=I. \quad (5.41)$$

Proof: The proof follows from (5.14), (5.23), (5.25), and (5.26) by a simple computation. ■

To obtain the formal expansion ''in powers of ρ'' of $\widetilde{M}$ we need of the expansions of $\widetilde{D},\widetilde{D}_j,\widetilde{h},\widetilde{V}_j$, $j=1,2$, that appear in the elements $((\widetilde{M}_{ij}))$, $i,j=1,2,3$, of $\widetilde{M}$. We have the following proposition.

Proposition 5.8: Let $\widetilde{D},\widetilde{D}_j,\widetilde{h},\widetilde{V}_j$, $j=1,2$, be given by (5.20), (5.21), (5.27), and (5.34). We denote with δ the functional differentiation with respect to $\rho(\underline{x})$. We have

$$\widetilde{D}=\sum_{m=0}^{\infty}\widetilde{D}_m, \quad \widetilde{D}_j=\sum_{m=0}^{\infty}\widetilde{D}_{j,m}, \quad \widetilde{V}_j=\sum_{m=0}^{\infty}\widetilde{V}_{j,m}, \quad \widetilde{h}=\sum_{m=0}^{\infty}\widetilde{h}_m, \quad j=1,2, \quad (5.42)$$

where

$$\widetilde{D}_m=\frac{1}{m!}\,(\delta^m\widetilde{D})[\rho], \quad \widetilde{D}_{j,m}=\frac{1}{m!}\,(\delta^m\widetilde{D}_j)[\rho], \quad \widetilde{V}_{j,m}=\frac{1}{m!}\,(\delta^m\widetilde{V}_j)[\rho], \quad (5.43)$$

$$\widetilde{h}_0=I, \quad \widetilde{h}_m=-\frac{1}{m!}\left(\widetilde{D}_{2,m-1}\,\frac{\partial\rho}{\partial x_2}+\widetilde{D}_{1,m-1}\,\frac{\partial\rho}{\partial x_1}\right), \quad m=1,2,\ldots\,. \quad (5.44)$$

In particular the first two terms of these expansions ''in powers of ρ'' are given by

$$\widetilde{D}_0=\iota\widetilde{q}, \quad \widetilde{D}_1=(\rho(\iota\widetilde{q})-(\iota\widetilde{q})\rho)(\iota\widetilde{q}), \quad (5.45)$$

$$\widetilde{D}_{j,0}=\widetilde{q}^{-1}\widetilde{q}_j, \quad \widetilde{D}_{j,1}=(\rho(\widetilde{q}^{-1}\widetilde{q}_j)-(\widetilde{q}^{-1}\widetilde{q}_j)\rho)(\iota\widetilde{q}), \quad j=1,2, \quad (5.46)$$

$$\widetilde{V}_{j,0}=\iota\widetilde{q}_j, \quad \widetilde{V}_{j,1}=(\rho(\iota\widetilde{q}_j)-(\iota\widetilde{q}_j)\rho)(\iota\widetilde{q}_j), \quad j=1,2, \quad (5.47)$$

$$\widetilde{h}_0^{-1}=I, \quad \widetilde{h}_1^{-1}=\widetilde{q}^{-1}\widetilde{q}_2\,\frac{\partial\rho}{\partial x_2}+\widetilde{q}^{-1}\widetilde{q}_1\,\frac{\partial\rho}{\partial x_1}. \quad (5.48)$$

Proof (formal): The formulas in (5.43) are obtained from Taylor's formula with base point $\rho=\rho_1(\underline{x})=0$, $\underline{x}=(x_1,x_2)^T\in\mathbf{R}^2$. We prove formulas (5.46) for $\widetilde{D}_j$, $j=1,2$. The (formal) proof of the expansion of $\widetilde{D}$ and $\widetilde{V}_j$, $j=1,2$, are analogous. The operators $\widetilde{D}_j$, $j=1,2$, satisfy the following relation:

$$\widetilde{D}_j\widetilde{Z}=\widetilde{Z}(\iota\widetilde{q})^{-1}(\iota\widetilde{q}_j),\quad j=1,2. \tag{5.49}$$

A variation in $\widetilde{Z}$ induces a variation in $\widetilde{D}_j$, $j=1,2$, as follows:

$$\delta\widetilde{D}_j=\delta\widetilde{Z}(\iota\widetilde{q})^{-1}(\iota\widetilde{q}_j)\widetilde{Z}^{-1}-\widetilde{D}_j\delta\widetilde{Z}\widetilde{Z}^{-1}=\delta\rho\widetilde{D}\widetilde{D}_j-\widetilde{D}_j\delta\rho\widetilde{D}+(\delta\rho\widetilde{D}_j\widetilde{D}-\delta\rho\widetilde{D}_j\widetilde{D}),\quad j=1,2. \tag{5.50}$$

From (5.50), applying Lemma 5.2 we obtain

$$\delta\widetilde{D}_j=(\delta\rho\widetilde{D}_j-\widetilde{D}_j\delta\rho)\widetilde{D},\quad j=1,2. \tag{5.51}$$

Using the Taylor's formula of $\widetilde{D}_j$, $j=1,2$, with base point $\rho=\rho_1(\underline{x})=0$, $\underline{x}=(x_1,x_2)^T\in\mathbf{R}^2$, that is,

$$\widetilde{D}_j[\rho_1+\delta\rho]=\widetilde{D}_j[\rho_1]+\delta\widetilde{D}_j+\cdots,\quad j=1,2, \tag{5.52}$$

and choosing $\delta\rho(x_1,x_2)=\rho(x_1,x_2)$, we have

$$\widetilde{D}_j[\rho]=\widetilde{D}_j[0]+(\delta\widetilde{D}_j)[0]+\tfrac{1}{2}(\delta^2\widetilde{D}_j)[0]+\cdots,\quad j=1,2. \tag{5.53}$$

Since $\widetilde{Z}[0]=I$, $\widetilde{D}[0]=\iota\widetilde{q}$, $\widetilde{D}_j[0]=\widetilde{q}^{-1}\widetilde{q}_j$, $j=1,2$, from (5.50) and (5.53) we obtain (5.46). Formula (5.44) follows from the definition of $\widetilde{h}$ and (5.43). Formula (5.48) is obtained by applying the Cauchy rule to the product of the series expansion ''in powers of ρ'' of the operators $\widetilde{h}$ and $\widetilde{h}^{-1}$.■

Proposition 5.9: Let $\widetilde{M}$ given by (5.14). Then $\widetilde{M}=\Sigma_{m=0}^{\infty}\widetilde{M}_m$, $\widetilde{M}_m=((\widetilde{M}_{ij,m}))$, $i,j=1,2,3$, $m=0,1,2,...$, where $((\widetilde{M}_{ij,m}))$, $i,j=1,2,3$, are obtained plugging the expansions in (5.42) into the formulas (5.35)–(5.41).

Proof (formal): The proof is a straightforward consequence of Lemma 5.7 and Proposition 5.8. ■

We note that due to the definitions of the operators $\widetilde{q},\widetilde{q}_j$, $j=1,2$, the computation of the expansion of the operator $\widetilde{M}$ involves only quadratures and is fully parallelizable.

Proposition 5.10: Let $\widetilde{M}=\Sigma_{m=0}^{\infty}\widetilde{M}_m$ be the formal expansion ''in powers of ρ'' of the operator $\widetilde{M}$ obtained in Proposition 5.9. The function $\underline{E}(\underline{x})$ solution of (1.6)–(1.9) can be (formally) expanded as follows:

$$\underline{E}(\underline{x})=\int_{\partial D}\mathrm{curl}_{\underline{x}}\{\Phi(\underline{x},\underline{y})\underline{g}(\underline{y})\}ds(\underline{y})+\frac{1}{k_0^2}\sum_{m=0}^{\infty}\int_{\partial D}\mathrm{curl}_{\underline{x}}\,\mathrm{curl}_{\underline{x}}\{\Phi(\underline{x},\underline{y})(\widetilde{M}_m\underline{g})(\underline{y})\}ds(\underline{y}),$$
$$\underline{x}\in D^c, \tag{5.54}$$

where Φ is given by (1.12).

Proof (formal): The proof follows immediately from (5.13), Proposition 5.9, and the integral representation formula (3.5) of Theorem 3.2. ■

Formula (5.54) can be used to approximate $\underline{E}(\underline{x})$ truncating the series on the right-hand side of (5.54) and using numerical quadrature formulas to compute the relevant integrals, so that the computation of $\underline{E}(\underline{x})$ is also fully parallelizable.

Finally we give the first two terms of the expansion ''in powers of ρ'' of the operator $\widetilde{M}$ that are used to obtain the numerical results of Sec. VI. A simple computation gives

$$\widetilde{M}_{11,0}=\iota\mathscr{F}^{-1}l_1p^{-1}l_2\mathscr{F}, \tag{5.55}$$

$$\widetilde{M}_{11,1}=+\mathscr{F}^{-1}l_1p^{-1}l_2\mathscr{F}\rho\mathscr{F}^{-1}p\mathscr{F}-\rho\mathscr{F}^{-1}l_1l_2\mathscr{F}+\iota\Bigg(\frac{\partial\rho}{\partial x_2}\mathscr{F}^{-1}l_1\mathscr{F}$$
$$+\mathscr{F}^{-1}l_1p^{-1}l_2\mathscr{F}\frac{\partial\rho}{\partial x_2}\mathscr{F}^{-1}p^{-1}l_2\mathscr{F}+\mathscr{F}^{-1}l_1p^{-1}l_1\mathscr{F}\frac{\partial\rho}{\partial x_1}\mathscr{F}^{-1}p^{-1}l_2\mathscr{F}$$
$$+\mathscr{F}^{-1}p\mathscr{F}\frac{\partial\rho}{\partial x_1}\mathscr{F}^{-1}p^{-1}l_2\mathscr{F}\Bigg), \tag{5.56}$$

$$\widetilde{M}_{12,0}=-\iota(\mathscr{F}^{-1}p\mathscr{F}+\mathscr{F}^{-1}l_1p^{-1}l_1\mathscr{F}), \tag{5.57}$$

$$\widetilde{M}_{12,1}=-\mathscr{F}^{-1}p\mathscr{F}\rho\mathscr{F}^{-1}p\mathscr{F}-\mathscr{F}^{-1}l_1p^{-1}l_1\mathscr{F}\rho\mathscr{F}^{-1}p\mathscr{F}+\rho k_0^2-\rho\mathscr{F}^{-1}l_2^2\mathscr{F}$$
$$+\iota\Bigg(-\mathscr{F}^{-1}l_1p^{-1}l_1\mathscr{F}\frac{\partial\rho}{\partial x_1}\mathscr{F}^{-1}p^{-1}l_1\mathscr{F}+\frac{\partial\rho}{\partial x_2}\mathscr{F}^{-1}l_2\mathscr{F}-\mathscr{F}^{-1}l_1p^{-1}l_2$$
$$\mathscr{F}\frac{\partial\rho}{\partial x_2}\mathscr{F}^{-1}p^{-1}l_1\mathscr{F}-\mathscr{F}^{-1}p\mathscr{F}\frac{\partial\rho}{\partial x_1}\mathscr{F}^{-1}p^{-1}l_1\mathscr{F}\Bigg), \tag{5.58}$$

$$\widetilde{M}_{21,0}=\iota(\mathscr{F}^{-1}p\mathscr{F}+\mathscr{F}^{-1}l_2p^{-1}l_2\mathscr{F}), \tag{5.59}$$

$$\widetilde{M}_{21,1}=+\mathscr{F}^{-1}p\mathscr{F}\rho\mathscr{F}^{-1}p\mathscr{F}+\mathscr{F}^{-1}l_2p^{-1}l_2\mathscr{F}\rho\mathscr{F}^{-1}p\mathscr{F}-\rho k_0^2+\rho\mathscr{F}^{-1}l_1^2\mathscr{F}$$
$$+\iota\Bigg(+\mathscr{F}^{-1}l_2p^{-1}l_2\mathscr{F}\frac{\partial\rho}{\partial x_2}\mathscr{F}^{-1}p^{-1}l_2\mathscr{F}-\frac{\partial\rho}{\partial x_1}\mathscr{F}^{-1}l_1\mathscr{F}+\mathscr{F}^{-1}l_1p^{-1}l_2\mathscr{F}\frac{\partial\rho}{\partial x_1}$$
$$\mathscr{F}^{-1}p^{-1}l_2\mathscr{F}+\mathscr{F}^{-1}p\mathscr{F}\frac{\partial\rho}{\partial x_2}\mathscr{F}^{-1}p^{-1}l_2\mathscr{F}\Bigg), \tag{5.60}$$

$$\widetilde{M}_{22,0}=-\iota\mathscr{F}^{-1}l_1p^{-1}l_2\mathscr{F}, \tag{5.61}$$

$$\widetilde{M}_{22,1}=-\mathscr{F}^{-1}l_1p^{-1}l_2\mathscr{F}\rho\mathscr{F}^{-1}p\mathscr{F}+\rho\mathscr{F}^{-1}l_1l_2\mathscr{F}+\iota\Bigg(-\frac{\partial\rho}{\partial x_1}\mathscr{F}^{-1}l_2\mathscr{F}$$
$$-\mathscr{F}^{-1}l_1p^{-1}l_2\mathscr{F}\frac{\partial\rho}{\partial x_1}\mathscr{F}^{-1}p^{-1}l_1\mathscr{F}-\mathscr{F}^{-1}l_2p^{-1}l_2\mathscr{F}\frac{\partial\rho}{\partial x_2}\mathscr{F}^{-1}p^{-1}l_1\mathscr{F}$$
$$-\mathscr{F}^{-1}p\mathscr{F}\frac{\partial\rho}{\partial x_2}\mathscr{F}^{-1}p^{-1}l_1\mathscr{F}\Bigg), \tag{5.62}$$

$$\widetilde{M}_{31,0}=0, \tag{5.63}$$

$$\widetilde{M}_{31,1}=\iota\frac{\partial\rho}{\partial x_1}\mathscr{F}^{-1}l_1p^{-1}l_2\mathscr{F}-\frac{\partial\rho}{\partial x_1}+\iota\frac{\partial\rho}{\partial x_2}\mathscr{F}^{-1}p\mathscr{F}+\iota\frac{\partial\rho}{\partial x_2}\mathscr{F}^{-1}l_2p^{-1}l_2\mathscr{F}, \tag{5.64}$$

$$\widetilde{M}_{32,0}=0, \tag{5.65}$$

$$\widetilde{M}_{32,1}=-\iota\frac{\partial\rho}{\partial x_2}\mathscr{F}^{-1}l_1p^{-1}l_2\mathscr{F}-\frac{\partial\rho}{\partial x_2}-\iota\frac{\partial\rho}{\partial x_1}\mathscr{F}^{-1}p\mathscr{F}-\iota\frac{\partial\rho}{\partial x_1}\mathscr{F}^{-1}l_1p^{-1}l_1\mathscr{F}, \tag{5.66}$$

$$\widetilde{M}_{13,0}=0, \tag{5.67}$$

$$\widetilde{M}_{13,1}=0, \tag{5.68}$$

$$\widetilde{M}_{23,0}=0, \tag{5.69}$$

$$\widetilde{M}_{23,1}=0, \tag{5.70}$$

$$\widetilde{M}_{33,0}=I, \tag{5.71}$$

$$\widetilde{M}_{33,1}=0. \tag{5.72}$$

VI. SOME NUMERICAL RESULTS

In this section we show some numerical results obtained computing the electric field $\underline{E}^2(\underline{x})$ of (1.10).

We compute an approximation of $\underline{E}^2(\underline{x})$ using formula (5.54) when $\Gamma_2=\partial D=\{x_3=\rho(x_1,x_2)\}$ [see (1.3)] and the reference surface is $\Gamma_1=\{x_3=0\}$. In particular, the first two terms of the expansion ''in powers of ρ'' of $\widetilde{M}$ are used [see (5.55)–(5.72)]. We remind the reader that the choice of the reference surface influences the numerical approximation of the electric field $\underline{E}^2(\underline{x})$. In fact, to obtain a good approximation using only a few terms of the expansion (5.54), we can choose $\Gamma_1=\{x_3=c\}$, where c is the constant solution of the following problem:

$$\min_{c\in\mathbf{R}} \max_{\underline{x}\in\mathbf{R}^2} |\rho(\underline{x})-c|. \tag{6.1}$$

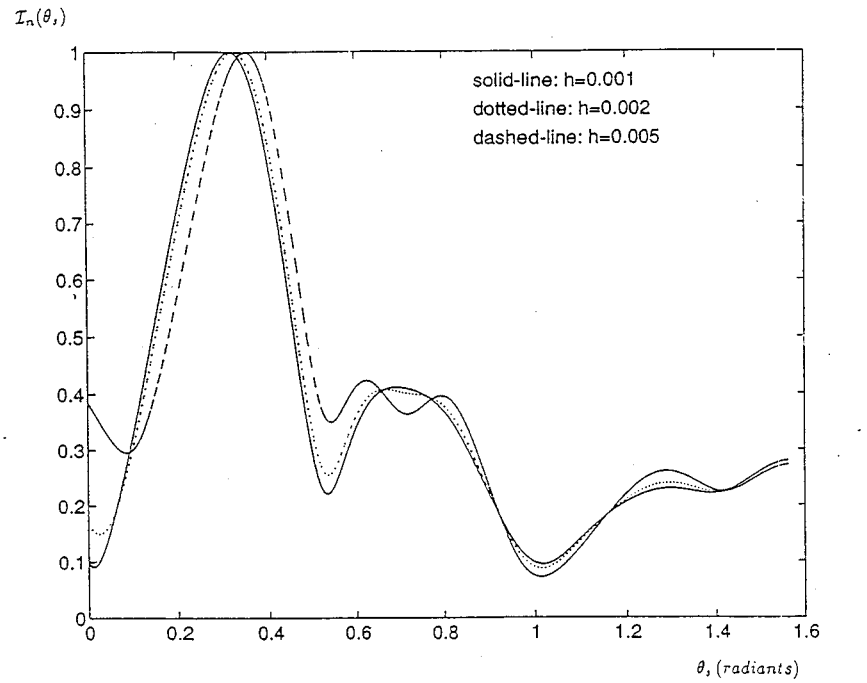

FIG. 1. Normalized scattering pattern as a function of the scattered angle θ_s.

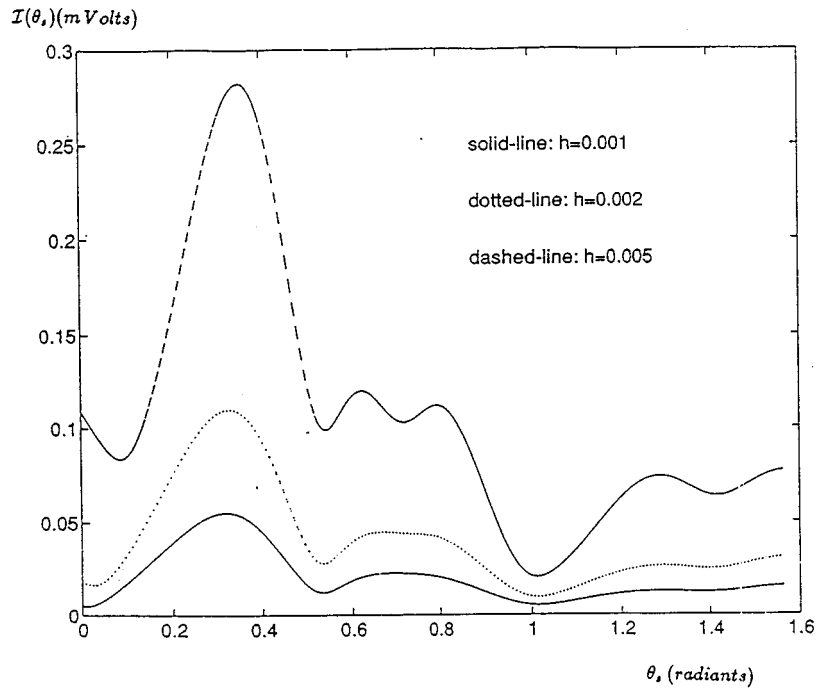

FIG. 2. This figure is analogous to Fig. 1 with the scattering intensity patterns instead of the normalized ones.

Formula (5.54) with the series truncated at $m=1$ has been implemented in a FORTRAN program. The computations are performed on a VAX-ALPHA 7000-610, using VMS ALPHA V1.5 double-precision arithmetic. We use quadrature formulas presented in Ref. 11.

In the numerical experiments we have chosen a plane linearly polarized incident wave; that is,

$$\underline{E}^i(\underline{x})=\underline{\Omega}e^{\iota k_0(\underline{x},\underline{\alpha})}, \quad \underline{x}\in\mathbf{R}^3, \tag{6.2}$$

where $\underline{\Omega}\in\mathbf{R}^3$ is the polarization vector, $\underline{\alpha}\in\mathbf{R}^3$, $\|\underline{\alpha}\|=1$, is the propagation direction of the incoming electric field, and $k_0>0$ is the wave number. Moreover, we assume $\operatorname{div}\underline{E}^i(\underline{x})=0$, $\underline{x}\in\mathbf{R}^3\backslash D$; that is,

$$(\underline{\Omega},\underline{\alpha})=0. \tag{6.3}$$

The function ρ [see (1.1)–(1.3)] is given by

$$\rho(x_1,x_2)=\begin{cases} h\ \sin(fx_1)e^{-1/(1-x_1^2-x_2^2)}, & x_1^2+x_2^2<1, \\ 0, & x_1^2+x_2^2\geqslant 1, \end{cases} \tag{6.4}$$

with f and h positive constants. The propagation direction $\underline{\alpha}$ is given by

$$\underline{\alpha}=(\cos\ \varphi_i\ \sin\ \theta_i,\sin\ \varphi_i\ \sin\ \theta_i,-\cos\ \theta_i)^T, \quad 0\leqslant\varphi_i<2\pi,0\leqslant\theta_i<\pi/2. \tag{6.5}$$

All of the calculations presented here are for normal incident $\theta_i=0$, and φ_i arbitrary, for the polarization vector $\underline{\Omega}=(1,1,0)^T$, for different values of the scattered angle θ_s and for $\varphi_s=\pi$.

The scattering intensity $\mathcal{I}(\theta_s)$ and the associated normalized intensity $\mathcal{I}_n(\theta_s)$ are defined by

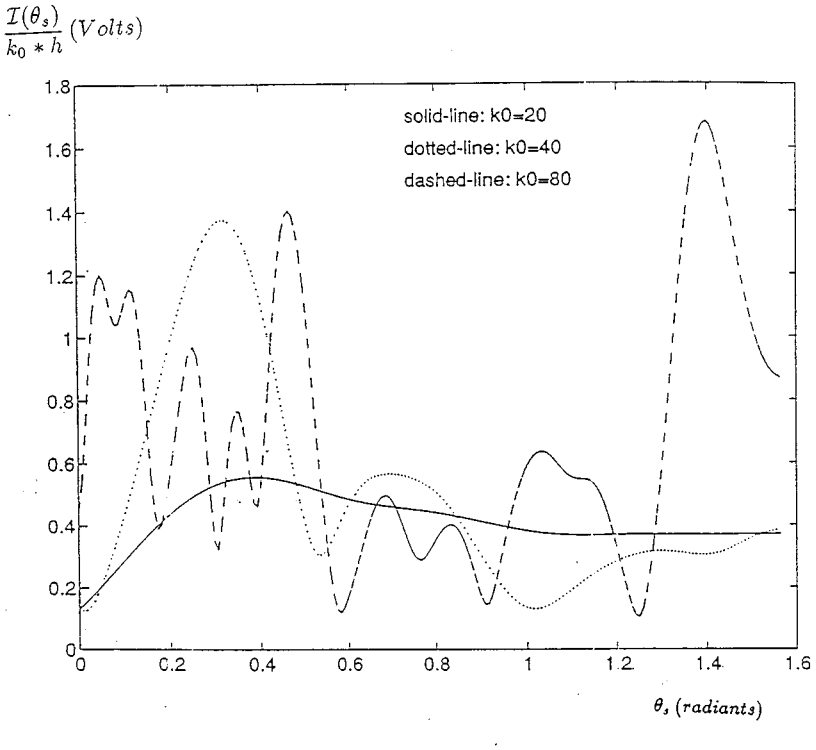

FIG. 3. Intensity patterns divided by k_0h as a function of the scattered angle θ_s.

$$\mathcal{I}(\theta_s) := \frac{|\underline{F}_0(\theta_s,\varphi_s)|}{k_0}, \quad \varphi_s=\pi, \quad 0\leqslant\theta_s<\frac{\pi}{2}, \tag{6.6}$$

$$\mathcal{I}_n(\theta_s) := \frac{|\underline{F}_0(\theta_s,\varphi_s)|}{\max_{\theta_s}|\underline{F}_0(\theta_s,\varphi_s)|}, \quad \varphi_s=\pi, \quad 0\leqslant\theta_s<\frac{\pi}{2}, \tag{6.7}$$

where $\underline{F}_0$ is the electric far field associated with $\underline{E}^2$ [see (3.6)], and $|\underline{F}_0|^2 = (\underline{F}_0, \overline{\underline{F}_0})$. We note that three parameters determine the behavior of the scattered field $\underline{E}_2$: the roughness h, the period $L=2\pi/f$ of the corrugation of the surface ∂D, and the incident wave number k_0.

The following figures show that for sufficiently large values of k_0 when $h\ll 2\pi/k_0$, a Bragg-like structure is presented with periodicity L and split depth h.

Figure 1 shows normalized scattering patterns as a function of the scattered angle θ_s, calculated for $\varphi_s=\pi$, $k_0=40$, $f=48$, and various values of the roughness $h=0.001$, 0.002, and 0.005. These scattering intensity patterns show that the peaks of the intensity are more or less independent of the value of the roughness h.

Figure 2 is analogous to Fig. 1 with the scattering intensity patterns instead of the normalized ones. We can see that the intensity increases when the roughness increases.

Figure 3 shows the intensity patterns divided by k_0h as a function of the scattered angle θ_s for $h=0.001$, $k_0=20$, 40, and 80, and $f=8$. We note that the peaks are located at $\theta_s\approx\theta_{s,m}$, where $\theta_{s,m}$ according to Bragg law is given by $\theta_{s,m}=\arcsin(mf/k_0)$, $m=1,2,\ldots$.

Figure 4 shows the normalized intensity for $\theta_s=0$, i.e., the backscattering direction, as a function of the incident wave number, k_0, and for different values of f [see (6.4)], $f=128$, 192,

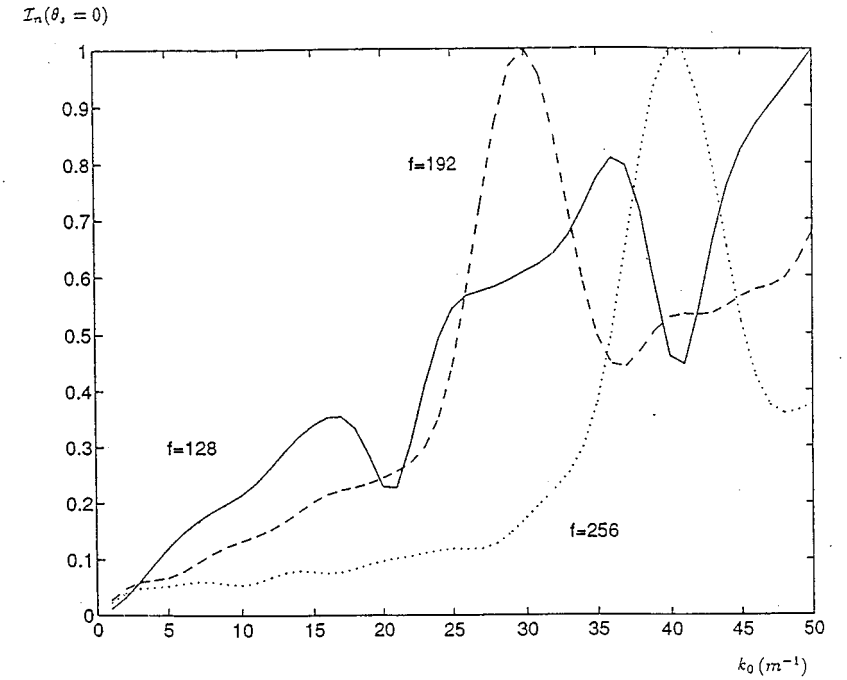

FIG. 4. Normalized intensity for $\theta_s=0$.

and 256. We note that a resonance phenomenon occurs, i.e., the first peak of each scattering pattern appears when $k_0/f \approx 0.15$.

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On group invariant solutions of the Boltzmann equation

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After reviewing the complete Lie group for the full Boltzmann equation, it is shown that projective transformations play a special role in the general case, and the class of invariant solutions giving rise to homoenergetic affine flows is presented. Homoenergetic affine flows in the two-dimensional case [potential $U(r)\propto r^{-2}$] are considered in detail: It is shown that the general solution of this problem can be essentially simplified by projective transformations. © *1996 American Institute of Physics.* [S0022-2488(96)02505-9]

I. INTRODUCTION

The group analysis, which is one of the most powerful general methods in mathematical physics,[1,2] was recently applied to the full spatially inhomogeneous Boltzmann equation in Ref. 3, where the complete (with certain natural restrictions) Lie group was constructed.

As it occurs to many classical equations of mathematical physics (for example, Euler gas dynamics equations), almost all point symmetries of the Boltzmann equation can be easily found from physical considerations. The only exception, as in the case of Euler equations,[1] is perhaps the so-called *projective invariance*.[4,5] Many attempts to construct special classes of relatively simple solutions to the Boltzmann equation have been previously made by different authors[6–10] (see also Refs. 11 and 12 for a review) without any connection with group properties of the equation. However the well known results of Refs. 6–10 could be understood more deeply just on that basis. We should also mention Refs. 13–18, in which the related problems are treated by means of Lie group methods. However, all these articles are not concerned with the full Boltzmann equation, but with very special cases. In the present article we use the results of group analysis of the Boltzmann equation, with special attention to the projective symmetry and its consequences: the Lemma from Sec. II clarifies a very special role of projective transformations for the Boltzmann equation in its general form. Sections III–IV are mostly devoted to the application of projective transformations to the so-called *homoenergetic affine flows*.[11,19] The classification of such flows for the *most symmetric* two-dimensional Boltzmann equation in the case of a potential $U(r)\propto r^{-2}$ is given in Sec. IV. It is shown that arbitrary (with some restrictions) four-parameter solutions can be expressed through a simpler two-parameter solution by projective transformations.

II. COMPLETE LIE GROUP, PROJECTIVE TRANSFORMATIONS, AND CONSERVATION LAWS

We consider the Boltzmann equation (BE) for the distribution function $f(\mathbf{x},\mathbf{v},t)$ ($\mathbf{x}\in\mathbb{R}^n$ denotes position, $\mathbf{v}\in\mathbb{R}^n$ velocity, $n=2,3,...$, while $t>0$ is the time variable)

$$\frac{\partial f}{\partial t}+\mathbf{v}\cdot\frac{\partial f}{\partial \mathbf{x}}=I(f,f),$$

$$\mathbf{x}\equiv\{x_1,\ldots,x_n\},\quad \mathbf{v}\equiv\{\nu_1,\ldots,\nu_n\},$$

$$I(f,f)=\int_{\mathbb{R}^n\times S^{n-1}} d\mathbf{w}\,d\mathbf{n}\,u\sigma\left(u,\frac{\mathbf{u}\cdot\mathbf{n}}{u}\right)\{f(\mathbf{v}')f(\mathbf{w}')-f(\mathbf{v})f(\mathbf{w})\},\tag{1}$$

$$\mathbf{u}=\mathbf{v}-\mathbf{w},\quad u=|\mathbf{u}|,\quad |\mathbf{n}|=1,$$

$$\mathbf{v}'=\tfrac{1}{2}(\mathbf{v}+\mathbf{w}+u\mathbf{n}),\quad \mathbf{w}'=\tfrac{1}{2}(\mathbf{v}+\mathbf{w}-u\mathbf{n}),$$

where $\sigma(u,\mu=\cos\theta)$ denotes the differential cross section (we use the same terminology for all number of dimensions $n=2,3,\ldots$) at the scattering angle $0<\theta\leqslant\pi$. We note that for the powerlike intermolecular potential $U(r)\propto r^{-m}$, $m>1$, the cross section reads as

$$\sigma(u,\mu)=u^{\gamma-1}g_\gamma(\mu),\quad \gamma=\frac{m-2(n-1)}{m};$$

the limiting case $m=\infty$ ($\gamma=1$) corresponds to hard spheres. A detailed investigation of group properties of the BE (with respect to Lie transformations) is presented in Ref. 3. The results are summarized as follows.

The most important (from the physical point of view) class of Lie (i.e., point) transformations for the BE can be represented as a linear transformation of the distribution function

$$f_\theta(\mathbf{x},\mathbf{v},t)=\exp(\theta\hat{L})f(\mathbf{x},\mathbf{v},t),\tag{2}$$

where $\hat{L}$ is a first order differential operator, i.e.,

$$\hat{L}=\Omega(\mathbf{x},\mathbf{v},t)+\mathbf{X}(\mathbf{x},\mathbf{v},t)\cdot\frac{\partial}{\partial\mathbf{x}}+\mathbf{V}(\mathbf{x},\mathbf{v},t)\cdot\frac{\partial}{\partial\mathbf{v}}+T(\mathbf{x},\mathbf{v}.t)\frac{\partial}{\partial t},\tag{3}$$

θ (positive or negative) being the *group parameter*. The following theorem describes the complete symmetry group for the BE in this class of transformations.

Theorem:[3] The complete list of admissible operators $\hat{L}$ for the BE consists of the following operators (A)–(C),

$$\text{(A)}\quad \hat{L}_{ij}^{(0)}=\left(x_1\frac{\partial}{\partial x_j}-x_j\frac{\partial}{\partial x_i}\right)+\left(\nu_i\frac{\partial}{\partial\nu_j}-\nu_j\frac{\partial}{\partial\nu_1}\right),\quad i,j=1,\ldots,n,$$

$$\text{(B)}\quad \hat{L}_i^{(1)}=\frac{\partial}{\partial x_i},\quad \hat{L}_i^{(2)}=t\frac{\partial}{\partial x_i}+\frac{\partial}{\partial\nu_i},\quad i=1,\ldots,n,$$

$$\text{(C)}\quad \hat{L}^{(3)}=\frac{\partial}{\partial t},\quad \hat{L}^{(4)}=t\frac{\partial}{\partial t}+\mathbf{x}\cdot\frac{\partial}{\partial\mathbf{x}}+1,$$

of the additional symmetry operator (D):

$$\text{(D)}\quad \hat{L}^{(5)}=t\frac{\partial}{\partial t}+(1-\rho)\mathbf{x}\cdot\frac{\partial}{\partial\mathbf{x}}-\rho\mathbf{v}\cdot\frac{\partial}{\partial\mathbf{v}},\quad \rho=\frac{m}{m(n+1)-2(n-1)}$$

in the case of powerlike potential $U \propto r^{-m}$, $m>1$ (with or without angular cutoff), and, finally, of a special symmetry operator (E):

$$\text{(E)}\quad \hat{L}^{(6)} = t^2 \frac{\partial}{\partial t} + t\mathbf{x}\cdot \frac{\partial}{\partial \mathbf{x}} + (\mathbf{x}-\mathbf{v}t)\cdot \frac{\partial}{\partial \mathbf{v}},$$

valid for the case $m=2$ (i.e., for $U \propto r^{-2}$).

If we now introduce the group transformations $T_\theta = \exp(\theta \hat{L})$, it is easy to obtain the explicit representation of the above written (in infinitesimal form) transformations. In particular one has, corresponding to the operator (D), the special class of scaling transformations

$$f_\theta^{(5)} = f[e^{(1-\rho)\theta}\mathbf{x}, e^{-\rho\theta}\mathbf{v}, e^{\theta}t],$$

and, for the special symmetry operator (E):

$$f_\theta^{(6)} = f\left[\frac{\mathbf{x}}{1-\theta t}, \mathbf{v}+\theta(\mathbf{x}-\mathbf{v}t), \frac{t}{1-\theta t}\right],$$

i.e., the class of the so-called projective transformations.[1–3] This symmetry is valid only for potential $U(r) \propto r^{-2}$. We consider here a little bit more in detail these nontrivial symmetry transformations.

The specific role of projective transformations for different classical and quantum systems has been pointed out in Ref. 3. Its role for the Boltzmann equation is connected with the following lemma.

Lemma. Let $f(\mathbf{x},\mathbf{v},t)$ be a solution of the generalized Boltzmann equation (1) with time-dependent differential cross section $\sigma(u,\mu,t)$. Then the function

$$F(\mathbf{x},\mathbf{v},t) = f\left[\frac{\mathbf{x}}{1+at}, \mathbf{v}(1+at)-a\mathbf{x}, \frac{t}{1+at}\right]$$

also satisfies, for $0<t<(1/a)$, the generalized Boltzmann equation with another time-dependent cross section:

$$\sigma_a(u,\mu,t) = (1+at)^{n-1}\sigma\left[u(1+at), \mu, \frac{t}{1+at}\right].$$

This lemma generalizes the related results of Ref. 4. To prove it, it is sufficient to make direct calculations, which we omit for brevity.

Corollary. The function $F(\mathbf{x},\mathbf{v},t)$ satisfies the usual Boltzmann equation with powerlike cross section $\sigma^{(\gamma)}(u,\mu) = u^{\gamma-1} g_\gamma(\mu)$ if and only if the function $f(\mathbf{x},\mathbf{v},t)$ satisfies the generalized Boltzmann equation with the cross section $\sigma_a^{(\gamma)}(u,\mu,t) = (1-at)^{n+\gamma-2} u^{\gamma-1} g_\gamma(\mu)$.

Hence, the projective transformations (E) are the equivalence transformations for the whole class of generalized Boltzmann equations with a time-dependent cross section, i.e., they change only the cross section, not the general form of the Boltzmann equation. In the special case

$$\sigma(u,\mu,t) = g(\mu)u^{1-n},$$

which corresponds to the potential $U(r) \propto r^{-2}$, the cross section is invariant under these transformations. We notice that the invariant transformation

$$F(\mathbf{x},\mathbf{v},t) = f\left[\frac{\mathbf{x}}{|t|}, |t|\left(\mathbf{v}-\frac{\mathbf{x}}{t}\right), \text{const}-\frac{1}{t}\right]$$

for the potential $U(r)\propto r^{-2}$ was found for the first time by Nikol'skii;[8] its connection with the projective transformations is clear.

Two additional conservation laws can be derived immediately from the above lemma. We note that the fundamental conservation laws (mass, momentum, and energy) for the Boltzmann equation do not depend on the cross section. Therefore, for any solution $f(\mathbf{x},\mathbf{v},t)$, with finite total second moments, the integral

$$E_a=\frac{1}{2}\int_{\mathbb{R}^n\times\mathbb{R}^n} d\mathbf{x}\, d\mathbf{y}\, f\left[\frac{\mathbf{x}}{1+at},\mathbf{v}(1+at)-a\mathbf{x},\frac{t}{1+at}\right]\nu^2$$
$$=\frac{1}{2}\int_{\mathbb{R}^n\times\mathbb{R}^n} d\tilde{\mathbf{x}}\, d\tilde{\mathbf{y}}\, f(\tilde{\mathbf{x}},\tilde{\mathbf{v}},\tilde{t})[\tilde{\mathbf{v}}+a(\tilde{\mathbf{x}}-\tilde{\mathbf{v}}\tilde{t})]^2$$

does not depend on time for any value of the group parameter a. Noting that

$$2E_a=2E_0+2aI_1+a^2I_2,$$

where

$$I_1=\int d\mathbf{x}\, d\mathbf{v}\, \mathbf{v}\cdot(\mathbf{x}-\mathbf{v}t)f(\mathbf{x},\mathbf{v},t),$$

$$I_2=\int d\mathbf{x}\, d\mathbf{v}(\mathbf{x}-\mathbf{v}t)^2 f(\mathbf{x},\mathbf{v},t),$$

one can immediately conclude that $I_{1,2}=$const. These conservation laws are not new (see, for instance, Ref. 20), however their connection with projective transformations seems very important.

III. HOMOENERGETIC AFFINE FLOWS AND SOME APPLICATIONS OF PROJECTIVE TRANSFORMATIONS

The infinitesimal operators (A)–(E) determine a Lie algebra, as it can be verified after a straightforward calculation of Lie brackets. For all cases (A)–(E) we can construct group invariants and the simplest invariant solutions of the BE, which are functions of these invariants. In this way we can again find all well known classes of invariant solutions, so that their group nature can be clarified. However, all really interesting invariant solutions are invariant under multiparameter groups. Therefore we formally need to classify, for each p, all corresponding multidimensional (with dimension not greater than p) subalgebras of the above-mentioned Lie algebra. This problem is rather complicated even in one dimension.[2] At the same time, most of the solutions obtained in such a way have no physical meaning.

Just for this reason we restrict ourselves to an interesting example having clear physical sense. Let us consider a linear combination of vector operators $\hat{\mathbf{L}}^{(1)}$ and $\hat{\mathbf{L}}^{(2)}$, i.e.,

$$L=\mathbf{a}\cdot\hat{\mathbf{L}}^{(1)}+\mathbf{b}\cdot\hat{\mathbf{L}}^{(2)},$$

with arbitrary vector parameters $\mathbf{a}$ and $\mathbf{b}$. To pass to n-parameter groups, we put

$$\mathbf{b}=\mathscr{K}\mathbf{a}\Leftrightarrow b_i=\sum_j K_{ij}a_j$$

with any matrix $(n\times n)$ $\mathscr{K}\equiv(K_{ij})$. Then

$$L=\sum_j \left\{ a_j \left[\hat{L}_j^{(1)} + \sum_i K_{ij} \hat{L}_i^{(2)} \right] \right\}$$

is the n-parameter infinitesimal operator of the corresponding group.

We can obtain, in this case, the independent invariants

$$\psi_0(t)=t, \quad \boldsymbol{\psi}=(\psi_1,\ldots,\psi_n)=\mathbf{v}-\hat{K}(t)\mathbf{x}, \qquad \hat{K}(t)=(\mathfrak{I}+t\mathscr{K})^{-1}\mathscr{K}, \tag{4}$$

$\mathfrak{I}$ denoting the identity matrix operator. We note that $\hat{K}(t)$ is the solution of the Cauchy problem

$$\frac{d}{dt}\hat{K}(t)+\hat{K}^2(t)=0, \quad \hat{K}(0)=\mathscr{K}.$$

The corresponding invariant solution reads

$$f(\mathbf{x},\mathbf{v},t)=F[\mathbf{v}-\hat{K}(t)\mathbf{x},t], \tag{5}$$

where $F(\mathbf{v},t)$ satisfies the equation

$$\frac{\partial F}{\partial t}-[\hat{K}(t)\mathbf{v}]\cdot\frac{\partial F}{\partial \mathbf{v}}=I(F,F\ ). \tag{6}$$

This class of solutions to the Boltzmann equation is also well known.[19] It describes the so-called *homoenergetic affine flows* (in the absence of external forces), first observed in Refs. 6 and 7 for the moments of distribution function in the case of Maxwellian molecules.

The existence and uniqueness of the corresponding distribution function for the general molecular model were recently proven in Ref. 19. In that article the solutions (5) were introduced on the basis of homoenergetic affine flow properties. The above derivation of Eq. (5) on the basis of symmetry considerations are perhaps simpler and more natural. We shall return to these solutions later.

The simplest application of group invariant transformations is transforming known exact solutions into new ones. One can start with the simplest exact solution $f(\mathbf{x},\mathbf{v},t)=\exp(-\ \nu^2)$, and then apply to this distribution function any above described transformation. It is easy to show that we obtain in such a way the complete class of the local Maxwellian solutions.

Less trivial example is given by the Nikol'skii transformation[9] of arbitrary space homogeneous solutions for powerlike potentials. Let us show that this transformation is closely connected with the above considered projective invariance. We consider the Boltzmann equation (1) with the cross section $\sigma(u,\mu)=u^{\gamma-1}g_\gamma(\mu)$. In accordance with the Lemma from Sec. II (see also Corollary), one can construct the solution of Eq. (1) in the form

$$f(\mathbf{x},\mathbf{v},t)=F\left[\mathbf{v}(1+at)-a\mathbf{x},\ \frac{t}{1+at}\right],$$

where $F(\mathbf{v},\tau)$ satisfies the generalized space homogeneous Boltzmann equation

$$\frac{\partial F}{\partial \tau}=(1-a\tau)^{n+\gamma-2}I(F,F\ ).$$

Putting

$$S(\tau)=\int_0^\tau d\tau'(1-a\tau')^{n+\gamma-2}$$

we can replace $F(\mathbf{v},\tau)$ by any solution $\Phi[\mathbf{v},S(\tau)]$ of the space homogeneous Boltzmann equation. In conclusion, we obtain the following well known formula for the Nikol'skii solution (see, for example, Ref. 12):

$$f(\mathbf{x},\mathbf{v},t)=\Phi[\mathbf{v}(1+at)-a\mathbf{x},T_a(t)],$$

$$T_a(t)=\int_0^{t/(1+at)} d\tau(1-a\tau)^{n+\gamma-2}=\frac{(1+at)^{n+\gamma-1}-1}{a(n+\gamma-1)(1+at)^{n+\gamma-1}},\quad n+\gamma>1.$$

Hence, the Nikol'skii transformation can be introduced on the basis of projective invariance. Therefore, if we apply this transformation to the Nikol'skii solution in the special case $n+\gamma=2$, then we obtain the same solution with another value of the group parameter a.

Let us now try to apply this transformation to homoenergetic affine flows described above, i.e., to the distribution function (5). Then we obtain, after some calculations,

$$f_a(\mathbf{x},\mathbf{v},t)=F\left\{(1+at)[\mathbf{v}-\hat{K}_a(t)\mathbf{x}],\ \frac{t}{1+at}\right\}, \tag{7}$$

where the matrix $\hat{K}_a(t)$ is the solution of the Cauchy problem

$$\frac{d}{dt}\hat{K}_a(t)+\hat{K}_a^2(t)=0,\quad \hat{K}_a(0)=\hat{K}(0)+a\mathfrak{I}.$$

Hence, the total class of homoenergetic affine flows is invariant under projective transformations. For the special case $n+\gamma=2$, the above formula (7) defines a solution of the Boltzmann equation, provided that $F(\mathbf{v},t)$ satisfies Eq. (6). We note that the matrix $\hat{K}(0)$ is the main parameter of this class of solutions. Equation (7) establishes (for $n+\gamma=2$) the exact connection between solutions $f(\mathbf{x},\mathbf{v},t)$, with given matrix $\hat{K}(0)$, and solutions $f_a(\mathbf{x},\mathbf{v},t)$, with a one-parameter set of matrices $\hat{K}_a(0)=\hat{K}(0)+a\mathfrak{I}$.

In particular we obtain the following correspondence between velocity moments:

$$M_a^{(p)}(t)=\int_{\mathbb{R}^n} d\mathbf{v}\ f_a(\mathbf{x},\mathbf{v},t)[\mathbf{v}-\hat{K}_a(t)\mathbf{x}]^p=(1+at)^{-(n+p)}M_0^{(p)}\left(\frac{t}{1+at}\right),\quad p=0,1,\ldots\ .$$

We consider below these flows for the two-dimensional ($n=2$) case in more detail.

IV. CLASSIFICATION OF HOMOENERGETIC AFFINE FLOWS FOR THE TWO-DIMENSIONAL BOLTZMANN EQUATION

We note that in two dimensions the potential $U(r)\propto r^{-2}$ corresponds to the value $\gamma=0$ [see comment after formula (1)]. Therefore, the case $n=2$, $m=2$ corresponds to the largest number of symmetries. The Boltzmann equation for the function $F(\mathbf{v},t)$ in Eq. (5) in this case reads

$$\frac{\partial F}{\partial t}-(\hat{K}(t)\mathbf{v})\cdot\frac{\partial F}{\partial \mathbf{v}}=I(F,F)=\int_{\mathbb{R}^2\times S^1} d\mathbf{w}\ d\mathbf{n}\ g\left(\frac{\mathbf{u}\cdot\mathbf{n}}{u}\right)[f(\mathbf{v}')f(\mathbf{w}')-f(\mathbf{v})f(\mathbf{w})],$$
$$\mathbf{u}=\mathbf{v}-\mathbf{w},\quad \hat{K}(t)=[1+t\hat{K}(0)]^{-1}\hat{K}(0) \tag{8}$$

with any given (2×2) matrix $\hat{K}(0)$.

In general, the solution of Eq. (8) depends on four parameters (matrix elements) provided that the initial distribution function $F(\mathbf{v},0)$ is fixed. We show now how to simplify this four-parameter solution in the special case when eigenvalues $\lambda_{1,2}$ of the matrix $\hat{K}(0)$ are real. Moreover we assume that $\lambda_1 \geqslant \lambda_2 \geqslant 0$, so that the solution exists and is positive for all $t>0$.[19] We note also that any such matrix $\hat{K}(0)$ reduces by rotations to the form

$$\hat{K}'(0)=\begin{pmatrix} \lambda_1 & b \\ 0 & \lambda_2 \end{pmatrix}, \tag{9}$$

therefore we consider only such three-parameter matrices. One more reduction can be obtained by applying a projective transformation. In order to do it, we first write down the solution of Eq. (8) with the initial matrix (9) in the form

$$F(\mathbf{v},t)\equiv F(\mathbf{v},t|\lambda_1,\lambda_2,b).$$

Then the application of the equality (7) with $a=\lambda_2$ results in the following formula:

$$F(\mathbf{v},t|\lambda_1,\lambda_2,b)=F\left[(1+\lambda_2 t)\mathbf{v},\frac{t}{1+\lambda_2 t}\middle|\lambda_1-\lambda_2,0,b\right].$$

Hence, it is sufficient to consider the two-parameter row matrix

$$\hat{K}''(0)=\begin{pmatrix} \lambda & b \\ 0 & 0 \end{pmatrix}\Rightarrow \hat{K}''(t)=[\mathfrak{I}+t\hat{K}''(0)]^{-1}\hat{K}''(0)=\frac{1}{1+\lambda t}\,\hat{K}''(0).$$

Finally we obtain from Eq. (8) the following equation for the function $F(\mathbf{v},t|\lambda,0,b)$:

$$\frac{\partial F}{\partial t}-\frac{1}{1+\lambda t}\,(\lambda \nu_x+b\nu_y)\,\frac{\partial F}{\partial \nu_x}=I(F,F\,).$$

Putting

$$F(\mathbf{v},t)=\Psi[\mathbf{v},(1/\lambda)\ln(1+\lambda t)](1+\lambda t)^{-1},$$

we obtain the resulting equation for $\Psi(\mathbf{v},\tau)$:

$$\frac{\partial \Psi}{\partial \tau}-\frac{\partial}{\partial \nu_x}\,[(\lambda \nu_x+b\nu_y)\Psi]=I(\Psi,\Psi).$$

In the case of zero initial drift velocity (relaxing this condition would be only matter of technical complication), and omitting all details, the first moment equations read

$$\rho_0=\int_{\mathbb{R}^2} d\mathbf{v}\;\Psi=\text{const},\qquad \int_{\mathbb{R}^2} d\mathbf{v}\;\mathbf{v}\Psi=0,$$

$$\frac{\partial}{\partial \tau}\,p_{xy}+[\lambda p_{xy}+bp_{yy}]=-\rho_0 S p_{xy},$$

$$\frac{\partial}{\partial t}\,(p_{xx}-p_{yy})+2(\lambda p_{xx}+bp_{xy})=-\rho_0 S(p_{xx}-p_{yy}), \tag{10}$$

$$\frac{\partial}{\partial \tau}(p_{xx}+p_{yy})+2(\lambda p_{xx}+b p_{xy})=0,$$

where

$$p_{ij}=\int_{\mathbb{R}^2} d\mathbf{v}\ \Psi \nu_i \nu_j, \quad i,j=x,y;$$

$$S=\int d\mathbf{n}\ g\left(\frac{\mathbf{u}\cdot\mathbf{n}}{u}\right)\left[1-\left(\frac{\mathbf{u}\cdot\mathbf{n}}{u}\right)^2\right]=\int_0^{2\pi} d\theta\ g(\cos\ \theta)\sin^2\ \theta.$$

Substituting here $p_{ij}(t)=p_{ij}(0)e^{z\tau}$, we obtain the following algebraic equation for the eigenvalue z:

$$(z+\lambda+\rho_0 S)[(z+\lambda)(z+\lambda+\rho_0 S)-\lambda^2]=b^2\rho_0 S.$$

It is convenient to pass to dimensionless values

$$\tilde{b}=\frac{b}{\rho_0 S}, \quad \tilde{\lambda}=\frac{\lambda}{\rho_0 S}, \quad \tilde{z}=\frac{z}{\rho_0 S}, \quad \theta=\tilde{z}+\tilde{\lambda},$$

so that we obtain the simple equation

$$(\theta+1)[\theta(\theta+1)-\tilde{\lambda}^2]=\tilde{b}^2. \tag{11}$$

The general analysis of this equation is similar to the case $\tilde{\lambda}=0$ observed in Ref. 11. There is always one positive root $\theta=R(\tilde{\lambda}^2,\tilde{b}^2)$, which defines the large time asymptotics of the pressure tensor $p_{ij}(\tau)$ by the formulas

$$p_{ij}(\tau)=p_{ij}^*(0)\exp[(-\lambda+\theta\rho_0 S)\tau], \quad i,j=x,y, \tag{12}$$

where $p_{ij}^*(0)$ are the corresponding projections of initial data.

Finally we return to initial variables and obtain general formulas for density $\rho(t|\lambda_1,\lambda_2,b)$ and pressure $p_{ij}(t|\lambda_1,\lambda_2,b)$, which correspond to an arbitrary initial matrix (9):

$$\rho(t|\lambda_1,\lambda_2,b)=\frac{\rho_0}{(1+\lambda_1 t)(1+\lambda_2 t)},$$

$$p_{ij}(t|\lambda_1,\lambda_2,b)=\tilde{p}_{ij}\left(\frac{1}{\lambda}\ln\frac{1+\lambda_1 t}{1+\lambda_2 t}\right)\Big/[(1+\lambda_2 t)^3(1+\lambda_1 t)],$$

where $\tilde{p}_{ij}(t|\lambda_1,\lambda_2,b)$ are defined by Eqs. (10) with $\lambda=\lambda_1-\lambda_2$. In particular the asymptotic formula (12) results in the following general asymptotic formula:

$$p_{ij}(t|\lambda_1,\lambda_2,b)=\frac{p_{ij}^*(0)}{[(1+\lambda_1 t)(1+\lambda_2 t)]^2}\left(\frac{1+\lambda_1 t}{1+\lambda_2 t}\right)^{R/\tilde{\lambda}},$$

where $\tilde{\lambda}=(\lambda_1-\lambda_2)/(\rho_0 S)$, $\tilde{b}=b/(\rho_0 S)$, $R(\tilde{\lambda}^2,b^2)$ denotes the maximal positive root of Eq. (11).

The higher moments of the distribution function can be obtained by the same method. Thus, using projective transformations one can easily generalize the well known exact results[11,21] for the uniform shear flow to the case of arbitrary initial matrix $\hat{K}(0)$ with real eigenvalues. A similar approach in the three-dimensional case will be considered elsewhere.

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Exact solution of the Ising model on group lattices of genus $g>1$

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We discuss how to apply the dimer method to Ising models on group lattices having nontrivial topological genus g. We find that the use of group extension and the existence of both external and internal group isomorphisms greatly reduces the number of distinct Pfaffians and leads to explicit topological formulas for their sign and weight in the expansion of the partition function. The complete solution for the Ising model on the Klein lattice group $L(2,7)$ with $g=3$ is given. © *1996 American Institute of Physics.* [S0022-2488(96)04006-6]

I. INTRODUCTION

Among the known approaches to the exact evaluation of the $2D$ Ising partition function which have followed the celebrated Onsager solution,[1] the dimer method[2–4] fully exploits the combinatorial and group theoretical properties of the lattices by relating the partition function $\mathcal{Z}$ to the generating function $\mathcal{Z}_d$ of close-packed dimer configurations. Though the method is in principle independent from the dimensionality of the lattice, the corresponding analysis in three dimensions has never been developed, due to the difficulties in extending Kasteleyn's Theorem on lattice orientation. In this paper, we deal with the issue of generalizing the dimer approach to the case of non-Abelian $2D$ lattices of high topological genus which should in fact be equivalent to higher dimensional lattices. Indeed the $3D$ cubic lattice can be considered as a handlebody $2D$ lattice of genus $g=N/4$ where N is the number of sites of the lattice. This hints that a non vanishing ratio g/N may be related to an effective dimension $D>2$ of the lattice. The great difficulty of the problem suggests that a possible concrete way to analyze such lattices is to consider at first graphs possessing the largest possible symmetry group, and the best candidates appear to be the group graphs already well-known in the mathematical literature.[5–8] In this framework we may consider the $2D$ planar lattice with periodic boundary conditions as an example of Abelian lattice group (translational symmetry group) with genus $g=1$, whereas an example of finite non-Abelian lattice with $g=0$ is given by the fullerene-like lattice studied in Ref. 9.

The paper is organized as follows. In Sec. II we outline the basic ideas concerning application of the dimer method to group lattices. In Sec. III we define an extended lattice group H and relate it to the homology and cohomology groups (mod2) H_1, H^1 of the original lattice Λ, define the Grassmann algebra over the decorated lattice $\Lambda^{\#}$ and the Pfaffians as function on orbits of H^1. In Sec. IV we apply the results of Sec. III to discrete groups of particular interest such as the Klein group $L(2,7)$ (of order $N=168$ and genus $g=3$) and discuss the role of external automorphisms. In Sec. V we analyze in detail the orbits of H_1, H^1 under the action of H, define an invariant duality map $\varphi: H_1 \to H^1$ and auxiliary functions of relevant computational interest. Finally, in Sec. VI we construct explicitly the irreps of H, apply them to the harmonic analysis on $\Lambda^{\#}$ and derive the expansion for $\mathcal{Z}$. Few preliminary numerical results are also given.

II. GROUP LATTICES AS ISING LATTICES

We recall here key points of the dimer procedure which are specific to group lattices (see also Refs. 10) :

(1) A discrete group G is defined by a presentation given in terms of a set of p generators

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$A_k, k=1,\ldots,p$ and t relators $P_i, i=1,\ldots,t$. The P_i are words in the generators equivalent to the identity. Let $\mathscr{F}$ be the free group on the $A_k, k=1,\ldots,p$. Let $\mathscr{N}$ be the minimal normal subgroup of $\mathscr{F}$ containing all relators. Then by definition $G=\mathscr{F}/\mathscr{N}$.

(2) The Cayley lattice Λ for a group is defined by giving a map $L: G \to \mathbf{R}^3$ where $L(g) \in \mathbf{R}^3$ is the point of $\mathbf{R}^3$ corresponding to the group element $g \in G$. A bond of color k is then a line joining $L(g)$ to $L(A_k g)$. The genus g of Λ is that of the surface of minimal genus $S \subset \mathbf{R}^3$ on which Λ can be drawn. The Ising Hamiltonian is then defined as

$$E = -\sum_{h \in G} \sum_{k=1}^{p} J_k \sigma_h \sigma_{A_k h}, \tag{1}$$

where the $\{\sigma_h = \pm 1\}$ are the spin variables and $\{J_k\}$ the exchange interactions between connected spins.

(3) Each relator P_i is then represented on Λ as a closed circuit $\zeta(P_i)$ made of oriented colored bonds. If $\zeta(P_i)$ encloses a simply connected region (tile) on S then P_i is called local relator. If S has genus $g=0$ then all relators are local. Of particular interest are models where g is large.

(4) The group lattice Λ is interesting on its own but cannot be related directly to the partition function of an Ising model and to do this we must consider[4] a decorated lattice $\Lambda^{\#}$. This amounts to replace each site of coordination q $(q>2)$ of the original lattice by a sublattice containing $3(q-2)$ points and $4q-9$ decorating bonds. The Ising partition function is then related to the dimer covering generating function on the decorated lattice.

(5) In order to compute the generating function we orient $\Lambda^{\#}$ according to the Kasteleyn prescription by assigning arrows to each bond inherited from Λ in such a way that for any closed circuit ℓ on $\Lambda^{\#}$, the number of bonds of ℓ oriented clockwise is of opposite parity to the number of sites enclosed by ℓ. For the decorating bonds see Ref. 4 or Sec. V.

(6) The Kasteleyn rules define completely the orientation for lattices of genus $g=0$, whereas for lattices of higher genus we have to deal with further sign fixing for loops which are not homologically trivial, i.e., not the boundary of a union of tiles. The assignment of arrows to $\Lambda^{\#}$ (or Λ) is not invariant under the action of G but rather under an extension H of G closely related to the homology H_1 and cohomology H^1 groups of Λ.

(7) The dimer covering generating function of the lattice can be expressed as a weighted sum of Pfaffians $Pf(\phi)$, where $\phi \in H^1$ and with sign given explicitly by the H-invariant function $\theta(\zeta), \zeta \in H_1$ defined in Sec. V. Harmonic analysis on H allows us to factorize Pfaffians into determinants of lesser order and external automorphisms induce identifications between Pfaffians.

III. THE EXTENDED LATTICE GROUP

In this section we first discuss the group extension H of G. Next we show that H partitions the homology H_1 and the cohomology H^1 groups of Λ into nonintersecting orbits characterized in terms of sign functionals. Their role in the expansion of the dimer generating function is then analyzed.

A. The groups H, H_1 and H^1

The extended lattice group H can be obtained from G by replacing the relators P_i with new relators containing the following elements:

(**i**) If $P_i, P_j \in G$ are local, then $P_i P_j^{-1}, P_i^2, P_i A_k P_i^{-1} A_k^{-1}$ are relators in H;

(**ii**) For generic relators $P_i, P_j \in G$ then $P_i^2, P_j^2, P_i P_j P_i^{-1} P_j^{-1}$ are relators in H.

We can write then $P_j = Q$ $(Q^2 = 1)$ for all local relators P_j, with $A_k Q = Q A_k$, i.e. Q is a central element that we call central signature. Putting $Z_i = P_i Q$ the nonlocal relators will be written as $Z_i^2, Z_i Z_j Z_i^{-1} Z_j^{-1}$ where in general $A_k Z_i \neq Z_i A_k$. The $\{Z_i\}$ generate an Abelian normal subgroup $HZ \subset H$. Particular examples of this extension will be discussed further on.

Nontrivial loops form a chain group $C_1(\Lambda^{\#}, \mathbf{Z_2})$. The equivalence classes of $C_1(\Lambda^{\#}, \mathbf{Z}_2)$ modulo boundaries form the homology group $H_1(\Lambda^{\#}, \mathbf{Z}_2)$. The class of multiplicative functionals on $H_1(\Lambda^{\#}, \mathbf{Z}_2)$ with values ± 1 are then the elements of the cohomology group $H^1(\Lambda^{\#}, \mathbf{Z}_2)$. Notice that $H^1(\Lambda^{\#}, \mathbf{Z}_2) \sim H^1(\Lambda, \mathbf{Z}_2)$ and $H_1(\Lambda^{\#}, \mathbf{Z}_2) \sim H_1(\Lambda, \mathbf{Z}_2)$ and therefore we denote them briefly by the symbols H^1, H_1 respectively. When dealing with elements of HZ, H_1 we may use addition instead of the product as composition rule. We write $g \sim g'$ if $g, g' \in H$ define the same site on Λ.

H_1 is isomorphic to HZ. To see it consider the closed chain ℓ on Λ as defined by the sequence $g_0 = g, g_p = h_p g_{p-1}, p = 1, \ldots, n$ with $h_{n+p} = h_p$. $\zeta(\ell)$ is then defined as

$$\zeta(\ell) = g_0^{-1} h_n h_{n-1} \cdots h_1 g_0 = g_p^{-1} h_{p-1} h_{p-2} \cdots h_1 h_n h_{n-1} \cdots h_{p+1} g_p . \tag{2}$$

Starting from g_0 we move n steps across bonds in Λ and each bond defines an element $h_i \in H$, where $h_i = A_k^{\pm 1}$, A_k being a generator of H. If $g_n \sim g_0$, ℓ is closed, $\zeta(\ell) \in HZ$ does not depend on the choice of g_0 on ℓ and defines a map $\zeta: C_1(\Lambda, \mathbf{Z}_2) \to HZ$. Adding a boundary ℓ_0 to ℓ (i.e., adding the boundary of a union of tiles on the lattice) amounts to replace a sequence of bonds $h_{i_1}, \ldots, h_{i_n}$ by an equivalent one obtained by using local relators only, therefore $\zeta(\ell + \ell_0) = \zeta(\ell)$ and ζ induces the map $\kappa: H_1 \to HZ$. Given inversely an element $\zeta \in HZ$, expressed in terms of relators as $\zeta = h_n \cdots h_1$, a corresponding closed chain $\ell(\zeta) \in C_1(\Lambda, \mathbf{Z}_2)$, and therefore a cycle in $H_1(\Lambda, \mathbf{Z}_2)$, is given by a sequence of g_i, $i = 0, \ldots, n$, with $g_0 = \mathbf{1}$ and $h_i g_{i-1} = g_i$. Also if $\zeta = h_n \cdots h_1, \zeta' = h_{m+n} \cdots h_{1+n} \in HZ$ and $g_n \sim g_{m+n} \sim \mathbf{1}$ the chain $\ell(\zeta + \zeta') = \ell(\zeta) + \ell(\zeta') \in C_1(\Lambda, \mathbf{Z}_2)$ defined by $g_0 = \mathbf{1}$ and $h_i g_{i-1} = g_i, i = 1 \cdots m+n$ corresponds to the element $\zeta + \zeta' \in HZ$. Hence κ is a group isomorphism.

Right multiplication on Λ by an element $h \in H$ translates the group lattice and if we replace g_i with $g_i h$ in ℓ we obtain a closed path ℓ_h which is the right translation of ℓ by h and a corresponding element $\zeta(\ell_h) = h^{-1} \ell h$ which defines the action of H on $\ell \in HZ$. In this way H acts naturally on $\Lambda^{\#}$, H_1 and H^1 and partitions H^1, H_1 into nonintersecting orbits. The use of orbits greatly simplifies the computation of $\mathcal{Z}$.

B. Sign functionals and lattice orientation

We assign an orientation to $\Lambda^{\#}$ according to the Kasteleyn rules and to each site $h \in H$ a Grassmann variable $a(h)$, with an anticommuting wedge product $a(h) \wedge a(h') = -a(h) \wedge a(h')$. Reversing the arrows on all bonds sharing the same site i corresponds to the change $a(h) \to -a(h)$.

Let ℓ given by (2). Each h_i is of the form $A_{k_i}^{p_i}$ where $p_i = \pm 1$ determines the orientation of the arrow in the bond. Closing ℓ means that we must identify $a(g_0)$ and $a(g_n)$ as

$$a(g_0) = p_n a(g_n). \tag{3}$$

We define then

$$\eta(\zeta(\ell)) = -\prod_{i=1}^{n} p_i . \tag{4}$$

If ζ is trivial then $\eta(\zeta) = 1$. All $\eta(\zeta)$ defined in this way, hereafter called sign functionals, are characterized by a particular recursion relation which can be proved as follows. Following Ref. 4

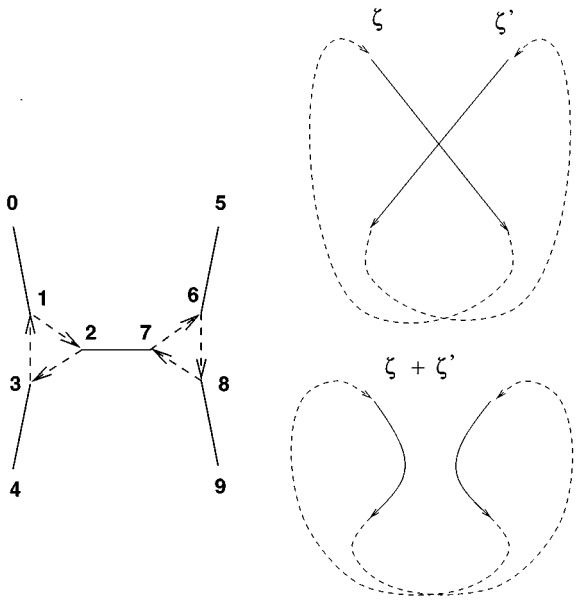

FIG. 1. Intersection between ℓ and ℓ' and schematic representation of ζ,ζ' and $\zeta+\zeta'$ (or ℓ,ℓ' and ℓ'').

we introduce a reference dimer configuration $\mathscr{C}_0$ on $\Lambda^{\#}$ consisting of all bonds of $\Lambda^{\#}$ inherited from Λ. By definition, any other dimer configuration $\mathscr{C}$ when superposed on $\mathscr{C}_0$ generates transition cycles $\zeta \in H_1$. In this proof we use transition cycles only. We consider representative chains $\ell,\ell',\ell'' \in C_1(\Lambda\#,\mathbf{Z}_2)$ of the pair of intersecting cycles ζ,ζ' and of the cycle $\zeta+\zeta'$ as in Fig. 1. Chains ℓ,ℓ' run over the sequence of sites P_i, $i=0,1,2,7,8,9$ and $i=5,6,7,2,3,4$ respectively, while ℓ'' runs over $i=0,1,3,4$ and $i=5,6,8,9$ but not $i=2,7$. We denote with B_{ij} the bonds joining P_i,P_j and with $n(\ell)$ the number of anticlockwise arrows on ℓ. The key point is that bonds B_{12},B_{13} are not contained in the intersection of ζ and $\zeta+\zeta'$ and thus $B_{12},B_{13}\notin\mathscr{C}_0$ whereas $B_{01}\in\mathscr{C}_0$. Similarly $B_{34},B_{27},B_{56},B_{89}\in\mathscr{C}_0$. By orienting $\Lambda^{\#}$ according to the Kasteleyn rules and counting arrows we see that $n(\ell'')\equiv n(\ell)+n(\ell')+1(\mathrm{mod}2)$. The general case where B_{ij} are replaced by sequences of bonds corresponds to the addition of boundaries to ℓ,ℓ',ℓ'' and leads to the same formula. Hence $n(\ell)$ is a function in H_1 and $\eta(\zeta+\zeta')=-\eta(\zeta)\eta(\zeta')$ if ζ,ζ' intersect and $\eta(\zeta+\zeta')=\eta(\zeta)\eta(\zeta')$ otherwise , i.e.,

$$\eta(\zeta+\zeta')=\eta(\zeta)\eta(\zeta')(-1)^{\Omega(\zeta,\zeta')}, \tag{5}$$

where $\Omega(\zeta,\zeta')=0,1$ is the intersection number (mod2) of ζ,ζ'. Given a sign functional $\eta(\zeta)$ then $\phi(\zeta)\eta(\zeta)$, $\phi\in H^1$, is another sign functional and so is the H-invariant function $\theta(\zeta),\zeta\in H_1$ defined in Sec. V.

C. Pfaffians and dimer covering generating function

Consider now the form

$$f=\frac{1}{2}\sum_{h,h'\in\Lambda^{\#}} x_{hh'}a(h)\wedge a(h'), \tag{6}$$

where $x_{hh'}=0$ if h and h' are not connected in $\Lambda^{\#}$ (neighbors). The factor $\frac{1}{2}$ is inserted in order to avoid double counting, the activity is given by $x_b=x_{hh'}=-x_{h'h}=\coth(\beta J_{hh'})$ if the bond b is oriented with the arrow from h to h', β is the inverse temperature and $J_{hh'}$ the exchange

interaction between spins (J_k in the previous notation) which depends only on the color k of the bond. Under the stated conditions decorating bonds have $x_{hh'}=1$. For the sole purpose of safe handling of signs we assume initially $x_b>0$. All arrows on $\Lambda^{\#}$ and all signs in (6) are then fixed by the sign functional η. The Pfaffian $Pf(\eta)$ is defined by

$$f^{M/2}=2^M M! Pf(\eta) a(1)\wedge a(2)\wedge\cdots\wedge a(M), \tag{7}$$

where $M=3(q-2)N$, N is the order of the group (or lattice size) and q is the lattice coordination. From (7) one derives the well-known relation

$$Pf(\eta)^2=Det(X(\eta)), \tag{8}$$

where $X(\eta)$ is the $M\times M$ matrix of elements x_{ij}. In general $Pf(\eta)$ is multilinear function of the x_b considered as independent variables. The partition function $\mathcal{Z}$ is then given by

$$\mathcal{Z}=\mathcal{Z}_d\, 2^N\prod_a \sinh(\beta J_a)^{1/2}, \tag{9}$$

where a runs on all the oriented bonds of the undecorated group lattice and

$$\mathcal{Z}_d=2^{-g}\sum_\eta s_\eta Pf(\eta), \quad s_\eta=\pm 1. \tag{10}$$

To each dimer configuration $\mathcal{C}$ we associate the contribution of $\mathcal{C}$ to $Pf(\eta)$, a monomial $M(\mathcal{C})=\Pi_b x_b$ where b runs over all oriented bonds of $\mathcal{C}$. Because of our conventions $M(\mathcal{C})$ has sign $\eta(\zeta)$ where ζ is the superposition of $\mathcal{C}$ and $\mathcal{C}_0$. In general ζ is the sum of nonintersecting cycles $\zeta=\Sigma_i\zeta_i$ so that $\eta(\zeta)=\Pi_i\eta(\zeta_i)$. The signs s_η must then be chosen in such a way as to set equal to 1 in (10) the coefficient of all $M(\mathcal{C})$ appearing in $\mathcal{Z}_d$. Once this is done in Sec. V the x_b can be given any sign.

IV. 2*D* ISING LATTICE AND THE *L*(2,7) LATTICE GROUP

The above group extension procedure can be naturally applied to a wide class of lattice groups. Here we discuss two examples: the Abelian $2D$ Ising lattice (of genus $g=1$) and the $L(2,7)$ Klein group. The latter is non-Abelian and of genus $g=3$, and its analysis should hopefully be of interest in the analysis of more general structures of dimension $D>2$.

A. 2*D* Ising lattice

The Onsager solution for the $2D$ Ising lattice made use of a rectangular $n\times m$ lattice with sites labelled by $i=1,\ldots,n$ and $j=1,\ldots,m$ (n even). In this lattice we identify opposite sides, giving it a toroidal ($g=1$) topology and turning in a group lattice G_{nm}. This last property makes it possible to apply harmonic analysis, i.e., Fourier transform methods, which eventually lead to the final formula. The group G_{nm} of the lattice is defined by the presentation

$$ST=TS, \quad S^n=\mathbf{1}, \quad T^m=\mathbf{1}, \tag{11}$$

for all integers n,m. However in order to satisfy the Kasteleyn rules we must use a central extension H_{nm} of (11) defined by

$$ST=QTS, \quad S^n=Z_1, \quad T^m=Z_2,$$

$$Q^2=Z_1^2=Z_2^2=1, \quad QZ_1=Z_1Q, \quad QZ_2=Z_2Q, \quad Z_1Z_2=Z_2Z_1. \tag{12}$$

Sites are labeled by elements $h\in H_{nm}$ with the condition

$$a(hQ) = -a(h). \tag{13}$$

The H_{nm} lattice is actually a covering of the G_{nm} lattice with corresponding variables $a(h)$ identified by the above condition which embodies the Kasteleyn rules.

Besides this condition we must set

$$a(hZ_1) = \epsilon_1 a(h), \quad a(hZ_2) = \epsilon_2 a(h), \tag{14}$$

where ϵ_1 and ϵ_2 take the values ± 1 in all the possible combinations. These correspond to the $2^{2g}=4$ possible choices of $\phi \in H^1$. It is tempting but misleading to label spin sites on the lattice by elements in G_{nm}. In this case the orientation would no longer be invariant under G_{nm}, a clear sign that the true symmetry is that of the extended group H_{nm}.

B. Non-Abelian group lattices of genus $g>1$

We examine now other types of symmetries which require non-central group extensions and which are of interest for models in $D>2$. The natural further step is provided by a vast array of discrete groups many of which are discussed in detail in the literature (see Refs. 5–8). Of particular interest are the Klein groups $L(2,p)$, where p is prime. The non-Abelian group of genus $g=0$ (the fullerene lattice) studied in Ref. 9 corresponds to $p=5$. The next interesting example which is at the same time non-Abelian and has a nontrivial topology is given by the lattice group $L(2,7)$ (also called $T(2,3,7)$ in the context of hyperbolic tessellations). The $L(2,7)$ group , briefly called G, has order 168 and is defined by the presentation

$$U^7 = \mathbf{1}, \quad V^2 = \mathbf{1}, \quad (UV)^3 = \mathbf{1}, \quad (VU^3)^4 = \mathbf{1}. \tag{15}$$

The analysis of a lattice possessing this kind of symmetry is one of the chief results of this paper which hopefully opens the way to the investigation of more general and interesting structures. The group lattice given by (15) has genus $g=3$ (produced by the nonlocal relator $(VU^3)^4$) and can be tessellated by 24 heptagons and 56 hexagons, for a total of 168 bonds of type U and 84 bonds of type V (see Ref. 11, pp. 539–549, for more details on the lattice).

The group G_{nm} given by (11) is Abelian and has a nontrivial genus $g=1$. On a lattice of genus g we expect that the Kasteleyn rule determines the orientation up to $2g$ signs with a total of 2^{2g} configurations. Each close path on the lattice Λ can be considered as an element of the homology group H_1 and an assignment of all remaining signs as an element of the cohomology group H^1. It is therefore sufficient to assign signs on a suitable basis of $2g$ elements of H_1. In the toroidal case this was done by giving ϵ_1, ϵ_2. In fact Z_1, Z_2 are central in the group G_{nm}.

The group G, as defined by (15), is non-Abelian and has a nontrivial genus, in particular the Z_i are no longer central elements and we deal with the discussed noncentral extension H of G defined by

$$U^7 = Q, \quad V^2 = Q, \quad (UV)^3 = Q, \quad W \equiv Q(VU^3)^4 = Z(\mathbf{1}), \tag{16}$$

and additional relators which can be expressed in term of the auxiliary elements

$$Z(h) = h^{-1} W h, \quad h \in H, \tag{17}$$

characterized by

$$Z(h_1)Z(h_2) = Z(h_2)Z(h_1), \quad (Z(h))^2 = 1, \quad \forall h_1, h_2, h \in H. \tag{18}$$

The $Z(h)$ are not all independent and can be expressed in terms of the subset of $2g=6$ elements

$$Z_n \equiv Z(U^n) = U^{-n} Z(\mathbf{1}) U^n. \tag{19}$$

Clearly $Z_n = Z_{n,(\mathrm{mod}7)}$ and $Z_0 = Z(\mathbf{1}) = Z_7$. The following identities equivalent under (18)

$$Z_5 Z_1 Z_4 Z_0 Z_3 Z_6 Z_2 = \mathbf{1}, \quad Z_1 Z_3 Z_5 Z_0 Z_2 Z_4 Z_6 = \mathbf{1}, \tag{20}$$

reduces to 6 the number of independent elements Z_i and can be proved by repeated application of relators (16) but not of (18).

A generic $\zeta \in H_1$can be always written in the additive form $\Sigma_i n_i Z_i$ where $n_i = 0,1$. Because of $\Sigma_{i=0}^{6} Z_i = 0$ we can always choose the n_i in such a way as to have $\Sigma_i n_i = 0$ or 1. All elements $Z(h), h \in H$, can be obtained by repeated conjugation of the Z_n by U and V. Conjugation by U is trivial, i.e. $U^{-1} Z_n U = Z_{n+1}$. Conjugation by V is less obvious. By using (16) and not (18) we find that

$$V^{-1} Z_0 V = Z_4, \quad V^{-1} Z_1 V = Z_3^{-1} Z_0^{-1}, \quad V^{-1} Z_2 V = Z_4^{-1} Z_2^{-1} Z_0^{-1},$$

$$V^{-1} Z_3 V = Z_4^{-1} Z_1^{-1}, \quad V^{-1} Z_4 V = Z_0, \quad V^{-1} Z_5 V = Z_5^{-1}, \quad V^{-1} Z_6 V = Z_6^{-1}, \tag{21}$$

which can be further simplified by using (18). In the additive form (21) and (19) can be written in full generality as

$$h^{-1} Z_i h = \sum_{k=0}^{6} P_{ik}(h) Z_k, \quad h \in H, \tag{22}$$

where $P(h)$is a representation mod 2 of H.

Moreover the group H has an external automorphism ν given by

$$\nu(V) = V^{-1} = -V, \quad \nu(U) = U^{-1}, \quad \nu(Z_p) = Z_{4-p}^{-1} = Z_{4-p}. \tag{23}$$

V. ORBITS OF HOMOLOGY AND COHOMOLOGY GROUPS

As anticipated, the analysis of orbits and of external automorphisms plays a central role in the computation of $\mathcal{Z}_d$. We thus give here the explicit construction of such orbits in H_1 and H_1, together with their duality map.

A functional $\phi \in H^1$ can be defined by the equivalent conditions:

$$a(gZ_i) = \epsilon_i a(g), \phi(Z_i) = \varepsilon_i, \quad i = 0, \ldots, 6; \quad \prod_{i=0}^{6} \epsilon_i = 1, \tag{24}$$

ϕ is then identified by $(\epsilon_0, \ldots, \epsilon_6)$. Let $\zeta \in H_1$ and let $h^{-1}\zeta h$ be the translated cycle. Then the translated functional ϕ_h is defined by

$$\phi_h(h^{-1}\zeta h) = \phi(\zeta). \tag{25}$$

We have then

$$\phi_U(U^{-1} Z_i U) = \phi(Z_i) = \epsilon_i = \phi_U(Z_{i+1}), \tag{26}$$

and hence

$$\phi_U(Z_i) = \epsilon_{i-1}, \quad \phi_{U_{-1}}(Z_i) = \epsilon_{i+1}. \tag{27}$$

Similarly we find

$$\phi_V(V^{-1} Z_0 V) = \phi(Z_0) = \epsilon_0 = \phi_V(Z_4), \tag{28}$$

and

$$\phi_V(Z_0)=\epsilon_4,\quad \phi_V(Z_3)=\epsilon_1\epsilon_4,\quad \phi_V(Z_2)=\epsilon_0\epsilon_4\epsilon_2,$$
$$\phi_V(Z_1)=\epsilon_3\epsilon_0,\quad \phi_V(Z_5)=\epsilon_5,\quad \phi_V(Z_6)=\epsilon_6. \tag{29}$$

There are $2^{2g}=64$ ($g=3$ denoting the genus of Λ) different elements in H^1 which fall in 5 different orbits containing 1,7,7,21,28 elements. We list these orbits with only one signature out of each cyclically permuted septet:

$$A:(1,1,1,1,1,1,1)\quad \text{(trivial)},$$
$$B:(1,1,-1,1,-1,-1,-1),$$
$$C:(-1,-1,-1,1,-1,1,1),$$
$$D:(-1,-1,-1,1,-1,-1,-1),(-1,-1,1,1,1,-1,-1),(1,1,-1,1,-1,1,1),$$
$$E:(-1,1,-1,1,-1,1,-1),(1,-1,-1,1,-1,-1,1),(-1,1,1,1,1,1,-1),(1,-1,1,1,1,-1,1). \tag{30}$$

The orbits B,C are mapped into each other by the action of ν. This proves incidentally that ν is external. We also list in similar fashion the dual orbits in H_1:

$$A:(0,0,0,0,0,0,0)\quad \text{(trivial)},$$
$$B:(1,1,0,0,1,0,1),$$
$$C:(1,0,1,0,0,1,1),$$
$$D:(0,0,1,0,1,0,0),(0,1,1,0,1,1,0),(0,1,0,0,0,1,0),$$
$$E:(1,0,0,0,0,0,1),(1,1,1,0,1,1,1),(1,1,0,0,0,1,1),(1,0,1,0,1,0,1), \tag{31}$$

as it can be checked by using (28)–(29).

For generic elements $\zeta,\zeta' \in H_1$ we use the additive form:

$$\zeta=\sum_{i=0}^{6} n_i Z_i,\quad \zeta'=\sum_{i=0}^{6} m_i Z_i, \tag{32}$$

and define the intersection number (mod2)

$$\tau(\zeta,\zeta')=\tau(\zeta',\zeta)=(-1)^{\Omega(\zeta,\zeta')}. \tag{33}$$

Ω is the $\mathbf{Z}_2$ valued form of Eq. (5) explicitly given by

$$\Omega(\zeta,\zeta')=\sum_{i,k=0}^{6} \chi(i-k)n_i m_k \tag{34}$$

with $\chi(i)=1$ if $i\equiv 1,2,5,6 \pmod 7$ and $\chi(i)=0$ otherwise, as it can be verified on the graph $\Lambda^{\#}$. $\tau(\zeta,\zeta')$ is invariant under conjugations by H, see (21), and is multiplicative, i.e.,

$$\tau(\zeta,\zeta'+\zeta'')=\tau(\zeta,\zeta')\tau(\zeta,\zeta''). \tag{35}$$

We define also

$$\theta(\zeta)=(-1)^{\frac{1}{2}\sum_{i,k=0}^{6}\chi(i-k)n_i n_k}, \tag{36}$$

so that $\theta(Z_i)=\theta(\mathbf{1})=1$ and $\theta(\zeta)$ is a sign functional as η in (5):

$$\theta(\zeta+\zeta')=\theta(\zeta)\theta(\zeta')\tau(\zeta,\zeta'). \tag{37}$$

All these definitions can be extended naturally to a wide class of lattice groups.

Then let

$$m_i=\sum_{k=0}^{6}\chi(i-k)n_k \tag{38}$$

and define the duality map $\varphi, H_1\to H^1$:

$$\varphi\left(\sum_{i=0}^{6} n_i Z_i\right)=((-1)^{m_0},\ldots,(-1)^{m_6}). \tag{39}$$

The 2^{2g} elements of H_1, H^1 are labeled as ζ_I, ϕ_I, where $\varphi(\zeta_I)=\phi_I$, by an index $I=1,\ldots,2^{2g}$ with ζ_1, ϕ_1 the trivial elements and sorted in such a way that in (31),(30) φ maps corresponding orbits in H_1, H^1. Clearly then $\phi_I(\zeta_K)=\tau(\zeta_I,\zeta_K)$. We set $\eta_I(\zeta)=\phi_I(\zeta)\theta(\zeta)$, $s_I=s_{\eta_I}$ so that we may label Pfaffians equally well with elements $\phi\in H^1$ and rewrite (10) as

$$\mathcal{Z}_d=2^{-g}\sum_I s_I Pf(\phi_I). \tag{40}$$

The importance of orbits should be clear once we realize that in (40) for elements ϕ_I, ϕ_J in the same orbit we have $Pf(\phi_I)=Pf(\phi_J)$. In this way the effective number of different terms in $\mathcal{Z}_d$ reduces to the number of orbits in H^1.

Further reductions arise from external automorphisms. When omitted, as in (40), we assume summation ranges on I,K to be $1\cdots 2^{2g}$. Since φ commutes with the group operations it maps orbits in H_1 into dual orbits in H^1 and we use the same label $A\cdots E$ for pairs of dual orbits. Moreover the $2^{2g}\times 2^{2g}$ matrix $\Phi=\Phi^T$ of elements $\Phi_{KI}=2^{-g}\tau(\zeta_I,\zeta_K)$ is orthogonal. First of all we have

$$\sum_I \Phi_{KI}^2=2^{-2g}\sum_I 1=1. \tag{41}$$

Next we have

$$\begin{aligned} p(K,K')=\sum_I \Phi_{KI}\Phi_{K'I}&=2^{-2g}\sum_I \phi_K(\zeta_I)\phi_{K'}(\zeta_I)\\ &=2^{-2g}\sum_I \phi_K(\zeta_I+\xi)\phi_{K'}(\zeta_I+\xi)\\ &=2^{-2g}\sum_I \phi_K(\zeta_I)\phi_{K'}(\zeta_I)\phi_K(\xi)\phi_{K'}(\xi)\\ &=p(K,K')\phi_K(\xi)\phi_{K'}(\xi) \end{aligned} \tag{42}$$

therefore $p(K,K')=0$ if $\exists\xi$: $\phi_K(\xi)\phi_{K'}(\xi)\neq 1$. But if $\forall\xi$: $\phi_K(\xi)\phi_{K'}(\xi)=1$ then $K=K'$ therefore $p(K,K')=0$ if $K\neq K'$. This proves that Φ is orthogonal and that $\Phi=\Phi^{-1}$.

We conclude this section with some rather technical formulas whose rôle will be crucial in what follows (Sec. VIII).

The sum $\Sigma_K\theta(\zeta_K)$ can be readily evaluated by using a standard basis for H_1 given by $X_i, Y_i, i=1\cdots g$ such that

$$\theta\left(\sum_i^g (p_iX_i+q_iY_i)\right)=(-1)^{\sum_{i=1}^g p_iq_i}, \tag{43}$$

where, for instance,

$$X_1=Z_0,\quad Y_1=Z_1,\quad X_2=Z_1+Z_5,\quad Y_2=Z_0+Z_2+Z_5,\quad X_3=Z_0+Z_3, Y_3=Z_1+Z_3+Z_6. \tag{44}$$

In this form $\Sigma_K\theta(\zeta_K)$ factors into g independent and equal sums each yielding a factor 2 and hence $\Sigma_K\theta(\zeta_K)=2^g$.

Furthermore,

$$2^{-g}\sum_K \tau(\zeta_I,\zeta_K)\theta(\zeta_K)=2^{-g}\theta(\zeta_I)\sum_K \theta(\zeta_K+\zeta_I)=\theta(\zeta_I) \tag{45}$$

since $\zeta_K+\zeta_I$ runs over the whole group H_1 taking every element once just as ζ_K and therefore $\Sigma_K\theta(\zeta_K+\zeta_I)=\Sigma_K\theta(\zeta_K)=2^g$.

VI. IRREPS OF *H*

The group H has $168\times 64=10752$ elements and in order to perform harmonic analysis and obtain partial block diagonalization of $X(\phi)$ and of Pfaffians we must find the unitary irreducible representations (irreps) of H.

The trivial functional (1,1,1,1,1,1) must be dealt with separately and requires the construction of the irreps of the factor group H_0 of H and central extension of G defined by

$$U^7=Q,\quad V^2=Q,\quad (UV)^3=Q,\quad (VU^3)^4=Q \tag{46}$$

(i.e., $Z_i=\mathbf{1}$) of order $168\times 2=336$. Therefore we have the relators

$$a(gZ_i)=a(g),\quad a(gQ)=-a(g). \tag{47}$$

Because of (47), only a subset of the unitary irreps of H_0 is actually used in the harmonic analysis. In order to see it let us write such irreps as $D^J_{\alpha\beta}(g)$ with J a convenient label and $\alpha,\beta=1,\ldots,d_J$ where d_J is the dimension of the irrep . The matrix elements satisfy the orthogonality relations:

$$\sum_{g\in H_0} D^J_{\alpha\beta}(g)^* D^{J'}_{\alpha'\beta'}(g)=\delta^{JJ'}\delta_{\alpha\alpha'}\delta_{\beta\beta'}. \tag{48}$$

Let us define

$$a^J_{\alpha\beta}=\sum_{g\in H_0} a(g)D^J_{\alpha\beta}(g). \tag{49}$$

Applying (49) to (47) we get

$$\sum_{g\in H_0} a(gQ)D^J_{\alpha\beta}(g) = -a^J_{\alpha\gamma} = a^J_{\alpha\gamma}D^J_{\gamma\beta}(Q). \tag{50}$$

But Q is a central element and $Q^2=\mathbf{1}$. Therefore by Schur lemma $D^J_{\gamma\beta}(Q)$ must be proportional to the identity, i.e.,

$$D^J_{\gamma\beta}(Q)=\kappa\delta_{\gamma\beta}, \quad \kappa=\pm 1, \tag{51}$$

therefore from (50)

$$\kappa a^J_{\alpha\gamma} = -a^J_{\alpha\gamma}, \tag{52}$$

i.e., $\kappa=-1$. It follows that only irreps having $\kappa=-1$ actually contribute to the Fourier expansion of $a(g)$. Those irreps which are also irreps of the original group G (i.e., those with $\kappa=1$) are absent from the expansion. There are only 5 irreps of H_0 with $\kappa=-1$ of dimension 4,4,6,6,8, satisfying separately the Burnside condition $4^2+4^2+6^2+6^2+8^2=168$. The detailed form is listed in Appendix A. The matrix elements of these irreps are polynomials in $K=\exp(i\pi/7)$ with $K^7=-1$. By abuse of language we may write

$$Q=-1, \quad U^7=-1, \quad V^2=-1, \quad (UV)^3=-1, \quad (VU^3)^4=-1, \tag{53}$$

instead of (46).

As for the remaining irreps of H the most convenient way is to obtain them as induced representations on the cosets of the subgroup L of H generated by

$$V, \quad U^{-1}VU^2, \quad U^{-6}VU^3, \quad U^{-4}VU^4, \quad U^{-5}VU^5, \tag{54}$$

as well as the cosets of the group $\nu(L)$ generated by

$$V^{-1}, \quad UV^{-1}U^{-2}, \quad U^6V^{-1}U^{-3}, \quad U^4V^{-1}U^{-4}, \quad U^5V^{-1}U^{-5}. \tag{55}$$

All generators and their inverses are of the form $U^{a(b)}VU^b, b=0,\ldots,6$. Let us briefly set $v=V$ and $t=U^{-1}VU^2$; we find then

$$\begin{gathered} U^{-6}VU^3=vt, \quad U^{-4}VU^4=Z_1(tv)^2=(tv)^2Z_4, \\ U^{-5}VU^5=vt(vt^{-1})^2Z_1=Z_2Z_6vt(vt^{-1})^2, \\ (vt)^4=QZ_3, \quad (tv)^4=QZ_1Z_4. \end{gathered} \tag{56}$$

It can be verified that $\{v,t,Z_i,Q\}$ generate the whole subgroup L. Let suppose that a representation $\lambda: L\to \mathrm{Hom}(\mathscr{S})$ is given on a linear space $\mathscr{S}$ of dimension n. Then λ can be extended to the induced representation μ: $H\to$ Hom$(\mathscr{H})$ where $\mathscr{H}\oplus_{p=0}^{6}\mathscr{S}_p$ and $\mathscr{S}_p$ are isomorphic to $\mathscr{S}$. Let ψ_i be a basis on $\mathscr{S}$, $\psi_{i,p}$ a basis on $\mathscr{S}_p$ and $\psi_{i,p+7}=-\psi_{i,p}$. The action of U on $\mathscr{H}$ is then defined by

$$U\psi_{i,p}=\psi_{i,p+1}, \tag{57}$$

hence $U^7=-1$. Moreover we set

$$w\psi_{i,0}=\psi_{k,p}\lambda_{k,i}(w), \quad w\in L. \tag{58}$$

From (56)–(58) derive the representation of V on $\mathscr{H}$ as follows:

$$V\psi_{i,b}=VU^b\psi_{i,0}=U^{a(b)}U^{-a(b)}VU^b\psi_{i,0}=U^{a(b)}\psi_{k,0}\lambda(U^{-a(b)}VU^b)_{k,i}$$
$$=\psi_{k,a(b)}\lambda(U^{-a(b)}VU^b)_{k,i}. \tag{59}$$

Since b can take all values $0,\ldots,6$ we deduce the complete representation of V on $\mathscr{H}$. The problem reduces now to that of finding a suitable representation of L on $\mathscr{L}$. Should we set $Q=Z_i=\mathbf{1}$, L becomes the octahedral group $T(2,3,4)$ of order 24. We are interested in irreps of L in which all $\lambda(Z_i)$ are diagonal and $\lambda(Z_i^2)=\mathbf{1}$. Each $\lambda(Z_i)$ is then a diagonal block matrix. In fact we have

$$Z_0\psi_{i,p}=Z_0U^p\psi_{i,0}=U^pZ_p\psi_{i,0}=U^p\lambda(Z_p)\psi_{i,0}=\lambda(Z_p)\psi_{i,p}. \tag{60}$$

It is then clear that $\mu(Z_s)$ is the diagonal matrix with entries $\lambda(Z_s)$, $\lambda(Z_{s+1}),\ldots,\lambda(Z_{s+6})$, where $\lambda(Z_s)$ has n eigenvalues $\xi_{i,s}=\pm1, i=1,\ldots,n, s=0,\ldots,6$. It follows also that each vector $\psi_{i,p}$ has eigenvalues

$$Z_s\psi_{i,p}=\xi_{i,s+p}\psi_{i,p}, \tag{61}$$

which define the element $\Xi\in H^1$:

$$\Xi=(\xi_{i,p},\xi_{i,p+1},\ldots,\xi_{i,p+6}). \tag{62}$$

For the group $\nu(L)$ the corresponding formulae are obtained by setting $v'=V^{-1}, t'=UV^{-1}U^{-2}$. We have then

$$U^6V^{-1}U^{-3}=v't', \quad U^4V^{-1}U^{-4}=Z_3(t'v')^2=(t'v')^2Z_0, \tag{63}$$

$$(v't')^4=QZ_0^{-1}, \quad (t'v')^4=QZ_0^{-1}Z_3^{-1}. \tag{64}$$

If an irrep of H contains a signature Ξ it contains also the whole orbit including its cyclical permutations. Nontrivial functionals have 7 distinct cyclical permutation of any Ξ corresponding to $p=0,\ldots,6$ in (62). The irrep μ of H generated by λ has dimension $7n$ and as many signatures. If it contains different orbits then is reducible. Therefore irreps can be grouped in disjoint subsets characterized by orbits. Irreps belonging to orbits A,D,E can be obtained either from L or $\nu(L)$ whereas B and C can be obtained only from L and $\nu(L)$ respectively. We list in Appendix B the explicit representations λ of the group L corresponding to each orbit by giving $\lambda(v),\lambda(t)$ and $\lambda(Z_1)$. In this way we obtain the irreps of the orbits A,B,D,E. Irreps of orbit C can be obtained by applying ν to irreps of B. Clearly orbits may appear in some irreps with multiplicities $m=1,2,4$ where n/m is the number of inequivalent signatures under cyclical permutations contained in the orbit. The method applied to orbits A yields representations which reduce into the irreps already discussed. The dimensions of the irreps satisfy a separate Burnside condition

$$\sum_{J\in O} d_J^2=n(O)N, \tag{65}$$

where $n(O)$ is the number of signatures belonging to a given orbit O.

VII. THE DECORATED LATTICE AND THE PARTITION FUNCTION

We need now a more explicit description of the decorated lattice $\Lambda^{\#}$ along lines already discussed in Ref. 9. Each element $h\in H$ identifies uniquely a site of Λ which we also label with h, being intended that $hQ\sim hZ_i\sim Z_ih$ identify the same site of Λ. h is connected to other 3 sites $Vh,Uh,U^{-1}h$ and is replaced in $\Lambda^{\#}$ by 3 sites h_a,h_b,h_c to which we associate Grasmann variables $a(h),b(h),c(h)$. The original oriented bonds $h\to Vh, h\to Uh$ are replaced by oriented

bonds $h_a \to Vh_a, h_b \to Uh_c$ (with exchange interaction J_V, J_U respectively) together with the additional decorating bonds $h_a \to h_c, h_c \to h_b, h_b \to h_a$. For each Pfaffian we need boundary conditions of the kind discussed above:

$$a(hZ_i) = \epsilon_i a(h), \quad a(Qh) = a(hQ) = -a(h) \tag{66}$$

and the corresponding conditions obtained by replacing a with b,c. Under these assumptions the 2-form (6) can be rewritten explicitly as

$$f = \sum_{h \in \Lambda} \left(a(h) \wedge c(h) + c(h) \wedge b(h) + b(h) \wedge a(h) + \frac{y}{2} a(h) \wedge a(Vh) + x b(h) \wedge c(Uh) \right), \tag{67}$$

where $y = \coth(\beta J_V)$, $x = \coth(\beta J_U)$.

Harmonic analysis on Λ can be performed by recalling the Fourier components of $a(h), b(h), c(h)$ given by $a(h) = \Sigma^J_{\alpha\beta} D^J_{\alpha\beta}(h)^* a^J_{\alpha\beta}$, etc. To this purpose we consider the matrices $\mathbf{a}^J, \mathbf{b}^J, \mathbf{c}^J$ of elements $a^J_{\alpha\beta}, b^J_{\alpha\beta}, c^J_{\alpha\beta}$ where $\alpha, \beta = 1 \cdots d_J$. By using the orthonormality relations (48) satisfied by the matrices $D^J_{\alpha\beta}(h)$ we rewrite $f = \Sigma_J f^J$ where

$$f^J = Tr \left(\mathbf{a}^{J\dagger} \wedge \mathbf{c}^J + \mathbf{c}^{J\dagger} \wedge \mathbf{b}^J + \mathbf{b}^{J\dagger} \wedge \mathbf{a}^J + \frac{y}{2} \mathbf{a}^{J\dagger} \wedge D^J(V) \mathbf{a}^J + x \mathbf{b}^{J\dagger} \wedge D^J(U) \mathbf{c}^J \right) \tag{68}$$

and $J^\dagger$ labels the complex conjugate irrep of J. The key point is that different pairs $J, J^\dagger$ lead to disjoint sets of Grassman variables, moreover $f^J + f^{J\dagger}$ separates into the sum of partial forms $\Sigma_\alpha (f^J)_{\alpha\alpha}$ + c.c. Therefore the final Pfaffian is the product of d_J partial (and identical) Pfaffians, which must be computed explicitly by use of (8). Once this is done we must determine the coefficients s_I appearing in (40). Since all the s_I and Pfaffians $Pf(\phi_I)$ sharing the same orbit O of ϕ_I are equal we can set $S_O = n(O) s_I, Pf(\phi_I) = pf(O), \forall \phi_I \in O$ and (40) reduces to

$$\mathcal{Z}_d = 2^{-g} \sum_O S_O pf(O). \tag{69}$$

The sign in $Pf(\phi_I)$ of a term associated with the path ζ is given by $\eta_I(\zeta) = \tau(\zeta_I, \zeta) \theta(\zeta)$. The s_I must be chosen in such a way as to set the final coefficient of ζ_K in the expansion (40):

$$2^{-g} \sum_I s_I \tau(\zeta_I, \zeta_K) \theta(\zeta_K) \tag{70}$$

equal to 1. Taking into account(45) we see that the condition

$$\forall I: 2^{-g} \sum_I s_I \tau(\zeta_I, \zeta_K) = \sum_I s_I \Phi_{IK} = \theta(\zeta_K) \tag{71}$$

has the simple solution

$$s_I = \theta(\zeta_I), \tag{72}$$

and thus $S_A = 1, S_B = S_C = 7, S_D = 21, S_E = -28$ and $S_A + S_B + S_C + S_D + S_E = 8 = 2^g$.

VIII. PFAFFIANS AND HARMONIC ANALYSIS ON THE LATTICE

The boundary conditions (66) on the Grassmann variables $a(h),b(h),c(h)$ imply strong restrictions on the Fourier components $a^J_{\alpha\beta},b^J_{\alpha\beta},c^J_{\alpha\beta}$ similar to those already derived for Q. Consider now $Pf(\phi)$ where $\phi=(\epsilon_0,\epsilon_1,\epsilon_2,\epsilon_3,\epsilon_4,\epsilon_5,\epsilon_6)$. From (66) we get

$$\sum_{h\in H} a(hZ_i)D^J_{\alpha\beta}(h)=\epsilon_i a^J_{\alpha\gamma}=a^J_{\alpha\gamma}D^J_{\gamma\beta}(Z_i). \tag{73}$$

In all the explicit representation of H listed in the Appendix B the matrices $D^J_{\gamma\beta}(Z_i)$ are diagonal and

$$D^J_{\gamma\beta}(Z_i)=\epsilon^J_i(\gamma)\,\delta_{\gamma\beta}. \tag{74}$$

Clearly $a^J_{\alpha\gamma},b^J_{\alpha\gamma},c^J_{\alpha\gamma}=0$ unless $\epsilon^J_i(\gamma)=\epsilon_i, i=0,\ldots,6$. The orbit O of ϕ identifies a subset of irreps and in (68) only a rectangular submatrix of $\mathbf{a}^J,\mathbf{b}^J,\mathbf{c}^J$ of dimension $d_J\times d_J/n(O)$ survives where d_J is the dimension of the irrep and $d_J/n(O)$the number of times a given signature in O appears in the irrep. The total number of surviving components of $a^J_{\alpha\gamma}$ among all irreps is in any case equal to the order N of the group G, i.e., 168.

Each $\mathbf{a}^J,\mathbf{b}^J,\mathbf{c}^J$ is therefore partitioned into $d_J/n(O)$ rectangular submatrices labeled by the signatures in O. Only one of these matrices needs to be used because they all yield the same final expression for the Pfaffian. Since in (68) all partial forms $f_{J\alpha}$ yield identical Pfaffians we may consider just one contribution and drop the index α. In this case the square of the partial Pfaffian can be written as the determinant of the block matrix Δ_J

$$\Delta_J=\begin{bmatrix} yD^J(V) & \mathbf{1} & -\mathbf{1} \\ -\mathbf{1} & 0 & \mathbf{1}-xD^J(U) \\ \mathbf{1} & -\mathbf{1}+xD^J(U^{-1}) & 0 \end{bmatrix}. \tag{75}$$

Notice that $\Delta_J^\dagger=-\Delta_J$. Upon multiplication of the last group of columns by $(\mathbf{1}-xD^J(U))^{-1}$ and the last group of rows by $(\mathbf{1}-xD^J(U^{-1}))^{-1}$ we find, as in Ref. 9,

$$Det(\Delta_J)=Det[y(\mathbf{1}-xD^J(U))D^J(V)(\mathbf{1}-xD^J(U^{-1}))+x(D^J(U)-D^J(U^{-1}))] \tag{76}$$

and therefore the effective dimension of the final determinant reduces to d_J. The dimer generating function $\mathcal{Z}_d$ is then

$$\mathcal{Z}_d=2^{-g}\sum_O S_O pf(O)=2^{-g}\sum_O S_O\prod_{J\in O} Pf_J^{d_J/n(O)}. \tag{77}$$

The degree of Pf_J in x,y is $d_J,d_J/2$ and therefore the total degree of $pf(O)$ in x is $\Sigma_{J\in O}d_J^2/n(O)=N$ because of the Burnside condition and half as much for y. Not all $Det(\Delta_J)$ are distinct, besides $Det(\Delta_J)=Det(\Delta_{J^\dagger})$ the external automorphism ν maps $pf(B)$into $pf(C)$and vice versa thus $pf(C)=pf(B)$. The number of independent Pfaffians is therefore further reduced to four $(64\to5\to4)$ by the existence of external automorphisms.

If $d_J/n(O)$ is odd the sign of $Pf_J=\pm\sqrt{Det(\Delta_J)}$ must be fixed unambiguously by computing it for instance in the limit $\beta\to0$. $\mathcal{Z}_d$ becomes then a polynomial in x,y of degree $N,N/2$.[12] In Fig. 2 we give the plot of the specific heat corresponding to a ferromagnetic choice of the exchange interactions, $(J_U=J_V=1)$. The specific heat presents a very sharp peak which prefigures the transition form and ordered ferromagnetic phase to a disordered paramagnetic one. When J_U,J_V have different signs or are both antiferromagnetic (i.e., negative) the model is totally frustrated and

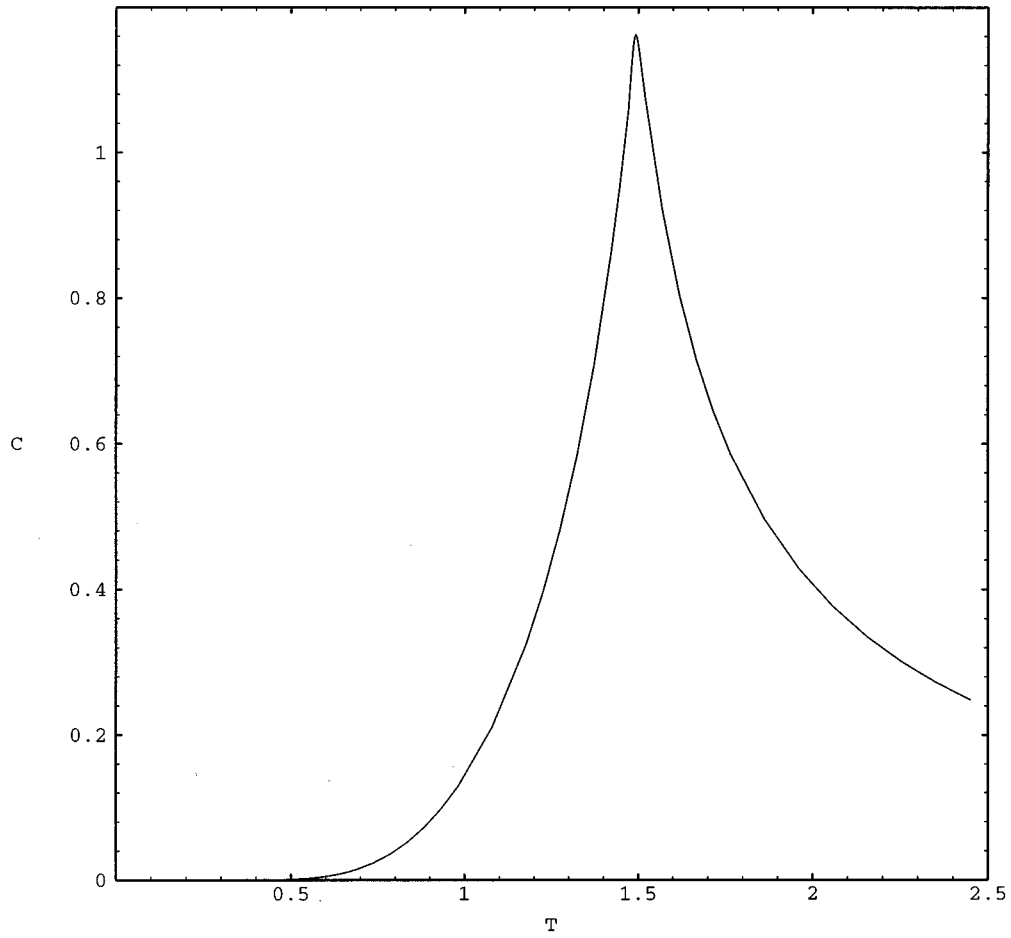

FIG. 2. Specific heat versus temperature for $J_U=J_V=1$.

the specific heat becomes smoother. Moreover, different finite values ($>\log\ 2/N$) of the ground state entropy are found, signaling an exponential degeneracy of the ground state.

IX. CONCLUSIONS

In this paper we have developed a formalism capable of dealing efficiently with Ising models defined on group lattices of nontrivial genus g. In particular we have applied the method to the Ising model on the Klein group $L(2,7)$ having $g=3$ and $N=168$. We found that the computation of the partition function $\mathcal{Z}$ is greatly simplified by use of symmetries of an extended group, both internal and external to the group, which reduce the number of and provide explicit formulas and topological interpretation for the sign and weight of Pfaffians in the expansion of $\mathcal{Z}$. We plan to apply this method to other lattices where N is large and g is comparable to N.

Note added in proof. A recent paper, to appear in Funct. Am. Appl. by N. P. Dolbilin, Yu. M. Zinoviev, A. S. Mishchenko, M. A. Slitan'ko, and M. I. Shtoprin contains results that partially overlap with ours.

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APPENDIX A

Fermionic irreps of H_0 :

$$U^{(1)}=\mathrm{diag}(-1,K,-K^2,-K^4),\quad U^{(2)}=(U^{(1)})^*,$$

$$U^{(3)}=\mathrm{diag}(K,-K^2,-K^4,-K^6,K^5,K^3),\quad U^{(4)}=(U^{(3)})^*,$$

$$U^{(5)}=\mathrm{diag}(K,-K^2,-K^4,-1,-K^6,K^5,K^3,-1).$$

$$V^{(1)}=\frac{2i}{\sqrt{7}}\begin{pmatrix} \frac{1}{2} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & c_1 & c_3 & c_2 \\ \frac{1}{\sqrt{2}} & c_3 & c_2 & c_1 \\ \frac{1}{\sqrt{2}} & c_2 & c_1 & c_3 \end{pmatrix}, \tag{A1}$$

with $c_k=\cos(2k\pi/7)$, $k=1,2,3$. $V^{(2)}=(V^{(1)})^*$.

$$V^{(3)}=\frac{2i}{7}\begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B} & -\mathbf{A} \end{pmatrix},$$

where

$$\mathbf{A}=\begin{pmatrix} s_2-\sqrt{2}s_3 & s_1-\sqrt{2}s_2 & s_3-\sqrt{2}s_1 \\ s_1-\sqrt{2}s_2 & s_3-\sqrt{2}s_1 & s_2-\sqrt{2}s_3 \\ s_3-\sqrt{2}s_1 & s_2-\sqrt{2}s_3 & s_1-\sqrt{2}s_2 \end{pmatrix},$$

$$\mathbf{B}=r\begin{pmatrix} s_3+(\sqrt{2}-1)s_1 & s_2+(\sqrt{2}-1)s_3 & s_1+(\sqrt{2}-1)s_2 \\ s_2+(\sqrt{2}-1)s_3 & s_1+(\sqrt{2}-1s_2 & s_3+(\sqrt{2}-1)s_1 \\ s_1+\sqrt{2}-1s_2 & s_3+(\sqrt{2}-1)s_1 & s_2+(\sqrt{2}-1)s_3 \end{pmatrix},$$

with $s_1=\sin(\pi/7)$, $s_2=-\sin(2\pi/7)$, $s_3=-\sin(4\pi/7)$ and $r=\sqrt{2+\sqrt{2}}$.

Finally $V^{(4)}=(V^{(3)})^*$ and

$$V^{(5)}=\frac{i}{7}\begin{pmatrix} \mathbf{C} & \mathbf{D} \\ \mathbf{D} & -\mathbf{C} \end{pmatrix},$$

where

$$\mathbf{C}=\begin{pmatrix} s_1+s_2 & s_1+s_3 & s_2+s_3 & \sqrt{\frac{3}{2}}(s_2-s_1) \\ s_1+s_3 & s_2+s_3 & s_1+s_2 & \sqrt{\frac{3}{2}}(s_1-s_3) \\ s_2+s_3 & s_1+s_2 & s_1+s_3 & \sqrt{\frac{3}{2}}(s_3-s_2) \\ \sqrt{\frac{3}{2}}(s_2-s_1) & \sqrt{\frac{3}{2}}(s_1-s_3) & \sqrt{\frac{3}{2}}(s_3-s_1) & \frac{1}{2}(s_1-2s_2+s_3) \end{pmatrix},$$

and

$$\mathbf{D}=2\sqrt{3}\begin{pmatrix} s_2 & s_1 & s_3 & \frac{1}{\sqrt{2}}(s_1-s_2) \\ s_1 & s_3 & s_2 & \frac{1}{\sqrt{2}}(s_3-s_1) \\ s_3 & s_2 & s_1 & \frac{1}{\sqrt{2}}(s_2-s_3) \\ \frac{1}{\sqrt{2}}(s_1-s_2) & \frac{1}{\sqrt{2}}(s_3-s_1) & \frac{1}{\sqrt{2}}(s_2-s_3) & \frac{1}{2}(s_1-s_3) \end{pmatrix}.$$

All these irreps are changed into equivalent and conjugate expressions by replacing K with $-K^2$.

APPENDIX B

Putting $\lambda(x)=x_O$ for the representations λ belonging to the orbit O we have Case B:

$$v_B=\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}, \quad t_B=\begin{pmatrix} \frac{(1+i\sqrt{2})}{2} & -\frac{1}{2} \\ \frac{1}{2} & \frac{(1-i\sqrt{2})}{2} \end{pmatrix}, \quad Z_{1,B}=\mathbf{I}_2\ ;$$

Case C: $v_C=v_B^{-1}$, $t_C=t_B^{-1}$, $Z_{1,C}=Z_{1,B}$;
Case D:

$$v_D^{(1)}=\frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -i & -i \\ 0 & 0 & 0 & 0 & -i & i \end{pmatrix}, \quad t_D^{(1)}=\frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 0 & \sqrt{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \sqrt{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & -i & -i \\ 0 & 0 & 0 & 0 & -i & i \\ -i & -i & 0 & 0 & 0 & 0 \\ -i & i & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$Z_{1,D}^{(1)}=\mathrm{diag}(1,1,1,1,-1,-1),$$

$$v_D^{(2)}=(v_D^{(1)})^*, \quad t_D^{(2)}=(t_D^{(1)})^*, \quad Z_{1,D}^{(2)}=Z_{1,D}^{(1)};$$

Case E :

$$v_E^{(1)}=\begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & -i & 0 & 0 \\ -i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \end{pmatrix}, \quad t_E^{(1)}=\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 0 & -i & 0 \\ 0 & 0 & 0 & 1 \\ 0 & -i & 0 & 0 \end{pmatrix},$$

$$Z_{1,E}^{(1)}=\mathrm{diag}(1,-1,1,-1), \quad v_E^{(2)}=(v_E^{(1)})^*, \quad t_E^{(2)}=(t_E^{(1)})^*, \quad Z_{1,E}^{(2)}=-Z_{1,E}^{(1)},$$

$$v_E^{(3)}=\begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & i & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -i & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & i & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -i \end{pmatrix},$$

$$t_E^{(3)}=\begin{pmatrix} \frac{1}{2} & \frac{-\sqrt{3}}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{3}}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{-\sqrt{3}}{2} & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & \frac{\sqrt{3}}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{3}}{2} & \frac{-1}{2} & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$Z_{1,E}^{(3)}=\mathrm{diag}(-1,-1,1,1,-1,-1,1,1).$$

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The successive reflection method in three dimensional particle transport

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The free streaming operator T is considered in a convex three dimensional region V, with diffusive multiplying boundary conditions. Some mathematical properties of T are examined by writing the particle density as an infinite series which takes into account successive reflections on ∂V, and by introducing an operator which in some sense annihilates the multiplying effect of ∂V. © *1996 American Institute of Physics.* [S0022-2488(96)01205-3]

I. INTRODUCTION

The basic mathematical properties of the streaming operator $T=-v\Omega\cdot\nabla$ usually are a first step in the study of abstract evolution problems in linear and nonlinear particle transport theory. In particular, whether or not T with suitable boundary conditions is the generator of a strongly continuous semigroup $\{\exp(tT),\ t\geqslant 0\}$ is a crucial question.[1] The behavior of $\|\exp(tT)\|$ as $t\to+\infty$ is also of interest because it leads to the asymptotic behavior of the total number of particles.

In this paper, we shall study the free streaming operator in a convex region $V\subset\mathbf{R}^3$, bounded by the closed C^1 surface ∂V, under the assumption that the following diffusive *multiplying* boundary condition holds

$$|\Omega\cdot\mathbf{n}(\mathbf{y})|f(\mathbf{y},\Omega)=\int_{\Omega'\cdot\mathbf{n}(\mathbf{y})>0}\alpha(\Omega,\Omega',\mathbf{y})\Omega'\cdot\mathbf{n}(\mathbf{y})f(\mathbf{y},\Omega')d\Omega',\quad \mathbf{y}\in\partial V,\quad \Omega\cdot\mathbf{n}(\mathbf{y})<0. \tag{1}$$

In relation (1), $f(\mathbf{y},\Omega)$ is the density of particles which are at $\mathbf{y}\in\partial V$ and have velocity $\mathbf{v}=v\Omega$, and $\mathbf{n}(\mathbf{y})$ is the (outward directed) normal unit vector at $\mathbf{y}$.

Furthermore, $\alpha(\Omega,\Omega',\mathbf{y})$ is a surface reflection kernel such that

$$\int_{\Omega\cdot\mathbf{n}(\mathbf{y})<0}\alpha(\Omega,\Omega',\mathbf{y})d\Omega=\alpha_0(\mathbf{y})>1\quad \text{at a.e.}\quad \mathbf{y}\in\partial V, \tag{2}$$

$$\alpha(\Omega,\Omega',\mathbf{y})=0\ \text{ if }\ 0\leqslant\Omega\cdot\mathbf{n}(\mathbf{y})<\epsilon_0\quad \text{at a.e.}\quad \mathbf{y}\in\partial V, \tag{3}$$

where ϵ_0 is an assigned positive number, with $\epsilon_0\ll 1$.

Relations (1) and (2) imply that particles, which impinge on ∂V at $\mathbf{y}$ with velocity $\mathbf{v}=v\Omega'$ $(\Omega'\cdot\mathbf{n}(\mathbf{y})>0)$, are reflected with velocity $\mathbf{v}=v\Omega$ $(\Omega\cdot\mathbf{n}(\mathbf{y})<0)$ and their number is multiplied by a factor larger than one. Such a multiplication phenomenon leads to some difficulties when one has to evaluate the norm of the evolution operator $\exp(tT)$. As it is shown in what follows, this difficulty may be overcome by introducing a suitable annihilation operator B.

Assumption (3) means that particles impinging on ∂V at $\mathbf{y}$ with velocity $\mathbf{v}$, such that the angle between $\mathbf{v}$ and $\mathbf{n}(\mathbf{y})$ is close to a right angle, are not reflected by ∂V. Hence, this (mainly technical)

condition cuts off the possibility of having two successive reflections at $\mathbf{y}$ and $\mathbf{y}'$ with $|\mathbf{y}-\mathbf{y}'|$ small. In any case, the number of this kind of reflections per unit time would be small compared with the total number of reflections at $\mathbf{y}\in\partial V$.

We finally remark that evolution problems with multiplying boundary conditions are certainly of mathematical interest.[2] However, they are also of physical interest because they may arise in connection with electron transport in photomultipliers, in algae or bacteria population problems, in neutron transport (in this case, ∂V may be the surface that bounds a moderator). The procedures that follow can also be used if multiplication is a volume phenomenon (i.e., if it occurs within V), such as in the case of neutron transport in a fissionable material.

II. THE SUCCESSIVE REFLECTION METHOD

In order to overcome the difficulties caused by the particle multiplication phenomenon on ∂V, we write the particle density $f(\mathbf{x},\Omega)$ as follows

$$f(\mathbf{x},\Omega)=\sum_{j=0}^{\infty} f_j(\mathbf{x},\Omega), \tag{4}$$

where $f_j(\mathbf{x},\Omega)$ is the density of the particles which ''remember'' just j reflections on the boundary surface ∂V. To explain the definition of f_j, we shall call ''mother'' a particle just before undergoing a reflection and ''daughters'' the particles generated by such a reflection. Assume that the daughters ''remember'' both the reflection during which they were generated and all the reflection events remembered by their mother. Then, f_j is composed of all particles which remember just j reflections.

According to definition (4) we introduce the Banach space X

$$X=\left\{ f: f=\begin{pmatrix} f_0 \\ f_1 \\ f_2 \\ \vdots \end{pmatrix}, \quad f_j\in L^1(V\times S), \quad \sum_{j=0}^{\infty} \|f_j\|_1<\infty \right\},$$

$$\|f\|=\sum_{j=0}^{\infty} \|f_j\|_1, \quad \|f_j\|_1=\int_V d\mathbf{x}\int_S |f_j(\mathbf{x},\Omega)|\,d\Omega, \tag{5}$$

and define the free streaming operator as follows

$$Tf=-v\begin{pmatrix} \Omega\cdot\nabla f_0 \\ \Omega\cdot\nabla f_1 \\ \Omega\cdot\nabla f_2 \\ \vdots \end{pmatrix},$$

$$D(T)=\{f: f\in X; Tf\in X; f \text{ satisfies the boundary conditions (7)}\} \tag{6}$$

$$|\Omega\cdot\mathbf{n}(\mathbf{y})|f_j(\mathbf{y},\Omega)=\int_{\Omega'\cdot\mathbf{n}(\mathbf{y})>0}\alpha(\Omega,\Omega',\mathbf{y})\Omega'\cdot\mathbf{n}(\mathbf{y})f_{j-1}(\mathbf{y},\Omega')d\Omega',$$

$$\mathbf{y}\in\partial V, \quad \Omega\cdot\mathbf{n}(\mathbf{y})<0, \quad j=0,1,2,\ldots\ . \tag{7}$$

In (5), S is the spherical surface of radius one, whereas $f_{-1}\equiv 0$ in the first of (7). Note that the boundary condition (7) shows that a reflection event changes f_{j-1} into f_j.

By using definitions (5), (6), and (7), we can write the abstract version of the free streaming problem in V:

$$\frac{d}{dt}u(t)=Tu(t), \quad t>0; \quad u(0)=u_0\in D(T)\cap X^+, \tag{8}$$

where $u(t)=u(\mathbf{x},\Omega;t)$ is now a function from $[0,+\infty)$ into the space X, $(d/dt)u$ is a strong derivative, and u_0 is an assigned initial particle distribution belonging to $D(T)$ and to the positive cone X^+.[3–5] We observe that (8) is in fact a system of infinite partial differential equations, coupled only because of the boundary conditions (7). In other words, (8) may be put into the form

$$\frac{d}{dt}u_j(t)=-v\Omega\cdot\nabla u_j, \quad t>0; \quad u_j(0)=u_{j0}\in X_1^+, \quad j=0,1,2,\ldots, \tag{9}$$

where the u_j's must satisfy (7) and be such that $-v\Omega\cdot\nabla u_j\in X_1=L^1(V\times S)$.

Equation (8) or system (9) are the mathematical formulation of the successive reflection method. Such a method has some similarity to the multiple collision technique[6] if multiplication occurs within V.

III. THE SEMIGROUP GENERATED BY *T*

To show that T is the generator of the strongly continuous semigroup $\{\exp(tT),\ t\geqslant 0\}$, we consider the equation

$$(zI-T)f=g, \tag{10}$$

where z is a positive constant, g is a given element of X, and the unknown must be sought in $D(T)$.

The solution $f\in D(T)$ of (10) has the form

$$f_j(\mathbf{x},\Omega)=\frac{1}{v}C_j(\mathbf{y},\Omega)\exp\left(-\frac{z}{v}s_0(\mathbf{x},\Omega)\right)+\frac{1}{v}\int_0^{s_0(\mathbf{x},\Omega)}\exp\left(-\frac{zs}{v}\right)g_j(\mathbf{x}-s\Omega,\Omega)ds, \tag{11}$$

where, given $\mathbf{x}$ and Ω, $s_0(\mathbf{x},\Omega)$ is such that $\mathbf{y}=\mathbf{x}-s_0(\mathbf{x},\Omega)\Omega\in\partial V$.

The constants $C_j(\mathbf{y},\Omega)$ can be evaluated by using the boundary condition (7) and assumption (3):

$$\begin{aligned}|\Omega\cdot\mathbf{n}(\mathbf{y})|C_j(\mathbf{y},\Omega)=&\int_{\Omega'\cdot\mathbf{n}(\mathbf{y})>\epsilon_0}d\Omega'\alpha(\Omega,\Omega',\mathbf{y})\Omega'\cdot\mathbf{n}(\mathbf{y})\left\{C_{j-1}(\mathbf{y}',\Omega')\exp\left(-\frac{z}{v}s_0(\mathbf{y},\Omega')\right)\right.\\&\left.+\int_0^{s_0(\mathbf{y},\Omega')}\exp\left(-\frac{zs}{v}\right)g_{j-1}(\mathbf{y}-s\Omega',\Omega')ds\right\},\\&\mathbf{y}\in\partial V, \quad \Omega\cdot n(\mathbf{y})<0, \quad j=0,1,2,\ldots,\end{aligned} \tag{12}$$

where $\mathbf{y}'=\mathbf{y}-s_0(\mathbf{y},\Omega')\Omega'\in\partial V$ and $C_{-1}\equiv 0$.

At any fixed $\mathbf{y}\in\partial V$, it follows from (12) and (2)

$$\begin{aligned}\int_{\Omega\cdot\mathbf{n}(\mathbf{y})<0}|\Omega\cdot\mathbf{n}(\mathbf{y})\|C_j(\mathbf{y},\Omega)|d\Omega\leqslant&\chi\exp\left(-\frac{z}{v}\delta\right)\int_{\Omega'\cdot\mathbf{n}(\mathbf{y})>0}\Omega'\cdot\mathbf{n}(\mathbf{y})|C_{j-1}(\mathbf{y}',\Omega')|d\Omega'\\&+\chi\int_{\Omega'\cdot\mathbf{n}(\mathbf{y})>0}d\Omega'\Omega'\cdot\mathbf{n}(\mathbf{y})\int_0^{s_0(\mathbf{y},\Omega')}|g_{j-1}(\mathbf{y}-s\Omega',\Omega')|ds,\end{aligned}$$

where

$$\chi=\sup\{\alpha_0(\mathbf{y}) \quad \mathbf{y}\in\partial V\}\geqslant 1, \quad \delta=\inf_{\mathbf{y}\in\partial V}\{\inf_{\Omega\cdot\mathbf{n}(\mathbf{y})\geqslant\epsilon_0}[s_0(\mathbf{y},\Omega)]\}>0 \tag{13}$$

(for example, if ∂V is a sphere of radius r, then $\delta=2r\epsilon_0$).

Integration over ∂V gives

$$\|C_j\|_b\leqslant\chi\,\exp\left(-\frac{z}{v}\,\delta\right)\|C_{j-1}\|_b+\chi\int_{\partial V}d\sigma_y\int_{\Omega'\cdot\mathbf{n}(\mathbf{y})>0}d\Omega'\,\Omega'\cdot\mathbf{n}(\mathbf{y})$$
$$\times\int_0^{s_0(\mathbf{y},\Omega')}|g_{j-1}(\mathbf{y}-s\Omega',\Omega')|ds, \tag{14}$$

where

$$\|\varphi\|_b=\int_{\partial V}d\sigma_y\int_{\Omega\cdot\mathbf{n}(\mathbf{y})<0}|\varphi(\mathbf{y},\Omega)|d\Omega,$$

and where we took into account that $\Omega'\cdot\mathbf{n}(\mathbf{y})d\sigma_y=|\Omega'\cdot\mathbf{n}(\mathbf{y}')|d\sigma_{y'}$. The second term on the right hand side of (45) can be written as follows:

$$\chi\int_S d\Omega'\int_{\partial V+(\Omega')}d\sigma_y\Omega'\cdot\mathbf{n}(\mathbf{y})\int_0^{s_0(\mathbf{y},\Omega')}|g_{j-1}(\mathbf{y}-s\Omega',\Omega')|ds$$
$$=\chi\int_S d\Omega'\int_V|g_{j-1}(\mathbf{x}',\Omega')|d\mathbf{x}'=\chi\|g_{j-1}\|_1,$$

where, $\mathbf{x}'=\mathbf{y}-s\Omega'$ and where, for each given Ω', $\partial V^+(\Omega')=\{\mathbf{y}:\mathbf{y}\in\partial V,\boldsymbol{\Omega}'\cdot\mathbf{n}(\mathbf{y})>0\}$.

Hence, (14) becomes

$$\|C_j\|_b\leqslant\chi\,\exp\left(-\frac{z}{v}\,\delta\right)\|C_{j-1}\|_b+\chi\|g_{j-1}\|_1, \tag{15}$$

and so:

$$\sum_{j=0}^{\infty}\|C_j\|_b\leqslant\eta(z)\|g\|, \tag{16}$$

where

$$\eta(z)=\frac{\chi}{1-\chi\,\exp(-(z/v)\,\delta)}, \tag{17}$$

provided that $\chi\exp(-(z/v)\,\delta)<1$, i.e., $z>z_0=(v/\delta)\ln\chi$.

On the other hand, we have from (11)

$$\|f_j\|_1\leqslant\frac{1}{v}\int_S d\Omega\int_V d\mathbf{x}\left\{|C_j(\mathbf{y},\Omega)|\exp\left(-\frac{z}{v}\,s_0(\mathbf{x},\Omega)\right)+\int_0^{s_0(\mathbf{x},\Omega)}\exp\left(-\frac{zs}{v}\right)|g_j(\mathbf{x}-s\Omega,\Omega)|ds\right\}.$$

By taking into account that $d\mathbf{x}=|\Omega\cdot\mathbf{n}(\mathbf{y})|d\sigma_y d\rho$ with $\Omega\cdot\mathbf{n}(\mathbf{y})<0$ for each fixed Ω, we obtain

$$\|f_j\|_1 \leqslant \frac{1}{v}\int_S d\Omega\Bigg\{\int_{\partial V^-(\Omega)} d\sigma_y |\Omega\cdot\mathbf{n}(\mathbf{y})\|C_j(\mathbf{y},\Omega)| \times \int_0^{s_0(\mathbf{y},-\Omega)} \exp\left(-\frac{z\rho}{v}\right)d\rho + \int_{\partial V^-(\Omega)} d\sigma_y|\Omega\cdot\mathbf{n}(\mathbf{y})| \times \int_0^{s_0(\mathbf{y},-\Omega)} d\rho\int_0^{\rho}\exp\left(z\,\frac{s'-\rho}{v}\right)|g_j(\mathbf{y}+s'\Omega,\Omega)|ds'\Bigg\},$$

where $\partial V^-(\Omega)=\{\mathbf{y}:\mathbf{y}\in\partial V,\ \Omega\cdot\mathbf{n}(\mathbf{y})<0\}$. Thus, we finally have

$$\|f_j\|_1 \leqslant \frac{1}{z}\{\|C_j\|_b+\|g_j\|_1\}, \tag{18}$$

and consequently

$$\|f\| \leqslant \frac{\eta(z)+1}{z}\|g\|, \quad z>z_0=\frac{v}{\delta}\ln\chi, \tag{19}$$

where we have used inequality (16).

We can summarize the preceding results as follows.

Lemma 1: Equation (10) has a unique solution $f=(zI-T)^{-1}g\in D(T)\forall g\in X$, provided that $z>z_0=(v/\delta)\ln\chi$. Moreover, $\|(zI-T)^{-1}\|\leqslant[\eta(z)+1]/z$ and $(zI-T)^{-1}[X^+]\subset X^+$.

Let now $g\in X^+$ and assume that $z>z_0$. Then, $f\in X^+$, $|f|=f$, and integration over S and V of the i-th component of (10) gives

$$z\|f_j\|_1+v\int_S d\Omega\int_V \Omega\cdot\nabla f_j(\mathbf{x},\Omega)d\mathbf{x}=\|g_j\|_1. \tag{20}$$

On the other hand, we have by using divergence theorem and condition (7)

$$\begin{aligned}\int_S d\Omega\Omega\cdot\int_V\nabla f_j(\mathbf{x},\Omega)d\mathbf{x} &= \int_S d\Omega\Omega\cdot\int_{\partial V} n(\mathbf{y})f_j(\mathbf{y},\Omega)d\sigma_y\\ &= \int_{\partial V}d\sigma_y\int_{\Omega\cdot\mathbf{n}(\mathbf{y})>0}\Omega\cdot\mathbf{n}(\mathbf{y})f_j(\mathbf{y},\Omega)d\Omega\\ &\quad -\int_{\partial V}d\sigma_y\int_{\Omega\cdot\mathbf{n}(\mathbf{y})<0}|\Omega\cdot\mathbf{n}(\mathbf{y})|f_j(\mathbf{y},\Omega)d\Omega\\ &= \int_{\partial V}d\sigma_y\int_{\Omega\cdot\mathbf{n}(\mathbf{y})>0}\Omega\cdot\mathbf{n}(\mathbf{y})f_j(\mathbf{y},\Omega)d\Omega\\ &\quad -\int_{\partial V}d\sigma_y\alpha_0(\mathbf{y})\int_{\Omega'\cdot\mathbf{n}(\mathbf{y})>0}\Omega'\cdot\mathbf{n}(\mathbf{y})f_{j-1}(\mathbf{y},\Omega')d\Omega'.\end{aligned}$$

Hence, (20) becomes

$$z\|f_j\|_1+v\int_{\partial V}d\sigma_y\int_{\Omega\cdot\mathbf{n}(\mathbf{y})>0}\Omega\cdot\mathbf{n}(\mathbf{y})f_j(\mathbf{y},\Omega)d\Omega$$

$$-v\int_{\partial V}d\sigma_y\alpha_0(\mathbf{y})\int_{\Omega'\cdot\mathbf{n}(\mathbf{y})>0}\Omega'\cdot\mathbf{n}(\mathbf{y})f_{j-1}(\mathbf{y},\Omega')d\Omega'=\|g_j\|_1.$$

As a consequence, we obtain

$$z\|f\|-v\int_{\partial V}d\sigma_y(\alpha_0(\mathbf{y})-1)\int_{\Omega\cdot\mathbf{n}(\mathbf{y})>0}\Omega\cdot\mathbf{n}(\mathbf{y})\sum_{j=0}^{\infty}f_j(\mathbf{y},\Omega)d\Omega=\|g\|.$$

Since $f=(zI-T)^{-1}g\in X^+$, we conclude that the resolvent operator satisfies the inequality

$$\|(zI-T)^{-1}g\|\geqslant\frac{\|g\|}{z},\quad z>z_0,\quad g\in X^+. \tag{21}$$

Note that $D(T)$ is dense in X; hence Lemma 1, inequality (20) and some results proved in Ref. 7 lead to the following theorem.

Theorem 1: $T\in\mathcal{G}(M,z_0;X)$, i.e., T is the infinitesimal generator of the strongly continuous semigroup $\{\exp(tT),\ t\geqslant 0\}$, such that $\|\exp(tT)\|\leqslant M\exp(z_0t)$, $\forall t\geqslant 0$. Moreover, $\exp(tT)[X^+]\subset[X^+]$, $\forall t\geqslant 0$.

We remark that, in Ref. 7, it is only shown that a suitable constant M exists, but no indication is given on how to evaluate it. This justifies the introduction of the ''annihilation'' operator B in the following section.

IV. THE ANNIHILATION OPERATOR

Due to Theorem 1, the unique strong solution of problem (8) has the form

$$u(t)=\exp(tT)u_0,\quad t\geqslant 0,\quad u_0\in D(T)\cap X^+, \tag{22}$$

and $u(t)\in D(T)\cap X^+$, $\forall t\geqslant 0$. Since $T\in\mathcal{G}(M,z_0;X)$, (22) gives

$$\|u(t)\|=\int_S d\Omega\int_V u(\mathbf{x},\Omega;t)d\mathbf{x}\leqslant M\ \exp(z_0t)\int_S d\Omega\int_V u_0(\mathbf{x},\Omega)d\mathbf{x}, \tag{23}$$

which is an upper bound for the total number of particles within V at time t. Note that inequality (23) depends on M, whose value is not easy to evaluate. On the other hand, the factor $\exp(z_0t)$ with $z_0=(v/\delta)\ln\chi$ has an interesting physical meaning. In fact, the ratio δ/v is the minimum time interval between two successive reflections on ∂V, whereas χ is the maximum multiplication factor. Hence, an upper bound for $\|u(t)\|$ can be obtained by assuming that all particles undergo their first collision at a time very close to $t=0$, the second at $t=\delta/v$, the third at $t=2\delta/v$,..., and that they are multiplied by χ each time. Then, the total number of particles at time t would be $\|u_0\|\chi\chi^{t/(\delta/v)}=\chi\exp((v/\delta)t\ln\chi)\|u_0\|=\chi\exp(z_0t)\|u_0\|$ because $1+tv/\delta$ is the number of reflection events during $[0,t]$.

In order to overcome the difficulty due to the constant M, we introduce the linear bounded operator

$$B\begin{pmatrix} 1 & 0 & 0 & \cdots \\ 0 & \chi^{-1} & 0 & \cdots \\ 0 & 0 & \chi^{-2} & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{pmatrix}, \quad D(B)=X \tag{24}$$

which is such that $B[X^+]\subset[X^+]$, $\|B\|=1$.

Assume now that $f\in D(T)$ and let $g=Bf$; then, $\Omega\cdot\nabla f_j\in X_1$ and f_j satisfies condition (7). Moreover, $g_j=f_j/\chi^j$ and so $\Omega\cdot\nabla g_j\in X_1$ and g_j satisfies the boundary condition

$$|\Omega\cdot\mathbf{n}(\mathbf{y})|g_j(\mathbf{y},\Omega)=\int_{\Omega'\cdot\mathbf{n}(\mathbf{y})>0}\hat{\alpha}(\Omega,\Omega',\mathbf{y})\Omega'\cdot\mathbf{n}(\mathbf{y})g_{j-1}(\mathbf{y},\Omega')d\Omega',$$

$$\mathbf{y}\in\partial V, \quad \Omega\cdot\mathbf{n}(\mathbf{y})<0, \quad j=0,1,2,\ldots, \tag{25}$$

where $\hat{\alpha}(\Omega,\Omega',\mathbf{y})=\alpha(\Omega,\Omega',\mathbf{y})/\chi$.

Condition (25) suggests to define a new streaming operator $\hat{T}$ as follows

$$\hat{T}g=-v\begin{pmatrix} \Omega\cdot\nabla g_0 \\ \Omega\cdot\nabla g_1 \\ \Omega\cdot\nabla g_2 \\ \vdots \end{pmatrix}, \tag{26a}$$

$$D(\hat{T})=B[D(T)]=\{g:g\in X;\hat{T}g\in X;g \text{ satisfies the boundary conditions (25)}\}. \tag{26b}$$

Since

$$\hat{\alpha}_0(\mathbf{y})=\int_{\Omega\cdot\mathbf{n}(\mathbf{y})<0}\hat{\alpha}(\Omega,\Omega',\mathbf{y})d\Omega=\alpha_0(\mathbf{y})/\chi\leqslant 1,$$

$$\hat{\chi}=\sup\{\hat{\alpha}(\mathbf{y}),\mathbf{y}\in\partial V\}=1,$$

Theorem 2 can be proved by using procedures similar to those of Sec. 2 (with $\hat{\alpha}_0$ and $\hat{\chi}=1$ instead of α_0 and χ). We remark that (20) and (25) lead to the relation

$$z\|f\|-v\int_{\partial V}d\sigma_y(\hat{\alpha}_0(\mathbf{y})-1)\int_{\Omega\cdot\mathbf{n}(\mathbf{y})>0}\Omega\cdot\mathbf{n}(\mathbf{y})\sum_{j=0}^{\infty}f_j(\mathbf{y},\Omega)d\Omega=\|g\|,$$

where $f=(zI-\hat{T})^{-1}g$ and $\hat{\alpha}_0(\mathbf{y})\leqslant 1$. Hence, we have

$$\|(zI-\hat{T})^{-1}g\|\leqslant\frac{\|g\|}{z}, \quad \forall z>\hat{z}_0=\frac{v}{\delta}\ln\hat{\chi}=0. \tag{27}$$

Furthermore, $D(\hat{T})$ is dense in X, and so (27) leads to the following theorem.

Theorem 2: $\hat{T}\in\mathcal{G}(1,0;X)$ i.e., $\hat{T}$ is the infinitesimal generator of the strongly continuous semigroup $\{\exp(t\hat{T}),\ t\geqslant 0\}$, such that $\|\exp(t\hat{T})\|\leqslant 1$, $\forall t\geqslant 0$. Moreover, $\exp(t\hat{T})[X^+]\subset[X^+]$, $\forall t\geqslant 0$.

We also observe that the following commutation property holds

$$BTf=\hat{T}Bf, \quad \forall f\in D(T). \tag{28}$$

In fact, $Bf\in B[D(T)]=D(\hat{T})\forall f\in D(T)$ and $\hat{T}Bf$ exists and belongs to X. Furthermore, given any $j=0,1,2,...$, we have

$$(BTf)_j=(Tf)_j/\chi^j=(-v\Omega\cdot\nabla f_j)/\chi^j,$$

$$(\hat{T}Bf)_j=-v\Omega\cdot\nabla(Bf)_j=(-v\Omega\cdot\nabla f_j/\chi^j),$$

and (28) is proved.

Consider now the following modified evolution problem

$$\frac{d}{dt}w(t)=\hat{T}w(t),\quad t>0;\quad w(0)=w_0\in D(\hat{T}),\tag{29}$$

whose unique strong solution has the form

$$w(t)=\exp(t\hat{T})w_0,\quad t\geqslant 0.\tag{30}$$

By applying the bounded operator B to both sides of equation (8), we have

$$\frac{d}{dt}Bu(t)=BTu(t),\quad t>0,\quad Bu(0)=Bu_0,$$

i.e.,

$$\frac{d}{dt}[Bu(t)]=\hat{T}[Bu(t)],\quad t>0;\quad [Bu(0)]=Bu_0,\tag{31}$$

where we used (28) and the relation $B(du/dt)=(dBu/dt)$, that holds because $B\in\mathscr{B}(X)$[3].

Comparison of (29) with (31) shows that $w(t)=Bu(t)$, provided that $w_0=Bu_0$. Hence, we have

$$\|Bu(t)\|=\|w(t)\|\leqslant\|w_0\|=\|Bu_0\|,\quad \forall t\geqslant 0,\tag{32}$$

because of (30) and Theorem 2.

Inequality (32) shows that $Bu(t)$ has the norm bounded by the norm of its initial value Bu_0. Note that $(Bu(t))_j=u_j(t)/\chi^j$, i.e., the j-th component of $Bu(t)$ is the density of particles, which remember j reflections, divided by χ^j (which in some sense, annihilates the multiplying effect of the j reflections). Moreover, we may obviously take $(Bu_0)_j=0\forall j=1,2,...$ and $(Bu_0)_0=u_{00}\in X_1^+$, with $u_{00}(\mathbf{y},\Omega)=0\forall\mathbf{y}\in\partial V$, where u_{00} is the particle density at $t=0$ (under the assumption that at $t=0$, no particle has yet undergone any reflection). Then, (32) reads as follows

$$\sum_{j=0}^{\infty}\chi^{-j}\int_S d\Omega\int_V u_j(\mathbf{x},\Omega;t)d\mathbf{x}\leqslant\int_S d\Omega\int_V u_{00}(\mathbf{x},\Omega)d\mathbf{x}.\tag{33}$$

V. CONCLUDING REMARKS

We can summarize the preceding results as follows.

Theorem 3: If T is defined by (6) and $\hat{T}$ by (26), then $T\in\mathscr{G}(M,z_0;X)$,$\hat{T}\in\mathscr{G}(1,0;X)$ and relation (28) holds. Moreover, the (positive) semigroups generated by T and $\hat{T}$ are such that

$$B\exp(tT)u_0=\exp(t\hat{T})Bu_0,\quad t\geqslant 0,\quad u_0\in D(T),\tag{34}$$

where B is defined by (24). Since $D(T)$ is dense in X, (34) may be extended to the whole X.

Relation (34) is of mathematical and physical interest because it shows that an evolution problem with particle multiplication may be studied by means of a suitable modified problem without multiplication. Furthermore, (34) leads to the definition of B-bounded semigroups.[8]

Inequality (33) indicates that

$$\int_S d\Omega \int_V u_j(\mathbf{x},\Omega;t)d\mathbf{x} \leqslant \chi^j \int_S d\Omega \int_V u_{00}(\mathbf{x},\Omega)d\mathbf{x}, \quad j=0,1,2,\ldots,$$

because $u \in X^+$ and so all the terms of the infinite series are non-negative. Finally, let $\overline{s_0}=\sup\{s_0(\mathbf{x},\Omega),\mathbf{x}\in V,\Omega\in S\}$ be the diameter of V. Then if $t>n\overline{s_0}/v$, $u_j \equiv 0 \forall j=0,1,2,\ldots,n-1$ and (33) becomes

$$\sum_{j=n}^{\infty} \chi^{-(j-n)} \int_S d\Omega \int_V u_j(\mathbf{x},\Omega;t)d\mathbf{x} \leqslant \chi^n \int_S d\Omega \int_V u_{00}(\mathbf{x},\Omega)d\mathbf{x}.$$

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Nonlinear discrete systems with nonanalytic dispersion relations

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A discrete system of coupled waves (with nonanalytic dispersion relation) is derived in the context of the spectral transform theory for the Ablowitz–Ladik spectral problem (discrete version of the Zakharov–Shabat system). This 3-wave evolution problem is a discrete version of the *stimulated Raman scattering* equations, and it is shown to be solvable for arbitrary boundary value of the two *radiation fields* and initial value of the *medium state*. The spectral transform is constructed on the basis of the $\bar{\partial}$-approach. © *1996 American Institute of Physics.*
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I. INTRODUCTION

This paper relates the study of the following discrete coupled system for the three fields $A_1(\theta,n,t)$, $A_2(\theta,n,t)$ and $q(n,t)$

$$\begin{aligned} &A_1(\theta,n,t)-A_1(\theta,n-1,t)=e^{-in\theta}q(n,t)A_2(\theta,n,t),\\ &A_2(\theta,n,t)-A_2(\theta,n-1,t)=-e^{in\theta}\overline{q(n,t)}A_1(\theta,n,t),\\ &q_t(n,t)=\frac{\rho(n,t)}{2\pi}\int_{-\pi}^{+\pi}d\theta e^{in\theta}(A_1*A_2)(\theta,n,t), \end{aligned} \tag{1}$$

where $\theta\in[-\pi,+\pi]$, $n\in\mathbf{Z}$ and $t\in\mathbf{R}^+$. The interaction term here above is defined as the *coupling* factor

$$(A_1*A_2)(\theta,n,t)=g(\theta,t)A_1(\theta,n-1,t)\overline{A_2}(\theta,n,t)+\overline{g(}\theta,t)A_1(\theta,n,t)\overline{A_2}(\theta,n-1,t), \tag{2}$$

where $g(\theta,t)$ is an arbitrary function in $L^2([-\pi,+\pi])$ (which could also be time dependent), and where the *energy ratio* $\rho(n,t)$ at the site n (it will be shown that this quantity is actually θ -independent) is defined as

$$\rho(n,t)=\frac{|I_1(\theta,t)|^2+|I_2(\theta,t)|^2}{|A_1(\theta,n,t)|^2+|A_2(\theta,n,t)|^2} \tag{3}$$

for the following definition of the boundary values $I_1(\theta,t)$ and $I_2(\theta,t)$ (input data)

$$I_1=\lim_{n\to+\infty}A_1(\theta,n,t),\qquad I_2=\lim_{n\to+\infty}A_2(\theta,n,t). \tag{4}$$

One of the main results is the proof that the system (1) with data (*initial-boundary value problem*)

$$q(n,0),\qquad I_1(\theta,t),\qquad I_2(\theta,t) \tag{5}$$

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is integrable. In particular this work provides the first instance of an integrable nonlinear discrete system with *nonanalytic dispersion relation*.

An interesting limit of the above equation arises when the arbitrary distribution $g(\theta)$ goes to a Dirac delta function, for instance $\delta(\theta)$. Then the system reads (now $A_j(n,t)$ denotes $A_j(\theta,n,t)|_{\theta=0}$)

$$A_1(n,t)-A_1(n-1,t)=q(n,t)A_2(n,t),$$

$$A_2(n,t)-A_2(n-1,t)=-\overline{q(}n,t)A_1(n,t), \tag{6}$$

$$q_t(n,t)=\rho(n,t)[A_1(n-1,t)\overline{A_2}(n,t)+A_1(n,t)\overline{A_2}(n-1,t)],$$

and it is called the *sharp line limit* of (1). Although a definite physical application of such an equation does not exist by now, it still can be understood in the following way. A_1 and A_2 are the two envelopes of some high frequency (HF) oscillations (say at frequency ω_1 and ω_2) which interact resonantly on each site n with a medium constituted of oscillators of envelope $q(n)$ and frequency $\Omega=\omega_1-\omega_2$, with a coupling intensity proportional to the relative amount $\rho(n)$ of the *total HF energy* which has reached the site n. Then the physical data are the input values $A_{1,2}(\theta,n,t)$ at $n=\infty$ of the HF external excitations, and the initial state of the medium oscillators.

The method used to build and solve (1) is the *inverse spectral* (or *scattering*) *transform* (IST) well known also as the *nonlinear Fourier transform*.[1] Indeed the method, in its principle, works like a Fourier transform. It associates to the field, solution of a nonlinear evolution equation, its *spectral transform* which evolves linearly. Then the field at time t is reconstructed from the spectral transform at time t by solving the *inverse spectral problem*. This method has been widely studied and extended to various interesting nonlinear evolution problems. We are particularly interested in three types of extension which will be used all three together.

The first extension involved here is the use of *discrete* spectral problems to solve discrete (in space) nonlinear evolution equations. Famous instances of integrable discrete systems are the Toda lattice[2] and a special discrete version of the nonlinear Schrödinger equation which has been proposed and integrated by Ablowitz and Ladik by using a discrete version of the Zakharov–Shabat spectral problem.[3] This so called Ablowitz–Ladik spectral problem and the related nonlinear differential–difference equations with polynomial dispersion relations have been extensively studied (see Refs. 4–17). Recently a different version of the discrete Zakharov–Shabat system has been proposed in order to keep the canonical Poisson structure of the continuous case.[18]

The second domain considered here concerns the extension of the spectral transform to the case of *nonanalytic dispersion relations*.[19,20] The first instance of such an integrable system is the self-induced transparency (SIT) equations of McCall–Hahn[21] which was shown to possess a Lax pair in Ref. 22 was given a N-soliton solution in Ref. 23 and later studied and completely solved in Ref. 24. These systems generically describe wave–wave interactions for which some boundary value are prescribed. These boundary values are strongly dependent on the physical problem under consideration. For instance the problem of superfluorescence in two-level media results in the same equation as SIT but with different boundary values and consequently quite different generic properties resulting mainly from a linear but *nonhomogeneous* evolution of the spectral transform.[25]

The third extension used is the generalization of the solution of an evolution equation with a nonanalytic dispersion relation to the case of *arbitrary boundary values*.[26] In this case, the evolution of the spectral transform can be not only nonhomogeneous but also *nonlinear* and still has interesting physical application. In particular the problem of stimulated Raman scattering of a high energy long laser pulse in a gas has been solved by this technique.[27,28]

The paper is organized as follows. In Sec. II we summarize the method of solution of the system (1) and provide there only the resulting formulae.

In Sec. III the principal Lax operator or, more precisely, the associated spectral problem (a special reduction of the Ablowitz–Ladik spectral problem) is used to define the spectral data (or nonlinear Fourier transform). This is done by selecting the basic set of Jost solutions and then proving that they obey a Riemann–Hilbert problem in the spectral parameter.

The inverse spectral problem is then solved in Sec. IV by means of the $\bar{\partial}$-formulation of the spectral problem, which means that the *potentials* are reconstructed from the *spectral data*. There the compatible *reductions* are also considered, which will allow in particular to obtain simpler integrable equations with an easier interpretation.

Section V is devoted to the formulation of the inverse spectral transform on the basis of the $\overline{\partial}$-problem. More precisely, having previously shown that the spectral problem (for the principal Lax operator) leads naturally to a ∂-problem, we prove here the reverse statement. This is useful in the following for considering the ∂-problem itself as the starting tool.

The general discrete integrable system with nonanalytic dispersion relations is then constructed by requiring a time evolution of the spectral transform with a *nonanalytic* dispersion law and a *nonhomogeneous* term.

These results are used in Sec. VI to prove that indeed the system (1) with the arbitrary boundary values (4) is solvable. That means that we obtain the time evolution of the spectral data in terms of the boundary values and the spectral transform of the initial datum $q(n,0)$. An interesting case corresponds to the growth of the field $q(n,t)$ on an initial medium at rest, that is for $q(n,0)\equiv 0$. The method furnishes in such a case the explicit output values of the HF fields $A_1(\theta,n,t)$ and $A_2(\theta,n,t)$ for $n=-\infty$.

II. SOLUTION OF THE SYSTEM. A SUMMARY

The general method to generate solutions of (1) is sketched hereafter. The starting point is the *spectral transform* of the initial datum $q(n,0)$, namely, the set of two scalar functions α and β defined on the unit circle, a sequence of N discrete points k_j outside the unit disc to each of which are associated N complex constants C_j. This set is given at $t=0$ as

$$\alpha(\zeta,0), \qquad \beta(\zeta,0), \qquad \zeta=e^{i\theta}; \qquad C_j(0), \qquad k_j, \qquad |k_j|>1, \qquad j=1,\ldots,N. \tag{7}$$

In the language of the scattering theory, α is called the *reflection coefficient*, β the *transmission coefficient*, N the number of *bound states* k_j, and C_j the related *normalization coefficients*. The effective construction of these data from $q(n,0)$ is displayed in Sec. III, but here we just consider that the set (7) is given and we show how to build from it a solution of (1). It is worth mentioning that in the linear limit case of *small* $q(x,0)$, $\alpha(\zeta,0)$ becomes the Fourier transform of q (with parameter 2ζ), $\beta(\zeta,0)$ become 1 and all the C_j's vanish (no discrete spectrum, or else no solitons in the linear limit).

The first step is to construct the *spectral transform* at time t by solving

$$\partial_t\alpha=\alpha\frac{g+\overline{g}}{2}(|I_1(\theta,t)|^2-|I_2(\theta,t)|^2)-(g+\overline{g})\overline{I_1}I_2 \tag{8}$$

$$-\alpha\frac{1}{2\pi i}P\oint_{\mathscr{C}}\frac{d\zeta'}{\zeta'-\zeta}(g+\overline{g})(|I_1|^2-|I_2|^2) \tag{9}$$

$$+\alpha\frac{1}{2\pi i}\oint_{\mathscr{C}}\frac{d\zeta'}{\zeta'}(g|I_1|^2-\overline{g}|I_2|^2), \tag{10}$$

$$\partial_t k_j=0, \tag{11}$$

$$\partial_t C_j(t) = -C_j(t)\frac{1}{2\pi i}P\oint_{\mathscr{C}}\frac{d\zeta'}{\zeta'-k_j}(g+\overline{g})(|I_1|^2-|I_2|^2) \tag{12}$$

$$+C_j(t)\frac{1}{2\pi i}\oint_{\mathscr{C}}\frac{d\zeta'}{\zeta'}(g|I_1|^2-\overline{g}|I_2|^2). \tag{13}$$

Unlike in the continuum case, the transmission coefficient $\beta(\zeta,t)$ cannot be computed directly from $\alpha(\zeta,t)$ and it becomes necessary to solve the equation

$$\beta(\zeta,t)^{-1}\partial_t\beta(\zeta,t) = -\frac{1}{2}\frac{\partial_t|\alpha|^2}{1+|\alpha|^2}+\frac{1}{2i\pi}P\oint_{\mathscr{C}}\frac{\zeta}{\zeta'}\frac{d\zeta'}{\zeta'-\zeta}\frac{\partial_t|\alpha|^2}{1+|\alpha|^2}. \tag{14}$$

In the integrals here, P denotes the Cauchy principal value and $\mathscr{C}$ the unit circle in the complex plane.

Although not elementary, in the case when I_1 and I_2 are given independently of α and β the above system of equations is *linear* and can in principle be explicitly solved as soon as the *initial data* (7) and the boundary values (4) are known. Before going further, it is already worth remarking that if the quantity I_1I_2 does not vanish, then the evolution for the reflection coefficient $\alpha(\zeta,t)$ has a nonhomogeneous term. Consequently the solution can grow on the *initial vacuum* $q(n,0)=0$ which has the spectral transform

$$\alpha(\zeta,0)=0, \qquad \beta(\zeta,0)=1; \quad N=0. \tag{15}$$

The second step consists in solving the following system of linear integral equations for the unknowns $\phi_i(k,n,t)$ for $|k|<1$

$$\begin{pmatrix}\phi_1(k)\\ \phi_2(k)\end{pmatrix} = \begin{pmatrix}1\\0\end{pmatrix}+\frac{1}{2i\pi}\oint_{\mathscr{C}}\frac{d\zeta'}{\zeta'-k}\frac{k}{\zeta'}(\zeta')^{-n}\alpha(\zeta')\begin{pmatrix}-\overline{\phi_2}(\zeta')\\ \overline{\phi_1}(\zeta')\end{pmatrix}$$
$$+\sum_{j=1}^{N}\frac{C_j}{k_j-k}\frac{k}{k_j}(k_j)^{-n}\begin{pmatrix}-\overline{\phi_2}(1/\overline{k_j})\\ \overline{\phi_1}(1/\overline{k_j})\end{pmatrix}. \tag{16}$$

The solution of (1) then reads (last step) for $\zeta=e^{i\theta}$

$$\begin{pmatrix}A_1\\ A_2\end{pmatrix} = I_1\begin{pmatrix}\phi_1(\zeta)\\ \zeta^n\phi_2(\zeta)\end{pmatrix}+I_2\begin{pmatrix}-\zeta^{-n}{}_2(\zeta)\\ \overline{\phi}_1(\zeta)\end{pmatrix}, \tag{17}$$

$$q(n+1,t) = -\overline{\phi}_2^{(-1)}(n,t), \tag{18}$$

with $\phi_2^{(-1)}$ the coefficient of k^{-1} in the Laurent expansion of the solution $\phi_2(k,n,t)$. This achieves the solution of the nonlinear system (1) with the arbitrary boundary values (4) as a sequence of *linear* operations.

An interesting information here is the output values (vs the input values) of the fields A_j (values for $n\to-\infty$) which will be proved to be

$$\begin{pmatrix}A_1\\ A_2\end{pmatrix}\xrightarrow[n\to-\infty]{}\frac{1}{1+|\alpha|^2}\begin{pmatrix}I_1\beta+I_2\overline{\alpha\beta}\\ -I_1\alpha\overline{\beta}+I_2\overline{\beta}\end{pmatrix} \tag{19}$$

for the input

$$\begin{pmatrix} A_1 \\ A_2 \end{pmatrix} \xrightarrow[n\to+\infty]{} \begin{pmatrix} I_1 \\ I_2 \end{pmatrix} \tag{20}$$

(note the necessity to compute not only the reflection coefficient α at time t but also the transmission coefficient β). This result, besides having a physical interest, has the nice property of being *explicit*. Indeed it does not require solving the integral equations (16). Actually, when the system (1) is viewed as describing the interaction of radiation components A_j with matter, the relevant (measured) physical information is the output values of the radiation components.

Now we can compute the ratio $\rho(-\infty,t)$ of transmitted *photon number*, defined in (3), as

$$\rho(n,t) \xrightarrow[n\to-\infty]{} \frac{1+|\alpha|^2}{|\beta|^2}, \tag{21}$$

while we have obviously

$$\rho(n,t) \xrightarrow[n\to+\infty]{} 1. \tag{22}$$

This is unlike in the continuous case for which we would find $\rho(-\infty,t)=1$, and results effectively from the discrete nature of (1). Indeed a direct calculation leads to the following *total photon number* nonconservation

$$|A_1(\zeta,n-1)|^2+|A_2(\zeta,n-1)|^2=(1+|q(n)|^2)(|A_1(\zeta,n)|^2+|A_2(\zeta,n)|^2). \tag{23}$$

As a consequence we obtain from (3) and the above relation

$$\rho^{-1}(n,t)=\prod_{i=n+1}^{\infty}(1+|q(i,t)|^2) \tag{24}$$

which proves in particular that the energy ratio $\rho(n,t)$ indeed does not depend on the variable θ.

III. THE SPECTRAL PROBLEM

In the case of the discrete variable, a spectral problem is understood as a difference equation for some unknown $\mu(n)$, which involves explicitly an external parameter, the *spectral parameter*, and a set of given n-dependent coefficients, the *potentials*. Solving a spectral problem results in defining the set of *spectral data* (functions of the parameter k) in such a way that they are in bijection with the set of potentials (in some given class of functions). We shall work here in the space of 2×2 matrices and adopt an equivalent form of the reduced Ablowitz–Ladik spectral problem used in Ref. 3 to integrate the discrete nonlinear Schrödinger equation. In our case we are able to write the spectral transform as a ∂-problem for the matrix $\mu(k,n)$, which results in a simple formulation of the inverse problem together with a very convenient tool for building and solving nonlinear evolutions, in particular those with nonanalytic dispersion relations and boundary value data.

A. Equation and Jost solutions

Let us consider the discrete spectral problem

$$\mu(k,n+1)-\Lambda^{-1}\mu(k,n)\Lambda=Q(n+1)\mu(k,n+1), \tag{25}$$

with the following definitions

$$\Lambda(k)=\begin{pmatrix} 1/z & 0 \\ 0 & z \end{pmatrix}, \qquad z^2=k, \qquad Q(n)=\begin{pmatrix} 0 & q(n) \\ r(n) & 0 \end{pmatrix}, \tag{26}$$

where k is the spectral parameter which belongs to the domain $\mathscr{D}=\mathbf{C}-\{0,\infty\}$. Up to a change of $n\to -n$, $k\to 1/k$ and a rescaling by convenient powers of z of the matrix elements of μ it is just the special reduction of the Ablowitz–Ladik spectral problem associated to the integrable discrete nonlinear Schrödinger equation. The solution of (25) possesses the property

$$\det\{\mu(k,n-1)\}=\det\{\mu(k,n)\}[1-r(n)q(n)]. \tag{27}$$

The solution of this spectral problem goes through the construction of some well chosen solutions (the Jost solutions) out of some particular asymptotic behaviors. These solutions are denoted by $\mu^{\pm}$ and are defined by the following discrete integral equations

$$\begin{pmatrix} \mu_{11}^{-}(k,n) \\ \mu_{21}^{-}(k,n) \end{pmatrix}=\begin{pmatrix} 1 \\ 0 \end{pmatrix}+\begin{pmatrix} -\sum_{i=n+1}^{+\infty} q(i)\mu_{21}^{-}(k,i) \\ \sum_{i=-\infty}^{n} k^{i-n}r(i)\mu_{11}^{-}(k,i) \end{pmatrix}, \tag{28}$$

$$\begin{pmatrix} \mu_{11}^{+}(k,n) \\ \mu_{21}^{+}(k,n) \end{pmatrix}=\begin{pmatrix} 1 \\ 0 \end{pmatrix}+\begin{pmatrix} -\sum_{i=n+1}^{+\infty} q(i)\mu_{21}^{+}(k,i) \\ -\sum_{i=n+1}^{+\infty} k^{i-n}r(i)\mu_{11}^{+}(k,i) \end{pmatrix}, \tag{29}$$

$$\begin{pmatrix} \mu_{12}^{-}(k,n) \\ \mu_{22}^{-}(k,n) \end{pmatrix}=\begin{pmatrix} 0 \\ 1 \end{pmatrix}+\begin{pmatrix} -\sum_{i=n+1}^{+\infty} k^{n-i}q(i)\mu_{22}^{-}(k,i) \\ -\sum_{i=n+1}^{+\infty} r(i)\mu_{12}^{-}(k,i) \end{pmatrix}, \tag{30}$$

$$\begin{pmatrix} \mu_{12}^{+}(k,n) \\ \mu_{22}^{+}(k,n) \end{pmatrix}=\begin{pmatrix} 0 \\ 1 \end{pmatrix}+\begin{pmatrix} \sum_{i=-\infty}^{n} k^{n-i}q(i)\mu_{22}^{+}(k,i) \\ -\sum_{i=n+1}^{+\infty} r(i)\mu_{12}^{+}(k,i) \end{pmatrix}. \tag{31}$$

We will make use also of the notation

$$\mu_1^{\pm}=\begin{pmatrix} \mu_{11}^{\pm} \\ \mu_{21}^{\pm} \end{pmatrix}, \qquad \mu_2^{\pm}=\begin{pmatrix} \mu_{12}^{\pm} \\ \mu_{22}^{\pm} \end{pmatrix}. \tag{32}$$

The above integral equations allow us to obtain, for some given class of potentials, the analytical properties of the solutions in the domain $\mathscr{D}$ of the complex k-plane, for all n. The function $\mu_1^{+}(k,n)$ is holomorphic inside the unit circle, the function $\mu_2^{-}(k,n)$ is holomorphic outside the unit circle, the function $\mu_1^{-}(k,n)$ is meromorphic outside the unit circle where it has a finite number N^{-} of simple poles k_j^{-}, the function $\mu_2^{+}(k,n)$ is meromorphic inside the unit circle where it has a finite number N^{+} of simple poles k_j^{+}. Moreover the two solutions $\mu^{\pm}$ are continuous on the unit circle.

B. Riemann–Hilbert problem and spectral data

The method to obtain from the integral equations defining $\mu^{\pm}$ the related Riemann–Hilbert problem is standard. We proceed through direct computation of the difference of the two column vectors μ_1^+ and μ_1^- and obtain the integral equation for this difference. It obeys the same equation as the quantity $-\alpha^-(k)k^{-n}\mu_2^-(k,n)$ (the quantity α^- is defined below) and, based on the uniqueness of the solution of such equations, we conclude

$$\mu_1^+(k,n)-\mu_1^-(k,n)=-\alpha^-(k)k^{-n}\mu_2^-(k,n), \qquad |k|=1. \tag{33}$$

The same approach is applied to $\mu_2^{\pm}$ and we get

$$\mu_2^+(k,n)-\mu_2^-(k,n)=\alpha^+(k)k^{n}\mu_1^+(k,n), \qquad |k|=1, \tag{34}$$

where the *reflection coefficients* $\alpha^-(k)$ and $\alpha^+(k)$ are defined (still for $|k|=1$) as

$$\alpha^-(k)=\sum_{-\infty}^{+\infty} k^i r(i)\mu_{11}^-(k,i), \qquad \alpha^+(k)=\sum_{-\infty}^{+\infty} k^{-i} q(i)\mu_{22}^+(k,i). \tag{35}$$

For future use we define also

$$\beta^-(k)=1-\sum_{-\infty}^{+\infty} q(i)\mu_{21}^-(k,i), \qquad \beta^+(k)=1-\sum_{-\infty}^{+\infty} r(i)\mu_{12}^+(k,i) \tag{36}$$

which are called the *transmission coefficients*. Note that, due to the analytical properties of μ_{21}^- (resp. μ_{12}^+), $\beta^-(k)$ can be continued analytically in $|k|\geqslant 1$ (resp. $\beta^+(k)$ in $|k|\leqslant 1$). Actually the vectors μ_1^- and μ_2^+ have poles where the transmission coefficients $\beta^{\pm}(k)$ have poles and we derive from the integral equations (after multiplication by $k-k_j^{\pm}$ and limit $k\to k_j^{\pm}$)

$$\operatorname*{Res}_{k_j^-}\{\mu_1^-(k,n)\}=\begin{pmatrix}0\\1\end{pmatrix}(k_j^-)^{-n}C_j^- +\begin{pmatrix} -\displaystyle\sum_{i=n+1}^{+\infty} q(i)\operatorname*{Res}_{k_j^-}\{\mu_{21}^-(k,i)\} \\ -\displaystyle\sum_{i=n+1}^{+\infty} (k_j^-)^{i-n} r(i)\operatorname*{Res}_{k_j^-}\{\mu_{11}^-(k,i)\}\end{pmatrix}, \tag{37}$$

$$\operatorname*{Res}_{k_j^+}\{\mu_2^+(k,n)\}=\begin{pmatrix}1\\0\end{pmatrix}(k_j^+)^{n}C_j^+ +\begin{pmatrix} -\displaystyle\sum_{i=n+1}^{+\infty} (k_j^+)^{n-i} q(i)\operatorname*{Res}_{k_j^+}\{\mu_{22}^+(k,i)\} \\ -\displaystyle\sum_{i=n+1}^{+\infty} r(i)\operatorname*{Res}_{k_j^+}\{\mu_{12}^+(k,i)\}\end{pmatrix} \tag{38}$$

with the following definitions of the $C_j^{\pm}$'s

$$C_j^-=\sum_{i=-\infty}^{+\infty} (k_j^-)^i r(i)\operatorname*{Res}_{k_j^-}\{\mu_{11}^-(k,i)\}, \tag{39}$$

$$C_j^+=\sum_{i=-\infty}^{+\infty} (k_j^+)^{-i} q(i)\operatorname*{Res}_{k_j^+}\{\mu_{22}^+(k,i)\} \tag{40}$$

which are called the *normalization coefficients*.

Since the vectors μ_1^+ and μ_2^- are holomorphic, we can write down their integral equations evaluated respectively in k_j^+ and k_j^- and compare them to the above integral equations for the residues. We obtain

$$\operatorname*{Res}_{k_j^-}\{\mu_1^-(k,n)\}=(k_j^-)^{-n}C_j^-\mu_2^-(k_j^-,n), \tag{41}$$

$$\operatorname*{Res}_{k_j^+}\{\mu_2^+(k,n)\}=(k_j^+)^{n}C_j^+\mu_1^+(k_j^+,n). \tag{42}$$

Finally the Riemann–Hilbert problem (33) and (34) is completed by the behaviors of the solution $\mu^{\pm}$ on the boundaries $|k|=0$ and $|k|=\infty$ of $\mathscr{D}$, which read

$$\mu_1^+(k,n)\xrightarrow[k\to 0]{}\begin{pmatrix}1\\0\end{pmatrix},\qquad \mu_2^-(k,n)\xrightarrow[k\to\infty]{}\begin{pmatrix}0\\1\end{pmatrix}. \tag{43}$$

The vectorial Riemann–Hilbert problem (33), (34) with singular points given by (41), (42) and the boundary behaviors (43) constitutes a closed problem which will be solved in the next section.

The behaviors of $\mu_1^-(k,n)$ at large k and of $\mu_2^+(k,n)$ at small k will be useful for the following and we define

$$\mu_{11}^-(k,n)\xrightarrow[k\to\infty]{} f(n). \tag{44}$$

Then

$$\mu_{21}^-(k,n)\xrightarrow[k\to\infty]{} r(n)f(n) \tag{45}$$

and one easily gets that $f(n)$ satisfies the integral equation

$$f(n)=1-\sum_{n+1}^{+\infty} q(i)r(i)f(i), \tag{46}$$

the solution of which is

$$f(n)=\prod_{n+1}^{+\infty}[1-q(i)r(i)]. \tag{47}$$

The same computation holds for $\mu_2^+(k,n)$ and we have finally

$$\mu^-(k,n)\xrightarrow[k\to\infty]{}\begin{pmatrix}f(n) & 0\\ r(n)f(n) & 1\end{pmatrix}, \tag{48}$$

$$\mu^+(k,n)\xrightarrow[k\to\infty]{}\begin{pmatrix}1 & q(n)f(n)\\ 0 & f(n)\end{pmatrix}. \tag{49}$$

It can be shown easily by using (33) and (34) that the determinant of the matrix $\mu(k,n)$ is analytic in the whole domain $\mathscr{D}$. Hence it follows from the Liouville theorem and the boundary values (48), (49) that

$$\det\{\mu(k,n)\}=f(n). \tag{50}$$

Note that, within the reduction $r=-\overline{q},\ f(n)=\rho(n)^{-1}$ as given by (24).

C. Asymptotic behaviors and unitarity relation

By taking the limit at large n directly on the integral equations, the functions $\mu^{\pm}$ obey for $|k|=1$

$$\mu^{-}(k,n)\xrightarrow[n\to+\infty]{}\begin{pmatrix}1 & 0\\ k^{-n}\alpha^{-}(k) & 1\end{pmatrix}, \tag{51}$$

$$\mu^{-}(k,n)\xrightarrow[n\to-\infty]{}\begin{pmatrix}\beta^{-}(k) & -k^{n}\hat{\alpha}^{-}(k)\\ 0 & \hat{\beta}^{-}(k)\end{pmatrix}, \tag{52}$$

$$\mu^{+}(k,n)\xrightarrow[n\to+\infty]{}\begin{pmatrix}1 & k^{n}\alpha^{+}(k)\\ 0 & 1\end{pmatrix}, \tag{53}$$

$$\mu^{+}(k,n)\xrightarrow[n\to-\infty]{}\begin{pmatrix}\hat{\beta}^{+}(k) & 0\\ -k^{-n}\hat{\alpha}^{+}(k) & \beta^{+}(k)\end{pmatrix}, \tag{54}$$

where the following *alternative scattering data* are defined as

$$\hat{\alpha}^{-}(k)=\sum_{-\infty}^{+\infty}k^{-i}q(i)\mu_{22}^{-}(k,i),\qquad \hat{\alpha}^{+}(k)=\sum_{-\infty}^{+\infty}k^{i}r(i)\mu_{11}^{+}(k,i), \tag{55}$$

$$\hat{\beta}^{-}(k)=1-\sum_{-\infty}^{+\infty}r(i)\mu_{12}^{-}(k,i),\qquad \hat{\beta}^{+}(k)=1-\sum_{-\infty}^{+\infty}q(i)\mu_{21}^{+}(k,i). \tag{56}$$

The quantities $\hat{\alpha}^{\pm}$ are also called the reflection coefficients *to the left* (referring to the limit $n\to-\infty$) when $\alpha^{\pm}$ are the reflection coefficients *to the right*.

It is easy to prove the following relations

$$\hat{\alpha}^{-}=\frac{\alpha^{+}\beta^{-}}{1-\alpha^{-}\alpha^{+}},\qquad \hat{\alpha}^{+}=\frac{\alpha^{-}\beta^{+}}{1-\alpha^{-}\alpha^{+}}, \tag{57}$$

$$\hat{\beta}^{-}=\frac{\beta^{+}}{1-\alpha^{-}\alpha^{+}},\qquad \hat{\beta}^{+}=\frac{\beta^{-}}{1-\alpha^{-}\alpha^{+}}. \tag{58}$$

Indeed, by using the Riemann–Hilbert problems (33) and (34) for μ (still for $|k|=1$) we have

$$\hat{\alpha}^{-}=\sum_{-\infty}^{+\infty}k^{-i}q(i)\mu_{22}^{+}(k,i)-\alpha^{+}\sum_{-\infty}^{+\infty}q(i)\mu_{21}^{+}(k,i)$$

$$=\alpha^{+}\left(1-\sum_{-\infty}^{+\infty}q(i)\mu_{21}^{+}(k,i)\right)=\alpha^{+}\hat{\beta}^{+}, \tag{59}$$

$$\hat{\beta}^+ = 1 - \sum_{-\infty}^{+\infty} q(i)\mu_{21}^-(k,i) + \alpha^- \sum_{-\infty}^{+\infty} k^{-i} q(i)\mu_{22}^-(k,i)$$

$$= \beta^- + \alpha^- \hat{\alpha}^-, \tag{60}$$

and so on for the other relations.

Now from (27) the determinant of $\mu(k,n)$ as $n \to -\infty$ can be computed and, by using the behaviors of $\mu(k,n)$, it leads to the relation

$$\beta^- \beta^+ = (1 - \alpha^- \alpha^+) \prod_{-\infty}^{+\infty} [1 - r(i)q(i)] \tag{61}$$

which is called the *unitarity relation*.

D. Reduction

A *reduction* denotes a simple (possibly algebraic) relation between the potentials (here $r(n)$ and $q(n)$) for which one can derive the counterpart relations for the spectral data. In other word a reduction is a relation which conserves the bijection between potentials and spectral data.

In the case

$$r(n) = -\overline{q(n)} \quad \Leftrightarrow \quad \overline{Q(n)} = \sigma_2 Q(n) \sigma_2, \tag{62}$$

it is easy to check that the function

$$\nu(k,n) = \sigma_2 \overline{\mu}(1/\overline{k},n)\sigma_2, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \tag{63}$$

obeys the same equation as $\mu(k,n)$. To compare them it is enough to consider their behaviors as $n \to \pm\infty$. Since

$$\sigma_2 \overline{\mu}^-(1/\overline{k},n)\sigma_2 \xrightarrow[n \to +\infty]{} \begin{pmatrix} 1 & -k^n \overline{\alpha^-}(1/\overline{k}) \\ 0 & 1 \end{pmatrix}, \tag{64}$$

we conclude that

$$\sigma_2 \overline{\mu}^-(1/\overline{k},n)\sigma_2 = \mu^+(k,n), \tag{65}$$

$$\overline{\alpha}^-(1/\overline{k}) = -\alpha^+(k). \tag{66}$$

The same calculation at $n \to -\infty$ gives

$$\overline{\beta}^-(1/\overline{k}) = \beta^+(k), \tag{67}$$

and also that the alternative scattering data obey similar relations.

For the discrete spectrum, the relation (65) implies

$$\operatorname*{Res}_{k_j^+} \{\mu_2^+(k,i)\} = \operatorname*{Res}_{k_j^+} \begin{pmatrix} -\overline{\mu_{21}}(1/\overline{k},i) \\ \overline{\mu_{11}}(1/\overline{k},i) \end{pmatrix}. \tag{68}$$

Using the basic relations

$$\operatorname*{Res}_{k_0}\{f(1/\overline{k})\}=-(\overline{k_0})^2\operatorname*{Res}_{1/\overline{k_0}}\{f(k)\},\quad \operatorname*{Res}_{k_0}\{\overline{g(k)}\}=\overline{\operatorname*{Res}_{k_0}\{g(k)\}},\tag{69}$$

the equation (68) becomes

$$\operatorname*{Res}_{k_j^+}\{\mu_2^+(k,i)\}=-(\overline{k}_j^+)^2\overline{\operatorname*{Res}_{1/\overline{k}_j^+}\begin{pmatrix}-\overline{\mu_{21}^-}(k,i)\\ \overline{\mu_{11}^-}(k,i)\end{pmatrix}}.\tag{70}$$

This last equation holds if

$$N^+=N^-,\qquad k_j^+=\frac{1}{\overline{k_j^-}}\tag{71}$$

for which it reads

$$\operatorname*{Res}_{k_j^+}\{\mu_2^+(k,i)\}=-(\overline{k}_j^+)^2\overline{\operatorname*{Res}_{k_j^-}\begin{pmatrix}-\overline{\mu_{21}^-}(k,i)\\ \mu_{11}^-(k,i)\end{pmatrix}}.\tag{72}$$

The above relation together with (65) and (71) then implies

$$\frac{C_j^+}{k_j^+}=\frac{\overline{C_j^-}}{\overline{k_j^-}}.\tag{73}$$

In the case of the reduction (62) we will use the following simplified notations (already used in Sec. II)

$$\alpha=\alpha^-,\qquad \beta=\beta^-,\qquad C_j=C_j^-,\qquad k_j=k_j^-,\qquad N=N^+=N^-.\tag{74}$$

In order to not over complicate this paper, we do not consider the other reduction $r=\overline{q}$ for which similar results can be easily obtained, but which corresponds to a spectral problem without discrete spectrum.

Last, it is useful for the following to rewrite the asymptotic boundary behaviors (51)–(54) within the reduction (and with the above notations) and for $|\zeta|=1$ as

$$\begin{pmatrix}\beta & \zeta^n\overline{\alpha}\gamma\\ 0 & \overline{\gamma}\end{pmatrix}\underset{n\to-\infty}{\longleftarrow}\mu^-(\zeta,n)\xrightarrow[n\to+\infty]{}\begin{pmatrix}1 & 0\\ \zeta^{-n}\alpha & 1\end{pmatrix},\tag{75}$$

$$\begin{pmatrix}\gamma & 0\\ -\zeta^{-n}\alpha\overline{\gamma} & \overline{\beta}\end{pmatrix}\underset{n\to-\infty}{\longleftarrow}\mu^+(\zeta,n)\xrightarrow[n\to+\infty]{}\begin{pmatrix}1 & -\zeta^n\overline{\alpha}\\ 0 & 1\end{pmatrix},\tag{76}$$

$$\gamma=\frac{\beta}{1+|\alpha|^2}.\tag{77}$$

Similarly, the unitarity relation (61) together with the definition (47) reads

$$|\beta|^2=(1+|\alpha|^2)f(-\infty).\tag{78}$$

IV. THE INVERSE SPECTRAL PROBLEM

The *inverse spectral problem* consists in reconstructing the potentials $q(n)$ and $r(n)$ from the spectral data

$$\alpha^{\pm}(k), \qquad \beta^{\pm}(k), \qquad |k|=1;$$

$$C_j^{\pm}, \qquad k_j^{\pm}, \qquad |k_j^{+}|<1, \qquad j=1,\ldots,N^{+}, \qquad |k_j^{-}|>1, \qquad j=1,\ldots,N^{-}. \tag{79}$$

A simple way of doing this is to reformulate the analytical properties of the matrix $\mu(k,n)$ in the domain $\mathscr{D}$ as a $\bar{\partial}$-problem.

A. Inverse problem as a $\bar{\partial}$-problem

Indeed, the set of fundamental relations (33), (34), (41) and (42), which contain all the information about the analytical properties of $\mu(k,n)$, can be summarized in the formula

$$\frac{\partial}{\partial \bar{k}}\mu(k,n)=\mu(k,n)R(k,n), \qquad k\in\mathscr{D}, \tag{80}$$

where the *spectral transform* contains all the information and reads

$$R(k,n)=\begin{pmatrix} 0 & \alpha^{+}(k)\,\delta^{+}(k,1) \\ -\alpha^{-}(k)\,\delta^{-}(k,1) & 0 \end{pmatrix}\begin{pmatrix} k^{-n} & 0 \\ 0 & k^{n} \end{pmatrix} -2i\pi\begin{pmatrix} 0 & \sum_{j=1}^{N^{+}} C_j^{+}\,\delta(k-k_j^{+}) \\ \sum_{j=1}^{N^{-}} C_j^{-}\,\delta(k-k_j^{-}) & 0 \end{pmatrix}\begin{pmatrix} k^{-n} & 0 \\ 0 & k^{n} \end{pmatrix}. \tag{81}$$

The distributions $\delta^{\pm}(k,1)$ are defined in the Appendix and the distribution $\delta(k)$ is normalized by requiring that $\int\int dk \wedge dk\,\delta(k)=1$. Using the method and tools described in the Appendix, and for the behaviors

$$\mu_1(k,n) \xrightarrow[k\to 0]{} \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \mu_2(k,n) \xrightarrow[k\to\infty]{} \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \tag{82}$$

we have the following solution of this $\bar{\partial}$-problem

$$\mu(k,n)=1+\frac{1}{2i\pi}\iint_{\mathscr{D}}\frac{d\lambda\wedge d\bar{\lambda}}{\lambda-k}\mu(\lambda,n)R(\lambda,n)\begin{pmatrix} k/\lambda & 0 \\ 0 & 1 \end{pmatrix}. \tag{83}$$

Due to the particular structure (81) of $R(k)$, the above matrix valued equation has actually to be understood as two vectorial integral equations, for $\mu_1^{+}(k,n)$ and for $\mu_2^{-}(k,n)$. As will be seen hereafter, the knowledge of these two vectors is sufficient for completely solving the problem.

B. Reconstruction of the potentials

The potentials are obtained from the asymptotic expansion of the Jost solutions μ_2^{-} and μ_1^{+} of (25) via the formulae

$$q(n+1)=-\mu_{12}^{-(-1)}(n), \qquad r(n+1)=-\mu_{21}^{+(1)}(n), \tag{84}$$

where $\mu_{12}^{-(-1)}(n)$ is the coefficient of k^{-1} in the Laurent expansion for $k\to\infty$ of $\mu_{12}^{-}(k,n)$, and $\mu_{21}^{+(1)}(n)$ the coefficient of k in the Taylor expansion for $k\to 0$ of $\mu_{21}^{+}(k,n)$. In particular from (83) we get

$$r(n+1)=\frac{1}{2i\pi}\oint_{\mathscr{C}} d\zeta\alpha^{-}(\zeta)\zeta^{-n-2}\mu_{22}^{-}(\zeta,n)-\sum_{j=1}^{N^{-}} C_j^{-}(k_j^{-})^{-n-2}\mu_{22}^{-}(k_j^{-},n), \tag{85}$$

$$q(n+1)=\frac{1}{2i\pi}\oint_{\mathscr{C}} d\zeta\alpha^{+}(\zeta)\zeta^{n}\mu_{11}^{+}(\zeta,n)+\sum_{j=1}^{N^{+}} C_j^{+}(k_j^{+})^{n}\mu_{11}^{+}(k_j^{+},n). \tag{86}$$

One could easily check that the potentials given by (86) and (85) do obey the reduction (62) when $\mu(k,n)$ obeys (65), $\alpha(k)$ obeys (66), $C_j^{\pm}$ obeys (73) and $k_j^{\pm}$ obeys (71).

Finally the transmission coefficients $\beta^{-}(k)$ and $\beta^{+}(k)$ are computed from their definitions (36), where the entries $\mu_{21}^{-}(k,n)$ and $\mu_{12}^{+}(k,n)$ are obtained from the solution μ_1^{+} and μ_2^{-} by using the explicit relations (33), (34). Equivalently one can use the relations (58) and the behaviors (52) and (54) to get ($|\zeta|=1$)

$$\beta^{+}(\zeta)=[1-\alpha^{+}\alpha^{-}]\lim_{n\to-\infty}\mu_{22}^{-}(\zeta,n), \tag{87}$$

$$\beta^{-}(\zeta)=[1-\alpha^{+}\alpha^{-}]\lim_{n\to-\infty}\mu_{11}^{+}(\zeta,n). \tag{88}$$

Remark: From the other components of μ_1^{+} and μ_2^{-} we obtain in (25) the following relations

$$\mu_{22}^{-(-1)}(n)=\sum_{n+1}^{\infty} r(i)q(i+1), \qquad \mu_{11}^{+(1)}(n)=\sum_{n+1}^{\infty} r(i+1)q(i). \tag{89}$$

V. THE METHOD OF THE $\bar{\partial}$-PROBLEM

We have shown in the preceding sections that the spectral problem (25) can be mapped to the ∂-problem (80), namely,

$$\frac{\partial}{\partial k}\mu(k)=\mu(k)R(k), \qquad k\in\mathscr{D}, \tag{90}$$

with the boundary behaviors (82). The solution of such a boundary value problem in the complex plane solves the Cauchy–Green integral equation

$$\mu(k)=1+\frac{1}{2i\pi}\iint_{\mathscr{D}}\frac{d\lambda\wedge d\bar{\lambda}}{\lambda-k}\mu(\lambda)R(\lambda)\begin{pmatrix} k/\lambda & 0\\ 0 & 1\end{pmatrix}. \tag{91}$$

The purpose of the following is to show that the above integral equation, for the unknown μ and the datum R, can be taken as the *starting tool*. More precisely we shall show how a parametric dependence of R (on an integer n and on a real t) induces the spectral problem (25) and a nonlinear evolution equation.

A. The principal spectral problem

We restrict this study to off-diagonal matrices $R(k)$ and consider the integral equation (91) as the given tool. If $R(k)$ depends now on an external integer n, the solution $\mu(k,n)$ solves then the ∂-problem (90) with the behaviors

$$\mu(k,n) \xrightarrow[k\to\infty]{} \begin{pmatrix} 1 & g(n) \\ 0 & f(n) \end{pmatrix} + k\mu^{(1)}(n) + \cdots, \tag{92}$$

$$\mu(k,n) \xrightarrow[k\to\infty]{} \begin{pmatrix} f'(n) & 0 \\ h(n) & 1 \end{pmatrix} + \frac{1}{k}\mu^{(-1)}(n) + \cdots, \tag{93}$$

where the functions f, f', g and h have to be evaluated. The determinant of $\mu(k,n)$ is analytic in $\mathscr{D}$ as indeed the off-diagonal structure of $R(k,n)$ implies

$$\frac{\partial}{\partial k}\det\{\mu(k,n)\} = 0, \tag{94}$$

and from the above behavior the Liouville theorem implies

$$\det\{\mu(k,n)\} = f(n) = f'(n). \tag{95}$$

We chose now the following explicit dependence of $R(k,n)$ on the discrete variable n

$$R(k,n+1) = \Lambda(k)^{-1} R(k,n) \Lambda(k), \tag{96}$$

with $\Lambda(k)$ defined in (26). The basic fundamental property which allows us to derive from the choice (96) a *difference* equation for μ in the variable n is the following

$$\frac{\partial}{\partial k} H(k,n) = 0, \qquad H(k,n) = \mu(k,n+1)\Lambda(k)^{-1}\mu(k,n)^{-1}\Lambda(k). \tag{97}$$

The above function $H(k,n)$ can then be reconstructed from its behaviors on the boundary of $\mathscr{D}$ ($k=\infty$ and $k=0$) which read from (92) and (93)

$$H(k,n) \xrightarrow[k\to\infty]{} \frac{1}{f(n)} \begin{pmatrix} f(n) - g(n+1)\mu_{21}^{(1)}(n) & g(n+1) \\ -f(n+1)\mu_{21}^{(1)}(n) & f(n+1) \end{pmatrix}, \tag{98}$$

$$H(k,n) \xrightarrow[k\to\infty]{} \frac{1}{f(n)} \begin{pmatrix} f(n+1) & -f(n+1)\mu_{12}^{(-1)}(n) \\ h(n+1) & f(n) - h(n+1)\mu_{12}^{(-1)}(n) \end{pmatrix}. \tag{99}$$

Since $H(k,n)$ is analytic, these two behaviors are equal, which implies the following four equations

$$\begin{gathered} f(n+1) = f(n) - g(n+1)\mu_{21}^{(1)}(n), \quad f(n+1) = f(n) - h(n+1)\mu_{12}^{(-1)}(n), \\ g(n+1) = -f(n+1)\mu_{12}^{(-1)}(n), \quad h(n+1) = -f(n+1)\mu_{21}^{(1)}(n), \end{gathered} \tag{100}$$

which are solved by first *defining* the *potentials* as

$$q(n+1) = -\mu_{12}^{(-1)}(n), \qquad r(n+1) = -\mu_{21}^{(1)}(n), \tag{101}$$

and hence

$$g(n) = q(n)f(n), \qquad h(n) = r(n)f(n), \tag{102}$$

with the recursion relation for $f(n)$

$$f(n)=f(n+1)[1-r(n+1)q(n+1)] \tag{103}$$

of which the solution is indeed given by (47).

Finally, the solution of the ∂-problem (97) reads

$$H(k,n)=\frac{1}{1-r(n+1)q(n+1)}\begin{pmatrix}1 & q(n+1)\\ r(n+1) & 1\end{pmatrix} \tag{104}$$

which can be written with (97) as the *discrete spectral problem*

$$\mu(k,n+1)\Lambda(k)^{-1}\mu(k,n)^{-1}\Lambda(k)=[1-Q(n+1)]^{-1}, \tag{105}$$

where

$$Q(n)=\begin{pmatrix}0 & q(n)\\ r(n) & 0\end{pmatrix}. \tag{106}$$

It is convenient for the following to define the quantity

$$U(n)=[1-Q(n+1)]^{-1} \tag{107}$$

such that the equation for $\mu(k,n)$ reads

$$\mu(k,n+1)=U(n)\Lambda(k)^{-1}\mu(k,n)\Lambda(k) \tag{108}$$

which is precisely the spectral problem (25).

B. Nonanalytic dispersion relations. A theorem

We consider now that $R(k,n)$ depends also on an external real t and address the problem of computing the expression of the time dependence of the solution μ of (91). The result can be stated as a theorem.

Theorem: *When the spectral transform $R(k,n,t)$ evolves according to*

$$R_t(k,n,t)=[R(k,n,t),\Omega(k,t)]+M(k,n,t), \tag{109}$$

where

$$M(k,n+1,t)=\Lambda(k)^{-1}M(k,n,t)\Lambda(k), \qquad [\Lambda(k),\Omega(k,t)]=0, \tag{110}$$

and where $\Omega(k,t)$ is the nonanalytic dispersion relation

$$\Omega(k,t)=\frac{1}{2i\pi}\iint_{\mathscr{D}}\frac{d\lambda\wedge d\bar{\lambda}}{\lambda-k}\frac{\partial\Omega(\lambda,t)}{\partial\bar{\lambda}}\begin{pmatrix}k/\lambda & 0\\ 0 & 1\end{pmatrix} \tag{111}$$

the potential Q obeys the following evolution

$$Q_t(n+1,t)=\left[\sigma_3,\frac{1}{2i\pi}\iint_{\mathscr{D}}\frac{d\lambda\wedge d\bar{\lambda}}{2\lambda}T(\lambda,n,t)\right], \tag{112}$$

where

$$T(k,n,t)=\Lambda(k)^{-1}\mu(k,n,t)\left\{M(k,n,t)-\frac{\partial\Omega(k,t)}{\partial\overline{k}}\right\}\Lambda(k)\mu^{-1}(k,n+1,t). \tag{113}$$

This theorem is proved hereafter.

1. The auxiliary spectral problem

Let us define the matrix

$$V(k,n,t)=\{\mu_t(k,n,t)-\mu(k,n,t)\Omega(k,t)\}\mu^{-1}(k,n,t), \tag{114}$$

and compute its $\overline{\partial}$-derivative which, from (80), (109) and (110), obeys

$$\frac{\partial V(k,n,t)}{\partial\overline{k}}=\mu(k,n,t)\left\{M(k,n,t)-\frac{\partial\Omega(k,t)}{\partial\overline{k}}\right\}\mu^{-1}(k,n,t). \tag{115}$$

To solve the above $\overline{\partial}$-problem we need the behaviors of V_1 as $k\to 0$ and V_2 as $k\to\infty$. Since

$$\mu(k,n,t)\xrightarrow[k\to 0]{}\begin{pmatrix}1 & q(n,t)f(n,t)\\ 0 & f(n,t)\end{pmatrix}+k\mu^{(1)}(n,t)+\cdots, \tag{116}$$

$$\mu(k,n,t)\xrightarrow[k\to\infty]{}\begin{pmatrix}f(n,t) & 0\\ r(n,t)f(n,t) & 1\end{pmatrix}+\frac{1}{k}\mu^{(-1)}(n,t)+\cdots, \tag{117}$$

it is easy to obtain, thanks also to the choice (111) (it would not be so in the case of a regular dispersion relation)

$$V_1(k,n,t)\xrightarrow[k\to 0]{}\begin{pmatrix}0\\ 0\end{pmatrix},\quad V_2(k,n,t)\xrightarrow[k\to\infty]{}\begin{pmatrix}0\\ 0\end{pmatrix}. \tag{118}$$

Consequently the solution reads

$$V(k,n,t)=\frac{1}{2i\pi}\iint_{\mathscr{D}}\frac{d\lambda\wedge d\overline{\lambda}}{\lambda-k}S(\lambda,n,t)\begin{pmatrix}k/\lambda & 0\\ 0 & 1\end{pmatrix}, \tag{119}$$

where we have defined

$$S(k,n,t)=\mu(k,n,t)\left\{M(k,n,t)-\frac{\partial\Omega(k,t)}{\partial\overline{k}}\right\}\mu^{-1}(k,n,t). \tag{120}$$

Now, with the above value of V, the definition (114) can be written as the *auxiliary spectral problem*

$$\mu_t(k,n,t)=V(k,n,t)\mu(k,n,t)+\mu(k,n,t)\Omega(k,t). \tag{121}$$

2. Fundamental property of V(k,n,t)

For simplicity of notations, we omit from now on the variable t. By direct computation the matrix S obeys the equation

$$S(k,n+1)U(n)=U(n)\Lambda(k)^{-1}S(k,n)\Lambda(k). \tag{122}$$

The next step consists in seeking an analogous property for $V(k,n)$, by computing the quantities $U(n)^{-1}V(k,n+1)$ on one side and $\Lambda(k)^{-1}V(k,n)\Lambda(k)U(n)^{-1}$ on the other side. Using

$$\Lambda(\lambda)^{-1}S(\lambda,n)\Lambda(\lambda)U(n)^{-1}\begin{pmatrix} k/\lambda & 0 \\ 0 & 1 \end{pmatrix}-\Lambda(k)^{-1}S(\lambda,n)\begin{pmatrix} k/\lambda & 0 \\ 0 & 1 \end{pmatrix}\Lambda(k)U(n)^{-1}$$

$$=\frac{\lambda-k}{\lambda}\begin{pmatrix} 0 & -q(n+1)s_{11}(\lambda,n)+\lambda s_{12}(\lambda,n) \\ r(n+1)s_{22}(\lambda,n)-(1/\lambda)s_{21}(\lambda,n) & 0 \end{pmatrix},$$

we obtain finally the required property of $V(k,n)$

$$U(n)^{-1}V(k,n+1)-\Lambda(k)^{-1}V(k,n)\Lambda(k)U(n)^{-1}=P(n), \tag{123}$$

$$P(n)=\frac{1}{2i\pi}\iint_{\mathscr{D}}\frac{d\lambda\wedge d\bar{\lambda}}{2\lambda}[\sigma_3,T(\lambda,n)], \tag{124}$$

$$T(k,n)=\Lambda(k)^{-1}S(k,n)\Lambda(k)U(n)^{-1}=U(n)^{-1}S(k,n+1). \tag{125}$$

We have used here above (122) to rewrite T in a more convenient form, and finally from the definition (120) of $S(k,n)$ and the spectral problem (25) it reads

$$T(k,n)=\Lambda(k)^{-1}\mu(k,n)\left\{M(k,n)-\frac{\partial\Omega(k)}{\partial\bar{k}}\right\}\Lambda(k)\mu^{-1}(k,n+1). \tag{126}$$

Note that the matrix $T(k,n)$ obeys a property similar to $S(k,n)$ since it can be checked directly that

$$U(n-1)T(k,n-1)=\Lambda(k)T(k,n)U(n)\Lambda(k)^{-1}. \tag{127}$$

3. The evolution equation

The nonlinear evolution of $Q(n,t)$ is now obtained in the usual way by requiring the compatibility between (108) and (121) which reads

$$\frac{\partial}{\partial t}\mu(k,n+1,t)=\frac{\partial}{\partial t}\{U(n)\Lambda(k)^{-1}\mu(k,n)\Lambda(k)\}$$

$$=V(k,n+1,t)\mu(k,n+1,t)+\mu(k,n+1,t)\Omega(k,t). \tag{128}$$

By means of (123) it is then easy to obtain the equation

$$U_t(n)=U(n)P(n)U(n), \tag{129}$$

which readily gives the evolution (112) since $U(n)=[1-Q(n+1)]^{-1}$. This ends the proof of the theorem.

C. Reduction

If we consider the reduction $r(n)=-\overline{q(n)}$ the matrices

$$\Omega(k,t)=\begin{pmatrix} \omega_1(k,t) & 0 \\ 0 & \omega_2(k,t) \end{pmatrix}, \tag{130}$$

$$M(k,n,t)=\begin{pmatrix} 0 & m_2(k,t) \\ m_1(k,t) & 0 \end{pmatrix}\begin{pmatrix} k^{-n} & 0 \\ 0 & k^n \end{pmatrix} \tag{131}$$

must be compatible with the preservation of the structure of $R(n)$ in the time evolution equation (109). We choose, therefore, ω_1 and ω_2 analytic inside and outside the unite circle with limit values on the two sides of the circle satisfying the symmetry properties ($\zeta=e^{i\theta}$)

$$\omega_1^-(\zeta,t)=\overline{\omega_2^+}(\zeta,t), \quad \omega_2^-(\zeta,t)=\overline{\omega_1^+}(\zeta,t), \tag{132}$$

and we choose m_1 and m_2 as

$$\begin{aligned} m_1(k,t)&=m^-(k,t)\,\delta^-(k,1)\equiv m(\zeta,t)\,\delta^-(k,1),\\ m_2(k,t)&=m^+(k,t)\,\delta^+(k,1)\equiv \overline{m(\zeta,t)}\,\delta^+(k,1), \end{aligned} \tag{133}$$

where

$$\zeta=\frac{k}{|k|}$$

and $m(\zeta,t)$ is a given *function* defined on the circle $|k|=1$. Note that the discontinuity of ω_1

$$p(\zeta,t)\equiv\omega_1^+(\zeta,t)-\omega_1^-(\zeta,t) \tag{134}$$

is related to the discontinuity of ω_2 by the formula

$$\omega_2^+(\zeta,t)-\omega_2^-(\zeta,t)=-\overline{p(\zeta,t)}. \tag{135}$$

The analytic properties of ω_1 and ω_2 are summarized by the formulae ($\zeta=k/|k|$)

$$\frac{\partial\omega_1}{\partial\bar{k}}=p(\zeta)\,\delta(k,1), \tag{136}$$

$$\frac{\partial\omega_2}{\partial\bar{k}}=-\overline{p(\zeta)}\,\delta(k,1), \tag{137}$$

where the distribution $\delta(k,1)$ is defined in the Appendix. Requiring that $\omega_1\to 0$ for $k\to 0$ and $\omega_2\to 0$ for $k\to\infty$, $\Omega(k)$ is defined by the following Cauchy–Green formula

$$\Omega(k)=\frac{1}{2\pi i}\oint_{\mathscr{C}}\frac{d\zeta}{\zeta-k}\begin{pmatrix} p(\zeta,t) & 0 \\ 0 & -\overline{p(\zeta,t)} \end{pmatrix}\begin{pmatrix} k/\zeta & 0 \\ 0 & 1 \end{pmatrix}. \tag{138}$$

It results that

$$\omega_1(k)=\overline{\omega_2(1/\bar{k})} \tag{139}$$

in agreement with the conditions on the boundaries (132).

It can be shown that with the choices indicated in (132) and (133) the evolution equation (112) is compatible with the reduction $r=-\bar{q}$. This evolution reads

$$q_t(n+1,t)=\frac{1}{2\pi}\,\frac{1}{f(n+1,t)}\int_{-\pi}^{+\pi}d\theta\;\gamma(\theta,n,t), \tag{140}$$

where

$$\gamma(\theta,n)=-\omega_1^-(\zeta)\mu_{11}^-(\zeta,n)\mu_{12}^-(\zeta,n+1)+\omega_1^+(\zeta)\mu_{11}^+(\zeta,n)\mu_{12}^+(\zeta,n+1)$$
$$+\omega_2^-(\zeta)\zeta\mu_{12}^-(\zeta,n)\mu_{11}^-(\zeta,n+1)-\omega_2^+(\zeta)\zeta\mu_{12}^+(\zeta,n)\mu_{11}^+(\zeta,n+1)+\alpha(\zeta)(\omega_1^-(\zeta)$$
$$-\omega_2^-(\zeta))\zeta^{-n}\mu_{12}^-(\zeta,n)\mu_{12}^-(\zeta,n+1)+\overline{\alpha}(\zeta)(\omega_1^+(\zeta)-\omega_2^+(\zeta))\zeta^{n+1}\mu_{11}^+(\zeta,n)\mu_{11}^+(\zeta,n+1)$$
$$-m(\zeta)\zeta^{-n}\mu_{12}^-(\zeta,n)\mu_{12}^-(\zeta,n+1)+\overline{m(\zeta)}\zeta^{n+1}\mu_{11}^+(\zeta,n)\mu_{11}^+(\zeta,n+1) \tag{141}$$

with $\zeta=e^{i\theta}$ (remember that $\alpha\equiv\alpha^-$ and $\alpha^+(\zeta)=-\overline{\alpha(\zeta)}$). Note that in computing $T(\lambda,n)$ in (112) the term containing $\Omega(k,t)$ must be written as follows

$$\Lambda^{-1}\mu(n)\frac{\partial\Omega}{\partial k}\Lambda\mu^{-1}(n+1)=\frac{\partial}{\partial k}(\Lambda^{-1}\mu(n)\Omega\Lambda\mu^{-1}(n+1))$$
$$-\Lambda^{-1}\mu(n)[R(n),\Omega]\Lambda\mu^{-1}(n+1) \tag{142}$$

which is a well defined local formulation of a $\bar{\partial}$ -problem for a sectionally holomorphic function.

It is convenient, by using equations (33) and (34), to rewrite (141) in terms of μ_1^+ and μ_2^-

$$\gamma(\theta,n)=p(\zeta)\mu_{11}^+(\zeta,n)\mu_{12}^-(\zeta,n+1)+\overline{p(\zeta)}\zeta\mu_{12}^-(\zeta,n)\mu_{11}^+(\zeta,n+1)$$
$$-m(\zeta)\zeta^{-n}\mu_{12}^-(\zeta,n)\mu_{12}^-(\zeta,n+1)+\overline{m(\zeta)}\zeta^{n+1}\mu_{11}^+(\zeta,n)\mu_{11}^+(\zeta,n+1) \tag{143}$$

which shows explicitly that the evolution equation depends only on the discontinuity of $\Omega(k)$ on the unit circle.

VI. INTEGRABLE DISCRETE INITIAL-BOUNDARY VALUE PROBLEM

By using the tools previously developed we prove now that the nonlinear system (1) is integrable when it is related to the initial boundary value (5). We rewrite hereafter this system in the variable $\zeta=e^{i\theta}$ and with the relation (24) as

$$q_t(n,t)\prod_{i=n+1}^{\infty}(1+|q(i,t)|^2)=\frac{1}{2\pi}\int_{-\pi}^{+\pi}d\theta\, e^{in\theta}(A_1*A_2)(\zeta,n,t), \tag{144}$$

$$A_1(\zeta,n,t)-A_1(\zeta,n-1,t)=\zeta^{-n}q(n,t)A_2(\zeta,n,t), \tag{145}$$

$$A_2(\zeta,n,t)-A_2(\zeta,n-1,t)=-\zeta^n\overline{q(n,t)}A_1(\zeta,n,t), \tag{146}$$

where the interaction term is defined as

$$(A_1*A_2)(\zeta,n,t)=g(\theta,t)A_1(\zeta,n-1,t)\overline{A_2}(\zeta,n,t)+\overline{g(\theta,t)}A_1(\zeta,n,t)\overline{A_2}(\zeta,n-1,t). \tag{147}$$

Theorem: *With the datum of the initial value* $q(n,0)$ *and the following arbitrary boundary values as* $n\to+\infty$

$$A_1(\zeta,n,t)\to I_1(\zeta,t),\qquad A_2(\zeta,n,t)\to I_2(\zeta,t), \tag{148}$$

the above system is solvable by the spectral transform method.

A. Proof of integrability

The proof is performed by showing that the evolution (144) can actually be written under the form (140). This then gives a unique definition of the functions $m(k)$ and $\omega(k)+\overline{\omega(}k)$ for which the two equations (140) and (144) are *identical*. Hence the evolution (109) of the spectral transform $R(k,t)$ is uniquely given via (132) and (133).

The first useful property is that *the following 5 vectors*

$$\begin{pmatrix} A_1(\zeta,n) \\ \zeta^{-n}A_2(\zeta,n) \end{pmatrix}, \qquad \begin{pmatrix} \mu_{11}^{\pm}(\zeta,n) \\ \mu_{21}^{\pm}(\zeta,n) \end{pmatrix}, \qquad \zeta^{-n}\begin{pmatrix} \mu_{12}^{\pm}(\zeta,n) \\ \mu_{22}^{\pm}(\zeta,n) \end{pmatrix}, \tag{149}$$

solve the equation (146). Then, by comparison of their asymptotic behaviors as $n\to+\infty$ given in (148) and in (53)–(52), we get

$$\begin{pmatrix} A_1(\zeta,n) \\ \zeta^{-n}A_2(\zeta,n) \end{pmatrix} = I_1(\zeta)\begin{pmatrix} \mu_{11}^{+}(\zeta,n) \\ \mu_{21}^{+}(\zeta,n) \end{pmatrix} + I_2(\zeta)\zeta^{-n}\begin{pmatrix} \mu_{12}^{-}(\zeta,n) \\ \mu_{22}^{-}(\zeta,n) \end{pmatrix}. \tag{150}$$

Next, to compute the product $(A_1*A_2)(\zeta,n)$ we make use of the Riemann–Hilbert relations

$$\mu_1^-(\zeta,n)-\mu_1^+(\zeta,n)=\alpha^-(\zeta)\zeta^{-n}\mu_2^-(\zeta,n), \tag{151}$$

$$\mu_2^-(\zeta,n)-\mu_2^+(\zeta,n)=-\alpha^+(\zeta)\zeta^{n}\mu_1^+(\zeta,n), \tag{152}$$

and rewrite it in terms only of μ_1^+ and μ_2^-

$$\begin{aligned}\zeta^{n+1}&(A_1*A_2)(\zeta,n+1)\\ &=-[g|I_1|^2-\overline{g|}I_2|^2]\mu_{11}^+(n)\mu_{12}^-(n+1)-[\overline{g|}I_1|^2-g|I_2|^2]\zeta\mu_{12}^-(n)\mu_{11}^+(n+1)\\ &\quad-(g+\overline{g)}\overline{I_1}I_2\zeta^{-n}\mu_{12}^-(n)\mu_{12}^-(n+1)+(g+\overline{g)}I_1\overline{I_2}\zeta^{n+1}\mu_{11}^+(n)\mu_{11}^+(n+1).\end{aligned} \tag{153}$$

Then, thanks to the expression (47), the two equations (140) and (144) are *identical* if and only if

$$p(\zeta,t)=-g(\theta,t)|I_1(\theta,t)|^2+\overline{g(}\theta,t)|I_2(\theta,t)|^2, \tag{154}$$

$$m(\zeta,t)=(g(\theta,t)+\overline{g(}\theta,t))\overline{I_1(}\theta,t)I_2(\theta,t). \tag{155}$$

Finally the theorem is proved and it remains to compute the evolution of the spectral transform.

B. Evolution of the spectral transform

1. Evolution of $\alpha(\zeta,t)$

The time evolution of $R(k,n,t)$ is given by (109) with M and Ω defined in (133) and in (138). Taking into account the structure (81) of $R(k,n,t)$ we have

$$\partial_t\alpha(\zeta,t)=[\omega_1^-(\zeta,t)-\omega_2^-(\zeta,t)]\alpha(\zeta,t)-m(\zeta,t), \tag{156}$$

$$\partial_t k_j=0, \qquad \partial_t C_j(t)=[\omega_1(k_j,t)-\omega_2(k_j,t)]C_j(t), \tag{157}$$

where from (138) and the Sokhotski–Plemelj formula we have

$$\omega_1^-(\zeta,t)-\omega_2^-(\zeta,t)=-\frac{1}{2}p(\zeta,t)-\frac{1}{2}\overline{p(\zeta,t)}+\frac{1}{2\pi i}P\oint_{\mathscr{C}}\frac{d\zeta'}{\zeta'-\zeta}p(\zeta',t)\frac{\zeta}{\zeta'}$$

$$+\frac{1}{2\pi i}P\oint_{\mathscr{C}}\frac{d\zeta'}{\zeta'-\zeta}\overline{p(\zeta',t)}, \tag{158}$$

$$\omega_1(k_j,t)-\omega_2(k_j,t)=\frac{1}{2\pi i}\oint_{\mathscr{C}}\frac{d\zeta'}{\zeta'-k_j}p(\zeta',t)\frac{k_j}{\zeta'}$$

$$+\frac{1}{2\pi i}\oint_{\mathscr{C}}\frac{d\zeta'}{\zeta'-k_j}\overline{p(\zeta',t)}, \tag{159}$$

and the functions $p(\zeta,t)$ and $m(\zeta,t)$ are given in (154) and (155).

As a result the evolution equation of α and C_j can be written

$$\partial_t\alpha=\alpha\frac{g+\overline{g}}{2}(|I_1(\theta,t)|^2-|I_2(\theta,t)|^2)-(g+\overline{g})\overline{I_1}I_2$$

$$-\alpha\frac{1}{2\pi i}P\oint_{\mathscr{C}}\frac{d\zeta'}{\zeta'-\zeta}(g+\overline{g})(|I_1|^2-|I_2|^2)$$

$$+\alpha\frac{1}{2\pi i}\oint_{\mathscr{C}}\frac{d\zeta'}{\zeta'}(g|I_1|^2-\overline{g}|I_2|^2), \tag{160}$$

$$\partial_t C_j(t)=-C_j(t)\frac{1}{2\pi i}P\oint_{\mathscr{C}}\frac{d\zeta'}{\zeta'-k_j}(g+\overline{g})(|I_1|^2-|I_2|^2)$$

$$+C_j(t)\frac{1}{2\pi i}\oint_{\mathscr{C}}\frac{d\zeta'}{\zeta'}(g|I_1|^2-\overline{g}|I_2|^2). \tag{161}$$

2. Evolution of $\beta(\zeta,t)$

The definition (58) allows us to obtain readily

$$\frac{\hat{\beta}_t^+}{\hat{\beta}^+}-\frac{\beta_t}{\beta}=-\frac{(|\alpha|^2)_t}{1+|\alpha|^2}, \tag{162}$$

which actually can be understood as a Riemann–Hilbert problem on the unit circle. Its solution reads

$$|k|>1:\quad \frac{\hat{\beta}_t^+}{\hat{\beta}^+}=\frac{\partial}{\partial t}\left(\frac{|\beta|^2}{1+|\alpha|^2}\right)\frac{1+|\alpha|^2}{|\beta|^2}-\frac{1}{2\pi i}\oint_{\mathscr{C}}\frac{d\zeta'}{\zeta'-k}\frac{(|\alpha(\zeta')|^2)_t}{1+|\alpha(\zeta')|^2}, \tag{163}$$

$$|k|<1:\quad \frac{\beta_t}{\beta}=-\frac{1}{2\pi i}\oint_{\mathscr{C}}\frac{d\zeta'}{\zeta'-k}\frac{k}{\zeta'}\frac{(|\alpha(\zeta')|^2)_t}{1+|\alpha(\zeta')|^2}. \tag{164}$$

Hence, writing the above equation for $k=\zeta(1-0)$, we get the evolution (14).

C. Evolution of the spectral transform from the Lax pair

For completeness, we rederive hereafter the preceding formula (evolution of α and β, in the absence of bound states for simplicity), by using the traditional approach for which the starting tool is the Lax pair (25), (121). The method consists simply in evaluating the asymptotic boundary values as $n\to\pm\infty$ on the auxiliary spectral problem (121), in which (forget for a while the (n,t)-dependence)

$$V(k)=\frac{1}{2i\pi}\iint_{\mathscr{D}}\frac{d\lambda\wedge d\bar{\lambda}}{\lambda-k}\mu(\lambda)\left(M(\lambda)-\frac{\partial\Omega(\lambda)}{\partial\bar{\lambda}}\right)\mu^{-1}(\lambda)\begin{pmatrix}k/\lambda & 0\\ 0 & 1\end{pmatrix}. \tag{165}$$

By using the identity (142), the equation (121) can be more conveniently written as

$$\mu_t(k,n,t)=X(k,n,t)\mu(k,n,t), \tag{166}$$

where

$$X(k)=\frac{1}{2i\pi}\iint_{\mathscr{D}}\frac{d\lambda\wedge d\bar{\lambda}}{\lambda-k}\mu(\lambda,n,t)(M(\lambda)+[R(\lambda),\Omega(\lambda)])\mu^{-1}(\lambda)\begin{pmatrix}k/\lambda & 0\\ 0 & 1\end{pmatrix}. \tag{167}$$

By inserting in the above equation the explicit forms of $R(k,n,t)$ given in (81) with (66) and no bound states, of $\Omega(k,t)$ given in (138), and of $M(k,n,t)$ given in (131) with (133), we get finally

$$X(k,n,t)=\frac{1}{2i\pi}\oint\frac{d\zeta'}{\zeta'-k}\frac{1}{f(n)}\chi(\zeta',n,t)\begin{pmatrix}k/\zeta' & 0\\ 0 & 1\end{pmatrix}, \tag{168}$$

with the following definition

$$\chi(\zeta)=\zeta^n[\overline{m}+(\omega_1^+-\omega_2^+)\overline{\alpha}]\begin{pmatrix}-\mu_{11}^+\mu_{21}^+ & (\mu_{11}^+)^2\\ -(\mu_{21}^+)^2 & \mu_{11}^+\mu_{21}^+\end{pmatrix}$$

$$+\zeta^{-n}[m-(\omega_1^--\omega_2^-)\alpha]\begin{pmatrix}\mu_{12}^-\mu_{22}^- & -(\mu_{12}^-)^2\\ (\mu_{22}^-)^2 & -\mu_{12}^-\mu_{22}^-\end{pmatrix}. \tag{169}$$

The main tool is now the asymptotic boundary behaviors (75) and (76) of $\mu^{\pm}$ which allows us to obtain, by taking the limit as $n\to+\infty$ of $\zeta^n\partial_t\mu_{21}^-(\zeta,n,t)$, the relations

$$\alpha_t(k)=-\frac{1}{2}[m-(\omega_1^--\omega_2^-)\alpha](k)+\lim_{n\to\infty}\frac{1}{2\pi i}P\oint\frac{d\zeta}{\zeta-k}\left(\frac{k}{\zeta}\right)^{n+1}[m-(\omega_1^--\omega_2^-)\alpha](\zeta),$$

$$0=-\frac{1}{2}[\overline{m}+(\omega_1^+-\omega_2^+)\overline{\alpha}](k)+\lim_{n\to\infty}\frac{1}{2\pi i}P\oint\frac{d\zeta}{\zeta-k}\left(\frac{\zeta}{k}\right)^{n}[\overline{m}+(\omega_1^+-\omega_2^+)\overline{\alpha}](\zeta).$$

Consequently, with the formula (see Appendix)

$$\lim_{n\to\infty}\frac{1}{2\pi i}P\oint\frac{d\zeta}{\zeta-k}\left(\frac{k}{\zeta}\right)^{n}\Phi(\zeta)=-\frac{1}{2}\Phi(k),\qquad |k|=1, \tag{170}$$

the preceding relations result precisely in the required evolution (156).

In the same way, by taking the limit as $n\to-\infty$ of $\partial_t\mu_{11}^-(\zeta,n,t)$, we readily obtain the required evolution (14) of the transmission coefficient $\beta(\zeta,t)$ (note that there, one should use also the unitarity relation (78)).

D. Time evolution of $f(n)$

It could be useful to have also explicitly the time evolution of the quantity $f(n)$. From (50) we have

$$f_t(n)=f(n)\ \mathrm{tr}\{\mu_t(k,n)\mu^{-1}(k,n)\} \tag{171}$$

and then using the auxiliary spectral problem (171)

$$f_t(n)=f(n)\ \mathrm{tr}\{X(k,n)\}. \tag{172}$$

From the expression (173) we obtain that the trace of $X(k,n)$ is k-independent and reads

$$\mathrm{tr}\{X(k,n)\}=\frac{1}{f(n)}\frac{1}{2i\pi}\oint\frac{d\zeta}{\zeta}\{\zeta^n\overline{m}\mu_{11}^+\mu_{21}^+-\zeta^{-n}m\mu_{12}^-\mu_{22}^-+(p+\overline{p})\mu_{12}^-\mu_{21}^+ -(\omega_1^+-\omega_2^+)\mu_{12}^+\mu_{21}^++(\omega_1^--\omega_2^-)\mu_{12}^-\mu_{21}^-. \tag{173}$$

Due to the analyticity of the function

$$\frac{1}{k}(\omega_1(k)-\omega_2(k))\mu_{12}(k)\mu_{21}(k)$$

inside and outside of the circle the last two terms in the r.h.s. vanish and we obtain for the evolution equation of $f(n)$

$$f_t(n)=\int_{-\pi}^{+\pi}d\theta\{\zeta^n\overline{m}\mu_{11}^+\mu_{21}^+-\zeta^{-n}m\mu_{12}^-\mu_{22}^-+(p+\overline{p})\mu_{12}^-\mu_{21}^+\}. \tag{174}$$

This result can also be expressed in terms of the physical quantities A_j and I_j by inverting (150) to get on the unit circle

$$\mu_{11}^+=\overline{\mu}_{22}^-=\frac{A_1\overline{I_1}+\overline{A_2}I_2}{|I_1|^2+|I_1|^2},$$

$$\mu_{21}^+=-\overline{\mu}_{12}^-=-\zeta^{-n}\frac{\overline{A_1}I_2-A_2\overline{I_1}}{|I_1|^2+|I_1|^2}$$

and then by inserting these formulae and those for $p+\overline{p}$ and m in (154) and (155) into (179). We obtain finally

$$f_t(n)=\frac{1}{2\pi}\int_{-\pi}^{\pi}d\vartheta(g+\overline{g})\frac{|I_1|^2|A_2|^2-|I_2|^2|A_1|^2}{|I_1|^2+|I_2|^2}. \tag{175}$$

Note that $f(n)$ is conserved if g is pure imaginary.

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APPENDIX: MATHEMATICAL TOOLS

1. Basic distributions

The distributions $\delta^{\pm}(\lambda,1)$ and $\delta(\lambda,1)$ have support on the circle $\mathscr{C}$ of radius 1 in the complex λ-plane and are defined by the following formulae

$$\iint_{\mathscr{D}} d\lambda\wedge d\bar{\lambda}\,\delta^{\pm}(\lambda,1)f(\lambda)=\oint_{\mathscr{C}} d\zeta\; f((1\mp 0)\zeta), \tag{A1}$$

$$\iint_{\mathscr{D}} d\lambda\wedge d\bar{\lambda}\,\delta(\lambda,1)f(\lambda)=\oint_{\mathscr{C}} d\zeta\; f(\zeta), \tag{A2}$$

or, equivalently, by

$$\iint_{\mathscr{D}} d\lambda\wedge d\bar{\lambda}\,\delta^{\pm}(\lambda,1)f(\lambda)=i\int_{-\pi}^{\pi} d\theta\; e^{i\theta}f((1\mp 0)e^{i\theta}), \tag{A3}$$

$$\iint_{\mathscr{D}} d\lambda\wedge d\bar{\lambda}\,\delta(\lambda,1)f(\lambda)=i\int_{-\pi}^{\pi} d\theta\; e^{i\theta}f(e^{i\theta}). \tag{A4}$$

Note that the distributions $\delta^{\pm}(\lambda,1)$ can operate on functions which have defined left or right limit on $\mathscr{C}$, while the distribution $\delta(\lambda,1)$ can operate on functions continuous on $\mathscr{C}$ or with support on $\mathscr{C}$.

By complex conjugation of the equation (A3) and by the change of variable $\theta\to-\theta$, we obtain

$$\iint_{\mathscr{D}} d\lambda\wedge d\bar{\lambda}\;\overline{\delta^{\pm}(\lambda,1)}f(\lambda)=i\int_{-\pi}^{\pi} d\theta\; e^{i\theta}f((1\mp 0)e^{-i\theta}). \tag{A5}$$

Next, by means of the change of variable $\lambda\to 1/\lambda$ (remember that the domain $\mathscr{D}$ does not contain the point $\lambda=0$) and $\theta\to-\theta$, we obtain

$$\iint_{\mathscr{D}} d\lambda\wedge d\bar{\lambda}\,\delta^{\pm}\left(\frac{1}{\lambda},1\right)f(\lambda)=i\int_{-\pi}^{\pi} d\theta\; e^{i\theta}f((1\pm 0)e^{-i\theta}), \tag{A6}$$

and consequently

$$\delta^{\pm}\left(\frac{1}{\lambda},1\right)=\overline{\delta^{\mp}(\lambda,1)}. \tag{A7}$$

Now, through the change of variable $\lambda\to\bar{\lambda}$, we obtain

$$\iint_{\mathscr{D}} d\lambda\wedge d\bar{\lambda}\,\delta^{\pm}(\bar{\lambda},1)f(\lambda)=i\int_{-\pi}^{\pi} d\theta\; e^{i\theta}f((1\mp 0)e^{-i\theta}) \tag{A8}$$

which implies the second symmetry property

$$\delta^{\pm}(\bar{\lambda},1)=\overline{\delta^{\pm}(\lambda,1)}. \tag{A9}$$

These two relation naturally leads to

$$\delta^+(\lambda,1)=\delta^-\left(\frac{1}{\lambda},1\right). \tag{A10}$$

Similar symmetry properties can be obtained for $\delta(\lambda,1)$.

2. The generalized $\bar{\partial}$-formula

Let $F^+ \in C^1(\overline{D^+})$ where D^+ is the open disk of radius 1 centered in the origin and $F^- \in C^1(\mathscr{C}D^+)$, let F^+ and F^- satisfy the Hölder condition on the circle $\mathscr{C}$ of radius 1 and let F^- vanish at large z. Then by noting $F(z)$ the function defined as $F^+(z)$ for $z \in D^+$ and as $F^-(z)$ for $z \in D^- \equiv \mathscr{C}\overline{D^+}$ we have

$$F(z)=\frac{1}{2\pi i}\oint_{\mathscr{C}}\frac{F^+(\zeta)-F^-(\zeta)}{\zeta-z}d\zeta+\frac{1}{2\pi i}\iint_{D^+}\frac{\partial F/\partial\bar{\lambda}}{\lambda-z}d\lambda\wedge d\bar{\lambda}+\frac{1}{2\pi i}\iint_{D^-}\frac{\partial F/\partial\bar{\lambda}}{\lambda-z}d\lambda\wedge d\bar{\lambda}, \tag{A11}$$

where the circle $\mathscr{C}$ is anticlockwise oriented.

If we define the $\bar{\partial}$–derivative of a function $F(z)$ discontinuous on $\mathscr{C}$ as follows

$$\frac{\partial F}{\partial\bar{z}}=(F^+(\zeta)-F^-(\zeta))\,\delta(z,1)+\phi_{D^+}(z)\frac{\partial F}{\partial\bar{z}}+\phi_{D^-}(z)\frac{\partial F}{\partial\bar{z}} \qquad \zeta=\frac{z}{|z|}, \tag{A12}$$

where $\phi_A(z)=1$ for $z \in A$ and $\phi_A(z)=0$ for $z \notin A$ the generalized $\bar{\partial}$–formula (191) can be rewritten as

$$F(z)=\frac{1}{2\pi i}\iint_{\overline{D^+\cup D^-}}\frac{\partial F/\partial\bar{\lambda}}{\lambda-z}d\lambda\wedge d\bar{\lambda}. \tag{A13}$$

Formula (A1) can be considered as the local formulation of the generalized Cauchy–Green formula (A1).

Subtracting formula (A1) at $z=a$ we obtain

$$\begin{aligned}F(z)=F(a)&+\frac{1}{2\pi i}\int_{\mathscr{C}}\frac{F^+(\zeta)-F^-(\zeta)}{\zeta-z}\left(\frac{z-a}{\zeta-a}\right)d\zeta+\frac{1}{2\pi i}\iint_{D^+_{a,0}}\frac{\partial F/\partial\bar{\lambda}}{\lambda-z}\left(\frac{z-a}{\lambda-a}\right)d\lambda\wedge d\bar{\lambda}\\&+\frac{1}{2\pi i}\iint_{D^-}\frac{\partial F/\partial\bar{\lambda}}{\lambda-z}\left(\frac{z-a}{\lambda-a}\right)d\lambda\wedge d\bar{\lambda}\end{aligned} \tag{A14}$$

if $a \in D^+$ and an analogous formula if $a \in D^-$. The second integral on the right hand side is obtained first by computing it on the set $D_{a,\epsilon}=\{\lambda:\lambda \in D,|\lambda-a|>\epsilon\}$ and then by taking the limit $\epsilon\to 0$. Note that the formula remains valid also if $F(z)$ is going to a constant different from 0 for $z\to\infty$.

If for $z\to\infty$ $F(z)\to F(\infty)$ we can apply (A1) to $F(z)-F(\infty)$ getting

$$\begin{aligned}F(z)=F(\infty)&+\frac{1}{2\pi i}\int_{\mathscr{C}}\frac{F^+(\zeta)-F^-(\zeta)}{\zeta-z}d\zeta+\frac{1}{2\pi i}\iint_{D^+}\frac{\partial F/\partial\bar{\lambda}}{\lambda-z}d\lambda\wedge d\bar{\lambda}\\&+\frac{1}{2\pi i}\iint_{D^-}\frac{\partial F/\partial\bar{\lambda}}{\lambda-z}d\lambda\wedge d\bar{\lambda}.\end{aligned} \tag{A15}$$

Finally let us note that the Sokhotski-Plemelj formula on the circle reads

$$\oint_{\mathscr{C}} \frac{d\zeta'}{\zeta'-(1\mp 0)\zeta} f(\zeta') = \pm i\pi f(\zeta) + P \oint_{\mathscr{C}} \frac{d\zeta'}{\zeta'-\zeta} f(\zeta'), \qquad |\zeta| = 1, \tag{A16}$$

where $P\oint$ denote the Cauchy principal value integral.

3. Limits of integrals

Let us prove that

$$\lim_{n\to\infty} \frac{1}{2\pi i} P \oint \frac{d\zeta}{\zeta-k} \left(\frac{k}{\zeta}\right)^n \Phi(\zeta) = -\frac{1}{2}\Phi(k), \qquad |k| = 1. \tag{A17}$$

Under the following successive changes of variables

$$\zeta = e^{i\vartheta}, \qquad k = e^{i\varphi}, \qquad \alpha = \vartheta - \varphi, \qquad x = n\alpha, \tag{A18}$$

we derive

$$\frac{1}{2\pi i} P \oint \frac{d\zeta}{\zeta-k} \left(\frac{k}{\zeta}\right)^n \Phi(\zeta) = \frac{1}{4\pi i} P \int_{-(\pi+\varphi)n}^{(\pi-\varphi)n} dx \frac{e^{-ix}}{n \sin(x/2n)} e^{ix/2n} \Phi(e^{i(x/n+\varphi)}) \tag{A19}$$

and taking the limit, for $-\pi < \varphi < \pi$,

$$\begin{aligned} \lim_{n\to\infty} \frac{1}{2\pi i} P \oint \frac{d\zeta}{\zeta-k} \left(\frac{k}{\zeta}\right)^n \Phi(\zeta) &= \frac{1}{2\pi i} P \int_{-\infty}^{\infty} dx \frac{e^{-ix}}{x} \Phi(e^{i\varphi}) \\ &= -\frac{1}{2\pi} \int_{-\infty}^{\infty} dx \frac{\sin x}{x} \Phi(e^{i\varphi}) = -\frac{1}{2}\Phi(e^{i\varphi}). \end{aligned}$$

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Multi-Hamiltonian structures for a class of degenerate completely integrable systems

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In this paper, a class of degenerate (i.e., associated to a degenerate Poisson structure) completely integrable systems is studied which generalizes the so-called odd and even master systems introduced and studied by Mumford and by Vanhaecke. It is shown that all these completely integrable systems, called the generalized master systems, admit a multi-Hamiltonian formulation, and a systematic construction of this multi-Hamiltonian structure is described. © *1996 American Institute of Physics.* [S0022-2488(96)01406-5]

I. INTRODUCTION

A dynamical system is said to be *bi-Hamiltonian* if it can be written in Hamiltonian form with respect to two different Poisson structures $\{\cdot,\cdot\}_1$ and $\{\cdot,\cdot\}_2$, i.e.,

$$\dot{x}=\{x,H_1\}_1=\{x,H_2\}_2,$$

for some functions $H_1,H_2\in C^\infty(M)$, under the additional assumption that the Poisson brackets $\{\cdot,\cdot\}_1$ and $\{\cdot,\cdot\}_2$ are *compatible*, i.e., their sum is also a Poisson bracket. The existence of bi-Hamiltonian structures was first observed by Magri[1] in the case of the Korteweg–de Vries equation, and it was remarked by the same author (see, e.g., Ref. 2) that the existence of a bi-Hamiltonian structure for a mechanical system is closely related to the complete integrability of the system. In view of this remark, the study of bi-Hamiltonian structures for finite-dimensional Hamiltonian systems has received considerable interest in the recent literature. It turns out that, in contrast to the nondegenerate case (where it was shown in Refs. 3–5 that there exists only a limited number of completely integrable bi-Hamiltonian systems), many degenerate completely integrable systems admit a bi-Hamiltonian structure (see, e.g., Ref. 6), and a number of techniques for constructing these structures (e.g., R-matrices,[7] master symmetries,[8] and reductions of infinite-dimensional systems[9,10]) were discovered.

In Ref. 11, Mumford introduced a completely integrable system on the space $\mathbf{R}^{3g+1}$, whose (complexified) invariant manifolds can be completed (by adjoining a divisor) into the Jacobian of a hyperelliptic curve of genus g, given by an equation

$$y^2=f(x),\quad f(x)=x^{2g+1}+h_1x^{2g}+\cdots+h_{2g+1}, \tag{1}$$

where h_i are the values of certain constants of motion H_i of the completely integrable system. The construction of these completely integrable systems was later adapted to the case where

$$f(x)=x^{2g+2}+h_1x^{2g}+\cdots+h_{2g+1} \tag{2}$$

by Vanhaecke,[6] who also made a detailed study of the systems associated to (1) and (2), which he called the (*odd* and *even*) *master systems*, and who constructed a multi-Hamiltonian formulation for these systems (in the two-dimensional case).

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In Ref. 12, Vanhaecke constructs, starting from an arbitrary nonzero polynomial $\varphi(x,y)\in\mathbf{R}[x,y]$, a Poisson bracket $\{\cdot,\cdot\}^{\varphi}$ on $\mathbf{R}^{2d}$. Taking the product of this Poisson manifold with a trivial Poisson manifold $(\mathbf{R}^{k+1},\{\cdot,\cdot\}_0)$ (with standard coordinates $c_0,\ldots,c_k$), one obtains a Poisson bracket $\{\cdot,\cdot\}_0^{\varphi}$ on $\mathbf{R}^{2d+k+1}$ which has the functions $c_0,\ldots,c_k$ as Casimir functions. Considering a deformation family of polynomials of the form

$$F(x,y,c)=F(x,y)-x^d c(x),\quad c(x)=c_0x^k+\cdots+c_k,$$

where $F(x,y)$ is a polynomial depending explicitly on y, it turns out that the coefficients $H_1,\ldots,H_d$ of the polynomial

$$H(\lambda)=H_1\lambda^{d-1}+\cdots+H_d=(F(\lambda,v(\lambda))-\lambda^d c(\lambda))\bmod u(\lambda)$$

are in involution with respect to the Poisson bracket $\{\cdot,\cdot\}_0^{\varphi}$ (for every polynomial φ), and hence determine a completely integrable system on the Poisson manifold $(\mathbf{R}^{2d+k+1},\{\cdot,\cdot\}_0^{\varphi})$.

In the special case where $\varphi=1$, $d=k=g$, and

$$F(x,y)=y^2+x^{2g+1}\quad\text{or}\quad F(x,y)=y^2+x^{2g+2},$$

these completely integrable systems turn out to be the odd and even master systems, and all systems $(\mathbf{R}^{2d+k+1},\{\cdot,\cdot\}_0^{\varphi},H_1)$ constructed above will therefore be called *generalized master systems*.

The aim of this paper is to construct a multi-Hamiltonian formulation for the generalized master systems. To do this, we start by constructing, for each $0<i\leqslant k+1$, a new Poisson bracket $\{\cdot,\cdot\}_i^{x^i\varphi}$. Next, we show that the Hamiltonian vector fields of the generalized master system $(\mathbf{R}^{2d+k+1},\{\cdot,\cdot\}_0^{\varphi},H_1)$ can be written in Hamiltonian form with respect to this new Poisson bracket. Finally, we prove that the Poisson brackets $\{\cdot,\cdot\}_i^{x^i\varphi}$, $i=0,\ldots,k+1$, are compatible.

The paper is organized as follows. In Sec. II, we collect some preliminary material concerning bi-Hamiltonian structures and completely integrable systems, and we fix some notation which will be used in the rest of the paper. In Sec. III, we briefly describe the (two-dimensional) odd master system and its multi-Hamiltonian structure. In Sec. IV we review the results from Ref. 12 and we introduce the generalized master systems, and in Sec. V we describe the multi-Hamiltonian structure for these generalized master systems.

II. PRELIMINARIES

A *Poisson manifold* $(M,\{\cdot,\cdot\})$ is a smooth manifold M, endowed with an antisymmetric $\mathbf{R}$-bilinear mapping

$$\{\cdot,\cdot\}:C^{\infty}(M)\times C^{\infty}(M)\to C^{\infty}(M),$$

called a *Poisson bracket*, which is a derivation in both of its arguments, and which satisfies the *Jacobi identity*

$$\{\{f,g\},h\}+\{\{g,h\},f\}+\{\{h,f\},g\}=0$$

for all $f,g,h\in C^{\infty}(M)$. Two functions $f,g\in C^{\infty}(M)$ are said to *Poisson commute*, or to be *in involution*, if $\{f,g\}=0$, and a function f which Poisson commutes with *all* functions $g\in C^{\infty}(M)$ is called a *Casimir function*. As the Poisson bracket $\{\cdot,\cdot\}$ is a derivation in its arguments, every function $f\in C^{\infty}(M)$ determines a vector field X_f on M, given by

$$X_f(g)=\{g,f\}$$

for all $g \in C^\infty(M)$. If $H \in C^\infty(M)$ generates a nonzero vector field (i.e., H is not a Casimir function), H is said to be a *Hamiltonian*, X_H its *Hamiltonian vector field*, and the triple $(M,\{\cdot,\cdot\},H)$ is called a *Hamiltonian system*.

Let $(M,\{\cdot,\cdot\})$ be a Poisson manifold of dimension n which admits k (independent) Casimir functions (i.e., it is of rank $2d=n-k$). A Hamiltonian system $(M,\{\cdot,\cdot\},H)$ on this Poisson manifold is said to be *completely integrable* if (apart from the Casimir functions $C_1,\ldots,C_k$) it admits d independent first integrals (sometimes called the *Hamiltonians* of the system) $H_1=H,H_2,\ldots,H_d$, which are in involution with respect to the Poisson bracket $\{\cdot,\cdot\}$.

Two Poisson brackets $\{\cdot,\cdot\}_1$ and $\{\cdot,\cdot\}_2$ on a manifold M are said to be *compatible* if their sum is again a Poisson bracket, and a set of Poisson brackets are said to be compatible if they are pairwise compatible. Finally, a Hamiltonian system $(M,\{\cdot,\cdot\}_1,H_1)$ is said to be *multi-Hamiltonian* if its Hamiltonian vector field can be written in Hamiltonian form with respect to a set of *compatible* Poisson brackets, i.e.,

$$X_{H_1}=\{\cdot,H_1\}_1=\{\cdot,H_2\}_2=\cdots=\{\cdot,H_n\}_n$$

for some functions $H_2,\ldots,H_n \in C^\infty(M)$.

In the rest of this paper, we will use the following notational conventions. Let $u(x)=x^d+u_1x^{d-1}+\cdots+u_d$ be a polynomial of degree d such that $u_d\neq 0$, and let α be an integer. Then any polynomial $P(x)$ can be decomposed, in a unique way, as $P(x)=Q(x)u(x)+x^\alpha R(x)$, where $\deg R(x)<d$, and we will denote

$$Q(x)=\left[\frac{P(x)}{u(x)}\right]_\alpha, \quad x^\alpha R(x)=P(x)\bmod_\alpha u(x).$$

In the case where $\alpha=0$ we will, in analogy with the notation in Ref. 12, denote

$$P(x)\bmod_0 u(x)=P(x)\bmod u(x), \quad \left[\frac{P(x)}{u(x)}\right]_0=\left[\frac{P(x)}{u(x)}\right]_+,$$

and we have the following.

Lemma 1: Let i be an integer, $P(x)$ be an arbitrary polynomial, and $u(x)=x^d+u_1x^{d-1}+\cdots+u_d$ be a polynomial such that $u_d\neq 0$. Then

$$(x^iP(x))\bmod_i u(x)=x^i(P(x)\bmod u(x)).$$

Proof: If $P(x)=u(x)Q(x)+R(x)$, where $\deg R(x)<\deg u(x)$, then

$$x^iP(x)=u(x)x^iQ(x)+x^iR(x),$$

and the result follows immediately.

III. MULTI-HAMILTONIAN FORMULATION FOR THE ODD MASTER SYSTEM

In Ref. 11, Mumford constructs a completely integrable system on the space $\mathbf{R}^{3g+1}$, whose (complexified) invariant manifolds can be completed into the Jacobian of a hyperelliptic curve of genus g. In the case where $g=2$, this completely integrable system is determined by the vector field

$$X=\begin{cases}\dot{u}_1=2v_1,\\ \dot{u}_2=2v_2,\\ \dot{v}_1=w_2-u_2-u_1w_1+u_1^2,\\ \dot{v}_2=w_3-w_1u_2+u_1u_2,\\ \dot{w}_1=-2v_1,\\ \dot{w}_2=-2v_2-2v_1w_1+2v_1u_1,\\ \dot{w}_3=2u_1v_2-2v_2w_1,\end{cases} \tag{3}$$

and a straightforward computation yields that the functions

$$H_1=-u_1-w_1,\quad H_2=-u_2-u_1w_1-w_2,$$

$$H_3=v_1^2-u_2w_1-u_1w_2-w_3,\quad H_4=2v_1v_2-u_2w_2-u_1w_3,\quad H_5=v_2^2-u_2w_3,$$

are first integrals of this dynamical system.

In Ref. 6 Vanhaecke shows that this system admits a multi-Hamiltonian structure, which is constructed as follows. The Poisson structure $\{\cdot,\cdot\}_1$, given with respect to the coordinates (u,v,w) by

$$\begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 & 0\\ 0 & 0 & 1 & u_1 & 0 & 0 & 2v_1\\ 0 & -1 & 0 & 0 & 0 & 1 & w_1-u_1\\ -1 & -u_1 & 0 & 0 & 1 & w_1 & w_2-u_2\\ 0 & 0 & 0 & -1 & 0 & 0 & 0\\ 0 & 0 & -1 & -w_1 & 0 & 0 & -2v_1\\ 0 & -2v_1 & u_1-w_1 & u_2-w_2 & 0 & 2v_1 & 0 \end{pmatrix},$$

has the functions H_1, H_2, and H_3 as Casimir functions, and $X=\{\cdot,H_4\}_1$, showing that the system is Hamiltonian with respect to the Poisson structure $\{\cdot,\cdot\}_1$. Further, the Poisson bracket $\{\cdot,\cdot\}_2$, given by

$$\begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & -u_2 & 0 & 0 & -2v_2\\ -1 & 0 & 0 & 0 & 1 & w_1-u_1 & 0\\ 0 & u_2 & 0 & 0 & 0 & -u_2 & -w_3\\ 0 & 0 & -1 & 0 & 0 & 0 & 0\\ 0 & 0 & u_1-w_1 & u_2 & 0 & 0 & 2v_2\\ 0 & 2v_2 & 0 & w_3 & 0 & -2v_2 & 0 \end{pmatrix},$$

has the functions H_1, H_2, and H_5 as Casimir functions, and $X=\{\cdot,H_3\}_2$, showing the Hamiltonian form of (3) with respect to this second bracket. A similar computation yields that the Poisson bracket $\{\cdot,\cdot\}_3$, given by

$$\begin{pmatrix} 0 & 0 & -u_1 & -u_2 & 0 & -2v_1 & -2v_2 \\ 0 & 0 & -u_2 & 0 & 0 & -2v_2 & 0 \\ u_1 & u_2 & 0 & 0 & -u_1 & -w_2 & -w_3 \\ u_2 & 0 & 0 & 0 & -u_2 & -w_3 & 0 \\ 0 & 0 & u_1 & u_2 & 0 & 2v_1 & 2v_2 \\ 2v_1 & 2v_2 & w_2 & w_3 & -2v_1 & 0 & 0 \\ 2v_2 & 0 & w_3 & 0 & -2v_2 & 0 & 0 \end{pmatrix},$$

has H_1, H_4, and H_5 as Casimir functions and that (3) can be written in Hamiltonian form with respect to this new bracket (with Hamiltonian H_2), and that the Poisson bracket $\{\cdot,\cdot\}_4$, given by

$$\begin{pmatrix} A & B \\ -{}^tB & C \end{pmatrix},$$

where

$$A=\begin{pmatrix} 0 & 0 & u_1^2-u_2 & u_1u_2 \\ 0 & 0 & u_1u_2 & u_2^2 \\ -u_1^2+u_2 & -u_1u_2 & 0 & 0 \\ -u_1u_2 & -u_2^2 & 0 & 0 \end{pmatrix}, \quad B=\begin{pmatrix} -2v_1 & 2u_1v_1-2v_2 & 2v_2u_1 \\ -2v_2 & 2u_2v_1 & 2v_2u_2 \\ -w_2+w_1u_1 & -w_3+u_1w_2 & u_1w_3 \\ -w_3+w_1u_2 & u_2w_2 & u_2w_3 \end{pmatrix},$$

and

$$C=\begin{pmatrix} 0 & -2v_1w_1 & -2v_2w_1 \\ 2v_1w_1 & 0 & 2v_1w_3-2v_2w_2 \\ 2v_2w_1 & 2v_2w_2-2v_1w_3 & 0 \end{pmatrix},$$

has H_3, H_4, and H_5 as Casimir functions, while the vector field (3) can be written in Hamiltonian form with respect to this bracket (with Hamiltonian H_1). Finally, it was shown in Ref. 6 that the Poisson brackets introduced in this section are compatible, proving that the odd master system is multi-Hamiltonian.

IV. GENERALIZED MASTER SYSTEMS

It was shown in Ref. 12 that one can associate, to an arbitrary (nonzero) polynomial $\varphi(x,y)$, a Poisson bracket $\{\cdot,\cdot\}^{\varphi}$ on the space $\mathbf{R}^{2d}$ and that, moreover, every polynomial $F(x,y)$ (depending explicitly on y) determines a completely integrable system on the Poisson manifold $(\mathbf{R}^{2d},\{\cdot,\cdot\}^{\varphi})$ (for any φ). We start this section by reviewing this construction. To this purpose, we consider the space $\mathbf{R}^{2d}$ as the space of pairs of polynomials

$$u(\lambda)=\lambda^d+u_1\lambda^{d-1}+\cdots+u_d,$$

$$v(\lambda)=v_1\lambda^{d-1}+\cdots+v_d,$$

i.e., the coefficients of the polynomials u,v serve as coordinates on $\mathbf{R}^{2d}$, and we write, e.g.,

$$\{u(\lambda),v_j\}=\sum_{i=1}^{d}\{u_i,v_j\}\lambda^{d-i}.$$

The following result gives explicit expressions for a family of Poisson brackets, indexed by the space of (nonzero) polynomials in two variables:

Proposition 2: Let $\varphi(x,y)$ be a nonzero polynomial in $\mathbf{R}[x,\ y]$. Then the bracket $\{\cdot,\cdot\}^{\varphi}$, given in terms of the coordinates u_i, v_i by

$$\{u_i,u_j\}^{\varphi}=\{v_i,v_j\}^{\varphi}=0,$$

$$\{u(\lambda),v_j\}^{\varphi}=\{u_j,v(\lambda)\}^{\varphi}=\varphi(\lambda,v(\lambda))\left[\frac{u(\lambda)}{\lambda^{d+1-j}}\right]_{+} \bmod u(\lambda), \tag{4}$$

$i,j=1,\ldots,d$, defines a (polynomial) Poisson structure on the space $\mathbf{R}^{2d}$. Moreover, all these Poisson brackets $\{\cdot,\cdot\}^{\varphi}$ are compatible.

The next step is the construction, for every Poisson bracket given by (4), of a collection of completely integrable systems on $\mathbf{R}^{2d}$. This is the purpose of the following proposition.

Proposition 3: Let $F(x,y)\in\mathbf{R}[x,\ y]\backslash\mathbf{R}[x]$. Then the coefficients $H_1,\ldots,H_d$ of the polynomial

$$H(\lambda)=H_1\lambda^{d-1}+\cdots+H_d=F(\lambda,v(\lambda)) \bmod u(\lambda)$$

define, for any nonzero polynomial $\varphi(x,y)$, a completely integrable system on the Poisson manifold $(\mathbf{R}^{2d},\{\cdot,\cdot\}^{\varphi})$.

Next, we consider the space $\mathbf{R}^{k+1}$ with standard coordinates $(c_0,\ldots,c_k)$, and we define a (trivial) Poisson bracket $\{\cdot,\cdot\}_0$ on this space by putting $\{f,g\}_0=0$ for all $f,g\in C^{\infty}(\mathbf{R}^{k+1})$. Considering the space $\mathbf{R}^{2d+k+1}$ as the product of the Poisson manifolds $(\mathbf{R}^{2d},\{\cdot,\cdot\}^{\varphi})$ and $(\mathbf{R}^{k+1},\{\cdot,\cdot\}_0)$, we obtain a (product) Poisson structure $\{\cdot,\cdot\}_0^{\varphi}$ on $\mathbf{R}^{2d+k+1}$, which has the coordinate functions $c_0,\ldots,c_k$ as Casimir functions. Denoting by $F(x,y,c_0,\ldots,c_k)$ a deformation family of polynomials (i.e., a family of polynomials depending on the parameters $c_0,\ldots,c_k$), it is easily seen that Proposition 3 immediately implies the following.

Proposition 4: The coefficients $H_1,\ldots,H_d$ of the polynomial

$$H(\lambda)=F(\lambda,v(\lambda),c_0,\ldots,c_k) \bmod u(\lambda)$$

are in involution with respect to the Poisson bracket $\{\cdot,\cdot\}_0^{\varphi}$, and hence determine a completely integrable Hamiltonian system $(\mathbf{R}^{2d+k+1},\{\cdot,\cdot\}_0^{\varphi},H_1)$, on the degenerate Poisson manifold $(\mathbf{R}^{2d+k+1},\{\cdot,\cdot\}_0^{\varphi})$.

The explicit expressions for the Hamiltonian vector fields of this system are given by the following.

Proposition 5: The Hamiltonian vector fields $X_{H_i}=\{\ \cdot\ ,H_i\}_0^{\varphi}, i=1,\ldots,d$, of the completely integrable system $(\mathbf{R}^{2d+k+1},\{\cdot,\cdot\}_0^{\varphi},H_1)$, are given by (the coefficients in μ^{d-i} of)

$$X_{H(\mu)}u_a=\frac{\partial F}{\partial y}(\mu,v(\mu),c)\{u_a,v(\mu)\}^{\varphi} \bmod u(\mu),$$

$$X_{H(\mu)}v_a=\left[\frac{F(\mu,v(\mu),c)}{u(\mu)}\right]_{+}\{u_a,v(\mu)\}^{\varphi} \bmod u(\mu),$$

$$X_{H(\mu)}c_b=0, \tag{5}$$

for all $a=1,\ldots,d$, and $b=0,\ldots,k$.

Remark 1: Putting $d=k=2$ and $\varphi(x,y)=1$, and letting $F(x,y,c)$ denote the special deformation family

$$F(x,y,c)=y^2+x^5-x^2c(x),\quad c(x)=c_0x^2+c_1x+c_2,$$

the construction described in this section yields a completely integrable system whose Hamiltonian vector field $\{\cdot,H_1\}_0^\varphi$ is given by

$$\dot{u}_1=2v_1, \quad \dot{u}_2=2v_2, \quad \dot{v}_1=2c_0u_1-c_1+3u_1^2-2u_2,$$

$$\dot{v}_2=c_0(2u_2-u_1^2)+c_1u_1-c_2-u_1^3+4u_1u_2+v_1^2,$$

$$\dot{c}_1=0, \quad \dot{c}_2=0, \quad \dot{c}_3=0.$$

Defining the functions (w_1,w_2,w_3) by

$$\lambda^3+w_1\lambda^2+w_2\lambda+w_3=\left[\frac{F(\lambda,v(\lambda))-\lambda^2c(\lambda)}{u(\lambda)}\right]_+,$$

we see that these differential equations determine the odd master system (3) and that, moreover, the Poisson structure $\{\cdot,\cdot\}_0^1$ and the invariants c_0,c_1,c_2,H_1,H_2 are exactly the Poisson structure $\{\cdot,\cdot\}_1$ and the invariants $H_1,\ldots,H_5$ described in Sec. III. In what follows, the completely integrable systems associated to a special deformation family of polynomials of the form

$$F(x,y,c)=F(x,y)-x^dc(x),$$

will therefore be called *generalized master systems.*

V. MULTI-HAMILTONIAN FORMULATION FOR THE GENERALIZED MASTER SYSTEMS

The aim of this section is to construct a multi-Hamiltonian formulation for the generalized master systems $(\mathbf{R}^{2d+k+1},\{\cdot,\cdot\}_0^\varphi,H_1)$ introduced in Sec. IV. To this purpose, let φ be a nonzero polynomial, $F(x,y,c)=F(x,y)-x^dc(x)$ be a deformation family of polynomials as above, and denote by

$$G(\lambda)=\lambda^dc(\lambda)+H(\lambda)=c_0\lambda^{d+k}+\cdots+c_k\lambda^d+H_1\lambda^{d-1}+\cdots+H_d$$

the polynomial whose coefficients are given by the Casimir functions of the Poisson bracket $\{\cdot,\cdot\}_0^\varphi$ and the first integrals $H_1,\ldots,H_d$ of the generalized master system $(\mathbf{R}^{2d+k+1},\{\cdot,\cdot\}_0^\varphi,H_1)$ associated to φ and F. Choosing any integer $0<i\leqslant k+1$, we can write the polynomial $G(\lambda)$ in the form

$$G(\lambda)=f_0\lambda^{d+k}+\cdots+f_{k-i}\lambda^{d+i}+\lambda^i(g_1\lambda^{d-1}+\cdots+g_d)+f_{k-i+1}\lambda^{i-1}+\cdots+f_k, \tag{6}$$

and, inspired by the choice of the Casimir functions of the different Poisson structures for the odd master system (Sec. III and Remark 1), we now construct a new Poisson bracket $\{\cdot,\cdot\}_i^\varphi$ which has the functions $f_0,\ldots,f_k$ as Casimir functions.

To do this, we start by remarking that

$$G(\lambda)=F(\lambda,v(\lambda))\text{mod } u(\lambda)+u(\lambda)\left[\frac{\lambda^dc(\lambda)}{u(\lambda)}\right]_+. \tag{7}$$

On the other hand, denoting

$$f(\lambda)=f_0\lambda^{d+k}+\cdots+f_{k-i}\lambda^{d+i}+f_{k-i+1}\lambda^{i-1}+\cdots f_k,$$

$$g(\lambda)=g_1\lambda^{d-1}+\cdots+g_d,$$

(6) takes the form

$$G(\lambda)=f(\lambda)+\lambda^i g(\lambda), \tag{8}$$

and comparing (7) and (8) we obtain

$$\left[\frac{\lambda^d c(\lambda)}{u(\lambda)}\right]_+=\left[\frac{f(\lambda)-(F(\lambda,v(\lambda))\text{mod } u(\lambda))}{u(\lambda)}\right]_i,$$

which yields

$$c(\lambda)=\left[\frac{u(\lambda)}{\lambda^d}\left[\frac{f(\lambda)-(F(\lambda,v(\lambda))\text{mod } u(\lambda))}{u(\lambda)}\right]_i\right]_+.$$

The right-hand side of this equation is defined on the subspace $u_d\neq 0$. As a consequence, the mapping

$$\phi:\mathbf{R}^{2d+k+1}\to\mathbf{R}^{2d+k+1}:(u,v,c)\mapsto(u,v,f(u,v,c))$$

is bijective on $M=\mathbf{R}^{2d+k+1}\backslash\{u_d=0\}$, and we can define a new Poisson bracket $\{\cdot,\cdot\}_i^\varphi$ on M by

$$\{f,g\}_i^\varphi=\{f\circ\phi^{-1},g\circ\phi^{-1}\}_0^\varphi\circ\phi.$$

This Poisson bracket has the functions $f_i=c_i\circ\phi$, $i=0,\ldots,k$, as Casimir functions and, moreover, it is easily seen that

$$\{u_i,u_j\}_i^\varphi=\{u_i,u_j\}_0^\varphi,\quad \{u_i,v_j\}_i^\varphi=\{u_i,v_j\}_0^\varphi,\quad \{v_i,v_j\}_i^\varphi=\{v_i,v_j\}_0^\varphi, \tag{9}$$

for all $i,j=1,\ldots,d$.

Our next step is to show that the Hamiltonian vector fields (5) of the generalized master system $(\mathbf{R}^{2d+k+1},\{\cdot,\cdot\}_0^\varphi,H_1)$ can be written in Hamiltonian form with respect to the Poisson brackets $\{\cdot,\cdot\}_i^{x^i\varphi}$, $i=1,\ldots,k+1$, the Hamiltonians being given by the remaining coefficients $g_1,\ldots,g_d$ of the polynomial $G(\lambda)$. To this purpose, we need the following two lemmas.

Lemma 6: The functions $c_0,\ldots,c_k,H_1,\ldots,H_d$ are in involution with respect to the Poisson bracket $\{\cdot,\cdot\}_i^\varphi$.

Proof: For the sake of simplicity, we use matrix notations in the proof of this theorem. In particular, we denote

$$\mathbf{u}=(u_1,\ldots,u_d,v_1,\ldots,v_d),\quad c=(c_0,\ldots,c_k),$$

$$f=(f_0,\ldots,f_k),\quad h=(H_1,\ldots,H_d).$$

For all $A,B\in\{\mathbf{u},f,c,h\}$, we denote by $\{A,B\}$ the matrix whose entries are given by $\{A_i,B_j\}$, and for all $A\in\{f,h\}$ and all $B\in\{\mathbf{u},c\}$, we write the Jacobian matrix of the functions A_i with respect to the coordinates B_j as A_B.

As the functions $c_0,\ldots,c_k$ are Casimir functions of the Poisson bracket $\{\cdot,\cdot\}_0^\varphi$, the Poisson matrix [with respect to the coordinates $(\mathbf{u},c)$] of the bracket $\{\cdot,\cdot\}_0^\varphi$ is of the form

$$\begin{pmatrix} A & 0\\ 0 & 0\end{pmatrix},$$

where A is the (skew-symmetric) $(2d\times 2d)$ matrix given by $\{\mathbf{u},\mathbf{u}\}^\varphi$.

Next, we compute the Poisson matrix of the bracket $\{\cdot,\cdot\}_i^\varphi$ with respect to the coordinates $(\mathbf{u},c)$. It follows immediately from (9) that this Poisson matrix is of the form

$$\begin{pmatrix} A & B \\ -{}^tB & C \end{pmatrix},$$

and taking into account that the functions f_i, $i=0,\ldots,k$, are Casimir functions of the bracket $\{\cdot,\cdot\}_i^\varphi$, we obtain that

$$\begin{pmatrix} A & B \\ -{}^tB & C \end{pmatrix}\begin{pmatrix} f_{\mathbf{u}} \\ f_c \end{pmatrix}=0,$$

which, together with the fact that $\det f_c\neq 0$ on M, yields that

$$B=-Af_{\mathbf{u}}f_c^{-1},\quad C={}^tf_c^{-1\,t}f_{\mathbf{u}}Af_{\mathbf{u}}f_c^{-1}.$$

The functions f_i are first integrals of the generalized master system $(\mathbf{R}^{2d+k+1},\{\cdot,\cdot\}_0^\varphi,H_1)$. Hence, they Poisson commute with respect to the bracket $\{\cdot,\cdot\}_0^\varphi$, implying that

$$\{f,f\}_0^\varphi={}^tf_{\mathbf{u}}Af_{\mathbf{u}}=0,$$

and consequently

$$C=0.$$

Summarizing, the Poisson matrix of the bracket $\{\cdot,\cdot\}_i^\varphi$ is of the form

$$\begin{pmatrix} A & -Af_{\mathbf{u}}f_c^{-1} \\ -{}^tf_c^{-1\,t}f_{\mathbf{u}}A & 0 \end{pmatrix},$$

and we see that

$$\{h,h\}_i^\varphi=({}^th_{\mathbf{u}}\,{}^th_c)\begin{pmatrix} A & -Af_{\mathbf{u}}f_c^{-1} \\ -{}^tf_c^{-1\,t}f_{\mathbf{u}}A & 0 \end{pmatrix}\begin{pmatrix} h_{\mathbf{u}} \\ h_c \end{pmatrix}=\{h,h\}_0^\varphi-{}^th_c\;{}^tf_c^{-1}\{f,h\}_0^\varphi-\{h,f\}_0^\varphi f_c^{-1}h_c=0.$$

Analogous computations yield that $\{c,h\}_i^\varphi=0$ and $\{c,c\}_i^\varphi=0$, which concludes the proof of the lemma.

Lemma 7: Let $\varphi(x,y)$, $F(x,y,c)$, and i be as above. Then

$$\{u_a,v(\mu)\}^{x^i\varphi}\bmod_i u(\mu)=\mu^i\{u_a,v(\mu)\}^\varphi,$$

for all $a=1,\ldots,d$.

Proof: A straightforward computation using (4) and Lemma 1 yields

$$\begin{aligned}\{u_a,v(\mu)\}^{x^i\varphi}\bmod_i u(\mu)&=\left(\mu^i\varphi(\mu,v(\mu))\left[\frac{u(\mu)}{\mu^{d+1-a}}\right]_+\bmod u(\mu)\right)\bmod_i u(\mu)\\&=\left(\mu^i\varphi(\mu,v(\mu))\left[\frac{u(\mu)}{\mu^{d+1-a}}\right]_+\right)\bmod_i u(\mu)\\&=\mu^i\left(\varphi(\mu,v(\mu))\left[\frac{u(\mu)}{\mu^{d+1-a}}\right]_+\bmod u(\mu)\right)=\mu^i\{u_a,v(\mu)\}^\varphi.\end{aligned}$$

We are now ready to prove the following theorem.

Theorem 8: Let $\varphi(x,y)$, $F(x,y,c)$, i, and $G(\lambda)$ be as above. Then we have, for all $a=1,\ldots,d$, that

$$\{\cdot,H_a\}_0^\varphi=\{\cdot,g_a\}_i^{x^i\varphi}.$$

Proof: As the functions $f_0,\ldots,f_n$ are Casimir functions of the Poisson bracket $\{\cdot,\cdot\}_i^{x^i\varphi}$, (6) yields

$$\{\cdot,G(\mu)\}_i^{x^i\varphi}=\mu^i(\{\cdot,g_1\}_i^{x^i\varphi}\mu^{d-1}+\cdots+\{\cdot,g_d\}_i^{x^i\varphi}). \tag{10}$$

On the other hand, we can rewrite $G(\mu)$ as

$$G(\mu)=F(\mu,v(\mu))-u(\mu)\left[\frac{F(\mu,v(\mu))-\mu^d c(\mu)}{u(\mu)}\right]_+,$$

which implies that

$$\{\cdot,G(\mu)\}_i^{x^i\varphi}=\{\cdot,v(\mu)\}_i^{x^i\varphi}\frac{\partial F}{\partial y}(\mu,v(\mu))-\{\cdot,u(\mu)\}_i^{x^i\varphi}\left[\frac{F(\mu,v(\mu))-\mu^d c(\mu)}{u(\mu)}\right]_+$$
$$-u(\mu)\left\{\cdot,\left[\frac{F(\mu,v(\mu))-\mu^d c(\mu)}{u(\mu)}\right]_+\right\}_i^{x^i\varphi}. \tag{11}$$

Comparing (10) and (11), we see that

$$\mu^i(\{\cdot,g_1\}_i^{x^i\varphi}\mu^{d-1}+\cdots+\{\cdot,g_d\}_i^{x^i\varphi})$$
$$=\left(\{\cdot,v(\mu)\}_i^{x^i\varphi}\frac{\partial F}{\partial y}(\mu,v(\mu))-\{\cdot,u(\mu)\}_i^{x^i\varphi}\left[\frac{F(\mu,v(\mu))-\mu^d c(\mu)}{u(\mu)}\right]_+\right)\mathrm{mod}_i\ u(\mu). \tag{12}$$

It follows immediately from (4) and (12) that, for all $b=1,\ldots,d$,

$$\mu^i(\{u_b,g_1\}_i^{x^i\varphi}\mu^{d-1}+\cdots+\{u_b,g_d\}_i^{x^i\varphi})=\left(\{u_b,v(\mu)\}^{x^i\varphi}\frac{\partial F}{\partial y}(\mu,v(\mu))\right)\mathrm{mod}_i\ u(\mu),$$

and Lemmas 1 and 7 then yield that

$$\mu^i(\{u_b,g_1\}_i^{x^i\varphi}\mu^{d-1}+\cdots+\{u_b,g_d\}_i^{x^i\varphi})=\mu^i\left(\{u_b,v(\mu)\}^\varphi\frac{\partial F}{\partial y}(\mu,v(\mu))\right)\mathrm{mod}\ u(\mu),$$

which, together with Proposition 5, implies that, for $a,b=1,\ldots,d$,

$$\{u_b,g_a\}_i^{x^i\varphi}=\{u_b,H_a\}_0^\varphi.$$

In a similar way, one proves that, for $a,b=1,\ldots,d$,

$$\{v_b,g_a\}_i^{x^i\varphi}=\{v_b,H_a\}_0^\varphi,$$

and we see from Lemma 6 that, for $b=0,\ldots,k$ and $a=1,\ldots,d$,

$$\{c_b,g_a\}_i^{x^i\varphi}=0=\{c_b,H_a\}_0^\varphi,$$

which concludes the proof of the theorem.

Finally, we show that the Poisson brackets $\{\cdot,\cdot\}_i^{x^i\varphi}, i=0,\ldots,k+1$, are compatible. To this purpose, it suffices to prove the following.

Theorem 9: Let φ be an arbitrary polynomial, and suppose that α and i are integers such that $\alpha+i\leqslant k+1$. Then the Poisson brackets $\{\cdot,\cdot\}_\alpha^\varphi$ and $\{\cdot,\cdot\}_{\alpha+i}^{x^i\varphi}$ are compatible.

Proof: To simplify the notation, we denote $\{\cdot,\cdot\}_1=\{\cdot,\cdot\}_\alpha^\varphi$ and $\{\cdot,\cdot\}_2=\{\cdot,\cdot\}_{\alpha+i}^{x^i\varphi}$. Further, we write the polynomial $G(\lambda)$ as

$$G(\lambda)=H_0\lambda^{d+k}+\cdots+H_{d+k},$$

and we denote by

$$\{\cdot,\cdot\}=\{\cdot,\cdot\}_1+\{\cdot,\cdot\}_2$$

the sum of the two brackets.

To prove the compatibility of $\{\cdot,\cdot\}_1$ and $\{\cdot,\cdot\}_2$, it suffices to prove the Jacobi identity

$$\{\{f,g\},h\}+\{\{g,h\},f\}+\{\{h,f\},g\}=0 \tag{13}$$

for all functions $f,g,h\in\{u_1,\ldots,u_d,v_1,\ldots,v_d,H_0,\ldots,H_{d+k}\}$. Using the fact that $\{\cdot,\cdot\}_1$ and $\{\cdot,\cdot\}_2$ are Poisson brackets and hence satisfy the Jacobi identity, (13) reduces to the ''mixed Jacobi identity''

$$\{\{f,g\}_2,h\}_1+\{\{g,h\}_2,f\}_1+\{\{h,f\}_2,g\}_1+\{\{f,g\}_1,h\}_2+\{\{g,h\}_1,f\}_2+\{\{h,f\}_1,g\}_2=0. \tag{14}$$

From Proposition 2 we know that $\{\cdot,\cdot\}^\varphi$ and $\{\cdot,\cdot\}^{x^i\varphi}$ are compatible. Hence, (14) holds if $f,g,h\in\{u_1,\ldots,u_d,v_1,\ldots,v_d\}$, and we only have to prove (14) in the case where at least one function (say, h) belongs to $\{H_0,\ldots,H_{d+k}\}$. As Theorem 8 implies that, for all $i=0,\ldots,d+k$, we have

$$\{\cdot,H_i\}_2=\{\cdot,H_j\}_1,\quad \{\cdot,H_i\}_1=\{\cdot,H_k\}_2,$$

for some j and k, we see that

$$\begin{aligned}&\{\{f,g\}_2,H_i\}_1+\{\{g,H_i\}_2,f\}_1+\{\{H_i,f\}_2,g\}_1+\{\{f,g\}_1,H_i\}_2+\{\{g,H_i\}_1,f\}_2+\{\{H_i,f\}_1,g\}_2\\&\quad=\{\{f,g\}_2,H_k\}_2+\{\{g,H_j\}_1,f\}_1+\{\{H_j,f\}_1,g\}_1+\{\{f,g\}_1,H_j\}_1+\{\{g,H_k\}_2,f\}_2\\&\qquad+\{\{H_k,f\}_2,g\}_2=0,\end{aligned}$$

as $\{\cdot,\cdot\}_1$ and $\{\cdot,\cdot\}_2$ satisfy the Jacobi identity.

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A completely integrable Hamiltonian system

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The dynamical system characterized by the Hamiltonian $H(\boldsymbol{q},\boldsymbol{p}) = \Sigma_{j,k=1}^{n}\, p_j p_k f(q_j - q_k)$ with $f(x)=\lambda+\mu\,\cos(\nu x)+\mu'\,\sin(\nu|x|)$ is completely integrable. Here n is an arbitrary positive integer and λ,μ,μ',ν are 4 arbitrary constants (λ and μ real, μ' and ν both real or both imaginary). © *1996 American Institute of Physics.* [S0022-2488(96)02805-8]

I. INTRODUCTION

It has been recently pointed out that the dynamical system characterized by the Hamiltonian

$$H(\boldsymbol{q},\boldsymbol{p})=\sum_{j,k=1}^{n}\, p_j p_k\, \exp(-|q_j-q_k|) \tag{1.1}$$

is completely integrable.[1] (Actually in Ref. 1 it was shown that the evolution of the coordinates $q_j(t)$ entailed by the Hamiltonian (1.1) coincides with the motion of the solitons of an integrable PDE,[2,1] which features ''peaked'' solitons whose position can be precisely defined. Thereby a Lax pair representation for these equations of motion was found, and n independent integrals of motion exhibited. Although it was not proven that these n integrals are in involution, these results suggested quite convincingly that the Hamiltonian (1.1) is integrable; as it is now demonstrated, see below.)

Motivated by this remarkable discovery, one of us investigated the integrability of the Hamiltonian

$$H(\boldsymbol{q},\boldsymbol{p})=\sum_{j,k=1}^{n}\, p_j p_k f(q_j-q_k), \tag{1.2}$$

and found[3] that this system is integrable (indeed, explicitly solvable) if

$$f(x)=\lambda+\mu\,\cos(\nu x). \tag{1.3}$$

The purpose and scope of this paper is to point out that the Hamiltonian (1.2) is completely integrable also in the more general case

$$f(x)=\lambda+\mu\,\cos(\nu x)+\mu'\,\sin(\nu|x|), \tag{1.4}$$

with λ,μ,μ',ν being 4 arbitrary constants. (To keep H real, we assume hereafter that λ and μ are real, μ' and ν both real or both imaginary). Of course special cases of the Hamiltonian (1.2) with (1.4) are the Hamiltonian (1.1) (corresponding to $\lambda=0$, $\mu=1$, $\mu'=\mathrm{i}$, $\nu=\mathrm{i}$), as well as the Hamiltonian (1.2) with (1.3) or with

$$f(x)=\alpha+\beta|x|+\gamma x^2, \tag{1.5}$$

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α, β, and γ being 3 arbitrary (real) constants (this corresponds to $\lambda = \alpha + 2\gamma/\epsilon^2$, $\mu = -2\gamma/\epsilon^2$, $\mu' = \beta/\epsilon$, $\nu = \epsilon$, $\epsilon \to 0$).

In Sec. II we show that the equations of motion entailed by the Hamiltonian (1.2) with (1.4) can be put in ''Lax pair'' form, and we thereby obtain n constants of motion for this system.

In Sec. III we prove that these n constants of motion are in involution; this entails the complete (''Liouville'') integrability of the Hamiltonian (1.2) with (1.4).

In Sec. IV we indicate how the problem can be reformulated via a convenient canonical transformation.

These findings suggest several avenues of additional research, which are outlined in Sec. V.

We end this introductory section with a remark on Arnol'd–Liouville integrability (with thanks to an anonymous referee for raising this issue).

A Hamiltonian system is termed *integrable in Liouville sense* if there exists n (n = number of degrees of freedom) globally defined constants of motion generically independent and in involution (one of them is of course the Hamiltonian itself).

If the n constants of motion in involution are of class C^1, and some other conditions hold, the Arnol'd–Liouville theorem affirms the global existence of torii on which the flow generated by the Hamiltonian (or by any one of the constants of motion) is *linear* (''actions-angles'' representation of the motion).

But the Hamiltonian (1.2) with (1.4) is not of class C^1, nor are the other $n-1$ constants of motion in involution of class C^1 (see below). Neither are they analytic. Indeed these features constitute perhaps the most remarkable characteristic of this model.

Hence the classical Arnol'd–Liouville theorem is not applicable to the Hamiltonian (1.2) with (1.4). Of course the existence of an integrable model of this type (neither C^1 nor analytic) underlies the interest of investigating extensions of the Arnol'd–Liouville theorem to include such systems.

II. LAX PAIR AND CONSTANTS OF MOTION

It was pointed out in Ref. 3 that the equations of motion entailed by (1.2), namely,

$$\dot{q}_j = 2\sum_{k=1}^{n} p_k f(q_j - q_k), \tag{2.1a}$$

$$\dot{p}_j = -2p_j \sum_{k=1}^{n} p_k f'(q_j - q_k), \tag{2.1b}$$

correspond to the $(n\times n)$-matrix Lax equation

$$\dot{\mathbf{L}} = [\mathbf{L}, \mathbf{A}] \tag{2.2}$$

provided the two $(n\times n)$-matrices $\mathbf{L}$ and $\mathbf{A}$ have the form

$$L_{jk} = (p_j p_k)^{1/2} \alpha(q_j - q_k), \tag{2.3}$$

$$A_{jk} = (p_j p_k)^{1/2} \gamma(q_j - q_k), \tag{2.4}$$

and the two (*a priori* arbitrary) functions $\alpha(x)$, $\gamma(x)$, together with the even function $f(x)$,

$$f(x) = f(-x), \tag{2.5}$$

satisfy the functional equation

$$2\alpha'(x+y)[f(x)-f(y)] - \alpha(x+y)[f'(x)-f'(y)] = \alpha(x)\gamma(y) - \alpha(y)\gamma(x). \tag{2.6}$$

[The ansatz (2.4) is actually less general than Eq. (4.9) of Ref. 3, and correspondingly this functional equation (2.6) is a special case of Eq. (3.4) of Ref. 3; but it is adequate for our present purposes.]

The first main result of this paper is to exhibit two functions, $\alpha(x)$ and $\gamma(x)$, that satisfy this functional equation, together with the function $f(x)$ given by (1.4). They read

$$\alpha(x)=(\Delta+\mu)^{1/2}\cos(\nu x/2)+(\Delta-\mu)^{1/2}\sin(\nu|x|/2), \tag{2.7}$$

$$\gamma(x)=\nu\mu'\ \mathrm{sign}(x)\{\cos(\nu x/2)-[\Delta+\mu)/(\Delta-\mu)]^{1/2}\sin(\nu|x|/2)\}, \tag{2.8}$$

with

$$\Delta^2=\mu^2+\mu'^2,\quad \Delta>0. \tag{2.9}$$

Several remarks are now in order.

Remark 2.1: The verification that these expressions of $\alpha(x)$ and $\gamma(x)$, together with the expression (1.4) of $f(x)$, satisfy the functional equation (2.6), requires an elementary if tedious computation, which must cover the three cases: (i) $x>0$, $y>0$; (ii) $x>0$, $y<0$, $x+y>0$; (iii) $x>0$, $y<0$, $x+y<0$ [all other possible cases are then automatically covered due to the obvious invariance of (2.6) under the interchange of x and y, as well as under the simultaneous change of sign of x and y if $\alpha(x)$ and $f(x)$ are even functions and $\gamma(x)$ is odd, as it is indeed implied by (1.4), (2.7), and (2.8)].

Remark 2.2: The expression (2.8) of $\gamma(x)$ could be generalized by adding to it $a\,\alpha(x)$, with a any arbitrary constant, since such an addition clearly does not affect the functional equation (2.6).

Remark 2.3: Both $f(x)$, see (1.4), and $\gamma(x)$, see (2.8), can be neatly related to $\alpha(x)$, see (2.7):

$$f(x)=\lambda-\Delta+\alpha^2(x), \tag{2.10}$$

$$\gamma(x)=2\mu'(\Delta-\mu)^{1/2}\alpha'(x). \tag{2.11}$$

Remark 2.4: The functional equation (2.6) can be rewritten as follows:

$$\alpha^2(x+y)\left[\frac{\partial}{\partial x}+\frac{\partial}{\partial y}\right]\{[f(x)-f(y)]/\alpha(x+y)\}=-\alpha(x)\gamma(y)+\alpha(y)\gamma(x). \tag{2.12}$$

Moreover, if one makes the assumption

$$\gamma(x)=c\,\alpha'(x), \tag{2.13}$$

which is *a priori* arbitrary, but *a posteriori* correct [in our case; see (2.11)], then the right-hand side of (2.12) can also be conveniently rewritten:

$$-\alpha(x)\gamma(y)+\alpha(y)\gamma(x)=c\left[\frac{\partial}{\partial x}-\frac{\partial}{\partial y}\right][\alpha(x)\alpha(y)] \tag{2.14a}$$

$$=c\,\alpha^2(y)\left[\frac{\partial}{\partial x}+\frac{\partial}{\partial y}\right][\alpha(x)/\alpha(y)] \tag{2.14b}$$

$$=-c\,\alpha^2(x)\left[\frac{\partial}{\partial x}+\frac{\partial}{\partial y}\right][\alpha(y)/\alpha(x)], \tag{2.14c}$$

entailing various possible reformulations of the functional equation (2.6) with (2.13), such as

$$\left[\frac{\partial}{\partial x}+\frac{\partial}{\partial y}\right]\{[f(x)-f(y)]/\alpha(x+y)\}=c\left[\frac{\partial}{\partial x}-\frac{\partial}{\partial y}\right][\alpha(x)\alpha(y)/\alpha^2(x+y)]. \tag{2.15}$$

Remark 2.5: In the special case $\mu'=0$ the function $f(x)$ takes of course the form (1.3), while $\alpha(x)$ and $\gamma(x)$ become

$$\alpha(x)=(2\mu)^{1/2}\cos(\nu x/2), \tag{2.16a}$$

$$\gamma(x)=-2\mu\nu\sin(\nu|x|/2). \tag{2.16b}$$

This is a different solution of the functional equation (2.6) than that given in Ref. 2, which reads instead (up to a convenient redefinition of the multiplicative constant)

$$\alpha(x)=(2\mu)^{1/2}\sin(\nu x/2), \tag{2.17a}$$

$$\gamma(x)=0. \tag{2.17b}$$

Note that in this case the matrix $\mathbf{L}$ is time-independent [see (2.2), (2.4), and (2.17b)]. It is of course trivial to verify that both these solutions, (2.16) and (2.17), satisfy (2.6) with (1.3).

Let us conclude this section by recalling that the possibility to rewrite the equations of motion (2.1) with (1.4) in the Lax pair form (2.2) [with (2.3)–(2.4) and (2.7)–(2.9)] yields n constants of motion, in the guise of the n eigenvalues of the Lax matrix (1.3), or equivalently of its n symmetrical invariants (the n coefficients of the polynomial $\det[\mathbf{L}-x\mathbf{I}]$, or of the traces of $\mathbf{L}^m$ with $m=1,2,\ldots,n$. We focus in the following on these latter quantities:

$$T_m=m^{-1}\,\mathrm{trace}[\mathbf{L}^m], \quad m=1,2,\ldots,n. \tag{2.18}$$

Note that (2.3), with (2.7) and (2.10), implies the relations

$$T_1=(\Delta+\mu)^{1/2}P, \tag{2.19}$$

$$T_2=(1/2)[H+(\Delta-\lambda)P^2], \tag{2.20}$$

with

$$P=\sum_{j=1}^{n}p_j \tag{2.21}$$

and H defined by (1.2).

In the special case $\mu'=0$ the matrix $\mathbf{L}$ is separable of rank 2 [see (2.3) with (2.16a)] and it therefore possesses only 2 nontrivial eigenvalues (all the others vanish); hence all T_m's with $m>2$ can be expressed in terms of T_1 and T_2. In this special case, however, there exists an alternative Lax matrix, which has the property that not only its eigenvalues, but indeed each of its $n(n-1)/2$ matrix elements, are constants of motion [see the *Remark 2.5* above; this Lax matrix is antisymmetrical, see (2.3) and (2.17a)]. Of course, for $n>3$, not all these constants of motion are independent; but there exist appropriate linear combinations of them (or rather of their squares), which provide *n independent* constants of motion *in involution*.[3] This implies the complete (''Liouville'') integrability of (1.2) with (1.3); a result which is however hardly interesting, since in this special case the time evolution of the Hamiltonian system can be exhibited in explicit form in terms of elementary functions (hence this system is not only *completely integrable*; it is *explicitly solvable*).[3]

Hereafter we focus on the general case with $\mu'\neq 0$. Then the Lax matrix [see (2.3) with (2.7) and (2.9)] is not separable, hence the quantities T_m, see (2.18), generally do provide *n indepen-*

dent integrals of motion. To demonstrate that this system is completely integrable it must moreover be shown that these n constants of motion are *in involution*. This is the second main result of this paper. The next section is devoted to its proof.

III. PROOF OF INVOLUTIVITY

Our task is to prove that the Poisson brackets,

$$\{T_m, T_{m'}\} = \sum_{i=1}^{n} \left[\left(\frac{\partial T_m}{\partial q_i} \right) \left(\frac{\partial T_{m'}}{\partial p_i} \right) - \left(\frac{\partial T_m}{\partial p_i} \right) \left(\frac{\partial T_{m'}}{\partial q_i} \right) \right], \tag{3.1}$$

vanish:

$$\{T_m, T_{m'}\} = 0; \quad m, m' = 1,2,\ldots,n. \tag{3.2}$$

For $m=1$ (or $m'=1$) this result is trivial; hereafter we assume $m>1$ (and $m'>1$).

The definition (2.18) implies the following formulas:

$$\frac{\partial T_m}{\partial q_i} = \sum_{i_1 \cdots i_m = 1}^{n} \left(\frac{\partial L_{i_1 i_2}}{\partial q_i} \right) L_{i_2 i_3} \cdots L_{i_m i_1}, \tag{3.3a}$$

$$\frac{\partial T_m}{\partial p_i} = \sum_{i_1 \cdots i_m = 1}^{n} \left(\frac{\partial L_{i_1 i_2}}{\partial p_i} \right) L_{i_2 i_3} \cdots L_{i_m i_1}. \tag{3.3b}$$

The definition (2.3) implies the following formulas:

$$\frac{\partial L_{jk}}{\partial q_i} = (p_j p_k)^{1/2} (\delta_{ij} - \delta_{ik}) \alpha'(q_j - q_k), \tag{3.4a}$$

$$\frac{\partial L_{jk}}{\partial p_i} = (1/2)(p_j p_k)^{1/2} (\delta_{ij} + \delta_{ik}) \alpha(q_j - q_k)/p_i. \tag{3.4b}$$

Hence, after a little algebra,

$$\begin{aligned} \{T_m, T_{m'}\} = (1/2) \sum_{i_1 \cdots i_m i'_1 \cdots i'_{m'} = 1}^{n} & ((1 \cdots m 1' \cdots m'))(23) \\ & \times (34) \cdots (m1)(2'3')(3'4') \cdots (m'1') \\ & \times \{\delta_{i_1 i'_1} [(12)'(1'2') - (1'2')'(12)]/p_{i_1} + (1 \leftrightarrow 2) \\ & + (1' \leftrightarrow 2') + (1 \leftrightarrow 2, 1' \leftrightarrow 2')\}. \end{aligned} \tag{3.5}$$

Here, we have introduced the convenient notations

$$((1 \cdots m 1' \cdots m')) \equiv p_{i_1} \cdots p_{i_m} p_{i'_1} \cdots p_{i'_{m'}}, \tag{3.6}$$

$$(12) \equiv \alpha(q_{i_1} - q_{i_2}), \quad (1'2') \equiv \alpha(q_{i'_1} - q_{i'_2}) \quad \text{and so on,} \tag{3.7a}$$

$$(12)' \equiv \alpha'(q_{i_1} - q_{i_2}), \quad (1'2')' \equiv \alpha'(q_{i'_1} - q_{i'_2}) \quad \text{and so on.} \tag{3.7b}$$

The notation $(1\leftrightarrow 2)$ indicates of course the exchange of the (summation) indices i_1, i_2; likewise $(1'\leftrightarrow 2')$ indicates the exchange of i'_1, i'_2.

Clearly the product $((1\cdots m1'\cdots m'))$ is invariant under any exchange of summation indices. Moreover the product $(23)(34)\cdots(m1)$ is invariant under the transformation $(1\leftrightarrow 2, m\leftrightarrow 3, m-1\leftrightarrow 4,...)$ [due to the evenness of $\alpha(x)=\alpha(-x)$, see (2.7), which implies $(12)=(21)$ and so on, see (3.7a)]. Likewise the product $(2'3')(3'4')\cdots(m'1')$ is invariant under the transformation $(1'\leftrightarrow 2', m\leftrightarrow 3', m'-1\leftrightarrow 4',...)$. Hence

$$\{T_m,_{m'}\}=2\sum_{i_1\cdots i_m i'_2\cdots i'_{m'}=1}^{n}((1\cdots m2'\cdots m'))(23)(34)\cdots(m1)(1m')$$
$$\times(m'm'-1)\cdots(3'2')[(12)'(12')-(12')'(12)]. \tag{3.8}$$

Note that the transition from (3.5) to (3.8) has involved two steps: the elimination of the 3 additional terms inside the curly bracket in the r.h.s. of (3.5) [compensated by the replacement of (1/2) by 2 in front of the sum], and then the sum over the index i'_1 (using the Kronecker $\delta_{i_1 i'_1}$).

Let us now consider the transformation $(2'\leftrightarrow 2,\ 3'\leftrightarrow 3,...,1\leftrightarrow h,...)$, under which the product $(23)(34)\cdots(m1)(1m')(m'm'-1)\cdots(3'2')$ is clearly invariant [as well, of course, as $(1\cdots m2'\cdots m')$]; incidentally, it would be easy to identify h, or more precisely the corresponding summation index i_h (which might or might not be a primed index), but this is not needed in the following. Hence,

$$\{T_m,T_{m'}\}=\sum_{i_1\cdots i_m i'_2\cdots i'_{m'}=1}^{n}((1\cdots m2'\cdots m'))(23)(34)\cdots(m1)(1m')(m'm'-1)\cdots(3'2')$$
$$\times[(12)'(12')-(12')'(12)+(h2')'(h2)-(h2)'(h2')]. \tag{3.9}$$

We now use the remarkable ''functional'' equality

$$(12)'(12')-(12')'(12)+(h2')'(h2)-(h2)'(h2')$$
$$=(\nu/2)(\Delta-\mu)^{1/2}(22')[s_{12}+s_{2h}+s_{h2'}+s_{2'1}], \tag{3.10}$$

which is proven below. Here we have introduced the convenient notation

$$s_{12}\equiv\mathrm{sign}(q_{i_1}-q_{i_2}), s_{h2'}\equiv\mathrm{sign}(q_{i_h}-q_{i'_2}) \text{ and so on.} \tag{3.11}$$

Note that this definition entails oddness of s_{12} under exchange of its two indices, $s_{12}=-s_{21}$, and likewise, of course, $s_{2h}=-s_{h2}$, $s_{h2'}=-s_{2'h}$, $s_{2'1}=-s_{12'}$.

Using (3.10) we get from (3.9)

$$\{T_m,T_{m'}\}=\sum_{i_1\cdots i_m i'_2\cdots i'_{m'}=1}^{n}S_{i_1\cdots i_m i'_2\cdots i'_{m'}}[s_{12}+s_{2h}+s_{h2'}+s_{2'1}], \tag{3.12a}$$

$$S_{i_1\cdots i_m i'_2\cdots i'_{m'}}=(\nu/2)(\Delta-\mu)^{1/2}((1\cdots m2'\cdots m'))(23)(34)\cdots(m1)(1m')$$
$$\times(m'm'-1)\cdots(3'2')(2'2). \tag{3.12b}$$

Note that $S_{i_1\cdots i_m i'_2\cdots i'_{m'}}$ depends cyclically on all $m+m'-1$ indices $i_1,...,\ i_m,\ i'_2,...,\ i'_{m'}$. Hence there clearly exists a transformation which interchanges any two chosen indices, and, in a suitable manner, all other indices pairwise (except one of two which might be

left unchanged, namely, get transformed into themselves), and leaves S invariant (it is actually easy to identify such a transformation; for instance, if the chosen pair are 1 and 2, the appropriate transformation is $(1\leftrightarrow 2, m'\leftrightarrow 2', m'-1\leftrightarrow 3', \ldots, m\leftrightarrow 3, m-1\leftrightarrow 4, \ldots)$. But s_{12} changes sign under any transformation that exchanges 1 and 2 (namely, the summation indices i_1 and i_2); likewise s_{2h} changes sign under any transformation that exchanges 2 and h, and so on for $s_{h2'}$ and $s_{2'1}$. It is thus shown that the sum in the r.h.s. of (3.12a) vanishes, and this implies (3.2.) Q.E.D.

There remains to prove the functional equation (3.10), namely, [see (3.7)]

$$\alpha'(q_1-q_2)\alpha(q_1-q_3)-\alpha'(q_1-q_3)\alpha(q_1-q_2)+\alpha'(q_0-q_3)\alpha(q_0-q_2)-\alpha'(q_0-q_2)\alpha(q_0-q_3)=(\nu/2)(\Delta-\mu)^{1/2}\alpha(q_2-q_3)[s_{12}+s_{20}+s_{03}+s_{31}], \tag{3.13}$$

where, for notational convenience, we have set $q_{i_1}=q_1$, $q_{i_2}=q_2$, $q_{i_h}=q_0$, $q_{i'_2}=q_3$ and of course $s_{jk}\equiv \mathrm{sign}(q_j-q_k)$. It is now a matter of trivial algebra to verify this formula, using the definition (2.7) of $\alpha(x)$, namely,

$$\alpha(q_j-q_k)=(\Delta+\mu)^{1/2}\cos[\nu(q_j-q_k)/2]+(\Delta-\mu)^{1/2}s_{jk}\sin[\nu(q_j-q_k)/2], \tag{3.14}$$

as well as the identity

$$s_{12}s_{13}+s_{23}s_{21}+s_{31}s_{32}=1, \tag{3.15}$$

whose validity is easily checked by considering all possible orderings of q_1, q_2, and q_3.

Note that these results clearly imply the following:

Proposition 3.1: Let the (nxn)-matrix $\mathbf{L}(\mathbf{q},\mathbf{p})$ be defined by (2.3), with $\alpha(x)$ *a priori* arbitrary except for the requirement that it be even, $\alpha(x)=\alpha(-x)$. Then the n quantities T_m defined by (2.18) are in involution [see (3.1,2)], provided $\alpha(x)$ satisfies the following functional equation:

$$\alpha'(x)\alpha(x+y+z)-\alpha'(x+y+z)\alpha(x)+\alpha'(y)\alpha(z)+\alpha'(z)\alpha(y)=\alpha(y+z)[\beta_1(x)+\beta_2(y)+\beta_3(z)+\beta_4(x+y+z)], \tag{3.16}$$

where the 4 functions $\beta_s(x)$ are also *a priori* arbitrary except for the requirement that they be all odd, $\beta_s(-x)=-\beta_s(x)$, $s=1,2,3,4$.

This functional equation is of course inferred from (3.13) via the positions $x=q_1-q_2$, $y=q_2-q_0$, $z=q_0-q_3$, implying $x+y+z=q_1-q_3$, $x+y=q_1-q_0$.

IV. A CANONICAL TRANSFORMATION

In this section we introduce new canonical coordinates x_j, y_j via the transformation

$$x_j=(2\mathrm{i}p_j/\nu)^{1/2}\exp(-\mathrm{i}\nu q_j/2), \tag{4.1a}$$

$$y_j=(2\mathrm{i}p_j/\nu)^{1/2}\exp(\mathrm{i}\nu q_j/2), \tag{4.1b}$$

$$p_j=(2\mathrm{i})^{-1}\nu x_j y_j, \tag{4.2a}$$

$$q_j=\nu^{-1}\arctan[\mathrm{i}(y_j{}^2-x_j{}^2)/(y_j{}^2+x_j{}^2)]. \tag{4.2b}$$

It is easy to check that this transformation is canonical:

$$\{x_j,y_k\}=\delta_{jk}. \tag{4.3}$$

In the new canonical variables the total momentum P, see (2.21), and the Hamiltonian H, see (1.2) with (1.4), read as follows:

$$P=(2\mathrm{i})^{-1}\sum_{j=1}^{n} x_j y_j ,$$

$$H=\lambda P^2-(\nu^2/8)\sum_{j,k=1}^{n}[\mu(x_j{}^2y_k{}^2+x_k{}^2y_j{}^2)-\mathrm{i}\mu' s_{jk}(x_j{}^2y_k{}^2-x_k{}^2y_j{}^2)], \tag{4.4}$$

where we are of course using the convenient notation

$$s_{jk}\equiv\mathrm{sign}(q_j-q_k). \tag{4.5}$$

Note the extreme simplicity of this Hamiltonian in the $\mu'=0$ case, when it takes the separable form

$$H=\lambda P^2-(\nu^2\mu/4)XY, \tag{4.6}$$

$$X=\sum_{j=1}^{n} x_j{}^2, \tag{4.7a}$$

$$Y=\sum_{j=1}^{n} y_j{}^2. \tag{4.7b}$$

This simplicity allows to solve in completely explicit form the equations of motion entailed by this Hamiltonian, which read

$$\dot{x}_j=-\mathrm{i}\lambda\nu P x_j-(1/2)\nu^2\mu X y_j , \tag{4.8a}$$

$$\dot{y}_j=\mathrm{i}\lambda\nu P y_j+(1/2)\nu^2\mu Y x_j , \tag{4.8b}$$

and which imply

$$\dot{P}=0, \tag{4.9}$$

$$\dot{X}=-2\mathrm{i}\nu(\lambda+\mu)PX, \tag{4.10a}$$

$$\dot{Y}=2\mathrm{i}\nu(\lambda+\mu)PY. \tag{4.10b}$$

This is left as an exercise for the diligent reader, who may thereby reobtain the results of Ref. 3.

Let us end this section by reporting (for the general case with $\mu'\neq 0$) the expressions, in the new canonical variables, of the matrices **L** and **A**:

$$L_{jk}=(\nu/4)[-\mathrm{i}(\Delta+\mu)^{1/2}(x_j y_k+x_k y_j)+(\Delta-\mu)^{1/2}s_{jk}(x_j y_k-x_k y_j)], \tag{4.11}$$

$$A_{jk}=(\nu^2\mu'/4)[-\mathrm{i}s_{jk}(x_j y_k+x_k y_j)-[(\Delta+\mu)/(\Delta-\mu)]^{1/2}(x_j y_k-x_k y_j)]. \tag{4.12}$$

V. OUTLOOK

In this final section we outline directions of research which are suggested by these findings.

There is the task to utilize them in order to explore the behavior of the dynamical system characterized by the Hamiltonian (1.2) with (1.4). While we do not expect an explicit solution to be obtainable in the general case with $\mu'\neq 0$, it should be possible to exploit the integrability of the system to evince much information on its behavior, in both cases: μ' and ν real, μ' and ν imaginary. A related problem arises from the ''geometrical'' interpretation naturally associated to

a Hamiltonian of type (1.2), which may be viewed as representing the kinetic energy of a particle moving on an n-dimensional manifold, whose metric is characterized via the function $f(x)$. This question may be enriched by performing canonical (or other) transformations before seeking a geometrical interpretation. In this connection we note that, in the special case $\mu'=0$, the Hamiltonian (4.4) includes the description of geodesic motion on the sphere.[4]

Several other questions are suggested by our findings. There exists an integrable nonlinear PDE whose solitons move according to the Hamiltonian (1.1);[1] is this also true in the general case [(1.2) with (1.4), $\mu'\neq 0$]? In the special case $\mu'=0$ there exists a quantized version of the Hamiltonian (1.2) with (1.3) which can be rather fully solved;[5] is this also true in the general case [(1.2) with (1.4), $\mu'\neq 0$]?

And what about possible (integrable) generalizations? For instance, one of us (F.C.) found that the Hamiltonian (1.2) with (1.3) remains solvable after addition of a term H',

$$H'(\mathbf{q},\mathbf{p})=c\sum_{j,k=1}^{n}(p_j-p_k)\sin[\nu(q_j-q_k)]. \tag{5.1}$$

It is likely that integrable generalizations of (1.2) with (1.4) also exist, corresponding to ''other root systems'' [if one associates (1.2) with the root system A_n], or obtainable via ''duplications,''[6] or involving the addition to the Hamiltonian of ''one-body terms,'' or including ''internal degrees of freedom'' (matrix models), or amounting to ''discretizations'' of the space variables (lattice models) or of the time variable (mappings). And what about complex or multidimensional extensions?

It is moreover evident that, for all models invariant under the translation $q_j\rightarrow q_j+q_0$, for which P is therefore a constant of the motion, the term P^2 in the Hamiltonian can rather trivially be replaced by a largely arbitrary function $F(P)$, without causing other than cosmetic changes. On the other hand it is rather clear[3] that the Hamiltonian

$$H=\lambda P^2+\sum_{j,k=1}^{n}p_jp_k[\mu_1\cos(\nu q_j)\cos(\nu q_k)+\mu_2\sin(\nu q_j)\sin(\nu q_k)] \tag{5.2}$$

is solvable in terms of elliptic functions.[7] Note that this model is not invariant under the translation $q_j\rightarrow q_j+q_0$, except in the special case $\mu_1=\mu_2=\mu$, when it reduces to (1.2) with (1.3).

And we end with the still extant, and most interesting, question: which is the most general function $f(x)$ such that the Hamiltonian (1.2) is integrable?

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Supertraces on the algebras of observables of the rational Calogero model with harmonic potential

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We define a complete set of supertraces on the algebra $SH_N(\nu)$, the algebra of observables of the N-body rational Calogero model with harmonic interaction. This result extends the previously known results for the simplest cases of $N=1$ and $N=2$ to arbitrary N. It is shown that $SH_N(\nu)$ admits $q(N)$ independent supertraces, where $q(N)$ is a number of partitions of N into a sum of odd positive integers, so that $q(N)>1$ for $N\geqslant 3$. Some consequences of the existence of several independent supertraces of $SH_N(\nu)$ are discussed, such as the existence of ideals in associated W_∞-type Lie superalgebras. © *1996 American Institute of Physics.*
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I. INTRODUCTION

In this paper we investigate some properties of the associative algebras that were shown in Refs. 1–3 to underlie the rational Calogero model[4] and were denoted as $SH_N(\nu)$ in Ref. 5. Algebra $SH_N(\nu)$ is the associative algebra of polynomials constructed from arbitrary elements σ of the symmetric group S_N and the generating elements a_i^α obeying the following relations:

$$\sigma a_i^\alpha = a_{\sigma(i)}^\alpha \sigma, \tag{1}$$

$$[a_i^\alpha, a_j^\beta] = \epsilon^{\alpha\beta} A_{ij}, \tag{2}$$

where $i,j=1,\ldots,N$, $\alpha,\beta=0,1$, $\epsilon^{\alpha\beta}=-\epsilon^{\beta\alpha}$, $\epsilon^{01}=1$, and

$$A_{ij}=\delta_{ij}+\nu\widetilde{A}_{ij}, \quad \widetilde{A}_{ij}=\delta_{ij}\sum_{l=1}^{N} K_{il}-K_{ij}. \tag{3}$$

Here $K_{ij}\in S_N$ with $i,j=1,\ldots,N$, $i\neq j$, are the elementary permutations $i\leftrightarrow j$ satisfying the relations

$$K_{ij}=K_{ji}, \quad K_{ij}K_{ij}=1, \quad K_{ij}K_{jl}=K_{jl}K_{li}=K_{li}K_{ij},$$

for $i\neq j\neq l\neq i$ and

$$K_{ij}K_{kl}=K_{kl}K_{ij},$$

if i,j,k,l are pairwise different. Note that in this paper repeated Latin indices $i,j,k,\ldots$, do not imply summation.

The defining relations (1)–(3) are consistent. In particular, the Jacobi identities,

$$[a_i^\alpha,[\alpha_j^\beta,a_k^\gamma]]+[a_j^\beta[a_k^\gamma,a_i^\alpha]]+[a_k^\gamma,[a_i^\alpha,a_j^\beta]]=0, \tag{4}$$

are satisfied.

An important property of $SH_N(\nu)$ that allows one to solve the Calogero model[4] is that this algebra possesses inner sl_2 automorphisms with the generators

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$$T^{\alpha\beta}=\frac{1}{2}\sum_{i=1}^{N}(a_i^\alpha a_i^\beta+a_i^\beta a_i^\alpha), \tag{5}$$

$$[T^{\alpha\beta},T^{\gamma\delta}]=\epsilon^{\alpha\gamma}T^{\beta\delta}+\epsilon^{\alpha\delta}T^{\beta\gamma}+\epsilon^{\beta\gamma}T^{\alpha\delta}+\epsilon^{\beta\delta}T^{\alpha\gamma}, \tag{6}$$

which act on the generating elements a_i^α as on sl_2 vectors,

$$[T^{\alpha\beta},a_i^\gamma]=\epsilon^{\alpha\gamma}a_i^\beta+\epsilon^{\beta\gamma}a_i^\alpha. \tag{7}$$

The Calogero Hamiltonian is identified with the Cartan element T^{01} which, according to (7), induces Z gradation of $SH_N(\nu)$. The latter property allows one[2] to construct wave functions via the standard Fock procedure with the Fock vacuum $|0\rangle$, such that $a_i^0|0\rangle=0$. Thus, the elements a_i^α serve as generalized oscillators underlying the Calogero problem. The concrete realization of these oscillators in terms of Dunkl differential-difference operators[6] was presented in Refs. 1 and 2.

These properties characterize the algebra $SH_N(\nu)$ as a natural generalization of the Heisenberg–Weyl algebra, the associative algebra of harmonic oscillators. Since the Lie algebra of quantum operators in the harmonic oscillator problem can be identified with the $W_{1+\infty}$ algebra,[7] the Lie (super)algebras constructed from $SH_N(\nu)$ with the aid of supercommutators give rise to a class of the $W_{1+\infty}$-type algebras, which have been denoted as $W_{N,\infty}(\nu)$ in Ref. 8, where it was shown that all these algebras contain the Virasoro algebra as a subalgebra. The latter observation indicates that the algebras $SH_N(\nu)$ and $W_{N,\infty}(\nu)$ can be related to conformal models as well as to other classes of models in the range from the quantum Hall effect[9] to higher-spin gauge theories[10] and KP hierarchy[11] where W_∞-type algebras prove to be important. An additional argument in favor of the relationship of $SH_N(\nu)$ to the quantum Hall effect is due to the known fact that the Calogero model can be interpreted as a one-dimensional reduction of the full anyonic problem.[12,3]

For lower values of N, a nature of $SH_N(\nu)$ is rather well understood. $SH_1(\nu)$ is the ordinary Heisenberg–Weyl algebra (since ν dependence is artificial in this case we will use the notation SH_1). Properties of this algebra are very well studied (see, e.g., Ref. 13). Note that since the center of mass coordinates $1/N\Sigma_{i=1}^N a_i^\alpha$ decouple from everything else in the defining relations (1)–(3), the associative algebra $SH_N(\nu)$ has the structure $SH_N(\nu)=SH_1\otimes SH_N'(\nu)$ where, by definition, $SH_N'(\nu)$ is the algebra of elements depending only on the relative coordinates $a_i^\alpha-a_j^\alpha$.

The properties of $SH_2'(\nu)$ are well studied too.[14] The algebra $SH_2'(\nu)$ is defined by the relations

$$[a^\alpha,a^\beta]=\epsilon^{\alpha\beta}(1+2\nu K), \tag{8}$$

where K is the only nontrivial element of S_2, while a^α are the relative motion oscillators. For the particular case of $\nu=0$, one recovers the algebra SH_1 in the sector of the K independent elements.

In Ref. 14 it was shown that $SH_2'(\nu)$ admits a unique supertrace operation defined by the simple formula

$$\mathrm{str}(1)=1,\quad \mathrm{str}(K)=-2\nu,\quad \mathrm{str}(W)=\mathrm{str}(WK)=0, \tag{9}$$

for any polynomial $W\in SH_2'$ of the form

$$W=\sum_{n=1}^{\infty}W_{\alpha_1\cdots\alpha_n}a^{\alpha_1}\cdots a^{\alpha_n}, \tag{10}$$

with arbitrary totally symmetric multispinors $W_{\alpha_1\cdots\alpha_n}$. For the particular case of $\nu=0$ one recovers the supertrace on SH_1.

Furthermore, it was shown in Ref. 14 by explicit evaluation of the invariant bilinear form $B(x,y)\overset{\text{def}}{=}\mathrm{str}(xy)$ that for $\nu=l+(1/2)$ (l is any integer) $SH_2'(\nu)$ reduces to finite-dimensional matrix algebras up to some infinite-dimensional ideals $\mathscr{I}$ that decouple from everything under the supertrace operation (9), i.e., $\mathrm{str}(xy)=0$, $\forall x\in\mathscr{I}$.

In Ref. 15 it was then observed that $SH_2'(\nu)$ is isomorphic to the factor of the enveloping algebra $U(\mathrm{osp}(1;2))$ of osp(1;2) over its ideal generated by the quadratic Casimir operator C_2 by factoring out all elements of the form $(C_2-c_2)U(\mathrm{osp}(1;2))$, where $c_2=\frac{1}{16}(4\nu^2-1)$ is an arbitrary constant. In its turn this observation clarified the origin of the ideals of $SH_2'(\nu)$ at $\nu=l+\frac{1}{2}$ as corresponding to the finite-dimensional representations of osp(1;2).

Although the algebra $SH_N(\nu)$ is getting interesting applications for any N, until now understanding of its algebraic properties for $N>2$ is far from being satisfactory. In particular, there is no interpretation of $SH_N(\nu)$ in terms of enveloping algebras of finite-dimensional superalgebras, and nothing is known about ideals of $SH_N(\nu)$ which information is very important in applications.

In this paper we analyze the existence of the invariant supertrace operation on $SH_N(\nu)$ i.e., such a complex-valued linear function $\mathrm{str}(f)$ on $SH_N(\nu)$ that

$$\mathrm{str}([f,g\})=0,\quad \forall f,g\in SH_N(\nu), \tag{11}$$

with the convention that

$$[f,g\}=fg-(-1)^{\pi(f)\pi(g)}gf, \tag{12}$$

where the parity π in $SH_N(\nu)$ is defined as follows:

$$\pi(a_i^\alpha)=1,\quad \pi(K_{ij})=0. \tag{13}$$

Let us note that an attempt to define differently graded traces like, e.g., an ordinary trace ($\pi\equiv 0$) unlikely leads to interesting results.

Knowledge of the supertrace operations on $SH_N(\nu)$ is useful in various respects. One of the most important applications of the supertrace is that it gives rise to n-linear invariant forms,

$$\mathrm{str}(a_1a_2\cdots a_n), \tag{14}$$

that allows one to work with the algebra essentially in the same way as with the ordinary finite-dimensional matrix algebras, and, for example, construct Lagrangians when working with dynamical theories based on $SH_N(\nu)$. Another useful property is that since null vectors of any invariant bilinear form span a both-side ideal of the algebra, this gives a powerful device for investigating ideals that decouple from everything under the supertrace operation as it occurs in $SH_2(\nu)$ for half-integer ν. It is also worth mentioning that having an explicit form of the trilinear form in one or another basis is practically equivalent to defining a star-product law in the algebra.

An important motivation for the analysis of the supertraces of $SH_N(\nu)$ is due to its deep relationship with the analysis of the representations of this algebra, which in its turn gets applications to the analysis of the wave functions of the Calogero model. For example, given representation of $SH_N(\nu)$, one can speculate that it induces some supertrace on this algebra as (appropriately regularized) supertrace of (infinite) representation matrices. When the corresponding bilinear form degenerates this would imply that the representation becomes reducible.

As we show, the situation for $SH_N(\nu)$ is very interesting, since starting from $N=3$ it admits more than one independent supertrace in contrast to the cases of $N=1$ and $N=2$. This fact is in agreement with the results of Ref. 5, where it was shown that there exist many inequivalent lowest-weight-type representations of $SH_N(\nu)$ for higher N (these representations are classified

according to the representations of S_N). Another important consequence of this phenomenon is that the Lie superalgebras $W_{N,\infty}(\nu)$ are not simple, while appropriate, their simple subalgebras possess nontrivial outer automorphisms.

The paper is organized as follows. In Sec. II we analyze consequences of S_N and sl_2 automorphisms of $SH_N(\nu)$. In Sec. III we discuss general properties of the supertraces and consequences of the existence of several independent supertraces. In Sec. IV we study the restrictions on supertraces of the group algebra of S_N considered as a subalgebra of $SH_N(\nu)$, which follow from the defining relations of $SH_N(\nu)$. These restrictions are called ground level conditions (GLC). They play a fundamental role in the problem, since, as we show in Sec. V, every solution of GLC admits a unique extension to some supertrace on $SH_N(\nu)$. In Appendix A it is shown that the number of independent supertraces on $SH_N(\nu)$ equals the number of partitions of N into a sum of odd positive integers. Some technical details of the proof of Sec. V are collected in Appendices B and C.

II. FINITE-DIMENSIONAL GROUPS OF AUTOMORPHISMS

The group algebra of S_N is the finite-dimensional subalgebra of $SH_N(\nu)$. The elements $\sigma\in S_N$ induce inner automorphisms of $SH_N(\nu)$. It is well known that any $\sigma\in S_N$ can be expanded into a product of pairwise commuting cycles,

$$\sigma=c_1c_2c_3\cdots c_t, \tag{15}$$

where $c_\mathfrak{m}$, $\mathfrak{m}=1,...,t$, are cyclic permutations acting on distinct subsets of values of indices i. For example, a cycle that acts on the first s indices as $1\to2\to\cdots\to s\to1$ has the form

$$c=K_{12}K_{23}\cdots K_{(s-1)s}. \tag{16}$$

We use the notation $|c|$ for the length of the cycle c. For the cycle (16), $|c|=s$. We take a convention that the cycles of unit length are associated with all values of i such that $\sigma(i)=i$, so that the relation $\Sigma_\mathfrak{m}|c_\mathfrak{m}|=N$ is true.

Given permutation $\sigma\in S_N$, we introduce a new set of basis elements $\mathfrak{B}_\sigma=\{b^I\}$ instead of $\{a_i^\alpha\}$ in the following way. For every cycle $c_\mathfrak{m}$ in the decomposition (15) ($\mathfrak{m}=1,...,t$), let us fix some index $l_\mathfrak{m}$, which belongs to the subset associated with the cycle $c_\mathfrak{m}$. The basis elements $b^\alpha_{\mathfrak{m}j}$, $j=1,...,|c_\mathfrak{m}|$, which realize one-dimensional representations of the commutative cyclic group generated by $c_\mathfrak{m}$, have the form

$$b^\alpha_{\mathfrak{m}j}=\frac{1}{\sqrt{|c_\mathfrak{m}|}}\sum_{k=1}^{|c_\mathfrak{m}|}(\lambda_\mathfrak{m})^{jk}a^\alpha_{l(\mathfrak{m},k)}, \tag{17}$$

where $l(\mathfrak{m},k)=c_\mathfrak{m}^{-k}(l_\mathfrak{m})$ and

$$\lambda_\mathfrak{m}=\exp(2\pi i/|c_\mathfrak{m}|). \tag{18}$$

From the definition (17), it follows that

$$c_\mathfrak{m}b^\alpha_{\mathfrak{m}j}=(\lambda_\mathfrak{m})^jb^\alpha_{\mathfrak{m}j}c_\mathfrak{m}, \tag{19}$$

$$c_\mathfrak{m}b^\alpha_{\mathfrak{n}j}=b^\alpha_{\mathfrak{n}j}c_\mathfrak{m}, \quad \text{for } \mathfrak{n}\neq\mathfrak{m}, \tag{20}$$

and therefore

$$\sigma b^\alpha_{\mathfrak{m}j}=(\lambda_\mathfrak{m})^jb^\alpha_{\mathfrak{m}j}\sigma. \tag{21}$$

In what follows, instead of writing $b^\alpha_{\mathfrak{m}j}$ we use the notation b^I with the label I accounting for the full information about the index α, the index $\mathfrak{m}$ enumerating cycles in (15), and the index j, which enumerates various elements $b^\alpha_{\mathfrak{m}j}$ related to the cycle $c_\mathfrak{m}$, i.e., $I(I=1,\ldots,2N)$ enumerates all possible triples $\{\alpha,\mathfrak{m},j\}$. We denote the index α, the cycle and the eigenvalue in (19) corresponding to some fixed index I as $\alpha(I)$, $c(I)$, and $\lambda_I=(\lambda_\mathfrak{m})^j$, respectively. The notation $\sigma(I)=\sigma_0$ implies that $b^\alpha_I \in \mathfrak{B}_{\sigma_0}$. $\mathfrak{B}_\mathbf{1}$ is the original basis of the generating elements a^α_i (here $\mathbf{1}$ is the unit permutation).

Let $\mathfrak{M}(\sigma)$ be the matrix that maps $\mathfrak{B}_\mathbf{1}\to\mathfrak{B}_\sigma$ in accordance with (17),

$$b^I=\sum_{i,\alpha}\mathfrak{M}^I_{i\alpha}(\sigma)a^\alpha_i. \tag{22}$$

Obviously this mapping is invertible. Using the matrix notations one can rewrite (21) as

$$\sigma b^I\sigma^{-1}=\sum_{J=1}^{2N}\Lambda^I_J(\sigma)b^J,\quad \forall b^I\in\mathfrak{B}_\sigma, \tag{23}$$

where $\Lambda^J_I(\sigma)=\delta^J_I\lambda_I$.

Every polynomial in $SH_N(\nu)$ can be expanded into a sum of monomials of the form

$$b^{I_1}b^{I_2}\cdots b^{I_s}\sigma, \tag{24}$$

where all $\sigma(I_k)=\sigma$. Every monomial of this form realizes some one-dimensional representation of the Abelian group generated by all cycles $c_\mathfrak{m}$ in the decomposition (15).

The commutation relations for the generating elements b^I follow from (2) and (3):

$$[b^I,b^J]=F^{IJ}=\mathscr{C}^{IJ}+\nu f^{IJ}, \tag{25}$$

where

$$\mathscr{C}^{IJ}=\epsilon^{\alpha(I)\alpha(J)}\delta_{c(I)c(J)}\delta_{\lambda_I\lambda_J^{-1}} \tag{26}$$

and

$$f^{IJ}=\sum_{i,j,\alpha,\beta}\mathfrak{M}^I_{i\alpha}(\sigma)\mathfrak{M}^J_{j\beta}(\sigma)\epsilon^{\alpha\beta}\widetilde{A}_{ij}. \tag{27}$$

The indices I,J are raised and lowered with the aid of the symplectic form $\mathscr{C}^{IJ}$

$$\mu^I=\sum_J\mathscr{C}^{IJ}\mu_J,\quad \mu_I=\sum_J\mu^J\mathscr{C}_{JI};\quad \sum_M\mathscr{C}_{IM}\mathscr{C}^{MJ}=-\delta^J_I. \tag{28}$$

Note that the elements b^I are normalized in (17) in such a way that the ν-independent part in (25) has the form (26).

Another important finite-dimensional algebra of inner automorphisms of $SH_N(\nu)$ is the sl_2 algebra that acts on the indices α. It is spanned by the S_N-invariant second-order polynomials (5). Evidently, $SH_N(\nu)$ decomposes into the infinite direct sum of only finite-dimensional irreducible representations of this sl_2 spanned by various homogeneous polynomials (24).

From the defining relations (1)–(3), it follows that $SH_N(\nu)$ is Z_2 graded with respect to the automorphism

$$f(a^\alpha_j)=-a^\alpha_j,\quad f(K_{ij})=K_{ij}, \tag{29}$$

which gives rise to the parity π (13). In applications to higher-spin models, this automorphism distinguishes between bosons and fermions.

The algebra $SH_N(\nu)$ admits the antiautomorphism ρ,

$$\rho(a_k^\alpha)=ia_k^\alpha, \quad \rho(K_{ij})=K_{ij}, \tag{30}$$

which leaves invariant the basic relations (1)–(3), provided that an order of operators is reversed according to the defining property of antiautomorphisms: $\rho(AB)=\rho(B)\rho(A)$. From (15), (16), and (21) it follows that

$$\rho(\sigma)=\sigma^{-1}, \quad \rho(b^I)=ib^J, \tag{31}$$

where J is related to I in such a way that $\alpha(J)=\alpha(I)$, $\sigma(J)=(\sigma(I))^{-1}$, $c(J)=(c(I))^{-1}$, and $\lambda_J=\lambda_I^{-1}$. Note that in higher-spin theories the counterpart of ρ distinguishes between odd and even spins.[16]

III. GENERAL PROPERTIES OF SUPERTRACE

In this section we summarize some general properties to be respected by any supertrace in $SH_N(\nu)$.

Let A be an arbitrary associative Z_2-graded algebra with the parity function $\pi(x)=0$ or 1. Suppose that A admits some supertrace operations str_p, where the label p enumerates different nontrivial supertraces. We call a supertrace str even (odd) if $\mathrm{str}(x)=0$, $\forall x\in A$ such that $\pi(x)=1(0)$. Let T_A be a linear space of supertraces on A. We say that $\dim T_A$ is the number of supertraces on A.

Given parity-preserving (anti) automorphism τ and supertrace operation str on A, $\mathrm{str}(\tau(x))$ is some supertrace as well. For inner automorphisms τ, $(\tau(x)=pxp^{-1}$, $\pi(p)=0)$, it follows from the defining property of the supertrace that $\mathrm{str}(\tau(x))=\mathrm{str}(x)$. Thus, T_A forms a representation of the factor group of the parity preserving automorphisms and antiautomorphisms of A over the normal subgroup of the inner automorphisms of A. Applying this fact to the original parity automorphism $(-1)^\pi$, one concludes that T_A can always be decomposed into a direct sum of subspaces of even and odd supertraces, $T_A=T_A^0\oplus T_A^1$ and that $T_A^1=0$ if the parity automorphism is inner.

In the sequel we only consider the case where $\dim T_A<\infty$ and there are no nontrivial odd supertraces. Let $A=A_1\otimes A_2$ with the associative algebras A_1 and A_2 endowed with some even supertrace operations t_1 and t_2, respectively. The supertrace on A can be defined by setting $\mathrm{str}(a_1\otimes a_2)=t_1(a_1)t_2(a_2)$, $\forall a_1\in A_1$, $\forall a_2\in A_2$. As a result, one concludes that $T_A=T_{A_1}\otimes T_{A_2}$. In the case of $SH_N(\nu)$, one thus can always separate out a contribution of the center of mass coordinates as an overall factor (SH_1 admits the unique supertrace).

If A is finite dimensional then the existence of two different supertraces indicates that A admits nontrivial both-side ideals. Actually, consider the bilinear form $B(f,g)=\alpha_1\,\mathrm{str}_1(fg)+\alpha_2\,\mathrm{str}_2(fg)$ with arbitrary parameters α_1, $\alpha_2\in\mathbb{C}$ and elements $f,g\in A$. The determinant of this bilinear form is some polynomial of α_1 and α_2. Therefore it vanishes for certain ratios α_1/α_2 or α_2/α_1 according to the central theorem of algebra. Thus, for these values of the parameters the bilinear form B degenerates and admits nontrivial null vectors x, $B(x,g)=0$, $\forall g\in A$. It is easy to see that the linear space $\mathcal{I}$ of all null vectors x is some both-side ideal of A. For infinite-dimensional algebras the existence of several supertraces does not necessarily imply the existence of ideals. As mentioned in the Introduction, the existence of several supertrace operations may be related to the existence of inequivalent representations. Also, it is worth mentioning that for the case of infinite-dimensional algebras and representations under investigation, it can be difficult to use the standard (i.e., matrixwise) definition of the supertrace. In this situation the formal definition of the supertraces on the algebra we implement in this paper is the only rigorous one.

Let l_A be the Lie superalgebra that is isomorphic to A as a linear space and is endowed with the product law (12). It contains the subalgebra $sl_A \in l_A$ spanned by elements g, such that $\mathrm{str}_p(g)=0$ for all p. Evidently sl_A forms the ideal of l_A. The factor algebra $t_A=l_A/sl_A$ is a commutative Lie algebra isomorphic to T_A^* as a linear space. Elements of t_A different from the unit element of A (which exist if $\dim T_A>1$) can induce outer automorphisms of sl_A. Let us note that it is this sl_A Lie superalgebra that usually has physical applications. For the case of $SH_N(\nu)$ under consideration, the algebra $l_{SH_N(\nu)}$ is identified with the algebra $W_{N,\infty}(\nu)$ introduced in Ref. 8. We therefore conclude that these algebras are not simple for $N>2$ because it is shown below that $SH_N(\nu)$ admits several supertraces for $N>2$. Instead, one can consider the algebras $sW_{N,\infty}(\nu)$.

Let l_A contain some subalgebra $\mathscr{L}$ such that A decomposes into a direct sum of irreducible representations of $\mathscr{L}$ with respect to the adjoint action of $\mathscr{L}$ on A via supercommutators. Then, only trivial representations of $\mathscr{L}$ can contribute to any supertrace on A. Actually, consider some nontrivial irreducible representation R of $\mathscr{L}$. Any $r \in R$ can be represented as

$$r=\sum_j [l_j, r_j\}, \quad l_j \in \mathscr{L}, \quad r_j \in R, \tag{32}$$

since elements of the form (32) span the invariant subspace in R. From (11) it follows then that $\mathrm{str}(r)=0$, $\forall r \in R$.

From the definition of the supertrace, it follows that

$$\mathrm{str}(a_1 a_2)+\mathrm{str}(a_2 a_1)=0, \tag{33}$$

for arbitrary odd elements a_1 and a_2 of A. A simple consequence of this relation is that

$$\mathrm{str}(a_1 a_2 \cdots a_n + a_2 \cdots a_n a_1 + \cdots + a_n a_1 \cdots a_{n-1})=0 \tag{34}$$

is true for an arbitrary even n if all a_i are some odd elements of A. Since we assume that the supertrace is even, (34) is true for any n. This simple property turns out to be practically useful because, when odd generating elements are subject to some commutation relations with the right-hand sides expressed via even generating elements like in (2), it often allows one to reduce evaluation of the supertrace of a degree-n polynomial of a_i to supertraces of lower degree polynomials.

Another useful property is that in order to show that the characteristic property of the supertrace (11) is true for any $x,g \in A$, it suffices to show this for a particular case where x is arbitrary while g is an arbitrary generating element of some fixed system of generating elements. Then (11) for general x and g will follow from the properties that A is associative and str is linear. For the particular case of $SH_N(\nu)$, this means that it is enough to set either $g=a_i^\alpha$ or $g=K_{ij}$.

Let us now turn to some specific properties of $SH_N(\nu)$ as a particular realization of A.

By identifying $\mathscr{L}$ with sl_2 (5) and taking into account that $SH_N(\nu)$ decomposes into a direct sum of irreducible finite-dimensional representations of sl_2, one arrives at the following.

Lemma 1: str(x) can be different from zero only when x is sl_2 singlet, i.e. $[T^{\alpha\beta}, x]=0$.

Corollary: Any supertrace on $SH_N(\nu)$ is even.

Analogously one deduces consequences of the S_N symmetry. In particular, one proves the following.

Lemma 2: Given $c \in S_N$ such that $cF=\mu Fc$ for some element F and any constant $\mu \neq 1$, str$(F)=0$. Given monomial $F = b^{I_1} b^{I_2} \cdots b^{I_s} \sigma$ with $b^{I_k} \in \mathfrak{B}_\sigma$ and a cycle c_0 in the decomposition (15) of σ, one concludes that str$(F)=0$ if $\Pi_{k:c(I_k)=c_0} \lambda_{I_k} \neq 1$, where λ_{I_k} are the eigenvalues (21) of b^{I_k}.

IV. GROUND LEVEL CONDITIONS

Let us analyze restrictions on a form of $\mathrm{str}(a), a \in S_N$, which follow from the defining relations of $SH_N(\nu)$.

First, we describe supertraces on the group algebra of S_N. Let some permutation σ decompose into n_1 cycles of length 1, n_2 cycles of length 2,... and n_N cycles of length N. The non-negative integers n_k satisfy the relation

$$\sum_{k=1}^{N} k n_k = N \tag{35}$$

and fix σ up to some conjugation $\sigma \to \tau\sigma\tau^{-1}$, $\tau \in S_N$. Thus

$$\mathrm{str}(\sigma) = \varphi(n_1, n_2, \ldots, n_N), \tag{36}$$

where $\sigma(n_1, n_2, \ldots, n_N)$ is an arbitrary function. Obviously the linear space of invariant functions on S_N [i.e., such that $f(\tau\sigma\tau^{-1}) = f(\sigma)$] coincides with the linear space of supertraces on the group algebra of S_N. Therefore, the dimension of the linear space of supertraces is equal to the number $p(N)$ of independent solutions of (35), the number of conjugacy classes of S_N. One can introduce the generating function for $p(N)$ as $P(q) = \Sigma_{n=0}^{\infty} p(n) q^n = \Pi_{k=1}^{\infty} 1/(1-q^k)$. The properties of this generating function and of the quantities $p(N)$ are discussed in detail, e.g., in Ref. 17.

According to the general argument of the previous section, the existence of several independent traces implies that the group algebra of S_N must have some ideals. Indeed, it can be shown to decompose into a direct sum of matrix algebras Mat_n.

Since the group algebra of S_N is embedded into $SH_N(\nu)$, some additional restrictions on the functions $\varphi(n_1, n_2, \ldots, n_N)$ follow from (11) and the defining relations (2)–(3) of $SH_N(\nu)$. Actually, consider some elements b^I such that $\lambda_I = -1$. Then, one finds from (11) and (21) that $\mathrm{str}(b^I b^J \sigma) = -\mathrm{str}(b^J \sigma b^I) = \mathrm{str}(b^J b^I \sigma)$, and therefore

$$\mathrm{str}([b^I, b^J]\sigma) = 0. \tag{37}$$

Since these conditions restrict supertraces of degree-0 polynomials of a_i^α, we call them ground level conditions (GLC). Thus, for every permutation σ and any even integer $2k$ such that there exists some cycle c of length $|c| = 2k$ in the decomposition (15), we have GLC (37) with b^I such that $c(I) = c$. Note, however, that if $\lambda_J \neq -1$ or $c(J) \neq c(I)$, then the relation $\mathrm{str}([b^I, b^J]\sigma) = 0$ is trivially satisfied as a consequence of *Lemma 2*.

It is convenient to rewrite GLC in the following form:

$$\mathrm{str}(c_0\sigma_0) = -\mathrm{str}(([b_{0k}^0, b_{0k}^1] - 1)c_0\sigma_0), \tag{38}$$

where c_0 is any cycle of even length $2k$ in the decomposition of the permutation $\sigma = c_0\sigma_0$ and b_{0k}^α is the corresponding variable (17) with $(\lambda_0)^k = -1$, i.e., $c_0 b_{0k}^\alpha = -b_{0k}^\alpha c_0$, $\sigma_0 b_{0k}^\alpha = b_{0k}^\alpha \sigma_0$ and $\lambda_0 = \exp(2\pi i/|c_0|)$.

To work out the explicit form of the restrictions on the functions $\varphi(n_1, n_2, \ldots, n_N)$ that follow from GLC, one has to use the following simple facts from the theory of the symmetric group.

Lemma 3: Let c_1 and c_2 be two distinct cycles in the decomposition (15). Let indices i_1 and i_2 belong to the subsets of indices associated with the cycles c_1 and c_2, respectively. Then the permutation $c = c_1 c_2 K_{i_1 i_2}$ is a cycle of length $|c| = |c_1| + |c_2|$.

Lemma 4: Given cyclic permutation $c \in S_N$, let $i \neq j$ be two indices such that $c^k(i) = j$, where k is some positive integer, $k < |c|$. Then $cK_{ij} = c_1 c_2$, where $c_{1,2}$ are some noncoinciding mutually commuting cycles such that $|c_1| = k$ and $|c_2| = |c| - k$.

Using the definition (17), the commutation relations (1)–(3) and *Lemmas 3* and *4*, one reduces GLC to the following system of equations:

$$n_{2k}\varphi(n_1,\dots,n_{2k},\dots,n_N) = -\nu n_{2k}\Bigg(2\sum_{s\neq k,s=1}^{2k-1} O_s\varphi(n_1,\dots,n_s+1,\dots,n_{2k-s}+1,\dots,n_{2k}-1;\dots,n_N)$$
$$+2O_k\varphi(n_1,\dots,n_k+2,\dots,n_{2k}-1,\dots,n_N)$$
$$+\sum_{s\neq 2k;s=1}^{N} sn_s\varphi(n_1,\dots,n_s-1,\dots,n_{2k}-1,\dots,n_{2k+s}+1,\dots,n_N)$$
$$+2k(n_{2k}-1)\varphi(n_1,\dots,n_{2k}-2,\dots,n_{4k}+1,\dots,n_N)\Bigg), \tag{39}$$

where $O_k=0$ for k even and $O_k=1$ for k odd.

Let us note that by virtue of the substitution

$$\varphi(n_1,\dots,n_N)=\nu^{E(\sigma)}\tilde{\varphi}(n_1,\dots,n_N), \tag{40}$$

where $E(\sigma)$ is the number of cycles of even length in the decomposition of σ (15), i.e.

$$E(\sigma)=n_2+n_4+\cdots, \tag{41}$$

one can get rid of the explicit dependence of ν from GLC (39). As a result, there are two distinguishing cases, $\nu=0$ and $\nu\neq 0$.

For lower N the conditions (39) take the form

$$\varphi(0,1)+2\nu\varphi(2,0)=0 \tag{42}$$

for $N=2$ [cf. (9)],

$$\varphi(1,1,0)+2\nu\varphi(3,0,0)+\nu\varphi(0,0,1)=0, \tag{43}$$

for $N=3$ and

$$\varphi(2,1,0,0)+2\nu\varphi(4,0,0,0)+2\nu\varphi(1,0,1,0)=0,$$

$$\varphi(0,2,0,0)+2\nu\varphi(2,1,0,0)+2\nu\varphi(0,0,0,1)=0,$$

$$\varphi(0,0,0,1)+4\nu\varphi(1,0,1,0)=0,$$

for $N=4$. As a result one finds 1-parametric families of solutions for $N=1$ and $N=2$ and 2-parametric families of solutions for $N=3$ and $N=4$.

Let G_N be the number of independent solutions of (39). As we show in the next section $G_N=\dim T_{SH_N(\nu)}$ for all ν. In other words, all other conditions on the supertrace do not impose any restrictions on the functions $\varphi(n_1,\dots,n_N)$ but merely express supertraces of higher-order polynomials of a_i^α in terms of $\varphi(n_1,\dots,n_N)$.

In the Appendix A we prove the following.

Theorem 1: *$G_N=q(N)$, where $q(N)$ is a number of partitions of N into a sum of odd positive integers, i.e. the number of the solutions of the equation $\Sigma_{k=0}^{\infty}(2k+1)n_k=N$ for non-negative integers n_i.*

One can guess this result from the particular case of $\nu=0$, where GLC tell us that $\varphi(n_1,\dots,n_N)$ can be nonvanishing (and arbitrary) only when all $n_{2k}=0$. Interestingly enough, G_N remains the same for $\nu\neq 0$.

V. SUPERTRACE FOR GENERAL ELEMENTS

In this section we prove the following.

Theorem 2: $\dim T_{SH_N(\nu)} = G_N$, *where* G_N *is the number of independent solutions of the ground level conditions (39).*

The proof of the *Theorem 2* will be given in a constructive way by virtue of the following double induction procedure.

(i) Assuming that GLC are true and $\mathrm{str}\{b^I, P_p(a)\sigma\} = 0$, $\forall P_p(a)$, σ and I provided that $b^I \in \mathfrak{B}_\sigma$ and

$$\lambda(I) \neq -1; \quad p \leqslant k,$$

or

$$\lambda(I) = -1, \quad E(\sigma) \leqslant l, \quad p \leqslant k,$$

or

$$\lambda(I) = -1; \quad p \leqslant k-2,$$

where $P_p(a)$ is an arbitrary degree p polynomial of a_i^α (p is odd) and $E(\sigma)$ is the number of cycles of even length in the decomposition (15) of σ, one proves that there exists such a unique extension of the supertrace that the same is true for $l \to l+1$.

(ii) Assuming that $\mathrm{str}\{b^I, P_p(a)\sigma\} = 0$, $\forall P_p(a)$, σ and b^I, such that $\sigma(I) = \sigma$, $p \leqslant k$ one proves that there exists such a unique extension of the supertrace that the assumption (i) is true for $k \to k+2$ and $l = 0$.

As a result this inductive procedure extends uniquely any solution of GLC to some supertrace on the whole $SH_N(\nu)$. [Let us remind ourselves that the supertrace of any odd element of $SH_N(\nu)$ is trivially zero by sl_2 invariance].

The inductive proof of *Theorem 2* is based on the S_N covariance of the whole setting and the following important lemma.

Lemma 5: Given permutation σ, *which has* $E(\sigma)$ *cycles of even length in the decomposition (15), the quantity* $f^{IJ}\sigma$ *for* $\sigma(I) = \sigma(J) = \sigma$ *and* $\lambda_I = \lambda_J = -1$ *can be uniquely expanded as* $f^{IJ}\sigma = \Sigma_q \alpha_q \sigma_q$, *where* α_q *are some coefficients and* $E(\sigma_q) = E(\sigma) - 1, \forall q$.

Lemma 5 is a simple consequence of the particular form of the structure coefficients f^{IJ} (27) and *Lemmas 3* and *4*. The proof is straightforward. Let us stress that it is *Lemma 5* that accounts for the specific properties of the algebra $SH_N(\nu)$ in the analysis of this section.

In practice, it is convenient to work with the exponential generating functions

$$\Psi_\sigma(\mu) = \mathrm{str}(e^S \sigma), \quad S = \sum_{L=1}^{2N} (\mu_L b^L), \tag{44}$$

where σ is some fixed element of S_N, $b^L \in \mathfrak{B}_\sigma$, and $\mu_L \in \mathbb{C}$ are independent parameters. By differentiating over μ_L, one can obtain an arbitrary polynomial of b^L in front of σ. The exponential form of the generating functions implies that these polynomials are Weyl ordered. In these terms the induction on a degree of polynomials is equivalent to the induction on a degree of homogeneity in μ of the power series expansions of $\Psi_\sigma(\mu)$.

As a consequence of the general properties discussed in the preceding sections, the generating function $\Psi_\sigma(\mu)$ must be invariant under the S_N similarity transformations,

$$\Psi_{\tau\sigma\tau^{-1}}(\mu) = \Psi_\sigma(\tilde{\mu}), \tag{45}$$

where the S_N transformed parameters are of the form

$$\tilde{\mu}_I = \sum_J \left(\mathfrak{M}(\tau\sigma\tau^{-1})\mathfrak{M}^{-1}(\tau)\Lambda^{-1}(\tau)\mathfrak{M}(\tau)\mathfrak{M}^{-1}(\sigma)\right)_I^J \mu_J, \tag{46}$$

and matrices $\mathfrak{M}(\sigma)$ and $\Lambda(\sigma)$ are defined in (22) and (23).

In accordance with the general argument of Sec. III, the necessary and sufficient conditions for the existence of even supertrace are the S_N-covariance conditions (45) and the condition that

$$\mathrm{str}\{b^L, (\exp S)\sigma\} = 0, \quad \text{for any } \sigma \quad \text{and} \quad L. \tag{47}$$

To transform (47) to an appropriate form, let us use the following two general relations, which are true for arbitrary operators X and Y and the parameter $\mu \in \mathbb{C}$:

$$X \exp(Y+\mu X) = \frac{\partial}{\partial \mu} \exp(Y+\mu X) + \int t_2 \exp(t_1(Y+\mu X))[X,Y]\exp(t_2(Y+\mu X))D^1t, \tag{48}$$

$$\exp(Y+\mu X)X = \frac{\partial}{\partial \mu} \exp(Y+\mu X) - \int t_1 \exp(t_1(Y+\mu X))[X,Y]\exp(t_2(Y+\mu X))D^1t, \tag{49}$$

with the convention that

$$D^{n-1}t = \delta(t_1+\cdots+t_n-1)\,\theta(t_1)\cdots\theta(t_n)dt_1\cdots dt_n. \tag{50}$$

The relations (48) and (49) can be derived with the aid of the partial integration (e.g., over t_1) and the following formula:

$$\frac{\partial}{\partial \mu} \exp(Y+\mu X) = \int \exp(t_1(Y+\mu X))X \exp(t_2(Y+\mu X))D^1t, \tag{51}$$

which can be proven by expanding in a power series. The well-known formula

$$[X, \exp(Y)] = \int \exp(t_1 Y)[X,Y]\exp(t_2 Y)D^1t, \tag{52}$$

is a consequence of (48) and (49).

With the aid of (48), (49), and (21), one rewrites (47) as

$$(1+\lambda_L)\frac{\partial}{\partial \mu_L}\Psi_\sigma(\mu) = \int (\lambda_L t_1 - t_2)\mathrm{str}(\exp(t_1 S)[b^L, S]\exp(t_2 S)\sigma)D^1t. \tag{53}$$

This condition should be true for any σ and L and plays the central role in the analysis of this section.

There are two essentially distinguishing cases, $\lambda_L \neq -1$ and $\lambda_L = -1$. In the latter case, the equation (53) takes the form

$$0 = \int \mathrm{str}(\exp(t_1 S)[b^L, S]\exp(t_2 S)\sigma)D^1t, \quad \lambda_L = -1. \tag{54}$$

In Appendix B we show by induction that the equations (53) and (54) are consistent in the following sense:

$$(1+\lambda_K)\frac{\partial}{\partial\mu_K}\int(\lambda_L t_1-t_2)\mathrm{str}(\exp(t_1S)[b^L,S]\exp(t_2S)\sigma)D^1t-(L\leftrightarrow K)=0,$$

$$\lambda_L\neq-1,\quad \lambda_K\neq-1 \tag{55}$$

and

$$(1+\lambda_K)\frac{\partial}{\partial\mu_K}\int\mathrm{str}(\exp(t_1S)[b^L,S]\exp(t_2S)\sigma)D^1t=0,\quad \lambda_L=-1. \tag{56}$$

Note that this part of the proof is quite general and does not depend on a concrete form of the commutation relations of a_i^α in (2).

By expanding the exponential e^S in (44) into power series in μ_K (equivalently b^K) one concludes that the equation (53) uniquely reconstructs the supertrace of monomials containing b^K with $\lambda_K\neq-1$ (from now on called regular polynomials) via supertraces of some lower-order polynomials. The consistency conditions (55) and (56) then guarantee that (53) does not impose any additional conditions on the supertraces of lower degree polynomials and allow one to represent the generating function in the form

$$\Psi_\sigma=\Phi_\sigma(\mu)+\sum_{L:\lambda_L\neq-1}\int_0^1\frac{\mu_L\,d\tau}{1+\lambda_L}\int D^1t(\lambda_L t_1-t_2)\mathrm{str}(e^{t_1(\tau S''+S')}[b^L,(\tau S''+S')]e^{t_2(\tau S''+S')}\sigma), \tag{57}$$

where we have introduced the generating functions Φ_σ for the supertrace of special polynomials, i.e. the polynomials depending only on b^L with $\lambda_L=-1$,

$$\Phi_\sigma(\mu)\overset{\text{def}}{=}\mathrm{str}(e^{S'}\sigma)=\Psi_\sigma(\mu)|_{(\mu_I=0,\quad\forall I:\lambda_I\neq-1)} \tag{58}$$

and

$$S'=\sum_{L:b^L\in\mathfrak{B}_\sigma,\lambda_L=-1}(\mu_L b^L);\quad S''=S-S'. \tag{59}$$

The relation (57) successively expresses the supertrace of higher-order regular polynomials via the supertraces of lower-order polynomials.

One can see that the arguments above prove effectively the inductive hypotheses (i) and (ii) for the particular case where either the polynomials $P_p(a)$ are regular and/or $\lambda_I\neq-1$. Note that for this case the induction on the number of cycles of even length (i) is trivial: one simply proves that a power of polynomial can be increased by 2.

Let us now turn to the less trivial case of the special polynomials:

$$\mathrm{str}\{b^I,(\exp S')\sigma\}=0,\quad \lambda_I=-1. \tag{60}$$

Consider the part of $\mathrm{str}\{b^I,(\exp S')\sigma\}$, which is of order k in μ, and suppose that $E(\sigma)=l+1$. According to (54), the conditions (60) give

$$0=\int\mathrm{str}(\exp(t_1S')[b^I,S'']\exp(t_2S')\sigma)D^1t. \tag{61}$$

Substituting $[b^I,S']=\mu^I+\nu\Sigma_M f^{IM}\mu_M$, where the quantities f^{IJ} and μ^I are defined in (25)–(28), one can rewrite the equation (61) in the form

$$\mu^I\Phi_\sigma(\mu)=-\nu\int \mathrm{str}\Big(\exp(t_1S')\sum_M f^{IM}\mu_M\,\exp(t_2S')\sigma\Big)D^1t. \tag{62}$$

Now we use the inductive hypothesis (i). The right-hand side of (62) is a supertrace of at most a degree $k-1$ polynomial of a_i^α in the sector of degree k polynomials in μ. Therefore one can use the inductive hypothesis (i) to obtain

$$\int \mathrm{str}\Big(\exp(t_1S')\sum_M f^{IM}\mu_M\,\exp(t_2S')\sigma\Big)D^1t=\int \mathrm{str}\Big(\exp(t_2S')\exp(t_1S')\sum_M f^{IM}\mu_M\sigma\Big)D^1t,$$

where we made use of the simple fact that $\mathrm{str}(S'F\sigma)=-\mathrm{str}(F\sigma S')=\mathrm{str}(FS'\sigma)$ due to the definition of S'.

As a result, the inductive hypothesis allows one to transform (60) to the following form:

$$X^I\equiv\mu^I\Phi_\sigma(\mu)+\nu\,\mathrm{str}\Big(\exp(S')\sum_M f^{IM}\mu_M\sigma\Big)=0. \tag{63}$$

By differentiating this equation with respect to μ_J, one obtains, after symmetrization,

$$\frac{\partial}{\partial\mu_J}(\mu^I\Phi_\sigma(\mu))+(I\leftrightarrow J)=-\nu\int \mathrm{str}\Big(e^{t_1S'}b^Je^{t_2S'}\sum_M f^{IM}\mu_M\sigma\Big)D^1t+(I\leftrightarrow J). \tag{64}$$

An important point is that the system of equations (64) is equivalent to the original equations (63), except for the ground level part $\Phi_\sigma(0)$. This can be easily seen from the simple fact that the general solution of the system of equations $(\partial/\partial\mu_J)X^I(\mu)+(\partial/\partial\mu_I)X^J(\mu)=0$ for entire functions $X^I(\mu)$ is of the form $X^I(\mu)=X^I(0)+\Sigma_J c^{IJ}\mu_J$, where $X^I(0)$ and $c^{JI}=-c^{IJ}$ are some constants. The part of (63) linear in μ is, however, equivalent to the ground level conditions analyzed in the previous section. Thus (64) contains all information additional to (39). For this reason we will, from now on, analyze the equation (64).

Using again the inductive hypothesis we move b^1 to the left and to the right with equal weights to get

$$\begin{aligned}\frac{\partial}{\partial\mu_J}\mu^I\Phi_\sigma(\mu)+(I\leftrightarrow J)=&-\frac{\nu}{2}\sum_M \mathrm{str}(\exp(S')\{b^J,f^{IM}\}\mu_M\sigma)\\&-\frac{\nu}{2}\int\sum_{L,M}(t_1-t_2)\mathrm{str}(\exp(t_1S')F^{JL}\mu_L\,\exp(t_2S')f^{IM}\mu_M\sigma)\\&\times D^1t+(I\leftrightarrow J).\end{aligned} \tag{65}$$

The last term on the right-hand side of this expression can be shown to vanish under the supertrace operation due to the factor of (t_1-t_2), so that one is left with the equation

$$L^{IJ}\Phi_\sigma(\mu)=-\frac{\nu}{2}R^{IJ}(\mu), \tag{66}$$

where

$$R^{IJ}(\mu)=\sum_M \mathrm{str}(\exp(S')\{b^J,f^{IM}\}\mu_M\sigma)+(I\leftrightarrow J) \tag{67}$$

and

$$L^{IJ}=\frac{\partial}{\partial\mu_J}\mu^I+\frac{\partial}{\partial\mu_I}\mu^J. \tag{68}$$

The differential operators L^{IJ} satisfy the standard $sp(2E(\sigma))$ commutation relations

$$[L^{IJ},L^{KL}]=-(\mathscr{C}^{IK}L^{JL}+\mathscr{C}^{IL}L^{JK}+\mathscr{C}^{JK}L^{IL}+\mathscr{C}^{JL}L^{IK}). \tag{69}$$

We show by induction in Appendix C that this algegra is consistent with the right-hand side of the basic relation (66), i.e. that

$$[L^{IJ},R^{KL}]-[L^{KL},R^{IJ}]=-(\mathscr{C}^{IK}R^{JL}+\mathscr{C}^{JL}R^{IK}+\mathscr{C}^{JK}R^{IL}+\mathscr{C}^{IL}R^{JK}). \tag{70}$$

Generally, these consistency conditions guarantee that the equations (66) express $\Phi_\sigma(\mu)$ in terms of R^{IJ} in the following way:

$$\Phi_\sigma(\mu)=\Phi_\sigma(0)+\frac{\nu}{8E(\sigma)}\sum_{I,J=1}^{2E(\sigma)}\int_0^1\frac{dt}{t}\,(1-t^{2E(\sigma)})(L_{IJ}R^{IJ})(t\mu), \tag{71}$$

provided that

$$R^{IJ}(0)=0. \tag{72}$$

The latter condition must hold for the consistency of (66), since its left-hand side vanishes at $\mu_I=0$. In the formula (71) it guarantees that the integral on t converges. In the case under consideration the property (72) is indeed true as a consequence of the definition (67).

Taking into account *Lemma 5* and the explicit form of R^{IJ} (67), one concludes that the equation (71) expresses uniquely the supertrace of special polynomials via the supertraces of polynomials of lower degrees or via the supertraces of special polynomials of the same degree with a lower number of cycles of even length, provided that the μ-independent term $\Phi_\sigma(0)$ is an arbitrary solution of GLC. This completes the proof of *Theorem 2*.

Comment 1: The formulas (57) and (71) can be effectively used in practical calculations of supertraces of particular elements of $SH_N(\nu)$.

Comment 2: Any supertrace on $SH_N(\nu)$ is determined unambiguously in terms of its values on the group algebra of S_N.

Corollary: Any supertrace on $SH_N(\nu)$ is ρ invariant, $\mathrm{str}(\rho(x))=\mathrm{str}(x)$, $\forall x\in SH_N(\nu)$, for the antiautomorphism ρ (30).

This is true, due to *Comment 2*, because σ and $\sigma^{-1}=\rho(\sigma)$ belong to the same conjugacy class of S_N so that $\mathrm{str}(\rho(\sigma))=\mathrm{str}(\sigma)$.

VI. CONCLUSIONS

In this paper we have shown that the algebras $SH_N(\nu)$ can be endowed with $q(N)$-independent supertrace operations, where $q(N)$ is the number of partitions of N into a sum of odd positive integers. We hope to apply the supertraces constructed in this paper to the analysis of the invariant forms of $SH_N(\nu)$. Although a definition of the supertraces on $SH_N(\nu)$ behaves regularly with the parameter ν [in particular, the number of supertraces $q(N)$ is ν independent], one can expect that this is not the case for the related bilinear forms, which can degenerate for some special values of ν, thus giving rise to ideals of $SH_N(\nu)$ as it happens[14] for the simplest case of $N=2$. The analysis of the structure of these ideals is a challenging problem important for various applications of $SH_N(\nu)$, including an analysis of its representations. We are going to study this problem for some lower values of $N>2$ in the future publication.

In conclusion, let us note that the method of the analysis of supertraces presented in this paper is rather general. Practically the only information of the specific structure of $SH_N(\nu)$ is that *Lemma 5* is true. Hopefully one can use the analogous methods for the analysis of supertraces of other associative algebras.

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APPENDIX A: INDEPENDENCE G_N OF ν

For the case $\nu=0$ it was argued in Sec. IV that (39) possesses $q(N)$ independent solutions. Let us now consider the case $\nu\neq 0$. By induction on a number of cycles of even length $e=E(\sigma)$, we show that given σ with $E(\sigma)=e\geqslant 1$ there is only one independent equation on $\mathrm{str}(\sigma)$, provided that all equations (39) with $E(\sigma)=e'<e$ are resolved. In this proof we set $\nu=1$, which does not lead to the loss of generality due to the scaling property (40). The first step of the induction consists of the observation that there are no equations for the case $E(\sigma)=0$.

Let us consider the case where there are two equations (38) on $\mathrm{str}(\sigma)$ for some σ. This is only possible if $\sigma=c_1c_2\sigma'$, where c_1 and c_2 are some cycles in the decomposition of σ, such that $|c_1|=2k$, $|c_2|=2l$, and $k\neq l$. Note that $E(\sigma')=E(\sigma)-2=e-2$.

Without loss of generality, let us set

$$c_1=K_{12}K_{23}\cdots K_{(2k-1)2k}, \quad c_2=K_{(2k+1)(2k+2)}\cdots K_{(2k+2l-1)(2k+2l)}, \tag{A1}$$

$$b_1^\alpha=\frac{1}{\sqrt{2k}}\,(a_1^\alpha-a_2^\alpha+\cdots-a_{2k}^\alpha), \quad b_2^\alpha=\frac{1}{\sqrt{2l}}\,(a_{2k+1}^\alpha-a_{2k+1}^\alpha+\cdots-a_{2k+2l}^\alpha). \tag{A2}$$

Also, we introduce

$$c=K_{1(2k+1)}c_1c_2=K_{12}K_{23}\cdots K_{(2k+2l-1)(2k+2l)} \tag{A3}$$

and

$$b^\alpha=\frac{1}{\sqrt{2k+2l}}\,(\sqrt{2k}b_1^\alpha+\sqrt{2l}b_2^\alpha)=\frac{1}{\sqrt{2k+2l}}\,(a_1^\alpha-a_2^\alpha+\ldots-a_{2k+2l}^\alpha). \tag{A4}$$

The corresponding equations (38) take the form

$$\mathrm{str}(\sigma)=-\mathrm{str}(([b_1^0,b_1^1]-1)\sigma) \tag{A5}$$

and

$$\mathrm{str}(\sigma)=-\mathrm{str}(([b_2^0,b_2^1]-1)\sigma). \tag{A6}$$

Using the following simple identity that holds for any trace on S_N,

$$\mathrm{str}\left(\frac{1}{2k}\sum_{p=1}^{2k}\sum_{q=2k+1}^{2k+2l}K_{pq}\sigma\right)=2l\ \mathrm{str}(K_{1(2k+1)}\sigma),$$

one can rewrite the right-hand side of (A5) as

$$\mathrm{str}(([b_1^0,b_1^1]-1)\sigma)=\mathrm{str}\left(\left([b_1^0,b_1^1]-1-\frac{1}{2k}\sum_{p=1}^{2k}\sum_{q=2k+1}^{2k+2l}K_{pq}\right)\sigma\right)+2l\ \mathrm{str}(K_{1(2k+1)}\sigma). \tag{A7}$$

The direct analysis based on the commutation relations (2) and (3) then shows that the first term on the right-hand side of (A7) is the supertrace of a linear combination of permutations, which all contain the cycle c_2 in their decompositions. The second term is the supertrace of the permutation that contains the cycle c (A3) in its decomposition. It is easy to see that for each of these terms the number of cycles of even length is $E(\sigma)-1$. This allows us to apply the equation (38) to each of these terms due to the inductive hypothesis. We identify c_0 with c_2 and c, respectively, for the first and second terms on the right-hand side of (A7). As a result the equation (A5) turns out to be transformed to the form

$$\mathrm{str}(\sigma)=\mathrm{str}\left(([b_2^0,b_2^1]-1)\left([b_1^0,b_1^1]-1-\frac{1}{2k}\sum_{p=1}^{2k}\sum_{q=2k+1}^{2k+2l}K_{pq}\right)\sigma\right)$$
$$+\mathrm{str}(([b^0,b^1]-1)2lK_{1(2k+1)}\sigma). \tag{A8}$$

Analogously, one obtains for (A6),

$$\mathrm{str}(\sigma)=\mathrm{str}\left(([b_1^0,b_1^1]-1)\left([b_2^0,b_2^1]-1-\frac{1}{2l}\sum_{p=1}^{2k}\sum_{q=2k+1}^{2k+2l}K_{pq}\right)\sigma\right)$$
$$+\mathrm{str}(([b^0,b^1]-1)2kK_{1(2k+1)}\sigma) \tag{A9}$$

Let us prove that the difference of the right-hand sides of (A8) and (A9) vanishes. With the aid of the simple consequence of the S_N invariance,

$$\frac{1}{4kl}\,\mathrm{str}\left([b_i^0,b_i^1]\sum_{p=1}^{2k}\sum_{q=2k+1}^{2k+2l}K_{pq}\sigma\right)=\mathrm{str}([b_i^0,b_i^1]K_{1(2k+1)}\sigma),\quad i=1,2,$$

this difference can be transformed to the form

$$X=\mathrm{str}((2k[b_1^0,b_1^1]-2l[b_2^0,b_2^1])K_{1(2k+1)}\sigma), \tag{A10}$$

where we have taken into account that

$$\mathrm{str}([b^0,b^1]K_{1(2k+1)}\sigma)=0, \tag{A11}$$

as a consequence of the inductive hypothesis and GLC (37), and that

$$\mathrm{str}([([b_2^0,b_2^1]-1),([b_1^0,b_1^1]-1)]\sigma)=0, \tag{A12}$$

since each term in the commutator belongs to the group algebra of S_N and commutes with σ so that (A12) vanishes for any supertrace on the group algebra of S_N.

Using the relation $b_1^\alpha=1/\sqrt{2k}(\sqrt{2k+2l}b^\alpha-\sqrt{2l}b_2^\alpha)$ one transforms X to the form

$$X=2\,\mathrm{str}((k+l)[b^0,b^1]-\sqrt{l(k+l)}[b^0,b_2^1]-\sqrt{l(k+l)}[b_2^0,b^1])K_{1(2k+1)}\sigma). \tag{A13}$$

Due to the S_N invariance the second term on the right-hand side of (A13) can be rewritten as

$$
\begin{aligned}
&-2\sqrt{l(k+l)}\,\mathrm{str}([b^0,b_2^1]K_{1(2k+1)}\sigma)\\
&\quad=-\frac{\sqrt{l(k+l)}}{k+l}\sum_{p=1}^{2k+2l}\mathrm{str}(c^p[b^0,b_2^1]c^{-p}K_{1(2k+1)}\sigma)\\
&\quad=-\frac{\sqrt{l}}{\sqrt{k+l}}\,\mathrm{str}\left(\left[b^0,\sum_{p=1}^{2k+2l}(-1)^p c^p b_2^1 c^{-p}\right]K_{1(2k+1)}\sigma\right)\\
&\quad=-2l\ \mathrm{str}([b^0,b^1]K_{1(2k+1)}\sigma). \qquad \text{(A14)}
\end{aligned}
$$

Analogously, one can transform the third term on the right-hand side of (A13). Using again (A11), one concludes that $X=0$.

Thus, it is shown that the number of solutions of (39) is equal to the number of the conjugacy classes in S_N with $E(\sigma)=0$. This completes the proof of *Theorem 1*.

APPENDIX B: CONSISTENCY FOR $\lambda\neq-1$

Let us prove by induction that the equations (55) are true for any two $\mu_1\equiv\mu_{K_1}$ and $\mu_2\equiv\mu_{K_2}$, such that both $\lambda_1\equiv\lambda_{K_1}\neq-1$ and $\lambda_2\equiv\lambda_{K_2}\neq-1$. To implement induction one selects from (47) a part of order k in μ and observes that it contains the anticommutator of b^L with a degree k polynomial in b^M, while the part on the right-hand side of the differential version (53) of (47), which is of the same order in μ has the order $k-1$ as the polynomial of b^M. This happens because of the presence of the commutator $[b^L,S]$, which is a degree zero polynomial due to the basic relations (2) and (3). As a result, the inductive hypothesis allows one to use the properties of the supertrace, provided that the above commutator is always handled as the right-hand side of (2) (i.e., it is not allowed to represent it again as a difference of the second-order polynomials).

Direct differentiation with the aid of (51) gives

$$
\begin{aligned}
&(1+\lambda_2)\frac{\partial}{\partial\mu_2}\int(\lambda_1 t_1-t_2)\mathrm{str}(e^{t_1 S}[b^1,S]e^{t_2 S}\sigma)D^1t-(1\leftrightarrow2)\\
&\quad=\left(\int(1+\lambda_2)(\lambda_1 t_1-t_2)\mathrm{str}(e^{t_1 S}[b^1,b^2]e^{t_2 S}\sigma)D^1t-(1\leftrightarrow2)\right)\\
&\qquad+\left(\int(1+\lambda_2)(\lambda_1(t_1+t_2)-t_3)\mathrm{str}(e^{t_1 S}b^2e^{t_2 S}[b^1,S]e^{t_3 S})D^2t-(1\leftrightarrow2)\right)\\
&\qquad+\left(\int(1+\lambda_2)(\lambda_1 t_1-t_2-t_3)\mathrm{str}(e^{t_1 S}[b^1,S]e^{t_2 S}b^2e^{t_3 S}\sigma)D^2t-(1\leftrightarrow2)\right). \qquad \text{(B1)}
\end{aligned}
$$

We have to show that the right-hand side of (B1) vanishes. Let us first transform the second and the third terms on the right-hand side of (B1). The idea is to move the operators b^2 through the exponentials toward the commutator $[b^1,S]$ so that to use then Jacobi identities for the double commutators. This can be done in two different ways inside the supertrace so that one has to fix appropriate weight factors for each of these processes. The correct weights turn out to be

$$
D^2t(\lambda_1(t_1+t_2)-t_3)b^2\equiv D^2t(\lambda_1-t_3(1+\lambda_1))b^2=D^2t\left(\left(\frac{\lambda_1\lambda_2}{1+\lambda_2}-t_3(1+\lambda_1)\right)\overrightarrow{b^2}+\frac{\lambda_1}{1+\lambda_2}\overleftarrow{b^2}\right) \qquad \text{(B2)}
$$

and

$$D^2t(\lambda_1 t_1 - t_2 - t_3)b^2 \equiv D^2t((\lambda_1+1)t_1 - 1)b^2 = D^2t\left(\left(t_1(1+\lambda_1) - \frac{1}{1+\lambda_2}\right)\overleftarrow{b^2} - \frac{\lambda_2}{1+\lambda_2}\,\overrightarrow{b^2}\right) \tag{B3}$$

in the second and third terms on the right-hand side of (B1), respectively. Here the notations $\vec{A}$ and $\overleftarrow{A}$ imply that the operator A has to be moved from its position to the right and to the left, respectively. Using (52) along with the simple formula

$$\int \phi(t_3,\ldots,t_{n+1})D^n t = \int t_1\phi(t_2,\ldots,t_n)D^{n-1}t \tag{B4}$$

one finds that all terms that involve both $[b^1,S]$ and $[b^2,S]$ cancel pairwise after antisymmetrization $1\leftrightarrow 2$.

As a result, one is left with some terms involving double commutators, which by virtue of Jacobi identities and antisymmetrization all reduce to

$$\int (\lambda_1\lambda_2 t_1 + t_2 - t_1 t_2(1+\lambda_1)(1+\lambda_2))\,\mathrm{str}(\exp(t_1 S)[S,[b^1,b^2]]\exp(t_2 S)\sigma)D^1 t. \tag{B5}$$

Finally, one observes that this expression can be equivalently rewritten in the form

$$\int (\lambda_1\lambda_2 t_1 + t_2 - t_1 t_2(1+\lambda_1)(1+\lambda_2))\left(\frac{\partial}{\partial t_1} - \frac{\partial}{\partial t_2}\right)\mathrm{str}(\exp(t_1 S)[b^1,b^2]\exp(t_2 S)\sigma)D^1 t, \tag{B6}$$

and after integration by parts cancel the first term on the right-hand side of (B1). Thus it is shown that the equations (53) are mutually compatible for the case $\lambda_{1,2}\neq -1$.

Analogously one can show that the equations (53) are consistent with (54). Actually, let $\lambda_1 = -1$, $\lambda_2 \neq -1$. Let us prove that

$$\frac{\partial}{\partial \mu_2}\,\mathrm{str}([b^1,\exp(S)]\sigma) = 0, \tag{B7}$$

provided that the supertrace is well defined for the lower-order polynomials. The explicit differentiation gives

$$\begin{aligned}\frac{\partial}{\partial \mu_2}\,\mathrm{str}([b^1,\exp(S)]\sigma) &= \int \mathrm{str}([b^1,\exp(t_1 S)b^2\,\exp(t_2 S)]\sigma)D^1 t \\ &= (1+\lambda_2)^{-1}\,\mathrm{str}([b^1,(b^2\,\exp(S) + \lambda_2\,\exp(S)b^2)]\sigma) + \cdots,\end{aligned} \tag{B8}$$

where dots denote some terms of the form $\mathrm{str}([b^1,B]\sigma)$ involving further commutators inside B, which therefore amount to some lower-order polynomials and vanish by the inductive hypothesis. As a result, one finds

$$\begin{aligned}\frac{\partial}{\partial \mu_2}\,\mathrm{str}([b^1,\exp(S)]\sigma) &= (1+\lambda_2)^{-1}\,\mathrm{str}((b^2[b^1,\exp(S)] + \lambda_2[b^1,\exp(S)]b^2)\sigma) \\ &\quad + (1+\lambda_2)^{-1}\,\mathrm{str}(([b^1,b^2]\exp(S) + \lambda_2\,\exp(S)[b^1,b^2])\sigma),\end{aligned} \tag{B9}$$

which expression vanishes by the inductive hypothesis as well.

APPENDIX C: CONSISTENCY FOR $\lambda=-1$

In order to prove (70) we use the inductive hypothesis (i). In this appendix we use the convention that any upper or lower indices denoted by the same letter are automatically symmetrized, e.g. $F^{II}\stackrel{\text{def}}{=}1/2(F^{I_1I_2}+F^{I_2I_1})$. Let us write the identity

$$0=\sum_M \ \mathrm{str}([\exp(S')\{b^I,f^{IM}\}\mu_M,b^Jb^J]\sigma)-(I\leftrightarrow J), \tag{C1}$$

which holds due to *Lemma 5* for all terms of degree $k-1$ in μ with $E(\sigma)\leqslant l+1$ and for all lower-order polynomials in μ (one can always move f^{IJ} to σ, combining them into a combination of elements of S_N analyzed in *Lemma 5*).

The straightforward calculation of the commutator on the right-hand side of (C1) gives $0=X_1+X_2+X_3$, where

$$X_1=-\sum_{M,L}\int \mathrm{str}(\exp(t_1S')\{b^J,F^{JL}\}\mu_L\ \exp(t_2S')\{b^I,f^{IM}\}\mu_M\sigma)D^1t-(I\leftrightarrow J),$$

$$X_2=\sum_M \ \mathrm{str}(\exp(S')\{\{b^J,F^{IJ}\},f^{IM}\}\mu_M\sigma)-(I\leftrightarrow J), \tag{C2}$$

$$X_3=\sum_M \ \mathrm{str}(\exp(S')\{b^I,\{b^J,[f^{IM},b^J]\}\}\mu_M\sigma)-(I\leftrightarrow J).$$

The terms bilinear in f in X_1 cancel due to the antisymmetrization $(I\leftrightarrow J)$ and the inductive hypothesis (i). As a result, one can transform X_1 to the form

$$X_1=(-\tfrac{1}{2}[L^{JJ},R^{II}]+2\ \mathrm{str}(e^{S'}\{b^I,f^{IJ}\}\mu^J\sigma))-(I\leftrightarrow J). \tag{C3}$$

Substituting $F^{IJ}=\mathscr{C}^{IJ}+\nu f^{IJ}$ and $f^{IM}=\nu^{-1}([b^I,b^M]-\mathscr{C}^{IM})$, one transforms X_2 to the form

$$X_2=2\mathscr{C}^{IJ}R^{IJ}-2(\mathrm{str}(e^{S'}\{b^J,f^{IJ}\}\mu^I\sigma)-(I\leftrightarrow J))+Y, \tag{C4}$$

where

$$Y=\mathrm{str}(e^{S'}\{\{b^J,f^{IJ}\},[b^I,S']\}\sigma)-(I\leftrightarrow J). \tag{C5}$$

Using that

$$\mathrm{str}(\exp(S')[Pf^{IJ}Q,S']\sigma)=0, \tag{C6}$$

provided that the inductive hypothesis can be used, one transforms Y to the form

$$Y=\mathrm{str}(e^{S'}(-[f^{IJ},(b^IS'b^J+b^JS'b^I)]-b^I[f^{IJ},S']b^J-b^J[f^{IJ},S']b^I+[f^{IJ},\{b^I,b^J\}]S')\sigma). \tag{C7}$$

Let us rewrite X_3 in the form $X_3=X_3^s+X_3^q$, where

$$X_3^s=\frac{1}{2}\sum_M \ \mathrm{str}(e^{S'}(\{b^I,\{b^J,[f^{IM},b^J]\}\}+\{b^J,\{b^I,[f^{IM},b^J]\}\})\mu_M\sigma)-(I\leftrightarrow J),$$

$$X_3^a=\frac{1}{2}\sum_M \ \mathrm{str}(e^{S'}(\{b^I,\{b^J,[f^{IM},b^J]\}\}-\{b^J,\{b^I,[f^{IM},b^J]\}\})\mu_M\sigma)-(I\leftrightarrow J).$$

With the aid of the Jacobi identities $[f^{IM},b^J]-[f^{JM},b^I]=[f^{IJ},b^M]$, one expresses X_3^s in the form

$$X_3^s=\tfrac{1}{2}\,\mathrm{str}(e^{S'}(\{b^I,b^J\}[f^{IJ},S']+[f^{IJ},S']\{b^I,b^J\}+2b^I[f^{IJ},S']b^J+2b^J[f^{IJ},S']b^I)\sigma).$$

X_3^a can be transformed to the form

$$X_3^a=\frac{1}{2}\sum_M \ \mathrm{str}(e^{S'}[F^{IJ},[f^{IM},b^J]]\mu_M\sigma)-(I\leftrightarrow J). \tag{C8}$$

By virtue of the substitutions $F^{IJ}=\mathscr{C}^{IJ}+\nu f^{IJ}$ and $f^{IM}=\nu^{-1}([b^I,b^M]-\mathscr{C}^{IM})$ in (C8) one finds after simple transformations that $Y+X_3=0$. From (C3) and (C4) it follows then that the right-hand side of (C1) equals $1/2([L^{II},R^{JJ}]-[L^{JJ},R^{II}])+2\mathscr{C}^{IJ}R^{IJ}$. This completes the proof of the consistency conditions (70).

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The nonsimultaneous nature of the Schwarzschild *R=0* singularity

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The relationship between the two well-behaved coordinate systems of Lemaître–Tolman–Novikov, and Kruskal–Szekeres–Penrose indicates that the Schwarzschild $R=0$ singularity is intrinsically nonsimultaneous. It follows that the simultaneous synchronous coordinates of Wald and Yip do not exist on the complete Schwarzschild manifold. In the process, the coordinate transformations between the Schwarzschild exterior model in its various common coordinate systems and the vacuum Lemaître–Tolman model (which includes Novikov coordinates and the closed Kantowski–Sachs model) is derived. It is also shown that, contrary to statements in the literature, the closed Kantowski–Sachs model is well-behaved limit of the Lemaître–Tolman model. © *1996 American Institute of Physics.* [S0022-2488(96)01605-9]

I. INTRODUCTION AND NOTATION

The spherically symmetric vacuum space–time is most commonly represented by the Kruskal–Szekeres and Penrose diagrams. The former represents the $R=0$ singularity as a right hyperbola, and the latter as a pair of parallel lines; the former shape implies a gradual emergence of the space–time from the past singularity, with the asymptotically flat regions appearing first and the neck appearing last, and the converse at the future singularity, whereas the latter suggests an instantaneous and simultaneous appearance or disappearance of the entire manifold. Although the $R=0$ surfaces are entirely spacelike, and although every point on, say, the past singularity is equivalent to every other point under T translations, this only establishes local equivalence. If white holes are generated by the big bang, and we can measure emerging signals, do there exist observers for whom it would look simultaneous, or at least homogeneous? The transformation between the causal coordinates of Kruskal–Szekeres and the geodesic coordinates of Lemaître–Tolman will show that $R=0$ is intrinsically nonsimultaneous.

The Schwarzschild[1] exterior metric is

$$ds^2=-\left(1-\frac{2M}{R}\right)dT^2+\frac{dR^2}{\left(1-\frac{2M}{R}\right)}+R^2\,d\Omega^2, \tag{1}$$

where

$$d\Omega^2=d\theta^2+\sin^2\theta\,d\phi^2. \tag{2}$$

The Schwarzschild to Kruskal–Szekeres[2,3] and Penrose[4–6] transformations are

$$U=\tan u=e^{(T+R)/4M}\sqrt{\frac{R}{2M}-1}, \tag{3}$$

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$$V=\tan v=-e^{(R-T)/4M}\sqrt{\frac{R}{2M}-1}, \tag{4}$$

where (U,V) and (u,v) are the Kruskal–Szekeres and Penrose coordinates, respectively. The resulting metrics are

$$ds^2=\frac{-32M^3}{Re^{R/2M}}dU\ dV+R^2\ d\Omega^2, \tag{5}$$

$$ds^2=\frac{-32M^3}{Re^{R/2M}}\frac{du\ dv}{\cos^2 u\ \cos^2 v}+R^2\ d\Omega^2, \tag{6}$$

where R is the solution of

$$e^{R/2M}\left(\frac{R}{2M}-1\right)=-UV=-\tan u\ \tan v. \tag{7}$$

The Lemaître–Tolman metric[7,8] represents spherically symmetric inhomogeneous dust in synchronous comoving coordinates,

$$ds^2=-dt^2+\frac{R'^2}{1+f}dr^2+R^2\ d\Omega^2, \tag{8}$$

where $'\equiv\partial/\partial r$, and $f=f(r)$ is an arbitrary function of coordinate radius that gives both the local spatial geometry, and the energy of the dust particles as a function of r. The areal radius $R=R(t,r)$ is the solution of

$$\dot{R}^2=\frac{2M}{R}+f, \tag{9}$$

where $\dot{}\equiv\partial/\partial t$, and the gravitational mass contained within a comoving sphere of radius r is $M=M(r)$. We will also need

$$\ddot{R}=-\frac{M}{R^2}, \tag{10}$$

$$2\dot{R}\dot{R}'=\frac{2M'}{R}-\frac{2MR'}{R^2}+f', \tag{11}$$

and the identity

$$R'=\left(\frac{M'}{M}-\frac{f'}{f}\right)R-\left[a'+\left(\frac{M'}{M}-\frac{3f'}{2f}\right)(t-a)\right]\dot{R}, \tag{12}$$

which holds for all f (See Refs. 9 and 10). The three (nontrivial) solutions are

elliptic—$f<0$:

$$R=\frac{M}{(-f)}(1-\cos\ \eta), \tag{13}$$

$$(\eta-\sin\ \eta)=\frac{(-f)^{3/2}(t-a)}{M}; \tag{14}$$

parabolic—$f=0$:

$$R=\left(\frac{9M(t-a)^2}{2}\right)^{1/3}; \tag{15}$$

hyperbolic—$f>0$:

$$R=\frac{M}{f}(\cosh\ \eta-1), \tag{16}$$

$$(\sinh\ \eta-\eta)=\frac{f^{3/2}(t-a)}{M}, \tag{17}$$

where $a=a(r)$ is a third arbitrary function that gives the time at which $R=0$—the big bang in cosmology, or the past singularity in vacuum.

The density is given by

$$8\pi\rho=\frac{2M'}{R^2R'}, \tag{18}$$

and since the pressure is zero, the dust particles (and therefore the constant r, θ, ϕ curves) follow geodesics of the space–time.

Obviously from (18) we have vacuum if M is a constant, and this must be equivalent to the Schwarzschild/Kruskal–Szekeres manifold, since it is spherically symmetric. In a previous paper—''P1''[11]—the vacuum Lemaître–Tolman models were discussed, and the wormhole topology of Kruskal–Szekeres was then extended to models that have nonvanishing density everywhere including the wormhole. In addition to constant M, complete coverage of the vacuum manifold requires that $f=-1$ at the narrowest part of the wormhole, where $R'=0$ permanently, and f must approach 0 or positive values as $r\to\infty$. The obvious choice for a, at least in models with $f\leqslant 0$ everywhere, is

$$a=-\frac{\pi M}{(-f)^{3/2}}, \tag{19}$$

since this makes the past and future singularities time symmetric. For models or regions where $f>0$, time symmetry is not possible, and this choice has no particular advantage. The set of all possible choices for $f(r)$ and $a(r)$ corresponds to all the possible families of radial geodesic coordinates for Schwarzschild, which have t as a global proper time along the geodesics. In other words the geodesics are orthogonal to the surfaces of constant proper time. A model where f goes from -1 to ∞ corresponds to the inner geodesics expanding and recollapsing from past to future singularities and the outer geodesics escaping to infinity, i^+ (or collapsing from infinity, i^-) (see Fig. 5 of P1 and below). To obtain Novikov's coordinates (Ref. 12, but see Ref. 13 or 14) for Schwarzschild from the Lemaître–Tolman form (see Fig. 4 of P1), we choose

$$M=\text{const}, \tag{20}$$

$$f=\frac{-1}{1+r^2}, \tag{21}$$

$$a=-\pi M(1+r^2)^{3/2}. \tag{22}$$

II. THE KANTOWSKI–SACHS LIMIT

It is usually stated[15,16] that the closed Kantowski–Sachs model[15] must be derived from the spherically symmetric field equations separately from the Lemaître–Tolman case. This is because $R=R(t)$ only in the former, but in the latter $R'=R'(t,r)\neq 0$. This is not true. We shall show that the Kantowski–Sachs model is a well-behaved limit of the Lemaître–Tolman model.

The closed Kantowski–Sachs metric, which describes a homogeneous, synchronous, comoving dust model, is

$$ds^2=-dt^2+X^2(t)dr^2+R^2(t)d\Omega^2, \tag{23}$$

where

$$t-t_0=\frac{A}{2}(\eta-\pi-\sin\ \eta), \tag{24}$$

$$R=\frac{A}{2}(1-\cos\ \eta), \tag{25}$$

$$X=E+\left(\frac{E}{2}(\pi-\eta)-B\right)\frac{\sin\ \eta}{(1-\cos\ \eta)}, \tag{26}$$

and the density is

$$8\pi\rho=\frac{4E}{A^2(1-\cos\ \eta)^2\left[E+\left(\frac{E}{2}(\pi-\eta)-B\right)\frac{\sin\ \eta}{(1-\cos\ \eta)}\right]}, \tag{27}$$

and A,E and B are constants. The η used here, which runs from 0 to 2π, is related to the one used by Kantowski and Sachs by

$$\eta_{\mathrm{KS}}=\frac{(\eta-\pi)}{2}, \tag{28}$$

and they also specified $E=0$ or 1, thus disallowing rescaling of the r coordinate. They identified the case $E=0$ as the region inside the horizon of the vacuum Schwarzschild model.

It is certainly true that R' must be zero everywhere, but this does not necessarily make the line element (8) degenerate, provided $\sqrt{1+f}$ also goes to zero, i.e., $f=-1$. It was first pointed out by Zel'dovich and Grishchuk[17] that many spatially closed Lemaître–Tolman model necessarily has points where $R(t=\mathrm{const},r)$ is a maximum and thus $R'=0$ there. Hellaby and Lake[10] further showed that, for either extremum to be a regular space–time point, $R'=0$ also requires $a'=0$, $f'=0$, and $M'=0$ at these points if shell crossings are to be avoided, as well as $f=-1$ if a surface layer is to be avoided. It turns out that there is no reason why these conditions cannot hold everywhere. So, let us set

$$\frac{R'}{\sqrt{1+f}}=X(t) \tag{29}$$

and then establish what extra conditions are required to reduce the evolution of (12) for the elliptic case, $f<0$, to that of (26). Substituting (13), (14), and (12) into (29) gives

$$\frac{R'}{\sqrt{1+f}} = \frac{1}{(1-\cos\,\eta)}\left[\frac{M}{(-f)\sqrt{1+f}}\left(\frac{M'}{M}-\frac{f'}{f}\right)(1-\cos\,\eta)^2 - \frac{M}{(-f)\sqrt{1+f}}\left(\frac{M'}{M}-\frac{3f'}{2f}\right)\sin\,\eta(\eta-\sin\,\eta) - \frac{a'\sqrt{-f}}{\sqrt{1+f}}\sin\,\eta\right]$$
$$= X(t) = \frac{1}{(1-\cos\,\eta)}\left[E(1-\cos\,\eta)+\left(\frac{E\pi}{2}-B\right)\sin\,\eta-\left(\frac{E}{2}\right)\eta\sin\,\eta\right]. \tag{30}$$

Identifying coefficients of $\cos^2\,\eta$ leads to

$$f' \to 0 \tag{31}$$

as expected, while identification of the remaining coefficients of $\eta\sin\,\eta$, $\sin\,\eta$, $\cos\,\eta$, and 1 yields

$$E = \frac{2M'}{(-f)\sqrt{1+f}}, \tag{32}$$

$$B = \frac{\pi M' + a'(-f)^{3/2}}{(-f)\sqrt{1+f}}. \tag{33}$$

To complete the transition of $R'/\sqrt{1+f}$ to a finite function of t only, we require M' and a' to also go to zero, so that E and B are finite,

$$M' = M_1\sqrt{1+f}, \tag{34}$$

$$\Rightarrow M = M_1\int \sqrt{1+f}\,dr + M_0, \tag{35}$$

$$a' = a_1\sqrt{1+f}, \tag{36}$$

$$\Rightarrow a = a_1\int \sqrt{1+f}\,dr + a_0, \tag{37}$$

$$f \to -1. \tag{38}$$

In summary, then, we choose the arbitrary Lemaître–Tolman functions of M and a to be as in (35) and (37), and then take the limit $f\to -1$ to arrive at the Kantowski–Sachs metric with

$$E = 2M_1, \tag{39}$$

$$B = \pi M_1 + a_1, \tag{40}$$

$$A = 2M_0, \tag{41}$$

$$t_0 = a_0 + \pi M_0. \tag{42}$$

In terms of the Lemaître–Tolman variables we then have

$$X = 2M_1 - (M_1\eta + a_1)\frac{\sin\,\eta}{(1-\cos\,\eta)}, \tag{43}$$

$$8\pi\rho=\frac{2M_1}{M_0^2(1-\cos\ \eta)^2X}. \tag{44}$$

Two specific examples of the function $f(r)$ with the appropriate limit are

$$f=-1+f_1\ \cos^2(r),\quad 0\leqslant f_1<1,\quad f_1\to 0, \tag{45}$$

$$f=\frac{-(1+f_2r^2)}{(1+f_3r^2)},\quad f_2\leqslant f_3,\quad f_2\to f_3 \tag{46}$$

III. DERIVING THE *(r,t)–(U,V)* TRANSFORMATION

It is convenient to find the transformation into Schwarzschild coordinates first. In order to transform the Schwarzschild metric to Lemaître–Tolman form, we write

$$T=T(t,r),\quad R=R(t,r). \tag{47}$$

Substituting the derivatives of the above into (1) and setting it equal to (8) results in

$$-\dot{T}^2\left(1-\frac{2M}{R}\right)+\frac{\dot{R}^2}{\left(1-\frac{2M}{R}\right)}=-1, \tag{48}$$

$$-2\dot{T}T'\left(1-\frac{2M}{R}\right)+\frac{2\dot{R}R'}{\left(1-\frac{2M}{R}\right)}=0, \tag{49}$$

$$-\left(1-\frac{2M}{R}\right)T'^2+\frac{R'^2}{\left(1-\frac{2M}{R}\right)}=\frac{R'^2}{1+f}. \tag{50}$$

Eliminating $\dot{T}$ and T' between these three equations leads to exactly the Lemaître–Tolman evolution equation (9), confirming that the vacuum Lemaître–Tolman model is just Schwarzschild in geodesic coordinates.

Substituting for $\dot{R}^2$ from (9) in (48) we find

$$\dot{T}=\frac{\sqrt{1+f}}{\left(1-\frac{2M}{R}\right)}, \tag{51}$$

and this in (49) gives

$$T'=\frac{R'\dot{R}}{\left(1-\frac{2M}{R}\right)\sqrt{1+f}}, \tag{52}$$

and one can check using (9)–(11) that both give the same $\dot{T}'$. Note, however, that if the mass is not held constant, $M=M(r)$, then these equations are not integrable. For regions where $f<0$, (51) may be transformed, by means of (13), the derivative of (14), and

$$\dot{T}=\frac{\partial T}{\partial\eta}\frac{\partial\eta}{\partial t} \tag{53}$$

into

$$\frac{\partial T}{\partial \eta}=\frac{M\sqrt{1+f}}{(-f)^{3/2}}\frac{(1-\cos\ \eta)^2}{(1-\cos\ \eta+2f)}, \tag{54}$$

which integrates with respect to η giving

$$T-J=\frac{M\sqrt{1+f}}{(-f)^{3/2}}[(\eta-\pi)(1-2f)-\sin\ \eta]$$
$$-2M\ln\left|\frac{1-(1+2f)\cos\ \eta+2\sqrt{(-f)(1+f)}\sin\eta}{1-\cos\ \eta+2f}\right| \tag{55}$$

where $J=J(r)$ is a function of integration (cf. Khuri,[18] and Misner, Thorne, and Wheeler[19]). Eliminating the parameter η once more with (13) and substituting from (9) converts this to

$$T-J=\frac{M\sqrt{1+f}(1-2f)}{(-f)^{3/2}}\cos^{-1}\left(1-\frac{(-f)R}{M}\right)-\frac{R\dot{R}\sqrt{1+f}}{(-f)}-2M\ \ln\left|\frac{(\dot{R}+\sqrt{1+f})^2}{\left(1-\frac{2M}{R}\right)}\right|, \tag{56}$$

and a very similar procedure for the case $f>0$ gives

$$T-J=-\frac{M\sqrt{1+f}(1-2f)}{f^{3/2}}\cosh^{-1}\left(1+\frac{fR}{M}\right)+\frac{R\dot{R}\sqrt{1+f}}{f}-2M\ \ln\left|\frac{(\dot{R}+\sqrt{1+f})^2}{\left(1-\frac{2M}{R}\right)}\right|. \tag{57}$$

Note that

$$\ln\left|\frac{(\dot{R}+\sqrt{1+f})^2}{\left(1-\frac{2M}{R}\right)}\right|=-\ln\left|\frac{(\dot{R}-\sqrt{1+f})^2}{\left(1-\frac{2M}{R}\right)}\right|.$$

A simpler version for $f=0$ gives

$$T-J=\sqrt{\frac{2R}{M}}\left(\frac{R+6M}{3}\right)-2M\ \ln\left|\frac{(\dot{R}+1)^2}{\left(1-\frac{2M}{R}\right)}\right|, \tag{58}$$

and one may verify, using Taylor expansions, that this is the $f\to 0$ limit of (56) and (57). Finally, substituting from (14) or (17) as appropriate converts (56) and (57) to

$$T-J=(1-2f)\sqrt{1+f}(t-a)+2R\dot{R}\sqrt{1+f}-2M\ \ln\left|\frac{(\dot{R}+\sqrt{1+f})^2}{\left(1-\frac{2M}{R}\right)}\right|, \tag{59}$$

which is valid for all values of f, and this is confirmed by straight differentiation of (59) with respect to t (holding r constant) to retrieve (51) again after applying (9) and (10).

It must now be checked that the solution also satisfies (52), which involves evaluating $J(r)$. Partial differentiation with respect to r and substitution from (9) and (11) leads to

$$T'-J'=\frac{1}{2\sqrt{1+f}R\dot{R}\left(1-\frac{2M}{R}\right)}\left\{f'\left[(1+2f)R\left(1-\frac{2M}{R}\right)(2R-3(t-a)\dot{R})\right]\right.$$
$$\left.+R'[4(1+f)(M+fR-2fM)]a'\left[2(1+f)(2f-1)R\dot{R}\left(1-\frac{2M}{R}\right)\right]\right\}. \tag{60}$$

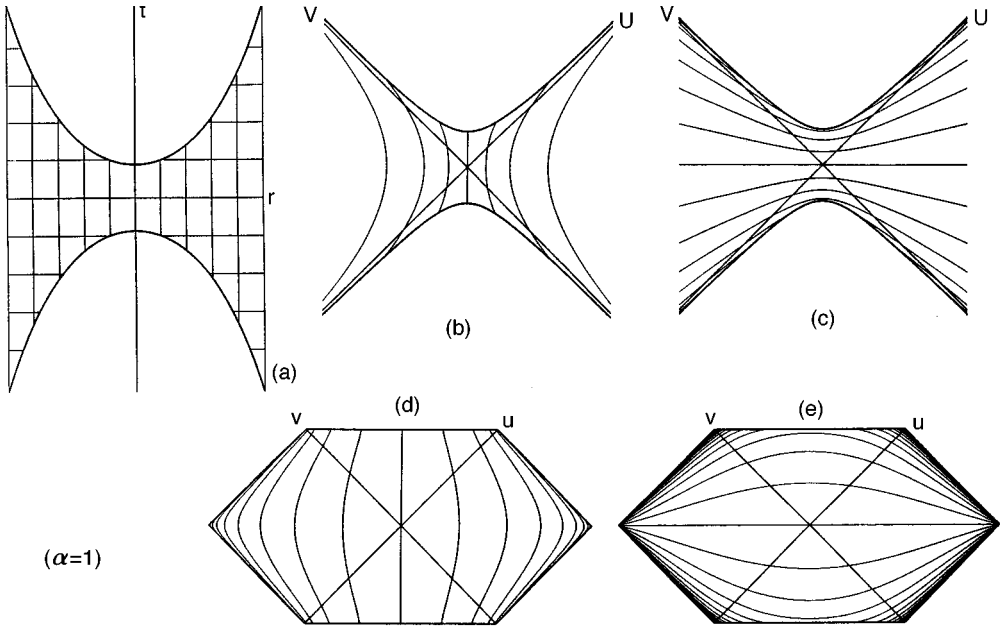

FIG. 1. The (a) Lemaître–Tolman, (b) and (c), Kruskal–Szekeres, and (d) and (e) Penrose diagrams, showing the constant t [(a), (b), and (d)] and constant r [(a), (c), and (e)] surfaces for Novikov coordinates.

Now (12) for constant M leads to

$$[3(t-a)\dot{R}-2R]f'=2fR'+2f\dot{R}a', \tag{61}$$

which may be used to eliminate f' in (60), yielding

$$T'-J'=\frac{\dot{R}R'}{\sqrt{1+f}\left(1-\frac{2M}{R}\right)}-\frac{a'}{\sqrt{1+f}}. \tag{62}$$

This clearly satisfies (52), once we have identified

$$J=\int\frac{a'dr}{\sqrt{1+f}}+J_0, \tag{63}$$

where J_0 is a constant.

The final transformation from vacuum Lemaître–Tolman to Schwarzschild coordinates then is

$$T=(1-2f)\sqrt{1+f}(t-a)+2R\dot{R}\sqrt{1+f}-2M\ \ln\left|\frac{(\dot{R}+\sqrt{1+f})^2}{\left(1-\frac{2M}{R}\right)}\right|+\int\frac{a'\ dr}{\sqrt{1+f}}+J_0, \tag{64}$$

combined with one of (13)+(14), (15), or (16)+(17), which cannot be made independent of the value of f. From (3) and (4) the vacuum Lemaître–Tolman to Kruskal–Szekeres transformation is

$$U=\sqrt{\frac{R}{2M}}(\sqrt{1+f}-\dot{R})\exp\left\{\frac{R+\sqrt{1+f}[(1-2f)(t-a)+2R\dot{R}]+J}{4M}\right\}, \tag{65}$$

$$V=-\sqrt{\frac{R}{2M}}(\sqrt{1+f}+\dot{R})\exp\left\{\frac{R-\sqrt{1+f}[(1-2f)(t-a)+2R\dot{R}]-J}{4M}\right\}. \tag{66}$$

Here $\dot{R}$ is just shorthand for $\sqrt{2M/R+f}$. A change in the value of the constant J_0 merely generates a constant translation of T and constant rescalings of U and V, so it may safely be set to zero. The transformations are illustrated in Fig. 1 for the Novikov choice of Lemaître–Tolman arbitrary functions.

IV. THE SHAPE OF THE *R=0* SINGULARITY

In Kruskal–Szekeres and Novikov coordinates the future singularity forms at the middle of the wormhole and succeeding shells collapse onto it at later times, the covers holding for the past singularity, whereas the Penrose diagram shows the past and future Schwarzschild singularities as simultaneous. In Lemaître–Tolman coordinates one is free to specify $a(r)$ and therefore can choose to make one, but not both, of the singularities simultaneous. We define the following family of Lemaître–Tolman arbitrary functions

$$M=\text{const}, \tag{67}$$

$$f=\frac{-1}{1+r^2}, \tag{68}$$

$$a=-\pi M\alpha(1+r^2)^{3/2}, \tag{69}$$

where the parameter α determines the degree of curvature of the past and future singularities—$\alpha=0$ makes the past singularity simultaneous at $t=0$, $\alpha=2$ makes the future singularity simultaneous at $t=0$, and $\alpha=1$ is the standard Novikov choice with the two singularities time symmetric about $t=0$. The corresponding transformations for various α values are shown in Fig. 2. It is apparent that, as the past singularity is brought closer and closer to being simultaneous, the geodesics crowd ever more tightly about $r=0,t=a$, and at $\alpha=0$ they all emerge from a single point on the past singularity, leaving large regions of the manifold uncharted by the coordinates. The envelope geodesic is obtained from the $r\to\infty$ limit with $a'=J=a=0$. In this limit the evolution is parabolic (15), and defining

$$y=\left(\frac{3t}{4M}\right)^{1/3} \tag{70}$$

gives the envelope in parametric form:

$$U=(y-1)\exp\left\{\frac{y^2}{2}+y\left(1+\frac{y^2}{3}\right)\right\}, \tag{71}$$

$$V=-(y+1)\exp\left\{\frac{y^2}{2}-y\left(1+\frac{y^2}{3}\right)\right\}. \tag{72}$$

The next model, defined by the choices

$$M=\text{const}, \tag{73}$$

$$f=-1+r^2, \tag{74}$$

$$a=0, \tag{75}$$

attempts to fill the uncovered regions with geodesics that escape to infinity, by extending f to positive values, but still keeping $a=0$. Although there is slightly greater coverage of the $U-V$ diagram, the curves still all start at the same $U-V$ event. The new envelope is given by the $f\to\infty$ limit of (65) and (66), holding R finite so that ($\cosh\eta-1\sim f$), i.e., $\eta\to\infty$ also. Replacing $\sqrt{1+f}$ with f gives

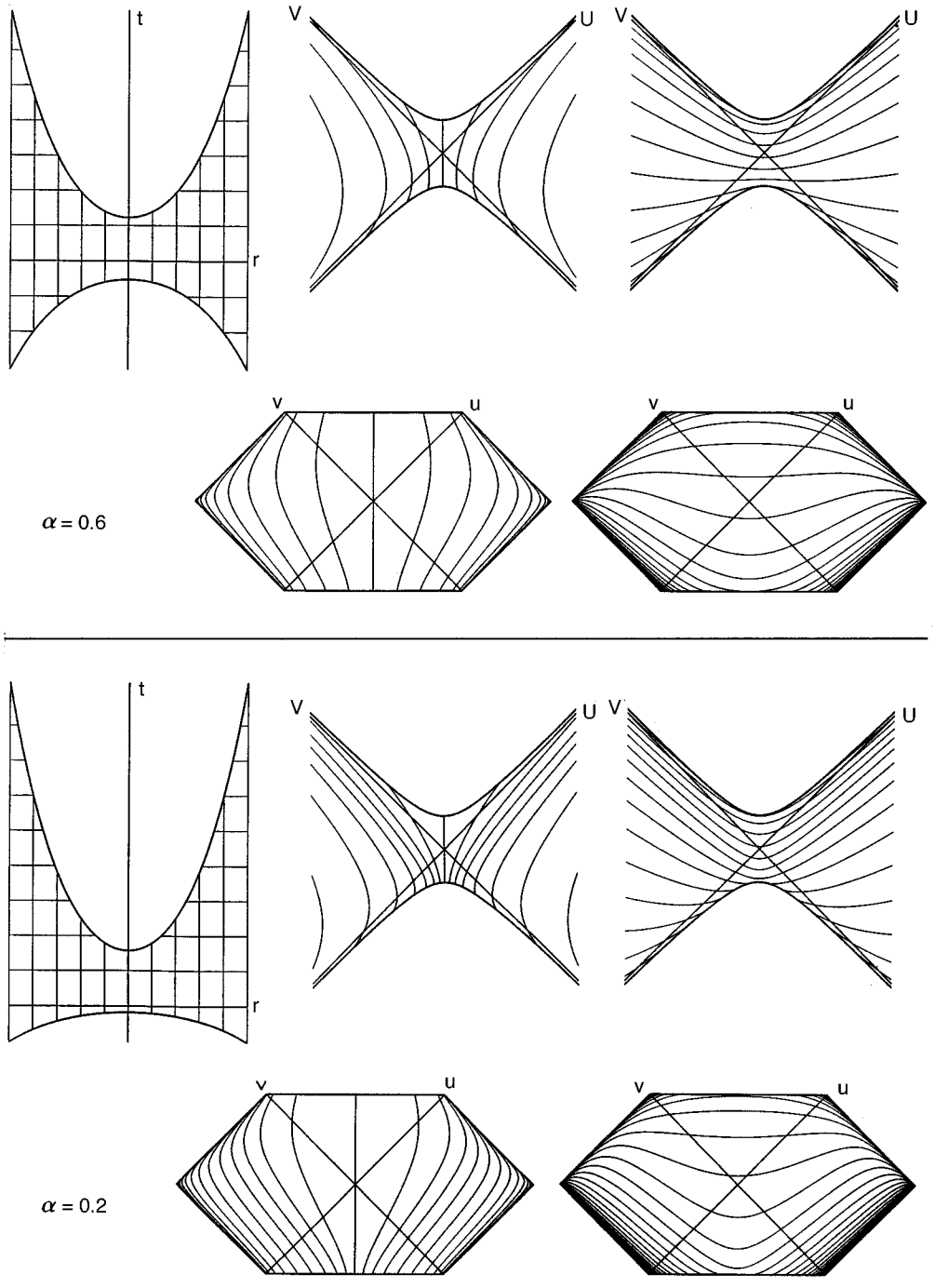

FIG. 2. The Lemaître–Tolman, Kruskal–Szekeres, and Penrose diagrams, showing the constant t and constant r surfaces for various values of α in the family of Lemaître–Tolman models given by the arbitrary functions (67)–(69).

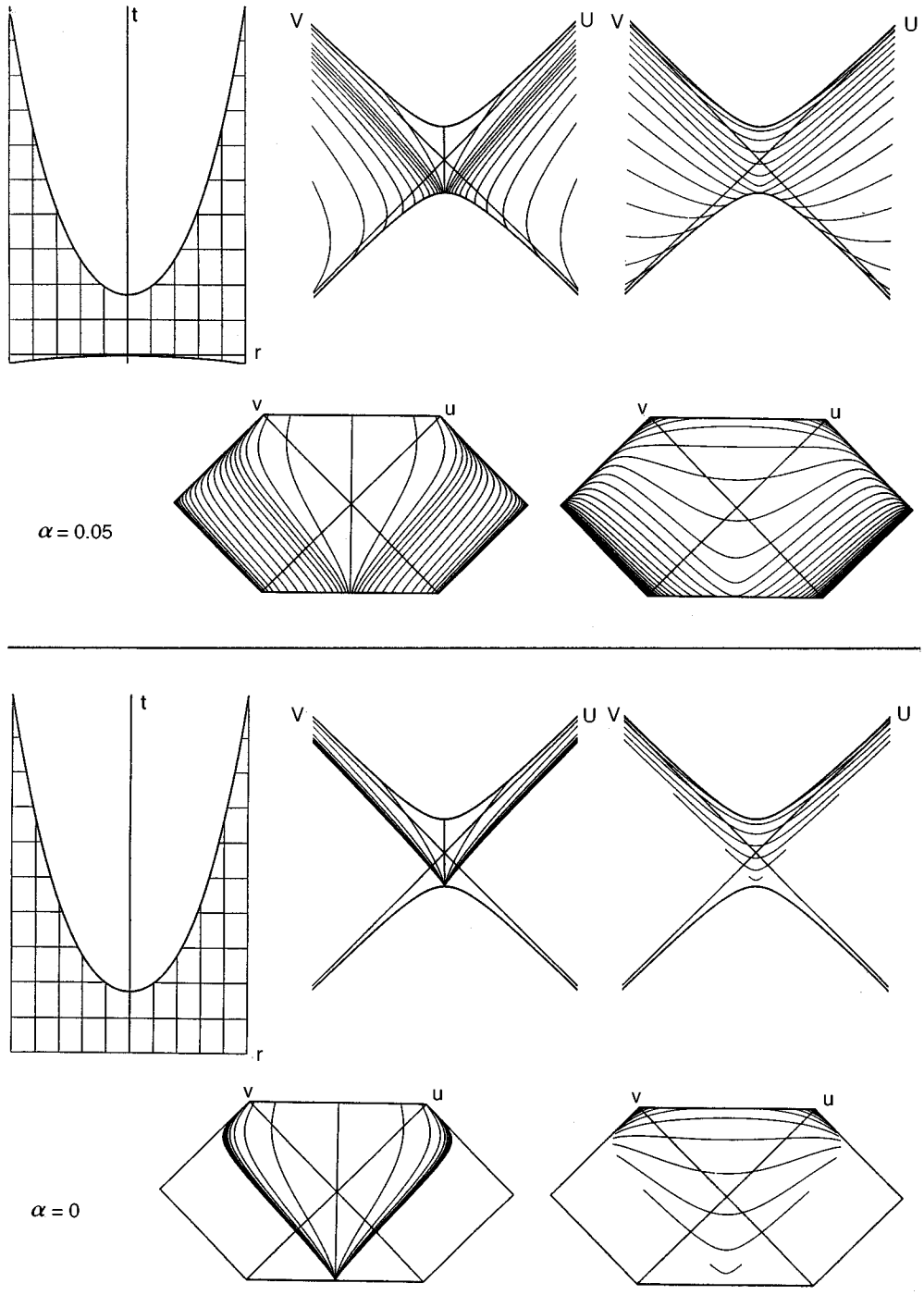

FIG. 2. (*Continued.*)

$$U=\left(\sqrt{\frac{\cosh\ \eta-1}{2}}-\sqrt{\frac{\cosh\ \eta+1}{2}}\right)\exp\left\{\frac{\cosh\ \eta-1}{4f}+\frac{\eta}{2}+\frac{J}{4M}\right\}, \tag{76}$$

$$V=-\left(\sqrt{\frac{\cosh\ \eta-1}{2}}+\sqrt{\frac{\cosh\ \eta+1}{2}}\right)\exp\left\{\frac{\cosh\ \eta-1}{4f}-\frac{\eta}{2}-\frac{J}{4M}\right\}, \tag{77}$$

so letting $a'=0=J$ and $\eta\to\infty$ gives

$$U \text{ undetermined}, \quad V=-1, \quad \text{or vice versa}, \tag{78}$$

which are the light rays emanating from $r=0$ on the past singularity, and reaching future null infinity.

In order to establish the same result in general, we take the $t\to a$, $R\to 0$, $\dot{R}\to\sqrt{2M/R}$ limit in the general expressions (65) and (66), arriving at

$$U\to -e^{J}, \quad V\to -e^{-J}, \tag{79}$$

which holds for arbitrary r, $f(r)$, and $a(r)$. Thus if $J\neq J(r)$, which is the case if $a'=0$ everywhere, then all constant r curves radiate from one $U-V$ point on the past singularity.

The one possibility we have not yet considered is the closed Kantowski–Sachs metric, which is well known to have R constant on all its constant t surfaces, so that both past and future singularities are simultaneous. Inserting the Kantowski–Sachs limit of the Lemaître–Tolman arbitrary functions into (64)–(66) gives

$$T=J_0+a_1 r-2M_0 \ln\left|\frac{\dot{R}^2}{\left(1-\frac{2M_0}{R}\right)}\right|, \tag{80}$$

$$U=-\dot{R}\sqrt{\frac{R}{2M_0}}\exp\left\{\frac{R+a_1 r+J_0}{4M_0}\right\}, \tag{81}$$

$$V=-\dot{R}=\sqrt{\frac{R}{2M_0}}\exp\left\{\frac{R-a_1 r-J_0}{4M_0}\right\}. \tag{82}$$

As expected, $t=\text{const}\to R=\text{const}$, and $r=\text{const}\to T=\text{const}$, so all coordinate geodesics pass through the neck (middle of the wormhole) at its moment of maximum expansion, and the metric is degenerate there, since there is a global shell crossing at that moment. Although these coordinates do cover the whole of the $R=0$ singularity and make it look simultaneous, they are not geodesically complete, and more importantly the coordinate geodesics are always in relative proper motion.

V. OBSERVER COORDINATES

In order to set up reasonable ''observer coordinates,'' which represent proper distance and time measurements, at least locally, we must start with a surface of simultaneity over a finite region, set up parallel timelike geodesics orthogonal to it, and then extend these geodesics a finite distance off the surface, using proper time along them for the fourth coordinate. Lemaître–Tolman coordinates already satisfy all but two of these requirements. A mere rescaling of the r coordinate,

$$\tilde{r}(r)=\int_0^r \frac{R'(t=\text{const},r)}{\sqrt{1+f}}\,dr \tag{83}$$

makes $\tilde{r}$ a local proper distance, and the coordinate geodesics are made parallel by requiring

$$\partial_t\sqrt{g_{rr}}=0\to\dot{R}'=0. \tag{84}$$

Inserting this and (12) into (11) and setting $M'=0$ for vacuum gives

$$a' = \frac{f'}{2Mf}(3M(t-a) - R^2\dot{R}), \tag{85}$$

which is always possible to satisfy *locally*, since the quantities in the brackets depend on a, f, and M but not directly on a' or f'. If $a'=0$ is required at some point, this in general requires $f'=0$, making it the locus of an extremum in the areal radius with $f=-1$.[10] Such a point necessarily occurs at one r value, and the corresponding geodesic is then a constant T curve, never quite emerging from the horizon. If, however, $a=$const is required, then $R'=0$ everywhere, and we have the $E=0=M_1$ closed Kantowski–Sachs model again, for which the coordinate geodesics cannot be made locally parallel away from $R=0$, since

$$\partial_t\sqrt{g_{rr}} = \dot{X} = \frac{2B}{A(1-\cos\,\eta)^2} = \frac{a_1}{M_0(1-\cos\,\eta)^2} \neq 0. \tag{86}$$

If both $E=0$ and $B=0$, then $X=0$, making the metric (23) degenerate.

VI. SIMULTANEOUS SYNCHRONOUS COORDINATES

Wald and Yip[20] considered conditions for the existence of simultaneous synchronous coordinates (SSCs) at spacelike singularities, as assumed in the Belinskii, Lifschitz, and Khalatnikov (BKL) approach to studying singularities (see Ref. 21). Wald and Yip's theorem 2 gives three conditions which allow one to find a Cauchy surface Σ such that Gaussian normal (i.e., synchronous) coordinates set up at Σ represent the singularity as simultaneous. In other words, the timelike geodesics of these coordinates all reach the singularity in the same proper time τ_Σ from Σ. Having set them up, the constant τ surfaces are a foliation that approaches the singularity as $\tau\to 0$. The conditions are, roughly speaking, (i) the (geodesic proper) time τ from Σ to the singularity (future causal boundary) is finite and nonzero; (ii) τ is a C^1 function throughout the future of $\Sigma(\mathrm{D}^+(\Sigma))$; (iii) every causal curve hits the singularity ($\tau\to 0$ along all causal curves).

We have shown that in the Schwarzschild/Kruskal–Szekeres manifold the following obtain

(a) Synchronous coordinates that cover the entire space–time manifold represent both future and past singularities as nonsimultaneous. Their $t=$const surfaces are Cauchy surfaces since $f\to 0$ or positive values as $r\to\infty$, thus covering the asymptotic regions, $R\to\infty$.

(b) Synchronous coordinates that make one or both singularities simultaneous do not cover the whole space–time. (Usually they do not even cover more than one $U-V$ point on the singularity that they make simultaneous.) Their $t=$const surfaces are not (complete) Cauchy surfaces.

(c) The nonexistence of SSCs for Schwarzschild black holes is due to the fact that the singularities, while entirely spacelike, are not all encompassing—they do not swallow all possible causal curves. The condition of Wald and Yip's theorem 2 that fails is condition (i), which requires τ_Σ (the maximum lifetime function of the Cauchy surface) to remain finite.

VII. CONCLUSION

We have found the transformation from the general vacuum Lemaître–Tolman model to Schwarzschild coordinates, and hence to Kruskal–Szekeres coordinates. Unfortunately this cannot be extended to nonempty Lemaître–Tolman models, since the system of partial differential equations (pdes) (51) and (52) are not integrable if M is not a constant. Similarly, equivalent expressions for $\dot{U}$ and U' are no longer integrable once $M=M(r)$, so the Lemaître–Tolman metric in double null coordinates cannot be expressed in the form (5)/(6), and probably contains nonzero coefficients of dU^2 and/or dV^2.

The vacuum Lemaître–Tolman model allows all possible families of radial geodesic coordinates to be set up, including those which generate observer coordinates in any given locality, as

well as those, such as the closed vacuum Kantowski–Sachs case, which never have a simultaneous surface on which the orthogonal timelike geodesics are parallel. Of course most arbitrary choices will have shell crossings, where the geodesics cross each other, at some time during their evolution, but this is only a coordinate problem in vacuum. Also there will be many choices that do not cover the full manifold, including all these that make $R=0$ simultaneous.

We have shown that it is impossible to find any reasonable set of ''observer coordinates,'' extended over a finite region of space–time, for which the Schwarzschild $R=0$ singularity is simultaneous. Furthermore, all possible global synchronous geodesic coordinates that cover the full spherically symmetric vacuum manifold represent $R=0$ as nonsimultaneous. Therefore we conclude that the Schwarzschild singularity is intrinsically nonsimultaneous, despite the appearance of the Penrose diagram. It would be interesting to determine whether this is a property of the spherically symmetric vacuum, or a property of the spatial topology. Nonempty Lemaître–Tolman models with the Kruskal–Szekeres topology were investigated in P1 where the horizons were shown to be split, and it has been shown[22] that the Lemaître–Tolman $R=0$ singularities are spacelike everywhere (unless a censorship violating singularity[23,24] is present, an impossibility in this topology which lacks an origin of spherical coordinates) but the detailed behavior of the light rays is not known.

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Qualitative analysis of causal cosmological models

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The Einstein's field equations of Friedmann–Robertson–Walker universes filled with a dissipative fluid described by both the *truncated* and *non-truncated* causal transport equations are analyzed using techniques from dynamical systems theory. The equations of state, as well as the phase space, are different from those used in the recent literature. In the de Sitter expansion both the hydrodynamic approximation and the non-thermalizing condition can be fulfilled simultaneously. For $\Lambda=0$ these expansions turn out to be stable provided a certain parameter of the fluid is lower than 1/2. The more general case $\Lambda>0$ is studied in detail as well. © *1996 American Institute of Physics.* [S0022-2488(96)03205-6]

I. INTRODUCTION

Recently, isotropic spatially homogeneous viscous cosmological models have been investigated using the causal (truncated and nontruncated) Israel–Stewart theory of irreversible processes, to modelize the bulk viscous transport.[1–3] It is known that dissipative processes may play a crucial role in the evolution of relativistic fluids both in cosmology and in high-energy astrophysical phenomena. The most oftenly used theory to describe such irreversible processes has been long since the first-order non-causal Eckart's theory[4] which however suffers from serious pathologies and drawbacks, i.e., superluminal velocities and instabilities.[5,6] In the late sixties Müller[7] proposed a second order theory in which the entropy flow depended on the dissipative variables besides the equilibrium ones. Israel and Stewart[8,9] and Pavón *et al.*[10] developed a fully relativistic formulation on that basis, the so-called *extended* or *transient* thermodynamics (see Ref. 11 for a recent and comprehensive review of the state of the art).

Shortly after Israel's paper appeared, Belinskii *et al.*[12] applied it to a viscous cosmological fluid using the so-called *truncated* version, in which some divergence terms in the transport equations were neglected. Most of the papers dealing with viscous and/or heat conducting cosmological models make use of such a truncated transport equation without stating clearly what the implications of such a simplification may be. Recently, some effort has been invested in analyzing to what extent the neglecting of the divergence terms can be justified from a physical point of view.[3,13] As far as we know, Hiscock and Salmonson[14] were the first to raise this point in the cosmological context. These authors stressed the key importance of the usually neglected divergence terms when obtaining viscosity-driven inflationary solutions. However, it is now clear that to get realistic solutions to the Einstein's field equations, the role played by the equations of state relating the different thermodynamic quantities is crucial. Hence the claim in Ref. 14 applies only to a Boltzmann gas.[15] In fact, the difficulty in using the extended transport equations lies mainly in the occurrence of some additional unknown coefficients, whose explicit expressions must be obtained from techniques other than those coming from thermodynamics, either kinetic or fluctuation theory,[16] more than in their intrinsic complexity.

Few exact solutions have been found to the Einstein's field equations with a non-perfect fluid described by extended thermodynamics[17,18] (ET for short). However, they were obtained under severe restrictions on the values for the free parameters in the transport equations. Obviously, any further attempt to get a deeper insight on the possible behavior of the solutions must rely on an approximate analysis of the equations. In this paper, we apply qualitative analysis techniques to the study of causal viscous Friedmann–Robertson–Walker (FRW) models with and without a

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positive cosmological constant. It is organized as follows. In section II we state the basic equations governing the models and discuss the equations of state to be used. In section III we apply the truncated version of ET whereas in section IV a corresponding analysis is carried out using the *full* version. In both cases a null and a positive cosmological constant are considered in turn. In section V we explore their dynamical consequences, and finally in section VI we summarize the main conclusions of the paper.

II. BASIC EQUATIONS

We restrict ourselves to a FRW space-time filled with a bulk viscous fluid and a positive cosmological constant Λ. The stress-energy tensor is

$$T_{ab}=(\rho+p+\Pi)u_a u_b+(p+\Pi-\Lambda)g_{ab}, \tag{1}$$

where u_a is the four velocity, ρ the energy density, p the equilibrium pressure, Π the bulk viscous pressure. Einstein's field equations for the spatially flat case (the only one we adress in this paper) are

$$H^2=\frac{\kappa}{3}\rho+\frac{\Lambda}{3}, \quad 3(\dot{H}+H^2)=-\frac{\kappa}{2}(\rho+3P_{eff})+\Lambda, \tag{2}$$

where $H\equiv\dot{R}/R$ is the Hubble factor, $R(t)$ the cosmic scale factor of the Robertson–Walker metric, $P_{eff}=p+\Pi$ and $\kappa=8\pi G/c^4$. An overdot denotes differentiation respect to time t. We assume the fluid obeys equations of state of the form

$$\zeta=\alpha\rho^m, \quad p=(\gamma-1)\rho, \quad \tau=\frac{\zeta}{\rho}, \tag{3}$$

where α is a positive constant, and γ the adiabatic index lying in the range $1<\gamma<2$ as the sound velocity $v_s/c=\gamma-1$ in the fluid must be lower than the speed of light. $\tau(\geqslant 0)$ is the relaxation time for transient bulk viscous effects, i.e., the time the system takes in going back to equilibrium once the divergence of the four-velocity has been switched off. The causal evolution equation for bulk viscous pressure can be cast into the form[3]

$$\Pi+\tau\dot{\Pi}=-3\zeta H-\frac{b}{2}\tau\Pi\left(3H+\frac{\dot{\tau}}{\tau}-\frac{\dot{T}}{T}-\frac{\dot{\zeta}}{\zeta}\right), \tag{4}$$

where $b=0$ for the truncated theory and $b=1$ for the full one. Since a dissipative expansion is non-thermalizing, the relaxation time must exceed the expansion rate H^{-1}. This leads to

$$\tau^{-1}<H, \tag{5}$$

which is a condition that reduces the interval of values of γ for which the model holds. As we shall see this restriction may be violated in the truncated theory as well as in the full theory when an ideal gas equation of state is assumed. This conflict can be circumvented by resorting to the expression for the speed of the viscous signals $a\equiv v^2/c^2\sim\zeta/\tau\rho$, which roughly implies[3,13]

$$\tau=\frac{\zeta}{a\rho}, \qquad 0<a<1, \tag{6}$$

and using (6) instead of (3c).

Most of the stability analysis below will be carried out for the de Sitter solutions, $H=$ const. As the universe undergoes a de Sitter expansion it could be argued that the hydrodynamic de-

scription (absolutely needed in our study if the results are to hold) might break down. In order for the fluid approach remains valid the mean collision time t_{col} must be less (in fact much less) than the expansion rate, i.e., $t_{col}<H^{-1}$. From kinetic theory one has $t_{col}=1/n\sigma$ where n is the particle number density and σ the cross section for collisions. In general $\sigma(T)$ is an increasing function of the temperature whereas, for a FRW universe, $n \propto 1/R^3 (=e^{-3H_0 t}$ for a de Sitter universe). From equations (2a), (3a) and (6) the non-thermalizing condition (5) and the condition for the hydrodynamic approximation imply

$$\frac{e^{3H_0 t}}{n_0 \sigma} < H_0^{-1} < \frac{\alpha}{a}\left(\frac{3}{\kappa}\right)^{m-1} H_0^{2m-2}, \tag{7}$$

where n_0 is a positive but otherwise arbitrary integration constant. Later it will be shown that the second inequality in (7) can be fulfilled when suitable values for the arbitrary parameters are chosen. Moreover, the first inequality may hold for sufficiently early times (when the inflation era supposedly took place). As the temperature remains constant during this period the cross section σ can be taken approximately constant.[19]

Recently in performing the qualitative analysis of imperfect fluid cosmological models (see for instance Refs. 1,2,20,21) dimensionless equations of state were used in terms of the dimensionless variables x and y, defined as

$$x \equiv 3\rho/\Theta^2, \qquad y \equiv 9\Pi/\Theta^2. \tag{8}$$

The equations of state [Eq. (3.4a), (3.4b) in Ref. 20)]

$$p/\Theta^2 = p_0 x^l, \qquad \zeta/\Theta = \zeta_0 x^m, \tag{9}$$

with $\Theta(\equiv 3H)$ the expansion factor, coincide with (3a), (3b) only for $l=m=1/2$. Furthermore, for the spatially flat FRW metric with $\Lambda=0$, the case we are interested in, we have $x=1$. Then the bulk viscous coefficient ζ varies as Θ irrespective of m, which restricts (9) to just one case: $m=1/2$ in (3a). In this paper we shall consider only the *spatially flat* case ($k=0$) which allows us to take $(\dot{H},H)$ as suitable dynamical variables in the phase space. In this case it appears to be more natural, especially when the above comments are taking into account, to adopt the oftenly used equations of state (3) rather than (9) in order to be able to compare our results with those in the literature for $m=1/2$. Consequently, all the fixed points to be analyzed will correspond to either de Sitter or static spacetimes ($X \equiv \dot{H}=0$) the former being physically relevant in inflationary models. If one is interested in studying non-flat FRW models, the variables $(\dot{H},H)$ become no longer appropriate and an approach similar to that of Coley[20] should by adopted.

III. QUALITATIVE ANALYSIS USING THE TRUNCATED THEORY

From equations (2), (3) and the expression (6) for τ we find for the Hubble factor the equation

$$\ddot{H} + 3\gamma H\dot{H} + \frac{a}{\delta}\left(H^2 - \frac{\Lambda}{3}\right)^{1-m}\dot{H} + \frac{(3H^2-\Lambda)a}{2}\left[\frac{\gamma}{\delta}\left(H^2-\frac{\Lambda}{3}\right)^{1-m} - 3H\right] = 0, \tag{10}$$

where $\delta = \alpha(3/\kappa)^{m-1}$. Equation (10) can be recast into the form

$$\dot{H} = P(H,X), \quad \dot{X} = Q(H,X), \tag{11}$$

where

$$P(H,X) = X, \tag{12}$$

$$Q(H,X)=-3\gamma HX-\frac{a}{\delta}\left(H^2-\frac{\Lambda}{3}\right)^{1-m}X-\frac{(3H^2-\Lambda)a}{2}\left[\frac{\gamma}{\delta}\left(H^2-\frac{\Lambda}{3}\right)^{1-m}-3H\right]. \tag{13}$$

The qualitative analysis begins by linearizing the system (11) for small perturbations–where the linear theory holds. Then the Jacobian matrix

$$\mathbf{L}=\begin{pmatrix} P_H & P_X \\ Q_H & Q_X \end{pmatrix}, \text{ with } P_H\equiv\frac{\partial P}{\partial H}, \text{ etc.,} \tag{14}$$

can be constructed. The elements of this matrix must be evaluated at the equilibrium points (h_i,X_i) (de Sitter and static solutions) which are found by solving the system $P(h_i,X_i)=Q(h_i,X_i)=0$. After diagonalizing $\mathbf{L}$ and obtaining its eigenvalues we can decide about the type of fixed points and their stability.

The analysis of the system (12), (13) for the two cases with $\Lambda=0$ and $\Lambda>0$ will be carried out in turn.

i. $\Lambda=0$

- $m=1/2$

We have the trivial fixed point,

$$(0,0),$$

which corresponds to an unstable static model. However, this case does not make sense as, by Einstein's equation (2a), $\rho=0$. If γ and δ fulfill the restriction

$$\gamma/\delta=3, \tag{15}$$

there exists an infinity of fixed points $(h_0,0)$, where h_0 denotes an arbitrary positive real constant. In this case the fixed points are parallel stable straight lines.

- $m\neq 1/2$

In the intervals $0\leqslant m<1/2$, $1/2<m<2$ there are two fixed points,

$$(0,0), \qquad (h_0,0), \tag{16}$$

with

$$h_0=\left(\frac{3\delta}{\gamma}\right)^{1/(1-2m)}, \tag{17}$$

whereas for $m\geqslant 2$ there is only one fixed point $(h_0,0)$. The discussion for the point $(0,0)$ mimics that for $m=1/2$.

Let us define the auxiliar parameter,

$$\Sigma_1=\frac{1}{4a}\left(\gamma+\frac{a}{\gamma}\right)^2.$$

For $m<\frac{1}{2}-\Sigma_1$ the equilibrium point $(h_0,0)$ is an asymptotically stable focus, for $m=\frac{1}{2}-\Sigma_1$ it is an asymptotically stable degenerate node, whereas for $m>\frac{1}{2}-\Sigma_1$ two cases arise. If $\frac{1}{2}-\Sigma_1<m<\frac{1}{2}$, then the equilibrium point is an asymptotically stable node, whereas if $m>1/2$ it is a unstable saddle point.

In the paper by Pavón *et al.*[22] slightly different techniques were used to analyze the case $m=1/2$ and $a=1$. Their relevant parameter was our Σ_1 with $a=1$. Our results agree with those of the mentioned reference (see Sec. 3.1 of Ref. 22) providing a more accurate classification of the stability points.

ii. $\Lambda>0$

As we shall see, there are two fixed points: $(h_0^\Lambda,0)$ and $(h_1^\Lambda,0)$. From (10) it follows the equation for the fixed points,

$$(3h_i^2-\Lambda)\left[\frac{\gamma}{\delta}\left(h_i^2-\frac{\Lambda}{3}\right)^{1-m}-3h_i\right]=0, \tag{18}$$

which must be solved for different values of m. However, (18) has an obvious solution independent of m, $h_0^\Lambda=\sqrt{\Lambda/3}$, which can be shown to correspond to a saddle point. This solution will be ruled out however since it would imply that the energy density vanishes identically. The other solution h_1^Λ will be analyzed for $m=0,\frac{1}{2},1$, in turn.

● $m=0$

Setting to zero the big square parenthesis in (18) and solving the resulting equation, one obtains

$$h_1^\Lambda=\frac{3\delta}{2\gamma}+\frac{1}{2}\sqrt{\frac{9\delta^2}{\gamma^2}+\frac{4\Lambda}{3}}.$$

We define

$$\Sigma_1^\Lambda=\frac{2-2\Sigma_1}{2\Sigma_1-1}, \qquad \Lambda_0=\frac{27\delta^2}{\gamma^2}\frac{1+\Sigma_1^\Lambda}{(\Sigma_1^\Lambda)^2}.$$

For $\Lambda<\Lambda_0$ the fixed point $(h_1^\Lambda,0)$ is an asymptotically stable node. If $\Lambda=\Lambda_0$ the fixed point is an asymptotically stable degenerate node whereas for $\Lambda>\Lambda_0$ it is an asymptotically stable focus.

● $m=1/2$

Now h_1^Λ is given by

$$h_1^\Lambda=\sqrt{\frac{\Lambda/3}{1-9\delta^2/\gamma^2}}.$$

For $0<9\delta^2/\gamma^2<1$, $(h_1^\Lambda,0)$ is an asymptotically stable node whereas for $9\delta^2/\gamma^2>1$ the fixed point is an asymptotically stable focus for any $\Lambda>0$.

● $m=1$

Now $h_1^\Lambda=\gamma/3\delta$. For $\Lambda<\gamma^2/3\delta^2$ we have a saddle fixed point, whereas for $\gamma^2/3\delta^2<\Lambda<\Lambda_1$, where

$$\Lambda_1=\frac{\gamma^2}{3\delta^2}\Sigma_2^\Lambda>0, \text{ with } \Sigma_2^\Lambda=\frac{1}{2a}\left(\gamma+\frac{a}{\gamma}\right)^2+1,$$

the fixed point is an asymptotically stable node. For $\Lambda=\Lambda_1$, it is an asymptotically stable degenerate node whereas for $\Lambda>\Lambda_1$, it is an asymptotically stable focus.

IV. QUALITATIVE ANALYSIS USING THE FULL THEORY

Actually, a proper study of viscous phenomena in the frame of ET requires the use of the full equation (4) (i.e., $b=1$). The physical implications of neglecting the second term of (4) have been

analyzed in detail in Refs. 3,13. The use of (4) requires an explicit expression for the temperature T in terms of other variables such as ρ and/or n. So far (with the exception of Ref. 14) the expression adopted for T has been a power-law

$$T=\beta\rho^r, \tag{19}$$

where $r\geqslant 0$ and $\beta>0$ are constants, which is the simplest way to guarantee a positive heat capacity.[23] However, we shall see that standard thermodynamic relations restrict the range of r. Cãlvao *et al.*[24] found a general equation for the evolution of temperature when two equations of state,

$$\rho=\rho(T,n), \quad p=p(T,n), \tag{20}$$

are given. However, their equation was obtained in the context of matter creation where Π is reinterpreted as a non-equilibrium pressure associated to particle production. The same equation has been carefully analyzed in Ref. 13, it reads as

$$\frac{\dot{T}}{T}=-\Theta\left[\frac{(\partial p/\partial T)_n}{(\partial\rho/\partial T)_n}+\frac{\Pi}{T(\partial\rho/\partial T)_n}\right]. \tag{21}$$

Obviously, when the equations of state (20) are known the evolution of T is no longer free but fixed by (21). However, only in very few cases these equations are explicitly known, as for instance in the case of a radiation gas or an ideal gas.[25] Equation (19) generalizes in a simple way the Stefan–Boltzmann ($R=1/4$) equation which holds for a radiation-dominated fluid in equilibrium. Thus, in that case we get that both equations of state ρ and p (when a γ-law is used) have T as the only independent variable, i.e., $\partial\rho(p)/\partial T=d\rho(p)/dT$. A useful and interesting relation follows from considering the standard thermodynamic relation[26]

$$\left(\frac{\partial\rho}{\partial n}\right)_T=\frac{\rho+p}{n}-\frac{T}{n}\left(\frac{\partial p}{\partial T}\right)_n, \tag{22}$$

which, by virtue of (3b) and (19), yields

$$r=\frac{\gamma-1}{\gamma}\left(\Rightarrow 0<r<\frac{1}{2}\right), \tag{23}$$

i.e., r is no longer an independent parameter (we are indebted to Roy Maartens for pointing us out this restriction). It has been argued[2] that the inequality $r<1$ is reasonable from a physical point of view, since ultrarelativistic and cold non-relativistic matter have $r=1/4$ and $r\sim 2/3$, respectively.

However, an alternative equation can be used for T instead of (19). It is well-known that a relativistic ideal monoatomic gas is described by the two equations of state $p=nT$ and $\rho=3nT+m^2M$, where m is the mass of the particles and M the zeroth-order moment of the Maxwell–Boltzmann distribution function (we use units $k_B=1$, k_B being the Boltzmann constant). We see that the γ-law (γ constant) is *not* compatible with the equations of state of a monoatomic gas in *equilibrium* except for radiation ($m=0$). In that case we have $n\propto T^3$ and the two equations of state for p and ρ reduce to the Stefan–Boltzmann equation and the γ-law with $\gamma=4/3$.

In the remainder of this section the full viscous transport equation will be analyzed resorting to the two expressions for the temperature mentioned above: a power-law given by (19) and an ideal gas equation for p together with the γ-law defining ρ, i.e.

$$p=nT, \qquad \rho=\frac{nT}{\gamma-1}. \tag{24}$$

Note that now both T and n are independent variables and only in the equilibrium limit the particle number density depends exclusively on the temperature, $n=n(T)$ (see comments above). It must be stressed that the Stefan–Boltzmann equation together with an ideal gas equation of state (with $n \propto T^3$) implies $\Pi=0$. So we conclude that out of equilibrium we are forced to adopt one of the two possibilities: (i) a power-law for T with no dependence on n at all; (ii) an ideal gas equation of state for the pressure together a γ-law, with n an independent variable on the same footing as T. Both approaches will be considered in turn.

A. Potential law for the temperature

Using equations (2), (3), (6), (19) and (23) the equation governing the evolution of the Hubble factor reduces to

$$\ddot{H}+\frac{3}{2}[1+\gamma(1-r)]H\dot{H}+\frac{a}{\delta}\left(H^2-\frac{\Lambda}{3}\right)^{1-m}\dot{H}+\frac{(3H^2-\Lambda)a}{2}$$
$$\times\left[\frac{\gamma}{\delta}\left(H^2-\frac{\Lambda}{3}\right)^{1-m}-3\left(1-\frac{\gamma}{2}\right)H\right]-3(r+1)\frac{H\dot{H}^2}{3H^2-\Lambda}=0. \tag{25}$$

i. $\Lambda=0$

● $m=1/2$

As in Section III only the case with γ and δ fulfilling the restriction

$$\frac{\gamma}{\delta}=\frac{3}{2}(2-\gamma), \tag{26}$$

is physically meaningful. In such instance there exists an infinity of stable fixed points $(h_1,0)$, with h_1 an arbitrary positive real number. The phase portrait are parallel stable straight lines.

● $m\neq 1/2$

There are two fixed points, $(0,0)$ and $(h_1,0)$, in the interval $m \in [0,\frac{1}{2})\cup(\frac{1}{2},2)$, where

$$h_1=\left(\frac{3\delta(2-\gamma)}{2\gamma}\right)^{1/(1-2m)}. \tag{27}$$

For $m\geqslant 2$ only the $(h_1,0)$ fixed point occurs, which we analyze next as nothing new arises about the point $(0,0)$.

Let us define the parameter

$$\Sigma_2=\frac{[\gamma(2-a)+2a]^2}{8a\gamma^2(2-\gamma)}>0.$$

For $m<\frac{1}{2}-\Sigma_2$ the equilibrium point is an attractor in the phase space (asymptotically stable focus). For $\frac{1}{2}-\Sigma_2\leqslant m<\frac{1}{2}$ we have asymptotically stable nodes instead. Finally if $m>1/2$, the fixed point is a saddle.

ii. $\Lambda>0$

From Eq. (25) it follows the equation for the fixed points,

$$(3h_i^2-\Lambda)\left[\frac{\gamma}{\delta}\left(h_i^2-\frac{\Lambda}{3}\right)^{1-m}-3\left(1-\frac{\gamma}{2}\right)h_i\right]=0, \tag{28}$$

where, as in the truncated case, only the solutions vanishing the big square parentheses make sense from a physical point of view. Equation (28) will be solved only for three different values of m. In this case we must take into account the constraint (23).

- $m=0$

The fixed point is $(h_2^\Lambda,0)$ with

$$h_2^\Lambda=\frac{3\delta}{2\gamma}\left(1-\frac{\gamma}{2}\right)+\frac{1}{2}\sqrt{\frac{9\delta^2}{\gamma^2}\left(1-\frac{\gamma}{2}\right)^2+\frac{4\Lambda}{3}}.$$

Defining the two new parameters,

$$\Sigma_3^\Lambda=\frac{2(1-\gamma/2)}{1/a[1-a/2+a/\gamma]^2-2(1-\gamma/2)}-1.$$

and

$$\Lambda_2=\frac{27\delta^2}{\gamma^2}\left(1-\frac{\gamma}{2}\right)^2\frac{1+\Sigma_3^\Lambda}{(\Sigma_3^\Lambda)^2},$$

we see that for $\Lambda\leqslant\Lambda_2$ the fixed point is an asymptotically stable node, whereas for $\Lambda>\Lambda_2$ it is an asymptotically stable focus.

- $m=1/2$

The fixed point is

$$h_2^\Lambda=\sqrt{\frac{\Lambda/3}{1-(9\delta^2/\gamma^2)(1-\gamma/2)^2}},$$

so

$$\delta<\frac{2\gamma}{3(2-\gamma)}.$$

Let us introduce

$$\delta_0=\frac{2\gamma}{3(2-\gamma)}(1-\Sigma_2)^{1/2}.$$

For $\delta>\delta_0$, $(h_2^\Lambda,0)$ is found to be an asymptotically stable node, however if $\delta=\delta_0$ it is an asymptotically stable degenerate node, whereas for $\delta<\delta_0$ the fixed point is an asymptotically stable focus. In the radiation case—i.e. $\gamma=4/3$- $\delta_0<0$ and the fixed point is a stable node.

- $m=1$

In this case

$$h_2^\Lambda=\frac{\gamma}{3\delta(1-\gamma/2)}.$$

Let us define the parameter

$$\Lambda_3=\frac{\gamma^2(1+2\Sigma_2)}{3\delta^2(1-\gamma/2)^2}>0.$$

For $\Lambda > \Lambda_3$ the fixed point is an asymptotically stable focus, and for $\Lambda = \Lambda_3$ an asymptotically stable degenerate node.

Finally, when $\Lambda < \Lambda_3$ we can distinguish two subcases. Defining

$$\Lambda_3^* = \frac{\gamma^2}{3\delta^2(1-\gamma/2)^2},$$

we have a saddle point for

$$\Lambda < \Lambda_3^*,$$

and an asymptotically stable node for

$$\Lambda_3^* < \Lambda < \Lambda_3.$$

B. Ideal gas equation for the temperature

In this section we shall study the specific behavior of the equilibrium points, making use of the state equations (24). As neither particle production nor annilation occurs, n obeys the conservation equation

$$\dot{n} + 3Hn = 0, \tag{29}$$

which leads to $n \propto R^{-3}$. The expression for the temperature,

$$T = \frac{3}{\kappa}\frac{\gamma-1}{n_0} R^3 \left(H^2 - \frac{\Lambda}{3} \right), \tag{30}$$

where $n_0 > 0$ is a constant, follows easily. Using (2), (3a), (3b), (4), (6) and (30) we get the equation

$$\ddot{H} + \frac{a}{\delta}\left(H^2 - \frac{\Lambda}{3} \right)^{1-m} \dot{H} + \frac{(3H^2-\Lambda)a}{2}\left[\frac{\gamma}{\delta}\left(H^2 - \frac{\Lambda}{3} \right)^{1-m} - 3\left(1 - \frac{\gamma}{2} \right) H \right] - 6\frac{H\dot{H}^2}{3H^2-\Lambda} = 0, \tag{31}$$

i. $\Lambda = 0$

We have the same fixed points as in the truncated theory [see equation (17)].

In the case $m = 1/2$ the discussion runs along the same lines as that of the truncated theory. After linearizing the system and introducing the parameter

$$\Sigma_3 = \frac{a}{4\gamma^2},$$

the following will be discussed. For $m < \frac{1}{2} - \Sigma_3$ the eigenvalues are complex and the equilibrium point is an attractor (asymptotically stable focus). For $m = \frac{1}{2} - \Sigma_3$ there is a bifurcation point which is an asymptotically stable degenerate node. For $m > 1/2$ one has a saddle point. Finally, if $\frac{1}{2} - \Sigma_3 < m < 1/2$ the fixed point results an asymptotically stable node.

ii. $\Lambda > 0$

Now the fixed points $(h_2^\Lambda, 0)$ are again the same as in the full theory using a power law for the temperature.

- $m = 0$

For any $\Lambda > 0$ the fixed point is an asymptotically stable focus.

- $m=1/2$

Defining

$$\delta_1=\frac{\gamma}{3}\sqrt{1-\frac{1}{2\gamma^2}},$$

we note that if δ lies in the interval $0<\delta<\delta_1$ the fixed point is an asymptotically stable focus. If $\delta=\delta_1$ it is an asymptotically stable degenerate node, and if $\delta_1<\delta<\gamma/3$ an asymptotically stable node for any $\Lambda>0$.

- $m=1$

Let us define

$$\Lambda_4=\frac{\gamma^2}{3\delta^2}(1+2\Sigma_3).$$

If $\Lambda<\gamma/3\delta^2$ then the fixed point is a saddle point, but if $\gamma/3\delta^2<\Lambda<\Lambda_4$ it is an asymptotically stable node. For $\Lambda=\Lambda_4$ it is an asymptotically stable degenerate node, and for $\Lambda>\Lambda_4$ an asymptotically stable focus.

1. Non-thermalizing condition for dissipative de Sitter expansion

i. $\Lambda=0$

From (5) and (2) one finds

$$H^{1-2m}<\delta/a\,. \tag{32}$$

For the truncated and full theory using an ideal gas equation for T this condition reduces to $\gamma>3a$ by virtue of (17). On the other hand, as the velocity of the viscous pulses, as well as the speed of sound, cannot exceed the speed of light ($1<\gamma<2$) we obtain the restrictions on γ and a. If a lies in the range $0<a<\frac{1}{3}$, the two mentioned conditions amount to $1<\gamma<2$; whereas if $\frac{1}{3}<a<\frac{2}{3}$ these restrictions imply $3a<\gamma<2$. Finally, if $\frac{2}{3}<a<1$, no γ can fulfill both conditions.

For the full theory with a power law for temperature one obtains the restriction $\gamma>\gamma_c$ where

$$\gamma_c=\frac{6a}{3a+2}.$$

Two conditions must be fulfilled simultaneously by γ: $1<\gamma<2$ and $\gamma>\gamma_c$. For $0<a<\frac{2}{3}$, these restrictions imply $1<\gamma<2$ (since $\gamma_c<1$); whereas for $\frac{2}{3}<a<1$ one has $1<\gamma_c<\gamma<2$. So for $a<1$ the full theory with a power law for temperature always holds.

ii. $\Lambda>0$

Instead of (32) we now have

$$\frac{a}{\delta}\left(H^2-\frac{\Lambda}{3}\right)^{1-m}<H, \tag{33}$$

when a positive cosmological constant is present.

For the fixed point $(h_1^\Lambda,0)$ (that of the truncated theory) the restrictions for γ are the same that in the truncated case with $\Lambda=0$, whereas for the full theory the restriction (33), when applied to the point $(h_2^\Lambda,0)$, coincides with that of the full theory using a power law for the temperature with vanishing Λ.

V. DYNAMICAL CONSEQUENCES

In this section we study the dynamical implications of linearizing the equation for H. This linearization allows one to obtain an analytical solution for $R(t)$ near the equilibrium points. The matrix $\mathbf{L}$ is given by (14) and the system of differential equations to solve is

$$\begin{pmatrix} \dot{h} \\ \dot{X} \end{pmatrix} = \begin{pmatrix} P_H & P_X \\ Q_H & Q_X \end{pmatrix} \begin{pmatrix} h \\ X \end{pmatrix}, \tag{34}$$

where $h \equiv H - h_i$ and $\overline{X} \equiv X - X_i = X$ being $(h_i, X_i = 0)$ the fixed points. Equation (34) can be written as

$$\ddot{h} - Q_X \dot{h} - Q_H h = 0, \tag{35}$$

where in our model $P_H = 0$ and $P_X = 1$. The corresponding characteristic equation reads as

$$\lambda_{\pm} = \frac{Q_X \pm \sqrt{Q_X^2 + 4Q_H}}{2},$$

which coincides with the equation for the eigenvalues of $\mathbf{L}$. We perturb the system around the de Sitter solution for $t = 0$, i.e., $H(t=0) = h_i + \epsilon(0)$ and take $\dot{H}(t=0) = \dot{\epsilon}(0)$ as initial condition.

A. Saddle points and nodes

In the neighborhood of these points the discriminant Δ is positive and the eigenvalues $\lambda_{\pm}$ are real and different. For $det(\mathbf{L}) < 0$ one has a saddle point, and for $det(\mathbf{L}) > 0$ a node. The solution of (35) is

$$h = c_1 e^{\lambda_+ t} + c_2 e^{\lambda_- t},$$

with

$$c_1 = -\frac{\dot{\epsilon}(0) - \epsilon(0)\lambda_-}{\lambda_- - \lambda_+}, \quad c_2 = \frac{\dot{\epsilon}(0) - \epsilon(0)\lambda_+}{\lambda_- - \lambda_+}.$$

Upon integration, one has for the scale factor

$$R(t) \propto e^{h_i t} \exp\left[\frac{c_1}{\lambda_+} e^{\lambda_+ t} + \frac{c_2}{\lambda_-} e^{\lambda_- t}\right], \tag{36}$$

which shows superinflationary expansion if initial conditions are taken such that c_1, c_2 are positive. This type of evolution for $R(t)$ on time has been obtained previously in a different context.[27] In this case the fluid when submitted to a small perturbation, goes away from the equilibrium point expanding much more rapidly than the de Sitter's. In the case of nodes, and when $\lambda_+ + \lambda_- = Q_X$ is positive (negative), the node will be unstable (stable).

B. Attractors and repellors

We study here the behavior of the scale factor near a sink (an asymptotically stable attractor) and a source (an asympotically unstable repellor). The solutions of the characteristic equation are complex,

$$\lambda_{\pm} = \frac{Q_X \pm i\sqrt{|\Delta|}}{2},$$

where $\Delta = Q_X^2 + 4Q_H$. Then the solution of (35) is

$$h = c_1 e^{\frac{Q_X}{2}t} \sin \frac{\sqrt{|\Delta|}}{2}(t + c_2).$$

The integration constants can be determined through the initial conditions. They read as

$$c_2 = \frac{2}{\sqrt{|\Delta|}} \tan^{-1}\left[\frac{\epsilon(0)\sqrt{|\Delta|}}{2\dot{\epsilon}(0) - \epsilon(0)Q_x}\right]$$

and

$$c_1 = \frac{\epsilon(0)}{\sin\,(\sqrt{|\Delta|}/2)c_2}.$$

Integrating the equation for h, one follows that

$$R(t) \propto e^{h_i t} \exp\left[\frac{2c_1}{Q_x^2 + |\Delta|}\left(Q_x \sin\frac{\sqrt{|\Delta|}}{2}(t + c_2) - \sqrt{|\Delta|}\cos\frac{\sqrt{|\Delta|}}{2}(t + c_2)\right)\right]. \tag{37}$$

For $Q_X < 0$ we have an attractor (the scale factor undergoes an oscillatory approach to the de Sitter solution) and for $Q_X > 0$ it is a source, i.e., the scale factor deviates from the de Sitter solution.

C. Degenerate nodes

In this case $\Delta = 0$ and $\lambda_+ = \lambda_- = \lambda = Q_X/2$. The solution of (35) is

$$h = c_1 e^{\lambda t} + c_2 t e^{\lambda t}.$$

Because of the initial conditions the integration constants are

$$c_1 = \epsilon(0), \quad \text{and} \quad c_2 = \dot{\epsilon}(0) - \lambda\epsilon(0).$$

Integration of the expression for h leads to

$$R(t) \sim e^{h_i t} \exp\left[\frac{e^{\lambda t}}{\lambda}\left(\epsilon(0) + (\dot{\epsilon}(0) - \lambda\epsilon)\left(t - \frac{1}{\lambda}\right)\right)\right], \tag{38}$$

hence $R(t)$ approaches to or separates from the de Sitter solution depending on the sign of λ. The rate of evolution is faster than in the de Sitter case.

D. Energy conditions

The weak energy condition (WEC) states that $T_{ab}W^aW^b \geq 0$, where T_{ab} is the energy-momentum tensor given by (1) and W^a a generic timelike vector. In our model this condition reduces to

$$\rho + \Lambda \geq 0. \tag{39}$$

The dominant energy condition (DEC) imposes $T_{ab}W^aW^b \geq 0$ and $-T^{ab}W_a$ to be a non-spacelike vector which is equivalent to $T_{00} \geq |T_{ab}|$.[28] This conditions is fulfilled in our case solely if

$$-\rho \leq p + \Pi \leq \rho + 2\Lambda. \tag{40}$$

Finally, the strong energy condition (SEC) requires that $T_{ab}W^aW^b+\frac{1}{2}T^a_a\geqslant 0$ which amounts to

$$\rho-2\Lambda+3p+3\Pi\geqslant 0. \tag{41}$$

These conditions can be rewritten in terms of H and $\dot{H}$ as

$$\begin{aligned}&\text{WEC:}\quad H^2\geqslant 0,\\ &\text{SEC:}\quad H^2+\dot{H}\leqslant 0,\\ &\text{DEC:}\quad \dot{H}\leqslant 0\quad\text{and}\quad 3H^2+\dot{H}\geqslant 0.\end{aligned}$$

As occurs in the standard inflationary scenarios the de Sitter solutions with $\Lambda\geqslant 0$ satisfy the WEC and DEC but not SEC.

VI. CONCLUSIONS

We have carried out a detailed analysis on the stability of de Sitter and static cosmological models, both in the truncated and full theory for the viscous transport equation (with and without a cosmological constant). We have shown that the conditions for the hydrodynamic approach and the nonthermalizing condition in a de Sitter expansion can be fulfilled simultaneously for sufficiently early times. When *no* cosmological constant is considered the stability analysis for the de Sitter solutions leads to similar results in all the cases, i.e., the models are *unstable* only for $m>1/2$. It is remarkable that this result holds for both the truncated and the full version of ET. On the other hand, when a *positive* cosmological constant is included we see that the models can be stable for $m=1$ if Λ is bounded from below. It remains to be proved that this result holds for a generic $m>1/2$ other than 1.

We have stressed the fact that for a radiation gas a different thermodynamic approach exists, depending on whether the particle number density is taken as an independent variable or not. In the case of a power-law for the temperature it exists a relationship between γ and r.

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Bounds on number of cusps due to point mass gravitational lenses

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Generic caustics in gravitational lensing occur locally either as folds or cusps. This paper rigorously proves that the total number of cusps, N_{cusps}, due to g point masses on a single plane having non-normalized external shear $\gamma>0$ and continuous matter with constant density σ_c, is bounded as follows: $0\leqslant N_{cusps}\leqslant 12g^2$. For vanishing shear $\gamma=0$ we obtain the result $0\leqslant N_{cusps}\leqslant 12g(g-1)$. Consequences of these bounds for the global geometry of caustics are discussed. It is also shown that if $\gamma\geqslant 0$ and σ_c is sufficiently large, then all cusps can be eliminated, that is, $N_{cusps}=0$. The paper also includes equations for calculating all the bi-caustics (i.e., curves yielding the positions of cusps during a one-parameter evolution) of a single point-mass lens with continuous matter and shear. The methods of the paper are based on a new approach to point-mass gravitational lensing using complex quantities and the theory of resultants. © *1996 American Institute of Physics.*
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I. INTRODUCTION

This paper is part of a series of mathematical studies aimed at investigating the global properties of caustics in gravitational lensing. The global geometry of caustics produced by general multiplane gravitational lens systems has recently been studied by Petters.[1] The latter gave counting formulas for general cusps as well as cusps of the first and second kinds. Currently, however, very little is known concerning the range of possible values for the number of cusps. In this paper, we determine bounds on the number of cusps due to single plane point-mass lens systems with continuous matter and external shear. We add that the overall issue of counting cusps is not only of mathematical interest, but also physically relevant. For example, Wambsganss, Witt, and Schneider[2] have shown that for point-mass lens systems with low surface mass density as much as 40% of all magnification events in a light curve are due to point sources passing outside cusps.

II. BOUNDS ON NUMBER OF CUSPS

Let $\mathbf{x}_1,\ldots,\mathbf{x}_g$ be distinct points in the plane and let γ, σ_c, and $m_1,\ldots,m_g$ be non-negative real numbers. The map $\eta:\mathbf{R}^2-\{\mathbf{x}_1,\ldots,\mathbf{x}_g\}\to\mathbf{R}^2$ given by

$$\eta(\mathbf{x})=\mathbf{x}-\sum_{i=1}^{g} m_i\frac{\mathbf{x}-\mathbf{x}_i}{|\mathbf{x}-\mathbf{x}_i|^2}-\begin{pmatrix}\sigma_c-\gamma & 0\\ 0 & \sigma_c+\gamma\end{pmatrix}\mathbf{x}$$

is a single-plane *lensing map* due to point masses m_i on a plane with non-normalized shear γ acting along one of the coordinate axes, and continuous matter having constant density σ_c (in units of the critical density). This lens system is called *underfocused* (resp., *overfocused*) if $0\leqslant\sigma_c<1$ (resp., if $\sigma_c>1$).

The central result of the paper is the following theorem.

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Theorem 1: *Let N_{cusps} be the total number of cusps of η.*
(*i*) *If $\gamma=0$, then $0\leqslant N_{cusps}\leqslant 12g(g-1)$.*
(*ii*) *If $\gamma>0$, then $0\leqslant N_{cusps}\leqslant 12g^2$.*
(*iii*) *If $\gamma\geqslant 0$ and σ_c is sufficiently large, then $N_{cusps}=0$.*

The upper bounds in Theorem 1 apply to the sum of the maximum number of cusps for the under– and overfocused cases. A detailed discussion of this point is deferred to Section IV and the Appendix. Theorem 1 and its proof are also illustrated explicitly in the Appendix for the case of a single point mass with continuous matter and shear.

Theorem 1 can be used to obtain bounds on the total curvature of the caustics due to single plane point mass lens systems with continuous matter and shear. Recently, Petters[3] showed that the total curvature K_{tot} of the caustics due to these lens systems is given by:

$$K_{tot}=-2\pi g+\pi N_{cusps}.$$

By Theorem 1(i,ii) the total curvature is then bounded as follows:

$$-2\pi g\leqslant K_{tot}\leqslant\begin{cases}2\pi g(6g-1) & \text{if } \gamma>0\\ 2\pi g(6g-7) & \text{if } \gamma=0.\end{cases} \tag{1}$$

The upper bounds in Theorem 1 apply to the sum of the maximum number of cusps for the under– and overfocused cases. A discussion of this point is deferred to Section IV. In addition, Theorem 1 and its proof are illustrated explicitly in the Appendix for the case of a single point mass with continuous matter and shear.

Theorem 1(iii) yields that *for σ_c sufficiently large, all cusps of the lensing map η can be eliminated.* The general issue of cusp elimination for differentiable maps was investigated by Levine[4] in 1965 and later by Eliashberg,[5] culminating in the Levine–Eliashberg theorem: a locally stable map from a compact, oriented, boundaryless n-manifold M into the plane is homotopic to a locally stable map with 0 or 1 cusp depending on whether the Euler characteristic of M is even or not. However, this theorem cannot be directly applied in lensing because if one starts with a generic lensing map, there is no guarantee that each stage of the theorem's homotopy is a lensing map. An immediate consequence of cusp elimination is that *for σ_c sufficiently large, the caustics consist of g ovals (Petters[6]) and, hence, the high-tail magnification cross-section is determined only by folds.*

III. PROOF OF MAIN THEOREM

The proofs of Theorem 1(i-ii) and Theorem 1(iii) are given in Section III.B and Section III.A, respectively. Throughout the sequel, suppose that $\sigma_c\neq 1$ unless stated to the contrary.

A. Elimination of Cusps

Whitney's singularity theory yields explicit equations characterizing cusp points in terms of derivatives of η (e.g., Lu[7]). Unfortunately, these equations are very complicated and hence difficult to analyze in order to investigate cusp elimination or to determine upper bounds for N_{cusps}. On the other hand, the natural ''rational form'' of the lensing map makes it readily accessible to complex variable techniques. Thus, following Witt[8] we express $\eta(\mathbf{x})$ in complex form ($z=x+iy$, $\mathbf{x}_i=z_i$) as follows:

$$\zeta(z)=(1-\sigma_c)z+\gamma\overline{z}+\sum_{\ell=1}^{g}\frac{m_\ell}{\overline{z}_\ell-\overline{z}}.$$

Critical curves of η are determined by the vanishing of the Jacobian determinant of the complex lensing map $\zeta(z)$:

$$\det\ J(z,\overline{z})=\frac{\partial\zeta}{\partial z}\frac{\overline{\partial\zeta}}{\partial z}-\frac{\partial\zeta}{\partial\overline{z}}\frac{\overline{\partial\zeta}}{\partial\overline{z}}=0.$$

Since $\partial\zeta/\partial z$ is real and $a^2=w\overline{w}$ ($a\in\mathbf{R}$, $w\in\mathbf{C}$) implies $w=|a|e^{i\varphi}$, we see that the above equation is solved by

$$\frac{\partial\zeta}{\partial\overline{z}}=\left|\frac{\partial\zeta}{\partial z}\right|e^{i\varphi},\varphi\in[0,2\pi),$$

or, equivalently,

$$|1-\sigma_c|e^{i\varphi}=\gamma+\sum_{\ell=1}^{g}\frac{m_\ell}{(\overline{z_\ell}-\overline{z})^2}. \tag{2}$$

Equation (2) can be rewritten as follows:

$$F(\overline{z})\equiv\prod_{\ell=1}^{g}(\overline{z_\ell}-\overline{z})^2+\sum_{\ell=1}^{g}\left(\hat{m}_\ell\prod_{\substack{r=1\\r\neq\ell}}^{g}(\overline{z_r}-\overline{z})^2\right),$$

where

$$\hat{m}_\ell=\frac{m_\ell}{(|1-\sigma_c|e^{i\varphi}-\gamma)}.$$

Set

$$P(\overline{z})=\prod_{\ell=1}^{g}(\overline{z_\ell}-\overline{z})^2.$$

Since

$$\lim_{\sigma_c\to\infty}F(\overline{z})=P(\overline{z})$$

the coefficients of $F(\overline{z})$ approach those of $P(\overline{z})$ as $\sigma_c\to\infty$. Hence, in the latter limit the zeros of $F(\overline{z})$ are in one-to-one correspondence with the zeros of $P(\overline{z})$, where zeros are counted with multiplicity, and approach the double zeros $z_1,\ldots,z_g$ of $P(\overline{z})$. This follows from the fact that the zeros of a complex polynomial are continuous functions of the coefficients of the polynomial.[9]

For σ_c sufficiently large, the critical curves lie in small discs about each of the points $z_1,\ldots,z_g$. Consider any such disc, say, $D(z_j;r_j)$ with radius r_j and centered at z_j. The larger the value of σ_c, the smaller one can choose r_j. Now, write the lensing map as

$$\zeta(z)=(1-\sigma_c)z+\gamma\overline{z}+\frac{m_j}{\overline{z_j}-\overline{z}}+R(\overline{z}),$$

where

$$R(\overline{z})=\sum_{\substack{\ell=1\\\ell\neq j}}^{g}\frac{m_\ell}{\overline{z_i}-\overline{z}}$$

Restricting $\zeta(z)$ to $D(z_j;r_j)$ and making r_j sufficiently small, we can approximate $\zeta(z)$ arbitrarily close by

$$\zeta_j(z)=(1-\sigma_c)z+\gamma\overline{z}+\frac{m_j}{\overline{z_j}-\overline{z}}.$$

However, $\zeta_j(z)$ is the Chang–Refsdal lens of mass m_i at position z_j. Witt and Petters[10] have shown that for $\sigma_c>\sqrt{4/3}\gamma+1$ the Chang–Refsdal lens has a single simple closed caustic curve with no cusps, while cusps exist (and more than one caustic is possible) for $\sigma_c\leqslant\sqrt{4/3}\gamma+1$. Observe that the caustic of $\zeta_j(z)$ is stable[11] if $\sigma_c>\sqrt{4/3}\gamma+1$. Thus, for large enough σ_c the caustics of $\zeta(z)$ have no cusps and consist of g simple closed curves.

B. Upper Bounds

1. Resultants and Equations for Cusps

We now show that cusps generated by the lensing map η can be characterized as common solutions of two polynomial equations. Resultants are then used to give a necessary and sufficient condition for these common solutions. See Erdl and Schneider[12] for applications of resultants to the study of double point-mass lenses on distinct planes.

A point z is mapped by ζ to a cusp point if and only if $(z,\overline{z})$ satisfies both of the following equations:

$$\det J(z,\overline{z})=0 \quad \text{and} \quad H_\zeta(z,\overline{z})=0,$$

where $H_\zeta(z,\overline{z})$ is the (complex) tangential vector at the caustic. It is given by

$$H_\zeta(z,\overline{z})=\frac{\partial\zeta}{\partial z}H_z+\frac{\partial\zeta}{\partial\overline{z}}\overline{H_z},$$

where

$$H_z=2i\frac{\partial\,\det J}{\partial\overline{z}}=-2i\frac{\partial\overline{\zeta}}{\partial\overline{z}}\frac{\partial^2\zeta}{\partial\overline{z}^2}$$

is the (complex) tangential vector at the critical curve. The partial derivatives are given as follows:

$$\frac{\partial\zeta}{\partial z}=(1-\sigma_c);\quad \frac{\partial\zeta}{\partial\overline{z}}=\gamma+\sum_{\ell=1}^{g}\frac{m_\ell}{(\overline{z_\ell}-\overline{z})^2};\quad \frac{\partial^2\zeta}{\partial\overline{z}^2}=\sum_{\ell=1}^{g}\frac{2m_\ell}{(\overline{z_\ell}-\overline{z})^3}.$$

Now let us denote

$$p_{\zeta,1}(\overline{z})=\frac{\partial\zeta}{\partial\overline{z}}\prod_{\ell=1}^{g}(\overline{z_\ell}-\overline{z})^2=\gamma\prod_{\ell=1}^{g}(\overline{z_\ell}-\overline{z})^2+\sum_{\ell=1}^{g}m_\ell\prod_{\substack{r=1\\r\neq\ell}}^{g}(\overline{z_r}-\overline{z})^2$$

and

$$p_{\zeta,2}(\overline{z})=\frac{\partial^2\zeta}{\partial\overline{z}^2}\prod_{\ell=1}^{g}(\overline{z_\ell}-\overline{z})^4=\prod_{\ell=1}^{g}(\overline{z_\ell}-\overline{z})\left(\sum_{\ell=1}^{g}m_\ell\prod_{\substack{r=1\\r\neq\ell}}^{g}(\overline{z_r}-\overline{z})^3\right).$$

Direct computation shows that the equations $\det J(z,\overline{z})=0$ and $H_{\zeta}(z,\overline{z})=0$ are equivalent, respectively, to

$$P_J(z,\overline{z})\equiv(\det J)\prod_{\ell=1}^{g}(\overline{z_\ell}-\overline{z})^2(z_\ell-z)^2=\left\{(1-\sigma_c)^2\prod_{\ell=1}^{g}(\overline{z_\ell}-\overline{z})^2\right\}\prod_{\ell=1}^{g}(z_\ell-z)^2-p_{\zeta,1}(\overline{z})$$
$$\times\left\{\gamma\prod_{\ell=1}^{g}(z_\ell-z)^2+\sum_{\ell=1}^{g}m_\ell\prod_{\substack{r=1\\r\neq\ell}}^{g}(z_r-z)^2\right\}=0, \tag{3}$$

and

$$P_H(z,\overline{z})\equiv\frac{i}{4}H_{\zeta}(z,\overline{z})\prod_{\ell=1}^{g}(z_\ell-z)^3(\overline{z_\ell}-\overline{z})^4=(1-\sigma_c)p_{\zeta,2}(\overline{z})$$
$$\times\left\{\gamma\prod_{\ell=1}^{g}(z_\ell-z)^3+\prod_{\ell=1}^{g}(z_\ell-z)\sum_{\ell=1}^{g}m_\ell\prod_{\substack{r=1\\r\neq\ell}}^{g}(z_r-z)^2\right\}$$
$$-p_{\zeta,1}^2(\overline{z})\sum_{\ell=1}^{g}m_\ell\prod_{\substack{r=1\\r\neq\ell}}^{g}(z_r-z)^3=0. \tag{4}$$

Next, consider any two polynomials in x_1 and x_2:

$$p(x_1,x_2)=a_0(x_2)+a_1(x_2)x_1+\ldots+a_m(x_2)x_1^m$$

and

$$q(x_1,x_2)=b_0(x_2)+b_1(x_2)x_1+\ldots+b_n(x_2)x_1^n.$$

The x_1-Sylvester resultant of p and q is defined by

$$\mathrm{Res}(x_2)=\det(\mathbf{A}_{m+n}),$$

where

$$\mathbf{A}_{m+n}=\begin{bmatrix}
a_m & a_{m-1} & a_{m-2} & \cdot & \cdot & \cdot & a_0 & 0 & 0 & \cdot\cdot & 0\\
0 & a_m & a_{m-1} & \cdot & \cdot & \cdot & a_1 & a_0 & 0 & \cdot\cdot & 0\\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots\\
0 & \cdots & 0 & a_m & a_{m-1} & a_{m-2} & \cdot & \cdot & \cdot & a_1 & a_0\\
b_n & b_{n-1} & \cdot & \cdot & \cdot & b_0 & 0 & \cdot & \cdot & \cdot & 0\\
0 & b_n & b_{n-1} & \cdot & \cdot & \cdot & b_0 & \cdot & \cdot & \cdot & 0\\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots\\
0 & \cdot & \cdot & \cdot & 0 & b_n & b_{n-1} & \cdot & \cdot & \cdot & b_0
\end{bmatrix}. \tag{5}$$

Note that the exact location of the nth and mth columns relative to each other depends on the values of n and m. The matrix $\mathbf{A}_{m+n}$ is described explicitly as follows: The ℓth–row of $\mathbf{A}_{m+n}$, where $1\leqslant\ell\leqslant n$, consists of $\ell-1$ zeros, followed by $a_m,a_{m-1},\ldots,a_0$, and the remainder of the row filled with zeros. For $n+1\leqslant\ell\leqslant m+n$, the ℓth–row has $\ell-n-1$ zeros followed

by $b_n, b_{n-1}, \ldots, b_0$, and the remaining slots having zeros. Note that $\mathrm{Res}(x_2)$ is a polynomial in x_2. The Resultant Theorem (e.g., Abhyankar[13,14]) yields that β satisfies $\mathrm{Res}(\beta)=0$ if and only if either $a_m(\beta)=0=b_n(\beta)$, or, $p(\alpha,\beta)=0=q(\alpha,\beta)$ for some α.

Using Eqs. (3) and (4), we can express $P_J(z,\overline{z})$ and $P_H(z,\overline{z})$ as polynomials in z with coefficients that are polynomials in $\overline{z}$:

$$P_J(z)=a_0(\overline{z})+a_1(\overline{z})z+\cdots+a_{2g}(\overline{z})z^{2g}$$

and

$$P_H(z)=b_0(\overline{z})+b_1(\overline{z})z+\cdots+b_{3g}(\overline{z})z^{3g}.$$

Note that if $\gamma=0$, then $b_{3g}=b_{3g-1}=0$.

Notation: *In order to capture the cases* $\gamma=0$ *and* $\gamma>0$ *simultaneously, let* $n(\gamma)=3g-2$ *if* $\gamma=0$ *and let* $n(\gamma)=3g$ *if* $\gamma>0$.

Rewrite P_H as:

$$P_H(z)=b_0(\overline{z})+b_1(\overline{z})z+\cdots+b_{n(\gamma)}(\overline{z})z^{n(\gamma)}.$$

The z-Sylvester resultant of P_J and P_H is then given by

$$\mathrm{Res}(\overline{z})=\det[\mathbf{A}_{2g+n(\gamma)}].$$

By the Resultant Theorem, $\overline{z_0}$ satisfies $\mathrm{Res}(\overline{z_0})=0$ if and only if either

$$a_{2g}(\overline{z_0})=0=b_{n(\gamma)}(\overline{z_0}),$$

or,

$$P_J(z_0,\overline{z_0})=0=P_H(z_0,\overline{z_0}).$$

Consequently, the cusps of the lensing map η form a subset of the zeros of $\mathrm{Res}(\overline{z})$.

2. Upper bounds for the degree of Res ($\overline{z}$)

By the Resultant Theorem we have $N_{cusps}\leqslant \deg[\mathrm{Res}(\overline{z})]$. To find an upper bound for the degree of $\mathrm{Res}(\overline{z})$, first write

$$\begin{aligned}\mathrm{Res}(\overline{z})&=\sum W_{i_0\ldots i_{2g}j_0\ldots j_{n(\gamma)}}a_0^{i_0}\ldots a_{2g}^{i_{2g}}b_0^{j_0}\ldots b_{n(\gamma)}^{j_{n(\gamma)}}\\&\equiv \mathrm{Res}(a_0,\ldots,a_{2g},b_0,\ldots,b_{n(\gamma)}).\end{aligned}\tag{6}$$

This expresses the resultant as a polynomial in the variables $a_0,\ldots,a_{2g},b_0,\ldots,b_{n(\gamma)}$ with integer coefficients $W_{i_0\ldots i_{2g}j_0\ldots j_{n(\gamma)}}$. Using the fact[15] that the resultant is homogeneous of degree $n(\gamma)$ in the coefficients a_ℓ and degree $2g$ in b_ℓ, we get:

$$\mathrm{Res}(ta_0,\ldots,ta_{2g},\lambda b_0,\ldots,\lambda b_{n(\gamma)})=t^{n(\gamma)}\lambda^{2g}\,\mathrm{Res}(a_0,\ldots,a_{2g},b_0,\ldots,b_{n(\gamma)}).\tag{7}$$

Hence:

$$\deg[\,\mathrm{Res}(\overline{z})]\leqslant[n(\gamma)]r+(2g)s,$$

where r and s are, respectively, the largest of the degrees of the polynomials $a_\ell(\overline{z})$ and $b_\ell(\overline{z})$.

We now determine r and s for $\gamma>0$ and $\gamma=0$. The coefficients in curly brackets in Eq. (3) are all of degree $2g$ for $\gamma\geqslant 0$. The first curly bracketed coefficient in Eq. (4) is of degree $4g-3$ if $\gamma>0$; the coefficient vanishes for $\gamma=0$. The second curly bracketed coefficient is of degree $4g-3$ independent of the value of γ. When $\gamma>0$ the third curly bracketed coefficient is of degree $4g$ (it is of degree $4g-4$ for $\gamma=0$). Hence, if $\gamma=0$, then $r=2g$ and $s=4g-3$. If $\gamma>0$, we get $r=2g$ and $s=4g$. Thus,

$$N_{cusps}\leqslant \deg[\ \mathrm{Res}(\overline{z})]\leqslant [n(\gamma)]r+(2g)s=\begin{cases}14g^2 & \text{if } \gamma>0\\ 14g^2-10g & \text{if } \gamma=0.\end{cases} \tag{8}$$

Remark: Computations of the resultant for $g=2$ with Mathematica[16] yield a degree of $56=14(2)^2$ for $\gamma>0$ and 32 for $\gamma=0$. In the latter case, Eq. (8) predicts an upper bound of $14(2)^2-10(2)=36$ for the degree of the resultant. This overestimates the degree by 4 for $g=2$.

We now show that for $\gamma=0$ the result of Eq. (8) improves as follows:

$$N_{cusps}\leqslant \deg[\ \mathrm{Res}(\overline{z})]\leqslant 14g^2-12g, \text{ if } \gamma=0. \tag{9}$$

Note that for $g=2$, Eq. (9) yields $14(2)^2-12(2)=32$ (see Remark above). Closer inspection of the coefficients a_ℓ and b_ℓ of the polynomials P_J and P_H reveals the following structure:

$$a_\ell(\overline{z})=a_{\ell,1}(\overline{z})+p_{\zeta,1}(\overline{z})a_{\ell,2} \quad \text{and} \quad b_r(\overline{z})=b_{r,1}(\overline{z})+p^2_{\zeta,1}(\overline{z})b_{r,2},$$

where $\ell=0,\ldots,2g$ and $r=0,\ldots,n(\gamma)$. Note that $a_{\ell,2}$ and $b_{r,2}$ are complex constants. Equations (3) and (4) imply:

$$P_J(z_j,\overline{z})=\sum_{\ell=0}^{2g} a_\ell(\overline{z})z_j^\ell=-p_{\zeta,1}(\overline{z})m_j\prod_{\substack{\ell=1\\ \ell\neq j}}^{g}(z_\ell-z_j)^2$$

and

$$P_H(z_j,\overline{z})=\sum_{\ell=0}^{n(\gamma)} b_\ell(\overline{z})z_j^\ell=-p^2_{\zeta,1}(\overline{z})m_j\prod_{\substack{\ell=1\\ \ell\neq j}}^{g}(z_\ell-z_j)^3.$$

Since $p_{\zeta,1}(\overline{z})$ (resp., $p^2_{\zeta,1}(\overline{z})$) is not a factor of

$$\sum_{\ell=0}^{2g} a_{\ell,1}(\overline{z})z_j^\ell \quad \left(\text{resp.,}\sum_{\ell=0}^{n(\gamma)} b_{\ell,1}(\overline{z})z_j^\ell\right),$$

we get

$$\sum_{\ell=0}^{2g} a_{\ell,1}(\overline{z})z_j^\ell=0 \quad \text{and} \quad \sum_{\ell=0}^{n(\gamma)} b_{\ell,1}(\overline{z})z_j^\ell=0.$$

The Resultant Theorem implies that if two single-variable polynomials have a common root, then their resultant vanishes.[17] Thus, $\mathrm{Res}(a_{0,1}(\overline{z}),\ldots,a_{2g,1}(\overline{z});b_{0,1}(\overline{z}),\ldots,b_{n(\gamma),1}(\overline{z}))=0$.

Now, Eq. (6) implies:

$$\begin{aligned}&\mathrm{Res}(a_0(\overline{z}),\ldots,a_{2g}(\overline{z});b_0(\overline{z}),\ldots,b_{n(\gamma)}(\overline{z}))\\&=\mathrm{Res}(a_{0,1}(\overline{z}),\ldots,a_{2g,1}(\overline{z});b_{0,1}(\overline{z}),\ldots,b_{n(\gamma),1}(\overline{z}))+(\text{sum of terms each containing at least one factor with a }(\ell,2)\text{–index})\\&=(\text{sum of terms each containing at least one factor with a }(\ell,2)\text{–index}).\end{aligned}\tag{10}$$

In addition,

$$\max[\deg\{a_{\ell,1}(\overline{z}):\ell=0,\ldots,2g\}]=2g,$$

$$\max[\deg\{p_{\zeta,1}^2(\overline{z})b_{\ell,2}:\ell=0,\ldots,n(\gamma)\}]=4g-4\ \text{for}\ \gamma=0,$$

$$\max[\deg\{p_{\zeta,1}(\overline{z})a_{\ell,2}:\ell=0,\ldots,2g\}]=2g-2\ \text{for}\ \gamma=0,$$

and

$$\max[\deg\{b_{\ell,1}(\overline{z}):\ell=0,\ldots,n(\gamma)\}]=4g-3.$$

Hence, the maximum of the degrees of the terms in Eq. (10) coincides with the degree of one of the following terms:

$$a_{0,1}^{i_0}\cdots a_{2g,1}^{i_{2g}}(p_{\zeta,1}^2b_{0,2})^{j_0}\cdots(p_{\zeta,1}^2b_{n(\gamma),2})^{j_{n(\gamma)}},\tag{11}$$

$$(p_{\zeta,1}a_{0,2})^{i_0}\cdots(p_{\zeta,1}a_{2g,2})^{i_{2g}}b_{0,1}^{j_0}\cdots b_{n(\gamma),1}^{j_{n(\gamma)}},$$

and

$$(p_{\zeta,1}a_{0,2})^{i_0}\cdots(p_{\zeta,1}a_{2g,2})^{i_{2g}}(p_{\zeta,1}^2b_{0,2})^{j_0}\cdots(p_{\zeta,1}^2b_{n(\gamma),2})^{j_{n(\gamma)}}.$$

By Eq. (7) we get $i_0+\cdots+i_{2g}=n(\gamma)$ and $j_0+\cdots+j_{n(\gamma)}=2g$, where $n(\gamma)=3g-2$ since $\gamma=0$. Of the above listed terms, the one at Eq.(11) has the largest degree:

$$(2g)(3g-2)+(4g-4)(2g)=14g^2-12g.$$

This establishes Eq.(9).

3. The polynomial $p_{\zeta,1}^g(\bar{z})$ is a factor of Res $(\bar{z})$

We begin with the following lemma:

Lemma 2: Let $p(z)=a_0+a_1z+\cdots+a_mz^m$ and $q(z)=b_0+b_1z+\cdots+b_nz^n$ be polynomials over **C**. If $p(\alpha)=C_0C_1\neq 0$ and $q(\alpha)=C_0C_2\neq 0$, then:

$$\mathrm{Res}(a_0,\ldots,a_{2g};b_0,\ldots,b_{n(\gamma)})=C_0\ \mathrm{Res}(C_1,a_1,\ldots,a_{2g};C_2,b_1,\ldots,b_{n(\gamma)}).$$

Proof: First, note that

$$\begin{aligned}&\mathrm{Res}(a_0,a_1,\ldots,a_m;b_0,b_1,\ldots,b_n)\\&\quad=\mathrm{Res}\left(C_0C_1-\sum_{\ell=1}^{m}a_\ell\alpha^\ell,a_1,\ldots,a_m;C_0C_2-\sum_{\ell=1}^{n}b_\ell\alpha^\ell,b_1,\ldots,b_n\right).\end{aligned}$$

Since the last column of the resultant matrix of p and q contains a_0 and b_0 with zeros everywhere else (see Eq.(5)), we can expand the resultant in the coefficients a_0 and b_0. This yields:

$$\begin{aligned}&\mathrm{Res}(a_0,a_1,\ldots,a_m;b_0,b_1,\ldots,b_n)\\&\quad=\mathrm{Res}(C_0C_1,a_1,\ldots,a_m;C_0C_2,b_1,\ldots,b_n)\\&\qquad+\mathrm{Res}\left(-\sum_{\ell=1}^{m}a_\ell\alpha^\ell,a_1,\ldots,a_m;-\sum_{\ell=1}^{n}b_\ell\alpha^\ell,b_1,\ldots,b_n\right).\end{aligned}$$

The last Resultant vanishes because the polynomials

$$p_1(z)=\left(-\sum_{\ell=1}^{m}a_\ell\alpha^\ell\right)+a_1z+\cdots+a_mz^m$$

and

$$q_1(z)=\left(-\sum_{\ell=1}^{n}b_\ell\alpha^\ell\right)+b_1z+\cdots+b_nz^n$$

satisfy $p_1(\alpha)=q_1(\alpha)=0$. The lemma now follows since

$$\mathrm{Res}(C_0C_1,a_1,\ldots,a_m;C_0C_2,b_1,\ldots,b_n)=C_0\mathrm{Res}(C_0,a_1,\ldots,a_m;C_2,b_1,\ldots,b_n).$$

Q.E.D. Lemma

Applying Lemma 2 to P_J and P_H with $C_1=1$ yields that

$$C_0=-p_{\zeta,1}(\overline{z})m_j\prod_{\substack{\ell=1\\ \ell\neq j}}^{g}(z_\ell-z_j)^2$$

factorizes out of $\mathrm{Res}(a_0(\overline{z}),\ldots,a_{2g}(\overline{z});b_0(\overline{z}),\ldots,b_{n(\gamma)}(\overline{z}))$ for $j=1,\ldots,g$. Hence

$$(-1)^gp_{\zeta,1}^g(\overline{z})\prod_{j=1}^{g}m_j\prod_{\substack{\ell=1\\ \ell\neq j}}^{g}(z_\ell-z_j)^2$$

is a factor of the resultant.

4. Eliminating zeros of Res $(\bar{z})$ that do not map to cusps

By the Resultant Theorem not all the zeros of $\mathrm{Res}(\overline{z})=\mathrm{Res}(a_0(\overline{z}),\ldots,a_{2g}(\overline{z});b_0(\overline{z}),\ldots,b_{n(\gamma)}(\overline{z}))$ may correspond to cusps. On a critical curve with $\sigma_c\neq 1$, we have $|\partial\zeta/\partial\overline{z}|=|1-\sigma_c|\neq 0$. Consequently, the zeros of the polynomial $p_{\zeta,1}(\overline{z})=0$ cannot lie on a critical curve with $\sigma_c\neq 1$. This implies that the upper bound on the number of cusps reduces as follows:

$$N_{cusps}\leqslant\deg[\,\mathrm{Res}(\overline{z})]\leqslant\begin{cases}14g^2-(2g)g=12g^2 & \text{if } \gamma>0\\ 14g^2-12g-(2g-2)g=12g^2-10g & \text{if } \gamma=0.\end{cases}\tag{12}$$

There can also be common zeros of $a_{2g}(\overline{z})$ and $b_{n(\gamma)}(\overline{z})$ that are not cusp points. In fact, if $\gamma=0$, then

$$a_{2g}(\overline{z})=(1-\sigma_c)^2\prod_{\ell=1}^{g}(\overline{z_\ell}-\overline{z})^2,$$

$$a_{2g-1}(\overline{z})=(1-\sigma_c)^2\left[-2\sum_{\ell=1}^{g}z_\ell\right]\prod_{\ell=1}^{g}(\overline{z_\ell}-\overline{z})^2,$$

and

$$b_{3g-2}(\overline{z})=(1-\sigma_c)\prod_{\ell=1}^{g}(\overline{z_\ell}-\overline{z})\left(\sum_{\ell=1}^{g}m_\ell\prod_{\substack{r=1\\r\neq\ell}}^{g}(\overline{z_r}-\overline{z})^3\right).$$

The coefficients a_{2g}, a_{2g-1} and b_{3g-2} have a common factor. If we now consider the Sylvester matrix (see Eq.(5)) and expand its determinant by the first two columns, then:

$$\begin{aligned}\det[\mathbf{A}_{2g+3g-2}]&=a_{2g}\det[\mathbf{A}_{1,1}]+b_{3g-2}\det[\mathbf{A}_{3g-2,1}]\\&=a_{2g}\det[\mathbf{A}_{1,1}]+b_{3g-2}[a_{2g-1}\det[\mathbf{A}_{3g-2,1}(1,1)]\\&\quad+a_{2g}\det[\mathbf{A}_{3g-2,1}(2,1)]+b_{3g-2}\det[\mathbf{A}_{3g-2,1}(3g-3,1)]],\end{aligned}\tag{13}$$

where $\mathbf{A}_{i,j}$ is the submatrix of $\mathbf{A}_{2g+3g-2}$ obtained by removing the ith row and jth column. Here, $\mathbf{A}_{i,j}(r,s)$ is the submatrix of $\mathbf{A}_{i,j}$ obtained by removing the rth row and sth column. We observe that in the expansion of Eq. (13) the factor

$$(1-\sigma_c)^2\prod_{\ell=1}^{g}(\overline{z_\ell}-\overline{z})^2$$

must factorize out of the resultant for the case $\gamma=0$. Hence, $\overline{z_1},\ldots,\overline{z_g}$ yield double zeros of the resultant. But no $\overline{z_\ell}$ ($\ell=1,\ldots,g$) can be mapped to a cusp point because as $\overline{z}\to\overline{z_\ell}$ the lensing map satisfies $|\zeta(\overline{z})|\to\infty$. Thus, for $\gamma=0$ we can exclude an additional $2g$ zeros from $\mathrm{Res}(\overline{z})$. The latter and Eq. (12) imply:

$$N_{cusps}\leqslant\begin{cases}12g^2 & \text{if } \gamma>0\\ 12g(g-1) & \text{if } \gamma=0\end{cases}.\tag{14}$$

IV. DISCUSSION

A comparison of Eq.(14) with some special well-studied cases (cf. Witt and Petters[18]) reveals that our upper bounds seem much higher than the actual maximum number of cusps for certain special configurations. The reason for this lies in Eq. (2), the parametric representation of critical curves. Two configurations of caustics always occur, namely, the underfocusing case ($0\leqslant\sigma_c<1$) and overfocusing one ($\sigma_c>1$). These two configurations have the same critical curves due to the factor $|1-\sigma_c|$ in the parametric representation. Assuming the same position of the stars, all models with $\sigma_c=t$ and $\sigma_c=2-t$, where $0\leqslant t<1$, have identical critical curves. Since we only set upper bounds on the number of points on the critical curves that are mapped to cusps, Eq. (14) apply simultaneously to the under– and overfocused cases. It is not known *a priori* whether a point on a critical curve is mapped to a cusp for the under– or overfocused situation. Hence, *the results of Eq. (14) yield upper bounds on the sum of the maximum number of cusps for the under- and overfocused cases.*

Example: If $g=1$ and $\gamma>0$, we obtain exactly 4 cusps (see Fig. 2a) for the underfocused case with $0\leqslant\sigma_c<1-\gamma$ (see Fig. 1), and a maximum of 8 cusps (see Fig. 2c) for the overfocused case

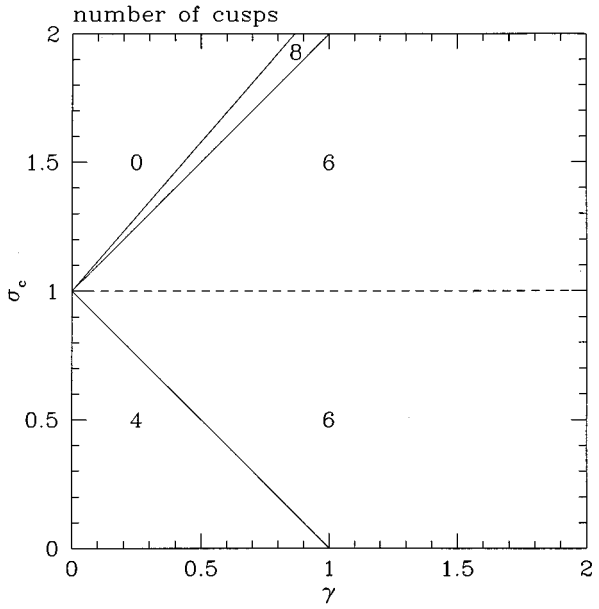

FIG. 1. Parameter space for the number of cusps for the one-point mass gravitational lens with shear γ and continuously distributed matter σ_c. The dashed line divides the under- and overfocused regions. The solid line below the dashed one is given by $\sigma_c = 1-\gamma$, while the line separating 8 and 6 cusps regions is $\sigma_c = 1+\gamma$. The boundary between the 0 and 8 cusps regions is $\sigma_c = 1+\sqrt{4/3}\gamma$.

with $1+\gamma < \sigma_c$ (cf. Witt and Petters[19]). For $1-\gamma < \sigma_c < 1+\gamma$ (note $\sigma_c \neq 1$) we get 6 cusps in the under– and overfocused cases (see Fig. 2b and 2d). The total sum agrees with our upper bound of 12: $4+8=12$ for $0 \leqslant \sigma_c < 1-\gamma$ ($\sigma_c > 1+\gamma$, respectively) and $6+6=12$ for $1-\gamma < \sigma_c < 1+\gamma$ (with $\sigma_c \neq 1$). The one-point mass lens with continuous matter and shear is detailed in the Appendix. We show that each zero z_0 of the resultant Res $(\overline{z})$ (see Eq. (A1)) is mapped by η in such a way that either $\eta(z_0)$ is a cusp for the underfocusing case, a cusp for the overfocusing case, or, is not a cusp point. For this reason, our upper bound on the number of cusps applies simultaneously to all three cases. In addition, we believe it is extremely difficult to separate cusps according to the under- and overfocused cases (see the Appendix), and, hence, to derive an upper bound for each such case. Therefore, it is not surprising that there are situations for which our upper bounds cannot be achieved. For instance, if $g=2$ and $\gamma=0$, then a maximum of 10 cusps occur for the separate cases of under– and overfocused lensing (Witt and Petters[20]). This yields a combined maximum of 20 cusps. But Eq.(14) predicts a combined maximum of 24.

Finally, the equations presented in Section III.B can be useful tools in the study of positions of cusps for the binary point-mass lens. Since there are already two binary events observed (Udalski *et al.*,[21] Alard, Mao and Guibert[22]), it is important to estimate the number of events that are passing close to cusps and to compute the corresponding cross section for the cusps (cf. Mao[23] and Schneider and Weiss[24]). This analysis is important because events passing outside a cusp of a binary lens can have a symmetrically shaped light curve, which is similar to events for a single point mass lens. Such cusp events can fake a single point mass event. This may lead to an underestimation of the fraction of binary or planetary systems in our galaxy (for an estimate about the expected fraction of binary events cf. Mao and Paczński[25]). Therefore, a careful analysis of the number or fraction of cusp-like events caused by binaries is needed. For such analysis we have to know the positions of the cusps in terms of the model parameters (e.g. mass of the star, separation of the binary etc.). The curves where cusps are located during a one-parameter evolution are called *bi-caustics* (see Petters[26]). For the case of the one-point mass lens with shear the bi-caustics (as a

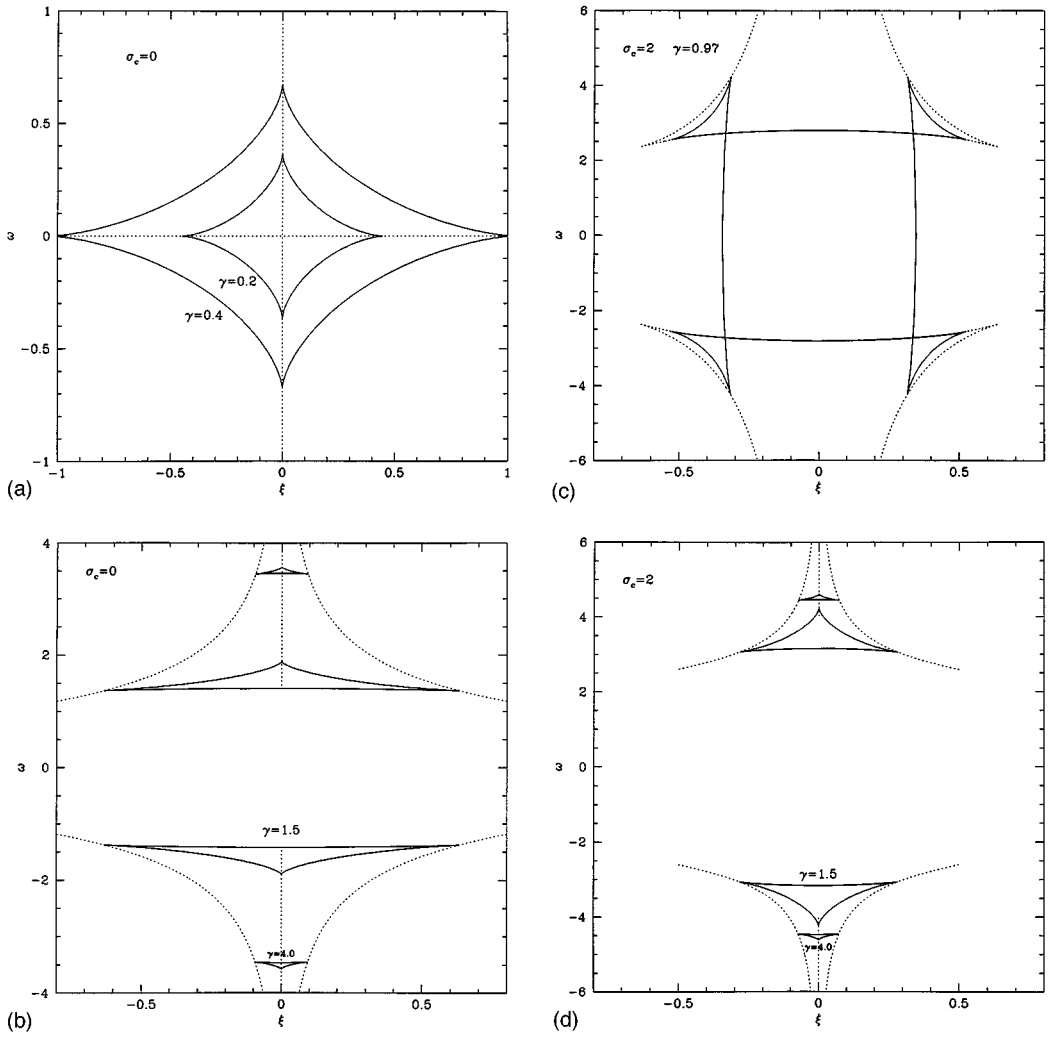

FIG. 2. Different caustics for the one point mass lens with different shears γ are shown. Each configuration corresponds to a parameter space in Fig. 1. The dotted lines indicate the bi-caustic curves where cusps may be located when γ is varied. The top (a) and (b) show the underfocused cases and the botton (c) and (d) show the overfocused cases. (Note that the case for 0 cusps is not shown in (c) but for $\gamma=\sqrt{3/4}$ the cusps merge at the point where the two bi-caustic curves merge. For smaller γ we obtain simply oval caustics.)

function of γ) are indicated as dotted lines in Fig. 2. Such curves can be evaluated with the tools presented here.

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APPENDIX: ONE-POINT MASS LENS WITH CONTINUOUS MATTER AND SHEAR

In order to make Theorem 1 and its proof more transparent, we shall discuss the one-point mass lens with continuous matter $\sigma_c \geqslant 0$ and shear $\gamma > 0$. The lensing map is given by

$$\zeta(z)=(1-\sigma_c)z+\gamma\overline{z}-\frac{m}{\overline{z}},$$

where we set $m_1=m$ and $z_1=0$ for convenience. The derivatives of the lensing map are:

$$\frac{\partial\zeta}{\partial z}=(1-\sigma_c),\quad \frac{\partial\zeta}{\partial\overline{z}}=\gamma+\frac{m}{\overline{z}^2},\quad \frac{\partial^2\zeta}{\partial\overline{z}^2}=-\frac{2m}{\overline{z}^3}.$$

The points in the deflector plane that are mapped by ζ to cusps are the common solutions of

$$P_J(z,\overline{z})=[(1-\sigma_c)^2-\gamma^2)\overline{z}^2-\gamma m]z^2-m(m+\gamma\overline{z}^2)=0$$

and

$$P_H(z,\overline{z})=[(1-\sigma_c)\gamma m\overline{z}]z^3+[(1-\sigma_c)m^2\overline{z}]z-m(m+\gamma\overline{z}^2)^2=0.$$

Note that P_J is a polynomial of degree 2 in z, while P_H is of degree 3 in z. To solve these two polynomial equations simultaneously, we take the z-resultant of P_J and P_H in order to eliminate the z variable from the equations (see Section III.B(1)):

$$\begin{aligned}\mathrm{Res}(\overline{z})=&\gamma m^2[\overline{z}^4((1-\sigma_c)^2-\gamma^2)-2\gamma m\overline{z}^2-m^2][\overline{z}^2\gamma+m] \\ &\times[\overline{z}^8\gamma^2((1-\sigma_c)^2-\gamma^2)^2+\overline{z}^6\gamma m(3(1-\sigma_c)^4-7\gamma^2(1-\sigma_c)^2+4\gamma^4) \\ &+\overline{z}^4m^2(3(1-\sigma_c)^4-8\gamma^2(1-\sigma_c)^2+6\gamma^4)-\gamma m^3(3(1-\sigma_c)^2-4\gamma^2)\overline{z}^2+\gamma^2m^4].\end{aligned}\tag{A1}$$

The resultant polynomial is of degree 14. The two zeros of $p_{\zeta,1}(\overline{z})=\overline{z}^2\gamma+m$ cannot be mapped to cusps. At such zeros, the derivative $\partial\zeta/\partial\overline{z}$ vanishes, which is not allowed for points mapped to cusps (see Section III.B(4)). Hence, the under– and overfocused cases have a combined maximum of at most 12 cusps. Note that since the term $(1-\sigma_c)$ appears as a quadratic expression in Eq. (A1), the 12 zeros may be mapped to cusps for either the under– or overfocused case.

We emphasize that a zero $\overline{z}_0$ of the resultant cannot be mapped simultanously to a cusp for the under– and the overfocused cases. In fact, the tangential vector at the caustic is $H_\zeta=(1-t)H_z+(\partial\zeta/\partial\overline{z})\overline{H}_z$ for the case $\sigma_c=t$, and $H_\zeta=(t-1)H_z+(\partial\zeta/\partial\overline{z})\overline{H}_z$ for the case $\sigma_c=2-t$, where $0\leqslant t<1$ (see Section III.B(1)). Since $H_z,\overline{H}_z$, and $\partial\zeta/\partial\overline{z}$ are independent of t, both equations cannot vanish simultanously unless we require $H_z=0$. This can happen at a point z_0 on a critical curve only when $\partial^2\zeta/\partial\overline{z}^2=0$ at z_0. Such solutions z_0 are mapped by η to beak-to-beak singularities (Witt and Petters[27]), which result from the merger of two cusps. Thus, zeros of the resultant that may seem to map simultanously to cusps for the under– and the overfocused cases, are actually mapped to beak-to-beak singularities. The latter may be viewed as degenerate cusps.

The combined maximum of 12 cusps can readily be checked using Fig. 1. To each configuration (γ,σ_c) for the underfocused case $\sigma_c=t$, there exist a configuration for the overfocused case $\sigma_c=2-t$ with the same critical curve. The corresponding configuration is determined by reflecting about the dashed line. The sum of the number of cusps of both configurations cannot exceed 12 as is shown by Fig. 1. However, for some configurations the total sum is less than 12 which means that not all solutions of the resultant are necessarily mapped on a cusp. (We note that we have restricted ourselves to $\gamma>0$ and $\sigma_c>0$ because of physical reasons. However, in mathematical terms the values and Fig. 1 may also be expanded to negative values.)

For completeness we show that the polynomial of degree 8 in Eq. (A1) can be solved analytically as well when we split up the complex quantities $z=x+iy$ in real and imaginary parts. (Note that the polynomial of degree 4 can be readily solved.) The vanishing of the real and imaginary parts of Eq. (A1) yields solutions whose x-component satisfies

$$16\gamma^2[(1-\sigma_c)^2-\gamma^2]x^4+4\gamma m[3(1-\sigma_c)^2+2(1-\sigma_c)\gamma-4\gamma^2]x^2+3(1-\sigma_c)^2m^2=0 \quad \text{(A2)}$$

and y-component obeys

$$y^2=(2m+(1-\sigma_c+2\gamma)x^2)/(2\gamma-1+\sigma_c). \quad \text{(A3)}$$

We note that Eq. (A3) is directly obtained from the imaginary part of Eq. (A1), while we get Eq. (A2) after substituting (A3) into the real part of Eq. (A1). The solutions of (A2) and (A3) yield the eight positions in the deflector plane that might be mapped to cusps for the under- or overfocusing case.

Finally, Eqs. (A2) and (A3) can also be used to derive the so-called bi-caustic curves, which give the cusp locations. The off-axis cusps $\zeta_{cusp}=\xi_{cusp}+i\omega_{cusp}$ are given by

$$16\gamma^2[\gamma-(1-\sigma_c)]\xi_{cusp}^4+8\gamma^2m[8\gamma^2-9(1-\sigma_c)^2]\xi_{cusp}^2-27(1-\sigma_c)^4m^2[\gamma+(1-\sigma_c)]=0.$$

The equation for ω_{cusp} can be obtained by replacing ξ_{cusp} by ω_{cusp} and γ by $-\gamma$. The resulting bi-caustics relative to γ are indicated as dotted lines in Fig. 2. The bi-caustics equations are derived by eliminating x and y from the lens equation $(\xi-(1-\sigma_c)x-\gamma x)(x^2+y^2)+m=0$ with Eq.(A2) and Eq.(A3), via the resultant.

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Abstract carrier space formalism for the irreducible tensor operators of compact quantum group algebras

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Defining conditions for irreducible tensor operators associated with the unitary irreducible corepresentations of compact quantum group algebras are deduced within the framework of the abstract carrier space formalism. It is shown that there are *two* types of irreducible tensor operator, which may be called 'ordinary' and 'twisted'. The consistency of the definitions is demonstrated, and various consequences are deduced, including generalizations of the Wigner–Eckart theorem for both the ordinary and twisted operators. Examples of irreducible tensor operators for the standard deformation of the function algebra of the compact Lie group SU(2) are described to demonstrate the applicability of the new definitions. © *1996 American Institute of Physics.* [S0022-2488(96)03005-3]

I. INTRODUCTION

Most of the applications to physics of the theories of groups and Lie algebras depend on the Wigner–Eckart theorem, and so it is of great interest to see how this theorem generalizes to other algebraic structures. In a previous paper,[1] hereafter referred to as Paper I, a study of the definitions and properties of irreducible tensor operators for a *compact quantum group algebra* $\mathscr{A}$ was initiated by examining the case of the right regular and left regular coaction formalisms, and was extended to the case of operators associated with the corresponding quantum homogeneous spaces of $\mathscr{A}$. In the present paper this will be further extended to the case of operators acting in the abstract carrier spaces of irreducible corepresentations of $\mathscr{A}$.

The plan of the present paper is as follows. The remainder of this section will be devoted to putting the analysis that follows into context, first by reviewing briefly the situation for compact Lie groups, and then by indicating the background for the generalization of compact Lie groups to compact quantum group algebras. In the next section the most relevant properties of compact quantum group algebras will be summarized, particular attention being devoted to the essential role played by corepresentations. This summary is continued in Section III, where the two different types of tensor product of corepresentations and their associated Clebsch–Gordan coefficients are briefly discussed. The heart of the paper is reached in Section IV, where the irreducible tensor operators are defined and some of their immediate properties are deduced. In particular, it will be shown there that there are *two* types of irreducible tensor operators, which will be described as being *ordinary* and *twisted* respectively. The *motivations* for the definitions of Section IV are deliberately relegated to the Appendix in order to emphasize that the treatment given for the compact quantum group algebras in Sections IV and V are entirely self-contained. In Section V it is shown that there are *two* theorems of the Wigner–Eckart type, one for the 'ordinary' and one for the 'twisted' irreducible tensor operators. To illustrate the applicability of the new definitions of Section IV, examples of irreducible tensor operators for the standard deformation of the function algebra of the compact Lie group SU(2) are described in Section VI. Unless otherwise stated, the notations, definitions, and terminology are exactly the same as those given in Paper I, which also contains an account of the relationship of the present line of study to previous work on the applicability of the Wigner–Eckart theorem to quantum groups.

Because the space of functions defined on a compact Lie group $\mathscr{G}$ is a special example of a compact quantum group algebra, all the well-known results for compact Lie groups naturally

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reappear in this particular case. However, as the detailed analysis shows, the theory in the general situation is rather more subtle, and exhibits various complications. Nevertheless, the point of view of the present communication is best introduced by considering first the abstract carrier space formalism in this very well established and familiar context of a compact Lie group $\mathscr{G}$ (cf. Refs. 2, 3). Let V^p be a carrier space for a unitary irreducible representation $\mathbf{\Gamma}^p$ of $\mathscr{G}$, and let $\psi_1^p, \psi_2^p, \ldots, \psi_{d_p}^p$ be an ortho-normal basis for V^p. Define for each $T \in \mathscr{G}$ a linear operator $\Phi^p(T)$ that acts on V^p by the requirement that

$$\Phi^p(T)(\psi_n^p) = \sum_{m=1}^{d_p} \Gamma^p(T)_{mn} \psi_m^p \tag{1}$$

for all $T \in \mathscr{G}$ and all $n = 1,2,\ldots,d_p$. Let $\mathbf{\Gamma}^p$, $\mathbf{\Gamma}^q$, and $\mathbf{\Gamma}^r$ be any three unitary irreducible representations of $\mathscr{G}$. Then one can consider a set of irreducible tensor operators $Q_1^q, Q_2^q, \ldots, Q_{d_q}^q$ that each map V^p into V^r and which are such that

$$\Phi^r(T) Q_n^q \Phi^p(T)^{-1} = \sum_{m=1}^{d_q} \Gamma^q(T)_{mn} Q_m^q \tag{2}$$

for all $T \in \mathscr{G}$ and all $n = 1,2,\ldots,d_q$. In this case the Wigner–Eckart theorem deals with inner products $\langle , \rangle$ defined on V^r and states that the j,k, and ℓ dependence of $\langle \psi_\ell^r, Q_k^q(\psi_j^p) \rangle$ depends only on Clebsch–Gordan coefficients for the reduction of the tensor product $\mathbf{\Gamma}^p \otimes \mathbf{\Gamma}^q$ into its irreducible constituents $\mathbf{\Gamma}^r$.

In a minor extension of this formalism, one could introduce an inner product space V that is a direct sum of carrier spaces of certain unitary irreducible representations of $\mathscr{G}$ and which contains at least $V^p \oplus V^r$ (and which, in the extreme case, may contain one carrier space for every inequivalent irreducible representation of $\mathscr{G}$). Then, for each $T \in \mathscr{G}$ an operator $\Phi(T)$ can be defined which maps elements of V into V, and which acts as $\Phi^p(T)$ on V^p, as $\Phi^r(T)$ on V^r, and so on. The irreducible tensor operators are then required to each map V into V and to be such that $\Phi(T) Q_n^q \Phi(T)^{-1} = \Sigma_{m=1}^{d_q} \Gamma^q(T)_{mn} Q_m^q$ for all $T \in \mathscr{G}$ and all $n = 1,2,\ldots,d_q$. In this case the Wigner–Eckart theorem deals with inner products $\langle , \rangle$ defined on V, but is otherwise the same as above.

As emphasized in Paper I, one most important lesson that can be drawn from these simple group theoretical considerations concerns the *consistency* of the definitions of the basis vectors *and* of the irreducible tensor operators. As $\Phi^p(T)\Phi^p(T') = \Phi^p(TT')$ and $\mathbf{\Gamma}^p(T)\mathbf{\Gamma}^p(T') = \mathbf{\Gamma}^p(TT')$ for all $T, T' \in \mathscr{G}$, it follows that if (1) is valid for T and for T', then it is also valid for their product TT'. Similarly, and very significantly, by defining for each $T \in \mathscr{G}$ an operator $\Psi(T)$ by

$$\Psi(T)(Q) = \Phi^r(T) Q \Phi^p(T)^{-1} \tag{3}$$

for every operator Q that maps V^p into V^r, the definition (2) can be recast as

$$\Psi(T)(Q_n^q) = \sum_{m=1}^{d_q} \Gamma^q(T)_{mn} Q_m^q \tag{4}$$

for all $T \in \mathscr{G}$ and all $n = 1,2,\ldots,d_q$. As $\Psi(T)\Psi(T') = \Psi(TT')$ for all $T, T' \in \mathscr{G}$, it follows that if (4) is valid for T and for T', then it is also valid for their product TT'. Put another way, because of the similarity in form between (1) and (4), the *consistency* of the definition (2) of the irreducible tensor operators Q_n^q is ensured by the fact that they too form a basis for a carrier space, this time for $\mathbf{\Gamma}^q$. In the analysis that follows (cf. Section IV), essentially this argument will be used to

justify the definitions that will be given for the irreducible tensor operators of the compact quantum group algebras, the only essential difference being that the argument has to be cast in terms of *corepresentations* instead of representations.

As is well known, the set of functions defined on a Lie group $\mathscr{G}$ form a Hopf algebra, $\mathscr{A}$, and the dual $\mathscr{A}'$ of $\mathscr{A}$ is the universal enveloping algebra of the Lie algebra $\mathscr{L}$ of $\mathscr{G}$. Moreover, the structure of $\mathscr{G}$ can be encoded into the structure of $\mathscr{A}$, and, in particular, $\mathscr{A}$ is commutative. A 'deformation' (or 'quantization') of $\mathscr{A}'$ induces a corresponding deformation of $\mathscr{A}$, and will make $\mathscr{A}$ non-commutative as well as being non-cocommutative. Although most attention has been focused on the deformed Hopf algebras $\mathscr{A}'$, it has been demonstrated by the pioneering work of Woronowicz,[4–6] which itself has been refined and developed by Dijkhuizen and Koornwinder,[7–12] that it is of very great interest to produce a self-contained and direct study of generalizations of the Hopf algebras $\mathscr{A}$. This can be done by assuming that they have certain characteristic properties, and the resulting structures have been called *compact matrix pseudogroups* by Woronowicz,[4–6] and *compact quantum group algebras* by Dijkhuizen and Koornwinder.[7–12] It is these that provide the framework for the present paper, which, as intimated above, is devoted to the study of the irreducible tensor operators for compact quantum group algebras in the abstract carrier space formalism.

II. COREPRESENTATIONS OF COMPACT QUANTUM GROUP ALGEBRAS

It should be recalled (cf. Refs. 1, 7–12) that a *right* $\mathscr{A}$*-comodule* consists of a vector space V and a linear mapping π_V from V to $V\otimes\mathscr{A}$ such that

$$(\pi_V\otimes id)\circ\pi_V=(id\otimes\Delta)\circ\pi_V \tag{5}$$

and

$$((id\otimes\epsilon)\circ\pi_V)(v)=v\otimes 1_C \tag{6}$$

for all $v\in V$. The operation π_V is then said to be a *right coaction* and provides a *corepresentation* of $\mathscr{A}$ with carrier space V.

Of great importance are the finite-dimensional *irreducible* corepresentations, which, for a compact quantum group algebra $\mathscr{A}$, are assumed to form a *countable* set (up to equivalence). Moreover each such irreducible corepresentation is equivalent to a *unitary* corepresentation. Let π^p, for $p=1,2,\ldots$, denote the set of unitary irreducible corepresentations of $\mathscr{A}$ (one being chosen from every equivalence class), and let V^p be a carrier space of π^p, assumed to be of finite dimension d_p, with basis $v_1^p, v_2^p, \ldots, v_{d_p}^p$. Then there exists a uniquely determined set of elements π_{jk}^p of $\mathscr{A}$ (for $j,k=1,2,\ldots,d_p$), called the *matrix coefficients* of π^p, which are such that

$$\pi^p(v_j^p)=\sum_{k=1}^{d_p} v_k^p\otimes\pi_{kj}^p \tag{7}$$

for all $j=1,2,\ldots,d_p$. The requirements (5) and (6) then imply that

$$\Delta(\pi_{jk}^p)=\sum_{\ell=1}^{d_p}\pi_{j\ell}^p\otimes\pi_{\ell k}^p \tag{8}$$

and

$$\epsilon(\pi_{jk}^p)=\delta_{jk} \tag{9}$$

(for $j,k=1,2,\ldots,d_p$). The unitary requirement on π^p implies that

$$S(\pi^p_{jk}) = \pi^{p*}_{kj}, \tag{10}$$

$$\sum_{\ell=1}^{d_p} M(\pi^{p*}_{\ell j} \otimes \pi^p_{\ell k}) = \delta_{jk} 1_{\mathscr{A}}, \tag{11}$$

and

$$\sum_{\ell=1}^{d_p} M(\pi^p_{j\ell} \otimes \pi^{p*}_{k\ell}) = \delta_{jk} 1_{\mathscr{A}} \tag{12}$$

(for all $j,k=1,2,\ldots,d_p$). For a compact quantum group algebra $\mathscr{A}$ this set of matrix coefficients is assumed (cf. Refs. 1, 7–12) to form a basis for $\mathscr{A}$.

Let $\mathscr{P}^p_{ij}$ be a set of projection operators for V^p that are defined by

$$\mathscr{P}^{\,p}_{ij}(v^p_k) = \delta_{ik} v^p_j \tag{13}$$

for all $i,j,k=1,2,\ldots,d_p$. Let π^r be another unitary irreducible corepresentation of $\mathscr{A}$, and let $\mathscr{L}^{pr}$ be the set of linear operators that map elements of V^p into V^r. A basis for $\mathscr{L}^{pr}$ is provided by the set of operators $\mathscr{P}^{\,pr}_{ij}$ that are defined by

$$\mathscr{P}^{\,pr}_{ij}(v^p_k) = \delta_{ik} v^r_j \tag{14}$$

for all $i,k=1,2,\ldots,d_p$ and all $j=1,2,\ldots,d_r$. Then

$$\mathscr{P}^{\,r}_{mn} \circ \mathscr{P}^{\,pr}_{k\ell} \circ \mathscr{P}^{\,p}_{ij} = \delta_{kj}\delta_{m\ell}\mathscr{P}^{\,pr}_{in} \tag{15}$$

for all $i,j,k=1,2,\ldots,d_p$ and all $\ell,m,n=1,2,\ldots,d_r$. If Q is any element of $\mathscr{L}^{pr}$, then

$$Q(v^p_k) = \sum_{j=1}^{d_r} q_{jk} v^r_j \tag{16}$$

for all $k=1,2,\ldots,d_p$, where q_{jk} are the complex numbers that are defined by

$$q_{jk} = \langle v^r_j, Q(v^p_k) \rangle \tag{17}$$

for all $k=1,2,\ldots,d_p$ and all $j=1,2,\ldots,d_r$, $\langle,\rangle$ being the inner product of V^r. Moreover one can write

$$Q = \sum_{i=1}^{d_p} \sum_{j=1}^{d_r} q_{ji} \mathscr{P}^{\,pr}_{ij}. \tag{18}$$

III. TENSOR PRODUCTS AND CLEBSCH–GORDAN COEFFICIENTS

A. Ordinary and twisted tensor products

With the *ordinary tensor product* of two irreducible corepresentations π^p and π^q of $\mathscr{A}$ (with carrier spaces V^p and V^q respectively) being defined as the mapping $\pi^p \boxtimes \pi^q$ from $V^p \otimes V^q$ to $V^p \otimes V^q \otimes \mathscr{A}$ that is such that

$$\pi^p \boxtimes \pi^q = (id \otimes id \otimes M) \circ (id \otimes \sigma \otimes id) \circ (\pi^p \otimes \pi^q), \tag{19}$$

it is easily shown from (7) that the corresponding matrix coefficients are given by

$$(\pi^p \boxtimes \pi^q)_{st,jk} = M(\pi^p_{sj} \otimes \pi^q_{tk}) \tag{20}$$

for all $j,s = 1,2,\ldots,d_p$ and all $k,t = 1,2,\ldots,d_q$.

Similarly, with the *twisted tensor product* of π^p and π^q being defined as the mapping $\pi^p \widetilde{\boxtimes} \pi^q$ from $V^p \otimes V^q$ to $V^p \otimes V^q \otimes \mathscr{A}$ that is such that

$$\pi^p \widetilde{\boxtimes} \pi^q = (id \otimes id \otimes M) \circ (id \otimes id \otimes \sigma) \circ (id \otimes \sigma \otimes id) \circ (\pi^p \otimes \pi^q), \tag{21}$$

it is also easily shown from (7) that the corresponding matrix coefficients are given by

$$(\pi^p \widetilde{\boxtimes} \pi^q)_{st,jk} = M(\pi^q_{tk} \otimes \pi^p_{sj}) \tag{22}$$

for all $j,s = 1,2,\ldots,d_p$ and all $k,t = 1,2,\ldots,d_q$.

B. Clebsch–Gordan coefficients

Suppose that the ordinary tensor product $\pi^p \boxtimes \pi^q$ is reducible [and hence is completely reducible (cf. Refs. 1, 7–12)], and that n^r_{pq} is the number of times that the irreducible corepresentation π^r (or a corepresentation equivalent to it) appears in its reduction. If the carrier spaces V^p and V^q have basis elements $v^p_1, v^p_1, \ldots, v^p_{d_p}$ and $v^q_1, v^q_1, \ldots, v^q_{d_q}$ respectively, then the set of elements $v^p_j \otimes v^q_k$ form a basis for $V^p \otimes V^q$, the carrier space of $\pi^p \boxtimes \pi^q$, and consequently appropriate linear combinations form bases for all the irreducible corepresentations π^r that appear in the reduction of the tensor product. Let $w^{r,\alpha}_{\ell}$ be such a combination, so that

$$w^{r,\alpha}_{\ell} = \sum_{j=1}^{d_p} \sum_{k=1}^{d_q} \left(\begin{matrix} p & q \\ j & k \end{matrix} \middle| \begin{matrix} r & , & \alpha \\ \ell & & \end{matrix} \right) v^p_j \otimes v^q_k, \tag{23}$$

for $\ell = 1,2,\ldots,d_r$, and $\alpha = 1,2,\ldots,n^r_{pq}$, and

$$(\pi^p \boxtimes \pi^q)(w^{r,\alpha}_{\ell}) = \sum_{u=1}^{d_r} w^{r,\alpha}_u \otimes \pi^r_{ul}, \tag{24}$$

for $u = 1,2,\ldots,d_r$, and $\alpha = 1,2,\ldots,n^r_{pq}$. The inverse of (23) is

$$v^p_j \otimes v^q_k = \sum_r \sum_{\alpha=1}^{n^r_{pq}} \sum_{\ell=1}^{d_r} \left(\begin{matrix} r & , & \alpha \\ \ell & & \end{matrix} \middle| \begin{matrix} p & q \\ j & k \end{matrix} \right) w^{r,\alpha}_{\ell}, \tag{25}$$

for $j = 1,2,\ldots,d_p$ and $k = 1,2,\ldots,d_q$. The *Clebsch–Gordan coefficients* defined in (23) form the elements of a $d_p \times d_q$ matrix $\mathbf{C}$, while the inverse coefficients defined in (25) form the elements of $\mathbf{C}^{-1}$, where

$$\mathbf{C}^{-1}(\pi^p \boxtimes \pi^q)\mathbf{C} = \sum_r \oplus n^r_{pq} \pi^r. \tag{26}$$

This implies that

$$(\pi^p \boxtimes \pi^q)_{is,jt} = \sum_r \sum_{\alpha=1}^{n^r_{pq}} \sum_{\ell,u=1}^{d_r} \left(\begin{matrix} p & q \\ i & s \end{matrix} \middle| \begin{matrix} r & , & \alpha \\ u & & \end{matrix} \right) \pi^r_{u\ell} \left(\begin{matrix} r & , & \alpha \\ \ell & & \end{matrix} \middle| \begin{matrix} p & q \\ j & t \end{matrix} \right) \tag{27}$$

for $i,j = 1,2,\ldots,d_p$, and $s,t = 1,2,\ldots,d_q$.

Thus, by (20), the product of any two basis elements of $\mathscr{A}$ can be expressed in terms of Clebsch–Gordan coefficients, for

$$M(\pi^p_{ij}\otimes\pi^q_{st})=\sum_r\sum_{\alpha=1}^{n^r_{pq}}\sum_{\ell,u=1}^{d_r}\left(\begin{matrix}p & q & r & , & \alpha\\ i & s & u & & \end{matrix}\right)\pi^r_{u\ell}\left(\begin{matrix}r & , & \alpha & p & q\\ \ell & & & j & t\end{matrix}\right) \tag{28}$$

for $i,j=1,2,\ldots,d_p$, and $s,t=1,2,\ldots,d_q$. This is essentially the converse of the relation (I.137),[1] that is, of

$$\begin{aligned}h(\pi^r_{ul}{}^{*}\pi^q_{tk}\pi^p_{sj}) \quad = \quad & \sum_{\alpha=1}^{n^r_{qp}}\sum_{v=1}^{d_r}\left(\begin{matrix}r & , & \alpha & q & p\\ \ell & & & k & j\end{matrix}\right)\left(\begin{matrix}q & p & r & , & \alpha\\ t & s & v & & \end{matrix}\right)\\ & \times\{((\mathbf{F}^r)^{-1})_{vu}/tr((\mathbf{F}^r)^{-1})\}\end{aligned} \tag{29}$$

for all $j=1,2,\ldots,d_p$, $k=1,2,\ldots,d_q$, and $l=1,2,\ldots,d_r$. Here h is the Haar functional and $\mathbf{F}^r$ is a non-singular $d_r\times d_r$ matrix with the property that

$$\sum_{k=1}^{d_r}F^r_{jk}\pi^r_{k\ell}=\sum_{k=1}^{d_r}\pi^{r\ddagger}_{jk}F^r_{k\ell} \tag{30}$$

(for all $j,\ell=1,2,\ldots,d_r$), where $\pi^{r\ddagger}$ is the doubly contragredient partner of π^r.

IV. THE IRREDUCIBLE TENSOR OPERATORS

A. Introduction

Let π^p,π^q, and π^r be unitary irreducible right coactions of $\mathscr{A}$ of dimensions d_p, d_q, and d_r respectively, and with matrix coefficients π^p_{jk}, π^q_{jk}, and π^r_{jk} respectively. Let $\mathscr{L}^{pr}$ be the vector space of operators introduced in Section II. It will be shown that there exist two types of irreducible tensor operators that are members of $\mathscr{L}^{pr}$ and which belong to the corepresentation π^q. These will be denoted by Q^q_j and $\widetilde{Q}^q_j$ (for $j=1,2,\ldots,d_q$), and will be called *ordinary* and *twisted* irreducible tensor operators respectively. Naturally the two types of irreducible tensor operators coincide in the special case in which $\mathscr{A}$ is commutative.

It will also be shown that the definitions of both of these types of irreducible tensor operators are easily extended to the case in which V is a vector space that is a direct sum of carrier spaces of unitary irreducible corepresentations of $\mathscr{A}$ and which contains at least $V^p\oplus V^r$.

B. Definitions of irreducible tensor operators

1. Definition of the ordinary irreducible tensor operators Q^q_j

The *ordinary irreducible tensor operators* Q^q_j belonging to the unitary irreducible right coaction π^q of $\mathscr{A}$ are *defined* to be members of $\mathscr{L}^{pr}$ that satisfy the condition

$$((id\otimes M)\circ(\pi^r\otimes id)\circ(Q^q_j\otimes S)\circ\pi^p)(v^p)=\sum_{k=1}^{d_q}Q^q_k(v^p)\otimes\pi^q_{kj} \tag{31}$$

for all $v^p\in V^p$ and all $j=1,2,\ldots,d_q$. Clearly this definition involves *only* quantities defined for $\mathscr{A}$ and its coactions. Both sides (31) are members of $V^r\otimes\mathscr{A}$. [The motivation behind the definition (32) is explained in Section 2 of the Appendix.]

It will now be shown that (31) provides a *consistent* definition, in that it can be re-expressed by saying that the operators Q^q_j (for $j=1,2,\ldots,d_q$) form the basis of an irreducible subspace of

a carrier space for a certain right coaction of $\mathscr{A}$. This right coaction will be denoted by $\pi_{\mathscr{L}^{pr}}$, as its carrier space is $\mathscr{L}^{pr}$. The *definition* of $\pi_{\mathscr{L}^{pr}}$ is then that it is the mapping of $\pi_{\mathscr{L}^{pr}}$ into $\pi_{\mathscr{L}^{pr}}\otimes\mathscr{A}$ specified by

$$\pi_{\mathscr{L}^{pr}}(Q)=\sum_{i,j=1}^{d_p}\sum_{m,n=1}^{d_r}(q_{ni}\mathscr{P}^{pr}_{jm})\otimes M(\pi^{\ r}_{mn}\otimes S(\pi^{\ p}_{ij})), \tag{32}$$

for all $Q\in\mathscr{L}^{pr}$, where q_{ni} and $\mathscr{P}^{pr}_{jm}$ are defined in (17) and (14). [The motivation for the definition (33) is given in Section 2 of the Appendix.]

It is then quite easily shown that $\pi_{\mathscr{L}^{pr}}$ satisfies (5) and (6) (with π_V and V replaced by $\pi_{\mathscr{L}^{pr}}$ and $\mathscr{L}^{pr}$ respectively), and hence $\pi_{\mathscr{L}^{pr}}$ is indeed a right coaction with carrier space $\mathscr{L}^{pr}$. Moreover, it is easily demonstrated that

$$(\pi_{\mathscr{L}^{pr}}(Q))(v^p\otimes 1_{\mathscr{A}})=((id\otimes M)\circ(\pi^r\otimes id)\circ(Q\otimes S)\circ\pi^p)(v^p) \tag{33}$$

for all $v^p\in V^p$ and all $Q\in\mathscr{L}^{pr}$. Thus (31) and (33) imply that the definition (31) can be written equivalently as

$$\pi_{\mathscr{L}^{pr}}(Q^q_j)=\sum_{k=1}^{d_q}Q^q_k\otimes\pi^q_{kj} \tag{34}$$

(for all $j=1,2,\ldots,d_q$). Because (34) is similar in form to (7), and as $\pi_{\mathscr{L}^{pr}}$ is a right coaction with carrier space $\mathscr{L}^{pr}$, the consistency of the definition (31) is now ensured.

Now consider the situation in which V is a vector space that is a direct sum of carrier spaces of unitary irreducible corepresentations of $\mathscr{A}$ and which contains at least $V^p\oplus V^r$. Let π be the mapping of V into $V\otimes\mathscr{A}$ that coincides with π^p on V^p and with π^r on V^r, and which acts similarly on any other carrier spaces that might be contained in V. Then the generalization of (31) is clearly

$$((id\otimes M)\circ(\pi\otimes id)\circ(Q^q_j\otimes S)\circ\pi)(v)=\sum_{k=1}^{d_q}Q^q_k(v)\otimes\pi^q_{kj} \tag{35}$$

for all $v\in V$ and all $j=1,2,\ldots,d_q$. [The consistency of the definition (35) is an immediate consequence of the consistency of (31)].

2. Definition of the twisted irreducible tensor operators $\tilde{Q}^q_j$

The *twisted irreducible tensor operators* $\widetilde{Q}^q_j$ belonging to the unitary irreducible right coaction π^q of $\mathscr{A}$ are *defined* to be members of $\mathscr{L}^{pr}$ that satisfy the condition

$$((id\otimes M)\circ(id\otimes\sigma)\circ(\pi^r\otimes id)\circ(\widetilde{Q}^{qR}_j\otimes S^{-1})\circ\pi^p)(v^p)=\sum_{k=1}^{d_q}\widetilde{Q}^q_k(v^p)\otimes\pi^q_{kj} \tag{36}$$

for all $v^p\in V^p$ and all $j=1,2,\ldots,d_q$. This definition (36) differs from the corresponding definition (31) only in the replacement of M by $M\circ\sigma$ *and* S by S^{-1} (neither of which have any effect in the special case in which $\mathscr{A}$ is commutative). (See Section 2 of the Appendix for further discussion of this pair of substitutions. It should be recorded that Rittenberg and Scheunert[13] noted previously, in the context of what was essentially the abstract carrier space formalism of Section I as generalized to irreducible *representations* of the dual $\mathscr{A}'$, that these substitutions do produce another type of irreducible tensor operator, but they did not pursue this observation.)

The demonstration that (36) provides a *consistent* definition again involves showing that it can be re-expressed by saying that the operators $\widetilde{Q}_j^q$ (for $j=1,2,\ldots,d_q$) form the basis of an irreducible subspace of a carrier space for another right coaction $\widetilde{\pi}_{\mathscr{L}^{pr}}$ of $\mathscr{A}$. This right coaction is *defined* as the mapping of $\mathscr{L}^{pr}$ into $\mathscr{L}^{pr}\otimes\mathscr{A}$ specified by

$$\widetilde{\pi}_{\mathscr{L}^{pr}}(Q)=\sum_{i,j=1}^{d_p}\sum_{m,n=1}^{d_r}(q_{ni}\mathscr{P}^{pr}_{jm})\otimes M(S^{-1}(\pi^p_{ij}\otimes\pi^r_{mn})) \tag{37}$$

for all $Q\in\mathscr{L}^{pr}$. [The motivation for the definition (37) is given in Section 3 of the Appendix]. Then

$$(\widetilde{\pi}_{\mathscr{L}^{pr}}(Q))(v^p\otimes 1_{\mathscr{A}})=((id\otimes M)\circ(id\otimes\sigma)\circ(\pi^r\otimes id)\circ(Q\otimes S^{-1})\circ\pi^p)(v^p) \tag{38}$$

for all $v^p\in V^p$ and all $Q\in\mathscr{L}^{pr}$. Thus (37) and (39) imply that the definition (37) can be written equivalently as

$$\widetilde{\pi}_{\mathscr{L}^{pr}}(\widetilde{Q}_j^{qR})=\sum_{k=1}^{d_q}\widetilde{Q}_k^{qR}\otimes\pi^q_{kj} \tag{39}$$

(for all $j=1,2,\ldots,d_q$), which then ensures its consistency.

In the situation in which V is a vector space that is a direct sum of carrier spaces of unitary irreducible corepresentations of $\mathscr{A}$ and which contains at least $V^p\oplus V^r$, and with the mapping π from V into $V\otimes\mathscr{A}$ that is defined in the end of the previous subsubsection, the generalization of (36) is clearly

$$((id\otimes M)\circ(id\otimes\sigma)\circ(\pi\otimes id)\circ(\widetilde{Q}_j^{qR}\otimes S^{-1})\circ\pi)(v)=\sum_{k=1}^{d_q}\widetilde{Q}_k^q(v)\otimes\pi^q_{kj} \tag{40}$$

for all $v\in V$ and all $j=1,2,\ldots,d_q$. [Again, the consistency of the definition (40) is an immediate consequence of the consistency of (36)].

C. Properties of irreducible tensor operators

1. The identity operator as an irreducible tensor operator

Suppose that V is a vector space that is a direct sum of carrier spaces of unitary irreducible corepresentations of $\mathscr{A}$ and which contains at least $V^p\oplus V^r$, and that π is the mapping of V into $V\otimes\mathscr{A}$ that is defined in the previous subsection. Suppose that Q is the *identity operator* id of V [so that $Q(v)=v$ for all $v\in V$]. Then, on using (5) and (6), together with the Hopf algebra properties $M\circ(id\otimes S)\circ\Delta=u\circ\epsilon$ and $u(1_C)=1_{\mathscr{A}}$, it follows that

$$((id\otimes M)\circ(\pi\otimes id)\circ(id\otimes S)\circ\pi)(v)=v\otimes 1_{\mathscr{A}} \tag{41}$$

for all $v\in V$, which, by (35), leads to the conclusion that the identity operator id is an *ordinary* irreducible tensor operator for the one-dimensional *identity* corepresentation whose sole matrix coefficient is $1_{\mathscr{A}}$.

It is easily checked [using (40) in place of (35)], that id is also a *twisted* irreducible tensor operator for this identity corepresentation.

The same conclusions for identity operators follow directly from (31) and (36) in the special case in which $p=r$.

2. Two useful identities for the ordinary irreducible tensor operators Q_j^q and $\tilde{Q}_j^q$

If Q_k^q is an *ordinary* irreducible tensor operator belonging to the unitary irreducible corepresentation π^q of $\mathscr{A}$ (as defined in (31)), and v_j^p (for $j=1,2,\ldots,d_p$) provides a basis for the carrier space V^p of the unitary irreducible corepresentation π^p of $\mathscr{A}$, then

$$\pi^r(Q_k^q(v_j^p))=\sum_{s=1}^{d_p}\sum_{t=1}^{d_q}(Q_t^q(v_s^p))\otimes(M(\pi_{tk}^q\otimes\pi_{sj}^p)), \tag{42}$$

for all $j=1,2,\ldots,d_p$, and $k=1,2,\ldots,d_q$. By contrast, if $\tilde{Q}_k^q$ is a *twisted* irreducible tensor operator belonging π^q, then

$$\pi^r(\tilde{Q}_k^q(v_j^p))=\sum_{s=1}^{d_p}\sum_{t=1}^{d_q}(\tilde{Q}_t^q(v_s^p))\otimes(M(\pi_{sj}^p\otimes\pi_{tk}^q)), \tag{43}$$

for all $j=1,2,\ldots,d_p$ and $k=1,2,\ldots,d_q$. It should be noted that the factors in the second term of the right-hand side of (43) are interchanged relative to those of (42).

The proof of (42) is as follows. On applying (7) and the relation $S(\pi_{ks}^p)=\pi_{sk}^{p*}$, the left-hand side of (31) (with $v^p=v_s^p$) becomes

$$((id\otimes M)\circ(\pi^r\otimes id))\left(\sum_{k=1}^{d_p}(Q_j^q(v_k^p))\otimes\pi_{sk}^{p*}\right).$$

On multiplying from the right with $id\otimes\pi_{si}^p$, summing over s, and applying the relation $M(\pi_{sk}^{p*}\otimes\pi_{si}^p)=\delta_{ik}1_{\mathscr{A}}$, this reduces to $\pi^r(Q_i^q(v_j^p))$. However, multiplication of the right-hand side of (31) from the right with $id\otimes\pi_{si}^p$ and summing over s produces $\Sigma_{s=1}^{d_p}\Sigma_{t=1}^{d_q}(Q_t^q(v_s^p))\otimes(M(\pi_{tk}^q\otimes\pi_{sj}^p))$. The line of proof for (43) is similar.

3. Identification of the corepresentations $\pi_{\mathscr{L}^{pr}}$ and $\tilde{\pi}_{\mathscr{L}^{pr}}$ of $\mathscr{A}$

It is easily shown from the definition (33) of $\pi_{\mathscr{L}^{pr}}$ that

$$\pi_{\mathscr{L}^{pr}}(\mathscr{P}_{ij}^{pr})=\sum_{m=1}^{d_p}\sum_{n=1}^{d_r}\mathscr{P}_{mn}^{pr}\otimes(\pi^r\boxtimes\overline{\pi^p})_{nm,ji}, \tag{44}$$

where $\mathscr{P}_{ij}^{pr}$ are the operators defined in (14), and where $\overline{\pi^p}$ is the corepresentation of $\mathscr{A}$ that is *conjugate* to π^p, so that its matrix coefficients are given by $\overline{\pi}_{jk}^p=(\pi_{jk}^p)^*$. Then, by (20) and (22),

$$\pi_{\mathscr{D}^{pr}}(\mathscr{P}_{ij}^{pr})=\sum_{m=1}^{d_p}\sum_{n=1}^{d_r}\mathscr{P}_{mn}^{pr}\otimes(\overline{\pi^p}\tilde{\boxtimes}\pi^r)_{mn,ij}. \tag{45}$$

This shows that $\pi_{\mathscr{D}^{pr}}$ is actually the right coaction that is given by the *twisted* tensor product $\overline{\pi^p}\tilde{\boxtimes}\pi^r$, and that the operators $\mathscr{P}_{ij}^{pr}$ are the basis vectors of the carrier space $\mathscr{L}^{pr}$ of this coaction.

Taken with (34), this indicates that the irreducible tensor operators Q_j^q of the definition (31) exist only if π^q is contained in the reduction of $\overline{\pi^p}\tilde{\boxtimes}\pi^r$. As $\overline{\pi^p}\tilde{\boxtimes}\pi^r$ and $\pi^r\boxtimes\overline{\pi^p}$ are equivalent,[1] this implies that Q_j^q exists only if $n_{rp}^q>0$. But $n_{rp}^q=n_{qp}^r$ [cf. (I.125), Ref. 1], so Q_j^q exists only if $n_{qp}^r>0$. [These observations are confirmed by the explicit expressions for the irreducible tensor operators given in (47) below and by the Wigner–Eckart theorem of (50) below.]

Similarly, one can show from the definition (37) of $\tilde{\pi}_{\mathscr{D}^{pr}}$ that

$$\tilde{\pi}_{\mathscr{L}^{pr}}(\mathscr{P}^{\,pr}_{ij}) = \sum_{m=1}^{d_p} \sum_{n=1}^{d_r} \mathscr{P}^{\,pr}_{mn} \otimes (\overline{\pi^{p\ddagger}} \boxtimes \pi^r)_{mn,ij}\,, \tag{46}$$

where $\overline{\pi^{p\ddagger}}$ is the corepresentation of $\mathscr{A}$ that is *conjugate* to the corepresentation $\pi^{p\ddagger}$ that is itself *doubly contragredient* to π^p. This shows that $\tilde{\pi}_{\mathscr{L}^{pr}}$ is the right coaction that is given by the ordinary tensor product $\overline{\pi^{p\ddagger}} \boxtimes \pi^r$, and that the operators $\mathscr{P}^{\,pr}_{ij}$ are the basis vectors of the carrier space $\mathscr{L}^{\,pr}$ of this coaction.

Taken with (39), this shows that the twisted irreducible tensor operators $\tilde{Q}^q_j$ of the definition (36) exist only if π^q is contained in the reduction of $\overline{\pi^{p\ddagger}} \boxtimes \pi^r$. As $\overline{\pi^{p\ddagger}}$ and $\overline{\pi^p}$ are equivalent,[7–12] this implies that $\tilde{Q}^q_j$ exists only if $n^{\overline{q}}_{pr} > 0$. But $n^{\overline{q}}_{pr} = n^r_{pq}$ [cf. (I.125), Ref. 1], so $\tilde{Q}^q_j$ exists only if $n^r_{pq} > 0$. [These observations are confirmed by the explicit expressions for the twisted irreducible tensor operators given in (49) below and by the Wigner–Eckart theorem of (52) below].

4. Explicit expressions for the irreducible tensor operators

If $n^r_{qp} > 0$ there exist n^r_{qp} linearly independent *ordinary* irreducible tensor operators that satisfy (31). These are given by

$$Q^{q,\alpha}_j = \sum_{i=1}^{d_p} \sum_{\ell=1}^{d_r} \left(\begin{matrix} r & \overline{p} \\ \ell & i \end{matrix} \middle| \begin{matrix} q & , & \alpha \\ j & & \end{matrix} \right) \mathscr{P}^{\,pr}_{i\ell}\,, \tag{47}$$

for $\alpha = 1,2,\ldots,n^r_{qp}$ and $j = 1,2,\ldots,d_q$. Here the label $\overline{p}$ in the Clebsch–Gordan coefficients relates to the corepresentation $\overline{\pi^p}$ that is conjugate to π^p. As noted in the previous subsubsection, $n^{\overline{q}}_{rp} = n^r_{qp}$ [cf. (I.125)].

The proof of (47) is as follows. The analogue of (I.130) for the tensor product $\pi^r \boxtimes \overline{\pi^p}$ is

$$\sum_{\ell=1}^{d_r} \sum_{i=1}^{d_p} (\pi^r \boxtimes \overline{\pi^p})_{nm,\ell i} \left(\begin{matrix} r & \overline{p} \\ \ell & i \end{matrix} \middle| \begin{matrix} q & , & \alpha \\ j & & \end{matrix} \right) = \sum_{k=1}^{d_q} \left(\begin{matrix} r & \overline{p} \\ n & m \end{matrix} \middle| \begin{matrix} q & , & \alpha \\ k & & \end{matrix} \right) \pi^q_{kj} \tag{48}$$

for $m = 1,2,\ldots,d_p$, $j = 1,2,\ldots,d_q$, $n = 1,2,\ldots,d_r$, and $\alpha = 1,2,\ldots,n^r_{qp}$. However, by (32), (44), and (47),

$$\pi_{\mathscr{L}^{pr}}(Q^{q,\alpha}_j) = \sum_{i,m=1}^{d_p} \sum_{\ell,n=1}^{d_r} \left(\begin{matrix} r & \overline{p} \\ \ell & i \end{matrix} \middle| \begin{matrix} q & , & \alpha \\ j & & \end{matrix} \right) \mathscr{P}^{\,pr}_{mn} \otimes (\pi^r \boxtimes \overline{\pi^p})_{nm,\ell i}\,.$$

On applying (48) and (47), this reduces to

$$\pi_{\mathscr{L}^{pr}}(Q^{q,\alpha}_j) = \sum_{k=1}^{d_q} Q^{q,\alpha}_k \otimes \pi^q_{kj}$$

(for all $j = 1,2,\ldots,d_q$ and $\alpha = 1,2,\ldots,n^r_{qp}$). That is, the operators $Q^{q,\alpha}_j$ defined in (47) satisfy (35), which is equivalent to (32).

Similarly, if $n^r_{pq} > 0$ there exist n^r_{pq} linearly independent *twisted* irreducible tensor operators that satisfy (32). These are given by

$$\tilde{Q}^{q,\alpha}_j = \sum_{i=1}^{d_p} \sum_{\ell=1}^{d_r} \left(\begin{matrix} \overline{p^\ddagger} & r \\ i & \ell \end{matrix} \middle| \begin{matrix} q & , & \alpha \\ j & & \end{matrix} \right) \mathscr{P}^{\,pr}_{i\ell}\,, \tag{49}$$

for $\alpha=1,2,\ldots,n^r_{pq}$ and $j=1,2,\ldots,d_q$. Here the label $\overline{p^{\ddagger}}$ in the Clebsch–Gordan coefficients relates to the corepresentation $\overline{\pi^{p\ddagger}}$ that is conjugate to the corepresentation $\pi^{p\ddagger}$ that is itself doubly contragredient to π^p. It should be noted that $n^q_{p\overline{r}}=n^r_{pq}=n^q_{\overline{p^{\ddagger}}r}$ [c.f. (I.125)].

The proof of (49) is similar to that of (47), but uses the right coaction $\widetilde{\pi}_{\mathscr{D}^{pr}}$ in the place of $\pi_{\mathscr{D}^{pr}}$. Also needed is the relation

$$(\overline{\pi^{p\ddagger}})_{ij}=\sum_{k,\ell=1}^{d_p}\overline{F^p_{ik}}(\overline{\pi^p})_{k\ell}\overline{((\mathbf{F}^p)^{-1})_{\ell j}},$$

which follows from (30), and the corresponding relation

$$\left(\begin{matrix}\overline{p} & r\\ i & \ell\end{matrix}\middle|\begin{matrix}q & , & \alpha\\ j & & \end{matrix}\right)=\sum_{k=1}^{d_p}\overline{((\mathbf{F}^p)^{-1})_{ik}}\left(\begin{matrix}\overline{p^{\ddagger}} & r\\ k & \ell\end{matrix}\middle|\begin{matrix}q & , & \alpha\\ j & & \end{matrix}\right).$$

V. THEOREMS OF THE WIGNER–ECKART TYPE

If π^p, π^q, and π^r are unitary irreducible corepresentations of $\mathscr{A}$ of dimensions d_p, d_q, and d_r respectively, v^p_j and v^r_ℓ are basis vectors belonging to the carrier spaces V^p and V^r of π^p and π^r respectively, and Q^q_k is an *ordinary* irreducible tensor operator belonging to π^q [as defined in (31)], then

$$\langle v^r_\ell,Q^q_k(v^p_j)\rangle=\sum_{\alpha=1}^{n^r_{qp}}\left(\begin{matrix}r & , & \alpha\\ \ell & & \end{matrix}\middle|\begin{matrix}q & p\\ k & j\end{matrix}\right)(r|Q^q|p)_\alpha, \tag{50}$$

for all $j=1,2,\ldots,d_p$, all $k=1,2,\ldots,d_q$, and all $\ell=1,2,\ldots,d_r$. Here the *reduced matrix elements* $(r|Q^q|p)_\alpha$ are given by

$$(r|Q^q|p)_\alpha=\sum_{s=1}^{d_p}\sum_{t=1}^{d_q}\sum_{u,v=1}^{d_r}\langle v^r_u,Q^q_t(v^p_s)\rangle\left(\begin{matrix}q & p\\ t & s\end{matrix}\middle|\begin{matrix}r & , & \alpha\\ v & & \end{matrix}\right)\times\{((\mathbf{F}^r)^{-1})_{vu}/tr((\mathbf{F}^r)^{-1})\} \tag{51}$$

for $\alpha=1,2,\ldots,n^r_{qp}$, and $\langle,\rangle$ denotes the inner product of V^r. Here $\mathbf{F}^r$ is the matrix defined in (30).

On the other hand, if $\widetilde{Q}^q_k$ is a *twisted* irreducible tensor operator belonging to π^q [as defined in (36)], then

$$\langle v^r_\ell,\widetilde{Q}^q_k(v^p_j)\rangle=\sum_{\alpha=1}^{n^r_{pq}}\left(\begin{matrix}r & , & \alpha\\ \ell & & \end{matrix}\middle|\begin{matrix}p & q\\ j & k\end{matrix}\right)(r|\widetilde{Q}^q|p)_\alpha, \tag{52}$$

for all $j=1,2,\ldots,d_p$, all $k=1,2,\ldots,d_q$, and all $\ell=1,2,\ldots,d_r$, where the reduced matrix elements $(r|\widetilde{Q}^q|p)_\alpha$ are given by

$$(r|\widetilde{Q}^q|p)_\alpha=\sum_{s=1}^{d_p}\sum_{t=1}^{d_q}\sum_{u,v=1}^{d_r}\langle v^r_u,\widetilde{Q}^q_t(v^p_s)\rangle\left(\begin{matrix}p & q\\ s & t\end{matrix}\middle|\begin{matrix}r & , & \alpha\\ v & & \end{matrix}\right)\times\{((\mathbf{F}^r)^{-1})_{vu}/tr((\mathbf{F}^r)^{-1})\} \tag{53}$$

for $\alpha=1,2,\ldots,n^r_{pq}$.

The results (50) and (52) again exhibit the classic Wigner–Eckart theorem behavior, in that they show that the j, k, and ℓ dependences of the inner products $\langle v^r_\ell,Q^q_k(v^p_j)\rangle$ and

$\langle v^r_\ell, \widetilde{Q}^q_k(v^p_j)\rangle$ are determined only by Clebsch−Gordan coefficients, but it should be noted that in the general case in which $\mathscr{A}$ is non-commutative, the inner products for the *ordinary* and *twisted* irreducible tensor operators involve *different* sets of Clebsch−Gordan coefficients.

The proof of (50) is as follows. The condition for a corepresentation π_V of $\mathscr{A}$ to be unitary is that

$$\sum_{[v]} \langle w, v_{[1]},\rangle S(v_{[2]}) = \sum_{[w]} \langle w_{[1]}, v\rangle (w_{[2]})^* \tag{54}$$

for all $v, w \in V$, the carrier space of π_V, where

$$\pi_V(v) = \sum_{[v]} v_{[1]} \otimes v_{[2]}, \tag{55}$$

with $v_{[1]} \in V$ and $v_{[2]} \in \mathscr{A}$ [cf. (I.51)]. Thus with $v = Q^q_j(v^p_i)$ and $w = v^r_\ell$, (54), (55), (42), and (7) imply that

$$\sum_{s=1}^{d_p} \sum_{t=1}^{d_q} \langle v^r_\ell, Q^q_t(v^p_s)\rangle S(M(\pi^q_{tj} \otimes \pi^p_{si})) = \sum_{u=1}^{d_r} \langle v^r_u, Q^q_j(v^p_i)\rangle (\pi^r_{u\ell})^*. \tag{56}$$

But $(\pi^r_{u\ell})^* = S(\pi^r_{\ell u})$, so acting on both sides with S^{-1} (which is well defined for a compact quantum group algebra[7–12]), multiplying through from the left by $(\pi^r_{\ell k})^*$, summing over ℓ, and using the relation $\Sigma_\ell M((\pi^r_{\ell k})^* \otimes (\pi^r_{\ell u})) = \delta_{uk} 1_{\mathscr{A}}$, (56) reduces to

$$\sum_{\ell=1}^{d_r} \sum_{s=1}^{d_p} \sum_{t=1}^{d_q} \langle v^r_\ell, Q^q_t(v^p_s)\rangle ((\pi^r_{\ell k})^* \pi^q_{tj} \otimes \pi^p_{si}) = \langle v^r_k, Q^q_j(v^p_i)\rangle 1_{\mathscr{A}}. \tag{57}$$

On acting with the Haar functional h, and applying (29) and the relation $h(1_{\mathscr{A}}) = 1$, (50) follows immediately. The proof of (52) is similar.

VI. EXAMPLE: IRREDUCIBLE TENSOR OPERATORS FOR THE STANDARD DEFORMATION OF THE FUNCTION ALGEBRA OF THE COMPACT LIE GROUP SU(2)

It is particularly interesting to study the foregoing theory for the case in which $\mathscr{A}$ is the standard deformation of the function algebra of the compact Lie group SU(2),because both this Hopf algebra $\mathscr{A}$ and its dual $\mathscr{A}'$ have been very extensively investigated, the former in the language of 'compact matrix pseudogroups' and the latter as the deformation $U_q(sl(2))$ of the universal enveloping algebra $U(sl(2))$ of the simple Lie algebra $sl(2)$.

A. Structure of the standard deformation of the function algebra of the compact Lie group *SU*(2)

It is well known (cf. Ref. 14) that the irreducible representations of the deformation $U_q(sl(2))$ (for generic q) can be labelled by a single index j, which takes values $0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$, the irreducible representation corresponding to j being $(2j+1)$-dimensional, with rows and columns that may be labeled by indices m' and m that take values $-j, -j+1, \ldots, j-1, j$, exactly as for the simple Lie algebra $sl(2)$. To each of these representations corresponds a *co*representation of the dual Hopf algebra $\mathscr{A}$. Consequently the labels for corepresentations of $\mathscr{A}$ will henceforth always be denoted by j (possibly with a prime or subscript attached) and the rows and columns of the corresponding matrix coefficients will be labelled by these indices m and m' (possibly with subscripts attached). (Although q was used in all the other sections of this paper to indicate an irreducible representation or corepresentation, in this section it will be employed to denote the standard deformation parameter.)

All of the irreducible corepresentations π^j (for $j=0,\frac{1}{2},1,\frac{3}{2},\ldots$) may be taken to be unitary, and their matrix coefficients $\pi^j_{m'm}$ form a basis for $\mathscr{A}$. Moreover *every* matrix coefficient $\pi^j_{m'm}$ for $j\geqslant 1$ can be written as a polynomial in the matrix coefficients of $\pi^{1/2}$, while $\pi^0_{00}=1_{\mathscr{A}}$. Let

$$\boldsymbol{\pi}^{1/2}=\begin{pmatrix} X & U \\ V & Y \end{pmatrix}, \tag{58}$$

where the entries are assumed to satisfy the relations

$$\begin{gathered} XU=q^{-1}UX, XV=q^{-1}VX, YU=qUY, YV=qVY, \\ UV=VU, XY-q^{-1}UV=1_{\mathscr{A}}, YX-qUV=1_{\mathscr{A}}. \end{gathered} \tag{59}$$

In the language of 'matrix pseudogroups' the matrix coefficients $\pi^j_{m'm}$ are called 'quantum d-functions' and are denoted by $d^j_{m'm}$. The work of Nomura[15] then implies that

$$\begin{aligned} \pi^j_{m'm}=q^{(m'-m)(2j-m'+m)/2}&\{[j+m']![j-m']![j+m]![j-m]!\} \\ &\times\sum_a \frac{q^{a(2j-m'+m-a)}X^{j+m-a}U^{m'-m+a}V^aY^{j-m'-a}}{[a]![j+m-a]![m'-m+a]![j-m'-a]!}, \end{aligned} \tag{60}$$

where $[n]=(q^n-q^{-n})/(q-q^{-1})$ and $[n]!=[n][n-1][n-2]\ldots[2][1]$, and where the sum over a is over all integers such that the expressions in the q-factorials are non-negative. (The present quantity q is actually $q^{1/2}$ in the notation of Nomura[15,16]). Then, for example

$$\boldsymbol{\pi}^1=\begin{pmatrix} X^2 & q^{1/2}[2]^{1/2}XU & U^2 \\ q^{1/2}[2]^{1/2}XV & XY+qUV & q^{1/2}[2]^{1/2}UY \\ V^2 & q^{1/2}[2]^{1/2}VY & Y^2 \end{pmatrix} \tag{61}$$

and

$$\boldsymbol{\pi}^{3/2}=\begin{pmatrix} X^3 & q[3]^{1/2}X^2U & q[3]^{1/2}XU^2 & U^3 \\ q[3]^{1/2}X^2V & X^2Y+q^2[2]XUV & q[2]XUY+q^2U^2V & q[3]^{1/2}U^2Y \\ q[3]^{1/2}XV^2 & q[2]XVY+q^2UV^2 & XY^2+q^2[2]UVY & q[3]^{1/2}UY^2 \\ V^3 & q[3]^{1/2}V^2Y & q[3]^{1/2}VY^2 & Y^3 \end{pmatrix}. \tag{62}$$

The product of any two matrix coefficients can (at least in principle) be deduced from the expressions.

An alternative way of getting the product of any two matrix coefficients is to invoke (28), for the Clebsch–Gordan coefficients are known for this $\mathscr{A}$. Indeed for this $\mathscr{A}$ the Clebsch–Gordan coefficients exhibit two simplifying features. First, the multiplicity is always just 1, so the index α in the Clebsch–Gordan coefficients of (23) may be omitted, and second, the Clebsch–Gordan coefficients can be taken to be purely real. As the Clebsch–Gordan series for $\pi^{j_1}\boxtimes\pi^{j_2}$ is the direct sum of π^j with $j=j_1+j_2, j_1+j_2-1,\ldots,|j_1-j_2|$, (28) reduces in this case to

$$M(\pi^{j_1}_{m_1'm_1}\otimes\pi^{j_2}_{m_2'm_2})=\sum_{j=|j_1-j_2|}^{j_1+j_2}\sum_{m',m=-j}^{j}\left(\begin{array}{cc|c} j_1 & j_2 & j \\ m_1' & m_2' & m' \end{array}\right)\left(\begin{array}{cc|c} j_1 & j_2 & j \\ m_1 & m_2 & m \end{array}\right)\pi^j_{m'm}. \tag{63}$$

Various equivalent expressions for the Clebsch–Gordan coefficients appear in the literature, but the most convenient for application here is that given by Nomura,[16] which, in the present notation, is

$$\left(\begin{array}{cc|c} j_1 & j_2 & j \\ m_1 & m_2 & m \end{array}\right)$$
$$= \Delta(j_1,j_2,j) q^{\{x(j_1)+x(j_2)-x(j)+2(j_1j_2+j_1m_2-j_2m_1)\}/2}$$
$$\times \{[j_1+m_1]![j_1-m_1]![j_2+m_2]![j_2-m_2]![j+m]![j-m]![2j+1]\}^{1/2}$$
$$\times \sum_a \frac{(-1)^a q^{-a(j_1+j_2+j+1)/2}}{[a]![j_1+j_2-j-a]![j_1-m_1-a]![j_2+m_2-a]![j-j_2+m_1+a]![j-j_1-m_2+a]!}, \tag{64}$$

where $\Delta(a,b,c)=\{[-a+b+c]![a-b+c]![a+b-c]!/[a+b+c+1]!\}^{1/2}$ and $x(a)=a(a+1)$, and where the sum over a is over all integers such that the expressions in the q-factorials are non-negative. In particular

$$\left(\begin{array}{cc|c} j+\frac{1}{2} & j & \frac{1}{2} \\ m+\frac{1}{2} & -m & \frac{1}{2} \end{array}\right) = (-1)^{j-m} q^{-j+\frac{1}{2}+\frac{3}{2}m} [j+m+1]^{1/2} \{[2][2j]!/[2j+2]!\}^{1/2} \tag{65}$$

and

$$\left(\begin{array}{cc|c} j+\frac{1}{2} & j & \frac{1}{2} \\ m-\frac{1}{2} & -m & -\frac{1}{2} \end{array}\right) = (-1)^{j-m} q^{\frac{1}{2}+\frac{3}{2}m} [j-m+1]^{1/2} \{[2][2j]!/[2j+2]!\}^{1/2}. \tag{66}$$

The action of the coproduct Δ and counit ϵ of $\mathscr{A}$ on the generators of $\mathscr{A}$ is given by

$$\Delta(X)=X\otimes X+U\otimes V, \quad \Delta(Y)=V\otimes U+Y\otimes Y,$$
$$\Delta(U)=X\otimes U+U\otimes Y, \quad \Delta(V)=V\otimes X+Y\otimes V,$$

and

$$\epsilon(X)=1, \epsilon(Y)=1, \quad \epsilon(U)=0, \epsilon(V)=0.$$

Moreover, the action of the star-operation * of $\mathscr{A}$ on the generators of $\mathscr{A}$ may be taken to be

$$X^*=Y, \quad Y^*=X, \quad U^*=-q^{-1}V, \quad V^*=-qU, \tag{67}$$

which implies[15] that its action on any matrix coefficient is given by

$$(\pi^j_{m'm})^* = (-1)^{m-m'} q^{m-m'} \pi^j_{-m',-m}. \tag{68}$$

As $S(\pi^j_{m'm})=(\pi^j_{mm'})^*$ [cf. (I.52), Ref. 1], it follows that

$$S(\pi^j_{m'm}) = (-1)^{-(m-m')} q^{-(m-m')} \pi^j_{-m,-m'}. \tag{69}$$

Thus

$$S^2(\pi^j_{m'm}) = q^{-2(m-m')} \pi^j_{m'm}. \tag{70}$$

As the matrix coefficients of the doubly contragredient corepresentation $\pi^{j\ddagger}$ are given by $(\pi^j_{m'm})^{\ddagger}=S^2\pi^j_{m'm}$ [cf. (I.57), Ref. 1], it follows that the $(2j+1)\times(2j+1)$ matrix of (30) (which appears in the expressions for the reduced matrix elements (51) and (53) of the Wigner–Eckart type theorems) is *diagonal* and that its elements are given by

$$F^j_{m'm}=\delta_{m'm}q^{-2(j-m)}. \tag{71}$$

B. Bosonic creation and annihilation operators as irreducible tensor operators

Let $b_1^\dagger, b_1$ and $b_2^\dagger, b_2$ be two pairs of 'deformed' bosonic creation and annihilation operators and N_1 and N_2 the associated number operators whose action on the infinite-dimensional Fock space spanned by the occupation number vectors $|n_i\rangle$ is given (cf. Refs. 17, 18) by

$$b_i^\dagger|n_i\rangle=[n_i+1]^{1/2}|n_i+1\rangle,$$

$$b_i|n_i\rangle=[n_i]^{1/2}|n_i-1\rangle, \quad N_i|n_i\rangle=n_i|n_i\rangle, \tag{72}$$

for $i=1,2$, where it is assumed that the vacuum state vectors $|0\rangle$ are such that $b_i|0\rangle=0$ for $i=1,2$. It is also assumed that every member of the set $\{b_1^\dagger, b_1, N_1\}$ commutes with every member of the set $\{b_2^\dagger, b_2, N_2\}$. In the deformed generalization of the Jordan–Schwinger realization of $sl(2)$ (cf. Refs. 17, 18), the basis vectors of the carrier spaces of the irreducible representations of $U_q(sl(2))$ are given by

$$v^j_m=|j+m, j-m\rangle, \tag{73}$$

and these, of course, are also the basis vectors of the carrier spaces of the irreducible *corepresentations* of $\mathscr{A}$.

Then

$$Q^{1/2}_{1/2}=b_1^\dagger q^{-(1/2)N_2}, \quad Q^{1/2}_{-1/2}=b_2^\dagger q^{(1/2)N_1}, \tag{74}$$

and

$$Q^{1/2}_{1/2}=qb_2q^{(1/2)N_1}, \quad Q^{1/2}_{-1/2}=-b_1q^{-(1/2)N_2}, \tag{75}$$

are two sets of pairs of *ordinary* irreducible tensor operators that belong to the 2-dimensional irreducible corepresentation $\pi^{1/2}$ of $\mathscr{A}$.

This will now be demonstrated for the *first* pair (74), starting from the definition (35), and taking V to be the direct sum of all the carrier spaces of all the irreducible corepresentations of $\mathscr{A}$ (with just one such irreducible corepresentation being included from each equivalence class). Define the right coaction π of $\mathscr{A}$ by

$$\pi(v^j_m)=\sum_{m'=-j}^{j} v^j_{m'}\otimes\pi^j_{m'm}, \tag{76}$$

for all $j=0,\frac{1}{2},1,\ldots$ and $m=j,j-1,\ldots,-j$. Then in this case (36) becomes

$$((id\otimes M)\circ(\pi\otimes id)\circ(Q^{1/2}_k\otimes S)\circ\pi)(v^j_m)=\sum_{\ell=-1/2}^{1/2} Q^{1/2}_\ell(v^j_m)\otimes\pi^{1/2}_{\ell k}, \tag{77}$$

for all $j=0,\frac{1}{2},1,\ldots$ and $m=j,j-1,\ldots,-j$. It will now be shown that this is indeed satisfied for $k=\frac{1}{2}$. (The proof for $k=-\frac{1}{2}$ is similar.) By (72), (69), (74), and (76), the left-hand side of (77) for $k=\frac{1}{2}$ is

$$\sum_{m''=-j-1}^{j}\sum_{m'=-j}^{j}[j+m'+1]^{1/2}q^{-(1/2)(j-m')-(m-m')}(-1)^{-(m-m')}$$
$$\times v^{j+(1/2)}_{m''+(1/2)}\otimes M(\pi^{j+(1/2)}_{m''+(1/2),m'+(1/2)}\otimes\pi^{j}_{-m,-m'}). \tag{78}$$

Similarly, by (72), (74), and (76), the right-hand side of (77) for $k=\frac{1}{2}$ is

$$[j+m+1]^{1/2}q^{-(1/2)(j-m)}v^{j+(1/2)}_{m+(1/2)}\otimes\pi^{1/2}_{1/2,1/2}+[j-m+1]^{1/2}q^{(1/2)(j+m)}v^{j+(1/2)}_{m-(1/2)}\otimes\pi^{1/2}_{-(1/2),(1/2)}, \tag{79}$$

so it remains to show that (78) reduces to (79). However, by (63) and (65), (78) reduces to

$$\sum_{m''=-j-1}^{j}\sum_{m'=-j}^{j}\sum_{j'=1/2}^{2j+(1/2)}\{[2][2j]!/[2j+2]!\}^{1/2}q^{((1/2)j-m-(1/2))}(-1)^{(j-m)}$$
$$\times\begin{pmatrix} j+\frac{1}{2} & j & \frac{1}{2}\\ m'+\frac{1}{2} & -m' & \frac{1}{2}\end{pmatrix}\begin{pmatrix} j+\frac{1}{2} & j & j'\\ m''+\frac{1}{2} & -m & m''+\frac{1}{2}-m\end{pmatrix}$$
$$\times\begin{pmatrix} j+\frac{1}{2} & j & j'\\ m'+\frac{1}{2} & -m' & \frac{1}{2}\end{pmatrix}v^{j+(1/2)}_{m''+(1/2)}\otimes\pi^{j'}_{m''+(1/2)-m,1/2}\,. \tag{80}$$

On invoking the Clebsch–Gordan orthogonality relation

$$\sum_{m'=-j}^{j}\begin{pmatrix} j+\frac{1}{2} & j & \frac{1}{2}\\ m'+\frac{1}{2} & -m' & \frac{1}{2}\end{pmatrix}\begin{pmatrix} j+\frac{1}{2} & j & j'\\ m'+\frac{1}{2} & -m' & \frac{1}{2}\end{pmatrix}=\begin{cases}1, & \text{if} \quad j'=\frac{1}{2}\\ 0, & \text{i} \quad \text{f}j'\neq\frac{1}{2}\end{cases}, \tag{81}$$

(80) [and hence (78)] reduces to

$$\sum_{m''=-j-1}^{j}\{[2][2j]!/[2j+2]!\}^{1/2}q^{((1/2)j-m-(1/2))}(-1)^{(j-m)}$$
$$\times\begin{pmatrix} j+\frac{1}{2} & j & \frac{1}{2}\\ m''+\frac{1}{2} & -m & m''+\frac{1}{2}-m\end{pmatrix}v^{j+(1/2)}_{m''+(1/2)}\otimes\pi^{j'}_{m''+1/2-m,1/2}. \tag{82}$$

However, the remaining Clebsch–Gordan coefficients are zero if $m''+\frac{1}{2}-m>\frac{1}{2}$, i.e. if $m''>m$, and are zero if $m''+\frac{1}{2}-m<-\frac{1}{2}$, i.e. if $m''<m-1$, so these Clebsch–Gordan coefficients are non-zero only for $m''=m,m-1$. Thus (82) [and hence (78)] becomes

$$\{[2][2j]!/[2j+2]!\}^{1/2}q^{(1/2j-m-1/2)}(-1)^{(j-m)}$$
$$\times\left\{\begin{pmatrix} j+\frac{1}{2} & j & \frac{1}{2}\\ m-\frac{1}{2} & -m & -\frac{1}{2}\end{pmatrix}v^{j+(1/2)}_{m-(1/2)}\otimes\pi^{1/2}_{-(1/2),1/2}+\begin{pmatrix} j+\frac{1}{2} & j & \frac{1}{2}\\ m+\frac{1}{2} & -m & \frac{1}{2}\end{pmatrix}v^{j+(1/2)}_{m+(1/2)}\otimes\pi^{1/2}_{1/2,1/2}\right\},$$

which, by (65) and (66), reduces to (79).

Similarly

$$\tilde{Q}^{1/2}_{1/2}=b_1^{\dagger}q^{(1/2)N_2},\quad \tilde{Q}^{1/2}_{-1/2}=b_2^{\dagger}q^{-(1/2)N_1}, \tag{83}$$

and

$$\tilde{Q}^{1/2}_{1/2}=q^{-1}b_2q^{-(1/2)N_1},\quad \tilde{Q}^{1/2}_{-1/2}=-b_1q^{(1/2)N_2}, \tag{84}$$

are two sets of pairs of *twisted* irreducible tensor operators belonging to the 2-dimensional irreducible corepresentation $\pi^{1/2}$ of $\mathscr{A}$. [This is easily deduced from (78) and (79), because in the special case of this algebra $\mathscr{A}$, (59) and (69) imply that the substitutions $M\rightarrow M\bigcirc\sigma$ and $S\rightarrow S^{-1}$ merely correspond to the replacement of q by q^{-1}].

It has been observed previously by Biedenharn and Tarlini[19] that (78) provide a pair of irreducible tensor operators for the 2-dimensional irreducible representation of $U_q(sl(2))$, their argument essentially using (A10) and the generalized Jordan-Schwinger realization of the generators of $U_q(sl(2))$, together with various identities involving the creation and annihilation operators. The object of the above analysis in this subsection is to give an explicit demonstration of the applicability of the *new* definitions (A10) and (A11) for $\mathscr{A}$, which, of course, apply not merely to this example but to *any* compact quantum group algebra.

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APPENDIX: MOTIVATION FOR DEFINITIONS

1. Introduction

The purpose of this Appendix is to *motivate* the definitions that are given in the main body of the paper for the irreducible tensor operators. This will be done by considering the simple special case in which the Hopf algebra $\mathscr{A}$ is the set of functions defined on a *finite* group $\mathscr{G}$ of order g, so that the dual $\mathscr{A}'$ of $\mathscr{A}$ is the group algebra of $\mathscr{G}$. Of course, as $\mathscr{A}$ is commutative in this special case, the resulting expressions are to some extent ambiguous, in that in this special case M is indistinguishable from $M\circ\sigma$ and S is indistinguishable from S^{-1}. The demonstration of the correctness, consistency, and usefulness of the definitions that are actually employed for the *general* case are the subject matter of the self-contained arguments of the main body of this paper.

A summary of the basic facts concerning the relationship of $\mathscr{A}$ and $\mathscr{A}'$ may be found in the Introduction to the Appendix of Paper I.

B. Motivation for definitions of irreducible tensor operators

The starting point of the present argument is (2), which of course also applies to finite groups, and which may be rewritten as

$$\hat{\pi}'^r(x)Q^q_j\hat{\pi}'^p(x^{-1})=\sum_{k=1}^{d_q}\Gamma^q(x)_{kj}Q^q_k \tag{A1}$$

for all $x\in\mathscr{G}$ and all $j=1,2,\ldots,d_q$. Here the operators $\hat{\pi}'^p(x)$ are defined by

$$\hat{\pi}'^p(x)(v^p_j)=\sum_{k=1}^{d_p}\Gamma^p(x)_{kj}v^p_k, \tag{A2}$$

and are related to the corresponding left action π'^p of $\mathscr{A}'$ (a mapping of the carrier space V^p into $V^p\otimes\mathscr{A}'$) by the prescription

$$\hat{\pi}'^p(x)(v^p_j)=\pi'^p(x\otimes v^p_j). \tag{A3}$$

As here $S_{\mathscr{A}'}(x)=x^{-1}$ and $\Delta_{\mathscr{A}'}(x)=x\otimes x$, (A1) can be rewritten in purely Hopf algebraic terms (for $\mathscr{A}'$) as

$$(\pi'^{r}\circ(id\otimes Q_j^q)\circ(id\otimes\pi'^{p})\circ(id\otimes S_{\mathscr{A}'}\otimes id)\circ(\Delta_{\mathscr{A}'}\otimes id))(x\otimes v^p)=\sum_{k=1}^{d_q}\Gamma^q(x)_{kj}Q_k^q(v^p) \quad \text{(A4)}$$

for all $x\in\mathscr{A}'$, all $v^p\in V^p$, and all $j=1,2,\ldots,d_q$. [Here the $\Gamma^q(x)_{kj}$ are now matrix elements of the irreducible representation π'^q of the Hopf algebra $\mathscr{A}'$].

This condition can be recast entirely in terms of quantities defined for the Hopf algebra $\mathscr{A}$ in the following way. As noted in equation (I.214), the relationship between a right coaction π_V of $\mathscr{A}$ and the corresponding left action π'_V of $\mathscr{A}'$ (with the same carrier space V) is

$$\pi'_V(a'\otimes v)=(M_{V,C}\circ(id\otimes ev)\circ(\sigma\otimes id)\circ(id\otimes\pi_V))(a'\otimes v) \quad \text{(A5)}$$

for all $a'\in\mathscr{A}'$ and all $v\in V$, where the evaluation map ev (from $\mathscr{A}'\otimes\mathscr{A}$ to C) is defined [cf. (I.41)] by

$$ev(a'\otimes a)=\langle a',a\rangle \quad \text{(A6)}$$

for all $a'\in\mathscr{A}'$ and all $a\in\mathscr{A}$. On applying this twice (once with with $\pi'_V=\pi'^{r}$ and once with $\pi'_V=\pi'^{p}$), the left-hand side of (A4) becomes

$$(M_{V^r,C}\circ(id\otimes ev)\circ(\sigma\otimes id)\circ(id\otimes\pi^r)\circ(id\otimes Q_j^q)\circ(id\otimes\pi^p)\circ(id\otimes M_{V^p,C})$$

$$\circ(id\otimes id\otimes ev)\circ(id\otimes\sigma\otimes id)\circ(id\otimes S_{\mathscr{A}'}\otimes\pi^p)\circ(\Delta_{\mathscr{A}'}\otimes id)(x\otimes v^p). \quad \text{(A7)}$$

As (I.209) and (I.210) can be rewritten as

$$(M_C\circ(ev\otimes ev)\circ(id\otimes\sigma\otimes id)\circ(\Delta_{\mathscr{A}'}\otimes id))(a'\otimes a\otimes b)=(ev\circ(id\otimes M))(a'\otimes a\otimes b)$$

for all $a,b\in\mathscr{A}$ and all $a'\in\mathscr{A}'$, and

$$(ev\circ(S_{\mathscr{A}'}\otimes id))(a'\otimes a)=(ev\circ(id\otimes S))(a'\otimes a)$$

for all $a\in\mathscr{A}$ and all $a'\in\mathscr{A}'$, (96) can be re-expressed as

$$(M_{V^r,C}\circ(id\otimes ev)\circ(\sigma\otimes id)\circ(id\otimes id\otimes M)\circ(id\otimes\pi^r\otimes id)\circ(id\otimes Q_j^q\otimes S)\circ(id\otimes\pi^p))(x\otimes v^p). \quad \text{(A8)}$$

However, the right-hand side of (A4) can be rewritten using (I.217) as $\Sigma_{k=1}{}^{d_q}\langle x,\pi_{kj}^q\rangle Q_k^q(v^p)$, and hence as

$$\sum_{k=1}^{d_q}(M_{V^r,C}\circ(id\otimes ev)\circ(\sigma\otimes id)\circ(id\otimes Q_k^q\otimes id))(x\otimes v^p\otimes\pi_{kj}^q). \quad \text{(A9)}$$

On equating (A8) and (A9), as the first three terms are common to both expressions, they can be removed. The remaining terms act simply as the identity on the factor x, so on removing this now trivial effect on x, it follows that (A4) is equivalent to

$$((id\otimes M)\circ(\pi^r\otimes id)\circ(Q_j^q\otimes S)\circ\pi^p)(v^p)=\sum_{k=1}^{d_q}Q_k^q(v^p)\otimes\pi_{kj}^q$$

for all $v^p \in V^p$ and all $j=1,2,\ldots,d_q$. As this involves *only* quantities defined for $\mathscr{A}$, it provides the desired criterion (32).

Now consider the situation in which V is a vector space that is a direct sum of carrier spaces of unitary irreducible corepresentations of $\mathscr{A}$ and which contains at least $V^p \oplus V^r$. Let π be the mapping of V into $V\otimes\mathscr{A}$ that coincides with π^p on V^p and with π^r on V^r, and which acts similarly on any other carrier spaces that might be contained in V. Of course V is also is the direct sum of carrier spaces of unitary irreducible representations of $\mathscr{A}'$. Then the generalization of (A4) to this situation is

$$(\pi'\circ(id\otimes Q_j^q)\circ(id\otimes\pi')\circ(id\otimes S_{\mathscr{A}'}\otimes id)\circ(\Delta_{\mathscr{A}'}\otimes id))(x\otimes v)=\sum_{k=1}^{d_q}\Gamma^q(x)_{kj}Q_k^q(v) \quad \text{(A10)}$$

for all $x \in \mathscr{A}'$, all $v \in V$, and all $j=1,2,\ldots,d_q$. (Here π' is the mapping of $V\otimes\mathscr{A}'$ into V that coincides with π'^p on V^p and with π'^r on V^r, and which acts similarly on any other carrier spaces that might be contained in V.) The generalization of (31) to this situation is obviously

$$((id\otimes M)\circ(\pi\otimes id)\circ(Q_j^q\otimes S)\circ\pi)(v)=\sum_{k=1}^{d_q}Q_k^q(v)\otimes\pi_{kj}^q \quad \text{(A11)}$$

for all $v \in V$ and all $j=1,2,\ldots,d_q$.

Because M is indistinguishable from $M\circ\sigma$ and S is indistinguishable from S^{-1} in the situation being considered here, the above arguments would equally well apply with each of the following 3 substitutions:

(1) replace M by $M\circ\sigma$, but leave S unchanged;
(2) leave M unchanged, but replace S by S^{-1};
(3) replace M by $M\circ\sigma$ *and* replace S by S^{-1}.

However, in the general case in which $\mathscr{A}$ is non-commutative, the possibilities (1) and (2) are *excluded* because with them, and in the situation discussed in the previous paragraph, the identity operator would not be an irreducible tensor operator belonging to the identity corepresentation. With the substitution (3), (31) changes into (36), which is the defining condition for a *twisted* irreducible tensor operator $\widetilde{Q}_j^q$. (Of course the corresponding substitutions for $\mathscr{A}'$ are $\Delta_{\mathscr{A}'}\to\sigma\circ\Delta_{\mathscr{A}'}$ and $S_{\mathscr{A}'}\to(S'_{\mathscr{A}})^{-1}$, so that the analogues of (A4) and (A10) are

$$(\pi'^r\circ(id\otimes\widetilde{Q}_j^q)\circ(id\otimes\pi'^p)\circ(id\otimes(S'_{\mathscr{A}})^{-1}\otimes id)\circ(\sigma\otimes id)\circ(\Delta_{\mathscr{A}'}\otimes id))(x\otimes v^p)$$
$$=\sum_{k=1}^{d_q}\Gamma^q(x)_{kj}\widetilde{Q}_k^q(v^p) \quad \text{(A12)}$$

(for all $x \in \mathscr{A}'$, all $v^p \in V^p$, and all $j=1,2,\ldots,d_q$), and

$$(\pi'\circ(id\otimes\widetilde{Q}_j^q)\circ(id\otimes\pi')\circ(id\otimes(S'_{\mathscr{A}})^{-1}\otimes id)\circ(\sigma\otimes id)\circ(\Delta_{\mathscr{A}'}\otimes id))(x\otimes v)=\sum_{k=1}^{d_q}\Gamma^q(x)_{kj}\widetilde{Q}_k^q(v) \quad \text{(A13)}$$

(for all $x \in \mathscr{A}'$, all $v \in V$, and all $j=1,2,\ldots,d_q$).

It is worth noting that (A4), (A10), (A12), and (A13) provide the appropriate definitions for irreducible tensor operators not merely for the context in which they have been derived here (i.e. for the case in which $\mathscr{A}'$ is the group algebra of a finite group $\mathscr{G}$), but also for the case in which $\mathscr{A}'$ is the universal enveloping algebra $U(\mathscr{L})$ of a Lie algebra $\mathscr{L}$ (with $S_{\mathscr{A}'}(a)=-a$ and $\Delta_{\mathscr{A}'}(a)=a\otimes 1+1\otimes a$ for all $a(\mathscr{L})$, and for deformations of such universal enveloping algebras.

[Of course in the case $\mathscr{A}'=\mathscr{U}(\mathscr{L})$, the criteria (A4) and (A12) coincide and the criteria (A10) and (A13) also coincide, but this will not be true for deformations of $U(\mathscr{L})$].

3. Derivation of the right coactions $\pi_{\mathscr{L}^{pr}}$ and $\tilde{\pi}_{\mathscr{L}^{pr}}$

Consideration of (3) suggests that one first defines an operator $\pi'_{\mathscr{L}^{pr}}$ to be the mapping of $\mathscr{A}'\otimes\mathscr{L}^{pr}$ into $\mathscr{L}^{pr}$ that is given by

$$\pi'_{\mathscr{L}^{pr}}(x\otimes Q)=\hat{\pi}'^{r}(x)Q\hat{\pi}'^{p}(x^{-1}), \tag{A14}$$

where the operators $\hat{\pi}'^{p}(x)$ were defined (A2) [and the $\hat{\pi}'^{r}(x)$ are defined similarly], and where Q is any member of $\mathscr{L}^{pr}$. If $a^1,a^2,\ldots$ form a basis for $\mathscr{A}'$, (A14) can be re-expressed in purely Hopf algebra terms (with $x=a^k$) as

$$\begin{aligned}&\pi'_{\mathscr{L}^{pr}}(a^k\otimes Q)\\&\quad=(\hat{M}\circ(id\otimes\hat{M})\circ(\hat{\pi}'^{r}\otimes id\otimes\hat{\pi}'^{p})\circ(id\otimes\sigma)\circ(id\otimes S_{\mathscr{A}'}\otimes id)\circ(\Delta_{\mathscr{A}'}\otimes id))(a^k\otimes Q).\end{aligned} \tag{A15}$$

[Here the operator multiplication operation $\hat{M}$ is defined by $\hat{M}(Q\otimes Q')=Q\circ Q'$ for all $Q,Q'\in\mathscr{L}^{pr}$.] It is then easily demonstrated that $\pi'_{\mathscr{L}^{pr}}$ is a *left action* of $\mathscr{A}'$ with carrier space $\mathscr{L}^{pr}$.

After some algebra, it can be shown that (A15) can be rewritten in terms of components as

$$\pi'_{\mathscr{L}^{pr}}(a^k\otimes Q)=\sum_{i,j=1}^{d_p}\sum_{m,n=1}^{d_r}\langle a^k,M(\pi^{r}_{mn}\otimes S(\pi^{\ p}_{ij}))\rangle q_{ni}\mathscr{P}^{pr}_{jm}, \tag{A16}$$

where the operators $\mathscr{P}^{pr}_{bi}$ are defined in (14) and the matrix elements q_{ja} are defined in (17). The corresponding right coaction $\pi_{\mathscr{L}^{pr}}$ of $\mathscr{A}$ is then given [cf. (I.213)] by

$$\pi_{\mathscr{L}^{pr}}(Q)=\sum_k \pi'_{\mathscr{L}^{pr}}(a^k\otimes Q)\otimes a_k \tag{A17}$$

for all $Q\in\mathscr{L}^{pr}$, where $a_1,a_2,\ldots$ is the dual basis of $\mathscr{A}$. Thus, by (A16) and (A17),

$$\pi_{\mathscr{L}^{pr}}(Q)=\sum_{i,j=1}^{d_p}\sum_{m,n=1}^{d_r}(q_{ni}\mathscr{P}^{pr}_{jm})\otimes M(\pi^{\ r}_{mn}\otimes S(\pi^{\ p}_{ij})),$$

which is (32).

On replacing M by $M\circ\sigma$ and S by S^{-1}, the definition (32) changes into the definition (37) for $\tilde{\pi}_{\mathscr{L}^{pr}}$.

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Quaternions and special relativity

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We reformulate Special Relativity by a quaternionic algebra on reals. Using *real linear quaternions*, we show that previous difficulties, concerning the appropriate transformations on the 3+1 space–time, may be overcome. This implies that a complexified quaternionic version of Special Relativity is a choice and not a necessity. © *1996 American Institute of Physics.* [S0022-2488(96)01106-1]

I. INTRODUCTION

''*The most remarkable formula in mathematics is:*

$$e^{i\theta}=\cos\ \theta+i\ \sin\ \theta. \tag{1}$$

This is our jewel. We may relate the geometry to the algebra by representing complex numbers in a plane

$$x+iy=re^{i\theta}.$$

This is the unification of algebra and geometry.''—Feynman.[1]

We know that a rotation of α-angle around the z axis, can be represented by $e^{i\alpha}$, in fact,

$$e^{i\alpha}(x+iy)=re^{i(\theta+\alpha)}.$$

In 1843, Hamilton in the attempt to generalize the complex field in order to describe the rotation in the three-dimensional space, discovered quaternions. Quaternions, as used in this paper, will always mean ''real quaternions''

$$q=a+ib+jc+kd,\quad a,b,c,d\in\mathscr{R}.$$

Today a rotation about an axis passing trough the origin and parallel to a given unitary vector $\mathbf{u}\equiv(u_x,u_y,u_z)$ by an angle α can be obtained taking the transformation

$$e^{(iu_x+ju_y+ku_z)\alpha/2}(ix+jy+kz)e^{-(iu_x+ju_y+ku_z)\alpha/2}. \tag{2}$$

Therefore, if we wish to represent rotations in the three-dimensional space and complete ''*the unification of algebra and geometry*,'' we need quaternions.

The quaternionic algebra has been expounded in a series of papers[2] and books[3] with particular reference to quantum mechanics; the reader may refer to these for further details. For convenience we repeat and develop the relevant points in the following section, where the terminology is also defined.

Nothing that U(1,q) is algebraically isomorphic to SU(2,c), the imaginary units i,j,k can be realized by means of the 2×2 Pauli matrices through

$$(i,j,k)\leftrightarrow(i\sigma_3,-i\sigma_2,-i\sigma_1)$$

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(this particular representation of the imaginary units i,j,k has been introduced in Ref. 4). So a quaternion q can be represented by a 2×2 complex matrix

$$q\leftrightarrow\mathcal{Q}=\begin{pmatrix} z_1 & -z_2^* \\ z_2 & z_1^* \end{pmatrix}, \tag{3}$$

where

$$z_1=a+ib, \quad z_2=c-id\in\mathcal{C}(1,i),$$

$$z_1^*=a-ib, \quad z_2^*=c+id.$$

It follows that a quaternion with unitary norm is identified by a unitary 2×2 matrix with unit determinant. This gives the correspondence between unitary quaternions $\mathrm{U}(1,q)$ and $\mathrm{Su}(2,c)$ [in a recent paper[5] the representation theory of the group $\mathrm{U}(1,q)$ has been discussed in detail]. Let us consider the transformation law of a spinor (two-dimensional representations of the rotation group)

$$\psi'=\mathcal{U}\psi, \tag{4}$$

where

$$\psi=\begin{pmatrix} z_1 \\ z_2 \end{pmatrix}, \quad \mathcal{U}\in\mathrm{SU}(2,c).$$

We can immediately verify that

$$\tilde{\psi}=\begin{pmatrix} -z_2 \\ z_1 \end{pmatrix}$$

transforms as follows,

$$\tilde{\psi}'=\mathcal{U}^*\tilde{\psi}, \tag{5}$$

so

$$\begin{pmatrix} z_1 & -z_2^* \\ z_2 & z_1^* \end{pmatrix}'=\mathcal{U}\begin{pmatrix} z_1 & -z_2^* \\ z_2 & z_1^* \end{pmatrix}$$

represents again the transformation law of a spinor.

Thanks to the identification (3) we can write the previous transformations by real quaternions as follows

$$q'=\mathcal{U}q,$$

with $q=z_1+jz_2$ and $\mathcal{U}$ quaternion with unitary norm $[N(\mathcal{U})=\mathcal{U}^+\mathcal{U}=1]$. Note that we do not need right operators to indicate the transformation law of a spinor.

Now we can obtain the transformation law of a three-dimensional vector $\mathbf{r}\equiv(x,y,z)$ by product of spinors; in fact, if we consider the purely imaginary quaternion

$$\omega=qiq^+=ix+jy+kz, \quad (i,j,k)^+\equiv-(i,j,k),$$

or the corresponding traceless 2×2 complex matrix

$$\Omega = \psi i \psi^{+} = \begin{pmatrix} ix & -y - iz \\ y - iz & -ix \end{pmatrix},$$

a rotation in the three-dimensional space can be written as follows:[6]

$$\omega' = \mathscr{U}\omega\mathscr{U}^{+} \quad \text{(quaternions)},$$

$$\Omega' = \mathscr{U}\Omega\mathscr{U}^{+} \quad (2\times 2 \text{ complex matrices}).$$

For infinitesimal transformations, $\mathscr{U}=1+\mathbf{Q}\cdot\boldsymbol{\theta}$, we find

$$\mathbf{Q}\cdot\mathbf{r}' = \mathbf{Q}\cdot\mathbf{r} + \mathbf{Q}\cdot\boldsymbol{\theta}\,\mathbf{Q}\cdot\mathbf{r} - \mathbf{Q}\cdot\mathbf{r}\mathbf{Q}\cdot\boldsymbol{\theta},$$

where

$$\mathbf{Q}\equiv(i,j,k), \quad \boldsymbol{\theta}\equiv(\alpha,\beta,\gamma).$$

If we rewrite the above mentioned transformation in the following form,

$$\mathbf{Q}\cdot\mathbf{r}' = [1 + \boldsymbol{\theta}\cdot(\mathbf{Q} - 1|\mathbf{Q})]\mathbf{Q}\cdot\mathbf{r}, \tag{6}$$

barred operators $\mathscr{O}|q$ act on quaternionic objects Φ as in $(\mathscr{O}|q)\Phi=\mathscr{O}\Phi q$.
We identify

$$\frac{i-1|i}{2}, \quad \frac{j-1|j}{2}, \quad \frac{k-1|k}{2},$$

as the generators for rotations in the three-dimensional space. The factor $\frac{1}{2}$ guarantees that our generators satisfy the usual algebra:

$$[A_m, A_n] = \epsilon_{mnp}A_p, \quad m,n,p = 1,2,3.$$

Up until now, we have considered only particular operations on quaternions. A quaternion q can also be multiplied by unitary quaternions $\mathscr{V}$ from the right. A possible transformation which preserves the norm is given by

$$q' = \mathscr{U}q\mathscr{V}, \quad (\mathscr{U}^{+}\mathscr{U} = \mathscr{V}^{+}\mathscr{V} = 1). \tag{7}$$

Since left and right multiplications commute, the group is locally isomorphic to SU(2)×SU(2), and so to O(4), the four-dimensional Euclidean rotation group.

As far as here we can recognize only particular real linear quaternions, namely,

$$1, \quad i, \quad j, \quad k, \quad 1|i, \quad 1|j, \quad 1|k.$$

Real linear and complex linear quaternion operators were first systematically discussed in the paper by Horwitz and Biedenharn.[7]

We have to hope of describing the Lorentz group if we use only previous objects. Analyzing the most general transformation on quaternions (see Sec. IV), we introduce new real linear quaternions which allow us to overcome the above difficulty and so obtain a quaternionic version of the Lorentz group, without the use of complexified quaternions. This result appears, to the best of our knowledge, for the first time in print.

First we briefly recall the standard way to rewrite special relativity by a quaternionic algebra on complex (see Sec. III).

In Sec. V, we present a quaternionic version of the special group SL(2,c), which is as well-known collected to the Lorentz group. Our conclusions are drawn in the final section.

II. QUATERNIONIC ALGEBRAS

A quaternionic algebra over a field $\mathscr{F}$ is a set

$$\mathscr{H}=\{\alpha+i\beta+j\gamma+k\delta|\,\alpha,\beta,\gamma,\delta\in\mathscr{F}\},$$

with multiplication operations defined by following rules for imaginary units i,j,k:

$$i^2=j^2=k^2=-1,\quad jk=-kj=i,\quad ki=-ik=j,\quad ij=-ji=k.$$

In our paper we will work with quaternionic algebras defined on reals and complex, so in this section we give a panoramic review of such algebras.

We start with a quaternionic algebra on reals

$$\mathscr{H}_R=\{\alpha+i\beta+j\gamma+k\delta|\,\alpha,\beta,\gamma,\delta\in\mathscr{R}\}.$$

We introduce the quaternion conjugation denoted by $^+$ and defined by

$$q^+=\alpha-i\beta-j\gamma-k\delta.$$

The previous definition implies

$$(\psi\varphi)^+=\varphi^+\psi^+,$$

for ψ, φ quaternionic functions. A conjugation operation which does not reverse the order of ψ, φ factors is given, for example, by

$$\tilde{q}=\alpha-i\beta+j\gamma-k\delta.$$

An important difference between quaternions and complexified quaternions, as remarked by Adler in his recent book[8] (pag. 8), is based on the concept of *division algebra*, which is a finite-dimensional algebra for which $a\neq0$, $b\neq0$ implies $ab\neq0$, in others words, which has no nonzero divisors of zero. A classical theorem[9] states that the only division algebras over the reals are algebras of dimension 1, 2, 4, and 8; the only associative algebras over the reals are $\mathscr{R}$, $\mathscr{C}$, and $\mathscr{H}_{\mathscr{R}}$;[10] the nonassociative division algebras include the octonions $\mathscr{O}$ (but there are others as well; see Ref. 11).

A simple example of a *nondivision* algebra is provided by the algebra of complexified quaternions

$$\mathscr{H}_{\mathscr{C}}=\{\alpha+i\beta+j\gamma+k\delta|\,\alpha,\beta,\gamma,\delta\in\mathscr{C}(1,\mathscr{I})\},$$

$$[\mathscr{I},\,i]=[\mathscr{I},\,j]=[\mathscr{I},\,k]=0.$$

In fact, since

$$(1+i\mathscr{I})(1-i\mathscr{I})=0,$$

there are nonzero divisors of zero.

For complexified quaternions we have different opportunities to define conjugation operations; we shall use the following terminology:

(1) The *complex* conjugate of $q_{\mathscr{C}}$ is

$$q_{\mathbb{C}}^{*}=\alpha^{*}+i\beta^{*}+j\gamma^{*}+k\delta^{*}.$$

Under this operation

$$(\mathscr{I},i,j,k)\rightarrow(-\mathscr{I},i,j,k)$$

and

$$(q_{\mathbb{C}}p_{\mathbb{C}})^{*}=q_{\mathbb{C}}^{*}p_{\mathbb{C}}^{*}.$$

(2) The *quaternion* conjugate of $q_{\mathbb{C}}$ is

$$q_{\mathbb{C}}^{\star}=\alpha-i\beta-j\gamma-k\delta.$$

Here

$$(\mathscr{I},i,j,k)\rightarrow(\mathscr{I},-i,-j,-k)$$

and

$$(q_{\mathbb{C}}p_{\mathbb{C}})^{\star}=p_{\mathbb{C}}^{\star}q_{\mathbb{C}}^{\star}.$$

(3) In the absence of standard terminology, we call that formed by combining these operations the *full* conjugate:

$$q_{\mathbb{C}}^{+}=\alpha^{*}-i\beta^{*}-j\gamma^{*}-k\delta^{*}.$$

Under this operation

$$(\mathscr{I},i,j,k)\rightarrow-(\mathscr{I},i,j,k)$$

and

$$(q_{\mathbb{C}}p_{\mathbb{C}})^{+}=p_{\mathbb{C}}^{+}q_{\mathbb{C}}^{+}.$$

Note that for real quaternions we have

$$q^{\star}\equiv q^{+}.$$

III. COMPLEXIFIED QUATERNIONS AND SPECIAL RELATIVITY

We begin this section by recalling a sentence of Anderson and Joshi[12] about the quaternionic reformulation of special relativity:

''There has been a long tradition of using quaternions for Special Relativity... The use of quaternions in special relativity, however, is not entirely straightforward. Since the field of quaternions is a four-dimensional Euclidean space, complex components for the quaternions are required for the 3+1 space–time of special relativity.''

In the following section, we will demonstrate that a reformulation of special relativity by a quaternionic algebra on reals is possible.

In the present section, we use complexified quaternions to reformulate special relativity (for further details the reader may consult the papers of Edmonds,[13] Gough,[14] Abonyi,[15] Gürsey,[16] and the book of Synge[17]).

A space–time point can be represented by complexified quaternions as follows:

$$\mathscr{X}=\mathscr{I}ct+ix+jy+kz. \tag{8}$$

The Lorentz invariant in this formalism is given by

$$\mathscr{X}^{*}.\mathscr{X}=(ct)^2-x^2-y^2-z^2. \tag{9}$$

If we consider the standard Lorentz transformation (boost $ct-x$)

$$ct'=\gamma(ct-\beta x),\quad x'=\gamma(x-\beta ct),\quad y'=y,\quad z'=z$$

and note that the first two equations may be rewritten as

$$ct'=ct\ \cosh\ \theta-x\ \sinh\ \theta,$$

$$x'=x\ \cosh\ \theta-ct\ \sinh\ \theta,$$

where $\cosh\ \theta=\gamma$ and $\sinh\ \theta=\beta\gamma$.

We can represent an infinitesimal transformation by

$$\mathscr{X}'=\mathscr{T}(ct-x\theta)+i(x-ct\theta)+jy+kz=\mathscr{X}+\mathscr{T}\frac{i+1|i}{2}\ \theta.\mathscr{X}.$$

We thus recognize, in the previous transformation, the generator

$$\mathscr{T}\frac{i+1|i}{2}.$$

It is now very simple to complete the translation. The set of generators of the Lorentz group is provided with

$$\text{boost}\ \ (ct,x)\quad \mathscr{T}\frac{i+1|i}{2},$$

$$\text{boost}\ \ (ct,y)\quad \mathscr{T}\frac{j+1|j}{2},$$

$$\text{boost}\ \ (ct,z)\quad \mathscr{T}\frac{k+1|k}{2},$$

$$\text{rotation around}\ \ x\quad \frac{i-1|i}{2},$$

$$\text{rotation around}\ \ y\quad \frac{j-1|j}{2},$$

$$\text{rotation around}\ \ z\quad \frac{k-1|k}{2}.$$

Therefore a general finite Lorentz transformation is given by

$$e^{\mathscr{T}(i\alpha_b+j\beta_b+k\gamma_b)+i\alpha_r+j\beta_r+k\gamma_r}(\mathscr{T}ct+ix+jy+kz)e^{\mathscr{T}(i\alpha_b+j\beta_b+k\gamma_b)-i\alpha_r-j\beta_r-k\gamma_r}.$$

The previous results can be elegantly summarized by the relation

$$\mathscr{X}'=\Lambda.\mathscr{X}\Lambda^{+},\quad \Lambda^{*}\Lambda=1, \tag{10}$$

where Λ is obviously a complexified quaternion. In this or a similar way many authors have reformulated special relativity with complex quaternions.

We remark that the complex component for the quaternions represent a choice and not a necessity.

IV. A NEW POSSIBILITY

We think that quaternions are the natural candidates to describe special relativity. It is simple to understand why: quaternions are characterized by four real numbers (whereas complexified quaternions by eight), thus we can collect these four real quantities with a point (ct,x,y,z) in the space–time. In quaternionic notation we have

$$\mathscr{X}=ct+ix+jy+kz. \tag{11}$$

In the first section we have introduced particular *real linear quaternions*, namely,

$$1, \quad \mathbf{Q}, \quad 1|\mathbf{Q},$$

where

$$\mathbf{Q}\equiv(i,j,k).$$

In order to write the most general real linear quaternions we must consider the following quantities:

$$\mathbf{Q}|i, \quad \mathbf{Q}|j, \quad \mathbf{Q}|k.$$

In fact, the most general transformation on quaternions is represented by

$$q+p|i+r|j+s|k, \tag{12}$$

with

$$q,p,r,s\in\mathscr{H}_{\mathscr{R}}.$$

New objects like

$$k|j, \quad j|k, \quad i|k, \quad k|i, \quad j|i, \quad i|j$$

will be essential to reformulate special relativity with real quaternions. They represent the wedges which permit us to overcome the difficulties which in the past did not allow a (real) quaternionic version of special relativity.

Returning to Lorentz transformations, let us start with the following infinitesimal transformation (boost $ct-x$):

$$\mathscr{X}'=ct-x\theta+i(x-ct\theta)+jy+kz=\mathscr{X}+\frac{k|j-j|k}{2}\,\theta\mathscr{X}.$$

We can immediately note that the generator which substitutes

$$\mathscr{I}\,\frac{i+1|i}{2}$$

is

$$\frac{k|j-j|k}{2}.$$

So we have the possibility of listing the generators of the Lorentz group without the need to work with complexified quaternions:

$$\text{boost } (ct,x) \quad \frac{k|j-j|k}{2},$$

$$\text{boost } (ct,y) \quad \frac{i|k-k|i}{2},$$

$$\text{boost } (ct,z) \quad \frac{j|i-i|j}{2},$$

$$\text{rotation around } x \quad \frac{i-1|i}{2},$$

$$\text{rotation around } y \quad \frac{j-1|j}{2},$$

$$\text{rotation around } z \quad \frac{k-1|k}{2}.$$

In Appendix A we explicitly prove that the action of previous generators leaves

$$\text{Re } \mathscr{Q}^2=(ct)^2-x^2-y^2-z^2 \tag{13}$$

invariant.

In Appendix B we will give an alternate but equivalent presentation of special relativity by a quaternionic algebra on reals. There we introduce a real linear quaternion g which substitutes the metric tensor $g^{\mu\nu}$.

V. A QUATERNIONIC VERSION OF THE COMPLEX GROUP SL(2)

In analogy to the connection between the rotation group O(3) to the special unitary group SU(2), there is a natural correspondence[18] between the Lorentz group O(3,1) and the special linear group SL(2). In fact, SL(2) is the universal covering group of O(3,1) in the same way that SU(2) is of O(3).

The aim of this Section is to give, by extending the consideration with which we collect the special unitary group SU(2) with unitary real quaternions (as shown in Sec. I), a quaternionic version of the special linear group SL(2). Once more the aim will be achieved with help of real linear quaternions.

A Lorentz spinor is a complex object which transforms under Lorentz transformations as

$$\psi'=\mathscr{A}\psi,$$

where $\mathscr{A}$ is a SL(2) matrix. When we restrict ourselves to the three-dimensional space and to rotations, this definition gives the usual Pauli spinors

$$\psi'=\mathscr{U}\psi,$$

where $\mathscr{U}$ is a SU(2) matrix.

Now we shall derive the generators of rotations and Lorentz boosts in the spinor representation by using real linear quaternions.

The action of generators of the special group SL(2),

$$\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}, \quad \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}, \quad \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

on the spinor

$$\psi = \begin{pmatrix} \xi \\ \eta \end{pmatrix}$$

can be represented by the action of real linear quaternions

$$i, \quad j, \quad k, \quad i|i, \quad j|i, \quad k|i$$

on the quaternion

$$q = \xi + j\,\eta.$$

In Sec. I we have obtained a three-dimensional vector (x,y,z) by product of Pauli spinors $q_{\mathscr{P}}$:

$$q_{\mathscr{P}}\, i q_{\mathscr{P}}^{+} = ix + jy + kz \quad (q'_{\mathscr{P}} = \mathscr{U} q_{\mathscr{P}}, \quad \mathscr{U}^{+}\mathscr{U} = 1).$$

Consequently, we have written its transformation law as follows:

$$(q_{\mathscr{P}}\, i q_{\mathscr{P}}^{+})' = \mathscr{U} q_{\mathscr{P}} i q_{\mathscr{P}}^{+} \mathscr{U}^{+}.$$

Now we start with a Lorentz spinor $q_{\mathscr{L}}$

$$q'_{\mathscr{L}} = \mathscr{A} q_{\mathscr{L}},$$

and construct a four-vector (ct,x,y,z) by-product of such spinors:

$$q_{\mathscr{L}}(1+i)q_{\mathscr{L}}^{+} = ct + ix + jy + kz.$$

The transformation law is then given by

$$(q_{\mathscr{L}}(1+i)q_{\mathscr{L}}^{+})' = (\mathscr{A} q_{\mathscr{L}})(1+i)(\mathscr{A} q_{\mathscr{L}})^{+}.$$

If we consider infinitesimal transformations

$$\mathscr{A} = 1 + \frac{\mathbf{Q}}{2} \cdot (\boldsymbol{\theta} + \boldsymbol{\zeta} | i),$$

with $\boldsymbol{\theta} \equiv (\alpha,\beta,\gamma)$ and $\boldsymbol{\zeta} \equiv (\tilde{\alpha},\tilde{\beta},\tilde{\gamma})$,
we have

$$\mathscr{T}' = \mathscr{T} + \frac{\alpha}{2}[i, \mathscr{T}] + \frac{\beta}{2}[j, \mathscr{T}] + \frac{\gamma}{2}[k, \mathscr{T}] + \frac{\tilde{\alpha}}{2}\{i, \tilde{\mathscr{T}}\} + \frac{\tilde{\beta}}{2}\{j, \tilde{\mathscr{T}}\} + \frac{\tilde{\gamma}}{2}\{k, \tilde{\mathscr{T}}\},$$

where

$$\mathscr{T}=q_{\mathscr{Z}}(1+i)q_{\mathscr{Z}}^{+}$$

and

$$\tilde{\mathscr{T}}=q_{\mathscr{Z}}i(1+i)q_{\mathscr{Z}}^{+}=\mathscr{T}-2q_{\mathscr{Z}}q_{\mathscr{Z}}^{+}.$$

In order to simplify next considerations we pose

$$\mathscr{T}=ix+jy+kz+ct=.\mathscr{T}_i+.\mathscr{T}_j+.\mathscr{T}_k+.\mathscr{T}_1,$$

$$\tilde{\mathscr{T}}=ix+jy+kz-ct=.\mathscr{T}_i+.\mathscr{T}_j+.\mathscr{T}_k-.\mathscr{T}_1,$$

so the standard Lorentz transformations are given by

$$.\mathscr{T}_1\to.\mathscr{T}_1+\tilde{\alpha}i.\mathscr{T}_i+\tilde{\beta}j.\mathscr{T}_j+\tilde{\gamma}k.\mathscr{T}_k,\quad .\mathscr{T}_i\to.\mathscr{T}_i-\tilde{\alpha}i.\mathscr{T}_1+\beta j.\mathscr{T}_k-\gamma k.\mathscr{T}_j,$$

$$.\mathscr{T}_j\to.\mathscr{T}_j-\tilde{\beta}j.\mathscr{T}_1-\alpha i.\mathscr{T}_k+\gamma k.\mathscr{T}_i,\quad .\mathscr{T}_k\to.\mathscr{T}_k-\tilde{\gamma}k.\mathscr{T}_1+\alpha i.\mathscr{T}_j-\beta j.\mathscr{T}_i.$$

In this way we obtain a quaternionic version of the special group SL(2) and demonstrate (in contrast with the opinion of Penrose)[6] that, if real linear quaternions appear, a ''trick'' similar to that one of rotations works to relate the full four-vector (ct,x,y,z) with real quaternions.

VI. CONCLUSIONS

The study of special relativity with a quaternionic algebra on reals has yielded a result of interest. While we cannot demonstrate in this paper that one number system (quaternions) is preferable to another (complexified quaternions), we have pointed out the advantages of using real linear quaternions which naturally appear when we work with a noncommutative number system, such as the quaternionic field. As seen in this paper these objects are very useful if we wish to rewrite special relativity by a quaternionic algebra on reals. The complexified quaternionic reformulation of special relativity is thus a choice and not a necessity. This affirmation is in contrast with the standard folklore (see, for example, Ref. 12).

Our principal aim in this work is to underline the potentialities of real linear quaternions. We wish to remember that many difficulties have been overcome thanks to these objects (which in our colorful language we have named generalized objects).[4]

To remark on their potentialities let us list the situations which have requested their use.

(i) The need of such objects naturally appears, for example, in the construction of quaternion group theory and tensor product group representations.[5] Also starting with only standard quaternions i,j,k in order to represent the generators of the group U(1,q), we find generalized quaternions when we analyze quaternionic tensor products.

$$\text{Spin } \frac{1}{2} \text{ generators: } \quad \frac{i}{2},\quad \frac{j}{2},\quad \frac{k}{2}.$$

$$\text{Spin } 1\oplus 0 \text{ generators: } \begin{pmatrix} \dfrac{i+1|i}{2} & 0 \\ 0 & \dfrac{i-1|i}{2} \end{pmatrix},\quad \begin{pmatrix} j & 1|i \\ 1|i & j \end{pmatrix},\quad \begin{pmatrix} k & -1 \\ 1 & k \end{pmatrix}.$$

(ii) If we desire to extend the isomorphism of SU(2,c) with U(1,q) to the group U(2,c), we must introduce the additional real linear quaternion ''$1|i$.'' In this way there exists at least one

version of quaternionic quantum mechanics in which a ''partial'' set of translations may be defined;[4] in fact, thanks to real linear operators, a translation between $2n\times 2n$ complex and $n\times n$ quaternionic matrices is possible.

(iii) In the work of Ref. 19 a quaternion version of the Dirac equation was derived in the form

$$\gamma_\mu \partial^\mu \psi i = m\psi,$$

where the γ_μ are two-by-two quaternionic matrices satisfying the Dirac condition

$$\{\gamma_\mu, \gamma_\nu\} = 2g_{\mu\nu}.$$

In Rotelli's formalism the momentum operator must be defined as

$$p^\mu = \partial^\mu |i,$$

which is also a generalized object.

(iv) In this paper, contrary to the common opinion, we have given a real quaternionic formulation of special relativity. In order to obtain that, we have introduced the following real linear quaternions:

$$\mathbf{Q}|i, \quad \mathbf{Q}|j, \quad \mathbf{Q}|k, \quad \mathbf{Q}\equiv(i,j,k).$$

A quaternionic version of the special group SL(2) has also been given.

We finally note that the process of generalization can be extended also to complexified quaternions. In a recent paper[20] we gave an elegant one-component formulation of the Dirac equation and, thanks to our generalization, we overcame previous difficulties concerning the doubling of solutions[12–14] in the complexified quaternionic Dirac equation.

In seeking a better understanding of the success of mathematical abstraction in physics and in particular of the wide applicability of quaternionic numbers in theories of physical phenomena, we found that generalized quaternions should *not* be undervalued. We think that there are good reasons to hope that these generalized structures provide new possibilities concerning physical applications of quaternions.

''The most powerful method of advance that can be suggested at present is to employ all the resources of pure mathematics in attempts to perfect and generalize the mathematical formalism that forms the existing basis of theoretical physics, and after each success in this direction, to try to interpret the new mathematical features in terms of physical entities...''—Dirac.[21]

APPENDIX A: QUATERNIONIC LORENTZ INVARIANT

In this Appendix we prove that the Lorentz invariant[8] is

$$\mathrm{Re}\ \mathscr{X}'^2 = \mathrm{Re}\ \mathscr{X}^2, \tag{A1}$$

where

$$\mathscr{X} = ct + ix + jy + kz.$$

Under an infinitesimal transformation, we have

$$\mathscr{X}' = \left(1 + \theta\,\frac{k|j - j|k}{2} + \alpha\,\frac{i-1|i}{2} + \cdots\right)\mathscr{X},$$

so, neglecting second-order terms,

$$\mathscr{X}'^2=\mathscr{X}^2+\frac{\theta}{2}\{\mathscr{X},k\mathscr{X}j-j\mathscr{X}k\}+\frac{\alpha}{2}\{\mathscr{X},i\mathscr{X}-\mathscr{X}i\}+\cdots .$$

Equation (14) is then satisfied since

$$\{\mathscr{X},i\mathscr{X}-\mathscr{X}i\}=(i-1|i)\mathscr{X}^2,$$

$$\{\mathscr{X},k\mathscr{X}j-j\mathscr{X}k\}=(1|j-j)\mathscr{X}k\mathscr{X}+(k-1|k)\mathscr{X}j\mathscr{X}$$

are purely imaginary quaternions.

Obviously we can derive the generators of the Lorentz group by starting from the infinitesimal transformation

$$\mathscr{X}'=\mathscr{X}+\mathscr{A}\mathscr{X}$$

and imposing that they satisfy the relation

$$\mathrm{Re}\{\mathscr{X},\mathscr{A}\mathscr{X}\}=0$$

$$(\mathrm{Re}\,\mathscr{X}'^2=\mathrm{Re}\,\mathscr{X}^2\Rightarrow\mathrm{Re}\{\mathscr{X},\mathscr{A}\mathscr{X}\}=0). \tag{A2}$$

With straightforward mathematical calculus we can find the generators requested. In order to simplify the following considerations let us pose

$$\mathscr{X}=a+ib+jc+kd,\quad \mathscr{A}=q_0+q_1|i+q_2|j+q_3|k$$

where $q_m=\alpha_m+i\beta_m+j\gamma_m+k\delta_m$ $(m=0,1,2,3)$ are real quaternions.

The only quantities which we must calculate are

$$\mathrm{Re}\{\mathscr{X},\mathscr{X}\},\quad \mathrm{Re}\{\mathscr{X},i\mathscr{X}i\},\quad \mathrm{Re}\{\mathscr{X},i\mathscr{X}\},\quad \mathrm{Re}\{\mathscr{X},k\mathscr{X}j\};$$

in fact, the other quantities can be obtained from previous ones, by simple manipulations:

$$\mathrm{Re}\{\mathscr{X},\mathscr{X}\}=2(+a^2-b^2-c^2-d^2),\quad \mathrm{Re}\{\mathscr{X},i\mathscr{X}i\}=2(-a^2+b^2-c^2-d^2),$$

$$\mathrm{Re}\{\mathscr{X},j\mathscr{X}j\}=2(-a^2-b^2+c^2-d^2),\quad \mathrm{Re}\{\mathscr{X},k\mathscr{X}k\}=2(-a^2-b^2-c^2+d^2),$$

$$\mathrm{Re}\{\mathscr{X},i\mathscr{X}\}=\mathrm{Re}\{\mathscr{X},\mathscr{X}i\}=-4ab,\quad \mathrm{Re}\{\mathscr{X},k\mathscr{X}j\}=\mathrm{Re}\{\mathscr{X},j\mathscr{X}k\}=4cd,$$

$$\mathrm{Re}\{\mathscr{X},j\mathscr{X}\}=\mathrm{Re}\{\mathscr{X},\mathscr{X}j\}=-4ac,\quad \mathrm{Re}\{\mathscr{X},j\mathscr{X}i\}=\mathrm{Re}\{\mathscr{X},i\mathscr{X}j\}=4bc,$$

$$\mathrm{Re}\{\mathscr{X},k\mathscr{X}\}=\mathrm{Re}\{\mathscr{X},\mathscr{X}k\}=-4ad,\quad \mathrm{Re}\{\mathscr{X},i\mathscr{X}k\}=\mathrm{Re}\{\mathscr{X},k\mathscr{X}i\}=4bd.$$

The previous relations imply the following conditions on the real parameters of the generator $\mathscr{A}$:

$$\alpha_0=0,\quad \beta_1=0,$$

$$\gamma_2=0,\quad \delta_3=0,$$

$$\beta_0=-\alpha_1=\alpha,\quad \gamma_0=-\alpha_2=\beta,$$

$$\delta_0=-\alpha_3=\gamma,\quad \delta_2=-\gamma_3=\theta,$$

$$\gamma_1=-\beta_2=\varphi,\quad \beta_3=-\delta_1=\eta.$$

We can immediately recognize the Lorentz generators given in Sec. IV.

APPENDIX B: QUATERNIONIC METRIC TENSOR

We introduce the usual four-vector x^μ by the following quaternion,

$$\mathscr{X}=x^0+ix^1+jx^2+kx^3,$$

and define a scalar product of two vectors $\mathscr{X}$, $\mathscr{Y}$ by

$$(\mathscr{X},g\mathscr{Y})_{\mathscr{R}}=\mathrm{Re}(\mathscr{X}^{+}g\mathscr{Y})=x^\mu g_{\mu\nu}y^\nu, \tag{B1}$$

where g is the generalized quaternion

$$-\tfrac{1}{2}(1+i|i+j|j+k|k).$$

We can define a real norm (or metric)

$$(\mathscr{X},g\mathscr{X})_{\mathscr{R}}=\mathrm{Re}(\mathscr{X}^{+}g\mathscr{X})=x^\mu g_{\mu\nu}x^\nu.$$

The vectors which transform under a Lorentz transformation $\mathscr{L}$ will be denoted by

$$\mathscr{X}'=\mathscr{L}\mathscr{X},$$

with $\mathscr{L}$ real linear operators [see Eq. (12)]. From the postulated invariance of the norm we can deduce the generators of Lorentz group.

If we consider infinitesimal transformations

$$\mathscr{L}=1+\mathscr{A},$$

we have

$$\mathrm{Re}(\mathscr{X}'^{+}g\mathscr{X}')=\mathrm{Re}(\mathscr{X}^{+}g\mathscr{X}+\mathscr{X}^{+}(\mathscr{A}^{+}g+g\mathscr{A})\mathscr{X})=\mathrm{Re}(\mathscr{X}^{+}g\mathscr{X}),$$

and therefore

$$\mathscr{A}^{+}g+g\mathscr{A}=0. \tag{B2}$$

Using real scalar products, given an operator

$$\mathscr{A}=q+p|i+r|j+s|k,\quad q,p,r,s\in\mathscr{H}_{\mathscr{R}},$$

we can write its Hermitian conjugate as follows:

$$\mathscr{A}^{+}=q^{+}-p^{+}|i-r^{+}|j-s^{+}|k.$$

Then Eq. (17) can be rewritten as

$$g\mathscr{A}+h.c.=0.$$

If we pose

$$g\mathscr{A}=B=\tilde{q}+\tilde{p}|i+\tilde{r}\,|j+\tilde{s}\,|k,$$

we obtain the following conditions on the operator B:

$$\mathrm{Re}\;\tilde{q}=\mathrm{Vec}\;\tilde{p}=\mathrm{Vec}\;\tilde{r}=\mathrm{Vec}\;\tilde{s}=0.$$

Noting that $\mathscr{A}=gB$ we can quickly write the generators of Lorentz group. We give explicitly an example

$$\mathscr{A}_1=g(1|i)=-\tfrac{1}{2}(-i+1|i+j|k-k|j),$$

$$\mathscr{A}_2=gi=-\tfrac{1}{2}(i-1|i+j|k-k|j),$$

$$\mathscr{A}=\mathscr{A}_1-\mathscr{A}_2=\frac{i-1|i}{2},\quad \tilde{\mathscr{A}}=\mathscr{A}_1+\mathscr{A}_2=\frac{k|j-j|k}{2}.$$

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Simple waves and invariant solutions of quasilinear systems

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The solutions of a system of homogeneous first-order quasilinear evolution equations for which the propagation velocity depends only on the field value are characterized by their invariance under a particular type of flow. All simple wave solutions are shown to have this property. The local images of simple wave solutions are the integral curves of a system of ordinary differential equations on the field space. The model for barotropic compressible flow is an example of a system that has invariant solutions of higher rank. A solution of this system is invariant under the flow of the convective derivative if and only if it is divergence-free. The evolution of initial data is shown to be divergence-free if and only if its differential is nilpotent. © *1996 American Institute of Physics.* [S0022-2488(96)02006-3]

I. INTRODUCTION

In this paper we study systems of differential equations of the form

$$\frac{\partial u^\alpha}{\partial t}+\sum_{i=1}^{n}\sum_{\beta=1}^{q} A_\beta^{i\alpha}(u)\,\frac{\partial u^\beta}{\partial x^i}=0,\quad \alpha=1,\ldots,q. \tag{1.1}$$

in $p=n+1$ independent variables t, $x^1,\ldots,x^n$ and q dependent variables $u^1,\ldots,u^q$. We write (1.1) as a vector equation,

$$\frac{\partial u}{\partial t}+A^1(u)\,\frac{\partial u}{\partial x^1}+\cdots+A^n(u)\,\frac{\partial u}{\partial x^n}=0,$$

or simply

$$\left(\frac{\partial}{\partial t}+A(u)\cdot\,\frac{\partial}{\partial x}\right)u=0, \tag{1.2}$$

where $A^1,\ldots,A^n$ are $q\times q$ matrix functions. The equation (1.2) is a system of coupled homogeneous first-order quasilinear evolution equations, typical of those encountered in fluid dynamics.[1–3] A function $u(t,x)$ is a q-component field defined on an n-dimensional spatial domain parametrized by coordinates $x^1,\ldots,x^n$, evolving according to a time parameter t. The identification of a function $u(t,x)$ with its graph $\{(t,x,u(t,x))\}$ is a local correspondence between functions and p-dimensional submanifolds of $\mathbb{R}^p\times\mathbb{R}^q$ transverse to the projection onto $\mathbb{R}^p$. The equation (1.2) is a geometric condition on the tangent spaces of the submanifold. Its form is invariant under arbitrary change of field variables and affine change of space variables.

In this work all manifolds, functions, and transformations are C^∞ and all considerations are local. The equation (1.2) is autonomous and translation invariant, so we restrict our attention to solutions $u(t,x)$ defined on a neighborhood of the point $t=0$, $x=0$. The relevant initial value problem consists of solving (1.2) subject to initial data defined on an open subset of the hyper-

plane $t=0$. For sufficiently small initial data there exists a time interval $[0,T]$ in which a gradient catastrophe for the solution of (1.2) does not occur and the solution does not blow up.[4–6] This fact makes it possible to use the method of characteristics to solve the problems of propagation and nonlinear superposition of waves over the time interval $[0,T]$. Using this method, existence, uniqueness, and the continuous dependence of solutions on initial data have been proved by many authors.[7–9] However, the results thus far obtained are mainly limited to hyperbolic systems with two independent variables. In this case the solution was constructed in the entire domain, where its existence was expected.

Exhibiting generic solutions of (1.2) is practically impossible, except for the characteristic equations discussed in Sec. II. A characteristic equation is simply an invariance condition, and its general solution is easily described in the implicit form. This suggests that we look for invariant solutions of the general equation (1.2). We discuss this approach in Sec. III. In Sec. IV all rank 1 solutions of the general equation are shown to be invariant. The equations that model barotropic compressible flow are discussed in Sec. V, as an example of a system with higher rank invariant solutions.

II. CHARACTERISTIC EQUATIONS

The simplest equations (1.2) are those with scalar matrices. This is always the case if $q=1$. If $A^1=a^1I,\ldots,A^n=a^nI$, where I is the $q\times q$ identity matrix, then (1.2) is the *characteristic* equation,

$$\left(\frac{\partial}{\partial t}+a(u)\cdot\frac{\partial}{\partial x}\right)u=0, \tag{2.1}$$

of the vector field

$$V=\frac{\partial}{\partial t}+a(u)\cdot\frac{\partial}{\partial x}, \tag{2.2}$$

on the space $\{(t,x,u)\}$ of independent and dependent variables. A function $u(t,x)$ is a solution of (2.1) if and only if V is tangent to its graph $\{(t,x,u(t,x))\}$, i.e., if and only if its graph is locally invariant under the flow of V. The independent invariants,

$$x^1-a^1(u)t,\ldots,x^n-a^n(u)t,u^1,\ldots,u^q,$$

of V provide a complete local description of the invariant submanifolds. We find that the local solutions of (2.1) near $t=0$ are defined implicitly by the equations

$$u=f(x-a(u)t), \tag{2.3}$$

where $f:\mathbb{R}^n\to\mathbb{R}^q$ is an arbitrary locally defined function. The general solution (2.3) of the characteristic equation (2.1) is well known.[10] Note that for each function f there is a unique solution $u=u(t,x)$ of (2.3) defined near $t=0$ with $u(0,x)=f(x)$ on the domain of f. Thus the initial value problem for (2.1) has a unique solution. Geometrically, the solution manifold is foliated by the trajectories of V, i.e., by the characteristic lines $t\mapsto(t,x+a(u)t,u)$. In physical terms, the initial signal $f(x)$ propagates through space at constant velocity $dx/dt=a(f(x))$. Note that V is a trivial symmetry of its characteristic equation in that the flow of V carries any solution manifold of (2.1) into itself, by construction.

III. THE GENERAL PROBLEM

The equation (1.2) is less tractable when the matrices $A^1,\ldots,A^n$ are not scalar. We look for solutions that are invariant under a vector field (2.2), i.e., for solutions given implicitly by an equation (2.3). Geometrically, we want solution manifolds of (1.2) that are foliated by the char-

acteristic lines of a vector field with the special form (2.2). In physical terms, we want solutions of (1.2) for which the signal propagation velocity depends only on the field value. Analytically, we want solutions of the overdetermined system,

$$\left(\frac{\partial}{\partial t}+A(u)\cdot\frac{\partial}{\partial x}\right)u=0,\quad \left(\frac{\partial}{\partial t}+a(u)\cdot\frac{\partial}{\partial x}\right)u=0, \tag{3.1}$$

for some functions $a^1,\ldots,a^n$.

For arbitrary functions a there is no reason to expect that the system (3.1) has any nonconstant solutions, i.e., for an arbitrary vector field (2.2) there is no reason to expect that the original equation (1.2) has nonconstant V-invariant solutions. The problem is to find vector fields (2.2) that are compatible with the equation (1.2) in the sense that nonconstant V-invariant solutions exist. The invariance condition (2.1) imposes constraints on initial data so that its unique evolution along the flow of V will be a solution of (1.2). For example, if the components a of V are constant then V is a symmetry of (1.2), and the constraint on initial data is simply a classical symmetry reduction of (1.2). The resulting invariant solutions are unidirectional waves propagating at constant velocity a, independent of the field value. In general, there is no certainty that nonconstant solutions of this type exist. We are not even assured the existence of nonconstant stationary solutions of (1.2) (the case $a=0$), e.g., consider the case $n=1$ where A is nonsingular. If V is not a symmetry of (1.2) then the constraint on initial data obtained by adjoining all compatibility conditions of the overdetermined system (3.1) is called a weak symmetry reduction,[11–13] because V is a (trivial) symmetry of the entire system of evolution equations and compatibility conditions. We do not yet have a satisfactory understanding of the compatibility conditions in the general case.

The *rank* of a function $u(t,x)$ at a point of its domain is the rank of its differential there, as a linear map from $\mathbb{R}^p$ to $\mathbb{R}^q$. For example, the rank of the solution (2.3) of the characteristic equation (2.1) is equal to the rank of the initial data f, hence is at most equal to $\min(n,q)$ at each point of its domain. Note that invariance ensures that its rank is less than p. The rank of a function is generically constant, so we restrict ourselves to functions with constant rank. The local image of a function with constant rank m is an m-dimensional manifold: the local image of a rank 0 function is a point, the local image of a rank 1 function is a curve, the local image of a rank 2 function is a surface, etc. The rank 0 functions are trivial solutions of (1.2), invariant under any vector field (2.2). We show in Theorem 1 that any rank 1 solution of (1.2) is invariant under some vector field (2.2). At the other extreme, there are no invariant solutions with rank p. Of course, all solutions of a characteristic equation are invariant. The system of Sec. V is not characteristic, but nevertheless has invariant solutions of each possible rank.

IV. SIMPLE WAVES

Much of the study of the equation (1.2) has focused on rank 1 solutions, also called *simple wave* solutions.[2,14,15] The structure of higher rank solutions is considerably more subtle.

Theorem 1: Any rank 1 solution of the equation

$$\left(\frac{\partial}{\partial t}+A(u)\cdot\frac{\partial}{\partial x}\right)u=0, \tag{4.1}$$

is locally invariant under a vector field of the form

$$\frac{\partial}{\partial t}+a(u)\cdot\frac{\partial}{\partial x}. \tag{4.2}$$

Proof: If $u(t,x)$ is a rank 1 solution, then there are locally defined regular functions $r:\mathbb{R}^p\to\mathbb{R}$ and $g:\mathbb{R}\to\mathbb{R}^q$, such that $u(t,x)$ is locally equal to $g(r(t,x))$, and

$$\left(\left(\frac{\partial r}{\partial t}\,I+\frac{\partial r}{\partial x}\cdot A(g(r))\right)g'(r)\right)(t,x)=0. \tag{4.3}$$

There is a smooth $p\times q$ matrix function $B(u)$ on a neighborhood of the local image of g such that the rows of $B(g(r))$ are transpositions of the q-component column vectors,

$$g'(r),\quad A^1(g(r))g'(r),\ldots,A^n(g(r))g'(r).$$

The condition (4.3) is then

$$(Dr\ B(g(r)))(t,x)=0.$$

We use the coefficients of B to define vector fields

$$V_\alpha=b^0_\alpha(u)\,\frac{\partial}{\partial t}+b^i_\alpha(u)\,\frac{\partial}{\partial x^i},\quad \alpha=1,\ldots,q.$$

On the solution manifold $\mathscr{S}=\{(t,x,u(t,x))\}$, we have

$$\begin{aligned}V_\alpha u(t,x)&=\left(b^0_\alpha(g(r))\,\frac{\partial u}{\partial t}+b^i_\alpha(g(r))\,\frac{\partial u}{\partial x^i}\right)(t,x)\\&=\left(\left(b^0_\alpha(g(r))\,\frac{\partial r}{\partial t}+b^i_\alpha(g(r))\,\frac{\partial r}{\partial x^i}\right)g'(r)\right)(t,x)\\&=((Dr\ B(g(r)))_\alpha g'(r))(t,x)=0.\end{aligned}$$

This implies that $\mathscr{S}$ is invariant under the vector fields V. Note that $b^0_\alpha\neq 0$ for some α because $g^1(r)\neq 0$. $\mathscr{S}$ is also invariant under the vector field

$$\frac{\partial}{\partial t}+\left(\frac{b^i_\alpha}{b^0_\alpha}\right)(u)\,\frac{\partial}{\partial x^i}.$$

□

An arbitrary rank 1 function need not be invariant under any vector field of the form (4.2), hence need not be a solution of any equation of the form (4.1). Note also that a rank 1 solution of (4.1) may be invariant under more than one vector field (4.2). For a given equation (4.1) and vector field V of the form (4.2), define

$$\Delta(V)_u=\bigcup_{0\neq\lambda\in\mathbb{R}^n}\ker(\lambda\cdot A(u)-\lambda\cdot a(u)I),$$

for each u in the domain of A. For example, if (4.1) is a characteristic equation and $n\geqslant 2$ then $\Delta(V)_u=\mathbb{R}^q$ for any V. In general, $\Delta(V)_u$ is a union of lines in $T_u\mathbb{R}^q$, well defined with respect to arbitrary change of field variables and affine change of space variables. We interpret $\Delta(V)$ as a system of ordinary differential equations on the domain of A. The *integral curves* of $\Delta(V)$ are the one-dimensional submanifolds of this domain, which are tangent at each point to $\Delta(V)$. Thus a locally defined regular function $g:\mathbb{R}\to\mathbb{R}^q$ is a parametrization of an integral curve if and only if the linear system,

$$(\lambda\cdot A(g(r))-\lambda\cdot a(g(r))I)g'(r)=0, \tag{4.4}$$

has a nonzero solution λ for each value of r. An integral curve is *generic* if the rank of the system (4.4) is constant as r varies, in which case there are smooth vector functions $\lambda^1(r),\ldots,\lambda^l(r)$ that form a basis of solutions. This definition does not depend on the particular parametrization $g(r)$.

Theorem 2: If a rank 1 solution of the equation

$$\left(\frac{\partial}{\partial t}+A(u)\cdot\frac{\partial}{\partial x}\right)u=0,$$

is invariant under the vector field

$$V=\frac{\partial}{\partial t}+a(u)\cdot\frac{\partial}{\partial x};$$

then its local image is an integral curve of $\Delta(V)$. Conversely, a generic integral curve of $\Delta(V)$ is locally the image of a rank 1 V-invariant solution.

Proof: If $u(t,x)$ is a rank 1 solution then there are locally defined regular functions $r:\mathbb{R}^p\to\mathbb{R}$ and $g:\mathbb{R}\to\mathbb{R}^q$ such that $u(t,x)$ is locally equal to $g(r(t,x))$, and

$$\left(\left(\frac{\partial r}{\partial t}I+\frac{\partial r}{\partial x}\cdot A(g(r))\right)g'(r)\right)(t,x)=0. \tag{4.5}$$

If $u(t,x)$ is V-invariant then

$$\left(\frac{\partial r}{\partial t}+a(g(r))\cdot\frac{\partial r}{\partial x}\right)(t,x)=0. \tag{4.6}$$

Fix a point (t,x) in the domain of r, and define $\lambda=\partial r/\partial x(t,x)$. Then

$$\frac{\partial r}{\partial t}(t,x)=-\lambda\cdot a(g(r(t,x))),$$

by (4.6), so we have

$$((\lambda\cdot A(g(r))-\lambda\cdot a(g(r))I)g'(r))(t,x)=0,$$

by (4.5). Note that (4.5) implies $\lambda\neq 0$ because r and g are regular, hence

$$g'(r(t,x))\in\Delta(V)_{g(r(t,x))}.$$

This proves that the local image of $u(t,x)$ is an integral curve of $\Delta(V)$. The converse follows from Theorem 3. □

Theorem 3: Fix an equation,

$$\left(\frac{\partial}{\partial t}+A(u)\cdot\frac{\partial}{\partial x}\right)u=0; \tag{4.7}$$

a vector field,

$$V=\frac{\partial}{\partial t}+a(u)\cdot\frac{\partial}{\partial x};$$

and a generic integral curve of $\Delta(V)$ parametrized by a function $g(r)$. The rank 1 V-invariant solutions of (4.7) defined at $t=0$, $x=0$ that map into this curve are locally the functions $u(t,x)=g(r(t,x))$, where $r(t,x)$ is implicitly defined by an equation

$$r=\phi(\lambda^1(r)\cdot(x-a(g(r))t),\ldots,\lambda^l(r)\cdot(x-a(g(r))t)),$$

where ϕ is an arbitrary regular function of l variables defined on a neighborhood of $0\in\mathbb{R}^l$ such that $\phi(0)$ is in the domain of g, and where $\lambda^1(r),\ldots,\lambda^l(r)$ form a smooth basis of solutions of the linear system,

$$(\lambda\cdot A(g(r))-\lambda\cdot a(g(r))I)g'(r)=0.$$

Proof: Any rank 1 solution that maps into the curve is given locally by $g(r(t,x))$, where

$$\left(\left(\frac{\partial r}{\partial t}I+\frac{\partial r}{\partial x}\cdot A(g(r))\right)g'(r)\right)(t,x)=0.$$

We assume that r is defined at $t=0$, $x=0$. The solution is V-invariant if and only if

$$\frac{\partial r}{\partial t}(t,x)=-\left(a(g(r))\cdot\frac{\partial r}{\partial x}\right)(t,x). \tag{4.8}$$

Combining these conditions, we find that

$$\left(\left(\frac{\partial r}{\partial x}\cdot A(g(r))-\frac{\partial r}{\partial x}\cdot a(g(r))I\right)g'(r)\right)(t,x)=0.$$

Therefore $\partial r/\partial x$ is a linear combination of $\lambda^1(r),\ldots,\lambda^l(r)$ at each point (t,x). In conjunction with (4.8), this implies that $dr(t,x)$ is a linear combination of the covectors,

$$\lambda^j(r(t,x))\cdot(dx-a(g(r(t,x)))dt),\quad j=1,\ldots,l.$$

Hence at each point on the submanifold $\mathscr{S}=\{r=r(t,x)\}$ of the space $\{(t,x,r)\}$ the differential $d(r-r(t,x))$ is a linear combination of dr and $dr^1,\ldots,dr^l$, where

$$r^j(t,x,r)=\lambda^j(r)\cdot(x-a(g(r))t),\quad j=1,\ldots,l.$$

Therefore the differentials $dr,dr^1,\ldots,dr^l$ are dependent on $\mathscr{S}$, i.e., the functions $r,r^1,\ldots,r^l$ are dependent on $\mathscr{S}$, because $d(r-r(t,x))=0$ on $\mathscr{S}$. But the functions $r^1,\ldots,r^l$ are independent on $\mathscr{S}$, because $\lambda^1,\ldots,\lambda^l$ are independent. Hence we have

$$r=\phi(r^1,\ldots,r^l) \tag{4.9}$$

on a neighborhood of the point $r=r(0,0)$ on $\mathscr{S}$, for some function ϕ. The implicit function theorem provides a unique solution $r=r(t,x)$ of (4.9) on a neighborhood of $t=0$, $x=0$ for any function ϕ defined on a neighborhood of $0\in\mathbb{R}^l$, and r is regular at $t=0$, $x=0$ if and only if ϕ is regular at $0\in\mathbb{R}^l$. If $\phi(0)$ is in the domain of g, then $u(t,x)=g(r(t,x))$ is a rank 1 function defined at $t=0$, $x=0$ that maps into the given integral curve. Reversing the preceeding arguments proves that $u(t,x)$ is a V-invariant solution. □

The case of one space variable is well known.[1,2,4,15] The equation (4.1) is then simply

$$\frac{\partial u}{\partial t}+A(u)\frac{\partial u}{\partial x}=0, \tag{4.10}$$

where A is a single $q\times q$ matrix. Fix a vector field,

$$V=\frac{\partial}{\partial t}+a(u)\ \frac{\partial}{\partial x}.$$

The subspace

$$\Delta(V)_u=\ker(A(u)-a(u)I)$$

is nonzero if and only if $a(u)$ is a characteristic value of $A(u)$. The integral curves of $\Delta(V)$ are the characteristic curves of the matrix function $A(u)$ with characteristic value $a(u)$. The regular V-invariant solutions map into these curves, by Theorem 2. Any integral curve is generic, hence, is locally the image of a rank 1 solution, again by Theorem 2. If $g(r)$ is a parametrization of an integral curve then the rank 1 solutions defined at $t=0$, $x=0$ that map into this curve are locally the functions $u(t,x)=g(r(t,x))$, where $r(t,x)$ is implicitly defined by an equation,

$$r=\phi(x-a(g(r))t),$$

where ϕ is an arbitrary regular function of a single variable such that $\phi(0)$ is in the domain of g, by Theorem 3. Theorem 1 tells us that this accounts for all rank 1 solutions. The existence of rank 1 solutions of the equation (4.10) is thus related to the existence of characteristic curves of the matrix A. In the cases $n\geqslant 2$ the equation (4.4) is the relevant generalization of the characteristic equation of a single matrix, and the integral curves of $\Delta(V)$ for the various vector fields V are generalizations of the characteristic curves of a single matrix function.

V. BAROTROPIC FLOW

We now discuss a system that is not characteristic yet has invariant solutions of each possible rank. The equations

$$\left(\frac{\partial}{\partial t}+u\cdot\frac{\partial}{\partial x}\right)u=0,\quad \frac{\partial\rho}{\partial t}+\frac{\partial}{\partial x}\cdot(\rho u)=0,\quad \rho>0, \tag{5.1}$$

describe n-dimensional ideal compressible fluid flow at constant pressure with no external forces.[3] We assume that dissipative effects such as viscosity and thermal conductivity are negligible. There are $n+1$ independent variables $t,x^1,\ldots,x^n$ and $n+1$ dependent variables $u^1,\ldots,u^n,\rho$. The field variables u and ρ denote the velocity and density of the fluid, and the equations (5.1) represent conservation of momentum and of mass. Writing (5.1) in the form (1.2), we find that

$$A^1=\begin{pmatrix} u^1 & & & & \\ & u^1 & & & \\ \vdots & & \ddots & & \\ \rho & 0 & \cdots & 0 & u^1 \end{pmatrix},\ldots,A^n=\begin{pmatrix} u^n & & & & \\ & u^n & & & \\ \vdots & & \ddots & & \\ 0 & \cdots & 0 & \rho & u^n \end{pmatrix}.$$

We will solve the initial value problem for (5.1), and then characterize the solutions invariant under the convective derivative,

$$V=\frac{\partial}{\partial t}+u\cdot\frac{\partial}{\partial x}. \tag{5.2}$$

The overdetermined system (3.1) is equivalent to the equations

$$\left(\frac{\partial}{\partial t}+u\cdot\frac{\partial}{\partial x}\right)u=0,\quad \frac{\partial\rho}{\partial t}+\frac{\partial}{\partial x}\cdot(\rho u)=0,\quad \frac{\partial}{\partial x}\cdot u=0,\quad \rho>0,$$

so a solution of (5.1) is invariant under the vector field (5.2) if and only if its velocity field is divergence-free. It can be shown that (5.2) is not a symmetry of (5.1).

The change of coordinates,

$$\overline{t}=t,\quad \overline{x}=x-ut,\quad \overline{u}=u,\quad \overline{\rho}=\rho$$

transforms (5.1) to the system

$$\frac{\partial\overline{u}}{\partial\overline{t}}=0,\quad \frac{\partial\overline{\rho}}{\partial\overline{t}}+\overline{\rho}\,\mathrm{tr}\left(\left(I+\overline{t}\,\frac{\partial\overline{u}}{\partial\overline{x}}\right)^{-1}\frac{\partial\overline{u}}{\partial\overline{x}}\right)=0,\quad \overline{\rho}>0. \tag{5.3}$$

The general solution of the condition $\partial\overline{u}/\partial\overline{t}=0$ is $\overline{u}(\overline{t},\overline{x})=f(\overline{x})$, where $f:\mathbb{R}^n\to\mathbb{R}^n$ is an arbitrary locally defined function. Then

$$\mathrm{tr}\left(\left(I+\overline{t}\,\frac{\partial\overline{u}}{\partial\overline{x}}(\overline{t},\overline{x})\right)^{-1}\frac{\partial\overline{u}}{\partial\overline{x}}(\overline{t},\overline{x})\right)=\frac{\partial}{\partial\overline{t}}\ln(\det(I+\overline{t}\overline{D}f(\overline{x}))),$$

so the condition on $\overline{\rho}(\overline{t},\overline{x})$ is

$$\frac{\partial}{\partial\overline{t}}\ln(\overline{\rho}(\overline{t},\overline{x})\det(I+\overline{t}\overline{D}f(\overline{x})))=0,$$

which holds if and only if

$$\overline{\rho}(\overline{t},\overline{x})=g(\overline{x})/\det(I+\overline{t}\overline{D}f(\overline{x})),$$

for some positive locally defined function $g:\mathbb{R}^n\to\mathbb{R}$. Thus, the unique solution $u(t,x),\rho(t,x)$ of (5.1) with initial conditions,

$$u(0,x)=f(x),\quad \rho(0,x)=g(x),$$

is defined implicitly by the equations

$$u=f(x-ut),\quad \rho(t,x)=g(x-u(t,x)t)/\det(I+tDf(x-u(t,x)t)).$$

The initial data f and $g>0$ are arbitrary functions defined on the same open subset of $\mathbb{R}^n$. This solution is known for the cases $n=1,2$.[16,17]

Note that $V=\partial/\partial\overline{t}$, so the invariance conditions are $\partial\overline{u}/\partial\overline{t}=0$, $\partial\overline{\rho}/\partial\overline{t}=0$, with the general solution

$$\overline{u}(\overline{t},\overline{x})=f(\overline{x}),\quad \overline{\rho}(\overline{t},\overline{x})=g(\overline{x}). \tag{5.4}$$

Augmenting (5.3) with the invariance conditions gives us the system

$$\frac{\partial\overline{u}}{\partial\overline{t}}=0,\quad \frac{\partial\overline{\rho}}{\partial\overline{t}}=0,\quad \mathrm{tr}\left(\left(I+\overline{t}\,\frac{\partial\overline{u}}{\partial\overline{x}}\right)^{-1}\frac{\partial\overline{u}}{\partial\overline{x}}\right)=0,\quad \overline{\rho}>0,$$

with solution (5.4), where $g>0$ is arbitrary and

$$\frac{\partial}{\partial t}\det(I+\overline{tD}f(\overline{x}))=0,$$

or

$$\det(I+\overline{tD}f(\overline{x}))=1.$$

This holds if and only if the characteristic polynomial of Df is

$$\det(\epsilon I+Df\ )=\epsilon^n.$$

Hence the V-invariant solutions of (5.1) are defined implicitly by the equations

$$u=f(x-ut),\quad \rho(t,x)=g(x-u(t,x)t),$$

where the initial data f and $g>0$ are defined on the same open subset of $\mathbb{R}^n$ and Df is nilpotent. The requirement that Df be nilpotent is a constraint on the initial data, which ensures that its evolution along the flow of V is a solution of (5.1). In the case $n=1$ the invariant solutions are density waves,

$$u(t,x)=c,\quad \rho(t,x)=g(x-ct),$$

propagating at constant velocity. In the case $n=2$ the local invariant solutions are defined implicitly by the equations

$$u=\frac{\partial\phi}{\partial s}(x-ut,y-vt),\quad v=-\frac{\partial\phi}{\partial r}(x-ut,y-vt),$$

$$\rho(t,x)=g(x-u(t,x,y)t,y-v(t,x,y)t),$$

where ϕ and $g>0$ are defined on the same open subset of $\mathbb{R}^2$ and $\phi(r,s)$ satisfies the Monge–Ampere equation,

$$\left(\frac{\partial^2\phi}{\partial r\ \partial s}\right)^2=\frac{\partial^2\phi}{\partial r^2}\frac{\partial^2\phi}{\partial s^2}.$$

For arbitrary n we obtain explicit invariant solutions,

$$u(t,x)=(I+tC)^{-1}Cx,\quad \rho(t,x)=g((I+tC)^{-1}x),$$

where g is arbitrary and C is a constant $n\times n$ matrix with $C^n=0$. These solutions can have any rank from 0 to n.

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Two relativistic boson models in the Schrödinger picture in three space–time dimensions

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A family of unitary representations of the Poincaré group is constructed, which describes two relativistic quantum bosons with weak interaction in three space–time dimensions. The mathematical formalism is the Schrödinger picture of quantum mechanics in the momentum space. The eigenvalue equation for the bound states is given and compared with the Schrödinger equation. © *1996 American Institute of Physics.* [S0022-2488(96)02706-5]

I. INTRODUCTION

Since the discovery of the Schrödinger equation in 1926, its relativistic generalization remains an open problem (see Ref. 1 for an overview of this question). In the present paper we propose a family of models for two relativistic quantum bosons with interaction in three space–time dimensions, in which the bound state equation (playing the role of a relativistic Schrödinger equation) agrees with what could be called an elementary (or naïve) relativistic generalization of the two-particle Schrödinger equation (with the kinetic term replaced by its relativistic counterpart and with a nonlocal interaction term). These models have been suggested by a new approach to the bound state problem in bosonic quantum field theory (QFT) in two space–time dimensions. The mathematical formalism is the Schrödinger picture of quantum mechanics (QM) in the momentum space, as in the standard representation of the two free boson models. More precisely, we start from such a free model and introduce an interaction by modifying the Hamiltonian and the Lorentz generators in such a way that the commutation rules of the Poincaré algebra remain satisfied. The interaction terms are constructed in terms of an ''interaction kernel,'' which can be chosen, in a center-of-mass frame, within a large class of functions. At the present state of this theory, however, the standard potential interaction used in QM cannot be obtained from this class.

Let us explain how this model has been found. In 1973 a rigorous mathematical construction for bosonic QFT models with weak coupling in two space–time dimensions has been obtained by Glimm, Jaffe, and Spencer[2] [the so-called weakly coupled $\mathscr{P}(\varphi)_2$ models]. Existence of bound states in some of these models have been established and the conditions for such states to occur completely specified (see Ref. 3 for a complete review of the question). Because of the mathematical construction of these models, other questions about the bound states than just their existence can be asked for. In particular, their eigenspaces can be investigated. A variational perturbation method has been established to construct an eigenvector by varying suitable combinations of zero-time vectors.[4] This construction has revealed the existence (at first perturbation orders) of stable subspaces under the Poincaré transformations, describing two particles with interaction, in the Schrödinger picture (because of the restriction to zero-time vectors) (Sec. III of Ref. 5). Such representations of the Poincaré group can be studied for themselves, without reference to QFT. We have obtained in Ref. 6 the complete set of such representations, in the weak-coupling regime, by a nonperturbative construction. They are given from an ''interaction kernel,'' which, in a center-of-mass frame, can be chosen arbitrarily. Such very simple models can be used to study in detail the phenomenology of quantum and relativistic particles at low energy, and in particular the bound state problem (high energy is without interest because particle creation does not occur). Moreover, the generalization to an arbitrary number of particles has been obtained[7] (so

the phenomena of particle creation could be introduced by taking suitable combinations of models with different particle numbers).

In the present article we are concerned with the generalization, for the two-particle case, to three space–time dimensions. The difficulty comes from the higher dimension of the Poincaré group (passing from 3 to 6) and from the number of commutation relations (passing from 3 to 15), which must hold simultaneously.

We consider first a two free boson representation of the Poincaré group in three space–time dimensions, acting on functions $f(\mathbf{p}_1,\mathbf{p}_2)$ of two momenta $(\mathbf{p}_1,\mathbf{p}_2)\in\mathbb{R}^2\times\mathbb{R}^2$. The infinitesimal generators are well known and given by unbounded self-adjoint operators satisfying the commutation rules of the Lie algebra of the Poincaré group. In this representation, the time variable does not appear explicitly, and this feature is what we call the ''Schrödinger picture.'' So we have the QM picture of a fixed state space, the time being a parameter introduced by the Hamiltonian evolution. Interaction is introduced by modifying the Hamiltonian and the Lorentz generators, in terms of an ''interaction kernel'' $h(\mathbf{P},\mathbf{Q},\mathbf{Q}')$ where $\mathbf{P}\in\mathbb{R}^2$ is the total momentum and $\mathbf{Q},\mathbf{Q}'\in\mathbb{R}^2$ are relative momenta. The Hilbert space of the representation is not changed. The commutation rules lead to several conditions on h, which reduce to a single equation, provided $h(\mathbf{P},\mathbf{Q},\mathbf{Q}')$ is a function of the norms $\|\mathbf{P}\|,\|\mathbf{Q}\|,\|\mathbf{Q}'\|$ only (this last requirement, which excludes the standard potential interactions of QM, cannot be removed at the present state of this theory). By the Banach fixed point theorem this equation can be completely solved in the weak-coupling regime. The solutions are parametrized by arbitrary functions of the relative momenta $c(\|\mathbf{Q}\|,\|\mathbf{Q}'\|)$, which are nothing else than the interaction kernel in a center-of-mass frame: $c(\|\mathbf{Q}\|,\|\mathbf{Q}'\|)=h(0,\mathbf{Q},\mathbf{Q}')$.

To investigate the physical content of these models, the asymptotic states have to be constructed, which assures that they really describe two-particle systems. Moreover, the equation for the bound states can be written down (consisting of the eigenvalue equation for the mass operator). This equation plays the role of a *relativistic Schrödinger equation*. It can be used to show the existence of bound states (for suitable functions c), which ensures that this theory is not trivial.

The connection between these models and QFT is not as simple as in two space–time dimensions, because of their particular interaction term and because in three space–time dimensions there are few available bosonic models in which bound states are known to exist. Such a connection could perhaps be obtained at a formal level, for theories admitting point interaction at first perturbation order.

Let us recall that the idea of modifying the free Poincaré representation in order to introduce interaction has been proposed in the 1940s by Dirac,[8] but for classical systems. By modifying only the Hamiltonian and the Lorentz generators he gets what he called an ''instant form dynamics.'' Dirac's conclusion was that it provides too complicated equations. In fact, what we have obtained is a set of solutions to these equations, in the quantum case and in three space–time dimensions, leading to explicit examples of such dynamics.

In Sec. II we recall the operators of the representation of the Poincaré group for two free bosons in the Schrödinger picture. The interaction is introduced by modifying some of these operators, by adding to them new terms obtained from an ''interaction operator'' $\mathcal{O}$. The commutation rules impose three conditions on $\mathcal{O}$, which, under a particular condition, reduce to a unique ''fundamental equation'' for the kernel of $\mathcal{O}$. In Sec. III we give the complete set of solutions of this equation, in the weak-coupling regime, by applying the Banach fixed point theorem. In Sec. IV we show that the operators we have obtained are really the infinitesimal generators of unitary, continuous representations of the Poincaré group, by applying a theorem by Fröhlich. In Sec. V the bound state equation is written down and compared with the two-body Schrödinger equation. The existence of a bound state is shown in an example. Finally, in Sec. VI we conclude by summing up what we have found: a family of two-particle models (by giving the construction of asymptotic states) with interaction having a (somewhat weak) link with (formal) QFT.

II. TWO-PARTICLE REPRESENTATIONS OF THE POINCARÉ ALGEBRA

The Lie algebra $\mathcal{G}$ of the Poincaré group $\mathcal{P}_+^\uparrow$ in three space–time dimensions is generated by the six operators H (Hamiltonian), $\mathbf{P}=(P_1,P_2)$ (momentum), J (angular momentum), and $\mathbf{L}=(L_1,L_2)$ (generators of the Lorentz transformations), satisfying the commutation rules

$$[P_1,P_2]=0, \quad [P_1,J]=-iP_2, \quad [P_2,J]=iP_1, \tag{1}$$

$$[P_j,H]=0, \quad [H,J]=0, \tag{2}$$

$$[P_j,L_k]=i\ \delta_{j,k}H, \quad [L_1,J]=-iL_2, \quad [L_2,J]=iL_1, \tag{3}$$

$$[H,L_j]=iP_j, \quad [L_1,L_2]=-iJ, \tag{4}$$

for all $1\leqslant j,\ k\leqslant 2$, where $\delta_{i,j}$ is the Kronecker tensor. This operator algebra admits two Casimir operators (i.e., operators that commute with all generators), the square mass operator M^2, and the Pauli–Lubanski operator E, given by

$$M^2:=H^2-P^2, \quad E:=-HJ+P_1L_2-P_2L_1. \tag{5}$$

The representation that describes one spinless particle of mass $m>0$, in the Schrödinger picture, is given by the following choice of operators:

$$\begin{gathered} P_j\phi(\mathbf{p})=p_j\phi(\mathbf{p}), \quad H\phi(\mathbf{p})=\omega(\mathbf{p})\phi(\mathbf{p}), \\ J\phi(\mathbf{p})=-i(p_1\partial_2-p_2\partial_1)\phi(\mathbf{p}), \quad L_j\phi(\mathbf{p})=-i\omega(\mathbf{p})\partial_j\phi(\mathbf{p}), \end{gathered} \tag{6}$$

for all $j\in\{1,2\}$, $\mathbf{p}=(p_1,p_2)\in\mathbb{R}^2$ and suitable functions $\phi:\mathbb{R}^2\to\mathbb{C}$, where we have put $\omega(\mathbf{p}):=\sqrt{\mathbf{p}^2+m^2}$. These operators define a representation of the algebra $\mathcal{G}$, which can be integrated to give an irreducible, unitary, and continuous representation of $\mathcal{P}_+^\uparrow$ in $L^2(\mathbb{R}^2,\sigma)$ (complex-valued functions), where σ is the measure $d\sigma(\mathbf{p}):=d\mathbf{p}[2\omega(\mathbf{p})]^{-1}$ (see Appendix A). In this representation the Casimir operators (5) are simply $M^2=m^2Id$ and $E=0$.

The representation that describes two identical bosons of mass $m>0$ without interaction, in the Schrödinger picture, is given by the symmetrical tensor product of two copies of the one-particle representation. By the properties of the tensor product we get a unitary continuous representation of $\mathcal{P}_+^\uparrow$ given by the generators

$$\begin{gathered} P_j\phi(\mathbf{p}_1,\mathbf{p}_2)=((\mathbf{p}_1)_j+(\mathbf{p}_2)_j)\phi(\mathbf{p}_1,\mathbf{p}_2), \\ H_0\phi(\mathbf{p}_1,\mathbf{p}_2)=(\omega(\mathbf{p}_1)+\omega(\mathbf{p}_2))\phi(\mathbf{p}_1,\mathbf{p}_2), \\ J\phi(\mathbf{p}_1,\mathbf{p}_2)=-i\left[\sum_{j=1}^{2}((\mathbf{p}_j)_1\partial_{(\mathbf{p}_j)_2}-(\mathbf{p}_j)_2\partial_{(\mathbf{p}_j)_1})\right]\phi(\mathbf{p}_1,\mathbf{p}_2), \\ L_{0,j}\phi(\mathbf{p}_1,\mathbf{p}_2)=-i(\omega(\mathbf{p}_1)\partial_{(\mathbf{p}_1)_j}+\omega(\mathbf{p}_2)\partial_{(\mathbf{p}_2)_j})\phi(\mathbf{p}_1,\mathbf{p}_2), \end{gathered} \tag{7}$$

for all $j\in\{1,2\}$, $(\mathbf{p}_1,\mathbf{p}_2)\in\mathbb{R}^4$ and suitable functions $\phi:\mathbb{R}^4\to\mathbb{C}$. The space of the representation is

$$\mathcal{H}:=L^2_{\mathrm{Sym}}(\mathbb{R}^2\times\mathbb{R}^2,\sigma_2) \tag{8}$$

[made of symmetrical functions $\phi(\mathbf{p}_1,\mathbf{p}_2)=\phi(\mathbf{p}_2,\mathbf{p}_1)$], where $\sigma_2:=\sigma\otimes\sigma$. It describes two particles without interaction (therefore we have put an index 0 to H_0 and $L_{0,j}$).

The Casimir operators are more complicated, given now by

$$M_0^2\phi(\mathbf{p}_1,\mathbf{p}_2)=[(\omega(\mathbf{p}_1)+\omega(\mathbf{p}_2))^2-(\mathbf{p}_1+\mathbf{p}_2)^2]\phi(\mathbf{p}_1,\mathbf{p}_2), \tag{9}$$

$$E_0\phi(\mathbf{p}_1,\mathbf{p}_2)=-i[\omega(\mathbf{p}_1)\mathbf{p}_2-\omega(\mathbf{p}_2)\mathbf{p}_1]\wedge\nabla_{\mathbf{p}_1-\mathbf{p}_2}\phi(\mathbf{p}_1,\mathbf{p}_2), \tag{10}$$

with the notation $(a_1,a_2)\wedge(b_1,b_2):=a_1b_2-a_2b_1$ for all $\mathbf{a},\mathbf{b}\in\mathbb{R}^2$ and $\nabla_{\mathbf{p}_1-\mathbf{p}_2}:=(\partial_{(\mathbf{p}_1)_1}-\partial_{(\mathbf{p}_2)_1},\partial_{(\mathbf{p}_1)_2}-\partial_{(\mathbf{p}_2)_2})$.

Now we want to modify these operators in order to introduce interaction. To remain in the Schrödinger picture we keep $\mathbf{P}$ and J unchanged and modify only H_0 and $\mathbf{L}_0$. Let $\mathscr{O}$ be a self-adjoint operator (the *interaction operator*) on which we only impose, for the moment, the formal commutation relations

$$[\mathscr{O},\mathbf{P}]=0,\quad [\mathscr{O},J]=0. \tag{11}$$

We define the interaction representation as follows:

$$\mathbf{P},J,\quad \text{as in (7)},\quad H:=H_0+\{\mathscr{O},H_0\},\quad L_j:=L_{0,j}+\{\mathscr{O},L_{0,j}\}, \tag{12}$$

for $j\in\{1,2\}$, where we have used the notation $\{A,B\}=AB+BA$. The Hilbert space of the representation is still given by (8). The particular form of the ''interaction terms'' of (12) together with the commutation rules (11) have the following nice consequence.

Lemma 1: The operators (12) satisfy formally the commutation rules (1), (2), and (3) of the algebra $\mathscr{G}$.

The proof is purely algebraic: (1) has not been changed; (2) is an immediate consequence of (11); (3) follows from a simple algebraic calculation (for more details, see Ref. 6 or 7). Note that (3) could be used to establish (12) once we impose the change of $L_{1,0}$ only. Until now, no condition on $\mathscr{O}$ except (11) was needed. But the last commutation rules (4) impose the following complicated equations:

$$0=[\{\mathscr{O},H_0\},L_{0,j}]+[H_0,\{\mathscr{O},L_{0,j}\}]+[\{\mathscr{O},H_0\},\{\mathscr{O},L_{0,j}\}], \tag{13}$$

$$0=[\{\mathscr{O},L_{0,1}\},L_{0,2}]+[L_{0,1},\{\mathscr{O},L_{0,2}\}]+[\{\mathscr{O},L_{0,1}\},\{\mathscr{O},L_{0,2}\}], \tag{14}$$

for all $j\in\{1,2\}$. This gives three equations for $\mathscr{O}$ of the same form (made of a linear term plus a bilinear term), which must hold simultaneously. We have now to find nontrivial solutions $\mathscr{O}\neq 0$ to this system.

In order to have a better physical understanding we make the change of variables $(\mathbf{p}_1,\mathbf{p}_2)\to(\mathbf{P},\mathbf{Q})$, given by

$$\begin{aligned}\mathbf{P}&:=\mathbf{p}_1+\mathbf{p}_2,\\ \mathbf{Q}&:=\frac{1}{2}(\mathbf{p}_1-\mathbf{p}_2)-\frac{1}{2}\mathbf{P}\frac{\omega(\mathbf{p}_1)-\omega(\mathbf{p}_2)}{M_0(\mathbf{p}_1,\mathbf{p}_2)+\omega(\mathbf{p}_1)+\omega(\mathbf{p}_2)},\end{aligned} \tag{15}$$

where $M_0(\mathbf{p},\mathbf{p}_2):=[(\omega(\mathbf{p}_1)+\omega(\mathbf{p}_2))^2-\mathbf{P}^2]^{1/2}$. The variable $\mathbf{P}$ is the total momentum while $\mathbf{Q}$ is the relative momentum, defined as the momentum in a center-of-mass frame [more precisely, $\mathbf{Q}$ is the transform of $\frac{1}{2}(\mathbf{p}_1-\mathbf{p}_2)$ under a Lorentz transformation leading to a center-of-mass frame; see Appendix B].

Under this change of variables the free representation (7) becomes

$$\begin{aligned}P_j\phi(\mathbf{P},\mathbf{Q})&=P_j\phi(\mathbf{P},\mathbf{Q}),\\ H_0\phi(\mathbf{P},\mathbf{Q})&=\Omega(\mathbf{P},\mathbf{Q})\phi(\mathbf{P},\mathbf{Q}),\end{aligned} \tag{16}$$

$$J\phi(\mathbf{P},\mathbf{Q}) = -i(P_1\partial_{P_2} - P_2\partial_{P_1} + J^{\mathbf{Q}})\phi(\mathbf{P},\mathbf{Q}),$$

$$L_{0,j}\phi(\mathbf{P},\mathbf{Q}) = -i(\Omega(\mathbf{P},\mathbf{Q})\partial_{P_j} + L^{\mathbf{Q}}_{0,j})\phi(\mathbf{P},\mathbf{Q}),$$

for all $j \in \{1,2\}$, where we have put

$$J^{\mathbf{Q}}\phi(\mathbf{P},\mathbf{Q}) := -i(Q_1\partial_{Q_2} - Q_2\partial_{Q_1})\phi(\mathbf{P},\mathbf{Q}),$$

$$L^{\mathbf{Q}}_{0,1}\phi(\mathbf{P},\mathbf{Q}) := \frac{P_2}{\Omega(\mathbf{P},\mathbf{Q}) + 2\omega(\mathbf{Q})}\, J^{\mathbf{Q}}\phi(\mathbf{P},\mathbf{Q}), \tag{17}$$

$$L^{\mathbf{Q}}_{0,2}\phi(\mathbf{P},\mathbf{Q}) := -\frac{P_1}{\Omega(\mathbf{P},\mathbf{Q}) + 2\omega(\mathbf{Q})}\, J^{\mathbf{Q}}\phi(\mathbf{P},\mathbf{Q}),$$

for all suitable functions ϕ, where $\Omega(\mathbf{P},\mathbf{Q}) = \sqrt{\mathbf{P}^2 + 4\omega(\mathbf{Q})^2}$ (see the calculation in Appendix B). As for (7), these operators define a representation of the algebra $\mathscr{G}$ that can be integrated to give a unitary and continuous representation of the Poincaré group $\mathscr{P}^{\uparrow}_{+}$, in the same function space (8), which can be written $\mathscr{H} = L^2_{Ev\cdot\mathbf{Q}}(\mathbb{R}^2 \times \mathbb{R}^2, \mu)$, made of functions even in $\mathbf{Q}$ [that is $\phi(\mathbf{P},\mathbf{Q}) = \phi(\mathbf{P}, -\mathbf{Q})$], where $d\mu(\mathbf{P},\mathbf{Q}) := d\sigma(\mathbf{Q})d\mathbf{P}\Omega(\mathbf{P},\mathbf{Q})^{-1}$ (see Appendix B). In these variables the Casimir operators (9), (10) concern only the $\mathbf{Q}$ variable,

$$M_0^2\phi(\mathbf{P},\mathbf{Q}) = 4\omega(\mathbf{Q})^2\phi(\mathbf{P},\mathbf{Q}), \tag{18}$$

$$E_0\phi(\mathbf{P},\mathbf{Q}) = 2\omega(\mathbf{Q})J^{\mathbf{Q}}\phi(\mathbf{P},\mathbf{Q}). \tag{19}$$

We call (17) the *relative terms* because without them [i.e., if we replace formally $J^{\mathbf{Q}}$ by 0 in (16)] we also get a representation of $\mathscr{G}$, which is nonequivalent to (7) (because with $E = 0$). Note that this particular representation is defined by the same formula as the one-particle representation (6), with $\mathbf{p}$ replaced by $\mathbf{P}$ and m replaced by $2\omega(\mathbf{Q})$. In the two space–time dimension case, the two free boson representation has such a property (Refs. 6 and 7). For this reason the relative terms (17) appear as the main difference between the two- and three-dimensional cases.

To find solutions to (13)–(14) we write $\mathscr{O}$ in the following general form:

$$\mathscr{O}\phi(\mathbf{P},\mathbf{Q}) := \int \frac{d\sigma(\mathbf{Q}')}{\Omega(\mathbf{P},\mathbf{Q}')}\, \phi(\mathbf{P},\mathbf{Q}')\, \frac{h(\mathbf{P},\mathbf{Q},\mathbf{Q}')}{\Omega(\mathbf{P},\mathbf{Q}) + \Omega(\mathbf{P},\mathbf{Q}')}, \tag{20}$$

where $h(\mathbf{P},\mathbf{Q},\mathbf{Q}')$ is *a priori* a function of norms $\|\mathbf{P}\|,\|\mathbf{Q}\|,\|\mathbf{Q}'\|$ and of the scalar products $\mathbf{P}\cdot\mathbf{Q},\mathbf{P}\cdot\mathbf{Q}',\mathbf{Q}\cdot\mathbf{Q}'$ only, and satisfies the symmetry condition

$$h(\mathbf{P},\mathbf{Q},\mathbf{Q}') = h(\mathbf{P},\mathbf{Q}',\mathbf{Q})^*, \tag{21}$$

together with $h(\mathbf{P},\mathbf{Q},\mathbf{Q}') = h(\mathbf{P},\mathbf{Q},-\mathbf{Q}') = h(\mathbf{P},-\mathbf{Q},\mathbf{Q}')$, for all $\mathbf{P},\mathbf{Q},\mathbf{Q}' \in \mathbb{R}^2$, where the star * denotes the complex conjugation. Note that $\mathscr{O}$ is a symmetric operator that formally satisfies (11).

We establish in Appendix C that, if $h(\mathbf{P},\mathbf{Q},\mathbf{Q}')$ is a function of norms $\|\mathbf{P}\|,\|\mathbf{Q}\|,\|\mathbf{Q}'\|$ only, the three equations (13)–(14) reduce to a single nonlinear integro differential equation for h. With the differential operator D given by

$$Dh(\mathbf{P},\mathbf{Q},\mathbf{Q}') := \frac{\Omega(\mathbf{P},\mathbf{Q})\Omega(\mathbf{P},\mathbf{Q}')}{\Omega(\mathbf{P},\mathbf{Q}) + \Omega(\mathbf{P},\mathbf{Q}')}\, \partial_{\|\mathbf{P}\|}h(\mathbf{P},\mathbf{Q},\mathbf{Q}'), \tag{22}$$

this equation can be written as follows:

$$0=2\,Dh(\mathbf{P},\mathbf{Q},\mathbf{Q}')+\int\frac{d\sigma(\mathbf{Q}'')}{\Omega(\mathbf{P},\mathbf{Q}'')^2}\left\{-\frac{\|\mathbf{P}\|}{\Omega(\mathbf{P},\mathbf{Q}'')}\,h(\mathbf{P},\mathbf{Q},\mathbf{Q}'')h(\mathbf{P},\mathbf{Q}'',\mathbf{Q}')\right.$$
$$\left.+Dh(\mathbf{P},\mathbf{Q},\mathbf{Q}'')h(\mathbf{P},\mathbf{Q}'',\mathbf{Q}')+h(\mathbf{P},\mathbf{Q},\mathbf{Q}'')Dh(\mathbf{P},\mathbf{Q}'',\mathbf{Q}')\right\}. \tag{23}$$

This is the fundamental equation that guarantees the relativistic structure of the theory. Let us sum up what we have found in the following statement.

Proposition 2: Let $h(\mathbf{P},\mathbf{Q},\mathbf{Q}')$ *be a function of* $\|\mathbf{P}\|,\|\mathbf{Q}\|,\|\mathbf{Q}'\|$ *only, which satisfies (21) and (23). Then the operators (12), with* $\mathscr{O}$ *given by (20), are symmetric and satisfy algebraically the commutation rules (1) to (4) of the algebra* $\mathscr{G}$.

III. EXISTENCE OF SOLUTIONS OF THE FUNDAMENTAL EQUATION

In this section we are concerned with the solutions to the equation (23).

Definition: Let $\mathscr{B}$ be the Banach space made of bounded, continuous functions $f:(\mathbb{R}_+)^3\to\mathbb{C}$, where $\mathbb{R}_+=[0,\infty)$, such that the following derivative $df(u,x,y):=r(u,x)r(u,y)[r(u,x)+r(u,y)]^{-1}\partial_u f(u,x,y)$ (with right derivation at $u=0$), where $r(u,v):=(u^2+4v^2+4m^2)^{1/2}$, exists and is also bounded and continuous, given the norm

$$|h|_{\mathscr{B}}:=\|h\|_\infty+\|dh\|_\infty. \tag{24}$$

The following result assures the existence of a large class of solutions of (23).

Proposition 3: There exists $0<K_1<\infty$ *such that, for all continuous bounded functions* $c:\mathbb{R}_+^2\to\mathbb{C}$ *satisfying* $\|c\|_\infty<K_1$, *there exists one and only one function* $f\in\mathscr{B}$ *satisfying*

(1) $|f|_{\mathscr{B}}<2K_1$,

(2) $f(0,x,y,)=c(x,y)$,

(3) $h(\mathbf{P},\mathbf{Q},\mathbf{Q}')=f(\|\mathbf{P}\|,\|\mathbf{Q}\|,\|\mathbf{Q}'\|)$ satisfies (23) for all $\mathbf{P},\mathbf{Q},\mathbf{Q}'\in\mathbb{R}^2$.

Moreover, h satisfies (21) if $c(x,y)=c(y,x)^*$.

Note that $h(\mathbf{P}=0,\mathbf{Q},\mathbf{Q}')=c(\|\mathbf{Q}\|,\|\mathbf{Q}'\|)$ is an arbitrary function, i.e. there is no restriction on the interaction kernel h for $\mathbf{P}=0$, that is in a center-of-mass frame. The proof is based on the Banach fixed point theorem. It gives not only existence and uniqueness, as stated in the Proposition, but also a formula for the solution h in terms of c.

Proof: Let us introduce a bilinear operator b,

$$b(f,g)(u,x,y):=\pi\int_0^u dv\left(\frac{1}{r(v,x)}+\frac{1}{r(v,y)}\right)\int_0^\infty\frac{z\,dz}{r(0,z)r(v,z)^2}\left\{-df(v,x,z)g(v,z,y)\right.$$
$$\left.-f(v,x,z)dg(v,z,y)+\frac{v}{r(v,z)}\,f(v,x,z)g(v,z,y)\right\}, \tag{25}$$

where $u,x,y\in\mathbb{R}_+$. By derivation of b (in the sense used in the definition of $\mathscr{B}$), one gets simply

$$db(f,g)(u,x,y)=\pi\int_0^\infty\frac{z\,dz}{r(0,z)r(u,z)^2}\left\{-df(u,x,z)g(u,z,y)-f(u,x,z)dg(u,z,y)\right.$$
$$\left.+\frac{u}{r(u,z)}\,f(u,x,z)g(u,z,y)\right\}. \tag{26}$$

The fundamental equation (23) can be written as $df-db(f,f)=0$, where $h(\mathbf{P},\mathbf{Q},\mathbf{Q}')=f(\|\mathbf{P}\|,\|\mathbf{Q}\|,\|\mathbf{Q}'\|)$. By integration, this equation becomes

$$f(u,x,y)=c(x,y)+b(f,f)(u,x,y):=A(f)(u,x,y), \tag{27}$$

where $c(x,y)$ is an arbitrary function (the integration ''constant''). This is a fixed point equation that can be solved by applying the Banach fixed point theorem (Ref. 9, Sec. 1.1) in the Banach space $\mathscr{B}$. From a standard analysis and a simple estimate, it follows that $b\colon \mathscr{B}\to\mathscr{B}$ and satisfies

$$|b(f,g)|_{\mathscr{B}} < K_1' |f|_{\mathscr{B}} |g|_{\mathscr{B}}, \tag{28}$$

where K_1' is the constant given by

$$K_1' = \pi \int_0^\infty \frac{2\,dv}{r(v,0)} \int_0^\infty \frac{z\,dz}{r(0,z)r(v,z)^2} + \pi \int_0^\infty \frac{z\,dz}{r(0,z)^3}.$$

Let us take $K_1 = (4K_1')^{-1}$ and $c(x,y) \in \mathscr{B}$ with $|c|_{\mathscr{B}} = \|c\|_\infty < K_1$. Then the operator $A(f)$ sends the ball $B(2K_1) := \{g \in \mathscr{B} \,|\, |g|_{\mathscr{B}} < 2K_1\}$ into itself and is a strict contraction on $B(2K_1)$ (see Ref. 6 or 7 for more details). In such a case, it follows from the Banach fixed point theorem that the equation $f = A(f)$ has one and only one solution in $B(2K_1)$, given by the limit of convergent sequence $f = \lim_{n\to\infty} A^n(0)$.

Let us suppose that c satisfies $c(x,y) = c(y,x)^*$. So does $A(0) = c$. If $g \in \mathscr{B}$ satisfies $g(u,x,y) = g(u,y,x)^*$, so does $b(g,g)$ and $A(g)$. By an induction argument it follows that $\lim_{n\to\infty} A^n(0)$ satisfies this symmetry, too. □

Remark 1: As previously mentioned, the proof gives a formula for the solution h in terms of c, given by a uniformly convergent sequence,

$$h(\mathbf{P},\mathbf{Q},\mathbf{Q}') = \lim_{n\to\infty} \mathscr{A}^n(0)(\mathbf{P},\mathbf{Q},\mathbf{Q}'), \tag{29}$$

for all $(\mathbf{P},\mathbf{Q},\mathbf{Q}') \in \mathbb{R}^6$, where

$$\mathscr{A}(g)(\mathbf{P},\mathbf{Q},\mathbf{Q}') := c(\|\mathbf{Q}\|,\|\mathbf{Q}'\|) + b(g,g)(\|\mathbf{P}\|,\|\mathbf{Q}\|,\|\mathbf{Q}'\|),$$

for all $g(\|\mathbf{P}\|,\|\mathbf{Q}\|,\|\mathbf{Q}'\|) \in \mathscr{B}$. The first terms of this sequence are

$$\mathscr{A}(0) = c, \quad \mathscr{A}^2(0) = \mathscr{A}(c) = c + b(c,c), \tag{30}$$

$$\mathscr{A}^3(0) = c + b(c,c) + b(b(c,c),c) + b(c,b(c,c)) + b(b(c,c),b(c,c)),$$

etc. The limit can be seen as a power series of c that converges uniformly. It is nonzero if $c \neq 0$ because it is continuous and satisfies $h(0,\mathbf{Q},\mathbf{Q}') = c(\|\mathbf{Q}\|,\|\mathbf{Q}'\|)$.

Remark 2: Proposition 3 ensures the existence of solutions only in a ball of a Banach space, that is, in the weak-coupling regime. However, the constant K_1 that limits the supremum of c can be taken of the order of m. A small calculation gives

$$K_1' = \frac{\pi}{4m}\left[\int_0^\infty \frac{u}{\cosh u}\,du + \frac{1}{2}\right] = \frac{1.8315\ldots}{m},$$

and thus $K_1 = m/7.3259\ldots$. In what follows we will take simply $K_1 = m/8$.

IV. UNITARY REPRESENTATIONS OF THE POINCARÉ GROUP

We have established the existence of a large class of operators $\mathscr{O}$ for which (12) gives rise to formal representations of the Lie algebra $\mathscr{G}$ (we call them formal because the problem of operator domains have not yet been considered). The natural question arises, under which conditions these

formal representations can be really defined and can be integrated to provide unitary and continuous representations of the Poincaré group. By imposing a new condition on c we can specify the domain of our operators.

Proposition 4: Let c: $\mathbb{R}_+^2 \to \mathbb{C}$ *satisfy* $c(x,y)=c(y,x)^*$ *and the hypothesis of Proposition 3 and, moreover,*

$$\sup_{(x,y)\in\mathbb{R}_+^2} |(x^2+m^2)^{3/4}(y^2+m^2)^{3/4}c(x,y)| < K_2, \tag{31}$$

for some $K_2>0$ *sufficiently small. Let* $h(\mathbf{P},\mathbf{Q},\mathbf{Q}')=f(\|\mathbf{P}\|,\|\mathbf{Q}\|,\|\mathbf{Q}'\|)$, *where* f *is the function deduced from* c *in Proposition 3. Then the following conditions are satisfied.*

(1) *The operators* H, $\mathbf{P}$, J, *and* $\mathbf{L}$ *are self-adjoint.*

(2) *The operator* $\Delta=m^{-2}(H^2+\mathbf{P}^2)+J^2+\mathbf{L}^2$ *is self-adjoint and there exists a dense domain* $\mathscr{D}$ *which is a common core for all operators* Δ, H, $\mathbf{P}$, J, *and* $\mathbf{L}$.

(3) *Let* A,B *be any pair of operators* H, P_1, P_2, J, L_1, L_2. *Then* A *is defined and symmetric on* $B\mathscr{D}$. *Moreover the commutation rules (1) to (4) hold on* $\mathscr{D}$.

This proposition gives a precise sense to our Lie algebra representations and to the commutation rules. Moreover, according to a theorem by Fröhlich[10] (see remark 2, after the proof), these conditions are sufficient to ensure the integrability of the algebra representations, leading, by the exponential map, to unitary, continuous representations of the universal cover of the Poincaré group. The interest of Fröhlich's theorem is that it does not require the domain $\mathscr{D}$ to be invariant under all operators, as in Nelson's classic theorem (Ref. 11, Theorem 5). The construction of a common invariant domain for operators as different as ours (multiplication, derivations, and kernel operators) is a difficult problem that has been achieved in the one-dimensional space case only at the price of strong conditions on c (in Ref. 6, c is a C^∞ fast decreasing function, which does not agree with the corresponding kernel in QFT). It is probable that with appropriate conditions on c, Nelson's theorem can also be used in the present case.

Proof: We proceed in three steps.

First step. We deduce from (31) two properties of h. Let $g\in\mathscr{B}$ such that $|g(u,x,y)|+|dg(u,x,y)|\leqslant k_1 s(x)^{-3/2}s(y)^{-3/2}$ for some $k_1\in(0,\infty)$ for all $(u,x,y,)\in\mathbb{R}_+^3$, where $s(t)=(t^2+m^2)^{1/2}$. By using this inequality in the integrals (25)–(26) and the methods leading to (28), we get

$$|b(g,g)(u,x,y)|+|db(g,g)(u,x,y)| \leqslant K_1' \frac{k_1^2}{m^3} \frac{1}{s(x)^{3/2}s(y)^{3/2}}.$$

Let c be a function satisfying the hypothesis of the proposition with K_2 small enough to have $4K_1'K_2/m^3 < 1$. Let us suppose that for some $n\in\mathbb{N}^*$ we know that $|A^n(0)(u,x,y)|+|dA^n(0)(u,x,y)|<C_n s(x)^{-3/2}s(y)^{-3/2}$ for some constant $C_n<2K_2$ and for all $(u,x,y)\in\mathbb{R}_+^3$ (this is true for $n=1$). Then

$$\begin{aligned}
&|A^{n+1}(0)(u,x,y)|+|dA^{n+1}(0)(u,x,y)| \\
&\quad = |c(x,y)+b(A^n(0),A^n(0))(u,x,y)| \\
&\qquad + |db(A^n(0),A^n(0))(u,x,y)| \\
&\quad \leqslant \left(K_2+K_1'\frac{C_n^2}{m^3}\right)\frac{1}{s(x)^{3/2}s(y)^{3/2}} = \frac{C_{n+1}}{s(x)^{3/2}s(y)^{3/2}},
\end{aligned}$$

with $C_{n+1} = K_2 + K_1'C_n^2/m^3 < 2K_2$. Thus, for such c all terms of the sequence $\{|A^n(0)(u,x,y)|+|dA^n(0)(u,x,y)|\}_{n=1}^\infty$ is bounded by $2K_2[s(x)s(y)]^{-3/2}$, and so are their limit. We have shown that for all $(\mathbf{P},\mathbf{Q},\mathbf{Q}')\in\mathbb{R}^6$,

$$\omega(\mathbf{Q})^{3/2}\omega(\mathbf{Q}')^{3/2}(|h(\mathbf{P},\mathbf{Q},\mathbf{Q}')|+|Dh(\mathbf{P},\mathbf{Q},\mathbf{Q}')|)<2K_2. \tag{32}$$

For the next step we also need to know that $\omega(\mathbf{Q})^{3/2}\omega(\mathbf{Q}')^{3/2}|\|\mathbf{P}\|\partial_{\|\mathbf{P}\|}\, Dh\|\mathbf{P}\|^{-1}|$ is bounded. Now $\|\mathbf{P}\|\partial_{\|\mathbf{P}\|}\, Dh\|\mathbf{P}\|^{-1} = \partial_{\|\mathbf{P}\|}\, Dh - \|\mathbf{P}\|^{-1}\, Dh$. A bound for the second term can be obtained from the equation (23) and the inequality (32), as follows. Let $g(\mathbf{P},\mathbf{Q},\mathbf{Q}')=\omega(\mathbf{Q})^{3/2}\omega(\mathbf{Q}')^{3/2}\|\mathbf{P}\|^{-1}\,\mathrm{Dh}(\mathbf{P},\mathbf{Q},\mathbf{Q}')$. From (23) we have

$$2g(\mathbf{P},\mathbf{Q},\mathbf{Q}')=\int \frac{d\mathbf{Q}''}{2\omega(\mathbf{Q}'')^4\Omega(\mathbf{P},\mathbf{Q}'')^3}\,\hat{h}(\mathbf{P},\mathbf{Q},\mathbf{Q}'')\hat{h}(\mathbf{P},\mathbf{Q}'',\mathbf{Q}')$$
$$-\int \frac{d\mathbf{Q}''}{2\omega(\mathbf{Q}'')^4\Omega(\mathbf{P},\mathbf{Q}'')^2}\,(g(\mathbf{P},\mathbf{Q},\mathbf{Q}'')\hat{h}(\mathbf{P},\mathbf{Q}'',\mathbf{Q}')+\hat{h}(\mathbf{P},\mathbf{Q},\mathbf{Q}'')g(\mathbf{P},\mathbf{Q}'',\mathbf{Q}')),$$

where $\hat{h}(\mathbf{P},\mathbf{Q},\mathbf{Q}'):=\omega(\mathbf{Q})^{3/2}\omega(\mathbf{Q}')^{3/2}h(\mathbf{P},\mathbf{Q},\mathbf{Q}')$ for all $(\mathbf{P},\mathbf{Q},\mathbf{Q}')\in\mathbb{R}^6$. From this relation and from (32) follows the estimate for the the sup-norm $\|g\|_\infty$:

$$2\|g\|_\infty<4K_2^2\int \frac{d\mathbf{Q}''}{16\omega(\mathbf{Q}'')^7}+\|g\|_\infty 4K_2\int \frac{d\mathbf{Q}''}{8\omega(\mathbf{Q}'')^6}.$$

Now $\int d\mathbf{Q}''\,\omega(\mathbf{Q}'')^{-6}<2m^{-4}$. Thus we obtain a bound for $\|g\|_\infty(2-K_2m^{-4})$. Now $2 - K_2m^{-4} > 2 - 1/(4mK_1') > 2 - \frac{1}{8}$ is positive, so we get a bound for $\|g\|_\infty$ (we have used the value of K_1' given in Remark 2, after the proof of Proposition 3).

The existence of $\partial_{\|\mathbf{P}\|}\, Dh$ is obtained as follows. In the sequence (29) the variable $\|\mathbf{P}\|$ appears only in the kernels $\Omega(\mathbf{P},\mathbf{Q})^{-1}$ or as the limit of integration on a variable u appearing only in such kernels or as a limit of integration, etc.. It follows that (29) is a sequence of analytic functions of $\|\mathbf{P}\|$ in a strip along the real axis. To study the convergence we replace u by $u+i\eta$ in the integrals (25) and (26), with $|\eta|$ small enough for the inequality (28) to be still satisfied (or for a smaller constant K_1' if necessary). Let us denote by b_η and db_η the bilinear operators on $\mathscr{B}$ we get, for suitable fixed η. The fixed-point equation (27), written for b_η, can be solved by the fixed-point theorem and leads to a sequence like (29), convergent in the same ball of $\mathscr{B}$. Because all the bounds are independent of η the convergence is also uniform wrt η. Thus, the limit $h(\mathbf{P},\mathbf{Q},\mathbf{Q}')$ is analytic for $\|\mathbf{P}\|$ in a neighborhood of the real axis, for all fixed $\mathbf{Q}$, $\mathbf{Q}'$.

To see that $\partial_{\|\mathbf{P}\|}\, Dh$ is bounded, we first note that Dh is also given by a convergent sequence like (29), where b is sometimes replaced by db. Let us write $b(g_1,g_2)=\int dz[\,\kappa_1^1 g_1 g_2 + \kappa_2^1\, dg_1 g_2+\kappa_3^1 g_1\, dg_2]$ and $db(g_1,g_2)=\int dz[\,\kappa_1^2 g_1 g_2+\kappa_2^2\, dg_1 g_2+\kappa_3^2 g_1\, dg_2]$, where the κ_i^j are functions of u,x,y,z, which are easily deduced from (25), (26). Let k_2 be a constant such that $\|\int dz[(\partial_u^n\kappa_1^j)g_1g_2+(\partial_u^n\kappa_2^j)dg_1g_2+(\partial_u^n\kappa_3^j)g_1\, dg_2\|_\infty<k_2|g_1|_{\mathscr{B}}|g_2|_{\mathscr{B}}$ for all $n\in\{0,1\}$ and $j\in\{1,2\}$. Let us consider the sequence for $\partial_{\|\mathbf{P}\|}\, Dh$ similar to (29) as a power series in c, as suggested by (30). The sum of n-order terms is bounded, in the sup norm, by $k_2K_1'^{n-2}n\mathscr{N}_n|c|_{\mathscr{B}}^n$ for all $n\in\mathbb{N}$, where $\mathscr{N}_n$ is the number of terms of order n in the limit of (30). This number can be calculated by applying the fixed point theorem to the trivial equation on $\mathbb{C}$: $x=k+x^2$, and from this explicit expression we get the estimate $\mathscr{N}_n<4^n$. This ensures the convergence of the series, in the sup norm, for all $|c|_{\mathscr{B}}<(4K_1')^{-1}$. Thus $\partial_{\|\mathbf{P}\|}\, Dh$ is bounded.

Let us introduce the function $\tilde{c}(\|\mathbf{Q}\|,\|\mathbf{Q}'\|)=m^{-3}\omega(\mathbf{Q})^{3/2}\omega(\mathbf{Q}')^{3/2}c(\|\mathbf{Q}\|,\|\mathbf{Q}'\|)$. From (31) and the condition on K_2 already used, it follows that $|\tilde{c}|_{\mathscr{B}}<(4K_1')^{-1}$, and so $\tilde{c}$ is an acceptable function. Now the series for $\partial_{\|\mathbf{P}\|}\, Dh(\mathbf{P},\mathbf{Q},\mathbf{Q}')$ can be bounded as follows: for all c we use $|c(\|\mathbf{Q}''\|,\|\mathbf{Q}'''\|)|\leq|\tilde{c}(\|\mathbf{Q}''\|,\|\mathbf{Q}'''\|)|$, except for the first and last factors, which we bound as follows: $|c(\|\mathbf{Q}\|,\|\mathbf{Q}''\|)|\leq\omega(\mathbf{Q})^{-3/2}|\tilde{c}(\|\mathbf{Q}\|,\|\mathbf{Q}''\|)|$, $|c(\|\mathbf{Q}''\|,\|\mathbf{Q}'\|)|\leq\omega(\mathbf{Q}')^{-3/2}|\tilde{c}(\|\mathbf{Q}''\|,\|\mathbf{Q}'\|)|$, respectively. We get an overall factor $\omega(\mathbf{Q})^{-3/2}\omega(\mathbf{Q}')^{-3/2}$ times a series that converges uniformly because each term can be bounded, as explained above. As a consequence of all these results the following estimate holds:

$$\omega(\mathbf{Q})^{3/2}\omega(\mathbf{Q}')^{3/2}|\|\mathbf{P}\|\partial_{\|\mathbf{P}\|}\, Dh(\mathbf{P},\mathbf{Q},\mathbf{Q}')\|\mathbf{P}\|^{-1}|<k_3, \tag{33}$$

for some $k_3 \in (0,\infty)$, for all $(\mathbf{P},\mathbf{Q},\mathbf{Q}') \in \mathbb{R}^6$.

Second step. We show that Δ is self-adjoint, using theorems by Nelson and Kato-Rellich. Because $\{\mathbf{P},H_0,J,\mathbf{L}_0\}$ are the infinitesimal generators of a unitary continuous representation of a Lie group (by Appendix A and the properties of the tensor product), it follows from a theorem by Nelson (see Ref. 11, Theorem 3) that all these operators and $\Delta_0 = m^{-2}(H_0^2+\mathbf{P}^2)+J^2+\mathbf{L}_0^2$ are self-adjoint and that there exists a domain $\mathscr{D}_0$ that is a common invariant domain and a common core for all of them. However, the largest common invariant domain is

$$\mathscr{D} = \{\phi \in \mathscr{H} | H_0^{n_1} P_1^{n_2} P_2^{n_3} J^{n_4} L_{0,1}^{n_5} L_{0,2}^{n_6} \Delta_0^{n_7} \phi \in \mathscr{H}, \quad \text{for all } n_1,\ldots,n_7 \in \mathbb{N}\}; \tag{34}$$

thus $\mathscr{D}$ is also a common core. By the Kato-Rellich theorem (Theorem X.12 of Ref. 12), Δ is essentially self-adjoint on $\mathscr{D}$ if

$$\|(\Delta-\Delta_0)\phi\| \leqslant k_4\|\Delta_0\phi\| + k_5\|\phi\|, \tag{35}$$

for all $\phi \in \mathscr{D}$, for some $0<k_4<1$ and $0<k_5<\infty$.

The bound (35) turns out to be a condition on the interaction terms of H and $\mathbf{L}$. To establish such a bound we need a general estimate of the norm of vectors like

$$\phi_\xi(\mathbf{P},\mathbf{Q}) := \int \frac{d\sigma(\mathbf{Q}')}{\Omega(\mathbf{P},\mathbf{Q}')}\, \phi(\mathbf{P},\mathbf{Q}')\xi(\mathbf{P},\mathbf{Q},\mathbf{Q}'),$$

for $\phi \in \mathscr{D}$ and a suitable kernel ξ. By using the Cauchy–Schwarz inequality and the Fubini theorem, as explained in detail in Ref. 6, we obtain

$$\|\phi_\xi\| \leqslant k_6\|\xi\|_{1/2,\infty}\|\phi\|, \tag{36}$$

where $k_6 := \sup \int d\sigma(\mathbf{Q})/(\Omega(\mathbf{P},\mathbf{Q})\omega(\mathbf{Q})) = \frac{1}{2}\int d\sigma(\mathbf{Q})\omega(\mathbf{Q})^{-2} = \pi/(2m)$ and

$$\|\xi\|_{\alpha,\infty} := \sup_{(\mathbf{P},\mathbf{Q},\mathbf{Q}') \in \mathbb{R}^6} \omega(\mathbf{Q})^\alpha \omega(\mathbf{Q}')^\alpha |\xi(\mathbf{P},\mathbf{Q},\mathbf{Q}')|, \tag{37}$$

for any $\alpha \in \mathbb{R}$. Now

$$\Delta - \Delta_0 = m^{-2}(H^2 - H_0^2) + \mathbf{L}^2 - \mathbf{L}_0^2.$$

For all $\phi \in \mathscr{D}$,

$$(H^2-H_0^2)\phi(\mathbf{P},\mathbf{Q}) = \int \frac{d\sigma(\mathbf{Q}')}{\Omega(\mathbf{P},\mathbf{Q}')}\, \phi(\mathbf{P},\mathbf{Q}')\Xi(\mathbf{P},\mathbf{Q},\mathbf{Q}'),$$

where

$$\Xi(\mathbf{P},\mathbf{Q},\mathbf{Q}') := (\Omega(\mathbf{P},\mathbf{Q})+\Omega(\mathbf{P},\mathbf{Q}'))h(\mathbf{P},\mathbf{Q},\mathbf{Q}') + \int \frac{d\sigma(\mathbf{Q}'')}{\Omega(\mathbf{P},\mathbf{Q}'')}\, h(\mathbf{P},\mathbf{Q}',\mathbf{Q}'')h(\mathbf{P},\mathbf{Q}'',\mathbf{Q}'). \tag{38}$$

By the following inequality: $\Omega(\mathbf{P},\mathbf{Q})+\Omega(\mathbf{P},\mathbf{Q}') \leqslant 2(\|\mathbf{P}\|+\omega(\mathbf{Q})+\omega(\mathbf{Q}')) \leqslant 2(\|\mathbf{P}\|+2\omega(\mathbf{Q})\omega(\mathbf{Q}')/m)$ and the estimate (36), we obtain

$$\|(H^2-H_0^2)\phi\| < 2k_6\|h\|_{1/2,\infty}\|(\|\mathbf{P}\|)\phi\| + \left[\frac{4k_6}{m}\|h\|_{3/2,\infty} + k_6^2\|h\|_{1/2,\infty}^2\right]\|\phi\|. \tag{39}$$

Because the coefficient of $\|\phi\|$ has not to be bounded, we omit to estimate it explicitly henceforth. Now let us put $\mathbf{L}_h := \mathbf{L} - \mathbf{L}_0$. We have to control the action of $\mathbf{L}^2 - \mathbf{L}_0^2 = \mathbf{L}_0 \cdot \mathbf{L}_h + \mathbf{L}_h \cdot \mathbf{L}_0 + \mathbf{L}_h^2$ on vectors $\phi \in \mathscr{D}$. Because $h(\mathbf{P},\mathbf{Q},\mathbf{Q})$ is only a function of the norms $\|\mathbf{P}\|,\|\mathbf{Q}\|,\|\mathbf{Q}\|$, we have $J^{\mathbf{Q}} h = J^{\mathbf{Q}'} h = 0$, and thus the terms $L_{0,j}^{\mathbf{Q}}$ of $L_{0,j}$ give no contribution. Thus, for the vector $\mathbf{L}_h \phi$, we find

$$\mathbf{L}_h \phi(\mathbf{P},\mathbf{Q}) = \int \frac{d\sigma(\mathbf{Q}')}{\Omega(\mathbf{P},\mathbf{Q}')} [\mathbf{L}_0 \phi(\mathbf{P},\mathbf{Q}')] \frac{h(\mathbf{P},\mathbf{Q},\mathbf{Q}')}{\Omega(\mathbf{P},\mathbf{Q}')} - i \int \frac{d\sigma(\mathbf{Q}')}{\Omega(\mathbf{P},\mathbf{Q}')} \phi(\mathbf{P},\mathbf{Q}') \times \left[\frac{\mathbf{P}}{\|\mathbf{P}\|} \frac{Dh(\mathbf{P},\mathbf{Q},\mathbf{Q}')}{\Omega(\mathbf{P},\mathbf{Q}')} - \frac{\mathbf{P}}{\Omega(\mathbf{P},\mathbf{Q}')^2} h(\mathbf{P},\mathbf{Q},\mathbf{Q}') \right], \tag{40}$$

for all $\phi \in \mathscr{D}$. Using the bound (36) we obtain

$$\|L_{h,j}\phi\| < \frac{k_6}{2m} \|h\|_{1/2,\infty} \|L_{0,j}\phi\| + \frac{k_6}{2m} \|(|h| + |Dh|)\|_{1/2,\infty} \|\phi\|, \tag{41}$$

for all $j \in \{1,2\}$. Replacing ϕ by $\mathbf{L}_0 \phi$ in (40) leads to the estimate

$$\|\mathbf{L}_h \cdot \mathbf{L}_0 \phi\| < \frac{k_6}{2m} \left\{ \|h\|_{1/2,\infty} \|\mathbf{L}_0^2 \phi\| + \|(|h| + |Dh|)\|_{1/2,\infty} \sum_{j=1}^{2} \|L_{0,j}\phi\| \right\}. \tag{42}$$

On the other hand, applying $\mathbf{L}_0$ to (40) gives

$$\begin{aligned} \mathbf{L}_0 \cdot \mathbf{L}_h \phi(\mathbf{P},\mathbf{Q}) = & \int \frac{d\sigma(\mathbf{Q}')}{\Omega(\mathbf{P},\mathbf{Q}')} \frac{\Omega(\mathbf{P},\mathbf{Q})}{\Omega(\mathbf{P},\mathbf{Q}')} [\mathbf{L}_0^2 \phi(\mathbf{P},\mathbf{Q}')] \frac{h(\mathbf{P},\mathbf{Q},\mathbf{Q}')}{\Omega(\mathbf{P},\mathbf{Q}')} \\ & - i \int \frac{d\sigma(\mathbf{Q}')}{\Omega(\mathbf{P},\mathbf{Q}')} \frac{\Omega(\mathbf{P},\mathbf{Q})}{\Omega(\mathbf{P},\mathbf{Q}')} [\mathbf{P} \cdot \mathbf{L}_0 \phi(\mathbf{P},\mathbf{Q}')] \\ & \times \left[-3 \frac{h(\mathbf{P},\mathbf{Q},\mathbf{Q}')}{\Omega(\mathbf{P},\mathbf{Q}')^2} + \left(\frac{2}{\Omega(\mathbf{P},\mathbf{Q}')} + \frac{1}{\Omega(\mathbf{P},\mathbf{Q})} \right) \frac{Dh(\mathbf{P},\mathbf{Q},\mathbf{Q}')}{\|\mathbf{P}\|} \right] \\ & - \Omega(\mathbf{P},\mathbf{Q}) \int d\sigma(\mathbf{Q}') \phi(\mathbf{P},\mathbf{Q}') (2 + \|\mathbf{P}\| \partial_{\|\mathbf{P}\|}) \\ & \times \left[\frac{Dh(\mathbf{P},\mathbf{Q},\mathbf{Q}')}{\|\mathbf{P}\| \Omega(\mathbf{P},\mathbf{Q}')^2} - \frac{h(\mathbf{P},\mathbf{Q},\mathbf{Q}')}{\Omega(P,q')^3} \right], \end{aligned}$$

for all $\phi \in \mathscr{D}$. We note in the last term the factor $\|\mathbf{P}\| \partial_{\|\mathbf{P}\|} Dh \|\mathbf{P}\|^{-1}$, the control of which requires the estimate (33). By $\Omega(\mathbf{P},\mathbf{Q})/\Omega(\mathbf{P},\mathbf{Q}') \leqslant (\omega(\mathbf{Q}) + \omega(\mathbf{Q}'))/m \leqslant 2\omega(\mathbf{Q})\omega(\mathbf{Q}')/m^2$, the inequality (36) and some trivial algebra, we obtain

$$\|\mathbf{L}_0 \cdot \mathbf{L}_h \phi\| \leqslant \frac{k_6}{m^3} \left(\|h\|_{3/2,\infty} \|\mathbf{L}_0^2 \phi\| + 3 \|(|h| + |Dh|)\|_{3/2,\infty} \sum_{i=1}^{2} \|L_{0,i}\phi\| \right) + k_7 \|\phi\|, \tag{43}$$

for some $k_7 \in (0,\infty)$ in which the constant k_3 of (33) is involved. By applying $\mathbf{L}_h$ to the expression (40) and by using (43) we get an estimate of the last term

$$\|\mathbf{L}_h^2\phi\| \leqslant \frac{k_6}{2m}\,\|(|h|+|Dh|)\|_{1/2,\infty}\left(\|\mathbf{L}_0\cdot\mathbf{L}_h\phi\|+\sum_{j=1}^{2}\|L_{h,j}\phi\|\right)$$
$$\leqslant \frac{k_6^2}{2m^6}\,(\|(|h|+|Dh|)\|_{3/2,\infty})^2\left(\|\mathbf{L}_0^2\phi\|+\frac{7}{2}\sum_{j=1}^{2}\|L_{0,j}\phi\|\right)+k_8\|\phi\|, \tag{44}$$

for some $k_8\in(0,\infty)$, where we have used $\|h\|_{1/2,\infty}\leqslant m^{-2}\|h\|_{3/2,\infty}$. More generally, from the definition (37) and the bound (32), it follows that

$$\|(|h|+|Dh|)\|_{1/2,\infty}\leqslant m^{-2}\|(|h|+|Dh|)\|_{3/2,\infty}<\frac{2K_2}{m^2}. \tag{45}$$

Finally, by collecting the estimates (39) and (42) to (45), we obtain

$$\|(\Delta-\Delta_0)\phi\|\leqslant 7(a+a^2)\left(\left\|\frac{\|\mathbf{P}\|}{m}\,\phi\right\|1+\sum_{j=1}^{2}\|L_{0,j}\phi\|\right)+(3a+2a^2)\|\mathbf{L}_0^2\phi\|+k_9\|\phi\|, \tag{46}$$

for some $k_9\in(0,\infty)$ and all $\phi\in\mathscr{D}$, where $a:=k_6K_2/m^3$. It remains to find a bound on $\|(\|P\|)\phi\|,\|L_{0,j}\phi\|,\|\mathbf{L}_0^2\phi\|$ of the type $k_{10}\|\Delta_0\phi\|+k_{11}\|\phi\|$ for constants k_{10} and k_{11}. Following Nelson (Ref. 11, proof of Lemma 6.1), we find

$$\left\|\frac{\|\mathbf{P}\|}{m}\,\phi\right\|+\sum_{j=1}^{2}\|L_{0,j}\phi\|\leqslant\sqrt{3}\left(\left\|\frac{\|\mathbf{P}\|}{m}\,\phi\right\|^2+\|\mathbf{L}_0\phi\|^2+\left\|\frac{H_0}{m}\,\phi\right\|^2+\|J\phi\|^2\right)^{1/2}$$
$$=\sqrt{3}(\phi,\Delta_0\phi)^{1/2}$$

$$<\sqrt{3}(\phi,(\tfrac{1}{2}\,\Delta_0^2+\Delta_0+\tfrac{1}{2})\phi)^{1/2}$$
$$=\sqrt{\tfrac{3}{2}}\|(\Delta_0+1)\phi\|\leqslant\sqrt{\tfrac{3}{2}}(\|\Delta_0\phi\|+\|\phi\|). \tag{47}$$

The bound on $\|\mathbf{L}_0^2\phi\|$ needs more development. Following Ref. 11 (proof of Lemma 6.1) again, we try to write $\Delta_0^2-(\mathbf{L}_0^2)^2$ as a sum of positive and negative operators. For that we use the commutation rules (1)–(4), which imply

$$\mathbf{P}^2\mathbf{L}^2+\mathbf{L}^2\mathbf{P}^2=\sum_{i,j=1}^{2}(P_iL_j^2P_i+L_iP_j^2L_i)-\mathbf{P}^2-4H^2,$$

$$H^2\mathbf{L}^2+\mathbf{L}^2H^2=H\mathbf{L}^2H+\mathbf{L}\cdot H^2\mathbf{L}-2\mathbf{P}^2-2H^2,$$

$$J^2\mathbf{L}^2+\mathbf{L}^2J^2=J\mathbf{L}^2J+\mathbf{L}\cdot J^2\mathbf{L}-\mathbf{L}^2,$$

$$J^2\mathbf{P}^2+\mathbf{P}^2J^2=J\mathbf{P}^2J+\mathbf{P}\cdot J^2\mathbf{P}-\mathbf{P}^2.$$

From these relations it follows that $\Delta_0^2-(\mathbf{L}_0^2)^2+m^{-2}(4\mathbf{P}^2+6H_0^2)+\mathbf{L}_0^2$ is a positive operator, and thus

$$(\mathbf{L}_0^2)^2 < \Delta_0^2 + m^{-2}(4\mathbf{P}^2 + 6H_0^2) + \mathbf{L}_0^2 < \Delta_0^2 + 6\Delta_0 + 9 = (\Delta_0 + 3)^2,$$

and finally $\|\mathbf{L}_0^2\phi\| < \|(\Delta_0+3)\phi\| \leqslant \|\Delta_0\phi\| + 3\|\phi\|$. By collecting all these results, the estimate (46) becomes

$$\|(\Delta - \Delta_0)\phi\| < (a + a^2)\left(3 + 7\sqrt{\frac{3}{2}}\right)\|\Delta_0\phi\| + k_{12}\|\phi\|,$$

for some constant $k_{12} \in (0,\infty)$ and all $\phi \in \mathscr{D}$. Let us compare this with the requirement (35). The necessary condition $k_4 := (a + a^2)(3 + 7\sqrt{3/2}) < 1$ is satisfied for $a \leqslant \pi/40$. Because $a = k_6 K_2/m^3 = \pi K_2/(2m^4)$ we get $K_2 \leqslant m^4/20$.

Third step. We show the essential self-adjointness of H, $\mathbf{P}$, J, and $\mathbf{L}$ on $\mathscr{D}$ and establish the Conclusion 3). We already know that H_0, $\mathbf{P}$, J, and $\mathbf{L}_0$ are essentially self-adjoint on $\mathscr{D}$ (second step). Then H is also essentially self-adjoint on $\mathscr{D}$ because

$$(H - H_0)\phi(\mathbf{P},\mathbf{Q}) = \int \frac{d\sigma(\mathbf{Q}')}{\Omega(\mathbf{P},\mathbf{Q}')}\,\phi(\mathbf{P},\mathbf{Q}')h(\mathbf{P},\mathbf{Q},\mathbf{Q}') \tag{48}$$

is well defined for all $\phi \in \mathscr{H}$ [because of (36) and because, by (31), $\|h\|_{1/2,\infty} < K_2/(4m^2)$]. Note the bound on the operator norm: $\|H - H_0\|_{\mathrm{op}} \leqslant k_6\|h\|_{1/2,\infty}$. For $\mathbf{L}$ we consider the bound (41). From the Kato-Rellich theorem (Theorem X.12 of Ref. 12) it follows that $\mathbf{L}$ is essentially self-adjoint on $\mathscr{D}$, provided $k_6\|h\|_{1/2,\infty}/(2m) < 1$ (note that this condition leads to $\|H - H_0\|_{\mathrm{op}} < 2m$ and thus implies the positivity of H), which holds, because by (45): $k_6\|h\|_{1/2,\infty}/(2m) \leqslant K_2 k_6/m^3 = a$ and because $a \leqslant \pi/40$ (see the second step).

By using the methods of the second step it is easy (but tedious) to check that all products AB with $A \neq B$, where A,B are any pair of operators H, P_1, P_2, J, L_1, L_2, are well defined on $\mathscr{D}$ because of (32) and (33) (the second step of this proof concerned the squares A^2 and can be taken as examples). For more details see similar estimates in Ref. 7 in the one space dimension case. These calculations give clear, explicit expressions that make evident the symmetry property stated in the Conclusion 3), and on which the commutation rules, which already hold on an algebraical level by proposition 2, can be verified analytically. □

Remark 1: From the explicit estimate of the constants K_1 and K_2 given in the previous proof, it follows that the function

$$c(x,y) = \lambda(x^2 + m^2)^{-3/4}(y^2 + m^2)^{-3/4}, \tag{49}$$

for all $x,y \in \mathbb{R}_+$ and all $|\lambda| < m^4/20$, satisfies all the hypotheses of Propositions 3 and 4.

Remark 2: Let us explain how Proposition 4 leads to the integrability condition of Ref. 10. We first verify the hypothesis of the commutation theorem (Ref. 12, Theorem X.37) or (Ref. 10, Theorem 0′). By (2) the operator $N := \Delta + 1$ is essentially self-adjoint on the domain $\mathscr{D}$ given by (34). The first hypothesis follows then from Nelson's argument used to establish (47) (without the index 0). Now by (3) the following calculation makes sense on $\mathscr{D}$:

$$
\begin{aligned}
(H\phi,N\phi)-(N\phi,H\phi)&=(H\phi,\mathbf{L}^2\phi)-(\mathbf{L}\phi,H\phi)\\
&=\sum_{j=1}^{2}(L_jH\phi,L_j\phi)-(L_j\phi,L_jH\phi)\\
&=\sum_{j=1}^{2}(HL_j\phi,L_j\phi)+i(P_j\phi,L_j\phi)-(L_j\phi,HL_j\phi)+i(L_j\phi,P_j\phi)\\
&=i(\phi,(\mathbf{P}\cdot\mathbf{L}+\mathbf{L}\cdot\mathbf{P})\phi),
\end{aligned}
$$

where we have taken the case of H as an example. Now for all $\phi\in\mathscr{D}$:

$$
0\leqslant\|(m^{-1}P_j\pm L_j)\phi\|^2=(\phi,(m^{-1}P_j\pm L_j)^2\phi)=(\phi,(m^{-2}P_j^2+L_j^2)\phi))\pm m^{-1}(\phi,(P_jL_j+L_jP_j)\phi),
$$

for all $j\in\{1,2\}$, from which it follows

$$
m^{-1}|(\phi,(\mathbf{P}\cdot\mathbf{L}+\mathbf{L}\cdot\mathbf{P})\phi)|\leqslant(\phi,(m^{-2}\mathbf{P}^2+\mathbf{L}^2)\phi)<(\phi,N\phi),
$$

and then the hypotheses of the commutation theorem are satisfied. The integrability of our algebra representation follows then from Ref. 10, Corollary 4.

V. THE CASIMIR OPERATORS

We study the modification of the Casimir operators [defined by (5) and given in the two free particle representations by (18)–(19)] due to the introduction of interaction. From the operators of the interaction representation (12) and the commutation rules (11) for $\mathscr{O}$, it follows that the Pauli–Lubanski operator E takes the form

$$
E=E_0+\{\mathscr{O},E_0\},
$$

where E_0 is the Pauli–Lubanski operator of the free representation, given by (19). Now the condition that the kernel $h(\mathbf{P},\mathbf{Q},\mathbf{Q}')$ of the operator $\mathscr{O}$ depends only on the norms $\|\mathbf{P}\|,\|\mathbf{Q}\|,\|\mathbf{Q}'\|$ has the consequence that

$$
J^{\mathbf{Q}}\mathscr{O}=\mathscr{O}J^{\mathbf{Q}}=0, \tag{50}
$$

from which it follows that $E_0\mathscr{O}=\mathscr{O}E_0=0$, and thus

$$
E=E_0. \tag{51}
$$

Thus, the introduction of interaction has no effect on the Pauli–Lubanski operator. On the other hand, the square mass operator M^2 takes the form

$$
M^2\phi(\mathbf{P},\mathbf{Q})=4(\mathbf{Q}^2+m^2)\phi(\mathbf{P},\mathbf{Q})+\int\frac{d\sigma(\mathbf{Q}')}{\Omega(\mathbf{P},\mathbf{Q}')}\,\phi(\mathbf{P},\mathbf{Q}')\Xi(\mathbf{P},\mathbf{Q},\mathbf{Q}'), \tag{52}
$$

for all $\phi\in\mathscr{D}$, where the kernel Ξ is given by (38). Note that the spectrum of M_0^2, the square-mass operator of the two free particle representations, given by (18), is absolutely continuous, made of the complete interval $[4m^2,\infty)$. The introduction of interaction has the important effect that an isolated eigenvalue may occur.

Proposition 5: Let c: $\mathbb{R}_+^2\to\mathbb{C}$ *satisfying the hypothesis of Proposition 4 and* h *as there. Then the operator* M^2 *is self-adjoint. Moreover, let* c *be given by (49); then for all* $0>\lambda>-m^4/20$, M^2 *has an eigenvalue* $0<m_B^2<4m^2$, *and its spectrum is* $\{m_B^2\}\cup[4m^2,\infty)$.

Proof: Because H and $\mathbf{P}$ commute they admit a simultaneous spectral measure $dE(\rho,\mathbf{P})$, where $\rho>0$ is the spectral variable associated to H. In this representation M^2 becomes simply the multiplication operator by $\rho^2-\mathbf{P}^2$, and thus is self-adjoint. Moreover, the invariant subspaces are limited in the $(\rho,\mathbf{P})$ space by the half-hyperboloids $\{\rho = \sqrt{\mathbf{P}^2+K^2}\}$ with $K>0$, and so is the support of dE.

Let us consider the one-parameter group of operators $\{U_1(\gamma)\}_{\gamma\in\mathbb{R}}$ defined by

$$U_1(\gamma)\phi(\rho,\mathbf{P}) := \phi(\rho\ \cosh\ \gamma + P_1\ \sinh\ \gamma, P_1\ \cosh\ \gamma + \rho\ \sinh\ \gamma, P_2),$$

for all $\phi\in L^2(\mathbb{R}^3,dE)$ with compact support [note that $U_1(\gamma)$ is not necessarily $\exp(i\gamma L_1)$]. In the $(\rho,\mathbf{P})$ space, $U_1(\gamma)$ translates a point $(\rho_0,\mathbf{P}_0)$ on the hyperboloid $\{\rho=(\mathbf{P}^2+\rho_0^2-\mathbf{P}_0^2)^{1/2}\}$ restricted to the $P_2=P_{0,2}$ plane, from a ''hyperbolic angle'' γ. Obviously $U_1(\gamma)$ commutes with M^2. In the same way we define the one-parameter group $\{U_2(\gamma)\}_{\gamma\in\mathbb{R}}$, acting on the P_2 variable. Thus, by suitable applications of these groups we can reduce the study of the spectrum of M to a neighborhood of $\mathbf{P}=0$, that is to the restriction of M to the subspace,

$$\mathscr{H}_\epsilon := \text{closure}_{\mathscr{H}}\{\phi\in\mathscr{H}\,|\,\phi(\mathbf{P},\mathbf{Q})=0, \quad \text{for all } \|\mathbf{P}\|>\epsilon\}, \tag{53}$$

for arbitrary small $\epsilon>0$.

On the other hand, let us consider the operator $M_{\mathbf{P}}^2$ (i.e, for fixed $\mathbf{P}$), given by

$$M_p^2\varphi(\mathbf{Q}) := 4(\mathbf{Q}^2+m^2)\varphi(\mathbf{Q}) + \int d\sigma_{\mathbf{P}}(\mathbf{Q}')\varphi(\mathbf{Q}')\Xi(\mathbf{P},\mathbf{Q},\mathbf{Q}'), \tag{54}$$

for suitable φ in the space $\mathscr{H}_{\mathbf{P}}=L^2(\mathbb{R},d\sigma_{\mathbf{P}})$, where $d\sigma_{\mathbf{P}}(\mathbf{Q})=d\sigma(\mathbf{Q})\Omega(\mathbf{P},\mathbf{Q})^{-1}$. Here $\mathbf{P}\in\mathbb{R}^2$ is just a set of two parameters.

Let $H_{\mathbf{P}}$ be the restriction of H for fixed $\mathbf{P}$, as an operator on $\mathscr{H}_{\mathbf{P}}$. Because $M_{\mathbf{P}}^2 = H_{\mathbf{P}}^2 - \mathbf{P}^2$ the spectrum of $M_{\mathbf{P}}^2$ is easily deduced from the spectrum of $H_{\mathbf{P}}$. We write $H_{\mathbf{P}} = \Omega + H_{h,\mathbf{P}}$ where $H_{h,\mathbf{P}}\varphi(\mathbf{Q}) := \int d\sigma_{\mathbf{P}}(\mathbf{Q}')\varphi(\mathbf{Q}')h(\mathbf{P},\mathbf{Q},\mathbf{Q}')$ for all $\varphi\in\mathscr{H}_{\mathbf{P}}$. Because $\int|h(\mathbf{P},\mathbf{Q},\mathbf{Q}')|^2\,d\sigma_{\mathbf{P}}(\mathbf{Q})d\sigma_{\mathbf{P}}(\mathbf{Q}')$ is well defined [by (32)], $H_{h,\mathbf{P}}$ is compact. By the ''classical Weyl theorem'' (Ref. 13, Sec. XIII.4) the essential spectrum of $\mathscr{H}_{\mathbf{P}}$ is the same as of $\Omega(\mathbf{P},\mathbf{Q})$ (for fixed $\mathbf{P}$), that is the interval $[\Omega(\mathbf{P},\mathrm{O}),\infty)$. It may exist a finite number of eigenvalues in $(0,\Omega(\mathbf{P},0))$, with finite-dimensional eigenspaces. Moreover, $\mathbf{P}\to H_{h,\mathbf{P}}$ is an analytic family of compact operators in a $\mathbb{C}^2$ neighborhood of the real axis [because by giving a small imaginary value to $\mathbf{P}$ the integral $\int|h(\mathbf{P},\mathbf{Q},\mathbf{Q}')|^2\,d\sigma_{\mathbf{P}}(\mathbf{Q})d\sigma_{\mathbf{P}}(\mathbf{Q}')$ is still defined]. Thus $H_{\mathbf{P}}$ is an ''analytic family of type (A)'' and by Theorem XII.13 of Ref. 13 the eigenvalues, if there are any, are continuous functions of $\mathbf{P}$. Returning to the operator $M_{\mathbf{P}}^2 = H_{\mathbf{P}}^2 - \mathbf{P}^2$ we conclude that its spectrum is made of the interval $[4m^2,\infty)$ and of a finite number of possible eigenvalues in the interval $(0,4m^2)$, which are continuous with respect to $\mathbf{P}$.

Now let us consider the case where an eigenvalue exists. By the theory of Ref. 13, Sec. XIII.16, and more precisely by the point (d) of theorem XIII.85 of this reference, follows that the spectrum of M^2 restricted to the subspace $\mathscr{H}_\epsilon$ given by (53), has, in fact, a gap. By the geometrical form of the support of dE this property passes on to the operator M^2 itself.

Let us take now the functions c given by (49). Because the eigenvalues of $H_{\mathbf{P}}$ are continuous in $\mathbf{P}$, they are eigenvalues of H_0 for $\mathbf{P}=0$, that is, solutions of the equation

$$2\sqrt{\mathbf{Q}^2+m^2}\varphi(\mathbf{Q}) + \lambda\,\omega(\mathbf{Q})^{-3/2}\int \frac{d\mathbf{Q}'}{4(\mathbf{Q}'^2+m^2)}\,\varphi(\mathbf{Q}')\omega(\mathbf{Q}')^{-3/2} = m_B\varphi(\mathbf{Q}),$$

which admits one and only one eigenvalue $0<m_B<2m$, with eigenvector $\varphi(\mathbf{Q})=\omega(\mathbf{Q})^{-3/2}(2\omega(\mathbf{Q})-m_B)^{-1}$, where m_B is the unique solution of the implicit equation

$$1=-\lambda\int\frac{d\mathbf{Q}}{4(\mathbf{Q}^2+m^2)^{5/2}}\frac{1}{2\sqrt{\mathbf{Q}^2+m^2}-m_B},$$

for $0>\lambda>-m^4/20$. From the geometrical form of the support of dE, it follows that the spectrum of M^2 is made of only one isolated eigenvalue m_B^2 and of the continuous interval $[2m,\infty]$. □

Remark: The eigenvalue equation for M^2, given by (51), takes the form

$$m_B^2\phi(\mathbf{P},\mathbf{Q})=4(\mathbf{Q}^2+m^2)\phi(\mathbf{P},\mathbf{Q})+\int\frac{d\sigma(\mathbf{Q}')}{\Omega(\mathbf{P},\mathbf{Q}')}\phi(\mathbf{P},\mathbf{Q}')\Xi(\mathbf{P},\mathbf{Q},\mathbf{Q}'),\tag{55}$$

where Ξ is given by (38) and m_B is expected to lie in $(0,2m)$. (55) can be considered as a *relativistic Schrödinger equation* because it generates the discrete structure of the bound states. Note that, due to the variables (15), it has the same general form as the Schrödinger equation, but with two important differences: the interaction is nonlocal and depends on $\mathbf{P}$. Contrary to the nonrelativistic case, this dependence cannot be removed, unless a particular referential frame is chosen, a center-of-mass frame. In that case, i.e. for $\mathbf{P}=0$, (55) reduces to

$$(m_B^2-4m^2)\varphi(\mathbf{Q})=4\mathbf{Q}^2\varphi(\mathbf{Q})+\int\frac{d\sigma(\mathbf{Q}')}{2\omega(\mathbf{Q}')}\varphi(\mathbf{Q}')\Xi(0,\mathbf{Q},\mathbf{Q}'),\tag{56}$$

which, except for the nonlocal interaction, is a Schrödinger-like equation. Moreover, for $\mathbf{P}=0$ the operator M^2 is the square of H, so that the eigenvalue equation (56) can be written for H, and becomes

$$m_B\varphi(\mathbf{Q})=2\sqrt{\mathbf{Q}^2+m^2}\varphi(\mathbf{Q})+\int\frac{d\sigma(\mathbf{Q}')}{2\omega(\mathbf{Q}')}\varphi(\mathbf{Q}')c(\|\mathbf{Q}\|,\|\mathbf{Q}'\|),\tag{57}$$

where $c(\|\mathbf{Q}\|,\|\mathbf{Q}'\|)=h(0,\mathbf{Q},\mathbf{Q}')$ is a center-of-mass interaction kernel (which can be chosen arbitrarily). Note that (57) corresponds to some kind of elementary (or naïve) generalization of the Schrödinger equation to the relativistic case.

VI. CONCLUSION

Let us sum up what we have found. We have constructed a family of unitary, continuous representations of the Poincaré group in three space–time dimensions, as perturbations of the two free boson model. These perturbations are nontrivial, in the sense that isolated eigenvalues of the Casimir operator M may appear (but the Casimir operator E, the Pauli–Lubanski operator, remains unchanged). To affirm that we have really obtained models for two bosons with interaction, it remains to construct the asymptotic states. For that we only need to show the existence of the generalized wave operators (Ref. 14, Sec. XI.3). This can be obtained from Cook's method (Theorem XI.4 of Ref. 14), with $A=H$ and $B=H_0$, and from the further assumption that $c\in C^2(\mathbb{R}_+^2)$ (with right derivation at 0), with first and second derivatives also bounded [the example (49) satisfies these conditions]. Let us consider the functions

$$F(t,\mathbf{P},\mathbf{Q})=\int\frac{d\sigma(\mathbf{Q}')}{\Omega(\mathbf{P},\mathbf{Q}')}\phi(\mathbf{P},\mathbf{Q}')h(\mathbf{P},\mathbf{Q},\mathbf{Q}')e^{-it\Omega(\mathbf{P},\mathbf{Q}')},\tag{58}$$

for $\phi\in\mathscr{S}(\mathbb{R}^4)$ (the Schwartz space) satisfying $\phi(\mathbf{P},0,Q_2)=\partial_{Q_1}^{\nu}\phi(\mathbf{P},0,Q_2)=0$ for $\nu\in\{1,...,4\}$. Such vectors ϕ generate a dense subspace of $\mathscr{H}$. On the other hand, from the techniques of the first step of the proof of Proposition 4 [used to establish (33)] and from the new conditions on c, it follows that $h\in C^2(\mathbb{R}^6)$ with all derivatives bounded. Performing then two integrations by parts wrt Q_1' leads to

$$F(t,\mathbf{P},\mathbf{Q})=-\frac{1}{32t^2}\int d\mathbf{Q}'\ e^{-it\Omega(\mathbf{P},\mathbf{Q}')}\partial_{Q_1'}\left(\frac{\Omega(\mathbf{P},\mathbf{Q}')}{Q_1'}\,\partial_{Q_1'}\,\frac{\phi(\mathbf{P},\mathbf{Q}')h(\mathbf{P},\mathbf{Q},\mathbf{Q}')}{Q_1'\omega(\mathbf{Q}')}\right),$$

from which it follows that the function

$$t\mapsto\left[\int\frac{d\mathbf{P}\,d\sigma(\mathbf{Q}')}{\Omega(\mathbf{P},\mathbf{Q}')}\,|F(t,\mathbf{P},\mathbf{Q})|^2\right]^{1/2}=\|(H-H_0)e^{-itH_0}\phi\|, \tag{59}$$

is in $L^1([1,\infty))$, as required by Cook's method. In conclusion, provided c satisfies these new conditions, our models describe really two-particle systems.

However, the connection of these models with other physical theories, like QFT, is a difficult point. First, because of their particular interaction form, which by (50) can be formulated as follows: the image of the interaction operator $\mathscr{O}$ is contained in the subspace of states with vanishing relative angular momentum (the so-called ''s waves''). Second, because in three-dimensional space–time QFT there are few available bosonic models in which bound states are known to exist (see Ref. 3, Sec. IV). Following the example of the two space–time dimension case, we could find a connection for constant kernel c, with QFT models admitting point interaction (i.e., with a $\lambda\phi_3^4$ term in the Hamiltonian) at first perturbation orders. But these models are defined only for $\lambda\geqslant 0$, in which case bound states are absent. On the other hand, a constant c may satisfy the hypothesis of Proposition 3, but not of Proposition 4.

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APPENDIX A: ONE-PARTICLE REPRESENTATION

We show that the operators (6) are the infinitesimal generators of a unitary, continuous and irreducible representation of the universal covering of the Poincaré group $\mathscr{P}_+^\uparrow$. Such a representation is a good candidate for a theory describing a quantum relativistic spinless particle of mass $m>0$. To that purpose, and for the next appendix, we need the Lorentz transform $\Lambda_{\mathbf{v}}$ for an arbitrary velocity $\mathbf{v}\in\mathbb{R}^2$. It is given by a rotation (putting $\mathbf{v}$ parallel to the first axis) followed by a Lorentz boost (along this axis) and then by the inverse rotation. More precisely, if $\mathbf{v}=\|\mathbf{v}\|(\cos\alpha,\sin\alpha)$, we get

$$\Lambda_{\mathbf{v}}=\begin{pmatrix}1&0&0\\0&\cos\alpha&-\sin\alpha\\0&\sin\alpha&\cos\alpha\end{pmatrix}\begin{pmatrix}\gamma&\beta\gamma&0\\\beta\gamma&\gamma&0\\0&0&1\end{pmatrix}\begin{pmatrix}1&0&0\\0&\cos\alpha&\sin\alpha\\0&-\sin\alpha&\cos\alpha\end{pmatrix}$$

$$=\begin{pmatrix}\gamma&\beta_1\gamma&\beta_2\gamma\\\beta_1\gamma&1+\dfrac{\beta_1^2}{\beta^2}(\gamma-1)&\dfrac{\beta_1\beta_2}{\beta^2}(\gamma-1)\\\beta_2\gamma&\dfrac{\beta_1\beta_2}{\beta^2}(\gamma-1)&1+\dfrac{\beta_2^2}{\beta^2}(\gamma-1)\end{pmatrix},$$

where we have put $\boldsymbol{\beta}=(\beta_1,\beta_2)=\mathbf{v}/c$, c being the speed of light, $\beta=\|\boldsymbol{\beta}\|$, and $\gamma=(1-\beta^2)^{-1/2}$. By applying this transformation to a three-dimensional vector $(p^0,\mathbf{p})=(p^0,p_1,p_2)\in\mathbb{R}^3$, we get a more compact expression,

$$\Lambda_{\mathbf{v}}\begin{pmatrix} p^0 \\ \mathbf{p} \end{pmatrix} = \begin{pmatrix} \gamma(p^0 + \boldsymbol{\beta}\cdot\mathbf{p}) \\ \gamma\left(p^0 + \dfrac{\boldsymbol{\beta}\cdot\mathbf{p}}{\beta^2}\right)\boldsymbol{\beta} + \dfrac{\mathbf{p}\wedge\boldsymbol{\beta}}{\beta^2}\,\boldsymbol{\beta}^{\perp} \end{pmatrix}, \tag{A1}$$

where $\boldsymbol{\beta}\cdot\mathbf{p} := \beta_1 p_1 + \beta_2 p_2$, $\boldsymbol{\beta}^{\perp} := (\beta_2, -\beta_1)$, and $\mathbf{p}\wedge\boldsymbol{\beta} = \mathbf{p}\cdot\boldsymbol{\beta}^{\perp} = p_1\beta_2 - p_2\beta_1$. Let us take $c=1$ again. The Poincaré representation describing one particle of mass $m>0$ without spin is given by the following result.

Lemma 6: The operators (6) are the infinitesimal generators of a unitary, continuous and irreducible representation of the universal covering of the Poincaré group $\mathscr{P}_+^{\uparrow}$ in the space $L^2(\mathbb{R}^2,\sigma)$.

We recall that $d\sigma(\mathbf{p}) = d\mathbf{p}[2\omega(\mathbf{p})]^{-1}$, where $\omega(\mathbf{p}) = \sqrt{\mathbf{p}^2+m^2}$.

Proof: Let us consider the following transformations of functions $\phi\in L^2(\mathbb{R},\sigma)$:

$$(\boldsymbol{\xi},\tau,\alpha,\boldsymbol{\beta})\cdot\phi(\mathbf{p}) := e^{i(\boldsymbol{\xi}\cdot\mathbf{p}+\tau\omega(\mathbf{p}))}\phi(\lambda_{\boldsymbol{\beta}}\,R_{\alpha}\mathbf{p}), \tag{A2}$$

for all $\tau\in\mathbb{R}$, ξ, $\beta\in\mathbb{R}^2$, $\alpha\in[0,2\pi)$ and almost all $\mathbf{p}\in\mathbb{R}^2$, where R_{α} is the matrix of the rotation of $\mathbb{R}^2$ of angle α and $\lambda_{\boldsymbol{\beta}}\mathbf{p}$ is the ''spatial'' component of the Lorentz transform of $(\omega(\mathbf{p}),\mathbf{p})$ of speed $\boldsymbol{\beta}$, more precisely, from (A1):

$$\lambda_{\boldsymbol{\beta}}\mathbf{p} := \gamma\left(\omega(\mathbf{p}) + \frac{\boldsymbol{\beta}\cdot\mathbf{p}}{\beta^2}\right)\boldsymbol{\beta} + \frac{\mathbf{p}\wedge\boldsymbol{\beta}}{\beta^2}\,\boldsymbol{\beta}^{\perp}. \tag{A3}$$

We claim that these transformations define a unitary, continuous, and irreducible representation in $L^2(\mathbb{R}^2,\sigma)$ of the Poincaré group $\mathscr{P}_+^{\uparrow}$, the infinitesimal generators of which are given by (6).

The unitarity and the group law are easily seen by introducing a third variable p^0 together with a Dirac-delta function in the measure, that is, by replacing $L^2(\mathbb{R}^2,\sigma)$ by $L^2(\mathbb{R}^3,\Sigma)$, where $d\Sigma(p^0,p_1,p_2) = dp^0\,dp_1\,dp_2\,\delta(p^{02}-p_1^2-p_2^2-m^2)\,\theta(p^0)$, θ being the Heaviside function. Because of the Σ measure, a vector $\phi(p^0,p_1,p_2)$ is not distinguished from $\phi(\sqrt{p_1^2+p_2^2+m^2},p_1,p_2)$. The transformation (A2) becomes, after Fourier transformation,

$$(\boldsymbol{\xi},\tau,\alpha,\boldsymbol{\beta})\cdot\tilde{\phi}(t,\mathbf{x}) = \tilde{\phi}((\boldsymbol{\xi},\tau,\alpha,\boldsymbol{\beta})^{-1}\cdot(t,\mathbf{x}))$$

(where $\tilde{\phi}$ is the Fourier transform of ϕ) that is, given in terms of the ordinary Poincaré transformation on space–time. The group law is now obvious. The unitarity follows from the Poincaré invariance of the measure Σ.

The continuity of the representation is easily seen in $L^2(\mathbb{R}^2,\sigma)$, by standard analysis methods. The irreducibility is obtained as follows. Let ϕ be a continuous, nonzero function in $L^2(\mathbb{R}^2,\sigma)$. Let us show that the only vector orthogonal to $\{e^{i\boldsymbol{\xi}\cdot\mathbf{p}}\phi(\lambda_{\boldsymbol{\beta}}\mathbf{p})\,|\,\boldsymbol{\xi},\boldsymbol{\beta}\in\mathbb{R}^2\}$ is 0. By the Fourier theory,

$$\int_{\mathbb{R}^2} d\sigma(\mathbf{p})\,\psi(\mathbf{p})^* e^{i\boldsymbol{\xi}\cdot\mathbf{p}}\phi(\lambda_{\boldsymbol{\beta}}\mathbf{p}) = 0, \quad \text{for all } \boldsymbol{\xi}\in\mathbb{R}^2, \tag{A4}$$

implies that $\psi(\mathbf{p})=0$ for almost all $\mathbf{p}$, such that $\phi(\lambda_{\boldsymbol{\beta}}\mathbf{p})\neq 0$. Without loss of generality, we may assume that $\phi(0)\neq 0$. From (A3) follows that the vector $\boldsymbol{\beta} = -\mathbf{p}/\omega(\mathbf{p})$ satisfies $\lambda_{\boldsymbol{\beta}}\mathbf{p}=0$, for all $\mathbf{p}\in\mathbb{R}^2$. Thus, if moreover we impose that (A4) holds for all $\boldsymbol{\beta}\in\mathbb{R}^2$ we get $\psi=0$.

After an elementary calculation, the operators (6) turn out to be the infinitesimal generators of the representation (61). □

APPENDIX B: THE RELATIVE MOMENTUM

We explain the change of variable $(\mathbf{p}_1,\mathbf{p}_2)\to(\mathbf{P},\mathbf{Q})$ given in (15) and establish some useful formulas.

The meaning of $\mathbf{P}=\mathbf{p}_1+\mathbf{p}_2$, the total momentum, is clear. The notion of relative momentum is more subtle. Physically it must be related to the momentum of one of the particles in a center-of-mass frame.

Let $p_1=(\omega(\mathbf{p}_1),\mathbf{p}_1)$ and $p_2=(\omega(\mathbf{p}_2),\mathbf{p}_2)$ be the energy momenta of two free particles, of the same mass to simplify. We define first

$$P=(P^0,\mathbf{P})=p_1+p_2, \quad q=(q^0,\mathbf{q})=\tfrac{1}{2}(p_1-p_2).$$

Note the useful relation $\mathbf{P}\cdot\mathbf{q}=P^0q^0$. Let $\Lambda_{\boldsymbol{\beta}}$ be a Lorentz transformation such that $\Lambda_{\boldsymbol{\beta}}P=(M_0,\mathbf{0})$, where $M_0=[(P^0)^2-\mathbf{P}^2]^{1/2}$. Physically, $\Lambda_{\boldsymbol{\beta}}$ is associated with a change of referential frame, which put the two particles of momenta $\mathbf{p}_1,\mathbf{p}_2$ on one of their center-of-mass frames. Then we define the relative momentum $\mathbf{Q}$ as the spatial projection of $\Lambda_{\boldsymbol{\beta}}q$ [the relative momentum just defined (as the center-of-mass frame itself), is not unique because in its definition $\Lambda_{\boldsymbol{\beta}}$ could be followed by a fixed space rotation without consequence]. The calculation of a $\Lambda_{\boldsymbol{\beta}}$ i.e. of a $\boldsymbol{\beta}$, is obtained from (A3). The condition that the spatial component of $\Lambda_{\boldsymbol{\beta}}P$ vanishes gives

$$(1-\beta^2)^{-1/2}\left(P^0+\frac{\boldsymbol{\beta}\cdot\mathbf{P}}{\beta^2}\right)\boldsymbol{\beta}+\frac{\mathbf{P}\wedge\boldsymbol{\beta}}{\beta^2}\,\boldsymbol{\beta}^{\perp}=0.$$

If we choose the direction of $\boldsymbol{\beta}$ parallel to $\mathbf{P}$, we get the unique solution $\boldsymbol{\beta}=-\mathbf{P}/P^0$. After some calculation one gets $\Lambda_{-\mathbf{P}/P^0}q=(0,\mathbf{Q})$, where

$$\mathbf{Q}=\frac{q^0M_0}{\mathbf{P}^2}\,\mathbf{P}-\frac{\mathbf{q}\wedge\mathbf{P}}{\mathbf{P}^2}\,\mathbf{P}^{\perp}.$$

If we write it in the form $\mathbf{Q}=\mathbf{q}+\xi\mathbf{P}$, the calculation of $\mathbf{P}\cdot\mathbf{Q}$ leads to $\xi=-q^0[P^0+M_0]^{-1}$ and we finally get the formula (15).

Let us calculate the operators of the two free boson representation (7) in these variables, to establish (16). The norm $\|\mathbf{Q}\|$ is obtained by the initial definition of $\mathbf{Q}$ and the properties of the Lorentz transform, which gives $\mathbf{Q}^2=(q^0)^2-\mathbf{q}^2$. From the trivial identity $(P^0)^2-\mathbf{P}^2=4m^2+4[(q^0)^2-\mathbf{q}^2]$, it follows that $M_0=2\omega(\mathbf{Q})$, and then

$$P^0=\omega(\mathbf{p}_1)+\omega(\mathbf{p}_2)=M_0^2+\mathbf{P}^2=\sqrt{\mathbf{P}^2+4\mathbf{Q}^2+4m^2},$$

which is denoted by $\Omega(\mathbf{P},\mathbf{Q})$ in (16). The angular momentum J is easily obtained because a rotation of the system $\mathbf{p}_1,\mathbf{p}_2$ leads to the same rotation of $\mathbf{P},\mathbf{Q}$, which is an obvious consequence of the formula (15). The Lorentz generator $L_{0,1}$ is obtained as follows. Under an infinitesimal Lorentz transform of hyperbolic angle γ in the first direction (of unit vector $\mathbf{e}_1$), the fundamental quantities become

$$\mathbf{P}\to\mathbf{P}+\gamma P^0\mathbf{e}_1, \quad \mathbf{q}\to\mathbf{q}+\gamma q^0\mathbf{e}_1,$$

$$P^0\to P^0+\gamma P_1, \quad q^0\to q^0+\gamma q_1.$$

Under such a transformation, $\mathbf{Q}$ becomes

$$\mathbf{Q}\to\mathbf{q}+\gamma q^0\mathbf{e}_1-\frac{q^0+\gamma q_1}{M_0+P^0+\gamma P_1}\,(\mathbf{P}+\gamma P^0\mathbf{e}_1)\approx\mathbf{Q}+\gamma\,\frac{P_2}{M_0+P^0}\,\mathbf{Q}^{\perp},$$

where we have performed a first-order development. The formula for $L_{0,1}$ given in (16) is then easily deduced. $L_{0,2}$ is obtained in the same way.

The Jacobian of the transformation $(\mathbf{p}_1,\mathbf{p}_2)\to(\mathbf{P},\mathbf{Q})$ is calculated in two steps. First we perform the transformation $(\mathbf{p}_1,\mathbf{p}_2)\to(\mathbf{P},\mathbf{q})$, with Jacobian 1, and then the transformation $(\mathbf{P},\mathbf{q})\to(\mathbf{P},\mathbf{Q})$ with

Jacobian

$$\left| \det\begin{pmatrix} \frac{\partial Q_1}{\partial q_1} & \frac{\partial Q_1}{\partial q_2} \\ \frac{\partial Q_2}{\partial q_1} & \frac{\partial Q_2}{\partial q_2} \end{pmatrix} \right|^{-1} = \left[1 - \left(P_1 \frac{\partial}{\partial q_1} + P_2 \frac{\partial}{\partial q_2} \right) \frac{q^0}{M_0 + P^0} \right]^{-1},$$

which, after a long and tedious calculation, gives $4\omega(\mathbf{p}_1)\omega(\mathbf{p}_2)[M_0 P^0]^{-1}$. Thus, the measure σ_2 becomes $d\sigma_2(\mathbf{p}_1,\mathbf{p}_2) = d\mu(\mathbf{P},\mathbf{Q}) = d\mathbf{P}\, d\sigma(\mathbf{Q})\Omega(\mathbf{P},\mathbf{Q})^{-1}$.

APPENDIX C: THE FUNDAMENTAL EQUATION

The fundamental equation (23) is the condition on a kernel $h(\mathbf{P},\mathbf{Q},\mathbf{Q}')$, depending only on the norms $\|\mathbf{P}\|,\|\mathbf{Q}\|,\|\mathbf{Q}'\|$, for the relation (13) and (14) to hold. This norm dependence leads to (50) and thus to $L_{0,j}\mathscr{O} = L_{0,j}^{\mathbf{P}}\mathscr{O}$ and $\mathscr{O}L_{0,j} = \mathscr{O}L_{0,j}^{\mathbf{P}}$, where $L_{0,j}^{\mathbf{P}} := -i\Omega(\mathbf{P},\mathbf{Q})\partial_{P_j}$ for all $j \in \{1,2\}$.

Let us calculate the jth equation of (13). The linear part in $\mathscr{O}$ can be written as

$$A_j := [\{H_0,\mathscr{O}\},L_{0,j}] + [H_0,\{L_{0,j},\mathscr{O}\}] = 2(H_0\mathscr{O}L_{0,j} - L_{0,j}\mathscr{O}H_0 + iP_j\mathscr{O}),$$

where we have used $[H_0,L_{0,j}] = iP_j$ and the fact that P_j and $\mathscr{O}$ commute. By applying this operator to a vector $\phi \in \mathscr{D}$ [the domain given by (34)] we obtain, in obvious symbolic notation,

$$\begin{aligned} A_j\phi(\mathbf{P},\mathbf{Q}) &= -2i\Omega \int d\sigma(\mathbf{Q}')\, \frac{\partial_{P_j}\phi h}{\Omega+\Omega'} + 2i\Omega\partial_{P_j}\int d\sigma(\mathbf{Q}')\, \frac{\phi h}{\Omega+\Omega'} + 2iP_j \int \frac{d\sigma(\mathbf{Q}')}{\Omega'}\, \frac{\phi h}{\Omega+\Omega'} \\ &= 2i\int d\sigma(\mathbf{Q}')\phi\left(\Omega\partial_{P_j}\frac{h}{\Omega+\Omega'} + \frac{P_j}{\Omega'}\frac{h}{\Omega+\Omega'} \right) \\ &= 2i\int d\sigma(\mathbf{Q}')\phi(\mathbf{P},\mathbf{Q}')\, \frac{\Omega(\mathbf{P},\mathbf{Q})\partial_{P_j}(\mathbf{P},\mathbf{Q},\mathbf{Q}')}{\Omega(\mathbf{P},\mathbf{Q}) + \Omega(\mathbf{P},\mathbf{Q}')}. \end{aligned}$$

To study the bilinear part, we rewrite (48) and (40):

$$\{H_0,\mathscr{O}\}\phi(\mathbf{P},\mathbf{Q}) = \int \frac{d\sigma(\mathbf{Q}')}{\Omega(\mathbf{P},\mathbf{Q}')}\, \phi(\mathbf{P},\mathbf{Q}')h(\mathbf{P},\mathbf{Q},\mathbf{Q}'),$$

$$\begin{aligned} \{L_{0,j}\mathscr{O}\}\phi(\mathbf{P},\mathbf{Q}) &= -i\int \frac{d\sigma(\mathbf{Q}')}{\Omega(\mathbf{P},\mathbf{Q}')}\, (\partial_{P_j}\phi(\mathbf{P},\mathbf{Q}'))h(\mathbf{P},\mathbf{Q},\mathbf{Q}) \\ &\quad -i\Omega(\mathbf{P},\mathbf{Q})\int d\sigma(\mathbf{Q}')\phi(\mathbf{P},\mathbf{Q}')\partial_{P_j}\frac{h(\mathbf{P},\mathbf{Q},\mathbf{Q}')}{\Omega(\mathbf{P},\mathbf{Q}')(\Omega(\mathbf{P},\mathbf{Q}) + \Omega(\mathbf{P},\mathbf{Q}'))} \end{aligned}$$

Thus, the bilinear part in $\mathscr{O}$ gives, in symbolic notation,

$$
\begin{aligned}
B_j\phi(\mathbf{P},\mathbf{Q}) :=& [\{H_0,\mathscr{O}\},\{L_0,\mathscr{O}\}]\phi(\mathbf{P},\mathbf{Q}) \\
=& \int \frac{d\sigma''}{\Omega''} h^{Q,Q''}\Bigg[-i\int \frac{d\sigma'}{\Omega'} (\partial_j\phi') h^{Q'',Q'} - i\Omega''\int d\sigma'\ \phi'\partial_j \frac{h^{Q'',Q'}}{\Omega'(\Omega''+\Omega')} \\
&+ i\partial_j \int \frac{d\sigma'}{\Omega'}\ \phi' h^{Q'',Q'}\Bigg] + i\Omega\int d\sigma''\left(\partial_j \frac{h^{Q,Q''}}{\Omega''(\Omega+\Omega'')}\right)\int \frac{dq'}{\Omega'}\ \phi' h^{Q'',Q'} \\
=& i\int d\sigma''\int d\sigma'\,\phi' \\
&\times\left(-h^{Q,Q''}\partial_j \frac{h^{Q''Q'}}{\Omega'(\Omega''+\Omega')} + \frac{h^{Q,Q''}}{\Omega''}\ \partial_j \frac{h^{Q'',Q'}}{\Omega'} + \frac{\Omega}{\Omega'}\left(\partial_j \frac{h^{Q,Q''}}{\Omega''(\Omega+\Omega'')}\right) h^{Q'',Q'}\right) \\
=& i\int \frac{d\sigma(\mathbf{Q}')}{\Omega(\mathbf{P},\mathbf{Q}')}\ \phi(\mathbf{P},\mathbf{Q}')\int \frac{d\sigma(\mathbf{Q}'')}{\Omega(\mathbf{P},\mathbf{Q}'')^2}\Bigg\{ -\frac{P_j}{\Omega(\mathbf{P},\mathbf{Q}'')}\ h(\mathbf{P},\mathbf{Q},\mathbf{Q}'')h(\mathbf{P},\mathbf{Q}'',\mathbf{Q}') \\
&+ \frac{\Omega(\mathbf{P},\mathbf{Q})\Omega(\mathbf{P},\mathbf{Q}'')\partial_{P_j}h(\mathbf{P},\mathbf{Q},\mathbf{Q}'')}{\Omega(\mathbf{P},\mathbf{Q})+\Omega(\mathbf{P},\mathbf{Q}'')}\ h(\mathbf{P},\mathbf{Q}'',\mathbf{Q}') \\
&+ h(\mathbf{P},\mathbf{Q},\mathbf{Q}'')\ \frac{\Omega(\mathbf{P},\mathbf{Q}'')\Omega(\mathbf{P},\mathbf{Q}')\partial_{P_j}h(\mathbf{P},\mathbf{Q}'',\mathbf{Q}')}{\Omega(\mathbf{P},\mathbf{Q}'')+\Omega(\mathbf{P},\mathbf{Q}')}\Bigg\}.
\end{aligned}
$$

Because h depends on $\mathbf{P}$ only through $\|\mathbf{P}\|$ we can replace ∂_{P_j} everywhere by $P_j\|\mathbf{P}\|^{-1}\partial_{\|\mathbf{P}\|}$. The condition $A_j+B_j=0$, which must hold for all $\phi\in\mathscr{D}$, leads to the fundamental equation (23), for all $j\in\{1,2\}$.

The equation (14) is slightly more difficult. By using $J^{\mathbf{Q}}\mathscr{O}=0$ and by putting $J^{\mathbf{P}}:=J-J^{\mathbf{Q}}$, the linear part can be written in symbolic notations:

$$
\begin{aligned}
C\phi(\mathbf{P},\mathbf{Q}) :=& 2(L^{\mathbf{P}}_{0,1}\mathscr{O}L^{\mathbf{P}}_{0,2} - L^{\mathbf{P}}_{0,2}\mathscr{O}L^{\mathbf{P}}_{0,1} - i\mathscr{O}J^{\mathbf{P}})\phi(\mathbf{P},\mathbf{Q}) \\
=& -2\Omega\int d\sigma'[(\partial_2\phi')\partial_1 - (\partial_1\phi')\partial_2]\ \frac{h}{\Omega+\Omega'} \\
&-2\int \frac{d\sigma'}{\Omega'}\,[(P_1\partial_2 - P_2\partial_1)\phi']\ \frac{h}{\Omega+\Omega'} \\
=& -\frac{2i}{\|\mathbf{P}\|}\int \frac{d\sigma(\mathbf{Q}')}{\Omega(\mathbf{P},\mathbf{Q}')}\ (J^{\mathbf{P}}\phi(\mathbf{P},\mathbf{Q}'))Dh(\mathbf{P},\mathbf{Q},\mathbf{Q}').
\end{aligned}
$$

The bilinear part gives

$$
\begin{aligned}
D\phi(\mathbf{P},\mathbf{Q}) :=& \left(\frac{1}{2}\,(C\mathscr{O}+\mathscr{O}C) + L^{\mathbf{P}}_{0,1}\mathscr{O}^2L^{\mathbf{P}}_{0,2} - L^{\mathbf{P}}_{0,2}\mathscr{O}^2L^{\mathbf{P}}_{0,1} + i\mathscr{O}^2J^{\mathbf{P}}\right)\phi(\mathbf{P},\mathbf{Q}) \\
=& -\frac{i}{\|\mathbf{P}\|}\int \frac{d\sigma'}{\Omega'}\ J^{\mathbf{P}}\phi'\int \frac{d\sigma''}{\Omega''}\left(Dh^{\mathbf{Q},\mathbf{Q}''}\ \frac{h^{\mathbf{Q}'',\mathbf{Q}'}}{\Omega'+\Omega''} + \frac{h^{\mathbf{Q},\mathbf{Q}''}}{\Omega+\Omega''}\ Dh^{\mathbf{Q}'',\mathbf{Q}'}\right) \\
&\times(-i)^2\int \frac{d\sigma'}{\Omega'}\ \Omega\Omega'[(\partial_2\phi')\partial_1 - (\partial_1\phi')\partial_2]\int \frac{d\sigma''}{\Omega''}\ \frac{h^{\mathbf{Q},\mathbf{Q}''}}{\Omega+\Omega''}\ \frac{h^{\mathbf{Q}'',\mathbf{Q}'}}{\Omega'+\Omega''}
\end{aligned}
$$

$$+\int \frac{d\sigma'}{\Omega'}\,[(P_1\partial_2-P_2\partial_1)\phi']\int \frac{d\sigma''}{\Omega''}\,\frac{h^{\mathbf{Q},\mathbf{Q}''}}{\Omega+\Omega''}\,\frac{h^{\mathbf{Q}'',\mathbf{Q}'}}{\Omega'+\Omega''}$$

$$=-\frac{i}{\|\mathbf{P}\|}\int \frac{d\sigma'}{\Omega'}\,J^{\mathbf{P}}\phi'\int \frac{d\sigma''}{\Omega''^2}\,(Dh^{\mathbf{Q},\mathbf{Q}''}h^{\mathbf{Q}'',\mathbf{Q}'}+h^{\mathbf{Q},\mathbf{Q}''}Dh^{\mathbf{Q}'',\mathbf{Q}'})$$

$$+i\int \frac{d\sigma'}{\Omega'}\,J^{\mathbf{P}}\phi'\int \frac{d\sigma''}{\Omega''^3}\,h^{\mathbf{Q},\mathbf{Q}''}h^{\mathbf{Q}'',\mathbf{Q}'}.$$

The condition $C+D=0$, which must hold for all $J^{\mathbf{P}}\phi$, leads to the fundamental equation (23) again.

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Toward discrete wavelets with irrational scaling factor

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Scaling equations determining Haar-type wavelets are considered for three Pisot numbers $\beta=(1+\sqrt{5})/2,\ 1+\sqrt{2},\ 2+\sqrt{3}$ appearing as dilation factors in scale invariance of observed diffraction patterns of quasicrystals. Simple summation formulas for exponentials of the corresponding β integers are derived. © *1996 American Institute of Physics.* [S0022-2488(96)03006-X]

I. INTRODUCTION

Wavelets have found many applications in modern science.[1,2] They are useful in signal processing, numerical solution of differential equations, analysis of fractals, etc. From a quantum mechanical point of view wavelets represent coherent states of the affine groups defining bases of Hilbert spaces. A particular interest is paid to such bases built by discrete dilations and translations of one (or few) function(s). A self-consistent procedure (multiresolution analysis) of constructing the latter generating function has been developed for rational dilation factors β (see, e.g., Refs. 1–3 and references therein). Analysis of the irrational factor cases, both algebraic and transcendental ones, is one of the motivations of the present investigation. Although our consideration is far from complete, the summation formulas derived below may be useful in the description of some fractals and quasicrystals.

We shall consider three cases:

$$\beta=\frac{1+\sqrt{5}}{2}=2\cos\frac{2\pi}{10};$$

$$\beta=1+\sqrt{2}=1+2\cos\frac{2\pi}{8};$$

$$\beta=2+\sqrt{3}=2+2\cos\frac{2\pi}{12}. \tag{1}$$

Powers of these numbers appear as dilation factors in scale invariance of observed diffraction patterns of quasicrystalline alloys.[4] The numbers (1) are known to be unitary Pisot numbers. Let us give some necessary definitions. A number β is called an algebraic integer if it satisfies the equation

$$x^n+a_{n-1}x^{n-1}+\cdots+a_0=0, \tag{2}$$

where the coefficients a_k, $k=0,\ldots,n-1$ are integers. Note that the highest power of x appears in (2) with the coefficient 1. A solution of (2) β is called a Pisot, or a Pisot–Vijayaraghavan number if $\beta>1$ and all other roots of (2) have modulus less than 1 [it is assumed that all roots of (2) are

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simple]. A Pisot number is called unitary if $|a_0|=1$. Ordinary integers are Pisot numbers but the rational numbers are not. An interesting property of Pisot numbers β is that the powers β^n are not uniformly distributed modulo 1 (more precisely, this sequence converges to 0 modulo 1). The Lebesgue measure of numbers with such a property is 0; astonishingly, it is not known whether fractional numbers belong to this set or not, i.e., in this respect they are more complicated than some irrational numbers. Pisot numbers form a closed set bounded from below and the lower bound $\beta_0 \approx 1.32$ is the real root of polynomial x^3-x-1.[5] Within this set lies the closed subset of totally real (i.e., all conjugated roots are real) Pisot numbers, which is bounded from below by the golden mean $(1+\sqrt{5})/2$. The existence of such bounds should have physical consequences in the sense that there should be some principal differences between the objects built by the scalings with the help of $\beta \geqslant \beta_0$ and $\beta < \beta_0$.

Let us briefly present the main wavelet construction formulas for the scaling factor equal to 2. The basic equation called the scaling equation (sometimes it is referred to as the refining equation),

$$\chi(x)=\sum_k c_k \chi(2x-k), \quad k \in \mathbf{Z}, \tag{3}$$

has compact support solutions when the number of nonzero coefficients in (3) is finite. The simplest representative of such systems appears from the equation

$$\chi(x)=\chi(2x)+\chi(2x-1), \tag{4}$$

determining the Haar scaling function

$$\chi(x)=\begin{cases} 1, & \text{for } x \in [0,1]; \\ 0, & \text{for } x \notin [0,1]. \end{cases} \tag{5}$$

An orthonormal basis of $L^2(\mathbf{R})$ is built from the wavelet function

$$h(x)=\sum_k (-1)^k c_{1-k} \chi(2x-k), \tag{6}$$

by discrete dilations and translations,

$$h_{j,k}(x)=2^{j/2} h(2^j x-k), \quad j,k \in \mathbf{Z}. \tag{7}$$

The scaling factor 2 in the given formulas plays the central role, the whole construction being based on the dyadic property $1/2^j = 1/2^{j+1} + 1/2^{j+1}$. However, the base of scaling 2 is too specific, in many cases dilations by arbitrary real numbers play an important role, e.g., such a situation takes place for the self-similar potentials discussed in Ref. 6, which are determined by the mixed differential and q-difference equations. It is expected that the wavelets provide a relevant tool for analysis of solutions of such equations. In the following sections we discuss how far one can go in the building of wavelets if the base of scaling is an irrational number.

II. GOLDEN MEAN SCALING FACTOR

Recently, a generalization of the Haar wavelet has been proposed in Ref. 7. It uses the τ-adic property of the ''golden mean'' number $\tau=(1+\sqrt{5})/2 \approx 1.62$:

$$\frac{1}{\tau^j}=\frac{1}{\tau^{j+1}}+\frac{1}{\tau^{j+2}} \quad \text{or} \quad \tau^2=\tau+1. \tag{8}$$

The number τ is the simplest irrational algebraic integer, by some properties it is quite close to the number 2. Equation (8) provides a subdivision of the unit interval into two parts $[0,1]=[0,1/\tau]\cup[1/\tau,1]$. The importance of scalings by τ and of the Fibonacci numbers associated with that in various domains of physics (and biology) is well known. It is especially relevant in geometrical studies of five-fold and ten-fold structures.

It is easy to see that the Haar scaling function (5) satisfies the equation

$$\chi(x)=\chi(\tau x)+\chi(\tau^2 x-\tau). \tag{9}$$

The τ wavelet of Haar[7] has the form

$$h^\tau(x)=\tau^{-1/2}\chi(\tau x)-\tau^{1/2}\chi(\tau^2 x-\tau). \tag{10}$$

An orthonormal basis of $L^2(\mathbf{R})$ is constructed in similarity with (7):

$$\{h^\tau_{j,b}(x),h^\tau_{j,-b-1}(x)\},\quad j\in\mathbf{Z},\quad b\in\tau\mathbf{Z}^+_\tau,$$

where

$$h^\tau_{j,b}(x)=\tau^{j/2}h^\tau(\tau^j x-b). \tag{11}$$

Here $\mathbf{Z}^+_\tau$ denotes the set of positive τ integers (including zero), i.e. real numbers that can be represented in the form

$$b=\sum_{l=0}^{j}\epsilon_l\tau^l,\quad \epsilon_l=\{0,1\},\quad \epsilon_l\epsilon_{l-1}=0. \tag{12}$$

The first τ integers are $0,1,\tau,\tau^2,\tau^2+1,\tau^3$, etc; they tile quasiperiodically positive real line by two tiles with respective lengths 1 and $1/\tau$, forming what is called the Fibonacci quasilattice. By $\tau\mathbf{Z}^+_\tau$ we denote the set of positive ''even'' τ integers b that do not have 1 as the last digit, i.e. $\epsilon_0(b)\neq 1$. Some additional information about the general β-numeration systems is given in the next section.

The Fourier transformation of (9) yields

$$\phi(\xi)=\frac{1}{\tau}\,\phi\left(\frac{\xi}{\tau}\right)+\frac{e^{-i\xi/\tau}}{\tau^2}\,\phi\left(\frac{\xi}{\tau^2}\right),\quad \phi(\xi)=\int_{-\infty}^{\infty}\chi(x)e^{-i\xi x}\,dx. \tag{13}$$

Fourier transform of the Haar scaling function is known explicitly,

$$\phi(\xi)=\int_0^1 e^{-i\xi x}\,dx=\frac{1-e^{-i\xi}}{i\xi}, \tag{14}$$

in particular, $\phi(0)=1$. Iterating relation (13) $N-1$ times one derives the equation (cf. with Ref. 8)

$$\phi(\xi)=\frac{F_{N+1}}{\tau^N}\,\phi\left(\frac{\xi}{\tau^N}\right)+\frac{F_N e^{-i\xi/\tau^N}}{\tau^{N+1}}\,\phi\left(\frac{\xi}{\tau^{N+1}}\right), \tag{15}$$

where the coefficients $F_N(\xi)$ satisfy the three-term recurrence relation

$$F_{N+2}(\xi)=F_{N+1}(\xi)+e^{-i\xi/\tau^N}F_N(\xi),\quad F_1=F_2=1. \tag{16}$$

Note that $F_N(0)$ coincide with the Fibonacci numbers.

Denote as $\{b_N\}$ the set of τ integers (12) that are strictly less than τ^N. From the general representation (12) one can deduce that $\{b_N\}=\{\tau b_{N-1}\}\cup\{1+\tau^2 b_{N-2}\}$. As a result, one can see that solution of the equation (16) is given by the following sum:

$$F_N(\xi)=\sum_{b\in\{b_{N-2}\}} e^{-i\xi b/\tau^{N-2}}. \tag{17}$$

The Fibonacci numbers $F_N(0)$ thus count the τ integers satisfying $0\leqslant b<\tau^{N-2}$. Since in the limit $N\to\infty$ one has $\phi(\xi/\tau^N)\to 1$, the relation (15) generates an interesting summation formula mentioned in Ref. 7,

$$e^{-i\xi/2}\frac{\sin\,\xi/2}{\xi/2}=\frac{1+\tau^2}{\tau^3}\lim_{N\to\infty}\frac{1}{\tau^N}\sum_{b\in\{b_N\}} e^{-i\xi b/\tau^N}. \tag{18}$$

A real part of the lhs of this equality is given by the function $\mathrm{sinc}\,\xi=\sin\xi/\xi$. Expanding both sides of the equation (18) into a Taylor series and equating coefficients in front of the powers of ξ, we get the following estimate of the growth of sums of powers of τ integers:

$$\sum_{0\leqslant b<\tau^N} b^n\to\frac{\tau^{N(n+1)+3}}{(n+1)(1+\tau^2)}. \tag{19}$$

For $n=1$ this may be compared with the sum of ordinary integers,

$$\sum_{0\leqslant k<2^N} k=2^{N-1}(2^N-1)\to 2^{2N-1}.$$

It would be interesting to find similar exact formulas for the sums (19). Repetition of the derivation of (18) for the standard scaling Eq. (4) results in the formula

$$e^{-i\xi/2}\frac{\sin\,\xi/2}{\xi/2}=\prod_{j=1}^{\infty}\left(\frac{1+e^{-i\xi/2^j}}{2}\right)=\lim_{N\to\infty}\frac{1}{2^N}\sum_{0\leqslant k<2^N} e^{-i\xi k/2^N}, \tag{20}$$

where the summation goes over the ordinary positive integers. In Fig. 1 we depict the function $\mathrm{sinc}\,\pi t$ versus the real parts of the rhs of (18) for $N=6$ ($\xi=\pi t$) and the rhs of (20) for $N=4$.

For arbitrary integer scaling factor p, the rhs of (20) is replaced by

$$\prod_{j=1}^{\infty}\left(\frac{1+e^{-i\xi/p^j}+\cdots+e^{-i\xi(p-1)/p^j}}{p}\right)=\lim_{N\to\infty}\frac{1}{p^N}\sum_{0\leqslant k<p^N} e^{-i\xi k/p^N}, \tag{21}$$

which follows from the evident identity $1=1/p+\cdots+1/p$ with p terms in the sum. However, it is not clear how to generalize this relation to the fractional scaling factors.

III. SUMMATION FORMULA FOR THE OCTONACCI NUMBER

Consider now another algebraic integer $\beta=1+\sqrt{2}\approx 2.41$, solution of the equation $\beta^2=2\beta+1$, which is sometimes called the octonacci number. This is the simplest unitary Pisot number in the extension ring $\mathbf{Z}[1,2\cos 2\pi/8]$ and such that $\mathbf{Z}[1,\beta]=\mathbf{Z}[1,2\cos 2\pi/8]$. Before considering properties of this specific number, we would like to describe briefly the general β-numeration algorithm.[9,10]

For a given real number $\beta>1$ any positive real number x can be represented in the form of series over β:

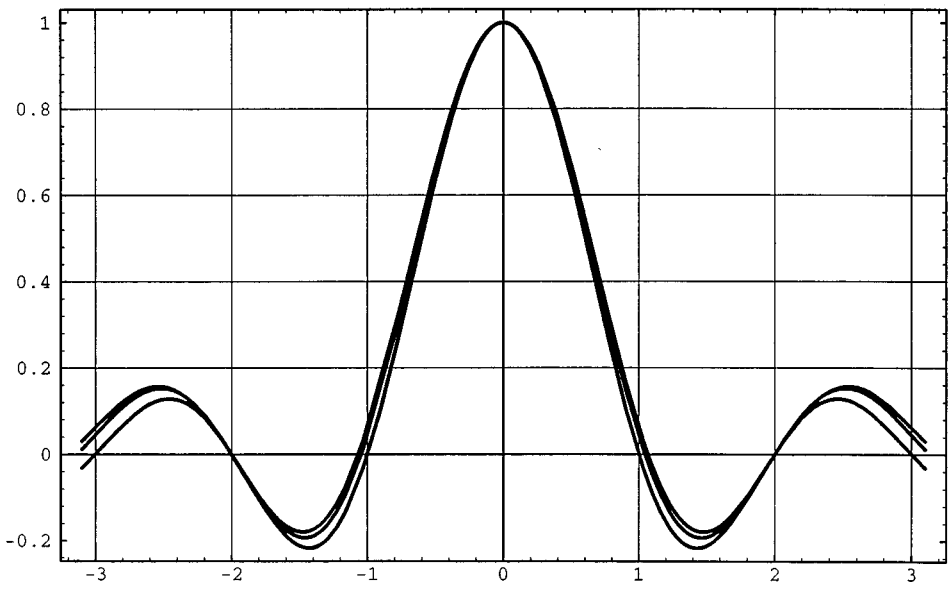

FIG. 1. The function sinc πt and real parts of the rhs of (18) for $N=6$ (the middle curve) and of the rhs of (19) for $N=4$ in appropriate units. The errors at $t=3$ are less than 5% of the maximum at $t=0$.

$$x=\sum_{l=-\infty}^{j} \epsilon_l \beta^l, \quad \epsilon_l=\{0,1,..,d\}, \tag{22}$$

where $d=\beta-1$ if β is an integer and otherwise $d=[\beta]$ the integer part of β. This representation, denoted symbolically as $x=\epsilon_j\cdots\epsilon_0.\epsilon_{-1}\cdots$, is unique if the digits ϵ_l are restricted in such a way that for any k one has $\Sigma_{l<k}\epsilon_l\beta^l<\beta^k$. For $\beta=\tau$ this means that there are no two successive digits equal to 1. When the expansion (22) contains only non-negative powers of β, x is said to be a β integer; β integers can be characterized by a finite algorithm only in special cases.

The above unique decomposition can be obtained by the so-called ''greedy'' algorithm. For any $x>0$ there is $k\in\mathbf{Z}$ such that $\beta^k\leqslant x<\beta^{k+1}$. Then put $\epsilon_k=[x/\beta^k]$ and $r_k=\{x/\beta^k\}$ (curled brackets $\{x\}$ denote the fractional part of x). Other digits ϵ_l, $l<k$ are determined recursively, $\epsilon_l=[\beta r_{l+1}]$, where $r_l=\{\beta r_{l+1}\}$. A simple characterization of the constraints upon digits uses the Rényi expansion of 1 denoted $d(1,\beta)=0.\epsilon_{-1}\cdots\epsilon_{-l}\cdots$ and obtained through the recursion $\epsilon_{-k-1}=[\beta T_\beta^k 1]$, where $T_\beta x\equiv(\beta x) \bmod 1$ for any $x\in[0,1]$.[9] For example, one has $d(1,\tau)=0.11$.

A number β is called a beta number if the corresponding Rényi expansion of 1 is eventually periodic [i.e., there exists an integer k such that for $l>k$ all digits ϵ_{-l} in $d(1,\beta)$ are obtained by periodic repetition of some finite set of digits]. For these numbers the notion of β integers is well defined in the sense that one can describe them by using a finite algorithm. An important fact is that any Pisot number is a beta number,[10] but there are beta numbers that are non-Pisot algebraic integers. Pisot numbers are important for building quasicrystals due to some additional properties (e.g., local inflationary properties) that we do not discuss here.

Returning to the octonacci number, we see that $\epsilon_l=\{0,1,2=[\beta]\}$, and in the corresponding β numeration the pairs $\{\epsilon_l,\epsilon_{l-1}\}$ are forbidden to be $\{2,1\}$ and $\{2,2\}$ since the Rényi expansion of 1 is $d(1,\beta)=0.21$. The first β integers are $0,1,2,\beta,\beta+1,\beta+2,2\beta,\beta^2,\ldots$. These numbers cover the real line quasiperiodically by two tiles with respective lengths 1 and $\beta-2=1/\beta$.

The equation satisfied by β determines a subdivision of the unit interval into three pieces such that the ratio of their lengths is equal to a power of β:

$$1=\frac{1}{\beta}+\frac{1}{\beta}+\frac{1}{\beta^2}. \tag{23}$$

This allows one to write a new equation for the Haar scaling function,

$$\chi(x)=\chi(\beta x)+\chi(\beta x-1)+\chi(\beta^2 x-2\beta), \tag{24}$$

Fourier transformation of which yields the following ''q-difference'' equation:

$$\phi(\xi)=\frac{1+e^{-i\xi/\beta}}{\beta}\,\phi\left(\frac{\xi}{\beta}\right)+\frac{e^{-i2\xi/\beta}}{\beta^2}\,\phi\left(\frac{\xi}{\beta^2}\right). \tag{25}$$

Iteration of this equation $N-1$ times results in

$$\phi(\xi)=\frac{G_{N+1}}{\beta^N}\,\phi\left(\frac{\xi}{\beta^N}\right)+\frac{e^{-i2\xi/\beta^N}G_N}{\beta^{N+1}}\,\phi\left(\frac{\xi}{\beta^{N+1}}\right), \tag{26}$$

where the coefficients $G_N(\xi)$ are determined from the recurrence relation

$$G_{N+2}=G_{N+1}(1+e^{-i\xi/\beta^{N+1}})+G_N e^{-i2\xi/\beta^N}, \quad G_0=0, \quad G_1=1. \tag{27}$$

In similarity with the previous case, solution of this recurrence is given by the sum

$$G_N(\xi)=\sum_{b\in\{b_N\}} e^{-i\xi b/\beta^{N-1}}, \tag{28}$$

where the summation goes over the set of β integers $\{b_N\}$ satisfying the constraints $0\leqslant b_N<\beta^N$ and $\epsilon_0(b_N)\neq 2$ (i.e., 2 is excluded as the last digit). The proof of (28) goes by induction. Indeed, $\{b_N\}$ can be split into three groups:

$$\{b_N\}=\{\beta b_{N-1}\}\cup\{1+\beta b_{N-1}\}\cup\{2\beta+\beta^2 b_{N-2}\}, \tag{29}$$

in self-explanatory notations. It is not difficult to see that (29) corresponds exactly to the rule of addition of exponentials in (27), (28). As a result, in the limit $N\to\infty$, one gets from (26) the summation formula

$$e^{-i\xi/2}\,\frac{\sin\,\xi/2}{\xi/2}=\frac{1+\beta^2}{\beta^2}\,\lim_{N\to\infty}\frac{1}{\beta^N}\sum_{b\in\{b_N\}} e^{-i\xi b/\beta^N}. \tag{30}$$

This formula differs from (18) and (20) by the presence of the constraint upon the last digit of β integers entering the sum. In Fig. 2 we depict $\mathrm{sinc}\,\pi t$ and the real part of the rhs of (30) for $N=3$ in the appropriate units. Analogously to (19), we can estimate from (30) the growth of the sum of powers of the β integers belonging to $\{b_N\}$,

$$\sum_{b\in\{b_N\}} b^n\to\frac{\beta^{N(n+1)+2}}{(n+1)(1+\beta^2)}.$$

Since we have a subdivision of $[0,1]$ into three intervals, there are two wavelet functions of the Haar type obtained by orthonormalization of $\chi(x)$, $\chi(\beta x)$, and $\chi(\beta x-1)$:

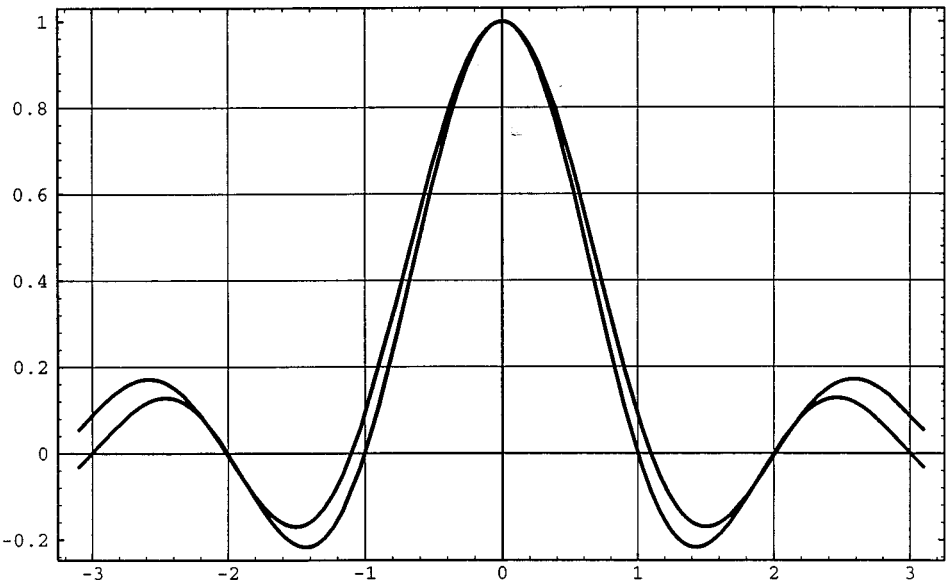

FIG. 2. The function sinc πt and the real part of the rhs of (30) for $N=3$. The approximation is less accurate than in Fig. 1.

$$h^{(1)}(x)=\sqrt{\beta-1}\,\chi(\beta x)-\frac{1}{\sqrt{\beta-1}}\,(\chi(\beta x-1)+\chi(\beta^2 x-2\beta)),$$
$$h^{(2)}(x)=\frac{1}{\sqrt{\beta-1}}\,(\chi(\beta x-1)-\beta\chi(\beta^2 x-2\beta)). \tag{31}$$

Splitting of the β integers into two sets, $\epsilon_0(b)\neq 2$ (''even'') and $\epsilon_0(b)=2$ (''odd'') appears naturally in the translations of (31) without overlaps. One can check that $h^{(l)}_{j,b}(x)=\beta^{j/2}h^{(l)}(\beta^j x-b)$ and $h^{(l)}_{j,-b-1}(x)$ define orthonormal vectors of $L^2(\mathbf{R})$, provided $\epsilon_0(b)\neq 2$. In order to prove that this sequence forms a basis of the Hilbert space, it is necessary to verify that it is dense that we do not pursue here.

IV. INFINITE PARTITION OF THE UNIT INTERVAL CASE

There are infinitely many algebraic integers for which one can derive summation formulas similar to (18) and (20). However, for some of these numbers subdivision of the unit interval contains infinitely many terms. For example, such a situation takes place for $\beta=2+\sqrt{3}\approx 3.73$, $\beta^2=4\beta-1$, when

$$1=\frac{3}{\beta}+2\sum_{j=2}^{\infty}\frac{1}{\beta^j},\quad \text{or}\quad d(1,\beta)=0.322\,222\ldots\,. \tag{32}$$

This β is the simplest unitary Pisot number in the extension ring $\mathbf{Z}[1,2\cos 2\pi/12]$, such that $\mathbf{Z}[1,\beta]=\mathbf{Z}[1,2\cos 2\pi/12]$. The β integers are defined similar to (12), with ϵ_l varying from 0 to $[\beta]=3$ and the constraint that between any two digits $\epsilon_l=3$ of the β numeration of arbitrary number, there should be at least one 0 or 1 (i.e., combinations {3,3}, {3,2,3}, etc. are forbidden). These numbers tile the positive real line by two tiles with respective lengths 1 and $\beta-3$; the first few β integers are $0,1,2,3,\beta,\beta+1,\beta+2,\beta+3,2\beta,\ldots$.

Using (32) one constructs a scaling equation for the characteristic function (5):

$$\chi(x)=\chi(\beta x)+\chi(\beta x-1)+\chi(\beta x-2)+\chi(\beta^2 x-3\beta)+\chi(\beta^2 x-3\beta-1)$$
$$+\sum_{k=3}^{\infty}\left[\chi(\beta^k x-3\beta^{k-1}-2\beta^{k-2}-\cdots-2\beta)+\chi(\beta^k x-3\beta^{k-1}-2\beta^{k-2}-\cdots-2\beta-1)\right], \tag{33}$$

or, after Fourier transformation,

$$\phi(\xi)=\frac{1}{\beta}\,(1+e^{-i\xi/\beta}+e^{-i\xi 2/\beta})\,\phi\left(\frac{\xi}{\beta}\right)+\frac{e^{-3i\xi/\beta}}{\beta^2}\,(1+e^{-i\xi/\beta^2})\,\phi\left(\frac{\xi}{\beta^2}\right)$$
$$+e^{-i\xi}\sum_{k=3}^{\infty}\frac{1}{\beta^k}\,(e^{-i\xi(1-\beta)/\beta^k}+e^{-i\xi(2-\beta)/\beta^k})\,\phi\left(\frac{\xi}{\beta^k}\right). \tag{34}$$

Let us write the result of successive iterations of this relation in the form

$$\phi(\xi)=\sum_{k=0}^{\infty}\frac{G_N^k(\xi)}{\beta^{N+k}}\,\phi\left(\frac{\xi}{\beta^{N+k}}\right), \tag{35}$$

where $N\geqslant 1$ and $G_1^k(\xi)$ are fixed in (34). Using the scaled form of (34) and substituting $\phi(\xi/\beta^N)$ into (35), we derive the following recurrence relation:

$$G_{N+1}^k(\xi)=G_N^0(\xi)G_1^k(\xi/\beta^N)+G_N^{k+1}(\xi). \tag{36}$$

For $k=0$ the first few steps of iteration of this relation allow us to see that $G_N^0(\xi)$ forms the pattern

$$G_N^0(\xi)=\sum_{b\in\{b_N\}}e^{-i\xi b/\beta^N}, \tag{37}$$

where $\{b_N\}$ are the β integers satisfying $0\leqslant b_N<\beta^N$, with the exception of those forming the left edge of tiles with length $\beta-3$. The latter means that $\epsilon_0(b_N)\neq 3$, but since we are dealing with the infinite partition of 1 there are other forbidden numbers as well. Namely, $3\beta+2$ and all other β integers having as the last digits the sequence {3,2,2,...} do not belong to $\{\beta_N\}$.

The summation formula we are interested in arises from (35) in the limit $N\to\infty$,

$$e^{-i\xi/2}\,\frac{\sin\,\xi/2}{\xi/2}=\lim_{N\to\infty}\sum_{k=0}^{\infty}\frac{G_N^k(\xi)}{\beta^{N+k}}. \tag{38}$$

For $N\to\infty$ the recursion (36) simplifies

$$G_{N+1}^0=3G_N^0+G_N^1,\quad G_{N+1}^k=2G_N^0+G_N^{k+1},\quad k\geqslant 1. \tag{39}$$

Since $G_N^0(\xi)$ is known (37), one may invert (39) in order to determine $G_N^k(\xi)$, $k>0$:

$$G_N^k=G_{N+k}^0-3G_{N+k-1}^0-2G_{N+k-2}^0-\cdots-2G_N^0,\quad k>0. \tag{40}$$

Substituting this formula into (38), we find the partial sum

$$S_l=\sum_{k=0}^{l}\lim_{N\to\infty}\frac{G_N^k(\xi)}{\beta^{N+k}}=\lim_{N\to\infty}\left(\frac{G_N^0}{\beta^N}\left(1-\frac{3}{\beta}-\frac{2}{\beta^2}-\cdots-\frac{2}{\beta^l}\right)+\frac{G_{N+1}^0}{\beta^{N+1}}\left(1-\frac{3}{\beta}-\frac{2}{\beta^2}-\cdots-\frac{2}{\beta^{l-1}}\right)\right.$$

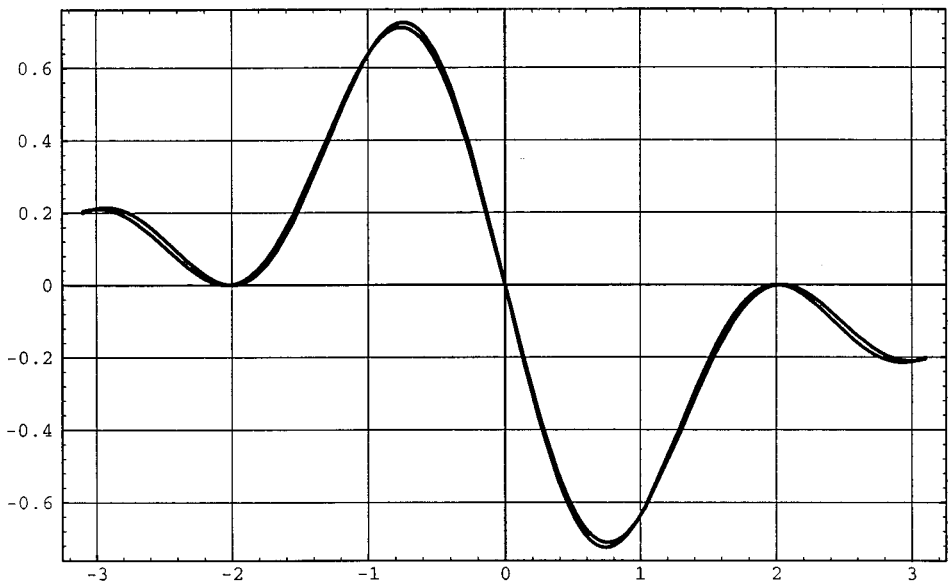

FIG. 3. The function $(\cos \pi t-1)/\pi t$ and the imaginary part of the rhs of (42) at $N=3$. Two curves almost coincide.

$$+\cdots+\frac{G^0_{N+l-1}}{\beta^{N+l-1}}\left(1-\frac{3}{\beta}\right)+\frac{G^0_{N+l}}{\beta^{N+l}}\Bigg)=\left(\frac{\beta+1}{\beta}-\frac{1}{\beta^l}\right)\lim_{N\to\infty}\frac{G^0_N(\xi)}{\beta^N}. \tag{41}$$

Taking the limit $l\to\infty$ in S_l, we find the summation formula

$$e^{-i\xi/2}\,\frac{\sin\,\xi/2}{\xi/2}=\frac{1+\beta}{\beta}\lim_{N\to\infty}\frac{1}{\beta^N}\sum_{b\in\{b_N\}}e^{-i\xi b/\beta^N}. \tag{42}$$

This formula looks similar to the previous ones, but its derivation is not rigorous because we did not verify that the recursion (36) corresponds indeed to the law of addition of exponents in (37) for arbitrary N. In Fig. 3 we depict imaginary parts of the lhs of (42) and the rhs for $N=3$ in the variable $t=\xi/\pi$ (the real part looks very close to the middle curve in Fig. 1). We are reminded that β integers from $\{b_N\}$ do not include left edges of the short $(\beta-3)$ tiles. It would be interesting to understand why for the golden mean number the sum (18) goes over all τ integers, whereas in the last two cases only the long tiles are relevant. If one takes inverse Fourier transforms of the derived summation formulas, one will find that the characteristic function of the unit interval can be approximated as a homogeneous sum of weighted Dirac delta functions located at the β-adic points and, again, it is not clear why one has to abandon some of these points for $\beta=1+\sqrt{2}$ and $2+\sqrt{3}$.

V. DISCUSSION OF THE MULTIRESOLUTION ANALYSIS

Wavelets are known to be related to iterative interpolation. In the case of interpolation of functions given on the lattice points $\mathbf{Z}$ the standard procedure consists in fixing the value of function on the dyadic (for the base 2), or, more generally, on the p-adic points of the real line. The rule of interpolation usually takes into account values of the function in several neighboring points (with some weights) in which the function was fixed at the previous steps of interpolation.[11] Due to the translational invariance the interpolation takes place homogeneously over the space. This is not so for the quasilattices.

Suppose that values of a function are fixed in the points of the Fibonacci quasiperiodic lattice Γ formed by the τ integers. Now there are two tiles with lengths 1 and $1/\tau$. The first step of subdivision process splits only the long tiles into two parts and the short tiles are left untouched. In this case the interpolation rule should be more involved than in the $\Gamma=\mathbf{Z}$ case, but the principle procedure remains the same.

Now let us discuss briefly a possible form of the multiresolution analysis associated with quasiperiodic tilings of a Euclidean space. Denote by Γ a set of points in $\mathbf{R}^n$ satisfying the Delaunay property. This means that (a) the distance between any two points of Γ is larger than a fixed real $r>0$, and (b) there exists a real number $R>0$ such that any ball of radius R contains at least one point from Γ. Such a set is said to form a quasilattice if it is equipped with additional properties (Meyer quasiaddition, local self-similarity,...). Assume that there exists an invertible matrix A whose eigenvalues have modulus larger than 1 and such that $A\Gamma\subset\Gamma$ for all points from Γ. A multiresolution analysis of the Hilbert space $L^2(\mathbf{R}^n)$ is a decomposition of it into a chain of subspaces V_j that satisfy the following set of conditions.

(1) $V_j\subset V_{j+1}$, $j\in\mathbf{Z}$.

(2) The closure of $\cup_{j\in\mathbf{Z}}V_j$ coincides with $L^2(\mathbf{R}^n)$.

(3) $\cap_{j\in\mathbf{Z}}V_j=\{0\}$.

(4) If $f(x)\in V_j$ then $f(Ax)\in V_{j+1}$ and $f(A^{-1}x)\in V_{j-1}$.

(5) There is a finite number of scaling functions $\chi^{(k)}(x)\in V_0$, $k=1,\ldots,K$, such that the set $\{\chi^{(k)}(x-\gamma),\ \gamma\in\Gamma\}$ is an orthonormal basis of V_0.

When Γ is a crystallographic lattice, e.g. $\mathbf{Z}^n$, and $K=1$, such definition is known to have nontrivial solutions for integer-valued matrices A.[12] In the one-dimensional space the above definition is valid for fractional dilation factors, but there are no compact support scaling functions in this case.[3] When β is irrational and $\Gamma=\mathbf{Z}$ only the $\sin c\, x$-type scaling functions are admissible.[3] For $K>1$ the scaling equation acquires a matrix form,[13] and the corresponding theory is referred to as a multiwavelet theory. The multidimensional multiwavelets were considered to some extent in Ref. 14.

Consider how scaling equations for Haar wavelets with an irrational scaling factor described earlier fit into the multiresolution scheme of $L^2(\mathbf{R})$. For $\beta=\tau$ the subspace V_0 is spanned by two functions[7] $\{\chi(x-b),\chi(x+b+1)\}$, with $b\in\tau\mathbf{Z}_\tau^+$ and $\{\chi(\tau x-b),\chi(\tau x+b+1)\}$ with $b\in\tau\mathbf{Z}_\tau^{+\mathrm{odd}}$ (a τ integer is odd if its last digit is 1, i.e. if it coincides with the left edge of a short tile). Despite the fact that the second scaling function is obtained from the first one by dilation, it is different from it, and this hints on the multiwavelets. Note however, that in the decomposition $V_1=V_0\oplus W_0$, the subspace W_0 is covered only by one wavelet function and the elements of W_0 have support only on the tiles of length 1. The latter means that the support of functions from W_j in the decomposition $V_{j+1}=V_j\oplus W_j$ never covers the whole line. This is an interesting property of the τ-multiresolution analysis—it subdivides only ''large'' tiles into the smaller ones.

Actually all three scaling equations considered by us can be represented in the 2×2 matrix form:

$$\chi^{(k)}(x)=\sum_{r=1}^{2}\sum_{m=0}^{[\beta]}c_m^{kr}\chi^{(r)}(\beta x-m), \tag{43}$$

where $\chi^{(1)}(x)=\chi(x)$, i.e. we indeed have multiwavelets. Note that only translations by integers are entering the sum in (43), but in the span of V_0 the functions $\chi^{(k)}(x)$ are translated by the β integers. For $\beta=\tau$ one has (unnormalized) $\chi^{(2)}(x)=\chi(\tau x)$ and

$$M(z)=\sum_{m=0}^{1}c_m z^m=\begin{pmatrix}1 & z\\ 1 & 0\end{pmatrix}. \tag{44}$$

For $\beta=1+\sqrt{2}$ one has $\chi^{(2)}(x)=\chi(\beta x)$ and

$$M(z)=\sum_{m=0}^{2} c_m z^m=\begin{pmatrix} 1+z & z^2 \\ 1 & 0 \end{pmatrix}. \tag{45}$$

A more interesting situation takes place for the infinite partition of 1 case, since the new scale intervenes the scene

$$\chi^{(2)}(x)=\chi\left(\frac{x}{\beta-3}\right),$$

so that

$$M(z)=\sum_{m=0}^{3} c_m z^m=\begin{pmatrix} 1+z+z^2 & z^3 \\ 1+z & z^2 \end{pmatrix}. \tag{46}$$

The choice $z=1$ in $M(z)$ corresponds to setting $\xi=0$ in the Fourier transform of the scaling equations. We remark that in all three cases $M(1)$ coincides with the matrix of substitutions of letters used in the construction of corresponding quasiperiodic tilings (for the Fibonacci case this is the celebrated $a\to ab$, $b\to a$ two letter algorithm). This observation should be relevant for building Haar-type wavelets for an arbitrary beta number.

The subdivision process in the octonacci number case is similar to the golden mean one—at each step only the long tiles are split into three pieces and the short ones are left untouched so that at any step of the subdivision only two types of tiles are present (also, it can be seen that the support of wavelets in W_j does not cover the whole line). In the $\beta=2+\sqrt{3}$ case the situation is different. As it is seen from the matrix form of the scaling equation, the long tiles are split into four pieces and the short ones into three, so that at each step of the subdivision one has again only two tiles with respective lengths $1/\beta^j$ and $(\beta-3)/\beta^j$. Such a picture of refining of the quasilattice may happen to be relevant for the quasicrystals growth process.

For completeness we give three Haar-type wavelets necessary for building an orthonormal basis of W_0 for $\beta=2+\sqrt{3}$:

$$h^{(1)}(x)=\sqrt{\beta-1}\,\chi(\beta x)-\frac{1}{\sqrt{\beta-1}}\,(\chi(x)-\chi(\beta x)),$$

$$h^{(2)}(x)=\sqrt{\frac{\beta(\beta-2)}{\beta-1}}\,\chi(\beta x-1)-\sqrt{\frac{\beta}{\beta+1}}\,(\chi(x)-\chi(\beta x)-\chi(\beta x-1)), \tag{47}$$

$$h^{(3)}(x)=\sqrt{\frac{2\beta}{\beta+1}}\left(\chi(\beta x-2)-\frac{\beta}{\beta-1}\,(\chi(x)-\chi(\beta x)-\chi(\beta x-1)-\chi(\beta x-2))\right).$$

In the splitting of length 1 tiles all three functions are appearing, whereas for the $(\beta-3)$ tiles only $h^{(2)}(x)$ and $h^{(3)}(x)$ are relevant, since their support is less than or equal to $\beta-3$.

With any beta number one can associate a tiling of the real line by a finite number of tiles. Therefore it is natural to expect that for an arbitrary beta-number scaling factor one will need only a finite number of Haar-type wavelets. If the dilation parameter is not a beta number (this does not necessarily mean that it is transcendental), probably there will always be an infinity of wavelets of compact support. Certainly this diminishes an economy reached by the discrete wavelets with respect to the continuous ones. For example, such a situation seems to take place for the fractional scaling factors since the Rényi expansion for them is not eventually periodic (this contradicts the intuition that fractional numbers are simple objects). Because the noncompact support wavelets

are less sensitive to the origin of the scaling factor, it may occur that there are finitely many discrete wavelets for some of the nonbeta number scaling factors (e.g., for some kind of fractions of beta numbers).

It should be stressed that in principle one can use a split of the unit interval into two subintervals with the help of arbitrary scaling factor $\beta>1$. This subdivision can be written tautologically as $1=1/\beta+1/\alpha$, $\alpha=\beta/(\beta-1)$. One may take the Fourier transform of the obvious equality $\chi(x)=\chi(\beta x)+\chi(\alpha x-\alpha/\beta)$ for the characteristic function $\chi(x)$ and iterate the resulting relation as we did it above. This would give a representation of the Fourier transform of $\chi(x)$ as an infinite sum of exponentials with arguments scaled by powers of β and α. However, the coefficients in front of these exponentials are not simple and the numbers entering the exponents are difficult to characterize. The importance of beta numbers, for any of which one can derive summation formulas similar to the discussed ones, stems from the fact that for them there is a finite algorithm for determining β integers following from the finite or eventually periodic form of the Rényi expansion of 1. Note that the scalings by arbitrary integer p lead to the infinite product representations of the sinc function, admitting a probabilistic interpretation. The summation formulas we have derived do not have a similar infinite product representation, but there should be some probabilistic meaning of them too.

The key difference between lattices and quasilattices is that the sum of two points of the lattice remains in the lattice, whereas for quasilattices $\{\gamma_1+\gamma_2\}\not\subset\Gamma$, $\gamma_{1,2}\in\Gamma$. Therefore for quasilattices one actually has the orthogonality relations with the larger number of points than those in Γ:

$$\int_{-\infty}^{\infty}\chi^{(j)}(x-\gamma_1)\chi^{(k)}(x-\gamma_2)dx=\delta_{\gamma_1,\gamma_2}\delta_{jk}=\delta_{0,\gamma_1-\gamma_2}\delta_{jk}, \tag{48}$$

which is valid, even if $\gamma_1-\gamma_2\notin\Gamma$. Note that there is a correlation between the indices j,k and $\gamma_{1,2}$ in (48). When β is a Pisot number the points of difference set either belong to Γ or they are close but not arbitrarily close to the quasilattice, i.e. the difference set obeys the Delaunay property[15] (such sets Γ are called Meyer sets). E.g., for $\beta=\tau$ its points either lie in Γ or they are obtained from Γ by adding $1/\tau$ or $1/\tau^2$.[16] Whether this requires further specification of the form of multiresolution analysis is not yet clear. However, most of the tools used for derivation of discrete wavelet bases from the multiresolution analysis disappear in the nonperiodic setting.

It is worth it to draw attention to the recent work,[14] where the crystallographic Coxeter groups were applied to the construction of wavelets. It is natural to expect that in the context of irrational scaling factors the higher-dimensional quasicrystallographic structures become relevant and, again, one may expect strong dependence of the multiresolution analyses on the nature of irrationality of the dilation parameter.

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Moduli-space structure of knots with intersections

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It is well known that knots are countable in ordinary knot theory. Recently, knots *with intersections* have raised a certain interest, and have been found to have physical applications. We point out that such knots—equivalence classes of loops in R^3 under diffeomorphisms—are not countable; rather, they exhibit a moduli-space structure. We characterize these spaces of moduli and study their dimension. We derive a lower bound (which we conjecture being actually attained) on the dimension of the (nondegenerate components) moduli spaces, as a function of the valence of the intersection. © *1996 American Institute of Physics.*
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I. INTRODUCTION

At the end of his delicious booklet on catastrophe theory,[1] Arnold notices the following. Consider a set of n lines through the origin in the plane. Call two such sets equivalent if they can be mapped into each other by a linear transformation of the plane. The equivalence classes are discrete for $n=1,2,3$; but for $n=4$, a moment of reflection shows that the equivalence classes are parametrized by a continuous parameter. Precisely this phenomenon is at the root of the emergence of a rich moduli space structure in the spaces of knots with intersections.

Knots play an increasingly important role in various areas of mathematics and physics.[2–4] Classical knot theory[5] deals with knots without intersections, but recent applications of knot theory require knots *with intersections* to be considered as well.[6] For instance, quantum states of the gravitational field are labeled by knots with intersections in the loop representation approach to quantum gravity.[7,8] Knots can be defined in two ways: as equivalence classes of loops in R^3 under continuous deformations (ambient isotopy) of the image of the loop—''c knots;'' or as equivalence classes (of unparametrized loops) under invertible smooth transformations (diffeomorphisms) of R^3-''d knots.'' For the non-self-intersecting loops, the two definitions are equivalent, and there is no distinction between c knots and d knots. But the two definitions cease to be equivalent in the case with intersections. Intersecting d knots are different than intersecting c knots. The case of intersecting d knots is of particular interest in physics;[7] these knots display a remarkable novel phenomenon, which, to our knowledge, has been rarely noticed (the only mention to this phenomenon we could find in the literature is in Ref. 9): unlike ordinary knot spaces, the space $\mathcal{K}_d$ of the intersecting d knots is not countable.

The continuous dimensions of the space $\mathcal{K}_d$ come from the differential structure of the underlying manifold. The differential structure gives rise to a tangent space T_p at intersection points, loops define lines in T_p, and diffeomorphisms act linearly on T_p. Equivalence under diffeomorphisms imply equivalence under linear transformations of T_p. We are therefore precisely in the situation of Arnold's example—one dimension up. For a large enough number of lines, linear transformations of T_p fail to be able to align all the lines, and a moduli space structure emerge. Let us illustrate more in detail how this comes about by means of an example. Consider a smooth loop α in R^3, with a self-intersection point $p \in R^3$, and assume that α goes through p five times, so that it has five tangents $\mathbf{v}_1,...,\mathbf{v}_5$ at p (assume any three of the five are linearly indepen-

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dent). Let us denote by $K_c[\alpha]$ the c knot to which α belongs. Consider a loop β in the same c knot $K_c[\alpha]$. The loop β will have an intersection point as well, say q, and five tangents $\mathbf{w}_1,...,\mathbf{w}_5$ at q. In order for α and β to be in the same d knot, there must be a *diffeomorphism* $f:R^3\to R^3$ sending α into β. In particular, f maps p to q. The tangent map f^* maps the tangent space at p, T_p, to the tangent space at q, T_q, and it should align the tangents $\mathbf{v}_i$ $(i=1,...,5)$ to the tangents $\mathbf{w}_i$. But f^* is a *linear* map between three-dimensional spaces, given by the Jacobian matrix of f at p; it is a $GL(3)$ transformation depending on nine parameters. Since the directions of five vectors $\mathbf{v}_i$ depend on ten parameters, it is clear that generically no linear transformation exists that aligns five given vectors $\mathbf{v}_i$ to five given vectors $\mathbf{w}_i$. Generically, α and β will not belong to to the same d knot. There will be—at least—one continuous parameter λ—function of the angles between the five tangents—which is invariant under diffeomorphisms and distinguishes α from β. Actually, as we shall see, in this example there are two such parameters, λ_1 and λ_2; we will give them explicitly below. d knots are distinguished by such continuous parameters, and therefore fail to be countable. The space of all d knots in $K_c[\alpha]$ is a finite-dimensional space obtained by quotienting the infinite-dimensional space $K_c[\alpha]$ by the infinite-dimensional group Diff_{R^3}. Namely, it is a moduli space, coordinated by the two moduli, λ_1 and λ_2.

The same phenomenon repeats in the higher jets—namely for derivatives of the loops higher than the tangents—in a more intricate manner. Derivatives of order n transform under diffeomorphisms according to (nontrivial) transformation formulas that depend only on the derivatives of order $n-1$ (or lower) of the Jacobian matrix. Since the last have a finite number of components, a sufficiently high number of segments crossing one intersection will always give rise to new moduli. Thus, d knots are not countable and exhibit a very rich moduli space structure, coming from the jets of all orders.

In this paper, we make the above observation precise, we define the moduli spaces of intersecting d knots, and study their general structure and their dimension. We derive some general results on these dimensions. In particular, our main result is a formula for the dimension of the (generic components) of these spaces. We show that this formula gives a lower bound on the dimension of these spaces as a function of the valence of the intersection, and we conjecture that the formula gives indeed the correct dimension. Our original motivations came from quantum gravity, and we expect, in particular, that our results could be of interest for that field.

II. STRUCTURE OF THE INTERSECTING *d*-KNOT SPACE

By loop, we indicate here a smooth map α: $S_1\to M$ from the circle S_1 to a three-dimensional manifold M, which we assume for simplicity having the topology of R^3. We indicate loops by Greek letters $\alpha,\beta,...$, and denote the space of the loops in R^3 as $\mathscr{L}$. We consider two equivalence relations in $\mathscr{L}$. We say that α and β are c equivalent, and write $\alpha\sim_c\beta$ if there exist a smooth one-parameter family $c_t, t\in[0,1]$ of smooth, invertible maps from the image of α to R^3 such that $c_0\alpha=\alpha$ and $c_1\alpha=\beta$. Namely, if the image of α can be smoothly deformed to the image of β. This is clearly an equivalence relation; we call the corresponding equivalence classes in $\mathscr{L}$ c knots, and denote them as K_c. We denote the equivalence class to which α belongs as $K_c[\alpha]$ and the space of c knots as $\mathscr{K}_c$. Next we say that α and β are d equivalent, and we write $\alpha\sim_d\beta$, if there exist a diffeomorphism t of S_1 and a diffeomorphism f of M—connected to the identity—such that $\alpha=f\circ\beta\circ t$. This too is an equivalence relation. We call the corresponding d-equivalence classes in $\mathscr{L}$ d knots, and denote them as K_d. We denote the equivalence class to which α belongs as $K_d[\alpha]$, and the space of d knots as $\mathscr{K}_d$. Thus

$$\mathscr{K}_c=\frac{\mathscr{L}}{\sim_c},\quad \mathscr{K}_d=\frac{\mathscr{L}}{\sim_d}. \tag{1}$$

Our aim is to study the structure of $\mathscr{K}_d$. In particular, we want to investigate its continuous dimensions. d knots can be labeled by a set of discrete parameters k_j and continuous parameters

λ_j. We will use a Dirac-like notation $K_d=|k_j,\lambda_j\rangle$, suggested by the fact that d knots label quantum state of space–time in loop quantum gravity. We are interested in studying the appearance and the number of continuous parameters λ_j, namely the dimensions of the d-knot moduli spaces.

The space of the c knots $\mathscr{K}_c$ is countable. Since every diffeomorphism in the connected component of the identity induces a smooth deformation of the image of the loop, $\alpha\sim_d\beta$ implies $\alpha\sim_c\beta$, and therefore every d knot is contained inside a single c knot. Thus, we have a well-defined map $i:\mathscr{K}_d\to\mathscr{K}_c$ sending $K_d[\alpha]$ to $K_c[\alpha]$. As the example of the introduction shows, the map i is not injective: a c knot is formed, in general, by many d knots. We call $\mathscr{K}_d^{(K_c)}$ the inverse image of K_c under i, namely the set of the d knots that correspond to the c-knot K_c. The space $\mathscr{K}_d$ is thus the union of a countable number of components $\mathscr{K}_d^{(K_c)}$, one for every c knot K_c,

$$\mathscr{K}_d=\bigcup_{K_c\in\mathscr{K}_c}\mathscr{K}_d^{(K_c)}. \tag{2}$$

In other words, the first discrete parameter that characterizes a d-knot K_d is the c-knot K_c to which it belongs, and we can write $K_d=|K_c,\text{ other parameters}\rangle$.

Let us consider one of the components $K_d^{(K_c)}$. A continuous map cannot change the number of intersections I of a loop. Therefore this number is well defined for a c-knot K_c. Each intersection i is further characterized by the number N_i of times the loop crosses it, which we call the valence of the intersection, following the literature. Thus, a set of integers N_i, $i=1...I$—the valence of its intersections—is associated with every c knot. Imagine now that three segments cross at the intersection i, namely $N_i=3$. Imagine that the corresponding three tangents at the intersection are linearly dependent. A continuous transformation can alter this linear dependence, but a diffeomorphism cannot. Thus, the presence of linear dependency between tangents distinguishes the d knot. We denote an intersection of valence three with linearly dependent tangents as a degenerate intersection. Similarly, we denote an intersection of higher valence degenerate if at least one triple of its tangents is linearly dependent. As we shall better illustrate below, degeneracy of this kind—a relation between derivatives of the loop that cannot be removed by a diffeomorphism—may occur for higher than first derivatives of the loops as well. The information about the presence of degeneracy is discrete, and we represent it collectively by a discrete parameter k_i for every intersection i. We write $K_d=|K_c,k_i,\text{ other parameters}\rangle$ and denote the set of d knots in the same c knot and with the same degeneracies as $\mathscr{K}_d^{(K_c,k_i)}$. We shall write $k_i=0$, or just omit the k_i to indicate that the i intersection has no degeneracies.

This exhausts the discrete parameters that characterize d knots. The remaining parameters distinguishing d knots are continuous moduli parameters. Thus, the space of intersecting d knots $\mathscr{K}_d$ can be written as the union of a denumerable set of components $\mathscr{K}_d^{(K_c,k_i)}$ as

$$\mathscr{K}_d=\bigcup_{K_c\in\mathscr{K}_c}\bigcup_{k_i}\mathscr{K}_d^{(K_c,k_i)}, \tag{3}$$

where the spaces $\mathscr{K}_d^{(K_c,k_i)}$ are finite-dimensional moduli spaces, whose dimensions we are now going to study.

Let us consider one of these moduli spaces $\mathscr{K}_d^{(K_c,k_i)}$. A moment of reflection shows that each modulus is attached to one of the intersections, and that there is no relation between moduli of different intersections. As we will show below, the number of moduli that characterize a d knot at one intersection depends on the valence N_i of the intersection, and the possible presence of degeneracies described by k_i. Let $d(N_i,k_i)$ be the number of moduli that characterize an intersection i. Then, there will be $d(N_i,k_i)$ continuous parameters $\lambda_j^{(i)}$, $j=1...d(N_i,k_i)$ characterizing each intersection i. The d knot is then fully characterized by all these parameter for each of its intersections. Namely

$$K_d = |K_c, k_i, \lambda_{j_i}^{(i)}\rangle, \tag{4}$$

where $i = 1...I$ and $j_i = 1...d(N_i, k_i)$. In other words, the moduli space $\mathscr{K}_d^{(K_c, k_i)}$ is the Cartesian product of one moduli space per each intersection. We denote the moduli space of an intersection of valence N and (possible) degeneracy k, by $\mathscr{K}_{N,k}$. We thus have

$$\mathscr{K}_d = \bigcup_{K_c \in \mathscr{K}_c} \bigcup_{k_i} \otimes_{i \in K_c} \mathscr{K}_{N_i, k_i}. \tag{5}$$

It follows that it is sufficient to study intersections (of any valence N and with any degeneracy k) in order to fully determine the general structure of $\mathscr{K}_d$. Below, we will discuss the moduli space $\mathscr{K}_N = \mathscr{K}_{N,0}$ of the intersections of arbitrary valence, but with no degeneracy. The case with degeneracy $k \neq 0$ can be treated along similar lines.

III. THE MODULI SPACE $\mathscr{K}_N$

Let p be a nondegenerate intersection point of valence N (we drop the suffix i since we deal here with a single intersection) in a loop α. We denote by s (or $t, u, ...$) a coordinate on the circle S_1 and use coordinates x^a with $a = 1,2,3$ from an atlas of M. Thus p^a will be the coordinates of p and we write $\alpha: s \mapsto \alpha^a(s)$. There are N segments of α crossing p (the intersection between α and a sufficiently small M neighborhood of p); we denote them by $\alpha_i^a(s)$, where $i = 1...N$, and we call s_i the N points in S_1 defined by $\alpha(s_i) = p$. Similarly, we consider a second loop β in the same moduli space, namely in the same c knot and with the same degeneracies as α. Let q be its intersection point (corresponding to p) and $\beta_i^a(s)$ the coordinates of the segments crossing in q. The two loops are in the same d knot if there is a diffeomorphism of the three manifold $f: x^a \mapsto f^a(x)$ and a diffeomorphism of the circle $t: s \mapsto t(s)$, such that

$$f^a(\alpha(t(s))) = \beta^a(s). \tag{6}$$

If we Taylor expand this condition around the intersection point, for each of the N segments, we obtain

$$\begin{aligned}
&\beta^a(s_i) + \frac{d}{ds}\,\beta^a(s)\Big|_{s_i}(s - s_i) + \cdots + \frac{1}{n!}\,\frac{d^n}{ds^n}\,\beta^a(s)\Big|_{s_i}(s - s_i)^n + \cdots \\
&\quad = f^a(\alpha(t(s_i))) + \frac{d}{ds}\,f^a(\alpha(t(s)))\Big|_{s_i}(s - s_i) + \cdots \\
&\qquad + \frac{1}{n!}\,\frac{d^n}{ds^n}\,f^a(\alpha(t(s)))\Big|_{s_i}(s - s_i)^n + \cdots .
\end{aligned} \tag{7}$$

From here on, the following notation will be used (for the sake of tradition and brevity):

$$\begin{aligned}
&\dot{\alpha}_i^a = \frac{d}{ds}\,\alpha^a(s)\Big|_{s_i}, \quad \alpha_i^{(n)a} = \frac{d^n}{ds^n}\,\alpha^a(s)\Big|_{s_i}, \\
&f^a_{b_1 \ldots b_n} = \frac{\partial^n f^a}{\partial x^{b_1} \ldots, \partial x^{b_n}}\Big|_p, \quad t_i^{(n)} = \frac{d^n}{ds^n}\,t(s)\Big|_{s_i}.
\end{aligned} \tag{8}$$

We now consider each term of the expansion (7) separately. To zero order, we have

$$f^a(p)=q^a. \tag{9}$$

To first order

$$f^a_b\dot{\alpha}^b_i t^{(1)}_i=\dot{\beta}^a_i\,. \tag{10}$$

Indices are summed if repeated on different levels. To second order we have

$$f^a_{bc}\dot{\alpha}^b_i\dot{\alpha}^c_i(t^{(1)}_i)^2+f^a_b\dot{\alpha}^b_i t^{(2)}_i=-f^a_b\alpha^{(2)b}_i(t^{(1)}_i)^2+\beta^{(2)a}_i\,. \tag{11}$$

And, for any order $n\geqslant 2$,

$$f^a_{b_1\cdots b_n}\dot{\alpha}^{b_1}_i\cdots\dot{\alpha}^{b_n}_i(t^{(1)}_i)^n+f^a_b\alpha^{(n)b}_i(t^{(1)}_i)^n+f^a_b\dot{\alpha}^b_i t^{(n)}_i+F^a_i=\beta^{(n)a}_i\,, \tag{12}$$

or

$$f^a_{b_1\cdots b_n}\dot{\alpha}^{b_1}_i\cdots\dot{\alpha}^{b_n}_i(t^{(1)}_i)^n+f^a_b\dot{\alpha}^b_i t^{(n)}_i=\beta^{(n)a}_i-f^a_b\alpha^{(n)b}_i(t^{(1)}_i)^n-F^a_i\,, \tag{13}$$

where F^a_i is a function of the derivatives of f, α^a_i, and t of orders lower than n (namely of $f^a_{b_1\cdots b_k},\ldots;\alpha^{(k)a}_i,\ldots;t^{(k)}_i,\ldots$, with $k=1,\ldots,n-1$). Equation (7) is equivalent to the infinite system (9)–(13).

Now, the two loops α and β are d equivalent if this system can be solved for the functions f and t, namely for the infinite tower of variables $f^a_{b_1\cdots b_n},t^{(n)}_i$. Therefore, we may regard (9)–(13) as a system of equations for the unknowns $f^a_{b_1\cdots b_n},t^{(n)}_i$. If the system can be solved for every α and β, then all such loops are in the same d knot and there are no moduli. Namely, the moduli space has zero dimension. This is the case, for instance, if $N=2$ (the lowest valence intersection, formed by a single crossing). In fact, one can check in this case that for each order n the number of unknowns is larger than the number of equations, and the system can be solved. For higher valence intersections, however, the system cannot be solved for arbitrary α and β. This means that there are loops that are not in the same d knot, and we have a moduli space structure.

A moment of reflection shows that the dimension of the moduli space is equal to the number of (independent) equations that overdetermine the system. To clarify this point, imagine that the system is solvable for general α and β only if we leave, say, d (independent) equations out. By inserting f and t that solve the rest of the system into these equations we obtain d equations relating α and β. If we imagine that β is fixed, we obtain then d conditions on α, determining the set of α's d equivalent to β. Thus, this set has codimension d in the space of the α's. This means that a d knot has codimension d in the space of the loops in $\mathscr{K}_N$, and therefore that there is a d parameters space of d knots in $\mathscr{K}_N$. Namely $\mathscr{K}_N$ is d dimensional.

Our task is therefore to find—for every given N—the number of d of independent equations by which the system (9)–(13) is overdetermined. This may seem a hard task, given that the system has an infinite number of equations, but there is a key observation that simplifies the matter. First, observe that the system has a rather simple structure. As we increase the order n, at each new order there are only a finite number of new unknowns that appear. Indeed the unknowns $f^a_{b_1\cdots b_n}$ and $t^{(n)}_i$ appear only at order n or higher. We denote them as unknowns of order n. For instance, at order zero, the only unknowns are the three f^a. At order unity, we have the new unknowns f^a_b (nine of them) and $t^{(1)}_i$ (N of them), and so on. Now, at each other n, we have the same number $3N$ of equations in the system. But the number of unknowns increases rapidly, because the number of components of $f^a_{b_1\cdots b_n}$ increases with n. Indeed, $f^a_{b_1\cdots b_n}$ has $3\times I_n$ independent entries, where

$$I_n = \frac{(n+1)(n+2)}{2} \tag{14}$$

is the number of independent components in a completely symmetrized $3\times3\times\cdots\times3$ n-dimensional matrix. It is then easy to see that (for fixed N) the equations of sufficiently high order can always be solved. More precisely, for every N, there is a number m, which we determine below, such that all equations of order higher than m can always be solved, and we can safely forget them. This fact essentially reduces the system to a finite-dimensional system, making the problem treatable.

A. A gauge

One is now tempted to immediately proceed to determine the number of equations by which the system is overdetermined by naively counting equations and unknowns order by order, and subtracting. Unfortunately, there is a complication. At every order n, the actual number of unknowns is less than what a simple count would suggest, because of the particular structure of our equations. Consider first Eq. (10). The unknowns are the nine components of f^a_b and the N quantities $t^{(1)}_i$. However, if $f^a_b, t^{(1)}_i$ solve (10), so do

$$\tilde{f}^a_b = T f^a_b, \quad \tilde{t}^{(1)}_i = T^{-1} T^{(1)}_i, \tag{15}$$

for every nonvanishing T. Therefore, the overall scale T can never be determined by Eq. (10). In other words, Eq. (10) depends on only $(9+N-1)$ functions of the $(9+N)$ quantities $f^a_b, t^{(1)}_i$. The remaining one cannot be determined by this equation.

The same happens at higher orders. It is easy to verify that if $f^a_{b_1\cdots b_n}, t^{(n)}_i$ solve the equation of order n, so do

$$\tilde{f}^a_{b_1\cdots b_n} = f^a_{b_1\cdots b_n} + f^a_{(b_1} T_{b_2\cdots b_n)},$$

$$\tilde{t}^{(n)}_i = t^{(n)}_i - T_{a_1\cdots a_{n-1}} \dot{\alpha}^{a_1}_i \cdots \dot{\alpha}^{a_{n-1}}_i (t^{(1)}_i)^2, \tag{16}$$

for every symmetric tensor $T_{a_1\cdots a_{n-1}}$. This tensor has I_{n-1} components. We call this transformation the n-order gauge of the system. Because of the gauge, if we cut off the system at order n, we have indeed I_{n-1} less unknowns entering the system than what a naive counting would suggest. Are there other degeneracies beside the gauge we have just described? We suspect there are not, but we have not been able to prove this in general. Because of this incompleteness, we cannot claim that the number we compute below is in fact the dimension of the moduli space, but only that it is the dimension's lower bound.

B. Size of the space of solutions

Consider the order $n=0$, Eq. (9). We have three unknowns (f^a) and three equations there. The system is linear and can obviously always be solved. Consider next the order $n=1$, Eq. (10). There are $9+N$ unknowns, and $3N$ equations. But, because of the gauge described above, only $9+N-1$ unknowns can be determined by the equations. Generically, the system can be solved if the number of equations is less than or equal to the number of unknowns, namely if

$$3N \leqslant 9 + N - 1. \tag{17}$$

In this case, if $N\leqslant4$. A simple inspection of the equation confirms that for $N\leqslant4$ the three equations can indeed be solved, and thus they do not give rise to any continuous dimension (since we assumed an absence of degeneracies at the beginning of our analysis). What happens if $N=5$?

In this case we have 15 equations and 13 (independent) unknowns. Which means that the system is overdetermined by two equations. Again, inspection shows that this is indeed the case. Correspondingly, we expect to have at least a two-dimensional moduli space for $N=5$.

Let us study this $N=5$. At order 2 we have $3N=15$ equations and $3I_2+N-I_{2-1}+I_{1-1}=21$ unknowns, where the term I_{2-1} represents the number of irrelevant variables (the ones that cannot be solved for) because of the gauge of order 2, and the term I_{1-1} represents the gauge unknown of order 1 that becomes relevant (can be solved for) at order 2. We have more unknowns than equations and so we expect the system to be solvable. Indeed, it is solvable. The same happens for higher orders, and thus we can conclude that the only equations for which the system is overdetermined are the two of order 1. Thus, an intersection of valence 5 has a two-dimensional moduli space. In the next section, we will study this example in detail for illustration. Here let us continue the general analysis.

At any given order n, we have $3N$ equations and $3I_n+N-I_{n-1}+I_{n-2}$ new unknowns, where again the term I_{n-1} is for the gauge terms of order n (that are not being solved for at order n) and the term I_{n-2} is for the gauge terms of order $n-1$ (that can be solved for in order n as opposed to order $n-1$). Generically, the system can be solved if the number of equations is less than the number of unknowns:

$$3N \leqslant 3I_n+N-I_{n-1}+I_{n-2}, \tag{18}$$

which yields

$$N \leqslant \frac{3n^2+7n+6}{4}. \tag{19}$$

Solving this for n, we find that the system is solvable at any order $n>m(N)$, where

$$m(N) =: \mathrm{Int}^-\left(\frac{\sqrt{48N-23}-7}{6}\right), \tag{20}$$

where $\mathrm{Int}^-(x)$ is the largest integer smaller than x. Thus we can forget all equations of order larger than $m(N)$ in the system [(9)–(13)]. The remaining system is formed by the $3N\times m$ equations of order $n \leqslant m(N)$. (We do not count the three equations of order zero and the three unknowns f^a, which can always be found.) At each order n (less or equal to m), the number d_n of overdetermined equations is

$$d_n = \#\text{ equations} - \#\text{ unknowns} = 3N-(3I_n+N-I_{n-1}+I_{n-2}), \tag{21}$$

(where $I_0=I_{-1}=0$), and the total number of equations by which the system is overdetermined is

$$d=\sum_{n=1,m} d_n = \sum_{n=1,m} 2N-3I_n+I_{n-1}-I_{n-2} = 2mN+I_{n-1}-3\sum_{n=1,m} I_n. \tag{22}$$

Since we are under the assumption that the intersection is nondegenerate, there are no additional degeneracies in the linear system, and the d equations by which the system is overdetermined are independent. Thus d gives the lower bound on the dimension of the moduli space that we are searching. Performing the sum, we get

$$d(N)=(2N-5)m-\frac{5}{2}m^2-\frac{1}{2}m^3, \tag{23}$$

where m is a function of N, given in Eq. (20). Equation (23) is our main result. It gives (a lower bound on) the dimension of the moduli space of a single nondegenerate intersection of order N.

IV. AN EXAMPLE: $N=5$

Let us consider again the simplest nondegenerate case in which a moduli space appear, which is $N=5$. Thus, we have an intersection point p crossed by the loop α five times. From Eq. (20) we have $m=1$ and from Eq. (23) $d=2$, as anticipated. It is instructive to identify the two continuous degrees of freedom of the knot space. We will do this in two different ways. First, we give a geometrical construction of these two degrees of freedom, and then we give an explicit algebraic expression for the two moduli.

Let us fix an arbitrary coordinate chart in the neighborhood of p, and let $\dot\alpha_i^a$ for $i=1,2,3,4,5$ be the components of the five tangents of α at p. Let us (arbitrarily) pick three of these five tangents, say $\dot\alpha_k^a$ for $k=1,2,3$. The three vectors $\dot\alpha_k^a$ define a basis in the tangent space at p. Clearly the components of the other two tangents, $\dot\alpha_4^a$ and $\dot\alpha_5^a$ on this basis, are quantities that do not depend on the coordinate chosen, and are consequently invariant under diffeomorphisms. If we indicate by $(\dot\alpha^{-1})_a^k$ the 3×3 matrix inverse to the 3×3 matrix $\dot\alpha_k^a$, such components are given by

$$\beta_4^k=(\dot\alpha^1)_a^k\dot\alpha_4^a, \quad \beta_5^k=(\dot\alpha^1)_a^k\dot\alpha_5^a. \tag{24}$$

The quantities β_4^k and β_5^k are invariant under diffeomorphisms. They transform under a reparametrization of the loop as $\beta_4^k\mapsto t_4t_k^{-1}\beta_4^k$, where t_i are the five derivatives of the reparametrization in the intersection point. Assuming, for instance, that the components of β_4^k are positive, we can always choose these derivatives in such a way that, say, $\beta_4^k=(1,1,1)$. The length of the last vector, β_5^k, can be arbitrarily rescaled, by fixing t_5, but its direction is uniquely determined. This direction gives the two dimensions of the moduli space.

Notice that the sign of the components of β_4^k determine eight disconnected sectors of the moduli space, at the boundary of which are degenerate intersections. This is a general feature: the moduli spaces in general have disconnected components, separated by the degenerate cases.

Given the above discussion, it is not too hard to write the two moduli explicitly. This can be done, for instance, in the following manner:

$$\lambda_1=\frac{(\dot\alpha^{-1})_a^1\dot\alpha_4^a(\dot\alpha^{-1})_b^2\dot\alpha_5^b}{(\dot\alpha^{-1})_c^2\dot\alpha_4^c(\dot\alpha^{-1})_d^1\dot\alpha_5^d}, \quad \lambda_2=\frac{(\dot\alpha^{-1})_a^1\dot\alpha_4^a(\dot\alpha^{-1})_b^3\dot\alpha_5^b}{(\dot\alpha^{-1})_c^3\dot\alpha_4^c(\dot\alpha^{-1})_d^1\dot\alpha_5^d}. \tag{25}$$

It is easy to see that these two quantities are independent and are invariant under diffeomorphisms of the manifold and reparametrization of the loops.

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Bicrossproduct Hopf superalgebras and $D=4$ κ-deformed Poincaré supergroup

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The general framework of bicrossproduct Hopf algebras given by Majid is extended to Z_2-graded bicrossproduct Hopf superalgebras. As examples of bicrossproduct Hopf superalgebras we provide the graded algebras of functions on undeformed as well as κ-deformed $D=4$ Poincaré supergroups. © *1996 American Institute of Physics.* [S0022-2488(96)01806-3]

I. INTRODUCTION

The inhomogeneous groups G described by means of the semidirect product $G=H\ltimes A$ of a simple Lie group H and the Abelian group A are very important in physical applications (see, e.g., Ref. 1). The most important example is given by the $D=4$ Poincaré group $\mathscr{P}_4=\mathrm{SO}(3,1)\ltimes T^4$, where $H=\mathrm{SO}(3,1)$ is the Lorentz group and $A=T^4$ describes four Abelian translations. The Poincaré group as a semidirect product can be supersymmetrized in two ways.

(i) We keep the factor $H=\mathrm{SO}(3,1)$ unchanged but we replace the Abelian subgroup $A=T^4$ by its superextension $T^{4;4}$, with the $D=4$ superalgebra generators $(\overline{Q_{\dot\alpha}}=(Q_\alpha)^+)$,

$$\begin{gathered}\{Q_\alpha,\overline{Q_{\dot\beta}}\}=2(\sigma_\mu)_{\alpha\dot\beta}P^\mu,\quad \{Q_\alpha,Q_\beta\}=\{\overline{Q_{\dot\alpha}},\overline{Q_{\dot\beta}}\}=0,\\ [Q_\alpha,P_\mu]=[\overline{Q_{\dot\alpha}},P_\mu]=0,\quad [P_\mu,P_\nu]=0.\end{gathered}\tag{1.1}$$

The $D=4$ Poincaré group $\mathscr{P}_{4;1}$ can be written therefore as (see, e.g., Ref. 2)

$$\mathscr{P}_{4;1}=\mathrm{SO}(3,1)\ltimes T^{4;4},\tag{1.2}$$

where both factors in (1.2) are non-Abelian.

(ii) One can attach to the factor $H=\mathrm{SO}(3,1)$ only two complex supertranslations, e.g., generated by Q_α ($\alpha=1,2$). In such a way we introduce the graded Lorentz group SO(3,1;2) with the Lorentz generators $M_{\mu\nu}$ and two anticommuting odd generators Q_α, satisfying the relations

$$[M_{\mu\nu},Q_\alpha]=\frac{i}{2}(\sigma_{\mu\nu})_\alpha{}^\beta Q_\beta.\tag{1.3}$$

Denoting the graded Abelian group generated by generators $(P_\mu,\overline{Q_{\dot\alpha}})$ by $\overline{T_{4;2}}$, one can write

$$\mathscr{P}_{4;1}=\mathrm{SO}(3,1;2)\ltimes\overline{T_{4;2}}.\tag{1.4a}$$

In fact, there is still another possibility, obtained by substituting in SO(3,1;2) the generators Q_α by $Q_{\dot\alpha}(\mathrm{SO}(3,1;2)\to\overline{\mathrm{SO}(3,1;2)})$ and replacing in $T_{4;2}$ the generators $Q_{\dot\alpha}$ by $Q_\alpha(T_{4;2}\to T_{4;2})$. One gets

$$\mathscr{P}_{4;1}=\overline{\mathrm{SO}(3,1;2)}\ltimes T_{4;2}. \tag{1.4b}$$

The advantage of the semidirect products (1.4a)–(1.4b) is the preservation of the graded Abelian nature of the second factor. It appears that this graded Abelian structure will be preserved also after the κ deformation (compare with Ref. 9, where the four-momenta for κ-deformed Poincaré algebra commute).

The main result of this paper is the description of quantum κ deformation of $D=4$ Poincaré supergroup in the framework of bicrossproduct Hopf superalgebras. It appears that for the standard (''bosonic'') quantum groups the bicrossproduct Hopf algebra $H_1\triangleright\!\blacktriangleleft H_2$ provides an attractive proposal for the general framework of quantum deformations of the classical semidirect product of H_1 and H_2 supplemented by consistent coalgebra structure.[3–5] Indeed, recently it has been shown that the dual pair of κ-deformed Poincaré algebra[6,7] and κ-deformed Poincaré group[8] can be very well incorporated[9–11] into the bicrossproduct scheme (the general approach proposed recently by Podleś and Woronowicz[12] can be also put into the general bicrossproduct framework). Our aim here is to extend such a framework to the ''super'' case.

Our presentation contains two parts.

(i) It appears that the signature factors that enter into the defining properties of graded bicrossproduct Hopf algebras are not known in the literature, and appear in several formulas in a way that is far from obvious. In Sec. II we describe the general framework describing graded bicrossproduct Hopf algebras, extending to the super case results presented by Majid.[3–5]

(ii) In Sec. III we describe the $D=4$ κ-deformed Poincaré supergroup, presented first in Ref. 13, as the graded bicrossproduct Hopf algebra, i.e. we provide the example of our general scheme. In this description the graded Hopf algebra is the algebra of functions on a quantum supergroup with a graded set of generators.

It should be stressed that the bicrossproduct description of Hopf algebra, $H=H_1\triangleright\!\blacktriangleleft H_2$, implies the bicrossproduct structure of dual Hopf algebra, $\tilde H=\tilde H_2\triangleright\!\blacktriangleleft\tilde H_1$, where the ''tilde'' describes the dual object. Indeed, the first complete proof of duality between $D=4$ κ-Poincaré quantum algebra and $D=4$ κ-Poincaré quantum group was obtained in Ref. 11 after using the bicrossproduct form of both dual structures. In the present paper it is first demonstrated that the $D=4$ κ-Poincaré supergroup is an example of graded bicrossproduct Hopf algebra. Because the bicrossproduct structure of $D=4$ κ-Poincaré quantum superalgebra is already known,[14] we believe that it is only a technical matter to extend the proof given in Ref. 11 to the supersymmetrized case.

II. BICROSSPRODUCT HOPF ALGEBRAS

First, we shall recall the general definition of bicrossproduct Hopf algebra, due to Majid.[3–5] Let H_1, H_2 ($a\in H_1$, $h\in H_2$) are two Hopf algebras, with the coproducts $\Delta(a)=a_{(1)}\otimes a_{(2)}$, $\Delta(h)=h_{(1)}\otimes h_{(2)}$. We assume further that the following occurs.

(i) H_2 is a right H_1 module algebra, i.e., there exists an action α: $H_2\otimes H_1\to H_2$ denoted by

$$\alpha(a\otimes h)=a\triangleleft h, \tag{2.1}$$

defining the crossproduct $H_1\ltimes H_2$.

(ii) H_1 is a left H_2-comodule coalgebra, i.e. there exists a coaction β: $H_1\to H_2\otimes H_1$, such that

$$\beta(h)=h^{(1)}\otimes h^{(2)}, \tag{2.2}$$

where $h^{(1)}\in H_2$, $h^{(2)}\in H_1$, which defines the crossproduct $H_1\blacktriangleright\!\blacktriangleleft H_2$.

The following statement is valid.

Theorem 1: *(see Ref. 3, Theorem 3.3)*
The linear space $H_1 \otimes H_2$ is endowed with the Hopf algebra structure and defines the right–left bicrossproduct Hopf algebra $H_1 \triangleright\!\blacktriangleleft H_2$ if the action α and coaction β satisfy the following compatibility conditions:

$$\epsilon(a \triangleleft h) = \epsilon(a)\epsilon(h), \quad \beta(1) = 1 \otimes 1, \tag{2.3a}$$

$$\Delta(a \triangleleft h) = (a_{(1)} \triangleleft h_{(1)}) h_{(2)}{}^{(1)} \otimes a_{(2)} \triangleleft h_{(2)}{}^{(2)}, \tag{2.3b}$$

$$\beta(hg) = (h^{(1)} \triangleleft g_{(1)}) g_{(2)}{}^{(1)} \otimes h^{(2)} g_{(2)}{}^{(2)}, \tag{2.3c}$$

$$h_{(1)}{}^{(1)}(a \triangleleft h_{(2)}) \otimes h_{(1)}{}^{(2)} = (a \triangleleft h_{(1)}) h_{(2)}{}^{(1)} \otimes h_{(2)}{}^{(2)}. \tag{2.3d}$$

The multiplication structure in $H_1 \triangleright\!\blacktriangleleft H_2$ is defined by

$$(h \otimes a) \cdot (g \otimes b) = h g_{(1)} \otimes (a \triangleleft g_{(2)}) b, \tag{2.4}$$

and the comultiplication looks as follows:

$$\Delta(h \otimes a) = (h_{(1)} \otimes h_{(2)}{}^{(1)} a_{(1)}) \otimes (h_{(2)}{}^{(2)} \otimes a_{(2)}). \tag{2.5}$$

The antipode and the counit are given by the formulas

$$S(h \otimes a) = (1 \otimes S(h^{(1)} a)) \cdot (S(h^{(2)}) \otimes 1), \tag{2.6a}$$

$$\epsilon(h \otimes a) = \epsilon(h)\epsilon(a). \tag{2.6b}$$

The simplest examples of bicrossproduct Hopf algebras are the following.

(i) Semidirect product of simple Lie algebra and the Abelian algebra, e.g. $\mathscr{P}_4 = \mathrm{SO}(3,1) \triangleright\!\blacktriangleleft T^4$, considered a Hopf algebra with a primitive coproduct. In such a case ($M_{\mu\nu} \in \mathrm{SO}(3,1)$, $P_\mu \in T^4$),

$$\alpha(P_\mu \otimes M_{\rho\tau}) = P_\mu \triangleleft M_{\rho\tau} = [P_\mu, M_{\rho\tau}], \quad \beta(M_{\mu\nu}) = 1 \otimes M_{\mu\nu}. \tag{2.7}$$

(ii) If H_1 is commutative and H_2 is cocommutative, the bicrossproduct $H_1 \triangleright\!\blacktriangleleft H_2$ describes the Hopf algebra extension in the sense of Singer.[15]

(iii) The quantum κ deformation of $D=4$ Poincaré algebra $\mathscr{U}(so(3,1)) \triangleright\!\blacktriangleleft \mathscr{U}_\kappa(T^4)$[9,10] as well as the quantum κ deformation od $D=4$ Poincaré group $C(\mathrm{SO}(3,1)) \blacktriangleright\!\triangleleft C_\kappa(\widetilde{T}^4)$,[9–11] where $C(\mathrm{SO}(3,1))$ and $C_\kappa(\widetilde{T}^4)$ describe, respectively, the algebra of functions on the Lorentz group and the algebra of functions on the Abelian translation group [$C_\kappa(\widetilde{T}^4)$ is dual to $\mathscr{U}_\kappa(T^4)$].

III. Z_2-GRADED BICROSSPRODUCT HOPF SUPERALGEBRA

A. Z_2-graded Hopf superalgebras

Let us assume that $\mathscr{H}$ is a Z_2-graded algebra, i.e., as a vector space $\mathscr{H} = \mathscr{H}_0 \oplus \mathscr{H}_1$. We define the parity of an element $h \in \mathscr{H}$ as follows:

$$p(h) = 0, \quad \text{if } h \in \mathscr{H}_0; \quad p(h) = 1, \quad \text{if } h \in \mathscr{H}_1. \tag{3.1}$$

We introduce the tensor product of two Z_2-graded algebras $\mathscr{H} \otimes \mathscr{H}'$ as Z_2-graded algebra, with the following multiplication rule:

$$(h \otimes h') \cdot (g \otimes g') = (-1)^{p(h')p(g)} hg \otimes h'g', \tag{3.2}$$

where $h,g \in \mathscr{H}$ and $h',g' \in \mathscr{H}'$. Let us introduce the following definitions:[16–18]
Definition 1: The Hopf superalgebra $(\mathscr{H},\Delta,\epsilon,S)$ *is given by the following axioms*:

(i) $\mathscr{H}$ *is a* Z_2*-graded algebra.*

(ii) *The comultiplication map* Δ*:* $\mathscr{H}\to\mathscr{H}\otimes\mathscr{H}$ *is a homomorphism of* $\mathscr{H}$ *and is superassociative, i.e.*

$$(\Delta\otimes 1)\Delta(h)=(1\otimes\Delta)\Delta(h), \tag{3.3}$$

where the tensor product is defined by (3.2); besides $\Delta(1) = 1 \otimes 1$.

(iii) *The counit* ϵ *is linear map* $\mathscr{H}\to C$*, where*

$$\epsilon(hh')=\epsilon(h)\epsilon(h'), \quad (\epsilon\otimes 1)\Delta(h)=(1\otimes\epsilon)\Delta(h)=h. \tag{3.4}$$

(iv) *The antipode* S *is defined as linear antiisomorphism* $\mathscr{H}\to\mathscr{H}$ *with the property* $(m(h\otimes h')=h\cdot h')$

$$m\circ(S\otimes 1)\circ\Delta(h)=m\circ(1\otimes S)\circ\Delta(h)=\epsilon(h)\cdot 1. \tag{3.5}$$

If we introduce the graded flip operation:

$$\sigma(h\otimes h')=(-1)^{p(h)p(h')}h'\otimes h, \tag{3.6}$$

and the graded opposite coproduct,

$$\Delta'(h)=\sigma\circ\Delta(h), \tag{3.7}$$

we also obtain that

$$(S\otimes S)\Delta(h)=\Delta'(S(h)), \tag{3.8}$$

as well as

$$S(hh')=(-1)^{p(h)p(h')}S(h')S(h). \tag{3.9}$$

Remark 1: The Hopf superalgebra is a special case of anionic Hopf algebras, with Z_n grading, for the special case $n=2$.[19] The anionic algebras are the special case of braided Hopf algebras.[20–21]

Remark 2: The well-known examples of noncommutative and noncocommutative Hopf superalgebras are the quantum deformations of universal enveloping algebras of simple Lie superalgebras (see, e.g., Refs. 17–19), as well as the quantum-deformation of the algebra of functions on a simple Lie supergroups (see, e.g., Ref. 22).

B. Bicrossproduct Hopf superalgebras

Let us assume that $\mathscr{H}_1$, $\mathscr{H}_2$ are two Hopf superalgebras (we put $h,g,f \in \mathscr{H}_1$, $a,b,c \in \mathscr{H}_2$). We assume further the following.

(i) $\mathscr{H}_2$ is a right $\mathscr{H}_1$ module, with the action α [see (2.1)], satisfying the grading property

$$ab\triangleleft h=(-1)^{p(h_{(1)})p(b)}(a\triangleleft h_{(1)})(b\triangleleft h_{(2)}), \tag{3.10a}$$

$$a\triangleleft(hg)=(a\triangleleft h)\triangleleft g. \tag{3.10b}$$

(ii) $\mathscr{H}_1$ is a left $\mathscr{H}_2$-comodule cosuperalgebra with the action β [see (2.2)], satisfying $\beta(1)=1\otimes 1$ and the following properties:

$$(1\otimes\beta)\circ\beta=(\Delta\otimes 1)\circ\beta, \tag{3.11a}$$

$$(\epsilon\otimes 1)\circ\beta(h)=1_{\mathscr{H}_1}\otimes h, \tag{3.11b}$$

$$(1\otimes\Delta)\beta(h)=m_{12}\sigma_{23}(\beta\otimes\beta)\Delta. \tag{3.11c}$$

Theorem 2: *The linear Z_2-graded space (superspace) $\mathscr{H}_1\otimes\mathscr{H}_2$ is endowed with the Hopf superalgebra structure and defines the Z_2-graded bicrossproduct Hopf superalgebra $\mathscr{H}_1\bowtie\mathscr{H}_2$ with the following definitions of multiplication, comultiplication, counit and antipode,*

$$(h\otimes a)(g\otimes b)=(-1)^{p(a)p(g_{(1)})}hg_{(1)}\otimes(a\triangleleft g_{(2)})b, \tag{3.12}$$

$$\Delta(h\otimes a)=(-1)^{p(h_{(2)}{}^{(2)})p(a_{(1)})}h_{(1)}\otimes h_{(2)}{}^{(1)}a_{(1)}\otimes h_{(2)}{}^{(2)}\otimes a_{(1)}, \tag{3.13}$$

$$\epsilon(h\otimes a)=\epsilon(h)\cdot\epsilon(a), \tag{3.14}$$

$$S(h\otimes a)=(-1)^{p(h^{(2)})[p(h^{(1)})+p(a)]}(1\otimes S(h^{(1)}a))(S(h^{(2)})\otimes 1), \tag{3.15}$$

if the following compatibility conditions are satisfied [compare with (2.3a)–(2.3d)]:

$$\epsilon(a\triangleleft h)=\epsilon(a)\epsilon(h), \tag{3.16a}$$

$$\Delta(a\triangleleft h)(-1)^{p(a_{(2)})[p(h_{(1)})+p(h_{(2)}{}^{(1)})]}(a_{(1)}\triangleleft h_{(1)})h_{(2)}{}^{(1)}\otimes a_{(2)}\triangleleft h_{(2)}{}^{(2)}, \tag{3.16b}$$

$$\beta(hg)=(-1)^{p(h^{(2)})[p(g_{(1)})+p(g_{(2)}{}^{(1)})]}(h^{(1)}\triangleleft g_{(1)})g_{(2)}{}^{(1)}\otimes h^{(2)}g_{(2)}{}^{(2)}, \tag{3.16c}$$

$$h_{(1)}{}^{(1)}(a\triangleleft h_{(2)})\otimes h_{(1)}{}^{(2)}=(-1)^{p(a)p(h_{(2)}{}^{(1)})+p(h_{(1)})p(h_{(2)}{}^{(2)})}(a\triangleleft h_{(1)})h_{(2)}{}^{(1)}\otimes h_{(2)}{}^{(2)}. \tag{3.16d}$$

In the proof we check directly that with the definitions (3.12)–(3.15) and the properties (3.16a)–(3.16d) the axioms of the graded bicrossproduct $\mathscr{H}_1\bowtie\mathscr{H}_2$ being a Hopf superalgebra are satisfied. In particular, we have to check the associativity of the multiplication (3.12), i.e.

$$[(h\otimes a)(g\otimes b)](f\otimes c)=(h\otimes a)[(g\otimes b)(f\otimes c)], \tag{3.17}$$

the coassociativity of the coproduct (3.13) [see (3.3)] and, what is the most complicated part, the homomorphism property of the coproduct,

$$\Delta((h\otimes a)(g\otimes b))=\Delta(h\otimes a)\Delta(g\otimes b). \tag{3.18}$$

The graded bicrossproducts described in this section can be used for the description of quantum deformations of inhomogeneous supergroups.

IV. AN EXAMPLE: $D=4$ κ-DEFORMED POINCARÉ SUPERGROUP IN BICROSSPRODUCT FORM

The $D=4$ κ-deformed Poincaré supergroup has been obtained in Ref. 13 by quantization of the r-matrix Poisson bracket, with the following choice of the classical r matrix for $D=4$ Poincaré superalgebra (see also Ref. 23),

$$r=N_i\wedge P_i-\frac{i}{4}\,Q_\alpha\wedge\overline{Q_{\dot\alpha}}, \tag{4.1}$$

where $M_{\mu\nu}=(M_i,N_i)$ are Lorentz generators, P_μ describe the four-momenta and $Q_\alpha,\overline{Q_{\dot\alpha}}$ are four supercharges described by the doublet of Weyl 2-spinors. The Hopf superalgebra of the functions on $D=4$ κ-deformed Poincaré supergroup is described by the following relations (see Ref. 13).

(a) Algebra

(i) Lorentz sector $(A_\alpha^\beta,A_{\dot\alpha}^{\dot\beta})$ (we use the spinorial representation of the Lorentz generators, e.g. $L_i=\frac{1}{4}[(\sigma_i)_\alpha^\beta L_\beta^\alpha+(\overline{\sigma_i})_{\dot\alpha}^{\dot\beta}L_{\dot\beta}^{\dot\alpha}]$):

The Lorentz subgroup parameters are classical, i.e.

$$[A_\alpha^\beta,A_\gamma^\delta]=[A_\alpha^\beta,A_\gamma^{\dot\delta}]=[A_{\dot\alpha}^{\dot\beta},A_{\dot\gamma}^{\dot\beta}]=0. \tag{4.2}$$

(ii) Translations (X_μ) [we denote $\theta=\begin{pmatrix}\theta_1\\ \theta_2\end{pmatrix}$, $\overline{\theta}=\begin{pmatrix}\theta^{\dot1}\\ \theta^{\dot2}\end{pmatrix}$]:

$$[X^i,X^j]=\frac{i}{8\kappa}\,\theta^T\sigma^i(\mathbf{1}-(AA^+)^{-1})\sigma^j\overline{\theta}-\frac{i}{8\kappa}\,\theta^T\sigma^j(\mathbf{1}-(AA^+)^{-1})\sigma^i\overline{\theta}, \tag{4.3}$$

$$[X^0,X^j]=-\frac{i}{\kappa}\,X^j+\frac{i}{8\kappa}\,\theta^T[\sigma^j,(AA^+)^{-1}]\overline{\theta},$$

$$[A_\alpha^\beta,X^i]=\frac{1}{2\kappa}\,((A\sigma_n)_\alpha^\beta\Lambda_n^i(A)-(\sigma^i\cdot A)_\alpha^\beta), \tag{4.4}$$

$$[A_\alpha^\beta,X^0]=\frac{1}{2\kappa}\,(A\sigma_i)_\alpha^\beta\Lambda_i^0(A).$$

(iii) Supertranslations,

$$\{\theta^\alpha,\theta^\beta\}=\{\theta^{\dot\alpha},\theta^{\dot\beta}\}=0,\quad \{\theta^\alpha,\theta^{\dot\beta}\}=\frac{i}{2\kappa}\,(\mathbf{1}-(AA^+)^{-1})^{\dot\beta\alpha}, \tag{4.5}$$

$$\{X^i,\theta_\alpha\}=\frac{1}{4\kappa}\,(\theta^T\sigma^i)_\gamma(\mathbf{1}_2-(AA^+)^{-1})_\alpha^\gamma, \tag{4.6}$$

$$\{X^0,\theta_\alpha\}=-\frac{1}{4\kappa}\,\theta_\gamma^T(\mathbf{1}+(AA^+)^{-1})_\alpha^\gamma,\quad \{A_\alpha^\beta,\theta^\gamma\}=\{A_{\dot\alpha}^{\dot\beta},\theta^\gamma\}=0. \tag{4.7}$$

(b) Coalgebra,

$$\Delta(X_\mu)=X_\mu\otimes 1+\Lambda_\mu^\nu(A)\otimes X_\nu-\frac{i}{2}\,(A_\alpha^{-1\beta}\sigma_{\beta\dot\gamma}^\mu\theta^{\dot\gamma}\otimes\theta^\alpha+\theta^\alpha\sigma_{\alpha\dot\beta}^\mu A_{\dot\gamma}^{-1\beta}\otimes\theta^{\dot\gamma}),$$

$$\Delta(\theta_\alpha)=\theta_\alpha\otimes 1+(A^{-1})_\alpha^\beta\otimes\theta_\beta,\quad \Delta(A_\alpha^\beta)=A_\alpha^\gamma\otimes A_\gamma^\beta. \tag{4.8}$$

(c) Antipodes:

$$S(X^\mu)=-\Lambda_\nu^\mu(A^{-1})X^\nu,\quad S(A_\alpha^\beta)=(A^{-1})_\alpha^\beta,\quad S(\theta^\alpha)=-A_\beta^\gamma\theta^\beta. \tag{4.9}$$

In such a way, we have obtained the complete set of relations describing the κ deformation of $N=1$ Poincaré supergroup.

In order to put the Hopf superalgebra (4.2)–(4.9) in the bicrossproduct algebra form, we should introduce the complexified chiral superspace coordinates (see, e.g., Ref. 24) as follows:

$$z_\mu = x_\mu + \frac{i}{2}\,\theta_\alpha (\sigma_\mu)^{\alpha\dot\beta}\overline{\theta_{\dot\beta}}. \tag{4.10}$$

Let us introduce the following two κ-deformed Hopf superalgebras.

(i) The algebra of functions $C(z_\mu,\theta_\alpha)$ on κ-deformed chiral superspace (z_μ,θ_α), with the following Hopf superalgebra relations:

$$[z_i,z_j]=0, \quad [z_0,z_i]=-\frac{i}{\kappa}\,z_i,$$

$$[z_0,\theta_\alpha]=-\frac{i}{2\kappa}\,\theta_\alpha, \quad [z_i,\theta_\alpha]=0, \quad \{\theta_\alpha,\theta_\beta\}=0, \tag{4.11}$$

and

$$\Delta(z_\mu)=z_\mu\otimes 1+1\otimes z_\mu, \quad \Delta(\theta_\alpha)=\theta_\alpha\otimes 1+1\otimes\theta_\alpha. \tag{4.12}$$

(ii) The classical Hopf superalgebra of functions $C(A_{\alpha\beta},A_{\dot\gamma\beta},\overline{\theta_{\dot\alpha}})$ on the superextension of the classical Lorentz group, with the following defining relations:

$$[A_{\alpha\beta},A_{\gamma\delta}]=[A_{\alpha\beta},A_{\dot\gamma\dot\delta}]=[A_{\dot\alpha\dot\beta},A_{\dot\gamma\dot\delta}]=0,$$
$$[A_{\alpha\beta},\overline{\theta_{\dot\gamma}}]=[A_{\dot\alpha\dot\beta},\overline{\theta_{\dot\gamma}}]=0, \quad \{\overline{\theta_{\dot\alpha}},\overline{\theta_{\dot\beta}}\}=0, \tag{4.13}$$

and

$$\Delta(A_{\alpha\beta})=A_{\alpha\gamma}\otimes A_{\gamma\beta}, \quad \Delta(A_{\dot\alpha\dot\beta})=A_{\dot\alpha\dot\gamma}\otimes A_{\dot\gamma\dot\beta},$$
$$\Delta(\overline{\theta_{\dot\alpha}})=\overline{\theta_{\dot\alpha}}\otimes 1+(A_{\dot\alpha\dot\beta})^{-1}\otimes\overline{\theta_{\dot\beta}}. \tag{4.14}$$

One can prove the following statement.

Theorem 3: *The $D=4$ κ-deformed Poincaré supergroup can be described as the graded bicrossproduct Hopf superalgebra,*

$$C_\kappa(\mathscr{P}_{4;1})=C(z_\mu,\theta_\alpha)\triangleright\!\blacktriangleleft C(A_{\alpha\beta},A_{\dot\alpha\dot\beta},\overline{\theta_{\dot\alpha}}), \tag{4.15}$$

with the following definition of the action α:

$$\overline{\theta_{\dot\alpha}}\triangleleft z_i=-\frac{i}{2\kappa}\,[\mathbf{1}-(A^+A)^{-1}]_{\dot\alpha}{}^{\dot\beta}\overline{\theta_{\dot\beta}}, \quad \overline{\theta_{\dot\alpha}}\triangleleft z_0=-\frac{i}{2\kappa}\,(A^+A)_{\dot\alpha}{}^{\dot\beta}\overline{\theta_{\dot\beta}},$$

$$\overline{\theta_{\dot\alpha}}\triangleleft\theta_\beta=-\frac{i}{2\kappa}\,[\mathbf{1}-(AA^+)^{-1}]_{\dot\alpha\beta},$$

$$A_{\alpha\beta}\triangleleft z_i=\frac{1}{2\kappa}\,[(A\sigma_k)_{\alpha\beta}\Lambda_{ik}(A,\overline{A})-(\sigma_iA)_{\alpha\beta}],$$
$$\overline{A_{\dot\alpha\dot\beta}}\triangleleft z_i=\frac{1}{2\kappa}\,[(\sigma_i\overline{A})_{\dot\alpha\dot\beta}\Lambda_{lk}(A,\overline{A})-(\overline{A\sigma}_i)_{\dot\alpha\dot\beta}], \tag{4.16}$$

$$A_{\alpha\beta}\triangleleft z_0=\frac{1}{2\kappa}\,(A\sigma_i)_\alpha{}^\beta\Lambda_{i0}(A,\overline{A}), \quad \overline{A_{\dot\alpha\dot\beta}}\triangleleft z_0=\frac{1}{2\kappa}\,(\sigma_i\overline{A})_{\dot\alpha}{}^{\dot\beta}\Lambda_{i0}(A,\overline{A}),$$

$$\overline{A}_{\alpha\beta} \triangleleft \theta_\gamma = A_{\dot{\alpha}\dot{\beta}} \triangleleft \theta_\gamma = 0,$$

and coaction β,

$$\beta(z_\mu) = \Lambda_\mu{}^\nu (A, \overline{A}) \otimes z_\nu - i(A^{-1}\sigma_\mu)_{\alpha\dot{\beta}} \overline{\theta}_{\dot{\beta}} \otimes \theta_\alpha,$$

$$\beta(\theta_\alpha) = (A^{-1})_{\beta\alpha} \otimes \theta_\beta. \tag{4.17}$$

The proof is obtained by performing the transformation (4.10) of the superalgebra basis (4.2)–(4.9) and showing that the resulting Hopf superalgebra fits into the graded bicrossproduct superalgebra framework.

V. FINAL REMARKS

In this paper we give the not known in the literature general definition of graded bicrossproduct Hopf superalgebra and we provided as well an example. Such a scheme can be extended to the case of anionic groups[19] and braided groups.[20,21] To our knowledge only the crossproducts of braided cocommutative Hopf algebra with the quasitriangular Hopf algebras have been considered.[25] It is an interesting task to introduce the general braided bicrossproduct of braided Hopf algebras and provide some nontrivial examples.

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Preliminary classification of $q_t = f(q, q_x, q_{xx}, q_{xxx})$

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The preliminary classification of $q_t = f(q, q_x, q_{xx}, q_{xxx})$ is given. The results are compared with Fokas's symmetry and Mikhailov–Shabat–Sokolov formal symmetry approaches. © *1996 American Institute of Physics.* [S0022-2488(96)01005-0]

I. INTRODUCTION

There are several methods[1] to examine the integrability of nonlinear partial differential equations, although in two dimensions most of these methods imply each other.[2] The existence of infinitely many conserved quantities is too strong. For example, Burger's equation has only one conservation law.[3] One can say that many integrable differential equations can be put into a bilinear form.[4] The converse, however, is not true, since a bilinear form can be constructed for equations that are not integrable. There are integrable equations like the Harry–Dym equation, which does not pass the Painlevé test.[5] Several authors[6,7] have considered the existence of bi-Hamiltonian formulation as the fundamental criteria to integrability.

Another approach to integrability is linearization technique.[8] If the linearized equation of a given differential equation supports an eigenvalue equation, then the given differential equation is integrable. The advantage of using this technique is the following: One member of the associated linear equation is known by virtue of the nonlinear partial differential equation itself. Unlike the Painlevé analysis, the given nonlinear equation can be of any form. We can classify nonlinear partial differential equations.

II. LINEARIZATION

We can describe the linearization method for evolutionary equations

$$q_t = f(q, q_x, q_{xx}, \ldots) \tag{1}$$

in the following way. First we linearize the given differential equation. In other words, we replace q (and its derivatives) in (1) by $q + \epsilon\Psi$ differentiate both sides of the resulting expression with respect to ϵ:

$$\Psi_t = D_f(\Psi), \tag{2}$$

where D_f is the Fréchet derivative.[3] The equation above can also be written as

$$\Psi_t = \sum_{i=0}^{N} f_i \Psi_i = \sum_{i=0}^{N} \frac{\partial f}{\partial q_i} \Psi_i, \tag{3}$$

where N is the order of differential equation, $q_0 = q$, $q_1 = q_x$, $q_2 = q_{xx}$, $\Psi_0 = \Psi$, $\Psi_1 = \Psi_x$, $\Psi_2 = \Psi_{xx}$, and so on. In the symmetry approach (2) is the main equation, Ψ is the symmetry of the differential equation, and it is a function of q_i.

The compatible eigenvalue equation is

$$H\Psi = 0, \tag{4}$$

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where H depends on q_i and a parameter k. If its order (highest derivative in H) is N, then (4) may be written as

$$\Psi_N=\sum_{i=0}^{N-1} A_i\Psi_i, \tag{5}$$

where $A_0,A_1,\ldots,A_{N-1}$ are functions of q_i and the parameter k. We assume the order of dependence of A_is on q_i in advance, similar to the symmetry approach. Compatibility condition of (5) and (2),

$$\Psi_{N,t}-\Psi_{t,N}=0, \tag{6}$$

using (2) gives

$$\sum_{i=0}^{N-1} \Psi_i W_i=0, \tag{7}$$

where W_is are functions of f_i, A_i, and their partial derivatives. Letting

$$W_i=0, \tag{8}$$

we obtain a system of differential equations among f_i, A_i, and their partial derivatives. Expanding A_is in terms of the parameter k will give

$$A_i=\sum_{j=0}^{N} A_{ij}k^j, \tag{9}$$

where A_{ij}s are functions of q_i. Now substituting (9) into (8) we obtain an overdetermined system of differential equations. Letting each coefficient of k^i vanish results in first (i) a set of algebraic equations among A_{ij} and f_i and, second (ii) a set of a system of differential equations. The solution of this system will determine the eigenvalue equation (5) which can be integrated to give

$$\Phi\Psi=k\Psi, \tag{10}$$

where Φ is the recursion operator.[9] Letting

$$\Psi=\sum k^n\Psi_n, \tag{11}$$

then one obtains

$$\Phi\Psi_n=\Psi_{n-1}. \tag{12}$$

Hence Φ is transforming a symmetry into another one. Suppose the given differential equation has Hamiltonian structure so that $\Psi=\Theta_1\gamma$, where Θ_1 is the Hamiltonian operator and γ is the conserved covariant. Then from (10) we obtain

$$(\Phi\Theta_1-k\Theta_1)\gamma=0. \tag{13}$$

Expanding $\gamma=\Sigma k^n\gamma_n$ we find

$$\Phi\Theta_1\gamma_n=\Theta_1\gamma_{n-1}. \tag{14}$$

Hence $\Phi\Theta_1$ is a candidate for the second Hamiltonian operator. In a sense the integrability in linearization is equivalent (for the scalar case) to the existence of a recursion operator which satisfies the eigenvalue equation. In this approach, the order of eigenvalue equation N, the order of dependence of A_is on the derivative of the dependent variable q, and the order of the spectral parameter are the key factors in the classification.[10]

Classification of integrable nonlinear differential equations started almost two decades ago.[11–13] So far the attempts for complete classification have been done for some evolutionary equations.[1,14,15] In this work, the preliminary classifications of $q_t=f(q,q_x,q_{xx})$ and $q_t=f(q,q_x,q_{xx},q_{xxx})$ are given and the results are compared with Olver–Fokas symmetry[3,12] and Mikhailov–Shabat–Sokolov (MSS)[14] formal symmetry approaches.

III. CLASSIFICATION OF $q_t=f(q,q_x,q_{xx})$

We consider differential equations of the following form:

$$q_t=f(q,q_x,q_{xx}). \tag{15}$$

The linearized form of the equation above can be given as

$$\Psi_t=\gamma\Psi_{xx}+\alpha\Psi_x+\beta\Psi, \tag{16}$$

where α,β,γ are functions of q,q_x,q_{xx}. We assume an eigenvalue equation having the same order as (15):

$$\Psi_{xx}=A\Psi_x+B\Psi. \tag{17}$$

With the expansion of A, B, and C as

$$A=A_0+A_1k+A_2k^2, \quad B=B_0+B_1k+B_2k^2, \tag{18}$$

here A_i and B_i $(i=0,1,2)$ are functions of q,q_x,q_{xx}. The highest power of k is related to the order of the given partial differential equation. [A different approach from Ref. 8 is used in this work. The order of the parameter (k) can take any integer value.] Compatibility of (16) and (17) give the following algebraic equations,

$$A_2=\frac{E_2}{\sqrt{\gamma}}, \quad A_1=\frac{E_1}{\sqrt{\gamma}}, \quad B_2=B_1\frac{E_2}{E_1}, \tag{19}$$

and evolution equations

$$\begin{aligned}A_{0,t}=&\alpha_{xx}+\alpha_xA_0+\gamma_{xx}A_0+2\gamma_xA_{0,x}+\gamma_xA_0^2+2\gamma_xB_0\\&+2\beta_x+A_{0,xx}\gamma+A_{0,x}\alpha+2A_{0,x}\gamma A_0+2B_{0,x}\gamma,\end{aligned} \tag{20}$$

$$\begin{aligned}B_{0,t}=&2\alpha_xB_0+\gamma_{xx}B_0+2\gamma_xB_{0,x}+\gamma_xA_0B_0+\beta_{xx}-\beta_xA_0\\&+2A_{0,x}\gamma B_0+B_{0,xx}\gamma+B_{0,x}\alpha,\end{aligned} \tag{21}$$

$$B_{1,t}=\frac{1}{\sqrt{\gamma}}\,(2\sqrt{\gamma}\alpha_xB_1+\sqrt{\gamma}\gamma_{xx}B_1+2\sqrt{\gamma}\gamma_xB_{1,x}+\sqrt{\gamma}\gamma_xA_0B_1 \tag{22}$$

$$-\beta_xE_1+2\gamma^{3/2}A_{0,x}B_1+\gamma^{3/2}B_{1,xx}+\gamma^{1/2}B_{1,x}), \tag{23}$$

$$\gamma_t = -\frac{1}{2E_1}(4\alpha_x \gamma E_1 + 2\gamma_{xx}\gamma E_1 - \gamma_x^2 \gamma E_1 + 8\gamma^{3/2}\gamma_x B_1 - 2\gamma_x \alpha E_1 + 4\gamma_x \gamma A_0 E_1 + 8A_{0,x}\gamma^2 E_1 + 8\gamma^{5/2} B_{1,x}). \tag{24}$$

A. Case (1)

The first type of integrable equation is given by the linearized equation

$$\Psi_t = \eta \Psi_{xx} - \left[\frac{2\eta r_q}{r} q_x - \frac{\eta_1}{E_1}\right]\Psi_x + \left[\frac{\eta(r_q^2 - r_{qq} r)}{r^2} q_x^2 - \frac{\eta_1 r_q}{\sqrt{\eta}}\right]\Psi, \tag{25}$$

with compatible eigenvalue equation

$$\Psi_{xx} = \left[-\frac{\sqrt{\eta} q_{xx}}{-\sqrt{\eta} q_x + E_1 r} + \frac{\sqrt{\eta} q_x^2 r_q}{r(-\sqrt{\eta} q_x + E_1 r)} + \frac{2E_1 r_q q_x}{-\sqrt{\eta} q_x + E_1 r} + \frac{E_1}{\sqrt{\eta}} k + \frac{E_2}{\sqrt{\eta}} k^2\right]\Psi_x + \left[\frac{E_1 r_q q_{xx}}{-\sqrt{\eta} q_x + E_1 r} + \frac{r_{qq} q_x^2}{r} - \frac{r_q^2 q_x^2}{r} - \frac{E_1 r_q^2 q_x^2}{r(-\sqrt{\eta} q_x + E_1 r)} - \frac{E_1(-\sqrt{\eta} q_{xx} + E_1 r_q q_x)}{-\sqrt{\eta} q_x + E_1 r} k - \frac{E_2(-\sqrt{\eta} q_{xx} + E_1 r_q q_x)}{-\sqrt{\eta} q_x + E_1 r} k^2\right]\Psi. \tag{26}$$

In linearization, the eigenvalue equation determines the recursion operator for the corresponding partial differential equation. Equation (26) can be integrated,

$$\Phi = D - \frac{r_q q_x}{r}, \tag{27}$$

to give the recursion operator. The integrable equation can be written as

$$q_t = \eta q_{xx} - \frac{\eta r_q q_x^2}{r} + \frac{\eta_1 q_x}{E_1} - \frac{\eta_1 r}{\sqrt{\eta}}, \tag{28}$$

where η, η_1, E_1, E_2 are constants and r is a function of q.

B. Case (2)

The second class can be given with linearized equation

$$\Psi_t = \eta \Psi_{xx} + \left[\frac{2\eta r_{qq}}{r_q} q_x + 2\eta r + \eta_1\right]\Psi_x + \left[\frac{\eta(r_{qqq} r_q - r_{qq}^2)}{r_q^2} q_x^2 + 2\eta r_q q_x\right]\Psi \tag{29}$$

and compatible eigenvalue equation

$$\Psi_{xx} = \left[\frac{q_{xx}}{q_x} - \frac{q_x r_{qq}}{r_q} - r + \frac{E_1}{\sqrt{\eta}} k + \frac{E_2}{\sqrt{\eta}} k^2\right]\Psi_x + \left[\frac{r q_{xx}}{q_x} - \frac{(r_{qqq} r_q - r_{qq}^2) q_x^2}{r_q^2} - 2 r_q q_x - \frac{E_1 q_{xx}}{\sqrt{\eta} q_x} k - \frac{E_2 q_{xx}}{\sqrt{\eta} q_x} k^2\right]\Psi. \tag{30}$$

The equation above can be integrated,

$$\Phi = D + \frac{r_{qq}q_x}{r_q} + r + q_x D^{-1} r_q, \tag{31}$$

where $(D^{-1}f)(x)=\int_{-\infty}^{x} f(\zeta)d\zeta$. The integrable equation can be written as

$$q_t = \eta q_{xx} + \frac{\eta r_{qq} q_x^2}{r_q} + (2\eta r + \eta_1) q_x. \tag{32}$$

Here η,η_1 are constants and r is a function of q. The equations (28) and (32) correspond to the integrable equations of Fokas,[12] Ibragimov–Shabat[11] and recursion operators (27) and (31) are obtained by the integration of the eigenvalue equations.

IV. CLASSIFICATION OF $q_t=f(q,q_x,q_{xx},q_{xxx})$

We consider differential equations of the general form

$$q_t = f(q,q_x,q_{xx},q_{xxx}). \tag{33}$$

The linearization of the equation above takes the following form:

$$\Psi_t = \alpha\Psi_{xxx} + \beta\Psi_{xx} + \gamma\Psi_x + \delta\Psi. \tag{34}$$

Here $\alpha,\beta,\gamma,\delta$ are functions of q,q_x,q_{xx},q_{xxx}. We consider an eigenvalue equation having the same order as (33),

$$\Psi_{xxx} = A\Psi_{xx} + B\Psi_x + C\Psi, \tag{35}$$

using the expansion of A, B, and C as

$$A = A_0 + A_1 k + A_2 k^2, \quad B = B_0 + B_1 k + B_2 k^2, \quad C = C_0 + C_1 k + C_2 k^2, \tag{36}$$

where A_i, B_i, and C_i are functions of $q,q_x,q_{xx},q_{xxx},q_{xxxx}$. The compatibility of (34) and (35) will give us for $q_t=f(q,q_x,q_{xx},q_{xxx})$ four classes:[14,15]

(1) $q_t = L_1 q_{xxx} + L_2$,
(2) $q_t = (L_1 q_{xxx} + L_2)^{-2} + L_3$,
(3) $q_t = (L_1 q_{xxx} + L_2)^{-1/2} + L_3$, and
(4) $q_t = (2L_1 q_{xxx} + L_2)(L_1 q_{xxx}^2 + L_2 q_{xxx} + L_3)^{-1/2} + L_4$,

where L_1, L_2, L_3, and L_4 are functions of q,q_x,q_{xx}.

A. Classification of $q_t=L_1q_{xxx}+L_2$

The classification will determine algebraic equations,

$$\begin{gathered} A_1=0, \quad A_2=0, \quad B_0=-\frac{2\gamma}{3\eta}, \quad B_1=E_1, \quad B_2=E_2, \\ C_0=-\frac{1}{3\eta}(\gamma_x - 2\gamma A_0 + 2\delta), \quad C_1=-E_1A_0, \quad C_2=-E_2A_0, \end{gathered} \tag{37}$$

and evolution equations as follows:

$$A_{0,t} = \gamma_x A_0 + \delta_x + A_{0,xxx}\eta + 3A_{0,xx}\eta A_0 + 3A_{0,x}^2\eta + A_{0,x}\gamma + 3A_{0,x}\eta A_0^2, \tag{38}$$

$$\gamma_t=\tfrac{1}{2}(2\gamma_{xxx}\eta-3\gamma_{xx}\eta A_0-3\gamma_x A_{0,x}\eta+2\gamma_x\gamma-3\delta_{xx}\eta+6\delta_x\eta A_0+6A_{0,x}\delta\eta), \tag{39}$$

$$\begin{aligned}\delta_t=\tfrac{1}{4}(&3\gamma_{xxx}\eta A_0-6\gamma_{xx}\eta A_0^2-3\gamma_x A_{0,xx}\eta-12\gamma_x A_{0,x}\eta A_0\\&+4\gamma_x\delta+\delta_{xxx}\eta-6\delta_{xx}\eta A_0+4\delta_x\gamma+12\delta_x\eta A_0^2+6A_{0,xx}\delta\eta+24A_{0,x}\delta\eta A_0),\end{aligned} \tag{40}$$

where η,E_1,E_2 are constants.

B. Case (1)

The linearized form of the first subclass is in the form

$$\Psi_t=\eta\Psi xxx+\left[\frac{\rho_1}{2}q_x^2+\rho\right]\Psi_x+\rho_q q_x\Psi \tag{41}$$

with compatible eigenvalue equation

$$\begin{aligned}\Psi xxx=&\frac{q_{xx}}{q_x}\Psi_{xx}+\left[-\frac{\rho_1}{3\eta}q_x^2-\frac{2\rho}{3\eta}+E_1k+E_2k^2\right]\Psi_x\\&+\left[-\frac{-2\rho q_{xx}+3\rho_q q_x^2}{3\eta q_x}-\frac{E_1q_{xx}}{q_x}k-\frac{E_2q_{xx}}{q_x}k^2\right]\Psi,\end{aligned} \tag{42}$$

where ρ_1 is constant and ρ is a function of q with the condition

$$\rho_{qqq}+\frac{4\rho_1}{3\eta}\rho_q=0. \tag{43}$$

The recursion operator can be obtained by integration:

$$\Phi=D^2+\frac{\rho}{3\eta}+\frac{\rho_1}{3\eta}q_x^2-\frac{\rho_1}{3\eta}q_xD^{-1}q_{xx}+\frac{q_x}{\eta}D^{-1}\rho_q. \tag{44}$$

The integrable equation is in the form

$$q_t=\eta q_{xxx}+\frac{\rho_1}{6}q_x^3+\rho q_x. \tag{45}$$

C. Case (2)

The second subclass is given by the linearized equation

$$\Psi_t=\eta\Psi xxx+\left[\frac{\epsilon_1}{2}q_x^2+\epsilon_1\epsilon_2q_x+\epsilon_3\right]\Psi_x, \tag{46}$$

with compatible eigenvalue equation

$$\begin{aligned}\Psi xxx=&\frac{q_{xx}}{q_x+\epsilon_2}\Psi_{xx}+\left[-\frac{\epsilon_1}{3\eta}q_x^2-\frac{2\epsilon_1\epsilon_2}{3\eta}q_x-\frac{2\epsilon_3}{3\eta}+E_1k+E_2k^2\right]\Psi_x\\&+\left[-\frac{(\epsilon_2^2\epsilon_1-2\epsilon_3)q_{xx}}{3\eta(q_x+\epsilon_2)}-\frac{E_1q_{xx}}{q_x+\epsilon_2}k-\frac{E_2q_{xx}}{q_x+\epsilon_2}k^2\right]\Psi,\end{aligned} \tag{47}$$

where $\epsilon_1,\epsilon_2,\epsilon_3$ are constants. The recursion operator can be obtained by integration

$$\Phi=D^2+\frac{2\epsilon_3}{3\eta}+\frac{\epsilon_1}{3\eta}q_x^2+\frac{2\epsilon_1\epsilon_2}{3\eta}q_x-\frac{\epsilon_1}{3\eta}(q_x+\epsilon_2)D^{-1}q_{xx}. \tag{48}$$

The integrable equation is in the form

$$q_t=\eta q_{xxx}+\frac{\epsilon_1}{6}q_x^3+\frac{\epsilon_1\epsilon_2}{2}q_x^2+\epsilon_3 q_x. \tag{49}$$

Equations (45) and (49) are classified by Fokas,[12] Ibragimov–Shabat,[11] and recursion operators (44) and (48) are obtained by the integration of the eigenvalue equations.

D. Case (3)

The eigenvalue equation is

$$\begin{aligned}\Psi_{xxx}=&\left[\frac{q_{xxx}+\lambda_1 q_{xx}+\lambda_2 q_x}{q_{xx}+\lambda_1 q_x+\lambda_2 q}-\lambda_3\right]\Psi_{xx}+\left[\frac{\lambda_3(q_{xxx}+\lambda_1 q_{xx}+\lambda_2 q_x)}{q_{xx}+\lambda_1 q_x+\lambda_2 q}-\lambda_4+\frac{E_1}{\lambda_5^{2/3}}k+\frac{E_2}{\lambda_5^{2/3}}k^2\right]\Psi_x\\&+\left[\frac{\lambda_4(q_{xxx}+\lambda_1 q_{xx}+\lambda_2 q_x)}{q_{xx}+\lambda_1 q_x+\lambda_2 q}-\frac{E_1(q_{xxx}+\lambda_1 q_{xx}+\lambda_2 q_x)}{\lambda_5^{2/3}(q_{xx}+\lambda_1 q_x+\lambda_2 q)}k-\frac{E_2(q_{xxx}+\lambda_1 q_{xx}+\lambda_2 q_x)}{\lambda_5^{2/3}(q_{xx}+\lambda_1 q_x+\lambda_2 q)}k^2\right]\Psi,\end{aligned} \tag{50}$$

and the linearized equation has the form

$$\Psi_t=\lambda_5\Psi_{xxx}+\tfrac{3}{2}\lambda_3\lambda_5\Psi_{xx}+\tfrac{3}{2}\lambda_4\lambda_5\Psi_x+\lambda_6\Psi. \tag{51}$$

The recursion operator is

$$\Phi=D^2+\lambda_3 D+\lambda_4. \tag{52}$$

The integrable equation is

$$q_t=\lambda_5 q_{xxx}+\tfrac{3}{2}\lambda_3\lambda_5 q_{xx}+\tfrac{3}{2}\lambda_4\lambda_5 q_x+\lambda_6 q, \tag{53}$$

where E_1, E_2, λ_1, λ_2, λ_3, λ_4, λ_5, and λ_6 are constants. Rabelo and Tanenblat also obtained linear equation using the classification method of pseudo-spherical surfaces with Gaussian curvature (-1).[16]

E. New integrable equation in the form $q_t=(L_1 q_{xxx}+L_2)^{-2}+L_3$

The classification will give the following algebraic equations,

$$\begin{aligned}A_1&=\frac{E_1}{\alpha^{1/3}},\\C_1&=-\tfrac{1}{3}(\alpha_x\alpha^{-4/3}E_1+\beta\alpha^{-4/3}E_1+3A_0\alpha^{-1/3}E_1-\alpha^{-2/3}E_2),\end{aligned} \tag{54}$$

and evolution equations

$$\alpha_t = -\frac{1}{9E_1\alpha}\,(27\alpha^{2/3}A_{0,x}E_2\alpha^2 + 18\alpha^{2/3}\beta_x E_2\alpha + 9\alpha^{2/3}\alpha_{xx}E_2\alpha - 6\alpha^{2/3}\alpha_x^2E_2 + 9\alpha^{2/3}\alpha_x E_2A_0\alpha$$
$$- 12\alpha^{2/3}\alpha_x E_2\beta + 81\alpha^{1/3}C_{1,x}\alpha^3 + 81\alpha^{1/3}\alpha_x C_1\alpha^2 + 81B_{0,x}E_1\alpha^3 - 27A_{0,x}E_1\beta\alpha^2 + 27\beta_{xx}E_1\alpha^2$$
$$- 27\beta_x\alpha_x E_1\alpha - 27\beta_x E_1A_0\alpha^2 - 36\beta_x E_1\beta\alpha + 27\gamma_x E_1\alpha^2 - 9\alpha_{xxx}E_1\alpha^2 + 9\alpha_{xx}\alpha_x E_1\alpha$$
$$- 18\alpha_{xx}E_1\beta\alpha - 4\alpha_x^3E_1 + 24\alpha_x^2E_1\beta + 54\alpha_x E_1B_0\alpha^2 + 9\alpha_x E_1A_0\beta\alpha + 24\alpha_x E_1\beta^2 - 9\alpha_x E_1\gamma\alpha), \tag{55}$$

$$\beta_t = -\frac{1}{9\alpha^{7/3}E_1^2}\,(-18\alpha^{2/3}A_{0,x}E_2^2\alpha^3 + 81\alpha^{2/3}A_{0,x}E_1C_1\alpha^4 + 81\alpha^{2/3}C_{1,x}E_1A_0\alpha^4 + 162\alpha^{2/3}C_{1,x}E_1\beta\alpha^3$$
$$- 12\alpha^{2/3}\beta_x E_2^2\alpha^2 + 81\alpha^{2/3}\beta_x E_1C_1\alpha^3 - 6\alpha^{2/3}\alpha_{xx}E_2^2\alpha^2 + 4\alpha^{2/3}\alpha_x^2E_2^2\alpha - 6\alpha^{2/3}\alpha_x E_2^2A_0\alpha^2$$
$$+ 8\alpha^{2/3}\alpha_x E_2^2\beta\alpha + 108\alpha^{2/3}\alpha_x E_1A_0C_1\alpha^3 + 108\alpha^{2/3}\alpha_x E_1C_1\beta\alpha^2 + 81\alpha^{1/3}C_{0,x}E_1^2\alpha^4$$
$$+ 27\alpha^{1/3}B_{0,x}\alpha_x E_1^2\alpha^3 + 81\alpha^{1/3}B_{0,x}E_1^2A_0\alpha^4 + 135\alpha^{1/3}B_{0,x}E_1^2\beta\alpha^3 + 27\alpha^{1/3}A_{0,x}\beta_x E_1^2\alpha^3$$
$$- 36\alpha^{1/3}A_{0,x}\alpha_x E_1^2\beta\alpha^2 + 81\alpha^{1/3}A_{0,x}E_1^2B_0\alpha^4 - 54\alpha^{1/3}A_{0,x}E_1^2A_0\beta\alpha^3 - 54\alpha^{1/3}A_{0,x}E_1^2\beta^2\alpha^2$$
$$- 54\alpha^{1/3}C_{1,x}E_2\alpha^4 + 27\alpha^{1/3}\delta_x E_1^2\alpha^3 - 9\alpha^{1/3}\beta_{xxx}E_1^2\alpha^3 + 18\alpha^{1/3}\beta_{xx}\alpha_x E_1^2\alpha^2 + 27\alpha^{1/3}\beta_{xx}E_1^2A_0\alpha^3$$
$$+ 36\alpha^{1/3}\beta_{xx}E_1^2\beta\alpha^2 + 9\alpha^{1/3}\beta_x^2E_1^2\alpha^2 + 27\alpha^{1/3}\beta_x\alpha_{xx}E_1^2\alpha^2 - 36\alpha^{1/3}\beta_x\alpha_x^2E_1^2\alpha$$
$$- 36\alpha^{1/3}\beta_x\alpha_x E_1^2A_0\alpha^2 - 72\alpha^{1/3}\beta_x\alpha_x E_1^2\beta\alpha + 54\alpha^{1/3}\beta_x E_1^2B_0\alpha^3 - 27\alpha^{1/3}\beta_x E_1^2A_0^2\alpha^3$$
$$- 81\alpha^{1/3}\beta_x E_1^2A_0\beta\alpha^2 - 48\alpha^{1/3}\beta_x E_1^2\beta^2\alpha - 9\alpha^{1/3}\beta_x E_1^2\gamma\alpha^2 + 27\alpha^{1/3}\gamma_{xx}E_1^2\alpha^3 + 18\alpha^{1/3}\gamma_x E_1^2\beta\alpha^2$$
$$- 36\alpha^{1/3}\alpha_{xx}\alpha_x E_1^2\beta\alpha + 27\alpha^{1/3}\alpha_{xx}E_1^2B_0\alpha^3 - 36\alpha^{1/3}\alpha_{xx}E_1^2A_0\beta\alpha^2 - 36\alpha^{1/3}\alpha_{xx}E_1^2\beta^2\alpha$$
$$+ 32\alpha^{1/3}\alpha_x^3E_1^2\beta + 36\alpha^{1/3}\alpha_x^2E_1^2A_0\beta\alpha + 60\alpha^{1/3}\alpha_x^2E_1^2\beta^2 - 54\alpha^{1/3}\alpha_x E_2C_1\alpha^3 + 81\alpha^{1/3}\alpha_x E_1^2C_0\alpha^3$$
$$+ 81\alpha^{1/3}\alpha_x E_1^2B_0A_0\alpha^3 + 54\alpha^{1/3}\alpha_x E_1^2B_0\beta\alpha^2 + 36\alpha^{1/3}\alpha_x E_1^2A_0\beta^2\alpha + 32\alpha^{1/3}\alpha_x E_1^2\beta^3$$
$$- 27B_{0,x}E_2E_1\alpha^4 + 18A_{0,x}\alpha_x E_2E_1\alpha^3 + 54A_{0,x}E_2E_1A_0\alpha^4 + 72A_{0,x}E_2E_1\beta\alpha^3 - 9\beta_{xx}E_2E_1\alpha^3$$
$$+ 24\beta_x\alpha_x E_2E_1\alpha^2 + 45\beta_x E_2E_1A_0\alpha^3 + 48\beta_x E_2E_1\beta\alpha^2 + 6\alpha_{xx}\alpha_x E_2E_1\alpha^2 + 18\alpha_{xx}E_2E_1A_0\alpha^3$$
$$+ 30\alpha_{xx}E_2E_1\beta\alpha^2 - 4\alpha_x^3E_2E_1\alpha - 6\alpha_x^2E_2E_1A_0\alpha^2 - 34\alpha_x^2E_2E_1\beta\alpha - 18\alpha_x E_2E_1B_0\alpha^3$$
$$+ 18\alpha_x E_2E_1A_0^2\alpha^3 - 6\alpha_x E_2E_1A_0\beta\alpha^2 - 32\alpha_x E_2E_1\beta^2\alpha), \tag{56}$$

$$A_{0,t} = 3C_{0,x}\alpha + 3B_{0,xx}\alpha + 6B_{0,x}\alpha_x + 3B_{0,x}A_0\alpha + 2B_{0,x}\beta + A_{0,xxx}\alpha + 3A_{0,xx}\alpha_x + 3A_{0,xx}A_0\alpha + A_{0,xx}\beta$$
$$+ 3A_{0,x}^2\alpha + 3A_{0,x}\beta_x + 3A_{0,x}\alpha_{xx} + 7A_{0,x}\alpha_x A_0 + 3A_0B_0\alpha + 3A_{0,x}A_0^2\alpha + 2A_{0,x}A_0\beta + A_{0,x}\gamma$$
$$+ 3\delta_x + \beta_{xxx} + 2\beta_{xx}A_0 + 2\beta_x B_0 + \beta_x A_0^2 + 3\gamma_{xx} + \gamma_x A_0 + \alpha_{xxx}A_0 + 3\alpha_{xx}B_0 + 2\alpha_{xx}A_0^2$$
$$+ 3\alpha_x C_0 + 3\alpha_x B_0A_0 + \alpha_x A_0^3, \tag{57}$$

$$B_{0,t} = 3C_{0,xx}\alpha + 6C_{0,x}\alpha_x + 2C_{0,x}\beta + B_{0,xxx}\alpha + 3B_{0,xx}\alpha_x + B_{0,xx}\beta + 3B_{0,x}A_{0,x}\alpha + 3B_{0,x}\beta_x$$
$$+ 3B_{0,x}\alpha_{xx} + B_{0,x}\alpha_x A_0 + 3B_{0,x}B_0\alpha + B_{0,x}\gamma + 3A_{0,xx}B_0\alpha + 6A_{0,x}\alpha_x B_0 + 3A_{0,x}C_0\alpha$$
$$+ 3A_{0,x}B_0A_0\alpha + 2A_{0,x}B_0\beta + 3\delta_{xx} - 2\delta_x A_0 + 3\beta_{xx}B_0 + 3\beta_x C_0 + \beta_x B_0A_0 + \gamma_{xxx} - \gamma_{xx}A_0$$
$$+ 2\gamma_x B_0 + \alpha_{xxx}B_0 + 3\alpha_{xx}C_0 + 2\alpha_{xx}B_0A_0 + \alpha_x C_0A_0 + 2\alpha_x B_0^2 + \alpha_x B_0A_0^2, \tag{58}$$

$$C_{0,t} = -(-C_{0,xxx}\alpha - 3C_{0,xx}\alpha_x - C_{0,xx}\beta - 3C_{0,x}A_{0,x}\alpha - 3C_{0,x}\beta_x - 3C_{0,x}\alpha_{xx} - C_{0,x}\alpha_x A_0 - C_{0,x}\gamma - 3B_{0,x}C_0\alpha - 3A_{0,xx}C_0\alpha - 6A_{0,x}\alpha_x C_0 - 3A_{0,x}C_0A_0\alpha - 2A_{0,x}C_0\beta - \delta_{xxx} + \delta_{xx}A_0 + \delta_x B_0 - 3\beta_{xx}C_0 - \beta_x C_0 A_0 - 3\gamma_x C_0 - \alpha_{xxx}C_0 - 2\alpha_{xx}C_0A_0 - 2\alpha_x C_0 B_0 - \alpha_x C_0 A_0^2), \tag{59}$$

$$C_{1,t} = -\frac{1}{3\alpha^{4/3}}(\alpha^{2/3}\delta_x E_2 - 9\alpha^{1/3}B_{0,x}C_1\alpha^2 - 9\alpha^{1/3}A_{0,xx}C_1\alpha^2 - 9\alpha^{1/3}A_{0,x}C_{1,x}\alpha^2 - 18\alpha^{1/3}A_{0,x}\alpha_x C_1\alpha - 9\alpha^{1/3}A_{0,x}A_0C_1\alpha^2 - 6\alpha^{1/3}A_{0,x}C_1\beta\alpha - 3\alpha^{1/3}C_{1,xxx}\alpha^2 - 9\alpha^{1/3}C_{1,xx}\alpha_x\alpha - 3\alpha^{1/3}C_{1,xx}\beta\alpha - 9\alpha^{1/3}C_{1,x}\beta_x\alpha - 9\alpha^{1/3}C_{1,x}\alpha_{xx}\alpha - 3\alpha^{1/3}C_{1,x}\alpha_x A_0\alpha - \alpha^{1/3}C_{1,x}\gamma\alpha - 9\alpha^{1/3}\beta_{xx}C_1\alpha - 3\alpha^{1/3}\beta_x A_0C_1\alpha - 9\alpha^{1/3}\gamma_x C_1\alpha - 3\alpha^{1/3}\alpha_{xxx}C_1\alpha - 6\alpha^{1/3}\alpha_{xx}A_0C_1\alpha - 6\alpha^{1/3}\alpha_x B_0C_1\alpha - 3\alpha^{1/3}\alpha_x A_0^2C_1\alpha + 3\delta_{xx}E_1\alpha - \delta_x\alpha_x E_1 - 3\delta_x E_1A_0\alpha - \delta_x E_1\beta). \tag{60}$$

The linearized equation is given by

$$\Psi_t = \left[-\frac{8(2q_{xx}E_2 + 9q_xE_1V_1)^3E_2^6}{27(2q_{xxx}E_2^2 + 27q_{xx}E_2E_1V_1 + 81q_xE_1^2V_1^2)^3E_1^3}\right]\Psi_{xxx} + \left[\frac{4(2q_{xxx}E_2 + 9q_{xx}E_1V_1)(2q_{xx}E_2 + 9q_xE_1V_1)^2E_2^6}{9(2q_{xxx}E_2^2 + 27q_{xx}E_2E_1V_1 + 81q_xE_1^2V_1^2)^3E_1^3}\right]\Psi_{xx} + \frac{\left[\begin{array}{c}(2((8E_2^4 + 2187E_1^4V_1E_3)q_{xx}^2E_2^2 + 18(4E_2^4 + 729E_1^4V_1E_3)q_{xx}q_xE_2E_1V_1 \\ + 81(2E_2^4 + 243E_1^4V_1E_3)q_x^2E_1^2V_1^2)q_{xxx}E_2^2V_1 + 324(q_{xx}E_2 + 3q_xE_1V_1)q_{xxx}^2E_2^4E_1^3V_1E_3 \\ + 2187(q_{xx}E_2 + q_xE_1V_1)(2E_2^4 + 243E_1^4V_1E_3)q_x^2E_1^3V_1^4 + 3(40E_2^4 + 6561E_1^4V_1E_3) \\ \times q_{xx}^3E_2^3E_1V_1^2 + 81(16E_2^4 + 2187E_1^4V_1E_3)q_{xx}^2q_xE_2^2E_1^2V_1^3 + 8q_{xxx}^3E_2E_1^2E_3)\end{array}\right]}{(2q_{xxx}E_2^2 + 27q_{xx}E_2E_1V_1 + 81q_xE_1^2V_1^2)^3E_1^2} \times \Psi_x + U_1\Psi \tag{61}$$

and the eigenvalue equation is

$$\Psi_{xxx} = \left[\frac{(4q_{xxx}E_2^2 - 81q_xE_1^2V_1^2)}{(2(2q_{xx}E_2 + 9q_xE_1V_1)E_2)} - \frac{3E_1^2(2q_{xxx}E_2^2 + 27q_{xx}E_2E_1V_1 + 81q_xE_1^2V_1^2)}{2E_2^2(2q_{xx}E_2 + 9q_xE_1V_1)}k\right]\Psi_{xx} + \left[\frac{9(2q_{xxx}E_2 + 9q_{xx}E_1V_1)E_1V_1}{2(2q_{xx}E_2 + 9q_xE_1V_1)E_2} + \frac{\left[\begin{array}{c}-3(4q_{xxxx}q_{xx}E_2^3 + 18q_{xxxx}q_xE_2^2E_1V_1 - 8q_{xxx}^2E_2^3] \\ -90q_{xxx}q_{xx}E_2^2E_1V_1 - 81q_{xxx}q_xE_2E_1^2V_1^2 \\ -324q_{xx}^2E_2E_1^2V_1^2 - 729q_{xx}q_xE_13V_1^3)E_1^2\end{array}\right]}{2(2q_{xx}E_2 + 9q_xE_1V_1)^2E_2^2}k\right] \times \Psi_x. \tag{62}$$

The eigenvalue equation can be integrated:

$$D^2 + \frac{9E_1V_1}{2E_2}D = -k\frac{3E_1^2(2q_{xxx}E_2^2 + 27q_{xx}E_2E_1V_1 + 81q_xE_1^2V_1^2)}{2E_2^2(2q_{xx}E_2 + 9q_xE_1V_1)}D. \tag{63}$$

The new integrable equation is in the form

$$q_t=\frac{2E_2^4(2q_{xx}E_2+9q_xE_1V_1)^3}{27E_1^3(2q_{xxx}E_2^2+27q_{xx}E_2E_1V_1+81q_xE_1^2V_1^2)^2}+E_3q_x+U_1q, \tag{64}$$

where E_1, E_2, E_3, U_1, and V_1 are constants. The equation above is a new integrable equation which is included in the MSS classification.[14]

F. $q_t=(L_1q_{xxx}+L_2)^{-1/2}+L_3$

The leading order term gives the differential equation as

$$-3f_{q_{xxx},3}f_{q_{xxx}}+5(f_{q_{xxx},2})^2=0. \tag{65}$$

The solution to (65) is given by

$$q_t=(L_1q_{xxx}+L_2)^{-1/2}+L_3, \tag{66}$$

where L_1, L_2, and L_3 are functions of q,q_x,q_{xx}. The classification has not been finished yet due to computer limitations. One integrable equation in this class is given by eigenvalue equation

$$\Psi_{xxx}=\left[-D_1+\frac{E_1}{2^{1/2}E_2^{2/3}}(E_2q_{xxx}+E_2D_1q_x+E_2^{2/3}D_2)k\right]\Psi_x+\left[\frac{E_1E_2^{1/3}}{2^{1/3}}(q_{xxx}+D_1q_{xx})k\right]\Psi \tag{67}$$

and linearized equation

$$\Psi_t=-\frac{E_2}{(E_2q_{xxx}+E_2D_1q_x+E_2^{2/3}D_2)^{3/2}}\Psi_{xxx}-\frac{E_2D_1}{(E_2q_{xxx}+E_2D_1q_x+E_2^{2/3}D_2)^{3/2}}\Psi_x. \tag{68}$$

The eigenvalue equation (67) can be integrated to give the recursion operator

$$\Phi=D^2+D_1. \tag{69}$$

The integrable equation is given by

$$q_t=\frac{1}{(E_2q_{xxx}+E_2D_1q_x+E_2^{2/3}D_2)^{1/2}}+E_3q_x, \tag{70}$$

where E_1, E_2, E_3, D_1, and D_2 are constants. This integrable equation is included in S-integrable equations of Calogero.[17]

G. $q_t=(2L_1q_{xxx}+L_2)(L_1q_{xxx}^2+L_2q_{xxx}+L_3)^{-1/2}+L_4$

The differential equation coming from the leading order is

$$-3f_{q_{xxx},3}f_{q_{xxx}}+5(f_{q_{xxx},2})^2+3\frac{f_{q_{xxx},2}f_{q_{xxx}}}{q_{xxx}+K_1}=0, \tag{71}$$

where $K_1=K_1(q,q_x,q_{xx})$. The general solution is given by

$$q_t=(2L_1q_{xxx}+L_2)(L_1q_{xxx}^2+L_2q_{xxx}+L_3)^{-1/2}+L_4; \tag{72}$$

here L_1,L_2,L_3,L_4 are functions to be determined. The classification of the type of nonlinear partial differential equations above has not been finished yet due to present limitations in the computing system; we hope to have an extension of the system in the near future.

V. CONCLUSION AND COMPARISON

According to Fokas,[1] an integrable equation possess infinitely many generalized symmetries. Although there exist algorithmic ways of finding symmetries, it is better to use another approach. One can obtain one symmetry and using the recursion operator infinitely many symmetries can be generated. Therefore the first step in finding out the integrability of an equation is to find a Lie–Bäcklund symmetry. Apparently, there exists an intimate connection between linearization and Fokas' symmetry approach. The existence of generalized symmetry manifests itself in the existence of a Lie–Bäcklund operator. The existence of infinitely many symmetries is expressed by the existence of a recursion operator. There is also a close relationship[12] between a Lie–Bäcklund operator and a linearized equation. Because, if Fokas' admissible Lie–Bäcklund operator is applied on the evolution equation, we obtain the Fréchet derivative of the equation under consideration or linearized form of our equation. The recursion operator in linearization is obtained by the integration of the eigenvalue equation.

Let us briefly recall Olver's symmetry approach, linearization test, and Mikhailov–Shabat–Sokolov formal symmetry method:

Olver's symmetry test: The equation $u_t=f[u]$ is integrable if there exists infinitely many non-Lie point symmetries or, equivalently, one non-Lie point symmetry and a recursion operator. The recursion operator and time-independent part of the linearized equation form a Lax pair $\Phi_t+[\Phi,D_f]=0$.

Linearization test: The equation $u_t=f[u]$ is integrable if there exists an eigenvalue equation $H\Psi=0$ such that it is compatible with linearized equation $\Psi_t=D_f(\Psi)$. The compatibility condition is $H_t+[H,\ D_f]=0$.

Mikhailov–Shabat–Sokolov formal symmetry test: The equation $u_t=f[u]$ is integrable if there exists a pseudo-differential operator L such that $L_t+[L,\ D_f]=0$ holds up to sufficiently low orders.

In all three approaches the crucial point is the existence of the recursion operator. In MSS formal symmetry and Olver–Fokas symmetry approaches, to get a recursion operator is not as easy as in the linearization test. These methods are useful for classification purposes, because they can be applied to arbitrary equations (without polynomial restriction).

We must also mention that our classification is up to a change of variables. There are partial differential equations which are not included in the classification (IV.), but they can be obtained by a transformation.[17] [For example, Eq. (3.13) in Ref. 1 by extended hodograph transformation.] On the other hand, there are equations which appear in the same class, and are related to each other by a Miura-type transformation. Moreover, there may be other integrable equations that do not appear in the classification (IV.), because of a different eigenvalue problem.

The main idea in this work is to give a new definition of integrability. We conjecture that a partial differential equation is integrable if its linearized equation can support an eigenvalue equation. This definition implements a method to check whether a given partial differential equation is integrable. In addition, one can search an integrable subclass of a given class of partial differential equation. Linearization is also compared with Fokas's symmetry and Mikhailov–Shabat–Sokolov formal symmetry approaches.

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A Rodriguez formula and integration measure for the quantum deformed Legendre functions

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Quantum deformed analogs of the Legendre functions are constructed from shift operator representations of the quantum deformed orbital angular momentum operators. A Rodriguez formula is found as well as the measure used to orthonormalize the functions. © *1996 American Institute of Physics.*
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I. INTRODUCTION

The representations of quantum deformed Lie algebras in terms of difference operators shows a rich variety of structure that can be traced to the nonuniqueness of the representations.[1] For example, recent work[2] on quantum su(2) has produced analytical realizations whose basis functions are rational rather than polynomial in nature. These functions do not conform simply to the standard classes of quantum deformed orthogonal polynomials but are interesting in their own right. The classical Legendre polynomials do have well known but not widely used rational forms. These do not appear naturally as eigenfunctions of differential operators in physics in the commonly used coordinate systems. In this paper we will show that the quantum deformed orbital angular momentum operators possess quantum analogs of these verions of the Legendre functions as their representation basis functions. From this knowledge a Rodriguez formula will be found and used to orthonormalize the functions.

II. AN OPERATOR REPRESENTATION OF $so(3)_q$

It is a simple matter to construct a difference operator representation of the angular momentum operators much in the spirit of Ref. 1. The product relations for the algebra are

$$[J_z, J_+]=J_+, \tag{1}$$

$$[J_z, J_-]=-J_-, \tag{2}$$

$$[J_+, J_-]=\frac{q^{2J_z}-q^{-2J_z}}{q-q^{-1}}. \tag{3}$$

In the hope that a realization in terms of operators acting on functions over the sphere S^2 can be found, we require that

$$J_z=\frac{1}{i}\frac{\partial}{\partial\phi}, \tag{4}$$

in which ϕ is the azimuthal angle on the sphere. The first two commutators essentially state that

$$J_+=e^{i\phi}o_+ \tag{5}$$

and

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$$J_- = e^{-i\phi} o_- , \tag{6}$$

in which the two operators o_+ and o_- have no ϕ dependence. For now we think of them as acting on a remaining variable x which must be a function of the polar angle θ. We define the deformation parameter q to be

$$q = e^s . \tag{7}$$

The remaining product (3) suggests the forms

$$J_+ = e^{i\phi}(A(x)e^{is\partial_\phi} + B(x)e^{-is\partial_\phi} + c(x)), \tag{8}$$

$$J_- = e^{-i\phi}(A^+(x)e^{is\partial_\phi} + B^+(x)e^{-is\partial_\phi} + c^+(x)), \tag{9}$$

in which for now $(+)$ does not necessarily mean adjoint. We further imagine that c and c^+ must contain difference operators that provide derivatives with respect to θ as q approaches 1, and so we define

$$c = ue^{is\partial_x}, \tag{10}$$

$$c^+ = u^+ e^{is\partial_x}. \tag{11}$$

Substitution into the products (1)–(3) gives six relations on the operators A, B, c, A^+, B^+, c^+ that seem to have only exponential solutions. A convenient set of solutions is

$$A = -B^+ = \frac{e^{-ix}}{q - q^{-1}}, \tag{12}$$

$$B = -A^+ = \frac{e^{ix}}{q - q^{-1}}, \tag{13}$$

$$u = -u^+ = -\frac{e^{ix} + e^{-ix}}{q - q^{-1}}. \tag{14}$$

This last choice of u is made to cancel terms of order s^{-1} as the limit q approaches 1. The limits of these operators as q goes to 1 do not agree with the standard orbital angular momentum operators and so we define

$$x = i \ln \tan \frac{\theta}{2}, \tag{15}$$

which gives the operators the correct undeformed limit. The full set of q-deformed angular momentum operators can now be displayed in terms of θ and ϕ:

$$J_z = \frac{1}{i}\frac{\partial}{\partial \phi}, \tag{16}$$

$$J_+ = \frac{e^{i\phi}}{q - q^{-1}}\left(\tan\frac{\theta}{2} e^{is\partial_\phi} + \cot\frac{\theta}{2} e^{-is\partial_\phi} - \frac{2}{\sin\theta} e^{s \sin\theta \partial_\theta}\right), \tag{17}$$

$$J_- = \frac{e^{-i\phi}}{q - q^{-1}}\left(-\cot\frac{\theta}{2} e^{is\partial_\phi} - \tan\frac{\theta}{2} e^{-is\partial_\phi} + \frac{2}{\sin\theta} e^{s \sin\theta \partial_\phi}\right). \tag{18}$$

These are in agreement with the results of Ref. 2.

III. HIGHEST WEIGHT EIGENFUNCTIONS

The highest weight eigenfunctions in the $2j+1$-dimensional subspace is the function annihilated by J_+:

$$(q^{-j}e^{-ix}+q^{j}e^{ix}-(e^{ix}+e^{-ix})e^{-is\partial_x})e^{ij\phi}\psi_{jj}=0. \tag{19}$$

This suggests the unusual form

$$\psi_{jj}=\frac{1}{\Sigma_n a_n e^{inx}}, \tag{20}$$

in which the coefficients have the recursion relation

$$a_{m+1}=-\frac{1-q^{j-m-1}}{1-q^{-(j+m+1)}}\,a_{m-1}. \tag{21}$$

This separates the solutions into even and odd cases; for example, in the even case the coefficients become

$$a_{2n}(q)=a_{-2n}(-q)=(-1)^n\prod_{m=0}^{n-1}\frac{1-q^{j-2m}}{1-q^{-(j+2m+2)}}, \tag{22}$$

and in both cases the q-binomial theorem allows the series solution to be expressed as

$$\psi_{jj}=\frac{e^{ij\phi}e^{ijx}}{\Pi_{m=1}^{j}(1+q^{2m}e^{2ix})}. \tag{23}$$

IV. THE q-LEGENDRE FUNCTIONS

The states annihilated by J_z would correspond to a q-analog of the Legendre functions. The most expedient way to build them is by solving the eigenvalue equation for the quadratic Casimir operator with the appropriate eigenvalue. The operator C_2 can be written as

$$\begin{aligned}(q-q^{-1})C_2=&(e^{ix}+e^{-ix})(q^{-1}e^{ix}+qe^{-ix})(q^{i\partial_x-i\partial_\phi}+q^{i\partial_x+i\partial_\phi}-q^{2i\partial_x})\\&-(q^{-1}e^{2ix}+qe^{-2ix}+2)\end{aligned} \tag{24}$$

and it has eigenvalues

$$\frac{(q^{j+1/2}-q^{-(j+1/2)})^2}{(q-q^{-1})^2}. \tag{25}$$

The issue of adjoint formation will be addressed in the section on the orthogonality of the eigenfunctions. Application of the Casimir operator to the sought-after function ψ_{j0} results in the equation

$$(2e^{is\partial_x}-e^{2is\partial_x})\psi_{j0}=\frac{q^{2j+1}+q^{-(2j+1)}+q^{-1}e^{2ix}+qe^{-2ix}}{(q^{-1}e^{2ix}+q+q^{-1}+qe^{-2ix})}\,\psi_{j0}. \tag{26}$$

Let $z=e^{ix}$ and extract the denominator from ψ_{j0} by defining

$$\psi_{j0}=\frac{f_j(z)}{\Pi_{n=1}^{j}(1+q^{2n}z^2)}, \tag{27}$$

and the result is that the numerator satisfies a difference equation

$$2(1+z^2)f_j(z)-(1+q^{2j}z^2)f_j(q^{-1}z)=(1+q^{-2j}z^2)f_j(qz), \tag{28}$$

which can be solved recursively for the series

$$f_j(z)=\sum_{m=0}^{j}(-1)^m\prod_{p=1}^{m}\left(\frac{q^{j-(p-1)}-q^{-(j-(p-1))}}{q^p-q^{-p}}\right)^2 z^{2m}. \tag{29}$$

The coefficients of z^{2m} are simply related to the Gaussian polynomials. Let

$$\binom{n}{m}_q=\frac{(q-q^{-1})(q^2-q^{-2})\cdots(q^n-q^{-n})}{(q-q^{-1})\cdots(q^m-q^{-m})(q-q^{-1})\cdots(q^{n-m}-q^{-(n-m)})}, \tag{30}$$

which reduces to the binomial coefficient as q goes to 1. Then our final expression for the q-Legendre function

$$\psi_{j0}=\frac{\Sigma_{m=0}^{j}(-1)^m\binom{j}{m}_q^2 z^{2m}}{\Pi_{m=1}^{j}(1+q^{2m}z^2)}, \tag{31}$$

is an obvious q-analog of a common rational expression for the Legendre functions

$$P_n(t)=\frac{\Sigma_{m=0}^{n}\binom{n}{m}^2 t^{2m}}{(1-t)^n}. \tag{32}$$

The substitution $x=(1+t)/(1-t)$ reduces this to the standard Legendre polynomial which can be shown by computing the generating function

$$2\pi\sum_{n=0}^{\infty}P_n(t)u^n=\int_0^{\infty}\sum_{n=0}^{\infty}\left(\frac{u(1+e^{i\theta}\sqrt{t})(1+e^{-i\theta}\sqrt{t})}{(1-t)}\right)^n d\theta=\frac{2\pi}{\sqrt{1-2u((1+t)/(1-t))+u^2}}. \tag{33}$$

In the classical case the Rodriguez formula is the equation

$$P_n=P_{n0}=(J_-)^nP_{nn}=\left[(1+t)^2\frac{d}{dt}\right]^n\left(\frac{t}{(1-t)^2}\right)^n, \tag{34}$$

in the rational representation, up to a normalization factor. The same route to a Rodriguez formula for the q-deformed functions can be followed. We define scale operators

$$d_+F(z)=F(qz), \tag{35}$$

$$d_-F(z)=F(q^{-1}z), \tag{36}$$

and the Jackson derivatives

$$\nabla_-F(z)=\frac{F(z)-F(q^{-1}z)}{z(1-q^{-1})}=\frac{1-d_-}{z(1-q^{-1})}F(z), \tag{37}$$

$$\nabla_+ F(z) = \frac{1-d_+}{z(1-q)} F(z), \tag{38}$$

change variables $z = e^{ix}$, and extract the ϕ dependence from ψ_{jm},

$$\psi_{jm} = e^{im\phi} g_{jm}(z). \tag{39}$$

The action of the lowering operators on the functions g_{jm} can be expressed as

$$g_{j(j-1)} = -z^{-1}[q^j(1+q^{-2j}z^2) - (1+z^2)d_-]g_{jj}, \tag{40}$$

$$g_{j(m-1)} = -z^{-1}[q^m(1+q^{-2m}z^2) - (1+z^2)d_-]g_{jm}. \tag{41}$$

The operator identity

$$\begin{aligned}(1-q^{-1})z^{-j}q^j(1+z^2)\cdots(1+q^{-2j}z^2)\nabla_- \frac{z^j F(z)}{(1+z^2)\cdots(1+q^{-2j+2}z^2)} \\ = z^{-1}[q^j(1+q^{-2j}z^2) - (1+z^2)d_-]F(z)\end{aligned} \tag{42}$$

allows us to write g_{j0} as the result of a q-power of an operator on g_{jj} by defining

$$D_m = q^m[-z^{-1}(1+q^{-2m}z^2)(1+q^{-2m+2}z^2)\nabla_-], \tag{43}$$

and by writing out repeated applications of J_- to g_{jj} we see cancellations of most of the binomials in the operator identity result in the compact expression

$$g_{j0} = D_1 D_2 \cdots D_j \left[\frac{z^j g_{jj}}{(1+z^2)\cdots(1+q^{-2j+2}z^2)}\right]. \tag{44}$$

This form will be particularly useful in the section in which the normalization integral is computed.

V. ORTHOGONALITY AND MEASURE

The functions g_{j0} are the q-Legendre functions but in an unnormalized state. They can be shown to be an orthogonal set with respect to a suitably chosen measure $\mu(z)$ on the positive z axis. Actual construction of the measure is simpler in the present case than in the examples of Refs. (3)–(5) because of the availability of the Rodriguez formula. The measure should be chosen if any ambiguity in its construction arises to have the expected classical limit as q approaches 1. The appropriate measure can be gotten quickly from the requirement that g_{00} be orthogonal to all g_{j0} for $j>0$. We write this condition as

$$\int_0^\infty \mu(z)(-z^{-1}(1+z^2)(1+q^{-2}z^2))\nabla_- \left[\frac{z^2 g_{j1}}{(1+z^2)(1+q^2z^2)}\right] dz = 0, \tag{45}$$

and now q-integrate by parts

$$\int_0^\infty \frac{z^2 g_{j1}}{(1+z^2)(1+q^2z^2)} \nabla_+ [q\mu(z)z^{-1}(1+z^2)(1+q^{-2}z^2)] dz = 0, \tag{46}$$

from which we see that

$$\mu(z)=\frac{z}{(1+z^2)(1+q^{-2}z^2)}, \tag{47}$$

up to a multiplicative factor. This does reduce to the correct classical limit. Now the orthogonality proof can proceed in the same way as in the classical case: express each function in terms of the Rodriguez formula and integrate by parts to move lowering operators from one function onto the other where they act as raising operators. This continues until a sufficient number act on the target function to annihilate it. An expedient would be a similar set of operator identities for the raising operator, such as the following:

$$g_{j1}=[(z+z^{-1})-(z+z^{-1})d_-]g_{j0}=(1+z^2)\nabla_- g_{j0}, \tag{48}$$

$$g_{j2}=[(zq+z^{-1}q^{-1})-(z+z^{-1})d_-]g_{j1}=q^{-1}z\nabla_- z^{-1}(1+q^2z^2)g_{j1}, \tag{49}$$

$$g_{j3}=[(zq^2+z^{-1}q^{-2})-(z+z^{-1})d_-]g_{j2}=\frac{q^{-2}z^2}{(1+q^2z^2)}\,(\nabla_- z^{-2}(1+q^2z^2)(1+q^4z^2))g_{j2}. \tag{50}$$

We now illustrate with an example, showing g_{20} and g_{10} are orthogonal. An operator O is interposed on the possibility that it may be needed and to facilitate simplification of the resulting expression:

$$\begin{aligned}&\int_0^\infty \mu(z)\left[qz^{-1}(1+z^2)(1+q^{-2}z^2)\nabla_- \frac{z}{(1+z^2)}\right]\\&\quad\times[q^2z^{-2}(1+z^2)(1+q^{-2}z^2)(1+q^{-4}z^2)\nabla_- \frac{z^2g_{22}}{(1+z^2)(1+q^2z^2)}]Og_{10}\,dz\\&\quad=-q\int_0^\infty\left[q^3z^{-1}(1+q^{-4}z^2)\nabla_- \frac{z^2g_{22}}{(1+z^2)(1+q^2z^2)}\right]\\&\qquad\times(1+q^{-2}z^2)\nabla_+ Og_{10}\,dz.\end{aligned} \tag{51}$$

If this process is to be the q-analog of the classical version, then we must have

$$(1+q^{-2}z^2)\nabla_+ Og_{10}=Og_{11}, \tag{52}$$

from which it is evident that the operator O decomposes into

$$O=d_-I, \tag{53}$$

in which the operator I transforms q into q^{-1} so that

$$(1+q^{-2}z^2)\nabla_+ d_-Ig_{10}=d_-I(1+z^2)\nabla_- g_{10}=d_-Ig_{11}. \tag{54}$$

Subsequent integrations by parts have the desired effect of raising d_-Ig_{11} past the point of no return:

$$\begin{aligned}&q^2\int_0^\infty q^3\,\frac{zg_{22}}{(1+z^2)(1+q^2z^2)}\,z\nabla_+ z^{-1}(1+q^{-4}z^2)d_-Ig_{11}dz\\&\quad=q^5\int_0^\infty\frac{zg_{22}}{(1+z^2)(1+q^2z^2)}\,d_-I[z\nabla_- z^{-1}(1+q^2z^2)g_{11}]dz=0,\end{aligned} \tag{55}$$

by the use of Eq. (49). The proof that the functions g_{j0} are orthogonal can now proceed as in the classical case along with a proof that J_+ and J_- are formal adjoints. First define the action of J_+ and J_- on g_{jm} in terms of the step operators

$$g_{j(m-1)}=J^m_{m-1}g_{jm}, \tag{56}$$

$$g_{j(m)}=J^{m-1}_{m}g_{j(m-1)}. \tag{57}$$

Now we develop by use of the operator identities

$$J^0_1=(1+z^2)\nabla_-, \tag{58}$$

$$J^1_2=q^1z\nabla_-z^{-1}(1+q^2z^2), \tag{59}$$

$$J^m_{m+1}=q^{-m}\frac{z^m}{(1+q^2z^2)\cdots(1+q^{2(m-1)}z^2)}\nabla_-z^{-m}(1+q^2z^2)\cdots(1+q^{2m}z^2), \tag{60}$$

$$J^1_0=qz^{-1}(1+z^2)(1+q^2z^2)\nabla_-\frac{z}{(1+z^2)}, \tag{61}$$

$$J^m_{m-1}=q^mz^{-m}(1+z^2)\cdots(1+q^{-2m}z^2)\nabla_-\frac{z^m}{(1+z^2)\cdots(1+q^{-2m+2}z^2)}, \tag{62}$$

a shorthand notation for the step operators.
Let

$$U_m=z^{-m}\prod_{n=1}^{m}(1+q^{2n}z^2), \tag{63}$$

$$V_m=z^{-m}\prod_{n=0}^{m}(1+q^{-2n}z^2), \tag{64}$$

with $U_0=1$ and $V_0=(1+z^2)$. Then the step operators can be written as

$$J^m_{m+1}=q^{-m}zU^{-1}_{m-1}\nabla_-U_m, \tag{65}$$

$$J^m_{m+1}=q^mV_m\nabla_-zV^{-1}_{m-1}. \tag{66}$$

The additional operator identity is trivial to prove:

$$d_-IV_m=q^mz^{-1}(1+z^2)(1+q^{-2}z^2)U_{m-1}d_-I. \tag{67}$$

Now apply this to $\Pi^j_1J^n_{n-1}$:

$$d_-I\prod_{n=2}^{j}J^n_{n-1}=z^{-1}(1+z^2)(1+q^{-2}z^2)\left[\prod_{n=2}^{j}(-q^{-n}U_{n-1}\nabla_+U^{-1}_{n-2})\right]\times\frac{z}{(1+z^2)(1+q^{-2}z^2)}d_-I. \tag{68}$$

Apply it to J^1_0:

$$d_-Iqz^{-1}(1+z^2)(1+q^{-2}z^2)\nabla_- \frac{z}{(1+z^2)}$$

$$=q^{-1}z^{-1}(1+z^2)(1+q^{-2}z^2)\nabla_+ \frac{z}{(1+q^{-2}z^2)}\, d_-I. \tag{69}$$

Put the two pieces together and use the definition of $\mu(z)$ to obtain

$$d_-I\prod_{n=1}^{j} J_{n-1}^n = q^{-1}\mu^{-1}(z)\prod_{n=2}^{j} (-q^{-n}U_{n-1}\nabla_+ zU_{n-2}^{-1})\mu(z)d_-I. \tag{70}$$

The factors in the product are precisely the transposes of the step-up operators and will be converted into J_{n+1}^n in turn upon integration by parts. In addition we have shown how to construct adjoints

$$\int_0^\infty \mu(z)F(z)d_-IJ_{m-1}^m G(z)dz = \int_0^\infty \mu(z)F(z)\mu^{-1}(z)q^{-m}U_{m-1}\nabla_+ zU_{m-2}^{-1}d_-IG(z)dz$$

$$=-\int_0^\infty U_{m-2}^{-1}z\nabla_- U_{m-1}q^{-m}F(z)\mu(z)d_-IG(z)dz$$

$$=\int_0^\infty \mu(z)J_m^{m-1}F(z)d_-IG(z)dz. \tag{71}$$

The proof of orthogonality is now obvious, partial integrations move lowering operators from g_{0j} onto g_{0k} and in the process makes them into raising operators. If $j>k$, this results in the annihilation of g_{0k}.

VI. THE NORMALIZATION INTEGRAL

The norm of g_{j0} can also be computed from the Rodriguez formula. Notice that the norm of g_{00} is well defined in the limit as q approaches 1 and $\mu(z)dz$ reduces correctly to $\sin\theta\, d\theta$ in that limit,

$$N_{00}=\int_0^\infty \frac{q^{-2}\, dy}{(1+y)(1+q^{-2}y)}=\frac{2\ln q}{(1-q^{-2})}. \tag{72}$$

We now demonstrate that

$$D_1D_2\cdots D_j \frac{z^{2j}}{\Pi_{n=1}^{2j}(1+q^{2n}z^2)}=q^{-j^2}\frac{(1-q^{-2})\cdots(1-q^{-2j})\Sigma_{n=0}^{j}(-1)^n(\begin{smallmatrix}j\\n\end{smallmatrix})_q{}^2 z^{2n}}{(1-q^{-1})\cdots(1-q^{-1})\Pi_{n=1}^{j}(1+q^{2n}z^2)}. \tag{73}$$

That this is true up to an overall multiplicative factor has already been established; now that factor is to be determined. The fastest path to this end is to notice that the numerator of the left-hand size of (73) always contains a term of order z^{2j}. The coefficient can be found by tracking its value with each application of a D_k operator with the result

$$q^{-j^2}\frac{(1-q^{-2})\cdots(1-q^{-2j})}{(1-q^{-1})\cdots(1-q^{-1})}, \tag{74}$$

as the coefficient of z^{2j}. The operators D_n to the right of d_-I in the expression

$$N_{jj}=\int_0^\infty \mu(z)\left[D_1\cdots D_j\left(\frac{z^j g_{jj}}{\Pi_0^{j-1}(1+q^{-2n}z^2)}\right)\right]d_-I\left[D_1\cdots D_j\left(\frac{z^j g_{jj}}{\Pi_0^{j-1}(1+q^{2n}z^2)}\right)\right]dz \quad (75)$$

are now passed through d_-I and moved by partial integration onto the first factor in the integral resulting in

$$N_{jj}=(-q)^j\int_0^\infty \mu(z)\left[D_{-j}\cdots D_{-1}D_1\cdots D_j\left(\frac{z^j g_{jj}}{\Pi_0^{j-1}(1+q^{-2n}z^2)}\right)\right]$$
$$\times d_-I\left[\left(\frac{z^j g_{jj}}{\Pi_0^{j-1}(1+q^{2n}z^2)}\right)\right]dz, \quad (76)$$

where

$$D_{-m}=q^{-m}z^{-1}(1+q^{2m-2}z^2)(1+q^{2m}z^2)\nabla_-. \quad (77)$$

The evaluation of the long string of D_{-k} operators on g_{j0} can be accomplished recursively by writing

$$g_{j0}=\frac{\Sigma_{n=0}^j A_n^{(0)}z^{2n}}{\Pi_{n=1}^j(1+q^{2n}z^2)}, \quad (78)$$

$$D_{-1}g_{j0}=\frac{\Sigma_{n=0}^j A_n^{(1)}z^{2n}}{\Pi_{n=2}^j(1+q^{2n}z^2)}, \quad (79)$$

$$\vdots$$

$$D_{-k}\cdots D_{-1}g_{j0}=\frac{\Sigma_{n=0}^j A_n^{(k)}z^{2n}}{\Pi_{n=k+1}^j(1+q^{2n}z^2)}. \quad (80)$$

Since the coefficients $A_m^{(0)}$ are already known, this recursive tower can be solved for

$$A_m^{(1)}=\frac{(-1)^m}{1-q^{-1}}\begin{pmatrix} j \\ m \end{pmatrix}_q^2 \frac{(1-q^{-2m})(1-q^{2j+2})}{(1-q^{2j+2-2m})}, \quad (81)$$

$$A_m^{(2)}=\frac{(-1)^m}{(1-q^{-1})^2}\begin{pmatrix} j \\ m \end{pmatrix}_q^2 \frac{(1-q^{-2m})(1-q^{2-2m})(1-q^{2j+2})(1-q^{2j+4})}{(1-q^{2j+2-2m})(1-q^{2j+4-2m})}, \quad (82)$$

$$\vdots.$$

The process terminates in

$$A_j^{(j-1)}=q^{-(j+2)(j-1)}\frac{(1-q^{2j})(1-q^{2j+2})\cdots(1-q^{4j-2})}{(1-q^2)(1-q^{-1})^{j-1}} \quad (83)$$

and

$$D_{-(j-1)}\cdots D_{-1}g_{j0}=A_j^{(j-1)}\frac{(1-z^2)}{(1+q^{2j}z^2)}. \quad (84)$$

The final expression for N_{jj} is

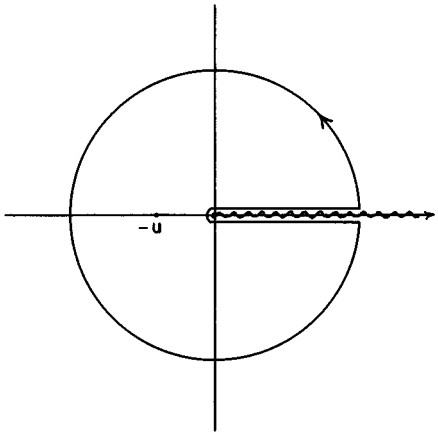

FIG. 1. Path of integration for (87).

$$N_{jj}=\frac{(1-q^{-2})\cdots(1-q^{-4j})}{(1-q^{-1})\cdots(1-q^{-1})}\int_0^\infty \frac{z^{2j+1}\,dz}{(1+q^{-2j}z^2)(1+q^{-2j+2}z^2)\cdots(1+q^{2j+2}z^2)}, \tag{85}$$

$$N_{jj}=2q^{2j(j+1)}\,\frac{(1-q^{-2})\cdots(1-q^{-4j})}{(1-q^{-1})\cdots(1-q^{-1})}\int_0^\infty \frac{y^j\,dy}{(1+y)\cdots(1+q^{4j+2}y)}. \tag{86}$$

This integral is of the form

$$I_{k,N}=\int_0^\infty \frac{y^{k-1}\,dy}{\Pi_{n=0}^N(u^n+y)}, \tag{87}$$

which can be evaluated by contour integration using the contour shown in the figure with branch cut extending to infinity, with result

$$I_{k,N}=\frac{2\pi i(-1)^{N+k-1}}{1-e^{2\pi ik}}\sum_{p=0}^{N}\frac{u^{-pN+p(p-1)/2+pk}(-1)^p}{(u)_p(u)_{N-p}}. \tag{88}$$

The sum can be performed using the q-binomial theorem

$$I_{k,N}=\frac{2\pi i}{1-e^{2\pi ik}}\,(-1)^{N+k-1}\,\frac{(u^{k-N})_N}{(u)_N}, \tag{89}$$

in which

$$(u)_N=(1-u)(1-u^2)\cdots(1-u^N). \tag{90}$$

For the case in which k is an integer, L'Hopital's rule gives

$$I_{k,N}=\frac{\ln u}{(1-u^N)\binom{N-1}{k-1}_u}. \tag{91}$$

The present usage of this integral has $u=q^{-2}$, $k=j+1$, and $N=2j+1$ with the conclusion that the functions

$$N_j D_1 \cdots D_j \left(\frac{z^{2j}}{\Pi_{n=1}^{2j}(1+q^{2n}z^2)} \right), \tag{92}$$

with

$$N_j = \sqrt{\frac{(1-q^{-2(2j+1)})(1-q^{-1})^{2j}}{2(1-q^{-2})^2 \cdots (1-q^{-2j})^2 \ln q^{-2}}}, \tag{93}$$

form an orthonormal set of rational functions on the positive ray that are q deformations of the rational form of the Legendre functions. The normalization coefficient N_j correctly reduces to

$$N_j = \frac{1}{2^j j!} \sqrt{\frac{2j+1}{2}}, \tag{94}$$

in the limit as q approaches 1.

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Abstract space–times and their Lorentz groups

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It has recently been discovered [A. A. Ungar, Am. J. Phys. **59**, 824 (1991); **60**, 815 (1992)] that the set $\mathbb{R}_c^3=\{\mathbf{v}\in\mathbb{R}^3 : \|\mathbf{v}\|<c\}$ of all relativistically admissible velocities in Euclidean three-space $\mathbb{R}^3$, with a binary operation $\oplus$ given by relativistic velocity addition, forms a gyrogroup $(\mathbb{R}_c^3,\oplus)$. The gyrogroup $(\mathbb{R}_c^3,\oplus)$ reduces to the group $(\mathbb{R}^3,+)$ in the limit $c\to\infty$, $+$ being the prerelativistic velocity addition (that is, the ordinary vector addition in the Euclidean three-space $\mathbb{R}^3$). The binary operation $\oplus$ in $\mathbb{R}_c^3$ is *gyroassociative* and *gyrocommutative*, as opposed to the binary operation $+$ in $\mathbb{R}^3$ which is associative and commutative. In this article we extend the study of gyrogroups into that of Lorentz groups. In particular, we find that a gyrogroup must be equipped with a *cocycle form* in order to be extendible into a Lorentz group. We thus study gyrogroups that are equipped with a cocycle form, and their resulting Lorentz groups. Interestingly, the cocycle form needed for the extension of gyrogroups into Lorentz groups involves a *cocycle identity* which is known to be useful in various branches of mathematics [B. R. Ebanks and C. T. Ng, Aequat. Math. **46**, 76 (1993)]. © *1996 American Institute of Physics.* [S0022-2488(96)01606-6]

I. INTRODUCTION

The relevance of gyrogroup theory to the study of real and complex Lorentz groups has been demonstrated in Refs. 1–4. The use of the real $(1+3)$-dimensional Lorentz group in the special theory of relativity (STR) is well known; and a use of a complex Lorentz group in quantum mechanics is presented in Ref. 5. The Lorentz group of STR is parametrizable by (i) relativistically admissible velocities and (ii) orientations. The values of the orientation parameter form a group, SO(3), under rotation composition; and the values of the velocity parameter form a nongroup *gyrogroup*, $(\mathbb{R}_c^3, \oplus)$, under relativistic velocity addition $\oplus$. The gyrogroup operation $\oplus$ in $\mathbb{R}_c^3=\{\mathbf{v}\in\mathbb{R}^3 : \|\mathbf{v}\|<c\}$ turns out to be *gyrocommutative* and *gyroassociative*, as opposed to the prerelativistic velocity addition $+$ in $\mathbb{R}^3$ which is both commutative and associative.

The prefix *gyro-* that we extensively use stems from analogies shared with *Thomas gyration*. Thomas gyration, in turn, is an abstraction of the common Thomas precession of STR. Unfortunately, Thomas precession is commonly studied in STR as an isolated peculiarity. In this article, however, we will see that Thomas gyration plays a central role in STR and in its abstraction, giving rise to the gyrogroup concept. In fact, it is the notion of the gyrogroup that allows the abstraction of the Lorentz group acting on spacetime. It was found that the gyrogroup structure is closely related to that of the so-called *K loop*,[3] which was discovered in 1965 by Karzel,[4] and is extensively studied in some areas of geometry.[6]

In Sec. II we introduce the gyrogroup definition, as well as the definition of the *cocycle form* that a gyrogroup must possess in order to be extendible into a Lorentz group. It thus turns out that the study of gyrogroups equipped with a cocycle form is fruitful, giving rise to elegant identities and exposing previously unknown structure underlying Lorentz groups. Of particular interest is the special case of the real and complex relativistic gyrogroups and their cocycle forms, presented in Sec. III. In that section a nonstandard relativistic gyrogroup that results in a nonstandard Lorentz group is also presented.

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The real and complex gyrogroups described in Sec. III are extended in Sec. IV into real and complex space–times. The action of abstract Lorentz transformations on these abstract space–times is then explored in Sec. V. The *gyrosemidirect product* presented in Sec. VI enables us in Sec. VII to study the abstract real and complex Lorentz transformation groups. In particular, we obtain Lorentz transformation composition laws that generalize the ones discovered in Refs. 7 and 8. Finally, group theoretical interpretation is presented in Sec. VIII.

Remarkably, although the cocycle identity is useful in several branches of mathematics,[9] the role it plays in the structure of the Lorentz group has gone unnoticed, along with the fact that the form $1+\mathbf{u}\cdot\mathbf{v}/c^2$ satisfies the cocycle identity in the relativistic gyrogroup $(\mathbb{R}^3_c,\oplus)$. The role played by the cocycle form in the abstract Lorentz group, described in this article, is indicated by the appearance of the relativistic cocycle form $1+\mathbf{u}\cdot\mathbf{v}/c^2$ in the expressions describing both the Lorentz transformation in STR and the relativistic velocity addition $\oplus$ in STR.

II. GYROGROUPS AND THEIR COCYCLE FORMS

Definition 2.1 (Groupoids and their automorphism groups): A groupoid $(S,+)$ is a nonempty set S with a binary operation $+$. An *automorphism* of the groupoid $(S,+)$ is a bijection of S that respects the binary operation $+$ in S. The set of all automorphisms of $(S,+)$ forms a group denoted by $\mathrm{Aut}(S,+)$.

Definition 2.2 (Gyrogroups): A groupoid $(P,+)$ is a gyrogroup if P contains an element, denoted by 0, such that

(G1) $\quad 0+x=x+0=x$

for any $x\in P$; and any element $x\in P$ has an inverse, denoted by $-x$, satisfying

(G2) $\quad -x+x=x+(-x)=0.$

Moreover, if for any x, $y\in P$ we define the map $\mathrm{gyr}[x;y]$ of P by the equation

$$\mathrm{gyr}[x;y]z=-(x+y)+(x+(y+z)),\quad z\in P,$$

then the following hold:

(G3)	$\mathrm{gyr}[x;y]\in\mathrm{Aut}(P,+)$,	gyroautomorphism,
(G4)	$x+y=\mathrm{gyr}[x;y](y+x)$,	gyrocommutative law,
(G5a)	$x+(y+z)=(x+y)+\mathrm{gyr}[x;y]z$,	right gyroassociative law,
(G5b)	$(x+y)+z=x+(y+\mathrm{gyr}[y;x]z)$,	left gyroassociative law,
(G6)	$\mathrm{gyr}[0;y]=I$,	identity gyroautomorphism,
(G7)	$\mathrm{gyr}[x+y;y]=\mathrm{gyr}[x;y]$,	loop property.

The gyroautomorphism $\mathrm{gyr}[x;y]$ of the gyrogroup $(P,+)$ is given in Definition 2.2 by its effect on any $z\in P$. Alternatively, if $L(a)$ denotes left gyrotranslation by a in $(P,+)$,

$$L(a)x=a+x$$

for all $a,x\in(P,+)$, then the inverse $L^{-1}(a)$ of $L(a)$ is $L^{-1}(a)=L(-a)$, and

$$\mathrm{gyr}[x;y]=L^{-1}(x+y)L(x)L(y). \tag{2.1}$$

In the particular case of the special-relativistic gyrogroup, the action of a gyroautomorphism $\mathrm{gyr}[x;y]$ is a rotation known as Thomas precession or *Thomas gyration*. Ambiguously, we say that the gyroautomorphisms $\mathrm{gyr}[x;y]$ are gyrations (or, rotations in the special relativistic case) of the gyrogroup P.

We will now present the definition and some properties of the cocycle form. In the sequel, these will prove useful in understanding the structure of Lorentz groups.

Definition 2.3 (The positive ray and the right-half complex plane): $\mathbb{R}$ and $\mathbb{C}$ denote, respectively, the real line and the complex plane. The *positive* ray is $\mathbb{R}^+=\{r\in\mathbb{R} : r>0\}$, and the *right-half complex plane* is $\mathbb{C}^+=\{z\in\mathbb{C} : \mathrm{Re}\, z>0\}$.

Definition 2.4R (A real cocycle form in a gyrogroup): A *real cocycle form* in a gyrogroup $(P,+)$ is a map

$$F : P\times P\to\mathbb{R}^+$$

possessing the following properties. For all $a,b,u,\nu,w\in P$,

(C1) $F(u,\nu+w)F(\nu,w)=F(\nu+u,w)F(u,\nu)$, cocycle identity,[9]

(C2) $F(u,\nu)=F(\mathrm{gyr}[a;b]u,\mathrm{gyr}[a;b]\nu)$, gyroinvariance, invariance under gyrations,

(C3R) $F(u,\nu)=F(\nu,u)$, symmetry,

(C4) $F(0,0)=1$, normalization condition.

If, in addition, F satisfies the condition

(C5) $F(-u,-\nu)=F(u,\nu)$, even cocycle form,

we say that F is *even*. The definition of a complex cocycle form is similar.

Definition 2.4C (Complex cocycle form in a gyrogroup): A *complex cocycle form* in a gyrogroup $(P,+)$ is a map

$$F : P\times P\to\mathbb{C}^+$$

possessing properties (C1)–(C4) of Definition 2.4R, but with property (C3R) replaced by the following property (C3C):

(C3C) $F(u,\nu)=\overline{F(\nu,u)}$, complex symmetry.

Clearly, if $F(u,\nu)$ is a complex cocycle form, then its modulus $|F(u,\nu)|$ is a real cocycle form.

Theorem 2.1: Let F be a real or complex cocycle form in a gyrogroup $(P,+)$. Then, for any $\nu,x\in P$,

(i) $F(0,\nu)=1$,

(ii) $F(\nu,-\nu)=F(\nu+x,-\nu)F(x,\nu)$,

(iii) $F(\nu,-\nu)$ is real, satisfying $F(\nu,-\nu)=F(-\nu,\nu)$.

Proof: The cocycle identity (C1) with $u=0$ and $\nu=-w$ gives

$$F(0,0)F(-w,w)=F(-w,w)F(0,-w)$$

implying, by means of (C4), that $F(0,-w)=1$ for any $w\in P$, thus verifying (i). Property (ii) follows from the cocycle identity (C1) with $u=x$ and $w=-\nu$, and from (i). The equality in (iii) follows from (i) and from (ii) with $x=-\nu$. If F is a complex cocycle form, then the reality of $F(\nu,-\nu)$ follows from (C3C).

Definition 2.5 (Gyrogroups with a cocycle form): A gyrogroup $(P,+)$ possessing a cocycle form F is denoted by $(P,+,F)$.

Definition 2.6 (The Lorentz factor γ): Let $(P,+,F)$ be a gyrogroup with a cocycle form F. For any $\nu\in P$, the Lorentz factor γ_ν is given by the equation

$$\gamma_\nu^{-2}=F(\nu,-\nu).$$

We will see in Sec. III that the relativistic gyrogroup possesses an even cocycle form, $S(\mathbf{u},\mathbf{v})$, such that its Lorentz factor $\gamma_{\mathbf{v}}$ [with $\gamma_{\mathbf{v}}^{-2}=S(\mathbf{v},-\mathbf{v})$] is the common Lorentz factor of STR.

Theorem 2.2R: Let $F(u,\nu)$ be an even real cocycle form in a gyrogroup $(P,+,F)$. Then

$$F(u,\nu)=\frac{\gamma_{u+\nu}}{\gamma_u\gamma_\nu} \tag{2.2}$$

for any $u,\nu\in P$.

Proof: By the cocycle identity

$$F(u+\nu,w)=\frac{F(\nu,u+w)F(u,w)}{F(\nu,u)}$$

with $w=-(u+\nu)$, noting that $u+w=-\nu$, we have

$$F(u+\nu,-(u+\nu))=\frac{F(\nu,-\nu)}{F(\nu,u)}\,F(u,-(u+\nu)). \tag{2.3}$$

By the identity (ii) in Theorem 2.1 with $x=u$, and by the symmetry of F, we have

$$F(\nu,-\nu)=F(\nu+u,-\nu)F(u,\nu)=F(\nu,u)F(\nu+u,-\nu),$$

implying

$$\frac{F(\nu,-\nu)}{F(\nu,u)}=F(\nu+u,-\nu). \tag{2.4}$$

Substituting (2.4) into (2.3) we have, by properties (C3R) and (C5) of the even real cocycle form $F(u,\nu)$,

$$\begin{aligned}F(u+\nu,-(u+\nu))&=F(\nu+u,-\nu)F(u,-(u+\nu))\\&=F(\nu+u,-\nu)F(u+\nu,-u)\\&=F(u+\nu,-u)F(\nu+u,-\nu).\end{aligned} \tag{2.5}$$

By two applications of identity (ii) in Theorem 2.1 (introducing $x=x_1$ in the first application and $x=x_2$ in the second application), with $x_1=\nu$ and $x_2=u$, and by (2.5) we have

$$\begin{aligned}F(u,-u)F(\nu,-\nu)&=F(u+x_1,-u)F(x_1,u)F(\nu+x_2,-\nu)F(x_2,\nu)\\&=F^2(u,\nu)F(u+\nu,-u)F(\nu+u,-\nu)\\&=F^2(u,\nu)F(u+\nu,-(u+\nu)).\end{aligned} \tag{2.6}$$

By Definition 2.6, the extreme left- and right-hand sides of Eq. (2.6) yield

$$\gamma_u^{-2}\gamma_\nu^{-2}=F^2(u,\nu)\,\gamma_{u+\nu}^{-2},$$

thus verifying Theorem 2.2R.

A generalization of Theorem 2.2R to any real cocycle form, not necessarily even, is given in Theorem 4.2. To demonstrate an application of Theorem 2.2R we verify the following.

Lemma 2.1R: Let $F(u,\nu)$ be an even real cocycle form in a gyrogroup $(P,+,F)$. Then F satisfies the identity

$$\frac{F(-(a+b),a+(b+\nu))F(a,b+\nu)F(b,\nu)}{F(a+b,-(a+b))F(a,b)}=1$$

for all $a,b,\nu\in P$.

Proof: By Theorem 2.2R, the identity in Lemma 2.1R can be written as

$$\frac{\gamma_\nu}{\gamma_{a+b}\gamma_{a+(b+\nu)}}\,\frac{\gamma_{a+(b+\nu)}}{\gamma_a\gamma_{b+\nu}}\,\frac{\gamma_{b+\nu}}{\gamma_b\gamma_\nu}\Big/\frac{1}{\gamma_{a+b}^2}\,\frac{\gamma_{a+b}}{\gamma_a\gamma_b}=1,$$

noting that

$$-(a+b)+\{a+(b+\nu)\}=\mathrm{gyr}[a;b]\nu,$$

so that

$$\gamma_{-(a+b)+(a+(b+\nu))}=\gamma_{\mathrm{gyr}[a;b]\nu}=\gamma_\nu,$$

thus completing the proof.

Lemma 2.1R and its proof were presented as an instructive demonstration of an application of Theorem 2.2R. However, the result of the Lemma can be extended to both real and complex cocycle forms which need not be even. We, therefore, present below a generalization of Lemma 2.1R.

Lemma 2.1: Let $F(u,\nu)$ be a real or complex cocycle form in a gyrogroup $(P,+,F)$. Then F satisfies the identity

$$\frac{F(-(a+b),a+(b+\nu))F(a,b+\nu)F(b,\nu)}{F(a+b,-(a+b))F(a,b)}=1 \tag{2.7}$$

for all $a,b,\nu\in P$.

Proof: By Theorem 2.1 (ii) we have

$$F(a+b,-(a+b))=F((a+b)+x,-(a+b))F(x,a+b)$$

for any $x\in P$. Hence, in particular, for $x=\mathrm{gyr}[a;b]\nu$, we have by (C2), (G5a), (G4), and (C3C) and by part (iii) of Theorem 2.1,

$$F(a+b,-(a+b))=F(a+(b+\nu),-(a+b))F(\nu,b+a)=F(-(a+b),a+(b+\nu))F(b+a,\nu). \tag{2.8}$$

Eliminating $F(b+a,\nu)$ between identity (2.8) and the cocycle identity

$$F(a,b+\nu)F(b,\nu)=F(b+a,\nu)F(a,b)$$

yields (2.7) as desired.

We will now present the complex counterpart of Theorem 2.2R.

Theorem 2.2C: Let $F(u,v)$ be an even complex cocycle form in a gyrogroup $(P,+,F)$. Then

$$|F(u,v)| = \frac{\gamma_{u+v}}{\gamma_u \gamma_v}$$

for any $u,v \in P$. Hence,

$$F(u,v) = \mathrm{tgyr}[u;v]\ \frac{\gamma_{u+v}}{\gamma_u \gamma_v},$$

where

$$\mathrm{tgyr}[u;v] = \frac{F(u,v)}{|F(u,v)|},$$

for any $u,v \in P$.

Proof: The complex conjugate of Eq. (2.3), noting that $F(v,-v)$ is real, takes the form

$$F(u+v,-(u+v)) = \frac{F(v,-v)}{\overline{F(v,u)}}\ \overline{F(u,-(u+v))}. \tag{2.9}$$

By the second identity in Theorem 2.1 with $x=u$, and by the complex symmetry of F, we have

$$F(v,-v) = F(v+u,-v)F(u,v) = \overline{F(v,u)}F(v+u,-v),$$

implying

$$\frac{F(v,-v)}{\overline{F(v,u)}} = F(v+u,-v). \tag{2.10}$$

Substituting (2.10) into (2.9) we have, by properties (C3C) and (C5) of the cocycle form $F(u,v)$,

$$\begin{aligned} F(u+v,-(u+v)) &= F(v+u,-v)\overline{F(u,-(u+v))} \\ &= F(v+u,-v)F(u+v,-u) \\ &= F(u+v,-u)F(v+u,-v). \end{aligned} \tag{2.11}$$

By the second identity in Theorem 2.1, with $x=v$ and $y=u$, and by (2.11) we have

$$\begin{aligned} F(u,-u)F(v,-v) &= F(u+x,-u)F(x,u)F(v+y,-v)F(y,v) \\ &= |F(u,v)|^2 F(u+v,-u)F(v+u,-v) \\ &= |F(u,v)|^2 F(u+v,-(u+v)). \end{aligned} \tag{2.12}$$

By Definition 2.6, the extreme left- and right-hand sides of Eq. (2.12) yield

$$\gamma_u^{-2}\gamma_v^{-2} = |F(u,v)|^2 \gamma_{u+v}^{-2},$$

thus verifying Theorem 2.2C.

Theorem 2.2C suggests the following.

Definition 2.7 (The time gyration): Let F be a complex cocycle form in a gyrogroup $(P, +, F)$. The *time gyrooperator* tgyr is a map

$$\text{tgyr} \ : \ P \times P \to \mathbb{C}_0^+ ,$$

where $\mathbb{C}_0^+ = \{z \in \mathbb{C} \ : \ |z| = 1, \ \text{Re}\, z > 0\}$, given by

$$\text{tgyr}[u; v] = \frac{F(u, v)}{|F(u, v)|} \tag{2.13}$$

for any $u, v \in P$. The $\text{tgyr}[u; v]$ are called *time gyrations*. They represent *rotations* of the complex plane $\mathbb{C}$.

The real counterpart of tgyr vanishes. If $F(u, v)$ is a real cocycle form in a gyrogroup $(P, +, F)$, then clearly $\text{tgyr}[u; v] = 1$ for any $u, v \in P$. Therefore, the extension from gyrogroups with a real cocycle form to gyrogroups with a complex cocycle form is not trivial; time gyration of a gyrogroup with a complex cocycle form has no real counterpart. As suggested by its term, tgyr possesses properties similar to those of gyr, as indicated in the following.

Theorem 2.3: The time gyration tgyr in a gyrogroup $(P, +, F)$ with a complex cocycle form satisfies the identities

(i) $\text{tgyr}^{-1}[u; v] = \text{tgyr}[v; u]$,

(ii) $\text{tgyr}[0; v] = 1$,

and it possesses the two loop properties

$$\text{tgyr}[u + v; v] = \text{tgyr}[u; v], \quad \text{left loop property (LLP)},$$

$$\text{tgyr}[u; v + u] = \text{tgyr}[u; v], \quad \text{right loop property (RLP)}.$$

Proof: (i) and (ii) follow immediately from the definition of tgyr, from property (C3C) of F, and from Theorem (2.1) (i). To verify the right loop property, let us substitute $w = u$ in the cocycle identity (C1), obtaining the identity

$$F(u; v + u)F(v, u) = F(v + u, u)F(u, v). \tag{2.14}$$

It follows from (2.14), by the complex symmetry property (C3C) of F, that the product $F(u, v + u)F(v, u)$ in $\mathbb{C}$ is real. Hence, the conjugate $\overline{F(v, u)} = F(u, v)$ of $F(v, u)$ is real proportional to $F(u, v + u)$, that is,

$$F(u, v) = rF(u, v + u) \tag{2.15}$$

for some positive real constant r. Dividing each side of (2.15) by its magnitude gives the right loop property (RLP). Taking the complex conjugate of each side of (2.15) one similarly verifies the left loop property (LLP). The proof of the theorem is thus complete.

III. THE REAL AND COMPLEX RELATIVISTIC GYROGROUPS AND THEIR COCYCLE FORMS

Definition 3.1 [Einstein gyrogroup; the standard relativistic gyrogroup $(V_c, \oplus)$]: Let $(V_\infty, +, \cdot)$ be a (real or complex) inner product space, and let

$$V_c = \{\mathbf{v} \in V_\infty \ : \ \|\mathbf{v}\| < c\} \tag{3.1}$$

be its open c ball; c being an arbitrary fixed positive constant. The inner product $\langle \mathbf{u},\mathbf{v}\rangle$ in V_∞ is denoted by $\mathbf{u}\cdot\mathbf{v}$ or $\mathbf{v}\cdot\mathbf{u}$ if V_∞ is real, and by $\mathbf{u}\cdot\overline{\mathbf{v}}$ or $\overline{\mathbf{v}}\cdot\mathbf{u}$ if V_∞ is complex (we make no attempt to define $\overline{\mathbf{v}}$ alone). To avoid unnecessary repetitions, if V_∞ is real then $\mathbf{u}\cdot\overline{\mathbf{v}}=\mathbf{u}\cdot\mathbf{v}$. Under this notation, the groupoid *induced* by the inner product space $(V_\infty,+,\cdot)$ is the pair $(V_c,\oplus)$ where the binary operation $\oplus$ in V_c is given by the abstract relativistic velocity addition

$$\mathbf{u}\oplus\mathbf{v}=\frac{1}{1+\overline{\mathbf{u}}\cdot\mathbf{v}/c^2}\left\{\mathbf{u}+\frac{1}{\gamma_u}\,\mathbf{v}+\frac{1}{c^2}\,\frac{\gamma_u}{1+\gamma_u}\,(\overline{\mathbf{u}}\cdot\mathbf{v})\mathbf{u}\right\},\quad \mathbf{u},\mathbf{v}\in V_c, \tag{3.2a}$$

γ_u being the well-known Lorentz factor of STR (written here for a possibly complex $\mathbf{u}$),

$$\gamma_u=\frac{1}{\sqrt{1-\overline{\mathbf{u}}\cdot\mathbf{u}/c^2}}. \tag{3.2b}$$

The use of the symbol γ_u in Eq. (3.2b) and in Definition 2.6 is not ambiguous, as indicated in Eqs. (3.6) and in a paragraph above these equations.

The groupoid $(V_c,\oplus)$ forms a gyrogroup known as the *(real or complex) relativistic gyrogroup*.[7] Following Ref. 13, it is also called Einstein gyrogroup.

Theorem 3.1 (A complex cocycle form in the complex relativistic gyrogroup): Let $(V_\infty,+,\cdot)$ be a complex inner product space, and let $(V_c,\oplus)$ be the gyrogroup induced on its open c ball V_c. Then the map

$$S\ :\ V_c\times V_c\to\mathbb{C}^+$$

given by the equation

$$S(\mathbf{u},\mathbf{v})=1+\frac{\overline{\mathbf{u}}\cdot\mathbf{v}}{c^2} \tag{3.3}$$

is an even complex cocycle form in the gyrogroup $(V_c,\oplus)$, giving rise to the triple $(V_c,\oplus,S)$ (defined in Definition 2.5).

Proof: We have to verify that $S(\mathbf{u},\mathbf{v})$ possesses properties (C1)–(C5) of the cocycle form. Invariance of $S(\mathbf{u},\mathbf{v})$ under gyrations is obvious; gyrations in the gyrogroup $(V_c,\oplus)$ are unitary transformations of V_c and of V_∞, under which the inner product $\cdot$ in V_∞ is invariant. This verifies (C2).

The validity of properties (C3)–(C5) for $S(\mathbf{u},\mathbf{v})$ is immediate. It remains to verify the cocycle identity (C1).

The binary operation $\oplus$ in the gyrogroup V_c is given by Eq. (3.2), which can be written as

$$\mathbf{u}\oplus\mathbf{v}=A_{\mathbf{u},\mathbf{v}}\mathbf{u}+B_{\mathbf{u},\mathbf{v}}\mathbf{v} \tag{3.4a}$$

with

$$A_{\mathbf{u},\mathbf{v}}=\frac{1}{1+(\overline{\mathbf{u}}\cdot\mathbf{v}/c^2)}\left(1+\frac{1}{c^2}\,\frac{\gamma_u}{1+\gamma_u}\,\overline{\mathbf{u}}\cdot\mathbf{v}\right)$$

and

$$B_{\mathbf{u},\mathbf{v}}=\frac{1}{1+(\overline{\mathbf{u}}\cdot\mathbf{v}/c^2)}\,\frac{1}{\gamma_u}. \tag{3.4b}$$

Hence,

$$\overline{\mathbf{u}\cdot(\mathbf{v}\oplus\mathbf{w})}=A_{\mathbf{v},\mathbf{w}}\overline{\mathbf{u}\cdot\mathbf{v}}+B_{\mathbf{v},\mathbf{w}}\overline{\mathbf{u}\cdot\mathbf{w}}=\frac{1}{1+(\overline{\mathbf{v}\cdot\mathbf{w}}/c^2)}\left\{\left(1+\frac{1}{c^2}\frac{\gamma_v}{1+\gamma_v}\overline{\mathbf{v}\cdot\mathbf{w}}\right)\overline{\mathbf{u}\cdot\mathbf{v}}+\frac{1}{\gamma_v}\overline{\mathbf{u}\cdot\mathbf{w}}\right\}$$

and

$$\overline{\mathbf{w}\cdot(\mathbf{v}\oplus\mathbf{u})}=A_{\mathbf{v},\mathbf{u}}\overline{\mathbf{v}\cdot\mathbf{w}}+B_{\mathbf{v},\mathbf{u}}\overline{\mathbf{u}\cdot\mathbf{w}}=\frac{1}{1+(\overline{\mathbf{u}\cdot\mathbf{v}}/c^2)}\left\{\left(1+\frac{1}{c^2}\frac{\gamma_v}{1+\gamma_v}\overline{\mathbf{u}\cdot\mathbf{v}}\right)\overline{\mathbf{v}\cdot\mathbf{w}}+\frac{1}{\gamma_v}\overline{\mathbf{u}\cdot\mathbf{w}}\right\}.$$

With the above definition of $S(\mathbf{u},\mathbf{v})$ we have (taking $c=1$ without loss of generality)

$$\begin{aligned}S(\mathbf{u},\mathbf{v}\oplus\mathbf{w})S(\mathbf{v},\mathbf{w})&=\{1+\overline{\mathbf{u}\cdot(\mathbf{v}\oplus\mathbf{w})}\}(1+\overline{\mathbf{v}\cdot\mathbf{w}})\\&=\left(1+\frac{1}{1+\overline{\mathbf{v}\cdot\mathbf{w}}}\left\{\left(1+\frac{\gamma_v}{1+\gamma_v}\overline{\mathbf{v}\cdot\mathbf{w}}\right)\overline{\mathbf{u}\cdot\mathbf{v}}+\frac{1}{\gamma_v}\overline{\mathbf{u}\cdot\mathbf{w}}\right\}\right)(1+\overline{\mathbf{v}\cdot\mathbf{w}})\\&=1+\overline{\mathbf{v}\cdot\mathbf{w}}+\left(1+\frac{\gamma_v}{1+\gamma_v}\overline{\mathbf{v}\cdot\mathbf{w}}\right)\overline{\mathbf{u}\cdot\mathbf{v}}+\frac{1}{\gamma_v}\overline{\mathbf{u}\cdot\mathbf{w}}\end{aligned}$$

and

$$\begin{aligned}S(\mathbf{v}\oplus\mathbf{u},\mathbf{w})S(\mathbf{u},\mathbf{v})&=\{1+\mathbf{w}\cdot\overline{(\mathbf{v}\oplus\mathbf{u})}\}(1+\overline{\mathbf{u}\cdot\mathbf{v}})\\&=\left(1+\frac{1}{1+\overline{\mathbf{u}\cdot\mathbf{v}}}\left\{\left(1+\frac{\gamma_v}{1+\gamma_v}\overline{\mathbf{u}\cdot\mathbf{v}}\right)\overline{\mathbf{v}\cdot\mathbf{w}}+\frac{1}{\gamma_v}\overline{\mathbf{u}\cdot\mathbf{w}}\right\}\right)(1+\overline{\mathbf{u}\cdot\mathbf{v}})\\&=1+\overline{\mathbf{u}\cdot\mathbf{v}}+\left(1+\frac{\gamma_v}{1+\gamma_v}\overline{\mathbf{u}\cdot\mathbf{v}}\right)\overline{\mathbf{v}\cdot\mathbf{w}}+\frac{1}{\gamma_v}\overline{\mathbf{u}\cdot\mathbf{w}},\end{aligned}$$

implying

$$S(\mathbf{u},\mathbf{v}\oplus\mathbf{w})S(\mathbf{v},\mathbf{w})=S(\mathbf{v}\oplus\mathbf{u},\mathbf{w})S(\mathbf{u},\mathbf{v}) \tag{3.5}$$

so that $S(\mathbf{u},\mathbf{v})$ satisfies the cocycle identity (C1) as desired. The proof of Theorem 3.1 is thus complete.

Clearly, Theorem 3.1 implicitly presents, as a special case, a real cocycle form in the real relativistic gyrogroup.

Theorem 3.1 associates the real and complex relativistic gyrogroups with respective real and complex cocycle forms S. Accordingly, we may denote the real and complex relativistic gyrogroups $(V_c,\oplus)$ by $(V_c,\oplus,S)$. Furthermore, following Definition 2.6 the relativistic even real form $S(\mathbf{v},\mathbf{u})$ induces a Lorentz factor $\gamma_{\mathbf{v}}$, $\gamma_{\mathbf{v}}^{-2}=S(\mathbf{v},-\mathbf{v})$. The factor $\gamma_{\mathbf{v}}$ turns out to be the well-known Lorentz factor of STR, Eq. (3.2b).

Due to the important role that the cocycle form $S(\mathbf{u},\mathbf{v})$ plays in the relativistic gyrogroup $(V_c,\oplus)$, it seems appropriate to express the binary operation $\oplus$ in V_c in terms of $S(\mathbf{u},\mathbf{v})$ rather than $\overline{\mathbf{u}\cdot\mathbf{v}}$. Equation (3.2) then takes the form

$$\mathbf{u}\oplus\mathbf{v}=\frac{1}{1+\gamma_u}\left(\gamma_u+\frac{1}{S(\mathbf{u},\mathbf{v})}\right)\mathbf{u}+\frac{1}{\gamma_u}\frac{1}{S(\mathbf{u},\mathbf{v})}\mathbf{v}, \tag{3.6a}$$

$$\gamma_u=\frac{1}{\sqrt{S(\mathbf{u},-\mathbf{u})}}, \tag{3.6b}$$

demonstrating the importance of the conditions $S(\mathbf{u},\mathbf{v})\neq 0$ and $S(\mathbf{u},-\mathbf{u})>0$ for all $\mathbf{u},\mathbf{v}\in V_c$.

Definition 3.2 [Möbius gyrogroup; the nonstandard relativistic gyrogroup $(V_c,\boxplus)$]: Let $(V_\infty,+,\cdot)$ be a real inner product space, and let V_c be its open c ball, c being an arbitrary fixed positive constant. The nonstandard binary operation in V_c, $\boxplus$, is given by the equation

$$\mathbf{u}\boxplus\mathbf{v}=\frac{1}{N^2(\mathbf{u},\mathbf{v})}\left\{\left(1+\frac{2}{c^2}\,\mathbf{u}\cdot\mathbf{v}+\frac{1}{c^2}\,\|\mathbf{v}\|^2\right)\mathbf{u}+\left(1-\frac{1}{c^2}\,\|\mathbf{u}\|^2\right)\mathbf{v}\right\} \tag{3.7a}$$

where $N^2(\mathbf{u},\mathbf{v})=(N(\mathbf{u},\mathbf{v}))^2$, N being the map

$$\mathrm{N}\ :\ \mathrm{V_c}\times\mathrm{V_c}\to\mathbb{R}^+$$

given by

$$N(\mathbf{u},\mathbf{v})=\sqrt{1+\frac{2}{c^2}\,\mathbf{u}\cdot\mathbf{v}+\frac{1}{c^4}\,\|\mathbf{u}\|^2\|\mathbf{v}\|^2}. \tag{3.8a}$$

The pair $(V_c,\boxplus)$ forms a gyrogroup[10,11] called the *nonstandard* relativistic gyrogroup induced by the real inner product space $(V_\infty,+,\cdot)$. Following Ref. 13, it is also called the Möbius gyrogroup.

Theorem 3.2: Let $(V_\infty,+,\cdot)$ be a real inner product space whose open c ball is V_c. Then $(V_c,\boxplus,F)$ is a gyrogroup with a real cocycle form, where $\boxplus$ and N are given by Eqs. (3.7a) and (3.8a).

Similarly to the proof of Theorem 3.1, the proof of Theorem 3.2 is lengthy but straightforward.

Remark: If we use the vector product notation

$$\mathbf{x}\times\mathbf{y}\times\mathbf{z}=-(\mathbf{y}\cdot\mathbf{z})\mathbf{x}+(\mathbf{x}\cdot\mathbf{z})\mathbf{y}$$

and

$$(\mathbf{x}\cdot\mathbf{y})^2=\|\mathbf{x}\|^2\|\mathbf{y}\|^2-(\mathbf{x}\cdot\mathbf{y})^2,$$

then Eqs. (3.7a) and (3.8a) take the elegant form

$$\mathbf{u}\boxplus\mathbf{v}=\frac{1+(1/c^2)\mathbf{u}\cdot\mathbf{v}-(1/c^2)(\mathbf{u}\times\mathbf{v})\times}{[1+(1/c^2)\mathbf{u}\cdot\mathbf{v}]^2+(1/c^4)(\mathbf{u}\times\mathbf{v})^2}\,(\mathbf{u}+\mathbf{v}) \tag{3.7b}$$

and

$$N(\mathbf{u},\mathbf{v})=\sqrt{[1+(1/c^2)\mathbf{u}\cdot\mathbf{v}]^2+(1/c^4)(\mathbf{u}\times\mathbf{v})^2}. \tag{3.8b}$$

The resulting space–time is the *expanding Minkowski space*, studied in Ref. 10.

Equation (3.7b), as opposed to Eq. (3.7a), is elegant in the sense that it exhibits the formal structure

$$\mathbf{u}\boxplus\mathbf{v}=\frac{A-B}{A^2+B^2}\,(\mathbf{u}+\mathbf{v}),$$

where A and B^2 are scalars, but B is an operator. The elegance of the binary operation $\boxplus$, as presented in Eq. (3.7b), stems from the fact that it is a generalized Möbius transformation.[11]

In a real inner product space V_∞ the standard and the nonstandard relativistic gyrogroups $(V_c,\oplus)$ and $(V_c,\boxplus)$ of Definitions 3.1 and 3.2 are isomorphic in the gyrogroup isomorphism sense introduced by You and Ungar.[12] In fact, the two binary operations $\oplus$ and $\boxplus$ in V_c, representing standard and nonstandard relativistic velocity addition, are related by the gyrogroup identity

$$\tfrac{1}{2}\odot(\mathbf{u}\oplus\mathbf{v})=\tfrac{1}{2}\odot\mathbf{u}\boxplus\tfrac{1}{2}\odot\mathbf{v} \tag{3.9}$$

in V_c.[12] In identity (3.9) the map $\frac{1}{2}\odot$ of V_c takes $\mathbf{u}\in V_c$ to its unique ''half'' $\frac{1}{2}\odot\mathbf{u}$ satisfying $\frac{1}{2}\odot\mathbf{u}\oplus\frac{1}{2}\odot\mathbf{u}=\mathbf{u}$, the inverse of which is the map $2\odot$ of V_c that takes $\mathbf{u}\in V_c$ to $2\odot\mathbf{u}=\mathbf{u}\oplus\mathbf{u}$.[13] It thus follows from (3.9) that $\boxplus$ is expressible in terms of $\oplus$ as

$$\mathbf{u}\boxplus\mathbf{v}=\tfrac{1}{2}\odot(2\odot\mathbf{u}\oplus 2\odot\mathbf{v}) \tag{3.10}$$

in V_c. Interestingly, when $V_\infty=\mathbb{R}^3$, the resulting standard and nonstandard Lorentz groups, studied in Ref. 10, are experimentally equivalent, as pointed out by Urbantke.[14] Their equivalence for abstract V_∞ is established in Ref. 12.

IV. REAL AND COMPLEX SPACE–TIMES

Definition 4.1: Let $(A\times B,\cdot)$ be a gyrogroup whose underlying set is the Cartesian product of two nonempty sets A and B. The gyro-operator gyr of the gyrogroup $(A\times B,\cdot)$ is *A central* if the gyration

$$\mathrm{gyr}[(a_1,b_1);(a_2,b_2)]$$

generated by (a_1,b_1) and (a_2,b_2) is independent of a_1, $a_2\in A$ for all (a_1,b_1), $(a_2,b_2)\in A\times B$. In other words,

$$\mathrm{gyr}[(a_1,b_1);(a_2,b_2)](a,b)=(a,\mathrm{gyr}_B[b_1;b_2]b) \tag{4.1}$$

for all $a\in A$ and $b\in B$ and some map

$$\mathrm{gyr}_B[b_1;b_2]:B\to B.$$

The map gyr_B is said to be the map of B induced by the A-central gyro-operator of the gyrogroup $(A\times B,\cdot)$.

Theorem 4.1: Let $(P,+)$ be a groupoid and let $(\mathbb{R}^+\times P,\cdot)$ be a groupoid of pairs whose groupoid operation $\cdot$ is related to the groupoid operation $+$ in P by the equation

$$(s,u)\cdot(t,\nu)=[F(u,\nu)st,u+\nu] \tag{4.2}$$

for some map

$$F\ :\ P\times P\to\mathbb{R}^+.$$

Then, the groupoid $(\mathbb{R}^+\times P,\cdot)$ is a gyrogroup with an $\mathbb{R}^+$-central gyro-operator if and only if the groupoid $(P,+)$ is a gyrogroup with a cocycle form, $(P,+,F)$, for which F is a real cocycle form.

Proof: Let $(P,+,F)$ be a gyrogroup equipped with the real cocycle form $F(u,\nu)$. We will show that the groupoid $(\mathbb{R}^+\times P,\cdot)$ is a gyrogroup whose gyro-operator is $\mathbb{R}^+$ central. (G1): The neutral element is (1,0); and (G2): The inverse is

$$(t,\nu)^{-1}=\left(\frac{1}{F(\nu,-\nu)t},-\nu\right). \tag{4.3}$$

It remains to show that the groupoid $(\mathbb{F}^+\times P,\cdot)$ possesses a gyro-operator gyr given by the equation

$$\mathrm{gyr}[(s,u);(t,\nu)]=L^{-1}[(s,u)\cdot(t,\nu)]L[(s,u)]L[(t,\nu)], \tag{4.4}$$

where $L[(t,\nu)]$ denotes left multiplication by (t,ν).

Let us therefore study the operator gyr in Eq. (4.4) by its effect on $(t,\nu)\in(\mathbb{F}^+\times P,\cdot)$, and show that it is indeed a gyro-operator of $(\mathbb{F}^+\times P,\cdot)$. We have, by Eq. (4.4),

$$\begin{aligned}
\mathrm{gyr}[(r,a);(s,b)](t,\nu) &= ((r,a)\cdot(s,b))^{-1}\cdot((r,a)\cdot((s,b)\cdot(t,\nu)))\\
&= (F(a,b)rs,a+b)^{-1}\cdot((r,a)\cdot((s,b)\cdot(t,\nu)))\\
&= \left(\frac{1}{F(a+b,-(a+b))F(a,b)rs},-(a+b)\right)\cdot((r,a)\cdot(F(b,\nu)st,b+\nu))\\
&= \left(\frac{1}{F(a+b,-(a+b))F(a,b)rs},-(a+b)\right)\\
&\quad\cdot(F(a,b+\nu)F(b,\nu)rst,a+(b+\nu))\\
&= \left(F(-(a+b),a+(b+\nu))\,\frac{F(a,b+\nu)F(b,\nu)rst}{F(a+b,-(a+b))F(a,b)rs},\right.\\
&\quad\left.-(a+b)+\{a+(b+\nu)\}\right)\\
&= (t,\mathrm{gyr}[a;b]\nu),
\end{aligned}\tag{4.5}$$

where in the last equality, (i) the equality between the first entry of pairs follows from Lemma 2.1, and (ii) the equality between the second entry of pairs follows from the definition of the gyro-operator gyr of the gyrogroup $(P,+)$ in Eq. (2.1). All the other equalities in the above chain of equations are obtained by pair multiplication, as defined in (4.2). Hence, we have the $\mathbb{R}^+$-central gyrooperator gyr of the groupoid $(\mathbb{R}^+\times P,\cdot)$ given by

$$\mathrm{gyr}[(r,a);(s,b)](t,\nu)=(t,\mathrm{gyr}[a;b]\nu)=\pi_2(\mathrm{gyr}[a;b])(t,\nu)=\mathrm{Gyr}[a;b](t,\nu),\tag{4.6}$$

where

$$\mathrm{Gyr}[a;b]=\pi_2\mathrm{gyr}[a;b])\tag{4.7}$$

with the map π_2 from operators B of P into operators $\pi_2(B)$ of $\mathbb{F}^+\times P$ given by the equation

$$\pi_2(B)(t,\nu)=(t,B\nu).\tag{4.8}$$

We should notice that gyr on the extreme left-hand side of Eq. (4.6) is the gyro-operator of $(\mathbb{R}^+\times P,\cdot)$, while gyr on the right-hand side of Eq. (4.7) is the gyro-operator of $(P,+)$, as clearly indicated by the arguments of gyr in these equations.

Equation (4.6) reveals a relation between the gyration $\mathrm{gyr}[a;b]$ of the gyrogroup $(P,+)$ and the operator $\mathrm{gyr}[(r,a);(s,b)]$ of the groupoid $(\mathbb{R}^+\times P,\cdot)$. We will show below that it readily follows (i) from this relation and (ii) from properties of the real cocycle form F that gyr possesses in $(\mathbb{R}^+\times P,\cdot)$ the gyrooperator properties (G3)–(G7). Hence, the groupoid $(\mathbb{R}^+\times P,\cdot)$ is indeed a gyrogroup, the gyrooperator of which is the $\mathbb{R}^+$-central gyro-operator Gyr (It is appropriate to interject here that, with one exception, all the gyro-operator properties are valid also when the cocycle form is complex. It is only the gyrocommutative law which fails when the cocycle form F is complex rather than real. Hence from the gyrogroup theoretic point of view a complex cocycle form gives rise to an interesting example of a *nongyrocommutative gyrogroup*, that is, a ''gyrogroup'' in which the gyrocommutativity axiom has been deleted.)

Let us now verify the validity of properties (G3)–(G7) in the groupoid $(\mathbb{R}^+\times P,\cdot)$. Using the abbreviation $g_{a,b}=\mathrm{gyr}[a;b]$ whenever convenient, we have (G3):

$$\begin{aligned}\mathrm{gyr}[(r,a);(s,b)]((t_1,\nu_1)\cdot(t_2,\nu_2)) &= \mathrm{gyr}[(r,a);(s,b)](F(\nu_1,\nu_2)t_1t_2,\nu_1+\nu_2)\\ &= (F(\nu_1,\nu_2)t_1t_2,\mathrm{gyr}[a;b](\nu_1+\nu_2))\\ &= (F(\nu_1,\nu_2)t_1t_2,g_{a,b}\nu_1+g_{a,b}\nu_2)\\ &= (F(g_{a,b}\nu_1,g_{a,b}\nu_2)t_1t_2,g_{a,b}\nu_1+g_{a,b}\nu_2)\\ &= (t_1,g_{a,b}\nu_1)\cdot(t_2,g_{a,b}\nu_2)\\ &= \mathrm{gyr}[(r,a);(s,b)](t_1,\nu_1)\cdot\mathrm{gyr}[(r,a);(s,b)](t_2,\nu_2).\end{aligned}$$

Hence $\mathrm{gyr}[(r,a);(s,b)]$ is an endomorphism of the groupoid $(\mathbb{R}^+\times P,\cdot)$, i.e., it is a map of the groupoid into itself respecting the binary operation. Moreover, $\mathrm{gyr}[(r,a);(s,b)]$ is invertible: for all $(t,\nu)\in\mathbb{R}^+\times P$ we have

$$\begin{aligned}\mathrm{gyr}[(r,a);(s,b)]\cdot\mathrm{gyr}[(s,b);(r,a)](t,\nu) &= \mathrm{gyr}[(r,a);(s,b)](t,\mathrm{gyr}[b;a]\nu)\\ &= (t,\mathrm{gyr}[a;b]\mathrm{gyr}[b;a]\nu)=(t,\nu).\end{aligned}$$

Hence $\mathrm{gyr}[(r,a);(s,b)]$ is an automorphism of the groupoid $(\mathbb{R}^+\times P,\cdot)$, thus verifying (G3). (G4): By the symmetry of $F(u,\nu)$,

$$\begin{aligned}\mathrm{gyr}[(r,a);(s,b)]((s,b)\cdot(r,a)) &= \mathrm{gyr}[(r,a);(s,b)](F(a,b)rs,b+a)\\ &= (F(a,b)rs,\mathrm{gyr}[a;b](b+a))\\ &= (F(a,b)rs,a+b)=(r,a)\cdot(s,b),\end{aligned}$$

thus verifying (G4).

(G5a):

$$\begin{aligned}(r,a)\cdot((s,b)\cdot(t,c)) &= (r,a)\cdot(F(b,c)st,b+c)\\ &= (F(a,b+c)F(b,c)rst,a+(b+c))\\ &= (F(b+a,c)F(a,b)rst,a+(b+c))\\ &= (F(a+b,g_{a,b}c)F(a,b)rst,(a+b)+g_{a,b}c)\\ &= (F(a,b)rs,a+b)\cdot(t,\ \mathrm{gyr}[a;b]c)\\ &= ((r,a)\cdot(s,b))\cdot\mathrm{gyr}[(r,a);(s,b)](t,c).\end{aligned}$$

(G5b):

$$\begin{aligned}((r,a)\cdot(s,b))\cdot(t,c) &= (F(a,b)rs,a+b)\cdot(t,c)\\ &= (F(a+b,c)F(a,b)rst,(a+b)+c)\\ &= (F(b+a,g_{b,a}c)F(a,b)rst,(a+b)+c)\\ &= (F(a,b+g_{b,a}c)F(b,g_{b,a}c)rst,a+(b+g_{b,a}c))\\ &= (r,a)\cdot(F(b,g_{b,a}c)st,b+g_{b,a}c)\\ &= (r,a)\cdot((s,b)\cdot(t,g_{b,a}c))=(r,a)\cdot((s,b)\cdot\mathrm{gyr}[(s,b);(r,a)](t,c));\end{aligned}$$

(G6):

$$\mathrm{gyr}[(1,0);(s,b)](t,c)=(t,\mathrm{gyr}[0;b]c)=(t,c),$$

so that $\mathrm{gyr}[(1,0);(s,b)]$ is the identity automorphism of $(\mathbb{R}^+\times P,\cdot)$, as required for (G6).

(G7):

$$\begin{aligned}\mathrm{gyr}[(r,a)\cdot(s,b);(s,b)](t,c) &= \mathrm{gyr}[F(a,b)rs,a+b);(s,b)](t,c)\\ &= (t,\mathrm{gyr}[a+b;b]c)\\ &= (t,\mathrm{gyr}[a;b]c)\\ &= \mathrm{gyr}[(r,a);(s,b)](t,c)\end{aligned}$$

for all $(t,c)\in\mathbb{R}^+\times P$, as required for (G7).

By establishing the validity of properties (G1)–(G7) for the groupoid $(\mathbb{R}^+\times P,\cdot)$, we have demonstrated that this groupoid is a gyrogroup.

Conversely, let assume that the groupoid $(\mathbb{R}^+\times P,\cdot)$ is a gyrogroup whose gyro-operator is $\mathbb{R}^+$ central. We will show that $(P,+,F)$ is a gyrogroup possessing the real cocycle form F.

Let the neutral element of the gyrogroup $(\mathbb{R}^+\times P,\cdot)$ be denoted by (1,0), and let the inverse of $(t,\nu)\in(\mathbb{R}^+\times P,\cdot)$ be denoted by $(T,-\nu)$ for some $T\in\mathbb{R}^+$. Then clearly the pair $(P,+)$ is a groupoid with a neutral element 0 and the inversion operation $-$.

To show that $(P,+,F)$ is a gyrogroup with F being its cocycle form, we have to establish the validity of properties (G1)–(G7) for the gyrogroup $(P,+)$, as well as the validity of properties (C1)–(C4) for its cocycle form F.

(G1): The neutral element of $(P,+)$ is 0.

(G2): The inverse of ν in $(P,+)$ is $-\nu$.

(C4): Since (1,0) is the neutral element of the product (4.2), we clearly have $F(0,\nu)=F(u,0)=1$ for any $u,\nu\in P$, and, in particular, $F(0,0)=1$.

The gyro-operator gyr of the gyrogroup $(\mathbb{R}^+\times P,\cdot)$ is given by Eq. (4.4), where the product $(s,u)\cdot(t,\nu)$ is given by Eq. (4.2). Hence, according to the fifth equality in the chain of equations (4.5), we have

$$\mathrm{gyr}[(r,a);(s,b)](t,\nu)=(G(a,b,\nu)t,\mathrm{gyr}[a;b]\nu), \tag{4.9}$$

where G is the map $G : P\times P\times P\to\mathbb{F}^+$ given by

$$G(a,b,\nu)=\frac{F(-(a+b),a+(b+\nu))F(a,b+\nu)F(b,\nu)}{F(a+b,-(a+b))F(a,b)}, \tag{4.10}$$

and where $\mathrm{gyr}[a;b]$ is the map of P given by

$$\mathrm{gyr}[a;b]=-(a+b)+\{a+(b+\nu)\}.$$

But the gyro-operator gyr of $(\mathbb{R}^+\times P,\cdot)$ in Eq. (4.9) is $\mathbb{R}^+$ central by assumption. Hence, it follows from Eq. (4.9) that $G(a,b,\nu)=1$, so that we have, by Eq. (4.10),

$$G(a,b,\nu)=\frac{F(-(a+b),a+(b+\nu))F(a,b+\nu)F(b,\nu)}{F(a+b,-(a+b))F(a,b)}=1, \tag{4.11}$$

and Eq. (4.9) can be written as

$$\mathrm{gyr}[(r,a);(s,b)](t,\nu)=(t,\mathrm{gyr}[a;b]\nu). \tag{4.12}$$

The gyrocommutative law in the gyrogroup $(\mathbb{F}^+\times P,\cdot)$ takes the form

$$(r,a)\cdot(s,b)=\mathrm{gyr}[(r,a);(s,b)]((s,b)\cdot(r,a)). \tag{4.13}$$

It can be written, by Eqs. (4.2) and (4.12), as

$$(F(a,b)rs,a+b)=\mathrm{gyr}[(r,a);(s,b)](F(b,a)rs,b+a)=(F(b,a)rs,\mathrm{gyr}[a;b](b+a)).$$

By equating each of the two entries of this equation we thus have (C3R): $F(a,b)=F(b,a)$ and (G4): $a+b=\mathrm{gyr}[a;b](b+a)$. *(G3):* $\mathrm{gyr}[a;b]$, *$a,b\in P$, is an automorphism of P.* To show this, we consider the following chain of equations. By means of Eqs. (4.12) and (4.2) we have

$$\begin{aligned}(F(\nu_1,\nu_2)t_1t_2,\mathrm{gyr}[a;b](\nu_1+\nu_2))&=\mathrm{gyr}[(r,a);(s,b)](F(\nu_1,\nu_2)t_1t_2,\nu_1+\nu_2)\\&=\mathrm{gyr}[(r,a);(s,b)]((t_1,\nu_1)\cdot(t_2,\nu_2))\\&=\mathrm{gyr}[(r,a);(s,b)](t_1,\nu_1)\cdot\mathrm{gyr}[(r,a);(s,b)](t_2,\nu_2)\\&=(t_1,\mathrm{gyr}[a;b]\nu_1)\cdot(t_2,\mathrm{gyr}[a;b]\nu_2)\\&=(F(\mathrm{gyr}[a;b]\nu_1,\mathrm{gyr}[a;b]\nu_2)t_1t_2,\mathrm{gyr}[a;b]\nu_1+\mathrm{gyr}[a;b]\nu_2),\end{aligned}$$

implying

$$\text{(C2):}\quad F(\nu_1,\nu_2)=F(\mathrm{gyr}[a;b]\nu_1,\mathrm{gyr}[a;b]\nu_2)$$

and

$$\mathrm{gyr}[a;b](\nu_1+\nu_2)=\mathrm{gyr}[a;b]\nu_1+\mathrm{gyr}[a;b]\nu_2. \tag{4.14}$$

Hence, by Eq. (4.14), $\mathrm{gyr}[a;b]$ is a homomorphism from P into itself for any $a,b\in P$. To verify that $\mathrm{gyr}[a;b]$ is an automorphism of P we will show that $\mathrm{gyr}[a;b]$ has an inverse, $\mathrm{gyr}^{-1}[a;b]=\mathrm{gyr}[b;a]$.

The inverse of the gyro-operator $\mathrm{gyr}[(r,a);(s,b)]$ is $\mathrm{gyr}[(s,b);(r,a)]$. Hence, by Eq. (4.12) we have

$$\begin{aligned}(t,\nu)&=\mathrm{gyr}[(r,a);(s,b)]\mathrm{gyr}[(s,b);(r,a)](t,\nu)\\&=\mathrm{gyr}[(r,a);(s,b)](t,\mathrm{gyr}[b;a]\nu)\\&=(t,\mathrm{gyr}[a;b]\mathrm{gyr}[b;a]\nu).\end{aligned}$$

Thus

$$\mathrm{gyr}[a;b]\mathrm{gyr}[b;a]=I \tag{4.15}$$

for any $a,b\in P$, I being the identity automorphism of P. It follows from Eq. (4.15) that the inverse of $\mathrm{gyr}[a;b]$ is $\mathrm{gyr}[b;a]$, as desired.

(G5a): Let us now establish the right gyroassociative law for $\mathrm{gyr}:P\times P\to\mathrm{Aut}(P,+)$. By the right gyroassociative law in the gyrogroup $(\mathbb{F}^+\times P,\cdot)$ and by Eqs. (4.2) and (4.12) we have

$$\begin{aligned}(F(u,\nu+w)F(\nu,w)rst,u+(\nu+w))&=(r,u)\cdot((s,\nu)\cdot(t,w))\\&=((r,u)\cdot(s,\nu))\cdot\mathrm{gyr}[(r,u);(s,\nu)](t,w)\\&=(F(u,\nu)rs,u+\nu)\cdot(t,\mathrm{gyr}[u;\nu]w)\\&=(F(u+\nu,\mathrm{gyr}[u;\nu]w)F(u,\nu)rst,u+\nu+\mathrm{gyr}[u;\nu]w),\end{aligned}$$

implying

$$F(u+\nu,\mathrm{gyr}[u;\nu]w)F(u,\nu)=F(u,\nu+w)F(\nu,w) \tag{4.16}$$

and

$$u+(\nu+w)=(u+\nu)+\mathrm{gyr}[u;\nu]w \tag{4.17}$$

for all $u,\nu,w\in P$. Equation (4.17) establishes the right gyroassociative law for gyr in $(P,+)$.

(G5b): We now wish to verify the left gyroassociative law for gyr:$P\times P\to\mathrm{Aut}(P,+)$. By the left gyroassociative law in the gyrogroup $(\mathbb{F}^+\times P,\cdot)$ and by Eqs. (4.2) and (4.12) we have

$$\begin{aligned}(F(u+\nu,w)F(u,\nu)rst,(u+\nu)+w)&=((r,u)\cdot(s,\nu)\cdot(t,w)\\&=(r,u)\cdot((s,\nu)\cdot\mathrm{gyr}[(s,\nu);(r,u)](t,w))\\&=(r,u)\cdot((s,\nu)\cdot(t,\mathrm{gyr}[\nu;u]w))\\&=(r,u)\cdot(F(\nu,\mathrm{gyr}[\nu;u]w)st,\nu+\mathrm{gyr}[\nu;u]w)\\&=(F(\nu,\mathrm{gyr}[\nu;u]w)F(u,\nu+\mathrm{gyr}[\nu;u]w)rst,u\\&\quad+(\nu+\mathrm{gyr}[\nu;u]w)),\end{aligned}$$

implying

$$F(\nu,\mathrm{gyr}[\nu;u]w)F(u,\nu+\mathrm{gyr}[\nu;u]w)=F(u+\nu,w)F(u,\nu) \tag{4.18}$$

and

$$(u+\nu)+w=u+(\nu+\mathrm{gyr}[\nu;u]w). \tag{4.19}$$

Equation (4.19) establishes the left gyroassociative law for gyr in $(P,+)$.

(G6): Since $\mathrm{gyr}[(s,u);(1,0)]=J$ is the identity automorphism of the gyrogroup $(\mathbb{F}^+\times P,\cdot)$, we have by Eq. (4.12)

$$(t,\nu)=\mathrm{gyr}[(r,a);(1,0)](t,\nu)=(t,\mathrm{gyr}[a;0]\nu)$$

implying

$$\mathrm{gyr}[a;0]\nu=\nu \tag{4.20}$$

for any $\nu\in P$. Hence

$$\mathrm{gyr}[a;0]=I, \tag{4.21}$$

I being the identity automorphism of P.

(G7): The (left) loop property (G7) for the gyrooperator gyr of the gyrogroup $(\mathbb{R}^+\times P,\cdot)$ takes the form

$$\mathrm{gyr}[(r,a)\cdot(s,b);(s,b)](t,\nu)=\mathrm{gyr}[(r,a);(s,b)](t,\nu)$$

for any $r,s,t\in\mathbb{F}^+$ and any $a,b,\nu\in P$. Hence by Eqs. (4.2) and (4.12) we have

$$\begin{aligned}(t,\mathrm{gyr}[a;b]\nu)&=\mathrm{gyr}[(r,a);(s,b)](t,\nu)\\&=\mathrm{gyr}[(r,a)\cdot(s,b);(s,b)](t,\nu)\\&=\mathrm{gyr}[(F(a,b)rs,a+b);(s,b)](t,\nu)\\&=(t,\mathrm{gyr}[a+b;b]\nu).\end{aligned}$$

Thus

$$\mathrm{gyr}[a+b;b]=\mathrm{gyr}[a;b] \tag{4.22}$$

for any $a,b,\nu\in P$. Equation (4.22) verifies (G7).

(C1): The cocycle identity follows from Eq. (4.16) and from (G4) and (C2):

$$\begin{aligned}F(u,\nu+w)F(\nu,w)&=F(u+\nu,\mathrm{gyr}[u;\nu]w)F(u,\nu)\\&=F(\mathrm{gyr}[u;\nu](\nu+u),\mathrm{gyr}[u;\nu]w)F(u,\nu)\\&=F(\nu+u,w)F(u,\nu),\end{aligned}$$

thus completing the proof of Theorem 4.1.

Definition 4.2 (Extended gyrogroups): The gyrogroup $(\mathbb{R}^+\times P,\cdot)$ of Theorem 4.1 is said to be the gyrogroup *over* a gyrogroup $(P,+,F)$, or the gyrogroup *extended* from a gyrogroup $(P,+,F)$.

Some properties of a real cocycle form F in a gyrogroup can be established by means of its extended gyrogroup. A real cocycle form F in a gyrogroup $(P,+,F)$ gives rise to its extended gyrogroup $(\mathbb{R}^+\times P,\cdot)$. The gyrogroup structure of the extended gyrogroup $(\mathbb{R}^+\times P,\cdot)$, in turn, reveals properties of F some of which are not easily detectable in $(P,+,F)$ itself. An example is provided by the proof of Theorem 4.2 below, a theorem that generalizes Theorem 2.2R.

Theorem 4.2: A real cocycle form F in a gyrogroup satisfies the identity

$$F(u,\nu)F(-u,-\nu)=\frac{F(u,-u)F(\nu,-\nu)}{F(u+\nu,-u-\nu)}=\frac{\gamma_{u+\nu}^2}{\gamma_u^2\gamma_\nu^2} \tag{4.23}$$

for all $u,\nu\in\mathbb{R}^+$.

Proof: In any gyrogroup $(G,+)$ we have [Ref. 15, Theorem 5.2]

$$-(a+b)=-a-b \tag{4.24}$$

for all $a,b\in G$. In the gyrogroup $(\mathbb{R}^+\times P,\cdot)$ extended from the gyrogroup $(P,+,F)$ with the real cocycle form F, Eq. (4.24) takes the form

$$(s,u)^{-1}\cdot(t,\nu)^{-1}=(F(u,\nu)st,u+\nu)^{-1}. \tag{4.25}$$

But, by Eqs. (4.3) and (4.2), we have

$$(s,u)^{-1}\cdot(t,\nu)^{-1}=\left(\frac{1}{F(u,-u)s},-u\right)\cdot\left(\frac{1}{F(\nu,-\nu)t},-\nu\right)=\left(\frac{F(-u,-\nu)}{F(u,-u)F(\nu,-\nu)st},-u-\nu\right) \tag{4.26}$$

and

$$(F(u,\nu)st,u+\nu)^{-1}=\left(\frac{1}{F(u+\nu,-u-\nu)F(u,\nu)st},-u-\nu\right). \tag{4.27}$$

Hence, by Eq. (4.25), the right-hand sides of Eqs. (4.26) and (4.27) are equal. From the equality of their first entries, we obtain the left identity in (4.23). The right identity in (4.23) follows from the definition of the factor γ in Definition 2.6. The proof is thus complete.

Clearly, if the real cocycle form F is even, then identity (4.23) specializes to (2.2).

V. REAL AND COMPLEX BOOSTS

In STR a boost is a pure Lorentz transformation; that is, a Lorentz transformation without rotation. The boosts discussed in this section result from abstraction of the relativistic boosts, and are restricted to the forward cone.

Definition 5.1 (Boosts of space–time): Let $(\mathbb{R}^+\times P,\cdot)$ be the gyrogroup extended from a gyrogroup $(P,+,F)$. Left multiplication of any $(t,\nu)\in(\mathbb{R}^+\times P,\cdot)$ by $B(u)=(\gamma_u,u)\in(\mathbb{R}^+\times P,\cdot)$ is called a *boost* of (t,ν) by $u\in P$. $B(u)$ is called a *boost of the space–time* $(\mathbb{R}^+\times P,\cdot)$, *parametrized by the gyrogroup* $(P,+)$. Thus

$$B(u)(t,\nu)=(\gamma_u,u)\cdot(t,\nu), \tag{5.1}$$

where the gyrogroup operation $\cdot$ in Eq. (5.1) is given by Eq. (4.2).

We will now show that the boosts of the space–time (forward cone) $(\mathbb{R}^+\times V_c,\oplus)$ parametrized by the relativistic gyrogroup $(V_c,\oplus,S)$ are the special relativistic Lorentz boosts (also known as *pure* Lorentz transformations, or Lorentz transformations *without rotation*).

Since the cocycle form S in the relativistic gyrogroup $(V_c,\oplus,S)$ is, by (3.3),

$$S(\mathbf{u},\mathbf{v})=1+\frac{\mathbf{u}\cdot\mathbf{v}}{c^2}, \tag{5.2}$$

multiplication in $(\mathbb{R}^+\times V_c,\oplus)$ takes the form

$$(r,\mathbf{u})\cdot(s,\mathbf{v})=\left(rs\left(1+\frac{\mathbf{u}\cdot\mathbf{v}}{c^2}\right),\mathbf{u}\oplus\mathbf{v}\right), \tag{5.3}$$

where no confusion should arise in the use of a dot to denote both a gyrogroup operation in a gyrogroup of pairs and an inner product in a vector space.

Let us introduce new notation in which we write the pair $(t,\mathbf{v})\in\mathbb{R}^+\times V_c$ as

$$(t,\mathbf{v})=\begin{pmatrix} t\\ \mathbf{v}t\end{pmatrix}=\begin{pmatrix} t\\ \mathbf{x}\end{pmatrix} \tag{5.4}$$

with $\mathbf{x}=\mathbf{v}t$. The right-hand side of Eq. (5.4) represents a forward time-like event.

Let $B(\mathbf{v})=(\gamma_\mathbf{v},\mathbf{v})$ be a boost of $(\mathbb{R}^+\times V_c,\oplus)$. Then the boost application to a space–time event $(t,\mathbf{v})\in(\mathbb{R}^+\times V_c,\oplus)$:

$$B(\mathbf{u})(t,\mathbf{v})=(\gamma_\mathbf{u},\mathbf{u})\cdot(t,\mathbf{v})=\left(\gamma_\mathbf{u}t\left(1+\frac{\mathbf{u}\cdot\mathbf{v}}{c^2}\right),\mathbf{u}\oplus\mathbf{v}\right),$$

takes the following form in the new notation:

$$B(\mathbf{u})\begin{pmatrix} t \\ \mathbf{x} \end{pmatrix} = \begin{pmatrix} \gamma_u t\left(1+\frac{1}{c^2}\,\mathbf{u}\cdot\mathbf{v}\right) \\ (\mathbf{u}\oplus\mathbf{v})\,\gamma_{\mathbf{u}} t\left(1+\frac{1}{c^2}\,\mathbf{u}\cdot\mathbf{v}\right) \end{pmatrix}$$

$$= \begin{pmatrix} \gamma_{\mathbf{u}}\left(t+\frac{1}{c^2}\,\mathbf{u}\cdot\mathbf{x}\right) \\ \frac{1}{1+\mathbf{u}\cdot\mathbf{v}/c^2}\left\{\mathbf{u}+\frac{1}{\gamma_u}\,\mathbf{v}+\frac{1}{c^2}\,\frac{\gamma_u}{1+\gamma_u}\,(\mathbf{u}\cdot\mathbf{v})\mathbf{u}\right\}\gamma_{\mathbf{u}} t\left(1+\frac{1}{c^2}\,\mathbf{u}\cdot\mathbf{v}\right) \end{pmatrix}$$

$$= \begin{pmatrix} \gamma_v\left(t+\frac{1}{c^2}\,\mathbf{u}\cdot\mathbf{x}\right) \\ \gamma_{\mathbf{u}}\mathbf{u}t+\mathbf{x}+\frac{1}{c^2}\,\frac{\gamma_u^2}{1+\gamma_u}\,(\mathbf{u}\cdot\mathbf{x})\mathbf{u} \end{pmatrix}. \tag{5.5}$$

This *real* boost application agrees with the *complex* boost application in Eq. (2.5) of Ref. 8.

Definition 5.2R (The norm of a real forward time-like space–time event): Let $(\mathbb{R}^+\times P,\cdot)$ be a space–time over the gyrogroup $(P,+,F)$ with a real cocycle form F, and let $(t,\nu)\in(\mathbb{R}^+\times P,\cdot)$ be an event. The norm $\|(t,\nu)\|$ of (t,ν) is given by

$$\|(t,\nu)\|^2 = t^2 F(\nu,-\nu).$$

Definition 5.2C (The norm of a complex forward time-like space–time event): Let $(\mathbb{C}^+\times P,\cdot)$ be a space–time over the gyrogroup $(P,+,F)$ with a complex cocycle form F, and let $(t,\nu)\in(\mathbb{C}^+\times P,\cdot)$ be an event. The norm $\|(t,\nu)\|$ of (t,ν) is given by

$$\|(t,\nu)\|^2 = |t|^2 F(\nu,-\nu).$$

Theorem 5.1R: Real boosts preserve the norm.

Proof: Let $(t',\nu')=B(u)(t,\nu)$. Then

$$(t',\nu')=B(u)(t,\nu)=(\gamma_u,u)\cdot(t,\nu)=(F(u,\nu)\,\gamma_u t, u+\nu)$$

and, hence,

$$\|(t',\nu')\|^2 = F^2(u,\nu)\,\gamma_u^2 t^2 F(u+\nu,-u-\nu)$$

$$= t^2\,\frac{\gamma_{u+\nu}^2}{\gamma_u^2\gamma_\nu^2}\,\gamma_u^2\,\frac{1}{\gamma_{u+\nu}^2} \qquad \text{(by Theorem 2.2R)}$$

$$= t^2\,\frac{1}{\gamma_\nu^2} = t^2 F(\nu,-\nu) = \|(t,\nu)\|^2.$$

Theorem 5.1C: Complex boosts preserve the norm.

Proof: Let $(t',\nu')=B(u)(t,\nu)$. Then,

$$(t',\nu')=B(u)(t,\nu)=(\gamma_u,u)\cdot(t,\nu)=(F(u,\nu)\,\gamma_u t, u+\nu)$$

and, hence,

$$\begin{aligned}\|(t',\nu')\|^2 &= |F^2(u,\nu)\gamma_u^2 t^2| F(u+\nu,-u-\nu)\\ &= |t|^2 \frac{\gamma_{u+\nu}^2}{\gamma_u^2\gamma_\nu^2}\,\gamma_u^2\,\frac{1}{\gamma_{u+\nu}^2} \qquad \text{(by Theorem 2.2C)}\\ &= |t|^2 \frac{1}{\gamma_\nu^2} = |t|^2 F(\nu,-\nu) = \|(t,\nu)\|^2.\end{aligned}$$

Theorem 5.2R: The real boost composition law is given by the equation

$$B(u)B(\nu) = B(u+\nu)\mathrm{Gyr}[u;\nu]. \tag{5.6}$$

Proof: Let $(\mathbb{R}^+\times P,\cdot)$ be the gyrogroup over a gyrogroup $(P,+,F)$ with a real cocycle form F. Then

$$\begin{aligned}B(u)B(\nu)(t,w) &= (\gamma_u,u)\cdot((\gamma_\nu,\nu)\cdot(t,w))\\ &= (\gamma_u,u)\cdot(F(\nu,w)\gamma_\nu t,\nu+w)\\ &= (F(u,\nu+w)F(\nu,w)\gamma_u\gamma_\nu t, u+(\nu+w))\\ &= (F(\nu+u,w)F(u,\nu)\gamma_u\gamma_\nu t,(u+\nu)+\mathrm{gyr}[u;\nu]w) \quad \text{[by (C1)]}\\ &= (F(\nu+u,w)\gamma_{u+\nu}t,(u+\nu)+\mathrm{gyr}[u;\nu]w) \qquad \text{(by Theorem 2.2.R)}\\ &= (F(\mathrm{gyr}[u;\nu](\nu+u),\ \mathrm{gyr}[u;\nu]w)\gamma_{u+\nu}t,(u+\nu)+\mathrm{gyr}[u;\nu]w)\\ &= (F(u+\nu,\ \mathrm{gyr}[u;\nu]w)\gamma_{u+\nu}t,(u+\nu)+\mathrm{gyr}[u;\nu]w)\\ &= (\gamma_{u+\nu},u+\nu)\cdot(t,\mathrm{gyr}[u;\nu]w)\\ &= (\gamma_{u+\nu},u+\nu)\cdot\mathrm{Gyr}[u;\nu](t,w)\\ &= B(u+\nu)\mathrm{Gyr}[u;\nu](t,w)\end{aligned}$$

for all $(t,w)\in(\mathbb{R}^+\times P,\cdot)$, as desired.

Similarly to the definition of π_2 in (4.8), we now define the map π_1 from transformations A of $\mathbb{C}$ into transformations $\pi_1(A)$ of $\mathbb{C}^+\times P$ by the equation

$$\pi_1(A)(t,\nu) = (At,\nu). \tag{5.7}$$

Similarly to Eq. (4.7), we define the map tGyr : $P\times P\to\mathrm{Aut}(\mathbb{C}^+\times P)$ by the equation

$$\mathrm{tGyr}[u;\nu] = \pi_1(\mathrm{tgyr}[u;\nu]). \tag{5.8}$$

Theorem 5.2C: The complex boost composition law is given by the equation

$$B(u)B(\nu) = B(u+\nu)\mathrm{tGyr}[u;\nu]\mathrm{Gyr}[u;\nu]. \tag{5.9}$$

Proof: Let $(\mathbb{C}^+\times P,\cdot)$ be a gyrogroup over $(P,+,F)$ with a complex cocycle form F.

We should remark here that the definition of $(\mathbb{C}^+\times P,\cdot)$ over $(P,+,F)$ for F complex is analogous to the definition of $(\mathbb{R}^+\times P,\cdot)$ over $(P,+,F)$ for real F in Definition 4.1. The resulting complex gyrogroup $(\mathbb{C}^+\times P,\cdot)$ satisfies all the gyrogroup axioms with one exception; it does not obey the gyrocommutative law. Thus, as opposed to the real gyrogroup $(\mathbb{R}^+\times P,\cdot)$ over $(P,+,F)$, its complex counterpart is a groupoid that may be called a nongyrocommutative gyrogroup.

Then we have

$$
\begin{aligned}
B(u)B(v)(t,w) &= (\gamma_u,u)\cdot((\gamma_v,v)\cdot(t,w)) \\
&= (\gamma_u,u)\cdot(F(v,w)\gamma_v t, v+w) \\
&= (F(u,v+w)F(v,w)\gamma_u\gamma_v t, u+(v+w)) \\
&= (F(v+u,w)F(u,v)\gamma_u\gamma_v t,(u+v)+\mathrm{gyr}[u;v]w) \quad [\text{by (C1)}] \\
&= (F(v+u,w)\gamma_{u+v}\,\mathrm{tgyr}[u;v]t,(u+v)+\mathrm{gyr}[u;v]w) \\
&\qquad\qquad (\text{by Theorem 2.2C}) \\
&= (F(\mathrm{gyr}[u;v](v+u),\mathrm{gyr}[u;v]w)\gamma_{u+v}\,\mathrm{tgyr}[u;v]t,(u+v)+\mathrm{gyr}[u;v]w) \\
&= (F(u+v,\ \mathrm{gyr}[u;v]w)\gamma_{u+v}\,\mathrm{tgyr}[u;v]t,(u+v)+\mathrm{gyr}[u;v]w) \\
&= (\gamma_{u+v},u+v)\cdot(\mathrm{tgyr}[u;v]t,\mathrm{gyr}[u;v]w) \\
&= (\gamma_{u+v},u+v)\cdot\mathrm{tGyr}[u;v]\mathrm{Gyr}[u;v](t,w) \\
&= B(u+v)\mathrm{tGyr}[u;v]\mathrm{Gyr}[u;v](t,w)
\end{aligned}
$$

for all $(t,w)\in(\mathbb{C}^+\times P,\cdot)$, as desired.

It is clear from Theorems 5.2R and 5.2C that the boost inverse to $B(u)$ is $B(-u)$. These theorems reveal an important distinction between real and complex boosts. While real boost compositions produce only space gyrations, complex boost compositions produce both space gyrations and time gyrations. As a result, in Sec. VII, real Lorentz transformations will be parametrized by two parameters, while complex Lorentz transformations will be parametrized by three parameters.

Definition 5.3 (Gyrogroup automorphisms): Let $(P,+,F)$ be a gyrogroup with a cocycle form. An *automorphism* A of $(P,+,F)$ is a bijection of P that respects $+$ and preserves F, that is, $A(a+b)=Aa+Ab$ and $F(Aa,Ab)=F(a,b)$ for any $a,b\in P$. The set of all automorphisms of $(P,+,F)$ forms a group denoted by $\mathrm{Aut}(P,+,F)$. Subgroups of $\mathrm{Aut}(P,+,F)$ containing all the gyrations $\mathrm{gyr}[a;b]$ of $P(a,b\in P)$ are denoted generically by $\mathrm{Aut}_0(P,+,F)$.

Theorem 5.3: Boosts ''commute'' with automorphisms according to the equation

$$\pi_2(A)B(u)=B(Au)\pi_2(A).$$

Proof: Let $\mathbb{F}^+$ denote either $\mathbb{R}^+$ or $\mathbb{C}^+$, let $(\mathbb{F}^+\times P,\cdot)$ be the real or complex space–time (forward cone) gyrogroup over a gyrogroup $(P,+,F)$ with a real or complex cocycle form F, and let $u\in P$ and $A\in\mathrm{Aut}(P,+,F)$. Then for any $(t,w)\in(\mathbb{F}^+\times P,\cdot)$ we have

$$
\begin{aligned}
\pi_2(A)B(u)(t,w) &= \pi_2(A)(\gamma_u,u)\cdot(t,w) \\
&= \pi_2(A)(F(u,w)\gamma_u t,u+w) \\
&= (F(u,w)\gamma_u t,A(u+w)) \\
&= (F(Au,Aw)\gamma_{Au}t,Au+Aw) \\
&= ((\gamma_{Au},Au)\cdot(t,Aw)) \\
&= B(Au)\pi_2(A)(t,w),
\end{aligned}
$$

and, hence, the result.

VI. THE GYROSEMIDIRECT PRODUCT GROUP

Definition 6.1 (The gyrosemidirect product): Let $(P,+)$ be a gyrogroup, the gyrooperator of which is denoted by gyr, and let $\mathrm{Aut}_0(P,+)$ be a subgroup of its automorphism group containing all its gyrations. The *gyrosemidirect product group*

$$(P,+)\times_g \mathrm{Aut}_0(P,+) \tag{6.1}$$

is a group of pairs $(a,A)\in P\times \mathrm{Aut}_0(P,+)$ with composition law given by

$$(a,A)(b,B)=(a+Ab,\mathrm{gyr}[a;Ab]AB). \tag{6.2}$$

It is anticipated in Definition 6.1 that the gyrosemidirect product (6.2) is a group operation in the Cartesian product $P\times\mathrm{Aut}_0(P,+)$ of a gyrogroup $P=(P,+)$ and an automorphism group. To show that this is indeed the case, we view any pair

$$(a,A)\in(P,+)\times_g\mathrm{Aut}_0(P,+) \tag{6.3}$$

as a bijection of P, given by

$$(a,A)x=a+Ax \tag{6.4}$$

for any $x\in P$. The inverse of the bijection (a,A) is clearly $(-A^{-1}a,A^{-1})$. The gyrosemidirect product (6.2) then emerges as a bijection composition and, hence, a group operation:

$$\begin{aligned}(a,A)(b,B)x&=(a,A)(b+Bx)\\&=a+A(b+Bx)\\&=a+(Ab+ABx)\\&=(a+Ab)+\mathrm{gyr}[a;Ab]ABx\\&=(a+Ab,\mathrm{gyr}[a;Ab]AB)x\end{aligned} \tag{6.5}$$

for all $x\in P$.

A slightly different gyrosemidirect product, that will be used with the complex Lorentz group, is the following.

Definition 6.2 (The complex gyrosemidirect product): Let $(P,+,F)$ be a gyrogroup with a complex cocycle form F, and let gyr and tgyr be its gyro-operator and its time gyro-operator, respectively. Moreover, let $\mathbb{C}_0$ be the group of all unimodular complex numbers. The *complex gyrosemidirect product*

$$(P,+,F)\times_g\{\mathbb{C}_0\times\mathrm{Aut}_0(P,+,F)\} \tag{6.6}$$

is a group of triples $(a,\alpha,A)\in P\times\mathbb{C}_0\times\mathrm{Aut}_0(P,+,F)$ with composition law given by

$$(a,\alpha,A)(b,\beta,B)=(a+Ab,\mathrm{tgyr}[a;Ab]\alpha\beta,\mathrm{gyr}[a;Ab]AB). \tag{6.7}$$

We are now in a position to present the real (complex) Lorentz transformation groups acting on the real (complex) space–time $(\mathbb{F}^+\times P,\cdot)$ over a gyrogroup $P=(P,+,F)$ with a real (complex) cocycle form F.

VII. ABSTRACT REAL AND COMPLEX LORENTZ TRANSFORMATION GROUPS

Our approach to the study of Lorentz groups by relativistic velocity spaces and the gyrogroups to which they give rise emphasizes analogies shared with Galilei relativity. These analogies are

partially summarized in the introductory section of Ref. 8. In particular, a $(1+n)$-dimensional Lorentz group in our approach appears as the gyrosemidirect product (see Sec. VI) of (i) a velocity gyrogroup and (ii) a rotation group. This is in full analogy with the $(1+n)$-dimensional Galilei group which is known to be the semidirect product of (i) a velocity group and (ii) a rotation group.

Our new approach became possible following the discovery in Ref. 1 of the symmetries concealed in Thomas precession, the abstraction of which is called Thomas gyration allowing us to introduce the prefix ''gyro.'' Following our approach to employ analogies shared with Galilean relativity and symmetries hidden in Thomas gyration, we treat the time coordinate on a different footing from the space coordinates, as we commonly do in Galilean relativity. Hence, in particular, the pair (t,ν) represents a (generalized) time–space as explained in Eq. (5.4), and should not be confused with the common energy-momentum space of STR. The pair (t,ν) represents a ''generalized'' or an ''abstract'' time–space in the sense that ν is an element of an abstract gyrogroup rather than a three-dimensional velocity.

Using techniques developed in the previous sections we generalize in this section results that were obtained in Refs. 7 and 8 for some special gyrogroups.

Definition 7.1R (The real Lorentz transformation): Let $(\mathbb{R}^+\times P,\cdot)$ be the space–time gyrogroup over a gyrogroup $(P,+,F)$ with a real cocycle form F, and let $\mathrm{Aut}_0(P,+,F)$ be a subgroup of $\mathrm{Aut}(P,+,F)$ containing all the gyroautomorphisms of P. For any $(u,U)\in(P,+,F)\times_g \mathrm{Aut}_0(P,+,F)$, the *real Lorentz transformation* $L\{u;U\}$ acting on the space–time $(\mathbb{R}^+\times P,\cdot)$ is given by

$$L\{u;U\}=B(u)\pi_2(U).$$

It follows from Definitions 5.1 and 6.1 that

$$\begin{aligned} L\{u;U\}(t,\nu)&=B(u)\pi_2(U)(t,\nu)\\ &=(\gamma_u,u)\cdot(t,U\nu)\\ &=(F(u,U\nu)\gamma_u t,u+U\nu) \end{aligned} \tag{7.1R}$$

for any $u\in(P,+,F)$, $U\in\mathrm{Aut}_0(P,+,F)$ and $(t,\nu)\in(\mathbb{R}^+\times P,\cdot)$.

Theorem 7.1R: Real Lorentz transformations preserve the norm.

Proof: By definition, the real Lorentz transformation

$$L\{u;U\}\ :\ (\mathbb{R}^+\times P,\cdot)\to(\mathbb{R}^+\times P,\cdot)$$

is given by a boost preceded by an automorphism,

$$L\{u;U\}=B(u)\pi_2(U).$$

Both $B(u)$ and $\pi_2(U)$ preserve the squared norm $\|(t,\nu)\|^2=t^2F(\nu,-\nu)$ in $(\mathbb{R}^+\times P,\cdot)$: $B(u)$ preserves the norm by Theorem 5.1R, and $\pi_2(U)$ preserves the norm, since it preserves the cocycle form $F(\nu,-\nu)$ by Definition 5.3. The proof is thus complete.

Theorem 7.2R (The real Lorentz transformation composition law):

The real Lorentz transformations of the space–time $(\mathbb{R}^+\times P,\cdot)$ over a gyrogroup $(P,+,F)$ with a real cocycle form, form a group with group operation given by

$$L\{u;U\}L\{\nu;V\}=L\{u+U\nu,\mathrm{gyr}[u;U\nu]UV\} \tag{7.2R}$$

for any $u,\nu\in P$ and $U,V\in\mathrm{Aut}(P,+,F)$.

Proof: Let $(\mathbb{R}^+\times P,\cdot)$ be a space–time gyrogroup over the gyrogroup $(P,+,F)$ with a real cocycle form F, and let $u,\nu\in P$ and $U,V\in\mathrm{Aut}(P,+,F)$. Then, the product of two successive real Lorentz transformations of $(\mathbb{R}^+\times P,\cdot)$ is

$$
\begin{aligned}
L\{u;U\}L\{\nu;V\} &= B(u)\pi_2(U)B(\nu)\pi_2(V) \\
&= B(u)B(U\nu)\pi_2(UV) && \text{(by Theorem 5.3)} \\
&= B(u+U\nu)\mathrm{Gyr}[u;U\nu]\pi_2(UV) && \text{(by Theorem 5.2R)} \\
&= B(u+U\nu)\pi_2(\mathrm{gyr}[u;U\nu]UV) \\
&= L\{u+U\nu);\mathrm{gyr}[u;U\nu]UV),
\end{aligned}
$$

as desired.

Theorem 7.2R presents the real Lorentz transformation composition law in terms of parameter composition, where the parameter composition is the gyrosemidirect product (6.2). Unlike its real counterpart, the complex Lorentz transformation involves three parameters.

Definition 7.1C (The complex Lorentz transformation):

Let $(\mathbb{C}^+\times P,\cdot)$ be the space–time gyrogroup over a gyrogroup $(P,+,F)$ with a complex cocycle form F, and let $\mathrm{Aut}_0(P,+,F)$ be a subgroup of $\mathrm{Aut}(P,+,F)$ containing all the gyroautomorphisms of P. For any $(u,\alpha,U)\in(P,+,F)\times_g\{\mathbb{C}_0\times\mathrm{Aut}_0(P,+,F)\}$, the *complex Lorentz transformation* $L\{u;\alpha;U\}$ acting on the space–time $(\mathbb{C}^+\times P,\cdot)$ is given by

$$L\{u;\alpha;U\}=B(u)\pi_1(\alpha)\pi_2(U).$$

It follows from Definitions 5.1 and 6.2 that

$$L\{u;\alpha;U\}(t,\nu)=B(u)\pi_1(\alpha)\pi_2(U)(t,\nu)=(\gamma_u,u)\cdot(\alpha t,U\nu)=(F(u,U\nu)\gamma_u\alpha t,u+U\nu) \tag{7.1C}$$

for any $u\in(P,+,F)$, $\alpha\in\mathbb{C}_0$, $U\in\mathrm{Aut}_0(P,+,F)$ and $(t,\nu)\in(\mathbb{C}^+\times P,\cdot)$.

Theorem 7.1C: Complex Lorentz transformations preserve the norm.

Proof: By definition, the complex Lorentz transformation

$$L\{u;\alpha;U\}\ :\ (\mathbb{C}^+\times P,\cdot)\to(\mathbb{C}^+\times P,\cdot)$$

is given by a boost preceded by two automorphisms of $(\mathbb{C}^+\times P,\cdot)$,

$$L\{u;\alpha;U\}=B(u)\pi_1(\alpha)\pi_2(U).$$

All $B(u)$, $\pi_1(\alpha)$ and $\pi_2(U)$ preserve the squared norm $\|(t,\nu)\|^2=|t|^2F(\nu,-\nu)$ in $(\mathbb{C}^+\times P,\cdot)$: $B(u)$ preserves the norm by Theorem 5.1C, $\pi_1(\alpha)$ preserves the norm since $\alpha\in\mathbb{C}_0$, and $\pi_2(U)$ preserves the norm since U preserves the cocycle form $F(\nu,-\nu)$ by Definition 5.3. The proof is thus complete.

Theorem 7.2C (The complex Lorentz transformation composition law): The complex Lorentz transformations of a complex space–time $(\mathbb{C}^+\times P,\cdot)$ over a gyrogroup $(P,+,F)$ form a group with group operation given by

$$L\{u;\alpha;U\}L\{\nu;\beta;V\}=L\{u+U\nu;\mathrm{tgyr}[u;U\nu]\alpha\beta;\mathrm{gyr}[u;U\nu]UV\} \tag{7.2C}$$

for any $u,\nu\in P$, $\alpha,\beta\in\mathbb{C}_0$, and $U,V\in\mathrm{Aut}(P,+,F)$.

Proof: Let $(\mathbb{C}^+\times P,\cdot)$ be the space–time gyrogroup over a gyrogroup $(P,+,F)$ with a complex cocycle form F, and let $u,\nu\in P$ and $U,V\in\mathrm{Aut}(P,+,F)$. Then, the product of two successive real Lorentz transformations of $(\mathbb{C}^+\times P,\cdot)$ is

$$
\begin{aligned}
L\{u;\alpha;U\}L\{\nu;\beta;V\} &= B(u)\pi_1(\alpha)\pi_2(U)B(\nu)\pi_1(\beta)\pi_2(V) \\
&= B(u)B(U\nu)\pi_1(\alpha\beta)\pi_2(UV) && \text{(by Theorem 5.3)} \\
&= B(u+U\nu)\mathrm{tGyr}[u;U\nu]\mathrm{Gyr}[u;U\nu]\pi_1(\alpha\beta)\pi_2(UV) && \text{(by Theorem 5.2C)} \\
&= B(u+U\nu)\pi_1(\mathrm{tgyr}[u;U\nu]\alpha\beta)\pi_2(\mathrm{gyr}[u;U\nu]UV \\
&= L\{u+U\nu;\mathrm{tgyr}[u;U\nu]\alpha\beta;\mathrm{gyr}[u;U\nu]UV\}
\end{aligned}
$$

as desired.

Theorem 7.2C presents the complex Lorentz transformation composition law in terms of parameter composition, where the parameter composition is the complex gyrosemidirect product (6.7). Unlike its real counterpart, the complex Lorentz transformation involves three parameters.

VIII. GROUP-THEORETICAL INTERPRETATION

The constructions used in this paper may be interpreted in terms of group theory. The group-theoretical interpretation is analogous in some ways to the useful interpretation of complex numbers $a+ib$ as 2×2 matrices

$$
\begin{pmatrix} a & -b \\ b & a \end{pmatrix}.
$$

Using this interpretation one may reduce complex analysis to matrix theory. For example, the square of the absolute value becomes the determinant, the real part is half the trace, and conjugation is matrix transposition. Of course, one does not normally view the complex numbers in this way since the matrix notation is excessively cumbersome for the purposes of complex analysis. By the same token, the gyrogroup approach, as presented in this article, is the most direct and convenient for computations in STR. In particular, the gyrogroup formalism stays very close to the familiar formalism of abelian groups. Thus the useful group-theoretical interpretation is of more purely mathematical interest.[16,17]

Specifically, our basic idea is to view the abstraction of the well-known relation

$$
\frac{(1-(u\oplus\nu))^2}{(1-u^2)(1-\nu^2)} = \frac{1}{(1+u\cdot\nu)^2}
$$

in STR, where $\oplus$ is the relativistic velocity addition (3.2), as a cocycle identity, Eq. (2.2); that is, the squared *coboundary* on the left is equal to the squared cocycle on the right. This identity is the fundamental relation used to extend the velocity addition law into a Lorentz transformation. In fact, this extension can be recast using the language of cohomologically trivial central extension of the Lorentz group. Furthermore, the present work may also have applications to areas of mathematical physics outside the foundations of special relativity, since it involves a new approach to polar decompositions and their relation to Grassmann varieties which occur frequently in various twistor constructions. As illustrative examples, we show below the relationship between our Theorems 4.1 and 2.2R and common group-theoretical considerations.

The gyrosemidirect product of Definition 6.1 shows how to embed a gyrogroup P into a group $G=P\times_g \mathrm{Aut}_0(P)$, a subgroup of the group $\widetilde{G}=P\times_g \mathrm{Aut}(P)$. The inversion map $J : P\to P$, $x\to -x$ is an automorphism of P, and conjugation by the element $(0, J)$ of $\widetilde{G}$ gives an involutory automorphism ϕ of G. Setting $P_0=\{(x, I)|x\in P\}$ and $K=\{(0, A)|A\in \mathrm{Aut}_0(P)\}$, one has $\phi(x,I)=(x,I)^{-1}$, $G=P_0K$, $P\cap K=\{(0, I)\}$, and P_0 is invariant under conjugation by elements of K. Moreover, elements of K are fixed by ϕ.

Conversely, consider a group G with an involutory automorphism ϕ. Suppose that $G=P_0K$ with $P_0\cap K=\{I\}$. Suppose that the elements of K are fixed points of ϕ. Suppose ϕ acts on P_0 by $\phi : P_0\to P_0;\ x\to x^{-1}$, and suppose that P_0 is invariant under conjugation by elements of K. Suppose x,y in P imply xyx in P_0, and suppose that $P_0\to P_0;\ x\to x^2$ is bijective, with two-sided inverse $x\to\sqrt{x}$. Then P becomes a gyrogroup $(P,+)$ under $x+y=\sqrt{x}y\sqrt{x}$. Indeed, for $xy=(x+y)k$, one has $\mathrm{gyr}[x;y]z=kzk^{-1}$.[17]

Now embed a gyrogroup P in a gyrosemidirect product group G, $G=PK$ as above. Since the inverse of a gyration is a gyration, the group generated by gyrations is just the set of products of gyrations. Thus the cocycle form $F : P\times P\to\mathbb{R}^+$ satisfying the gyroinvariance may be extended to a cocycle form on G by $F(\phi_1k_1,\phi_2k_2)=F(\phi_1,k_1\phi_2k_1^{-1})$. By the standard theory of central extensions for groups,[18] one obtains a central extension $\hat{G}$ of G by $\mathbb{R}^+$. The extension gyrogroup $(\mathbb{R}^+\times P,\cdot)$ of Theorem 4.1 may then be recovered from the extension group $\hat{G}$ as above. Conversely, if $(\mathbb{R}^+\times P,\cdot)$ is a gyrogroup, then $(P,+)$ is, too, by virtue of being a quotient. Theorem 2.2R corresponds to the case where the exact sequence

$$1\to\mathbb{R}^+\to\hat{G}\to G\to 1$$

splits.

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Comment on: The Itzykson–Zuber integral for $U(m|n)$ [J. Math. Phys. 36, 3085–3093 (1995)]

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In their recent work, Alfaro, Medina, and Urrutia evaluate the supersymmetric version of the Harish–Chandra–Itzykson–Zuber (HCIZ) integral[1,2] by generalizing the diffusion equation method of Itzykson and Zuber.[2] This integral is of considerable interest in quantum chaos and the theory of random matrices. In the case $n=m$, this integral was already calculated,[3] also by generalizing the diffusion equation method of Ref. 2. By using this integral, a new derivation of the correlation functions of the Gaussian unitary ensemble (GUE) was given which can be viewed as an irreducible integral representation.[3] For the discussion of transitions between ensembles, those integrals are the essential tool. By applying the ordinary HCIZ integral, Mehta and Pandey[4] calculated all correlations for the statistical model of gradually broken time reversal invariance. Employing the supersymmetric HCIZ integral, the correlations for the statistical model of a gradually broken quantum number were evaluated in Ref. 5.

After the angular integration over the unitary group, usually further integrations over the eigenvalues, i.e., the s-variables in Refs. 3 and 5 or the λ-variables in the work of Alfaro, Medina, and Urrutia, are required. Here, two important remarks are in order: First, all permutations in the determinant yield the same result because of the antisymmetry of the integration measure of the eigenvalues. This is why one needs only the trace term if further integrations are required.[3] Second, boundary contributions to the integral emerge which have no counterparts in the ordinary case. In Ref. 3, the most important one of those, the Efetov–Wegner term[6,7] was given. In the case of the group $U(1|1)$, a complete formula was constructed[8] using a very general theory developed by Rothstein.[9]

Obviously, the supersymmetric HCIZ has much to do with harmonic analysis in superspaces. For the group $U(1|1)$, graded or super spherical harmonics were derived[10] in which anticommuting indices formally play the role of an angular momentum. The corresponding representations in terms of graded or super Wigner functions were discussed in Ref. 11. In the general case $U(k_1|k_2)$, such representations involving anticommuting indices were constructed in Ref. 12 by generalizing the Gelfand–Tzetlin method to supersymmetry. These results have also been used in Ref. 12 to evaluate the supersymmetric HCIZ integral for $n\neq m$, including all permutation and exchange terms.

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Reply to the Comment on: The Itzykson–Zuber integral for $U(m|n)$

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This note is to observe that the integral (B3) calculated in the Appendix B of Ref. 1 is not the supersymmetric IZ integral for the particular case $m=n$, but it rather corresponds to the expression that survives when the IZ integral is subsequently integrated over all the eigenvalues and after some symmetry properties are taken into account. Since some applications do not require a further integration over the eigenvalues, the difference between the two expressions is of basic importance.

The above remark is most easily illustrated with the standard IZ integral, in the case of ordinary $n\times n$ matrices. In this situation, the result given in Eq. (B3) of Ref. 1 would read

$$\int \exp\left(-\frac{1}{2t}\mathrm{tr}(\sigma-\rho)^2\right)d\mu(V)=A\frac{t^{n(n-1)/2}}{\Delta(R)\Delta(S)}\exp\left(-\frac{1}{2t}\mathrm{tr}(S-R)^2\right), \tag{1}$$

where $\Delta(R)$ denotes the Vandermonde determinant of the eigenvalues. The numerical constant A is independent of t and also of the eigenvalues. From the above expression we would conclude, according to Ref. 1, that the IZ integral is given by

$$\int \exp\left(\frac{1}{t}\mathrm{tr}(RVSV^{-1})\right)d\mu(V)=A\frac{t^{n(n-1)/2}}{\Delta(R)\Delta(S)}\exp\left(\frac{1}{t}\mathrm{tr}(RS)\right). \tag{2}$$

Nevertheless, we know from Ref. 2 that the correct answer for this integral is

$$\int \exp\left(\frac{1}{t}\mathrm{tr}(RVSV^{-1})\right)d\mu(V)=B\frac{t^{n(n-1)/2}}{\Delta(R)\Delta(S)}\det\left(\exp\frac{1}{t}r_i s_j\right). \tag{3}$$

The left-hand side of Eq. (2) corresponds only to the diagonal term in the expansion of the complete determinant which produces the correct answer in Eq. (3). Only under a further integration over all the eigenvalues, can the remaining n^2-1 terms reduce to the diagonal one. In other words, the result (1) is correct only under a symmetric integration over the eigenvalues

$$\int \exp\left(-\frac{1}{2t}\mathrm{tr}(\sigma-\rho)^2\right)d\mu(V)\Delta^2(R)d[R]=A\frac{t^{n(n-1)/2}}{\Delta(S)}\int \exp\left(-\frac{1}{2t}\mathrm{tr}(S-R)^2\right)\Delta(R)d[R]. \tag{4}$$

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An analogous situation occurs in the supersymmetric case, when comparing the expression (B3) of Ref. 1 with the formula (9) of Ref. 3, in the case $m=n$.

Summarizing, even though the methods used by Guhr and the authors coincide, the results obtained are different in the same sense that the corresponding calculations of Ref. 2 and 4 are not equivalent to each other. Besides, nowhere in Ref. 1 can the expression for the supersymmetric IZ integral, given in Eq. (9) of Ref. 3, be found, even for the particular case $m=n$.

In relation to the interesting observation of Ref. 1 about the existence of Efetov–Wegner terms, we only observe that such terms will appear when the supersymmetric IZ integral is further integrated over the eigenvalues. They reflect the existence of singularities due to the contribution of the Berezinian, which need to be regularized. If the regulator chosen is not explicitly supersymmetric, the Efetov–Wegner terms will be needed to restore a supersymmetric result.

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Antisymmetric tensor fields on spheres: Functional determinants and non-local counterterms

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The Hodge–de Rham Laplacian on spheres acting on antisymmetric tensor fields is considered. Explicit expressions for the spectrum are derived in a quite direct way, confirming previous results. Associated functional determinants and the heat kernel expansion are evaluated. Using this method, new non-local counterterms in the quantum effective action are obtained, which can be expressed in terms of Betti numbers. © *1996 American Institute of Physics.* [S0022-2488(96)02507-8]

I. INTRODUCTION

Modern interest in antisymmetric tensor fields is connected with supergravity theories where these fields appear as members of a supermultiplet. Kaluza–Klein compactification of higher dimensional supergravities leads to backgrounds of the form $S^d \times R^4$, where S^d is the d-dimensional sphere. Quantum effects on such backgrounds were considered e.g. in Refs. 1,2. Some general mathematical statements about p-forms—very useful in this context—can be found in the monography by Gilkey.[3] Typically, the action for an antisymmetric tensor field B reads as

$$S = \int \sqrt{g} dx F_{ij\ldots k} F^{ij\ldots k}, \quad F = dB, \tag{1}$$

where d denotes external differentiation of forms. The action (1) for the p-form B^p is invariant under gauge transformations,

$$B^p \to B^p + dB^{p-1}. \tag{2}$$

All quantum corrections in a theory described by the action (1), including the contribution of ghosts, can be expressed in terms of determinants of the Hodge–de Rham Laplacian,

$$\Delta_{HdR} = -(d^*d + dd^*). \tag{3}$$

The spectrum of Δ_{HdR} is the same for p- and $(d\text{-}p)$-forms. Consequently, it is enough to evaluate the determinant of Δ_{HdR} for $p \leqslant d/2$. Due to the gauge invariance under the transformation (2) and to the factorization property,

$$\det_p(-\Delta_{HdR}) = \det_{pT}(-\Delta_{HdR}) \times \det_{(p-1)T}(-\Delta_{HdR}) \tag{4}$$

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—where the subscript T means that the determinant is taken over the space of transversal forms—we can restrict our considerations to transversal p-forms. We will assume in all those expressions, as in (4), that zero modes (harmonic p-forms) are excluded from the determinants.

In Sec. II we will obtain the spectrum of the Hodge–de Rham Laplace operator on the unit sphere S^d, for any dimension d, acting on transversal p-forms. In Sec. III we will calculate explicitly the determinants for the sphere, and in Sec. IV the heat kernel coefficients. A complete list will be given up to $d=7$, a dimension that is important in the compactification of supersymmetric theories. Finally, a discussion on the transversal Laplacian and non-local counterterms will be provided in Sec. V. It is proven there that the heat kernel expansion for the Hodge–de Rham Laplacian on transversal p-forms contains a constant term, even in the case of odd-dimensional spaces. The new non-local counterterms in the quantum effective action will be expressed in terms of Betti numbers.

II. SPECTRUM OF THE LAPLACE OPERATOR

In this section we define the spectrum of the Laplace operator Δ_{HdR} on the unit sphere S^d acting on transversal p-forms. For $p=0,1$ this spectrum is well known[4]:

$$b_l^0=-l(l+d-1), \quad D_l^0=\frac{(2l+d-1)(l+d-2)!}{l!(d-1)!}, \quad l=0,1,2,\ldots,$$
$$b_l^1=-l(l+d-1)+2-d, \quad D_l^1=\frac{l(l+d-1)(2l+d-1)(l+d-3)!}{(d-2)!(l+1)!}, \quad l=1,2,3,\ldots, \tag{5}$$

where b_l^p denote the eigenvalues and D_l^p their degeneracies. For higher forms the spectrum of the Laplace operator on S^d can be obtained by using standard group theoretical techniques.[5–7]

For any homogeneous space G/H a field Φ_A belonging to an irreducible representation $D(H)$ can be expanded as[8]

$$\Phi_A(x)=V^{-\frac{1}{2}}\sum_{n,\zeta,q}\sqrt{\frac{d_n}{d_D}}D^{(n)}_{A\zeta,q}(g_x^{-1})\phi^{(n)}_{q,\zeta}, \tag{6}$$

where V is the volume of G/H and $d_D=$ dim $D(H)$. We sum over representations $D^{(n)}$ of G which give $D(H)$ after reduction to H. Here ζ labels the multiple components $D(H)$ in the branching $D^{(n)}\downarrow H$, $d_n=$ dim $D^{(n)}$. The matrix elements of $D^{(n)}$ have the following orthogonality property

$$\int_{G/H}dx\sqrt{g}D^{(n)*}_{A\zeta,q}(g_x^{-1})D^{(n')}_{A\xi,p}(g_x^{-1})=Vd_n^{-1}d_D\delta_{\zeta\xi}\delta_{pq}\delta_{nn'}. \tag{7}$$

Consider, for example, the case when $d=5$: $S^5=SO(6)/SO(5)$. The representations $D(H)=D(SO(5))$ describing antisymmetric tensors are just antisymmetric tensor powers of the vector representation of $SO(5)$:

$$p=0, \quad D(SO(5))=[0,0], \quad p=1, \quad D(SO(5))=[1,0],$$
$$p=2, \quad D(SO(5))=[1,1], \quad p=3, \quad D(SO(5))=[1,1]. \tag{8}$$

We label the representations by their Dynkin indices in square brackets. Notice that we use here the slightly non-standard definition of the Dynkin indices from the book by Barut and Raezka.[9] These indices are more convenient for the reduction of representations. Owing to duality, the representations in the last two lines of (8) are equivalent.

In order to construct the harmonic expansion (6) one must find all the representations of $SO(6)$ which give the representations (8) after reduction to $SO(5)$. For a given irreducible representation $[q_1,q_2]$ of $SO(5)$ with integer Dynkin indices q_1 and q_2, the representations $[m_1,m_2,m_3]$ of $SO(6)$ containing $[q_1,q_2]$ are defined by the conditions[9]

$$m_1 \geqslant q_1 \geqslant m_2 \geqslant q_2 \geqslant |m_3|, \tag{9}$$

where all m_A are integers and m_1 and m_2 are non-negative. Any representation satisfying the nonequality (9) contains the single representation $[q_1,q_2]$. Summation over ζ in (6) may be omitted. One can easily find all the representations of $SO(6)$ that are needed

$$\begin{gathered} p=0,\ D^{(l)}(SO(6))=[l,0,0],\ \ l=0,1,\ldots, \\ p=1,\quad D^{(l)}(SO(6))=[l,1,0],\ \ l=1,2,\ldots=[l,0,0], l=1,2,\ldots, \\ p=2,3,\quad D^{(l)}(SO(6))=[l,1,0],\ \ l=1,2,\ldots,=[l,1,1], l=1,2,\ldots,=[l,1,-1], l=1,2,\ldots\ . \end{gathered} \tag{10}$$

External differentiation maps transversal $p-1$ forms to longitudinal p-forms. This mapping can be traced back to the corresponding spherical harmonics. Hence, for the transversal forms only the following representations contribute to the harmonic expansion:

$$\begin{gathered} p=0,\quad D^{(l)}(SO(6))=[l,0,0], \\ p=1,\quad D^{(l)}(SO(6))=[l,1,0], \\ p=2,\quad D^{(l)}(SO(6))=[l,1,1],=[l,1,-1], \\ p=3,\quad D^{(l)}(SO(6))=[l,1,0], l=1,2,3,\ldots\ . \end{gathered} \tag{11}$$

The scalar mode with $l=0$ belongs to the kernel of the Laplace operator and should be regarded as a harmonic zero-form.

In the space of p-forms there are two main second-order differential operators, namely the Hodge–de Rham Laplacian, $-\Delta_{HdR}=dd^*+d^*d$, and the ordinary Laplacian, $\Delta=\nabla^i\nabla_i$. On the sphere S^d these two operators differ by a constant, namely

$$-\Delta_{HdR}=\Delta+p^2-dp. \tag{12}$$

In any homogeneous space G/H the Laplace operators can be expressed in terms of the quadratic Casimir operators of G and H:

$$\Delta=C_2(G)-C_2(H), -\Delta_{HdR}=C_2(G). \tag{13}$$

Using the harmonic expansion (11), (8), and standard expressions[9] for the Casimir operators in (13), we obtain the eigenvalues b_l^p of the Laplace operator Δ_{HdR} acting on transversal p-forms on S^5. The corresponding degeneracies D_l^p are equal to the dimensions of the representations of $SO(6)$.

$$\begin{gathered} b_l^2=-l(l+4)-4,\quad D_l^2=\frac{1}{2}l(l+1)(l+3)(l+4),\quad l=1,2,\ldots, \\ b_l^3=-l(l+4)-3,\quad D_l^3=\frac{1}{3}l(l+2)^2(l+4),\quad l=1,2,\ldots\ . \end{gathered} \tag{14}$$

For $p=0,1$ our result coincides with (5). Other spheres can be dealt with along the same lines. For $d=3$ we have:

$$b_l^2=-l(l+2), \quad D_l^2=(l+1)^2, \quad l=1,2,\ldots \ . \tag{15}$$

For $d=4$:

$$b_l^2=-l(l+3)-2, \quad D_l^2=\frac{1}{2}l(2l+3)(l+3), \quad l=1,2,\ldots \ . \tag{16}$$

For $d=6$:

$$b_l^2=b_l^3=-l(l+5)-6, \quad D_l^2=D_l^3=\frac{1}{12}l(l+1)(l+4)(l+5)(2l+5), \quad l=1,2,3,\ldots \ . \tag{17}$$

For $d=7$:

$$\begin{aligned} b_l^2&=-l(l+6)-8, \quad D_l^2=\frac{1}{24}l(l+1)(l+3)^2(l+5)(l+6), \\ b_l^3&=-l(l+6)-9, \quad D_l^3=\frac{1}{18}l(l+1)(l+2)(l+4)(l+5)(l+6), \quad l=1,2,3,\ldots \ . \end{aligned} \tag{18}$$

Owing to duality, the spectrum of Δ_{HdR} on transversal 4-forms on S^7 is the same as on longitudinal 3-forms. The latter one coincides with that on transversal 2-forms. Continuing in this way, one can define the spectrum for higher values of p. The remarkable property of equivalence of the spectra for $p=2$ and $p=3$ on S^6 holds only for transversal forms. In the above equations we have listed some spectra for $p>d/2$. They are useful in some applications not considered in this paper. For example, they are needed for the computation of the spectrum of the Laplacian on a ball.[10,7,11]

There is a general function for the eigenvalues and their multiplicities, which have been obtained above for some particular cases. It is the following:

$$\begin{aligned} D_l(d,p)&=\frac{(2l+d-1)(l+d-1)!}{p!(d-p-1)!(l-1)!(l+p)(l+d-p-1)}, \\ b_l(d,p)&=-l(l+d-1)-p(d-p-1). \end{aligned} \tag{19}$$

These equations can be obtained by means of lengthy but straightforward calculations repeating step by step the above derivation of the spectrum on S^5. All group theoretical techniques that are needed can be learned from Chaps. 9 and 10 of Ref. 9. Note that an explicit derivation for the case of the ordinary Laplacian had been carried out, e.g., in Ref. 5, and that previous results already existed in the mathematical literature.[12,13] Our method is similar to the one in the papers.[12,13] However, explicit expressions for the eigenvalues and degeneracies can be found in Ref. 5 only, where reduction of the harmonic polynomials from R^{d+1} was used. It is noticeable that a mistake in previous calculations was reported in Ref. 5, which shows that the computation is not trivial at all. It thus seems useful to present an alternative derivation of the spectrum, which turns out to be in complete agreement with Ref. 5 Note that the eigenvalues of the Laplace operator on transversal p-forms are denoted in Ref. 5 by ${}^{p+1}\lambda_k$, where $k=l-1=0,1,\ldots$.

III. CALCULATION OF THE DETERMINANTS FOR THE SPHERE

Here we are going to calculate the determinants corresponding to the Hodge–de Rham Laplacian on spheres of different dimensions, $d=2,3,4,5,6,7$, and for forms of different orders $p=1,2,3,4$. We shall make use of the formulas (see above)

$$\det(-\Delta_{HdR})^{(d)}=\det(-\Delta_{HdR})_{p^T}^{(d)}\times\det(-\Delta_{HdR})_{(p-1)^T}^{(d)}, \tag{20}$$

and employ the definition of determinant through the zeta function of the corresponding operator, that is

$$\det A=\exp(-\zeta_A'(0)). \tag{21}$$

Owing to the multiplicative property of the determinant—which is obviously fulfilled for the operators we are going to consider (see Ref. 14 for a discussion of more general cases)—at the level of the zeta functions the product in (20) transforms into a sum of the corresponding zeta functions (even before taking the derivative). We shall arrange our calculations according to this observation. The general methods employed in Refs. 15,16 will be used (see Ref. 17 for more references to these techniques). Related calculations have been carried out in Ref. 18.

Using the general formulas (19) for the spectrum and its degeneracy, one can write the expression of the zeta function corresponding to a p-form in any dimension d $(p\leqslant(d+1)/2)$, namely

$$\begin{aligned}\zeta_{-\Delta_{p^T}^{(d)}}(s)&=\sum_{l=1}^{\infty}D_l(d,p)[-b_l(d,p)]^{-s}\\&=\frac{1}{p!(d-p-1)!}\sum_{l=1}^{\infty}\frac{(2l+d-1)(l+d-1)!}{(l-1)!(l+p)(l+d-p-1)}\left[\left(l+\frac{d-1}{2}\right)^2-\left(p-\frac{d-1}{2}\right)^2\right]^{-s}.\end{aligned} \tag{22}$$

To continue, we notice that the degeneracy is a polynomial in l of order $d-1$, and we expand it in powers of $l+(d-1)/2$:

$$D_l(p,d)=\sum_{\alpha=0}^{d-1}e_\alpha(d,p)\left(l+\frac{d-1}{2}\right)^\alpha. \tag{23}$$

Formally, we can write

$$e_\alpha=\frac{1}{\alpha}\frac{d^\alpha}{dl^\alpha}D_l(p,d)|_{l=(1-d/2)}. \tag{24}$$

The sum over l can be evaluated easily, e.g.

$$\begin{aligned}\zeta_{-\Delta_{p^T}^{(d)}}(s)&=\sum_{\alpha=0}^{d-1}e_\alpha(d,p)\sum_{l=1}^{\infty}\left(l+\frac{d-1}{2}\right)^\alpha\left[\left(l+\frac{d-1}{2}\right)^2-\left(p-\frac{d-1}{2}\right)^2\right]^{-s}\\&=\sum_{\alpha=0}^{d-1}e_\alpha(d,p)\sum_{l=1}^{\infty}\left(l+\frac{d-1}{2}\right)^{\alpha-2s}[1-[p-(d-1)/2]^2[l+(d-1)/2]^2]^{-s}\\&=\frac{1}{\Gamma(s)}\sum_{\alpha=0}^{d-1}e_\alpha(d,p)\sum_{k=0}^{\infty}\frac{\Gamma(k+s)}{k!}\left(p-\frac{d-1}{2}\right)^{2k}\zeta_H\left(2s+2k-\alpha,\frac{d+1}{2}\right),\end{aligned} \tag{25}$$

where we have used the binomial expansion. Note that this expansion is absolutely convergent, since $[p-(d-1)/2]^2/[l+(d-1)/2]^2<1$ for $p\leqslant(d+1)/2$. The indetermined number 0^0 when $p=(d-1)/2$ is consistently defined to be one. Here $\zeta_H(s,\nu)$ is the Hurwitz zeta-function. For ν a natural number, this zeta-function can be directly related to the Riemann zeta-function through the formula[15–17]

$$\zeta_H(s,m)=\zeta_R(s)-\sum_{l=1}^{m} l^{-s}. \tag{26}$$

For ν a half-integer, we can correspondingly subtract terms from $\zeta_H(s,1/2)$, which is again related to the Riemann zeta-function,

$$\zeta_H(s,1/2)=(2^s-1)\zeta_R(s). \tag{27}$$

For d even, $e_\alpha=0$ for $\alpha=0,2,\ldots,d-2$, and for d odd, $e_\alpha=0$ for $\alpha=1,3,\ldots,d-2$. When we differentiate the zeta-function (25) we must distinguish between these two cases. For d odd, we get

$$\zeta'_{-\Delta_{pT}^{(d)}}(0)=\sum_{a=0}^{(d-1)/2} e_{2a}\left[2\zeta'_H\left(-2a,\frac{d+1}{2}\right)+\sum_{k=1}^{\infty}\frac{[p-(d-1)/2]^{2k}}{k}\zeta_H\left(2k-2a,\frac{d+1}{2}\right)\right]. \tag{28}$$

While for d even the expression is a bit more complicated since the Hurwitz zeta-function has a pole when its argument is one. Using the Laurent series expansion

$$\zeta_H(2s+1,\nu)=\frac{1}{2s}-\Psi(\nu)+\mathcal{O}(s), \tag{29}$$

we obtain, for d even,

$$\begin{aligned}\zeta'_{-\Delta_{pT}^{(d)}}(0)=\sum_{a=0}^{\frac{d}{2}-1} e_{2a+1}\Bigg[&2\zeta'_H\left(-2a-1,\frac{d+1}{2}\right)+\sum_{k=1}^{a}\frac{[p-(d-1)/2]^{2k}}{k}\zeta_H\left(2k-2a-1,\frac{d+1}{2}\right)\\&+\frac{(p-(d-1)/2)^{2a+2}}{a+1}\left(\frac{1}{2}\sum_{l=1}^{a} l^{-1}-\Psi\left(\frac{d+1}{2}\right)\right)\\&+\sum_{a+2}^{\infty}\frac{[p-(d-1)/2]^{2k}}{k}\zeta_H\left(2k-2a-1,\frac{d+1}{2}\right)\Bigg].\end{aligned} \tag{30}$$

Continuing in this way and substituting for the derivatives of the Riemann zeta function the values[19]

$$\begin{gathered}\zeta'(0)=-\frac{1}{2}\ln(2\pi),\zeta'(-1)=-0.1654211437,\zeta'(-2)=-0.0304484571,\\ \zeta'(-3)=0.0053785764,\zeta'(-4)=0.0079838115,\\ \zeta'(-5)=-0.0005729860,\zeta'(-6)=-0.0058997591,\ldots,\end{gathered} \tag{31}$$

we have obtained the following numerical results for the determinants:

$$\det(-\Delta_{HdR})_4^{(7)}=0.088786,\det(-\Delta_{HdR})_3^{(7)}=0.088786,\det(-\Delta_{HdR})_2^{(7)}=1.858601,$$

$$\det(-\Delta_{HdR})_1^{(7)}=0.775194,\det(-\Delta_{HdR})_3^{(6)}=7.103758,\det(-\Delta_{HdR})_2^{(6)}=1.726306,$$

$$\det(-\Delta_{HdR})_1^{(6)}=0.835544,\det(-\Delta_{HdR})_3^{(5)}=11.090330,\det(-\Delta_{HdR})_2^{(5)}=11.090330, \quad (32)$$

$$\det(-\Delta_{HdR})_1^{(5)}=0.581303,\det(-\Delta_{HdR})_2^{(4)}=0.128002,\det(-\Delta_{HdR})_1^{(4)}=0.621433,$$

$$\det(-\Delta_{HdR})_2^{(3)}=0.095528,\det(-\Delta_{HdR})_1^{(3)}=0.095528,\det(-\Delta_{HdR})_1^{(2)}=10.210016.$$

IV. CALCULATION OF THE HEAT KERNEL COEFFICIENTS

The heat-kernel coefficients B_k are given from the small$-t$ expansion of the heat kernel $K(t)$,

$$K(t)=(4\pi t)^{-d/2}\sum_{k=0,1/2,1,\ldots} B_k t^k. \quad (33)$$

When we consider a manifold without boundaries, as is the case for the sphere, the coefficients with a half-integer k vanish. There is a close connection between the coefficients for an operator and its zeta-function. This connection is given by the formulas

$$\mathrm{Res}\zeta(s)=\frac{B_{d/2-s}}{(4\pi)^{d/2}\Gamma(s)}, \quad (34)$$

at $s=m/2,(m-1)/2,\ldots,1/2;-(2l+1)/2$ for $l=0,1,2\ldots$, and

$$\zeta(-m)=(-1)^m m!\frac{B_{d/2+m}}{(4\pi)^{d/2}}, \quad (35)$$

for $m=0,1,2,\ldots$. These formulas constitute a very powerful approach to the determination of the heat kernel coefficients (see, for instance, Refs. 20,21 and the references therein). Again we consider separately the cases d odd and d even. When d is odd we only have to calculate the residues, since there are only integer coefficients. The residues matching integer coefficients are located at $s=d/2-m$, $m=0,1,2\ldots$. When $m\leqslant(d-1)/2$,

$$\mathrm{Res}\zeta_{-\Delta_{p^T}^{(d)}}\left(\frac{d}{2}-m\right)=\frac{1}{2}\sum_{a=(d-1)/2-m}^{(d-1)/2} e_{2a}\frac{\Gamma(1/2+a)}{\Gamma(d/2-m)(1-d)/2+m+a)!}\left(p-\frac{d-1}{2}\right)^{1-d+2m+2a}, \quad (36)$$

and when $m>(d-1)/2$,

$$\mathrm{Res}\zeta_{-\Delta_{p^T}^{(d)}}\left(\frac{d}{2}-m\right)=\frac{1}{2}\sum_{a=0}^{(d-1)/2} e_{2a}\frac{\Gamma(1/2+a)}{\Gamma\left(\frac{d}{2}-m\right)(1-d)/2+m+a)!}\left(p-\frac{d-1}{2}\right)^{1-d+2m+2a}. \quad (37)$$

For even dimension we must consider the point values at $s=-m$ and the residues at $s=d/2-l$, $l=0,1,\ldots,d/2-1.$,

$$\zeta_{-\Delta_{p^T}^{(d)}}(-m)=\sum_{a=0}^{d/2-1} e_{2a+1}\left[\sum_{k=0}^{m}\frac{(-1)^k m!}{(m-k)!k!}\left(p-\frac{d-1}{2}\right)^{2k}\zeta_H\left(2k-2a-1-2m,\frac{d+1}{2}\right)\right.$$
$$\left.+\frac{(-1)^m m!a!}{2(1+a+m)!}\left(p-\frac{d-1}{2}\right)^{2+2a+2m}\right], \tag{38}$$

and we get

$$\mathrm{Res}\zeta_{-\Delta_{p^T}^{(d)}}\left(\frac{d}{2}-l\right)=\frac{1}{2}\sum_{a=d/2-1-l}^{d/2-1} e_{2a+1}\frac{a!}{\Gamma\left(\frac{d}{2}-l\right)\left(1-\frac{d}{2}+l+a\right)!}\left(p-\frac{d-1}{2}\right)^{2-d+2a+2l}. \tag{39}$$

As the actual zeta-functions are sums of the zeta-functions for the transversal field, the heat kernel coefficients are also just sums of the corresponding coefficients for the transversal fields. Using the two equations (34) and (35) we immediately obtain the coefficients from the formulas given above.

For $d=7$, $p=4$ and $p=3$, we have

$$B_0=\frac{35\,\pi^4}{3},B_1=\frac{-175\,\pi^4}{3},B_2=\frac{2009\pi^4}{18},B_3=\frac{-553\,\pi^4}{6},B_4=\frac{159\,\pi^4}{8},B_5=\frac{167\pi^4}{24},$$
$$B_6=\frac{1289\pi^4}{720},B_7=\frac{613\pi^4}{1680},B_8=\frac{71\pi^4}{1152},B_9=\frac{461\pi^4}{51840},B_{10}=\frac{271\pi^4}{241920}. \tag{40}$$

For $d=7$, $p=2$:

$$B_0=7\,\pi^4,B_1=-21\,\pi^4,B_2=\frac{133\pi^4}{10},B_3=\frac{371\pi^4}{30},B_4=\frac{-229\pi^4}{40},B_5=\frac{-1213\pi^4}{120},$$
$$B_6=\frac{-2807\pi^4}{720},B_7=\frac{6483\pi^4}{2800},B_8=\frac{132847\pi^4}{28800}, \tag{41}$$
$$B_9=\frac{1050881\pi^4}{259200},B_{10}=\frac{3147083\pi^4}{1209600}.$$

For $d=7$, $p=1$:

$$B_0=\frac{7\,\pi^4}{3},B_1=\frac{7\,\pi^4}{3},B_2=\frac{-301\pi^4}{90},B_3=\frac{-203\pi^4}{30},B_4=\frac{-43\pi^4}{40},B_5=\frac{949\pi^4}{120},$$
$$B_6=\frac{6839\pi^4}{720},B_7=\frac{9823\pi^4}{8400},B_8=\frac{-282271\pi^4}{28800},B_9=\frac{-3734393\pi^4}{259200}, \tag{42}$$
$$B_{10}=\frac{-3734393\pi^4}{403200}.$$

For $d=6$, $p=3$:

$$B_0=\frac{64\,\pi^3}{3},B_1=\frac{-256\,\pi^3}{3},B_2=128\,\pi^3,B_3=\frac{-75008\pi^3}{945},B_4=\frac{1472\pi^3}{135},B_5=\frac{256\pi^3}{99},$$

$$B_6=\frac{373376\pi^3}{405405},B_7=\frac{40448\pi^3}{81081},B_8=\frac{1373248\pi^3}{3828825}, \tag{43}$$

$$B_9=\frac{167651072\pi^3}{535687425},B_{10}=\frac{65263383424\pi^3}{206239658625}.$$

For $d=6$, $p=2$:

$$B_0=16\,\pi^3,B_1=-48\,\pi^3,B_2=\frac{128\,\pi^3}{3},B_3=\frac{176\pi^3}{315},B_4=\frac{-48\,\pi^3}{5},B_5=\frac{-1360\pi^3}{297},$$

$$B_6=\frac{-171328\pi^3}{405405},B_7=\frac{80096\pi^3}{81081},B_8=\frac{37236464\pi^3}{34459425}, \tag{44}$$

,

$$B_9=\frac{52062832\pi^3}{59520825},B_{10}=\frac{2616564224\pi^3}{3618239625}.$$

For $d=6$, $p=1$:

$$B_0=\frac{32\,\pi^3}{5},B_1=0,B_2=\frac{-128\pi^3}{15},B_3=\frac{-1408\pi^3}{315},B_4=\frac{352\pi^3}{75},$$

$$B_5=\frac{11008\pi^3}{1485},B_6=\frac{5982208\pi^3}{2027025},B_7=\frac{-164096\pi^3}{57915}, \tag{45}$$

$$B_8=\frac{-952002848\pi^3}{172297125},B_9=\frac{-337870336\pi^3}{72747675},$$

$$B_{10}=\frac{-8650820224\pi^3}{4464061875}.$$

For $d=5$, $p=3$ and $p=2$:

$$B_0=10\,\pi^3,B_1=\frac{-80\,\pi^3}{3},B_2=\frac{70\,\pi^3}{3},B_3=\frac{-14\,\pi^3}{3},B_4=\frac{-29\pi^3}{18},B_5=\frac{-37\pi^3}{90},$$

$$B_6=-\frac{\pi^3}{12},B_7=\frac{-53\pi^3}{3780},B_8=\frac{-61\pi^3}{30240},B_9=\frac{-23\pi^3}{90720},B_{10}=\frac{-11\pi^3}{388800}. \tag{46}$$

For $d=5$, $p=1$:

$$B_0=5\,\pi^3,B_1=\frac{-10\,\pi^3}{3},B_2=\frac{-10\,\pi^3}{3},B_3=\frac{2\,\pi^3}{3},B_4=\frac{35\pi^3}{18},B_5=\frac{91\pi^3}{90},$$

$$B_6=\frac{-\pi^3}{12},B_7=\frac{-2101\pi^3}{3780},B_8=\frac{-3289\pi^3}{6048},B_9=\frac{-32791\pi^3}{90720},B_{10}=\frac{-104873\pi^3}{544320}. \tag{47}$$

For $d=4$, $p=2$:

$$B_0=16\,\pi^2, B_1=-32\,\pi^2, B_2=\frac{304\pi^2}{15}, B_3=\frac{-160\pi^2}{63}, B_4=\frac{-176\pi^2}{315}, B_5=\frac{-608\pi^2}{3465},$$
$$B_6=\frac{-11104\pi^2}{135135}, B_7=\frac{-448\pi^2}{8775}, B_8=\frac{-443504\pi^2}{11486475}, \tag{48}$$
$$B_9=\frac{-467045792\pi^2}{13749310575}, B_{10}=\frac{-2327539744\pi^2}{68746552875}.$$

For $d=4$, $p=1$:

$$B_0=\frac{32\,\pi^2}{3}, B_1=\frac{-32\,\pi^2}{3}, B_2=\frac{-32\pi^2}{45}, B_3=\frac{352\pi^2}{189}, B_4=\frac{928\pi^2}{945},$$
$$B_5=\frac{1952\pi^2}{10395}, B_6=\frac{-38848\pi^2}{405405}, B_7=\frac{-262336\pi^2}{2027025}, \tag{49}$$
$$B_8=\frac{-3454688\pi^2}{34459425}, B_9=\frac{-3024736672\pi^2}{41247931725}, B_{10}=\frac{-12244948288\pi^2}{206239658625}.$$

For $d=3$, $p=2$ and $p=1$:

$$B_0=6\,\pi^2, B_1=-6\,\pi^2, B_2=\pi^2, B_3=\frac{\pi^2}{3}, B_4=\frac{\pi^2}{12}, B_5=\frac{\pi^2}{60},$$
$$B_6=\frac{\pi^2}{360}, B_7=\frac{\pi^2}{2520}, B_8=\frac{\pi^2}{20160}, B_9=\frac{\pi^2}{181440}, B_{10}=\frac{\pi^2}{1814400}. \tag{50}$$

And for $d=2$, $p=1$:

$$B_0=8\,\pi, B_1=\frac{-16\,\pi}{3}, B_2=\frac{8\,\pi}{15}, B_3=\frac{32\,\pi}{315}, B_4=\frac{8\,\pi}{315}, B_5=\frac{32\,\pi}{3465},$$
$$B_6=\frac{3056\,\pi}{675675}, B_7=\frac{1856\,\pi}{675675}, B_8=\frac{22664\,\pi}{11486475}, B_9=\frac{4481632\,\pi}{2749862115}, B_{10}=\frac{104409808\,\pi}{68746552875}. \tag{51}$$

V. TRANSVERSAL LAPLACIAN AND NON-LOCAL COUNTERTERMS

In this section we see that the heat kernel expansion for the Hodge–de Rham Laplacian on transversal p-forms contains a constant term in odd–dimensional spaces. Call $\kappa(t)=\Sigma_{k=1}^{\infty}\exp(-tk^2)$. The asymptotic behavior of κ in the limit $t\to 0$ is $\kappa(t)=\frac{1}{2}(\sqrt{(\pi/t)}-1)$, where corrections are exponentially small and can be neglected in the computation of power-low asymptotics. The transversal heat kernel,

$$K(t;p,d)=\sum_{l=1}^{\infty} D_l(p,d)\exp[tb_l(p,d)], \tag{52}$$

on odd-dimensional spheres can be put in terms of κ using D_l and b_l of Sec. 2:

$$K(t;0,3)=-1-\kappa'(t),$$

$$K(t;1,3)=-2[\kappa'(t)+\kappa(t)],$$

$$K(t;0,5)=-1+\frac{1}{12}e^{4t}[\kappa''(t)+\kappa'(t)],$$

$$K(t;1,5)=1+\frac{1}{3}e^{t}[\kappa''(t)+4\kappa'(t)],$$

$$K(t;2,5)=\frac{1}{2}[\kappa''(t)+5\kappa'(t)+4\kappa(t)], \tag{53}$$

$$K(t;0,7)=-1-\frac{e^{9t}}{360}[\kappa'''(t)+5\kappa''(t)+4\kappa'(t)],$$

$$K(t;1,7)=1-\frac{e^{4t}}{60}[\kappa'''(t)+10\kappa''(t)+9\kappa'(t)],$$

$$K(t;2,7)=-1-\frac{e^{t}}{24}[\kappa'''(t)+13\kappa''(t)+36\kappa'(t)],$$

$$K(t;3,7)=-\frac{1}{18}[\kappa'''(t)+14\kappa''(t)+41\kappa'(t)+36\kappa(t)],$$

where the prime denotes differentiation. One can evaluate the coefficient $a_{d/2}$ before t^0 in the small-t expansion of $K(t;p,d)$. Derivatives of κ do not contribute and one obtains

$$a_{d/2}=(-1)^{p+1}. \tag{54}$$

At first sight this relation contradicts the general theory[22] of the heat kernel, which precludes integer powers of t on odd-dimensional manifolds without boundary. In fact, the relation (54) is well known and can be derived from general formulae.[22] Consider an odd-dimensional manifold M without boundary. The space of p-forms, Λ^p can be decomposed in a direct sum of eigenspaces of the Hodge–de Rham Laplacian:

$$\Lambda^p=\Lambda^{pT}\oplus\Lambda^{pL}\oplus H^p, \tag{55}$$

where Λ^T and Λ^L are transversal and longitudinal p-forms, respectively. H^p denotes the space of harmonic p-forms spanned by zero modes of the Hodge–de Rham Laplacian. The Laplace operator on *all* p-forms satisfies the whole set of requirements in Ref. 22 and, hence, the corresponding coefficient in front of t^0 in the heat kernel expansion should vanish. On the other hand, this coefficient is just the sum of the coefficients in front of t^0 for the same operator restricted to the spaces on the right hand side of (55). But this immediately gives

$$0=a^p_{d/2}+a^{p-1}_{d/2}+\beta_p, \tag{56}$$

where, as above, $a_{d/2}$ denotes the constant term in the heat kernel expansion for transversal p-forms. Here $\beta_p=$ dim H^p is the Betti number. For 0-forms we have

$$a^0_{d/2} = -\beta_0 . \tag{57}$$

The two equations (56) and (57) can be solved, giving

$$a^p_{d/2} = \sum_{q=0}^{p} (-1)^{p-q+1} \beta_q . \tag{58}$$

The relation (54) is a particular case of (58). What happens in odd dimensions is that the Betti numbers ''propagate'' up the chain leading to the formula (58).

Consider now the quantum path integral for an antisymmetric tensor field with the action (1). The partition function Z_p can be expressed in terms of the determinants of the Hodge–de Rham Laplacian on transversal forms[23,24]

$$Z_p = \prod_{q=0}^{p} \det{}_{qT}(-\Delta_{HdR})^{-(1/2)(-1)^{p-q}}. \tag{59}$$

To avoid possible ambiguities in treating the zero modes we suppose that $\beta_p = 0$. The ''total'' heat kernel for Z_p is an alternated sum of heat kernels for transversal forms. As the coefficient multiplying t^0 leads to a logarithmic divergence in the path integral, on an odd-dimensional manifold without boundary, we have that this divergence is proportional to

$$\sum_{q=0}^{p} (p-q+1)(-1)^{p-q+1} \beta_q . \tag{60}$$

Such divergence cannot be canceled by means of an integral of a local invariant constructed from the Riemann tensor and, hence, it requires a non–local counterterm. Some topological effects in quantum theories of antisymmetric tensor field were discussed in Ref. 24 These effects are, however, related to the Gauss–Bonnet term, which can be expressed in the function of local densities and vanishes for odd-dimensional spheres. In the context of three-dimensional Chern–Simons theory, Eq. (58) has been obtained in Ref. 25.

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Proper time and path integral representations for the commutation function

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On the example of the quantized spinor field, interacting with arbitrary external electromagnetic field, the commutation function is studied. It is shown that a proper time representation is available in any dimensions. Using it, all the light cone singularities of the function are found explicitly, generalizing the Fock formula in four dimensions, and a path integral representation is constructed. © *1996 American Institute of Physics.* [S0022-2488(96)03806-6]

I. INTRODUCTION

It is known that the solution of quantum field theory problems involves as a rule different singular functions, e.g., commutation functions, Green functions, and so on. These functions are well studied for free fields (see, for example, Ref. 1). Problems appear when an interaction is presented. In particular, it is important to study singular functions in external backgrounds such as external fields and curved spaces and in arbitrary dimensions. The latter may be important for multidimensional version of field theories, which are considered now in relation with the unification of all the interactions. One ought to say that the commutation functions play an important role in QFT with external backgrounds. In contrast with the case without external backgrounds, the perturbation theory, which takes into account a background exactly, uses complicated (matrix) propagators. Such propagators contain as component parts, besides the causal and anticausal Green functions, the commutation functions as well.[2,3] Here, we present proper time and path integral representations for the commutation function and for some related functions in external fields. On the basis of the proper time representation we study, in particular, light cone singularities of the function in arbitrary dimensions. Traditionally QED is a testing ground where new procedures and methods are worked through, not infrequently creating new ideas and more profound understanding of the structure of QFT. That is why we consider here the case of QED with an arbitrary external electromagnetic field, bearing in mind that the results can be extend to other theories and backgrounds.

Fock for the first time[4] introduced an integral over the proper time to present the regular on the light cone part of the commutation function $S(x,x')$ (in $3+1$ dimensions) of the spinor fields, interacting with an external electromagnetic field $A_\mu(x)$,

$$S(x,x') = i[\psi(x), \overline{\psi}(x')]_+ , \tag{1}$$

where $\psi(x)$ and $\overline{\psi}(x')$ are the electron–positron field operators. This function obeys the Dirac equation

$$\begin{gathered}(\hat{\mathscr{P}}_\nu \gamma^\nu - m) S(x,x') = 0, \quad \hat{\mathscr{P}}_\nu = i\partial_\nu - g A_\nu(x), \\ [\gamma^\mu, \gamma^\nu]_+ = 2\eta^{\mu\nu}, \quad \eta^{\mu\nu} = \mathrm{diag}(1,-1,-1,-1),\end{gathered} \tag{2}$$

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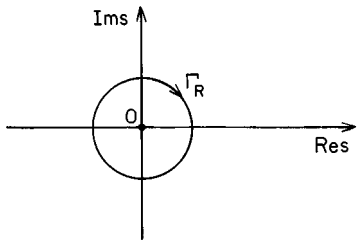

FIG. 1. Contour of integration for Δ_R function.

and the initial condition

$$S(x,x')|_{x_0=x_0'}=i\gamma^0\delta(\mathbf{x}-\mathbf{x}'). \tag{3}$$

The commutation function $S(x,x')$ is at the same time the propagation function of the Dirac equation, i.e., it connects solutions $\psi(x)$ of the equation in two different time instants,

$$\psi(x_0,\mathbf{x})=-i\int S(x,x')\gamma^0\psi(x_0',\mathbf{x}')d\mathbf{x}'. \tag{4}$$

Thus the Cauchy problem can be solved by means of the function. Squaring Eq. (2) one gets

$$S(x,x')=(\hat{\mathscr{P}}_\nu\gamma^\nu+m)\Delta(x,x'), \tag{5}$$

where the function $\Delta(x,x')$ obey the equation

$$[(\hat{\mathscr{P}}_\nu\gamma^\nu)^2-m^2]\Delta(x,x')=0, \tag{6}$$

and the initial conditions

$$\Delta(x,x')|_{x_0=x_0'}=0, \quad \partial_0\Delta(x,x')|_{x_0=x_0'}=\delta(\mathbf{x}-\mathbf{x}'). \tag{7}$$

Fock's solution of Eqs. (6) and (7) reads

$$\begin{gathered}\Delta(x,x')=\epsilon(x_0-x_0')\left[\Theta((x-x')^2)\Delta_R(x,x')+\frac{1}{2\pi}e^{ig\Lambda}\delta((x-x')^2)\right],\\ \epsilon(x_0-x_0')=\mathrm{sign}(x_0-x_0').\end{gathered} \tag{8}$$

The function Λ is the line integral of the potentials,

$$\Lambda=-\int_{x'}^{x}A_\mu(\tilde{x})d\tilde{x}^\mu; \tag{9}$$

$\Delta_R(x,x')$ is the Riemann function, which is presented by means of a proper time integral

$$\Delta_R(x,x')=\int_{\Gamma_R}f(x,x',s)ds \tag{10}$$

over the closed path Γ_R, (see Fig. 1) which is a clockwise circle around the point $s=0$ with a small enough radius, inside of which the function $f(x,x',s)$ has not any singularities besides the essential singularity $s=0$. The function $f(x,x',s)$ obeys the ''Schrödinger equation''

$$i\frac{d}{ds}f(x,x',s)=[m^2-(\hat{\mathscr{P}}_\nu\gamma^\nu)^2]f(x,x',s), \tag{11}$$

and the boundary condition

$$\lim_{s\to+0} f(x,x',s)=i\delta(x-x'). \tag{12}$$

One has to remark that the same function $f(x,x',s)$ appears in the Schwinger representation[5] for the causal Green function $S^c(x,x')$ (propagator) of the Dirac equation,

$$(\hat{\mathscr{P}}_\nu\gamma^\nu-m)S^c(x,x')=-\delta(x-x'). \tag{13}$$

Namely,

$$S^c(x,x')=(\hat{\mathscr{P}}_\nu\gamma^\nu+m)\int_0^\infty f(x,x',s)ds, \tag{14}$$

where at $s\to\infty$ one has to enter into the complex plane s, so that $\lim_{s\to\infty} f(x,x',s)=0$. Extension of the Schwinger representation to the curved space case was made by DeWitt[2] and then, developing his technics, to the gauge theory.[6]

The Schwinger representation for $S^c(x,x')$ and the Fock representation for $S(x,x')$ differ essentially in sense of possibilities of generalization. Thus the Schwinger representation retains its form for any space–time dimensionality d. Moreover, the inverse operator S^c can be easily presented via an exponent by means of the Schwinger proper time representation (super-proper time representation[7]), so that the path integral representations follows.[7,8] At the same time the Fock representation has the specific form (8) for $\Delta(x,x')$ in $d=3+1$. Besides, the form (8), which separates the light cone singular part from the regular one, does not give any leading consideration to write a path integral for the commutation function, similar to one for the propagator.

Below we propose a proper time representation for the commutation function, which has an universal form in any dimensions. Using it, we find explicitly all the light cone singularities of the commutation function in arbitrary dimensions, generalizing the Fock's formula (8). Moreover, such a representation allows one to write a path integral for the commutation function. In the conclusion we present similar representations for some other singular functions of the Dirac equation on the basis of the results obtained.

II. PROPER TIME REPRESENTATION FOR THE COMMUTATION FUNCTION

Here, we are going to write a proper time representation for the function $\Delta(x,x')$ from formula (5) in arbitrary space–time dimensions $d\geqslant 2$. To this end we need to find first the behavior of the function $f(x,x',s)$ at $s\to 0$. We will use Eqs. (11) and (12) in d-dimensions, where

$$[\gamma^\mu,\gamma^\nu]_+=2\eta^{\mu\nu},\quad \eta^{\mu\nu}=\mathrm{diag}\underbrace{(1,-1,\ldots,-1)}_{d}.$$

Similar to Schwinger[5] we present $f(x,x's)$ as a matrix element of an evolution operator $U(s)$,

$$\begin{aligned} f(x,x',s)&=i\langle x|U(s)|x'\rangle,\\ U(s)&=e^{-iHs},\quad H=m^2-(\Pi_\nu\gamma^\nu)^2, \end{aligned} \tag{15}$$

where $|x\rangle$ are eigenfunctions for some hermitian operators of coordinates X^μ, the corresponding canonically conjugate operators of momenta are P_μ, so that

$$X^\mu|x\rangle = x^\mu|x\rangle, \quad \langle x|x'\rangle = \delta(x-x'), \quad \int |x\rangle\langle x|dx = I,$$

$$[P_\mu, X^\nu]_- = -i\delta_\mu^\nu, \quad \langle x|P_\mu|x'\rangle = -i\partial_\mu\delta(x-x'), \tag{16}$$

$$\Pi_\mu = -P_\mu - gA_\mu(X), \quad [\Pi_\mu, \Pi_\nu]_- = -igF_{\mu\nu}(X), \quad F_{\mu\nu}(X) = \partial_\mu A_\nu(X) - \partial_\nu A_\mu(X).$$

The matrix element obeys the conditions

$$\left(i\frac{\partial}{\partial x^\mu} - gA_\mu(x)\right)\langle x|U(s)|x'\rangle = \langle x|\Pi_\mu U(s)|x'\rangle,$$

$$\left(-i\frac{\partial}{\partial x'^\mu} - gA_\mu(x')\right)\langle x|U(s)|x'\rangle = \langle x|U(s)\Pi_\mu|x'\rangle. \tag{17}$$

Introducing the operators

$$X^\mu(s) = U^{-1}(s)X^\mu U(s), \quad \gamma^\mu(s) = U^{-1}(s)\gamma^\mu U(s), \quad \Pi_\mu(s) = U^{-1}(s)\Pi_\mu U(s),$$

we come to the equations

$$\frac{d}{ds}X^\mu(s) = i[H, X^\mu(s)]_- = 2\Pi^\mu(s),$$

$$\frac{d}{ds}\gamma^\mu(s) = i[H, \gamma^\mu(s)]_-, \quad \frac{d}{ds}\Pi_\mu(s) = i[H, \Pi_\mu(s)]_-. \tag{18}$$

Using the decomposition in powers of s, one can get for H

$$H = -\frac{1}{4s}[X(s)X(s) - 2X(s)X(0) - X(0)X(0)] - i\frac{d}{2s} + O(1).$$

Then the solution of Eqs. (11), (12), and (17) has a form

$$f(x,x',s)|_{s\to 0} = f_0(x,x',s)[1+O(s)],$$

$$f_0(x,x',s) = \frac{1}{(4\pi s)^{d/2}}\exp\left\{-i\frac{\pi}{4}(d-4) + ig\Lambda - \frac{i}{4s}(x-x')^2\right\}, \tag{19}$$

where Λ is the d-dimensional line integral (9). Thus one can conclude that $f(x,x',s)$ has no singularities in a small enough neighborhood of the point $s=0$ (excluding this point). Based on this one can make a key observation in $3+1$ dimensions. Namely, let us consider the Fock representation (5) and (8) beyond the light cone $(x-x')^2 \neq 0$. In this case the relation holds

$$\Theta((x-x')^2)\int_{\Gamma_R} f(x,x',s)ds = \int_\Gamma f(x,x',s)ds, \tag{20}$$

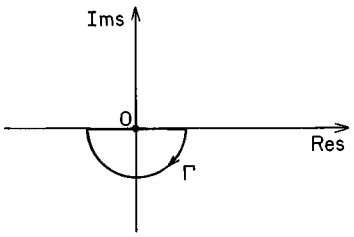

FIG. 2. Contour of integration for Δ function.

where Γ (see Fig. 2) is a contour, which connects the points $s=+0$ and $s=e^{-i\pi}0$, and passes in the lower part of complex plane s in a small enough neighborhood of the point $s=0$ so that Eq. (19) is still valid inside the contour Γ. Then the function $\Delta(x,x')$ can be written in $3+1$ dimensions at $(x-x')^2\neq 0$ in the following form:

$$\Delta(x,x')=\epsilon(x_0-x_0')\int_\Gamma f(x,x',s)ds. \tag{21}$$

It turns out that Eq. (21) is valid on the light cone as well and, moreover, in any dimensions. Below we are going to prove this statement.

First of all one can remark that Eq. (19) implies

$$\lim_{s\to e^{-i\pi_0}} f(x,x',s)=-i\delta(x-x'). \tag{22}$$

Together with Eqs. (11), (12), and (22) this allows one to verify that expression (21) obeys Eq. (6) at $x_0\neq x_0'$.

Now we have to study the behavior of function (21) at $x_0\to x_0'$. Using the representation (19) let us select all the light cone singularities in Eq. (21),

$$\Delta(x,x')=I_R(x,x')+\sum_{n=0}^{[d/2]-1} I^{(n)}(x,x'), \tag{23}$$

$$I_R(x,x')=\epsilon(x_0-x_0')\int_\Gamma f_R(x,x',s)ds, \tag{24}$$

$$f_R(x,x',s)=f(x,x',s)-\sum_{n=0}^{[d/2]-1} f^{(n)}(x,x',s),$$

$$I^{(n)}(x,x')=\epsilon(x_0-x_0')\int_\Gamma f^{(n)}(x,x',s)ds, \tag{25}$$

$$f^{(n)}(x,x',s)=\frac{1}{n!}\frac{d^n}{ds^n}\left[\frac{f(x,x',s)}{f_0(x,x',s)}\right]_{s=0} s^n f_0(x,x',s).$$

Here, $I_R(x,x')$ is a regular on the light cone function, which is zero at $(x-x')^2\leqslant 0$. All the singularities are concentrated in the functions $I^{(n)}(x,x')$. It is convenient to make a change of variables $t=s^{-1}$ in expression (25) to present the latter in the following form:

$$I^{(n)}(x,x')=\epsilon(x_0-x_0')a^{(n)}(x,x')\left(\frac{d}{d\tau}\right)^{[(d-2)/2]-n} Y(\tau-(\mathbf{x}-\mathbf{x}')^2)|_{\tau=(x_0-x_0')^2},$$
$$a^{(n)}(x,x')=\pi^{-[(d-1)/2]}e^{ig\Lambda}(4i)^{-n}\frac{1}{4n!}\frac{d^n}{ds^n}\left[\frac{f(x,x',s)}{f_0(x,x',s)}\right]_{s=0}, \tag{26}$$

where the function $Y(\tau-(\mathbf{x}-\mathbf{x}')^2)$ has different forms for even and for odd d. Namely, for even d,

$$Y(\tau-(\mathbf{x}-\mathbf{x}')^2)=Y_{\text{even}}(\tau-(\mathbf{x}-\mathbf{x}')^2)=2\Theta(\tau-(\mathbf{x}-\mathbf{x}')^2), \tag{27}$$

and for odd d,

$$Y(\tau-(\mathbf{x}-\mathbf{x}')^2)=Y_{\text{odd}}(\tau-(\mathbf{x}-\mathbf{x}')^2)$$
$$=e^{i(\pi/4)}\int_{e^{i\pi}\infty}^{\infty}(4\pi t)^{1/2}\exp\left\{-\frac{i}{4}[\tau-(\mathbf{x}-\mathbf{x}')^2]t\right\}dt. \tag{28}$$

Now one can see that for even d the function $I^{((d/2)-1)}(x,x')$ can be expressed via the Θ-function (27), whereas the rest functions $I^{(n)}(x,x')$ are concentrated on the light cone. Thus function (23) is zero for points, which cannot be causally connected, i.e., for $(x-x')^2<0$.

Consider the contribution of distributions (27) and (28) to an integral with some continuous functions on the coordinates $(\mathbf{x}-\mathbf{x}')$ in the case $(x_0-x_0')\to 0$. In this case the distributions are zero beyond the sphere of the radius $|x_0-x_0'|+0$, thus formula (27) can be written in the form

$$Y_{\text{even}}(\tau-(\mathbf{x}-\mathbf{x}')^2)=2V(\sqrt{\tau})\delta(\mathbf{x}-\mathbf{x}'), \tag{29}$$

where $V(r)$ is the volume of the $d-1$ sphere with the radius r,

$$V(r)=cr^{d-1},\quad c=\pi^{(d-1)/2}\Gamma^{-1}\left(\frac{d+1}{2}\right), \tag{30}$$

and $\Gamma(x)$ is the gamma-function. The least power of (x_0-x_0') in expression (23) comes from $I^{(0)}(x,x')$, the latter can be derived from Eqs. (26) and (29) and has the form $I^{(0)}(x,x')=e^{ig\Lambda}(x_0-x_0')\delta(\mathbf{x}-\mathbf{x}')$. In case $d\geqslant 4$, the next power of (x_0-x_0') comes from the function $I^{(1)}(x,x')\sim e^{ig\Lambda}(x_0-x_0')^3\delta(\mathbf{x}-\mathbf{x}')$. At $d=2$ the same power of (x_0-x_0') comes from the function $I_R(x,x')$ defined by Eq. (24). Thus we can write for any even d at $(x_0-x_0')\to 0$

$$\Delta(x,x')|_{x_0\to x_0'}=e^{ig\Lambda}[x_0-x_0'+O((x_0-x_0')^3)]\delta(\mathbf{x}-\mathbf{x}'). \tag{31}$$

One can see that Eq. (31) is a continuous function of the time (x_0-x_0') together with its first derivatives, and obeys Eq. (6) at $(x_0-x_0')\to 0$, and the initial conditions (7).

Expression (28) at $(x_0-x_0')\to 0$ (d is odd) can be presented in the form

$$Y_{\text{odd}}(\tau-(\mathbf{x}-\mathbf{x}')^2)=B(\tau)\delta(\mathbf{x}-\mathbf{x}'), \tag{32}$$

where

$$B(\tau)=\int_{V(r_0)}Y_{\text{odd}}(\tau-\mathbf{y}^2)d\mathbf{y}. \tag{33}$$

The integration in Eq. (33) is going over the volume of $d-1$ sphere with the radius $r_0=|x_0-x_0'|+0$. Integral (33) is reducing to one over the radius r only,

$$B(\tau)=(d-1)c\int_0^{r_0}Y_{\rm odd}(\tau-r^2)r^{d-2}\,dr, \tag{34}$$

where c was defined in Eq. (30) and we remember that $r_0>\tau$. The former can be calculated and presented in the form

$$B(\tau)=e^{i\pi d/4}\pi^{(d-2)/2}\int_{e^{i\pi}\infty}^{\infty}t^{-d/2}e^{-i\tau t}\,dt. \tag{35}$$

Similar to the even case the least power of (x_0-x_0') in Eq. (23) comes from the function $I^{(0)}(x,x')$. By means of Eqs. (32) and (35) the latter can be written as

$$I^{(0)}(x,x')=\epsilon(x_0-x_0')\,\delta(\mathbf{x}-\mathbf{x}')\,\frac{e^{i3\pi/4}e^{ig\Lambda}}{4\sqrt{\pi}}\int_{e^{i\pi}\infty}^{\infty}t^{-3/2}e^{-i(x_0-x_0')^2t}\,dt. \tag{36}$$

Using the representation

$$t^{-1/2}=e^{-i\pi/4}\frac{2}{\sqrt{\pi}}\left(\int_0^{\sqrt{(x_0-x_0')^2-0}}e^{iz^2t}\,dz+\int_{\sqrt{(x_0-x_0')^2+0}}^{\infty}e^{iz^2t}\,dz\right)$$

in Eq. (36) and changing the order of the integration over t and z, we get finally $I^{(0)}(x,x')=e^{ig\Lambda}(x_0-x_0')\,\delta(\mathbf{x}-\mathbf{x}')$. In the same manner one can verify that the next power of (x_0-x_0') at $d\geqslant 5$ comes from the function $I^{(1)}(x,x')\sim e^{ig\Lambda}(x_0-x_0')^3\delta(\mathbf{x}-\mathbf{x}')$. In the case $d=3$ the same power of (x_0-x_0') comes from function (24). That is why the same dependence Eq. (31) holds at any odd d.

Thus we have shown that function (21) obeys Eq. (6) and the initial conditions (7) in any dimensions d. Then the commutation function can be written in an universal form in any dimensions [by means of Eqs. (5) and (21)],

$$S(x,x')=\epsilon(x_0-x_0')(\hat{\mathscr{P}}_\nu\gamma^\nu+m)\int_\Gamma f(x,x',s)ds. \tag{37}$$

Here, we have used the initial conditions (7) to put $\epsilon(x_0-x_0')$ before the operator $\hat{\mathscr{P}}_\nu\gamma^\nu+m$.

It was already seen from Eqs. (23)–(28) that the representation (21) is convenient to select the light cone singularities. In case of even d one can also get d-dimensional generalization of the Fock representation. To this end let us write the function $I_R(x,x')$ from Eq. (24) by means of an integral over the closed path Γ_R, defined in Eq. (10),

$$I_R(x,x')=\epsilon(x_0-x_0')\Theta((x-x')^2)\int_{\Gamma_R}f_R(x,x',s)ds. \tag{38}$$

From $f_R(x,x',s)$ only the term $f^{(n)}(x,x',s)$ with $n=(d/2)-1$ gives nonzero contribution, namely,

$$\Theta((x-x')^2)\int_{\Gamma_R}f^{(d/2-1)}(x,x',s)ds=\int_\Gamma f^{(d/2-1)}(x,x',s)ds.$$

That allows one to rewrite Eq. (23) for even d in the form

$$\Delta(x,x')=\epsilon(x_0-x_0')\Bigg[\Theta((x-x')^2)\Delta_R(x,x')+\sum_{n=0}^{(d-4)/2} 2a^{(n)}(x,x')\left(\frac{d}{d\tau}\right)^{(d-4)/2-n}$$

$$\times\delta(\tau-(\mathbf{x}-\mathbf{x}')^2)\Big|_{\tau=(x_0-x_0')^2}\Bigg], \tag{39}$$

where $a^{(n)}(x,x')$ are defined in Eq. (26), and $\Delta_R(x,x')$ is d-dimensional Riemann function, defined by integral (10). At $d=4$ this expression coincides with the Fock's one (8).

The expression for the commutation function $i[\phi(x),\phi^\dagger(x')]_-$ of the scalar fields $\phi(x)$ and $\phi^\dagger(x')$ one can derive from representation (21) for the function $\Delta(x,x')$, putting formally all the γ-matrices to zero. We do not also see any difficulties to extend the results obtained to the curved space and gauge theories using the Schwinger–DeWitt technics.[2,6]

III. PATH INTEGRAL REPRESENTATION FOR THE COMMUTATION FUNCTION

Here, we are going to discuss a path integral representation for the commutation function at $d=4$. For our purpose, it is convenient to deal with the transformed by $\gamma^5=\gamma^0\gamma^1\gamma^2\gamma^3$ function $\widetilde{S}(x,x') = S(x,x')\gamma^5$, which obeys the properly transformed Dirac equation

$$(\hat{\mathscr{P}}_\nu\widetilde{\gamma}^\nu-m\gamma^5)\widetilde{S}(x,x')=0, \tag{40}$$

and the initial condition

$$\widetilde{S}(x,x')|_{x_0=x_0'}=-i\widetilde{\gamma}^0\delta(\mathbf{x}-\mathbf{x}'), \tag{41}$$

where $\hat{\mathscr{P}}_\nu=i\partial_\nu-gA_\nu(x)$, and $\widetilde{\gamma}^\nu=\gamma^5\gamma^\nu$. The matrices $\widetilde{\gamma}^\nu$ have the same commutation relations as initial ones γ^ν, $[\widetilde{\gamma}^\mu,\widetilde{\gamma}^\nu]_+=2\eta^{\mu\nu}$. For all the γ-matrices ($\widetilde{\gamma}^5=\gamma^5$) we have $[\widetilde{\gamma}^m,\widetilde{\gamma}^n]_+=2\eta^{mn}$, m, $n=\overline{0,3}$,5; $\eta^{mn}=\mathrm{diag}(1,-1,-1,-1,-1)$.

If one presents the function $\widetilde{S}(x,y)$ in the form

$$\widetilde{S}(x,x')=-(\hat{\mathscr{P}}_\nu\widetilde{\gamma}^\nu-m\gamma^5)\widetilde{\Delta}(x,x'), \tag{42}$$

then the function $\widetilde{\Delta}$ obeys the equation

$$(\hat{\mathscr{P}}_\nu\widetilde{\gamma}^\nu-m\gamma^5)^2\widetilde{\Delta}(x,x')=[(\hat{\mathscr{P}}_\nu\gamma^\nu)^2-m^2]\widetilde{\Delta}(x,x')=0. \tag{43}$$

One can remark that according to the definition and to Eqs. (6) and (7) there is a relation $\widetilde{\Delta}(x,x')=-\gamma^5\Delta(x,x')\gamma^5$, which allows on to conclude that the functions $\widetilde{\Delta}(x,x')$ and $\Delta(x,x')$ obey the same initial conditions. Because they obey also the same equation they coincide. Thus one can write, using the results obtained before Eq. (37),

$$\widetilde{S}(x,x')=-\epsilon(x_0-x_0')\int_\Gamma(\hat{\mathscr{P}}_\nu\widetilde{\gamma}^\nu-m\gamma^5)f(x,x',s)ds. \tag{44}$$

By means of the representation (15) for the function $f(x,x',s)$, where one can replace the operator $[(\Pi_\nu\gamma^\nu)^2-m^2]$ by one $(\Pi_\nu\widetilde{\gamma}^\nu-m\gamma^5)^2$, and introducing the operator $(\hat{\mathscr{P}}_\nu\widetilde{\gamma}^\nu-m\gamma^5)$ under the sign of the matrix element, we get

$$\widetilde{S}(x,x')=-i\epsilon(x_0-x_0')\int_\Gamma\langle x|(\Pi_\nu\widetilde{\gamma}^\nu-m\gamma^5)\exp\{i(\Pi_\nu\widetilde{\gamma}^\nu-m\gamma^5)^2\}|x'\rangle ds. \tag{45}$$

The operator $(\Pi_\nu\widetilde{\gamma}^\nu-m\gamma^5)$ can be presented via a Grassmannian integral,

$$(\Pi_\nu\tilde{\gamma}^\nu - m\gamma^5) = i\int e^{i\chi(\Pi_\nu\hat{\gamma}^\nu - m\gamma^5)}d\chi,$$

where χ is a Grassmann variable, which anticommutes with γ matrices by the definition. Here, and in what follows, integrals over Grassmann variables are understood as Berezin's integrals.[9] Thus the commutation function (45) takes the form

$$\tilde{S} = \tilde{S}(x_{\rm out}, x_{\rm in}) = \epsilon(x^0_{\rm out}, x^0_{\rm in}) \int_\Gamma ds \int \langle x_{\rm out}| e^{-i.\hat{\mathscr{H}}(s,\chi)} |x_{\rm in}\rangle d\chi, \tag{46}$$

where

$$\hat{\mathscr{H}}(s,\chi) = s\left(m^2 - \Pi^2 + \frac{ig}{2} F_{\alpha\beta}\tilde{\gamma}^\alpha\tilde{\gamma}^\beta\right) + (\Pi_\nu\tilde{\gamma}^\nu - m\tilde{\gamma}^5)\chi. \tag{47}$$

Now one can present the matrix element entering in expression (46) by means of a path integral. First, we write $\exp(-i.\hat{\mathscr{H}}) = (\exp(-i.\hat{\mathscr{H}}/N))^N$, and then insert $(N-1)$ resolutions of identity $\int |x\rangle\langle x| dx = I$ between all the operators $\exp(-i.\hat{\mathscr{H}}/N)$. Besides, we introduce N additional integrations over s and χ to transform then the ordinary integrals over these variables into the corresponding path-integrals,

$$\tilde{S} = \epsilon(x^0_{\rm out}, x^0_{\rm in}) \lim_{N\to\infty} \int_\Gamma ds_0 \int d\chi_0\, dx_1 \cdots dx_{N-1}\, ds_1 \cdots ds_N\, d\chi_1 \cdots d\chi_N$$

$$\times \prod_{k=1}^{N} \langle x_k| e^{-i.\hat{\mathscr{H}}(s_k,\chi_k)\Delta\tau} |x_{k-1}\rangle \delta(s_k - s_{k-1})\,\delta(\chi_k - \chi_{k-1}), \tag{48}$$

where $\Delta\tau = 1/N$, $x_0 = x_{\rm in}$, $x_N = x_{\rm out}$. Bearing in mind the limiting process, one can calculate the matrix elements from Eq. (48) approximately,

$$\langle x_k| e^{-i.\hat{\mathscr{H}}(s_k,\chi_k)\Delta\tau} |x_{k-1}\rangle \approx \langle x_k| 1 - i.\hat{\mathscr{H}}(s_k,\chi_k)\Delta\tau |x_{k-1}\rangle, \tag{49}$$

using the resolution of identity $\int |p\rangle\langle p| dp$, where

$$P_\mu|p\rangle = p_\mu|p\rangle, \quad \langle p|p'\rangle = \delta(p-p'), \quad \langle x|p\rangle = \frac{1}{(2\pi)^2} e^{ipx}.$$

In this connection it is important to notice that the operator $\hat{\mathscr{H}}(s_k,\chi_k)$ has originally the symmetric form in the operators $\hat{x}$ and $\hat{p}$. Indeed, the only one term in $\hat{\mathscr{H}}(s_k,\chi_k)$, which contains products of these operators is $[P_\alpha, A^\alpha(X)]_+$. One can verify that this is maximal symmetrized expression, which can be combined from entering operators (see remark in Ref. 10). Thus one can write $\hat{\mathscr{H}}(s,\chi) = \mathrm{Sym}_{(\hat{x},\hat{p})}\, \mathscr{H}(s,\chi,\hat{x},\hat{p})$, where $\mathscr{H}(s,\chi,x,p)$ is the Weyl symbol of the operator $\hat{\mathscr{H}}(s,\chi)$ in the sector of coordinates and momenta, $\mathscr{H}(s,\chi,x,p) = s(m^2 - \mathscr{P}^2 + ig/2F_{\alpha\beta}\tilde{\gamma}^\alpha\tilde{\gamma}^\beta) + (\mathscr{P}_\nu\tilde{\gamma}^\nu - m\gamma^5)\chi$, and $\mathscr{P}_\nu = -p_\nu - gA_\nu(x)$. That is a general statement,[11] which can be easily checked in that concrete case by direct calculations, that the matrix elements (49) are expressed in terms of the Weyl symbols in the middle point $\overline{x_k} = (x_k + x_{k-1})/2$. Taking all that into account, one can see that in the limiting process the matrix elements (49) can be replaced by the expressions

$$\int \frac{dp_k}{(2\pi)^4} \exp\left(i\left[p_k \frac{x_k - x_{k-1}}{\Delta\tau} - \mathscr{H}(s_k,\chi_k,\overline{x_k},p_k)\right]\right)\Delta\tau, \tag{50}$$

which are noncommutative due to the γ-matrix structure and are situated in Eq. (48) so that the numbers k increase from right to left. For the two δ-functions, accompanying each matrix element (49) in expression (48), we use the integral representations

$$\delta(s_k-s_{k-1})\,\delta(\chi_k-\chi_{k-1})=\frac{i}{2\pi}\int e^{i[\pi_k(s_k-s_{k-1})+\nu_k(\chi_k-\chi_{k-1})]}d\pi_k\,d\nu_k,$$

where ν_k are odd variables. Then we attribute formally to γ-matrices, entering into Eq. (50), index k, and then we attribute to all quantities the ''time'' τ_k, according the index k they have, $\tau_k=k\Delta\tau$, so that $\tau\in[0,1]$. Introducing the T-product, which acts on γ-matrices, it is possible to gather all the expressions, entering in Eq. (48), in one exponent and deal then with the γ-matrices like with odd variables. Thus we get for the right side of Eq. (48)

$$\widetilde{S}=\epsilon(x^0_{\rm out},x^0_{\rm in})T\int_\Gamma ds_0\int d\chi_0\int_{x_{\rm in}}^{x_{\rm out}}Dx\int Dp\int_{s_0}Ds\int_{\chi_0}D\chi\int D\pi\int D\nu$$
$$\times\exp\left\{i\int_0^1\left[s\left(\mathscr{P}^2-m^2-\frac{ig}{2}F_{\alpha\beta}\widetilde{\gamma}^\alpha\widetilde{\gamma}^\beta\right)+(m\gamma^5-\mathscr{P}_\nu\widetilde{\gamma}^\nu)\chi+p\dot{x}+\pi\dot{s}+\nu\dot{\chi}\right]d\tau\right\},\quad(51)$$

where x, p, s, π, are even and χ, ν are odd trajectories, obeying the boundary conditions $x(0)=x_{\rm in}$, $x(1)=x_{\rm out}$, $s(0)=s_0$, $\chi(0)=\chi_0$. The operation of T-ordering acts on the γ-matrices, which suppose formally to depend on time τ. Expression (51) can be reduced to

$$\widetilde{S}=\epsilon(x^0_{\rm out},x^0_{\rm in})\int_\Gamma ds_0\int d\chi_0\int_{x_{\rm in}}^{x_{\rm out}}Dx\int Dp\int_{s_0}Ds\int_{\chi_0}D\chi\int D\pi\int D\nu$$
$$\times\exp\left\{i\int_0^1\left[s\left(\mathscr{P}^2-m^2-\frac{ig}{2}F_{\alpha\beta}\frac{\delta_l}{\delta\rho_\alpha}\frac{\delta_l}{\delta\rho_\beta}\right)+\left(m\frac{\delta_l}{\delta\rho_5}-\mathscr{P}_\nu\frac{\delta_l}{\delta\rho_\nu}\right)\chi+p\dot{x}+\pi\dot{s}+\nu\dot{\chi}\right]d\tau\right\}$$
$$\times T\exp\int_0^1\rho_n(\tau)\widetilde{\gamma}^n\,d\tau\Big|_{\rho=0},$$

where five odd sources $\rho_n(\tau)$ are introduced, which anticommute with the γ-matrices by definition. One can present the quantity $T\exp\int_0^1\rho_n(\tau)\widetilde{\gamma}^n\,d\tau$ via a path integral over odd trajectories,[7]

$$T\exp\int_0^1\rho_n(\tau)\widetilde{\gamma}^n\,d\tau=\exp\left(i\widetilde{\gamma}^n\frac{\partial_l}{\partial\theta^n}\right)$$
$$\times\int_{\psi(0)+\psi(1)=\theta}\exp\left[\int_0^1(\psi_n\dot{\psi}^n-2i\rho_n\psi^n)d\tau+\psi_n(1)\psi^n(0)\right]\mathscr{D}\psi|_{\theta=0},$$

$$\mathscr{D}\psi=D\psi\left[\int_{\psi(0)+\psi(1)=0}D\psi\exp\left\{\int_0^1\psi_n\dot{\psi}^n\,d\tau\right\}\right]^{-1},\quad(52)$$

where θ^n are odd variables, anticommuting with γ-matrices, and $\psi^n(\tau)$ are odd trajectories of integration, obeying the boundary conditions, which are pointed out below the signs of integration. Using Eq. (52) we get the Hamiltonian path integral representation for the commutation function

$$\widetilde{S}=\epsilon(x^0_{\rm out},x^0_{\rm in})\exp\left(i\widetilde{\gamma}^n\frac{\partial_l}{\partial\theta^n}\right)\int_\Gamma ds_0\int d\chi_0\int_{s_0}Ds\int_{\chi_0}D\chi\int_{x_{\rm in}}^{x_{\rm out}}Dx\int Dp\int D\pi\int D\nu$$
$$\times\int_{\psi(0)+\psi(1)=\theta}\mathscr{D}\psi\,\exp\left\{i\int_0^1[s(\mathscr{P}^2-m^2+2igeF_{\alpha\beta}\psi^\alpha\psi^\beta)+2i(\mathscr{P}_\alpha\psi^\alpha-m\psi^5)\chi-i\psi_n\dot{\psi}^n\right.$$
$$\left.+p\dot{x}+\pi\dot{s}+\nu\dot{\chi}]d\tau+\psi_n(1)\psi^n(0)\right\}\Bigg|_{\theta=0}.$$

Integrating over momenta in the path integral, we get

$$\widetilde{S}=\epsilon(x^0_{\rm out},x^0_{\rm in})\exp\left(i\widetilde{\gamma}^n\frac{\partial_l}{\partial\theta^n}\right)\int_\Gamma de_0\int d\chi_0\;G(e_0,\chi_0,x^0_{\rm out},x^0_{\rm in}),\tag{53}$$

$$G(e_0,\chi_0,x^0_{\rm out},x^0_{\rm in})=\int_{e_0}De\int_{\chi_0}D\chi\int_{x_{\rm in}}^{x_{\rm out}}Dx\int D\pi\int D\nu\int_{\psi(0)+\psi(1)=\theta}\mathscr{D}\psi$$
$$\times M(e)\exp\left\{i\int_0^1\left[-\frac{\dot{x}^2}{2e}-\frac{e}{2}m^2-g\dot{x}A(x)+iegF_{\mu\nu}(x)\psi^\mu\psi^\nu\right.\right.$$
$$\left.\left.+i\left(\frac{\dot{x}_\mu\psi^\mu}{e}-m\psi^5\right)\chi-i\psi_n\dot{\psi}^n+\pi\dot{e}+\nu\dot{\chi}\right]d\tau+\psi_n(1)\psi^n(0)\right\}\Bigg|_{\theta=0},\tag{54}$$

where $M(e)$ is the integration measure,

$$M(e)=\int Dp\;\exp\left\{\frac{i}{2}\int_0^1 ep^2\,d\tau\right\}.\tag{55}$$

The exponent in integrand (54) can be considered as an effective and nondegenerate Lagrangian action of a spinning particle in an external field. It consists of two principal parts. The first one, which unites two summand with the derivatives of e and χ, can be treated as a gauge fixing term and corresponds to the gauge conditions $\dot{e}=\dot{\chi}=0$. The rest part of the effective action, in fact, coincides with the gauge invariant action[12] of a spinning particle. One can interpret the pair e_0, χ_0 in representation (53) as a super proper time.

Comparing the path integral representation (53) for the commutation function with one[7] for the Dirac propagator (causal Green function), one can remark that they are quite similar, one of the differences is in the contour of integration over s_0. Namely, the path integral representation for the Dirac propagator $\widetilde{S}^c$ (transformed by γ^5) reads

$$\widetilde{S}^c=\exp\left(i\widetilde{\gamma}^n\frac{\partial_l}{\partial\theta^n}\right)\int_\Gamma de_0\int d\chi_0\;G(e_0,\chi_0,x^0_{\rm out},x^0_{\rm in}),\tag{56}$$

where the function $G(e_0,\chi_0,x^0_{\rm out},x^0_{\rm in})$ has the same form (54). Thus in case of the commutation function the c-number component of the super proper time is complex in contrast with the case of the propagator.

IV. CONCLUSION

The results obtained for the commutation function allows one to get also similar proper time representation for some other singular functions. For example, it is easy to get for the retarded, $S^{\rm ret}(x,x')=\Theta(x_0-x_0')S(x,x')$, and advanced, $S^{\rm adv}(x,x')=-\Theta(x_0'-x_0)S(x,x')$, functions the following representations, in which one has to understand $\Theta(0)=1/2$:

$$S^{\rm ret}(x,x')=\Theta(x_0-x_0')(\hat{\mathscr{P}}_\nu\gamma^\nu+m)\int_\Gamma f(x,x',s)ds, \tag{57}$$

$$S^{\rm adv}(x,x')=\Theta(x_0'-x_0)(\hat{\mathscr{P}}_\nu\gamma^\nu+m)\int_\Gamma f(x,x',s)ds. \tag{58}$$

Combining the Schwinger representation (14) for the causal Green function and the representation (37) for the commutation function, one can get proper time representations for positive and negative frequency functions $S^{\mp}(x,x')$. Namely, let us define them via the Schwinger representation of the causal Green function,

$$S^{\mp}(x,x')=\pm S^c(x,x'),\quad \pm(x_0-x_0')>0. \tag{59}$$

Using the completeness relation

$$S(x,x')=S^-(x,x')+S^+(x,x'), \tag{60}$$

we get for any x,x'

$$S^{\mp}(x,x')=\Theta(\mp[x_0-x_0'])S(x,x')\pm S^c(x,x'). \tag{61}$$

In this connection one ought to remark that there is a problem with the causal Green function definition in case of an arbitrary external field. From the one hand, there exists the Feynman definition, based on the definition of the inverse operator to the Dirac equation by means of the prescription $m^2\to m^2-i\epsilon$. On the other hand, in the perturbation theory there appears a field theoretical definition of the propagator in the form

$$S^c(x,x')=i\langle 0|T\psi(x)\overline{\psi}(x')|0\rangle. \tag{62}$$

In the absence of the external field or in fields of special form, which do not violate the vacuum stability [then the operators of the spinor fields in Eq. (62) have to be taken in the Furry representation], it is possible to verify that the Feynman causal Green function and the propagator (14) coincide. In the same case one can establish that the former function can be defined via the Schwinger proper time representation. In external fields, which violate the vacuum stability (create pairs from the vacuum), the situation is not so clear. In this case does not exist an unique vacuum for all the time instances. One has to distinguish the initial $|0,\text{in}\rangle$ and final $|0,\text{out}\rangle$ vacua.[2,3,13] In virtue of that, one has also to use different kinds of propagators in the perturbation theory,

$$S^c(x,x')=i\,\frac{\langle 0,\text{out}|T\psi(x)\overline{\psi}(x')|0,\text{in}\rangle}{\langle 0,\text{out}|0,\text{in}\rangle}, \tag{63}$$

$$S^c_{\rm in}(x,x')=i\langle 0,\text{in}|T\psi(x)\overline{\psi}(x')|0,\text{in}\rangle, \tag{64}$$

and the positive and negative frequency commutation functions,

$$\begin{aligned} S^-(x,x')&=i\,\frac{\langle 0,\text{out}|\psi(x)\overline{\psi}(x')|0,\text{in}\rangle}{\langle 0,\text{out}|0,\text{in}\rangle},\\ S^+(x,x')&=i\,\frac{\langle 0,\text{out}|\overline{\psi}(x')\psi(x)|0,\text{in}\rangle}{\langle 0,\text{out}|0,\text{in}\rangle}. \end{aligned} \tag{65}$$

It was shown that in special cases of external fields, violating the vacuum stability, the Feynman causal Green function, presented by means of the Schwinger proper time integral, gives, namely, the propagator (63), whereas the propagator (64) demands a modification of the Schwinger contour in the proper time integration.[14] At the present time does not exist a proof of the equivalence between of the Feynman causal Green function and the propagator (63) for any external fields. Nevertheless, there is a strong believe that they are equivalent. If one excepts such an equivalence, then the positive and negative frequency commutation functions (65) have the representation (61) in arbitrary external fields.

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Quantum Lobachevsky planes

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We classify all $SL(2,\mathbb{R})$-covariant Poisson structures on the Lobachevsky plane with respect to all multiplicative Poisson structures on $SL(2,\mathbb{R})$ and describe quantizations for all these Poisson structures. © *1996 American Institute of Physics.* [S0022-2488(96)01507-1]

I. INTRODUCTION

A first step into the direction of a quantization of the notions of algebraic geometry (cf. Ref. 1) is the quantization of the three fundamental one-dimensional complex domains: the complex plane, the Riemannian sphere, and the complex upper half-plane. Quantum planes were considered in Ref. 2. Quantum Riemannian spheres are discussed in Refs. 3 and 4. A quantum upper half-plane appears first in Ref. 5 (for certain other quantizations of the upper half-plane, see also Remark 7). In this letter we consider the case of the quantum complex upper half-plane.

In the theory of quantum groups the classification of certain Poisson structures gives generally a good insight into the problem of the classification of quantum structures. At first we give the full solution of the classification problem in the classical limit [i.e., the description of all possible $SL(2,\mathbb{R})$-covariant Poisson structures for the upper half-plane with respect to the action of all possible multiplicative Poisson structures on $SL(2,\mathbb{R})$). Further, we describe classes of quantum structures, which reproduce all listed Poisson structures in the classical limit. We obtain two-parameter quantizations of the upper half-plane for every action of one of the quantum groups $SL_q(2,\mathbb{R})$, $SU_q(1,1)$, and $SL_h(2,\mathbb{R})$.

II. PRELIMINARIES

In this section we introduce the basic concepts (see also Refs. 5–7). Let (A,Δ,ϵ) be a Hopf algebra. A *left quantum space* (H,ϕ) is an algebra H along with an algebra homomorphism $\phi: H\to A\otimes H$ such that $(\Delta\otimes\mathrm{id})\phi=(\mathrm{id}\otimes\phi)\phi$ and $(\epsilon\otimes\mathrm{id})\phi=\mathrm{id}$. Two left quantum spaces (H_1,ϕ_1) and (H_2,ϕ_2) are *isomorphic* if there is an algebra isomorphism $h: H_1\to H_2$, such that $\phi_2\circ h=(\mathrm{id}\otimes h)\circ\phi_1$. Further consider commutative Hopf algebras and commutative quantum spaces. We say that the Poisson bracket $\{.,.\}$ on A is *multiplicative* if $\{\Delta(x),\Delta(y)\}_{A\otimes A}=\Delta(\{x,y\})$, where $A\otimes A$ carries the Poisson structure of the direct product. We call a Poisson bracket $\{.,.\}$ on H *covariant* if $\{\phi(x),\phi(y)\}_{A\otimes H}=\phi(\{x,y\})$, where $A\otimes H$ carries the direct product structure from A and H. We say that two multiplicative or covariant, respectively, Poisson brackets on A and, respectively, H are *equivalent* if they intertwine with an automorphism of A and, respectively, H.

III. THE CLASSICAL CASE

A. Poisson structures on SL(2,$\mathbb{R}$)

Let $A=\mathbb{R}[a,b,c,d]/(ad-bc-1)$ be the commutative unital algebra of polynomial functions in the coordinates of

$$\mathrm{SL}(2,\mathbb{R})=\left\{\left.\begin{pmatrix} a & b \\ c & d \end{pmatrix}\right| a,b,c,d\in\mathbb{R},\ \ ad-bd=1\right\}.$$

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Here A becomes a Hopf algebra with respect to the Hopf multiplication

$$\Delta\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} a\otimes a + b\otimes c & a\otimes b + b\otimes d \\ c\otimes a + d\otimes c & c\otimes b + d\otimes d \end{pmatrix}$$

and the counit ϵ with

$$\epsilon\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

Here A has the coinverse κ with

$$\kappa\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}.$$

We consider three types of multiplicative Poisson algebras A_λ^A, A_λ^K, and A^N:
(1) $A_\lambda^A=(A,\{,\}_\lambda)$, $\lambda\in\mathbb{R}$, $\lambda\neq 0$, with

$$\{a,b\}_\lambda=\lambda ab,\quad \{a,c\}_\lambda=\lambda ac,\quad \{a,d\}_\lambda=2\lambda bc,$$

$$\{b,c\}_\lambda=0,\quad \{b,d\}_\lambda=\lambda bd,\quad \{c,d\}_\lambda=\lambda cd;$$

(2) $A_\lambda^K=(A,\{,\}_\lambda)$, $\lambda>0$, with

$$\{a,b\}_\lambda=\lambda(1-a^2-b^2),\quad \{a,c\}_\lambda=\lambda(a^2+c^2-1),\quad \{a,d\}_\lambda=\lambda(a-d)(b-c),$$

$$\{b,c\}_\lambda=\lambda(a+d)(b+c),\quad \{b,d\}_\lambda=\lambda(b^2+d^2-1),\qquad \{c,d\}_\lambda=\lambda(1-c^2-d^2);$$

and
(3) $A^N=(A,\{,\})$ with

$$\{a,b\}=(1-a^2),\quad \{a,c\}=c^2,\quad \{a,d\}=c(d-a),$$

$$\{b,c\}=c(d+a),\quad \{b,d\}=(d^2-1),\quad \{c,d\}=-c^2.$$

We shortly denote $A_\lambda^A(\lambda\in\mathbb{R},\ \lambda\neq 0)$, $A_\lambda^K(\lambda>0)$, and A^N by A_λ^I $(I=A,K,N)$.

Remark 1: The notation A_λ^I with $I=A,K,N$ is justified by the fact that the Poisson brackets of A_λ^A, A_λ^K, and A^N, respectively, vanish on the subgroups of the KAN-decomposition

$$G_A=\left\{\begin{pmatrix} e^x & 0 \\ 0 & e^{-x} \end{pmatrix}\middle|\, e\in\mathbb{R}\right\},$$

$$G_K=\left\{\begin{pmatrix} \cos x & \sin x \\ -\sin x & \cos x \end{pmatrix}\middle|\, x\in[0,2\pi)\right\},$$

and

$$G_N=\left\{\begin{pmatrix} 1 & x \\ 0 & 1 \end{pmatrix}\middle|\, x\in\mathbb{R}\right\},$$

respectively.

Proposition 1: Every nontrivial multiplicative Poisson structure on A is equivalent to one of the structures $A_\lambda^A(\lambda\neq 0)$, $A_\lambda^K(\lambda>0)$, A^N. All these structures are nonequivalent.

Proof: We give a sketch proof. Set $g=\mathrm{sl}(2,\mathbb{R})$. Because $H^1(g,g\wedge g)=0$, every Poisson structure on $\mathrm{SL}(2,\mathbb{R})$ arises from a classical r-matrix, $r\in g\wedge g$, which satisfies the modified classical Yang–Baxter equation (MCYBE) $(\wedge_1^3 ad_x)C(r)=0$, $\forall x\in g$ with a certain element $C(r)\in g\wedge g\wedge g$ (cf. Ref. 6). Because $g=\mathrm{sl}(2,\mathbb{R})$ is a simple Lie algebra, the one-dimensional representation $\wedge_1^3 ad$ is trivial. That is, the MCYBE is satisfied for every $r\in g$.

To show that two structures are equivalent, it is enough to show that their r-matrices are connected by an automorphism of $\mathrm{sl}(2,\mathbb{R})$. All automorphisms are generated by inner automorphisms [i.e., the adjoint action of $\mathrm{SL}(2,\mathbb{R})$] and the automorphism α with

$$\alpha\begin{pmatrix} a & b \\ c & d \end{pmatrix}=\begin{pmatrix} a & -b \\ -c & d \end{pmatrix}.$$

Let

$$e_{-1}=\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix},\quad e_0=\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},\quad e_1=\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

and $r=\alpha e_1\wedge e_{-1}+\beta e_0\wedge e_1+\gamma e_0\wedge e_{-1}$. Studying the adjoint action $\wedge_1^2 Ad$ of $\mathrm{SL}(2,\mathbb{R})$ and the action of α on $r\in g\wedge g$, we recognize that r is equivalent to one of the following elements:

$$r_\lambda^A=\lambda e_1\wedge e_{-1},\quad \lambda\in\mathbb{R},\lambda\neq 0,$$

$$r_\lambda^K=\lambda(e_0\wedge e_1+e_0\wedge e_{-1}),\quad \lambda>0,$$

$$r^N=e_0\wedge e_1.$$

All these elements are nonequivalent.

Because A consists of the matrix elements of the finite-dimensional representations $\rho:\mathrm{SL}(2,\mathbb{R})\to\mathbb{R}^n$, one can give the Poisson structures by the formula

$$\{l_1(\rho_1(g)v_1),l_2(\rho_2(g)v_2)\}=(l_1\otimes l_2)([(\rho_1\otimes\rho_2)(r_0),\rho_1(g)\otimes\rho_2(g)]v_1\otimes v_2)$$

[$v\in\mathbb{R}^d$, $l\in(\mathbb{R}^d)^*$, cf. Ref. 8]. The structures A_λ^A, A_λ^K, and A^N correspond to the above normal forms r_λ^A, r_λ^K, and r^N for r. □

B. Poisson structures on the upper half-plane

Further consider the subalgebra $H\subseteq A$ generated by the elements $A=a^2+b^2$, $B=ac+bd$, $D=c^2+d^2$ (cf. Ref. 5) and the left coaction $\phi=\Delta|_H:H\to A\otimes H$ with

$$\phi(A)=a^2\otimes A+b^2\otimes D+2ab\otimes B,$$

$$\phi(D)=c^2\otimes A+d^2\otimes D+2cd\otimes B,$$

$$\phi(B)=ac\otimes A+bd\otimes D+(ad+bc)\otimes B.$$

By the next Proposition we give a complete classification of all possible covariant Poisson structures on H with respect to A_λ^I.

Proposition 2: (1) All with respect to A_λ^I covariant Poisson structures are given by the one-parameter series:

(i) $H_{\lambda,\mu}^A$($\lambda\in\mathbb{R}$, $\lambda\neq 0$, $\mu\in\mathbb{R}$):

$$\{A,B\}=2\lambda A(B+\mu),\quad \{A,D\}=4\lambda B(B+\mu),\quad \{B,D\}=2\lambda D(B+\mu);$$

(ii) $H^K_{\lambda,\mu}(\lambda>0,\ \mu\in\mathbb{R})$:

$$\{A,B\}=2\lambda A(A+D+\mu),$$

$$\{A,D\}=4\lambda B(A+D+\mu),$$

$$\{B,D\}=2\lambda D(A+D+\mu);$$

(iii) $H^N_{\mu}(\mu\in\mathbb{R})$:

$$\{A,B\}=2A(D+\mu),\quad \{A,D\}=4B(D+\mu),\quad \{B,D\}=2D(D+\mu)$$

for $I=n$.

(2) Two Poission algebras H^I_{λ,μ_i} and H^I_{λ,μ_2} are equivalent if and only if $|\mu_1|=|\mu_2|$.

Proof: (1) All left invariant Poisson structures [i.e., $\phi(\{x,y\})=\{\phi(x),\phi(y)\}$, $\forall x,y\in H$, where $A\otimes H$ carries a Poisson structure which is the direct product of the zero structure on A and of the structure on H] are given by

$$\{A,B\}=2\mu A,\quad \{A,D\}=4\mu B,\quad \{B,D\}=2\mu D$$

($\mu\in\mathbb{R}$). We obtain the above formulas by the calculation for a fixed μ (for example, $\mu=0$) and from the fact that the difference of two left covariant structures is left invariant (cf. Ref. 7).

(2) The proof of the equivalence follows from the fact that (H,ϕ) has the unique automorphism $x\to -x,\forall x\in H$. □

The following Proposition shows that we can realize the Poisson algebras $H^I_{\lambda,\mu}$ as subalgebras of A^I_λ.

Consider subalgebras $H_{\alpha,\beta,\gamma}\subset A$ generated by elements $\overline{A},\overline{B},\overline{D}\in A$ with

$$\overline{A}:=\alpha a^2+\beta b^2+2\gamma ab,$$

$$\overline{B}:=\alpha ac+\beta bd+\gamma(ad+bc),$$

$$\overline{D}:=\alpha c^2+\beta d^2+2\gamma cd.$$

We have $H_{1,1,0}=H$, and the correspondence between A, B, D, and the overlined elements arranges an isomorphism $H_{\alpha,\beta,\gamma}\cong H$ (i.e., $\overline{AD}-\overline{B}^2=1$), if and only if $\alpha\beta-\gamma^2=1$.

Proposition 3: Let $\alpha\beta-\gamma^2=1$. Then $H_{\alpha,\beta,\gamma}$ is a Poisson subalgebra of A^I_λ and we have

$$\text{(i)}\quad H_{\alpha,\beta,\gamma}\cong H^A_{\lambda,-\gamma},$$

$$\text{(ii)}\quad H_{\alpha,\beta,\gamma}\cong H^K_{\lambda,-\alpha-\beta},\ \text{and}$$

$$\text{(iii)}\quad H_{\alpha,\beta,\gamma}\cong H^N_{\lambda,-\beta}.$$

Proof: The isomorphies can be verified by an explicit calculation.

Remark 2: The preceding Proposition admits the realization of all $H^I_{\lambda,\mu}$ by $H_{\alpha,\beta,\gamma}$ with real α,β,γ, except the cases H^N_0 and $H^K_{\lambda,\mu}$, $|\mu|<2$. For example, $H^A_{\lambda,\mu}\cong H_{1,1+\mu^2,\mu}$, $H^K_{\lambda,\mu}\cong H_{(\mu+\sqrt{\mu^2-4})/2,(\mu-\sqrt{\mu^2-4})/2,0}$ and $H^N_\mu\cong H_{-1/\mu,-\mu,0}$. In the other cases we have only complex realizations, for example, $H^K_{\lambda,\mu}\cong H_{(\mu+i\sqrt{4-\mu^2})/2,(\mu-i\sqrt{4-\mu^2})/2,0}$ and $H^N_0\cong H_{0,0,i}$. The realizations are not unique.

C. Geometric interpretation

There is an interpretation of the parameter μ in terms of fixed points z_0 of the upper half-plane.

Let $z\to(az+b)/(cz+d)$ be the usual action of $\mathrm{SL}(2,\mathbb{R})$ on the complex coordinate $z=+iy$, $y>0$, of the upper half-plane, i.e.,

$$x\to\frac{ac(x^2+y^2)+(ad+bc)x+bd}{c^2(x^2+y^2)+2cdx+d^2},$$

$$y\to\frac{y}{c^2(x^2+y^2)+2cdx+d^2}.$$

Further let G_{z_0} be the subgroup of $\mathrm{SL}(2,\mathbb{R})$, which fixes the point $z_0=x_0+iy_0$, $y_0>0$. It follows that the functions

$$x=x(a,b,c,d)=\frac{ac(x_0^2+y_0^2)+(ad+bc)x_0+bd}{c^2(x_0^2+y_0^2)+2cdx_0+d^2}$$

and

$$y=y(a,b,c,d)=\frac{y_0}{c^2(x_0^2+y_0^2)+2cdx_0+d^2}$$

are left G_{z_0}-invariant and can be identified with functions on $G_{z_0}G$. We recognize that $\overline{B}=xy^{-1}$, $\overline{D}=y^{-1}$ generate $H_{y_0+x_0^2/y_0,x_0/y_0,1/y_0}$ For the parameter μ we get the interpretation

$$\mu=\mathrm{ctg}(\arg(z_0))=\frac{\mathrm{Re}\ z_0}{\mathrm{Im}\ z_0},\quad \text{if } I=A,$$

$$\mu=-\frac{1+|z_0|^2}{\mathrm{Im}\ z_0},\quad \text{if } I=K,$$

$$\mu=-\frac{1}{\mathrm{Im}\ z_0},\quad \text{if } I=N.$$

We remark that $x,y\notin H=\mathbb{R}[\overline{A,B,D}]$ and $\overline{A,B,D}\notin H':=\mathbb{R}[x,y]$, but H and H' are dense subalgebras of the algebra of smooth functions on the upper half-plane (H and H' are dense on every compact subset). With respect to the xy coordinates the Poisson brackets have the form

$$\{x,y\}=-2\lambda(xy+\mu y^2)$$

if $I=A$,

$$\{x,y\}=-2\lambda(x^2y+y+y^3+\mu y^2)$$

if $I=K$, and

$$\{x,y\}=-2(y+\mu y^2)$$

if $I=N$.

IV. THE QUANTUM CASE

A. The quantum groups $\mathscr{A}_h^I$

First we recall the definition of the three known quantum deformations of SL(2,$\mathbb{R}$).

The Poisson algebras A_λ^I correspond to the quantum algebras $\mathscr{A}_h^A$ ($h\in\mathbb{R}$, $h\neq 2\pi n$, $n\in\mathbb{N}$), $\mathscr{A}_h^K$ ($h>0$), and $\mathscr{A}^N$. For all these algebras we write shortly $\mathscr{A}_h^I$ ($I=A,K,N$). The algebras $\mathscr{A}_h^I$ are generated by elements a,b,c,d and relations

$$ab=e^{\mathbf{i}h}ba,\quad ac=e^{\mathbf{i}h}ca,\quad bd=e^{\mathbf{i}h}db,$$

$$cd=e^{\mathbf{i}h}dc,\quad bc=cb,\quad ad-da=(e^{\mathbf{i}h}-e^{-\mathbf{i}h})bc,$$

$$ad-e^{\mathbf{i}h}bc=da-e^{\mathbf{i}h}cb=1,\quad h\neq 2\pi n,$$

for $I=A$;

$$ab-ba=\mathbf{i}h(1-a^2-b^2),\quad ac-ca=\mathbf{i}h(a^2+c^2-1),$$

$$bd-db=\mathbf{i}h(b^2+d^2-1),\quad cd-dc=\mathbf{i}h(1-c^2-d^2),$$

$$ad-da=\mathbf{i}h(ab+ba+ac+ca+bd+db+cd+dc),$$

$$bc-cb=\mathbf{i}h(ab+ba-ac-ca-bd-db+cd+dc),$$

$$ad+da-bc-cb=2+h(2-a^2-b^2-c^2-d^2),\quad h>0,$$

for $I=K$; and

$$ab-ba=\mathbf{i}(1-a^2),\quad ac-ca=\mathbf{i}c^2,\quad bd-db=\mathbf{i}(d^2-1),$$

$$cd-dc=-\mathbf{i}c^2,\quad ad-da=\mathbf{i}c(d-a),\quad bc-cb=\mathbf{i}(dc+ca),$$

$$ad-bc+\mathbf{i}ac=da-cb-\mathbf{i}ca=1$$

for $I=N$.

The algebras $\mathscr{A}_h^I$ become Hopf algebras with respect to the Hopf multiplication

$$\Delta\begin{pmatrix}a & b\\ c & d\end{pmatrix}=\begin{pmatrix}a\otimes a+b\otimes c & a\otimes b+b\otimes d\\ c\otimes a+d\otimes c & c\otimes b+d\otimes d\end{pmatrix}$$

and Hopf *-algebras with respect to the involution

$$a^*:=a,\quad b^*:=b,\quad c^*:=c,\quad d^*:=d.$$

The counit ϵ is given by

$$\epsilon\begin{pmatrix}a & b\\ c & d\end{pmatrix}=\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$$

and the coinverse κ is given by

$$\kappa\begin{pmatrix}a & b\\ c & d\end{pmatrix}=\begin{pmatrix}d & -q^{-1}b\\ -qc & a\end{pmatrix}$$

for $I=A$;

$$\kappa(a)=\frac{1}{4}\left(\left(2-\frac{2-2h^2}{1+h^2}\right)a+\left(2+\frac{2-2h^2}{1+h^2}\right)d-\frac{2h}{1+h^2}\,b-\frac{2h}{1+h^2}\,c\right),$$

$$\kappa(b)=\frac{1}{4}\left(\frac{2}{1+h^2}\,a-\frac{2}{1+h^2}\,d-\left(2+\frac{2-2h^2}{1+h^2}\right)b+\left(2-\frac{2-2h^2}{1+h^2}\right)c\right),$$

$$\kappa(c)=\frac{1}{4}\left(\frac{2}{1+h^2}\,a-\frac{2}{1+h^2}\,d+\left(2-\frac{2-2h^2}{1+h^2}\right)b-\left(2+\frac{2-2h^2}{1+h^2}\right)c\right),$$

$$\kappa(d)=\frac{1}{4}\left(\left(2+\frac{2-2h^2}{1+h^2}\right)a+\left(2-\frac{2-2h^2}{1+h^2}\right)d+\frac{2h}{1+h^2}\,b+\frac{2h}{1+h^2}\,c\right),$$

for $I=K$; and

$$\kappa\begin{pmatrix}a & b\\ c & d\end{pmatrix}=\begin{pmatrix}d+c & -b+(d-a+c)\\ -c & a-c\end{pmatrix}$$

for $I=N$.

Remark 3: $\mathscr{A}_h^K$ is equivalent to the quantum group $\mathrm{SU}_q(1,1)$, $q\in\mathbb{R}$, which is given by elements $\alpha,\alpha^*,\beta,\beta^*$ and relations

$$\alpha\beta=q\beta\alpha,\quad \alpha\beta^*=q\beta^*\alpha,$$

$$\beta\beta^*=\beta^*\beta,\quad \beta\alpha^*=q\alpha^*\beta,\quad \beta^*\alpha^*=q\alpha^*\beta^*,$$

$$\alpha\alpha^*-q^2\beta\beta^*=\alpha^*\alpha-\beta^*\beta=1.$$

The formulas of $\mathrm{SU}_q(1,1)$ and $\mathscr{A}_h^K$ are connected by the transformation of the deformation parameter $h=(1-q)/(1+q)$ and by the ''quantum Cayley transformation'' of the matrix elements

$$\alpha:=\tfrac{1}{2}(a+d+\mathbf{i}(b-c)),$$

$$\alpha^*=\tfrac{1}{2}(a+d+\mathbf{i}(-b+c)),$$

$$\beta:=\tfrac{1}{2}(a-d-\mathbf{i}(b+c)),$$

$$\beta^*=\tfrac{1}{2}(a-d+\mathbf{i}(b+c)).$$

Remark 4: Instead of $\mathscr{A}^N$ one considers Hopf *-algebras $\mathrm{SL}_h(2,\mathbb{R})$ $(h\neq 0)$, where the algebra structure is replaced by

$$ab-ba=\mathbf{i}h(1-a^2),\quad ac-ca=\mathbf{i}hc^2,\quad bd-db=\mathbf{i}h(d^2-1),$$

$$cd-dc=-\mathbf{i}hc^2,\quad ad-da=\mathbf{i}hc(d-a),\quad bc-cb=\mathbf{i}h(dc+ca),$$

$$ad-bc+\mathbf{i}hac=da-cb-\mathbf{i}hca=1.$$

(cf. Refs. 9 and 10). All these structures are equivalent to $\mathscr{A}^N$ by the Hopf *-algebra isomorphism $a\to a$, $b\to hb$, $c\to(1/h)c$, $d\to d$.

B. The quantum spaces ($\mathscr{H}^I_{h,k,d}$,ϕ)

1. The algebras $\mathscr{H}^I_{h,k,d}$

The Poisson algebras $H^I_{\lambda,\mu}$ correspond to the algebras $\mathscr{H}^a_{h,k,d}(h\neq 2\pi n)$, $\mathscr{H}^k_{h,k,d}$ $(h>0)$, $\mathscr{H}^n_{k,d}$, $k,d\in\mathbb{R}$. For all these algebras we write shortly $\mathscr{H}^I_{h,k,d}$.

We define the $\mathscr{H}^I_{h,k,d}$ as algebras which are generated by elements A,B,C,D and relations

$$C=e^{-\mathbf{i}h}B+k(1-e^{-\mathbf{i}h}),\quad AB=e^{2\mathbf{i}h}BA+k(1-e^{2\mathbf{i}h})A,$$

$$BD=e^{2\mathbf{i}h}DB+k(1-e^{2\mathbf{i}h})D,\quad AD-e^{2\mathbf{i}h}BC=d+k(1-e^{2\mathbf{i}h})B,$$

$$DA-e^{-2\mathbf{i}h}CB=d+k(1-e^{-2\mathbf{i}h})B,\quad h\neq 2\pi n$$

for $I=A$;

$$C=B-\mathbf{i}h(A+D+k),\quad AB-BA=\mathbf{i}h(2kA+2A^2+AD+BC),$$

$$BD-DB=\mathbf{i}h(2kD+2D^2+AD+CB),$$

$$AD-B^2=d+\mathbf{i}h(kB+AB+BD),$$

$$DA-C^2=d-\mathbf{i}h(kC+CA+DC),\quad h>0,$$

for $I=K$; and

$$C=B-\mathbf{i}(D+k),$$

$$AB-BA=2\mathbf{i}A(D+k)-2B(D+k),$$

$$BD-DB=2\mathbf{i}D(D+k),$$

$$AD-BC=d+2\mathbf{i}B(D+k),$$

$$DA-CB=d-2\mathbf{i}(D+k)C$$

for $I=N$.

The algebras $\mathscr{H}^I_{h,k,d}$ become *-algebras with respect to the involutions

$$A^*:=A,\quad D^*:=D,\quad B^*:=C=e^{-\mathbf{i}h}B+k(1-e^{-\mathbf{i}h}),\quad C^*:=B$$

for $I=A$;

$$A^*:=A,\quad D^*:=D,\quad B^*:=C=B-\mathbf{i}h(A+D+k),\quad C^*:=B$$

for $I=K$; and

$$A^*:=A,\quad D^*:=D,\quad B^*:=C=B-\mathbf{i}(D+k),\quad C^*:=B$$

for $I=N$.

Remark 5: Formally we recover the Poisson structures of Sec. III B in the limit $t\to\infty$, if we set $B=C$, $q=\lambda t$, $k=\mu$, $d=1$, and $\{x,y\}:=\lim(1/it)[x,y]$.

Next we show that we can realize the *-algebras $\mathscr{H}^I_{h,k,d}$ as *-subalgebras of $\mathscr{A}^I_h$. Let

$$\overline{A}:=\alpha a^2+\beta b^2+\gamma(ab+ba),$$

$$\overline{B}:=\alpha ac+\beta bd+\gamma(ad+bc),$$

$$\overline{C}:=\alpha ca+\beta db+\gamma(da+cb),$$

$$\overline{D}:=\alpha c^2+\beta d^2+\gamma(cd+dc).$$

Proposition 4: Let $\alpha,\ \beta,\ \gamma\in\mathbb{R}$, and $\overline{A,B,C,D}$ satisfy the relations of

(i) $\mathscr{H}^A_{h,\gamma,\alpha\beta-\gamma^2}$,
(ii) $\mathscr{H}^K_{h,-\alpha-\beta,\alpha\beta-\gamma^2}$, and
(iii) $\mathscr{H}^N_{h,-\beta,\alpha\beta-\gamma^2}$.

Proof: The proof can be given by an explicit calculation.

Remark 6: Proposition 4 admits the realization of all $\mathscr{H}^I_{h,k,d}$, with real α,β,γ without the cases $\mathscr{H}^K_{h,0,d}$, $|k|<2$, and $\mathscr{H}^N_{h,0,d}$, $d>0$. For example, $\mathscr{H}^A_{h,k,d}\cong\mathscr{H}_{\mathbf{1},d+k^2,k}$, $\mathscr{H}^K_{h,k,d}\cong\mathscr{H}_{(k+\sqrt{k^2-4})/2,(k-\sqrt{k^2-4})/2,0}$ and $\mathscr{H}^N_{h,k,d}\cong\mathscr{H}_{-d/k,-k,0}$. In other cases we have only complex realizations; for example, $H^K_{h,k,d}\cong H_{(k+i\sqrt{4-k^2})/2,(k-i\sqrt{4-k^2})/2,0}$ and $\mathscr{H}_{0,0,\mathbf{i}\backslash d}\cong\mathscr{H}^N_{h,0,d}$.

Remark 7: (1) The special case $\mathscr{H}_{\mathbf{1},\mathbf{1},0}\cong\mathscr{H}^A_{h,\mathbf{0},\mathbf{1}}$ was first mentioned in Ref. 5, p. 188.

(2) The formulas for $\mathscr{H}^A_{h,k,d}$ are similar those from Podles' sphere $C(X_{\mu,\lambda,\rho})$ (cf. Ref. 4). Both can be specified from the complex quantum space $\Xi_{q,\lambda,\rho}$ of $\mathrm{SL}_q(2,\mathbb{C})$ from Ref. 11 by fixing certain involutions.

(3) In Ref. 12 the quantum spaces $\mathscr{H}_{\alpha,\beta,0}\cong\mathscr{H}^A_{h,0,\alpha\beta}$, $\alpha,\beta\geqslant 0$, were considered.

(4) The quantum spaces $\mathscr{H}^K_{h,k,d}$ correspond to one-parameter series of quantum discs $C_{\mu,q}(\overline{U})$ in Ref. 13. Formally the correspondence is arranged by the quantum Cayley transformation (cf. Remark 3).

2. The coaction of $\mathscr{A}^I_h$ on $\mathscr{H}^I_{h,k,d}$

We will describe an coaction ϕ, i.e., a homomorphism $\phi:\mathscr{H}^I_{h,k,d}\to\mathscr{A}^I_h\otimes\mathscr{H}^I_{h,k,d}$ with $(\Delta\otimes\mathrm{id})\phi=(\mathrm{id}\otimes\phi)\phi$ and $(\epsilon\otimes\mathrm{id})\phi=\mathrm{id}$ such that we can call $(\mathscr{H}^I_{h,k,d},\phi)$ a quantum space with respect to $\mathscr{A}^I_h$.

According to Remark 6, consider $\mathscr{H}^I_{h,k,d}$ as a subalgebra of $\mathscr{A}^I_h$, i.e., we identify A,B,C,D with A,B,C,D. We obtain (independent from I,h,k,d)

$$\Delta(A)=a^2\otimes A+b^2\otimes D+ab\otimes B+ba\otimes C,$$

$$\Delta(D)=c^2\otimes A+d^2\otimes D+cd\otimes B+dc\otimes C,$$

$$\Delta(B)=ac\otimes A+bd\otimes D+ad\otimes B+bc\otimes C,$$

$$\Delta(C)=ca\otimes A+db\otimes D+cb\otimes B+da\otimes C.$$

That is, $\mathscr{H}^I_{h,k,d}$ is a left coideal of $\mathscr{A}^I_h$ and we have proven the following proposition.

Proposition 5: The homomorphism $\phi:\mathscr{H}^I_{h,k,d}\to\mathscr{A}^I_h\otimes\mathscr{H}^I_{h,k,d}:\phi:=\Delta|_{\mathscr{H}^I_{h,k,d}}$ defines a left coaction, that is, $(\mathscr{H}^I_{h,k,d},\phi)$ are left quantum spaces.

Remark 8: Every $\mathscr{H}^I_{h,k,d}$ is equivalent to one of the quantum spaces

$$\mathscr{H}^I_{h,k,\pm 1},\mathscr{H}^I_{h,k,0}$$

with $k\geqslant 0$.

Proof: We achieve $k\in[0,\infty)$ because of the automorphism $X\to -X$, $X\in\mathscr{H}^I_{h,k,d}$, and we achieve $d=0,\pm 1$ by the reparametrization $X\to(1/\sqrt{|d|})X$, $X\in\mathscr{H}^I_{h,k,d}$. ∎

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On localization and regularization

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Different regularizations are studied in localization of path integrals. We discuss the effect of the choice of regularization by evaluating the partition functions for the harmonic oscillator and the Weyl character for SU(2). In particular, we solve the Weyl shift problem that arises in path integral evaluation of the Weyl character by using the Atiyah–Patodi–Singer η-invariant and the Borel–Weil theory. © *1996 American Institute of Physics.* [S0022-2488(96)01107-3]

I. INTRODUCTION

Quantum localization is a generalization Duistermaat–Heckman theorem[1] to infinite dimensions. This theorem states that if the Hamiltonian H generates a global circle, or, more generally, a torus action in the phase space Γ, then the canonical partition function is given exactly by the saddle-point approximation around the critical points of H. Extensions to calculation of quantum mechanical partition functions using phase space path integrals have been represented in, e.g., Ref. 2.

We shall first consider basic ideas of localization. Then we shall carefully regularize the pertinent functional determinants arising from the path integrals. There is an ambiguity in choosing the regularization scheme because of the spectral asymmetry of first-order differential operators. Therefore, the result depends on the regularization as in the case of quantum mechanical anomalies.

Finally, we are going to apply our localization to the quantization of the simple harmonic oscillator and to the evaluation of the Weyl character of spin. We shall notice that different regularizations give different energy spectra for the harmonic oscillator. We also show that the continuum coherent state path integral yields directly the correct character for spin if we choose an appropriate regularization. In particular, we will consider the relation of character formulas to the Borel–Weil theory which constructs the irreducible representations of a Lie group as holomorphic functions. Using this theory we relate the character formulas to the equivariant index of the Dolbeault complex. The result is that the path integral yields directly the correct character without an explicit Weyl shift of the highest weight.

II. LOCALIZATION OF PHASE SPACE PATH INTEGRALS

We are interested in exact evaluation of phase space path integrals (partition functions) of the form

$$Z(T)=\int_{L\Gamma}\mathscr{D}xPf\|\omega_{ab}(x)\|\exp\left(i\int_0^T dt[\vartheta_a\dot{x}^a-H(x)]\right), \tag{1}$$

where $\{x^a\}$ are local coordinates in Γ, $Pf\|\omega_{ab}\|$ is the Liouville measure factor, ϑ_a is the symplectic potential, and $\omega_{ab}=\partial_a\vartheta_b-\partial_b\vartheta_a$. The integration is performed over the loop space $L\Gamma$ consisting of the phase space loops. The integrability condition[3] requires that

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$$\int_\Sigma \omega = 2\pi n$$

for any two-cycle Σ in Γ so that the path integral is single valued. We introduce anticommuting variables ψ^a to write $Pf\|\omega_{ab}\|$ as a path integral:

$$Z(T) = \int \mathscr{D}x \mathscr{D}\psi \, \exp\left(i \int_0^T dt \left[\vartheta_a \dot{x}^a - H(x) + \frac{1}{2} \psi^a \omega_{ab} \psi^b \right] \right). \tag{2}$$

The boundary conditions are periodic also for the fermions, since they are a realization of the differentials of the bosonic coordinates.

We interpret the path integral (2) in terms of equivariant cohomology in $L\Gamma$. From the bosonic part of the action we obtain a Hamiltonian vector field in $L\Gamma$,

$$\chi_S^a = \dot{x}^a - \omega^{ab} \partial_b H,$$

whose zeroes define the Hamilton's equations. The equivariant exterior derivative in $L\Gamma$ is

$$d_S = d + \iota_S,$$

where ι_S denotes the contraction along the vector field χ_S. The square of d_S is the loop space Lie derivative

$$\mathscr{L}_S = d\iota_S + \iota_S d \sim \frac{d}{dt} - \mathscr{L}_H.$$

The action $S_B + S_F$ is supersymmetric under the infinitesimal loop space supersymmetry transformations that are parametrized by a gauge fermion $\delta\Psi$:

$$x^a \to x^a + \delta\Psi \, d_S x^a = x^a + \delta\Psi \, \psi^a, \qquad \psi^a \to \psi^a + \delta\Psi \, d_S \psi^a = \psi^a + \delta\Psi \, \chi_S^a. \tag{3}$$

This implies that the action is equivariantly closed:

$$d_S(S_B + S_F) = 0.$$

By an analog of Fradkin–Vilkovisky theorem[4] one can show that the path integral remains intact if we modify the action by $S \to S + d_S\Psi$, where Ψ satisfies the Lie derivative condition

$$d_S^2 \Psi = \mathscr{L}_S \Psi = 0. \tag{4}$$

In the limit $\lambda \to 0$ the path integral

$$Z_\lambda(T) = \int \mathscr{D}x^a \mathscr{D}\psi^a \, \exp\left(i \int_0^T dt \left[\vartheta_a \dot{x}^a - H(x^a) + \frac{1}{2} \psi^a \omega_{ab} \psi^b + \lambda d_S \Psi \right] \right) \tag{5}$$

reduces to (2) and $\lambda \to \infty$ gives localization.

To construct a gauge fermion Ψ we need a metric g in the phase space. The loop space Lie derivative condition (4) is satisfied if the metric g in Γ is invariant under the Hamiltonian action of H

$$\mathscr{L}_H g = 0, \tag{6}$$

which means that χ_H is a Killing vector field. This is a very restrictive condition for the Hamiltonian: it must generate a global U(1)-action in Γ. We can choose any metric which satisfies the condition (6) and average it over the group action.

We will consider the following selections for the gauge fermion:

$$\Psi_1 = \tfrac{1}{2} g_{ab} \dot{x}^a \psi^b$$

gives localization to the constant modes, which are points of the manifold;

$$\Psi_2 = \tfrac{1}{2} g_{ab} \chi_H^a \psi^b$$

to the zeroes of χ_H, which we assume to be nondegenerate and isolated; and

$$\Psi_3 = \tfrac{1}{2} g_{ab} \chi_S^a \psi^b$$

to the classical trajectories. For simplicity we use subscripts 1,2,3 in the actions and partition functions corresponding to the gauge fermions $\Psi_{1,2,3}$. The actions become

$$S_1 = \int_0^T dt \left[\left(\vartheta_a - \frac{\lambda}{2} g_{ab} \chi_H^b \right) \dot{x}^a - H + \frac{\lambda}{2} g_{ab} \dot{x}^a \dot{x}^b + \frac{\lambda}{2} \psi^a (g_{ab} \partial_t + \dot{x}^c g_{bd} \Gamma^d_{ac}) \psi^b + \frac{1}{2} \psi^a \omega_{ab} \psi^b \right],$$

$$S_2 = \int_0^T dt \left[\vartheta_a \dot{x}^a - H + \frac{\lambda}{2} g_{ab} \chi_H^a (\dot{x}^b - \chi_H^b) + \frac{\lambda}{2} \psi^a \partial_a (g_{cb} \chi_H^c) \psi^b + \frac{1}{2} \psi^a \omega_{ab} \psi^b \right],$$

$$S_3 = \int_0^T dt \left[\vartheta_a \dot{x}^a - H + \frac{\lambda}{2} g_{ab} \chi_S^a \chi_S^b + \frac{\lambda}{2} \psi^a \partial_a (g_{cb} \chi_S^c) \psi^b + \frac{1}{2} \psi^a \omega_{ab} \psi^b \right]. \tag{7}$$

To take the limit $\lambda \to \infty$ in path integrals we make the decomposition to constant modes x_0^a, ψ_0^a and to nonconstant modes x_t^a, ψ_t^a and scale the nonconstant modes by $1/\sqrt{\lambda}$:

$$x^a(t) = \psi_0^a + \frac{1}{\sqrt{\lambda}} x_t^a, \quad \psi^a(t) = \psi_0^a + \frac{1}{\sqrt{\lambda}} \psi_t^a. \tag{8}$$

The Jacobi determinant is unity. An expansion to a quadratic order around the constant modes and the limit $\lambda \to \infty$ gives a Gaussian path integral

$$Z_1 = \int dx_0^a d\psi_0^a \exp\left[-iT \left(H - \frac{1}{2} \psi_0^a \omega_{ab} \psi_0^b \right) \right] Z_{\mathrm{fl},1}(T), \tag{9}$$

where the fluctuation path integral $Z_{\mathrm{fl}}(T)$ is a product of fermionic and bosonic parts:

$$\begin{aligned} Z_{F,1} &= \int \prod_t d\psi_t^a \exp\left\{ -\frac{i}{2} \int_0^T dt \ \psi_t^a g_{ab} \partial_t \psi_t^b \right\}, \\ Z_{B,1} &= \int \prod_t dx_t^a \exp\left\{ \frac{i}{2} \int_0^T dt \ x_t^a [\mathscr{R}_{ab} \partial_t - g_{ab} \partial_t^2] x_t^b \right\}. \end{aligned} \tag{10}$$

Here

$$\mathscr{R}_{ab} = R_{ab} + \tilde{\Omega}_{ab}$$

is the equivariant curvature with R_{ab} the Riemannian curvature two-form and

$$\tilde{\Omega}_{ab}=\tfrac{1}{2}[\nabla_b(g_{ac}\chi_H^c)-\nabla_a(g_{bc}\chi_H^c)]$$

the momentum map[5] corresponding to χ_H, ∇ being the covariant derivative. Here H, ω, g and $\mathscr{R}$ are evaluated at the constant modes. The path integral Z_2 is given by a sum over the critical points $\{x_i\}$ of the Hamiltonian:

$$Z_2=\sum_{x_i}\frac{\exp[-iTH]}{\mathrm{Pf}\|\partial_a\chi_H^b\|}Z_{\mathrm{fl},2}(T). \tag{11}$$

Here $Z_{\mathrm{fl},2}$ is also a product of fermionic and bosonic parts:

$$Z_{F,2}(T)=\int\prod_t d\psi_t^a\,\exp\left\{\frac{i}{2}\int_0^T dt\;\psi_t^a\partial_a(g_{bc}\chi_H^c)\psi_t^b\right\},$$

$$Z_{B,2}(T)=\int\prod_t dx_t^a\,\exp\left\{\frac{i}{2}\int_0^T dt\;x_t^a\partial_a(g_{bc}\chi_H^c)(\delta_d^b\partial_t-\partial_d\chi_H^b)x_t^d\right\}. \tag{12}$$

Here g and χ_H are again evaluated at the constant modes. Finally, the path integral Z_3 reduces to a sum over the T-periodic classical trajectories

$$Z_3=\sum_{x_{cl}}\frac{1}{Pf\|\delta_b^a\partial_t-\partial_b\chi_H^a\|}\exp[iS_{cl}]. \tag{13}$$

In practice, it is usually a highly nontrivial problem to find the T-periodic classical trajectories of a dynamical system.[6]

III. REGULARIZATION OF FLUCTUATION PATH INTEGRALS

In the following all the path integrals and determinants are evaluated over periodic configurations for both the bosonic and fermionic degrees of freedom. The primes will denote that we exclude the constant modes. In real polarization the fluctuation parts in $Z_{1,2}$ become

$$Z_{\mathrm{fl},1}=\frac{1}{\sqrt{\mathrm{Det}'\|\delta_b^a\partial_t-\mathscr{R}_b^a\|}},\quad Z_{\mathrm{fl},2}=\frac{1}{\sqrt{\mathrm{Det}'\|\delta_b^a\partial_t-\partial_b\chi_H^a\|}}. \tag{14}$$

It is quite important to notice that in the reduced determinants one index is covariant and another contravariant.

In Kähler polarization the fluctuations parts are, using the additional symmetries of the metric and the Riemann curvature tensor,[7]

$$Z_{\mathrm{fl},1}=\frac{1}{\mathrm{Det}'\|\delta_a^b\partial_t-\mathscr{R}_a^b\|},\quad Z_{\mathrm{fl},2}=\frac{1}{\mathrm{Det}'\|\delta_a^b\partial_t-\partial_a\chi_H^b\|}. \tag{15}$$

These determinants are taken over the holomorphic indices. By this we mean the following: The relevant matrices can be block diagonalized

$$A=\mathrm{diag}(A_1,A_2,\ldots,A_N)$$

with blocks

$$A_k=\begin{pmatrix}a_k^+ & 0\\ 0 & a_k^-\end{pmatrix}\equiv\begin{pmatrix}a_k & 0\\ 0 & -a_k\end{pmatrix}.$$

The symbols a_k^+ and a_k^- denote the holomorphic and antiholomorphic eigenvalues of A, and we consider only the eigenvalues corresponding to the holomorphic indices to the determinant.

We have to choose a regularization scheme for the determinants. A standard method is to apply ζ- and η-functions. The ζ-function regularization does not directly apply to first-order operators because they have an infinite number of negative eigenvalues. To take them into account we define the η-function for the first-order operator B by

$$\eta_B(s)=\sum_{b_n\neq 0}\operatorname{sign}(b_n)|b_n|^{-s}+\dim\operatorname{Ker} B=\frac{1}{\Gamma((s+1)/s)}\int_0^\infty dt\ t^{(s-1)/2}\operatorname{Tr}[B\ \exp(-tB^2)].$$

Analytical continuation to $s=0$ gives the Atiyah–Patodi–Singer η-invariant[8] of B that measures the spectral asymmetry of B and specifies the phase of $\mathrm{Det}(B)$. The absolute value $|\mathrm{Det}(B)|$ is regularized using the formula

$$|\mathrm{Det}(B)|=+\sqrt{\mathrm{Det}(B^2)}=+\exp\left[-\frac{1}{2}\,\zeta'_{B^2}(0)\right].$$

In real polarization we have to evaluate the square root of a determinant of the antisymmetric operator $B=\partial_t-A$ where A is an antisymmetric matrix. In our case A is $\|\mathscr{P}_a^b\|$ or $\|\partial_a\chi_H^b\|$. By determining the spectrum of B and applying ζ-function regularization we obtain, up to an inessential numerical normalization, the result

$$\frac{1}{\sqrt{\mathrm{Det}'(\partial_t-A)}}=\prod_{n=1}^{N}\left|\frac{a_n/2}{\sin(a_nT/2)}\right|=\frac{1}{T^N}\,\hat{A}(TA), \tag{16}$$

where we have defined the function of the matrix X

$$\hat{A}(X)=\prod_n\ \frac{x_n/2}{\sin(x_n/2)},$$

where x_n are the skew-eigenvalues of X. The result is non-negative since the negative and positive skew-eigenvalues appear in pairs. Therefore there is no ambiguity with the spectral asymmetry.

Now we consider the determinants in Kähler polarization. It is sufficient to consider the determinant of a block. Earlier we noticed that the fluctuation path integrals reduce to the determinant of the operator $B=i\partial_t-a$. The functional Pfaffian in (13) is also similar to this determinant. To regularize

$$\mathrm{Det}'(B)=\prod_{n\neq 0}\left(\frac{2\pi n}{T}-a\right)$$

properly we have to take into account that B has an infinite number of negative eigenvalues. Thus there is a problem with the spectral asymmetry.

Therefore, we have to choose a regularization prescription which has a relation to quantum mechanical anomalies. In the regularization of the determinants it is not possible to maintain all the symmetries that are present in the classical theory. For example, Elitzur *et al.*[9] considered the corresponding fermionic problem with antiperiodic boundary conditions. They evaluated the quantum mechanical partition function for a Dirac fermion in an external gauge field $A(t)$ in $0+1$-dimensions,

$$Z(T)=\int \mathscr{D}\overline{\psi}\mathscr{D}\psi\ \exp\left[i\int_0^T dt\ \overline{\psi}(i\partial_t-a)\psi\right]=\mathrm{Det}(i\partial_t-a), \tag{17}$$

where, because of the gauge invariance of the action, only the constant mode a of $A(t)$ contributes. The classical action has both the invariance under large gauge transformations

$$a\to a+n2\pi/T,\quad \psi\to\psi, \tag{18}$$

and the charge conjugation invariance

$$a\leftrightarrow -a,\quad \psi\leftrightarrow -\overline{\psi}. \tag{19}$$

However, when regularizing the determinant one has to choose which symmetry one wants to maintain, which leads to a global anomaly. Here we have an analogous situation. It is not *a priori* clear what the result of the regularization should be, and there is a genuine ambiguity.

Since the zeroes of the determinant are at $aT=2\pi n$, the determinant must be proportional to

$$\frac{\sin(aT/2)}{a/2}.$$

The proportionality factor can be any function without zeroes, that is, the exponent function. The determinant is, therefore, up to an irrelevant constant,

$$\mathrm{Det}(i\partial_t-a)=\frac{\sin(aT/2)}{a/2}\exp(i\phi aT),$$

with a phase ϕ whose natural values turn out to be 0 and $\pm\frac{1}{2}$ since they yield the (anti)symmetries of the product under $a\leftrightarrow -a$ and $a\to a+2\pi n/T$. However, there is a minor subtlety: in our localization formulas the zero modes are absent and this destroys these symmetries. Nevertheless, we may still consider the residual symmetries. The choice $\phi=0$ corresponds to neglecting the spectral asymmetry and choosing the (anti)symmetry $a\to -a$ to be unbroken. In this regularization scheme the inverse determinant is simply

$$\frac{1}{\mathrm{Det}'(\partial_t-A)}=\frac{1}{T^N}\hat{A}(TA).$$

This is the result that usually appears in literature. However, there is another possibility. The values $\phi=\pm\frac{1}{2}$ correspond to maintaining the symmetry $a\to a+2\pi n/T$ and taking into account the spectral asymmetry by the Atiyah–Patodi–Singer η-invariant. This yields

$$\frac{1}{\mathrm{Det}'(\partial_t-A)}=\prod_{n=1}^{N}\frac{a_n/2}{\sin(a_nT/2)}\exp\left(\frac{ia_nT}{2}\right)=\frac{1}{T^N}\,\mathrm{Td}(TA), \tag{20}$$

where we have defined the following function of the matrix X:

$$\mathrm{Td}(X)=\prod_n\frac{x_n/2}{\sin(x_n/2)}\,e^{ix_n/2}.$$

We take only the eigenvalues corresponding to the holomorphic indices to the determinant.

Let us now write down the resulting localization formulas. The localization to constant modes yields the expression

$$Z_1(T)=\frac{1}{T^N}\int dx_0^a d\psi_0^a \ \mathrm{Ch}[-iT(H-\omega)]\begin{Bmatrix}\hat{A}(T\mathscr{R})\\ \mathrm{Td}(T\mathscr{R})\end{Bmatrix}. \tag{21}$$

We have defined equivariant generalizations[10] of the conventional characteristic classes known as equivariant $\hat{A}$ and Todd genus, and identified the exponential with the equivariant Chern class. When $H=0$ they reduce to the conventional characteristic classes and the result is a topological invariant. The localization to the critical points $\{x_i\}$ of the Hamiltonian gives the result

$$Z_2(T)=\frac{1}{T^N}\sum_{x_i}\ \frac{\exp(-iTH)}{\mathrm{Pf}(\partial\chi_H)}\begin{Bmatrix}\hat{A}(T\partial\chi_H)\\ \mathrm{Td}(T\partial\chi_H)\end{Bmatrix}. \tag{22}$$

We must use local coordinates in the evaluation of the determinants when localizing to the critical points of the Hamiltonian. Finally, the localization to T-periodic classical trajectories yields

$$Z^3(T)=\frac{1}{T^N}\sum_{x_{\mathrm{cl}}}\ \exp(iS_{\mathrm{cl}})\begin{Bmatrix}\hat{A}(T\partial\chi_H)\\ \mathrm{Td}(T\partial\chi_H)\end{Bmatrix}. \tag{23}$$

IV. HARMONIC OSCILLATOR

Now we show that the localization formulas yield the correct partition function for the harmonic oscillator in a flat phase space. The path integral for it is Gaussian and in principle there is no reason to apply localization to it. However, it is reasonable to check by some simple examples that our assumptions and derivations are valid. In particular, we will show that the choice of the metric in the phase space is not relevant, contrary to claims in literature.[11] It is also illustrative to consider the significance of the regularization schemes we have used.

In real polarization the Hamiltonian is $H=\frac{1}{2}(p^2+q^2)$ and the symplectic two-form is $dq\wedge dp$. The coherent state representation (Kähler polarization) requires some further investigation, since we have to fix an operator ordering prescription. In terms of creation and annihilation operators the normal and symmetric-ordered Hamiltonians are, respectively,

$$H_n=:\tfrac{1}{2}(a^\dagger a+aa^\dagger):=a^\dagger a,\quad H_s=a^\dagger a+\tfrac{1}{2}. \tag{24}$$

The symmetric-ordered Hamiltonian has an explicit zero point energy $E_0=\frac{1}{2}$.

To apply the localization formulas we must choose a metric in the phase space and calculate the equivariant curvature and the derivatives of the Hamiltonian vector field. If the Lie derivative condition $\mathscr{L}_H g=0$ is satisfied, we can start from an any smooth metric in the phase space and average it. So we may choose a constant metric

$$g=\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}.$$

The nonzero components of the equivariant curvature are

$$\mathscr{R}^p_q=-\mathscr{R}^q_p=1.$$

The localization formula (21) yields the result

$$Z(T)=\int dpdqd\psi^q d\psi^p \exp\left[-iT\left(\frac{1}{2}p^2+\frac{1}{2}q^2-\psi^p\psi^q\right)\right]\frac{1}{2\sin(T/2)}$$
$$\sim\frac{1}{2\sin(T/2)}$$
$$=\sum_{n=0}^{\infty}\exp[i(n+1/2)T], \tag{25}$$

which is the correct partition function with the zero-point energy $E_0=\frac{1}{2}$.

Let us now digress slightly to discuss the result. In Ref. 11 Dykstra, Lykken, and Reiten analyzed this problem and they noticed a dependence on the metric. What they did not notice was that the index structure of the equivariant curvature is $\mathscr{R}_a^b$ and, therefore, it is invariant under global scalings of the metric. Furthermore, they used a metric which in polar coordinates near the origin behaves like

$$ds^2=dr^2+cr^2\,d\phi^2.$$

This is a metric on a cone, not on a plane when $c\neq 1$ and is not smooth, nor even continuous at the origin. Therefore it is not surprising that their energy levels depend on the parameter c, which represents the tip angle of the cone. From this we see that we cannot choose an arbitrary invariant metric, since it has to respect the topology of the phase space.

The localization to the critical points of the Hamiltonian (22) yields also the correct result. The only zero of χ_H is the origin of the phase space, which gives

$$Z(T)=\frac{1}{\mathrm{Pf}\begin{pmatrix}0&1\\-1&0\end{pmatrix}}\frac{1/2}{\sin(T/2)}=\frac{1}{2\sin(T/2)}.$$

If we want to apply the localization the classical trajectories, we must classify all the T-periodic classical trajectories. If $T\neq 2\pi n$, the problem reduces to the localization to the critical points of the Hamiltonian. However, if $T=2\pi n$, the zeroes of χ_S are not isolated and we have to use a degenerate version of the localization formula to the classical trajectories.[12]

We now consider the harmonic oscillator in the Kähler polarization. We will only discuss the localization formulas to constant modes. The reasoning is similar to other formulas. There are four cases to consider: the localizations with the $\hat{A}$ genus and Todd genus using two different orderings. We will only list the spectra we obtain. The use of $\hat{A}$ genus yields the spectra $E_n=n+\frac{1}{2}$ (normal ordering) and $E_n=n+1$ (symmetric ordering). The Todd genus gives the results $E_n=n$ (normal ordering) and $E_n=n+\frac{1}{2}$ (symmetric ordering). The first and fourth results have the correct zero-point energy. From this example we see that to get correct results from the path integral we do need some additional information other than the classical action and boundary conditions: we must choose a regularization scheme that gives physically correct results.

V. CHARACTER FOR SU(2)

We shall now use our localization formulas to derive the Kirillov and Weyl character formulas for Lie groups.[10] The character formula for SU(2) has been widely discussed in literature.[13–15] However, there has been some controversy about the Weyl shift problem: the path integral usually gives almost the correct character up to the substitution $j\to j+\frac{1}{2}$. We show that the coherent state path integral and the localization formulas with the Todd genus directly yield the correct character. In this calculation we use the continuum version of the coherent state path integral and show that this also yields the correct result, contrary to discussions in literature.[16]

To motivate the use of Todd genus we relate the character of a simple Lie group G in the highest weight representation λ to the index of the twisted Dolbeault complex on the coadjoint orbit O_f (Ref. 17) of the group. The Borel–Weil theory[14,18] constructs the irreducible representations of G as holomorphic sections of a line bundle L that is associated to a principal bundle $G \to G/T_G \sim O_f$, where T_G is the Cartan torus of G.[18] The holomorphic sections of this line bundle (coherent states) form the basis for the irreducible representation. The connection one-form on L is the symplectic potential

$$\vartheta = \frac{\partial F}{\partial z^k}\, dz^k - \frac{\partial F}{\partial \overline{z^k}} d\overline{z^k},$$

where F is the Kähler potential on O_f. It can be shown that the twisted Dolbeault operator $\overline{\partial_L} = \partial + \vartheta_{\overline{z}}$ annihilates the normalized coherent states $|z\rangle$ and therefore $|z\rangle \in H^{0,0}(O_f, L)$. If we can prove that all the other cohomology groups are trivial, e.g., by Lichnerowicz vanishing theorem,[10] we conclude that the dimension of the highest weight representation R_λ is $\dim H^{0,0}(O_f, L)$. Consequently, this is equal to the index of the twisted Dolbeault complex. The Riemann–Roch–Hirzebruch index theorem relates this analytical index to the topological invariant

$$\text{ind}\ \overline{\partial_L} = \dim\ R_\lambda = \int_{O_f} \text{Td}(O_f) \wedge \text{Ch}(L). \tag{26}$$

Indeed, we notice that the localization formula (21) with $H=0$ represents this index provided we use the Todd class. For SU(2) we obtain the known result for the dimension of the spin-j-representation

$$\dim\ R_j = \text{ind}\ \overline{\partial_L} = 2j+1.$$

This is the correct result without the explicit Weyl shift by the Weyl vector $\rho = \frac{1}{2}$.

We shall now use an equivariant version of the index theorem to derive the character formulas. The character of an element in the Cartan subalgebra is the partition function for the Hamiltonian H that represents it on O_f:

$$\chi(\beta) = \text{Str}\ \exp[-iTH]. \tag{27}$$

To make a relation to the Dolbeault index we write this as an equivariant index (character index, G-index, Lefschetz number).[10] One can show that the Laplacians $\overline{\partial_L^\dagger \partial_L}$ and $\overline{\partial_L \partial_L^\dagger}$ have equal nonzero eigenvalues. If all other comohomology classes except $H^{0,0}$ are trivial, as we presume, $\overline{\partial_L^\dagger}$ does not have zero modes. Consequently, we can write the trace as an equivariant index:

$$\begin{aligned} \text{ind}_H(\overline{\partial_L}, T) &\equiv \lim_{\beta\to\infty}\ \text{Tr}\ e^{-iTH}(e^{-\beta \overline{\partial_L^\dagger \partial_L}} - e^{-\beta \overline{\partial_L \partial_L^\dagger}}) \\ &= \lim_{\beta\to\infty}\ \text{Str}\ \exp[-iTH] \exp\left[-\beta \begin{pmatrix} \overline{\partial_L^\dagger \partial_L} & 0 \\ 0 & \overline{\partial_L \partial_L^\dagger} \end{pmatrix}\right]. \end{aligned} \tag{28}$$

Only the zero modes contribute to the trace. The expression is also independent of β. Therefore, in the limit $\beta \to 0$, all we are left with are the zero modes of ∂_L. Consequently, the equivariant index is equal to the character

$$\text{ind}_H(\overline{\partial_L}, T) = \text{Str}\ \exp[-iTH].$$

Thus, the character is the equivariant index of the twisted Dolbeault complex and therefore we choose the localization with the Todd class.

To derive the character formulas we apply standard methods to write $\mathrm{Str}\exp[-iTH]$ as a coherent state path integral of the form (2). Since we can choose an invariant metric on a coadjoint orbit[17] we can localize the path integral to classical trajectories, to constant modes, or to critical points of the Hamiltonian. The two latter cases yield the Kirillov character formula[19] ($2N$ is the dimension of the orbit)

$$\chi(T)=\frac{1}{T^N}\int_{O_f}\mathrm{Ch}[-iT(H-\omega)]\mathrm{Td}(T\mathscr{R}^+), \tag{29}$$

and the Weyl character formula

$$\chi(T)=\frac{1}{T^N}\sum_{z_i}\frac{\exp(-iTH)}{\det{}^+(\partial\chi_H)}\,\mathrm{Td}(T\partial\chi_H), \tag{30}$$

respectively. In (30) we have identified the Pfaffian in the real polarization with the determinant over the holomorphic eigenvalues of $\|\partial_a\chi_H^b\|$ and the summation is over the critical points of the Hamiltonian or equivalently the Weyl group.

As the only example we evaluate the character for SU(2). We write the character as a coherent state path integral over the coadjoint orbit $\mathrm{SU}(2)/U(1)\sim S^2$. We choose complex coordinates by introducing the stereographic projection from the south pole. The Kähler potential on the orbit with radius j is $F=j\log(1+z\bar{z})$ from which we obtain the metric and the symplectic one- and two-forms in the standard fashion. The integrability condition requires j to be a multiple of $\frac{1}{2}$: this is the topological quantization of spin. The canonical realization for $H=J_3$ is

$$J_3=-j\,\frac{1-z\bar{z}}{1+z\bar{z}}$$

and the path integral for the character becomes (2),

$$\chi_j(T)=\int\mathscr{D}z\mathscr{D}\bar{z}\mathscr{D}\psi\mathscr{D}\bar{\psi}\exp\left[ij\int_0^T dt\left(i\,\frac{\dot{z}\bar{z}-z\dot{\bar{z}}}{1+z\bar{z}}+\frac{1-z\bar{z}}{1+z\bar{z}}+\frac{2i\psi\bar{\psi}}{(1+z\bar{z})^2}\right)\right], \tag{31}$$

with periodic boundary conditions. The Lie derivative condition (6) is satisfied for $H=J_3$. This path integral is given exactly by the WKB approximation.[2,16] The relevant quantities in the Kirillov formula (29) are

$$H-\omega=j\,\frac{1-z\bar{z}-\psi\bar{\psi}}{1+z\bar{z}+\psi\bar{\psi}},\quad \mathscr{R}^+=R^++\Omega^+=\frac{1-z\bar{z}-\psi\bar{\psi}}{1+z\bar{z}+\psi\bar{\psi}}. \tag{32}$$

Now one can use the Parisi–Sourlas integration formula

$$\int dzd\bar{z}d\psi d\bar{\psi}F(z\bar{z}+\psi\bar{\psi})=\pi[F(\infty)-F(0)],$$

which gives

$$\chi_j(T)=\frac{\sin(j+1/2)T}{\sin(T/2)}=\sum_{m=-j}^{j}\exp[imT]. \tag{33}$$

This is exactly the correct result without an explicit Weyl shift. Also the Weyl formula (30) gives the correct result when we use local coordinate charts in the vicinity of the critical points. To get the correct north pole contribution we invert the coordinates $z \to 1/z$, $\overline{z} \to 1/\overline{z}$. This also yields the correct character (33):

$$\begin{aligned}\chi_j(T) &= \frac{\exp[-ijT]}{2\sin(T/2)}\exp[-iT/2] + \frac{\exp[-ijT(-1)]}{2\sin(-T/2)}\exp[iT/2] \\ &= \frac{\sin(j+1/2)T}{\sin(T/2)} \\ &= \sum_{m=-j}^{j} \exp[imT].\end{aligned}$$

On the other hand, using $\hat{A}$ genus we obtain the result

$$\chi_j(T) = \frac{\sin(jT)}{\sin(T/2)},$$

which is the correct result up to the Weyl shift $j \to j+1/2$. So we see that in the character formulas we have to use the Todd genus instead of $\hat{A}$ genus to directly get the correct result.

VI. CONCLUSIONS

We have considered phase space path integrals with the property that the Hamiltonian generates an isometry of the phase space. Using equivariant cohomology in the loop space we were able to reduce the path integrals to finite-dimensional integrals and sums. We also noticed that the results were not uniquely defined because of spectral asymmetry. The choice of regularization yielded equivariant $\hat{A}$ and Todd classes.

We applied localization to the harmonic oscillator and to the quantization of coadjoint orbits. We showed that localization produces correct results for these systems. In addition, we derived Kirillov and Weyl character formulas that produce correct characters for Lie groups without the Weyl shift. We demonstrated this explicitly by evaluating the character for SU(2). The explanation for the Weyl shift was the same as in the case of the Coxeter shift[20] in Chern–Simons theory, the η-invariant.

It would be interesting to apply our formalism to more complicated systems such as loop groups and field theories. Also, it seems possible to use localization and equivariant cohomology to study quantum integrability, generic supersymmetric theories, and problems in classical mechanics, as well.

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One dimensional periodic Dirac Hamiltonians: Semiclassical and high-energy asymptotics for gaps

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In this article we consider a one-dimensional Dirac operator with a potential of Gevrey class α and study the semiclassical and high-energy asymptotics of the spectral gaps for a region of energies that in the Schrödinger case corresponds to unbounded motion. An exponential upper bound for the gap's widths as well as the asymptotic expansion of their positions are derived for both cases; the first two terms in the asymptotic expansions are explicitly written down for the scalar potential case. © *1996 American Institute of Physics.* [S0022-2488(96)02406-1]

I. INTRODUCTION

The asymptotics of the spectral gaps of the one-dimensional Schrödinger operators with periodic potentials, for both high-energy and semiclassical limits, is fairly well understood (for polynomial bounds on the error one can see Ref. 1, while for exponential bounds one can see Ref. 2, for an inverse scattering method, or Ref. 3 and references therein for WKB-type methods). The extension of this kind of results to more general systems of ordinary differential equations is far from being straightforward. In this paper we consider the problem of the high-energy asymptotics and of the semiclassical behavior of the spectral gaps for a general one-dimensional Dirac Hamiltonian with a periodic potential, as given by the formula (1). The class of potentials that we cover contains the Gevrey classes of any order α (in particular for $\alpha=1$ we recover the analytic case that is the one usually considered).

The method that we propose starts from the results in Ref. 4 about adiabatic expansions, that up to the end lead to a ''quantization rule'' precise enough to provide both the asymptotic expansion of the position of the spectral gaps, as well as the exponential decrease of their widths. Analogous results for the Schrödinger operator were written down, by using the same method, in the (partly unpublished) notes.[4] Let us notice that some of the results (e.g., the asymptotic expansion of the position of the gaps) seem to be new, even in the Schrödinger case (see, however, Ref. 1 for related results). Let us also point that the method we use allows us to extend some of the results below to more general systems of ordinary differential equations, e.g. to the linear Hamiltonian systems considered in Ref. 5. Our reason to restrict ourselves to the Dirac case were on the one hand to keep the length of the note to a reasonable level and on the other hand the fact the one-dimensional Dirac operator, apart from describing the physical three-dimensional situation when the periodic potential is actually constant along two spatial directions, appears also in other contexts. As an example, the so-called AKNS operator (recently studied in Ref. 6 by the inverse scattering method), which appeared[7,8] in connection with the ''generalized Fourier transform'' for nonlinear differential equations, is equivalent to a particular case of the Dirac Hamiltonian that we consider.

II. THE PROBLEM AND THE MAIN RESULTS

The one-dimensional Dirac Hamiltonian acting on $L^2(\mathbf{R};\mathbf{C}^2)$, has the following form:

$$H_{\mathrm{D}}(\hbar):=-i\hbar\sigma_1\partial+m\sigma_3+\mathbf{V}(s), \tag{1}$$

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where ∂ is the operator of derivation with respect to s on $\mathbf{R}$, $m \in \mathbf{R}_+$, σ_j for $j=1,2,3$ are the Pauli matrices:

$$\sigma_1=\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad \sigma_2=\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \quad \sigma_3=\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

and $\mathbf{V}(s)$ is a 2×2 Hermitian matrix-valued function. We assume that $\mathbf{V}(s)$ is C^∞ and periodic with period T:

$$\mathbf{V}(s+T)=\mathbf{V}(s). \tag{2}$$

Since the Pauli matrices are Hermitian and together with $\sigma_0=1$ they form a basis for the 2×2 Hermitian matrices one has

$$\mathbf{V}(s)=\sum_{j=0}^{3} V_j(s)\sigma_j, \tag{3}$$

where V_j are real C^∞ functions of period T. By Floquet theory one can show[9] that the spectrum $\sigma_{\mathrm{D}}(\hbar)$ of $H_{\mathrm{D}}(\hbar)$ has a ''band structure,'' a point $E \in \mathbf{R}$ being in $\sigma_{\mathrm{D}}(\hbar)$ if and only if the equation

$$H_{\mathrm{D}}(\hbar)f=Ef \tag{4}$$

admits a solution f that is uniformly bounded on $\mathbf{R}$. Multiplied by σ_1, (4) takes the form

$$i\hbar\ \partial f(s)=H_E(s)f(s); \quad H_E(s)=-im\sigma_2+\sigma_1\mathbf{V}(s)-E\sigma_1, \tag{5}$$

which is a linear ''evolution'' equation in $\mathbf{C}^2$, with a ''time'' dependent non-Hermitian generator $H_E(s)$. By the above discussion, if the ''motion'' generated by $H_E(s)$ is stable, then $E \in \sigma_{\mathrm{D}}(\hbar)$. We are thus led to study the stability of the ''motion'' generated by $H_E(s)$. For our method to work we need that

$$\sup_{s\in\mathbf{R}}\ \sup_{t\in\mathbf{R}} \|e^{itH_E(s)}\|<\infty. \tag{6}$$

Let

$$\lambda_{\pm}(s,E):=V_1(s)\pm\{(V_0(s)-E)^2-(m+V_3(s))^2-V_2(s)^2\}^{1/2} \tag{7}$$

be the eigenvalues of $H_E(s)$. Then (6) holds true for all $E \in \Sigma_d$, where

$$\Sigma_d:=\{E\in\mathbf{R}|\ \inf_{s\in\mathbf{R}}\{(V_0(s)-E)^2-(m+V_3(s))^2-V_2(s)^2\}\geqslant d\}, \tag{8}$$

where d is a strictly positive constant, since in this case $\lambda_{\pm}(s,E)$ are real and distinct.

In what follows we assume that $\mathbf{V}(s)$ belongs to the Gevrey class of order $\alpha\geqslant 1$. More exactly, we suppose the following.

Hypothesis V_α: There exist $M<\infty$ and $\alpha\geqslant 1$, such that

$$\sup_{s\in[0,T]} |\partial^k V_j(s)|\leqslant M^k(k!)^\alpha.$$

Remarks:

1. Since the functions V_j are bounded: $\Sigma_d\supset\mathbf{R}\backslash[-A,A]$ for sufficiently large A.

2. In the scalar case (8) reduces to

$$\Sigma_d=\{E\in\mathbf{R}|\ \inf_{s\in\mathbf{R}}\{(V_0(s)-E)^2-m^2\}\geqslant d\}.$$

Our results are summarized in the following.

Theorem: Suppose $\mathbf{V}(s)$ satisfies (2) and the hypothesis V_α. Let $\rho_{\mathrm{D}}(\hbar)$ be the resolvent set of $H_{\mathrm{D}}(\hbar)$.

A. (Semiclassical limit): There exists $\hbar_0>0$ depending upon M and d, such that for all $\hbar\in(0,\hbar_0]$ and all $E\in\Sigma_d$ there exist two real functions $\phi_\pm(s,\hbar,E)$, such that the following occurs.

(i) $\phi_\pm(s,\hbar,E)$ have asymptotic expansions in $\hbar$:

$$\phi_\pm(s,\hbar,E)\sim\hbar^{-1}\lambda_\pm(s,E)+\sum_{k=0}^{\infty}\hbar^k\phi_{\pm,k}(s,E).$$

More precisely, for any $n\in\mathbf{N}$ there exists $\hbar_n\in(0,\hbar_0]$ and a positive constant $C_{n,\hbar_n}$, depending only on n and $\hbar_n$ and such that for any $s\in[0,T]$ and any $\hbar\in(0,\hbar_n]$ one has the estimation

$$\left|\phi_\pm(s,\hbar,E)-\hbar^{-1}\lambda_\pm(s,E)-\sum_{k=0}^{n}\hbar^k\phi_{\pm,k}(s,E)\right|\leqslant C_{n,\hbar_1}\hbar^{n+1}.$$

(ii) If $K\subset\Sigma_d$ is a compact set and we denote

$$I(\hbar,E):=\int_0^T\{\phi_+(s,\hbar,E)-\phi_-(s,\hbar,E)\}ds,$$

$$\mathscr{E}(K;\hbar):=\{E\in K|\exists n\in\mathbf{Z}:I(\hbar,E)=2\pi n\},$$

then there exist constants $k_1<\infty$, $k_2>0$ depending only upon M and d, such that

$$\rho_{\mathrm{D}}(\hbar)\cap K\subset\{E\in K|\exists\widetilde{E}\in\mathscr{E}(K;\hbar):|E-\widetilde{E}|\leqslant k_1\ \exp(-k_2\hbar^{-1/\alpha})\}.$$

B. (High-energy limit): For sufficiently large E_0, there exist $n_0(E_0)$ and for any $n\geqslant n_0(E_0)$ there exist E_n, such that the following occurs.

(i) E_n have asymptotic expansions in n^{-1} of the form

$$E_n\sim\frac{\pi}{T}n+\sum_{k=0}^{\infty}F_{k+1}n^{-k}.$$

(ii) There exist constants $c_1<\infty$, $c_2>0$ depending only upon M and E_0, such that

$$\rho_{\mathrm{D}}(\hbar)\cap[E_0,\infty)\subset\{E\in[E_0,\infty)|\exists n\geqslant n_0:|E-E_n|\leqslant c_1\ \exp(-c_2n^{1/\alpha})\}.$$

Remarks:

(1) If $E_n(\hbar)$ are the solutions of the equation $I(\hbar,E)=2\pi n$, it follows from the proof of the theorem that $E_n(\hbar)-E_{n-1}(\hbar)$ is of order $\hbar$. Thus, for $\hbar\to0$ the gaps may accumulate, their separation diminishing like $\hbar$, but they shrink exponentially in $\hbar$.

(2) We would like to emphasize that our theorem does not provide a lower bound for the gap's width, so that some gaps may in fact be absent. A formula for the dominant term for the gap's width is much harder to obtain and not very much is known, even for the Schrödinger case (see Refs. 1, 3, 10, and references therein).

(3) The analog of the above theorem for the Schrödinger case was given in Ref. 4.

(4) From the results known for the Schrödinger case, one expects that the spectrum of $H_D(\hbar)$ contained in $\mathbf{R}\backslash\Sigma_0$ consists of energy bands that shrink exponentially as $\hbar\to 0$. The asymptotics of the first band has been obtained recently.[11]

(5) The functions $\phi_\pm(s,\hbar,E)$ and the constants F_k are easily computable for the case of the scalar potential ($V_1=V_2=V_3=0$), and the first three terms of the asymptotic expansions given in the above theorem are

$$\phi_{+,0}(s,E)=\phi_{-,0}(s,E)=0,$$

$$\phi_{+,1}(s,E)=\phi_{-,1}(s,E)=\frac{3}{8}\,m^2(\partial V_0(s))^2\{(V_0(s)-E)^2-m^2\}^{-5/2},$$

$$F_0=\pi/T \quad F_1=\frac{1}{T}\int_0^T V_0(s)ds, \quad F_2=-\frac{1}{2\pi}\int_0^T (3V_0(s)^2-m^2)ds.$$

One observes that the terms of order zero in the series of $\phi_\pm(s,\hbar,E)$, namely $\phi_{\pm,0}(s,E)$ (that are the leading terms of the Berry's phase) are zero. This is a general feature of the real Hamiltonians.

III. PROOF OF THE THEOREM

We give a detailed proof of part A of the theorem and we indicate the changes that one has to make in order to prove part B by a similar procedure. The proof combines the technique of quasi-invariant subspaces[4] for the time-dependent evolution (5) with methods from the theory of stability of motion for linear Hamiltonian systems.[12] For the sake of completeness we give in an Appendix the main definitions and results of Ref. 4 that we need. The proof is divided in a series of steps.

(1) Consider the Hamiltonian (1). As we already said, in view of (2) the Floquet theory[9] allows one to write a direct integral decomposition of $H_D(\hbar)$ and to show that $E\in\sigma_D(\hbar)$ if and only if (4) has a uniformly bounded solution on $\mathbf{R}$. The argument can be found in Ref. 9 in a rather abstract setting that covers our case.

(2) After multiplication with σ_1 (4) becomes [see (5)]

$$i\hbar\,\partial f(s)=H_E(s)f(s).$$

This equation can be viewed as an evolution equation for a classical system with a linear complex Hamiltonian. More precisely, if on $\mathbf{C}^2$ one considers the operator $J:=\sigma_1$ that satisfies

$$J=J^*=J^{-1},$$

and its associated nondegenerate, nondefinite scalar product:

$$\langle u,v\rangle:=(u,Jv), \tag{9}$$

with $(\cdot,\cdot)$ the usual scalar product on $\mathbf{C}^2$, one can verify that

$$H_E(s)=JH_E(s)^*J=:H_E(s)^\sharp, \tag{10}$$

which means that $H_E(s)$ is J Hermitian, i.e.

$$\langle u,H_E(s)v\rangle=\langle H_E(s)u,v\rangle.$$

As a consequence, if we denote by $U_\hbar(s,s_0;E)$ the evolution associated to (5):

$$i\hbar\,\partial_s U_\hbar(s,s_0;E)=H_E(s)U_\hbar(s,s_0;E); \quad U_\hbar(s_0,s_0;E)=\mathbf{1}, \tag{11}$$

then the following relation is verified:

$$U_\hbar(s,s_0;E)^\sharp U_\hbar(s,s_0;E)=\mathbf{1},$$

but due to the fact that the product $\langle\cdot,\cdot\rangle$ is not positive definite, this relation does not imply that $\|U_\hbar(s,s_0;E)\|\leqslant 1$, and our problem is precisely to find the values of E for which we have

$$\sup_{s\in\mathbf{R}}\|U_\hbar(s,s_0;E)\|=\infty. \tag{12}$$

(3) The condition $E\in\Sigma_d$ implies that $H_E(s)$ has two distinct real eigenvalues: $\lambda_\pm(s,E)$ given by (7). This implies that

$$H_E(s)=\sum_{\tau=\pm}\lambda_\tau(s,E)P_\tau(s,E), \tag{13}$$

where $P_\tau(s,E)$ are two projections in $\mathbf{C}^2$ satisfying the relations

$$P_\tau(s,E)^\sharp=P_\tau(s,E)=P_\tau(s,E)^2;\quad \sum_{\tau=\pm}P_\tau(s,E)=\mathbf{1},$$

$$P_+(s,E)P_-(s,E)=P_-(s,E)P_+(s,E)=0. \tag{14}$$

It follows that the associated eigenvectors satisfy the estimations

$$|\langle v_\tau(s),v_\tau(s)\rangle|\geqslant k(s)\|v_\tau(s)\|^2;\quad k(s)>0,$$

which, together with the fact that one can restrict s to the compact interval $[0,\ T]$, implies the existence of a strictly positive constant $k>0$, such that

$$|\langle v_\tau(s),v_\tau(s)\rangle|\geqslant k\|v_\tau(s)\|^2,\quad \forall s\in\mathbf{R},$$

i.e., the families of subspaces $P_\tau(s,E)\mathbf{C}^2$, $\tau=\pm$, are uniformly definite for $s\in\mathbf{R}$ (in the sense of Ref. 13). Indeed, let us fix $v_\pm\neq 0$ in $P_\pm(s,E)\mathbf{C}^2$ and suppose that $\langle v_-,v_-\rangle=0$. Any $v\in\mathbf{C}^2$ can be written as $v=\alpha v_-+\beta v_+$ and then $\langle v,v_-\rangle=0$, and since the product $\langle\cdot,\cdot\rangle$ is nondegenerate it follows that $v_-=0$. More precisely, let us observe that $\Sigma_d=\Sigma_d^+\cup\Sigma_d^-$, where

$$\Sigma_d^+:=[\sup_{s\in\mathbf{R}}\{V_0(s)+((V_3(s)+m)^2+V_2(s)+d)^{1/2}\},+\infty)\subset\mathbf{R},$$

$$\Sigma_d^-:=(-\infty,\inf_{s\in\mathbf{R}}\{V_0(s)-((V_3(s)+m)^2+V_2(s)+d)^{1/2}\}]\subset\mathbf{R},$$

and by some elementary algebra one can verify that $\langle v_+,v_+\rangle$ is positive for $E\in\Sigma_d^-$ and negative for $E\in\Sigma_d^+$, while $\langle v_-,v_-\rangle$ is positive for $E\in\Sigma_d^+$ and negative for $E\in\Sigma_d^-$.

(4) In order to apply the results from Ref. 4 taking $\hbar$ as the small parameter ϵ, one has to verify the ''gap'' and ''smoothness'' assumptions (see the hypothesis $\mathscr{H}_\alpha$ of the Appendix). The gap condition is evidently verified, since for $E\in\Sigma_d$

$$|\lambda_+(s,E)-\lambda_-(s,E)|\geqslant 2\sqrt{d}. \tag{15}$$

Let us now consider the smoothness condition. The condition $\mathscr{V}_\alpha$ implies directly that the family $H_E(s)$ satisfies for E in an arbitrary compact K:

$$\sup_{s\in[0,T]}\|\partial^k H_E(s)\|\leqslant N^k(k!)^\alpha, \tag{16}$$

where N depends only on M and the compact set K. The needed condition on the resolvent,

$$R_\hbar(s,E):=(H_E(s)-z)^{-1}, \tag{17}$$

follows from (16) and the following simple fact that can be proved by a slight modification of the argument in Ref. 14.

Lemma 1: Let f be a matrix-valued function with components of class $\mathbf{C}^\infty(\mathbf{R})$, satisfying: (i) f is of Gevrey class of order α, for some $\alpha\geqslant 1$, i.e. $\exists M\in\mathbf{R}_+$, such that

$$\sup_{s\in\mathbf{R}}\|\partial^k f(s)\|\leqslant M^k(k!)^\alpha,$$

(ii) $\exists\delta>0$, such that $|\det f(s)|\geqslant\delta$ for any $s\in\mathbf{R}$.

Then f is invertible for any $s\in\mathbf{R}$ and defines a function $\tilde{f}(s):=f(s)^{-1}$ that is also of the Gevrey class of order α, i.e. $\exists\tilde{M}\in\mathbf{R}_+$, such that

$$\sup_{s\in\mathbf{R}}\|\partial^k\tilde{f}(s)\|\leqslant\tilde{M}^k(k!)^\alpha.$$

(5) Following Ref. 4, for $\hbar$ small enough, one constructs (see the Appendix) for $\tau=\pm$ the J-orthogonal projections $P_{\tau,\hbar}(s,E)$ satisfying (14) with $P_\tau(s,E)$ replaced by $P_{\tau,\hbar}(s,E)$:

$$P_{\tau,\hbar}(s,E)\sim P_\tau(s,E)+\sum_{k=1}^{\infty}E_{\tau,k}(s,E)\hbar^k \tag{18}$$

(in the sense of an asymptotic series), and also satisfying the estimation

$$\|i\hbar\ \partial P_{\tau,\hbar}(s,E)-[H_E(s),P_{\tau,\hbar}(s,E)]\|\leqslant k_1\ \exp(-k_2\hbar^{-1/\alpha}), \tag{19}$$

where k_1,k_2 depend upon M,d, and K. In particular,

$$\lim_{\hbar\to 0}\|P_{\tau,\hbar}(s,E)-P_\tau(s,E)\|=0. \tag{20}$$

Moreover, from (20) and the fact that $P_\tau(s,E)\mathbf{C}^2$ are uniformly definite, it follows that $P_{\tau,\hbar}(s,E)\mathbf{C}^2$ are also uniformly definite, i.e., there exists $\kappa>0$, such that for all $v\in\mathbf{C}^2$,

$$|\langle P_{\tau,\hbar}(s,E)v,P_{\tau,\hbar}(s,E)v\rangle|\geqslant\kappa\|P_{\tau,\hbar}(s,E)v\|^2, \tag{21}$$

and the signs are the same as for $\langle P_\tau(s,E)v,P_\tau(s,E)v\rangle$. Notice also that due to the definitions given in the Appendix, $P_{\tau,\hbar}(s,E)$ are periodic functions of s with period T.

Consider $U^A_\hbar(s,s_0;E)$ associated to $P_{\tau,\hbar}(s,E)$, as given by Proposition A.5. In particular, it satisfies the intertwining property:

$$P_{\tau,\hbar}(s,E)=U^A_\hbar(s,s_0;E)P_{\tau,\hbar}(s_0,E)U^A_\hbar(s,s_0;E)^{-1}. \tag{22}$$

In spite of the fact that the operators $U^A_\hbar(s,s_0;E)$ are not unitary (they are J unitary), the intertwining property (22) allows us to control their norms. We remark first that from (21) it follows that there exist $c_1>0,c_2<\infty$ depending only upon κ, such that

$$c_1\|v\|^2\leqslant\sum_{\tau=\pm}|\langle P_{\tau,\hbar}(s,E)v,P_{\tau,\hbar}(s,E)v\rangle|\leqslant c_2\|v\|^2. \tag{23}$$

Using this relation and the J unitarity of the evolution, we can obtain an upper bound for the adiabatic evolution. In fact, for any $u \in \mathscr{H}$,

$$\|U_\hbar^A(s,s_0;E)u\|^2 \leqslant \frac{1}{c_1}\sum_{\tau=\pm}|\langle P_{\tau,\hbar}(s,E)U_\hbar^A(s,s_0;E)u, P_{\tau,\hbar}(s,E)U_\hbar^A(s,s_0;E)u\rangle|$$

$$= \frac{1}{c_1}\sum_{\tau=\pm}|\langle P_{\tau,\hbar}(s_0,E)v, P_{\tau,\hbar}(s_0,E)v\rangle| \leqslant \frac{c_2}{c_1}\|u\|^2, \tag{24}$$

so that we get the following estimation:

$$\|U_\hbar^A(s,s_0;E)\| \leqslant (c_2/c_1)^{1/2}, \tag{25}$$

where the constant c_2/c_1 does not depend on s and s_0, but only on d. A similar argument works for the inverse $U_\hbar^A(s,s_0;E)^{-1}$ so that the evolution $\{U_\hbar^A(s,s_0;E)\}_{s\in\mathbf{R}}$ is stable for any given $E \in \Sigma_d$ (with $d>0$).

(6) We want to estimate the difference between the two evolutions:

$$\{U_\hbar^A(s,s_0;E)\}_{s\in\mathbf{R}} \quad \text{and} \quad \{U_\hbar(s,s_0;E)\}_{s\in\mathbf{R}}.$$

Let us denote by $H_\hbar^A(s,E)$ the generator of the adiabatic evolution and let

$$B_\hbar(s,E) := H_E(s) - H_\hbar^A(s,E) \tag{26}$$

be the difference of the two generators. We consider the following factorization [(A17) in the Appendix]:

$$U_\hbar(s,s_0;E) = U_\hbar^A(s,s_0;E)\Omega_\hbar(s,s_0;E). \tag{27}$$

Using the results proved in Ref. 4 and reviewed in the Appendix, for each $s \in [0,T]$ one can find two constants $k(s)<\infty$ and $k_2(s)>0$, so that if we denote

$$\delta_\hbar(s) := k(s)\exp(-k_2(s)\hbar^{-1/\alpha}), \tag{28}$$

we have the estimation

$$\|B_\hbar(s,E)\| \leqslant \delta_\hbar(s), \quad \forall s \in \mathbf{R}. \tag{29}$$

By integration we obtain the following inequality:

$$\|\Omega_\hbar(s,s_0;E)-\mathbf{1}\| \leqslant \frac{1}{\hbar}\int_{s_0}^{s}\|U_\hbar^A(u,s_0;E)\|\|U_\hbar^A(u,s_0;E)^{-1}\|\|B_\hbar(u,E)\|du + \frac{1}{\hbar}\int_{s_0}^{s}\|U_\hbar^A(u,s_0;E)\|$$

$$\times\|U_\hbar^A(u,s_0;E)^{-1}\|\|B_\hbar(u,E)\|\|\Omega_\hbar(u,s_0;E)-\mathbf{1}\|du. \tag{30}$$

At this point we may use the following form of the Gronwall Lemma.

Lemma 2: Let $s_0 \in \mathbf{R}$ be fixed and $g,h \in L^\infty([s_0,\infty))$ be some positive functions with g nondecreasing on $[s_0,\infty)$. If $f \in L^\infty([s_0,\infty))$ satisfies

$$0 \leqslant f(t) \leqslant g(t) + \int_{s_0}^{t} h(s)f(s)ds$$

for almost all $t \in [s_0,\infty)$, then

$$f(t)\leqslant g(t)\exp\left(\int_{s_0}^{t} h(s)ds\right).$$

We obtain the following estimation:

$$\|\Omega_\hbar(s,s_0;E)-\mathbf{1}\|\leqslant\frac{c}{\hbar}\left(\int_{s_0}^{s}\delta_\hbar(u)du\right)\exp\left(\frac{c}{\hbar}\int_{s_0}^{s}\delta_\hbar(u)du\right). \tag{31}$$

(7) Due to the periodicity of $\mathbf{V}(s)$, we can study the stability of the evolution $\{U_\hbar(s,s_0;E)\}_{s\in\mathbf{R}}$ by looking only at the discrete evolution generated by the monodromy matrix:

$$M_\hbar(E):=U_\hbar(T,0;E). \tag{32}$$

Let us also define the adiabatic monodromy matrix:

$$M_\hbar^A(E):=U_\hbar^A(T,0;E) \tag{33}$$

and the factorization [similar to (27)]

$$M_\hbar(E)=M_\hbar^A(E)W_\hbar(E),\quad W_\hbar(E):=\Omega_\hbar(T,0;E), \tag{34}$$

so that

$$\|M_\hbar(E)-M_\hbar^A(E)\|\leqslant\frac{c}{\hbar}\left(\int_0^T\delta_\hbar(u)du\right)\exp\left(\frac{c}{\hbar}\int_0^T\delta_\hbar(u)du\right). \tag{35}$$

Due to the properties of $k(s)$ and $k_2(s)$ given in Ref. 4 and due to the fact that the interval $[0,T]$ is compact, there exist two positive constants $c_1<\infty$ and $c_2>0$ such that

$$\int_0^T\delta_\hbar(u)du\leqslant c_1\ \exp(-c_2\hbar^{-1/\alpha}). \tag{36}$$

In conclusion,

$$\|M_\hbar(E)-M_\hbar^A(E)\|\leqslant\frac{c}{\hbar}\exp(-c_2\hbar^{-1/\alpha}). \tag{37}$$

Moreover, the adiabatic evolution being stable [step (5)], it follows that it exists a finite constant c, such that

$$\|(M_\hbar^A(E))^n\|\leqslant c,\quad \forall n\in\mathbf{N}. \tag{38}$$

Let us now explicitly compute the eigenvalues of the adiabatic monodromy matrix. We choose a basis $\{v_\tau(E)\}_{\tau=\pm}$ in $\mathbf{C}^2$, such that $v_\tau(E)\in\mathscr{R}P_\tau(0,E)$ and

$$|\langle v_\tau(E),v_\tau(E)\rangle|=1,\quad \text{for } \tau=\pm.$$

We define the smooth (C^∞), periodic $\mathbf{C}^2$-valued functions:

$$v_\tau(s;E):=U_\hbar(s,0;E)v_\tau(E), \tag{39}$$

and we remark that they verify the relations

$$|\langle v_\tau(s;E),v_\tau(s;E)\rangle|=1,\quad \langle v_+(s;E),v_-(s;E)\rangle=0, \tag{40}$$

$$v_\tau(s;E) \in \mathscr{R}P_\tau(s,E), \quad \forall s \in \mathbf{R}. \tag{41}$$

For sufficiently small $\hbar$, we define the two $\mathbf{C}^2$-valued functions:

$$w_{\tau,\hbar}(s;E) := \left|\langle v_\tau(s;E), P_{\tau,\hbar}(s,E)v_\tau(s;E)\rangle\right|^{-1/2} P_{\tau,\hbar}(s,E)v_\tau(s;E), \tag{42}$$

that are periodic in s, and for fixed s and E take values in $\mathscr{R}P_{\tau,\hbar}(s,E)$. Taking into account that $U^A_\hbar$ is an intertwining family for the set of one-dimensional projections $\{P_{\tau,\hbar}(s,E)\}_{s\in\mathbf{R}}$ and making use of the differential equation satisfied by $\{U^A_\hbar(s,0;E)\}_{s\in\mathbf{R}}$, we can see that

$$U^A_\hbar(s,0;E)w_{\tau,\hbar}(s;E) = \exp\left(-i\int_0^s \phi_\tau(u,\hbar,E)du\right) w_{\tau,\hbar}(s;E), \tag{43}$$

where we have introduced the following functions:

$$\phi_\tau(u,\hbar,E) := \pm\frac{1}{\hbar}\langle w_{\tau,\hbar}(u;E), H^A_\hbar(u,E)w_{\tau,\hbar}(u;E)\rangle \mp i\left\langle w_{\tau,\hbar}(u;E), \frac{\partial}{\partial u} w_{\tau,\hbar}(u;E)\right\rangle. \tag{44}$$

These functions are real because of the evident identity:

$$\frac{\partial}{\partial u}\langle w_{\tau,\hbar}(u;E), w_{\tau,\hbar}(u;E)\rangle = 0,$$

and they are the functions appearing in part A of our theorem of Sec. I. The periodicity with respect to s implies the following form for the adiabatic monodromy matrix:

$$M^A_\hbar(E) = \exp(-i\Phi^+_n(E))P_{+,\hbar}(0,E) + \exp(-i\Phi^-_\hbar(E))P_{-,\hbar}(0,E), \tag{45}$$

$$\Phi^\tau_\hbar(E) := \int_0^T \phi_\tau(u,\hbar,E)du. \tag{46}$$

Thus $M^A_\hbar(E)$ has the eigenvalues $\mu^A_{\tau,\hbar}(E) \equiv \exp(-i\Phi^\tau_\hbar(E))$ and is evidently stable.

Let us remark here that due to the exponential estimation for the difference

$$B_\hbar(u,E) := H_E(u) - H^A_\hbar(u,E)$$

in deriving the asymptotic expansion for $\phi_\tau(u,\hbar,E)$, one can replace $H^A_\hbar(u,E)$ by $H_E(u)$. Now the asymptotic expansion for $\phi_\tau(u,\hbar,E)$ easily follows from that of the projections $P_{\tau,\hbar}(s,E)$ (theorem A.3 in the Appendix), and one can see that the leading term is $\hbar^{-1}\lambda_\tau(u,E)$.

(8) As remarked in the first step of our proof $E \in \sigma_{\mathrm{D}}(\hbar)$ if and only if Eq. (4) has a uniformly bounded solution on $\mathbf{R}$; thus, in order that $E \in K \subset \Sigma_d$ to belong to $\rho_{\mathrm{D}}(\hbar)$, it is necessary that the discrete evolution generated by $M_\hbar(E)$ should not be stable. The results of step (7) imply that the evolution generated by $M^A_\hbar(E)$ is stable for any $E \in \Sigma_d$. Moreover, for small $\hbar$, $M_\hbar(E)$ is very close to $M^A_\hbar(E)$ in the matrix norm. Observing that both $M_\hbar(E)$ and $M^A_\hbar(E)$ are J unitary, we make use of the following result:[12]

Lemma 3: Let M be a J-unitary matrix on $\mathbf{C}^2$ (with J unitary and self-adjoint), then its eigenvalues are symmetric with respect to the unit circle in $\mathbf{C}$.

Let $\{\mu_{\tau,\hbar}(E)\}_{\tau=\pm}$ be the two eigenvalues of $M_\hbar(E)$. We know that the eigenvalues of $M^A_\hbar(E)$ belong to the unit circle and let us suppose that

$$|\mu^A_{+,\hbar}(E) - \mu^A_{-,\hbar}(E)| = \epsilon_0 > 0. \tag{47}$$

Then for $\hbar$ small enough, we have

$$|\mu^A_{\tau,\hbar}(E)-\mu_{\tau,\hbar}(E)|\leqslant\|M^A_\hbar(E)-M_\hbar(E)\|\leqslant\frac{c}{\hbar}\exp(-c_2\hbar^{-1/\alpha})<\frac{\epsilon_0}{4}. \tag{48}$$

Using now Lemma 3, we conclude that the eigenvalues $\{\mu_{\tau,\hbar}(E)\}_{\tau=\pm}$ must also belong to the unit circle, the evolution generated by $M_\hbar(E)$ thus being stable. In conclusion, if (47) is true and $\hbar$ is sufficiently small, $E\in\sigma_{\mathrm{D}}(\hbar)$. Thus, in the limit $\hbar\to 0$, the necessary condition for E to belong to $\rho_{\mathrm{D}}(\hbar)$ is

$$\mu^A_{+,\hbar}(E)=\mu^A_{-,\hbar}(E). \tag{49}$$

Taking into account (45) and (46), condition (49) is precisely the condition

$$I(\hbar,E)=2\pi n,$$

defining the set $\mathscr{E}(\mathrm{K};\hbar)$ in the statement of part A of our theorem of Sec. I.

(9) In order to obtain the upper bound for the gap's width, we observe that for a small, fixed value of $\hbar$, we have

$$|\mu^A_{\tau,\hbar}(E)-\mu_{\tau,\hbar}(E)|\leqslant\frac{c}{\hbar}\exp(-c_2\hbar^{-1/\alpha}), \tag{50}$$

so that if

$$|\mu^A_{+,\hbar}(E)-\mu^A_{-,\hbar}(E)|\geqslant 2\frac{c}{\hbar}\exp(-c_2\hbar^{-1/\alpha}), \tag{51}$$

we conclude that the eigenvalues $\{\mu_{\tau,\hbar}(E)\}_{\tau=\pm}$ have to belong to the unit circle, so that $E\in\sigma_{\mathrm{D}}(\hbar)$. Hence, an upper bound for the gap's width can be derived from the condition

$$|\exp(-i\Phi^+_\hbar(E))-\exp(-i\Phi^-_\hbar(E))|\leqslant 2\frac{c}{\hbar}\exp(-c_2\hbar^{-1/\alpha}), \tag{52}$$

or equivalently

$$\left|\sin\left\{\int_0^T(\phi_+(u,\hbar,E)-\phi_-(u,\hbar,E))du\right\}\right|\leqslant\frac{c}{\hbar}\exp(-c_2\hbar^{-1/\alpha}). \tag{53}$$

As we explain in the Appendix, for fixed $\hbar$, the functions $\phi_\tau(u,\hbar,E)$ are differentiable with respect to E, their asymptotic series are differentiable term by term, and the derivatives of these series provide asymptotic expansions for the derivatives of $\phi_\tau(u,\hbar,E)$. The leading terms of these asymptotic expansions are $\hbar^{-1}\lambda_\tau(u,E)$ that has a nonzero derivative with respect to E, as one can easily see from the definition of $\lambda_\tau(u,E)$ in formula (7). The elementary inequality $|\sin x|\leqslant|x|$, $\forall x\in\mathbf{R}$, together with relation (53) imply the following upper bound for the gap's width:

$$|E-\widetilde{E}|\leqslant c_3\exp(-c_2\hbar^{-1/\alpha}),\quad \widetilde{E}\in\mathscr{E}(K), \tag{54}$$

for $\hbar$ small enough, as claimed in part A of our theorem in Sect. I.

(10) Concerning the second part of the theorem (the high-energy asymptotic expansion), we shall briefly comment on the changes one has to make in the above proof in order to get the desired conclusion. One has to fix $\hbar=1$ so that Eq. (5) becomes

$$i\,\partial f(s)=-im\sigma_2 f(s)+\sigma_1\mathbf{V}(s)f(s)-E\sigma_1 f(s). \tag{55}$$

By dividing with E, considering E large and denoting $\epsilon := E^{-1}$, we get the evolution equation:

$$i\epsilon\,\partial f(s) = -i\epsilon m\sigma_2 f(s) + \epsilon\sigma_1 \mathbf{V}(s) f(s) - \sigma_1 f(s) \equiv H_\epsilon(s) f(s). \tag{56}$$

In Ref. 4 it is observed that the general procedure elaborated for adiabatic expansions also works in the case when the generator $\{H(s)\}_{s\in\mathbf{R}}$ depends on the small parameter ϵ, as long as the generator $\{H_\epsilon(s)\}_{s\in\mathbf{R}}$, and all the derivatives of its resolvent are uniformly bounded for ϵ in a neighborhood of zero. The Hermitian nondefinite form $\langle\cdot,\cdot\rangle$ on $\mathbf{C}^2$ remains the same and one obtains two functions $\tilde{\phi}_\pm(s;\epsilon)$ given by a formula similar to (44). Then the same type of ''quantization rule'' is obtained and also similar asymptotic expansions.

Remark: We consider the scalar case $V_1(s) = V_2(s) = V_3(s) = 0$ and compute the first three terms of the asymptotic expansions for $\phi_\tau(u,\hbar,E)$ appearing in part A of the main theorem, and for the values E_n appearing in part B of the same theorem. Let us begin with $\phi_\tau(u,\hbar,E)$ and make use of the vector functions defined in step (7). We have

$$P_{\tau,\hbar}(s,E) = P_\tau(s,E) + \hbar E_{\tau,1}(s,E) + \hbar^2 E_{\tau,2}(s,E) + R, \tag{57}$$

with $\|R\| \leqslant c\hbar^3$ and c independent of s, $\hbar$, and E, but depending on the compact set $K \subset \Sigma_d$. We can easily see that

$$P_\tau(s,E) E_{\tau,1}(s,E) P_\tau(s,E) = 0, \tag{58}$$

$$P_\tau(s,E) E_{\tau,2}(s,E) P_\tau(s,E) = -P_\tau(s,E)[E_{\tau,1}(s,E)]^2 P_\tau(s,E). \tag{59}$$

Using these relations and the explicit formula for $E_{\tau,1}(s,E)$ [see (A6)], we obtain

$$E_{+,1}(s,E) = \frac{i}{\lambda_+ - \lambda_-}\{\langle \partial v_+, v_-\rangle |v_+\rangle\langle v_-| - \langle v_-, \partial v_+\rangle |v_-\rangle\langle v_+|\}, \tag{60}$$

$$\frac{1}{\hbar}\langle w_{\pm,\hbar}(u;E), H^A_\hbar(u,E) w_{\pm,\hbar}(u;E)\rangle = \pm\lambda_\pm(u,E)\frac{1}{\hbar} + \hbar\,\frac{|\langle \partial v_\pm(u,E), v_\mp\rangle|^2}{\lambda_+(u,E) - \lambda_-(u,E)}, \tag{61}$$

$$-i\left\langle w_{\tau,\hbar}(u;E),\ \frac{\partial}{\partial u} w_{\tau,\hbar}(u;E)\right\rangle = -i\left\langle v_\tau(u;E),\ \frac{\partial}{\partial u} v_\tau(u;E)\right\rangle + 2\hbar\,\frac{|\langle \partial v_\pm(u,E), v_\mp\rangle|^2}{\lambda_+(u,E) - \lambda_-(u,E)}. \tag{62}$$

In conclusion, we get

$$\phi_\pm(u,\hbar,E) = \lambda_\pm(u,E)\frac{1}{\hbar} \mp i\left\langle v_\tau(u;E),\ \frac{\partial}{\partial u} v_\tau(u;E)\right\rangle \pm 3\hbar\,\frac{|\langle \partial v_\pm(u,E), v_\mp\rangle|^2}{\lambda_+(u,E) - \lambda_-(u,E)} + r(\hbar^2). \tag{63}$$

With the leading term in the expansion being of order $\hbar^{-1}$, it is evident that the difference of two successive solutions E_n and E_{n+1} is of order $\hbar$. Now let us consider the scalar case and explicitly compute the first terms of the expansion. In this case

$$\lambda_\pm(u,E) = \pm\sqrt{(V_0(u) - E)^2 - m^2}, \tag{64}$$

$$v_\pm(u;E) = \sqrt{\frac{1}{2}}\begin{pmatrix} \dfrac{((V_0(u)-E)^2 - m^2)^{1/4}}{(V_0(u) - E + m)^{1/2}} \\ \\ \pm\dfrac{(V_0(u) - E + m)^{1/2}}{((V_0(u)-E)^2 - m^2)^{1/4}} \end{pmatrix}. \tag{65}$$

For the equation (56) by similar procedures, one obtains

$$\tilde{\lambda}_{\pm}(u,E)=\pm\sqrt{(\epsilon V_0(u)-1)^2-\epsilon^2 m^2}, \tag{66}$$

$$\tilde{v}_{\pm}(u;E)=\sqrt{\frac{1}{2}}\begin{pmatrix} \dfrac{((\epsilon V_0(u)-1)^2-\epsilon^2 m^2)^{1/4}}{(\epsilon V_0(u)-1+\epsilon m)^{1/2}} \\ \pm\dfrac{(\epsilon V_0(u)-1+\epsilon m)^{1/2}}{((\epsilon V_0(u)-1)^2-\epsilon^2 m^2)^{1/4}} \end{pmatrix}. \tag{67}$$

Introducing the relations (64), (65) into (63), we obtain the results given in remark 5 of Sec. I. Proceeding similarly with (66), (67) and solving for E up to order n^{-1}, we obtain the terms $F_k(s,E)$ for $k=0,1,2$.

APPENDIX A:

We gather here the main definitions and results from[4] that we have used in the proof of our main theorem of Sec. I. Suppose we are given a Hilbert space h with a sesquilinear Hermitian form $\langle\cdot,\cdot\rangle$ on it, defined by a Hermitian involution J on h. Let us consider a family of J-Hermitian operators $\{H(s)\}_{s\in\mathbf{R}}$ and the corresponding evolution equation:

$$i\epsilon\frac{\partial}{\partial s}U_\epsilon(s,s_0)=H(s)U_\epsilon(s,s_0), \tag{A1}$$

with a parameter $\epsilon\in[0,1)$. We are interested in the behavior of the solution $U_\epsilon(s,s_0)$ when $\epsilon\to 0$. Our procedure consists in considering ''quasi-invariant'' subspaces of $H(s)$ for ϵ small and to define a ''reduced evolution'' on these subspaces, that can be easily integrated. We denote

$$R_z(s):=(H(s)-z)^{-1}. \tag{A2}$$

$\mathscr{H}_\alpha$ *Hypothesis on* $H(s)$: For $s\in(a,b)\subset\mathbf{R}$, we consider a family of J-Hermitian operators $\{H(s)\}_{s\in(a,b)}$ satisfying the following.

(1.) For all $s\in(a,b)$, $H(s)$ has an isolated part of the spectrum $\sigma_0(s)$ such that

$$\sigma(s)=\sigma_0(s)\cup\sigma_1(s),\quad d(\sigma_0(s),\sigma_1(s)):=d(s)\geqslant d>0,$$

$$\operatorname{diam}(\sigma_0(s)):=D(s)\leqslant D<\infty.$$

(2.) Let $s\in(a,b)$ and let $\Gamma(s)$ be a contour enclosing $\sigma_0(s)$ in its interior and being at a distance $d(s)/2$ from $\sigma_0(s)$. We suppose there exists a neighborhood U of s, such that $\Gamma(s)\subset\rho(H(u))$ for $u\in U$ and there exists $\alpha\geqslant 1$ such that

$$\sup_{z\in\Gamma(s)}\left|\frac{\partial^k}{\partial s^k}R_z(s)\right|\leqslant b(s)c(s)^k(k!)^\alpha$$

for $k\in\mathbf{N}$, with $0\leqslant c(s),\ b(s)<\infty$.

We define the projection

$$P_0(s):=\frac{1}{2\pi i}\int_{\Gamma(s)}R_z(s)dz \tag{A3}$$

and build up some quasi-invariant associated subspaces and a corresponding reduced evolution. We denote

$$Q_0(s):=\mathbf{1}-P_0(s). \tag{A4}$$

Proposition A.1: Suppose that we are given a family $\{H(s)\}_{s\in(a,b)}$ of J-Hermitian operators on h, verifying the hypothesis $\mathscr{H}_\alpha$, and let P_0 be the projection given by (A3). Then the operators $\{E_j(s)\}_{j\in N}$ defined by

$$E_0(s):=P_0(s), \tag{A5}$$

$$E_j(s):=\sum_{m=1}^{j-1}E_m(s)E_{j-m}(s)-2P_0(s)\sum_{m=1}^{j-1}E_m(s)E_{j-m}(s)P_0(s)+\frac{1}{2\pi}\int_{\Gamma_{(s)}}R_z(s)$$
$$\times\{Q_0(s)\partial E_{j-1}(s)P_0(s)-P_0(s)\partial E_{j-1}(s)Q_0(s)\}R_z(s)dz \tag{A6}$$

are the unique solutions of the system of recurrent equations:

$$E_j(s)=\sum_{m=0}^{j}E_m(s)E_{j-m}(s), \tag{A7}$$

$$i\ \partial E_{j-1}(s)=[H(s),E_j(s)], \tag{A8}$$

and satisfy the estimations

$$\|E_j(s)\|\leqslant g(s)^j(j!)^\alpha, \tag{A9}$$

where $0\leqslant g(s)<\infty$ and $g(s)$ depends only on $c(s)$ and on the length of the contour $\Gamma(s)$.

We introduce the notation

$$N_\epsilon(s):=[(\epsilon g(s))^{-1/\alpha}]-1, \tag{A10}$$

where we have denoted by $[x]$ the entire part of x and we define

$$T_\epsilon(s):=\sum_{j=0}^{N_\epsilon(s)}\epsilon^jE_j(s). \tag{A11}$$

Proposition A.2: Suppose that we are given a family $\{H(s)\}_{s\in(a,b)}$ of J-Hermitian operators on h, verifying the hypothesis $\mathscr{H}_\alpha$, and let $T_\epsilon(s)$ be defined by (A11) and the family $\{E_j(s)\}_{j\in N}$ as given in Proposition A.1. Then we have that (i) for any $s\in(a,b)$, $\lim_{\epsilon\to0}\|T_\epsilon(s)-P_0(s)\|=0$; (ii) there exist two positive constants c_1 and c_2, such that

$$\|T_\epsilon(s)^2-T_\epsilon(s)\|\leqslant c_1b(s)\exp(-c_2(\epsilon g(s))^{-1/\alpha}).$$

Due to estimation (ii) of the above proposition, a procedure developed in Ref. 4 allows us to define the following projection:

$$P_\epsilon(s):=\frac{1}{2\pi i}\int_{\Gamma(s)}(T_\epsilon(s)-z)^{-1}\,dz, \tag{A12}$$

and its J-orthogonal projection: $Q_\epsilon(s):=\mathbf{1}-P_\epsilon(s)$.

Theorem A.3: Suppose that we are given a family $\{H(s)\}_{s\in(a,b)}$ of J-Hermitian operators on h, verifying the hypothesis $\mathscr{H}_\alpha$, then the following occurs.

(i) We have the asymptotic series $P_\epsilon(s)\sim\Sigma_{m=0}^{\infty}\epsilon^jE_j(s)$;

(ii) For any $s\in(a,b)$ there exist two positive constants $k_1(s)<\infty$ and $k_2(s)>0$, depending on $c(s)$ and the length of $\Gamma(s)$, such that

$$\|i\epsilon\,\partial P_\epsilon(s)-[H(s),P_\epsilon(s)]\|\leqslant b(s)k_1(s)\exp(-k_2(s)\epsilon^{-1/\alpha}).$$

Thus, we have obtained the quasi-invariant subspaces associated to the family $\{P_0(s)\}_{s\in(a,b)}$. Let us remark that the entire construction has been done pointwise, so that no integral over s is needed. We want to construct now an intertwining evolution for the family $\{P_\epsilon(s)\}_{s\in(a,b)}$, which, in addition, should have a J-Hermitian generator close to $H(s)$. As in Ref. 4 let us define

$$\begin{aligned}H^A_\epsilon(s):&=H(s)+(1-2P_\epsilon(s))\{i\epsilon\,\partial P_\epsilon(s)-[H(s),P_\epsilon(s)]\}\\&=P_\epsilon(s)H(s)P_\epsilon(s)+Q_\epsilon(s)H(s)Q_\epsilon(s)+(1-2P_\epsilon(s))(i\epsilon\,\partial P_\epsilon(s)),\end{aligned}\tag{A13}$$

$$B_\epsilon(s):=H(s)-H^A_\epsilon(s)\tag{A14}$$

and let $U^A_\epsilon(s,s_0)$ and $A_\epsilon(s,s_0)$ be the solutions of the following evolution equations:

$$i\epsilon\,\partial U^A_\epsilon(s,s_0)=H^A_\epsilon(s)U^A_\epsilon(s,s_0),\quad U^A_\epsilon(s_0,s_0)=\mathbf{1},\tag{A15}$$

$$\begin{gathered}i\,\partial A_\epsilon(s,s_0)=(1-2P_\epsilon(s))(i\epsilon\,\partial P_\epsilon(s))A_\epsilon(s,s_0),\\A_\epsilon(s_0,s_0)=\mathbf{1}.\end{gathered}\tag{A16}$$

Proposition A.4: The solution of the evolution equation (A16), which is called ''the parallel transport'' associated to the family $\{P_\epsilon(s)\}_{s\in(a,b)}$, is given by J-unitary operators and satisfies the relations

$$P_\epsilon(s)=A_\epsilon(s,s_0)P_\epsilon(s_0)A_\epsilon(s,s_0)^{-1},$$

$$P_\epsilon(s)(\partial A_\epsilon(s,s_0))P_\epsilon(s_0)=0.$$

Proposition A.5: The solution of the evolution equation (A15) is given by J-unitary operators, is an intertwining evolution for the family $\{P_\epsilon(s)\}_{s\in(a,b)}$, i.e.

$$P_\epsilon(s)=U^A_\epsilon(s,s_0)P_\epsilon(s_0)U^A_\epsilon(s,s_0)^{-1},$$

and we have the estimation

$$\|B_\epsilon(s)\|\leqslant b(s)k_1(s)\exp(-k_2(s)\epsilon^{-1/\alpha}),$$

with the same constants as in Theorem A.3.

If we define the factorization

$$U_\epsilon(s,s_0)=U^A_\epsilon(s,s_0)\Omega_\epsilon(s,s_0),\tag{A17}$$

one obtains for Ω_ϵ the following evolution equation:

$$\begin{gathered}i\epsilon\,\partial\Omega_\epsilon(s,s_0)=\{U^A_\epsilon(s,s_0)^{-1}B_\epsilon(s)U^A_\epsilon(s,s_0)\}\Omega_\epsilon(s,s_0),\\\Omega_\epsilon(s_0,s_0)=\mathbf{1}.\end{gathered}\tag{A18}$$

Propositions A.4 and A.5 imply that we can factorize $U^A_\epsilon(s,s_0)$ as the following product:

$$U^A_\epsilon(s,s_0)=A_\epsilon(s,s_0)U^r_\epsilon(s,s_0),\tag{A19}$$

where $\{U^r_\epsilon(s,s_0)\}_{s\in(a,b)}$ defines the ''reduced evolution'' on $P_\epsilon(s_0)h$ and satisfies the equation

$$[U^r_\epsilon(s,s_0),P_\epsilon(s_0)]=0. \tag{A20}$$

When $P_\epsilon(s_0)$ is of rank one, this evolution can be very easily integrated, and $U^r_\epsilon(s,s_0)$ is given by an operator of multiplication with a function $F_\epsilon(s,s_0)$.

Let us also remark that if $H(s)$ depends on a parameter E, taking values in some compact set and if one has uniform bounds on the E derivatives of all the s derivatives of the resolvent of $H(s)$ then all the procedures summarized in Theorem A.3 also work for the E derivatives of the projections $P_0(s;E)$. Thus, the asymptotic expansion for $P_\epsilon(s;E)$ can be differentiated term by term, and one obtains an asymptotic expansion for the E derivative of $P_\epsilon(s;E)$.

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The contraction of the SU(1,1) discrete series of representations by means of coherent states

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The group SU(1,1) is a deformation of the Poincaré group. This relationship is studied both at the classical level (coadjoint orbits) and at the quantum level (unitary representations). The contraction of the Lie algebras is written in such a way that the limit of coadjoint orbits, and hence of the classical mechanics, appears clearly. At the quantum level the representations are written on holomorphic functions Hilbert spaces and the contraction is realized by restricting these functions. It is shown that this restriction is a continuous operator. Moreover, using suitable coherent states, it is proved that the contraction extends to the representation of the whole enveloping algebras of the groups, hence it allows us to define the contraction of the quantum mechanics observables. © *1996 American Institute of Physics.* [S0022-2488(96)00106-5]

I. INTRODUCTION

It is well-known that the Lie algebra su(1,1) is a deformation of both the Lie algebra of the 1+1 Poincaré group $\mathcal{P}^{1,1}$ and the Lie algebra of the harmonic oscillator. In fact, writing

$$[X_0,X_1]=mc^2\kappa^2X_2,[X_2,X_0]=X_1/m,[X_2,X_1]=X_0/mc^2,$$

for su(1,1), one can see that the limit $\kappa\to 0$ gives the Poincaré Lie algebra and the limit $\kappa\to 0, c\to\infty, \kappa c=\omega$ gives the harmonic oscillator Lie algebra.[1] The contraction toward the harmonic oscillator has been studied in Ref. 2, we now study the contraction toward Poincaré group. Note that this contraction has another interpretation: The group SU(1,1) can be viewed as the relativity group of the anti-de Sitter space–time,[3] and the contraction is the zero curvature limit of a classical or quantum mechanics on a curved space–time. Both interpretations yield the same mathematical treatment that we now develop. This contraction has been studied by Refs. 4, 5 and 6, we shall follow the latter which constructs the contraction ''à la Dooley''[7] and obtains a deformation $\Pi_\kappa:\mathcal{P}^{1,1}\to\mathrm{SU}(1,1)$. If $\mathcal{B}_\kappa$ is the Hilbert space of the representation U of SU(1,1) and $\mathcal{H}$ the Hilbert space of the representation V of $\mathcal{P}^{1,1}$, one can define a precontraction map $i_\kappa:\mathcal{B}_\kappa\to\mathcal{H}$. The contraction is then realized formally by applying i_κ and, after that, by taking the limit $\kappa\to 0$. More precisely the essential result obtained in Ref. 6 is

$$\lim_{\kappa\to 0}\|i_\kappa U_{\Pi_\kappa(g)}i_\kappa^{-1}\psi-V_g\psi\|_{\mathcal{H}}=0, \tag{1}$$

where ψ belongs to a dense family in $\mathcal{H}$. The question of the continuity of the i_κ was not answered, we now give a positive answer. Moreover this construction was not satisfactory because the formula (1) is proved for ψ independent of κ. But the states of a relativistic harmonic oscillator are elements of $\mathcal{B}_\kappa$ and naturally depend on κ, hence it would be more natural to replace (1) by

$$\lim_{\kappa\to 0}\|i_\kappa U_{\Pi_\kappa(g)}\phi_\kappa-V_g i_\kappa\phi_\kappa\|_{\mathcal{H}}=0. \tag{2}$$

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This formula cannot be true for any $\phi_\kappa \in \mathcal{B}_\kappa$, and we have to look for the states in $\mathcal{B}_\kappa$ which contract, it means the states for which $\lim_{\kappa\to 0} i_\kappa \phi_\kappa$ exists in some sense. Moreover the mathematical elements that are physically relevant are the observables and their mean values, that is the reason why we define the contraction of the representation of the Lie algebra and even of the representation of the enveloping algebra. However there is some difficulty in defining the limit of operators that do not live on the same space. We shall overcome this difficulty by using coherent states. The states on which the mean values of the observables of SU(1,1) are calculated are usually the eigenvectors of the Hamiltonian, written $|n\rangle$ or the Berezin coherent states[8] written $|z\rangle$. They both form quantum frames:[9]

$$\mathrm{Id}=\sum_n |n\rangle\langle n| \quad \text{and} \quad \mathrm{Id}=\int_{\mathcal{D}} |z\rangle\langle z| d\mu,$$

where the last integral is taken on the unit disk of the complex plane which carries the representation of SU(1,1), with the invariant measure. Unfortunately these states do not contract in the sense defined above. This is not surprising because the map i_κ is the restriction of the states to the vertical axis of the disk whereas the states $|n\rangle$ have a circular symmetry and the states $|z\rangle$ are concentrated on the point z, and the latter contracts in a weak sense only for z with real part equal to zero. The representation of SU(1,1) is square-integrable, hence for any $\psi_\kappa \in \mathcal{B}_\kappa$, the $U_g\psi_\kappa$ form a frame of $\mathcal{B}_\kappa$. The problem is to choose ψ_κ in a convenient way. The above remark on i_κ suggests that ψ_κ must be concentrated as near to the vertical axis of $\mathcal{D}$ as possible. Moreover the property for a state of minimizing the uncertainty relations is equivalent to being the eigenvector for some element of the representation of the complexified Lie algebra. This property should be preserved by the contraction and we shall see that this is the case as well. Hence we shall look for coherent states, minimizing the uncertainty relation, and whose shape[10] is as near to the vertical axis as possible. Such a state exists, and using the square integrability of the representation it allows us to construct a quantum frame that we shall use to define the contraction of quantum observables. *We shall prove that for* $\mathfrak{a}$ *in the* SU(1,1) *enveloping algebra the operator* $U(\mathfrak{a})$ *contracts to* $V(C(\mathfrak{a}))$ *where* $C(\mathfrak{a})$ *is the contraction of* $\mathfrak{a}$.

Dooley has suggested the use of the scheme of geometric quantization to study the contraction,[7] however the usual definition of the contractions is written with a rather arbitrary identification of the Lie algebras. This identification induces an identification of the dual spaces for which there is no convergence of the orbits. We develop below a new way to define contractions for which this disadvantage disappears: the coadjoint orbits do converge. With this definition the process of contraction becomes very clear at the classical mechanics level: Indeed *the coadjoint orbits are interpreted as phase spaces and the phase space of the first system tends to the phase space of the second system as the parameter tends to* 0.

II. THE GROUPS AND THEIR REPRESENTATIONS

The contraction of groups, or more precisely of Lie algebras, has been introduced by Inonü and Wigner,[11] and has been studied, for instance, in Refs. 12 and 7. We shall use a definition which is a little bit different:

Definition 2.1: Let $\mathfrak{g}_1=(V_1,[,]_1)$ *and* $\mathfrak{g}_2=(V_2,[,]_2)$ *be two Lie algebras. We say that* $\mathfrak{g}_2$ *is a contraction of* $\mathfrak{g}_1$ *when there exists a family* $\Phi_\kappa, \kappa \in \mathbb{R}^{+*}$ *of invertible linear maps from* V_2 *to* V_1 *such that*

$$\lim_{\kappa\to 0} \Phi_\kappa^{-1}[\Phi_\kappa x, \Phi_\kappa y]_1=[x,y]_2, \quad \forall x,y \in \mathfrak{g}_2.$$

One also says that $\mathfrak{g}_1$ is a deformation of $\mathfrak{g}_2$, the link between contractions and deformations is discussed in Ref. 13. In the papers previously cited, the spaces V_1 and V_2 are identified as vector spaces in a somehow arbitrary way, but the map Φ_κ furnishes another identification between these spaces, and we shall see that this is more natural. In fact, we choose a basis f_i of V_2, and note

c_{ij}^k the corresponding structure constants. Let be $f_i^\kappa=\Phi_\kappa(f_i)$ and let $c_{ij}^k(\kappa)$ be the corresponding structure constants in $\mathfrak{g}_1$. From $[f_i^\kappa,f_j^\kappa]_1=c_{ij}^k(\kappa)f_k^\kappa$ and from the above definition we get

$$c_{ij}^k=\lim_{\kappa\to 0}c_{ij}^k(\kappa). \tag{3}$$

We can identify the spaces $\mathfrak{g}_1$ and $\mathfrak{g}_2$ by means of the map Φ_κ, if this space is of finite dimension, the equality (3) implies that the endomorphism $\mathrm{ad}_{f_i^\kappa}$ tends to ad_{f_i} when $\kappa\to 0$, in the sense of the finite dimensional vector spaces natural topology. The identification of the Lie algebras allows an identification of the groups G_1 and G_2, at least in the vicinity of the identity, by means of the exponential map. The continuity of this map implies that the adjoint and coadjoint representations of G_1 converge toward the corresponding representations of G_2. Hence we have also the convergence of coadjoint orbits: *The contraction of the relativity groups implies the convergence of the whole classical mechanics of the first system toward the classical mechanics of the second system.* This was not the case in the usual definition of the contraction.

Here are some useful results on SU(1,1) and on the Poincaré group $\mathcal{P}^{1,1}$. The group SU(1,1) is the following set of matrices:

$$g=\begin{pmatrix}\alpha & \beta\\ \overline{\beta} & \overline{\alpha}\end{pmatrix},\quad |\alpha|^2-|\beta|^2=1. \tag{4}$$

The Lie algebra is three dimensional, here is a basis of this space:

$$e_0=\frac{1}{2}\begin{pmatrix}i & 0\\ 0 & -i\end{pmatrix},\quad e_1=-\frac{1}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},\quad e_2=\frac{1}{2}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}.$$

The Poincaré group is the following set of matrices:

$$(a,\theta)=\begin{pmatrix}\cosh\theta & \sinh\theta & a^0\\ \sinh\theta & \cosh\theta & a^1\\ 0 & 0 & 1\end{pmatrix}.$$

The Lie algebra basis associated with this parameterization is written:

$$f_i=\frac{d}{da^i}(a,\theta)_{(a,\theta)=Id},i=0,1 \text{ and } f_2=\frac{d}{d\theta}(a,\theta)_{(a,\theta)=Id}.$$

We shall see now that the group SU(1,1) is a deformation of the Poincaré group, in fact we define:

$$\begin{array}{rccl}\Phi_\kappa: & p(1,1) & \to & \mathrm{su}(1,1),\\ & f_i & \mapsto & \kappa e_i,\quad i=0,1\\ & f_2 & \mapsto & e_2,\end{array}$$

and one can see that

$$\lim_{\kappa\to 0}\Phi_\kappa^{-1}[\Phi_\kappa f_i,\Phi_\kappa f_j]=[f_i,f_j].$$

This allows us to write the map which realizes the deformation

$$\begin{array}{rccc}\Pi_\kappa: & \mathcal{P}^{1,1} & \to & \mathrm{SU}(1,1)\\ & (a,\theta)=e^{a^0f_0+a^1f_1}e^{\theta f_2} & \mapsto & e^{\kappa(a^0e_0+a^1e_1)}e^{\theta e_2}.\end{array} \tag{5}$$

The SU(1,1) coadjoint orbit M_κ that we consider is defined by the equation

$$x_0^2-x_1^2-\kappa^2x_2^2=1, \quad x_0>0,$$

written in the dual basis $f_i^{\kappa *}$. This orbit is interpreted as the phase space of the system,[6] and using the above identification, it converges to M_0

$$x_0^2-x_1^2=1, \quad x_0>0,$$

when $\kappa\to 0$. The manifold M_0 is a coadjoint orbit of the Poincaré group and is interpreted as the phase space for a relativistic free particle on the two dimensional flat space–time. Then, following the argumentation of Ref. 6, one remarks that the curve C defined by

$$x_0^2-x_1^2=1, \quad x_2=0,$$

is a submanifold of all the M_κ, hence we shall write the quantum representation of the Poincaré group on a space of functions on C. This can be realized by means of a geometric quantization. Moreover the SU(1,1) representation corresponding to M_κ by geometric quantization can be more easily written on the unit disk of the plane, which is diffeomorphic to the orbits by means of a stereographic projection. By this projection, the curve C projects onto the imaginary axis of the disk and the precontraction will be realized by the restriction to this axis. More precisely, the SU(1,1) representations involved here are those of the discrete series. The Hilbert space is defined as follows:

$$\mathcal{B}_\kappa=\{f; f\in L^2(\mathcal{D},dP_\kappa); f \text{ holomorphic on } \mathcal{D}\},$$

where $\mathcal{D}=\{z\in\mathbb{C}; |z|<1\}$ and $dP_\kappa(z,\overline{z})=(2\kappa^{-1}-1)(1-z\overline{z})^{2\kappa^{-1}-2}dz\,d\overline{z}/\pi$ with $1/2<\kappa^{-1}\in\mathbb{N}/2$. The group representation is given by

$$U_g f(z)=(-\overline{\beta}z+\alpha)^{-2\kappa^{-1}} f\left(\frac{\overline{\alpha}z-\beta}{-\overline{\beta}z+\alpha}\right),$$

where g is as in (4). Note that this representation is defined on $\mathcal{D}$, which can be interpreted as the phase space, and the basis e_i of the Lie algebra can be used to define the three classical observables (see Ref. 2 for more details):

$$k_0=\frac{1+z\overline{z}}{1-z\overline{z}}, \quad k_1=i\frac{z-\overline{z}}{1-z\overline{z}}, \quad k_2=\frac{z+\overline{z}}{1-z\overline{z}}, \tag{6}$$

which are the classical version of the three quantum observables

$$K_i f=i\frac{d}{d\alpha}(U_{e^{\alpha e_i}}f)_{\alpha=0}.$$

We consider now the Poincaré group, the representation is defined on $L^2(]-1,1[;2dx/(1-x^2))=\mathcal{H}$ by

$$V_{(a,\theta)}f(x)=\exp\left(-i\frac{1+x^2}{1-x^2}a^0-i\frac{2x}{1-x^2}a^1\right)f\left(\frac{x\cosh(\theta/2)+\sinh(\theta/2)}{\cosh(\theta/2)+x\sinh(\theta/2)}\right).$$

This representation is equivalent to the usual Wigner one by the change of variable $x=p/(p_0+1)$. The observables corresponding to the basis f_i are given by

$$P_0=\frac{1+x^2}{1-x^2},\quad P_1=\frac{2x}{1-x^2},\quad P_2=i\frac{1-x^2}{2}\frac{d}{dx}. \tag{7}$$

Moreover the map Φ_κ allows us to define the contraction for the enveloping algebra in the following way. For E a vector space let TE be the tensor algebra of E, and for any algebra A, let

$$A[[\kappa]]=\oplus_{n\geqslant 0}(\kappa^n A)$$

be the set of formal power series with coefficients in A. This is an associative graded algebra. The map $T\Phi_\kappa: Tp(1,1)\to T\mathrm{su}(1,1)$ can be extended by linearity in

$$T_\kappa\Phi_\kappa: Tp(1,1)[[\kappa]]\to T\mathrm{su}(1,1)[[\kappa]],$$

which is injective and nonsurjective because of the definition of Φ_κ. Let E_κ be the image of $T_\kappa\Phi_\kappa$, this is the sub-algebra generated by the f_i^κ. One can see easily that we obtain the following commutative diagram:

$$\begin{array}{ccccc} Tsu(1,1)[[\kappa]] & \supset & E_\kappa & \xrightarrow{(T_\kappa\Phi_\kappa)^{-1}} & Tp(1,1)[[\kappa]] \\ \downarrow \pi_1 & & \downarrow \pi_2 & & \downarrow \pi_3 \\ \mathfrak{U}su(1,1)[[\kappa]] & \supset & \pi_1(E_\kappa) & \xrightarrow{C} & \mathfrak{U}p(1,1) \end{array}$$

where $\mathfrak{U}p(1,1)$ and $\mathfrak{U}\mathrm{su}(1,1)$ are the enveloping algebras, π_1 the natural projection, π_2 the restriction of π_1 and π_3 the projection composed with the operation $\kappa=0$. In fact one verifies easily that any element in the kernel of π_2 is also in the kernel of $\pi_3(T_\kappa\Phi_\kappa)^{-1}$, so there exists a linear application C which makes the diagramm commutative, C is the contraction map for the enveloping algebras.

Then one defines $K_i^\kappa=i(d/d\alpha)(U_{e^{\alpha f_i^\kappa}})_{\alpha=0}$. The representations U and V yield differential representations of the spaces in the previous diagram. We write again U and V for these differential representations. For any $\mathfrak{a}$ in $\pi_1(E_\kappa)$, the operator $U(\mathfrak{a})$ is of the form $P(K_0^\kappa,K_1^\kappa,K_2^\kappa,\kappa)$, where P is a polynomial. We shall see that this observable contracts in some sense toward $P(P_0,P_1,P_2,0)=V(C(\mathfrak{a}))$.

III. PRECONTRACTION

The precontraction is the following transformation. For $f\in\mathcal{B}_\kappa$ let

$$i_\kappa(f)(x)=(1-x^2)^{\kappa^{-1}}f(ix).$$

Then we have the following result.

Theorem 3.1: *The map i_κ is a continuous injection from $\mathcal{B}_\kappa$ to $\mathcal{H}$.*

Proof: The map i_κ is clearly injective, thanks to the analyticity of the elements of $\mathcal{B}_\kappa$. Let $f(z)=\Sigma_{n\geqslant 0}a_n z^n$ be in $\mathcal{B}_\kappa$, and let be

$$I=\|f\|^2_{\mathcal{B}_\kappa}=\sum_{n\geqslant 0}|a_n|^2\frac{\Gamma(2\kappa^{-1})\Gamma(n+1)}{\Gamma(2\kappa^{-1}+n)}:=\sum_{n\geqslant 0}b_n, \tag{8}$$

and

$$J=\|i_\kappa(f)\|^2_{\mathcal{H}}=2\int_{-1}^{1}|f(ix)|^2(1-x^2)^{2\kappa^{-1}-1}dx.$$

By a symmetry argument it will be enough to consider

$$J' := \int_0^1 |f(ix)|^2 (1-x^2)^{2\kappa^{-1}-1} dx.$$

Then

$$\begin{aligned} J' &= \lim_{\rho\to 1,\rho\leqslant 1} \int_0^\rho \sum_{n,m} a_n \overline{a_m} i^{n+m} (-1)^m x^{n+m} (1-x^2)^{2\kappa^{-1}-1} dx \\ &\leqslant \frac{1}{2}\sum_{n,m} |a_n||a_m| B\left(\frac{n+m+1}{2}, 2\kappa^{-1}\right) \\ &= \frac{1}{2}\sum_{p\geqslant 0} B\left(\frac{p+1}{2}, 2\kappa^{-1}\right) \sum_{n=0}^{p} |a_n||a_{n-p}| \\ &\leqslant \frac{1}{2}\sum_{p\geqslant 0} B\left(\frac{p+1}{2}, 2\kappa^{-1}\right) \sum_{n=0}^{p} |a_n|^2 \\ &= \frac{1}{2}\sum_{n\geqslant 0} |a_n|^2 \sum_{k\geqslant 1} B\left(\frac{n+k}{2}, 2\kappa^{-1}\right). \end{aligned}$$

Using the expression (8) and the identity $B(x,y)=\Gamma(x)\Gamma(y)/\Gamma(x+y)$, we obtain

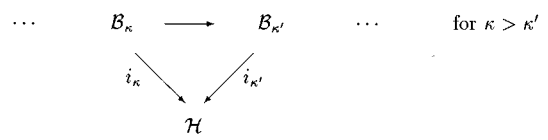
$$\begin{aligned} J' &\leqslant \frac{1}{2}\sum_{n\geqslant 0} b_n \frac{\Gamma(2\kappa^{-1}+n)}{\Gamma(n+1)\Gamma(2\kappa^{-1})} \sum_{k\geqslant 1} \frac{\Gamma((n+k)/2)\Gamma(2\kappa^{-1})}{\Gamma(2\kappa^{-1}+(n+k)/2)} \\ &= \frac{1}{2}\sum_{n\geqslant 0} b_n \frac{\Gamma(2\kappa^{-1}+n)}{\Gamma(n+1)} \sum_{p\geqslant n+1} \frac{1}{\Pi_{k=0}^{2\kappa^{-1}-1}\left(\frac{p}{2}+k\right)} \\ &\leqslant \frac{1}{2}\sum_{n\geqslant 0} b_n \frac{\Gamma(2\kappa^{-1}+n)}{\Gamma(n+1)} \int_{n+1}^{\infty} \frac{d\lambda}{((\lambda-1)/2)^{2\kappa^{-1}}} \\ &\leqslant \frac{(2\kappa^{-1})!\ 2^{2\kappa^{-1}-1}}{2\kappa^{-1}-1} I. \end{aligned}$$

This proves the theorem.

Remarks:

1. Let $\mathcal{C}_\kappa = i_\kappa(\mathcal{B}_\kappa)$. One can see easily that i_κ is injective and nonsurjective, moreover for $\kappa' < \kappa$ we have $\mathcal{B}_{\kappa'} \supset \mathcal{B}_\kappa$, hence $\mathcal{C}_{\kappa'} \supset \mathcal{C}_\kappa$ moreover $\mathcal{C}_1$ contains the functions $P(x)(1-x^2)$ where P is a polynomial which are dense in $\mathcal{H}$. This proves that $\mathcal{C}_\kappa$ is dense in $\mathcal{H}$ for any κ.

Hence we have the following commutative diagram:



The arrows represent continuous injections. In the contraction, a family of states ψ_κ covers the whole discrete series, but this will be written in $\mathcal{H}$ in which all the spaces $\mathcal{B}_\kappa$ are injected.

2. For $\kappa=1$ we obtain

Corollary 3.2: Let f be a holomorphic function on $\mathcal{D}$ which is square integrable for the Lebesgue measure on $\mathcal{D}$, then f is square integrable on any diameter of the disk, equipped with the measure $(1-r^2)dr$.

3. Let be $\mathcal{U}=\{f\in\mathcal{H}$; such that f can be analytically extended on $\mathcal{D}\}$ then $\cup_k\mathcal{C}_\kappa \neq \mathcal{U}$, this can be seen by considering the function $f(z)=e^{1/(1-z)}$.

The contraction of states is now defined in the following way:

Definition 3.3: A family of states $\psi_\kappa \in \mathcal{B}_\kappa$ contracts to $\psi \in \mathcal{H}$ iff $i_\kappa(\psi_\kappa)$ tends in some (possibly weak) sense to ψ.

IV. COHERENT STATES

In Ref. 2 we used the Berezin coherent states to study the contraction of SU(1,1) to the harmonic oscillator group. But these states cannot be used in the present contraction. In fact $i_\kappa(|z\rangle)$ has generally no limit when $\kappa\to 0$ except when $z=ia$ for $a\in\mathbb{R}$. In this case we have $\sqrt{(\pi\kappa)^{-1}}i_\kappa(|ia\rangle)\to\delta_a$ in a weak sense. This can be verified easily, let $\phi\in\mathcal{C}_0^\infty(]-1,1[)$, then we have

$$(\sqrt{(\pi\kappa)^{-1}}i_\kappa(|ia\rangle),\phi)_{\mathcal{H}}=\frac{\sqrt{\kappa^{-1}}}{\sqrt{\pi}}\int_{-1}^{1}\left(\frac{(1-x^2)(1-a^2)}{(1-ax)^2}\right)^{\kappa^{-1}}\phi(x)\frac{dx}{1-x^2}$$
$$=\frac{\sqrt{\kappa^{-1}}}{\sqrt{\pi}}\int_{-1}^{1}\left(1-\frac{(x-a)^2}{(1-ax)^2}\right)^{\kappa^{-1}}\phi(x)\frac{dx}{1-x^2}.$$

A straightforward calculation, using the dominated convergence theorem, proves that this expression tends to $\phi(a)$.

Turning to the coherent states, it is well-known that they have several definitions, which are not equivalent except for the Weyl group. One of them is to minimize the uncertainty relations for the group generators. In the case of SU(1,1), we can extract from the commutators the following uncertainty relation:

$$\frac{(\Delta K_1)(\Delta K_2)}{\langle K_0\rangle}\geqslant\frac{\kappa}{2},\tag{9}$$

where $(\Delta K_i)^2=\langle\psi|K_i^2|\psi\rangle-\langle\psi|K_i|\psi\rangle^2$ and $\langle K_0\rangle=\langle\psi|K_0|\psi\rangle$. One can see by an explicit calculation that the Berezin coherent states $|z\rangle$ do not minimize this relation (i.e., they do not realize the equality in (9)) except when $z=\overline{z}$. The Barut–Girardello coherent states[14] are defined as eigenvectors of the annihilator, they do minimize the relation but do not contract correctly. Following Nieto and Simmons,[10] we now look for states minimizing the uncertainty relations with a given ''shape.'' Suppose that a normalized state $|\psi_\alpha\rangle$ verifies

$$(AK_2+iK_1)|\psi_\alpha\rangle=\alpha|\psi_\alpha\rangle,\quad\text{where}\quad A\in\mathbb{R}_+\quad\text{and}\quad\alpha\in\mathbb{C},\tag{10}$$

then we have clearly $\alpha=A\langle K_2\rangle+i\langle K_1\rangle$ and calculating the square of the norm of (10), we obtain $A^2(\Delta K_2)^2+(\Delta K_1)^2=A\kappa\langle K_0\rangle$, and combined with (9) this gives $A\Delta K_2=\Delta K_1$, that is to say: $|\psi_\alpha\rangle$ has a given shape which does not depend on α. Moreover we have

$$\frac{(\Delta K_1)(\Delta K_2)}{\langle K_0\rangle}=\frac{\kappa}{2}.$$

The resolution of the equation (10) gives

for $A>1$

$$\psi_\alpha(z)=C_\alpha\left(z+i\sqrt{\frac{A+1}{A-1}}\right)^{-\kappa^{-1}+i\alpha(\kappa^{-1}/\sqrt{A^2-1})}\left(z-i\sqrt{\frac{A+1}{A-1}}\right)^{-\kappa^{-1}-i\alpha(\kappa^{-1}/\sqrt{A^2-1})}, \quad (11)$$

where C_α is a constant of normalization,

for $A=1$

$$\psi_\alpha(z)=C_\alpha e^{\kappa^{-1}\alpha z},$$

which are the Barut–Girardello coherent states,[14]

for $0<A<1$

$$\psi_\alpha(z)=C_\alpha\left(z+\sqrt{\frac{1+A}{1-A}}\right)^{-\kappa^{-1}+\alpha(\kappa^{-1}/\sqrt{A^2-1})}\left(z-\sqrt{\frac{1+A}{1-A}}\right)^{-\kappa^{-1}-\alpha(\kappa^{-1}/\sqrt{A^2-1})}.$$

Let us remark that the cases $A=0$ and $A=\infty$ give rise to solutions which are not square integrable. However, in view of the definition of the contraction, these states will have a good behavior during the contraction, only if they are concentrated in the vicinity of the vertical axis. This means that the classical observable k_2 (see(6)) must vanish in the limit $\kappa\to 0$. At the quantum level this means that $\Delta K_2\to 0$. Then it is natural to put $A=\kappa^{-1}$, and we define the state:

$$\psi_\kappa(z)=\left(z^2+\frac{1+\kappa}{1-\kappa}\right)^{-\kappa^{-1}},$$

obtained from (11) with $A=\kappa^{-1}$ and $\alpha=0$. The property of square integrability of the representation of SU(1,1) (Ref. 15) allows us to construct a quantum frame, i.e., a resolution of the identity in the following way. Let $\psi_{\kappa,g}=U_g\psi_\kappa$, we obtain

$$\mathrm{Id}=\int_{\mathrm{SU(1,1)}}|\psi_{\kappa,g}\rangle\langle\psi_{\kappa,g}|d\mu(g),$$

where $d\mu$ is the Haar measure on SU(1,1) conveniently normalized. The crucial point is the good behavior of these coherent states during the contraction.

V. CONVERGENCE RESULTS

We first need two lemmas:

Lemma 5.1: Let be $a\in\mathbb{R}$, $a>0$, $n_0\in\mathbb{N}$, $n>0$, $b\in\mathbb{R}$ *and A a non negative function defined for* $\kappa>0$ *such that* $0<\lim_{\kappa\to 0}A(\kappa)<\infty$, *and P a polynomial. Then for any* $x\in\,]-1,1[$ *and for* κ *small enough,*

$$P(x)\left(1+\frac{\kappa A(\kappa)}{1-x^2}\right)^{-a\kappa^{-1}+b+O(\kappa)}\frac{1}{(1-x^2)^{n_0}}\leqslant B(a,b,n_0), \quad (12)$$

where B does not depend on x nor on κ.

Proof: Even if it means changing a, it is sufficient to consider

$$\left(1+\frac{\kappa A(\kappa)}{1-x^2}\right)^{-a\kappa^{-1}}\frac{1}{(1-x^2)^{n_0}}.$$

Put $u=1/(1-x^2)\geqslant 1$, we have to prove that the function

$$\phi_\kappa(u)=n_0\ \log\ u-\frac{a}{\kappa}\log(1+\kappa A(\kappa)u),$$

is bounded uniformly in κ, for small enough κ. This is easily obtained by calculating the derivative of ϕ_κ, and proving that ϕ_κ has a maximum (depending on κ), with a finite limit when $\kappa\to 0$.

Definition 5.2: Let $\mathcal{A}$ be the set of functions on $]-1,1[$ which have the shape of the left hand side of (12).

Lemma 5.3: Let f_κ be in $\mathcal{H}$. Suppose that the family f_κ verify:

- $\lim_{\kappa\to 0} f_\kappa = f$ *almost everywhere on* $]-1,1[$,
- $f_\kappa(x)/(1-x^2)$ *is bounded on* $]-1,1[$, *uniformly in* κ,

then $f_\kappa\to f$ in the sense of the norm topology on $\mathcal{H}$.

Proof: From the second hypothesis, one can deduce that $|f_\kappa(x)|\leqslant M$ where M is a constant, hence we have $|f_\kappa(x)|^2/(1-x^2)\leqslant M^2$. As a consequence:

$$\frac{|f_\kappa(x)-f(x)|^2}{(1-x^2)}\leqslant\frac{|f_\kappa(x)|^2}{(1-x^2)}+2\frac{|f_\kappa(x)||f(x)|}{(1-x^2)}+\frac{|f(x)|^2}{(1-x^2)}\leqslant 4M^2.$$

Moreover $|f_\kappa(x)-f(x)|^2/(1-x^2)\to 0$ a.e. and by the dominated convergence theorem we obtain that

$$\int_{-1}^{1}\frac{|f_\kappa(x)-f(x)|^2}{(1-x^2)}dx\to 0.$$

Let

$$\tilde{\psi}_\kappa=i_\kappa\psi_\kappa\quad\text{and}\quad\tilde{\psi}_{\kappa,g}=i_\kappa\psi_{\kappa,\Pi_\kappa(g)}\quad\text{for } g\in\mathcal{P}^{1,1}.$$

One verifies easily that for any x: $\lim_{\kappa\to 0}\tilde{\psi}_\kappa(x)=e^{-2/(1-x^2)}=:\psi(x)$. Rewritten with the variable p on $L^2(\mathbb{R},dp/p_0)$ this state becomes $\psi(p)=Ce^{-p_0}$, called Gaussian probe in Ref. 9. This state stands out because, putting light velocity back and getting it to infinity, it becomes the ground state of the harmonic oscillator. We shall prove now that all the $\psi_{\kappa,g}=U_g(\psi_\kappa)$ contract in the sense of the norm. For this purpose, let us consider (a,θ) fixed in $\mathcal{P}^{1,1}$, then we have

$$\Pi_\kappa(a,\theta)=\begin{pmatrix}\alpha & \beta\\ \beta & \alpha\end{pmatrix}.$$

The coefficients can be calculated, using (5) and we obtain

$$\alpha=\alpha(\kappa)=\cosh\left(\frac{\theta}{2}\right)+\frac{i\kappa}{2}\left(a^0\cosh\left(\frac{\theta}{2}\right)-a^1\sinh\left(\frac{\theta}{2}\right)\right)+o(\kappa),$$

$$\beta=\beta(\kappa)=i\ \sinh\left(\frac{\theta}{2}\right)+\frac{\kappa}{2}\left(a^0\sinh\left(\frac{\theta}{2}\right)-a^1\cosh\left(\frac{\theta}{2}\right)\right)+o(\kappa).\tag{13}$$

Hence:

$$\tilde{\psi}_{\kappa,(a,\theta)}(x)=\left(1+\frac{2\kappa\left(x\sinh\left(\frac{\theta}{2}\right)+\cosh\left(\frac{\theta}{2}\right)\right)^2+i\kappa f(a,\theta,x)+P(a,\theta,x)o(\kappa)}{1-x^2}\right)^{-\kappa^{-1}},$$

where P is uniformly bounded with respect to x, that is to say $|P(a,\theta,x)|\leqslant M(a,\theta)$, and f is some function. One can easily verify that

$$\lim_{\kappa\to 0} i_\kappa U_{\Pi_\kappa(g)}\psi_\kappa(x)=V_g\psi(x)=:\psi_g(x) \quad \text{for any } x \text{ and for any } g \text{ in } \mathcal{P}^{1,1},$$

moreover,

$$|\tilde{\psi}_{\kappa,(a,\theta)}(x)|\leqslant\left(1+\frac{2\kappa(x\sinh(\theta/2)+\cosh(\theta/2))^2-|P(a,\theta,x)o(\kappa)|}{1-x^2}\right)^{-\kappa^{-1}}$$
$$\leqslant\left(1+\frac{2\kappa e^{-|\theta|}-M(a,\theta)o(\kappa)}{1-x^2}\right)^{-\kappa^{-1}}.$$

Then, using the first lemma we have $|\tilde{\psi}_{\kappa,(a\theta)}(x)|/(1-x^2)$ uniformly bounded in x and κ. Thanks to the second lemma we obtain:

Proposition 5.4: For a fixed (a,θ), $\lim_{\kappa\to 0} i_\kappa U_{\Pi_\kappa(a,\theta)}\psi_\kappa=V_{(a,\theta)}\psi$ in the sense of the norm topology on $\mathcal{H}$.

Note that this result generalizes (1) looking like (2). Now we are ready to state our definition of the contraction. Let A^κ be an observable on $\mathcal{B}_\kappa$, i.e., an essentially self adjoint operator whose domain contains the $\psi_{\kappa,g}$. Let

$$\tilde{A}^\kappa=i_\kappa A^\kappa i_\kappa^{-1}.$$

Here is the main definition.

Definition 5.5: Let A^κ be an observable on $\mathcal{B}_\kappa$, we say that A^κ contracts to an observable A on $\mathcal{H}$ iff

$$\lim_{\kappa\to 0}\langle\tilde{\psi}_{\kappa,g'}|\tilde{A}^\kappa|\tilde{\psi}_{\kappa,g}\rangle=\langle\psi_{g'}|A|\psi_g\rangle \forall g,g'\in\mathcal{P}^{1,1}.$$

The scalar product is the scalar product of $\mathcal{H}$.

We can now state the main result:

Theorem 5.6: *For any $\mathfrak{a}$ in $\pi_1(E_\kappa)$ and for any g,g' in $\mathcal{P}^{1,1}$ we have*

$$\lim_{\kappa\to 0}\langle\tilde{\psi}_{\kappa,g'}|\tilde{U}(\mathfrak{a})|\tilde{\psi}_{\kappa,g}\rangle=\langle\psi_{g'}|V(C(\mathfrak{a}))|\psi_g\rangle.$$

That is to say: Any polynomial expression in the K_i^κ contracts to the corresponding expression in the P_i.

Before proving this theorem, we need some intermediate results. The precontraction of the group generators gives the following results.

$$\tilde{K}_0^\kappa=\frac{1+x^2}{1-x^2}+\kappa x\frac{d}{dx},$$

$$\tilde{K}_1^\kappa=\frac{2x}{1-x^2}+\kappa\frac{1+x^2}{2}\frac{d}{dx},$$

$$\widetilde{K}_2^\kappa = i\frac{x^2-1}{2}\frac{d}{dx}.$$

Formally these formulas converge to (7), but we can obtain more. One can see easily that $\mathcal{A}$ (*cf.* definition 5.2) contains $\widetilde{\psi}_\kappa$ and moreover for any $f_\kappa \in \mathcal{A}$ which tends in norm to f for $\kappa \to 0$, one has $\widetilde{K}_i^\kappa f_\kappa \in \mathcal{A}$ and

$$\widetilde{K}_i^\kappa f_\kappa \overset{\mathcal{H}}{\to} P_i f.$$

As a consequence we have the following result:

Proposition 5.7: Let be $f_\kappa \in \mathcal{A}$ and P a polynomial, then $P(\widetilde{K}_0^\kappa, \widetilde{K}_1^\kappa, \widetilde{K}_2^\kappa) f_\kappa$ tends in the sense of the $\mathcal{H}$-norm to $P(P_0, P_1, P_2) f$ where f is the limit of f_κ.

Remark: A consequence of this proposition is that ψ minimizes the uncertainty relations:

$$\frac{(\Delta P_1)(\Delta P_2)}{\langle P_0 \rangle} \geqslant \frac{1}{2}.$$

In fact we have in $\mathcal{H}$,

$$(P_2 + iP_1)\psi = \lim_{\kappa\to 0}(\widetilde{K}_2^\kappa + i\widetilde{K}_1^\kappa)\widetilde{\psi}_\kappa = \lim_{\kappa\to 0} i_\kappa (K_2^\kappa + iK_1^\kappa)\psi_\kappa = 0.$$

Hence the property of minimizing the uncertainty relation is preserved by the contraction.

Now we consider the group action on $\mathcal{A}$, for any $f_\kappa \in \mathcal{A}$ we obtain

$$\widetilde{U}_g f_\kappa(x) = Z(x) f_\kappa\left(-i\frac{\overline{\alpha i}x - \beta}{-i\beta x + \alpha}\right),$$

where

$$Z(x) = (\alpha^2 + \beta^2)^{-\kappa^{-1}}\left(\frac{1-x^2}{1-2iFx-Ex^2}\right)^{\kappa^{-1}},$$

with

$$E = \frac{\overline{\alpha^2} + \overline{\beta^2}}{\alpha^2 + \beta^2} \quad \text{and} \quad F = \frac{\overline{\beta}\overline{\alpha} + \overline{\alpha}\overline{\beta}}{\alpha^2 + \beta^2}.$$

One can see easily that for any x, $\widetilde{U}_{\Pi_\kappa(a,\theta)} f_\kappa(x)$ tends to $V_{(a,\theta)} f(x)$, moreover one can show (Ref. 6) that Z is bounded by a constant which depends only on (a,θ). In view to obtaining the L^2-convergence, we have to control the second term, more precisely let

$$Y = \frac{1}{\left(1-\left(-i\left(\frac{\overline{\alpha i}x-\beta}{-i\beta x+\alpha}\right)\right)^2\right)^{n_0}}\left(1+\frac{\kappa A(\kappa)}{1-\left(-i\left(\frac{\overline{\alpha i}x-\beta}{-i\beta x+\alpha}\right)\right)^2}\right)^{-a\kappa^{-1}+b+O(\kappa)}.$$

Remark that, using (13) we obtain

$$\left(-i\left(\frac{\overline{\alpha i}x-\beta}{-i\beta x+\alpha}\right)\right)^2 = B + i\kappa C,$$

where $|B| < 1$ and for a^0, a^1, θ fixed, C is a bounded function of x and κ: $|C| \leqslant M$. Then

$$|Y| = \left(1 + \frac{(1-B)\kappa^{-1}+1}{((1-B)\kappa^{-1})^2 + C^2}\right)^{-\kappa^{-1}/2} \frac{\kappa^{-n_0}}{(((1-B)\kappa^{-1})^2 + C^2)^{n_0/2}}$$

$$\leqslant \left(1 + \frac{(1-B)\kappa^{-1}+1}{((1-B)\kappa^{-1})^2 + C^2}\right)^{-\kappa^{-1}/2} \kappa^{-n_0} \left(\frac{(1-B)\kappa^{-1}+1}{((1-B)\kappa^{-1})^2 + C^2}\right)^{n_0/2}.$$

And we can complete the demonstration as in the Lemma 5.1, verifying that $|Y|$ is bounded by a constant which depends only on (a,θ). Hence we have shown that

Proposition 5.8: $\forall (a,\theta) \in \mathcal{P}^{1,1}$ *and* $\forall f_\kappa \in \mathcal{A}$, $\widetilde{U}_{\Pi_\kappa(a,\theta)} f_\kappa$ *tends in the sense of the* $\mathcal{H}$*-norm to* $V_{(a,\theta)} f$ *where* f *is the* $\mathcal{H}$*-limit of* f_κ.

Turning to the demonstration of the Theorem 5.6, we remark that

$$P(\widetilde{K}_0^\kappa, \widetilde{K}_1^\kappa, \widetilde{K}_2^\kappa)\widetilde{\psi}_{\kappa,g} = \widetilde{U}_g \widetilde{U}_g^{-1} P(\widetilde{K}_0^\kappa, \widetilde{K}_1^\kappa, \widetilde{K}_2^\kappa)\widetilde{U}_g \widetilde{\psi}_\kappa = \widetilde{U}_g P(\tilde{\mathrm{a}}\mathrm{d}_g K_0^\kappa, \tilde{\mathrm{a}}\mathrm{d}_g K_1^\kappa, \tilde{\mathrm{a}}d_g K_2^\kappa)\widetilde{\psi}_\kappa .$$

We complete the demonstration, using the convergence of the structure constants and the above propositions.

VI. CONCLUSION

It was already known that SU(1,1) contracts to the Poincaré group. But in this paper we have proved that the classical and quantum mechanics described by this group contracts to the corresponding mechanics associated to the Poincaré group. This can be interpreted as the limit at null curvature of the anti-de Sitterian mechanics or as the limit of a relativistic harmonic oscillator to a free relativistic particle. We emphasize that this limit is not only for the representation but also for all the quantum observables. However this contraction is somehow singular, it is obtained by a restriction to a set of measure zero. Then it is not surprising that the frame $\psi_{\kappa,g}$ becomes at the limit a dense family which is no more a family of coherent states: it contains too many vectors. In fact $\psi \in D(P_0^{1/2})$ and one can deduce[9] that if $M = \mathcal{P}^{1,1}/e^{\mathbb{R}f_0}$ and if s is a Borelian section $M \to \mathcal{P}^{1,1}$, then the set of $V_{(s(z))}\psi$ where $z \in M$ is a frame of $\mathcal{H}$.

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Quantum mechanics of charged particles in random electromagnetic fields

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In this paper we consider the $\hbar \to 0$ asymptotics for the solutions to stochastic Schrödinger equations for quantum mechanical particles in random electromagnetic fields in R^n. We obtain semi-classical expansions for their solutions up to any order in $L^2(R^n)$ a.s. by using a stochastic Hamilton Jacobi equation and a stochastic continuity equation. We conclude that as $\hbar \to 0$ the stochastic quantum mechanics with random electromagnetic fields tends to stochastic classical mechanics. © *1996 American Institute of Physics.* [S0022-2488(96)04306-X]

I. INTRODUCTION

In this paper we consider the $\hbar \to 0$ asymptotics of the solution to the following stochastic Schrödinger equation in R^n

$$\frac{i}{\hbar} dH \psi_t + d\psi_t = 0, \tag{1.1}$$

where the Hamiltonian for random electromagnetic fields is given by the following Stratonovich type differential

$$\begin{aligned} dH = &\left(\frac{1}{2} \{ -\hbar^2 \Delta + 2i\hbar b \cdot \nabla + i\hbar (\nabla \cdot b) + b^2 \} + V \right) dt \\ &+ \frac{1}{2} \sum_{r=1}^{m_1} [2i\hbar A^r \cdot \nabla + i\hbar (\nabla \cdot A^r) + 2(b \cdot A^r)] \circ dw_t^{1r} + \sum_{r=1}^{m_2} K^r \circ dw_t^{2r} \end{aligned} \tag{1.2}$$

and $w_t^{(k)} = (w_t^{k1}, w_t^{k2}, \cdot, w_t^{km_k})$ $(k = 1,2)$ is m_k-dimensional Brownian motion with $w_t^{k_i}$ independent Wiener processes on probability space $(\Omega, \mathcal{F}, P)$, b, A^r $(r = 1,2, \cdots, m_1)$ are C^2 vector fields in R^n and V, K^r $(r = 1,2, \cdots, m_2)$ are C^2 functions. Here we denote the inner product in R^n by $- \cdot -$ or sometimes $\langle -, - \rangle$, the corresponding Euclidean metric being $|-| = \sqrt{-, -} = \sqrt{\langle -, - \rangle}$. This random operator dH can be considered as the stochastic generalization of the Schrödinger operators in electromagnetic fields considered by many people, such as Simon,[1] Cycon *et al.*,[2] Elworthy, Truman and Watling,[3] and Cartier and DeWitt-Morette,[4] to name but a few. Heuristically we have to consider random Schrödinger operators like

$$\frac{1}{2} \left(i\hbar \nabla + b + \sum_{r=1}^{m_1} A^r \circ \frac{dw_t^{1r}}{dt} \right)^2 + V + \sum_{r=1}^{m_2} K^r \circ \frac{dw_t^{2r}}{dt},$$

which leads to (1.2) as $dw_t^{(1)} \circ dw_t^{(1)} = 0$ for Stratonovich type differentials. The random electromagnetic field in R^3 is given by $\nabla \times (b + \Sigma_{r=1}^{m_1} A^r \circ dw_t^{1r}/dt) = \text{curl } b + \Sigma_{r=1}^{m_1} \text{curl } A^r \circ dw_t^{1r}/dt$ and $\nabla^k (b^l + \Sigma_{r=1}^{m_1} A^{lr} \circ dw_t^{1r}/dt) - \nabla^l (b^k + \Sigma_{r=1}^{m_1} A^{kr} \circ dw_t^{1r}/dt)$ in the general case with the electric field given by $-\nabla (V + \Sigma_{r=1}^{m_2} K^r \circ dw_t^{2r}/dt)$. The sort of noise we consider is white noise in time distributed locally in different directions. Since it is known that before an earthquake there are

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random fluctuations in the Earth's local electromagnetic field, equation (1.1) is a useful model for earthquake predictions. Clearly there are also potential defence applications.

Inspired by Maslov's quasi-classical asymptotics of quantum mechanics (Maslov[5]), Truman,[6] Elworthy and Truman[7,8] developed the path-space Hamilton Jacobi theory in order to treat deterministic heat equations (or Schrödinger equations) to get quasi-classical expansions for their solutions. Elworthy and Truman[7] considered the Schrödinger equation

$$\frac{i}{\hbar}H\psi_t^\hbar + \frac{\partial}{\partial t}\psi_t^\hbar = 0 \tag{1.3}$$

with $H = -\frac{1}{2}\hbar^2\Delta + V = \frac{1}{2}(i\hbar\nabla)^2 + V$ and initial condition $\psi_0^\hbar(x) = T_0(x)\exp\{iS_0(x)/\hbar\}$ and proved if $T_0 \in C_0^\infty(R^n)$ and $S_0 \in C^\infty(R^n)$ then as $\hbar \to 0$

$$\psi_t^\hbar(-)\exp\{-iS(-,t)/\hbar\} \to T_0(\Phi_t^{-1}-)\phi^{\frac{1}{2}}(-,t) \tag{1.4}$$

in $L^2(R^n)$ where $\Phi_t : R^n \to R^n$ is defined by the following second order classical mechanical equation

$$\ddot{\Phi}_t = -\nabla V(\Phi_t), \Phi_0(x) = x, \dot{\Phi}_t(x) = \nabla S_0(x), \tag{1.5}$$

and under a no-caustics condition, Φ_t^{-1} is the inverse of Φ_t and

$$S(x,t) = \frac{1}{2}\int_0^t |\dot{\Phi}_s(\Phi_t^{-1}(x))|^2 ds + S_0(\Phi_t^{-1}(x)) - \int_0^t V(\Phi_s(\Phi_t^{-1}(x)))ds$$

and $\phi(x,t) = |\det(\partial/\partial x)\,\Phi_t^{-1}(x)|$. Elworthy, Truman and Watling [3] generalized the above result to Schrödinger equations in the presence of electromagnetic fields. The Hamilton Jacobi theory has been used successfully in the study of the Feynman–Kac integral in curved space in obtaining small time and small $\hbar$ asymptotics for solutions of diffusion heat equations and Schrödinger equations as well as the classical mechanical limit of the quantum partition function (Elworthy, Ndumu and Truman[9]). These techniques have been applied by Elworthy[10,11] to linear heat equations, by Elworthy, Truman and Zhao[12] to nonlinear generalized KPP equations in which we have proved that the travelling wave front is given by a Hamilton Jacobi function, and to many other problems. Truman and Zhao[13–15] and Kolokoltsov[16] independently developed stochastic Hamilton Jacobi theory to include the stochastic heat equations such as the Zakai equation of nonlinear filtering, and stochastic Schrödinger equations arising in quantum filtering (Belavkin[17]) and the stochastic evolution equation in Hudson and Parthasarathy[18] and random wave processes in Dawson and Papanicolaou.[19]

The challenging question is to develop the stochastic Hamilton Jacobi theory to treat equations such as (1.1) with dH defined by (1.2) in random electromagnetic fields. This question also arises in study of stochastic heat equations with random vector drifts. In this paper we tackle this problem. In section II we consider the stochastic Hamiltonian system and solve the Hamilton Jacobi equations under a no-caustic condition (Theorem 2.2)

$$dS_t(x) + \frac{1}{2}|\nabla S_t(x) - b(x,t)|^2 dt - \sum_{r=1}^{m_1} \langle A^r(x,t), \nabla S_t(x) - b(x,t)\rangle \circ dw_t^{1r} + V(x,t)dt$$
$$+ \sum_{r=1}^{m_2} K^r(x,t)dw_t^{2r} = 0. \tag{1.6}$$

and stochastic continuity equation (Lemma 2.3)

$$d\phi(x,t)+\operatorname{div}\left\{\phi(x,t)\left[(\nabla S(x,t)-b(x,t))dt-\sum_{r=1}^{m_1}A^r(x,t)\circ dw_t^{1r}\right]\right\}=0. \tag{1.7}$$

These give the desired cancellations of orders $i\hbar^{-1}$ and $(i\hbar)^0$ when we consider the stochastic Schrödinger equation (1.1) in section III. In fact we obtain the semi-classical expansions for the solution to equation (1.1) up to any order in $L^2(R^n)$ a.s. The corresponding question for the deterministic equation was considered by Elworthy, Truman and Watling.[3] Nevertheless the proof we give in this paper is simpler and more straightforward than that in the previous paper. As a simple consequence of above we conclude that in the limit as $\hbar\to 0$ the probability of the quantum mechanical charged particle in random electromagnetic fields being in the set A at time t equals the probability of the quantum mechanical particle being in the set $\Phi_t^{-1}A$ in time 0, i.e. $\lim_{\hbar\to 0}\widetilde{P}^{\hbar}(t,A)=\widetilde{P}(0,\Phi_t^{-1}A)$ where Φ_t is the classical stochastic Hamiltonian flow in configuration space, $\widetilde{P}$ being the quantum mechanical probability, A any Borel set in R^n. In this sense stochastic quantum mechanics associated with the stochastic Schrödinger equation converges to the stochastic classical mechanics of the corresponding stochastic Hamiltonian system as $\hbar\to 0$. Furthermore, our results give the asymptotic expansions of $\widetilde{P}^{\hbar}(t,A)$.

In section IV we prove a result that the random map $\Phi_s:R^n\to R^n$ is almost surely a diffeomorphism for $0\leqslant s\leqslant T(\omega)$ and such $T(\omega)>0$ exists almost surely i.e. for some positive time the no caustic condition is satisfied.

We can immediately apply the stochastic Hamilton Jacobi theory to stochastic heat equations and Burgers' equations with random drifts. For these results see Truman and Zhao.[20] For the Schrödinger equations, the no caustic condition avoids the complications of Maslov indices. When caustics do occur we expect the original analysis of Maslov could be generalized to this stochastic setting but we have not investigated this in any detail.

II. THE STOCHASTIC HAMILTON JACOBI EQUATIONS

In this section we consider the stochastic Hamilton Jacobi equation and the stochastic continuity equation. These are two basic equations in stochastic Hamilton Jacobi theory. Indeed in the next section we will give the semi-classical expansions for the solution of stochastic Schrödinger equation (1.1) by applying the stochastic Hamilton Jacobi theory where the stochastic Hamilton Jacobi equation and the stochastic continuity equation give the right cancellations as required.

For given C^2 vector fields b,A^r $(r=1,2,\cdots,m_1)$ in R^n and C^2 functions V,K^r $(r=1,2,\cdots,m_2)$, S_0 and m_k dimensional Brownian motion $w_s^{(k)}=(w_s^{k1},w_s^{k2},\cdots,w_s^{km_k})$ $(k=1,2)$ on the probability space $(\Omega,\mathcal{F},P)$, consider the following stochastic Hamiltonian system of Stratonovich type written in phase space

$$\begin{cases} d\Phi_s^k=v_s^k ds-\sum_{r=1}^{m_1}A^{kr}(\Phi_s,s)\circ dw_s^{1r}, \\ dv_s^k=-\nabla^k V(\Phi_s,s)ds-\sum_{r=1}^{m_2}\nabla^k K^r(\Phi_s,s)dw_s^{2r}-\dfrac{\partial}{\partial s}b_k(\Phi_s,s)ds \\ \qquad +(\nabla^k b_l(\Phi_s,s)-\nabla^l b_k(\Phi_s,s))\left(v_s^l ds-\sum_{r=1}^{m_1}A^{lr}(\Phi_s,s)\circ dw_s^{1r}\right) \\ \qquad +v_s^l\sum_{r=1}^{m_1}\nabla^k A^{lr}(\Phi_s,s)\circ dw_s^{1r}, \\ \qquad k=1,2,\cdots,n \end{cases} \tag{2.1}$$

with $\Phi_0(x)=x, v_0(x)=\nabla S_0(x)-b(x,0)$. Here we use usual summation convention over Latin indices.

Let $\widetilde{S}:[0,+\infty)\times R^n\times\Omega\to R$ be defined by the following non-anticipating Itô's stochastic integral

$$\widetilde{S}_t(y)=\frac{1}{2}\int_0^t|v_s(y)|^2ds+S_0(y)-\int_0^t V(\Phi_s(y),s)ds-\sum_{r=1}^{m_2}\int_0^t K^r(\Phi_s(y),s)dw_s^{2r}$$
$$+\int_0^t\langle b(\Phi_s(y),s),d\Phi_s(y)\rangle. \tag{2.2}$$

Lemma 2.1: *For any $t\geqslant 0$ and a.e. $\omega\in\Omega$,*

$$(\nabla_y\Phi_t(y))^*[v_t(y)+b(\Phi_t(y),t)]=\nabla_y\widetilde{S}_t(y) \tag{2.3}$$

and

$$d\widetilde{S}_t(y)=\frac{1}{2}|v_t(y)|^2dt-V(\Phi_t(y),t)dt-\sum_{r=1}^{m_2}K^r(\Phi_t(y),t)dw_t^{2r}+\langle b(\Phi_t(y),t),d\Phi_t(y)\rangle. \tag{2.4}$$

Here by $-^*$ we denote the transpose of $-$.

Proof: Differentiating $\widetilde{S}_t(y)$ with respect to y_j $(j=1,2,\cdots,n)$ we obtain

$$\nabla_{y_j}\widetilde{S}_t(y)=\int_0^t(\nabla_{y_j}v_s(y))^*v_s(y)ds+\nabla_{y_j}S_0(y)-\int_0^t(\nabla_{y_j}\Phi_s(y))^*\nabla V(\Phi_s(y),s)ds$$
$$-\sum_{r=1}^{m_2}\int_0^t(\nabla_{y_j}\Phi_s(y))^*\nabla K^r(\Phi_s(y),s)dw_s^{2r}+\int_0^t b^l(\Phi_s(y),s)d\nabla_{y_j}\Phi_s^l(y)$$
$$+\int_0^t\nabla^k b^l(\Phi_s(y),s)\nabla_{y_j}\Phi_s^k(y)d\Phi_s^l(y), \tag{2.5}$$

by using the summation convention. The first term in (2.5) can be calculated by using equation (2.1) and the integration by parts formula

$$\int_0^t v_s^k(y)\nabla_{y_j}v_s^k(y)ds=\int_0^t v_s^k(y)\left[d\nabla_{y_j}\Phi_s^k(y)+\sum_{r=1}^{m_1}\nabla^l A^{kr}(\Phi_s,s)\nabla_{y_j}\Phi_s^l(y)\circ dw_s^{1r}\right]$$
$$=v_t^k(y)\nabla_{y_j}\Phi_t^k(y)-v_0^k(y)\nabla_{y_j}\Phi_0^k(y)-\int_0^t\nabla_{y_j}\Phi_s^k(y)dv_s^k(y)$$
$$+\sum_{r=1}^{m_1}\int_0^t v_s^k(y)\nabla^l A^{kr}(\Phi_s,s)\nabla_{y_j}\Phi_s^l(y)\circ dw_s^{1r}$$
$$=v_t^k(y)\nabla_{y_j}\Phi_t^k(y)-v_0^k(y)\,\delta_j^k-\int_0^t\nabla_{y_j}\Phi_s^k(y)dv_s^k$$
$$+\sum_{r=1}^{m_1}\int_0^t v_s^l(y)\nabla^k A^{lr}(\Phi_s,s)\nabla_{y_j}\Phi_s^k(y)\circ dw_s^{1r},$$

by commuting the positions of k and l in the last term. It turns out from the cancellations due to equation (2.1) that (2.5) is

$$\nabla_{y_j}\widetilde{S}_t(y)=(\nabla_{y_j}\Phi_t(y))^* v_t(y)+b^j(y,0)-\int_0^t\nabla_{y_j}\Phi_s^k(y)\Big[v_s^l(y)(\nabla^k b_l(\Phi_s,s)-\nabla^l b_k(\Phi_s,s))ds$$
$$-\frac{\partial}{\partial s}b_k(\Phi_s,s)ds\Big]-\int_0^t\nabla_{y_j}\Phi_s^k(y)\sum_{r=1}^{m_1}A^{lr}(\Phi_s,s)(\nabla^l b^k(\Phi_s,s)-\nabla^k b^l(\Phi_s,s))\circ dw_s^{1r}$$
$$+\int_0^t b^k(\Phi_s(y),s)d\nabla_{y_j}\Phi_s^k(y)+\int_0^t\nabla^k b^l(\Phi_s(y),s)\nabla_{y_j}\Phi_s^k(y)d\Phi_s^l(y). \tag{2.6}$$

By the integration by parts formula again we have

$$\int_0^t b^k(\Phi_s(y),s)d\nabla_{y_j}\Phi_s^k(y)=b^k(\Phi_t(y),t)\nabla_{y_j}\Phi_t^k(y)-b^k(y,0)\,\delta_k^j-\int_0^t\nabla_{y_j}\Phi_s^k(y)$$
$$\times\Big(\nabla^l b^k(\Phi_s(y),s)d\Phi_s^l+\frac{\partial}{\partial s}b^k(\Phi_s,s)ds\Big). \tag{2.7}$$

Cancellations in (2.6) and (2.7) using equation (2.1) again finally lead to

$$\nabla_{y_j}\widetilde{S}_t(y)=\nabla_{y_j}\Phi_t^k(y)((v_t^k(y)+b^k(\Phi_t(y),t))),$$

which is (2.3) as required. We can prove (2.4) by direct differentiation easily. ■

We assume a *no-caustic condition*: there exists $T(\omega)>0$ a.s. such that for $0\leqslant s\leqslant T(\omega)$, $\Phi_s(\omega):R^n\to R^n$ is a diffeomorphism for a.e. $\omega\in\Omega$. In section IV we will prove this is true for $V,K^r\in C_0^\infty(R^n)$ and $b,A^r\in C_0^\infty(R^n,R^n)$. It is noteworthy here that the diffeomorphism property for the Hamiltonian system in configuration space is different from that in phase space. Actually in phase space, equation (2.1) is a multidimensional first order stochastic differential equation in which case the diffeomorphism property is covered by stochastic flow theory in Kunita[21] and Elworthy.[10] Unfortunately the diffeomorphism of $(\Phi_s,v_s):R^{2n}\to R^{2n}$ does not imply the diffeomorphism of $\Phi_s:R^n\to R^n$ in configuration space.

The following is the main result of this section. It gives the solution of the stochastic Hamilton Jacobi equation with random vector potentials under the no caustic condition.

Theorem 2.2: *With no caustic assumption for* $0\leqslant s\leqslant T(\omega)$ *we define* $S_t(\omega):R^n\to R^1$ *for a.e.* $\omega\in\Omega$ *and* $0\leqslant t\leqslant T(\omega)$ *by*

$$S_t(x)=\widetilde{S}_t(\Phi_t^{-1}(x)). \tag{2.8}$$

Then for a.e. $\omega\in\Omega$, $0\leqslant t\leqslant T(\omega)$ *and any* $x\in R^n$

$$\nabla S_t(x)=v_t(\Phi_t^{-1}(x))+b(x,t), \tag{2.9}$$

and $S_t(x)$ *satisfies the following stochastic Hamilton Jacobi equation:*

$$dS_t(x)+\frac{1}{2}|\nabla S_t(x)-b(x,t)|^2dt-\sum_{r=1}^{m_1}\langle A^r(x,t),\nabla S_t(x)-b(x,t)\rangle\circ dw_t^{1r}+V(x,t)dt$$
$$+\sum_{r=1}^{m_2}K^r(x,t)dw_t^{2r}=0. \tag{2.10}$$

Proof: Differentiating $S_t(x)$ with respect to x_k for $k \in \{1,2,\cdots,n\}$ and using (2.3)

$$\begin{aligned}\nabla_{x_k} S_t(x) &= \nabla^j \widetilde{S}_t(\Phi_t^{-1}(x)) \nabla_{x_k} \Phi_t^{-1}(x)_j \\ &= \nabla^j \Phi_t^l(\Phi_t^{-1}(x))(v_t^l(\Phi_t^{-1}(x)) + b^l(x,t)) \nabla_{x_k} \Phi_t^{-1}(x)_j \\ &= \nabla_{x_k} \Phi_t^l(\Phi_t^{-1}(x))(v_t^l(\Phi_t^{-1}(x)) + b^l(x,t)) \\ &= \delta_k^l (v_t^l(\Phi_t^{-1}(x)) + b^l(x,t)) = v_t^k(\Phi_t^{-1}(x)) + b^k(x,t),\end{aligned}$$

gives (2.9). It will be used often in the following form that

$$\nabla_x S_t(x) - b(x,t) = v_t(\Phi_t^{-1}(x)). \tag{2.11}$$

Differentiating $S_t(x)$ with respect to t and using (2.3), (2.4) and (2.11) we deduce that

$$\begin{aligned}dS_t(x) &= d\widetilde{S}_t(\Phi_t^{-1}(x)) + \nabla^j \widetilde{S}_t(\Phi_t^{-1}(x)) d\Phi_t^{-1}(x)_j \\ &= \frac{1}{2}|v_t(\Phi_t^{-1}(x))|^2 dt + \langle b(x,t), d\Phi_t(\Phi_t^{-1}(x))\rangle - V(x,t)dt - \sum_{r=1}^{m_2} K^r(x,t) dw_t^{2r} \\ &\quad + \nabla^j \Phi_t^l(\Phi_t^{-1}(x))(v_t^l(\Phi_t^{-1}(x)) + b^l(x,t)) d\Phi_t^{-1}(x)_j \\ &= \frac{1}{2}|\nabla S(x,t) - b(x,t)|^2 dt - V(x,t)dt - \sum_{r=1}^{m_2} K^r(x,t) dw_t^{2r} - d\Phi_t^l(\Phi_t^{-1}(x)) v_t^l(\Phi_t^{-1}(x)).\end{aligned} \tag{2.12}$$

This is from differentiating the identity $\Phi_t^l(\Phi_t^{-1}(x)) = x^l$ with respect to t to obtain $d\Phi_t^l(\Phi_t^{-1}(x)) + \nabla^j \Phi_t^l(\Phi_t^{-1}(x)) d\Phi_t^{-1}(x)_j = 0$. But from the Hamiltonian system (2.1) and the identity (2.11) the last term in (2.12) is

$$\begin{aligned}-\langle v_t(\Phi_t^{-1}(x)), d\Phi_t(\Phi_t^{-1}(x))\rangle &= -\left\langle v_t(\Phi_t^{-1}(x)), v_t(\Phi_t^{-1}(x))dt - \sum_{r=1}^{m_1} A^r(x,t) \circ dw_t^{1r} \right\rangle \\ &= -|\nabla S(x,t) - b(x,t)|^2 dt \\ &\quad + \sum_{r=1}^{m_1} \langle \nabla S(x,t) - b(x,t), A^r(x,t)\rangle \circ dw_t^{1r}.\end{aligned}$$

By replacing this formula in (2.12), we obtain the stochastic Hamilton Jacobi equation (2.10) as required. ■

Lemma 2.3: *Assume that Φ_t satisfies the no caustic condition for $0 \leqslant t \leqslant T(\omega)$ for a.e. $\omega \in \Omega$. Let $S(x,t)$ be defined as above and define $\phi(x,t) = |\det[\partial \Phi_t^{-1}(x)/\partial x]| > 0$. Then for $0 \leqslant t \leqslant T(\omega)$ for a.e. $\omega \in \Omega$ and any $x \in R^n$, $\phi(x,t)$ satisfies the following stochastic continuity equation:*

$$d\phi(x,t) + \operatorname{div}\left\{ \phi(x,t) \left[(\nabla S(x,t) - b(x,t))dt - \sum_{r=1}^{m_1} A^r(x,t) \circ dw_t^{1r} \right] \right\} = 0. \tag{2.13}$$

Proof: We make repeated use of the rule for differentiating determinants $|A|$ with respect to an external parameter u:

$$d_u|A| = \sum_{\alpha,\beta=1}^{n} \frac{\partial |A|}{\partial a_{\alpha\beta}} d_u a_{\alpha\beta} = \sum_{\alpha,\beta=1}^{n} A_{\alpha,\beta} d_u a_{\alpha\beta}, \tag{2.14}$$

where $|A| = \Sigma_{\beta=1}^{n} a_{\alpha\beta} A_{\alpha\beta}$, $A_{\alpha\beta}$ being a cofactor of $a_{\alpha\beta}$ in $|A|$. As we consider the Stratonovich type equation, (2.14) is still valid. Writing

$$\phi = \sum_{\beta=1}^{n} \frac{\partial (\Phi_t^{-1}(x))_\alpha}{\partial x^\beta} X_\beta^\alpha,$$

gives

$$d\phi(x,t) = \sum_{\alpha,\beta=1}^{n} d\frac{\partial (\Phi_t^{-1}(x))_\alpha}{\partial x^\beta} X_\beta^\alpha = \sum_{\alpha,\beta=1}^{n} \frac{\partial d(\Phi_t^{-1}(x))_\alpha}{\partial x^\beta} X_\beta^\alpha. \tag{2.15}$$

Now we consider the equation $\Phi_t^\alpha(\Phi_t^{-1}(x)) = x^\alpha$ and differentiate it with respect to t to give

$$\nabla_\beta \Phi_t^\alpha(\Phi_t^{-1}(x)) d\Phi_t^{-1}(x)^\beta + d\Phi_t^\alpha(\Phi_t^{-1}(x)) = 0. \tag{2.16}$$

But differentiating it with respect to $x^{\alpha'}$ gives

$$\nabla_\beta \Phi_t^\alpha(\Phi_t^{-1}(x)) \frac{\partial \Phi_t^{-1}(x)_\beta}{\partial x^{\alpha'}} = \delta_{\alpha'}^\alpha.$$

Hence we obtain from above

$$[\nabla_\beta \Phi_t^\alpha(\Phi_t^{-1}(x))]_{\alpha\beta}^{-1} = \left[\frac{\partial \Phi_t^{-1}(x)_\beta}{\partial x_0^\alpha}\right]_{\beta\alpha}$$

and so we deduce that

$$\frac{\partial (\Phi_t^{-1}(x))^{\beta'}}{\partial x_\alpha} \nabla_\beta \Phi_t^\alpha(\Phi_t^{-1}(x)) = \delta_\beta^{\beta'},$$

giving in (2.16)

$$d(\Phi_t^{-1}(x))^{\beta'} = -\frac{\partial (\Phi_t^{-1}(x))^{\beta'}}{\partial x^\alpha} d\Phi_t^\alpha(\Phi_t^{-1}(x)). \tag{2.17}$$

Now it turns out from (2.15) that

$$d\phi(x,t) = \sum_{\alpha,\beta=1}^{n} \frac{\partial}{\partial x^\beta}[X_\beta^\alpha d\Phi_t^{-1}(x)_\alpha] - \sum_{\alpha,\beta=1}^{n} \frac{\partial X_\beta^\alpha}{\partial x^\beta} d\Phi_t^{-1}(x)_\alpha.$$

The second term on the right hand side is zero as we now demonstrate. We differentiate the identity

$$\delta_\beta^k \phi = \sum_{\alpha=1}^{n} X_\beta^\alpha \frac{\partial \Phi_t^{-1}(x)_\alpha}{\partial x^k}, \quad \beta,k = 1,2,\cdots,n,$$

partially with respect to x^β and then sum over β to deduce that

$$\frac{\partial}{\partial x^k}\phi=\sum_{\beta=1}^{n}\frac{\partial}{\partial x^\beta}(\delta_\beta^k\phi)=\sum_{\alpha,\beta=1}^{n}X_\beta^\alpha\frac{\partial^2\Phi_t^{-1}(x)_\alpha}{\partial x^\beta\partial x^k}+\sum_{\alpha,\beta=1}^{n}\frac{\partial X_\beta^\alpha}{\partial x^\beta}\frac{\partial\Phi_t^{-1}(x)_\alpha}{\partial x^k}=\sum_{\alpha,\beta=1}^{n}X_\beta^\alpha\frac{\partial^2\Phi_t^{-1}(x)_\alpha}{\partial x^\beta\partial x^k}.$$

Therefore for any $k=1,2,\cdots,n$,

$$\sum_{\alpha,\beta=1}^{n}\frac{\partial X_\beta^\alpha}{\partial x^\beta}\frac{\partial\Phi_t^{-1}(x)_\alpha}{\partial x^k}=0.$$

Multiplying above by $d\Phi_t^k(\Phi_t^{-1}(x))$ and summing over k we have

$$-\sum_{\alpha,\beta=1}^{n}\frac{\partial X_\beta^\alpha}{\partial x^\beta}d\Phi_t^{-1}(x)_\alpha=0,$$

by using (2.17). It turns out from (2.17) again that

$$d\phi(x,t)=\sum_{\alpha,\beta=1}^{n}\frac{\partial}{\partial x^\beta}[X_\beta^\alpha d\Phi_t^{-1}(x)_\alpha]=-\sum_{\alpha,\beta,k=1}^{n}\frac{\partial}{\partial x^\beta}\left(\frac{\partial(\Phi_t^{-1}(x))^\alpha}{\partial x^k}d\Phi_t^k(\Phi_t^{-1}(x))X_\beta^\alpha\right).$$

This gives by using equation (1.1) again and (2.11)

$$\begin{aligned}d\phi(x,t)&=-\sum_{\beta,k=1}^{n}\frac{\partial}{\partial x^\beta}\{\delta_\beta^k\phi(x,t)d\Phi_t^k(\Phi_t^{-1}(x))\}\\&=-\sum_{k=1}^{n}\frac{\partial}{\partial x^k}\{\phi(x,t)d\Phi_t^k(\Phi_t^{-1}(x))\}\\&=-\sum_{k=1}^{n}\frac{\partial}{\partial x^k}\left\{\phi(x,t)\left[v^k(\Phi_t^{-1}(x))dt-\sum_{r=1}^{m_1}A^{kr}(x,t)\circ dw_t^{1r}\right]\right\}\\&=-\operatorname{div}\left\{\phi(x,t)\left[(\nabla S(x,t)-b(x,t))dt-\sum_{r=1}^{m_1}A^r(x,t)\circ dw_t^{1r}\right]\right\}.\end{aligned}$$

Finally we arrive at the result

$$d\phi(x,t)+\operatorname{div}\left\{\phi(x,t)\left[(\nabla S(x,t)-b(x,t))dt-\sum_{r=1}^{m_1}A^r(x,t)\circ dw_t^{1r}\right]\right\}=0,$$

as required. ■

III. STOCHASTIC SCHRÖDINGER EQUATIONS, PASSAGE FROM QUANTUM MECHANICS IN RANDOM ELECTROMAGNETIC FIELDS TO STOCHASTIC CLASSICAL MECHANICS

In this section we consider the Schrödinger equation (1.1) with dH defined by (1.2). This corresponds to situations when quantum particles are subject to random magnetic fields $(\nabla^k b^l-\nabla^l b^k)dt+\Sigma_{r=1}^{m_1}(\nabla^k A^{lr}-\nabla^l A^{kr})\circ dw_t^{1r}$ and random electric fields $-\nabla V dt-\Sigma_{r=1}^{m_2}\nabla K^r\circ dw_t^{2r}$. Here b,A^r $(r=1,2,\cdots,m_1)$ and V,K^r $(r=1,2,\cdots,m_2)$ and $w_t^{(1)},w_t^{(2)}$ are the same as in section I. The sort of noise in our model is white noise in time distributed locally about different points in different directions if $A^r\in C_0^\infty(R^1\times R^n,R^n)$ and $K^r\in C_0^\infty(R^1\times R^n)$. It is this case that physicists are interested in. It could also be a useful model in defence applications.

The following lemma is based on the stochastic Hamilton Jacobi equation and stochastic continuity equations.

Lemma 3.1: *Assume* b, A^r $(r=1,2,\cdots,m_1)$ *and* S_0, V, K^r $(r=1,2,\cdots,m_2)$ *and* $w_t^{(1)}, w_t^{(2)}$ *as above and the stochastic classical flow* Φ_t *defined by (2.1) satisfies the no caustic condition for* $0\leqslant t\leqslant T(\omega)$. *For any* $f\in C^\infty(R^1\times R^n)$ *and for* $0\leqslant t\leqslant T(\omega)$ *define* θ_t *for a.e.* $\omega\in\Omega$ *by*

$$\theta_t(x)=\exp\{iS(x,t)/\hbar\}\phi^{1/2}(x,t)f_t[\Phi_t^{-1}(x)], \tag{3.1}$$

where $S(x,t)$ *and* $\phi(x,t)$ *are defined as above, then* $||\theta_t||_{L^2(R^n)}=||f_t||_{L^2(R^n)}$ *almost surely and for* $0\leqslant t\leqslant T(\omega)$ *and a.e.* $\omega\in\Omega$,

$$\begin{aligned} d\theta_t(x)=&\left[\frac{1}{2}\phi^{-1}(x,t)d\phi(x,t)+i\hbar^{-1}dS(x,t)+f_t^{-1}[\Phi_t^{-1}(x)]df_t[\Phi_t^{-1}(x)]\right]\theta_t(x)\\ &-\exp\{iS(x,t)/\hbar\}\phi^{1/2}(x,t)\nabla_x f_t[\Phi_t^{-1}(x)]\cdot\Bigg((\nabla_x S(x,t)-b(x,t))dt\\ &-\sum_{r=1}^{m_1}A^r(x,t)\circ dw_t^{1r}\Bigg). \end{aligned} \tag{3.2}$$

However $\theta_t\in\mathscr{D}(dH)$ *(the domain of the operator dH), and*

$$\begin{aligned} \frac{idH}{\hbar}\theta_t(-)+d\theta_t(-)=&-\frac{1}{2}i\hbar\exp\{iS(-,t)/\hbar\}\Delta(\phi^{1/2}(-,t)f_t(\Phi_t^{-1}-))dt\\ &+\exp\{iS(-,t)/\hbar\}\phi^{1/2}(-,t)df_t(\Phi_t^{-1}-), \end{aligned} \tag{3.3}$$

where the quantum mechanical Hamiltonian in white noise electromagnetic fields is given by

$$\begin{aligned} dH=&\left(\frac{1}{2}\{-\hbar^2\Delta+2i\hbar b\cdot\nabla+i\hbar(\nabla\cdot b)+b^2\}+V\right)dt+\frac{1}{2}\sum_{r=1}^{m_1}[2i\hbar A^r\cdot\nabla+i\hbar(\nabla\cdot A^r)\\ &+2(b\cdot A^r)]\circ dw_t^{1r}+\sum_{r=1}^{m_2}K^r\circ dw_t^{2r} \end{aligned} \tag{3.4}$$

terms such as $b\cdot\nabla, \nabla\cdot b, b^2(=b\cdot b)$ *and* $A^r\cdot\nabla, \nabla\cdot A^r, b\cdot A^r$ *being multiplication operators.*

In particular for $f_t\equiv T_0\in C^\infty(R^n)$ *being independent of* t, $\theta_t(x)$ *is an approximate solution of stochastic Schrödinger equation in the sense that almost surely*

$$\frac{idH}{\hbar}\theta_t(-)+d\theta_t(-)=-\frac{1}{2}i\hbar\exp\{iS(-,t)/\hbar\}\Delta(\phi^{1/2}(-,t)T_0(\Phi_t^{-1}-))dt,$$

with initial condition $\theta_0(x)=\exp\{iS_0(x)/\hbar\}T_0(x)$, *for* $0\leqslant t\leqslant T(\omega)$.

Proof: The claim $||\theta_t||_{L^2(R^n)}=||f_t||_{L^2(R^n)}$ follows from changing variables in integral $\int_{R^n}|\theta_t(x)|^2dx$ from $x\to x_0=\Phi_t^{-1}(x)$ and the definition of ϕ. To get formula (3.2), firstly

$$\begin{aligned} d\theta_t(x)=&\left[\frac{1}{2}\phi^{-1}(x,t)d\phi(x,t)+i\hbar^{-1}dS(x,t)+f_t^{-1}[\Phi_t^{-1}(x)]df_t[\Phi_t^{-1}(x)]\right]\theta_t(x)\\ &+\exp\{iS(x,t)/\hbar\}\phi^{1/2}(x,t)Df_t[\Phi_t^{-1}(x)]\cdot d\Phi_t^{-1}(x). \end{aligned}$$

We obtain (3.2) by applying formula (2.17) for $d\Phi_t^{-1}(x)$ proved in section II, equations (2.1) and (2.9).

For (3.3), we use the following operator identity:

$$\begin{aligned}\Delta_x \exp\{iS(x,t)/\hbar\}\phi^{1/2}(x,t)-= &\exp\{iS(x,t)/\hbar\}\Delta_x(\phi^{1/2}(x,t)-)+i\hbar^{-1}\exp\{iS(x,t)/\hbar\}\phi^{1/2}(x,t)\\ &\times[\phi^{-1}(x,t)\nabla_x S(x,t)\cdot\nabla_x\phi(x,t)+\Delta_x S(x,t)+i\hbar^{-1}|\nabla_x S(x,t)|^2\\ &+2\nabla_x S(x,t)\cdot\nabla_x]-, \qquad (3.5)\end{aligned}$$

which is easy to prove and gives a rigorous identity when each side is applied to a suitable smooth function such as $f_t(\Phi_t^{-1}(x))$. From above, using

$$dH=(\tfrac{1}{2}\{-\hbar^2\Delta+2i\hbar b\cdot\nabla+i\hbar(\nabla\cdot b)+b^2\}+V)dt+\tfrac{1}{2}\sum_{r=1}^{m_1}[2i\hbar A^r\cdot\nabla+i\hbar(\nabla\cdot A^r)$$

$$+2(b\cdot A^r)]\circ dw_t^{1r}+\sum_{r=1}^{m_2}K^r\circ dw_t^{2r},$$

we obtain

$$\begin{aligned}\frac{idH}{\hbar}\theta_t(x)+d\theta_t(x)=&-\frac{1}{2}i\hbar\exp\{iS(x,t)/\hbar\}\Delta(\phi^{1/2}(x,t)f_t[\Phi_t^{-1}(x)])dt\\ &+\frac{1}{2}\exp\{iS(x,t)/\hbar\}\phi^{1/2}[\phi^{-1}(x,t)\nabla_x S(x,t)\cdot\nabla_x\phi(x,t)+\Delta_x S(x,t)\\ &+i\hbar^{-1}|\nabla_x S(x,t)|^2+2\nabla_x S(x,t)\cdot\nabla_x]f_t[\Phi_t^{-1}(x)]dt-(b\cdot\nabla)\\ &\times\{\exp\{iS(x,t)/\hbar\}\phi^{1/2}(x,t)f_t[\Phi_t^{-1}(x)]\}dt+i\hbar^{-1}\Big\{\frac{i\hbar}{2}\mathrm{div}\,b(x,t)+V\\ &+\frac{b^2}{2}(x,t)\Big\}\exp\{iS(x,t)/\hbar\}\phi^{1/2}(x,t)f_t[\Phi_t^{-1}(x)]dt-\sum_{r=1}^{m_1}(A^r\cdot\nabla)\\ &\times\{\exp\{iS(x,t)/\hbar\}\phi^{1/2}(x,t)f_t[\Phi_t^{-1}(x)]\}\circ dw_t^{1r}+i\hbar^{-1}\Big\{\sum_{r=1}^{m_1}\Big(\frac{i\hbar}{2}\mathrm{div}\,A^r(x,t)\\ &+(b(x,t)\cdot A^r(x,t))\Big)\circ dw_t^{1r}\\ &+\sum_{r=1}^{m_2}K^r(x,t)\circ dw_t^{2r}\Big\}\exp\{iS(x,t)/\hbar\}\phi^{1/2}(x,t)f_t[\Phi_t^{-1}(x)]\\ &+\Big[\frac{1}{2}\phi^{-1}(x,t)d\phi(x,t)+i\hbar^{-1}dS(x,t)+f_t^{-1}[\Phi_t^{-1}(x)]df_t[\Phi_t^{-1}(x)]\Big]\\ &\times\exp\{iS(x,t)/\hbar\}\phi^{1/2}(x,t)f_t[\Phi_t^{-1}(x)]-\exp\{iS(x,t)/\hbar\}\phi^{1/2}\nabla_x f_t[\Phi_t^{-1}(x)]\\ &\cdot\Big((\nabla S(x,t)-b(x,t))dt-\sum_{r=1}^{m_1}A^r(x,t)\circ dw_t^{1r}\Big) \qquad (3.6)\end{aligned}$$

all differentiations ∇ being with respect to x. Now we have

$$(b(x,t)\cdot\nabla)\{\exp\{iS(x,t)/\hbar\}\phi^{1/2}(x,t)f_t[\Phi_t^{-1}(x)]\}dt$$
$$=\exp\{iS(x,t)/\hbar\}\phi^{1/2}(x,t)(b(x,t)\cdot\nabla f_t[\Phi_t^{-1}(x)])dt+(b(x,t)\cdot\nabla)$$
$$\times\{\exp\{iS(x,t)/\hbar\}\phi^{1/2}\}(x,t)f_t[\Phi_t^{-1}(x)]dt$$

and

$$(b\cdot\nabla)\{\exp\{iS/\hbar\}\phi^{1/2}\}dt=\left[i\hbar^{-1}(b\cdot\nabla S)+\frac{1}{2}\phi^{-1}(b\cdot\nabla\phi)\right]\exp\{iS/\hbar\}\phi^{1/2}dt,$$

as well as

$$(A^r(x,t)\cdot\nabla)\{\exp\{iS(x,t)/\hbar\}\phi^{1/2}(x,t)f_t[\Phi_t^{-1}(x)]\}\circ dw_t^{1r}$$
$$=\exp\{iS(x,t)/\hbar\}\phi^{1/2}(x,t)(A^r(x,t)\cdot\nabla f_t[\Phi_t^{-1}(x)])\circ dw_t^{1r}+(A^r(x,t)\cdot\nabla)$$
$$\times\{\exp\{iS(x,t)/\hbar\}\phi^{1/2}\}(x,t)f_t[\Phi_t^{-1}(x)]\circ dw_t^{1r}$$

and

$$(A^r\cdot\nabla)\{\exp\{iS/\hbar\}\phi^{1/2}\}\circ dw_t^{1r}=\left[i\hbar^{-1}(A^r\cdot\nabla S)+\frac{1}{2}\phi^{-1}(A^r\cdot\nabla\phi)\right]\exp\{iS/\hbar\}\phi^{1/2}\circ dw_t^{1r}.$$

Now we consider potentially difficult term in $(i\hbar^{-1})$ in (3.6). This is easily computed to be

$$\left(\frac{1}{2}|\nabla S|^2-b\cdot\nabla S+V+\frac{b^2}{2}\right)dt-\sum_{r=1}^{m_1}A^r\cdot(\nabla S-b)\circ dw_t^{1r}+\sum_{r=1}^{m_1}K^r\circ dw_t^{2r}+dS$$
$$=\left(\frac{1}{2}|\nabla S-b|^2+V\right)dt-\sum_{r=1}^{m_1}A^r\cdot(\nabla S-b)\circ dw_t^{1r}+\sum_{r=1}^{m_2}K^r\circ dw_t^{1r}+dS=0 \tag{3.7}$$

from the stochastic Hamilton Jacobi equation.

Apart from the desired first term in (3.6), the remaining terms in $(i\hbar)^0$ are

$$\frac{1}{2}\exp\{iS/\hbar\}\phi^{1/2}f_t(\Phi_t^{-1}(x))\left[\phi^{-1}\left((\nabla S-b)dt-\sum_{r=1}^{m_1}A^r\circ dw_t^{1r}\right)\cdot\nabla\phi+\left((\Delta S-\operatorname{div}b)dt\right.\right.$$
$$\left.\left.-\sum_{r=1}^{m_1}\operatorname{div}A^r\circ dw_t^{1r}\right)+\phi^{-1}d\phi+2f_t^{-1}(\Phi_t^{-1}(x))df_t(\Phi_t^{-1}(x))\right]$$
$$=\exp\{iS/\hbar\}\phi^{1/2}df_t(\Phi_t^{-1}(x)), \tag{3.8}$$

since ϕ satisfies stochastic continuity equation (2.13). Hence we have proved (3.3). The rest of the lemma follows immediately. ■

In Lemma 3.1 we allow f to be a function of space and time t. The time dependence of f gives us an opportunity to push the approximate solution in the sense of Lemma 3.1 further, i.e., up to any order. The proof works by choosing the right f_t associated with each order and applying (3.3) in Lemma 3.1 such that we have the right cancellations in the summation. We have the following lemma.

Lemma 3.2: *Assume all the conditions in Lemma 3.1 and the same dH. For any* $T_0 \in C^\infty(R^n)$ *being independent of t, define*

$$T_0(-,t)=T_0[-], \tag{3.9}$$

and for $j=1,2,\cdots,m$ *for certain integer* $m\geqslant 0$, *a.e.* $\omega\in\Omega$ *and* $0\leqslant t\leqslant T(\omega)$,

$$T_j(y,t)=\int_0^t(\phi^{-1/2}(-,s)\Delta(\phi^{1/2}(-,s)T_{j-1}(\Phi_s^{-1}-,s)))\Phi_s(y)ds, \tag{3.10}$$

and

$$\theta_t^{(m)}(x)=\exp\{iS(x,t)/\hbar\}\phi^{1/2}(x,t)\sum_{j=0}^{m}\frac{1}{2^j}T_j(\Phi_t^{-1}(x),t)(i\hbar)^j. \tag{3.11}$$

Then $\theta_t^{(m)}\in\mathscr{D}(dH)$ *and* $\theta_t^{(m)}$ *is an approximate solution of the stochastic Schrödinger equation in the sense that*

$$\frac{idH}{\hbar}\theta_t^{(m)}(-)+d\theta_t^{(m)}(-)=-\frac{1}{2^{m+1}}(i\hbar)^{m+1}\exp\{iS(-,t)/\hbar\}\Delta(\phi^{1/2}(-,t)T_m(\Phi_t^{-1}-,t))dt, \tag{3.12}$$

with initial condition $\theta_0(x)=\exp\{iS_0(x)/\hbar\}T_0(x)$ *for a.e.* $\omega\in\Omega$ *and* $0\leqslant t\leqslant T(\omega)$.

Proof: Writing

$$g_j(x,t)=\frac{1}{2^j}\exp\{iS(x,t)/\hbar\}\phi^{1/2}(x,t)T_j(\Phi_t^{-1}(x),t)$$

and applying formula (3.3) in Lemma 3.1 to $g_j(x,t)$ where $f_t(-)=(1/2^j)\,T_j(-,t)$, we obtain

$$\frac{i}{\hbar}dHg_0(x,t)+dg_0(x,t)=-\frac{1}{2}i\hbar\exp\{iS(x,t)/\hbar\}\Delta(\phi^{1/2}(x,t)T_0(\Phi_t^{-1}(x),t))dt,$$

and for $j=1,2,\cdots,m$

$$\begin{aligned}\frac{i}{\hbar}dHg_j(x,t)+dg_j(x,t)=&-\frac{1}{2^{j+1}}i\hbar\exp\{iS(x,t)/\hbar\}\Delta(\phi^{1/2}(x,t)T_j(\Phi_t^{-1}(x),t))dt\\&+\frac{1}{2^j}\exp\{iS(x,t)/\hbar\}\Delta(\phi^{1/2}(x,t)T_{j-1}(\Phi_t^{-1}(x),t))dt.\end{aligned}$$

Therefore it follows obviously that

$$\begin{aligned}&\frac{i}{\hbar}dH\left(\sum_{j=0}^{m}g_j(x,t)(i\hbar)^j\right)+d\left(\sum_{j=0}^{m}g_j(x,t)(i\hbar)^j\right)\\&\quad=-i\hbar\sum_{j=0}^{m}\frac{1}{2^{j+1}}\exp\{iS(x,t)/\hbar\}\Delta(\phi^{1/2}(x,t)T_j(\Phi_t^{-1}(x),t))(i\hbar)^jdt\\&\qquad+\sum_{j=1}^{m}\frac{1}{2^j}\exp\{iS(x,t)/\hbar\}\Delta(\phi^{1/2}(x,t)T_{j-1}(\Phi_t^{-1}(x),t))(i\hbar)^jdt\\&\quad=-\sum_{j=0}^{m}\frac{1}{2^{j+1}}\exp\{iS(x,t)/\hbar\}\Delta(\phi^{1/2}(x,t)T_j(\Phi_t^{-1}(x),t))(i\hbar)^{j+1}dt\end{aligned}$$

$$+\sum_{j=1}^{m}\frac{1}{2^j}\exp\{iS(x,t)/\hbar\}\Delta(\phi^{1/2}(x,t)T_{j-1}(\Phi_t^{-1}(x),t))(i\hbar)^j dt$$

$$=-\frac{1}{2^{m+1}}(i\hbar)^{m+1}\exp\{iS(x,t)/\hbar\}\Delta(\phi^{1/2}(x,t)T_m(\Phi_t^{-1}(x),t))dt.$$

Therefore we have (3.12) as $\theta_t^{(m)}(x)=\Sigma_{j=0}^{m}g_j(x,t)(i\hbar)^j$. ■

Lemma 3.2 does not give us the approximate solution properly. In the following theorem we are going to pass the approximation in Lemma 3.2 to an approximation in $L^2(R^n)$ a.s.

Theorem 3.3: *Assume there exists a unique solution of* $\psi^\hbar(x,t)=\exp\{-i\int_0^t dH/\hbar\}\psi_0^\hbar(x)$ *in* $L^2(R^n,dn)$, *where*

$$dH=(\tfrac{1}{2}\{-\hbar^2\Delta+2i\hbar b\cdot\nabla+i\hbar(\nabla\cdot b)+b^2\}+V)dt$$
$$+\tfrac{1}{2}\sum_{r=1}^{m_1}[2i\hbar A^r\cdot\nabla+i\hbar(\nabla\cdot A^r)+2(b\cdot A^r)]\circ dw_t^{1r}+\sum_{r=1}^{m_2}K^r\circ dw_t^{2r},$$

with $A_t^r(r=1,2,\cdots,m_1), b\in C_0^\infty(R^n,R^n)$ *for any* $t\geqslant 0$, *and* $\psi_0^\hbar(x)=\exp\{iS_0(x)/\hbar\}T_0(x)$, $T_0\in C_0^\infty(R^n)$, S_0,T_0 *being independent of* $\hbar$. *Assume the stochastic flow* $\Phi_s:R^n\to R^n$ *defined by (2.1) satisfies the no caustic condition for* $0\leqslant s\leqslant T(\omega)$ *for a.e.* $\omega\in\Omega$. *Then for each* $t\in[0,T(\omega))$, *as* $\hbar\to 0$

$$\exp\{-iS(x,t)/\hbar\}\psi^\hbar(x,t)\to\phi^{1/2}(x,t)T_0(\Phi_t^{-1}(x)) \tag{3.13}$$

in $L^2(R^n)$ *uniformly in* t *almost surely, if* $\Delta(\phi^{1/2}(-,t)T_0(\Phi_t^{-1}(-))\in L^2(R^n)$ *and* $\int_0^t||\Delta(\phi^{1/2}(-,s)T_0(\Phi_s^{-1}(-))||_{L^2(R^n)}ds<\infty$ *almost surely. Here* $S(x,t)$ *is defined by (2.2) and (2.8) and* $\Phi_t^{-1}(x)$ *is the inverse of the stochastic flow* $\Phi_t:R^n\to R^n$ *and* $\phi(x,t)=|\det(\partial\Phi_t^{-1}(x)/\partial x)|$.

Furthermore, define

$$T_0(-,t)=T_0[-],$$

and for $j=1,2,\cdots,m$ *for certain integer* $m\geqslant 0$ *and* $0\leqslant t\leqslant T(\omega)$

$$T_j(-,t)=\int_0^t(\phi^{-1/2}(-,s)\Delta(\phi^{1/2}(-,s)T_{j-1}(\Phi_s^{-1}-,s)))\Phi(y)ds.$$

Then for a.e. $\omega\in\Omega$ *and* $0\leqslant t\leqslant T(\omega)$,

$$\psi_t^\hbar(x)=\exp\{iS(x,t)/\hbar\}\left[\phi^{1/2}(x,t)\sum_{j=0}^{m}\frac{1}{2^j}T_j(\Phi_t^{-1}(x),t)(i\hbar)^j+R_m(x,t)(i\hbar)^{m+1}\right], \tag{3.14}$$

and

$$||R_m(-,t)||_{L^2(R^n)}\leqslant\frac{1}{2^{m+1}}\int_0^t||\Delta(\phi^{1/2}(-,s)T_m(\Phi_s^{-1}-,s))||_{L^2(R^n)}ds, \tag{3.15}$$

if $\Delta(\phi^{1/2}(-,s)T_m(\Phi_s^{-1}(-),s))\in L^2(R^n)$ *for* $0\leqslant s\leqslant t$ *and*
$\int_0^t||\Delta(\phi^{1/2}(-,s)T_m(\Phi_s^{-1}(-),s))||_{L^2(R^n)}ds<\infty$ *almost surely.*

Proof: For the semi-classical expansion (3.14) and estimate (3.15) first note

$$\frac{idH}{\hbar}(\theta_t^{(m)}-\psi_t)+d(\theta_t^{(m)}-\psi_t)=-\frac{1}{2^{m+1}}(i\hbar)^{m+1}\exp\{iS(-,t)/\hbar\}\Delta(\phi^{1/2}(-,t)T_m(\Phi_t^{-1}-,t))dt,$$

from Lemma 3.2. Therefore by the definition of $L^2(R^n)$ norm

$$\begin{aligned}
d(\theta_t^{(m)}-\psi_t,\theta_t^{(m)}-\psi_t)_{L^2(R^n)}&=d\left(\int_{R^n}(\theta_t^{(m)}-\psi_t)(\overline{\theta_t^{(m)}}-\overline{\psi_t})dx\right)\\
&=\int_{R^n}((d(\theta_t^{(m)}-\psi_t))(\overline{\theta_t^{(m)}}-\overline{\psi_t})+(\theta_t^{(m)}-\psi_t)d(\overline{\theta_t^{(m)}}-\overline{\psi_t}))dx\\
&=\int_{R^n}\frac{i}{\hbar}-(\overline{\theta_t^{(m)}}-\overline{\psi_t})dH(\theta_t^{(m)}-\psi_t)+(\theta_t^{(m)}-\psi_t)\overline{dH}(\overline{\theta_t^{(m)}}-\overline{\psi_t}))\\
&\quad-\frac{1}{2^{m+1}}(i\hbar)^{m+1}\int_{R^n}\exp\{iS(x,t)/\hbar\}\Delta(\phi^{1/2}(x,t)T_m(\Phi_t^{-1}(x),t))\\
&\quad\times(\overline{\theta_t^{(m)}}-\overline{\psi_t})dxdt-\frac{1}{2^{m+1}}(-i\hbar)^{m+1}\int_{R^n}\exp\{-iS(x,t)/\hbar\}\\
&\quad\times\Delta(\phi^{1/2}(x,t)T_m(\Phi_t^{-1}(x),t))(\theta_t^{(m)}-\psi_t)dxdt.
\end{aligned}$$

Here by $\overline{\theta,\psi}$ we denote the complex conjugate of functions θ and ψ and by $\overline{dH}$ we denote the complex conjugate of operator dH. But

$$\begin{aligned}
&\int_{R^n}(-(\overline{\theta_t^{(m)}}-\overline{\psi_t})dH(\theta_t^{(m)}-\psi_t)+(\theta_t^{(m)}-\psi_t)\overline{dH}(\overline{\theta_t^{(m)}}-\overline{\psi_t}))\\
&\quad=\int_{R^n}\frac{1}{2}\{\hbar^2((\overline{\theta_t^{(m)}}-\overline{\psi_t})\Delta(\theta_t^{(m)}-\psi_t)-(\theta_t^{(m)}-\psi_t)\Delta(\overline{\theta_t^{(m)}}-\overline{\psi_t}))\}dxdt\\
&\qquad+\int_{R^n}i\hbar\left(bdt+\sum_{r=1}^{m_1}A^r\circ dw_t^{1r}\right)(-(\overline{\theta_t^{(m)}}-\overline{\psi_t})\nabla(\theta_t^{(m)}-\psi_t)-(\theta_t^{(m)}-\psi_t)\nabla(\overline{\theta_t^{(m)}}-\overline{\psi_t}))dx\\
&\qquad+\int_{R^n}i\hbar\left(\operatorname{div}bdt+\sum_{r=1}^{m_1}\operatorname{div}A^r\circ dw_t^{1r}\right)(-(\theta_t^{(m)}-\psi_t)(\overline{\theta_t^{(m)}}-\overline{\psi_t}))dx\\
&\quad=\frac{1}{2}\hbar^2\int_{R^n}\operatorname{div}((\overline{\theta_t^{(m)}}-\overline{\psi_t})\nabla(\theta_t^{(m)}-\psi_t)-(\theta_t^{(m)}-\psi_t)\nabla(\overline{\theta_t^{(m)}}-\overline{\psi_t}))dxdt\\
&\qquad-i\hbar\int_{R^n}\operatorname{div}\left(\left(bdt+\sum_{j=1}^{m_1}A^r\circ dw_t^{1r}\right)((\theta_t^{(m)}-\psi_t)(\overline{\theta_t^{(m)}}-\overline{\psi_t}))\right)dx=0,
\end{aligned}$$

by the Divergence Theorem.

Now by the Cauchy–Schwarz inequality we have

$$d(\theta_t^{(m)}-\psi_t,\theta_t^{(m)}-\psi_t)_{L^2(R^n)}=-\frac{1}{2^m}\int_{R^n}\Delta(\phi^{1/2}(x,t)T_m(\Phi_t^{-1}(x),t))\mathrm{Re}\{(i\hbar)^{m+1}\exp\{iS(x,t)/\hbar\}$$
$$\times(\overline{\theta_t^{(m)}}-\overline{\psi_t})\}dxdt$$
$$\leqslant\frac{1}{2^m}||\Delta(\phi^{1/2}(-,t)T_m(\Phi_t^{-1}(x),t))||_{L^2(R^n)}$$
$$\times||\mathrm{Re}\{(i\hbar)^{m+1}\exp\{iS(x,t)/\hbar\}(\overline{\theta_t^{(m)}}-\overline{\psi_t})\}||_{L^2(R^n)}dt$$
$$\leqslant\frac{1}{2^m}\hbar^{m+1}||\theta_t^{(m)}-\psi_t||_{L^2(R^n)}$$
$$\times||\Delta(\phi^{1/2}(x,t)T_m(\Phi_t^{-1}(x),t))||_{L^2(R^n)}dt.$$

Therefore solving the ordinary differential equation we have

$$||\theta_t^{(m)}-\psi_t||_{L^2(R^n)}\leqslant\frac{1}{2^{m+1}}\hbar^{m+1}\int_0^t||\Delta(\phi^{1/2}(-,s)T_m(\Phi_s^{-1}(-),s))||_{L^2(R^n)}ds.$$

Note the unitary property of the operator $\exp\{-iS(x,t)/\hbar\}$, therefore

$$||\exp\{-iS(x,t)/\hbar\}(\theta_t^{(m)}-\psi_t)||_{L^2(R^n)}\leqslant\frac{1}{2^{m+1}}\hbar^{m+1}\int_0^t||\Delta(\phi^{1/2}(-,s)T_m(\Phi_s^{-1}(-),s))||_{L^2(R^n)}ds.$$

This leads to the semi-classical expansion (3.14) and estimate (3.15). Claim (3.13) is only a special case of the result proved above. ■

Now let A be any measurable subset of the configuration space R^n and $\tilde{P}^\hbar(A,t)$ be the quantum probability that the quantum mechanical particle is in A at time t. Rewrite (3.14) in Theorem 3.3 to give

$$\psi_t^\hbar(x)=\exp\{iS(x,t)/\hbar\}\Bigg[\phi^{1/2}(x,t)\Bigg(\sum_{j=0}^{r_1}\frac{(-1)^j}{2^{2j}}T_{2j}(\Phi_t^{-1}(x),t)\hbar^{2j}$$
$$+i\sum_{j=0}^{r_2}\frac{(-1)^j}{2^{2j+1}}T_{2j+1}(\Phi_t^{-1}(x),t)\hbar^{2j+1}\Bigg)+R_m(x,t)(i\hbar)^{m+1}\Bigg]. \tag{3.16}$$

Here the integers r_1 and r_2 are defined by: $r_1=\max\{r:2r\leqslant m\}$ and $r_2=\max\{r:2r+1\leqslant m\}$.

According to Born's probabilistic interpretation:

$$\tilde{P}^\hbar(A,t)=\int_A|\psi_\hbar(x,t)|^2dx.$$

We now have an asymptotic expansion of $\tilde{P}^\hbar(A,t)$ as follows:

$$\tilde{P}^\hbar(A,t)=\sum_{j=0}^{m}P_{2j}\hbar^{2j}+\int_A|R_m(x,t)|^2dx\hbar^{2(m+1)}. \tag{3.17}$$

Here $\int_A|R_m(x,t)|^2dx$ is bounded and P_{2j} $(j=0,1,\cdots)$ are given below:

$$P_0(A,t)=\int_{\Phi_t^{-1}A}T_0^2(y,t)dy,$$

$$P_2(A,t)=\int_{\Phi_t^{-1}A}\left(\frac{1}{2^2}T_1^2(y,t)-\frac{1}{2}T_0(y,t)T_2(y,t)\right)dy,$$

$$P_4(A,t)=\int_{\Phi_t^{-1}A}\left(\frac{1}{2^4}T_2^2(y,t)+\frac{1}{2^3}T_0(y,t)T_4(y,t)-\frac{1}{2^3}T_1(y,t)T_3(y,t)\right)dy.$$

In the limit as $\hbar\to 0$ we have

$$\lim_{\hbar\to 0}\widetilde{P}^{\hbar}(A,t)=P_0=\int_{\Phi_t^{-1}A}|\psi_0(y)|^2dy=\widetilde{P}(\Phi_t^{-1}A,0),$$

Φ_t being the classical Hamiltonian flow associated with the stochastic system (2.1). Hence, in the limit as $\hbar\to 0$, the quantum mechanical system in the configuration space R^n, as determined by

$$\frac{idH}{\hbar}\psi_t+d\psi_t=0$$

in random electromagnetic fields can quantum mechanically arrive at only these points which are accessible to the corresponding stochastic classical system. In this sense, stochastic quantum mechanics tends to stochastic classical mechanics on R^n as $\hbar$ tends to zero. This is a simple consequence of the result in this paper.

Moreover, $\hbar^2T_1$ is the integral along the classical sample path of the Bohm's first quantum potential (see Holland[22]). This quantity has the dimensions of action i.e. the dimensions of $\hbar$. The first term in $\hbar^2P_2$ is the ratio of $(\hbar^2T_1)^2$ to $\hbar^2$. By the same token, $\hbar^4T_2T_0$ will have the dimensions of $(\text{action})^2$ i.e. yet again of $\hbar^2$, and the ratio of this quantity to $\hbar^2$ is what appears in $\hbar^2P_2$. We therefore see that the correction to the quantum probability for finding the particle in A at the time t are significant only when these ratios are nonnegligible.

When $A=R^n$, we can prove $P_2(R^n,t)=P_4(R^n,t)=\cdots=P_{2m}(R^n,t)=0$ by using the definition of P_{2j} and T_j. Therefore we have $P^{\hbar}(R^n,t)=P_0(R^n,t)=P^{\hbar}(R^n,0)$. This shows that the semiclassical expansion gives a normalized solution of stochastic Schrödinger equations. Detailed proofs of this and related results will be published in the future.

It is also interesting to note that in a classical inaccessible region A, $P_0(A,t)=0$. Therefore $T_0(-)=0$ almost everywhere in $\Phi_t^{-1}A$. It turns out that $\frac{1}{4}\hbar^2\int_{\Phi_t^{-1}}T_1^2(y,t)dy$ gives us (if the higher order terms are negligible) the probability of finding a quantum mechanical particle in the classical inaccessible region A.

The results in this paper also give the quantization of the stochastic Hamiltonian mechanics studied in Albeverio,[23] Albeverio, Hilbert and Zehnder,[24] and by McKean,[25] Markus and Weerasinghe.[26]

IV. NO CAUSTIC CONDITION

We end this paper by discussing the no-caustic condition. As we have pointed out in section II, the diffeomorphism property of the (stochastic) Hamiltonian system in configuration space is different from that for first order (stochastic) differential equations. The latter equations have been discussed by many people, in particular by Kunita[21] and Elworthy[10] for stochastic differential equations. The Lipschitz condition guarantees the stochastic flow property up to explosion time for first order stochastic differential equations. Unfortunately this is not true for the (stochastic) Hamiltonian system in configuration space. The simplest example is the harmonic oscillator studied in Elworthy, Truman and Zhao:[12] $\ddot{\Phi}_s=-\Phi_s,\Phi_0(x)=x,\dot{\Phi}_0(x)=x$. The solution is given by $\Phi_s(x)=x\cos s+x\sin s$. At $s=\frac{3}{4}\pi$, $\Phi_s(x)=0$, for any $x\in R^1$. That is to say $\Phi_{(3/4)\pi}$ is not a diffeomorphism and the caustic time is $s=\frac{3}{4}\pi$. Therefore a diffeomorphism theorem for (stochastic)

Hamiltonian system in configuration space is needed as clearly caustics are a common feature. In fact we have showed in Truman and Zhao[15] that it is caustics which lead to the random shock waves for inviscid stochastic Burgers' equations. Here we include a simple theorem guaranteeing the absence of caustics.

Theorem 4.1: *Assume* $A_t^r, b_t, (\partial/\partial t)\, b_t \in C_0^\infty(R^n,R^n)$, $V_t, K_t^r, S_0 \in C_0^\infty(R^n)$. *Then there exists* $T(\omega)>0$ *a.s. such that* $\Phi_t(\omega):R^n\to R^n$ *defined by (2.1), is a diffeomorphism for* $0\leqslant s\leqslant T(\omega)$ *for a.e.* $\omega\in\Omega$.

Proof: Integrating second equation of (2.1) we have

$$v_t^k=\nabla^k S_0(x)-b^k(x,0)+Z_t^k+\int_0^t(\nabla^k b_l(\Phi_s,s)-\nabla^l b_k(\Phi_s,s))v_s^l ds$$
$$+\int_0^t\sum_{r=1}^{m_1}\nabla^k A^{lr}(\Phi_s,s)v_s^l\circ dw_s^{1r},$$

where

$$Z_t^k=-\int_0^t\left(\nabla^k V(\Phi_s,s)ds-\sum_{r=1}^{m_2}\nabla^k K^r(\Phi_s,s)dw_s^{2r}-\frac{\partial}{\partial s}b_k(\Phi_s,s)ds\right)-\int_0^t(\nabla^k b_l(\Phi_s,s)$$
$$-\nabla^l b_k(\Phi_s,s))\sum_{r=1}^{m_1}A^{lr}(\Phi_s,s)\circ dw_s^{1r}.$$

For any $T^*>0$, Z_t^k $(k=1,2,\cdots,n)$ is bounded almost surely for any $0\leqslant t\leqslant T^*$. Therefore v_t^k $(k=1,2,\cdots,n)$ is bounded almost surely for any $0\leqslant t\leqslant T^*$. Differentiating (2.1) with respect to space variable x, we know $(\nabla_j\Phi_s^k,\nabla_j v_s^k)$ satisfies stochastic ordinary differential linear equations with $\nabla_j\Phi_0^k(x)=\delta_j^k,\nabla_j v_0^k(x)=\nabla_j(\nabla^k S_0(x)-b^k(x,0))$. Therefore for $0\leqslant t\leqslant T^*$, $(\nabla_j\Phi_s^k,\nabla_j v_s^k)$ are bounded almost surely. Therefore there exists $T(\omega)>0$ a.s. such that for $0\leqslant t\leqslant T(\omega)$ the matrix norm $||\int_0^t\nabla v_s ds-\Sigma_{r=1}^{m_1}\int_0^t(\nabla\Phi_s)^*\nabla A^r(\Phi_s,s)\circ dw_s^{1r}||<1$ a.s. But

$$\nabla\Phi_s=I+\int_0^t\nabla v_s ds-\sum_{r=1}^{m_1}\int_0^t(\nabla\Phi_s)^*\nabla A^r(\Phi_s,s)\circ dw_s^{1r}.$$

By the similar argument to the one in Elworthy and Truman[7] we know for $0\leqslant t\leqslant T(\omega)$, $\Phi_t(\omega)$ is nonsingular a.s. The diffeomorphism follows from the global inverse theorem. (See Ref. 7 for example). ■

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Conditional symmetry and spectrum of the one-dimensional Schrödinger equation

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We develop an algebraic approach to studying the spectral properties of the stationary Schrödinger equation in one dimension based on its high-order conditional symmetries. This approach makes it possible to obtain in explicit form representations of the Schrödinger operator by $n\times n$ matrices for any $n\in\mathsf{N}$ and, thus, to reduce a spectral problem to a purely algebraic one of finding eigenvalues of constant $n\times n$ matrices. The connection to so-called quasiexactly solvable models is discussed. It is established, in particular, that the case, when conditional symmetries reduce to high-order Lie symmetries, corresponds to exactly solvable Schrödinger equations. A symmetry classification of Schrödinger equation admitting nontrivial high-order Lie symmetries is carried out, which yields a hierarchy of exactly solvable Schrödinger equations. Exact solutions of these are constructed in explicit form. Possible applications of the technique developed to multidimensional linear and one-dimensional nonlinear Schrödinger equations are briefly discussed.
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I. INTRODUCTION

Basic motivation for introducing conditional symmetries (the term ''conditional symmetry'' was suggested for the first time by Fushchych[1–3]), was a necessity to find a symmetry background of a quickly growing variety of exact solutions of nonlinear partial differential equations that could not be obtained within the framework of the classical Lie approach. An intensive search of such solutions was begun independently and almost simultaneously by Fushchych with collaborators (see, Refs. 4,5 and references therein), Clarkson and Kruskal (''the direct reduction method''[6]), Olver and Rosenau (''nonclassical reduction''[7]) and Winternitz and Levi.[8] A number of examples of nonlinear partial differential equations in two, three, and even four dimensions having nontrivial conditional symmetries is growing rapidly. In particular, it has been established by Fushchych, Zhdanov, and Revenko[9–13] that such fundamental equations of the modern quantum field theory as the four-dimensional nonlinear d'Alembert, Dirac, Levi–Leblond, Maxwell, and Yang-Mills equations possess *infinite* conditional symmetries, while their Lie symmetries are finite only.

On the other hand, much less attention is devoted to the study of conditional symmetries of linear differential equations (though the first example of conditional symmetry has been obtained by Bluman and Cole for the one-dimensional linear heat equation[14]). In view of the role played by conditional symmetries in the theory of nonlinear differential equations, one can expect that application of these to linear equations will also be rich in results. In the present paper we establish the rather unexpected (at least for the author) fact that conditional symmetries can be effectively applied to study spectral properties of the stationary Schrödinger equation,

$$\psi_{xx}=(\epsilon+V(x))\psi. \tag{1}$$

In particular, we will prove that it is conditional symmetry that is responsible for a phenom-

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enon of so-called ''quasiexact solvability'' of some specific class of equations (1).[15–17] And what is more, the case when conditional symmetries are equivalent to Lie symmetries will be shown to yield exactly solvable Schrödinger equations.

All principal approaches to a construction of (quasi)exactly solvable models (apart from the specific ways of an implementation of these) are based on a possibility to construct a basis $u_1(x)$, $u_2(x),\ldots,u_n(x)$ of some invariant space $\mathscr{V}_n$ of the Schrödinger operator $S=\partial_x^2-V(x)$. This means that there should exist constant $n\times n$ matrix $\|\Lambda_{jk}\|$ such that the following conditions are fulfilled:

$$Su_j(x)\equiv(\partial_x^2-V(x))u_j(x)=\sum_{k=1}^{n}\Lambda_{jk}u_k(x),\quad j=1,2,\ldots,n. \tag{2}$$

Given such functions $u_j(x)$, a procedure for calculating the spectrum of the Schrödinger operator (or, more precisely, a part of the spectrum) is completely algebraic. Let $\mathbf{a}^j=(a_1^j,a_2^j,\ldots,a_n^j)$, $j=1,\ldots,m,m\leqslant n$ be a complete system of eigenvectors of the $n\times n$ matrix $\Lambda=\|\Lambda_{jk}\|_{j,k=1}^{n}$ and $\lambda_1,\ldots,\lambda_m$ be their eigenvalues, namely

$$\sum_{j=1}^{n}\Lambda_{jk}a_j^l=\lambda_l a_k^l,\quad l=1,2,\ldots,m. \tag{3}$$

Then, the function

$$\psi_k(x)=\sum_{j=1}^{n}a_j^k u_j(x) \tag{4}$$

is easily seen to satisfy the equation (1) with $\epsilon=\lambda_k$ under arbitrary $k=1,2,\ldots,m$.

Saying it another way, after being restricted to a linear space $\mathscr{V}_n$ with basis functions $u_1(x),u_2(x),\ldots,u_n(x)$ the Schrödinger operator becomes a matrix operator. Thus, a reduction of a differential operator to a matrix operator takes place. But such a procedure is quite a common routine in the theory of Lie symmetries of differential equations. Indeed, if we restrict a partial differential equation having N independent variables to a subset of its solutions invariant under a one-parameter subgroup of the Lie group admitted by the equation in question, then it is reduced to a partial differential equation with $N-1$ independent variables. Such a procedure is called symmetry reduction of differential equations (for more details, see, e.g., Refs. 4, 18, and 19). Taking $N=1$ (the case of an ordinary differential equation) we obtain as a reduced equation a differential equation with $N=0$, i.e. an algebraic equation!

One of the main aims of the present paper is to show that the idea of symmetry reduction, when formulated in an appropriate way, can be applied effectively to an algebraization of the problem of describing spectrum of the Schrödinger operator.

As mentioned above classical Lie symmetries of partial differential equation do not give all possible reductions. More general symmetries responsible for a possibility of reducing the order of differential equations are conditional symmetries. Roughly speaking, the necessary and sufficient condition providing a possibility to reduce a number of variables in a given partial differential equation is a requirement of conditional invariance (Ref. 20). It will be established that a similar situation takes place for the Schrödinger equation (1). Symmetries providing reducibility of differential equation (1) to a system of algebraic equations of the form (2) are exactly the high-order conditional symmetries introduced independently by Zhdanov and Fushchych[21,22] and Fokas and Liu[23] (also see Refs. 24–26).

It should be emphasized that considerations of the present paper are purely *algebraic*. The method of conditional symmetries making it possible to study spectral properties of the Schrödinger operator S gives no information about analytical properties of the corresponding eigenfunc-

tions. In each specific case such properties of the eigenfunctions obtained as square integrability, asymptotic behavior, singularities, etc. should be studied independently (see, e.g., Ref. 27). The reason is that this method (and group-theoretical, symmetry methods in general) exploits algebraic properties of the solution set of Eq. (1) (or its part) as a whole and, roughly speaking, is independent of analytical properties of specific solutions.

II. CONDITIONAL SYMMETRY OF THE SCHRÖDINGER EQUATION

Consider the nth-order differential operator,

$$Q=\sum_{j=0}^{n} q_j(x)\partial_x^j, \tag{5}$$

where $\partial_x^0=1$, $\partial_x^{j+1}=(d/dx)\partial_x^j$, and functions $q_j(x)$ are supposed to be independent of ϵ.

Following Refs. 28 and 29 we say that Eq. (1) is conditionally invariant with respect to the operator Q if the following operator identity holds:

$$[Q,\partial_x^2-(\epsilon+V(x))]=RQ+P(\partial_x^2-(\epsilon+V(x)). \tag{6}$$

Here $[Q_1,Q_2]\equiv Q_1Q_2-Q_2Q_1$, R, P are some first- and nth-order differential operators, correspondingly. The above operator equality should be understood in the following way: the differential operators on the left- and right-hand sides give the same result when acting on arbitrary $(n+2)$-times continuously differentiable function $f(x)$.

Provided R vanishes, condition (6) is nothing else but a criterion for Eq. (1) to be invariant with respect to the operator Q. In such a case, the operator Q is a generalized (high-order) Lie symmetry operator. But given a condition $R\neq 0$, the operator Q corresponds to high-order conditional symmetry of the Schrödinger equation (1).

It is easy to see that if an equation is conditionally invariant with respect to the operator Q, then it is conditionally invariant with respect to the operator $q(x)Q$ with an arbitrary sufficiently smooth function $q(x)$. Consequently, without loss of generality we can suppose that in (5) $q_n(x)=1$ and consider differential operators of the form

$$Q=\partial_x^n+\sum_{j=0}^{n-1} q_j(x)\partial_x^j. \tag{7}$$

As the coefficients of the operator Q do not depend on ϵ, equality (6) is only possible if $R=r(x)$ and $P=0$ with some sufficiently smooth function $r(x)$. Consequently, the condition (6) is rewritten to become

$$[Q,\partial_x^2-V(x)]=r(x)Q. \tag{8}$$

We call the Schrödinger operator *reducible* if there exist linearly independent functions $u_1(x),\ldots,u_n(x)$ and constants Λ_{jk} such that the conditions (2) are fulfilled. Let us note that this terminology is justified both from the point of view of the classical representation theory and of the symmetry analysis of differential equations. Indeed, conditions (2) mean that the representation space of the operator S contains an invariant subspace and, consequently, the representation is reducible. On the other hand, conditions (2) ensure the reduction of the differential equation (1) to a system of algebraic equations. We will prove an assertion that shows that this is not a simple coincidence but a fundamental fact having a natural symmetry interpretation.

Theorem 1: *The Schrödinger operator $S=\partial_x^2-V(x)$ is reducible if and only if there exists an nth-order differential operator Q of the form (5) such that Eq. (1) is conditionally invariant with respect to Q.*

Proof: The necessity. Let the operator $S=\partial_x^2-V(x)$ be reducible. Then, the conditions (2) hold. As functions $u_j(x)$ are linearly independent, they form a fundamental system of solutions of some nth-order linear ordinary differential equation.[30]

We recall that the fundamental system of solutions of an ordinary differential equation is a maximal set of its particular solutions such that any smooth solution can be represented as a linear combination of these. Provided the order of the ordinary differential equation in question is equal to n, any n linearly independent solutions of it form a fundamental system. Furthermore, having a fundamental system of solutions we can reconstruct the corresponding ordinary differential equation within a multiplication by a function $r(x)$. Consequently, if we fix the coefficient of the nth-order derivative to be equal to 1, then this equation is unique.

Thus, there exists the nth-order differential equation,

$$u^{(n)}(x)+\sum_{j=0}^{n-1}\widetilde{q}_j(x)u^{(j)}(x)=0, \tag{9}$$

such that the functions $u_j(x)$ form a fundamental system of its solutions.

We will prove that Eq. (1) is conditionally invariant with respect to the operator

$$\widetilde{Q}=\partial_x^n+\sum_{j=0}^{n-1}\widetilde{q}_j(x)\partial_x^j.$$

By force of relations (2) the following equalities hold:

$$[\widetilde{Q},\partial_x^2-V(x)]u_j(x)=\widetilde{Q}\{(\partial_x^2-V(x))u_j(x)\}-(\partial_x^2-V(x))\{\widetilde{Q}u_j(x)\}=\widetilde{Q}\left\{\sum_{k=1}^{n}\Lambda_{jk}u_k(x)\right\}=0,$$

for any $j=1,2,\ldots,n$.

Thus, the functions $u_j(x)$ satisfy an ordinary differential equation,

$$[\widetilde{Q},\partial_x^2-(\epsilon+V(x))]u(x)=0, \tag{10}$$

whose order is easily established to be equal to n. Consequently, its fundamental system of solutions consists of n functions. Hence, we conclude that the functions $u_j(x)$ form a fundamental system of solutions of (10). As an ordinary differential equation is determined by its fundamental system uniquely within a multiplication by a function $r(x)$, the relation holds,

$$[\widetilde{Q},\partial_x^2-(\epsilon+V(x))]=r(x)\widetilde{Q},$$

which is the same as what was to be proved.

The sufficiency. Let the Schrödinger equation (1) be conditionally invariant with respect to the operator (7), which means that the condition (8) is fulfilled. Consider an equation,

$$Qu(x)\equiv\left(\partial_x^n+\sum_{j=0}^{n-1}q_j(x)\partial_x^j\right)u(x)=0, \tag{11}$$

as an ordinary differential equation for a function $u(x)$. Clearly, its general solution is represented in the form

$$u(x)=\sum_{j=1}^{n}C_ju_j(x), \tag{12}$$

where C_j are arbitrary constants and $u_1(x),\ldots,u_n(x)$ is a fundamental system of solutions of nth-order ordinary differential equation (11).

From the condition (8) it follows that the Schrödinger operator $S=\partial_x^2-V(x)$ is a symmetry operator for the equation (11), i.e., it transforms each solution of Eq. (11) into another solution of the same equation. Consequently, for any $j=1,2,\ldots,n$ the function $\widetilde{u}_j(x)=(\partial_x^2-V(x))u_j(x)$ satisfy (11). But by definition the fundamental system of solutions of nth-order ordinary differential equation forms a maximal set of its linearly independent solutions, which means that any solution can be represented as a linear combination of functions $u_j(x)$. Thus, there exist such constants Λ_{jk} that functions $u_j(x)$ satisfy relations (2), whence it follows that the corresponding Schrödinger equation is reducible. The theorem is proved.

Note that the proof of theorem is, in fact, independent of the specific form of the Schrödinger operator $S=\partial_x^2-V(x)$. It is straightforward to generalize Theorem 1 to the case of an arbitrary Nth-order differential operator,

$$\widetilde{S}=\sum_{j=0}^{N} f_j(x)\partial_x^j. \tag{13}$$

We give the corresponding assertion without proof.

Theorem 2: *The operator $\widetilde{S}$ in (13) is reducible if and only if there exists nth-order differential operator Q of the form (5) such that equation $\widetilde{S}\psi(x)=0$ is conditionally invariant with respect to Q.*

To illustrate the above statement we consider two examples.

Example 1: Consider the harmonic oscillator Schrödinger equation,

$$\psi_{xx}=(\epsilon+x^2)\psi. \tag{14}$$

As a direct check shows the nth-order differential operator,

$$Q=(\partial_x-x)^n, \tag{15}$$

satisfies the following commutation relation:

$$[Q,\partial_x^2-(\epsilon+x^2)]=2nQ$$

(the easiest way to prove the above formula is to use the mathematical induction method).

Consequently, Eq. (14) is conditionally invariant with respect to the operator Q and we can apply Theorem 1. Integrating equation $Q\psi(x)=0$ yields a basis of the invariant space $\mathscr{V}_n$ of the Schrödinger operator $\partial_x^2-x^2$,

$$e^{-x^2/2},\quad xe^{-x^2/2},\quad x^2e^{-x^2/2},\ldots,x^{n-1}e^{-x^2/2}.$$

It is readily seen that the above functions satisfy relations (2) with $V(x)=x^2$. Calculating eigenvalues (λ_j) and eigenvectors ($\vec{a}^j$) of the corresponding matrix $\|\Lambda_{jk}\|$, we obtain exact solutions of the Schrödinger equation (14) with $\epsilon=\lambda_1,\ldots,\lambda_m$ in the form (4).

Example 2: Let us generalize the previous example as follows. We are looking for the Schrödinger equations (1) conditionally invariant with respect to the nth-order operator, which can be represented as a power of the first-order differential operator, i.e.

$$Q=(a(x)\partial_x+b(x))^{n+1}. \tag{16}$$

By an appropriate transformation of the dependent and independent variables,

$$z=F(x), \quad \varphi(z)=\exp\left(-\int G(x)dx\right)\psi(x),$$

we can transform the operator Q as follows:

$$\widetilde{Q}=\partial_z^{n+1}.$$

After rewriting the initial Schrödinger equation in the new variables $z,\varphi(z)$ we get

$$f(z)\varphi_{zz}+g(z)\varphi_z+(h(z)-\epsilon)\varphi=0,$$

where

$$f(z)=(F'(x))^2, \quad g(z)=F''(x)+2F'(x)G(x),$$

$$h(z)=-V(x)+G'(x)+G^2(x).$$

Commutation relations (8) now read as

$$[\partial_z^{n+1}, f(z)\partial_z^2+g(z)\partial_z+h(z)-\epsilon]=r(z)\partial_z^{n+1}. \tag{17}$$

Computing the commutator on the left-hand side (which is a simple exercise in differential calculus) and equating coefficients of the linearly independent operators ∂_z^j we conclude that the equation (17) is consistent if and only if the functions f,g,h are polynomials in z of the following form:

$$h(z)=A_0-n(B_2+(n-1)C_3)z+C_4(n-1)nz^2,$$

$$g(z)=B_0+B_1z+B_2z^2+2C_4(1-n)z^3,$$

$$f(z)=C_0+C_1z+C_2z^2+C_3z^3+C_4z^4,$$

where $A_0,B_0,B_1,\ldots,C_4$ are arbitrary constants.

Returning back to the initial variables $x,u(x)$ we get the necessary and sufficient conditions for the Schrödinger equation (1) to be conditionally invariant with respect to an operator belonging to the class (16),

$$-V+G'+G^2=A_0-n(B_2+(n-1)C_3)F+C_4(n-1)nF^2,$$

$$F''+2F'G=B_0+B_1F+B_2F^2+2C_4(1-n)F^3,$$

$$(F')^2=C_0+C_1F+C_2F^2+C_3F^3+C_4F^4,$$

whence we derive the form of the potential $V(x)$,

$$V(x)=\frac{v_0+v_1\omega+v_2\omega^2+v_3\omega^3+v_4\omega^4}{16(C_0+C_1\omega+C_2\omega^2+C_3\omega^3+C_4\omega^4)}, \tag{18}$$

$$v_0=4B_0^2-16A_0C_0+8B_1C_0-8B_0C_1+3C_1^2-8C_0C_2,$$

$$v_1=8B_0B_1+16B_2C_0(n+1)-16A_0C_1-16B_0C_2+4C_1C_2+16B_2C_0n+8C_0C_3(2n^2-2n-3),$$

$$v_2=4B_1^2+8B_0B_2+8B_2C_1(2n+1)-16A_0C_2-8B_1C_2+4C_2^2-24B_0C_3+2C_1C_3(8n^2-8n-3)$$
$$-16C_0C_4n(n+2),$$

$$v_3=8B_1B_2-16A_0C_3-16B_1C_3-16B_0C_4(n+1)+16B_2C_2n-16B_0C_4n-8C_1C_4(2n^2+2n-1)$$
$$+4C_2C_3(4n^2-4n+1),$$

$$v_4=4B_2^2+8B_2C_3(2n-1)-16A_0C_4-8B_1C_4(2n+1)+C_3^2(16n^2-16n+3)+8C_2C_4(1-2n^2),$$

and of the function $G(x)$,

$$G(x)=\frac{2B_0-C_1+2(B_1-C_2)\omega+(2B_2-3C_3)\omega^2-4C_4n\omega^3}{4\sqrt{C_0+C_1\omega+C_2\omega^2+C_3\omega^3+C_4\omega^4}}.$$

In the above formulas, $\omega(x)$ is an elliptic function determined by the quadrature

$$\int^{\omega(x)}\frac{d\tau}{\sqrt{C_0+C_1\tau+C_2\tau^2+C_3\tau^3+C_4\tau^4}}=x.$$

Furthermore, exact solutions of the Schrödinger equation with the potential (18) read as

$$\psi(x)=\exp\left(\int G(x)dx\right)\sum_{j=0}^{n}a_j\omega(x)^j,$$

where $\mathbf{a}=(a_0,a_1,\ldots,a_n)$ is an eigenvector of some $(n+1)\times(n+1)$ constant matrix whose entries are linear combinations of the parameters $A_0,B_0,B_1,\ldots,C_4$ (we omit the corresponding formulas).

Thus, we arrived at the nine-parameter family of quasiexactly solvable Schrödinger equations obtained by Turbiner and Shifman within the framework of their Lie algebraic approach[15,16] and by Ushveridze by means of a more general analytic approach. A detailed account of properties of the Schrödinger equation with potentials (18) can be found in the monograph.[17] We restrict ourselves to noting that if we choose in the above formulas $B_2=C_3=C_4=0$, then the potential $V(x)$ does not depend on n (the order of the operator Q) and, consequently, the corresponding Schrödinger equation is exactly solvable. Thus, the well-known six-parameter family of exactly solvable Schrödinger equations is obtained. In particular, choosing $C_1=C_2=C_3=C_4=0$, $C_0=1$ yields the harmonic oscillator Schrödinger equation (14).

Now let us pass from particular examples to the general case in order to examine which constraints are imposed on the coefficients of the operator (7) by the requirement of conditional invariance (8). In order to compute the commutator on the left-hand side of (8) we use the following identity:

$$[\partial_x^k,f(x)]=\sum_{j=0}^{k-1}C_k^jf^{(k-j)}(x)\partial_x^j,\quad k\in\mathbf{N},\tag{19}$$

where $C_k^j=k!(j!(k-j)!)^{-1}$ are binomial coefficients, which is established by the mathematical induction method with the help of the evident identity,

$$[\partial_x^{k+1},f(x)]\equiv\partial_x[\partial_x^k,f(x)]+f'(x)\partial_x^k.$$

Taking into account formula (19) we rewrite relation (8) as follows:

$$-\sum_{j=0}^{n-1} C_n^j V^{(n-j)} \partial_x^j - \sum_{i=1}^{n-1} \sum_{j=0}^{i-1} q_i C_i^j V^{(i-j)} \partial_x^j - \sum_{j=0}^{n-1} (2q_j' \partial_x + q_j'') \partial_x^j = r(x) \left(\partial_x^n + \sum_{j=0}^{n-1} q_j \partial_x^j \right).$$

Comparing the coefficients of ∂_x^n on the left- and right-hand sides of the above equation we conclude that $r(x) = -2q_{n-1}'$. Comparing the coefficients of the linearly independent operators $\partial_x, \partial_x^2, \ldots, \partial_x^{n-1}$, we arrive at the following system of nonlinear ordinary differential equations for the functions $q_0(x), q_1(x), \ldots, q_{n-1}(x), V(x)$:

$$2q_{j-1}' + q_j'' + C_n^j V^{(n-j)} + \sum_{i=j+1}^{n-1} q_i C_i^j V^{(i-j)} - 2q_{n-1}' q_j = 0, \tag{20}$$

where $j = 0,1,\ldots,n-1$ and by convention $q_{-1} \overset{\text{def}}{=} 0$, $q_n \overset{\text{def}}{=} 1$.

Thus, we have n equations for $n+1$ functions, which means that the system (20) is underdetermined. As an immediate consequence of this fact we conclude that *any* Schrödinger equation (1) is reducible. Indeed, fixing in an arbitrary way a function $V = V(x)$ yields a second-order system of n ordinary differential equations for n functions $q_0(x), q_1(x), \ldots, q_{n-1}(x)$. Each solution of such a system gives rise to an operator Q satisfying by construction condition (8). Consequently, the conditions of Theorem 1 can be fulfilled with any choice of the potential $V(x)$.

Let us demonstrate how the results obtained can be used to study the spectral properties of the Schrödinger equation. Remarkably, to this end we do not need an explicit form of solution of the system of nonlinear ordinary differential equations (20). It suffices to know initial values of the functions $q_j(x)$ and of their first derivatives $q_j'(x)$ at some point $x = x_0 \in \mathbf{R}$. We denote these as follows:

$$q_j(x_0) = A_{j+1}, \quad q_j'(x_0) = B_{j+1}, \quad j = 0,1,\ldots,n-1. \tag{21}$$

All the information about spectral properties of the Schrödinger operator restricted to an invariant space $\mathscr{V}_n$ with basis elements $u_1(x), u_2(x), \ldots, u_n(x)$ is contained in the matrix $\|\Lambda_{jk}\|$, which determines a transformation law (2) for the functions $u_j(x)$ with respect to the action of the Schrödinger operator S.

Let Q be a differential operator of the order n satisfying condition (8) with some choice of the function $V(x)$. Then, by force of Theorem 1, an invariant space $\mathscr{V}_n$ of the corresponding Schrödinger operator S is spanned by the fundamental system of solutions of the nth-order ordinary differential equation,

$$u^{(n)}(x) + \sum_{j=0}^{n-1} q_j(x) u^{(j)}(x) = 0. \tag{22}$$

We denote this system as $\{u_1(x), u_2(x), \ldots, u_n(x)\}$. As any n linearly independent solutions of Eq. (22) form a fundamental system of solutions, there is a freedom in the choice of the functions $u_j(x)$. We fix these by imposing initial conditions.

Let $\|L_{jk}\|$ be a constant nonsingular $n \times n$ matrix. Consider the following n Cauchy problems:

$$u_k^{(n)}(x)+\sum_{j=0}^{n-1} q_j(x)u_k^{(j)}(x)=0, \quad k=1,\ldots,n,$$
$$u_k^{(j-1)}(x_0)=L_{kj}, \quad k,j=1,\ldots,n. \tag{23}$$

It is well known from the general theory of linear differential equations that the above system has a unique solution, and what is more, this solution yields a fundamental system of solutions of Eq. (22).

Differentiating relations (2) $n-1$ times with respect to x and excluding the nth and the $(n+1)$th derivatives of the functions $u_j(x)$ with the help of Eqs. (23) we arrive at the following relations:

$$\sum_{k=1}^{n} \Lambda_{jk}u_k^{(i)}=u_j^{(i+2)}-\sum_{k=0}^{i} C_i^k V^{(i-k)}u_j^{(k)},$$
$$\sum_{k=1}^{n} \Lambda_{jk}u_k^{(n-2)}=-\sum_{k=0}^{n-1} q_k u_j^{(k)}-\sum_{k=0}^{n-2} C_{n-2}^k V^{(n-k-2)}u_j^{(k)}, \tag{24}$$
$$\sum_{k=1}^{n} \Lambda_{jk}u_k^{(n-1)}=\sum_{k=0}^{n-1} (q_{n-1}q_k-q_k'-q_{k-1}-C_{n-1}^k V^{(n-k-1)})u_j^{(k)},$$

where $j=1,\ldots,n$, $i=0,\ldots,n-3$ and as above $q_{-1}\overset{\text{def}}{=}0$.

Choosing $x=x_0$ in (24) yields

$$\sum_{k=1}^{n} \Lambda_{jk}L_{ki}=\sum_{k=1}^{n} L_{jk}R_{ki}, \quad j,i=1,\ldots,n,$$

where

$$R_{ki}=\delta_{ki+2}-C_{i-1}^{k-1}V^{(i-k)}(x_0), \quad i=1,\ldots,n-2,$$
$$R_{kn-1}=-A_k-C_{n-2}^{k-1}V^{(n-k-1)}(x_0), \tag{25}$$
$$R_{kn}=A_nA_k-B_k-A_{k-1}-C_{n-1}^{k-1}V^{(n-k)}(x_0).$$

In formulas (25), the index k runs from 1 to n, A_k, B_k are constants defined by (21), and δ_{kj} is the Kronecker symbol.

Rewriting the formulas obtained in the matrix form, we have $\Lambda L=LR$, where Λ, L, R are constant $n\times n$ matrices with entries $\Lambda_{jk}, L_{jk}, R_{jk}$, respectively. Hence, we derive the explicit form of the matrix Λ,

$$\Lambda=LRL^{-1}. \tag{26}$$

Thus we have proved the following assertion.

Theorem 3: *Let L be an arbitrary invertible $n\times n$ matrix, and $A_1,\ldots,A_n,B_1,\ldots,B_n$ be arbitrary constants. Then, for any choice of the function $V(x)$ there exist n functions $u_1(x),\ldots,u_n(x)$ such that the relations (2) hold, Λ_{jk} being the entries of the $n\times n$ matrix given by formulas (25), (26).*

The above theorem has as a consequence the following important assertion that describes a finite part of the spectrum of the Schödinger operator S.

Theorem 4: *Let* $\lambda_1,...,\lambda_m$ *be distinct eigenvalues of the matrix* $\|R_{jk}\|$ *determined by formulas (25). Then, for any choice of parameters* A_j, B_j *there exist linearly independent functions* $\psi_1(x),\ldots,\psi_m(x)$ *satisfying the Schrödinger equation (1) with* $\epsilon=\lambda_1$, $\epsilon=\lambda_2,...,$ $\epsilon=\lambda_m$ *correspondingly*.

The proof follows from Theorem 2 if one takes into account that the matrix Λ is similar to R and, consequently, has the same eigenvalues λ_1, $\lambda_2,...,\lambda_m$. The explicit form of the functions $\psi_1(x),\ldots,\psi_m(x)$ is given by the formula (4), where $\mathbf{a}^j=(a_1^j,a_2^j,\ldots,a_n^j)$, $j=1,\ldots,m$ are eigenvectors of the matrix Λ corresponding to the eigenvalues λ_1, $\lambda_2,...,\lambda_m$.

Thus, using the conditional symmetry approach we were able not only to calculate the spectrum of the Schrödinger operator $S=\partial_x^2-V(x)$ but also to construct in an explicit form a $2n$-parameter family of matrix representations of S.

As is seen from formulas (25), (26), there is a large freedom in choice of the matrix Λ. First, it depends on $2n$ arbitrary constants A_j, B_j, which fix a fundamental system of solutions of ordinary differential equation (22). Consequently, choosing specific constants A_j, B_j means fixing a representation space $\mathscr{V}_n$. Second, it contains an arbitrary constant $n\times n$ matrix L. The appearance of the matrix L in the definition of Λ reflects a freedom in choosing a basis of the representation space $\mathscr{V}_n$. Indeed, if $u_1(x),\ldots,u_n(x)$ is a basis of the space $\mathscr{V}_n$, then the functions $\Sigma_{k=1}^n L_{jk}u_k(x)$ also form a basis with an arbitrary invertible constant $n\times n$ matrix $\|L_{jk}\|$. That is why choosing a specific matrix L results in fixing a basis of the representation space $u_1(x,\ldots,u_n(x)$. This freedom can be used, in particular, to obtain an orthogonal basis for $\mathscr{V}_n$ (to this end one should apply the standard Gram–Schmidt orthogonalization procedure).

But representations of the Schrödinger operator in these bases are equivalent, which is readily seen from the formula (26).

Thus, it is established that *any* Schrödinger equation has n-dimensional invariant spaces $\mathscr{V}_n$ with arbitrary $n\in\mathbf{N}$. Furthermore, we have constructed the $2n$-parameter family of matrix representations of the corresponding Schrödinger operator in these spaces [the formulas (25), (26)]. But to obtain an explicit form of the basis of $\mathscr{V}_n$ we still have

•to integrate system of nonlinear ordinary differential equations (20), and

•to construct the general solution of the nth-order ordinary differential equation (22).

We will demonstrate that using a simple trick we may avoid the necessity to integrate Eq. (22). The said trick is based on the fact that we need not all solutions of (22), but only those that simultaneously satisfy the initial Schrödinger equation (1). This means that we have to solve the following overdetermined system of two ordinary differential equations:

$$\psi_{xx}=(\epsilon+V(x))\psi, \quad \psi^{(n)}(x)+\sum_{j=0}^{n-1} q_j(x)\psi^{(j)}(x)=0. \tag{27}$$

Using the first equation and its differential consequences up to the order $n-2$ we can exclude from the second equation all the derivatives of the function ψ of the order $j>1$ and rewrite system (27) in the following equivalent form:

$$\psi_{xx}=(\epsilon+V(x))\psi, \quad \left(\sum_{i=0}^{N} a_i(x)\epsilon^i\partial_x+\sum_{i=0}^{N} b_i(x)\epsilon^i\right)\psi=0, \tag{28}$$

where $N=[n/2], a_i(x), b_i(x)$ are linear combinations of the functions $q_j(x)$ with coefficients depending on $V(x)$ and its derivatives (and, consequently, independent of ϵ), and, furthermore, $a_N=1$ if $n=2N+1$ and $a_N=0, b_N=1$ if $n=2N$.

The compatibility condition for the above system reads as

$$\left(\frac{\Sigma_{i=0}^N b_i(x)\epsilon^i}{\Sigma_{i=0}^N a_i(x)\epsilon^i}\right)_x-\left(\frac{\Sigma_{i=0}^N b_i(x)\epsilon^i}{\Sigma_{i=0}^N a_i(x)\epsilon^i}\right)^2+V(x)+\epsilon=0. \tag{29}$$

As functions a_i, b_i are independent of ϵ, coefficients of the powers of ϵ should be independent of x. This requirement yields the following.

(1) $2N+1$ ordinary differential equations,

$$\sum_{i+j=k}(b_i'a_j-b_ia_j'-b_ib_j+Va_ia_j)+\sum_{i+j=k-1}a_ia_j=C_k, \tag{30}$$

where $k=0,1,\ldots,2N$, for $2N+2$ functions $a_0,\ldots,a_{N-1},b_0,\ldots,b_N,V$, provided $n=2N+1$; or

(2) $2N$ ordinary differential equations of the form (30), with k taking the values $0,1,\ldots,2N-1$ for $2N+1$ functions $a_0,\ldots,a_{N-1},b_0,\ldots,b_{N-1},V$, provided $n=2N$.

In (30), C_j are arbitrary constants.

Provided conditions (30) are fulfilled, the compatibility condition (29) reduces to an algebraic equation,

(1) under $n=2N+1$,

$$\epsilon^{2N+1}+\sum_{j=0}^{2N}C_j\epsilon^j=0; \tag{31}$$

(2) under $n=2N$,

$$\epsilon^{2N}+\sum_{j=0}^{2N-1}C_j\epsilon^j=0; \tag{32}$$

and the general solution of system (28) is given by the quadrature

$$\psi(x)=\exp\left\{-\int\left(\frac{\sum_{i=0}^{N}b_i(x)\epsilon^i}{\sum_{i=0}^{N}a_i(x)\epsilon^i}\right)dx\right\}. \tag{33}$$

It should be noted that Eqs. (31), (32) are nothing else but characteristic equations for the matrix R defined by (25). Their solutions $\lambda_1,\ldots,\lambda_m$ are eigenvalues and $\psi_1(x)=\psi(x)|_{\epsilon=\lambda_1},\ldots,\psi_m(x)=\psi(x)|_{\epsilon=\lambda_m}$ are eigenfunctions of the corresponding Schrödinger operator $S=\partial_x^2-V(x)$.

III. SYMMETRY AND EXACT SOLVABILITY

To the best of our knowledge, the first paper, where a systematic study of high-order Lie symmetries of the Schrödinger equations with nonvanishing potentials has been undertaken, is the one by Nikitin, Onufriychuk, and Fushchych.[31] In particular, for several one-dimensional exactly solvable models third-order symmetry operators were constructed. Furthermore, it was conjectured that exact integrability of the Schrödinger equation (1) is intimately connected with its symmetry properties. This conjecture has been confirmed in Ref. 24, where a number of exactly solvable potentials were obtained by means of third-order symmetries of (1) and, furthermore, a method for integrating the corresponding Schrödinger equations was suggested. Using a technique developed in the previous section we will demonstrate how to derive exact integrability of Eq. (1) from its symmetry properties in the class of arbitrary order symmetry operators.

The nth-order operator Q of the form (5) is a symmetry operator of Eq. (1) if the condition (2) is satisfied with $r(x)=0$. As coefficients of Q are independent of ϵ, equality (2) is only possible when $P\equiv 0$. Computing the commutator on the left-hand side of (2) with $r=0$, $P=0$, and equating to zero the coefficients of ∂_x^{n+1} and ∂_x^n, we conclude that $q_n(x)=\text{const}$, $q_{n-1}(x)=\text{const}$. Consequently, any nth-order symmetry operator admitted by the Schrödinger equation (1) can be represented in the form (5) with $q_n=C=\text{const}\neq 0$, $q_{n-1}=C_0=\text{const}$.

First, following Ref. 24 we will consider in more detail the third-order symmetry operators admitted by the Schrödinger equation (1). These are the lowest-order symmetry operators not equivalent to usual first-order Lie symmetries. The general form of a third-order symmetry operator is as follows (we choose $C=1$):

$$Q=\partial_x^3+C_0\partial_x^2+q_1(x)\partial_x+q_0(x), \tag{34}$$

where $q_0(x),q_1(x)$ are sufficiently smooth functions to be determined from the invariance condition (2) with $n=3$, $r=P=0$. A short computation yields the following expressions for the coefficients of the operator Q:

$$q_0(x)=C_2-C_0V(x)-\tfrac{3}{4}V'(x), \quad q_1(x)=C_1-\tfrac{3}{2}V(x),$$

where $V(x)$ is an arbitrary solution of the third-order nonlinear ordinary differential equation,

$$-4C_1V'+6VV'-V^{(3)}=0. \tag{35}$$

Integrating twice the above equation we arrive at the first-order ordinary differential equation integrable in elliptic functions,

$$C_4+2C_3V(x)+4C_1V(x)^2-2V(x)^3+V'(x)^2=0. \tag{36}$$

It was established in Ref. 24 that particular cases of almost all exactly solvable potentials that can be expressed in elementary functions, such as the trigonometric and hyperbolic Pöschel–Teller, Eckart, Kratzer potentials, potential well of finite and infinite depth, are obtained as solutions of the equation (36).

This fact implies an existence of an intimate connection between high-order Lie symmetries and exact solvability of the Schrödinger equations. In what follows we will show that this is not simply a conjecture but a fundamental fact, making it possible to classify exactly solvable models and to construct their exact solutions in an explicit form (see, also Refs. 24 and 25).

It is straightforward to check that if Q is a Lie symmetry of the Schrödinger equation (1), then $\widetilde{Q}=Q+P(\partial_x^2-V(x)-\epsilon)$, where P is an arbitrary differential operator, is also its Lie symmetry. Furthermore, systems of ordinary differential equations,

$$(\partial_x^2-V(x)-\epsilon)\psi(x)=0, \quad Q\psi(x)=0,$$

and

$$(\partial_x^2-V(x)-\epsilon)\psi(x)=0, \quad \widetilde{Q}\psi(x)=0,$$

are equivalent in a sense that they have the same solutions. Making use of these facts we can reduce the nth-order symmetry operator Q to a first-order symmetry operator, the coefficients of which are Nth-order polynomials in ϵ (we will preserve the same designation Q for the reduced operator),

$$Q=a(x,\epsilon)\partial_x+b(x,\epsilon)\equiv\left(\sum_{j=0}^{N}a_j(x)\epsilon^j\right)\partial_x+\sum_{j=0}^{N}b_j(x)\epsilon^j. \tag{37}$$

From the invariance condition for the reduced operator,

$$[\partial_x^2-V(x)-\epsilon,a(x,\epsilon)\partial_x+b(x,\epsilon)]=R(x,\epsilon)(\partial_x^2-V(x)-\epsilon),$$

we get a system of determining equations for the coefficients of Q,

$$a''(x,\epsilon)+2b'(x,\epsilon)=0,$$

$$b''(x,\epsilon)+a(x,\epsilon)V'(x)+2a'(x,\epsilon)(V(x)+\epsilon)=0,$$

where primes denote differentiation with respect to x.

Splitting the above equations by powers of ϵ with subsequent integrating yields

$$b_j(x)=-\frac{1}{2}a_j'(x)+B_j, \quad a_N(x)=A_N,$$
$$a_{j-1}(x)=\frac{1}{4}a_j''(x)-V(x)a_j(x)+\frac{1}{2}\int V'(x)a_j(x)dx+A_{j-1}. \tag{38}$$

In (38), A_{-1},A_j,B_j are arbitrary constants, $j=0,1,\ldots,N$, $a_{-1}(x)\overset{\text{def}}{=}0$.

Thus, the problem of describing nth-order symmetry operators of the Schrödinger equation is reduced to solving the recurrent relations,

$$a_{j-1}(x)=\frac{1}{4}a_j''(x)-V(x)a_j(x)+\frac{1}{2}\int V'(x)a_j(x)dx+A_{j-1}, \tag{39}$$

with $a_N(x)=A_N=\text{const}$, $a_{-1}(x)\overset{\text{def}}{=}0$, $j=N,N-1,\ldots,0$.

The first N relations ($j=N,N-1,\ldots,1$) are solved by subsequent integrations yielding the expressions for the functions $a_0(x),\ldots,a_{N-1}(x)$ via the function $V(x)$ and its derivatives. Substituting these results into the last equation ($j=0$) we arrive at the $2N$th-order nonlinear ordinary differential equation for the function $V(x)$. It will be shown that any solution of this equation gives rise to an exactly solvable Schrödinger equation (1).

To reveal the structure of the equation in question we introduce the new functions $U_0(x),U_1(x),\ldots$, by the following recurrence relation:

$$U_j(x)=XU_{j-1}(x)\equiv(\tfrac{1}{4}\partial_x^2-V(x)+\tfrac{1}{2}\partial_x^{-1}V'(x))U_{j-1}, \quad j=0,1,\ldots, \tag{40}$$

where ∂_x^{-1} denotes integration with respect to x and $U_{-1}(x)\overset{\text{def}}{=}1$.

Formally, a definition of functions $U_j(x)$ contains a quadrature but integrating relations (40) successively we can get rid of it for any $j=1,2,3,\ldots$. Below, we adduce expressions of the functions $U_j(x)$ for $j=0,1,2,3$,

$$U_0(x)=-\frac{1}{2}V(x), \quad U_1(x)=\frac{1}{2^3}(3V(x)^2-V''(x)),$$

$$U_2(x)=\frac{1}{2^5}(-10V(x)^3+5V'(x)^2+10V(x)V''(x)-V^{(4)}(x)),$$

$$U_3(x)=\frac{1}{2^7}(35V(x)^4-70V(x)V'(x)^2-70V(x)^2V''(x)+21V''(x)^2+28V'(x)V^{(3)}(x)$$
$$+14V(x)V^{(4)}(x)-V^{(6)}(x)).$$

Now we can solve the first N relations of (39) in terms of the functions $U_j(x)$,

$$a_{N-j}(x)=\sum_{k=0}^{j-1}A_{N-k}U_{j-k-1}(x)+A_{N-j}, \quad j=1,\ldots,N. \tag{41}$$

Inserting the above expressions into the last equation of (39), we get

$$A_{-1}+\sum_{k=0}^{N} A_{N-k}U_{N-k}(x)=0 \tag{42}$$

[when deriving the above equation we take into account that by convention $a_{-1}(x)=0$].

Equation (42) is the necessary and sufficient condition for the Schrödinger equation (1) to be invariant with respect to the first-order operator (37), whose coefficients are polynomials in ϵ of the order N. But it is easy to see that given a condition (42), Eq. (1) admits an operator of the form (37), whose coefficients are polynomials in ϵ of an arbitrary order $N'>N$.

Indeed, the invariance conditions for the operator,

$$Q=\left(\sum_{j=0}^{N'} a_j(x)\epsilon^j\right)\partial_x+\sum_{j=0}^{N'} b_j(x)\epsilon^j,$$

have the form (38) with $N=N'$. Coefficients $a_j(x)$ with $j=N',N'-1,\ldots,N'-N$ are given by formulas (41), where one should replace N by N', and the remaining coefficients by force of relation (42) read as

$$a_j(x)=\sum_{k=0}^{N-1}\tilde{A}_{jk}U_k(x)+A_j, \quad j=0,1,\ldots,N'-N-1,$$

where $A_0,\ldots,A_{N'-N-1}$ are arbitrary constants, $\tilde{A}_{jk}$ are constants expressed via $A_{N'-N},\ldots,A_{N'}$.

Substituting these results into the last ($j=0$) equation from (41) yields

$$A_{-1}+A_0U_0(x)+\sum_{k=0}^{N-1}\tilde{A}_{0k}U_{k+1}(x)=0,$$

whence we conclude that, provided $A_{-1}=A_0=0$, $\tilde{A}_{0k}=0$, $k=0,1,\ldots,N-1$, the invariance conditions are satisfied.

Thus, if Eq. (42) is fulfilled with some $N\in\mathbf{N}$, then the corresponding Schrödinger equation admits arbitrary-order Lie symmetries and, consequently, is exactly solvable.

A general solution of the Schrödinger equation invariant under the operator Q is given by (33). Substituting formula (33) into Eq. (1), where $V(x)$ is an arbitrary solution of (42), results in a $(2N+1)$th-order algebraic equation for ϵ. Its solutions $\epsilon=\lambda_1,\ldots,\epsilon=\lambda_m$ are eigenvalues of the Schrödinger operator. Corresponding eigenfunctions are obtained if we insert $\epsilon=\lambda_1,\ldots,\epsilon=\lambda_m$ into (33).

Summing up, we conclude that any solution $V(x)$ of (42) gives rise to an exactly solvable Schrödinger equation. In what follows it will be established that the more strong assertion holds. Namely, if $V(x)$ is a solution of (42) with some N, then the corresponding Schrödinger equation may have an *arbitrary* spectrum.

Theorem 5: *Let $V=V(x)$ be a solution of ordinary differential equation (42) with some fixed $N\in\mathbf{N}$. Then, the Schrödinger equation (1) is exactly solvable and, moreover, the Schrödinger operator $S=\partial_x^2-V(x)$ may have an arbitrarily prescribed spectrum.*

Proof: We will give the principal steps of the proof, omitting technical details. As the potential $V(x)$ satisfies Eq. (42), the corresponding Schrödinger equation admits a Lie symmetry of the form (37). Excluding from (37) the parameter ϵ we recover symmetry operator Q of the order $n=2N+1$ that commutes with the Schrödinger operator S. Next, we construct an operator $Q_1=Q+f(\epsilon)$, where $f(\epsilon)$ is an arbitrary smooth function. Evidently, Q_1 commutes with S and,

consequently, is a symmetry operator of the Schrödinger equation. This means that conditions of Theorem 1 are fulfilled and a fundamental system of solutions of the ordinary differential equation,

$$Q_1 u(x)=0$$

forms a basis of the invariant space $\mathscr{V}_n$ of the corresponding Schrödinger operator S. Representation of S in the space V_n is given by the formulas (25), (26), where $A_1=a+f(\epsilon)$ and parameters $a,A_2,\ldots,A_n,B_1,\ldots,B_N$ are independent of $f(\epsilon)$. Eigenvalues of the operator S are solutions of the characteristic equation for the matrix R having the entries (25), i.e. of the equation

$$\det\|R_{jk}-\epsilon\delta_{jk}\|=0.$$

It is not difficult to become convinced of that the above equation can be represented in the form

$$p_0(\epsilon)+p_1(\epsilon)f(\epsilon)+p_2(\epsilon)f(\epsilon)^2=0,$$

where p_0,p_1,p_2 are polynomials in ϵ of the order not higher than n.

Consequently, zeros of the function

$$F(\epsilon)=p_0(\epsilon)+p_1(\epsilon)f(\epsilon)+p_2(\epsilon)f(\epsilon)^2$$

are eigenvalues of the Schrödinger operator.

As $f(\epsilon)$ is arbitrary, the function $F(\epsilon)$ may have an arbitrarily prescribed set of zeros and, thus, a spectrum of the initial Schrödinger equation (1) may be arbitrary.

As an illustration, we will consider the simplest case when there exists such N_1 that $U_{N_1}(x)=0$. In such a case, the coefficients of the symmetry operator (37) with $N=kN_1$, $k\in\mathbf{N}$ are easily shown to be

$$a(x,\epsilon)=\left(\sum_{j=-1}^{N_1-1}U_j(x)\epsilon^{N_1-j-1}\right)\left(\sum_{j=0}^{k}A_j\epsilon^j\right),$$

$$b(x,\epsilon)=-\frac{1}{2}\left(\sum_{j=-1}^{N_1-1}U_j'(x)\epsilon^{N_1-j-1}\right)\left(\sum_{j=0}^{k}A_j\epsilon^j\right)+\left(\sum_{j=0}^{N}B_j\epsilon^j\right),$$

where $A_0,\ldots,A_k,B_0,\ldots,B_N$ are arbitrary constants.

Inserting this result into (41) and integrating we come to the following Ansatz for the function $\psi(x)$:

$$\psi(x)=\left(\sum_{j=-1}^{N_1-1}U_j(x)\epsilon^{N_1-j-1}\right)^{1/2}\exp\left\{-f(\epsilon)\int\frac{dx}{\sum_{j=-1}^{N_1-1}U_j(x)\epsilon^{N_1-j-1}}\right\},\tag{43}$$

where $f(\epsilon)=(\Sigma_{j=0}^{N}B_j\epsilon^j)(\Sigma_{j=0}^{k}A_j\epsilon^j)^{-1}$.

Substitution of the expression (43) into the initial equation after some manipulations gives the following algebraic equation:

$$\epsilon^{2N_1+1}+\sum_{j=0}^{N_1-1}\mathscr{I}_j\epsilon^j-f(\epsilon)^2=0,\tag{44}$$

where $\mathscr{I}_j$ are integrals of the ordinary differential equation $U_{N_1}(x)=0$ and, consequently, are constant on the set of its solutions.

Thus, for an arbitrary $N_1 \in \mathbf{N}$ any solution $V=V(x)$ of the ordinary differential equation $U_{N_1}(x) = 0$ gives rise to an exactly solvable Schrödinger equation. Eigenvalues of the Schrödinger operator S are the roots of the algebraic equation (44) and the eigenfunctions are of the form (43), where ϵ is an arbitrary solution of (44).

It is instructive to consider in more detail the above formulas for the case $N=N_1=1$. With this choice of N the formula (43) reads as

$$\psi(x)=(2\epsilon-V(x))^{1/2}\exp\left\{-2\,f(\epsilon)\left(\int\frac{dx}{2\epsilon-V(x)}\right)\right\}, \tag{45}$$

where $f(\epsilon)=(A_1\epsilon+A_0)(B_1\epsilon+B_0)^{-1}$ and the function $V(x)$ is a solution of the ordinary differential equation $U_1(x)=0$, i.e.

$$-3V(x)^2+V''(x)=0. \tag{46}$$

Inserting the Ansatz (45) into (1) yields the following equality:

$$-8\epsilon^3+\mathscr{I}_0+8f(\epsilon)^2=0, \tag{47}$$

where

$$\mathscr{I}_0=V(x)^3-\tfrac{1}{2}V'(x)^2$$

is the first integral of Eq. (46). Note that an alternative derivation of the formulas (45)–(47) has been obtained in Ref. 25.

Now let us make an important remark. It is readily seen from formulas (45)–(47) that the function $f(\epsilon)$ is not obliged to be a ratio of two first-order polynomials. It may be arbitrary. And what is more, eigenvalues of the Schrödinger operator are the zeros of the function $F(\epsilon)=-8\epsilon^3+\mathscr{I}_0+8f(\epsilon)^2$. Choosing an arbitrary function $f(\epsilon)$ in a proper way we can get the function $F(\epsilon)$ having arbitrary prescribed set of zeros. This means that the Schrödinger equation (1) with $V(x)$ satisfying (47) may have an arbitrary spectrum.

For example, if we choose $f=\sqrt{\epsilon^3-\mathscr{I}_0/8}$, then the function (45) is a solution of the Schrödinger equation under arbitrary ϵ (the case of a continuous spectrum). Next, if we choose $f=\sqrt{\epsilon^3-\mathscr{I}_0/8+\Sigma_{j=0}^{N}A_j\epsilon^j}$, then a finite discrete spectrum is obtained (eigenvalues are roots of the Nth-order polynomial). At last, choosing $f=\sqrt{\epsilon^3-\mathscr{I}_0/8+\sin\epsilon}$ yields an infinite discrete spectrum (eigenvalues are zeros of the $\sin\epsilon$).

Similar results are obtained for $N=N_1=2$,

$$\psi(x)=(8\epsilon^2-4\epsilon V(x)+3V(x)^2-V''(x))^{1/2}\exp\left\{-8f(\epsilon)\left(\int\frac{dx}{8\epsilon^2-4\epsilon V(x)+3V(x)^2-V''(x)}\right)\right\},$$

where $f(\epsilon)$ is an arbitrary function, $V(x)$ is a solution of the ordinary differential equation,

$$10V(x)^3-5V'(x)^2-10V(x)V''(x)+V^{(4)}(x)=0, \tag{48}$$

and ϵ is a solution of the equation,

$$-128\epsilon^5-2\epsilon\mathscr{I}_1+\mathscr{I}_0+128f(\epsilon)^2=0.$$

Here $\mathscr{I}_0$, $\mathscr{I}_1$ are integrals of Eq. (48) of the form

$$\mathscr{I}_0=5V(x)^4-10V(x)V'(x)^2-V''(x)^2+2V'(x)V^{(3)}(x),$$

$$\mathscr{I}_1=-\frac{\mathscr{I}_0V(x)}{2}+\frac{19V(x)^5}{2}-\frac{\mathscr{I}_0^2}{8V'(x)^2}-\frac{5\mathscr{I}_0V(x)^4}{4V'(x)^2}-\frac{25V(x)^8}{8V'(x)^2}+\frac{5V(x)^2V'(x)^2}{2}-10V(x)^3V''(x)$$
$$-V'(x)^2V''(x)+\frac{5V(x)V''(x)^2}{2}+\frac{\mathscr{I}_0V''(x)^2}{4V'(x)^2}+\frac{5V(x)^4V''(x)^2}{4V'(x)^2}-\frac{V''(x)^4}{8V'(x)^2}.$$

Generically, if $V(x)$ is a solution of the $2N$th-order ordinary differential equation $U_N(x)=0$, then the corresponding Schrödinger operator S may have an arbitrary spectrum. Eigenvalues of S are obtained by solving the algebraic equation (44) and its eigenfunctions by substituting the corresponding values for ϵ into (43).

We will finish this section with one more puzzling property of the exactly integrable models obtained. Let us denote the total derivatives of the functions $U_j(x)$ with respect to x as $W_j(x)$ and consider an infinite set of evolution equations for a function $u=u(t,x)$,

$$\frac{\partial u(t,x)}{\partial t}=F_j[u(t,x)],\quad j>1, \tag{49}$$

where the functions F_j are obtained from $W_j(x)$ by formal replacement of $V(x)$ with $u(t,x)$. Now we see that equations obtained in this way form the famous integrable KdV hierarchy. Taking, for example, $j=2$ yields the KdV equation,

$$\frac{\partial u(t,x)}{\partial t}=\frac{1}{2^3}\left(6u(t,x)\,\frac{\partial u(t,x)}{\partial x}-\frac{\partial^3u(t,x)}{\partial x^3}\right).$$

Furthermore, differentiating the relations (40) we obtain the recurrence relations determining $W_j(x)$,

$$W_{j+1}(x)=YW_j(x)\equiv(\tfrac{1}{4}\,\partial_x^2-V(x)-\tfrac{1}{2}\,V'(x)\partial_x^{-1})W_j(x),\quad j=0,1,\ldots,$$

with $W_0(x)=0$. The operator Y above is nothing else but the well-known recurrence operator for the KdV hierarchy.[32]

Next, if we formally replace $V(x)$ by $u(t,x)$ in $U_j(x)$ determined by the recurrence relations (40), then the densities of motion constants of the KdV equation are obtained, X being the recursion operator connecting these densities.

Equations of the form (42) are known in the literature as the stationary Lax–Novikov equations. Equations of the stationary KdV hierarchy are particular cases of Eqs. (42) with $A_1=\cdots=A_{N-1}=0$. We have proved that any solution $V=V(x)$ of the stationary Lax–Novikov hierarchy (42) yields an exactly solvable Schrödinger equation. The correspondence between solutions of stationary KdV hierarchy and exactly solvable Schrödinger equations with reflectionless potentials is known (see, e.g., the paper[33] and references therein). Moreover, it has been established that the Schrödinger operators with so chosen potentials may have an arbitrarily prescribed spectrum. But the fact that solutions of the stationary Lax–Novikov hierarchy (42) have the same property seems to be new.

IV. CONCLUSION

In view of numerous excellent papers and monographs (see, e.g., Ref. 17 and the literature cited therein) devoted to developing algebraic methods for the investigation of spectral properties of Eq. (1), it is, of course, not enough to say that the problem of describing part of the spectrum of the Schrödinger equation is equivalent to computing its conditional symmetries in order to

justify a necessity of introducing a new complicated structure. Our principal motivation for looking for a symmetry interpretation of the results obtained in this field is that it may open a possibility

- to study the spectrum of two- and three-dimensional Schrödinger equations;
- to investigate ''spectral properties'' of nonlinear Schrödinger equations; and
- to study spectral properties of matrix differential operators (say, of the Dirac operator), by purely algebraic means.

For instance, there are strong evidences that a necessary condition for a three-dimensional Schrödinger equation to be exactly solvable is an invariance with respect to a three-dimensional Lie algebra of high-order symmetry operators. We can guess that one of the necessary conditions of ''quasiexact solvability'' of the three-dimensional Schrödinger equations is a nontrivial conditional symmetry admitted. The simplest possibility to move in this direction is to combine the technique developed in the present paper with the method of separation of variables.[34] In our paper[35] we have classified potentials $V(x_1,x_2)$ such that the corresponding two-dimensional Schrödinger equation,

$$i\psi_t+\psi_{x_1x_1}+\psi_{x_2x_2}=V(x_1,x_2)\psi$$

can be separated into three ordinary differential equations. One of these is a first-order equation and can always be integrated by quadratures. Two other are exactly of the form (1) and can be solved within the framework of the approach described in Secs. II and III.

Furthermore, the method of conditional symmetries is applicable not only to linear partial differential equations but also to nonlinear ones.[21,22] Let, for example, the one-dimensional nonlinear Schrödinger equation,

$$\psi_{xx}=(\epsilon+V(x)+F(\psi,\psi^*,\psi_x,\psi_x^*))\psi \tag{50}$$

be conditionally invariant with respect to an nth-order Lie–Bäcklund operator,

$$Q=\eta(x,\psi,\psi',\ldots,\psi^{(n)})\partial_\psi+\cdots,$$

in the sense of Ref. 22. Then, using a technique similar to that developed in Sec. II we can construct an Ansatz for a function $\psi(x)$, which gives a solution of (50), provided the energy parameter ϵ satisfy some algebraic equation $G(\epsilon)=0$. Solutions of this equation can be interpreted as eigenvalues of the nonlinear Schrödinger operator ∂_x^2-V-F.

An interesting example is a family of nonlinear Schrödinger equations suggested by Doebner and Goldin.[36] Taking the polar decomposition,

$$\psi(t,x)=e^{r(t,x)+is(t,x)}, \tag{51}$$

and fixing the gauge $\nu_1=-1$, $\nu_2=0$ (this is always possible[37]), we can represent the Doebner–Goldin model in the following way:

$$\begin{gathered} r_t+s_{xx}+2r_xs_x=0,\\ s_t+2\mu_2r_{xx}+\mu_1s_{xx}+4(\mu_2+\mu_5)r_x^2+2(\mu_1+\mu_4)r_xs_x+\mu_3s_x^2+\mu_0V(x)=0, \end{gathered} \tag{52}$$

where $\mu_0,\ldots,\mu_5$ are model parameters.

If we impose on the solutions of (52) an additional condition $s_x=0$ (which picks out a subset of stationary solutions), then the system obtained is consistent if and only if the conditions,

$$r=r(x), \quad s=-\epsilon t, \quad \epsilon=\text{const}\in\mathbf{R}, \tag{53}$$

are fulfilled.

With this choice of functions r and s, system (52) reduces to a single equation,

$$-\epsilon+2\mu_2 r''+4(\mu_2+\mu_5)(r')^2+\mu_0 V(x)=0, \tag{54}$$

which is either linear ($\mu_2+\mu_5=0$) or can be linearized by the substitution

$$\varphi(x)=\exp\left\{\frac{\mu_2}{2(\mu_2+\mu_5)}\, r(x)\right\}, \tag{55}$$

to become

$$\varphi''=\left(\frac{\epsilon}{4(\mu_2+\mu_5)}-\frac{\mu_0}{4(\mu_2+\mu_5)}\, V(x)\right)\varphi. \tag{56}$$

As established in Sec. II, any equation of the form (56) possesses a nontrivial high-order conditional symmetry. Since the nonlinear equation (54) is equivalent to (56), it possesses high-order conditional symmetry as well. Thus, the initial Doebner–Goldin equation has a subset of solutions with nontrivial conditional symmetry, which can be effectively applied to construct finite or even infinite (if the conditional symmetry can be reduced to a high-order Lie symmetry) set of its exact solutions.

We hope that the reasonings above are convincing enough to motivate a further study of high-order conditional symmetries of linear and nonlinear Schrödinger equations in one, two, and three dimensions. It may be also very interesting to study classical and conditional symmetries of the stationary Dirac equation in the presence of nonvanishing electromagnetic field and to apply these to derive a spectrum of the Dirac operator. These problems are under investigation now and will be a topic of our future publications.

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Integral equation methods for the inverse problem with discontinuous wave speed

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The recovery of the coefficient $H(x)$ in the one-dimensional generalized Schrödinger equation $d^2\psi/dx^2+k^2H(x)^2\psi=Q(x)\psi$, where $H(x)$ is a positive, piecewise continuous function with positive limits $H_\pm$ as $x\to\pm\infty$, is studied. The large-k asymptotics of the wave functions and the scattering coefficients are analyzed. A factorization formula is given expressing the total scattering matrix as a product of simpler scattering matrices. Using this factorization an algorithm is presented to obtain the discontinuities in $H(x)$ and $H'(x)/H(x)$ in terms of the large-k asymptotics of the reflection coefficient. When there are no bound states, it is shown that $H(x)$ is recovered from an appropriate set of scattering data by using the solution of a singular integral equation, and the unique solvability of this integral equation is established. An equivalent Marchenko integral equation is derived and is shown to be uniquely solvable; the unique recovery of $H(x)$ from the solution of this Marchenko equation is presented. Some explicit examples are given, illustrating the recovery of $H(x)$ from the solution of the singular integral equation and from that of the Marchenko equation. © *1996 American Institute of Physics.* [S0022-2488(96)02606-0]

I. INTRODUCTION

Consider the one-dimensional generalized Schrödinger equation,

$$\psi''(k,x)+k^2H(x)^2\psi(k,x)=Q(x)\psi(k,x), \quad x\in\mathbf{R}, \tag{1.1}$$

which describes the propagation of waves in a one-dimensional nonhomogeneous, nonabsorptive medium, where k^2 is energy, $1/H(x)$ is the wave speed, and $Q(x)$ is the restoring force density. The discontinuities of $H(x)$ correspond to abrupt changes in the properties of the medium in which the wave propagates. The prime denotes the derivative with respect to the spatial coordinate, and the coefficients $H(x)$ and $Q(x)$ are assumed to satisfy the following conditions:

(H1) $H(x)$ is strictly positive and piecewise continuous with jump discontinuities at x_n for $n=1,\ldots,N$, such that $x_1<\cdots<x_N$.
(H2) $H(x)\to H_\pm$ as $x\to\pm\infty$, where $H_\pm$ are positive constants.
(H3) $H-H_\pm\in L^1(\mathbf{R}^\pm)$, where $\mathbf{R}^-=(-\infty,0)$ and $\mathbf{R}^+=(0,+\infty)$.
(H4) H' is absolutely continuous on (x_n,x_{n+1}) and $2H''H-3(H')^2\in L^1_1(x_n,x_{n+1})$, for $n=0,\ldots,N$, where $x_0=-\infty$ and $x_{N+1}=+\infty$, and $L^1_\beta(I)$ denotes the space of measurable functions $f(x)$ on I, such that $\int_I dx\ (1+|x|)^\beta|f(x)|<+\infty$.
(H5) $Q(x)$ is real valued and belongs to $L^1_1(\mathbf{R})$.

The scattering solutions of (1.1) are those behaving like $e^{ikH_\pm x}$ or $e^{-ikH_\pm x}$ as $x\to\pm\infty$, and

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such solutions occur when $k^2>0$. Among the scattering solutions are the Jost solution from the left $f_l(k,x)$ and the Jost solution from the right $f_r(k,x)$ satisfying the boundary conditions

$$f_l(k,x)=\begin{cases} e^{ikH_+x}+o(1), & x\to+\infty, \\ \dfrac{1}{T_l(k)}\,e^{ikH_-x}+\dfrac{L(k)}{T_l(k)}\,e^{-ikH_-x}+o(1), & x\to-\infty, \end{cases}$$

$$f_r(k,x)=\begin{cases} \dfrac{1}{T_r(k)}\,e^{-ikH_+x}+\dfrac{R(k)}{T_r(k)}\,e^{ikH_+x}+o(1), & x\to+\infty, \\ e^{-ikH_-x}+o(1), & x\to-\infty, \end{cases}$$

where $T_l(k)$ and $T_r(k)$ are the transmission coefficients from the left and from the right, respectively, and $L(k)$ and $R(k)$ are the reflection coefficients from the left and from the right, respectively. For each fixed $x\in\mathbf{R}$, the Jost solutions have continuous extensions to the upper half complex plane $\mathbf{C}^+$, and they are analytic there.[1] The reduced transmission coefficient $\tau(k)$, the reduced reflection coefficients $\rho(k)$ from the right and $\check{\rho}(k)$ from the left, respectively, are defined as

$$\tau(k)=\sqrt{\frac{H_+}{H_-}}\,T_l(k)e^{ikA}=\sqrt{\frac{H_-}{H_+}}\,T_r(k)e^{ikA}, \tag{1.2}$$

$$\rho(k)=R(k)e^{2ikA_+}, \quad \check{\rho}(k)=L(k)e^{2ikA_-}, \tag{1.3}$$

where

$$A_\pm=\pm\int_0^{\pm\infty} ds[H_\pm-H(s)], \quad A=A_++A_-. \tag{1.4}$$

If $\tau(0)\neq0$, which is called the exceptional case, the Jost solutions $f_l(0,x)$ and $f_r(0,x)$ are linearly dependent. If $\tau(0)=0$, which is called the generic case, $f_l(0,x)$ and $f_r(0,x)$ are linearly independent, and in this case $\tau(k)$ vanishes linearly as $k\to0$. Usually these two cases need to be analyzed separately, and the small-k analysis of the scattering problem in the exceptional case requires tedious estimates. However, the fact[2] that an exceptional case can always be decomposed into two generic cases is expected to simplify the analysis of the scattering problem in the exceptional case.

In general, (1.1) may have bound states, i.e. nontrivial solutions belonging to $L^2(\mathbf{R},H(x)^2dx)$. Since the treatment of bound states requires many separate arguments, we do not consider them in this paper. Bound states were already studied in Ref. 1 and further results may appear in the future. Thus, we assume that (1.1) does not have any bound states. The number of bound states for (1.1) is equal[3] to the number of bound states for the Schrödinger equation,

$$\Phi''(k,x)+k^2\Phi(k,x)=Q(x)\Phi(k,x), \quad x\in\mathbf{R}, \tag{1.5}$$

and hence our assumption can be restated by saying that $Q(x)$ does not have any bound states.

The inverse scattering problem in which we are interested consists of the recovery of $H(x)$ in (1.1) from an appropriate set of scattering data. The analysis of the scattering problem in a discontinuous medium is the first step to analyze the inverse scattering problem, and we mention the relevant work[4–7] of Sabatier and his collaborators on the scattering in a discontinuous medium in one and three dimensions governed by $\{\alpha(x)^{-2}\nabla\cdot[\alpha(x)^2\nabla]+k^2-V(x)\}\phi(k,x)=0$. In Ref. 4 Sabatier estimated the large-k asymptotics of the scattering data and also briefly discussed the inverse scattering problem in such a medium. Various authors have studied inverse scattering problems for differential equations with discontinuous coefficients, as exemplified by Krueger's

work[8–10] and the bibliography of Ref. 1. Of more direct concern to us is the work by Sabatier[4] and Grinberg.[11,12] Grinberg, in the special (but still important) case $Q(x)=0$, developed a method to recover $H(x)$ using the solution of a singular integral equation; in this special case there are no bound states, the exceptional case occurs, and the norm of the associated singular integral operator is strictly less than unity so that the integral equation has a unique solution that can be obtained through iteration. The general case with nontrivial $Q(x)$ and with bound states was analyzed by a similar method in Ref. 1, and $H(x)$ was recovered from the solution of a singular integral equation under the assumption $Q\in L^1_{1+\alpha}(\mathbf{R})$ for some $\alpha\in(0,1]$. In Ref. 13 the scattering data leading to a unique solution of the inverse problem were specified.

In this paper, when there are no bound states, we develop a method to obtain $H(x)$ from the scattering data consisting of $Q(x)$, $\rho(k)$, and H_+. As already known,[13] H_+ must be omitted from the scattering data in the generic case, but in the exceptional case it needs to be specified in the scattering data in order to obtain $H(x)$ uniquely; this is also true in the method presented here. Note also that, in the scattering data, one can use $\measuredangle(k)$ instead of $\rho(k)$ and one can also use H_- instead of H_+. The method given here and the method of Ref. 1 have some similarities and differences. The method used here holds whenever $Q\in L^1_1(\mathbf{R})$, whereas in Ref. 1, for technical reasons, we needed $Q\in L^1_{1+\alpha}(\mathbf{R})$ for some $\alpha\in(0,1]$. In both methods a singular integral equation is formulated and from its solution $H(x)$ is recovered; however, in the present paper we exploit the large-k behavior of the reduced scattering coefficients, thus avoiding complications encountered in Ref. 1 as $k\to 0$. A crucial result here is Proposition 2.1, which strengthens the result of Theorem 2.4 in Ref. 1. From the solution at $k=0$ of the singular integral equation one finds $H(x)$ as the x-derivative of the solution $y(x)$ of a separable differential equation under the initial condition $y(0)=0$. Furthermore, when the reduced reflection coefficient $\rho(k)$ is an almost periodic function, the singular integral equation of the present paper becomes trivial, and so does the computation of $H(x)$; in Ref. 1, even this relatively simple case required extensive calculations.

When $H(x)$ and $H'(x)$ have no discontinuities, the large-k asymptotics of the reduced scattering coefficients defined in (1.2)–(1.3) are known to be of the form $\tau(k)-1=O(1/k)$, $\rho(k)=O(1/k)$, and $\measuredangle(k)=O(1/k)$. It is also known that each discontinuity of $H(x)$ contributes to the almost periodic part of the $O(1)$ terms in these asymptotics. We refer the reader to Refs. 1, 4, 11–13 for details. In this paper we show that the discontinuities in $H'(x)/H(x)$ are responsible for some of the $O(1/k)$ terms in these asymptotics; in fact, we develop an algorithm to recover the jumps in $H'(x)/H(x)$ from the large-k asymptotics of a reduced reflection coefficient.

This paper is organized as follows. In Sec. II we study the large-k asymptotics of the reduced scattering coefficients. In Sec. III we study the large-k asymptotics of certain wave functions defined in (3.1)–(3.2). In Sec. IV we present a factorization formula expressing the reduced scattering matrix as a matrix product of scattering matrices corresponding to potentials supported on a finite interval or on a half-line and those corresponding to discontinuities in $H(x)$ and $H'(x)/H(x)$. In Sec. V we present an algorithm to recover the discontinuities in $H(x)$ and $H'(x)/H(x)$ from the large-k asymptotics of the scattering data, thus generalizing the work of Ref. 13 regarding the discontinuities in $H(x)$. The results in Secs. II and III are used in Sec. VI in order to convert a key Riemann-Hilbert problem into a pair of uncoupled singular integral equations; in this section we also establish the unique solvability of these integral equations and show how to recover $H(x)$ from the solution of either singular integral equation. In Sec. VII we show that each singular integral equation can be converted into a Marchenko integral equation that is uniquely solvable, and we describe the recovery of $H(x)$ from the solution of a Marchenko equation. Hence, the inverse problem is solved by recovering $H(x)$ either by the method of Sec. VI or by that of Sec. VII. In Section VIII we present some examples illustrating the recovery of $H(x)$ using the solution of a singular integral equation and using the solution of a Marchenko equation; we also illustrate the algorithm of recovery of the discontinuities in $H'(x)/H(x)$.

II. SCATTERING COEFFICIENTS

In this section we analyze the large-k asymptotics of the reduced scattering coefficients defined in (1.2)–(1.3). Under the Liouville transformation

$$y=y(x)=\int_0^x ds\ H(s), \quad \psi(k,x)=\frac{1}{\sqrt{H(x)}}\,\phi(k,y), \tag{2.1}$$

the generalized Schrödinger equation (1.1) is transformed into

$$\frac{d^2\phi(k,y)}{dy^2}+k^2\phi(k,y)=V(y)\,\phi(k,y), \tag{2.2}$$

where

$$V(y(x))=\frac{H''(x)}{2H(x)^3}-\frac{3}{4}\,\frac{H'(x)^2}{H(x)^4}+\frac{Q(x)}{H(x)^2}. \tag{2.3}$$

Since $H(x)$ is assumed to have jump discontinuities at x_j for $j=1,\ldots,N$, the quantity $V(y)$ is undefined at $y_j=y(x_j)$. However, $V(y)$ is well defined in each of the intervals (y_j,y_{j+1}) for $j=0,\ldots,N$; thus, the Liouville transformation can be used on each interval (x_j,x_{j+1}) although it cannot be used on $\mathbf{R}$. Since $H(x)$ is strictly positive with positive limits as $x\to\pm\infty$, it follows that $y_0=y(x_0)=-\infty$ and $y_{N+1}=y(x_{N+1})=+\infty$. The constants q_j, defined by

$$q_j=\frac{H(x_j-0)}{H(x_j+0)}, \tag{2.4}$$

correspond to the relative jumps in the wave speed at the interfaces x_j, and y_j correspond to the times required for the wave to propagate from the fixed location $x=0$ to the interfaces x_j for $j=1,\ldots,N$.

Let $V_{j,j+1}(y)$ be the potential defined by

$$V_{j,j+1}(y)=\begin{cases} V(y), & y\in(y_j,y_{j+1}),\\ 0, & \text{elsewhere,}\end{cases} \tag{2.5}$$

where $V(y)$ is the quantity in (2.3). From (H4) it follows that $V_{j,j+1}\in L_1^1(\mathbf{R})$ for $j=0,\ldots,N$. Let $Y_{l;j,j+1}(k,y)$ and $Y_{r;j,j+1}(k,y)$ denote the Faddeev functions[1] from the left and from the right, respectively, associated with the potential $V_{j,j+1}(y)$. We have[1]

$$Y_{l;j,j+1}(k,y)=\begin{cases} \dfrac{1}{t_{j,j+1}(k)}\,[1+l_{j,j+1}(k)e^{-2iky}], & y\leqslant y_j, \quad j=1,\ldots,N, \quad k\in\overline{C^+},\\ \dfrac{1}{t_{0,1}(k)}\,[1+l_{0,1}(k)e^{-2iky}]+o(1), & y\to-\infty, \quad j=0, \quad k\in\mathbf{R},\end{cases} \tag{2.6}$$

$$Y_{r;j,j+1}(k,y)=\begin{cases} \dfrac{1}{t_{j,j+1}(k)}\,[1+r_{j,j+1}(k)e^{2iky}], & y\geqslant y_{j+1}, \quad j=0,\ldots,N-1, \quad k\in\overline{C^+},\\ \dfrac{1}{t_{N,N+1}(k)}\,[1+r_{N,N+1}(k)e^{2iky}]+o(1), & y\to+\infty, \quad j=N, \quad k\in\mathbf{R},\end{cases} \tag{2.7}$$

where $t_{j,j+1}(k)$, $r_{j,j+1}(k)$, and $l_{j,j+1}(k)$ denote the transmission coefficient and the reflection coefficients from the right and from the left, respectively, for the potential $V_{j,j+1}(y)$. Since $V_{j,j+1}\in L_1^1(\mathbf{R})$, it follows that for each fixed $y\in\mathbf{R}$ we have

$$Y_{l;j,j+1}(k,y)=1+O(1/k),\quad Y'_{l;j,j+1}(k,y)=o(1),\quad k\to\infty \text{ in } \overline{\mathbf{C}^+},\tag{2.8}$$

$$Y_{r;j,j+1}(k,y)=1+O(1/k),\quad Y'_{r;j,j+1}(k,y)=o(1),\quad k\to\infty \text{ in } \overline{\mathbf{C}^+}.\tag{2.9}$$

Using (2.1) it can be shown that the functions defined by

$$\eta_{j,j+1}(k,x)=\frac{1}{\sqrt{H(x)}}\,e^{iky}Y_{l;j,j+1}(k,y),\quad \xi_{j,j+1}(k,x)=\frac{1}{\sqrt{H(x)}}\,e^{-iky}Y_{r;j,j+1}(k,y),\tag{2.10}$$

are solutions of (1.1). Let us introduce the matrices

$$\Gamma_{j,j+1}(k,x)=\begin{bmatrix}\eta_{j,j+1}(k,x) & \xi_{j,j+1}(k,x)\\ \eta'_{j,j+1}(k,x) & \xi'_{j,j+1}(k,x)\end{bmatrix},\quad j=0,\ldots,N,\tag{2.11}$$

$$\mathcal{S}(k)=\prod_{n=1}^{N}\Gamma_{n-1,n}(k,x_n-0)^{-1}\Gamma_{n,n+1}(k,x_n+0).\tag{2.12}$$

It was shown in Ref. 1 that

$$\frac{1}{\tau(k)}=\frac{1}{t_{0,1}(k)}\,[1\ \ 0]\mathcal{S}(k)\begin{bmatrix}1\\0\end{bmatrix}=\frac{1}{t_{N,N+1}(k)}\,[0\ \ 1]\mathcal{S}(k)^{-1}\begin{bmatrix}0\\1\end{bmatrix},\tag{2.13}$$

$$\frac{\ell(k)}{\tau(k)}=\begin{bmatrix}\dfrac{l_{0,1}(k)}{t_{0,1}(k)} & 1\end{bmatrix}\mathcal{S}(k)\begin{bmatrix}1\\0\end{bmatrix},\tag{2.14}$$

$$\frac{\rho(k)}{\tau(k)}=\begin{bmatrix}1 & \dfrac{r_{N,N+1}(k)}{t_{N,N+1}(k)}\end{bmatrix}\mathcal{S}(k)^{-1}\begin{bmatrix}0\\1\end{bmatrix}.\tag{2.15}$$

Moreover,

$$\det\Gamma_{n,n+1}(k,x)=-\frac{2ik}{t_{n,n+1}(k)},\quad \det\mathcal{S}(k)=\frac{t_{0,1}(k)}{t_{N,N+1}(k)}.$$

Let

$$\alpha_n=\frac{1}{2}\left(\sqrt{q_n}+\frac{1}{\sqrt{q_n}}\right),\quad \beta_n=\frac{1}{2}\left(\sqrt{q_n}-\frac{1}{\sqrt{q_n}}\right),\tag{2.16}$$

$$E(k,x_n)=\begin{bmatrix}\alpha_n & \beta_n e^{-2iky_n}\\ \beta_n e^{2iky_n} & \alpha_n\end{bmatrix},\tag{2.17}$$

with q_n as in (2.4); let us also define $a(k)$ and $b(k)$ by

$$\begin{bmatrix}a(k) & b(k)\\ b(-k) & a(-k)\end{bmatrix}=\prod_{n=1}^{N}E(k,x_n).\tag{2.18}$$

Let AP^W (almost periodic functions with Wiener norm) stand for the algebra of all complex-valued functions $f(k)$ on $\mathbf{R}$ that are of the form $f(k)=\Sigma_{j=-\infty}^{\infty}f_j e^{ik\lambda_j}$, where $f_j\in\mathbf{C}$ and $\lambda_j\in\mathbf{R}$ for

all j and $\Sigma_j|f_j|<+\infty$. It is already known[1] that the functions $a(k)$, $b(k)$, $1/a(k)$, and $b(k)/a(k)$ belong to AP^W. In the next proposition we obtain the large-k asymptotics of the reduced scattering coefficients $\tau(k)$, $\rho(k)$, and $\ell(k)$.

Proposition 2.1: Under assumptions (H1)–(H5) we have

$$\tau(k)=\frac{1}{a(k)}+O\left(\frac{1}{k}\right), \quad k\to\infty \ \text{ in } \ \overline{\mathbf{C}^+}, \tag{2.19}$$

$$\rho(k)=-\frac{b(k)}{a(k)}+O\left(\frac{1}{k}\right), \quad k\to\pm\infty, \tag{2.20}$$

$$\ell(k)=\frac{b(-k)}{a(k)}+O\left(\frac{1}{k}\right), \quad k\to\pm\infty, \tag{2.21}$$

where $a(k)$ and $b(k)$ are the quantities defined in (2.18).

Proof: Using (2.8)–(2.10) we obtain

$$\Gamma_{n,n+1}(k,x_{n+1}-0)^{-1}\Gamma_{n+1,n+2}(k,x_{n+1}+0) = \begin{bmatrix} \alpha_{n+1}(1+O(1/k)) & \beta_{n+1}e^{-2iky_{n+1}}(1+O(1/k)) \\ \beta_{n+1}e^{2iky_{n+1}}(1+O(1/k)) & \alpha_{n+1}(1+O(1/k)) \end{bmatrix}, \quad k\to\infty \ \text{ in } \ \overline{\mathbf{C}^+}, \tag{2.22}$$

where α_n and β_n are the constants defined in (2.16). Furthermore, using (2.13)–(2.15) and the fact[14] that

$$t_{j,j+1}(k)=1+O(1/k), \quad k\to\infty \ \text{ in } \ \overline{\mathbf{C}^+},$$

$$r_{j,j+1}(k)=O(1/k), \quad l_{j,j+1}(k)=O(1/k), \quad k\to\pm\infty,$$

we obtain (2.19)–(2.21). ■

Proposition 2.1 is an improvement over Theorem 2.4 in Ref. 13, where the error terms in (2.19)–(2.21) were only shown to be $o(1)$. We refer the reader to Refs. 1 and 13 for various other properties of the reduced scattering coefficients.

III. ESTIMATES ON WAVE FUNCTIONS

In this section we analyze the large-k behavior of the scattering solutions of (2.2). As in (5.1)–(5.2) of Ref. 1, let us define the Faddeev functions $Z_l(k,y)$ and $Z_r(k,y)$, from the left and from the right, respectively, associated with (2.2):

$$Z_l(k,y)=\sqrt{\frac{H(x)}{H_+}}\,e^{-iky-ikA_+}f_l(k,x), \tag{3.1}$$

$$Z_r(k,y)=\sqrt{\frac{H(x)}{H_-}}\,e^{iky-ikA_-}f_r(k,x), \tag{3.2}$$

where y is the quantity defined in (2.1) and $A_\pm$ are the constants in (1.4). Note that $e^{iky}Z_l(k,y)$ and $e^{-iky}Z_r(k,y)$ are the Jost solutions from the left and from the right, respectively, of (2.2). In this section we analyze the large-k asymptotics of $Z_l(k,y)$ and $Z_r(k,y)$.

The next proposition shows that, for each fixed $y \in \mathbf{R}\backslash\{y_1,\ldots,y_N\}$, the Faddeev functions can be written as the sum of an almost periodic function and a continuous function, the latter vanishing as $k\to\infty$ in $\overline{\mathbf{C}^+}$.

Proposition 3.1: For each fixed $y \in \mathbf{R}\backslash\{y_1,\ldots,y_N\}$, we have

$$Z_l(k,y)=J_l(k,y)+O(1/k), \quad Z_r(k,y)=J_r(k,y)+O(1/k), \quad k\to\infty \ \text{ in } \ \overline{\mathbf{C}^+}, \tag{3.3}$$

where

$$J_l(k,y)=[1 \quad e^{-2iky}]\left(\prod_{n=j+1}^{N} E(k,x_n)\right)\begin{bmatrix}1\\0\end{bmatrix}, \quad y\in(y_j,y_{j+1}), \quad j=0,\ldots,N-1, \tag{3.4}$$

$$J_l(k,y)=1, \quad y\in(y_N,+\infty), \tag{3.5}$$

$$J_r(k,y)=1, \quad y\in(-\infty,y_1), \tag{3.6}$$

$$J_r(k,y)=[e^{2iky} \quad -1]\left(\prod_{n=j}^{1} E(k,x_n)\right)\begin{bmatrix}0\\-1\end{bmatrix}, \quad y\in(y_j,y_{j+1}), \quad j=1,\ldots,N, \tag{3.7}$$

with $E(k,x_n)$ defined in (2.17). The product notation in (3.7) means that n decreases from j to 1.

Proof: When $y\in(y_N,+\infty)$, from (3.13), (3.15), (3.21) of Ref. 1 and (2.10) and (3.1), we have

$$Z_l(k,y)=Y_{l;N,N+1}(k,y), \quad y\in(y_N,+\infty), \tag{3.8}$$

and hence $Z_l(k,y)=1+O(1/k)$ as $k\to\infty$ in $\overline{\mathbf{C}^+}$. Thus, we have (3.3) with $J_l(k,y)$ as in (3.5). Similarly, from (3.13), (3.15), (3.22) of Ref. 1 and (2.10) and (3.2), we get

$$Z_r(k,y)=Y_{r;0,1}(k,y), \quad y\in(-\infty,y_1), \tag{3.9}$$

and hence $Z_r(k,y)=1+O(1/k)$ as $k\to\infty$ in $\overline{\mathbf{C}^+}$. Thus, we have (3.3) with $J_r(k,y)$ as in (3.6).

When $y\in(y_j,y_{j+1})$ with $0\leqslant j\leqslant N-1$, from (3.25) of Ref. 1 and (3.1), we see that

$$\begin{aligned} Z_l(k,y)=&[1 \quad 0]\sqrt{H(x)}e^{-iky}\Gamma_{j,j+1}(k,x)\\ &\times\left(\prod_{n=j}^{N-1}\Gamma_{n,n+1}(k,x_{n+1}-0)^{-1}\Gamma_{n+1,n+2}(k,x_{n+1}+0)\right)\begin{bmatrix}1\\0\end{bmatrix}, \end{aligned}\tag{3.10}$$

where $\Gamma_{j,j+1}(k,x)$ is the matrix defined in (2.11). From (2.8)–(2.10) we have

$$[1 \quad 0]\sqrt{H(x)}e^{-iky}\Gamma_{j,j+1}(k,x)=[1+O(1/k) \quad e^{-2iky}(1+O(1/k))]. \tag{3.11}$$

Hence, using (2.22) and (3.11) in (3.10), we obtain

$$Z_l(k,y)=J_l(k,y)[1+O(1/k)], \quad k\to\infty \ \text{ in } \ \overline{\mathbf{C}^+}, \tag{3.12}$$

with $J_l(k,y)$ as in (3.4). Similarly, when $y\in(y_j,y_{j+1})$ with $1\leqslant j\leqslant N$, from (3.26) of Ref. 1 and (3.2), we see that

$$Z_r(k,y)=[1 \quad 0]\sqrt{H(x)}e^{iky}\Gamma_{j,j+1}(k,x)\left(\prod_{n=j}^{1}\Gamma_{n,n+1}(k,x_n+0)^{-1}\Gamma_{n+1,n+2}(k,x_n-0)\right)\begin{bmatrix}0\\1\end{bmatrix}. \tag{3.13}$$

From (2.8)–(2.10) we have

$$[1 \quad 0]\sqrt{H(x)}e^{iky}\Gamma_{j,j+1}(k,x)=[e^{2iky}(1+O(1/k)) \quad 1+O(1/k)]. \tag{3.14}$$

Using (2.22) and (3.14) in (3.13), we obtain

$$Z_r(k,y)=J_r(k,y)[1+O(1/k)], \quad k\to\infty \ \text{ in } \ \overline{\mathbf{C}^+}, \tag{3.15}$$

with $J_r(k,y)$ as in (3.7). Note that for each fixed $y\in\mathbf{R}\backslash\{y_1,\ldots,y_N\}$ the functions $J_l(k,y)$ and $J_r(k,y)$ are uniformly bounded in $\overline{\mathbf{C}^+}$, and hence we see that (3.12) and (3.15) imply (3.3). ■

Recall that the Hardy spaces $\mathbf{H}^p_\pm(\mathbf{R})$ are defined as the spaces of all functions $f(k)$ that are analytic in $k\in\mathbf{C}^\pm$ and satisfy $\sup_{\epsilon>0}\int_{-\infty}^{\infty}dk\ |f(k\pm i\epsilon)|^p<+\infty$.

Theorem 3.2: For each fixed $y\in\mathbf{R}\backslash\{y_1,\ldots,y_N\}$, the functions $Z_l(k,y)-J_l(k,y)$ and $Z_r(k,y)-J_r(k,y)$ belong to the Hardy space $\mathbf{H}^2_+(\mathbf{R})$.

Proof: It is proved in Theorem 2.1 of Ref. 1 that, for each fixed $x\in\mathbf{R}\backslash\{x_1,\ldots,x_N\}$, $f_l(k,x)$ and $f_r(k,x)$ are continuous functions of k in $\overline{\mathbf{C}^+}$ and analytic in $\mathbf{C}^+$; therefore, for each fixed $y\in\mathbf{R}\backslash\{y_1,\ldots,y_N\}$, the Faddeev functions $Z_l(k,y)$ and $Z_r(k,y)$ are continuous in $\overline{\mathbf{C}^+}$ and analytic in $\mathbf{C}^+$. From (3.4)–(3.7) we see that $J_l(k,y)$ and $J_r(k,y)$ are continuous in $\overline{\mathbf{C}^+}$ and analytic in $\mathbf{C}^+$. Hence, by Proposition 3.1 we can conclude that $Z_l(k,y)-J_l(k,y)$ and $Z_r(k,y)-J_r(k,y)$ belong to the Hardy space $\mathbf{H}^2_+(\mathbf{R})$. ■

Note that we can also conclude the analyticity in $\mathbf{C}^+$ and continuity in $\overline{\mathbf{C}^+}$ of $Z_l(k,y)$ and $Z_r(k,y)$ from (3.10) and (3.13), respectively, because the matrices there have these properties. At first the inverse matrices in (3.10) and (3.13) seem to have a $(1/k)$ singularity at $k=0$ in the exceptional case; however, if any $V_{n,n+1}(y)$ are exceptional potentials, we can divide each of those intervals (y_n,y_{n+1}) into two subintervals such that the fragments on the two subintervals are generic;[2] hence, even in the exceptional case, from (3.10) and (3.13), we can conclude that $Z_l(k,y)$ and $Z_r(k,y)$ are analytic in $\mathbf{C}^+$ and continuous in $\overline{\mathbf{C}^+}$.

Note that the matrix product $E(k,x_{j+1})\cdots E(k,x_N)$ in (3.4) can be explicitly evaluated in analogy to (2.28) of Ref. 13. Let us write

$$\prod_{n=j+1}^{N} E(k,x_n)=\begin{bmatrix} A_j(k) & B_j(k) \\ B_j(-k) & A_j(-k)\end{bmatrix},$$

where $A_j(k)$ and $B_j(k)$ will be explicitly evaluated. Thus, we can write (3.4)–(3.5) as

$$J_l(k,y)=[A_j(k)+e^{-2iky}B_j(-k)], \quad y\in(y_j,y_{j+1}), \tag{3.16}$$

with $A_N(k)=1$ and $B_N(k)=0$. Using induction, we can show that $A_j(k)$ and $e^{-2iky}B_j(-k)$ both are exponential polynomials having at most 2^{N-j} terms. All the coefficients in the exponential polynomials are real constants and all the exponentials are bounded by 1 in absolute value in $\overline{\mathbf{C}^+}$. For future reference, we list $A_j(k)$ and $B_j(k)$ for $j=N-1,\ N-2,\ N-3$.
If $j=N-1$,

$$A_{N-1}(k)=\alpha_N, \quad e^{2iky_N}B_{N-1}(k)=\beta_N.$$

If $j=N-2$,

$$A_{N-2}(k)=\alpha_{N-1}\alpha_N+\beta_{N-1}\beta_N e^{2ik(y_N-y_{N-1})},$$

$$e^{2iky_N}B_{N-2}(k)=\alpha_{N-1}\beta_N+\beta_{N-1}\alpha_N e^{2ik(y_N-y_{N-1})}.$$

If $j=N-3$,

$$A_{N-3}(k)=\alpha_{N-2}\alpha_{N-1}\alpha_N+\beta_{N-2}\beta_{N-1}\alpha_N e^{2ik(y_{N-1}-y_{N-2})}$$
$$+\alpha_{N-2}\beta_{N-1}\beta_N e^{2ik(y_N-y_{N-1})}+\beta_{N-2}\alpha_{N-1}\beta_N e^{2ik(y_N-y_{N-2})},$$

$$e^{2iky_N}B_{N-3}(k)=\alpha_{N-2}\alpha_{N-1}\beta_N+\beta_{N-2}\beta_{N-1}\beta_N e^{2ik(y_{N-1}-y_{N-2})}$$
$$+\alpha_{N-2}\beta_{N-1}\alpha_N e^{2ik(y_N-y_{N-1})}+\beta_{N-2}\alpha_{N-1}\alpha_N e^{2ik(y_N-y_{N-2})}.$$

We see that, for $j\leqslant N-1$, the term $e^{2iky_N}B_j(k)$ is obtained from $A_j(k)$ by interchanging β_N with α_N.

In a similar manner, using

$$E(k,x_j)^{-1}\cdots E(k,x_1)^{-1}=[E(k,x_1)\cdots E(k,x_j)]^{-1},$$

we can explicitly evaluate the matrix product $E(k,x_1)\cdots E(k,x_j)$ appearing in (3.7) in analogy to (2.28) of Ref. 13. Let us write

$$\prod_{n=1}^{j}E(k,x_n)=\begin{bmatrix}C_j(k) & D_j(k)\\ D_j(-k) & C_j(-k)\end{bmatrix},$$

where $C_j(k)$ and $D_j(k)$ will be explicitly evaluated. Thus, we can write (3.6)–(3.7) as

$$J_r(k,y)=[C_j(k)-e^{2iky}D_j(-k)],\quad y\in(y_j,y_{j+1}),\tag{3.17}$$

with $C_0(k)=1$ and $D_0(k)=0$. Using induction, we can show that $C_j(k)$ and $e^{2iky}D_j(-k)$ both are exponential polynomials having at most 2^j terms. All the coefficients in the exponential polynomials are real constants and all the exponentials are bounded by 1 in absolute value in $\overline{\mathbf{C}^+}$. For future reference, we list $C_j(k)$ and $D_j(k)$ for $j=1,\ 2,\ 3$.
If $j=1$,

$$C_1(k)=\alpha_1,\quad e^{2iky_1}D_1(k)=\beta_1.$$

If $j=2$,

$$C_2(k)=\alpha_1\alpha_2+\beta_1\beta_2e^{2ik(y_2-y_1)},\quad e^{2iky_2}D_2(k)=\alpha_1\beta_2+\beta_1\alpha_2e^{2ik(y_2-y_1)}.$$

If $j=3$,

$$C_3(k)=\alpha_1\alpha_2\alpha_3+\beta_1\beta_2\alpha_3e^{2ik(y_2-y_1)}+\alpha_1\beta_2\beta_3e^{2ik(y_3-y_2)}+\beta_1\alpha_2\beta_3e^{2ik(y_3-y_1)},$$

$$e^{2iky_3}D_3(k)=\alpha_1\alpha_2\beta_3+\beta_1\beta_2\beta_3e^{2ik(y_2-y_1)}+\alpha_1\beta_2\alpha_3e^{2ik(y_3-y_2)}+\beta_1\alpha_2\alpha_3e^{2ik(y_3-y_1)}.$$

We see that, for $j\geqslant 1$, the term $e^{2iky_j}D_j(k)$ is obtained from $C_j(k)$ by interchanging β_j with α_j.

IV. FACTORIZATION

In this section we generalize the factorization formula of Ref. 15 and show that the reduced scattering matrix corresponding to (1.1) can be expressed in terms of the scattering matrices corresponding to the potentials $V_{j,j+1}(y)$ defined in (2.5) and certain matrices associated with the discontinuities of $H(x)$ and $H'(x)/H(x)$. Using the scattering coefficients introduced in (2.6)–(2.7), let us define

$$\Lambda_{j,j+1}(k)=\begin{bmatrix} \dfrac{1}{t_{j,j+1}(k)} & -\dfrac{r_{j,j+1}(k)}{t_{j,j+1}(k)} \\ \dfrac{l_{j,j+1}(k)}{t_{j,j+1}(k)} & \dfrac{1}{t_{j,j+1}(-k)} \end{bmatrix}, \quad j=0,1,\ldots,N, \tag{4.1}$$

$$\Lambda(k)=\begin{bmatrix} \dfrac{1}{\tau(k)} & -\dfrac{\rho(k)}{\tau(k)} \\ \dfrac{\ell(k)}{\tau(k)} & \dfrac{1}{\tau(-k)} \end{bmatrix}, \tag{4.2}$$

$$F_j(k)=\begin{bmatrix} \alpha_j+\dfrac{\nu_j}{2ik} & \left(\beta_j+\dfrac{\nu_j}{2ik}\right)e^{-2iky_j} \\ \left(\beta_j-\dfrac{\nu_j}{2ik}\right)e^{2iky_j} & \alpha_j-\dfrac{\nu_j}{2ik} \end{bmatrix}, \quad j=1,\ldots,N, \tag{4.3}$$

where α_j and β_j are the constants defined in (2.16) and

$$\nu_j=\frac{1}{2\sqrt{H(x_j-0)H(x_j+0)}}\left[\frac{H'(x_j-0)}{H(x_j-0)}-\frac{H'(x_j+0)}{H(x_j+0)}\right]. \tag{4.4}$$

Note that $\nu_j=0$ if and only if $H'(x)/H(x)$ is continuous at x_j. Following Sabatier's terminology[4–7] we can refer to $F_j(k)$ as a ''hard scatterer'' and $\Lambda_{j,j+1}(k)$ as a ''soft scatterer.'' The following theorem shows how the matrices defined in (4.1)–(4.3) are related to one another.

Theorem 4.1: We have

$$\Lambda=\Lambda_{0,1}F_1\Lambda_{1,2}F_2\Lambda_{2,3}\cdots F_N\Lambda_{N,N+1}, \tag{4.5}$$

where Λ, $\Lambda_{j,j+1}$, and F_j are the matrices defined in (4.2), (4.1), and (4.3), respectively.

Proof: Note that we have $\Lambda_{j,j+1}=G_jD_j$, where we have defined

$$G_j=\begin{bmatrix} \dfrac{1}{t_{j,j+1}(k)} & 0 \\ \dfrac{l_{j,j+1}(k)}{t_{j,j+1}(k)} & 1 \end{bmatrix}, \quad D_j=\begin{bmatrix} 1 & -r_{j,j+1}(k) \\ 0 & t_{j,j+1}(k) \end{bmatrix}.$$

Using the displayed equation in Ref. 1 following (14.4), we can relate $\Lambda(k)$ and $\mathscr{G}(k)$ defined in (2.12) as $\Lambda=G_0\mathscr{G}D_N$. Inserting the identity matrices $G_jG_j^{-1}$ and $D_jD_j^{-1}$ in the appropriate places in (2.12), we obtain

$$\Lambda=G_0D_0\prod_{n=1}^{N}[D_{n-1}^{-1}\Gamma_{n-1,n}(k,x_n-0)^{-1}\Gamma_{n,n+1}(k,x_n+0)G_n^{-1}][G_nD_n]. \tag{4.6}$$

Using (2.11), it can be checked that

$$D_{n-1}^{-1}\Gamma_{n-1,n}(k,x_n-0)^{-1}\Gamma_{n,n+1}(k,x_n+0)G_n^{-1}=F_n, \tag{4.7}$$

where F_n are the matrices defined in (4.3). Thus, using (4.7) in (4.6), we get (4.5). ■

It is already known[13] that the function $H(x)$ given by

$$H(x)=\frac{h_{j,j+1}}{f_l(0,x)^2}, \quad x\in(x_j,x_{j+1}), \quad j=0,\ldots,N,$$

$$h_{N,N+1}=H_+; \quad h_{j-1,j}=q_j h_{j,j+1}, \quad j=0,\ldots,N,$$

corresponds to the scattering data $Q(x)$, $\rho(k)=-b(k)/a(k)$, and $\tau(k)=1/a(k)$; as seen from Proposition 2.1, the scattering coefficients in this case coincide with their asymptotic expressions as $k\to\pm\infty$. In this case, the matrix factorization given in (4.5) reduces to the factorization in (2.18). This is because in this case ν_j given in (4.4) vanishes, and hence the matrix $F_j(k)$ defined in (4.3) becomes equal to $E(k,x_j)$ defined in (2.17); in fact, $F_j(k)=E(k,x_j)$ if and only if $\nu_j=0$. Furthermore, in this case $V_{j,j+1}(y)=0$ and hence $\Lambda_{j,j+1}(k)=\mathbf{I}$; in fact, $\Lambda_{j,j+1}(k)=\mathbf{I}$ if and only if $V_{j,j+1}(y)=0$. In this case, we also have $Z_l(k,y)=J_l(k,y)$ and $Z_r(k,y)=J_r(k,y)$.

Now let us ask the following question. If we choose $V_{j,j+1}(y)=0$ for $j=0,1,\ldots,N$, but still allow $\nu_j\neq 0$, what is the corresponding $H(x)$? From the factorization formula (4.5), by letting $\Lambda_{j,j+1}(k)=\mathbf{I}$, we can explicitly evaluate the corresponding scattering matrix. In this case, the corresponding $H(x)$ is given by

$$\sqrt{H(x)}=\frac{1}{a_j f_l(0,x)+b_j f_r(0,x)}, \quad x\in(x_j,x_{j+1}), \quad j=0,\ldots,N, \tag{4.8}$$

$$a_N=\frac{1}{\sqrt{H_+}}, \quad b_N=0, \tag{4.9}$$

and a_j, b_j for $j=0,1,\ldots,N-1$, will be determined recursively by using the jumps in $H(x)$ and $H'(x)/H(x)$ according to (2.4) and (4.4), respectively. Using (4.8) in (2.4), we obtain

$$\frac{a_j f_l(0,x_j)+b_j f_r(0,x_j)}{a_{j-1} f_l(0,x_j)+b_{j-1} f_r(0,x_j)}=\sqrt{q_j}, \quad j=1,\ldots,N. \tag{4.10}$$

From (4.8) we have

$$\frac{H'(x)}{H(x)}=-2\,\frac{a_j f_l'(0,x)+b_j f_r'(0,x)}{a_j f_l(0,x)+b_j f_r(0,x)}, \tag{4.11}$$

and hence from (4.4) we get

$$\frac{a_{j-1} f_l'(0,x_j)+b_{j-1} f_r'(0,x_j)}{a_{j-1} f_l(0,x_j)+b_{j-1} f_r(0,x_j)}-\frac{a_j f_l'(0,x_j)+b_j f_r'(0,x_j)}{a_j f_l(0,x_j)+b_j f_r(0,x_j)}=-\nu_j\sqrt{H(x_j-0)H(x_j+0)}, \quad j=1,\ldots,N. \tag{4.12}$$

Solving the linear system (4.10) and (4.12) with unknowns a_{j-1} and b_{j-1} in terms of a_j and b_j and known quantities, and using (4.9), we obtain

$$a_{j-1}=\frac{a_j}{\sqrt{q_j}}+\frac{\nu_j f_r(0,x_j)\sqrt{H(x_j+0)}}{[f_l(0,x);f_r(0,x)]}, \quad j=1,\ldots,N; \quad a_N=\frac{1}{\sqrt{H_+}}, \tag{4.13}$$

$$b_{j-1}=\frac{b_j}{\sqrt{q_j}}-\frac{\nu_j f_l(0,x_j)\sqrt{H(x_j+0)}}{[f_l(0,x);f_r(0,x)]}, \quad j=1,\ldots,N; \quad b_N=0, \tag{4.14}$$

where $[f_l(0,x);f_r(0,x)]=f_l(0,x)f_r'(0,x)-f_l'(0,x)f_r(0,x)$ is the Wronskian, which is a constant completely determined by $Q(x)$ alone. We can also obtain the Jost solutions for (1.1) explicitly. In

this case, since $V_{j,j+1}(y)=0$, we have $Y_{l;j,j+1}(k,y)=1$ and $Y_{r;j,j+1}(k,y)=1$; thus, the matrix $\Gamma_{j,j+1}(k,x)$ defined in (2.11) is determined by using (2.10). Hence, using (3.8) and (3.10) the Faddeev function $Z_l(k,y)$ is determined, and using (3.9) and (3.13) the Faddeev function $Z_r(k,y)$ is determined. Then we obtain $f_l(k,x)$ and $f_r(k,x)$ as in (3.1)–(3.2).

Note that in the above procedure, in case $Q(x)$ is an exceptional potential, i.e., if $f_l(0,x)$ and $f_r(0,x)$ are linearly dependent, in (4.8)–(4.14) we need to replace $f_r(0,x)$ by a zero-energy solution of (1.5) linearly independent of $f_l(0,x)$, such as $\psi(x)=f_l(0,x)\int_0^x dy/f_l(0,y)^2$; with this choice of $\psi(x)$, we have $[f_l(0,x);\psi(x)]=1$. In the exceptional case, it turns out that although different choices for $\psi(x)$ lead to different coefficients a_j and b_j, the resulting $H(x)$ is independent of the choice of $\psi(x)$. Also note that, if $N=1$, it is necessary that the generic case occurs; however, for $N\geqslant 2$ the exceptional case may occur.

V. AN ALGORITHM TO RECOVER JUMPS IN $H'(x)/H(x)$

In Ref. 13 we described an algorithm to recover N, y_j, and q_j associated with the discontinuities of $H(x)$ in terms of the leading asymptotic behavior of the scattering data as $k\to\pm\infty$. In this section we will analyze the $O(1/k)$ terms in the scattering data and will describe an algorithm to recover the constants ν_j associated with the discontinuities of $H'(x)/H(x)$ from the almost periodic part of the $O(1/k)$ terms in the scattering data. The algorithm of Ref. 13 must be applied first to recover N, y_j, and q_j before the algorithm to recover ν_j is used. In order to use the algorithm, one also needs to know the value of $w_{N,N+1}$, where we have defined

$$w_{j,j+1}=\int_{y_j}^{y_{j+1}} dz\ V_{j,j+1}(z),$$

with $V_{j,j+1}(y)$ being the quantity defined in (2.5). The constant $w_{N,N+1}$ can be obtained from a reduced reflection coefficient in various ways without solving the entire inverse problem. For example, as we will see in Sec. VII, we have $w_{N,N+1}=2h_l(0+,y_N)$, where $h_l(t,y)$ is the solution of the Marchenko equation (7.7) that is uniquely solvable; hence the solution of (7.7) at the fixed point y_N gives us $w_{N,N+1}$.

Since $V_{j,j+1}\in L_1^1(\mathbf{R})$, the scattering coefficients associated with $V_{j,j+1}(y)$ satisfy[14]

$$\frac{1}{t_{j,j+1}(k)}=1+\frac{w_{j,j+1}}{2ik}+o\left(\frac{1}{k}\right),\quad k\to\pm\infty,$$

$$\frac{r_{j,j+1}(k)}{t_{j,j+1}(k)}=o\left(\frac{1}{k}\right),\quad \frac{l_{j,j+1}(k)}{t_{j,j+1}(k)}=o\left(\frac{1}{k}\right),\quad k\to\pm\infty,$$

and hence from (4.1) we have

$$\Lambda_{j,j+1}(k)=\mathbf{I}+\frac{w_{j,j+1}}{2ik}\,\mathbf{J}+o\left(\frac{1}{k}\right),\quad k\to\pm\infty,$$

where we have defined $\mathbf{J}=\mathrm{diag}(1,-1)$. Let us write (4.3) in the form

$$F_j=E_j+\frac{\nu_j}{2ik}\,U_j,$$

where E_j is the matrix $E(k,x_j)$ defined in (2.17) and

$$U_j=\begin{bmatrix} 1 & e^{-2iky_j} \\ -e^{2iky_j} & -1 \end{bmatrix}.$$

Thus, as $k\to\pm\infty$, from (4.5) we obtain $\Lambda=E_1E_2\cdots E_N+O(1/k)$ and

$$2ik[\Lambda-E_1E_2\cdots E_N]=w_{0,1}\mathbf{J}E_1E_2\cdots E_N+w_{1,2}E_1\mathbf{J}E_2\cdots E_N+\cdots+w_{N,N+1}E_1E_2\cdots E_N\mathbf{J}$$
$$+\nu_1U_1E_2\cdots E_N+\nu_2E_1U_2E_3\cdots E_N+\cdots+\nu_NE_1E_2\cdots E_{N-1}U_N+o(1). \tag{5.1}$$

Thus, from (2.18) and (4.2) we see that (5.1) allows us to express

$$2ik\left[\frac{1}{\tau(k)}-a(k)\right]=\Delta(k)+o(1),\quad k\to\pm\infty, \tag{5.2}$$

$$-2ik\left[\frac{\rho(k)}{\tau(k)}+b(k)\right]=\Omega(k)+o(1),\quad k\to\pm\infty, \tag{5.3}$$

where $\Delta(k)$ and $\Omega(k)$ are linear combinations of $w_{0,1},\ldots,w_{N,N+1}$ and $\nu_1,\ldots,\nu_N$ with almost periodic polynomials as coefficients.

Let us now explain how to compute ν_N. When $N=1$ we have

$$\Delta(k)=(w_{0,1}+w_{1,2})\alpha_1+\nu_1\equiv\Delta_1, \tag{5.4}$$

$$e^{2iky_1}\Omega(k)=(w_{0,1}-w_{1,2})\beta_1+\nu_1\equiv\Omega_1. \tag{5.5}$$

Multiplying (5.4) by β_1 and (5.5) by α_1, and subtracting the resulting equations, we obtain

$$\nu_1=\frac{1}{\alpha_1-\beta_1}[2w_{1,2}\alpha_1\beta_1+\alpha_1\Omega_1-\beta_1\Delta_1]. \tag{5.6}$$

When $N=2$, we have

$$\Delta(k)=\Delta_1+e^{2ik(y_2-y_1)}\Delta_2, \tag{5.7}$$

$$e^{2iky_2}\Omega(k)=\Omega_1+e^{2ik(y_2-y_1)}\Omega_2, \tag{5.8}$$

where we have defined

$$\Delta_1=(w_{0,1}+w_{1,2}+w_{2,3})\alpha_1\alpha_2+\nu_1\alpha_2+\nu_2\alpha_1, \tag{5.9}$$

$$\Omega_1=(w_{0,1}+w_{1,2}-w_{2,3})\alpha_1\beta_2+\nu_1\beta_2+\nu_2\alpha_1, \tag{5.10}$$

$$\Delta_2=(w_{0,1}-w_{1,2}+w_{2,3})\beta_1\beta_2+\nu_1\beta_2-\nu_2\beta_1,$$

$$\Omega_2=(w_{0,1}-w_{1,2}-w_{2,3})\beta_1\alpha_2+\nu_1\alpha_2-\nu_2\beta_1.$$

Multiplying (5.9) by β_2 and (5.10) by α_2 and subtracting the resulting equations, we obtain

$$\alpha_1(\beta_2-\alpha_2)\nu_2=-2w_{2,3}\alpha_1\alpha_2\beta_2+\beta_2\Delta_1-\alpha_2\Omega_1,$$

and hence

$$\nu_2=\frac{1}{\alpha_2-\beta_2}\left[2w_{2,3}\alpha_2\beta_2+\frac{\alpha_2\Omega_1-\beta_2\Delta_1}{\alpha_1}\right].$$

As can be seen from (5.4), (5.5), (5.7), and (5.8), and in general be proved by induction, the quantity $e^{2iky_N}\Omega(k)$ is obtained from $\Delta(k)$ by interchanging β_N with α_N and by changing the sign of $w_{N,N+1}$. It can also be shown that $\Delta(k)$ and $e^{2iky_N}\Omega(k)$ both are exponential polynomials having at most 2^{N-1} nonzero terms. To compute ν_N for arbitrary N, we let Δ_1 and Ω_1 denote the constant terms in the almost periodic polynomials $\Delta(k)$ and $e^{2iky_N}\Omega(k)$, respectively. From (5.1) we have

$$\Delta_1=\left(\sum_{j=0}^{N} w_{j,j+1}+\sum_{j=1}^{N}\frac{\nu_j}{\alpha_j}\right)\prod_{n=1}^{N}\alpha_n,$$

$$\Omega_1=\left(-2w_{N,N+1}\beta_N+\beta_N\sum_{j=0}^{N} w_{j,j+1}+\beta_N\sum_{j=1}^{N-1}\frac{\nu_j}{\alpha_j}+\nu_N\right)\prod_{n=1}^{N-1}\alpha_n.$$

Using

$$\beta_N\Delta_1-\alpha_N\Omega_1=2w_{N,N+1}\beta_N\prod_{j=1}^{N}\alpha_j+\nu_N(\beta_N-\alpha_N)\prod_{j=1}^{N-1}\alpha_j,$$

we get

$$\nu_N=\frac{1}{\alpha_N-\beta_N}\left[2w_{N,N+1}\alpha_N\beta_N+\frac{\alpha_N\Omega_1-\beta_N\Delta_1}{\Pi_{j=1}^{N-1}\alpha_j}\right].$$

After obtaining ν_N, we can recover ν_{N-1} as follows. The solution of the Marchenko equation in the interval $(y_N,+\infty)$ yields $V_{N,N+1}(y)$ by (7.9); thus also we have the matrix $\Lambda_{N,N+1}(k)$ defined in (4.1) because it is determined by the scattering matrix of the potential $V_{N,N+1}(y)$. Note that from the unitarity of the scattering matrix corresponding to the potential $V_{j,j+1}(y)$, we have $\det\Lambda_{j,j+1}(k)=1$. Using (2.16) it can be shown that $\det F_j(k)=1$. Thus, we can easily form the matrix $\Lambda\Lambda_{N,N+1}^{-1}F_N^{-1}$ and recover ν_{N-1} from this matrix, as we have recovered ν_N from the matrix Λ. Note that the reduced reflection coefficient from the right associated with the matrix $\Lambda\Lambda_{N,N+1}^{-1}F_N^{-1}$ is given by

$$\rho^{[N-1]}(k)=-\frac{[1\quad 0]\Lambda\Lambda_{N,N+1}^{-1}F_N^{-1}\begin{bmatrix}0\\1\end{bmatrix}}{[1\quad 0]\Lambda\Lambda_{N,N+1}^{-1}F_N^{-1}\begin{bmatrix}1\\0\end{bmatrix}}. \tag{5.11}$$

Once ν_{N-1} is obtained, we recursively get the remaining $\nu_{N-2},\ldots,\nu_1$.

VI. A SINGULAR INTEGRAL EQUATION

In this section, when there are no bound states, we formulate the singular integral equation (6.7) whose kernel and nonhomogeneous term are determined by the reduced reflection coefficient $\rho(k)$. We also show that (6.7) is uniquely solvable and its solution leads to the recovery of $H(x)$. In a similar manner, we formulate the singular integral equation (6.10) in terms of $\mathscr{l}(\mathrm{k})$ and prove its unique solvability and show that its solution also leads to the recovery of $H(x)$.

For each fixed $y\in\mathbf{R}\backslash\{y_1,\ldots,y_N\}$, from (5.11) of Ref. 1, we have

$$\begin{bmatrix}Z_l(-k,y)\\Z_r(-k,y)\end{bmatrix}=\begin{bmatrix}\tau(k) & -\rho(k)e^{2iky}\\-\mathscr{l}(k)e^{-2iky} & \tau(k)\end{bmatrix}\begin{bmatrix}Z_r(k,y)\\Z_l(k,y)\end{bmatrix},\quad k\in\mathbf{R}. \tag{6.1}$$

Using (2.19)–(2.21) and (3.3), we obtain

$$\begin{bmatrix} J_l(-k,y) \\ J_r(-k,y) \end{bmatrix} = \begin{bmatrix} \dfrac{1}{a(k)} & \dfrac{b(k)}{a(k)}\, e^{2iky} \\ -\dfrac{b(-k)}{a(k)}\, e^{-2iky} & \dfrac{1}{a(k)} \end{bmatrix} \begin{bmatrix} J_r(k,y) \\ J_l(k,y) \end{bmatrix}, \quad k \in \mathbf{R}. \tag{6.2}$$

Subtracting (6.2) from (6.1), we get

$$Z_l(-k,y) - J_l(-k,y) = \left[\tau(k) - \frac{1}{a(k)} \right] Z_r(k,y) + \frac{1}{a(k)} \left[Z_r(k,y) - J_r(k,y) \right] - \rho(k) e^{2iky} \left[Z_l(k,y) - J_l(k,y) \right] - \left[\rho(k) + \frac{b(k)}{a(k)} \right] e^{2iky} J_l(k,y), \tag{6.3}$$

$$Z_r(-k,y) - J_r(-k,y) = \left[\tau(k) - \frac{1}{a(k)} \right] Z_l(k,y) + \frac{1}{a(k)} \left[Z_l(k,y) - J_l(k,y) \right] - \ell(k) e^{-2iky} \left[Z_r(k,y) - J_r(k,y) \right] - \left[\ell(k) - \frac{b(-k)}{a(k)} \right] e^{-2iky} J_r(k,y). \tag{6.4}$$

Let us analyze (6.3). Using Propositions 2.1 and 3.1 and Theorem 3.2, for each fixed y, in the absence of bound states, of the four terms on the right-hand side, we see that the first two belong to the Hardy space $\mathbf{H}^2_+(\mathbf{R})$ and the last two belong to $L^2(\mathbf{R})$; the term on the left-hand side belongs to $\mathbf{H}^2_-(\mathbf{R})$. Let $\Pi_\pm$ denote the orthogonal projection operators from $L^2(\mathbf{R})$ onto $\mathbf{H}^2_\pm(\mathbf{R})$, i.e.

$$(\Pi_\pm f\,)(k) = \frac{\pm 1}{2\pi i} \int_{-\infty}^{\infty} \frac{ds}{s - k \mp i0}\, f(s).$$

Let us define

$$X_l(k,y) = Z_l(-k,y) - J_l(-k,y), \quad X_r(k,y) = Z_r(-k,y) - J_r(-k,y). \tag{6.5}$$

Applying the projection Π_- on both sides of (6.3), we obtain

$$X_l(\cdot\,,y) + \Pi_-(\rho e^{2i(\cdot)y} \mathscr{F} X_l(\cdot\,,y)) = -\Pi_- \left(\left[\rho + \frac{b}{a} \right] e^{2i(\cdot)y} J_l(\cdot\,,y) \right), \tag{6.6}$$

where $(\mathscr{F} f\,)(k) = f(-k)$. Note that (6.6) is a singular integral equation and can be written as

$$X_l(k,y) + (\mathscr{O}_l X_l)(k,y) = P_l(k,y), \quad k \in \mathbf{R}, \tag{6.7}$$

where we have defined

$$(\mathscr{O}_l X)(k) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{ds}{s + k - i0}\, \rho(-s) e^{-2isy} X(s), \quad k \in \mathbf{R}, \tag{6.8}$$

$$P_l(k,y) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{ds}{s - k + i0} \left[\rho(s) + \frac{b(s)}{a(s)} \right] e^{2isy} J_l(s,y). \tag{6.9}$$

Notice that the integral operator $\mathscr{O}_l$ defined in (6.8) is the same as the operator defined in (5.23) of Ref. 1. Comparing (5.21) of Ref. 1 and (6.7), we see that the kernels in these two integral equations differ by a minus sign. We also recall that the solution of the singular integral equation of Ref. 1 is given by $X_l(k,y) = [Z_l(-k,y) - Z_l(0,y)]/[k\sqrt{H(x)}]$, where $Z_l(k,y)$ is the quantity defined in (3.1), whereas the solution of the integral equation of this paper is given by (6.5). The factor $1/k$ in the expression for $X_l(k,y)$ used in Ref. 1 was introduced to ensure that $X_l(k,y)$ belongs to an appropriate Hardy space, namely to $\mathbf{H}_-^p(\mathbf{R})$ if $p<1/(1-\alpha)$. However, this factor, while providing the desired behavior as $k\to\infty$, introduced some complications at $k=0$. With the present definition (6.5) it is easy to show that $X_l(k,y)$ is continuous as $k\to 0$ in $\overline{\mathbf{C}^+}$ and $X_l(k,y)=O(1/k)$ as $k\to\infty$ in $\overline{\mathbf{C}^+}$, without imposing any stronger condition on $Q(x)$ than $Q\in L_1^1(\mathbf{R})$.

In a similar manner, in the absence of bound states, from (6.4) we obtain

$$X_r(\cdot,y)+\Pi_-(\mathscr{C}e^{-2i(\cdot)y}\mathscr{F}X_r(\cdot,y))=-\Pi_-\left(\left[\mathscr{C}-\frac{\mathscr{F}b}{a}\right]e^{-2i(\cdot)y}J_r(\cdot,y)\right),$$

which is equivalent to

$$X_r(k,y)+(\mathscr{O}_rX_r)(k,y)=P_r(k,y),\quad k\in\mathbf{R}, \tag{6.10}$$

where we have defined

$$(\mathscr{O}_rX)(k)=\frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{ds}{s+k-i0}\,\mathscr{C}(-s)e^{2isy}X(s),\quad k\in\mathbf{R},$$

$$P_r(k,y)=\frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{ds}{s-k+i0}\left[\mathscr{C}(s)-\frac{b(-s)}{a(s)}\right]e^{-2isy}J_r(s,y). \tag{6.11}$$

The solvability of (6.7) and (6.10) is analyzed in the next theorem.

Theorem 6.1: The singular integral equation (6.7) has a unique solution $X_l\in\mathbf{H}_-^2(\mathbf{R})$ for every nonhomogeneous term belonging to $\mathbf{H}_-^2(\mathbf{R})$, and the solution can be obtained through iteration. Similarly, (6.10) has a unique solution $X_r\in\mathbf{H}_-^2(\mathbf{R})$ for every nonhomogeneous term belonging to $\mathbf{H}_-^2(\mathbf{R})$ and the solution can be obtained through iteration.

Proof: The operator $\mathscr{O}_l$ defined in (6.8) is a strict contraction on $\mathbf{H}_-^2(\mathbf{R})$, which is proved in Theorem 7.1 of Ref. 1. Hence, (6.7) is uniquely solvable and its solution can be obtained through iteration. The proof for (6.10) is given in the same manner. ■

Next we will recover $H(x)$ from an appropriate set of scattering data. We will consider the generic and exceptional cases separately because the scattering data in these two cases are not the same.

Let us first consider the generic case; in this case an appropriate set of scattering data consists of $\{\rho(k),Q(x)\}$. We proceed as follows. Using the method of Ref. 16, from $\rho(k)$ we get $b(k)$ and $a(k)$; then from these we get N, $\{y_1,\ldots,y_N\}$, and $\{q_1,\ldots,q_N\}$ by using the method of Ref. 13. Hence, we have α_j and β_j for $j=1,\ldots,N$. Since $Q(x)$ is known, we also know the zero-energy Jost solutions of (1.5); these Jost solutions are identical to the zero-energy Jost solutions of (1.1). For example, we can get $f_l(0,x)$ by using (5.25) of Ref. 1. Next we obtain $J_l(k,y)$ using (3.4) and (3.5). Note that $J_l(k,y)$ is uniquely constructed from $\rho(k)$ because we already have y_j, α_j, and β_j for $j=1,\ldots,N$. From (3.1) and the fact that $H(x)=dy/dx$, we have

$$\frac{dy}{Z_l(0,y)^2}=H_+\,\frac{dx}{f_l(0,x)^2}. \tag{6.12}$$

Using $J_l(k,y)$ and $\rho(k)$ in (6.7), we obtain $X_l(k,y)$ uniquely. Then using (6.5), we write (6.12) in the form

$$\frac{dy}{[X_l(0,y)+J_l(0,y)]^2}=H_+\,\frac{dx}{f_l(0,x)^2}. \tag{6.13}$$

We get H_+ from (6.13) as

$$H_+=\frac{\int_{-\infty}^{0}dy/[X_l(0,y)+J_l(0,y)]^2}{\int_{-\infty}^{0}dx/f_l(0,x)^2}. \tag{6.14}$$

Note that both integrals in (6.14) converge because[17] in the generic case, $f_l(0,x)^2$ grows like x^2 as $x\to-\infty$ and $Z_l(0,y)^2$ grows like y^2 as $y\to-\infty$. Next, using a generalization of the method given in Theorem 5.1 of Ref. 13, we obtain $x_1,\ldots,x_N$. This is done as follows. If $N=1$ and $y_1=0$, then $x_1=0$. If $N=1$ and $y_1\neq0$, then we can proceed as in the case $N\geqslant2$. If $N\geqslant2$, then at least $N-1$ of the points $y_1,\ldots,y_N$ must be nonzero. If at least one of these is positive, we can pick the smallest of them, say y_p. Then x_p is uniquely determined by

$$\int_0^{y_p}\frac{dy}{[X_l(0,y)+J_l(0,y)]^2}=H_+\int_0^{x_p}\frac{dx}{f_l(0,x)^2}, \tag{6.15}$$

and we recursively determine $x_{p+1},\ldots,x_N$ using

$$\int_{y_p}^{y_{p+1}}\frac{dy}{[X_l(0,y)+J_l(0,y)]^2}=H_+\int_{x_p}^{x_{p+1}}\frac{dx}{f_l(0,x)^2}.$$

Similarly, we can determine $x_{p-1},x_{p-2},\ldots,x_1$. If all y_j are nonpositive, then we pick the one with the smallest absolute value that is nonzero (either y_N or y_{N-1}) and find the corresponding x_j by using the appropriate integral of the form (6.15). Having found each x_j corresponding to y_j, we obtain $y(x)$ by solving the first-order separable ordinary differential equation (6.13) with the initial condition $y(x_i)=y_i$. Having $y(x)$ in each interval (x_j,x_{j+1}), we get $H(x)=dy/dx$.

Now let us consider the exceptional case. In this case, we cannot use (6.14) to obtain H_+. In fact, for the unique recovery of $H(x)$ we need to include H_+ in the scattering data; otherwise, we get a one-parameter family of $H(x)$ corresponding to the set $\{\rho(k),Q(x)\}$. Thus, in the exceptional case, we recover $H(x)$ from the scattering data $\{\rho(k),H_+,Q(x)\}$ by the method outlined in the generic case.

Note that one can also recover $H(x)$ from the solution of the singular integral equation (6.10) using the scattering data $\{\mathscr{A}(k),Q(x)\}$ in the generic case and using $\{\mathscr{A}(k),Q(x),H_+\}$ in the exceptional case. One then needs to solve the analog of (6.12) given by

$$\frac{dy}{Z_r(0,y)^2}=H_-\,\frac{dx}{f_r(0,x)^2}, \tag{6.16}$$

with the condition $y(0)=0$. Note that from (6.5) we have $Z_r(0,y)=X_r(0,y)+J_r(0,y)$, and $f_r(0,x)$ is the zero-energy Jost solution from the right of (1.5) corresponding to $Q(x)$. The potential $Q(x)$ uniquely determines[14,18–20] $f_r(0,x)$, for example, by

$$f_r(0,x)=1+\int_{-\infty}^{x}dz\;(x-z)Q(z)f_r(0,z). \tag{6.17}$$

Once we obtain y as a function of x from (6.16), we recover $H(x)$ as

$$H(x)=H_- \frac{Z_r(0,y)^2}{f_r(0,x)^2}. \tag{6.18}$$

Note that, in the exceptional case, H_- can be expressed in terms of H_+ by using (5.29) of Ref. 1, namely,

$$H_-=H_+ \frac{1-\rho(0)}{1+\rho(0)} \left(\frac{1+R^{[0]}(0)}{T^{[0]}(0)} \right)^2, \tag{6.19}$$

where $R^{[0]}(k)$ and $T^{[0]}(k)$ are the reflection coefficient from the right and the transmission coefficient, respectively, associated with (1.5). Hence, in the exceptional case, one can use H_- in the scattering data instead of H_+ because of (6.19). Note also that in the exceptional case $f_l(0,x)$ and $f_r(0,x)$ are linearly dependent, and we have[17]

$$f_r(0,x)= \frac{1+R^{[0]}(0)}{T^{[0]}(0)} f_l(0,x). \tag{6.20}$$

Let $f_l^{[0]}(k,x)$ and $f_r^{[0]}(k,x)$ denote the Jost solutions of (1.5) from the left and from the right, respectively. In the generic case we have

$$f_r^{[0]}(k,x)=[f_l^{[0]}(k,x);f_r^{[0]}(k,x)]f_l^{[0]}(k,x) \int_{-\infty}^{x} \frac{dz}{f_l^{[0]}(k,z)^2}, \tag{6.21}$$

where the Wronskian $[f_l^{[0]}(k,x);f_r^{[0]}(k,x)]$ is equal to $-2ik/T^{[0]}(k)$. Hence, in the generic case from (6.21), after using the fact that $f_l^{[0]}(0,x)=f_l(0,x)$ and $f_r^{[0]}(0,x)=f_r(0,x)$, we have

$$f_r(0,x)= \left[\lim_{k\to 0} \frac{-2ik}{T^{[0]}(k)} \right] f_l(0,x) \int_{-\infty}^{x} \frac{dz}{f_l(0,z)^2}.$$

VII. MARCHENKO INTEGRAL EQUATION

In this section we show that the singular integral equation (6.7), with the use of the Fourier transform, can be transformed into the integral equation (7.7) generalizing the Marchenko integral equation[14,18–20] for the one-dimensional Schrödinger equation. We establish the unique solvability of (7.7) and describe how its solution leads to the recovery of $H(x)$.

Using (2.20) and the continuity of $\rho(k)$ and $b(k)/a(k)$, we see that $\rho+(b/a)\in L^p(\mathbf{R})$ for any $p\in(1,+\infty]$. We may then write

$$\rho(k)=-\frac{b(k)}{a(k)}+\int_{-\infty}^{\infty} dz\ e^{ikz}\varrho(z), \tag{7.1}$$

where $\varrho\in L^q(\mathbf{R})$ for $q\in[2,+\infty)$. The symmetry relation $F(-k)=\overline{F(k)}$ for $k\in\mathbf{R}$ valid for ρ, a, and b, implies that ϱ is real valued. Since b/a belongs to AP^W, we have $b(k)/a(k) = -\Sigma_s \gamma_s e^{ikb_s}$ where b_s are different real numbers and γ_s are real constants satisfying $\Sigma_s|\gamma_s|<+\infty$; thus we can write (7.1) in the form

$$\rho(k)=\sum_s \gamma_s e^{ikb_s}+\int_{-\infty}^{\infty} dz\ e^{ikz}\varrho(z). \tag{7.2}$$

Let us write (7.2) in the concise form

$$\rho(k)=\int_{-\infty}^{\infty} d\mu(t)\ e^{ikt}, \tag{7.3}$$

for a suitable real measure μ that is the sum of a discrete measure (with weights γ_s at the points b_s) and an absolutely continuous measure (with a Radon-Nikodym derivative ϱ). Let $\mathscr{F}$ denote the Fourier transform defined by

$$(\mathscr{F}g)(t)=\frac{1}{2\pi}\int_{-\infty}^{\infty} dk\ e^{ikt}g(k). \tag{7.4}$$

Since $X_l(\cdot,y)$ and $P_l(\cdot,y)$ appearing in (6.7) belong to $\mathbf{H}_-^2(\mathbf{R})$, their Fourier transforms are supported on the positive half-line; hence, we have

$$X_l(k,y)=\int_0^{\infty} dt\ e^{-ikt}h_l(t,y), \quad P_l(k,y)=\int_0^{\infty} dt\ e^{-ikt}h_{l0}(t,y), \tag{7.5}$$

where $h_l, h_{l0}\in L^q(\mathbf{R}^+)$ for any $q\in[2,+\infty)$. Furthermore, as seen from (3.16), $J_l(k,y)$ consists of a finite sum of exponential terms; hence we have $J_l(k,y)=\Sigma_s\omega_s(y)e^{ik\zeta_s(y)}$, where, in each interval (y_j,y_{j+1}), $\omega_s(y)$ is a constant and $\zeta_s(y)$ is either a constant or an affine function of y. Thus, from (6.9) we obtain

$$h_{l0}(t,y)=-\sum_s\ \omega_s(y)\varrho(-t-2y-\zeta_s(y)), \quad t\geqslant 0.$$

Now let us take the Fourier transform of both sides of (6.7). We have

$$h_l(\cdot,y)+(\mathscr{F}\mathscr{O}_l\mathscr{F}^{-1}h_l)(\cdot,y)=h_{l0}(\cdot,y). \tag{7.6}$$

Using (7.2) or (7.3) we can write (7.6) as the Marchenko-like integral equation

$$h_l(t,y)+\int_{-\infty}^{-(t+2y)} d\mu(z)\ h_l(-z-t-2y,y)=h_{l0}(t,y), \quad t\geqslant 0,$$

or equivalently

$$h_l(t,y)+\sum_{\{s:b_s<-t-2y\}}\gamma_s h_l(-t-2y-b_s,y)+\int_0^{\infty} ds\ \varrho(-s-t-2y)\ h_l(s,y)=h_{l0}(t,y), \quad t\geqslant 0. \tag{7.7}$$

We will call (7.7) a Marchenko equation. Note that when $N=0$, i.e. when $V(y)$ given in (2.3) is well defined for all $y\in\mathbf{R}$, the integral equation (7.7) reduces to

$$h_l(t,y)+\int_0^{\infty} ds\ \varrho(-s-t-2y)\ \ h_l(s,y)=-\varrho(-t-2y), \quad t\geqslant 0, \tag{7.8}$$

which is the Marchenko equation[14,18–20] for the ordinary Schrödinger equation. In a similar manner we can also obtain a Marchenko integral equation associated with the reflection coefficient ℓ(k), but we will not list it here. The next theorem shows that (7.7) is uniquely solvable.

Theorem 7.1: Equation (7.7) has a unique solution in $L^2(\mathbf{R}^+)$ for every nonhomogeneous term belonging to $L^2(\mathbf{R}^+)$, and the solution can be obtained through iteration.

Proof: The operator $\mathscr{O}_l$ in (7.6) is a strict contraction on $\mathbf{H}_-^2(\mathbf{R})$, as indicated in the proof of Theorem 6.1. Considering $L^2(\mathbf{R}^+)$ and $\mathbf{H}_-^2(\mathbf{R})$ as subspaces of $L^2(\mathbf{R})$, we see that $\sqrt{2\pi}\mathscr{F}$, where

$\mathscr{F}$ is the Fourier transformation defined in (7.4), is a unitary operator on $L^2(\mathbf{R})$ mapping $\mathbf{H}_-^2(\mathbf{R})$ onto $L^2(\mathbf{R}^+)$. Thus, the operator $\mathscr{F}\mathscr{O}_l\mathscr{F}^{-1}$ acting from $L^2(\mathbf{R}^+)$ into $L^2(\mathbf{R}^+)$ is a strict contraction. Hence, (7.7) is uniquely solvable and its solution can be obtained through iteration. ■

Let us now discuss the recovery of $H(x)$ from the solution of the Marchenko equation (7.7). Once $h_l(t,y)$ is obtained from (7.7), we can get $X_l(k,y)$ from (7.5) and recover $H(x)$ by repeating the procedure described in Sec. VI.

Let us also describe another way to recover $H(x)$. This is done in conjunction with the algorithm described in Sec. V, where N, y_j, q_j, are recovered first; recall that these are the parameters associated with the ''hard scatterers.'' Next we recover the quantities associated with the ''soft scatterers,'' namely we obtain $V_{j,j+1}(y)$. This is done recursively as follows. First we solve (7.7) only for $y>y_N$ and get $h_l(t,y)$ in the interval $(y_N,+\infty)$. Because of (3.8) we obtain[21]

$$V_{N,N+1}(y)=-2\,\frac{dh_l(0+,y)}{dy}, \quad y_N<y<+\infty, \tag{7.9}$$

$$Z_l(0,y)=1+\int_y^\infty dz\ (z-y)V_{N,N+1}(z)\ Z_l(0,z), \quad y_N<y<+\infty. \tag{7.10}$$

Then, as described in Sec. V, we form the new reduced reflection coefficient $\rho^{[N-1]}(k)$ defined in (5.11) and obtain $V_{N-1,N}(y)$ from the solution of the Marchenko equation corresponding to $\rho^{[N-1]}(k)$ by using the analog of (7.9). Continuing in this manner, we then recover $V_{j,j+1}(y)$ for $j=0,1,\ldots,N$. Then we obtain $Z_l(0,y)$ for $y\in\mathbf{R}\backslash\{y_1,\ldots,y_N\}$ as follows. From (3.1) we have

$$Z_l(k,y_j-0)=\sqrt{q_j}\ Z_l(k,y_j+0),$$

$$Z_l'(k,y_j-0)=\frac{Z_l'(k,y_j+0)}{\sqrt{q_j}}-2ik\left(\beta_j-\frac{\nu_j}{2ik}\right)Z_l(k,y_j+0),$$

as well as $Z_l(k,+\infty)=1$ and $Z_l'(k,+\infty)=0$. Hence, $Z_l(0,y)$ and $Z_l'(0,y)$ satisfy the following internal boundary conditions:

$$Z_l(0,y_j-0)=\sqrt{q_j}\ Z_l(0,y_j+0), \tag{7.11}$$

$$Z_l'(0,y_j-0)=\frac{Z_l'(0,y_j+0)}{\sqrt{q_j}}+\nu_j\ Z_l(0,y_j-0). \tag{7.12}$$

Thus, in each interval (y_j,y_{j+1}), we can uniquely obtain $Z_l(0,y)$ from $V_{j,j+1}(y)$ by using

$$Z_l(0,y)=(y-y_{j+1})Z_l'(0,y_{j+1}-0)+Z_l(0,y_{j+1}-0)+\int_y^{y_{j+1}}dz\ (z-y)V(z)\ Z_l(0,z). \tag{7.13}$$

Thus, using (7.10), (7.11)–(7.13) we obtain $Z_l(0,y)$ for $y\in\mathbf{R}\backslash\{y_1,\ldots,y_N\}$. Once we have $Z_l(0,y)$, we can recover $H(x)$ by using the procedure outlined starting with (6.12).

Note that although we assume that there are no bound states associated with (1.1), some of the $V_{j,j+1}(y)$ may have bound states. In terms of the factorization formula (4.5), this happens when the hard scatterers $F_j(k)$ in (4.5) overcome the bound states from the soft scatterers $\Lambda_{j,j+1}(k)$, resulting in no bound states for (1.1); in other words, the poles of $t_{j,j+1}(k)$ in $\mathbf{C}^+$ are canceled by the terms in $F_j(k)$, resulting in no poles in $\mathbf{C}^+$ for $\tau(k)$. The recovery of $V_{j,j+1}(y)$, even in the presence of bound states, is well understood;[22] since each $V_{j,j+1}(y)$ has support contained in a

half-line, the reflection coefficient $r_{j,j+1}(k)$ uniquely determines $V_{j,j+1}(y)$ without needing the bound state energies and the bound state norming constants; in fact, both the bound state energies and the norming constants are uniquely determined by $r_{j,j+1}(k)$ alone.

We can also obtain $H(x)$ by modifying the procedures described earlier. For example, using the reduced reflection coefficient from the left ℓ(k), the analog of (7.7) associated with ℓ(k) can be used to obtain $V_{j,j+1}(y)$ starting with the interval (y_0,y_1) and moving to the interval (y_1,y_2) and continuing in this manner. One can also solve the Marchenko equations associated with ℓ(k) and $\rho(k)$, respectively, simultaneously starting with the intervals (y_0,y_1) and (y_N,y_{N+1}), respectively, and moving to the intervals (y_1,y_2) and (y_{N-1},y_N), respectively, and continuing in this manner until all $V_{j,j+1}(y)$ are obtained. Then, using (7.11)–(7.13) one gets $Z_l(0,y)$ or $Z_r(0,y)$, from which $H(x)$ is obtained using (6.12) or (6.16).

VIII. EXAMPLES

In this section we illustrate the methods described in Secs. V–VII through explicitly solved examples. In Examples 8.1–8.3 we illustrate the recovery of $H(x)$ using the solution of the Marchenko integral equation (7.7). In Example 8.4 we illustrate the method of Sec. V to recover the discontinuities in $H'(x)/H(x)$. In Example 8.5 we illustrate the alternative procedure described in Sec. VII using (5.11). Finally, In Example 8.6 we illustrate the recovery of $H(x)$ in terms of the solutions of the singular integral equations (6.7) and (6.10).

Example 8.1: Let us demonstrate the Marchenko method of Sec. VII. As our scattering data, for a given $Q(x)$ with no bound states and a given H_+, let us use

$$\rho(k)=\epsilon\,\frac{k+i\alpha}{k+i\gamma}, \tag{8.1}$$

where ϵ, α, and γ are real constants satisfying $-1<\epsilon<1$, $\gamma>0$, and $\gamma^2>\alpha^2\epsilon^2$. It is straightforward but tedious to show that for $y\leqslant 0$ the denominator in (8.11) and (8.12) is nonzero if and only if $(\alpha+\beta)\epsilon\neq 0$. Thus, in this example, we assume $(\alpha+\beta)\epsilon\neq 0$ and postpone the case $(\alpha+\beta)\epsilon=0$ to Example 8.2. Using the method of Ref. 16 we construct $\tau(k)$ by solving the Wiener-Hopf factorization problem $\tau(k)\tau(-k)=1-|\rho(k)|^2$ for $k\in\mathbf{R}$, and we obtain

$$\tau(k)=\sqrt{1-\epsilon^2}\,\frac{k+i\beta}{k+i\gamma}, \tag{8.2}$$

where we have defined the positive constant

$$\beta=\sqrt{\frac{\gamma^2-\alpha^2\epsilon^2}{1-\epsilon^2}}. \tag{8.3}$$

It can be verified that $|\tau(k)|^2+|\rho(k)|^2=1$ and that $\tau(k)$ has no poles or zeros in $\mathbf{C}^+$. Since $\tau(0)\neq 0$, we are in the exceptional case. Using the method of Ref. 13, we obtain

$$N=1,\quad q_1=\frac{1-\epsilon}{1+\epsilon},\quad y_1=0,\quad a(k)=\frac{1}{\sqrt{1-\epsilon^2}},\quad b(k)=-\frac{\epsilon}{\sqrt{1-\epsilon^2}}. \tag{8.4}$$

From (3.16) we get

$$J_l(k,y)=\begin{cases}\dfrac{1-\epsilon e^{-2iky}}{\sqrt{1-\epsilon^2}}, & y<0,\\ 1, & y>0.\end{cases} \tag{8.5}$$

Thus, from (6.9) we obtain

$$P_l(k,y)=\begin{cases}\dfrac{i\epsilon}{k+i\gamma}\,(\alpha-\gamma)\sqrt{1-e^2}\,[e^{2\gamma y}-e^{2iky}], & y<0,\\ 0, & y>0.\end{cases} \tag{8.6}$$

Using (8.6) in (7.5) we have

$$h_{l0}(t,y)=\begin{cases}-\dfrac{\epsilon(\alpha-\gamma)}{\sqrt{1-\epsilon^2}}\,e^{\gamma(t+2y)}, & t>0, \quad t+2y<0,\\ 0, & t>0, \quad t+2y>0.\end{cases}$$

From (8.1) we see that we can write (7.2) as

$$\rho(k)=\epsilon+\int_{-\infty}^{\infty}dt\; e^{ikt}\varrho(t),$$

with

$$\varrho(t)=\begin{cases}0, & t<0\\ \epsilon(\alpha-\gamma)e^{-\gamma t}, & t>0,\end{cases} \tag{8.7}$$

and hence $\varrho(t)$ is supported only on $t\geqslant 0$. The Marchenko equation (7.7) has the following form:

$$h_l(t,y)=0, \quad t>0, \quad t+2y>0, \tag{8.8}$$

$$h_l(t,y)+\epsilon h_l(-t-2y,y)+\epsilon(\alpha-\gamma)e^{\gamma(t+2y)}\int_0^{-(t+2y)}ds\; e^{\gamma s}h_l(s,y)=-\frac{\epsilon(\alpha-\gamma)}{\sqrt{1-\epsilon^2}}\,e^{\gamma(t+2y)},$$

$$t>0, \quad t+2y<0. \tag{8.9}$$

Notice that from (8.8) we obtain $X_l(k,y)=0$ for $y>0$, and hence using (8.1) and (8.5), from (6.13) we conclude that

$$H(x)=\frac{H_+}{f_l(0,x)^2}, \quad y=H_+\int_0^x\frac{dz}{f_l(0,z)^2}, \quad x>0, \tag{8.10}$$

where $f_l(0,x)$ is the zero-energy Jost solution from the left associated with $Q(x)$. We can solve (8.9) exactly and obtain

$$h_l(t,y)=\frac{(\beta^2-\gamma^2)e^{\beta t}+\epsilon(\gamma-\beta)(\alpha+\beta)e^{-\beta(t+2y)}}{\sqrt{1-e^2}[(\alpha+\beta)\epsilon e^{-2\beta y}+\beta-\gamma]}, \quad t>0, \quad t+2y<0, \tag{8.11}$$

where β is the constant in (8.3) and the denominator does not vanish. Using (8.11) in (7.5), for $y<0$, we get

$$X_l(k,y)=\frac{(\beta+ik)(\beta^2-\gamma^2)[e^{2y(ik-\beta)}-1]+(\beta-ik)\epsilon(\gamma-\beta)(\alpha+\beta)e^{-2\beta y}[1-e^{2y(\beta+ik)}]}{(k^2+\beta^2)\sqrt{1-\epsilon^2}[(\alpha+\beta)\epsilon e^{-2\beta y}+\beta-\gamma]}. \tag{8.12}$$

Hence, using (8.5) and (8.12), we find

$$Z_l(0,y)=\sqrt{\frac{\gamma-\epsilon\alpha}{\gamma+\epsilon\alpha}}\,\frac{\epsilon(\alpha+\beta)e^{-2\beta y}+\gamma-\beta}{\epsilon(\alpha+\beta)e^{-2\beta y}-y+\beta}, \quad y<0. \tag{8.13}$$

Using (8.13) in (6.12), we obtain

$$\frac{\gamma+\epsilon\alpha}{\gamma-\epsilon\alpha}\left[y+\frac{2(\gamma-\beta)/\beta}{\epsilon(\alpha+\beta)+\gamma-\beta}-\frac{2(\gamma-\beta)/\beta}{\epsilon(\alpha+\beta)e^{-2\beta y}+\gamma-\beta}\right]=H_+\int_0^x\frac{dz}{f_l(0,z)^2}, \quad y<0, \tag{8.14}$$

$$H(x)=\frac{H_+}{f_l(0,x)^2}\,\frac{\gamma-\epsilon\alpha}{\gamma+\epsilon\alpha}\left[\frac{\epsilon(\alpha+\beta)e^{-2\beta y}+\gamma-\beta}{\epsilon(\alpha+\beta)e^{-2\beta y}-\gamma+\beta}\right]^2, \quad y<0, \tag{8.15}$$

where y in (8.15) is obtained in terms of x from (8.14).

Example 8.2: In this example we consider the same scattering data as in Example 8.1 but with the additional condition $(\alpha+\beta)\epsilon=0$, where β is the constant in (8.3). If $\epsilon=0$ then $\rho(k)=0$ and $\tau(k)=1$, and the Marchenko equation (7.7) gives us $h_l(t,y)=0$ for $t>0$ and $y\in\mathbf{R}$; thus, there are no discontinuities in $H(x)$ or $H'(x)/H(x)$, and we have

$$H(x)=\frac{H_+}{f_l(0,x)^2}, \quad x\in\mathbf{R}.$$

If $\beta=-\alpha$ but $\epsilon\neq0$, then $\gamma=\beta$; in this case we have

$$\rho(k)=\epsilon\,\frac{k-i\gamma}{k+i\gamma}, \quad \tau(k)=\sqrt{1-\epsilon^2}.$$

In this case, for $x>0$, (8.10) is still valid. When $x<0$, we proceed as follows. In the Marchenko equation (8.9), putting $\alpha=-\gamma$, we obtain

$$h_l(t,y)+\epsilon h_l(-t-2y,y)-2\gamma\epsilon e^{\gamma(t+2y)}\int_0^{-(t+2y)}ds\;e^{\gamma s}h_l(s,y)=\frac{2\epsilon\gamma}{\sqrt{1-\epsilon^2}}\,e^{\gamma(t+2y)},$$

$$t>0, \quad t+2y<0. \tag{8.16}$$

The solution of (8.16) is given by

$$h_l(t,y)=\frac{2\epsilon\gamma}{\sqrt{1-\epsilon^2}}\,\frac{e^{\gamma(t+2y)}}{1+\epsilon e^{2\gamma y}}, \quad t>0, \quad t+2y<0. \tag{8.17}$$

Using (6.5), (7.5), (8.5), (8.8), and (8.17), we obtain

$$Z_l(0,y)=\sqrt{\frac{1+\epsilon}{1-\epsilon}}\,\frac{1-\epsilon e^{2\gamma y}}{1+\epsilon e^{2\gamma y}}, \quad y<0. \tag{8.18}$$

Using (8.18) in (6.12), we obtain

$$\frac{1-\epsilon}{1+\epsilon}\left[y+\frac{2/\gamma}{1-\epsilon e^{2\gamma y}}-\frac{2/\gamma}{1-\epsilon}\right]=H_+\int_0^x\frac{dz}{f_l(0,z)^2}, \quad x<0, \tag{8.19}$$

$$H(x)=\frac{H_+}{f_l(0,x)^2}\,\frac{1+\epsilon}{1-\epsilon}\left(\frac{1-\epsilon e^{2\gamma y}}{1+\epsilon e^{2\gamma y}}\right)^2, \quad y<0, \tag{8.20}$$

where y in (8.20) is obtained in terms of x from (8.19).

Example 8.3: In this example, we consider the scattering data of Example 8.1 with $\gamma^2=\alpha^2\epsilon^2$. When $\gamma=\pm\alpha\epsilon$, we have $\beta=0$, and hence $\rho(k)=(\epsilon k\pm i\gamma)/(k+i\gamma)$. Since $\rho(0)=+1$ is not allowed (cf. Theorem 4.2 of Ref. 1), we cannot have $\gamma=+\alpha\epsilon$. Thus, the inverse scattering problem to be solved corresponds to the scattering data

$$\rho(k)=\frac{\epsilon k-i\gamma}{k+i\gamma}, \quad Q(x),$$

when there are no bound states. We have $\tau(k)=\sqrt{1-\epsilon^2}k/(k+i\gamma)$, and hence this corresponds to the generic case; thus H_+ cannot be specified arbitrarily in the scattering data, and it is determined as in (6.14). In this case, (8.8) still holds. Putting $\alpha=-\gamma/\epsilon$ in (8.9), we obtain

$$h_l(t,y)+\epsilon h_l(-t-2y,y)-\gamma(1+\epsilon)e^{\gamma(t+2y)}\int_0^{-(t+2y)} ds\; e^{\gamma s}h_l(s,y)=\frac{\gamma(1+\epsilon)}{\sqrt{1-\epsilon^2}}\,e^{\gamma(t+2y)},$$

$$t>0, \quad t+2y<0. \tag{8.21}$$

The solution of (8.21) is given by

$$h_l(t,y)=\frac{\gamma}{\sqrt{1-\epsilon^2}}, \quad t>0, \quad t+2y<0. \tag{8.22}$$

Using (7.5), (8.5), (8.8), and (8.22), we obtain

$$Z_l(0,y)=\frac{1-\epsilon-2\gamma y}{\sqrt{1-\epsilon^2}}, \quad y<0. \tag{8.23}$$

Using (8.23) in (6.12), we have

$$\frac{(1+\epsilon)y}{1-\epsilon-2\gamma y}=H_+\int_0^x\frac{dz}{f_l(0,z)^2}, \quad x<0. \tag{8.24}$$

Letting $x,y\to-\infty$ in (8.24), as in (6.14), we get

$$H_+=\frac{1+\epsilon}{2\gamma\int_{-\infty}^0 dz/f_l(0,z)^2}. \tag{8.25}$$

Thus, from (8.24) and (8.25) we find

$$y=\frac{1-\epsilon}{2\gamma}\,\frac{\int_0^x dz/f_l(0,z)^2}{\int_{-\infty}^x dz/f_l(0,z)^2}, \quad x<0,$$

$$H(x)=\frac{1-\epsilon}{2\gamma f_l(0,x)^2}\,\frac{\int_{-\infty}^0 dz/f_l(0,z)^2}{[\int_{-\infty}^x dz/f_l(0,z)^2]^2}, \quad x<0. \tag{8.26}$$

Alternatively, by using (6.21) we can write (8.26) as

$$H(x)=\frac{(1-\epsilon)[f_l^{[0]}(0,x);f_r^{[0]}(0,x)]^2}{2\gamma}\,\frac{\int_{-\infty}^{0} dz/f_l(0,z)^2}{f_r(0,x)^2},\quad x<0.$$

This expression agrees with that obtained in (6.51) of Example 6.2 in Ref. 1, but the method used here is simpler.

Example 8.4: In this example we describe how to obtain ν_j defined in (4.4) related to discontinuities in $H'(x)/H(x)$ using the method outlined in Sec. V. Let us use the scattering data of Example 8.1, and hence $\rho(k)$ is given by (8.1) and $\pi(k)$ is given by (8.2). We proceed as in Example 8.1 until (8.7); we then set up the Marchenko equation only for $y>0$, which, by (8.8), yields $h_l(t,y)=0$. At this point we can conclude that $V_{1,2}(y)=0$ and hence $w_{1,2}=0$. Using (5.2)–(5.5), we obtain

$$\Delta_1=\frac{2(\beta-\gamma)}{\sqrt{1-\epsilon^2}},\quad \Omega_1=\frac{2\epsilon(\alpha-\beta)}{\sqrt{1-\epsilon^2}}.$$

Thus, from (5.6) we get

$$\nu_1=\frac{2\epsilon(\alpha-\gamma)}{(1+\epsilon)\sqrt{1-\epsilon^2}}\,. \tag{8.27}$$

Hence, $H'(x)/H(x)$ is continuous at $x=0$ if and only if $\epsilon(\alpha-\gamma)=0$, i.e. if and only if $\rho(k)$ in (8.1) is a constant.

Example 8.5: In this example we illustrate the iterative method outlined in Sec. VII to recover $H(x)$, based on the matrix factorization in (4.5). Let us again use the scattering data of Example 8.1. We proceed as in Example 8.4 and get $H(x)$ given in (8.10) for $x>0$, $V_{1,2}(y)=0$, and ν_1 given in (8.27). Thus, we have $\Lambda_{1,2}=\mathbf{I}$ and

$$F_1(k)=\frac{1}{\sqrt{1-\epsilon^2}}\begin{bmatrix} 1+\dfrac{\epsilon(\alpha-\gamma)}{ik(1+\epsilon)} & -\epsilon+\dfrac{\epsilon(\alpha-\gamma)}{ik(1+\epsilon)} \\ -\epsilon-\dfrac{\epsilon(\alpha-\gamma)}{ik(1+\epsilon)} & 1-\dfrac{\epsilon(\alpha-\gamma)}{ik(1+\epsilon)} \end{bmatrix},$$

where $\Lambda_{j,j+1}(k)$ and $F_j(k)$ are the matrices defined in (4.1) and (4.3), respectively. From (4.1) and (4.5) we obtain $\Lambda_{0,1}(k)$. Note that, in this case, $\rho^{[0]}(k)$ defined in (5.11) and $r_{0,1}(k)$ corresponding to $V_{0,1}(y)$ coincide. We have

$$r_{0,1}(k)=\frac{-k_+k_-}{(k-k_+)(k-k_-)},\quad t_{0,1}(k)=\frac{k(k+i\beta)}{(k-k_+)(k-k_-)}, \tag{8.28}$$

where k_+ and k_- are the constants defined as

$$k_\pm=-\frac{i}{2}\,\frac{\gamma+\epsilon\alpha}{1+\epsilon}\,[1\pm\sqrt{1+E}],\quad E=\frac{4\epsilon(\gamma-\alpha)}{(1-\epsilon)(\gamma+\epsilon\alpha)}. \tag{8.29}$$

Next, we will solve the Marchenko equation (7.7) for $y<0$ with the input of (8.28) and (8.29). In fact, since there are no discontinuities associated with the reflection coefficient in (8.28), the Marchenko equation (7.7) reduces to (7.8). Note that the sign of E in (8.29) is the same as the sign

of $\epsilon(\gamma-\alpha)$. There are three cases to consider, namely $E=0$, $E<0$, and $E>0$. When $E=0$, i.e. when $\epsilon=0$ or $\alpha=\gamma$, we have $r_{0,1}(k)=0$, and hence $h_l(t,y)=0$. Thus $V_{0,1}(y)=0$, because in analogy to (7.9) we have

$$V_{0,1}(y)=-2\frac{dh_l(0+,y)}{dy}, \quad -\infty<y<0. \tag{8.30}$$

Thus $Y_{l;0,1}(k,y)=1$, and so $H(x)$ is given by (8.10) for all $x\in\mathbf{R}$. Next, we consider the case $E<0$. In this case both k_+ and k_- lie in $\mathbf{C}^-$, and hence using (8.28) in (7.1) we obtain

$$\varrho(t)=\begin{cases} 0, & t<0, \\ \dfrac{ik_+k_-}{k_+-k_-}[e^{-ik_+t}-e^{-ik_-t}], & t>0. \end{cases} \tag{8.31}$$

The solution of the Marchenko equation (7.8) with the integral kernel in (8.31) is given by

$$h_l(t,y)=\begin{cases} 0, & t>-2y, \\ \dfrac{k_+k_-}{\beta}\dfrac{(\beta+\gamma)[e^{\beta t}-e^{-2\beta y}]+\epsilon(\beta-\alpha)[1-e^{-\beta(t+2y)}]}{\epsilon(\beta-\alpha)+(\beta+\gamma)e^{-2\beta y}}, & t<-2y, \end{cases}$$

where β is the constant in (8.3). Again, using (8.30), we obtain

$$V_{0,1}(y)=\begin{cases} 0, & y>0, \\ -\dfrac{8\beta^2\epsilon(\beta-\alpha)(\beta+\gamma)e^{-2\beta y}}{[\epsilon(\beta-\alpha)+(\beta+\gamma)e^{-2\beta y}]^2}, & y<0. \end{cases} \tag{8.32}$$

Corresponding to $V_{0,1}(y)$ in (8.32), we have the zero-energy Jost solution from the right given by

$$Y_{r;0,1}(0,y)=\frac{-\epsilon(\beta-\alpha)+(\beta+\gamma)e^{-2\beta y}}{\epsilon(\beta-\alpha)+(\beta+\gamma)e^{-2\beta y}}, \quad y<0. \tag{8.33}$$

Using (3.9) we see that for $y<0$, $Z_r(0,y)$ is given by (8.33). Using (6.16)–(6.18) and (8.33) we obtain

$$y-\frac{2\epsilon(\beta-\alpha)/\beta}{\epsilon(\beta-\alpha)+\beta+\gamma}+\frac{2\epsilon(\beta-\alpha)/\beta}{\epsilon(\beta-\alpha)+(\beta+\gamma)e^{-2\beta y}}=H_-\int_0^x\frac{dz}{f_r(0,z)^2}, \quad x<0, \tag{8.34}$$

$$H(x)=\frac{H_-}{f_r(0,x)^2}\left[\frac{-\epsilon(\beta-\alpha)+(\beta+\gamma)e^{-2\beta y}}{\epsilon(\beta-\alpha)+(\beta+\gamma)e^{-2\beta y}}\right]^2, \quad x<0, \tag{8.35}$$

where y in (8.35) is obtained in terms of x from (8.34), and $f_r(0,x)$ is the zero-energy Jost solution from the right associated with $Q(x)$. Using (6.19) and (6.20), one can show that (8.34) and (8.35) are identical to (8.14) and (8.15), respectively. Finally, let us briefly consider the case where the constant E defined in (8.29) is positive. In this case, k_+ is in $\mathbf{C}^-$ and k_- is in $\mathbf{C}^+$. Thus, $V_{0,1}(y)$ has one bound state. However, since $V_{0,1}(y)$ is supported on a half-line, its bound state norming constant cannot be chosen arbitrarily and is determined by $r_{0,1}(k)$ alone.[22] Routine computations[21] lead us again to $H(x)$ as given in (8.14).

Example 8.6: In this example, we demonstrate the recovery of $H(x)$ by the method outlined in Sec. VI, namely by solving the singular integral equations (6.7) or (6.10). As our scattering data, let us use the same scattering data as in Example 8.1, with the same restrictions on the parameters ϵ, α, and γ. First, using the method of Ref. 13 we get the quantities given in (8.4). When $y>0$, we will solve (6.7); for this, using (3.16), we get $J_l(k,y)=1$ and from (6.9) we have

$P_l(k,y)=0$. Thus, the solution of (6.7) for $y>0$ is given by $X_l(k,y)=0$; hence from (6.13) we obtain $H(x)$ for $x>0$ as given in (8.10). Now let us consider the situation when $y<0$; in this case, it is easier to obtain ℓ(k) and solve (6.10). Using the method of Ref. 16 we construct $\tau(k)$ given in (8.2) and using $\ell(\mathrm{k})=-\rho(-\mathrm{k})\tau(\mathrm{k})/\tau(-\mathrm{k})$, we get

$$\ell(k)=-\epsilon\,\frac{k-i\alpha}{k+i\gamma}\,\frac{k+i\beta}{k-i\beta}. \tag{8.36}$$

Using (8.36) in (6.11), we obtain

$$P_r(k,y)=\frac{2i\epsilon\beta}{k-i\beta}\,\frac{\beta-\alpha}{\beta+\gamma}\,e^{2\beta y},\quad y<0. \tag{8.37}$$

Since $X_r(k,y)$ is analytic in $\mathbf{C}^-$, a contour integration along the boundary of $\mathbf{C}^-$ converts (6.10) into the algebraic equation,

$$X_r(k,y)-\frac{2i\epsilon\beta}{k-i\beta}\,\frac{\beta-\alpha}{\beta+\gamma}\,e^{2\beta y}X_r(-i\beta,y)=P_r(k,y),\quad y<0.$$

Using (8.37) and the analyticity requirement on $X_r(k,y)$ to evaluate $X_r(-i\beta,y)$, we get

$$X_r(k,y)=\frac{2i\epsilon\beta}{k-i\beta}\,\frac{\beta-\alpha}{\beta+\gamma}\,\frac{(\beta+\gamma)e^{2\beta y}}{\beta+\gamma+\epsilon(\beta-\alpha)e^{2\beta y}},\quad y<0. \tag{8.38}$$

From (3.17) we have $J_r(k,y)=1$ for $y<0$. Thus, using (6.5) and (8.38), we get

$$Z_r(0,y)=\frac{(\beta+\gamma)e^{-2\beta y}-\epsilon(\beta-\alpha)}{(\beta+\gamma)e^{-2\beta y}+\epsilon(\beta-\alpha)},\quad y<0.$$

Thus using (6.16) and (6.18)–(6.20), we obtain $H(x)$ given in (8.15).

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Generalization of the Bremmer coupling series

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An operator formalism is developed to expand the acoustic wave field in a multi-dimensionally smoothly varying medium, generated by a source localized in space and time, into a sum of constituents each of which can be interpreted as a wave that has traveled up and down with respect to a direction of preference a definite number of times. This expansion is a generalization of the Bremmer coupling series. The condition of smoothness of the medium relates to the width of the signature of the source in the configuration. Both the existence and the convergence (in the weak sense) of the expansion are discussed. The operator calculus involved leads to a natural generalization of the concept of slowness surface to multi-dimensionally smoothly varying media. The operator associated with the corresponding generalized vertical slowness induces the full one-way wave operator in the type of media under consideration. In addition, a wavefield decomposition operator as well as an interaction operator that couples the decomposed constituents, are derived. [S0022-2488(96)01407-7]

I. INTRODUCTION

In recent years, there has been an increasing interest in the use of one-way ''parabolic'' approximations to the wave operator in the application of seismic modeling and migration-inversion techniques,[1–3] and in the application of long-range waveguiding problems in ocean acoustics[4–6] and integrated optics.[7,8] The parabolic approximation arises in the decomposition (or ''splitting'') of the acoustic wave field into constituents that travel ''up'' and ''down'' with respect to a given direction of preference, such that the two constituents satisfy coupled partial differential equations of a specific type. In this paper, we shall discuss the mathematical theory underlying this decomposition technique. The theory builds on the work of Seeley,[9,10] Hörmander,[11] and Duistermaat and Guilleman,[12] and is based on the calculus of pseudo-differential operators. The use of such operators, in particular in the field of underwater acoustics where it yields the factorization of the Helmholtz operator, has been noticed by Fishman and McCoy,[13–17] Fishman,[18,19] Fishman and Wales,[20] McCoy and Frazer,[21] and Weston.[22] The interaction of up- and downgoing constituents has been discussed by McCoy, Fishman, and Frazer.[23] Within the parabolic approximations, Corones[24] has put the interaction in the context of the Bremmer series.

The direction of preference, which is assigned to the ''vertical'' direction, arises from the medium's variations. In its exact form, the decomposition procedure transforms the scattering problem in n dimensions into a continuous family of $(n-1)$-dimensional problems, such that the remaining scattering phenomenon can be solved with the aid of a Neumann series in the relative vertical changes in the medium parameters. This series is a generalization to multi-dimensionally varying media of the Bremmer coupling series that has been used in one-dimensional scattering problems (for an example, see Ref. 25).

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The decomposition introduced applies to media which vary smoothly on the scale of the irradiating pulse, and generalizes the standard decomposition to media that are no longer translationally invariant in the ''horizontal'' directions. Owing to this generalization, more refined mathematical tools are required, such as the calculus of pseudo-differential operators. The up/down decomposition does not allow any further decomposition into horizontal, right/left, directions. Media, in which discontinuities in their physical properties occur, should be smoothed on the scale of the irradiating pulse with the aid of equivalent medium averaging prior to the decomposition. With regard to media with discontinuities, we mention the alternative, quasi-decomposition into up- and downgoing waves in the neighborhood of a ''rough'' interface separating two homogeneous half-spaces with the aid of the modified Rayleigh hypothesis.[26,27]

The key applications of the Bremmer series are (i) an efficient way of numerically solving a direct scattering problem, (ii) identification of multiple scattered wave constituents, and (iii) formulations of various inverse scattering procedures. Fast numerical schemes require sparse matrix representations of the kernel associated with the relevant integral or pseudo-differential part of the one-way wave operator in space domain. The properties of the kernel, however, are such that generic bases in which its representation becomes sparse do not exist. Parabolic-type approximations of the kernel's symbol, on the other hand, lead to possible sparsifications. The validity of such approximations has been discussed in previous papers.[2,3] They typically capture the precritical angle phenomena in the wave propagation. Beyond this regime, matrix representations for the exact cokernel, acting in horizontal slowness space, have to be considered. A list of references to the development and applications of parabolic theories can be found in Ref. 2. Approximations of a different nature and with a different range of validity result from the method of phase screens.[28] Other numerical procedures are based on constructing a spectral representation of the pseudo-differential part of the one-way wave operator and relate to normal-mode summation.

The solution of the direct scattering problem in the form of a Bremmer series allows one to identify or predict multiple scattered constituents in the configuration. Applying this process to physical measurements, however, requires some knowledge about the medium in which the experiment has been carried out. In fact, the Bremmer series yields an expansion of the acoustic wavefield in terms of the spatial derivatives of the medium properties, as opposed to an expansion in the medium's contrast with respect to a given embedding through a contrast-source integral representation. The leading term in the former expansion is a high-frequency (Rytov-like) approximation to the wavefield; in the latter expansion, the leading term is the (distorted) Born approximation in the embedding. It is noted that, once the former procedure has led to a construction of the Green's function in the embedding, the latter procedure can be applied to the contrast (possibly with discontinuities).

The Bremmer coupling series essentially recomposes the solutions of the system of coupled one-way wave equations into a two-way solution. As such, it connects the one-way wave formulation of scattering to the Dirichlet-to-Neumann map formulation (see also Refs. 29 and 30), and also yields a solution of the associated invariant imbedding equations. We note that the decomposition of the direct scattering problem is an integral part of the layer stripping approach to the inverse scattering problem (see, for example, Ref. 31 for the one-dimensional formulation and Ref. 32, for a multi-dimensional formulation). In fact, the Bremmer series representation allows one to link the asymptotic single-scattering approach (see, for example, Ref. 33 and 34) with the mentioned multiple-scattering approach.

The Bremmer coupling series becomes a powerful tool in those configurations in which the complexity of the medium is such that ray-theoretic approaches become intractable or the approximation by homogeneous horizontal layers breaks down.

The remainder of this paper is organized as follows. In Sec. II, the principle of directional decomposition is explained. In Sec. III, the decomposition problem is related to the solution of an elliptic problem in one dimension less than the original scattering problem. In Sec. IV, the original system of two-way wave equations is transformed into a system of coupled one-way wave equa-

tions. The one-way wave equations define a generalization of the concept of slowness surface, which is discussed in Sec. V. In Sec. VI, the fundamental properties of the Green's functions of the one-way equations are derived. These functions are used in Sec. VII to transform the system of one-way integro-differential equations into a system of integral equations, which is then solved in terms of a Neumann series expansion. Finally, presented in Sec. VIII is a series expansion for the generalized slowness surface that yields an explicit solution of the elliptic problem posed in Sec. III. Section IX concludes the paper.

We note that our analysis differs slightly from the standard mathematical treatment of factorizing differential operators, since in our case the $(n-1)$-dimensional (''horizontal'') space is not assumed to be compact. However, with regard to the numerical implementation of the theory, periodic boundary conditions may be imposed in the horizontal directions. The causal acoustic waves are well defined on $\mathscr{T}^{n-1}\times\mathbb{R}$, where $\mathscr{T}^{n-1}$ denotes the $(n-1)$-dimensional torus, for a finite time window.

II. DIRECTIONAL DECOMPOSITION OF THE ACOUSTIC SCATTERING PROCESS

In each subdomain of the configuration where the acoustic properties vary continuously with position, the acoustic wavefield satisfies the hyperbolic system of partial differential equations

$$\partial_k p+\rho\partial_t v_k=f_k, \tag{II.1}$$

$$\kappa\partial_t p+\partial_r v_r=q, \tag{II.2}$$

where p=acoustic pressure (Pa), v_r=particle velocity (m/s), ρ=volume density of mass (kg/m^3), κ=compressibility (Pa^{-1}), q=volume source density of injection rate (s^{-1}), f_k=volume source density of force (N/m^3), and $\{x_1,x_2,x_3\}$ are the right-handed, orthogonal, Cartesian coordinates, t is the time, and the subscript notation and the summation convention for Cartesian tensors are employed. We assume that the coefficients ρ and κ are smooth, i.e., infinitely differentiable functions of position, and time independent. Furthermore, we assume that these functions are constant outside a sphere of finite radius. This provision enables us to formulate the acoustic wave propagation, when necessary, as a scattering problem in a homogeneous embedding. The smoothness entails that the singularities of the wavefield (in particular the ones on the wavefront) arise from the ones in the signatures of the source distributions. Further, causality of the wave motion is enforced. This implies that if the sources that generate the wavefield are switched on at the instant $t=0$, the wavefield quantities satisfy the initial conditions

$$p(x_m,t)=0 \quad \text{for } t<0 \quad \text{and all} \quad x_m, \tag{II.3}$$

$$v_r(x_m,t)=0 \quad \text{for } t<0 \quad \text{and all} \quad x_m. \tag{II.4}$$

Due to the time invariance of the medium, the causality of the wave motion can also be taken into account by carrying out a one-sided Laplace transformation with respect to time and requiring that the transform-domain wave quantities are bounded functions of position in all space when the time Laplace-transform parameter s, which is in general complex, lies in the right half $\mathrm{Re}\{s\}>0$ of the complex s plane. The limiting case of sinusoidal oscillations of angular frequency $\omega\in\mathbb{R}$ is covered by considering the limiting case $s\to i\omega$, in which i is the imaginary unit, the limit being taken via $\mathrm{Re}\{s\}>0$. In view of Lerch's theorem,[35] however, it is sufficient to consider values with $\mathrm{Im}\{s\}=0$ and $s\geqslant s_0>0$; s_0 will be specified at several stages in the analysis.

To show the notation, we give the expression for the acoustic pressure,

$$\hat{p}(x_m,s)=\int_{t=0}^{\infty}\exp(-st)p(x_m,t)dt. \tag{II.5}$$

Under this transformation, assuming zero initial conditions, we have $\partial_t \rightarrow s$. The transformed system of first-order equations follows from Eqs. (II.1) and (II.2) as

$$\partial_k \hat{p} + s\rho \hat{v}_k = \hat{f}_k, \tag{II.6}$$

$$s\kappa \hat{p} + \partial_r \hat{v}_r = \hat{q}. \tag{II.7}$$

The change of the wavefield in space along a direction of preference can now be expressed in terms of the changes of the wavefield in the plane perpendicular to it. The direction of preference is taken along the x_3 axis (or ''vertical'' axis) and the remaining (''horizontal'') coordinates are denoted by x_μ, $\mu=1,2$. The procedure requires a separate handling of the horizontal components of the particle velocity. From Eqs. (II.6) and (II.7) we obtain

$$\hat{v}_\kappa = -\rho^{-1} s^{-1} (\partial_\kappa \hat{p} - \hat{f}_\kappa), \tag{II.8}$$

leaving, upon substitution, the matrix differential equation

$$(\partial_3 \delta_{I,J} + s\hat{A}_{I,J})\hat{F}_J = \hat{N}_I, \quad I,J \in \{1,2\}, \tag{II.9}$$

in which the elements of the acoustic field matrix are given by [in Eq. (II.7) $r=\nu$,3]

$$\hat{F}_1 = \hat{p}, \tag{II.10}$$

$$\hat{F}_2 = \hat{v}_3, \tag{II.11}$$

the elements of the acoustic system's operator matrix are given by

$$\hat{A}_{1,1} = \hat{A}_{2,2} = 0, \tag{II.12}$$

$$\hat{A}_{1,2} = \rho, \tag{II.13}$$

$$\hat{A}_{2,1} = -s^{-1} \partial_\nu (\rho^{-1} s^{-1} \partial_\nu) + \kappa, \tag{II.14}$$

and the elements of the notional source matrix by

$$\hat{N}_1 = \hat{f}_3, \tag{II.15}$$

$$\hat{N}_2 = -s^{-1} \partial_\nu (\rho^{-1} \hat{f}_\nu) + \hat{q}. \tag{II.16}$$

It is observed that the right-hand side of Eq. (II.8) and $\hat{A}_{I,J}$ contain spatial derivatives with respect to the horizontal coordinates only. Further, it is noted that $\hat{A}_{1,2}$ is a multiplicative operator, whereas $\hat{A}_{2,1}$ is a partial differential operator. Equation (II.9) is sometimes called the *two-way* wave equation (Ref. 36).

To be able to solve the scattering process along the vertical direction separately from the scattering process in the (family of) planes perpendicular to it, we decouple the two operators on the left-hand side of Eq. (II.9). This procedure will possibly lead to an additional source term on the right-hand side that accounts for the coupling. To achieve this, we shall construct an appropriate linear operator $\hat{L}_{I,J}$ with

$$\hat{F}_I = \hat{L}_{I,J} \hat{W}_J \tag{II.17}$$

that, with the aid of the commutation relation

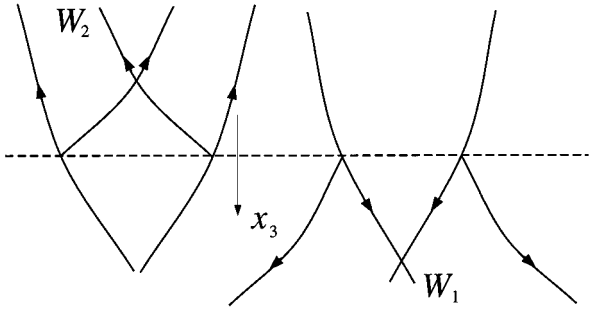

FIG. 1. Directional decomposition.

$$(\partial_3 \hat{L}_{I,J}) = [\partial_3, \hat{L}_{I,J}] \tag{II.18}$$

([.,.] denotes the commutator), transforms Eq. (II.9) into

$$\hat{L}_{I,J}(\partial_3 \delta_{J,M} + s\hat{\Lambda}_{J,M})\hat{W}_M = -(\partial_3 \hat{L}_{I,J})\hat{W}_J + \hat{N}_I, \tag{II.19}$$

so as to make $\hat{\Lambda}_{\mathrm{J,M}}$, satisfying

$$\hat{A}_{I,J}\hat{L}_{J,M} = \hat{L}_{I,J}\hat{\Lambda}_{J,M}, \tag{II.20}$$

a diagonal matrix of operators. We denote $\hat{L}_{I,J}$ as the composition operator and $\hat{W}_M$ as the wave matrix. The elements of the wave matrix represent the local weights of the down- and upgoing constituents (see also Fig. 1). The expression in parentheses on the left-hand side of Eq. (II.19) represents the two so-called *one-way* wave operators (Ref. 36). The first term on the right-hand side of Eq. (II.19) is representative for the scattering due to variations of the medium properties in the vertical direction. The scattering due to variations of the medium properties in the horizontal directions is contained in $\hat{\Lambda}_{\mathrm{J,M}}$ and, implicitly, in $\hat{L}_{I,J}$.

To investigate whether solutions $(\hat{L}_{I,J}, \hat{\Lambda}_{\mathrm{J,M}})$ of Eq. (II.20) exist, we introduce the column matrix, or generalized eigenvector, operators $\hat{L}_I^{(\pm)}$ according to

$$\hat{L}_I^{(+)} = \hat{L}_{I,1}, \tag{II.21}$$

$$\hat{L}_I^{(-)} = \hat{L}_{I,2}. \tag{II.22}$$

Upon writing the diagonal elements of $\hat{\Lambda}_{\mathrm{J,M}}$ as

$$\hat{\Lambda}_{1,1} = \hat{\Gamma}^{(+)}, \tag{II.23}$$

$$\hat{\Lambda}_{2,2} = \hat{\Gamma}^{(-)}, \tag{II.24}$$

Eq. (II.20) decomposes into the two systems of equations

$$\hat{A}_{I,J}\hat{L}_J^{(+)} = \hat{L}_I^{(+)}\hat{\Gamma}^{(+)}, \tag{II.25}$$

$$\hat{A}_{I,J}\hat{L}_J^{(-)} = \hat{L}_I^{(-)}\hat{\Gamma}^{(-)}. \tag{II.26}$$

By analogy with the case where the medium is translationally invariant in the horizontal directions, we shall denote $\hat{\Gamma}^{(\pm)}$ as the *vertical slowness* operators. Notice that the operators $\hat{L}_1^{(\pm)}$ compose the acoustic pressure and that the operators $\hat{L}_2^{(\pm)}$ compose the vertical particle velocity, whereas the elements of $\hat{W}_M$ may be physically ''nonobservable.''

Through mutual elimination, the equations for $\hat{L}_1^{(\pm)}$ and $\hat{L}_2^{(\pm)}$ can be decoupled as follows:

$$\hat{A}_{1,2}\hat{A}_{2,1}\hat{L}_1^{(\pm)}=\hat{L}_1^{(\pm)}\hat{\Gamma}^{(\pm)}\hat{\Gamma}^{(\pm)}, \tag{II.27}$$

$$\hat{A}_{2,1}\hat{A}_{1,2}\hat{L}_2^{(\pm)}=\hat{L}_2^{(\pm)}\hat{\Gamma}^{(\pm)}\hat{\Gamma}^{(\pm)}. \tag{II.28}$$

The partial differential operators on the left-hand sides, which are given by

$$\hat{A}_{2,1}\hat{A}_{1,2}=-s^{-1}\partial_\nu(\rho^{-1}s^{-1}\partial_\nu(\rho\ ))+\kappa\rho, \tag{II.29}$$

$$\hat{A}_{1,2}\hat{A}_{2,1}=-\rho s^{-1}\partial_\nu(\rho^{-1}s^{-1}\partial_\nu\ )+\rho\kappa, \tag{II.30}$$

are strongly elliptic in the horizontal plane $\mathbb{R}^2$ for each value of the vertical coordinate $x_3\in\mathbb{R}$ and all frequencies s under consideration; they differ from one another in case the volume density of mass does vary in the horizontal directions. To ensure that nontrivial solutions of Eqs. (II.27) and (II.28) exist, one equation must imply the other. To construct a formal solution, an Ansatz is introduced in the form of a commutation relation for one of the components $\hat{L}_J^{(\pm)}$ that restricts the freedom in the choice for the other component. Three choices will be considered.

A. Acoustic-pressure normalization analog

Our first Ansatz assumes that $\hat{L}_2^{(\pm)}$ can be chosen such that

$$[\hat{L}_2^{(\pm)},\hat{A}_{2,1}\hat{A}_{1,2}]=0. \tag{II.31}$$

In view of Eq. (II.28), the $\hat{\Gamma}^{(\pm)}$ must then satisfy

$$\hat{A}_{2,1}\hat{A}_{1,2}-\hat{\Gamma}^{(\pm)}\hat{\Gamma}^{(\pm)}=0. \tag{II.32}$$

The commutation relation for $\hat{L}_1^{(\pm)}$ follows as $[\hat{A}_{1,2}^{-1}\hat{L}_1^{(\pm)},\hat{A}_{2,1}\hat{A}_{1,2}]=0$ and a possible solution of Eqs. (II.25) and (II.26) is

$$\hat{L}_2^{(\pm)}=\hat{\Gamma}^{(\pm)},\quad \hat{L}_1^{(\pm)}=\hat{A}_{1,2}. \tag{II.33}$$

Since $\hat{L}_2^{(\pm)}$ as given by Eq. (II.33) satisfies Eq. (II.31), the Ansatz is justified. In view of the up/down symmetry, the solutions of Eq. (II.32) are written as

$$\hat{\Gamma}^{(+)}=-\hat{\Gamma}^{(-)}=\hat{\Gamma}=\hat{\mathrm{A}}^{1/2}, \tag{II.34}$$

where $\hat{\mathrm{A}}\equiv\hat{A}_{2,1}\hat{A}_{1,2}$. Thus, the composition operator becomes

$$\hat{L}=\begin{pmatrix}\hat{A}_{1,2} & \hat{A}_{1,2}\\ \hat{\Gamma} & -\hat{\Gamma}\end{pmatrix}. \tag{II.35}$$

In terms of the inverse vertical slowness operator, $\hat{\Gamma}^{-1}=\hat{\mathrm{A}}^{-1/2}$, the decomposition operator then follows as

$$\hat{L}^{-1}=\frac{1}{2}\begin{pmatrix}\hat{A}_{1,2}^{-1} & \hat{\Gamma}^{-1}\\ \hat{A}_{1,2}^{-1} & -\hat{\Gamma}^{-1}\end{pmatrix}. \tag{II.36}$$

In this normalization, the elements of the wave matrix correspond with pressures up to the action of $\hat{A}_{1,2}$; pressures are typically measured with hydrophones.

B. Vertical-particle-velocity normalization analog

A second Ansatz assumes that $\hat{L}_1^{(\pm)}$ can be chosen such that

$$[\hat{L}_1^{(\pm)},\hat{A}_{1,2}\hat{A}_{2,1}]=0. \tag{II.37}$$

Then, $\hat{\Gamma}^{(\pm)}$ must satisfy [cf. Eq. (II.27)]

$$\hat{A}_{1,2}\hat{A}_{2,1}-\hat{\Gamma}^{(\pm)}\hat{\Gamma}^{(\pm)}=0, \tag{II.38}$$

and a possible solution of Eqs. (II.25) and (II.26) is

$$\hat{L}_1^{(\pm)}=\hat{\Gamma}^{(\pm)},\quad \hat{L}_2^{(\pm)}=\hat{A}_{2,1}, \tag{II.39}$$

which satisfies the second Ansatz. The solutions of Eq. (II.38) are written as

$$\hat{\Gamma}^{(+)}=-\hat{\Gamma}^{(-)}=\hat{\Gamma}=\hat{\mathrm{A}}^{1/2}, \tag{II.40}$$

where $\hat{\mathrm{A}}\equiv\hat{A}_{1,2}\hat{A}_{2,1}$. Thus, the composition operator is given by

$$\hat{L}=\begin{pmatrix}\hat{\Gamma} & -\hat{\Gamma}\\ \hat{A}_{2,1} & \hat{A}_{2,1}\end{pmatrix}. \tag{II.41}$$

Now, the decomposition operator becomes

$$\hat{L}^{-1}=\frac{1}{2}\begin{pmatrix}\hat{\Gamma}^{-1} & \hat{\mathrm{A}}^{-1}\hat{A}_{1,2}\\ -\hat{\Gamma}^{-1} & \hat{\mathrm{A}}^{-1}\hat{A}_{1,2}\end{pmatrix}. \tag{II.42}$$

In this normalization, $\hat{A}_{2,1}$ acting on the elements of the wave matrix results in vertical particle velocities; particle velocities are typically measured with geophones.

C. Vertical-acoustic-power-flux normalization analog

It will appear to be advantageous to consider a third Ansatz, viz., the one arising from the acoustic-power-flux normalization. For this, the commutation relation

$$[\hat{A}_{1,2}^{-1/2}\hat{L}_1^{(\pm)},\ \hat{A}_{1,2}^{1/2}\hat{A}_{2,1}\hat{A}_{1,2}^{1/2}]=0 \tag{II.43}$$

is imposed on $\hat{L}_1^{(\pm)}$. Then the vertical slowness operators must satisfy the equation

$$\hat{A}_{1,2}^{1/2}\hat{A}_{2,1}\hat{A}_{1,2}^{1/2}-\hat{\Gamma}^{(\pm)}\hat{\Gamma}^{(\pm)}=0. \tag{II.44}$$

Note that the operator $\hat{\mathrm{A}}$,

$$\hat{\mathrm{A}}\equiv\hat{A}_{1,2}^{1/2}\hat{A}_{2,1}\hat{A}_{1,2}^{1/2}=-\rho^{1/2}s^{-1}\partial_\nu(\rho^{-1}s^{-1}\partial_\nu(\rho^{1/2}\,))+\kappa\rho, \tag{II.45}$$

is self-adjoint with respect to the standard real L^2 inner product in (almost all of) L^2. A possible solution of Eqs. (II.25) and (II.26) is now given by

$$\hat{L}_1^{(\pm)}=(\hat{A}_{1,2}/2)^{1/2}(\hat{\Gamma}^{(+)})^{-1/2},\quad \hat{L}_2^{(\pm)}=\pm(2\hat{A}_{1,2})^{-1/2}(\hat{\Gamma}^{(+)})^{1/2}. \tag{II.46}$$

The solutions of Eq. (II.44) are written as

$$\hat{\Gamma}^{(+)} = -\hat{\Gamma}^{(-)} = \hat{\Gamma} = \hat{A}^{1/2}. \tag{II.47}$$

Thus, the composition operator is given by

$$\hat{L} = \frac{1}{\sqrt{2}} \begin{pmatrix} \hat{A}_{1,2}^{1/2}\hat{\Gamma}^{-1/2} & \hat{A}_{1,2}^{1/2}\hat{\Gamma}^{-1/2} \\ \hat{A}_{1,2}^{-1/2}\hat{\Gamma}^{1/2} & -\hat{A}_{1,2}^{-1/2}\hat{\Gamma}^{1/2} \end{pmatrix}. \tag{II.48}$$

This composition operator $\hat{L}$: $(L^2)^2 \rightarrow (L^2)^2$ is normalized in the sense that [cf. Eq. (II.46)]

$$\hat{L}^T J \hat{L} = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \tag{II.49}$$

with

$$J = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}. \tag{II.50}$$

This normalization establishes the connection with asymptotic ray theory in the vicinity of the wavefronts.

Using Eq. (II.48), we can map the pressure to the vertical particle velocity, viz.,

$$\hat{F}_2 = \hat{\boldsymbol{Y}}^{(+)}\hat{F}_1 \quad \text{if} \quad \hat{W}_2 = 0, \tag{II.51}$$

$$\hat{F}_2 = \hat{\boldsymbol{Y}}^{(-)}\hat{F}_1 \quad \text{if} \quad \hat{W}_1 = 0, \tag{II.52}$$

where

$$\pm\hat{\boldsymbol{Y}}^{(\pm)} = \hat{\boldsymbol{Y}} = \hat{A}_{1,2}^{-1/2}\hat{\Gamma}\hat{A}_{1,2}^{-1/2} \tag{II.53}$$

has the interpretation of *admittance* operator. The latter operator discriminates the decomposed constituents. Note that $\hat{F}_1^T\hat{F}_2$ represents the vertical component of the Poynting vector.

The decomposition operator becomes

$$\hat{L}^{-1} = \frac{1}{\sqrt{2}} \begin{pmatrix} \hat{\Gamma}^{1/2}\hat{A}_{1,2}^{-1/2} & \hat{\Gamma}^{-1/2}\hat{A}_{1,2}^{1/2} \\ \hat{\Gamma}^{1/2}\hat{A}_{1,2}^{-1/2} & -\hat{\Gamma}^{-1/2}\hat{A}_{1,2}^{1/2} \end{pmatrix}. \tag{II.54}$$

It is observed that all the operators involved can be directly constructed from $\hat{\mathrm{A}}^{-1/4}$, viz., $\hat{\Gamma}^{-1/2} = \hat{\mathrm{A}}^{-1/4}$, $\hat{\Gamma}^{1/2} = \hat{\mathrm{A}}(\hat{\mathrm{A}}^{-1/4})^3$, and $\hat{\Gamma} = \hat{\mathrm{A}}(\hat{\mathrm{A}}^{-1/4})^2$. All these powers of $\hat{\mathrm{A}}$ are self-adjoint in (almost all of) L^2 as well as positive definite, since it has been assumed that $\mathrm{Im}\{s\} = 0$ and $\mathrm{Re}\{s\} > 0$.

Apparently a whole class of composition operators $\hat{L}_{I,J}$, all leading to different representations of the scattering process in the horizontal space, exists. The final results for the acoustic pressure and the vertical particle velocity, however, will not depend on a particular choice: in terms of observables the decomposition yields

$$\hat{F}_I^{(+)} = \hat{L}_I^{(+)}(\hat{L}^{-1})_{1,J}\hat{F}_J, \tag{II.55}$$

$$\hat{F}_I^{(-)} = \hat{L}_I^{(-)}(\hat{L}^{-1})_{2,J}\hat{F}_J. \tag{II.56}$$

For practical applications, one adjusts the normalization to the sensors being used; it is quite common that only one of the two relevant field components is being measured.

At this point, it is emphasized that $\hat{\Gamma}^{(\pm)}$ are still unknown. It is noted that the key property we have used so far is that the diagonal of the system's operator matrix $\hat{A}$ vanishes. For the evaluation

of $\hat{\Gamma}^{(\pm)}$, and $\hat{L}_J^{(\pm)}$, we need to introduce (fractional) powers of an elliptic partial differential operator in $\mathbb{R}^2$ for each value of $x_3 \in \mathbb{R}$ [cf. Eq. (II.32), (II.38), or (II.44)]. How this can be done will be discussed in Sec. III. In this respect it is noted that only a proper definition of a negative (fractional) power is needed, since positive fractional powers are constructed from the negative ones through the application of the operator itself an appropriate number of times. For the time being, the vertical coordinate will play the role of parameter, which will be indicated by writing $\mathbb{R}^3=\mathbb{R}^2\times\mathbb{R}$. In this framework, the wavefield is viewed as a map of x_3 with values in a function space on $\mathbb{R}^2$.

III. THE DIMENSIONALLY REDUCED SCATTERING PROBLEM

In this section we will consider the acoustic-pressure normalization analog. All the other normalizations lead to similar results. Thus, consider the partial differential operator $\hat{\mathrm{A}}=\hat{\mathrm{A}}_{2,1}\hat{\mathrm{A}}_{1,2}$ on $\mathbb{R}^2$ [cf. Eq. (II.29)] which is *elliptic with a parameter* yet to be specified. The dependence on x_3 will be suppressed in this section.

In the following analysis it is assumed that the field matrix $\hat{F}_I$ and the wave matrix $\hat{W}_M$ are contained in proper spaces, which, in view of the smoothness of the medium, is controlled by the source distributions [cf. Eqs. (II.6) and (II.7)]. The elliptic operator is clearly well-defined on the space C_0^∞ of smooth functions with compact support in $\mathbb{R}^2$. It can be extended as a bounded operator $\hat{A}$: $H^r \to H^{r-2}$ for any real r (Ref. 37, Theorem 8.9). Here, H^r is a reserved symbol for the Sobolev spaces. [Whenever we write H^r, we mean $H^r(\mathbb{R}^2)$; otherwise, the underlying space will be specified.] The norm on H^r will be denoted as $\|.\|_r$, and the norm of an operator $H^r \to H^{r'}$ as $\|.\|_{r,r'}$. The norms are implicitly scaled with the time Laplace-transform parameter s; we postpone the discussion of this aspect to Sec. V. In particular, when $r=0$, we have an operator $\hat{\mathrm{A}}$: $\mathrm{L}^2 \to \mathrm{H}^{-2}$, which is bounded. On the other hand, note that $\hat{\mathrm{A}}$: $L^2 \to L^2$ is unbounded in general.

First, we shall discuss the existence and integral representations of powers of $\hat{\mathrm{A}}$. To this end, we need to analyze the properties of its *resolvent*. The construction of the resolvent is, essentially, the solution to the reduced scattering problem and will be dealt with in Sec. VIII.

A. Properties of the resolvent

Let λ be a complex variable. The resolvent $\hat{R}_\lambda$ of $\hat{\mathrm{A}}$ is defined as

$$\hat{R}_\lambda = (\hat{\mathrm{A}} - \lambda I)^{-1}: \; H^r \to H^{r+l}, \quad 0 \leqslant l \leqslant 2. \tag{III.1}$$

It exists for $\lambda \notin \sigma(\hat{\mathrm{A}})$, which defines the spectrum $\sigma(\hat{\mathrm{A}})$ of $\hat{\mathrm{A}}$. We refer to this spectrum as the *horizontal spectrum*. Whenever confusion would arise, the resolvent will be denoted as $\hat{R}_\lambda^{(\mathrm{A})}$ rather than $\hat{R}_\lambda$ to explicitly show its relation to the operator $\hat{\mathrm{A}}$.

First, to analyze the spectrum of $\hat{\mathrm{A}}$, we consider the case $r=l=0$. We have $\hat{A}$: $L^2 \to L^2$. In accordance with the structure of our horizontal partial differential operators, we introduce a family of inner products on L^2 with respect to $\hat{u}=\hat{u}(x_\mu, s)$ and $\hat{v}=\hat{v}(x_\mu, s)$ as

$$\langle \hat{u}, \hat{v} \rangle_{0_p} = \int_{x_\mu \in \mathbb{R}} \hat{u}^* \hat{v} \rho^p dx_1 dx_2, \tag{III.2}$$

where * denotes complex conjugate (note that for s real all the quantities are, however, real) and corresponding L^2-norms as

$$\|\hat{u}\|_{0_p}^2 = \langle \hat{u}, \hat{u} \rangle_{0_p} \tag{III.3}$$

with $-1 \leqslant p \leqslant 1$. For the acoustic-pressure normalization analog we take $p=1$. (For the vertical-particle-velocity normalization analog we take $p=-1$ and for the vertical-acoustic-power-flux normalization analog we take $p=0$. When $p=0$ the subscript will be omitted.) Using

$$\int_{x_\mu\in\mathbb{R}}[-s^{-1}\partial_\nu(\rho^{-1}s^{-1}\partial_\nu(\rho\hat{u}))]^*\ \hat{v}\rho dx_1dx_2$$

$$=-\int_{x_\mu\in\mathbb{R}}\rho^{-1}[-s^{-1}\partial_\nu(\rho\hat{u})]^*(s^*)^{-1}\partial_\nu(\rho\hat{v})dx_1dx_2$$

$$=\int_{x_\mu\in\mathbb{R}}\hat{u}^*[-(s^*)^{-1}\partial_\nu(\rho^{-1}(s^*)^{-1}\partial_\nu(\rho\hat{v}))]\ \rho dx_1dx_2, \tag{III.4}$$

it is found that $\hat{\mathrm{A}}$ is self-adjoint in L^2, i.e.,

$$\langle\hat{\mathrm{A}}\hat{u},\hat{v}\rangle_{0_1}=\langle\hat{u},\hat{\mathrm{A}}\hat{v}\rangle_{0_1}. \tag{III.5}$$

In the derivation of Eq. (III.4) it was used that the sum of contributions from the boundaries in the horizontal plane at infinity vanishes. In fact, the proof is obvious on C_0^∞; subsequently, use that C_0^∞ is dense in L^2. Note that the self-adjointness [cf. Eq. (III.5)] in combination with the unboundedness is not in contradiction with the Hellinger–Toeplitz theorem,[38] since it only holds for functions that satisfy boundary conditions associated with causal solutions to the spectral-domain acoustic equations.

From Eq. (III.4) it also follows that (here, we need the condition $\mathrm{Im}\{s\}=0$)

$$\langle\hat{\mathrm{A}}\hat{u},\hat{u}\rangle_{0_1}=\int_{x_\mu\in\mathbb{R}}\rho^{-1}|s^{-1}\partial_\nu(\rho\hat{u})|^2\ dx_1dx_2+\int_{x_\mu\in\mathbb{R}}\kappa\rho|\hat{u}|^2\ \rho dx_1dx_2, \tag{III.6}$$

so that

$$\langle\hat{\mathrm{A}}\hat{u},\hat{u}\rangle_{0_1}\geqslant\langle c^{-2}\rangle\langle\hat{u},\hat{u}\rangle_{0_1}, \tag{III.7}$$

in which

$$\langle c^{-2}\rangle=\inf_{x_\mu\in\mathbb{R}}\{\kappa\rho\}>0. \tag{III.8}$$

This shows that $\hat{\mathrm{A}}$ is positive and semi-bounded from below in $\|.\|_{0_1}$. Again, these properties trivially hold, e.g., on C_0^∞. Since by Cauchy–Schwarz' inequality

$$\|(\hat{\mathrm{A}}-\lambda I)\hat{u}\|_{0_1}\|\hat{u}\|_{0_1}\geqslant|\langle(\hat{\mathrm{A}}-\lambda I)\hat{u},\hat{u}\rangle_{0_1}|, \tag{III.9}$$

while [cf. Eq. (III.7)]

$$|\langle\hat{\mathrm{A}}\hat{u},\hat{u}\rangle_{0_1}-\lambda^*\langle\hat{u},\hat{u}\rangle_{0_1}|\geqslant[(\langle c^{-2}\rangle-\mathrm{Re}\{\lambda\})^2+(\mathrm{Im}\{\lambda\})^2]^{1/2}\langle\hat{u},\hat{u}\rangle_{0_1}=|\langle c^{-2}\rangle-\lambda|\langle\hat{u},\hat{u}\rangle_{0_1} \tag{III.10}$$

if $\mathrm{Re}\{\lambda\}\leqslant\langle c^{-2}\rangle$, we obtain

$$\|(\hat{\mathrm{A}}-\lambda I)\hat{u}\|_{0_1}\|\hat{u}\|_{0_1}\geqslant|\langle c^{-2}\rangle-\lambda|\|\hat{u}\|_{0_1}^2. \tag{III.11}$$

Hence, when $\lambda\notin\sigma(\hat{\mathrm{A}})$ and $\mathrm{Re}\{\lambda\}\leqslant\langle c^{-2}\rangle$, we arrive at the estimate

$$\|\hat{R}_\lambda\|_{0_1,0_1}\leqslant|\langle c^{-2}\rangle-\lambda|^{-1} \tag{III.12}$$

for the operator norm of the resolvent as an operator $L^2\to L^2$. When λ is large enough, this implies that there exists a constant $C_{0,0}$ such that

$$\|\hat{R}_\lambda\|_{0_1,0_1} \leqslant C_{0,0}/|\lambda|. \tag{III.13}$$

Now, let the inner product on H^r using Parseval's formula be defined through

$$\langle .,. \rangle_{r_p} = \langle (\hat{\Gamma}_0)^r ., (\hat{\Gamma}_0)^r . \rangle_{0_p} \quad \text{with} \quad \hat{\Gamma}_0 = [-s^{-2}\partial_\sigma \partial_\sigma + \langle c^{-2} \rangle]^{1/2}.$$

Thus, the inner product and the corresponding norm contain the parameter s. The estimate for the norm of $\hat{R}_\lambda$ can be generalized following Ref. 9, Theorem 1, Corollary 1, and is given in Sec. VIII:

$$\|\hat{R}_\lambda\|_{r,r+l} \leqslant C_{r,l}/|\lambda|^{1-l/2}, \quad 0 \leqslant l \leqslant 2, \tag{III.14}$$

when λ is large enough and lies in the sector $\Lambda = \Lambda_0 \cup \Lambda_{sp}$ of the complex plane, where Λ_0 is defined as $\pi/2 < |\arg(\lambda)| \leqslant \pi$ and Λ_{sp} is defined as $0 < |\arg(\lambda)| \leqslant \pi/2$.

From Eq. (III.7) ($r=0$) it also follows that the spectrum must be real and positive and bounded from below, i.e., when $\lambda \in \sigma(\hat{A})$,

$$\lambda \geqslant \langle c^{-2} \rangle; \tag{III.15}$$

the ''smoothness'' of the possible eigenfunctions is estimated in their appropriate Sobolev space H^r. The property that the spectrum is semibounded from below extends to $\hat{A}$ as an unbounded operator $H^r \to H^r$ also for $r \neq 0$ (see also Ref. 37, Theorem 13.31). We have to ensure that the spectrum is strictly positive in H^r for $r \neq 0$. Since the multiplication operator, arising from the multiplicative part, say $\hat{\phi}$, of the elliptic operator $\hat{A}$ satisfies $(\hat{\Gamma}_0)^r \hat{\phi} (\hat{\Gamma}_0)^{-r} = \hat{\phi} - [\hat{\phi}, (\hat{\Gamma}_0)^r](\hat{\Gamma}_0)^{-r}$ while $[\hat{\phi}, \hat{\Gamma}_0] = O(s^{-1})$ as $s \to \infty$, it is found that $\langle \hat{\phi}\hat{u}, \hat{u} \rangle_{r_p} \geqslant 0$ if the medium is sufficiently smooth or s is large enough and $\hat{\phi} \geqslant 0$. Anyway, the spectrum can be controlled by imposing constraints on the compressibility or on the topology of the underlying horizontal space. In general, the spectrum will consist of absolute continuous (branch cut), pure point and possibly singular continuous contributions. By requiring that $\kappa \to \infty$ as $|\chi_\mu| \to \infty$, or by applying periodic boundary conditions in the horizontal directions, the operator $\hat{A}$ becomes compact, and its spectrum becomes discrete.

It is observed that the estimate in Eq. (III.14) and the properties of $\hat{A}$ hold at each depth level x_3, provided that $\langle c^{-2} \rangle$ is a positive and bounded function of x_3. How to obtain, via a parametrix, the resolvent, which is a two-dimensional problem, will be discussed at the end of this paper.

Given the resolvent $\hat{R}_\lambda$ for $\lambda \notin \sigma(\hat{A})$, we then construct general powers of the differential operator $\hat{A}$, following a standard procedure from functional analysis. This will be discussed in the next subsections.

B. Negative fractional powers of the elliptic operator

Let the power λ^z of a complex variable λ with $z \in \mathbb{R}$ be defined as

$$\lambda^z = |\lambda|^z \exp[iz \arg(\lambda)], \tag{III.16}$$

with $\arg(\lambda) \in (-\pi, \pi)$. With this definition, the branch cut of λ^z is along the negative real axis. Let $\mathscr{B}$ be a contour of integration in the λ plane around the branch cut, counter-clockwise oriented, staying away a small but finite distance from the origin (the branch point), not intersecting the spectrum $\sigma(\hat{A})$, and going to infinity in the sector Λ_0. Then, for $z \in \mathbb{R}_{<0}$, the Dunford integral

$$\hat{A}_z = \frac{1}{2\pi i} \int_{\lambda \in \mathscr{B}} \lambda^z \hat{R}_\lambda \, d\lambda \tag{III.17}$$

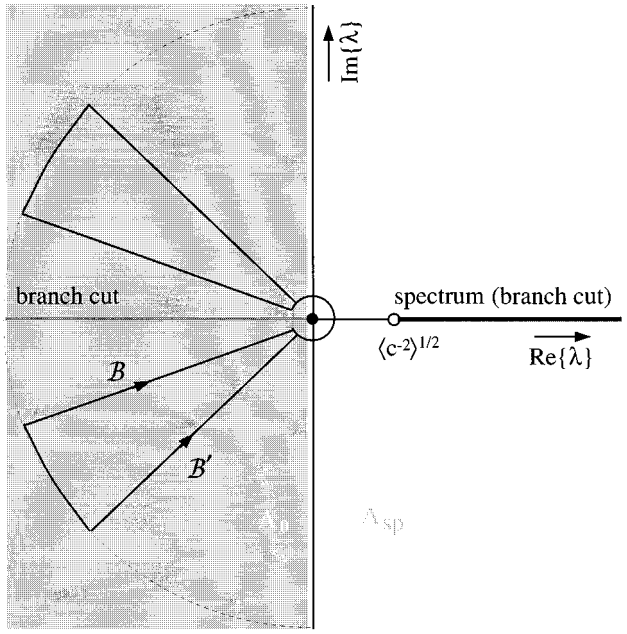

FIG. 2. Contours for the Dunford integral (Seeley's rays of minimal growth).

converges in the operator norm $\|.\|_{r,r-2z}$ on H^r (the proof relies on the symbol calculus of Secs. V and VIII for the parametrix of $\hat{A}-\lambda I$ for $\lambda\in\Lambda_0$ large, in combination with the knowledge about the spectrum $\sigma(\hat{A})$ near the origin). The integral satisfies the composition equation

$$\hat{A}_z\hat{A}_w=\hat{A}_{z+w} \tag{III.18}$$

for z, $w\in\mathbb{R}_{<0}$. To show this, consider another contour $\mathscr{B}'$ around the branch cut such that $\mathscr{B}$ is in between $\mathscr{B}'$ and the branch cut. The integral in Eq. (III.17) remains the same when the contour $\mathscr{B}$ is deformed into $\mathscr{B}'$ (see Fig. 2), since the contributions from the arcs connecting $\mathscr{B}$ and $\mathscr{B}'$ at infinity vanish. Using $\mathscr{B}'$ to evaluate $\hat{A}_z$ and $\mathscr{B}$ to evaluate $\hat{A}_w$, we get

$$\hat{A}_z\hat{A}_w=-\frac{1}{4\pi^2}\int_{\lambda\in\mathscr{B}'}\int_{\mu\in\mathscr{B}}\hat{R}_\lambda\hat{R}_\mu\lambda^z\mu^w\,d\lambda\,d\mu=-\frac{1}{4\pi^2}\int_{\lambda\in\mathscr{B}'}\int_{\mu\in\mathscr{B}}\frac{\lambda^z\mu^w}{\lambda-\mu}(\hat{R}_\lambda-\hat{R}_\mu)d\lambda\,d\mu, \tag{III.19}$$

in view of the Hilbert identity. Since for the first term we have owing to the theorem of residues

$$\int_{\lambda\in\mathscr{B}'}\left[\int_{\mu\in\mathscr{B}}\frac{\mu^w}{\lambda-\mu}\,d\mu\right]\lambda^z\hat{R}_\lambda\,d\lambda=2\pi i\int_{\lambda\in\mathscr{B}'}\lambda^{w+z}\hat{R}_\lambda\,d\lambda \tag{III.20}$$

and, upon changing the order of integration, for the second term

$$\int_{\mu\in\mathscr{B}}\left[\int_{\lambda\in\mathscr{B}'}\frac{\lambda^z}{\lambda-\mu}\,d\lambda\right]\mu^w\hat{R}_\mu\,d\mu=0, \tag{III.21}$$

in view of Cauchy's theorem, Eq. (III.19) reduces to

$$\hat{\mathrm{A}}_z\hat{\mathrm{A}}_w=\frac{1}{2\pi i}\int_{\lambda\in\mathscr{B}'}\lambda^{z+w}\hat{R}_\lambda\,d\lambda, \tag{III.22}$$

from which Eq. (III.18) is found.

C. The inverse operator

In the case $z=-1$, Eq. (III.17) implies

$$\hat{\mathrm{A}}_{-1}=\frac{1}{2\pi i}\int_{\lambda\in\mathscr{S}}\lambda^{-1}\hat{R}_\lambda\,d\lambda, \tag{III.23}$$

where $\mathscr{S}$ encircles the origin counter-clockwise (note that the contributions from the branch cut cancel). The spectrum of $\hat{\mathrm{A}}$ lies outside $\mathscr{S}$ in the λ plane. The change of variables $\mu=\lambda^{-1}$ leads to

$$\hat{\mathrm{A}}_{-1}=\frac{1}{2\pi i}\int_{\mu\in\mathscr{S}'}\mu\hat{R}_{\mu^{-1}}\mu^{-2}\,d\mu, \tag{III.24}$$

where $\mathscr{S}'$ denotes the contour in the μ plane corresponding to $\mathscr{S}$ in the λ plane, but also encircling the origin counter-clockwise. Notice that the spectrum of $\hat{\mathrm{A}}$ lies inside $\mathscr{S}'$ in the μ plane, hence $\hat{R}_{\mu^{-1}}$ is well defined on $\mathscr{S}'$. Since

$$\hat{R}_{\mu^{-1}}=\mu\hat{\mathrm{A}}^{-1}(\mu I-\hat{\mathrm{A}}^{-1})^{-1}, \tag{III.25}$$

certainly when $\mu\in\mathscr{S}'$, substitution in Eq. (III.24) yields

$$\hat{\mathrm{A}}_{-1}=\frac{1}{2\pi i}\,\hat{\mathrm{A}}^{-1}\int_{\mu\in\mathscr{S}'}\mu^{-1}(I-\mu^{-1}\hat{\mathrm{A}}^{-1})^{-1}\,d\mu. \tag{III.26}$$

Since the operator $\hat{\mathrm{A}}^{-1}$ must be bounded, $(I-\mu^{-1}\hat{\mathrm{A}}^{-1})^{-1}$ can be expanded in the Neumann series $(I-\mu^{-1}\hat{\mathrm{A}}^{-1})^{-1}=\Sigma_{n=0}^{\infty}\mu^{-n}\hat{\mathrm{A}}^{-n}$. In view of Cauchy's theorem, only the term $n=0$ in Eq. (III.26) contributes, from which it follows that

$$\hat{\mathrm{A}}_{-1}=\hat{\mathrm{A}}^{-1} \tag{III.27}$$

(see, e.g., Ref. 39, III Theorem 6.15). Equations (III.18) and (III.27) show that the operators $\hat{\mathrm{A}}_z$ behave like ordinary powers for negative values of z.

D. Non-negative fractional powers of the elliptic operator

With the aid of Eq. (III.17) a non-negative fractional power of $\hat{\mathrm{A}}$ can be readily introduced through

$$\hat{\mathrm{A}}^z=\hat{\mathrm{A}}^k\hat{\mathrm{A}}_{z-k}, \tag{III.28}$$

where k is an integer such that $k>z$. The resulting operators behave, again, like ordinary powers, i.e.,

$$\hat{\mathrm{A}}^z\hat{\mathrm{A}}^w=\hat{\mathrm{A}}^{z+w} \tag{III.29}$$

(note that $\hat{\mathrm{A}}$ and its resolvent commute).

In view of Eqs. (III.17), and (III.28) and (III.14), which are based on the results of Sec. VIII, it follows that $\hat{\mathrm{A}}^z$: $H^r\to H^{r-2z}$ is bounded for general r and for all $z\in\mathbb{R}$.

E. The Schrödinger problem

If $\hat{\mathrm{A}}$ is *compact* and self-adjoint, its eigenfunctions ψ and spectrum can be used to evaluate its negative fractional powers, viz., upon choosing the contour $\mathscr{B}$ in the Dunford integral equation (III.17) in Λ_{sp} around $\sigma(\hat{\mathrm{A}})$. Then, applying the theorem of residues leads to

$$\hat{\mathrm{A}}_z\psi_{[N]}=\frac{1}{2\pi i}\int_{\lambda\in\mathscr{B}}\lambda^z\hat{R}_\lambda\psi_{[N]}\,d\lambda=\frac{1}{2\pi i}\,\psi_{[N]}\int_{\lambda\in\mathscr{B}}\lambda^z(\lambda_{[N]}-\lambda)^{-1}\,d\lambda=\lambda^z_{[N]}\psi_{[N]}. \tag{III.30}$$

Expanding the components of the wave matrix into the eigenfunctions of $\hat{\mathrm{A}}$ leads to a diagonal representation of $\hat{\mathrm{A}}_z$, viz.,

$$\hat{\mathrm{A}}_z\hat{u}=\sum_{[N]}\lambda^z_{[N]}\hat{u}_{[N]}\psi_{[N]}\quad\text{with}\quad\hat{u}=\sum_{[N]}\hat{u}_{[N]}\psi_{[N]}. \tag{III.31}$$

Finding the horizontal spectrum and eigenfunctions, $\hat{\mathrm{A}}\psi=\lambda\psi$, is a Schrödinger problem in two dimensions; note that this spectrum may vary with x_3. The Dunford integral around the spectrum links the current methodology to the theory of waveguides in two dimensions, since $s^2\hat{\mathrm{A}}$ corresponds with a dimensionally reduced wave equation.

F. Vertical derivatives of powers of the elliptic operator

Consider, again, Eq. (II.19). We are now in a position to show that $(\partial_3\hat{L}_{I,J})$ exists. As before, it is sufficient to prove that the expression for $(\partial_3\hat{\mathrm{A}}_z)$ converges in operator norm when $z<0$. To this end, we consider the integral

$$\frac{1}{2\pi i}\int_{\lambda\in\mathscr{B}}\lambda^z\partial_3\hat{R}_\lambda\,d\lambda,$$

in which

$$\partial_3\hat{R}_\lambda=-\hat{R}_\lambda(\partial_3\hat{\mathrm{A}})\hat{R}_\lambda, \tag{III.32}$$

where ∂_3 in $(\partial_3\hat{\mathrm{A}})$ acts on the coefficients of $\hat{\mathrm{A}}$ only. In fact, $(\partial_3\hat{\mathrm{A}})$: $H^r\to H^r$ is a multiplication operator. Note that this operator is bounded, since the derivatives of the medium parameters are assumed to be continuous. Further, $\partial_3\hat{R}_\lambda$ vanishes in those regions where the medium properties are independent of x_3. The norm of $\partial_3\hat{R}_\lambda$ satisfies the estimate [cf. Eq. (III.14)]

$$\|\partial_3\hat{R}_\lambda\|_{r,r+l+m}\leqslant\|\hat{R}_\lambda\|_{r+l,r+l+m}\|(\partial_3\hat{\mathrm{A}})\|_{r+l,r+l}\|\hat{R}_\lambda\|_{r,r+l}\leqslant C_{r,l,m}/|\lambda|^{2-(l+m)/2} \tag{III.33}$$

for $0\leqslant l$, $m\leqslant 2$, and $\lambda\in\Lambda_0$ large. It then also follows that $(\partial_3\hat{\mathrm{A}}_z)$: $H^r\to H^{r-2(z-1)}$ exists and is bounded for $\mathrm{Re}\{z\}<0$ (the proof relies on the symbol expansions to be discussed in Sec. VIII). Now, use the relation

$$(\partial_3\hat{\mathrm{A}}^z)=(\partial_3\hat{\mathrm{A}}^k\hat{\mathrm{A}}_{z-k})=\sum_{q=0}^{k}\hat{\mathrm{A}}^q(\partial_3\hat{\mathrm{A}})\hat{\mathrm{A}}^{k-q}\hat{\mathrm{A}}_{z-k}+\hat{\mathrm{A}}^k(\partial_3\hat{\mathrm{A}}_{z-k})$$

to extend the result from $z<0$ to $z\geqslant 0$.

IV. THE SYSTEM OF ONE-WAY WAVE EQUATIONS IN THE TIME-LAPLACE-TRANSFORM DOMAIN

Next, we complete the directional decomposition procedure. Using any of the decomposition schemes, Eq. (II.19) transforms into

$$(\partial_3\delta_{I,M}+s\hat{\Lambda}_{I,M})\hat{W}_M=-(\hat{L}^{-1})_{I,M}(\partial_3\hat{L}_{M,K})\hat{W}_K+(\hat{L}^{-1})_{I,M}\hat{N}_M, \tag{IV.1}$$

which can be interpreted as a coupled system of one-way wave equations. The coupling between the components of $\hat{W}_M$ is apparent in the first sourcelike term on the right-hand side. In particular, we shall further investigate the decomposition operator associated with the vertical-power-flux normalization and given by Eq. (II.48). For this normalization, the coupling operator becomes

$$-\hat{L}^{-1}(\partial_3\hat{L})=\begin{pmatrix}\hat{T} & \hat{R}\\ \hat{R} & \hat{T}\end{pmatrix}, \tag{IV.2}$$

in which

$$\hat{T}=-\tfrac{1}{4}\hat{\Gamma}^{-1/2}[\hat{\Gamma},\,\hat{A}_{1,2}^{-1}(\partial_3\hat{A}_{1,2})]\hat{\Gamma}^{-1/2}-\tfrac{1}{2}[\hat{\Gamma}^{1/2},\,(\partial_3\hat{\Gamma}^{-1/2})], \tag{IV.3}$$

where we have used the property that $\hat{\Gamma}^{1/2}(\partial_3\hat{\Gamma}^{-1/2})=-(\partial_3\hat{\Gamma}^{1/2})\hat{\Gamma}^{-1/2}$, is the *transmission* operator that consists of commutators only, and

$$\begin{aligned}\hat{R}&=-\tfrac{1}{4}\hat{\Gamma}^{-1/2}([\hat{\Gamma},\,\hat{A}_{1,2}^{-1}(\partial_3\hat{A}_{1,2})]+2\hat{A}_{1,2}^{-1}(\partial_3\hat{A}_{1,2})\hat{\Gamma}-2(\partial_3\hat{\Gamma}))\hat{\Gamma}^{-1/2}\\&=-\tfrac{1}{4}\hat{\Gamma}^{-1/2}\{\hat{\Gamma},\hat{A}_{1,2}^{-1}(\partial_3\hat{A}_{1,2})\}\hat{\Gamma}^{-1/2}-\tfrac{1}{2}\{\hat{\Gamma}^{1/2},(\partial_3\hat{\Gamma}^{-1/2})\},\end{aligned} \tag{IV.4}$$

where {.,.} denotes the anticommutator, is the *reflection* operator. In the limit of a horizontally homogeneous medium (or as $s\to\infty$), the physical interpretation of Eq. (IV.1) simplifies since then $\hat{L}^{-1}(\partial_3\hat{L})$ becomes purely off-diagonal. In this case, therefore only counter-propagating constituents interact. This property reveals the consistency of the decomposition method with asymptotic ray theory.

The reflection and transmission operators are bounded and vanish, due to our initial assumption of a homogeneous, isotropic embedding, outside a closed interval along the x_3-direction. To show the boundedness, note that the multiplication operator,

$$\hat{A}_{1,2}^{-1}(\partial_3\hat{A}_{1,2}):\ H^s\to H^s\quad\text{with}\ \hat{A}_{1,2}^{-1}(\partial_3\hat{A}_{1,2})\in C_0^\infty, \tag{IV.5}$$

is bounded for all H^s. Further, $\hat{\Gamma}^{1/2}(\partial_3\hat{\Gamma}^{-1/2})=-(\partial_3\hat{\Gamma}^{1/2})\hat{\Gamma}^{-1/2}$: $H^r\to H^{r+l}$ with $0\leqslant l\leqslant 2$ are bounded. Thus, the norms of the reflection and transmission operators in $\mathbb{R}^2$ can be estimated as

$$\begin{aligned}\|\hat{T}\|_{r,r}\leqslant C_{r,1}^T\,[&\|\hat{\Gamma}^{-1/2}\|_{r-1/2,r}\|\hat{A}_{1,2}^{-1}(\partial_3\hat{A}_{1,2})\|_{r-1/2,r-1/2}\|\hat{\Gamma}^{1/2}\|_{r,r-1/2}\\&+\|\hat{\Gamma}^{1/2}\|_{r+1/2,r}\|\hat{A}_{1,2}^{-1}(\partial_3\hat{A}_{1,2})\|_{r+1/2,r+1/2}\|\hat{\Gamma}^{-1/2}\|_{r,r+1/2}]+C_{r,2}^T\,\|[\hat{\Gamma}^{1/2},(\partial_3\hat{\Gamma}^{-1/2})]\|_{r,r}\end{aligned} \tag{IV.6}$$

and

$$\begin{aligned}\|\hat{R}\|_{r,r}\leqslant C_{r,1}^R\,[&\|\hat{\Gamma}^{-1/2}\|_{r-1/2,r}\|\hat{A}_{1,2}^{-1}(\partial_3\hat{A}_{1,2})\|_{r-1/2,r-1/2}\|\hat{\Gamma}^{1/2}\|_{r,r-1/2}\\&+\|\hat{\Gamma}^{1/2}\|_{r+1/2,r}\|\hat{A}_{1,2}^{-1}(\partial_3\hat{A}_{1,2})\|_{r+1/2,r+1/2}\|\hat{\Gamma}^{-1/2}\|_{r,r+1/2}]+C_{r,2}^R\,\|\{\hat{\Gamma}^{1/2},(\partial_3\hat{\Gamma}^{-1/2})\}\|_{r,r}\end{aligned} \tag{IV.7}$$

uniformly in $s\geqslant s_0>0$.

So far we have replaced Eq. (II.9) by Eqs. (IV.1) and (II.17). Equation (IV.1) shows that at this stage the vertical derivative operator needs further analysis. To illustrate how the source distributions control the space to which the wave matrix belongs, suppose that $\hat{f}_k \in H^r$ and $\hat{q} \in H^{r-1}$. Then $\hat{N}_1 \in H^r$ and $\hat{N}_2 \in H^{r-1}$ [cf. Eqs. (II.15) and (II.16)]. In accordance with the matrix operator in Eq. (II.9), $\hat{F}_1 \in H^{r+1}$ and $\hat{F}_2 \in H^r$. Further, we have $\hat{A}_{1,2}$: $H^{r(+1)} \to H^{r(+1)}$, whereas $\hat{A}_{2,1}$: $H^{r+1} \to H^{r-1}$ [cf. Eqs. (II.12)–(II.14)]. In view of Eq. (II.48) we then arrive at $\hat{W}_M \in H^{r+1/2}$. In practice, we set $r = -\frac{1}{2}$.

A. Factorization of the "Helmholtz" operator

If we constrain our configuration to a vertically homogeneous (thin) slab, the directional decomposition implies a factorization of the Laplace-domain analog of the second-order wave equation. Using Eq. (II.40), we find that

$$(\partial_3 + s\hat{\Gamma}^{(+)})(\partial_3 + s\hat{\Gamma}^{(-)}) = \partial_3^2 - s^2\hat{\mathrm{A}}. \tag{IV.8}$$

Indeed, the pressure satisfies the equation [cf. Eq. (II.9)]

$$(\partial_3^2 - s^2\hat{A}_{1,2}\hat{A}_{2,1})\hat{F}_1 = \partial_3\hat{N}_1 - \hat{A}_{1,2}\ s\hat{N}_2. \tag{IV.9}$$

However, it is emphasized that the factorization does not hold in this form for vertically heterogeneous media.

V. THE GENERALIZED VERTICAL SLOWNESS

For the proofs of the basic results in Sec. III, for the evaluation of the resolvent $\hat{R}_\lambda^{(\mathrm{A})}$ and hence of $\hat{\Gamma}$ and $\hat{L}_{I,J}$, as well as in preparation of the evaluation (and the associated numerical implementation with respect to a Fourier basis) of the Green's functions belonging to the left-hand side of Eq. (IV.1), the calculus of pseudo-differential operators is employed. An overview of the pseudo-differential-operator calculus can be found in several textbooks.[11,40–42]

It is obvious that $\hat{\mathrm{A}}$: $H^r \to H^{r-2}$ can be interpreted as a pseudo-differential operator of order 2. The existence of the resolvent, via a parametrix, as a pseudo-differential operator has been shown by Seeley,[9] Section 6. As a consequence of this, the vertical slowness operator $\hat{\Gamma} = \hat{\mathrm{A}}^{1/2}$: $H^r \to H^{r-1}$ can be represented by a pseudo-differential operator of order 1.

A. General considerations

First, we present some rules for a general pseudo-differential operator $\hat{\Gamma}$: $H^r \to H^{r-d}$ of order d; later on, we will focus our attention on the particular case of the vertical slowness operator for which $d = 1$.

The Fourier transformation in the horizontal plane is defined as

$$\tilde{\hat{u}}(\alpha_\mu, x_3, s) = \int_{x_\mu \in \mathbb{R}} \hat{u}(x_m, s)\exp(is\alpha_\mu x_\mu)\,dx_1\,dx_2. \tag{V.1}$$

Here, $i\alpha_\mu$ are identified as the horizontal slownesses. Now, the Sobolev norm (with parameter s) on H^r is written as (in view of Plancherel's theorem)

$$\|\hat{u}\|_r^2 = \left(\frac{s}{2\pi}\right)^2 \int_{\alpha_\mu \in \mathbb{R}} [|\tilde{\hat{u}}(\alpha_\mu, x_3, s)|\ \ [(\langle c^{-2}\rangle + \alpha_\sigma\alpha_\sigma)^{1/2}]^r]^2\,d\alpha_1\,d\alpha_2. \tag{V.2}$$

In the space domain, $i\alpha_\lambda$ corresponds to the *horizontal slowness* operator

$$D_\lambda = -\frac{1}{s}\,\partial_\lambda. \tag{V.3}$$

Note that D_λ and the multiplication by x_κ do not commute, since

$$[x_\kappa,\, D_\lambda] = \frac{1}{s}\,\delta_{\kappa,\lambda}\,. \tag{V.4}$$

However, in the limit $s\to\infty$ the commutator vanishes. By letting the operator $\hat{\Gamma}$ act on a Fourier component $\exp(-is\alpha_\mu x_\mu)$ we introduce its left symbol $\hat{\gamma}(x_\kappa,\alpha_\lambda)$,

$$\hat{\Gamma}(x_\kappa,D_\lambda)\exp(-is\alpha_\mu x_\mu) = \hat{\gamma}(x_\kappa,\alpha_\lambda)\exp(-is\alpha_\mu x_\mu). \tag{V.5}$$

For a general test function $\hat{u}$ this implies

$$(\hat{\Gamma}(x_\kappa,D_\lambda)\hat{u})(x_\mu) = \int_{x'_\nu\in\mathbb{R}} \hat{\mathscr{C}}(x_\mu,x'_\nu)\hat{u}(x'_\nu)dx'_1dx'_2\,, \tag{V.6}$$

in which, with the use of Eq. (V.1),

$$\hat{\mathscr{C}}(x_\mu,x'_\nu) = \left(\frac{s}{2\pi}\right)^2 \int_{\alpha_\nu\in\mathbb{R}} \hat{\gamma}(x_\mu,\alpha_\nu)\exp[is\alpha_\nu(x'_\nu-x_\nu)]d\alpha_1d\alpha_2\,. \tag{V.7}$$

Here, $\hat{\mathscr{C}}$ is called the Schwartz kernel of the pseudo-differential operator $\hat{\Gamma}$. The left symbol and the Schwartz kernel are related through the Fourier transformation [cf. Eq. (V.7)]

$$\hat{\gamma}(x_\mu,\alpha_\lambda) = \int_{x'_\nu\in\mathbb{R}} \hat{\mathscr{C}}(x_\mu,x'_\nu)\exp[is(x_\lambda-x'_\lambda)\alpha_\lambda]dx'_1dx'_2\,. \tag{V.8}$$

In the horizontal space Fourier-transform domain Eq. (V.6) becomes

$$(\hat{\Gamma}\tilde{u})(\alpha_\mu) = \left(\frac{s}{2\pi}\right)^2 \int_{\alpha'_\nu\in\mathbb{R}} \tilde{\gamma}(\alpha_\mu-\alpha'_\mu,\alpha'_\nu)\tilde{u}(\alpha'_\nu)d\alpha'_1d\alpha'_2\,, \tag{V.9}$$

where $\tilde{\Gamma}$ is defined as

$$(\hat{\Gamma}\tilde{u})(\alpha_\mu) = \int_{x_\nu\in\mathbb{R}} \exp(is\alpha_\mu x_\mu)\hat{\Gamma}(x_\kappa,D_\lambda)\hat{u}(x_\nu)dx_1dx_2 \tag{V.10}$$

and $\tilde{\gamma}$ as

$$\tilde{\gamma}(\alpha_\mu,\alpha'_\nu) = \int_{x_\nu\in\mathbb{R}} \exp(is\alpha_\mu x_\mu)\,\hat{\gamma}(x_\mu,\alpha'_\nu)dx_1dx_2\,. \tag{V.11}$$

Equation (V.9) explicitly shows the interaction between the different Fourier components (see also Refs. 43–45). The quantity $\tilde{\gamma}$ is denoted as the *cokernel*[42] of $\hat{\Gamma}$. Its representation is useful for numerical computations.

The notation in Eq. (V.6) is justified by the fact that if $\hat{\gamma}$ would be a polynomial in α_λ, as is the case when $\hat{\Gamma}$ is a partial differential operator, then $\hat{\Gamma}$ would be obtained from $\hat{\gamma}$ by replacing $i\alpha_\lambda$ by D_λ put to the right of the coefficients. Still, we omit the dependencies of $\hat{\gamma}$ and $\hat{u}$ on x_3 and s for the time being. The integral in Eq. (V.6) converges with Eq. (V.7) even when $\hat{\gamma}$ becomes large, as long as $\hat{\gamma}$ oscillates more slowly than the exponential. The Schwartz kernel [cf. Eq. (V.7)] is a so-called oscillatory integral. To guarantee that the right-hand side of Eq. (V.7) exists as a distribution, the symbol $\hat{\gamma}$ must lie in a space $S^d(\mathbb{R}^2\times\mathbb{R}^2)$, d being a real number, which means that for all m_1,m_2,n_1,n_2 there exists a constant C_{m_1,m_2,n_1,n_2} such that (Ref. 11, Definition 18.1.1)

$$|(\partial_{\alpha_1}^{m_1}\partial_{\alpha_2}^{m_2}\partial_{x_1}^{n_1}\partial_{x_2}^{n_2}\hat{\gamma})(x_\kappa,\alpha_\lambda)| \leqslant C_{m_1,m_2,n_1,n_2}[(\langle c^{-2}\rangle+\alpha_\sigma\alpha_\sigma)^{1/2}]^{d-m_1-m_2} \tag{V.12}$$

for all $x_\kappa \in \mathbb{R}$, $\alpha_\lambda \in \mathbb{R}$. The constant C_{m_1,m_2,n_1,n_2} may depend on s but is $O(1)$ as $s\to\infty$. The number d is called the order of the space S^d. We write $S^{-\infty} = \cap_{d\in\mathbb{R}} S^d$. Under the condition Eq. (V.12) it follows that $\hat{\mathscr{C}}$ is a distribution of order $\leqslant k$ with $k>d+2$ (Ref. 46, Theorem 7.8.2 and Appendix A), while $\hat{\Gamma}$: $H^r\to H^{r-d}$ is continuous (Ref. 11, Theorem 18.1.13) and d is the so-called order of the operator; the corresponding operator norm associated with the Sobolev norm with parameter is $O(1)$ as $s\to\infty$ if the symbol is $O(1)$. Then the kernel is smooth outside the diagonal in $\mathbb{R}^2\times\mathbb{R}^2$. The space of pseudo-differential operators of which the left symbols are in S^d is denoted by Op S^d. It is observed that Op $S^{-\infty}$ is the space of operators the Schwartz kernels of which are in $C^\infty(\mathbb{R}^2\times\mathbb{R}^2)$. The expansions of symbols to be considered later on will all be mod $S^{-\infty}$.

B. The equation for the slowness surface

The left symbol $\hat{a}=\hat{a}(x_\mu,\alpha_\nu)$ of the normalized elliptic differential operator given in Eq. (II.45),

$$\begin{aligned}\hat{\mathrm{A}} &= -\rho^{1/2}s^{-1}\partial_\nu(\rho^{-1}s^{-1}\partial_\nu(\rho^{1/2}\,))+\kappa\rho \\ &= -s^{-2}\partial_\nu\partial_\nu+\kappa\rho+\tfrac{3}{4}\rho^{-2}s^{-2}(\partial_\nu\rho)^2-\tfrac{1}{2}\rho^{-1}s^{-2}(\partial_\nu\partial_\nu\rho),\end{aligned} \tag{V.13}$$

using Eq. (V.5), is obtained as

$$\hat{a}=\alpha_\nu\alpha_\nu+\kappa\rho+\tfrac{3}{4}\rho^{-2}s^{-2}(\partial_\nu\rho)^2-\tfrac{1}{2}\rho^{-1}s^{-2}(\partial_\nu\partial_\nu\rho). \tag{V.14}$$

The latter expression is real valued, while terms $O(s^{-1})$ do not occur. The symbol lies in S^2 (note that the third- and higher-order derivatives with respect to α_ν vanish and that the volume density of mass and the compressibility together with their derivatives are bounded functions of position in space). The corresponding Schwartz kernel is given by

$$\begin{aligned}\hat{\mathscr{C}}(x_\mu,x'_\mu) &= -s^{-2}\partial_\nu\partial_\nu\delta(x_\mu-x'_\mu) \\ &\quad +[\kappa\rho+\tfrac{1}{2}\rho^{-1}s^{-2}\{\tfrac{3}{2}\rho^{-1}(\partial_\nu\rho)^2-(\partial_\nu\partial_\nu\rho)\}](x_\mu)\,\delta(x_\mu-x'_\mu),\end{aligned} \tag{V.15}$$

with as its support $x_\mu = x'_\mu$, i.e., the diagonal in $\mathbb{R}^2\times\mathbb{R}^2$.

To transform the operator equation (II.44) into an equation for the corresponding left symbols, we consider the composition of two pseudo-differential operators. Representing the operators as in Eqs. (V.6) and (V.7), the composition rule for the respective left symbols is found (see the Appendix). Application of this rule yields the definition of the generalized slowness surface as the solutions $\hat{\gamma}^{(\pm)}\in S^1$ of [cf. Eq. (V.14)]

$$\begin{aligned}&-\left(\frac{s}{2\pi}\right)^2\int_{x'_\nu\in\mathbb{R}}\int_{\alpha'_\nu\in\mathbb{R}}\hat{\gamma}(x_\mu,\alpha'_\lambda)\exp[is(x_\sigma-x'_\sigma)(\alpha_\sigma-\alpha'_\sigma)]\,\hat{\gamma}(x'_\lambda,\alpha_\nu)\,d\alpha'_1 d\alpha'_2 dx'_1 dx'_2 \\ &+\alpha_\nu\alpha_\nu+\kappa\rho+\tfrac{3}{4}\rho^{-2}s^{-2}(\partial_\nu\rho)^2-\tfrac{1}{2}\rho^{-1}s^{-2}(\partial_\nu\partial_\nu\rho)=0.\end{aligned} \tag{V.16}$$

The branches are $\hat{\gamma}^{(\pm)}(x_\kappa,\alpha_\lambda)$ such that

$$\mathrm{Re}\{\hat{\gamma}^{(+)}(x_\mu,\alpha_\nu)\}\geqslant 0 \quad \text{and} \quad \mathrm{Re}\{\hat{\gamma}^{(-)}(x_\mu,\alpha_\nu)\}\leqslant 0.$$

Due to the isotropy (up/down symmetry) of the medium we have $\hat{\gamma}^{(+)}=-\hat{\gamma}^{(-)}$. Further, note that as $s\to\infty$ the composition of symbols tends to an ordinary multiplication. The solution of the

associated equation for the slowness surface yields the principal vertical slowness, which coincides pointwise with the vertical gradient of travel time along a characteristic.

So far, we had to assume that the medium properties (i.e., the coefficients in the elliptic operator) were smooth. This condition can be somewhat relaxed. Media, in which discontinuities in their physical properties occur, should be smoothed on the scale of the irradiating pulse width with the aid of equivalent medium averaging. To allow singularities in the medium and the volume source densities to coexist, however, requires a novel analysis of pseudo-differential operators.[47] Further, our analysis in the horizontal plane builds on the one on the torus; thus, we have chosen to use left symbols rather than Weyl symbols (Ref. 11, Sections 18.4 and 18.5) in this paper.

VI. THE GREEN'S FUNCTIONS OF THE ONE-WAY WAVE OPERATORS

We now subject the left-hand side of Eq. (IV.1) to a further investigation. In it, we recognize the operators

$$\partial_3+s\hat{\Gamma}^{(\pm)}\colon\ \mathscr{S}(\mathbb{R}_{\pm},H^r(\mathbb{R}^2))\rightarrow\mathscr{S}(\mathbb{R}_{\pm},H^{r-1}(\mathbb{R}^2)), \tag{VI.1}$$

where $\mathscr{S}(\mathbb{R}_{\pm},H^r(\mathbb{R}^2))$, denotes a Banach space of maps $\mathbb{R}_{\pm}\rightarrow H^r(\mathbb{R}^2)$. The operators in Eq. (VI.1) are the full one-way wave operators. A technical complication arises because the operators in Eq. (VI.1) cannot be identified as pseudo-differential operators $H^r(\mathbb{R}^2\times\mathbb{R})\rightarrow H^{r-1}(\mathbb{R}^2\times\mathbb{R})$ (see also Ref. 41).

To arrive at the coupled system of integral equations that is equivalent to Eq. (IV.1) and that can be solved in terms of a Neumann expansion, we have to invert the operator occurring on the left-hand side. The one-sided elementary kernels $\hat{\mathscr{G}}^{(\pm)}(x_\mu,x_3;x'_\nu,x'_3)$ associated with the operators

$$\hat{\mathrm{G}}^{(\pm)}=(\partial_3+s\hat{\Gamma}^{(\pm)})^{-1}\colon\ \mathscr{S}(\mathbb{R}_{\pm},H^r(\mathbb{R}^2))\rightarrow\mathscr{S}(\mathbb{R}_{\pm},H^r(\mathbb{R}^2))$$

in three-dimensional space are the so-called Green's functions. They satisfy the equations

$$\partial_3\hat{\mathscr{G}}^{(\pm)}+s\hat{\Gamma}^{(\pm)}\hat{\mathscr{G}}^{(\pm)}=\delta(x_\nu-x'_\nu)\,\delta(x_3-x'_3), \tag{VI.2}$$

together with the condition of causality.

We will consider the case $\hat{\mathrm{G}}=\hat{\mathrm{G}}^{(+)}$, $\hat{\mathscr{G}}=\hat{\mathscr{G}}^{(+)}$, and $\hat{\Gamma}=\hat{\Gamma}^{(+)}$ in detail. The operator $\hat{\mathrm{G}}$ acts on a test function $\hat{u}$ as

$$(\hat{\mathrm{G}}\hat{u})(x_\mu,x_3)=\int_{\zeta\in\mathbb{R}}\int_{x'_\nu\in\mathbb{R}}\hat{\mathscr{G}}(x_\mu,x_3;x'_\nu,\zeta)\hat{u}(x'_\nu,\zeta)dx'_1dx'_2d\zeta. \tag{VI.3}$$

Let us define the initial-value problem of determining the function $\hat{U}(x_\mu,x_3;\zeta)$ satisfying

$$(\partial_3+s\hat{\Gamma})\hat{U}=0\quad\text{for } x_3\geqslant\zeta,\quad \hat{U}(x_\mu,\zeta;\zeta)=\hat{u}(x_\mu,\zeta). \tag{VI.4}$$

Then it is observed that

$$(\hat{\mathrm{G}}\hat{u})(x_\mu,x_3)=\int_{\zeta=-\infty}^{x_3}\hat{U}(x_\mu,x_3;\zeta)d\zeta. \tag{VI.5}$$

A. Properties of the inverse one-way wave operator

Now, to estimate in a proper norm the operator $\hat{\mathrm{G}}$, let

$$\hat{\Gamma}=\hat{\mathrm{L}}+\hat{\mathrm{E}}, \tag{VI.6}$$

where

$$\hat{\mathrm{L}}=[-s^{-2}\partial_\sigma\partial_\sigma+c_L^{-2}]^{1/2} \tag{VI.7}$$

is an elliptic operator independent of x_3 (which can be identified as the vertical slowness operator of order 1 in a homogeneous medium with slowness c_L^{-1}) and where

$$\hat{\mathrm{E}}=\hat{\Gamma}-\hat{\mathrm{L}} \tag{VI.8}$$

is a pseudo-differential operator of order $\leqslant 0$. Note that [cf. Eq. (V.1) and below]

$$\|\hat{\mathrm{L}}\hat{u}\|_r\geqslant c_L^{-1}\|\hat{u}\|_r \tag{VI.9}$$

uniformly in s (and x_3). In this framework, our initial-value problem is written as

$$(\partial_3+s\hat{\mathrm{L}})\hat{U}=-s\hat{\mathrm{E}}\hat{U}\quad\text{for } x_3\geqslant x_3',\quad \hat{U}(x_\mu,x_3';x_3')=\hat{u}(x_\mu,x_3'). \tag{VI.10}$$

Thus, the causal or one-sided propagator $\hat{U}$ satisfies [cf. Eq. (VI.10)]

$$\hat{U}(x_3;x_3')=\exp[-s(x_3-x_3')\hat{\mathrm{L}}]\hat{U}(x_3';x_3')-s\int_{\zeta=x_3'}^{x_3}\exp[-s(x_3-\zeta)\hat{\mathrm{L}}]\ \hat{\mathrm{E}}(\zeta)\hat{U}(\zeta;x_3')d\zeta. \tag{VI.11}$$

Taking Sobolev norms on both sides yields on account of Eq. (VI.9)

$$\begin{aligned}\|\hat{U}(x_3;x_3')\|_r\leqslant&\exp[-s(x_3-x_3')c_L^{-1}]\|\hat{U}(x_3';x_3')\|_r\\&+s\int_{\zeta=x_3'}^{x_3}\exp[-s(x_3-\zeta)c_L^{-1}]\|\hat{\mathrm{E}}(\zeta)\|_{r,r}\|\hat{U}(\zeta;x_3')\|_r\,d\zeta.\end{aligned} \tag{VI.12}$$

Now, let

$$w(x_3)=\exp(sx_3c_L^{-1})\|\hat{U}(x_3;x_3')\|_r, \tag{VI.13}$$

then Eq. (VI.12) leads to

$$w(x_3)\leqslant w(x_3')+s\,\eta\int_{\zeta=x_3'}^{x_3}w(\zeta)d\zeta, \tag{VI.14}$$

where (note that $\hat{\mathrm{E}}$ must be bounded)

$$\eta(c_L^{-1})=\sup_{x_3\in\mathbb{R}}\|\hat{\mathrm{E}}(x_3)\|_{r,r}. \tag{VI.15}$$

(In view of the structure of $\hat{\Gamma}$ note that η depends on s but that an estimate can be given uniformly in s for values away from zero). Application of Gronwall's theorem (Ref. 48, p. 37) to Eq. (VI.14) yields

$$w(x_3)\leqslant w(x_3')\exp[s\,\eta\,(x_3-x_3')], \tag{VI.16}$$

for $x_3\geqslant x_3'$, so that upon using Eq. (VI.13) we have

$$\|\hat{U}(x_3;x_3')\|_r\leqslant\|\hat{U}(x_3';x_3')\|_r\exp[-s(x_3-x_3')(c_L^{-1}-\eta)] \tag{VI.17}$$

for $x_3 \geqslant x_3'$. To find a useful estimate for the norm of $\hat{\mathrm{G}}$, c_L^{-1} must be chosen such that $c_L^{-1} > \eta(c_L^{-1})$ uniformly in s for $s \geqslant s_0$. Let $\hat{e}$ denote the left symbol of $\hat{\mathrm{E}}$. An expansion for this symbol follows from Eq. (V.16) and the results of Sec. VIII:

$$\hat{e} = (\alpha_\nu \alpha_\nu + c^{-2})^{1/2} - (\alpha_\sigma \alpha_\sigma + c_L^{-2})^{1/2} + C^{(0)}, \tag{VI.18}$$

where $c^{-2} = \kappa\rho$, and $C^{(0)}$ is in S^d, $d \leqslant 0$ independent of c_L. Let

$$\mathsf{m} = \sup_{x_m \in \mathbb{R}^3} |c^{-1} - c_L^{-1}|. \tag{VI.19}$$

In a realistic medium, we can arrange the parameters such that there exists an estimate $\mathsf{m} \leqslant \mathsf{m}_0$ with m_0 independent of c_L. We have

$$|(\alpha_\nu \alpha_\nu + c^{-2})^{1/2} - (\alpha_\sigma \alpha_\sigma + c_L^{-2})^{1/2}| \leqslant \mathsf{m}.$$

Since $C^{(0)}$ is continuous, we find the estimate

$$|\hat{e}(x_m, \alpha_\lambda)| \leqslant \mathsf{m} + c^{(0)}. \tag{VI.20}$$

Further, we obtain

$$\partial_{\alpha_\mu} \hat{e} = \alpha_\mu \frac{(\alpha_\sigma \alpha_\sigma + c_L^{-2})^{1/2} - (\alpha_\nu \alpha_\nu + c^{-2})^{1/2}}{(\alpha_\nu \alpha_\nu + c^{-2})^{1/2} (\alpha_\sigma \alpha_\sigma + c_L^{-2})^{1/2}} + C^{(-1)}, \quad C^{(-1)} = \partial_{\alpha_\mu} C^{(0)}. \tag{VI.21}$$

Since $C^{(-1)} \in S^d$, $d \leqslant -1$, we find the estimate

$$|\partial_{\alpha_\mu} \hat{e}(x_m, \alpha_\lambda)| \leqslant (\mathsf{m} + c^{(-1)}) (\langle c^{-2} \rangle + \alpha_\sigma \alpha_\sigma)^{-1/2} \tag{VI.22}$$

with $c^{(-1)}$ independent of c_L. This way, we can continue to analyze estimates like Eq. (V.12) for $\hat{e}$ up to any order of differentiation. Let c_0 denote the supremum of all $c^{(d)}$ s; the calculus of symbols (and the proof of continuity of pseudo-differential operators[11]) then implies the estimate

$$\sup_{x_3 \in \mathbb{R}} \|\hat{\mathrm{E}}(x_3)\|_{r,r} \leqslant \beta \mathsf{m} + C_0, \quad C_0 = \beta c_0, \quad \beta > 1, \tag{VI.23}$$

where C_0 is independent of c_L. Now, choose c_L so that

$$c_L^{-1} > \beta \mathsf{m} + C_0 \geqslant \eta(c_L^{-1}) = \sup_{x_3 \in \mathbb{R}} \|\hat{\mathrm{E}}(x_3)\|_{r,r}. \tag{VI.24}$$

To be able to find a c_L^{-1}, C_0 must satisfy the inequalities [cf. Eq. (VI.24)]

$$0 < 2C_0 < -(\beta - 1) \sup_{x_m \in \mathbb{R}^3} c^{-1} + (\beta + 1) \inf_{x_m \in \mathbb{R}^3} c^{-1},$$

from which it follows that $\beta > 1$ must be chosen in accordance with the conditions

$$1 \leqslant \frac{\sup_{x_m \in \mathbb{R}^3} c^{-1}}{\inf_{x_m \in \mathbb{R}^3} c^{-1}} < \frac{\beta + 1}{\beta - 1}.$$

Let β_1 satisfy the conditions, and let $\beta=\beta_1+\beta_2$; then $\beta\,\mathsf{m}\leqslant\beta_1\mathsf{m}+\beta_2\mathsf{m}_0$, and $\beta\,\mathsf{m}_0$ can be absorbed in C_0 to recover an estimate of the type Eq. (VI.24). [In a horizontally homogeneous medium we find $\mathsf{m}(c_L^{-1}) = \sup_{x_3\in\mathbb{R}}|c^{-1} - c_L^{-1}|$, hence c_L^{-1} must be chosen in accordance with $c_L^{-1}>\beta(1+\beta)^{-1}\sup_{x_3\in\mathbb{R}}c^{-1}$.]

Now, take Sobolev norms on both sides of Eq. (VI.5):

$$\begin{aligned}\|(\hat{\mathrm{G}}\hat{u})(x_3)\|_r &\leqslant \int_{\zeta=-\infty}^{x_3} \|\hat{U}(x_3;\zeta)\|_r\, d\zeta \\ &\leqslant \int_{\zeta=-\infty}^{x_3} \exp[-s(x_3-\zeta)(c_L^{-1}-\eta)]\, \|\hat{U}(\zeta;\zeta)\|_r\, d\zeta \\ &= \int_{\zeta=-\infty}^{x_3} \exp[-s(x_3-\zeta)(c_L^{-1}-\eta)]\, \|\hat{u}(\zeta)\|_r\, d\zeta. \end{aligned} \tag{VI.25}$$

Apparently, a useful norm on $\mathscr{L}(\mathbb{R}_\pm, H^r(\mathbb{R}^2))$ for the wavefield in three-dimensional space is given by

$$\|\cdot\|_{r;3} = \sup_{x_3\in\mathbb{R}} \|\cdot\|_r . \tag{VI.26}$$

Then, from Eq. (VI.25) it follows that

$$\|\hat{\mathrm{G}}\|_{r;3,r;3} \leqslant \frac{1}{s(c_L^{-1}-\eta)}, \quad s\geqslant s_0 . \tag{VI.27}$$

This estimate has been made explicit for $r=0$ [cf. below Eq. (VI.17)]. Similar steps can be carried out upon replacing $(+)$ by $(-)$.

B. Path integral representations

With the vertical slowness symbols following from the resolvent, which represents the scattering process in the horizontal directions, we can construct the Green's functions $\hat{\mathscr{G}}^{(\pm)}$ using a Hamiltonian path integral representation.[49–51]

First, it is observed that the vertical slowness operators at different levels of x_3 do not necessarily commute with one another due to the heterogeneity of the medium. Thus we arrive at a ''time''-ordered product integral representation (see, e.g., Ref. 50) of the one-sided propagators [cf. Eq. (VI.4)] associated with the one-way wave equations, where ''time'' refers to the vertical coordinate x_3,

$$\hat{U}^{(\pm)}(.,x_3;x_3') = \pm H(\mp[x_3'-x_3]) \left\{ \prod_{\zeta=x_3'}^{x_3} \exp[-s\hat{\Gamma}^{(\pm)}(.,\zeta)d\zeta] \right\} \hat{u}(.,x_3'). \tag{VI.28}$$

In this expression, the operator ordering is initiated by $\exp[-s\hat{\Gamma}(.,x_3')d\zeta]$ acting on $\hat{u}(.,x_3')$ followed by applying $\exp[-s\hat{\Gamma}(.,\zeta)\mathrm{d}\zeta]$ to the result, successively for increasing ζ.

If the medium in the interval $[x_3', x_3]$ were weakly varying in the vertical direction, the Trotter product formula can be applied to the product integral in Eq. (VI.28). This results in the Hamiltonian path integral representations for the Green's functions,

$$\hat{\mathscr{G}}^{(\pm)}(x_\nu,x_3;x_\mu',x_3') = \pm H(\mp[x_3'-x_3]) \int_P \mathscr{D}(x_\nu'',\alpha_\nu'')$$

$$\times\exp\left[-s\int_{\zeta=x_3'}^{x_3}d\zeta\{i\alpha_\sigma''(d_\zeta x_\sigma'')+\hat{\gamma}^{(\pm)}(x_\mu'',\zeta,\alpha_\nu'',s)\}\right], \tag{VI.29}$$

P being a set of paths $(x_\mu''(\zeta),\alpha_\nu''(\zeta))$ in (horizontal) phase space satisfying

$$x_\nu''(\zeta=x_3')=x_\nu', \quad x_\nu''(\zeta=x_3)=x_\nu. \tag{VI.30}$$

Omitting the Heaviside function in the expression for the $\hat{\mathscr{G}}^{(\pm)}$ yields the kernel $\hat{g}^{(\pm)}$ of the so-called *phase shift operator* (Ref. 52). A perturbative approximation of the latter operator based on the split-step Fourier transform is discussed in Ref. 53. In Eq. (VI.29) we have restricted ourselves to causal solutions, since the conditions $\mathrm{Re}\{\hat{\gamma}^{(+)}\}\geqslant 0$ and $\mathrm{Re}\{\hat{\gamma}^{(-)}\}\leqslant 0$ imply that $\hat{\mathscr{G}}^{(\pm)}$ remain bounded as $|x_3|\to\infty$.

The path integral in Eq. (VI.29) is to be interpreted as the lattice multiple integral

$$\begin{aligned}&\hat{\mathscr{G}}^{(\pm)}(x_\nu,x_3;x_\mu',x_3')\\&\quad=\pm H(\mp[x_3'-x_3])\lim_{N\to\infty}\int\prod_{i=1}^{N}\left(\frac{s}{2\pi}\right)^2 d^2\alpha_\nu^{(i)}\prod_{j=1}^{N-1}d^2x_\nu^{(j)}\\&\qquad\times\exp\left[-s\sum_{k=1}^{N}\{i\alpha_\sigma^{(k)}(x_\sigma^{(k)}-x_\sigma^{(k-1)})+\hat{\gamma}^{(\pm)}(x_\mu^{(k)},\zeta_k-\tfrac{1}{2}N^{-1}\Delta x_3,\alpha_\nu^{(k)},s)N^{-1}\Delta x_3\}\right]\end{aligned} \tag{VI.31}$$

with

$$x_\nu^{(0)}=x_\nu', \quad x_\nu^{(N)}=x_\nu, \tag{VI.32}$$

and

$$\Delta x_3=x_3-x_3'. \tag{VI.33}$$

Note that the function

$$\tau(x_\nu,x_\nu')=\sum_{k=1}^{N}\{i\alpha_\sigma^{(k)}(x_\sigma^{(k)}-x_\sigma^{(k-1)})+\hat{\gamma}^{(\pm)}(x_\mu^{(k)},\zeta_k-\tfrac{1}{2}N^{-1}\Delta x_3,\alpha_\nu^{(k)},s)N^{-1}\Delta x_3\}$$

can be associated with travel time along a path. All the integrations are taken over the interval $(-\infty,\infty)$, $N^{-1}\Delta x_3$ is the step size in ζ, and $(x_\mu^{(j)},\alpha_\nu^{(j)})$ are the coordinates of a path at the discrete values ζ_j of ζ as $j=1,\ldots,N$. If Δx_3 is sufficiently small, the path integral reduces to

$$\begin{aligned}\hat{\mathscr{G}}^{(\pm)}(x_\mu,x_3;x_\nu',x_3')\simeq\pm H(\mp[x_3'-x_3])\int\left(\frac{s}{2\pi}\right)^2 d\alpha_1''d\alpha_2''\\\times\exp[-s\{i\alpha_\sigma''(x_\sigma-x_\sigma')+\hat{\gamma}^{(\pm)}(x_\mu,x_3-\tfrac{1}{2}\Delta x_3,\alpha_\nu'',s)\Delta x_3\}].\end{aligned} \tag{VI.34}$$

In the analysis $\hat{\gamma}^{(\pm)}$ may be interpreted as (nonstandard square-root) Hamiltonians.

If the medium varies strongly in the vertical direction, the interval $[x_3',\ x_3]$ is divided up into thinner slabs, and the product integral is used to arrive at a composition of one-sided propagators through these slabs, for which the lattice multiple integrals are then substituted. The resulting

multiple integral is similar to the one in Eq. (VI.31). It is conjectured that the stationary-phase approximation of the path integral in Eq. (VI.29) leads to the leading term of the asymptotic ray expansion[54,55] including the KMAH index,[55] in the presence of caustics.

The expression in Eq. (VI.34) serves as the basis for numerical computations based on Fourier transformations. Rather than using this thin-slab propagator, quasi-Monte Carlo methods can be applied to numerically calculate the propagator over larger vertical distances. Also techniques from the theory of symplectic integrators (Ref. 56) may prove to be useful in the propagation over long distances.

C. The Schwartz kernel

The one-sided Green's function is directly related to the Schwartz kernel associated with the vertical slowness operator. Since [cf. Eqs. (VI.3) and (VI.29)]

$$\partial_3(\hat{\mathrm{G}}\hat{u})(x_\mu,x_3)-\hat{u}(x_\mu,x_3)=\int_{\zeta=-\infty}^{x_3}\int_{x'_\nu\in\mathbb{R}}\partial_3\hat{\mathscr{G}}(x_\mu,x_3;x'_\nu,\zeta)\hat{u}(x'_\nu,\zeta)dx'_1dx'_2d\zeta, \tag{VI.35}$$

while [cf. Eq. (VI.5)]

$$\partial_3(\hat{\mathrm{G}}\hat{u})(x_\mu,x_3)-\hat{u}(x_\mu,x_3)=\int_{\zeta=-\infty}^{x_3}\partial_3\hat{U}(x_\mu,x_3;\zeta)d\zeta$$

for all x_3, we have [cf. Eq. (VI.4)]

$$-s\hat{\Gamma}(.,.;x_3)\hat{U}(.,x_3;\zeta)=\int_{x'_\nu\in\mathbb{R}}\partial_3\hat{\mathscr{G}}(.,x_3;x'_\nu,\zeta)\hat{u}(x'_\nu,\zeta)dx'_1dx'_2. \tag{VI.36}$$

Upon taking the limit $\zeta\uparrow x_3$, we thus obtain

$$-s(\hat{\Gamma}(.,.;x_3)\hat{u})(x_\mu,x_3)=\int_{x'_\nu\in\mathbb{R}}\lim_{\zeta\uparrow x_3}\partial_3\hat{\mathscr{G}}(x_\mu,x_3;x'_\nu,\zeta)\hat{u}(x'_\nu,\zeta)dx'_1dx'_2 \tag{VI.37}$$

so that

$$\hat{\mathscr{C}}(x_\mu,x'_\nu;x_3)=\lim_{\zeta\uparrow x_3}-\frac{1}{s}\,\partial_3\hat{\mathscr{G}}(x_\mu,x_3;x'_\nu,\zeta). \tag{VI.38}$$

This expression implies that, in the special case of a homogeneous medium, the Schwartz kernel reduces to the vertical particle velocity ($\hat{F}_2$) response due to a vertical point-force source [$\hat{f}_3=\delta(x_\mu-x'_\mu)\,\delta(x_3-x'_3)$] at zero vertical offset.

VII. THE BREMMER COUPLING SERIES

The resolvents $\hat{R}^{(\mathrm{A})}_\lambda$ fully describe the scattering in the level surfaces of x_3. From these resolvents the left vertical slowness symbols have been derived, which in their turn are used in constructing the Green's functions introduced in Sec. VI. Employing the Green's functions of the one-way operators, we are now able to formulate the scattering process along the vertical direction in terms of a coupled system of integral equations.

To simplify the notation, we set

$$\hat{X}_1=(\hat{L}^{-1})_{1,M}\hat{N}_M,\quad \hat{X}_2=(\hat{L}^{-1})_{2,M}\hat{N}_M. \tag{VII.1}$$

Using Eq. (VII.1), we rewrite Eq. (IV.1) as [cf. Eqs. (IV.3) and (IV.4)]

$$\partial_3 \hat{W}_1 + s\hat{\Gamma}^{(+)}\hat{W}_1 = \hat{X}_1 + \hat{T}\hat{W}_1 + \hat{R}\hat{W}_2, \tag{VII.2}$$

$$\partial_3 \hat{W}_2 + s\hat{\Gamma}^{(-)}\hat{W}_2 = \hat{X}_2 + \hat{R}\hat{W}_1 + \hat{T}\hat{W}_2. \tag{VII.3}$$

To derive an integral representation for $\hat{W}_{1,2}$, we introduce the *adjoint* Green's functions $\hat{\mathscr{G}}_\alpha^{(\pm)}$ satisfying

$$\partial_3 \hat{\mathscr{G}}_a^{(\pm)} - s[\hat{\Gamma}^{(\pm)}]^T \hat{\mathscr{G}}_a^{(\pm)} = \delta(x_\nu - x'_\nu)\,\delta(x_3 - x'_3), \quad \text{with } [\hat{\Gamma}^{(\pm)}]^T = \hat{\Gamma}^{(\pm)} \tag{VII.4}$$

since $\hat{\Gamma}^{(\pm)}$ is self-adjoint in L^2. Note that

$$\hat{\mathscr{G}}_a^{(\pm)}(x'_\nu, \zeta; x_\mu, x_3) = -\hat{\mathscr{G}}^{(\pm)}(x_\mu, x_3; x'_\nu, \zeta). \tag{VII.5}$$

In fact, in view of the up/down symmetry of the medium, we also have

$$\hat{\mathscr{G}}_a^{(\pm)}(x'_\nu, \zeta; x_\mu, x_3) = \hat{\mathscr{G}}^{(\mp)}(x'_\nu, \zeta; x_\mu, x_3). \tag{VII.6}$$

[Equations (VII.5) and (VII.6) constitute reciprocity relations.] Combining Eq. (VII.4) for the adjoint Green's functions with (VII.2) and (VII.3), it is found that

$$\partial_3 \langle \hat{\mathscr{G}}_a^{(+)}, \hat{W}_1 \rangle_0 = \langle \hat{\mathscr{G}}_a^{(+)}, \hat{X}_1 + \hat{T}\hat{W}_1 + \hat{R}\hat{W}_2 \rangle_0 + \hat{W}_1(x'_\nu, x'_3)\,\delta(x_3 - x'_3), \tag{VII.7}$$

$$\partial_3 \langle \hat{\mathscr{G}}_a^{(-)}, \hat{W}_2 \rangle_0 = \langle \hat{\mathscr{G}}_a^{(-)}, \hat{X}_2 + \hat{R}\hat{W}_1 + \hat{T}\hat{W}_2 \rangle_0 + \hat{W}_2(x'_\nu, x'_3)\,\delta(x_3 - x'_3). \tag{VII.8}$$

Now, we have

$$\langle \hat{\mathscr{G}}_a^{(+)}(.,x_3;x'_\mu,x'_3), \hat{W}_1(.,x_3) \rangle_0 = 0 \tag{VII.9}$$

as $x_3 \to \infty$ since $\hat{\mathscr{G}}_a^{(+)} = 0$ when $x_3 > x'_3$ while in view of the assumption that in some upper half-space the fluid is homogeneous, $\hat{W}_1 = 0$ as $x_3 \to -\infty$ on the basis of causality. A similar reasoning leads to

$$\langle \hat{\mathscr{G}}_a^{(-)}(.,x_3;x'_\mu,x'_3), \hat{W}_2(.,x_3) \rangle_0 = 0 \tag{VII.10}$$

as $x_3 \to \pm\infty$. Integration of Eqs. (VII.7) and (VII.8) over all x_3 then yields a coupled system of integral equations which can be written in operator form as [cf. Eq. (VII.5)]

$$(\delta_{I,J} - \hat{\mathrm{K}}_{I,J})\hat{W}_J = \hat{W}_I^0, \tag{VII.11}$$

in which

$$\begin{pmatrix} \hat{W}_1^0 \\ \hat{W}_2^0 \end{pmatrix} = \begin{pmatrix} \hat{\mathrm{G}}^{(+)} & 0 \\ 0 & \hat{\mathrm{G}}^{(-)} \end{pmatrix} \begin{pmatrix} \hat{X}_1 \\ \hat{X}_2 \end{pmatrix}, \tag{VII.12}$$

i.e.,

$$\hat{W}_1^0(x_\mu, x_3) = \int_{\zeta=-\infty}^{x_3} \int_{x'_\nu \in \mathbb{R}} \hat{\mathscr{G}}^{(+)}(x_\mu, x_3; x'_\nu, \zeta)\hat{X}_1(x'_\nu, \zeta)\,dx'_1 dx'_2 d\zeta, \tag{VII.13}$$

$$\hat{W}_2^0(x_\mu, x_3) = \int_{\zeta=x_3}^{\infty} \int_{x'_\nu \in \mathbb{R}} \hat{\mathscr{G}}^{(-)}(x_\mu, x_3; x'_\nu, \zeta)\hat{X}_2(x'_\nu, \zeta)\,dx'_1 dx'_2 d\zeta \tag{VII.14}$$

denote the directly transmitted waves, and

$$\hat{\mathrm{K}}=\begin{pmatrix}\hat{\mathrm{G}}^{(+)} & 0\\ 0 & \hat{\mathrm{G}}^{(-)}\end{pmatrix}\begin{pmatrix}\hat{T} & \hat{R}\\ \hat{R} & \hat{T}\end{pmatrix} \tag{VII.15}$$

(note that the second matrix operator acts in the horizontal directions only, whereas the first matrix operator acts in the full space), i.e.,

$$(\hat{\mathrm{K}}_{1,1}\hat{W}_1)(x_\mu,x_3)=\int_{\zeta=-\infty}^{x_3}\int_{x'_\nu\in\mathbb{R}}\hat{\mathscr{G}}^{(+)}(x_\mu,x_3;x'_\nu,\zeta)(\hat{T}\hat{W}_1)(x'_\nu,\zeta)dx'_1dx'_2d\zeta, \tag{VII.16}$$

$$(\hat{\mathrm{K}}_{1,2}\hat{W}_2)(x_\mu,x_3)=\int_{\zeta=-\infty}^{x_3}\int_{x'_\nu\in\mathbb{R}}\hat{\mathscr{G}}^{(+)}(x_\mu,x_3;x'_\nu,\zeta)(\hat{R}\hat{W}_2)(x'_\nu,\zeta)dx'_1dx'_2d\zeta, \tag{VII.17}$$

$$(\hat{\mathrm{K}}_{2,1}\hat{W}_1)(x_\mu,x_3)=\int_{\zeta=x_3}^{\infty}\int_{x'_\nu\in\mathbb{R}}\hat{\mathscr{G}}^{(-)}(x_\mu,x_3;x'_\nu,\zeta)(\hat{R}\hat{W}_1)(x'_\nu,\zeta)dx'_1dx'_2d\zeta, \tag{VII.18}$$

$$(\hat{\mathrm{K}}_{2,2}\hat{W}_2)(x_\mu,x_3)=\int_{\zeta=x_3}^{\infty}\int_{x'_\nu\in\mathbb{R}}\hat{\mathscr{G}}^{(-)}(x_\mu,x_3;x'_\nu,\zeta)(\hat{T}\hat{W}_2)(x'_\nu,\zeta)dx'_1dx'_2d\zeta \tag{VII.19}$$

are representative for the multiple scattering formalism. Now, consider the operators $\hat{\mathrm{K}}_{I,J}$: $\mathscr{S}(\mathbb{R}_{\pm},H^0(\mathbb{R}^2))\to\mathscr{S}(\mathbb{R}_{\pm},H^0(\mathbb{R}^2))$. In the space of wave matrices we introduce the norm [cf. Eq. (VI.26)]

$$\|\hat{W}\|=\left(\sum_{J=1}^{2}\|\hat{W}_J\|^2_{0;3}\right)^{1/2}. \tag{VII.20}$$

Hence, $\|\hat{\mathrm{K}}\|^2\leqslant\Sigma_{I,J=1}^{2}\|\hat{\mathrm{K}}_{I,J}\|^2_{0;3,0;3}$. Using the norm estimates of the preceding sections, it is found that $\|\hat{\mathrm{K}}\|=O(s^{-1})$ as $s\to\infty$, which implies that the norm of $\hat{\mathrm{K}}$ is less than 1 when $s\geqslant s_0$, for s_0 sufficiently large. In that case a convergent Neumann expansion of Eq. (VII.11) yields its solution.

Thus, the solution of Eq. (VII.11),

$$\hat{W}=\hat{R}^{(\mathrm{K})}\hat{W}^0, \tag{VII.21}$$

is found in the form of a sum of generalized-ray-like constituents, the Bremmer series,[57] upon employing the Neumann expansion for the resolvent of $\hat{\mathrm{K}}$:

$$\hat{R}^{(\mathrm{K})}=(I-\hat{\mathrm{K}})^{-1}=\sum_{n=0}^{\infty}\hat{\mathrm{K}}^n. \tag{VII.22}$$

To emphasize that we have found the solution of the direct scattering problem as a summation over multiple scattered constituents, we write

$$\hat{W}=\sum_{n=0}^{\infty}\hat{W}^{(n)}\quad\text{with}\quad\hat{W}^{(n)}=\hat{\mathrm{K}}\hat{W}^{(n-1)}. \tag{VII.23}$$

Figure 3 illustrates the decomposition procedure and the interrelation between the different resolvents. The analog of the series in a horizontally shift invariant medium can be found, e.g., in Refs. 58 and 59.

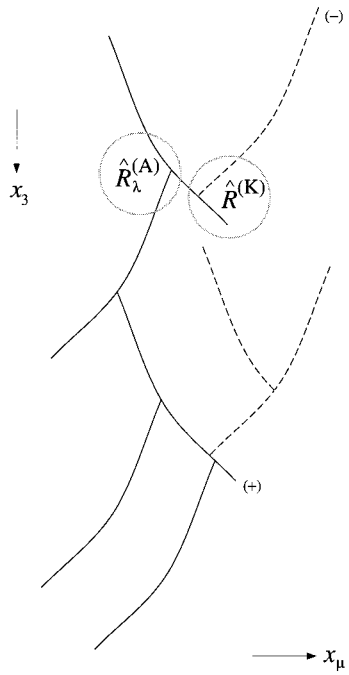

FIG. 3. The decomposition of the scattering process (the solid rays refer to one term in the series).

Upon substituting in $\hat{\mathrm{K}}$ the path integral representations for the Green's functions of Sec. VI, the recursion formula (VII.23) leads to path integral representations for all the constituents in the coupling series. Upon substituting for the transmission/reflection operators their Schwartz kernel representations, Eq. (VII.23) essentially composes path integrals at any level where interaction takes place. In particular, one finds a path integral representation for the leading order backscattered field, $\hat{W}^{(1)}$.

Finally, Eq. (II.17) must be employed to compose the acoustic field matrix per constituent [cf. Eq. (VII.21)], i.e., to obtain the observables. The uniqueness of the time-domain counterpart of this result for $s \geqslant s_0$ is guaranteed by Lerch's theorem (see Ref. 35). Note that the convergence of the series is guaranteed essentially in the time domain; the convergence criterium in the frequency or complex Laplace domain as described by Wing,[60] and earlier by Atkinson,[61] is different from ours. From the final representation of the acoustic field matrix, the associated representation for the Dirichlet-to-Neumann map can be obtained.[29]

VIII. ANALYSIS OF THE SYMBOLS

The scattering process in horizontal space is governed by a composition equation for the (unknown) resolvent of a (known) elliptic operator. Here, we shall discuss an asymptotic expansion for the left symbol of the resolvent belonging to $\hat{\mathrm{A}}$ introduced in Sec. III as the slowness vector becomes large to find the solution of the composition equation (V.16) as well as the other powers needed to transform Eq. (II.9) into Eq. (IV.1). Using the first few terms of the asymptotic expansion, a Neumann series is derived for the resolvent. The latter expansion is the counterpart in horizontal space of the Neumann expansion introduced in Sec. VII.

A natural decomposition of the left symbol of the partial differential operator $\hat{\mathrm{A}}$ is [cf. Eq. (V.14)]

$$\hat{a} = \hat{a}^{(\infty)} + \hat{a}^{(-2)}, \tag{VIII.1}$$

the first term being $O(1)$ and the second term being $O(s^{-2})$ as $s\to\infty$. We have

$$\hat{a}^{(\infty)}=\alpha_\nu\alpha_\nu+\check{c}^{-2}c_\infty^{-2},$$
$$\hat{a}^{(-2)}=\tfrac{3}{4}\rho^{-2}s^{-2}(\partial_\nu\rho)^2-\tfrac{1}{2}\rho^{-1}s^{-2}(\partial_\nu\partial_\nu\rho), \tag{VIII.2}$$

where

$$\check{c}^{-1}=(c/c_\infty)^{-1} \tag{VIII.3}$$

and

$$c^{-2}=\kappa\rho, \tag{VIII.4}$$

in which c_∞^{-1} is an appropriate parameter, introduced to enforce the correct asymptotic behavior. The differential equation for the symbol $\hat{r}_\lambda$ of the resolvent follows from the equation $(\hat{\mathrm{A}}-\lambda I)\hat{R}_\lambda=I$ as [cf. Eq. (VIII.2)]

$$(is^{-1}\partial_{x_\sigma}+\alpha_\sigma)^2\hat{r}_\lambda+(c^{-2}+\hat{a}^{(-2)}-\lambda)\hat{r}_\lambda-1=0. \tag{VIII.5}$$

This equation must be solved for $\hat{r}_\lambda\in S^{-2}$. The left symbols of the negative real powers then follow from [cf. Eq. (III.17)]

$$\hat{a}_z=\frac{1}{2\pi i}\int_{\mathscr{B}}\lambda^z\hat{r}_\lambda\,d\lambda. \tag{VIII.6}$$

The symbols of the positive real powers are obtained using the composition equation for left symbols repeatedly (see the Appendix).

A. The parametrix: asymptotic analysis

To carry out the asymptotic analysis, the symbol of the operator $\hat{\mathrm{A}}-\lambda I$ with parameter is written as

$$\hat{a}_\lambda=\hat{a}_{\lambda,2}+\hat{a}_{\lambda,0}, \tag{VIII.7}$$

where

$$\hat{a}_{\lambda,2}=\hat{a}^{(\infty)}-\lambda,\quad \hat{a}_{\lambda,0}=\hat{a}^{(-2)}. \tag{VIII.8}$$

The correct behavior of the symbol of the resolvent as λ and c_∞^{-1} become large is achieved by thinking of λ and c_∞^{-2} as the squares of the Fourier domain counterparts of two new independent variables. Actually, it is natural to treat the slowness of the medium as if it were a component of the slowness vector. This way, the term $-\lambda$ and the one linear in c_∞^{-2} are absorbed in the principal part of the symbol. It is noticed that $\hat{a}_{\lambda,2}$ is homogeneous of degree 2 in $(\alpha_\mu,\lambda^{1/2},c_\infty^{-1})$, i.e.,

$$\hat{a}_{t^2\lambda,2}(x_\mu,t\alpha_\nu,tc_\infty^{-1})=t^2\hat{a}_{\lambda,2}(x_\mu,\alpha_\nu,c_\infty^{-1}) \tag{VIII.9}$$

for $t>0$ such that $t^2\lambda\in\Lambda$, while $\hat{a}_{\lambda,0}$ is homogeneous of degree 0 in the same sense. Further, it follows that $\hat{a}_{\lambda,2}\neq 0$ for $\lambda\in\Lambda$ and $(\alpha_\sigma\alpha_\sigma)^{1/2}+|\lambda|^{1/2}+|c_\infty^{-1}|\neq 0$, where Λ is, again, the sector in the complex λ plane defined by $0<|\arg(\lambda)|\leqslant\pi$. Hence, the operator associated with $\hat{a}_\lambda$ is ''elliptic with parameters λ and c_∞^{-1},'' whereas the symbol itself is in $S^2_\Lambda(\mathbb{R}^2\times\mathbb{R}^2,\mathbb{R})$. The extension of this concept to anisotropic elastic media has been given by de Hoop and de Hoop.[62] In the following it is crucial to restrict λ to the sector Λ in the complex plane.

Consider the *parametrix* $\hat{B}_\lambda$, which is an approximation to the resolvent $\hat{R}_\lambda$ in the following sense. Let the symbol of the resolvent, too, be expanded in a sum of symbols $b_{\lambda,-2-j}$ which are homogeneous of degree $-2-j$ in $(\alpha_\mu,\lambda^{1/2},c_\infty^{-1})$; then this sum defines the parametrix, which resembles the resolvent up to an integral operator in Op $S^{-\infty}$ with an infinitely differentiable kernel (Ref. 63, p. 20). The successive terms in the series have increasingly smooth kernels. This way, a parametrix is constructed with the correct behavior as $|\lambda|\to\infty$ or $c_\infty^{-1}\to\infty$ (the latter corresponds to $s\to\infty$). Thus, the symbol of the parametrix is written as

$$\hat{b}_\lambda=\sum_{j=0}^{\infty}\hat{b}_{\lambda,-2-j}. \tag{VIII.10}$$

The terms $\hat{b}_{\lambda,-2-j}$, $j=0,1,...$, are determined as follows. Substitute the expansion Eq. (VIII.10) into Eq. (VIII.5) and collect terms of equal degrees. Then we arrive at

$$\begin{aligned}&\hat{a}_{\lambda,2}\hat{b}_{\lambda,-2}=1,\\ &\hat{a}_{\lambda,2}\hat{b}_{\lambda,-3}+2is^{-1}\alpha_\mu\partial_{x_\mu}\hat{b}_{\lambda,-2}=0,\\ &\hat{a}_{\lambda,2}\hat{b}_{\lambda,-2-j}+2is^{-1}\alpha_\mu\partial_{x_\mu}\hat{b}_{\lambda,-1-j}+[\hat{a}_{\lambda,0}-s^{-2}\partial_{x_\mu}\partial_{x_\mu}]\hat{b}_{\lambda,-j}=0,\quad j=2,3,\dots .\end{aligned} \tag{VIII.11}$$

It can be shown that the solutions must satisfy (following Ref. 9)

$$\begin{aligned}|(\partial_{\alpha_1}^{m_1}\partial_{\alpha_2}^{m_2}\partial_{x_1}^{n_1}\partial_{x_2}^{n_2}\hat{b}_{\lambda,-2-j})(x_\kappa,\alpha_\mu)|\le s^{-j}C_{m_1,m_2,n_1,n_2}&[(\langle c^{-2}\rangle+\alpha_\nu\alpha_\nu+c_\infty^{-2}+|\lambda|)^{1/2}]^{-2}\\ &\times[(\langle c^{-2}\rangle+\alpha_\sigma\alpha_\sigma)^{1/2}]^{-j-m_1-m_2}.\end{aligned} \tag{VIII.12}$$

For the asymptotic sum as following from Eq. (VIII.11), we have the estimate

$$\hat{b}_\lambda-\sum_{j=0}^{K-1}\hat{b}_{\lambda,-2-j}=O(|\alpha|^{-2-K})\quad\text{as }|\alpha|\to\infty \tag{VIII.13}$$

for $K=1,2,3,...$. Let $\hat{B}_{\lambda,-2-j}$ be the operator that corresponds to the symbol $\hat{b}_{\lambda,-2-j}$, and let

$$\hat{B}_\lambda^{(K)}=\sum_{j=0}^{K-1}\hat{B}_{\lambda,-2-j}. \tag{VIII.14}$$

From Eq. (VIII.12), using that for $l=0,1,2$ we have

$$[(\langle c^{-2}\rangle+\alpha_\nu\alpha_\nu+c_\infty^{-2}+|\lambda|)^{1/2}]^{-2}\le|\lambda|^{-1+l/2}\,[(\langle c^{-2}\rangle+\alpha_\nu\alpha_\nu+c_\infty^{-2})^{1/2}]^{-l}, \tag{VIII.15}$$

we obtain the estimate for $\hat{B}_\lambda^{(K)}$:

$$\|\hat{B}_\lambda^{(K)}\|_{r,r+l}\le C''_{r,l,K}/|\lambda|^{1-l/2} \tag{VIII.16}$$

with $l=0,1,2$ and $\lambda\in\Lambda$. With $\hat{B}_\lambda^{(K)}$ there is associated the truncated expansion of $\hat{A}$, viz., $\hat{A}^{(K)}=\Sigma_{j'=0}^{K-1}\hat{A}_{2-j'}$ (set $\hat{a}_2=\hat{a}^{(\infty)}$, $\hat{a}_0=\hat{a}^{(-2)}$, $\hat{a}_{j'}=0$ otherwise). In general, if $K\ge2$ we have $\hat{A}-\hat{A}^{(K)}\in\text{Op }S^0$, so that the latter difference is bounded and continuous as an operator $H^r\to H^r$; the same holds for $\hat{A}-\hat{A}^{(K)}$: $H^r\to H^{r+K-2}$. Using this and Eq. (VIII.16), it follows that for $K\ge2$

$$\|(\hat{A}-\lambda I)\hat{B}_\lambda^{(K)}-(\hat{A}^{(K)}-\lambda I)\hat{B}_\lambda^{(K)}\|_{r,r+l+K-2}\le C'_{r,l,K}/|\lambda|^{1-l/2}. \tag{VIII.17}$$

Using Eqs. (A15), (VIII.11), and (VIII.12), after some manipulations as in Refs. 9 and 10, we arrive at

$$\|I-(\hat{\mathrm{A}}-\lambda I)\hat{B}_{\lambda}^{(K)}\|_{r,r+l+K-2}\leqslant C_{r,l,K}/|\lambda|^{1-l/2} \tag{VIII.18}$$

with $l=0,1,2$ and $\lambda\in\Lambda$, whereas $C_{r,l,K}=O(s^{-K})$ as $s\to\infty$. Hence, for $K=2$, setting

$$\hat{C}_{\lambda}=I-(\hat{\mathrm{A}}-\lambda I)\hat{B}_{\lambda}^{(2)}, \tag{VIII.19}$$

we get for sufficiently large λ [cf. Eq. (VIII.18)]

$$\|\hat{C}_{\lambda}\|_{r,r}\leqslant\tfrac{1}{2}. \tag{VIII.20}$$

Thus, the resolvent follows as the convergent Neumann series

$$\hat{R}_{\lambda}=\hat{B}_{\lambda}^{(2)}\left(\sum_{n=0}^{\infty}\hat{C}_{\lambda}^{n}\right)\quad\text{for }\lambda\in\Lambda\text{ large.} \tag{VIII.21}$$

Now, using that

$$\sum_{n=0}^{\infty}\|\hat{C}_{\lambda}^{n}\|_{r+l,r+l}\leqslant 2, \tag{VIII.22}$$

in combination with Eq. (VIII.16), finally leads to the estimate in Eq. (III.14). Following Ref. 9 (Theorem 2), through the explicit evaluation of the symbols [cf. Eq. (VIII.6)] it can be shown that the integral in Eq. (III.17) defines a pseudo-differential operator of order $2z$.

Solving the system of equations (VIII.11) yields

$$\hat{b}_{\lambda,-2}=\hat{a}_{\lambda,2}^{-1}, \tag{VIII.23}$$

$$\hat{b}_{\lambda,-3}=2\alpha_{\mu}(is^{-1}\partial_{x_{\mu}}\hat{a}_{\lambda,2})\;\hat{a}_{\lambda,2}^{-3}, \tag{VIII.24}$$

while

$$\begin{aligned}\hat{b}_{\lambda,-4}=&-\hat{a}_{\lambda,0}\;\hat{a}_{\lambda,2}^{-2}-s^{-2}(\partial_{x_{\mu}}\partial_{x_{\mu}}\hat{a}_{\lambda,2})\;\hat{a}_{\lambda,2}^{-3}+[2s^{-2}(\partial_{x_{\mu}}\hat{a}_{\lambda,2})(\partial_{x_{\mu}}\hat{a}_{\lambda,2})\\&+4\alpha_{\mu}s^{-1}\alpha_{\nu}s^{-1}(\partial_{x_{\mu}}\partial_{x_{\nu}}\hat{a}_{\lambda,2})]\;\hat{a}_{\lambda,2}^{-4}-12(\alpha_{\mu}s^{-1}\partial_{x_{\mu}}\hat{a}_{\lambda,2})\\&\times(\alpha_{\nu}s^{-1}\partial_{x_{\nu}}\hat{a}_{\lambda,2})\;\hat{a}_{\lambda,2}^{-5}\end{aligned} \tag{VIII.25}$$

and so on.

It is observed that the Neumann series for the vertical scattering gives rise to a decomposition into constituents that have traveled up and down a definite number of times, while the Neumann series in Eq. (VIII.21) clearly does not separate the wavefield into constituents that travel from right to left or vice versa.

B. The vertical slowness

From a physical point of view, it is interesting to compare the contributions to the generalized slowness surface from the successive terms of the parametrix. For this, the integration over λ has to be carried out and the original elliptic operator has to be applied to the result. Using Eqs. (VIII.6), (VIII.23), and (VIII.24), we have

$$\hat{a}_{-1/2}(x_\mu,\alpha_\nu)=(c^{-2}+\alpha_\sigma\alpha_\sigma)^{-1/2}\,[1+\tfrac{3}{4}(c^{-2}+\alpha_\nu\alpha_\nu)^{-2}i\alpha_\mu s^{-1}(\partial_{x_\mu}c^{-2})+\cdots].$$

With this the left symbol for the vertical slowness becomes

$$\begin{aligned}\hat{\gamma}(x_\mu,\alpha_\nu)&=(is^{-1}\partial_{x_\sigma}+\alpha_\sigma)^2\hat{a}_{-1/2}+(c^{-2}+\hat{a}^{(-2)})\hat{a}_{-1/2}\\&=(c^{-2}+\alpha_\sigma\alpha_\sigma)^{1/2}\,[1+(c^{-2}+\alpha_\nu\alpha_\nu)^{-1}\hat{a}^{(-2)}+\tfrac{1}{2}(c^{-2}+\alpha_\nu\alpha_\nu)^{-2}\\&\quad\times\{-\tfrac{1}{2}i\alpha_\mu s^{-1}(\partial_{x_\mu}c^{-2})+s^{-2}(\partial_{x_\mu}\partial_{x_\mu}c^{-2})\}+\cdots].\end{aligned}\tag{VIII.26}$$

Note that this expansion is valid for real-valued α_μ; it is, however, nonuniform. In the complex radial horizontal slowness plane, a set of branch points, where the argument of the square root vanishes, has been introduced. Near the branch points the polyhomogeneous expansion does not behave properly, and a uniform expansion must be found. It is an open issue whether a parallel analytic continuation of the symbols into the complex radial horizontal slowness and complex Laplace planes exists and would be stable. However, in the angular frequency (ω) domain with $s=i\omega$ and $\alpha_\nu=-i\alpha_\nu^{(\omega)}$, $\omega\in\mathbb{R}$ and $\alpha_\nu^{(\omega)}\in\mathbb{R}$, a uniform expansion has been found by Fishman and Gautesen.[30]

Spectral theory (Sec. III) can also be employed to construct a convergent expansion for $\hat{a}_z$,

$$\hat{a}_z(x_\mu,\alpha_\nu)=\sum_{[N]}\frac{\lambda^z_{[N]}}{N_{[N]}}\,\psi_{[N]}(x_\mu)\int_{x'_\nu\in\mathbb{R}}\psi_{[N]}(x'_\nu)\exp[is(x_\sigma-x'_\sigma)\alpha_\sigma]dx'_1dx'_2\tag{VIII.27}$$

if

$$\int_{x_\mu\in\mathbb{R}}\psi_{[N]}(x_\mu)\,\psi_{[M]}(x_\mu)dx_1dx_2=N_{[N]}\delta_{[N],[M]}.\tag{VIII.28}$$

Upon taking $z=-\frac{1}{2}$ and composing the result with $\hat{a}$, the vertical slowness symbol is found, as before. The latter construction implies an explicit regularization of the vertical slowness operator. Numerical algorithms associated with a construction of this kind can be found in the literature on the Mode Expansion Method[64] (see also Ref. 65).

IX. DISCUSSION OF THE RESULTS

In this paper, we have generalized the Bremmer coupling series to configurations with multidimensionally varying media with properties that are up/down symmetric. The setup of the series required the introduction of the directional wavefield decomposition into, the one-way wave equations for, and the interaction of up/down constituents. The decomposition into ''up'' and ''down'' no longer permits a separation into ''left'' and ''right.'' The convergence of the series in space–time has been proved.

The solution of the direct scattering problem in smoothly varying media has been given in terms of two nested series expansions. Both expansions represent resolvents, one associated with the coupling of counter-propagating constituents, and the other associated with the evaluation of the generalized slowness surface and the (de)composition operators. For practical purposes, one hopes that just a few terms of both series suffice to describe the scattering phenomenon under investigation; particular numerical advantage is achieved when only a few frequencies are of physical importance. Smoothness of the medium is understood relative to the pulse width associated with the irradiating source.

The derivation of the generalized Bremmer coupling series implies two basically alternative numerical approaches: a spectral approach based upon the eigenfunctions of the elliptic operator,

and a phase space approach making direct use of the left symbols. The spectral approach is rigorous, but not as efficient as the phase space approach. The most straightforward way to develop a propagation algorithm of the first kind is based on a matrix representation of the elliptic operator on the torus in terms of a basis of pyramid-type functions (rather than a basis of eigenfunctions); this leads to a finite difference approximation of the partial differential operator. The matrix is then diagonalized with the aid of the Lanczos method[66] in which only the relevant eigenpairs are calculated and propagated. The remaining calculations make use of the diagonal form thus obtained.

The phase space approach lends itself for various different approximations to enhance its computational efficiency. Among those are the (rational) parabolic approximations and the phase-screen reduction of the vertical slowness symbol. The phase-screen approximation is only valid in relatively weakly heterogeneous media. In the rational approximation method, special care has to be taken to keep the associated, approximate vertical slowness operator self-adjoint; inherently, the distinction between the principal part of and the higher-order contributions to the vertical slowness symbol becomes obscure (see Ref. 67). The uniform expansion of Fishman and Gautesen[30] lends itself to a competing algorithm, and includes critical scattering-angle phenomena, unlike the rational approximation approach. We note that the generalized Bremmer coupling series as presented in this paper lends itself to understanding the limits of approximate one-way wave theories.

Several approaches exist for the transformation back to the time domain. A numerical inverse Laplace transform can be used under the assumption that we restrict our scattered field to a finite time window. It is emphasized that causility in this approach throughout the calculations is preserved. For a review of various algorithms we refer the reader to Ref. 68; pioneering work was carried out by Papoulis.[69] As a candidate, we mention the Stehfest algorithm.

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APPENDIX: THE CALCULUS OF PSEUDO-DIFFERENTIAL OPERATORS

1. The composition equation

In this subsection we consider the composition of two pseudo-differential operators, $\hat{\mathrm{B}}_3=\hat{\mathrm{B}}_1\hat{\mathrm{B}}_2$, say. Representing the operators as in Eqs. (V.6) and (V.7),

$$(\hat{\mathrm{B}}(x_\kappa,D_\lambda)\hat{u})(x_\mu)=\int_{x'_\nu\in\mathbb{R}}\hat{\mathscr{B}}(x_\mu,x'_\nu)\hat{u}(x'_\nu)dx'_1dx'_2, \tag{A1}$$

in which

$$\hat{\mathscr{B}}(x_\mu,x'_\nu)=\left(\frac{s}{2\pi}\right)^2\int_{\alpha_\nu\in\mathbb{R}}\hat{\beta}(x_\mu,\alpha_\nu)\exp[is\alpha_\nu(x'_\nu-x_\nu)]d\alpha_1d\alpha_2, \tag{A2}$$

a composition rule for the corresponding left symbols, $\hat{\beta}_1$, $\hat{\beta}_2$, and $\hat{\beta}_3$, is found. To begin with, the Schwartz kernels must satisfy the composition rule

$$\hat{\mathscr{B}}_3(x_\mu,x'_\nu)=\int_{x''_\nu\in\mathbb{R}}\hat{\mathscr{B}}_1(x_\mu,x''_\nu).\hat{\mathscr{B}}_2(x''_\nu,x'_\nu)dx''_1dx''_2. \tag{A3}$$

Hence,

$$\left(\frac{s}{2\pi}\right)^2\int_{\alpha_\nu\in\mathbb{R}}\hat{\beta}_3(x_\mu,\alpha_\nu)\exp[is\alpha_\sigma(x'_\sigma-x_\sigma)]d\alpha_1d\alpha_2=\int_{x''_\nu\in\mathbb{R}}\hat{\mathscr{B}}_1(x_\mu,x''_\nu).\hat{\mathscr{B}}_2(x''_\nu,x'_\nu)dx''_1dx''_2. \tag{A4}$$

Substituting in Eq. (A4) $u_\nu=x_\nu$ and $u_\nu=-(x'_\nu-x_\nu)$, we arrive at

$$\left(\frac{s}{2\pi}\right)^2\int_{\alpha_\nu\in\mathbb{R}}\hat{\beta}_3(u_\mu,\alpha_\nu)\exp(-is\alpha_\sigma v_\sigma)d\alpha_1d\alpha_2=\int_{x''_\nu\in\mathbb{R}}\hat{\mathscr{B}}_1(u_\mu,x''_\nu).\mathscr{B}_2(x''_\nu,u_\nu-v_\nu)dx''_1dx''_2. \tag{A5}$$

By inverse Fourier transformation it now follows that

$$\hat{\beta}_3(u_\mu,\alpha_\nu)=\int_{v_\nu\in\mathbb{R}}\int_{x''_\nu\in\mathbb{R}}\hat{\mathscr{B}}_1(u_\mu,x''_\nu).\hat{\mathscr{B}}_2(x''_\nu,u_\nu-v_\nu)\exp(is\alpha_\sigma v_\sigma)dx''_1dx''_2dv_1dv_2. \tag{A6}$$

Substituting Eq. (A2) twice yields

$$\begin{aligned}\hat{\beta}_3(u_\mu,\alpha_\nu)=\left(\frac{s}{2\pi}\right)^4&\int_{x''_\nu\in\mathbb{R}}\int_{\alpha'_\nu\in\mathbb{R}}\int_{\alpha''_\nu\in\mathbb{R}}\int_{v_\nu\in\mathbb{R}}\hat{\beta}_1(u_\mu,\alpha'_\nu)\hat{\beta}_2(x''_\nu,\alpha''_\nu)\\&\times\exp[is\{(\alpha_\sigma-\alpha''_\sigma)v_\sigma+(u_\sigma-x''_\sigma)(\alpha''_\sigma-\alpha'_\sigma)\}]\\&\times dv_1dv_2d\alpha''_1d\alpha''_2d\alpha'_1d\alpha'_2dx''_1dx''_2.\end{aligned} \tag{A7}$$

Upon performing four of the integrations, we arrive at ($u_\mu=x_\mu$)

$$\begin{aligned}\hat{\beta}_3(x_\kappa,\alpha_\lambda)=\left(\frac{s}{2\pi}\right)^2&\int_{x''_\nu\in\mathbb{R}}\int_{\alpha'_\nu\in\mathbb{R}}\hat{\beta}_1(x_\mu,\alpha'_\nu)\hat{\beta}_2(x''_\nu,\alpha_\nu)\\&\times\exp[is(x_\sigma-x''_\sigma)(\alpha_\sigma-\alpha'_\sigma)]d\alpha'_1d\alpha'_2dx''_1dx''_2.\end{aligned} \tag{A8}$$

This equation can also be written as a differential equation. To this end, we introduce the four-dimensional Fourier transformation in phase space

$$\tilde{\tilde{\beta}}(\xi_\mu,\eta_\nu)=\left(\frac{s}{2\pi}\right)^2\int_{x_\mu\in\mathbb{R}}\int_{\alpha_\nu\in\mathbb{R}}\hat{\beta}(x_\mu,\alpha_\nu)\exp[is(\xi_\kappa x_\kappa+\eta_\lambda\alpha_\lambda)]d\alpha_1d\alpha_2dx_1dx_2 \tag{A9}$$

and its inverse

$$\hat{\beta}(x_\mu,\alpha_\nu)=\left(\frac{s}{2\pi}\right)^2\int_{\xi_\mu\in\mathbb{R}}\int_{\eta_\nu\in\mathbb{R}}\tilde{\tilde{\beta}}(\xi_\mu,\eta_\nu)\exp[-is(\xi_\kappa x_\kappa+\eta_\lambda\alpha_\lambda)]d\eta_1d\eta_2d\xi_1d\xi_2. \tag{A10}$$

Using Eq. (A10), we have

$$\left(\frac{s}{2\pi}\right)^2\int_{x_\kappa\in\mathbb{R}}\int_{\alpha_\lambda\in\mathbb{R}}\hat{\beta}(x_\kappa,\alpha_\lambda)\exp(isx_\sigma\alpha_\sigma)d\alpha_1d\alpha_2dx_1dx_2$$

$$=\left(\frac{s}{2\pi}\right)^4\int_{\alpha_\lambda\in\mathbb{R}}\int_{x_\kappa\in\mathbb{R}}\int_{\xi_\kappa\in\mathbb{R}}\int_{\eta_\lambda\in\mathbb{R}}\tilde{\tilde{\beta}}(\xi_\kappa,\eta_\lambda)\exp[-is(\xi_\sigma x_\sigma+\eta_\sigma\alpha_\sigma$$

$$-x_\sigma\alpha_\sigma)]d\eta_1 d\eta_2 d\xi_1 d\xi_2 dx_1 dx_2 d\alpha_1 d\alpha_2$$

$$=\left(\frac{s}{2\pi}\right)^2\int_{\xi_\kappa\in\mathbb{R}}\int_{\eta_\lambda\in\mathbb{R}}\tilde{\tilde{\beta}}(\xi_\kappa,\eta_\lambda)\exp(-is\xi_\sigma\eta_\sigma)d\eta_1 d\eta_2 d\xi_1 d\xi_2$$

$$=\exp\left[\frac{i}{s}\,\partial_{\alpha_\sigma}\partial_{x_\sigma}\right]\hat{\beta}(x_\kappa,\alpha_\lambda)\big|_{(x_\kappa,\alpha_\lambda)=(0,0)}. \tag{A11}$$

Using this equality in Eq. (A8), it is found that

$$\hat{\beta}_3(x_\kappa,\alpha_\lambda)=\exp\left[\frac{i}{s}\,\partial_{\alpha'_\sigma}\partial_{x'_\sigma}\right]\hat{\beta}_1(x_\kappa,\alpha'_\nu)\hat{\beta}_2(x'_\mu,\alpha_\lambda)\Big|_{(x'_\kappa,\alpha'_\lambda)=(x_\kappa,\alpha_\lambda)}. \tag{A12}$$

The interpretation of the exponential operator follows upon analyzing

$$\hat{B}_3(x_\kappa,\alpha_\lambda,x'_\mu,\alpha'_\nu)=\exp\left[\frac{i}{s}\,\partial_{\alpha'_\sigma}\partial_{x'_\sigma}\right]\hat{\beta}_1(x_\kappa,\alpha'_\nu)\hat{\beta}_2(x'_\mu,\alpha_\lambda) \tag{A13}$$

introducing

$$\hat{\rho}_M(x_\kappa,\alpha_\lambda,x'_\mu,\alpha'_\nu)=\hat{B}_3(x_\kappa,\alpha_\lambda,x'_\mu,\alpha'_\nu)-\sum_{m=0}^{M-1}\frac{1}{m!}\left(\frac{i}{s}\right)^m(\partial_{\alpha'_\sigma}\partial_{x'_\sigma})^m\hat{\beta}_1(x_\kappa,\alpha'_\nu)\hat{\beta}_2(x'_\mu,\alpha_\lambda). \tag{A14}$$

Note that $\hat{\beta}_3(x_\kappa,\alpha_\lambda)=\hat{B}_3(x_\kappa,\alpha_\lambda,x_\kappa,\alpha_\lambda)$. Suppose that $\hat{\beta}_1$ lies in a space S^{s_1} and that $\hat{\beta}_2$ lies in a space S^{s_2}. Then the following estimate holds (see the proof of Theorem 18.1.8 in Ref. 11)

$$\begin{aligned}&|(\partial^{m_1}_{\alpha_1}\partial^{m_2}_{\alpha_2}\partial^{n_1}_{x_1}\partial^{n_2}_{x_2}\partial^{m'_1}_{\alpha'_1}\partial^{m'_2}_{\alpha'_2}\partial^{n'_1}_{x'_1}\partial^{n'_2}_{x'_2}\hat{\rho}_M)(x_\kappa,\alpha_\lambda,x'_\mu,\alpha'_\nu)|\\&\quad\leqslant C_{M,m_1,m_2,n_1,n_2,m'_1,m'_2,n'_1,n'_2}\,[(1+\alpha'_\rho\alpha'_\rho)^{1/2}]^{s_1-M-m'_1-m'_2}\\&\quad\quad\times[(1+\alpha_\sigma\alpha_\sigma)^{1/2}]^{s_2-m_1-m_2},\end{aligned} \tag{A15}$$

which implies that $\hat{\rho}_M(x_\mu,\alpha_\nu,x_\mu,\alpha_\nu)\in S^{s_1+s_2-M}$.

2. Continuity

We will review the proof of continuity of a pseudo-differential operator $\hat{\mathrm{B}}$: $H^r\to H^{r-d}$, given that its symbol $\hat{\beta}$ is contained in S^d. Let $\hat{\Gamma}$ be the pseudo-differential operator of order 1,

$$\hat{\Gamma}_0=[-D_\sigma\,D_\sigma+\langle c^{-2}\rangle]^{1/2}, \tag{A16}$$

which, by Fourier analysis, is trivially continuous as an operator $H^r\to H^{r-1}$. Then also

$$\hat{\Gamma}_0^d:\ H^r\to H^{r-d}\quad\text{continuous for}\quad d\in\mathbb{R}. \tag{A17}$$

Now, let $\hat{u}\in H^r$. Then $\hat{u}_0=\hat{\Gamma}_o^r\hat{u}\in L^2$; using the parametrix $\hat{\Gamma}_o^{-r}$ of $\hat{\Gamma}_o^r$, we can write

$$\hat{u}=\hat{\Gamma}_0^{-r}\hat{u}_0+\hat{v}_0 \quad \text{with } \hat{u}_0\in L^2 \text{ and } \hat{v}_0\in C^\infty.$$

The contribution from $\hat{v}_0$ is trivially dealt with. We obtain

$$\hat{\Gamma}_0^{r-d}\hat{\mathrm{B}}\hat{u}=\hat{\Gamma}_0^{r-d}\hat{\mathrm{B}}\hat{\Gamma}_0^{-r}\hat{u}_0. \tag{A18}$$

Hence, continuity of $\hat{\mathrm{B}}$ is proved, if

$$\hat{\mathrm{B}}_0\equiv\hat{\Gamma}_0^{r-d}\hat{\mathrm{B}}\hat{\Gamma}_0^{-r}:\ L^2\to L^2 \text{ continuous.} \tag{A19}$$

From the calculus of symbols, discussed in the preceding subsection, we find that the symbol $\hat{\beta}_0$ of the latter operator is contained in S^0.

Step 1: $\hat{\beta}\in S^{-n-1}$. Let $\mu=1,...,n$, and $\hat{\beta}\in S^{-n-1}$. Then

$$|\hat{\mathscr{B}}(x_\mu,x'_\nu)|\leqslant\left(\frac{s}{2\pi}\right)^2\int_{\alpha_\nu\in\mathbb{R}}|\hat{\beta}(x_\mu,\alpha_\nu)|^2 d\alpha_1\cdots d\alpha_n\leqslant C.$$

Note that

$$(x_\mu-x'_\mu)^{l_\mu}\hat{\mathscr{B}}(x_\mu,x'_\nu) \text{ corresponding with } i^{l_\mu}\partial_{\alpha_\mu}^{l_\mu}\hat{\beta}(x_\mu,\alpha_\nu)$$

must be bounded as well, hence

$$(1+[(x_\mu-x'_\mu)^2]^{1/2})^{n+1}\ |\hat{\mathscr{B}}(x_\mu,x'_\nu)|\leqslant C.$$

Schur's lemma states that if $\hat{\mathscr{B}}(x_\mu,x'_\nu)$ is continuous and

$$\sup_{x'_\nu}\int_{x_\mu\in\mathbb{R}}|\hat{\mathscr{B}}(x_\mu,x'_\nu)|dx_1\cdots dx_n\leqslant C \quad\text{and}\quad \sup_{x_\mu}\int_{x'_\nu\in\mathbb{R}}|\hat{\mathscr{B}}(x_\mu,x'_\nu)|dx'_1\cdots dx'_n\leqslant C, \tag{A20}$$

that then $\hat{\mathrm{B}}:L^2\to L^2$ is bounded with norm $\leqslant C$. (This is a consequence of Cauchy–Schwarz inequality.) Conditions (A20) are satisfied for $\hat{\beta}\in S^{-n-1}$.

Step 2: $\hat{\beta}\in S^m$, $m\leqslant -1$. Let $\hat{\beta}\in S^m$, $m\leqslant -1$. Let $\hat{\beta}^*\in S^m$ be the symbol of the adjoint operator $\hat{\mathrm{B}}^T$. Set $\hat{\mathrm{C}}\equiv\hat{\mathrm{B}}^T\hat{\mathrm{B}}$. Then

$$\|\hat{\mathrm{B}}\hat{u}\|^2\leqslant\|\hat{\mathrm{C}}\hat{u}\|\ \|\hat{u}\|.$$

Hence, if $\hat{\mathrm{C}}$ is continuous, then $\hat{\mathrm{B}}$ must be continuous. Let the symbol of $\hat{\mathrm{C}}$ be contained in S^{2m}. By induction, we find continuity for

$$m\leqslant-\frac{n+1}{2},\quad m\leqslant-\frac{1}{2}\frac{n+1}{2},\quad \ldots,\quad m\leqslant -1.$$

Step 3: $\hat{\beta}\in S^0$. Let $\hat{\beta}\in S^0$. Then there is an estimate

$$M>2\sup|\hat{\beta}(x_\mu,\alpha_\nu)|^2.$$

Set

$$\hat{\delta}(x_\mu,\alpha_\nu)\equiv[M-|\hat{\beta}(x_\mu,\alpha_\nu)|^2]^{1/2}\in S^0.$$

Since

$$M-|\hat{\beta}(x_\mu,\alpha_\nu)|^2\geqslant M/2,$$

the symbol $\hat{\delta}$ is well defined. Using the calculus of the previous subsection, form the operator $\hat{\mathrm{D}}^T\hat{\mathrm{D}}$; then

$$\hat{\mathrm{D}}^T\hat{\mathrm{D}}=M-\hat{\mathrm{B}}^T\hat{\mathrm{B}}+\hat{\mathrm{E}},\quad \hat{e}\in S^{-1}.$$

From this operator equality, we obtain

$$\|\hat{\mathrm{B}}\hat{u}\|^2\leqslant\|\hat{u}\|^2M+\langle\hat{\mathrm{E}}\hat{u},\hat{u}\rangle.$$

In the previous step we have shown that $\hat{\mathrm{E}}$ must be continuous ($\hat{e}\in S^{-1}$); hence $\hat{\mathrm{B}}$ must be continuous.

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Diffuse tomography modulo Grassmann and Laplace

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Complicated and unphysical families of modified transition probabilities for the 4×4 diffuse tomographic problem are presented. Grassmann–Plücker identities and Laplace expansions of determinants are used to simplify the initial transition probabilities. Besides restoring self-consistency to the system, enforcing range conditions eliminates one-half of the parameters. © *1996 American Institute of Physics.* [S0022-2488(96)01705-5]

I. INTRODUCTION

Applications in medical imaging motivated efforts to invert two-and three-dimensional versions of the Redheffer *-product.[1–7] One possible application is monitoring the brains of neonates, which are unable to withstand repeated x-ray irradiation. Brain hemorrhage is the leading cause of death among premature infants. The goal is to detect cranial bleeds without overexposing the infant to harmful radiation.

Range conditions were studied in Refs. 8 and 9 for very general two- and three-dimensional systems. Because of these range conditions the inverse problem is underdetermined. In Ref. 10 a recursive algorithm was sketched for recovering a p-parameter family of solutions to the inverse problem in the plane where the difference between the amount of independent data and number of unknowns is p. The purpose of this paper is to fill in the details.

The first section of this paper includes an introduction to the forward problem and a description of its range conditions. Each recursive level of the inversion scheme presented in Ref. 10 consists of two parts. The first part divides a system into four subsystems and computes families of data sets for the subsystems from the original data set. Unfortunately, this process introduces too many parameters. The superfluous parameters must be eliminated from the subsystems' data sets. This is done in Secs. II and III for the first level of the recursive scheme by enforcing range conditions upon the subsystems' data sets. Sections I C and I D give insight into the difficulty of enforcing the various range conditions. Because of the combinatorial nature of the problem, several different matrix identities are helpful. Grassmann–Plücker identities are used to derive some of them in Sec. II A. The solutions presented in Sec. I D are presented modulo the matrix identities in Sec. II B. These solutions are functions of the data and 64 parameters. That the range conditions which are simplest to enforce imply that eight of the parameters are identically zero is shown in Sec. III A. The rest of the relatively easily enforceable conditions are studied in Secs. III B 1 and III B 2. The remaining conditions are more difficult to enforce (Sec. III C). Additional matrix identities are required to reduce these remaining conditions to palatable form (Secs. III C 2 and 3). In Section III C 4 it is shown that these identities form a complete set. Sections III B 2 and III C 4 are quite technical and may be omitted without losing sight of the main objective—recursive subdivision of a diffuse tomographic system.

A. Description of the model

Consider an $n\times n$ array of pixels in the plane. On each outer face there are two devices. One device shoots photons across the outside edge into the neighboring pixel; the other device detects photons as they leave the system. For each of the $4n$ outside edges $4n$ pieces of data are collected.

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These data are stored as a $4n\times 4n$ transition matrix, Q. Within the system, photons travel either horizontally or vertically. Label the horizontal and vertical axes x_1 and x_2, respectively. A photon traveling parallel to the x_i axis in the positive direction moves with velocity x_i^+. Photons traveling in the opposite direction travel with velocity x_i^-. They do not interact and may be absorbed within a pixel. Photons move according to a Markov process.[11] The probabilities with which a photon moves to a neighboring pixel depend upon its previous, as well as present, location. In this two-step formulation the state space consists of locations. The state space may be redefined so that photons move according to a one-step Markov process. In the new state space a single state consists of the photon's location and direction of travel.

There are three different types of these Markov states: incoming, outgoing, and hidden. The probabilities with which photons move from one state to another are referred to as transition probabilities. For each pixel O and incident direction the sum of the absorption probability and the four possible transition probabilities must be identically one. The absorption probability is therefore neglected in the rest of this paper. Each pixel corresponds to 16 transition probabilities. For example, a photon which travels with velocity x_i^+ into pixel O and travels straight through pixel O does so with some probability, denoted by $x_i^+Ox_i^+$. The same photon travels to O's neighbor in the x_j^+ direction with probability $x_i^+Ox_j^+$. These probabilities are the nonzero entries of the Markov transition matrix M. M is sparse and may be written as a block matrix with nontrivial subblocks Pio, Pih, Pho, and Phh. Pio, for example, contains the probabilities with which photons in incoming states move directly to outgoing states. Pih contains the probabilities with which photons in incoming states move to hidden states. Pho and Phh are the transition matrices for photons starting in hidden states traveling to outgoing and hidden states, respectively. Pio and Phh are always square matrices.

B. Forward problem

The forward map takes $16n^2$ transition probabilities to the $4n\times 4n$ data matrix Q. The domain of the forward map lies in the unit cube in $\mathbb{R}^{16n^2}$ and is defined by

$$(x_i^{\pm}Ox_1^+ + x_i^{\pm}Ox_1^-) + (x_i^{\pm}Ox_2^+ + x_i^{\pm}Ox_2^-) \leqslant 1, \quad \pm = +,-, i = 1,2,$$

for each pixel O. Furthermore, none of these transition probabilities may be zero. Here Q_i^j represents the probability that a photon which enters the system at source i exits the system at detector j. Q provides no time-of-flight information. Because Q is a transition matrix, acceptable solutions lie in the unit cube in $\mathbb{R}^{16n^2}$ and satisfy

$$0 \leqslant \sum_{\lambda=1}^{4n} Q_i^{\lambda} \leqslant 1, \quad i = 1,2,\ldots,4n.$$

The forward map is given by the following matrix expression:

$$Q = Pio + Pih\sum_{n=0}^{\infty} Phh^n \;\; Pho = Pio + Pih(I - Phh)^{-1}Pho \tag{1}$$

C. Range conditions

Range conditions appear as rank-deficient submatrices of Q. Each of these rank-deficient submatrices represents travel from one ''side'' of the system to the other ''side.'' Let b be a (not necessarily straight) barrier of $\#b$ hidden states separating the ''sides.'' The Markovian nature of the system can be used to show that the corresponding submatrix is generically of rank $\#b$.[8] For the purposes of this paper it is only necessary to consider straight barriers.

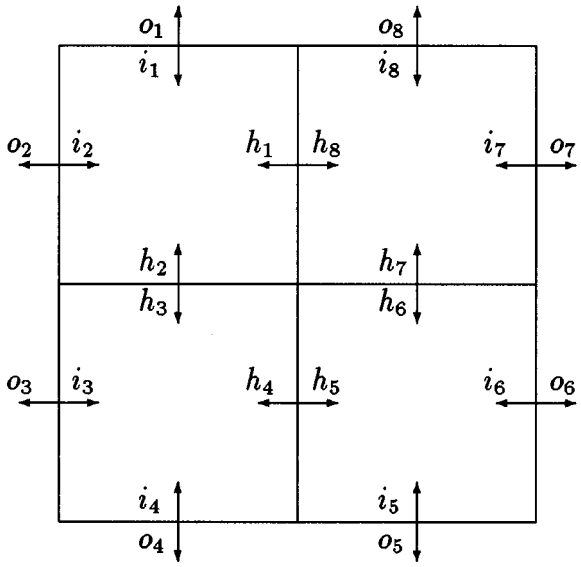

FIG. 1. Incoming, hidden, and outgoing states are labeled with is, hs, and os, respectively.

Notation: Let Q_r^c denote the submatrix of Q taken from rows **r** and columns **c**. Let dQ_r^c denote the determinant of this submatrix. Furthermore, let $a-b$ denote $a,a+1,\ldots,b$, where $a,b\in\mathbb{N}$.

For example, the data matrix for a 2×2 system has many rank-deficient submatrices. See Fig. 1. The 4×4 submatrix representing travel from left to right, Q_{1-4}^{5-8}, is generically rank two, as is Q_{5-8}^{1-4}. Similarly, the submatrices $Q_{3-6}^{1,2,7,8}$ and $Q_{1,2,7,8}^{3-6}$ are generically of rank two as well.

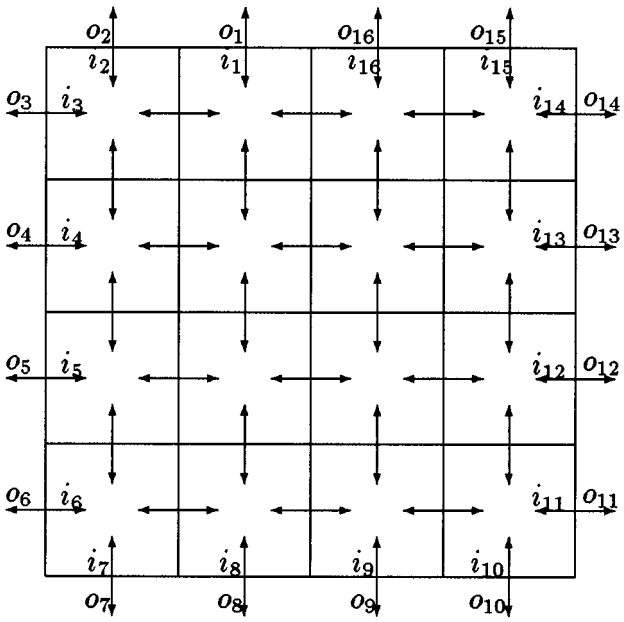

FIG. 2. A 4×4 system. The incoming and outgoing states are labeled; all unlabeled states are hidden states. There are 16 incoming and 16 outgoing states, but 48 hidden states.

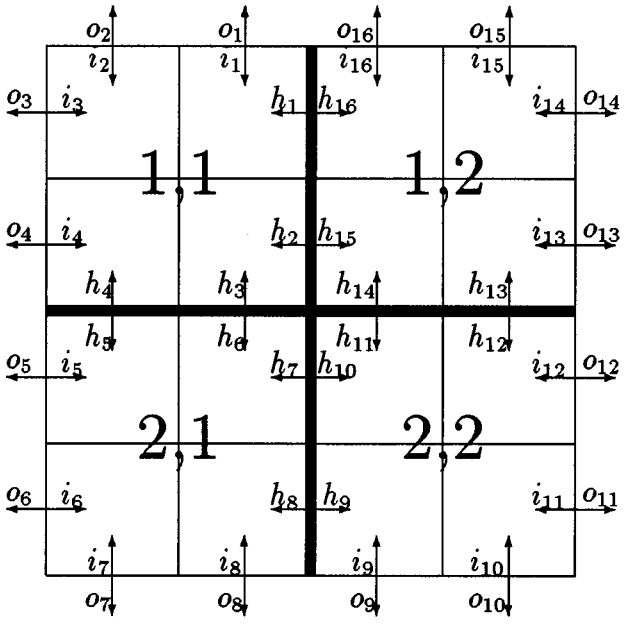

FIG. 3. Decomposition of a 4×4 system into four 2×2 subsystems. The thick lines separate the subsystems. The ''modified'' 4×4 system disregards individual pixels. Only the subsystems are relevant at the first level of this recursive procedure.

D. Modified transition matrices in terms of *A*

Although the final goal is to recover the microscopic transition probabilities for each pixel from boundary value data, the purpose of this section is more modest. A 32-parameter family of data sets for the subsystems shown in Fig. 3 are computed from the original data. Once the data sets for each of the subsystems are found, the 2×2 subsystems can be tackled in parallel.

The sparse block structures of Pio, Pho, Pih, and Phh were used in Ref. 10 to solve for nonzero blocks of Phh, Pio, and Pih in terms of $A \equiv Pho^{-1}$. This result is used here and requires the following.

Notation: $[M:N]$ denotes the concatenation of matrices M and N (where M and N have the same number of rows). Furthermore, let r_{a-b} denote any choice of one half of the natural numbers between a and b inclusive. ($b-a$ is always odd.) Finally, define $r_{\mathbf{l}} \equiv r_{1-8}$, $r_{\mathbf{b}} \equiv r_{5-12}$, $r_{\mathbf{r}} \equiv r_{9-16}$, and $r_{\mathbf{t}} \equiv r_{1-4,13-16}$, representing choices of rows from the left, bottom, right, and top of the system, respectively.

The following solutions will be used later to eliminate some of the A_i^js:

$$Phh_{1-4}^{5,6} = Pho_{1-4}^{1-4}(Q_{r_{\mathbf{r}}}^{1-4})^{-1} Q_{r_{\mathbf{r}}}^{5-8} A_{5-8}^{5,6}, \tag{2}$$

$$Phh_{1-4}^{15,16} = Pho_{1-4}^{1-4}(Q_{r_{\mathbf{b}}}^{1-4})^{-1} Q_{r_{\mathbf{b}}}^{13-16} A_{13-16}^{15,16}, \tag{3}$$

$$Pih_{1-4}^{5,6} = [Q_{1-4}^{5-8} - (Q_{1-4}^{1-4} - Pio_{1-4}^{1-4})(Q_{r_{\mathbf{r}}}^{1-4})^{-1} Q_{r_{\mathbf{r}}}^{5-8}] A_{5-8}^{5,6}, \tag{4}$$

$$Pih_{1-4}^{15,16} = [Q_{1-4}^{13-16} - (Q_{1-4}^{1-4} - Pio_{1-4}^{1-4})(Q_{r_{\mathbf{b}}}^{1-4})^{-1} Q_{r_{\mathbf{b}}}^{13-16}] A_{13-16}^{15,16}, \tag{5}$$

where

$$Pio_{1-4}^{1-4}=Q_{1-4}^{1-4}-[Q_{1-4}^{13-16}(Q_{r_{\mathbf{b}}}^{13-16})^{-1}Q_{r_{\mathbf{b}}}^{1-4}A_{1-4}^{1,2}:Q_{1-4}^{5-8}(Q_{r_{\mathbf{b}}}^{5-8})^{-1}Q_{r_{\mathbf{r}}}^{1-4}A_{1-4}^{3,4}]Pho_{1-4}^{1-4}. \quad (6)$$

Solutions for blocks within the same transition matrix have a common structure. Hidden–outgoing and hidden–hidden transitions can be expressed in terms of Q and A much more simply than incoming–outgoing and incoming–hidden transitions.

II. SIMPLIFYING THE SOLUTIONS

Although the above solutions are relatively compact, the solutions for Pio and Pih can be simplified. The Grassmann–Plücker identites found in classical algebraic geometry are used to derive matrix identities in the next section. The results are used to simplify the solutions for Pio and Pih in Sec. II B.

A. Matrix truisms

Since the inverse problem involves linear systems, it is not surprising that Grassmannians and the Grassmann–Plücker embedding come into play. The identities which embed Grassmannians $G(k,n)$ in $\mathbb{P}^{\binom{n}{k}-1}$ are derived below. A cursory explanation of the embedding can be found in Refs. 12 and 13. For a more thorough exposition see Refs. 14 and 15. Let Λ be any rectangular matrix with k rows and n columns where $k<n-1$ and $\Lambda=(a)_{ij}$. Let $I=(i_1,i_2,i_3,\ldots,i_{(k-1)})$ index $(k-1)$ distinct columns of Λ. Let $J=(j_1,j_2,j_3,\ldots,j_{(k+1)})$ index $(k+1)$ distinct columns of Λ. Then,

$$\sum_{\lambda=1}^{k+1}\pi_{(i_1,i_2,\ldots,i_{k-1},j_\lambda)}\pi_{(j_1,j_2,\ldots,j_{\lambda-1},j_{\lambda+1},\ldots,j_{k+1})}=0. \quad (7)$$

Equation (7) defines the Grassmann relations. Let $\alpha,\beta,\gamma,\eta,\kappa\in\mathbb{N}^k$. For any matrix Q, basic matrix properties imply

$$(Q_\alpha^\gamma)^{-1}Q_\alpha^\eta=\left(\frac{dQ_\alpha^{\gamma_1,\gamma_2,\ldots,\gamma_{i-1},\eta_j,\gamma_{i+1},\ldots,\gamma_n}}{dQ_\alpha^\gamma}\right)_{i,j}, \quad (8)$$

$$Q_\kappa^\gamma(Q_\alpha^\gamma)^{-1}Q_\alpha^\eta=Q_\kappa^\eta-\left(\frac{1}{dQ_\alpha^\gamma}\right)(dQ_{\kappa_i,\alpha}^{\eta_j,\gamma})_{i,j}. \quad (9)$$

The identity (8) combines with Grassmann-Plücker relations to imply

$$\begin{aligned}(dQ_{\kappa_i,\alpha}^{\gamma_k,\beta})_{i,k}(Q_\alpha^\gamma)^{-1}Q_\alpha^\eta&=(dQ_{\kappa_i,\alpha}^{\gamma_k,\beta})_{i,k}\left(\frac{dQ_\alpha^{\gamma_1,\gamma_2,\ldots,\gamma_{k-1},\eta_j,\gamma_{k+1},\ldots,\gamma_n}}{dQ_\alpha^\gamma}\right)_{k,j}\\&=\frac{-1}{dQ_\alpha^\gamma}\sum_{k=1}^{n}(-1)^k(dQ_{\kappa_i,\alpha}^{\gamma_k,\beta}dQ_\alpha^{\eta_j,\gamma_1,\gamma_2,\ldots,\gamma_{k-1},\gamma_{k+1},\ldots,\gamma_n})_{i,j}\\&=\left(dQ_{\kappa_i,\alpha}^{\eta_j,\beta}-\frac{dQ_\alpha^\beta}{dQ_\alpha^\gamma}dQ_{\kappa_i,\alpha}^{\eta_j,\gamma}\right)_{i,j}. \quad (10)\end{aligned}$$

These matrix identities can be used to simplify (4)–(6). Finally, note that

$$I=A_{1-4}^{1-4}Pho_{1-4}^{1-4}=A_{1-4}^{1,2}Pho_{1,2}^{1-4}+A_{1-4}^{3,4}Pho_{3,4}^{1-4}$$

because Pho is block diagonal and $A=Pho^{-1}$. This argument applies to other blocks on the diagonal.

B. Matrix solutions revisited

The solution for Pio_{1-4}^{1-4} can be simplified using (9) as follows:

$$
\begin{aligned}
Pio_{1-4}^{1-4} &= Q_{1-4}^{1-4} - \left[\left(Q_i^j - \frac{dQ_{i,r_5}^{j,13-16}}{dQ_{r_5}^{13-16}} \right)_{i,j} A_{1-4}^{1,2} : \left(Q_i^j - \frac{dQ_{i,r_9}^{j,5-8}}{dQ_{r_9}^{5-8}} \right)_{i,j} A_{1-4}^{3,4} \right] Pho_{1-4}^{1-4} \\
&= Q_{1-4}^{1-4} - [Q_{1-4}^{1-4} A_{1-4}^{1,2} : Q_{1-4}^{1-4} A_{1-4}^{3,4}] Pho_{1-4}^{1-4} \\
&\quad + \left[\left(\frac{dQ_{i,r_5}^{j,13-16}}{dQ_{r_5}^{13-16}} \right)_{i,j} A_{1-4}^{1,2} : \left(\frac{dQ_{i,r_9}^{j,5-8}}{dQ_{r_9}^{5-8}} \right)_{i,j} A_{1-4}^{3,4} \right] Pho_{1-4}^{1-4} \\
&= \left[\left(\frac{dQ_{i,r_5}^{j,13-16}}{dQ_{r_5}^{13-16}} \right)_{i,j} A_{1-4}^{1,2} : \left(\frac{dQ_{i,r_9}^{j,5-8}}{dQ_{r_9}^{5-8}} \right)_{i,j} A_{1-4}^{3,4} \right] Pho_{1-4}^{1-4} \\
&= \left(\frac{dQ_{i,r_5}^{j,13-16}}{dQ_{r_5}^{13-16}} \right)_{i,j} A_{1-4}^{1,2} Pho_{1,2}^{1-4} + \left(\frac{dQ_{i,r_9}^{j,5-8}}{dQ_{r_9}^{5-8}} \right)_{i,j} A_{1-4}^{3,4} Pho_{3,4}^{1-4} \\
&= \left(\frac{dQ_{i,r_5}^{j,13-16}}{dQ_{r_5}^{13-16}} - \frac{dQ_{i,r_9}^{j,5-8}}{dQ_{r_9}^{5-8}} \right)_{i,j} A_{1-4}^{1,2} Pho_{1,2}^{1-4} + \left(\frac{dQ_{i,r_9}^{j,5-8}}{dQ_{r_9}^{5-8}} \right)_{i,j} .
\end{aligned}
$$

Define the 4×4 matrices

$$
\mathbf{m} = \left(\frac{dQ_{i,r_5}^{j,13-16}}{dQ_{r_5}^{13-16}} - \frac{dQ_{i,r_9}^{j,5-8}}{dQ_{r_9}^{5-8}} \right)_{i,j} ,
$$

$$
\mathbf{M} = \mathbf{m}\, A_{1-4}^{1,2}\, Pho_{1,2}^{1-4} .
$$

Then the nonzero entries of Pio can be expressed (fairly) compactly, albeit nonuniquely:

$$
Pio_{1-4}^{1-4} = \mathbf{M} + \left(\frac{dQ_{i,r_9}^{j,5-8}}{dQ_{r_9}^{5-8}} \right)_{i,j} . \tag{11}
$$

Simpler solutions for Pio can be used to express Pih more succinctly. For instance, substituting the matrix identity (8) as well as (11) and

$$
\left(\frac{dQ_{i+12,5-8}^{j+12,9-12}}{dQ_{5-8}^{9-12}} \right)_{i,j} (Q_{5-8}^{13-16})^{-1} Q_{5-8}^{1-4} = \left(\frac{dQ_{i+12,5-8}^{j,9-12}}{dQ_{5-8}^{9-12}} - \frac{dQ_{i+12,5-8}^{j,13-16}}{dQ_{5-8}^{13-16}} \right)_{i,j} , \tag{12}
$$

$$
\left(\frac{dQ_{i+12,r_5}^{j+12,1-4}}{dQ_{r_5}^{1-4}} \right)_{i,j} (Q_{r_b}^{13-16})^{-1} Q_{r_b}^{1-4} = \left(\frac{dQ_{i+12,r_b}^{j,1-4}}{dQ_{r_b}^{1-4}} - \frac{dQ_{i+12,r_b}^{j,13-16}}{dQ_{r_b}^{13-16}} \right)_{i,j} \equiv - \left(\frac{dQ_{i+12,r_b}^{j,13-16}}{dQ_{r_b}^{13-16}} \right)_{i,j} \tag{13}
$$

into equations (4) and (5) yields

$$
Pih_{1-4}^{5,6} = \mathbf{M} (Q_{r_r}^{1-4})^{-1} Q_{r_r}^{5-8} A_{5-8}^{5,6} , \tag{14}
$$

$$Pih_{1-4}^{15,16}=\left[\left(\frac{dQ_{i,9-12}^{j+12,5-8}}{dQ_{9-12}^{5-8}}\right)_{i,j}+\mathbf{M}(Q_{9-12}^{1-4})^{-1}Q_{9-12}^{13-16}\right]A_{13-16}^{15,16}. \tag{15}$$

In (12) and (15) the choice of rows is dictated by the matrix identity (10). Similar computations give simple expressions for each block of Pio and Pih in terms of Q and the 64 nonzero entries of A.

III. REMOVING A_i^js

In this section range conditions are used to derive 32 independent conditions upon the A_i^js. The entries of Pho, Phh, Pio, and Pih are (almost) the data for each of the 2×2 subsystems. They do not obey the range conditions mentioned in Sec. I C, however. Range conditions for the 2×2 subsystems are zero-valued 3×3 minors of the subsystems' data sets. Enforcing these conditions yields polynomials in the A_i^js. These polynomials factor into products of several terms; the relevant term is always linear. Although there are many such conditions, only 32 of them are independent. Only half, therefore, of the parameters may be eliminated by virtue of range conditions upon the 2×2 subsystems.

Each of the four subsystems has an 8×8 data matrix. The data matrix for the 1,1 subsystem is shown below:

$$Q11=\begin{bmatrix} Pio_2^2 & Pio_2^3 & Pio_2^4 & Pih_2^5 & Pih_2^6 & Pih_2^{15} & Pih_2^{16} & Pio_2^1 \\ Pio_3^2 & Pio_3^3 & Pio_3^4 & Pih_3^5 & Pih_3^6 & Pih_3^{15} & Pih_3^{16} & Pio_3^1 \\ Pio_4^2 & Pio_4^3 & Pio_4^4 & Pih_4^5 & Pih_4^6 & Pih_4^{15} & Pih_4^{16} & Pio_4^1 \\ Pho_4^2 & Pho_4^3 & Pho_4^4 & Phh_4^5 & Phh_4^6 & Phh_4^{15} & Phh_4^{16} & Pho_4^1 \\ Pho_3^2 & Pho_3^3 & Pho_3^4 & Phh_3^5 & Phh_3^6 & Phh_3^{15} & Phh_3^{16} & Pho_3^1 \\ Pho_2^2 & Pho_2^3 & Pho_2^4 & Phh_2^5 & Phh_2^6 & Phh_2^{15} & Phh_2^{16} & Pho_2^1 \\ Pho_1^2 & Pho_1^3 & Pho_1^4 & Phh_1^5 & Phh_1^6 & Phh_1^{15} & Phh_1^{16} & Pho_1^1 \\ Pio_1^2 & Pio_1^3 & Pio_1^4 & Pih_1^5 & Pih_1^6 & Pih_1^{15} & Pih_1^{16} & Pio_1^1 \end{bmatrix}.$$

$Q11$ has four rank-deficient submatrices. They are 4×4 submatrices of rank two (or less). Two constraints are required to force a generic vector in $\mathbb{R}^4$ to lie in a given two-dimensional subspace. Four conditions are required, therefore, to force a generic 4×4 matrix to be of rank two. These conditions will be studied in order of increasing complexity. (Clearly, the conditions which involve variables from Pih are bound to be horrendous, so the are not considered until much later.) Eight of the conditions are identities of the form $A_i^j=0$. The rest reduce (at a generic point) to four term linear equations. Right–left, left–right, top–bottom, and bottom–top rank deficient submatrices are labeled as Qij_{rl}, Qij_{lr}, Qij_{tb}, and Qij_{bt}, where $i,j=1,2$. One such rank deficient submatrix whose entries are relatively simple expressions in A and Q is

$$Q11_{rl}=\begin{bmatrix} Q11_5^1 & Q11_5^2 & Q11_5^3 & Q11_5^4 \\ Q11_6^1 & Q11_6^2 & Q11_6^3 & Q11_6^4 \\ Q11_7^1 & Q11_7^2 & Q11_7^3 & Q11_7^4 \\ Q11_8^1 & Q11_8^2 & Q11_8^3 & Q11_8^4 \end{bmatrix}=\begin{bmatrix} Pho_3^2 & Pho_3^3 & Pho_3^4 & Phh_3^5 \\ Pho_2^2 & Pho_2^3 & Pho_2^4 & Phh_2^5 \\ Pho_1^2 & Pho_1^3 & Pho_1^4 & Phh_1^5 \\ Pio_1^2 & Pio_1^3 & Pio_1^4 & Pih_1^5 \end{bmatrix}.$$

Other relatively simple rank-deficient submatrices are the ''hidden–outgoing'' submatrices: $Q11_{bt}$, $Q12_{bt}$, $Q12_{lr}$, $Q21_{tb}$, $Q21_{rl}$, $Q22_{lr}$, and $Q22_{tb}$. The preponderance of their entries

represent hidden–outgoing transitions. Entries of ''incoming–hidden'' submatrices are predominantly incoming–hidden transitions. There are eight ''incoming–hidden'' submatrices: $Q11_{tb}$, $Q11_{lr}$, $Q21_{lr}$, $Q21_{bt}$, $Q22_{bt}$, $Q22_{rl}$, $Q12_{rl}$, and $Q12_{tb}$.

A. Identities

Since $Q11_{rl}$ is rank two, the determinant of any 3×3 minor is identically zero. Recall that A is a 16×16 block matrix, with 4×4 blocks on the diagonal. The upper left block of A is the inverse of the upper left block of Pho, and so

$$-A_4^1=\begin{vmatrix} Pho_1^2 & Pho_1^3 & Pho_1^4 \\ Pho_2^2 & Pho_2^3 & Pho_2^4 \\ Pho_3^2 & Pho_3^3 & Pho_3^4 \end{vmatrix} \Big/ dPho_{1-4}^{1-4}=\begin{vmatrix} Q11_5^1 & Q11_5^2 & Q11_5^3 \\ Q11_6^1 & Q11_6^2 & Q11_6^3 \\ Q11_7^1 & Q11_7^2 & Q11_7^3 \end{vmatrix} \Big/ dPho_{1-4}^{1-4}=0.$$

The same reasoning applies to $Q11_{bt}$ and shows that $A_1^4=0$. This argument also applies to the rank-deficient submatrices $Q21_{rl}$, $Q21_{tb}$, $Q12_{lr}$, $Q22_{tb}$, and $Q22_{lr}$ and yields the following identities:

$$A_1^4=0,\quad A_4^1=0,\quad A_5^8=0,\quad A_8^5=0,\quad A_9^{12}=0,\quad A_{12}^9=0,\quad A_{13}^{16}=0,\quad A_{16}^{13}=0. \tag{16}$$

B. ''Easy'' conditions

The rest of the equations used to removed parameters are linear in the A_i^js. The simplest result from forcing the other 3×3 minors of ''hidden–outgoing'' submatrices to be zero. In this section eight more conditions are derived by considering the 3×3 minors of ''hidden–outgoing'' submatrices whose entries are only hidden–outgoing and hidden–hidden transitions. Then it is shown that all other conditions upon the ''hidden–outgoing'' submatrices are redundant.

1. Hidden–outgoing and hidden–hidden conditions

Consider the 3×4 submatrix of $Q11_{rl}$:

$$\begin{bmatrix} Q11_5^1 & Q11_5^2 & Q11_5^3 & Q11_5^4 \\ Q11_6^1 & Q11_6^2 & Q11_6^3 & Q11_6^4 \\ Q11_7^1 & Q11_7^2 & Q11_7^3 & Q11_7^4 \end{bmatrix}=\begin{bmatrix} Pho_3^2 & Pho_3^3 & Pho_3^4 & Phh_3^5 \\ Pho_2^2 & Pho_2^3 & Pho_2^4 & Phh_2^5 \\ Pho_1^2 & Pho_1^3 & Pho_1^4 & Phh_1^5 \end{bmatrix}.$$

Since $Phh_{1-3}^5 = Pho_{1-3}^{1-4}(Q_{r_{\mathbf{r}}}^{1-4})^{-1}Q_{r_{\mathbf{r}}}^{5-8}A_{5-8}^5$, it helps to define

$$\mathbf{v}=(Q_{r_{\mathbf{r}}}^{1-4})^{-1}Q_{r_{\mathbf{r}}}^{5-8}A_{5-8}^5.$$

Then every 3×3 minor of

$$\begin{bmatrix} Pho_1^2 & Pho_1^3 & Pho_1^4 & \\ Pho_2^2 & Pho_2^3 & Pho_2^4 & Pho_{1-3}^{1-4}\mathbf{v} \\ Pho_3^2 & Pho_3^3 & Pho_3^4 & \end{bmatrix}$$

must be identically zero. Let $\{\alpha,\beta,\gamma\}=\{2,3,4\}$. Then

$$\begin{vmatrix} Pho_1^\alpha & Pho_1^\beta & \\ Pho_2^\alpha & Pho_2^\beta & Pho_{1-3}^{1-4}\mathbf{v} \\ Pho_3^\alpha & Pho_3^\beta & \end{vmatrix}=\begin{vmatrix} Pho_1^\alpha & Pho_1^\beta & Pho_1^1 \\ Pho_2^\alpha & Pho_2^\beta & Pho_2^1 \\ Pho_3^\alpha & Pho_3^\beta & Pho_3^1 \end{vmatrix} v_1+\begin{vmatrix} Pho_1^\alpha & Pho_1^\beta & Pho_1^\gamma \\ Pho_2^\alpha & Pho_2^\beta & Pho_2^\gamma \\ Pho_3^\alpha & Pho_3^\beta & Pho_3^\gamma \end{vmatrix} v_\gamma$$

$$= \pm A_4^{\gamma} v_1 / dA_{1-4}^{1-4} + \pm A_4^1 v_{\gamma} / dA_{1-4}^{1-4}$$
$$= \pm A_4^{\gamma} v_1 / dA_{1-4}^{1-4},$$

since $A_4^1 \equiv 0$. Furthermore, A_4^{γ} is generally nonzero, forcing $v_1 = 0$. The matrix identity (8) says that the first row of $(Q_{r_{\mathbf{r}}}^{1-4})^{-1} Q_{r_{\mathbf{r}}}^{5-8}$ equals $(dQ_{r_{\mathbf{r}}}^{j+4,2,3,4} / dQ_{r_{\mathbf{r}}}^{1-4})_{j=1,2,3,4}$ which implies

$$0 = \sum_{j=5}^{8} dQ_{r_{\mathbf{r}}}^{j,2,3,4} A_j^5 \equiv \sum_{j=5}^{7} dQ_{r_{\mathbf{r}}}^{j,2,3,4} A_j^5, \tag{17}$$

where the last equivalence holds by virtue of the fact that $A_8^5 \equiv 0$. The same reasoning applied to the other ''hidden–outgoing'' submatrices results in

$$0 = \sum_{j=1}^{3} dQ_{r_{\mathbf{b}}}^{j,14,15,16} A_j^1 = \sum_{j=2}^{4} dQ_{r_{\mathbf{r}}}^{j,5,6,7} A_j^4 = \sum_{j=6}^{8} dQ_{r_{\mathbf{t}}}^{j,9,10,11} A_j^8 = \sum_{j=9}^{11} dQ_{r_{\mathbf{t}}}^{j,6,7,8} A_j^9 = \sum_{j=10}^{12} dQ_{r_{\mathbf{l}}}^{j,13,14,15} A_j^{12}$$
$$= \sum_{j=13}^{15} dQ_{r_{\mathbf{l}}}^{j,10,11,12} As_j^{13} = \sum_{j=14}^{16} dQ_{r_{\mathbf{b}}}^{j,1,2,3} A_j^{16}. \tag{18}$$

2. Redundant hidden–outgoing conditions

In the previous section, a 3×4 submatrix of the 4×4 $Q11_{rl}$ was forced to be of rank two. This would not generally suffice to show that rank $Q11_{rl}=2$. In this section, however, it is shown that conditions (17) and (18) do in fact force rank $Q11_{rl}=2$. We start by checking that modulo (17) and (18) the first three columns of $Q11_{rl}$ are rank two. As mentioned in the Introduction, the reader may prefer to skip ahead to Sec. III C.

$$\begin{bmatrix} Q11_5^1 & Q11_5^2 & Q11_5^3 \\ Q11_6^1 & Q11_6^2 & Q11_6^3 \\ Q11_7^1 & Q11_7^2 & Q11_7^3 \\ Q11_8^1 & Q11_8^2 & Q11_8^3 \end{bmatrix} = \begin{bmatrix} Pho_3^2 & Pho_3^3 & Pho_3^4 \\ Pho_2^2 & Pho_2^3 & Pho_2^4 \\ Pho_1^2 & Pho_1^3 & Pho_1^4 \\ Pio_1^2 & Pio_1^3 & Pio_1^4 \end{bmatrix} = \begin{bmatrix} \begin{pmatrix} & & 1 \\ & 1 & \\ 1 & & \end{pmatrix} Pho_{1-3}^{2-4} \\ \mathbf{m}_1 A_{1-4}^{1,2} Pho_{1,2}^{1-4} + \mathbf{w} \end{bmatrix},$$

where

$$\mathbf{w} = \left(\frac{dQ_{i,r_{\mathbf{r}}}^{j,5-8}}{dQ_{r_{\mathbf{r}}}^{5-8}} \right)_{j=2,3,4} \quad \text{and} \quad \mathbf{m}_1 = \left(\frac{dQ_{1,r_{\mathbf{b}}}^{j,13-16}}{dQ_{r_{\mathbf{b}}}^{13-16}} - \frac{dQ_{1,r_{\mathbf{r}}}^{j,5-8}}{dQ_{r_{\mathbf{r}}}^{5-8}} \right)_{j,1,2,3,4}. \tag{19}$$

Then for $1 \leqslant \alpha < \beta \leqslant 3$,

$$0=\begin{vmatrix} Pho_{\alpha}^{2} & Pho_{\alpha}^{3} & Pho_{\alpha}^{4} \\ Pho_{\beta}^{2} & Pho_{\beta}^{3} & Pho_{\beta}^{4} \\ Pio_{1}^{2} & Pio_{1}^{3} & Pio_{1}^{4} \end{vmatrix}$$

$$=\left|\begin{bmatrix} \mathbf{e}_{\alpha} \\ \mathbf{e}_{\beta} \\ \mathbf{m}_{1}[A_{1-4}^{1,2}:0] \end{bmatrix} Pho_{1-3}^{2-4}\right| + \left|\begin{bmatrix} \mathbf{e}_{\alpha} \\ \mathbf{e}_{\beta} \end{bmatrix} Pho_{1-3}^{2-4} \\ \mathbf{w} \right|$$

$$=\left|\begin{matrix} \mathbf{e}_{\alpha} \\ \mathbf{e}_{\beta} \\ \mathbf{m}_{1}[A_{1-4}^{1,2}:0] \end{matrix}\right| |Pho_{1-3}^{2-4}| + \left|\begin{matrix} Pho_{\alpha,\beta}^{2-4} \\ \mathbf{w} \end{matrix}\right| = \mathbf{w}^{2} dPho_{\alpha,\beta}^{3,4} - \mathbf{w}^{3} dPho_{\alpha,\beta}^{2,4} + \mathbf{w}^{4} dPho_{\alpha,\beta}^{2,3}. \quad (20)$$

The last line follows from the fact that $|Pho_{1-3}^{2-4}| \equiv 0$. Since $A \equiv Pho^{-1}$, for $\{a,b,c,d\} = \{1,2,3,4\}$ and $\{\alpha,\beta,\gamma\} = \{1,2,3\}$, $dPho_{\alpha,\beta}^{a,b} = -1^{\alpha+\beta+a+b} dA_{c,d}^{\gamma,4} / dA_{1-4}^{1-4}$. Substituting this, (16), and (19) into (20) implies

$$0=\left|\begin{matrix} Pho_{\alpha,\beta}^{2-4} \\ \mathbf{w} \end{matrix}\right| = A_{1}^{\gamma}(A_{2}^{4} dQ_{1,r_{\mathbf{r}}}^{2,5-8} + A_{3}^{4} dQ_{1,r_{\mathbf{r}}}^{3,5-8} + A_{4}^{4} dQ_{1,r_{\mathbf{r}}}^{4,5-8}). \quad (21)$$

Generally $A_{1}^{\gamma} \neq 0$. The second term of (21) is really equivalent to the second equation in (18). Consider the Jacobian of both equations:

$$\begin{bmatrix} dQ_{1,r_{\mathbf{r}}}^{2,5-8} & dQ_{1,r_{\mathbf{r}}}^{3,5-8} & dQ_{1,r_{\mathbf{r}}}^{4,5-8} \\ dQ_{r_{\mathbf{r}}}^{2,5-7} & dQ_{r_{\mathbf{r}}}^{3,5-7} & dQ_{r_{\mathbf{r}}}^{4,5-7} \end{bmatrix}. \quad (22)$$

Let $j,k \in \{2,3,4\}$. Grassman relations imply

$$dQ_{1,r_{\mathbf{r}}}^{j,5-8} dQ_{r_{\mathbf{r}}}^{k,5-7} - dQ_{1,r_{\mathbf{r}}}^{k,5-8} dQ_{r_{\mathbf{r}}}^{j,5-7} = dQ_{r_{\mathbf{r}}}^{5-8} dQ_{1,r_{\mathbf{r}}}^{j,k,5-7} = 0. \quad (23)$$

The last equality follows because of range conditions. For any $j,k \in \{2,3,4\}$, $Q_{1,r_{\mathbf{r}}}^{j,k,5-7}$ represents travel across the barrier separating incoming states [1,8–16] from outgoing states [2–7]. This matrix is generally of rank four, so $dQ_{1,r_{\mathbf{r}}}^{j,k,5-7} \equiv 0$. Because of (23) the Jacobian (22) is rank one.

The only 3×3 minors of $Q11_{rl}$ which have not yet been shown to be zero by virtue of (17) and (18) are those which are functions in incoming–hidden transitions. For example,

$$\begin{vmatrix} Pho_{2}^{3} & Pho_{2}^{4} & Phh_{2}^{5} \\ Pho_{1}^{3} & Pho_{1}^{4} & Phh_{1}^{5} \\ Pio_{1}^{3} & Pio_{1}^{4} & Pih_{1}^{5} \end{vmatrix} \quad (24)$$

is an example of such a minor. Before showing that (24) is trivally zero we define **U** and **u** as follows:

$$\mathbf{U} \equiv (Q_{r_{\mathbf{r}}}^{1-4})^{-1} Q_{r_{\mathbf{r}}}^{5-8} A_{5-8}^{5} = \frac{1}{dQ_{r_{\mathbf{r}}}^{1-4}} \begin{bmatrix} dQ_{r_{\mathbf{r}}}^{2,3,4,5} & dQ_{r_{\mathbf{r}}}^{2,3,4,6} & dQ_{r_{\mathbf{r}}}^{2,3,4,7} \\ -dQ_{r_{\mathbf{r}}}^{1,3,4,5} & -dQ_{r_{\mathbf{r}}}^{1,3,4,6} & -dQ_{r_{\mathbf{r}}}^{1,3,4,7} \\ dQ_{r_{\mathbf{r}}}^{1,2,4,5} & dQ_{r_{\mathbf{r}}}^{1,2,4,6} & dQ_{r_{\mathbf{r}}}^{1,2,4,7} \\ -dQ_{r_{\mathbf{r}}}^{1,2,3,5} & -dQ_{r_{\mathbf{r}}}^{1,2,3,6} & -dQ_{r_{\mathbf{r}}}^{1,2,3,7} \end{bmatrix} A_{5-7}^{5} = \frac{1}{dQ_{r_{\mathbf{r}}}^{1-4}} \begin{bmatrix} 0 \\ \mathbf{u} \end{bmatrix},$$

where the first entry in the last equality is due to (17). Recall (19),

$$Phh^{5}_{1-2}=Pho^{1-4}_{1-2}(Q^{1-4}_{r_{\mathbf{r}}})^{-1}Q^{5-8}_{r_{\mathbf{r}}}A^{5}_{5-8}=\left(\frac{1}{dQ^{1-4}_{r_{\mathbf{r}}}}\right)Pho^{2-4}_{1-2}\mathbf{u},$$

$$Pih^{5}_{1}=\mathbf{M}_1(Q^{1-4}_{r_{\mathbf{r}}})^{-1}Q^{5-8}_{r_{\mathbf{r}}}A^{5}_{5-8}=\left(\frac{1}{dQ^{1-4}_{r_{\mathbf{r}}}}\right)\mathbf{m}_1A^{1,2}_{1-4}Pho^{2-4}_{1,2}\mathbf{u}, \tag{25}$$

$$Pio^{3,4}_{1}=\mathbf{M}^{3,4}_{1}+\mathbf{w}^{3,4}=\mathbf{m}_1A^{1,2}_{1-4}Pho^{3,4}_{1,2}+\mathbf{w}^{3,4}.$$

Furthermore, $\left|{}^{Pho^{2-4}_{1,2}}_{\mathbf{w}}\right| = 0$ because of the fact that (21) is equivalent to (18). Plugging this into (24) yields a 3×3 minor which is trivially zero because

$$\begin{aligned}
&\begin{vmatrix} Pho^{3,4}_{1,2} & : & Pho^{2-4}_{1,2}\mathbf{u} \\ \mathbf{m}_1A^{1,2}_{1-4}Pho^{3,4}_{1,2}+\mathbf{w}^{3,4} & : & \mathbf{m}_1A^{1,2}_{1-4}Pho^{2-4}_{1,2}\mathbf{u}\end{vmatrix} \\
&\quad=\begin{vmatrix} Pho^{3,4}_{1,2} & : & Pho^{2-4}_{1,2}\mathbf{u} \\ \mathbf{m}_1A^{1,2}_{1-4}Pho^{3,4}_{1,2} & : & \mathbf{m}_1A^{1,2}_{1-4}Pho^{2-4}_{1,2}\mathbf{u}\end{vmatrix}+\begin{vmatrix} Pho^{3,4}_{1,2} & : & Pho^{2-4}_{1,2}\mathbf{u} \\ \mathbf{w}^{3,4} & : & 0\end{vmatrix} \\
&\quad=\left|\begin{pmatrix} 1 & 0 \\ 0 & 1 \\ \mathbf{m}_1A^{1,2}_{1-4} & \end{pmatrix}Pho^{2-4}_{1,2}\begin{pmatrix} 0 & 0 & \mathbf{u}_1 \\ 1 & 0 & \mathbf{u}_2 \\ 0 & 1 & \mathbf{u}_3\end{pmatrix}\right|+\left|\begin{pmatrix} Pho^{2-4}_{1,2} \\ \mathbf{w}\end{pmatrix}\begin{pmatrix} 0 & 0 & \mathbf{u}_1 \\ 1 & 0 & \mathbf{u}_2 \\ 0 & 1 & \mathbf{u}_3\end{pmatrix}\right|=0.
\end{aligned}$$

The last line follows because of Eq. (21) and the fact that the determinant of a 3×2 matrix with a 2×3 matrix is zero. Therefore, forcing (24) to be zero yields no additional conditions upon the A^{j}_{i}s. Analogous computations hold for the rest of the range conditions upon $Q11_{rl}$, $Q11_{bt}$, $Q12_{bt}$, $Q12_{lr}$, $Q21_{tb}$, $Q21_{rl}$, $Q22_{lr}$, and $Q22_{tb}$. All of these conditions are equivalent to the identities (16)–(18), so only 16 of the possible 32 conditions are independent. In the next section, more conditions are found amongst the modified data for $Q11_{tb}$, $Q11_{lr}$, $Q21_{lr}$, $Q21_{bt}$, $Q22_{bt}$, $Q22_{rl}$, $Q12_{rl}$, and $Q12_{tb}$.

C. ''Hard'' conditions

Consider now the rank-deficient ''incoming–hidden'' submatrix

$$Q11_{tb}=\begin{bmatrix} Pih^{5}_{1} & Pih^{6}_{1} & Pih^{15}_{1} & Pio^{4}_{1} \\ Pih^{5}_{2} & Pih^{6}_{2} & Pih^{15}_{2} & Pio^{4}_{2} \\ Pih^{5}_{3} & Pih^{6}_{3} & Pih^{15}_{3} & Pih^{4}_{3} \\ Phh^{5}_{1} & Phh^{6}_{1} & Phh^{15}_{1} & Pho^{4}_{1}\end{bmatrix}. \tag{26}$$

In Sec. III C 1 range conditions upon $Q11_{tb}$ are derived. These conditions are simplified in Sec. III C 3. Finally, all other conditions upon the ''incoming–hidden'' submatrices are shown to be redundant in Sec. III C 4.

1. Derive ''hard'' conditions

In order to start with as few incoming–hidden transitions as possible, let $1\leqslant\alpha<\beta\leqslant3$ and consider the minor of (26) taken from rows $\alpha,\beta,4$ and columns 1,2,4:

$$\begin{vmatrix} \mathbf{M}_{\alpha,\beta}(Q_{r_{\mathbf{r}}}^{1-4})^{-1}Q_{r_{\mathbf{r}}}^{5-8}A_{5-8}^{5,6} & : & \mathbf{M}_{\alpha,\beta}e_4+\left(\dfrac{dQ_{i,r_{\mathbf{r}}}^{4-8}}{dQ_{r_{\mathbf{r}}}^{5-8}}\right)_{i,j} \\ Pho_1^{1-4}(Q_{r_{\mathbf{r}}}^{1-4})^{-1}Q_{r_{\mathbf{r}}}^{5-8}A_{5-8}^{5,6} & : & Pho_1^4 \end{vmatrix}. \tag{27}$$

Now define the 2×4 and 3×4 derivates and $\mathbf{m}$ and $\mathbf{N}$:

$$\mathbf{m}_{\alpha,\beta}\equiv\left(\begin{matrix} \dfrac{dQ_{\alpha,r_{\mathbf{b}}}^{j,13-16}}{dQ_{r_{\mathbf{b}}}^{13-16}}-\dfrac{dQ_{\alpha,r_{\mathbf{r}}}^{j,5-8}}{dQ_{r_{\mathbf{r}}}^{5-8}} \\ \dfrac{dQ_{\beta,r_{\mathbf{b}}}^{j,13-16}}{dQ_{r_{\mathbf{b}}}^{13-16}}-\dfrac{dQ_{\beta,r_{\mathbf{r}}}^{j,5-8}}{dQ_{r_{\mathbf{r}}}^{5-8}} \end{matrix}\right)_j, \quad \text{for } j\in\{1,2,3,4\}, \tag{28}$$

$$\mathbf{N}\equiv\begin{bmatrix} \mathbf{m}_{\alpha,\beta} & A_{1-4}^{1,2} \\ 1 & 0 \end{bmatrix}Pho_{1,2}^{1-4}, \tag{29}$$

and note that $\mathbf{N}$ is rank two. Substituting (28) and (29) into (27) yields the following form for the 3×3 determinants:

$$\begin{vmatrix} \mathbf{N}(Q_{r_{\mathbf{r}}}^{1-4})^{-1}Q_{r_{\mathbf{r}}}^{5-8}A_{5-8}^{5,6}:\mathbf{N}e_4+\dfrac{1}{dQ_{r\mathbf{r}}^{5-8}}\begin{pmatrix} dQ_{\alpha,r_{\mathbf{r}}}^{4-8} \\ dQ_{\beta,r_{\mathbf{r}}}^{4-8} \\ 0 \end{pmatrix} \end{vmatrix}$$

$$=\left|\mathbf{N}[(Q_{r_{\mathbf{r}}}^{1-4})^{-1}Q_{r_{\mathbf{r}}}^{5-8}A_{5-8}^{5,6}:e_4]\right|+\frac{1}{dQ_{r_{\mathbf{r}}}^{5-8}}\begin{vmatrix} \mathbf{N}(Q_{r_{\mathbf{r}}}^{1-4})^{-1}Q_{r_{\mathbf{r}}}^{5-8}A_{5-8}^{5,6}: & dQ_{\alpha,r_{\mathbf{r}}}^{4-8} \\ & dQ_{\beta,r_{\mathbf{r}}}^{4-8} \\ & 0 \end{vmatrix}$$

$$=\frac{1}{dQ_{r_{\mathbf{r}}}^{5-8}}\begin{vmatrix} \begin{bmatrix} \mathbf{m}_{\alpha,\beta} & : & A_{1-4}^{1,2} \\ 1 & : & 0 \end{bmatrix}Pho_{1,2}^{1-4}(Q_{r_{\mathbf{r}}}^{1-4})^{-1}Q_{r_{\mathbf{r}}}^{5-8}A_{5-8}^{5,6} & : & dQ_{\alpha,r_{\mathbf{r}}}^{4-8} \\ & & & & dQ_{\beta,r_{\mathbf{r}}}^{4-8} \\ & & & & 0 \end{vmatrix}$$

$$=\frac{1}{dQ_{r_{\mathbf{r}}}^{5-8}}\begin{vmatrix} \mathbf{m}_{\alpha,\beta} & A_{1-4}^{1,2} & \vdots & dQ_{\alpha,r_{\mathbf{r}}}^{4-8} \\ & & & dQ_{\beta,r_{\mathbf{r}}}^{4-8} \\ 1 & 0 & \vdots & 0 \end{vmatrix}\begin{vmatrix} Pho_{1,2}^{1-4}(Q_{r_{\mathbf{r}}}^{1-4})^{-1}Q_{r_{\mathbf{r}}}^{5-8}A_{5-8}^{5,6} & 0 \\ & 0 \\ 0 & 1 \end{vmatrix}$$

$$=C\left|\mathbf{m}_{\alpha,\beta}A_{1-4}^2:\begin{matrix} dQ_{\alpha,r_{\mathbf{r}}}^{4-8} \\ dQ_{\beta,r_{\mathbf{r}}}^{4-8} \end{matrix}\right|=C\sum_{j=1}^{4}\begin{vmatrix} \left(\dfrac{dQ_{\alpha,r_{\mathbf{b}}}^{j,13-16}}{dQ_{r_{\mathbf{b}}}^{13-16}}-\dfrac{dQ_{\alpha,r_{\mathbf{r}}}^{j,5-8}}{dQ_{r_{\mathbf{r}}}^{5-8}}\right) & dQ_{\alpha,r_{\mathbf{r}}}^{4-8} \\ \left(\dfrac{dQ_{\beta,r_{\mathbf{b}}}^{j,13-16}}{dQ_{r_{\mathbf{b}}}^{13-16}}-\dfrac{dQ_{\beta,r_{\mathbf{r}}}^{j,5-8}}{dQ_{r_{\mathbf{r}}}^{5-8}}\right) & dQ_{\beta,r_{\mathbf{r}}}^{4-8} \end{vmatrix}A_j^2$$

$$=\sum_{j=1}^{4}\left(\frac{1}{dQ_{r_{\mathbf{b}}}^{13-16}}(dQ_{\alpha,r_{\mathbf{b}}}^{j,13-16}dQ_{\beta,r_{\mathbf{r}}}^{4-8}-dQ_{\beta,r_{\mathbf{b}}}^{j,13-16}dQ_{\alpha,r_{\mathbf{r}}}^{4-8})-\frac{1}{dQ_{r_{\mathbf{r}}}^{5-8}}(dQ_{\alpha,r_{\mathbf{r}}}^{j,5-8}dQ_{\beta,r_{\mathbf{r}}}^{4-8}\right.$$

$$\left.-dQ_{\beta,r_{\mathbf{r}}}^{j,5-8}dQ_{\alpha,r_{\mathbf{r}}}^{4-8})\right)A_j^2$$

$$=\frac{C}{dQ_{r_{\mathbf{b}}}^{13-16}}\sum_{j=1}^{4}(dQ_{\alpha,r_{\mathbf{b}}}^{j,13-16}dQ_{\beta,r_{\mathbf{r}}}^{4-8}-dQ_{\beta,r_{\mathbf{b}}}^{j,13-16}dQ_{\alpha,r_{\mathbf{r}}}^{4-8}-dQ_{r_{\mathbf{b}}}^{13-16}dQ_{\alpha,\beta,r_{\mathbf{r}}}^{j,4-8})A_j^2, \tag{30}$$

where $C\equiv|\,Pho_{1,2}^{1-4}(Q_{r_{\mathbf{r}}}^{1-4})^{-1}Q_{r_{\mathbf{r}}}^{5-8}A_{5-8}^{5,6}|/dQ_{r_{\mathbf{r}}}^{5-8}$. The last equality holds because Grassman relations imply

$$dQ_{\alpha,r_{\mathbf{r}}}^{j,5-8}dQ_{\beta,r_{\mathbf{r}}}^{4-8}-dQ_{\beta,r_{\mathbf{r}}}^{j,5-8}dQ_{\alpha,r_{\mathbf{r}}}^{4-8}=dQ_{\alpha,\beta,r_{\mathbf{r}}}^{j,4-8}dQ_{r_{\mathbf{r}}}^{5-8}. \tag{31}$$

If $C\neq 0$, then forcing (27) to be zero gives three conditions upon the A_j^2s, since there are three ways to choose α,β in (30). The same argument applied to other ''incoming–outgoing'' submatrices yields similar conditions. These conditions are simplified in Sec. III C 3. However, first we must verify the following.

Claim: $C\neq 0$.

Proof: Define $\eta\equiv Pih(I-Phh)^{-1}$. Then $Q_{r_{\mathbf{r}}}^{1-4}=\eta_{r_{\mathbf{r}}}^{1-4}Pho_{1-4}^{1-4}$ and $Q_{r_{\mathbf{r}}}^{5-8}=\eta_{r_{\mathbf{r}}}^{5-8}Pho_{5-8}^{5-8}$. Since $A\equiv Pho^{-1}$,

$$C\equiv|Pho_{1,2}^{1-4}(Q_{r_{\mathbf{r}}}^{1-4})^{-1}Q_{r_{\mathbf{r}}}^{5-8}A_{5-8}^{5,6}|/dQ_{r_{\mathbf{r}}}^{5-8}$$

$$=\frac{1}{dQ_{r_{\mathbf{r}}}^{5-8}}\left|\begin{pmatrix}1&0&0&0\\0&1&0&0\end{pmatrix}(\eta_{r_{\mathbf{r}}}^{1-4})^{-1}\eta_{r_{\mathbf{r}}}^{5-8}\begin{pmatrix}1&0\\0&1\\0&0\\0&0\end{pmatrix}\right| \tag{32}$$

$$=-\begin{vmatrix}d\eta_{r_{\mathbf{r}}}^{2-5}&d\eta_{r_{\mathbf{r}}}^{2,3,4,6}\\d\eta_{r_{\mathbf{r}}}^{1,3,4,5}&d\eta_{r_{\mathbf{r}}}^{1,3,4,6}\end{vmatrix}\Big/(dQ_{r_{\mathbf{r}}}^{5-8}(d\eta_{r_{\mathbf{r}}}^{1-4})^2) \tag{33}$$

$$=d\eta_{r_{\mathbf{r}}}^{3-6}/(dQ_{r_{\mathbf{r}}}^{5-8}d\eta_{r_{\mathbf{r}}}^{1-4}). \tag{34}$$

Equation (32) follows from the definitions of $Q_{r_{\mathbf{r}}}^{1-4}$, $Q_{r_{\mathbf{r}}}^{5-8}$, and A in terms of η and Pho. Equation (8) implies (33), which combined with Grassmann relations yields (34). Since there is no barrier of less than four states separating incoming states 9, 10, 11, and 12 from hidden states 1, 2, 3, and 4, $d\eta_{r_{\mathbf{r}}}^{3-6}\neq 0$ in the generic case. □

2. More matrix identities

In the following section condition (30) is simplified using many matrix identities. First note that Grassmann relations imply

$$\begin{vmatrix}dQ_{14,15,5-8}^{i,9-13}&dQ_{14,15,5-8}^{j,9-13}\\dQ_{14,16,5-8}^{i,9-13}&dQ_{14,16,5-8}^{j,9-13}\end{vmatrix}=dQ_{14,5-8}^{9-13}dQ_{14-16,5-8}^{i,j,9-13} \tag{35}$$

and $dQ_{14-16,5-8}^{i,j,9-13}dQ_{15,16,5-8}^{k,9-13}-dQ_{14-16,5-8}^{i,k,9-13}dQ_{15,16,5-8}^{j,9-13}+dQ_{14-16,5-8}^{j,k,9-13}dQ_{15,16,5-8}^{i,9-13}=0$. Therefore,

$$\begin{vmatrix}dQ_{14,15,5-8}^{i,9-13}&dQ_{14,15,5-8}^{j,9-13}&dQ_{14,15,5-8}^{k,9-13}\\dQ_{14,16,5-8}^{i,9-13}&dQ_{14,16,5-8}^{j,9-13}&dQ_{14,16,5-8}^{k,9-13}\\dQ_{15,16,5-8}^{i,9-13}&dQ_{15,16,5-8}^{j,9-13}&dQ_{15,16,5-8}^{k,9-13}\end{vmatrix}$$

$$= dQ^{9-13}_{14,5-8}\left(dQ^{i,j,9-13}_{14-16,5-8}dQ^{k,9-13}_{15,16,5-8} - dQ^{i,k,9-13}_{14-16,5-8}dQ^{j,9-13}_{15,16,5-8} + dQ^{j,k,9-13}_{14-16,5-8}dQ^{i,9-13}_{15,16,5-8}\right)$$
$$\equiv 0. \tag{36}$$

Because Q^{9-16}_{1-8} is generically of rank four,

$$Q^{13-16}_{5-8} = Q^{9-12}_{5-8}(Q^{9-12}_{1-4})^{-1}Q^{13-16}_{1-4}. \tag{37}$$

This means that for $\alpha \in \{1,2,3,4\}$

$$\begin{aligned} dQ^{n,13-16}_{\alpha,5-8} &= \begin{vmatrix} Q^n_\alpha & \vdots & Q^{13-16}_\alpha \\ Q^n_{5-8} & \vdots & Q^{13-16}_{5-8} \end{vmatrix} = \begin{vmatrix} Q^n_\alpha & \vdots & Q^{13-16}_\alpha \\ Q^n_{5-8} & \vdots & Q^{9-12}_{5-8}(Q^{9-12}_{1-4})^{-1}Q^{13-16}_{1-4} \end{vmatrix} \\ &= \begin{vmatrix} Q^n_\alpha & \vdots & \mathbf{e}_\alpha \\ Q^n_{5-8} & \vdots & Q^{9-12}_{5-8}(Q^{9-12}_{1-4})^{-1} \end{vmatrix} \begin{vmatrix} 1 & \\ & Q^{13-16}_{1-4} \end{vmatrix} \\ &= \begin{vmatrix} Q^n_\alpha & \vdots & Q^{9-12}_\alpha \\ Q^n_{5-8} & \vdots & Q^{9-12}_{5-8} \end{vmatrix} \begin{vmatrix} 1 & \\ & (Q^{9-12}_{1-4})^{-1} \end{vmatrix} \begin{vmatrix} 1 & \\ & Q^{13-16}_{1-4} \end{vmatrix} \\ &= dQ^{n,9-12}_{\alpha,5-8}\frac{dQ^{13-16}_{1-4}}{dQ^{9-12}_{1-4}}. \end{aligned} \tag{38}$$

Similarly,

$$dQ^{n,4-8}_{\alpha,\beta,13-16} = dQ^{n,4,9-12}_{\alpha,\beta,13-16}\frac{dQ^{5-8}_{1-4}}{dQ^{9-12}_{1-4}} \quad \text{and} \quad dQ^{n,5-8}_{\alpha,13-16} = dQ^{n,9-12}_{\alpha,13-16}\frac{dQ^{5-8}_{1-4}}{dQ^{9-12}_{1-4}}. \tag{39}$$

Finally, Grassmann relations and range conditions combine with the above identities in the following:

$$\sum_{\sigma\in S_3}\frac{\operatorname{sgn}\sigma}{2}dQ^{\sigma_1,\sigma_2,9-13}_{14-16,5-8}dQ^{\sigma_3,13-16}_{\alpha,5-8}$$
$$= \frac{dQ^{13-16}_{1-4}}{dQ^{9-12}_{1-4}}\sum_{\sigma\in S_3}\frac{\operatorname{sgn}\sigma}{2}dQ^{\sigma_1,\sigma_2,9-13}_{14-16,5-8}dQ^{\sigma_3,9-12}_{\alpha,5-8} \tag{40}$$
$$= \frac{dQ^{13-16}_{1-4}}{dQ^{9-12}_{1-4}}\left(\pm dQ^{9-13}_{\alpha,5-8}dQ^{\sigma_1,\sigma_2,\sigma_3,9-12}_{14-16,5-8} + dQ^{9-12}_{5-8}dQ^{\sigma_1,\sigma_2,\sigma_3,9-13}_{\alpha,14-16,5-8}\right) \tag{41}$$
$$= \frac{dQ^{13-16}_{1-4}}{dQ^{9-12}_{1-4}}dQ^{9-12}_{5-8}dQ^{\sigma_1,\sigma_2,\sigma_3,9-13}_{\alpha,14-16,5-8} \tag{42}$$
$$= dQ^{13-16}_{5-8}dQ^{\sigma_1,\sigma_2,\sigma_3,9-13}_{\alpha,14-16,5-8}. \tag{43}$$

Equation (41) follows from (40) by Grassmann relations; (42) follows from (41) because consistency conditions force $dQ^{9-13}_{\alpha,5-8}\equiv 0$. Finally, (37) forces (43).

In the next section the following notation will also be used.

Notation: Define the matrix $\mathbf{C}$ with columns $\mathbf{c}^j$ and rows $\mathbf{c}_j$, i.e.,

$$\mathbf{C} = [\mathbf{c}^1 \quad \mathbf{c}^2 \quad \mathbf{c}^3 \quad \mathbf{c}^4] = \begin{bmatrix} \mathbf{c}_1 \\ \mathbf{c}_2 \end{bmatrix}.$$

3. Simplification of "hard" conditions

This section consists of a single

Claim: The conditions in (30) are equivalent to

$$0=\sum_{n=1}^{4} dQ^{n,9-13}_{\gamma,\delta,5-8}A_n^2 \quad \text{for } \gamma,\delta\in\{14,15,16\}. \tag{44}$$

Furthermore, Eqs. (30) and (44) constitute only two independent conditions upon the A_i^2s.

Proof: Due to (36), only two independent conditions upon the A_n^2s are given by (44). For convenience, consider (30) where $r_{\mathbf{b}}=5-8$ and $r_{\mathbf{r}}=13-16$. To finish the proof of this claim it is necessary to show that for $\alpha,\beta\in\{1,2,3\}$, the matrix $\mathbf{C}$

$$\mathbf{c}^j=\begin{pmatrix} dQ^{j,13-16}_{\alpha,5-8}dQ^{4-8}_{\beta,13-16}-dQ^{j,13-16}_{\beta,5-8}dQ^{4-8}_{\alpha,13-16}-dQ^{13-16}_{5-8}dQ^{j,4-8}_{\alpha,\beta,13-16} \\ dQ^{j,9-13}_{14,15,5-8} \\ dQ^{j,9-13}_{14,16,5-8} \end{pmatrix}_j \tag{45}$$

is also of rank two. Equations (35), (43), and (39) are combined to show that for $i,j,k\in\{1,2,3,4\}$ $|\mathbf{c}^i\ \ \mathbf{c}^j\ \ \mathbf{c}^k|=0$, forcing $\mathbf{C}$ to be rank two:

$$\begin{aligned}
\frac{|\mathbf{c}^i\ \ \mathbf{c}^j\ \ \mathbf{c}^k|}{dQ^{9-13}_{14,5-8}} &= ((dQ^{i,13-16}_{\alpha,5-8}dQ^{4-8}_{\beta,13-16}-dQ^{i,13-16}_{\beta,5-8}dQ^{4-8}_{\alpha,13-16}-dQ^{13-16}_{5-8}dQ^{i,4-8}_{\alpha,\beta,13-16})dQ^{j,k,9-13}_{14-16,5-8} \\
&\quad -(dQ^{j,13-16}_{\alpha,5-8}dQ^{4-8}_{\beta,13-16}-dQ^{j,13-16}_{\beta,5-8}dQ^{4-8}_{\alpha,13-16}-dQ^{13-16}_{5-8}dQ^{j,4-8}_{\alpha,\beta,13-16})dQ^{i,k,9-13}_{14-16,5-8} \\
&\quad +(dQ^{k,13-16}_{\alpha,5-8}dQ^{4-8}_{\beta,13-16}-dQ^{k,13-16}_{\beta,5-8}dQ^{4-8}_{\alpha,13-16}-dQ^{13-16}_{5-8}dQ^{k,4-8}_{\alpha,\beta,13-16})dQ^{i,j,9-13}_{14-16,5-8}) \\
&= \sum_{\sigma\in S_3(i,j,k)} \frac{\operatorname{sgn}\sigma}{2} dQ^{\sigma_1,\sigma_2,9-13}_{14-16,5-8}((dQ^{\sigma_3,13-16}_{\alpha,5-8}dQ^{4-8}_{\beta,13-16}-dQ^{\sigma_3,13-16}_{\beta,5-8}dQ^{4-8}_{\alpha,13-16}) \\
&\quad -dQ^{13-16}_{5-8}dQ^{\sigma_3,4-8}_{\alpha,\beta,13-16}) \qquad (46) \\
&= dQ^{13-16}_{5-8}\Bigg(dQ^{i,j,k,9-13}_{\alpha,14-16,5-8}dQ^{4-8}_{\beta,13-16}-dQ^{i,j,k,9-13}_{\beta,14-16,5-8}dQ^{4-8}_{\alpha,13-16} \\
&\quad -\sum_{\sigma\in S_3(i,j,k)} \frac{\operatorname{sgn}\sigma}{2} dQ^{\sigma_1,\sigma_2,9-13}_{14-16,5-8}dQ^{\sigma_3,4-8}_{\alpha,\beta,13-16}\Bigg) \qquad (47) \\
&= \frac{dQ^{13-16}_{5-8}dQ^{5-8}_{1-4}}{dQ^{9-12}_{1-4}}\Bigg(dQ^{i,j,k,9-13}_{\alpha,14-16,5-8}dQ^{4,9-12}_{\beta,13-16}-dQ^{i,j,k,9-13}_{\beta,14-16,5-8}dQ^{4,9-12}_{\alpha,13-16} \\
&\quad -\sum_{\sigma\in S_3(i,j,k)} \frac{\operatorname{sgn}\sigma}{2} dQ^{\sigma_1,\sigma_2,9-13}_{14-16,5-8}dQ^{\sigma_3,4,9-12}_{\alpha,\beta,13-16}\Bigg) \qquad (48) \\
&= \frac{dQ^{13-16}_{5-8}dQ^{5-8}_{1-4}}{dQ^{9-12}_{1-4}}(\pm dQ^{4,9-13}_{\alpha,\beta,13-16}\,dQ^{i,j,k,9-12}_{14-16,5-8}\pm dQ^{4,9-12}_{\alpha,\beta,14-16}\,dQ^{i,j,k,9-13}_{13-16,5-8}) \qquad (49) \\
&= 0. \qquad (50)
\end{aligned}$$

Equation (47) follows from (46) and (43). Equation (48) follows from (47), (38), and (39). Equation (49) is the result of another Grassmann relation. The last equation, (50), holds because consistency conditions force $dQ^{4,9-12}_{\alpha,\beta,13-16}=0=dQ^{4,9-13}_{\alpha,\beta,13-16}$. □

Similar calculations hold for $Q11_{lr}$, $Q21_{lr}$, $Q21_{bt}$, $Q22_{bt}$, $Q22_{rl}$, $Q12_{rl}$, and $Q12_{tb}$, yielding 16 independent conditions upon the A^j_is:

$$0=\sum_{n=1}^{4} dQ^{n,9-13}_{\alpha,\beta,5-8}A^2_n \quad \text{for } \alpha,\beta\in\{14,15,16\}, \tag{51}$$

$$0=\sum_{n=1}^{4} dQ^{n,8-12}_{\alpha,\beta,13-16}A^3_n \quad \text{for } \alpha,\beta\in\{5,6,7\}, \tag{52}$$

$$0=\sum_{n=5}^{8} dQ^{n,1,13-16}_{\alpha,\beta,9-12}A^6_n \quad \text{for } \alpha,\beta\in\{2,3,4\}, \tag{53}$$

$$0=\sum_{n=5}^{8} dQ^{n,12-6}_{\alpha,\beta,1-4}A^7_n \quad \text{for } \alpha,\beta\in\{9,10,11\}, \tag{54}$$

$$0=\sum_{n=9}^{12} dQ^{n,1-5}_{\alpha,\beta,13-16}A^{10}_n \quad \text{for } \alpha,\beta\in\{6,7,8\}, \tag{55}$$

$$0=\sum_{n=9}^{12} dQ^{n,1-4,16}_{\alpha,\beta,5-8}A^{11}_n \quad \text{for } \alpha,\beta\in\{13,14,15\}, \tag{56}$$

$$0=\sum_{n=13}^{16} dQ^{n,5-9}_{\alpha,\beta,1-4}A^{14}_n \quad \text{for } \alpha,\beta\in\{10,11,12\}, \tag{57}$$

$$0=\sum_{n=13}^{16} dQ^{n,4-8}_{\alpha,\beta,9-12}A^{15}_n \quad \text{for } \alpha,\beta\in\{1,2,3\}. \tag{58}$$

4. Redundant "hard" conditions

In the previous section two equations were derived which force the first, second, and fourth columns of $Q11_{tb}$ to be rank two. In this section conditions forcing the first three columns of $Q11_{tb}$ to be rank two are shown to be equivalent to conditions (51)–(58).

The reader is reminded that this section is quite technical and is included for the sake of completeness. Much of the notation of the previous section is retained. Here, however, $r_{\mathbf{b}}$ and $r_{\mathbf{r}}$ are fixed so that $r_{\mathbf{b}}\equiv 9-12\equiv r_{\mathbf{r}}$. For the sake of notation, define the 2×4 matrices $\mathbf{L}$ and $\mathbf{D}$:

$$\mathbf{L}^j\equiv\begin{pmatrix} dQ^{j+12,5-8}_{\alpha,r_{\mathbf{r}}} \\ dQ^{j+12,5-8}_{\beta,r_{\mathbf{r}}} \end{pmatrix} \quad \text{and} \quad \mathbf{D}\equiv\mathbf{m}_{\alpha,\beta}. \tag{59}$$

The minor taken from rows α, β, 4 and first three columns of $Q11_{tb}$ can be written as follows:

$$\begin{vmatrix} Pih^5_\alpha & Pih^6_\alpha & Pih^{15}_\alpha \\ Pih^5_\beta & Pih^6_\beta & Pih^{15}_\beta \\ Phh^5_1 & Phh^6_1 & Phh^{15}_1 \end{vmatrix}$$

$$
\begin{aligned}
&= \left| \mathbf{N}(Q^{1-4}_{9-12})^{-1} Q^{5-8}_{9-12} A^{5,6}_{5-8} \vdots \left(\mathbf{N}(Q^{1-4}_{9-12})^{-1} Q^{13-16}_{9-12} + \frac{1}{dQ^{5-8}_{9-12}} \begin{pmatrix} \mathbf{L} \\ 0 \end{pmatrix} \right) A^{15}_{13-16} \right| \\
&= |\mathbf{N}(Q^{1-4}_{9-12})^{-1} [Q^{5-8}_{9-12} A^{5,6}_{5-8} \vdots Q^{13-16}_{9-12} A^{15}_{13-16}]| + \frac{1}{dQ^{5-8}_{9-12}} \\
&\quad \times \left| \mathbf{N}(Q^{1-4}_{9-12})^{-1} Q^{5-8}_{9-12} A^{5,6}_{5-8} \vdots \begin{pmatrix} \mathbf{L} \\ 0 \end{pmatrix} A^{15}_{13-16} \right| \\
&= C \left| \begin{matrix} \mathbf{D} A^{1,2}_{1-4} \\ 1 \quad 0 \end{matrix} \vdots \begin{pmatrix} \mathbf{L} \\ 0 \end{pmatrix}_j A^{15}_{13-16} \right|, \quad \text{since } \mathbf{N} \text{ is rank two} \\
&= C |\mathbf{D} A^2_{1-4} \vdots \mathbf{L} A^{15}_{13-16}|. \qquad (60)
\end{aligned}
$$

At first blush this appears to be quadratic in A^j_is. Equation (30) can be used to factor the A^j_is out of (60). Now define the matrices **F** and **G** whose columns are

$$
\mathbf{f}^j \equiv \begin{pmatrix} dQ^{j,9-13}_{14,15,5-8} \\ dQ^{j,9-13}_{14,16,5-8} \end{pmatrix}, \quad \mathbf{g}^j \equiv \begin{pmatrix} dQ^{j+12,4-8}_{1,2,9-12} \\ dQ^{j+12,4-8}_{1,3,9-12} \end{pmatrix}.
$$

Then (51) and (58) imply

$$
0 = \mathbf{F} \begin{pmatrix} A^2_1 \\ A^2_2 \\ A^2_3 \\ A^2_4 \end{pmatrix} \quad \text{and} \quad 0 = \mathbf{G} \begin{pmatrix} A^{15}_{13} \\ A^{15}_{14} \\ A^{15}_{15} \\ A^{15}_{16} \end{pmatrix}
$$

or

$$
\begin{pmatrix} A^2_1 \\ A^2_2 \\ A^2_3 \\ A^2_4 \end{pmatrix} = \begin{pmatrix} -[\mathbf{f}^1 \ \mathbf{f}^2]^{-1} [\mathbf{f}^3 \ \mathbf{f}^4] \\ I \end{pmatrix} \begin{pmatrix} A^2_3 \\ A^2_4 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} A^{15}_{13} \\ A^{15}_{14} \\ A^{15}_{15} \\ A^{15}_{16} \end{pmatrix} = \begin{pmatrix} -[\mathbf{g}^1 \ \mathbf{g}^2]^{-1} [\mathbf{g}^3 \ \mathbf{g}^4] \\ I \end{pmatrix} \begin{pmatrix} A^{15}_{15} \\ A^{15}_{16} \end{pmatrix}. \qquad (61)
$$

Plugging (59) and (61) into (60) takes the previously found ''hard'' conditions into account and yields

$$
C \left| \mathbf{D} \begin{pmatrix} -[\mathbf{f}^1 \ \mathbf{f}^2]^{-1} [\mathbf{f}^3 \ \mathbf{f}^4] \\ I \end{pmatrix} \begin{pmatrix} A^2_3 \\ A^2_4 \end{pmatrix} \vdots \mathbf{L} \begin{pmatrix} -[\mathbf{g}^1 \ \mathbf{g}^2]^{-1} [\mathbf{g}^3 \ \mathbf{g}^4] \\ I \end{pmatrix} \begin{pmatrix} A^{15}_{15} \\ A^{15}_{16} \end{pmatrix} \right|. \qquad (62)
$$

Showing that (62) is zero requires several steps:

(1) Show that $\mathbf{D}\left(\begin{smallmatrix} -[\mathbf{f}^1 \ \mathbf{f}^2]^{-1}[\mathbf{f}^3 \ \mathbf{f}^4] \\ I \end{smallmatrix}\right)$ and $\mathbf{L}\left(\begin{smallmatrix} -[\mathbf{g}^1 \ \mathbf{g}^2]^{-1}[\mathbf{g}^3 \ \mathbf{g}^4] \\ I \end{smallmatrix}\right)$ are both rank one.
(2) Compute column vectors $\mathbf{c}, \overline{\mathbf{c}}$, such that $\mathbf{D}\left(\begin{smallmatrix} -[\mathbf{f}^1 \ \mathbf{f}^2]^{-1}[\mathbf{f}^3 \ \mathbf{f}^4] \\ I \end{smallmatrix}\right) = \mathbf{c}\mathbf{r}^T$ and $\mathbf{L}\left(\begin{smallmatrix} -[\mathbf{g}^1 \ \mathbf{g}^2]^{-1}[\mathbf{g}^3 \ \mathbf{g}^4] \\ I \end{smallmatrix}\right) = \overline{\mathbf{c}}\overline{\mathbf{r}^T}$ for some column vectors $\mathbf{r}$, and $\overline{\mathbf{r}}$.
(3) Check that $0 \equiv |\mathbf{c} : \overline{\mathbf{c}}|$.

Step One: The following identity for any 2×4 matrix **F** is helpful:

$$
[\mathbf{f}^1 \ \mathbf{f}^2]^{-1} [\mathbf{f}^3 \ \mathbf{f}^4] = \frac{1}{|\mathbf{f}^1 \ \mathbf{f}^2|} \begin{bmatrix} -|\mathbf{f}^2 \ \mathbf{f}^3| & |\mathbf{f}^2 \ \mathbf{f}^4| \\ |\mathbf{f}^1 \ \mathbf{f}^3| & -|\mathbf{f}^1 \ \mathbf{f}^4| \end{bmatrix}.
$$

Therefore,

$$\left|\mathbf{f}^1\ \mathbf{f}^2||\mathbf{d}^1\mathbf{d}^2|\right|-[\mathbf{f}^1\ \mathbf{f}^2|^{-1}[\mathbf{f}^3\ \mathbf{f}^4|+[\mathbf{d}^1\ \mathbf{d}^2|^{-1}[\mathbf{d}^3\ \mathbf{d}^4|\Bigg|$$

$$=|\mathbf{f}^1\ \mathbf{f}^2||\mathbf{d}^1\ \mathbf{d}^2|\begin{vmatrix} +\left(\left|\frac{\mathbf{f}^2\ \mathbf{f}^3}{\mathbf{f}^1\ \mathbf{f}^2}\right|-\left|\frac{\mathbf{d}^2\ \mathbf{d}^3}{\mathbf{d}^1\ \mathbf{d}^2}\right|\right) & -\left(\left|\frac{\mathbf{f}^2\ \mathbf{f}^4}{\mathbf{f}^1\ \mathbf{f}^2}\right|-\left|\frac{\mathbf{d}^2\ \mathbf{d}^4}{\mathbf{d}^1\ \mathbf{d}^2}\right|\right) \\ -\left(\left|\frac{\mathbf{f}^1\ \mathbf{f}^3}{\mathbf{f}^1\ \mathbf{f}^2}\right|-\left|\frac{\mathbf{d}^1\ \mathbf{d}^3}{\mathbf{d}^1\ \mathbf{d}^2}\right|\right) & +\left(\left|\frac{\mathbf{f}^1\ \mathbf{f}^4}{\mathbf{f}^1\ \mathbf{f}^2}\right|-\left|\frac{\mathbf{d}^1\ \mathbf{d}^4}{\mathbf{d}^1\ \mathbf{d}^2}\right|\right) \end{vmatrix} \tag{63}$$

$$=\frac{1}{|\mathbf{f}^1\ \mathbf{f}^2||\mathbf{d}^1\ \mathbf{d}^2|}\,((|\mathbf{f}^2\ \mathbf{f}^3||\mathbf{d}^1\ \mathbf{d}^2|-|\mathbf{f}^1\ \mathbf{f}^2||\mathbf{d}^2\ \mathbf{d}^3|)(|\mathbf{f}^1\ \mathbf{f}^4||\mathbf{d}^1\ \mathbf{d}^2|$$
$$-|\mathbf{f}^1\ \mathbf{f}^2||\mathbf{d}^1\ \mathbf{d}^4|)-(|\mathbf{f}^1\ \mathbf{f}^3||\mathbf{d}^1\ \mathbf{d}^2|-|\mathbf{f}^1\ \mathbf{f}^2||\mathbf{d}^1\ \mathbf{d}^3|)(|\mathbf{f}^2\ \mathbf{f}^4||\mathbf{d}^1\ \mathbf{d}^2|$$
$$-|\mathbf{f}^1\ \mathbf{f}^2||\mathbf{d}^2\ \mathbf{d}^4|))$$

$$=\frac{1}{|\mathbf{f}^1\ \mathbf{f}^2||\mathbf{d}^1\ \mathbf{d}^2|}\,(|\mathbf{d}^1\ \mathbf{d}^2|^2(|\mathbf{f}^1\ \mathbf{f}^4||\mathbf{f}^2\ \mathbf{f}^3|$$
$$-|\mathbf{f}^1\ \mathbf{f}^3||\mathbf{f}^2\ \mathbf{f}^4|)+|\mathbf{f}^1\ \mathbf{f}^2|^2(|\mathbf{d}^1\ \mathbf{d}^4||\mathbf{d}^2\ \mathbf{d}^3|-|\mathbf{d}^1\ \mathbf{d}^3||\mathbf{d}^2\ \mathbf{d}^4|)$$
$$+|\mathbf{d}^1\ \mathbf{d}^2||\mathbf{f}^1\ \mathbf{f}^2|(-|\mathbf{d}^1\ \mathbf{d}^4||\mathbf{f}^2\ \mathbf{f}^3|-|\mathbf{f}^1\ \mathbf{f}^4||\mathbf{d}^2\ \mathbf{d}^3|+|\mathbf{f}^1\ \mathbf{f}^3||\mathbf{d}^2\ \mathbf{d}^4|$$
$$+|\mathbf{d}^1\ \mathbf{d}^3||\mathbf{f}^2\ \mathbf{f}^4|)) \tag{64}$$

$$=\frac{1}{|\mathbf{f}^1\ \mathbf{f}^2||\mathbf{d}^1\ \mathbf{d}^2|}\,(-|\mathbf{d}^1\ \mathbf{d}^2|^2|\mathbf{f}^1\ \mathbf{f}^2||\mathbf{f}^3\ \mathbf{f}^4|-|\mathbf{f}^1\ \mathbf{f}^2|^2|\mathbf{d}^1\ \mathbf{d}^2||\mathbf{d}^3\ \mathbf{d}^4|$$
$$+|\mathbf{d}^1\ \mathbf{d}^2||\mathbf{f}^1\ \mathbf{f}^2|(-|\mathbf{d}^1\ \mathbf{d}^4||\mathbf{f}^2\ \mathbf{f}^3|-|\mathbf{f}^1\ \mathbf{f}^4||\mathbf{d}^2\ \mathbf{d}^3|+|\mathbf{f}^1\ \mathbf{f}^3||\mathbf{d}^2\ \mathbf{d}^4|$$
$$+|\mathbf{d}^1\ \mathbf{d}^3||\mathbf{f}^2\ \mathbf{f}^4|)) \tag{65}$$

$$=-(|\mathbf{d}^1\ \mathbf{d}^2||\mathbf{f}^3\ \mathbf{f}^4|-|\mathbf{d}^1\ \mathbf{d}^3||\mathbf{f}^2\ \mathbf{f}^4|+|\mathbf{d}^1\ \mathbf{d}^4||\mathbf{f}^2\ \mathbf{f}^3|+|\mathbf{d}^2\ \mathbf{d}^3||\mathbf{f}^1\ \mathbf{f}^4|$$
$$-|\mathbf{d}^2\ \mathbf{d}^4||\mathbf{f}^1\ \mathbf{f}^3|+|\mathbf{d}^3\ \mathbf{d}^4||\mathbf{f}^1\ \mathbf{f}^2|) \tag{66}$$

$$=-\left|\begin{matrix}\mathbf{D}\\ \mathbf{F}\end{matrix}\right| \tag{67}$$

$$=-\left|\begin{matrix}\mathbf{d}_1\\ \mathbf{d}_2\\ \mathbf{F}\end{matrix}\right|=\frac{1}{dQ_{5-8}^{13-16}dQ_{\alpha,13-16}^{4-8}}\left|\begin{matrix}\mathbf{d}_1\\ -dQ_{5-8}^{13-16}dQ_{\alpha,13-16}^{4-8}\,\mathbf{d}_2\\ \mathbf{F}\end{matrix}\right|$$

$$=\frac{1}{dQ_{5-8}^{13-16}dQ_{\alpha,13-16}^{4-8}}\left|\begin{matrix}\mathbf{d}_1\\ dQ_{5-8}^{13-16}(dQ_{\beta,13-16}^{4-8}\,\mathbf{d}_1-dQ_{\alpha,13-16}^{4-8}\mathbf{d}_2)\\ \mathbf{F}\end{matrix}\right|$$

$$=\frac{1}{dQ_{5-8}^{13-16}dQ_{\alpha,13-16}^{4-8}}\left|\begin{matrix}\mathbf{d}_1\\ \mathbf{C}\end{matrix}\right|=0 \tag{68}$$

so

$$\left|-[\mathbf{f}^1\ \mathbf{f}^2]^{-1}[\mathbf{f}^3\ \mathbf{f}^4]+[\mathbf{d}^1\ \mathbf{d}^2]^{-1}[\mathbf{d}^3\ \mathbf{d}^4]\right|=0$$

Line (65) follows from (64) by virtue of Grassmann relations; (66) is simply the Laplace expansion of (67).[16] In equation (68), $\mathbf{C}$ is the same rank two matrix defined in (45), so $|^{\mathbf{d}_1}_{\mathbf{C}}|$ is rank deficient. Now,

$$\begin{aligned}
&\left|\mathbf{D}\begin{pmatrix} -[\mathbf{f}^1\ \ \mathbf{f}^2]^{-1}[\mathbf{f}^3\ \ \mathbf{f}^4] \\ I \end{pmatrix}\right| \\
&\quad = |-[\mathbf{d}^1\ \ \mathbf{d}^2][\mathbf{f}^1\ \ \mathbf{f}^2]^{-1}[\mathbf{f}^3\ \ \mathbf{f}^4]+[\mathbf{d}^3\ \ \mathbf{d}^4]| \\
&\quad = |[\mathbf{d}^1\ \ \mathbf{d}^2](-[\mathbf{f}^1\ \ \mathbf{f}^2]^{-1}[\mathbf{f}^3\ \ \mathbf{f}^4]+[\mathbf{d}^1\ \ \mathbf{d}^2]^{-1}[\mathbf{d}^3\ \ \mathbf{d}^4])| \\
&\quad = |[\mathbf{d}^1\ \ \mathbf{d}^2]|\left|(-[\mathbf{f}^1\ \ \mathbf{f}^2]^{-1}[\mathbf{f}^3\ \ \mathbf{f}^4]+[\mathbf{d}^1\ \ \mathbf{d}^2]^{-1}[\mathbf{d}^3\ \ \mathbf{d}^4])\right| = 0
\end{aligned}$$

so

$$\mathbf{D}\begin{pmatrix} -[\mathbf{f}^1\ \ \mathbf{f}^2]^{-1}[\mathbf{f}^3\ \ \mathbf{f}^4] \\ I \end{pmatrix}$$

is rank one. A similar method works to show that

$$\mathbf{L}\begin{pmatrix} -[\mathbf{g}^1\ \ \mathbf{g}^2]^{-1}[\mathbf{g}^3\ \ \mathbf{g}^4] \\ I \end{pmatrix}$$

is also rank one. Recall (31) and the definition of $\mathbf{l}_\alpha$:

$$\mathbf{l}_\alpha = (dQ^{13,5-8}_{\alpha,9-12}\quad dQ^{14,5-8}_{\alpha,9-12}\quad dQ^{15,5-8}_{\alpha,9-12}\quad dQ^{16,5-8}_{\alpha,9-12}).$$

Furthermore, define

$$\mathbf{l}_{\alpha,\beta} = (dQ^{13,4-8}_{\alpha,\beta,9-12}\quad dQ^{14,4-8}_{\alpha,\beta,9-12}\quad dQ^{15,4-8}_{\alpha,\beta,9-12}\quad dQ^{16,4-8}_{\alpha,\beta,9-12})$$

and notice that

$$dQ^{4-8}_{\beta,9-12}\mathbf{l}_\alpha - dQ^{4-8}_{\alpha,9-12}\mathbf{l}_\beta = dQ^{5-8}_{9-12}\mathbf{l}_{\alpha\beta}.$$

The argument used to go from (63) to (67) and the fact that

$$\mathbf{L} = \begin{pmatrix} \mathbf{l}_\alpha \\ \mathbf{l}_\beta \end{pmatrix} \quad \text{and} \quad \mathbf{G} = \begin{pmatrix} \mathbf{l}_{1,2} \\ \mathbf{l}_{1,3} \end{pmatrix}$$

lead to the following:

$$\begin{aligned}
\left|\mathbf{L}\begin{pmatrix} -[\mathbf{g}^1\ \ \mathbf{g}^2]^{-1}[\mathbf{g}^3\ \ \mathbf{g}^4] \\ I \end{pmatrix}\right| &= |[\mathbf{l}^1\ \ \mathbf{l}^2]|\,|(-[\mathbf{g}^1\ \ \mathbf{g}^2]^{-1}[\mathbf{g}^3\ \ \mathbf{g}^4]+[\mathbf{l}^1\ \ \mathbf{l}^2]^{-1}[\mathbf{l}^3\ \ \mathbf{l}^4])| = |[\mathbf{l}^1\ \ \mathbf{l}^2]|\left|\begin{matrix}\mathbf{L}\\ \mathbf{G}\end{matrix}\right| \\
&= |[\mathbf{l}^1\ \ \mathbf{l}^2]|\begin{vmatrix} \mathbf{l}_\alpha \\ \mathbf{l}_\beta \\ \mathbf{l}_{1,2} \\ \mathbf{l}_{1,3} \end{vmatrix} = |[\mathbf{l}^1\ \ \mathbf{l}^2]|\begin{vmatrix} \mathbf{l}_\alpha \\ \mathbf{l}_\beta \\ dQ^{4-8}_{2,9-12}\mathbf{l}_1 - dQ^{4-8}_{1,9-12}\mathbf{l}_2 \\ dQ^{4-8}_{3,9-12}\mathbf{l}_1 - dQ^{4\times 8}_{1,9-12}\mathbf{l}_2 \end{vmatrix}
\end{aligned}$$

$$= |[\mathbf{l}^1 \ \ \mathbf{l}^2]| \left| \begin{pmatrix} & \mathbf{e}_\alpha & \\ & \mathbf{e}_\beta & \\ dQ^{4-8}_{2,9-12} & -dQ^{4-8}_{1,9-12} & 0 \\ dQ^{4-8}_{3,9-12} & 0 & -dQ^{4-8}_{1,9-12} \end{pmatrix} \begin{pmatrix} \mathbf{l}_1 \\ \mathbf{l}_2 \\ \mathbf{l}_3 \end{pmatrix} \right| = 0,$$

since the product of a 4×3 with a 3×4 matrix is a 4×4 rank-deficient matrix.

Step Two: Brute force suffices to find the column vector $\mathbf{c}$ where

$$\begin{aligned}
\mathbf{c}\mathbf{r}^T &= \mathbf{D}\begin{pmatrix} -[\mathbf{f}^1 \ \ \mathbf{f}^2]^{-1}[\mathbf{f}^3 \ \ \mathbf{f}^4] \\ I \end{pmatrix} \\
&= -[\mathbf{d}^1 \ \ \mathbf{d}^2][\mathbf{f}^1 \ \ \mathbf{f}^2]^{-1}[\mathbf{f}^3 \ \ \mathbf{f}^4] + [\mathbf{d}^3 \ \ \mathbf{d}^4] \\
&= -\frac{1}{|\mathbf{f}^1 \ \ \mathbf{f}^2|}[\mathbf{d}^1 \ \ \mathbf{d}^2]\begin{bmatrix} -|\mathbf{f}^2 \ \ \mathbf{f}^3| & -|\mathbf{f}^2 \ \ \mathbf{f}^4| \\ |\mathbf{f}^1 \ \ \mathbf{f}^3| & |\mathbf{f}^1 \ \ \mathbf{f}^4| \end{bmatrix} + [\mathbf{d}^3 \ \ \mathbf{d}^4] \\
&= -\frac{1}{|\mathbf{f}^1 \ \ \mathbf{f}^2|}[-|\mathbf{f}^2 \ \ \mathbf{f}^3|\mathbf{d}^1 + |\mathbf{f}^1 \ \ \mathbf{f}^3|\mathbf{d}^2 : -|\mathbf{f}^2 \ \ \mathbf{f}^4|\mathbf{d}^1 + |\mathbf{f}^1 \ \ \mathbf{f}^4|\mathbf{d}^2] + [\mathbf{d}^3 : \mathbf{d}^4] \\
&= \frac{1}{|\mathbf{f}^1 \mathbf{f}^2|}[(|\mathbf{f}^2 \ \ \mathbf{f}^3|\mathbf{d}^1 - |\mathbf{f}^1 \ \ \mathbf{f}^3|\mathbf{d}^2 + |\mathbf{f}^1 \ \ \mathbf{f}^2|\mathbf{d}^3) : (|\mathbf{f}^2 \ \ \mathbf{f}^4|\mathbf{d}^1 - |\mathbf{f}^1 \ \ \mathbf{f}^4|\mathbf{d}^2 + |\mathbf{f}^1 \ \ \mathbf{f}^2|\mathbf{d}^4)]
\end{aligned}$$

therefore set $\mathbf{c} \equiv [|\mathbf{f}^2 \ \mathbf{f}^3|\mathbf{d}^1 - |\mathbf{f}^1 \ \mathbf{f}^3|\mathbf{d}^2 + |\mathbf{f}^1 \ \mathbf{f}^2|\mathbf{d}^3]$. A similar calculation holds to show

$$\mathbf{L}\begin{pmatrix} -[\mathbf{g}^1 \ \ \mathbf{g}^2]^{-1}[\mathbf{g}^3 \ \ \mathbf{g}^4] \\ I \end{pmatrix} = \overline{\mathbf{c}\,\mathbf{r}^T} \quad \text{for} \quad \overline{\mathbf{c}} = [|\mathbf{g}^2 \ \ \mathbf{g}^3|\mathbf{l}^1 - |\mathbf{g}^1 \ \ \mathbf{g}^3|\mathbf{l}^2 + |\mathbf{g}^1 \ \ \mathbf{g}^2|\mathbf{l}^3].$$

Step Three: In order to show that (60) is trivially zero a few more identities are needed. Because Q^{1-8}_{9-16} is generically of rank four, $Q^{5-8}_{9-12} = Q^{1-4}_{9-12}(Q^{1-4}_{13-16})^{-1}Q^{5-8}_{13-16}$ and $dQ^{4-8}_{\alpha,9-12}$ can be expressed as a product of minors

$$\begin{aligned}
dQ^{4-8}_{\alpha,9-12} &= \begin{vmatrix} Q^4_\alpha & \vdots & Q^{5-8}_\alpha \\ Q^4_{9-12} & \vdots & Q^{5-8}_{9-12} \end{vmatrix} = \begin{vmatrix} Q^4_\alpha & \vdots & Q^{5-8}_\alpha \\ Q^4_{9-12} & \vdots & Q^{1-4}_{9-12}(Q^{1-4}_{13-16})^{-1}Q^{5-8}_{13-16} \end{vmatrix} \\
&= \begin{vmatrix} 1 & & \\ & Q^{1-4}_{9-12} & \end{vmatrix} \begin{vmatrix} Q^4_\alpha & \vdots & Q^{5-8}_\alpha \\ \mathbf{e}_4 & \vdots & (Q^{1-4}_{13-16})^{-1}Q^{5-8}_{13-16} \end{vmatrix} \\
&= \begin{vmatrix} 1 & & \\ & Q^{1-4}_{9-12} & \end{vmatrix} \begin{vmatrix} 1 & & \\ & (Q^{1-4}_{13-16})^{-1} & \end{vmatrix} \begin{vmatrix} Q^4_\alpha & \vdots & Q^{5-8}_\alpha \\ Q^4_{13-16} & \vdots & Q^{5-8}_{13-16} \end{vmatrix} \\
&= dQ^{4-8}_{\alpha,13-16}\frac{dQ^{1-4}_{9-12}}{dQ^{1-4}_{13-16}}.
\end{aligned} \tag{69}$$

The Grassmann relation

$$\sum_{\sigma\in S_3} \frac{\operatorname{sgn}\sigma}{2} dQ^{\sigma_1,\sigma_2,4-8}_{1-3,9-12} dQ^{\sigma_3,5-8}_{\alpha,9-12} = dQ^{\sigma_1,\sigma_2,\sigma_3,5-8}_{1-3,9-12} dQ^{4-8}_{\alpha,9-12},$$

as well as Grassmann relations for the minors

$$|\mathbf{f}^j \ \ \mathbf{f}^k| = dQ^{9-13}_{14,5-8} dQ^{j,k,9-13}_{14-16,5-8},$$

$$|\mathbf{g}^j \ \ \mathbf{g}^k| = dQ^{4-8}_{1,9-12} dQ^{j+12,k+12,4-8}_{1-3,9-12},$$

can be used to write $\overline{\mathbf{c}}$ fairly simply:

$$\begin{aligned}\overline{\mathbf{c}} &= \sum_{\sigma\in S_3} \frac{\operatorname{sgn}\sigma}{2} |\mathbf{g}^{\sigma_1} \ \mathbf{g}^{\sigma_2}| \mathbf{l}^{\sigma_3} \\ &= dQ^{4-8}_{1,9-12} \sum_{\sigma\in S_3(13,14,15)} \frac{\operatorname{sgn}\sigma}{2} dQ^{\sigma_1,\sigma_2,4-8}_{1-3,9-12} \begin{pmatrix} dQ^{\sigma_3,5-8}_{\alpha,9-12} \\ dQ^{\sigma_3,5-8}_{\beta,9-12} \end{pmatrix} \\ &= dQ^{4-8}_{1,9-12} dQ^{13,14,15,5-8}_{1-3,9-12} \begin{pmatrix} dQ^{4-8}_{\alpha,9-12} \\ dQ^{4-8}_{\beta,9-12} \end{pmatrix} = \tilde{\kappa} \begin{pmatrix} dQ^{4-8}_{\alpha,13-16} \\ dQ^{4-8}_{\beta,13-16} \end{pmatrix}.\end{aligned}$$

The last line follows from Eq. (69) for some $\overline{\kappa}\in\mathbb{R}$. Computing $\mathbf{c}$ is more complicated. First note that Eqs. (38) and (39) can be used to rewrite

$$\mathbf{d}^i \equiv \begin{pmatrix} \dfrac{dQ^{i,13-16}_{\alpha,5-8}}{dQ^{13-16}_{5-8}} - \dfrac{dQ^{i,5-8}_{\alpha,13-16}}{dQ^{5-8}_{13-16}} \\ \dfrac{dQ^{i,13-16}_{\beta,5-8}}{dQ^{13-16}_{5-8}} - \dfrac{dQ^{i,5-8}_{\beta,13-16}}{dQ^{5-8}_{13-16}} \end{pmatrix} = \begin{pmatrix} \dfrac{dQ^{i,9-12}_{\alpha,5-8}}{dQ^{9-12}_{5-8}} - \dfrac{dQ^{i,9-12}_{\alpha,13-16}}{dQ^{9-12}_{13-16}} \\ \dfrac{dQ^{i,9-12}_{\beta,5-8}}{dQ^{9-12}_{5-8}} - \dfrac{dQ^{i,9-12}_{\beta,13-16}}{dQ^{9-12}_{13-16}} \end{pmatrix} = \mathbf{d}^i_a - \mathbf{d}^i_b,$$

where

$$\mathbf{d}^i_a \equiv \frac{1}{dQ^{9-12}_{5-8}} \begin{pmatrix} dQ^{i,9-12}_{\alpha,5-8} \\ dQ^{i,9-12}_{\beta,5-8} \end{pmatrix} \quad \text{and} \quad \mathbf{d}^i_b \equiv \frac{1}{dQ^{9-12}_{13-16}} \begin{pmatrix} dQ^{i,9-12}_{\alpha,13-16} \\ dQ^{i,9-12}_{\beta,13-16} \end{pmatrix}.$$

A combination of Grassmann relations and range conditions are required now

$$\begin{aligned}\sum_{\sigma\in S_3} \frac{\operatorname{sgn}\sigma}{2} dQ^{\sigma_1,\sigma_2,9-13}_{14-16,5-8} dQ^{\sigma_3,9-12}_{\alpha,5-8} &= \pm dQ^{\sigma_1,\sigma_2,\sigma_3,9-12}_{14-16,5-8} dQ^{9-13}_{\alpha,5-8} + dQ^{\sigma_1,\sigma_2,\sigma_3,9-13}_{\alpha,14-16,5-8} dQ^{9-12}_{5-8} \\ &= dQ^{\sigma_1,\sigma_2,\sigma_3,9-13}_{\alpha,14-16,5-8} dQ^{9-12}_{5-8},\end{aligned}$$

since consistency conditions force $dQ^{9-13}_{\alpha,5-8} \equiv 0$. Another identity is useful:

$$\begin{aligned}\sum_{\sigma\in S_3} \frac{\operatorname{sgn}\sigma}{2} dQ^{\sigma_1,\sigma_2,9-13}_{14-16,5-8} dQ^{\sigma_3,9-12}_{\alpha,13-16} &= dQ^{9-12}_{13-16} \, dQ^{1-3,9-13}_{\alpha,14-16,5-8} + dQ^{9-13}_{\alpha,13-16} \, dQ^{1-3,9-12}_{14-16,5-8} \\ &\quad - dQ^{9-12}_{\alpha,14-16} \, dQ^{1-3,9-13}_{13-16,5-8}.\end{aligned}$$

Therefore,

$$\begin{aligned}\sum_{\sigma\in S_3} \frac{\operatorname{sgn}\sigma}{2} |\mathbf{f}^{\sigma_1} \mathbf{f}^{\sigma_2}| \mathbf{d}^{\sigma_3}_a &= \frac{dQ^{9-13}_{14,5-8}}{dQ^{9-12}_{5-8}} \sum_{\sigma\in S_3} \frac{\operatorname{sgn}\sigma}{2} dQ^{\sigma_1,\sigma_2,9-13}_{14-16,5-8} \begin{pmatrix} dQ^{\sigma_3,9-12}_{\alpha,5-8} \\ dQ^{\sigma_3,9-12}_{\beta,5-8} \end{pmatrix} \\ &= dQ^{9-13}_{14,5-8} \begin{pmatrix} dQ^{1-3,9-13}_{\alpha,14-16,5-8} \\ dQ^{1-3,9-13}_{\beta,14-16,5-8} \end{pmatrix} \qquad (70)\end{aligned}$$

and

$$\sum_{\sigma\in S_3}\frac{\operatorname{sgn}\sigma}{2}|\mathbf{f}^{\sigma_1}\ \mathbf{f}^{\sigma_2}|\mathbf{d}_b^{\sigma_3}=\frac{dQ^{9-13}_{14,5-8}}{dQ^{9-12}_{13-16}}\sum_{\sigma\in S_3}\frac{\operatorname{sgn}\sigma}{2}dQ^{\sigma_1,\sigma_2,9-13}_{14-16,5-8}\begin{pmatrix}dQ^{\sigma_3,9-12}_{\alpha,13-16}\\ dQ^{\sigma_3,9-12}_{\beta,13-16}\end{pmatrix}$$
$$=dQ^{9-13}_{14,5-8}\begin{pmatrix}dQ^{1-3,9-13}_{\alpha,14-16,5-8}\\ dQ^{1-3,9-13}_{\beta,14-16,5-8}\end{pmatrix}+\frac{dQ^{9-13}_{14,5-8}}{dQ^{9-12}_{13-16}}\left(dQ^{1-3,9-12}_{14-16,5-8}\begin{pmatrix}dQ^{9-13}_{\alpha,13-16}\\ dQ^{9-13}_{\beta,13-16}\end{pmatrix}\right.$$
$$\left.-dQ^{1-3,9-13}_{13-16,5-8}\begin{pmatrix}dQ^{9-12}_{\alpha,14-16}\\ dQ^{9-12}_{\beta,14-16}\end{pmatrix}\right).\tag{71}$$

Notice that thanks to range conditions

$$\begin{vmatrix}dQ^{9-13}_{\alpha,13-16} & dQ^{9-12}_{\alpha,14-16}\\ dQ^{9-13}_{\beta,13-16} & dQ^{9-12}_{\beta,14-16}\end{vmatrix}=\pm dQ^{9-13}_{\alpha,\beta,14-16}\,dQ^{9-12}_{13-16}=0,$$

which permits (71) to be written more simply. For some $\kappa,\hat{\kappa}\in\mathbb{R}$,

$$\sum_{\sigma\in S_3}\frac{\operatorname{sgn}\sigma}{2}|\mathbf{f}^{\sigma_1}\ \mathbf{f}^{\sigma_2}|\mathbf{d}_b^{\sigma_3}=dQ^{9-13}_{14,5-8}\begin{pmatrix}dQ^{1-3,9-13}_{\alpha,14-16,5-8}\\ dQ^{1-3,9-13}_{\beta,14-16,5-8}\end{pmatrix}+\hat{\kappa}\begin{pmatrix}dQ^{9-13}_{\alpha,13-16}\\ dQ^{9-13}_{\beta,13-16}\end{pmatrix}$$
$$=dQ^{9-13}_{14,5-8}\begin{pmatrix}dQ^{1-3,9-13}_{\alpha,14-16,5-8}\\ dQ^{1-3,9-13}_{\beta,14-16,5-8}\end{pmatrix}+\kappa\begin{pmatrix}dQ^{5-8,13}_{\alpha,13-16}\\ dQ^{5-8,13}_{\beta,13-16}\end{pmatrix}.\tag{72}$$

The last line follows from (39). Equations (70) and (72) imply

$$\mathbf{c}=\sum_{\sigma\in S_3}\frac{\operatorname{sgn}\sigma}{2}|\mathbf{f}^{\sigma_1}\ \mathbf{f}^{\sigma_2}|\mathbf{d}^{\sigma_3}=\sum_{\sigma\in S_3}\frac{\operatorname{sgn}\sigma}{2}|\mathbf{f}^{\sigma_1}\ \mathbf{f}^{\sigma_2}|(\mathbf{d}_a^{\sigma_3}-\mathbf{d}_b^{\sigma_3})=\kappa\begin{pmatrix}dQ^{5-8,13}_{\alpha,13-16}\\ dQ^{5-8,13}_{\beta,13-16}\end{pmatrix}.\tag{73}$$

The Grassmann relation

$$\begin{vmatrix}dQ^{5-8,13}_{\alpha,13-16} & dQ^{4-8}_{\alpha,13-16}\\ dQ^{5-8,13}_{\beta,13-16} & dQ^{4-8}_{\beta,13-16}\end{vmatrix}=\pm dQ^{4-8,13}_{\alpha,\beta,13-16}\,dQ^{5-8}_{13-16}$$

can be used to simplify

$$|\mathbf{c}\ \overline{\mathbf{c}}|=\hat{\kappa}\kappa\begin{vmatrix}dQ^{5-8,13}_{\alpha,13-16} & dQ^{4-8}_{\alpha,9-12}\\ dQ^{5-8,13}_{\beta,13-16} & dQ^{4-8}_{\beta,9-12}\end{vmatrix}=\pm\hat{\kappa}\kappa(dQ^{4-8,13}_{\alpha,\beta,13-16}\quad dQ^{5-8}_{13-16})=0.$$

The last equality follows from range conditions. Since $\alpha,\beta\in\{1,2,3\}$, rank $Q^{4-8,13}_{\alpha,\beta,14-16}\leqslant 4$. Therefore, rank $Q^{4-8,13}_{\alpha,\beta,13-16}\leqslant 5$, forcing $dQ^{4-8,13}_{\alpha,\beta,13-16}=0$. Finally, steps 1–3 imply

$$\begin{vmatrix}Pih^5_\alpha & Pih^6_\alpha & Pih^{15}_\alpha\\ Pih^5_\beta & Pih^6_\beta & Pih^{15}_\beta\\ Phh^5_1 & Phh^6_1 & Phh^{15}_1\end{vmatrix}=C|\mathbf{D}A^2_{1-4}:\mathbf{L}A^{15}_{13-16}|$$
$$=\left|\mathbf{D}\begin{pmatrix}-[\mathbf{f}^1\ \mathbf{f}^2]^{-1}[\mathbf{f}^3\ \mathbf{f}^4]\\ I\end{pmatrix}\begin{pmatrix}A^3_2\\ A^2_4\end{pmatrix}:\mathbf{L}\begin{pmatrix}-[\mathbf{g}^1\ \mathbf{g}^2]^{-1}[\mathbf{g}^3\ \mathbf{g}^4]\\ I\end{pmatrix}\begin{pmatrix}A^{15}_{15}\\ A^{15}_{16}\end{pmatrix}\right|$$
$$=\left|\mathbf{cr}^T\begin{pmatrix}A^2_3\\ A^2_4\end{pmatrix}:\overline{\mathbf{cr}}^T\begin{pmatrix}A^{15}_{15}\\ A^{15}_{16}\end{pmatrix}\right|\begin{vmatrix}Pih^5_\alpha & Pih^6_\alpha & Pih^{15}_\alpha\\ Pih^5_\beta & Pih^6_\beta & Pih^{15}_\beta\\ Phh^5_1 & Phh^6_1 & Phh^{15}_1\end{vmatrix}$$

$$= \left(\mathbf{r}^T \cdot \begin{pmatrix} A_3^2 \\ A_4^2 \end{pmatrix}\right) * \left(\overline{\mathbf{r}^T} \cdot \begin{pmatrix} A_{15}^{15} \\ A_{16}^{15} \end{pmatrix}\right) * |\mathbf{c}:\overline{\mathbf{c}}|$$

$$= 0.$$

Similar calculations hold to show that other minors of this ilk are trivially zero and force no additional conditions upon the A_i^js.

IV. CONCLUSION

Enforcing range conditions upon the solution of the ''modified problem,'' which subdivides a 4×4 system in to four subsystems, was done analytically in Sec. III. That it might prove computationally infeasible to eliminate excess parameters for larger systems has been one of the author's greatest fears for diffuse tomography. Some of the tricks used here carry over to larger systems. Others, however, do not. For example, the derivation of the condition (30) does not go through. The author's goal is to implement a recursive scheme which generates data for $n/2\times n/2$ subsystems from an $n\times n$ system's data set. In order to implement such a scheme a complete and computationally reasonable set of conditions analogous to (16)–(18) and (51)–(58) is required. Hopefully, they will be as succinct and linear as their counterparts for the 4×4 problem.

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On a hierarchy of macroscopic models for semiconductors

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This paper shows that various models of electron transport in semiconductors that have been previously proposed in the literature can be connected one with each other by the diffusion approximation methodology. We first investigate the diffusion limit of the semiconductor Boltzmann equation towards the so-called ''spherical harmonic expansion model,'' under the assumption of dominant elastic scattering. Then, this model is again connected, either to the energy-transport model or to a ''periodic spherical harmonic expansion model'' through a diffusion approximation, respectively making electron–electron or phonon scattering large. We provide the mathematical background which makes the Hilbert expansions associated with these various diffusion limits rigorous. © *1996 American Institute of Physics.* [S0022-2488(96)01306-0]

I. INTRODUCTION

This paper is concerned first with a mathematical derivation of the spherical harmonic expansion model of semiconductors from the Boltzmann equation and, second, with the connections of this model to other previously derived macroscopic models (energy-transport, drift-diffusion, and periodic spherical harmonic expansion models). Indeed, the search for macroscopic models which provide reliable but not too computationally expensive descriptions of hot electron transport in semiconductors is an important issue for industry. This paper intends to clarify the relations between the various models of semi-classical electron-transport that are now available.

In this paper, the hierarchy between the various models is outlined, together with the macroscopic limit which links two successive steps of the hierarchy. Each macroscopic limit is associated with a particular choice of space and time scales which makes a specific collision mechanism dominant. Figure 1 provides an overview of this hierarchy. Each of the considered models appears in a box together with its abbreviation and the physical unknown it is concerned with. An arrow between two boxes indicates a macroscopic limit which connects the corresponding models. Solid lines indicate which macroscopic limits will be detailed in this paper. Dashed arrows have already been dealt with in previous papers and will not be considered. Along the arrow is mentioned the dominant scattering mechanism which is used in the corresponding macroscopic limit.

The drift–diffusion limit (arrow 1) has first been investigated in Ref. 1 and successively by many authors.[2–5] The mathematical theory has been given in Refs. 6 and 7 in the framework of model collision operators for which the scattering matrix is assumed to be smooth. This direct arrow from the Boltzmann equation (BE) to the drift-diffusion model (DD) is well understood and will not be investigated here.

More recently, a new model based on the diffusion approximation of the Boltzmann equation subject to dominant scattering by optical phonons of constant energy has been proposed,[8–10] (arrow 2). This new model will further be referred to as the ''periodic spherical harmonic expansion model'' (PSHE) because of its analogy with the (unperiodic) spherical harmonic expansion model (SHE). Mathematically rigorous approximation theorems are given in Refs. 8 and 9; part of the analysis relies on properties of the optical phonon collision operator which were proved in Refs. 11–13. This arrow 2 will not be further investigated here.

The energy-transport model (ET) consists of a system of diffusion equations for the electron density and temperature. This extended drift-diffusion model can also be viewed as a hydrodynamic model in which the inertia terms in the momentum transport equation are neglected[14–16]

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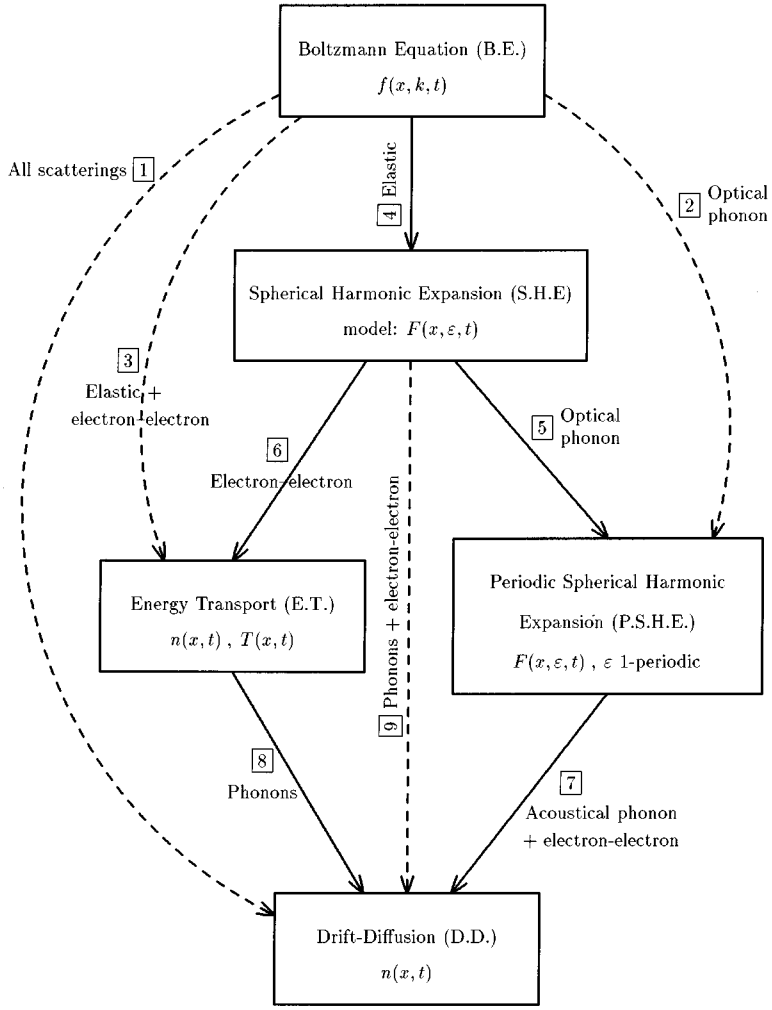

FIG. 1. The hierarchy of models.

(for the hydrodynamic model of semiconductors we refer the reader in particular to Refs. 17–19). The ET model first appeared in Refs. 20 and 21 and then has been widely used for numerical computations,[14,15,22,23] mostly with phenomenological transport coefficients. Its derivation from the Boltzmann equation may be found in Refs. 24 and 25. The dominant scatterings needed for this model to be valid are shown in Ref. 16 to be electron–electron and elastic collisions (arrow 3). Mathematically rigorous convergence results for this limit are in progress.[26] Again, this limit will not be further investigated in the present paper.

There are several drawbacks to the approaches of Ref. 10 (for the PSHE model) and of Ref. 16 (for the ET model). In neither case is the assumption on the dominant scattering realistic for hot electron transport. Indeed, the basic assumption of Ref. 10 is that the (constant) optical phonon energy is of order 1. However, at room temperature and for hot electrons this energy should rather be considered as small and both the impurity and phonon scatterings viewed (at leading order) as elastic. Also, in Ref. 16, the electron–electron collision operator is assumed of the same order of magnitude as the elastic operator, which is questionable. Therefore, in the present paper, we investigate the diffusion approximation of the Boltzmann equation subject to dominant elastic scattering, which yields the SHE model (arrow 4).

This question has first been investigated in Ref. 27. Another drawback of Refs. 10 and 16 is that the diffusion constants coming from these theories are not explicit. We shall see that both the PSHE model and the ET model can be obtained through relaxation limits of the SHE model (arrows 5 and 6) and that these limits yield more explicit expressions of the diffusion coefficients (even analytic in the most simple situations).

The SHE model first appeared in studies by Stratton.[20,21,28,29] Then, it was introduced as a numerical method in Refs. 30–37. The first derivation of this model from a diffusion approximation of the Boltzmann equation appears in Ref. 27 and we shall follow their approach. However, the analysis of Ref. 27 is restricted to isotropic scattering while that of Ref. 30 is restricted to spherically symmetric band diagrams. We shall derive the model in a general setting and show that it reduces to that of Refs. 27 and 30 under suitable assumptions. This more general approach applies particularly to III–V materials, for instance, for which the phonon collisions are highly anisotropic and the band diagrams not spherically symmetric. We shall also provide the necessary mathematical framework to make these analyses more rigorous. However, the proof of the convergence of the diffusion approximation will be deferred to future work.

The relaxation limits of the SHE model towards the PSHE model (arrow 5) and towards the ET model (arrow 6) will also be considered in detail. In Ref. 38, arrow 6 is investigated via a moment expansion method but needs phenomenological closure relations. In our ET model, the diffusion coefficients are the same as in Ref. 20. At variance, the investigation of arrow 5 is new and is proved directly via a coercivity estimate (contrary to Refs. 9 and 10 where the resolution of a recursion system is needed).

To be complete, the relaxation limits of both the PSHE model and the ET model towards the drift-diffusion (DD) model (arrows 7 and 8) will be outlined. Arrow 7 is treated by considering both acoustical phonon and electron–electron scattering. At variance, Ref. 10 treats such a limit by considering a second polar optical phonon scattering with an irrational phonon energy with respect to the first optical phonon energy. Finally the direct limit of the SHE model to the DD model (arrow 9) is not considered but would be rather straightforward. Note that the three limits (arrows 7–9) yield the same diffusion coefficient in the DD model and that its expression is different from what the direct limit from the Boltzmann equation (arrow 1) would give.

The paper is organized as follows: Sec. II is devoted to a presentation of the Boltzmann equation and of the appropriate scaling. Section III is concerned with the diffusion limit of the Boltzmann equation to the SHE model (arrow 4). In Sec. IV we deal with the relaxation limit of the SHE model to the ET model (arrow 6) and outline the relaxation limit of the latter to the DD model (arrow 8). In Sec. V, we perform a similar program going from the SHE model to the PSHE model and then to the DD model, via a sequence of relaxation limits (arrows 5 and 7).

II. THE BOLTZMANN EQUATION

The starting point is the Boltzmann equation for the electrons in the conduction band of the semiconductor. Let $f(x,k,t)$ be the distribution function depending on the position $x \in \mathbb{R}^3$, the wave vector $k \in B$, and the time $t \geqslant 0$. The Brillouin zone B is the elementary cell of the dual lattice L^* and is identified with the torus $\mathbb{R}^3/L^*$. Any function of k will thus be considered as L^* periodic.

The Boltzmann equation is written[25]

$$\frac{\partial f}{\partial t} + \frac{1}{\hbar}\,\nabla_k \varepsilon(k)\cdot\nabla_x f + \frac{q}{\hbar}\,\nabla_x V(x,t)\cdot\nabla_k f = Q_{\mathrm{ld}}(f) + Q_e(f), \tag{II.1}$$

where $\varepsilon: k \in B \mapsto \varepsilon(k) \in \mathbb{R}$ is the given energy band diagram, $V:(x,t) \in \mathbb{R}^3 \times [0,\infty) \mapsto \mathbb{R}$ is the electrostatic potential, q is the elementary charge, $\hbar$ is the reduced Planck constant, $Q_{\mathrm{ld}}(f)$ is the collision operator for lattice-defect collisions, and $Q_e(f)$ is the collision operator for electron–

electron collisions. The coupling of V to f through Poisson's equation need not be considered in the subsequent analysis. Therefore, $V(x,t)$ will be treated as a given function.

The main three classes of lattice-defects are impurities, acoustical phonons, and optical phonons:[39]

$$Q_{\rm ld}(f)=Q_{\rm imp}(f)+Q_{ac}(f)+Q_{\rm op}(f), \tag{II.2}$$

Because of the elastic character of impurity scattering, Pauli's exclusion terms in the gain and loss terms cancel and we obtain

$$Q_{\rm imp}(f)(k)=\int_B \Phi_{\rm imp}(x,k,k')\,\delta(\varepsilon'-\varepsilon)(f'-f)dk', \tag{II.3}$$

where $\varepsilon=\varepsilon(k)$, $\varepsilon'=\varepsilon(k')$, $f=f(k)$, $f'=f(k')$, δ is the delta measure, and $\Phi_{\rm imp}(x,k,k')=\Phi_{\rm imp}(x,k',k)$ is the impurity scattering matrix element. For optical phonons, we have

$$\begin{aligned} Q_{\rm op}(f)(k)=\int_B \Phi_{\rm op}(x,k,k')\{&[(N_{\rm op}+1)\delta(\varepsilon-\varepsilon'+\varepsilon_{\rm op})+N_{\rm op}\delta(\varepsilon-\varepsilon'-\varepsilon_{\rm op})]f'(1-f)\\ &-[(N_{\rm op}+1)\delta(\varepsilon'-\varepsilon+\varepsilon_{\rm op})+N_{\rm op}\delta(\varepsilon'-\varepsilon-\varepsilon_{\rm op})]f(1-f')\}dk', \end{aligned} \tag{II.4}$$

where $\Phi_{\rm op}(x,k,k')=\Phi_{\rm op}\,(x,k',k)$ is the matrix element, $\varepsilon_{\rm op}$ is the constant optical phonon energy, and $N_{\rm op}$ is optical phonon occupation number:

$$N_{\rm op}=(e^{\varepsilon_{\rm op}/k_{\rm B}T_L}-1)^{-1}$$

with $k_{\rm B}$ the Boltzmann constant and T_L the lattice temperature. The acoustical phonon collision operator is given by a similar expression (II.4) with the indices ''op'' replaced by ''ac.'' The only major difference between acoustical and optical scattering is that the acoustical phonon energy $\varepsilon_{\rm ac}=\varepsilon_{\rm ac}\,(k-k')$ is a nonconstant function of $k-k'$.

The electron–electron collision operator is given by[16,39]

$$\begin{aligned} Q_e(f)(k)=\int_{B^3}\Phi_e(k,k_1,k',k_1')\,\delta(\varepsilon'+\varepsilon_1'-\varepsilon-\varepsilon_1)\,\delta_p(k'+k_1'-k-k_1)\\ \times[f'f_1'(1-f)(1-f_1)-ff_1(1-f')(1-f_1')]dk_1dk'dk_1', \end{aligned} \tag{II.5}$$

where

$$\delta_p(k'+k_1'-k-k_1)=\sum_{g\,\epsilon L^*}\delta(k'+k_1'-k-k_1+g). \tag{II.6}$$

In (II.6), the terms with $g\neq 0$ account for umklapp processes and are necessary to preserve the periodic structure in k. Note that since the integral defining Q_e is taken on B^3, then only a finite number of terms of the sum in (II.6) need to be taken into account. The matrix element Φ_e is such that $\Phi_e(k,k_1,k',k_1')=\Phi_e(k_1,k,k',k_1')=\Phi_e(k',k_1',k,k_1)$. In all these operators, the normalizing factors $1/4\pi^3$ coming from the momentum density of states have been transferred to the ϕs and will be ignored in the remainder of the paper.

The Boltzmann equation (II.1) is scaled by introducing typical density and kinetic energy scales for electrons: n_0 is the typical density injected in the structure (which can be larger than the doping density if high injection effects are present) and ε_0 is the typical kinetic energy that the

electrons can gain in the structure ($\varepsilon_0 \approx qV_A$ if V_A is the applied bias). Let now k_0 be the typical norm of wave vectors k satisfying $\varepsilon(k)=\varepsilon_0$. The dimensionless parameter

$$\eta = \frac{4\pi^3 n_0}{k_0^3}$$

is the natural distribution function scale and measures the level of degeneracy of the electron gas. The velocity scale is given by $v_0=\varepsilon_0/\hbar k_0$ and the space scale x_0 is linked to the time scale t_0 through $x_0=v_0 t_0$. Finally the potential scale V_0 is connected to ε_0 by $qV_0=\varepsilon_0$ (i.e., $V_0 \approx V_A$).

Dimensionless parameters measuring the relative strength of the collision operators ν_{imp}, ν_{op}, ν_{ac}, ν_e, are given by

$$\nu_{\text{imp}} = \frac{\phi_{\text{imp},0} k_0^3}{\varepsilon_0} t_0, \quad \nu_e = \frac{\phi_{e,0} 4\pi^3 n_0 k_0^3}{\varepsilon_0} t_0,$$

where $\Phi_{\text{imp},0}$ and $\Phi_{e,0}$ are ''typical values'' of Φ_{imp} and Φ_e, and ν_{op} and ν_{ac} are given by similar expressions as ν_{imp} associated with ''typical values'' $\Phi_{\text{op},0}$ and $\Phi_{\text{ac},0}$. Here $\Phi_{\text{imp},0}$ is used to scale the matrix element Φ_{imp} in dimensionless form and similarly with the other scattering mechanisms.

Finally, let also $\varepsilon_{\text{ac},0}$ be the order of magnitude of the acoustical phonon energy and introduce the dimensionless parameters

$$\alpha^2 = \frac{\varepsilon_{\text{op}}}{\varepsilon_0}, \quad \beta^2 = \frac{\varepsilon_{\text{ac},0}}{\varepsilon_0}, \quad \gamma^2 = \frac{k_B T_L}{\varepsilon_0},$$

α^2 (resp. β^2) measures the typical energy gain or loss during an optical (resp. acoustical) phonon collision, while γ^2 quantifies how ''hot'' is the electron gas ($\gamma^2 \ll 1$ implies hot electron effects).

After scaling with the above units, the equations are written

$$\frac{\partial f}{\partial t} + \nabla_k \varepsilon(k) \cdot \nabla_x f + \nabla_x V \cdot \nabla_k f = \nu_{\text{imp}} Q_{\text{imp}}(f) + \nu_{\text{ac}} Q_{\text{ac}}^{\beta}(f) + \nu_{\text{op}} Q_{\text{op}}^{\alpha}(f) + \nu_e Q_e(f) \qquad \text{(II.7)}$$

with Q_{imp} given by (II.3) applied with the dimensionless quantities. Here $Q_{\text{op}}^{\alpha}(f)$ is obtained from (II.4) in the same manner, and by replacing ε_{op} by α^2, $(1-f)$ by $(1-\eta f)$, and $(1-f')$ by $(1-\eta f')$. To obtain $Q_{\text{ac}}^{\beta}(f)$ from (II.4), it is enough to replace Φ_{op} by the dimensionless form of Φ_{ac}, N_{op} by N_{ac}, ε_{op} by $\beta^2 \varepsilon_{\text{ac}}$, and $(1-f)$ by $(1-\eta f)$. This latter substitution is sufficient to yield the dimensionless form of $Q_e(f)$.

The equations are posed on a dilated Brillouin zone B/k_0. We recall that

$$N_{\text{op}} = (e^{\alpha^2/\gamma^2} - 1)^{-1}, \quad N_{\text{ac}} = (e^{\beta^2 \varepsilon_{\text{ac}}/\gamma^2} - 1)^{-1}.$$

We shall analyze the behavior of (II.7) at various time, length, and energy scales. First, we are interested in a high energy scale (i.e., for large applied biases) at which the relative energy gain or loss of electron energy during a phonon collision is very small. Therefore, we let, following Refs. 27 and 16,

$$\alpha^2 \ll 1, \quad \beta^2 \ll 1. \qquad \text{(II.8)}$$

Together with (II.8), we suppose that

$$\frac{\alpha^2}{\gamma^2} \approx \frac{\beta^2}{\gamma^2} = 0(1), \qquad \text{(II.9)}$$

which means that at the high energy scale, the acoustical phonon energy $\varepsilon_{ac,0}$, the optical phonon energy $\varepsilon_{op,0}$, and the lattice thermal energy $k_B T_L$ are all considered of the same order of magnitude, and very small compared with the electron energy ε_0. Of course, one knows that, physically, $\varepsilon_{ac,0}<K_B T_L<\varepsilon_{op,0}$,[39] but the differences in the magnitudes of these energies are only detectable on longer time scales. This point will be clarified in Secs. IV and V.

By expanding $Q^{\alpha}_{op}(f)$ and $Q^{\beta}_{ac}(f)$ in powers of α^2 and β^2 and using (II.8), we can write the global lattice-defect collision operator according to (see also Refs. 27 and 16):

$$Q_{ld}(f)=(\nu_{imp}+\nu_{ac}+\nu_{op})Q_0(f)+\beta^2\nu_{ac}Q^{\beta}_{ac,1}(f)+\alpha^2\nu_{op}Q^{\alpha}_{op,1}(f),$$

where $Q_0(f)$ is an elastic collision operator given by

$$\begin{aligned} Q_0(f)&=\int \Phi_0(x,k,k')\,\delta(\varepsilon'-\varepsilon)(f'-f)dk', \\ \Phi_0&=\Phi_{imp}+(2N_{op}+1)\Phi_{op}+(2N_{ac}+1)\Phi_{ac}, \end{aligned} \tag{II.10}$$

and $Q^{\beta}_{ac,1}$ (resp. $Q^{\alpha}_{op,1}$) is of order 1 when β (resp. α) tends to zero. We now choose the time scale to be such that $(\nu_{imp}+\nu_{ac}+\nu_{op})=1$. From (II.9), we let $\alpha^2=\beta^2$ and we assume that

$$\nu_e=0(\alpha^2), \quad \text{i.e.,}\ \nu_e=\alpha^2\overline{\nu_e},\ \ \overline{\nu_e}=0(1). \tag{II.11}$$

We define

$$Q^{\alpha}_1=\nu_{ac}Q^{\alpha}_{ac,1}(f)+\nu_{op}Q^{\alpha}_{op,1}(f)+\overline{\nu_e}Q_e(f)=0(1)\ \ \text{as}\ \ \alpha\to 0. \tag{II.12}$$

The final form of the scaled Boltzmann equation (II.7) is thus

$$\frac{\partial f}{\partial t}+\nabla_k\varepsilon(k)\cdot\nabla_x f+\nabla_x V(x,t)\cdot\nabla_k f=Q_0(f)+\alpha^2 Q^{\alpha}_1(f), \tag{II.13}$$

where $Q_0(f)$ is the elastic operator (II.10) and $Q^{\alpha}_1(f)$ is given by (II.12). The ordering between the collision operators is the same as in Ref. 27. In Ref. 16 electron–electron collisions are considered of order 1, instead of α^2, and are brought into the leading order collision operator. A precise discussion of the magnitude of $Q_e(f)$ compared with Q_0 is given in Refs. 28 and 29. It is shown that for large densities Q_0 and Q_e are of the same order of magnitude while at low densities Q_e is smaller than Q_0. The ordering displayed by (II.13) is then characteristic of a rather small density case.

III. FIRST MACROSCOPIC SCALE: THE "SPHERICAL" HARMONIC EXPANSION MODEL

A. Scaling

We are interested in the diffusion scaling for Eq. (II.13). Following Ref. 27 or 16, we let

$$x'=\alpha x, \quad t'=\alpha^2 t.$$

This leads to the following scaled version of (II.13):

$$\frac{\partial f^{\alpha}}{\partial t}+\frac{1}{\alpha}\,(\nabla_k\varepsilon\cdot\nabla_x f^{\alpha}+\nabla_x V\cdot\nabla_k f^{\alpha})=\frac{1}{\alpha^2}\,Q_0(f^{\alpha})+Q^{\alpha}_1(f^{\alpha}). \tag{III.1}$$

Inserting the Hilbert expansion of f^{α},

$$f^\alpha = f_0 + \alpha f_1 + \alpha^2 f_2 + \cdots ,$$

in (III.1), we find

$$Q_0(f_0) = 0, \tag{III.2}$$

$$Q_0(f_1) = \nabla_k \varepsilon \cdot \nabla_x f_0 + \nabla_x V \cdot \nabla_k f_0, \tag{III.3}$$

$$Q_0(f_2) = \frac{\partial f_0}{\partial t} + \nabla_k \varepsilon \cdot \nabla_x f_1 + \nabla_x V \cdot \nabla_k f_1 - Q_1^\alpha(f_0). \tag{III.4}$$

To solve these equations, we need to investigate the operator Q_0.

B. Properties of Q_0

We first recall the coarea formula:[40] for any C^1 function $\varepsilon: B \to \mathbb{R}$, and any test function $\psi \in C^0(B)$ [where $C^0(B)$ denotes the set of continuous functions on B], we have

$$\int_B \psi(k)\,dk = \int_{-\infty}^{+\infty} \left(\int_{\varepsilon^{-1}(e)} \psi(k)\, \frac{dS_e(k)}{|\nabla \varepsilon(k)|} \right) de, \tag{III.5}$$

where $dS_e(k)$ denotes the Euclidean surface element on the manifold $\varepsilon^{-1}(e)$. We shall denote $dN_e(k) = dS_e(k)/|\nabla \varepsilon(k)|$ and (III.5) will be formally written

$$\int_B \psi(k)\,dk = \int_{-\infty}^{+\infty} \left(\int_{\varepsilon} \psi(k)\, dN_\varepsilon(k) \right) d\varepsilon. \tag{III.6}$$

We let $N(e)$ be the density of states of energy e:

$$N(e) = \int_{\varepsilon^{-1}(e)} dN_e(k). \tag{III.7}$$

By duality, we have for any $\psi \in C^0(B)$

$$\int_B \psi(k)\, \delta(\varepsilon(k) - \varepsilon)\,dk = \int_\varepsilon \psi(k)\, dN_\varepsilon(k). \tag{III.8}$$

We now recall that

$$Q_0(f) = \int_B \phi_0(x,k,k')\, \delta(\varepsilon' - \varepsilon)(f' - f)\,dk',$$

and we note that

$$Q_0(\psi(\varepsilon) f) = \psi(\varepsilon) Q_0(f), \quad \forall \psi = \psi(\varepsilon), \ \forall f. \tag{III.9}$$

We introduce

$$Lf = Q_0\left(\frac{f}{N(\varepsilon(k))} \right) = \frac{1}{N(\varepsilon(k))}\, Q_0(f), \tag{III.10}$$

and we denote by L^2_N the weighted space

$$L_N^2=\left\{ f(k), \int_B f^2(k)N(\varepsilon(k))dk<+\infty \right\}.$$

We assume that $N(\varepsilon(k))\neq 0$ for k a.e. in B so that L_N^2 is a separable Hilbert space with the scalar product and norm

$$\langle f,g\rangle_N=\int_B f(k)g(k)N(\varepsilon(k))dk, \quad \|f\|_N^2=\langle f,f\rangle_N.$$

Proposition III.1: Assume $\exists C_1, C_2>0$, $C_1\leqslant\phi_0\leqslant C_2$. Then

(i) $-L$ is a self-adjoint bounded non-negative operator on L_N^2,
(ii) $\mathrm{Ker}\, L=\{f\in L_N^2 \text{ s.t.} \exists g\in L^2(\mathbb{R}),\ f(k)=g(\varepsilon(k))/N(\varepsilon(k))\}$,
(iii) $(\mathrm{Ker}\, L)^\perp=\{f\in L_N^2, \text{ s.t. } \int_\varepsilon f(k)dN_\varepsilon(k)=0, \text{ a.e.}\varepsilon\}$,
(iv) $\exists\mu>0$, $\langle -Lf,\ f\rangle_N\geqslant\mu\|f-Pf\|_N^2$, where Pf is the orthogonal projection on $\ker L$,
(v) $Pf(k)=1/N(\varepsilon)\int_\varepsilon f dN_\varepsilon(k)$ and $\forall\psi(\varepsilon)$, $P(\psi(\varepsilon)f)=\psi(\varepsilon)Pf$,
(vi) $R(L)=(\mathrm{Ker}\, L)^\perp$.

Here $\mathrm{Ker}\, L$ and $R(L)$ stand for the kernel and the range of the operator L.

Proof: (i) is easy using the boundedness of Φ_0 and the formula

$$\int \Phi_0(f)g dk=\langle Lf,g\rangle=-\frac{1}{2}\int\int_{B\times B}\Phi_0(x,k,k')\delta(\varepsilon'-\varepsilon)(f'-f)(g'-g)dk\ dk'. \tag{III.11}$$

(ii) and (iii) are obvious by the coarea formula. To prove (iv), we just have to prove that

$$\langle -Lf,f\rangle_N\geqslant\mu\|f\|_N^2, \quad \forall f\in(\mathrm{Ker}\, L)^\perp.$$

We have, with (III.11),

$$\begin{aligned}\langle -Lf,f\rangle_N&=\frac{1}{2}\int\int_{B\times B}\Phi_0(x,k,k')\delta(\varepsilon'-\varepsilon)|f'-f|^2\ dk\ dk'\\ &\geqslant C\int_{-\infty}^{+\infty}\int_{\varepsilon(k')=\varepsilon}\int_{\varepsilon(k)=\varepsilon}[|f(k)|^2\\ &\quad +|f(k')|^2-2f(k)f(k')]\cdot dN_\varepsilon(k)dN_\varepsilon(k')d\varepsilon.\end{aligned}$$

However, since $f\in(\mathrm{Ker}\, L)^\perp$,

$$\int_{\varepsilon(k')=\varepsilon}\int_{\varepsilon(k)=\varepsilon}f(k')f(k)dN_\varepsilon(k)dN_\varepsilon(k')=0$$

and therefore

$$\langle -Lf,f\rangle_N\geqslant C\int_0^{+\infty}\int_{\varepsilon(k')=\varepsilon}\int_{\varepsilon(k)=\varepsilon}(f(k)^2+f(k')^2)dN_\varepsilon(k)dN_\varepsilon(k')d\varepsilon\geqslant 2C\|f\|_N^2.$$

(v) is just a computation and (vi) is a direct consequence of (iv). ■

C. Resolution of the Hilbert expansion (3.2)–(3.4)

By Eq. (III.2) and proposition III.1 (ii), there exists a function $F(x,\varepsilon,t)$ such that

$$f_0(x,k,t)=F(x,\varepsilon(k),t). \tag{III.12}$$

Then, Eq. (III.3) is equivalently written

$$Lf_1=\frac{1}{N(\varepsilon(k))}\,\nabla_k\varepsilon(k)\left[\nabla_x F+\nabla_x V\,\frac{\partial F}{\partial\varepsilon}\right]. \tag{III.13}$$

Since $\nabla_x F+\nabla_x V\partial F/\partial\varepsilon$ only depends on k through $\varepsilon(k)$, it is clear that the right-hand side of (III.13) belongs to $(\mathrm{Ker}\,L)^{\perp}=R(L)$. Therefore, Eq. (III.13) is solvable in f_1. Moreover, we have the following obvious lemma, using (III.9).

Lemma III.2: Let $\boldsymbol{\lambda}(x,k)$ be the unique solution in $(\mathrm{Ker}\,L)^{\perp}$ of

$$-L(\boldsymbol{\lambda})=\frac{1}{N(\varepsilon(k))}\,\nabla_k\varepsilon. \tag{III.14}$$

Then the unique solution in $(\mathrm{Ker}\,L)^{\perp}$ of Eq. (III.13) is given by

$$f_1=-\boldsymbol{\lambda}(x,k)\cdot\left(\nabla_x F+\nabla_x V\,\frac{\partial F}{\partial\varepsilon}\right). \tag{III.15}$$

Remark III.3: $\boldsymbol{\lambda}$ depends on x through L because Φ_0 may depend on x. (In particular, the impurity scattering matrix element depends on the doping density). Here $\boldsymbol{\lambda}$ is a vector-valued function and Eq. (III.14) must be understood componentwise. Adding an element of $\ker L$ to f_1 would not modify the subsequent analysis. ■

Then, Eq. (III.4) can be written

$$Lf_2=\frac{1}{N(\varepsilon)}\left[\frac{\partial F}{\partial t}+\nabla_k\varepsilon\cdot\nabla_x f_1+\nabla_x V\cdot\nabla_k f_1-Q_1^{\alpha}(F)\right]. \tag{III.16}$$

By Proposition III.1 (vi) and (iii), the solvability condition for (III.16) is written

$$\int_{\varepsilon}\left[\frac{\partial F}{\partial t}+\nabla_k\varepsilon\cdot\nabla_x f_1+\nabla_x V\cdot\nabla_k f_1-Q_1^{\alpha}(F)\right]dN_{\varepsilon}(k)=0,\quad \text{a.e. } \varepsilon. \tag{III.17}$$

Setting

$$S^{\alpha}(F)=\int_{\varepsilon}Q_1^{\alpha}(F)\,dN_{\varepsilon}(k), \tag{III.18}$$

$$J(x,\varepsilon,t)=\int_{\varepsilon}\nabla_k\varepsilon\,f_1(x,k,t)\,dN_{\varepsilon}(k), \tag{III.19}$$

we find the following.

Theorem III.4: Let f_0 and f_1 be given by (III.12) and (III.15). Then, the solution f_2 of Eq. (III.4) exists if and only if $F\ (x,\varepsilon,t)$ satisfies

$$N(\varepsilon)\,\frac{\partial F}{\partial t}+\nabla_x\cdot J+\nabla_x V\cdot\,\frac{\partial J}{\partial\varepsilon}-S^{\alpha}(F)=0, \tag{III.20}$$

$$J(x,\varepsilon,t)=-D(x,\varepsilon)\left(\nabla_x F+\nabla_x V\,\frac{\partial F}{\partial\varepsilon}\right), \tag{III.21}$$

where

$$D(x,\varepsilon)=\int_{\varepsilon}\nabla_k\varepsilon\otimes\boldsymbol{\lambda}(x,k)\,dN_{\varepsilon}(k). \tag{III.22}$$

Proof: Equations (III.21) and (III.22) just come from (III.19) and (III.15). The first, second, and fourth terms of (III.20) obviously come from the corresponding terms in (III.17). For the third term, we proceed as in Ref. 10. We write, for any $\psi=\psi(\varepsilon)$,

$$\begin{aligned}\int_B \nabla_k f_1\psi(\varepsilon)\,dk &= -\int_B f_1\nabla_k\psi(\varepsilon)\,dk\\ &= -\int_B f_1\nabla_k\varepsilon\,\psi'(\varepsilon)\,dk\\ &= -\int_{\mathbb{R}}\psi'(\varepsilon)\left(\int_{\varepsilon} f_1\nabla_k\varepsilon\,dN_{\varepsilon}(k)\right)d\varepsilon\\ &= -\int_{\mathbb{R}}\psi'(\varepsilon)J(\varepsilon)\,d\varepsilon\\ &= \int_{\mathbb{R}}\psi(\varepsilon)J'(\varepsilon)\,d\varepsilon.\end{aligned}$$

It follows that

$$\int_{\varepsilon}\nabla_k f_1\,dN_{\varepsilon}(k)=\frac{\partial J}{\partial\varepsilon}.$$

■

Remark III.5: System (III.20) and (III.21) is in the form of Ref. 27 except for the expression of the diffusion matrix (see below). By the change of unknowns

$$F(x,\varepsilon,t)=G(x,\varepsilon-V(x,t),t),\quad J(x,\varepsilon,t)=I(x,\varepsilon-V(x,t),t),$$

system (III.20) and (III.21) is equivalent with

$$N(u+V(x,t))\left(\frac{\partial G}{\partial t}-\frac{\partial V}{\partial t}\,\frac{\partial G}{\partial u}\right)+\nabla_x\cdot I=S^{\alpha}(G), \tag{III.23}$$

$$I(x,t,u)=-D(x,u+V(x,t))\nabla_x G, \tag{III.24}$$

where u stands for the new variable $\varepsilon-V(x,t)$. System (III.23) and (III.24) is in the form of Ref. 30, except again for the expression of the diffusion matrix (see below). System (III.23) and (III.24) is a system of diffusion equations coupled by the transport term $N\,\partial V/\partial t\,\partial G/\partial u$ and by the collision operator S^{α}. In reference to Ref. 30, it will be called the ''spherical'' harmonic expansion model, the quotes indicating that, for arbitrary band diagrams, the expansion in no more ''spherical'' but rather on constant energy shells. ■

D. Properties of the diffusion matrix

Proposition III.6: $D(x,\varepsilon)$ is a symmetric non-negative 3×3 matrix. Moreover, $\exists C>0$ such that

$$D(x,\varepsilon)\geqslant \frac{C}{N(\varepsilon)} \int_{\varepsilon} \nabla_k\varepsilon\otimes\nabla_k\varepsilon \; dN_\varepsilon(k). \tag{III.25}$$

Remark III.7: The right-hand side of (III.25) is a symmetric non-negative 3×3 matrix which is degenerate at the critical points of ε. Estimate (III.25) is sharp as will further be shown by examples. ■

Proof: Let $\psi(\varepsilon)\in C^0(\mathbb{R})$. By definition (III.22) we have

$$\int_{\mathbb{R}} D_{ij}(\varepsilon)\psi(\varepsilon)d\varepsilon = \int_{\mathbb{R}}\left(\int_{\varepsilon}\partial_{k_i}\varepsilon\lambda_j \; dN_\varepsilon(k)\right)\psi(\varepsilon)d\varepsilon.$$

Then, by using the coarea formula and definition (III.14) of $\boldsymbol{\lambda}$, we have

$$\int_{\mathbb{R}} D_{ij}(\varepsilon)\psi(\varepsilon)d\varepsilon = -\int_B L(\lambda_i N(\varepsilon))\lambda_j\psi(\varepsilon)dk.$$

Now, using the self-adjointness of L and property (III.9),

$$\begin{aligned}
\int_{\mathbb{R}} D_{ij}(\varepsilon)\psi(\varepsilon)d\varepsilon &= -\int \lambda_i N(\varepsilon) L(\lambda_j\psi(\varepsilon))dk \\
&= -\int \lambda_i\psi(\varepsilon) L(\lambda_j N(\varepsilon))dk \\
&= \int \lambda_i\psi(\varepsilon)\partial_{k_j}\varepsilon \; dk \\
&= \int_{\mathbb{R}}\psi(\varepsilon)\left(\int_{\varepsilon}\lambda_i\partial_{k_j}\varepsilon dN_\varepsilon(k)\right)d\varepsilon \\
&= \int_{\mathbb{R}}\psi(\varepsilon)D_{ji}(\varepsilon)d\varepsilon,
\end{aligned}$$

which proves that $D_{ij}(\varepsilon)=D_{ji}(\varepsilon)$.

Now, we choose $\psi\in C^0(\mathbb{R})$, $\psi\geqslant0$, and we let $\xi=(\xi_1,\xi_2,\xi_3)\in\mathbb{R}^3$. Using Einstein's summation convention, we have

$$\begin{aligned}
\int_{\mathbb{R}}\psi(\varepsilon)D_{ij}(\varepsilon)\xi_i\xi_j \; d\varepsilon &= \int_{\mathbb{R}}\psi(\varepsilon)\left(\int_{\varepsilon}\partial_{k_i}\varepsilon\xi_i\lambda_j\xi_j \; dN_\varepsilon(k)\right)d\varepsilon \\
&= -\int_B L(\lambda_i\xi_i\sqrt{\psi(\varepsilon)})(\lambda_j\xi_j\sqrt{\psi(\varepsilon)})N(\varepsilon)dk.
\end{aligned}$$

Since $\lambda_i\xi_i\sqrt{\psi(\varepsilon)}\in(\mathrm{Ker}\ L)^\perp$, we have, by Proposition 3.1 (iv),

$$\int_{\mathbb{R}}\psi(\varepsilon)D_{ij}(\varepsilon)\xi_i\xi_j \; d\varepsilon \geqslant \mu\|\lambda_i\xi_i\sqrt{\psi(\varepsilon)}\|_N^2. \tag{III.26}$$

By the continuity of L, we deduce

$$\begin{aligned}\|\lambda_i\xi_i\sqrt{\psi(\varepsilon)}\|_N^2 &\geqslant C\|L(\lambda_i\xi_i)\sqrt{\psi(\varepsilon)}\|_N^2\\ &\geqslant C\|(1/N)\vec{\nabla}_k\varepsilon\cdot\boldsymbol{\xi}\sqrt{\psi(\varepsilon)}\|_N^2\\ &\geqslant C\int_{\mathbb{R}}\frac{\psi(\varepsilon)}{N(\varepsilon)}\left(\int_\varepsilon|\vec{\nabla}_k\varepsilon\cdot\boldsymbol{\xi}|^2dN_\varepsilon(k)\right)d\varepsilon.\end{aligned}\tag{III.27}$$

Inserting (III.26) in (III.27) leads to

$$\int_{\mathbb{R}}\psi(\varepsilon)(D_{ij}(\varepsilon)\xi_i\xi_j)d\varepsilon\geqslant C'\int_{\mathbb{R}}\psi(\varepsilon)\left(\frac{1}{N(\varepsilon)}\int_\varepsilon(\boldsymbol{\nabla}_k\varepsilon\otimes\boldsymbol{\nabla}_k\varepsilon)dN_\varepsilon(k)\right)_{ij}\xi_i\xi_j\,d\varepsilon$$

for all $\psi\in C^0(\mathbb{R})$, $\psi\geqslant 0$, which implies (III.25). ■

We now investigate simplifying assumptions which enable us to give more explicit expressions of $D(x,\varepsilon)$. First, we assume that $\Phi_0(x,k,k')=\Phi_0(x,\varepsilon(k))$ [we recall that Φ_0 needs only to be defined on the set $\varepsilon(k')=\varepsilon(k)$]. Then $Q_0(f)$ is equivalently written in the form of a relaxation operator:

$$Q_0(f)=-\frac{1}{\tau(x,\varepsilon)}\,(f-Pf)\tag{III.28}$$

with $\tau(x,\varepsilon)=(\Phi_0(x,\varepsilon)N(\varepsilon))^{-1}$ and P is the projection defined in Proposition 3.1 (v). Then, the solution of (III.10) can be written

$$\boldsymbol{\lambda}(x,k)=\tau(x,\varepsilon)\nabla_k\varepsilon\tag{III.29}$$

and can be referred to as the ''mean free path of particles of wave vector k.'' Therefore, we have

$$D(x,\varepsilon)=\tau(x,\varepsilon)\int_\varepsilon\vec{\nabla}_k\varepsilon\otimes\hat{\nabla}_k\varepsilon\;dN_\varepsilon(k).\tag{III.30}$$

This is the case explicitly treated in Ref. 27 and our results coincide. This case proves that estimate (III.25) is sharp, because it becomes an equality in the case of Ref. 27.

Another simplification is to consider a spherically symmetric band diagram (and therefore $B=\mathbb{R}^3$), together with Φ_0 being such that $\Phi_0(x,k,k')=\Phi_0(x,\varepsilon,(k/|k|)\cdot(k'/|k'|))$. In this case, the elastic collision operator is rotationally invariant. A relaxation time can be defined by (with S^2 being the unit sphere of $\mathbb{R}^3$)

$$\begin{aligned}\frac{1}{\tau(x,\varepsilon)}&=\frac{1}{4\pi}\left(\int_{S^2}\Phi_0(x,\varepsilon,\omega)(1-\omega_z)d\omega\right)N(\varepsilon),\\ N(\varepsilon)&=4\pi\sum_{\varepsilon(|k|)=\varepsilon}\frac{|k|^2}{|\varepsilon'(|k|)|}\end{aligned}\tag{III.31}$$

[we assume that for any $\varepsilon\in\mathbb{R}$, the set $\{|k|,\varepsilon(|k|)=\varepsilon\}$ is discrete.] Then a straightforward computation leads to

$$\boldsymbol{\lambda}(x,k)=\tau(x,\varepsilon)\varepsilon'(|k|)\mathbf{k}/|k|.\tag{III.32}$$

$$D(x,\varepsilon)=\frac{4\pi}{3}\,\tau(x,\varepsilon)\left(\sum_{\varepsilon(|k|)=\varepsilon}|\varepsilon'(|k|)|\;|k|^2\right)\mathrm{Id}\tag{III.33}$$

where Id is the identity matrix of $\mathbb{R}^3$. This expression can be further simplified if one assumes that ε is a strictly monotone (e.g., increasing) function of $|k|$. In such a case, the $\varepsilon(|k|)$ relation can be inverted, and, following Ref. 30, we can define a function γ such that

$$|k|^2=\gamma(\varepsilon).$$

All the functions of $|k|$ may be expressed as functions of ε, and we have

$$\varepsilon'(\varepsilon)=2\frac{\sqrt{\gamma(\varepsilon)}}{\gamma'(\varepsilon)},\quad N(\varepsilon)=2\pi\sqrt{\gamma(\varepsilon)}\gamma'(\varepsilon), \tag{III.34}$$

$$\boldsymbol{\lambda}(x,k)=\Lambda(x,\varepsilon)\mathbf{k}/|k|,\quad \Lambda(x,\varepsilon)=\tau(x,\varepsilon)\varepsilon'(\varepsilon), \tag{III.35}$$

and

$$D(x,\varepsilon)=\left(\frac{8\pi}{3}\,\tau(x,\varepsilon)\,\frac{\gamma(\varepsilon)^{3/2}}{\gamma'(\varepsilon)}\right)\ \mathrm{Id}=\frac{1}{3}\,(N(\varepsilon)\Lambda(x,\varepsilon)\varepsilon'(\varepsilon))\mathrm{Id}. \tag{III.36}$$

This is the case considered in Ref. 30 and our results coincide. Even more specifically, let us assume that $\Phi_0=\Phi_0(x)$ is independent of k, k', which is true for acoustical and nonpolar optical phonons. (Indeed, these are the main sources of scattering in Si at room temperature, since the impurity scattering can be neglected.) Let us also assume a parabolic band structure $\gamma(\varepsilon)=2m_*\varepsilon$ with m_* being the effective mass. Then, by (III.36),

$$D(x,\varepsilon)=\frac{2\varepsilon}{3\Phi_0(x)m_*}\,\mathrm{Id}. \tag{III.37}$$

IV. SECOND MACROSCOPIC SCALE DRIVEN BY ELECTRON–ELECTRON COLLISIONS: THE ENERGY-TRANSPORT MODEL

A. Scaling

The starting point is now the ''spherical'' harmonic expansion model (III.20) and (III.21). Going back to (II.12), the collision term $S^\alpha(f)$ is written

$$S^\alpha(F)=\frac{\nu_{\mathrm{ac}}}{\alpha^2}\,\mathrm{S}^\alpha_{\mathrm{ac}}(F)+\frac{\nu_{\mathrm{op}}}{\alpha^2}\,S^\alpha_{\mathrm{op}}(F)+\overline{\nu_e}S_e(F), \tag{IV.1}$$

where we have [because the elastic parts Q^0_{ac} and Q^0_{op} vanish on $F(\varepsilon)$]

$$S^\alpha_{\mathrm{ac}}(F)(\varepsilon)=\int_\varepsilon Q^\alpha_{\mathrm{ac}}(F)dN_\varepsilon(k),\quad S^\alpha_{\mathrm{op}}(F)(\varepsilon)=\int_\varepsilon Q^\alpha_{\mathrm{op}}(F)dN_\varepsilon(k), \tag{IV.2}$$

$$S_e(F)(\varepsilon)=\int_\varepsilon Q_e(F)dN_\varepsilon(k). \tag{IV.3}$$

We now assume that both phonon collision operators $\nu_{\mathrm{ac}}/\alpha^2S^\alpha_{\mathrm{ac}}(F)$ and $\nu_{\mathrm{op}}/\alpha^2S^\alpha_{\mathrm{op}}(F)$ are of the same order of magnitude, and we choose the time unit such that $\nu_{\mathrm{ac}}/\alpha^2\simeq\nu_{\mathrm{op}}/\alpha^2\simeq1$. We also assume that the electron–electron collision operator $\overline{\nu_e}S_e(F)$ is dominant and we let $\overline{\nu_e}=1/\beta$, $\beta\ll1$. This amounts to assuming that, for a distribution function which is constant on the energy surfaces, the energy loss due to phonon collision occurs on a longer scale than the thermalization

by electron–electron collisions. This hypothesis is certainly correct for hot-electron distribution functions F with a substantial high-energy tail. On the contrary, for ''cooler'' Fs, this hypothesis is more doubtful and we shall investigate this case in Sec. V.

Therefore, the evolution of a hot-electron energy distribution $F^\beta(x,\varepsilon,t)$ is ruled by the following equations:

$$N(\varepsilon)\,\frac{\partial F_\beta}{\partial t}+\nabla_x\cdot J^\beta+\nabla_x V\cdot\frac{\partial J^\beta}{\partial\varepsilon}=\frac{1}{\beta}\,S_e(F^\beta)+S_1(F^\beta), \tag{IV.4}$$

$$J^\beta(x,\varepsilon,t)=-D(x,\varepsilon)\left(\nabla_x F^\beta+\nabla_x V\cdot\frac{\partial F^\beta}{\partial\varepsilon}\right), \tag{IV.5}$$

with $S_e(F^\beta)$ given by (IV.3) and $S_1(F^\beta)=S_{\rm ac}(F^\beta)+S_{\rm op}(F^\beta)$ and $S_{\rm ac}$, $S_{\rm op}$ given by (IV.2). We are interested in the limit $\beta\to 0$. Again, we use a Hilbert expansion

$$F^\beta=F_0+\beta F_1+\cdots,\quad J^\beta=J_0+\beta J_1+\cdots\ .$$

Identifying equal powers of β, we obtain

$$S_e(F_0)=0, \tag{IV.6}$$

$$N(\varepsilon)\,\frac{\partial F_0}{\partial t}+\nabla_x\cdot J_0+\nabla_x V\,\frac{\partial J_0}{\partial\varepsilon}-S_1(F_0)=D_{F_0}S_e(F_1). \tag{IV.7}$$

Here $D_{F_0}S_e(F_1)$ denotes the derivative of S_e at F_0 applied to F_1. To solve (IV.6) and (IV.7), we first investigate the properties of S_e and $D_{F_0}S_e(F_1)$. We note that the scaling (IV.4) of the ''spherical'' harmonic expansion model is of hydrodynamic type and not of diffusion type. The reason is that the transport part (left-hand side of the equation) is already a diffusion model.

B. Properties of S_e and $D_{F_0}S_e$

For this section, we shall mainly rely on section 4 of Ref. 16. We have

Proposition IV.1: (i) Entropy inequality:

$$\int_{\mathbb{R}} S_e(F)\ln\left(\frac{F}{1-\eta F}\right)d\varepsilon\leqslant 0.$$

(i) $\int_{\mathbb{R}} S_e(F)\,\binom{1}{\varepsilon}d\varepsilon=0$

(ii) $S_e(F)=0\Leftrightarrow\exists\,\mu\varepsilon\mathbb{R},\ T>0$ such that

$$F=\mathscr{F}_{\mu,T}(\varepsilon)=\frac{1}{\eta+e^{(\varepsilon-\mu)/T}}. \tag{IV.8}$$

Proof: The proof is immediate from Ref. 16 by noting that, $\forall F(\varepsilon)$, $G(\varepsilon)$,

$$\begin{aligned}\int_{\mathbb{R}} S_e(F)G(\varepsilon)d\varepsilon&=\int_B Q_e(F(\varepsilon(k)))G(\varepsilon(k))dk\\&=-\frac{1}{4}\int_{B^4}\Phi_e\delta_\varepsilon\delta_k(G'+G_1'-G-G_1)\\&\quad\times(F'F_1'(1-\eta F)(1-\eta F_1)-FF_1(1-\eta F')(1-\eta F_1'))d^4k,\end{aligned}$$

where δ_ε stands for $\delta(\varepsilon' + \varepsilon_1' - \varepsilon - \varepsilon_1)$, δ_k for $\delta_p(k' + k_1' - k - k_1)$, and $d^4k = dk\ dk_1\ dk'\ dk_1'$.

We now define

$$\Sigma_{\mathscr{F}}(f) = N(\varepsilon)^{-1} D_{\mathscr{F}} S_e(f) \tag{IV.9}$$

and the Hilbert space

$$H_{\mathscr{F}} = \left\{ f(\varepsilon),\ \int_{\mathbb{R}} |f(\varepsilon)|^2 \frac{N(\varepsilon)}{\mathscr{F}(1-\eta\mathscr{F})}\, d\varepsilon < +\infty \right\},$$

provided with the obvious scalar product $\langle , \rangle_{\mathscr{F}}$ and norm $|\cdot|_{\mathscr{F}}$. We have the following.

Proposition IV.2: (i) $-\Sigma_{\mathscr{F}}$ is a bounded non-negative self-adjoint operator on $H_{\mathscr{F}}$.

(ii) $\ker \Sigma_{\mathscr{F}} = \mathrm{Span}\ (\mathscr{F}(1-\eta\mathscr{F}), \mathscr{F}(1-\eta\mathscr{F})\varepsilon)$.

(iii) $\langle -\Sigma_{\mathscr{F}}(f), f\rangle_{\mathscr{F}} \geqslant \mu |f - Pf|^2_{\mathscr{F}}$, where P is the orthogonal projection on $\mathrm{Ker}\ \Sigma_{\mathscr{F}}$ for $\langle , \rangle_{\mathscr{F}}$.

(iv) $R(\Sigma_{\mathscr{F}}) = (\mathrm{Ker}\ \Sigma_{\mathscr{F}})^{\perp} = \{ f \in H_{\mathscr{F}}, \int f\binom{1}{\varepsilon} N(\varepsilon) d\varepsilon = 0 \}$.

Proof: Again, the proof is immediate from Ref. 16. Indeed, we have

$$\langle -\Sigma_{\mathscr{F}}(f), g\rangle_{\mathscr{F}} = -\int_{\mathbb{R}} \Sigma_{\mathscr{F}}(f)(\varepsilon) g(\varepsilon) \frac{N(\varepsilon) d\varepsilon}{\mathscr{F}(1-\eta\mathscr{F})}.$$

However, differentiating (IV.3) with respect to $\mathscr{F}$ yields

$$N(\varepsilon)\Sigma_{\mathscr{F}}(f)(\varepsilon) = \int_{\varepsilon} D_{\mathscr{F}} Q_e(f)(k)\, dN_\varepsilon(k).$$

Therefore

$$\langle -\Sigma_{\mathscr{F}}(f), g\rangle_{\mathscr{F}} = -\int_B D_{\mathscr{F}} Q_e(f)(k) g(\varepsilon(k)) \frac{dk}{\mathscr{F}(\varepsilon(k))(1-\eta\mathscr{F}(\varepsilon(k)))}. \tag{IV.10}$$

Let $\mathscr{H}_{\mathscr{F}}$ be the Hilbert space

$$\mathscr{H}_{\mathscr{F}} = \left\{ \varphi(k), \int_B |\varphi(k)|^2 \frac{dk}{\mathscr{F}(\varepsilon(k))(1-\eta\mathscr{F}(\varepsilon(k)))} < +\infty \right\},$$

provided with the obvious scalar product $\ll , \gg_{\mathscr{F}}$ and norm $\|\cdot\|_{\mathscr{F}}$. In Ref. 16, the operator

$$-\mathscr{L}_{\mathscr{F}} = -D_{\mathscr{F}} Q_e - Q_0, \tag{IV.11}$$

where Q_0 is given by (II.10), is proved to be a bounded non-negative self-adjoint operator on $\mathscr{H}_{\mathscr{F}}$ for $\ll , \gg_{\mathscr{F}}$. However, since f only depends on ε, we have $Q_0(f) = 0$, so that (IV.10) can be written

$$\langle -\Sigma_{\mathscr{F}}(f), g\rangle_{\mathscr{F}} = -\ll \mathscr{L}_{\mathscr{F}} f, g(\varepsilon) \gg_{\mathscr{F}}.$$

Therefore, $-\Sigma_{\mathscr{F}}$ inherits of all the properties of $-\mathscr{L}_{\mathscr{F}}$. Proposition 4.2 follows from corollary 4.6, lemma 4.7, and proposition 4.8 of Ref. 16. ■

C. Resolution of the Hilbert expansion (4.6) and (4.7)

The solution of (IV.6) is obviously from proposition IV.1 (iii):

$$F_0(x, \varepsilon, t) = \mathscr{F}_{\mu(x,t), T(x,t)}(\varepsilon). \tag{IV.12}$$

Then, J_0 is given by (IV.5) with $\beta=0$, which yields

$$J_0(x,\varepsilon,t) = -D(x,\varepsilon)\mathscr{F}(1-\eta\mathscr{F})\left\{\left(\nabla_x\left(\frac{\mu}{T}\right)-\frac{\nabla_x V}{T}\right)-\varepsilon\nabla\left(\frac{1}{T}\right)\right\}. \tag{IV.13}$$

The search of a solution for (IV.7) leads to the following theorem.

Theorem IV.3: Let F_0 be given by (IV.12). Then, the solution of Eq. (IV.7) exists if and only if $\mu(x,t)$ and $T(x,t)$ satisfy the following set of diffusion equations:

$$\frac{\partial}{\partial t}\, n(\mu,T)-\nabla\cdot\left[\mathscr{D}_{11}\left(\nabla_x\left(\frac{\mu}{T}\right)-\frac{\nabla_x V}{T}\right)+\mathscr{D}_{12}\,\frac{\nabla_x T}{T^2}\right]=0, \tag{IV.14}$$

$$\begin{aligned}\frac{\partial}{\partial t}\, n\mathscr{E}(\mu,T)&-\nabla\cdot\left[\mathscr{D}_{21}\left(\nabla_x\left(\frac{\mu}{T}\right)-\frac{\nabla x V}{T}\right)+\mathscr{D}_{22}\,\frac{\nabla_x T}{T^2}\right]\\&+\nabla_x V\cdot\left[\mathscr{D}_{11}\left(\nabla_x\left(\frac{\mu}{T}\right)-\frac{\nabla_x V}{T}\right)+\mathscr{D}_{12}\,\frac{\nabla_x T}{T^2}\right]\\&=W(\mu,T,T_L),\end{aligned} \tag{IV.15}$$

where

$$\begin{pmatrix} n(\mu,T)\\ n\mathscr{E}(\mu,T)\end{pmatrix}=\int_{\mathbb{R}}\mathscr{F}_{\mu,T}(\varepsilon)\begin{pmatrix}1\\ \varepsilon\end{pmatrix}N(\varepsilon)\,d\varepsilon, \tag{IV.16}$$

$$\mathscr{D}_{ij}=\mathscr{D}_{ij}(x,\mu,T)=\int_{\mathbb{R}}D(x,\varepsilon)\mathscr{F}(1-\eta\mathscr{F})\chi_i\chi_j\;d\varepsilon,\quad i,j=1,2, \tag{IV.17}$$

with $\chi_1(\varepsilon)=1$, $\chi_2(\varepsilon)=\varepsilon$, and

$$W(\mu,T,T_L)=\int_{\mathbb{R}}S_1(\mathscr{F}_{\mu,T})\varepsilon\;d\varepsilon. \tag{IV.18}$$

We recall that T_L is the lattice temperature.

Proof: From Proposition IV.2 (iv), the condition for Eq. (4.7) to be solvable in F_1 is

$$\int\left[N(\varepsilon)\,\frac{\partial F_0}{\partial t}+\nabla_x J_0+\nabla x V\,\frac{\partial J_0}{\partial\varepsilon}-S_1(F_0)\right]\begin{pmatrix}1\\ \varepsilon\end{pmatrix}d\varepsilon=0.$$

With the expression (IV.13) of J_0, this immediately yields (IV.14) and (IV.15). ■

Remark IV.4: System (IV.14) and (IV.15) belongs to the class of energy-transport models. In Ref. 16, a similar model is directly derived from a diffusion approximation of the Boltzmann equation (II.13) in which the leading order collision operator is $Q_0(f)+Q_e(f)$. In that case, the diffusion matrix D_{ij} is given by a different (and more complicated) expression than (IV.16), namely,

$$\mathscr{D}_{ij}=\int_B(\chi_i\nabla_k\varepsilon)\otimes\boldsymbol{\psi}_j\;dk, \tag{IV.19}$$

where $\boldsymbol{\psi}_i$ is the unique solution in $(\ker\mathscr{L}_F)^\perp$ of

$$\mathscr{L}_{\mathscr{F}}\boldsymbol{\psi}_i=-(\chi_i\nabla_k\varepsilon)\mathscr{F}(1-\eta\mathscr{F})$$

and $\mathscr{L}_{\mathscr{T}}$ is the operator given by (IV.11). The expression (IV.17) is probably better because the electron–electron collisions in semiconductors are usually not as strong as the phonon collisions (in their elastic approximation). Therefore the relaxation towards a Fermi–Dirac distribution function is a multiscale phenomenon as described in the present paper rather than a single-scale process as implied by the analysis of Ref. 16. In Ref. 16, the connection between energy-transport models and hydrodynamic models is thoroughly investigated. We shall not develop this point here. ■

D. Properties of the diffusion matrix D and the energy relaxation term $W(\mu, T, T_L)$

From Ref. 16, Lemma 4.11, we immediately deduce the following lemma, which proves that W is a relaxation term of the electron temperature T to the lattice temperature T_L:

Lemma IV.5: $W(\mu,T,T_L)\cdot(T-T_L)\leqslant 0$.

Now, we let $\mathscr{D}$ be the block 6×6 matrix

$$\mathscr{D}=\begin{pmatrix}\mathscr{D}_{11} & \mathscr{D}_{12}\\ \mathscr{D}_{21} & \mathscr{D}_{22}\end{pmatrix}=\mathscr{D}(x,\mu,T).$$

We have the following.

Proposition IV.6:

(i) $\forall i,j\in\{1,2\}\ \mathscr{D}_{ij}^{T}=\mathscr{D}_{ij}$.

(ii) $\mathscr{D}_{12}=\mathscr{D}_{21}$.

(iii) Assume that the six functions $\partial_{k_1}\varepsilon$, $\partial_{k_2}\varepsilon$, $\partial_{k_3}\varepsilon$, $\varepsilon\partial_{k_1}\varepsilon$, $\varepsilon\partial_{k_2}\varepsilon$, $\varepsilon\partial_{k_3}\varepsilon$ are linearly independent. Then the matrix $\mathscr{D}(x,\mu,T)$ is symmetric positive definite for any $\mu\in(-\infty,+\infty)$, $T>0$.

Proof: (i) follows from the symmetry of $D(x,\varepsilon)$ and (ii) from the fact that $\chi_1\chi_2=\chi_2\chi_1$. For (iii), let ξ_1, ξ_2 be two vectors of $\mathbb{R}^3$ such that $|\xi_1|^2+|\xi_2|^2=1$, $\xi_i=(\xi_{ip})_{p=1,2,3}$. We have, using Einstein's summation convention,

$$(\mathscr{D}_{ij}\xi_i,\xi_j)=\int_{\mathbb{R}} D(x,\varepsilon).\mathscr{F}(1-\eta.\mathscr{F})\chi_i\xi_i\chi_j\xi_j\,d\varepsilon=\int_{\mathbb{R}} D_{pq}(x,\varepsilon).\mathscr{F}(1-\eta.\mathscr{F})\chi_i\xi_{ip}\chi_j\xi_{jq}\,d\varepsilon.$$

Then, by Proposition III.6, we have

$$(\mathscr{D}_{ij}\xi_i,\xi_j)\geqslant\frac{C}{N(\varepsilon)}\int_{\mathbb{R}}\left(\int_{\varepsilon}(\chi_i\partial_{k_p}\varepsilon)\xi_{ip}(\chi_j\partial_{k_q}\varepsilon)\xi_{jq}\,dN_{\varepsilon}(k)\right).\mathscr{F}(1-\eta.\mathscr{F})d\varepsilon$$

$$\geqslant\frac{C}{N(\varepsilon)}\int_{B}\left|\begin{pmatrix}\nabla_k\varepsilon\\ \varepsilon\nabla_k\varepsilon\end{pmatrix}\cdot\begin{pmatrix}\xi_1\\ \xi_2\end{pmatrix}\right|^2\mathscr{F}(1-\eta.\mathscr{F})dk. \tag{IV.20}$$

The minimal value of the right-hand side of (IV.20) for $(\xi_1,\xi_2)\in\mathbb{R}^6$, $|\xi_1|^2+|\xi_2|^2=1$ cannot be zero, otherwise it would be zero for a particular choice of (ξ_1,ξ_2), which would lead to a contradiction. ■

Remark IV.7: The assumptions on ε which appear in Proposition IV.6 are of geometric nature. They appear in the same form in the energy-transport model directly deduced from the Boltzmann equation derived in Ref. 16. ■

The diffusion matrix $\mathscr{D}$ can be explicitly computed under the simplifying assumption of the last paragraph of Sec. III D: if Φ_0 is independent of k, k' and in the case of a parabolic band structure $(\gamma(\varepsilon)=2m_*\varepsilon)$ and of a nondegenerate statistics [i.e., $\mathscr{F}(1-\eta\mathscr{F})\to\exp(-(\varepsilon-\mu)/T)$ when $\eta\to 0$], the diffusion matrix $\mathscr{D}(x,\mu,T)$ is given from (IV.17) and (III.37) by

$$\mathscr{D}(x,\mu,T)=\frac{2T^2e^{\mu/T}}{3\Phi_0(x)m_*}\begin{pmatrix}\mathrm{Id} & 2T\ \mathrm{Id}\\ 2T\ \mathrm{Id} & 6T^2\ \mathrm{Id}\end{pmatrix}.$$

Remark IV.8: (i) We have $(1/T)\mathscr{D}_{11}^{-1}\mathscr{D}_{12}-\frac{5}{2}\,\mathrm{Id}=-\frac{1}{2}\,\mathrm{Id}\neq 0$, which implies that nonvanishing cross effects such as a friction force of thermal origin (Soret effect) or a heat flux of friction origin (Peltier effect) should be expected in the hydrodynamic model of semiconductor (see Ref. 16, sections 5 and 6).

(ii) The heat conductivity κ and the electrical conductivity σ are given by[16,25]

$$\kappa=\frac{1}{T^2}\,(\mathscr{D}_{22}-\mathscr{D}_{21}\mathscr{D}_{11}^{-1}\mathscr{D}_{12}),\quad \sigma=\frac{1}{T}\,\mathscr{D}_{11}.$$

So that the Landau coefficient $\Lambda=\kappa/\sigma T=2$. In particular, Λ is constant which is the expression of the Wiedemann–Franz law. ■

E. The third macroscopic scale: The drift-diffusion model

If we look at an even longer time scale, the energy losses due to phonon collisions become important and we tend to an asymptotic regime where the electron and lattice temperatures are equal. To investigate this regime, time and space must be rescaled, and system (4.13) and (4.14) is put in the form:

$$\frac{\partial}{\partial t}\,n(\mu^\delta,T^\delta)+\boldsymbol{\nabla}\cdot I^\delta=0, \tag{IV.21}$$

$$\frac{\partial}{\partial t}\,n\mathscr{E}(\mu^\delta,T^\delta)+\boldsymbol{\nabla}\cdot I_W^\delta-\boldsymbol{\nabla}_x V\cdot I^\delta=\frac{1}{\delta}\,W(\mu^\delta,T^\delta,T_L), \tag{IV.22}$$

where $\delta\ll 1$ is a small parameter, and the current I^δ and the energy current I_w^δ are given by the constitutive relations

$$I^\delta=-\left[\mathscr{D}_{11}\left(\nabla_x\left(\frac{\mu^\delta}{T^\delta}\right)-\frac{\nabla_x V}{T^\delta}\right)+\mathscr{D}_{12}\,\frac{\nabla_x T^\delta}{(T^\delta)^2}\right], \tag{IV.23}$$

$$I_W^\delta=-\left[\mathscr{D}_{21}\left(\nabla_x\left(\frac{\mu^\delta}{T^\delta}\right)-\frac{\nabla_x V}{T^\delta}\right)+\mathscr{D}_{22}\,\frac{\nabla_x T^\delta}{(T^\delta)^2}\right]. \tag{IV.24}$$

We are now interested in the behavior of (IV.21) and (IV.22) when $\delta\to 0$. Again, a Hilbert expansion can be used:

$$\mu^\delta=\mu_0+\delta\mu_1+\cdots,\quad T^\delta=T_0+\delta T_1+\cdots,\quad I^\delta=I_0+\delta I_1+\cdots\ . \tag{IV.25}$$

The order δ^{-1} and δ^0 equations are thus written

$$W(\mu_0,T_0,T_L)=0, \tag{IV.26}$$

$$\frac{\partial}{\partial t}\,n(\mu_0,T_0)+\boldsymbol{\nabla}\cdot I_0=0, \tag{IV.27}$$

and I_0 is given by (IV.23) with μ^δ, T^δ replaced by μ_0, T_0. Then, using Lemma 4.11 of Ref. 16, we easily obtain the following.

Theorem IV.9: The solution μ_0, T_0 of system (IV.26) and (IV.27) is $T_0 = T_L$ and μ_0 given by the conventional drift-diffusion model:

$$\frac{\partial}{\partial t} n(\mu_0, T_L) + \nabla \cdot I_0 = 0, \tag{IV.28}$$

$$I_0 = -\left[\mathscr{D}_{11}(x, \mu_0, T_L) \left(\nabla_x \left(\frac{\mu_0}{T_L} \right) - \frac{\nabla_x V}{T_L} \right) + \mathscr{D}_{12}(x, \mu_0, T_L) \frac{\nabla_x T_L}{(T_L)^2} \right]. \tag{IV.29}$$

Remark IV.10: In particular, when T_L is independent of x, one recovers the more usual form

$$I_0 = -\mathscr{D}_{11}(x, \mu_0, T_L) \frac{\nabla_x (\mu_0 - V)}{T_L}, \tag{IV.30}$$

with $\mathscr{D}_{11}(x, \mu_0, T_L)$ given by formula (IV.17). ■

V. SECOND MACROSCOPIC SCALE DRIVEN BY OPTICAL PHONON COLLISIONS: THE "PERIODIZED SPHERICAL" HARMONIC EXPANSION MODEL

A. Scaling

We return to the "spherical" harmonic expansion model (3.20) and (3.21) and we investigate what happens when the optical phonon collision operator is supposed to be dominant instead of the electron–electron one as in Sec. IV. We recall that this is more likely to happen when the typical energy of the electron is of the order of the phonon energy (i.e., a few 10^{-2}–10^{-1} eV). Therefore, this assumes that the energy distribution function has no "high energy tail."

Going back to the notations of Sec. IV A, we assume $\nu_{\mathrm{ac}}/\alpha^2 \simeq \overline{\nu_e} \simeq 0(1)$ while $\nu_{\mathrm{op}}/\alpha^2 = 1/\beta$, $\beta \ll 1$. In this case, the evolution of the energy distribution function $F^\beta(x, \varepsilon, t)$ is governed by

$$N(\varepsilon) \frac{\partial F^\beta}{\partial t} + \nabla_x \cdot J^\beta + \nabla_x V \cdot \frac{\partial J^\beta}{\partial \varepsilon} = \frac{1}{\beta} S_{\mathrm{op}}(F^\beta) + S_1(F^\beta), \tag{V.1}$$

$$J^\beta(x, \varepsilon, t) = -D(x, \varepsilon) \left(\nabla_x F^\beta + \nabla_x V \frac{\partial F^\beta}{\partial \varepsilon} \right), \tag{V.2}$$

with $S_{\mathrm{op}}(F^\beta)$ given by (IV.2) and $S_1(F^\beta) = S_{\mathrm{ac}}(F^\beta) + S_e(F^\beta)$ and $S_{\mathrm{ac}}(F^\beta)$, $S_e(F^\beta)$ given by (IV.2) and (IV.3), respectively. We are again interested in the limit $\beta \to 0$ and again we use a Hilbert expansion:

$$F^\beta = F_0 + \beta F_1 + \cdots, \quad J^\beta = J_0 + \beta J_1 + \cdots .$$

Identifying equal powers of β yields

$$S_{\mathrm{op}}(F_0) = 0, \tag{V.3}$$

$$N(\varepsilon) \frac{\partial F^0}{\partial t} + \nabla_x \cdot J_0 + \nabla_x V \cdot \frac{\partial J_0}{\partial \varepsilon} - S_1(F_0) = D_{F_0} S_{\mathrm{op}}(F_1), \tag{V.4}$$

where $D_{F_0} S_{\mathrm{op}}(F_1)$ denotes the derivative of S_{op} at F_0 applied to F_1. As usual, we first investigate the properties of S_{op} and $D_{F_0} S_{\mathrm{op}}$.

B. Properties of S_{op} and $D_{F_0}S_{op}$

A straightforward computation gives (see also Ref. 10)

$$S_{\mathrm{op}}(F)=N(\varepsilon)\int_{\mathbb{R}}A(x,\varepsilon,\varepsilon')\sigma(\varepsilon,\varepsilon')(a^{-\varepsilon}F'(1-\eta F)-a^{-\varepsilon'}F(1-\eta F'))N(\varepsilon')d\varepsilon', \quad \text{(V.5)}$$

where $a=\exp(1/T_L)$,

$$\sigma(\varepsilon,\varepsilon')=a^{\varepsilon}\delta(\varepsilon'-\varepsilon+1)+a^{\varepsilon'}\delta(\varepsilon'-\varepsilon-1)=\sigma(\varepsilon',\varepsilon), \quad \text{(V.6)}$$

$$\begin{aligned}A(x,\varepsilon,\varepsilon')&=\frac{1}{N(\varepsilon)N(\varepsilon')}\int_{\varepsilon}\int_{\varepsilon'}\tilde{\Phi}_{\mathrm{op}}(x,k,k')dN_{\varepsilon}(k)dN_{\varepsilon'}(k'),\\&=A(x,\varepsilon',\varepsilon)\end{aligned} \quad \text{(V.7)}$$

and $\tilde{\Phi}_{\mathrm{op}}=\Phi_{\mathrm{op}}/(a-1)$. In (V.5), we have rescaled the energies so that the optical phonon energy is equal to 1. The form (V.5) is similar to (II.4). Following Ref. 13 or 10, we have the following.

Proposition V.1: (i) Entropy inequality: Let χ be a nondecreasing function on $\mathbb{R}_+$ and let $H(\varepsilon)$ be defined by $F(1-\eta F)^{-1}=Ha^{-\varepsilon}$. Then

$$\begin{aligned}\int_{\mathbb{R}}S_{\mathrm{op}}(F)\chi(H)d\varepsilon=-\frac{1}{2}\int_{\mathbb{R}}A(x,\varepsilon,\varepsilon')\sigma(\varepsilon,\varepsilon')(1-\eta F)(1-\eta F')a^{-\varepsilon-\varepsilon'}(H-H')\\\times(\chi(H)-\chi(H'))N(\varepsilon)N(\varepsilon')d\varepsilon d\varepsilon'\leq 0.\end{aligned}$$

(ii) We write a.e. $(N(\varepsilon)d\varepsilon)$ for ''almost everywhere with respect to the measure $N(\varepsilon)d\varepsilon$.'' For any function $q(\varepsilon)$, which is a.e. $(N(\varepsilon)d\varepsilon)$ one-periodic in ε, we have:

$$\int_{\mathbb{R}}S_{\mathrm{op}}(F)q(\varepsilon)d\varepsilon=0.$$

(iii) $S_{\mathrm{op}}(F)=0\Leftrightarrow\exists\mu(\varepsilon)$, a.e. $(N(\varepsilon)d\varepsilon)$ one-periodic function of ε such that

$$F(\varepsilon)=:\mathscr{F}_{\mu(\varepsilon),T_L}(\varepsilon)=:\mathscr{F}(\varepsilon,\mu(\varepsilon)),$$

where $\mathscr{F}_{\mu,T}(\varepsilon)$ is the Fermi–Dirac distribution (IV.8).

We now introduce the linearized operator about $\mathscr{F}(\varepsilon,\mu(\varepsilon))$:

$$L_{\mathscr{F}}(f)=\frac{1}{N(\varepsilon)}D_{\mathscr{F}}S_{\mathrm{op}}(f). \quad \text{(V.8)}$$

Following Ref. 10, we write

$$L_{\mathscr{F}}(f)=\int_{\mathbb{R}}A(x,\varepsilon,\varepsilon')\sigma(\varepsilon,\varepsilon')\sigma_{\mathscr{F}}(\varepsilon,\varepsilon')\left(\frac{f'}{\mathscr{G}'}-\frac{f}{\mathscr{G}}\right)N(\varepsilon')d\varepsilon', \quad \text{(V.9)}$$

where $\mathscr{G}=:\mathscr{F}(1-\eta\mathscr{F})$ and

$$\sigma_{\mathscr{F}}(\varepsilon,\varepsilon')=\sigma_{\mathscr{F}}(\varepsilon',\varepsilon)=a^{-\mu(\varepsilon)}\mathscr{F}\mathscr{F}', \quad \text{(V.10)}$$

where (V.10) is meaningful only for $\varepsilon'=\varepsilon\pm1$ and on Supp $(N(\varepsilon)N(\varepsilon'))$ (we denote by Supp the support of a function). Let us now assume that

$$\text{Supp } N(\varepsilon)=[0,\, b] \quad \text{and } \{N=0\}=]-\infty,0]\cup[b,+\infty[\tag{V.11}$$

and introduce the Hilbert space

$$K_{\mathscr{G}}=\left\{F(\varepsilon) \text{ s.t. } F=0 \quad \text{a.e. on } \{N=0\}, \quad \int_{\mathbb{R}}|F(\varepsilon)|^2\,\frac{N(\varepsilon)d\varepsilon}{\mathscr{G}(\varepsilon)}<+\infty\right\}, \tag{V.12}$$

provided with the obvious inner product $(,)_{\mathscr{G}}$ and norm $|\cdot|_{\mathscr{G}}$. We have the following.

Proposition V.2: (i) $-L_{\mathscr{F}}$ is a bounded non-negative self-adjoint operator on $K_{\mathscr{G}}$.

(ii) $\text{Ker } L_{\mathscr{F}}=\{p(\varepsilon)\mathscr{G}(\varepsilon)\in K_{\mathscr{G}},\ p(\varepsilon) \text{ one-periodic}\}$.

(iii) $(-L_{\mathscr{F}}f,f)_{\mathscr{G}}\geqslant \mu|f-Pf|^2_{\mathscr{G}}$, where P is the orthogonal projection on $\text{Ker } L_{\mathscr{F}}$ for $(,)_{\mathscr{G}}$.

(iv)

$$Pf(\varepsilon)=\frac{\Sigma_{i\in\mathbb{Z}}N(\varepsilon+i)f(\varepsilon+i)}{\Sigma_{i\in\mathbb{Z}}N(\varepsilon+i)\mathscr{G}(\varepsilon+i)}\,\mathscr{G}(\varepsilon).$$

(v)

$$R(L_{\mathscr{F}})=(\text{Ker } L_{\mathscr{F}})^{\perp}=\left\{f\in K_{\mathscr{G}} \text{ s.t. } \sum_{i\in\mathbb{Z}} f(\varepsilon+i)N(\varepsilon+i)=0\right\}.$$

Proof: By a straightforward computation, we have

$$\begin{aligned}-\int L_{\mathscr{F}}f(\varepsilon)g(\varepsilon)\,\frac{N(\varepsilon)d\varepsilon}{\mathscr{G}(\varepsilon)}&=(-L_{\mathscr{F}}f,g)_{\mathscr{G}}\\ &=\frac{1}{2}\int_{\mathbb{R}}\int_{\mathbb{R}}A(x,\varepsilon,\varepsilon')\sigma(\varepsilon,\varepsilon')\sigma_{\mathscr{F}}(\varepsilon,\varepsilon')\\ &\quad\times\left(\frac{f'}{\mathscr{G}'}-\frac{f}{\mathscr{G}}\right)\left(\frac{g'}{\mathscr{G}'}-\frac{g}{\mathscr{G}}\right)N(\varepsilon)N(\varepsilon')d\varepsilon d\varepsilon'\end{aligned} \tag{V.13}$$

which shows (i). (ii) follows directly from (V.13): $p(\varepsilon)$ is first an a.e. $(N(\varepsilon)d\varepsilon)$ one-periodic function but can be extended into a one-periodic function on $\mathbb{R}$ by the definition of $K_{\mathscr{G}}$ (V.12). For (iv), it is enough to prove that

$$(\text{Ker } L_{\mathscr{F}})^{\perp}=\left\{f\in K_{\mathscr{G}},\sum_{i\in\mathbb{Z}} f(\varepsilon+i)N(\varepsilon+i)=0\right\}. \tag{V.14}$$

Indeed, for $f\in(\text{Ker } L_{\mathscr{F}})^{\perp}$ and any $p(\varepsilon)\ \mathscr{G}(\varepsilon)\in\text{Ker } L_{\mathscr{F}}$, $p(\varepsilon)$ being one-periodic, we have

$$0=\int_{\mathbb{R}}f(\varepsilon)(p(\varepsilon)\mathscr{G}(\varepsilon))\,\frac{N(\varepsilon)d(\varepsilon)}{\mathscr{G}(\varepsilon)}=\int_0^1\left(\sum_{i\in\mathbb{Z}} f(\varepsilon+i)N(\varepsilon+i)\right)p(\varepsilon)d\varepsilon,$$

which gives (V.14). (v) directly follows from (iii) and (V.14). There remains to prove (iii). For that, we notice that

$$(-L_{\mathscr{F}}f,f)_{\mathscr{G}}=\int_{\mathbb{R}}A(\varepsilon,\varepsilon+1)\mathscr{F}(\varepsilon)\mathscr{F}(\varepsilon+1)a^{\varepsilon-\mu(\varepsilon)+1}\left|\frac{f(\varepsilon+1)}{\mathscr{G}(\varepsilon+1)}-\frac{f(\varepsilon)}{\mathscr{G}(\varepsilon)}\right|^2 N(\varepsilon)N(\varepsilon+1)d\varepsilon. \tag{V.15}$$

Hence

$$(-L_{\mathscr{F}}f,f)_{\mathscr{G}} \geqslant C\int_{\mathbb{R}}\left|\frac{f(\varepsilon+1)}{\mathscr{G}(\varepsilon+1)}-\frac{f(\varepsilon)}{\mathscr{G}(\varepsilon)}\right|^2 N(\varepsilon)N(\varepsilon+1)d\varepsilon.$$

Let $n=\mathrm{Int}(b)+1$, where b is defined by (V.11) and Int (b) is the integer part of the real number b. Then

$$(-L_F f,f)_{\mathscr{G}} \geqslant C\sum_{i=0}^{n-1}\int_0^1\left|\frac{f(\varepsilon+i+1)}{\mathscr{G}(\varepsilon+i+1)}-\frac{f(\varepsilon+i)}{\mathscr{G}(\varepsilon+i)}\right|^2 N(\varepsilon+i)N(\varepsilon+i+1)d\varepsilon. \tag{V.16}$$

Now let f be in $(\mathrm{Ker}\, L_{\mathscr{F}})^{\perp}$. Using the formula

$$\frac{f(\varepsilon+k)}{\mathscr{G}(\varepsilon+k)}-\frac{f(\varepsilon+l)}{\mathscr{G}(\varepsilon+l)}=\begin{cases}\displaystyle\sum_{j=l}^{k-1}\frac{f(\varepsilon+j+1)}{\mathscr{G}(\varepsilon+j+1)}-\frac{f(\varepsilon+j)}{\mathscr{G}(\varepsilon+j)}, & k>l,\\ \displaystyle-\sum_{j=k}^{l-1}\frac{f(\varepsilon+j+1)}{\mathscr{G}(\varepsilon+j+1)}-\frac{f(\varepsilon+j)}{\mathscr{G}(\varepsilon+j)}, & k<l,\end{cases}$$

which we multiply by $N\mathscr{G}(\varepsilon+l)$ and sum over all ''l''s, we find

$$h(\varepsilon)f(\varepsilon+k)=\sum_{l=-\infty}^{k-1}N(\varepsilon+l)\mathscr{G}(\varepsilon+l)\left(\sum_{j=l}^{k-1}\frac{f(\varepsilon+j+1)}{\mathscr{G}(\varepsilon+j+1)}-\frac{f(\varepsilon+j)}{\mathscr{G}(\varepsilon+j)}\right)$$
$$-\sum_{l=k+1}^{+\infty}N(\varepsilon+l)\mathscr{G}(\varepsilon+l)\left(\sum_{j=k}^{l-1}\frac{f(\varepsilon+j+1)}{\mathscr{G}(\varepsilon+j+1)}-\frac{f(\varepsilon+j)}{\mathscr{G}(\varepsilon+j)}\right)$$

where

$$h(\varepsilon)=\sum_{i\in\mathbb{Z}}N(\varepsilon+i)\mathscr{G}(\varepsilon+i).$$

Inverting the indices l and j in the above formula and taking the squares, we find

$$h^2(\varepsilon)|f(\varepsilon+k)|^2\leqslant 2\left|\sum_{j=-\infty}^{k-1}\left(\frac{f(\varepsilon+j+1)}{\mathscr{G}(\varepsilon+j+1)}-\frac{f(\varepsilon+j)}{\mathscr{G}(\varepsilon+j)}\right)\sum_{l=-\infty}^{j}N\mathscr{G}(\varepsilon+l)\right|^2$$
$$+2\left|\sum_{j=k}^{+\infty}\left(\frac{f(\varepsilon+j+1)}{\mathscr{G}(\varepsilon+j+1)}-\frac{f(\varepsilon+j)}{\mathscr{G}(\varepsilon+j)}\right)\left(\sum_{l=j+1}^{+\infty}N\mathscr{G}(\varepsilon+l)\right)\right|^2.$$

Now let $\varepsilon\in[0\ \ 1]$ and let us estimate

$$\sum_{k\in\mathbb{Z}}|f(\varepsilon+k)|^2N(\varepsilon+k)=\sum_{k=0}^{n-1}|f(\varepsilon+k)|^2N(\varepsilon+k).$$

Using the fact that $h(\varepsilon)\geqslant C>0$ and that the sums are over a finite number of indices, we deduce from the Cauchy–Schwartz inequality that

$$\sum_{k=0}^{n-1}N(\varepsilon+k)|f(\varepsilon+k)|^2\leqslant C\sum_{k=0}^{n-1}N(\varepsilon+k)\sum_{j=0}^{k-1}\left|\frac{f(\varepsilon+j+1)}{\mathscr{G}(\varepsilon+j+1)}-\frac{f(\varepsilon+j)}{\mathscr{G}(\varepsilon+j)}\right|^2\left|\sum_{l=0}^{j}N\mathscr{G}(\varepsilon+l)\right|^2$$
$$+C\sum_{k=0}^{n-1}N(\varepsilon+k)\sum_{j=k}^{n-2}\left|\frac{f(\varepsilon+j+1)}{\mathscr{G}(\varepsilon+j+1)}-\frac{f(\varepsilon+j)}{\mathscr{G}(\varepsilon+j)}\right|^2\left|\sum_{l=j+1}^{n-1}N\mathscr{G}(\varepsilon+l)\right|^2.$$

Now grouping the terms

$$\left|\frac{f(\varepsilon+j+1)}{\mathcal{G}(\varepsilon+j+1)}-\frac{f(\varepsilon+j)}{\mathcal{G}(\varepsilon+j)}\right|^2$$

corresponding to the same index j and taking a special care of terms with $j=0$ and $j=n-2$, we have

$$\begin{aligned}\sum_{k=0}^{N-1} N(\varepsilon+k)|f(\varepsilon+k)|^2 \leqslant & CN(\varepsilon)\left|\frac{f(\varepsilon+1)}{\mathcal{G}(\varepsilon+1)}-\frac{f(\varepsilon)}{\mathcal{G}(\varepsilon)}\right|^2 \\ & + CN(\varepsilon+n-1)\left|\frac{f(\varepsilon+n-1)}{\mathcal{G}(\varepsilon+n-1)}-\frac{f(\varepsilon+n-2)}{\mathcal{G}(\varepsilon+n-2)}\right|^2 \\ & + C\sum_{i=1}^{n-3}\left|\frac{f(\varepsilon+i+1)}{\mathcal{G}(\varepsilon+i+1)}-\frac{f(\varepsilon+i)}{\mathcal{G}(\varepsilon+i)}\right|^2.\end{aligned}$$

To get the above estimate, we used extensively the property $N \leqslant C$.

Using now the fact that $N(\varepsilon) \geqslant C$ on $[1, n-2]$ [see (V.11)], we finally obtain

$$\forall \varepsilon \in [0,1], \quad \sum_k N(\varepsilon+k)|f(\varepsilon+k)|^2 \leqslant C\sum_k N(\varepsilon+k)N(\varepsilon+k+1)\left|\frac{f}{\mathcal{G}}(\varepsilon+k+1)-\frac{f}{\mathcal{G}}(\varepsilon+k)\right|^2. \tag{V.17}$$

We then deduce from (V.16) that

$$\forall f \in \operatorname{Ker} L_{\mathcal{F}}^{\perp}, \quad (-L_{\mathcal{G}} f\cdot f)_{\mathcal{G}} \geqslant C\sum_k \int_0^1 N(\varepsilon+k)|f(\varepsilon+k)|^2\, d\varepsilon \geqslant C\int_{\mathbb{R}} N(\varepsilon)\left|\frac{f(\varepsilon)}{\mathcal{G}(\varepsilon)}\right|^2 d\varepsilon.$$

This ends the proof. ■

C. Resolution of the Hilbert Expansion (5.3) and (5.4)

From Proposition V.1 (iii), Eq. (V.3) implies that there exists $\mu(x,\varepsilon,t)$, a.e., $(N(\varepsilon)d\varepsilon)$ one-periodic in ε, such that

$$F_0(x,\varepsilon,t)=\mathcal{F}(\varepsilon,\mu(x,\varepsilon,t))\cdot \text{a.e.}(N(\varepsilon)d\varepsilon). \tag{V.18}$$

Then, $J_0(x,\varepsilon,t)$ is given by (V.2) with $\beta=0$, which yields

$$J_0(x,\varepsilon,t)=-D(x,\varepsilon)\mathcal{F}(1-\eta\mathcal{F})\left\{\left(\nabla_x\left(\frac{\mu}{T_L}\right)-\frac{\nabla_x V}{T_L}+\frac{\nabla_x V}{T_L}\frac{\partial\mu}{\partial\varepsilon}\right)-\varepsilon\nabla\left(\frac{1}{T_L}\right)\right\}. \tag{V.19}$$

The resolution of (V.4) leads to the following.

Theorem V.3: Let F_0 be given by (V.18). The solution of Eq. (V.4) exists if and only if $\mu(x,\varepsilon,t)$ satisfies the following system (with periodic boundary conditions on $\varepsilon\in[0,1]$):

$$\frac{\partial}{\partial t}\,\nu(\varepsilon,\mu(x,\varepsilon,t))+\nabla_x\cdot j+\nabla_x V\cdot\frac{\partial j}{\partial\varepsilon}=T_1(\mu), \tag{V.20}$$

$$j(x,\varepsilon,t)=-\left[\Delta_1(x,\varepsilon,\mu(x,\varepsilon,t))\left\{\nabla_x\left(\frac{\mu}{T_L}\right)-\frac{\nabla_x V}{T_L}+\frac{\nabla_x V}{T_L}\frac{\partial\mu}{\partial\varepsilon}\right\}+\Delta_2(x,\varepsilon,\mu(x,\varepsilon,t))\,\frac{\nabla T_L}{T_L^2}\right], \tag{V.21}$$

where for $\varepsilon\in[0,1]$, $\mu\in\mathbb{R}$, we set

$$\nu(\varepsilon,\mu)=\sum_{i\in\mathbb{Z}} N(\varepsilon+i)\mathscr{F}(\varepsilon+i,\mu), \tag{V.22}$$

$$\begin{aligned}\Delta_1(x,\varepsilon,\mu)&=\sum_{i\in\mathbb{Z}} D(x,\varepsilon+i)\mathscr{F}(\varepsilon+i,\mu)(1+\eta\mathscr{F}(\varepsilon+i,\mu)),\\ \Delta_2(x,\varepsilon,\mu)&=\sum_{i\in\mathbb{Z}} D(x,\varepsilon+i)(\varepsilon+i)\mathscr{F}(\varepsilon+i,\mu)(1+\eta\mathscr{F}(\varepsilon+i,\mu)),\end{aligned} \tag{V.23}$$

and for a one-periodic function $\mu(\varepsilon)$,

$$T_1(\mu)(\varepsilon)=\sum_{i\in\mathbb{Z}} S_1(\mathscr{F}(\varepsilon,\mu(\varepsilon)))(\varepsilon+i). \tag{V.24}$$

Proof: From Proposition V.2 (v), the condition for Eq. (V.4) to be solvable in F_1 is

$$\begin{aligned}&\sum_{i\in\mathbb{Z}}\left\{N(\varepsilon+i)\,\frac{\partial}{\partial t}\,\mathscr{F}(\varepsilon+i,\mu(x,\varepsilon,t))+\nabla_x\cdot J_0(x,\varepsilon+i,t)+\nabla_x V\cdot\frac{\partial J_0}{\partial\varepsilon}\,(x,\varepsilon+i,t)\right\}\\ &\quad=\sum_{i\in\mathbb{Z}} S_1(\mathscr{F}(\cdot,\mu(x,\cdot,t)))(\varepsilon+i),\end{aligned}$$

which obviously yields (V.20) and (V.21). ■

In (V.21), only Δ_1 acts as a diffusion coefficient. From proposition III.6, we have the following.

Proposition V.4: $\Delta_1(x,\varepsilon,\mu)$ is a symmetric non-negative 3×3 matrix. Moreover, $\exists C>0$ such that

$$\Delta_1(x,\varepsilon,\mu)\geqslant C\sum_{i\in\mathbb{Z}}\ \frac{1}{N(\varepsilon+i)}\left(\int_{\varepsilon+i}(\nabla_k\varepsilon\otimes\nabla_k\varepsilon)\,dN_{\varepsilon+i}(k)\right)\mathscr{F}(\varepsilon+i,\mu)(1-\eta\mathscr{F}(\varepsilon+i,\mu)). \tag{V.25}$$

In particular, if Q_0 is given by a relaxation time operator (III.28), the following expression of Δ_1 follows from (III.30):

$$\Delta_1(x,\varepsilon,\mu)=\sum_{i\in\mathbb{Z}}\tau(x,\varepsilon+i)\left(\int_{\varepsilon+i}(\nabla_k\varepsilon\otimes\nabla_k\varepsilon)\,dN_{\varepsilon+i}(k)\right)\mathscr{F}(\varepsilon+i,\mu)(1-\eta\mathscr{F}(\varepsilon+i,\mu)). \tag{V.26}$$

When $\Phi_0=\Phi_0(x)$ is independent of k, k', for a parabolic band structure $|k|^2=2m_*\varepsilon$ and a nondegenerate statistics $\mathscr{F}(1-\eta\mathscr{F})\to\exp-((\varepsilon-\mu)/T_L)$, we find from (III.37)

$$\begin{aligned}\Delta_1(x,\varepsilon,\mu)&=\frac{2}{3\Phi_0(x)m_*}\sum_{i\in\mathbb{N}}(\varepsilon+i)\exp\left(-\frac{(\varepsilon+i)-\mu}{T_L}\right)\\ &=\frac{2}{3\Phi_0(x)m_*}\,\frac{\varepsilon+e^{-1/T_L}(1-\varepsilon)}{(1+e^{-1/T_L})^2}\exp\left(-\frac{\varepsilon-\mu}{T_L}\right).\end{aligned} \tag{V.27}$$

D. The third macroscopic scale: The drift–diffusion model

Looking at a longer time scale, the effect of both acoustical phonon collisions and electron–electron collisions will be to relax the periodic function $\mu(x,\varepsilon,t)$ to a constant. We expect the conventional drift-diffusion model to be valid in this regime. After rescaling, system (V.20) and (V.21) is written

$$\frac{\partial}{\partial t}\,\nu(\varepsilon,\mu^{\delta}(x,\varepsilon,t))+\nabla_x\cdot j^{\delta}+\nabla_x V\cdot\frac{\partial j^{\delta}}{\partial\varepsilon}=\frac{1}{\delta}\,T_1(\mu^{\delta}), \tag{V.28}$$

$$j^{\delta}(x,\varepsilon,t)=-\left[\Delta_1(x,\varepsilon,\mu^{\delta}(x,\varepsilon,t))\left(\nabla_x\left(\frac{\mu^{\delta}}{T_L}\right)-\frac{\nabla_x V}{T_L}+\frac{\nabla_x V}{T_L}\,\frac{\partial\mu^{\delta}}{\partial\varepsilon}\right)+\Delta_2(x,\varepsilon,\mu^{\delta}(x,\varepsilon,t))\,\frac{\nabla T_L}{T_L^2}\right], \tag{V.29}$$

where $T_1(\mu^{\delta})=T_e(\mu^{\delta})+T_{\mathrm{ac}}(\mu^{\delta})$ and

$$T_e(\mu)(\varepsilon)=\sum_{i\in\mathbb{Z}} S_e(\mathscr{F}(\varepsilon,\mu(\varepsilon)))(\varepsilon+i),$$

$$T_{\mathrm{ac}}(\mu)(\varepsilon)=\sum_{i\in\mathbb{Z}} S_{\mathrm{ac}}(\mathscr{F}(\varepsilon,\mu(\varepsilon)))(\varepsilon+i),$$

and S_e and S_{ac} are given by (IV.2) and (IV.3).

For any one-periodic function $\psi(\varepsilon)$, we have, by straightforward computation,

$$\int_0^1 T_e(\mu)(\varepsilon)\psi(\varepsilon)d\varepsilon=-\frac{1}{4}\int_{B^4}\Phi_e\delta_\varepsilon\delta_k\pi(1-\eta\mathscr{F})a^{-(\varepsilon+\varepsilon_1)}(\psi'+\psi_1'-\psi-\psi_1)$$
$$\times(a^{(\mu(\varepsilon')+\mu(\varepsilon_1'))}-a^{(\mu(\varepsilon)+\mu(\varepsilon_1))})d^4k, \tag{V.30}$$

with the notations of the proof of Proposition IV.1,

$$a=e^{1/T_L},\quad \pi(1-\eta\mathscr{F})=(1-\eta\mathscr{F})(1-\eta\mathscr{F}_1)(1-\eta\mathscr{F}')(1-\eta\mathscr{F}_1'),$$

and

$$\int_0^1 T_{\mathrm{ac}}(\mu)(\varepsilon)\psi(\varepsilon)d\varepsilon=-\frac{1}{2}\int_{B^2}\frac{\Phi_{\mathrm{ac}}(x,k,k')}{a^{\varepsilon_{\mathrm{ac}}(k-k')}-1}\,\sigma_{\mathrm{ac}}(\varepsilon,\varepsilon')(1-\eta\mathscr{F})(1-\eta\mathscr{F}')$$
$$\times a^{-(\varepsilon+\varepsilon')}(\psi'-\psi)(a^{\mu(\varepsilon')}-a^{\mu(\varepsilon)})dk\,dk', \tag{V.31}$$

with Φ_{ac} and $\varepsilon_{\mathrm{ac}}$ defined in Sec. II and

$$\sigma_{\mathrm{ac}}(\varepsilon,\varepsilon')=a^{\varepsilon}\delta(\varepsilon'-\varepsilon+\varepsilon_{\mathrm{ac}}(k-k'))+a^{\varepsilon'}\delta(\varepsilon'-\varepsilon-\varepsilon_{\mathrm{ac}}(k-k'))=\sigma_{\mathrm{ac}}(\varepsilon',\varepsilon).$$

We deduce the following.

Proposition V.5:

(i) Entropy inequality:

$$\int_0^1 T_e(\mu)(\varepsilon)\mu(\varepsilon)d\varepsilon\leqslant 0,\quad \int_0^1 T_{\mathrm{ac}}(\mu)(\varepsilon)\mu(\varepsilon)d\varepsilon\leqslant 0.$$

(ii) $\int_0^1 T_e(\mu)(\varepsilon)d\varepsilon=0$, $\int_0^1 T_{\mathrm{ac}}(\mu)(\varepsilon)d\varepsilon=0$.

(iii) $T_e(\mu)+T_{\rm ac}(\mu)=0\Rightarrow\mu$ is constant.

Proof: Only the point (iii) needs to be commented on. By (i) this implies that $T_e(\mu)=0$ and thus that $\mu(\varepsilon)$ is an affine function (by the proof of proposition 4.4 of Ref. 16). However, it also needs to be one-periodic in ε, which implies that $\mu(\varepsilon)$ is constant. ■

Let now $\mu\in\mathbb{R}$ be a constant and define $\mathscr{T}_1=\mathscr{T}_{\rm ac}+\mathscr{T}_e$. With $\mathscr{T}_{\rm ac}=D_\mu T_{\rm ac}$, $\mathscr{T}_e=D_\mu T_e$ are the derivatives of $T_{\rm ac}$ and T_e about the constant function μ. By differentiating relations (V.30) and (V.31), we obtain for any ν, $\psi\in L^2(0,1)$

$$\int_0^1(\mathscr{T}_e\nu)(\varepsilon)\psi(\varepsilon)d\varepsilon=-\frac{1}{4}\int_{B^4}\Phi_e\delta_\varepsilon\delta_{\rm ac}\pi(1-\eta\mathscr{F})a^{-(\varepsilon+\varepsilon_1)}a^{2\mu}\ln a(\psi'+\psi_1'-\psi-\psi_1)\times(\nu'+\nu_1-\nu-\nu_1)d^4k \tag{V.32}$$

and

$$\int_0^1(\mathscr{T}_{\rm ac}\nu)(\varepsilon)\psi(\varepsilon)d\varepsilon=-\frac{1}{2}\int_{B^2}\tilde{\Phi}_{\rm ac}\sigma_{\rm ac}(1-\eta\mathscr{F})(1-\eta\mathscr{F}')a^{-(\varepsilon+\varepsilon')}a^{\mu}\ln a(\psi'-\psi)\times(\nu'-\nu)dk\,dk'. \tag{V.33}$$

The following proposition is a direct consequence of (V.32) and (V.33):

Proposition V.6:

(i) $\mathscr{T}_1$ is a bounded non-negative self-adjoint operator on $L^2(0,1)$.
(ii) $\mathrm{Ker}\,\mathscr{T}_1$ is spanned by the constant functions on $[0,1]$.
(iii) $-(\mathscr{T}_1\nu,\nu)_{L^2(0,1)}\geqslant C|\nu-\langle\nu\rangle|^2$, where $\langle\nu\rangle$ is the L^2 mean value.
(iv) $R(\mathscr{T}_1)=(\mathrm{Ker}\,\mathscr{T}_1)^\perp=\{\nu\in L(0,1)^2/\langle\nu\rangle=0\}$.

Proof: The only nonimmediate point is (iii) and it directly follows from Proposition IV.2 (iii). ■

The Hilbert expansion of μ^δ yields

$$\mu^\delta=\mu_0+\delta\mu_1+\cdots,\quad j^\delta=j_0+\delta j_1+\cdots,$$

and by identifying equal powers of δ, we obtain

$$T_1(\mu_0)=0, \tag{V.34}$$

$$\frac{\partial}{\partial t}\nu(\varepsilon,\mu_0(x,\varepsilon,t))+\nabla_x\cdot j_0+\nabla_x V\cdot\frac{\partial j_0}{\partial\varepsilon}=D_{\mu_0}T_1(\mu_1). \tag{V.35}$$

By Proposition V.5 (iii), (V.34) implies that $\mu_0=\mu_0(x,t)$ is independent of ε. Then by (V.29), we deduce

$$j_0(x,\varepsilon,t)=-\left[\Delta_1(x,\varepsilon,\mu_0(x,t))\left(\nabla_x\left(\frac{\mu_0}{T_L}\right)-\frac{\nabla_x V}{T_L}\right)+\Delta_2(x,\varepsilon,\mu_0(x,t))\frac{\nabla T_L}{T_L^2}\right]. \tag{V.36}$$

Proposition V.6 gives the condition for Eq. (V.35) to be solvable in μ_1 and yields the following.

Theorem V.7: Let $\mu_0(x,t)$ be independent of ε. There exists a solution μ_1 of Eq. (V.35) if and only if μ_0 satisfies the system

$$\frac{\partial}{\partial t}n(\mu_0,T_L)+\nabla_x\cdot I_0=0, \tag{V.37}$$

$$I_0 = -\left[\mathscr{D}_{11}(x,\mu_0,T_L)\left(\nabla_x\left(\frac{\mu_0}{T_L}\right) - \frac{\nabla_x V}{T_L}\right) + \mathscr{D}_{12}(x,\mu_0,T_L)\ \frac{\nabla T_L}{T_L^2}\right], \tag{V.38}$$

where $n(\mu,T)$ is defined by (IV.16) and the coefficients $\mathscr{D}_{1j}(x,\mu,T)$ are given by (IV.17).

Proof: By Proposition V.6 (iv), there exists a solution μ_1 of (V.35) if and only if

$$\int_0^1 \left(\frac{\partial}{\partial t}\ \nu(\varepsilon,\mu_0)(x,t)\right) + \nabla_x \cdot j_0 + \nabla_x V \cdot\ \frac{\partial J_0}{\partial \varepsilon} d\varepsilon = 0.$$

There remains to combine the integration on $[0,1]$ with the summation over $i \in \mathbb{Z}$ in formulas (V.22) and (V.24) to recover the formulae (IV.16) and (IV.17) and to obtain the result. ■

Remark V.8: Starting from the ''spherical'' harmonic expansion model, it is equivalent to recover the usual drift-diffusion model, either via the energy-transport model or via the ''periodized spherical'' harmonic expansion model: the expression of the diffusion coefficients is the same (compare Theorem V.7 with Theorem IV.9). ■

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Energy extremes and spin configurations for the one-dimensional antiferromagnetic Ising model with arbitrary-range interaction

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The one-dimensional antiferromagnetic spin-$\frac{1}{2}$ Ising model is investigated using the formalism of Maximally/Minimally Even sets. The salient features of Maximally/Minimally Even set theory are introduced. Energy and spin content vectors are defined to facilitate the use of interval spectra used in Maximally/Minimally Even set theory. It is shown that Maximally Even sets of up- and down-spins minimize the configurational energy per spin and that Minimally Even sets maximize configurational energy per spin. An exponentially decreasing antiferromagnetic pairwise interaction of arbitrary range is used as an example interaction. The asymptotic ($N\rightarrow\infty$) configurational energy per spin and the energy per spin calculated for seven-near neighbors are compared. © *1996 American Institute of Physics.* [S0022-2488(96)00107-7]

I. INTRODUCTION

The simplest description of the pairwise interaction of spins on a lattice is given by the Ising model which yields the following for the configurational energy of a lattice of spin-$\frac{1}{2}$ ''particles:''

$$\mathscr{H}=-4\sum_{\substack{i,j=0\\ i\neq j}}^{N-1}\mathscr{J}(|i-j|)s_{iz}s_{jz},$$

where N is the total number of lattice sites, and the sum is taken over all pairs of lattice sites. The function $\mathscr{J}(|i-j|)$ is the pairwise interaction energy, the absolute value of which decreases with distance. The s_z are the z-components of the spins which may take on the values of $\pm\frac{1}{2}$. (For a discussion of lattice gas models, see the excellent reference by Simon.[1])

In a one-dimensional system, it is convenient to invoke periodic boundary conditions which requires that $s_{0z}=s_{Nz}$. Therefore, a one-dimensional spin-$\frac{1}{2}$ lattice can be thought of as a cycle of lattice sites, some of which are occupied by up-spins ($+\frac{1}{2}$) and others by down-spins ($-\frac{1}{2}$). A simplification may be made by defining $\sigma_p=2s_{pz}$. Then, the configurational energy may be written as

$$\mathscr{H}=-\sum_{\substack{i,j=0\\ i\neq j}}^{N-1}\mathscr{J}(|i-j|)\sigma_i\sigma_j,$$

where the σ take on the values of ±1. By considering antiferromagnetic pairwise interactions only (i.e., $\mathscr{J}(|i-j|)<0$), a further simplification results, and the configurational energy is given by

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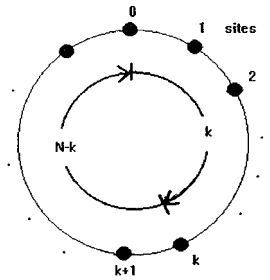

FIG. 1. Clockwise distances between pairs of lattice sites.

$$\mathscr{H}_{\text{anti}}=\sum_{\substack{i,j=0\\ i\neq j}}^{N-1} J(|i-j|)\sigma_i\sigma_j\,,$$

where $J(|i-j|)=|\mathscr{J}(|i-j|)|$.

For a given down-spin density (ratio of the number of down-spin sites to the total number of sites), the average configurational energy (energy per site) depends on the distribution of the up- and down-spin sites. Since there is a large number of sites, for a given down-spin density, there are many possible values for the average configurational energy. We will focus on the average energy extremes of this cyclic one-dimensional system by exploiting the formalism of Maximally Even and Minimally Even sets as described by Clough and Douthett[2] and Block and Douthett.[3]

Curiously, many of the tools employed in this paper have been developed in the music theory literature. Content vectors are routinely used in the analysis of twentieth-century music as well as in compositional design, and Lewin[4] was the first to explore the properties of these vectors in microtonal systems (systems that have other than 12 divisions to the octave). Block and Douthett[3] developed weighting vectors to be used in conjunction with content vectors to find pitch-class sets (collections of tones) whose members have particular pairwise intervallic relationships. In doing so, they developed a measure that compares the evenness between any two pitch-class sets of the same size. Clough and Myerson[5,6] developed interval spectra to explore combinatorial properties of diatonic scales (e.g., the white keys on the piano) and to extend these properties into microtonal systems. Clough and Douthett[2] expanded on this work and developed the theory of Maximally Even Sets. These sets, along with their iterations, model scale and chord structures in both the usual musical system (12 divisions to the octave) and microtonal systems.

II. ENERGY, CONTENT, AND SPIN CONTENT VECTORS

The method discussed in this section and the next in which the dot product of an energy vector and a content vector is used to determine the configurational energy of a particular lattice configuration is based on related work done by Block and Douthett.[3] To apply their method to the problem at hand, let N be the number of sites in the lattice, N_- be the number of these sites occupied by down-spins, and N_+ be the number occupied by up-spins. Assuming periodic boundary conditions, for each pair of sites, there are two *clockwise distances* (with respect to the number of sites that separate them) associated with this pair (Fig. 1). If the consecutive sites in the lattice are represented by the consecutive integers 0 through $N-1$, the two distances associated with site 0 and site k are k and $N-k$. Now assume J is a strictly convex function on the interval $(0,\infty)$. [Later the discussion will be restricted to pairwise interactions for which $\Sigma_{k=1}^{\infty}J(k)$ converges.] Then the absolute value of the energy contributed by a pair of sites at a distance k is

$$J_N(k)=J(k)+J(N-k).$$

Thus, if E_- is the sum of the J_N-functions over all down-spin pairs, E_+ is the sum of the J_N-functions over all the up-spin pairs, and E_0 is the sum over all the pairs with opposite orientations, the total energy of the lattice is

$$E = E_+ + E_- - E_0 .$$

It is convenient to construct vectors that allow computation of this energy via dot products. The first vector, the *energy vector*, is defined as follows:

$$W = (J_N(1), J_N(2), \ldots, J_N(\lfloor N/2 \rfloor)).$$

To construct the content vectors, consider the following example:

Suppose $N = 7$ and $N_- = 3$. (Hence, $N_+ = 4$.) Consider the distribution in Fig. 2(b) on the complete labeled graph K_7. Then the set of down-spins is $S_- = \{0,2,3\}$ and the set of up-spins is $S_+ = \{1,4,5,6\}$. Now consider the complete labeled subgraphs K_- [Fig. 2(a)] and K_+ [Fig. 2(c)]. The edges of these graphs are weighted as follows: Suppose an edge e has incident vertices whose labels are a and b. Then the weight of this edge is

$$w(e) = \min\{|a-b|, 7-|a-b|\}.$$

The *content vectors* of these graphs are three-tuples that have as their kth entries the number of edges that have weight k. Then the content vectors for K_-, K_7, and K_+ are $V_- = (1,1,1)$, $V_7 = (7,7,7)$, and $V_+ = (2,2,2)$, respectively.

It is possible to compute V_+ without its graph. Lewin[4] has shown

$$V_+ - V_- = (n,n,n),$$

where $n = N_+ - N_- = N - 2N_-$. In this case, $n = 7 - 2 \cdot 3 = 1$. Thus,

$$V_+ = (1,1,1) + V_- = (2,2,2).$$

This characterization will be useful when these results are generalized.

Now, consider the complement of $K_- \cup K_+$,

$$K_{-,+} = (K_- \cup K_+)^c$$

whose graph is illustrated in Fig. 2(d). This graph is a complete bipartite, and the edges in this graph are precisely those that are incident to one up-spin site and one down-spin site. By definition, the edge sets of K_-, K_+, and $K_{-,+}$ partition the edge set of K_7. The content vector V_0 of $K_{-,+}$ is computed as follows:

$$V_7 = V_- + V_+ + V_0, \quad V_0 = V_7 - V_- - V_+ = (4,4,4).$$

Note that this corresponds to the calculation by inspection of $K_{-,+}$ in Fig. 2(d). Finally the *spin content vector* is defined as

$$V = V_+ + V_- - V_0 = (1,1,1).$$

The above example may be extended to the general case. The lattice may be modelled with the complete labeled graph K_N whose labels range from 0 through $N-1$. Then the edge weight of an edge e whose incident vertices have labels a and b is

$$w(e) = \min\{|a-b|, N-|a-b|\}.$$

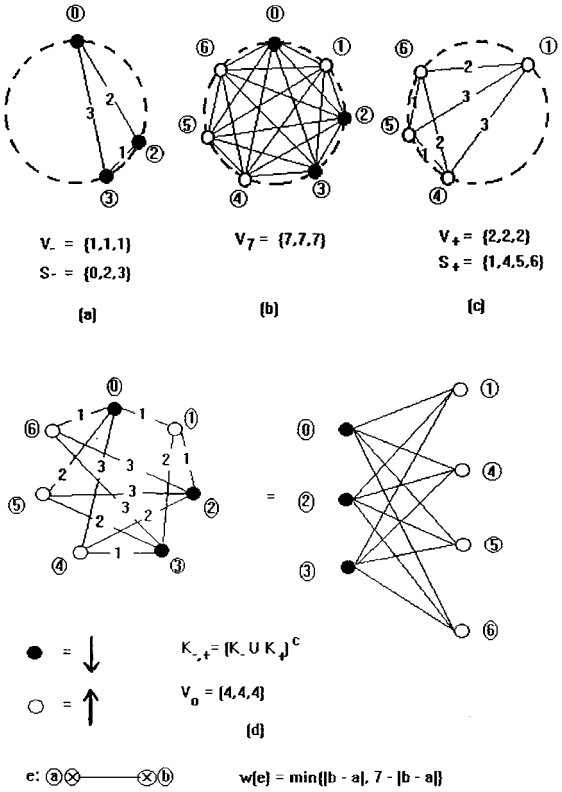

FIG. 2. Graphs and content vectors.

The notation $(\cdots n\cdots)$ indicates $a\lfloor N/2\rfloor$-tuple in which every entry is n. For convenience, assume N is odd. Then the content vector for K_N is $V_N=(\cdots N\cdots)$. [Note that if N is even, the last entry of this vector must be divided by 2. It is left to the reader to verify that the assumption that N is even will produce the same results as $N\to\infty$.]

Now let S_- and S_+ be the sets of labels of down-spins and up-spins, respectively. Then the complete labeled subgraphs K_- and K_+ on these sets and their corresponding content vectors V_- and V_+ are constructed in the same way as those in the above example. Because of symmetry, it can be assumed without loss of generality that $N_-<N/2$. Furthermore, since $N_-<N_+$, it can be shown that $V_+-V_-=(\cdots N-2N_-\cdots)$.[4] Thus,

$$V_+=(\cdots N-2N_-\cdots)+V_-. \tag{1}$$

Define the graph $K_{-,+}=(K_-\cup K_+)^c$ to be the complete bipartite graph with partitions S_- and S_+, and let its content vector be V_0. Then, since $V_N=(\cdots N\cdots)$, and the edge sets of K_-, K_+, and $K_{-,+}$ partition the edge set of K_N, (1) implies

$$V_-+V_++V_0=(\cdots N\cdots),\quad V_0=2(\cdots N_-\cdots)-2V_-. \tag{2}$$

Then, by (1) and (2),

$$V=V_++V_--V_0=4V_-+(\cdots N-4N_-\cdots).$$

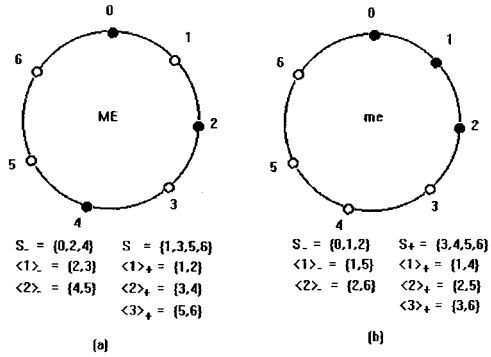

FIG. 3. ME and me distributions.

This means that the spin content vector of any configuration can be completely determined by the set of down-spin labels. The total energy can be found by taking the dot product of the spin content vector and the energy vector:

$$E=E_+ + E_- - E_0 = V_+ \cdot W + V_- \cdot W - V_0 \cdot W = (V_+ + V_- - V_0)\cdot W = V \cdot W.$$

In the previous example, $V_- = (1,1,1)$. Thus,

$$V = 4(1,1,1) + (\cdots 7 - 4(3) \cdots) = -(1,1,1).$$

So the total energy of the lattice is

$$E = V \cdot W = -(1,1,1)\cdot (J_7(1), J_7(2), J_7(3)) = -J_7(1) - J_7(2) - J_7(3).$$

III. MAXIMALLY AND MINIMALLY EVEN DISTRIBUTIONS

Consider the configurations in Fig. 3. The total energy for the configuration in Fig. 3(a) is $E=-5J_7(1)+3J_7(2)-J_7(3)$ and in Fig. 3(b), $E=3J_7(1)-J_7(2)-5J_7(3)$. For a given convex interaction J, the configuration in Fig. 3(a) will yield the least energy and in Fig. 3(b), the greatest. If J is strictly convex, the only other configurations yielding these energy extremes are rotations of the above. We now turn our attention to the unique properties of the classes of these configurations.

The *interval spectrum of near-neighbor down-spins (up-spins)* is defined to be the set of distinct clockwise distances between each pair of consecutive down-spins (up-spins). This set is denoted by $\langle 1\rangle_-(\langle 1\rangle_+)$. Thus, for the sets in Fig. 2, $\langle 1\rangle_- = \{1,2,4\}$ and $\langle 1\rangle_+ = \{1,2,3\}$; in Fig. 3(a), $\langle 1\rangle_- = \{2,3\}$ and $\langle 1\rangle_+ = \{1,2\}$; and in Fig. 3(b), $\langle 1\rangle_- = \{1,5\}$ and $\langle 1\rangle_+ = \{1,4\}$. This concept may be extended to sets of clockwise distances between pairs of next-neighbor down-spins (up-spins) [pairs that have precisely one down-spin (up-spin) site between them]. Then for the sets in Fig. 2, $\langle 2\rangle_- = \{3,5,6\}$ and $\langle 2\rangle_+ = \{2,3,4,5\}$; in Fig. 3(a), $\langle 2\rangle_- = \{4,5\}$ and $\langle 2\rangle_+ = \{3,4\}$; and in Fig. 3(b), $\langle 2\rangle_- = \{2,6\}$ and $\langle 2\rangle_+ = \{2,5\}$. In general, the *spectrum of* k, written $\langle k\rangle_\pm$, is the set of distinct clockwise distances between pairs of down-spins (up-spins) that have precisely $k-1$ down-spins (up-spins) between them. A pair of down-spins (up-spins) is *associated with* k if the pair has the above property. These spectra are defined for $1 \leqslant k \leqslant N_\pm - 1$, and they were originally defined by Clough and Myerson.[5,6] If the clockwise distances of all the pairs of sites of like spins associated with k are added together, their sum is Nk (Clough and Myerson[5,6] and Hubbard[7]). For example, in Fig. 3(a) where $\langle 2\rangle_+ = \{3,4\}$, there are two intervals of length 3 and two of length 4 associated with $k=2$. This corresponds to the equality $2\cdot 3 + 2\cdot 4 = 7\cdot 2$. Similarly, for $\langle 3\rangle_+ = \{5,6\}$, there are

three intervals of length 5 and one of length 6 associated with $k=3$, and $3\cdot5+1\cdot6=7\cdot3$. In general, if $l\in\langle k\rangle_{\pm}$ and $r_{k,l}$ is the number of down-spin (up-spin) pairs associated with k that have a clockwise distance of l, then

$$\sum_{l\in\langle k\rangle_{\pm}} r_{k,l}l=Nk.$$

Hubbard[7] observed that, for a given down-spin density, the minimum average energy occurs when each spectrum consists of one or two consecutive integers. Clough and Douthett[2] showed that, for such configurations,

$$\langle k\rangle_{\pm}=\left\{\left\lfloor\frac{Nk}{N_{\pm}}\right\rfloor,\left\lceil\frac{Nk}{N_{\pm}}\right\rceil\right\},$$

where $1\leqslant k\leqslant N_{\pm}-1$. In addition, they generated the classes of all configurations that have this property with their *maximally even (ME) algorithm*:[2]

> Let i be a fixed integer such that $0\leqslant i\leqslant N-1$, and assign down-spins (up-spins) to sites $\lfloor(Nk+i)/N_{\pm}\rfloor$ where $k=0,1,\ldots,N_{\pm}-1$. Assign up-spins (down-spins) to the remaining sites. Then each down- and up-spin spectrum consists of one or two consecutive integers. Conversely, if each down-spin (up-spin) spectrum consists of one or two consecutive integers, then there exists an i, $0\leqslant i\leqslant N-1$, such that the down-spins (up-spins) occupy the sites $\lfloor(Nk+i)/N_{\pm}\rfloor$, $k=0,1,\ldots,N_{\pm}-1$, and the up-spins (down-spins) occupy the rest.

[A slightly more restrictive form of this algorithm is discussed by Clough and Myerson[5,6] and Bak.[8]] A set of down-spins (up-spins) in which each spectrum consists of one or two consecutive integers is called a *ME set*. Clough and Douthett[2] showed that, for a given N and $N_{\pm}$, ME sets are equivalent under rotation and that the complement of a ME set is also a ME set. When S_{-} and S_{+} are ME sets, then the configuration is a *ME configuration.*

Minimally Even (me) Sets were first suggested by Block and Douthett.[3] A configuration is a *me configuration* when all the sites with like spin are clustered together, and the sets of down-spins and up-spins are called *me sets* as illustrated in Fig. 3(b). It is clear that the complement of a me set is me, and when $S_{\pm}$ is a me set then

$$\langle k\rangle_{\pm}=\{k,N-N_{\pm}+k\}$$

for all k, $1\leqslant k\leqslant N_{\pm}-1$. Moreover, for any configuration, ME, me, or otherwise, if $l\in\langle k\rangle_{\pm}$, then

$$k\leqslant l\leqslant N-N_{\pm}+k.$$

Note that the energy contributed to the lattice by the down-spins (up-spins) may be computed in the following way:

(1) For each k and each $l\in\langle k\rangle_{\pm}$, determine $r_{k,l}$.
(2) For each $l\in\langle k\rangle_{\pm}$, compute $r_{k,l}J(l)$.
(3) For each k, sum the products in (2) over $l\in\langle k\rangle_{\pm}$.
(4) Sum the results in (3) over k, $1\leqslant k\leqslant N_{\pm}-1$.

Thus,

$$E_{\pm}=\sum_{k}\sum_{l\in\langle k\rangle_{\pm}} r_{k,l}J(l).$$

This double sum is smallest when the set $S_{\pm}$ is a ME set and largest when it is a me set, and, for any strictly convex function J, the total energy E is minimum if and only if the configuration is ME and maximum precisely when the configuration is me (see Appendix A).

IV. SPIN CONTENT VECTORS AND AVERAGE ENERGY FOR ME CONFIGURATIONS

It should be noted that if J is convex but not strictly convex, for a given N and N_-, ME and me configurations still minimize and maximize total energy, respectively, but they may not have these properties uniquely. In what follows, we assume only that J is a convex function, although we will focus on ME and me configurations since much is known about their structures.

Let ρ be the down-spin density (i.e., $\rho=N_-/N$) and $\{x\}$ be the fractional part of x. It is not difficult to show that if $\rho=0$, the configurational energy per spin is $\Sigma_{k=1}^{N}J(k)$. Otherwise, for an equivalent problem. Clough and Douthett[2] have shown that, for a ME set and fixed integer k, $1\leqslant k\leqslant N_- -1$, there are $N\rho(1-\{k/\rho\})$ down-spin pairs associated with k that have length $\lfloor k/\rho\rfloor$ and $N\rho\{k/\rho\}$ down-spin pairs associated with k that have length $\lfloor k/\rho\rfloor+1$. Assuming $N_-<N/2$ and N is odd, the content vector for a ME set is

$$V_-=(\nu_1^-,\nu_2^-,\ldots,\nu_{(N-1)/2}^-)$$

where

$$\nu_j^-=\begin{cases} N\rho(1-\{k/\rho\}), & \text{if } j=\lfloor k/\rho\rfloor,\\ N\rho\{k/\rho\}, & \text{if } j=\lfloor k/\rho\rfloor+1,\\ 0, & \text{otherwise.}\end{cases}$$

Since $V=4V_-+(\cdots N-4N_-\cdots)$, the ME spin content vector is

$$V_{\mathrm{ME}}=(\nu_1,\nu_2,\ldots,\nu_{(N-1)/2}),$$

where

$$\nu_j=\begin{cases} N(1-4\rho\{k/\rho\}), & \text{if } j=\lfloor k/\rho\rfloor,\\ N(1+4\rho\{k/\rho\}-4\rho), & \text{if } j=\lfloor k/\rho\rfloor+1,\\ N(1-4\rho), & \text{otherwise.}\end{cases}$$

Then the minimum configurational energy for a given N and N_- is $E_{\min}=V_{\mathrm{ME}}\cdot W$; whence, the minimum average energy for a given down-spin density is

$$U_N^{\min}(\rho)=\frac{V_{\mathrm{ME}}\cdot W}{N}=4\rho\sum_{k=1}^{\lfloor N\rho/2\rfloor}[(1-\{k/\rho\})J_N(\lfloor k/\rho\rfloor)+\{k/\rho\}J_N(\lceil k/\rho\rceil)]+(1-4\rho)\sum_{k=1}^{N}J(k).$$

Now assume (in addition to the convexity of J) that $\Sigma_{k=1}^{\infty}J(k)$ converges, and define $U^{\min}$ as follows:

$$U^{\min}(\rho)=\begin{cases}\Sigma_{j=1}^{\infty}J(j), & \text{if } \rho=0,\\ \Sigma_{k=0}^{\infty}f_k(\rho), & \text{otherwise,}\end{cases}\tag{3}$$

where

$$f_k(\rho)=\begin{cases}(1-4\rho)\Sigma_{j=1}^{\infty}J(j), & \text{if } k=0,\\ 4\rho[(1-\{k/\rho\})J(\lfloor k/\rho\rfloor)+\{k/\rho\}J(\lceil k/\rho\rceil)], & \text{otherwise.}\end{cases}$$

Then $U_N^{\min} \to U^{\min}$ uniformly on $[0, \frac{1}{2}]$, $U^{\min}$ is uniformly continuous on $[0, \frac{1}{2}]$, and, for each $\rho \in [0, \frac{1}{2}]$, the series defining $U^{\min}(\rho)$ is absolutely convergent (Appendix B). Since this series is absolutely convergent, rearranging the terms in the series will not effect the sum. Let

$$U^{\min}(\rho) = a_1(\rho)J(1) + a_2(\rho)J(2) + a_3(\rho)J(3)\cdots$$

be a rearrangement of (3) with partial sums

$$u_n^{\min}(\rho) = a_1(\rho)J(1) + a_2(\rho)J(2) + a_3(\rho)J(3)\cdots + a_n(\rho)J(n).$$

Then, for each n, the coefficients of $u_n^{\min}$ are functions of ρ and can be determined by (3). For example, suppose the antiferromagnetic pairwise interaction is given by

$$\mathscr{J}(k) = -J_0 e^{-\alpha k}$$

where α and J_0 are positive constants. Then $J(k) = J_0 e^{-\alpha k}$, and the seventh partial sum is

$$u_7^{\min}(\rho) = a_1(\rho)J(1) + a_2(\rho)J(2) + \cdots + a_7(\rho)J(7), \tag{4}$$

where the coefficients are given below:

	a_1	a_2	a_3	a_4	a_5	a_6	a_7
$0 \leqslant \rho \leqslant \frac{1}{8}$	$1-4\rho$	$1-4\rho$	$1-4\rho$	$1-4\rho$	$1-4\rho$	$1-4\rho$	$1-4\rho$
$\frac{1}{8} < \rho \leqslant \frac{1}{7}$	$1-4\rho$	$1-4\rho$	$1-4\rho$	$1-4\rho$	$1-4\rho$	$1-4\rho$	$28\rho-3$
$\frac{1}{7} < \rho \leqslant \frac{1}{6}$	$1-4\rho$	$1-4\rho$	$1-4\rho$	$1-4\rho$	$1-4\rho$	$24\rho-3$	$5-28\rho$
$\frac{1}{6} < \rho \leqslant \frac{1}{5}$	$1-4\rho$	$1-4\rho$	$1-4\rho$	$1-4\rho$	$20\rho-3$	$5-24\rho$	$1-4\rho$
$\frac{1}{5} < \rho \leqslant \frac{1}{4}$	$1-4\rho$	$1-4\rho$	$1-4\rho$	$16\rho-3$	$5-20\rho$	$1-4\rho$	$1-4\rho$
$\frac{1}{4} < \rho \leqslant \frac{2}{7}$	$1-4\rho$	$1-4\rho$	$12\rho-3$	$5-16\rho$	$1-4\rho$	$1-4\rho$	$28\rho-7$
$\frac{2}{7} < \rho \leqslant \frac{1}{3}$	$1-4\rho$	$1-4\rho$	$12\rho-3$	$5-16\rho$	$1-4\rho$	$24\rho-7$	$9-28\rho$
$\frac{1}{3} < \rho \leqslant \frac{3}{8}$	$1-4\rho$	$8\rho-3$	$5-12\rho$	$1-4\rho$	$20\rho-7$	$9-24\rho$	$1-4\rho$
$\frac{3}{8} < \rho \leqslant \frac{2}{5}$	$1-4\rho$	$8\rho-3$	$5-12\rho$	$1-4\rho$	$20\rho-7$	$9-24\rho$	$1-4\rho$
$\frac{2}{5} < \rho \leqslant \frac{3}{7}$	$1-4\rho$	$8\rho-3$	$5-12\rho$	$16\rho-7$	$9-20\rho$	$1-4\rho$	$28\rho-11$
$\frac{3}{7} \leqslant \rho \leqslant \frac{1}{2}$	$1-4\rho$	$8\rho-3$	$5-12\rho$	$16\rho-7$	$9-20\rho$	$24\rho-11$	$13-28\rho$

Note that $u_7^{\min}$ is a continuous function made up of line segments whose end points are members of the Farey series F_8—the set of fractions between 0 and 1 inclusive whose denominators do not exceed 8. [In general, the endpoints of the line segments that make up $u_n^{\min}$ are points in the set $[0, \frac{1}{2}] \cap F_{n+1}$.] Shown in Fig. 4 is a plot of the minimum normalized energy per spin, $u_7^{\min}(\rho)/J_0$, versus the down-spin density, ρ, for a value of $\alpha = 0.01$. [A discussion of the significance of the value of α will be given in reference to Figs. 5–8 when the truncated series (4) is compared to the exact values for the minimum normalized energy per spin, which is derived below.] As inferred in

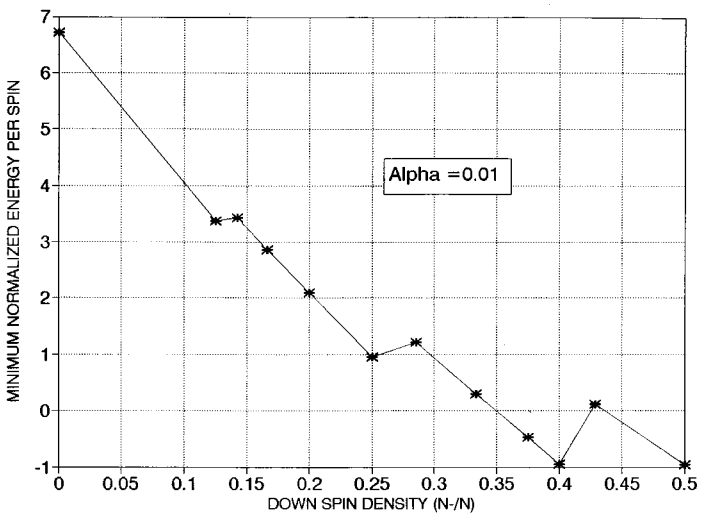

FIG. 4. Normalized configurational energy per spin verses down-spin density for a ME distribution of Ising spins with $\alpha=0.01$; seven nearest-neighbor interactions are included.

the list of coefficients above, the slope of each line segment in Fig. 4 depends on a particular subinterval of the interval $[0, \frac{1}{2}]$.

''Exact'' values can be computed for rational ρ. Let $\rho=p/q$, where p and q are integers. Then $\{k/\rho\}=\{qk/p\}$, and for $j\equiv k(\mathrm{mod}\, p)$, $\{qj/p\}=\{qk/p\}$. Whence, the coefficients, $a_k(\rho)$, cycle. Next, (3) is broken up to reflect this cycling:

$$U^{\min}\left(\frac{p}{q}\right)=\left(\frac{q-4p}{q}\right)\sum_{k=1}^{\infty} J(k)+\frac{4p}{q}\sum_{j=1}^{p}\sum_{k=1}^{\infty}\left[\left(1-\left\{\frac{qj}{p}\right\}\right)J\left(q(k-1)+\left\lfloor\frac{qj}{p}\right\rfloor\right)\right.$$
$$\left.+\left\{\frac{qj}{p}\right\}J\left(q(k-1)+\left\lceil\frac{qj}{p}\right\rceil\right)\right]. \tag{5}$$

Using (5), it is now possible to calculate the exact minimum average energy for a given rational ρ. For example, if $J(k)=J_0e^{-\alpha k}$ as above, then, for $\rho=2/7$, the exact minimum normalized energy per spin is

$$\frac{U^{\min}(\frac{2}{7})}{J_0}=-\frac{e^{-\alpha}}{7(1-e^{-\alpha})}+\frac{4e^{-3\alpha}+4e^{-4\alpha}+8e^{-7\alpha}}{7(1-e^{-7\alpha})}.$$

To compare the normalized energy per spin at the endpoints of the line segments in (4) to that calculated using (5), it is necessary to calculate the exact minimum normalized averages for $\rho\in[0, \frac{1}{2}]\cap F_8$. For $\alpha=0.01$, Fig. 5 compares the minimum normalized energy per spin versus down-spin density for the truncated series $u_7^{\min}(\rho)/J_0$ to the exact values as calculated from (5) for corresponding $p/q\in[0,\frac{1}{2}]\cap F_8$. The truncated series corresponds to approximating the minimum energy by accounting for interaction energies of the seven nearest neighbors only. As shown, for the relatively small value of $\alpha=0.01$, the seven near-neighbor approximation differs significantly from the exact result. The value of α reflects the range of the pairwise interaction. For small values of α the interaction is relatively long ranged. Therefore, more neighbors must be included to adequately approximate the average configurational energy. For $\alpha=0.01$ it is clear that more than seven neighbors are required.

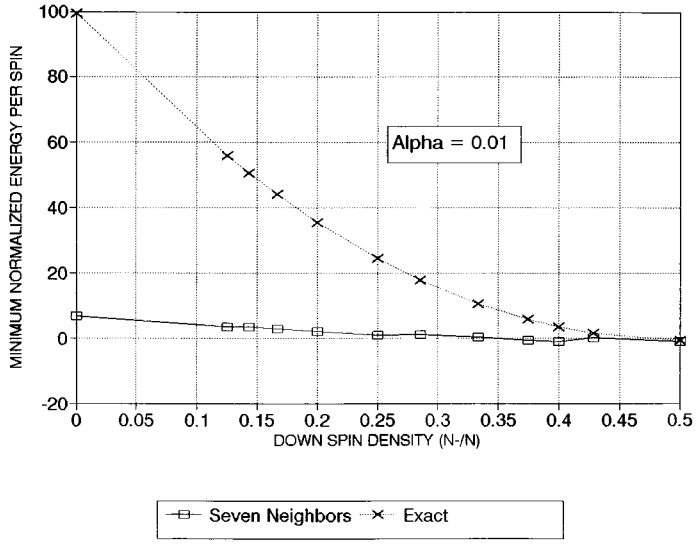

FIG. 5. Normalized configurational energy per spin verses down-spin density for a ME distribution of Ising spins with $\alpha=0.01$; exact calculations (all neighbors included in the limit as $N\rightarrow\infty$) compared to seven nearest-neighbor calculation.

In Fig. 6, the minimum normalized energy per spin versus down-spin density is shown for a value of $\alpha=0.1$. Again, the seven neighbor approximation is used for comparison to the exact values. The value of $\alpha=0.1$ corresponds to a shorter range interaction than that shown in Fig. 5. As expected, the approximate results are closer to the exact results. Figures 7 and 8 show similar results for larger values of α. In Fig. 7, $\alpha=0.5$, and in Fig. 8, the minimum normalized configurational energy per site is shown for a value of $\alpha=1.0$. Clearly, as the range of the interaction

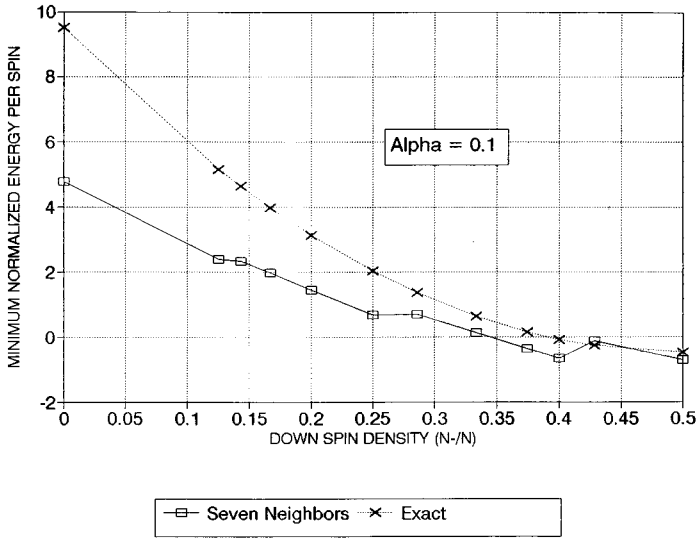

FIG. 6. Normalized configurational energy per spin verses down-spin density for a ME distribution of Ising spins with $\alpha=0.10$; exact calculations (all neighbors included in the limit as $N\rightarrow\infty$) compared to seven nearest-neighbor calculation.

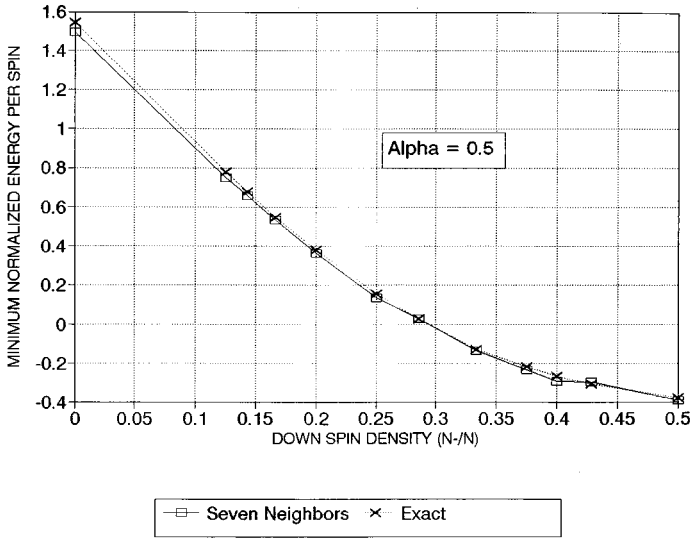

FIG. 7. Normalized configurational energy per spin verses down-spin density for a ME distribution of Ising spins with $\alpha=0.50$; exact calculations (all neighbors included in the limit as $N\rightarrow\infty$) compared to seven nearest-neighbor calculation.

becomes shorter, the truncated series approximation gets better. For large enough values of α, only near-neighbor interactions are relevant, and the minimum energy per spin is simply a linear function of the down-spin density:

$$U^{\min}(\rho)\approx u_1^{\min}(\rho)=J_0e^{-\alpha}(1-4\rho).$$

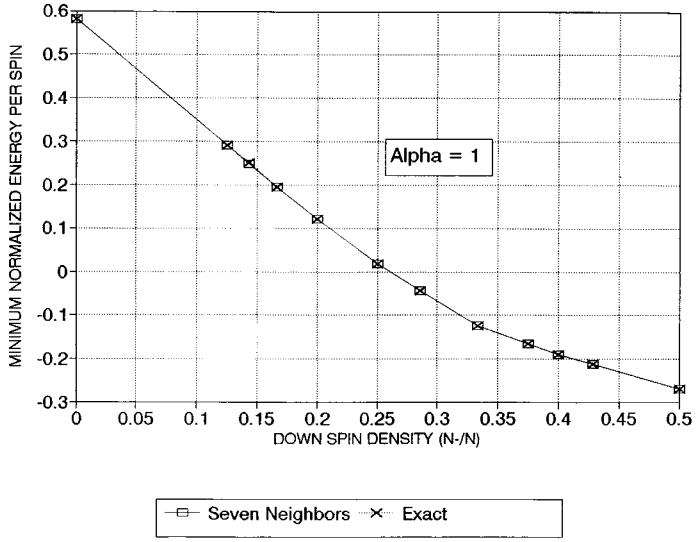

FIG. 8. Normalized configurational energy per spin verses down-spin density for a ME distribution of ising spins with $\alpha=1.00$; exact calculations (all neighbors included in the limit as $N\rightarrow\infty$) compared to seven nearest-neighbor calculation.

The specific relative error between the approximate value of the minimum energy per spin and the exact value may be used as the criterion for determining the number of pairwise neighbors needed to adequately describe the average configurational energy of the system.

V. SPIN CONTENT VECTORS AND AVERAGE ENERGY FOR me CONFIGURATIONS

Since the construction of me configurations is less complicated than that of ME configurations, a somewhat less formal approach will be taken in this section (as compared with Sec. IV and Appendix B).

For a me set with $N_- \geqslant 1$ and odd $N \geqslant 5$, it is easy to see that the content vector is

$$V_- = (\nu_1^-, \nu_2^-, \ldots, \nu_{(N-1)/2}^-),$$

where

$$\nu_k^- = \begin{cases} N_- - k, & \text{if } 1 \leqslant k \leqslant N_-, \\ 0, & \text{otherwise.} \end{cases}$$

Thus, the me spin content vector is

$$V_{\text{me}} = (\nu_1, \nu_2, \ldots, \nu_{(N-1)/2}),$$

where

$$\nu_k = \begin{cases} N - 4k, & \text{if } 1 \leqslant k \leqslant N_-, \\ N - 4N_-, & \text{otherwise.} \end{cases}$$

It follows that, for a me configuration and given N and N_-, the maximum configuration energy is

$$E_{\max} = V_{\text{me}} \cdot W = N \sum_{k=1}^{N} J(k) - 4 \sum_{k=1}^{N_-} k J_N(k) - 4N_- \sum_{k=N_-+1}^{N-N_--1} J(k).$$

Then the maximum average energy for a given down-spin density is

$$U_N^{\max}(\rho) = \frac{V_{\text{me}} \cdot W}{N} = \sum_{k=1}^{N} J(k) - \frac{4}{N} \sum_{k=1}^{N\rho} k J_N(k) - 4\rho \sum_{k=N\rho+1}^{N-N\rho-1} J(k). \tag{6}$$

A rather unexpected result turns up when the lattice has a me configuration; in the limit of large N, the configurational energy per spin is independent of the down-spin density, ρ. Let $U^{\max}(\rho) = \Sigma_{k=1}^{\infty} J(k)$. Then $U_N^{\max} \to U^{\max}$ uniformly since, as $N \to \infty$, the first sum in (6) converges to $\Sigma_{k=1}^{\infty} J(k)$ and the other two sums converge to 0. These convergences are clearly true for the first and second sums. To see that the third sum in (6) converges to 0, assume $\rho \in (0, \frac{1}{2}]$, and fix $\epsilon > 0$. Now let $\delta = \epsilon / 4\Sigma_{k=1}^{\infty} J(k)$, and choose N_0 large enough so that $\Sigma_{k=\lfloor \delta N \rfloor}^{\infty} J(k) < \epsilon/2$ whenever $N \geqslant N_0$. Then, if $\rho < \delta$,

$$4\rho \sum_{k=N\rho+1}^{N-N\rho-1} J(k) < 4\delta \sum_{k=1}^{\infty} J(k) = \epsilon.$$

On the other hand, if $\rho \geqslant \delta$, then

$$4\rho \sum_{k=N\rho+1}^{N-N\rho-1} J(k) \leqslant 2 \sum_{k=\lfloor \delta N \rfloor}^{\infty} J(k) < \epsilon$$

whenever $N \geqslant N_0$. Thus, the last sum in (6) converges to 0 independent of ρ, implying that $U_N^{\max} \to U^{\max}$ uniformly on the interval $(0, \frac{1}{2}]$. Moreover, if $\rho=0$, then me and ME configurations are identical (all spins are up), implying $U^{\max}(0)=U^{\min}(0)$. Whence, by (3), $U^{\max}(0)=\Sigma_{k=1}^{\infty} J(k)$. It follows that

$$U^{\max}(\rho)=\sum_{k=1}^{\infty} J(k),$$

for all $\rho \in [0, \frac{1}{2}]$. Thus, in the limit of large N, the maximum average energy depends only on the clustering of the down-spins and up-spins in the configuration and not on the down-spin density.

VI. SUMMARY

An analysis of the antiferromagnetic spin-$\frac{1}{2}$ Ising model with periodic boundary conditions has been carried out using the formalism of Maximally/Minimally Even sets first introduced by Clough and Douthett[2] and Block and Douthett[3] in the Music Theory literature.

Applying elementary graph theory (decomposition of complete graphs), the configurational energy of a system has been calculated by the dot product of a so-called energy vector and a spin content vector. Casting the configurational energy in this form is convenient for keeping track of the contribution to the configurational energy from each set of neighbor pairs separately. This formulation allowed us to use the theory of maximally/minimally even sets to calculate the interval spectra which is equivalent to the spin content vector.

It is shown that, for the antiferromagnetic case and fixed N and N_-, Maximally Even sets of up- and down-spins minimize the configurational energy for a given down-spin density while Minimally Even sets maximize the configurational energy (Appendix A). Furthermore, the configurational energy per site is calculated in the limit of large N (Appendix B) to yield the ''exact'' (asymptotic) expression.

In order to investigate the range on the configurational energy per site, a simple form of pairwise antiferromagnetic interaction is assumed that decreases exponentially with the distance. As expected, it is shown that the shorter the range of the interaction the fewer the number of neighbors needed to adequately describe the system. Our formulation allows the number of neighbor pairs necessary to approximate the configurational energy per site to be calculated to any desired precision.

Finally, it is shown that, for Minimally Even sets of up- and down-spins, the average configurational energy depends only on the clustering of like spins and not on the down-spin density in the limit of large N.

APPENDIX A: CONFIGURATIONS ASSOCIATED WITH ENERGY EXTREMES

Before developing the theorems and corollaries, it will be useful to summarize important properties discussed in Sec. III that are needed for our proofs. The first properties deal with interval spectra.

P1. For each k, if $l \in \langle k \rangle_{\pm}$, then $k \leqslant l \leqslant N-N_{\pm}+k$.

P2. For each k, $\Sigma_{l \in \langle k \rangle_{\pm}} r_{k,l} l = Nk$.

Properties P3–P6 involve definitions and properties of ME and me sets.

P3. The set $S_{\pm}$ is a ME set if and only if $\langle k \rangle_{\pm} = \{\lfloor Nk/N_{\pm} \rfloor, \lceil Nk/N_{\pm} \rceil\}$ for all k, $1 \leqslant k \leqslant N_{\pm}-1$.

P4. The set $S_{\pm}$ is a me set if and only if $\langle k \rangle_{\pm} = \{k, N-N_{\pm}+k\}$ for all k, $1 \leqslant k \leqslant N_{\pm}-1$.

P5. The complement of a ME set is ME.

P6. The complement of a me set is me.

The last property needed (discussed at the end of Sec. III) expresses the energy contributed by the set of down-spins (up-spins) in terms of the interval spectra and the pairwise interaction.

P7. $E_{\pm} = \Sigma_k \Sigma_{l \in \langle k \rangle_{\pm}} r_{k,l} J(l)$.

A corollary about convexity is needed to prove the assertions made in Sec. III about minimum and maximum energies. Before stating the ''Convex Corollary,'' it is necessary to state a well-known theorem[9] (without proof) to which the Convex Corollary belongs.

Theorem 1: Let J be a (strictly) convex function on the interval (a,b), and suppose that x_1, x_2, y_1, $y_2 \in (a,b)$ such that $x_1(<)\leqslant x_2<y_2$ and $x_1<y_1(<)\leqslant y_2$. Then

$$\frac{J(y_1)-J(x_1)}{y_1-x_1}\,(<)\leqslant \frac{J(y_2)-J(x_2)}{y_2-x_2}.$$

*Corollary 1 (***convex**): Let J be a (strictly) convex function on the interval $(0,\infty)$, and assume $0<h<p\leqslant q$. Then

$$J(p)+J(q)(<)\leqslant J(p-h)+J(q+h).$$

Proof: If p, q, and h are as defined above, then $p-h,p,q,q+h\in(0,\infty)$, $p-h<q<q+h$, and $p-h<p<q+h$. Thus, by the Theorem 1,

$$\frac{J(p)-J(p-h)}{p-(p-h)}\,(<)\leqslant \frac{J(q+h)-J(q)}{(q+h)-q}.$$

It follows that

$$J(p)+J(q)(<)\leqslant J(p-h)+J(q+h). \qquad \blacksquare$$

This result will be needed to prove the ''Stick Theorem,'' which, in turn, will allow us to show that the energy of the set of down-spins (up-spins) is minimum precisely when $S_{\pm}$ is a ME set and maximum when $S_{\pm}$ is a me set. Finally, the ''Energy Theorem,'' which will show that the total energy E of a lattice is minimized or maximized precisely when the lattice configuration is ME or me respectively, will be proved.

To prove the ''Stick Theorem,'' it is necessary to make the following construction.

Assume J is a strictly convex function, and let m and n be integers with $2\leqslant m\leqslant n$. Consider the sequence of sets

$$\mathbf{T}_j(n,m)=(T_1,T_2,T_3,\ldots,T_{m-1}),$$

where each set T_k, $1\leqslant k\leqslant m-1$, consists of m sticks with integer lengths. If t is a stick, the *length* of the stick will be denoted by $l_1(t)$. In addition, for each k, the set T_k has the following properties:

(1) for each $t\in T_k$, $k\leqslant l_1(t)\leqslant n-m+k$;
(2) $\Sigma_{t\in T_k} l_1(t)=nk$.

The *spectrum* $\langle k\rangle$ of the set T_k is the set of all distinct lengths of the sticks in T_k, $a_k=\min\langle k\rangle$, and $b_k=\max\langle k\rangle$. Define $\sigma_J(T_k)$ as follows:

$$\sigma_J(T_k)=\sum_{t\in T_k} J(l_1(t)).$$

Finally, define the sum $\Psi_J(n,m)$ as follows:

$$\Psi_J(n,m)=\sum_k \sigma_J(T_k).$$

Theorem 2 (stick): Let J be a strictly convex function on the interval $(0,\infty)$, and suppose $\mathbf{T}_J(n,m)$ is defined as above.

(1) The sum $\Psi_J(n,m)$ is minimum if and only if

$$\langle k\rangle=\left\{\left\lfloor \frac{nk}{m}\right\rfloor,\left\lceil \frac{nk}{m}\right\rceil\right\}$$

for all k, $1\leqslant k\leqslant m-1$.

(2) The sum $\Psi_J(n,m)$ is maximum if and only if

$$\langle k\rangle=\{k,n-m+k\}$$

for all k, $1\leqslant k\leqslant m-1$.

Proof: (1) For a given k, we say the set of sticks T_k can be *reduced* if there exists a set T_k^* such that $\sigma_J(T_k^*)<\sigma_J(T_k)$.

Now consider the family of sets of sticks

$$\mathscr{T}_k=\{T_k|b_k-a_k\geqslant 2\}.$$

Then for each $T_k\in\mathscr{T}_k$, there are sticks $t_1, t_2\in T_k$ such that $l_1(t_2)-l_1(t_1)\geqslant 2$. Replace these sticks with sticks t_1^* and t_2^* whose lengths are $l_1(t_1^*)=l_1(t_1)+1$ and $l_1(t_2^*)=l_1(t_2)-1$. Call the new set of sticks T_k^*. Thus, T_k^* is a set of m sticks and $\Sigma_{t\in T_k^*}l_1(t)=nk$. Moreover, from the Convex Corollary,

$$J(l_1(t_1^*))+J(l_1(t_2^*))<J(l_1(t_1))+J(l_1(t_2)).$$

It follows that $\sigma_J(T_k^*)<\sigma_J(T_k)$. Hence, if $T_k\in\mathscr{T}_k$, then T_k can be reduced by replacing sticks as described above.

Since $\mathscr{T}_k$ contains a finite number of sets, there exists a set $T_k^{\min}\in\mathscr{T}_k$ such that

$$\sigma_J(T_k^{\min})=\min\{\sigma_J(T_k)|T_k\in\mathscr{T}_k\}.$$

However, since $T_k^{\min}\in\mathscr{T}_k$, $T_k^{\min}$ can also be reduced by replacing sticks. Call this new set of sticks T_k^{**}. Then, for T_k^{**}, $b_k-a_k\leqslant 1$. Thus, the spectrum of T_k^{**} must contain either one or two consecutive integers. Since this is true for each k, $\Psi_J(n,m)$ is smallest precisely when

$$\langle k\rangle=\left\{\left\lfloor \frac{nk}{m}\right\rfloor,\left\lceil \frac{nk}{m}\right\rceil\right\}$$

for all k, $1\leqslant k\leqslant m-1$.

(2) For a given k we say the set of sticks T_k can be *increased* if there exists a set T_k^* such that $\sigma_J(T_k^*)>\sigma_J(T_k)$.

Note that if $m-k$ sticks have length k and k sticks have length $n-m+k$, then there is a total of m sticks, and the sum of the lengths of these sticks is nk. Let T_k^{**} be the set of these sticks.

Since, for each T_k, the sum of the lengths of the sticks in T_k is the constant nk, there are fewer than $m-k$ sticks with length k in T_k if and only if there are fewer than k sticks with length $n-m+k$. It follows that if $t_1\in T_k$ and $k<l_1(t_1)<n-m+k$, then there exists $t_2\in T_k$ such that $t_2\neq t_1$ and $k<l_1(t_2)<n-m+k$.

Now consider the family of sets of sticks

$$\mathscr{T}_k=\{T_k|\exists t\in T_k\ni:k<l_1(t)<n-m+k\}.$$

It follows that if $T_k \in \mathscr{T}_k$, then there exists t_1, $t_2 \in T_k$ such that $t_1 \neq t_2$ and $k < l_1(t_1) \leqslant l_1(t_2) < n-m+k$. Let t_1^* and t_2^* be sticks such that $l_1(t_1^*) = l_1(t_1) - 1$ and $l_1(t_2^*) = l_1(t_2) + 1$. Then by the Convex Corollary

$$J(l_1(t_1^*)) + J(l_1(t_2^*)) > J(l_1(t_1)) + J(l_1(t_2)).$$

Replace t_1 and t_2 with t_1^* and t_2^*, and call the new set of sticks T_k^*. Thus, $\sigma_J(T_k^*) > \sigma_J(T_k)$. Hence, if $T_k \in \mathscr{T}_k$, then T_k can be increased by replacing sticks as described above.

Since $\mathscr{T}_k$ contains a finite number of sets, there exists a set $T_k^{\max} \in \mathscr{T}_k$ such that

$$\sigma_J(T_k^{\max}) = \max\{\sigma_J(T_k) | T_k \in \mathscr{T}_k\}.$$

However, since $T_k^{\max} \in \mathscr{T}_k$, $T_k^{\max}$ can also be increased by replacing sticks. It follows that the new set must have sticks whose lengths are either k or $n-m+k$. Thus, this new set is T_k^{**}. Since this is true for each k, $\Psi_J(n,m)$ is maximum precisely when

$$\langle k \rangle = \{k, n-m+k\}$$

for all k, $1 \leqslant k \leqslant m-1$. ■

Corollary 2: For a fixed N and $N_\pm$,

(1) $E_\pm$ is minimum if and only if $S_\pm$ is a ME set.
(2) $E_\pm$ is maximum if and only if $S_\pm$ is a me set.
(3) *Proof:* For each length $l \in \langle k \rangle$, let $r_{k,l}$ be the number of sticks in T_k that have length l. Then

$$\sigma_J(T_k) = \sum_{l \in T_k} J(l_1(t)) = \sum_{l \in \langle k \rangle} r_{k,l} J(l).$$

It follows that

$$\Psi_J(n,m) = \sum_k \sigma_J(T_k) = \sum_k \sum_{l \in \langle k \rangle} r_{k,l} J(l).$$

Replace n with N, m with $N_\pm$, and $\langle k \rangle$ with $\langle k \rangle_\pm$. Then by properties P1, P2, and P7,

$$E_\pm = \Psi_J(N, N_\pm).$$

The corollary follows immediately from the Stick Theorem and from properties P3 and P4. ■

Theorem 3 (energy): For a fixed N (N odd) and $N_\pm$,

(1) E is minimum if and only if the lattice configuration is ME.
(2) E is maximum if and only if the lattice configuration is me.

Proof: Recall that $V_- + V_+ + V_0 = V_N = (\cdots N \cdots)$. Thus,

$$V_0 = V_N - (V_- + V_+) = (\cdots N \cdots) - (V_- + V_+).$$

However, then

$$E_0 = V_0 \cdot W = V_N \cdot W - (V_- \cdot W + V_+ \cdot W) = +N \sum_{k=1}^{N} J(k) - (E_- + E_+).$$

The first term in the last expression on the right is a constant, and by Corollary 2 and property P5 (P6), the sum $E_- + E_+$ is minimized (maximized) if and only if the lattice configuration is ME (me). It follows that E_0 is maximized (minimized). However, then the total energy

$$E = E_+ + E_- - E_0$$

is minimized (maximized). ■

We have assumed that J is strictly convex to illustrate the uniqueness of ME and me configurations. If it is only assumed that J is convex, then the configurational energy extremes still occur when the configurations are ME and me. However, these configurations no longer necessarily uniquely define these extreme states, and configurations other than ME and me may have the same average configurational energies.

APPENDIX B: THE CONVERGENCES AND CONTINUITY OF $U^{\min}$

Assume J is a convex function on the interval $(0,\infty)$ such that $\Sigma_{k=1}^{\infty} J(k)$ converges. From these restrictions, it is easy to see that $J(k)$ is a decreasing positive function, and, hence, $\Sigma_{k=1}^{\infty} J(k)$ is absolutely convergent. Now assume N is an odd positive integer, and let $\rho \in (0, 1/2]$. For notational convenience, set $p_\rho = \lfloor N\rho/2 \rfloor$ and $p_1 = (N-1)/2$. Note that p_ρ depends on N and ρ while p_1 depends only on N. Moreover, if $1 \leqslant k \leqslant p_\rho$, then $\lfloor k/\rho \rfloor$ and $\lceil k/\rho \rceil$ are both less than N; whence, $J(N - \lfloor k/\rho \rfloor)$ and $J(N - \lceil k/\rho \rceil)$ are defined.

Now let $J_N(k) = J(k) + J(N-k)$ where $1 \leqslant k \leqslant N-1$. Let $\rho \in [0, 1/2]$, and define $U_N^{\min}$ as follows:

$$U_N^{\min}(\rho) = \sum_{k=0}^{p_\rho} f_{N,k}(\rho),$$

where

$$f_{N,k}(\rho) = \begin{cases} (1-4\rho)\displaystyle\sum_{j=1}^{N} J(j), & \text{if } k = 0, \\ 4\rho[(1-\{k/\rho\})J_N(\lfloor k/\rho \rfloor) + \{k/\rho\}J_N(\lceil k/\rho \rceil)], & \text{otherwise.} \end{cases}$$

Next define $U^{\min}$ as follows:

$$U^{\min}(\rho) = \begin{cases} \displaystyle\sum_{j=1}^{\infty} J(j), & \text{if } \rho = 0, \\ \displaystyle\sum_{k=0}^{\infty} f_k(\rho), & \text{otherwise,} \end{cases}$$

where

$$f_k(\rho) = \begin{cases} (1-4\rho)\displaystyle\sum_{j=1}^{\infty} J(j), & \text{if } k = 0 \\ 4\rho[(1-\{k/\rho\})J(\lfloor k/\rho \rfloor) + \{k/\rho\}J(\lceil k/\rho \rceil)], & \text{otherwise.} \end{cases}$$

We will show that $U_N^{\min} \to U^{\min}$ uniformly on the interval $[0, 1/2]$, that $U^{\min}$ is uniformly continuous on $[0, 1/2]$, and that the series defining $U^{\min}(\rho)$ is absolutely convergent for every $\rho \in [0, 1/2]$.

Before beginning the theorems and proofs relevant to this paper, it is necessary to state a couple of well-known preliminary theorems. Although these theorems can be found in many analysis texts, we refer the reader to Rudin.[10]

Theorem 4: Suppose $f_n \to f$ uniformly on a set E in a metric space, and let x be a limit point of E. Then

$$\lim_{t\to x}\lim_{n\to\infty} f_n(t) = \lim_{n\to\infty}\lim_{t\to x} f_n(t).$$

Theorem 5: Suppose $\{f_n\}$ is a sequence of continuous functions and $f_n \to f$ uniformly on a set E in a metric space. Then f is continuous on E.

Theorem 6: For each positive integer N, the function $U_N^{\min}(\rho)$ is continuous on the interval $[0, 1/2]$.

Proof: We consider continuity at $\rho=0$ first. Let $\delta_0 = 2/N$. Then, $U_N^{\min}(\rho) = f_{N,0}(\rho)$ when $\rho < \delta_0$. Now choose $\epsilon > 0$, and let $\delta_1 = \epsilon/4\Sigma_{k=1}^{N} J(k)$. Now let $\delta = \min\{\delta_0, \delta_1\}$, and choose ρ such that $0 \leqslant \rho < \delta$. Then

$$|U_N^{\min}(\rho) - U_N^{\min}(0)| = 4\rho \sum_{k=1}^{N} J(k) < \epsilon.$$

Thus, $U_N^{\min}$ is continuous at $\rho=0$.

Now assume $\rho \in (0, 1/2]$. If it is shown that $f_{N,k}$ is continuous on $(0, 1/2]$ for all k, $0 \leqslant k \leqslant p_\rho$, then their sum is continuous.

It is clear that $f_{N,k}$, $1 \leqslant k \leqslant p_\rho$, is continuous on $(0, 1/2]$ except possibly when k/ρ is an integer. [If k/ρ is not an integer, then $f_{N,k}(\rho)$ is a linear function on some small neighborhood of ρ.] Fix k, and suppose $\rho_0 \in (0, 1/2]$ and k/ρ_0 is an integer, say $k_0 = k/\rho_0$. Let $\delta_0 = \rho_0^2/(k-\rho_0^2)$. Then $f_{N,k}(\rho_0) = 4\rho_0 J_N(k_0)$. Furthermore, for $\rho_0 < \rho < \rho_0 + \delta_0$, $\lfloor k/\rho \rfloor = k/\rho_0 - 1 = k_0 - 1$, and for $\rho_0 - \delta_0 < \rho < \rho_0$, $\lfloor k/\rho \rfloor = k/\rho_0 = k_0$. Choose $\epsilon > 0$, and let

$$\delta_1 = \frac{\epsilon}{4|k_0 J_N(k_0-1) - (k_0-1)J_N(k_0)|}$$

and

$$\delta_2 = \frac{\epsilon}{4|(k_0+1)J_N(k_0) - k_0 J_N(k_0+1)|},$$

where it is assumed that the denominators of δ_1 and δ_2 are not 0. Now let $\delta = \min\{\delta_0, \delta_1, \delta_2\}$, and choose ρ so that $|\rho - \rho_0| < \delta$. There are two cases.

Case 1: Suppose $\rho_0 < \rho < \rho_0 + \delta$. Noting that $\{k/\rho\} = k/\rho - \lfloor k/\rho \rfloor$,

$$\begin{aligned} |f_{N,k}(\rho) - f_{N,k}(\rho_0)| &= 4|[\rho(k_0-1) - k + \rho]J_N(k_0-1) - [\rho(k_0-1) - k]J_N(k_0) - \rho_0 J_N(k_0)| \\ &= 4|\rho - \rho_0||k_0 J_N(k_0-1) - (k_0-1)J_N(k_0)|. \end{aligned}$$

If the right side of the equation is 0 (i.e., if the denominator of δ_1 is 0), then $f_{N,k}(\rho) = f_{N,k}(\rho_0)$; otherwise, $|f_{N,k}(\rho) - f_{N,k}(\rho_0)| < \epsilon$. In either case, $\lim_{\rho \to \rho_0^+} f_{N,k}(\rho) = f_{N,k}(\rho_0)$.

Case 2: Suppose $\rho_0 - \delta < \rho < \rho_0$. Then

$$\begin{aligned} |f_{N,k}(\rho) - f_{N,k}(\rho_0)| &= 4|[\rho k_0 - k + \rho]J_N(k_0) - [\rho k_0 - k]J_N(k_0+1) - \rho_0 J_N(k_0)| \\ &= 4|\rho - \rho_0||(k_0+1)J_N(k_0) - k_0 J_N(k_0+1)|. \end{aligned}$$

Similar to case 1, if the right side of the equality is 0 (i.e., if the denominator of δ_2 is 0), then $f_{N,k}(\rho)=f_{N,k}(\rho_0)$; otherwise, $|f_{N,k}(\rho)-f_{N,k}(\rho_0)|<\epsilon$. Thus, $\lim_{\rho\to\rho_0^-} f_{N,k}(\rho) = f_{N,k}(\rho_0)$. It follows that, for each $k, f_{N,k}$ is continuous on the interval $[0, \frac{1}{2}]$. Whence, $U_N^{\min}$ is continuous on $[0, \frac{1}{2}]$. [In fact, $U_N^{\min}$ is uniformly continuous since the function is defined on a closed and bounded interval.] ■

Theorem 7: The sequence $U_N^{\min}\to U^{\min}$ uniformly on the interval $[0, \frac{1}{2}]$. Moreover, $U^{\min}$ is uniformly continuous on $[0, \frac{1}{2}]$.

Proof: For $\rho\in(0, \frac{1}{2}]$, we have

$$|U^{\min}(\rho)-U_N^{\min}(\rho)|\leqslant\left|\sum_{k=0}^{p_\rho}(f_k(\rho)-f_{N,k}(\rho))\right|+\left|\sum_{k=p_\rho+1}^{\infty} f_k(\rho)\right|. \tag{B1}$$

For the first sum in (B1),

$$\begin{aligned}\left|\sum_{k=0}^{p_\rho}(f_k(\rho)-f_{N,k}(\rho))\right| &= \left|(1-4\rho)\sum_{k=N+1}^{\infty} J(k)-4\rho\sum_{k=1}^{p_\rho}\left[\left(1-\left\{\frac{k}{\rho}\right\}\right)J\left(N-\left\lfloor\frac{k}{\rho}\right\rfloor\right)\right.\right.\\ &\qquad\left.\left.+\left\{\frac{k}{\rho}\right\}J\left(N-\left\lceil\frac{k}{\rho}\right\rceil\right)\right]\right|\\ &\leqslant\sum_{k=N+1}^{\infty} J(k)+4\sum_{k=1}^{p_\rho} J\left(N-1-\frac{k}{\rho}\right).\end{aligned}$$

Clearly, the first sum on the right side of the above goes to 0 as $N\to\infty$. To show the second sum does as well, note that if $k=p_\rho$, then $k\leqslant N\rho/2$, and, hence, $k/\rho\leqslant N/2$. It follows that

$$4\sum_{k=1}^{p_\rho} J(N-1-k/\rho)\leqslant 4p_\rho J(N-1-N/2)\leqslant 2N\rho J((N-2)/2)\leqslant NJ((N-2)/2)\to 0$$

as $N\to\infty$.

For the second sum in (B1),

$$\left|\sum_{k=p_\rho+1}^{\infty} f_k(\rho)\right| = 4\rho\sum_{k=p_\rho+1}^{\infty}\left[\left(1-\left\{\frac{k}{\rho}\right\}\right)J\left(\left\lfloor\frac{k}{\rho}\right\rfloor\right)+\left\{\frac{k}{\rho}\right\}J\left(\left\lceil\frac{k}{\rho}\right\rceil\right)\right]\leqslant 4\sum_{k=p_\rho+1}^{\infty} J\left(\frac{k}{\rho}-1\right).$$

To show the right side of the above inequality goes to 0 as $N\to\infty$, note that, for any non-negative integer m,

$$p_1-2+m<\frac{N+1}{2}-2+m=\frac{(N\rho/2)-(3\rho/2)+m\rho}{\rho}<\frac{\lfloor N\rho/2\rfloor+1-(3\rho/2)+m\rho}{\rho}<\frac{p_\rho+1+m}{\rho}-1.$$

Thus, since J is a decreasing function,

$$J\left(\frac{p_\rho+1+m}{\rho}-1\right)\leqslant J(p_1-2+m).$$

Finally, for any non-negative integer $M\geqslant p_1-2$,

$$4\sum_{k=p_\rho+1}^{M} J\left(\frac{k}{\rho}-1\right)\leqslant 4\sum_{k=p_1-2}^{M} J(k)\leqslant 4\sum_{k=p_1-2}^{\infty} J(k),$$

$$4\sum_{k=p_\rho+1}^{\infty} J\left(\frac{k}{\rho}-1\right)\leqslant 4\sum_{k=p_1-2}^{\infty} J(k).$$

Since the right side of the above inequality goes to zero as $N\to\infty$ (independent of ρ), the left side does as well. It follows that $U_N^{\min}\to U^{\min}$ uniformly on $(0, \frac{1}{2}]$. Moreover, since 0 is in the domain of $U_N^{\min}$, it is convenient to define $U^{\min}(0)$ as follows:

$$U^{\min}(0)=\lim_{\rho\to 0} U^{\min}(\rho)=\lim_{N\to\infty} U_N^{\min}(0)=\sum_{k=1}^{\infty} J(k)$$

(Theorem 4). Since $U_N^{\min}$ is continuous on $[0, \frac{1}{2}]$ for every N, $U^{\min}$ is continuous on $[0, \frac{1}{2}]$ (Theorem 5), and since $U^{\min}$ is defined on a closed and bounded interval, $U^{\min}$ is uniformly continuous on $[0, \frac{1}{2}]$. ■

Theorem 8: For each $\rho\in[0, \frac{1}{2}]$, the series defining $U^{\min}(\rho)$ is absolutely convergent.

Proof: Since $\rho\in[0, \frac{1}{2}]$ and $\Sigma_{k=1}^{\infty}J(k)<\infty$,

$$\sum_{k=0}^{\infty}|f_k(\rho)|\leqslant|1-4\rho|\sum_{k=1}^{\infty}J(k)+\sum_{k=1}^{\infty}|f_k(\rho)|\leqslant\sum_{k=1}^{\infty}J(k)+2\sum_{k=1}^{\infty}J(k)<\infty,$$

Whence, $U^{\min}(\rho)$ is absolutely convergent for every $\rho\in[0, \frac{1}{2}]$. ■

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On the Poisson integrals representation in the classical statistical mechanics of continuous systems

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Description of the grand canonical Gibbs ensemble for classical continuous systems in terms of the nonlocally perturbed infinite-divisible generalized random fields is presented. The equivalence of the traditional description with the ones presented here on the level of DLR equations is established. The antiferromagnetism for the purely repulsive interactions has been observed. Finally, the usefulness of our description for an analysis of the high-temperature cluster expansion has been demonstrated. © *1996 American Institute of Physics.* [S0022-2488(96)02106-8]

I. INTRODUCTION

Our everyday experience shows that several matter transformations like crystallization, liquid–vapour, etc. transformation are the most natural phenomena of the phase transition type. Their physical picture can be perfectly well understood on the basis of the molecular theory of matter.[1,2] Therefore it is reasonable to expect that the corresponding mathematical description of such basic phenomena should be encompassed by the highly developed apparatus of the modern statistical mechanics. But this is not true: the rigorous microscopic description of the most natural phase transitions that take place in nature does not exist.

The conceptual background for the statistical mechanics description of the real matter in the microworld is highly developed on a more or less sophisticated level of abstraction.[3–5] However, only the (noninteresting from the point of view of physics) high-temperature/low-density regime of couplings seems to be well understood[3–6] from the point of view of basic principles of classical statistical mechanics. It seems that one of the main reasons for the lack of progress in developing the rigorous methods enabling us to penetrate the low-temperature/high-density properties of realistic models of matter is the description of the corresponding Gibbs ensembles in terms of variables that are not well suited for that purpose. The discrete spin system models are much more appropriate[3,7,8] and powerful progress has been achieved in the last decades. The only class of continuous systems whose low-temperature properties are rather well known are the so-called Widom–Rowlison type of models.[9–11] However, from the point of view of the general theory these models are rather exceptional and exotic and moreover the methods developed for the analysis of the corresponding low-temperature phase diagrams do not extend to the more typical systems. The functional integral representation (the sine-Gordon representation) of the system interacting through the two-body potential of positive-definite type has been originated by Siegert[12] and significantly extended and explored in Refs. 13 and 14. In particular, the functional integral representation of the corresponding Gibbs ensembles in terms of the perturbed gently Gaussian measures opened the opportunity to apply the powerful methods of the constructive quantum field theory[15] to the analysis of low-temperature properties of such systems. This class of models contains extremely interesting, from the point of view of physics, systems like the regularized Coulomb gases, where some phase transitions (Debye screening, for example) take place,

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and indeed the methods of the constructive quantum field theory were successfully applied[16–21] to the analysis of these effects. Additionally, some further results pertaining the phase diagrams in the full range of the parameters have also been obtained.[22–25]

The above listed two classes of models for macroscopic real matter show how important a role might be played by the choice of the proper mathematical description of a given system, and this is our main motivation for writing this paper. We propose to introduce generalized random fields of the Poisson type and their nonlocal perturbations as an alternative to the existing description[3,4] of continuous systems. A large class of models for continuous systems is selected for which the description in terms of the Poisson functional integrals applies well. It is our hope that the introduced formalism will stimulate further progress on the basically open problem of low-temperature properties of continuous systems.

It is worth stressing that the Poisson functional integrals have been used in various contexts in the mathematical physics several times. For example, they were used in Refs. 26 and 27 while searching for the alternative to the conventional perturbation expansions around the Gaussian point in the quantum field theory. Recently the functional Poisson integrals have been used for the constructions of some four-dimensional 4-D quantum field-like structures[28,29] (also see Ref. 30 for a systematic approach to such constructions). Finally, they were used to describe quantum semi-relativistic statistical mechanics.[31] The systematic introduction of Poisson functional integral representations in quantum statistical mechanics of continuous systems as announced in Ref. 32 is now under preparation.[33]

Section II is devoted to the demonstration that the traditional description of the grand canonical Gibbs ensembles describing continuous systems of particles and the introduced here Poisson functional integral description are equivalent on the level of the corresponding DLR equations.

In Sec. III the lattice approximation is introduced and its convergence to the continuum is demonstrated. As a result we detect that for continuous systems of particles interacting through repulsive interaction antiferromagnetism holds.

In Sec. IV we shall demonstrate how the use of Poisson functional integrals simplifies the construction of the corresponding high-temperature cluster expansion. In particular a slight extension of the result of Ref. 34 is obtained.

II. POISSON INTEGRALS DESCRIPTION OF THE GRAND CANONICAL GIBBS ENSEMBLE

The material in this section is divided into three parts for better understanding. In the first part we collect some relevant data for the purposes of the present work properties of generalized random fields of the Poisson type. Some additional material concerning Poisson noise calculus[35–38] is included in the Appendix. In the second part of this section we recall the standard description of the grand canonical Gibbs ensemble for continuous systems of particles and then we express the finite volume quantities of the grand canonical Gibbs ensemble through the Poisson functional integrals. Finally, in the third part we shall demonstrate the equivalence of the standard description with the one introduced here in the thermodynamical limit.

A. Generalized random fields of Poisson type

Let $\mathscr{D}'(R^d)$ be the (real part of) the space of Schwartz distributions and let $\mathscr{D}(R^d)$ be the corresponding nuclear test function space. The Borel σ-algebra of sets in $\mathscr{D}'(R^d)$ will be denoted by $\mathscr{B}(\mathscr{D}'(R^d))$. A generalized random field will be identified with the corresponding probabilistic, Borel, cylindric measure on the standard measure space $(\mathscr{D}'(R^d)),\mathscr{B}(\mathscr{D}'(R^d))$. A given generalized random field μ is completely determined by its characteristic functional (Minlos theorem[39]),

$$F_\mu(f)=\int_{\mathscr{D}'(R^d)} d\mu(\varphi)e^{i\langle\varphi,f\rangle}, \tag{II.1}$$

where $f \in \mathscr{D}(R^d)$ and $\langle \varphi, f \rangle$ is the dualization between $\mathscr{D}'(R^d)$ and $\mathscr{D}(R^d)$. A given generalized random field μ is called an infinite divisible random field iff for any $f, g \in \mathscr{D}(R^d)$ with the disjoint supports we have

$$\int d\mu(\varphi) e^{i\langle \varphi, f \rangle} e^{i\langle \varphi, g \rangle} = \int d\mu(\varphi) e^{i\langle \varphi, f \rangle} \int d\mu(\varphi) e^{i\langle \varphi, g \rangle}. \tag{II.2}$$

There exists a so-called Levy–Kchintchine formula,[39] which gives the complete description of the whole class of infinitely divisible random fields in terms of their characteristic functionals, which must be of the form

$$\int_{\mathscr{D}'(R^d)} d\mu(\varphi) e^{i\langle \varphi, f \rangle} = e^{\Psi(f)},$$

where

$$\Psi(f) = \int_{R^d} dx \left(\int_{|\lambda|>0} d\sigma(\lambda)(e^{i\lambda f(x)} - \alpha(\lambda)(1 + i\lambda f(x))) + a_0 + i a_1 f(x) - a_2 \frac{(f(x))^2}{2!} \right), \tag{II.3}$$

for some positive constant a_2, any $a_1 \in R^d$, $a_0 \in R$ arbitrary, and the measure $d\sigma(\lambda)$ must fulfill certain regularity properties together with a function α (see Ref. 39 for details).

In particular, if λ is a sufficiently regular measure on R^1, then the functional

$$\Gamma(f) \equiv \exp\left\{ z \int dx \int d\lambda(\alpha)[e^{i\alpha f(x)} - 1] \right\}, \tag{II.4}$$

belongs to the class described by (II.3) for any $z > 0$. The corresponding generalized random field is called a Poisson random field with the intensity measure $z\, d\lambda$, and the corresponding measure will be denoted as $dP^{z,\lambda}$. For further use we shall collect here some basic properties of the Poisson generalized random fields.

1. Integration by parts formula

If $\int \alpha\, d\lambda(\alpha) < \infty$, then

$$\int_{\mathscr{D}'(R^d)} \langle q, f \rangle F(q) dP^{z,\lambda}(q) = z \int d\lambda(\alpha) \alpha \int_\Lambda dx\, f(x) \int F(q + \alpha \delta(-x)) dP^{z,\lambda}(dq). \tag{II.5}$$

2. Moments of $P^{z,\lambda}$

Under a suitable assumption made on $d\lambda$ the field $P^{z,\lambda}$ has moments of arbitrary order, and they are given by

$$\int_{\mathscr{D}'(R^d)} dP^{z,\lambda}(q) \prod_{i=1}^{N} \langle q, f_i \rangle = \sum_{1 \leqslant l \leqslant N_*} \sum_{\substack{m_1 v_1 + \cdots + m_l v_l = N \\ m_1 < \cdots < m_l}} z^{v_1 + \cdots + v_l} \times \sum_{\text{permut}} \hat{f}_{i_1^{(1)}, \ldots, i_{m_1}^{(1)}} \cdots \hat{f}_{i_1^{(r_l)}, \ldots, i_{m_l}^{(r_l)}} \cdots \hat{f}_{j_1^{(1)}, \ldots, j_{m_l}^{(l)}} \cdots \hat{f}_{j_l^{(r_l)}, \ldots, j_{m_l}^{(r_l)}}, \tag{II.6}$$

where $i_1^{(1)}, \ldots, j_{m_l}^{(r_l)} \in \{1, 2, \ldots, N\}$,

$$\hat{f}_{i_1,\ldots,i_{i_m}} \equiv \int dx \prod_{k=1}^{m} f_{i_k}(x) \int d\lambda(\alpha)\alpha^m \tag{II.7}$$

and

$$N_* = [\tfrac{1}{2}(8N+1)^{1/2} - 1], \tag{II.8}$$

where $[x]$ denotes the integer part of x.

3. Support property of $dP^{z,\lambda}$

Any Poisson field is supported on the set

$$\Xi_\infty = \sum_{i=1}^{\infty} \alpha_i \delta(x - x_i),$$

where $x_l \neq x_j$ for $l \neq j$ and the collection $\{x_1,\ldots,x_n,\ldots\}$ forms a locally finite configuration, $\alpha_i \in \operatorname{supp} d\lambda$ are chosen arbitrary, i.e. $P^{z,\lambda}(\Xi_\infty) = 1$.

4. Normal ordering of the Poisson fields (see Refs. 35–38)

For a given $q \in \Xi_\infty$ we shall write

$$\alpha(q) = (\alpha_1,\ldots,\alpha_n,\ldots), \quad \text{if } q = \sum_{i=1}^{\infty} \alpha_i \delta(x - x_i),$$

$$x(q) = (x_1,\ldots,x_n,\ldots), \quad \text{if } q = \sum_{i=1}^{\infty} \alpha_i \delta(x - x_i),$$

$$\alpha^2(q) = \sum_{l=1}^{\infty} \alpha_l^2, \quad \text{if } q = \sum_{i=1}^{\infty} \alpha_i \delta(x - x_i) \quad \text{and} \quad \sum_{l=1}^{\infty} \alpha_l^2 < \infty.$$

For any $q \in \Xi_\infty$ such that $q = \Sigma_i \alpha_i \delta(x - x_i)$ and all $x_i \in \Lambda$, where $\Lambda \in R^d$ is some bounded set, we define

$$:q(x)q(y): = q(x)q(y) - \delta(x-y)\alpha(q)q(y), \tag{II.9}$$

$$:qVq: = \int :q(x)V(x-y)q(y):dxdy = \int q(x)V(x-y)q(y)dxdy - \alpha(q)V(0)q(x), \tag{II.10}$$

if V is a locally integrable kernel and such that $V(0) < \infty$. If $V \in L^1_{\mathrm{loc}}(R^d)$ but $V(0) = \infty$, then we can define

$$:qVq: = \lim_{\epsilon \downarrow 0} :qV_\epsilon q:, \tag{II.11}$$

where the sequence of continuous kernels $V_\epsilon \to V$ locally in $L_1(R^d)$ as $\epsilon \downarrow 0$. See Refs. 35–38.

Also for q as above, we define

$$:q(x_1)q(x_2)q(x_3):=q(x_1)q(x_2)q(x_3)-\delta(x_1-x_2)q(x_1,\hat{\alpha}^2)q(x_3,\alpha)$$
$$-\delta(x_1-x_3)q(x_1,\alpha^2)q(x_2,\alpha)+2\,\delta(x_1-x_2)\,\delta(x_1-x_3)q(x_1,\alpha^3), \tag{II.12}$$

where for given $q(x)\equiv q(x,\alpha)=\Sigma_{i=1}\alpha_i\delta(x-x_i)$ localized in the bounded region $\Lambda\subset R^d$:

$$q(x,\hat{\alpha}^2)=\sum_{i=1}^{n}\alpha_i^2 q(x-x_i); \tag{II.13}$$

$$q(x,\alpha^p)=\sum_{i=1}^{n}\alpha_i^p q(x-x_i); \tag{II.14}$$

and similarly to (II.10) we can define define the random element: $qVqq$: for a suitably chosen kernel V on R^{3d}.

5. Conditional expectation values

For $\Lambda\subset R^d$ bounded we denote the $dP^{z,\lambda}$-completed σ-algebra $\Sigma(\Lambda)$ generated by the random elements $\{\langle q,f\rangle,\ q\in\Xi_\infty,\ f\in\mathscr{D}(\Lambda)\}$. Then we introduce the decomposition: for $q\in\Xi_\infty$: $q=\Sigma_{i=1}^{\infty}\alpha_i\delta(x-x_i)$ define

$$q_\Lambda\overset{df}{=}\sum_j \alpha_j\delta(x-x_j):x_j\in\Lambda$$

and

$$q_{\Lambda^c}=\sum_j \alpha_j\delta(x-x_j):x_j\in\Lambda^c.$$

The following formulas for the conditional expectation values are valid:

$$E_{P^{\lambda,z}}\{F|\Sigma(\Lambda^c)\}(q)=\int F(\eta_\Lambda,q_{\Lambda^c})dP^{z,\lambda}_{|\Sigma(\Lambda)}(\eta_\Lambda), \tag{II.15}$$

from which it follows rather easily that $dP^{z,\lambda}_\Lambda\equiv dP^{z,\lambda}_{|\Sigma(\Lambda)}$ is again ∞-divisible generalized random field on $\mathscr{D}'(\Lambda)$ with the characteristic functional [for $f\in\mathscr{D}(\Lambda)$],

$$\int e^{i\langle\varphi,f\rangle}dP^{z,\lambda}_\Lambda=e^{z\int_\Lambda\int(e^{i\alpha f(x)}-1)dx\,d\lambda(\alpha)} \tag{II.16}$$

and the set

$$\Xi_\Lambda=\left\{\sum_{i=1}^{n<\infty}\alpha_i\delta(x-x_i);x_i\in\Lambda,\alpha_i\in\text{supp }d\lambda\right\}$$

is the carrier set for $dP^{z,\lambda}_\Lambda$, i.e. $P^{z,\lambda}_\Lambda(\Xi_\Lambda)=1$.

B. Finite volume grand canonical Gibbs ensembles

Let Σ be a Borel subset of R^1 (in most of the applications we have in mind Σ is a discrete subset), which will be called the spaces of charges, and we shall assume that some ''*a priori*'' given regular measure λ is defined on Σ such that $\lambda(\Sigma)<\infty$ and λ has moments of all orders.

In the sets $(R^d\times\Sigma)^{\times k}$, $k=1,2,...,\infty$ the following equivalence relation is introduced: we will say that $\omega=((x_1,\alpha_1),\ldots,(x_k,\alpha_k))$ and $\omega' = ((x_1',\alpha_1'),\ldots,(x_k',\alpha_k'))$ are equivalent iff they differ only by permutations of pairs $(x_i,\alpha_i)\in R^d\times\Sigma$ composing them. Taking any $\Lambda\subset R^d$ and $\omega\in(R^d\times\Sigma)^{\times k}$, we shall denote by ω_Λ the element of $(\Lambda\times\Sigma)^{\times|\omega_\Lambda|}$ obtained from ω by removing those (x_i,α_i) for which $x_i\notin\Lambda$. The subset of $(R^d\times\Sigma)^\infty/\infty$ composing of those ω for which the following holds: *for any bounded* $\Lambda\subset R^d$, ω_Λ *belongs to some* $(\Lambda\times\Sigma)^{\times k}/\infty$ *for some finite* k will be called the set of locally finite configurations of the system and will be denoted by $C_{\mathrm{lf}}(R^d\times\Sigma)$. For a given $\Lambda\subset R^d$ we shall denote by $C(\Lambda\times\Sigma)\equiv\{\omega'=\omega_\Lambda$ for some $q\in C_{\mathrm{lf}}(R^d\times\Sigma)\}$.

Then we have

$$C_{\mathrm{lf}}(R^d\times\Sigma)\cong C_{\mathrm{lf}}(\Lambda\times\Sigma)\times C_{\mathrm{lf}}((R^d\backslash\Lambda)\times\Sigma),$$

for any $\Lambda\subset R^d$ and also $C(\Lambda\times\Sigma)=\cup_{n>0}C_n(\Lambda\times\Sigma)$ and $C_{\mathrm{lf}}(R^d\times\Sigma)=\cup_{n\geqslant 0}C_n(R^d\times\Sigma)$, where $C_n(\Lambda\times\Sigma)=\{\omega_\Lambda|\#\omega_\Lambda=n\}$, where $\#\omega_\Lambda\equiv$number of elements composing ω_Λ. The set $C_n(\Lambda\times\Sigma)$ can be identified with $(\Lambda\times\Sigma)^{\times n}/\infty$, therefore it is possible to transport the corresponding topological and measurable structures from $(\Lambda\times\Sigma)^r/\infty$ into the set $C_n(\Lambda\times\Sigma)$ and then into $C(\Lambda\times\Sigma)$ also. It is a result of Ref. 40 that the corresponding topological and measurable structures coincide on $C(\Lambda\times\Sigma)$. The corresponding σ-algebras will be denoted by $\Sigma_{(\Lambda)}$ and by $\Sigma(R^d)$ for $C_{\mathrm{lf}}(R^d\times\Sigma)$.

On the sets Δ_Λ^n defined by

$$\Delta_\Lambda^n\equiv\{\omega\in C_\Lambda(\Lambda\times\Sigma)|\#(\omega)=n,\omega=\omega_\Delta\},$$

we can define a map,

$$\Pi_{0,\Lambda}^{z,\lambda}(\Delta_\Lambda^n)\equiv\frac{z^n}{n!}\,\rho(\Delta)^n\left(\int_\Sigma\lambda(d\alpha)\right)^n \tag{II.17}$$

and then by standard construction we can extend this to a measure the σ-algebra generated by the sets Δ_Λ^n [coinciding with $\Sigma(\Lambda)$ for any Λ, including R^d also]. The corresponding measures will be called finite volume (if Λ is bounded) grand canonical free, Gibbs ensembles and will be denoted by $\tilde{\Pi}_\Lambda^{\lambda,z}$ and their corresponding normalized versions by $\Pi_\Lambda^{\lambda,z}$ and the infinite volume g.c. Gibbs free ensemble for $\Lambda=R^d$ with the notation $\tilde{\Pi}_\infty^{\lambda,z}$, respectively $\Pi_\infty^{\lambda,z}$, where $z>0$ stands for the chemical activity.

Let us define the map:

$$j_\Lambda:C(\Lambda\times\Sigma)\ni\omega=((x_1,\omega_1),\ldots,(x_n,\alpha_n))\to j_\Lambda(\omega)\equiv\Sigma_{i=1}^n\alpha_i\delta(x-x_i)\in\mathscr{D}'(\Lambda). \tag{II.18}$$

It follows easily that j_Λ is (weakly) $(\Sigma(\Lambda);\beta(\mathscr{D}'(\Lambda)))$ measurable and therefore the measure $\Pi_\Lambda^{\lambda,z}$ can be transported on the space $((\mathscr{D}'(\Lambda)),\beta(\mathscr{D}'(\Lambda)))$ by this map. Then for any bounded and measurable F on $\mathscr{D}'(\Lambda)$ we have

$$\int_{\mathscr{D}'(\Lambda)}d(j_\Lambda\circ\Pi_\Lambda^{z,\lambda})(q)F(q)=\int_{C(\Lambda\times\Sigma)}d\Pi_\Lambda^{z,\lambda}(\hat{\omega})(F\circ j_\Lambda)(\omega). \tag{II.19}$$

Taking $F(q)\equiv e^{\langle q,f\rangle}$ for $f\in\mathscr{D}(\Lambda)$ we obtain

$$\int_{\mathscr{D}'(\Lambda)}d(j_\Lambda\circ\Pi_\Lambda^{z,\lambda})(q)e^{i\langle q,f\rangle}=\exp\left\{z\int d\lambda(\alpha)\int dx(e^{i\alpha f(x)}-1)\right\} \tag{II.20}$$

by an easy $C(\Lambda\times\Sigma)$-calculation, in which we recognize a characteristic functional of Poisson g.r.f. $dP_{\Lambda}^{z,\lambda}$ on $\mathscr{D}'(\Lambda)$.

Any measurable function $\mathscr{E}^{\Lambda}:\hat{\Omega}(\Lambda)\to(-\infty,\infty]$ will be called interaction. We shall require that $\mathscr{E}^{\Lambda}$ is thermodynamically stable, i.e., there exists $B>0$ such that for any $\hat{\omega}\in\hat{\Omega}(\Lambda)$: $\mathscr{E}^{\Lambda}(\hat{\omega})\geqslant -|\hat{\omega}|B$ uniformly in Λ. Having in mind the decomposition $\hat{\Omega}(\Lambda)=\cup_{n\geqslant 0}^{\infty}\Omega_n(\Lambda)$ we can define a sequence of potentials $\mathscr{V}=(\widetilde{V}_1,\widetilde{V}_2,\ldots)$, which determines $\mathscr{E}^{(\Lambda)}$. To avoid the complicated notation, the following assumption on $\mathscr{V}$ will be made throughout this paper.

(H1) $\widetilde{\mathscr{V}}=(\widetilde{V}_2,\widetilde{V}_3,0,\ldots)$, i.e. we shall consider only two and three body forces, (H2) $\widetilde{V}_2,\widetilde{V}_3$ are of the following form:

$$\widetilde{V}_2(\hat{x},\hat{y})=\widetilde{V}_2((x,\alpha),(y,\beta))=\alpha\beta V_2(x,y),$$

$$\widetilde{V}_2((x,\alpha),(y,\beta),(z,\gamma))=\alpha\beta\gamma V_3(x,y,z).$$

The energy function is then given by

$$\mathscr{E}_{\mathscr{V}}^{\Lambda}:C(\Lambda\times\Sigma)\ni\hat{\omega}=(\hat{x}_1,\ldots,\hat{x}_n)\to\mathscr{E}_{\mathscr{V}}^{\Lambda}(\hat{\omega})$$

$$=\sum_{1\leqslant i<j\leqslant n}\alpha_i\alpha_j V_2(x_i,x_j)+\sum_{1\leqslant i<j<k\leqslant n}\alpha_i\alpha_j\alpha_k V_3(x_i,x_j,x_k) \quad \text{(II.21)}$$

The finite volume partition function $Z_{\Lambda}^{\lambda}(z,\beta)$ is given by

$$Z_{\Lambda}^{\lambda}(z,\beta)=\int_{C(\Lambda)}d\Pi_{\Lambda,0}^{z,\lambda}(\hat{\omega})\exp(-\beta\mathscr{E}_{\mathscr{V}}^{\Lambda}(\hat{\omega}), \quad \text{(II.22)}$$

and the (unconditioned) grand canonical Gibbs ensemble by the measure

$$d\Pi_{\Lambda}^{z,\lambda}(\hat{\omega})\equiv(Z_{\Lambda}^{\lambda}(z,\beta))^{-1}\exp\{-\beta\mathscr{E}_{\mathscr{V}}^{\Lambda}(\hat{\omega})\}d\Pi_{\Lambda,0}^{z,\lambda}(\hat{\omega}). \quad \text{(II.23)}$$

This measure is uniquely determined by the so-called correlation functions ρ_{Λ}. For our purposes, however, the more suitable objects are so-called reduced correlation functions $\hat{\rho}_{\Lambda}$, given by

$$\hat{\rho}_{\Lambda}(\hat{\omega}_n)=\exp\beta\mathscr{E}_{\mathscr{V}}^{\Lambda}(\hat{\omega}_n)\rho_{\Lambda}(\hat{\omega}_n)=z^n\sum_{m\geqslant 0}^{\infty}\frac{z^m}{m!}\int_{\Lambda}d\hat{y}|_1^m\frac{\exp\{-\beta\mathscr{E}_{\mathscr{V}}^{\lambda}(\hat{y}_1^n)\}\exp\{-\beta\mathscr{E}_{\mathscr{V}}^{\Lambda}(\hat{y}_1^n|\hat{x}_1^n)\}}{Z_{\Lambda}(z,\beta)}, \quad \text{(II.24)}$$

where

$$\hat{x}_1^n=(\hat{x}_1,\ldots,\hat{x}_n)=((x_1,\alpha_1),\ldots,(x_n,\alpha_n)), \quad \text{(II.25)}$$

$$\int_{\Lambda}d\hat{x}_1^n\equiv\int_{\Lambda}\prod_{i=1}^{n}dx_i\,d\lambda(\alpha_i); \quad \text{(II.26)}$$

$$\mathscr{E}_{\mathscr{V}}^{\Lambda}(\hat{y}_1^m|\hat{x}_1^n)=\mathscr{E}_{\mathscr{V}}^{\Lambda}(\hat{x}_1^n V\hat{y}_1^m)-\mathscr{E}_{\mathscr{V}}^{\Lambda}(\hat{x}_1^n)-\mathscr{E}_{\mathscr{V}}^{\Lambda}(\hat{y}_1^m). \quad \text{(II.27)}$$

For a moment we shall assume that the potentials V_2 and V_3 are bounded functions on R^{2d} and R^{3d}, respectively.

Let us consider first the case $V_3\equiv 0$.

Proposition II.1: Let us assume that $\widetilde{V}_2$ is stable, then the following formulas hold:

$$Z_\Lambda^\lambda(z,\beta)=\int_{\mathscr{D}'(\Lambda)} dP_\Lambda^{z,\lambda}(q)e^{-(\beta/2):V_2^\Lambda(q,q):} \tag{II.28}$$

(1) where

$$:V_2^\Lambda(q,q):\equiv\int_\Lambda dx\ dy:q(x)V_2(x,y)q(y):. \tag{II.29}$$

(2) The reduced, grand canonical correlation functions are given by

$$\hat\rho_\Lambda(\hat x_1^n)=z^n\int_{\mathscr{D}'(R^d)} d\mu_\Lambda^{z,\lambda}(q)\prod_{i=1}^n e^{-\beta V_2(q)(x_i)}, \tag{II.30}$$

where

$$e^{-\beta V_2(q)(x)}=e^{-\beta\int dy\ V_2(x-y)q(y)};$$

and

$$d\mu_\Lambda^{z,\lambda}(q)=\frac{\exp\left(-\frac{\beta}{2}\int_\Lambda :q(x)V(x-y)q(y):dx\ dy\right)}{Z_\Lambda^\lambda(z,\beta)}\,dP_{\Lambda,0}^{z,\lambda}. \tag{II.31}$$

(a) Proof: It follows by an easy $(C(\Lambda\times\Sigma),\Pi_{\Lambda,0}^{z,\lambda})$ calculation using the transport formula (II.20).

Similarly we obtain the following.

Proposition II.2: Let $(\widetilde V_2,\widetilde V_3)$ *be stable and such that*

$$\sup_x V_3(x,x,x)<\infty,\quad \sup_{x,y}V_3(x,x,y)<\infty,\quad V_2(0)<\infty.$$

Then the following formulas are valid:

$$Z_\Lambda^\lambda(z,\beta)=\int_{\mathscr{D}'(\Lambda)} dP_\Lambda^{z,\lambda}(q)e^{-\beta:\mathscr{E}_\Lambda^\nu(q,q,q):}, \tag{II.32}$$

(1) where

$$:\mathscr{E}_\Lambda^\nu(q):=\frac{1}{2}:V_2(q,q):+\frac{1}{3!}:V_3(q,q,q):.$$

(2) The corresponding reduced correlation functions are given by

$$\rho_\Lambda^n(\hat x_1^n)=z^n\int_{\mathscr{D}'(\Lambda)} d\mu_\Lambda(q)\prod_{i=1}^n e^{-\beta V_2(q)(x_i)}\prod_{1\le i<j\le n} e^{-\beta V_3^1(q)(x_i,x_j)}\prod_{i=1}^n e^{-\beta V_3^2(q)(x_i)}, \tag{II.33}$$

where

$$V_3^1(q)(x_i,x_j)=\int_\Lambda dy\ q(y)V_3(x_i,x_j,y);$$

$$V_3^2(q)(x)=\int_\Lambda dy\int_\Lambda dy' :q(x)q(y):V_3(x,y,y'); \tag{II.34}$$

$$d\mu_\Lambda(q)=(Z_\Lambda^\lambda(z,\beta))^{-1}e^{-\beta:\mathscr{E}_\Lambda^\nu:(q)}\ dP_\Lambda^{z,\lambda}.$$

(b) Proof: Again by passing to $(C(\Lambda\times\Sigma),\Pi_{\Lambda,0}^{z,\lambda})$ variables and the use of the normal product definition, as described in Sec. II A *4*.

Now let $(\chi_\epsilon)_{\epsilon>0}$ be a positive mollifier on R_+^d, i.e. $\chi_\epsilon(x)\in C_0^\infty(R^d)$; $\chi_\epsilon\geqslant 0$; $\sup\chi_\epsilon\subset B(0,\epsilon)$; $\|\chi_\epsilon\|_1=1$ and $\omega-\lim_{\epsilon\downarrow 0}\delta_\epsilon(x)=\delta$ (in the weak sense). Taking $V\in L^1_{\mathrm{loc}}(R^d)$ we see that $\chi_\epsilon * V\equiv V^\epsilon\epsilon C^\infty(R^d)$, and moreover, $\lim_{\epsilon\downarrow 0}V^\epsilon=V$ locally in the $L^1(R^d)$ sense.

Proposition II.3: Let $\mathscr{V}=(0,V_2,0,...)$ be such that $V_2\in L^1_{\mathrm{loc}}(R^d)$ is stable and translationally invariant.

(1) Then for any regularizing sequence χ_ϵ as above the following limit:

$$\hat\Gamma_\Lambda(f)=\lim_{\epsilon\downarrow 0}\hat\Gamma_\Lambda^\epsilon(f)=\int_{\mathscr{D}'(\Lambda)}dP_\Lambda^{z,\lambda}(q)e^{-\beta/2V_2^\epsilon(q,q)_\Lambda:}e^{i(q,f)} \tag{II.35}$$

exists and defines continuous and positively defined functional on $\mathscr{D}(\Lambda)$.

(2) For any $(\chi_\epsilon)_{\epsilon>0}$, any $p\geqslant 1$ the limit

$$\lim_{\epsilon\downarrow 0}e^{-:\beta/2V_2^\epsilon(q,q)_\Lambda:}\equiv e^{-:\beta/2V_2(q,q)_\Lambda:} \tag{II.36}$$

exist in the $L^p(\mathscr{D}'(\Lambda),dP_\Lambda^{z,\lambda})$ sense.

(3) For any $(\chi_\epsilon)\subset C_0^\infty(R^d)$ as above, the limits

$$\hat\rho_\Lambda^n(\hat x_1^n)=\lim_{\epsilon\downarrow 0}\frac{\int_{\mathscr{D}'(\Lambda)}d\mathscr{P}_\Lambda^{z,\lambda}(q)\Pi_{i=1}^n\exp(-\beta\Sigma_{i=1}^n(q*V_\epsilon)(x_i))\exp\{-\beta/2:V_\Lambda^\epsilon(q,q):\}}{\hat\Gamma_\Lambda^\epsilon(0)}, \tag{II.37}$$

exists pointwise on $(\Lambda\times\Sigma)^{\times n}/\infty$.

Remark: The same convergence results hold for many body interactions, provided they are not too singular.

As a simple corrolary, we obtain the following.

Corollary II.4: Let $V_2\in L^1_{\mathrm{loc}}(R^d)$ be stable and translationally invariant potential. Then there exists a probabilistic, Borel cylindric measure $d\mu_\Lambda^{(z,\lambda)}$ on $\mathscr{D}'(\Lambda)$, such that

$$\int_{\mathscr{D}'(\Lambda)}e^{i\langle q,f\rangle}d\mu_\Lambda^{(z,\lambda)}(q)=\frac{\hat\Gamma_\Lambda(f)}{\hat\Gamma_\Lambda(0)}\equiv\Gamma_\Lambda(f). \tag{II.38}$$

The measures $d\mu_\Lambda^{(z,\lambda)}$ are locally absolutely continuous with respect to $dP_\Lambda^{z,\lambda}$ and the corresponding Radon–Nikodym derivatives are given by

$$\frac{d\mu_\Lambda^{(z,\lambda)}(q)}{dP_\Lambda^{z,\lambda}(q)}=\exp\left\{-\frac{\beta}{2}:V_\Lambda(q,q):\right\}. \tag{II.39}$$

(c) Proof: By the $(C(\Lambda\times\Sigma);d\Pi_{\Lambda,0}^{z,\lambda})$ calculations, we have

$$\hat{\Gamma}^{\epsilon}_{\Lambda}(f)=\int_{\mathscr{D}'(\Lambda)} dP^{z,\lambda}_{\Lambda}(q)e^{i\langle q,f\rangle}\exp\left\{-\frac{\beta}{2}:V^{\epsilon}_{\Lambda}(q,q):\right\}$$
$$=e^{-z\lambda(\Sigma)|\Lambda|}\sum_{n\geqslant 0}^{\infty}\frac{z^n}{n!}\int d(\hat{x})^n_1\prod_{i=1}^{n}[e^{i\alpha_i f(x_i)}-1]e^{-\beta\mathscr{E}_{V^{\epsilon}_2}(\hat{x}^n_1)}, \tag{II.40}$$

where

$$\mathscr{E}_{V^{\epsilon}_2}(x^n_1)=\frac{1}{2}\sum_{1\leqslant i<j\leqslant n}\alpha_i\alpha_j V^{\epsilon}_2(x_i-x_j). \tag{II.41}$$

From the assumed stability of $\mathscr{E}_{V^{\epsilon}_2}$ follows the uniform (in ϵ) estimate

$$|\hat{\Gamma}^{\epsilon}_{\Lambda}(f)|\leqslant\exp\left\{z\int_{\Lambda}d(\hat{x})|e^{if(x)}|e^{\beta B}\right\}e^{-z|\lambda(\Sigma)||\Lambda|}, \tag{II.42}$$

which means that the series (II.40) is uniformly convergent in ϵ. The nth term of (II.40) can be estimated by the following inequality:

$$\left|\int_{\Lambda}d(\hat{x})^n_1\left(\prod_{i=1}^{n}e^{\alpha_i f(x_i)}e^{-\beta\mathscr{E}_{\nu^{\epsilon}_2}(\hat{x}^n_1)}-\prod_{i=1}^{n}e^{\alpha_i f(x_i)}e^{-\beta\mathscr{E}_{\nu^{\epsilon'}_2}(\hat{x}^n_1)}\right)\right|$$
$$\leqslant\int_0^1 ds\ se^{n\beta B}\sum_{1\leqslant i<j\leqslant n}\int_{\Lambda}d(\hat{x})^n_1\alpha_i\alpha_j|V^{\epsilon}_2(x_i-x_j)-V^{\epsilon'}_2(x_i-x_j)|. \tag{II.43}$$

Therefore, assuming $V_2\in L^1_{\mathrm{loc}}(R^d)$, we conclude that the nth term in (II.40) is convergent in ϵ to the corresponding expression with $\epsilon=0$.

Therefore $\lim_{\epsilon\downarrow 0}\hat{\Gamma}^{\epsilon}_{\Lambda}(f)=\Gamma_{\Lambda}(f)$ exists and is given by (II.35). From the estimate (II.42) the continuity of $\Gamma_{\Lambda}(f)$ on $\mathscr{D}'(\Lambda)$ follows easily.

Again, by $C(\Lambda\times\Sigma)$ calculations:

$$\int_{\mathscr{D}'(\Lambda)}\left|e^{-\beta/2:\nu^{\epsilon}_{2\Lambda}(q,q):}-e^{-\beta/2:\nu'_{2\Lambda}(q,q):}\right|^2 dP^{z,\lambda}_{\Lambda}(q)$$
$$=e^{-z|\lambda(\Sigma)||\Lambda|}\sum_{n\geqslant 0}^{\infty}\frac{z^n}{n!}\int_{\Lambda^n}d(\hat{x}^n_1)(e^{-2\beta\mathscr{E}_{\nu^{\epsilon}_2}(\hat{x}^n_1)}+e^{-2\beta\mathscr{E}_{\nu^{\epsilon'}_2}(\hat{x}^n_1)}-2e^{-\beta\mathscr{E}_{\nu^{\epsilon}_2}(\hat{x}^n_1)}e^{-\beta\mathscr{E}_{\nu^{\epsilon'}_2}(\hat{x}^n_1)})$$
$$\leqslant e^{-z|\lambda(\Sigma)||\Lambda|}2\sum_{n\geqslant 0}^{\infty}\frac{z^n}{n!}e^{2\beta Bn}\beta\int_{\Lambda^n}d(\hat{x})^n_1|\mathscr{E}_{\nu^{\epsilon}_2}(\hat{x}^n_1)-\mathscr{E}_{\nu^{\epsilon}_2}(\hat{x}^n_1)|. \tag{II.44}$$

The nth term of the last line is convergent to zero as $\epsilon\downarrow 0$, provided $V_2\in L^1_{\mathrm{loc}}(R^d)$. Moreover, the whole series appearing in the middle of (II.44) is uniformly convergent in ϵ as it follows from the stability of V^{ϵ}_2.

As an immediate application of our formulas we propose the following.

Corollary II.5: Let us assume that V_2 is superstable, i.e. $\mathscr{E}_{V_2}$ is superstable on $C_{\mathrm{lf}}(R^d\times\Sigma)$, that $V_2\in L^1_{\mathrm{loc}}$, and that $\mathscr{E}_{V_2}$ is lower regular on $C_{\mathrm{lf}}(R^d\times\Sigma)$ in the sense of Ruelle.[44] *Then the family of measures $(d\mu^{(z,\lambda)}_{\Lambda})_{\Lambda}$ indexed by bounded $\Lambda\subset R^d$ is precompact (in the topology of convergence of all finite-dimensional projections) in the space of measures on $(\mathscr{D}'(R^d),\mathscr{B}(\mathscr{D}'(R^d)))$.*

(d) Proof: For any $\zeta\in C$, $\zeta=t+is$ and using $C(\Lambda\times\Sigma)$ calculations, we obtain

$$\int_{\mathscr{D}'(\Lambda)} e^{\xi\langle q,f\rangle}\, d\mu_\Lambda^{(z,\lambda)}(q)=\sum_{n\geqslant 0}\frac{z^n}{n!}\int_\Lambda d(\hat{x})_1^n[e^{\xi f(x_i)}-1]\rho_\Lambda^n(\hat{x}_1^n). \tag{II.45}$$

From Ruelle's work[41] we conclude that there exists a constant C independent of z and Λ, such that

$$\operatorname*{ess\,sup}_{(\hat{x}_1^n)}|\rho_\Lambda^n(\hat{x}_1^n)|\leqslant C^n, \tag{II.46}$$

from which follows that

$$\left|\int_{\mathscr{D}'(\Lambda)} e^{\xi\langle g,f\rangle}\, d\mu_\Lambda^{(z,\lambda)}(q)\right|\leqslant\exp\left\{C|\zeta|\|f\|_1\int_0^1 e^{\xi s\|f\|_\infty}\, ds\right\}. \tag{II.47}$$

□

C. Infinite-volume grand canonical Gibbs measures

Let $\Xi_\infty\subset\mathscr{D}'(R^d)$ be the Borel subset consisting of those q that are of the form $q(x)=\Sigma_{i=1}^n\delta(x-x_i)$, where $x_i\neq x_j$ for $i\neq j$ and such that for any bounded $\Lambda\subset R^d$, the cardinality of the set of those x_i that belong to Λ is finite. The corresponding cardinality will be denoted by $\#(q_\Lambda)$. The smaller subset $\Xi_\infty^T\subset\Xi_\infty$ of so-called tempered configurations $q\in\mathscr{D}'(R^d)$ is defined by requiring that there exists a constant $a=a(q)$ such that for any $\square_r=\{x\in R^d|\mathrm{dist}(r,x)\leqslant 1\}$, we have $\#(q_{\square_r})\leqslant a\ \log_+ r$ for a sufficiently large r.

Taking a stable potential $\mathscr{V}$ we then define the following probabilistic kernels:

$${}^{\mathscr{V}}\Pi_\Lambda^{(\Lambda')}(-|-)(z,\beta,\mathscr{V})\mathscr{D}'(\Lambda)\times\Xi_{\Lambda'\setminus\Lambda}\to[0,1], \tag{II.48}$$

by

$$\begin{aligned}{}^{\mathscr{V}}\Pi_\Lambda^{(\Lambda')}(dq_\Lambda|\,\eta_{\Lambda'\setminus\Lambda})(z,\beta,\mathscr{V})&=(Z_\Lambda^{(\Lambda')}(\,\eta_{\Lambda'\setminus\Lambda}))^{-1}\ \exp\{-\beta\mathscr{E}_{\mathscr{V}}(q_\Lambda)\}\\&\quad\times\exp\{-\beta\mathscr{E}_{\mathscr{V}}^c(q_\Lambda|\,\eta_{\Lambda'\setminus\Lambda})\}dP_\Lambda^z(q_\Lambda),\end{aligned} \tag{II.49}$$

where $\Lambda\subset\Lambda'$ are bounded subsets of R^d,

$$\mathscr{E}_{\mathscr{V}}(q_\Lambda|\,\eta_{\Lambda'\setminus\Lambda})=\mathscr{E}_{\mathscr{V}}(q_\Lambda\cup\eta_{\Lambda'\setminus\Lambda})-\mathscr{E}_{\mathscr{V}}(q_\Lambda)-\mathscr{E}_V(\,\eta_{\Lambda'\setminus\Lambda}), \tag{II.50}$$

$$Z_\Lambda^{(\Lambda')}(\,\eta_{\Lambda'\setminus\Lambda})=\int_{\mathscr{D}'(R^d)}dP_\Lambda^z(q_\Lambda)\exp\{-\beta\mathscr{E}_{\mathscr{V}}(q_\Lambda)\}\exp\{-\beta\mathscr{E}_{\mathscr{V}}(q_\Lambda|\,\eta_{\Lambda'\setminus\Lambda})\}. \tag{II.51}$$

Let us define the following σ-algebras:

$$\widetilde{\Sigma}(\Lambda)\equiv\sigma\{(q,f\ )|f\in C_0^\infty(\Lambda);q\in\Xi_\Lambda\},$$

being subalgebras of the Borel σ-algebra in $\mathscr{D}'(R^d)$. For a given $\mathscr{V}$ we define $\Xi_\infty(\mathscr{V})$ as a Borel subset of Ξ_∞ consisting of those η for which

(i)

$$\lim_{\widetilde{\Lambda}\uparrow\Lambda^c} Z_\Lambda^{\widetilde{\Lambda}}(\,\eta_{\widetilde{\Lambda}})\equiv Z_\Lambda(\,\eta_{\Lambda^c}),$$

exists for any countably generated filter $\widetilde{\Lambda}$ tending to Λ^c and is filter independent and

(ii)

$$\lim_{\tilde{\Lambda}\uparrow\Lambda^c} \mathscr{E}_{\mathscr{T}}(q_\Lambda|\eta_{\tilde{\Lambda}}) \equiv \mathscr{E}_{\mathscr{T}}(q_\Lambda|\eta_{\Lambda^c}),$$

exists for any $q_\Lambda \in \Xi_\Lambda$ and any filter $(\tilde{\Lambda})$ as above, and the limit is filter independent.

Definition II.1 (after Dobrushin[42]): Any probabilistic Borel cylindric measure μ on $(\mathscr{D}'(R^d), \beta(\mathscr{D}'(R^d)))$, such that
(G0)

$$\mu(\Xi_\infty(\mathscr{T})) = 1;$$

(G1) for any bounded $\Lambda \subset R^d$, any bounded and $\Sigma(\Lambda)$-measurable function F,

$$\int_{\mathscr{D}'(P^d)} d\mu(\eta)\, {}^{\mathscr{P}}\Pi_\Lambda(F|\eta_{\Lambda^c})(z,\beta,\mathscr{T}) = \int_{\mathscr{D}'(R^d)} d\mu(q) F(q), \tag{II.52}$$

(LR)
where ${}^{P}\Pi_\Lambda(-|-)(z,\beta,\mathscr{T})$ is defined as the (weak) limit of $\Pi_\Lambda^{(\tilde{\Lambda})}(-|-)(z,\beta,\mathscr{T})$, will be called the functional, grand canonical Gibbs ensemble for a system $(\mathscr{T},\lambda,z,\beta)$. The set of all functional grand canonical Gibbs ensembles will be denoted by ${}^{\mathscr{P}}\mathscr{G}(z,\beta)$. The set of those $\mu \in {}^{\mathscr{P}}\mathscr{G}(z,\beta)$ that are supported on the tempered configurations will be denoted by ${}^{\mathscr{P}}\mathscr{G}^{T}(z,\beta)$ and will be called the set of tempered grand canonical Gibbs ensembles for $(\mathscr{T},\lambda,z,\beta)$.

There exists a corresponding notion of the grand canonical Gibbs ensembles in the language of the space $(C_{\mathrm{lf}}(R^d), \beta(C_{\mathrm{lf}}(R^d)))$ (see. e.g., Refs. 5, 6). The corresponding set of grand canonical (tempered) Gibbs ensembles for $(z,\mathscr{T},\lambda,\beta)$ will be denoted by $\mathscr{G}^{(T)}(z,\beta)$.

We extend the representation of the grand canonical Gibbs ensemble by functional integrals to the infinite volume limit situation by the following result.

Theorem II.6: *There exists a bijection $\mathscr{T}_\infty$ between the set ${}^{\mathscr{P}}\mathscr{G}(z,\beta)$ and $\mathscr{G}(z,\beta)$. The bijection $\mathscr{T}_\infty$ when restricted to the Martin–Dynkin boundary of ${}^{\mathscr{P}}\mathscr{G}(z,\beta)$ is still bijection between $\partial^{\mathscr{P}}\mathscr{G}(z,\beta)$ and $\partial\mathscr{G}(z,\beta)$.* (The existence of the Martin–Dynkin boundary and the corresponding integral decomposition follows from the general abstract arguments of Fölmer.[52])

(e) Proof: Let

$$\pi_\infty : C_{fl}(R^d) \ni \tilde{x} \to \pi_\infty(\tilde{x}) = \sum_{i=1}^{\infty} \alpha_i \delta(x - x_i) \in \mathscr{D}'(R^d). \tag{II.53}$$

It is easy to note that the map π_∞ is (weakly) measurable, and moreover, $\pi_\infty(C_{fl}(\mathscr{T})) = \Xi_\infty(\mathscr{T})$. Therefore any Borel measure $\tilde{\mu}$ concentrated on the set $C_{fl}(\mathscr{T})$ can be transported onto the Borel measure $\mu = \pi_\infty \circ \mu$ on $\beta(\mathscr{D}'(R^d))$, such that $\mu(\Xi_\infty(\mathscr{T})) = 1$.

Assuming that $\tilde{\mu} \in \mathscr{G}(z,\beta)$, it follows by an easy calculation that for any $\tilde{y} \in C_{fl}(\mathscr{T})$,

$$\begin{aligned} Z_\Lambda(\tilde{y}_{\Lambda^c}) &= \int_{C_{(\Lambda)}} d\Pi_{\Lambda,0}^{z,\lambda}(\tilde{x}) e^{-\beta \mathscr{E}_{\mathscr{T}}(\tilde{x})} e^{-\beta \mathscr{E}_{\mathscr{T}}(\tilde{x}|\tilde{y}_{\Lambda^c})} \\ &= \int_{\mathscr{D}'(R^d)} dP_\Lambda^z(q_\Lambda) \exp[-\beta \mathscr{E}_{\mathscr{T}}(q_\Lambda)] \exp[-\beta \mathscr{E}_{\mathscr{T}}(q|\pi_\infty(\tilde{y}_{\Lambda^c})], \end{aligned} \tag{II.54}$$

and for any $|\Lambda| < \infty$, $\tilde{y} \in C_{\mathrm{lf}}(\mathscr{T})$:

$$\pi_\infty \circ \Pi_\Lambda(d\tilde{x}|\tilde{y}_{\Lambda^c})(z,\beta,\mathscr{T}) = {}^{\mathscr{P}}\Pi(\pi_\infty(d\tilde{x}_\Lambda)|\pi_\infty(\tilde{y}_{\Lambda^c})). \tag{II.55}$$

Therefore, if we assume that $\tilde{\mu}$ fulfills the DLR equation on

$$(C_{\mathrm{lf}}(R^d);\beta(C_{\mathrm{lf}}(R^d))),$$

then the transported $\mu=\pi_\infty\circ\tilde{\mu}$ fulfills the corresponding DLR equation on $(\mathscr{D}'(R^d),\ \beta(\mathscr{D}'(R^d)))$, and vice versa. Thus, we have proved that $\pi_\infty\circ(\mathscr{G}(z,\beta))=^{\mathscr{P}}\mathscr{G}(z,\beta)$.

If now $\tilde{\mu}\in\partial\mathscr{G}(z,\beta)$, then the corresponding ''σ-algebra at infinity'' $\Sigma_\infty^{\tilde{\mu}}=\cap_{\Lambda\subset R^d}\Sigma_{\tilde{\mu}}(\Lambda^c)$ must be $\tilde{\mu}$-trivial (see, e.g., Refs. 3, 5, 8), and this is also sufficient for $\tilde{\mu}\in\partial\mathscr{G}(z,\beta)$.

From the formula

$$E_{\tilde{\mu}}\{F|\hat{\Sigma}(\Lambda^c)\}(\tilde{y}_{\Lambda C})=E_{\pi_\infty\circ\tilde{\mu}}\{F\circ\pi_\infty|\Sigma(\Lambda^c)\}(\pi_\infty(\tilde{y}_\Lambda c),\tag{II.56}$$

where

$$\hat{\Sigma}(\Lambda^c)\overset{df}{\equiv}\sigma\{\tilde{y}_{\Lambda^c}\}\subset\beta(C_{\mathrm{lf}}(R^d)),\tag{II.57}$$

it follows that $\pi_{\infty|\partial\mathscr{G}(z,\beta)}$ is still injective and is surjective on $^{\mathscr{P}}\mathscr{G}(z,\beta)$. □

Before closing this section let us remark that in the case of positive-definite two body potential V_2, such that $V_2(0)<\infty$ another interesting functional integral representation, that we call mixed Poisson-sine-Gordon representation exists. Let $d\mu_{V_2}$ denote the centered Gaussian measure on $\mathscr{D}'(R^d)$ with the covariance V_2. Then the following formulas are valid:

$$Z_\Lambda^\lambda(z,\beta)=\int_{\mathscr{D}'(\Lambda)\otimes\mathscr{D}'(R^d)}dP_\Lambda^{z,\lambda}(q)\otimes d\mu_V(\varphi)e^{i\sqrt{\beta}\langle\varphi,q\rangle}e^{(\beta/2)V(0)(\#(q))}\tag{II.58}$$

and

$$\rho_\Lambda^{(n)}((\hat{x})_1^n)=z^n\int_{\mathscr{D}'(\Lambda)\otimes\mathscr{D}'(R^d)}d\mu_\Lambda^{(z,\beta,\lambda)}(\varphi,q)\prod_{i=1}^n:e^{i\sqrt{\beta}\langle\varphi,q(x_i)\rangle}:,\tag{II.59}$$

where

$$d\mu_\Lambda^{(z,\beta,\lambda)}(\varphi,q)=\frac{:e^{i\sqrt{\beta}\langle\varphi,q\rangle}:d\mu_V(\varphi)\otimes dP_\Lambda^{z,\lambda}(q)}{Z_\Lambda^\lambda(z,\beta)},\tag{II.60}$$

$$:e^{i\sqrt{\beta}\langle\varphi,q(x_i)\rangle}:=\exp\left(\frac{\beta}{2}V(0)(\#q)\right)\exp(i\sqrt{\beta}\langle\phi,q(x_i)\rangle),\quad q(x_i)=q(.-x_i).\tag{II.61}$$

Whether the mixed Poisson-sine-Gordon representation might be useful remains to be investigated. (The picture arising is similar to those described in Ref. 43.)

III. CYLINDRICAL APPROXIMATIONS

For simplicity we take $\Sigma=\{1\}$ and $\lambda\{1\}=1$ in this section.

Let p_z denote the one-dimensional Poisson distribution on the real line R^1, with the intensity parameter $z>0$, i.e.

$$p_z(dx)=e^{-z}\sum_{n\geqslant 0}\frac{z^n}{n!}\delta(x-n).$$

Then the characteristic functional γ_z of p_z is given by

$$\gamma_z(\alpha)=\int e^{i\alpha x}p_z(dx)=e^{z(e^{i\alpha}-1)}. \tag{III.1}$$

Let $(\chi_\epsilon)_{\epsilon>0}$ be a positive mollifier on R^d, such that supp $\chi_\epsilon=B(0,\epsilon)$. Defining $q_\epsilon=(q*\chi_\epsilon)(x)$ and computing

$$\Gamma_\epsilon(f)\equiv\int_{\mathscr{D}'(R^d)} e^{i\langle q_\epsilon,f\rangle}\,dP^z_\Lambda(q)=\exp\left(z\int(e^{if_\epsilon(x)}-1)dx\right), \tag{III.2}$$

we see that

$$\Gamma^z_\epsilon(\alpha)\equiv\lim_{f\to\delta_x}\Gamma_\epsilon(f)=\int e^{i\langle q_\epsilon,\delta_x\rangle}\,d\mathscr{P}_\Lambda(q)=\exp z|B(0,\epsilon)|\exp z\left(\int e^{i\alpha\chi_\epsilon(y)}\,dy\right). \tag{III.3}$$

Let (B_i) be any measurable partitioning of $B(0,\epsilon)$. Then we can approximate Γ^z_ϵ by

$$\Gamma^z_\epsilon\equiv\prod_{i=1}^n\gamma_{z|B_i|}(\alpha\chi_\epsilon(y_i)), \tag{III.4}$$

where $y_i\in B_i$. Thus, if (B_{i_α}) in any family of measurable partitioning of $B(0,\epsilon)$ such that $\max\{\text{diam } B_{i_\alpha}\}\to 0$ as $m\to\infty$, then for any choice of $y_{i_\alpha}\in B_{i_\alpha}$ we have the equality

$$\Gamma^z_\epsilon=\lim_m\gamma_{i_m}|P_{z|B_{i_m}(0,\epsilon)|}(\alpha\chi_\epsilon(y_{i_m})). \tag{III.5}$$

The measure $p^z_\epsilon(dx)$ on R^1, defined by

$$\Gamma^{(z)}_\epsilon(\alpha)=\int e^{i\alpha x}p^\epsilon_z(dx), \tag{III.6}$$

will play the role of a single spin distribution in our cylindrical approximation to the measure $d\mu_\Lambda$, given by (II.34). It is easy to see that p^z_ϵ is concentrated on the real half-line $R_+=\{x\in R|x\geqslant 0\}$ and is given by a limit of an infinite divisible distribution,

$$P_{z|B_l(0,\epsilon)|}\left(\frac{dx}{\chi_\epsilon(y_i)}\right). \tag{III.7}$$

For a given small $\rho>0$, let Z^d_ρ denote the lattice of size ρ in R^d, i.e. $Z^d_\rho=\{(x_z,\ldots,x_d)|x_i=n_i\rho;n_i\in Z\}$ and we denote for a given $\Lambda\in R^d$; $\Lambda_\rho\equiv\Lambda\cap Z_\rho$. Taking $\rho>2\epsilon$ and using the independence properties of the field $P^z_\Lambda(dq)$, we can write down the following formula:

$$\begin{aligned}
&\int_{\mathscr{D}'(R^d)}dP^z_\Lambda(dq)\exp\left\{-\frac{\beta}{2}\sum_{n,n'\in\Lambda_\rho}\rho^{2d}q_\epsilon(n)V(n-n')q_\epsilon(n')\right\}\\
&\quad\times\exp\left\{\frac{\beta}{2}\sum_{n,n'\in\Lambda_\rho}\rho^{2d}\delta_\epsilon(n-n')q_\epsilon(n)V(n-n')\right\}\\
&\quad=\int_{R^{|\Lambda_\rho|}}\bigotimes_{n\in\Lambda_\rho}dp^\epsilon_z(s_n)\exp\left\{-\frac{\beta}{2}\sum_{n,n'\in\Lambda_\rho}\rho^{2d}s_nV(n-n')s_{n'}\right\}\\
&\qquad\times\exp\left\{\frac{\beta}{2}\sum_{n\in\Lambda_\rho}s_nh^\rho_\Lambda(n)\rho^d\right\},
\end{aligned} \tag{III.8}$$

where $h^{\rho}_{\Lambda}(n) \equiv \Sigma_{n' \in \Lambda_\rho} \delta_\epsilon(n-n')V(n-n')\rho^d$.

Lemma III.1: Let $V \in L_1(R^d)$ be stable and let $V(0)<\infty$. Then for any $z>0$, $\beta>0$, $|\Lambda|<\infty$ the following holds:

$$\lim_{\substack{(\epsilon,\rho)\to(0,0)\\ \epsilon>0}} \int_{\mathscr{D}'(R^d)} dP^z_\Lambda(q) \exp\left\{ -\frac{\beta}{2} \sum_{n,n' \in \Lambda_\rho} \rho^{2d} q_\epsilon(n) V(n-n') q_\epsilon(n') \right\}$$
$$\times \exp\left\{ -\frac{\beta}{2} \sum_{n,n' \in \Lambda_\rho} \rho^{2d} \delta_\epsilon(n-n') V(n-n') q_\epsilon(n) \right\}$$
$$= \int_{\mathscr{D}'(R^d)} dP^z_\Lambda(q) \exp\left\{ -\frac{\beta}{2} \int_\Lambda dx \int_\Lambda dy :q(x)q(y): V(x-y) \right\}. \tag{III.9}$$

(f) Proof: For the proof we proceed to the $C(\Lambda)$-integration picture,

$$\int_{\mathscr{D}'(R^d)} d\tilde{P}^z_\Lambda(q) \exp\left\{ -\frac{\beta}{2} \sum_{n,n' \in \Lambda_\rho} \rho^{2d} q_\epsilon(n) V(n-n') q_\epsilon(n') \right\}$$
$$\times \exp\left\{ \frac{\beta}{2} \sum_{n,n' \in \Lambda_\rho} \rho^{2d} q_\epsilon(n) \delta_\epsilon(n-n') V(n-n') \right\}$$
$$= \sum_{n \geqslant 0} \frac{z^n}{n!} \int_\Lambda d(x)^n_1 \exp\left\{ -\frac{\beta}{2} \sum_{n,n' \in \Lambda_\rho} \rho^{2d} \left(\sum_{i,j=1}^n \delta_\epsilon(n-x_i) V(n-n') \delta_\epsilon(n'-x_j) \right) \right\}$$
$$\times \exp\left\{ \frac{\beta}{2} \sum_{n,n'} \rho^{2d} \sum_{i=1}^n \delta_\epsilon(n-n') \delta_\epsilon(x_i-n) V(n-n') \right\}. \tag{III.10}$$

Noting that

$$\lim_{\substack{(\epsilon,\rho)\to(0,0)\\ e>0}} \left\{ \sum_{n,n' \in \Lambda_\rho} \rho^{2d} \sum_{i,j=1}^n \delta_\epsilon(n-x_i) V(n-n') \delta_\epsilon(n'-x_j) \right\} = \sum_{i,j=1}^n V(x_i, x_j) \tag{III.11}$$

and

$$\lim_{(\epsilon,\rho)\to(0,0)} \left\{ \sum_{n,n' \in \Lambda_\rho} \rho^{2d} \sum_{i=1}^n \delta_\epsilon(n-x_i) \delta_\epsilon(n-n') V(n-n') \right\} = nV(0). \tag{III.12}$$

Moreover, it is due to the stability of V that one can find easily a uniform [in (ρ,ϵ), $\epsilon>0$] bound on the nth term of the form

$$|(n\text{th term of rhs of (III.10)})| \leqslant \frac{z^n}{n!} e^{\beta C n} |\Lambda|^n, \tag{III.13}$$

for some constant C. This justifies the interchange of $\lim_{\substack{(\epsilon,\rho)\to(0,0)\\ \epsilon>0}}$ with the sum $\Sigma_{n\geqslant 0}$. □

If $V(0)=\infty$, then we regularize V; then we apply the above proof for V_ϵ and then we apply the proposition II.3.

Similar cylindrical approximations can be written for the (reduced) correlation functionals (II.24) also. For $\rho>2\epsilon$ the following formulas are valid:

$$\hat{\rho}_{\Lambda}^{(\rho,\epsilon)}(x_1,\ldots,x_n)=\int_{R^{|\Lambda_\rho|}}\bigotimes_{n\in\Lambda_\rho} dp^{\epsilon}_{z,\Lambda}(S_{\Lambda_\rho})\prod_{i=1}^{n}\exp\left\{-\beta\sum_{n^i\in\Lambda_\rho}\rho^d V(x_i-n^i)S(n)\right\}$$

$$=\int_{R^{|\Lambda_\rho|}} dp^{\epsilon}_{z,\Lambda_\rho}(S_{\Lambda_\rho})\prod_{n\in\Lambda_\rho}\exp\left\{-\beta\left(\sum_{i=1}^{n}\rho^d V(x_i-n)\right)S(n)\right\}, \quad \text{(III.14)}$$

where

$$dp^{\epsilon}_{z,\Lambda_\rho}(S_{\Lambda_\rho})=\exp\left\{-\frac{\beta}{2}\sum_{n,n'\in\Lambda_\rho}\rho^{2d}S(n)V(n-n')S(n')\right\},$$

$$\exp\left\{\frac{\beta}{2}\sum_{n\in\Lambda_\rho}\rho^d S(n)h^{\rho}_{\Lambda}(n)\right\}\frac{1}{Z^{\epsilon}_{\Lambda_\rho}(z,\beta)}\bigotimes_{n\in\Lambda_\rho}p^{\epsilon}_{z}(dS_n), \quad \text{(III.15)}$$

$$Z^{\epsilon}_{\Lambda_\rho}(z,\beta)=\int_{R^{|\Lambda_\rho|}}dP^{\epsilon}_{z,\Lambda_\rho}(S_{\Lambda_\rho}) \quad \text{(III.16)}$$

and

$$S_{\Lambda_\rho}=(S_n)_{n\in\Lambda_\rho}.$$

Lemma III.2: Let $V\in L_1(R^d)$ be a stable potential. Then for any $z>0$, $\beta>0$ we have

$$\lim_{\substack{(\epsilon,\rho)\to(0,0)\\ \epsilon>0}}\hat{\rho}_{\Lambda}^{(\epsilon,\rho)}(x_1,\ldots,x_n)=\hat{\rho}_{\Lambda}(x_1,\ldots,x_n),$$

pointwise on $\Lambda^{\times n}$.

In the region $\rho>2\epsilon$, the cylindric approximation to the Poisson integrals, introduced above gives the approximation of continuous systems by lattice spin systems, with unbounded spins, taking the values in the support of the measure $p^{\epsilon}_{z}(dx)$. The interaction in between spin variables is given by $\rho^{2d}V(n-n')$, and the counterterm has a meaning of an external magnetic field $h^{\delta}(n)$. Taking V to be positive, we realize that then our spin system is of an antiferromagnetic type.

IV. HIGH-TEMPERATURE CLUSTER EXPANSION

The construction of the high-temperature cluster expansion for the measure $d\mu_{\Lambda}^{(z,\lambda)}$ will be presented in this section. The cluster expansion of the Brydges–Federbush type (initiated in Ref. 44 and developed in Refs. 45, 46) is that which we would like to obtain. Demonstration of how the use of Poisson integral representations considerably simplifies the corresponding constructions is our main objective. We hope that the essential simplifications that appear in our construction can be very useful to analyze the corresponding low-temperature expansions[17–19] constructed for an analysis of the Debye screening in the (regularized) Coulomb systems.[17–21,47] Previously the corresponding high-temperature expansion has been described and analyzed by one of authors[34] for positive-definite two body potentials V_2, such that $V_2(0)<\infty$. Here we extend this construction and the convergence result for much larger class of two body interactions.

Notation in this section is very close to Refs. 45 and 34 (see also Ref. 47); therefore we refer to those papers if some confusions arise.

The reduced-correlation functions are objects for which the cluster expansion is supplied and the convergence will be demonstrated.

Let us fill up the space R^d with a set of disjoint lattice cubes of unit size. All the subsets of R^d that will appear are assumed to be unions of unit cubes. For a fixed $X_0=\{x_1,\ldots,x_m\}\subset R^{dm}$ we

define $X_1(X_0)\equiv Y_1$ to be the minimal union of lattice cubes covering X_0. Let $Y_2, Y_3,\ldots,Y_{n_\Lambda}$, where $n_\Lambda\equiv|\Lambda\backslash Y_1|+1$ will be disjoint unit cubes for which $\cup_{q\leqslant j\leqslant n_\Lambda} Y_j=\Lambda$, for a given bounded $\Lambda\subset R^d$.

Although the set V_1 is fixed, but the cubes $(Y_j)_{j=2,\ldots,n_\Lambda}$ being the variables of the corresponding series will change their positions. Let us define a new sequence (X_i) by the following recurrence:

$$X_n=Y_n\cup X_{n-1};\quad X_{n_\Lambda}=\Lambda;\quad X_n^c=\Lambda\backslash X_n. \tag{IV.1}$$

To simplify the notations we use the following abbreviations:

$$V_0(X)=V_0(X;q)=\sum_{j=1}^{n}\alpha_j\int_X V_2(x_j-y)q(y)dy, \tag{IV.2}$$

$$V(X',X'')=V(X',X'',q)=\int_X dx\int_{X''}dy\ q(x)V(x-y)q(y). \tag{IV.3}$$

Here we should stress that for X',X'' such that $X'\cap X''=\emptyset$, we have

$$:V(X',X''):=V(X',X''). \tag{IV.4}$$

Then we obtain for $\hat\rho_\Lambda(\hat x)_m^1$,

$$\rho_\Lambda(\hat x_m^1)=Z_\Lambda^\lambda(z,\beta)^{-1}\int dP_\Lambda^{z,\lambda}(q)e^{-\beta V_0(\Lambda)-1/2:V(\Lambda,\Lambda):}. \tag{IV.5}$$

To construct the cluster expansion let us introduce the following sequences:

$$V_0(X_n;(S)_{n-1})=\sum_{a\leqslant j\leqslant m}S_1\cdots S_{j-1}V_0(Y_j); \tag{IV.6}$$

$$V_1(X_n;(S)_{n-1})=\frac{1}{2}\sum_{a\leqslant j\leqslant m}V(Y_i,Y_j)+\sum_{i\leqslant i<j\leqslant n}S_i\cdots S_{j-1}V(Y_i,Y_j). \tag{IV.7}$$

The interpolation parameters $0\leqslant S_i\leqslant 1$, $i=1,\ldots,n-1$ specify the intensity of interactions between the particles lying in $X-I$ and $X_i^c=\Lambda\backslash X_i$. Equation (IV.7) corresponds to the sequence of covariances of sine-Gordon measure in Ref. 18. In our case it appears, after factorization of $e^{-\beta/2:V(\Lambda,\Lambda):}$ in (IV.5) at every step of expansion as a result of repeated application of the Newton–Leibnitz formula (see Refs. 18, 47 for details). Then taking into account (II.2) we obtain the cluster expansion in the form

$$\hat\rho_\Lambda(\hat x_1^m)=\sum_{1\leqslant n\leqslant n_\Lambda}\ \sum_{Y_2,\ldots,Y_n\subset\Lambda}b_n(X_n)f_\Lambda(X_n), \tag{IV.8}$$

where

$$b_n(X_n)=(-\beta)^{n-1}\int_0^1 d(S)_1^n\int P_\Lambda^{z,\lambda}(q)\prod_{q\leqslant j\leqslant n}\sum_{k=1}^{j-1}s_k\cdots s_{j-2}V_{kj}(q)$$
$$\times\exp(-\beta V_0(X_n;(s)_{n-1})-\beta:V(X_n;(s)_1^{n-1}):), \tag{IV.9}$$

with

$$V_{1,j}(q)=V_0(Y_j)+V(Y_1,Y_j),$$
$$V_{ij}(g)=V(Y_i,Y_j), \quad \text{if } i<1. \tag{IV.10}$$

Finally, the product of sums in (IV.9) leads to the tree-graph representation (see Refs. 45–47 for details):

$$b_n(X_n)=(-\beta)^n\sum_{\eta}\int_0^1 d(s)_1^{n-1} f_\eta((s)_1^{n-2})\int dP_\Lambda^{z,\lambda}(q)\prod_{2\leqslant j\leqslant n} V_{\eta(j),j}(q)$$
$$\times\exp\{-\beta V_0(X_n,(s)_1^{n-1})-\beta:V(X_n;(s)_1^{n-1}):\}. \tag{IV.11}$$

Now we are ready to formulate the main result of this section.

Theorem IV.1: *Let the interaction potential be stable (on* $(R^d\times\Sigma)^{\times 2}$*) and satisfy the following integrability conditions:*

$$V\equiv\max_{Y'}\sum_{Y\subset R^d}\tilde{V}_{Y',Y}<\infty;$$
$$\tilde{V}_{Y',Y}\equiv\max_{x\in Y'}\sqrt{\int_Y dy|V_2(x-y)|^2}<\infty, \tag{IV.12}$$

where Y, Y', *are unit cubes from our lattice. Then there exists a constant* $C=C(\beta,z)$ *independent of* Λ, *such that for sufficiently large* $1/\beta$ *that satisfies the condition*

$$64C\beta V<1, \tag{IV.13}$$

the infinite-volume limit $\hat{\rho}_\infty((x_1)^m)$ *of* $\hat{\rho}_\Lambda((x_1)^m)$ *exists and can be represented by the series (IV.8) with* $\Lambda=R^d$, $n_\Lambda=\infty$, *and*

$$f(X_n)=\lim_{\Lambda\uparrow R^d} f_\Lambda(X_n), \quad \text{instead of } f_\Lambda(X_n).$$

(g) Proof: We shall start with an estimation of $b_n(X)$. For this we apply the Schwartz inequality to the integrals in (IV. 11) with respect to $dP_\Lambda^{z,\lambda}$:

$$|b_n(X_n)|\leqslant\beta^{n-1}\sum_{\eta}\int_0^1 d(s)_1^{n-1} f_\eta((s)_1^{n-1})\left(\int dP_\Lambda^{z,\lambda}(q)\prod_{q\leqslant j\leqslant n} V^2_{\eta(j),j}(q)\right)^{1/2}$$
$$\times\left(\int dP_\Lambda^{z,\lambda}(q)\exp[-4\beta V_0(X_n,s_{n-1})]\right)^{1/4}$$
$$\times\left(\int dP_\Lambda^{z,\lambda}(q)\exp[-4\beta:V(X_n,(s)_1^{n-1}):]\right)^{1/4}. \tag{IV.14}$$

To estimate the last factor we define (following Brydges and Federbuch[45])

$$W_0^{X_0} = V(X_n,(s)1n-1)_{|s_1=\cdots=s_{n-1}=1};$$

$$W_i^{X_n} = (1-s_i)W_{i-1}^{X_n,X_i} + s_i W_{i-1}^{X_n};$$

$$i = 1,2,\ldots,n-2;$$

$$W_{n-1}^{X_n} = V(X_n;(s)_1^{n-1});$$

$$W_{i-1}^{X_n,X_i} = W_{i-1}^{X_i} + W_0^{X_n X_i}. \tag{IV.15}$$

Then in terms of q fields the stability condition for $V(X_n,X_n)$ is

$$:V(X_n,X_n):=:W_0^{X_n}:\geqslant -\beta\#(q)X_n \tag{IV.16}$$

[where $\#(q)X_n$ is the number of $x_1,\ldots,x_n$ composing $\Sigma\alpha_i\delta(x-x_i)$, which are located in the set X_n]. It is clear from (IV.17) and induction procedure that (IV.15) is true for $W_{i-1}^{X_n,X_i}$ for every $i=1,2,\ldots,n-1$. Noting that the induction step in (IV.15) for the construction of $W_i^{X_n}$ satisfies the inequality (IV.16) for all i, as it is a convex sum of terms that do so. So, we have

$$:V(X_n;(s)_1^{n-1}):\geqslant -\beta\#(q)X_n\,. \tag{IV.17}$$

Therefore we have

$$\begin{aligned}\int\ dP_\Lambda^{z,\lambda}(q)e^{-4\beta:V(X_n(s)_1^{n-1}):} &\leqslant \int dP_\Lambda^{z,\lambda}(q)e^{4\beta B(\#q)X_n}\\ &= e^{-z|X_n||\lambda(\sigma)|}\sum_{k\geqslant 0}\ \frac{z^k}{k!}\left(\int_\Sigma d\lambda(\alpha)\int_{X_n}dx\right)^k\\ &= e^{z(4\beta B-1)|X_1|\Lambda(\Sigma)}.\end{aligned} \tag{IV.18}$$

The integral in the middle bracket of (IV.14) can be estimated in the same way as in Ref. 46. This gives

$$\begin{aligned}&\int\ dP_\Lambda^{z,\lambda}(q)e^{-4\beta V_0(X_n,(s)_1^{n-1})} \leqslant e^{zme^{mB}c(4\beta)};\\ &c(4\beta) = \sup_{\alpha'}\int_R^d |e^{-4\beta\alpha\alpha' V(x)}-1|dx\ d\lambda(\alpha).\end{aligned} \tag{IV.19}$$

Using Lemma 1 of Ref. 34 and the Battle–Federbush estimate,[48] we finally obtain

$$|b_n(X_n)| \leqslant (64\beta z)^n \max_\eta \prod_{q\leqslant j\leqslant n} \widetilde{V}_{Y_{n(j)},Y_j}. \tag{IV.20}$$

Now the proof of the theorem follows from the estimate:

$$|f_\Lambda(X_n)| \leqslant e^{cn}, \tag{IV.21}$$

which is the consequence of the well-known method of the Kirkwood–Salsburg type of equation for the function $f_\Lambda(X_n)$ on the subsets of Λ.[44] Collecting all together, we get the convergence of the cluster expansion (IV.8) in the region $64C\beta V<1$, with

$$C = e^{z(e^{4\beta B}-1)\lambda(\Sigma)+\overline{c}}. \tag{IV.22}$$

□

Similar cluster expansions can be supplied and analyzed also for many body interactions. However, already on the the level of three body interactions it appears that for typical V_3, although individual terms of the cluster expansion converge, however, the whole expansion diverges in the limit $\Lambda \uparrow R^3$, being in some cases Borel summable.[48]

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Lagrangian dynamics for classical, Brownian, and quantum mechanical particles

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In the framework of Nelson's stochastic mechanics [E. Nelson, *Dynamical Theories of Brownian Motion* (Princeton University, Princeton, 1967); F. Guerra, Phys. Rep. **77**, 263 (1981); E. Nelson, *Quantum Fluctuations* (Princeton University, Princeton, 1985)] we seek to develop the particle counterpart of the hydrodynamic results of M. Pavon [J. Math. Phys. **36**, 6774 (1995); Phys. Lett. A **209**, 143 (1995)]. In particular, a *first form* of Hamilton's principle is established. We show that this variational principle leads to the correct equations of motion for the classical particle, the Brownian particle in thermodynamical equilibrium, and the quantum particle. In the latter case, the critical process q satisfies a stochastic Newton law. We then introduce the momentum process p, and show that the pair (q,p) satisfies canonical-like equations. © *1996 American Institute of Physics.* [S0022-2488(96)03507-4]

I. INTRODUCTION

In a recent paper,[1] we established the stochastic mechanics counterpart of the second (hydrodynamic) form of Hamilton's principle. The resulting variational picture is much richer and of a different nature with respect to the one previously considered in the literature. This paper deals with the first (particle) form of Hamilton's principle. Our principle may be viewed as a strengthening of Ref. 2 (pp. 73–75) which in turn was a modification of Yasue's original work.[3] Further related work may be found in Ref. 4 (Chap. 5). We adopt kinematical variables and stochastic derivatives different from Refs. 3 and 2. The critical stochastic process is not Markovian, but becomes Markovian if we adjoin certain mean-forward and mean-backward velocities. This picture is consistent with the classical mechanical picture.

For the purpose of later reference and comparison, we outline below one of the main results of Ref. 1. Assume that the motion of a nonrelativistic, spinless particle can be described by a stochastic process $q=\{q(t);t_0\leqslant t\leqslant t_1\}$, taking the values in $\mathbb{R}^3$ and having a stochastic differential of the form

$$dq(t)=\beta(t)dt+\left(\frac{\hbar}{m}\right)^{1/2}dw_+, \tag{1}$$

where the *forward drift* $\beta(t)$ is a measurable function of $\{q(\tau);t_0\leqslant\tau\leqslant t\}$, w_+ is a *Wiener process* with increments independent at each time of the past of q satisfying $E\{dw_+dw_+^T\}=I_3dt$. If the diffusion has finite kinetic energy

$$E\left\{\int_{t_0}^{t_1}\beta(t)\cdot\beta(t)d\tau\right\}<\infty,$$

then we also have the reverse-time representation[5]

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$$dq(t)=\gamma(t)dt+\left(\frac{\hbar}{m}\right)^{1/2}dw_-, \tag{2}$$

where γ, called the *backward drift*, depends at each time only on the future of the process q and w_- is another Wiener process whose increments are, at each time, independent of the future of the process q and satisfy $E\{dw_-dw_-^T\}=I_3dt$. When $\hbar$ tends to zero, both β and γ tend to the classical velocity. Hence, the *current velocity* $v(t):=\frac{1}{2}[\beta(t)+\gamma(t)]$ corresponds to the classical velocity, and the *osmotic velocity* $u(t):=\frac{1}{2}[\beta(t)-\gamma(t)]$ tends to zero in the semiclassical limit. In order to develop the Lagrangian and Hamiltonian formalism in stochastic mechanics in a way that naturally extends the classical case we are then naturally led[1,6] to introduce the *complex-valued* velocity (quantum velocity) $v_q(t):=v(t)-iu(t)$ that simultaneously captures $v(t)$ and $u(t)$. From Eqs. (1) and (2) we get

$$dq(t)=v(t)dt+\frac{1}{2}\left(\frac{\hbar}{m}\right)^{1/2}[dw_++dw_-], \tag{3}$$

$$0=u(t)dt+\frac{1}{2}\left(\frac{\hbar}{m}\right)^{1/2}[dw_+-dw_-]. \tag{4}$$

Multiplying the second equation by $-i$, and then adding it to the first, we finally get

$$dq(t)=[v(t)-iu(t)]dt+dw, \tag{5}$$

where

$$dw=\frac{1}{2}\left(\frac{\hbar}{m}\right)^{1/2}[(1-i)dw_++(1+i)dw_-].$$

For the properties of the *quantum noise* dw see Ref. 1 (Sec. VII). The differential (5) of q, differently from Eqs. (1) and (2), enjoys the *time reversal invariance* property, see Ref. 6.

Consider the situation where the particle is subject to an external conservative force deriving from the sufficiently regular potential $V(x)$. Let $L(x,y):=\frac{1}{2}my\cdot y-V(x)$ be the Lagrangian defined on $\mathbb{R}^3\times\mathbb{C}^3$, and let $\mathscr{T}$ denote the family of finite-energy, $\mathbb{C}^3$-valued stochastic processes on $[t_0,t_1]$. For ϕ_0 a complex-valued function on $\mathbb{R}^3$ such that $\psi_0(x):=\exp i/\hbar\,\varphi_0(x)$ has L^2 norm 1, consider the variational problem

$$\text{extremize}_{v_q\in\mathscr{T}}E\left\{\int_{t_0}^{t_1}L(x(t),v_q(t))dt+\varphi_0(x(t_0))\right\} \tag{6}$$

subject to the constraint that the finite-energy, possibly non-Markovian diffusion x has quantum velocity v_q and a prescribed probability density ρ_1 at time t_1. We then have the following result (Ref. 1, Sec. VIII).

Theorem 1: *Suppose that the solution* $\{\psi(x,t),t\in[t_0,t_1]\}$ *of the Schrödinger equation*

$$\frac{\partial\psi}{\partial t}=\frac{i\hbar}{2m}\Delta\psi-\frac{i}{\hbar}V(x)\psi, \tag{7}$$

with initial condition $\psi(x,t_0)=\psi_0(x)$ *never vanishes and satisfies*

$$E\left\{\int_{t_0}^{t_1}|\nabla \log \psi(x(t),t)|^2 dt\right\}<\infty$$

for each finite-energy diffusion x *on* $[t_0,t_1]$. *In Problem (6), let* $\rho_1(x)=|\psi(x,t_1)|^2$. *Then, there exists a stochastic process* $\{x^*(t);t_0\leqslant t\leqslant t_1\}$, *called the Nelson process, solving together with its quantum drift* $1/m\nabla\hbar/i \log \psi(x^*(t),t)$ *Problem (6).*

It is worthwhile to observe that the Markov property of the extremal process is a *result* of the variational principle. Also notice that the probability density $\rho(x,t)$ of $q(t)$ satisfies Born's relation $\rho(x,t)=|\psi(x,t)|^2$. The existence of the Nelson process corresponding to a given solution $\psi(x,t)$ of the Schrödinger equation is, in the general case where $\psi(x,t)$ can vanish, a challenging question that has generated considerable interest, see, e.g., Refs. 7, 4 (Chap IV), and 8, and references therein. The existence of the Nelson probability measure is established in Ref. 1 under the present assumptions by means of the Girsanov transformation theory, cf., e.g., Ref. 9 (Chap 6). The quantum Hamilton principle just recalled was also shown in Ref. 1 to be a consequence of two other variational principles of the min–max type. The first one, called the *saddle-point action principle*, contains as special cases both the Guerra–Morato variational principle[10] and Schrödinger original variational derivation of the time-independent equation, see, e.g., Ref. 11 (p. 118). The second, called the *saddle-point entropy production principle*, concerns the production of configurational entropy. The Nelson process appears then as a *saddle-point equilibrium solution* for both stochastic differential games.

In this paper, we develop the *first (particle) form* of Hamilton's principle in stochastic mechanics. We then show that this variational principle can be applied to a variety of conservative systems such as the classical particle, the Brownian particle in thermodynamical equilibrium, and the quantum particle by simply changing the family of trial motions.

The paper is outlined as follows. In Sec. II we collect some basic facts about the kinematics of stochastic processes. In Sec. III, we develop a stochastic calculus of variations. The corresponding Hamilton's principle is then applied in Sec. IV to various conservative systems. In Sec. V, we develop some basic elements of the Hamilton–Jacobi theory in stochastic mechanics.

II. BACKGROUND ON THE KINEMATICS OF STOCHASTIC PROCESSES

Let $(\Omega,\mathcal{E},\mathbf{P})$ be a complete probability space, and let $\mathcal{A}:=(\mathcal{A}_t)$, $t\in[t_0,t_1]$, be a nondecreasing family of sub σ-algebras of $\mathcal{E}$. Let $x:=\{x(t);t\in[t_0,t_1]\}$ be an $\mathbb{R}^n$-valued, second-order, $\mathcal{A}$-adapted stochastic process, namely the components of $x(t)$ are $\mathcal{A}_t$-measurable for all t in $[t_0,t_1]$. Suppose that x is a.s. and mean-square continuous. We say that x is *mean-forward differentiable* with respect to the filtration $\mathcal{A}$ if the limit

$$(D_+^{\mathcal{A}}x)(t)=\lim_{h\searrow 0} E\left\{\frac{x(t+h)-x(t)}{h}\,\middle|\,\mathcal{A}_t\right\}$$

exists for $t\in[t_0,t_1)$, and forms a continuous curve in $L_n^2(\Omega,\mathcal{E},\mathbf{P})$. In this case, it may be shown along the lines of Ref. 12 (Sec. 11) that x is a continuous semimartingale of the form

$$x(t)=x(t_0)+\int_{t_0}^{t}(D_+^{\mathcal{A}}x)(s)ds+m_+^{\mathcal{A}}(t), \tag{8}$$

where the integral is a Riemann integral in $L_n^2(\Omega,\mathcal{E},\mathbf{P})$ (Ref. 13 p. 10), and $m_+^{\mathcal{A}}$ is a square-integrable, continuous $\mathcal{A}_t$-martingale with $m_+^{\mathcal{A}}(t_0)=0$ a.s. (for the definitions, see, e.g., Ref. 14, p. 78). Similarly, if $\mathcal{B}:=(\mathcal{B}_t)$, $t\in[t_0,t_1]$, is a nonincreasing family of sub σ-algebras of $\mathcal{E}$ to which x is adapted, we say that x is *mean-backward differentiable* with respect to $\mathcal{B}$ if the limit

$$(D_-^{\mathscr{B}}x)(t)=\lim_{h\searrow 0} E\left\{ \frac{x(t)-x(t-h)}{h} \,\middle|\, \mathscr{B}_t \right\}$$

exists for $t\in(t_0,t_1]$, and forms a continuous curve in $L_n^2(\Omega,\mathscr{E},\mathbf{P})$. In that case, x admits the backward semimartingale representation

$$x(t)=x(t_1)+\int_{t_1}^{t}(D_-^{\mathscr{B}}x)(s)ds-m_-^{\mathscr{B}}(t), \tag{9}$$

where $m_-^{\mathscr{B}}$ is a reverse-time, square-integrable, continuous, $\mathscr{B}_t$-martingale with $m_-^{\mathscr{B}}(t_1)=0$ a.s. Notice that $D_+^{\mathscr{A}}x$ and $D_-^{\mathscr{B}}x$ depend crucially on the filtrations $\mathscr{A}$ and $\mathscr{B}$. Obviously, for x to be mean-square differentiable, $\mathscr{A}_t$ must contain $\mathscr{F}_t:=\sigma\{x(s);t_0\leqslant s\leqslant t\}$ and $\mathscr{B}_t$ must contain $\mathscr{G}_t:=\sigma\{x(s);t\leqslant s\leqslant t_1\}$. If x is mean-forward and mean-backward differentiable with respect to $\mathscr{F}:=(\mathscr{F}_t)$ and $\mathscr{G}:=(\mathscr{G}_t)$, respectively, we call $\beta(t):=(D_+^{\mathscr{F}}x)(t)$ the *forward drift* of x and $\gamma(t):=(D_-^{\mathscr{G}}x)(t)$ the *backward drift* of x. Of course, for mean-square differentiable processes, we have $\beta(t)=\gamma(t)=\dot{x}(t)$.

For stochastic processes that are simultaneously mean-forward and mean-backward differentiable with respect to the filtrations $\mathscr{A}$ and $\mathscr{B}$, we can introduce two more stochastic derivatives (using the notation introduced in Ref. 15) by

$$(D^{\mathscr{A},\mathscr{B}}x)(t):=\frac{(D_+^{\mathscr{A}}x)(t)+(D_-^{\mathscr{B}}x)(t)}{2},$$

$$(\delta D^{\mathscr{A},\mathscr{B}}x)(t):=\frac{(D_+^{\mathscr{A}}x)(t)-(D_-^{\mathscr{B}}x)(t)}{2}.$$

In particular, $v(t):=(D^{\mathscr{F},\mathscr{G}}x)(t)=(\beta(t)+\gamma(t))/2$ and $u(t):=(\delta D^{\mathscr{F},\mathscr{G}}x)(t)=(\beta(t)-\gamma(t))/2$ are the *current drift* and the *osmotic drift* of x, respectively. Representations (8) and (9) now give

$$x(t)-x(s)=\int_s^t(D^{\mathscr{A},\mathscr{B}}x)(\sigma)d\sigma+\frac{1}{2}[m_+^{\mathscr{A}}(t)-m_+^{\mathscr{A}}(s)+m_-^{\mathscr{B}}(t)-m_-^{\mathscr{B}}(s)], \tag{10}$$

$$0=\int_s^t(\delta D^{\mathscr{A},\mathscr{B}}x)(\sigma)d\sigma+\frac{1}{2}[m_+^{\mathscr{A}}(t)-m_+^{\mathscr{A}}(s)-m_-^{\mathscr{B}}(t)+m_-^{\mathscr{B}}(s)]. \tag{11}$$

Multiplying Eq. (11) by $-i$, and then adding it to Eq. (10), we finally get a generalization of Eq. (5),

$$x(t)-x(s)=\int_s^t((D-i\,\delta D)^{\mathscr{A},\mathscr{B}}x)(\sigma)d\sigma+m^{\mathscr{A},\mathscr{B}}(t)-m^{\mathscr{A},\mathscr{B}}(s), \tag{12}$$

where

$$m^{\mathscr{A},\mathscr{B}}(t):=\tfrac{1}{2}[(1-i)m_+^{\mathscr{A}}(t)+(1+i)m_-^{\mathscr{B}}(t)].$$

As for the diffusion processes of Sec. I, we call $v_q(t):=((D-i\,\delta D)^{\mathscr{F},\mathscr{G}}x)(t)$ the *quantum drift* of x and $dm^{\mathscr{F},\mathscr{G}}(t)$ the *quantum noise*.

Remark 1: Notice that when $((D-i\,\delta D)^{\mathscr{A},\mathscr{B}}x)=f(x(t),t)$, *$x$ is a Markov process. Indeed, it admits a forward differential given by*

$$dx=[\mathfrak{R}f(x(t),t)-\mathfrak{F}f(x(t),t)]dt+dm_+^{\mathscr{A}},$$

where $\Re$ and $\Im$ denote real and imaginary part, respectively.

We now state Nelson's product rule.

Lemma 1: Let $x,y:[t_0,t_1]\to L_n^2(\Omega,\mathcal{E},\mathbf{P})$ be two a.s. *and mean-square continuous stochastic processes. Suppose that x and y are simultaneously mean-forward and mean-backward differentiable with respect to the filtrations $\mathcal{A}$ and $\mathcal{B}$, respectively. Suppose, moreover, that the processes $D_+^{\mathcal{A}}x$, $D_-^{\mathcal{B}}x$, $D_+^{\mathcal{A}}y$, and $D_-^{\mathcal{B}}y$ have continuous paths. Then*

$$E\{x(t_1)\cdot y(t_1)-x(t_0)\cdot y(t_0)\}=E\left\{\int_{t_0}^{t_1}[(D_+^{\mathcal{A}}x)(t)\cdot y(t)+x(t)\cdot(D_-^{\mathcal{B}}y)(t)]dt\right\}. \tag{13}$$

Exchanging the roles of x and y in Eq. (13), adding and subtracting, we get two more formulas corresponding to Eqs. (10) and (11).

Corollary 1: Let x and y be as in the previous lemma. Then

$$E\{x(t_1)\cdot y(t_1)-x(t_0)\cdot y(t_0)\}=E\left\{\int_{t_0}^{t_1}[(D^{\mathcal{A},\mathcal{B}}x)(t)\cdot y(t)+x(t)\cdot(D^{\mathcal{A},\mathcal{B}}y)(t)]dt\right\}, \tag{14}$$

$$0=E\left\{\int_{t_0}^{t_1}[(\delta D^{\mathcal{A},\mathcal{B}}x)(t)\cdot y(t)+x(t)\cdot(\delta D^{\mathcal{A},\mathcal{B}}y)(t)]dt\right\}. \tag{15}$$

Multiplying Eq. (15) by $-i$, and then adding it to the first, we finally get a fundamental integration by parts formula related to representation (12).

Corollary 2: Let x and y be as in the above lemma. Then

$$\begin{aligned}&E\{x(t_1)\cdot y(t_1)-x(t_0)\cdot y(t_0)\}\\&\quad=E\left\{\int_{t_0}^{t_1}[((D-i\,\delta D)^{\mathcal{A},\mathcal{B}}x)(t)\cdot y(t)+x(t)\cdot((D+i\,\delta D)^{\mathcal{A},\mathcal{B}}y)(t)]dt\right\}.\end{aligned} \tag{16}$$

So far we have dealt with $\mathbb{R}^n$-valued stochastic processes. A moment's thought, however, reveals that everything we have done holds true if the processes are $\mathbb{C}^n$-valued.

We now consider the case where the process x is an n-dimensional, finite-energy Markovian diffusion with constant diffusion coefficient $\sigma^2 I_n$. We denote by $b_+(x(t),t)$ and $b_-(x(t),t)$ its forward and backward drifts, respectively. Moreover, let

$$v(x(t),t)=\frac{b_+(x(t),t)+b_-(x(t),t)}{2}$$

and

$$u(x(t),t)=\frac{b_+(x(t),t)-b_-(x(t),t)}{2}$$

denote the current and osmotic drifts. We then have Nelson's relation

$$u(x,t)=\frac{\sigma^2}{2}\,\nabla\,\log\,\rho(x,t), \tag{17}$$

where $\rho(x,t)$ is the sufficiently smooth probability density of $x(t)$ [set $u(x,t)$ equal to zero whenever $\rho(x,t)=0$]. Moreover, the Fokker–Planck equation governing the evolution of ρ

$$\frac{\partial\rho}{\partial t}+\nabla\cdot(b_+\rho)=\frac{\sigma^2}{2}\,\Delta\rho,$$

may be rewritten as a *continuity equation* of fluid dynamics

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (v\rho) = 0. \tag{18}$$

As before, let $\mathscr{F}_t := \sigma\{x(s); t_0 \leqslant s \leqslant t\}$ and $\mathscr{G}_t := \sigma\{x(s); t \leqslant s \leqslant t_1\}$. Also let $f(x,t): \mathbb{R}^n \times [t_0, t_1] \to \mathbb{R}$ be a function with compact support of class $C^{2,1}$. From the two changes of variables formulas (Ito's rules) corresponding to the forward and backward representations for the increments of x [Eqs. (1) and (2)] we get (Ref. 12, p. 104)

$$(D_+^{\mathscr{F}} f(x(t),t)) = \left[\left(\frac{\partial}{\partial t} + b_+ \cdot \nabla + \frac{\sigma^2}{2}\Delta\right) f\right](x(t),t), \tag{19}$$

$$(D_-^{\mathscr{G}} f(x(t),t)) = \left[\left(\frac{\partial}{\partial t} + b_- \cdot \nabla - \frac{\sigma^2}{2}\Delta\right) f\right](x(t),t). \tag{20}$$

The semisum and the semidifference of Eqs. (19) and (20) give

$$(D^{\mathscr{F},\mathscr{G}} f(x(t),t)) = \left[\frac{\partial}{\partial t} + v(t) \cdot \nabla\right] f(x(t),t), \tag{21}$$

$$(\delta D^{\mathscr{F},\mathscr{G}} f(x(t),t)) = \left[u(t) \cdot \nabla + \frac{\sigma^2}{2}\Delta\right] f(x(t),t). \tag{22}$$

We can now establish a rather interesting formula.

Lemma 2: Let $x(t)$ be a finite-energy Markovian diffusion whose never vanishing probability density ρ is of class $C^{2,1}$. Then

$$[D_+^{\mathscr{F}}(D_+^{\mathscr{F}} x)](t) - [D_-^{\mathscr{G}}(D_-^{\mathscr{G}} x)](t) = 2\{[D^{\mathscr{F},\mathscr{G}}(\delta D^{\mathscr{F},\mathscr{G}} x)](t) + [\delta D^{\mathscr{F},\mathscr{G}}(D^{\mathscr{F},\mathscr{G}} x)](t)\} = 0, \text{ a.s.} \tag{23}$$

for all $t \in [t_0, t_1]$.

Proof: From Eq. (18), we get

$$\frac{\partial \log \rho}{\partial t} = -\nabla \cdot v - v \cdot \nabla \log \rho.$$

Using Eq. (17), we get

$$\frac{\partial u}{\partial t} = -\frac{\sigma^2}{2}\Delta v - u \cdot \nabla v - v \cdot \nabla u. \tag{24}$$

In view of Eqs. (21) and (22), Eq. (24) can now be written as

$$(D^{\mathscr{F},\mathscr{G}} u)(t) + (\delta D^{\mathscr{F},\mathscr{G}} v)(t) = [D^{\mathscr{F},\mathscr{G}}(\delta D^{\mathscr{F},\mathscr{G}} x)](t) + [\delta D^{\mathscr{F},\mathscr{G}}(D^{\mathscr{F},\mathscr{G}} x)](t) = 0, \tag{25}$$

which is Eq. (23). □

Equation (24) was derived by Nelson in his early work [Ref. 12, Eq. (5) on p. 106]. Curiously, nobody seems to have noticed the straightforward reformulation of Eq. (24) given by Eqs. (25) and (23). The corresponding hydrodynamical equation (Madelung equation) occurs in the context of the *saddle-point entropy production principle*, cf. Ref. 1, Sec. V.

III. STOCHASTIC CALCULUS OF VARIATIONS

Let $\mathscr{X}(x_0,x_1)$ denote the family of $\mathbb{R}^n$-valued, mean-square continuous processes $x=\{x(t);t\in[t_0,t_1]\}$ such that $x(t_0)=x_0$ a.s., $x(t_1)=x_1$ a.s., and satisfying the following two properties.

(i) x is mean-forward and mean-backward differentiable with respect to its past and future filtrations $\mathscr{F}=(\mathscr{F}_t)$ and $\mathscr{G}=(\mathscr{G}_t)$, respectively; we denote by $X(t)$ the augmented process

$$X(t)=\begin{pmatrix} x(t) \\ \beta(t) \\ \gamma(t) \end{pmatrix}.$$

(ii) The process X is a simultaneously mean-forward and mean-backward differentiable with respect to the filtrations $\mathbf{F}=(\mathbf{F}_t)$ and $\mathbf{G}=(\mathbf{G}_t)$, where $\mathbf{F}_t:=\sigma\{X(s);t_0\leqslant s\leqslant t\}$ and $\mathbf{G}_t:=\sigma\{X(s);t\leqslant s\leqslant t_1\}$.

Obviously, $\mathscr{F}_t\subseteq\mathbf{F}_t$ and $\mathscr{G}_t\subseteq\mathbf{G}_t$. In order to avoid any confusion, we stress the fact that, in general, $(D_+^{\mathbf{F}}x)(t)\neq(D_+^{\mathscr{F}}x)(t)=\beta(t)$ and $(D_-^{\mathbf{G}}x)(t)\neq(D_-^{\mathscr{G}}x)(t)=\gamma(t)$. Consequently, $(D^{\mathbf{F},\mathbf{G}}x)\times(t)\neq v(t)$ and $(\delta D^{\mathbf{F},\mathbf{G}}x)(t)\neq u(t)$. Also notice that $\mathscr{X}(x_0,x_1)$ contains as a proper subset the family of finite-energy, *Markovian* diffusions with the prescribed end-point marginals.

For each $x\in\mathscr{X}(x_0,x_1)$, we define the family of *variations* y of x to be the set $\mathscr{Y}(x)$ of $\mathbb{R}^n$-valued, mean-square continuous processes $y=\{y(t);t\in[t_0,t_1]\}$ satisfying the two properties: (i) $y(t_0)=y(t_1)=0$ a.s.; (ii) y is simultaneously mean-forward and mean-backward differentiable with respect to the filtrations $\mathbf{F}$ and $\mathbf{G}$, respectively.

Remark 2: Let $f:\mathbb{R}^n\times[t_0,t_1]\to\mathbb{R}^n$, having compact support in $\mathbb{R}^n\times(t_0,t_1)$, be of class $C^{2,1}$. Then, $y(t):=f(x(t),t)$ belongs to $\mathscr{Y}(x)$. These are precisely the variations considered by Nelson in Ref. 3.

Let $L:\mathbb{R}^n\times\mathbb{C}^n\times\mathbb{C}^n\times[t_0,t_1]\to\mathbb{C}^n$ be a sufficiently regular function. Namely, $L(x,z_1,z_2,t)$ is continuously differentiable with respect to x and t, entirely as a function of z_1 and entirely as a function of z_2. Define $I:\mathscr{X}(x_0,x_1)\to\mathbb{C}$ by

$$I(x)=E\left\{\int_{t_0}^{t_1}L(x(t),((D-i\,\delta D)^{\mathbf{F},\mathbf{G}}x)(t),((D+i\,\delta D)^{\mathbf{F},\mathbf{G}}x)(t),t)dt\right\}.$$

Notice that in this action integral appear the conditional derivatives relative to the pair of filtrations $(\mathbf{F},\mathbf{G})$ rather than with respect to $(\mathscr{F},\mathscr{G})$. Also notice that our choice of kinematical variables differs from those previously considered in the literature [Refs. 3, 2 (pp. 73–75), and 4 (Chap. 5). Let dom I denote the subset of x in $\mathscr{X}(x_0,x_1)$ such that $I(x)<\infty$.

Definition 1: The process $x\in\mathrm{dom}\,I$ is critical for I if for all processes $y\in\mathscr{Y}(x)$ we have

$$I(x+y)-I(x)=o(\|y\|),$$

where

$$\|y\|^2:=E\left\{\int_{t_0}^{t_1}[y(t)\cdot y(t)+(D^{\mathbf{F},\mathbf{G}}y)(t)\cdot(D^{\mathbf{F},\mathbf{G}}y)(t)+(\delta D^{\mathbf{F},\mathbf{G}}y)(t)\cdot(\delta D^{\mathbf{F},\mathbf{G}}y)(t)]dt\right\}.$$

We are now ready for the fundamental theorem of stochastic calculus of variations.

Theorem 2: *The stochastic process $x\in\mathrm{dom}\,I$ is critical for I if and only if it satisfies the Euler–Lagrange equations*

$$\left[(D+i\delta D)^{\mathbf{F,G}}\frac{\partial L}{\partial z_1}+(D-i\delta D)^{\mathbf{F,G}}\frac{\partial L}{\partial z_2}-\frac{\partial L}{\partial x}\right]=0 \quad \text{a.s.} \tag{26}$$

for almost all $t\in[t_0,t_1]$.

Proof: Let $x\in\operatorname{dom} I$ be critical for I, and let $y\in\mathscr{Y}(x)$ be a variation of x. By Taylor's formula

$$I(x+y)-I(x)=o(\|y\|)+E\left\{\int_{t_0}^{t_1}\left[\frac{\partial L}{\partial x}\cdot y+\frac{\partial L}{\partial z_1}\cdot((D-i\delta D)^{\mathbf{F,G}}y)+\frac{\partial L}{\partial z_2}\cdot((D+i\delta D)^{\mathbf{F,G}}y)\right]dt\right\}.$$

Applying Eq. (16), and taking into account the fact that y vanishes at the end points, we get

$$I(x+y)-I(x)=o(\|y\|)+E\left\{\int_{t_0}^{t_1}\left[\frac{\partial L}{\partial x}-(D+i\delta D)^{\mathbf{F,G}}\left(\frac{\partial L}{\partial z_1}\right)-(D-i\delta D)^{\mathbf{F,G}}\left(\frac{\partial L}{\partial z_2}\right)\right]\cdot y\,dt\right\}. \tag{27}$$

Since the expectation in Eq. (27) must vanish for all $y\in\mathscr{Y}(x)$, it follows that both the real and the imaginary parts of

$$\left[\frac{\partial L}{\partial x}-(D+i\delta D)^{\mathbf{F,G}}\left(\frac{\partial L}{\partial z_1}\right)-(D-i\delta D)^{\mathbf{F,G}}\left(\frac{\partial L}{\partial z_2}\right)\right]$$

must vanish. Conversely, if Eq. (26) holds, x is critical because of Eq. (27). □

Corollary 3: Let $L(x,z_1,z_2,t):=\frac{1}{2}mz_1\cdot z_2-V(x)$, *where* V *is of class* C^1. *Then* $x\in\operatorname{dom} I$ *is critical for* I *if and only if the stochastic Newton law*

$$m[((D^{\mathbf{F,G}}D^{\mathbf{F,G}}-\delta D^{\mathbf{F,G}}\delta D^{\mathbf{F,G}})x)(t)]=-\nabla V(x(t)) \quad \text{a.s.} \tag{28}$$

for all $t\in[t_0,t_1]$.

Proof: Notice that in this case

$$\frac{\partial L}{\partial z_1}(x(t),((D-i\delta D)^{\mathbf{F,G}}x)(t),((D+i\delta D)^{\mathbf{F,G}}x)(t),t)=\frac{m}{2}((D+i\delta D)^{\mathbf{F,G}}x)(t),$$

$$\frac{\partial L}{\partial z_2}(x(t),((D-i\delta D)^{\mathbf{F,G}}x)(t),((D+i\delta D)^{\mathbf{F,G}}x)(t),t)=\frac{m}{2}((D-i\delta D)^{\mathbf{F,G}}x)(t).$$

From Eq. (26), we get that x is critical for I if and only if

$$\frac{m}{2}[((D+i\delta D)^{\mathbf{F,G}}(D+i\delta D)^{\mathbf{F,G}}+(D-i\delta D)^{\mathbf{F,G}}(D-i\delta D)^{\mathbf{F,G}})x)](t)=-\nabla V(x(t)), \quad \text{a.s.} \tag{29}$$

and Eq. (28) follows. □

Remark 3: Notice that Eqs. (28) and (29) can also be written in the form

$$\frac{m}{2}[((D_+^{\mathbf{F}}D_-^{\mathbf{G}}+D_-^{\mathbf{G}}D_+^{\mathbf{F}})x)(t)]=-\nabla V(x(t)). \tag{30}$$

The comparison between the left-hand sides of Eqs. (29) and (30) gives the long sought probabilistic meaning for the Nelson stochastic acceleration, cf. Ref. 2, Problem 6, p. 133. Nelson's acceleration may also be viewed as the real part of $((D-i\delta D)^{\mathbf{F,G}}(D-i\delta D)^{\mathbf{F,G}})x)$ *which occurs in the global Newton's law (40) below.*

IV. HAMILTON'S PRINCIPLE

We now require that the conservative motion of a particle of mass m be critical for the action I introduced in Sec. III.

A. Classical particle

Consider a classical particle subject to an external conservative force induced by the potential function V. As trajectories we take deterministic, C^2 functions. Hence, $\mathscr{F}_t=\mathbf{F}_t=\mathscr{G}_t=\mathbf{G}_t=\{\Omega,\varnothing\}$, namely the trivial σ field. In particular, x_0 and x_1 are two points in $\mathbb{R}^3$. Moreover, $(D^{\mathbf{F},\mathbf{G}}x)(t)=\dot{x}(t)$, $(\delta D^{\mathbf{F},\mathbf{G}}x)(t)=0$, and $(D^{\mathbf{F},\mathbf{G}}\dot{x})(t)=\ddot{x}(t)$. Thus, Corollary 2 gives that x is critical for I if and only if Newton's law

$$m\ddot{x}(t)=-\nabla V(x(t)) \tag{31}$$

is satisfied for all $t\in[t_0,t_1]$.

B. Classical particle with uncertain end points

Suppose we have a classical (C^2 trajectories) particle with uncertain initial and terminal positions. This uncertainty is described through initial and final probability densities ρ_0 and ρ_1, respectively. Let x_0 and x_1 be distributed according to ρ_0 and ρ_1, respectively. Then, for all admissible motions x we have $\mathscr{F}_t=\mathbf{F}_t=\sigma(x_0)$ and $\mathscr{G}_t=\mathbf{G}_t=\sigma(x_1)$. As before, $\mathscr{D}^{\mathbf{F},\mathbf{G}}x(t)=\dot{x}(t)$, and $\delta\mathscr{D}^{\mathbf{F},\mathbf{G}}x(t)=0$. Thus, by Corollary 2, the stochastic process x satisfying $x(t_0)=x_0$ a.s., $x(t_1)=x_1$ a.s. with C^2 paths is critical for I if and only if Eq. (31) holds for all times with probability one.

C. Brownian particle

Consider a Brownian particle in thermodynamical equilibrium. We assume that its motion may be described by a stochastic process x with differentiable sample paths and that forms a diffusion with constant diffusion coefficient together with its derivative $\dot{x}$. Hence, we have $\dot{x}(t)=\beta(t)=\gamma(t)=\mathscr{D}^{\mathbf{F},\mathbf{G}}x$, and $\delta\mathscr{D}^{\mathbf{F},\mathbf{G}}x=0$. Moreover, $\mathbf{F}_t=\sigma\{x(s),\dot{x}(s);t_0\leqslant s\leqslant t\}$ and $\mathbf{G}_t=\sigma\{x(s),\dot{x}(s);t\leqslant s\leqslant t_1\}$. By Corollary 2, x is critical for I if and only if

$$m(D^{\mathbf{F},\mathbf{G}}\dot{x})(t)=-\nabla V(x(t)) \quad \text{a.s.} \tag{32}$$

for all $t\in[t_0,t_1]$. It follows, in particular, that the critical process x is such that $(x,\dot{x})$ is Markovian (see Remark 1).

Theorem 3: *The stochastic process x in the above described class is critical for I if and only if the forward drift of $\dot{x}$ is given by*

$$(D^{\mathbf{F}}\dot{x})(t)=-\lambda\dot{x}(t)-\frac{1}{m}\nabla V(x(t)), \quad \text{a.s.}, \tag{33}$$

where $\lambda=\sigma^2 m/(2kT)$ and σ^2 is the diffusion coefficient of $\dot{x}$.

Proof: By the Gibbsian postulate, the equilibrium distribution is the Maxwell–Boltzmann distribution

$$\rho(x.\dot{x})=c\ \exp\left\{\frac{-\frac{1}{2}m\dot{x}\cdot\dot{x}-V(x)}{kT}\right\}. \tag{34}$$

Moreover, since

$$\begin{pmatrix} x(t) \\ \dot{x}(t) \end{pmatrix}$$

is Markovian, Nelson's relation (17) between the forward and the backward drift of $\dot{x}$ yields

$$(D^{\mathbf{F},\mathbf{G}}\dot{x})(t) = (D_+^{\mathbf{F}}\dot{x})(t) - \frac{\sigma^2}{2}\nabla_{\dot{x}} \log \rho(x(t),\dot{x}(t)). \tag{35}$$

Equations (34) and (35) now give

$$(D^{\mathbf{F},\mathbf{G}}\dot{x})(t) = (D_+^{\mathbf{F}}\dot{x})(t) + \sigma^2 \frac{m}{2kT}\dot{x}(t). \tag{36}$$

If x is critical, then Eqs. (32) and (36) give Eq. (33). Conversely, if the process x has forward drift of $\dot{x}$ given by Eq. (33), and has the invariant density (34), then it satisfies the Newton law (32), see Refs. 1 (p. 102) and 16. □

Remark 4: It follows, in particular, that the Markovianess of $(x,\dot{x})$*, the form of the forward drift of* $\dot{x}$ *in the Ornstein–Uhlenbeck model of physical Brownian motion (Ref. 12, Chaps. 9 and 10), and its relation to the diffusion coefficient* (Einstein's fluctuation–dissipation relation) *are consequences of the Gibbsian postulate and of the Newton law (34). Conversely, given that the forward drift of* $\dot{x}$ *lies in a certain class, necessary and sufficient conditions can be given for the particle to obey the Maxwell–Boltzmann distribution in equilibrium, see Ref. 17, Sec. III.*

D. Quantum particle

Consider a nonrelativistic, spinless quantum mechanical particle moving in a force field. As class of motions we take the subclass of $\mathscr{X}(x_0,x_1)$ of the finite-energy diffusions with constant diffusion coefficient $\sigma^2=\hbar/m$. In this case, the action is given by

$$I(x) = \int_{t_0}^{t_1}\left[\frac{1}{2}m((D-i\delta D)^{\mathbf{F},\mathbf{G}}x)(t)\cdot((D+i\delta D)^{\mathbf{F},\mathbf{G}}x)(t) - V(x(t))\right]dt. \tag{37}$$

Then x satisfies Hamilton's principle if and only if it satisfies the stochastic Newton law (28) or, equivalently, Eq. (29) which may be rewritten as follows

$$m\Re[((D-i\delta D)^{\mathbf{F},\mathbf{G}}(D-i\delta D)^{\mathbf{F},\mathbf{G}}x)](t) = -\nabla V(x(t)), \quad \text{a.s.} \tag{38}$$

Next we postulate

$$[(D^{\mathbf{F},\mathbf{G}}\delta D^{\mathbf{F},\mathbf{G}} + \delta D^{\mathbf{F},\mathbf{G}}D^{\mathbf{F},\mathbf{G}})x](t) \equiv 0. \tag{39}$$

Putting together Eqs. (39) with (38), we get

$$m[((D-i\delta D)^{\mathbf{F},\mathbf{G}}(D-i\delta D)^{\mathbf{F},\mathbf{G}}x)](t) = -\nabla V(x(t)), \quad \text{a.s.} \tag{40}$$

Assumption (39) simply means that the acceleration in the left-hand side of Eq. (40) must be real. Also notice that Eq. (39) is precisely Eq. (23) for the position process x. Finally notice that the extremizing process x is such that the augmented process

$$\begin{pmatrix} x(t) \\ ((D-i\delta D)^{\mathbf{F},\mathbf{G}}x)(t) \end{pmatrix} \tag{41}$$

is Markovian. To see this, recall Remark 1 and observe that

$$\left((D-i\delta D)^{\mathbf{F},\mathbf{G}}\begin{pmatrix} x(t) \\ ((D-i\delta D)^{\mathbf{F},\mathbf{G}}x) \end{pmatrix}\right)(t)=\begin{pmatrix} ((D-i\delta D)^{\mathbf{F},\mathbf{G}}x)(t) \\ -\frac{1}{m}\nabla V(x(t)) \end{pmatrix}.$$

The process x by itself, however, is in general *non Markovian*.

We are now ready to introduce the *momentum process* corresponding to such a process by

$$p(t):=\frac{\partial L}{\partial z_2}(x(t),((D-i\delta D)^{\mathbf{F},\mathbf{G}}x)(t),((D+i\delta D)^{\mathbf{F},\mathbf{G}}x)(t),t)=m((D-i\delta D)^{\mathbf{F},\mathbf{G}}x)(t),$$

$$\overline{p(t)}:=\frac{\partial L}{\partial z_1}(x(t),((D-i\delta D)^{\mathbf{F},\mathbf{G}}x)(t),((D+i\delta D)^{\mathbf{F},\mathbf{G}}x)(t),t)=m((D+i\delta D)^{\mathbf{F},\mathbf{G}}x)(t).$$

Then Eq. (40) reads

$$((D-i\delta D)^{\mathbf{F},\mathbf{G}}p)(t)=-\nabla V(x(t)),\text{a.s.} \tag{42}$$

or equivalently

$$((D+i\delta D)^{\mathbf{F},\mathbf{G}}\overline{p)}(t)=-\nabla V(x(t)),\text{a.s.} \tag{43}$$

Let $H(x,y):=(1/2m)y\cdot y+V(x)$ be the *Hamiltonian function* defined on $\mathbb{R}^3\times\mathbb{C}^3$, and write $q(t)$ instead of $x(t)$ for the position of the quantum particle. We then get the *canonical-like equations*

$$((D-i\delta D)^{\mathbf{F},\mathbf{G}}q)(t)=\nabla_y(q(t),p(t)), \tag{44}$$

$$((D-i\delta D)^{\mathbf{F},\mathbf{G}}p)(t)=-\nabla_x(q(t),p(t)), \tag{45}$$

or equivalently

$$((D+i\delta D)^{\mathbf{F},\mathbf{G}}q)(t)=\nabla_y H(q(t),\overline{p(t)}), \tag{46}$$

$$((D+i\delta D)^{\mathbf{F},\mathbf{G}}\overline{p)}(t)=-\nabla_x H(q(t),\overline{p(t)}). \tag{47}$$

The closest in spirit previous attempt to define the momentum process within stochastic mechanics is Ref. 18. See Ref. 2, pp. 95–98 and Ref. 4, pp. 117–119] for further work and discussion on this topic.

We close the section with a comment. In Ref. 19 (p. 110), Bohm and Hiley write concerning Nelson's stochastic acceleration: ''*If it could be made clear that this definition is physically or kinematically plausible then Nelson's approach would evidently have an important advantage*.'' As observed in Remark 3, the Nelson acceleration may be viewed as the real part of the second-order stochastic derivative $((D-i\delta D)^{\mathbf{F},\mathbf{G}}(D-i\delta D)^{\mathbf{F},\mathbf{G}})x)$ which occurs in Eq. (40).

In Sec. V, we show that indeed the Nelson process associated with a particular solution of the Schrödinger equation satisfies the global Newton's law (40). Hence, we feel that the results of this paper, together with Refs. 12, 15, 2, 1, 6, clearly demonstrate the physical and kinematical plausibility of Nelson's acceleration.

V. ELEMENTS OF HAMILTON–JACOBI THEORY

Following Ref. 6, we now develop the basic elements of a Hamilton–Jacobi theory of stochastic mechanics (see Ref. 15, Sec. 1 for a beautiful account of the classical theory). Suppose $\{\psi(x,t);t_0\leqslant t\leqslant t_1\}$ is a never vanishing solution of the *Schrödinger equation*

$$\frac{\partial \psi}{\partial t} = \frac{i\hbar}{2m}\nabla\psi - \frac{i}{\hbar}V(x)\psi.$$

Then $S_q(x,t) := \hbar/i \log \psi(x,t)$ satisfies

$$\frac{\partial S_q}{\partial t} + \frac{1}{2m}\nabla S_q \cdot \nabla S_q + V(x) - \frac{i\hbar}{2m}\Delta S_q = 0. \tag{48}$$

This is the *Hamilton–Jacobi equation* of stochastic mechanics. Indeed, we can now rephrase Theorem 1 as follows. Suppose $\{S_q(x,t); t_0 \leqslant t \leqslant t_1\}$ solves Eq. (48) with the initial condition $S_q(x,t_0) = \phi_0(x)$, and satisfies

$$E\left\{\int_{t_0}^{t_1} |\nabla S_q(x(t),t)|^2 dt\right\} < \infty$$

for all finite-energy diffusions x on $[t_0,t_1]$. Let $\rho_1(x) = |\exp(i/\hbar)S_q(x,t_1)|^2$. Then, there is a stochastic process $\{q(t); t_0 \leqslant t \leqslant t_1\}$, called the Nelson process, solving together with its quantum drift $(1/m)\nabla S_q(q(t),t)$ Problem (6). Corresponding to such an S_q, we define the *momentum field* by $p(x,t) = \nabla S_q(x,t)$, and the momentum process by $p(t) := p(q(t),t) = \nabla S_q(q(t),t)$. In Ref. 6 it was shown that the process $p(t)$ has the same first and second moments as the quantum momentum operator. It was also shown that the uncertainty relations admit a simple stochastic interpretation in terms of the pair $(q(t),p(t))$.

Theorem 4: *The pair* $(q(t),p(t))$ *satisfies the stochastic Hamilton equations (44) and (45).*

Proof: Let us first notice that $(D_+^{\mathbf{F}}q)(t) = (D_+^{\mathscr{F}}q)(t) = b_+(q(t),t)$. Indeed, since $q(t)$ is Markovian, so is

$$X(t) = \begin{pmatrix} q(t) \\ b_+(q(t),t) \\ b_-(q(t),t) \end{pmatrix}.$$

We then have

$$\begin{aligned}
(D_+^{\mathbf{F}}q)(t) &= \lim_{h \searrow 0} E\left\{ \frac{q(t+h)-q(t)}{h} \,\middle|\, \mathbf{F}_t \right\} \\
&= \lim_{h \searrow 0} E\left\{ \frac{q(t+h)-q(t)}{h} \,\middle|\, \begin{pmatrix} q(t) \\ b_+(q(t),t) \\ b_-(q(t),t) \end{pmatrix} \right\} \\
&= \lim_{h \searrow 0} E\left\{ \frac{q(t+h)-q(t)}{h} \,\middle|\, q(t) \right\} \\
&= (D_+^{\mathscr{F}}q)(t) = b_+(q(t),t).
\end{aligned}$$

Similarly, we get $(D_-^{G}q)(t) = (D_-^{C}q)(t) = b_-(q(t),t)$. Hence, $(D^{\mathbf{F},\mathbf{G}}q)(t) = (D^{\mathscr{F},\mathscr{G}}q)(t) = v(q(t),t)$ and $(\delta D^{\mathbf{F},\mathbf{G}}q)(t) = (\delta D^{\mathscr{F},\mathscr{G}}q)(t) = u(q(t),t)$. We then have $((D - i\delta D)^{\mathbf{F},\mathbf{G}}q)(t) = ((D - i\delta D)^{\mathscr{F},\mathscr{G}}q)(t) = v(q(t),t) - iu(q(t),t) = v_q(q(t),t) = (1/m)\nabla S_q(q(t),t) = \nabla_y H(q(t), p(q(t),t)) = \nabla_y H(q(t),p(t))$. To prove Eq. (45), recall from Ref. 1, Sec. VII that if $\phi(x,t)$ is a complex-valued function with sufficiently regular real and imaginary parts, then

$$d[\phi(q(t),t)] = \left[\frac{\partial}{\partial t} + v_q(q(t),t)\cdot\nabla - \frac{i\hbar}{2m}\Delta\right]\phi(q(t),t)dt + \nabla\phi(q(t),t)\cdot dw, \tag{49}$$

where $dw = dq - v_q(q(t),t)dt$ is the quantum noise corresponding to q. Applying Eq. (49) to $p(q(t),t) = \nabla S_q(q(t),t)$, we get

$$d[p(q(t),t)]=\left[\frac{\partial}{\partial t}+v_q(q(t),t)\cdot\nabla-\frac{i\hbar}{2m}\nabla\right]\nabla S_q(q(t),t)dt+D(q(t),t)dw, \tag{50}$$

where the 3×3 matrix D has ijth entry $d_{ij}(q(t),t)=(\partial^2/\partial x_i\partial x_j)S_q(q(t),t)$. Replacing $v_q(q(t),t)$ in Eq. (50) with $(1/m)\nabla S_q(q(t),t)$, and then employing Eq. (48), we get

$$d[p(q(t),t)]=-\nabla V(q(t))dt+D(q(t),t)dw. \tag{51}$$

Hence, the quantum drift of $p(t)$ is $-\nabla V(q(t))$ and Eq. (45) holds. □

By the same procedure, we can handle more general (sufficiently regular) Hamiltonian functions $H(x,y,t)$ if $S_q(x,t)$ now satisfies

$$\frac{\partial S_q}{\partial t}+H(x,\nabla S_q,t)-\frac{i\hbar}{2m}\Delta S_q=0,$$

and if we can construct a Markov process q with quantum drift

$$v_q(q(t),y)=\nabla_y H(q(t),\nabla S_q(q(t),t),t),$$

and prescribed initial condition.

We now isolate a crucial step in the proof of Theorem 4. In view of Eq. (49), define the *quantum acceleration field* by the substantial derivative

$$a_q(x,t):=\left[\frac{\partial}{\partial t}+v_q(x,t)\cdot\nabla-\frac{i\hbar}{2m}\Delta\right]v_q(x,t), \tag{52}$$

where $v_q(x,t)=(1/m)\nabla S_q(x,t)$. Using Eq. (48) in Eq. (52), we finally get

$$a_q(x,t)=-\frac{1}{m}\nabla V(x). \tag{53}$$

Equation (53) is the local form counterpart of Eq. (40).

Remark 5: Let $\{\psi(x,t);t_0\leqslant t\leqslant t_1\}$ be a never vanishing solution of the Schrödinger equation satisfying Carlen's finite-energy condition (Ref. 7). Then the corresponding Nelson process satisfies Eq. (40) with end points distributed according to $\rho_0(x)=|\psi(x,t_0)|^2$ and $\rho_1(x)=|\psi(x,t_1)|^2$.

VI. DISCUSSION

In this paper, we have developed a particle form of Hamilton's principle. We have then applied the principle to various conservative systems only changing the class of admissible motions. In the case of a quantum particle, we have seen that the critical process x satisfies the stochastic Newton law (40). This process is not Markovian, but the corresponding augmented process (41) is Markovian.

In Ref. 1, see also the outline in Sec. I, we have developed the second, hydrodynamic version of Hamilton's principle in the context of stochastic mechanics. The critical process q is there Markovian. Indeed, it is the Nelson process. Introducing the momentum field, and then the momentum process p as in Sec. V, we have obtained a pair of stochastic processes satisfying the stochastic Hamilton equations (44) and (45).

If we agree that in a deterministic context Markovian means ''satisfies a first-order differential equation,'' we see that the similarity with classical mechanics is striking. Much remains to be done, however, to develop a satisfactory Lagrangian and Hamiltonian formalism in stochastic mechanics even in the simplest case considered in this paper.

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On the geometry of non-holonomic Lagrangian systems

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We present a geometric framework for non-holonomic Lagrangian systems in terms of distributions on the configuration manifold. If the constrained system is regular, an almost product structure on the phase space of velocities is constructed such that the constrained dynamics is obtained by projecting the free dynamics. If the constrained system is singular, we develop a constraint algorithm which is very similar to that developed by Dirac and Bergmann, and later globalized by Gotay and Nester. Special attention to the case of constrained systems given by connections is paid. In particular, we extend the results of Koiller for Čaplygin systems. An application to the so-called non-holonomic geometry is given. © *1996 American Institute of Physics.* [S0022-2488(96)02407-3]

I. INTRODUCTION

A non-holonomic Lagrangian system consists of a regular Lagrangian $L(q^A,\dot{q}^A)$ defined on the phase space of velocities TQ of a configuration manifold Q with local coordinates $(q^A),1\leqslant A\leqslant n=\dim Q$, subjected to constraints defined by m local functions $\phi_i(q^A,\dot{q}^A)$. That means that the only allowable velocities are those verifying that $\phi_i=0$. We only consider the case of linear constraints, say those of the form $\phi_i(q^A,\dot{q}^A)=(\mu_i)_A(q)\dot{q}^A$. By applying a suitable Hamilton's principle, we arrive to the constrained Euler–Lagrange equations,

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}^A}\right)-\frac{\partial L}{\partial q^A}=-\lambda^i(\mu_i)_A,$$

where λ^i, $1\leqslant i\leqslant m$, are some Lagrange multipliers to be determined (see, for instance, Valcovici,[1] Pars,[2] Neimark and Fufaev,[3] Vershik and Faddeev,[4] Saletan and Cromer,[5] Rumiantsev,[6] Pironneau,[7] Vershik and Gershkovich,[8] Massa and Pagani[9,10]). In some of them, a more general type of constraints was discussed. We notice that Hamilton's principle in the non-holonomic framework is not a variational principle. We remit to the excellent book by Rosenberg[11] for a detailed discussion on that subject.

In the last years, there is an increasing interest in non-holonomic mechanics, and other approaches from a geometrical point of view have appeared: Weber,[12] Pitanga,[13,14] Marle,[15] Massa and Pagani,[9,10] Bates and Śniatycki,[16] Giachetta,[17] Koiller,[18] Cariñena and Rañada,[19] Rañada,[20] Dazord,[21] Cariñena and Rañada,[22] Sarlet, Cantrijn and Saunders,[23,24] Sarlet,[25,26] de León and M. de Diego.[27–31]

Our approach is a globalization of the one by Cariñena and Rañada.[19] In order to globalize their picture, we will consider a distribution D of codimension m defined on Q. The constraints

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imply that the motion is only allowable for some values of velocities, those belonging to the distribution D. The constrained motion equations can be written out by modifying the motion equations for the associated free Lagrangian system as follows:

$$(i_X\omega_L - dE_L) \in (D^v)^0, \quad X \in D^c, \tag{1}$$

along the points of D, where ω_L is the symplectic Poincaré–Cartan two-form, E_L is the energy associated with L, and D^v and D^c are the lifts of D to TQ. Notice that we do not need to invoke Lagrange multipliers. This approach is the dual version (i.e., in terms of distributions) of the one by Cartan using exterior systems.

Under some regularity hypothesis we construct an almost product structure $(\mathscr{P},\mathscr{Q})$ on TQ along the linear submanifold D such that the dynamics are obtained by projecting the Euler-Lagrange vector field ξ_L which solves the motion equations of the free problem,

$$i_{\xi_L}\omega_L = dE_L .$$

That is, the solutions of the constrained dynamics are just the solutions of the second order differential equation $\xi = \mathscr{P}(\xi_L)$ (Section II).

If the constrained system is not regular, we develop in Section III a constraint algorithm which is remarkably similar to that developed by Dirac and Bergmann for singular Lagrangian systems.[32–34] We obtain the local and global aspects of the constraint algorithm. By the way, we introduce the notion of first and second class constraints in this framework.

In Section IV we consider a very important kind of constrained systems, those called generalized Čaplygin systems. A generalized Čaplygin system consists of a Lagrangian function $L:TQ\to\mathbb{R}$ and a connection Γ in a fibration $\rho:Q\to M$ such that L is invariant by the horizontal lift operation. The particular case when $\rho:Q\to M$ is a principal bundle with structure group G, L is G-invariant and Γ is a principal connection, i.e., the horizontal subspaces are G-invariant, was considered by Koiller.[18] We extend the results by Koiller, and prove that there exists a well-defined Lagrangian function $L^*:TM\to\mathbb{R}$, such that the generalized Čaplygin system (L,Γ) is equivalent to a non-conservative system on TM with Lagrangian function L^* and external force α. Here, α is an one-form on TM related with the curvature of the connection Γ. Roughly speaking, the curvature is just the force of constraint. Several examples are studied.

Finally, in Section V, we apply our procedure to give a new insight to an old problem in the so-called non-holonomic geometry. Let Q be a Riemannian manifold with Riemannian metric g and Levi-Civita connection ∇ and suppose that a distribution D on Q is given. The goal is to obtain a new linear connection ∇^* on Q such that the geodesics of ∇^* are the extremals of the variational problem subjected to these linear constraints (see Synge,[35] Vranceanu,[36] Neimark and Fufaev[3] and the references therein). We define a connection Γ^* along D by using our procedure and the relations between non-homogeneous connections and second order differential equations on TQ obtained by Grifone.[37] If the constraints are holonomic, Γ^* induces a linear connection in the vector bundle $D\to Q$.

II. NON-HOLONOMIC LAGRANGIAN SYSTEMS

Let $L:TQ\to\mathbb{R}$ be a Lagrangian function defined on the phase space of velocities TQ of a n-dimensional configuration manifold Q. Denote by (q^A,v^A) the fibered coordinates on TQ. (Sometimes we will use the notation $v^A=\dot{q}^A$.)

The motion equations for L can be derived by a variational procedure. In fact, the extremals of the action,

$$\int L(q^A,\dot{q}^A)dt,$$

where $\dot{q}^A = dq^A/dt$ are just the solutions of the Euler–Lagrange equations,

$$\frac{d}{dt}\left(\frac{\partial L}{\partial v^A}\right) - \frac{\partial L}{\partial q^A} = 0, \quad v^A = \frac{dq^A}{dt}. \tag{2}$$

Alternatively, there exists a symplectic formulation. Indeed, let $\omega_L = -d\alpha_L$ be the Poincaré-Cartan 2-form, where $\alpha_L = J^*(dL)$. Here, J is the canonical almost tangent structure on TQ. That is, J is a tensor field of type (1,1) on TQ such that $J^2 = 0$ and rank $J = n$; J is locally defined by

$$J = \frac{\partial}{\partial v^A} \otimes dq^A.$$

The energy associated with L is defined by $E_L = CL - L$, where $C = v^A(\partial/\partial v^A)$ is the Liouville vector field on TQ. That is, C is the infinitesimal generator of the dilations along the fibers.

The global motion equation for the free problem is (see Ref. 38)

$$i_X \omega_L = dE_L. \tag{3}$$

We say that the Lagrangian L is regular if the Hessian matrix $(\partial^2 L/\partial v^A \partial v^B)$ is non-singular. In such a case, the form ω_L is symplectic and, thus, (3) has a unique solution ξ_L (the Euler–Lagrange vector field) which is a second order differential equation (SODE for short). Further, the solutions of ξ_L coincide with the solutions of the Euler–Lagrange equations. More precisely, the projections onto Q of the integral curves of ξ_L are the extremals for L.

Now, we suppose that a family of linear constraints is given. In the local picture, L is subjected to constraints defined by m local functions of the form $\phi_i(q^A, v^A) = (\mu_i)_A(q)v^A$. That means that the only allowable velocities are those verifying that $\phi_i = 0$.

The purpose of this paper is to give a global picture of Lagrangian systems subjected to linear constraints.

Definition II.1: A non-holonomic Lagrangian system is given by the following data:
(i) A regular Lagrangian $L: TQ \to \mathbb{R}$*;*
(ii) An $(n-m)$*-dimensional distribution* D *on the* n*-dimensional configuration manifold* Q*.*
The constraints are said to be holonomic if D *is involutive.*

This means that the only allowable velocities are the tangent vectors belonging to D, i.e., the motion is constrained to the submanifold D. Notice that D can be viewed as a vector subbundle of $\tau_Q: TQ \to Q$, and, so, D is a submanifold of TQ.

Define two distributions D^c and D^v on TQ as follows. Suppose that $\{\mu_i; 1 \leqslant i \leqslant m\}$ is a local basis of 1-forms of the annihilator D^0 of D. Then D^c and D^v are, respectively, defined by

$$(D^c)^0 = \langle \mu_i^v, \mu_i^c \rangle, \quad (D^v)^0 = \langle \mu_i^v \rangle, \tag{4}$$

where μ_i^v (resp., μ_i^c) denotes the vertical (resp., complete) lift of the 1-form μ_i to TQ (see Refs. 38,39).

If $\{\overline{\mu_i}\}$ is another local basis of D we have

$$\overline{\mu_i} = \Lambda_i^j \mu_j,$$

where (Λ_i^j) is a regular matrix defined on the overlapping of the two local neighborhoods. Since

$$\overline{\mu_i^c} = (\Lambda_i^j)^c \mu_j^v + (\Lambda_i^j)^v \mu_j^c, \quad \overline{\mu_i^v} = (\Lambda_i^j)^v \mu_j^v, \tag{5}$$

we deduce that D^c and D^v are well-defined. Here f^v (resp., f^c) denotes the vertical (resp., complete) lift of a function f on Q to TQ (see Refs. 39, 38).

Since the allowable velocities have to belong to D, we deduce that the motion equations for the constrained mechanical systems would be

$$(i_X\omega_L - dE_L) \in (D^v)^0, \quad X \in D^c, \tag{6}$$

along the points of D.

In fact, suppose that $\mu_i = (\mu_i)_A dq^A$. Hence we have

$$\mu_i^v = (\mu_i)_A dq^A,$$
$$\mu_i^c = (\mu_i)_A^c dq^A + (\mu_i)_A dv^A,$$
$$\hat{\mu}_i = (\mu_i)_A v^A,$$

where $\hat{\mu}_i$ is the function on TQ defined by $\hat{\mu}_i(q^A, v^A) = \mu_i(v^A(\partial/\partial q^A))$.

Notice that there are many solutions of the first equation in (6), since ω_L is symplectic. Moreover, every solution of (6) is a SODE. In fact, let μ_i be a local basis of D. Then, (6) can be locally written as follows:

$$i_X\omega_L - dE_L = \lambda^i \mu_i^v, \quad \mu_i^v(X) = 0, \quad \mu_i^c(X) = 0, \tag{7}$$

for some Lagrange multipliers λ^i to be determined. If we apply i_J to the first equation in (7), we have

$$i_J i_X \omega_L - i_J(dE_L) = 0,$$

which implies $i_{JX}\omega_L = i_C\omega_L$ and, then, $JX = C$. Here, i_J denotes the derivation of type i_* in the sense of Frölicher–Nijenhuis associated with J, that is, i_J is completely defined by the formulas $i_J f = 0$ and $i_J(df) = J^*(df)$ for any function f on TQ.[38] Therefore, we deduce that the local expression of X is

$$X = v^A \frac{\partial}{\partial q^A} + X^A \frac{\partial}{\partial v^A}.$$

Thus, the solutions of X satisfy the following constrained Euler–Lagrange equations:

$$\frac{d}{dt}\left(\frac{\partial L}{\partial v^A}\right) - \frac{\partial L}{\partial q^A} = -\lambda^i (\mu_i)_A, \quad v^A = \frac{dq^A}{dt}.$$

By the way, notice that $\mu_i^v(X) = \hat{\mu}_i$ and $\mu_i^c(X) = X(\hat{\mu}_i)$. Then the second set of equations in (7) defines the submanifold D, and the third one means that X has to be tangent to D. Given the symplectic form ω_L we have the associated musical isomorphisms,

$$\flat_L : T(TQ) \to T^*(TQ)$$

and

$$\#: T^*(TQ) \to T(TQ),$$

where for any $X \in T(TQ)$, $\flat_L(X) = i_X\omega_L$, and for any $\alpha \in T^*(TQ)$, $\#\alpha = X_\alpha$ is the unique tangent vector to TQ such that $b_L(X_\alpha) = \alpha$. From $(D^v)^0$ and by using the isomorphism $\#$, we obtain a distribution S on TQ. A vector $v \in T_xTQ$ belongs to S_x if $i_v\omega_L(x) \in (D^v)_x^0$. It is clear that $\dim S = m$.

Let Z_i be the local vector field defined by

$$i_{Z_i}\omega_L=\mu_i^v, \quad 1\leqslant i\leqslant m.$$

A direct computation shows that

$$Z_i=-W^{AB}(\mu_i)_B\frac{\partial}{\partial v^A},$$

where (W^{AB}) is the inverse matrix of the Hessian matrix $(W_{AB}=\partial^2L/\partial v^A\partial v^B)$. Therefore, Z_i is vertical.

We have that S is locally generated by the vector fields $\{Z_i,\ 1\leqslant i\leqslant m\}$.

Definition II.2: The constrained system will be called regular if

$$T_xD\cap S_x=0, \quad for\ \ any\ \ x\in D.$$

The meaning of the regularity of the constrained system will become clear in a while. Notice that the regularity of the constrained system is closely related with the nature of the Lagrangian function.

Suppose that the constrained system is regular. Since for any $x\in D$, we have $\dim S_x=m$, and $\dim T_xD=2n-m$, we obtain that

$$T_xTQ=T_xD\oplus S_x, \quad \forall x\in D.$$

Thus, each tangent vector $v\in T_xTQ$ splits in a unique way as $v=v_1+v_2$, where $v_1\in T_xD$ and $v_2\in S_x$. Then, we can construct two complementary projectors $\mathscr{P}$ and $\mathscr{Q}$ as follows: $\mathscr{P}(v)=v_1$, and $\mathscr{Q}(v)=v_2$. In fact, $(\mathscr{P},\mathscr{Q})$ is a well-defined almost product structure on TQ along the points of D.

Take now the codistribution $\langle dE_L\rangle\oplus(D^v)^0$. By using the isomorphism #, we obtain a distribution S_L on TQ locally generated by $\{\xi_L,Z_1,\cdots,Z_m\}$. That is,

$$S_L=\#(\langle dE_L\rangle\oplus(D^v)^0).$$

Then, $\dim(T_xD\cap(S_L)_x)=1$, $\forall x\in D$. Moreover, there exists a unique generator ξ of the distribution $TD\cap S_L$ along the points of D such that $(J\xi=C)_{/D}$.

The vector field $\xi\in\mathscr{X}(D)$ is the solution of the Lagrangian system subjected to constraints given by a distribution D. This vector field ξ is precisely $P(\xi_{L/D})$, the projection of the Euler-Lagrange vector field of the free Lagrangian system. In fact, along the points of D, we have

$$\begin{aligned} i_{\mathscr{P}(\xi_L)}\omega_L-dE_L&=i_{\xi_L-\mathscr{Q}(\xi_L)}\omega_L-dE_L\\ &=-i_{\mathscr{Q}(\xi_L)}\omega_L\in(D^v)^0. \end{aligned}$$

Moreover, we deduce that $\mathscr{P}(\xi_L)(x)\in T_xD$ or, equivalently, $\mathscr{P}(\xi_L)\in D^c$.

In order to perform an explicit computation of the vector field ξ, we proceed as follows. Take a local basis $\{\mu_i,1\leqslant i\leqslant m\}$ of D and define $\mathscr{C}_{ij}=Z_i(\hat{\mu}_j)$. We deduce that

$$\mathscr{C}_{ij}=-W^{AB}(\mu_i)_A(\mu_j)_B. \tag{8}$$

Proposition II.3: The constrained system is regular iff *the matrices* $(\mathscr{C}_{ij})$ *are non-singular on* D.

Proof: Suppose that the constrained system is regular. Take an arbitrary linear combination of columns of $\mathscr{C}$ at some point $x\in D$ such that

$$\sum_{i=1}^{m} \lambda^i Z_i(x)(\hat{\mu}_j)=0.$$

Thus, $\Sigma\lambda^i Z_i(x)\in T_xD$ which implies that $\Sigma\lambda^i Z_i(x)=0$ and hence $\lambda^1=\lambda^2=\cdots\lambda^m=0$.

Conversely, suppose $\mathscr{C}$ ia non-singular and take $X\in S_x\cap T_xD$. Thus, $X=\Sigma\lambda^i Z_i(x)$ and $X(\hat{\mu}_j)=0$, $\forall j$, $1\leqslant j\leqslant m$ which implies that $\Sigma\lambda^i Z_i(\hat{\mu}_j)=0$. Therefore we deduce that $\lambda^1=\cdots=\lambda^m=0$ and $X=0$.

■

Thus, if D is regular, we obtain an explicit expression for the projector $\mathscr{Q}$:

$$\mathscr{Q}=\mathscr{C}^{ij}Z_j\otimes d\hat{\mu}_i,$$

where $(\mathscr{C}^{ij})$ denotes the inverse matrix of $(\mathscr{C}_{ij})$.

Then, we get

$$\xi=\mathscr{P}(\xi_L)=\xi_L-\mathscr{C}^{ij}\xi_L(\hat{\mu}_i)Z_j.$$

Proposition II.4: If the Hessian matrix

$$\left(\frac{\partial^2 L}{\partial v^A \partial v^B}\right),$$

is positive or negative definite at each point $x\in D$, then the constrained system is regular.

Proof: The result follows from (8) (see also Cariñena and Rañada[19]).

■

Remark II.5: Proposition II.4 clarifies the usual assumption on the positive or negative character of the Hessian matrix of L. It is nothing but that a sufficient condition to ensure the regularity of the constrained system. Of course, if the Lagrangian L is natural, that is, $L=T-V$, where T is the kinetic energy of a Riemannian metric g on Q and V is a potential energy, then the constrained system would be regular.

Remark II.6: From the regularity of the matrices $\mathscr{C}$, we deduce that $(\mathscr{P},\mathscr{Q})$ may be extended (in many ways) to an open neighborhood of D. Consequently, $\mathscr{P}(\xi_L)$ may also be extended to an open neighborhood of D (see Ref. 27 for more details).

By using the almost product structure $(\mathscr{P},\mathscr{Q})$ and the musical isomorphisms, we can construct the following linear mapping $\overline{\mathscr{Q}}_x:T^*_x(TQ)\to T^*_x(TQ)$:

$$\overline{\mathscr{Q}}_x(\alpha_x)=\flat_L(\mathscr{Q}_x(\#(\alpha_x))),\quad \forall\alpha_x\in T^*_x(TQ),\quad x\in D.$$

Since $\overline{\mathscr{Q}}_x^2=\mathrm{id}$ and $Im\overline{\mathscr{Q}}_x=(D^v)^o_x$, we obtain the following splitting:

$$T^*_x(TQ)=(D^v)^o_x\oplus\overline{S_x},\quad \forall x\in D,$$

where $\overline{S_x}=Im\overline{\mathscr{P}}_x$, $\overline{\mathscr{P}}_x=\mathrm{id}-\overline{\mathscr{Q}}_x$ being the complementary projector. In fact, $\overline{\mathscr{P}}$ and $\overline{\mathscr{Q}}$ may be interpreted as tensor fields of type (1,1) on TQ defined along D.

Notice that $\overline{S}$ is the annihilator of the distribution along D locally generated by the vector fields $\{X_{\hat{\mu}_i},1\leqslant i\leqslant m\}$, where $X_{\hat{\mu}_i}$ is the Hamiltonian vector field of the function $\hat{\mu}_i$ with respect to the symplectic form ω_L.

The following result tells us that one could add the constraint forces to the energy to obtain a global force acting on the system.

Theorem II.7: *The solution of the constrained dynamics is the unique vector field ξ on D such that*

$$(i_X\omega_L=\overline{\mathscr{P}}(dE_L))_{/D}.$$

Proof: By the construction of $\overline{\mathscr{Q}}$ we have that

$$\overline{\mathscr{Q}}(dE_L)=i_{\mathscr{Q}(\xi_L)}\omega_L.$$

On the other hand, $\xi=\mathscr{P}(\xi_L)$ is the solution of the constrained dynamics. Thus, we deduce that

$$i_{\mathscr{P}(\xi_L)}\omega_L=i_{\xi_L}\omega_L-i_{\mathscr{Q}(\xi_L)}\omega_L=dE_L-\overline{\mathscr{Q}}(dE_L)=\overline{\mathscr{P}}(dE_L).$$

Since ω_L is symplectic, we conclude that the solution of the equation

$$(i_X\omega_L=\overline{\mathscr{P}}(dE_L))_{/D}$$

is unique. ■

A direct computation shows that the local expression of $\overline{\mathscr{Q}}$ is

$$\overline{\mathscr{Q}}=-\mathscr{C}^{ij}X_{\hat{\mu}_i}\otimes\mu_j^v.$$

Therefore, we obtain that

$$\overline{\mathscr{P}}(dE_L)=dE_L-\mathscr{C}^{ij}\xi_L(\hat{\mu}_i)\mu_j^v.$$

The following lemmas will be used in Section IV.

Lemma II.8: Given a regular constrained system with Lagrangian function L and linear constraints D, the vector field ξ solving the constrained dynamics satisfies

$$\mathscr{L}_\xi\alpha_L=dL-L_{\mathscr{Q}(\xi_L)}\alpha_L,$$

where $\mathscr{L}_\xi$ denotes the Lie derivative with respect to ξ.

Proof: It follows since $\xi=\mathscr{P}(\xi_L)=\xi_L-\mathscr{Q}(\xi_L)$ and $\mathscr{L}_{\xi_L}\alpha_L=dL$. ■

Lemma II.9: Under the same hypothesis as in Lemma II.8, we have

$$\mathscr{L}_{\mathscr{Q}(\xi_L)}\alpha_L\in(D^v)^0.$$

Proof: Since $\mathscr{Q}(\xi_L)=\Sigma_{j=1}^m\Lambda^jZ_j$, with $\Lambda^j=\mathscr{C}^{ij}\xi_L(\hat{\mu}_i)$, we deduce that

$$\begin{aligned}\mathscr{L}_{\mathscr{Q}(\xi_L)}\alpha_L&=\mathscr{L}\sum_{j=1}^m\Lambda^jZ_j\alpha_L\\&=i\sum_{j=1}^m\Lambda^jZ_jd\alpha_L+d(i\sum_{j=1}^m\Lambda^jZ_j\alpha_L)\\&=-i\sum_{j=1}^m\Lambda^jZ_j\omega_L=-\sum_{j=1}^m\Lambda^j\mu_j^v,\end{aligned}$$

since the vector fields Z_j are vertical and α_L is semibasic. ■

III. THE SINGULAR CASE

In this section we shall describe what happens if the given constrained system is not regular, or, in other words, $T_xD\cap S_x=0$, for some points x in D. Notice that this fact is equivalent to the non-regularity of the local matrices $(\mathscr{C}_{ij})$.

For any point $x\in D$, we have the obvious inclusion

$$T_xD\cap S_x\subset T_xD\cap(S_L)_x.$$

In the regular case, this inclusion is strict, and the jump of dimension is just 1. This jump allows us to obtain the dynamics by taking a basis ξ of $(TD\cap S_L)_{/D}$ normalized in order to get $J\xi=C$. The above remarks illuminate the way to proceed in the singular case.

Define a submanifold D_2 of TQ as follows:

$$D_2=\{x\in D/T_xD\cap S_x\subsetneqq T_xD\cap(S_L)_x\}.$$

This implies that for any point $x\in D_2$, there exists some tangent vector

$$X=\xi_L(x)+\lambda^iZ_i(x)\in T_xD\cap(S_L)_x,$$

such that $X\notin S_x$. Thus, X is a solution of the constrained equation, but, in general, it is not necessarily tangent to D_2.

Therefore, we define a new submanifold D_3 of D_2 as follows:

$$D_3=\{x\in D_2/T_xD_2\cap S_x\subsetneqq T_xD_2\cap(S_L)_x\}.$$

Proceeding further, we obtain a sequence of constraint submanifolds,

$$\cdots\to D_k\to\cdots\to D_2\to D_1=D.$$

$D=D_1$ will be called the primary constraint submanifold, D_2 the secondary constraint submanifold and so on.

As in the Gotay and Nester algorithm for singular Lagrangian systems[33,34] we also have three possibilities

(i) There exists an integer $k\geqslant 1$ such that $D_k=\varnothing$. This means that the equations (6) are not consistent.

(ii) There exists an integer $k\geqslant 1$ such that $D_k=\varnothing$ but $\dim D_k=0$. In this case, there are no dynamics. D_k consists in isolated points and the solution of the constrained dynamics is $X=0$.

(iii) There exists an integer $k\geqslant 1$ such that $D_{k+1}=D_k$ and $\dim D_k>0$. In this case the algorithm stabilizes at the final constraint submanifold $D_f=D_k$. So, there exists at least a vector field ξ on D_f satisfying the SODE condition $((J\xi=C)_{/D_f})$ and such that

$$i_\xi\omega_L-dE_L\in(D^v)^0.$$

Assume that the algorithm ends at some final constraint submanifold D_f. Thus, we have

$$T_xD_f\cap S_x\subsetneqq T_xD_f\cap(S_L)_x,\quad\forall x\in D_f.$$

We will suppose that the distribution $TD_f\cap S$ along D has constant dimension, say r, that is,

$$\dim(T_xD_f\cap S_x)=r,\quad\text{for all } x\in D_f.$$

Lemma III.1: We have that $\xi_L(x)\in T_xD_f+S_x$ for any $x\in D_f$.

Proof: Since $T_xD_f\cap S_x\subsetneqq T_xD_f\cap(S_L)_x$ for any $x\in D_f$, we deduce that there exists a tangent vector $X\in T_xD_f\cap(S_L)_x$ such that $X\notin T_xD_f\cap S_x$. Thus, $X=\xi_L(x)+\lambda^iZ_i(x)$ which implies that

$\xi_L(x)=X-\lambda^i Z_i\in T_xD_f+S_x$. ■

In order to determine the dynamics, we split S_x as a direct sum of two subspaces, say

$$S_x=\check{S}_x\oplus(T_xD_f\cap S_x). \tag{9}$$

Obviously, there are many choices for a complementary subspace of $T_xD_f\cap S_x$ into S_x. From (9) we deduce that $\check{S}_x\cap T_xD_f=0$, and we can then split $T_x(TQ)$ as follows:

$$T_x(TQ)=\check{S}_x\oplus T_xD_f\oplus M_x,\quad x\in D_f,$$

where M_x is a suitable complementary subspace. Take the corresponding three complementary projectors:

$$\mathcal{Q}_x:T_x(TQ)\to\check{S}_x,$$

$$(\mathcal{P}_1)_x:T_x(TQ)\to T_xD_f,$$

$$(\mathcal{P}_2)_x:T_x(TQ)\to M_x.$$

Consider the projector $(\mathcal{P})_x=(\mathcal{P}_1)_x+(\mathcal{P}_2)_x$. Hence, we have (along the points of D_f)

$$\begin{aligned} i_{\mathcal{P}_x(\xi_L(x))}\omega_L(x)-(dE_L)_x&=i_{\xi_L(x)-\mathcal{Q}_x(\xi_L(x))}\omega_L(x)-i_{\xi_L(x)}\omega_L(x)\\ &=-i_{\mathcal{Q}_x(\xi_L(x))}\omega_L(x)\in(D^v)^0_x. \end{aligned}$$

Moreover, for any $x\in D_f$, we deduce that

$$\mathcal{P}_x(\xi_L(x))=(\mathcal{P}_1)_x(\xi_L(x))\in T_xD_f,$$

since $\xi_L(x)\in T_xD_f+S_x$ by Lemma III.1.

A differentiable choice of both distributions $\check{S}$ and M allows us to construct an almost product structure $(\mathcal{P}_1,\mathcal{P}_2,\mathcal{Q})$ [or $(\mathcal{P},\mathcal{Q})$, where $\mathcal{P}=\mathcal{P}_1+\mathcal{P}_2$] along D_f such that $\mathcal{P}(\xi_{L/D_f})$ is a solution of the constrained dynamics. Notice that a general solution is of the form

$$\mathcal{P}(\xi_{L/D_f})+TD_f\cap S.$$

We have chosen complementary distributions $\check{S}$ and M in order to obtain the dynamics. Notice that it is possible to realize both decompositions, say $S=\check{S}\oplus(T_xD_f\cap S)$ and $T(TQ)=\check{S}\oplus TD_f\oplus M$. In fact, take a local basis $\{\mu_i\}$ of D^0 and denote by ϕ_I the constraint functions which define D_f, where $1\leqslant I\leqslant 2n-\dim D_f$. Notice that $\phi_I=\hat{\mu}_I$, for $1\leqslant I\leqslant m$. We have assumed that $TD_f\cap S$ has constant rank r. Thus, the matrix $(\mathcal{C}_{iJ})=(Z_i(\hat{\phi}_J))$ has also constant rank $m-r$. Indeed, take a local basis $Y_1,\ldots,Y_r$ of $TD_f\cap S$ such that $Y_a=\mathcal{A}^i_aZ_i$. Since Y_a is tangent to D_f, we get

$$\mathcal{A}^i_aZ_i(\phi_J)=0,\quad \text{for all } J.$$

But this implies that rank $\mathcal{C}=m-r$. The converse is proved by reversing the argument.

Assume that the submatrix $\mathcal{C}'=(\mathcal{C}_{I'J'})$, $(1\leqslant I',J'\leqslant m-r)$ is regular. In that case, we define a projector $\mathcal{Q}$ by putting

$$\mathcal{Q}=\mathcal{C}^{I'J'}Z_{J'}\otimes d\phi_{I'},$$

where $(\mathscr{C}^{I'J'})$ is the inverse matrix of $(\mathscr{C}_{I'J'})$. Notice that $\check{S}=\langle Z_{I'}\rangle$. If we put $\mathscr{P}=\mathrm{id}-\mathscr{Q}$ we obtain an almost product structure $(\mathscr{P},\mathscr{Q})$ along D_f. The decomposition $\mathscr{P}=\mathscr{P}_1+\mathscr{P}_2$ is obtained by choosing a complementary M of $\check{S}\oplus TD_f$. This choice corresponds to the ambiguity in the determination of the other Lagrange multipliers. Indeed, if we compute $\mathscr{P}(\xi_L)$ we obtain

$$\mathscr{P}(\xi_L)=\xi_L-\mathscr{C}^{I'J'}\xi_L(\phi_{I'})Z_{J'},$$

and a general solution is of the form

$$\mathscr{P}(\xi_L)+Y,$$

where $Y\in TD_f\cap S$. So, the only Lagrange multipliers determined are just the components of the $Z_{J'}$'s.

Remark III.2: A solution of (6) has the general form $X=\xi_L+\lambda^i Z_i$, where Z_i are the symplectic gradients of the 1-forms μ_i^v. The tangency condition may now be written as

$$\xi_L(\hat{\mu}_j)+\lambda^i Z_i(\hat{\mu}_j)=0,\quad 1\leqslant j\leqslant m, \tag{10}$$

or, equivalently,

$$\xi_L(\hat{\mu}_j)+\lambda^i\mathscr{C}_{ij}=0,\quad 1\leqslant j\leqslant m. \tag{11}$$

If the matrix $\mathscr{C}_{ij}$ is regular, the system of equations (11) have a solution which is obtained by the well-known Crame rule, or, in a more sophisticated way, by constructing the local almost product structure $(\mathscr{P},\mathscr{Q})$.

If the constrained system is singular, Equation (10) can be analyzed as in the Dirac-Bergmann algorithm.[32] In fact,

$$\xi_L(\hat{\mu}_j)+\lambda^i\mathscr{C}_{ij}=0,\quad 1\leqslant j\leqslant m,$$

is a system of m equations with m unknowns, the Lagrange multipliers. The system is consistent if the ranks of the matrices $(\mathscr{C}_{ij})$ and $(\mathscr{C}_{ij};-\xi_L(\hat{\mu}_j))$ coincide. (Of course, they are equal if the constrained system is regular.) Therefore, we select the points where the ranks coincide. Denote by D_2 the collection of all these points. At the points in D_2 there are solutions, but they are not necessarily tangent to D_2. By the way, new constraints may appear. In fact, notice that, if the matrix $(\mathscr{C}_{ij})$ has rank, say r, then the matrix $(\mathscr{C}_{ij};-\xi_L(\hat{\mu}_j))$ has rank greater or equal to r. Suppose that $\mathscr{M}$ is a submatrix of $(\mathscr{C}_{ij})$ of rank r. The determinants of the submatrices of $(\mathscr{C}_{ij};-\xi_L(\hat{\mu}_j))$ obtained from $\mathscr{M}$ by adding elements of the column $\xi_L(\hat{\mu}_j)$ are the new possible constraints. These secondary constraints ϕ_α have to be added to the motion equations which become

$$\begin{aligned}\xi_L(\hat{\mu}_j)+\lambda^i Z_i(\hat{\mu}_j)&=0,\\ \xi_L(\phi_\alpha)+\lambda^i Z_i(\phi_\alpha)&=0.\end{aligned} \tag{12}$$

The procedure is now repeated, and we obtain a sequence of submanifolds

$$\cdots\to\overline{D_k}\to\cdots\to\overline{D_2}\to D,$$

which are just the same that the ones previously obtained. More precisely, $\overline{D_k}$ is the intersection of D_k with the tangent bundle of the open neighborhood where the local basis μ_i is defined.

Remark III.3: We started with linear constraints, or, in the present terminology, the primary constraints are linear. However, the secondary constraints are not necessarily linear.

If we denote by $\{,\}_L$ the Poisson bracket on TQ defined from the symplectic form ω_L, we have $\{f,E_L\}_L=\xi_L(f)$, for any function f on TQ. Thus, (10) can be written as follows:

$$\{\hat{\mu}_j,E_L\}_L+\lambda^i Z_i(\hat{\mu}_j)=0, \quad 1\leqslant j\leqslant m.$$

As in the Dirac–Bergmann approach,[32] we can distinguish two different classes of constraints. A constraint f will be called first class if $\{f,\Psi\}_L\sim 0$, that is, $\{f,\Psi\}_L$ vanishes on the final constraint submanifold D_f. Otherwise, f will be called a second class constraint. We deduce that the Hamiltonian vector fields corresponding to first class constraints are tangent to D_f, and the Hamiltonian vector fields corresponding to second class constraints are transversal to D_f.

Example III.4: Consider the following Lagrangian function L defined on $T\mathbb{R}^3$ by

$$L=\frac{1}{2}((v^1)^2+(v^2)^2-(v^3)^2+(q^1)^2),$$

subjected to linear constraints given by a distribution D on $\mathbb{R}^3$ whose annihilator is

$$D^0=\langle dq^1+dq^3\rangle.$$

Here (q^1,q^2,q^3) denote the standard coordinates on $\mathbb{R}^3$, and $(q^1,q^2,q^3,v^1,v^2,v^3)$ the induced ones on $T\mathbb{R}^3$. Thus, the submanifold $D\subset T\mathbb{R}^3$ consists in those points in $T\mathbb{R}^3$ such that $v^1+v^3=0$.

The distribution S is generated by the vector field

$$Z=-\frac{\partial}{\partial v^1}+\frac{\partial}{\partial v^3}.$$

We have

$$S_x\cap T_xD=S_x,$$

for any $x\in D$. Therefore, the constrained system is singular.

Applying the constraint algorithm, we get

$$D_2=\{x\in D/T_xD\cap S_x\subsetneqq T_xD\cap(S_L)_x\},$$

so that

$$D_2=\{(q^A,v^A)\in T\mathbb{R}^3/v^1+v^3=0,\ q^1=0\}.$$

We proceed further, and obtain

$$\begin{aligned}D_3&=\{x\in D/T_xD_2\cap S_x\subsetneqq T_xD_2\cap(S_L)_x\},\\&=\{(q^A,v^A)\in T\mathbb{R}^3/v^3=0,\ q^1=0,\ v^1=0\}.\end{aligned}$$

Now, since

$$T_xD_3\cap S_x\subsetneqq T_xD_3\cap(S_L)_x,$$

for any $x\in D_3$, we deduce that D_3 is the final constraint submanifold.

The dynamics is given by the vector field $(\xi_L+\lambda Z)_{/D_3}$, for any function λ on D_3.

IV. CONSTRAINTS DEFINED BY CONNECTIONS. GENERALIZED ČAPLYGIN SYSTEMS

One of the most appealing instances of non-holonomic Lagrangian systems are those given by the existence of a connection.

Suppose that Q is a fibered manifold over a manifold M, say, $\rho:Q\to M$ is a surjective submersion. Assume that a connection Γ in $\rho:Q\to M$ is given, such that the allowable motions of a Lagrangian function $L:TQ\to\mathbb{R}$ have to be horizontal curves with respect to that connection. In other words, the allowable velocities are horizontal tangent vectors. Thus, D is just the horizontal distribution H such that

$$TQ=H\oplus V\rho.$$

Let us recall that Γ may be considered as a tensor field of type (1,1) on Q such that $\Gamma^2=\mathrm{id}$ and the eigenspaces corresponding to the eigenvalue -1 are just the vertical subspaces. Take fibered coordinates $(q^A)=(q^a,q^i)$, $1\leqslant a\leqslant n-m$, $1\leqslant i\leqslant m$, $n=\dim Q$. The horizontal distribution is locally spanned by the local vector fields

$$H_a=\left(\frac{\partial}{\partial q^a}\right)^H=\frac{\partial}{\partial q^a}-\Gamma^i_a(q^A)\frac{\partial}{\partial q^i},$$

where Y^H stands for the horizontal lift to Q of a vector field Y on M, and $\Gamma^i_a=\Gamma^i_a(q^b,q^j)$ are the Christoffel components of Γ. Thus, we obtain a local basis of vector fields on Q,

$$\left\{H_a,V_i=\frac{\partial}{\partial q^i}\right\}.$$

Its dual basis of 1-forms is

$$\{\eta_a=dq^a,\eta_i=\Gamma^i_a dq^a+dq^i\}.$$

We deduce that H^0 is locally spanned by the 1-forms $\{\eta_i\}$.

Define the curvature of Γ as the tensor field of type (1,2) on Q given by

$$R=\frac{1}{2}[\mathbf{h},\mathbf{h}],$$

where $\mathbf{h}=(1/2)(\mathrm{id}+\Gamma)$ is the horizontal projector associated with Γ, and $[\mathbf{h},\mathbf{h}]$ is its Nijenhuis tensor (see Ref. 38). Thus,

$$R(\mathbf{h}(u_1),\mathbf{h}(u_2))=v([\mathbf{h}(u_1),\mathbf{h}(u_2)]),$$

$$R(\mathbf{h}(u_1),\mathbf{v}(u_2))=0,$$

$$R(\mathbf{v}(u_1),\mathbf{v}(u_2))=0,$$

for any $u_1,u_2\in T_xQ$, where $\mathbf{v}=\mathrm{id}-\mathbf{h}$ is the complementary vertical projector. Since

$$\mathbf{h}\left(\frac{\partial}{\partial q^a}\right)=\frac{\partial}{\partial q^a}-\Gamma^i_a\frac{\partial}{\partial q^i},$$

$$\mathbf{h}\left(\frac{\partial}{\partial q^i}\right)=0,$$

we obtain

$$R\left(\frac{\partial}{\partial q^a},\frac{\partial}{\partial q^b}\right)=R^i_{ab}\frac{\partial}{\partial q^i},$$

where

$$R^i_{ab}=\frac{\partial\Gamma^i_a}{\partial q^b}-\frac{\partial\Gamma^i_b}{\partial q^a}+\Gamma^j_a\frac{\partial\Gamma^i_b}{\partial q^j}-\Gamma^j_b\frac{\partial\Gamma^i_a}{\partial q^j}.$$

We say that Γ is flat if the curvature R identically vanishes. In this case, the constrained system is holonomic.

Notice that this kind of non-holonomic constrained systems is very special, since the local constraints are of the form

$$v^i=-\Gamma^i_a(q^A)v^a,$$

that is, some velocities are explicitly written in terms of the others.

We will consider a very special kind of such constrained systems, those called generalized Čaplygin systems.

Definition IV.1: A generalized Čaplygin system consists of a Lagrangian function $L:TQ\to\mathbb{R}$ *and a connection* Γ *in a fibration* $\rho:Q\to M$ *such that*

$$L((Y^H)_q)=L((Y^H)_{\tilde{q}}),$$

for any $Y\in T_yM$, *where* $q,\tilde{q}\in Q$ *are such that* $\rho(q)=\rho(\tilde{q})=y$.

Remark IV.2: Notice that the Čaplygin systems considered by Koiller[18] are particular cases. In fact, in that case, $\rho:Q\to M$ is a principal bundle with structure group G, L is G-invariant, and Γ is a principal connection, i.e., the horizontal subspaces are G-invariant. The 1-forms η_i are just the components of the connection form. If the group G is Abelian, then the last condition implies that the Christoffel components do not depend on the fiber coordinates. So, we recover the classical setting of Čaplygin systems[18].

From the definition, one easily see that there exists a well-defined Lagrangian function $L^*:TM\to\mathbb{R}$, by setting

$$L^*(Y)=L((Y^H)_q),$$

for any $Y\in T_yM$, where q is an arbitrary point in the fiber over y. In local coordinates we have

$$L^*(q^a,v^a)=L(q^a,q^i,v^a,-\Gamma^i_a v^a).$$

Since L^* does not depend on q^i we deduce that

$$\frac{\partial L}{\partial q^i}=\frac{\partial L}{\partial v^j}\frac{\partial\Gamma^j_a}{\partial q^i}v^a. \tag{13}$$

The constrained Euler–Lagrange equations for L are the following:

$$\frac{d}{dt}\left(\frac{\partial L}{\partial v^a}\right)-\frac{\partial L}{\partial q^a}=-\sum_i\lambda^i\Gamma^i_a,$$

$$\frac{d}{dt}\left(\frac{\partial L}{\partial v^i}\right)-\frac{\partial L}{\partial q^i}=-\lambda^i,$$

$$v^a=\frac{dq^a}{dt},\quad v^i=\frac{dq^i}{dt}.$$

After some calculations, and using (13), we obtain that

$$\frac{d}{dt}\left(\frac{\partial L^*}{\partial v^a}\right)-\frac{\partial L^*}{\partial q^a}=\frac{\partial L}{\partial v^i}v^b\left(\frac{\partial \Gamma_b^i}{\partial q^a}-\frac{\partial \Gamma_a^i}{\partial q^b}+\Gamma_b^j\frac{\partial \Gamma_a^i}{\partial q^j}-\Gamma_a^j\frac{\partial \Gamma_b^i}{\partial q^j}\right),$$

where $v^a=dq^a/dt$.

As we have proved in Section II, the intrinsic motion equations are

$$\begin{gathered}(i_X\omega_L-dE_L)\in(H^v)^0,\\ X\in H^c,\end{gathered}\tag{14}$$

along H.

If we assume that the constrained system is regular (for instance, if the Lagrangian L is natural) then there exists an almost product structure $(\mathscr{P},\mathscr{Q})$ on TQ along H such that the vector field $\xi=\mathscr{P}(\xi_L)$ gives the constrained dynamics. Let us recall that ξ is a vector field defined on H, that is, $\xi\in\mathfrak{X}(H)$.

Define a 1-form $\alpha_{L,\Gamma}$ on TM as follows:

$$(\alpha_{L,\Gamma})_u(U)=-(\alpha_L)_x(\widetilde{X}),$$

for any $U\in T_u(TM)$, for any $u\in T_yM$, where $\widetilde{X}\in T_x(TQ)$ is a tangent vector which projects onto the tangent vector $R((u^H)_q,(T\tau_M(U))_q^H)\in T_qQ$, $\rho(q)=y$, and $x\in D$ with $\tau_Q(x)=q$. [Notice that there is a unique point $x\in D$ such that $\tau_Q(x)=q$ and $T\rho(x)=u$.] In local coordinates, we get

$$\alpha_{L,\Gamma}=\left[\frac{\partial L}{\partial v^i}v^bR_{ab}^i\right]dq^a.$$

It should be remarked that $\alpha_{L,\Gamma}$ is not a *bona fide* 1-form on TM, but it is a 1-form along the mapping $T\rho_{/H}:H\to TM$. For the sake of simplicity, we will assume that $\alpha_{L,\Gamma}$ is well-defined on TM, which is the case in most of the examples.

Now, consider the non-conservative Lagrangian system with Lagrangian function L and external force $\alpha_{L,\Gamma}$. The intrinsic motion equation is

$$i_Y\omega_{L^*}=dE_{L^*}+\alpha_{L,\Gamma},\tag{15}$$

on TM. We will study its solutions. Notice that the corresponding Euler–Lagrange equations are

$$\begin{gathered}\frac{d}{dt}\left(\frac{\partial L^*}{\partial v^a}\right)-\frac{\partial L^*}{\partial q^a}=-\frac{\partial L}{\partial v^i}v^bR_{ab}^i,\\ v^a=\frac{dq^a}{dt}.\end{gathered}\tag{16}$$

Theorem IV.3: *(1) The generalized Čaplygin system* (L,Γ) *is regular* iff L^* *is regular;*
(2) In this case, the vector field ξ *is projectable onto* TM, *and its projection* Y *is just the solution of (15).*

Dynamical proof: We first show how the result can be derived by using a pure dynamical argument. As we have shown, if $(q^a(t),q^i(t))$ is a solution of the constrained motion equations (14) then it is a horizontal curve, and its projection is a solution of the non-conservative equations (16). Conversely, if $(q^a(t))$ is a solution of (16), then its horizontal lift to Q is a solution of (14). Now, assume that the generalized Čaplygin system (L,Γ) is regular so that there exists one and only one solution with a fixed initial data in TM. Take an initial data in TM. Its horizontal lift

gives an initial data in TQ for which there exists one and only one solution of (14). Its projection will be a solution of (15) for the given initial data, and, furthermore, it will be the unique solution with that data. The converse is proved by a similar argument.

The same procedure proves that ξ is projectable, and its projection Y is just a solution of (15). In fact, the solutions of ξ project onto the solutions of Y, and, conversely, the horizontal lifts of the solutions of Y are just the solutions of ξ.

Next, we exhibit an alternative proof based on the geometrical ingredients of the theory. First of all, we will prove the following lemma.

Lemma IV.4: Let Γ be an arbitrary connection in a fibration $\rho:Q\to M$ with horizontal projector $\mathbf{h}$. *If μ_1 and μ_2 are two 1-forms and X is a horizontal vector field on Q such that*

$$\mathscr{L}_X\mu_1=\mu_2,$$

then we have

$$\mathscr{L}_X(\mathbf{h}^*\mu_1)=\mathbf{h}^*\mu_2-\alpha,$$

where $\mathbf{h}^*$ *is the transpose operator of* $\mathbf{h}$, *and α is the 1-form on Q defined by*

$$\alpha(Y)=-\mu_1(R(X,Y)-\mathbf{h}([X,\mathbf{v}Y])),$$

R being the curvature of Γ.

Proof: Assume that $\mathscr{L}_X\mu_1=\mu_2$ and X is a horizontal vector field. Let Y be an arbitrary vector field on Q. We have

$$\begin{aligned}(\mathscr{L}_X(\mathbf{h}^*\mu_1))(Y)&=\mathscr{L}_X(\mathbf{h}^*\mu_1)(Y)-(\mathbf{h}^*\mu_1)([X,Y])\\&=X(\mu_1(\mathbf{h}Y))-\mu_1(\mathbf{h}([X,Y])\\&=\mu_2(\mathbf{h}Y)+\mu_1([X,\mathbf{h}Y])-\mu_1(\mathbf{h}[X,Y])\\&=\mathbf{h}^*\mu_2(Y)+\mu_1(R(X,Y)-\mathbf{h}([X,\mathbf{v}Y])).\end{aligned}$$

■

Geometrical proof of the theorem: First of all, we will prove that the generalized Čaplygin system (L,Γ) is regular if L^* is regular. In fact, denote by

$$W=(W^{AB})=\begin{pmatrix}W^{ab} & W^{aj}\\ W^{ib} & W^{ij}\end{pmatrix}$$

the inverse matrix of the Hessian matrix $(\partial^2L/\partial v^A\partial v^B)$. We have

$$\mathscr{C}_{ij}=-W^{ab}\Gamma^i_a\Gamma^j_b-W^{ja}\Gamma^i_a-W^{ib}\Gamma^j_b-W^{ij},$$

or, equivalently,

$$\mathscr{C}=-(\gamma,I_{m\times m})W(\gamma,I_{m\times m})^t,$$

where γ is a matrix $m\times(n-m)$ with entries $\gamma_{ia}=\Gamma^i_a$, $1\leqslant i\leqslant m$, $1\leqslant a\leqslant n-m$, and the superindex t means that we are taking the transpose matrix.

On the other hand, the entries of the Hessian matrix $\mathscr{M}$ of L^* are

$$\frac{\partial^2L^*}{\partial v^a\partial v^b}=\frac{\partial^2L}{\partial v^a\partial v^b}-\Gamma^i_a\frac{\partial^2L}{\partial v^i\partial v^b}-\Gamma^j_b\frac{\partial^2L}{\partial v^j\partial v^a}+\Gamma^i_a\Gamma^j_b\frac{\partial^2L}{\partial v^i\partial v^j},$$

or, equivalently,

$$\mathscr{M}=(I_{(n-m)\times(n-m)},-\gamma^t)W^{-1}(I_{(n-m)\times(n-m)},-\gamma^t)^t.$$

If we put $\mathscr{A}=(\gamma,I_{m\times m})$ and $\mathscr{B}=(I_{(n-m)\times(n-m)},-\gamma^t)$, it is no hard to show that either $\mathscr{C}$ or $\mathscr{M}$ are regular, then the square matrices

$$\begin{pmatrix}\mathscr{A}\\ \mathscr{B}W^{-1}\end{pmatrix} \text{ and } \begin{pmatrix}W\mathscr{A}^t\\ \mathscr{B}^t\end{pmatrix}$$

are also regular.

The result follows taking into account that

$$\begin{pmatrix}\mathscr{A}\\ \mathscr{B}W^{-1}\end{pmatrix}\cdot\begin{pmatrix}W\mathscr{A}^t\\ \mathscr{B}^t\end{pmatrix}=\begin{pmatrix}\mathscr{A}W\mathscr{A}^t & 0\\ 0 & \mathscr{B}W^{-1}\mathscr{B}^t\end{pmatrix}.$$

Therefore, we have proved the first part of the theorem.

Next, we will prove the second part.

Given a connection Γ in the fibration $\rho:Q\to M$ we define a connection $\overline{\Gamma}$ in the fibration $T\rho:TQ\to TM$ along the submanifold H as follows. The horizontal distribution $\overline{H}$ of $\overline{\Gamma}$ is locally spanned by the vector fields

$$\left(\frac{\partial}{\partial q^a}\right)^{\overline{H}}=\frac{\partial}{\partial q^a}-\Gamma^i_a\frac{\partial}{\partial q^i}-v^b\left(\frac{\partial\Gamma^i_b}{\partial q^a}-\Gamma^j_a\frac{\partial\Gamma^i_b}{\partial q^j}\right)\frac{\partial}{\partial v^i},$$

$$\left(\frac{\partial}{\partial v^a}\right)^{\overline{H}}=\frac{\partial}{\partial v^a}-\Gamma^i_a\frac{\partial}{\partial v^i}.$$

Along H, we obtain a local basis of vector fields on TQ,

$$\left\{\left(\frac{\partial}{\partial q^a}\right)^{\overline{H}},\left(\frac{\partial}{\partial v^a}\right)^{\overline{H}},\frac{\partial}{\partial q^i},\frac{\partial}{\partial v^i}\right\}.$$

Its dual basis of 1-forms is

$$\{dq^a,dv^a,\eta^v_i,d\hat{\eta}_i\}.$$

Thus, the set $\{\eta^v_i,d\hat{\eta}_i\}$ is the annihilator of $\overline{H}$. A simple computation shows that $\overline{H}$ is globally defined along H.

If $\mathbf{h}$ is the horizontal projector associated with $\overline{\Gamma}$ we have $\overline{\mathbf{h}}^*(dq^a)=dq^a$, $\overline{\mathbf{h}}^*(dv^a)=dv^a$, $\overline{\mathbf{h}}^*(\eta^v_i)=0$ and $\overline{\mathbf{h}}^*(d\hat{\eta}_i)=0$.

Consider the pull-backs of the 1-forms α_{L*} and $dL*$ to TQ by means of $T\rho$. Along H we deduce that

$$\overline{\mathbf{h}}^*(\alpha_L)=(T\rho)^*\alpha_{L*},$$

$$\overline{\mathbf{h}}^*(dL)=(T\rho)^*dL^*.$$

From Lemma II.8 we have

$$\mathscr{L}_\xi\alpha_L=dL-\mathscr{L}_{\mathscr{Q}(\xi_L)}\alpha_L, \tag{17}$$

and from Lemma IV.4, we get

$$\mathscr{L}_{\xi}(\overline{\mathbf{h}}^{*}\alpha_L)=\overline{\mathbf{h}}^{*}(dL)-\overline{\mathbf{h}}^{*}(\mathscr{L}_{\mathcal{Q}(\xi_L)}\alpha_L)-\overline{\alpha}, \tag{18}$$

where $\overline{\alpha}$ is the 1-form on TQ along H defined by

$$\overline{\alpha}(Z)=-\alpha_L(\overline{R}(\xi,Z)-\overline{\mathbf{h}}([\xi,\overline{\mathbf{v}}(Z)])),$$

$\overline{R}$ being the curvature of $\overline{\Gamma}$. Since α_L is semibasic and $\overline{\Gamma}$ is a connection in the fibration $T\rho:TQ\to TM$ (along H), we deduce that $\alpha_L(\overline{\mathbf{h}}([\xi,\overline{\mathbf{v}}(Z)])=0$, and hence we get

$$\overline{\alpha}(Z)=-\alpha_L(\overline{R}(\xi,Z)).$$

In local coordinates we obtain

$$\overline{\alpha}=\frac{\partial L}{\partial v^i}v^b\left(\frac{\partial\Gamma^i_a}{\partial q^b}-\frac{\partial\Gamma^i_b}{\partial q^a}-\Gamma^j_b\frac{\partial\Gamma^i_a}{\partial q^j}+\Gamma^j_a\frac{\partial\Gamma^i_b}{\partial q^j}\right)dq^a.$$

Therefore, we deduce that $\overline{\alpha}$ is projectable, and its projection is just the 1-form $\alpha_{L,\Gamma}$ on TM.

From Lemma II.9 we have

$$\overline{\mathbf{h}}^{*}(\mathscr{L}_{\mathcal{Q}(\xi_L)}\alpha_L)=0,$$

and therefore (18) becomes

$$\mathscr{L}_{\xi}(T\rho)^{*}\alpha_{L^{*}}=(T\rho)^{*}(dL^{*})-\overline{\alpha}.$$

Let Y be a vector field on TM which is a solution of the equation

$$\mathscr{L}_{Y}\alpha_{L^{*}}=dL^{*}-\alpha_{L,\Gamma}.$$

Then every vector field $\widetilde{Y}$ on TQ which projects onto Y verifies

$$\mathscr{L}_{\widetilde{Y}}(T\rho)^{*}\alpha_{L^{*}}=(T\rho)^{*}(dL^{*})-\overline{\alpha}. \tag{19}$$

In particular, the horizontal lift $Y^{\overline{H}}$ with respect to $\overline{\Gamma}$ verifies (19). Since ξ also verifies (19) and $\xi\in\overline{H}$, we deduce that $Y^{\overline{H}}=\xi$.

■

Thus, we have the following.

Corollary IV.5: The generalized Čaplygin system (L,Γ) *is equivalent to a non-conservative system on* TM *with Lagrangian function* L^{*} *and external force* $\alpha_{L,\Gamma}$.

Remark IV.6: The above procedure is a sort of reduction, but not in the sense of Marsden and Weinstein.[40] In fact, we could consider the general case of a constrained Lagrangian system subjected to linear constraints given by a distribution D on Q, and such that L and D are invariant by the action of a Lie group G. This is just the case of Čaplygin systems as were considered by Koiller.

Remark IV.7: The distribution H^c satisfies the following relation:

$$T(TQ)=H^c\oplus V(T\rho),$$

along the points of H. Thus, H^c defines a connection Γ^c in the fibration $T\rho:TQ\to TM$ along the submanifold H, which could be considered as the tangent lift of the original connection Γ in the fibration $\rho:Q\to M$. We have proved that the vector field ξ is horizontal with respect to $\overline{\Gamma}$. A

similar device proves that ξ is also horizontal with respect to Γ^c, and moreover $\xi = Y^{H^c}$. The relationship between both connections $\overline{\Gamma}$ and Γ^c is the following: they coincide if and only Γ is flat, or, in other words, the constrained system is holonomic.

Remark IV.8: Assume that the constrained system is not regular. From Theorem IV.3 we deduce that L^* is a singular Lagrangian function. Thus, Equation (15) has no, in general, solution. However, we can develop a constraint algorithm as follows. Put $K_1 = TM$ and define K_2 be the submanifold of points in TM for which there exists at least a solution of (15). On K_2 there is a solution, but it is not necessarily tangent to K_2. So, we consider the submanifold K_3 consisting in those points in K_2 where a tangent solution to K_2 exists.

Proceeding further we obtain a sequence of constraint submanifolds,

$$\cdots \to K_k \to \cdots \to K_2 \to K_1 = TM.$$

On the other hand, there exists a sequence of constraint submanifolds,

$$\cdots \to H_k \to \cdots \to H_2 \to H_1 = H,$$

obtained by applying the constraint algorithm developed in Section III. It is almost obvious that both algorithms are related by the projection mapping $T\rho : TQ \to TM$, that is, we have

$$T\rho(H_r) = M_r, \quad r \geqslant 1.$$

Example IV.9 (The sleigh of Čaplygin and Carathéodory):

Consider a sleigh, that is, a body having three points of contact with a plane where two of them slide freely but the third A is subjected to a force which does not allow transversal velocity. The configuration manifold is $Q = \mathbb{R}^2 \times S^1$ with coordinates (x, y, ϕ), where (x, y) are the coordinates of the center of mass C of the sleigh, and ϕ is the angle between the x-axis and the line AC (see Ref. 18). If we denote by a the distance from A to C, by J the moment of inertia and by $m = 1$ the mass of the sleigh, the Lagrangian function is given by

$$L = \frac{1}{2}(\dot{x}^2 + \dot{y}^2) + \frac{1}{2} J \dot{\phi}^2,$$

Observe that L is a natural Lagrangian obtained from the Riemannian metric

$$g = \frac{1}{2}(dx^2 + dy^2 + J d\phi^2),$$

on $\mathbb{R}^2 \times S^1$.

Consider the fibration

$$\rho : \mathbb{R}^2 \times S^1 \to \mathbb{R}^2,$$

defined by

$$\rho(x, y, \phi) = (x, y).$$

Define a connection Γ in ρ by

$$\Gamma\left(\frac{\partial}{\partial x}\right)=\frac{\partial}{\partial x}-2\frac{\sin\phi}{a}\frac{\partial}{\partial\phi},$$

$$\Gamma\left(\frac{\partial}{\partial y}\right)=\frac{\partial}{\partial y}+2\frac{\cos\phi}{a}\frac{\partial}{\partial\phi},$$

$$\Gamma\left(\frac{\partial}{\partial\phi}\right)=-\frac{\partial}{\partial\phi}.$$

The curvature R of Γ is

$$R=\frac{1}{a^2}\frac{\partial}{\partial\phi}\otimes(dx\wedge dy).$$

The horizontal distribution of Γ is generated by

$$\left\langle\frac{\partial}{\partial x}-\frac{\sin\phi}{a}\frac{\partial}{\partial\phi},\quad\frac{\partial}{\partial y}+\frac{\cos\phi}{a}\frac{\partial}{\partial\phi}\right\rangle,$$

and the annihilator of H is generated by the 1-form

$$\eta=d\phi-\frac{\cos\phi}{a}dy+\frac{\sin\phi}{a}dx.$$

In fact, η is the connection 1-form of Γ. Therefore, the linear constraints are

$$\dot\phi-\frac{\cos\phi}{a}\dot y+\frac{\sin\phi}{a}\dot x=0.$$

Notice that ρ is a principal S^1-bundle. However, Γ is no a principal connection, since the horizontal subspaces are not S^1-invariant. Thus, (L,Γ) is not a generalized Čaplygin system. However, we can apply the general procedure developed in Section II.

Since L is natural, the constrained system is regular, and then there exists a well-defined solution of the constrained dynamics along the submanifold H of TQ.

The distribution S is generated by the vector field

$$Z=-\frac{1}{J}\frac{\partial}{\partial\dot\phi}+\frac{\cos\phi}{a}\frac{\partial}{\partial\dot y}-\frac{\sin\phi}{a}\frac{\partial}{\partial\dot x},$$

along the points of H.

The almost product structure $(\mathscr{P},\mathscr{Q})$ is given by

$$\mathscr{Q}=-\frac{Ja^2}{a^2+J}\left(-\frac{1}{J}\frac{\partial}{\partial\dot\phi}+\frac{\cos\phi}{a}\frac{\partial}{\partial\dot y}-\frac{\sin\phi}{a}\frac{\partial}{\partial\dot x}\right)$$
$$\otimes\left(\left(\frac{\sin\phi}{a}\dot y+\frac{\cos\phi}{a}\dot x\right)d\phi+\frac{\sin\phi}{a}d\dot x-\frac{\cos\phi}{a}d\dot y+d\dot\phi\right),$$

$$\mathscr{P}=\mathrm{id}-\mathscr{Q}.$$

Thus, the only vector field ξ such that $\xi_x \in (S_L)_x \cap T_x H$ and $J_x(\xi_x) = C_x$, for any $x \in H$, is given by

$$\xi = \mathscr{P}(\xi_L) = \dot{x}\frac{\partial}{\partial x} + \dot{y}\frac{\partial}{\partial y} + \dot{\phi}\frac{\partial}{\partial \phi} - \frac{J}{a^2+J}\sin\phi(\sin\phi\dot{y} + \cos\phi\dot{x})\frac{\partial}{\partial \dot{x}}$$

$$+ \frac{J}{a^2+J}\cos\phi(\sin\phi\dot{y} + \cos\phi\dot{x})\frac{\partial}{\partial \dot{y}} - \frac{a}{a^2+J}(\sin\phi\dot{y} + \cos\phi\dot{x})\frac{\partial}{\partial \dot{\phi}},$$

along the points of H.

Example IV.10 (The ''two-wheeled carriage''):

The configuration space of the ''two-wheeled carriage'' is $Q = \mathbb{R}^2 \times S^1 \times T^2$, with coordinates $(x, y, \phi, \Phi_1, \Phi_2)$ (see Refs. 18,3).

Let $2r$ be the lateral length, a the radius of the wheels, C_0 the center of mass, situated at distance l from a point (x,y). If we denote by m_0 the mass of the body without wheels, k_0 the radius of gyration about the vertical through (x,y), m_1 the mass of a wheel, C the axial moments of inertia and A its moment of inertia about a diameter, then the Lagrangian function is given by

$$L = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2) + m_0 l\dot{\phi}(\dot{y}\cos\phi - \dot{x}\sin\phi) + \frac{1}{2}J\dot{\phi}^2 + \frac{1}{2}C(\dot{\Phi}_1^2 + \dot{\Phi}_2^2),$$

where $m = m_0 + 2m_1$ and $J = m_0 k_0^2 + 2m_1 r^2 + 2A$.

Consider now the fibration

$$\rho : \mathbb{R}^2 \times S^1 \times T^2 \to T^2,$$

defined by $\rho(x, y, \phi, \Phi_1, \Phi_2) = (\Phi_1, \Phi_2)$.

Define a connection Γ in ρ by

$$\Gamma\left(\frac{\partial}{\partial \Phi_1}\right) = \frac{\partial}{\partial \Phi_1} - a\cos\phi\frac{\partial}{\partial x} - a\sin\phi\frac{\partial}{\partial y} - \frac{a}{r}\frac{\partial}{\partial \phi},$$

$$\Gamma\left(\frac{\partial}{\partial \Phi_2}\right) = \frac{\partial}{\partial \Phi_2} - a\cos\phi\frac{\partial}{\partial x} - a\sin\phi\frac{\partial}{\partial y} + \frac{a}{r}\frac{\partial}{\partial \phi},$$

$$\Gamma\left(\frac{\partial}{\partial x}\right) = -\frac{\partial}{\partial x}, \quad \Gamma\left(\frac{\partial}{\partial y}\right) = -\frac{\partial}{\partial y}, \quad \Gamma\left(\frac{\partial}{\partial \phi}\right) = -\frac{\partial}{\partial \phi}.$$

The horizontal distribution H of Γ is generated by

$$\left\langle \frac{\partial}{\partial \Phi_1} - \frac{a}{2}\cos\phi\frac{\partial}{\partial x} - \frac{a}{2}\sin\phi\frac{\partial}{\partial y} - \frac{a}{2r}\frac{\partial}{\partial \phi}, \quad \frac{\partial}{\partial \Phi_2} - \frac{a}{2}\cos\phi\frac{\partial}{\partial x} - \frac{a}{2}\sin\phi\frac{\partial}{\partial y} + \frac{a}{2r}\frac{\partial}{\partial \phi} \right\rangle.$$

Thus, the annihilator of H is generated by the 1-forms

$$\eta_x = dx + \frac{a\cos\phi}{2}d\Phi_1 + \frac{a\cos\phi}{2}d\Phi_2,$$

$$\eta_y = dy + \frac{a\sin\phi}{2}d\Phi_1 + \frac{a\sin\phi}{2}d\Phi_2,$$

$$\eta_\phi = d\phi + \frac{a}{2r} d\Phi_1 - \frac{a}{2r} d\Phi_2 .$$

The linear constraints are then

$$\dot{x} = -\frac{a\cos\phi}{2}\dot{\Phi}_1 - \frac{a\cos\phi}{2}\dot{\Phi}_2 ,$$

$$\dot{y} = -\frac{a\sin\phi}{2}\dot{\Phi}_1 - \frac{a\sin\phi}{2}\dot{\Phi}_2 ,$$

$$\dot{\phi} = -\frac{a}{2r}\dot{\Phi}_1 + \frac{a}{2r}\dot{\Phi}_2 .$$

The curvature of the connection is given by the vector 2-form,

$$R = \frac{a^2}{2r}\left(-\sin\phi \frac{\partial}{\partial x} + \cos\phi \frac{\partial}{\partial y}\right) \otimes (d\Phi_1 \wedge d\Phi_2).$$

The fibration $\rho : \mathbb{R}^2 \times S^1 \times T^2 \to T^2$ is a principal $\mathbb{R}^2 \times S^1$-bundle, and Γ is a principal connection with connection 1-form

$$\eta = (\eta_x, \eta_y, \eta_\phi),$$

taking values into the Lie algebra of $\mathbb{R}^2 \times S^1$. Notice that $\mathbb{R}^2 \times S^1$ may be identified with the group of Euclidean motions of the plane (see Koiller[18]).

Thus, the system (L, Γ) is a generalized Caplygin system. By applying the general theory developed in this section, we obtain a Lagrangian function $L^* : T^2 \to \mathbb{R}$ as follows:

$$L^*(\Phi_1, \Phi_2, \dot{\Phi}_1, \dot{\Phi}_2) = \frac{1}{8} m a^2 (\dot{\Phi}_1^2 + \dot{\Phi}_2^2) + \frac{J a^2}{8 r^2} (\dot{\Phi}_2 - \dot{\Phi}_1)^2 + \frac{1}{2} C (\dot{\Phi}_1^2 + \dot{\Phi}_2^2).$$

From Corollary IV.5, we know that the constrained system (L, D) is equivalent to the nonconservative system given by L^* and the external force

$$\alpha_{L,\Gamma} = \frac{m_0 l a^3}{4 r^2} (\dot{\Phi}_2 - \dot{\Phi}_1) \dot{\Phi}_2 d\Phi_1 - \frac{m_0 l a^3}{4 r^2} (\dot{\Phi}_2 - \dot{\Phi}_1) \dot{\Phi}_1 d\Phi_2 .$$

From a tedious but straightforward computation we have that the solution Y of the equation

$$i_Y \omega_{L^*} = dE_{L^*} + \alpha_{L,\Gamma} ,$$

is the vector field,

$$Y = \dot{\Phi}_1 \frac{\partial}{\partial \Phi_1} + \dot{\Phi}_2 \frac{\partial}{\partial \Phi_2} + K_1 (\dot{\Phi}_1 - \dot{\Phi}_2)(K_2 \dot{\Phi}_2 - J a^2 \dot{\Phi}_1) \frac{\partial}{\partial \dot{\Phi}_1} + K_1 (\dot{\Phi}_2 - \dot{\Phi}_1)(K_2 \dot{\Phi}_1 - J a^2 \dot{\Phi}_2) \frac{\partial}{\partial \dot{\Phi}_2},$$

where $K_1 = m_0 l a^3 / (m^2 a^4 r^4 + 8 m a^2 r^4 C + 2 m a^4 r^2 J + 16 r^4 C^2 + 8 J C a^2 r^2)$ and $K_2 = m a^2 r^2 + 4 C r^2 + J a^2$.

We obtain the solution on TQ by taking the horizontal lift of the vector field Y by the connection $\overline{\Gamma}$.

V. AN APPLICATION: EQUATIONS OF CONSTRAINED GEODESICS

Let Q be a Riemannian manifold with Riemannian metric g and Levi-Civita connection ∇ and suppose that a distribution D on Q is given. A very old problem in the literature is to obtain a new linear connection ∇^* on Q such that the geodesics of ∇^* are the extremals of the variational problem subjected to these linear constraints (see Synge,[35] Vranceanu,[36] Neimark and Fufaev[3] and the references therein.) We shall apply our method to give a new look at Synge's paper.

The Lagrangian function is

$$L(q^A,v^A)=\frac{1}{2}g_{AB}v^Av^B,$$

that is, L is the kinetic energy of g. Take an orthonormal local basis $\{\mu_i\}$ of D. Since $E_L=L$, we obtain

$$\xi_L=v^A\frac{\partial}{\partial q^A}-\Gamma^C_{AB}v^Av^B\frac{\partial}{\partial v^C},$$

where Γ^C_{AB} are the Christoffel components of ∇. In fact, ξ_L is the geodesic spray.

A direct computation shows that

$$Z_i=-g^{AB}(\mu_i)_B\frac{\partial}{\partial v^A},$$

$$\hat{\mu}_i=(\mu_i)_Av^A,$$

$$\mathscr{C}_{ij}=Z_i(\hat{\mu}_j)=-g^{AB}(\mu_i)_A(\mu_j)_B=-\delta_{ij}.$$

Therefore, the constrained system is regular.

From Proposition II.4 there exists a unique almost product structure $(\mathscr{P},\mathscr{Q})$ such that $\mathscr{P}_x(X)\in T_xD$ and $\mathscr{Q}_x(X)\in S_x$, where $X\in T_xTQ$. We have

$$\begin{aligned}\mathscr{P}(\xi_L)&=v^A\frac{\partial}{\partial q^A}-v^Av^B\left(\Gamma^C_{AB}+\frac{\partial(\mu_i)_B}{\partial q^A}g^{CR}(\mu_i)_R-\Gamma^E_{AB}(\mu_i)_Eg^{CR}(\mu_i)_R\right)\frac{\partial}{\partial v^C}\\&=v^A\frac{\partial}{\partial q^A}-v^Av^B\left(\Gamma^C_{AB}+\left(\frac{\partial(\mu_i)_B}{\partial q^A}-\Gamma^E_{AB}(\mu_i)_E\right)g^{CR}(\mu_i)_R\right)\frac{\partial}{\partial v^C}\\&=v^A\frac{\partial}{\partial q^A}-v^Av^B(\Gamma^C_{AB}+(\mu_i)_{A;B}(\mu_i)^C)\frac{\partial}{\partial v^C},\end{aligned}$$

where

$$(\mu_i)_{A;B}=\frac{\partial(\mu_i)_A}{\partial q^B}-\Gamma^E_{AB}(\mu_i)_E$$

denote the components of the covariant derivative of μ_i, and $(\mu_i)^C=g^{CR}(\mu_i)_R$.

Since $\mathscr{P}(\xi_L)$ is a SODE and tangent to D, we know that for each tangent vector $z\in D$ there is a curve σ on Q which is a solution of $\mathscr{P}(\xi_L)$ with that initial data, i.e., $\sigma(0)=x$, $\dot{\sigma}(0)=z$ and $\dot{\sigma}$ is an integral curve of $\mathscr{P}(\xi_L)$. In fact, the solutions of $\mathscr{P}(\xi_L)$ are just the solutions of the following system of differential equations:

$$\frac{d^2q^C}{dt^2}+(\Gamma^*)^C_{AB}\frac{dq^A}{dt}\frac{dq^B}{dt}=0, \tag{20}$$

where

$$(\Gamma^*)^C_{AB}=\Gamma^C_{AB}+(\mu_i)_{A;B}(\mu_i)^C.$$

Notice that (20) are just the differential equations obtained by Synge in Ref. 35. Of course, (20) have no solutions for arbitrary initial data, since only the velocities in D are allowable.

Notice that $(\Gamma^*)^A_{BC}$ are not the Christoffel components of a linear connection ∇^* on Q. They define a more general geometric object, an spray defined on a submanifold D of TQ. Indeed, let us recall that there exists a one-to-one correspondence between sprays on TQ and linear connections on Q (see Ref. 38). In fact, if ξ is an spray, then $\Gamma=-\mathscr{L}_\xi J$ is a linear connection on Q, and, conversely, if Γ is a linear connection on Q, then its associated SODE is an spray.

The vector field $\mathscr{P}(\xi_L)$ can be extended to a vector field defined on some open neighborhood of D in TQ. Of course, there are many extensions of $\mathscr{P}(\xi_L)$. Choose an arbitrary extension and define

$$\Gamma^*=-\mathscr{L}_{P(\xi_L)}J.$$

So, Γ^* is a tensor field of type (1,1) defined on some open neighborhood of D, and its local expression is as follows:

$$\Gamma^*\left(\frac{\partial}{\partial q^A}\right)=\frac{\partial}{\partial q^A}-2(\Gamma^*)^C_{AB}v^B\frac{\partial}{\partial v^C},$$

$$\Gamma^*\left(\frac{\partial}{\partial v^A}\right)=-\frac{\partial}{\partial v^A}.$$

A direct computation shows that $(\Gamma^*)^2=\mathrm{id}$, and the vector eigenspace corresponding to the eigenvalue -1 at a point of D is just the vertical subspace at that point. Moreover, given another extension of $\mathscr{P}(\xi_L)$, we obtain that the new tensor field Γ^* coincides with the former on D.

Thus, Γ^* defines a connection on some open neighborhood of D and all these connections coincide on D.

We define the horizontal and vertical projectors of Γ^* in the usual way:

$$h^*=\frac{1}{2}(\mathrm{id}+\Gamma^*),\quad v^*=\frac{1}{2}(\mathrm{id}-\Gamma^*).$$

Their local expressions are the following ones:

$$h^*\left(\frac{\partial}{\partial q^A}\right)=\frac{\partial}{\partial q^A}-(\Gamma^*)^C_{BA}v^B\frac{\partial}{\partial v^C},$$

$$h^*\left(\frac{\partial}{\partial v^A}\right)=0,$$

$$v^*\left(\frac{\partial}{\partial q^A}\right)=(\Gamma^*)^C_{BA}v^B\frac{\partial}{\partial v^C},$$

$$v^*\left(\frac{\partial}{\partial v^A}\right)=\frac{\partial}{\partial v^A}.$$

Using the standard procedures for connections on TQ (see Refs. 37,38), we define a covariant derivative as follows. Let X be a vector field on Q and Y be a vector field which is tangent to D. In other words, X is a section of $\tau_Q:TQ\to Q$ and Y a section of $\tau_{Q/D}:D\to Q$. Define

$$(\nabla^*_X Y)(x)=\phi_{Y(x)}(v^*(dY(x)(X(x))),\quad \forall x\in Q,$$

where $\phi_{Y(x)}$ is the linear isomorphism,

$$\phi_{Y(x)}:V_{Y(x)}\tau_Q\to T_xQ$$

from the vertical subspace at $Y(x)$ onto T_xQ.

If $X=X^A(\partial/\partial q^A)$ and $Y=Y^A(\partial/\partial q^A)$, we deduce that

$$\nabla^*_X Y=X^A\left[\frac{\partial Y^C}{\partial q^A}+(\Gamma^*)^C_{AB}Y^B\right]\frac{\partial}{\partial q^C}.$$

We look for a condition which ensures that $\nabla^*_X Y\in D$. We have

$$\begin{aligned}\mu_i(\nabla^*_X Y)&=(\mu_i)_D dq^D\left[\left(X^A\frac{\partial Y^C}{\partial q^A}+X^A(\Gamma^*)^C_{AB}Y^B\right)\right]\\&=X^A\left[(\mu_i)_C\frac{\partial Y^C}{\partial q^A}+(\mu_i)_C(\Gamma^*)^C_{AB}Y^B\right].\end{aligned}$$

Since

$$(\Gamma^*)^A_{BC}=\Gamma^C_{AB}+(\mu_i)_{A;B}(\mu_i)^C,$$

we deduce that

$$\begin{aligned}(\mu_i)_C(\Gamma^*)^C_{AB}&=(\mu_i)_C\Gamma^C_{AB}+(\mu_i)_C\frac{\partial(\mu_J)_A}{\partial q^B}(\mu_j)^C-(\mu_i)^C\Gamma^E_{AB}(\mu_i)_E(\mu_j)^C\\&=\frac{\partial(\mu_i)_A}{\partial q^B}.\end{aligned}$$

Thus, we obtain that

$$\mu_i(\nabla^*_X Y)=X^A\left[(\mu_i)_B\frac{\partial Y^B}{\partial q^A}+\frac{\partial(\mu_i)_A}{\partial q^B}Y^B\right]. \tag{21}$$

But $Y\in D$, and therefore we get

$$0=\mu_i(Y)=(\mu_i)_B Y^B.$$

By deriving this last formula, we have

$$(\mu_i)_B\frac{\partial Y^B}{\partial q^A}+\frac{\partial(\mu_i)_B}{\partial q^A}Y^B=0. \tag{22}$$

From (21) and (22) we deduce the following result.

Proposition V.1: ∇^* *defines a connection in the vector bundle* $\tau_Q:D\to Q$ *if and only if* D *is involutive.*

As a consequence, if the system is holonomic, ∇^* is a derivation in the vector bundle $D \to Q$. In the general case, we only get that

$$\nabla^* : \mathfrak{X}(Q) \times \mathrm{Sec}(D) \to \mathfrak{X}(Q)$$

behaves as a derivation.

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On the asymptotic integrability of a higher-order evolution equation describing internal waves in a deep fluid

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A higher-order nonlocal evolution equation describing internal waves in a deep fluid is shown to be asymptotically integrable only if the coefficients of the higher-order terms satisfy certain constraints. In this case, the nonlocal equation can be transformed to the integrable Benjamin–Ono equation. The asymptotic integrability of the reductions of the higher-order evolution equation to a complex Burgers equation, to an envelope-wave equation, and to a finite-dimensional dynamical system is also considered. © *1996 American Institute of Physics.*
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I. INTRODUCTION

The evolution of small amplitude waves of certain nonlinear dispersive systems can be studied asymptotically using the so-called multiscale expansion method (see, e.g., Ref. 1). This method yields a basic evolution equation which is formally valid at the leading asymptotic order, as well as a sequence of evolution equations at higher asymptotic orders. It turns out that for many important physical systems the basic evolution equation is an *integrable* equation (see Ref. 2 for a discussion of this remarkable fact). Each integrable evolution equation is a member of a hierarchy of infinitely many integrable equations. It is interesting that the evolution equation valid at the next asymptotic order, differs from the next member of the associated integrable hierarchy, only in the value of the numerical coefficients of the nonlinear terms. For example, idealized unidirectional water waves of small amplitude and large wave length satisfy[3] the equation

$$\eta_t+\eta_{xxx}+6\,\eta\,\eta_x+\epsilon(\alpha_1\,\eta_{xxxxx}+\alpha_2\,\eta\,\eta_{xxx}+\alpha_3\,\eta_x\,\eta_{xx}+\alpha_4\,\eta^2\,\eta_x)+O(\epsilon^2)=0, \tag{1.1}$$

where $\alpha_1,...,\alpha_4$ are certain numbers. As $\epsilon\to 0$, this equation becomes the Korteweg–deVries (KdV) equation, which is an integrable equation. Furthermore, if $\alpha_2=10\alpha_1$, $\alpha_3=20\alpha_1$, $\alpha_4=30\alpha_1$, then the $O(\epsilon)$ term of Eq. (1.1) becomes the right-hand side of the next member of the hierarchy of integrable equations associated with the KdV equation.

If the basic evolution equation is integrable, we say that the underlying physical system is *asymptotically integrable* to $O(\epsilon)$. It turns out that in certain cases it is possible to formally extend the asymptotic integrability of the system to $O(\epsilon^2)$. For example, in the case of water waves Kodama found[4] an explicit transformation which maps Eq. (1.1) to the integrable equation obtained by Eq. (1.1) when $\alpha_2=10\alpha_1$, $\alpha_3=20\alpha_1$, and $\alpha_4=30\alpha_1$. A generalization of Kodama's transformation which actually maps Eq. (1.1) to KdV equation itself, and an extension of this result to the case of water waves without the unidirectionalization assumption, are given in Ref. 5. It is also shown in Ref. 5 that the concept of the mastersymmetries (see Ref. 6 and references therein) provides an algorithmic approach to finding the transformations which map the physical equations to the integrable ones. Similar results are valid for the case that the basic evolution equation is the nonlinear Schrödinger (NLS) equation.

In this paper we study the asymptotic integrability of the systems whose basic equation is the Benjamin–Ono (BO) equation, i.e., we study the equation

$$u_t = 2uu_x + Hu_{xx} + \epsilon[\alpha u_{xxx} + \beta_1(uHu_x)_x + \beta_2 uHu_{xx} + \beta_3 H(uu_x)_x + \gamma u^2 u_x] + O(\epsilon^2), \quad (1.2)$$

where ϵ is the small parameter of the multiscale expansion, H is the Hilbert transform,

$$(Hf)(x) = \frac{1}{\pi} \int\!\!\!\!\!\!- _{-\infty}^{\infty} \frac{f(\xi)}{\xi - x}\, d\xi, \quad (1.3)$$

and $\int\!\!\!\!\!\!-$ denotes the principal value integral.

Equation (1.2) occurs in the modeling of long internal waves in a deep continuously stratified fluid, and was recently derived in Ref. 7. In this case u denotes the horizontal velocity of the fluid and the coefficients $\alpha,\ldots,\gamma$ can be expressed through the parameters of the fluid stratification. The particular case that the stratification profile can be approximated by a two-layer model with density ρ_1 in the upper (shallow) layer and ρ_2 in the lower (deep) layer, was studied in Ref. 8 and is described by Eq. (1.2) with

$$\alpha = \frac{27}{4}\left(\frac{4\delta^2}{9} - 1\right), \quad \beta_1 = 6, \quad \beta_2 = \frac{3}{2}, \quad \beta_3 = \frac{27}{2}, \quad \gamma = -3, \quad (1.4)$$

where $\delta = \rho_1/\rho_2 < 1$.

The structure of our paper is as follows. In Sec. II we present two main results for Eq. (1.2). (a) We show that if the coefficients satisfy the numerical constraints

$$3\alpha + \beta_1 + \beta_2 + \beta_3 = 0, \quad (1.5)$$

and

$$\beta_1 + \beta_3 - \gamma = 0, \quad (1.6)$$

then Eq. (1.2) is asymptotically integrable to $O(\epsilon^2)$ (see Propositions 2.1 and 2.2).

(b) We study the pole-decomposition solution of Eq. (1.2) and establish that if Eqs. (1.5) and (1.6) are satisfied, then the system describing these solutions is asymptotically integrable to $O(\epsilon^2)$ (see Proposition 2.3). This implies that in this case the algebraic solitary waves interact without a phase shift to $O(\epsilon^2)$.

Unfortunately, in the physically important case that the coefficients of Eq. (1.2) are given by Eq. (1.4), the constraints (1.5) and (1.6) are not satisfied. This is consistent with the fact that in this case the interaction of the algebraic solitary waves exhibits phase shifts to $O(\epsilon^2)$.[9]

Although we have only shown that the validity of Eqs. (1.5) and (1.6) is a sufficient condition for asymptotic integrability, we conjecture that it is also a necessary condition. This conjecture is supported by the following arguments. There exists an exact reduction from Eq. (1.2) to a complex perturbed Burgers equation. In this case, if the coefficients of Eq. (1.2) satisfy a single constraint, denoted here by $\nu = 0$, then the perturbed Burgers equation can be mapped to the integrable Burgers equation. Furthermore, it was shown in Ref. 7 that there exists an asymptotic limit from Eq. (1.2) to a certain modulation equation for envelope waves. This equation contains a free parameter, denoted by χ and is an integrable equation if $\chi = 0$.[10] It is remarkable that the equations $\nu = 0$ and $\chi = 0$ are equivalent to Eqs. (1.5) and (1.6). The reductions related to Eq. (1.2) are discussed in Sec. III.

II. MAIN RESULTS

Proposition 2.1: Let $v(x,t)$ satisfy the BO equation,

$$v_t = 2vv_x + Hv_{xx}. \quad (2.1)$$

Let $u(x,t)$ be defined by

$$u=v+\frac{\epsilon}{2}(\lambda_1 v^2+\lambda_2 Hv_x+\lambda_3 x[2vv_x+Hv_{xx}]). \tag{2.2}$$

Then, u solves Eq. (1.2) where the coefficients of Eq. (1.2) satisfy the constraints given by Eqs. (1.5) and (1.6). Actually, these coefficients can be parametrized by λ_1, λ_2, λ_3 through the equations

$$\alpha=\lambda_3, \quad \beta_1=-\lambda_2, \quad \beta_2=\lambda_1-\lambda_3, \quad \beta_3=-\lambda_1+\lambda_2-2\lambda_3, \quad \gamma=-\lambda_1-2\lambda_3. \tag{2.3}$$

Proof: This result can be verified by a direct calculation. However, we choose to derive a more general result which contains the above as a particular case.

Let $\mathscr{H}(v)$ denote the ring consisting of smooth functions of $v(x,t)$, of its x derivatives, of the action of H on these functions, and of the multiplication by x on these functions. Let v solve the equation,

$$v_t=K(v)+\epsilon\tilde{K}(v), \tag{2.4}$$

where $K,\tilde{K}\in\mathscr{H}$. Define u by the transformation,

$$u=v+\epsilon\tilde{\tau}(v), \tag{2.5}$$

where $\tilde{\tau}\in\mathscr{H}$. Then by direct substitution it follows that u solves the equation,

$$u_t=K(u)+\epsilon(\tilde{K}(u)+[\tilde{\tau}(u),K(u)]_L)+O(\epsilon^2). \tag{2.6}$$

Here $[A,B]_L$ denotes the Lie bracket of $A,B\in\mathscr{H}$, defined by

$$[A(u),B(u)]_L=A'[B](u)-B'[A](u), \tag{2.7}$$

and where prime denotes Frechet differentiation, i.e.,

$$A'[B](u)=\frac{\partial}{\partial\epsilon}A[u+\epsilon B(u)]\Big|_{\epsilon=0}. \tag{2.8}$$

In the particular case when $\tilde{K}=0$, $\tilde{\tau}$ is given by the $O(\epsilon)$ terms of Eq. (2.2), and K is the right-hand side of the BO equation, i.e.,

$$K(v)=2vv_x+Hv_{xx}, \tag{2.9}$$

then Eq. (2.6) becomes Eq. (1.2) with its parameters given by Eq. (2.3). Eliminating the λ's from (2.3) we obtain Eqs. (1.5) and (1.6).

Proposition 2.2: Let v satisfy the integrable equation

$$v_t=K(v)+\epsilon\alpha K_1(v), \tag{2.10}$$

where $K(v)$ is given by Eq. (2.9), and $K_1(v)$ is defined by

$$K_1(v)=[v_{xx}-\tfrac{3}{2}(vHv_x+Hvv_x)-v^3]_x. \tag{2.11}$$

Define u by

$$u=v+\frac{\epsilon}{2}(\mu_1 v^2+\mu_2 Hv_x). \tag{2.12}$$

Then, u solves Eq. (1.2), where the coefficients satisfy the constraints given by Eqs. (1.5) and (1.6). Actually, these coefficients can be parametrized by

$$\beta_1=-\tfrac{3}{2}\alpha-\mu_2,\quad \beta_2=\mu_1,\quad \beta_3=-\tfrac{3}{2}\alpha-\mu_1+\mu_2,\quad \gamma=-3\alpha-\mu_1. \tag{2.13}$$

Proof: This result is a particular case of the more general result presented in the proof of Proposition 2.1.

Remark 2.1: (a) Equation (2.10) is integrable because K_1 is the first commuting flow of the BO equation, i.e.,

$$[K,K_1]_L=0. \tag{2.14}$$

(b) Let $\tau(u)\in\mathscr{H}$ be defined by

$$\tau=u^2+\tfrac{3}{2}Hu_x+x[2uu_x+Hu_{xx}]. \tag{2.15}$$

This function is the *mastersymmetry* of the BO equation.[6] It has the defining property that

$$K_1(u)=\tfrac{1}{2}[\tau,K]_L. \tag{2.16}$$

The terms of $K_1(u)$ differ from the $O(\epsilon)$ terms of Eq. (1.2) only in their numerical coefficients. Thus, in order to find the form of the transformation $\tilde{\tau}(u)$ in (2.5) it is natural to replace the numerical coefficients of $\tau(u)$ by arbitrary constants; in this way $\tau(u)$ becomes the $O(\epsilon)$ term of Eq. (2.2).

(c) If the coefficients of Eq. (1.2) are defined by Eq. (1.4), the constraints (1.5) and (1.6) are not satisfied. However, even in this case, Eq. (2.2) defines a three parameter group of infinitesimal transformations which maps Eq. (1.2) to itself. Using this group of transformations it is possible to show that the equations for the velocity amplitude, and for the fluid interface displacement, derived in Refs. 7 and 8 respectively, are equivalent.

Proposition 2.3: Let $a_j(t)$ and $X_j(t)$ be complex valued scalar functions of t, $a_j^*(t)$ and $X_j^*(t)$ denote their complex conjugation, $j=1,\ldots,N$, and assume that $\mathrm{Im}\,X_j<0$. Equation (1.2) admits the pole-decomposition solution

$$u=\sum_{j=1}^{N}\left[\frac{ia_j(t)}{x-X_j(t)}-\frac{ia_j^*(t)}{x-X_j^*(t)}\right], \tag{2.17}$$

if and only if: (a) The coefficients of Eq. (1.2) satisfy Eqs. (1.5) and (1.6);

(b) a_j is given by

$$a_j=1-\frac{\epsilon\beta_2}{2}\dot{X}_j+O(\epsilon^2); \tag{2.18}$$

(c) X_j satisfy the perturbed Calogero–Moser dynamical system,

$$\ddot{X}_j=8{\sum_k}'\frac{1}{(X_j-X_k)^3}+12\epsilon\alpha{\sum_k}'\frac{\dot{X}_j+\dot{X}_k}{(X_j-X_k)^3}+O(\epsilon^2), \tag{2.19}$$

where $\dot{X}_j=dX_j/dt$, $\ddot{X}_j=d^2X_j/dt^2$, and the sign Σ_k' denotes summation over k from 1 to N excluding j.

Proof: Substituting the pole expansion (2.17) into (1.2) one finds a fourth-order polynomial in terms of $(x-X_j)^{-n}$. Equating the coefficients of the terms with $n=4$ and $n=1$ to zero it follows that

$$6\alpha+3\beta_1+2\beta_2+3\beta_3-\gamma=0, \tag{2.20}$$

and

$$[\beta_1+\beta_2+\beta_3-\gamma]\ddot{X}_j-8\beta_2\sum_k{}' \frac{1}{(X_j-X_k)^3}=0. \tag{2.21}$$

The $O(1)$ term of Eq. (1.2) is the BO equation, thus to the leading order $\ddot{X}_j = 8\Sigma_k'(X_j - X_k)^{-3}$.[11] Substituting this expression into Eq. (2.21), we find that Eqs. (2.20) and (2.21) yield (1.5) and (1.6). Using these two equations, the coefficient of the term $(x-X_j)^{-n}$ with $n=3$ implies Eq. (2.18), while that with $n=2$ implies

$$\begin{aligned} i\dot{X}_j=&2\sum_k{}' \frac{1}{X_j-X_k}-2\sum_k \frac{1}{X_j-X_k^*}+i\epsilon\Bigg[-3\alpha\Bigg(\sum_k \sum_l{}'' \frac{1}{(X_j-X_k)(X_j-X_l)} \\ &-2\sum_k{}' \sum_l \frac{1}{(X_j-X_k)(X_j-X_l^*)}+\sum_k \sum_l \frac{1}{(X_j-X_k^*)(X_j-X_l^*)}\Bigg) \\ &+(\beta_3-\beta_1-3\beta_2)\sum_k \frac{1}{(X_j-X_k^*)^2}\Bigg]+O(\epsilon^2); \end{aligned} \tag{2.22}$$

the sign $\Sigma_k\Sigma_l''$ denotes summation over all k and l from 1 to N which are not equal to j and to each other. Equations (2.22) are different from those derived by Case[11] from the integrable equation (2.10) where the last $O(\epsilon)$ term in Eq. (2.22) is absent. However, differentiating (2.22) with respect to t and using the pole-decomposition technique discussed in Ref. 12, it can be shown that this term cancels out to $O(\epsilon^2)$, and Eq. (2.22) reduces to (2.19).

Remark 2.2: (a) Let Y_j, $j=1,\ldots,N$, satisfy the integrable Calogero–Moser dynamical system,

$$\ddot{Y}_j=8\sum_k{}' \frac{1}{(Y_j-Y_k)^3}. \tag{2.23}$$

Define X_j by

$$X_j=Y_j+\frac{\epsilon\alpha}{2}Y_j\dot{Y}_j. \tag{2.24}$$

Then, X_j satisfy Eq. (2.19) to $O(\epsilon^2)$. We note that the transformation (2.24) also follows from Proposition 2.1. Indeed, since v satisfies the BO equation (2.1), it admits the pole decomposition,

$$v=\sum_{j=1}^{N}\left[\frac{i}{x-Y_j(t)}-\frac{i}{x-Y_j^*(t)}\right]. \tag{2.25}$$

Substituting this expansion and the corresponding one for u [see (2.17)] into (2.2) with $\lambda_1=\alpha+\beta_2$, $\lambda_2=-\beta_1$, and $\lambda_3=\alpha$ we find that Eq. (2.2) reduces to (2.24).

(b) The pole decomposition of Eq. (1.2) yields an integrable dynamical systems if the coefficients satisfy the constraints given by Eq. (1.5) and (1.6). This provides further evidence that these constraints are necessary and sufficient conditions for the asymptotic integrability of Eq. (1.2). Furthermore, explicit soliton and periodic wave solutions of this equation can be found in the integrable case by means of the pole-decomposition representation (2.17) (see Ref. 11).

III. RELATED REDUCTIONS

In this section we discuss the integrability of certain equations related to Eq. (1.2).

Reduction 3.1: Let u be analytic in the upper half plane of the complex extension of x. Then $Hu=iu$, and Eq. (1.2) reduces to the complex perturbed Burgers equation

$$u_t=2uu_x+iu_{xx}+\epsilon[\alpha u_{xxx}+i(\beta_1+\beta_3)u_x^2+i(\beta_1+\beta_2+\beta_3)uu_{xx}+\gamma u^2u_x]+O(\epsilon^2). \quad (3.1)$$

It can be shown that if v satisfies the complex Burgers equation

$$v_t=2vv_x+iv_{xx}, \quad (3.2)$$

and if u is defined by

$$u=v+\frac{\epsilon}{2}(\nu_1v^2+\nu_2v_x\partial^{-1}v+\nu_3x[2vv_x+iv_{xx}]), \quad (3.3)$$

then u satisfies Eq. (3.1), where the coefficients of Eq. (3.1) satisfy the single constraint

$$\nu=3\alpha+3\beta_1+\beta_2+3\beta_3-2\gamma=0. \quad (3.4)$$

We note that the constraint (3.4) does not coincide with either Eq. (1.5) or (1.6). Moreover, Eq. (3.3) contains a nonlocal term, which is absent in Eq. (2.2). However, if the coefficients of Eq. (1.2) satisfy Eqs. (1.5) and (1.6), then both $\nu_2=0$ and $\nu=0$ are valid.

Reduction 3.2: Let u be expanded in the asymptotic form

$$u=\sqrt{\epsilon}[\Psi(X,T)\exp[i(x-t)]+\text{c.c.}]+O(\epsilon), \quad X=\epsilon(x-2t), \quad T=\epsilon^2t, \quad (3.5)$$

where c.c. denotes complex conjugation. Then, it can be shown[7] that the function $\Psi(X,T)$ satisfies the equation

$$i\Psi_T+\Psi_{XX}+\Psi[i+H](|\Psi|^2)_X+\chi|\Psi|^2\Psi=0, \quad (3.6)$$

where

$$\chi=3\alpha+2\beta_1+\beta_2+2\beta_3-\gamma. \quad (3.7)$$

It was shown in Ref. 10 that if $\chi=0$ then Eq. (3.6) is integrable. [If one applies the ansatz (3.5) to the BO equation instead of Eq. (1.2), one finds Eq. (3.6) with $\chi=0$.] We note that if Eqs. (1.5) and (1.6) are valid, then $\chi=0$. Furthermore, Eqs. (3.4) and (3.7) are equivalent to Eqs. (1.5) and (1.6).

Reduction 3.3: Let the function u be represented asymptotically as $t\to\pm\infty$ by

$$u=u_0(\theta_1^{\pm};a_1)+u_0(\theta_2^{\pm};a_2)+O(\epsilon), \quad \theta_j^{\pm}=a_j(x+v_jt+\epsilon X_j^{\pm}), \quad j=1,2, \quad (3.8)$$

where $u_0(\theta_j^{\pm};a_j)$ is the profile of the BO (algebraic) soliton solution. The parameters a_j, v_j, and $X_j^{\pm}$ describe the amplitude, the velocity, and the phase shift of the j soliton, respectively. Assume that $a_1<a_2$, which implies $v_1<v_2$. Then, the velocities of the individual BO solitons are expressed through their amplitudes by the equations

$$v_j=a_j-\frac{\epsilon a_j^2}{4}(6\alpha+7\beta_1+6\beta_2+5\beta_3-5\gamma)+O(\epsilon^2). \quad (3.9)$$

Furthermore, the total phase shifts of the BO soliton interactions, $\Delta X_j=X_j^+-X_j^-$, are given by

$$\Delta X_1 = -\frac{\pi}{(a_1+a_2)^2}\,[(3\alpha+\beta_1+\beta_2+\beta_3)(2a_1^2+4a_1a_2-2a_2^2) + (\beta_1+\beta_2-\gamma)(3a_1^2+6a_1a_2-a_2^2)], \tag{3.10}$$

$$\Delta X_2 = -\frac{\pi}{(a_1+a_2)^2}\,[(3\alpha+\beta_1+\beta_2+\beta_3)(-2a_1^2+4a_1a_2+2a_2^2) + (\beta_1+\beta_2-\gamma)(-a_1^2+6a_1a_2+3a_2^2)]. \tag{3.11}$$

When the coefficients of Eq. (1.2) are given by Eqs. (1.4), the total phase shifts (3.10) and (3.11) reduce to those found by Matsuno.[9] Here we have generalized his result to show that the total phase shifts exactly vanish only if the coefficients in (1.2) satisfy Eqs. (1.5) and (1.6). This is consistent with the fact that in this case, the interaction of the BO (algebraic) solitons is described by the integrable Calogero–Moser system (2.23) which does not produce any phase shifts of the algebraic soliton interactions.

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Soliton solutions and nontrivial scattering in an integrable chiral model in (2+1) dimensions

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The behavior of solitons in integrable theories is strongly constrained by the integrability of the theory; i.e., by the existence of an infinite number of conserved quantities that these theories are known to possess. One usually expects the scattering of solitons in such theories to be rather simple, i.e., trivial. By contrast, in this paper we generate new soliton solutions for the planar integrable chiral model whose scattering properties are highly nontrivial; more precisely, in head-on collisions of N indistinguishable solitons the scattering angle (of the emerging structures relative to the incoming ones) is π/N. We also generate soliton–antisoliton solutions with elastic scattering; in particular, a head-on collision of a soliton and an antisoliton resulting in 90° scattering. © *1996 American Institute of Physics.* [S0022-2488(96)02007-5]

I. INTRODUCTION

In this paper we study certain exact soliton solutions of an integrable system. Before any detailed discussion, and to avoid confusion later on, it is worthwhile clearing up a small point of terminology: the word *solitons* was introduced by mathematicians to describe lumps of energy that were stable to perturbations and did not change either velocity or shape when colliding with each other. However, in recent literature all sorts of localized energy configurations have been called solitons. We shall go along this looser definition. By a soliton we shall mean a lump of energy that moves but we shall not imply stability of the shape or the velocity or a simple behavior in collision.

An interesting problem is to look at the scattering properties of two or more solitons colliding. In some known systems with nontrivial topology, the collision of two solitons is inelastic (some radiation is emitted) and nontrivial (a head-on collision results in 90° scattering); all this has been observed analytically[1,2] and numerically.[3–6] One can construct explicit time-dependent solutions only in very special, so-called integrable models. Usually in these models extended objects interact trivially, in the sense that they pass through each other with no lasting change in velocity or shape (i.e., they behave as genuine solitons). Some examples in (2+1) dimensions are the Kadomtsev–Petviashvili equation[7] and the integrable chiral model.[8] The last system is the subject of this paper and will be described below. Until now, nontrivial scattering of solitons occurs mostly in nonintegrable systems, which is far from simple. The question that arises is whether this type of scattering can occur in integrable models too. There are some limited examples of integrable systems where soliton dynamics can be nontrivial. In (1+1) dimensions there are many models that possess nontrivial soliton-like solutions (cf. Ref. 9); like the boomeron solutions,[10] which are solitons with time-dependent velocities. In (2+1) dimensions there are the dromion solutions[11] of the Davey–Stewartson equation, which decay exponentially in both spatial coordinates and interact in a nontrivial manner;[12] and the soliton solutions[13] of the Kadomtsev–Petviashvili equations, whose scattering properties are highly nontrivial.

In the present work we are going to construct families of soliton solutions for the integrable (2+1)-dimensional chiral model and observe the occurrence of different types of behavior. This happens since the solitons in this system have internal degrees of freedom that determine their orientation in space; do not affect the initial energy density; and are important in understanding the

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evolution as a whole. Therefore, they can interact either trivially or nontrivially, depending on the orientation of these internal parameters and on the values of the impact parameter defined as the distance of closest of approach between their centers in the absence of interaction. Namely, if two initial soliton-like structures are sent toward each other at zero impact parameter, then, as most numerical simulations have shown, the outgoing structures emerge at 90°.

To proceed further let us specify the system. The modified SU(2) chiral model studied by Ward[8] is given by the field equation

$$\partial^{\mu}(J^{-1}J_{\mu})-\tfrac{1}{2}V_{\alpha}\epsilon^{\alpha\mu\nu}[J^{-1}J_{\mu},J^{-1}J_{\nu}]=0. \tag{1}$$

Here J takes values in the SU(2) group and is thought of as a 2×2 unitary matrix of functions of the space–time coordinates on $\mathbf{R}^{2+1}$: $x^{\mu}=(x^0,x^1,x^2)=(t,x,y)$ with $\det J=1$. Greek letters are space–time indices, taking values 0, 1, 2, ∂_{μ} denotes partial differentiation with respect to x^{μ}, while gaps $J_{\mu}\equiv\partial_{\mu}J$. The quantity $\epsilon^{\alpha\mu\nu}$ is the alternating tensor of three indices with $\epsilon^{012}=1$. Finally, V_{α} is a unit vector in space–time. The conformal properties of V_{α} determine whether the symmetry group is SO(2) or SO(1,1) (depending on whether V_{α} is time-like or space-like).

Ward[8] chooses V_{α} to have the components $V_{\alpha}=(0,1,0)$, the space-like case, so that (1) is a chiral equation with torsion term and has the same conserved energy-momentum vector as the chiral field equation. In fact, the corresponding energy density is

$$\mathscr{E}=-\tfrac{1}{2}\ \mathrm{tr}\ [(J^{-1}J_t)^2+(J^{-1}J_x)^2+(J^{-1}J_y)^2]. \tag{2}$$

Here tr denotes the matrix trace. It should be emphasized that $\mathscr{E}$ is a positive-defined functional of J, and hence a conserved energy exists that is the integral of the energy density over the space-like plane $x^0=$const. The boundary conditions are chosen so that the field configuration has finite energy. Consequently, we require that J be everywhere smooth and that

$$J=J_0+J_1(\theta)r^{-1}+O(r^{-2}), \tag{3}$$

at spatial infinity, with $x+iy=re^{i\theta}$. Here J_0 is a constant matrix, and J_1 depends only on θ (no time dependence).

The ensuing system when V_a is i times a time-like vector instead of space-like has been studied in Ref. 14. Equation (1) admits solitons, localized in two dimensions, with trivial scattering, i.e., each soliton suffers no change in velocity and no phase shift upon scattering.[8,14] It is the purpose of this paper to construct new soliton solutions for (1), and investigate their scattering behavior. Such solutions are localized along the direction of motion; they are not, however, of constant size: their height, which corresponds to the maximum of the energy density $\mathscr{E}$, is time dependent.

The rest of the paper is arranged as follows. In the next section we shall briefly discuss the integrability properties of (1), and write down a family of multisoliton solutions as configurations that are the limiting cases of the ones already obtained using the standard method of *Riemann problem with zeros*.[8] In Sec. III we construct two families of multisoliton solutions with nontrivial scattering; in particular, for the first one we prove that in all head-on collisions the N moving structures undergo π/N scattering. In Sec. IV we construct a mixture of soliton–antisoliton solutions, and in Sec. V we discuss their dynamics and scattering properties. We finish the paper with a short section containing our conclusions.

II. CONSTRUCTION OF SOLITON SOLUTIONS

The integrable nature of Eq. (1) means that there is a variety of methods for constructing exact solutions. Together with *Riemann problem with zero*,[8] both *twistor techniques*[15] and a full *inverse scattering formalism*[16] have been applied to the model. In this section we indicate a general

method for constructing soliton solutions of the integrable chiral model (1). The technique is a variation of that Ref. 8, 17, following a pioneering idea of Zakharov and his collaborators.[18]

The nonlinear equation (1) is integrable in a sense that it may be written as the compatibility condition for the following linear system:

$$\begin{aligned} L\psi &\equiv (\lambda\partial_x - \partial_u)\psi = A\psi, \\ M\psi &\equiv (\lambda\partial_v - \partial_x)\psi = B\psi. \end{aligned} \tag{4}$$

Here $\lambda \in \mathbf{C}$, (u,v,x) are coordinates on $\mathbf{R^{2+1}}$ with $u=(t+y)/2$, $v=(t-y)/2$, A and B are 2×2 anti-Hermitian trace-free matrices depending only on (u,v,x), and $\psi(\lambda,u,v,x)$ is an unimodular 2×2 matrix function satisfying the reality condition

$$\psi(\lambda,u,v,x)\psi(\overline{\lambda},u,v,x)^{\dagger} = I, \tag{5}$$

where the overbar denotes the complex conjugate, † denotes the complex conjugate transpose matrix, and I is the 2×2 identity matrix. The system (4) is overdetermined, and in order for a solution ψ to exist, A and B have to satisfy the integrability conditions, which are

$$B_x = A_v, \quad A_x - B_u - [A,\, B] = 0. \tag{6}$$

If we put $J(u,v,x) = \psi(\lambda=0,u,v,x)^{-1}$, where ψ is a solution of the system (4), we get by comparing (4) and (6) that

$$A = J^{-1}J_v, \quad B = J^{-1}J_x. \tag{7}$$

Therefore, the integrability condition for (4) implies that there exists a field J that satisfies the equation of motion (1); and moreover, the reality condition on ψ ensures that J is unitary.

Using the standard method of *Riemann problem with zeros*, in order to construct the multi-soliton solution, one may assume that the function ψ has simple poles in λ, or in other words, must possess the form

$$\psi(\lambda) = I + \sum_{k=1}^{n} \frac{M_k}{\lambda - \mu_k}, \tag{8}$$

where M_k are 2×2 matrices independent of the complex parameter λ, n is the number of solitons, and the complex parameter μ_k determines the velocity of the kth soliton. The components of the matrix M_k are given in terms of a rational function f_k of the complex variable, $\omega_k = x + \mu_k u + \mu_k^{-1} v$. [Roughly speaking, $f_k(\omega_k)$ describes the shape of the kth soliton.] In fact, the matrix M_k (cf. Ref. 8) has the form

$$M_k = -\sum_{l=1}^{n} (\Gamma^{-1})^{kl} \overline{m_a^l} m_b^k, \tag{9}$$

with Γ^{-1} the inverse of

$$\Gamma^{kl} = \sum_{a=1}^{2} (\overline{\mu_k} - \mu_l)^{-1} \overline{m_a^k} m_a^l. \tag{10}$$

Here m_a^k are holomorphic functions of ω_k, given by $m_a^k = (m_1^k, m_2^k) = (1,\, f_k)$. These solitons pass each other without any change of direction or phase shift. Infinite energy extended wave solutions[19] may be constructed by taking f_k to be an exponential function of ω_k. Such extended wave solutions suffer a phase shift upon scattering, although again there is no change in velocity.

All this assumes that the parameters μ_k are distinct, and also $\overline{\mu_k} \neq \mu_l$ for all k, l. In this paper examples are given of two generalizations of these constructions: one involving higher-order poles in μ_k and the other where $\overline{\mu_k} = \mu_l$.

Let us look at an example in which the function ψ has a a double pole in λ, and no other poles. So we take ψ to have the form

$$\psi = I + \sum_{k=1}^{2} \frac{R_k}{(\lambda - \mu)^k}, \tag{11}$$

where R_k are 2×2 matrices independent of λ. (This hypothesis can be generalized by taking the function ψ to have a pole of order n in λ.)

It has been proved[17] that ψ given by (11) satisfies the reality condition (5) if and only if it factorizes as

$$\psi(\lambda) = \left(I - \frac{(\overline{\mu} - \mu)}{(\lambda - \mu)} \frac{q_1^\dagger \otimes q_1}{\|q_1\|^2} \right) \left(I - \frac{(\overline{\mu} - \mu)}{(\lambda - \mu)} \frac{q_2^\dagger \otimes q_2}{\|q_2\|^2} \right), \tag{12}$$

where q_k are two-dimensional row vectors and $\|q_k\|^2 = q_k \cdot q_k^\dagger$.

The q_k have to satisfy a condition, which amounts to saying the matrices $A = (L\psi)\psi^{-1}$ and $B = (M\psi)\psi^{-1}$ are independent of λ. One way of obtaining q_k with this property is as a limit of the simple-pole case (8) with $n=2$. The idea is to take a limit $\mu_k \to \mu$. In order to end up with a smooth solution ψ for all (u,v,x), it is necessary that $f_2(\omega_2) - f_1(\omega_1) \to 0$ in this limit.

In our case, with $n=2$, we put $\mu_1 = \mu + \epsilon$, $\mu_2 = \mu - \epsilon$, and write $f_1(\omega_1) = f(\omega_1)$, $f_2(\omega_2) = f(\omega_2)$, with f being a rational function of one variable. In the limit $\epsilon \to 0$, ψ has the form (12), with

$$\begin{aligned} q_1 &= (1 + |f|^2)(1, f) + \varphi(\overline{\mu} - \mu)(\overline{f}, -1), \\ q_2 &= (1, f). \end{aligned} \tag{13}$$

Here f is a rational function of $\omega = x + \mu u + \mu^{-1} v$, $\varphi = (u - \mu^{-2} v) f'(\omega)$, while $f'(\omega)$ denotes the derivative of $f(\omega)$ with respect to its argument. As a result, we have a solution $J = \psi(\lambda = 0)^{-1}$ depending on the complex parameter μ and on the arbitrary function f. In fact, it has the form of the following product:

$$J = \left(I + \frac{(\overline{\mu} - \mu)}{\mu} \frac{q_2^\dagger \otimes q_2}{\|q_2\|^2} \right) \left(I + \frac{(\overline{\mu} - \mu)}{\mu} \frac{q_1^\dagger \otimes q_1}{\|q_1\|^2} \right), \tag{14}$$

with q_k given by (13). Notice that J takes values in $SU(2)$; is smooth everywhere on $\mathbf{R}^{2+1}$ (mainly because the two vectors q_1 and q_2 are nowhere zero); it satisfies the boundary condition (3); and the equation of motion (1).

To start with, and in order to illustrate the above family of soliton solutions, let us examine two simple cases, by giving specific values to the parameters μ and $f(\omega)$. (The complex parameter μ determines the velocity of the ''center-of-mass'' of the system.)

• Let us take $\mu = i$ (which corresponds to the ''center-of-mass'' of the system being stationary) and $f(\omega) = \omega$, thus $\omega = z$ and $\varphi = t$, where $z = x + iy$; $r^2 = z\overline{z}$. Therefore the row vectors (13) become

$$\begin{aligned} q_1 &= (1 + r^2)(1, z) - 2it(\overline{z}, -1), \\ q_2 &= (1, z). \end{aligned} \tag{15}$$

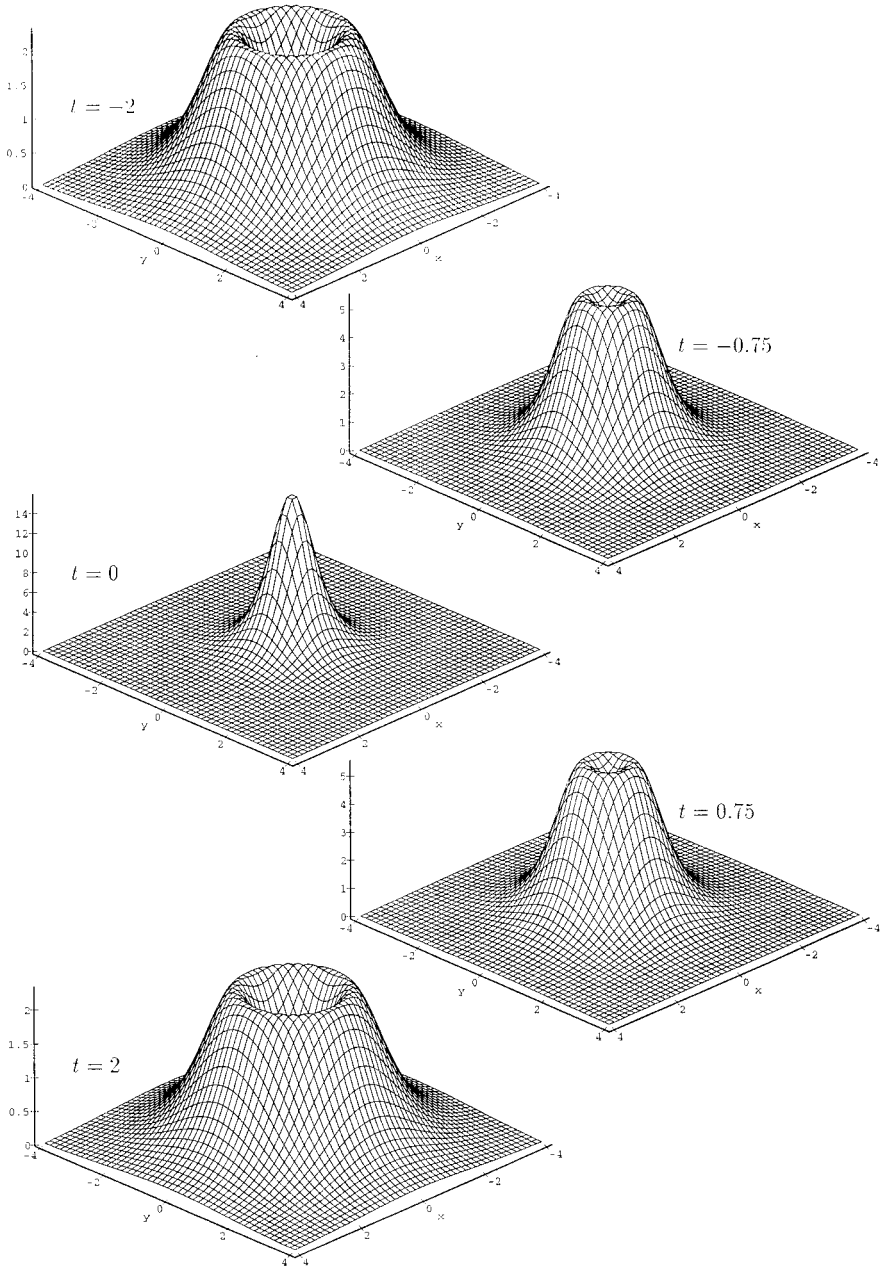

FIG. 1. The energy density $\mathscr{E}$ (16) at increasing times.

In this time-dependent solution, for t negative, a ring structure with reducing radius is obtained, which deforms to a single peak at $t=0$ and thereafter expands again to a ring. Figure 1 presents few pictures of the corresponding energy density at some representative values of time. Ring structures occur in the soliton scattering of many nonintegrable planar systems[3,5] and are an approximation of two solitons.

This picture can be confirmed by looking at the energy density of the solution, which is

$$\mathscr{E}=16\,\frac{r^4+2r^2+4t^2(2r^2+1)+1}{(r^4+2r^2+4t^2+1)^2}. \tag{16}$$

Notice that the energy density is time reversible and rotationally symmetric (see below). For large (positive) t, the height of the ring (maximum of $\mathscr{E}$) is proportional to $1/t$, while its radius is proportional to $\sqrt{t}$.

• Accordingly, let us take $\mu=i$ and $f(\omega)=\omega^2$. Thus, the row vectors (13) are

$$\begin{aligned} q_1&=(1+r^4)(1,\,z^2)-4itz(\overline{z^2},-1),\\ q_2&=(1,\,z^2). \end{aligned} \tag{17}$$

Here, for negative t, a single peak occurs with an additional ring, which changes to a ring structure at $t=0$ and reverts back to the original form, for positive t (see Fig. 2). However, these rings are not radiation since they travel with speed less than that of light. In fact, for large (positive) t, their velocity is approximately proportional to $t^{-2/3}$. (Note that we have set the velocity of the light, c, equal to the unity, so that in all our calculations we can use dimensionless quantities.)

This leads to an energy density, which is

$$\mathscr{E}=64\,\frac{r^{10}+18t^2r^8+2r^6+4t^2r^4+r^2+2t^2}{(r^8+2r^4+16t^2r^2+1)^2}. \tag{18}$$

Again, $\mathscr{E}$ has the same symmetries as in (16). For large (positive) t, the height of the soliton peak is proportional to t^2 and its radius is proportional to $1/t$; while the soliton ring spread out, becoming broader and broader, with height proportional to $t^{-2/3}$ and radius proportional to $t^{1/3}$.

Finally, a general concluding remark should be made. Although (1) is not rotationally symmetric in the xy plane; when $f(z)=z^p$ the field J (13,14) is invariant under the transformation $z\to e^{i\phi}z$, since

$$J\;\to\;J'=\begin{pmatrix} e^{i\phi p/2} & 0\\ 0 & e^{-i\phi p/2}\end{pmatrix} J \begin{pmatrix} e^{-i\phi p/2} & 0\\ 0 & e^{i\phi p/2}\end{pmatrix}. \tag{19}$$

This transformation does not affect the equation of motion (1) due to the chiral symmetry $J\to\kappa J\tau$, where κ and τ are constant $SU(2)$ matrices. The main features of this time-dependent solution may be inferred as follows. If r is large, the field J is close to its asymptotic value J_0, as long as $2tf'/|f|^2\to 0$. But as $2t|f'|/|f|^2\approx 1$, J departs from its asymptotic value J_0 and a ring structure emerges with radius proportional to $(2tp)^{1/(p+1)}$.

III. SOLITON–SOLITON SCATTERING

We now move on to the more interesting question of scattering processes. In fact, we will use the method of Sec. II to construct solutions of (1) representing scattering solitons. We will see that, in all head-on collisions of N moving solitons the scattering angle is π/N. Moreover, when the N solitons are very close together, and in particular, when they are on top of each other, the N lumps that represent them merge together to form a ring-like structure. Then, instead of moving toward the center, they emerge from the ring in a direction that bisects the angle formed by the incoming ones. As we have already mentioned this nontrivial scattering is not usual in an integrable theory, but is exceptional.

The scattering solutions arise if we take a solution of the simple-pole case (8) with $n=2$, put $\mu_1=\mu+\epsilon$, $\mu_2=\mu-\epsilon$, and take the limit $\epsilon\to 0$. The constraint $f_2(\omega_2)-f_1(\omega_1)\to 0$ as $\epsilon\to 0$ has to be imposed, in order for the resulting solution ψ to be smooth for all (u,v,x). So let us write

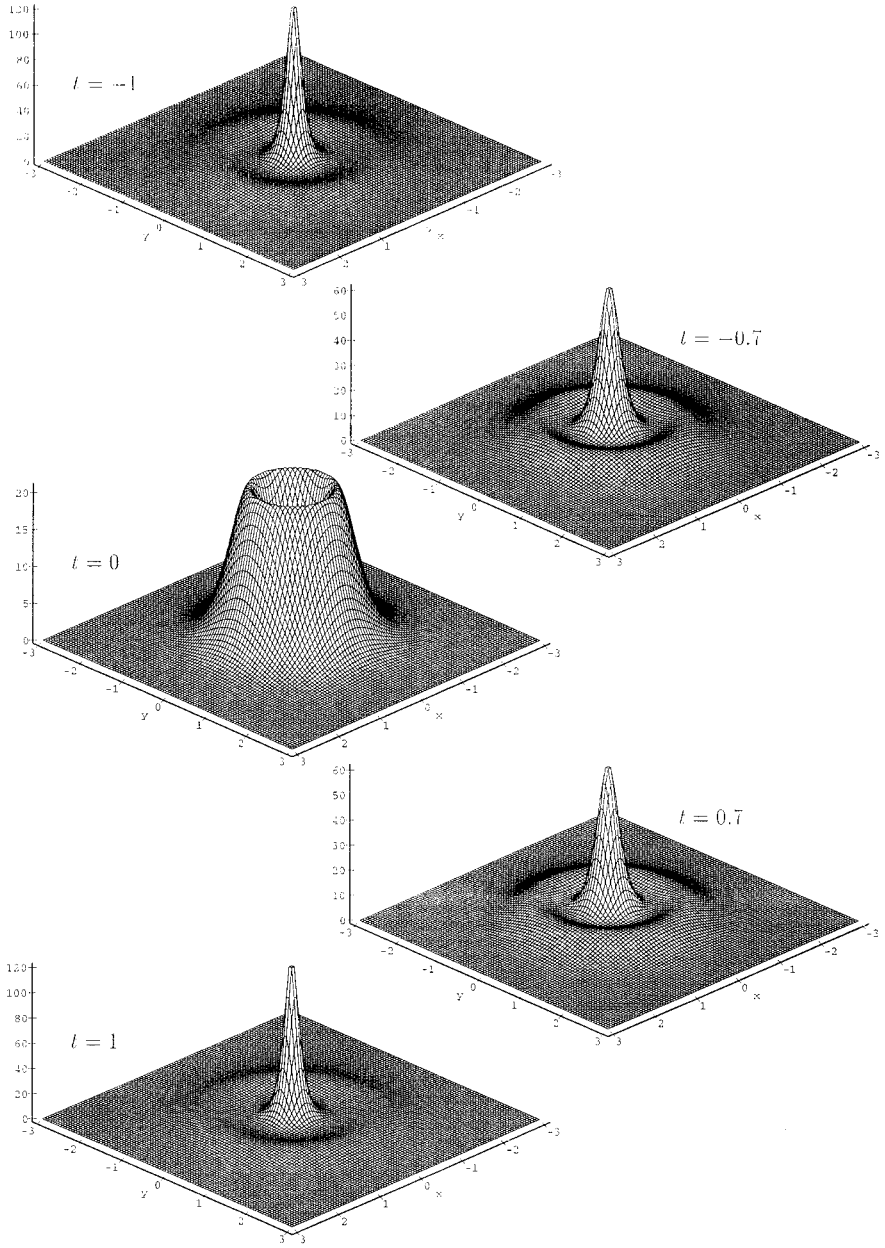

FIG. 2. The energy density $\mathscr{E}$ (18) at various times.

$f_1(\omega_1)=f(\omega_1)+\epsilon h(\omega_1)$, $f_2(\omega_2)=f(\omega_2)-\epsilon h(\omega_2)$, where f and h are both rational functions of one variable (the examples of the previous section had $h=0$). Once again J is given by (14), with the two-vectors q_k given by

$$q_1=(1+|f|^2)(1,\ f\ )+\vartheta(\overline{\mu}-\mu)(\overline{f},-1),$$
$$q_2=(1,\ f\ ), \tag{20}$$

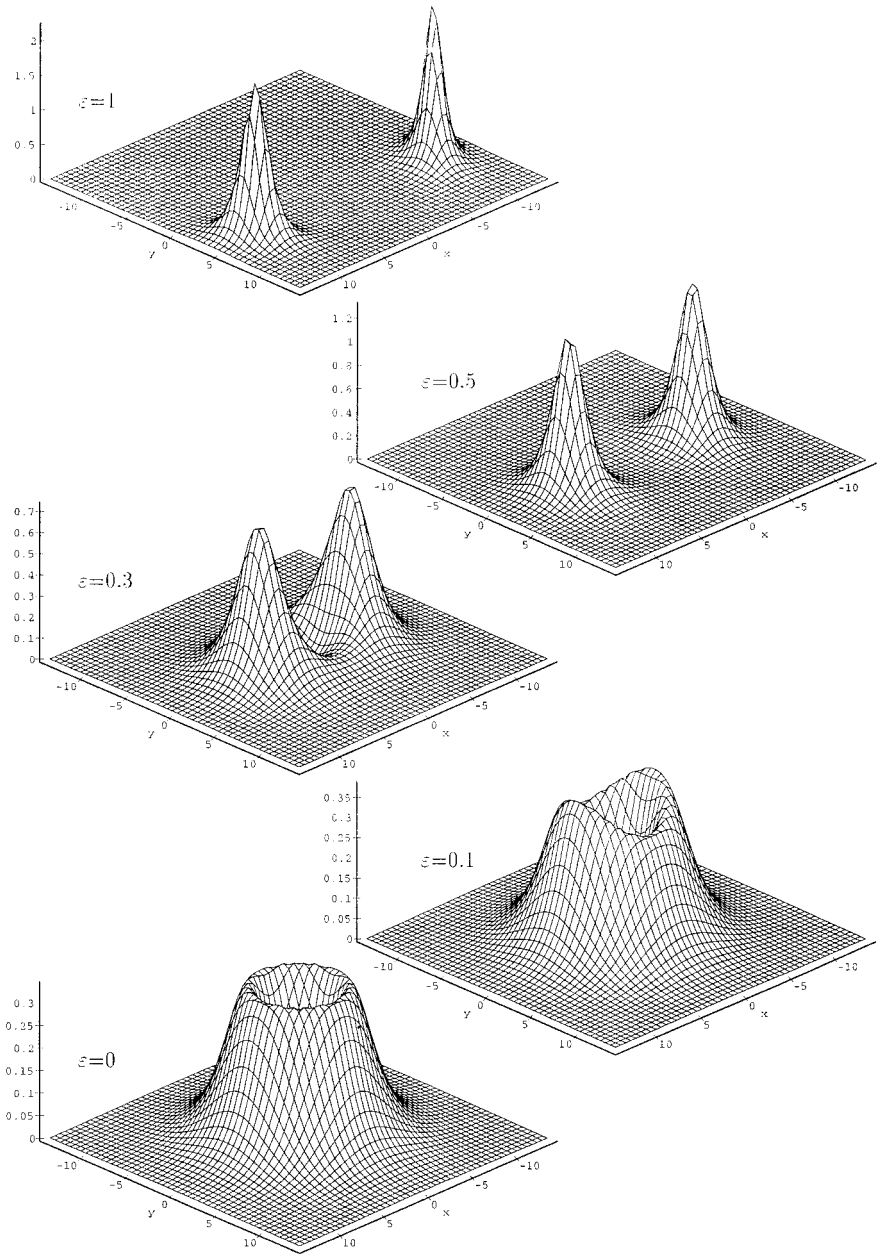

FIG. 3. Energy density at various values of ϵ for a system of two solitons ($t=-15$).

where $\vartheta=\varphi+h(\omega)$. So this solution belongs to a large family, since one may take f and h to be any rational meromorphic functions of ω. Note that J is smooth on $\mathbf{R}^{2+1}$ and satisfies its boundary condition, irrespective of the choice of f and h.

It may seem strange that one can take the limit of a family of soliton solutions with trivial scattering, and obtain a new one with nontrivial scattering. Thus, it is interesting to study how the solitons are affected by varying ϵ. To do so, let us take a solution of the simple-pole case (8) with $n=2$, put $\mu_1=i+\epsilon$, $\mu_2=i-\epsilon$, while taking $f_k=\omega_k$; and study how the configuration of the two initial well-separated solitons changes as $\epsilon\to 0$ at a fixed time ($t=-15$). Figure 3 shows that as

$\epsilon \to 0$ the solitons disperse, shift, and interact with each other. In other words, their internal degrees of freedom as well as the impact parameter change in this limit, making the process highly nontrivial.

As an example, let us present two typical cases.

• Let us take $\mu=i$, $f(\omega)=\omega$, and $h(\omega)=\omega^3$, thus $\vartheta=t+z^3$. For r large, J is equal to its asymptotic value J_0, as long as $\vartheta/z^3=1+t/z^3\approx 1$, but as z approaches any of the three cube roots of $-t$, then $\vartheta\to 0$, while J departs from J_0, and three localized solitons emerge. For t negative, the three solitons are approximately at the points $((-t)^{1/3},0)$, $(-(-t)^{1/3},\pm\sqrt{3}(-t)^{1/3})$; while for t positive, the solitons are at $(-t^{1/3},0)$, $(t^{1/3},\pm\sqrt{3}t^{1/3})$.

More information can be deduced from the energy density, which is

$$\mathcal{E}=16[2r^8+16r^6+19r^4+2r^2(1+8xy^2t)+4t^2(1+2r^2)+1+8xy^4t-8x^5t \\ -16tx(x^2-y^2)]/[4r^6+r^4+2r^2+4t^2+1+8tx(x^2-3y^2)]^2. \tag{21}$$

The density $\mathcal{E}$ is symmetric under the interchange $t\mapsto -t$, $x\mapsto -x$, and $y\mapsto -y$. For small (negative) t, the solitons form an intermediate state having the shape of a ring with three maxima on the direction of the incoming solitons that deforms to a circularly symmetric ring at $t=0$ and then energy seems to flow around, until three other maxima are formed in the transverse direction, for small (positive) t.

Figure 4 shows clearly the intermediate states with three maxima. The three new maxima then give rise to three new solitons emerging at 60° to the original direction of motion. During the intermediate phase solitons lose their identity.

Finally, something has to be said about their size. For large (positive) t, their height is proportional to $t^{-4/3}$, their radius is proportional to $t^{1/3}$, while their speed is proportional to $t^{-2/3}$: therefore, they spread out and slow down.

• Accordingly, let us take $\mu=i$ while we choose $f(\omega)=\omega^2$ and $h(\omega)=\omega^3$. Here J departs from its asymptotic value J_0 when z approaches the values $\pm\sqrt{-2t}$ or zero [since $\vartheta=z(2t+z^2)\to 0$]; and (again) three localized solitons emerge. In this case though, if t is negative, all three of them are on the x axis at $x\approx\pm\sqrt{-2t}$ and at the origin; while if t is positive, they are on the y axis at $y\approx\pm\sqrt{2t}$ and at the origin. So the picture consists of three solitons: a static one at the origin, with the other two accelerating toward the origin, scattering at right angles and then decelerating as they separate.

This can be observed from the energy density, which is

$$\mathcal{E}=32[r^{12}+2r^2(r^8+r^6+1)+36t^2r^8+4r^6+9r^4+8t^2r^4+4t^2 \\ +12t(x^{10}-y^{10})+4t(x^2-y^2)(3+2x^2y^2+6x^4y^4) \\ +4t(x^6-y^6)(9x^2y^2-2)-y^{10}]/[r^8+4r^6+2r^4+16tr^2(t+x^2-y^2)+1]^2. \tag{22}$$

Here $\mathcal{E}$ is symmetric under the interchange $t\mapsto -t$, $x\rightleftharpoons y$; therefore the collision is time symmetric, with the only effect the 90° scattering (no phase shift; no radiation). For large (positive) t, the height of the static soliton is proportional to t^2 and its radius is proportional to $1/t$; while the moving solitons expand with height proportional to $t^{-2/3}$ and radius proportional to $t^{1/3}$.

In Fig. 5 we present some pictures of the total energy densities of three solitons during a typical nontrivial evolution.

In principle one should be able to visualize the emerging soliton structures when $f(\omega)=\omega^p$ and $h(\omega)=\omega^q$, i.e., are rational of degree p, $q\in\mathbf{N}$, respectively. In fact, for $q>p$ the configuration consists of $(p-1)$ static solitons at the ''center-of-mass'' of the system (if more than one, a ring structure is formed) accompanied by $N=q-p+1$ solitons accelerating toward the ones in the middle, scattering at an angle of π/N, and then decelerating as they separate. This follows from the

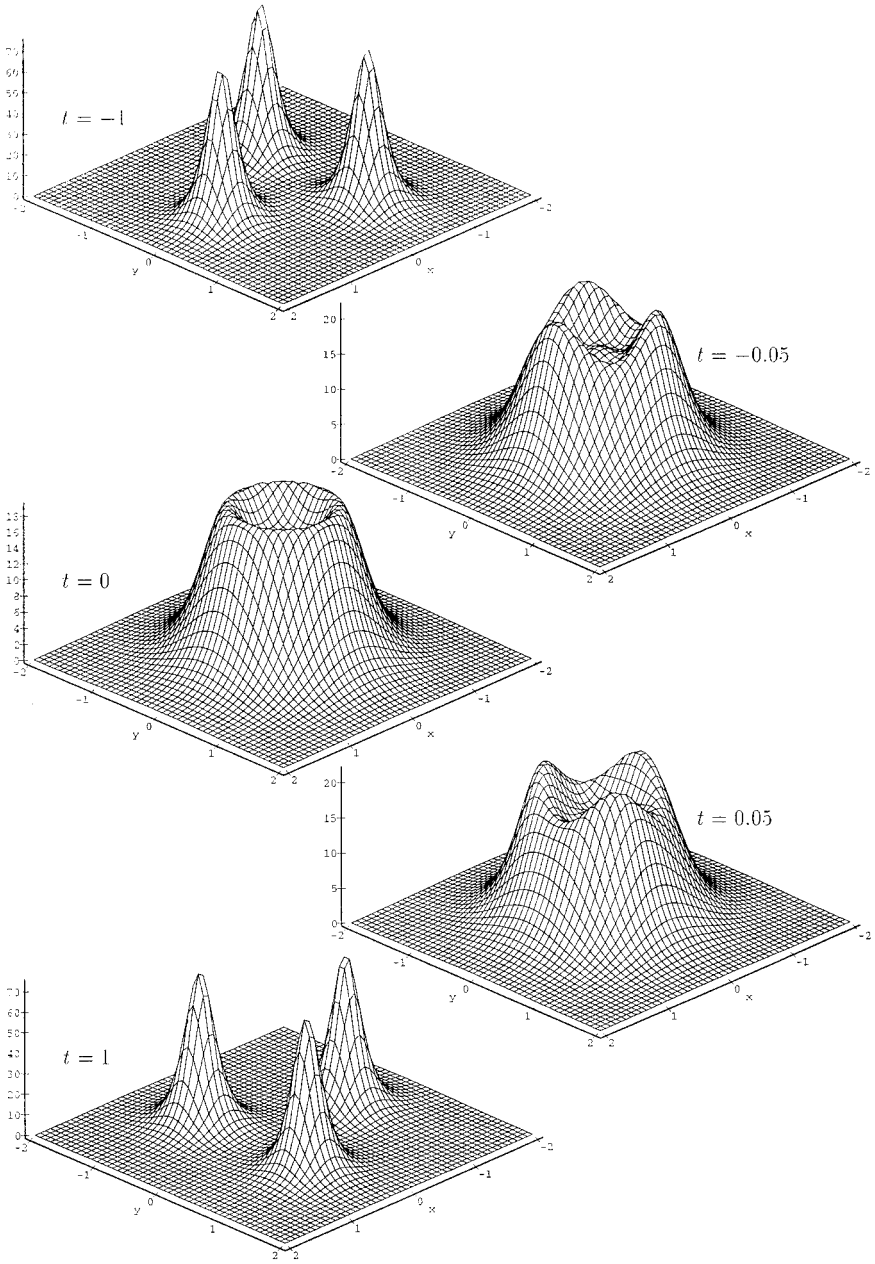

FIG. 4. Energy density at increasing times for a system of three solitons with 60° angle scattering.

fact that the field J departs from its asymptotic value J_0 when $\vartheta=\omega^{(p-1)}(p(u-\mu^{-2}v)+\omega^N)\to 0$, which is true when either $\omega^{(p-1)}=0$ or $\omega^N+p(u-\mu^{-2}v)=0$; and this is approximately where the solitons are located.

We conclude this section by investigating the corresponding case where $\psi(\lambda)$ has a triple pole (and no others). Therefore, it is taken to have the form

$$\psi(\lambda)=I+\sum_{k=1}^{3}\frac{\mathscr{R}_2}{(\lambda-\mu)^k}. \tag{23}$$

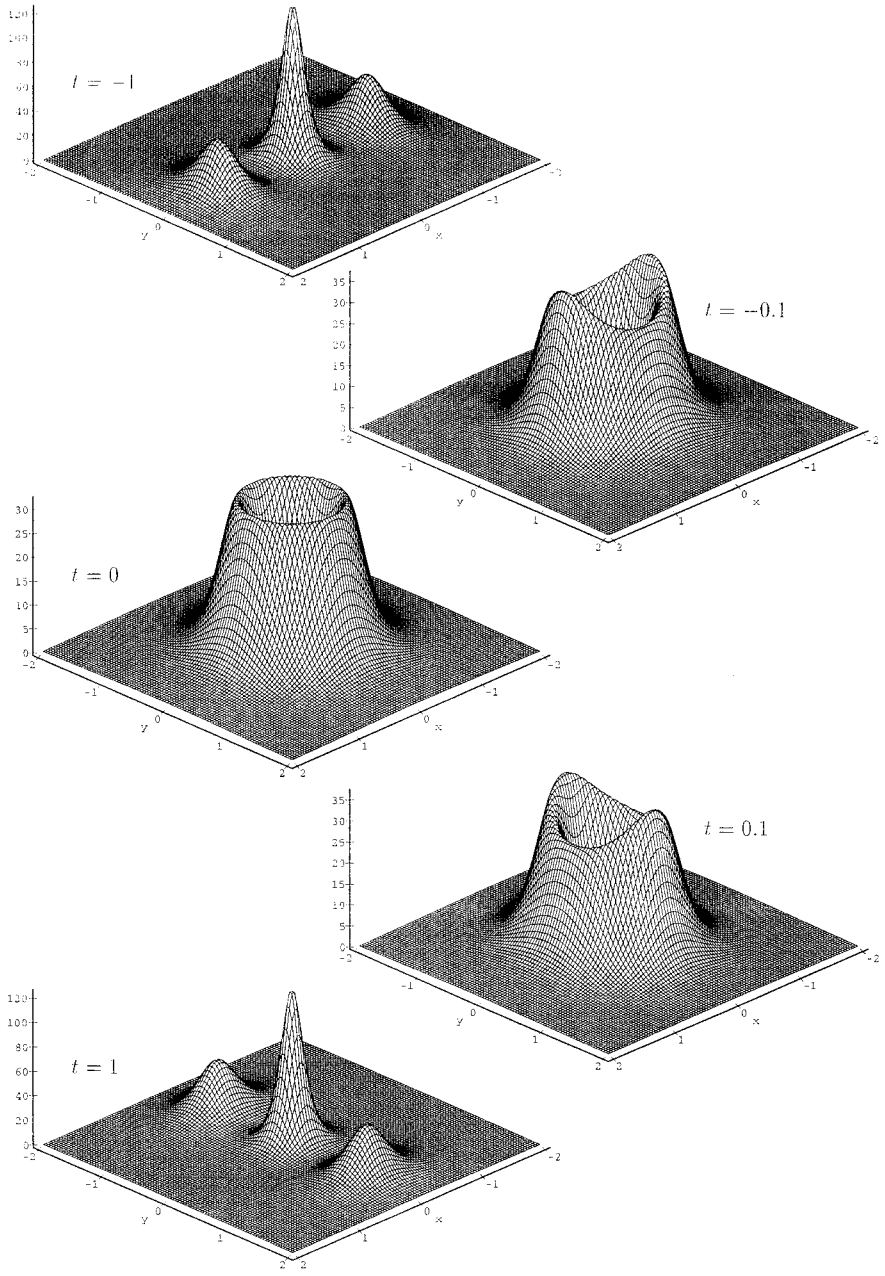

FIG. 5. Energy density at various times for the scattering of three solitons, with one being static at the origin.

As we have already mentioned, the reality condition (5) is satisfied if and only if ψ factorizes into three simple factors of the following type:

$$\psi(\lambda)=i\left(I-\frac{(\overline{\mu}-\mu)}{(\lambda-\mu)}\frac{q_1^{\dagger}\otimes q_1}{\|q_1\|^2}\right)\left(I-\frac{(\overline{\mu}-\mu)}{(\lambda-\mu)}\frac{q_2^{\dagger}\otimes q_2}{\|q_2\|^2}\right)\left(I-\frac{(\overline{\mu}-\mu)}{(\lambda-\mu)}\frac{q_3^{\dagger}\otimes q_3}{\|q_3\|^2}\right), \tag{24}$$

for some two-vectors q_k. The requirement that the matrices $A=(L\psi)\psi^{-1}$ and $B=(M\psi)\psi^{-1}$ should be independent of λ imposes differential equations on q_k; which are three nonlinear equations, and it seems difficult to find their general solution.

One way of proceeding is to take a solution for the simple-pole case (8) with $n=3$, put $\mu_1=i+\epsilon$, $\mu_2=i$, $\mu_3=i-\epsilon$, and take the limit $\epsilon\to 0$. In order to obtain a smooth solution ψ for all (u,v,x), it is necessary that $f_1(\omega_1)-f_2(\omega_2)\to 0$, $f_1(\omega_1)-f_3(\omega_3)\to 0$, $f_2(\omega_2)-f_3(\omega_3)\to 0$ as $\epsilon\to 0$. So let us write $f_1(\omega_1)=f(\omega_1)+\epsilon h(\omega_1)+\epsilon^2 g(\omega_1)$, $f_2(\omega_2)=f(\omega_2)$, $f_3(\omega_3)=f(\omega_3)-\epsilon h(\omega_3)+\epsilon^2 g(\omega_3)$, where f, h, and g are rational functions of one variable. On taking the limit, we obtain a ψ of the form (24), smooth on $\mathbf{R^{2+1}}$ and such that the matrices A and B are independent of λ.

Consequently, $J=\psi(0)^{-1}$ is a smooth solution of (1) of the form

$$J=i\left(I-\frac{2q_3^{\dagger}\otimes q_3}{\|q_3\|^2}\right)\left(I-\frac{2q_2^{\dagger}\otimes q_2}{\|q_2\|^2}\right)\left(I-\frac{2q_1^{\dagger}\otimes q_1}{\|q_1\|^2}\right), \tag{25}$$

with q_k being in terms of $f(z)$, $h(z)$, and $g(z)$ by

$$\begin{aligned} q_1&=(1+|f|^2)^2(1,f)-4i(b+id)(1+|f|^2)(\overline{f},-1)-4b^2(\overline{f}^2,-\overline{f}-2i\overline{b})-8id\overline{b}(1,f),\\ q_2&=(1+|f|^2)(1,f)-2ib(\overline{f},-1),\\ q_3&=(1,f), \end{aligned} \tag{26}$$

where $b=tf'(z)+h(z)$ and $d=t^2f''(z)/2+i(t-y)f'(z)/2+th'(z)+g(z)$. Note that the two-vectors q_2, q_3 here correspond to the ones given by (20) for $\mu=i$, respectively.

Let us examine a sample example of this solution, since we may take f, h, and g to be any rational meromorphic function of z.

• Let us take $f(z)=0$, $h(z)=z$ and $g(z)=z^2$; thus $b=z$ and $d=t+z^2$. This solution consists of two solitons coming in along the y axis merging to form a peak at the origin and then two new solitons emerging along the x axis. Figure 6 illustrates what happens near $t=0$.

The energy density of the system is

$$\mathscr{E}=32\,\frac{80r^4+32(r^2+t^2)+256t^2r^2-64t(x^2-y^2)+128tyr^2-8y+3}{[32r^4+12r^2-16yr^2+16t^2+16ty+32t(x^2-y^2)+1]^2}, \tag{27}$$

which has a reflection symmetry around the x axis. For large (positive) t, $\mathscr{E}$ is peaked at two points on the y axis, namely $y\approx\pm\sqrt{t}$. Moreover, the height of the corresponding solitons is proportional to $1/t$, and their radius is proportional to $\sqrt{t}$; which means that the y axis asymmetry vanishes at $t\to\infty$.

IV. CONSTRUCTION OF SOLITON–ANTISOLITON SOLUTIONS

In this section we construct a large family of solutions, which, as we will argue later, can be though of as representing soliton–antisoliton field configurations. Roughly speaking, solitons correspond to f being a function of the variable z, and antisolitons correspond to a function of $\overline{z}$.

One way to generate a soliton–antisoliton solution of (1), is to assume that $\psi(\lambda)$ has the form

$$\psi(\lambda)=I+\frac{n^1\otimes m^1}{(\lambda-i)}+\frac{n^2\otimes m^2}{(\lambda+i)}. \tag{28}$$

Here n^k, m^k for $k=1,2$ are complex-valued two-vector functions of $(t,z,\overline{z})$ (not depending on λ).

The idea is to find the $n_1^1,\ldots,m_1^1,\ldots$, such that the reality condition (5) holds, and such that the matrices $A=(L\psi)\psi^{-1}$ and $B=(M\psi)\psi^{-1}$ are independent of λ. One way of proceeding is to take

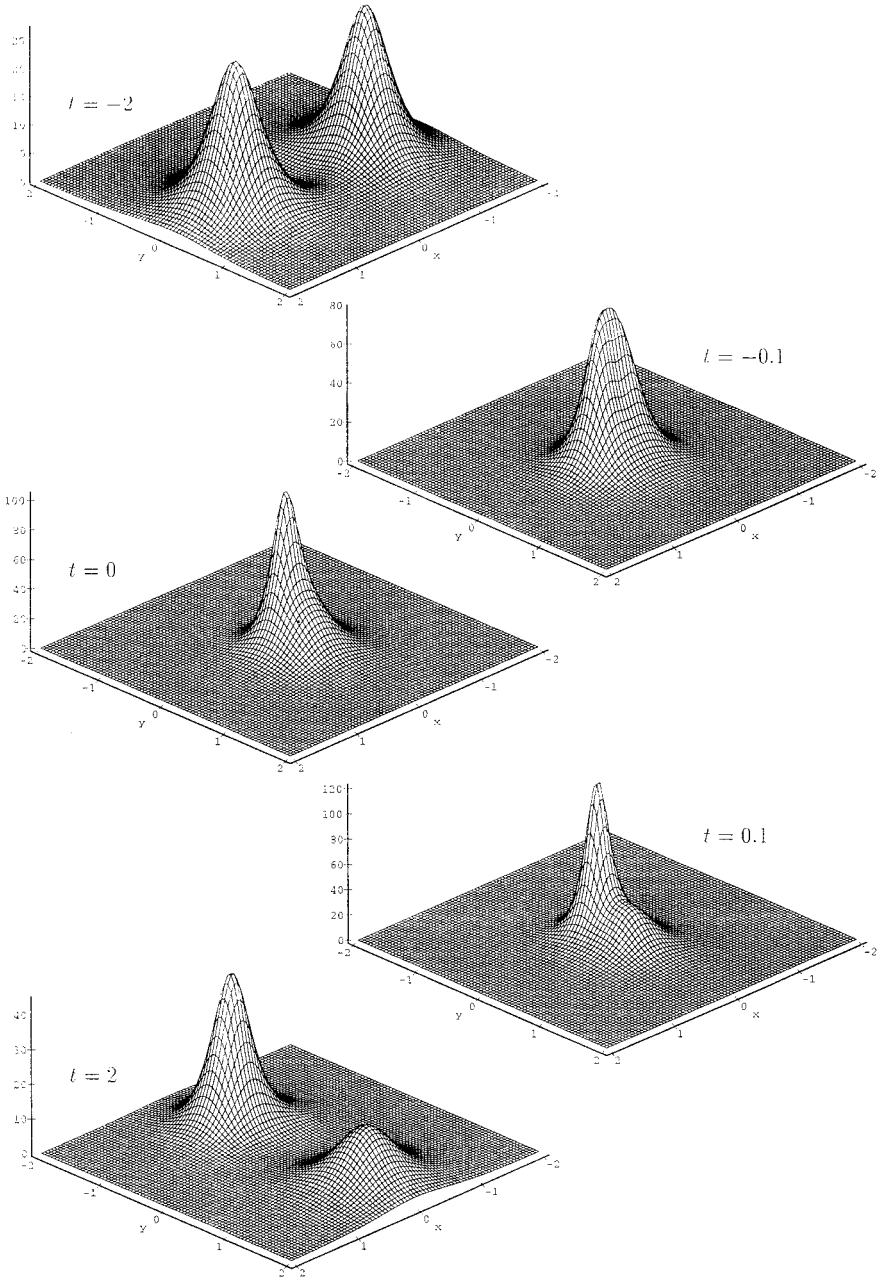

FIG. 6. Energy density at increasing times when $\psi(\lambda)$ has a triple pole (and no others).

the solution (8) with $n=2$, put $\mu_1=i+\epsilon$, $\mu_2=-i-\epsilon$, and take the limit $\epsilon\to 0$. In order for the resulting ψ to be smooth on $\mathbf{R}^{2+1}$, it is necessary to take $f_1=f(\omega_1)$, $f_2=-1/f(\omega_2)-\epsilon h(\omega_2)$, where f and h are rational functions of one variable. On taking the limit $\epsilon\to 0$, we then obtain a ψ as in (28) with $m^k=(m_1^k,m_2^k)$ being holomorphic functions of z (or $\overline{z}$), through the relations $m^1=(1,f)$, $m^2=(-f,1)$, while

$$n^1=\frac{2i(1+|f|^2)}{(1+|f|^2)^2+|w|^2}\,\overline{m^1}+\frac{2\overline{w}}{(1+|f|^2)^2+|w|^2}\,\overline{m^2},$$

$$n^2=-\frac{2w}{(1+|f|^2)^2+|w|^2}\,\overline{m^1}-\frac{2i(1+|f|^2)}{(1+|f|^2)^2+|w|^2}\,\overline{m^2}, \tag{29}$$

with

$$w\equiv\overline{hf}^2+2tf'. \tag{30}$$

So we generate a solution $J=\psi(\lambda=0)^{-1}$, which depends on the two arbitrary rational functions $f=f(z)$ and $h=h(\overline{z})$. This solution has the form

$$J=\frac{1}{(1+|f|^2)^2+|w|^2}\begin{bmatrix}|w|^2+2i(f\overline{w}+\overline{fw})-(1+|f|^2)^2 & -2i(w-f^2\overline{w})\\ -2i(\overline{w}-\overline{f}^2w) & |w|^2-2i(f\overline{w}+\overline{fw})-(1+|f|^2)^2\end{bmatrix}, \tag{31}$$

with w given by (30). In general, by taking $f(z)=z^p$ and $h(\overline{z})=\overline{z}^q$, where p is a positive integer and q is a non-negative integer; the energy, obtained by integrating (2), is $E=(2p+q)8\pi$. Roughly speaking, the solution looks like $(2p+q)$ lumps at arbitrary positions in the xy plane; which as we are going to see are a combination of solitons and antisolitons.

A topological charge may be defined for the field J (31) by exploiting the connection of it with the $O(3)$ σ-model. The unmodified chiral model [i.e., (1) with $V_\alpha=(0,0,0)$] is equivalent to the $O(4)$ σ-model[20] through the relation

$$J=I\phi_0+\mathbf{i}\boldsymbol{\sigma}\cdot\boldsymbol{\phi}, \tag{32}$$

where $\boldsymbol{\sigma}$ are the usual Pauli matrices and $(\phi_0,\boldsymbol{\phi})=(\phi_0,\phi_1,\phi_2,\phi_3)$ is a four vector of real fields that are constrained to lie on $\mathbf{S^3}$, i.e., $\phi_0^2+\boldsymbol{\phi}\cdot\boldsymbol{\phi}=1$. The only static finite energy solutions of the $O(4)$ σ- model correspond to the embedding of the $O(3)$ σ model.[21] Therefore the only static solutions of (1) are the $O(3)$ embeddings that we shall describe. This is because for the one-soliton solution (static or Lorentz boosted in the y axis) the term in (1) proportional to V_α is zero, so the system behaves like the $O(4)$ model, for which the $O(3)$ embedding is totally geodesic. [However, for time-dependent configurations, the term proportional to V_α is nonzero and will affect the evolution of the field, which will in general not lie in an $O(3)$ subspace of $O(4)$.]

To proceed further, let us mention the topological aspects of the $O(3)$ and $O(4)$ σ-models. In studying soliton-like solutions, we require that the field configuration has finite energy. This implies that the field must take the same value at all points of spatial infinity, so that space is compactified from $\mathbf{R^2}$ to $\mathbf{S^2}$. At fixed time, the field is a map from $\mathbf{S^2}$ into the target space. Now for the $O(3)$ model, the field is a map $\boldsymbol{\phi}$: $\mathbf{S^2}\to\mathbf{S^2}$, and due to the homotopy relation

$$\pi_2(\mathbf{S^2})=\mathbf{Z}, \tag{33}$$

such maps are classified by an integer winding number $\mathcal{N}$, which is a conserved topological charge. An expression for this charge is given by

$$\mathcal{N}=(8\pi)^{-1}\int \epsilon_{ij}\boldsymbol{\phi}\cdot(\partial_i\boldsymbol{\phi}\wedge\partial_j\boldsymbol{\phi})\;\; d^2x, \tag{34}$$

where $i=1,2$ with $x^i=(x,y)$.

Although, for the $O(4)$ model [the same argument is valid for (1) due to the topological aspects of the theory], the field at fixed time is a map $(\phi_0,\boldsymbol{\phi})$: $\mathbf{S^2}\to\mathbf{S^3}$ and the corresponding homotopy relation is

$$\pi_2(\mathbf{S^3})=0, \tag{35}$$

so there is no winding number. However, for soliton solutions that correspond to some initial embedding of $O(3)$ space into $O(4)$, there is a useful topological quantity, as we are going to see.

Consider the $O(4)$ configuration, which at some time corresponds to an $O(3)$ embedding, which we choose to be $\phi_0=0$ for definiteness. At this time the field is restricted to an $\mathbf{S^2}$ equator of the possible $\mathbf{S^3}$ target space. Suppose that the field never maps to the antipodal points $\{\mathscr{A}_1, \mathscr{A}_2\}=\{\phi_0=1,\ \phi_0=-1\}$ at any time, so the target space is $\mathbf{S_0^3}=\mathbf{S^3}-\{\mathscr{A}_1, \mathscr{A}_2\}$. Now $\mathbf{S_0^3}\approx\mathbf{S^2}\times\mathbf{R}$, and thus we have the homotopy relation

$$\pi_2(\mathbf{S_0^3})=\pi_2(\mathbf{S^2}\times\mathbf{R})=\pi_2(\mathbf{S^2})\oplus\pi_2(\mathbf{R})=\mathbf{Z}, \tag{36}$$

and therefore a topological winding number exists. An expression for this winding number is easy to give, since it is the winding number of the map after projection onto the chosen $\mathbf{S^2}$ equator, i.e.,

$$\mathscr{N}'=(8\pi)^{-1}\int \epsilon_{ij}\boldsymbol{\phi}'\cdot(\partial_i\boldsymbol{\phi}'\wedge\partial_j\boldsymbol{\phi}')\ d^2x, \tag{37}$$

where $\boldsymbol{\phi}'=\boldsymbol{\phi}/|\boldsymbol{\phi}|$. If the field does map to the antipodal points $\{\mathscr{A}_1, \mathscr{A}_2\}$ at some time the winding number is ill defined at this time, and if considered as a function of time $\mathscr{N}'$ will be integer valued but may suffer discontinuous jumps as the field moves through the antipodal points. In the following examples, before comparing the solution J given by (31) with the $O(3)$ embedding it is convenient to perform the transformation $J\to MJ$ with

$$M=(\sqrt{2})^{-1}\begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}, \tag{38}$$

so that the evolution of the field remains close to the $O(3)$ embedding.

V. SOLITON–ANTISOLITON SCATTERING

Usually in the nonintegrable models, there is an attractive force between solitons of opposite topological charge. In fact, if the solitons and antisolitons are well separated, then they attract each other and eventually annihilate into a wave of pure radiation, which spreads with the velocity of light.[3,4] However, the interaction forces between solitons and antisolitons do depend on their configuration; in particular, they depend on the relative orientation between them in the internal space. Therefore, the cross section for the soliton–antisoliton elastic scattering is nonzero. (In the real world, the proton–antiproton elastic scattering is seen in a reasonable fraction of cases.) This is the first example for which there has been constructed an explicit (since the system is integrable) solution of elastic soliton–antisoliton scattering in either integrable or nonintegrable model. As a result, it provides a major link between soliton dynamics in integrable and nonintegrable systems.

The evolution is initially similar to the numerical results obtained through the connection of the integrable chiral model (1) with the $O(3)$ σ-model.[20] In particular, a soliton and an antisoliton are moving along the x axis toward each other at an accelerating rate until they merge at the origin and form a peak. Note that a peak is formed rather than a ring since the energy is mainly kinetic when a soliton and an antisoliton merge. However, rather than the peak dissipating in a wave of radiation it now reforms into two new structures that undergo 90° scattering. In general, in all head-on collisions of N moving soliton and antisoliton objects, the scattering angle is π/N degrees relative to the initial direction of motion.

Next we looked at two cases corresponding to the mixtures of solitons and antisolitons. [The configurations given by (31) when $h(\overline{z})=0$ are equivalent to the ones obtained from **(13), (14)** when $f(z)=z^p$.]

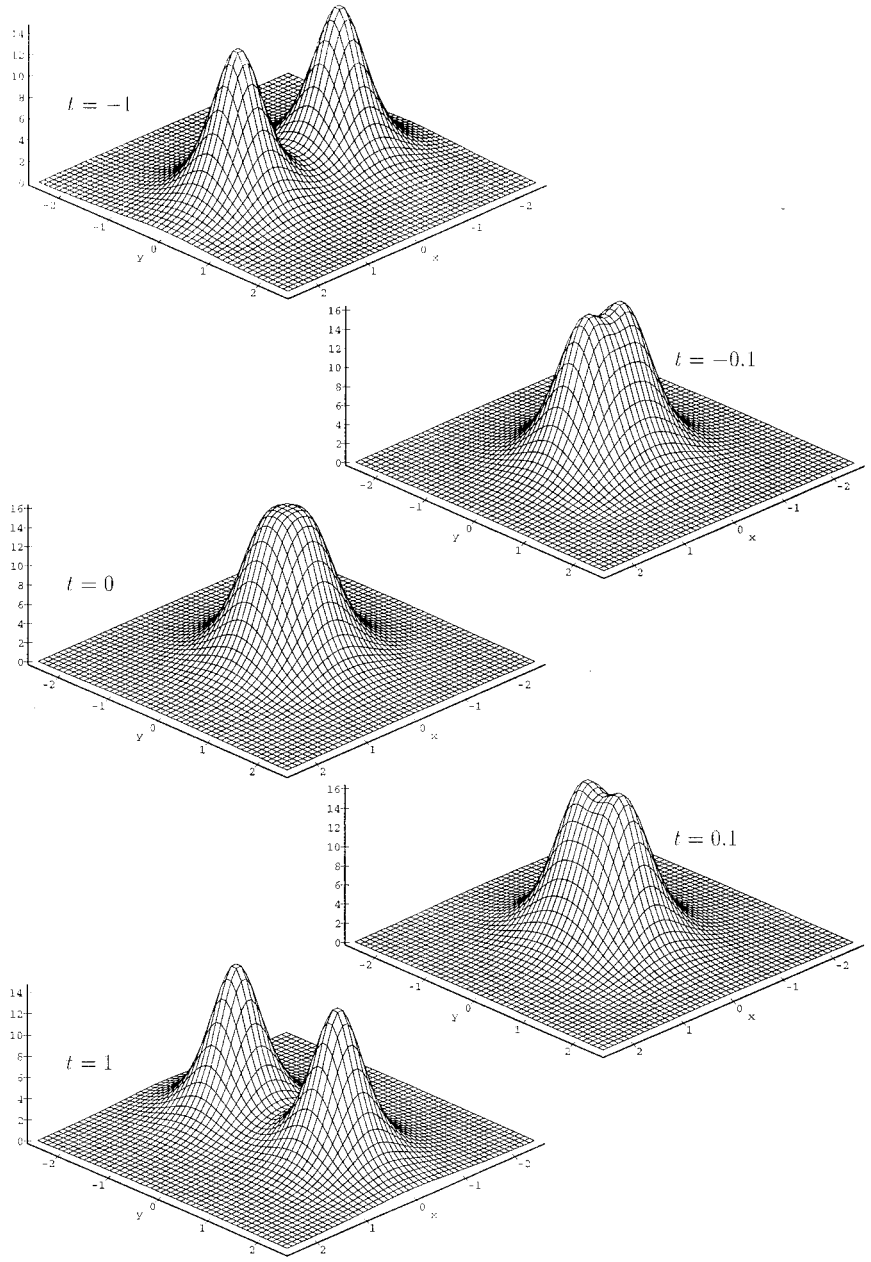

FIG. 7. Energy density at increasing times showing a 90° scattering between a soliton and an antisoliton.

• First, let us take $f(z)=z$ and $h(\overline{z})=1$. Roughly speaking, if r is large, J is close to its asymptotic value J_0, as long as $w/z^2=1+2t/z^2\approx 1$; but as z approaches $\pm\sqrt{-2t}$ then $w\to 0$, and J departs from its asymptotic value: this is where the two structures are located. More precisely, for negative t, the two objects are on the x axis, approximately at $x\approx\pm\sqrt{-2t}$; while for positive t, they are on the y axis, approximately at $y\approx\pm\sqrt{2t}$. Figure 7 illustrates what happens near $t=0$.

The picture is consistent with the properties of the energy density of the solution, which is

$$\mathscr{E}=16\,\frac{2r^4+4r^2+4t^2(1+2r^2)-4t(x^2-y^2)+1}{[2r^4+2r^2+4t(x^2-y^2)+4t^2+1]^2}. \tag{39}$$

Note the symmetry of $\mathscr{E}$ under the interchange $t\mapsto -t$, $x\rightleftharpoons y$; the time symmetry of the density confirms the lack of radiation. The corresponding localized structures are not, however, of constant size: for large (positive) t, their height is proportional to $1/t$, while their radius is proportional to $\sqrt{t}$.

The projected topological charge $\mathscr{N}'$ is zero throughout the scattering process; while the projected topological density q', i.e.,

$$\mathscr{N}'=\int q'\,dx\,dy, \tag{40}$$

has an almost identical distribution (up to a scale) to that of the energy density [see Fig. 8(a)]. Therefore, the configuration represents a soliton and an antisoliton that are clearly visible as distinct structures having, respectively, $+1$ and -1 units of topological charge concentrated in a singe lump.

Equation (1) is not Lorentz invariant and indeed is not even radially symmetric due to the presence of the vector V_a, which picks out a particular direction in space, and therefore one may expect to find different scattering behavior for more general solutions; e.g., when the soliton and the antisoliton are moving along the x axis rather that the y axis. However, this is not true since (1) is a reduction of the self-dual Yang–Mills equation in $\mathbf{R}^{2+2}$, which does have an SO(1,2) symmetry. Therefore, the SO(2) symmetry of the Yang–Mills system means that any given solution J, can, in principle, be converted to gauge fields by performing a coordinate rotation (together with a gauge transformation) and then recover the corresponding J' that will describe the same solution as J, but with a rotated coordinate system. Indeed, this is what happens by taking

$$f(z)=e^{(2i\phi)}z, \quad h(\overline{z})=1, \tag{41}$$

where ϕ is an angle in the xy-plane. This picture presents a rotated version through any angle ϕ in the xy plane of the original one (i.e., Fig. 7).

• Finally, let us take $f(z)=z$, and $h(\overline{z})=\overline{z}$. The corresponding configuration consists of one soliton and two antisolitons [see Fig. 8(b)].

It is interesting to look at the time dependence of various energies in each process. The total energy, of course, is constant and it is the spatial integral of the following energy density:

$$\mathscr{E}=8[r^8+8r^6+11r^4+4r^2-8x^5t+16ty^2(x^3+t)+8t^2+48xy^2t+2-16x^2t(x-t)+24xty^4]/$$
$$[r^6+r^4+2r^2+4t^2+4tx^3-12xy^2t+1]^2. \tag{42}$$

Obviously, the energy density $\mathscr{E}$ is symmetric under the interchange $t\mapsto -t$, $x\mapsto -x$, and $y\mapsto -y$, only. Again all three structures come together, forming a bell-like structure, and then emerge at an angle of 60° with respect to the original direction. However, by looking at the maximum of $\mathscr{E}$ we observe that, for large (positive) t, the height of the localized structures is proportional to $t^{-4/3}$, while their radius is proportional to $t^{1/3}$; thus they spread out as they move apart.

Figure 9 shows the results of a head-on collision of the one-soliton two-antisoliton system.

Let us conclude with the observation that, by taking $f(z)=z^p$ and $h(\overline{z})=\overline{z}^{\,q}$, J departs from its asymptotic value J_0 when $w=z^{p-1}(2tp+z^N)\to 0$ with $N=p+q+1$, which is true when either $z^{(p-1)}=0$ or $2tp+z^N=0$: this is approximately where the lumps are located. Therefore, J represents a family of a soliton–antisoliton solution, which consists of $(p-1)$ static soliton-like objects at the origin, with N others accelerating toward them, scattering at an angle of π/N, and then decelerating as they separate.

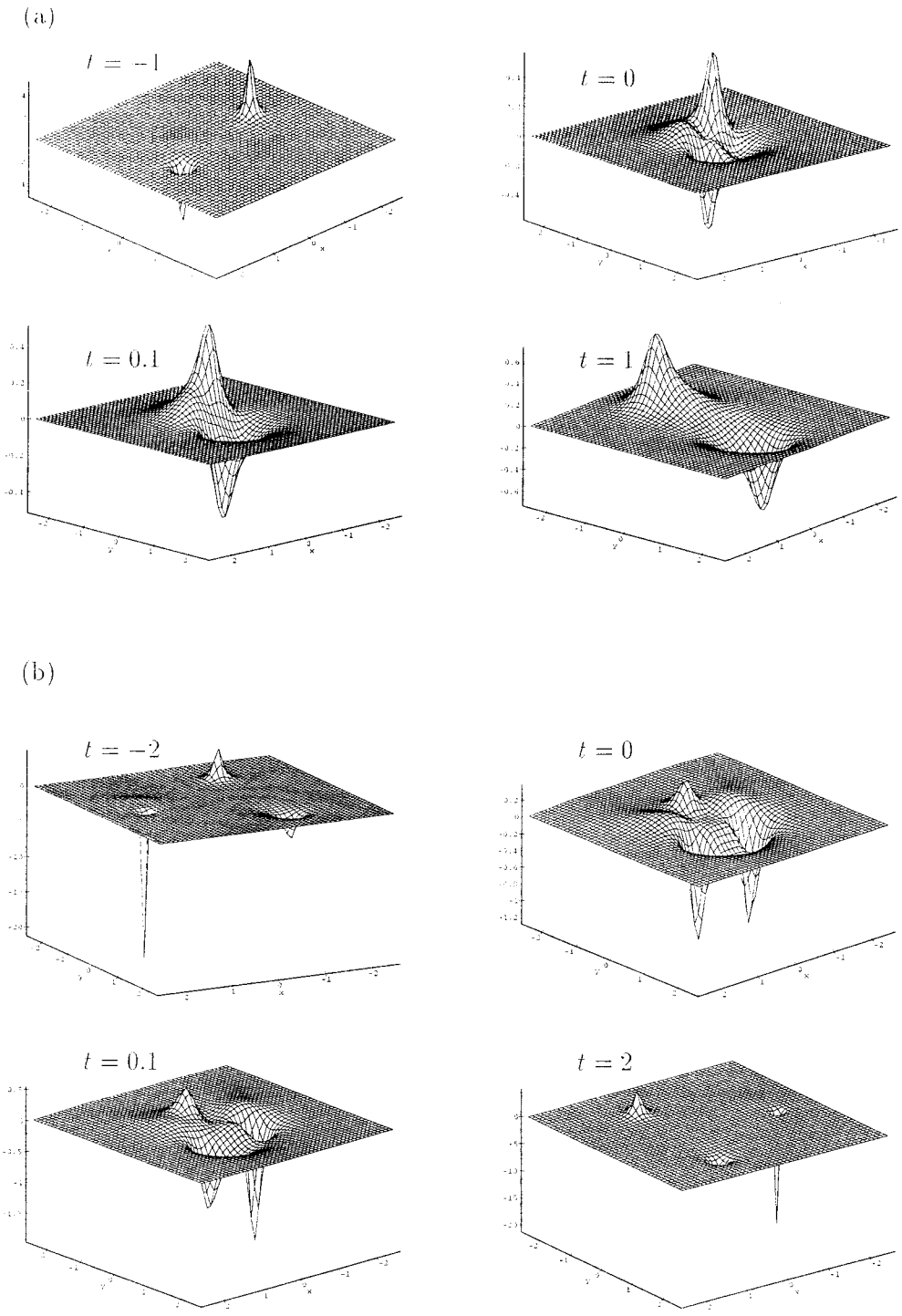

FIG. 8. Topological charge density at increasing times for (a) soliton–antisoliton scattering and (b) one-soliton two-antisoliton scattering.

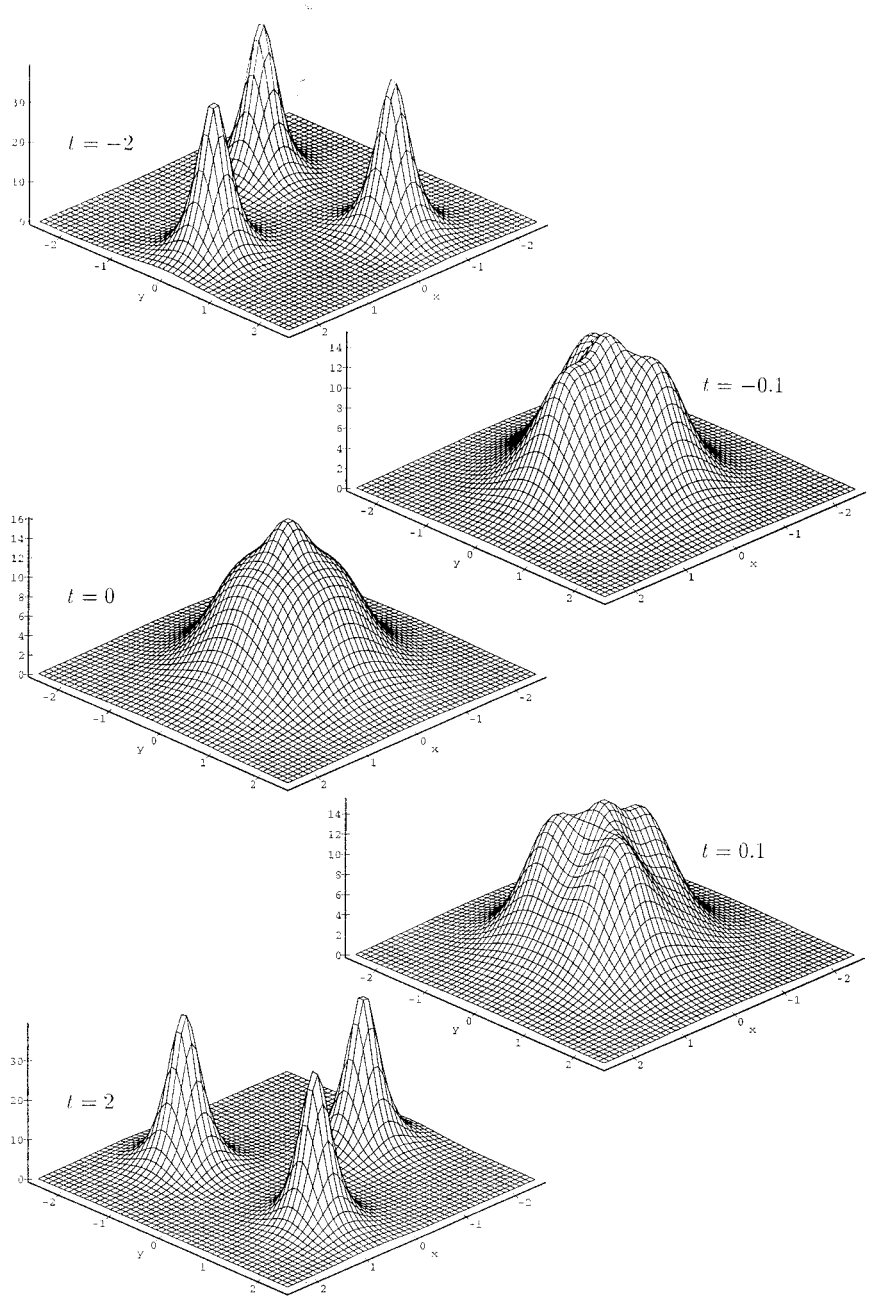

FIG. 9. Energy density of a system consisting of a soliton and two antisolitons at various times.

VI. CONCLUSION

The infinite number of conservation laws associated with a given integrable system place severe constraints upon possible soliton dynamics. The construction of exact analytic multisoliton solutions with trivial scattering properties is a result of such integrability properties. In this paper new soliton and soliton–antisoliton solutions have been obtained for the planar integrable chiral model (1). These structures travel with nonconstant velocity; their size is nonconstant; and they

interact nontrivially. Such results might be useful for connecting integrable and nonintegrable systems, which possess soliton solutions. In addition, they indicate the likely occurrence of new phenomena in higher-dimensional soliton theory that are not present in $(1+1)$ dimensions.

It seems likely that there are many more interesting solutions still to be found; an open question being what is the general form of the function ψ when it has a higher-order pole in λ. One could, for example, investigate the case $n=3$ for $\psi(\lambda)$ with a single and a double pole; and determine the scattering properties of the emerging structures, in terms of their initial velocity and of the values of the impact parameter. Finally, it would be of great interest to deduce the general form of the function $\psi(\lambda)$ for the soliton–antisoliton case (28) with the only constraint to satisfy the reality condition (5) and the requirement that the matrices $A=(L\psi)\psi^{-1}$ and $B=(M\psi)\psi^{-1}$ be independent of λ.

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Variational method: How it can generate false instabilities

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When the variational method is applied to nonlinear evolution equations for determining solitary wave dynamics, it is possible for the method to predict the pulse to be unstable when in fact it is stable. We determine the necessary conditions for this to occur as well as give sufficient conditions for avoiding such false instabilities. We also discuss the general problem of applying the method to a general evolution equation. © *1996 American Institute of Physics.* [S0022-2488(96)03406-8]

I. INTRODUCTION

In this work we determine the necessary conditions under which the Rayleigh–Ritz variational method could give rise to false instabilities when applied to the study of the dynamics of solitary waves propagating in one spatial dimension. We also give sufficient conditions in order to avoid such false instabilities.

The variational method was probably first used to study the dynamics of a solitary wave in Ref. 1. First we will briefly describe the essence of this method. Suppose one is given an evolutional partial differential equation (PDE)

$$\vec{u}_t + \vec{N}[\vec{u}] = 0, \tag{1.1}$$

where $\vec{u}(x,t) = (u_1(x,t),\ldots,u_n(x,t))^T$, $\vec{N}$ is a nonlinear operator containing derivatives with respect to the space coordinate, x, and t is the evolutional coordinate. In most cases, one is unable to obtain an exact solution of (1.1), other than the trivial solution, analytically. Then one can employ the variational method to obtain an approximate analytical solution to the equation of interest. Here we will only be concerned with the solitary wave, or pulse solutions, $\vec{u}_0(x,t)$, such that $|\vec{u}_0(x,t)|$ depends only on the single variable $\theta = (x - Vt)$, with V being constant, and $\vec{u}_0(|\theta| \to \infty) \to 0$ (the center of the pulse is at $\theta = 0$). To apply the variational method, one first takes a trial function, also called an ansatz, which is not necessarily a solution of (1.1) but still has the main characteristics of a pulse. Namely, it is usually bell-shaped (for example, a Gaussian), where its parameters can be put into correspondence with the pulse's amplitude, width, phase, etc. These parameters, called the ''variational parameters,'' are allowed to change with the time. Then one inserts the ansatz into the Lagrangian density corresponding to Eq. (1.1) and integrates it over x. The resulting function is a reduced Lagrangian, which depends explicitly on the variational parameters and possibly on the time. Finally, one uses the reduced Lagrangian to derive the Euler–Lagrange equations for the variational parameters. Thus, the study of the dynamics of the solitary pulse of the original PDE is reduced to solving a finite number of *ordinary* differential equations (ODE) and/or algebraic equations.

It is clear that the variational method is merely an optimization procedure: It allows one to determine the ''optimal'' parameters of a pulse, with the ansatz for the pulse's shape being prescribed by the researcher. The limitations of the variational method do not clearly follow from the initial assumption, as is the case with ''rigorous'' methods, such as perturbation methods.

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Thus, it is the purpose of this paper to expose possible ''dangers'' which can arise in applications of the variational method as well as to show how these ''dangers'' can be avoided.

After Ref. 1, where the variational method was applied to the analysis of the dynamics of the soliton of the nonlinear Schrödinger equation (NLS), this method has been used in many other works (see, for example, Ref. 2 and references therein). It has been mostly applied to the NLS-type equations (or systems of coupled equations); its results were usually checked against a numerical solution or a solution obtained by other means, and the variational method has been found to work reasonably well. However in Ref. 3, Malomed and Tasgal reported that they had applied the variational method to the equations of the Massive Thirring Model (MTM) [see Eqs. (3.1) in Sec. III] and discovered that in a certain sector of the parameter space, the method failed to give reasonable results for any, even small, times. Namely, they took an ansatz which was a sum of the exact one-soliton solution of the MTM *plus* some small variation localized around the soliton, with this variation being of a rather general form. For some range of the soliton's parameters they found that certain components of this variation grew exponentially in time. Thus, the variational method indicated that the MTM soliton was unstable. However, since the MTM is integrable by the method of the inverse scattering transform (IST) in $1+1$ dimensions (with the ground state $u=v\equiv 0$ being stable), this is known to be untrue. In fact, our own numerical integration of Eqs. (3.1) with different near-soliton initial conditions revealed no instability. For this reason, the instability obtained in Ref. 3 can be called a ''*false* instability.''

It is of interest to understand how and why such false instabilities of a solitary wave can arise with the variational method. It is also important to determine the conditions which one needs to impose on the ansatz in order to avoid the false instability, if such occurs. Thus, let us now give a definition of stability or instability of a solitary wave, which we will use in this paper.

When one linearizes (1.1) about an exact solution, $\vec{u}_0(x,t)$, there results a linear PDE of the form:

$$\vec{\mathbf{v}}_t + L\vec{\mathbf{v}} = 0, \tag{1.2}$$

where $\vec{\mathbf{v}} = (\delta u_1, \delta u_1^*, \ldots, \delta u_n, \delta u_n^*)^T$, and the linear operator $L = (\delta \vec{N}[\vec{u}]/\delta \vec{u})|_{\vec{u}=\vec{u}_0}$. One needs to include the complex conjugates, δu_j^*, in $\vec{\mathbf{v}}$, because, in general, $\vec{N}[\vec{u}]$ may depend on $\vec{u}^*$. Letting then $\vec{\mathbf{v}}(x,t) = \vec{\mathbf{v}}(x)e^{-i\lambda t}$, one obtains from (1.2) an equation defining the eigenmode corresponding to the eigenvalue λ. These eigenmodes fall into two general classes. First, for real λ, there is a continuous spectrum, where far from the solitary wave, the modes become plane waves, $e^{ik(\lambda)x}$. Second, there is also the discrete spectrum consisting of several localized (square integrable) modes, which exist, usually, for $\lambda = 0$, and may also exist for some complex λ. The former discrete spectrum modes are the so-called ''neutral'' modes, and they correspond to the shift of the solitary wave's parameters. If in the spectrum of (1.2) there is a localized mode with $\mathrm{Im}\,\lambda > 0$, we will call both this mode and the solitary wave unstable; otherwise, they will be called stable.

Let us now state the assumptions that we make in our analysis. First, we consider a force-free motion of a solitary wave, thus all the nontrivial dynamics is due to the difference of the pulse's initial profile from the exact solution. Second, throughout the paper we assume that the form of the exact solution is known and consider only *small* (in L_2-norm) ''perturbations'' about it. Thus, expansion of such ''perturbations'' over the set of eigenmodes of (1.2) becomes relevant. In the concluding section we discuss how our analysis can be generalized if the above two assumptions are relaxed.

A general form of the ansatz representing a solution close to the exact solution $\vec{u}_0(x,t)$ is

$$\vec{u}_{\mathrm{close}}(x,t) = \vec{u}_0(x,t;\alpha_1(t),\ldots,\alpha_n(t)), \tag{1.3}$$

where one obtains $\vec{u}_0(x,t)$ upon setting all the variational parameters $\alpha_j(t)$ to zero. Without loss of generality, the α's may be taken to be real. By assumption, the α's are to be small, and then we have

$$\vec{u}_{\text{close}}(x,t)-\vec{u}_0(x,t)\approx\sum_{j=1}^{n}\alpha_j(t)\left.\frac{\partial\vec{u}}{\partial\alpha_j}\right|_{(\alpha_1,\ldots\alpha_n)=0}\equiv\sum_{j=1}^{n}\alpha_j(t)\vec{u}_{,j}(x). \tag{1.4}$$

Thus we will take the ansatz in the form:

$$\vec{u}_{\text{var}}(x,t)=\sum_{j=1}^{n}\alpha_j(t)\vec{u}_{,j}(x). \tag{1.5}$$

The quantities $\vec{u}_{,j(x)}$ will be referred to as variations. Since the α_j's are small, then the resulting Euler–Lagrange equations will be linear ODEs, with the coefficients being fixed by the choice of the variations. If this system has complex normal frequencies, it means that, according to the variational method, the solitary wave solution in question is unstable. Suppose one can prove by some means, other than the variational method, that the spectrum of the corresponding equation (1.2) does not contain eigenvalues with Im $\lambda>0$. Then we pose the following questions: (1) what is the mechanism by which the variational method can introduce a false instability for a given evolution equation? and (2) if a false instability can occur in a given problem, then how can one choose the ansatz in order to avoid the false instability?

We show that there are two mechanisms (one or the other is necessary, but neither is sufficient) by which a variational ansatz could introduce a false instability. First, any variation, $\vec{u}_{,j}(x)$, will always be some linear combination of the discrete and/or continuous modes of (1.2). Then, (1.5) requires that every mode contained in a given variation execute a common motion with the others, bound in the same variation. Consequently, we find that one mechanism by which an ansatz could introduce a *false* instability is for the variations to couple discrete modes to continuous modes. An example of this will be given later. Fortunately, this type of a false instability is easy to avoid or eliminate, as we shall see later.

The second mechanism for generating a false instability requires that a certain inner product of the continuous spectrum eigenfunctions be sign indefinite. In this case, there are two ''spaces'' of (the continuous spectrum) eigenfunctions, distinguished by the sign of that inner product. Thus, a false instability can occur via the second mechanism if a variation in the ansatz mixes the eigenfunctions from the two ''spaces.'' We remark here that the importance of having certain functionals positive definite, when studying stability of solitary wave solutions, was emphasized in a number of works.[4–6] However, in those works, no connection was established with the variational method in the form being discussed in this paper.

The rest of the paper is organized as follows. In Sec. II, we consider the case of the NLS. Here we show that if a variation couples discrete and continuous modes, then a false instability can occur via the first mechanism. However, in the case of the NLS it was shown (Ref. 7) that all the discrete spectrum modes are neutral modes, i.e., they correspond to the shifts of each of the soliton's independent parameters. Then we prove that, by allowing each and every of the soliton's parameters to vary independently of the others, one decouples the continuous and discrete spectrum modes, thereby eliminating the possibility for a false instability to occur via the first mechanism. This fact also explains why a false instability has never been found for the NLS-type equations, although the explicit decomposition of the discrete and continuous spectra was never done in the previous studies. Finally in this section we sketch a procedure by which one can construct a variational ansatz that does not contain the neutral modes. This procedure allows one to reduce the number of variational parameters in the ansatz by, naturally, exactly the number of the neutral modes.

In Sec. III, we analyze the MTM equations. Here we have an example where the continuous modes form two ''spaces.'' Therefore, a false instability for the MTM could arise via the second mechanism. This is the source of the result which Malomed and Tasgal found in Ref. 3. Conse-

quently, a simple method for avoiding false instabilities in this case would be to separate the eigenmodes belonging to the different ''spaces'' into different variations of the ansatz.

One should note that we have considered in this paper only equations integrable by the IST. This fact enabled us to completely determine the spectra of the corresponding linearized equations. In particular, we knew beforehand that there were no unstable modes. We address the general case, i.e., when the latter may be present, in the concluding section.

In Sec. IV, we show that there is a method to avoid false instabilities which could arise via the second mechanism, *without* being forced to separate the two ''spaces'' of the eigenfunctions. However, for nonlinear evolutional equations, the application of this simple method is tantamount to having the exact solution before one begins to construct a variational solution. Also in Sec. IV, we obtain a formula which elucidates the meaning of the results produced by the variational method for a particular choice of the ansatz.

In the concluding section we discuss how one can apply our approach when the exact solitary wave solution is not known, as well as what information one can glean if completeness of the corresponding set of eigenfunctions is not established. In the latter case we show that the variational method can be used to detect a *true* instability of the solitary wave. We also mention the generalization of our analysis when a solitary wave is driven by an external force.

II. THE NLS CASE

First, we consider the NLS in the following form:

$$iu_t+u_{xx}+2u|u|^2=0. \tag{2.1}$$

Its exact one-soliton solution is well known:

$$\begin{gathered} u_0(x,t|V)=A\ \text{sech}\ \theta\ \exp\left\{\frac{iV}{2A}\ \theta+i\left(A^2+\frac{V^2}{4}\right)t+i\varphi_0\right\}, \\ \theta=A(x-Vt-x_0), \end{gathered} \tag{2.2}$$

where the parameters A,V,x_0,φ_0 are constants. One can always eliminate V by the Galilean transformation, so we will take $V=0$ in what follows and denote $u_0(x,t)\equiv u_0(x,t|0)$. We still will need expression (2.2) with $V\neq 0$ later on in this section.

A variational ansatz which is usually taken to study small oscillations of the exact soliton of the NLS is the following:

$$u_{\text{var}}(x,t)=\epsilon u_0(x,t)[\,\delta\eta(t)+i\,\delta\varphi(t)+\delta A(t)\,\theta\ \tanh\ \theta+i\,\delta c(t)\,\theta^2], \tag{2.3a}$$

where $\epsilon\ll 1$; compare (2.3a) with (1.5). Here, $\delta\eta(t)$ is the variational parameter for the soliton's amplitude, $\delta\varphi(t)$—the variational parameter for its overall phase, $\delta A(t)$—the variational parameter for the width, and $\delta c(t)$ is the variational parameter for the chirp. The variations corresponding to these parameters are:

$$\begin{gathered} \delta u_{(\delta\eta)}=1\cdot u_0, \quad \delta u_{(\delta A)}=\theta\ \tanh\ \theta\cdot u_0, \\ \delta u_{(\delta\varphi)}=i\cdot u_0, \quad \delta u_{(\delta c)}=i\,\theta^2\cdot u_0. \end{gathered} \tag{2.3b}$$

Two other parameters, the coefficient of the linear phase (frequency shift) and the soliton's center coordinate are not included in (2.3) because the equations for them decouple from those for $\delta\eta,\delta\varphi,\delta A,\delta c$. At the end of this section we will show how, basing on our method, one can construct an ansatz with only *two* parameters, which, however, provides more correct description of the soliton oscillations.

The Lagrangian density for Eq. (2.1) is

$$\mathscr{L}\equiv\mathscr{L}^{\mathrm{NLS}}=\frac{i}{2}\,(u_t^*u-u^*u_t)-|u_x|^2+|u|^4. \tag{2.4}$$

With the aim in mind to study the dynamics of small variations on the background of soliton (2.2), we substitute in (2.4) $u=u_0+\delta u(x,t)$, with $|\delta u|\ll|u_0|$. Then in the main order in δu we obtain:

$$\mathscr{L}_2\equiv\mathscr{L}_2^{\mathrm{NLS}}=\tfrac{1}{2}\,\vec{\mathbf{v}}^{\dagger}\sigma_3(i\partial_t+A^2L)\vec{\mathbf{v}}, \tag{2.5}$$

where

$$\vec{\mathbf{v}}\equiv\begin{pmatrix}\mathbf{v}_1\\ \mathbf{v}_2\end{pmatrix}=\begin{pmatrix}\delta u\ e^{-iA^2t}\\ \delta u^*\ e^{iA^2t}\end{pmatrix}, \tag{2.6a}$$

$$L\equiv L^{\mathrm{NLS}}=\sigma_3(\partial_\theta^2-1)+2\,\mathrm{sech}^2\,\theta\ \ (2\sigma_3+i\sigma_2). \tag{2.6b}$$

If $u(x,t)=u_0+\delta u$ is a solution of (2.1), then the vector $\vec{\mathbf{v}}$ satisfies the equation

$$(i\partial_t+A^2L)\vec{\mathbf{v}}=0, \tag{2.7}$$

which is the linearization of (2.1) on the background of the soliton. Therefore we seek a solution of (2.7) as an expansion over the set of the eigenfunctions of the following eigenvalue problem:

$$L\vec{\mathbf{v}}=\lambda\vec{\mathbf{v}}, \tag{2.8}$$

with L given by (2.6b). The solution to this problem was given in Ref. 7 and is as follows. The basis in the class of functions which are sufficiently smooth and decay sufficiently rapidly at infinity (i.e., in the Schwartz class) is formed by the continuous spectrum of the operator L:

$$\psi_1(k)=\left[\left(1-\frac{2ike^{-\theta}}{(k+i)^2\,\cosh\,\theta}\right)\begin{pmatrix}0\\1\end{pmatrix}+\frac{1}{(k+i)^2\,\cosh^2\,\theta}\begin{pmatrix}1\\1\end{pmatrix}\right]e^{ik\theta},$$

$$\psi_2(k)=\left[\left(1+\frac{2ike^{-\theta}}{(k-i)^2\,\cosh\,\theta}\right)\begin{pmatrix}1\\0\end{pmatrix}+\frac{1}{(k-i)^2\,\cosh^2\,\theta}\begin{pmatrix}1\\1\end{pmatrix}\right]e^{-ik\theta},$$

$$\text{for real}\ \ k, \tag{2.9a}$$

such that

$$L\psi_1=(k^2+1)\psi_1,\quad L\psi_2=-(k^2+1)\psi_2; \tag{2.9b}$$

and also the discrete spectrum of L:

$$\phi_1=\begin{pmatrix}1\\-1\end{pmatrix}\mathrm{sech}\,\theta,\quad \phi_2=\begin{pmatrix}1\\1\end{pmatrix}\mathrm{sech}\,\theta\,\tanh\,\theta, \tag{2.10a}$$

where

$$L\phi_1=L\phi_2=0, \tag{2.10b}$$

and

$$\phi_1^{\mathscr{J}}=\begin{pmatrix}1\\1\end{pmatrix}(\theta\tanh\theta-1)\operatorname{sech}\theta,\quad \phi_2^{\mathscr{J}}=\begin{pmatrix}1\\-1\end{pmatrix}\theta\operatorname{sech}\theta, \tag{2.11a}$$

with

$$L\phi_j^{\mathscr{J}}=-2\phi_j,\quad j=1,2. \tag{2.11b}$$

An arbitrary two-component vector $\vec{\mathbf{w}}(\theta)=(\mathbf{w}_1,\mathbf{w}_2)^T$ from $L_2(-\infty,\infty)$ can be expanded over this basis as follows:[7]

$$\vec{\mathbf{w}}(\theta)=\int_{-\infty}^{\infty}dk(g_1(k)\psi_1(k,\theta)+g_2(k)\psi_2(k,\theta))+\sum_{j=1,2}(\beta_j\phi_j+\gamma_j\phi_j^{\mathscr{J}}), \tag{2.12}$$

where $g_j(k),\beta_j,\gamma_j$, $j=1,2$, are the scalar expansion coefficients. We note that $\phi_{1,2}^{\mathscr{J}}$, as it is seen from (2.11b), are not eigenfunctions of the operator L. They are the so-called associate, or derivative states (see Ref. 7), and are required for completeness because the operator L is not self-adjoint.

The fact that one was able to find the explicit form of the eigenfunctions of (2.8), as well as to prove the completeness of the corresponding set, has its origin in that the NLS is integrable by the IST. In general, for the operator L corresponding to an arbitrary nonlinear evolution equation, one is not able to find the eigenfunctions explicitly. However, in what follows it will be clear that for our purpose the only essential information, furnished by the IST, is that the set of eigenfunctions of L (including the associate states) forms a basis in the appropriate space of functions. The rest of the required information can be extracted from the asymptotics (for $|\theta|\to\infty$) of L. The latter does not depend on the integrability of the evolution equation under study and therefore can be found for an equation of a rather general form, with the only possible information missing being the completeness of the corresponding set of eigenfunctions. In Sec. V we will discuss how one can proceed with our approach if one does not know whether the set of eigenfunctions is complete or not.

Thus, we will come back to Eq. (2.8) and proceed as though if we did not know the explicit form of the eigenfunctions. The purpose of doing this is to demonstrate how our procedure can be applied to evolution equations, for which an exact form of the eigenfunctions is not available. To this end, let us first notice that the operator L has the following symmetry:

$$\sigma_1 L\sigma_1=-L=-L^*. \tag{2.13}$$

Let us emphasize that this symmetry exists since, from the definition of $\vec{\mathbf{v}}$, it follows that

$$\vec{\mathbf{v}}=\sigma_1\vec{\mathbf{v}}^*. \tag{2.14}$$

Consequently, if ψ is a solution of (2.8) with the eigenvalue λ, then

$$\psi_2(k)=\sigma_1\psi_1(k)^* \tag{2.15}$$

is another solution with the eigenvalue $-\lambda$. (Since L is real valued, we could have as well used $\psi_2=\sigma_1\psi_1$; we used (2.15) instead because it will be a convenient form later.) From the asymptotics of L, one finds the asymptotic form of the eigenfunctions, say, at $\theta\to-\infty$:

$$\underline{\theta\to-\infty}\quad \psi_1\to\begin{pmatrix}0\\1\end{pmatrix}e^{ik\theta},\quad \psi_2\to\begin{pmatrix}1\\0\end{pmatrix}e^{-ik\theta}. \tag{2.16}$$

Also from the asymptotics, one finds the eigenvalues corresponding to real k:

$$\lambda \equiv \lambda_{\psi_1} = k^2 + 1, \quad \lambda_{\psi_2} = -(k^2+1), \tag{2.17}$$

which is consistent with (2.9). The asymptotics of $\psi_{1,2}$ at the other end, $\theta \to +\infty$, can be obtained from the asymptotics of L only in the following general form:

$$\underline{\theta \to +\infty} \quad \psi_1 \to a(k) \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{ik\theta} + b(k) \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{-ik\theta}, \tag{2.18}$$

with some coefficients $a(k)$, $b(k)$. [Note that the first component of ψ_1 must be zero in order that the first equation of (2.9b) be satisfied.] We address the general case (2.18) in Appendix A. Below in this section we will make use of the well-known fact that the soliton (2.2) is a reflectionless potential in the corresponding scattering problem in the IST. Then it follows that in (2.18) $|a(k)| = 1$, $|b(k)| = 0$. This is of course consistent with the explicit form (2.9) of $\psi(k)$, with $a(k) = [(k-i)/(k+i)]^2$. Using this will significantly simplify the calculations. The result found in Appendix A is qualitatively the same as that of this section.

As for the discrete spectrum, this can be easily found explicitly. Let us denote $\overline{u_{(0)}} = u_0(x,t)e^{-iA^2t}$. Then, by differentiating the equation for $\overline{u_0}$, one observes that

$$\phi_1 \equiv \left(-i \frac{\partial}{\partial \varphi_0} \overline{u_0}, \ \text{c.c.} \right)^T, \quad \phi_2 \equiv \left(\frac{\partial}{\partial x_0} \overline{u_0}, \ \text{c.c.} \right)^T \tag{2.19a}$$

satisfy (2.10b), and

$$\phi_1^{\mathscr{D}} \equiv \left(\frac{\partial}{\partial A} \overline{u_0}, \ \text{c.c.} \right)^T, \quad \phi_2^{\mathscr{D}} \equiv \left(-i \frac{\partial}{\partial V} \overline{u(x,t|V)} \Big|_{V=0}, \ \text{c.c.} \right)^T \tag{2.19b}$$

satisfy (2.11b). We remark that in the last expression in (2.19b) one should set $\partial_V \theta \equiv 0$. Thus, the discrete spectrum modes correspond to the shift of the soliton's parameters.

Inserting (2.12) into (1.5), one has

$$\vec{\mathbf{v}}_{\text{var}} = \sum_{j=1}^{n} \alpha_j(t) \left\{ \int_{-\infty}^{\infty} dk [g_{1j}(k)\psi_1(k,\theta) + g_{2j}(k)\psi_2(k,\theta)] + \sum_{m=1,2} (\beta_{mj}\phi_j + \gamma_{mj}\phi_j^{\mathscr{D}}) \right\}. \tag{2.20}$$

From (2.14), (2.15), and (2.20), one finds

$$g_{2j}(k) = g_{1j}^*(k), \quad j = 1,\ldots n;$$

$$\text{Re}(\beta_{1j}) = \text{Re}(\gamma_{2j}) = 0 = \text{Im}(\beta_{2j}) = \text{Im}(\gamma_{1j}). \tag{2.21}$$

To calculate the reduced Lagrangian

$$\langle \mathscr{L}_2 \rangle \equiv \int_{-\infty}^{\infty} dx \ \mathscr{L}_2,$$

we need certain inner products between the eigenfunctions of L. These can be obtained in a standard manner from the Wronskian relation. Namely, from the equation

$$\phi^A(\lambda', \theta)L = \lambda' \phi^A(\lambda', \theta),$$

which is adjoint to (2.8), Eq. (2.8) itself, and (2.6b) one finds

$$\partial_\theta W(\phi^A(\lambda',\theta),\phi(\lambda,\theta)) \equiv \partial_\theta(\partial_\theta\phi^A(\lambda',\theta)\sigma_3\phi(\lambda,\theta) - \phi^A(\lambda',\theta)\sigma_3\partial_\theta\phi(\lambda,\theta))$$
$$= (\lambda'-\lambda)\phi^A(\lambda',\theta)\phi(\lambda,\theta), \tag{2.22}$$

where $\phi(\lambda,\theta)$ is a solution of (2.8). From the explicit form of L it follows that one can choose

$$\phi^A(\lambda,\theta) = \phi^\dagger(\lambda,\theta)\sigma_3. \tag{2.23}$$

Then from (2.22)–(2.23), (2.16)–(2.17), and (2.10)–(2.11), one obtains that the only nonzero inner products between the eigenfunctions of L are the following ones:

$$\langle\psi_1^\dagger(k')|\sigma_3|\psi_1(k)\rangle = -\langle\psi_2^\dagger(k')|\sigma_3|\psi_2(k)\rangle = -2\pi\delta(k-k'), \tag{2.24a}$$

$$\langle\phi_1^\dagger|\sigma_3|\phi_1^{\mathscr{S}}\rangle = -\langle\phi_2^\dagger|\sigma_3|\phi_2^{\mathscr{S}}\rangle = -2, \tag{2.24b}$$

where

$$\langle\psi_1^\dagger(k')|\sigma_3|\psi_1(k)\rangle = \int_{-\infty}^{\infty} d\theta\ \psi_1^\dagger(k',\theta)\sigma_3\psi_1(k,\theta),$$

etc. Using (2.5), (2.20), (2.24), and (2.21), one finds

$$\langle\mathscr{S}_2\rangle = \sum_{j,l=1}^{n}\{i\alpha_l\dot{\alpha}_j(\langle g_{1j}|g_{1l}\rangle - \langle g_{1l}|g_{1j}\rangle) - \alpha_l\alpha_j A^2(\langle g_{1j}|\lambda|g_{1l}\rangle + \langle g_{1l}|\lambda|g_{1j}\rangle)$$
$$+ i\alpha_l\dot{\alpha}_j(\beta_{1l}\gamma_{1j} - \beta_{1j}\gamma_{1l} + \beta_{2l}\gamma_{2j} - \beta_{2j}\gamma_{2l}) + 2\alpha_l\alpha_j A^2(\gamma_{1l}\gamma_{1j} + \gamma_{2l}\gamma_{2j})\}, \tag{2.25}$$

where now

$$\langle f|h\rangle = \pi\int_{-\infty}^{\infty} dk\ f^*(k)h(k), \quad \langle f|m|h\rangle = \pi\int_{-\infty}^{\infty} dk\ f^*(k)m(k)h(k).$$

From (2.25) one sees that the variations in the ansatz can be chosen so that to decouple the discrete and continuous modes of the operator L in the reduced Lagrangian. This is analogous to the well-known fact that the evolutions of the discrete and continuous scattering data in the framework of the IST are decoupled in the first-order perturbation theory. If the decomposition of the two parts of the spectrum is achieved in (2.25), then the reduced Lagrangian splits into two parts, with one corresponding to the continuous spectrum and the other, to the discrete spectrum. The latter part [which has all $g_{1j}(k)=0$, $j=1,\ldots n$] yields trivial evolution of its parameters: All the time derivatives are either zero or constant in time. Indeed, this second part of the reduced Lagrangian is due to the variations composed entirely from the neutral modes, which correspond to the shift of the soliton's parameters, see (2.19). But it is obvious that in the absence of a driving force, which is the case we consider, one can ''zero out'' the trivial dynamics of the soliton's parameters by re-adjusting the parameters of the background solution $u_0(x,t)$. In other words, by properly choosing the background solution $u_0(x,t)$, one can set $\beta_{mj}=\gamma_{mj}=0$, $j=1,\ldots n$, $m=1,2$.

Considering then only the continuous spectrum part in (2.25) and letting $\alpha_j(t)=\overline{\alpha_j}e^{i\omega t}$, $j=1,\ldots N$, with $\overline{\alpha_j}$'s being independent of t, we arrive at the following set of Euler–Lagrange equations:

$$\sum_{j=1}^{n}\overline{\alpha_j}\{2\omega(\langle g_{1j}|g_{1l}\rangle - \langle g_{1l}|g_{1j}\rangle) + A^2(\langle g_{1j}|\lambda|g_{1l}\rangle + \langle g_{1l}|\lambda|g_{1j}\rangle)\} = 0, \tag{2.26}$$

for $l=1,\ldots n$. In a matrix form, this reads as follows:

$$(M+\omega N)\vec{\alpha}=0, \tag{2.27}$$

where $\vec{\alpha}=(\overline{\alpha_1},\ldots\overline{\alpha_n})^T$ and M and N are Hermitian matrices (see below). It is known (see, e.g., Ref. 8 and Secs. 10.5 and 10.8 of Ref. 9) that if either M or N is sign definite, then all the ω's are real valued. If neither M or N is sign definite, then one cannot determine whether ω's are real or complex valued. In our case, N is clearly not sign definite since it is Hermitian and antisymmetric. However, the matrix M with the entries

$$M_{jl}=(\langle g_{1j}|\lambda|g_{1l}\rangle+\langle g_{1l}|\lambda|g_{1j}\rangle) \tag{2.28}$$

is the Gram matrix (see, e.g., Sec. 9.5 of Ref. 9) and thus is positive definite, provided that all the functions $g_{1j}(k)$, $j=1,\ldots n$ are linearly independent (cf. Ref. 10). The standard proof of this fact goes as follows. For n arbitrary complex numbers c_i, define $\vec{\mathbf{x}}=(c_1 g_{11}(k),\ldots c_n g_{1n}(k))^T$, $\vec{\mathbf{y}}=(c_1^* g_{11}(k),\ldots c_n^* g_{1n}(k))^T$, $\vec{\mathbf{c}}=(c_1,\ldots c_n)^T$, and then consider

$$\vec{\mathbf{c}}^\dagger M\vec{\mathbf{c}}=\sum_{lj} c_l c_j^*(\langle g_{1j}|\lambda|g_{1l}\rangle+\langle g_{1l}|\lambda|g_{1j}\rangle)=\left\|\sum_{j=1}^{n}\mathbf{x}_j\sqrt{\lambda}\right\|^2+\left\|\sum_{j=1}^{n}\mathbf{y}_j\sqrt{\lambda}\right\|^2, \tag{2.29}$$

which is positive if $g_{1j}(k)$, $j=1,\ldots n$ are linearly independent. Hence M is positive definite. Thus, we have proved that if the ansatz for the NLS does not contain components of the discrete spectrum (or decouples them from the continuous spectrum), then a false instability can never occur.

We will shortly present an example showing how one can construct an ansatz not containing the discrete spectrum. But at this moment, let us note that one can effectively achieve the decomposition by simply allowing *each* of the soliton parameters to vary, even if the variations in the ansatz mix the components of the discrete and continuous spectra. Let us consider a variational ansatz of the form

$$\vec{\mathbf{v}}_{\text{var}}=[\text{r.h.s. of (2.20)}]+\nu_1(t)i\phi_1(\theta)+\nu_2(t)\phi_2(\theta)+\mu_1(t)\phi_1^{\mathscr{D}}(\theta)+\mu_2(t)i\phi_2^{\mathscr{D}}(\theta), \tag{2.30}$$

where $\nu_{1,2}$ and $\mu_{1,2}$ are real [see (2.21)]. Thus, we have allowed each of the soliton parameters to vary independently of each other and of the continuous modes. Note that variations corresponding to variational parameters α_j's still may contain the components of the discrete spectrum. Then the reduced Lagrangian can be shown, after some straightforward algebra, to be of the form:

$$\begin{aligned}\langle\mathscr{L}_2\rangle-&[\text{r.h.s. of (2.25) with all } \beta_{mj}=\gamma_{mj}=0]\\ &=2A^2(\mu_1+\langle\alpha|\gamma_1\rangle)^2+2A^2(i\mu_2+\langle\alpha|\gamma_2\rangle)^2+2\dot{\nu}_1(\mu_1+\langle\alpha|\gamma_1\rangle)\\ &\quad-2i\dot{\nu}_2(i\mu_2+\langle\alpha|\gamma_2\rangle)-2i\langle\dot{\alpha}|\beta_1\rangle(\mu_1+\langle\alpha|\gamma_1\rangle)-2i\langle\dot{\alpha}|\beta_2\rangle(i\mu_2+\langle\alpha|\gamma_2\rangle).\end{aligned} \tag{2.31}$$

In Eq. (2.31) and Eq. (2.32) below we use the bracket notations as follows:

$$\langle\alpha|\gamma_1\rangle\equiv\sum_{j=1}^{n}\alpha_j(t)\gamma_{1j},$$

etc. From (2.31) one sees that $\nu_{1,2}$ are cyclic coordinates, so the corresponding momenta are constants of the motion, and then

$$\dot{\mu}_1+\langle\dot{\alpha}|\gamma_1\rangle=0,\quad i\dot{\mu}_2+\langle\dot{\alpha}|\gamma_2\rangle=0. \tag{2.32}$$

Then the first two terms on the r.h.s. of (2.31) are constants while the others are total time derivatives. Thus the reduced Lagrangian (2.31), calculated for the ansatz (2.30), is equivalent to one calculated without the contribution from the discrete spectrum.

It is clear that mixing components of the discrete and continuous spectra, without allowing the soliton parameters to vary independently, is only a *necessary* condition for the ansatz to produce a false instability. A false instability can be expected to occur if the coupling between the discrete and continuous spectra in the ansatz is, in a certain sense, strong enough. Below we present an example of such an ansatz:

$$u(x,t)=u_0\cdot[\,\delta\eta(t)+\delta\varphi(t)\,\theta+i\,\delta\varphi(t)\,]. \tag{2.33}$$

The corresponding Euler–Lagrange equations for $\delta\eta(t),\delta\varphi(t)$ reveal oscillations with $\omega^2=-(28/9-8\pi^2/27)A^4<0$, which are therefore unstable.

To conclude this section, we will demonstrate how one can construct an ansatz which does not contain the neutral modes. Let us take ansatz (2.3a) as a starting point. By calculating the inner products, defined by formulae (2.24), of its variations (2.3b) with the discrete spectrum (2.10), (2.11) and inspecting them, one finds that the following combinations:

$$\begin{aligned}
&\vec{\mathbf{v}}_{(\delta\eta)}-\vec{\mathbf{v}}_{(\delta A)}\equiv W_1=(1-2\,\theta\,\tanh\,\theta)\operatorname{sech}\,\theta\,\begin{pmatrix}1\\1\end{pmatrix},\\
&\vec{\mathbf{v}}_{(\delta\varphi)}+\frac{12}{\pi^2}\,\vec{\mathbf{v}}_{(\delta c)}\equiv W_2=i\left(1+\frac{12}{\pi^2}\,\theta^2\right)\operatorname{sech}\,\theta\,\begin{pmatrix}1\\-1\end{pmatrix},
\end{aligned} \tag{2.34}$$

are orthogonal (with weight function σ_3) to the discrete spectrum. Thus, the ansatz

$$u(x,t)=u_0\cdot\left[\,\alpha_1(t)(1-2\,\theta\,\tanh\,\theta)+i\,\alpha_2(t)\left(1+\frac{12}{\pi^2}\,\theta^2\right)\right] \tag{2.35}$$

does not contain the neutral modes. This ansatz has only two variational parameters instead of four in ansatz (2.3a). Still, using (2.35) one can match any initial condition allowed by ansatz (2.3a), if one adjusts the background soliton's parameters properly. To see this, it is enough to notice that

$$\begin{aligned}
&\vec{\mathbf{v}}_{(\delta\eta)}=-W_1-2\,\phi_1^{\mathscr{D}},\quad \vec{\mathbf{v}}_{(\delta\varphi)}=i\,\phi_1,\\
&\vec{\mathbf{v}}_{(\delta A)}=-W_1-\phi_1^{\mathscr{D}},\quad \vec{\mathbf{v}}_{(\delta c)}=\frac{\pi^2}{12}\,(W_2-i\,\phi_1).
\end{aligned} \tag{2.36}$$

Finally, we note that the results produced by (2.3a) and (2.36) are equivalent, which is in agreement with the result proven above for the ansatz of the form (2.30); here $\mu_1=(\delta A-\delta\eta)$, $\nu_1=\delta\varphi$, $\mu_2=\nu_2=0$.

In summary, in this section we have shown that in order to guarantee that the ansatz will not give a false instability for the NLS, it is sufficient to require that the discrete and continuous spectrum modes be decoupled in the ansatz.

III. THE MTM CASE

The considerations in this section are very similar to those in the previous one, so we present here only the most necessary details. We consider the equations of the MTM in the laboratory coordinates:

$$i(u_x+u_t)+v+|v|^2u=0,\quad i(-v_x+v_t)+u+|u|^2v=0. \tag{3.1}$$

Its one-soliton solution is given by[11]:

$$u_0(x,t|V)=\left(\frac{1+V}{1-V}\right)^{1/4}\sin Q\ \mathrm{sech}\left(\theta\sin Q-\frac{iQ}{2}\right)\cdot\exp\{-it\sqrt{1-V^2}\cos Q+iV\theta\cos Q+i\varphi_0\},$$

$$v_0(x,t|V)=-\left(\frac{1-V}{1+V}\right)^{1/4}\sin Q\ \mathrm{sech}\left(\theta\sin Q+\frac{iQ}{2}\right)\cdot\exp\{-it\sqrt{1-V^2}\cos Q+iV\theta\cos Q+i\varphi_0\}, \tag{3.2}$$

where $\theta=(x-x_0-Vt)/\sqrt{1-V^2}$, x_0, φ_0 are arbitrary constants, and the constants Q and V satisfy: $0<Q<\pi$, $-1<V<1$. Equations (3.1) are Lorentz-invariant, so one can consider only the solution with $V=0$, which we will denote as $u_0(x,t)$, $v_0(x,t)$.

The Lagrangian density for Eqs. (3.1) is

$$\mathscr{L}\equiv\mathscr{L}^{\mathrm{MTM}}=\frac{i}{2}\left[(u^*u_t+u^*u_x+v^*v_t-v^*v_x)-\mathrm{c.c.}\right]+(u^*v+v^*u)+|u|^2|v|^2. \tag{3.3}$$

We substitute into (3.3) $u=u_0+\delta u$, $v=v_0+\delta v$ with $|\delta u|\ll|u_0|$, $|\delta v|\ll|v_0|$, and find

$$\mathscr{L}_2\equiv\mathscr{L}_2^{\mathrm{MTM}}=\frac{1}{2}\,\vec{\mathbf{w}}^{\dagger}\begin{pmatrix}\sigma_3 & 0\\ 0 & \sigma_3\end{pmatrix}(i\partial_t+L)\vec{\mathbf{w}}, \tag{3.4a}$$

where

$$\vec{\mathbf{w}}=\begin{pmatrix}\delta u\ e^{it\cos Q}\\ \delta u^*\ e^{-it\cos Q}\\ \delta v\ e^{it\cos Q}\\ \delta v^*\ e^{-it\cos Q}\end{pmatrix}. \tag{3.4b}$$

In (3.4a),

$$L\equiv L^{\mathrm{MTM}}=i\begin{pmatrix}I_2 & 0\\ 0 & -I_2\end{pmatrix}\frac{\partial}{\partial\theta}+\begin{pmatrix}\cos Q+|u_0|^2 & 0 & 1+\overline{u_0v_0^*} & \overline{u_0v_0}\\ 0 & -(\cos Q+|u_0|^2) & -\overline{u_0^*v_0^*} & -(1+\overline{u_0^*v_0})\\ 1+\overline{u_0^*v_0} & \overline{u_0v_0} & \cos Q+|u_0|^2 & 0\\ -\overline{u_0^*v_0^*} & -(1+\overline{u_0v_0^*}) & 0 & -(\cos Q+|u_0|^2)\end{pmatrix}, \tag{3.5}$$

where $\overline{u_0}=u\exp(it\cos Q)$, $\overline{v_0}=v\exp(it\cos Q)$. If the pair (u_0,v_0) is a solution of (3.1), then the vector $\vec{\mathbf{w}}$ satisfies the equation:

$$(i\partial_t+L)\vec{\mathbf{w}}=0, \tag{3.6}$$

which is the linearization of (3.1) on the background of the soliton (3.2). Then we have to consider the eigenvalue problem

$$L\vec{\mathbf{w}}=\lambda\vec{\mathbf{w}}, \tag{3.7}$$

with L given by (3.5). Its solution was found by the present authors in Ref. 12. Here, however, we will proceed by using the asymptotic form of L and the corresponding eigenfunctions, with the reason being the same as in Sec. II. The only result from Ref. 12 which we will use here will be the completeness of a certain set of the eigenfunctions of (3.7). In Appendix B we present the explicit form of these eigenfunctions, found in Ref. 12.

Equation (3.7) has four linearly independent solutions with the following asymptotics, say, at $\theta\to-\infty$:

$$\underline{\theta\to-\infty}\quad \psi_1\to\begin{pmatrix}1\\0\\r(k)\\0\end{pmatrix}e^{ik\theta},\quad \psi_2\to\begin{pmatrix}0\\1\\0\\r(k)\end{pmatrix}e^{-ik\theta},$$
$$\psi_3\to\begin{pmatrix}1\\0\\-r(-k)\\0\end{pmatrix}e^{ik\theta},\quad \psi_4\to\begin{pmatrix}0\\1\\0\\-r(-k)\end{pmatrix}e^{-ik\theta}, \tag{3.8}$$

for real k, where

$$r(k)=k+\sqrt{k^2+1}. \tag{3.9}$$

Also from the asymptotic form of L, one finds that

$$L\psi_1=\lambda(k)\psi_1,\quad L\psi_2=-\lambda(k)\psi_2,\quad L\psi_3=\mu(k)\psi_3,\quad L\psi_4=-\mu(k)\psi_4, \tag{3.10a}$$

with

$$\lambda(k)=\cos Q+\sqrt{k^2+1},\quad \mu(k)=\cos Q-\sqrt{k^2+1}. \tag{3.10b}$$

In complete analogy with (2.13)–(2.15), one obtains

$$\begin{pmatrix}\sigma_1&0\\0&\sigma_1\end{pmatrix}L\begin{pmatrix}\sigma_1&0\\0&\sigma_1\end{pmatrix}=-L^*, \tag{3.11}$$

$$\psi_2(k,\theta)=\begin{pmatrix}\sigma_1&0\\0&\sigma_1\end{pmatrix}\psi_1^*(k,\theta),\quad \psi_4(k,\theta)=\begin{pmatrix}\sigma_1&0\\0&\sigma_1\end{pmatrix}\psi_3^*(k,\theta). \tag{3.12}$$

Notice that no involution can be established between ψ_1 and ψ_3.

Considering the asymptotics allows one only to obtain the general form of the eigenfunctions at $\theta\to+\infty$ [cf. (2.18)]. Here, as in the case of the NLS, we will make use of the fact that soliton (3.2) is the reflectionless potential in the corresponding scattering problem. This allows one to state that

$$\underline{\text{for }\ \theta\to+\infty}\quad \psi_1\to a(k)\begin{pmatrix}1\\0\\r(k)\\0\end{pmatrix}e^{ik\theta},\quad \psi_3\to\tilde{a}(k)\begin{pmatrix}1\\0\\-r(-k)\\0\end{pmatrix}e^{ik\theta}, \tag{3.13}$$

with $|a(k)|=|\tilde{a}(k)|=1$ for real k, and the asymptotics of ψ_2, ψ_4 at $\theta\to+\infty$ are then found from (3.12).

In Sec. II it was explained how the neutral modes of L can be found. So here we will only state that these modes, together with the set $\{\psi_i(k)\}_{i=1,\ldots,4}$ for all real k, form a basis in the space of four-component vector functions with entries from the Schwartz class; see Appendix B for details. Now, as was also discussed in Sec. II, the contributions from the continuous and discrete spectra of L can be decoupled in the averaged Lagrangian, with it being possible to effectively ''zero out'' the contribution of the discrete spectrum. Thus, below we will only consider the variations which do not contain the discrete spectrum components. Then, similarly to (2.20), any ansatz with smooth entries can be represented as follows:

$$\vec{\mathbf{w}}(\theta)=\sum_{j=1}^{n}\alpha_j\int_{-\infty}^{\infty}dk\sum_{m=1}^{4}g_{mj}(k)\psi_m(k,\theta). \tag{3.14}$$

From (3.14) and (3.12) one obtains an analog of (2.21):

$$g_{2j}(k)=g_{1j}^{*}(k),\quad g_{4j}(k)=g_{3j}^{*}(k),\quad j=1,\ldots n. \tag{3.15}$$

However, there is no relation between $g_{1j}(k)$ and $g_{3j}(k)$ because, as mentioned earlier, no involution exists between ψ_1 and ψ_3.

Using the same technique as for the NLS, we obtain the following inner products (defined in the x space):

$$\begin{aligned}
&\langle\psi_1^{\dagger}(k')|\begin{pmatrix}\sigma_3 & 0\\ 0 & \sigma_3\end{pmatrix}|\psi_1(k)\rangle=4\pi\sqrt{k^2+1}(\sqrt{k^2+1}+k)\,\delta(k-k'),\\
&\langle\psi_2^{\dagger}(k')|\begin{pmatrix}\sigma_3 & 0\\ 0 & \sigma_3\end{pmatrix}|\psi_2(k)\rangle=-4\pi\sqrt{k^2+1}(\sqrt{k^2+1}+k)\,\delta(k-k'),\\
&\langle\psi_3^{\dagger}(k')|\begin{pmatrix}\sigma_3 & 0\\ 0 & \sigma_3\end{pmatrix}|\psi_3(k)\rangle=4\pi\sqrt{k^2+1}(\sqrt{k^2+1}-k)\,\delta(k-k'),\\
&\langle\psi_4^{\dagger}(k')|\begin{pmatrix}\sigma_3 & 0\\ 0 & \sigma_3\end{pmatrix}|\psi_4(k)\rangle=-4\pi\sqrt{k^2+1}(\sqrt{k^2+1}-k)\,\delta(k-k').
\end{aligned} \tag{3.16}$$

Let us note that the eigenfunctions $\{\psi_i(k)\}_{i=1,\ldots,4}$ can be divided into two ''spaces,'' $S^{+}=\{\psi_1(k),\psi_2(k)\}$ and $S^{-}=\{\psi_3(k),\psi_4(k)\}$, depending on the sign of the following inner product:

$$\langle\psi^{\dagger}(k')|\begin{pmatrix}\sigma_3 & 0\\ 0 & \sigma_3\end{pmatrix}L|\psi(k)\rangle; \tag{3.17}$$

(we consider the δ function to be positive). Also notice that in the case of Eq. (2.1), there is only one ''space.''

Inserting (3.14) into (3.4a) and using (3.10), (3.15), and (3.16), one obtains the reduced Lagrangian for Eqs. (3.1):

$$\begin{aligned}
\langle\mathscr{L}_2\rangle=\sum_{jl}\{&i\alpha_l\dot{\alpha}_j(\langle h_l|h_j\rangle-\langle h_j|h_l\rangle+\langle\tilde{h}_l|\tilde{h}_j\rangle-\langle\tilde{h}_j|\tilde{h}_l\rangle)\\
&+\alpha_l\alpha_j(\langle h_j|\lambda|h_l\rangle+\langle h_l|\lambda|h_j\rangle+\langle\tilde{h}_l|\mu|\tilde{h}_j\rangle+\langle\tilde{h}_j|\mu|\tilde{h}_l\rangle)\},
\end{aligned} \tag{3.18}$$

where

$$h_j = g_{1j}(k)\sqrt{2(k^2+1+k\sqrt{k^2+1})},$$

$$\tilde{h}_j = g_{3j}(k)\sqrt{2(k^2+1-k\sqrt{k^2+1})}.$$

The corresponding Euler–Lagrange equations for $\overline{\alpha_j} = \alpha_j e^{-i\omega t}$, $j=1,\ldots n$, have the following matrix form [compare with (2.27)]:

$$((M_1 - M_2) + \omega(N_1 + N_2))\vec{\alpha} = 0, \tag{3.19}$$

where

$$(M_1)_{lj} = \langle h_j|\lambda|h_l\rangle + \langle h_l|\lambda|h_j\rangle, \quad (M_2)_{lj} = \langle h_j||\mu||\tilde{h}_l\rangle + \langle \tilde{h}_l||\mu||\tilde{h}_j\rangle,$$

$$(N_1)_{lj} = 2(\langle h_l|h_j\rangle - \langle h_j|h_l\rangle), \quad (N_2)_{lj} = 2(\langle \tilde{h}_l|\tilde{h}_j\rangle - \langle \tilde{h}_j|\tilde{h}_l\rangle).$$

In the expression for $(M_2)_{lj}$ we wrote $|\mu|$ in order to stress that $\mu(k)$ is always negative, while $\lambda(k)$ is always positive. The matrix $N = N_1 + N_2$ is, as for the NLS, not sign definite. M_1 and M_2 separately are positive definite, but $M = M_1 - M_2$ is not sign definite since the entries of M_1 are not related to those of M_2 [see the note (3.15)]. Therefore, the normal frequencies ω in (3.19) could be real or complex. One can show that, because N is Hermitian and anti-symmetric, the corresponding characteristic polynomial contains only even powers of ω. So, if there is a normal frequency ω with Im $\omega > 0$, then there necessarily is another normal frequency $(-\omega)$ with Im $(-\omega) < 0$. Thus the variational method could (incorrectly) predict that the soliton solution of the MTM equations is unstable. Thus, we conclude that if the ansatz for Eqs. (3.1) ''mixes'' the components corresponding to the two sets S^+ and S^-, then it may produce a false instability.

Let us remark that the ansatz used in Ref. 3 *did* contain components of the discrete spectrum, so the instability found there could be due to that reason. However, we performed the calculations with a similar ansatz from which the discrete spectrum was excluded, and we still found an instability setting in for $Q \approx 1$ [see (3.2)], which is close to the result of Ref. 3. Therefore we conclude that the instability found in Ref. 3 can be attributed to ''mixing of the spaces'' S^+ and S^-.

One would like to have some methods for choosing the variational ansatz so as to avoid such false instabilities. One simple way which would guarantee that the frequencies ω produced by the variational method would always be real would be to choose the ansatz in such a form so as to have: $h_j(k) \cdot \tilde{h}_j(k) = 0$, $j = 1,\ldots n$. Then all variations would be expandable over either the set S^+ or S^-, but not the whole set $S = \{\psi_1(k), \psi_2(k), \psi_3(k), \psi_4(k)\}$. In this case, Eq. (3.19) would decompose into two equations:

$$(M^{\pm} + \omega N^{\pm})\vec{\alpha}^{\pm} = 0, \tag{3.20}$$

where $M^{\pm} = \pm M_{1,2}$, $N^{\pm} = N_{1,2}$. Then one would be able to guarantee that the corresponding ω's would be real valued, and thus false instabilities will not occur.

Let us then observe that when the soliton parameter $Q \ll 1$, and the variations are expanded mainly over the eigenmodes with $|k| \ll 1$, it is possible to construct variations which *almost* entirely consist of the eigenfunctions from only one of the spaces. First, notice that these two limits, $Q \ll 1$ and $|k| \ll 1$, are compatible in the following sense: a soliton with $Q \ll 1$ has a large width, and the corresponding variations, whose scale is usually taken to be of the same order of magnitude as that of the soliton, are expandable mostly over the eigenmodes with $|k| \ll 1$. Next, from (3.4b) one has:

$$\delta u = \int_{-\infty}^{\infty} dk (g_1(k)\psi_1^{(1)}(k,\theta) + g_3(k)\psi_3^{(1)}(k,\theta)),$$

$$\delta v = \int_{-\infty}^{\infty} dk (g_1(k)\psi_1^{(3)}(k,\theta) + g_3(k)\psi_3^{(3)}(k,\theta)),$$

where $\psi_{1,3}^{(j)}$ is the jth entry of $\psi_{1,3}(k,\theta)$. But from (3.5) and (3.8) one can see that for $Q \ll 1$, $|k| \ll 1$, the ratios $\psi_1^{(3)}(k,\theta)/\psi_1^{(1)}(k,\theta)$ and $\psi_3^{(3)}(k,\theta)/\psi_3^{(1)}(k,\theta)$ are approximately $+1$ and -1, respectively. Then, taking the variations in the ansatz to be either symmetric ($\delta u = \delta v$, $g_3(k) \approx 0$) or anti-symmetric ($\delta u = -\delta v$, $g_1(k) \approx 0$), one can, in the considered limit, attain approximate decoupling of S^+ and S^- and thus avoid false instabilities more easily than by simply using an arbitrary guess. This conclusion is in excellent agreement with the results of Ref. 3.

In summary, in this section we have considered the MTM equation and have concluded that the false instability, found in Ref. 3, is due to the coupling of eigenfunctions from two different ''spaces'' in the ansatz.

IV. A CASE WHEN ANSATZ HAS ONLY TWO VARIATIONAL PARAMETERS

The purpose of this section is twofold. First, taking the ansatz in a simple form, we provide a justification to the intuitive idea that the variational method gives, in a sense, an averaged description of the pulse's dynamics. Second, for the same simple form of the ansatz, we introduce a method which allows one to avoid false instabilities, arising due to the second mechanism, *without* separation of the two ''spaces'' of the eigenfunctions.

For definiteness, let us restrict our consideration to Eqs. (3.1). Similar results can be obtained for any other evolution equation. Let the ansatz contain only two variations:

$$\begin{aligned}\vec{\mathbf{w}}_{\text{var}} &= \alpha(t)\vec{\mathbf{w}}_\alpha(\theta) + \beta(t)\vec{\mathbf{w}}_\beta(\theta) \\ &\equiv \alpha(t)\int_{-\infty}^{\infty}\sum_{j=1}^{4} g_{j\alpha}(k)\psi_j(k,\theta)dk + \beta(t)\int_{-\infty}^{\infty}\sum_{j=1}^{4} g_{j\beta}(k)\psi_j(k,\theta)dk, \end{aligned} \tag{4.1}$$

where $\alpha(t)$, $\beta(t)$ are the (real) variational parameters. As before, we exclude the discrete spectrum. We will denote the eigenvalues $\lambda(k) \equiv \lambda_1(k)$ and $\mu(k) \equiv \lambda_3(k)$. Then from (3.15) and (3.18) one obtains the Euler–Lagrange equations for ansatz (4.1). Using them, we arrive, after some involved algebra, at the following expression for the frequency ω:

$$\begin{aligned} -\omega^2 &\left[\int_{-\infty}^{\infty} dk \sum_{j=1,3} \nu_j(k)(g_{j\alpha}^*(k)g_{j\beta}(k) - g_{j\alpha}(k)g_{j\beta}^*(k))\right]^2 \\ &= \int\int_{-\infty}^{\infty} dk\, dk' \sum_{\{j,m\}=\{1,3\}} \lambda_j(k)\lambda_m(k')\nu_j(k)\nu_m(k') \\ &\quad \times (|g_{j\alpha}^*(k)g_{m\beta}(k') - g_{m\alpha}(k')g_{j\beta}^*(k)|^2 + |g_{j\alpha}(k)g_{m\beta}(k') - g_{m\alpha}(k')g_{j\beta}(k)|^2), \end{aligned} \tag{4.2}$$

where $\nu_j(k) = (k^2 + 1 + (-1)^{(j-1)/2}k\sqrt{k^2+1})$, $j = 1,3$. The l.h.s. of (4.2) is always non-negative since the integrand is purely imaginary. Since $\lambda_1(k) > 0$ and $\lambda_3(k) < 0$, the expansion coefficients $g_{j\alpha}(k)$, $g_{j\beta}(k)$ can be chosen so that to make the r.h.s. of (4.2) negative. That would yield $\omega^2 < 0$, which implies a false instability. Thus we see that it is *always* possible to construct an ansatz which would introduce a false instability when the linearized evolution equation has two ''spaces'' of the eigenfunctions.

Let us now choose $g_{j\beta}(k) = ig_{j\alpha}(k)$ ($j = 1,3$) for all k in the expansion. Then the second term in the r.h.s. of (4.2) vanishes, and (4.2) becomes

$$\omega^2\left[\int_{-\infty}^{\infty}\sum_{j=1,3} dk\ \nu_j(k)|g_{j\alpha}(k)|^2\right]^2=\left[\int_{-\infty}^{\infty}\sum_{j=1,3} dk\ \lambda_j(k)\nu_j(k)|g_{j\alpha}(k)|^2\right]^2. \tag{4.3}$$

This implies that (i) $\omega^2\geqslant 0$, i.e. the ansatz with $g_{j\beta}(k)=ig_{j\alpha}(k)$ will never produce a false instability, even though the two ''spaces'' S^+ and S^- are not separated; and (ii) the frequency given by the variational method is simply a weighed average of $\lambda(k)$.

Now let us note that *away* from the center of the soliton,

$$\psi_j(k,\theta)=\hat{\sigma}_3\psi_j(k,\theta), \tag{4.4}$$

where $\hat{\sigma}_3=\mathrm{diag}(\sigma_3,\sigma_3)$ [see (3.8)]. Equation (4.4), together with the assumption $g_{j\beta}(k)=ig_{j\alpha}(k)$, implies that

$$\vec{\mathbf{w}}_\beta=i\hat{\sigma}_3\vec{\mathbf{w}}_\alpha. \tag{4.5}$$

However, near the center of the soliton, Eq. (4.4) and, consequently, Eq. (4.5) do not hold. This is the key reason why it is not straightforward to use the above method to construct an ansatz which would guarantee absence of false instabilities. Namely, when one is designing an ansatz, one knows the θ dependence of the variations but not the expansion coefficients $g(k)$. Obviously, if one knows $\psi(k,\theta)$, then having an expansion coefficient is equivalent to having the explicit form of the corresponding variation. The question of whether this simple method could be applied without using the eigenfunctions remains open.

V. CONCLUSION AND GENERAL DISCUSSION

The main result of this paper has been to present the necessary conditions for the variational method to give rise to false instabilities, and also to give sufficient conditions in order to avoid such false instabilities.

For a false instability to occur, it is necessary (but not sufficient) that the variational ansatz satisfy at least one of the following two conditions:

(1) At least one of the variations contains both neutral and continuous spectrum modes. This is the first mechanism via which false instabilities can occur; it was discussed in Sec. II.
(2) There are two different ''spaces'' of the continuous spectrum eigenfunctions, and at least one of the variations contains eigenfunctions from both spaces. This is the second mechanism, which was discussed in Sec. III.

Note that if a background solution of the evolution equation is a reflectionless potential for the continuous spectrum eigenfunctions, as it was in all the examples considered here, then the existence of the two ''spaces'' is manifested by sign indefiniteness of the ''natural'' inner product (3.17). We emphasize that this condition is not equivalent to the condition of sign definiteness of the continuous spectrum of the Hermitian operator $\hat{\sigma}_3 L$, where $\hat{\sigma}_3=\mathrm{diag}(\sigma_3,\sigma_3,...)$, because $\psi(k)$ in (3.17) are eigenfunctions of the non-Hermitian operator L. In a more general case of a nonintegrable equation, the existence of the two ''spaces'' is equivalent to nonsign definiteness of the matrix M introduced in Sec. II; see Appendix A for technical details of how one can determine whether M is or is not sign definite.

Consequently, in order to guarantee that false instabilities will never occur, it is sufficient (but not necessary) to impose on the ansatz the following restrictions:

(1) Either no variation in the ansatz contains the neutral modes, or each and every one of the solitary wave's *independent* parameters is allowed to vary.
(2) If there are two different spaces of the eigenfunctions in the continuous spectrum, then each variation contains components from only one of the two spaces.

In a particular case when the ansatz contains only two real variational parameters, $\alpha(t)$ and $\beta(t)$, we proved in Sec. IV that the second necessary condition above can be replaced by the following requirement on the corresponding expansion coefficients: $g_\beta(k)=ig_\alpha(k)$. Even though the variations in this case may contain eigenfunctions from the two different ''spaces,'' the ansatz so constructed will never produce a false instability.

Let us now address the application of these results to a general (and usually nonintegrable) nonlinear evolution equation. It is obvious that these results are only strictly true for small variations about a solitary wave. However, if variations are not so small that nonlinear effects can be ignored, then one certainly should insure that the corresponding linear limit is free of false instabilities. With this said, for the rest of the discussion, we shall only consider the case where the variations are small.

First we consider the case when the exact solitary wave solution of this evolution equation is known. One starts by constructing, by either of the methods presented in Sec. II, an ansatz which either does not contain the neutral modes or, which is effectively the same, includes variations corresponding to each and every solitary wave's parameter. The neutral modes are found by varying the independent solitary wave's parameters. Note that there can also exist additional discrete spectrum modes, different from the neutral ones; as it is known, not only their form, but also their very presence in the spectrum, can be determined analytically only in exceptional cases (see, for example, Ref. 13). Such modes may or may not make the solitary wave unstable, depending on their time evolution in the linearized evolution equation.

Next, one follows the outline of Sec. II and determines whether the corresponding matrix M is sign definite (see Appendix A for technical details). If it is not, then the ansatz can produce a false instability, unless one can separate S^+ and S^- (see, for example, the discussion at the end of Sec. III). If a false instability can arise via the second mechanism, then the results of the variational method might be questionable, and in this case one cannot say anything about the existence of any unstable modes in the discrete spectrum.

Now, suppose that the matrix M can be shown to be sign definite or to separate into two sign-definite matrices, as in (3.20). Let us then discuss the possibility of detecting, by means of the variational method, an unstable mode in the discrete spectrum. In the case considered, the variational method can either produce or not, an instability. If the former is the case, then one can claim that the linearized operator has an unstable eigenmode in the discrete spectrum, because it would be the only manner in which an instability can arise in this case. Then it follows that the solitary wave is truly linearly unstable. Thus, the variational method provides an analytical means of detecting the existence of an unstable mode in the spectrum of a linearized evolution equation. However, the opposite statement, namely: ''if under the above specified conditions an instability does not arise, then the solitary wave is linearly stable,'' is not true. The trivial counterexample here is that of the ansatz which simply does not contain the unstable mode. But even if we exclude this trivial possibility, then calculations analogous to those presented in Appendix A did not give us any affirmative answer. So it would be interesting to compare the results of the variational method, applied to the problem of linear stability of a solitary wave, with those obtained by other methods.

Now, suppose that the exact solution of the evolution equation in question is not available. Then one may take an ansatz (usually a Gaussian) and determine the stationary points of the corresponding Euler–Lagrange equations, written for the ansatz' parameters. This yields a profile approximating the exact solitary wave. This profile will have the analogues of the soliton parameters, and then one can obtain the ''approximate neutral modes'' by an analog of formula (2.19). The rest is then similar to the consideration in the above paragraphs.

If the equation has a perturbation such that a Lagrangian density of the perturbed equation still exists, then the variational ansatz must contain both the continuous and discrete spectra, but the two should not be coupled in the same variation.

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APPENDIX A: THE CASE OF NLS-TYPE EQUATION WITH ARBITRARY NONLINEARITY

Here we present the details of the proof that for a general one-component NLS-type equation, i.e., the equation with the same linear but different nonlinear part, a false instability does not occur. We assume that the ansatz does not contain components of the discrete spectrum.

From (2.22) it follows that $\partial_\theta W(\psi_1(k),\psi_1(k))=0$. Then using asymptotics (2.16), (2.18) and comparing the values of $W(\psi_1(k),\psi_1(k))$ at $\theta\to-\infty$ and $\theta\to+\infty$, one finds

$$|a(k)|^2=1+|b(k)|^2. \tag{A1}$$

Denoting by $\phi_1(k)$ a solution of (2.8) with the asymptotics

$$\underline{\theta\to+\infty} \quad \phi_1(k)\to\begin{pmatrix}0\\1\end{pmatrix}e^{ik\theta},$$

one finds from (2.18):

$$\psi_1(k)=a(k)\phi_1(k)+b(k)\phi_1(-k). \tag{A2}$$

We assume the corresponding operator L to be real, which is so if the nonlinearity in the evolution equation is of the form $uV(|u|^2)$. Then

$$\psi_1^*(-k)=\psi_1(k), \quad \phi_1^*(-k)=\phi_1(k). \tag{A3}$$

and from (A2) and (A3) one obtains:

$$a^*(-k)=a(k), \quad b^*(-k)=b(k). \tag{A4}$$

Using (A1) and (A4) one obtains a generalization of (2.24a):

$$\langle\psi_1^\dagger(k')|\sigma_3|\psi_1(k)\rangle=-2\pi(|a(k)|^2\delta(k-k')+a(k)b(k)\delta(k+k')), \tag{A5a}$$

$$\langle\psi_2^\dagger(k')|\sigma_3|\psi_2(k)\rangle=2\pi(|a(k)|^2\delta(k-k')+a^*(k)b^*(k)\delta(k+k')). \tag{A5b}$$

Then from (A4) and (A5) it is straightforward to obtain a generalization of (2.27). Namely, the matrices M, N now have the entries:

$$N_{jl}=\langle g_j||a|^2|g_l\rangle+\langle g_j(-k)|ab|g_l\rangle-\text{c.c.}; \tag{A6a}$$

$$M_{jl}=\langle g_j|\lambda|a|^2|g_l\rangle+\langle g_j(-k)|\lambda ab|g_l\rangle+\text{c.c.} \tag{A6b}$$

In (A6) we have omitted the subindex ''1'' of g_{1j}, and we also omit the argument of functions if it is k. As before, N is Hermitian with $\mathrm{Tr}\,N=0$, so in order to guarantee that $\omega^2\geqslant 0$, one needs to prove that M is positive definite. Similar to (2.29), denote $\vec{\mathbf{x}}=\sqrt{\lambda}(c_1g_1,\ldots c_ng_n)^T$, $\vec{\mathbf{y}}=\sqrt{\lambda}(c_1^*g_1,\ldots c_n^*g_n)^T$, $\vec{\mathbf{c}}=(c_1,\ldots c_n)^T$, and then consider $\vec{\mathbf{c}}^\dagger M\vec{\mathbf{c}}$. Taking into account the identity

$$\langle g_j(-k)|\lambda ab|g_l\rangle=\langle g_j(k)|\lambda a^*b^*|g_l(-k)\rangle$$

and (A1) and (A4) one obtains that

$$\vec{\mathbf{c}}^{\dagger}M\vec{\mathbf{c}}=(\vec{\mathbf{x}}\ \text{part})+(\vec{\mathbf{y}}\ \text{part}), \tag{A7}$$

where

$$\begin{aligned}(\vec{\mathbf{x}}\ \text{part})=\frac{1}{2}\Bigg[&\left\|\sum_{j=1}^{n}x_j(k)|a(k)|\right\|^2+\left\|\sum_{j=1}^{n}x_j(k)|b(k)|\right\|^2+\left\|\sum_{j=1}^{n}x_j(k)\right\|^2\\&+\sum_{j,l}\langle\mathbf{x}_j^*(-k)|a(k)b(k)|\mathbf{x}_l(k)\rangle+\sum_{j,l}\langle\mathbf{x}_j^*(k)|a^*(k)b^*(k)|\mathbf{x}_l(-k)\rangle\Bigg]\\=\frac{1}{2}\Bigg[&\left\|\sum_{j=1}^{n}(\mathbf{x}_j(-k)a(-k)+\mathbf{x}_j(k)b(k))\right\|^2+\left\|\sum_{j=1}^{n}\mathbf{x}_j(k)\right\|^2\Bigg]>0.\end{aligned}$$

Similarly, the $\vec{\mathbf{y}}$ part in (A7) is positive, thus M is positive definite.

APPENDIX B: COMPLETENESS OF THE SET OF SOLUTIONS OF EQ. (3.7)

Below we present the explicit expressions of the eigenfunctions of Eq. (3.7), which form a complete set in the Schwartz class. Let us first introduce the notations. Let $f(\xi,\theta)=(f_1(\xi,\theta),f_2(\xi,\theta))^T$ be an arbitrary vector function with the entries f_1, f_2 bounded for any real θ and for Im $\xi^2=0$, and the pair $u\equiv u(x,t)$, $v\equiv v(x,t)$ be a solution of (3.1). Denote

$$Y(f(\xi,\theta))\equiv(Y_1,Y_2,Y_3,Y_4)^T, \tag{B1a}$$

where

$$\begin{aligned}Y_1=\frac{1}{\xi}f_2^2+uf_1f_2,\quad Y_2=\frac{1}{\xi}f_1^2-u^*f_1f_2,\\Y_3=-\xi f_2^2-vf_1f_2,\quad Y_4=-\xi f_1^2+v^*f_1f_2.\end{aligned} \tag{B1b}$$

Let now $f(\xi,\theta)$ be a Jost solution of the x-operator in the Lax pair corresponding to Eq. (3.1) (Refs. 11 and 12). Then in Ref. 12 a result was proven which, in terms relevant to this paper, is the following. The function Y defined in (B1) is a solution of Eq. (3.7) with $\lambda(\xi)=\cos Q-\frac{1}{2}(\xi^2+\xi^{-2})$. Moreover, a certain set of these functions is complete. In particular, when the pair (u,v) is the exact one-soliton solution (3.2), then the two linearly independent Jost solutions with oscillatory asymptotics at $|\theta|\to\infty$ are

$$\begin{aligned}\chi(\xi,\theta)=\begin{pmatrix}0\\1\end{pmatrix}e^{-iA(\theta)-i/2\,k(\xi)\theta}-\frac{\sin Q e^{-(i/2)k(\xi)\theta}}{\xi^2-\xi_1^{*2}}\\\cdot\begin{pmatrix}\xi\ \operatorname{sech}\left(\theta\sin Q+\dfrac{iQ}{2}\right)\cdot\ \exp(-iB-iQ+iA(\theta))\\i\ \operatorname{sech}\left(\theta\sin Q-\dfrac{iQ}{2}\right)\cdot\ \exp(\theta\sin Q-iA(\theta)-iQ/2)\end{pmatrix},\end{aligned} \tag{B2a}$$

and

$$\overline{\chi(}\xi,\theta)=\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}\chi^*(\xi^*,\theta), \tag{B2b}$$

where Q was defined in Sec. III,

$$A(\theta)=\arctan\left(\tan\left(\frac{Q}{2}\right)\tanh(\theta\ \sin\ Q)\right)+\frac{Q}{2},$$

$$\xi_1=\exp\left(\frac{i}{2}\,Q\right),\quad B=-t\ \cos\ Q,\quad k(\xi)=\frac{1}{2}\,(\xi^2-\xi^{-2}).$$

The two Jost solutions vanishing at $|\theta|\to\infty$ are

$$\chi_1(\theta)\equiv\chi(\xi_1,\theta)=\frac{1}{2}\begin{pmatrix} i\ \mathrm{sech}\left(\theta\ \sin\ Q+\dfrac{iQ}{2}\right)\cdot\ \exp(-iB+iA(\theta)+(\theta\ \sin\ Q-iQ)/2)\\ \mathrm{sech}\left(\theta\ \sin\ Q-\dfrac{iQ}{2}\right)\cdot\ \exp(-iA(\theta)-(\theta\ \sin\ Q-iQ)/2)\end{pmatrix}, \tag{B3a}$$

and

$$\overline{\chi_1}(\theta)\equiv\overline{\chi(}\xi_1^*,\theta). \tag{B3b}$$

Then any four-component vector $\vec{\mathbf{w}}$ with the entries from the Schwartz class can be expanded as follows:

$$\vec{\mathbf{w}}(\theta)=\int_0^\infty d\xi[c_1(\xi)Y(\chi(i\xi,\theta))+c_2(\xi)Y(\overline{\chi(}i\xi,\theta))+c_3(\xi)Y(\chi(\xi,\theta))+c_4(\xi)Y(\overline{\chi(}\xi,\theta))]$$
$$+d_1Y(\chi_1(\theta))+d_2Y(\overline{\chi_1}(\theta))+d_3\,\frac{\partial}{\partial\xi}\,Y(\chi(\xi,\theta))\Big|_{\xi_1}+d_4\,\frac{\partial}{\partial\xi}\,Y(\overline{\chi(}\xi,\theta))\Big|_{\xi_1}. \tag{B4}$$

Finally, from (B1) and (B2) and (3.8) one observes that

$$Y(\chi(i\xi,\theta))=-\frac{i}{\xi}\,\psi_1(k(\xi),\theta),\quad Y(\overline{\chi(}i\xi,\theta))=-\frac{i}{\xi}\,\psi_2(k(\xi),\theta),$$

$$Y(\chi(\xi,\theta))=\frac{1}{\xi}\,\psi_3(-k(\xi),\theta),\quad Y(\overline{\chi(}\xi,\theta))=\frac{1}{\xi}\,\psi_4(-k(\xi),\theta), \tag{B5}$$

with in (B5) $\xi>0$. Notice that (B5) is in accordance with (3.13). Thus formula (3.14) is justified.

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Stationary problems for equation of the KdV type and dynamical *r*-matrices

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We study a new quite general family of dynamical r-matrices for an auxiliary loop algebra $\mathscr{L}(su(2))$ related to restricted flows for equations of the KdV type. This underlying r-matrix structure allows us to reconstruct Lax representations and to find variables of separation for a wide set of the integrable natural Hamiltonian systems. © *1996 American Institute of Physics.* [S0022-2488(96)01906-8]

I. INTRODUCTION

The main aim of this paper is to study the r-matrix formulation for mechanical systems embedded as restricted flows into KdV type equations and to investigate its connection with Lax representations and with the method of separation of variables. Lax representations are essential for solving these mechanical systems either by linearization on the Jacobian of determinant curve of the Lax matrix or by determining variables of separation through the functional Bethe ansatz.[1,2]

Restricted flows are easiest understood as stationary flows of soliton hierarchies with sources.[3] Many well known integrable mechanical systems, such as Henon-Heiles, Garnier, Neumann (and many others) can be embedded into the KdV and other soliton hierarchies as restricted flows.[4]

The main advantage of such embedding is that important structure elements for restricted flows, such as Lax representation, bi-Hamiltonian formulation, Newton parametrization[5] can be systematically derived from the underlying soliton hierarchies. But it is not the case, as yet, for the r-matrix formulation of these mechanical systems. There is no direct way of transporting the well known r-matrix formulation for soliton hierarchies[6] to their stationary and restricted flows. The underlying r-matrix structure for finite-dimensional systems appears to be more complicated than for integrable PDE's. A new type of, so called, dynamical r-matrices depending both on the spectral parameter and on dynamical variables has to be considered. The first example of such an r-matrix has been found for the Calogero–Moser system[7] and then for the parabolic and elliptic separable potentials.[8,9,10]

It appears that the parabolic and elliptic r-matrices belong to a quite general family of dynamical r-matrices which we introduce in this paper through a convenient ansatz which generalizes our r-matrix from Refs. 9 and 10. We study the general algebraic properties of these r-matrices and derive Lax representations through proper specializations. These specializations are guided by the known integrable cases of natural Hamiltonian systems related to restricted flows for equations of the KdV type.[3,9] Further we use these Lax representations for finding variables of separation and explain how starting with variables of separation these Lax representations can be reconstructed by using the Sklyanin approach.[1,2]

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The paper is organized as follows.

In section II we consider additive algebraic deformations of linear r-matrix algebras on an auxiliary loop algebra $\mathbf{g}=\mathscr{L}(\mathrm{su}(2))$. Kernels of these r-matrices have either rational, trigonometric and elliptic dependence on the spectral parameter.[6,11,12] We consider deformations $L(\lambda)=L_0(\lambda)+F(\lambda)\in\mathscr{L}(\mathrm{su}(2))$ of a certain Lax matrix $L_0(\lambda)\in\mathscr{L}(su(2))$, which satisfies the standard r-matrix brackets. These deformed Lax matrices obey a dynamical rs-matrix algebra. From dynamical point of view the deformed Lax matrices correspond to systems with additively shifted integrals of motion,

$$I_k^{new}=I_k^{old}+f_k.$$

Further, for r-matrices of the XXX and XXZ type we consider projection of deformations $F(\lambda)$ on finite-dimensional Poisson (ad_R^*-invariant) subspaces $\mathscr{L}_{M,N}(\mathrm{su}(2))$. Their Lax matrices $L_{MN}(\lambda)$ obey the rs-matrix brackets as well. At the end of section II we construct Lax pairs from the rs-matrix algebra and prove that these Lax pairs are related to stationary flows for equations of the KdV type.

In section III we express matrix elements of the matrices $L_0(\lambda)$ and $L_{MN}(\lambda)$, defined on a direct sum of loop algebras $\oplus\mathscr{L}(\mathrm{su}(2))$, through canonically conjugated variables of separation and prove that these matrices obey the rs-matrix brackets. Such matrices describe a geodesic motion and a potential motion on a Riemannian manifold with complex diagonal meromorphic Riemannian metrices of a special type. Corresponding potentials are the finite gap potentials on these manifolds. The problem of quantization is discussed briefly.

In section IV we consider finite-dimensional integrable systems of natural type and investigate three types of canonical transformations of variables prescribed by the linear r-matrix structure. Two of these are pure coordinate transformations to generalized elliptic coordinates and to Jacobi coordinates, while the third one provides an example of a momentum dependent change of variables. We exemplify our approach with a quartic potential of two degrees of freedom.

In the concluding remarks we discuss shortly an application of our constructions to other nonlinear integrable PDE's such as the AKNS and the sine-Gordon hierarchies.

II. DEFORMATIONS OF LINEAR *r*-MATRIX ALGEBRA

We shall use basic algebraic constructions in the r-matrix scheme for loop algebras in accordance with Refs. 12 and 13.

In this paper we consider the loop algebra $\mathscr{L}(\mathbf{a})$ under Lie algebra $\mathbf{a}=\mathrm{su}(2)$ only and shall use tensor form of r-brackets which is more common in the inverse scattering method.[6,11,14] We also fix the representation of the algebra su(2) and shall work in the matrix notation, although the underlying constructions are independent of particular matrix representation. In the following we shall consider spin one half representations of su(2) or shall use the direct sum of these representations. This means that we restrict ourselves to two-dimensional auxiliary space in which su(2) matrices act.

There are two important Lie–Poisson brackets (R-brackets)[12,13] which can be considered as linear classical limit of the fundamental commutator relations in the quantum inverse scattering method.[15,11] They are the r-bracket,

$$\{\overset{1}{L}(\lambda),\overset{2}{L}(\mu)\}=[r(\lambda,\mu),\overset{1}{L}(\lambda)+\overset{2}{L}(\mu)], \tag{II.1}$$

and the rs-bracket,

$$\{\overset{1}{L}(\lambda),\overset{2}{L}(\mu)\}=[r(\lambda,\mu),\overset{1}{L}(\lambda)+\overset{2}{L}(\mu)]+[s(\lambda,\mu),\overset{1}{L}(\lambda)-\overset{2}{L}(\mu)], \tag{II.2}$$

which is related to the reflection equations.[15,10] Here we use the standard notations $\overset{1}{L}(\lambda) = L(\lambda) \otimes I$, $\overset{2}{L}(\mu) = I \otimes L(\mu)$. The brackets (II.1)–(II.2) are Lie–Poisson brackets, if the matrices $r(\lambda,\mu)$ and $s(\lambda,\mu)$ satisfy the modified classical Yang–Baxter equations.[12,13]

For a traceless 2×2 matrix $L_0(\lambda)$ (which we shall call Lax matrix),

$$L_0(\lambda)=\sum_{k=1}^{3} s_k(\lambda)\cdot\sigma_k, \tag{II.3}$$

which obeys the linear r-matrix algebra (II.1) the r-matrix is an antisymmetric function of one argument $r(\lambda,\mu)\equiv r(\lambda-\mu)$ and $r(\lambda)=-r(-\lambda)$. Namely, put

$$r(\lambda)=\sum_{k=1}^{3} w_k(\lambda)\cdot\sigma_k\otimes\sigma_k. \tag{II.4}$$

The σ_k are Pauli matrices and coefficients $w_k(\lambda)$ are functions of spectral parameter only. They are determined by construction of the R-matrix on loop algebra $\mathcal{L}(\mathbf{a})$[12,13] or by the requirement that the r-matrix obeys classical Yang–Baxter equations.[6,11,14] In the quantum inverse scattering method r-matrices with rational, trigonometric and elliptic dependence on the spectral parameter are called r-matrices of XXX, XXZ and XYZ types, respectively.[6,11,14]

It follows from the algebra (II.1) that the determinant $d_0(\lambda)\equiv\det L_0(\lambda)$ can be taken as a generating function of commuting integrals of motion I_k since

$$\{d_0(\lambda),d_0(\mu)\}=0,\quad d_0(\lambda)=\sum_k I_k\lambda^k,\quad \lambda,\mu\in\mathbf{C}\ \text{ implies }\ \{I_k,I_j\}=0. \tag{II.5}$$

A similar property is valid for the rs-algebra (II.2) too.

Here we consider deformations $L(\lambda)\in\mathcal{L}(\mathbf{a})^*$ of the Lax matrix $L_0(\lambda)\in\mathcal{L}(\mathbf{a})^*$ with $\mathbf{a}=su(2)$. The main stimulus for considering such deformations has been inspired by the study of Lax representation and r-matrix formulation for restricted flows of the KdV and coupled KdV hierarchies,[3,9] which describe many physically interesting integrable natural Hamiltonian systems such as Neumann, Garnier, Henon-Heiles systems and an infinite family of integrable polynomial potentials.[16]

Now we find a new natural generalization of this result where the deformed matrix $L(\lambda)$ belongs the same phase space. The additive deformation of $L_0(\lambda)$ has the form

$$L(\lambda)=\sum_{k=1}^{3}\left(s_k(\lambda)+\alpha_k(\lambda)\cdot\frac{f(\lambda)}{2\tilde{b}(\lambda)}\right)\cdot\sigma_k=L_0(\lambda)+F(\lambda), \tag{II.6}$$

where

$$\tilde{b}(\lambda)=\sum_{i=1}^{3}\alpha_i(\lambda)s_i(\lambda), \tag{II.7}$$

and

$$\alpha_1^2(\lambda)+\alpha_2^2(\lambda)+\alpha_3^2(\lambda)=0. \tag{II.8}$$

Here functions $\alpha_j(\lambda)$ and the arbitrary function $f(\lambda)$ are complex-valued functions of the spectral parameter λ only. The condition (II.8) guarantees that determinant of $L(\lambda)$ has the additive property

$$d(\lambda)=d_0(\lambda)+f(\lambda),$$

which means that integrals of the motion $d(\lambda)=\Sigma\ I_k\lambda^k$ of the deformed integrable systems differ by some constants,

$$I_k^{new}=I_k^{old}+f_k, \quad f_k\in\mathbf{C}.$$

The requirement that the deformed Lax matrix $L(\lambda)$ satisfy the rs-bracket (II.2) with the same r-matrix $r(\lambda-\mu)$ yields four algebraic equations for the unknown functions $\alpha_k(\lambda)$, $k=1,2,3$ and a certain function $g(\lambda,\mu)$.

Theorem 1: *The deformed Lax matrix (II.6)–(II.8) satisfies the linear rs-algebra (II.2), if*

$$w_j(\lambda,\mu)\alpha_j(\mu)\alpha_i(\lambda)-w_i(\lambda,\mu)\alpha_i(\mu)\alpha_j(\lambda)=g(\lambda,\mu)\cdot\alpha_k(\lambda), \tag{II.9}$$

where (j,i,k) *are cyclic permutations of indices* $(1,2,3)$ *and the scale function* $g(\lambda,\mu)$ *depends only on the spectral parameters* λ *and* μ. *The corresponding matrix* $s(\lambda,\mu)$ *is given by*

$$s(\lambda,\mu)=\sum_{i,j=1}^{3}\alpha_{ij}(\lambda,\mu)\sigma_i\otimes\sigma_j, \tag{II.10}$$

with

$$\alpha_{ij}(\lambda,\mu)=w_i(\lambda,\mu)\cdot g(\lambda,\mu)\cdot\frac{\alpha_i(\mu)\alpha_j(\mu)f(\mu)}{\tilde{b}^2(\mu)}-w_j(\lambda,\mu)\cdot g(\mu,\lambda)\cdot\frac{\alpha_i(\lambda)\alpha_j(\lambda)f(\lambda)}{\tilde{b}^2(\lambda)}. \tag{II.11}$$

Proof: The proof is a direct but lengthy computation.

Notice that the function $f(\lambda)$ is quite arbitrary here. A compact form of the equation (II.9) follows from the ideas of Sklyanin in Ref. 1:

Lemma 1: The condition (II.9) of Theorem 1 for the coefficients $\alpha_k(\lambda)$ *is equivalent to the equation*

$$\{\tilde{b}(\lambda),\tilde{b}(\mu)\}=g(\lambda,\mu)\cdot\tilde{b}(\lambda)-g(\mu,\lambda)\cdot\tilde{b}(\mu). \tag{II.12}$$

Proof: This lemma is proved by direct substitution of the equality (II.9) into the equation (II.12) and vice versa.

Let us present some of the best known[6,11,14] r-matrices and the related solutions for $\alpha_k(\lambda)$ and $g(\lambda,\mu)$. The r-matrix of the XXX and XXZ types are

$$w_1=w_2\equiv w(\lambda)=\frac{\eta}{\varphi(\lambda)} \quad \text{and} \quad w_3(\lambda)=\frac{\eta\varphi'(\lambda)}{\varphi(\lambda)},$$

with

$$\varphi(\lambda)=\lambda \quad \text{in the } XXX \text{ case}, \tag{II.13}$$

and

$$\varphi(\lambda)=\sinh\lambda \quad \text{in the } XXZ \text{ case}; \tag{II.14}$$

here η is constant and $\varphi'(\lambda)$ denotes the derivative with respect to λ.

An interesting particular class of solutions to equations (II.8)–(II.9) is distinguished by the conditions

$$\alpha_3=0, \quad \alpha_1^2+\alpha_2^2=0. \tag{II.15}$$

They represent two points on the circle in complex plane with the phase difference equal to $\pi/2$, for instance $\alpha_1=1$, $\alpha_2=i$. For these solutions the function $g(\lambda,\mu)$ is equal to zero ($g(\lambda,\mu)=0$). A different example of solutions for r-matrix of XXZ type is

$$\alpha_1=\cosh\lambda, \quad \alpha_2=i\sinh\lambda, \quad \alpha_3=i.$$

Usually one uses the following rational parametrization for an r-matrix of the XXZ type:

$$w_1(u-v)=w_2(u-v)=\eta\frac{2uv}{u^2-v^2}, \quad w_3(u-v)=\eta\frac{u^2+v^2}{u^2-v^2}, \tag{II.16}$$

$$\varphi(u)=u-\frac{1}{u}, \quad \text{with } u=e^{\lambda}, \quad v=e^{\mu},$$

as, for example, in the description of the sine-Gordon equation.[6]

An elliptic r-matrix of the XYZ type has

$$w_1(\lambda)=\eta\frac{\Theta_{11}'}{\Theta_{10}}\frac{\Theta_{10}(\lambda,k)}{\Theta_{11}(\lambda,k)}, \quad w_2(\lambda)=\eta\frac{\Theta_{11}'}{\Theta_{00}}\frac{\Theta_{00}(\lambda,k)}{\Theta_{11}(\lambda,k)}, \tag{II.17}$$

$$w_3(\lambda)=\eta\frac{\Theta_{11}'}{\Theta_{01}}\frac{\Theta_{01}(\lambda,k)}{\Theta_{11}(\lambda,k)},$$

with

$$\alpha_1=-1; \quad \alpha_2=\frac{i}{k}\frac{\mathrm{dn}(\lambda,k)}{\mathrm{cn}(\lambda,k)}, \quad \alpha_3=\frac{k'}{k}\frac{1}{\mathrm{cn}(\lambda,k)}.$$

Here k and k' denote modulus of the Jacobi elliptic functions and $\Theta_{ij}(\lambda,k)$ are the elliptic theta function in the notation of Ref. 15. We have to emphasize that the functions $\tilde{b}(\lambda)$ (II.7) with the coefficients $\alpha_k(\lambda)$ (II.17) and the function $g(\lambda,\mu)$ were introduced in Ref. 1 for the quadratic r-matrix algebra as a solution of the equation (II.12). The function $g(\lambda,\mu)$ is independent from the second parameter μ function and it is equal to

$$g(\lambda,\mu)=\eta\frac{\Theta_{11}'}{\Theta_{10}}\frac{\Theta_{10}(\lambda-K,k)}{\Theta_{11}(\lambda-K,k)}.$$

This solution has a natural relation with a similar transformation of the Lax matrix $L_0(\lambda)$ introduced in Ref. 15.

It is well known that r-brackets (II.1) are the Lie–Poisson brackets if the r-matrix obeys the classical Yang–Baxter equations.[6,12,13] The Yang–Baxter equation is an equation on matrices in the space $\mathbf{C}^2\otimes\mathbf{C}^2\otimes\mathbf{C}^2$. We use the familiar tensor notations L_j for the matrix acting as matrix L in the j's factor of the product and trivially acting in the remaining factors, for example $L_1=L\otimes I\otimes I$. In similar way a matrix r_{ij} is acting trivially in the third k's factor and it works as a matrix r in the product of the other ij's factors. The classical Yang–Baxter equation for pure numerical r-matrices has the form

$$[d_{12}^{\pm}(\lambda,\mu),d_{13}^{\pm}(\lambda,\nu)]+[d_{12}^{\pm}(\lambda,\mu),d_{23}^{\pm}(\mu,\nu)]+[d_{32}^{\pm}(\nu,\mu),d_{13}^{\pm}(\lambda,\nu)]=0. \tag{II.18}$$

Following[7,8] we introduce dynamical Yang–Baxter equations for this new family of a dynamical rs-matrix. Let us consider matrices $d^{\pm}\equiv r\pm s$ corresponding to a particular class of solutions α_k (II.15).

Theorem 2: *For the rs-algebra (II.2) with matrices (II.4)–(II.11), the following equations are valid:*

$$[d^{\pm}_{12}(\lambda,\mu),d^{\pm}_{13}(\lambda,\nu)]+[d^{\pm}_{12}(\lambda,\mu),d^{\pm}_{23}(\mu,\nu)]+[d^{\pm}_{32}(\nu,\mu),d^{\pm}_{13}(\lambda,\nu)]+[L_2(\mu),d^{\pm}_{13}(\lambda,\nu)]$$
$$-[L_3(\nu),d^{\pm}_{12}(\lambda,\mu)]+[X(\lambda,\mu,\nu),L_2(\mu)-L_3(\nu)]=0. \tag{II.19}$$

The matrix $X(\lambda,\mu,\nu)$ *is*

$$X(\lambda,\mu,\nu)=\beta(\lambda,\mu,\nu)\cdot\sigma_-\otimes\sigma_-\otimes\sigma_-,$$
$$\beta(\lambda,\mu,\nu)=\frac{f(\lambda)b^{-3}(\lambda)\cdot(\mu-\nu)+f(\mu)b^{-3}(\mu)\cdot(\nu-\lambda)+f(\nu)b^{-3}(\nu)\cdot(\lambda-\mu)}{(\lambda-\mu)(\mu-\nu)(\nu-\lambda)}. \tag{II.20}$$

The other two equations are obtained from (II.19) by cyclic permutation.

Proof: This Theorem also can be proved by a straightforward computation.

Tensor $X(\lambda,\mu,\nu)$ is a completely symmetric tensor with respect to any permutations of auxiliary spaces. For the quite arbitrary solutions α_k to the equations (II.8)–(II.9) we can introduce an asymmetric tensor $X^{(i,j,k)}(\lambda,\mu,\nu)$. Then dynamical Yang–Baxter equations take the general form introduced in Ref. 7.

Now we consider the special deformations of the XXX and XXZ cases using the list of formulas collected in Refs. 8, 9, 10 and on meaning its in general rs-matrix approach to loop algebras.

Our purpose is to apply the rs-matrix formulation for description of natural Hamiltonian systems in order to solve them through separation of variables. For separating variables we shall apply the functional Bethe ansatz.[1,2] Using similar transformations of the Lax matrix $L_0(\lambda)$ and corresponding renormalization of the Baker–Akhiezer vector-function we can restrict ourselves to a particular class of deformations obtained by certain projections of the matrix,

$$L(\lambda)=\begin{pmatrix} a & b \\ f(\lambda)b^{-1}+c & -a\end{pmatrix}(\lambda)=L_0(\lambda)+\begin{pmatrix} 0 & 0 \\ f(\lambda)b^{-1} & 0\end{pmatrix}. \tag{II.21}$$

Also, we shall require that entries of $L_0(\lambda)$ be the absolutely convergent Laurent series in the XXX case or the absolutely convergent Fourier series in the XXZ case,

$$a(\lambda)=\sum_k a_k\lambda^k \quad \text{or} \quad a(\lambda)=\sum_k a_k\exp(k\cdot\lambda) \tag{II.22}$$

for XXX and XXZ cases, respectively, and similarly for $b(\lambda)$ and $c(\lambda)$.

It is well known[12] that the standard R-bracket on $\mathcal{S}(\mathbf{a})^*$ associated with a general R-brackets has a large collection of finite-dimensional Poisson (ad^*_R-invariant) subspaces,

$$\mathcal{S}_{M,N}=\oplus_{j=-M}^{N}\mathbf{a}^*\lambda^j, \quad \text{provided } M\geqslant 0;\ N\geqslant -1. \tag{II.23}$$

In other words the subspaces $\mathcal{S}_{M,0}$ and $\mathcal{S}_{1,N}$ are invariant under the coadjoint action of the subalgebras $\mathbf{g}_+$ and $\mathbf{g}_-$.[12].

Let us introduce the following projection operators $[\cdot]_{MN}$ on these Poisson subspaces:

$$[z]_{MN}=\left[\sum_{k=-\infty}^{+\infty} z_k\lambda^k\right]_{MN}\equiv\sum_{k=-M}^{N} z_k\lambda^k,$$
$$[z]_{MN}=\left[\sum_{k=-\infty}^{+\infty} z_k\exp(k\cdot\lambda)\right]_{MN}\equiv\sum_{k=-M}^{N} z_k\exp(k\cdot\lambda), \tag{II.24}$$

for the Laurent and for the Fourier series.

We shall define a new additive deformation of $L_0(\lambda)$ as

$$L_{MN}(\lambda)=L_0(\lambda)+F_{MN}(b,\lambda)\equiv\begin{pmatrix} a & b \\ G_{MN}(b,\lambda)+c & -a\end{pmatrix}(\lambda), \tag{II.25}$$

where $G_{MN}(b,\lambda)$ is a function of the spectral parameter λ and of the entry $b(\lambda)$. It reads as

$$G_{MN}(b,\lambda)=[f(\lambda)\cdot b^{-1}(\lambda)]_{MN}, \tag{II.26}$$

$$f(\lambda)=\sum_{k=-\infty}^{\infty} f_k\lambda^k,\quad \text{or}\quad f(\lambda)=\sum_{k=-\infty}^{\infty} f_k\exp(k\lambda). \tag{II.27}$$

The essential feature of this deformation is, in comparison with (II.6), that the determinant of the modified matrix $L_{MN}(\lambda)$ is different from $d_0(\lambda)+f(\lambda)$,

$$d(\lambda)=d_0(\lambda)+b\cdot G_{MN}\neq d_0(\lambda)+f(\lambda),$$

and therefore integrals of motion I_k^{new} of the deformed system are functionally different from the undeformed integrals I_k^{old}, and yet the $L_{MN}(\lambda)$ matrix belongs to a certain rs-algebra.

Theorem 3: *The matrix $L_{MN}(\lambda)$ (II.25) satisfies the linear rs-matrix algebra (II.2), with the matrix $s_{MN}(\lambda,\mu)$ given by*

$$s(\lambda,\mu)=\alpha_{MN}(\lambda,\mu)\sigma_-\otimes\sigma_-,\quad \sigma_-=\begin{pmatrix}0&0\\1&0\end{pmatrix}.$$

The function $\alpha_{MN}(\lambda,\mu)$ is defined by

$$\alpha_{MN}(\lambda,\mu)=-w(\lambda-\mu)([f(\lambda)b^{-2}(\lambda)]_{MN}-[f(\mu)b^{-2}(\mu)]_{MN}), \tag{II.28}$$

where $w(\lambda)\equiv w_1(\lambda)=w_2(\lambda)$.

Proof: The proof is a straightforward calculation.

The Theorem 3 has a transparent meaning in the framework of the general r-matrix approach to loop algebras. The Theorem 3 asserts that the matrix $s(\lambda,\mu)$ can be restricted to subspaces $\mathscr{S}_{M,N}$ (II.23) and subspaces $\mathscr{S}_{M,N}$ is a common Poisson subspace for the rs-brackets (II.2) with matrix $s_{MN}=[s(\lambda,\mu)]_{MN}$. Since the deformations (II.3) are directly connected with the KdV equation,[9] matrices $d^{\pm}=r\pm s_{MN}$ obey dynamical Yang–Baxter equations, which are obtained by restriction of the equation (II.19)–(II.20) to the corresponding subspace $\mathscr{S}_{MN}$. For certain matrices $L_{MN}(\lambda)$ and s_{MN} this proposition has been proved in Ref. 8.

In order to describe Lax representations for integrable Hamiltonian systems related to matrices $L_0(\lambda)$ and $L_{MN}(\lambda)$ we introduce matrices[12,13]

$$d_{12}(\lambda,\mu)=r(\lambda,\mu)+s(\lambda,\mu),\quad \text{and}\quad d_{21}(\lambda,\mu)=r(\lambda,\mu)-s(\lambda,\mu).$$

In terms of these matrices the Lie–Poisson rs-brackets read as

$$\{\overset{1}{L}(\lambda),\overset{2}{L}(\mu)\}=[d_{12}(\lambda,\mu),\overset{1}{L}(\lambda)]+[d_{21}(\lambda,\mu),\overset{2}{L}(\mu)]. \tag{II.29}$$

For constructing Lax representations we shall make use of the following lemma.[6]

Lemma 2: If matrix $L(\lambda)$ *obeys the Lie–Poisson algebra (II.29) then the spectral invariants,*

$$H_n(\lambda)=\mathrm{tr}(L^n), \quad n=1,2,\ldots;, \tag{II.30}$$

are integrals of motion in involution $\{H_n,H_m\}=0$ *and the Lax equation are given by*

$$\dot{L}(\mu)=\{H_n(\lambda),L(\mu)\}=[M_n(\lambda,\mu),L(\mu)], \tag{II.31}$$

with

$$M_n(\lambda,\mu)=n\ \mathrm{tr}_1(\overset{1}{L}{}^{n-1}(\lambda)d_{21}(\lambda,\mu)), \quad n=1,2\ldots, \tag{II.32}$$

where tr_1 *means a trace in the first auxiliary space and a dot over L means a derivative with respect to time corresponding to the Hamiltonian* $H_n(\lambda)$. In two dimensional auxiliary space $d(\lambda)\equiv\det L(\lambda)=-\frac{1}{2}(\mathrm{tr}(L^2)=-\frac{1}{2}H_2(\lambda))$.

In order to get a Hamiltonian H, which does not depend on the spectral parameter, one needs a linear functional (a projection) Φ_λ which selects, for example (in the *XXX* case), a coefficient at certain power of λ,

$$H=\tfrac{1}{2}\,\Phi_\lambda[H_2(\lambda)]=\Phi_\lambda[d(\lambda)]. \tag{II.33}$$

For instance, it can be defined as a residue of order m at λ_0,

$$\Phi_\lambda[z]=\mathrm{Res}^m_{\lambda_0} z(\lambda)=\frac{1}{(m-1)!}\,\frac{d^{m-1}}{d\lambda^{m-1}}\,((\lambda-\lambda_0)^m z(\lambda))\bigg|_{\lambda=\lambda_0}. \tag{II.34}$$

Then the Lax representation for the Lax matrices [(II.3) or (II.21)] with the Hamiltonian (II.33) has the form

$$\begin{gathered}\dot{L}(\mu)=\{H,L(\mu)\}=\{\tfrac{1}{2}\,\Phi_\lambda[\mathrm{tr}_1\overset{1}{L}{}^2(\lambda)],L(\mu)\}=[M(\mu),L(\mu)],\\ M(\mu)=\Phi_\lambda[\mathrm{tr}_1(\overset{1}{L}(\lambda)\cdot d_{21}(\lambda,\mu))]=\Phi_\lambda[M(\lambda,\mu)].\end{gathered} \tag{II.35}$$

In particular, for the initial Lax matrix L_0 (II.3) one gets $s=0$; $d_{21}(\lambda,\mu)=r(\lambda-\mu)$ and then

$$\dot{L}_0(\mu)=[M_0(\mu),L_0(\mu)] \quad \text{and} \quad M_0(\mu)=\Phi_\lambda\left[2\sum_{k=1}^{3} s_k(\lambda)\cdot w_k(\lambda-\mu)\cdot\sigma_k\right]. \tag{II.36}$$

In this paper we start with the requirement that

$$M_0=\sigma_+\equiv\begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix} \tag{II.37}$$

and choose $L_0(\lambda)$ and Φ_λ appropriately. It is a rather strong restriction for the matrices L_0 (II.3) and for the corresponding Hamiltonians. This requirement comes from the study of rs-representations for natural Hamiltonian systems related to stationary flows for equations of KdV type.[9,10]

As an immediate consequence of the Lax representation (II.35) with the matrix M_0 (II.37) we can rewrite the Lax matrix L_0 in the form

$$L_0(\mu)=\begin{pmatrix} -\frac{b_x}{2} & b \\ -\frac{b_{xx}}{2} & \frac{b_x}{2} \end{pmatrix}, \quad b_x=\{H_0,b\}, \tag{II.38}$$

where H_0 is a Hamiltonian corresponding to L_0. Since the determinant of $L_0(\lambda)$ is a generating function of integrals of motion, we see that it obeys the equation

$$-\{H_0,d_0(\lambda)\}=-d_{0,x}(\lambda)=\partial_x^3\cdot b=b_{xxx}=0. \tag{II.39}$$

Now for a fixed triad (L_0,M_0,Φ_λ) we introduce a modified matrix $L(\lambda)$ (II.21). In this case the matrix $M(\mu)$ is constructed according to (II.35) with $d_{21}(\lambda,\mu)=r-s$ and with the use of the same projector Φ_λ. It reads as

$$M(\mu)=\begin{pmatrix} 0 & 1 \\ -u(\mu) & 0 \end{pmatrix}, \quad u(\mu)=f(\mu)b^{-2}(\mu), \tag{II.40}$$

due to the linearity of Φ_λ,

$$\begin{aligned}&\Phi_\lambda[w_1\cdot(-f(\lambda)b^{-1}(\lambda)+c(\lambda)+(f(\lambda)b^{-2}(\lambda)-f(\mu)b^{-2}(\mu))\cdot b(\lambda))]\\ &\quad=-f(\mu)b^{-2}(\mu)=-u(\mu).\end{aligned} \tag{II.41}$$

Then from the Lax representation (II.35) it follows that the deformed matrix $L(\lambda)$ has to be equal to

$$L(\lambda)=\begin{pmatrix} -\frac{b_x}{2} & b \\ -b(\lambda)u(\lambda)-\frac{b_{xx}}{2} & \frac{b_x}{2} \end{pmatrix}, \quad b_x=\{H,b\}, \tag{II.42}$$

where the Hamiltonian $H=\Phi_\lambda[d(\lambda)]$ is obtained by applying the old projector Φ_λ to the modified determinant. The determinant $d(\lambda)$ of the modified matrix $L(\lambda)$ obeys the equation

$$-d_x(\lambda)=\left(\frac{1}{4}\,\partial_x^3+u\partial_x+\frac{1}{2}\,u_x\right)\cdot b=B_1[u]\cdot b=0. \tag{II.43}$$

Here $B_1[u]$ is the Hamiltonian pencil operator for the coupled KdV equation.[4,3]

For the deformed [according to (II.25)] matrix $L_{MN}(\lambda)$ the Lax equation is constructed analogously (II.40)–(II.42) and (II.43). One has to replace $u(\mu)=f(\mu)b^{-2}(\mu)$ with the potential $u_{MN}(\mu)=[f(\mu)b^{-2}(\mu)]_{MN}$.

Equation (II.43) shows that our deformation is connected to the stationary problems for equations of the KdV type. The Hamiltonian and some properties of motion for the finite-dimensional integrable systems connected with stationary flows of the KdV equations were considered in Refs. 17, 18. Lax representations, bi-Hamiltonian structures, Newton representations

and some other properties for these systems were introducing in Refs. 4, 5 through the method of the restricted flows for nonlinear equations. Some particular systems were studied in the r-matrix approach.[8,9,10] In the next section we tie these different methods to the Lie algebraic method of constructing matrices $L(\lambda)$ on the loop algebras.

In the next section we shall assume that the Lax matrix M_0 has the form

$$M_0=\begin{pmatrix} v_0 & u_0 \\ 0 & -v_0 \end{pmatrix}. \tag{II.44}$$

It introduces certain technical complications without influence on the conceptual structure.

III. CONSTRUCTION OF LAX MATRICES $L(\lambda)$ FOR SEPARABLE SYSTEMS

The main problem for a given integrable Hamiltonian system with a complete set of functionally independent and commuting integrals of motion $H_1,\ldots,H_n$ is to determine its solutions. The construction in the Liouville theorem has a local character and there is no general way to describe solutions globally unless some additional information about the system is known, such as a complete, spectral parameter dependent Lax representation or variables of separation.

For the Lax matrices $L_0(\lambda)$ satisfying r-matrix algebra with the r-matrix of the XXX, XXZ and XYZ types the problem of determining variables of separation has been essentially solved by Sklyanin.[2]

Proposition 1 (Sklyanin[1,2]): Take the poles of the properly normalized Baker–Akhiezer function and the corresponding eigenvalues of the Lax matrix and you obtain the separation of variables. It turns out that in the case of the $GL(N)$-invariant r-matrix the normalization of the Baker–Akhiezer function corresponding to any constant numeric vector produces separation of variables.

In our case $N=2$ and coordinates u_k, v_k, $k=1,\ldots,n$ defined as

$$b(\lambda=u_k)=0, \quad v_k=a(\lambda=u_k), \tag{III.1}$$

are canonically conjugate variables of separation and corresponding separation equations are

$$v_k^2=-d(u_k), \tag{III.2}$$

where $d(\lambda)\equiv\det L(\lambda)$.

A general construction of matrices $L_0(\lambda)$ with multiple poles on a direct sum of loop algebras $\oplus\mathscr{L}(su(2))$ has been presented in detail in Ref. 12. The Lax matrix is assumed in the form

$$L_0(\lambda)=\sum_{\alpha=1}^{3}\sum_{j}^{N} s_j^{\alpha} w_{\alpha}(\lambda-\nu_j)\sigma_{\alpha}, \tag{III.3}$$

where σ_α are Pauli matrices, $w_\alpha(\lambda)$ are coefficients of the corresponding r-matrix and ν_j are simple poles of the fixed divisor $D=\{\nu_1,\ldots,\nu_N\}$. Residues s_j^α are the standard linear coordinates on $su(2)^*$ with Lie-Poisson brackets,

$$\{s_j^{\alpha},s_k^{\beta}\}=\delta_{jk}\epsilon_{\alpha\beta\gamma}\cdot s_j^{\gamma}.$$

The corresponding phase space is the direct sum of N copies $su(2)^*$. These matrices describe systems of N interacting Euler tops. The case of higher order of poles can be treated as a degeneration of (III.3). It describes different tops[12] as well. For all these system we can apply a procedure of separation of variables.

In contrast to Ref. 12, we provide a solution of the converse problem of how to construct Lax matrices $L(\lambda)$ satisfying the rs-matrix algebra for an integrable system given in terms of variables

of separation. We express first $L(\lambda)$ in terms of variables of separation (u_k, v_k), $k=1,\ldots,n$ and then we shall use the canonical transformations naturally determining from the r-matrix structure to the ''physical'' variables (x_k, p_k), $k=1,\ldots,n$.

Let us take the meromorphic matrix-function $L_0(\lambda)$ and consider the coefficients $w_1(\lambda)=w_2(\lambda)$ of the r-matrices (II.13)–(II.14) with one distinguished point at infinity (it is zero by both arguments and their residues at infinity are equal to -1). Let us choose the linear functional Φ_λ as the higher residue fixed order K at infinity,

$$\Phi_\lambda[z] = -\mathrm{Res}_\infty^K z(\lambda). \tag{III.4}$$

Then (II.35) and (II.44) gives

$$-\mathrm{Res}_\infty^K\left[\frac{b(\lambda)}{\varphi(\lambda-\mu)}\right]=u_0, \quad -\mathrm{Res}_\infty^K\left[\frac{c(\lambda)}{\varphi(\lambda-\mu)}\right]=0, \tag{III.5}$$

$$-\mathrm{Res}_\infty^K\left[\frac{a(\lambda)\varphi'(\lambda-\mu)}{\varphi(\lambda-\mu)}\right]=v_0. \tag{III.6}$$

In particular $u_0=1$, $v_0=0$ for the matrix M_0 (II.37). In the XXX case it means that entries $b(\lambda)$ and $a(\lambda)$ have the highest in λ terms in power $K+1$ equal to u_0 and v_0, respectively. The entry $c(\lambda)$ has the highest term of order K only. Note that the conditions for the entry $a(\lambda)$ and $c(\lambda)$ (III.5)–(III.6) in the Lax pair (L_0, M_0) (II.37) follow from the first condition (III.5) for entry $b(\lambda)$ and from the definitions $a(\lambda)=-b_x/2=-\partial_x b/2$ and $c(\lambda)=-b_{xx}/2$, since the derivative ∂_x commutes with the functional Φ_λ.

Just as in Ref. 12 we can fix one divisor D consisting of poles in the matrix-function $L_0(\lambda)$ and a second divisor U consisting of zeroes of the entry $b(\lambda)$. Let them have the form

$$\begin{gathered} D=\{(e_j,m_j)j=1,\ldots,\tilde{m};\}, \quad U=\{(u_k,n_k)k=1,\ldots,\tilde{n};\}, \\ u_k\neq\infty, \quad \text{and} \quad e_j\neq u_k, \forall j,k, \end{gathered} \tag{III.7}$$

where D, $U\subset \mathbf{CP_1}=\mathbf{C}\cup\{\infty\}$ for the XXX model and D, $U\subset \mathbf{CP_1}/2\pi\mathbf{Z}$ for the XXZ model. We consider the simple zeroes u_k, $n_k\equiv 1$; $k=1,\ldots,n$, only. This restriction is related to the r-matrix structure. The poles at e_j can be multiple poles and their orders m_j are fixed. In the formulae below each pole is counted according to its multiplicity and we do not use special indices when it is clear from a context.

Now we introduce the following ansatz for the entry $b(\lambda)$:

$$\begin{gathered} b(\lambda)=u_0\cdot\frac{\Pi_{k=1}^n\varphi(\lambda-u_k)}{\Pi_{j=1}^m\varphi(\lambda-e_j)}, \\ \varphi(\lambda)\equiv w^{-1}(\lambda)=\lambda \quad \text{in the } XXX \text{ case}, \\ \varphi(\lambda)=\sinh\lambda \quad \text{in the } XXZ \text{ case}, \end{gathered} \tag{III.8}$$

where u_0 is either a constant or a dynamical variable. The function $\varphi(\lambda)$ depends from the type of the r-matrix and the functional Φ_λ (III.4) is residue with $K=1$ for $n<m$ and $K=n-m+1$ for $n\geqslant m$.

The entry $a(\lambda)$ has m poles at points e_j of the divisor D and its values at n points u_k are given $(a(\lambda=u_k)=v_k)$ (III.1). The asymptotic behavior at infinity is fixed by Lax representation (III.5). By a Lagrange interpolation formula the entry $a(\lambda)$ can be represented as

$$a(\lambda)=b(\lambda)\cdot\left(v_0+\sum_{i=1}^{n} v_i\cdot w_3(\lambda-u_i)\cdot g_{ii}\right),$$

where

$$g_{ii}=\left[\left.\frac{\partial b}{\partial\lambda}\right|_{\lambda=u_i}\right]^{-1}=\mathrm{Res}_{u_i}b^{-1}(\lambda)=\frac{\Pi_{j=1}^{m}\varphi(u_i-e_j)}{\Pi_{k\neq i}^{n}\varphi(u_i-u_k)}. \tag{III.9}$$

The $w_3(\lambda)=\varphi'(\lambda)/\varphi(\lambda)$ is the coefficient in the definition of the corresponding r-matrix. Variables u_0, v_0 are connected to the Lax matrix M_0 (II.44).

Further, from the Lax representation (II.38) for the initial matrix $L_0(\lambda)$, we can construct the entry $a(\lambda)$. It reads as

$$a(\lambda)=-\frac{b_x}{2}=\frac{b(\lambda)}{2}\cdot\left(-\frac{\dot u_0}{u_0}+\sum_{i=1}^{n}\dot u_i\cdot w_3(\lambda-u_i)\right), \tag{III.10}$$

where

$$\dot u_k\equiv u_{k,x}=\partial_x u_k,\quad \text{and}\quad w_3(\lambda)=\frac{\varphi'(\lambda)}{\varphi(\lambda)}. \tag{III.11}$$

We set now, for simplicity, $u_0=1$ and $v_0=0$ as in the Lax matrix (II.37). Definition of entry $c(\lambda)$ follows from (II.38) as well,

$$c(\lambda)=-\frac{b_{xx}}{2}=-\frac{a^2(\lambda)}{b(\lambda)}+\frac{b(\lambda)}{2}\cdot\sum_{i=1}^{n}\left(\ddot u_i w_3(\lambda-u_i)-\dot u_i^2\,\frac{\partial w_3(\lambda-u_i)}{\partial u_i}\right), \tag{III.12}$$

where $\ddot u_i$ and $\dot u_i$ are defined below.

From comparison of two forms of the entry $a(\lambda)$ (III.9) and (III.10) we can introduce the following Hamiltonian:

$$H_0=\sum_{i=1}^{n} v_i^2\cdot g_{ii}=\sum_{i=1}^{n} v_i^2\cdot\left[\left.\frac{\partial b(\lambda)}{\partial\lambda}\right|_{\lambda=u_i}\right]^{-1}, \tag{III.13}$$

using the Hamilton–Jacobi equations.

The remaining symbols in the entry $c(\lambda)$ are defined as

$$\dot u_i\equiv\frac{\partial H_0}{\partial v_i}=2\cdot v_i\cdot g_{ii},$$

$$\ddot u_i=2\sum_{j=1}^{m} v_i^2\cdot g_{ii}^2\cdot\frac{\varphi'(u_i-e_j)}{\varphi(u_i-e_j)}+2\sum_{k=1}^{n}\left[(v_k+v_i)^2 g_{ii}g_{kk}-v_i^2(g_{kk}-g_{ii})g_{ii}\right]\varphi(u_i-u_k)\varphi'(u_i-u_k),$$

where $\varphi(\lambda)=w_1^{-1}(\lambda)=\lambda$ or $\varphi(\lambda)=\sinh(\lambda)$. Then a direct calculation shows that the Hamiltonian (III.13) is equal to the Hamiltonian (II.33) $H_0=\Phi_\lambda[d_0(\lambda)]$.

The matrix $L_0(\lambda)$ with entries (III.8)–(III.9) and (III.12) obeys the r-matrix structure (II.1) as we can check it directly using the additive theorems for $\varphi(\lambda)$.

So, we have constructed the initial matrix $L_0(\lambda)$ in terms of variables of separation. From the initial matrices $L_0(\lambda)$ we can construct modified matrices $L_{MN}(\lambda)$ (II.25). These matrices describe integrable Hamiltonian system with the Hamiltonian $H=\Phi_\lambda[d(\lambda)]$ and a complete set of

the integrals of motion can be obtained from determinants of these matrices as well. The determinant $d(\lambda)$ is a meromorphic function with the divisors of poles determined by divisors of the entries of $L_0(\lambda)$ or of $L_{MN}(\lambda)$. Therefore the rational algebraic functions $d(\lambda)$ can be written as a quotient of two products or it can be decomposed into a simple fraction according to the Mittag-Leffler theorem,

$$d(\lambda)=\frac{P_d^N(\lambda)}{Q_d^m(\lambda)}=\frac{\Pi_{k=1}^N\varphi(\lambda-h_k)}{\Pi_{j=1}^m\varphi(\lambda-e_j)}=P_d^{N-m}(\lambda)+\sum_{j,i} H_{ji}\cdot\varphi^{-i}(\lambda-e_j)$$
$$=\prod_{k=1}^{N-m}\varphi(\lambda-H_k)+\sum_{j,i} H_{ji}\cdot\varphi^{-i}(\lambda-e_j), \qquad \text{(III.14)}$$

where $N=n$ for the initial matrix $L_0(\lambda)$. Both decompositions provide us with sets of integrals of motion.

So, zeroes h_k of the function $P_d^N(\lambda)$ can be chosen as a first set of integrals of motion in involution for the Hamiltonian systems related to the Lax matrices $L_0(\lambda)$ and $L_{MN}(\lambda)$. Zeroes H_k of the function $P_d^{N-m}(\lambda)$ and the residues H_{ji} at points e_j constitute a second set of the integrals of motion in involution. Integrals of motion I_k^{new} of the deformed system are functionally different from the undeformed integrals I_k^{old} and it reads as

$$I_k^{new}=I_k^{old}+V_k^{MN}(u_1,\ldots,u_n),$$

where $V_k^{MN}(u_1,\ldots,u_n)$ are functions on coordinates only. The proof of involutivity of I_k^{new} is based on the equality (II.5) and completeness and functional independence of these integrals follow from completeness and functional independence of I_k^{old}, which have been proved by Mishchenko and Fomenko (see the review[12]).

We summarize these considerations as the following.

Proposition 2: The Lax matrix $L_0(\lambda)$ (III.8), (III.9), (III.12) describes geodesic motions on the Riemannian manifold with the complex diagonal meromorphic Riemannian metrics,

$$g^{kj}=\delta_k^j\cdot\left[\frac{\partial b(\lambda)}{\partial\lambda}\bigg|_{\lambda=u_i}\right]^{-1}\cdot=\delta_k^j\cdot\frac{\Pi_{j=1}^m\varphi(u_i-e_j)}{\Pi_{k\neq i}^n\varphi(u_i-u_k)}, \qquad \text{(III.15)}$$

defined on moduli of n-dimensional Jacobi varieties in terms of complex elliptic (root) coordinates u_k. The Hamiltonian system (III.13),

$$H_0=\sum_i^n v_i^2 g_{ii},$$

has a complete system of first integrals v_k and it defines a Lagrangian submanifold of the phase space $\mathbf{C}^{2n}$ which has the form of symmetric product $((\Gamma\times\ldots\times\Gamma)/\sigma_n)$ of n copies of Riemannian surfaces,[18]

$$\Gamma: v_k^2=-d(\lambda)|_{\lambda=u_k}=-\left[\frac{P_d(\lambda)}{Q_d(\lambda)}\right]_{\lambda=u_k}. \qquad \text{(III.16)}$$

A modified Lax matrix $L_{MN}(\lambda)$ (II.25) describes potential motion on the same Riemannian manifold with a Hamiltonian of a natural type,

$$H=H_0+V_{MN}(u_1,u_2\ldots,u_n;f_{-M},f_{-M+1},\ldots,f_N), \qquad \text{(III.17)}$$

f_j are coefficients of the function $f(\lambda)=\Sigma\ f_k\lambda^k$ or of $f(\lambda)=\Sigma\ f_k e^{k\lambda}$. These matrices obey the rs-matrix structure (II.2) with the s_{MN}-matrix given by the Theorem 3.

For these systems we can define a Riemann matrix of periods of holomorphic differentials and by using the Abel–Jacobi map we can find the action-angle variables. The potentials V_{MN} are the finite gap potentials on these manifolds.[17,18] For details about geodesic and potential motion with metric (III.15) in the *XXX* case see Refs. 17,18.

Thus we have constructed initial matrices L_0 and modified matrices L_{MN} (II.21)–(II.25) which correspond to a geodesic motion and a potential motion on Riemannian manifolds with metric (III.15), respectively. For the *XXX* case the initial matrix $L_0(\lambda)$ (III.8), (III.9), (III.12) was considered in Ref. 19 and the Hamiltonian H_0 (III.13) describes free motion on Riemannian spaces of constant curvature.

The above results describe motions on a Jacobi variety $((\Gamma\times\ldots\times\Gamma)/\sigma_n)$ which is a symmetric product of uniform Riemannian surfaces,

$$\Gamma: v_k^2=-d(\lambda)|_{\lambda=u_k}. \tag{III.18}$$

This scheme can be generalized to the case of the more general Jacobi variety $((\Gamma_1\times\Gamma_2\ldots\times\Gamma_n))$ with different Riemannian surfaces,

$$\Gamma_k^{(j)}: v_k^{(j)2}=-d^{(j)}(\lambda)|_{\lambda=u_k},\quad k=1,\ldots,n_j, j=1,\ldots,n, \tag{III.19}$$

where k and j are two numbers indexing curves. Motion on such manifolds can be described with the use of the block matrices,

$$L(\lambda)=\oplus_j^n L^{(j)}(\lambda,v_1^{(j)},u_1^{(j)};\ldots;v_{n_j}^{(j)},u_{n_j}^{(j)}), \tag{III.20}$$

acting in the auxiliary space,

$$V_{aux}=\oplus_j V_{aux}^{(j)}. \tag{III.21}$$

Here j denotes numbers of blocks and k denotes the number of degrees of freedom related to each block. Each block,

$$L^{(j)}(\lambda,v_1^{(j)},u_1^{(j)};\ldots;v_{n_j}^{(j)},u_{n_j}^{(j)}),$$

is a matrix of type $L_0(\lambda)$ or $L_{MN}(\lambda)$ (II.21), respectively. These manifolds have been investigated in Ref. 20 and such block matrices were considered in Ref. 10.

In the *XYZ* case parametrization of the entry $b(\lambda)$ is more complicated. For instance, it has to comply with the equality (II.12),

$$\{\tilde{b}(\lambda),\tilde{b}(\mu)\}=g(\lambda,\mu)\cdot\tilde{b}(\lambda)-g(\mu,\lambda)\cdot\tilde{b}(\mu).$$

In order to bypass this difficulty we can use two-dimensional lattice averaging[6] for the constructing matrices $L_0(\lambda)$ from the corresponding matrices of the rational model.

IV. CANONICAL TRANSFORMATIONS OF VARIABLES

We can represent meromorphic matrix-functions $L(\lambda)$ by means of generators of various Lie groups, which one can consider as the various phase spaces for the integrable systems. This leads to links among different integrable systems: the Neumann problem, Gaudin magnets and Euler tops.[12,19] In this paper we shall consider finite-dimensional integrable systems of the natural type and shall investigate three types of canonical transformations of variables prescribed by a linear r-matrix structure (II.1), (II.2).

A. Generalized elliptic coordinates

If the limit orders of poles m_j at the points e_j are fixed, then the Poisson brackets at different poles are independent and the corresponding orbits are a direct product of orbits of algebra $su(2)$. This factorization is independent of the points e_j.[12] By the Mittag–Leffler theorem we can decompose rational functions $b(\lambda)$ (III.8) and $a(\lambda)$ (III.9) into partial fractions,

$$b(\lambda)=P_b^{n-m}(\lambda)+\sum_{j,i} b_{ji}\cdot\varphi^{-i}(\lambda-e_j)=\prod_{k=1}^{n-m}\varphi(b_k-\lambda)+\sum_{j,i} b_{ji}\cdot\varphi^{-i}(\lambda-e_j),$$
$$a(\lambda)=P_a^{n-m-1}(\lambda)+\sum_{j,i} a_{ji}\cdot\varphi^{-i}(\lambda-e_j)=\prod_{k=1}^{n-m-1}\varphi(a_k-\lambda)+\sum_{ji} a_{ji}\cdot\varphi^{-i}(\lambda-e_j), \tag{IV.1}$$

where b_k and a_k are zeroes of the polynomials $P_b^{n-m}(\lambda)$ and $P_a^{n-m-1}(\lambda)$, respectively. The residues b_{ji} and a_{ji} at the points e_j are linear coordinates on the algebra $su(2)^*$ (III.3). We use the later two representations for generators of this algebra in terms of canonical variables,

$$b_j=x_j^2,\quad a_j=x_jp_j,\quad c_j=p_j^2, \tag{IV.2}$$

$$b_j=2x_jX_j,\quad a_j=x_jp_j+X_jP_j,\quad c_j=2p_jP_j. \tag{IV.3}$$

We omit here the double indexes ji which are necessary for higher order poles and we used notation c_j for residues of entry $c(\lambda)$. Variables x_j, p_j and X_j, P_j are canonically conjugate coordinates and momenta. Generalized elliptic coordinates correspond to the first representation (IV.2) and in our scheme they are a simple consequence of the Mittag–Leffler theorem for meromorphic functions.

The other $(n-m)$ variables can be chosen as zeroes of the polynomial $P_b^{n-m}(\lambda=x_k)$ and as the values of function $P_a^{n-m-1}(\lambda)$ at these zeroes x_k,

$$P_b^{n-m}(\lambda=x_k)=0,\quad p_k=P_a^{n-m-1}(\lambda=x_k). \tag{IV.4}$$

Variables x_k, $k=m+1,\ldots,n$ are calculated from the coefficients of the polynomial $P_b^{n-m}(\lambda)=\Sigma\ B_k\lambda^k$. For instance, in the XXX case with simple poles these coefficients are equal to

$$B_k=\frac{1}{(k-1)!}\frac{d^{k-1}}{d\lambda^{k-1}}\,b(\lambda)\bigg|_{\lambda=0}+(-1)^k\sum_{j=1}^{m}\frac{x_j^2}{e_j^{k+1}}, \tag{IV.5}$$

then the conjugate (to the x_k) momenta p_k, $k=m+1,\ldots,n$ are

$$p_k=a(\lambda)|_{\lambda=x_k}-\sum_{j=1}^{m}\frac{x_jp_j}{x_k-e_j}. \tag{IV.6}$$

Lemma 3: Variables x_j,p_j $j=1,\ldots,m$ and x_k,p_k $k=m+1,\ldots,n$ are a system of canonically conjugate variables.

Proof: The Mittag–Leffler theorem defines a unique, invertible map between old n pairs of variables (u_k,v_k), $k=1,\ldots,n$ and the new n pairs of variables (x_k,p_k), $k=1,\ldots,n$. The proof of canonical conjugation of these variables is based on the r-matrix structure. The technique developed by Sklyanin (see Ref. 1) has to be employed.

In the case of higher order poles we have an additional freedom in representing residues through canonical variables. There are two approaches to this problem. The first one is connected with standard degenerations of simple divisors, for example $e_j \to e_{j+1}$ or $e_j \to \infty$. This approach is developed in Refs. 9,21. Our approach is different.

We shall show how the variables (q_j, p_j) are connected to Newton type variables for stationary flows of KdV type equations introduced in Ref. 5. We shall consider the XXX case but generalization for the XXZ case is transparent. The r-matrix algebra is associative; a linear combination of any two matrices L_1 and L_2 satisfying (II.1) satisfies (II.1) too. Let us consider the polynomial part of $L_0(\lambda)$ corresponding to poles at infinity. The determinants of $L_0(\lambda)$ and $L(\lambda)$ from (II.39)–(II.43) are

$$d_0(\lambda) = \frac{b \cdot b_{xx}}{2} - \frac{b_x^2}{4}, \quad d(\lambda) = \frac{b \cdot b_{xx}}{2} - \frac{b_x^2}{4} + b^2 \cdot u_{MN}(\lambda). \tag{IV.7}$$

They are integrated forms of the KdV recursion relations.[5]

A simple substitution for the entries of matrix $L_0(\lambda)$,

$$b(\lambda) = \mathscr{B}^2, \quad a(\lambda) = -b_x/2 = -\mathscr{B}\mathscr{B}_x, \qquad c(\lambda) = -b_{xx}/2 = -\mathscr{B}_x^2 - \mathscr{B}\mathscr{B}_{xx}, \tag{IV.8}$$

turns determinants (IV.7) into the form

$$d_0(\lambda) = \mathscr{B}^3 \mathscr{B}_{xx}, \quad d(\lambda) = \mathscr{B}^3 \mathscr{B}_{xx} + \mathscr{B}^4 \left[\frac{f(\lambda)}{\mathscr{B}^4} \right]_{MN}, \tag{IV.9}$$

if we use an explicit formula for the potential $u_{MN}(\lambda)$. These equations have the form of Newton equations for $\mathscr{B}$,

$$\mathscr{B}_{xx} = d_0(\lambda) \mathscr{B}^{-3}, \quad \mathscr{B}_{xx} = d(\lambda) \mathscr{B}^{-3} - \mathscr{B} \left[\frac{f(\lambda)}{\mathscr{B}^4} \right]_{MN}. \tag{IV.10}$$

If we assume that $\mathscr{B} = \Sigma_{j=0}^{N} q_{N-j} \lambda^j$ is a polynomial then its coefficients q_j obey the Newton equation of motion (IV.10) with $d(\lambda) = \Sigma\, I_k \lambda^k$, where I_k are integrals of motion. It becomes clear in terms of variables q_j that deformation of integrals of motion I_k affects only the potential (q-dependent) part. The kinetic (momentum dependent) part of I_k remains unchanged.

Coefficients of all entries $a(\lambda)$, $b(\lambda)$ and $c(\lambda)$ are easily expressed in terms of coefficients of $\mathscr{B}$. Let us fix the highest order of λ in entry as K, then

$$b(\lambda) = \sum_{j=0}^{K} b_j \lambda^j, \quad a(\lambda) = \sum_{j=0}^{K} a_j \lambda^j, \quad c(\lambda) = \sum_{j=0}^{K} c_j \lambda^j, \tag{IV.11}$$

with

$$b_K = 1, \quad a_K = 0, \quad c_K = 0, \tag{IV.12}$$

due to the definition of M_0 and Φ_λ. Let

$$\mathscr{B}(\lambda) = \sum_{j=0}^{K} q_{K-j} \lambda^j, \quad \text{with } q_0 = 1,$$

where the set $\mathscr{B}$ we consider as a formal set. After substitution of these definitions into (IV.8) we obtain

$$b_j=\sum_{i=0}^{K-j} q_i q_{K-j-i}, \quad a_j=-\sum_{i=0}^{K-j} q_{i,x} q_{K-j-i},$$
$$c_j=-\sum_{i=0}^{K-j} q_{i,x} q_{K-j-i,x}-\sum_{i=0}^{K-j} q_{i,xx} q_{K-j-i}, \tag{IV.13}$$

where q_x is derivate with respect to x, and we used the Newton formulae for a product of sets. From $q_0=1$ and the definitions (IV.13) the restrictions (IV.12) for the higher coefficients of entries of matrix L_0 follow automatically. Canonically conjugate (to the coordinates q_j) momenta p_j can be derived from the r-matrix algebra (II.1) and from the definitions (IV.11)–(IV.13),

$$p_j=q_{K+1-j,x}, \quad \{p_j,q_k\}=\delta_{jk}.$$

As an example, we present first polynomials,

$$K=1, \quad b(\lambda)=\lambda+2q_1, \quad -a(\lambda)=p_1,$$
$$K=2, \quad b(\lambda)=\lambda^2+2\lambda x_1+(2x_2+x_1^2), \quad -a(\lambda)=\lambda p_2+(p_1+p_2 x_1), \tag{IV.14}$$
$$K=3, \quad b(\lambda)=\lambda^3+2\lambda^2 x_1+\lambda(2x_2+x_1^2)+2(x_3+x_1 x_2),$$
$$-a(\lambda)=\lambda^2 p_3+\lambda(p_2+p_3 x_1)+(p_1+p_2 x_1+p_3 x_2).$$

All integrals of motion can be expressed in terms of new variables directly from the equations (IV.9) by taking residues. Notice that the kinetic part of the Hamiltonian $H=\Phi_\lambda[d(\lambda)]$ has the nondiagonal form

$$T=\sum_{j=1}^{K+1} p_j p_{K-j}. \tag{IV.15}$$

Definition of the variables of separation is not changed by deforming the Lax matrix $L_0(\lambda)$ (II.21). For instance, the free motion Hamiltonian $H=T$ (IV.15) and the corresponding Hamiltonian with potential terms $H=T+V_{MN}$ separate in the same coordinate systems.

A. Jacobi coordinates

Let us take a simplest matrix $L_0^{(k)}(\lambda)$ with the entry $b(\lambda)$ of (III.8) which has only one zero,

$$L_0^{(k)}(\lambda,v_k,u_k)=\begin{pmatrix} -v_k & \varphi(\lambda-u_k) \\ 0 & v_k \end{pmatrix}. \tag{IV.16}$$

It obeys the linear r-matrix algebra (II.1) with the r-matrix (II.13) or (II.14). Let

$$L_0(\lambda)=\oplus_k^n L_0^{(k)}(\lambda,v_k,u_k), \tag{IV.17}$$

which means that we associate to our system a matrix L, which has blocks structure, and each block $L_0^{(k)}$ obeys the r-algebra with the same r-matrix.

A modified matrix $L(\lambda)$ (II.21) is equal to

$$L(\lambda)=\oplus_k^n L_{MN}^{(k)}(\lambda,v_k,u_k), \tag{IV.18}$$

where blocks $L_{MN}^{(k)}(\lambda,v_k,u_k)$ are

$$L_{MN}^{(k)}(\lambda,v_k,u_k)=\begin{pmatrix} -v_k & \varphi(\lambda-u_k) \\ \left[\dfrac{f(\lambda)}{\varphi(\lambda-u_k)}\right]_{MN} & v_k \end{pmatrix}. \tag{IV.19}$$

These matrices are deformations of the initial matrices $L_0(\lambda,v_k,u_k)$ (IV.16) and each block $L_{MN}^{(k)}$ obeys the rs-algebra with a common r-matrix but different (since they depend on u_k) matrices $s_{MN}^{(k)}$ constructed according to (II.28).

The matrix L_0 (IV.16) and the modified matrix L_{MN} (IV.19) have an internal structure,[21]

$$\begin{aligned} L_0(\lambda,v_k,u_k)&=\begin{pmatrix} -v_k & \varphi(\lambda-u_k) \\ 0 & v_k \end{pmatrix}=\begin{pmatrix} -\Sigma\alpha_j p_j^{(k)} & \varphi(\lambda-\Sigma\alpha_j^{-1}q_j^{(k)}) \\ 0 & \Sigma\alpha_j p_j^{(k)} \end{pmatrix}, \\ L_{MN}(\lambda,v_k,u_k)&=\begin{pmatrix} -\Sigma\alpha_j p_j^{(k)} & \varphi(\lambda-\Sigma\alpha_j^{-1}q_j^{(k)}) \\ \left[\dfrac{f(\lambda)}{\varphi(\lambda-\Sigma\alpha_j^{-1}q_j^{(k)})}\right]_{MN} & \Sigma\alpha_j p_j^{(k)} \end{pmatrix}, \end{aligned} \tag{IV.20}$$

if variables v_k and u_k are considered as linear combinations of certain canonical variables $p_j^{(k)}$, $q_j^{(k)}$ $j=1,\ldots,K$. If we consider a system with an n degree of freedom and require that the Hamiltonian has a natural canonical form with the kinetic energy form,

$$T^{(n)}=\sum_{k=1}^{n} v_k^2=\sum\ q_j^2;$$

then the internal structure of (IV.20) leads to the Jacobi transformations for a n-degrees of freedom systems. It is then a pure coordinate change of variables. As before free motion equations corresponding to the undeformed matrix and motion with potential corresponding to the modified matrix separate in the same system of coordinates.

B. Momentum dependent change of variables

Let us consider functions $B_j(\lambda)$ and $A_j(\lambda)$, which are algebraic functions of entries of the matrix $L(\lambda)$ and which satisfy suitable Poisson brackets, for example

$$\{A_j(\lambda),A_k(\mu)\}=\{B_j(\lambda),B_k(\mu)\}=0,$$

$$\{A_j(\lambda),B_k(\mu)\}=\delta_{jk}\cdot g(\lambda,\mu)\cdot(B_j(\lambda)-B_k(\mu)).$$

We shall require that zeroes of the functions $B_j(\lambda)$ and values of functions $A_j(\lambda)$ at these zeroes define a new system of coordinates. Because functions $B_j(\lambda)$ and $A_j(\lambda)$ are meromorphic functions it will also be interesting to consider the corresponding residues. The first example of the such transformations associated to Henon-Heiles system has been considered in Ref. 10.

Now we present new transformation related to the two particles quartic potential.[22] In the same way as for the Jacobi transformations we consider the block matrices $L(\lambda)$ (IV.18) with the two simplest blocks (IV.19).[10]

Lemma 4: The map $(u_1,u_2,v_1,v_2)\to(x,p,p_x,p_y)$ *given by*

$$x^2=\alpha\frac{d_1(\lambda)-d_2(\lambda)}{b_1^2(\lambda)-b_2^2(\lambda)}\bigg|_{\lambda=0};\quad \alpha\in\mathbf{R},\quad p_x=\frac{a_1(\lambda)b_1(\lambda)-a_2(\lambda)b_2(\lambda)}{b_1^2(\lambda)-b_2^2(\lambda)}\bigg|_{\lambda=0}\cdot x;$$
$$y^2=\beta(b_1^2(\lambda)+b_2^2(\lambda))_{\lambda=0}-\frac{\alpha\beta p_x^2}{2x^2}+\frac{x^2}{2},\quad \beta\in\mathbf{R};\tag{IV.21}$$
$$p_y y=\frac{1}{4\beta}(a_1(\lambda)b_1(\lambda)+a_2(\lambda)b_2(\lambda))_{\lambda=0}+\alpha\beta\frac{p_x}{x}\left(1+\frac{p_x^2}{x^2}\right)+p_x x;$$

where $a_k(\lambda)$ *and* $b_k(\lambda)$ *are the entries of matrices* $L_{MN}(\lambda,v_k,u_k)$; $k=1,2$ (IV.19) *and* $d_k(\lambda)$ *are the corresponding determinants, is a canonical transformation.* Proof is based on the undeformed r-matrix algebra and on the following relation:

$$\{d_k(\lambda),d_j(\mu)\}=0,$$

which is given by the rs-algebra (II.2) with $s_{MN}^{(k)}$-matrices (II.28).

We emphasize that it is a non-pure coordinate change of variables and that a free motion on the manifold and a potential motion on it separate in different systems of coordinates.

V. CONCLUSIONS

We have developed here the rs-matrix scheme for natural finite-dimensional integrable systems connected to the KdV and the coupled KdV hierarchies. But it applies to other hierarchies of integrable nonlinear evolution equations as well. For the hierarchy of the KdV type equations the Lax matrix M_0 (II.37) is independent of the spectral parameter. The corresponding matrices for the AKNS hierarchy and for the SG hierarchy have one pole at infinity or two poles at infinity and at zero correspondingly.[6] For applying our scheme in these cases one has to redefine the projector Φ_λ:

$$\Phi_{\lambda\mu}=\varphi(\mu)\cdot\mathrm{Res}_{\lambda=\infty}^{K}+\mathrm{Res}_{\lambda=\infty}^{K-1},\quad \varphi(\mu)=\mu\ \text{ or }\ \varphi(\mu)=\mu+\frac{1}{\mu}.\tag{V.1}$$

These two choices of the function $\varphi(\mu)$ correspond to the AKNS and to the SG hierarchy if we use the second rational parametrization for the r-matrix of XXZ type (II.16) for the SG equation. The Hamiltonians in terms of the root variables u_k of finite-dimensional systems connected with stationary flows for this hierarchies were introduced in Refs. 17, 18.

In order to apply our approach to restricted flows of the AKNS hierarchy of equations[23] we have to fix the form of the matrix M_0 as

$$M_0(\mu)=\begin{pmatrix}\mu & w\\ u & -\mu\end{pmatrix},$$

and to choose the projector $\Phi_{\lambda\mu}$ in the form (V.1).

In the next step one has to consider the undeformed matrix $L_0(\lambda)$ corresponding to this choice of M_0 and $\Phi_{\lambda\mu}$ and prove that it obeys the r-matrix algebra. Let the matrix $L_0(\lambda)$ have the form

$$L_0(\lambda)=L_0^{\infty}(\lambda)+L_0^{D}(\lambda),$$

where we split $L_0(\lambda)$ into the polynomial (pole at infinity) part and the D-divisor part corresponding to finite poles. One finds the following sequence of L_0^{∞} matrices yielding the prescribed M_0 and $\Phi_{\lambda\mu}$ and satisfying the r-matrix algebra (II.1):

$$L_0^{\infty}(\lambda)=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix},$$

$$L_0^{\infty}(\lambda)=\begin{pmatrix}\lambda & q_1\\ p_1 & -\lambda\end{pmatrix}, \quad \{p_1,q_1\}=1,$$

$$L_0^{\infty}(\lambda)=\begin{pmatrix}\lambda^2-\dfrac{q_1q_2}{2} & \lambda q_1-2p_2\\ \lambda q_2-2p_1 & -\lambda^2+\dfrac{q_1q_2}{2}\end{pmatrix}, \quad \{p_2,q_2\}=1.$$

The analog of the parametrization related to the Newton representation (IV.14)[5] for the recurrent construction of these matrices is not known as yet. In this case the Hamiltonians are equal to $H=\Phi_{\lambda\mu}[d(\lambda)]$, but they do not depend on the spectral parameter μ since the corresponding residues are equal to zero.

The matrix M_0 is more symmetric by its entries in this case and respective integrable systems are of the non-natural type[23] one can use various solutions of the equations (II.15) for the deformation coefficients α_j. Systems with such deformations will be investigated in detail in the forthcoming publications.

Finally, we remark that the rs-matrix scheme presented in this paper applies to the discrete time analogs of soliton hierarchies. It yields an rs-matrix description of integrable symplectic maps.

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On the huge Lie superalgebra of pseudo-superdifferential operators and super KP-hierarchies

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Lie superalgebraic methods are used to establish a connection between the huge Lie superalgebra Ξ of super- (pseudo-) differential operators and various super KP-hierarchies. We show in particular that Ξ splits into $5=2\times2+1$ graded algebras expected to correspond to five classes of super-KP-hierarchies generalizing the well-known Manin–Radul and Figueroa–Mas–Ramos supersymmetric KP-hierarchies. © *1996 American Institute of Physics.* [S0022-2488(96)02506-6]

I. INTRODUCTION

Recently, there has been much interest in studying two-dimensional integrable models.[1,2] Known as the generalized KdV-hierarchies, these models are incorporated into a much larger integrable system, namely the KP-hierarchy.[3] This is defined as a set of multitime evolution equations, which read in the Lax form as

$$\frac{\partial L}{\partial t_r}=[L_+^r,L],\quad r=1,2,3,\dots, \tag{1}$$

where L is a pseudo-differential operator given by

$$L=\partial+\sum_{i\geqslant1} U_i(z)\partial^{1-i},\quad \partial=\frac{\partial}{\partial z}. \tag{2}$$

There are various remarkable properties of the KP-hierarchy. The most essential ones are its bi-Hamiltonian structures[1,4] and the fact that it admits a Lax formulation.[1,5] Several extensions of the standard KP-hierarchy, Eqs. (1), (2), are possible. The more known ones, given by the supersymmetric extensions of the hierarchy, Eqs. (1), (2), are based on the Manin–Radul odd pseudo-superdifferential operator,[6]

$$L=D+\sum_{i\geqslant0} U_{(i+1)/2}(\hat{z})D^{-i}, \tag{3}$$

and the Figueroa O'Farrill–Mas–Ramos even pseudo-superdifferential operator,[7]

$$L=D^2+\sum_{i\geqslant0} U_{(i+2)/2}(\hat{z})D^{-i}, \tag{4}$$

with $D=\partial_\theta+\theta\partial$.

In this Letter we propose a consistently algebraic formulation of the extended KP-integrable systems. We will present a systematic description of the Lie superalgebra Ξ of supersymmetric

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pseudo-differential operators and we will show, in particular, that it splits into $6=3\times2$ Lie superalgebras. To establish a connection with the supersymmetric extensions of the KP-hierarchy, Eqs. (1), (2), we will define $5=2\times2+1$ graded spaces of pseudo-superdifferential operators containing as a particular element the Figueroa–Mas–Ramos, Eq. (4), and the Manin–Radul, Eq. (3), superdifferential Lax operators, and we will conclude by expecting that these five graded spaces correspond to five classes of supersymmetric KP-hierarchies.

II. THE ALGEBRA Ξ OF SUPER-PSEUDO-DIFFERENTIAL OPERATORS

A. The ring $\mathscr{R}$ of analytic superfields

Let us first consider the ring of analytic superfields $U_{k/2}(\hat{z})$, $k\in\mathbf{Z}$, which depend on $(1|1)$ superspace coordinates $\hat{z}=(z,\theta)$. In this supercommutative $\mathbf{Z}_2$-graded ring $\mathscr{R}$, one can define an odd superderivative $D=\partial_\theta+\theta\partial$, the $N=1$ supercovariant derivative that obeys the $N=1$ supersymmetric algebra $D^2=\partial$ with $\theta^2=0$ and $\partial_\theta=\int d\theta$. Following the analysis developed in Ref. 8, the ring $\mathscr{R}$ can be decomposed as

$$\mathscr{R}=\bigoplus_{k\in\mathbf{Z}}\mathscr{R}_{k/2}^{(0,0)}, \tag{5}$$

where $\mathscr{R}_{k/2}^{(0,0)}$ is the set of superfields $U_{k/2}(\hat{z})$ labeled by half-integer conformal spin $k/2$, $K\in\mathbf{Z}$. The upper indices (0,0), carried by $\mathscr{R}$ and that we shall drop whenever no confusion can arise, are special values of general indices (p,q) to be introduced later on. One can also define the following product:

$$\langle U_{k/2},U_{l/2}\rangle=\delta_{k+l,1}\int d\hat{z}\,\frac{U_k}{2}(\hat{z})U_{(1-k)/2}(\hat{z}), \tag{6}$$

showing that the one-dimensional subspaces $\mathscr{R}_{k/2}$ and $\mathscr{R}_{(1-k)/2}$ are dual to each other. Using dimensional arguments, it is not difficult to see that the product $\langle\cdot,\cdot\rangle$, Eq. (6), carries a conformal spin $\Delta=-\frac{1}{2}$. Later on, we shall introduce a combined scalar product $\langle\langle\cdot,\cdot\rangle\rangle$ built out of Eq. (6) and the pairing product (,) of conformal spin $\Delta=1/2$, so that we get $\Delta[\langle\langle,\rangle\rangle]=0$.

Since the conformal spin product, Eq. (6), gets induced here, we have that $\mathscr{R}=\mathscr{H}_+\oplus\mathscr{H}_-$, where $\mathscr{H}_+$ and $\mathscr{H}_-$ are two dual semi-infinite tensor subspaces characterized, respectively, by positive and negative conformal spin as shown here below,

$$\mathscr{H}_+=\bigoplus_{k>0}\mathscr{R}_{k/2},\quad \mathscr{H}_-=\bigoplus_{k>0}\mathscr{R}_{(1-k)/2}. \tag{7}$$

We learn, in particular, that the space $\mathscr{R}_0$ of vanishing conformal spin superfields $U_0(\hat{z})$, is the dual of the space $\mathscr{R}_{1/2}$ generated by the superfield $U_{1/2}(\hat{z})$ of conformal spin 1/2. We remark, also, that the conformal spin product, Eq. (6), agrees with the $\mathbf{Z}_2$-grading,

$$\mathscr{R}=\mathscr{R}_{\bar{0}}\oplus\mathscr{R}_{\bar{1}}, \tag{8a}$$

with

$$\mathscr{R}_{\bar{0}}=\mathscr{H}_{+\bar{0}}\oplus\mathscr{H}_{-\bar{0}},\quad \mathscr{R}_{\bar{1}}=\mathscr{H}_{+\bar{1}}\oplus\mathscr{H}_{-\bar{1}}, \tag{8b}$$

where $\mathscr{H}_{\pm,0}$ and $\mathscr{H}_{\pm,1}$ are subspaces related to each other by the duality conjugation,

$$[\mathscr{H}_\pm]_0^*=[\mathscr{H}_\mp]_{\bar{1}}. \tag{8c}$$

B. The superspace $\Xi_{m/2}^{(p,q)}$ and super Lax operators

Consider the superspace $\Xi_{m/2}^{(p,q)}$ labeled by three quantum numbers $m/2$, p, and q defining, respectively, the conformal spin, the lowest, and the highest degrees. Typical elements of this superspace are given by

$$L_{m/2}^{(p,q)}[u]=\sum_{i=p}^{q} U_{(m-i)/2}(\hat{z})D^i, \quad p,q,m\in\mathbf{Z}, \tag{9}$$

where $U_{(m-i)/2}/(\hat{z})$ are an analytic superfield of conformal spin $(m-i)/2\cdot\Xi_{m/2}^{(p,q)}$ behaves then as a $(1+q-p)$-dimensional superspace generated by $L_{m/2}^{(p,q)}$ and whose superspace decomposition is given by the linear sum

$$\Xi_{m/2}^{(p,q)}=\bigoplus_{i=p}^{q}\Xi_{m/2}^{(i,i)}, \tag{10a}$$

with

$$\Xi_{m/2}^{(i,i)}=\mathscr{R}_{(m-i)/2}\oplus D^i, \tag{10b}$$

where $\mathscr{R}_{k/2}=\Xi_{k/2}^{(0,0)}$ is the ring of analytic superfields $U_{k/2}(\hat{z})$ introduced previously. For any element $L_{m/2}^{(p,q)}$ of the superspace $\Xi_{m/2}^{(p,q)}$, one can introduce the conformal spin Δ, the degrees (deg), and the grading $|\cdot|$, properties, which are summarized in the following table:

$$\begin{array}{ccccc} & \Delta & \deg & |\cdot| \\ U_{i/2}\ D^j & \dfrac{i+j}{2} & (j,j) & (i+j)\bmod 2 \\ \Xi_{m/2}^{(p,q)} & \dfrac{m}{2} & (p,q) & m(\mathrm{mod}\ 2) \end{array} \tag{11}$$

An element $L_{m/2}^{(p,q)}$ is called a super Lax operator, if it is homogeneous under the $\mathbf{Z}_2$-grading,

$$|x|=\begin{cases} 0, & \text{for } x \text{ even}, \\ 1, & \text{for } x \text{ odd}, \end{cases} \tag{12}$$

and have the following form at order $m,m\in\mathbb{N}$,

$$L_{m/2}^{(0,m)}=D^m+\sum_{i=1}^{m} U_{i/2}(\hat{z})D^{m-i}. \tag{13}$$

The homogeneity condition simply states that the $\mathbf{Z}_2$-grading of the analytic superfield $U_{i/2}(\hat{z})$ is defined as

$$|U_{i/2}(\hat{z})|=i(\mathrm{mod}\ 2). \tag{14}$$

Setting $m=2n$, $p=1$, and $q=2n$ into Eq. (9), one recovers the Inami Kanno super Lax operator of $2n$th order,[9] associated to the affine Lie superalgebra $A(n-1|n-1)^{(1)}$, namely

$$L_n^{(1,2n)}[u]=D^{2n}+\sum_{i=1}^{n-1}[U_i(\hat{z})D^{2(n-i)}+U_{(2i+1)/2}(\hat{z})D^{2(n-i)-1}]. \tag{15}$$

The space of supersymmetric Lax operators, Eq. (13), is given by the coset space

$$\mathscr{M}^{(m-1)}=\Xi^{(0,m)}_{m/2}/\Xi^{(m-1/m-1)}_{m/2}, \tag{16}$$

which exhibits a dimension $m-1$.

To define a Lie algebraic structure on the superspace $\Xi^{(p,q)}_{m/2}$, one needs to introduce a Lie bracket defined for two arbitrary operators X and Y as

$$[X,Y]=XY-(-)^{|X|\cdot|Y|}YX. \tag{17}$$

It follows then that $\Xi^{(p,q)}_{m/2}$ defines a Lie superalgebra, provided that

$$m=0 \qquad \text{and} \quad p\leqslant q\leqslant 1. \tag{18}$$

The multiplication of operators in $\Xi^{(p,q)}_{m/2}$ is given by the generalized Leibnitz rule,[6]

$$D^i\phi(\hat{z})=\sum_{k=0}^{\infty}\begin{bmatrix} i \\ i-k \end{bmatrix}(-)^{|\phi|(i-k)}\phi^{(k)}(\hat{z})D^{i-k}, \tag{19}$$

where $\phi^{(k)}=D^k\phi$ and $[{}^{i}_{i-k}]$, $i\in\mathbf{Z}$, is the superbinomial coefficient given by

$$\begin{bmatrix} i \\ k \end{bmatrix}=\begin{cases} 0, & \text{for } k>i \quad \text{or} \quad (i,k)\equiv(0,1) \mod 2, \\ \begin{pmatrix} [i/2] \\ [k/2] \end{pmatrix} & \text{otherwise.} \end{cases} \tag{20}$$

The symbol $[x]$ stands for the integer part of $x\in(1/2)\mathbf{Z}$ and $\binom{i}{j}$ is the usual binomial coefficient.

C. The huge Lie superalgebra Ξ

A larger set of supersymmetric pseudo-differential operators than $\Xi^{(p,q)}_{m/2}$ is give by the infinite-dimensional vector space $\Xi^{(p,q)}$ of superdifferential operators with given degrees $(p,q),p,q\in\mathbf{Z}$, but indefinite conformal spins,

$$\Xi^{(p,q)}=\bigoplus_{m\in\mathbf{Z}}\Xi^{(p,q)}_{m/2}. \tag{21}$$

The set $\Xi^{(p,q)}$ exhibits a Lie superalgebra structure wth respect to the bracket, Eq. (17), provided that

$$p\leqslant q\leqslant 1. \tag{22}$$

Using the conformal spin product, Eq. (6), it follows that $\Xi^{(p,q)}$ decomposes as

$$\Xi^{(p,q)}=\Lambda^{(p,q)}_{+}\oplus\Lambda^{(p,q)}_{-}, \tag{23a}$$

with

$$\Lambda^{(p,q)}_{+}=\bigoplus_{k>0}\Xi^{(p,q)}_{k/2}, \quad \Lambda^{(p,q)}_{-}=\bigoplus_{k>0}\Xi^{(p,q)}_{(1-k)/2}. \tag{23b}$$

Setting $(p,q)=(0,0)$, Eqs. (21) and (23) reduce, respectively, to Eqs. (5) and (7) with $\Xi^{(0,0)}=\mathscr{R}$ and $\Lambda^{(0,0)}_{\pm}=\mathscr{H}_{\pm}$.

A huge Lie superalgebra is obtained by summing from Eq. (21) over all the allowed values of the degrees (p,q). It is defined by

$$\Xi=\bigoplus_{p\leqslant q}\Xi^{(p,q)}, \tag{24a}$$

or equivalently

$$\Xi = \bigoplus_{p\in\mathbf{Z}}\Big[\bigoplus_{n\in\mathbb{N}}\Xi^{(p,p+n)}\Big]. \tag{24b}$$

Remark that the infinite-dimensional superspace Ξ is closed under the Lie bracket, Eq. (17), without any constraint. Remark also that combining the conformal spin and the degrees quantum numbers, one can write

$$\Xi = \bigoplus_{p\in\mathbf{Z}}\bigoplus_{n\in\mathbb{N}}\bigoplus_{m\in\mathbf{Z}}\Xi^{(p,q)}_{m/2}. \tag{25}$$

Let us now consider $L^{(p,q)}$ and $P^{(r,s)}$, two super-(pseudo-) differential operators with fixed degrees but indefinite conformal spin. The degree pairing product $(\cdot,\cdot)$ associated to $L^{(p,q)}$ and $P^{(r,s)}$ is defined as

$$(L^{(p,q)},P^{(r,s)}) = \delta_{p+s+1,0}\delta_{q+r+1,0}\delta\ \mathrm{res}(L^{(p,q)}\cdot P^{(r,s)}), \tag{26}$$

where $(\delta\,\mathrm{res})$ is the super-residue operation given by

$$\delta\ \mathrm{res}\ D^i = \delta_{i+1,0}. \tag{27}$$

Using Eqs. (25) and (26), one can easily check that $\Delta[(\cdot,\cdot)]=\frac{1}{2}$. Combining the conformal spin and the degree pairing products Eqs. (6) and (26), one defines the following combined scalar product:

$$\langle\langle L^{(p,q)}_{m/2},P^{(r,s)}_{m/2}\rangle\rangle = \delta_{p+s+1,0}\delta_{q+r+1,0}\delta_{n+m,0}\int d\hat{z}\ \delta\ \mathrm{res}[L^{(p,q)}_{m/2}\circ P^{(r,s)}_{n/2}], \tag{28}$$

so that $\Delta[\langle\langle\cdot,\rangle\rangle]=0$.

The combined scalar product we have defined in Eq. (28) plays an important role in the construction of the supersymmetric Gelfand–Dickey (SGD) Poisson bracket; see Ref. 10.

As shown in the bosonic case,[8] we note that the superspaces $\Xi^{(p,q)}$ and $\Xi^{(-q-1,-p-1)}$ are dual to each other, with respect to the degree pairing product, Eq. (26). It is then straightforward to see that the Lie superalgebra Ξ decomposes as

$$\Xi = \Xi^{+}\oplus\Xi^{-}, \tag{29a}$$

with

$$\Xi^{+} = \bigoplus_{p\geqslant 0}\bigoplus_{n\in\mathbb{N}}\Xi^{(p,p+n)},\quad \Xi^{-} = \bigoplus_{p\geqslant 0}\bigoplus_{n\in\mathbb{N}}\Xi^{(-p-n-1,-p-1)}, \tag{29b}$$

or equivalently, by using the combined scalar product, Eq. (28),

$$\Xi^{+} = \bigoplus_{p\geqslant 0}\bigoplus_{n\in\mathbb{N}}\bigoplus_{m\in\mathbf{Z}}\Xi^{(p,p+n)}_{m/2},\quad \Xi^{-} = \bigoplus_{p\geqslant 0}\bigoplus_{n\in\mathbb{N}}\bigoplus_{m\in\mathbf{Z}}\Xi^{(-p-n-1,-p-1)}_{m/2}. \tag{29c}$$

Next, we introduce the graded algebras Σ^{k}_{ij} and their dual $(\Sigma^{k}_{ij})^{*}=\Sigma^{-k}_{-i,j}$, with respect to Eq. (28), where the indices $k=\pm$, $i=0,\pm$, and $j=0,1(\mathrm{mod}\ 2)$ refer, respectively, to the degrees, the conformal spin, and the grading quantum numbers. As an example, Σ^{+}_{+0} is the bosonic Lie algebra of superdifferential operators of positive definite spins and degrees and Σ^{-}_{-0}, its dual, the Lie algebra of super pseudo-differential operators of negative definite spins and degrees. Σ^{+}_{+0} is just

the Lie algebra of Lorentz scalar differential operators containing the Lie algebra of vector fields on the circle, namely, diff(S^1) and its dual is $\Sigma^{-}_{-\,0}$. The graded Lie algebras Σ^{k}_{ij} are related to the superalgebras $\Xi^{\pm}$, Eqs. (29), as

$$\Xi^{+} \oplus \bigoplus_{i=0,\pm} \bigoplus_{j=\overline{0,1}} \Sigma^{+}_{i,j}, \quad \Xi^{-} \oplus \bigoplus_{i=0,\pm} \bigoplus_{j=\overline{0,1}} \Sigma^{-}_{-i,j}. \tag{30}$$

A remarkable property of the infinite-dimensional Lie superalgebra Ξ is that it splits into a linear sum of $6=3\times 2$ graded subalgebras given by

$$\Xi = \bigoplus_{i=0,\pm} (S_i \oplus S_i^{*}), \tag{31}$$

where the graded Lie subalgebra S_i and its dual S_i^{*} split for a fixed conformal spin index i into

$$S_i = \Sigma^{+}_{i,0} \oplus \Sigma^{+}_{i,1}, \quad S_i^{*} = \Sigma^{-}_{-i,0} \oplus \Sigma^{-}_{-i,1}, \tag{32a}$$

or equivalently,

$$S_{-} = \Sigma^{+}_{-,0} \oplus \Sigma^{+}_{-,1} \quad S_0 = \Sigma^{+}_{0,0}, \quad S_{+} = \Sigma^{+}_{+,0} \oplus \Sigma^{+}_{+,1}, \tag{32b}$$

and

$$S_{+}^{*} = \Sigma^{-}_{-,0} \oplus \Sigma^{-}_{-,1}, \quad S_0^{*} = \Sigma^{-}_{0,0}, \quad S_{-}^{*} = \Sigma^{-}_{+,0} \oplus \Sigma^{-}_{+,1}. \tag{32c}$$

III. THE HUGE LIE SUPERALGEBRA Ξ AND SUPER-KP-HIERARCHIES

Motivated by the well-known idea that the Lie (super) algebra methods allow for a unifying treatment of nonlinear integrable systems, we try in this section to find a relation between the Lie superalgebra Ξ of supersymmetric (pseudo-) differential operators discussed previously and the various (super-) KP integrable hierarchies. We first briefly review what is known about KP-hierarchy. The latter can be thought of as a dynamical system defined on a space whose functions $U_j(z)$ are elements of the ring $\mathscr{R}_j$ of analytic fields of conformal spin $j \in \mathbf{Z}$. It is also defined as the universal family of isospectral deformations of the pseudo-differential operator,[3]

$$L = \partial + \sum_{i \geqslant 1} U_i(z)\, \partial^{1-i}. \tag{33}$$

The evolution of L is given by a commuting family of flows $\partial_i = \partial/\partial t$, in terms of which we have

$$\partial_i L_1 = [(L^i)_{+}, L] = -[(L^i)_{-}, L]. \tag{34}$$

The subscript $+$(resp., $-$) means taking the purely differential (resp., pseudo-differential) part of L^i and $t=\{t_i\}$ an infinite system of time variables. The flows, Eq. (34), are bi-Hamiltonians in the sense that there exist two Poisson bracket structures $\{.,\}_{1,2}$ such that we can rewrite Eq. (34) as

$$\partial_i L = \{H_i, L\}_2 = \{H_{i+1}, L\}_1. \tag{35}$$

Here the Hamiltonians for the KP-hierarchy are $H_r = 1/r \int \mathrm{res}\, L^r$, with $\mathrm{res}\, \partial^{-1} = 1$.

There are two usual supersymmetric extensions of the standard KP-hierarchy, Eqs. (33),(34). The first one is given by the Manin–Radul supersymmetric KP-hierarchy associated to the odd super Lax operator,[6]

$$L=D+\sum_{i\geqslant 0} U_{(i+1)/2}(\hat{z})D^{-i}. \tag{36}$$

The second one is given by the supersymmetric KP-hierarchy associated to the even super Lax operator,[7]

$$L=D^2+\sum_{i\geqslant 0} U_{(i+2)/2}(\hat{z})D^{-i}. \tag{37}$$

The interesting consequence of the choice of L, Eq. (37), is that under a suitable choice of reduction, it reduces to the Inami–Kanno super Lax operator describing the generalized $N=2$ super KdV-hierarchy.[9]

Using the $6=3\times 2$ decomposition of the Lie superalgebra Ξ, Eqs. (31),(32), one suspects that there exist $5=2\times 2+1$ classes of supersymmetric KP-hierarchies. The origin of these hierarchies can be traced to the fundamental fact that there exist precisely five graded algebras,

$$\begin{aligned}
&\text{(a)}\quad g_1=(S_+\oplus S_-^*)_{\overline{0}}=\Sigma^{+}_{+0}\oplus\Sigma^{-}_{+0},\\
&\text{(b)}\quad g_2=(S_+\oplus S_-^*)_{\overline{1}}=\Sigma^{+}_{+1}\oplus\Sigma^{-}_{+1},\\
&\text{(c)}\quad g=(S_0\oplus S_0^*)_{\overline{0}}=\Sigma^{+}_{00}\oplus\Sigma^{-}_{00},\\
&\text{(d)}\quad g_2^*=(S_-\oplus S_+^*)_1=\Sigma^{-}_{-1}\oplus\Sigma^{+}_{-1},\\
&\text{(e)}\quad g_1^*=(S_-\oplus S_+^*)_{\overline{0}}=\Sigma^{-}_{0}\oplus\Sigma^{+}_{-0},
\end{aligned} \tag{38}$$

where $g_1=\Sigma^{+}_{+0}\oplus\Sigma^{-}_{+0}$, Eq. (38a), is the Lie algebra containing as a particular element, the even super Lax operator, Eq. (37), of the Figueroa–Mas–Ramos super KP-hierarchy. $g_2=\Sigma^{+}_{+1}\oplus\Sigma^{-}_{+1}$ is the graded space generated by elements like the odd super Lax operator, Eq. (36), corresponding to the Manin–Radul super KP-hierarchy. The graded spaces g_2^* and g_1^* are just the dual of g_2 and g_1 with respect to the combined scalar product, Eq. (28). Note also that the self-dual Lie algebra $g=\Sigma^{+}_{00}\oplus\Sigma^{-}_{00}$, Eq. (38c), containing the superdifferential operators of vanishing conformal spin type,

$$L=U_{-1/2}(\hat{z})D+\sum_{i\geqslant 0} U_{i/2}(\hat{z})D^{-i}, \tag{39}$$

necessitate in itself a particular interest, as it can lead to a new class of super KP-hierarchy. A more explicit description of these five super KP-hierarchies will be considered in a future paper.

IV. CONCLUSION

Using the huge Lie superalgebra Ξ of pseudo-superdifferential operators that splits into $6=3\times 2$ Lie superalgebras, Eqs. (31),(32), we have defined $5=2\times 2+1$ graded algebras, Eqs. (38). These graded algebras are expected to correspond to five classes of super KP-hierarchies generalizing the usual Manin–Radul and Figueroa–Mas–Ramos supersymmetric KP-hierarchies. We expect moreover that these $5=2\times 2+1$ super KP-hierarchies will provide a unified framework that exhibits the underlying structure of $2d$ quantum supergravity.

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Prolongation approach to Bäcklund transformation of Zhiber–Mikhailov–Shabat equation

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The prolongation structure of Zhiber–Mikhailov–Shabat (ZMS) equation is studied by using Wahlquist–Estabrook's method. The Lax pair for ZMS and Riccati equations for pseudopotentials are formulated respectively from linear and nonlinear realizations of the prolongation structure. Based on nonlinear realization of the prolongation structure, an auto-Bäcklund transformation of ZMS equation is obtained. © *1996 American Institute of Physics.* [S0022-2488(96)03007-1]

I. INTRODUCTION

The off-conformally integrable models in two-dimensional space-time have some common features. They have spectrum-dependent Lax pairs, an infinite number of conserved currents and the underlying nonlinear symmetries, and can be solved by means of inverse scattering method. The $a_2^{(2)}$ Toda model, i.e. Zhiber–Mikhailov–Shabat (ZMS) model, is of such a fascinating class of integrable two-dimensional field theories. It is the third and last relativistic single scalar Toda model (the others are Liouville and sine-Gordon models),[1,2] and has significant applications in physical context. To our knowledge, the equation of motion of ZMS model (ZMS equation) governs the propagation of resonant ultra-short plane wave optical pulses in certain *degenerate* media.[3] The integrability of ZMS model has been confirmed for a long time. The soliton solutions of the ZMS equation by means of inverse scattering method were given in Ref. 4. The S-matrix approach to the quantum version of the model was seriously investigated by Izergin and Korepin[5] in terms of the quantum inverse scattering method, and by Smirnov[6] and Efthimiou[7] in the framework of perturbative conformal field theory. Recently, we have studied the infinitesimal dressing transformations and Lie–Poisson structure hidden in ZMS model.[8] Nevertheless, there would not seem to be a good knowledge of the finite nonlinear symmetries (such as the dressing group symmetry and Bäcklund transformation) of the model. In order to fill in the gap, we study the prolongation structure of ZMS equation in the spirit of Wahlquist–Estabrook's (WE's) prolongation approach[9,10] in the present paper. Owing to the so-called prolongation structure, we discover an auto-Bäcklund transformation of ZMS equation, which turns out to be a set of Riccati-type differential equations of the so-called pseudopotentials.

II. PROLONGATION STRUCTURE OF ZMS EQUATION

WE's prolongation structure is a very useful medium for searching Bäcklund transformation of nonlinear differential equations. To obtain the prolongation structure of ZMS equation:

[a)]Mailing address.

$$\partial_+\partial_-\phi-2(e^{\phi}-e^{-2\phi})=0, \tag{2.1}$$

we define the following two-forms on a four-dimensional manifold with coordinates associated with Eq. (2.1),

$$\begin{cases}\alpha_1=d\phi\wedge dx^+-\pi_\phi dx^-\wedge dx^+,\\ \alpha_2=d\pi_\phi\wedge dx^-+2(e^{\phi}-e^{-2\phi})dx^-\wedge dx^+.\end{cases} \tag{2.2}$$

These two-forms constitute a closed ideal and would become null on the solution manifold $(\phi(x^+,x^-),\pi_\phi(x^+,x^-),x^+,x^-)$. They are the Pfaff forms of ZMS equation. For the above Pfaff forms we will assume that prolongation forms can be given by some one-forms $\Omega^a(a=1,2,3,\ldots,\ N)$,

$$\Omega^a=-dq^a+F^a(\phi,\pi_\phi,q)dx^-+G^a(\phi,\pi_\phi,q)dx^+, \tag{2.3}$$

where N is an outstanding integer, q^a are the so-called pseudopotentials, and F^a and G^a are functionals of fields π_ϕ, ϕ and q^a.

The concept of pseudopotential plays a crucial role in the discussions of Bäcklund transformations and Lax pairs in WE's prolongation method. As a matter of fact, the expected Bäcklund transformation and the first-order differential equations satisfied by Lax pair of ZMS Eq. (2.1) will be formulated as the differential equations for suitably defined pseudopotentials q^a. The integrability of pseudopotentials q^a requires that the ideal generated by the form sets $\{\alpha^a\}$ and $\{\Omega^a\}$ is closed, i.e.,

$$d\Omega^a=\eta_b^a\wedge\Omega^b+f^{a,i}\alpha_i, \tag{2.4}$$

where η_b^a and $f^{a,i}$ are some one-forms and zero-forms respectively. When (2.4) is explicitly written out by using (2.2) and (2.3), it splits up into a set of partial differential equations:

$$\begin{gathered}\partial_\phi F^a=0,\quad \partial_{\pi_\phi}G^a=0,\\ F^b\partial_b G^a-G^b\partial_b F^a+\pi_\phi\partial_\phi G^a-2(e^{\phi}-e^{-2\phi})\partial_{\pi_\phi}F^a=0,\end{gathered} \tag{2.5}$$

where the derivative $\partial/\partial q^a$ is abbreviated to ∂_a. Analyzing these equations we find,

$$F^a=X_0^a+X_1^a\pi_\phi,\quad G^a=2Y_0^a e^{\phi}+2Y_1^a e^{-2\phi}. \tag{2.6}$$

In the ansatz (2.6) X_i^a and Y_i^a $(i=0,1)$ are assumed to be functions of q^a only.

For the convenience of the later discussions we now introduce some vector fields (Lie derivatives) X_i and Y_i in N-dimensional space of pseudopotentials (q-space),

$$X_i=X_i^a\partial_a,\quad Y_i=Y_i^a\partial_a. \tag{2.7}$$

It is then a direct consequence of (2.5)–(2.7) that,

$$[X_0,Y_0]=X_1,\ [X_0,Y_1]=-X_1,\ [X_1,Y_0]=-Y_0,\ [X_1,Y_1]=2Y_1. \tag{2.8}$$

Because of the absence of $[X_0,X_1]$ and $[Y_0,Y_1]$, the set of Lie brackets given by (2.8) does not form a closed linear algebra. It is obviously impossible that one may close the algebra by setting the unknown commutators to be linear combinations of the given generators such that the results are consistent with the Jacobi identities. This is a big difference between the prolongation structure of ZMS equation and those of sine-Gordon equation, Ernst equation and chiral model.[10,11] However, the algebra can be closed by assigning new generators to the unknown commutators and

repeating the process of working through the Jacobi identities. After a tedious but straightforward computation, we see that the enlarged algebra becomes an infinite-dimensional algebra $a_2^{(2)}$ (without center), which coincides with a well-known fact that ZMS model is the Toda field theory over the twisted Kac–Moody algebra $a_2^{(2)}$.[1,2] Let $\{H_i^{(m)}, E_{\pm\alpha}^{(m)}\}$ be the Cartan–Weyl basis of $a_2^{(2)}$, which obeys the following commutation relations:

$$
\begin{aligned}
[H_i^{(m)}, E_{\pm\beta}^{(n)}] = & \pm \delta_{i1}\delta_{\beta 1} E_{\pm 1}^{(m+n)} \mp 2\,\delta_{i1}\delta_{\beta 2} E_{\pm 2}^{(m+n)} \mp \delta_{i1}\delta_{\beta 3} E_{\pm 3}^{(m+n)} \\
& \pm 3\,\delta_{i2}\delta_{\beta 1} E_{\mp 3}^{(m+n)} \mp 3\,\delta_{i2}\delta_{\beta 3} E_{\mp 1}^{(m+n)},
\end{aligned}
$$

$$
[E_{\pm\alpha}^{(m)}, E_{\pm\beta}^{(n)}] = \mp \delta_{\alpha 1}\delta_{\beta 2} E_{\pm 3}^{(m+n)} \pm \delta_{\alpha 1}\delta_{\beta 3} H_2^{(m+n)}, \tag{2.9}
$$

$$
\begin{aligned}
[E_{\alpha}^{(m)}, E_{-\beta}^{(n)}] = & (\delta_{\alpha 1}\delta_{\beta 1} - \delta_{\alpha 2}\delta_{\beta 2} - \delta_{\alpha 3}\delta_{\beta 3}) H_1^{(m+n)} - \delta_{\alpha 3}\delta_{\beta 2} E_1^{(m+n)} - \delta_{\alpha 2}\delta_{\beta 3} E_{-1}^{(m+n)} \\
& + 2\,\delta_{\alpha 3}\delta_{\beta 1} E_2^{(m+n)} + 2\,\delta_{\alpha 1}\delta_{\beta 3} E_{-2}^{(m+n)},
\end{aligned}
$$

where $(m, n = 0, \pm 1, \pm 2, \pm 3, \ldots; i = 1, 2; \alpha, \beta = 1, 2, 3)$. Then we have the following identifications,

$$
X_0 = E_1^{(-1)} + E_2^{(0)}, \quad X_1 = H_1^{(0)}, \quad Y_0 = E_{-1}^{(1)}, \quad Y_1 = E_{-2}^{(0)}. \tag{2.10}
$$

Now we study the linear realizations of the vector fields X_i and Y_i in an infinite-dimensional q-space which has coordinate variables $\{q_j^{(m)}; j = 1, 2, 3; m = 0, \pm 1, \pm 2, \pm 3, \ldots\}$. Following Omote,[10] we introduce some auxiliary vector fields $\{A_{ij}^{(m)}\}$:

$$
A_{ij}^{(m)} = \sum_{n=-\infty}^{+\infty} q_i^{(m+n)} \frac{\partial}{\partial q_j^{(n)}}. \tag{2.11}
$$

They can be shown to satisfy commutator relations

$$
[A_{ij}^{(m)}, A_{kl}^{(n)}] = \delta_{jk} A_{il}^{(m+n)} - \delta_{il} A_{kj}^{(m+n)}. \tag{2.12}
$$

This fact implies that the set of vector fields $\{A_{ij}^{(m)}\}$ provide an operator version of graded matrices $\{e_{ij}^{(m)} = e_{ij} \otimes \lambda^m\}$ (λ is a gradation parameter). Therefore, the Cartan–Weyl basis of $a_2^{(2)}$ under consideration has the following linear realization[8] in a triplicated infinite-dimensional q-space:

$$
\begin{cases}
H_1^{(m)} = A_{11}^{(m)} - A_{33}^{(m)}, \\
H_2^{(m)} = A_{11}^{(m)} - 2A_{22}^{(m)} + A_{33}^{(m)}, \\
E_2^{(m)} = A_{31}^{(m)}, \\
E_{-2}^{(m)} = A_{13}^{(m)},
\end{cases}
\qquad
\begin{cases}
E_1^{(m)} = A_{12}^{(m)} - A_{23}^{(m)}, \\
E_{-1}^{(m)} = A_{21}^{(m)} - A_{32}^{(m)}, \\
E_3^{(m)} = A_{32}^{(m)} + A_{21}^{(m)}, \\
E_{-3}^{(m)} = A_{12}^{(m)} + A_{23}^{(m)}.
\end{cases}
$$

Explicitly,

$$
\begin{aligned}
X_0 &= \sum_{n=-\infty}^{+\infty}\left[q_1^{(n-1)}\frac{\partial}{\partial q_2^{(n)}} - q_2^{(n-1)}\frac{\partial}{\partial q_3^{(n)}} + q_3^{(n)}\frac{\partial}{\partial q_1^{(n)}}\right],\\
X_1 &= \sum_{n=-\infty}^{+\infty}\left[q_1^{(n)}\frac{\partial}{\partial q_1^{(n)}} - q_3^{(n)}\frac{\partial}{\partial q_3^{(n)}}\right],\\
Y_0 &= \sum_{n=-\infty}^{+\infty}\left[q_2^{(n+1)}\frac{\partial}{\partial q_1^{(n)}} - q_3^{(n+1)}\frac{\partial}{\partial q_2^{(n)}}\right],\\
Y_1 &= \sum_{n=-\infty}^{+\infty}\left[q_1^{(n)}\frac{\partial}{\partial q_3^{(n)}}\right],
\end{aligned}
\tag{2.13}
$$

i.e., the components of F^a and G^a are assigned to the following linear representations in a triplicated infinite-dimensional q-space :

$$
\begin{aligned}
&F_1^{(n)} = q_3^{(n)} + q_1^{(n)}\pi_\phi, \qquad F_2^{(n)} = q_1^{(n-1)}, \qquad F_3^{(n)} = -q_2^{(n-1)} - q_3^{(n)}\pi_\phi,\\
&G_1^{(n)} = 2q_2^{(n+1)}e^{\phi}, \qquad G_2^{(n)} = -2q_3^{(n+1)}e^{\phi}, \qquad G_3^{(n)} = 2q_1^{(n)}e^{-2\phi}.
\end{aligned}
\tag{2.14}
$$

Relying on the one-form (2.3), we see that the pseudopotentials introduced in (2.14) satisfy equations

$$
\partial_-\begin{bmatrix} q_1^{(n)} \\ q_2^{(n)} \\ q_3^{(n)} \end{bmatrix} = \begin{bmatrix} \partial_-\phi & 0 & 1 \\ 0 & 0 & 0 \\ 0 & -1 & -\partial_-\phi \end{bmatrix}\begin{bmatrix} q_1^{(n)} \\ q_2^{(n-1)} \\ q_3^{(n)} \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}\begin{bmatrix} q_1^{(n-1)} \\ q_2^{(n)} \\ q_3^{(n)} \end{bmatrix},
$$

$$
\partial_+\begin{bmatrix} q_1^{(n)} \\ q_2^{(n)} \\ q_3^{(n)} \end{bmatrix} = \begin{bmatrix} 0 & 2e^{\phi} & 0 \\ 0 & 0 & -2e^{\phi} \\ 2e^{-2\phi} & 0 & 0 \end{bmatrix}\begin{bmatrix} q_1^{(n)} \\ q_2^{(n+1)} \\ q_3^{(n+1)} \end{bmatrix},
\tag{2.15}
$$

on the solution surface $(\phi(x^+,x^-),\pi_\phi(x^+,x^-),x^+,x^-)$ of ZMS Eq. (2.1). Let us define a parameter-dependent potential $\Psi(\lambda)$ by

$$
\Psi(\lambda) \equiv \begin{bmatrix} \psi_1(\lambda) \\ \psi_2(\lambda) \\ \psi_3(\lambda) \end{bmatrix} = \sum_{n=-\infty}^{+\infty}\lambda^n\begin{bmatrix} q_1^{(n)} \\ q_2^{(n)} \\ q_3^{(n)} \end{bmatrix}.
\tag{2.16}
$$

Then we get from (2.15) the partial differential equations for $\Psi(\lambda)$: $\partial_\pm\Psi = A_\pm\Psi$, where

$$
\begin{cases} A_+ = \dfrac{2}{\lambda}e^{\phi}E_1 + 2e^{-2\phi}E_2, \\ A_- = \partial_-\phi H_1 + \lambda E_{-1} + E_{-2}. \end{cases}
\tag{2.17}
$$

Such $A_\pm$ do just constitute a Lax pair representation of ZMS Eq. (2.1), which gives Eq. (2.1) as the zero-curvature equation $[\partial_+ - A_+, \partial_- - A_-] = 0$, the consistency condition of the equations for Ψ. In (2.17), H_1, $E_{\pm1}$ and $E_{\pm2}$ are some 3×3 matrices defined as $H_1 = e_{11} - e_{33}$, $E_1 = e_{12} - e_{23}$, $E_2 = e_{31}$, $E_{-1} = e_{21} - e_{32}$ and $E_{-2} = e_{13}$ respectively. These matrices are among the independent generators of $SL(3,\mathscr{R})$ group.[8]

Another aspect of the prolongation structure is the nonlinear realizations of the vector fields X_i and Y_i $(i = 0, 1)$ in a finite-dimensional q-space. In Refs. 10 and 11, the authors cited some

instances in illustration of the fact that the linear realizations of the vector fields are relevant to Lax representation while the nonlinear realizations of these fields associate themselves with the Bäcklund transformation of the considered nonlinear differential equation. We will show that this conclusion is also true for ZMS Eq. (2.1).

It is worthwhile to indicate that there does not exist an unpenetrable barrier between the linear realizations and the nonlinear realizations of the vector fields. In fact, there is a standard method to get the nonlinear realizations of the vector fields from their linear realizations, in which the Lax pair plays the crucial role.[12] Let us apply the method to ZMS model. Defining $q_1=\psi_1/\psi_2, q_2=-\psi_3/\psi_2$ as new pseudopotentials, we see from Lax pair (2.17) and auxiliary linear equations that these pseudopotentials[13] satisfy a set of Riccati-type equations:

$$\begin{aligned} &\partial_+ q_1=\frac{2}{\lambda}(1-q_1q_2)e^{\phi}, \qquad \partial_+ q_2=-2q_1e^{-2\phi}-\frac{2}{\lambda}q_2^2e^{\phi}, \\ &\partial_- q_1=-(q_2+\lambda q_1^2)+q_1\pi_\phi, \quad \partial_- q_2=\lambda(1-q_1q_2)-q_2\pi_\phi, \end{aligned} \tag{2.18}$$

where $\pi_\phi=\partial_-\phi$. On the other hand, it follows from (2.3) and (2.6) that

$$\begin{aligned} &\partial_+ q_1=2Y_0^1e^{\phi}+2Y_1^1e^{-2\phi}, \quad \partial_+ q_2=2Y_0^2e^{\phi}+2Y_1^2e^{-2\phi}, \\ &\partial_- q_1=X_0^1+X_1^1\pi_\phi, \qquad \partial_- q_2=X_0^2+X_1^2\pi_\phi, \end{aligned} \tag{2.19}$$

in two-dimensional q-space. Therefore, the vector fields acquire the following nonlinear realizations:

$$\begin{cases} X_0=-(q_2+\lambda q_1^2)\partial_1+\lambda(1-q_1q_2)\partial_2, \\ X_1=q_1\partial_1-q_2\partial_2, \\ Y_0=\dfrac{1}{\lambda}(1-q_1q_2)\partial_1-\dfrac{1}{\lambda}q_2^2\partial_2, \\ Y_1=-q_1\partial_2. \end{cases} \tag{2.20}$$

Simultaneously, the prolongated algebra $a_2^{(2)}$ is nonlinearly realized as,

$$\begin{cases} H_1^{(m)}=\lambda^{-m}(q_1\partial_1-q_2\partial_2), \\ H_2^{(m)}=3\lambda^{-m}(q_1\partial_1+q_2\partial_2), \\ E_2^{(m)}=-\lambda^{-m}q_2\partial_1, \\ E_{-2}^{(m)}=-\lambda^{-m}q_1\partial_2, \end{cases} \quad \begin{cases} E_1^{(m)}=-\lambda^{-m}[q_1^2\partial_1-(1-q_1q_2)\partial_2], \\ E_{-1}^{(m)}=\lambda^{-m}[(1-q_1q_2)\partial_1-q_2^2\partial_2], \\ E_3^{(m)}=\lambda^{-m}[(1+q_1q_2)\partial_1+q_2^2\partial_2], \\ E_{-3}^{(m)}=-\lambda^{-m}[q_1^2\partial_1+(1+q_1q_2)\partial_2]. \end{cases} \tag{2.21}$$

In (2.20) and (2.21), λ is an arbitrary spectral parameter and m takes integer value. Notably, the vector fields (2.20) are not among a finite-dimensional subalgebra of $a_2^{(2)}$ unless λ equals to *one*. This is another important difference in the prolongation structure of ZMS equation from those of sine-Gordon equation, Ernst equation and chiral model.[10]

III. THE BÄCKLUND TRANSFORMATION OF ZMS EQUATION

The aim of this section is to search the auto-Bäcklund transformation of ZMS Eq. (2.1) on the basis of the prolongation structure. We assume that the new ZMS field variables $\tilde{\phi}$ and $\tilde{\pi}$ are functions of the old ϕ, π_ϕ and the pseudopotentials q^a. The new forms $\alpha_i(i=1,2)$ which are gotten from the old ones by replacing ϕ and π_ϕ with $\tilde{\phi}(\phi,\pi_\phi,q^a)$ and $\tilde{\pi}(\phi,\pi_\phi,q^a)$ should vanish modulo the old α_i and the prolongation one-forms Ω^a; i.e., there should exist some zero-forms g_{ij} and one-forms ν_i^a such that

$$\tilde{\alpha}_i(\tilde{\phi},\tilde{\pi}_\phi)=g_{ij}\alpha_j(\phi,\pi_\phi)+\nu_i^a\wedge\Omega^a. \tag{3.1}$$

This is the condition for the existence of Bäcklund transformations. In terms of (2.2) and (2.3), the condition can be recast as

$$\partial_{\pi_\phi}\tilde{\phi}=0,\ \ \partial_\phi\tilde{\pi}_\phi=0,\ \ \tilde{\pi}_\phi=\pi_\phi(\partial_\phi+X_1)\tilde{\phi}+X_0\tilde{\phi} \tag{3.2}$$

and

$$e^{\tilde{\phi}}-e^{-2\tilde{\phi}}=(e^{\phi}-e^{-2\phi})\partial_{\pi_\phi}\tilde{\pi}+(e^{\phi}Y_0+e^{-2\phi}Y_1)\tilde{\pi}_\phi. \tag{3.3}$$

The special expressions of Eqs. (3.2) lead to the following ansatz solutions for the new ZMS field variables $\tilde{\phi}$ and $\tilde{\pi}_\phi$

$$\begin{cases}\tilde{\phi}=c\phi+f(q^a),\\ \tilde{\pi}_\phi=\pi_\phi[c+X_1f(q^a)]+X_0f(q^a),\end{cases} \tag{3.4}$$

where c is an outstanding constant. Substituting (3.4) into (3.3) we get,

$$X_1f(q^a)=c_1, \tag{3.5}$$

and

$$e^{c\phi}e^{f(q^a)}-e^{-2c\phi}e^{-2f(q^a)}=e^{\phi}[c+c_1+Y_0X_0f(q^a)]-e^{-2\phi}[c+c_1-Y_1X_0f(q^a)]. \tag{3.6}$$

where c_1 is another constant.

We now apply the nonlinear expressions (2.20) of the vector fields X_i and Y_i $(i=0, 1)$ in the two-dimensional q-space to Eqs. (3.4)–(3.6). In this case, (3.5) becomes a first-order quasi-linear differential equation whose general solution reads:

$$f(q_1,q_2)=c_1\ln q_1+\omega(q_1q_2), \tag{3.7}$$

where $\omega(q_1q_2)$ is an arbitrary differentiable function of its variable q_1q_2. Generally speaking, Eq. (3.5) would have another particular solution beyond (3.7). But we quit finding such a particular solution here. One of the reason is that there is no systematic method for searching it. What is more, even if we happened to find out a particular solution for Eq. (3.5), it would be excessive to expect this solution satisfying Eq. (3.6) further. If the Bäcklund transformation of ZMS equation exists, it is bound to connect with the general solution (3.7).

To determine the function $\omega(q_1q_2)$ in (3.7) and then resolve completely the Bäcklund transformation for ZMS Eq. (2.1), Eq. (3.6) must be taken into account. After a simple and straightforward calculation we find,

$$c=1,\quad c_1=0,\quad \omega(q_1q_2)=\ln(2q_1q_2-1). \tag{3.8}$$

Namely, the auto-Bäcklund transformation of ZMS Eq. (2.1) is as follows:

$$\tilde{\phi}=\phi+\ln(2q_1q_2-1), \tag{3.9}$$

where the auxiliary pseudopotentials are determined by Riccati equations

$$\begin{aligned}\partial_+q_1&=\frac{2}{\lambda}(1-q_1q_2)e^{\phi}, &\partial_+q_2&=-2q_1e^{-2\phi}-\frac{2}{\lambda}q_2^2e^{\phi},\\ \partial_-q_1&=-(q_2+\lambda q_1^2)+q_1\partial_-\phi, &\partial_-q_2&=\lambda(1-q_1q_2)-q_2\partial_-\phi,\end{aligned} \tag{3.10}$$

for a given ϕ. One can easily justify that $\tilde{\phi}$ is a solution of ZMS Eq. (2.1) once ϕ fulfills Eq. (2.1) and vice versa. The problem of Bäcklund transformation of ZMS equation was ever discussed in Refs. 14 and 15. The Bäcklund transformation obtained by Sharipov and Yamilov[14] is a set of second order differential equations, which is very cumbersome for solving single soliton solutions[15] and is difficult to turn to our Bäcklund transformation (3.9)–(3.10).

IV. DISCUSSIONS

In the previous sections we have studied the prolongation structure of Zhiber–Mikhailov–Shabat equation. The prolongation structure yields an incomplete set of commutators of vector fields in the pseudopotential space. Following Omote[10] and Ablowitz *et al.*,[12] we have found out the linear and nonlinear differential realizations of the vector fields respectively. It is shown that the linear realizations of the vector fields give the linear auxiliary equations (Lax pair) of ZMS equation, while their nonlinear realizations are connected with the Bäcklund transformation of the equation. Nevertheless, the application of this Bäcklund transformation to constructing new analytical solutions of ZMS equation from some old ones, e.g., constructing the single-soliton solution from vacuum solution, remains an open problem. It is easy to see that ZMS Eq. (2.1) has an analytical solution governed by the first-order equations $\partial_{\pm}\phi=\mu^{\pm}\sqrt{2(2e^{\phi}+e^{-2\phi}-3)}$ (μ is an arbitrary constant). But we have not driven out these equations from the Bäcklund transformation laws yet. Another even more interesting problem is perhaps to study the dressing group symmetry in ZMS model by virtue of prolongation structure. By some naive perception we conjecture that the finite dressing transformations of ZMS equation may be exposed through a slightly different nonlinear realization of the prolongation structure. The dressing procedure is a useful method for solving single soliton solution. The detail for such problems are now in preparation.

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Curvature collineations of some static spherically symmetric space–times

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Curvature collineations of some static spherically symmetric space–times are derived and compared with isometries and Ricci collineations for corresponding space–times. © *1996 American Institute of Physics.* [S0022-2488(96)04106-0]

I. INTRODUCTION

Over the past few years there has been much interest in the classification of solutions of the Einstein field equations in terms of their isometries. These isometries are given by Killing vectors (KVs), along which the Lie derivative of the metric tensor is zero, admitted by the space–time. Each independent KV gives rise to a conservation law for the spacetime. The classification by Petrov[1,2] was incomplete in that it did not provide a list of metrics for a given set of isometries, though a complete list of isometries was available. In an extensive study of spherically symmetric spacetimes, Takeno[3] used the curvature invariants of such space–times to classify them according to their isometries and these invariants. Following a different approach Qadir *et al.*[4] obtained a classification of such space–times by their isometries and provided a complete list of distinct space–time metrics. It appears that Takeno missed some metrics (for example, nonstatic spacetime like the Einstein universe but with the role of t and r inter changed, so that the isometry group is SO(1,3)XR instead of SO(4)XR).

Though the classification of space–times in terms of their isometries is important, Katzin, Davies, and Lavine[5,6] argue that the symmetries of the matter field would be given by Ricci collineations (RCs), along which the Lie derivative of the Ricci tensor is zero. A complete classification of spherically symmetric, static metrics in terms of RCs has been obtained[7,8] and is being extended to the nonstatic cases.[9]

Katzin *et al.* also argue that the symmetries of the Riemann tensor, called curvature collineations (CCs), would also provide insights into general relativity. Though they give a theorem on connection between RCs and CCs, no explicit attempt to classifying spacetimes according to their CCs has been given. Keeping this point in mind and the complexity of the system of CC equations, we consider some specific spacetimes to obtain their CCs using some special methods. It is hoped that this would enable one to extend these methods to obtain a classifications of general space–times according to their CCs.

In the next section we give the set of coupled quadratic CC equations and their form for spherically symmetric static space–times. In the third section we solve this set of equations for various specific cases. A summary and conclusion is given in the last section.

II. CC EQUATIONS

A CC, $\boldsymbol{\xi}$, satisfies the equation

$$\mathop{\mathscr{L}}_{\boldsymbol{\xi}} R = 0, \tag{1}$$

where R is the Riemann Christoffel curvature tensor. In a torsion free space, in a coordinate basis, this equation reduces to the set of partial differential equations (PDEs)

$$R^{\alpha}{}_{bcd,f}\xi^{f} + R^{\alpha}{}_{fcd}\xi^{f}{}_{,b} + R^{\alpha}{}_{bfd}\xi^{f}{}_{,c} + R^{\alpha}{}_{bcf}\xi^{f}{}_{,d} - f^{f}{}_{bcd}\xi^{\alpha}{}_{,f} = 0. \tag{2}$$

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In a given 4-dimensional space–time there are actually 256 coupled PDEs to be solved for four unknown functions of four variables. However, for spherically symmetric static space–times in which at the most only six independent components (3 $R^0{}_{i0i}$, where $i=1,...,3$, 2 $R^1{}_{\alpha1\alpha}$, where $\alpha=1$, 2, and 1 $R^2{}_{323}$) of the Riemann tensor can survive, the system of CC equations reduces to 22 sets of coupled CC equations consisting of *54* PDEs to be solved only. These coupled CC equations (without requiring summation over repeated indices) are given by

$$R^i{}_{1i1}\xi^1{}_{,0}+R^\alpha{}_{0\alpha0}\xi^0{}_{,1}=0, \quad (i,\alpha)=(0,1),(2,2),(3,3), \tag{3}$$

$$R^i{}_{2i2}\xi^2{}_{,0}+R^\alpha{}_{0\alpha0}\xi^0{}_{,2}=0, \quad (i,\alpha)=(0,2),(1,1),(3,3), \tag{4}$$

$$R^i{}_{3i3}\xi^3{}_{,0}+R^\alpha{}_{0\alpha0}\xi^0{}_{,3}=0, \quad (i,\alpha)=(0,3),(1,1),(2,2), \tag{5}$$

$$R^i{}_{1i1,f}\xi^f+2R^i{}_{1i1}\xi^1{}_{,1}=0, \quad i=0,2,3 \text{ and } f=1 \text{ or } 2, \tag{6}$$

$$R^i{}_{1i1}\xi^1{}_{,2}+R^\alpha{}_{2\alpha2}\xi^2{}_{,1}=0, \quad (i,\alpha)=(0,0),(2,1),(3,3), \tag{7}$$

$$R^i{}_{1i1}\xi^1{}_{,3}+R^\alpha{}_{3\alpha3}\xi^3{}_{,1}=0, \quad (i,\alpha)=(0,0),(3,1),(2,2), \tag{8}$$

$$R^i{}_{2i2}\xi^2{}_{,3}+R^\alpha{}_{3\alpha3}\xi^3{}_{,2}=0, \quad (i,\alpha)=(0,0),(1,1),(3,2), \tag{9}$$

$$R^i{}_{2i2,f}\xi^f+2R^i{}_{2i2}\xi^2{}_{,2}=0, \quad i=0,1,3 \text{ and } f=1 \text{ or } 2, \tag{10}$$

$$R^i{}_{3i3,f}\xi^f+2R^i{}_{3i3}\xi^3{}_{,3}=0, \quad i=0,1,2 \text{ and } f=1 \text{ or } 2, \tag{11}$$

$$R^i{}_{0i0,f}\xi^f+2R^i{}_{0i0}\xi^0{}_{,0}=0, \quad i=1,2,3 \text{ and } f=1 \text{ or } 2, \tag{12}$$

$$(R^0{}_{i0i}-R^\alpha{}_{i\alpha i})\xi^0{}_{,\alpha}=0, \quad (i,\alpha)=(1,3),(2,3),(1,2),(3,2),(2,1),(3,1), \tag{13}$$

$$(R^0{}_{i0i}-R^\alpha{}_{i\alpha i})\xi^\alpha{}_{,0}=0, \quad (i,\alpha)=(1,3),(2,3),(1,2),(3,2),(2,1),(3,1), \tag{14}$$

$$(R^\alpha{}_{i\alpha i}-R^\beta{}_{i\beta i})\xi^\alpha{}_{,\beta}=0, \quad (i,\alpha,\beta)=(0,1,2),(3,1,2),(0,1,3),(2,1,3), \tag{15}$$

$$(R^\alpha{}_{i\alpha i}-R^\beta{}_{i\beta i})\xi^\beta{}_{,\alpha}=0, \quad (i,\alpha,\beta)=(0,1,2),(3,1,2),(0,3,2),(1,3,2), \tag{16}$$

$$(R^\alpha{}_{i\alpha i}-R^\beta{}_{i\beta i})\xi^\beta{}_{,\alpha}=0, \quad (i,\alpha,\beta)=(0,1,3),(2,1,3),(0,2,3),(1,2,3). \tag{17}$$

III. SOLUTION OF THE CC EQUATIONS

We solve the CC equations for Minkowski, De Sitter (anti-De Sitter), Einstein (anti-Einstein), Schwarzschild, and Reissner–Nordstrom metrics along with three Bertotti–Robinson-like metrics.[10] However, since the problem of solving CC equations is trivial in Minkowski space–time, we do not solve this case explicitly and only give results. The CC equations in the De Sitter and anti-De Sitter metrics reduce to the Killing equations. We therefore only quote results without giving details for these two cases. We present the complete procedure for solving the CC equations for the Einstein metric. As the same methods apply for the anti-Einstein, Schwarzschild, Reissner–Nordstrom, and Bertotti–Robinson-like metrics, we again only quote the results for them.

For the Einstein metric

$$ds^2=dt^2-\frac{dr^2}{1-r^2/R^2}-r^2(d\vartheta^2+\sin^2\vartheta\, d\phi^2), \tag{18}$$

the nonzero Riemann tensor components are given by

$$R^1{}_{212}=r^2/R^2, \quad R^1{}_{313}=\frac{r^2}{R^2}\sin^2\vartheta=R^2{}_{323}. \tag{19}$$

With these values in the CC equations, some of the equations [Eqs: (3)–(5), (8), and (15)–(17)] are identically satisfied, while Eqs. (13) and (14), respectively, yield

$$\left.\begin{aligned}\xi^0{}_{,\alpha}&=0 \quad (\alpha=1,2,3),\\ \xi^\alpha{}_{,0}&=0 \quad (\alpha=1,2,3).\end{aligned}\right\} \tag{20}$$

Now using Eqs. (20), Eqs. (6)–(11), respectively, yield

$$r\xi^1+R^2(1-r^2/R^2)\xi^1{}_{,1}=0, \tag{21}$$

$$\xi^1{}_{,2}+r^2(1-r^2/R^2)\xi^2{}_{,1}=0, \tag{22}$$

$$\xi^1{}_{,3}+r^2(1-r^2/R^2)\sin^2\vartheta\,\xi^3{}_{,1}=0, \tag{23}$$

$$\xi^2{}_{,3}+\sin^2\vartheta\,\xi^3{}_{,2}=0, \tag{24}$$

$$\xi^1+r\xi^2{}_{,2}=0, \tag{25}$$

$$\xi^1+r\cot\vartheta\,\xi^2+r\xi^3{}_{,3}=0. \tag{26}$$

To solve this system of PDEs we first consider Eq. (21), writing it in the form

$$\xi^1{}_{,1/\xi^1}=\frac{r/R^2}{(1-r^2/R^2)}. \tag{27}$$

In view of Eq. (20), Eq. (27) yields

$$\xi^1=\sqrt{1-r^2/R^2}A(\vartheta,\phi), \tag{28}$$

where $A(\vartheta,\phi)$ is a function of integration. Now differentiating Eq. (28) with respect to ϑ comparing with Eq. (22) and solving while using Eq. (20), gives

$$\xi^2=\frac{\sqrt{1-r^2/R^2}}{r}A_\vartheta(\vartheta,\phi)+B(\vartheta,\phi), \tag{29}$$

where $B(\vartheta,\phi)$ is some function of integration. Now using Eqs. (28) and (29), Eq. (25) yields

$$\frac{\sqrt{1-r^2/R^2}}{r}(A_{\vartheta\vartheta}(\vartheta,\phi)+A(\vartheta,\phi))+B_\vartheta(\vartheta,\phi)=0, \tag{30}$$

which is satisfied only when

$$B_\vartheta(\vartheta,\phi)=0=A_{\vartheta\vartheta}(\vartheta,\phi)+A(\vartheta,\phi). \tag{31}$$

These equations can be easily solved to give

$$\left.\begin{aligned}A&=A_1(\phi)\cos\vartheta+A_2(\phi)\sin\vartheta,\\ B&=B_1(\phi),\end{aligned}\right\}, \tag{32}$$

where $A_1(\phi)$, $A_2(\phi)$ and $B_1(\phi)$ are again functions of integration. Now using Eqs. (28), (29), and (32), Eq. (23) give

$$\xi^3=\frac{\sqrt{1-r^2/R^2}}{r\ \sin^2\ \vartheta}\ (A_{1\phi}(\phi)\cos\ \vartheta+A_{2\phi}(\phi)\sin\ \vartheta)+D(\vartheta,\phi), \tag{33}$$

where $D(\vartheta,\phi)$ is some function of integration. At this stage we substitute these values of ξ^1, ξ^2, and ξ^3 into Eq. (24). It turns out that this is satisfied only when

$$A_{1\phi}=0=D_{\vartheta}(\vartheta,\phi)+\frac{1}{\sin^2\ \vartheta}\ B_{1\phi}(\phi). \tag{34}$$

This equation can be easily solved to obtain,

$$\left.\begin{aligned} &A_1=\alpha_1\\ &D(\vartheta,\phi)=\cot\ \vartheta B_{1\phi}(\phi)+E(\phi),\end{aligned}\right\} \tag{35}$$

where α_1 is a constant and $E(\phi)$ some integration function. Inserting Eqs. (35) into Eq. (26) and requiring consistency give

$$\left.\begin{aligned} &A_{2\phi\phi}(\phi)+A_2(\phi)=0,\\ &B_{1\phi\phi}(\phi)+B_1(\phi)=0=E_{\phi}(\phi).\end{aligned}\right\} \tag{36}$$

These equations can again be easily solved to give

$$\left.\begin{aligned} &A_2=\alpha_2\ \cos\ \phi+\alpha_3\ \sin\ \phi,\\ &B_1=\alpha_4\ \cos\ \phi+\alpha_5\ \sin\ \phi,\\ &E=\alpha_6,\end{aligned}\right\} \tag{37}$$

where α_2 to α_6 are integration constants. Inserting Eqs. (32) and (34)–(37), the CCs become

$$\left.\begin{aligned} &\xi^1=\sqrt{1-r^2/R^2}(\alpha_1\ \cos\ \vartheta+(\alpha_2\ \cos\ \phi+\alpha_3\ \sin\ \phi)\sin\ \vartheta],\\ &\xi^2=\frac{\sqrt{1-r^2/R^2}}{r}\ (-\alpha_1\ \sin\ \vartheta+(\alpha_2\ \cos\ \phi+\alpha_3\ \sin\ \phi)\cos\ \vartheta]+(\alpha_4\ \cos\ \phi+\alpha_5\ \sin\ \phi),\\ &\xi^3=\frac{\sqrt{1-r^2/R^2}}{r\ \sin\ \vartheta}\ [-\alpha_2\ \sin\ \phi+\alpha_3\ \cos\ \phi]+\cot\ \vartheta[(-\alpha_4\ \sin\ \phi+\alpha_5\ \cos\ \phi)]+\alpha_6,\\ &\xi^0=\xi^0(t).\end{aligned}\right\} \tag{38}$$

Notice that these are six CCs for the spatial components of $\boldsymbol{\xi}$ and the temporal component of, $\boldsymbol{\xi}$, is an arbitrary function of t only. Similarly for the anti-Einstein metric ''R^2'' is replaced by ''$-R^2$'' in the metric. It is easily verified that the number of CCs in the anti-Einstein metric turn out to be the same as the number of CCs in the Einstein metric with the only difference that R^2 in Eqs. (38) is replaced by $-R^2$.

For the Schwarzschild metric

$$ds^2=\left(1-\frac{2m}{r}\right)dt^2-\left(1-\frac{2m}{r}\right)^{-1}\ dr^2-r^2\ d\Omega^2$$

the surviving Riemann Christoffel curvature tensor components are

$$R^0{}_{101}=\frac{2m}{r^3\left(1-\frac{2m}{r}\right)}, \quad R^0{}_{202}=-\frac{m}{r}=R^1{}_{212},$$

$$R^0{}_{303}=-\frac{m}{r}\sin^2\vartheta=R^1{}_{313}, \quad R^2{}_{323}=-\frac{2m}{r}\sin^2\vartheta.$$

The CCs in this case turn out to be the same as four KVs for this metric,

$$\xi^\alpha=\{\alpha_0,0,(\alpha_1\cos\phi+\alpha_2\sin\phi),-\cot\vartheta(\alpha_1\sin\phi-\alpha_2\cos\phi)+\alpha_3\}. \tag{39}$$

In the Reissner–Nordstrom spacetime

$$ds^2=\left(1-\frac{2m}{r}+\frac{4\pi Q^2}{r^2}\right)-\left(1-\frac{2m}{r}+\frac{4\pi Q^2}{r^2}\right)^{-1}dr^2-r^2\,d\Omega^2,$$

the nonzero Riemann tensor components are given by

$$R^0{}_{101}=\frac{(2Mr-12\pi Q^2)}{r^2(r^2-2Mr+4\pi Q^2)}, \quad R^0{}_{202}=-\frac{(2Mr-4\pi Q^2)}{r^2},=R^1{}_{212},$$

$$R^0{}_{303}=-\frac{(2Mr-4\pi Q^2)}{r^2}\sin^2\vartheta=R^1{}_{313}, \quad R^2{}_{323}=\left(\frac{2Mr-4\pi Q^2}{r^2}\right)\sin^2\vartheta.$$

The CCs in this case are again same as four KVs of Schwarzschild metric given by Eq. (39).

The De Sitter and anti-De Sitter space–times, respectively, have their metrics given by

$$ds^2=\left(1\mp\frac{r^2}{R^2}\right)dt^2-\left(1\mp\frac{r^2}{R^2}\right)^{-1}dr^2-r^2\,d\Omega^2.$$

In this case the surviving Riemann Christoffel curvature tensor component are given by

$$R^0{}_{101}=\frac{1/R^2}{1\mp r^2/R^2}, \quad R^0{}_{202}=\frac{r^2}{R^2}=R^1{}_{212},$$

$$R^0{}_{303}=\frac{r^2}{R^2}\sin^2\vartheta=-R^1{}_{313}=R^2{}_{323}.$$

If we write the CC equations for the above metrics, it is seen that the CC equations become same as Killing equations, hence in both cases the CCs are same as ten KVs there.[3]

There exists three Bertotti–Robinson-like metrics in the literature. In the first case the metric is given by

$$ds_1^2=(B+r)^2\,dt^2-dr^2-a^2\,d\Omega^2.$$

Here, only one Riemann tensor component given by

$$R^2{}_{323}=\sin^2\vartheta$$

survives and CCs in this case become

TABLE I. Comparison of KVs, RCs, and CCs for some specific spherically symmetric static metrics.

	KVs	RCs	CCs
Minkowski	10	Arbitrary	Arbitrary
De Sitter/anti	10	10	10
Einstein/anti	7	$6+\xi^0$ (arbt) (x^α)	$6+\xi^0$ (arbt) (t)
Bertotti–Robinson$_{\rm I}$	6	$3+\xi^0$ (x^α) & ξ^1 (x^α),	$3+\xi^0$ (t,r), ξ^1 (t,r)
Bertotti–Robinson$_{\rm II}$	6	6	6
Bertotti–Robinson$_{\rm III}$	6	6	6
Schwarzschild	4	Arbitrary	4
Reissner–Nordstrom	4	4	4

$$\xi^0=f(t,r), \quad \xi^1=g(t,r),$$

$$\xi^2=(C_1\cos\phi+C_2\sin\phi), \quad \xi^3=\cot\vartheta(-C_1\sin\phi+C_2\cos\phi)+C_3.$$

In the other two Bertotti–Robinson-like metrics given by

$$ds^2_{\rm II}=\cos^2(c+\sqrt{\alpha}r)dt^2-dr^2-a^2\,d\Omega^2,$$

$$ds^2_{\rm III}=\cosh^2(C+\sqrt{\alpha}r)dt^2-dr^2-a^2\,d\Omega^2$$

only $R^0{}_{101}$ and $R^2{}_{323}$ survive. Here, $R^0{}_{101_{\rm II}}=-R^0{}_{101_{\rm III}}=\alpha$ (constant), whereas, $R^2{}_{323_{\rm II}}=R^2{}_{323_{\rm III}}$. The CCs in both cases again turn out to be same as six KVs of these metrics.[3]

IV. CONCLUSION

In the hope of understanding how the information about the symmetries implicit in the geometry, and relevant for the matter–energy field (through the Einstein equations), is distributed between the metric tensor, the Ricci tensor, and the Riemann tensor, we have explicitly computed the CCs for some specific spherically symmetric static metrics. We discuss our results in the light of Table I for KVs, RCs, and CCs of the corresponding space–times.

While the isometries must always be definite, collineations can be unlimited. This is due to the fact that the metric tensor is nondegenerate while the Ricci tensor and Riemann tensor need not be nondegenerate. Where degeneracy arises there are arbitrary many collineations possible. In particular, if the relevant tensor is zero all vectors are collineations. Since there is a unique space–time that is Riemann flat (the Minkowski space–time) every vector is a CC. Any vacuum space–time is Ricci flat and hence has all vectors as RCs. In the same way there is a greater freedom of RCs than of CCs in the Einstein and anti-Einstein spaces. For the former there is one arbitrary function of four variables (i.e., α^4) while for the latter it depends on only one variable (i.e., α^1). Similarly, for the flat Bertotti–Robinson-like metric there are two arbitrary functions. For RCs we have $(\alpha^4)^2$ while for CCs we have $(\alpha^2)^1$. The most striking case is for the Schwarzschild metric where the CCs are identical with the KVs but *every vector* is an RC. Clearly, the CCs are closer to the more restricted KVs than are the RCs.

It would be important to develop general methods of classifying space–times with some minimal symmetry group in terms of their CCs and seeing how this general classification compares with KVs and RCs. The easiest for this purpose is the class of all spherically symmetric static space–times (of which only the generic case remains to be dealt with). Then one could hope to extend the discussion by dropping the requirement of staticity, going over to cylindrical or plane symmetry, and then reducing the minimal symmetry group further. Finally, it would be necessary to compare the results with other classification schemes, such as Petrov classification.

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The symplectic geometry of a parametrized scalar field on a curved background

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We study the real, massive Klein–Gordon field on a C^∞ globally-hyperbolic background space–time with compact Cauchy hypersurfaces. In particular, the parametrization of this system as initiated by Dirac and Kuchař is put on a rigorous basis. The discussion is focussed on the structure of the set of spacelike embeddings of the Cauchy manifold into the space–time, and on the associated e-tensor density bundles and their tangent and cotangent bundles. The dynamics of the field is expressed as a set of automorphisms of the space of initial data in which each pair of embeddings defines one such automorphism. Using these results, the extended phase space of the system is shown to be a weak-symplectic manifold, and the Kuchař constraint is shown to define a smooth constraint submanifold which is foliated smoothly by the constraint orbits. The pull-back of the symplectic form to the constraint surface is a presymplectic form which is singular on the tangent spaces to the constraint orbits. Thus, the geometric structure of this infinite-dimensional system is analogous to that of a finite-dimensional, first-class parametrized system, and hence many of the results for the latter can be transferred to the infinite-dimensional case without difficulty. © *1996 American Institute of Physics.* [S0022-2488(96)02807-1]

I. INTRODUCTION

The long history of studies of quantum field theory in a background space–time peaked sharply in the seventies (for reviews from that era, see Refs. 1 and 2) following Hawking's discovery of the quantum radiation produced by a black hole.[3] In those days, the main aim was to find a direct quantization of the true physical degrees of freedom of the system. However, much earlier, Dirac had reformulated this system in a parametrized form so that it could be used as a model for general relativity proper.[4] The idea is to treat embeddings of Cauchy hypersurfaces in the space–time as additional degrees of freedom of the system. Together with their conjugate momenta and the Cauchy data of the scalar field on the embeddings, they define an extended phase space. To retrieve the original dynamics one has to impose constraints. This procedure was studied in some detail in Refs. 5, 6 and 7; a shorter exposition can be found in Ref. 8. The resulting system can be classified as a ''first-class parametrized system.''

A method of quantizing first-class parametrized systems was initiated by Dirac; in particular, he studied a system of massive particles in Minkowski space–time.[9] A generalization of this method to any *finite*-dimensional first-class parametrized system was given by Hájíček[10] using a combination of Dirac's ideas with the group quantization method of Isham[11] and the algebraic quantization method of Ashtekar.[12] In what follows, this generalization will be referred to as the ''perennial formalism.''

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If one is interested in extending the perennial formalism to infinite-dimensional systems, the scalar field on a fixed space–time offers itself naturally as a well-understood and much-discussed model. However, the perennial formalism is based on a geometrical form of Hamiltonian dynamics, whereas the existing formulations of the parametrized scalar field are non-geometrical. The main purpose of the present article is to recast the classical theory of a parametrized scalar field in a fixed background into the geometrical, Hamiltonian form for infinite-dimensional systems developed by Marsden and collaborators (see Ref. 13). The ensuing results are of interest in themselves and are also used in the accompanying article[14] dealing with the application of the perennial formalism to the quantum theory of a field propagating on a curved background.

Marsden's techniques have been applied to a variety of systems, including general relativity itself.[15] In all these examples, the extended phase space is an (open) subset of a linear space, and hence the tangent space at any point in the phase space can be naturally identified with this linear space. The resulting significant simplifications have been thoroughly exploited in the literature (for example, see Ref. 15). However, in our case, the space of embeddings is a genuine manifold, not just a subspace of a linear space. Of course, the rough idea of how the theory is to be applied in general to such cases is well-known,[13] but—as we shall see—the specific system of interest to us possesses some crucial additional structure that is very helpful in the detailed analysis.

The plan of the article is as follows. In section II, the theory of the Cauchy problem of a hyperbolic, partial differential equation (as reviewed, for example, in Ref. 15) is applied to the dynamics of a massive scalar field in a globally hyperbolic space–time. The Cauchy hypersurfaces are assumed to be compact, but it seems likely that—if desired—the proofs (which are relegated to the Appendix) could be adapted to deal with asymptotically flat Cauchy hypersurfaces. The set of all Cauchy data is given the structure of a topological vector space Γ_ϕ, and an automorphism of this space is associated with each oriented pair of embeddings of the Cauchy manifold in the space–time, thereby producing a rather generalized concept of ''time evolution.''

In section III, we extend the phase space from Γ_ϕ to $\Gamma_\phi \times T^*\mathscr{E}$, where $\mathscr{E}$ is the space of embeddings introduced by Kuchař in Ref. 5. This way of parametrizing the system was discussed in detail by Isham and Kuchař.[7] The structure of the e-tensor density bundles over $\mathscr{E}$ is described, and their tangent and cotangent bundles are studied; this is where we lay the foundation for the subsequent mathematical developments. Our approach to the resulting infinite-dimensional Hamiltonian system is based on the geometrical ideas of Chernov, Fischer, and Marsden.[13,15] The constructions of the phase space manifold, the symplectic structure, and the Poisson brackets are all described explicitly.

In section IV, we show that (i) the constraint set is a submanifold of the phase space; (ii) the constraint orbits are submanifolds of the constraint surface; and (iii) the vector space defined by the right hand side of the evolution equation coincides with the tangent space of a constraint orbit. For the model we study, the proofs (which are adapted from Ref. 15) are straightforward. The resulting structure is analogous to a high degree to that of a finite-dimensional first-class parametrized system, and hence the application of the perennial formalism is relatively unproblematic.

II. FIELD DYNAMICS

We are interested in the theory of a relativistic field propagating on a fixed background space–time $\mathscr{M}$. The associated dynamical equation defines an evolution map between Cauchy data along two arbitrary Cauchy hypersurfaces. We shall need various properties of these maps that can be derived from results concerning the Cauchy problem for linear hyperbolic systems as described—for example—in Refs. 15 and 16.

The following properties of the space–time $(\mathscr{M},g)$ will be assumed:

(1) The space–time $\mathscr{M}$ is equipped with a C^∞ differential structure. In particular, this means that diffeomorphisms do not mix the different Sobolev structures that will be placed on various function spaces associated with Σ and $\mathscr{M}$.

(2) The Lorentzian metric g is such that the pair $(\mathscr{M},g)$ is globally hyperbolic. Thus the four-manifold $\mathscr{M}$ is necessarily diffeomorphic to $\Sigma\times\mathbb{R}$ where the three-manifold Σ is a model for any Cauchy hypersurface in $\mathscr{M}$.

(3) The three-manifold Σ is compact. This assumption is made for the sake of simplicity, but we expect that similar results can be obtained for asymptotically flat space–times using analogous—but more laborious—methods; see Ref. 15).

The relativistic wave equation of interest is the Klein–Gordon equation for a real scalar field:

$$|\det g|^{-1/2}\partial_\mu(|\det g|^{1/2}g^{\mu\nu}\partial_\nu\phi)+m^2\phi=0 \tag{1}$$

where the real, non-negative constant m is the mass parameter.

A central role in the theory is played by C^{r+1} $(r>2)$ embeddings $X:\Sigma\to\mathscr{M}$ that are spacelike with respect to g. We shall refer to any such X simply as an ''embedding,'' and denote by $\mathrm{Emb}_g(\Sigma,\mathscr{M})$ the space of all such (see Refs. 5 and 7). Each embedding X determines a positive-definite C^r-metric γ on Σ as the pull-back X^*g of g by X; i.e., in local coordinates on both Σ and $\mathscr{M}$,

$$\gamma_{ab}(x):=g_{\mu\nu}(X(x))X^\mu{}_{,a}(x)X^\nu{}_{,b}(x). \tag{2}$$

The map X also determines a future-oriented, unit normal vector $n(X(x))$ at each point of the hypersurface $X(\Sigma)$ in $\mathscr{M}$.

Any embedding $X\in\mathrm{Emb}_g(\Sigma,\mathscr{M})$ defines a ''Cauchy datum'' for ϕ along the hypersurface $X(\Sigma)$. This is a pair (φ,π) of fields on Σ, where the scalar φ and the density (of weight $w=1$) π are defined by

$$\varphi(x):=\phi(X(x)), \tag{3}$$

$$\pi(x):=(\det\gamma)^{1/2}(x)n^\mu(X(x))\partial_\mu\phi(X(x)), \tag{4}$$

for all $x\in\Sigma$, and where γ is defined in Eq. (2).

We shall need certain Sobolev spaces of tensor-density fields on Σ (for more details see Ref. 16). The first step is to introduce a fixed, auxiliary C^r Riemannian metric f_{kl} on Σ. Let $I,J,K,\ldots$ denote multiple indices, and let $|I|$ be the number of simple indices within I. Let f_{IJ} be the abbreviation for the tensor product of $|I|=|J|$ copies of the covariant tensors f_{ij}, and—similarly—f^{IJ} denotes the appropriate tensor product of contravariant fields f^{ij}. If T^J_I is a C^r tensor-density field on Σ of type $(|I|,|J|,w)$ (w is the weight), $T^J_{I|K}$ will denote the tensor-density field obtained from T^J_I by a $|K|$-fold covariant derivative (covariant with respect to the auxiliary metric f). Then the Sobolev space scalar product $(T,S)^s_f$ between two tensor-density fields T^J_I and S^J_I is defined by

$$(T,S)^s_f:=\sum_{|M|=|N|=0}^{s}\int_\Sigma d^3x(\det f)^{1/2-w}f^{IK}f^{MN}f_{JL}T^J_{I|M}S^L_{K|N} \tag{5}$$

where $s\leqslant r$. We denote the corresponding Sobolev space by $H^s_{|I||J|w}(\Sigma)$, or simply $H^s_w(\Sigma)$ if no confusion can result. Note that the topology of these spaces is independent of the auxiliary metric f provided that Σ is compact (which we are assuming).

Using this notation, we can introduce the space Γ^s_ϕ of Cauchy data:

$$\Gamma^s_\phi:=H^s_0(\Sigma)\times H^{s-1}_1(\Sigma) \tag{6}$$

with $\varphi \in H_0^s(\Sigma)$ and $\pi \in H_1^{s-1}(\Sigma)$. The dynamics of the field ϕ as determined by Eq. (1) defines maps between the spaces of Cauchy data corresponding to different embeddings. The relevant facts about these maps (which are more or less well-known; see Ref. 15) are listed in Appendix 1, and culminate in the following theorem:

Theorem: Let X_1 and X_2 be two arbitrary C^{r+1} embeddings with $r \geqslant 4$. Then each pair $(\varphi_1, \pi_1) \in \Gamma_\phi^s$ (with $2 \leqslant s \leqslant r-2$) defines a unique solution ϕ of the field equation (1) such that

(1) the Cauchy datum associated with the embedding X_1 is the given pair (φ_1, π_1);

(2) the embedding X_2 gives a well-defined Cauchy datum (φ_2, π_2) that belongs to Γ_ϕ^s

(3) the map $\rho_{X_1 X_2}: \Gamma_\phi^s \to \Gamma_\phi^s$ thus defined is an automorphism of the Sobolev space Γ_ϕ^s.

Note that we obtain a maximal classical solution in the sense that the embedding X_2 can be chosen to map Σ so that it passes through any given point of $\mathscr{M}$.

The theorem above implies that a differentiable solution is obtained if s is sufficiently large. Indeed, the famous Sobolev lemma asserts that $H_w^s(\Sigma) \subset C_w^{s'}(\Sigma)$ if $s > s' + \frac{1}{2} \dim \Sigma$. For example, ϕ will be C^2 if $s = 4$. The index s can be taken as large as one wishes if r is sufficiently large. In particular, for $r = \infty$, one can take the intersection Γ_ϕ^∞ of the Hilbert spaces Γ_ϕ^s, $s = 4,5, \ldots$, to give the space of all pairs of C^∞-functions and densities that is equipped with the structure of a countably Hilbert nuclear space (see Ref. 17).

III. THE EXTENDED PHASE SPACE

The theory of a scalar field on a curved background was rewritten in the form of a parametrized system in Refs. 7 and 18. In this section, we shall reformulate a part of this work so that it becomes compatible with the mathematical formalism of Fischer and Marsden.[15] First however, the studies in Refs. 5 and 7 of the differential geometry of the space of embeddings $\mathscr{E}$ must be extended to include certain bundles over $\mathscr{E}$.

The construction of a smooth differential structure on a space of continuous maps between two finite-dimensional manifolds was described as early as 1958 by Eells,[19] but we shall use the method developed more recently in Ref. 20. Recall that, in a pair of local charts

$$(U,h) \text{ of } \Sigma \text{ and } (\overline{V,h}) \text{ of } \mathscr{M} \tag{7}$$

[where $X(U) \cap \overline{V} \neq \varnothing$], a given embedding $X: \Sigma \to \mathscr{M}$ can be represented by the function $\overline{h} \circ X \circ h^{-1}: h(U) \to \mathbb{R}^4$. We say that X belongs to the space $H^s(\Sigma, \mathscr{M})$ if these local representatives are in the Sobolev space $H^s(h(U), \mathbb{R}^4)$ for all such pairs of local charts. This notion can be shown to be atlas-independent for $s > 3/2$ [which means that X is continuous since, according to the Sobolev lemma, $X \in C^r(\mathscr{N}, \mathscr{M})$ if $s > r + \dim(\mathscr{N})/2$].

In what follows, a major role is played by the tangent and cotangent bundles to the infinite-dimensional manifold of embeddings. In the differential geometry of a finite-dimensional manifold $\mathscr{N}$, a tangent vector τ at a point $p \in \mathscr{N}$ can be defined in several different ways. One algebraic approach is to view τ as a derivation at p of the ring $C^\infty(\mathscr{N})$ of smooth functions on $\mathscr{N}$: i.e., $\tau: C^\infty(\mathscr{N}) \to \mathbb{R}$ is a linear map with the property that if $f, g \in C^\infty(\mathscr{N})$, then $\tau(fg) = f(p)\tau(g) + g(p)\tau(f)$. A more geometrical approach is to define τ as an equivalence class of local curves $\sigma: (-\epsilon, \epsilon) \to \mathscr{N}$ where (i) $\epsilon > 0$ (and can be σ-dependent); (ii) $\sigma(0) = p$; and (iii) two local curves σ_1 and σ_2 are regarded as being equivalent if their tangent vectors at $p \in \mathscr{N}$ are equal as computed in a local coordinate system around p (the equivalence classes are independent of choice of coordinate system).

In the finite-dimensional case, these two definitions can be shown to be equivalent. However, the situation in infinite dimensions is quite different since complicated functional-analytical problems need to be resolved before the algebraic definition can even be posed. Fortunately, the geometrical definition of a tangent vector as an equivalence class of curves still works well and, when applied to the case of interest, leads naturally to the definition of the tangent space

$T_X H^s(\Sigma,\mathscr{M})$ to $H^s(\Sigma,\mathscr{M})$ at the embedding X as the set of maps $V:\Sigma\to T\mathscr{M}$ with the property that the image $V(x)$ of a point $x \in \Sigma$ is a tangent vector on $\mathscr{M}$ at the point $X(x)$; i.e., $V(x) \in T_{X(x)}\mathscr{M}$; more formally, V satisfies the relation $X=\chi\circ V$, where $\chi:T\mathscr{M}\to\mathscr{M}$ is the bundle projection of the tangent bundle $T\mathscr{M}$ of $\mathscr{M}$.

This defining property of $V \in T_X H^s(\Sigma,\mathscr{M})$ can be expressed in another way that will be useful later. Namely, we recall that if $\rho:E\to\mathscr{M}$ is the projection map of any fibre bundle E over a manifold $\mathscr{M}$, and if $f:\mathscr{N}\to\mathscr{M}$ is a map from another manifold $\mathscr{N}$ into $\mathscr{M}$, then the pull-back bundle f^*E over $\mathscr{N}$ is defined as

$$f^*E:=\{(x,e)\in\mathscr{N}\times E\,|\,f(x)=\rho(e)\}, \tag{8}$$

and a cross-section of this bundle is given by any map $\psi:\mathscr{N}\to E$ such that $\rho(\psi(x))=f(x)$. It follows therefore that a vector $V \in T_X H^s(\Sigma,\mathscr{M})$ can be regarded as a cross-section of the bundle $X^*(T\mathscr{M})$.

Note that the vector space $T_X H^s(\Sigma,\mathscr{M})$ can be given an H^s-structure so that the function space $H^s(\Sigma,\mathscr{M})$ becomes a Banach manifold modelled on the Banach space $T_X H^s(\Sigma,\mathscr{M})$ (for example, via an exponential map in $\mathscr{M}$). We shall assume from now on that this has been done, and we shall consider only embeddings that lie in $H^s(\Sigma,\mathscr{M})$, and (with the value s of the Sobolev class understood) denote the set of all such by $\mathscr{E}$; i.e., $\mathscr{E}:=\mathrm{Emb}_g(\Sigma,\mathscr{M})\cap H^s(\Sigma,\mathscr{M})$. It can be shown that $\mathscr{E}$ is an open subset of $H^s(\Sigma,\mathscr{M})$, and hence $\mathscr{E}$ is a Banach manifold with the same tangent spaces and analogous manifold structure as that of $H^s(\Sigma,\mathscr{M})$ itself.

The above definition of a tangent vector leads immediately to the definition of the tangent bundle $T\mathscr{E}$ of $\mathscr{E}$. More generally, if ${}^R_S T\mathscr{M}$ is the tensor bundle of type (R,S) over $\mathscr{M}$ (R times contravariant and S times covariant), we obtain an ''e-tensor bundle'' ${}^R_S T\mathscr{E}$ over $\mathscr{E}$ by defining an e-tensor at the point $X \in \mathscr{E}$ to be a map $\psi:\Sigma\to{}^R_S T\mathscr{M}$ such that $\psi(x) \in {}^R_S T_{X(x)}\mathscr{M}$; i.e., $X=\chi\circ\psi$, where χ now denotes the bundle projection of ${}^R_S T\mathscr{M}$. Equivalently, ψ can be regarded as a cross-section of the bundle $X^*({}^R_S T\mathscr{M})$ over Σ.

We shall need an even more general e-tensor of the type defined in Ref. 5 which transforms as a tensor density of type (r,s,w) with respect to a coordinate change in Σ around x, and as a tensor of type (R,S) with respect to a coordinate change in $\mathscr{M}$ around the point $X(x) \in \mathscr{M}$. The precise definition of such an e-tensor is that it is a cross-section ψ of the bundle ${}^{r,w}_{s} T\Sigma\otimes X^*({}^R_S T\mathscr{M})$ over Σ, where ${}^{r,w}_{s} T\Sigma$ is the bundle of tensors over Σ that are r times contravariant, s times covariant, and of tensor-density weight w. It follows that, for all $x \in \Sigma$, we have $\psi(x) \in {}^{r,w}_{s} T_x\Sigma\otimes{}^R_S T_{X(x)}\mathscr{M}$, and hence $\psi(x)$ can be represented by its components $\psi^{k_1\ldots k_r\mu_1\ldots\mu_R}_{l_1\ldots l_s\nu_1\ldots\nu_S}(x)$ on Σ defined with respect to an appropriate pair of coordinate charts on Σ and $\mathscr{M}$.

There is another way of representing e-tensors which is particularly useful for discussing tangent vectors to the collection of all e-tensors of a certain type. Namely, recall that if V and W are any pair of finite-dimensional vector spaces, then there is a canonical isomorphism of $V^*\otimes W$ with the space $L(V,W)$ of linear maps from V to W in which the linear map $L_{\ell\otimes w}$ associated with $\ell\otimes w \in V^*\otimes W$ is defined by $L_{\ell\otimes w}(v):=\langle\ell,v\rangle w$ for all $v \in V$. In particular, we note that ${}^{r,w}_{s} T_x\Sigma$ is the algebraic dual of ${}^{s,-w}_{r} T_x\Sigma$, and hence it follows that if ψ is an e-tensor with $\psi(x) \in {}^{r,w}_{s} T_x\Sigma\otimes{}^R_S T_{X(x)}\mathscr{M}$, then we can identify $\psi(x)$ as a linear map $\psi(x):{}^{s,-w}_{r} T_x\Sigma\to{}^R_S T_{X(x)}\mathscr{M}$. This can be summarized rather neatly by defining an e-tensor to be a vector bundle map ψ from ${}^{s,-w}_{r} T\Sigma$ to ${}^R_S T\mathscr{M}$, i.e., the following diagram is commutative

$$\begin{array}{ccc} {}^{s,-w}_{r} T\Sigma & \overset{\psi}{\to} & {}^R_S T\mathscr{M} \\ \downarrow\rho & & \downarrow\chi \\ \Sigma & \overset{X}{\to} & \mathscr{M} \end{array} \tag{9}$$

where ρ and χ are the projection maps in the indicated tensor bundles over Σ and $\mathscr{M}$, respectively. Thus if $\tau \in {}^{s,-w}_{r}T_{x}\Sigma$, we have $\psi(\tau) \in {}^{R}_{S}T_{X(x)}\mathscr{M}$.

We shall denote the bundle of such e-tensors by ${}^{R,r,w}_{S,s}T\mathscr{E}$. The linear space ${}^{R,r,w}_{S,s}T_{X}\mathscr{E}$ can be given a Sobolev structure with an arbitrary Sobolev class (not necessarily the same as that of $\mathscr{E}$). An easy, ''covariant'' method for doing so can be obtained by using an auxiliary Riemannian metric on $\mathscr{M}$ in addition to that on Σ. This enables covariant derivatives of e-tensors to be defined (see Ref. 5). However, a ''coordinate dependent'' method is even easier to define, and is more general in the sense that it can also be used for objects of higher rank, like the elements of $T_{(X,P)}(T^{*}\mathscr{E})$ (see below). This is based on pairs of charts Eq. (7), which will associate a map of $h(X^{-1}(X(U)\cap V))\subset\mathbb{R}^{3}$ into $\mathbb{R}^{m}$ with any e-tensor. One can then define a Sobolev scalar product by patching together the integrands within each set $h(X^{-1}(X(U)\cap V))$ with the aid of a partition of unity corresponding to a covering of Σ by these sets. This scalar product depends on the system of charts chosen, but the topology does not and is equivalent to that obtained using the covariant method.

It is clear that the usual tensor operations, such as linear combination, tensor product, and contraction at a point $x \in \Sigma$ or $X(x) \in \mathscr{M}$, define corresponding operations on the e-tensors (for details see Ref. 5). The result is an e-tensor whose Sobolev class coincides with the lowest class involved in the operation.

There is one more operation of importance that we shall call ''pairing.'' Let $\xi \in {}^{R,r,w}_{S,s}T_{X}\mathscr{E}$ and $\eta \in {}^{S,s,1-w}_{R,r}T_{X}\mathscr{E}$. The pairing $\langle \xi,\eta\rangle$ is defined by

$$\langle \xi,\eta\rangle := \int_{\Sigma} d^{3}x\,\xi(x)\cdot\eta(x) \tag{10}$$

where $\xi(x)\cdot\eta(x)$ denotes the contractions at x and $X(x)$ such that all indices of ξ are contracted with those of η in the order in which they appear. Then $\xi(x)\cdot\eta(x)$ is a scalar density on Σ, and hence $\langle \xi,\eta\rangle$ is a coordinate independent real number.

A particularly important example of a bundle of e-tensors is the tangent bundle $T\mathscr{E} := {}^{1,0,0}_{0,0}T\mathscr{E}$ whose points ξ are pairs (X,V) where $X \in \mathscr{E}$, and V is a $T\mathscr{M}$-valued function on Σ with $V(x) \in T_{X(x)}\mathscr{M}$; equivalently, V is a cross-section of $X^{*}(T\mathscr{M})$. Even more important for our purposes is the cotangent bundle $T^{*}\mathscr{E}$. To define cotangent vectors we have to identify $T^{*}_{X}\mathscr{E}$ with a particular topological vector space of real-valued, linear functions on $T_{X}\mathscr{E}$. The appropriate choice for our purposes is the space ${}^{0,0,1}_{1,0}T_{X}\mathscr{E}$ of Sobolev class s', the linear operation being the pairing (the class parameter s' must satisfy the condition $s'\leqslant s$, where s is the class parameter of $\mathscr{E}$, but can otherwise be arbitrary). Thus, $P \in T^{*}_{X}\mathscr{E} := {}^{0,0,1}_{1,0}T_{X}\mathscr{E}$ is a cross-section of the bundle $\mathscr{D}^{1}\Sigma\otimes X^{*}(T^{*}\mathscr{M})$ where, in general, $\mathscr{D}^{w}\Sigma$ is shorthand for the real-line bundle ${}^{0,w}_{0}T\Sigma$ of scalar densities on Σ of weight w. Thus $P(x) \in \mathscr{D}^{1}_{x}\Sigma\otimes T^{*}_{X(x)}\mathscr{M}$; equivalently, P is a bundle map from $\mathscr{D}^{-1}\Sigma$ to $T^{*}\mathscr{M}$ that ''covers'' X in the sense that $P(\tau) \in T^{*}_{X(x)}\mathscr{M}$ for all $\tau \in \mathscr{D}^{-1}_{x}\Sigma$.

With respect to a local coordinate chart y^{μ}, $\mu=0,1,2,3$, on $\mathscr{M}$, the pair $(X,P) \in T^{*}\mathscr{E}$ is represented by local functions (X^{μ},P_{ν}) on Σ, where X^{μ} is defined by

$$X^{\mu}(x) := y^{\mu}(X(x)), \tag{11}$$

and where the four scalar-density functions P_{ν}, $\nu=0,1,2,3$, on Σ are defined by the expansion

$$P(x) = P_{\nu}(x)\,dy^{\nu}|_{X(x)} \tag{12}$$

using the differentials dy^{ν} associated with the local coordinate system y^{ν} on $\mathscr{M}$ (as usual, summation over repeated indices is understood) and using a local coordinate system on Σ to locally trivialize the line bundle $\mathscr{D}^{-1}\Sigma$. In terms of these local functions, the pairing operation is

$$\langle (X,P),(X,V)\rangle = \int_\Sigma d^3x P_\mu(x) V^\mu(x) \tag{13}$$

where the functions V^μ on Σ are defined by the equation

$$V(x) = V^\mu(x)\left(\frac{\partial}{\partial y^\mu}\right)_{X(x)}. \tag{14}$$

The e-tensor bundles can be given a manifold structure based on that of $\mathscr{E}$. A point in such a bundle ${}^{R,r,w}_{S,s}T\mathscr{E}$ is represented by a pair (X,ψ) where $X \in \mathscr{E}$, and $\psi \in {}^{R,r,w}_{S,s}T_X\mathscr{E}$ is a cross-section of the bundle ${}^{r,w}_{s}T\Sigma \otimes X^*({}^R_S T\mathscr{M})$ or—better for our purposes—the pair (X,ψ) fits into the commutative diagram Eq. (9). A tangent vector is defined as an equivalence classes of curves $t \mapsto (X_t,\psi_t)$, and it is clear from this geometrically that a tangent vector at (X,ψ) consists of a pair of objects (V,W) where (i) $V \in T_X\mathscr{E}$ (i.e., $V(x) \in T_{X(x)}\mathscr{M}$); (ii) W is a bundle map from ${}^{s,-w}_{r}T\Sigma$ to $T({}^R_S T\mathscr{M})$ such that, for all $\tau \in {}^{s,-w}_{r}T_x\Sigma$, we have $W(\tau) \in T_{\psi(\tau)}({}^R_S T\mathscr{M})$; and (iii) $\chi_*(W(\tau)) = V(x)$ where $\chi_*: T({}^R_S T\mathscr{M}) \to T\mathscr{M}$ is induced from the bundle projector $\chi: {}^R_S T\mathscr{M} \to \mathscr{M}$ in Eq. (9). Note that V and W both take their values in vector spaces, and hence the collection of all such pairs (V,W) can be given an appropriate Sobolev structure to become Banach spaces. By this means, the bundle of e-tensors over $\mathscr{E}$ becomes a Banach manifold.

Now, in general, if E is any vector bundle over $\mathscr{M}$, the tangent space T_pE splits into a direct sum $E_{\pi(p)} \oplus T_{\pi(p)}\mathscr{M}$ where $E_{\pi(p)}$ denotes the fiber of E over the point $\pi(p) \in \mathscr{M}$. However, in the absence of any connection on E there is no natural way of performing such a split. Note that in our case, where $E = {}^R_S T\mathscr{M}$, this (non-canonical) split means that the vector $W(\tau) \in T_{\psi(\tau)}({}^R_S T\mathscr{M})$ (with $\tau \in {}^{s,-w}_{r}T_x\Sigma$) can be written as a sum of an element of ${}^R_S T_{X(x)}\mathscr{M}$ (the analogue of $E_{\pi(p)}$) and an element [in fact, $V(x)$] of $T_{X(x)}\mathscr{M}$. This means that, using a local coordinate system on $\mathscr{M}$, the vector $W(\tau)$ can be written as a collection of numbers associated with the point $X(x) \in \mathscr{M}$, namely the components $V^\mu(x)$ of the vector $V(x)$, and the components of the space–time object in ${}^R_S T_{X(x)}\mathscr{M}$, which we shall write as $W^{\mu_1 \cdots \mu_R}_{\nu_1 \cdots \nu_S}(\tau)$.

A particularly simple example is the tangent bundle $T(T^*\mathscr{E})$. The bundle $T^*\mathscr{E}$ consists of pairs (X,P) where $X \in \mathscr{E}$, and where P is a bundle map $P: \mathscr{D}^{-1}\Sigma \to T^*\mathscr{M}$ that covers $X: \Sigma \to \mathscr{M}$, i.e., $P(\tau) \in T^*_{X(x)}\mathscr{M}$ for all $\tau \in \mathscr{D}_x^{-1}\Sigma$. Then, according to the discussion above, a tangent vector to $T^*\mathscr{E}$ at the point (X,P) consists of a pair (V,W) where $V \in T_X\mathscr{E}$ and where $W: \mathscr{D}^{-1}\Sigma \to T(T^*\mathscr{M})$ satisfies $W(\tau) \in T_{P(\tau)}(T^*\mathscr{M})$ with $\pi_*(W(\tau)) = V(x)$ for all $\tau \in \mathscr{D}_x^{-1}\Sigma$, where $\pi: T^*\mathscr{M} \to \mathscr{M}$ is the bundle projection.

The problem occasioned by the non-canonical split can be seen by looking at the situation using a local coordinate system. The element $(X,P) \in T^*\mathscr{E}$ is represented by the local functions (X^μ, P_ν) on Σ, and a transformation of coordinates in $\mathscr{M}$ from y^μ to y'^α leads to new functions (X'^α, P'_β) satisfying

$$X'^\alpha(x) = y'^\alpha(X(x)), \tag{15}$$

$$P'_\beta(x) = J^\nu_{\beta'}(X(x)) P_\nu(x), \tag{16}$$

where $J^\nu_{\beta'}$ denotes the matrix $\partial y^\mu / \partial y'^\beta$. As emphasized earlier, a tangent vector in infinite-dimensional differential geometry is defined as an equivalence class of curves and, with respect to the pair of charts Eq. (7), a curve in $T^*\mathscr{E}$ is represented by functions $(t,x) \mapsto (X^\mu(x,t), P_\nu(x,t))$. Hence the tangent vector to this curve is represented by the functions $\dot{X}^\mu$ and $\dot{P}_\nu$ on Σ where

$$\dot{X}^{\mu}(x) := \left.\frac{\partial X^{\mu}(x,t)}{\partial t}\right|_{t=0}, \quad \dot{P}_{\nu}(x) := \left.\frac{\partial P_{\nu}(x,t)}{\partial t}\right|_{t=0}. \tag{17}$$

Note that $P_{\mu}(x,t)$ are components with respect to coordinates at the point $X(x,t)$ of $\mathscr{M}$ while $P_{\mu}(x,t+dt)$ are those at another point $X(x,t+dt)$ of $\mathscr{M}$.

Differentiating formula Eq. (15) along the curve with respect to t, we obtain

$$\dot{X}'^{\alpha}(x) := \left.\frac{\partial X'^{\alpha}(x,t)}{\partial t}\right|_{t=0} = \left.\frac{\partial y'^{\alpha}(X(x,t))}{\partial t}\right|_{t=0} = \frac{\partial y'^{\alpha}}{\partial y^{\mu}}(X(x)) \left.\frac{\partial y^{\mu}(X(x,t))}{\partial t}\right|_{t=0}$$

$$= J^{\alpha'}_{\mu}(X(x))\dot{X}^{\mu}(x), \tag{18}$$

which shows that, as expected, the derivatives $\dot{X}^{\mu}(x)$ transform on $\mathscr{M}$ in a tensorial way. On the other hand, the analogous calculations for Eq. (16) yield

$$\dot{P}'_{\beta}(x) = J^{\nu}_{\beta'\mu}(X(x))\dot{X}^{\mu}(x)P_{\nu}(x) + J^{\nu}_{\beta'}(X(x))\dot{P}_{\nu}(x) \tag{19}$$

where $J^{\nu}_{\beta'\mu}$ denotes the derivative of the matrix $J^{\nu}_{\beta'}$ with respect to the original coordinates y^{μ}. This shows that the four quantities $\dot{P}'_{\beta}(x)$ cannot be regarded as the components of any tensorial object on $\mathscr{M}$. In general, a tangent vector to $(X,P) \in T^*\mathscr{E}$ can be represented by the functions (V^{μ},W_{ν}) on Σ which transform under a change of coordinates on $\mathscr{M}$ as

$$\begin{pmatrix} V'^{\alpha}(x) \\ W'_{\beta}(x) \end{pmatrix} = \begin{pmatrix} J^{\alpha'}_{\mu}(X(x)) & 0 \\ J^{\rho}_{\beta'\mu}(X(x))P_{\rho}(x) & J^{\nu}_{\beta'}(X(x)) \end{pmatrix} \begin{pmatrix} V^{\mu}(x) \\ W_{\nu}(x) \end{pmatrix}. \tag{20}$$

We shall often need to work with the cotangent vectors from $T^*(T^*\mathscr{E})$. Let us describe their most important properties. As discussed above, a vector in $T_{(X,P)}(T^*\mathscr{E})$ is a pair (V,W) where $V \in T_X\mathscr{E}$, and $W:\mathscr{D}^{-1}\Sigma \to T(T^*\mathscr{M})$ is such that $\pi_*(W(\tau)) = V(x) \in T_{X(x)}\mathscr{M}$ for all $\tau \in \mathscr{D}_x^{-1}\Sigma$, where $\pi:T^*\mathscr{M} \to \mathscr{M}$ is the bundle projection. By definition, the kernel of the map $\pi_*:T(T^*\mathscr{M}) \to T\mathscr{M}$ is the set of vertical vectors in $T(T^*\mathscr{M})$, and at each $k \in T^*\mathscr{M}$ there is a natural isomorphism ι of $V_k(T^*\mathscr{M})$ (the vertical tangent vectors at k) with $T^*_{\pi(k)}\mathscr{M}$. In fact, at each $k \in T^*\mathscr{M}$, the map π_* fits into the short exact sequence

$$0 \to T^*_{\pi(k)}\mathscr{M} \xrightarrow{\iota} T_k(T^*\mathscr{M}) \xrightarrow{\pi_*} T_{\pi(k)}\mathscr{M} \to 0. \tag{21}$$

The dual of this sequence is the short exact sequence

$$0 \to T^*_{\pi(k)}\mathscr{M} \xrightarrow{\pi^{\dagger}_*} T^*_k(T^*\mathscr{M} \xrightarrow{\iota^{\dagger}} T^{**}_{\pi(k)}\mathscr{M} \to 0 \tag{22}$$

where a † superscript denotes the adjoint of the linear map to which it is attached. Note that, since $\mathscr{M}$ is finite-dimensional, the third term in Eq. (22) (i.e., $T^{**}_{\pi(k)}\mathscr{M}$) is (non-canonically) isomorphic to $T_{\pi(k)}\mathscr{M}$.

Using the ideas above, it is natural to define an element of $T^*_{(X,P)}(T^*\mathscr{E})$ as a pair (A,B) where $B:\Sigma \to T^{**}\mathscr{M} \simeq T\mathscr{M}$, and where the bundle map $A:\mathscr{D}^{-1}\Sigma \to T^*(T^*\mathscr{M})$ satisfies $A(\tau) \in T^*_{P(\tau)}(T^*\mathscr{M})$ with $\iota^{\dagger}(A(\tau)) = B(x)$ for all $\tau \in \mathscr{D}_x^{-1}\Sigma$. In local coordinates on $\mathscr{M}$, an element $(A,B) \in T^*_{(X,P)}(T^*\mathscr{E})$ can be represented by a set of local functions (A_{μ},B^{ν}) on Σ (each A_{μ} is actually a scalar density on Σ; B^{ν} are genuine scalar functions). The pairing of such an object with a vector (V,W) in $T_{(X,P)}(T^*\mathscr{E})$ is defined by

$$\langle (A,B),(V,W)\rangle := \int_\Sigma d^3x (A_\mu(x)V^\mu(x) + B^\mu(x)W_\mu(x)). \tag{23}$$

The condition that the result be independent of coordinates on $\mathscr{M}$ determines the transformation of $(A_\mu(x), B^\nu(x))$ to be

$$\begin{pmatrix} A'_\alpha(x) \\ B'^\beta(x) \end{pmatrix} = \begin{pmatrix} J^\mu_{\alpha'} & -J^\rho_{\alpha'\nu}(X(x))P_\rho(x) \\ 0 & J^{\beta'}_\nu(X(x)) \end{pmatrix} \begin{pmatrix} A_\mu(x) \\ B^\nu(x) \end{pmatrix}. \tag{24}$$

Thus $V^\mu(x)$ and $B^\mu(x)$ represent tensorial objects on $\mathscr{M}$, but $W_\mu(x)$ and $A_\mu(x)$ do not.

A key observation is the following. If the transformation law Eq. (20) is compared with Eq. (24), it is clear that the quantity $(G^\mu, -F_\mu)$ formed from the ''components'' of a covector on $T^*\mathscr{E}$ transforms as a tangent vector on $T^*\mathscr{E}$. Thus we have a map $J_{\mathscr{E}}: T^*(T^*\mathscr{E}) \to T(T^*\mathscr{E})$ defined in local coordinates on the component functions by

$$J_{\mathscr{E}}(A_\alpha, B^\nu) = (B^\mu, -A_\alpha). \tag{25}$$

We can choose the Sobolev classes so that the classes of the functions V^α, X^α and B^α coincide, and so do those of P_β, W_β and A_β. Then $J_{\mathscr{E}}$ is a Sobolev space isomorphism.

More abstractly, we recall that if Q is any finite-dimensional manifold there is a canonical isomorphism $j: T^*_p(T^*Q) \to T_p(T^*Q)$ defined on any cotangent vector ℓ at the point p in T^*Q by

$$\omega(j(\ell), v) = \langle \ell, v\rangle_p \quad \text{for all} \quad v \in T_p(T^*Q) \tag{26}$$

where ω is the canonical two-form on the cotangent bundle T^*Q. In the context of the embedding space, if $(A,B) \in T^*_{(X,P)}(T^*\mathscr{E})$, then $A(\tau) \in T^*_{P(\tau)}(T^*\mathscr{M})$, and hence we can use the isomorphism $j: T^*_{P(\tau)}(T^*\mathscr{M}) \to T_{P(\tau)}(T^*\mathscr{M})$ to define a map $J: T^*_{(X,P)}(T^*\mathscr{E}) \to T_{(X,P)}(T\mathscr{E})$ by requiring that $J(A,B)(\tau) := j(A(\tau))$. This is the coordinate-free definition of the object given in Eq. (25).

The phase space Γ_ϕ of the scalar field ϕ was introduced in section II. We note now that Γ_ϕ can be considered as the cotangent bundle $T^*\mathscr{Q}$, where $\mathscr{Q}$ is the space H^∞_0 of all C^∞-scalar fields on Σ. As $\mathscr{Q}$ is a linear space, there is a natural identification between the spaces $T^*\mathscr{Q}$ and $\mathscr{Q} \times T^*_\varphi\mathscr{Q}$ for any $\varphi \in \mathscr{Q}$. Also, $T^*_\varphi\mathscr{Q} = H^\infty_1$ is itself a linear space, and so there is an identification between the spaces $T_{(\varphi,\pi)}(T^*\mathscr{Q})$ and $T^*\mathscr{Q} \simeq H^\infty_0 \times H^\infty_1$. Similarly, $T^*_{(\varphi,\pi)}(T^*\mathscr{Q}) \simeq H^\infty_1 \times H^\infty_0$. More precisely, if $(\xi,\eta) \in T_{(\varphi,\pi)}(T^*\mathscr{Q})$ and $(f,h) \in H^\infty_1 \times H^\infty_0$, then the pairing $(f,h): T_{(\varphi,\pi)}(T^*\mathscr{Q}) \to \mathbb{R}$ is defined by

$$\langle (f,h),(\xi,\eta)\rangle := \int_\Sigma d^3x (f\xi + h\eta). \tag{27}$$

The extended phase space Γ of the parametrized scalar field of Ref. 7 is defined as $\Gamma := \Gamma_\phi \times T^*\mathscr{E}$. Hence $\Gamma \simeq T^*(\mathscr{Q} \times \mathscr{E})$, so that the extended phase space is again a cotangent bundle. In the context of the full space Γ, a tangent vector from $T_{(\varphi,\pi,X,P)}\Gamma$ can be specified by its ''components'' (Φ,Π,V,W), where $(V,W) \in T_{(X,P)}(T^*\mathscr{E})$ and $(\Phi,\Pi) \in T_{(\varphi,\pi)}(T^*\mathscr{Q})$. Similarly, a cotangent vector from $T^*_{(\varphi,\pi,X,P)}\Gamma$ can be specified by (A_φ, A_π, A, B), where $(A,B) \in T^*_{(X,P)}(T^*\mathscr{E})$ and $(A_\varphi, A_\pi) \in T^*(T^*\mathscr{Q})$. The natural pairing is

$$\langle (A_\varphi, A_\pi, A, B),(\Phi,\Pi,V,W)\rangle := \int_\Sigma d^3x (A_\varphi\Phi + A_\pi\Pi + A_\mu V^\mu + B^\mu W_\mu). \tag{28}$$

There is an isomorphism $J: T^*_{(\varphi,\pi,X,P)}\Gamma \to T_{(\varphi,\pi,X,P)}\Gamma$ (if the Sobolev classes are chosen to match each other) given by

$$J(A_\varphi, A_\pi, A_X, A_P) := (A_\pi, -A_\varphi, A_P, -A_X). \tag{29}$$

Using this isomorphism, a symplectic structure Ω on Γ can be defined as follows. Let v_1 and v_2 be two vectors in $T_{(\varphi,\pi,X,P)}\Gamma$. Then

$$\Omega(v_1, v_2) := -\langle J^{-1} v_1, v_2 \rangle \tag{30}$$

or, in ''component'' form,

$$\Omega((\Phi_1,\Pi_1,V_1,W_1),(\Phi_2,\Pi_2,V_2,W_2)) = \int_\Sigma d^3x (\Pi_1\Phi_2 - \Phi_1\Pi_2 + W_{1\mu}V_2^\mu - V_1^\mu W_{2\mu}). \tag{31}$$

It follows at once that (i) $\Omega(v_1,v_2) = -\Omega(v_2,v_1)$; (ii) Ω is weakly non-degenerate (see Ref. 13); and (iii) Ω is not only closed but also exact.

As Ω is only a weak symplectic form, not every differentiable function on Γ will have a Hamiltonian vector field. The class of functions that do can be characterized as follows. If $F:\Gamma\to\mathbb{R}$, we say that F has a gradient if the following two conditions are satisfied:

(1) the Fréchet derivative, $\mathrm{D}F|_{(\varphi,\pi,X,P)}: T_{(\varphi,\pi,X,P)}\Gamma \to \mathbb{R}$ is a bounded linear map;

(2) there exists $\mathrm{grad}F \in T^*_{(\varphi,\pi,X,P)}\Gamma$ such that $\langle \mathrm{grad}F, v\rangle = \mathrm{D}F|_{(\varphi,\pi,X,P)}(v)$ for all $v \in T_{(\varphi,\pi,X,P)}\Gamma$. The ''components'' of this gradient will be denoted by the collection of functions $(\mathrm{grad}_\varphi F, \mathrm{grad}_\pi F, (\mathrm{grad}_X F)_\mu, (\mathrm{grad}_P F)^\nu)$.

Condition (2) means that DF must be regular (no distributions are accepted!), and hence we have to work with smeared objects. This will not lead to any real loss of generality. The quantity grad F is calculated from DF as usual by integration by parts (if F contains derivatives).

For a differentiable function with a gradient, we can define an associated ''Hamiltonian vector field.'' Specifically, if F is such a function, then $\xi_F \in T_{(\varphi,\pi,X,P)}\Gamma$ is defined by the relation

$$\langle \mathrm{grad}\ F, v\rangle = \Omega(v, \xi_F) \quad \text{for all} \quad v \in T_{(\varphi,\pi,X,P)}\Gamma. \tag{32}$$

Hence, because of Eq. (30), we see that $\langle \mathrm{grad}F, v\rangle = \langle J^{-1}\xi_F, v\rangle$ for all v, and so $\xi_F = J(\mathrm{grad}\ F)$.

Finally, the Poisson bracket of a pair of differentiable functions F and G is defined as $\{F,G\} := -\Omega(\xi_F, \xi_G)$, and we see immediately that

$$\{F,G\} = \langle \mathrm{grad}\ F, \xi_G\rangle. \tag{33}$$

This Poisson bracket is antisymmetric and, since Ω is closed, it satisfies the Jacobi identity.

IV. THE CONSTRAINT MANIFOLD

The parametrized scalar field theory possesses a set of constraints $\mathscr{H}_\mu = 0$ on the Cauchy data (φ,π,X,P). These constraints are contained in the map

$$C:\Gamma \to T^*\mathscr{E}, \tag{34}$$

$$(\varphi,\pi,X,P) \mapsto (X, \mathscr{H}(\varphi,\pi,X,P)) \tag{35}$$

where $\mathscr{H}(\varphi,\pi,X,P) \in T^*_X\mathscr{E}$, i.e., $\mathscr{H}(\varphi,\pi,X,P)(x) \in T^*_{X(x)}(\mathscr{M})$ for all $x \in \Sigma$, so that $\mathscr{H}(\varphi,\pi,X,P)(x) = \mathscr{H}(\varphi,\pi,X,P)_\mu(x) dy^\mu|_{X(x)}$ in a coordinate system y^μ on $\mathscr{M}$. The specific form of the constraints $\mathscr{H}_\mu(x)$ is given in Ref. 7 as

$$\mathscr{H}_\mu = P_\mu + \mathscr{H}^\phi_\mu, \tag{36}$$

$$\mathscr{H}^\phi_\mu = -\mathscr{H}^\phi_\perp n_\mu + \mathscr{H}^\phi_k X^k_\mu, \tag{37}$$

where $n_\mu(x)$ is the unit normal space–time vector at $X(x)\in\mathscr{M}$, and where $X^k_\mu(x):=g_{\mu\nu}(x)\gamma^{kl}(X(x))X,^\nu_l(x)$. The components $\mathscr{H}^\phi_\mu(\varphi,\pi,X)$ can be projected normal, and tangential, to the hypersurface $X(\Sigma)$ to give

$$\mathscr{H}^\phi_\perp=\tfrac{1}{2}(\det\ \gamma)^{1/2}\left(\frac{\pi^2}{\det\gamma}+\gamma^{kl}\varphi_k\varphi_l+m^2\varphi^2\right), \tag{38}$$

$$\mathscr{H}^\phi_k=\pi\varphi,_k\,. \tag{39}$$

The goal of this section is to explore the pre-symplectic structure of the manifold $\widetilde{\Gamma}$ of solutions to these constraints, i.e., $\widetilde{\Gamma}:=\{(\varphi,\pi,X,P)\in\Gamma|C(\varphi,\pi,X,P)=(X,0)\}$. In particular, we have the following theorem.

Theorem 2: Let the Sobolev class of all spaces involved be ∞. Then, $\widetilde{\Gamma}$ is a C^∞-submanifold of Γ in a neighborhood of any of its points. This constraint manifold $\widetilde{\Gamma}$ is given by $\widetilde{\Gamma}=\widetilde{C}(\Gamma_\phi\times\mathscr{E})$, where $\widetilde{C}:\Gamma_\phi\times\mathscr{E}\to\Gamma$ is defined by $\widetilde{C}(\varphi,\pi,X):=(\varphi,\pi,X,-\mathscr{H}^\phi(\varphi,\pi,X))$.

Proof: The proof is similar to that in Ref. 15, but requires less sophisticated functional analysis because our constraints are available in an explicit form; in particular—unlike the case in Ref. 15—we do not need to use the Fredholm alternative theorem.

We start by assuming that $T^*\Gamma$ is C^∞, and postulate that the Sobolev class of Π and W is $s-1$, where s is the class of X, Φ and V. Consider the map $\mathrm{D}C|_{(\varphi,\pi,X,P)}:T_{(\varphi,\pi,X,P)}\Gamma\to T_{\mathscr{H}(\varphi,\pi,X,P)}(T^*\mathscr{E})$. To use the implicit function theorem, this map must be a surjection with a splitting kernel (see, e.g., Ref. 21). However, $\mathrm{D}C|_{(\varphi,\pi,X,P)}$ is trivially surjective. Moreover, its kernel in $T_{\widetilde{C}(X,\varphi,\pi)}\Gamma$ is given by $\mathrm{D}\widetilde{C}|_{(\varphi,\pi,X)}(T_{(\varphi,\pi,X)}(\Gamma_\phi\times\mathscr{E}))$. We shall now show that $\mathrm{D}C|_{(\varphi,\pi,X)}$ is injective with a splitting image.

The map $\mathrm{D}\widetilde{C}|_{(\varphi,\pi,X)}:T_{(\varphi,\pi,X)}(\Gamma_\phi\times\mathscr{E})\to T_{\widetilde{C}(\varphi,\pi,X)}\Gamma$ between the Sobolev spaces $T_{(\varphi,\pi,X)}(\Gamma_\phi\times\mathscr{E})\simeq\Gamma^s_\phi\times H^s_0$ and $T_{\widetilde{C}(\varphi,\pi,X)}\Gamma\simeq\Gamma^s_\phi\times H^s_0\times H^{s-1}_1$ has a derivative given by

$$\mathrm{D}\widetilde{C}|_{(\varphi,\pi,X)}(\Phi,\Pi,V)=(\Phi,\Pi,V,-\mathrm{D}\mathscr{H}^\phi|_{(\varphi,\pi,X)}(\Phi,\Pi,V)), \tag{40}$$

where

$$\mathrm{D}\mathscr{H}^\phi|_{(\varphi,\pi,X)}(\Phi,\Pi,V)=\mathrm{D}_\varphi\mathscr{H}^\phi|_{(\varphi,\pi,X)}(\Phi)+\mathrm{D}_\pi\mathscr{H}^\phi|_{(\varphi,\pi,X)}(\Pi)+\mathrm{D}_X\mathscr{H}^\phi|_{(\varphi,\pi,X)}(V). \tag{41}$$

Using the results of Ref. 7 and Eqs. (37)–(39), we find after some calculation that

$$\mathrm{D}_\varphi\mathscr{H}^\phi_\mu|_{(\varphi,\pi,X)}(\Phi)=(\det\ \gamma)^{1/2}(L^k_\mu\Phi_{\|k}-n_\mu m^2\varphi\Phi), \tag{42}$$

$$\mathrm{D}_\pi\mathscr{H}^\phi_\mu|_{(\varphi,\pi,X)}(\Pi)=L^\perp_\mu\Pi, \tag{43}$$

$$\mathrm{D}_X\mathscr{H}^\phi_\mu|_{(\varphi,\pi,X)}(V)=\frac{1}{2}(\det\ \gamma)^{1/2}K^k_{\mu\nu}V^\nu_{\|k}+\mathscr{H}^\phi_\kappa\Gamma^\kappa_{\mu\nu}V^\nu, \tag{44}$$

where

$$L^k_\mu=-\gamma^{kl}\varphi_{\|l}n_\mu+\frac{\pi}{(\det\ \gamma)^{1/2}}X^k_\mu, \tag{45}$$

$$L^\perp_\mu=-\frac{\pi}{(\det\ \gamma)^{1/2}}n_\mu+\varphi_{\|k}X^k_\mu, \tag{46}$$

$$K^m_{\mu\nu}=\left(\frac{\pi^2}{\det\ \gamma}-\gamma^{kl}\varphi_{\|k}\varphi_{\|l}-m^2\varphi^2\right)n_\mu X^m_\nu+\left(\frac{\pi^2}{\det\ \gamma}+\gamma^{kl}\varphi_{\|k}\varphi_{\|l}+m^2\varphi^2\right)$$

$$\times X^m_\mu n_\nu+2\ \varphi_{\|k}\varphi_{\|l}\gamma^{km}n_\mu X^k_\nu-2\frac{\pi}{(\det\ \gamma)^{1/2}}\varphi_{\|k}(\gamma^{km}n_\mu n_\nu+X^k_\nu X^m_\mu), \tag{47}$$

and ''$\|$'' denotes the bi-covariant derivative, for example $Y^\mu_{k\|l}=Y^\mu_{k,l}+\Gamma^\mu_{\rho\sigma}Y^\rho_k X^\sigma_l-\gamma^m_{kl}Y^\mu_m$, where $\Gamma^\mu_{\rho\sigma}$ is the Christoffel symbol of the metric $g_{\mu\nu}$ on M, and γ^m_{kl} is the Christoffel symbol of the pull-back of g to Σ by X. By inspection, these formulas imply the crucial result that the map $\mathrm{D}\mathscr{H}^\phi|_{(\varphi,\pi,X)}:H^s_0\times\Gamma^s_\phi\to H^{s-1}_1$ is continuous and bounded (recall that φ, π and X are C^∞). Hence, for all $(\Phi,\Pi,V)\in\Gamma^s_\phi\times H^s_0$, the map $\mathrm{D}\widetilde{C}|_{(\varphi,\pi,X)}$ is continuous and bounded, and—by inspection—injective. It follows from the closed graph theorem that the image $\mathrm{D}\widetilde{C}|_{(\varphi,\pi,X)}(\Gamma^s_\phi\times H^s_0)$ is therefore closed in $\Gamma^s_\phi\times H^s_0\times H^{s-1}_1$. However, a closed subspace of a Hilbert space splits, which proves the theorem. **QED**

By abuse of language, we will often call $\Gamma_\phi\times\mathscr{E}$ the ''constraint manifold.''

For each fixed value of x and μ, the quantity $\mathscr{H}_\mu(x)$ can be viewed as a function on the phase space, but it has no gradient; in particular, the Poisson bracket of a pair of such functions is not well-defined. Constraint functions with gradients can be constructed by ''smearing.'' Specifically, if $N\in T_X\mathscr{E}$ [i.e., $N(x)\in T_{X(x)}\mathscr{M}$], then $\mathscr{H}_N$ is defined as

$$\mathscr{H}_N:=\int_\Sigma d^3x N^\mu(x)\mathscr{H}_\mu(x). \tag{48}$$

It is clear that the equations $\mathscr{H}_N=0$ for all $N\in T_X\mathscr{E}$ are equivalent to $\mathscr{H}_\mu(x)=0$ for all μ,x. In particular, let U be a C^∞ vectorfield on $\mathscr{M}$. Then each embedding X determines an element, $x\mapsto U^\mu(X(x))(\partial/\partial y^\mu)_{X(x)}$, of $T_X\mathscr{E}$. This is the type of smearing used in Ref. 7.

Let us calculate the gradient of $\mathscr{H}_N$. Starting from Eq. (37), using Eqs. (42), (43) and (44), and integrating by parts, we obtain

$$\mathrm{grad}_\varphi\mathscr{H}_N=(\det\gamma)^{1/2}[-(N^\mu L^k_\mu)_{\|k}-m^2\varphi n_\mu N^\mu], \tag{49}$$

$$\mathrm{grad}_\pi\mathscr{H}_N=L^\perp_\mu N^\mu, \tag{50}$$

$$(\mathrm{grad}_X\mathscr{H}_N)_\nu=N^\mu_{\|\nu}\mathscr{H}_\mu-\tfrac{1}{2}(\det\ \gamma)^{1/2}(N^\mu K^k_{\mu\nu})_{\|k}-P_\kappa\Gamma^\kappa_{\mu\nu}N^\mu, \tag{51}$$

$$(\mathrm{grad}_P\mathscr{H}_N)^\nu=N^\nu, \tag{52}$$

where $L^\perp_\mu, L^k_\mu$ and $K^k_{\mu\nu}$ are given by Eqs. (45), (46) and (47). In Ref. 7, the following theorem was shown:

Theorem 3: Let M and N be two C^∞ vector fields on $\mathscr{M}$. Then

$$\{\mathscr{H}_M,\mathscr{H}_N\}=-\mathscr{H}_{[M,N]}, \tag{53}$$

where $[M,N]$ is the Lie bracket of the fields M^μ and N^μ.

Substituting the expressions Eqs. (49)–(52) for the gradients into the Poisson brackets (53) we obtain an identity that plays an important role in some proofs:

$$\frac{1}{2}\int_\Sigma d^3x(\det\gamma)^{1/2}[(M^\mu K^k_{\mu\nu})_{\|k}N^\nu-(N^\mu K^k_{\mu\nu})_{\|k}M^\nu]$$

$$=\int_\Sigma d^3x(\mathrm{grad}_\varphi\mathscr{H}_M\mathrm{grad}_\pi\mathscr{H}_N-\mathrm{grad}_\pi\mathscr{H}_M\mathrm{grad}_\varphi\mathscr{H}_N). \tag{54}$$

The following theorem was essentially shown in Ref. 7:

Theorem 4: Let ϕ satisfy the Klein–Gordon equation (1) on $\mathscr{M}$. Then for each curve $\lambda \mapsto X_\lambda$ with the tangent vector field N on $\mathscr{E}$, the initial data $(\varphi_\lambda, \pi_\lambda)$ for ϕ on $X_\lambda(\Sigma)$ satisfy the evolution equation

$$(\dot{\varphi}, \dot{\pi}, \dot{X}, \dot{P}) = J(\text{grad}\, \mathscr{H}_N). \tag{55}$$

The equation for $\dot{P}$ is a consequence of the first three equations and the constraints $\mathscr{H}_N = 0$ for all $N \in T_X\mathscr{E}$.

Conversely, if a curve $\lambda \mapsto (\varphi_\lambda, \pi_\lambda, X_\lambda)$ on $\Gamma_\phi \times \mathscr{E}$ satisfies the evolution equations (55), then it defines a unique solution ϕ of the Klein–Gordon equation.

Thus the Hamiltonian vector fields $J(\text{grad}\, \mathscr{H}_N)$ of the functions $\mathscr{H}_N$ are tangential to $\widetilde{\Gamma}$, and hence the system is first class, according to the definition given in Ref. 10.

A simple consequence of theorem 4 is that the pull-back of the vector field (55) to $\Gamma_\phi \times \mathscr{E}$ is given by

$$\dot{\varphi} = \text{grad}_\pi \mathscr{H}_N, \tag{56}$$

$$\dot{\pi} = -\text{grad}_\varphi \mathscr{H}_N, \tag{57}$$

$$\dot{X} = N. \tag{58}$$

Let us denote the space of longitudinal vectors at $(\varphi, \pi, X) \in \Gamma_\phi \times \mathscr{E}$ by $\Xi_{(\varphi,\pi,X)}$, i.e.,

$$\Xi_{(\varphi,\pi,X)} := \{(\Phi, \Pi, V) \in T_{(\varphi,\pi,X)}\widetilde{\Gamma} \,|\, \Phi = \text{grad}_\pi \mathscr{H}_N, \Pi = -\text{grad}_\varphi \mathscr{H}_N, V = N \in T_X\mathscr{E}\}. \tag{59}$$

The map $(\text{grad}_\pi \mathscr{H}_N, -\text{grad}_\varphi \mathscr{H}_N): T_X\mathscr{E} \to T_{(\varphi,\pi)}\Gamma_\phi$ is continuous and hence, by the closed graph theorem, $\Xi_{(\varphi,\pi,X)}$ is a *closed* subspace of $T_{(\varphi,\pi,X)}\widetilde{\Gamma}$.

Another consequence of theorem 4 is that the Fréchet derivative of the map $\rho_{XX'}$ with respect to X' is given by

$$\mathrm{D}_{X'}\rho_{XX'}|_{(\varphi,\pi)}(V) = (\text{grad}_\pi \mathscr{H}_V(\varphi', \pi', X'), -\text{grad}_\varphi \mathscr{H}_V(\varphi', \pi', X')), \tag{60}$$

where $(\varphi', \pi') := \rho_{XX'}(\varphi, \pi)$.

We shall need the pull-back of the symplectic form to the constraint manifold. This is given by the following theorem.

Theorem 5: The pull-back $\widetilde{\Omega}$ of the form Ω is given by the formula

$$\begin{aligned}\widetilde{\Omega}((\Phi_1, \Pi_1, V_1), (\Phi_2, \Pi_2, V_2)) \\ = \int_\Sigma d^3x [(\Pi_1 + \text{grad}_\varphi \mathscr{H}_{V_1})(\Phi_2 - \text{grad}_\pi \mathscr{H}_{V_2}) \\ - (\Pi_2 + \text{grad}_\varphi \mathscr{H}_{V_2})(\Phi_1 - \text{grad}_\pi \mathscr{H}_{V_1})].\end{aligned} \tag{61}$$

Proof: The pull-back by the map $\widetilde{C}$ of the form Ω is given by

$$\widetilde{\Omega}((\Phi_1, \Pi_1, V_1), (\Phi_2, \Pi_2, V_2)) := \Omega(\mathrm{D}\widetilde{C}(\Phi_1, \Pi_1, V_1), \mathrm{D}\widetilde{C}(\Phi_2, \Pi_2, V_2)). \tag{62}$$

Substituting into this equation the expressions for $\mathrm{D}\widetilde{C}$ from Eqs. (40) and (41), and using Eq. (54), one easily arrives at Eq. (61). **QED**

Thus, $\widetilde{\Omega}$ is degenerate, and the degeneracy subspace at the point $(\varphi, \pi, X) \in \widetilde{\Gamma}$ coincides with $\Xi_{(\varphi,\pi,X)}$.

The last important notion involving the constraint submanifold is that of a ''c-orbit,'' defined to be the set of points in $\tilde{\Gamma}$ that correspond to just one maximal classical solution (see Ref. 10). Let $\tilde{\gamma}_{(\varphi,\pi,X)}$ be the map $\tilde{\gamma}_{(\varphi,\pi,X)}:\mathscr{E}\to\Gamma_\phi\times\mathscr{E}$ defined by

$$\tilde{\gamma}_{(\varphi,\pi,X)}(X'):=(\rho_{XX'}(\varphi,\pi),X'). \tag{63}$$

Then the c-orbit $\gamma_{(\varphi,\pi,X)}$ through the point $(\varphi,\pi,X)\in\Gamma_\phi\times\mathscr{E}$ is defined as

$$\gamma_{(\varphi,\pi,X)}:=\tilde{\gamma}_{(\varphi,\pi,X)}(\mathscr{E}) \tag{64}$$

i.e., $\gamma_{(\varphi,\pi,X)}$ is the collection of all embeddings, and Cauchy data on such, induced by the unique solution to the field equations whose Cauchy data on $X(\Sigma)$ is (φ,π).

We shall show that the c-orbits are smooth submanifolds of $\tilde{\Gamma}$ and that their tangent spaces coincide with $\Xi_{(\varphi,\pi,X)}$; the proof is analogous to that of theorem 2.

The tangent space to γ at $\tilde{\gamma}_{(\varphi,\pi,X)}(X')$ is the image of the map $\mathrm{D}\tilde{\gamma}_{(\varphi,\pi,X)}|_{X'}:T_{X'}\mathscr{E}\to T_{(\varphi',\pi',X')}(\Gamma_\phi\times\mathscr{E})$, where $(\varphi',\pi'):=\rho_{XX'}(\varphi,\pi)$. Using Eq. (60) we obtain, for all $V\in T_{X'}\mathscr{E}$,

$$\begin{aligned}\mathrm{D}\tilde{\gamma}_{(\varphi,\pi,X)}|_{X'}(V)&=(\mathrm{D}\rho_{XX'}(\varphi,\pi)|_{X'}(V),V)\\&=(\mathrm{grad}_{\pi'}\mathscr{H}_V(\varphi',\pi',X'),-\mathrm{grad}_{\varphi'}\mathscr{H}_V(\varphi',\pi',X'),V).\end{aligned} \tag{65}$$

Hence, $\mathrm{D}\tilde{\gamma}_{(\varphi,\pi,X)|_{X'}}$ is injective, and a comparison of Eq. (65) with Eqs. (56)–(58) shows that $\mathrm{D}\tilde{\gamma}_{(\varphi,\pi,X)}|_{X'}(T_{X'}\mathscr{E})=\Xi_{(\varphi,\pi,X)}$. As Ξ is a closed subspace of a Hilbert space, it splits, and the claims above are proved.

V. CONCLUSIONS

We have shown that, with proper functional-analytical care, the geometrical structure of an infinite-dimensional parametrized system can be developed in a way that is analogous to that of a finite-dimensional system. In particular, for the model considered, the extended phase space is a (weak-)symplectic infinite-dimensional manifold, the constraint set is a submanifold of the phase space, and the c-orbits are submanifolds of the constraint set. The criteria for a constrained system to be first class are of the same form as those of a finite-dimensional system. Many constructions available for a finite-dimensional system can now be performed in the infinite-dimensional case. The only difference is that the symplectic form is only weakly non-degenerate. However, physicists usually work with a restricted class of functions so that the Poisson brackets are still well-defined.

We anticipate that our main results are broadly generalizable. For example, an extension to the case where the Cauchy hypersurfaces are asymptotically flat is likely to be relatively straightforward. We hope that our results will be useful for a number of purposes. In particular, our main goal was to apply the perennial formalism to the scalar field system; this is be done in the accompanying article.

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APPENDIX: CAUCHY PROBLEM

We collect together some well-known results about the Cauchy problem of linear hyperbolic systems and then use them to sketch a proof of the theorem 1 in section II.

First, we state some lemmas about the space–time $(\mathscr{M},g)$.

Lemma 1: Let X and X' be two embeddings in $\mathscr{E}$ such that $X'(\Sigma)\subset I^+(X(\Sigma))$. Then, given $T>0$ and $\epsilon>0$, there is a one-dimensional family $\{X_t\}$, $t\in(-\epsilon,T+\epsilon)$, of embeddings such that:

(a) $X_0=X$, $X_T(\sigma)=X'(\Sigma)$;

(b) if (U,h) is a chart of Σ $[h(U)\subset\mathbb{R}^3]$, then $(\cup_{t\in(-\epsilon,T+\epsilon)}X_t(U),[X_t(h^{-1}(x))]^{-1})$ is a C^{r+1} chart in $\mathscr{M}$, where $X_t(h^{-1}(x))$ is considered as a map

$$X_t((h^{-1}(x))):(-\epsilon,T+\epsilon)\times h(U)\to\mathscr{M}; \tag{A1}$$

(c) the components $g_{\alpha\beta}(t,x)$ of the metric in any such chart satisfy the equations

$$g_{00}(t,x)<0 \tag{A2}$$

in $(-\epsilon,T+\epsilon)\times h(U)$ (the t-curves are everywhere timelike), and

$$\begin{aligned} g_{00}(0,x) &= g_{00}(T,x) = -1, \\ g_{0i}(0,x) &= g_{0i}(T,x) = 0, \end{aligned} \tag{A3}$$

for all $x\in h(U)$.

The proof is simple. Observe that g^{00} is negative and g_{kl} is positive-definite everywhere in $(-\epsilon,T+\epsilon)\times h(U)$; this is because any $X_t(U)$ hypersurface is a part of a Cauchy hypersurface, and hence spacelike. Then the condition that g^{kl} is also positive-definite everywhere is equivalent to Eq. (A2). Hence, for any $t\in[0,T]$ and $x\in h(U)$, we have

$$|g^{00}|>c_1, \tag{A4}$$

$$g^{kl}\xi_k\xi_l>c_2e^{kl}\xi_k\xi_l, \tag{A5}$$

where c_1 and c_2 are positive constants, e_{kl} is a positive-definite C^∞ metric on Σ, and ξ_k is an arbitrary covector field on Σ.

The proof of the following lemma can be found in Ref. 16:

Lemma 2: If Σ_1 and Σ_2 are two Cauchy hypersurfaces in $(\mathscr{M},g)$, then there is a Cauchy hypersurface Σ_3 such that

$$\Sigma_3\subset[I^+(\Sigma_1)\cap I^-(\Sigma_2)]. \tag{A6}$$

Thus, $\Sigma_1\cap\Sigma_3=\Sigma_2\cap\Sigma_3=\varnothing$.

Next, consider the Klein–Gordon equation (1) for the field ϕ, and the associated Cauchy problem. In the chart described in lemma I, Eq. (1) has the form

$$\begin{aligned} -g^{00}\frac{\partial^2\phi}{\partial t^2} &= g^{kl}\frac{\partial^2\phi}{\partial x^k\partial x^l}+2g^{0k}\frac{\partial^2\phi}{\partial t\partial x^k}+|\det g|^{-1/2}\partial_\mu(|\det g|^{1/2}g^{0\mu})\frac{\partial\phi}{\partial t} \\ &\quad +|\det g|^{-1/2}\partial_\mu(|\det g|^{1/2}g^{k\mu})\frac{\partial\phi}{\partial x^k}+m^2\phi. \end{aligned} \tag{A7}$$

An initial datum for ϕ at the time t is the pair of scalar fields $(\varphi_t,\dot\varphi_t)$ on Σ given by

$$\varphi_t(x)=\phi(t,x), \tag{A8}$$

$$\dot\varphi_t(x)=\frac{\partial\phi}{\partial t}, \tag{A9}$$

where $\varphi_t(x)$ coincides with the Cauchy datum for $X_t(\Sigma)$ as defined by Eq. (4). For $t=0$ and $t=T$, we have also

$$(\det\ \gamma)^{1/2}\dot{\varphi}_0(x)=\pi_0(x), \tag{A10}$$

$$(\det\ \gamma)^{1/2}\dot{\varphi}_T(x)=\pi_T(x), \tag{A11}$$

where $\pi_0(x)$ and $\pi_T(x)$ are the pieces of Cauchy data defined by Eq. (3) for $X_0(\Sigma)$ and $X_T(\Sigma)$.

Consider the coefficient functions of Eq. (A7). They define tensor fields on Σ. Indeed,

$$a^{00}(t,x)=-g^{00}(t,x), \tag{A12}$$

$$a^{0}(t,x)=|\det\ g|^{-1/2}\partial_\mu(|\det\ g|^{1/2}g^{0\mu})|_{t,x}, \tag{A13}$$

$$a(t,x)=m^2, \tag{A14}$$

are scalar fields on Σ for each t, whereas

$$a^{0k}(t,x)=g^{0k}(t,x), \tag{A15}$$

$$a^{k}(t,x)=|\det\ g|^{-1/2}\partial_\mu(|\det\ g|^{1/2}g^{k\mu})|_{t,x}, \tag{A16}$$

are contravariant vector fields for each t, and

$$a^{kl}(t,x)=g^{kl}(t,x) \tag{A17}$$

is a contravariant tensor of second rank on Σ for each t.

The C^{r+1}-differentiability of X implies the following properties of these tensor fields:

$$\begin{aligned} &a^{\alpha\beta}\in \mathrm{Lip}([0,T];H_0^{r-1}(\Sigma))\subset L^\infty([0,T];H_0^r(\Sigma)),\\ &a^{\alpha}\in \mathrm{Lip}([0,T];H_0^{r-2}(\Sigma))\subset L^\infty([0,T];H_0^{r-1}(\Sigma)),\\ &a\in \mathrm{Lip}([0,T];H_0^{\infty}(\Sigma))=L^\infty([0,T];H_0^r(\Sigma)). \end{aligned} \tag{A18}$$

Moreover, according to Eqs. (A4) and (A5), we have $a^{00}(t,x)\geqslant c_1$ for all $t\in[0,T]$ and $x\in\Sigma$, and

$$a^{kl}(t,x)\xi_k(x)\xi_l(x)\geqslant c_2' e^{kl}(x)\xi_k(x)\xi_l(x), \tag{A19}$$

for all $t\in[0,T]$ and $x\in\Sigma$. The relations above enable us to use ''localized'' forms of the theorems 4.15 and 4.13 in Ref. 15, and to apply them to construct unique local evolution systems $F_{t,s}$ which can be ''patched together.'' By this means we are able to prove the following lemma (for further details see Ref. 15):

Lemma 3: Let the assumptions of Lemma 1 be satisfied, and let $r\geqslant 4$. Then, each initial datum $(\varphi_0(x),\dot{\varphi}_0(x))\in H_0^{s+1}(\Sigma)\times H_0^s(\Sigma)$ on $X_0(\Sigma)$, where $1\leqslant s\leqslant r-1$, defines a unique solution ϕ to the equation (1) in U whose initial datum $(\varphi_T(X),\dot{\varphi}_T(x))$ on $X_T(\Sigma)$ belongs to the Sobolev space $(\varphi_T(X),\dot{\varphi}_T(x))\in H_0^{s+1}(\Sigma)\times H_0^s(\Sigma)$. Furthermore, the maps $U(0,T):H_0^{s+1}(\Sigma)\times H_0^s(\Sigma)\to H_0^{s+1}(\Sigma)\times H_0^s(\Sigma)$ are automorphisms of Banach spaces.

Note that it is a trivial matter to pass from the initial data $(\varphi,\dot{\varphi})$ to the Cauchy data (φ,π): since $(\det\gamma)^{1/2}$ is C^∞ and bounded below by zero in U, the definition $\pi(x):=(\det\gamma)^{1/2}\dot{\varphi}(x)$ describes an isomorphism between the Banach spaces $H_0^s(\Sigma)$ and $H_1^s(\Sigma)$ for any $s\leqslant r$.

Finally, given any pair of arbitrary embeddings X_1 and X_2, we can use lemma 2 to find an ''intermediate'' embedding X_3. To be able to apply lemma 1 to the pairs $\{X_1,X_3\}$ and $\{X_3,X_2\}$, we must find two embeddings X_3' and X_3'' such that the corresponding t-curves are

timelike, and with $X_3'(\Sigma)=X_3''(\Sigma)=X_3(\Sigma)$. Then, we can use lemma 3 and the diffeomorphism invariance of B to prove the theorem 1. **QED**

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Perennials and the group-theoretical quantization of a parametrized scalar field on a curved background

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The perennial formalism is applied to the real, massive Klein–Gordon field on a globally-hyperbolic background space–time with compact Cauchy hypersurfaces. The parametrized form of this system is taken over from the accompanying paper. Two different algebras $\mathscr{S}_{\rm can}$ and $\mathscr{S}_{\rm loc}$ of elementary perennials are constructed. The elements of $\mathscr{S}_{\rm can}$ correspond to the usual creation and annihilation operators for particle modes of the quantum field theory, whereas those of $\mathscr{S}_{\rm loc}$ are the smeared fields. Both are shown to have the structure of a Heisenberg algebra, and the corresponding Heisenberg groups are described. Time evolution is constructed using transversal surfaces and time shifts in the phase space. Important roles are played by the transversal surfaces associated with embeddings of the Cauchy hypersurface in the space–time, and by the time shifts that are generated by space–time isometries. The automorphisms of the algebras generated by this particular type of time shift are calculated explicitly. The construction of the quantum theory using the perennial formalism is shown to be equivalent to the Segal quantization of a Weyl system if the time shift automorphisms of the algebra $\mathscr{S}_{\rm can}$ are used. In this way, the absence of any timelike Killing vector field in the background space–time leads naturally to the ''problem of time'' for quantum field theory on a background space–time. Within the perennial formalism, this problem is formally identical to the problem of time for any parametrized system, including general relativity itself. Two existing strategies—the ''scattering'' approach, and the ''algebraic'' approach—for dealing with this problem in quantum field theory on a background space–time are translated into the language of the perennial formalism in the hope that this may give some insight into how the general problem can be solved. The non-unitary time evolution typical of the Hawking effect is shown to be due to global properties of the corresponding phase space: specifically, the time shifts map a global transversal surface to a non-global one. Thus, the existence of this effect is closely related to the global time problem. [S0022-2488(96)02707-7]

I. INTRODUCTION

In the canonical approach to quantum gravity, much emphasis is placed on three particular issues: the conceptual problems that arise in the interpretation of the theory, especially the problem of time; the role of the space–time diffeomorphism group; and the construction of non-perturbative quantization methods (for reviews, see Refs. 1–3). The Dirac method of imposing

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operator constraints on the allowed state vectors (which, in the case of gravity, leads to the Wheeler-DeWitt equation) has become particularly popular because of its manifest relation to the idea of invariance under the action of space–time diffeomorphisms.

However, diffeomorphism invariance can also be secured by adopting a method in which only ''gauge-invariant'' objects are quantized; Dirac himself laid the foundations[4] for a powerful approach of this sort. A generalization of the Dirac method to include all finite-dimensional, first-class parametrized systems was presented by Hájíček.[5] The resulting theory, which combines the group-theoretic[6] and algebraic[7] methods of quantization with that of Dirac, is called the ''perennial formalism,'' following the terminology introduced by Kuchař in his analysis[8] of the problem of observables in canonical quantum gravity. The key idea of this method is to find an algebra of phase-space functions whose Poisson brackets with all the first-class constraints vanish; such functions are therefore constant on the phase-space orbits of the (function) group generated by the constraints. Furthermore, this algebra is required to be large enough to generate all gauge-invariant functions in an appropriate sense. Quantization of the system then consists in finding irreducible self-adjoint representations of this algebra of ''physical observables'' or, essentially equivalently, finding irreducible, unitary representations of the associated ''canonical'' group.

In the present article we develop the perennial formalism in the context of a field system, namely a linear, massive scalar field propagating on a fixed, globally-hyperbolic space–time with compact Cauchy hypersurfaces.

Various motivations lie behind such a study. To begin with, infinite-dimensional systems are qualitatively different from finite-dimensional ones, and it is an important—and mathematically non-trivial—challenge to see how the perennial formalism can be extended to this case. We shall show how the scalar field theory can be rewritten in such a way as to become a simple example of a system with perennials. However, quantum field theory in a fixed background has been much studied in the past using standard methods, and hence it provides a useful model for exploring the perennial formalism for an infinite-dimensional system. As we shall see, new problems *do* appear, the most important of which concerns the choice of the operator representation for the group/algebra generated by the perennials.

In the standard approach to quantum field theory on a background space–time, the normal way of addressing the problem of operator representation makes extensive use of the classical time evolution of the system. Thus the time evolution and associated Hamiltonian are considerably more important for infinite-dimensional systems than they are in the finite-dimensional case. Specifically, if there is no timelike isometry group, then the physical representation for the quantum system is not determined and—at the same time—the time evolution and Hamiltonian of the classical system are not well-defined (by the perennial formalism). Such a lack of a Hamiltonian was identified in Ref. 5 as the general form taken by the problem of time within the perennial formalism. However, studies of quantum field theory on a background space–time have produced several possible strategies for dealing with this problem, and one can hope that some of these ideas may be applicable to other situations, especially if a common language—in our case, that of the perennial formalism—has been developed.

The perennial formalism enables us to reformulate the dynamics of a scalar field in a background space–time in terms of properties of the system's phase space. In this reformulation, an important role is played by the idea of a *transversal surface*, defined in general for a system with a gauge group as a submanifold in the phase space that cuts orbits of the gauge group transversally; the *domain* of a transversal surface is the set of points in the constraint submanifold that can be joined to the transversal surface by the orbits of the constraints; see Ref. 5. Global problems may arise: for example, there may not exist any global transversal surface (i.e., one whose domain is the whole constraint surface); or there might be a symmetry transformation that maps a global transversal surface onto a transversal surface that is not global. Indeed, we shall show that the latter situation arises in the particular case of a space–time with a black hole. This leads to an information loss in which the quantum evolution associated with the symmetry sends pure states

to mixed states (the Hawking effect). A situation with somewhat similar features can occur if a system has no global transversal surfaces (the so-called ''global'' time problem); in particular, an analogous non-unitarity is exhibited by the quantum time evolution. Toy models exhibiting such behavior were studied in Refs. 9 and 10. Thus, the ideas developed in the present article may be of use in finding a physical interpretation in general situations in which the global time problem arises.

Another motivation for our present work is that our understanding of quantum field theory on a fixed background might itself profit from the use of the language of perennials. For example, the symmetries and transversal surfaces that have been employed in the past in studies of such quantum field theories are of a very special nature: namely, transformations of phase space that are generated in a particular way by space–time transformations, and surfaces associated with space–time hypersurfaces. The perennial formalism permits more general types of symmetry and transversal surface, and suggests how these can be found. The question then is if these symmetries can be utilized in the quantum theory, and—if not—why not.

The plan of the paper is as follows. In section II, we summarize the results of the companion work[11] where the dynamics and the symplectic geometry of the parametrized scalar field was cast into the standard form of a first-class parametrized system so that the perennial formalism can be applied. In section III, two different kinds of perennials are constructed and each of them is shown to form an algebra of elementary perennials, both of which are versions of the infinite Heisenberg algebra. We show that each isometry of the background space–time defines a map of the phase space that is a symmetry. We calculate the action of these symmetries on the elementary perennials and find that they define automorphisms of the algebras. Then we show how the theory of time evolution as described in Ref. 5 can be applied to the present case.

In the final section we show how the group and algebraic quantization that is performed as the next step reduces to the familiar problem of finding a physically appropriate representation of the Weyl group. We briefly summarize the relevant results of the theory of Weyl systems in connection with quantum field theory on a background space–time, and we show that our quantization method leads to a quantum theory that is equivalent to the usual one. Finally, we discuss the problem of time in a quantum field theory in a fixed background. We study a ''scattering approach'' to quantization that makes use of an isolated symmetry that is defined on only a small subset of the phase space. In the context of the perennial formalism, such a generalized symmetry is sufficient to define a time evolution. We show that the resulting quantum evolution is nonunitary if the symmetry does not preserve the domains of the transversal surfaces involved in the construction, and we apply the results to the Hawking effect. We also briefly describe the ''algebraic approach'' to quantization in which the states are defined as functionals on the algebras of perennials.

II. STRUCTURE OF THE EXTENDED PHASE SPACE

In this section, we shall summarize the results of the companion work[11] so that the present paper becomes self-contained. For more details, one should consult.[11]

We work with a curved background space–time $(\mathscr{M},g)$ and assume that it is C^∞ and globally hyperbolic; the Cauchy surface Σ is assumed to be compact. The real scalar field ϕ satisfies the Klein–Gordon equation

$$|\det g|^{-1/2}\partial_\mu(|\det g|^{1/2}g^{\mu\nu}\partial_\nu\phi)+m^2\phi=0. \tag{1}$$

Consider a C^∞ embedding $X:\Sigma\to\mathscr{M}$ that is spacelike with respect to the metric g. Let $\mathscr{E}$ denote the space of all such embeddings. Each embedding X determines a positive-definite metric γ_X on Σ and a unit normal vector field n_X to $X(\Sigma)$ in $\mathscr{M}$. The embedding X also defines a Cauchy datum for the field ϕ along the hypersurface $X(\Sigma)$. This is a pair (φ,π) of fields on Σ, where the scalar φ and the density (of weight $w=1$) π are defined by

$$\varphi(x) := \phi(X(x)), \tag{2}$$

$$\pi(x) := (\det\ \gamma)^{1/2}[X(x)]n^{\mu}(X(x))\partial_{\mu}\phi(X(x)). \tag{3}$$

The space of all C^{∞} Cauchy data will be denoted by Γ_{ϕ}—a linear space that can be equipped with a Sobolev structure (for details, see Ref. 11). The dynamical equation (1) defines a mapping between Cauchy data corresponding to different embeddings. Specifically, let X and X' be two arbitrary spacelike embeddings and let $(\varphi,\pi) \in \Gamma_{\phi}$. Then there is a unique solution ϕ of Eq. (1) whose Cauchy datum at $X(\Sigma)$ is (φ,π), and this induces a well-defined Cauchy datum (φ',π') on $X'(\Sigma)$. Thus we get a map $(\varphi,\pi)\rightarrow(\varphi',\pi')$, which we denote by $\rho_{XX'}$. One can show that $\rho_{XX'}$ is an automorphism of the Sobolev space Γ_{ϕ}.

The space Γ_{ϕ} is the phase space of the (non-constrained) scalar field ϕ on the curved background $(\mathscr{M},g)$. If we extend this space by adding all spacelike embeddings X and their conjugate momenta P, and if we impose suitable constraints, we obtain a constrained system that is dynamically equivalent to the original one. The points of the resulting extended phase space Γ are collections of fields, $x\mapsto(\varphi(x),\pi(x),X(x),P(x))$ on Σ. These fields can be characterized by their transformation properties with respect to a pair of local charts

$$(U,h)\ \text{of}\ \Sigma \quad \text{and} \quad (\overline{V,h})\ \text{of}\ \mathscr{M} \tag{4}$$

(where $X(U)\cap\overline{V} \neq \emptyset$). In particular, $P_{\mu}(x)$ is a covector with respect to the transformation of (V,h) on $\mathscr{M}$ and a quadruple of scalar densities with respect to the transformation of (U,h) on Σ. Quantities of this type were called ''e-tensor densities'' by Kuchař.[12]

The phase space Γ can be given a structure of an infinite-dimensional differentiable manifold with tangent and cotangent vectors described as follows. Consider a curve $\lambda\rightarrow(\varphi_{\lambda},\pi_{\lambda},X_{\lambda},P_{\lambda})$ whose tangent vector components $(\Phi,\Pi,V,W)\equiv(\dot{\varphi}_{\lambda},\dot{\pi}_{\lambda},\dot{X}_{\lambda},\dot{P}_{\lambda})$ can be calculated by differentiating with respect to λ the coordinate representatives associated with the pair of charts (4). The fields $\Phi(x)$, $\Pi(x)$, $V(x)$ and $W(x)$ are again characterized by their transformation properties: the first three are e-tensors, but the fourth transforms in a more complicated way (see Ref. 11). The space $T_{(\varphi,\pi,X,P)}\Gamma$ of all such vectors can be given the C^{∞} structure of a Fréchet space. A cotangent vector at a point (φ,π,X,P) of Γ will be a quadruple $(A_{\varphi},A_{\pi},A,B)$ of fields on Σ such that the pairing

$$\langle(A_{\varphi},A_{\pi},A,B),(\Phi,\Pi,V,W)\rangle := \int_{\Sigma} d^3x(A_{\varphi}\Phi + A_{\pi}\Pi + A_{\mu}V^{\mu} + B^{\mu}W_{\mu}) \tag{5}$$

with vectors from $T_{(\varphi,\pi,X,P)}\Gamma$ gives a coordinate independent number. This requirement determines the transformation properties of the fields $(A_{\varphi},A_{\pi},A,B)$.

One can show that $(A_{\pi},-A_{\varphi},B,-A)$ transforms as a tangent vector. Thus, there is a map $J:T^{*}_{(\varphi,\pi,X,P)}\Gamma\rightarrow T_{(\varphi,\pi,X,P)}\Gamma$ given by $J(A_{\varphi},A_{\pi},A_X,A_P) := (A_{\pi},-A_{\varphi},A_P,-A_X)$. The C^{∞} structure of the space $T^{*}_{(\varphi,\pi,X,P)}\Gamma$ can be chosen in such a way that J is an isomorphism. Using this isomorphism, a symplectic structure Ω on Γ can be defined as follows. If v_1 and v_2 are two vectors in $T_{(\varphi,\pi,X,P)}\Gamma$ then

$$\Omega(v_1,v_2) := -\langle J^{-1}v_1,v_2\rangle. \tag{6}$$

It follows at once that (i) $\Omega(v_1,v_2) = -\Omega(v_2,v_1)$; (ii) Ω is weakly non-degenerate (see Ref. 13); and (iii) Ω is not only closed but also exact.

As Ω is only a weak symplectic form, not every differentiable function on Γ will have an associated Hamiltonian vector field. The class of functions that do can be characterized as follows. If $F:\Gamma\rightarrow\mathbb{R}$, we say that F has a *gradient* if the following two conditions are satisfied:

(1) the Fréchet derivative, $DF|_{(\varphi,\pi,X,P)}:T_{(\varphi,\pi,X,P)}\Gamma\rightarrow\mathbb{R}$ is a bounded linear map;

(2) there exists $\mathrm{grad}F \in T^*_{(\varphi,\pi,X,P)}\Gamma$ such that $\langle \mathrm{grad}F, v\rangle = \mathrm{D}F|_{(\varphi,\pi,X,P)}(v)$ for all $v \in T_{(\varphi,\pi,X,P)}\Gamma$.

The quantity $\mathrm{grad}F$ is calculated from DF as usual by integration by parts (if F contains derivatives). The ''components'' of this gradient will be denoted by the collection of functions $(\mathrm{grad}_\varphi F, \mathrm{grad}_\pi F, (\mathrm{grad}_X F)_\mu, (\mathrm{grad}_P F)^\nu)$.

For a differentiable function with a gradient, we can define the associated ''Hamiltonian vector field.'' Specifically, if F is such a function, then $\xi_F \in T_{(\varphi,\pi,X,P)}\Gamma$ is defined by the relation $\langle \mathrm{grad}F, v\rangle = \Omega(v, \xi_F)$, for all $v \in T_{(\varphi,\pi,X,P)}\Gamma$. Hence, because of Eq. (6), we see that $\langle \mathrm{grad}F, v\rangle = \langle J^{-1}\xi_F, v\rangle$ for all v, and so $\xi_F = J(\mathrm{grad}F)$. Finally, the Poisson bracket of a pair of differentiable functions F and G is defined as $\{F,G\} := -\Omega(\xi_F, \xi_G)$, and we see immediately that

$$\{F,G\} = \langle \mathrm{grad}F, \xi_G\rangle. \tag{7}$$

This Poisson bracket is antisymmetric and, since Ω is closed, it satisfies the Jacobi identity.

The constraints that must be imposed on the extended phase space Γ are

$$\mathscr{H}_\mu = P_\mu + \mathscr{H}^\phi_\mu, \tag{8}$$

$$\mathscr{H}^\phi_\mu = -\mathscr{H}^\phi_\perp n_\mu + \mathscr{H}^\phi_k X^k_\mu, \tag{9}$$

where $\mathscr{H}^\phi_\perp = \frac{1}{2}(\det\ \gamma)^{1/2}[(\pi^2/\det\ \gamma) + \gamma^{kl}\varphi_{,k}\varphi_{,l} + m^2\varphi^2]$, and $\mathscr{H}^\phi_k = \pi\varphi_{,k}$. One can show that the constraint set $\tilde{\Gamma}$ defined by $\mathscr{H}_\mu = 0$ is a smooth submanifold in a neighborhood of any of its points. Moreover, $\tilde{\Gamma} = \tilde{C}(\Gamma_\phi \times \mathscr{E})$, where $\tilde{C}: \Gamma_\phi \times \mathscr{E} \to \Gamma$ is defined by $\tilde{C}(\varphi,\pi,X) := (\varphi,\pi,X, -\mathscr{H}^\phi(\varphi,\pi,X))$. We shall often refer to $\tilde{\Gamma}$ as $\Gamma_\phi \times \mathscr{E}$.

If we smear $\mathscr{H}_\mu$ to get $\mathscr{H}_N := \int_\Sigma d^3x N^\mu(x)\mathscr{H}_\mu(x)$, where $N \in T_X\mathscr{E}$ [i.e., $N(x) \in T_{X(x)}\mathscr{M}$], we obtain a differentiable function with a gradient. Such a function defines a Hamiltonian vector field, and one can proceed in complete analogy with the theory of finite-dimensional systems. For example, let ϕ satisfy the Klein–Gordon equation (1) on $\mathscr{M}$. Then for each curve $\lambda \mapsto X_\lambda$ with the tangent vector field N on $\mathscr{E}$, the initial data $(\varphi_\lambda, \pi_\lambda)$ for ϕ on $X_\lambda(\Sigma)$ satisfy the evolution equation

$$(\dot{\varphi}, \dot{\pi}, \dot{X}, \dot{P}) = J(\mathrm{grad}\mathscr{H}_N). \tag{10}$$

Thus the Hamiltonian vector fields $J(\mathrm{grad}\mathscr{H}_N)$ of the functions $\mathscr{H}_N$ are tangential to $\tilde{\Gamma}$, and the system is first class according to the definition given in Ref. 5. The pull-back of the vector field (10) to $\Gamma_\phi \times \mathscr{E}$ is given by

$$\dot{\varphi} = \mathrm{grad}_\pi \mathscr{H}_N, \tag{11}$$

$$\dot{\pi} = -\mathrm{grad}_\varphi \mathscr{H}_N, \tag{12}$$

$$\dot{X} = N. \tag{13}$$

Let us denote the space of longitudinal vectors at $(\varphi,\pi,X) \in \Gamma_\phi \times \mathscr{E}$ by $\Xi_{(\varphi,\pi,X)}$, i.e.,

$$\Xi_{(\varphi,\pi,X)} := \{(\Phi,\Pi,V) \in T_{(\varphi,\pi,X)}\tilde{\Gamma} \,|\, \Phi = \mathrm{grad}_\pi \mathscr{H}_N, \Pi = -\mathrm{grad}_\varphi \mathscr{H}_N, V = N \in T_X\mathscr{E}\}. \tag{14}$$

The space $\Xi_{(\varphi,\pi,X)}$ is a closed subspace of $T_{(\varphi,\pi,X)}\tilde{\Gamma}$. Moreover, there is a submanifold of $\tilde{\Gamma}$ whose tangent space coincides with $\Xi_{(\varphi,\pi,X)}$ at each point of the submanifold. Let us denote the maximal submanifold of this kind passing through a point $(\varphi,\pi,X) \in \tilde{\Gamma}$ by $\gamma_{(\varphi,\pi,X)}$. This subset $\gamma_{(\varphi,\pi,X)}$ is called a ''c-orbit through (φ,π,X),'' in complete analogy with the situation for a finite-dimensional system.

Finally, the pull-back $\tilde{\Omega}$ of the form Ω to $\tilde{\Gamma}$ is given by the formula

$$\tilde{\Omega}((\Phi_1,\Pi_1,V_1),(\Phi_2,\Pi_2,V_2))$$

$$= \int_\Sigma d^3x[(\Pi_1 + \mathrm{grad}_{\varphi'}\mathscr{H}_{V_1})(\Phi_2 - \mathrm{grad}_{\pi'}\mathscr{H}_{V_2})$$

$$-(\Pi_2 + \mathrm{grad}_{\varphi'}\mathscr{H}_{V_2})(\Phi_1 - \mathrm{grad}_{\pi'}\mathscr{H}_{V_1})]. \tag{15}$$

Clearly, $\tilde{\Omega}$ is a presymplectic form and $\Xi_{(\varphi,\pi,X)}$ is its singular subspace.

III. PERENNIALS, SYMMETRIES AND TIME EVOLUTION

In section II we showed that the geometrical structure of the phase space, constraint submanifold and the c-orbits of our infinite-dimensional system are all analogous to those of the corresponding objects in a finite-dimensional system as studied, for example, in Ref. 5. The application of the perennial formalism is now straightforward.

A crucial role in the perennial formalism is played by quantities that are reparametrization and gauge invariant. In particular, a *perennial* is defined as a function $o:\Gamma\to\mathbb{R}$ that is constant along the c-orbits; or, equivalently,

$$\{o,H_N\}|_{\tilde{\Gamma}} = 0, \text{ for all } N. \tag{16}$$

In most physical applications of a field theory, one deals with a restricted class of functions on the phase space—the so-called ''local functionals.'' Each local functional has the form $\int_\Sigma d^3x F(x)$, where the value of $F(x)$ at $x \in \Sigma$ is a polynomial function of values of the fields and their x-derivatives taken at the same point. It is easy to show that (i) all local functionals possess gradients; (ii) the Poisson bracket of two local functionals is again a local functional, so that multiple Poisson brackets are well-defined; and (iii) they satisfy the Jacobi identity. Since the smeared constraint $\mathscr{H}_N$ is itself a local functional it follows that the set of all local functionals that are perennials forms a Poisson algebra $\mathscr{P}_{\mathrm{lf}}$.

Let us now construct a particular class of local functional perennials for the case of scalar field theory on a background space–time. The idea is to associate a perennial o_ϕ with each maximal solution ϕ of the classical field equations. Specifically, let (ξ,η,X,P) be an arbitrary point of Γ and let (φ,π) be the Cauchy datum of ϕ at X. Then o_ϕ is defined by

$$o_\phi(\xi,\eta,X,P) := \int_\Sigma d^3x(\varphi\eta - \xi\pi). \tag{17}$$

The main task is to show that o_ϕ is constant along c-orbits.

Let $\gamma_{(\xi,\eta,X)}$ be a c-orbit and let ψ be the associated maximal classical solution, i.e., (ξ,η) is the Cauchy datum of ψ on $X(\Sigma)$. Let $(\xi',\eta',X',P') \in \gamma_{(\xi,\eta,X)}$ be an arbitrary point on the c-orbit. Then

$$o_\phi(\xi',\eta',X',P') = \int_\Sigma d^3x(\varphi'\eta' - \xi'\pi'), \tag{18}$$

where (φ',π') and (ξ',η') are the Cauchy data of ϕ and ψ respectively at X'. Using Eqs. (2) and (3), we can rewrite this as

$$o_\phi(\xi',\eta',X',P') = \int_\Sigma d^3x(\det\,\gamma')^{1/2}n'^{\mu}(\phi\psi_{,\mu} - \psi\phi_{,\mu})_{X'(\Sigma)}, \tag{19}$$

where γ' is the induced metric on $X'(\Sigma)$, and n'^{μ} is the unit normal vector to $X'(\Sigma)$. However, the integral on the right hand side is just the familiar ''Klein–Gordon inner product'' $(\phi,\psi)_{\mathrm{KG}}$ of the two solutions ϕ and ψ, and this is well-known to be independent of the Cauchy surface $X'(\Sigma)$. Hence o_ϕ is constant, as claimed.

The perennial o_ϕ has the following properties.

(1) Suppose that o_ϕ is constant along the whole of the constraint set $\tilde{\Gamma}$. Then ϕ must have the same Klein–Gordon product with any other solution, which is only possible if $\phi=0$.

(2) Let ϕ and ψ be two maximal solutions with corresponding perennials o_ϕ and o_ψ. Then the definition (17) implies immediately that

$$o_\phi + o_\psi = o_{\phi+\psi}, \tag{20}$$

$$r o_\phi = o_{r\phi} \text{ for all } r \in \mathbb{R}, \tag{21}$$

where the linearity of the field equation (1) guarantees that the solutions $\phi+\psi$ and $r\phi$ are again maximal.

(3) The Poisson bracket of o_ϕ and o_ψ can be obtained from Eq. (7). To calculate it we need the gradients, and using Eqs. (11) and (12) we obtain

$$\langle \mathrm{grad}\, o_\phi|_{(\xi,\eta,X,P)}, (\Phi,\Pi,V,W)\rangle$$

$$= \int_\Sigma d^3x [\varphi\Pi - \pi\Phi + \xi \mathrm{grad}_\varphi H_V|_{(\varphi,\pi,X,P)} + \eta \mathrm{grad}_\pi H_V|_{(\varphi,\pi,X,P)}]. \tag{22}$$

Thus,

$$\mathrm{grad}_\varphi o_\phi|_{(\xi,\eta,X,P)} = -\pi,$$

$$\mathrm{grad}_\pi o_\phi|_{(\xi,\eta,X,P)} = \varphi,$$

$$\mathrm{grad}_P o_\phi|_{(\xi,\eta,X,P)} = 0,$$

where (φ,π) is the Cauchy datum of ϕ at X. It follows that

$$J(\mathrm{grad} o_\phi) = (\varphi,\pi,0,A), \tag{23}$$

where A_μ are functions of ξ, η, X, P and ϕ. Then

$$\{o_\phi, o_\psi\}(\xi,\eta,X,P) = \int_\Sigma d^3x (\det\,\gamma)^{1/2} n^\mu (\phi\psi_{,\mu} - \psi\phi_{,\mu})_{X(\Sigma)} = (\phi,\psi)_{\mathrm{KG}}, \tag{24}$$

where γ and n^μ are the induced metric and unit normal vector at $X(\Sigma)$. Thus the Poisson bracket is independent of (ξ,η,X,P) and is hence a constant real function on the phase space Γ.

(4) Let ϕ and ψ be two different maximal solutions representing two different orbits γ_ϕ and γ_ψ. Then there is a third solution, χ, such that $(\chi,\phi-\psi)_{\mathrm{KG}} \neq 0$, and hence o_χ has different values at γ_ϕ and γ_ψ.

Let $\mathcal{S}_\phi$ denote the set of perennials of the form o_ϕ where ϕ runs over the set of all C^∞ solutions to the field equations. Then, because of the second property above, $\mathcal{S}_\phi$ is a linear space. Let $\mathcal{R}\cong\mathbb{R}$ denote the set of the constant real functions on Γ, and consider the linear space $\mathcal{S}_{\mathrm{can}} := \mathcal{S}_\phi \oplus \mathcal{R}$. This space $\mathcal{S}_{\mathrm{can}}$ is closed with respect to Poisson bracket operations because of the third property above. Moreover, $\mathcal{S}_{\mathrm{can}} \subset \mathcal{P}_{\mathrm{lf}}$. Thus $\mathcal{S}_{\mathrm{can}}$ is a Lie subalgebra of $\mathcal{P}_{\mathrm{lf}}$. According to the fourth property above, it separates the c-orbits in $\tilde{\Gamma}$. It follows that $\mathcal{S}_{\mathrm{can}}$ can play the role of an ''algebra of elementary perennials'' for our system—the basic ingredient in the ''algebraic

method of quantization'' in which the quantum theory is associated with a self-adjoint representation of $\mathscr{S}_{\text{can}}$ on a Hilbert space (see Ref. 5). The relations (20), (21) and (24) imply that $\mathscr{S}_{\text{can}}$ is an infinite-dimensional Heisenberg algebra. Specifically, as a linear space it is a direct sum of $\mathscr{R}$ and the space $\mathscr{S}_\phi$ that is equipped with the (weakly) non-degenerate skew-symmetric form $(\cdot,\cdot)_{\text{KG}}$; the Lie bracket is then defined by

$$[(\phi_1,r_1),(\phi_2,r_2)]:=(0,(\phi_1,\phi_2)_{\text{KG}}). \tag{25}$$

The corresponding Lie group is the so-called ''Heisenberg group'' $\mathscr{G}_{\text{can}}$ defined on $\mathscr{S}_\phi\times\mathbb{R}$ by the group law

$$(\phi_1,r_1)\cdot(\phi_2,r_2):=\left(\phi_1+\phi_2,r_1+r_2+\frac{1}{2}(\phi_1,\phi_2)_{\text{KG}}\right). \tag{26}$$

The action of $\mathscr{G}_{\text{can}}$ on Γ can be deduced from the action of its generators o_ϕ given by Eq. (17): namely, the point (ξ,η,X,P) maps to $(\xi+\varphi,\eta+\pi,X,P')$, where (φ,π) is the initial datum of ϕ at $X(\Sigma)$ and P' is a function of ξ,η,X,P, and ϕ such that $(\xi+\varphi,\eta+\pi,X,P')\in\widetilde{\Gamma}$ if $(\xi,\eta,X,P)\in\widetilde{\Gamma}$. The action is not faithful since the subgroup $(0,\mathbb{R})$ acts trivially, and hence the group $\mathscr{G}_{\text{can}}$ is a central extension of a group of symmetries on Γ (see Ref. 6). Thus $\mathscr{G}_{\text{can}}$ satisfies all the conditions for a so-called ''first-class canonical group'' whose irreducible, unitary representations can be associated with a quantization of the system.[6]

There is an alternative choice for the algebra of elementary perennials in which the perennials are associated with ''smeared fields;'' as such, they form the basis for a different (but ultimately equivalent) quantization of the scalar field. The construction goes as follows. Let $D(\mathscr{M})$ be the space of C^∞ test functions with compact support on the space–time $\mathscr{M}$, let $f\in D(\mathscr{M})$ and $(\varphi,\pi,X,P)\in\Gamma$. Then there is a unique maximal classical solution ϕ with the Cauchy datum (φ,π) at $X(\Sigma)$, and we define the perennial $\kappa_f:\Gamma\to\mathbb{R}$ by the equation

$$\kappa_f(\varphi,\pi,X,P):=\int_{\mathscr{M}} d^4y|\det g|^{1/2}\phi f. \tag{27}$$

Note that κ_f does not depend on P, and it is a perennial because the same classical solution leads to the same value of κ_f. Let us list some important properties of this type of perennial.

(1) Clearly, κ_f can be constant along $\widetilde{\Gamma}$ only if $f=0$, and then $\kappa_f=0$.

(2) Let f and f' be two elements of $D(\mathscr{M})$ with corresponding perennials κ_f and $\kappa_{f'}$. Then the definition (27) implies immediately that

$$\kappa_f+\kappa_{f'}=\kappa_{f+f'},$$

$$r\kappa_f=\kappa_{rf}\text{ for all }r\in\mathbb{R}.$$

(3) We can find an explicit expression for κ_f if we use the Cauchy propagator $G(x,y)$ for Eq. (1) [$G(x,y)$ is sometimes known as the ''Pauli–Jordan function'']. The existence and uniqueness of such a propagator for space–times of the type with which we are dealing was shown by Choquet-Bruhat.[14] The basic properties of the Cauchy propagator (for example, see Ref. 15) are (i) $G(x,y)=-G^r(x,y)+G^a(x,y)$, where G^r and G^a are respectively the retarded and advanced propagators; (ii) $G(x,y)$ is real and skew-symmetric in x and y; and (iii) $G(x,y)$ satisfies the identity

$$\phi(x)=(G(x,\cdot),\phi(\cdot))_{\text{KG}}, \tag{28}$$

where $\phi(x)$ is any C^∞ solution to Eq. (1). From Eq. (28), it follows immediately that

$$(G(x,\cdot),G(\cdot,y))_{\mathrm{KG}}=G(x,y). \tag{29}$$

If the Klein–Gordon product on the right hand side of Eq. (28) is written out along Σ, we obtain an expression for the solution ϕ at any point $y \in \mathscr{M}$ in terms of its Cauchy data at $X(\Sigma)$. Substituting for $\phi(y)$ in Eq. (27) from Eq. (28) then gives the desired formula:

$$\kappa_f=-\int_\Sigma d^3x(\det\ \gamma)^{1/2}n^\mu \frac{\partial G(f,y)}{\partial y^\mu}|_{X(x)}\varphi(x)+\int_\Sigma d^3xG(f,X(x))\pi(x), \tag{30}$$

where

$$G(f,x):=\int_{\mathscr{M}} d^4y|\det g|^{1/2}f(y)G(y,x). \tag{31}$$

Thus, κ_f belongs to the class of local functionals.

(4) We have the relation $\{\kappa_f,\kappa_{f'}\}=-G(f,f')$, whose derivation is simple: read off the gradient of κ_f from the formula (30), insert it in Eq. (7), and use the identity (29).

The smeared perennials generate a Lie algebra, which we denote by $\mathscr{S}_{\mathrm{loc}}$. Properties (2) and (4) above imply that $\mathscr{S}_{\mathrm{loc}}$ is a Heisenberg algebra on $D(\mathscr{M})\times\mathbb{R}$ with the skew-symmetric form $-G(f,f')$. The corresponding Heisenberg group $\mathscr{G}_{\mathrm{loc}}$ can be used as a first-class canonical group for the system.

The next important step is to consider the role played by symmetries, where—in complete analogy with the finite-dimensional case (see Ref. 5)—a symmetry is defined as a symplectic diffeomorphism of Γ that preserves the constraint surface $\tilde{\Gamma}$. In particular, it can be shown that each symmetry maps c-orbits onto c-orbits.

We shall describe a particular class of symmetries that play an important role in the study of quantum field theory on a curved space–time. Any isometry $\vartheta:\mathscr{M}\to\mathscr{M}$ defines a map $\theta:\Gamma\to\Gamma$ as follows. Let $(\varphi,\pi,X,P) \in \Gamma$ be arbitrary and set $X':=\vartheta\circ X$. Since ϑ is an isometry, the embedding X' is spacelike, and hence a Cauchy surface for $\mathscr{M}$. The fields φ, π and P are e-tensor densities at $X \in \mathscr{E}$, and so can be considered as $\mathscr{M}$-tensors at points in $X(\Sigma)$ [note that $\varphi(x)$ and $\pi(x)$ are scalars, and $P(x)$ is a covector]. Set $(\varphi',\pi',P'):=(\vartheta^{*-1}\varphi,\vartheta^{*-1}\pi,\vartheta^{*-1}P)$, where ϑ^* is the usual pull-back of differential forms on $\mathscr{M}$. Finally, define $\theta(\varphi,\pi,X,P):=(\varphi',\pi',X',P')$.

A simple way of showing that θ is a symmetry is to use the ϑ-shifted chart. Each pair of local charts of the type $(U,h),(V,h)$ in Eq. (4) can be ''shifted'' by ϑ to become the chart (U,h) on Σ and the chart $(\vartheta(V),h\circ\vartheta^{-1})$ on $\mathscr{M}$. The functions that represent (φ',π',X',P') in the shifted charts coincide numerically with those that represent (φ,π,X,P) in the original charts. Moreover, the metric $g'_{\mu\nu}$ in $\vartheta(V)$ coincides with $g_{\mu\nu}$ in $\vartheta(V)$. Thus, if (φ,π,X,P) satisfies the constraints, then (φ',π',X',P') will also do so. Furthermore, any curve $\lambda\mapsto(\varphi_\lambda,\pi_\lambda,X_\lambda,P_\lambda)$ on Γ defines a curve $\lambda\mapsto\theta(\varphi_\lambda,\pi_\lambda,X_\lambda,P_\lambda)$ that has the same form in the respective coordinate systems. Thus the tangent vectors of these two curves must have the same components. It follows that θ is differentiable and—moreover—symplectic since the values of the symplectic form at (φ,π,X,P) and at (φ',π',X',P') must coincide numerically in the respective coordinate systems. Hence θ is a symmetry.

Let us list some of the important properties of θ.

(1) The restriction $\tilde{\theta}:\Gamma_\phi\times\mathscr{E}\to\Gamma_\phi\times\mathscr{E}$ of θ to $\tilde{\Gamma}$, is given by

$$\tilde{\theta}(\varphi,\pi,X)=(\varphi,\pi,\vartheta\circ X). \tag{32}$$

This follows immediately from the idea of a shifted chart and the fact that φ and π are scalar fields. Thus we obtain the same Cauchy datum at the shifted Cauchy surface.

(2) Let ϕ be a global solution of the field equation, with a Cauchy datum in the Sobolev space Γ_ϕ. Then $\phi\circ\vartheta^{-1}$ is again such a solution since ϑ is an isometry. If ϕ has the Cauchy datum (φ,π) at X, then $\phi\circ\vartheta^{-1}$ has the datum (φ,π) at $\vartheta\circ X$. It follows that the map $\rho_{XX'}$ defined earlier satisfies $\rho_{\theta\circ X\theta\circ X'}(\varphi,\pi)=\rho_{XX'}(\varphi,\pi)$.

(3) The definition of θ implies immediately that it maps c-orbits onto c-orbits. In particular, if γ_ϕ is an orbit corresponding to a maximal solution ϕ, then $\theta(\gamma_\phi)=\gamma_{\phi\circ\vartheta^{-1}}$.

(4) Let o_ϕ be a perennial in $\mathscr{S}_{\rm can}$. The θ-shifted perennial $s_\vartheta(o_\phi)$ was defined in Ref. 5 as $s_\vartheta(o_\phi):=o_\phi\circ\theta^{-1}$. Then we have the relation

$$s_\vartheta(o_\phi)=o_{\phi\circ\vartheta^{-1}}. \tag{33}$$

Indeed, $o_\phi(\theta^{-1}(\xi,\eta,X,P))=o_\phi(\xi,\eta,X',P')=\int_\Sigma d^3x(\varphi'\eta-\pi'\xi)$ where (φ',π') is the Cauchy datum of ϕ at $X'=\vartheta^{-1}\circ X$. However, (φ',π') is also the Cauchy datum of $\phi\circ\vartheta^{-1}$ at X. Thus, $o_\phi(\theta^{-1}(\xi,\eta,X,P))=o_{\phi\circ\vartheta^{-1}}(\xi,\eta,X,P)$, and this is equivalent to Eq. (33). A straightforward calculation gives the θ-shift for $\mathscr{S}_{\rm loc}$ as $s_\vartheta(\kappa_f)=\kappa_{f\circ\vartheta^{-1}}$.

The relation in Eq. (33) implies that s_ϑ is an automorphism of the algebra $\mathscr{S}_{\rm can}$ since the map $\phi\mapsto\phi\circ\vartheta^{-1}$ is a linear transformation of solutions that preserves the Klein–Gordon product, and the constant functions on Γ are left invariant by s_ϑ. Similarly, s_ϑ is an automorphism of the algebra $\mathscr{S}_{\rm loc}$ because the map $f\to f\circ\vartheta$ is linear and preserves the quadratic form $G(\cdot,\cdot)$. In fact, s_ϑ induces a transformation of perennials from $\mathscr{S}_{\rm can}$ that is directly related to the Bogoliubov transformations that arise in the study of quantum field theory on a curved background. Indeed, if we choose a complex orthonormal basis $\{\phi_m,\phi_m^*\}$ for the space of solutions (for example, see Ref. 15), then the coefficients $\{a_m,a_m^*\}$ of the expansion of any solution ϕ in terms of this basis have the form of our perennials: namely $a_m=(\phi_m^*,\phi)_{\rm KG}$. The transformation s_ϑ of perennials thus defines new coefficients a_m, and the expansion of these in terms of the old ones is what is normally called a ''Bogoliubov transformation.''

Let us observe that the perennial formalism allows a more general type of symmetry that is not necessarily associated with transformations of space–time. For example, the group $\mathscr{G}_{\rm can}$ is a group of such symmetries. This raises the interesting question of whether other symmetries that are not associated with space–time transformations can be found, and—if so—if they can be helpful in the study of quantum field theory on a curved background.

Finally, let us construct the time evolution of the system. In the finite-dimensional case, such a construction is based on a transversal surface Γ_0 and a one-dimensional symmetry group $\{h(t)\}$ that moves Γ_0 (see Ref. 5). A transversal surface Γ_0 is defined to be a smooth submanifold of $\widetilde{\Gamma}$ that (i) intersects each c-orbit γ in at most one point $p=\Gamma_0\cap\gamma$; and (ii) has the property that each such intersection is transversal, i.e., $T_p\Gamma_0\cap T_p\gamma=\{0\}$, where 0 is the zero vector. A transversal surface is said to be ''global'' if it intersects each c-orbit. All these definitions can be extended without change to the infinite-dimensional case.

Similarly, the projections of perennials and of symmetries can be defined as for finite-dimensional systems. Thus, let $i_0:\Gamma_0\to\Gamma$ be the submanifold injection, and let $\pi_0:\widetilde{\Gamma}\to\Gamma_0$ be the projection that is defined by $\pi_0(p):=\gamma_p\cap\Gamma_0$, where γ_p is the c-orbit through the point $p\in\widetilde{\Gamma}$. If o is a perennial, then its projection $o_0:\Gamma_0\to R$ is defined by

$$o_0:=i_0^*o=o\circ i_0=o|_{\Gamma_0}. \tag{34}$$

If $\psi:\Gamma\to\Gamma$ is a symmetry, then $a_0(\psi):\Gamma_0\to\Gamma_0$ is defined by

$$a_0(\psi):=\pi_0\circ\psi|_{\Gamma_0}. \tag{35}$$

One can easily show that i_0^* is a Poisson algebra isomorphism, and that $a_0(\psi)$ is a symmetry of Γ_0.

We shall use a special type of transversal surface that is associated with embeddings as follows. For any spacelike embedding $X:\Sigma\to\mathscr{M}$, define the subset $\Gamma_X\subset\widetilde{\Gamma}$ by

$$\Gamma_X:=\{(\varphi,\pi,X)\in\widetilde{\Gamma}|(\varphi,\pi)\in\Gamma_\phi\}. \tag{36}$$

In the following steps we shall show that Γ_X is a transversal surface.

(1) The subset Γ_X can be considered as the image of the map $i_X:\Gamma_\phi\to\Gamma$ defined by $i_X(\varphi,\pi):=(\varphi,\pi,X,P)$ where P is given by Eq. (9). Note that $\mathrm{D}i_X|_{(\varphi,\pi)}$ is given by

$$\mathrm{D}i_X|_{(\varphi,\pi)}(\Phi,\Pi,V,W)=(\Phi,\Pi,0,W)\in T_{\widetilde{C}(\varphi,\pi,X)}\widetilde{\Gamma}, \tag{37}$$

and hence the linear map $\mathrm{D}i_X|_{(\varphi,\pi)}$ is injective and splits as

$$T_{\widetilde{C}(\varphi,\pi,X)}\widetilde{\Gamma}=\{(\Phi,\Pi,0,W)|(\Phi,\Pi)\in T_{(\varphi,\pi)}\Gamma_\phi, W=-\mathrm{D}H^\phi(\Phi,\Pi,0)\}$$

$$\times\{(0,0,V,W)|V\in H_0^s, W=-\mathrm{D}H^\phi(0,0,V)\}. \tag{38}$$

Hence, Γ_X is a smooth submanifold of Γ.

(2) Any tangent vector to Γ_X at $(\varphi,\pi,X)\in\Gamma_\phi\times\mathscr{E}$ has the form $(\Phi,\Pi,0)$, where $(\Phi,\Pi)\in T_{(\varphi,\pi)}\Gamma_\phi\simeq\Gamma_\phi$. The tangent space to $\gamma_{(\varphi,\pi,X)}$ at (φ,π,X) is the space $\Xi_{(\varphi,\pi,X)}$ given by Eq. (14), and the only vector (Φ,Π,V) in $\Xi_{(\varphi,\pi,X)}$ with $V=0$ is the zero vector. Thus the condition for transversality is satisfied.

(3) Any c-orbit γ_ϕ intersects Γ_X, and the point of intersection is (φ,π,X), where (φ,π) is the (unique) Cauchy datum of ϕ at X. Thus Γ_X is a global transversal surface.

Note that the injection i_X gives Γ_X the structure of a linear (Fréchet) space. Hence we can identify $T_{(\varphi,\pi)}\Gamma_X$ with Γ_X itself.

The pull-back Ω_X of $\widetilde{\Omega}$ by $i_X|_{\widetilde{\Gamma}}$ can easily be calculated from Eq. (15) as

$$\Omega_X((\Phi_1,\Pi_1),(\Phi_2,\Pi_2))=\int_\Sigma d^3x(\Phi_2\Pi_1-\Phi_1\Pi_2). \tag{39}$$

This is a constant, weakly nondegenerate form on $T_{(\varphi,\pi)}\Gamma_\phi\times T_{(\varphi,\pi)}\Gamma_\phi$ that can be identified with the following one on $\Gamma_\phi\times\Gamma_\phi$:

$$\Omega_X((\varphi_1,\pi_1),(\varphi_2,\pi_2))=\int_\Sigma d^3x(\pi_1\varphi_2-\varphi_1\pi_2). \tag{40}$$

This form can be used to equip Γ_ϕ with the structure of a linear, weak-symplectic space.

Note that the perennial formalism allows for more general transversal surfaces that are not necessarily associated with surfaces in space–time. An intriguing—and open—question is if an explicit example of such a surface can be found and, if so, if it can be used to construct a quantum field theory on a generic space–time with no timelike Killing vectors (see later).

Let us suppose next that there is a one-dimensional group of isometries $\vartheta(t)$ in the space–time $\mathscr{M}$ such that, for all t, $\vartheta(t)(X(\Sigma))\neq X(\Sigma)$ and $\vartheta(t)$ is generated by an everywhere timelike Killing vector in $\mathscr{M}$. The corresponding one-dimensional group $\{\theta(t)\}$ of symmetries of Γ, together with the transversal surface Γ_X, form a basis for the construction of an ''auxiliary rest frame'' with ''time levels'' given by $\Gamma_t:=\theta(t)\Gamma_X$ and ''rest trajectories'' given by θ-orbits $\{\theta(t)p\}$, $p\in\Gamma_0$. Any c-orbit γ defines a curve, $t\mapsto\eta_\gamma(t):=\Gamma_t\cap\gamma$, and the motion with respect to the auxiliary rest frame can be defined in a complete analogy to the finite-dimensional case by comparing the curve $\eta_\gamma(t)$ with the rest trajectories $\theta(t)p$. ''The same measurement at different

times'' can again be defined as the set of time-shifted perennials $o \to o_t := s_{\vartheta(t)} o$, and the construction of the classical Schroedinger or Heisenberg pictures by means of the projection to Γ_0 is straightforward (for details see Ref. 5).

However, note that the procedure described here differs in one respect from that described in Ref. 5. Namely, the symmetry group $\{\theta(t)\}$ we have chosen to generate the time evolution is *not* a subgroup of the first-class canonical group $\mathcal{G}_{\rm can}$ or $\mathcal{G}_{\rm loc}$. Thus, the construction of the quantum mechanical time evolution as given in Ref. 5 has to be generalized. This will be done in the next section.

IV. QUANTUM THEORY

In this section, the construction of the quantum theory described in Ref. 5 for finite-dimensional systems will be extended to the scalar field on a fixed background. The construction uses a representation of the first-class canonical group $\mathcal{G}$ by unitary operators $R(g)$, $g \in \mathcal{G}$, on a Hilbert space $\mathcal{K}$. The generators of $\mathcal{G}$—the elements of the Lie algebra $\mathcal{S}$—are represented by self-adjoint operators on $\mathcal{K}$. Then the automorphism $s_{\vartheta(t)}$ of the algebra $\mathcal{S}$ defines an automorphism $\hat{s}_{\vartheta(t)}$ of the corresponding operator algebra by the commutative diagram:

$$\begin{array}{ccc} \mathcal{S} & \overset{s_{\vartheta(t)}}{\rightarrow} & \mathcal{S} \\ \downarrow R & & \downarrow R \\ R(\mathcal{S}) & \overset{\hat{s}_{\vartheta(t)}}{\rightarrow} & R(\mathcal{S}). \end{array} \tag{41}$$

We arrive at a unitary evolution if we can implement the automorphism $\hat{s}_{\vartheta(t)}$ by a unitary map $U(t): \mathcal{K} \to \mathcal{K}$; that is, $\hat{s}_{\vartheta(t)}(\hat{O}) = U^{-1}(t) \hat{O} U(t)$.

The classical constructions in the previous sections—in particular, the choice of the algebras of elementary perennials—were performed in such a way that the rules of the algebraic or group-theoretical approaches to quantization as described above lead directly to well-known approaches to the quantization of a scalar field on a fixed space–time background. In particular, $\mathcal{S}_{\rm can}$ leads to the Segal theory (for example, see Refs. 16 and 17).

Let us concentrate on $\mathcal{S}_{\rm can}$. As was explained in the previous section, $\mathcal{S}_{\rm can}$ is an infinite-dimensional version of the Heisenberg algebra, and it determines an abstract infinite-dimensional Heisenberg group $\mathcal{G}_{\rm can}$ (in fact, a ''nuclear group,'' see Ref. 18) that is a central extension of the corresponding symmetry group of the phase space Γ and which acts transitively on the c-orbits. The group $\mathcal{G}_{\rm can}$, together with a unitary representation (which must satisfy certain additional conditions in order to guarantee the existence of ''quantum observables;'' see Ref. 16) is called a ''Weyl system'' in the literature. If we apply the theory of Weyl systems to the present case, we can draw the following conclusions:

(1) The group-theoretical approach to the quantization of an infinite-dimensional system differs significantly from the finite-dimensional case in the following respects. As a rule, a finite-dimensional Lie group has only relatively few representations—indeed, the Heisenberg group of n dimensions has just one (up to unitary equivalence) for any n. Many finite-dimensional canonical groups arise naturally as semi-direct products in which the ''non-Abelian'' factor is sufficiently large that there are only a few inequivalent orbits in the dual of the abelian factor (see Ref. 6). However, an infinite-dimensional Heisenberg group has a huge number of non-equivalent representations. Many of these have no obvious physical application, while others have a meaning in relation to external parameters. For example, in quantum field theory at a finite temperature each value of the temperature is associated with a particular representation (and non-zero temperature representations are not even irreducible).

(2) The most difficult part of the construction of a linear quantum field theory is therefore the choice of a ''physical'' representation. In the Segal theory, the key object on which such a choice is based is the time evolution automorphism $s_{\vartheta(t)}$ of the Heisenberg algebra $\mathscr{S}_{\rm can}$. For example, a cyclic state (generating the representation by a Gel'fand–Neumark–Segal construction) might be selected using the Kubo–Martin–Schwinger condition with $\hat{s}_{\vartheta(t)}$. Another approach based on $s_{\vartheta(t)}$ is described in Ref. 17.

Thus a new problem arises here, analogous perhaps to the ''Hilbert space problem'' of Kuchař's classification[3] of different aspects of the problem of time in canonical quantum gravity. In fact, quantum field theory in a curved background has a time problem of its own: most interesting background space–times do not possess a one-dimensional group of timelike isometries $\vartheta(t)$ (i.e., there is no time-like Killing vector), so that $s_{\vartheta(t)}$ is not available. However, several methods have been developed for (at least, partly) bypassing this problem and thereby enabling a number of interesting questions to be addressed. These methods are not as mathematically rigorous as those based on a timelike Killing vector but, nevertheless, they may give some hints about the problem of time in the full theory of canonical quantum gravity. We shall consider two different strategies that we shall call the ''scattering approach'' and the ''algebraic approach'' to quantization. Let us describe how they can be applied in the context of the perennial formalism.

A. Scattering approach

The scattering approach to quantization is based on an isolated symmetry whose domain is a small subset of the phase space Γ. Let us consider first an (idealized) example in which $(\mathscr{M},g)$ is a space–time that satisfies the conditions of section II and which contains open subsets U' and U'' with the following properties:

(1) Both U' and U'' are locally stationary: i.e., there are local flows $\vartheta'(t,X)$ and $\vartheta''(t,X)$ generated by timelike Killing generators that are defined everywhere on U' and U'' respectively.

(2) Both U' and U'' contain Cauchy hypersurfaces: i.e., there are spacelike embeddings X' and X'' such that $X'(\Sigma)\subset U'$ and $X''(\Sigma)\subset U''$.

(3) There is an isometry $\vartheta: U'\to U''$ such that $X''=\vartheta\circ X'$.

Finally, let $\mathscr{S}_{\rm can}$ denote the algebra of elementary perennials as discussed in section III.

The local flows ϑ' and ϑ'' may not induce global symmetries of Γ, but they will define perennials h' and h'' in some neighborhood of $\Gamma_{X'}$ and $\Gamma_{X''}$ that correspond to the generators of ϑ' and ϑ'' respectively. These perennials can be used to construct representations $(R',\mathscr{K}')$ and $(R'',\mathscr{K}'')$ of $\mathscr{S}_{\rm can}$ such that $-h'$ and $-h''$ are represented by positive, self-adjoint operators $\hat{H}'$ and $\hat{H}''$ (see, e.g. Ref. 19). Following the procedure described in Ref. 9, one could now try to implement the map $\rho_{X'X''}:\Gamma_{X'}\to\Gamma_{X''}$, which is a symplectic diffeomorphism (see section II), by a unitary map $U(\rho):\mathscr{K}'\to\mathscr{K}''$. This would leave us with only one Hilbert space (a ''pasting'' of $\mathscr{K}'$ and $\mathscr{K}''$).

However, the literature on the quantum theory of a scalar field has proceeded in a different direction than can be related to the Heisenberg picture in the perennial formalism, as described in Ref. 5. The first observation is that the discrete isometry ϑ induces a symmetry θ that is defined in some neighborhood of $\Gamma_{X'}$ in Γ; in turn, θ determines a well-defined automorphism $s_\vartheta:\ \mathscr{S}_{\rm can}\to\mathscr{S}_{\rm can}$ of the space of perennials. Indeed, for this it is sufficient that θ maps a globally transversal surface $\Gamma_{X'}$ onto another such $\Gamma_{X''}$. The θ-shifted perennials are then completely determined by their values on $\Gamma_{X''}$, and these are given by the θ-maps of the restrictions of the original perennials to $\Gamma_{X'}$. Note that θ is not a symmetry in the sense of Ref. 5 (it is not globally defined); we shall refer to such a map as a ''time shift.''

The next step is to define the map $\hat{s}'_\vartheta: R'(\mathscr{S}_{\rm can})\to R'(\mathscr{S}_{\rm can})$ by the obvious analogue of the commutative diagram (41), and then to see whether or not it can be implemented by a unitary map $U(\vartheta):\mathscr{K}'\to\mathscr{K}'$. If the Cauchy hypersurface is compact, this is always possible.[20] Thus one can again work with just a single Hilbert space. The interpretation of the various mathematical objects

is then that $R'(\mathscr{S}_{\rm can})$ contains the Heisenberg observables at the ''time'' $\Gamma_{X'}$; $R'(s_\vartheta(\mathscr{S}_{\rm can}))$ contains those at the ''time'' $\Gamma_{X''}$; the elements of $\mathscr{K}'$ are the Heisenberg states; and $U(\vartheta)$ is the unitary scattering matrix.

If $U(\vartheta)$ does *not* exist, a Heisenberg-picture dynamics can still be used to calculate the expectation values of time-shifted operators that are well-defined in certain states. For example, in this way one can calculate the number of particles within a given finite energy range and a finite volume that are created from the vacuum of $\mathscr{K}'$ in the region between $X'(\Sigma)$ and $X''(\Sigma)$, even though the *total* number of created particles diverges.

Note that the scattering approach will work even if there is only the ''rudiments'' of a symmetry, but it will give only information on what comes ''out'' if we let something go ''in''; what happens ''inside'' remains quite undetermined.

B. The Hawking effect

An example of the scattering approach is the calculation of the Hawking effect.[19] In this section, we shall reformulate this calculation in terms of the perennial formalism. Our motivation is *not* to present a new and conceptually better derivation of the effect but rather to use this model of the scalar field on a black-hole background to suggest a possible meaning of a time shift that does not preserve the domains of transversal surfaces.

In a general system, a transversal surface Γ_X will not be global (i.e., it will not cut *all* the c-orbits transversally), and the time shift that is available will not preserve the domains of these surfaces [the domain $\mathscr{D}(\Gamma_1)$ of a transversal surface Γ_1 is the subset of $\widetilde{\Gamma}$ such that the c-orbit through any point of $\mathscr{D}(\Gamma_1)$ intersects Γ_1; see Ref. 5].

For example, the toy models studied in Refs. 9 and 10 do not possess global transversal surfaces, but there are some that are almost global in the sense that the closure of the domain contains the whole constraint surface $\widetilde{\Gamma}$. The results of Ref. 9 suggest that there is no difference between global and almost global surfaces as far as the quantum theory is considered. In Ref. 10, two almost global surfaces Γ_1 and Γ_2 were chosen, each with two components, $\Gamma_1^\pm$ and $\Gamma_2^\pm$ respectively, giving a total of four, closed transversal surfaces. There is a discrete symmetry θ that maps Γ_1^+ onto Γ_2^+, but $\mathscr{D}(\Gamma_1^+) \neq \mathscr{D}(\Gamma_2^+)$. The Hilbert spaces $\mathscr{K}_1$ and $\mathscr{K}_2$ corresponding to the transversal surfaces Γ_1^+ and Γ_2^+ were constructed, and a unitary map $U(\vartheta):\mathscr{K}_1\to\mathscr{K}_2$ of these Hilbert spaces was found that corresponds to the classical map θ. However, the pasting map $\rho:\Gamma_1^+\to\Gamma_2^+$ is defined (by the c-orbits; see Ref. 9) only between some proper subsets of Γ_1^+ and Γ_2^+; the corresponding map $U(\rho)$ is defined only on a proper subspace $\mathscr{K}_{12}\subset\mathscr{K}_1$, and $\mathscr{K}_{21}=U(\rho)\mathscr{K}_{12}$ is a proper subset of $\mathscr{K}_2$. Although the map $U(\rho):\mathscr{K}_{12}\to\mathscr{K}_{21}$ itself is unitary, the corresponding time evolution operator $U(\rho)\circ U^{-1}(\vartheta):\mathscr{K}_1\to\mathscr{K}_1$ is defined only on the subspace $\mathscr{K}_{12}$ and so it is not a unitary operator on $\mathscr{K}_1$. This leads to a time evolution that can change the norms of states, the only physical interpretation of which is that the system can be ''lost'' or ''found'' during the time evolution—this can in fact happen already in the classical theory of this (bizarre) system.

A similar situation can arise in the context of quantum field theory on a curved background. Suppose first that there is a Cauchy surface Σ that consists of two components Σ_1 and Σ_2, so that $\Sigma=\Sigma_1\cup\Sigma_2$. Then both Σ_1 and Σ_2 are closed surfaces in $\mathscr{M}$, and the space Γ_ϕ of Cauchy data on Σ splits into the direct sum of $\Gamma_{\phi 1}$ and $\Gamma_{\phi 2}$, where

$$\Gamma_{\phi i}=\{(\varphi,\pi)\in\Gamma_\phi|\,\mathrm{supp}(\varphi,\pi)\subset\Sigma_i\}, \tag{42}$$

$i=1,2$. Both $\Gamma_{\phi 1}$ and $\Gamma_{\phi 2}$ are Fréchet spaces, and $\Gamma_\phi=\Gamma_{\phi 1}\otimes\Gamma_{\phi 2}$. For a given spacelike embedding $X:\Sigma_1\cup\Sigma_2\to\mathscr{M}$, a pair of transversal surfaces Γ_{Xi}, $i=1,2$, can be defined by

$$\Gamma_{Xi}:=\{(\varphi,\pi,X)\in\widetilde{\Gamma}|\,\mathrm{supp}(\varphi,\pi)\subset\Sigma_i\}. \tag{43}$$

The proof that Γ_{Xi} is transversal is analogous to that for Γ_X in section III, with the relation Eq. (38) being replaced by

$$T_{\tilde{C}(\varphi,\pi,X)}\tilde{\Gamma}=\{(\Phi,\Pi,0,W)|(\Phi,\Pi)\in\Gamma_{\phi 1},W=-\mathrm{D}H^{\phi}(\Phi,\Pi,0)\}$$
$$\times\{(\Phi,\Pi,0,W)|(\Phi,\Pi)\in\Gamma_{\phi 2},W=-\mathrm{D}H^{\phi}(\Phi,\Pi,0)\}$$
$$\times\{(0,0,V,W)|V\in T_X\mathscr{E},W=-\mathrm{D}H^{\phi}(0,0,V)\}. \tag{44}$$

Of course, the surface Γ_{X1} is not even almost globally-transversal: we have the relation $\Gamma_X=\Gamma_{X1}\times\Gamma_{X2}$, and only Γ_X is a global transversal surface.

The Poisson algebra $\mathscr{P}$ of perennials contains ideals $\mathscr{P}_1$ and $\mathscr{P}_2$ of perennials associated with the transversal surfaces Γ_{X1} and Γ_{X2}, where

$$\mathscr{P}_i:=\{o\in\mathscr{P}|\text{supp } o\subset\mathscr{D}(\Gamma_{Xi})\}. \tag{45}$$

These ideals $\mathscr{P}_1$ and $\mathscr{P}_2$ generate $\mathscr{P}$. Similarly, the Lie algebra of elementary perennials $\mathscr{S}$ contains two ideals $\mathscr{S}_1$ and $\mathscr{S}_2$ defined by analogous equations, and $\mathscr{S}=\mathscr{S}_1\oplus\mathscr{S}_2$ is a Lie algebra decomposition. Indeed, each function $o\in\mathscr{S}$ has a restriction o_X to Γ_X, and there are unique $o_{X1}\in\mathscr{S}_1$ and $o_{X2}\in\mathscr{S}_2$ such that $o_X=o_{X1}+o_{X2}$. Observe that o_{Xi} vanishes at Γ_{Xi}, so that we have $\{o_{X1},o_{X2}\}=0$ as desired.

Suppose that the physical representations of the algebras $\mathscr{S}$, $\mathscr{S}_1$ and $\mathscr{S}_2$ on Hilbert spaces $\mathscr{K}$, $\mathscr{K}_1$ and $\mathscr{K}_2$ respectively have the property $\mathscr{K}=\mathscr{K}_1\otimes_s\mathscr{K}_2$, where $\otimes_s$ denotes the symmetrized tensor product. Let $|a\rangle$ be an arbitrary element of $\mathscr{K}$. Then it is well-known that there is a density operator $\hat{a}_1$ in $\mathscr{K}_1$ such that

$$\langle a|\hat{o}_1|a\rangle=\mathrm{tr}(\hat{a}_1\hat{o}_1),\quad \text{for } all\ \hat{o}_1\in L(\mathscr{K}_1) \tag{46}$$

(for example, see Ref. 19). Suppose finally that there is an isometry $\vartheta:X'(\Sigma)\to X(\Sigma_1)$, where $X'(\Sigma)$ is a Cauchy hypersurface and $X(\Sigma_1)$ is defined as above. The corresponding time shift $\theta:\Gamma_{X'}\to\Gamma_{X1}$ maps a global transversal surface onto a non-global one. Let us define s_ϑ by

$$s_\vartheta o|_{\Gamma_{X1}}=o\circ\theta^{-1},$$

$$s_\vartheta o|_{\Gamma_{X2}}=0\quad \text{for all } o\in\mathscr{S}.$$

We see immediately that $s_\vartheta(\mathscr{S})=\mathscr{S}_1$.

Now we can apply the Heisenberg picture method as described in subsection IV A. The elements of $\mathscr{K}$ are considered as Heisenberg states, and the algebra $R(\mathscr{S})$ contains the Heisenberg observables at the ''time'' $\Gamma_{X'}$ and $R(\mathscr{S}_1)$ contains those at the ''time'' Γ_{X1}. The result is that the time-evolution operator $\hat{s}_\vartheta$ maps the algebra $R(\mathscr{S})$ onto its own proper subalgebra $R(\mathscr{S}_1)$ so that the representation R of $\mathscr{S}_1$ is not irreducible, and a Heisenberg state $|a\rangle$ that is pure with respect to the algebra $R(\mathscr{S})$ is a mixed state $\hat{a}_1$ with respect to the time shifted algebra $R(\mathscr{S}_1)$.

An example in which ϑ maps a global transversal surface onto a non-global one is the Hawking radiation produced by the spherically-symmetric, asymptotically flat space–time associated with a collapsing star (see Ref. 19) (actually, it is a limiting case of the procedure above; moreover, the assumption must be made that the theory in Ref. 11 can be generalized to an asymptotically-flat spacetime). In this example, the scalar field is chosen to have a vanishing mass-parameter m, and hence the dynamics is determined completely by the conformal structure of the space–time $(\mathscr{M},g)$. The past and future null infinities $\mathscr{T}^+$ and $\mathscr{T}^-$ are null hypersurfaces in the conformal completion, $\mathscr{M}$, of $\mathscr{M}$. The hypersurfaces $\mathscr{T}^-$ and $\mathscr{T}^+\cup\mathscr{H}$ are Cauchy hypersurfaces for a zero rest mass field, where $\mathscr{H}$ is the event horizon in $\mathscr{M}$ (see Ref. 21). They can be considered as limits of time-like Cauchy hypersurfaces. Both $\mathscr{H}$ and $\mathscr{T}^+$ are closed hypersurfaces

in $\bar{\mathscr{M}}$. Note that Σ and $X_\pm$ can be chosen such that $X_-(\Sigma)=\mathscr{I}^-$ and $X_+(\Sigma)=\mathscr{I}^+$. The maps ϑ, ϑ_+ and ϑ_- which were (effectively) used in Ref. 19 can be described by means of the Eddington-Finkelstein coordinates (u,r,α,β) and (v,r,α,β) in some neighborhoods of $\mathscr{I}^-$ and $\mathscr{I}^+$ as follows: ϑ_- is defined by $(v,\infty,\alpha,\beta)\to(v+t,\infty,\alpha,\beta)$, ϑ_+ by $(u,\infty,\alpha,\beta)\to(u+t,\infty,\alpha,\beta)$, and ϑ by $u(v,\alpha,\beta)=v$, $r=\infty$, $dr\to -dr$, $\alpha(v,\alpha,\beta)=\alpha$, and $\beta(v,\alpha,\beta)=\beta$ (in-coming modes are mapped into out-going ones). This time shift ϑ is not uniquely determined because u and v are defined up to an additive constant, but most of the physically interesting results do not depend on the choice made. In this situation, the considerations above are applicable, and the result is again a non-unitary evolution that sends pure states into mixed states. This time, the normalization of states is preserved: some information is lost, but the system itself is not.

C. Algebraic approach

Hilbert spaces play a less direct role in this approach in which the basic objects are elements of some algebra of local observables on which states are defined as linear functionals. One can reformulate the algebraic approach in terms of the perennial formalism using the algebra of the smeared fields, $\mathscr{S}_{\rm loc}$. We shall not go into detail here, but just sketch the main ideas.

The local observables are polynomials in the smeared field operators

$$\hat{\kappa}_f, \quad \hat{\kappa}_f\hat{\kappa}_h, \ldots, \tag{47}$$

as well as the regularized stress-energy tensor components $\hat{T}^{\mu\nu}(p)$ at arbitrary points p of the space–time $\mathscr{M}$. The stress-energy tensor has an immediate physical interpretation whereas the smeared field operators play only an auxiliary role.

The states are defined as certain linear functionals on the above algebra, with the value of such a state σ on an operator $\hat{o}$ having the physical meaning of the expected value. Attention is restricted to so-called ''quasifree Hadamard states,'' whose value on any polynomial of the smeared fields is determined by its value on the following second-order polynomial

$$G_\sigma(f,h)=\sigma(\hat{\kappa}_f\hat{\kappa}_h+\hat{\kappa}_h\hat{\kappa}_f). \tag{48}$$

The bilinear form $G_\sigma(f,h)$ has a kernel $G_\sigma(y_1,y_2)$, so that

$$G_\sigma(f,h)=\int_{\mathscr{M}} \mathrm{d}^4y_1\,\mathrm{d}^4y_2 G_\sigma(y_1,y_2)f(y_1)h(y_2), \tag{49}$$

which satisfies the field equation in each argument y_1 and y_2. This leads to the crucial observation that the state can be ''calculated'' by solving the wave equation. For a Hadamard state, the short-distance behavior of $G_\sigma(y_1,y_2)$ as $y_1\to y_2$ is such that the expected value in the state σ of the stress-energy tensor is well-defined and can be calculated from $G_\sigma(y_1,y_2)$.

The quasifree Hadamard states do not form a Hilbert space: neither a scalar product—nor a linear combination—of a pair of them is well-defined. However, to obtain a physical interpretation of such a state it is only necessary to calculate the expected value of the stress-energy tensor, and this is feasible. For more details see Ref. 22.

V. CONCLUSIONS

We have found an intriguing result: canonical quantization of a system can lead to a non-unitary time evolution. The result has been derived by a careful analysis of global properties of the physical phase space: an aspect that has been rather neglected heretofore. However, more work is

necessary to understand the relations between the global properties and the time evolution in some generality. Also, the physical interpretation of the time evolution in parametrized systems needs to be developed further.

In the course of our calculations we have seen that the central commandment of the perennial formalism—to work only with perennials—is in reality not too restrictive since almost everything can be viewed as a perennial. In particular, the usual particle variables of the quantum field theory—for example, creation and annihilation operators—can be considered as perennials ($\mathscr{I}_{\rm can}$), as can the more local, smeared fields in $\mathscr{I}_{\rm loc}$.

However, these and other insights gained in our article have only a relative value in so far as their derivation exploited two special features of our model—the linearity of the field equations, and the existence of a background space–time. A question left for future research is if these structures can be replaced with something that will work in more complicated cases.

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Separation of the massless field equations for arbitrary spin in the Robertson–Walker space–time

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The massless spin 2 free-field equation is studied in the Robertson–Walker space–time via the Newman–Penrose formalism and separated by using a Chandrasekhar–Teukolski method. The resulting temporal and angular equations are explicitly integrated. The radial equations are solved in the flat universe case. The closed universe case shows, in principle, the existence of a discrete spectrum of the energy of the massless particles. In the general case of spin greater than 2 the massless field equations are shown to be separable by induction. The separated equations admit the same recurrence structure and analog interpretation properties of the spin 2 and less than 2 cases. © *1996 American Institute of Physics.* [S0022-2488(96)00307-6]

I. INTRODUCTION

After the pioneer paper by Newman and Penrose[1] the spinor formalism represents the natural tool to formulate in general relativity the (massless and massive) field equations. In this context the massless free-field equation for a field of spin $s=\frac{1}{2}(n+1)$ can be written[2]

$$\nabla_{AA'}\phi^{A}_{A_1A_2\cdots A_n}=0, \quad \phi_{AA_1A_2\ldots A_n}=\phi_{(AA_1A_2\ldots A_n)}. \tag{1}$$

The equations (1) are consistent in a curved space–time for $n=0$ (Weyl's equation) and $n=1$ (homogeneous Maxwell equations).[2] For $n>1$, they are consistent only if the space–time is conformally flat[2–5] (Inconsistencies arise already in Minkowski space–time for $s>1$ in the case of electromagnetic interaction[6]). To overcome these difficulties in arbitrary curved space–time, alternative formulations have been proposed in terms of symmetrized field equations stronger than Eq. (1).[7–9]

In the case of conformally flat space–time the equation (1) can be solved in a general way for arbitrary spin.[2]

In this paper we propose an alternative general solution in the case of the (conformally flat) Robertson–Walker geometry.[2] The solution is obtained by separating Eq. (1) for arbitrary spin. The proof of the result is done by induction over n in the context of the Newman–Penrose formalism.

We first completely solve the case $s=2$ by a separation method already applied to the $s=\frac{1}{2}$ and $s=1$ cases[10,11] and that is similar to the Chandrasekhar–Teukolski method employed to solve the Dirac equation in the Kerr metric.[12] The time and angular equations relative to this case are integrated in the flat, closed, and open universe. The radial equations, which are explicitly integrated in case of flat space–time, imply a restriction on the minimum possible eigenvalue of the angular equations. In the case of a closed universe, the structures of the radial equations suggest that the energy of the massless particles takes purely discrete values, a compatibility problem, however, being open.

The induction is then completed by taking into account the recursive separated structure of the angular and radial equations of the case $s=2$. A central role in the proof is played by the special structure that the spin coefficients take in the null tetrad frame that has been employed to perform the calculations.

II. THE MASSLESS SPIN 2 EQUATIONS

We now develop the field equation (1) by the Newman–Penrose formalism in the case of a spin 2 field. Since the field is represented by a symmetric spinor, its independent components can be characterized by setting

$$\phi_h \equiv \phi_{AA_1A_2A_3} \Leftrightarrow A+A_1+A_2+A_3=h, \quad h=0,1,2,3,4. \tag{2}$$

With this simplified notation we now develop the content of Eq. (1) by applying the Newman–Penrose formalism.[1] By using the expressions of the covariant spinorial derivatives in terms of the generalized Dirac matrices, $\nabla_{\mathbf{AX}'} = \sigma^a_{\mathbf{AX}'}\nabla_a$, by expressing the covariant derivatives by means of the tabulated spin coefficients[2,12] and with the usual identification $D\equiv\partial_{00'}$, $\delta\equiv\partial_{01'}$, $\delta^*\equiv\partial_{10'}$, $\Delta\equiv\partial_{11'}$ relative to the directional derivatives, we get from Eq. (1)

$$(D-2\epsilon-4\rho)\phi_1-(\delta^*+\pi-4\alpha)\phi_0+3\kappa\phi_2=0, \tag{3.1}$$

$$(D-3\rho)\phi_2-(\delta^*+2\pi-2\alpha)\phi_1+2\kappa\phi_3+\lambda\phi_0=0, \tag{3.2}$$

$$(D-2\epsilon-2\rho)\phi_3-(\delta^*+3\pi)\phi_2+\kappa\phi_4+2\lambda\phi_1=0, \tag{3.3}$$

$$(D+4\epsilon-\rho)\phi_4-(\delta^*+4\pi+2\alpha)\phi_3+3\lambda\phi_2=0, \tag{3.4}$$

$$(\Delta+\mu-4\gamma)\phi_0-(\delta-4\tau-2\beta)\phi_1-3\sigma\phi_2=0, \tag{3.5}$$

$$(\Delta+2\mu-2\gamma)\phi_1-(\delta-3\tau)\phi_2-2\sigma\phi_3-\nu\phi_0=0, \tag{3.6}$$

$$(\Delta+3\mu)\phi_2-(\delta+2\beta-2\tau)\phi_3-2\nu\phi_1-\sigma\phi_4=0, \tag{3.7}$$

$$(\Delta+4\mu+2\gamma)\phi_3-(\delta+4\beta-\tau)\phi_4+3\nu\phi_2=0, \tag{3.8}$$

that are the massless spin 2 equations. It is a standard result that these equations are formally identical with the Bianchi identities in vacuum.[13] We have written down eight equations because for any one of the equations (3.2), (3.3), (3.6), and (3.7) we obtain also, by the above procedure, two replicas of them.

III. SPIN 2 IN THE ROBERTSON–WALKER GEOMETRY

The object is now to separate Eqs. (3) in the Robertson–Walker space–time whose metric is given by

$$ds^2=dt^2-R^2(t)\left[\frac{dr^2}{1-ar^2}+r^2(d\theta^2+\sin^2\theta\, d\varphi^2)\right], \quad a=0,\pm1. \tag{4}$$

In connection with the Newman–Penrose formalism we choose the null tetrad frame $\{l^i,n^i,m^i,m^{\star i}\}$, whose associated directional derivatives are given by

$$\begin{aligned} D&\equiv l^i\partial_i=(\partial_t+R^{-1}\sqrt{1-ar^2}\partial_r)/\sqrt{2},\\ \Delta&\equiv n^i\partial_i=(\partial_t-R^{-1}\sqrt{1-ar^2}\partial_r)/\sqrt{2},\\ \delta&\equiv m^i\partial_i=(\partial_\theta+i\ \csc\ \theta\partial_\phi)/(\sqrt{2}rR),\\ \delta^*&\equiv m^{*i}\partial_i=(\partial_\theta-i\ \csc\ \theta\partial_\phi)/(\sqrt{2}rR), \end{aligned} \tag{5}$$

to which there correspond the nonzero spin coefficients[10]

$$\begin{aligned}\rho&=-(r\dot{R}+\sqrt{1-ar^2})/(\sqrt{2}rR),\\ \mu&=(r\dot{R}-\sqrt{1-ar^2})/(\sqrt{2}rR),\\ \beta&=-\alpha=\cot\,\theta/(2\sqrt{2}rR),\\ \epsilon&=-\gamma=\dot{R}/(2\sqrt{2}R).\end{aligned}\tag{6}$$

Owing to the symmetry of the metric, the φ dependence in Eqs. (3) can be separated, by the substitution $\phi_h\rightarrow\phi_h\exp(im\varphi)$, $m=0,\pm1,\pm2,\pm3,\ldots$. By using the above results and by setting

$$\phi_h(r,\theta,\varphi,t)=\exp(im\varphi)\,\phi_h(r,t)S_h(\theta),\quad h=0,1,2,3,4,\quad m=0,\pm1,\pm2,\ldots,\tag{7}$$

in Eqs. (3), the φ dependence factors out and the θ dependence can be separated to obtain

$$\frac{rR\sqrt{2}}{\phi_0}(D-2\epsilon-4\rho)\phi_1=\frac{1}{S_1}L_2^-S_0=\lambda_0,\tag{8.1}$$

$$\frac{rR\sqrt{2}}{\phi_1}(D-3\rho)\phi_2=\frac{1}{S_2}L_1^-S_1=\lambda_1,\tag{8.2}$$

$$\frac{rR\sqrt{2}}{\phi_2}(D+2\epsilon-2\rho)\phi_3=\frac{1}{S_3}L_0^-S_2=\lambda_2,\tag{8.3}$$

$$\frac{rR\sqrt{2}}{\phi_3}(D+4\epsilon-\rho)\phi_4=\frac{1}{S_4}L_{-1}^-S_3=\lambda_3,\tag{8.4}$$

$$\frac{rR\sqrt{2}}{\phi_1}(\Delta+\mu-4\gamma)\phi_0=\frac{1}{S_0}L_{-1}^+S_1=\lambda_4,\tag{8.5}$$

$$\frac{rR\sqrt{2}}{\phi_2}(\Delta+2\mu-2\gamma)\phi_1=\frac{1}{S_1}L_0^+S_2=\lambda_5,\tag{8.6}$$

$$\frac{rR\sqrt{2}}{\phi_3}(\Delta+3\mu)\phi_2=\frac{1}{S_2}L_1^+S_3=\lambda_6,\tag{8.7}$$

$$\frac{rR\sqrt{2}}{\phi_4}(\Delta+4\mu+2\gamma)\phi_3=\frac{1}{S_3}L_2^+S_4=\lambda_7,\tag{8.8}$$

λ_i, $i=0,1,\ldots,7$, being the corresponding separation constants and where use has been made of the definition

$$L_n^{\pm}=\partial_\theta\mp m\,\csc\,\theta+n\,\cot\,\theta.\tag{9}$$

By further setting

$$\phi_h(r,t)=\psi_h(r)T(t),\quad h=0,1,2,3,4,\tag{10}$$

also the r,t dependence can be separated in Eqs. (8) to obtain

$$ik=\sqrt{1-ar^2}\,\frac{\psi_1'}{\psi_1}+\frac{4}{r}\,\sqrt{1-ar^2}-\frac{\lambda_0}{r}\,\frac{\psi_0}{\psi_1}, \tag{11.1}$$

$$ik=\sqrt{1-ar^2}\,\frac{\psi_2'}{\psi_2}+\frac{3}{r}\,\sqrt{1-ar^2}-\frac{\lambda_1}{r}\,\frac{\psi_1}{\psi_2}, \tag{11.2}$$

$$ik=\sqrt{1-ar^2}\,\frac{\psi_3'}{\psi_3}+\frac{2}{r}\,\sqrt{1-ar^2}-\frac{\lambda_2}{r}\,\frac{\psi_2}{\psi_3}, \tag{11.3}$$

$$ik=\sqrt{1-ar^2}\,\frac{\psi_4'}{\psi_4}+\frac{1}{r}\,\sqrt{1-ar^2}-\frac{\lambda_3}{r}\,\frac{\psi_3}{\psi_4}, \tag{11.4}$$

$$ik=-\sqrt{1-ar^2}\,\frac{\psi_0'}{\psi_0}-\frac{1}{r}\,\sqrt{1-ar^2}-\frac{\lambda_4}{r}\,\frac{\psi_1}{\psi_0}, \tag{11.5}$$

$$ik=-\sqrt{1-ar^2}\,\frac{\psi_1'}{\psi_1}-\frac{2}{r}\,\sqrt{1-ar^2}-\frac{\lambda_5}{r}\,\frac{\psi_2}{\psi_1}, \tag{11.6}$$

$$ik=-\sqrt{1-ar^2}\,\frac{\psi_2'}{\psi_2}-\frac{3}{r}\,\sqrt{1-ar^2}-\frac{\lambda_6}{r}\,\frac{\psi_3}{\psi_2}, \tag{11.7}$$

$$ik=-\sqrt{1-ar^2}\,\frac{\psi_3'}{\psi_3}-\frac{4}{r}\,\sqrt{1-ar^2}-\frac{\lambda_7}{r}\,\frac{\psi_4}{\psi_3}, \tag{11.8}$$

$$ik=-R\,\frac{\dot{T}}{T}-3\dot{R}, \tag{11.9}$$

where ik is the separation constant, k being assumed to be a real number as a consequence of the physical interpretation that will be given later on.

The time dependence can be obtained by integrating Eq. (11.9) to obtain

$$T(t)=T(0)\,\frac{R^3(0)}{R^3(t)}\,\exp\left[-ik\int_0^t\frac{dt'}{R(t')}\right]. \tag{12}$$

The result clearly depends on the assumed cosmological background.

IV. THE ANGULAR EQUATIONS

From the first-order angular equations (8) one derives 14 second-order equations: 8 of them are in only one of the functions S_0,S_1,S_2,S_3,S_4, 2 of them are in the pair S_0,S_2, 2 are in the pair S_1,S_3, and 2 are in the pair S_2,S_4. However, by taking into account the identities

$$L_2^-L_{-1}^+=L_0^+L_1^-+2, \tag{13.1}$$

$$L_1^-L_0^+=L_1^+L_0^-, \tag{13.2}$$

$$L_2^+L_{-1}^-=L_0^-L_1^++2, \tag{13.3}$$

and by assuming the separation constants satisfy the relations

$$\lambda_0\lambda_4=\lambda_1\lambda_5+2, \tag{14.1}$$

$$\lambda_1\lambda_5=\lambda_2\lambda_6, \tag{14.2}$$

$$\lambda_2\lambda_6=\lambda_3\lambda_7-2, \tag{14.3}$$

one is left with only five independent equations

$$L^+_{-1}L^-_2S_0=\lambda_0\lambda_4S_0, \tag{15.1}$$

$$L^-_2L^+_{-1}S_1=\lambda_0\lambda_4S_1, \tag{15.2}$$

$$L^-_1L^+_0S_2=(\lambda_0\lambda_4-2)S_2, \tag{15.3}$$

$$L^+_2L^-_{-1}S_3=\lambda_0\lambda_4S_3, \tag{15.4}$$

$$L^-_{-1}L^+_2S_4=\lambda_0\lambda_4S_4. \tag{15.5}$$

The remaining equations are automatically satisfied by the solutions of Eqs. (15). For what concerns Eqs. (15) we are looking for solutions that are regular in $\theta=0$ and $\theta=\pi$. Since Eqs. (15.4) and (15.5) can be obtained, respectively, from Eqs. (15.2) and (15.1) by the substitution $m\rightarrow -m$, we can reduce ourselves to the study of Eqs. (15.1)–(15.3). By setting

$$\lambda_0\lambda_4=-\lambda^2 \tag{16}$$

and by taking into account Eq. (13.2), one can check that the equations (15.3) and (15.2) coincide directly with two of the angular equations of the spin 1 case, once the substitution $\lambda^2+2\rightarrow\lambda^2$ is performed.[11] Therefore, the solutions of Eq. (15.3) are

$$S_1(\theta)=(1-\xi^2)^{|m|/2}P^m_{l_1}(\xi), \quad \xi=\cos\,\theta, \tag{17}$$

corresponding to $\lambda^2+2=l_1(l_1+1)$ with $l_1=|m|,|m|+1,|m|+2,\ldots$.

The solutions of Eq. (15.2), expressed in terms of the Jacobi polynomials[14] for $m\geqslant 1$, $m\leqslant -1$, $m=0$, respectively, are

$$S_1(\theta)=(1-\cos\,\theta)^{(m-1)/2}(1+\cos\,\theta)^{(m+1)/2}P^{(m+1,m-1)}_{l_1-m}(\cos\,\theta), \tag{18.1}$$

$$S_1(\theta)=(1+\cos\,\theta)^{(|m|-1)/2}(1-\cos\,\theta)^{(|m|+1)/2}P^{(|m|-1,|m|+1)}_{l_1-|m|}(\cos\,\theta), \tag{18.2}$$

$$S_1(\theta)=\sin\,\theta P^{(1,1)}_{l_1+2}(\cos\,\theta), \tag{18.3}$$

corresponding to $\lambda^2+2=l_1(l_1+1)$ in every case with $l_1=|m|,|m|+1,|m|+2,\ldots$, for $|m|\geqslant 1$ and $l_1=1,2,3,\ldots$, for $m=0$.

The solutions of Eq. (15.1) require some elaboration. By using the definition (9) and then by setting $\xi=\cos\,\theta$ it becomes

$$S_0''+\frac{2\xi}{\xi^2-1}S_0'+\frac{(\lambda^2+2)(1-\xi^2)-m^2-4-4m\xi}{(1-\xi^2)^2}S_0=0. \tag{19}$$

If now $m\geqslant 2$, by setting

$$S_0=(1-\xi)^{(m+2)/2}(1+\xi)^{(m-2)/2}f(\xi), \quad \xi=\cos\,\theta, \tag{20}$$

in (20) and then $\xi=2x-1$ in the resulting equation, one finds for f the equation

$$x(1-x)f''+[m-1-2x(m+1)]f'-[m(m+1)-(\lambda^2+2)]f=0, \tag{21}$$

whose acceptable solutions, in terms of the Jacobi polynomials, are

$$\begin{gathered} S_0(\theta)=(1-\xi)^{(m+2)/2}(1+\xi)^{(m-2)/2}P_{l_0-m}^{(m-2,m+2)}(\xi), \quad m\geqslant 2, \\ \lambda^2+2=l_0(l_0+1), \quad l_0=m,m+1,m+2,\ldots . \end{gathered} \tag{22.1}$$

The case $m\leqslant -2$ can be obtained from the case $m\geqslant 2$ by the substitution $\xi\to-\xi$, $m\to -m$, so that

$$\begin{gathered} S_0(\theta)=(1+\xi)^{(|m|+2)/2}(1-\xi)^{(|m|-2)/2}P_{l_0-|m|}^{(|m|+2,|m|-2)}(\xi), \quad m\leqslant -2, \\ \lambda^2+2=l_0(l_0+1), \quad l_0=|m|,|m|+1,|m|+2,\ldots . \end{gathered} \tag{22.2}$$

By a similar procedure we have for $m=1,-1,0$, respectively,

$$S_0(\theta)=(1-\xi)^{3/2}(1+\xi)^{1/2}P_{l_0-2}^{(1,3)}(\xi), \tag{22.3}$$

$$S_0(\theta)=(1+\xi)^{3/2}(1-\xi)^{1/2}P_{l_0-2}^{(3,1)}(\xi), \tag{22.4}$$

$$S_0(\theta)=(1-\xi)^{2}P_{l_0-2}^{(2,2)}(\xi), \quad \xi=\cos\,\theta, \tag{22.5}$$

all corresponding to $\lambda^2+2=l_0(l_0+1)$ with $l_0=2,3,4,\ldots$.

By comparing all the results of the angular equations one finds that the common eigenvalue have the form $\lambda^2+2=l(l+1)$ with $l=2,3,4,\ldots$.

V. THE RADIAL EQUATIONS

To simplify the study of the radial equations we introduce the operators

$$A_b=\sqrt{1-ar^2}\,\frac{d}{dr}+\frac{b}{r}\,\sqrt{1-ar^2}-ik, \quad k,b\in R. \tag{23}$$

They satisfy, among others, the identities

$$A_2 r A_3^{\star}=A_2^{\star} r A_3, \tag{24.1}$$

$$r A_3 r A_2^{\star}=r A_1^{\star} r A_4+2. \tag{24.2}$$

Accordingly, the radial equations (11) can be compactly written

$$r A_4\psi_1=\lambda_0\psi_0, \quad r A_1^{\star}\psi_0=-\lambda_4\psi_1, \tag{25.1}$$

$$r A_3\psi_2=\lambda_1\psi_1, \quad r A_2^{\star}\psi_1=-\lambda_5\psi_2, \tag{25.2}$$

$$r A_2\psi_3=\lambda_2\psi_2, \quad r A_3^{\star}\psi_2=-\lambda_6\psi_3, \tag{25.3}$$

$$r A_1^{\star}\psi_4=\lambda_3\psi_3, \quad r A_4^{\star}\psi_3=-\lambda_7\psi_4. \tag{25.4}$$

Also here one obtains 14 second-order equations for the radial functions ψ_h, $h=0,1,2,3,4$, that can be shown to be compatible by using the assumptions (14) and the identities (24). By this procedure one is left with the following five independent equations:

$$rA_4 rA_1^\star \psi_0 = \lambda^2 \psi_0, \tag{26.1}$$

$$rA_1^\star rA_4 \psi_1 = \lambda^2 \psi_1, \tag{26.2}$$

$$rA_2 rA_3^\star \psi_2 = (\lambda^2+2)\psi_2, \tag{26.3}$$

$$rA_1 rA_4^\star \psi_3 = \lambda^2 \psi_3, \tag{26.4}$$

$$rA_4^\star rA_1 \psi_4 = \lambda^2 \psi_4. \tag{26.5}$$

The solutions of these equations must satisfy also the condition

$$\psi_h(0)=0, \quad h=0,1,2,3,4, \tag{27}$$

as a consequence of the very structure of the radial equations. The number of equations to solve is reduced by remarking that if ψ_0 and ψ_1 satisfy Eqs. (26.1) and (26.2), then $\psi_0^\star$ and $\psi_1^\star$ satisfy Eqs. (26.5) and (26.4), respectively.

By using the definitions (23), Eqs. (26.1), (26.2), (26.3) become, respectively,

$$r(1-ar^2)\psi_0'' + (6-7ar^2)\psi_0' + \left[r(k^2-5a) + \frac{4-\lambda^2}{4} + 4ik\sqrt{1-ar^2} \right]\psi_0 = 0, \tag{28.1}$$

$$r(1-ar^2)\psi_1'' + (6-7ar^2)\psi_1' + \left[r(k^2-8a) + \frac{4-\lambda^2}{r} + 2ik\sqrt{1-ar^2} \right]\psi_1 = 0, \tag{28.2}$$

$$r(1-ar^2)\psi_2'' + (6-7ar^2)\psi_2' + \left[r(k^2-9a) + \frac{4-\lambda^2}{r} \right]\psi_2 = 0, \quad a=0,\pm 1. \tag{28.3}$$

Near $r=0$ the acceptable solutions of the Fuchs class equations (28) have the behavior

$$\psi_d(r) = r^{(\sqrt{4\lambda^2+9}-5)/2} f_d(r,k^2), \quad d=0,1,2, \tag{29}$$

f_d being a regular function in $r=0$. Therefore, as a consequence of (27), the eigenvalues of the angular equations are $\lambda^2+2=l(l+1)$ with now $l\geqslant 3$.

We are able to solve Eqs. (28) only in the flat universe case. By inserting

$$\psi_d(r) = r^{(\sqrt{4\lambda^2+9}-5)/2} e^{ikr} Z_d(r), \quad d=0,1,2, \tag{30}$$

in Eqs. (28) with $a=0$ and then by setting $\xi=-2ikr$, one finds for Z_d the confluent hypergeometric equation[14]

$$\xi Z_d'' + (1+\sqrt{4\lambda^2+9}-\xi)Z_d' - \tfrac{1}{2}[\sqrt{4\lambda^2+9}+5(1-d)]Z_d = 0, \tag{31}$$

whose solution $Z_d = \phi(\frac{1}{2}\sqrt{4\lambda^2+9} + \frac{5}{2}(1-d); 1+\sqrt{4\lambda^2+9}; r)$, $d=0,1,2$, corresponds to the acceptable ψ_d satisfying Eq. (27).

Finally we remark that as a consequence of Eq. (11) (λ_i and k being independent constants), we have also the constraints to be imposed to the wave functions

$$\psi_h(1)=0, \quad h=0,1,2,3,4. \tag{32}$$

Therefore $f_d(1,k^2)=0$ for $d=0,1,2$, and hence there is the possible existence of a discrete spectrum of values of k^2 that is common to the three cases. It is an open problem whether this is indeed possible and what are such values.

VI. GENERALIZATION TO ARBITRARY SPIN

We now show that the results of the previous sections relative to $s=2$ can be extended to hold for arbitrary spin $s>2$. By generalizing the procedure of Sec. II the general equation (1) can be developed to give

$$\partial_{AA'}\phi^{A}_{A_1A_2\cdots A_n}+\phi^{X}_{A_1A_2\cdots A_n}\Gamma^{A}_{AA'X}-\phi^{A}_{XA_2\cdots A_n}\Gamma^{X}_{AA'A_1}-\phi^{A}_{A_1\cdots XA_n}\Gamma^{X}_{AA'A_{n-1}}-\phi^{A}_{A_1\cdots A_{n-1}X}\Gamma^{X}_{AA'A_n}=0. \tag{33}$$

Let now the indexes $A_1A_2\cdots A_{n-1}$ be taken fixed, denote by ϕ_h the obvious generalization of Eq. (2), and let h be so chosen that $h=A_1+A_2+\cdots+A_{n-1}$.

Suppose $A_n=0$. Then the equation (33) contains in principle $\phi_h,\phi_{h+1},\phi_{h-1}$ [corresponding to the order $(n-1)$] plus four terms originating from

$$-\phi^{A}_{A_1\cdots A_{n-1}X}\Gamma_{AA'0}{}^{X}, \tag{34}$$

which are of the form $\phi_h\Gamma_{1A'0}{}^{0},\phi_{h+1}\Gamma_{0A'0}{}^{0},\phi_{h+1}\Gamma_{1A'0}{}^{1},\phi_{h+2}\Gamma_{0A'0}{}^{1}$.
However, $\Gamma_{0A'0}{}^{1}=0$ because it corresponds to the spin coefficients[2] κ and σ that are zero in our scheme [see Eq. (6)]. Therefore the term (34) introduces no new function with respect to the case $n-1$. Since ϕ_{h-1} is not present in the case $n=3$ [see Eqs. (3), where $\kappa=\lambda=\pi=\tau=\sigma=\nu=0$], by induction it is not present even in the equation (33) which therefore contains only ϕ_h,ϕ_{h+1}. Moreover one can check that the surviving terms originating from (34) are such that $\rho,\mu,\epsilon,D,\Delta$ are associated to one of the functions ϕ_h,ϕ_{h+1} while $\alpha,\beta,\delta,\delta^{\star}$ to the other.

Suppose now $A_n=1$. By the same argument of the case $A_n=0$ the term (34) add terms containing only ϕ_{h+1},ϕ_{h+2} to those relative to the order $(n-1)$ that are now $\phi_h,\phi_{h+1},\phi_{h+2}$. By induction, the term ϕ_h is not present because it is not present in the case $n=3$ [see again Eq. (3)]. Also here the association of the spin coefficients with the directional derivatives is the same of the case $A_n=0$.

By induction, the equations (33) have therefore the recursive structure of Eqs. (3), each equation containing only two functions.

The equations (33) are therefore not only separable, but, by applying by induction the procedure of the previous sections, they are such that the corresponding angular, radial, and time equations can be written down as the natural generalization of Eqs. (8) and (11).

The recursive structure of the equations resulting from (33) holds also to the cases $s=\frac{1}{2}$ and $s=1$ that have been previously studied.[10,11]

VII. CONCLUDING REMARKS

In the previous sections the constants λ^2 and k have been introduced by the separation procedure.

The constant λ^2 is directly connected, for $s=2$, to the eigenvalues of the angular equations [see (18) and (22)]. After the generalization of Sec. VI, the same interpretation holds for the other values of the spin.

In connection with the result (12) we interpret k^2 as the energy of the (massless) particles, even if the radial equations do not have the explicit form of a Schrödinger-like eigenvalue problem as it directly happens for $s=\frac{1}{2}$ (Ref. 10) and for the Dirac equation in the Kerr geometry.[12] The given interpretation can be extended to the arbitrary spin case because the time equation that generalizes Eq. (11.9) implies a solution with always the same exponential factor of Eq. (12).

According to this interpretation, the closed universe case implies discrete levels for the energy of the particle. The determination of the energy levels is in general difficult, the difficulty increasing with increasing spin because there are problems of mathematical compatibility already evident for $s=2$ as remarked in Sec. V. The simple case relative to $s=\frac{1}{2}$ has been studied and gives energy levels whose values are, however, very far from the present experimental sensitivity.[10]

Since also the (massive) Dirac equation shows the existence of discrete energy levels,[15] such a property seems to be a characteristic feature of the closed universe case of the standard cosmology.

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A quantum analog of the $\mathcal{Z}$ algebra

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We define a natural quantum analog for the $\mathcal{Z}$ algebra, and which we refer to as the $\mathcal{Z}_q$ algebra, by modding out the Heisenberg algebra from the quantum affine algebra $U_q(\widehat{sl(2)})$ with level k. We discuss the representation theory of this $\mathcal{Z}_q$ algebra. In particular, we exhibit its reduction to a group algebra, and to a tensor product of a group algebra with a quantum Clifford algebra when $k=1$, and $k=2$, and thus we recover the explicit constructions of $U_q(\widehat{sl(2)})$-standard modules as achieved by Frenkel–Jing and Bernard, respectively. Moreover, for arbitrary nonzero level k, we show that the explicit basis for the simplest $\mathcal{Z}$-generalized Verma module as constructed by Lepowsky and Primc is also a basis for its corresponding $\mathcal{Z}_q$-module, i.e., it is invariant under the q-deformation for generic q. We expect this $\mathcal{Z}_q$ algebra [associated with $U_q(\widehat{sl(2)})$ at level k] to play the role of a dynamical symmetry in the off-critical Z_k statistical models. © *1996 American Institute of Physics.* [S0022-2488(96)01506-X]

I. INTRODUCTION

One of the major recent developments in the field of integrable models has been the realization by the Kyoto school[1,2] of the important role played by non-Abelian and dynamical symmetries in the resolution of integrable systems. Prior to this and besides conformal field theory, the main approach in the analysis of integrable models has been based on Abelian symmetries together with the Bethe *ansatz*. However, this approach, despite its success of being more systematic in handling the spectra of most integrable systems, has its limitations as far as concrete computations of physical quantities are concerned such as form factors and correlation functions. The reason is that the latter quantities are based on scalar products of the eigenvectors of the Hamiltonians or transfer matrices of the systems; however, the eigenspaces in the physically interesting thermodynamic limit are infinite-dimensional, and hence it is not easy to define their structures, and much less the scalar products on them. However, since some non-Abelian infinite-dimensional algebras have well-defined scalar products on their infinite-dimensional modules, then if we succeed in establishing that the Hamiltonian or the transfer matrix of an integrable system commutes with one of these algebras, we automatically know not only its eigenspaces, which are the modules of this algebra, but also the scalar product on them. We might even describe the local operators and the creation and annihilation operators of the eigenvectors in terms of some operators related to this algebra, such as the intertwiners of its modules, and hence we might be able to compute exactly the form factors and correlation functions. In fact, this is precisely the program that has been behind the enormous success in the resolution of conformal field theories, and more recently in the resolution of the XXZ quantum spin chain model (which is equivalent to the six-vertex classical model) in the antiferromagnetic regime by the Kyoto school. We should, however, mention Ref. 3 where another approach to the calculation of correlation functions is developed.

It is then an interesting program to build as many infinite-dimensional algebras as possible, hoping that one of them turns out to be a non-Abelian or a dynamical symmetry of an integrable model, and vice versa. The main point of this paper is precisely to define a new infinite-dimensional algebra, which, as explained in the next paragraph, should be the dynamical symmetry of the off-critical Z_k models.

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It is known that the $\widehat{\mathrm{sl}(2)}$ affine Lie algebra is a dynamical symmetry in conformal field theory (the continuum critical limit of the XXX model)[4] and a non-Abelian symmetry of the antiferromagnetic (off-critical) XXX model.[2] Moreover, its deformation, the $\mathrm{U}_q(\widehat{\mathrm{sl}(2)})$ algebra, is also a non-Abelian symmetry of the antiferromagnetic (off critical) XXZ model. It is also known that the critical Z_k models, such as the Ising model ($k=2$) and the Potts model ($k=3$), have as a dynamical symmetry the parafermionic algebra,[5] which is ironically related to the $\mathcal{Z}$ algebra.[6] The latter algebra, in turn, is obtained from the quotient of the $\widehat{\mathrm{sl}(2)}$ algebra with level k by its Heisenberg subalgebra.

From all the above known results, it is therefore natural to consider a similar construction for a quantum analogue of the $\mathcal{Z}$ algebra, denoted by $\mathcal{Z}_q$, from the $\mathrm{U}_q(\widehat{\mathrm{sl}(2)})$ algebra, and to expect it to play the same role of a dynamical symmetry for the off-critical Z_k models. In fact, such a program is already and implicitly implemented in the simplest case of the off-critical Ising model ($k=2$), where the $\mathcal{Z}_q$ algebra (to be precise, the corresponding quantum parafermionic algebra) reduces simply to a quantum Clifford algebra.[7]

This paper is organized as follows: in Sec. II, we recall basic definitions about the $\mathrm{U}_q(\widehat{\mathrm{sl}(2)})$ quantum affine algebra, using the formal variable approach. In Sec. III, we gradually introduce the $\mathcal{Z}_q$ algebra by modding out the Heisenberg subalgebra from $\mathrm{U}_q(\widehat{\mathrm{sl}(2)})$ with level k. We derive two defining relations, called ''the quantum generalized commutation relations,'' for this algebra, as well as the relations between its elements and those of $\mathrm{U}_q(\widehat{\mathrm{sl}(2)})$. In Sec. IV, we discuss the reduction of $\mathcal{Z}_q$ in the simpler cases $k=1$ and $k=2$ to a group algebra $\mathbb{C}[Q]$, with Q being the root lattice of the sl(2) Lie algebra,[8] and to a tensor product of $\mathbb{C}[Q]$ with a quantum deformation of a Clifford algebra,[9] respectively. In Sec. V, we provide one of the main new results of this paper: an explicit construction of the basis of the simplest $\mathcal{Z}_q$ modules, and hence $\mathrm{U}_q(\widehat{\mathrm{sl}(2)})$ modules, for arbitrary nonzero level k. These are the so-called generalized Verma modules.[10,11] We show that the spanning vectors of the basis of a generalized Verma module, as constructed in the ''classical'' $\mathcal{Z}$ algebra case in Refs. 11 and 12, do still form a basis for a $\mathcal{Z}_q$-generalized Verma module. In Sec. VI, we give more quantum generalized commutation relations satisfied by polynomials of $\mathcal{Z}_q$ elements and discuss their potential applications. Finally, Sec. VII is devoted to our conclusions.

II. THE $\mathrm{U}_q(\widehat{\mathrm{sl}(2)})$ QUANTUM AFFINE ALGEBRA

The $\mathrm{U}_q(\widehat{\mathrm{sl}(2)})$ affine algebra is a unital associative algebra with elements $\{e_{\pm\alpha_i},\ k_i^{\pm},\ q^{\pm d};\ i=0,1\}$ and defining relations in the homogeneous gradation[13,14]

$$
\begin{gathered}
[k_i,\ k_j]=0, \quad k_i k_i^{-1}=k_i^{-1}k_i=1,\\
q^{-d}q^{d}=q^{d}q^{-d}=1,\\
q^{d}k_i q^{-d}=k_i, \quad q^{d}e_{\pm\alpha_i}q^{-d}=q^{\pm\delta_{i0}}e_{\pm\alpha_i},\\
k_i e_{\pm\alpha_j}k_i^{-1}=q^{\pm(\alpha_i,\alpha_j)}e_{\pm\alpha_j},\\
[e_{\alpha_i},\ e_{-\alpha_j}]=\delta_{ij}\,\frac{k_i-k_i^{-1}}{q-q^{-1}},\\
(e_{\pm\alpha_i})^3 e_{\pm\alpha_j}-[3](e_{\pm\alpha_i})^2 e_{\pm\alpha_j}e_{\pm\alpha_i}+[3]e_{\pm\alpha_i}e_{\pm\alpha_j}(e_{\pm\alpha_i})^2-e_{\pm\alpha_j}(e_{\pm\alpha_i})^3=0,
\end{gathered}
\tag{1}
$$

where $[x]=(q^x-q^{-x})/(q-q^{-1})$, $q=e^{t/2}$ is a complex number called a deformation parameter, and $\{\alpha_i, i=0,1\}$ is the set of positive simple roots of $\widehat{\mathrm{sl}(2)}$ affine Lie algebra with the invariant symmetric bilinear form $(\alpha_i,\alpha_j)=a_{i,j}$ (see Sec. IV). Here $a_{i,i}=2$ and $a_{i,1-i}=-2$, $i=0,1$ are the elements of the $\widehat{\mathrm{sl}(2)}$ affine Cartan matrix. Note that the special element $\gamma=k_0k_1$ is in the center of $\mathrm{U}_q(\widehat{\mathrm{sl}(2)})$ and acts as q^k on its highest weight representations, with k referred to as the level. We also refer to the above elements generating $\mathrm{U}_q(\widehat{\mathrm{sl}(2)})$ as the Chevalley generators.

The Chevalley generators are associated with the simple roots only. One would like to describe the commutation relations of all the elements associated with the infinite-dimensional set of roots $\{\pm\alpha+n\delta; n\in\mathbb{Z}\}\cup\{n\delta; n\in\mathbb{Z}\backslash 0\}\}$, with $\alpha=\alpha_1$ and $\delta=\alpha_0+\alpha_1$, and where the Serre relation [i.e., the last relation in (1)] becomes redundant. Drinfeld succeeded in finding such a set of generators, which we refer to as the Drinfeld generators.[15] This set is $\{x_u^{\pm}, \alpha_m, K^{\pm 1}, q^{\pm d}, \gamma^{\pm 1/2}; n\in\mathbb{Z}, m\in\mathbb{Z}^*=\mathbb{Z}\backslash 0\}\}$ with defining relations

$$\gamma^{1/2}\gamma^{-1/2}=\gamma^{-1/2}\gamma^{1/2}=1, \quad [\gamma^{\pm 1/2}, y]=0, \quad \forall y\in \mathrm{U}_q(\widehat{\mathrm{sl}(2)}), \tag{2}$$

$$KK^{-1}=K^{-1}K=1, \tag{3}$$

$$K_{\alpha_n}K^{-1}=\alpha_n, \tag{4}$$

$$Kx_n^{\pm}K^{-1}=q^{\pm 2}x_n^{\pm}, \tag{5}$$

$$q^dq^{-d}=q^{-d}q^d=1, \quad Kq^{\pm d}K^{-1}=q^{\pm d}, \tag{6}$$

$$q^dx_n^{\pm}q^{-d}=q^nx_n^{\pm}, \tag{7}$$

$$q^d\alpha_nq^{-d}=q^n\alpha_n, \tag{8}$$

$$[\alpha_n, \alpha_m]=\frac{(q^{2n}-q^{-2n})(\gamma^n-\gamma^{-n})}{nt^2}\,\delta_{n+m,0}, \tag{9}$$

$$[\alpha_n, x_m^{\pm}]=\pm\,\frac{\gamma^{\mp|n|/2}(q^{2n}-q^{-2n})}{nt}\,x_{n+m}^{\pm}, \tag{10}$$

$$[x_n^+, x_m^-]=\frac{\gamma^{(n-m)/2}\Psi_{n+m}-\gamma^{(m-n)/2}\Phi_{n+m}}{q-q^{-1}}, \tag{11}$$

$$x_{n+1}^{\pm}x_m^{\pm}-q^{\pm 2}x_m^{\pm}x_{n+1}^{\pm}=q^{\pm 2}x_n^{\pm}x_{m+1}^{\pm}-x_{m+1}^{\pm}x_n^{\pm}, \tag{12}$$

where Ψ_n and Φ_n are given by the mode expansions of the fields $\Psi(z)$ and $\Phi(z)$, which are themselves defined by

$$\begin{aligned}\Psi(z)&=\sum_{n\geqslant 0}\Psi_nz^{-n}=K\,\exp\left\{t\sum_{n>0}\alpha_nz^{-n}\right\},\\ \Phi(z)&=\sum_{n\leqslant 0}\Phi_nz^{-n}=K^{-1}\,\exp\left\{-t\sum_{n<0}\alpha_nz^{-n}\right\}.\end{aligned} \tag{13}$$

Here z is a formal variable and

$$K=\Psi_0=\Phi_0^{-1}\equiv q^{\alpha_0}, \tag{14}$$

where we mean identification by the symbol $\equiv$.

The isomorphism ρ between $U_q(\widehat{sl(2)})$ with the Chevalley generators and $U_q(\widehat{sl(2)})$ with the Drinfeld generators is given explicitly by

$$\begin{gathered}\rho: k_0 \to \gamma K^{-1}, \quad \rho: k_1 \to K, \\ \rho: e_{\pm\alpha_1} \to x_0^{\pm}, \quad \rho: e_{\alpha_0} \to x_1^{-} K^{-1}, \quad \rho: e_{-\alpha_0} \to K x_{-1}^{+}.\end{gathered} \tag{15}$$

For later purposes we will use the formal variable approach[16] (instead of the usual operator product expansion method) to reexpress the algebra as a quantum current algebra with elements $\{\Psi(z), \Phi(z), x^{\pm}(z), \gamma^{\pm 1/2}, q^{\pm d}\}$, where[8]

$$x^{\pm}(z) = \sum_{n \in \mathbb{Z}} x_n^{\pm} z^{-n}, \tag{16}$$

and with defining relations

$$\gamma^{1/2}\gamma^{-1/2} = \gamma^{-1/2}\gamma^{1/2} = 1, \quad [\gamma^{\pm 1/2}, y] = 0, \quad \forall y \in U_q(\widehat{sl(2)}), \tag{17}$$

$$[\Psi(z), \Psi(w)] = 0, \tag{18}$$

$$[\Phi(z), \Phi(w)] = 0, \tag{19}$$

$$\Psi(z)\Phi(w) = g(wz^{-1}\gamma) g(wz^{-1}\gamma^{-1})^{-1} \Phi(w)\Psi(z), \tag{20}$$

$$\Psi(z) x^{\epsilon}(w) = g(wz^{-1}\gamma^{-\epsilon/2})^{-\epsilon} x^{\epsilon}(w)\Psi(z), \tag{21}$$

$$\Phi(z) x^{\epsilon}(w) = g(zw^{-1}\gamma^{-\epsilon/2})^{\epsilon} x^{\epsilon}(w)\Phi(z), \tag{22}$$

$$[x^{\epsilon}(z), x^{-\epsilon}(w)] = \epsilon \frac{\delta(zw^{-1}\gamma^{-\epsilon})\Psi(w\gamma^{\epsilon/2}) - \delta(zw^{-1}\gamma^{\epsilon})\Phi(z\gamma^{\epsilon/2})}{q - q^{-1}}, \tag{23}$$

$$(z - wq^{2\epsilon}) x^{\epsilon}(z) x^{\epsilon}(w) = (zq^{2\epsilon} - w) x^{\epsilon}(w) x^{\epsilon}(z), \tag{24}$$

$$q^d x^{\epsilon}(z) = x^{\epsilon}(zq^{-1}) q^d, \tag{25}$$

$$q^d \Psi(z) = \Psi(zq^{-1}) q^d, \tag{26}$$

$$q^d \Phi(z) = \Phi(zq^{-1}) q^d. \tag{27}$$

Here $\epsilon = \pm 1$ and $g(z)$ is meant to be the following formal power series in z:

$$g(z) = \sum_{n \in \mathbb{Z}_+} c_n z^n, \tag{28}$$

where the coefficients c_n, $n \in \mathbb{Z}_+$ are determined from the Taylor expansion of the function

$$f(\xi) = \frac{q^2\xi - 1}{\xi - q^2} = \sum_{n \in \mathbb{Z}_+} c_n z^n \tag{29}$$

at $\xi = 0$.[8] In the above relations we have also introduced the δ-function $\delta(z)$ which is defined as the formal Laurent series

$$\delta(z)=\sum_{n\in\mathbb{Z}} z^n, \tag{30}$$

and which plays a key role in the formal calculus approach (see Ref. 16 for its properties).

The three relations (25), (26) and (27) translate the fact that $x_n^{\pm}$, Ψ_n, and Φ_n are homogeneous of the same degree n.

III. THE $\mathcal{Z}_q$ ALGEBRA

It is well known that the Heisenberg subalgebra of $\widehat{\mathrm{sl}(2)}$ plays a crucial role in the construction of vertex operators and highest weight representations. One would like to extend this role to the quantum case. Note that in the sequel, the unit element and $q^{\pm d}$ are meant to be in all the (sub)algebras defined below, so we will not consider them unless stated otherwise. Let $\mathrm{U}_q(\hat{h})$ be the quantum analog of the enveloping Heisenberg algebra, referred to as q-Heisenberg algebra. It is a subalgebra of $\mathrm{U}_q(\widehat{\mathrm{sl}(2)})$ generated by $\{\alpha_n,\ \gamma^{\pm 1/2},\ n\in\mathbb{Z}^*\}$ with relations

$$[\alpha_n,\ \gamma^{\pm 1/2}]=0,\quad \gamma^{1/2}\gamma^{-1/2}=\gamma^{-1/2}\gamma^{1/2}=1, \tag{31}$$

$$[\alpha_n,\ \alpha_m]=\delta_{n+m,0}\,\frac{(q^{2n}-q^{-2n})(\gamma^n-\gamma^{-n})}{2nt^2}. \tag{32}$$

Let $\mathrm{U}_q(\hat{h}^+)$ and $\mathrm{U}_q(\hat{h}^{-1})$ denote the commutative subalgebras of $\mathrm{U}_q(\hat{h})$ generated by $\{\alpha_n,\ \gamma^{\pm 1/2};\ n>0\}$ and $\{\alpha_n,\ n<0\}$, respectively. By the Poincaré–Birkhoff–Witt theorem for, $\mathrm{U}_q(\hat{h})$, we have

$$\mathrm{U}_q(\hat{h})=\mathrm{U}_q(\hat{h}^+)\mathrm{U}_q(\hat{h}^-), \tag{33}$$

and, consequently, the following induced $\hat{h}$-module,

$$I(q^k)=\mathrm{U}_q(\hat{h})\otimes_{\mathrm{U}_q(\hat{h}^+)}\mathbb{C}[q^k], \tag{34}$$

is irreducible (for $k\neq 0$ which is understood in the sequel) and isomorphic to $\mathrm{U}_q(\hat{h}^-)$ and hence to the symmetric algebra $\mathrm{S}(\hat{h}^-)$.[8] In this formula, $\mathbb{C}[q^k]$ denotes the field of complex numbers considered as the one-dimensional $\mathrm{U}_q(\hat{h}^+)$-module and on which γ acts as multiplication by q^k, and α_n, $n>0$ acts trivially. This means that $\mathrm{S}(\hat{h}^-)$ is a canonical $\mathrm{U}_q(\hat{h})$-module on which γ acts as multiplication by q^k, α_n $(n<0)$ acts as a creation (multiplication) operator, and α_n $(n>0)$ acts as an (derivation) annihilation operator satisfying the relation (32). The latter actions are given by

$$\gamma^{\pm 1}: x\to q^{\pm k}x,$$

$$\alpha_n: x\to \alpha_n x,\quad n<0,\quad \alpha_n: x\to[\alpha_n,\ x],\quad n>0, \tag{35}$$

where x is any element in $S(\hat{h}^-)$. Moreover, the action of $q^{\pm d}$ on $S(\hat{h}^-)$ is defined by

$$q^{\pm d}: x\to q^{\pm d}xq^{\mp d}. \tag{36}$$

The action of α_0 and hence the action of $\Psi_0 = q^{\alpha_0}$ (and Φ_0) on $S(\hat{h}^-)$ will be defined later.

Now we would like to show that the highest weight modules of the whole quantum affine algebra $\mathrm{U}_q(\widehat{\mathrm{sl}(2)})$ must be constructed as tensor products of the form $S(\hat{h}^-)\otimes W$. Here W are certain vector spaces to be defined later and which are trivial as $\mathrm{U}_q(\hat{h})$-module. *La raison d'être* of W stems from the fact that $S(\hat{h}^-)$ is only a $\mathrm{U}_q(\hat{h})$-module and in general cannot be upgraded to a $\mathrm{U}_q(\widehat{\mathrm{sl}(2)})$-module, which is especially true here since we are considering $\mathrm{U}_q(\widehat{\mathrm{sl}(2)})$ in the homogeneous gradation. Therefore, we have to ''correct'' $S(\hat{h}^-)$ by tensoring it with additional

new spaces which do not overlap with it, so that the resulting tensor product remains as a $U_q(\hat{h})$-module. Of course, this correction will be performed by considering a minimum number of extra spaces.

It is well known in the case of affine algebras that these constructions can be achieved by means of vertex operators. The most famous vertex construction of the quantum affine algebras is the Frenkel–Jing one, which is, however, valid only for the simply laced algebras and with the central element γ acting as q (i.e., $k=1$) on their highest weight modules.[8] In this case, which will be recovered explicitly later for $U_q(\widehat{sl(2)})$ when we set $k=1$ in our general construction, it turns out that W is identified with a group algebra associated with the weight lattice of the Lie algebra corresponding to the quantum affine algebra in question. If $k=2$, W is identified with a tensor product of a group algebra and an exterior (Clifford) algebra. Such a construction has been achieved in the case of $U_q(so(2n+1))$ with level 1 by Bernard.[9] For $k>2$ it was shown in Ref. 17 that one needs to introduce, besides the group algebra, a certain quantum parafermionic algebra (though the representation theory was not discussed there).

Although we are concerned with $U_q(\widehat{sl(2)})$ for $k>1$, the form of the vertex operators used by Frenkel and Jing for $k=1$ led us to introduce the following vertex operators:

$$S_{\epsilon}^{\pm}(z)=\exp\left\{\pm\epsilon t\sum_{n>0}\frac{\alpha_{\pm n}}{q^{nk}-q^{-nk}}\,q^{-\epsilon nk/2}z^{\mp n}\right\},\quad \epsilon=\pm, \tag{37}$$

which are viewed as formal Laurent series in z with coefficients acting on $S(\hat{h}^{-})$. Using (32) and the usual formal rule

$$e^A e^B=e^B e^A e^{[A,B]}\quad \text{if } [A,[A,B]]=[B,[A,B]]=0, \tag{38}$$

for some operators A and B, we find

$$\begin{aligned} S_{\epsilon}^{+}(z)S_{\epsilon'}^{-}(w)&=\frac{(q^{k-2-(\epsilon+\epsilon')k/2}wz^{-1};q^{2k})_{\infty}^{\epsilon\epsilon'}}{(q^{k+2-(\epsilon+\epsilon')k/2}wz^{-1};q^{2k})_{\infty}^{\epsilon\epsilon'}}\,S_{\epsilon'}^{-}(w)S_{\epsilon}^{+}(z),\\ S_{\epsilon}^{\pm}(z)S_{\epsilon'}^{\pm}(w)&=S_{\epsilon'}^{\pm}(w)S_{\epsilon}^{\pm}(z), \end{aligned} \tag{39}$$

where as usual $(x;y)_{\infty}$ means

$$(x;y)_{\infty}=\prod_{n=0}^{\infty}(1-xy^n). \tag{40}$$

Each factor $(1-\omega z^{-1}q^{x})^{-1}$ in (39) is understood as the formal power series $\Sigma_{n\geqslant 0}w^n z^{-n}q^{xn}$. Moreover, using (32) and the formal rule

$$[A,e^B]=[A,B]e^B,\quad \text{if } [B,[A,B]]=0, \tag{41}$$

for some operators A and B, we obtain

$$\begin{aligned} &[\alpha_n,S_{\epsilon}^{+}(z)]=0,\quad [\alpha_{-n}S_{\epsilon}^{+}(z)]=-\frac{\epsilon q^{-\epsilon nk/2}z^{-n}(q^{2n}-q^{-2n})}{nt}\,S_{\epsilon}^{+}(z),\\ &[\alpha_{-n},S_{\epsilon}^{-}(z)]=0,\quad [\alpha_n,S_{\epsilon}^{-}(z)]=-\frac{eq^{-\epsilon nk/2}z^{n}(q^{2n}-q^{-2n})}{nt}\,S_{\epsilon}^{-}(z), \end{aligned} \tag{42}$$

where $n>0$ and $\epsilon=\pm$. For future purposes let us note here that one can easily show that the commutation relations (21) and (22) are equivalent to

$$[\alpha_n, x^{\epsilon}(z)]=\frac{\epsilon q^{-\epsilon|n|k/2} z^n (q^{2n}-q^{-2n})}{nt}\, x^{\epsilon}(z), \quad \epsilon=\pm; \quad n\in\mathbb{Z}\backslash\{0\}. \tag{43}$$

Let us now define the main new objects of this paper, which we refer to as the ''$\mathcal{Z}_q$ operators $\mathcal{Z}_n^{\epsilon}$,'' as the Laurent modes in

$$\mathcal{Z}^{\epsilon}(z)=\sum_{n\in\mathbb{Z}} \mathcal{Z}_n^{\epsilon} z^{-n}, \tag{44}$$

where

$$\mathcal{Z}^{\epsilon}(z)=S_{\epsilon}^{-}(z)x^{\epsilon}(z)S_{\epsilon}^{+}(z). \tag{45}$$

These operators $\mathcal{Z}_n^{\epsilon}$ are the quantum analogs of the (classical, $q=1$) $\mathcal{Z}$ operators that have been extensively studied in the literature (see, for example, Ref. 12). By abuse of terminology, we refer also to the ''currents $\mathcal{Z}^{\epsilon}(z)$'' as $\mathcal{Z}_q$ operators, but strictly speaking they are the generating functions of the latter operators. Let us denote by $\mathcal{Z}_q$ the algebra generated by $\{\Psi_0,\Phi_0,\mathcal{Z}_n^{\epsilon};n\in\mathbb{Z}\}$. The defining relations of this algebra, which we refer to as ''the quantum generalized commutation relations,'' will be given shortly below.

The space W on which this algebra acts nontrivially is the necessary space to be tensored with $S(\hat{h}^-)$ such that $S(\hat{h}^-)\otimes W$ is a $U_q(\widehat{\mathrm{sl}(2)})$-module. Therefore W will be defined if we know all the properties of the $\mathcal{Z}_q$ operators, that is, their relations with $U_q(\widehat{\mathrm{sl}(2)})$ itself and their algebra.

By definition, the relation between $\mathcal{Z}_q$ operators is given through their generating functions by (45). Next, it can easily be checked that the relations (42) and (43) imply that they commute with the quantum Heisenberg algebra $U_q(\hat{h})$, i.e.,

$$[\alpha_n,\ \mathcal{Z}^{\epsilon}(z)]=0, \quad n\in\mathbb{Z}\backslash\{0\}, \quad [\gamma^{\pm 1/2},\mathcal{Z}^{\epsilon}(z)]=0, \quad \epsilon=\pm. \tag{46}$$

This is a very important result, which is, in fact, the main motivation behind the particular choice for the forms of $S_{\epsilon'}^{\epsilon}(z)$ as given by (37). This is because the symmetric algebra $S(\hat{h}^-)$ realizes already the quantum Heisenberg subalgebra $U_q(\hat{h})$ and since the $\mathcal{Z}_q$ operators commute with $U_q(\hat{h})$, we can define then the actions of $U(\hat{h})$ and $\mathcal{Z}_q$ as follows on $S(\hat{h}^-)\otimes W$:

$$x: u\otimes v\to xu\otimes v, \quad y: u\otimes v\to u\otimes yv, \tag{47}$$

where $x\in U_q(\hat{h})$, $y\in\mathcal{Z}_q$, $u\in S(\hat{h}^-)$, and $v\in W$. From the Laurent expansion in zw^{-1} of both sides of (21) and (22), we obtain the relation

$$\Psi_0 x^{\epsilon}(w)=q^{2\epsilon}x^{\epsilon}(w)\Psi_0, \tag{48}$$

which, because of (5), amounts to

$$\Psi_0\mathcal{Z}^{\epsilon}(w)=q^{2\epsilon}\mathcal{Z}^{\epsilon}(w)\Psi_0. \tag{49}$$

Combining this relation with (46) and

$$\begin{aligned}\Psi(z)&=\Psi_0 S_{\epsilon}^{+}(zq^{-3\epsilon k/2})S_{-\epsilon}^{+}(zq^{3\epsilon k/2}),\\ \Phi(z)&=\Phi_0 S_{\epsilon}^{-}(zq^{3\epsilon k/2})S_{-\epsilon}^{-}(zq^{-3\epsilon k/2}), \quad \epsilon=\pm,\end{aligned} \tag{50}$$

we arrive finally at

$$\begin{aligned}\Psi_n \mathscr{Z}^{\epsilon}(w) &= q^{2\epsilon}\mathscr{Z}^{\epsilon}(w)\Psi_n, \quad n\geqslant 0,\\ \Phi_n \mathscr{Z}^{\epsilon}(w) &= q^{-2\epsilon}\mathscr{Z}^{\epsilon}(w)\Phi_n, \quad n\leqslant 0.\end{aligned} \tag{51}$$

In the sequel, however, we will only consider the relations (46) and (49) but not (51) since the latter is an immediate consequence of the former and (50).

Clearly, the action of the generating functions $x^{\epsilon}(z)$ on $S(\hat{h}^-)\otimes W\otimes\mathbb{C}[z, z^{-1}]$ decomposes then as

$$x^{\epsilon}(z)=S^-_{-\epsilon}(zq^{-\epsilon k})S^+_{-\epsilon}(zq^{\epsilon k})\otimes\mathscr{Z}^{\epsilon}(z), \quad \epsilon=\pm, \tag{52}$$

where we have used

$$(S^{\pm}_{\epsilon}(z))^{-1}=S^{\pm}_{-}(zq^{\pm\epsilon k}), \quad \epsilon=\pm, \tag{53}$$

and (42) to express $x_{\epsilon}(z)$ in terms of $\mathscr{Z}^{\epsilon}(z)$. We now define the actions of $q^{\pm d}$ and $\gamma^{\pm 1}$ on $S(\hat{h}^-)\otimes W$ as

$$q^{\pm d}: u\otimes v\to q^{\pm d}u\otimes q^{\pm d}v, \quad \gamma^{\pm 1}: u\otimes v\to q^{\pm k}u\otimes v, \tag{54}$$

where $u\in S(\hat{h}^-)$ and $v\in W$. The relation between $\mathscr{Z}^{\epsilon}(z)$ and $q^{\pm d}$, which reads as

$$q^d\mathscr{Z}^{\epsilon}(z)=\mathscr{Z}^{\epsilon}(zq^{-1})q^d, \tag{55}$$

can easily be derived from (25) and

$$q^d S^{\epsilon}_{\epsilon'}(z)=S^{\epsilon}_{\epsilon'}(zq^{-1})q^d, \tag{56}$$

which, in turn, can be obtained from (38). Relation (55) means that the $\mathscr{Z}_q$ algebra is graded [it inherits the gradation of $\mathrm{U}_q(\widehat{\mathrm{sl}(2)})$] and that the $\mathscr{Z}_q$ operators $\mathscr{Z}^{\epsilon}_n$ are homogeneous of degree n.

Let us now turn to the derivation of the defining relations [besides (14) and (49)] of the $\mathscr{Z}_q$ algebra, that is, the quantum generalized commutation relations. They simply follow from the substitution of $x^{\epsilon}(z)$ as given by (52) in (23) and (24). We find

$$\begin{aligned}&\frac{(q^{k+2}wz^{-1};q^{2k})_{\infty}}{(q^{k-2}wz^{-1};q^{2k})_{\infty}}\,\mathscr{Z}^{\epsilon}(z)\mathscr{Z}(-\epsilon|w)-\frac{(q^{k+2}zw^{-1};q^{2k})_{\infty}}{(q^{k-2}zw^{-1};q^{2k})_{\infty}}\,\mathscr{Z}^{-\epsilon}(w)\mathscr{Z}^{\epsilon}(z)\\ &\quad=\frac{\epsilon}{q-q^{-1}}\,(\Psi_0\delta(zw^{-1}q^{-\epsilon k})-\Phi_0\delta(zw^{-1}q^{\epsilon k}))\\ &\quad=\frac{1}{q-q^{-1}}\,(q^{\epsilon\alpha_0}\delta(zw^{-1}q^{-k})-q^{-\epsilon\alpha_0}\delta(zw^{-1}q^{k})),\end{aligned} \tag{57}$$

$$\begin{aligned}&(z-q^{2\epsilon}w)\,\frac{(q^{k-2-k\epsilon}wz^{-1};q^{2k})_{\infty}}{(q^{k+2-k\epsilon}wz^{-1};q^{2k})_{\infty}}\,\mathscr{Z}^{\epsilon}(z)\mathscr{Z}^{\epsilon}(w)\\ &\quad=(q^{2\epsilon}z-w)\,\frac{(q^{k-2-k\epsilon}zw^{-1};q^{2k})_{\infty}}{(q^{k+2-k\epsilon}zw^{-1};q^{2k})_{\infty}}\,\mathscr{Z}^{\epsilon}(w)\mathscr{Z}^{\epsilon}(z).\end{aligned} \tag{58}$$

In summary, in addition to the latter quantum generalized commutation relations, the $\mathscr{Z}_q$ fields $\mathscr{Z}^{\epsilon}(z)$ must satisfy the following relations with the elements of $\mathrm{U}_q(\widehat{\mathrm{sl}(2)})$ when they act on the W part of the tensor product $S(\hat{h}^-)\otimes W$:

$$[\alpha_n, \mathscr{Z}^{\epsilon}(z)]=0, \quad n\in\mathbb{Z}\backslash\{0\}, \tag{59}$$

$$\Psi_0\mathscr{Z}^{\epsilon}(z)=q^{2\epsilon}\mathscr{Z}^{\epsilon}(z)\Psi_0, \tag{60}$$

$$x^{\epsilon}(z)=S^{-}_{-\epsilon}(zq^{-\epsilon k})S^{+}_{-\epsilon}(zq^{\epsilon k})\otimes\mathscr{Z}^{\epsilon}(z), \tag{61}$$

$$q^d\mathscr{Z}^{\epsilon}(z)=\mathscr{Z}^{\epsilon}(zq^{-1})q^d, \tag{62}$$

$$[\gamma^{\pm},\mathscr{Z}^{\epsilon}(z)]=0. \tag{63}$$

All these relations will be useful in the explicit construction of the space W from the operators $\mathscr{Z}^{\epsilon}_n$. This is illustrated in Sec. IV.

IV. EXPLICIT CONSTRUCTIONS OF SOME $U_q(\widehat{sl(2)})$-STANDARD MODULES

Let us briefly recall the definition of some $U_q(\widehat{sl(2)})$-modules.[2,11,18] For this, we still need some notions from $\widehat{sl(2)}$ affine algebra, which is generated by $\{e_i,f_i,h_i,d;i=0,1\}$. We define on its Cartan subalgebra $\hat{h}=\mathbb{C}h_0+\mathbb{C}h_1+\mathbb{C}d$ an invariant symmetric bilinear form $(\ ,\ )$ by

$$(h_i,h_i)=2, \quad (h_i,h_{1-i})=-2, \quad (h_i,d)=\delta_{i,0}, \quad (d,d)=0, \quad i=0,1. \tag{64}$$

Let $\hat{h}^*=\mathbb{C}\Lambda_0+\mathbb{C}\Lambda_1+\mathbb{C}\delta=\mathbb{C}\alpha_0+\mathbb{C}\alpha_1+\mathbb{C}\Lambda_0$ be the dual space to h with

$$\langle\Lambda_i,h_j\rangle=\delta_{i,j}, \quad \langle\delta,d\rangle=1, \quad \langle\Lambda_i,d\rangle=0, \quad \langle\delta,h_i\rangle=0, \tag{65}$$

where

$$\langle\ ,\ \rangle:\hat{h}^*\otimes\hat{h}\to\mathbb{C} \tag{66}$$

is the natural pairing, the vectors Λ_i are the fundamental weights, α_i are the positive roots, and $\delta=\alpha_0+\alpha_1$ is the null root. One can induce a symmetric bilinear form $(\ ,\ )$ on $\hat{h}^*$ by

$$\begin{aligned}&(\Lambda_i,\Lambda_j)=\tfrac{1}{2}\delta_{i,1}\delta_{j,1}, \quad (\Lambda_i,\delta)=1, \quad (\delta,\delta)=0, \quad (\alpha_i,\alpha_i)=2,\\ &(\alpha_i,\alpha_{1-i})=2, \quad (\alpha_i,\Lambda_0)=\delta_{i,0}, \quad (\Lambda_0,\Lambda_0)=0, \quad i,j=0,1.\end{aligned} \tag{67}$$

The weights $\lambda\in\hat{h}^*$ such that

$$\lambda=n_0\Lambda_0+n_1\Lambda_1, \quad n_0,n_1\in\mathbb{N}\backslash\{0\}, \tag{68}$$

are called regular dominant integral weights, and $n_0+n_1=k$ is the level that we have introduced previously.

As defined in Sec. II the algebra $U_q(\widehat{sl(2)})$ is generated by $\{e_i, f_i, K^{\pm1}, \gamma^{\pm1}, q^{\pm d}, i=0,1\}$. Let V be a $U_q(\widehat{sl(2)})$-module and $\mu\in\hat{h}$, the subspace $V_\mu\subset V$ defined by

$$V_\mu=\{v\in V/K^{\pm1}v=q^{\pm\langle\mu,h_1\rangle}v, \quad \gamma^{\pm1}v=q^{\pm k}v, \quad q^{\pm d}v=q^{\pm\langle\mu,d\rangle}v\}, \tag{69}$$

is called a μ-weight space, and any $v\in V_\mu$ is referred to as a μ-weight vector. The module V becomes a weight module if it is the direct sum of its weight spaces. A $U_q(\widehat{sl(2)})$ highest weight vector v_λ in V is a λ-weight vector which satisfies the additional condition

$$e_iv_\lambda=0, \quad i=0,1. \tag{70}$$

The space V is called a $U_q(\widehat{sl(2)})$ highest weight module if it generated from a λ highest weight vector v_λ. In this case, v_λ is unique (up to a multiplication by a scalar), and hence we label V by the weight λ as $V(\lambda)$. The $U_q(\widehat{sl(2)})$-module $V(\lambda)$ is called standard if it is generated from a highest weight vector v_λ with a dominant integral weight λ and such that

$$f_i^{\langle \lambda, h_i\rangle+1} v_\lambda = 0, \quad i=0,1, \tag{71}$$

in which case it is irreducible.

Let us now address the explicit constructions of the standard modules in the cases $k=1$ and $k=2$. As explained previously, we should address only the explicit constructions of the space W in terms of the $\mathcal{Z}_q$ operators since the $S(\hat{h}^-)$ part is already constructed in terms of polynomials of α_n. Consequently, in the sequel we will mainly concentrate on the W part of the $U_q(\widehat{sl(2)})$-modules.

Case I: $k=1$.[8] In this case, the relations (58)–(63) satisfied by the $\mathcal{Z}_q$ operators $\mathcal{Z}^\epsilon(z)$ simplify significantly and reduce to the following relations:

$$\begin{aligned}
&\frac{\mathcal{Z}^\epsilon(z)\mathcal{Z}^{-\epsilon}(w)}{(1-q^{-1}wz^{-1})(1-qwz^{-1})} - \frac{\mathcal{Z}^{-\epsilon}(w)\mathcal{Z}^\epsilon(z)}{(1-q^{-1}zw^{-1})(1-qzw^{-1})} \\
&\quad = \frac{\epsilon}{q-q^{-1}}\left(\Psi_0 \delta(zw^{-1}q^{-\epsilon}) - \Phi_0 \delta(zw^{-1}q^{\epsilon})\right) \\
&\quad = \frac{1}{q-q^{-1}}\left(q^{\epsilon\alpha(0)}\delta(zw^{-1}q^{-1}) - q^{-\epsilon\alpha(0)}\delta(zw^{-1}q)\right),
\end{aligned} \tag{72}$$

$$w^2 \mathcal{Z}^\epsilon(z)\mathcal{Z}^\epsilon(w) = z^2 \mathcal{Z}^\epsilon(w)\mathcal{Z}^\epsilon(z), \tag{73}$$

$$[\alpha_n,\ \mathcal{Z}^\epsilon(z)] = 0, \quad n \in \mathbb{Z}\backslash\{0\}, \tag{74}$$

$$\Psi_0 \mathcal{Z}^\epsilon(z) = q^{2\epsilon}\mathcal{Z}^\epsilon(z)\Psi_0, \tag{75}$$

$$\Phi_0 \mathcal{Z}^\epsilon(z) = q^{-2\epsilon}\mathcal{Z}^\epsilon(z)\Phi_0, \tag{76}$$

$$x^\epsilon(z) = S^-_{-\epsilon}(zq^{-\epsilon k})S^+_{-\epsilon}(zq^{\epsilon k}) \otimes \mathcal{Z}^\epsilon(z), \tag{77}$$

$$q^d \mathcal{Z}^\epsilon(z) = \mathcal{Z}^\epsilon(zq^{-1})q^d, \tag{78}$$

$$[\gamma^\pm,\ \mathcal{Z}^\epsilon(z)] = 0. \tag{79}$$

It can easily be checked that these equations are solved by

$$\mathcal{Z}^\epsilon(z) = e^{\epsilon\alpha} z^{\epsilon\alpha_0 + (1/2)(\alpha,\alpha)} = e^{\epsilon\alpha} z^{\epsilon\alpha_0 + 1}, \quad \epsilon = \pm, \tag{80}$$

where α is the sl(2) positive simple root and $e^\alpha \in \mathbb{C}[P]$. Here $P = Q \cup (Q + \alpha/2)$ and Q are the sl(2) weight and root lattices, while $\mathbb{C}[P]$ and $\mathbb{C}[Q]$ are the corresponding Abelian group algebras, respectively. The elements z^{α_0} and q^d act on $\mathbb{C}[P]$ as

$$z^{\alpha_0} e^\beta = z^{(\alpha,\beta)} e^\beta z^{\alpha_0}, \quad q^d e^\beta = e^\beta q^d q^{-\beta_0 - (\beta,\beta)/2}, \quad \beta \in P. \tag{81}$$

As a conclusion, $x^\epsilon(z)$ acts on $S(\hat{h}^-)\otimes\mathbb{C}[P]$ as $S^-_{-\epsilon}(zq^{-\epsilon})S^+_{-\epsilon}(zq^{\epsilon}) \otimes e^{\epsilon\alpha} z^{\epsilon\alpha_0+1}$ and is single valued. Moreover, the subspaces $S(\hat{h}^-)\otimes\mathbb{C}[Q]$ and $S(\hat{h}^-)\otimes e^{\alpha/2}\mathbb{C}[Q]$, whose direct sum is

$S(\hat{h}^-)\otimes\mathbb{C}[P]$, are invariant and irreducible. They are, in fact, isomorphic to the standard (basic) modules $V(\Lambda_0)$ and $V(\Lambda_1)$ with highest weight vectors realized as $1\otimes 1$ and $1\otimes e^{\alpha/2}$, respectively.

Case II: $k=2$.[9] In this case, the relations (58)–(63) satisfied by the $\mathcal{Z}_q$ operators reduce to

$$\frac{\mathcal{Z}^{\epsilon}(z)\mathcal{Z}^{-\epsilon}(w)}{1-wz^{-1}}-\frac{\mathcal{Z}^{-\epsilon}(w)\mathcal{Z}^{\epsilon}(z)}{1-zw^{-1}}=\frac{\epsilon}{q-q^{-1}}\left(\Psi_0\delta(zw^{-1}q^{-2\epsilon})-\Phi_0\delta(zw^{-1}q^{2\epsilon})\right)$$

$$=\frac{1}{q-q^{-1}}\left(q^{\epsilon\alpha_0}\delta(zw^{-1}q^{-2})-q^{-\epsilon\alpha_0}\delta(zw^{-1}q^{2})\right), \quad (82)$$

$$(z-wq^{2\epsilon})(1-wz^{-1}q^{-2\epsilon})\mathcal{Z}^{\epsilon}(z)\mathcal{Z}^{\epsilon}(w)=(zq^{2\epsilon}-w)(1-zw^{-1}q^{-2\epsilon})\mathcal{Z}^{\epsilon}(w)\mathcal{Z}^{\epsilon}(z), \quad (83)$$

$$[\alpha_n,\ \mathcal{Z}^{\epsilon}(z)]=0, \quad n\in\mathbb{Z}\backslash\{0\}, \quad (84)$$

$$\Psi_0\mathcal{Z}^{\epsilon}(z)=q^{2\epsilon}\mathcal{Z}^{\epsilon}(z)\Psi_0, \quad (85)$$

$$\Phi_0\mathcal{Z}^{\epsilon}(z)=q^{-2\epsilon}\mathcal{Z}^{\epsilon}(z)\Phi_0, \quad (86)$$

$$x_{\epsilon}(z)=S^{-}_{-\epsilon}(zq^{-2\epsilon})S^{+}_{-\epsilon}(zq^{2\epsilon})\otimes\mathcal{Z}^{\epsilon}(z), \quad (87)$$

$$q^d\mathcal{Z}^{\epsilon}(z)=\mathcal{Z}^{\epsilon}(zq^{-1})q^d, \quad (88)$$

$$[\gamma^{\pm},\ \mathcal{Z}^{\epsilon}(z)]=0. \quad (89)$$

Let the operator z^{α_0} act on $\mathbb{C}[P]$ and $\mathbb{C}[Q]$ as in the case $k=1$ and q^d act as

$$q^d e^{\beta}=e^{\beta}q^d q^{-\beta_0/2-(\beta,\beta)/4}, \quad \beta\in P. \quad (90)$$

The above equations are then satisfied by

$$\mathcal{Z}^{\epsilon}(z)=e^{\epsilon\alpha}z^{\epsilon\alpha_0/2+(1/4)(\alpha,\alpha)}\psi(z)=e^{\epsilon\alpha}z^{\epsilon\alpha_0/2+1/2}\psi(z), \quad \epsilon=\pm, \quad (91)$$

where

$$\{\psi(z),\psi(w)\}=\delta(zw^{-1}q^{-2})+\delta(zw^{-1}q^{2}),$$

$$\text{if } z^{\alpha_0/2}\in\mathrm{End}(e^{\alpha/2}\mathbb{C}[Q]\otimes\mathbb{C}[z,\ z^{-1}]), \quad (92)$$

$$\{\psi(z),\psi(w)\}=(zw^{-1})^{1/2}(q^{-1}\delta(zw^{-1}q^{-2})+q\,\delta(zw^{-1}q^{2})),$$

$$\text{if } z^{\alpha_0/2}\in\mathrm{End}(\mathbb{C}[Q])\otimes\mathbb{C}[z,\ z^{-1}]. \quad (93)$$

Relation (92) means that the fermion field $\psi(z)$ has the Laurent expansion

$$\psi(z)=\sum_{n\in\mathbb{Z}}\psi_n z^{-n}. \quad (94)$$

Substituting this expansion back in (92) and comparing the coefficients of powers of zw^{-1}, we obtain the following anticommutation relations for the modes ψ_n:

$$\{\psi_n,\psi_m\}=(q^{2n}+q^{-2n})\,\delta_{n+m,0}, \quad \text{if } z^{\alpha_0/2}\in\mathrm{End}(e^{\alpha/2}\mathbb{C}[Q]\otimes\mathbb{C}[z,\ z^{-1}]). \quad (95)$$

This is the usual Rammond (R) sector for the modes ψ_n, $n\in\mathbb{Z}$. Similarly (93) enforces the following expansion:

$$\psi(z)=\sum_{r\in\mathbb{Z}+1/2}\psi_r z^{-r}. \tag{96}$$

As in the (R) sector, relation (93) leads to the following anticommutation relations for the modes ψ_n:

$$\{\psi_r,\psi_s\}=(q^{2r}+q^{-2r})\,\delta_{r+s,0},\quad \text{if } z^{\alpha_0/2}\in \mathrm{End}(\mathbb{C}[Q]\otimes\mathbb{C}[z,z^{-1}]). \tag{97}$$

This is the familiar Neuveu–Schwarz (NS) sector for the modes ψ_r. The Clifford algebra with the anticommutation relations (95) and (97) first appeared in the work of Bernard on the explicit construction of $U_q(so(2n+1))$-standard modules with level $k=1$.[9] Then, it was used in Refs. 18 and 19 for the calculation of the N-point correlation functions for the spin-1 XXZ model.

Let $T^{\mathrm{R}}(T^{\mathrm{NS}})$, $T^{\mathrm{R}}_{\mathrm{even}}(T^{\mathrm{NS}}_{\mathrm{even}})$, $T^{\mathrm{R}}_{\mathrm{odd}}(T^{\mathrm{NS}}_{\mathrm{odd}})$ be the Fock space spanned by the modes $\{\psi_n, n<0\}$ ($\{\psi_r, r<0\}$), a subspace of $T^{\mathrm{R}}(T^{\mathrm{NS}})$ spanned by an even number of modes $\psi_n(\psi_r)$, and a subspace of $T^{\mathrm{R}}(T^{\mathrm{NS}})$ spanned by an odd number of modes $\psi_n(\psi_r)$, respectively. Note that in the (R) sector the zero mode ψ_0 acts trivially on T^{R}, and so to make its action nontrivial we extend the Fock space T^{R} by $\mathbb{C}^2$, with basis $\{v_+=\binom{1}{0}, v_-=\binom{0}{1}\}$ such that $\psi_n(n\neq 0)$ and ψ_0 act as $\psi_n\otimes 1$ and $1\otimes\left(\begin{smallmatrix}0&1\\1&0\end{smallmatrix}\right)$ on $T^{\mathrm{R}}\otimes\mathbb{C}^2$, respectively. Putting all the pieces together, we conclude that $x^{\epsilon}(z)$ acts as

$$x^{\epsilon}(z)=S^{-}_{-\epsilon}(zq^{-2\epsilon})S^{+}_{-\epsilon}(zq^{2\epsilon})\otimes\psi(z)\otimes e^{\epsilon\alpha}z^{\epsilon\alpha_0/2+1/2} \tag{98}$$

on the space $S(\hat{h}^-)\otimes(T^{\mathrm{R}}\otimes\mathbb{C}^2)\otimes e^{\alpha/2}\mathbb{C}[Q]$ in the (R) sector, and on the space $S(\hat{h}^-)\otimes(T^{\mathrm{NS}})\otimes\mathbb{C}[Q]$ in the (NS) sector. Moreover, the $U_q(\widehat{sl(2)})$-standard modules $V(2\Lambda_0)$, $V(2\Lambda_1)$, and $V(\Lambda_0+\Lambda_1)$ are isomorphic to the following subspaces of the latter spaces

$$\begin{aligned}
V(2\Lambda_0)&\sim S(\hat{h}^-)\otimes T^{\mathrm{NS}}_{\mathrm{even}}\otimes\mathbb{C}[2Q]\oplus S(\hat{h}^-)\otimes T^{\mathrm{NS}}_{\mathrm{odd}}\otimes e^{\alpha}\mathbb{C}[2Q],\\
V(2\Lambda_1)&\sim S(\hat{h}^-)\otimes T^{\mathrm{NS}}_{\mathrm{even}}\otimes e^{\alpha}\mathbb{C}[2Q]\oplus S(\hat{h}^-)\otimes T^{\mathrm{NS}}_{\mathrm{odd}}\otimes\mathbb{C}[2Q],\\
V(\Lambda_0+\Lambda_1)&\sim S(\hat{h}^-)\otimes(T^{\mathrm{R}}_{\mathrm{even}}\otimes v_+\oplus T^{\mathrm{R}}_{\mathrm{odd}}\otimes v_-)\otimes e^{\alpha/2}\mathbb{C}[2Q]\oplus S(\hat{h}^-)\otimes(T^{\mathrm{R}}_{\mathrm{odd}}\otimes v_+\oplus T^{\mathrm{R}}_{\mathrm{even}}\otimes v_-)\\
&\quad\otimes e^{3\alpha/2}\mathbb{C}[2Q],
\end{aligned} \tag{99}$$

and their respective highest weight vectors are given by

$$\begin{aligned}
v_{2\Lambda_0}&=1\otimes 1\otimes 1,\\
v_{2\Lambda_1}&=1\otimes 1\otimes e^{\alpha},\\
v_{\Lambda_0+\Lambda_1}&=1\otimes 1\otimes v_+\otimes e^{\alpha/2}.
\end{aligned} \tag{100}$$

V. CONSTRUCTION OF A $U_q(\widehat{sl(2)})$-GENERALIZED MODULE

Let $U_q(sl(2))$ be a subalgebra of $U_q(\widehat{sl(2)})$ generated by $\{e_1,f_1,K^{\pm 1}\}$ and let $M=\mathbb{C}v_0$ be the trivial one-dimensional $U_q(sl(2))$ weight module. We also introduce $U_q(\widehat{sl(2)})_{\geqslant 0}$, $U_q(\widehat{sl(2)})_{>0}$, and $U_q(\widehat{sl(2)})_{<0}$ as three subalgebras $U_q(\widehat{sl(2)})$ generated by all elements with non-negative, positive, and negative degrees with respect to q^d, respectively. We equip M with a $U_q(\widehat{sl(2)})_{\geqslant 0}$-module structure by

$$q^{\pm d}v_0=q^{\pm a}v_0,\quad a\in\mathbb{C},$$

$$\gamma^{\pm 1} v_0 = q^{\pm k} v_0, \tag{101}$$

$$x v_0 = 0, \quad \forall x \in \mathrm{U}_q(\widehat{\mathrm{sl}(2)})_{>0}.$$

Here a is scalar, which can be set to 0 without loss of generality. From M, we induce the following $\mathrm{U}_q(\widehat{\mathrm{sl}(2)})$-module:

$$G(M) = \mathrm{U}_q(\widehat{\mathrm{sl}(2)}) \otimes_{\mathrm{U}_q(\widehat{\mathrm{sl}(2)})_{\geqslant 0}} M, \tag{102}$$

which is called a generalized Verma module.[10,11] In fact, since M is a one-dimensional $\mathrm{U}_q(\mathrm{sl}(2))$-module, $G(M)$ is the simplest example of a $\mathrm{U}_q(\widehat{\mathrm{sl}(2)})$-generalized Verma module. Slightly more complicated examples of generalized Verma modules can be constructed from higher-dimensional M modules. We define the module $W(M)$ through the following isomorphism of $\mathrm{U}_q(\widehat{\mathrm{sl}(2)})$-modules:

$$G(M) \simeq \mathrm{U}_q(\widehat{\mathrm{sl}(2)})_{<0} \otimes_{\mathbb{C}} M \simeq S(\hat{h}^-) \otimes_{\mathbb{C}} W(M). \tag{103}$$

Both modules $G(M)$ and $W(M)$ are q^d weight modules with weight space decompositions:

$$G(M) = \oplus_{n \leqslant 0} G(M)_n,$$

$$W(M) = \oplus_{n \leqslant 0} W(M)_n. \tag{104}$$

From the work of Lusztig,[20] we know that for generic q the dimensions of weight spaces of $\mathrm{U}_q(\widehat{\mathrm{sl}(2)})$-modules are the same as those of the weight spaces of the $\widehat{\mathrm{sl}(2)}$-modules. The characters $\chi(G(M))$ and $\chi(W(M))$ of $G(M)$ and $W(M)$ have been computed in the $\widehat{\mathrm{sl}(2)}$ case in Refs. 6 and 11 and are given by

$$\begin{aligned} \chi(G(M)) &= \sum_{n \geqslant 0} \dim(G(M)_n) p^n = \frac{1}{\Pi_{n>0}(1-p^n)^3}, \\ \chi(W(M)) &= \sum_{n \geqslant 0} \dim(W(M)_n) p^n = \frac{1}{\Pi_{n>0}(1-p^n)^2}, \end{aligned} \tag{105}$$

where $p \in \mathbb{C}^*$ is a formal variable. The second character will allow us to prove the linear independence of a particular set of vectors constructed from the $\mathcal{Z}_q$ operators $\mathcal{Z}_n^{\epsilon}$ and which span $W(M)$. This means that the latter set of vectors is a basis for $W(M)$.

Here, we will not untwist the $\mathcal{Z}_q$ algebra into a tensor product of a group algebra and a new algebra, which is parafermionic in nature and has been partially described in Ref. 17. We will rather construct the $W(M)$ module in terms of the $\mathcal{Z}_q$ operators themselves. This will be sufficient to find an explicit realization of the $\mathrm{U}_q(\widehat{\mathrm{sl}(2)})$-generalized Verma module $G(M) = S(\hat{h}^-) \otimes W(M)$ since the $S(\hat{h}^-)$ is already constructed in terms of symmetric polynomials of α_n. To this end, we first define

$$\mathcal{Z}(\epsilon, \epsilon' | z, w) = f(\epsilon, \epsilon' | wz^{-1}) \mathcal{Z}^{\epsilon}(z) \mathcal{Z}^{\epsilon'}(w), \tag{106}$$

$$f(\epsilon, \epsilon' | z) = \frac{(q^{-(\epsilon+\epsilon')k/2+k-2} z; q^{2k})_{\infty}^{\epsilon\epsilon'}}{(q^{-(\epsilon+\epsilon')k/2+k+2} z; q^{2k})_{\infty}^{\epsilon\epsilon'}}. \tag{107}$$

Next, following some ideas in Ref. 6 in the case of $\widehat{\mathrm{sl}(2)}$ algebra, and which have been well summarized in Ref. 21 in the case of the elliptic algebra, we introduce the following formal Laurent and power series:

$$\mathcal{Z}(\epsilon,\epsilon'|z,w)=\sum_{n_1,n_2\in\mathbb{Z}}\mathcal{Z}(\epsilon,\epsilon'|n_1,n_2)z^{-n_1}w^{-n_2}, \tag{108}$$

$$\mathcal{Z}^{\epsilon}(z)=\sum_{n\in\mathbb{Z}}\mathcal{Z}_n^{\epsilon}z^{-n}, \tag{109}$$

$$f(\epsilon,\epsilon'|z)=\frac{1}{\Sigma_{n\geqslant 0}\tilde{a}_n^{\epsilon,\epsilon'}z^n}=\sum_{n\geqslant 0}a_n^{\epsilon,\epsilon'}z^n. \tag{110}$$

Relation (107) and (110) imply that

$$\begin{gathered}a_0^{\epsilon,\epsilon'}=\tilde{a}_0^{\epsilon,\epsilon'}=1,\\ \Sigma_{n\geqslant 0}\tilde{a}_n^{\epsilon,\epsilon'}a_{m-n}^{\epsilon,\epsilon'}=\delta_{m,0},\quad m\geqslant 0,\\ a_n^{\epsilon,\epsilon'}=\tilde{a}_n^{\epsilon,\epsilon'}=0,\quad n<0.\end{gathered} \tag{111}$$

Substituting the above expansions back in (106), and comparing the coefficients of the powers of wz^{-1}, we obtain

$$\mathcal{Z}_{n_1}^{\epsilon}\mathcal{Z}_{n_2}^{\epsilon'}=\sum_{n\geqslant 0}\tilde{a}_n^{\epsilon,\epsilon'}\mathcal{Z}(\epsilon,\epsilon'|n_1-n,n_2+n), \tag{112}$$

$$\mathcal{Z}(\epsilon,\epsilon'|n_1,n_2)=\sum_{n\geqslant 0}a_n^{\epsilon,\epsilon'}\mathcal{Z}_{n_1-n}^{\epsilon}\mathcal{Z}_{n_2+n}^{\epsilon'}. \tag{113}$$

Furthermore, substituting the latter expansions in the quantum generalized relations (57) and (58) and using (113), we arrive at

$$\mathcal{Z}(\epsilon,-\epsilon|n_1,n_2)=\mathcal{Z}(-\epsilon,\epsilon|n_2,n_1)+Y(\epsilon|n_1)\delta_{n_1+n_2,0}, \tag{114}$$

$$\mathcal{Z}(\epsilon,\epsilon|n_1,n_2)=q^{2\epsilon}\mathcal{Z}(\epsilon,\epsilon|n_1-1,n_2+1)+q^{2\epsilon}\mathcal{Z}(\epsilon,\epsilon|n_2,n_1)-\mathcal{Z}(\epsilon,\epsilon|n_2+1,n_1-1), \tag{115}$$

respectively, and where

$$Y(\epsilon|n)=\frac{1}{q-q^{-1}}\,(q^{kn+\epsilon\alpha_0}-q^{-kn-\epsilon\alpha_0}). \tag{116}$$

Relations (114) and (115) are useful in the normal ordering of products of $\mathcal{Z}_q$ operators by moving any operator $\mathcal{Z}_{n_1}^{\epsilon}$ with $n_1>n_2$ to the right of $\mathcal{Z}_{n_2}^{\epsilon'}$, and the operator $\mathcal{Z}_n^{+}$ to the right of $\mathcal{Z}_n^{-}$. To see this, let us examine the normal ordering of $\mathcal{Z}_{n_1}^{\epsilon}\mathcal{Z}_{n_2}^{\epsilon'}$ in the following three nontrivial cases:

A. $n_1 > n_2$, $\epsilon = -\epsilon'$

Using (112) and (114), we obtain

$$\mathcal{Z}^{\epsilon}_{n_1}\mathcal{Z}^{-\epsilon}_{n_2} = \sum_{n\geqslant 0} \tilde{a}^{\epsilon,-\epsilon}_{n}\mathcal{Z}(\epsilon,-\epsilon|n_1-n,n_2+n) = \sum_{0\leqslant n\leqslant (n_1-n_2-x)/2} \tilde{a}^{\epsilon,-\epsilon}_{n}\mathcal{Z}(-\epsilon,\epsilon|n_2+n,n_1-n)$$
$$+ \sum_{0\leqslant (n_1-n_2-x)/2<n} \tilde{a}^{\epsilon,-\epsilon}_{n}\mathcal{Z}(\epsilon,-\epsilon|n_1-n,n_2+n)$$
$$+ \sum_{0\leqslant n\leqslant (n_1-n_2-x)/2} \tilde{a}^{\epsilon,-\epsilon}_{n} Y(\epsilon|n_1)\,\delta_{n_1+n_2,0}\,, \tag{117}$$

where x is equal to 0 or 1 depending on whether n_1-n_2 is even or odd, respectively. It is therefore clear from the latter relation and (113) that the product $\mathcal{Z}^{\epsilon}_{n_1}\mathcal{Z}^{-\epsilon}_{n_2}$ with $n_1>n_2$ can be normal ordered.

B. $n_1 = n_2$, $\epsilon = -\epsilon' = +$

Like the previous case, we have

$$\mathcal{Z}^{+}_{n_1}\mathcal{Z}^{-}_{n_1} = \sum_{h\geqslant 0} \tilde{a}^{+,-}_{n}\mathcal{Z}(+,-|n_1-n,n_1+n),$$
$$= \mathcal{Z}(-,+|n_1,n_1) + Y(+|0)\,\delta_{n_1,0}$$
$$+ \sum_{n>0} \tilde{a}^{+,-}_{n}\mathcal{Z}(-\epsilon,\epsilon|n_1-n,n_1+n). \tag{118}$$

The same argument as in case A holds, and hence the product $\mathcal{Z}^{+}_{n_1}\mathcal{Z}^{-}_{n_1}$ can be normal ordered as well.

C. $n_1 > n_2$, $\epsilon = \epsilon'$

This case is less straightforward. First, (112) implies that

$$\mathcal{Z}^{\epsilon}_{n_1}\mathcal{Z}^{\epsilon}_{n_2} = \sum_{n\geqslant 0} \tilde{a}^{\epsilon,\epsilon}_{n}\mathcal{Z}(\epsilon,\epsilon|n_1-n,n_2+n), \tag{119}$$

which according to (113) means that the product $\mathcal{Z}^{\epsilon}_{n_1}\mathcal{Z}^{\epsilon}_{n_2}$ can be normal ordered if we can normal order also any operator $\mathcal{Z}(\epsilon,\epsilon|n_1,n_2)$ with $n_1>n_2$ by writing it as a linear combination of operators $\mathcal{Z}(\epsilon,\epsilon|m_1,m_2)$ with $m_1\leqslant m_2$. Relation (115) allows indeed this second type of normal ordering. The reason is that repeated use of this relation leads to

$$\mathcal{Z}(\epsilon,\epsilon|n_1+2p,n_1) = q^{2\epsilon}\mathcal{Z}(\epsilon,\epsilon|n_1,n_1+2p) + q^{2(p-1)\epsilon}(q^{2\epsilon}-1)\mathcal{Z}(\epsilon,\epsilon|n_1+p,n_1+p)$$
$$+ \sum_{n=1}^{p-1} q^{2(n-1)\epsilon}(q^{4\epsilon}-1)\mathcal{Z}(\epsilon,\epsilon|n_1+n,n_1+2p-n), \quad p>0,$$
$$\mathcal{Z}(\epsilon,\epsilon|n_1+2p+1,n_1) = q^{2\epsilon}\mathcal{Z}(\epsilon,\epsilon|n_1,n_1+2p+1) + \sum_{n=1}^{p} q^{2(n-1)\epsilon}(q^{4\epsilon}-1)$$
$$\times \mathcal{Z}(\epsilon,\epsilon|n_1+n,n_1+2p+1-n), \quad p>0, \tag{120}$$

where all the operators $\mathcal{Z}(\epsilon,\epsilon|m_1,m_2)$ on the right-hand sides of the above equations have $m_1 \leqslant m_2$. Consequently, the product $\mathcal{Z}^{\epsilon}_{n_1}\mathcal{Z}^{\epsilon}_{n_2}$ with $n_1 > n_2$ can also be normal ordered.

Since $x^{\epsilon}(z)$ acts as $S^{-}_{-\epsilon}(zq^{-2\epsilon})S^{+}_{-\epsilon}(zq^{2\epsilon})\otimes\mathcal{Z}^{\epsilon}(z)$ on $S(\hat{h}^{-})\otimes W(M)\otimes\mathbb{C}[z, z^{-1}]$, it is clear that $W(M)$ is spanned by the vectors in the set

$$\{\mathcal{Z}^{\epsilon_1}_{n_1}\cdots\mathcal{Z}^{\epsilon_s}_{n_s}v_0, \quad \epsilon_i=\pm, \quad n_i<0, \quad i=1,\ldots,s; \quad s>0\}. \tag{121}$$

The condition $n_i<0$ guarantees that the above vectors have negative degrees as they should (otherwise they are null) since $S(h^{-})\otimes W(M)$ is a graded $U_q(\widehat{sl(2)})$-highest weight module. Because of the normal ordering of the $\mathcal{Z}^{\epsilon}_{n}$ operators discussed above, the above spanning set for $W(G)$ can be reduced further to the smaller set

$$H=\{\mathcal{Z}^{\epsilon_1}_{n_1}\cdots\mathcal{Z}^{\epsilon_s}_{n_s}v_0, \quad \epsilon_i=\pm, \quad n_i\leqslant n_{i+1}; \quad \epsilon_i\leqslant\epsilon_{i+1} \quad \text{if} \quad n_i=n_{i+1}, \quad i=1,\ldots,s; \quad s>0\}, \tag{122}$$

where the order $-<+$ is meant. It can easily be seen that the set H is a basis for $W(M)$ since its character coincides with the one of $W(G)$ as given by (105). Therefore, we have an explicit construction of the $U_q(\widehat{sl(2)})$-generalized Verma module $G(M)$ with nonzero level k.

VI. RELATIONS IN THE $\mathcal{Z}_q$ ENVELOPING ALGEBRA

In this section, we extend the quantum generalized commutation relations (57) and (58) to relations satisfied by arbitrary polynomials of $\mathcal{Z}^{\epsilon}(z)$. For this purpose let us consider the following operators:

$$\mathcal{Z}(\epsilon_1,\ldots,\epsilon_s|z_1,\ldots,z_s)=S^{-}_{\epsilon_1}(z_1)\cdots S^{-}_{\epsilon_s}(z_s)x^{\epsilon_1}(z_1)\cdots x^{\epsilon_s}(z_s)S^{+}_{\epsilon_1}(z_1)\cdots S^{+}_{\epsilon_s}(z_s), \quad s>0, \tag{123}$$

which are a generalization of (45). They are expressed in terms of the operators $\mathcal{Z}^{\epsilon}(z)$ introduced in (45) as

$$Z(\epsilon_1,\ldots,\epsilon_s|z_1,\ldots,z_s)=\prod_{1\leqslant i<j\leqslant s}\frac{(q^{-(\epsilon_i+\epsilon_j)k/2+k-2}z_jz_i^{-1};q^{2k})^{\epsilon_i\epsilon_j}_{\infty}}{(q^{-(\epsilon_i+\epsilon_j)k/2+k+2}z_jz_i^{-1}q^{2k})^{\epsilon_i\epsilon_j}_{\infty}}\,\mathcal{Z}^{\epsilon_1}(z_1)\mathcal{Z}^{\epsilon_1}(z_2)\cdots\mathcal{Z}^{\epsilon_s}(z_s) \tag{124}$$

$$=\prod_{2\leqslant i\leqslant s}\frac{(q^{-(\epsilon_1+\epsilon_i)k/2+k-2}z_iz_1^{-1};q^{2k})^{\epsilon_1\epsilon_s}_{\infty}}{(q^{-(\epsilon_1+\epsilon_i)k/2+k+2}z_iz_1^{-1};q^{2k})^{\epsilon_1\epsilon_i}_{\infty}}\,\mathcal{Z}^{\epsilon_1}(z_1)\mathcal{Z}(\epsilon_2,\ldots\epsilon_s|z_2,\ldots,z_s). \tag{125}$$

The above relations can easily be derived from

$$S^{+}_{\epsilon}(z_1)x^{\epsilon'}(z_2)=\frac{(q^{-(\epsilon+\epsilon')k/2+k+2}z_2z_1^{-1};q^{2k})^{\epsilon\epsilon'}_{\infty}}{(q^{-(\epsilon+\epsilon')k/2+k-2}z_2z_1^{-1};q^{2k})^{\epsilon\epsilon'}_{\infty}}\,x^{\epsilon'}(z_2)S^{+}_{\epsilon}(z_1), \tag{126}$$

$$S^{-}_{\epsilon}(z_1)x^{\epsilon'}(z_2)=\frac{(q^{-(\epsilon+\epsilon')k/2+k-2}z_1z_2^{-1};q^{2k})^{\epsilon\epsilon'}_{\infty}}{(q^{-(\epsilon+\epsilon')k/2+k+2}z_1z_2^{-1};q^{2k})^{\epsilon\epsilon'}_{\infty}}\,x^{\epsilon'}(z_2)S^{-}_{\epsilon}(z_1). \tag{127}$$

Relations (46) and (124) imply that the operators $Z(\epsilon_1,\ldots,\epsilon_s|z_1,\ldots,z_s)$ commute also with $U_q(\hat{h})$.

Let us now derive the first type of the quantum generalized commutation relations in the $\mathcal{Z}_q$ enveloping algebra, which is valid only if $\epsilon_r=-\epsilon_{r+1}$:

$$
\begin{aligned}
&\mathscr{Z}(\epsilon_1,\ldots,\epsilon_r,\epsilon_{r+1},\ldots,\epsilon_s|z_1,\ldots,z_r,z_{r+1},\ldots,z_s)-\mathscr{Z}(\epsilon_1,\ldots,\epsilon_{r+1},\epsilon_r,\ldots,\epsilon_s|z_1,\ldots,z_{r+1},z_r,\ldots,z_s)\\
&\quad=S^-_{\epsilon_1}(z_1)\cdots S^-_{\epsilon_s}(z_s)x^{\epsilon_1}(z_1)\cdots x^{\epsilon_{r-1}}(z_{r-1})\\
&\qquad\times[x^{\epsilon_r}(z_r),x^{\epsilon_{r+1}}(z_{r+1})]x^{\epsilon_{r+2}}(z_{r+2})\cdots x^{\epsilon_s}(z_s)S^+_{\epsilon_1}(z_1)\cdots S^+_{\epsilon_s}(z_s)\\
&\quad=\frac{\epsilon_r}{q-q^{-1}}\,S^-_{\epsilon_1}(z_1)\cdots S^-_{\epsilon_s}(z_s)x^{\epsilon_1}(z_1)\cdots x^{\epsilon_{r-1}}(z_{r-1})(\Psi(z_{r+1}q^{\epsilon_r k/2})\,\delta(z_r z_{r+1}^{-1}q^{-\epsilon_r k})\\
&\qquad-\Phi(z_r q^{\epsilon_r k/2})\,\delta(z_r z_{r+1}^{-1}q^{\epsilon_r k}))x^{\epsilon_{r+2}}(z_{r+2})\cdots x^{\epsilon_s}(z_s)S^+_{\epsilon_1}(z_1)\cdots S^+_{\epsilon_s}(z_s)\\
&\quad=\frac{\epsilon_r}{q-q^{-1}}\,\mathscr{Z}(\epsilon_1,\ldots\hat{\epsilon}_r,\hat{\epsilon_{r+1}}\cdots\epsilon_s|z_1,\ldots,\hat{z}_r,\hat{z_{r+1}},\ldots,z_s)\\
&\qquad+\left\{\Psi_0\,\delta(z_r z_{r+1}^{-1}q^{-\epsilon_r k})q^{2\Sigma_{i>r+1}\epsilon_i}\prod_{i>r+1}\left(\frac{1-q^{-2-(\epsilon_i+\epsilon_r)k/2}z_i z_{r+1}^{-1}}{1-q^{2-(\epsilon_i+\epsilon_r)k/2}z_i z_{r+1}^{-1}-1}\right)^{\epsilon_i}\right.\\
&\qquad\left.-\Phi_0\,\delta(z_r z_{r+1}^{-1}q^{\epsilon_r k})q^{-2\Sigma_{i>r+1}\epsilon_i}\prod_{i<r}\left(\frac{1-q^{-2-(\epsilon_i+\epsilon_r)k/2}z_{r+1}z_i^{-1}-1}{q^{2-(\epsilon_i+\epsilon_r)k/2}z_{r+1}z_i^{-1}-1}\right)^{\epsilon_i}\right\},\\
&\qquad\epsilon_r=\epsilon_{r+1},
\end{aligned}
\tag{128}
$$

where we have used (48), (50), (53), and (127). Above, we have also introduced the notation

$$
\mathscr{Z}(\epsilon_1,\ldots,\hat{\epsilon}_r,\hat{\epsilon_{r+1}},\ldots,\epsilon_s|z_1,\ldots,\hat{z}_r,\hat{z_{r+1}},\ldots,z_s)=S^-xS^+,
\tag{129}
$$

with

$$
\begin{aligned}
S^\pm&=S^\pm_{\epsilon_1}(z_1)\cdots S^\pm_{\epsilon_{r-1}}(z_{r-1})S^\pm_{\epsilon_{r+2}}(z_{r+2})\cdots S^\pm_{\epsilon_s}(z_s),\\
x&=x^{\epsilon_1}(z_1)\cdots x^{\epsilon_{r-1}}(z_{r-1})x^{\epsilon_{r+2}}(z_{r+2})\cdots x^{\epsilon_s}(z_s),
\end{aligned}
\tag{130}
$$

and where the hat on $\hat{\epsilon}$ means that the symbol ϵ is omitted.

Using the formal power series

$$
\begin{aligned}
&\left(\frac{1-a}{1-b}\right)^{\epsilon}=(1-a^{(1+\epsilon)/2}b^{(1-\epsilon)/2})\sum_{n\geqslant 0}a^{n(1-\epsilon)/2}b^{n(1+\epsilon)/2},\\
&\prod_{i=1}^{s}(1-z_i z^{-1}q^{a_i})=\sum_{j_1,\ldots,j_i=0,1}(-1)^{\Sigma_{i=1}^s j_i}q^{\Sigma_{i=1}^s a_i}z_1^{j_1}\cdots z_s^{j_s}z^{-\Sigma_{i=1}^s j_i},
\end{aligned}
\tag{131}
$$

we can expand the products in (128) as

$$
\begin{aligned}
&\prod_{i>r+1}\left(\frac{1-q^{-2-(\epsilon_i+\epsilon_r)k/2}z_i z_{r+1}^{-1}}{1-q^{2-(\epsilon_i+\epsilon_r)k/2}z_i z_{r+1}^{-1}-1}\right)^{\epsilon_i}\\
&\quad=\sum_{j_{r+2},\ldots,j_s=0,1}\ \sum_{m_{r+2}\geqslant j_{r+2},\ldots,m_s\geqslant j_s}(-1)^{\Sigma_{i>r+1}j_i}q^{\Sigma_{i>r+1}m_i(2\epsilon_i-(\epsilon_i+\epsilon_r)k/2)-4\epsilon_i j_i}\\
&\qquad\times z_{r+1}^{-\Sigma_{i>r+1}m_i}z_{r+2}^{m_{r+2}}\cdots z_s^{m_s},
\end{aligned}
\tag{132}
$$

and

$$\prod_{i<r}\left(\frac{1-q^{-2-(\epsilon_i+\epsilon_r)k/2}z_{r+1}z_i^{-1}-1}{q^{2-(\epsilon_i+\epsilon_r)k/2}z_{r+1}z_i^{-1}-1}\right)^{\epsilon_i}$$
$$=\sum_{j_1,\ldots,j_{r-1}=0,1}\ \sum_{m_1\geqslant j_1,\ldots,m_{r-1}\geqslant j_{r-1}}(-1)^{\Sigma_{i<r}j_i}q^{\Sigma_{i<r}m_i(2\epsilon_i-(\epsilon_i+\epsilon_r)k/2)-4\epsilon_i j_i}z_1^{-m_1}\cdots$$
$$\times z_{r-1}^{-m_{r-1}}z_{r+1}^{\Sigma_{i<r}m_i}. \tag{133}$$

Substituting these expansions in (128) and taking into account the formal Laurent expansions

$$\mathcal{Z}(\epsilon_1,\ldots,\epsilon_s|z_1,\ldots,z_s)=\sum_{n_1,\ldots,n_s\in Z}\mathcal{Z}(\epsilon_1,\ldots,\epsilon_s|n_1,\ldots,n_s)z_1^{-n_1}\cdots z_s^{-n_s},$$
$$\mathcal{Z}(\epsilon_1,\ldots\hat{\epsilon}_r,\hat{\epsilon_{r+1}},\ldots,\epsilon_s|z_1,\ldots,\hat{z}_r,\hat{z_{r+1}},\ldots z_s) \tag{134}$$
$$=\sum_{n_1,\ldots,n_{r-1},n_{r+2},\ldots,n_s\in Z}\mathcal{Z}(\epsilon_1,\ldots,\hat{\epsilon}_r,\hat{\epsilon_{r+1}},\ldots,\epsilon_s|n_1,\ldots,\hat{n}_r,\hat{n_{r+1}},\ldots,n_s)$$
$$\times z_1^{-n_1}\cdots z_{r-1}^{-n_{r-1}}z_{r+2}^{-n_{r+2}}\cdots z_s^{-n_s},$$

we obtain the first quantum generalized commutation relation satisfied by the Laurent modes:

$$\mathcal{Z}(\epsilon_1,\ldots,\epsilon_r,\epsilon_{r+1},\ldots,\epsilon_s|n_1,\ldots,n_r,n_{r+1},\ldots,n_s)$$
$$-\mathcal{Z}(\epsilon_1,\ldots,\epsilon_{r+1},\epsilon_r,\ldots,\epsilon_s|n_1,\ldots,n_{r+1},n_r,\ldots,n_s)$$
$$=\frac{\epsilon_r}{q-q^{-1}}\left(\sum_{j_{r+2},\ldots,j_s=0,1}\ \sum_{m_{r+2}\geqslant j_{r+2},\ldots,m_s\geqslant j_s}\delta_{n_r+n_{r+1},\Sigma_{i>r+1}m_i}(-1)^{\Sigma_{i>r+1}j_i}\right.$$
$$\left.\times q^{n_r\epsilon_r k+\Sigma_{i>r+1}m_i(2\epsilon_i-(\epsilon_i+\epsilon_r)k/2)+2\epsilon_i(1-2j_i)}\right)$$
$$\times\mathcal{Z}(\epsilon_1,\ldots,\hat{\epsilon}_r,\hat{\epsilon_{r+1}},\ldots,\epsilon_s|n_1,\ldots,n_{r-1},\hat{n}_r,\hat{n_{r+1}},n_{r+2}+m_{r+2},\ldots,n_s+m_s)\Psi_0$$
$$-\sum_{j_1,\ldots,j_{r-1}=0,1}\ \sum_{m_1\geqslant j_1,\ldots,m_{r-1}\geqslant j_{r-1}}\delta_{n_r+n_{r+1},-\Sigma_{i<r}m_i}$$
$$\times(-1)^{\Sigma_{i<r}j_i}q^{-n_r\epsilon_r k-2\Sigma_{i>r+1}\epsilon_i+\Sigma_{i<r}m_i(2\epsilon_i-(\epsilon_i+\epsilon_r)k/2)-4\epsilon_i j_i}\mathcal{Z}(\epsilon_1,\ldots,\hat{\epsilon}_r,\hat{\epsilon_{r+1}},\ldots,\epsilon_s|n_1$$
$$+m_1,\ldots,n_{r-1}+m_{r-1},\hat{n}_r,\hat{n_{r+1}},n_{r+2},\ldots,n_s)\Phi_0,\quad \epsilon_r=-\epsilon_{r+1}. \tag{135}$$

We remark that in the above formula the following relations are meant:

$$\delta_{n_r+n_{r+1},\Sigma_{i>r+1}m_i}=\delta_{n_r+n_{r+1},0},\quad \text{if } r=1,$$
$$\delta_{n_r+n_{r+1},-\Sigma_{i<r}m_i}=\delta_{n_r+n_{r+1},0},\quad \text{if } r=s-1. \tag{136}$$

The second type of quantum generalized commutation relations in the $\mathcal{Z}_q$ enveloping algebra is derived in the case $\epsilon_r=\epsilon_{r+1}$ as follows:

$$
\begin{aligned}
&(z_r - z_{r+1}q^{2\epsilon_r})\mathscr{Z}(\epsilon_1,\ldots,\epsilon_r,\epsilon_{r+1},\ldots,\epsilon_s|z_1,\ldots,z_r,z_{r+1},\ldots,z_s)\\
&\quad-(z_r q^{2\epsilon_r} - z_{r+1})\mathscr{Z}(\epsilon_1,\ldots,\epsilon_{r+1},\epsilon_r,\ldots,\epsilon_s|z_1,\ldots,z_{r+1},z_r,\ldots,z_s)\\
&\quad=S^-_{\epsilon_1}(z_1)\cdots S^-_{\epsilon_s}(z_s)X_{\epsilon_1}(z_1)\cdots X_{\epsilon_{r-1}}(z_{r-1})((z_r - z_{r+1}q^{2\epsilon_r})X_{\epsilon_r}(z_r)X_{\epsilon_{r+1}}(z_{r+1})\\
&\qquad-(z_r q^{2\epsilon_r} - z_{r+1})X_{\epsilon_{r+1}}(z_{r+1})X_{\epsilon_r}(z_r))X_{\epsilon_{r+2}}(z_{r+2})\cdots X_{\epsilon_s}(z_s)S^+_{\epsilon_1}(z_1)\cdots S^+_{\epsilon_1}(z_s)\\
&\quad=0,\quad \epsilon_r=\epsilon_{r+1}.
\end{aligned}
\tag{137}
$$

Substituting the Laurent expansion (134) in this relation we obtain this second quantum generalized commutation relation satisfied by the Laurent modes

$$
\begin{aligned}
&\mathscr{Z}(\epsilon_1,\ldots,\epsilon_r,\epsilon_{r+1},\ldots,\epsilon_s|n_1,\ldots,n_{r-1},1+n_r,n_{r+1},\ldots,n_s)\\
&\quad-q^{2\epsilon_r}\mathscr{Z}(\epsilon_1,\ldots,\epsilon_{r+1},\epsilon_r,\ldots,\epsilon_s|n_1,\ldots,n_{r-1},n_{r+1},1+n_r,\ldots,n_s)\\
&\quad=q^{2\epsilon_r}\mathscr{Z}(\epsilon_1,\ldots,\epsilon_r,\epsilon_{r+1},\ldots,\epsilon_s|n_1,\ldots,n_{r-1},n_r,1+n_{r+1},\ldots,n_s)\\
&\qquad-\mathscr{Z}(\epsilon_1,\ldots,\epsilon_{r+1},\epsilon_r,\ldots,\epsilon_s|n_1,\ldots,n_{r-1},1+n_{r+1},n_r,\ldots,n_s),\quad \text{if } \epsilon_r=\epsilon_{r+1}.
\end{aligned}
\tag{138}
$$

Although the first quantum generalized commutation relation looks completely different from its classical analog due to the appearance of various sums over the indices j_i and m_i instead of a single sum over a single index in the classical case,[12] we have checked that in the limit $q\to 1$ this quantum generalized commutation relation does indeed reduce to its classical analog, which in our notation reads simply as follows:

$$
\begin{aligned}
&\mathscr{Z}(\epsilon_1,\ldots,\epsilon_r,\epsilon_{r+1},\ldots,\epsilon_s|n_1,\ldots,n_r,n_{r+1},\ldots,n_s)\\
&\quad-\mathscr{Z}(\epsilon_1,\ldots,\epsilon_{r+1},\epsilon_r,\ldots,\epsilon_s|n_1,\ldots,n_{r+1},n_r,\ldots,n_s)\\
&\quad=(n_r k+2\epsilon_r(\epsilon_{r+2}+\cdots+\epsilon_s)+\epsilon_r h)\\
&\qquad\times\mathscr{Z}(\epsilon_1,\ldots,\hat{\epsilon}_r,\hat{\epsilon_{r+1}},\ldots,\epsilon_s|n_1,\ldots,n_{r-1},\hat{n}_r,\hat{n_{r+1}},n_{r+2},\ldots,n_s),\\
&\qquad\text{if } n_r+n_{r+1}=0,\quad \epsilon_r=-\epsilon_{r+1},\\
&\quad=2\epsilon_r\sum_{i>r+1}\epsilon_i\mathscr{Z}(\epsilon_1,\ldots,\hat{\epsilon}_r,\hat{\epsilon_{r+1}},\epsilon_s|n_1,\ldots,n_{r-1},\hat{n}_r,\hat{n_{r+1}},n_{r+2},\ldots,n_i+n_r+n_{r+1},\ldots,n_s),\\
&\qquad\text{if } n_r+n_{r+1}>0,\quad \epsilon_r=-\epsilon_{r+1},\\
&\quad=-2\epsilon_r\sum_{i<r}\epsilon_i\mathscr{Z}(\epsilon_1,\ldots,\hat{\epsilon}_r,\hat{\epsilon_{r+1}},\ldots,\epsilon_s|n_1,\ldots,n_i+n_r+n_{r+1},\ldots,n_{r-1},\hat{n}_r,\hat{n_{r+1}},n_{r+2},\ldots,n_s),\\
&\qquad\text{if } n_r+n_{r+1}<0,\quad \epsilon_r=-\epsilon_{r+1}.
\end{aligned}
\tag{139}
$$

The classical analog of the second quantum generalized commutation relation is simpler and is given by

$$
\begin{aligned}
&\mathscr{Z}(\epsilon_1,\ldots,\epsilon_r,\epsilon_{r+1},\ldots,\epsilon_s|n_1,\ldots,n_r,n_{r+1},\ldots,n_s)\\
&\qquad-\mathscr{Z}(\epsilon_1,\ldots,\epsilon_{r+1},\epsilon_r,\ldots,\epsilon_s|n_1,\ldots,n_{r+1},n_r,\ldots,n_s)=0,\quad \text{if } \epsilon_r=\epsilon_{r+1}.
\end{aligned}
\tag{140}
$$

In the case $q=1$, the above formulas were used in Refs. 11 and 12 to construct bases for Verma modules and standard modules. We think that their explicit dependence on q might allow for the crystallization of these modules (i.e., $q\to 0$), and also for their treatment when q is a root of unity.

Moreover, since from the physical point of view, one is rather interested in the computation of traces and matrix elements of the intertwiners between the standard modules, a concrete realization of these modules in terms of the Z_q might be very useful for this purpose. Although it is not yet known how to achieve this program even when $q=1$, we think that the above formulas are a starting point in this direction, especially when $q=0$ where one expects some simplifications compared to $q=1$.

VII. CONCLUSIONS

In this paper, we have introduced a natural quantum analog of the Z_q algebra with arbitrary level k. In the special cases $k=1$ and $k=2$, our Z_q algebra simplifies considerably and reduces to the well-known results. Moreover, as a new example of a Z_q module, that is, with $k>2$, we provide an explicit construction of the basis for a generalized Verma module. One would like to diagonalize the off-critical Z_k statistical models by the elements of the quantum parafermionic algebra, which is obtained from the quotient of the Z_q algebra by its subalgebra $\mathbb{C}[Q]$, in the same way that the off-critical Ising model has been diagonalized by the quantum Clifford algebra (i.e., the special case $k=2$ of the quantum parafermionic algebra).[7]

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Two parameter deformation of Grassmann matrix group and supergroup

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The two parameter quantum deformations of 2×2 Grassmann matrices, Gr(2), and supermatrices, Gr(1|1), are presented. Gr(2) whose matrix elements are all Grassmannian variables is called the superdual of the general linear group GL(2), and Gr(1|1) whose diagonal matrix elements are Grassmannian variables is called the superdual of the supergroup GL(1|1) whose nondiagonal elements are Grassmannian. Noncentral dual superdeterminant for Grassmann supermatrices belonging to $\mathrm{Gr}_{p,q}(1|1)$ is constructed. As with the 2×2 quantum matrices, the relations satisfied by the matrix elements of the Grassmann matrices and supermatrices are expressed in terms of an $\hat{R}$ matrix. The properties of the nth power of a Grassmann supermatrix are given as an Appendix. © *1996 American Institute of Physics.*
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I. INTRODUCTION

Quantum groups are a generalization of the concept of groups. More precisely, a quantum group is a deformation of a group that, for particular values of the deformation parameter, coincides with the group. The theory and applications of quantum groups have attracted a lot of attention among mathematicians and physicists. The main physical motivation for quantum groups is that when nonlinear physical systems which are classically completely integrable are quantized, the classical symmetry group should be replaced by the corresponding quantum group.[1] On the other hand, most of the difficulties involving the divergences of quantum field theories which lie at the heart of all interactions require supersymmetry and thus the introduction of supergroups.[2] The algebraic structure underlying quantum groups extends the theory of the supergroups.[3–8] In Ref. 9, the q analog, $\mathrm{Gr}_q(1|1)$, of the dual supermatrices Gr(1|1) is presented. $\mathrm{Gr}_q(1|1)$ is the superdual of the quantum group $\mathrm{GL}_q(1|1)$ and the properties of the quantum dual supermatrices are discussed. In this paper we present a two parameter deformation, $\mathrm{Gr}_{p,q}(2)$ and $\mathrm{Gr}_{p,q}(1|1)$, of the Grassmann matrices and supermatrices, respectively and give an $\hat{R}$ matrix for this deformation.

We will say that Grassmann matrices are the dual matrices in GL(2) and Grassmann supermatrices are the dual supermatrices in GL(1|1). To study the two parameter extension of the Grassmann matrices and supermatrices, we follow the approach of Manin[3] in Sec. II. In the following section we get an $\hat{R}$ matrix which gives the relations between the matrix elements of a dual matrix in GL(1|1). The properties of the nth power of a dual supermatrix which are more compact than the single deformation parameter case are given in Appendix.

II. THE QUANTUM GRASSMANN MATRIX GROUP $\mathrm{Gr}_{p,q}(2)$

Before discussing the two parameter deformation of the dual matrices in the general linear group GL(2), we give some notations and useful formulas.

A. Notations

Consider 2×2 matrices with Grassmannian entries. We will say that such matrices form the Grassmann matrix group and denote it by Gr(2). Explicitly, a Grassmannian 2×2 matrix $\hat{A}$ is of the form

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$$\hat{A}=\begin{pmatrix}\alpha & \beta\\ \gamma & \delta\end{pmatrix}, \tag{2.1}$$

where all entries are Grassmannian.

Since the matrix elements of $\hat{A}$ are all Grassmannian, for the conventional tensor products

$$\hat{A}_1=\hat{A}\otimes I \quad \text{and} \quad \hat{A}_2=I\otimes\hat{A}, \tag{2.2}$$

one can write (no-grading)

$$(\hat{A}_1)^{ij}{}_{kl}=\hat{A}^i{}_k\delta^j{}_l, \tag{2.3a}$$

$$(\hat{A}_2)^{ij}{}_{kl}=\delta^i{}_k\hat{A}^j{}_l \tag{2.3b}$$

where δ denotes the Kronecker delta.

B. Two parameter deformation of Gr(2)

The one parameter deformation of Grassmann matrices was given by Corrigan *et al.*[4] In this section, we will give a two parameter deformation of Grassmann matrices, i.e., of Gr(2). Let $R_p[2|0]$ be a quantum vector space which is two dimensional. The coordinates of a vector $V=(x,y)^T\in R_p[2|0]$ satisfy the bilinear product relation

$$xy-pyx=0. \tag{2.4}$$

We consider a dual quantum vector space $R_q[0|2]$, the generators of which are Grassmannian. The coordinates of a (dual) vector $\hat{V}=(\xi,\eta)^T\in R_q[0|2]$ satisfy the relations

$$\xi^2=0=\eta^2, \quad \eta\xi+q\xi\eta=0 \tag{2.5}$$

as introduced in Ref. 3.

Now we want to define a two parameter deformation of the algebra of functions on the Grassmann matrix group Gr(2) as an associative algebra with unit, generated by the generators α, β, γ, and δ. For this, we consider linear transformations $\hat{A}$ with the following properties:

$$\hat{A}:R_p[2|0]\to R_q[0|2], \tag{2.6a}$$

$$\hat{A}:R_q[0|2]\to R_p[2|0]. \tag{2.6b}$$

We assume that the matrix elements of $\hat{A}$ commute with the coordinates of $R_p[2|0]$ and anti-commute with the coordinates of $R_q[0|2]$. Then the endomorphisms in (2.6) impose the following (p,q)-anti-commutation relations among the matrix elements of $\hat{A}$:

$$\begin{gathered}\alpha\beta+p^{-1}\beta\alpha=0, \quad \alpha\gamma+q^{-1}\gamma\alpha=0,\\ \gamma\delta+p^{-1}\delta\gamma=0, \quad \beta\delta+q^{-1}\delta\beta=0,\\ \alpha\delta+\delta\alpha=0, \quad \alpha^2=\beta^2=\gamma^2=\delta^2=0,\\ \beta\gamma+pq^{-1}\gamma\beta=(p-q^{-1})\delta\alpha,\end{gathered} \tag{2.7}$$

where p and q are nonzero complex numbers and $pq\pm1\neq0$.

Since the entries of $\hat{A}$ are all Grassmannian, a proper inverse cannot exist. However, the left and right inverses of $\hat{A}$ can be constructed. Let

$$\Delta_L=\beta\gamma+q^{-1}\delta\alpha, \tag{2.8a}$$

$$\Delta_R=\gamma\beta-p^{-1}\alpha\delta. \tag{2.8b}$$

Then at least the formally, the left and right inverses of $\hat{A}$ become

$$\hat{A}_L^{-1}=\begin{pmatrix} q^{-1}\delta & \beta \\ -pq^{-1}\gamma & -p\alpha \end{pmatrix}, \tag{2.9}$$

$$\hat{A}_R^{-1}=\begin{pmatrix} -q\delta & \beta \\ -qp^{-1}\gamma & p^{-1}\delta \end{pmatrix}. \tag{2.10}$$

Indeed, it is easy to show that

$$\hat{A}_L^{-1}\hat{A}=\Delta_L I, \tag{2.11a}$$

$$\hat{A}\hat{A}_R^{-1}=\Delta_R I, \tag{2.11b}$$

where I is the 2×2 unit matrix. In this case, Δ_L may be considered as a left quantum (dual) determinant and Δ_R as a right quantum (dual) determinant. Note that, one can write

$$\Delta_L\hat{A}_R^{-1}=\hat{A}_L^{-1}\Delta_R \tag{2.12}$$

using (2.8)–(2.10) and associativity of the algebra (2.7).

The algebra (2.7) is associative under multiplication and the relations in (2.7) may be also expressed in a tensor product form

$$\hat{R}(1)\hat{A}_1\hat{A}_2=-\hat{A}_2\hat{A}_1\hat{R}(1), \tag{2.13}$$

where

$$\hat{R}(x)=(p+q^{-1})\sum_i e^i{}_i\otimes e^i{}_i+2x\sum_{i\neq j}(pq^{-1})^{i-1}e^i{}_i\otimes e^j{}_j+(p-q^{-1})\left(\sum_{i>j}-\sum_{i<j}\right)e^i{}_j\otimes e^j{}_i. \tag{2.14}$$

Here the elements of the matrix $e^k{}_l$ are

$$(e^k{}_l)^i{}_j=\delta^i{}_k\delta^j{}_l. \tag{2.15}$$

The explicit form of $\hat{R}(x)$ is

$$\hat{R}(x)=\begin{pmatrix} p+q^{-1} & 0 & 0 & 0 \\ 0 & 2x & q^{-1}-p & 0 \\ 0 & p-q^{-1} & 2xpq^{-1} & 0 \\ 0 & 0 & 0 & p+q^{-1} \end{pmatrix}. \tag{2.16}$$

In terms of the matrix elements Eq. (2.13) is of the form

$$\hat{R}^{ij}{}_{kl}\hat{A}^k{}_m\hat{A}^l{}_n=-\hat{A}^j{}_l\hat{A}^i{}_k\hat{R}^{kl}{}_{mn}. \tag{2.17}$$

Finally, we note that the algebra (2.7) and the $\hat{R}$ matrix in (2.16) with $p=q$ and $x=-1$ was given in Ref. 4 (Sec. III).

III. TWO PARAMETER DEFORMATION OF THE GRASSMANN MATRIX SUPERGROUP

In this section, we consider 2×2 supermatrices whose diagonal elements are Grassmannian. We remark that the supergroup GL(1|1) whose nondiagonal elements are Grassmannian is (p,q) deformed in Refs. 7 and 8. We will say that such supermatrices form the Grassmann supermatrix group and denote it by Gr(1|1). Explicitly, a Grassmann 2×2 supermatrix $\hat{\mathscr{A}}$ is of the form

$$\hat{\mathscr{A}}=\begin{pmatrix}\alpha & b\\ c & \delta\end{pmatrix} \tag{3.1}$$

with two odd (greek letters) and two even (latin letters) matrix elements. Even matrix elements commute with everything and odd matrix elements anti-commute among themselves.

We begin with Manin's approach.[3] To do this, we consider the endomorphisms of a two-dimensional quantum superplane and its dual, denoted by $R_p[1|1]$ and $R_q^*[1|1]$, respectively.

$$U=\begin{pmatrix}x\\ \xi\end{pmatrix}\in R_p[1|1]\Leftrightarrow x\xi-p\xi x=0,\quad \xi^2=0, \tag{3.2}$$

and its dual

$$\hat{U}=\begin{pmatrix}\eta\\ y\end{pmatrix}\in R_q^*[1|1]\Leftrightarrow \eta^2=0,\quad \eta y-q^{-1}y\eta=0. \tag{3.3}$$

Suppose that the matrix elements of $\hat{\mathscr{A}}$ (anti-)commute with the coordinates of $R_p[1|1]$ and $R_q^*[1|1]$. Then, the endomorphisms

$$\hat{\mathscr{A}}:\quad R_p[1|1]\rightarrow R_q^*[1|1], \tag{3.4a}$$

$$\hat{\mathscr{A}}:\quad R_q^*[1|1]\rightarrow R_p[1|1] \tag{3.4b}$$

impose the following bilinear product relations among the generators of $\hat{\mathscr{A}}$:

$$\alpha b=p^{-1}b\alpha,\quad \alpha c=q^{-1}c\alpha, \tag{3.5a}$$

$$\delta b=p^{-1}b\delta,\quad \delta c=q^{-1}c\delta, \tag{3.5b}$$

$$\alpha\delta+\delta\alpha=0,\quad \alpha^2=0=\delta^2, \tag{3.5c}$$

$$bc=pq^{-1}cb+(p-q^{-1})\delta\alpha \tag{3.5d}$$

where p and q are nonzero complex numbers and $pq\pm1\neq0$. These relations may be considered as a two parameter deformation of a Grassmann superalgebra on four elements (α,b,c,δ) where α and δ are Grassmannian elements. This deformed algebra denoted by $\mathrm{Gr}_{p,q}(1|1)$. For $p=q$, one obtains the one parameter deformation of the generators of $\hat{\mathscr{A}}$ that was given in Ref. 9.

The inverse of $\hat{\mathscr{A}}$ can be found as in Ref. 9 and it is of the form

$$\hat{\mathscr{A}}^{-1}=\begin{pmatrix}-c^{-1}\delta b^{-1} & c^{-1}+c^{-1}\delta b^{-1}\alpha c^{-1}\\ b^{-1}+b^{-1}\alpha c^{-1}\delta b^{-1} & -b^{-1}\alpha c^{-1}\end{pmatrix} \tag{3.6}$$

provided that b and c are invertible. It is easy to verify that this is the proper right and left inverse of $\hat{\mathscr{A}}$, i.e.,

$$\hat{\mathscr{A}}\hat{\mathscr{A}}^{-1}=I=\hat{\mathscr{A}}^{-1}\hat{\mathscr{A}}.$$

Let

$$\hat{\mathscr{A}}^{-1}=\begin{pmatrix}\alpha' & b'\\ c' & \delta'\end{pmatrix}.$$

Then, the matrix elements of $\hat{\mathscr{A}}^{-1}$ satisfy the following relations

$$\begin{gathered}\alpha' b'=pb'\alpha', \quad \alpha' c'=qc'\alpha',\\ \delta' b'=pb'\delta', \quad \delta' c'=qc'\delta',\\ \alpha'\delta'+\delta'\alpha'=0, \quad \alpha'^2=0=\delta'^2,\\ b'c'=qp^{-1}c'b'+(q-p^{-1})\delta'\alpha'.\end{gathered} \tag{3.7}$$

Therefore, the matrix elements of $\hat{\mathscr{A}}^{-1}$ satisfy the (p^{-1},q^{-1})-commutation relations while the matrix elements of $\hat{\mathscr{A}}$ satisfy the (p,q)-commutation relations.

The quantum (dual) superdeterminant of $\hat{\mathscr{A}}$ is defined as

$$s\hat{D}_{p,q}(\hat{\mathscr{A}})=\hat{D}=c^{-1}b-c^{-1}\alpha c^{-1}\delta=pq^{-1}(bc^{-1}-\alpha c^{-1}\delta c^{-1}), \tag{3.8}$$

which for $p=q$ is the same as $s\hat{D}_q(\hat{\mathscr{A}})$ in Ref. 9. The factor pq^{-1} in (3.8) appeared because of the relation (3.5d). Note that the second equality in (3.8) is obtained by using the relation

$$bc^{-1}=qp^{-1}c^{-1}b-(q-p^{-1})c^{-1}\delta\alpha c^{-1}, \tag{3.9}$$

which in turn is obtained from Eq. (3.5d).

In general $\hat{D}$, the quantum (dual) superdeterminant of $\hat{\mathscr{A}}$, is not central but obeys the following commutation relations

$$\begin{gathered}\hat{D}\alpha=pq^{-1}\alpha\hat{D}, \quad \hat{D}\delta=pq^{-1}\delta\hat{D},\\ \hat{D}b=pq^{-1}b\hat{D}, \quad \hat{D}c=pq^{-1}c\hat{D}.\end{gathered} \tag{3.10}$$

It is interesting that the quantum (dual) superdeterminant $\hat{D}$ is not central while the quantum superdeterminant of a matrix $\mathrm{GL}_{p,q}(1|1)$ is 7. However, it becomes central for $p=q$ as noted down in Ref. 9.

Before passing to the next section, we remark that the interesting point in the construction of (3.6) is the fact that the dual superdeterminant $\hat{D}$ is not necessarily central.

IV. THE $\hat{R}$ MATRIX

In this section, we give an $\hat{R}$ matrix to obtain the relations (3.5). The algebra (3.5) is associative under multiplication and the relation (3.5) may be expressed in terms of a graded $\hat{R}$-matrix condition, as with the quantum supermatrix. To this end, we use the tensoring convention

$$(\hat{\mathscr{A}}_1)^{ij}{}_{kl}=(\hat{\mathscr{A}}\otimes I)^{ij}{}_{kl}=(-1)^{k(j+l)}\hat{\mathscr{A}}^i{}_k\delta^j{}_l=\hat{\mathscr{A}}^i{}_k\delta^j{}_l, \tag{4.1a}$$

$$(\hat{\mathscr{A}}_2)^{ij}{}_{kl}=(I\otimes\hat{\mathscr{A}})^{ij}{}_{kl}=(-1)^{i(j+l)}\hat{\mathscr{A}}^j{}_l\delta^i{}_k. \tag{4.1b}$$

The explicit form of $\hat{\mathscr{A}}_1$ and $\hat{\mathscr{A}}_2$ is

$$\hat{\mathscr{A}}_1=\begin{pmatrix} \alpha & 0 & b & 0 \\ 0 & \alpha & 0 & b \\ c & 0 & \delta & 0 \\ 0 & c & 0 & \delta \end{pmatrix}, \tag{4.2a}$$

$$\hat{\mathscr{A}}_2=\begin{pmatrix} -\alpha & -b & 0 & 0 \\ -c & -\delta & 0 & 0 \\ 0 & 0 & -\alpha & b \\ 0 & 0 & c & -\delta \end{pmatrix}. \tag{4.2b}$$

Then the associative algebra (3.5) is equivalent to equation

$$\hat{R}(-1).\hat{\mathscr{A}}_1.\hat{\mathscr{A}}_2=-\hat{\mathscr{A}}_2.\hat{\mathscr{A}}_1\hat{R}(-1), \tag{4.3}$$

where

$$\hat{R}(-1)=\begin{pmatrix} p+q^{-1} & 0 & 0 & 0 \\ 0 & -2 & q^{-1}-p & 0 \\ 0 & p-q^{-1} & -2pq^{-1} & 0 \\ 0 & 0 & 0 & p+q^{-1} \end{pmatrix}. \tag{4.4}$$

This $\hat{R}(-1)$ matrix obtained from (2.14) with $x=-1$. Here a 4×4 matrix in the form (4.2a) is labeled in the following way

$$M=\begin{pmatrix} M^{11}{}_{11} & M^{11}{}_{12} & M^{11}{}_{21} & M^{11}{}_{22} \\ M^{12}{}_{11} & M^{12}{}_{12} & M^{12}{}_{21} & M^{12}{}_{22} \\ M^{21}{}_{11} & M^{21}{}_{12} & M^{21}{}_{21} & M^{21}{}_{22} \\ M^{22}{}_{11} & M^{22}{}_{12} & M^{22}{}_{21} & M^{22}{}_{22} \end{pmatrix} \tag{4.5}$$

similar to Ref. 6.

We have given the (p,q)-commutation relations which satisfied by the matrix elements of a Grassmannian matrix and a Grassmannian supermatrix, i.e., we made a two parameter deformation of the Grassmann matrix group Gr(2) and the supermatrix group Gr(1|1). We obtained the Grassmannian quantum superdeterminant of a Grassmannian quantum supermatrix (p,q)-deformed case. However, it reduces to the case discussed in Ref. 9 for $p=q$. We have given an $\hat{R}$ matrix which by use of a tensor product gives the (p,q)-commutation relations between the matrix elements of a Grassmannian supermatrix.

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APPENDIX: THE PROPERTIES OF THE *n*th POWER OF GRASSMANN SUPERMATRICES

Here we will discuss the properties of the nth power of a Grassmann supermatrix. First we note that the product of two Grassmann supermatrices is not a Grassmann supermatrix, i.e., the matrix elements of a product $M=\hat{M}\hat{M}'$ do not satisfy (3.5). However, $\hat{M}\hat{M}'\in \mathrm{GL}_{p,q}(1|1)$ if $\hat{M}$ and

$\hat{M}'$ are two Grassmann supermatrices and (b,c) $((\alpha,\delta))$ pairwise commute (anti-commute) with (b',c') $((\alpha',\delta'))$. So, we must consider the matrix elements of $\hat{M}^n$ with respect to even and odd values of n. Let the $(2n-1)$th power of $\hat{M}\in \mathrm{Gr}_{p,q}(1|1)$ be

$$\hat{M}^{2n-1}=\begin{pmatrix} A_{2n-1} & B_{2n-1} \\ C_{2n-1} & D_{2n-1} \end{pmatrix}, \quad n\geqslant 1. \tag{A1}$$

After some algebra, one obtains

$$\begin{aligned} A_{2n-1}&=\{\langle n\rangle_{pq}\alpha+p\langle n-1\rangle_{pq}\delta\}(bc)^{n-1},\\ B_{2n-1}&=\{bc+p\langle n-1\rangle_{p^2q^2}\alpha\delta\}(bc)^{n-2}b,\\ C_{2n-1}&=\{cb+q\langle n-1\rangle_{p^2q^2}\delta\alpha\}(cb)^{n-2}c,\\ D_{2n-1}&=\{\langle n\rangle_{pq}\delta+q\langle n-1\rangle_{pq}\alpha\}(cb)^{n-1}, \end{aligned} \tag{A2}$$

where

$$\langle N\rangle_{pq}=\frac{1-p^Nq^N}{1-pq}. \tag{A3}$$

Now it is easy to show the following relations are satisfied:

$$\begin{aligned} A_{2n-1}B_{2n-1}&=p^{-(2n-1)}B_{2n-1}A_{2n-1},\\ A_{2n-1}C_{2n-1}&=p^{-(2n-1)}C_{2n-1}A_{2n-1},\\ D_{2n-1}B_{2n-1}&=q^{-(2n-1)}B_{2n-1}D_{2n-1},\\ D_{2n-1}C_{2n-1}&=q^{-(2n-1)}C_{2n-1}D_{2n-1},\\ A_{2n-1}D_{2n-1}+D_{2n-1}A_{2n-1}&=0,\\ A_{2n-1}^2=0&=D_{2n-1}^2,\\ B_{2n-1}C_{2n-1}&=p^{2n-1}q^{-(2n-1)}C_{2n-1}B_{2n-1}+(p^{2n-1}-q^{-(2n-1)})A_{2n-1}D_{2n-1}. \end{aligned} \tag{A4}$$

Thus, $\hat{M}^{2n-1}$ is a Grassmann supermatrix with deformation parameters p^{2n-1} and q^{2n-1}, i.e., $\hat{M}^{2n-1}\in \mathrm{Gr}_{p^{2n-1},q^{2n-1}}(1|1)$.

Similarly, if we write the matrix $\hat{M}^{2n}$, the $(2n)$th power of $\hat{M}\in \mathrm{Gr}_{p,q}(1|1)$, as

$$\hat{M}^{2n}=\begin{pmatrix} A_{2n} & B_{2n} \\ C_{2n} & D_{2n} \end{pmatrix}, \quad n\geqslant 1 \tag{A5}$$

where

$$\begin{aligned} A_{2n}&=\left\{bc+p\,\frac{1-pq}{1+pq}\,\langle n\rangle_{pq}\langle n-1\rangle_{pq}\alpha\delta\right\}(bc)^{n-1},\\ B_{2n}&=\langle n\rangle_{pq}\{\alpha+p\,\delta\}(bc)^{n-1}b,\\ C_{2n}&=\langle n\rangle_{pq}\{\delta+q\,\alpha\}(cb)^{n-1}c, \end{aligned}$$

$$D_{2n}=\left\{cb+q\,\frac{1-pq}{1+pq}\,\langle n\rangle_{pq}\langle n-1\rangle_{pq}\delta\alpha\right\}(cb)^{n-1}, \tag{A6}$$

then the elements of $\hat{M}^{2n}$ obey the following relations

$$A_{2n}B_{2n}=q^{2n}B_{2n}A_{2n}, \quad A_{2n}C_{2n}=p^{2n}C_{2n}A_{2n},$$

$$D_{2n}B_{2n}=q^{2n}B_{2n}D_{2n}, \quad D_{2n}C_{2n}=p^{2n}C_{2n}D_{2n},$$

$$B_{2n}C_{2n}+p^{n}q^{-n}C_{2n}B_{2n}=0,$$

$$B_{2n}^{2}=0=C_{2n}^{2},$$

$$A_{2n}D_{2n}-D_{2n}A_{2n}=(p^{2n}-q^{-2n})C_{2n}B_{2n}. \tag{A7}$$

Thus the matrix $\hat{M}^{2n}$ is a supermatrix in the form of

$$T=\begin{pmatrix}\alpha & \beta\\ \gamma & d\end{pmatrix} \tag{A8}$$

with the deformation parameters p^{2n} and q^{2n}. Such supermatrices T form the supergroup GL(1|1) whose deformation was given in Refs. 7 and 8. The nth power of such a supermatrix and the relations between the matrix elements of T^n can be found in Ref. 10 (Sec. 3).

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Algebraic proof of the symmetric space theorem

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I give a relatively elementary proof of the symmetric space theorem, due to Goddard, Nahm and Olive [Phys. Lett. B **160**, 111–116 (1985)]. Unlike their original proof, which involves the quark-model construction, I only use elementary algebraic techniques. © *1996 American Institute of Physics.*
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I. INTRODUCTION

In 1985 Goddard, Nahm and Olive[1] proved an interesting theorem, which has been called the symmetric space theorem. It relates the vanishing of certain coset Virasoro algebras to the existence of symmetric spaces. This has further interesting mathematical consequences in representation theory of affine Kac–Moody algebras, since the vanishing of the coset Virasoro algebra is the condition for finite reducibility of representations of affine algebras restricted to certain affine subalgebras.

The original proof by the above authors involved the use of physical concepts, such as quarks. The purpose of the present paper is to state and prove the symmetric space theorem, by using purely algebraic concepts. In particular, I shall carry out the proof following an idea used by Witt,[2] thereby using only elementary algebraic transformations.

In section II I introduce relevant definitions and notations. In section III I first prove three auxiliary lemmas and two corollaries, then state and prove the theorem.

II. DEFINITIONS AND NOTATIONS

A. Affine algebras

The *affine Kac–Moody algebra*, affine algebra for short,

$$\tilde{\mathcal{G}}(\mathfrak{g}) = (\mathbb{C}[t,t^{-1}] \otimes_{\mathbb{C}} \mathfrak{g}) \oplus \mathbb{C}\mathcal{K}, \tag{1}$$

associated to an underlying simple Lie algebra $\mathfrak{g}$ is defined by the following commutation relations:

$$[t^m \otimes x, t^n \otimes y] = t^{m+n} \otimes [x,y] + m\,\delta_{m,-n}(x|y)\mathcal{K}, \tag{2}$$

where $\mathcal{K}$ spans the center of $\tilde{\mathcal{G}}(\mathfrak{g})$ and is called the central term, and $(.|.)$ is the *normalized invariant form* on $\mathfrak{g}$. The term invariant means that

$$([x,y]|z) = (x|[y,z]), \quad \forall x,y,z \in \mathfrak{g}. \tag{3}$$

It is well known (see for example Ref. 3), that two invariant symmetric bilinear forms on a simple Lie algebra differ only by a scalar factor. The normalized invariant form, which will be used henceforth, is defined such that the highest root has length $\sqrt{2}$.

The affine algebra for an underlying Abelian algebra $\mathfrak{g}$ can be defined similarly, by (1) and (2). However, for Abelian $\mathfrak{g}$ any nondegenerate symmetric form $(.|.)$ is invariant. In contrast to the case of a simple algebra, such a form cannot be further determined by algebraic constraints derived from the Lie algebra structure. In this article Abelian algebras will almost always appear

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as subalgebras of the simple algebra $so(n)$. Therefore, there will be a natural choice of $(.|.)$, namely the restriction of the normalized invariant form of $so(n)$ to $\mathfrak{g}$. In the definitions, where an Abelian algebra is not given as a subalgebra of $so(n)$, $(.|.)$ may be any fixed nondegenerate symmetric form.

When the central element $\mathscr{K}$ of the affine algebra $\widetilde{\mathscr{L}}(\mathfrak{g})$ acts as a scalar k id in a representation, then k is called the *level of this representation.*

For a reductive Lie algebra,

$$\mathfrak{u}=\mathfrak{u}_0\oplus\mathfrak{u}_1\oplus\ldots\oplus\mathfrak{u}_S, \tag{4}$$

with center $\mathfrak{u}_0$ and simple ideals $\mathfrak{u}_1,\ldots,\mathfrak{u}_S$, the affine algebra $\widetilde{\mathscr{L}}(\mathfrak{u})$ is the direct sum of the affine algebras associated to the ideals $\mathfrak{u}_0,\ldots,\mathfrak{u}_S$:

$$\widetilde{\mathscr{L}}(\mathfrak{u})=\bigoplus_{s=0}^{S}\widetilde{\mathscr{L}}(\mathfrak{u}_s)=\bigoplus_{s=0}^{S}((\mathbb{C}[t,t^{-1}]\otimes\mathfrak{u}_s)\oplus\mathbb{C}\mathscr{K}_s). \tag{5}$$

The affine algebra associated to a finite-dimensional reductive Lie algebra $\mathfrak{u}$ is thus a S-dimensional central extension of the *loop algebra* $\mathbb{C}[t,t^{-1}]\otimes\mathfrak{u}$ *associated to* $\mathfrak{u}$. (In the case of an underlying semi-simple Lie algebra the affine algebra is indeed the universal central extension of the loop algebra.) The loop algebra can be identified with the Lie algebra of polynomial maps of S^1 into $\mathfrak{u}$.

B. The Virasoro algebra and the Sugawara construction

The *Virasoro algebra,*

$$\mathrm{Vir}=\bigoplus_{n\in\mathbb{Z}}\mathbb{C}d_n\oplus\mathbb{C}c,$$

is defined by the following commutation relations:

$$\begin{aligned}&[c,d_n]=0,\\ &[d_m,d_n]=(m-n)d_{m+n}+\delta_{m,-n}\frac{m^3-m}{12}c,\quad \forall m,n\in\mathbb{Z}.\end{aligned} \tag{6}$$

Let $\mathfrak{g}$ be a simple Lie algebra. Let $\{u_i\}$ and $\{u^i\}$ be dual bases of $\mathfrak{g}$. The *quadratic Casimir operator* is the following element of the universal enveloping algebra $\mathfrak{U}(\mathfrak{g})$ of $\mathfrak{g}$:

$$\Omega=\sum_{i=1}^{\dim\mathfrak{g}}u_iu^i. \tag{7}$$

Ω commutes with any element of $\mathfrak{g}$, therefore, by the Schur lemma it acts as a scalar, denoted by ω_ρ, on any irreducible representation ρ of $\mathfrak{g}$. Given a representation of the affine algebra $\widetilde{\mathscr{L}}(\mathfrak{g})$ of level $k\neq-1/2\omega_{ad}$, where ω_{ad} denotes the scalar value of the quadratic Casimir operator in the adjoint representation, one can construct a representation of Vir by using the following *Sugawara operators* (cf. Ref. 4), where the notation $x^{(n)}\equiv t^n\otimes x$ is used:

$$L_0 := \frac{1}{(2k+\omega_{ad})}\left(\sum_i u_i u^i + 2\sum_{n=1}^{\infty}\sum_i u_i^{(-n)} u^{i(n)}\right),$$
$$L_n := \frac{1}{(2k+\omega_{ad})}\sum_{m\in\mathbb{Z}}\sum_i u_i^{(-m)} u^{i(m+n)}, \quad \forall n\in\mathbb{Z}\backslash\{0\}. \tag{8}$$

The operators L_n obey the commutation relations (6), where the central element of the Virasoro algebra takes the scalar value

$$c = \frac{2k\ \dim\ \mathfrak{g}}{2k+\omega_{ad}}. \tag{9}$$

For an underlying abelian algebra the same equations hold with $\omega_{ad}=0$. In this case (9) yields $c=\dim\ \mathfrak{g}$. The Sugawara operators L_m and the elements $x^{(n)}$ of the affine algebra obey the following commutation relations:

$$[L_m, x^{(n)}] = -n x^{(m+n)}, \quad \forall m,n\in\mathbb{Z}, x\in\mathfrak{g}. \tag{10}$$

For a reductive Lie algebra as in (4), the Sugawara operators corresponding to $\tilde{\mathscr{Z}}(\mathfrak{u})$ in a representation of levels $k_s \neq -1/2\omega_{ad_s}$, are given by

$$L_n^{\mathfrak{u}} := \sum_{s=0}^{S} L_n^{\mathfrak{u}_s},$$

where $L_n^{\mathfrak{u}_s}$ is the Sugawara operator for the individual ideal $\mathfrak{u}_s$. The $L_n^{\mathfrak{u}_s}$ provide a representation of the Virasoro algebra with central value

$$c_{\mathfrak{u}} = \sum_{s=0}^{S} \frac{2k_s\ \dim\ \mathfrak{u}_s}{2k_s+\omega_{ad_s}}. \tag{11}$$

Again, the $L_n^{\mathfrak{u}}$ satisfy a commutation relation similar to (10), where $x\in\mathfrak{u}$.

C. The coset construction

Let U be a compact Lie subgroup of the orthogonal group $SO(n)$. Then the complexified Lie algebra of U is a reductive algebra $\mathfrak{u}$ as in (4), which is a subalgebra of the orthogonal algebra $so(n)$.

The inclusion of $\mathfrak{u}$ in $so(n)$ gives rise to a homomorphism of the associated affine algebras:

$$\tilde{\mathscr{Z}}(\mathfrak{u}) = \bigoplus_{s=0}^{S}((\mathbb{C}[t,t^{-1}]\otimes\mathfrak{u}_s)\oplus\mathbb{C}\mathscr{K}_s) \to \tilde{\mathscr{Z}}(so(n)) = (\mathbb{C}[t,t^{-1}]\otimes so(n))\oplus\mathbb{C}\mathscr{K}. \tag{12}$$

The obvious inclusion homomorphism of the loop algebras is lifted consistently to a homomorphism of the affine algebras in (12) by letting

$$\mathscr{K}_s \mapsto j_s\mathscr{K}, \quad \text{for } s=0,\ldots,S, \tag{13}$$

where for the simple ideals $\mathfrak{u}_s$, $s\geq 1$, the factor j_s is the *Dynkin index*, which is defined as the ratio of the normalized invariant form $(.|.)_{so(n)}$ on $so(n)$ (restricted to $\mathfrak{u}_s$) and the normalized invariant form $(.|.)_s$ on $\mathfrak{u}_s$, i.e.

$$(x|y)_{so(n)} = j_s(x|y)_s, \quad \forall x,y\in\mathfrak{u}_s. \tag{14}$$

For $s=0$ we choose $(.|.)_0$ to be the restriction of $(.|.)_{so(n)}$ to $\mathfrak{u}_0$. Then, by letting $j_0=1$, equation (14) holds also for $s=0$.

In this situation the Sugawara construction can be applied to both $so(n)$ and $\mathfrak{u}$ to obtain Sugawara operators $L_n^{so(n)}$ and $L_n^{\mathfrak{u}}$ which are different in general and form representations of Vir. We can calculate their central values by using (9) and (11). We get

$$c_{so(n)}=\frac{k_{so(n)}n(n-1)}{2k_{so(n)}+2n-4} \tag{15}$$

and

$$c_{\mathfrak{u}}=\sum_{s=0}^{S}\frac{2k_{so(n)}j_s\dim\,\mathfrak{u}_s}{2k_{so(n)}j_s+\omega_{ad_s}}, \tag{16}$$

respectively. In (15) I substituted $\dim(so(n))=n(n-1)/2$ and

$$\omega_{ad_{so(n)}}=2n-4. \tag{17}$$

[The expression (17) can be computed, for example, by using the relation $\omega_{ad}=2\check{h}$, where $\check{h}$ is the *dual Coxeter number*. A table of dual Coxeter numbers can be found in Ref. 4.] In (16) I used $k_s=j_sk_{so(n)}$, which follows from (13).

By (10) we have

$$[L_l^{so(n)},x^{(m)}]=-mx^{(m+l)},\quad \forall l,m\in\mathbb{Z},\quad x\in so(n). \tag{18}$$

$$[L_l^{\mathfrak{u}},x^{(m)}]=-mx^{(m+l)},\quad \forall l,m\in\mathbb{Z},\quad x\in\mathfrak{u}. \tag{19}$$

Therefore, the difference operators,

$$K_l:=L_l^{so(n)}-L_l^{\mathfrak{u}},$$

commute with each $x^{(m)}\in\widetilde{\mathscr{G}}(\mathfrak{u})$ individually,

$$[K_l,x^{(m)}]=0,\quad \forall l,m\in\mathbb{Z},\quad x\in\mathfrak{u}, \tag{20}$$

and consequently, by (8), with the corresponding Sugawara operator,

$$[K_l,L_m^{\mathfrak{u}}]=0,\quad \forall l,m\in\mathbb{Z}. \tag{21}$$

It follows that

$$[K_l,K_m]=[L_l^{so(n)},L_m^{so(n)}]-[L_l^{\mathfrak{u}},L_m^{\mathfrak{u}}],\quad \forall l,m\in\mathbb{Z}. \tag{22}$$

We deduce that the K_m, like the $L_m^{so(n)}$ and the $L_m^{\mathfrak{u}}$, define a representation of Vir, whose central charge is equal to the difference of the Sugawara values,

$$c_K=c_{so(n)}-c_{\mathfrak{u}}=\frac{k_{so(n)}n(n-1)}{2k_{so(n)}+2n-4}-\sum_{s=0}^{S}\frac{2k_{so(n)}j_s\ \dim\,\mathfrak{u}_s}{2k_{so(n)}j_s+\omega_{ad_s}}. \tag{23}$$

The above construction of representations of the Virasoro algebra is called the *coset construction.* It was introduced by Goddard and Olive in Ref. 5. It can be applied similarly for any simple (or even reductive) Lie algebra $\mathfrak{g}$ instead of $so(n)$ and a reductive subalgebra $\mathfrak{u}\subseteq\mathfrak{g}$, but in this article I shall only consider the case $\mathfrak{g}=so(n)$.

An important property of all the above constructions is that they preserve the unitarity of the involved representations, i.e., a unitary representation of the affine algebra $\tilde{\mathscr{L}}(so(n))$, induces a unitary representation of its subalgebra $\tilde{\mathscr{L}}(\mathfrak{u})$. Then by the Sugawara construction applied to the unitary representations of $\tilde{\mathscr{L}}(\mathfrak{u})$ and $\tilde{\mathscr{L}}(so(n))$ we get two different unitary representations of Vir. Finally, the resulting coset representation of Vir is again unitary.

The Virasoro algebra has no nontrivial unitary representations with zero central charge, so that the coset Virasoro algebra vanishes iff $c_K=0$. Furthermore, as was first shown in Ref. 5, the representation of $\tilde{\mathscr{L}}(\mathfrak{u})$ induced by a unitary highest weight representation of $\tilde{\mathscr{L}}(so(n))$ is finitely reducible, if and only if the coset Virasoro algebra vanishes.

It can be shown that $c_K=0$ is only possible for level 1 representations of $\tilde{\mathscr{L}}(so(n))$ (see, e.g., Ref. 6). In this case (23) reduces to

$$c_K=\frac{n}{2}-\sum_{s=0}^{S}\frac{2j_s \dim \mathfrak{u}_s}{2j_s+\omega_{ad_s}}, \quad \text{for } k_{so(n)}=1. \tag{24}$$

D. Indices of representations

The *index* κ_ρ *of a representation* ρ of a simple Lie algebra is defined as the ratio between the trace form of the representation and the normalized invariant form on the algebra, i.e.,

$$Tr(\rho(x)\rho(y))=\kappa_\rho(x|y). \tag{25}$$

For a simple Lie algebra $\mathfrak{g}$ or an Abelian subalgebra of a simple Lie algebra in an n-dimensional representation ρ of $\mathfrak{g}$, on which the Casimir operator is a scalar multiple of the identity, $\rho(\Omega)=\omega_\rho \mathrm{id}_n$ one gets by using (7) and (25):

$$\kappa_\rho \dim \mathfrak{g}=\omega_\rho n. \tag{26}$$

In particular, if ρ is the adjoint representation of a simple Lie algebra, then (26) yields for its index,

$$\kappa_{ad}=\omega_{ad}. \tag{27}$$

This equation also holds (trivially) for an Abelian Lie algebra, since in this case $\kappa_{ad}=\omega_{ad}=0$.

It can be shown that the index of the natural representation of $so(n)$ [i.e., the representation of $so(n)$ by antisymmetric $n\times n$-matrices] is 2 (see, e.g., Ref. 6). Let $\mathfrak{u}$ be a reductive subalgebra of $so(n)$ as in subsection II C. Then the index κ_{ρ_s} of the representation ρ_s of the ideal $\mathfrak{u}_s$ obtained by restricting the natural representation of $so(n)$ to $\mathfrak{u}_s$ is determined by

$$Tr(\rho_s(x)\rho_s(y))=2(x|y)_{so(n)}=2j_s(x|y)_s, \quad \forall x,y\in\mathfrak{u}_s,$$

i.e.

$$\kappa_{\rho_s}=2j_s. \tag{28}$$

Note that with our choice of $(.|.)_0$ the definition of the index makes sense also for the Abelian subalgebra $\mathfrak{u}_0$ in the representation ρ_0 and we get $\kappa_0=2$.

E. Infinitesimal symmetric spaces

Let $\mathfrak{g}$ be a semi-simple Lie algebra and let σ be an *involution* of $\mathfrak{g}$, i.e. an automorphism of $\mathfrak{g}$ of order 2: $\sigma^2=\mathrm{id}$. Let

$$\mathfrak{g}=\mathfrak{g}_0\oplus\mathfrak{g}_1$$

be the decomposition of $\mathfrak{g}$ into eigenspaces of σ,

$$\mathfrak{g}_0=\{x\in\mathfrak{g}|\sigma(x)=x\},\quad \mathfrak{g}_1=\{x\in\mathfrak{g}|\sigma(x)=-x\},$$

then $\mathfrak{g}/\mathfrak{g}_0\cong\mathfrak{g}_1$ is called an *infinitesimal symmetric space.*

Under the above conditions the following relations hold:

$$[\mathfrak{g}_0,\mathfrak{g}_0]\subseteq\mathfrak{g}_0,\quad [\mathfrak{g}_0,\mathfrak{g}_1]\subseteq\mathfrak{g}_1,\quad [\mathfrak{g}_1,\mathfrak{g}_1]\subseteq\mathfrak{g}_0. \tag{29}$$

This means that the Lie algebra $\mathfrak{g}$ is $\mathbb{Z}/2\mathbb{Z}$-graded. On the other hand, given a $\mathbb{Z}/2\mathbb{Z}$-gradation on $\mathfrak{g}$ [i.e., a decomposition $\mathfrak{g}=\mathfrak{g}_0\oplus\mathfrak{g}_1$ such that (29) holds], then an involution σ of $\mathfrak{g}$ is defined by letting $\sigma(x)=x$ for all $x\in\mathfrak{g}_0$ and $\sigma(x)=-x$ for all $x\in\mathfrak{g}_1$. Thus the infinitesimal symmetric spaces can equivalently be defined by (29).

Since the Killing form is invariant under automorphisms, we have

$$Tr(ad(x)ad(y))=Tr(ad(\sigma(x))ad(\sigma(y)))=-Tr(ad(x)ad(y)),\quad \forall x\in\mathfrak{g}_0,y\in\mathfrak{g}_1. \tag{30}$$

Thus $\mathfrak{g}_0$ and $\mathfrak{g}_1$ are orthogonal with respect to the Killing form on $\mathfrak{g}$ and the restriction of the Killing form to $\mathfrak{g}_0$, respectively, to $\mathfrak{g}_1$ is nondegenerate.

The list of all symmetric spaces is due to Cartan. A derivation based on Kac's classification of finite order automorphisms of semisimple Lie algebras can be found in Ref. 7; cf. also Ref. 1.

F. The underlying real representation of an orthogonal representation

A complex representation of a compact Lie group U is called *orthogonal* if there exists a nondegenerate symmetric bilinear form $(.|.)$ on the representation space $\mathfrak{p}$, such that

$$(g(x)|g(y))=(x|y),\quad \forall g\in U,x,y\in\mathfrak{p}, \tag{31}$$

i.e. the form is *invariant* under U. By choosing an orthonormal base of $\mathfrak{p}$ with respect to $(.|.)$ we get a matrix representation of U by orthogonal matrices. If U is connected and the orthogonal representation is faithful, this gives an embedding of U in $SO(n)$.

On the Lie algebra level the invariance property is the following:

$$(u(x)|y)=-(x|u(y)),\quad \forall u\in\mathfrak{u},\quad x,y\in\mathfrak{p}, \tag{32}$$

for example (3) is equivalent to this equation in the special case of the adjoint representation. Since the Killing form is invariant under the adjoint action and since it is nondegenerate for a semisimple Lie algebra, the adjoint representation of a semisimple Lie algebra $\mathfrak{g}$ is an orthogonal representation.

In the case of a $\mathbb{Z}/2\mathbb{Z}$-graded Lie algebra, the representation of $\mathfrak{g}_0$ on $\mathfrak{g}_1$ is an orthogonal representation, the restriction of the Killing form to $\mathfrak{g}_1$ being an invariant form.

It is well known (see, e.g., Ref. 8, Prop. (6.4)), that every complex orthogonal representation of a compact Lie group U is the complexification of a real representation of U. This means that there exists a real subspace $\mathfrak{p}^{\mathbb{R}}$ of $\mathfrak{p}$, invariant under the group action $[U(\mathfrak{p}^{\mathbb{R}})\subseteq\mathfrak{p}^{\mathbb{R}}]$, such that

$$\mathfrak{p}=\mathfrak{p}^{\mathbb{R}}\oplus i\mathfrak{p}^{\mathbb{R}}$$

as a real vector space, (i.e., each element of $p\in\mathfrak{p}$ can be uniquely decomposed as $p=x+iy$ with $x,y\in\mathfrak{p}^{\mathbb{R}}$) and such that

$$u(x+iy)=u(x)+iu(y),\quad \forall u\in U,\quad x,y\in\mathfrak{p}^{\mathbb{R}}.$$

Although $\mathfrak{p}^{\mathbb{R}}$ is in general not uniquely determined as a real subspace of $\mathfrak{p}$, its isomorphic type as a real U-module is uniquely determined by the isomorphic type of the complex U-module $\mathfrak{p}$, since $\mathfrak{p}$ is isomorphic to $\mathfrak{p}^{\mathbb{R}} \oplus \mathfrak{p}^{\mathbb{R}}$ as a real U-module.

III. THE SYMMETRIC SPACE THEOREM

The following assumptions and notations shall be valid for the whole section: Let U be a compact Lie group and let the reductive Lie algebra $\mathfrak{u} = \mathfrak{u}_0 \oplus \mathfrak{u}_1 \oplus \ldots \oplus \mathfrak{u}_S$ with center $\mathfrak{u}_0$ and simple ideals $\mathfrak{u}_1, \ldots, \mathfrak{u}_S$ be the complexification of the Lie algebra of U. Let $\{u^i\}_{i=1,\ldots,\dim \mathfrak{u}}$ be a base for $\mathfrak{u}$ consisting of anti-Hermitian elements, which is the union of bases $\{u^i\}_{i \in I_s}$ for the ideals $\mathfrak{u}_s$ such that $(u^i | u^j) = -\delta_{ij}$ for $i, j \in I_s$. (This is possible since on the real subalgebra of anti-Hermitian elements the normalized invariant form is negative definite.) For $i \in \{1, \ldots, \dim \mathfrak{u}\}$ let $s(i)$ denote the index of the ideal, which contains the element u^i, $u^i \in \mathfrak{u}_{s(i)}$, such that $0 \leqslant s(i) \leqslant S$.

Before stating the theorem I shall prove three lemmas, which will be needed for its proof, but can also be useful by themselves.

Lemma 1: The following equation holds in the universal enveloping algebra $\mathfrak{U}(\mathfrak{u})$ *and thus in any representation of* $\mathfrak{u}$*:*

$$2 \sum_{i \in I_s} u^i u^j u^i = -2\Omega_s u^j + \delta_{s(j),s} \omega_{ad_s} u^j, \quad \text{for } 0 \leqslant s \leqslant S, \quad 1 \leqslant j \leqslant \dim \mathfrak{u}, \tag{33}$$

where Ω_s *denotes the quadratic Casimir operator of the ideal* $\mathfrak{u}_s$.

Proof: The quadratic Casimir operator of $\mathfrak{u}_s$ can be written as

$$\Omega_s = -\sum_{i \in I_s} (u^i)^2.$$

Applying $ad_{\mathfrak{u}}(\Omega_s)$ to u^j gives $\omega_{ad_s} u^j$, if $u^j \in \mathfrak{u}_s$ and 0 otherwise, since $[u^i, u^j] = 0$ for $s(i) \neq s(j)$. Therefore,

$$\begin{aligned} ad_{\mathfrak{u}}(\Omega_s) u^j = \delta_{s(j)s} \omega_{ad_s} u^j &= -\sum_{i \in I_s} ad(u^i)^2 (u^j) \\ &= -\sum_{i \in I_s} [u^i [u^i, u^j]] \\ &= -\sum_{i \in I_s} (u^i (u^i u^j - u^j u^i) - (u^i u^j - u^j u^i) u^i) \\ &= -\sum_{i \in I_s} ((u^i)^2 u^j - u^i u^j u^i - u^i u^j u^i + u^j (u^i)^2) \\ &= 2\Omega_s u^j + 2 \sum_{i \in I_s} u^i u^j u^i, \end{aligned}$$

where we used that Ω_s commutes with u^j. □

Applying (33) again to u^j and summing over j, we immediately get the following corollary.

Corollary 1: *The sum of the elements* $(u^i u^j)^2$ *lies in the center of* $\mathfrak{U}(u)$ *and is given in terms of the quadratic Casimir operators as follows:*

$$2 \sum_{i \in I_s} \sum_{j \in I_t} (u^i u^j)^2 = (2\Omega_t - \delta_{st} \omega_{ad_s}) \Omega_s, \quad \text{for } 0 \leqslant s, t \leqslant S. \tag{34}$$

By taking the trace of equation (34) we immediately get the following corollary, which will be used in the proof of the next lemma.

Corollary 2: *In any n-dimensional matrix representation of* $\mathfrak{u}$, *such that the operators* u^i *are represented by matrices* M^i *and such that the quadratic Casimir operator* Ω_s *of the ideal* $\mathfrak{u}_s$ *acts as a scalar* $\omega_s id_n$ *for* $s=0,\ldots,S$, *the following identity holds:*

$$2\sum_{i\in I_s}\sum_{j\in I_t} Tr((M^iM^j)^2)=(2\omega_t-\delta_{st}\omega_{ad_s})\omega_s n, \quad \text{for } 0\leqslant s,t\leqslant S. \tag{35}$$

The following further assumptions and notations shall again be valid in the sequel.

Let $\mathfrak{p}$ be a faithful n-dimensional orthogonal complex representation of the compact group U. This defines an embedding of U into $SO(n)$ and we shall thus view U as a subgroup of $SO(n)$. Let $\{p_\alpha\}_{\alpha=1,\ldots,n}$ be an orthonormal base of $\mathfrak{p}^{\mathbb{R}}$. Let the application of the operators u^i on the basis p_α be described by the real antisymmetric matrices M^i, as follows:

$$u^i(p_\alpha)=\sum_{\gamma=1}^{n} M^i_{\gamma\alpha}p_\gamma. \tag{36}$$

Furthermore let y_s denote the index of the representation of $\mathfrak{u}_s$ on $\mathfrak{u}\oplus\mathfrak{p}$.

To evaluate y_s we note that (a) the index of a direct sum of representations is the sum of the indices of the direct summands and (b) the index of the adjoint action of $\mathfrak{u}_s$ on $\mathfrak{u}$ is ω_{ad_s}, because of (27), and since the adjoint action of $\mathfrak{u}_s$ on the sum of the $\mathfrak{u}_t$ with $t\neq s$ is trivial. Denoting the index of the representation of the ideal $\mathfrak{u}_s$ on $\mathfrak{p}$ by κ_s (instead of κ_{ρ_s}), we get

$$y_s=\omega_{ad_s}+\kappa_s=\omega_{ad_s}+2j_s. \tag{37}$$

It follows that $y_s>0$ for $s=0,\ldots,S$.

We assume that the underlying real representation $\mathfrak{p}^{\mathbb{R}}$ of $\mathfrak{p}$ is irreducible. This holds, for example, if $\mathfrak{p}$ is itself irreducible, but $\mathfrak{p}$ can also decompose as $\mathfrak{p}\cong\mathfrak{q}\oplus\mathfrak{q}^*$, where $\mathfrak{q}$ is some irreducible complex representation, such that $\mathfrak{q}\ncong\mathfrak{q}^*$. [The theorem also holds when $\mathfrak{p}^{\mathbb{R}}$ is reducible, and it can be derived from the irreducible case (see, e.g., Ref. 6).]

It can be shown that under the assumption that $\mathfrak{p}^{\mathbb{R}}$ is irreducible as a U-module, the Casimir operators Ω_s act as real positive scalars on $\mathfrak{p}$, although $\mathfrak{p}$ is not irreducible as a module over $\mathfrak{u}_s$,

$$\rho(\Omega_s)=\omega_s \mathrm{id}_n, \quad \text{with } \omega_s>0. \tag{38}$$

Therefore, (26) and (35) hold in this situation.

Lemma 2: *Let V be a level one representation space of the affine algebra* $\tilde{\mathfrak{L}}(so(n))$. *Let* $c_{\mathfrak{u}}$ *denote the central element of the Virasoro algebra constructed from* $\tilde{\mathfrak{L}}(\mathfrak{u})$ *by the Sugawara construction on V and let* c_K *denote the central element of the coset Virasoro algebra on V. Furthermore, let*

$$J_{\alpha\beta\gamma\delta}:=\sum_{s=0}^{S}\frac{1}{y_s}\sum_{i\in I_s}(M^i_{\gamma\beta}M^i_{\delta\alpha}+M^i_{\beta\alpha}M^i_{\delta\gamma}+M^i_{\alpha\gamma}M^i_{\delta\beta}), \tag{39}$$

where M is defined in (36), then the following identity holds:

$$\sum_{\alpha\beta\gamma\delta}(J_{\alpha\beta\gamma\delta})^2=\frac{6}{n}c_{\mathfrak{u}}c_K. \tag{40}$$

Proof: First let us bring c_K and $c_{\mathfrak{u}}$ in the form that is most adequate to the following calculations. Substituting (28) in (24) we get

$$c_K=\frac{n}{2}-\sum_{s=0}^{S}\frac{\kappa_s \dim \mathfrak{u}_s}{\kappa_s+\omega_{ad_s}} \overset{(26)(37)}{=} \frac{n}{2}-\sum_{s=0}^{S}\frac{n\omega_s}{y_s}. \tag{41}$$

For $c_{\mathfrak{u}}$ alone we have

$$c_{\mathfrak{u}}=\sum_{s=0}^{S}\frac{n\omega_s}{y_s}>0. \tag{42}$$

The sums

$$J^i_{\alpha\beta\gamma\delta}:=M^i_{\gamma\beta}M^i_{\delta\alpha}+M^i_{\beta\alpha}M^i_{\delta\gamma}+M^i_{\alpha\gamma}M^i_{\delta\beta}, \tag{43}$$

are invariant under cyclic permutation of the indices α,β,γ: $J^i_{\alpha\beta\gamma\delta}=J^i_{\gamma\alpha\beta\delta}=J^i_{\beta\gamma\alpha\delta}$, so that

$$\begin{aligned}\frac{1}{3}\sum_{\alpha,\beta,\gamma,\delta}J^i_{\alpha\beta\gamma\delta}J^i_{\alpha\beta\gamma\delta}&=\sum_{\alpha,\beta,\gamma,\delta}J^i_{\alpha\beta\gamma\delta}M^j_{\gamma\beta}M^j_{\delta\alpha}\\&=\sum_{\alpha,\beta,\gamma,\delta}(M^i_{\gamma\beta}M^i_{\delta\alpha}+M^i_{\beta\alpha}M^i_{\delta\gamma}+M^i_{\alpha\gamma}M^i_{\delta\beta})M^j_{\gamma\beta}M^j_{\delta\alpha}\\&=(Tr(M^iM^j))^2-2Tr((M^iM^j)^2)\\&=\delta_{ij}\kappa^2_{s(i)}-2Tr((M^iM^j)^2),\end{aligned} \tag{44}$$

where κ_s is the index of the representation of $\mathfrak{u}_s$ on $\mathfrak{p}$. For the third equality I used the antisymmetry of the matrices M^i. Using (44) we get

$$\begin{aligned}\frac{1}{3}\sum_{\alpha,\beta,\gamma,\delta}(J_{\alpha\beta\gamma\delta})^2&=\frac{1}{3}\sum_{s,t=0}^{S}\frac{1}{y_sy_t}\sum_{i\in I_s,j\in I_t}\sum_{\alpha,\beta,\gamma,\delta}J^i_{\alpha\beta\gamma\delta}J^j_{\alpha\beta\gamma\delta}\\&\overset{(44)}{=}\sum_{s=0}^{S}\frac{\kappa_s^2\dim\mathfrak{u}_s}{y_s^2}-\sum_{s,t=0}^{S}\frac{2}{y_sy_t}\sum_{i\in I_s,j\in I_t}Tr((M^iM^j)^2)\\&\overset{(26)(35)}{=}\sum_{s=0}^{S}\left(\frac{\kappa_s\omega_sn}{y_s^2}-\sum_{t=0}^{S}\frac{(2\omega_t-\delta_{st}\omega_{ad_s})\omega_sn}{y_sy_t}\right)\\&\overset{(37)}{=}\sum_{s=0}^{S}\frac{\omega_sn}{y_s}\left(\frac{\kappa_s+\omega_{ad_s}}{y_s}-\sum_{t=0}^{S}\frac{2\omega_t}{y_t}\right)\\&=\left(\sum_{s=0}^{S}\frac{\omega_sn}{y_s}\right)\left(1-\sum_{t=0}^{S}\frac{2\omega_t}{y_t}\right)\\&\overset{(41)}{=}c_{\mathfrak{u}}\cdot\frac{2c_K}{n}.\end{aligned}$$

□

The following lemma was shown in Ref. 1.

Lemma 3: Suppose that $\mathfrak{g}\equiv\mathfrak{u}\oplus\mathfrak{p}$ *forms a* $\mathbb{Z}/2\mathbb{Z}$*-graded algebra, as in (29) with* $\mathfrak{g}_0=\mathfrak{u}$ *and* $\mathfrak{g}_1=\mathfrak{p}$*, which is related to the given orthogonal* $\mathfrak{u}$*-module-structure on* $\mathfrak{u}\oplus\mathfrak{p}$ *as follows.*

• *The Killing form of* $\mathfrak{g}$ *coincides on* $\mathfrak{p}\times\mathfrak{p}$ *with the given orthogonal inner product, i.e.,* $Tr(ad_{\mathfrak{g}}(p_\alpha)ad_{\mathfrak{g}}(p_\beta))=\delta_{\alpha,\beta}$, $\forall 1\leqslant\alpha,\beta\leqslant n$.

• *The restriction of the adjoint representation of* $\mathfrak{g}$ to $\mathfrak{u}$ *coincides with the given* $\mathfrak{u}$*-module structure of* $\mathfrak{u}\oplus\mathfrak{p}$*, i.e.,*

$$[u^i,u^j+p_\alpha]_{\mathfrak{g}}=[u^i,u^j]_{\mathfrak{u}}+u^i(p_\alpha)=[u^i,u^j]_{\mathfrak{u}}+\sum_\gamma M^i_{\gamma\alpha}p_\gamma,\quad \forall 1\leqslant i,j\leqslant \dim\,\mathfrak{u},\quad 1\leqslant\alpha\leqslant n, \tag{45}$$

where $[.,.]_{\mathfrak{g}}$ *and* $[.,.]_{\mathfrak{u}}$ *denote the Lie products on* $\mathfrak{g}$ and $\mathfrak{u}$, *respectively. Then the Lie product on* $\mathfrak{p}$ *is given by*

$$[p_\alpha,p_\beta]_{\mathfrak{g}}=\sum_{i=1}^{\dim\,\mathfrak{u}}\frac{1}{y_{s(i)}}M^i_{\alpha\beta}u^i. \tag{46}$$

Proof: The invariance (3) of the Killing form means that

$$Tr(ad(u^i)ad([p_\alpha,p_\beta]))=Tr(ad([u^i,p_\alpha])ad(p_\beta)). \tag{47}$$

Since $[\mathfrak{g}_1,\mathfrak{g}_1]\subseteq\mathfrak{g}_0$ by assumption, we must have $[p_\alpha,p_\beta]=\sum_{j=1}^{\dim\,\mathfrak{u}}X^j_{\alpha\beta}u^j$, where the $X^j_{\alpha\beta}$ are some constants, such that $X^j_{\alpha\beta}=-X^j_{\beta\alpha}$. These constants can be determined by equating the l.h.s. of (47),

$$\sum_{j=1}^{\dim\,\mathfrak{u}}X^j_{\alpha\beta}Tr(ad(u^i)ad(u^j))=\sum_{j=1}^{\dim\,\mathfrak{u}}-X^j_{\alpha\beta}y_{s(i)}\delta_{ij}=-X^i_{\alpha\beta}y_{s(i)},$$

with the r.h.s. of (47),

$$Tr(ad([u^i,p_\alpha])ad(p_\beta))=\sum_{\gamma=1}^{n}M^i_{\gamma\alpha}Tr(ad(p_\gamma)ad(p_\beta))=\sum_{\gamma=1}^{n}M^i_{\gamma\alpha}\delta_{\gamma\beta}=M^i_{\beta\alpha}.$$

It follows that

$$X^i_{\alpha\beta}=-\frac{1}{y_{s(i)}}M^i_{\beta\alpha}=\frac{1}{y_{s(i)}}M^i_{\alpha\beta}. \qquad \square$$

Symmetric Space Theorem (Goddard, Nahm, Olive): *Let U be a compact Lie group with a faithful n-dimensional orthogonal representation on* $\mathfrak{p}$. *Consider the Lie algebra* $\mathfrak{u}$ *of U as a subalgebra of so(n) with the inclusion of* $\mathfrak{u}$ *in so(n) induced by the representation on* $\mathfrak{p}$. *Let* c_K *denote the central element of the coset Virasoro algebra on a level one representation space of* $\widetilde{\mathscr{L}}(so(n))$.

Then c_K vanishes if and only if $\mathfrak{g}\equiv\mathfrak{u}\oplus\mathfrak{p}$ carries the structure of a $\mathbb{Z}/2\mathbb{Z}$-graded Lie algebra with $\mathfrak{g}_0=\mathfrak{u}$ and $\mathfrak{g}_1=\mathfrak{p}$, which is related to the given orthogonal $\mathfrak{u}$-module-structure on $\mathfrak{u}\oplus\mathfrak{p}$ as in Lemma 3.

Proof: The conditions of the theorem, in view of Lemma 3, leave no freedom in defining the Lie product $[.,.]_{\mathfrak{g}}$, if it exists: This is because these conditions already uniquely determine a bilinear antisymmetric product on $\mathfrak{g}=\mathfrak{u}\oplus\mathfrak{p}$, as follows:

$$[u^i,u^j]_{\mathfrak{g}}=[u^i,u^j]_{\mathfrak{u}},$$

$$[u^i,p_\alpha]_{\mathfrak{g}}=\sum_{\gamma=1}^{n}M^i_{\gamma\alpha}p_\gamma=-[p_\alpha,u^i]_{\mathfrak{g}},$$

$$[p_\alpha,p_\beta]_{\mathfrak{g}}=\sum_{i=1}^{\dim\,\mathfrak{u}}\frac{1}{y_{s(i)}}M^i_{\alpha\beta}u^i$$

(cf. Lemma 3). Therefore, the proof of the theorem boils down to showing, that c_K vanishes if and only if this bilinear antisymmetric product on $\mathfrak{g}$ obeys the Jacobi identity.

It can easily be shown from the assumptions that the Jacobi identity holds for any three elements, if at least one of them lies in $\mathfrak{u}$. Therefore, $\mathfrak{g}$ is a Lie algebra iff the Jacobi identity holds on its $\mathfrak{p}$ part, i.e., iff

$$0=[p_\alpha,[p_\beta,p_\gamma]]+[p_\gamma,[p_\alpha,p_\beta]]+[p_\beta,[p_\gamma,p_\alpha]]=\sum_{\delta=1}^{n} J_{\alpha\beta\gamma\delta}p_\delta, \quad \forall\,\alpha,\beta,\gamma, \tag{48}$$

where we used the equation

$$[p_\alpha,[p_\beta,p_\gamma]]=\sum_{\delta=1}^{n}\left(\sum_{i=1}^{\dim \mathfrak{u}} \frac{M^i_{\gamma\beta}M^i_{\delta\alpha}}{y_{s(i)}}\right)p_\delta,$$

which follows from Lemma 3.

Thus, the Jacobi identity (48) is equivalent to the condition

$$J_{\alpha\beta\gamma\delta}=0, \quad \forall\,\alpha,\beta,\gamma,\delta. \tag{49}$$

But since the M^i are real, the $J_{\alpha\beta\gamma\delta}$ are also real. Therefore, each individual $J_{\alpha\beta\gamma\delta}$ vanishes if and only if the sum of the squares $(J_{\alpha\beta\gamma\delta})^2$ on the l.h.s. of (40) vanishes. But since by Lemma 2 this sum is equal to $(6/n)c_{\mathfrak{u}}c_K$ and $c_{\mathfrak{u}}$ is always positive, it follows that (49) is equivalent to the vanishing of c_K:

$$c_K=0, \quad \text{iff } J_{\alpha\beta\gamma\delta}=0, \quad \forall\,\alpha,\beta,\gamma,\delta. \tag{50}$$

□

The equivalence (50) was shown in Ref. 5 using the quark model construction. This result and the observation that (49) is equivalent to a Jacobi identity led to the symmetric space theorem.[1]

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The Kazhdan–Lusztig conjecture for $\mathscr{W}$ algebras

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The main result in this paper is the character formula for arbitrary irreducible highest weight modules of $\mathscr{W}$ algebras. The key ingredient is the functor provided by quantum Hamiltonian reduction, which constructs the $\mathscr{W}$ algebras from affine Kac–Moody (KM) algebras and in a similar fashion $\mathscr{W}$ modules from KM modules. Assuming certain properties of this functor, the $\mathscr{W}$ characters are subsequently derived from the Kazhdan–Lusztig conjecture for KM algebras. The result can be formulated in terms of a double coset of the Weyl group of the KM algebra: the Hasse diagrams give the embedding diagrams of the Verma modules and the Kazhdan–Lusztig polynomials give the multiplicities in the characters. © *1996 American Institute of Physics.* [S0022-2488(96)00607-X]

I. INTRODUCTION

The $\mathscr{W}$ algebras were introduced more than a decade ago as (higher spin) extensions of the Virasoro algebra in the context of two-dimensional conformal field theory.[1] Analogous to the Virasoro algebra, one expects that the representation theory of $\mathscr{W}$ algebras plays a crucial role in applications such as in conformal field theories with $\mathscr{W}$ symmetry, and in theories where the $\mathscr{W}$ symmetry is gauged ($\mathscr{W}$ strings and $\mathscr{W}$ gravity) (see Refs. 2 and 3 for reviews). For these applications, the relevant representations are highest weight modules. A basic goal is therefore to describe the irreducible modules, and more specifically to compute their characters.

There exists a general approach to find the irreducible characters from the characters of Verma modules. Any Verma module $M(x)$ can be decomposed into irreducible highest weight modules $L(y)$ (local composition series). This gives rise to character formulas of the form

$$\mathrm{ch}\ M(x)=\sum_y m_{xy}\ \mathrm{ch}\ L(y), \tag{1}$$

where m is a matrix whose entries m_{xy} count the number of times that $L(y)$ appears in the decomposition of $M(x)$. Doing this for all $M(x)$ such that m can be inverted gives

$$\mathrm{ch}\ L(x)=\sum_y m^{-1}_{xy}\ \mathrm{ch}\ M(y). \tag{2}$$

The characters of Verma modules are in general easy to compute, hence the computation of the characters of the irreducible modules boils down to determining the multiplicities m_{xy}.

This general program has been applied successfully to the Virasoro algebra.[4] The key ingredient there is that every submodule of a Verma module is a sum of Verma modules. Since there is at most one embedding between Verma modules, this implies that the multiplicities m_{xy} are 0 or 1, and the irreducible characters follow directly from the embedding pattern of the Verma modules. These embedding patterns are completely classified, and, consequently for the Virasoro algebra, the characters of *all* irreducible highest weight modules are known.

For $\mathscr{W}$ algebras the submodule structure of Verma modules is much more complicated: in general submodules are not sums of Verma modules. Therefore the embedding patterns of the Verma modules do not determine the irreducible characters. This is directly related to the occurrence of multiplicities $m_{xy}>1$.

There are, of course, also other approaches. For instance, for the $\mathscr{W}_N$ minimal models, the irreducible character $\mathrm{ch}\,L(x)$ (for x inside the Kac table) has been determined directly, using free-field methods.[5] In terms of the multiplicities this amounts to having computed a single row of m^{-1}. It does not appear to be possible to apply these methods to compute the other rows, which is necessary to determine the characters of all irreducible highest weight modules (i.e., also for x outside or on the boundary of the Kac table). In a way, the results of Ref. 5 for $\mathscr{W}_N$ algebras amount to having the $\mathscr{W}$ analog of the Weyl–Kac character formula for affine Kac–Moody (KM) algebras.

For affine KM algebras the characters are known beyond the Weyl–Kac character formula. For $k+h^\vee\neq 0$ the program described above has been fully completed. The result can be summarized as follows:

(i) The weights y appearing in the decomposition (1) are determined by a subgroup of the affine Weyl group, and the associated Bruhat ordering [the Kac–Kazhdan (KK) condition[6]].

(ii) The multiplicities m_{xy} are given in terms of the Kazhdan–Lusztig polynomials associated to the affine Weyl group [the Kazhdan–Lusztig (KL) conjecture[7,8]].

The main ingredient in the proof of (i) is the Jantzen filtration, whereas (ii) has been proven using the intersection cohomology of Schubert varieties (only for integral weights; for other weights it is still a conjecture). Neither of these concepts seems to have been worked out for $\mathscr{W}$ algebras.

It is now interesting to note that $\mathscr{W}$ algebras and KM algebras are intimately related. In particular, a large class of $\mathscr{W}$ algebras can be obtained from affine KM algebras by (quantum) Hamiltonian reduction, where one imposes certain constraints on the KM generators (see Ref. 9 for a review). In this way a $\mathscr{W}$ algebra can be constructed for every embedding of sl_2 into the simple Lie algebra underlying the affine KM algebra.[10] The quantum construction naturally allows for a Becchi–Rouet–Stora–Tyutin (BRST) formulation, in which the $\mathscr{W}$ algebra arises as the BRST cohomology of a complex involving the KM algebra.[11–13] Of course, given an sl_2 embedding, one can also compute the cohomology of a KM module. By construction, the result will be a module of the corresponding $\mathscr{W}$ algebra. Thus, one obtains in a natural way a functor from KM modules to $\mathscr{W}$ modules. The action of this ''reduction functor'' is, in general, hard to compute. In Ref. 12, the action on (resolutions of) admissible KM modules was computed for principal sl_2 embeddings, assuming certain properties of the reduction functor. This way the characters of the W_N minimal models are recovered.

The main new idea in this paper is to apply the reduction functor to ''arbitrary'' KM modules, to find the analogs of the general results (i) and (ii) for $\mathscr{W}$ algebras. The result is a natural generalization of the KL conjecture to $\mathscr{W}$ algebras associated to arbitrary sl_2 embeddings. We show how this ''KL conjecture for $\mathscr{W}$ algebras'' can be derived from the KL conjecture for KM algebras, assuming similar properties as in Ref. 12 of the reduction functor. These assumptions are motivated by the results[14] for finite $\mathscr{W}$ algebras. The upshot is that *all* irreducible characters for such $\mathscr{W}$ algebras are thereby determined. We verified the conjecture for a nontrivial set of $\mathscr{W}_3$ modules.

The setup of this paper is as follows. In Sec. II, we review the representation theory and KL conjectures of affine KM algebras, including a discussion of the translation functor that serves as a helpful analogy with the reduction functor. Then in Sec. III, after some remarks on the representation theory of general $\mathscr{W}$ algebras, we present the main result of this paper in Sec. III C, the KL conjecture for $\mathscr{W}$ algebras. We also give an idea of how it can be derived using the reduction

functor. Several applications of the conjecture are discussed in Sec. IV. Properties of Coxeter groups and their KL polynomials are given in the Appendix.

II. THE KAZHDAN–LUSZTIG CONJECTURES FOR AFFINE KAC–MOODY ALGEBRAS

We first present a collection of results concerning affine KM algebras and their highest weight modules, leading to the KL conjectures. Virtually everything stated here can be found somewhere in the mathematical literature on the subject, or can be concluded directly from it. We have avoided a rigorous presentation, but instead focussed on the line of thought, and made clear what is well established and what is conjectured. For background and explanations on KM algebras and the structure of the highest weight modules we refer to Refs. 15 and 16, and for Weyl groups and KL polynomials to Ref. 17.

A. Composition series and character formulas

Let g be an affine KM algebra, and fix a triangular decomposition $g=n_+\oplus h\oplus n_-$ in positive root generators, Cartan subalgebra (CSA), and negative root generators. A singular vector v_λ is an eigenvector of the generators of the Cartan subalgebra h with weight $\lambda\in h^*$, and is annihilated by the positive root generators. A highest weight module is a module that is generated from a singular vector, the highest weight vector, by the action of the negative root generators. There are two important examples of highest weight modules. The first is the Verma module $M(\lambda)$, which is uniquely defined by the property that it is generated freely from v_λ. The second is the quotient of $M(\lambda)$ by its maximal proper submodule, which gives the unique irreducible highest weight module $L(\lambda)$.

Highest weight modules themselves are special examples of modules in the so-called category $\mathscr{O}$.[8,18] In general this category consists of modules V which have a weight space decomposition

$$V=\oplus_{\mu\leqslant\lambda}V_\mu, \tag{3}$$

where the μs satisfy $\mu\leqslant\lambda$ for λ in some finite subset of h^* (recall that $\mu\leqslant\lambda$ iff $\lambda-\mu$ is on the positive root lattice Q_+ of g) and $\dim V_\mu<\infty$. The category $\mathscr{O}$ contains highest weight modules, tensor products, submodules, quotients, etc.

For every module V in $\mathscr{O}$, one can define a (formal) character $\mathrm{ch}\,V$,

$$\mathrm{ch}\,V=\sum_\mu \dim V_\mu e^\mu, \tag{4}$$

where the formal exponentials satisfy $e^\lambda e^\mu=e^{\lambda+\mu}$ and $e^0=1$. The character of the Verma module $M(\lambda)$ is given by

$$\mathrm{ch}\,M(\lambda)=e^\lambda\sum_{\gamma\in Q_+}P(\gamma)e^{-\gamma}=e^\lambda\prod_{\alpha\in\Delta_+}(1-e^{-\alpha})^{-\dim g_\alpha}, \tag{5}$$

where g_α is the root space of root α, Δ_+ is the set of positive roots, and $P(\gamma)$ is the (generalized) Kostant partition function. One of the central problems of representation theory is to find the characters of the irreducible highest weight modules $L(\lambda)$. The strategy is to relate these to the explicit characters of Verma modules (5). This is possible due to the following general structure theorem, which also illustrates that $\mathscr{O}$ is natural in the context of highest weight modules [in particular, the $L(\lambda)$s are the only irreducibles in $\mathscr{O}$]. Every module V in the category $\mathscr{O}$ has a local composition series at any weight λ of V. A local composition series for V at λ is a sequence of submodules of V, $V=V_0\supset V_1\supset\cdots\supset V_{n-1}\supset V_n=0$, such that either $V_i/V_{i+1}\cong L(\mu)$ for some $\mu\geqslant\lambda$, or $(V_i/V_{i+1})_\mu=0$ for all $\mu\geqslant\lambda$. One denotes by $[V:L(\mu)]$ the number of times that $L(\mu)$ appears in the local composition series of V at λ. It is called the multiplicity of $L(\mu)$ in V. It is independent of the particular sequence of submodules one chooses. We stress that $[V:L(\mu)]$ does

not count the number of singular vectors at weight μ in V: the statement that $V_i/V_{i+1}\cong L(\mu)$ only requires that there is a vector v_μ which is singular in the quotient V_i/V_{i+1} but not necessarily singular in V_i, let alone V. A vector that is singular in a quotient of submodules is called primitive, and the corresponding weight is called a primitive weight. Obviously, a singular vector is also primitive, but it is important to realize that there are also other types of primitive vectors. We also stress that the multiplicities $[M:L]$ can be larger than 1, contrary to what was initially thought based on the known trivial multiplicities of the simple Lie algebras $\overline{g} = \overline{\mathrm{sl}}_2, \overline{\mathrm{sl}}_3$ and the affine KM algebra $g=\mathrm{sl}_2$.

At the level of characters, the local composition series implies that (4) is given by a sum over the irreducible characters: $\mathrm{ch}\, V=\Sigma_\mu [V:L(\mu)]\mathrm{ch}\, L(\mu)$, where the sum runs over the weights of V (of course, only the primitive weights give a nonvanishing contribution). This applies in particular to Verma modules, leading to

$$\mathrm{ch}\, M(\lambda)=\sum_{\mu\leqslant\lambda} [M(\lambda):L(\mu)]\mathrm{ch}\, L(\mu). \tag{6}$$

Note that the composition series starts with $[M(\lambda):L(\lambda)]=1$, since $\dim M(\lambda)_\lambda=1$. Ordering the set of weights $\mu\leqslant\lambda$ as $\lambda=\mu_0, \mu_1, \mu_2,...$, such that $j\geqslant i$ whenever $\mu_j\leqslant\mu_i$, one has the following set of equations:

$$\mathrm{ch}\, M(\mu_i)=\sum_{\mu_j\leqslant\mu_i} [M(\mu_i):L(\mu_j)]\mathrm{ch}\, L(\mu_j).$$

The matrix $[M(\mu_i):L(\mu_j)]$, called the Jantzen matrix (for λ), is upper triangular with ones on the main diagonal. Therefore, it can be inverted. Denoting the inverse matrix elements by $(L(\mu_i):M(\mu_j))$ (which are possibly negative integers), one finds

$$\mathrm{ch}\, L(\mu_i)=\sum_{\mu_j\leqslant\mu_i} (L(\mu_i):M(\mu_j))\mathrm{ch}\, M(\mu_j).$$

In conclusion, from (6) one finds the character formula

$$\mathrm{ch}\, L(\lambda)=\sum_{\mu\leqslant\lambda} (L(\lambda):M(\mu))\mathrm{ch}\, M(\mu). \tag{7}$$

Here $\mathrm{ch}\, M(\mu)$ is given through (5). Computing $\mathrm{ch}\, L(\lambda)$ boils down to computing the numbers $(L(\lambda):M(\mu))$ for all $\mu\leqslant\lambda$ or, equivalently, the Jantzen matrix $[M(\mu_i):L(\mu_j)]$ for λ.

B. The Kac–Kazhdan conditions

The first step in determining the multiplicities $[M(\lambda):L(\mu)]$ is to find all pairs λ,μ such that $[M(\lambda):L(\mu)]\neq 0$. The general solution to this problem has been given by Kac and Kazhdan,[6] using the generalized Casimir of g and the Jantzen filtration of Verma modules.[15] For the purposes of this paper it is sufficient to consider only weights λ with $\langle\lambda+\rho,\delta\rangle=k+h^\vee\neq 0$. In that case the result of Ref. 6 can be rephrased in terms of properties of the affine Weyl group.[19]

The affine Weyl group W is a Coxeter group, generated by the simple reflections s_i where $s_i(\lambda)=\lambda-\langle\lambda,\alpha_i^\vee\rangle\alpha_i$ are the reflections in the simple roots α_i of g. Arbitrary elements $w\in W$ correspond to expressions $w = s_{i_1}s_{i_2}\cdots s_{i_k}$. The minimal number of simple reflections needed to generate w is called the length $\ell(w)$ of w. An expression of minimal length is called reduced. If $w,w'\in W$ are two reduced expressions, then we denote $w<w'$ if the reduced expression for w can be obtained by dropping simple reflections from a reduced expression for w'. The resulting relation $w\leqslant w'$ is a partial ordering of W, called the Bruhat ordering.

An important ingredient in what follows is the subgroup $W_\lambda \subset W$: it is the group generated by reflections $r_{\hat{\alpha}}$ with $\hat{\alpha} \in \Delta^{re}_{\lambda,+} = \{\alpha \in \Delta^{re}_+ | \langle \lambda+\rho, \alpha^\vee \rangle \in \mathbf{Z}\}$. Clearly, only if λ is integral, $W_\lambda = W$ (recall that $\rho \in h^*$ satisfies $\langle \rho, \alpha_i^\vee \rangle = 1$), otherwise W_λ will be a proper subgroup of W (which for affine W may be isomorphic to W). It can be shown that W_λ is again a Weyl group; it is generated by simple reflections $\hat{s}_i = r_{\hat{\alpha}_i}$ (simple in W_λ) where $\hat{\alpha}_i$ are the simple roots of the rootsystem $\Delta^{re}_{\lambda,+}$. The length function on W_λ is denoted $\ell_\lambda(w)$. Obviously, the relation between λ and W_λ is many-to-one; for instance, $W_\lambda = W_{\lambda+\mu}$ for arbitrary integral weight μ. In fact, up to isomorphisms, there is only a finite number of W_λ.[20]

The groups W_λ organize the nonvanishing multiplicities in the following way: the primitive weights of $M(\lambda)$ are on the shifted Weyl orbit $W_\lambda.\lambda$, where

$$w.\lambda \equiv w(\lambda+\rho) - \rho, \tag{8}$$

and vice versa. Only the lower weights (with respect to Bruhat ordering) on the orbit are primitive weights of $M(\lambda)$. In the remainder of this section we describe this in more detail.

First consider $k + h^\vee > 0$. Then every orbit $W_\mu.\mu$ has precisely one maximal element λ, the dominant weight, such that $w.\lambda \leqslant \lambda$ for all $w \in W_\mu$. Using (8) it is easy to see that such a dominant weight λ is characterized by

$$\langle \lambda+\rho, \hat{\alpha}_i^\vee \rangle \geqslant 0. \tag{9}$$

Clearly, there is a one-to-one correspondence between dominant weights λ and orbits $W_\lambda.\lambda$. There may not be a one-to-one correspondence between elements of W_λ and the weights on the orbit $W_\lambda.\lambda$. This happens precisely if there is a subgroup W^0_λ of W_λ which leaves λ invariant. Here W^0_λ is a finite parabolic subgroup of W_λ, generated by the simple reflections $r_{\hat{\alpha}_i}$ with $\hat{\alpha}_i$ satisfying $\langle \lambda+\rho, \hat{\alpha}_i^\vee \rangle = 0$. A dominant weight is called regular if W^0_λ is trivial, and it is called singular otherwise. Thus, weights on the orbit $W_\lambda.\lambda$ of a dominant weight are in one-to-one correspondence with elements of the coset

$$W_\lambda / W^0_\lambda, \tag{10}$$

i.e., any weight μ can be written uniquely as $\mu = w.\lambda$ with λ dominant and $w \in W_\lambda / W^0_\lambda$. This coset will be crucial in what follows: in particular *the multiplicities depend on* λ *only through the coset* W_λ / W^0_λ!

Denote $M_w = M(w.\lambda)$ and $L_w = L(w.\lambda)$. Then the Kac–Kazhdan condition for $k + h^\vee > 0$ can be described as follows:

$$[M_w : L_{w'}] \neq 0 \quad \text{iff} \quad w \leqslant w' \ \text{ with } \ w, w' \in W_\lambda / W^0_\lambda. \tag{11}$$

Here, the ordering on the coset W_λ / W^0_λ is induced from the Bruhat ordering on W_λ:

$$w \leqslant w' \ \text{ with } \ w, w' \in W_\lambda / W^0_\lambda \quad \text{iff} \quad \underline{w} \leqslant \underline{w}' \ \text{ with } \ \underline{w}, \underline{w}' \in W_\lambda. \tag{12}$$

[Here $\underline{w}$ is the minimal coset representative of w in the coset, defined through $\ell(\underline{ws}) > \ell(\underline{w})$ for all $s \in W^0_\lambda$. Of course we could also have chosen the maximal representatives $\overline{w}$ which have $\ell(\overline{ws}) < \ell(\overline{w})$ for all $s \in W^0_\lambda$.]

For the character formulas (6) and (7) the Kac–Kazhdan result implies the following. First of all, the sum over the weight space in (6) reduces to a sum over $w' \in W_\lambda / W^0_\lambda$:

$$\mathrm{ch}\, M_w = \sum_{w' \geqslant w} [M_w : L_{w'}] \mathrm{ch}\, L_{w'}. \tag{13}$$

Second, using transitivity of the Bruhat order this can be inverted

$$\mathrm{ch}\, L_w = \sum_{w' \geqslant w} (L_w : M_{w'})\, \mathrm{ch}\, M_{w'}\,. \tag{14}$$

Unlike the sum in (13) not all terms in this sum have to be nonvanishing.

For weights with $k+h^\vee<0$, the result can be rephrased analogously. We note that weights with $k+h^\vee<0$ are the image of weights with $k+h^\vee>0$ under the shifted inversion

$$\sigma.\lambda = -\lambda - 2\rho. \tag{15}$$

Clearly, $W_{\sigma.\lambda} = W_\lambda$, so σ is also a one-to-one map between the orbits on either side (orbits always belong to one side only as W leaves $k+h^\vee$ invariant). Since σ reverses the order of weights, every orbit now will have a minimal weight, called antidominant, which is of the form $\sigma.\lambda$ with λ dominant. In terms of these antidominant weights one has the analog of (11) describing the full KK condition for $k+h^\vee<0$:

$$[M_w : L_{w'}] \neq 0 \quad \text{iff} \quad w \geqslant w' \quad \text{with} \quad w, w' \in W_\lambda / W_\lambda^0. \tag{16}$$

Thus one finds the same character formulas (13) and (14), but with the sum over $w' \leqslant w$.

C. Embeddings of Verma modules

In the previous section we have discussed the role of the cosets W_λ / W_λ^0 in finding the primitive weights of a Verma module $M(\lambda)$. In this section we discuss how the same cosets also describe the embeddings between Verma modules.

This is based on the property of KM Verma modules that at every primitive weight there is at least one singular vector.[6] Since a singular vector v_μ in a Verma module $M(\lambda)$ gives rise to a homomorphism $M(\mu) \hookrightarrow M(\lambda)$ (embedding) between Verma modules, this statement implies that there is a homomorphism iff the multiplicity $[M(\lambda):L(\mu)]$ is nonvanishing. Hence

$$M_{w'} \hookrightarrow M_w \quad \text{iff} \quad w \leqslant w' \quad \text{with} \quad w, w' \in W_\lambda / W_\lambda^0. \tag{17}$$

In other words: the diagram representing the embeddings of the Verma modules is given by the Hasse diagram of the coset W_λ / W_λ^0: the vertices of this diagram are the elements of the coset and the links between the vertices connect the adjacent elements (two coset elements x,y are called adjacent if there is no third coset element z such that $x<z<y$). Since one can classify the Hasse diagrams, this gives a classification of embedding diagrams.

In fact, if $k+h^\vee \neq 0$, the relation between embeddings and the Hasse diagram is even stronger, because in that case there is at most one singular vector at every primitive weight. This implies that the homomorphism $M(\mu) \hookrightarrow M(\lambda)$ is unique, or

$$\dim \mathrm{Hom}(M(\mu), M(\lambda)) \leqslant 1. \tag{18}$$

This can be argued as follows. If there is a sequence $M(\mu_1) \hookrightarrow M(\mu_2) \hookrightarrow M(\mu_3)$ of homomorphisms, the embedding property implies that

$$\dim \mathrm{Hom}(M(\mu_1), M(\mu_3)) \geqslant \dim \mathrm{Hom}(M(\mu_2), M(\mu_3)). \tag{19}$$

For $k+h^\vee<0$, any Verma module contains always a lowest primitive weight (the antidominant weight). At this weight, there is precisely one singular vector (because any two embedded Verma modules necessarily overlap). This immediately implies (18).

For $k+h^\vee>0$, there is no lowest primitive weight. In that case (18) follows from the result for $k+h^\vee<0$ through the ''reflection principle'' of semi-infinite homology,[21]

$$\mathrm{Hom}(M(\mu), M(\lambda)) \simeq \mathrm{Hom}(M(\sigma.\lambda), M(\sigma \cdot \mu)). \tag{20}$$

D. Jantzen's translation functor

In this section we discuss how the multiplicities for *arbitrary* dominant weights follow from the multiplicities for *regular* dominant weights. The idea is to use Jantzen's translation functor[8,15] to map modules with regular weights (trivial W_λ^0) to modules with singular weights (nontrivial W_λ^0). The reason for highlighting this ingredient here is the striking similarity between this derivation and the derivation of $\mathscr{W}$ multiplicities from KM multiplicities using the reduction functor in Sec. III B.

Let λ' be a singular dominant weight, and let λ be a regular dominant weight such that $\lambda-\lambda'$ is an integral weight. Clearly, $W_\lambda = W_{\lambda'}$, but W_λ^0 is trivial whereas $W_{\lambda'}^0$ is not. The tensorproduct with the irreducible module associated with $\lambda'-\lambda$ gives rise to an exact functor[8,15,22] (the translation functor) that maps

$$M(w.\lambda) \overset{t}{\mapsto} M(w.\lambda'). \tag{21}$$

To obtain the action of the translation functor on irreducible modules, observe that for Verma modules $M(w'.\lambda) \hookrightarrow M(w.\lambda)$ with w,w' in the same coset, the functor maps the quotient $M(w.\lambda)/M(w'.\lambda)$ [which contains $L(w.\lambda')$] to zero, so it immediately follows that

$$L(w.\lambda) \overset{t}{\mapsto} L(w.\lambda')\,\delta_{\overline{w},w}\,. \tag{22}$$

(Here $\overline{w}$ is the maximal representative of w in the coset $W_\lambda / W_{\lambda'}^0$.) The maps (21) and (22) determine the multiplicities for singular weights from the multiplicities of the regular weights:

$$[M(w.\lambda'):L(w'.\lambda')] = [M(\overline{w}.\lambda):L(\overline{w'}.\lambda)]. \tag{23}$$

Another useful application of the translation functor is the computation of the character of the irreducible module L_e for regular dominant weights λ (without having to determine the full Jantzen matrix). For such weights namely, the sum in (14) runs over all the elements of W_λ. Applying (21) and (22) to it for a translation chosen such that $W_{\lambda'}^0$ contains just one reflection gives that the coefficients are given by $\varepsilon_w = (-1)^{l_\lambda(w)}$,[22] hence

$$\text{ch}\, L_e = \sum_{w \in W_\lambda} \varepsilon_w\, \text{ch}\, M_w\,. \tag{24}$$

This is the generalization of the Weyl–Kac formula[16] to arbitrary regular dominant weights. The same trick cannot be applied to obtain arbitrary characters (i.e., ch L_w or for λ singular). It is this particular character formula (for admissible λ) that forms the starting point of Ref. 12 for generalization to $\mathscr{W}$ algebras.

E. The KL conjectures

Now we are ready to describe the final step, i.e., to give the Kahdan–Lusztig formula for the multiplicities. In Ref. 7, Kazhdan and Lusztig defined for an arbitrary Coxeter group W a set of polynomials $P_{x,y}(q)$, labelled by pairs of elements x,y in W, and depending on a single variable q. For details and properties about the definition of these polynomials, see the Appendix. Important for us is that they can be computed explicitly from a recursion relation [see (A18)]

$$P_{x,ys} = q^{1-c} P_{xs,y} + q^c P_{x,y} - q \sum_{\substack{x \leqslant z < y \\ zs < z}} P_{x,z} P_{z,y}\,. \tag{25}$$

The simple reflection s is chosen such that $y<ys$, such that the polynomials $P_{x,y}$ are expressed in terms of polynomials $P_{x',y'}$ with $l(y')<l(y)$.

Similarly, one defines a set of inverse polynomials $Q_{x,y}(q)$ through

$$\sum_{x\leqslant z\leqslant w} P_{x,z}(q)Q_{z,y}(q)\epsilon_z\epsilon_y=\delta_{x,y}\,, \tag{26}$$

which can also be computed directly from a recursion relation [see (A18)]

$$Q_{x,ys}=cQ_{xs,y}+(-q)^cQ_{x,y}+cq\sum_{\substack{x<z\leqslant y\\ zs>z}}\mathcal{P}_{x,z}Q_{z,y}\,. \tag{27}$$

Analogously, one may also associate KL polynomials P^I,Q^I to a coset W/W_I for W_I a parabolic subgroup of W. If W_I is finite, these are related to the KL polynomials on W as follows:

$$P^I_{x,y}=P_{\underline{x},y},\quad Q^I_{x,y}=Q_{x,y}. \tag{28}$$

Here $\underline{z}$ and $\overline{z}$ are the minimal and maximal representatives of z in the coset $[z]$. In general, the polynomials P^I and Q^I are not each other's inverse. The inverse polynomials of P^I, Q^I are denoted $\widetilde{Q}^I$, $\widetilde{P}^I$; they are defined through

$$\sum_{x\leqslant z\leqslant y}\widetilde{Q}^I_{x,z}P^I_{z,y}=\sum_{x\leqslant z\leqslant y}Q^I_{x,z}\widetilde{P}^I_{z,y}=\delta_{x,y}\,. \tag{29}$$

They can also be expressed in terms of the polynomials on W:

$$\widetilde{P}^I_{x,y}=\sum_{z\in[x]}P_{z,y}\epsilon_z\epsilon_y,\quad \widetilde{Q}^I_{x,y}=\sum_{z\in[y]}Q_{\overline{x},z}\epsilon_{\overline{x}}\epsilon_z\,. \tag{30}$$

The KL conjectures relate the multiplicities in the character formulas to the value of these polynomials at $q=1$. Let λ be a dominant weight with coset W_λ/W^0_λ, $P_{w,w'}$ be the KL polynomials for W_λ, and $Q_{w,w'}$ be the associated inverse KL polynomials. Then the multiplicities are given by[7,8,15,23]

$$\begin{aligned} &k+h^\vee>0:\quad [M_w:L_{w'}]=P^I_{w,w'}(1),\quad (L_w:M_{w'})=\widetilde{Q}^I_{w,w'}(1)\\ &k+h^\vee<0:\quad [M_w:L_{w'}]=Q^I_{w',w}(1),\quad (L_w:M_{w'})=\widetilde{P}^I_{w',w}(1)\end{aligned}, \tag{31}$$

(the superscript I refers to the subgroup W^0_λ). These conjectures have been proven for integral weights, in Ref. 24 for $k+h^\vee>0$, and Ref. 25 for $k+h^\vee<0$. It is inconceivable that the conjectures for $k+h^\vee>0$ are related to the conjecture for $k+h^\vee<0$ through the semi-infinite cohomology of affine KM algebras.

The conjectures naturally fit in a circle of ideas generally referred to as Kazhdan–Lusztig theory. This theory interrelates many different problems, such as the classification of primitive ideals in enveloping algebras, the computation of the multiplicities in composition series, and the intersection cohomology of Schubert varieties (see Ref. 26 for an overview). It applies in particular to simple Lie algebras, affine KM algebras, and quantum groups. In Sec. III we show that it also applies to $\mathscr{W}$ algebras.

III. THE KL CONJECTURES FOR $\mathscr{W}$ ALGEBRAS

Compared to the situation for affine Kac–Moody algebras, relatively little is known about the representation theory of $\mathscr{W}$ algebras. The fact that a classification of such algebras is still lacking

makes it harder to give a general approach to this problem. We claim, however, that for the class of $\mathscr{W}$ algebras obtained through Hamiltonian reduction of affine KM algebras, the analog of most results described in Sec. II exists. In particular, we formulate the KL conjecture for such $\mathscr{W}$ algebras.

A. Some generalities on $\mathscr{W}$ algebras and modules

Let us first consider a general $\mathscr{W}$ algebra, generated by the modes of a finite set of quasiprimary fields (for a precise definition see Ref. 2). The $\mathscr{W}$ algebra will have a CSA h, i.e., a maximal Abelian subalgebra of the zero modes. Unlike for KM algebras, the adjoint action of h on the generators of the $\mathscr{W}$ algebra is, in general, not diagonalizable (e.g., the zero-mode W_0 of the spin three field of $\mathscr{W}_3$); therefore the ''triangular'' decomposition of $\mathscr{W}=\mathscr{W}_+\oplus h\oplus\mathscr{W}_-$, in positive root generators, Cartan subalgebra, and negative root generators is given with respect to a subalgebra $h'\subset h$:

$$\mathscr{W}=\oplus_{a'}\mathscr{W}_{-a'}\oplus h\oplus_{a'}\mathscr{W}_{a'}, \tag{32}$$

where a' runs over the set of positive roots Δ'_+. By assumption $\mathscr{W}_{-a'}\cong\mathscr{W}_{a'}$ as vector spaces, paired by an involutive map $\sigma:\mathscr{W}_{-a'}\to\mathscr{W}_{a'}$.

The setup of representation theory is similar to that of affine KM algebras, in the following sense. A singular vector v_a is an eigenvector of the generators of h with weight $a\in h^*$, and v_a is annihilated by all positive root generators. A highest weight module V is generated from v_a by the action of the negative root generators. Similarly, one introduces a category $\mathscr{O}$, which consists of modules V which have a weight space decomposition into a direct sum of weight spaces of the subalgebra h',

$$V=\oplus_{b'\leqslant a'}V_{b'}, \tag{33}$$

where the sum is over weights b' satisfying $b'\leqslant a'$ for a' in some finite subset of h'^*, and $\dim V_{b'}<\infty$ (note that $b'\leqslant a'$ iff $a'-b'$ is on the positive root lattice Q'_+ of h').

The category $\mathscr{O}$ again contains Verma modules $M(a)$, irreducible quotients $L(a)$, submodules, etc. (but no tensor products as, in general, the tensor product of two $\mathscr{W}$ modules is not a $\mathscr{W}$ module).

For every module V in $\mathscr{O}$ one can define a (formal) character ch V,

$$\mathrm{ch}\ V=\sum_{b'}\dim V_{b'}e^{b'}. \tag{34}$$

The Verma module $M(a)$ has character formula

$$\mathrm{ch}\ M(a)=e^{a'}\sum_{b'\in Q'_+}P(b')e^{-b'}=e^{a'}\prod_{b'\in\Delta'_+}(1-e^{-b'})^{-\dim\mathscr{W}_{b'}}, \tag{35}$$

where $P(b')$ is some generalized Kostant partition function.

The finite dimensionality of the weight spaces $V_{b'}$ implies that the action of the generators of the CSA h outside h' is reasonably well behaved: every weight space $V_{b'}$ can be decomposed into a finite number of Jordan blocks U_b,

$$V_{b'}=\oplus_b U_b. \tag{36}$$

This implies that one can make local composition series in $\mathscr{O}$, where the irreducible quotients are again the highest weight modules $L(b)$, occurring with multiplicities $[V:L(b)]$. This leads to

character formulas ch $V=\Sigma_b[V:L(b)]$ch $L(b)$, where of course b can only appear in the sum if b' is a weight of V. This applies in particular to a Verma module $M(a)$, leading to

$$\text{ch } M(a)=\sum_{b'\leqslant a'}[M(a):L(b)]\text{ch } L(b), \tag{37}$$

where clearly $[M(a):L(a)]=1$. Once again, this character formula can be inverted, such that the characters of irreducible modules can be expressed in characters of Verma modules

$$\text{ch } L(a)=\sum_{b'\leqslant a'}(L(a):M(b))\text{ch } M(b). \tag{38}$$

To conclude: also for $\mathscr{W}$ algebras, the general strategy to find character formulas is to compute the multiplicities $[M(a):L(b)]$. This is what we will do in the next section.

B. $\mathscr{W}$ modules from sl_2 reductions

A large class of $\mathscr{W}$ algebras can be obtained through a procedure of (quantum) Hamiltonian reduction of affine KM algebras.[9] A particularly nice set of reductions are those related to sl_2 embeddings.[10] For every sl_2 embedding into the simple Lie algebra underlying the untwisted affine KM algebra, one can define a BRST complex such that the associated cohomology is nonvanishing only in the zeroth term. This cohomology is a $\mathscr{W}$ algebra.[11–13]

Similarly, on the level of the representation theory, the cohomology of a complex associated to a KM module gives a $\mathscr{W}$ module. This defines a functor from the category of KM modules to the category of $\mathscr{W}$ modules. We assume the following properties of this reduction functor:[12,14] (1) the cohomology of the BRST complex associated to the KM module is nonvanishing only in the zeroth term, (2) KM Verma modules $M(\lambda)$ are mapped to $\mathscr{W}$ Verma modules $M(a(\lambda))$, and (3) a local composition series of a KM Verma module is mapped to a local composition series of the corresponding $\mathscr{W}$ Verma module.

From these assumptions it immediately follows that, when acting on KM irreducible modules, the reduction functor maps

$$L(\lambda)\to L(a(\lambda)) \quad \text{or} \quad L(\lambda)\to 0. \tag{39}$$

If one knows which $L(\lambda)$ have vanishing or nonvanishing cohomology, then the multiplicities of $\mathscr{W}$ Verma modules are determined. The main result of this paper is an explicit formula for these multiplicities, in terms of KL polynomials associated to a double coset which is completely fixed by the reduction data. Note that the reduction only gives rise to a $\mathscr{W}$ algebra for $k+h^\vee\neq 0$, i.e., precisely those weights for which the KM multiplicities are given by the KL conjecture. This implies that one has the complete KL conjecture for this class of $\mathscr{W}$ algebras, so that the characters of all irreducible highest weight $\mathscr{W}$ modules are known.

Let us explain how this should work. Associated to the particular sl_2-reduction is a regular subalgebra g_r of the finite-dimensional simple Lie algebra $\overline{g}$ underlying the affine Kac–Moody algebra g.[14] The sl_2 subalgebra is principally embedded into g_r. This embedding determines a set of constraints which can be chosen in such a way that they involve only positive roots. This is necessary to get nonvanishing cohomology from KM Verma modules. In explicit examples it is possible to verify that this cohomology is given by a Verma module of the corresponding $\mathscr{W}$ algebra.[12,14] We assume that this holds in general. From the results of Ref. 14 we expect that the parametrization $a(\lambda)$ of the $\mathscr{W}$ weight is invariant under the shifted action of the Weyl group W^r of g_r (which is a finite parabolic subgroup of W). More precisely,

$$a(w.\lambda)=a(\lambda) \quad \text{iff} \quad w\in W^r, \tag{40}$$

so there is a one-to-one correspondence between the $\mathscr{W}$ weights and the invariants of the Weyl group W^r. Using this parametrization we will from now on denote Verma modules and irreducible modules for the $\mathscr{W}$ algebra by $M^r(\lambda)$ and $L^r(\lambda)$ with λ a weight of g. Up to W^r invariance, the labelling by g weights fixes the $\mathscr{W}$ weights uniquely.

Let λ be a dominant weight. From the existence of the composition series it follows that the set of primitive weights in a $\mathscr{W}$ Verma module $M^r(\lambda)$ is contained in the orbit of the double coset

$$W^r_\lambda \backslash W_\lambda / W^0_\lambda, \tag{41}$$

where $W^r_\lambda = W^r \cap W_\lambda$. From the embedding property (17) of KM Verma modules it now follows that for each weight on this orbit there is an embedding of $\mathscr{W}$ Verma modules, thus there is a one-to-one correspondence between primitive weights and weights on the orbit of the double coset (41).

It is instructive to note the analogy with the translation functor discussed in Sec. II D: the translation functor maps regular KM Verma modules $M(\lambda)$ to arbitrary KM Verma modules $M(\lambda')$, such that the relevant cosets W_λ are mapped to $W_{\lambda'}/W^0_{\lambda'}$. Similarly, the reduction functor maps arbitrary KM Verma modules $M(\lambda)$ to arbitrary $\mathscr{W}$ Verma modules $M^r(\lambda)$, such that the relevant cosets W_λ/W^0_λ are mapped to $W^r_\lambda \backslash W_\lambda / W^0_\lambda$. Indeed, the derivation of the $\mathscr{W}$ multiplicities from KM multiplicities from this point on goes completely analogous to the derivation in Sec. II D.

The irreducible $\mathscr{W}$ module $L^r(\mu)$ may arise only as the cohomology of the KM modules $L(w.\mu)$ with $w \in W^r$. Obviously, the cohomology of the associated KM Verma modules $M(w.\mu)$ are identical. Therefore, the cohomology of $L(\mu)$ must vanish when there is a $w \in W^r_\mu$ such that $M(w.\mu) \subset M(\mu)$ with $w.\mu \neq \mu$. On every W^r_μ orbit of μ, only the lowest weight contributes therefore.

It follows that the reduction functor maps

$$M_w \to M^r_w, \quad L_w \to L^r_w \delta_{w,\overline{w}}, \tag{42}$$

where again $M^r_w = M^r(w.\lambda)$, $L^r_w = L^r(w.\lambda)$, and $\overline{w}$ is the maximal representative of w in the double coset (41).

Thus we observe that again the way to associate KL polynomials with the double coset (41) is to take maximal representatives.

To summarize, consider the $\mathscr{W}$ algebra associated with the regular subalgebra g_r. Let λ be a dominant weight, and let $w, w' \in W^r_\lambda \backslash W_\lambda / W^0_\lambda$. Denote the double coset of w by $[w]$, the minimal representatives by $\underline{w}$ and the maximal representative by $\overline{w}$, and define the following polynomials:

$$P^{IJ}_{w,w'} = P_{\overline{w},\overline{w'}}, \quad Q^{IJ}_{w,w'} = Q_{\underline{w},\underline{w}'}.$$
$$\widetilde{P}^{IJ}_{w,w'} = \sum_{x \in [w]} P_{x,\underline{w}'} \epsilon_x \epsilon_{\underline{w}'}, \quad \widetilde{Q}^{IJ}_{w,w'} = \sum_{x \in [w']} Q_{\overline{w},x} \epsilon_{\overline{w}} \epsilon_x. \tag{43}$$

Conjecture 1 (KL conjecture for $\mathscr{W}$ algebras): The multiplicities in Verma modules are given by the KL polynomials associated with the double coset (41):

$$\begin{aligned} k + h^\vee > 0: \quad & [M^r_w : L^r_{w'}] = P^{IJ}_{w,w'}(1), \quad (L^r_w : M^r_{w'}) = \widetilde{Q}^{IJ}_{w,w'}(1), \\ k + h^\vee < 0: \quad & [M^r_w : L^r_{w'}] = Q^{IJ}_{w',w}(1), \quad (L^r_w : M^r_{w'}) = \widetilde{P}^{IJ}_{w',w}(1). \end{aligned} \tag{44}$$

Hence the character formula for irreducible $\mathscr{W}$ modules is given by

TABLE I. Classification of embedding patterns of the Virasoro algebra.

Feigin–Fuchs	coset
I	trivial
$\mathrm{II}_{\pm}$	a_1
II^{0}	a_1/a_1
$\mathrm{III}_{\pm}$	$\hat{a}_1$
$\mathrm{III}^{0}_{\pm}$	$\hat{a}_1/a_1$
$\mathrm{III}^{00}_{\pm}$	$a_1\backslash\hat{a}_1/a_1$

$$k+h^\vee>0: \quad \mathrm{ch}\, L^r_w=\sum_{w'\geqslant w}\widetilde{Q}^{IJ}_{w,w'}(1)\mathrm{ch}\, M^r_{w'},$$
$$k+h^\vee<0: \quad \mathrm{ch}\, L^r_w=\sum_{w'\leqslant w}\widetilde{P}^{IJ}_{w',w}(1)\mathrm{ch}\, M^r_{w'}. \tag{45}$$

Conjecture 2: The embedding diagram of Verma modules corresponds to the Hasse diagram of the double coset (41):

$$\left.\begin{array}{ll} k+h^\vee>0: & M^r_{w'}\hookrightarrow M^r_w \\ k+h^\vee<0: & M^r_w\hookrightarrow M^r_{w'} \end{array}\right\} \quad \text{iff} \quad w\leqslant w' \quad \text{with} \quad w,w'\in W^r_\lambda\backslash W_\lambda/W^0_\lambda. \tag{46}$$

Moreover, we expect that also for $\mathscr{W}$ algebras there is just one singular vector at any given weight. The KL conjecture supports this as follows. For $k+h^\vee<0$, there is an antidominant weight, so here the proof is identical to the case discussed in Sec. II C. Barring a reflection principle for $\mathscr{W}$ algebras, a general proof for $k+h^\vee>0$ is lacking. However, in the examples we studied, the polynomials appear to have the property that at arbitrary length $l(w)$ one can always find a w such that polynomial $P_{e,w}=1$. This provides an upperbound for the number of singular vectors at that weight and, consequently, also at every primitive weight $w'.\lambda$ for any $w'\leqslant w$ [see (19)]. So we expect that also for $\mathscr{W}$ algebras, $\dim \mathrm{Hom}\,(M^r(\lambda), M^r(\mu))\leqslant 1$.

IV. EXAMPLES AND APPLICATIONS

In this section we discuss some examples that on the one hand provide evidence for the validity of the conjectures and, on the other, are an illustration of their effectiveness for actual computations. In particular, the (explicit) calculation of $\mathscr{W}$ characters for irreducible highest weight modules is now reduced to combinatorics on the Weyl group of g. For simplicity we restrict to $g=\mathrm{sl}_N$. If $\lambda=\Sigma_{i=0}^{l}\lambda_i\Lambda_i$ is a dominant weight (where Λ_i are the fundamental weights of $\mathrm{sl}_N, \langle\Lambda_i,\alpha_j^\vee\rangle=\delta_{ij}$), then the level $k=\Sigma_{i=0}^{l}\lambda_i$, P_+^k is the set of dominant integral weights of level k, and P_{++}^k are the regular weights in P_+^k. The finite part $\bar{\lambda}\in\bar{h}^*$ is $\bar{\lambda}=\Sigma_{i=1}^{l}\lambda_i\Lambda_i$ and finally $h^\vee=N$.

A. Comparison with known results

The first check is provided by the Virasoro algebra, which is the quantum Hamiltonian reduction of the affine KM algebra $g=\mathrm{sl}_2$. In that case, it is a straightforward exercise to show that the conjectures agree with the results of Feigin and Fuchs: (1) the embedding diagrams are classified by the double cosets of the reflection subgroups of the affine Weyl group $\hat{a}_1$ (see Table I) and 2 the multiplicities in the characters are given by the corresponding KL polynomials: $P_{x,y}=Q_{x,y}=1$ for all $x\leqslant y$.

TABLE II. Classification of $\mathscr{W}_3$ modules with W_λ isomorphic to $\hat{a}_2$.

W^r_λ	W^0_λ	t	Λ^+	Λ^-	c	h	w	Table
a_2	a_2	1	(1,0,0)	(0,0,0)	2	0	0	V
a_2	a_2'	1	(0,1,0)	(0,0,0)	2	$\frac{1}{3}$	$\frac{2}{27}$	VI
a_2	a_1	2	(1,1,0)	(0,0,0)	-10	$-\frac{1}{3}$	$\frac{1}{27}$	VII
a_2	a_1'	2	(0,1,1)	(0,0,0)	-10	0	0	VIII
a_2	$\cdots$	3	(1,1,1)	(0,0,0)	-30	-1	0	IX
a_1	a_1	3/2	(2,1,0)	(0,1,0)	-2	$-\frac{1}{9}$	$-\frac{1}{81}$	X
a_1	a_1'	3/2	(2,0,1)	(0,1,0)	-2	$\frac{2}{9}$	$\frac{10}{81}$	XI
a_1	$\cdots$	3/2	(1,1,1)	(0,1,0)	-2	0	0	XII
$\cdots$	$\cdots$	4/3	(2,1,1)	(0,1,1)	0	0	0	XIII

TABLE III. The KL polynomials $P_{x,y}$ for the Weyl group $\hat{a}_2$ of the affine KM algebra $g=\mathrm{sl}_3$, up to $l(y)=15$. To find $P_{x,y}$ for arbitrary pairs x,y [with $l(y)\leqslant 15$] use that (1) $P_{x,y}=0$ unless $x\leqslant y$, (2) $P_{x,y}=P_{x^{-1},y^{-1}}$, (3) $P_{x,y}=P_{\tau(x),\tau(y)}$ with τ an automorphism of the Dynkin diagram, (4) $P_{x,y}=P_{x',y}$ for $x\leqslant x'$ and $P_{x',y}(1)$ maximal, (5) if (1)–(4) do not apply, then $P_{x,y}=1$. So, given a pair x,y with $x\leqslant y$, one first fixes i,j,k and an order (i.e., reading from left-to-right or from right-to-left) such that y is in the table. Second, one searches for an x' (in the fixed order) in the table such that $x\leqslant x'$ and $P_{x',y}(1)$ is maximal; then $P_{x,y}=P_{x',y}$. If either of the two steps fail, then $P_{x,y}=1$.

$\ell(y)$	y	x	$P_{x,y}-1$	$\ell(y)$	y	x	$P_{x,y}-1$	$\ell(y)$	y	x	$P_{x,y}-1$
4	ijki	i	q			ijk	$3q^2+3q$	14	ijikijikijikij	ijikijikijk	q
5	ijkij	ij	q		ijkijikijki	ijikijki	q			ijikijikiji	q
	ijkji	i	q			ikijkij	q			ijikijikij	$2q$
6	ijikij	iji	q			ijkijki	$2q$			ijikijk	q^2+2q
	ijkijk	iki	q			ijiki	q^2+2q			ijikiji	q^2+2q
		ijk	q		ijkijkijkij	ijkijkij	q			ijikij	$2q^2+2q$
7	ijikiji	iji	q	12	ijikijikijik	ijikijiki	q			iji	q^3+2q^2+2q
	ijkijik	ijik	q			ijikijik	$2q$		ijikijikijkijk	ijikijkijki	q
		iki	q			ijiki	q^2+2q			ijikijikijk	q
		ijk	$2q$			ijik	$2q^2+2q$			ijikijkijk	$2q$
	ijkijki	ijki	q		ijikijikijki	ijikijkij	q			ijikijk	q^2+2q
8	ijikijik	ijiki	q			ijikijiki	q		ijikijkijkijki	ijikijkijki	q
		ijik	$2q$			ijikijki	$2q$		ijkijkijkijkij	ikijkijkijk	q
	ijikijki	ijiki	q			ijiki	q^2+2q			ijkijkijkij	q
	ijkijkij	ikijk	q		ijikijkijkij	ijikijkij	q	15	ijikijikijikiji	ijikijikiji	q
		ijkij	q		ijkijkijkijk	ikijkijki	q			ijikiji	q^2+q
9	ijikijiki	ijiki	q			ijkijkijk	q			iji	q^3+q^2+q
	ijkijikij	ijikij	q	13	ijikijikijiki	ijikijiki	q		ijikijikijikijk	ijikijikijk	q
		ikijk	q			ijiki	q^2+q			ijikijk	q^2+q
		ijkij	$2q$		ijikijikijkij	ijikijkij	q		ijikijikijkijki	ijikijkijki	q
		iji	q^2+2q		ijkijikijikij	ijkijikijk	q		ijkijikijikijk	ijkijikijiki	q
	ijkijikji	ijikji	q			ijikijikij	q			ijikijikijik	q
		ijkji	$3q$			ikijikijk	$2q$			ikijikijiki	$2q$
		ijiki	$2q$			ijkijikij	$3q$			ijkijikijik	$3q$
		iji	q^2+3q			ijikijkij	$2q$			ijikijikijk	$2q$
		i	$2q^2+3q$			ijikijk	q^2+3q			ikijkijki	q^2+2q
	ijkijkijk	ijkijk	q			ijikiji	q^2+2q			ijikijikj	q^2+2q
10	ijikijikij	ijikijk	q			ijikij	$2q^2+3q$			ijikijiki	q^2+3q
		ijikiji	q			ikijk	$2q^2+3q$			ijkijiki	$2q^2+3q$
		ijikij	$2q$			ijkij	$3q^2+3q$			ijikijik	$2q^2+3q$
		iji	q^2+2q			iji	q^3+3q^2+3q			ikijiki	$3q^2+3q$
	ijikijkijk	ijikijk	q		ijkijikijikji	ijikijikji	q			ijkijik	$4q^2+3q$
	ijkijkijki	ikijkij	q			ijkijikji	$3q$			ijikijk	$3q^2+3q$
		ijkijki	q			ijikijiki	$2q$			ijikj	q^3+3q^2+3q
11	ijikijikiji	ijikiji	q			ijikjik	q^2+2q			ijiki	q^3+4q^2+3q
		iji	q^2+q			ijikiji	q^2+3q			ijik	$2q^3+4q^2+3q$
	ijikijikijk	ijikijk	q			ijikji	$2q^2+3q$			iki	$2q^3+4q^2+3q$
	ijkijikijk	ijkijiki	q			ijkji	$4q^2+3q$			ijk	$3q^3+4q^2+3q$
		ijikijik	q			ijiki	$3q^2+3q$		ijkijikijikijki	ijkijikijkij	q
		ikijiki	$2q$			iji	q^3+4q^2+3q			ijkijikijki	q
		ijkijik	$3q$			i	$2q^3+4q^2+3q$			ikijikijkij	$2q$
		ijkijk	$2q$		ijkijikijkijk	ijikijkijk	q			ijkijikijki	$3q$
		ijikj	q^2+2q			ikijkijki	q			ijikijkijki	$2q$
		ijiki	q^2+3q			ijkijkijk	$2q$			ijikijkij	q^2+3q
		ijik	$2q^2+3q$			ijikijk	q^2+2q			ijikijiki	q^2+2q
		iki	$2q^2+3q$		ijkijkijkijki	ijkijkijki	q			ijikijki	$2q^2+3q$

TABLE IV. Inverse KL polynomials $Q_{x,y}$ for the Weyl group $\hat{a}_2$ of the affine KM algebra $g=\mathrm{sl}_3$, up to $l(x)=14$. To find $Q_{x,y}$ for arbitrary pairs x,y [with $l(x)\leqslant 14$] use the rules of TABLE III with x,y interchanged and the ordering reversed.

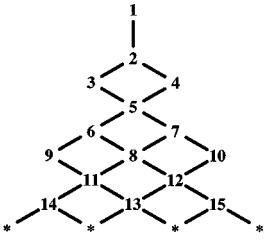
$\ell(x)$	x	y	$Q_{x,y}-1$	$\ell(x)$	x	y	$Q_{x,y}-1$	$\ell(x)$	x	y	$Q_{x,y}-1$
1	i	ijki	q			jikijkijk	$2q$			jikijkijkij	$2q$
		ijkijki	q^2+q			ijkijkijki	$3q$			ijkijkijkijk	$3q$
		ijkijkijki	q^3+q^2+q			ikjikjikji	q			ijkjikijikij	q^2+3q
		ijkijkijkijki	$q^4+q^3+q^2+q$			ijkijikijik	q^2+3q			ijkjikijkijk	q^2+3q
2	ij	ijkij	q			ijkijijikji	q^2+3q			jikijikijikij	q^2+2q
		ikjikj	q			ikjikjikjik	$2q$			jkijkijkijkij	q^2+3q
		ijkijkij	q^2+q			jikijikijik	q^2+2q			ijikijikijikij	$2q^2+3q$
		ikjikjikj	q^2+q			jkijkijkijk	q^2+3q			ijikijikijkijk	$2q^2+3q$
		ijkijkijkij	q^3+q^2+q			ijikijikijik	$2q^2+3q$			ijkijkijkijkij	$2q^2+3q$
		ikjikjikjikj	q^3+q^2+q			ijikijikijki	$2q^2+3q$			ikjikjikjikjik	q
		ijkijkijkijkij	$q^4+q^3+q^2+q$			ijkijkijkijk	$2q^2+3q$	ijkijik		ijkijikijik	q
3	iji	ijikij	q			jikjikijkjik	$3q$			ijkijkijkijk	q
		ikjikj	q			ijikijikijiki	$4q^2+3q$			ikjikjikjikjik	q
		ijikiji	$3q$			ijkijikijikji	$3q^2+3q$	ijkijki		ijkijkijki	q
		ijkijki	$2q$			ijkijikijkijk	$3q^2+3q$			ijkijkijkijki	q^2+q
		ijkjikj	$2q$			ijkijkijkijki	$4q^2+3q$	8	ijikijik	ijkijikijik	q
		ijkijkij	$3q$			ikjikjikjikji	q^2+3q			ijikijikijik	$2q$
		ijkijikij	q^2+3q			jikijikijkjik	$3q^2+3q$			ikjikjikjikjik	q
		ijkijikji	q^2+3q			jikijikijkjik	q^2+3q	ijkikji		ijkijikijki	q
		ikjikjikj	q^2+3q			ikjikjikjikjik	$2q^2+3q$			jikijikijki	q
		ijkijikij	$2q^2+3q$			jkijkijkijkijk	q^3+3q^2+3q			ijkikijikijki	$2q$
		ijkijkijki	$2q^2+3q$	ijkij		ijkijkij	q			jkijkijkijki	q
		ijikijikiji	$4q^2+3q$			ijkijkijkij	q^2+q			ijkijkijkijki	$2q$
		ijkijikijki	$3q^2+3q$			ikjikjikjikj	q	ijkijkij		ijkijkijkij	q
		ijkijikjikj	$3q^2+3q$			ijkijkijkijkij	q^3+q^2+q			ijkjkijkijkij	q^2+q
		ijkijkijkij	$4q^2+3q$	ijkji		ijkijikji	q	9	ijikijiki	ijkikijikijk	q
		ikjikjikjikj	q^3+3q^2+3q			ijkijkijki	q			ijkijikijki	q
		ijkjikijikij	q^3+4q^2+3q			ijkijikjikji	q^2+q			ijkikijikjiki	$3q$
		ijkijikijikji	q^3+4q^2+3q			ijkijkijkijki	q^2+q			ijkijikijikji	$2q$
		ijkijkijkijki	$2q^3+4q^2+3q$	6	ijikij	ijkijikij	q			jikijikijkijk	$2q$
		ijkjikijkijkj	q^3+4q^2+3q			jikijikij	q			jkijkijkijkijk	q
		ijkijikijikij	$2q^3+4q^2+3q$			ijkijikij	$2q$	ijkikijkij		ijkikijikijk	q
		ijkijkijkijkij	$4q^3+4q^2+3q$			jkijkijkij	q			ijkijkijkij	q
	ijk	ijkijk	q			ijkjkijkij	$2q$			jkijkijkijki	q
		ikjikjik	q			ikjikjikjikj	q			ijkikjikijkij	$3q$
		ijkijkijk	q^2+q			ijkijkijikij	q^2+2q			ijkijikijikij	$2q$
		ikjikjikjik	q^2+q			jikijikijikj	q^2+2q			ijkikjkijkijki	$2q$
		ijkijkijkijk	q^3+q^2+q			jikjikjikjikj	$2q$			jikijkijkijki	$2q$
		ikjikjikjikjik	q^3+q^2+q			jkijkijkijkij	q^2+2q			ijkijkijkijkij	$3q$
4	ijik	ijkijik	q			ijikijikijikij	$2q^2+2q$	ijkijikij		ijkijikijikij	q
		ijikijik	$2q$			ijkijkijkijkij	$2q^2+2q$			ijkijkijkijkij	q
		ikjikjik	q	ijkijk		ijkijkijk	q	ijkijikji		ijkijikijikji	q
		ijkijkijk	$2q$			ijkijkijkijk	q^2+q	ijkijkijk		ijkijkijkijk	q
		ikjikjikjikj	q^2+2q			ikjikjikjikjik	q	10	ijikijikij	ijkijikijikij	q
		ikjikjikjik	q^2+2q	7	ijikiji	ijikijikij	q			jikijikijikij	q
		ijikijikijik	$2q^2+2q$			ijikijikiji	$3q$			ijikijikijikij	$2q$
		ijkijkijkijk	$2q^2+2q$			ijkijkijkij	$2q$	ijikijkijk		ijkijikijkijk	q
		ikjikjikjikjik	q^3+2q^2+2q			ikjikjikjikj	q			jikijikijkijk	q
	ijki	ijkijki	q			ijkijikijikij	q^2+2q			ijkijkijkijkij	$2q$
		ijkijkijki	q^2+q			ijkijikijikji	q^2+3q			jkijkijkijkijk	q
		ikjikjikji	q			ijkijkijkijkij	$3q$	ijkijkijki		ijkijkijkijki	q
5	ijiki	ijikijik	q	ijikijk		ijkijikij	q			ijkijikijkijk	q
		ijikijki	q			ijkijkijk	q	ijikijkijki		ijkijikijkijk	q
		jkijkijk	q			jkijkijkij	q			ijkijkijkijki	q
		ijkijiki	$3q$			ijkijikijk	$3q$			jkijkijkijkijk	q
		ijkijikji	$2q$			ijkijikijik	$2q$	ijkijkijkij		ijkijkijkijkij	q
		ijkijkijk	$2q$			ijkijkijkij	$2q$				

A second check is provided by the $\mathscr{W}_N$ minimal models, which are the quantum Hamiltonian reduction of the affine KM algebra $g=\mathrm{sl}_N$ with respect to the principal sl_2 embedding. Consider the dominant weights λ with W_λ isomorphic to W,[22]

$$\lambda+\rho=w(\Lambda^+-t\Lambda^-), \tag{47}$$

TABLE V. Multiplicities $P^{IJ}_{x,y}(1)$ and Hasse diagram for the coset $a_2\backslash\hat{a}_2/a_2$.

P^{IJ}	$\{2,3\},\{2,3\}$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	(h,w)
1	e	1	2	1	1	3	2	2	4	1	1	3	3	5	2	2	$(0,0)$
2	1	·	1	1	1	2	2	2	3	1	1	3	3	4	2	2	$(1,0)$
3	1231	·	·	1	·	1	2	1	2	1	1	3	2	3	2	2	$(3,-2)$
4	1321	·	·	·	1	1	1	2	2	1	1	2	3	3	2	2	$(3,2)$
5	12321	·	·	·	·	1	1	1	2	1	1	2	2	3	2	2	$(4,0)$
6	1231231	·	·	·	·	·	1	·	1	1	·	2	1	2	2	1	$(7,-6)$
7	1321321	·	·	·	·	·	·	1	1	·	1	1	2	2	1	2	$(7,6)$
8	123121321	·	·	·	·	·	·	·	1	·	·	1	1	2	1	1	$(9,0)$
9	1231231231	·	·	·	·	·	·	·	·	1	·	1	·	1	2	·	$(12,-16)$
10	1321321321	·	·	·	·	·	·	·	·	·	1	·	1	1	·	2	$(12,16)$
11	12312131231	·	·	·	·	·	·	·	·	·	·	1	·	1	1	·	$(13,-12)$
12	12321321321	·	·	·	·	·	·	·	·	·	·	·	1	1	·	1	$(13,12)$
13	1231213121321	·	·	·	·	·	·	·	·	·	·	·	·	1	·	·	$(16,0)$
14	1231231231231	·	·	·	·	·	·	·	·	·	·	·	·	·	1	·	$(19,-30)$
15	1321321321321	·	·	·	·	·	·	·	·	·	·	·	·	·	·	1	$(19,30)$



where $t=p/p'(p,p'$ relative prime integers), $\Lambda^+\in P^p_{++}$, $\Lambda^- \in P^{p'-1}_{++}$, and w is an arbitrary element of the Weyl group W of $\overline{g}$. The simple roots of $\Delta^{re}_{\lambda,+}$ are given by $\hat{\alpha}_i=w(\alpha_i)+\Lambda_i^-\delta$. Let $\hat{s}_i=r_{\hat{\alpha}_i}$. Then

(1) W_λ is generated by the simple reflections $\hat{s}_i$,
(2) W^0_λ is generated by the $\hat{s}_i$ for which $\Lambda_i^+=0$,
(3) W^r_λ is generated by the $\hat{s}_i$ for which $\Lambda_i^-=0$ and α_i is a simple root of g_r.

The $\mathscr{W}_N$ minimal models arise from dominant weights (47) which have trivial W^0_λ and W^r_λ, hence $\Lambda^+-\rho\in P^{p-N}_{++}$ and $\Lambda^- - \overline{\rho} \in P^{p'-N}_{++}$. The multiplicities $Q_{e,w}$ for these regular dominant weights are easily read off from the recursion relation (27) for $x=e$, since in that case $Q_{e,ys}=Q_{e,y}$ for all $sy>y$, so it follows that $Q_{e,w}=1$. This reproduces the character formulas of Refs. 5 and 12 for the $\mathscr{W}_N$ minimal models. Similarly, admissible modules for arbitrary $\mathscr{W}$ algebras can be obtained. As should be clear from above, the only difference will be in the domain of Λ^-.

New test cases for weights λ with $W_\lambda\cong W$ arise when one considers nontrivial subgroups W^0_λ and/or W^r_λ and nondominant highest weights. In the next section we will do this for the case of the $\mathscr{W}_3$ algebra.

B. Classification of $\mathscr{W}_3$ modules

The Zamolodchikov algebra $\mathscr{W}_3$ (Ref. 1) is the quantum Hamiltonian reduction of the affine KM algebra sl_3 with respect to the principal sl_2 subalgebra.[27] The W_3 weights are (h,w,c), the eigenvalues of the zero modes L_0W_0, and c, respectively. The parametrization of the $\mathscr{W}_3$ weights in terms of the sl_3 weight λ that follows from the BRST construction is

TABLE VI. Multiplicities $P^{IJ}_{x,y}(1)$ and Hasse diagram for the coset $a_2\backslash\hat{a}_2/a'_2$.

P^{IJ}	$\{2,3\},\{1,3\}$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	(h,w)
1	e	1	1	2	2	1	3	1	3	2	4	2	1	4	3	1	$(\frac{1}{3},\frac{2}{27})$
2	12	·	1	1	2	1	2	1	3	2	3	2	1	4	3	1	$(\frac{4}{3},-\frac{16}{27})$
3	132	·	·	1	1	1	2	1	2	2	3	2	1	3	3	1	$(\frac{7}{3},\frac{20}{27})$
4	12312	·	·	·	1	·	1	1	2	1	2	2	1	3	2	1	$(\frac{13}{3},-\frac{70}{27})$
5	132132	·	·	·	·	1	1	·	1	2	2	1	1	2	3	1	$(\frac{16}{3},\frac{128}{27})$
6	1232132	·	·	·	·	·	1	·	1	1	2	1	1	2	2	1	$(\frac{19}{3},\frac{56}{27})$
7	12312312	·	·	·	·	·	·	1	1	·	1	2	·	2	1	1	$(\frac{25}{3},-\frac{250}{27})$
8	123121312	·	·	·	·	·	·	·	1	·	1	1	·	2	1	1	$(\frac{28}{3},-\frac{160}{27})$
9	132132132	·	·	·	·	·	·	·	·	1	1	·	1	1	2	·	$(\frac{31}{3},\frac{308}{27})$
10	12312132132	·	·	·	·	·	·	·	·	·	1	·	·	1	1	·	$(\frac{37}{3},\frac{110}{27})$
11	12312312312	·	·	·	·	·	·	·	·	·	·	1	·	1	·	1	$(\frac{43}{3},-\frac{520}{27})$
12	132132132132	·	·	·	·	·	·	·	·	·	·	·	1	·	1	·	$(\frac{49}{3},\frac{686}{27})$
13	1231213121312	·	·	·	·	·	·	·	·	·	·	·	·	1	·	·	$(\frac{49}{3},-\frac{286}{27})$
14	1232132132132	·	·	·	·	·	·	·	·	·	·	·	·	·	1	·	$(\frac{52}{3},\frac{52}{27})$
15	12312312312312	·	·	·	·	·	·	·	·	·	·	·	·	·	·	1	$(\frac{64}{3},\frac{64}{27})$

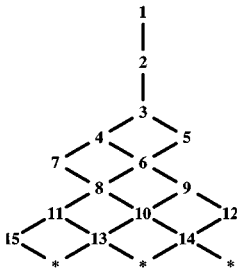
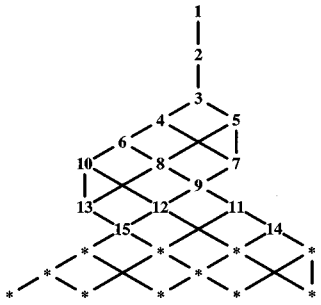


TABLE VII. Multiplicities $P^{IJ}_{x,y}(1)$ and Hasse diagram for the coset $a_2\backslash\hat{a}_2/a_1$.

P^{IJ}	$\{2,3\},\{3\}$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	(h,w)
1	e	1	1	2	2	1	2	1	2	4	1	2	3	1	2	4	$(-\frac{1}{3},\frac{1}{27})$
2	1	·	1	1	1	1	2	1	2	3	1	2	2	1	2	4	$(\frac{2}{3},\frac{10}{27})$
3	12	·	·	1	1	1	1	1	1	3	1	2	2	1	2	3	$(\frac{5}{3},-\frac{35}{27})$
4	132	·	·	·	1	·	1	1	1	2	1	1	2	1	2	3	$(\frac{8}{3},\frac{28}{27})$
5	1231	·	·	·	·	1	·	1	1	2	·	2	1	1	2	2	$(\frac{11}{3},-\frac{125}{27})$
6	1321	·	·	·	·	·	1	·	1	1	1	1	1	1	1	3	$(\frac{14}{3},\frac{154}{27})$
7	12312	·	·	·	·	·	·	1	·	1	·	1	1	·	2	1	$(\frac{20}{3},-\frac{260}{27})$
8	12321	·	·	·	·	·	·	·	1	1	·	1	1	1	1	2	$(\frac{17}{3},\frac{55}{27})$
9	123121	·	·	·	·	·	·	·	·	1	·	1	1	·	1	1	$(\frac{23}{3},-\frac{143}{27})$
10	132132	·	·	·	·	·	·	·	·	·	1	·	1	1	·	2	$(\frac{23}{3},\frac{343}{27})$
11	1231231	·	·	·	·	·	·	·	·	·	·	1	·	·	1	·	$(\frac{32}{3},-\frac{440}{27})$
12	1232132	·	·	·	·	·	·	·	·	·	·	·	1	·	·	1	$(\frac{29}{3},\frac{91}{27})$
13	1321321	·	·	·	·	·	·	·	·	·	·	·	·	1	·	1	$(\frac{35}{3},\frac{595}{27})$
14	12312312	·	·	·	·	·	·	·	·	·	·	·	·	·	1	·	$(\frac{44}{3},-\frac{836}{27})$
15	12321321	·	·	·	·	·	·	·	·	·	·	·	·	·	·	1	$(\frac{38}{3},\frac{442}{27})$



$$h=\frac{1}{2t}\,|\overline{\lambda}+\overline{\rho}|^2+\frac{c-2}{24},\quad w=\frac{1}{27t(t-1)}\,(\overline{\lambda}+\overline{\rho},\Lambda_1)(\overline{\lambda}+\overline{\rho},\Lambda_2)(\overline{\lambda}+\overline{\rho},\Lambda_1-\Lambda_2),\tag{48}$$

with $c=50-24t-24/t$ for $t=k+3$. The character of a $\mathscr{W}_3$ Verma module is given by $\mathrm{ch}\,M^r(\lambda)=q^h\eta(q)^2$ [note that if $t=1$, the parametrization (48) is singular, in that case one replaces $w\to(t-1)w$].

Up to isomorphism, there are two nontrivial parabolic subgroups of the affine Weyl group $\hat{a}_2$ of sl_3, namely $a_1\simeq Z_2$ and $a_2\simeq D_3$. This gives rise to nine inequivalent double cosets [we eliminated the invariance of the $\mathscr{W}_3$ weights under $(t,\lambda)\to(1/t,-\lambda/t)$, which interchanges W^0_λ and W^r_λ] (see Table II). For each of these double cosets, we computed the multiplicities $P^{IJ}_{w,w'}(1)$ (for the first 15 elements) from the KL polynomials $P_{w,w'}(q)$ of sl_3. Together with the KL polynomials $Q_{w,w'}(q)$ these are given in Tables III and IV.[28] Together with the associated Hasse diagrams, they are given in Tables V–XIII.

To check if the polynomials and Hasse diagrams correspond with multiplicities and embedding diagrams of $\mathscr{W}$ Verma modules, we subsequently calculated (parts of) the irreducible characters and embedding patterns directly on the Verma module.

This goes as follows. Starting from a highest weight vector v_a (eigenvector of L_0, W_0, c with eigenvalues h,w,c, and annihilated by the L_n, W_n for $n>0$) a basis $M(a)_{h+N}$ of the Verma

TABLE VIII. Multiplicities $P^{IJ}_{x,y}(1)$ and Hasse diagram for the coset $a_2'\backslash\hat{a}_2/a_1$.

P^{IJ}	$\{2,3\},\{1\}$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	(h,w)
1	e	1	1	1	1	1	3	2	2	2	2	2	2	5	1	1	(0,0)
2	12	·	1	·	1	1	2	2	1	2	2	2	2	4	1	1	(1,−1)
3	13	·	·	1	1	1	2	1	2	2	2	2	2	4	1	1	(1,1)
4	123	·	·	·	1	·	1	1	1	2	1	2	1	3	1	1	(3,−3)
5	132	·	·	·	·	1	1	1	1	1	2	1	2	3	1	1	(3,3)
6	1232	·	·	·	·	·	1	1	1	1	1	1	1	3	1	1	(4,0)
7	12312	·	·	·	·	·	·	1	·	1	·	1	1	2	1	·	(6,−6)
8	13213	·	·	·	·	·	·	·	1	·	1	1	1	2	·	1	(6,6)
9	123123	·	·	·	·	·	·	·	·	1	·	1	·	1	1	·	(9,−15)
10	132132	·	·	·	·	·	·	·	·	·	1	·	1	1	·	1	(9,15)
11	1231213	·	·	·	·	·	·	·	·	·	·	1	·	1	·	·	(10,−10)
12	1232132	·	·	·	·	·	·	·	·	·	·	·	1	1	·	·	(10,10)
13	12312132	·	·	·	·	·	·	·	·	·	·	·	·	1	·	·	(12,0)
14	12312312	·	·	·	·	·	·	·	·	·	·	·	·	·	1	·	(13,−27)
15	13213213	·	·	·	·	·	·	·	·	·	·	·	·	·	·	1	(13,27)

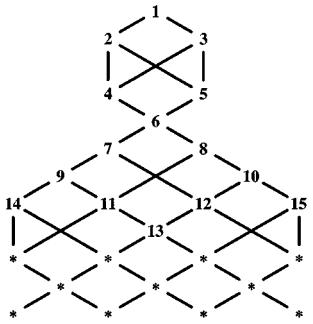
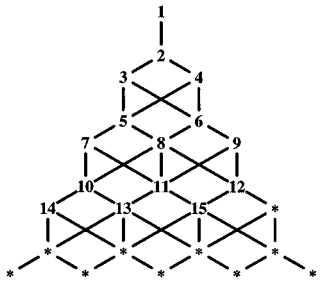


TABLE IX. Multiplicities $P^{IJ}_{x,y}(1)$ and Hasse diagram for the coset $a_2\backslash\hat{a}_2$.

P^{IJ}	$\{2,3\},\emptyset$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	(h,w)
1	e	1	1	1	1	2	2	1	2	1	2	3	2	2	1	2	$(-1,0)$
2	1	·	1	1	1	1	1	1	1	1	2	3	2	2	1	2	$(0,0)$
3	12	·	·	1	·	1	1	1	1	1	2	2	1	2	1	1	$(1,-1)$
4	13	·	·	·	1	1	1	1	1	1	1	2	2	1	1	2	$(1,1)$
5	123	·	·	·	·	1	·	1	1	·	1	1	1	1	1	1	$(3,-2)$
6	132	·	·	·	·	·	1	·	1	1	1	1	1	1	1	1	$(3,2)$
7	1231	·	·	·	·	·	·	1	·	·	1	1	·	1	1	1	$(5,-5)$
8	1232	·	·	·	·	·	·	·	1	·	1	1	1	1	1	1	$(4,0)$
9	1321	·	·	·	·	·	·	·	·	1	·	1	1	1	·	1	$(5,5)$
10	12312	·	·	·	·	·	·	·	·	·	1	·	·	1	1	·	$(8,-8)$
11	12321	·	·	·	·	·	·	·	·	·	·	1	·	1	·	1	$(7,0)$
12	13213	·	·	·	·	·	·	·	·	·	·	·	1	·	·	1	$(8,8)$
13	123121	·	·	·	·	·	·	·	·	·	·	·	·	1	·	·	$(9,-5)$
14	123123	·	·	·	·	·	·	·	·	·	·	·	·	·	1	·	$(11,-14)$
15	123213	·	·	·	·	·	·	·	·	·	·	·	·	·	·	1	$(9,5)$



module at depth N is constructed. The rank of the innerproduct matrix (Shapovalov form) at depth N gives the dimension of the irreducible character at depth N, and the eigenvectors of W_0 in the kernel of L_1, L_2, and W_1 gives the singular vectors.

In practice, even at modest depth these calculations require much computer time: with the Mathematica routines we had available, the singular vectors could generically be determined up to depth 9, and the characters up to depth 6. To appreciate the effectiveness of the KL conjecture: applying Table III to the vacuum module for $c=0$ the characters are already determined beyond depth 200, where the Verma module has of the order of 10^{20} states. To verify the predictions of the conjectures, we selected a dominant weight with every coset such that the singular vectors in the associated Verma module occur at the lowest possible levels (see Table II). For every coset we computed the characters of the first 15 submodules, and reconstructed the embedding patterns. We found complete agreement with the KL conjecture.

C. Closed character formulas

The practical upshot of the KL conjectures is that characters of $\mathscr{W}$ algebras can be computed using only the combinatorics of double cosets of affine Weyl groups. In general, however, the word problem posed by the recursion relation (27) is too complicated to solve in closed form. Only in certain special cases, one does get a closed expression for character formulas, as in the case of the Virasoro algebra ($Q_{x,y}=1$ for $x\leqslant y$) and the $\mathscr{W}_N$ minimal models ($Q_{e,y}=1$). We end this section by discussing two more examples where a closed formula can be obtained: cosets of type $W\backslash W$ and of type $W\backslash W/W$.

TABLE X. Multiplicities $P^{IJ}_{x,y}(1)$ and Hasse diagram for the coset $a_1\backslash\hat{a}_2/a_1$.

P^{IJ}	$\{3\},\{3\}$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	(h,w)
1	e	1	1	1	2	2	2	1	1	2	2	2	2	2	2	2	$(-\frac{1}{9},-\frac{1}{81})$
2	1	·	1	·	1	1	1	1	1	2	2	1	1	2	2	1	$(\frac{17}{9},-\frac{55}{81})$
3	2	·	·	1	1	1	1	1	1	1	1	2	2	2	1	2	$(\frac{8}{9},-\frac{29}{81})$
4	12	·	·	·	1	·	1	1	·	1	1	1	1	2	1	1	$(\frac{35}{9},-\frac{595}{81})$
5	21	·	·	·	·	1	1	·	1	1	1	1	1	1	1	1	$(\frac{44}{9},\frac{836}{81})$
6	121	·	·	·	·	·	1	·	·	1	1	1	1	1	1	1	$(\frac{53}{9},\frac{323}{81})$
7	132	·	·	·	·	·	·	1	·	·	1	1	·	1	1	1	$(\frac{44}{9},-\frac{136}{81})$
8	231	·	·	·	·	·	·	·	1	1	·	·	1	1	1	1	$(\frac{62}{9},-\frac{190}{81})$
9	1231	·	·	·	·	·	·	·	·	1	·	·	·	1	1	·	$(\frac{107}{9},-\frac{2755}{81})$
10	1321	·	·	·	·	·	·	·	·	·	1	·	·	·	1	·	$(\frac{98}{9},\frac{2618}{81})$
11	2132	·	·	·	·	·	·	·	·	·	·	1	·	·	·	1	$(\frac{80}{9},\frac{1760}{81})$
12	2312	·	·	·	·	·	·	·	·	·	·	·	1	1	·	1	$(\frac{89}{9},-\frac{1729}{81})$
13	12312	·	·	·	·	·	·	·	·	·	·	·	·	1	·	·	$(\frac{152}{9},-\frac{5320}{81})$
14	12321	·	·	·	·	·	·	·	·	·	·	·	·	·	1	·	$(\frac{134}{9},-\frac{406}{81})$
15	21312	·	·	·	·	·	·	·	·	·	·	·	·	·	·	1	$(\frac{107}{9},-\frac{325}{81})$

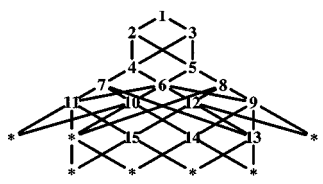
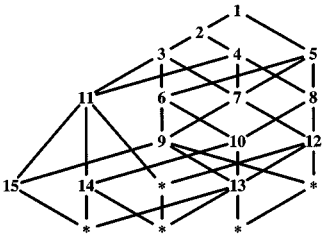


TABLE XI. Multiplicities $P^{IJ}_{x,y}(1)$ and Hasse diagram for the coset $a_1\backslash\hat{a}_2/a_1'$.

P^{IJ}	$\{3\},\{2\}$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	(h,w)
1	e	1	1	1	1	1	1	2	1	2	2	1	2	3	1	1	$(\frac{2}{9},\frac{10}{81})$
2	1	·	1	1	1	·	1	1	1	1	2	1	1	3	1	1	$(\frac{20}{9},-\frac{260}{81})$
3	13	·	·	1	·	·	1	1	·	1	1	1	1	2	1	1	$(\frac{29}{9},\frac{91}{81})$
4	21	·	·	·	1	·	·	1	1	1	1	1	1	2	1	1	$(\frac{38}{9},\frac{442}{81})$
5	23	·	·	·	·	1	1	1	1	2	2	·	2	2	1	1	$(\frac{11}{9},-\frac{125}{81})$
6	123	·	·	·	·	·	1	·	·	1	1	·	·	1	1	1	$(\frac{47}{9},-\frac{665}{81})$
7	213	·	·	·	·	·	·	1	·	1	·	·	1	1	·	1	$(\frac{65}{9},\frac{1495}{81})$
8	231	·	·	·	·	·	·	·	1	·	1	·	1	1	1	·	$(\frac{68}{9},-\frac{935}{81})$
9	1213	·	·	·	·	·	·	·	·	1	·	·	·	1	·	1	$(\frac{74}{9},\frac{874}{81})$
10	1231	·	·	·	·	·	·	·	·	·	1	·	·	1	1	·	$(\frac{119}{9},-\frac{3689}{81})$
11	1321	·	·	·	·	·	·	·	·	·	·	1	·	·	1	1	$(\frac{83}{9},\frac{2197}{81})$
12	2131	·	·	·	·	·	·	·	·	·	·	·	1	1	·	·	$(\frac{89}{9},\frac{253}{81})$
13	12131	·	·	·	·	·	·	·	·	·	·	·	·	1	·	·	$(\frac{128}{9},-\frac{2852}{81})$
14	12321	·	·	·	·	·	·	·	·	·	·	·	·	·	1	·	$(\frac{137}{9},-\frac{2015}{81})$
15	13213	·	·	·	·	·	·	·	·	·	·	·	·	·	·	1	$(\frac{128}{9},\frac{3952}{81})$



1. The coset $\overline{W}\backslash W$

Consider a coset of the form $\overline{W}\backslash W$, with W the affine Weyl group and $\overline{W}$ the corresponding finite Weyl group. These cosets correspond to modules on the boundary of the Kac table (type III^0 of the Virasoro), where the characters are given by finite sums over Verma characters.

For the $\mathscr{W}_3$ algebra $W=\hat{a}_2$ and $W=a_2$. The KL polynomials $P^{IJ}_{x,y}$ and Hasse diagram of $a_2\backslash\hat{a}_2$ are given in Table IX. In that case it can be shown that there are two different character formulas, depending only on the length of $\underline{w}$ (the minimal representative of w in the coset). If the length $l(\underline{w})$ is odd, there are precisely two adjacent elements of $\underline{w}$ of length $l(\underline{w})+1$, of the form $\underline{w}.j$ and $\underline{w}.k$ (where j and k are distinct simple reflections). Let a_2 denote the a_2 generated by j and k. Then the character reads

$$\mathrm{ch}\, L(w.\lambda)=\sum_{x\in a_2}\epsilon_x\,\mathrm{ch}\, M(w.x.\lambda). \tag{49}$$

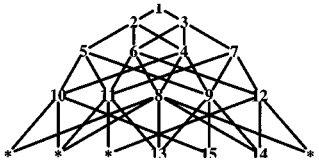
If the length $l(\underline{w})$ is even, there are at most three adjacent elements of $\underline{w}$ of length $l(\underline{w})+1$, and there is precisely one of the form $\underline{w}.i$ (for i a simple reflection). Then we find

$$\mathrm{ch}\, L(w.\lambda)=\sum_{x\in a_2}\epsilon_x(\mathrm{ch}\, M(w.i.x.i.\lambda)-\mathrm{ch}\, M(w.i.x.\lambda)), \tag{50}$$

where again the a_2 is generated by j,k (i,j,k are distinct simple reflections).

TABLE XII. Multiplicities $P^{IJ}_{x,y}(1)$ and Hasse diagram for the coset $a_1\backslash\hat{a}_2$.

P^{IJ}	$\{3\},\emptyset$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	(h,w)
1	e	1	1	1	1	1	1	1	1	2	1	2	1	2	2	1	(0,0)
2	1	·	1	·	1	1	1	·	1	1	1	1	1	1	2	1	(1,−1)
3	2	·	·	1	1	·	1	1	1	1	1	1	1	1	1	1	(1,1)
4	12	·	·	·	1	·	·	·	1	1	1	·	·	1	1	1	(3,−5)
5	13	·	·	·	·	1	·	·	·	1	1	1	·	1	1	1	(2,2)
6	21	·	·	·	·	·	1	·	1	·	·	1	1	1	1	·	(3,5)
7	23	·	·	·	·	·	·	1	·	1	·	1	1	1	1	1	(2,−2)
8	121	·	·	·	·	·	·	·	1	·	·	·	·	1	1	·	(4,0)
9	123	·	·	·	·	·	·	·	·	1	·	·	·	1	1	1	(6,−14)
10	132	·	·	·	·	·	·	·	·	·	1	·	·	·	·	1	(5,5)
11	213	·	·	·	·	·	·	·	·	·	·	1	·	1	·	·	(6,14)
12	231	·	·	·	·	·	·	·	·	·	·	·	1	·	1	·	(5,−5)
13	1213	·	·	·	·	·	·	·	·	·	·	·	·	1	·	·	(8,0)
14	1231	·	·	·	·	·	·	·	·	·	·	·	·	·	1	·	(10,−30)
15	1232	·	·	·	·	·	·	·	·	·	·	·	·	·	·	1	(7,−7)



It appears that these two formulas are related to the generic decomposition patterns of Weyl modules, studied in Ref. 29. Similarly, there is 1 formula in the case of A_1, 4 different formulas for B_2, and 12 for G_2.

These character formulas apply in particular to the $(p,1)$ topological minimal models. The admissible weights (47) in that case are integral, hence $W_\lambda^r = W$. The regular integral weights

$$(\lambda+\rho,\alpha_i^\vee) \neq 0 \bmod p \tag{51}$$

are on the orbit of the coset $\overline{W}\backslash W$, with dominant weights $\lambda \in P_{++}^p$. For $\mathscr{W}_3$ therefore, provided $p \geqslant 3$, (49) and (50) give the character formulas for all the regular weights. We observe that (51) is exactly the condition for the physical states in $(p,1)$ topological minimal matter coupled to W-gravity.[30] An interesting open question is whether the nontrivial multiplicities indicate the presence of extra physical states.

The character formulas (49) and (50) apply in other cases as well, for instance (i) for regular integral weights on the boundary of the (p,p') Kac table, (ii) for weights with $W_\lambda^0 = W$ and W_λ^r trivial (interchanging left and right multiplication), and (iii) for the other $g = \mathrm{sl}_3$ related $\mathscr{W}$ algebras ($W_3^{(2)}$ and sl_3 itself).

2. The coset $\overline{W}\backslash W/\overline{W}$

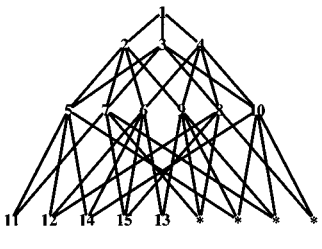
Consider a coset of the form $\overline{W}\backslash W/\overline{W}$, with W an affine Weyl group and $\overline{W}$ a subgroup isomorphic to the finite Weyl group W. These cosets correspond to modules in a corner of the Kac table (type III^{00} of the Virasoro), where again the characters are given by finite sums over Verma characters, but in addition they are now grouped in $\overline{g}$ multiplets. Specifically, the multiplicities $P_{x,y}^{IJ}(1)$ are related to the dimension of weight spaces in finite-dimensional modules of the simple Lie algebra $\overline{g}$.[31] The correspondence is as follows. First consider the case where the embedding of the left and right subgroups is the same and given by W (depending on g there may be more ways to embed W in W). Since $W = W \cdot Q$ (semidirect product) and in Q there is a unique dominant element α on each W orbit, it follows that there is a one-to-one correspondence between coset elements $w \in W\backslash W/W$ and dominant roots $\overline{\alpha}_w \in P_+ \cap Q$. More generally, if the embeddings are chosen differently, this correspondence is between coset elements $w \in W\backslash W/W'$ and dominant weights $\lambda \in P_+ \cap Q + \Lambda_i$, where Λ_i is the fundamental weight that determines the embedding: W' is generated by the set of simple reflections s_j for $j \neq i$. Then the result of Ref. 31 states that

$$P_{w,w'}^{IJ}(1) = \dim L(\overline{\lambda}_{w'})_{\overline{\lambda}_w}, \tag{52}$$

where $L(\overline{\lambda})_{\overline{\mu}}$ is the weight space of weight $\overline{\mu}$ in the (finite dimensional) irreducible $\overline{g}$ module of highest weight λ.

TABLE XIII. Multiplicities $P_{x,y}^{IJ}(1)$ and Hasse diagram for $\hat{a}_2$.

P^{IJ}	$\emptyset,\emptyset$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	(h,w)
1	e	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	$(0,0)$
2	1	·	1	·	·	1	1	1	·	1	·	1	1	1	1	1	$(2,0)$
3	2	·	·	1	·	1	·	1	1	·	1	1	1	·	1	1	$(1,-1)$
4	3	·	·	·	1	·	1	·	1	1	1	·	1	1	1	1	$(1,1)$
5	12	·	·	·	·	1	·	·	·	·	·	1	1	·	1	·	$(4,-10)$
6	13	·	·	·	·	·	1	·	·	·	·	·	1	1	1	1	$(4,10)$
7	21	·	·	·	·	·	·	1	·	·	·	1	·	·	·	1	$(5,15)$
8	23	·	·	·	·	·	·	·	1	·	·	·	1	·	·	1	$(3,-7)$
9	31	·	·	·	·	·	·	·	·	1	·	·	·	1	·	·	$(5,-15)$
10	32	·	·	·	·	·	·	·	·	·	1	·	·	·	1	·	$(3,7)$
11	121	·	·	·	·	·	·	·	·	·	·	1	·	·	·	·	$(6,6)$
12	123	·	·	·	·	·	·	·	·	·	·	·	1	·	·	·	$(8,-22)$
13	131	·	·	·	·	·	·	·	·	·	·	·	·	1	·	·	$(6,-6)$
14	132	·	·	·	·	·	·	·	·	·	·	·	·	·	1	·	$(8,22)$
15	213	·	·	·	·	·	·	·	·	·	·	·	·	·	·	1	$(9,35)$



This result applies in particular to the $\mathscr{W}_N$ algebras with $c=\mathrm{rank}(\overline{g})$, i.e., with $k+h^\vee=1$. From (47) it follows that the dominant weight is determined by a level 1 weight, i.e., $\lambda+\rho=\Lambda_i$. Here $W^r_\lambda=W$ and $W^0_\lambda=W'$. Using the correspondence described above, to every primitive weight $\mu=w.\lambda$ one associates the dominant weight $\lambda_w=\overline{\mu}+\overline{\rho}$. Then the sum $w'\geqslant w$ can be rewritten as follows:

$$\mathrm{ch}\ M^r(\mu)=\sum_{\overline{\mu'}\geqslant\overline{\mu}}\dim L(\overline{\mu'}+\overline{\rho})_{\overline{\mu+\rho}}\,\mathrm{ch}\ L^r(\mu'). \tag{53}$$

Inverting this [using the basis transformation from Verma modules $M(\overline{\mu})$ to singlets $e^{\overline{\mu}}$] gives

$$\mathrm{ch}\ L^r(\mu)=\sum_{x\in W}\epsilon_x\ \mathrm{ch}\ M^r(\mu+\rho-x(\rho)). \tag{54}$$

This character formula was first proposed in Ref. 32, where it was obtained as a limit of the characters of the $\mathscr{W}_N$ minimal models.[5] The inverse formula (53) was obtained for $\mathscr{W}_3$ in Ref. 33, using an explicit construction of the singular vectors in the Fock space and comparison of the characters for each side. Again, this character formula applies more generally, in particular to the weights in a corner of the (p,p') Kac table [in that case one replaces $\rho\to p\rho$ everywhere on the rhs of (54)].

V. CONCLUDING REMARKS

In this paper we have formulated the KL conjecture for $\mathscr{W}$ algebras associated with arbitrary sl_2 reductions. The result can be described in terms of a double coset $W^r_\lambda\backslash W_\lambda/W^0_\lambda$: the Hasse diagram gives the embedding diagram of the Verma modules, and the KL polynomials give the multiplicities in the characters.

The conjectures also apply to finite $\mathscr{W}$ algebras, which are the Hamiltonian reduction of simple Lie algebras $\overline{g}$.[13] In that case one simply takes W to be the Weyl group W of $\overline{g}$. The character formulas for this class of algebras are given in Ref. 14 (for regular integral weights only) and the results agree completely.

We remark that the conjecture is also a useful tool to analyze the structure of the Verma modules in more detail. This is particularly important if one attempts to construct a resolution of the irreducible modules by Verma modules. The physical motivation for doing so is the application to $\mathscr{W}$ gravity/strings: it is much simpler to compute the (string) BRST cohomology on Verma modules than on irreducible modules. The problem is that it is not always possible to find a resolution by Verma modules. For instance, for the $\mathscr{W}_3$ string at $c=2$ it is found by explicit construction[33] that there is no resolution by Verma modules, but instead one is forced to introduce generalized Verma modules. This is directly linked to the existence of primitive vectors that are pseudo-singular rather than singular (they are not an eigenvector of W_0). For such an analysis it is convenient to have the data presented by the KL conjecture. This way, for instance, one can easily show that the character (50) of the $(p,1)$ topological minimal models for $\mathscr{W}_3$ cannot be reproduced by a resolution by (generalized) Verma modules. This is due to the occurrence of subsingular vectors.[14] It would be very interesting to know what type of modules are needed to build such a resolution, since these modules are going to carry the cohomology of the topological $\mathscr{W}_3$ string. Work on this is in progress.

APPENDIX

1. KL Polynomials on Coxeter groups

In this Appendix, we summarize the definition and some of the properties of KL polynomials $P_{x,y}$ for a Coxeter group W, (for details see Refs. 7 and 17). The starting point is the Hecke algebra $\mathscr{H}$ with generators T_y (one for each $y\in W$) and defining relations

$$T_x T_y = T_{xy} \quad \text{if } l(xy) = l(x) + l(y), \tag{A1}$$

$$(T_s + 1)(T_s - q) = 0 \quad \text{if } s \in S, \tag{A2}$$

where S is the set of simple reflections that generate W. The elements T_y are invertible in $\mathscr{H}$, and one can write

$$T_{y^{-1}}^{-1} = \sum_{x \leqslant y} \epsilon_x \epsilon_y R_{x,y}(q) q^{-l(y)} T_x, \tag{A3}$$

where $\epsilon_y = (-1)^{l(y)}$, and $R_{x,y}(q)$ is a polynomial in q of degree $l(y) - l(x)$ for $x \leqslant y$, uniquely defined by (A3). The map ι defined by

$$\iota(q) = q^{-1}, \quad \iota(T_y) = T_{y^{-1}}^{-1} \tag{A4}$$

is an automorphism of $\mathscr{H}$. The KL polynomials are associated with the invariants of ι. For any pair $x \leqslant y$ in W, there is a uniquely defined polynomial $P_{x,y}$ of degree $\leqslant (l(y) - l(x) - 1)/2$ if $x < y$, and $P_{x,x} = 1$, such that

$$C_y = \sum_{x \leqslant y} \epsilon_x \epsilon_y q^{l(y)/2 - l(x)} P_{x,y}(q^{-1}) T_x \tag{A5}$$

satisfies

$$\iota(C_y) = C_y \quad \text{for all } y \in W. \tag{A6}$$

Equivalently, the P-polynomials satisfy

$$q^{l(y)-l(x)} P_{x,y}(q^{-1}) = \sum_{x \leqslant z \leqslant y} R_{x,z} P_{z,y}(q) \quad \text{for all } x \leqslant y. \tag{A7}$$

From this, one can extract a recursion relation (expressing the polynomials $P_{x,y}$ in terms of the polynomials $P_{x',y'}$ with $y' < y$). Namely, for $ys > y$ one has[7]

$$P_{x,ys} = q^{1-c} P_{xs,y} + q^c P_{x,y} - q \sum_{\substack{x \leqslant z < y \\ zs < z}} P_{x,z} \not{P}_{z,y}. \tag{A8}$$

Here $c = 1$ if $xs < x$ and 0 otherwise, and $\not{P}_{z,y}$ is the term in $P_{z,y}$ of (maximal) degree $\frac{1}{2}(l(y) - l(z) - 1)$. The initial values of the recursion relation are $P_{x,e}(q) = \delta_{x,e}$. This implies in particular that $P_{x,y}(q) = 0$ unless $x \leqslant y$. From (A8) it also follows that $P_{x,y}(0) = 1$ if $x \leqslant y$. In the case of crystallographic Coxeter groups [which includes (affine) Weyl groups], the coefficients of $P_{x,y}$ give the dimensions of stalks of cohomology sheaves of the intersection cohomology complexes associated to Schubert varieties.[34] This implies, in particular, that these coefficients are non-negative integers.

Similarly, if $ys < y$ it can be shown that $C_y T_s = -C_y$, which implies that

$$P_{x,y} = P_{xs,y} \quad \text{for } x \leqslant y \text{ and } ys < y. \tag{A9}$$

For finite Coxeter groups (where there is a unique longest element w_0) it easily follows that

$$P_{x,w_0} = 1. \tag{A10}$$

2. Inverse KL polynomials on Coxeter groups

The KL polynomials $P_{y,w}$ form an upper triangular matrix with ones on the main diagonal, which naturally can be inverted. Thus, one can define for each $x \leqslant y$ in W a polynomial $Q_{x,y}$ such that

$$\sum_{x \leqslant z \leqslant y} \epsilon_x \epsilon_z P_{x,z} Q_{z,y} = \delta_{x,y} \quad \text{for all } x \leqslant y. \tag{A11}$$

It is clear that $Q_{x,x}(q)=1$ and that $Q_{x,y}(q)$ has degree $\leqslant (l(y)-l(x)-1)/2$ for $x<y$, and $\mathbb{Q}_{x,y}=\mathbb{P}_{x,y}$. It also follows that

$$q^{l(y)-l(x)} Q_{x,y}(q^{-1}) = \sum_{x \leqslant z \leqslant y} Q_{x,z} R_{z,y}(q) \quad \text{for all } x \leqslant y. \tag{A12}$$

The Q-polynomials are also associated to invariants of ι. Define elements S_x, D_x of $\mathscr{H}^*$ by

$$\langle S_x, \iota(T_y) \rangle = \langle D_x, C_y \rangle = \delta_{x,y^{-1}}, \tag{A13}$$

and let $\langle \iota(u), h \rangle = \iota(\langle u, \iota(h) \rangle)$. It follows that $\iota(D_x)=D_x$ and

$$D_x = \sum_{x \geqslant y} q^{l(x)/2-l(y)} Q_{x,y} S_y, \tag{A14}$$

with $Q_{x,y}$ the inverse polynomials (A11). From the right $\mathscr{H}$-action on $\mathscr{H}^*$ given by $\langle u \cdot h, h' \rangle = \langle u, hh' \rangle$ one can conclude that $D_x \cdot T_s = qD_x$ if $xs>x$. This implies

$$Q_{x,ys} = Q_{x,y} \quad \text{for } x \leqslant y \text{ and } xs>x. \tag{A15}$$

From this it easily follows that

$$Q_{e,y}=1 \quad \text{for all } y \in W. \tag{A16}$$

The analog of (A8) for the Q-polynomials is (for $xs<x$)

$$Q_{xs,y} = q^{1-c} Q_{x,ys} + q^c Q_{x,y} - q \sum_{\substack{x<z \leqslant y \\ zs>y}} \mathbb{Q}_{x,z} Q_{z,y}, \tag{A17}$$

with $c=1$ for $ys>y$ and $c=0$ for $ys<y$. In this form (A17) cannot be used to solve for the Q-polynomials (at least not in the case of infinite Coxeter groups). But, combining (A17) and (A15) for $ys>y$, one obtains a useful relation (expressing $Q_{z,w}$ in terms of $Q_{z',w'}$ with $w'<w$)

$$Q_{x,ys} = cQ_{xs,y} + (-q)^c Q_{x,y} + cq \sum_{\substack{x<z \leqslant y \\ zs>z}} \mathbb{Q}_{x,z} Q_{z,y}, \tag{A18}$$

with $c=1$ for $xs<x$ and $c=0$ for $xs>x$. In the case of (affine) Weyl groups the coefficients of $Q_{x,y}$ are again non-negative integers.

In the case of a finite Coxeter group, the KL polynomials P are related to the inverse polynomials Q through

$$Q_{x,y} = P_{w_0 y, w_0 x}. \tag{A19}$$

On the other hand, if the group is not finite, P and Q do not appear to be related in any such way.

3. KL polynomials on cosets

Similar as for ordinary Coxeter groups W, one can also construct KL polynomials on cosets W/W_I (or $W_I\backslash W$), where W_I is a parabolic subgroup of W.[35] In particular, one finds that again there are recursion relations for the associated polynomials $P^I_{x,y}$ and $Q^I_{x,y}$. If the subgroup W_I is finite (which is sufficient for our purposes), the polynomials P^I, Q^I and their inverses $\widetilde{Q}^I$, $\widetilde{P}^I$, defined through

$$\sum_{x\leqslant z\leqslant y} \widetilde{Q}^I_{x,z}P^I_{z,y}=\sum_{x\leqslant z\leqslant y} Q^I_{x,z}\widetilde{P}^I_{z,y}=\delta_{x,y}\,, \tag{A20}$$

can be expressed in terms of the KL polynomials of W:

$$\begin{aligned} &P^I_{x,y}=P_{\overline{x,y}}\,, \quad Q^I_{x,y}=Q_{\underline{x},\underline{y}},\\ &\widetilde{P}^I_{x,y}=\sum_{z\in[x]} P_{\underline{z},\underline{y}}\epsilon_z\epsilon_{\underline{y}}, \quad \widetilde{Q}^I_{x,y}=\sum_{z\in[y]} Q_{\overline{x},z}\epsilon_{\overline{x}}\epsilon_z\,. \end{aligned} \tag{A21}$$

Here $\underline{z}$ is the minimal and $\overline{z}$ is the maximal representative of the coset $[z]$ of z. (Note that this notation is slightly different from the notation used in Ref. 14.)

However, the cosets that play a role in this paper are two-sided cosets $W_I\backslash W/W_J$, with respect to parabolic subgroups W_I and W_J. There does not appear to be an abstract setup for double-sided cosets. In particular, the partial ordering on these cosets is more complicated than in the case of one-sided cosets (for example, the length of adjacent elements may differ by more than 1). So instead of defining KL polynomials through a recursion relation, we take (A21) as our starting point, i.e., we define

$$\begin{aligned} &P^{IJ}_{w,w'}=P_{\overline{w,w'}}\,, \quad Q^{IJ}_{w,w'}=Q_{\underline{w},\underline{w'}}\,,\\ &\widetilde{P}^{IJ}_{w,w'}=\sum_{x\in[w]} P_{x,\underline{w'}}\epsilon_x\epsilon_{\underline{w'}}\,, \quad \widetilde{Q}^{IJ}_{w,w'}=\sum_{x\in[w']} Q_{\overline{w},x}\epsilon_{\overline{w}}\epsilon_x\,, \end{aligned} \tag{A22}$$

where the polynomials $\widetilde{P}^{IJ}$, $\widetilde{Q}^{IJ}$ are again the inverse polynomials

$$\sum_{x\leqslant z\leqslant y} \widetilde{Q}^{IJ}_{x,z}P^{IJ}_{z,y}=\sum_{x\leqslant z\leqslant y} Q^{IJ}_{x,z}\widetilde{P}^{IJ}_{z,y}=\delta_{x,y}\,. \tag{A23}$$

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A noncommutative Hopf structure on $\mathscr{C}^\infty$[SL(2,C)] as a quantum Lorentz group

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We introduce a ''classical'' Fréchet Hopf algebra $\mathscr{A}$ containing the quantum deformation of the enveloping Lorentz algebra of Ogievestky and Wess *et al.* (as a dense Hopf subalgebra). We also show that $\mathscr{A}$ is isomorphic to a quasitriangular twisted topological tensor product Hopf algebra. By duality, we recover on the topological dual space of $\mathscr{A}$, the non-commutative algebra structure introduced by Podles and Woronowicz. Finally, this non-commutative product can be extended to $\mathscr{C}^\infty(SL(2,\mathbb{C}))$ which then becomes a topological Hopf algebra for its natural Fréchet topology. © *1996 American Institute of Physics.* [S0022-2488(96)02306-7]

I. INTRODUCTION

Quantum group theory[1] and the star-product approach to quantum mechanics[2] have a common basis: non-commutative deformations of a commutative algebra. This was made mathematically explicit in the results of Refs. 3–5: for example, every F.R.T. quantum group[6] (corresponding to a semi-simple real Lie group G) is realized as a subalgebra of $\mathscr{C}^\infty(G)$ endowed with a non-commutative product which is a deformation of the usual product of functions. Thus, the idea that the symmetry properties in Quantum Theory are described by a ''quantum group'' is very attractive: some of the failures of the constructive quantum field theory could be explained by the introduction of a ''quantum Poincaré group.''

A first step in such a program is the construction of a well-defined quantum Lorentz group (and its dual version). Taking into account the physical aim, this quantum Lorentz group must contain a Hopf subalgebra $SU_t(2)(q=e^t)$. Consequently, the Drinfeld–Jimbo deformation[1,7] of the enveloping algebra of the Lorentz Lie algebra is not appropriate.

A few years ago, Podles and Woronowiz,[8] Carow-Watamura *et al.*,[9] respectively, have introduced a quantum Lorentz group while a quantum Lorentz enveloping algebra was defined by Ogievestky *et al.*[10] Let us give a brief overview of each of these models.

- The P. W. model is the topological Hopf algebra of the continuous functions on the Lorentz quantum group. The latter is constructed by generators and relations from the fundamental representation of the Woronowicz model $SU_t(2)$ and its Pontryagin dual.
- The C. W. model is obtained from two copies of $SL_t(2)$ in its fundamental representation and a cross relation between the generators of each of them. It is the F.R.T. view.[6]
- The O. S. W. Z. model is a subalgebra of $\mathscr{U}_t(\mathfrak{sl}(2))\otimes\mathscr{U}_t(\mathfrak{sl}(2))(q=e^t)$ which carries an ad-hoc coproduct.

This raises several problems.

1. First, it is not proved that these models are some deformations (for the usual notion[11]) of the corresponding classical model. We only can assert that the quantum relations give the classical relations for $q\to 1$. Thus we cannot directly use the results of Drinfeld on quantum deformations nor those of Refs. 3 and 4.

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2. What relations do there exist between these three models: ''isomorphism,'' ''duality'' (the meaning of these words remaining to be precised)?

3. What is the structure of the O. S. W. Z. model (resp., C. W. model) with respect to the tensor product Hopf algebra $\mathscr{U}_t(\mathfrak{sl}(2))\otimes\mathscr{U}_t(\mathfrak{sl}(2))$ [resp., $SL_t(2)\otimes SL_t(2)$]?

Part of the answers to these questions was more or less given in Ref. 12, Majid asserts that the C. W. model is a double cross product of two copies of $SL_t(2)$; in Ref. 13, the authors obtain the Hopf structure of the O. S. W. Z. model, starting from the algebraic Hopf structure of the P. W. model. Let us remark that all these models are defined by generators and relations.

In this paper, we do not only answer the previous questions but we also realize the above mentioned model either as a classical topological algebra, or, as its topological dual vector space, endowed with various topological Hopf algebra structures. We are reminded that these classical topological models for ''quantum groups'' have been introduced in Refs. 3 and 4 and that one of its features is to define the q-deformed structure together with the classical structure on the same classical topological vector space.

To be more precise, we start with the O. S. W. Z. Hopf algebra,[10] or, more exactly, the Hopf algebra $\mathscr{U}_t\mathscr{L}$ generated by the basis of Schirrmacher and relations[14] (which is larger than the initial O. S. W. Z. model). We introduce a Fréchet topological algebra $\mathscr{A}$ by ''classical'' methods and its topological dual space $\mathscr{H}(G)$ where G is $SL(2,\mathbb{C})\times SL(2,\mathbb{C})$ (the classical algebra of coefficient functions on G for the holomorphic finite-dimensional representations) but we must take into account Problem 1. These topological models provide us the following results.

(i) The algebra $\mathscr{A}$ can be endowed with various topological Hopf structures so that the Hopf algebra $\mathscr{U}_t\mathscr{L}$ and the tensor product Hopf algebra $\mathscr{U}_t(\mathfrak{sl}(2))\otimes\mathscr{U}_t(\mathfrak{sl}(2))$ (including the classical cases $t=0$) are dense Hopf subalgebras of $\mathscr{A}$.

(ii) Denote by Δ_t (resp., δ_t) the coproduct of $\mathscr{U}_t\mathscr{L}$ [resp., $\mathscr{U}_t(\mathfrak{sl}(2))$] and by A_1 (resp., A_2) the topological model of $(\mathscr{U}_t(\mathfrak{sl}(2)),\delta_t)$ [resp., $(\mathscr{U}_t(\mathfrak{sl}(2)),\delta_t^{op})$] introduced in Ref. 3. We construct an element W of $A_2\hat{\otimes}A_1$ such that $(\mathscr{A},\Delta_t)$ is the twisting of the topological tensor product Hopf algebra $A_1\hat{\otimes}A_2$ by W. Thus $(\mathscr{A},\Delta_t)$ is isomorphic to a quasitriangular Hopf algebra: we give a quasitriangular R-matrix in $\mathscr{A}\hat{\otimes}\mathscr{A}$.

(iii) By duality, the coproduct Δ_t induces onto $\mathscr{H}(G)$ the non-commutative structure (noted $\star_t$) of the algebra introduced by Podles and Woronowicz.[8] The product $\star_t$ is given in term of the usual product of functions.

(iv) Dualizing the results of Point (ii), the Hopf algebra $(\mathscr{H}(G),\star_t)$ is isomorphic to the double cross product of two copies of $SL_t(2)$ with the same cross relations as defined in Ref. 12. We obtain the C. W. model.[9]

(v) The introduction of the real structure of Ref. 10 on $\mathscr{U}_t\mathscr{L}$ ($t\in\mathbb{R}$) is tantamount to considering the topological Hopf subalgebra $(\underline{H}(G_0),\star_t)$ of $(H(G),\star_t)$, where G_0 is a real Lie subgroup of G conjugate to the subgroup $\{(T,{}^tT^{-1}),T\in SL(2,\mathbb{C})\}$. We then prove from Ref. 5, $\mathscr{C}^{\infty}(G_0)$ with its natural Fréchet topology can be endowed with a topological Hopf algebra structure which is the extension of the Hopf structure defined by $\star_t$ on $\mathscr{H}(G_0)$.

In particular, Points (i), (iii) and (iv) answer Question 2 while Points (ii) and (iv) solve Question 3. Moreover, a unique topological classical model $(\mathscr{A},H(G))$ carries all q-deformed structures introduced by the previously mentioned authors. Finally, Point (v) completes the total parallelism between quantum group theory and the star-product approach to quantum mechanics. The paper is organized as follows.

In Section II we introduce some definitions and notations for the various Hopf algebras needed here and we recall some of their properties. Section III is devoted to the construction (up to equivalence) of all the finite-dimensional representations of the Hopf algebra $\mathscr{U}_t\mathscr{L}$: this classification is needed for the proof of Point (i). In Section IV, we construct the topological algebra $\mathscr{A}$ and we prove the results claimed in Points (i) and (ii). Section V deals with duality: The

topological dual space $\mathscr{H}(G)$ of $\mathscr{A}$ is introduced and the various properties of Points (iii), (iv) and (v) are obtained.

II. $\mathscr{U}_t(\mathfrak{sl}(2,\mathbb{C}))$ AND $\mathscr{U}_t(\mathfrak{so}(4))$: DEFINITIONS AND NOTATIONS

II.1. Let $\mathscr{L}$ be the complex Lie algebra of $\mathfrak{so}(3,1)$ or $\mathfrak{so}(4)$. $\mathscr{L}$ can be written as the direct sum of Lie algebras $\mathfrak{g}_1 \oplus \mathfrak{g}_2$ where the Lie algebra $(\mathfrak{g}_i)_{i=1,2}$ is isomorphic to $\mathfrak{sl}(2)$. A basis of $\mathfrak{g}_i$ is $\{Y_i, F_i, G_i\}$ with the relations.

$$[Y_i, F_i] = F_i, \quad [Y_i, G_i] = -G_i, \quad [F_i, G_i] = 2Y_i, \quad i = 1,2. \tag{1}$$

Let $\mathscr{U}\mathscr{L} = \mathscr{U}\mathfrak{g}_1 \otimes \mathscr{U}\mathfrak{g}_2$ be the enveloping algebra of $\mathscr{L}$. Its center is generated by the two elements:

$$Q_i = F_i G_i - Y_i + Y_i^2 = G_i F_i + Y_i + Y_i^2, \quad i = 1,2. \tag{2}$$

II.2. According to Refs. 10 and 14, we denote by $\mathscr{U}_t\mathscr{L}$ or $\mathscr{U}_t\mathfrak{sl}(2,\mathbb{C})$ the complex associative algebra ($q = e^t, q \in \mathbb{C}$) generated by $\{L_+, L_-, l, l^{-1}, K_1, K_2, k, \tilde{k}\}$ and the relations ($\lambda = q - q^{-1}$):

$$L_+ l = q l L_+, \quad L_- l = q^{-1} l L_-, \quad [L_+, L_-] = q^{-1}\lambda^{-1}(l^{-2} - l^2), \tag{3}$$

$$\begin{aligned} &kK_1 = qK_1 k, \quad \tilde{k}K_1 = q^{-1}K_1\tilde{k}, \quad kK_2 = qK_2 k, \quad \tilde{k}K_2 = q^{-1}K_2\tilde{k}, \\ &K_1K_2 = K_2K_1, \quad k\tilde{k} = \tilde{k}k - q\lambda^3 K_1K_2, \quad k\tilde{k} + q^2\lambda^2 K_1K_2 = 1, \end{aligned} \tag{4}$$

$$\begin{aligned} &kL_+ = q^{-1}L_+k + q^{-1}\lambda l^{-1}K_2, && kL_- = q^{-1}L_-k + q^{-1}\lambda l K_1, \\ &\tilde{k}L_+ = qL_+\tilde{k} - \lambda K_2 l, && \tilde{k}L_- = qL_-\tilde{k} - \lambda K_1 l^{-1}, \\ &kl = lk, && \tilde{k}l = l\tilde{k}, \\ &K_1L_+ = L_+K_1 - q^{-1}\lambda^{-1}(l^{-1}\tilde{k} - lk), && K_1L_- = L_-K_1, \\ &K_2L_+ = L_+K_2, && K_2L_- = L_-K_2 + q^{-1}\lambda(kl^{-1} - l\tilde{k}), \\ &K_1 l = q^{-1} l K_1, && K_2 l = q l K_2. \end{aligned} \tag{5}$$

Set $C = \frac{1}{2}(l + l^{-1}) \quad S = \lambda^{-1}(l - l^{-1}) \quad C' = \frac{1}{2}(k + \tilde{k}) \quad S' = \lambda^{-1}(k - \tilde{k})$.

Then $\{L_+, L_-, C, S, K_1, K_2, C', S'\}$ is a system of generators of $\mathscr{U}_t\mathscr{L}$ with relations [deduced from (3), (4), (5)] well defined for any q in $\mathbb{C}$. To simplify notations , we write here the elements of this last basis of $\mathscr{U}_t\mathscr{L}$ without subscript t.

If $\{L_{+,0}, L_{-,0}, C_0, S_0, K_{1,0}, K_{2,0}, C_0', S_0'\}$ denotes the basis of $\mathscr{U}_0\mathscr{L}$, set

$$\begin{aligned} &H_3 = -S_0C_0, \quad H_+ = C_0L_{+,0}, && H_- = C_0L_{-,0}, \\ &F_3 = iC_0'S_0', \quad F_+ = 2iK_{2,0}C_0' - iL_{+,0}C_0, && F_- = -2iK_{1,0}C_0' + iL_{-,0}C_0, \end{aligned} \tag{6}$$

and

$$\begin{aligned} &2Y_1 = H_3 - iF_3, && 2F_1 = H_+ - iF_+, \quad 2G_1 = H_- - iF_-, \\ &2Y_2 = -(H_3 + iF_3), && 2G_2 = H_+ + iF_+, \quad 2F_2 = H_- + iF_-, \end{aligned} \tag{7}$$

Then $\{Y_1, F_1, G_1, Y_2, F_2, G_2, C_0, C_0'\}$ is a system of generators of $\mathscr{U}_0\mathscr{L}$ where the six first elements generate the classical enveloping algebra $\mathscr{U}\mathscr{L}$ as defined in paragraph II.1., C_0 and C_0' commute with all the other ones and verify $C_0^2 = C'^2_0 = 1$. Then

$$\mathscr{U}_0\mathscr{L} = \mathscr{U}\mathscr{L} \otimes \frac{\mathbb{C}[X,Y]}{\langle X^2 - 1, Y^2 - 1\rangle}.$$

$\mathscr{U}_t\mathscr{L}$ has the two following central elements:

$$\begin{aligned} Q_1' &= qK_2L_- + \lambda^{-2}(q^{-1}kl^{-1} + q\tilde{k}l), \\ Q_2' &= qK_1L_+ + \lambda^{-2}(q^{-1}kl + q\tilde{k}l^{-1}). \end{aligned} \tag{8}$$

Remark II.2.1: The generators H_3, H_+, H_- (resp., F_3, F_+, F_-) defined by formulas (6) are the rotation generators (resp., boost generators) of $\mathscr{L}$ in the notations of Naimark (Ref. 15, p. 87, Sec. 2).

Moreover $\mathscr{U}_t\mathscr{L}$ has a Hopf algebra structure defined by Refs. 10 and 14:

- coproduct Δ_t,

$$\begin{aligned} &\Delta_t(l) = l\otimes l, \quad \Delta_t(L_+) = L_+\otimes l^{-1} + l\otimes L_+, \quad \Delta_t(L_-) = L_-\otimes l^{-1} + l\otimes L_-, \\ &\Delta_t(k) = k\otimes k - q\lambda^2 K_1\otimes K_2, \quad \Delta_t(\tilde{k}) = \tilde{k}\otimes\tilde{k} - q\lambda^2 K_2\otimes K_1, \\ &\Delta_t(K_1) = K_1\otimes\tilde{k} + k\otimes K_1, \quad \Delta_t(K_2) = K_2\otimes k + \tilde{k}\otimes K_2; \end{aligned} \tag{9}$$

- counit ε_t,

$$\begin{aligned} &\varepsilon_t(l) = \varepsilon_t(l^{-1}) = \varepsilon_t(k) = \varepsilon_t(\tilde{k}) = 1, \\ &\varepsilon_t(L_+) = \varepsilon_t(L_-) = \varepsilon_t(K_1) = \varepsilon_t(K_2) = 0; \end{aligned} \tag{10}$$

- antipode J_t,

$$\begin{aligned} &J_t(l) = l^{-1}, \quad J_t(l^{-1}) = l, \quad J_t(L_+) = -qL_+, \quad J_t(L_-) = -q^{-1}L_-, \\ &J_t(k) = \tilde{k}, \quad J_t(\tilde{k}) = k, \quad J_t(K_1) = -q^{-1}K_1, \quad J_t(K_2) = -qK_2. \end{aligned} \tag{11}$$

Introduce the algebra isomorphism φ of $\mathscr{U}_t\mathscr{L}$ into $\mathscr{U}_t\mathscr{L}$ as follows:

$$\varphi(l) = l^{-1}, \quad \varphi(k) = k, \quad \varphi(\tilde{k}) = \tilde{k}, \quad \varphi(K_1) = -qK_2, \quad \varphi(L_+) = -q^{-1}L_-; \tag{12}$$

and

$$\varphi\circ\varphi = id.$$

Thus, we have

$$\Delta_t\circ\varphi = (\varphi\otimes\varphi)\circ\tau\Delta_t, \quad (\varphi\circ J_t)^2 = 1, \quad \varepsilon_t\circ\varphi = \varepsilon_t,$$

where τ is the flip automorphism of $\mathscr{U}_t\mathscr{L}\otimes\mathscr{U}_t\mathscr{L}$ defined by $\tau(x\otimes y) = y\otimes x$.

Remark II.2.2: The q-Lorentz Hopf algebra as introduced in Ref. 10 can be seen as a Hopf subalgebra of the Hopf algebra $\mathscr{U}_t\mathscr{L}$. Actually, if $\{\tau_3, T_+, T_-, \tau_1, \sigma_2, S_1, T_2\}$ is a basis of Ref. 10, we have

$$\begin{aligned} &\tau_3 = l^4, \quad \tau_3^{-1} = (l^{-1})^4, \quad T_+ = q^{-1}L_+l, \quad T_- = q^2L_-l, \\ &\tau_1 = kl^{-1}, \quad \sigma_2 = \tilde{k}l, \quad S_1 = -qK_1l, \quad T_2 = K_2l^{-1}. \end{aligned}$$

II.3. We remark that $\mathscr{U}_t\mathscr{L}$ is not the usual quantum deformation of $\mathscr{U}\mathscr{L}$ as defined by Jimbo[7] from the Cartan matrix of $\mathscr{L}$. The Jimbo quantum deformation of the algebra $\mathscr{U}\mathscr{L}$ is the Hopf algebra $\mathscr{U}_t(\mathfrak{sl}(2))\otimes\mathscr{U}_t(\mathfrak{sl}(2))$ considered as the tensor product of two Hopf algebras. If m_t, δ_t, e_t, j_t are, respectively, the product, coproduct, counit, and antipode of $\mathscr{U}_t(\mathfrak{sl}(2))$, then the product m_t', coproduct Δ_t', counit ε_t' and antipode J_t' on $\mathscr{U}_t(\mathfrak{sl}(2))\otimes\mathscr{U}_t(\mathfrak{sl}(2))$ are

$$\begin{aligned}
&\Delta_t' = (I\otimes\tau\otimes I)\circ(\delta_t\otimes\delta_t),\\
&m_t' = (m_t\otimes m_t)\circ(I\otimes\tau\otimes I),\\
&\varepsilon_t' = e_t\otimes e_t,\\
&J_t' = j_t\otimes j_t .
\end{aligned} \tag{13}$$

A system of generators of $\mathcal{U}_t(\mathfrak{sl}(2))\otimes\mathcal{U}_t(\mathfrak{sl}(2))$ is $\{K_1', K_1'^{-1}, F_1', G_1', K_2', K_2'^{-1}, F_2', G_2'\}$ with the relations for $i=1,2$:

$$\begin{aligned}
&K_i'F_i' = qF_i'K_i', \quad K_i'G_i' = q^{-1}G_i'K_i',\\
&[F_i', G_i'] = \lambda^{-1}(K_i'^{2} - K_i'^{-2}),\\
&\Delta_t'(F_i') = F_i'\otimes K_i' + K_i'^{-1}\otimes F_i', \quad \Delta_t'(G_i') = G_i'\otimes K_i' + K_i'^{-1}\otimes G_i',\\
&\Delta_t'(K_i') = K_i'\otimes K_i' .
\end{aligned} \tag{14}$$

We also introduce the Hopf algebra $\mathcal{U}_t(\mathfrak{sl}(2))\otimes\mathcal{U}_t(\mathfrak{sl}(2))^{op}$ where $\mathcal{U}_t(\mathfrak{sl}(2))^{op}$ is the algebra $\mathcal{U}_t(\mathfrak{sl}(2))$ with the opposite Hopf structure $(\delta_t^{op},\ e_t,\ j_t^{-1})$. We set

$$\Delta_t'' = (I\otimes\tau\otimes I)\circ(\delta_t\otimes\delta_t^{op}), \quad J_t'' = j_t\otimes j_t^{-1} .$$

As $\mathcal{U}_t(\mathfrak{sl}(2))$ is a quasi-triangular Hopf algebra, the Hopf algebra $\mathcal{U}_t(\mathfrak{sl}(2))\otimes\mathcal{U}_t(\mathfrak{sl}(2))$ [resp., $\mathcal{U}_t(\mathfrak{sl}(2))\otimes\mathcal{U}_t(\mathfrak{sl}(2))^{op}$] also is quasi-triangular. Its universal R-matrix $\mathcal{R}'$ (resp., $\mathcal{R}''$) is given by

$$\mathcal{R}' = (1\otimes\tau\otimes 1)(R\otimes R), \quad \mathcal{R}'' = (1\otimes\tau\otimes 1)(R\otimes\tau R);$$

where R is the universal R-matrix of $\mathcal{U}_t(\mathfrak{sl}(2))$.

II.4 Let us introduce the following elements of $\mathcal{U}_t(\mathfrak{sl}(2))\otimes\mathcal{U}_t(\mathfrak{sl}(2))$:

$$\begin{aligned}
&l = K_1'^{-1}K_2', && l^{-1} = K_1'K_2'^{-1},\\
&k = K_1'K_2', && \tilde{k} = K_1'^{-1}K_2'^{-1} - q\lambda^2F_1'F_2',\\
&K_1 = K_1'F_2', && K_2 = K_2'F_1',\\
&L_+ = F_1'K_2'^{-1} + q^{-1}K_1'^{-1}G_2', && L_- = K_1'^{-1}F_2' + q^{-1}G_1'K_2'^{-1}.
\end{aligned}$$

Then, these elements verify Formulas (3), (4) and (5) so that the algebra $\mathcal{U}_t\mathcal{S}$ is a strict subalgebra of $\mathcal{U}_t(\mathfrak{sl}(2))\otimes\mathcal{U}_t(\mathfrak{sl}(2))$. In Section IV, we shall see that $\mathcal{U}_t\mathcal{S}$, $\mathcal{U}_t(\mathfrak{sl}(2))\otimes\mathcal{U}_t(\mathfrak{sl}(2))$ and the algebra introduced in Remark II.2.2 can be identified with dense subalgebras of the same topological algebra.

III. FINITE DIMENSIONAL REPRESENTATIONS OF $\mathcal{U}_t\mathcal{S}$ ($q^n\neq 1, \forall n\in\mathbf{N}$)

III.1. Let (m_0,p_0) be an element of $\mathbb{N}/2\times\mathbb{N}/2$ and let V_{m_0,p_0} be a $(2m_0+1)(2p_0+1)$ dimensional vector-space with a basis $\{f_{m,p,};m=0,1,\ldots,2m_0;p=0,1,\ldots,2p_0\}$. Let us introduce the operators defined on V_{m_0,p_0} by the formulas

$$
\begin{aligned}
&l f_{m,p} = \varepsilon_1 q^{m_0 - p_0 - m + p} f_{m,p},\\
&k f_{m,p} = \varepsilon_2 q^{-(m_0+p_0)+m+p} f_{m,p},\\
&\tilde{k} f_{m,p} = \varepsilon_2^{-1} q^{p_0+m_0-p-m} f_{m,p} - \varepsilon_2 q \lambda^2 [2m_0 - m][2p_0 - p] f_{m+1,p+1},\\
&L_+ f_{m,p} = \varepsilon_1 (q^{m_0-m-1}[p] f_{m,p-1} + q^{p_0-p}[2m_0 - m] f_{m+1,p}),\\
&L_- f_{m,p} = \varepsilon_1 (q^{p_0-p-1}[m] f_{m-1,p} + q^{m_0-m}[2p_0 - p] f_{m,p+1}),\\
&K_1 f_{m,p} = \varepsilon_2 q^{-m_0+m}[2p_0 - p] f_{m,p+1},\\
&K_2 f_{m,p} = \varepsilon_2 q^{-p_0+p}[2m_0 - m] f_{m+1,p},
\end{aligned}
\tag{15}
$$

where

$$
\varepsilon_1^2 = \varepsilon_2^2 = \pm 1, \quad [n] = \frac{q^n - q^{-n}}{q - q^{-1}}, \quad \forall n \in \mathbb{N}.
$$

Thus these operators on V_{m_0,p_0} verify the relations (3), (4), (5) of $\mathscr{U}_t\mathscr{L}$. Denote by $\rho^{m_0,p_0,\varepsilon_1,\varepsilon_2}$ the representation of $\mathscr{U}_t\mathscr{L}$ defined by Formulas (15) in the vector-space V_{m_0,p_0}.

Remark III.1.1: The representations $\rho^{m_0,p_0,\varepsilon_1,\varepsilon_2}$ with $\varepsilon_1^2 = \varepsilon_2^2 = -1$ have no limit for $q \to 1$.

III.2. Using (8) we have

$$
\begin{aligned}
&\rho^{m_0,p_0,\varepsilon_1,\varepsilon_2}(Q_1') = \varepsilon_1 \varepsilon_2^{-1} \left([m_0][m_0+1] + \frac{q + q^{-1}}{\lambda^2} \right),\\
&\rho^{m_0,p_0,\varepsilon_1,\varepsilon_2}(Q_2') = \varepsilon_1 \varepsilon_2 \left([p_0][p_0+1] + \frac{q + q^{-1}}{\lambda^2} \right).
\end{aligned}
\tag{16}
$$

Theorem III.2.1:

1. Every finite dimensional irreducible representation ρ of the complex algebra $\mathscr{U}_t\mathscr{L}$ in the vector-space V is equivalent to the representation $\rho^{m_0,p_0,\varepsilon_1,\varepsilon_2}$ in the $(2m_0+1)(2p_0+1)$ finite dimensional space $V_{m_0,p_0}, (m_0,p_0) \in \mathbb{N}/2 \times \mathbb{N}/2, \varepsilon_1^2 = \varepsilon_2^2 = \pm 1$.

2. Two representations $\rho^{m_0,p_0,\varepsilon_1,\varepsilon_2}$ and $\rho^{m_0',p_0',\varepsilon_1',\varepsilon_2'}$ of $\mathscr{U}_t\mathscr{L}$ are equivalent if and only if $m_0 = m_0', p_0 = p_0', \varepsilon_1 = \varepsilon_1', \varepsilon_2 = \varepsilon_2'$.

We must prove the two following Lemmas.

Lemma A: *There exists in V an eigenvector v of l and k with respective eigenvalues α and β. For such a vector, $\alpha\beta$ necessarily is different of zero.*

Proof: The relations $kl = lk$ and $ll^{-1} = 1$, the finite dimension of V imply the existence of v with α non zero. Suppose, for a contradiction, β equal to zero. We then prove

$k\tilde{k}^n v = (1 - q^{2n})\tilde{k}^{n-1} v$.

As q^n is different of 1 for any n, we obtain a contradiction with the finite dimension of V.

Lemma B: *We can choose v_0 as in Lemma A such that there exist two integers m_1 and p_1 with the property $\{K_2^m K_1^p v_0, m \in \{0,1,\cdots m_1\}, p \in \{0,1,\cdots p_1\}\}$ is a basis of V.*

Proof: (a) Let v be as in Lemma A. Thus $K_2^m K_1^p v ((m,p) \in \mathbb{N}^2)$ is zero or an eigenvector of l, k, lk^{-1}, lk with respective eigenvalues $\alpha q^{p-m}, \beta q^{p+m}, \beta\alpha^{-1} q^{2m}, \beta\alpha q^{2p}$ and $\alpha\beta$ non-zero.
We have the relations

$$
\begin{aligned}
&l(kl^{-1}L_- - K_1) = q(kl^{-1}L_- - K_1) l,\\
&k(kl^{-1}L_- - K_1) = q^{-1}(kl^{-1}L_+ - K_1) k,
\end{aligned}
\tag{17}
$$

$$\begin{aligned} l(klL_+ - K_2) &= q^{-1}(klL_+ - K_2)l, \\ k(klL_+ - K_2) &= q^{-1}(klL_+ - K_2)k. \end{aligned} \tag{18}$$

We define a subset of $\mathbb{Z}^2$ as follows:

$$P = \{(m,p) \in \mathbb{Z}^2 / \exists v_{m,p} \in V \text{ with } lv_{m,p} = \alpha q^{p-m} v_{m,p}, kv_{m,p} = \beta q^{p+m} v_{m,p}\}.$$

P contains $(0,0)$ and is finite. Set

$$m_0 = \inf\{m \in \mathbb{Z} / \exists p \in \mathbb{Z} \text{ with } (m,p) \in P\}, \quad p_0 = \inf\{p \in \mathbb{Z} \text{ with } (m_0,p) \in P\}.$$

We denote by v_0 a common eigenvector of l and k with the respective eigenvalues,

$$\alpha_0 = \alpha q^{p_0 - m_0} \quad \text{and} \quad \beta_0 = \beta q^{p_0 + m_0}.$$

Thus Formulas (17) and (18) imply

$$(kl^{-1}L_- - K_1)v_0 = 0 \quad \text{and} \quad (klL_+ - K_2)v_0 = 0\ . \tag{19}$$

Consider the subspace W of V generated by $\{K_2^m K_1^p v_0, (m,p) \in \mathbb{N} \text{ with } K_2^m K_1^p v_0 \neq 0\}$.

(b) We want to prove that W is V. The stability of W by l, l^{-1}, k, K_1, K_2 is evident. Using $\widetilde{k}k = 1 - \lambda^2 K_1 K_2$ and Lemma A, we deduce the stability of W by $\widetilde{k}$. Using Q_1' and Q_2' (8) which are represented by scalar operators on V, we deduce the stability of W by $K_2 L_-$ and $K_1 L_+$. The equality $l\widetilde{k}(kl^{-1}L_- v_0) = L_- v_0 - \lambda^2 K_1 (K_2 L_- v_0)$ together with (19) gives

$$L_- v_0 \in W.$$

A similar argument allows to conclude that $L_+ v_0$ is in W. The stability of W by L_+ and L_- results from relations (5). The irreducibility of the representation of $\mathscr{U}_t\mathscr{L}$ in V permits to assert that W is equal to V.

(c) Now we claim that

$$\{(m,p) \in \mathbb{N}^2 \text{ with } K_2^m K_1^p v_0 \neq 0\} = \{0,1,\cdots m_1\} \times \{0,1,\cdots p_1\},$$

where

$$m_1 = \sup\{m \in \mathbb{N} \text{ with } K_2^m v_0 \neq 0\}, \quad p_1 = \sup\{p \in \mathbb{N} \text{ with } K_1^p v_0 \neq 0\}.$$

Evidently, $K_2^m K_1^p v_0 = 0$ if $m > m_1$ or $p > p_1$. Now pick out an integer $m (m \leqslant m_1)$ and suppose there exists an integer $p' (1 \leqslant p' \leqslant p_1)$ such that $K_2^m K_1^{p'} v_0$ is zero and $K_2^m K_1^{p'-1} v_0$ is non-zero. From (17) we have

$$(kl^{-1}L_- - K_1)^m K_2^m K_1^{p'-1} v_0 = \mu K_1^{p'-1} v_0, \quad \mu \neq 0.$$

Applying K_1 we obtain $K_1^{p'} v_0 = 0$, in contradiction with the definition of p_1. Hence

$$\forall (m,p) \in \{0,1\cdots m_1\} \times \{0,1\cdots p_1\}, \quad K_1^m K_2^p v_0 \neq 0.$$

Lemma 2 is proved.

Proof of the theorem: Lemma 2 gives a basis of V and the action of $l, l^{-1}, K_1, K_2, k, \widetilde{k}$ on the elements of this basis, in a function of the two non-zero parameters α_0, β_0. From (19) we deduce easily $L_- v_0$ and $L_+ v_0$. The relations between L_-(resp., L_+) and K_1, L_-(resp., L_+) and K_2 give by induction the action of L_- and L_+ on the basis and the conditions

$$\alpha_0\beta_0^{-1}=\varepsilon q^{m_1},\quad \varepsilon^2=1(\text{ resp.},\ \alpha_0\beta_0=\varepsilon' q^{p_1},\quad \varepsilon'^2=1)$$

or

$$\alpha_0=\varepsilon_1 q^{(m_1-p_1)/2},\quad \beta_0=\varepsilon_2 q^{(-p_1-m_1)/2},\quad \varepsilon_1\varepsilon_2=\varepsilon',\quad \varepsilon_1\varepsilon_2^{-1}=\varepsilon.$$

Set for (m,p) in $\{0,1,\cdots m_1\}\times\{0,1,\cdots p_1\}$:

$$f_{m,p}=\varepsilon_2^{-p-m}\alpha_{mp}K_2^m K_1^p v_0\ ,$$

$$\alpha_{mp}=\frac{q^{(p_1 m+m_1 p)/2}-mp}{[m_1]\cdots[m_1-m+1][p]\cdots[p_1-p+1]}\ .$$

Then the action of $l,k,\tilde{k},K_1,K_2,L_+,L_-$ on the basis $\{f_{m,p}\}$ is given by formulas (15) where we have $2m_0=m_1$ and $2p_0=p_1$.
Part (b) of the theorem results from formulas (16) and from the spectrum of l and k in the representation $\rho^{m_0,p_0,\varepsilon_1,\varepsilon_2}$ (together with $q^n\neq 1,\forall n\in\mathbb{N}$).

We can introduce in $\mathscr{U}_t\mathscr{S}$ the following central elements:

$$Q_1(\varepsilon_1,\varepsilon_2)=Q_1'-\varepsilon_1\varepsilon_2^{-1}\lambda^{-2}(q+q^{-1}),$$
$$Q_2(\varepsilon_1,\varepsilon_2)=Q_2'-\varepsilon_1\varepsilon_2\lambda^{-2}(q+q^{-1}),$$
$$\text{with } \varepsilon_1^2=\varepsilon_2^2=\pm 1.$$

Theorem III.2.2: *Every finite dimensional representation of $\mathscr{U}_t\mathscr{S}$ is completely reducible.*
The proof is the same as for Theorem 1, Sec. IV, in Ref. 16

Corollary III.2.3: We have the following equivalences between representations of $\mathscr{U}_t\mathscr{S}$:

$$(a)\ \rho^{m_0,0,\varepsilon_1,\varepsilon_2}\otimes\rho^{0,p_0,\varepsilon_1',\varepsilon_2'}\circ\Delta_t=\rho^{m_0,p_0,\varepsilon_1\varepsilon_1',\varepsilon_2\varepsilon_2'},$$
$$(b)\ \rho^{0,p_0,\varepsilon_1',\varepsilon_2'}\otimes\rho^{m_0,0,\varepsilon_1,\varepsilon_2}\circ\Delta_t\simeq\rho^{m_0,p_0,\varepsilon_1\varepsilon_1',\varepsilon_2\varepsilon_2'},$$
$$(c)\ \rho^{m_0,0,\varepsilon_1,\varepsilon_2}\otimes\rho^{0,p_0,\varepsilon_1',\varepsilon_2'}\circ\tau\Delta_t\simeq\rho^{m_0,p_0,\varepsilon_1\varepsilon_1',\varepsilon_2\varepsilon_2'},$$
$$(d)\ \rho^{0,p_0,\varepsilon_1',\varepsilon_2'}\otimes\rho^{m_0,0,\varepsilon_1,\varepsilon_2}\circ\tau\Delta_t\simeq\rho^{m_0,p_0,\varepsilon_1\varepsilon_1',\varepsilon_2\varepsilon_2'},$$
$$(e)\ \rho^{m,p,\varepsilon_1,\varepsilon_2}\circ\varphi\simeq\rho^{p,m,\varepsilon_1^{-1},\varepsilon_2}.$$

Proof: For each case (a) to (d), it is easy to prove the irreducibility of the tensor product of the two considered representations of $\mathscr{U}_t\mathscr{S}$. Theorem III.2.1, together with the spectrum of the representants of Q_1, Q_2, l and k, gives the results. A direct calculation proves the equivalence of $\rho^{m,0,\varepsilon_1,\varepsilon_2}\circ\varphi$ and $\rho^{0,m,\varepsilon_1^{-1},\varepsilon_2}$. Then (e) is deduced from (a) and the property $\Delta_t\circ\varphi=(\varphi\otimes\varphi)\circ(\tau\Delta_t)$.

Corollary III.2.4: We have

$$\text{(a) } \rho^{m_0,p_0,\varepsilon_1,\varepsilon_2}\otimes\rho^{m_0',p_0',\varepsilon_1',\varepsilon_2'}\circ\Delta_t\simeq\bigoplus_{\substack{i=|m_0-m_0'|,\ldots,m_0+m_0'\\ j=|p_0-p_0'|,\ldots,p_0+p_0'}}\rho^{i,j,\varepsilon_1\varepsilon_1',\varepsilon_2\varepsilon_2'};$$

$$\text{(b) } \rho^{m_0,p_0,\varepsilon_1,\varepsilon_2}\otimes\rho^{m_0',p_0',\varepsilon_1'\varepsilon_2'}\circ\tau\Delta_t\simeq\bigoplus_{\substack{i=|m_0-m_0'|,\ldots,m_0+m_0'\\ j=|p_0-p_0'|,\ldots,p_0+p_0'}}\rho^{i,j,\varepsilon_1\varepsilon_1',\varepsilon_2\varepsilon_2'}.$$

IV. A COMMON MODEL FOR THE HOPF ALGEBRA $\mathcal{U}_t\mathcal{L}$ and $\mathcal{U}_t(\mathfrak{sl}(2))\otimes\mathcal{U}_t(\mathfrak{sl}(2))$ ($q^n\neq 1, \forall n\in\mathbb{N}$)

In this Section we construct a classical topological algebra $\mathcal{A}$ using the finite dimensional representations of the Lorentz Lie algebra. Then, the algebras $\mathcal{U}_t\mathcal{L}$ and $\mathcal{U}_t(sl(2))\otimes\mathcal{U}_t(sl(2))$ can be densely realized in $\mathcal{A}$ (Paragraph IV.1). Moreover, in Paragraph IV.2, the Hopf structures of $\mathcal{U}_t\mathcal{L}$ and $\mathcal{U}_t(sl(2))\otimes\mathcal{U}_t(sl(2))$ are extended onto the topological algebra $\mathcal{A}$ which then carries various topological Hopf structures. In particular Theorem IV.2.1 proves, the first Hopf structure on $\mathcal{A}$ is the twisting of the second one and consequently, it is quasi-triangular. Explicit formulas are given for the twisting element and the quasi-triangular R-matrix in $\mathcal{A}\hat{\otimes}\mathcal{A}$. As $\mathcal{U}_t\mathcal{L}$ is not a Drinfeld-Jimbo deformation, we need to prove Corollary IV.2.2 whose the result is basic for Paragraph V.3.

IV.1 The topological algebra $\mathcal{A}$

We use the results of Refs. 3 and 4. Consequently this common model is constructed from the set of finite dimensional irreducible representations of $\mathcal{U}\mathcal{L}=\mathcal{U}\mathfrak{g}_1\otimes\mathcal{U}\mathfrak{g}_2$ (paragraph II.1.). If (ρ_n, V_n) denotes the irreducible representation of $\mathfrak{sl}(2)$ of dimension $2n+1$, n in $\mathbb{N}/2$, each finite dimensional irreducible of $\mathcal{U}\mathcal{L}$ is equivalent to $(\rho_n\otimes\rho_p, V_n\otimes V_p),(n,p)$ in $\mathbb{N}/2\times\mathbb{N}/2$. To simplify, we denote

$$\rho_{n,p}=\rho_n\otimes\rho_p, \quad V_{n,p}=V_n\otimes V_p.$$

We introduce the Fréchet algebra $\mathcal{A}$ defined as follows:

(i) $\mathcal{A}=\Pi_{(n,p)\in\mathbb{N}/2\times\mathbb{N}/2}\mathcal{L}(V_n\otimes V_p)=\Pi_{(n,p)\in\mathbb{N}/2\times\mathbb{N}/2}\mathcal{L}(V_n)\otimes\mathcal{L}(V_p)$. $\mathcal{A}$ is endowed with the product topology.

(ii) If $a=(a_{n,p})$ and $b=(b_{n,p})$ are two elements of $\mathcal{A}$, then $a.b=(a_{n,p}b_{n,p})$.

(iii) Then, $\mathcal{A}$ is the projective tensor product $A_1\hat{\otimes}A_2$ where $A_i(i=1,2)$ is defined as in Ref. 3 (i.e., $A_1=\Pi_{n\in\mathbb{N}/2}\mathcal{L}(V_{n,0})$, [resp., $A_2=\Pi_{p\in\mathbb{N}/2}\mathcal{L}(V_{0,p})$] endowed with the product topology and the evident algebra structure).

Similarly to Ref. 3, we have the following properties:

i. $\mathcal{U}\mathcal{L}$ can be identified with a subalgebra of $\mathcal{A}$ via the injective morphism:

$u\in\mathcal{U}\mathcal{L}\rightarrow(\rho_{n,p}(u))_{(n,p)\in\mathbb{N}/2\times\mathbb{N}/2}\in\mathcal{A}$

ii. $\overline{\mathcal{U}\mathcal{L}}=\mathcal{A}$ (Jacobson density theorem).

iii. $\rho_{n,p}:\mathcal{U}\mathcal{L}\rightarrow\mathcal{L}(V_{n,p})$ is continuous and can be extended to a representation of $\mathcal{A}$, which we shall still denote $\rho_{n,p}$.

Now, let us introduce the following elements in $\mathcal{A}$:

$$\begin{aligned}
&\Lambda_1=(\Lambda_{1,n,p}), \quad \text{with } \Lambda_{1,n,p}=n\mathbb{1}_{V_n}\otimes\mathbb{1}_{V_p},\\
&\Lambda_2=(\Lambda_{2,n,p}), \quad \text{with } \Lambda_{2,n,p}=\mathbb{1}_{V_n}\otimes p\mathbb{1}_{v_p},\\
&C_1=(C_{1,n,p}), \quad \text{with } C_{1,n,p}=(-1)^{2n}\mathbb{1}_{V_n}\otimes\mathbb{1}_{V_p},\\
&C_2=(C_{2,n,p}), \quad \text{with } C_{2,n,p}=(-1)^{2p}\mathbb{1}_{V_n}\otimes\mathbb{1}_{V_p}.
\end{aligned} \tag{20}$$

Let us give the classical representation ρ_{n_0,p_0} of $\mathcal{U}\mathcal{L}$ on a standard basis $\{f_{n,p}, n=0,\ldots,2n_0, p=0,\ldots,2p_0\}$ of V_{n_0,p_0}:

$$\begin{aligned}
&Y_1f_{n,p}=(-n_0+n)f_{n,p}, \quad && Y_2f_{n,p}=(-p_0+p)f_{n,p},\\
&F_1f_{n,p}=(2n_0-n)f_{n+1,p}, \quad && F_2f_{n,p}=(2p_0-p)f_{n,p+1},\\
&G_1f_{n,p}=nf_{n-1,p}, && G_2f_{n,p}=pf_{n,p-1}.
\end{aligned} \tag{21}$$

Taking into account the identification of $\mathscr{U}\mathscr{L}$ as a subalgebra of $\mathscr{A}$, the following elements are well defined in the algebra $\mathscr{A}$:

$$
\begin{aligned}
&l = C_1 C_2 q^{(Y_2 - Y_1)}, \quad l^{-1} = C_1 C_2 q^{(Y_1 - Y_2)}, \\
&k = C_2 q^{(Y_2 + Y_1)}, \quad \tilde{k} = C_2 \left(q^{-(Y_1 + Y_2)} - \lambda^2 q \frac{[Y_1 - \Lambda_1 - 1][Y_2 - \Lambda_2 - 1]}{(Y_1 - \Lambda_1 - 1)(Y_2 - \Lambda_2 - 1)} F_1 F_2 \right), \\
&K_1 = C_2 q^{Y_1} \frac{[Y_2 - \Lambda_2 - 1]}{(Y_2 - \Lambda_2 - 1)} F_2, \quad K_2 = C_2 q^{Y_2} \frac{[Y_1 - \Lambda_1 - 1]}{(Y_1 - \Lambda_1 - 1)} F_1, \\
&L_- = C_1 C_2 \left(q^{-Y_2 - 1} \frac{[Y_1 + \Lambda_1 + 1]}{(Y_1 + \Lambda_1 + 1)} G_1 + q^{-Y_1} \frac{[Y_2 - \Lambda_2 - 1]}{(Y_2 - \Lambda_2 - 1)} F_2 \right), \\
&L_+ = C_1 C_2 \left(q^{-Y_1 - 1} \frac{[Y_2 + \Lambda_2 + 1]}{(Y_2 + \Lambda_2 + 1)} G_2 + q^{-Y_2} \frac{[Y_1 - \Lambda_1 - 1]}{(Y_1 - \Lambda_1 - 1)} F_1 \right),
\end{aligned}
\tag{22}
$$

$$
\begin{aligned}
&K_1' = C_1 q^{Y_1}, \quad K_1'^{-1} = C_1 q^{-Y_1}, \\
&F_1' = C_1 \frac{[Y_1 - \Lambda_1 - 1]}{(Y_1 - \Lambda_1 - 1)} F_1, \\
&G_1' = C_1 \frac{[Y_1 + \Lambda_1 + 1]}{(Y_1 + \Lambda_1 + 1)} G_1,
\end{aligned}
\tag{23a}
$$

$$
\begin{aligned}
&K_2' = C_2 q^{Y_2}, \quad K_2'^{-1} = C_2 q^{-Y_2}, \\
&F_2' = C_2 \frac{[Y_2 - \Lambda_2 - 1]}{(Y_2 - \Lambda_2 - 1)} F_2, \\
&G_2' = C_2 \frac{[Y_2 + \Lambda_2 + 1]}{(Y_2 + \Lambda_2 + 1)} G_2 \ .
\end{aligned}
\tag{23b}
$$

Denote by $\mathscr{A}_t$ (resp., $\mathscr{A}_t'$, $A_{1,t}$, $A_{2,t}$) the subalgebra of $\mathscr{A}$ generated by the elements of $\mathscr{A}$ defined by Formulas (22) [resp., (23a), (23b)]. Then, $\mathscr{A}_t'$ is the tensor product of algebras $A_{1,t} \otimes A_{2,t}$. From Ref. 3, $A_{1,t}$ (resp., $A_{2,t}$) is a dense subalgebra of A_1 (resp., A_2), which is isomorphic to $\mathscr{U}_t(\mathfrak{sl}(2))$.

We have

$$
\begin{aligned}
&l = K_1'^{-1} K_2', && l^{-1} = K_1' K_2'^{-1}, \\
&k = C_1 K_1' K_2', && \tilde{k} = C_1 (K_1'^{-1} K_2'^{-1} - q\lambda^2 F_1' F_2'), \\
&K_1 = C_1 K_1' F_2', && K_2 = C_1 K_2' F_1', \\
&L_+ = F_1' K_2'^{-1} + q^{-1} K_1'^{-1} G_2', && L_- = K_1'^{-1} F_2' + q^{-1} G_1' K_2'^{-1} \ .
\end{aligned}
\tag{24}
$$

Then we can claim the following.

Theorem IV.1.1: *$\mathscr{A}_t$ (resp., $\mathscr{A}_t'$) is a subalgebra of $\mathscr{A}$ isomorphic to $\mathscr{U}_t\mathscr{L}$* [resp., $\mathscr{U}_t(\mathfrak{sl}(2)) \otimes \mathscr{U}_t(\mathfrak{sl}(2))$]. Moreover we have $\mathscr{A}_t = \mathscr{A}$ (resp., $\mathscr{A}_t' = \mathscr{A}$).

Proof: Let X be one of the elements of $\mathscr{A}_t$ defined by Formulas (22). Then, we have $X = (\rho_{n,p}(X))$ and $\rho_{n,p}(X) = \rho^{n,p,(-1)^{2(n+p)},(-1)^{2p}}(X)$ where $\rho^{n,p,(-1)^{2(n+p)},(-1)^{2p}}(X)$ is defined by Formulas (15). Then the application $X \in \mathscr{A}_t \to X \in \mathscr{U}_t\mathscr{L}$ defines a morphism of $\mathscr{A}_t$ into $\mathscr{U}_t\mathscr{L}$. The injectivity of this morphism is deduced from the property that the set of representations of $U_t\mathscr{L}$, $\{\rho^{n,p,(-1)^{2n+2p},(-1)^{2p}}, (n,p) \in \mathbb{N}/2 \times \mathbb{N}/2\}$ is a complete set of representations of $\mathscr{U}_t\mathscr{L}$.

From now on, $\mathscr{U}_t\mathscr{L}$ can be identified with $\mathscr{A}_t$ and, consequently, $\rho^{n,p,(-1)^{2n+2p},(-1)^{2p}}$ with $\rho_{n,p}$ on $\mathscr{A}_t$. The density of $\mathscr{A}_t$ in $\mathscr{A}$ is given by the Jacobson density theorem applied to the $\mathscr{A}$-module $V=\Sigma_{(n,p)\in(\mathbb{N}/2)^2}V_{n,p}$ and to the semi-simple representation ρ of $\mathscr{A}_t, \rho=\Sigma_{(n,p)\in(\mathbb{N}/2)^2}\rho_{n,p}$.

The proof for $\mathscr{A}'_t$ is evident. We just have to remark that any finite-dimensional irreducible representation is equivalent to $\rho_n\otimes\rho_p$ and to use the results of Ref. 3 for $A_{i,t}(i=1,2)$.

Remark IV.1.2: (a) Part (e) of Corollary III.2.3, together with the density of $\mathscr{A}_t$ in $\mathscr{A}$ imply that the morphism φ defined on $\mathscr{A}_t$ [Formulas (12)] has a unique continuous extension on $\mathscr{A}$. We have

$$\begin{aligned}&\varphi(C_1)=C_1,\quad \varphi(C_2)=C_2,\\&\varphi(K'_1)=C_1C_2K'_2,\quad \varphi(F'_1)=-q^{-1}C_1C_2F'_2,\quad \varphi(G'_1)=-qC_1C_2G'_2\ .\end{aligned}\tag{25}$$

(b) The initial q-Lorentz algebra introduced in Ref. 10 (see Remark II.2.2) is a subalgebra of $\mathscr{A}$ which also is dense in $\mathscr{A}$.

IV.2 Various topological Hopf structures on $\mathscr{A}$

For that, we need to introduce $\mathscr{A}\hat{\otimes}\mathscr{A}$, the completion of $\mathscr{A}\otimes\mathscr{A}$ for the projective topology. Then

$$\mathscr{A}\hat{\otimes}\mathscr{A}=\prod_{\substack{(n,p)\\(n',p')\in(\mathbb{N}/2)^2}}\mathscr{L}(V_{np})\otimes\mathscr{L}(V_{n'p'})$$

Take into account Theorem IV.1.1, its consequences and Corollaries IV.2.3 and IV.2.4 and let us apply the methods of Refs. 3 and 4 to extend the Hopf structure $(\Delta_t,\varepsilon_t,J_t)$ [resp., $(\Delta'_t,\varepsilon'_t,J'_t)$ or $(\Delta''_t,\varepsilon'_t,J''_t)$] of $\mathscr{A}_t$ (resp., $\mathscr{A}'_t$) to $\mathscr{A}$. To be self contained we shall recall how this is done.

• The counit ε_t (resp., ε'_t) of $\mathscr{A}_t$ (resp., $\mathscr{A}'_t$) (equal to $\rho_{0,0}$) obviously extends to $\mathscr{A}$. The antipode J_t (resp., J'_t or J''_t) of $(\mathscr{A}_t,\ \Delta_t)$ [resp., $(\mathscr{A}'_t,\ \Delta'_t)$ or $(\mathscr{A}'_t,\ \Delta''_t)$] has a continuous extension to $\mathscr{A}$ given by (for J_t)

$$\forall a\in\mathscr{A},\quad (J_t(a))_{n,p}={}^t\hat{\rho}_{np}(a),\quad \forall(n,p)\in\mathbb{N}/2\times\mathbb{N}/2\ ,$$

where $\hat{\rho}_{np}(a)={}^t\rho_{np}\circ J_t(a)$ is the contragradient representation of $\rho_{n,p}$ of $\mathscr{A}$.

• The extension of Δ_t (resp., Δ'_t or Δ''_t) of $\mathscr{A}_t$ (resp., $\mathscr{A}'_t$) to $\mathscr{A}$ results from the existence of an element $\mathscr{P}(t)$ [resp., $\mathscr{P}'(t)$ or $\mathscr{P}''(t)$] of $\mathscr{A}\hat{\otimes}\mathscr{A}$ such that

$$\Delta_t=\mathscr{P}(t)\Delta_0\mathscr{P}(t)^{-1},\Delta'_t=\mathscr{P}'(t)\Delta_0\mathscr{P}'(t)^{-1},\Delta''_t=\mathscr{P}''(t)\Delta_0\mathscr{P}''(t)^{-1}.\tag{26}$$

The existence of $\mathscr{P}'(t)$ [resp., $\mathscr{P}''(t)$] (the Drinfeld twist) is proved in Ref. 17. In particular, denote by $P^{(i)}(t)$ the element of $(\mathscr{U}(\mathfrak{sl}(2))\otimes\mathscr{U}(\mathfrak{sl}(2)))[[t]]$ (Ref. 17) in the model $A_i(i=1,2)$ of Ref. 3 such that

$$\delta_t=P^{(i)}(t)\,\delta_0P^{(i)}(t)^{-1}\ .$$

Then we have

$$\mathscr{P}'(t)=P^{(1)}(t)_{1,3}P^{(2)}(t)_{2,4},\quad \mathscr{P}''(t)=P^{(1)}(t)_{1,3}P^{(2)}(t)_{4,2}\ .\tag{27}$$

Using Refs. 3 and 4, Theorem IV.1.1, Corollaries III.2.3 and III.2.4, $\mathcal{P}(t)$ can be constructed as follows:

$$(\rho_{n,p}\otimes\rho_{n',p'})\circ\Delta_t=\sum_{i=|n-n'|}^{n+n'}\sum_{j=|p-p'|}^{p+p'}\rho_{i,j}\ .$$

and

$$V_{n,p}\otimes V_{n',p'}=\sum_{i=|n-n'|}^{n+n'}\sum_{j=|p-p'|}^{p+p'}V_{i,j}(t)\ .$$

Then $\mathcal{P}_{(n,p),(n',p')}(t)$ is defined as the element of $\mathcal{L}(V_{np}\otimes V_{n'p'})$ which sends the basis of $V_{ij}(0)$ [Formulas (21)] onto the basis of $V_{i,j}(t)$ [Formulas (15)]. We have

$$(\rho_{n,p}\otimes\rho_{n',p'})\circ\Delta_t=(\Delta_t)_{(n,p),(n',p')}=\mathcal{P}_{(n,p),(n',p')}(t)\Delta_0(\mathcal{P}_{(n,p),(n',p')}(t))^{-1}\ .$$

Thus, Formulas (26) can be extended to $\mathcal{A}$ and provide an extension of Δ_t, (resp., Δ'_t, Δ''_t), still denoted by the same symbol. These extensions are continuous morphisms of $\mathcal{A}$ into $\mathcal{A}\hat{\otimes}\mathcal{A}$.

Now, in order to prove that the Hopf structure $(\mathcal{A},\ \Delta_t,\ \varepsilon_t,\ J_t)$ is a twisting of $(\mathcal{A},\ \Delta''_t,\ \varepsilon_t,\ J''_t)$, let us introduce the following element W of $A_2\hat{\otimes}A_1$:

$$W=e^{-2t(Y_2\otimes Y_1)}\sum_{i\in\mathbb{N}}\frac{\lambda^i}{[i]!}q^{i(3i+1)/2}F_2'^iK_2'^i\otimes F_1'^iK_1'^i\ . \tag{28}$$

Using Formulas (24), we remark that

$$W_{p,n}=\rho_{0,p}\otimes\rho_{n,0}(W)=\rho_{0,p}\otimes\rho_{n,0}(R_{21})\ , \tag{29}$$

where $R=R_{12}$ is the universal R-matrix of the Hopf subalgebra $\mathcal{U}_t(\mathfrak{sl}(2))$ of $\mathcal{U}_t(\mathcal{L})$ generated by $\{L_+,L_-,l,l^{-1}\}$. Recall that R is given by[18]

$$R=e^{2t(Y_1-Y_2\otimes Y_1-Y_2)}\sum_{i\in\mathbb{N}}\frac{\lambda^i}{[i]!}q^{i(3i+1)/2}L_+^il^{-i}\otimes L_-^il^i\ .$$

Formulas (29) implies the existence of W^{-1}. We have

$$(W^{-1})_{p,n}=(W_{p,n})^{-1}=\rho_{0,p}\otimes\rho_{n,0}(R_{21}^{-1})=\rho_{0,p}\otimes\rho_{n,0}[(J_t^{-1}\otimes id)R_{21}]=\rho_{0,p}\otimes\rho_{n,0}[(id\otimes J_t)R_{21}].$$

Theorem IV.2.1:

1. The Hopf algebra $(\mathcal{A},\ \Delta_t,\ \varepsilon_t,\ J_t)$ *is the twisting*[18] *of the Hopf algebra* $(\mathcal{A},\ \Delta''_t,\ \varepsilon'_t,\ J''_t)$ *by the element* $W_{23}=(1\otimes W\otimes 1)$ *of* $\mathcal{A}\hat{\otimes}\mathcal{A}$ *[W defined by Formula (28)].*

2. The Hopf algebra $(\mathcal{A},\ \Delta_t,\ \varepsilon_t,\ J_t)$ *has an R-matrix* $\mathcal{R}$ *given by*

$$\mathcal{R}=W_{41}R_{31}^{(1)-1}R_{42}^{(2)}W_{23}{}^{-1}, \tag{30}$$

where $R^{(i)}$ *is the universal R-matrix of* A_i $(i=1,2)$ *given in Ref. 18*

Sketch of the proof: Part 1 of the Theorem will be proved after having verified

$$\begin{aligned}\Delta_t&=W_{23}\Delta''_tW_{23}{}^{-1},\\ J_t&=W_{21}{}^{-1}(j_t\otimes j_t^{-1})W_{21},\end{aligned} \tag{31}$$

For that, we need to prove the following.

Lemma A:

$$1.\ \rho_{n,0}\otimes\rho_{0,p}\circ\Delta_t=\rho_{n,0}\otimes\rho_{0,p}\circ\Delta_t''=\rho_{np},\quad \forall(n,p)\in\mathbb{N}/2\times\mathbb{N}/2,$$
$$2.\ \rho_{n,0}\otimes\rho_{n',0}\circ\Delta_t=\rho_{n,0}\otimes\rho_{n',0}\circ\Delta_t'',\quad \forall(n,n')\in\mathbb{N}/2\times\mathbb{N}/2,$$
$$3.\ \rho_{0,p}\otimes\rho_{0,p'}\circ\Delta_t=\rho_{0,p}\otimes\rho_{0,p'}\circ\Delta_t'',\quad \forall(p,p')\in\mathbb{N}/2\times\mathbb{N}/2.$$

This lemma is easily obtained from Corollary III.2.3 (a) , Formulas (15) and (24).

Call τ_{np} the linear map of $V_n\otimes V_p$ into $V_p\otimes V_n$ which exchanges V_n and V_p.

Lemma B:

$$1.\ \rho_{0,p}\otimes\rho_{n,0}\circ\Delta_t''=\tau_{np}\rho_{np}\tau_{np}^{-1},\quad \forall(p,n)\in\mathbb{N}/2\times\mathbb{N}/2,$$
$$2.\ \rho_{0,p}\otimes\rho_{n,0}\circ\Delta_t=W_{p,n}(\rho_{0,p}\otimes\rho_{n,0}\circ\Delta_t'')W_{p,n}^{-1},\quad \forall(p,n)\in\mathbb{N}/2\times\mathbb{N}/2\ .$$

Proof: Theorem IV.1.1 and its consequences, together with Corollary III.2.3 (resp., the definition of Δ_t'') imply the equivalence of the representation $\rho_{0,p}\otimes\rho_{n,0}\circ\Delta_t$ (resp., $\rho_{0,p}\otimes\rho_{n,0}\circ\Delta_t''$) of $\mathcal{A}$ with the representation $\rho_{n,p}$ of $\mathcal{A}$. Now Lemma B (2) follows from a direct calculation on the basis of the dense subalgebra $\mathcal{U}_t\mathcal{L}$ of $\mathcal{A}$ and from the continuity of Δ_t and Δ_t'' on $\mathcal{A}$.

Now we want to prove the first identity of (31).

Lemma A (1) and Lemma B, with the coassociativity of Δ, imply

$$\rho_{n,p}\otimes\rho_{n',p'}\circ\Delta_t=(1\otimes W_{p,n'}\tau_{n',p}\otimes 1)[(\rho_{n,0}\otimes\rho_{n',0}\otimes\rho_{0,p}\otimes\rho_{0,p'})\circ(\Delta_t\otimes\Delta_t)\circ\Delta_t]$$
$$\times(1\otimes\tau_{n',p}{}^{-1}W_{p,n'}{}^{-1}\otimes 1).$$

Using Corollary III.2.4 (b) and Lemma A, we can replace Δ_t by Δ''_t in the right hand side of the previous equality. The first Formula of (31) now follows from Lemma B (1). We similarly prove the second identity of (31).

The previous result implies the existence of a R-matrix $\mathcal{R}$ for the Hopf algebra $(\mathcal{A},\Delta_t,\varepsilon_t, J_t)$ which verifies Formulas (30): here A_1 is endowed with the quasitriangular structure $(\tau R^{(1)})^{-1}$.

Theorem (IV.2.1), Formulas (27) and (28) together with the results of Ref. 17 $\{P^{(i)}(t)$ belongs to $(\mathcal{U}(\mathfrak{sl}(2))\otimes\mathcal{U}(\mathfrak{sl}(2)))[[t]]\}$ allow us to deduce

Corollary IV.2.2: *Let $\mathcal{P}(t)$ be the element of $\mathcal{A}\hat{\otimes}\mathcal{A}$ given by*

$$\mathcal{P}(t)=W_{23}\mathcal{P}''(t)=W_{23}P_{13}^{(1)}(t)P_{42}^{(2)}(t).$$

Then $\mathcal{P}(t)$ belongs to $[\mathcal{U}\mathcal{L}\otimes\mathcal{U}\mathcal{L}][[t]]$ [$\mathcal{U}\mathcal{L}$ defined in (1.1)] and verifies

$$\Delta(t)=\mathcal{P}(t)\Delta_0\mathcal{P}(t)^{-1}.$$

Now we consider the Hopf algebra (A_1,δ_t,e_t,j_t) and introduce the twisted topological tensor product Hopf algebra $A_1\hat{\otimes}_{\tau R^{(1)}}A_1$ which is the twisting[18] of the topological tensor product Hopf algebra $A_1\hat{\otimes}A_1$ by $(\tau R^{(1)})_{23}$. Moreover $A_1\hat{\otimes}_{\tau R^{(1)}}A_1$ has a quasitriangular structure given by Ref. 19:

$$\mathcal{R}_1=(\tau R^{(1)})_{41}(\tau R^{(1)})_{13}^{-1}R_{24}^{(1)}(\tau R^{(1)})_{23}^{-1}$$
$$=R_{14}^{(1)}(R^{(1)})_{31}^{-1}R_{24}^{(1)}(R^{(1)})_{32}^{-1}\ .$$

Call s the isomorphism of the Hopf algebra (A_1,δ_t) onto the Hopf algebra (A_2,δ_t^{op}) given by

$$X_1\in A_1\rightarrow s(X_1)=(S_p\rho_{p,0}(X_1)S_p^{-1})_{p\in\mathbb{N}/2}$$

$$S_p=\begin{pmatrix} 0 & \dots & \dots & 0 & q^{-2p} \\ \vdots & & & \iddots & 0 \\ \vdots & & \iddots & & \vdots \\ 0 & q^{-1} & & & \vdots \\ 1 & 0 & \dots & \dots & 0 \end{pmatrix}\ .$$

Set $\mathcal{S}=1\otimes s$.

Then, from Theorem IV.2.1, we can easily deduce the following.

Corollary IV.2.3: *$\mathcal{S}^{-1}$ realizes an isomorphism of the Hopf algebra $(\mathcal{A},\Delta_t,\varepsilon_t,J_t)$ onto the quasitriangular twisted tensor product Hopf algebra $A_1\hat{\otimes}_{\tau R^{(1)}}A_1$. Then $(\mathcal{A},\Delta_t,\varepsilon_t,J_t)$ has a quasitriangular structure given by $(\mathcal{S}\otimes\mathcal{S})(\mathcal{R}_1)$ which is equal to the R-matrix $\mathcal{R}$ [Formula (30)].*

Remark IV.2.4: The Hopf algebra $(\mathcal{A},\Delta_t,\varepsilon_t,J_t)$ has another quasitriangular *R*-matrix $\overline{\mathcal{R}}$ given by

$$\overline{\mathcal{R}}=W_{41}(R_{31}^{(1)})^{-1}(R_{24}{}^{(2)})^{-1}W_{23}{}^{-1}.$$

IV.3 $*$-structures on $(\mathcal{A},\Delta_t)$

In Refs. 10 and 14, the authors introduce a conjugate-linear map Φ on the Hopf algebra $\mathcal{U}_t\mathcal{L}$ (or $\mathcal{A}_t$) as follows :

$$\Phi(l)=l,\quad \Phi(k)=\tilde{k},\quad \Phi(\tilde{k})=k,\quad \Phi(K_1)=K_2,\quad \Phi(L_+)=L_-,$$

$$\Phi\circ\Phi=id.$$

After having chosen q real (equivalent to t real), Φ becomes an anti-involution of the algebra $\mathcal{A}_t$, which also is a morphism of the coalgebra structure. Then for t real, Formulas (11) and (12) permit us to prove that

$$\Phi=\overline{\varphi}\circ J_t|_{\mathcal{A}_t}\ , \tag{32}$$

where $\overline{\varphi}$ is the conjugate map of φ.

Taking into account Remark IV.1.2 (a) and the results of Section III. 2, Φ has a unique continuous extension on $\mathcal{A}$ (for t real), which is given by the preceding Formula. Thus, for t real, $(\mathcal{A},\Delta_t,\varepsilon_t,J_t,\varphi)$ is a *-Hopf algebra.

V. DUAL FORMALISM AND REAL STRUCTURES

In this section, we first construct the topological dual vector space of $\mathscr{A}$, $H(G)$ (G as defined in V.1) which coincides with the algebra of the coefficient functions on G (for the holomorphic finite-dimensional representations of G). In Sec. V.1 we also give the non-commutative Hopf algebra structure on $(H(G),\star_t)$ dual to the Hopf structure on $\mathscr{A}$ defined by $\mathscr{U}_t\mathscr{L}$: we obtain the non-commutative algebra structure of Podles-Woronowicz in term of the classical product of functions. Now, we introduce a *-structure on $(H(G),\star_t)$ which is equivalent to consider the Hopf subalgebra $(H(G_0),\star_t)$ (where G_0 is a real Lie subgroup of G isomorphic to $SL(2,\mathbb{C})$) (Sec. V.2). Then, the main result of this Section is to extend the Hopf structure of $(H(G_0),\star_t)$ to $\mathscr{C}^{\infty}(G_0)$ (which contains $H(G_0)$), endowed with its usual Fréchet topology. Such a result is proved in Ref. 5 for any real semi-simple Lie group G' and any deformation of the commutative algebra $H(G')$ which is inherited from a deformation of the coalgebra structure on the enveloping algebra of the Lie algebra of G'. In our case, the product $\star_t$ on $H(G_0)$ is inherited from the coproduct Δ_t on $\mathscr{A}$ with values in $\mathscr{A}\hat{\otimes}.\mathscr{A}$ and $\mathscr{A}\hat{\otimes}.\mathscr{A}$ strictly containing $(\mathscr{U}\mathscr{L}\otimes\mathscr{U}\mathscr{L})[[t]]$. Fortunately, the Formula $\Delta_t=\mathscr{P}(t)\Delta_0\mathscr{P}(t)^{-1}$ and Corollary IV.2.2. which asserts that $\mathscr{P}(t)$ belongs to $(\mathscr{U}\mathscr{L}\otimes\mathscr{U}\mathscr{L})[[t]]$, permits us to apply the result of Ref. 5 and to conclude (Sec. V.3).

V.1 Dual Hopf algebra of $(\mathscr{A},\Delta_t)$

Set

$$G=SL(2,\mathbb{C})\times SL(2,\mathbb{C}).$$

This group is imbedded in $\mathscr{A}$ by the following identification:

$$x=(T,\tilde{T})\in G\xrightarrow{i}a=(a_{n,p})_{(n,p)\in(\mathbb{N}/2)^2}\in\mathscr{A},$$

where

$$a_{n,p}=\rho_n(T)\otimes\rho_p(\tilde{T})=\rho_{n,p}(x).$$

i is an injective morphism. Using the same argument as for the density of $\mathscr{U}\mathscr{L}$ in $\mathscr{A}$ (Jacobson density Theorem), we get

$$\overline{\text{span } i(G)}=\mathscr{A}.$$

Let us consider the topological dual space $\mathscr{A}^{\star}$ of $\mathscr{A}$. $\mathscr{A}^{\star}$ can be identified with $\mathscr{H}(G)=\oplus_{(n,p)\in(\mathbb{N}/2)^2}\mathscr{L}(V_{n,p})$ (endowed by the inductive topology) as follows :

$$a=(a_{n,p})\in\mathscr{A},\quad b=\sum_{\text{finite}}b_{np}\in\mathscr{H},\quad \langle b|a\rangle=\sum_{\text{finite}}\text{Tr}(b_{np}a_{np})\ .$$

Then the density of G in $\mathscr{A}$ allows us to consider $\mathscr{H}(G)$ as an algebra of functions on G .

Using Corollary III.2.4, $\mathscr{H}(G)$ is exactly the algebra of functions on G generated by the coefficient functions, i.e.

$$\mathscr{H}(G)=\mathbb{C}[a,b,c,d,a',b',c',d']/\langle ad-bc=a'd'-b'c'=1\rangle,$$

where the element x of G is given by

$$x=(T,\tilde{T}),\quad \text{with } T=\begin{pmatrix}a & b\\ c & d\end{pmatrix}=\rho_{1/2,0}(x),\quad \tilde{T}=\begin{pmatrix}\tilde{a} & -\tilde{b}\\ -\tilde{c} & \tilde{d}\end{pmatrix}=\rho_{0,1/2}(x).$$

By duality, the results of Section IV give various topological Hopf structures on $\mathscr{H}$. The coproduct is always the mapping $h(x)\to h(x.y)$ if h is in $\mathscr{H}(G)$. But $\mathscr{H}(G)$ is endowed with different associative, non-commutative products. Denote by $\star_t$ (resp., $\star_t', \star_t''$) the product on $\mathscr{H}(G)$ induced by the coproduct Δ_t (resp., Δ_t', Δ_t'') of $\mathscr{A}$. Theorem IV.2.1 and Corollary IV.2.2 together with Formulas (26) and (27) allow us to express the products $\star_t, \star_t', \star_t''$ on $\mathscr{H}(G)$ in term of the classical product of functions.
Set $(.\otimes.)\circ\Delta_t=.\otimes_t.$ and $(.\otimes.)\circ\tau\Delta_t=.\otimes_t^{op}.$
We obtain

$$
\begin{aligned}
&\text{(a)}\quad T\underset{t}{\otimes}T=P^{(1)}_{1/2,\,1/2}(t)T\otimes_0 T(P^{(1)}_{1/2,\,1/2}(t))^{-1},\\
&\text{(b)}\quad T\underset{t}{\otimes}^{op}T=R^{(1)}_{1/2,\,1/2}(t)T\otimes_t T(R^{(1)}_{1/2,\,1/2}(t))^{-1},\\
&\text{(c)}\quad \widetilde{T}\underset{t}{\otimes}\widetilde{T}=\tau P^{(2)}_{1/2,\,1/2}(t)\widetilde{T}\otimes_0\widetilde{T}(\tau P^{(2)}_{1/2,\,1/2}(t))^{-1},\\
&\text{(d)}\quad \widetilde{T}\underset{t}{\otimes}^{op}\widetilde{T}=\tau R^{(2)}_{1/2,\,1/2}(t)\widetilde{T}\otimes_t\widetilde{T}(\tau R^{(2)}_{1/2,\,1/2}(t))^{-1};
\end{aligned}
\tag{33}
$$

$$
\begin{aligned}
&\text{(a)}\quad T\underset{t}{\otimes}\widetilde{T}=T\otimes_0\widetilde{T},\\
&\text{(b)}\quad \widetilde{T}\underset{t}{\otimes}T=\hat{R}_{(1/2,0),(0,1/2)}T\otimes_t\widetilde{T}(\hat{R}_{(1/2,0),(0,1/2)})^{-1},
\end{aligned}
\tag{34}
$$

or explicitly,

$$a^{\star 2}=a^2,\quad b^{\star 2}=b^2,\quad c^{\star 2}=c^2,\quad d^{\star 2}=d^2,$$

$$\widetilde{a}^{\,\star 2}=\widetilde{a}^{\,2},\quad \widetilde{b}^{\star 2}=\widetilde{b}^{\,2},\quad \widetilde{c}^{\,\star 2}=\widetilde{c}^{\,2},\quad \widetilde{d}^{\star 2}=\widetilde{d}^{\,2},$$

$$b\star_t a=qa\star_t b=q^{\frac{1}{2}}ab,\quad \widetilde{b}\star_t\widetilde{a}=q^{-1}\widetilde{a}\star_t\widetilde{b}=q^{\frac{-1}{2}}\widetilde{a}\widetilde{b},$$

$$c\star_t a=qa\star_t c=2q^{\frac{1}{2}}(q+q^{-1})^{-1}ac,\quad \widetilde{c}\star_t\widetilde{a}=q^{-1}\widetilde{a}\star_t\widetilde{c}=2q^{-\frac{1}{2}}(q+q^{-1})^{-1}\widetilde{a}\widetilde{c},$$

$$d\star_t b=qb\star_t d=2q^{\frac{1}{2}}(q+q^{-1})^{-1}bd,\quad \widetilde{d}\star_t\widetilde{b}=q^{-1}\widetilde{b}\star_t\widetilde{d}=2q^{\frac{-1}{2}}(q+q^{-1})^{-1}\widetilde{b}\widetilde{d},\tag{33$'$}$$

$$d\star_t c=qc\star_t d=2q^{\frac{1}{2}}cd,\quad \widetilde{d}\star_t\widetilde{c}=q^{-1}\widetilde{c}\star_t\widetilde{d}=2q^{\frac{-1}{2}}\widetilde{c}\widetilde{d},$$

$$c\star_t b=b\star_t c=2(q+q^{-1})^{-1}bc,\quad \widetilde{c}\star_t\widetilde{b}=\widetilde{b}\star_t\widetilde{c}=2(q+q^{-1})^{-1}\widetilde{b}\widetilde{c},$$

$$a\star_t d=ad-(q-q^{-1})(q+q^{-1})^{-1}bc,\quad \widetilde{a}\star_t\widetilde{d}=ad+(q-q^{-1})(q+q^{-1})^{-1}\widetilde{b}\widetilde{c},$$

$$d\star_t a=ad+(q-q^{-1})(q+q^{-1})^{-1}bc,\quad \widetilde{d}\star_t\widetilde{a}=ad-(q-q^{-1})(q+q^{-1})^{-1}\widetilde{b}\widetilde{c},$$

$$a\star_t\widetilde{a}=\widetilde{a}\star_t a+q\lambda\widetilde{c}\star_t c=a\widetilde{a},\quad a\star_t\widetilde{d}=\widetilde{d}\star_t a=a\widetilde{d},$$

$$b\star_t\widetilde{b}=\widetilde{b}\star_t b-q\lambda(\widetilde{a}\star_t a-d\star_t\widetilde{d})=b\widetilde{b},\quad b\star_t\widetilde{c}=\widetilde{c}\star_t b=b\widetilde{c},$$

$$c\star_t\widetilde{c}=\widetilde{c}\star_t c=c\widetilde{c},\quad c\star_t\widetilde{b}=\widetilde{b}\star_t c=c\widetilde{b},$$

$$d\star_t\tilde{d}=\tilde{d}\star_t d-q\lambda\tilde{c}\star_t c=d\tilde{d},\quad d\star_t\tilde{a}=\tilde{a}\star_t d=d\tilde{a},$$

$$c\star_t\tilde{a}=q^{-1}\tilde{a}\star_t c=\tilde{a}c,\quad a\star_t\tilde{c}=q^{-1}\tilde{c}\star_t a=\tilde{c}a,$$

$$c\star_t\tilde{d}=q\tilde{d}\star_t c=\tilde{d}c,\quad d\star_t\tilde{c}=q\tilde{c}\star_t d=\tilde{c}d, \tag{34'}$$

$$b\star_t\tilde{d}=q^{-1}\tilde{d}\star_t b-\lambda\tilde{c}\star_t a=b\tilde{d},\quad d\star_t\tilde{b}=q^{-1}\tilde{b}\star_t d-\lambda\tilde{a}\star_t c=d\tilde{b},$$

$$a\star_t\tilde{b}=q\tilde{b}\star_t a+q^2\lambda\tilde{d}\star_t c=a\tilde{b},\quad b\star_t\tilde{a}=q\tilde{a}\star_t b+q^2\lambda\tilde{c}\star_t d=b\tilde{a}.$$

Remark V.1.1 : We recognize in Formulas (33′) and (34′) the relations obtained by Podles and Woronowicz.[8]

Set

$$H=\mathbb{C}[a,b,c,d]/\langle ad-bc=1\rangle;\quad \tilde{H}=\mathbb{C}[\tilde{a},\tilde{b},\tilde{c},\tilde{d}]/\langle\tilde{a}\tilde{d}-\tilde{b}\tilde{c}=1\rangle\ .$$

From Theorem IV.2.1, the product $\star_t''$ (resp., $\star_t'$) coïncides with the product $\star_t$ (resp., $\star_t$) on H and with the product $\star_t$ (resp., $\star_{-t}$) on $\tilde{H}$.
The dual translation of Theorem IV.2.1 and Corollary IV.2.3 is the following one.

Proposition V.1.2:

(*a*) H and $\tilde{H}$ are two Hopf subalgebras of $(\mathscr{H}(G),\star_t')$ [which is isomorphic to $SL_t(2,\mathbb{C})$] and $(\mathscr{H}(G),\star_t')$ is $H\otimes\tilde{H}$ as the tensor product of Hopf algebras.

(*b*) H (resp., $\tilde{H}$) is a Hopf subalgebra of $(\mathscr{H}(G),\star_t)$ isomorphic to $SL_t(2)$ [resp., $SL_{-t}(2)$]. Moreover $(\mathscr{H}(G),\star_t)$ is isomorphic to the double cross product of two Hopf algebras $SL_t(2)$ as defined by Majid in Ref. 12.

Proof: Part (a) and the first affirmation of Part (b) summarize the above claimed properties. Using Corollary IV.2.3 and the injection of G in $\mathscr{A}$, Formula (34b) is equivalent by $\mathscr{S}$ to

$$\hat{R}_{(1/2,0),(1/2,0)}T\otimes_t s^{-1}(\tilde{T})=s^{-1}(\tilde{T})\otimes_t T\hat{R}_{(1/2,0),(1/2,0)}\ . \tag{35}$$

We recognize the Formula which is used for the definition of the q-Lorentz group in Ref. 12. Taking into account the results of Refs. 9 and 12, the Hopf algebra ${}^t\mathscr{S}^{-1}[\mathscr{H}(G)]$ is the double cross product of two Hopf algebras isomorphic to $SL_t(2)$ (or $H,\star_t$): Formula (35) gives the action of each of these algebras on the other one.

V.2 Real structure on $(\mathscr{H},\star_t)$ (for q real)

The anti-involution Φ of the algebras $\mathscr{A}$ [Formula (32)] defines by duality an anti-involution Φ^* of the algebra $(\mathscr{H}(G),\star_t)$:

$$\Phi^*={}^t(\Phi\circ J_t^{-1})={}^t\overline{\varphi}.$$

We have

$$\overline{\varphi(x)}=\begin{pmatrix}\begin{pmatrix}\overline{\tilde{a}} & q^{-1}\overline{\tilde{b}}\\ q\overline{\tilde{c}} & \overline{\tilde{d}}\end{pmatrix},\begin{pmatrix}\overline{a} & -q\overline{b}\\ -q^{-1}\overline{c} & \overline{d}\end{pmatrix}\end{pmatrix}.$$

A real structure on $\mathscr{H}$ is defined by

$$\Phi^*=J_t\ \Leftrightarrow\ \tilde{T}=\Gamma{}^t\overline{T^{-1}}\Gamma^{-1}, \tag{36}$$

where

$$\Gamma=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}.$$

Set $G_0=\{(T,\Gamma^t\overline{T^{-1}}\Gamma^{-1}),T\in SL(2,\mathbb{C})\}$.
G_0 is a subgroup of $SL(2,\mathbb{C})\times SL(2,\mathbb{C})$, isomorphic to the real Lie group $SL(2,\mathbb{C})$. Then the real form given by Formula (36) of the $*$-Hopf algebra $(\mathscr{H}(G),\star_t,\Phi^*)$ is $\mathscr{H}(G_0)$. We remark that $\{(T,\Gamma T\Gamma^{-1}),T\in SU(2)\}$ is a subgroup of G_0 isomorphic to $SU(2)$. Thus $\mathscr{H}(SU(2))$ [or $SU_t(2)$] is a Hopf subalgebra of $\mathscr{H}(G_0)$.

V.3 $\star$-product on $C^\infty(G_0)$

Let us introduce $C^\infty(G_0)$ with its usual Fréchet topology and its dual space $A(G_0)$ (the space of compactly supported distributions on G_0) with the strong dual topology. Thus $C^\infty(G_0)$ and $A(G_0)$ are topological Hopf algebras with dual Hopf structures. Moreover, $C^\infty(G_0)$ [resp., $A(G_0)$] contains $H(G_0)$ (resp., $\mathscr{U}\mathscr{L}$) as Hopf subalgebra and $A(G_0)$ is a subalgebra of $\mathscr{A}$. Now, as noticed at the beginning of Section V, the results of Corollary IV.2.2 allows us to apply Theorem IV.3 of Ref. 5. The latter one with Remark V.1.1 allows to assert the following.

Proposition V.3.1: *There exists a topological Hopf deformation of* $\mathscr{C}^\infty(G_0)$ [resp., $A(G_0)$] *which extends the topological Hopf deformation* $[\mathscr{H}(G_0),\star_t]$ *[resp., which is a restriction of the topological Hopf deformation* $(\mathscr{A},\Delta_t)$*]. Moreover, this product* $\star_t$ *induces on* $\mathscr{H}(G_0)$ *the noncommutative algebra structure introduced by Podles and Woronowicz.*[8]

To conclude, in this paper we show that the topological Hopf algebras $(\mathscr{C}^\infty(G_0),\star_t)$ and $(A(G_0),\Delta_t)$ are the good topological models for (respectively) $SL_t(2,\mathbb{C})$ and $\mathscr{U}_t\mathscr{L}$ in our approach to quantum group theory, which is based on deformation quantization.

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Inclusion of gauge bosons in the tensor formulation of the Dirac theory

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A recent article characterized all classical tensor systems which admit Fermi quantization as those having unitary Lie–Poisson brackets. Examples include Euler's tensor equation for a rigid body and Dirac's bispinor equation in tensor form. It was further shown that the tensor form of Dirac's bispinor Lagrangian can be derived from a tetrad formulation of a Kaluza–Klein model, which unifies the Dirac and Einstein Lagrangians. Thus, fermions, like bosons, are represented as gauge fields in the tensor formulation of the Dirac theory. In this article boson gauge fields are added to the unified Dirac–Einstein Lagrangian by defining the gauge group of the Kaluza–Klein model to be a semi-direct product. It is shown that the semi-direct product structure uniquely prescribes the usual ''minimal coupling'' between bosons and fermions. © *1996 American Institute of Physics.*
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I. INTRODUCTION

Ever since Dirac introduced his celebrated bispinor equation in 1928, there has been continued interest in its tensor formulation. Recently, Takahashi and Zhelnorovich investigated the tensor form of the Dirac Lagrangian.[1] Following this work, we showed that the tensor Dirac Lagrangian is equal to a constrained Yang–Mills Lagrangian in the limit of an infinitely large coupling constant.[2] We also showed that the tensor form of Dirac's partial differential bispinor equation is a classical Hamiltonian system with (noncanonical) unitary Lie–Poisson brackets.[3] Such Lie–Poisson brackets occur classically for systems with gauge symmetry such as Euler's equation for a rigid body.[4] Fermi quantization was derived for both the Dirac and Euler tensor equations by representing the classical Lie–Poisson brackets as commutators of Heisenberg operators.[3]

A belief that a 360° rotation alters the state of a fermion particle has for a long time supported the view in quantum field theory that fermions can be represented only by bispinor fields, and not by tensor fields. However, recent studies of particle localization show that 360° rotation of bispinor fields, whose energy spectrum is bounded from below, produces no observable effects.[2,5,6] Moreover, experiments designed to observe the rotation properties of bispinors, in fact, described the rotation properties of constrained tensor fields.[3]

More recently we showed that the tensor form of the Dirac Lagrangian and its constraint could be derived from a tetrad formulation of a Kaluza–Klein model which unifies the Dirac and Einstein Lagrangians. In this tetrad formulation, both the fermion field and the gravitational field arise from a tetrad of vector fields v_K, where $K=0,1,2,3$, and a complex scalar field ρ. We showed that the isometric modes of the tetrad propagate as fermions, whereas the self-adjoint modes propagate as gravitons.[7]

Introducing a tetrad to describe both fermion and gravitational fields addresses an important problem posed by current theories of fermion–graviton interaction. To define bispinor fields on a space–time, reference tetrad fields (or equivalent soldering forms) must be defined.[8,9] The implied dynamics of these reference fields have been, at best, partially modelled. We found that such tetrad fields themselves, used as dynamical variables, give rise to both fermions and gravitons.

In this article we introduce gauge bosons into the Kaluza–Klein model based on the constrained Yang–Mills formulation of the Dirac theory. In this formulation fermions are represented

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as constrained gauge potentials and bosons are represented as unconstrained gauge potentials. As discussed below, the two sets of gauge potentials are associated with a semi-direct product gauge group which precisely produces the usual coupling between bosons and fermions.

In the constrained Yang–Mills formulation of the Dirac theory, bispinor fields are mapped to $SL(2,R)\times U(1)$ gauge potentials F_α^K and a complex scalar field ρ which satisfy the orthogonal constraint[3,7]

$$F_\alpha^K F_{K\beta} = |\rho|^2 g_{\alpha\beta}, \tag{1.1}$$

where $g_{\alpha\beta}$ is the Minkowski space–time metric. The gauge index $K=0,1,2,3$ is contracted using a metric with Minkowski signature which will be denoted η_{JK} [note that the gauge group $SL(2,R)\times U(1)$ is a four-dimensional Lie group for which η_{JK} is an invariant metric]. The covariant derivative in the Yang–Mills formulation of the Dirac theory can be expanded symmetrically to include electromagnetic and chiral interactions by the addition of four $SL(2,R)\times U(1)$ unconstrained boson gauge potentials V_α^K which act on the four constrained fermion $SL(2,R)\times U(1)$ gauge potentials. This gives the gauge potentials V_α^K and F_α^K a hierarchical structure, whereby one set of gauge potentials acts on the second set, and not vice versa. This is precisely the hierarchical structure of gauge potentials associated with a gauge group which is a semi-direct product. Thus we show that the set of gauge potentials $\{F_\alpha^K, V_\alpha^K\}$ are associated with the semi-direct product gauge group $\Gamma = G_\varphi \times G$, where $G = SL(2,R)\times U(1)$ and φ denotes the adjoint action of G on G (see Sec. II). That is, in the tensor formulation the usual coupling between bosons and fermions results from the semi-direct product structure of the gauge group Γ.

As shown in Sec. II, the four boson gauge potentials V_α^K are also defined in the bispinor theory. The electromagnetic gauge potential V_α^0 and the chiral gauge potential V_α^3 correspond to a maximal compact subgroup $U(1)\times U(1)$ of $SL(2,R)\times U(1)$. The gauge potentials V_α^1 and V_α^2 correspond to noncompact one-parameter subgroups of $SL(2,R)\times U(1)$ which, acting on F_α^K or bispinor fields Ψ, mix positive and negative energy states. Thus only the compact gauge potentials V_α^0 and V_α^3 appear to be physical. Hence, as in the bispinor theory, we set V_α^1 and V_α^2 to zero by restricting the boson gauge group to a maximal compact subgroup of $SL(2,R)\times U(1)$.

The derivations presented in Sec. II suggest that the tensor formulation of the Dirac theory extends to more than one fermion flavor, and hence to further applications in particle physics. In Sec. II we show that the Dirac–Yang–Mills Lagrangian for the gauge group $SL(2,R)\times U(1)$ extends to the larger gauge group $SL(2,C)\times U(1)$, which contains the electroweak gauge group $SU(2)\times U(1)$ as a maximal compact subgroup. Application of the extended Lagrangian to electroweak theory is presently being considered.

In this paper we introduce two new notions which have application to Kaluza–Klein theories. First, we consider Kaluza–Klein theories for which the gauge group is a semi-direct product, which, as previously discussed, allows us to define boson gauge potentials which act on the fermion gauge potentials.

Second in the Kaluza–Klein formulation of the tensor Dirac theory, the fermion field, boson field, and the gravitational field are described by a scalar field ρ and a tetrad of vector fields v_K on a smooth manifold $M = X\times\Gamma$, where X is a space–time and $\Gamma = G_\varphi \times G$ is the semi-direct product gauge group defined previously. The tetrad v_K together with a (fixed) basis of right-invariant vector fields on Γ defines a metric, denoted as $\langle , \rangle$, and hence a volume form, denoted as dv, and also a curvature two-form, denoted as $R(,)$ on M (see Sec. III). The unified action, S, for the gravitational, boson, and fermion fields is given by

$$S = \int L\, dv, \tag{1.2}$$

where the unified Lagrangian, L, is (see Sec. III)

$$L=\frac{g}{16\pi\kappa_0}R[v]+\overline{v_K(\rho+m)}v^K(\rho+m)-\frac{1}{2}g^2|\rho|^4, \tag{1.3}$$

where κ_0 is Newton's gravitational constant, g is a coupling constant, and m is the fermion mass. In formula (1.3), we employ the sum of sectional curvatures restricted to the subspace spanned by the tetrad v_K:

$$R[v]=\sum_{J=0}^{3}\sum_{K=0}^{3}\langle R(v_J,v_K)v^J,v^K\rangle. \tag{1.4}$$

This both avoids unphysical terms such as the cosmic constant arising from the scalar curvature of Γ, and removes previously assumed restrictions on the gauge group, such as a bi-invariant metric.[10] Furthermore, by formulating the Kaluza–Klein Lagrangian (1.3) with the tetrad v_K, the constraint (1.1) is eliminated.

In Sec. II we include boson gauge fields in the derivation of the tensor form of the Dirac bispinor equation. Then in Sec. III we derive a Kaluza–Klein model based on the tensor Dirac theory. We express the usual equations for the gravitational field $g_{\alpha\beta}$, the electromagnetic and chiral fields V_α^K, and the Dirac bispinor field Ψ in terms of new variables (v_K,ρ), and thereby unify these fields within a simple conceptual framework at a classical level.

II. TENSOR FORM OF THE DIRAC BISPINOR LAGRANGIAN INCLUDING BOSON GAUGE POTENTIALS

In this section we include boson gauge potentials in the derivation of the tensor form of the Dirac bispinor Lagrangian. We will show that the tensor form of the Dirac Lagrangian unifies boson and fermion fields as gauge potentials belonging to a semi-direct product gauge group. We will further show that the semi-direct product structure of the gauge potentials produces the usual minimal coupling between boson and fermion fields. As in previous work,[3,7] the derivation exploits the SL(2,R)×U(1) gauge symmetry of Dirac's bispinor Lagrangian.

Consider the SL(2,R)×U(1) gauge transformations, acting on the bispinor field Ψ, with the infinitesimal generators τ_K for $K=0,1,2,3$ defined by

$$\begin{aligned}&\tau_0\Psi=-i\Psi, \quad \tau_1\Psi=i\Psi^C,\\ &\tau_2\Psi=\Psi^C, \quad \tau_3\Psi=i\gamma_5\Psi,\end{aligned} \tag{2.1}$$

where Ψ^C denotes the charge conjugate of Ψ and γ_5 is the fifth Dirac matrix.[6] Note that the action of SL(2,R)×U(1) on Ψ is *real* linear, whereas usually only complex linear gauge transformations of bispinors are considered. The infinitesimal gauge generators τ_0, τ_1, and τ_2 generate SL(2,R) and τ_3 generates U(1).

The SL(2,R)×U(1) gauge transformations generated by τ_K commute with Lorentz transformations.[6] From formula (2.1) the commutation relations of the gauge generators τ_K are given by

$$[\tau_0,\tau_1]=2\tau_2, \quad [\tau_0,\tau_2]=-2\tau_1, \quad [\tau_1,\tau_2]=-2\tau_0, \tag{2.2}$$

and τ_3 commutes with all the τ_K. Formula (2.2) can be written more compactly as

$$[\tau_J,\tau_K]=2f_{JK}^L\tau_L, \tag{2.3}$$

which defines the Lie algebra structure constants f_{JK}^L for the gauge group SL(2,R)×U(1).

From formula (2.2) the Minkowski metric η_{JK}, with diagonal elements $\{1,-1,-1,-1\}$ and zeros off the diagonal, is an invariant metric[11] for the gauge group $\mathrm{SL}(2,R)\times\mathrm{U}(1)$. Gauge indices $J,K,L=0,1,2,3$ will be raised and lowered using the Minkowski metric η_{JK}. As in formula (2.3), repeated gauge indices are to be summed.

We define the Yang–Mills covariant derivative $\hat{D}_\alpha$ acting on bispinor fields as follows:

$$\hat{D}_\alpha=\partial_\alpha+qV_\alpha^K\tau_K, \tag{2.4}$$

where $\alpha=0,1,2,3$ is a Lorentz index, ∂_α denote partial derivatives with respect to space–time coordinates, q is a Yang–Mills coupling constant, and V_α^K are boson gauge potentials associated with the gauge generators τ_K. Associated with the gauge potentials V_α^K is the Yang–Mills curvature tensor $V_{\alpha\beta}^K$ defined by the formula

$$[\hat{D}_\alpha,\hat{D}_\beta]=qV_{\alpha\beta}^K\tau_K. \tag{2.5}$$

From formulas (2.3) and (2.4) we obtain the explicit expression

$$V_{\alpha\beta}^L=\partial_\alpha V_\beta^L-\partial_\beta V_\alpha^L+2qf_{JK}^L V_\alpha^J V_\beta^K. \tag{2.6}$$

Dirac's bispinor Lagrangian, L_{D}, is given by

$$L_{\mathrm{D}}=\mathrm{Re}[i\overline{\Psi}\gamma^\alpha\hat{D}_\alpha\Psi-m_0 s]-\tfrac{1}{4}V_K^{\alpha\beta}V_{\alpha\beta}^K, \tag{2.7}$$

where s is the complex scalar field defined by

$$\mathrm{Re}[s]=\overline{\Psi}\Psi,\quad \mathrm{Im}[s]=i\overline{\Psi}\gamma_5\Psi, \tag{2.8}$$

where $\overline{\Psi}$ is the dual conjugate of the bispinor field Ψ, the γ^α are Dirac matrices,[6] and m_0 denotes the fermion mass. Lorentz indices α, $\beta=0,1,2,3$ are raised and lowered using the (Minkowski) space–time metric, which we will denote as $g_{\alpha\beta}$. Repeated Lorentz indices are to be summed.

Apart from the mass term, the Dirac Lagrangian (2.7) is invariant under the $\mathrm{SL}(2,R)\times\mathrm{U}(1)$ gauge transformations (2.1). From formula (2.8), s is invariant under $\mathrm{SL}(2,R)$ gauge transformations, and transforms as a complex scalar under the U(1) gauge transformations generated by τ_3. To make the Lagrangian (2.7) invariant for *all* $\mathrm{SL}(2,R)\times\mathrm{U}(1)$ gauge transformations, it suffices that m_0 transform like $\overline{s}$ (the complex conjugate of s). Since m_0 appears in the Lagrangian (2.7) without derivatives, the assumption that m_0 transforms like $\overline{s}$ under U(1) gauge transformations has no effect on the Dirac equation.

Expanding the covariant derivative $\hat{D}_\alpha$ in the Dirac Lagrangian (2.7), we obtain the following interaction term coupling the boson and fermion fields:

$$L_I=qV_\alpha^K j_K^\alpha, \tag{2.9}$$

where the fermion Noether currents j_K^α are defined by

$$j_K^\alpha=\mathrm{Re}[i\overline{\Psi}\gamma^\alpha\tau_K\Psi]. \tag{2.10}$$

The Noether currents (2.10) satisfy an orthogonal constraint known as a Fierz identity given by[1,3]

$$j_\alpha^K j_{K\beta}=|s|^2 g_{\alpha\beta}, \tag{2.11}$$

where, as previously stated, $g_{\alpha\beta}$ is the (Minkowski) space–time metric.

We then map a set of $\mathrm{SL}(2,R)\times\mathrm{U}(1)$ gauge potentials F_α^K and a complex scalar field ρ into (j_α^K,s) by setting

$$j^K_\alpha = 4|\rho|^2 F^K_\alpha, \quad s = 4|\rho|^2\overline{\rho.} \tag{2.12}$$

Note that by formulas (2.8), (2.10), and (2.12), the fields F^K_α transform as SL(2,R)×U(1) gauge potentials; whereas ρ is invariant under SL(2,R) gauge transformations, and transforms as a complex scalar under the U(1) gauge transformations generated by τ_3. For the fields (F^K_α,ρ), the Fierz identity (2.11) becomes the orthogonal constraint:

$$F^K_\alpha F_{K\beta} = |\rho|^2 g_{\alpha\beta}. \tag{2.13}$$

Note that the space–time metric $g_{\alpha\beta}$ has the same signature as the metric η_{JK}. The tetrad model presented in Sec. III will explicate both the constraint (2.13) and the equality of the metric signatures.

Now, consider (F^K_α, V^K_α) as gauge potentials for the gauge group Γ whose infinitesimal generators (S_K, T_K) satisfy the following semi-direct product commutation relations:[12]

$$[S_J,\ S_K] = f^L_{JK} S_L, \quad [T_J,\ S_K] = f^L_{JK} S_L, \quad [T_J,\ T_K] = f^L_{JK} T_L, \tag{2.14}$$

where f^L_{JK} are the previously defined SL(2,R)×U(1) structure constants.

We define the Yang–Mills covariant derivative for the semi-direct product gauge group Γ by

$$D_\alpha = \partial_\alpha + g F^K_\alpha S_K + 2q V^K_\alpha T_K, \tag{2.15}$$

where we set $T_K = \frac{1}{2}\tau_K$ [compare formulas (2.3) and (2.14)], g is a Yang–Mills coupling constant, and q is the previously defined coupling constant in formula (2.4). Note that the covariant derivative (2.15) can also be written as

$$D_\alpha = \hat{D}_\alpha + g F^K_\alpha S_K, \tag{2.16}$$

where we denote

$$\hat{D}_\alpha = \partial_\alpha + 2q V^K_\alpha T_K, \tag{2.17}$$

which often simplifies derivations. Formula (2.17) agrees with (2.4) since $T_K = \frac{1}{2}\tau_K$. No confusion results from using the same symbol, $\hat{D}_\alpha$, for the covariant derivative (2.17) acting on bispinor or tensor fields. Associated with the semi-direct product gauge potentials (F^K_α, V^K_α) is the Yang–Mills curvature tensor $(F^K_{\alpha\beta}, V^K_{\alpha\beta})$ defined by the formula

$$[D_\alpha,\ D_\beta] = g F^K_{\alpha\beta} S_K + 2q V^K_{\alpha\beta} T_K. \tag{2.18}$$

From formulas (2.14) and (2.15) we obtain the explicit expression

$$F^L_{\alpha\beta} = \hat{D}_\alpha F^L_\beta - \hat{D}_\beta F^L_\alpha + g f^L_{JK} F^J_\alpha F^K_\beta, \tag{2.19}$$

where we denote

$$\hat{D}_\alpha F^L_\beta = \partial_\alpha F^L_\beta + 2q f^L_{JK} V^J_\alpha F^K_\beta, \tag{2.20}$$

whereas $V^K_{\alpha\beta}$ is given as in formula (2.6).

Furthermore, we define the metric on the gauge group Γ to be the block matrix

$$\eta = (\eta_{ab}) = \begin{bmatrix} \eta_{JK} & 0 \\ 0 & -g\,\eta_{JK} \end{bmatrix}, \tag{2.21}$$

whose components we denote as η_{ab}. Let F^a_α and $F^a_{\alpha\beta}$ denote the components of (F^K_α, V^K_α) and $(F^K_{\alpha\beta}, V^K_{\alpha\beta})$, respectively. Furthermore, let the gauge indices a,b be raised and lowered using the metric η_{ab}. Then, with the orthogonal constraint (2.13), Dirac's equation is obtained from the following Yang–Mills Lagrangian, L_g, in the limit of an infinitely large Yang–Mills coupling constant g:

$$L_g = \tfrac{1}{4} F^{\alpha\beta}_a F^a_{\alpha\beta} + \overline{D_\alpha(\rho+m)} D^\alpha(\rho+m) - \tfrac{1}{2} g^2 |\rho|^4, \tag{2.22}$$

where $m_0 = \frac{1}{2} mg$ is the fermion mass, and, from formula (2.16),

$$D_\alpha(\rho+m) = \hat{D}_\alpha(\rho+m) + igF^3_\alpha(\rho+m), \tag{2.23}$$

where from formula (2.17)

$$\hat{D}_\alpha(\rho+m) = \partial_\alpha \rho + 2iqV^3_\alpha(\rho+m). \tag{2.24}$$

Recall that s and m_0, and hence ρ and m, transform as complex scalars under the U(1) gauge transformations generated by S_3 and T_3. [Note: The part of the Lagrangian (2.22) for the scalar field ρ is not unique. An alternative Lagrangian from which Dirac's bispinor Lagrangian can also be obtained was previously presented.[2,3] However, the Lagrangian (2.22) has unique additional properties discussed in Ref. 7.]

Note that the boson gauge potentials V^K_α occur in the Yang–Mills Lagrangian L_g via the minimal substitution of $\hat{D}_\alpha = \partial_\alpha + 2qV^K_\alpha T_K$ for ∂_α [see formulas (2.17), (2.19), (2.20), (2.23), and (2.24)]. This ''minimal coupling'' was shown by formulas (2.15) and (2.18) to be uniquely prescribed by the semi-direct product commutation relations (2.14). In the following theorem we derive the Dirac bispinor Lagrangian L_{D} from the Yang–Mills Lagrangian L_g, and thereby obtain the usual minimal coupling between boson gauge potentials V^K_α and bispinor fields Ψ.

Theorem 1: Dirac's bispinor Lagrangian (2.7) equals

$$L_{\mathrm{D}} = \lim_{g\to\infty} g^{-1} L_g. \tag{2.25}$$

Proof: The derivation is greatly simplified by embedding the F^K_α and V^K_α into SL(2,C)×U(1) gauge potentials A^K_α and W^K_α as follows:

$$\begin{gathered} A^0_\alpha = -F^3_\alpha, \quad W^0_\alpha = -V^3_\alpha, \quad A^1_\alpha = -iF^2_\alpha, \quad W^1_\alpha = -iV^2_\alpha, \\ A^2_\alpha = iF^1_\alpha, \quad W^2_\alpha = iV^1_\alpha, \quad A^3_\alpha = -F^0_\alpha, \quad W^3_\alpha = -V^0_\alpha, \end{gathered} \tag{2.26}$$

where now A^0_α and W^0_α are the U(1) gauge potentials, and $\mathbf{A}_\alpha = (A^1_\alpha, A^2_\alpha, A^3_\alpha)$ and $\mathbf{W}_\alpha = (W^1_\alpha, W^2_\alpha, W^3_\alpha)$ are complex SL(2,C) gauge potentials.[3] Substituting (2.26) into formula (2.22), L_g becomes

$$L_g = -\tfrac{1}{4}\,\mathrm{Re}[A^{\alpha\beta}_a A^a_{\alpha\beta}] + \overline{D_\alpha(\rho+m)} D^\alpha(\rho+m) - \tfrac{1}{2} g^2 |\rho|^4, \tag{2.27}$$

where $A^a_{\alpha\beta} = (A^K_{\alpha\beta}, W^K_{\alpha\beta})$ and

$$\begin{aligned} A^0_{\alpha\beta} &= \hat{D}_\alpha A^0_\beta - \hat{D}_\beta A^0_\alpha, \\ W^0_{\alpha\beta} &= \partial_\alpha W^0_\beta - \partial_\beta W^0_\alpha, \\ \mathbf{A}_{\alpha\beta} &= \hat{D}_\alpha \mathbf{A}_\beta - \hat{D}_\beta \mathbf{A}_\alpha - g\mathbf{A}_\alpha \times \mathbf{A}_\beta, \end{aligned} \tag{2.28}$$

$$\mathbf{W}_{\alpha\beta}=\partial_\alpha\mathbf{W}_\beta-\partial_\beta\mathbf{W}_\alpha-2q\mathbf{W}_\alpha\times\mathbf{W}_\beta,$$

$$D_\alpha(\rho+m)=\hat{D}_\alpha(\rho+m)+igA^0_\alpha(\rho+m),$$

where

$$\hat{D}_\alpha A^0_\beta=\partial_\alpha A^0_\beta,$$

$$\hat{D}_\alpha\mathbf{A}_\beta=\partial_\alpha\mathbf{A}_\beta-2q\mathbf{W}_\alpha\times\mathbf{A}_\beta, \tag{2.29}$$

$$\hat{D}_\alpha(\rho+m)=\partial_\alpha\rho+2iqW^0_\alpha(\rho+m).$$

The index a in formula (2.27) is contracted using the SL(2,C)×U(1) invariant metric η_{ab} defined just as in formula (2.21).

Furthermore, the orthogonal constraint (2.13) becomes

$$A^K_\alpha A_{K\beta}=-|\rho|^2 g_{\alpha\beta}. \tag{2.30}$$

With this constraint, a straightforward derivation using formulas (2.27) and (2.28) shows that formula (2.25) becomes

$$\lim_{g\to\infty} g^{-1}L_g=-\mathrm{Re}[(\hat{D}_\alpha\mathbf{A}_\beta)\cdot\mathbf{A}^\alpha\times\mathbf{A}^\beta+2i\overline{\rho A}^0_\alpha\hat{D}^\alpha\rho+4m_0|\rho|^2\overline{\rho}]-\tfrac{1}{4}V^{\alpha\beta}_K V^K_{\alpha\beta}. \tag{2.31}$$

Apart from the term $-\frac{1}{4}V^{\alpha\beta}_K V^K_{\alpha\beta}$ and the minimal substitution of $\hat{D}_\alpha$ for the partial derivatives, ∂_α, formula (2.31) is precisely the tensor form of the free Dirac bispinor Lagrangian.[1,3] By expanding $\hat{D}_\alpha$ in formula (2.31), and using formulas (2.12), (2.26), (2.29), and (2.30), we obtain the interaction term (2.9). Q.E.D.

Note that the embedding (2.26) is derived from embedding the gauge group SL(2,R)×U(1) as a subgroup of the gauge group SL(2,C)×U(1). Thus, the SL(2,C) gauge potentials $\mathbf{A}_\alpha$ and $\mathbf{W}_\alpha$ are restricted to an SL(2,R) subset of gauge potentials, which by formula (2.26) satisfy

$$\mathrm{Re}[A^1_\alpha]=\mathrm{Re}[A^2_\alpha]=\mathrm{Im}[A^3_\alpha]=0,$$

$$\mathrm{Re}[W^1_\alpha]=\mathrm{Re}[W^2_\alpha]=\mathrm{Im}[W^3_\alpha]=0. \tag{2.32}$$

The Euler–Lagrange equation for the Lagrangian (2.27) with the constraint (2.30), expressed using Lagrange multipliers, commutes with the restriction (2.32). Hence, the $\mathbf{A}_\alpha$ and $\mathbf{W}_\alpha$ can be used to denote either SL(2,C) or the subset of SL(2,R) gauge potentials. By regarding SL(2,R) as embedded in the complex analytic group SL(2,C), we are able to use familiar vector operations to express the Lie algebra structure constants, as, for example, the vector cross product in formulas (2.28) and (2.29), and the vector triple product in formula (2.31). The vector operations greatly simplify derivations.

Also, note from formula (2.1) that V^0_α is the electromagnetic gauge potential and V^3_α is the chiral gauge potential associated with the infinitesimal generators $\tau_0=-i$ and $\tau_3=i\gamma_5$, respectively. Here τ_0 and τ_3 generate a maximal compact U(1)×U(1) subgroup of SL(2,R)×U(1). The noncompact generators τ_1 and τ_2 by formula (2.1) mix positive and negative energy states. Thus, the associated boson gauge potentials V^1_α and V^2_α are unphysical, and hence must vanish for both the bispinor and tensor theories. Thus, the gauge group $\Gamma=G_\varphi\times K$, where G=SL(2,R)×U(1) and K=U(1)×U(1), and where φ denotes the adjoint representation[12] of K on G. This case is handled similarly to the case where $\Gamma=G_\varphi\times G$, which we considered previously, and is equivalent to setting V^1_α and V^2_α equal to zero in formulas (2.4) and (2.17).

III. UNIFICATION OF GRAVITONS, FERMIONS, AND BOSONS IN A TETRAD MODEL

In this section we add boson gauge potentials to the tetrad formulation of the Kaluza–Klein model, which previously contained only gravitational and fermion fields.[7] For simplicity, we will associate the boson gauge potentials V_α^K with the same gauge group $G=\mathrm{SL}(2,R)\times\mathrm{U}(1)$ as for the fermion gauge potentials F_α^K. However, this will not prevent us from restricting V_α^K to a compact subgroup of G, as discussed at the end of Sec. II.

Let X be a four-dimensional space–time, and let dx^α, with $\alpha=0,1,2,3$, denote local coordinate one-forms on an open chart $U\subset X$. The gravitational field, which here we denote as $\tilde{\gamma}$ on X, is expressed locally on U by

$$\tilde{\gamma}=g_{\alpha\beta}\,dx^\alpha\otimes dx^\beta. \tag{3.1}$$

The fermion and boson fields on X we denote as (F^K,ρ) and V^K, where F^K and V^K with $K=0,1,2,3$ are tetrads of one-forms, expressed locally on U by

$$F^K=F_\alpha^K\,dx^\alpha,\quad V^K=V_\alpha^K\,dx^\alpha, \tag{3.2}$$

and ρ is a complex scalar field. In this section we unify the gravitational field $\tilde{\gamma}$, the fermion field (F^K,ρ) and the boson field V^K by deriving the Einstein and Dirac–Yang–Mills Lagrangians from a tetrad formulation of a Kaluza–Klein model. The constraint (2.13) of the fermion field (F^K,ρ) will be shown to be a consequence of the tetrad model.

On the semi-direct product gauge group $\Gamma=G_\varphi\times G$ (see Sec. II) we fix two tetrads of right-invariant vector fields c_K and d_K with commutation relations given by [compare with formula (2.14)]:

$$[c_J,\,c_K]=\lambda f_{JK}^L c_L,\quad [d_J,\,c_K]=\hat{\lambda} f_{JK}^L c_L,\quad [d_J,\,d_K]=\hat{\lambda} f_{JK}^L d_L, \tag{3.3}$$

where f_{JK}^L are the previously defined $\mathrm{SL}(2,R)\times\mathrm{U}(1)$ structure constants, λ and $\hat{\lambda}$ are real scale factors given by

$$\lambda=g/\varepsilon,\quad \hat{\lambda}=2q/\varepsilon, \tag{3.4}$$

where g and q are the previously defined Yang–Mills coupling constants, and

$$\varepsilon=\sqrt{\frac{16\pi\kappa_0}{3g}}, \tag{3.5}$$

where κ_0 is Newton's gravitation constant. Since Γ is an eight-dimensional Lie group, the right-invariant vector fields $\{c_K,d_K\}$ span the Lie algebra of Γ. From formula (3.3), the vector fields $\{c_K,d_K\}$ are orthogonal with respect to the right-invariant metric η defined by

$$\eta=\eta_{JK}(\pi^J\otimes\pi^K-g\sigma^J\otimes\sigma^K), \tag{3.6}$$

where $\{\pi^K,\sigma^K\}$ are right-invariant one-forms on Γ dual to $\{c_K,d_K\}$ and η_{JK} has diagonal elements $\{1,-1,-1,-1\}$ and zeros off the diagonal. [Note that all Lie groups have right-invariant metrics, but only a restricted class of Lie groups have invariant (i.e., bi-invariant) metrics.[11] Note also that the metrics in this paper, such as the bi-invariant metric η_{JK} on $\mathrm{SL}(2,R)\times\mathrm{U}(1)$ which has a Minkowski signature, are not positive definite.]

On the space–time X, we assume the existence of a global nonsingular tetrad of smooth vector fields e_K. Let θ^K denote the tetrad of one forms on X dual to the vector fields e_K. Thus, on the Kaluza–Klein manifold $M=X\times\Gamma$, we can define the following tetrad of vector fields:

$$v_K=(e_K,\varepsilon|\rho|c_K,\varepsilon v_K^J d_J), \tag{3.7}$$

where now ρ is a complex scalar field on M, v_K^J are coefficients associated with the boson field [see formula (3.17)], and ε is the previously defined constant (3.5). We define the metric γ on M with respect to the basis $\{v_K, c_K, d_K\}$ to be

$$\gamma = \begin{bmatrix} \eta_{JK} & 0 \\ 0 & \eta_{ab} \end{bmatrix}, \tag{3.8}$$

where η_{ab} denote the components of the metric η defined in formula (3.6). We also denote the metric γ as $\langle , \rangle$. Thus, with respect to the metric $\langle , \rangle$, the tetrad v_K is orthonormal, and orthogonal to Γ.

The manifold $M = X \times \Gamma$ has a natural right action of Γ. For v_K to be right-invariant, it is necessary and sufficient that e_K, $|\rho|$, and v_K^J depend only on the space–time coordinates $x \in X$. Also, ρ is a complex U(1) scalar field. Specifically, in a local coordinate system (x^α, y^K, z^K) on M, ρ has the form

$$\rho = e^{i(\lambda y + \hat{\lambda} z)} \tilde{\rho}(x), \tag{3.9}$$

where $y = y^3$ and $z = z^3$ are the normal coordinates for the U(1) subgroups of Γ generated by c_3 and d_3 [see formula (3.3)].

Our goal in this section is to derive the Einstein and Dirac–Yang–Mills Lagrangians from the following Lagrangian for the fields (v_K, ρ):

$$L = \frac{g}{16\pi\kappa_0} R[v] + \overline{v_K(\rho + m)} v^K (\rho + m) - \frac{1}{2} g^2 |\rho|^4, \tag{3.10}$$

where the mass m is defined on M by

$$m = \frac{2m_0}{g} e^{i(\lambda y + \hat{\lambda} z)}, \tag{3.11}$$

and $R[v]$, at each point of M, is the sum of sectional curvatures over the four-dimensional subspace spanned by the orthonormal tetrad v_K, defined by

$$R[v] = \sum_{J=0}^{3} \sum_{K=0}^{3} \langle R(v_J, v_K) v^J, v^K \rangle, \tag{3.12}$$

where $R(\,,\,)$ is the curvature two-form[11] associated with the semi-Riemannian metric $\langle\,,\,\rangle$. We express the action for the fields (v_K, ρ) by

$$S = \int L \, dv, \tag{3.13}$$

where dv is the volume form on M associated with the metric $\langle\,,\,\rangle$.

We now show that the Lagrangian (3.10) equals the Hilbert–Einstein Lagrangian for the gravitational field plus the Dirac–Yang–Mills Lagrangian (2.22). The constraint (2.13) of the fermion gauge potentials will be shown to be a consequence of the tetrad v_K. Using a simplified notation, we can write v_K in formula (3.7) as

$$v_K = e_K + \varepsilon |\rho| c_K + \varepsilon v_K^J d_J, \tag{3.14}$$

where $e_K = (e_K, 0, 0)$, $c_K = (0, c_K, 0)$, and $d_K = (0, 0, d_K)$ on M, and similar notation for the dual one-forms θ^K, π^K, and σ^K induced on M.

From formula (3.14), the basis of one-forms on M dual to the basis of vector fields $\{v_K, c_K, d_K\}$ is given by $\{\theta^K, \omega^K, \mu^K\}$, where

$$\omega^K = \pi^K - \varepsilon|\rho|\,\theta^K, \quad \mu^K = \sigma^K - \varepsilon v_J^K \theta^J, \tag{3.15}$$

and the metric (3.8) is expressed by

$$\gamma = \eta_{JK}\theta^J \otimes \theta^K + \eta_{ab}\omega^a \otimes \omega^b, \tag{3.16}$$

where $\omega^a = (\omega^K, \mu^K)$.

Let us define with respect to the basis $\{\partial/\partial x^\alpha, c_K, d_K\}$ the following fields on $\mathrm{U}\times\Gamma$:

$$g_{\alpha\beta} = \eta_{JK}\theta_\alpha^J \theta_\beta^K, \quad F_\alpha^K = |\rho|\,\theta_\alpha^K, \quad V_\alpha^K = v_J^K \theta_\alpha^J. \tag{3.17}$$

By definition of θ^K and using formulas (3.15) and (3.17):

$$\theta^K = \theta_\alpha^K\, dx^\alpha, \quad \omega^K = \pi^K - \varepsilon F_\alpha^K\, dx^\alpha, \quad \mu^K = \sigma^K - \varepsilon V_\alpha^K\, dx^\alpha. \tag{3.18}$$

Moreover, writing $\pi^a = (\pi^K, \sigma^K)$ and $F_\alpha^a = (F_\alpha^K, V_\alpha^K)$, formula (3.18) can be expressed more simply by

$$\theta^K = \theta_\alpha^K\, dx^\alpha, \quad \omega^a = \pi^a - \varepsilon F_\alpha^a\, dx^\alpha. \tag{3.19}$$

On substituting formulas (3.17) and (3.19) into (3.16), the metric γ becomes

$$\gamma = \begin{bmatrix} g_{\alpha\beta} + \varepsilon^2 \eta_{ab} F_\alpha^a F_\beta^b & -\varepsilon F_\alpha^a \eta_{ab} \\ -\varepsilon\, \eta_{ab} F_\beta^b & \eta_{ab} \end{bmatrix}. \tag{3.20}$$

Thus, γ is precisely the Kaluza–Klein metric[10] for the gravitational field $g_{\alpha\beta}$ and the gauge potentials $F_\alpha^a = (F_\alpha^K, V_\alpha^K)$. Also, by formula (3.17),

$$\eta_{JK} F_\alpha^J F_\beta^K = |\rho|^2 g_{\alpha\beta}, \tag{3.21}$$

which is precisely the constraint (2.13). Furthermore, by formula (3.17), the gravitational metric $g_{\alpha\beta}$ has the same (Minkowski) signature as the invariant metric η_{JK} on $\mathrm{SL}(2,R)\times\mathrm{U}(1)$.

A straightforward derivation using the Kaluza–Klein metric γ in formula (3.20) shows that[7,10]

$$R[v] = \widetilde{R} + \tfrac{3}{4}\varepsilon^2 F_a^{\alpha\beta} F_{\alpha\beta}^a, \tag{3.22}$$

where $\widetilde{R}$ denotes the scalar curvature of X, and $F_{\alpha\beta}^a = (F_{\alpha\beta}^K, V_{\alpha\beta}^K)$ is defined as in formulas (2.6) and (2.19). We can now prove the following theorem:

Theorem 2: The total Lagrangian L given in formula (3.10) equals the Hilbert–Einstein Lagrangian for the gravitational field plus the Dirac–Yang–Mills Lagrangian L_g given in formula (2.22), and similarly for the action (3.13).

Proof: The theorem follows by substituting formula (3.22) into (3.10), and by noting from formula (3.8) that the volume form dv on M depends only on the one-forms θ^K. By expressing the gravitational field $g_{\alpha\beta}$, the fermion field (F_α^K, ρ), and the boson field V_α^K in terms of the new variables θ_α^K, ρ, and V_α^K as in formula (3.17), the constraint (2.13) is eliminated. Q.E.D.

(Note that the gravitational field $g_{\alpha\beta}$ and a bispinor field Ψ, which together have $10+8=18$ real components, are equivalent to θ_α^K and ρ, which also have $16+2=18$ real components.[7])

The following observations can be made about the proof of Theorem 2. First, the unphysical cosmic constant, which is the scalar curvature of the gauge group Γ occurring in the Lagrangian of the usual Kaluza–Klein model, does not occur in the Lagrangian (3.10) because in formula

(3.12) we restricted $R[v]$ to the tetrad v_K. Second, for the same reason, Theorem 2 does not require that the right-invariant metric η given in formula (3.6) be bi-invariant,[11] which, in the usual Kaluza–Klein model, places restrictions on the gauge group.[10]

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Random perturbations of iterated maps

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Random perturbations of Markov processes on systems of contractive maps are considered. The existence of a unique invariant measure for the randomly perturbed process is proved under a very weak assumption on perturbations. In particular, the proof holds for the full class of translationally invariant perturbations. © *1996 American Institute of Physics.* [S0022-2488(96)00907-3]

The Markov operator $\mathscr{M}:\mathscr{P}(X)\to\mathscr{P}(X)$ defined by a set $\{w_i:X\to X\}$ of N Lipschitz maps in given by[1]

$$(\mathscr{M}\nu)(A)=\sum_{i=1}^{N} p_i\nu(w_i^{-1}A), \quad \text{for } A \text{ measurable}, \tag{1}$$

where $\mathscr{P}(X)$ denotes the set of normalized Borel measures on a compact space X, each w_i has Lipschitz constant $s_i<1$, and each p_i is non-negative and $\Sigma_{i=1}^{N}p_i=1$. The operator $\mathscr{M}$ formalizes the iteration dynamics on X given by choosing an i at random with probability p_i and then applying w_i. The dynamics on $\mathscr{P}(X)$ is deterministic with a unique invariant measure. Next, we consider random perturbations of the dynamics just defined. When any w_i is applied to a point x in X, in the presence of noise, the result is not necessarily $w_i(x)$. Instead, it only makes sense to give the probability $\mathscr{N}(A|w_i(x))$ for x to land in $A\subset X$ by the perturbed action of w_i, for each set A which belongs to the family $\mathscr{B}(X)$ of Borel measurable sets. In the noiseless limit $\mathscr{N}(\cdot|w_i(x))$ is a Dirac delta distribution located at $w_i(x)$. Therefore a random perturbation is a map $\mathscr{N}:\mathscr{B}(X)\times X\to[0,1]$. The effect of noise on measures is given by a map $\mathscr{S}:\mathscr{P}(X)\to\mathscr{P}(X)$, where $\mathscr{S}\nu$ is the measure onto which a given measure ν is taken by the perturbation, independent of the Markovian process $\mathscr{M}$. In terms of the pertubation $\mathscr{N}$, $\mathscr{S}$ is given by

$$\mathscr{S}\nu(A)=\int \mathscr{N}(A|\cdot)\,d\nu.$$

The function $\mathscr{N}(A|\cdot)$ is measurable for each $A\in\mathscr{B}(X)$. This condition is satisfied for the most commonly studied noises.

Under noise, the evolution is governed by the *perturbed Markov operator* $\mathscr{R}=(\mathscr{S}\circ\mathscr{M})$. In terms of the perturbation $\mathscr{N}$, the perturbed Markov operator $\mathscr{R}$ is

$$\mathscr{R}\nu(A)=\int \mathscr{N}(A|\cdot)\,d[\mathscr{M}\nu], \tag{2}$$

with operator $\mathscr{M}$ is defined in Eq. (1). Using in Eq. (2) the defining set of Lipschitz maps, $\{w_i\}$, the perturbed operator is written as

$$\mathscr{R}\nu(A)=\int \sum_{i=1}^{N} p_i \mathscr{N}(A|\cdot)\circ w_i d\nu. \tag{3}$$

The perturbed Markov operator $\mathscr{R}$ has a unique invariant measure if it is contractive in a suitable metric. We consider *Hutchinson* metric. Given any two measures $\mu,\ \nu\in\mathscr{P}(X)$, their distance $h(\mu,\nu)$ in the Hutchinson metric is given by $\min\{|\int f d\mu-\int f d\nu|: f\in\mathscr{F}\}$, where $\mathscr{F}$ is the set of real-valued functions on X with Lipschitz constant not bigger than one. Under a very weak assumption on $\mathscr{N}$, the following claim states that the perturbed operator $\mathscr{R}$ is contractive in the Hutchinson metric.

Lemma 1: Let a perturbation map $\mathscr{N}$ satisfy the inequality

$$\left|\int f d\mathscr{N}(\cdot|x)-\int f d\mathscr{N}(\cdot|y)\right|\leqslant d(x,y)$$

for each $x,\ y\in X$ and $f\in\mathscr{F}$. Then the perturbed Markov operator $\mathscr{R}$ is contractive in the Hutchinson metric for any Markov operator $\mathscr{M}$.

Proof: Let $\mu,\nu\in\mathscr{P}(X)$. From the form of $\mathscr{R}$ in Eq. (3) and the definition of the Hutchinson metric, we have

$$h(\mathscr{R}\mu,\mathscr{R}\nu)=\sup_{f\in\mathscr{F}}\left\{\left|\sum_{i=1}^{N} p_i\left(\int F_i\, d\mu-\int F_i\, d\nu\right)\right|\right\}\leqslant\sum_{i=1}^{N} p_i \sup_{g\in\mathscr{F}}\left\{\left|\int F_i\, d\mu-\int F_i\, d\nu\right|\right\}$$
$$=s\sum_{i=1}^{N} p_i \sup_{g\in\mathscr{F}}\left\{\left|\int \frac{1}{s}F_i\, d\mu-\int \frac{1}{s}F_i\, d\nu\right|\right\},$$

where $F_i: X\to R$ is defined by $F_i(x)=\int g d\mathscr{N}(\cdot|w_i(x))$, and $s=\max\{s_i\}$. By hypothesis, for all $g\in\mathscr{F}$ and all i, we have

$$\left|\frac{1}{s}\int g d\mathscr{N}(\cdot|w_i(x))-\frac{1}{s}\int g d\mathscr{N}(\cdot|w_i(y))\right|\leqslant\frac{1}{s}d(w_i(x),w_i(y))\leqslant\frac{1}{s}sd(x,y),$$

from which $(1/s)F_i\in\mathscr{F}$ for all i and each $g\in\mathscr{F}$. Therefore it follows that

$$h(\mathscr{R}\mu,\mathscr{R}\nu)\leqslant s\sum_{i=1}^{N} p_i h(\mu,\nu)=sh(\mu,\nu).$$

The most frequent kind of physical random perturbation is the homogeneous, or *translationally invariant*, noise. Let X be a compact subspace of a vector space [Hutchinson's function is a metric on $\mathscr{P}(X)$ only if X is compact]. A homogeneous perturbation $\mathscr{N}$ satisfies the condition $\mathscr{N}(A|x)=\mathscr{N}(A+(y-x)|y)$ for each $x,y\in X$ and each measurable A. Our claim is that the hypothesis of Lemma 1 holds for such a noise. Let $\{A_i\}$ be a partition of $\operatorname{supp}\mathscr{N}(\cdot|x)$, and let $x_i\in A_i$. The integral of any continuous function, and in particular of any $f\in\mathscr{F}$ with respect to the measure $\mathscr{N}(\cdot|x)$, can be approximated with an arbitrary degree of precision as $\Sigma_i\mathscr{N}(A_i|x)f(x_i)$ by making the diameter of the sets A_i sufficiently small. The same is true for the integral of f with respect to the measure $\mathscr{N}(\cdot|y)$, this time using the sets $B_i=A_i+(y-x)$ and the points $y_i=x_i+(y-x)$, and therefore the difference of the integrals of f with respect to $N(\cdot|x)$ and $N(\cdot|y)$ is arbitrarily close to $|\Sigma_i\mathscr{N}(A_i|x)f(x_i)-\Sigma_i\mathscr{N}(B_i|y)f(y_i)|$. Since $\mathscr{N}(A_i|x)=\mathscr{N}(B_i|y)$ for each i, this number is not bigger than $\Sigma_i\mathscr{N}(A_i|x)|f(y_i)-f(x_i)|$, and this cannot be bigger than $d(x,y)=|y-x|$ since $\Sigma_i\mathscr{N}(A_i|x)=1$ and each $|f(y_i)-f(x_i)|$ is not bigger than $|y_i-x_i|=|y-x|$ since $f\in\mathscr{F}$. Therefore we have proved the following.

Theorem 1: Let a Markov operator $\mathscr{M}$ be subjected to a translationally invariant random perturbation. Then the perturbed operator $\mathscr{R}$ is a contractive operator with a unique measure μ which satisfies $\mathscr{R}\mu=\mu$.

We remark that Theorem 1 is a very general result. The underlying space X is an arbitrary compact subset of a vector space; the mappings w_i are arbitrary contractive functions and the noise associated to each point is also arbitrary, provided that it is translationally invariant and that $\mathscr{N}(A|\cdot)$ is measurable for each $A\in\mathscr{B}(X)$. For instance, this measurability condition holds when X is contained in R^n and $\mathscr{N}(\cdot|x)$ defines a distribution function. In a related result, Garcia-Pelayo and Schieve[2] proved the existence of a unique invariant measure of a dynamical system subjected to external noise. Their treatment is restricted to R^n, the noise they study corresponds to a normal distribution centered in x for $\mathscr{N}(\cdot|x)$, and they only consider mappings w_i which are contractive affine transformations on X.

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Comments on Hamiltonian structures for the *n*-dimensional Lotka–Volterra equations [J. Math. Phys. 36, 3520–3534 (1995)]

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In a recent paper, Plank presents results on first integrals for the Lotka–Volterra system (LVS) and their use as possible Hamiltonians. Since he was not acquainted with already published results, we feel that an embedding of his results in those of previous papers can clarify some of his statements. We concentrate our comments on the results presented in his paragraphs III and IV. © *1996 American Institute of Physics.* [S0022-2488(96)02207-4]

(A) 2d LVS. The idea of associating a Hamiltonian to a 2d ODE system was first introduced by Nutku[2] for the particular Lotka–Volterra system (LVS) studied by Volterra corresponding to the equations[1,1] (the two numbers refer respectively to the reference of the paper and the formula number) when $a_{11}=a_{22}=0$. A generalization was provided by Cairó and Feix[3] who showed that, if a system possess a first integral (invariant) I not depending explicitly on time, then I can be considered as Hamiltonian through a time rescaling. It must be pointed out that the relation given in theorem 3.1 (p. 3523) in order to allow the system to have a Hamiltonian structure is just the relation $R_{12}=0$ given in Ref. 4 to obtain invariant III (note that a and b are inverted in Refs. 1 and 4.

(B) First integrals for *n*-dimensional LVS. Plank mentioned four types of first integral on the top of p. 3525. (i) concerns the n-dimensional Volterra case (for $a_{ii}=0$), (ii) and (iii) are, respectively, invariant III and II of Cairó and Feix and (iv) is claimed to be new. In fact (iv) is a limiting case of invariant III. To fix ideas we look at the conditions of existence for Plank's first integral (iv) in the case $n=3$. These conditions are given at the bottom of p. 3531. The first one is $b_1=0$ for $B_0\neq 0$ (below we consider the case $B_0=0$). Let us take then $B_0=1$. Then from (iv) $B_2=a_{12}/b_2$ and $B_3=a_{13}/b_3$. Moreover, taking $i=k=2$ and $i=k=3$ in condition (iii) we obtain, respectively, $a_{12}=a_{22}$ and $a_{13}=a_{33}$. Using this result and taking for instance $i=2$, $k=3$, we obtain $a_{22}(a_{23}-a_{33})/b_2+a_{33}(a_{32}-a_{22})/b_3=0$, which is exactly our relation[4,26] $R_{23}=0$. On the other hand $b_1=0$ together with $a_{12}=a_{22}$ implies $R_{12}=0$ and $b_1=0$ and $a_{13}=a_{33}$ implies $R_{13}=0$. Consequently the conditions of existence of the first integral (iv) of Plank are a special case of those for invariant III of Cairó and Feix. Note that $B_0=0$ implies all b_i equal and we recover the invariant II conditions. One can easily prove that, indeed, invariant III takes the form given by the first integral (iv) of Plank. Moreover the conditions (i) to (iv) given at the bottom of p. 3527 are our conditions to obtain invariant III. In fact condition (iv) is automatically fulfilled if n is even. If n is odd, this condition is not necessary and actually the first integral is time-dependent through a factor e^{st}. Another point which needs further explanation is the expression of $K(x)$ and the conditions to be fulfilled given at the top of p. 3530. Conditions (i) are our conditions[4,17] and Plank's relation (ii) is identical to our relations.[4,19] Condition (iv) is automatically satisfied if n is odd and, if n is even, we do not need this condition if we introduce a factor e^{st} in the first integral. However, in that case we need a rescaling (see Ref. 5) both of the x_i and t of the form $x_i=e^{bt}\overline{x_i}$ and $\overline{dt}=e^{bt}dt$, where $b\equiv b_i$. So in all cases we can obtain a time-independent first integral

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without condition (iv). On the other hand Plank's condition (iii) is misleading. We have $n(n-1)/2$ equations and n unknowns. Since the system is homogeneous, we need $n(n-1)/2-n+1=(n-1)(n-2)/2$ relations between the a_{ij}. These relations appear in our paper.[4,15] where an explanation of this number of constraints is provided. The extension of the Hamiltonian formalism to systems of dimension greater than two possessing first integrals was also considered in Refs. 6–9.

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Erratum: Solution of the one-dimensional *N*-body problems with quadratic and/or inversely quadratic pair potentials [J. Math. Phys. 12, 419–436 (1971)]

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In the right-hand side of Eq. (4.5) c_{kq} should be replaced by $c_{kq}p^{-(1/2)(N-3)}$. Since the quantities c_{kq} are defined throughout up to an arbitrary multiplicative constant c, it might appear that this change is irrelevant. This is not the case, because in the argument that follows Eq. (4.5) the fact that c_{kq} does not depend on p (in particular, on the sign of p) plays an essential role. Note that, *after this replacement*, c_{kq} is indeed independent of p, as it is clearly implied (for dimensional reasons) by (4.8), or rather by the identification of the right-hand-sides of (4.8) (of course with c_{kq} replaced by $c_{kq}p^{-(1/2)(N-3)}$) and (4.10), an identification which constitutes the defining property of the quantities c_{kq}. The rest of the proof following Eq. (4.5) proceeds then as given, with these consequential changes: In the right-hand-sides of (4.14), (4.10), and (4.8), A should be replaced by $A' \equiv A - \frac{1}{2}(N-3) = \frac{1}{2}N(N-1)(a+\frac{1}{2})$; likewise c_{kq} should be replaced by $c_{kq}p^{-(1/2)(N-3)}$ in the right-hand-sides of (4.5) and (4.8) (as already mentioned), as well as (4.9) and (4.18) (in this latter equation, one might then also wish to replace the newly inserted factor $p^{-(1/2)(N-3)}$ with $(\overline{p})^{-(1/2)(N-3)}$, as well as the first factor in the right-hand-side, $e^{-i\pi A}$, with $e^{-i\pi A'}$; since $\overline{p} = -p$, see (4.19), these latter changes are merely notational ones; but they are appropriate for the argument which is subsequently made).

Note that these adjustments do not affect the main conclusion, see Eq. (4.23). Moreover, they entail that the overall ''phase shift'' $\eta \equiv -iA' = -\frac{1}{2}N(N-1)i\pi(a+\frac{1}{2})$ can now be naturally interpreted as resulting from the addition of $\frac{1}{2}N(N-1)$ equal phase shifts due to as many two-body collisions (the ''factorization,'' or ''solitonic,'' property).

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Surface-embeddability approach to the dynamics of the inhomogeneous Heisenberg spin chain

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The surface-embeddability approach of Lund and Regge is applied to the classical, inhomogeneous Heisenberg spin chain to study the class of inhomogeneity functions f for which the spin evolution equation and its gauge-equivalent generalized nonlinear Schrödinger equation (GNLSE) are exactly solvable. Writing the spin vector $\mathbf{S}(x,t)$ as $\partial_x\mathbf{r}$ and identifying $\mathbf{r}(x,t)$ with a position vector generating a surface, we show that the kinematic equation satisfied by $\mathbf{r}$ implies certain constraints on the admissible geometries of this surface. These constraints, together with the Gauss–Mainardi–Codazzi equations, enable us to express the coefficient of the second fundamental form as well as f in terms of the metric coefficients G and its derivatives, for arbitrary time-independent G. Explicit solutions for the GNLSE can also be found in terms of the same quantities. Of the admissible surfaces generated by $\mathbf{r}$, a special class that emerges naturally is that of surfaces of revolution: Explicit solutions for $\mathbf{r}$ and $\mathbf{S}$ are found and discussed for this class of surfaces. © *1996 American Institute of Physics.* [S0022-2488(96)01307-2]

I. INTRODUCTION

Over a decade ago, one of us proposed[1] a model Hamiltonian for the inhomogeneous Heisenberg spin chain and showed that the spin evolution equation in the continuum description is given by the nonlinear equation

$$\mathbf{S}_t=(f\mathbf{S}\times\mathbf{S}_x)_x, \quad \mathbf{S}^2=1, \tag{1.1}$$

where $\mathbf{S}$ denotes the spin vector, f is the site-dependent exchange interaction between spins, and the subscripts denote partial derivatives. Further, by using the moving space curve formalism,[2] it was shown[1] that Eq. (1.1) is gauge equivalent to a generalized nonlinear Schrödinger equation (GNLSE) of the form

$$iq_t+(fq)_{xx}+2q\left\{f|q|^2+\int_{-\infty}^{x}f_x|q|^2\,dx\right\}=0, \tag{1.2a}$$

where

$$q=\frac{\kappa}{2}\exp\int_{-\infty}^{x}\tau\,dx \tag{1.2b}$$

with the curvature κ and the torsion τ of the curve being given by

$$\kappa^2=(\mathbf{S}_x)^2; \quad \tau=\mathbf{S}.(\mathbf{S}_x\times\mathbf{S}_{xx})/\kappa^2. \tag{1.2c}$$

Equations (1.1) and (1.2a) have applications in fluid dynamics as well, where they appear in the study of the motion of an inhomogeneous vortex filament in an incompressible inviscid fluid.[3] The

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dynamics of the model and its higher dimensional analogs have attracted further attention in recent years.[4,5] For the homogeneous chain (corresponding to $f=$const), Eq. (1.2a) reduces[6] to the well-known completely integrable nonlinear Schrödinger equation[7] solvable by the (isospectral) inverse scattering transform (IST) method.[8] When f is a linear function of x, Eq. (1.2a) yields a slightly modified version of an integrable equation studied by Calogero and Degasperis,[9] and the IST in this case has been discussed by Lakshmanan and Bullough.[10] Here, the spectral parameter is a function of time. These are the only two classes of $f(x)$ for which the conventional IST method is directly applicable, and the corresponding GNLSEs are expected to pass the conventional integrability tests. All other $f(x)$ fall into a separate class, in the sense that the spectral parameter now becomes a function of both space and time.[1] Some years ago, Burtsev *et al.*[11] showed that if a nonlinear evolution equation has an associated spectral parameter with a certain prescribed functional form for its space–time dependence, it is possible to develop a conventional IST scheme to obtain strict soliton solutions. We note that the spin evolution of a chain with linear inhomogeneity belongs to this class. For certain other inhomogeneities, we have shown that if the space–time dependence of the spectral parameter has a separable product form, it becomes possible to use an approach[1] based on the Ablowitz–Kaup–Newell–Segur[8] formalism to analyze Eq. (1.2a) in terms of a transformed spatial variable to obtain localized solutions. However, more general questions such as integrability, strict solitons, etc., could not be addressed in this approach. Another point to be noted is that while knowing a solution $\mathbf{S}$ of Eq. (1.1) enables one to find the solution q of Eq. (1.2a) in a straightforward fashion by using Eqs. (1.2b) and (1.2c), the inverse procedure, i.e., the construction of $\mathbf{S}$ from q, is computationally not so easy. On the other hand, *if* q satisfies a completely integrable equation, the soliton-surfaces approach pioneered by Sym[12] can be adopted to construct $\mathbf{S}$, using the solution to the associated isospectral Lax pair system. This has been carried out for the homogeneous chain (the case $f=$const).[13] It is also possible to find soliton solutions for $\mathbf{S}$ by solving Eq. (1.1) directly, using the IST method,[14] for the homogeneous chain.

Recently, in a very interesting paper, Cieśliński, Sym, and Wesselius[5] have used some ideas from Sym's surface approach[12] to find exact solutions of Eq. (1.1) for several other inhomogeneity functions by a somewhat different route: Representing $\mathbf{S}$ as the spatial derivative of a vector $\mathbf{r}$, i.e., setting

$$\mathbf{S}=\mathbf{r}_x, \tag{1.3}$$

it is seen that the kinematic equation

$$\mathbf{r}_t=f(\mathbf{r}_x\times\mathbf{r}_{xx}), \quad \mathbf{r}_x^2=1, \tag{1.4}$$

for a vector $\mathbf{r}$ implies Eq. (1.1).

Assuming the surface generated by the position vector $\mathbf{r}(x,t)$ to be equipped with a metric of the geodesic form, they showed[5] that the Gauss–Mainardi–Codazzi (GMC) equations[15] for this surface can be cast in the same form as Eq. (1.2a), upon making appropriate identifications between q and f on the one hand and the coefficients of the first and second fundamental forms (i.e., the metric and the extrinsic curvature respectively) on the other. By specializing to surfaces of revolution, they demonstrated that the equations for the geodesics on the surface can be integrated explicitly for certain cases, and gave an algorithm for obtaining both f and the corresponding solution $\mathbf{S}$. Choosing the simplest geodesic coordinates on a surface of revolution ("parallels" and "meridians"), the solutions called "spins-on-meridians" could be found for a wide variety of time-independent, bounded, positive functions $f(x)$, i.e., inhomogeneous ferromagnetic couplings. However, for more general geodesic coordinates on surfaces of revolutions, the solutions turned out to correspond to time-dependent functions $f(x,t)$ which were either unbounded or negative in all typical examples. Both these characteristics are unphysical, and for the latter ($f<0$), an anti-

ferromagnetic coupling is implied, causing the nearest-neighbor spin vectors to be almost antiparallel for low energies, and therefore the continuum equation (1.1) is itself quite inappropriate to describe low-energy dynamics.

In view of what has been said above, we confine ourselves to the ferromagnetic case $f>0$ in this paper. Our geometric formulation differs form that of Cieśliński *et al.*[5] in the sense that although we also identify $\mathbf{r}(x,t)$ with a position vector that generates a surface, we do not compare the GMC equations to Eq. (1.2a), nor do we use the general equations of geodesics. We adopt the strategy suggested by Lund and Regge[16] in a different context, and regard the kinematic equation (1.4) as a *constraint* on the surface generated. Such a constraint is expected to permit only certain special geometries for the surface.[16] Indeed, for the model under investigation, the surface metric is shown to be *necessarily* of the geodesic form and, further, certain coefficients of the two fundamental forms get related through the function f. Using these results in the GMC equations, and *restricting* our discussion to the case of time-independent metrics, it becomes possible to "integrate" them. This enables us to find the expressions for L, M, and N (the coefficients of the second fundamental form) as well as the corresponding function f in terms of the metric coefficient G, its x derivatives, and two (arbitrary) integration constants. It is then demonstrated that the solution q of Eq. (1.2a) can also be written in terms of the above-mentioned quantities, by simply reexpressing the moving curve parameters κ and τ [appearing in Eq. (1.2b) and defined in Eq. (1.2c)] in terms of surface coefficients by using the Gauss–Weingaraten (GW) equations[15] for the surface. Thus we see that given an arbitrary metric coefficient, the explicit solution for q along with the corresponding f can be written down. This solution q is a *complex* function in general, and is interesting in its own right since it contains information[1] on the energy and momentum densities along the chain. Furthermore, on inspecting the expressions for L, M, and N obtained from the GMC equations, it is readily seen that they correspond to those of surfaces of revolution,[15] when one of the two integration constants referred to above vanishes. Also, $G^{1/2}$ plays the role of the generator of revolution, and the explicit solution of $\mathbf{r}(x,t)$ can be written down in this limiting case. In this limit, our expression for $f(x)$ reduces to the result obtained[5] in the geodesic approach, for the spins-on-meridian solutions. The corresponding solutions for q are necessarily *real*. For certain common surfaces of revolution like the torus and the catenoid, the solution $\mathbf{S}$ of Eq. (1.1) can be expressed solely as a functional of f that appears in the equation, essentially because the surface metric can be written down as a functional of the function f for these surfaces. Some illustrative examples are discussed at the end.

II. THE MODEL

We begin by briefly describing the physical system under consideration and outline the derivation of Eq. (1.1).

The inhomogeneous, isotropic Heisenberg spin chain is described by the following Hamiltonian:[1]

$$H=-\sum_i f_i \mathbf{S}_i \cdot \mathbf{S}_{i+1}. \tag{2.1}$$

Here f_i denotes a site-dependent nearest-neighbor interaction and $\mathbf{S}_i$ is the classical spin vector at site i; $(\mathbf{S}_i)^2=S^2=\text{const}$. A classical treatment for spins is justified from experimental results[17] for spins $S\geq\frac{3}{2}$. Hereafter, $\mathbf{S}_i^2$ is normalized to unity for convenience. For the conventional Heisenberg Hamiltonian, the exchange interaction which couples nearest-neighbor spins is a constant (say, f_0) everywhere along the chain. However, it is possible to fabricate systems in which (a) the distance between neighboring atoms varies along the chain so that the overlap of identical electronic wavefunctions (which is a measure of the exchange coupling f) varies as well, or (b) the atoms may be equally spaced, but the wavefunction may be made to change from site to site by the deliberate introduction of impurities or organic complexes in a controlled manner,[17] without

causing lattice distortions. The spin evolution equation for the system is found using $(d\mathbf{S}_i/dt)=\{H,\mathbf{S}_i\}$, where $\{,\}$ denotes the Poisson bracket, and the Cartesian spin-components S_i^α satisfy the angular momentum algebra $\{S_i^\alpha,S_j^\beta\}=\delta_{ij}\epsilon_{\alpha\beta\gamma}S_j^\gamma$. Using Eq. (2.1) for the Hamiltonian, we obtain[1]

$$\frac{d\mathbf{S}_i}{dt}=f_i(\mathbf{S}_i\times\mathbf{S}_{i+1})+f_{i-1}(\mathbf{S}_i\times\mathbf{S}_{i-1}). \tag{2.2}$$

A continuum version of Eq. (2.2) is suitable when $\mathbf{S}_i$ and f_i vary slowly over one lattice separation a. This would be a good description at low temperature for a ferromagnetic coupling, $f>0$. Hence we write $\mathbf{S}_i\to\mathbf{S}(x,t)$, $f_i\to f(x)$ and use Taylor expansions for $\mathbf{S}(x\pm a,t)$ and $f(x-a,t)$ to order a^2 to obtain

$$\mathbf{S}_t=f(\mathbf{S}\times\mathbf{S}_{xx})+f_x(\mathbf{S}\times\mathbf{S}_x), \tag{2.3}$$

on rescaling the time variable by a factor a^2. The two terms on the right-hand side can be combined easily to yield the spin evolution equation (1.1).

III. KINEMATIC RESTRICTIONS ON THE SURFACE GEOMETRY

Our starting point is the kinematic equation for $\mathbf{r}(x,t)$ given Eq. (1.4), which (as already stated) implies Eq. (1.1), when $\mathbf{r}_x=\mathbf{S}$. Let us identify $\mathbf{r}(x,t)$ with a position vector generating a smooth surface in E^3, with local coordinates x and t. Let the metric, i.e., the first fundamental form of this surface, be given by[15]

$$I=d\mathbf{r}^2=E\,dx^2+2F\,dxdt+G\,dt^2, \tag{3.1}$$

where by definition $E=\mathbf{r}_x^2$, $F=\mathbf{r}_x\cdot\mathbf{r}_t$ and $G=\mathbf{r}_t^2$. However, $\mathbf{S}^2=\mathbf{r}_x^2=1$ in the model and from Eq. (1.4) it is readily verified that $\mathbf{r}_x\cdot\mathbf{r}_t=0$. Therefore, $E=1$ and $F=0$, and the metric (3.1) is *necessarily* constrained to be of the geodesic form given below:

$$I=dx^2+G(x,t)dt^2. \tag{3.2}$$

The unit normal $\mathbf{n}$ to the surface is given by

$$\mathbf{n}=(\mathbf{r}_x\times\mathbf{r}_t)/G^{1/2}. \tag{3.3}$$

As usual, the extrinsic curvature (second fundamental form) is defined as

$$II=-d\mathbf{r}.d\mathbf{n}=L\,dx^2+2M\,dxdt+N\,dt^2, \tag{3.4}$$

where

$$L=\mathbf{r}_{xx}.\mathbf{n},\quad M=\mathbf{r}_{xt}.\mathbf{n},\quad\text{and}\quad N=\mathbf{r}_{tt}.\mathbf{n}. \tag{3.5}$$

As is well known in surface theory, the Gauss–Weingarten (GW) equations for surface can be written in terms of L,M,N and the usual Christoffel symbols Γ_{ij}^k.[15] For the metric given in Eq. (3.2), the latter reduce to

$$\begin{gathered}\Gamma_{11}^1=\Gamma_{11}^2=\Gamma_{12}^1=0;\\ \Gamma_{12}^2=\tfrac{1}{2}G_x/G,\quad \Gamma_{22}^1=-\tfrac{1}{2}G_x,\quad\text{and}\quad \Gamma_{22}^2=\tfrac{1}{2}G_t/G.\end{gathered} \tag{3.6}$$

Using these, the GW equations read

$$\mathbf{r}_{xx}=L\mathbf{n}, \tag{3.7a}$$

$$\mathbf{r}_{xt}=\tfrac{1}{2}(G_x/G)\mathbf{r}_t+M\mathbf{n}, \tag{3.7b}$$

$$\mathbf{r}_{tt}=-\tfrac{1}{2}G_x\mathbf{r}_x+\tfrac{1}{2}(G_t/G)\mathbf{r}_t+N\mathbf{n}, \tag{3.7c}$$

$$\mathbf{n}_x=-L\mathbf{r}_x-(M/G)\mathbf{r}_t, \tag{3.7d}$$

$$\mathbf{n}_t=-M\mathbf{r}_x-(N/G)\mathbf{r}_t. \tag{3.7e}$$

Further, for this surface it is easy to show that

$$(\mathbf{r}_x\times\mathbf{r}_{xx})=L(\mathbf{r}_x\times\mathbf{n})=(L/G^{1/2})\mathbf{r}_t, \tag{3.8}$$

where we have used Eq. (3.3) in Eq. (3.7a), along with $F=0$. Comparing this with the given equation (1.4), we get the constraint

$$f=-G^{1/2}/L, \tag{3.9}$$

for $L\neq 0$. In other words, given f, Eq. (1.4) can have a solution only if the coefficients G and L are related through f as in Eq. (3.9).

For coordinates with $E=1$ and $F=0$, the compatibility conditions $(\mathbf{r}_{xx})_t=(\mathbf{r}_{xt})_x$ and $(\mathbf{r}_{tt})_x=(\mathbf{r}_{xt})_t$ yield the following Gauss–Mainardi–Codazzi (GMC)[15] equations:

$$-(LN-M^2)/G=(\Gamma^2_{12})_x-(\Gamma^2_{11})_t+\Gamma^1_{12}\Gamma^2_{11}-\Gamma^1_{11}\Gamma^2_{12}+\Gamma^2_{12}\Gamma^2_{12}-\Gamma^2_{11}\Gamma^2_{22}, \tag{3.10a}$$

$$L_t-M_x=L\Gamma^1_{12}+M(\Gamma^2_{12}-\Gamma^1_{11})-N\Gamma^2_{11}, \tag{3.10b}$$

$$M_t-N_x=L\Gamma^1_{22}+M(\Gamma^2_{22}-\Gamma^1_{12})-N\Gamma^2_{12}. \tag{3.10c}$$

On using the expressions for Γ^k_{ij} given in Eq. (3.6), and the following definition for the Gaussian curvature K,

$$K=(LN-M^2)/G, \tag{3.11}$$

Eqs. (3.10) reduce to

$$-K=(G_x/2G)_x+(G_x/2G)^2, \tag{3.12a}$$

$$L_t-M_x=M(G_x/2G), \tag{3.12b}$$

$$M_t-N_x=-L(G_x/2)+M(G_t/2G)-N(G_x/2G). \tag{3.12c}$$

Now, the fundamental theorem of surfaces[15] states that if we can identify functions G, L, M and N which satisfy the Gauss equation [Eq. (3.12a)] and the Mainardi–Codazzi equations [Eqs. (3.12b) and (3.12c)], then there exists a surface $\mathbf{r}(x,t)$. In other words, an exact solution of Eq. (1.4) exists, provided, of course, if the additional constraint $f=-G^{1/2}/L$ is satisfied. [Further, the knowledge of these functions G, L, M, and N will also immediately enable us to find explicit solutions q of Eq. (1.2a), as will be demonstrated in Sec. V.]

Before concluding this section, we note that Eq. (3.12a) can be written in the more convenient form

$$(G^{1/2})_{xx}=-KG^{1/2}. \tag{3.13}$$

IV. EXPRESSIONS FOR L, M, AND N SATISFYING GMC EQUATIONS AND THE CORRESPONDING FORMULA FOR f

The task ahead of us is to determine the coefficients L, M, and N of the second fundamental form which satisfy the GMC equations (3.12) in a manner consistent with the given evolution. The most convenient starting point is the Gauss equation (3.13). It involves only x derivatives, suggesting the simplest nontrivial choice $G(x,t)=G(x)$. Further, if $f=f(x)$, then $L_t=0$, since $L=-G^{1/2}/f$ from Eq. (3.9). Thus Eq. (3.12b) yields $M_x=-MG_x/2G$, which (for a given G) has the solution

$$M=C_oG^{-1/2}, \tag{4.1}$$

where C_o is an arbitrary constant, taken to be independent of time. Hence $M_t=0$ on using $G_t=0$, and Eq. (3.12c) becomes

$$N_x-NG_x/2G=LG_x/2=-G^{1/2}G_x/2\,f, \tag{4.2}$$

where Eq. (3.9) has been used to express L in terms of G and f.

This has a solution

$$N=G^{1/2}\left\{C_1-\int \frac{G_x}{2f}\,dx\right\}, \tag{4.3}$$

where C_1 is a (time-independent) integration constant. However, we also have an expression for N arising from the definition of K given in Eq. (3.11), giving

$$N=(KG+M^2)/L=-f(KG+M^2)/G^{1/2}, \tag{4.4}$$

where we have used Eq. (3.9). Substituting for M from Eq. (4.1) yields

$$N=-fG^{1/2}(K+C_oG^{-2}). \tag{4.5}$$

Equating the expressions for N given in Eqs. (4.3) and (4.5) for consistency, we obtain

$$f(K+C_oG^{-2})=\left\{\int \frac{G_x}{2f}\,dx-C_1\right\}. \tag{4.6}$$

Interestingly, this equation can be solved for f in terms of $G^{1/2}$ as follows: Differentiating both sides of Eq. (4.6) gives

$$G_x=2f[f(K+C_oG^{-2})]_x. \tag{4.7}$$

Multiplying both sides of Eq. (4.7) by $(K+C_oG^{-2})$ and integrating with respect to x, we obtain

$$A_o+\int G_x(K+C_oG^{-2})dx=f^2(K+C_oG^{-2})^2, \tag{4.8}$$

where A_o is an arbitrary constant of integration. Equation (4.8) is solved for f to give

$$f=\pm(K+C_oG^{-2})^{-1}\left\{\int (K+C_oG^{-2})G_x\,dx+A_o\right\}^{1/2}, \tag{4.9}$$

where, from Eq. (3.13), $K=-(G^{1/2})_{xx}/G^{1/2}$. Another curious fact that emerges is that the integration in Eq. (4.9) can be carried out exactly, to give f as a function of $G^{1/2}$: To show this, define

$$G^{1/2}=\phi. \tag{4.10}$$

This yields $G=\phi^2$, $G_x=2\phi\phi_x$, and $K=-\phi_{xx}/\phi$. Substituting these in Eq. (4.9) and evaluating the integral we get the expression for the inhomogeneity function to be

$$f=\pm\phi\,\frac{(2A_o-\phi_x^2-C_o\phi^{-2})^{1/2}}{C_o\phi^{-3}-\phi_{xx}}. \tag{4.11}$$

On using this expression for f in Eqs. (3.9), (4.1), and (4.5) and setting $G=\phi^2$, we obtain the corresponding expressions for L, M, and N as

$$L=\frac{-\phi}{f}=\frac{\phi_{xx}-C_o\phi^{-3}}{(2A_o-\phi_x^2-C_o\phi^{-2})^{1/2}}, \tag{4.12}$$

$$M=C_o\phi^{-1}, \tag{4.13}$$

$$N=f(\phi_{xx}-C_o\phi^{-3})=-\phi(2A_o-\phi_x^2-C_o\phi^{-2})^{1/2}. \tag{4.14}$$

These clearly satisfy the GMC equations since they have been obtained by essentially integrating the equations. The point to be noted is that the quantities L,M,N as well as f depend on ϕ and its derivatives. Thus *given* an arbitrary function ϕ [with the provision that $(2A_o-\phi_x^2-C_o\phi^{-2})>0$] we can use Eqs. (4.11)–(4.14) to find the quantities explicitly. Combining this result with the fundamental theorem of surfaces discussed at the end of Sec. III, we conclude that for inhomogeneity functions f determined from Eq. (4.11) in this fashion, exact solutions $\mathbf{r}(x,t)$ of Eq. (1.4) exist. In addition, the solution q of Eq. (1.2a) corresponding to such functions can be explicitly found as will be shown in Sec. V. Explicit solutions of $\mathbf{r}$ can also be found for a special subclass of f. It can be verified that Eqs. (4.11)–(4.14) represent a special case (corresponding to a time-independent metric) of the formulas (29) in Ref. 5.

V. EXACT DYNAMICAL SOLUTIONS AND THEIR ASSOCIATED GEOMETRY

In this section, we show that the solution q for the GNLSE [Eq. (1.2a)] can be expressed in terms of the surface coefficients and can therefore be explicitly found for a given metric. Explicit solutions for $\mathbf{r}$ and $\mathbf{S}$ are written down in the case $G=G(x)$, $M=0$ corresponding to "spins on meridians" (Ref. 5).

A. Solutions for the GNLSE

As mentioned in the Introduction, the solution q of Eq. (1.2a) can be expressed in terms of the curvature κ and torsion τ, the parameters of a (moving) curve as $q=\frac{1}{2}\kappa\exp(i\int_{-\infty}^{x}\tau\,dx)$, where κ and τ are defined in Eq. (1.2c). Using these definitions together with the GW equations (3.7), we obtain

$$\kappa=(\mathbf{S}_x.\mathbf{S}_x)^{1/2}=(\mathbf{r}_{xx}.\mathbf{r}_{xx})=L; \tag{5.1}$$

τ can also be expressed in terms of the surface coefficients as follows:

$$\tau=\mathbf{S}.(\mathbf{S}_x\times\mathbf{S}_{xx})/\kappa^2=\mathbf{r}_x.(\mathbf{r}_{xx}\times\mathbf{r}_{xxx})/L^2. \tag{5.2}$$

However, from Eqs. (3.7a) and (3.7d),

$$\mathbf{r}_{xxx}=L_x\mathbf{n}+L\mathbf{n}_x=L_x\mathbf{n}-L^2\mathbf{r}_x-(LM/G)\mathbf{r}_t,$$

giving

$$(\mathbf{r}_{xx}\times\mathbf{r}_{xxx})=L^3(\mathbf{r}_x\times\mathbf{n})+(L^2M/G)(\mathbf{r}_t\times\mathbf{n}).$$

On using the definition of $\mathbf{n}$ given in Eq. (3.3), we obtain

$$(\mathbf{r}_{xx}\times\mathbf{r}_{xxx})=-(L^2/G^{1/2})(L\mathbf{r}_t-M\mathbf{r}_x). \tag{5.3}$$

Using Eq. (5.3) in (5.2) yields

$$\tau=M/G^{1/2}. \tag{5.4}$$

Substituting Eqs. (5.1) and (5.4) in Eq. (1.2b) gives the following solution for q in terms of L, M, and G:

$$q=\frac{1}{2}L\exp i\int MG^{-1/2}\,dx. \tag{5.5}$$

In Sec. IV we have shown that L and M are given by Eqs. (4.12) and (4.13), for $G=G(x)$. Substituting for them in Eq. (5.5) and setting $G^{-1/2}=\phi^{-1}$ leads to

$$q=\tfrac{1}{2}\frac{\phi_{xx}-C_o\phi^{-3}}{(2A_o-\phi_x^2-C_o\phi^{-2})^{1/2}\exp iC_o\int\phi^{-2}\,dx}. \tag{5.6}$$

Note that the torsion $\tau=C_0\phi^{-2}$ for this system. Summarizing, we have the following result: For any arbitrary ϕ [such that $(2A_0-\phi_x^2-C_o\phi^{-2})>0$], the inhomogeneity function f can be found from Eq. (4.11), and for that f, the corresponding solution q of Eq. (1.2a) is given in Eq. (5.6).

We parenthetically remark that Eq. (5.5) agrees with the result obtained by Sym and Wesselius.[4] However, their procedure involved showing essentially that when Eq. (5.5) is substituted into the GNLSE (1.2a) and real and imaginary terms are equated, GMC equations are obtained, on setting $f=\sqrt{G}/L$. We also note from Eq. (5.5) that while surfaces with $M=0$ pick out purely real solutions of (1.2a), those with $M\neq0$ correspond to complex solutions q.

The solution for q is physically interesting, since it has been shown[1] that the energy and momentum densities along the chain have the form $E(x,t)=2f|q|^2$ and $P(x,t)=4f^2|q|^2(\arg q)_x$. From Eqs. (4.1) and (5.5), we obtain the relation $E(x,t)=(2fG)^{-1}P(x,t)=(2f\phi^2)^{-1}P(x,t)$, where the general expression for f is given in Eq. (4.11). An interesting observation is that if the product (fG) is a constant, then the total (integrated) energy $\mathscr{E}=\int E(x,t)dx$ is proportional to the total momentum $\mathscr{P}=\int P(x,t)dx$, leading to the linear dispersion relation $\mathscr{E}\sim\mathscr{P}$. This is reminiscent of the dispersion relation for the basic excitations in other physical systems such as photons, linearized antiferromagnetic magnons in a *homogeneous* chain, etc. Unfortunately, the solutions for ϕ obtained by setting $f\sim\phi^{-2}$ in Eq. (4.11) are not expressible in terms of elementary functions, even if $C_o=0$. Nevertheless, the observation that $f(x)$ may be "tuned" to control the energy-momentum dispersion relation is of significance.

B. Solutions for r

In Sec. IV expressions for L, M, N, and f were obtained in terms of $\phi=G^{1/2}$ and two arbitrary constants C_o and A_o. Let us consider the two possible classes of surfaces corresponding to $M=0$ and $M\neq0$ one by one:

(i) $M=0$: From Eq. (4.13), we see that C_o must vanish when M vanishes. Using this, Eqs. (4.12) and (4.14) yield L and N respectively as

$$L=\phi_{xx}/(2A_o-\phi_x^2)^{1/2}\quad\text{and}\quad N=-\phi(2A_o-\phi_x^2)^{1/2}. \tag{5.7}$$

It is easily verified that these extrinsic curvature coefficients correspond to the following *surface of revolution*:

$$\mathbf{r}=\left(\int (2A_o-\phi_x^2)^{1/2}\,dx,\phi\cos t,\phi\sin t\right). \tag{5.8}$$

Thus ϕ plays the role of the generator of a surface of revolution. Further, since $\mathbf{r}_x^2=\mathbf{S}^2=1$, Eq. (5.8) leads to $2A_o=1$. By computing $\mathbf{r}_{xx}$ from Eq. (5.8), we find $L^2=(\mathbf{r}_{xx}.\mathbf{r}_{xx})=2A_o\phi_{xx}^2/(2A_o-\phi_x^2)$, which agrees with the expression for L given in (5.7), on setting $2A_o=1$. (The expression for N can be verified similarly).

Using this value of A_0 in Eq. (4.11) and setting $C_o=0$, we get

$$f=\pm\phi(1-\phi_x^2)^{1/2}/\phi_{xx}. \tag{5.9}$$

Note that this expression for f was also obtained by Cieśliński *et al.*[5] essentially by integrating the equations for geodesics on a surface of revolution. [See Eq. (37) of Ref. 5]. Thus we see that their result for spins on meridians corresponds to the limit $M=C_o=0$ of the expression for f given in Eq. (4.11), which we derived as the inhomogeneity function supporting an exact dynamical solution for a time-independent metric. From Eq. (5.6), $q=\frac{1}{2}\phi_{xx}/(2A_o-\phi_x^2)^{1/2}$.

(ii) $M\neq0$: This corresponds to $C_0\neq0$ [see Eq. (4.13)]. The construction of $\mathbf{r}$ corresponding to Eqs. (4.12)–(4.14) with $C_o\neq0$ is nontrivial and is an open problem. The solution of q for $C_o\neq0$ can be found from Eq. (5.6).

C. Solutions of S and illustrative examples

Returning to Eq. (5.9), many examples of $\phi(x)$ and the corresponding function $f(x)$ have been presented in Table I of Ref. 5 for which $\mathbf{r}$ and $\mathbf{S}$ can be found. In what follows, we study the problem from a different angle and present a discussion in terms of the Gaussian curvature K. Equation (3.13) for K can be written as

$$K=-\phi_{xx}/\phi. \tag{5.10}$$

Using this in Eq. (5.9) we obtain

$$Kf=(1-\phi_x^2)^{1/2}. \tag{5.11}$$

Substituting Eq. (5.11) in the expression for $\mathbf{r}$ given in Eq. (5.8) with $2A_o=1$ and computing $\mathbf{r}_x$ yields

$$\mathbf{S}=\mathbf{r}_x=((1-\phi_x^2)^{1/2},\phi_x\cos t,\phi_x\sin t)=(Kf,(1-K^2f^2)^{1/2}\cos t,(1-K^2f^2)^{1/2}\sin t). \tag{5.12}$$

Hence $\mathbf{S}$ is given as a functional of the product Kf.

Illustrative Examples: It is instructive to consider well-known surfaces of revolution as possible examples for finding $\mathbf{r}(x,t)$, keeping in mind the requirement that the corresponding inhomogeneity function should be positive definite (i.e., ferromagnetic) and bounded everywhere on the chain. Note that surfaces with $K=0$ [leading to $\phi_{xx}=0$—see Eq. (5.10)] must be excluded since f becomes unbounded. We give below three examples where the solution $\mathbf{S}$ of Eq. (1.1) can be written *solely* as a functional of f.

(i) *Torus*: $\mathbf{r}=(\sin x,(R+\cos x)\cos t,(R+\cos x)\sin t)$ gives $\phi=(R+\cos x)$, $f=\phi=G^{1/2}$, $K=(1-R\phi^{-1})=(1-Rf^{-1})$. Hence, using this K in Eq. (5.12),

$$\mathbf{S}=\mathbf{r}_x=((f-R),[1-(f-R)^2]^{1/2}\cos t,[1-(f-R)^2]^{1/2}\sin t).$$

(ii) *Sphere of radius* λ^{-1}: $\mathbf{r}=\lambda^{-1}(\sin\lambda x,\cos\lambda x\cos t,\cos\lambda x\sin t)$ gives $\phi=\cos\lambda x$, $f=\phi=G^{1/2}$, $K=1$. Note that $f=\cos\lambda x$ can be arranged to remain positive for $-L_0\leqslant x\leqslant L_0$, L_0 being the length of the chain, by choosing $\lambda=\pi/2L_0$. Thus

$$\mathbf{S}=(f,(1-f^2)^{1/2}\cos t,(1-f^2)^{1/2}\sin t).$$

(iii) *Catenoid:* $\mathbf{r}=(\sinh^{-1}x,(1+x^2)^{1/2}\cos t,(1+x^2)^{1/2}\sin t)$ gives $\phi=(1+x^2)^{1/2}$, $f=\phi^3=G^{3/2}$, $K=-\phi^{-4}=-f^{-4/3}$. Since $|x|<L_0$, f is bounded. Hence

$$\mathbf{S}=(-f^{-1/3},(1-f^{-2/3})^2\cos t,(1-f^{-2/3})^2\sin t).$$

Note that for these simple surfaces, $\mathbf{S}$ involves only f and no derivatives of f. This feature is obviously not true in general. As is clear from Eq. (5.12), if we choose the surface metric $G=\phi^2$ to be a functional of f (and its derivatives), $\mathbf{S}$ can also be expressed in terms of those quantities. This can be easily verified for the simple surfaces given above where ϕ is a functional of f. On the other hand, for example, consider a surface with the generator $\phi=\alpha\exp(-x^2)$, where $\alpha=$const. On using Eq. (5.9), we obtain $f=\pm[1-4x^2\exp(-2x^2)]^{1/2}/2(1-2x^2)=\pm[1-4(\ln\alpha-\ln\phi)\phi^2/\alpha^2]^{1/2}/2(1-\ln\alpha^2-\ln\phi^2)$ (f can remain positive by an appropriate choice of the length scale). Equation (5.10) yields $K=2(1-2x^2)=2(1-\ln\alpha^2-\ln\phi^2)$. Note that it is not possible to invert the expression for f to write ϕ as a simple functional of f, as was possible for the torus, etc. Therefore, for this example $\mathbf{S}$ cannot be written in terms of f, but only in terms of ϕ, since $Kf=[1-4(\ln\alpha\text{-}\ln\phi)\phi^2/\alpha^2]^{1/2}$ [see Eq. (5.9)].

It is interesting to investigate whether the completely integrable homogeneous chain with $f=f_0=$const (see the Introduction) has a class of special solutions of the surface of revolution class as well. A short calculation shows that, for this case, Eq. (5.9) can be solved to give special solutions for ϕ which are elliptic functions. On the other hand, for the other integrable example $f(x)=ax+b$, a and b being constants, Eq. (5.9) is a nonlinear ODE with x-dependent coefficients and its solution is nontrivial and the question remains open at present. However, it is pertinent to add that using the geodesic approach with cylindrical surfaces,[5] it is possible to obtain solutions for $\mathbf{r}$ for time-dependent functions $f(x,t)=a(t)x+b(t)$. However, as already mentioned there,[5] its physical interpretation as a model for a ferromagnet would present difficulties.

VI. CONCLUDING REMARKS

In this paper, we have used a surface-embeddability approach pioneered by Lund and Regge to analyze the nonlinear dynamics of an inhomogeneous ferromagnetic chain to find exact solutions of the spin evolution equation. Our approach is distinct from the existing one[5] which consists of calculating geodesics on surfaces of revolution. However, the surface considered in both the approaches is the same, viz, that generated by the position vector $\mathbf{r}(x,t)$ where $\mathbf{r}_x$ is the spin vector. We have given the formalism for surfaces with arbitrary time-independent metrics $G(x)$. Our emphasis has been on the determination of inhomogeneities $f(x)$ for which exact solutions of the dynamical system exist. In addition, the corresponding solutions for the GNLSE [Eq. (1.2a)] can be found explicitly for these inhomogeneities. Surfaces of revolution with simplest geodesic coordinates ("parallels" and "meridians") emerge as a subclass for which the corresponding solution for $\mathbf{r}$ can also be written down explicitly.

Extension of our procedure to include space–time-dependent metrics $G(x,t)$ and thereby enlarge the class of functions $f(x)$ amenable to exact solution in a consistent fashion would be of interest. However, since $G_t\neq0$ and $L=-G^{1/2}/f$, we have $L_t\neq0$ in this case. As a result, all the terms appearing in the GMC equations [Eqs. (3.12)] get retained, and the analysis for the determination of f becomes quite involved.

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The Casimir energy of the twisted string loop: Uniform and two segment loops

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We calculate the Casimir energy of a two segment loop of string with one normal boundary point and one twisted boundary point. The energy is renormalized relative to the twisted uniform loop. The use of the twisted loop in simplifying untwisted loop calculations is discussed. © *1996 American Institute of Physics.* [S0022-2488(96)01908-1]

I. INTRODUCTION

Oscillating loops of cosmic strings have been suggested as a possible seed for galaxy formation in the early universe.[1] In these models, matter condenses about the oscillating string loops which radiate into the surrounding matter as they decay. String loops have been reviewed by Vilenkin[2] who discusses their radial oscillations and gives examples of the kinds of density fluctuations that could be seeded by decaying loops of various structures. In early models loops were created in a symmetry breaking phase transition[2] but more recently, Basu, Guth, and Vilenkin[3] have discussed spontaneous nucleation processes that create loops and other defects during the early universe inflationary period and the effects of these more persistent defects on galaxy seeding. A theory relating quantum fluctuations to the evolution of loops and other defects has been developed by Garriga and Vilenkin[4] and Basu and Vilenkin.[5]

Several kinds of radiation can be associated with an oscillating string, such as electromagnetic, gravitational or goldstone-boson emission. The importance of the latter type of radiation in galaxy formation models has been emphasized by Davis[6] and Vilenkin and Vachasspati.[7] Oscillations associated with strings have also been discussed by Rosenzweig and Srivastava[8] who consider the bulk vibrations associated with the Higgs field surrounding a string and point out that this contribution to the radiation emission might be dominant in string decay processes. They also point out an interesting aspect of twisted strings and string loops; one of the models discussed in this paper is a straight string threading a string loop and it is found that the interaction energy is absent when the configuration is twisted. Other complex loop arrangements are also possible.

One possibility for a more complex loop is a loop with segments. Davis,[6] for example, mentions that when formed a vortex loop could be made of many segments coming from previously casually disconnected regions so that oscillating segmented string loops could be considered. Pagels,[9] in a calculation of loop correlation functions, assumed that the initial loop in a loop decay process was segmented. There has also been considerable interest in the Casimir or zero point energy of oscillation segmented loops.[10–13] This particular aspect of loop behavior is interesting and important, given the possible importance of oscillating loops in galaxy formation processes and the role of fluctuations in the evolution of loop dynamics.[14] The segmented loop is also a relatively simple system on which to perform Casimir calculations and thus provides a useful testing ground for various renormalization methods. It may also be applicable to the vacuum states of two dimensional field theories.[10] The models so far discussed in the literature have had two building blocks, ϕ_i $(i=1,2)$ segments, each of a different density and tension but

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with the same wave speed $v=c$. The segments are joined alternatingly at points $x_{\bar{N}}$ to create segmented loops. The boundary condition is

$$\Phi_1(x_N)=\Phi_2(x_{\bar{N}}), \tag{1}$$

with a similar tension relation for the derivatives. $\bar{N}$ is the number of segments. In the literature, the energies for the segmented string have been renormalized by the energy of the uniform string joined to itself, a system with one boundary point. The boundary conditions at this point for the uniform string are analogous to (1).

In this paper, we will consider a string loop in which one of the boundary points, x_1, is twisted, where the fields obey the boundary conditions

$$\Phi_1(x_1)=-\Phi_2(x_1), \quad \Phi_1(x_{\bar{N}})=\Phi_2(x_{\bar{N}}) \quad \bar{N}\neq 1. \tag{2}$$

The tension relations for the derivatives at the boundary points are similar. For the uniform loop with one boundary point only, we are obviously creating a Möbius loop.

Twisted fields have been discussed generally by Isham.[15] In Minkowski space, DeWitt[16] has considered the Casimir energy of both twisted and untwisted scalar fields with a periodicity along the z-axis. Using cylindrical polar coordinates in Minkowski space, Ford[17] has treated the Casimir energy of a twisted string. Both DeWitt and Ford found the twisted scalar field to have a positive energy compared to a negative energy for the untwisted string. The twisted loop is an interesting problem because one can compare the energy to that of the untwisted loop to discover if it is energetically more favorable for a straight string to join in a simple or a twisted topology, because the differing loop topologies make Casimir energy comparisons quite valuable and because the twisted loop may offer a way of simplifying the untwisted string with a large number of segments.

The Casimir energy for the twisted uniform loop is calculated in the next section. A comparison is made to the untwisted uniform string. Twisted strings with two segments are discussed in the third part of the paper. The energies in these sections are renormalized using the Euler-MacLaurin sum formula and a cut off function. In the fourth section we compare this method to regularizing using point splitting and the generalized zeta function. It is potentially instructive to calculate the result by all three methods. There are many regularization methods, each with its advantages and problems. A comparison insures that a problem specific to one method has not influenced the result of the calculation. There are situations, usually involving a boundary, where the three methods do not agree and a study of the divergence behavior causing the disagreement can be insightful.[18] A comparison between the two segment twisted string and the four segment untwisted loop is discussed in the last section.

II. UNIFORM LOOPS

A. Twisted loop-anti periodic boundary condition

Let the field on the loop be described by both clockwise and counterclockwise moving waves,

$$\Phi(x)=\xi e^{i\omega x}+\eta e^{-i\omega x}. \tag{3}$$

The boundary conditions are

$$\Phi(x)=-\Phi(x+L), \quad \Phi'(x)=-\Phi'(x+L). \tag{4}$$

Using (3) and (4), the allowed frequencies are

$$\cos(\omega L)=-1, \quad \omega=\frac{2\pi}{L'}\left(n+\frac{1}{2}\right). \tag{5}$$

The energy associated with the zero point twisted string oscillations is found from the $\alpha \to 0$ limit of the sum with cutoff function

$$E_t = 2 \times \frac{1}{2} \sum_{n=0}^{\infty} \frac{2\pi}{L}\left(n+\frac{1}{2}\right)\exp\left(\frac{-2\pi\alpha(n+\frac{1}{2})}{L}\right). \tag{6}$$

Evaluating the sum using the Euler-McLaurin sum formula and taking the limit one finds

$$E_t = \frac{L}{2\pi\alpha^2} + \frac{\pi}{12L} + O(\alpha^2). \tag{7}$$

This could be compared to the energy for the untwisted uniform string given by Brevik and Nielsen,[10]

$$E_u = \frac{L}{2\pi\alpha^2} - \frac{\pi}{6L} + O(\alpha^2). \tag{8}$$

The first term in both Eqs. (7) and (8) can be identified as the energy of the string with no boundary.[19] Subtracting off the energy of the unbounded string one finds the renormalized energies,

$$E_{t,r} = \frac{\pi}{12L}, \quad E_{u,r} = -\frac{\pi}{6L}. \tag{9}$$

One sees that, relative to the unbounded string, the untwisted string represents the lower energy state. This is similar to the results of DeWitt[16] and Ford.[17]

B. Another boundary condition for the uniform string

More complex twists can be constructed using the boundary conditions

$$\begin{aligned} \Phi(x) &= \phi(x+L)\exp\left[\frac{2\pi i}{N}\right], \\ \Phi'(x) &= \Phi'(x+L)\exp\left[\frac{2\pi i}{N}\right], \end{aligned} \tag{10}$$

where N is the number of circuits needed to complete the field. $N=1$ is the uniform untwisted string, $N=2$ is the uniform twisted string treated in the previous section.

Applying the boundary conditions one finds that the allowed frequencies are given by

$$\cos\left(\omega L + \frac{2\pi}{N}\right) = 1, \tag{11}$$

$$\omega = \frac{2\pi}{L}\left(n+\frac{1}{N}\right). \tag{12}$$

The associated Casimir energy calculated with the sum formula and a cut off is

$$E_t - \frac{L}{2\pi\alpha^2} = \frac{2\pi}{L}\left(\frac{-1}{12} + \frac{1}{2N} - \frac{1}{2N^2}\right). \tag{13}$$

For integer N this is always greater than the untwisted string energy E_u given in (9). For $0<N<1$ the twisted uniform string energy can be less than that of the untwisted string.

III. THE TWO SEGMENT TWISTED STRING

A. Allowed frequencies

The two segment string has two scalar fields, one moving on each of the two kinds of string,

$$\Phi_1(x)=\xi_1 e^{i\omega x}+\eta_1 e^{-i\omega x},$$
$$\Phi_2(x)=\xi_2 e^{i\omega x}+\eta_2 e^{-i\omega x}. \tag{14}$$

We will take the twisted boundary point to be $x=0(L)$ and the normal boundary point to be $x=L_1$, where we allow for the possibility that the segments are of different lengths.

The boundary conditions on the fields gives

$$O(L):\xi_1 e^{0}+\eta_1 e^{-0}=\xi_2 e^{i\omega L}+\eta_2 e^{-i\omega L},$$
$$L_1:\xi_1 e^{i\omega L_1}+\eta_1 e^{-i\omega L_1}=\xi_2 e^{i\omega L_1}+\eta_2 e^{-i\omega L_1}. \tag{15}$$

The derivative conditions are

$$O(L):R(\xi_1 e^{0}-\eta_1 e^{-0})=\xi_2 e^{i\omega L}-\eta_2 e^{-i\omega L},$$
$$L_1:R(\xi_1 e^{i\omega L_1}-\eta_1 e^{-i\omega L_1})=\xi_2 e^{i\omega L_1}-\eta_2 e^{-i\omega L_1}, \tag{16}$$

where $R=T_1/T_2$, the ratio of the tensions in the two segments. Brevik and Nielsen[10] use x for this ratio.

From the coefficient determinent we can find the dispersion relation giving the allowed frequencies,

$$(1-R)^2\cos(\omega(L-2L_1))-(1+R)^2\cos(\omega L)-4R=0, \tag{17a}$$

which can be written as

$$(1-R)^2\cos(\omega(s-1)L_1)-(1+R)^2\cos(\omega(s+1)L_1)-4R=0. \tag{17b}$$

Another equivalent but useful form is

$$\sin(s\omega L_1)\sin(\omega L_1)=\frac{4R}{(1-R)^2}\cos^2\left(\frac{(s+1)\omega L_1}{2}\right), \tag{18}$$

where $s=L_2/L_1$, the ratio of the lengths of the two possible segments and $L=L_1+L_2$.

B. Some special cases

1. $R=1$ (equal tensions)

This is the same as the uniform twisted string treated in the second part of the paper.

2. $R=0$ ($T_2=\infty$ or $T_1=0$)

From the dispersion relation (18) we find

$$\omega_{n1}=\frac{\pi n_1}{L},\quad \omega_{n2}=\frac{\pi n_2}{L}. \tag{19}$$

This is the same result as for the $R=0$ untwisted string and has an identical Casimir energy.[10] Since we started with a twisted string, this is an interesting result but may be understood by realizing that the infinite T_2, implies infinite density since the wave speed is unity so that the second string blocks passage of the wave in the first string segment, effectively turning the boundary points of passage into points of reflection. The fact that the $R=0$ point is the same in both the twisted and untwisted loops may also identify this point as a common or double point between the two different loop topological phases. The zero tension limit has been discussed by Lindström.[20]

C. General energies and frequencies-odd *s*

1. The Casimir energy

The dispersion relation can be written as a polynomial in $\sin^{(s+1)}(\omega L_1)$. There will be $((s+1)/2)$ double branches, i.e., solutions to the equation for $\sin^2(\omega L_1)$. Each root is an allowed frequency. Each double branch has roots $\pi\beta_i$. There are $((s+1)/2)$ values of β_i. For each β_i the frequency spectrum is

$$\omega L_1=\begin{cases}\pi(\beta+n), \\ \pi(1-\beta+n),\end{cases} \quad 0\leqslant\beta\leqslant\tfrac{1}{2}. \tag{20}$$

There is no degeneracy to consider.

Using the Euler MacLaurin Sum formula with a cut off as in the uniform string case, the Casimir energy for a single β is

$$E(\beta)=\frac{L_1}{2\pi\alpha^2}-\frac{\pi}{2L_1}\left(\frac{\beta^2}{2}+\frac{(1-\beta)^2}{2}\right)+\frac{\pi}{6L_1}. \tag{21}$$

Summing over the $((s+1)/2)$ double branches we have

$$E=\frac{L}{2\pi\alpha^2}-\frac{\pi(s+1)}{4L}\sum_{i=1}^{(s+1)/2}(\beta_i^2+(1-\beta_i)^2)+\frac{\pi(s+1)^2}{12L}. \tag{22}$$

Once s is chosen, β can be determined from the dispersion relation (17) or (18) and numerical values for the energies found.

The energy in Eq. (22) is not yet renormalized. The prescription that we shall use is analogous to that used by Brevik and Nielsen for the untwisted string loop:

$$E_r=E \text{ (renormalized)}=E-E \text{ (uniform twisted loop)}. \tag{23}$$

Using this prescription and Eq. (22) we find the energy as

$$E_r=\frac{\pi(s^2+2s)}{12L}-\frac{\pi(s+1)}{4L}\sum_{i=1}^{(s+1)/2}(\beta_i^2+(1-\beta_i)^2). \tag{24}$$

We will now consider some special cases.

2. $s=1$ ($L_1=L_2$)

From the dispersion relation (18) we find one double branch for $s=1$,

$$\sin^2(\omega L_1)=\frac{4R}{(1+R)^2}. \tag{25}$$

TABLE I. Some energies for the twisted string loop renormalized to the unform twisted loop.

R	$E_r(s=1)$	$E_r(s=2)$	$E_r(s=3)$
0	$\frac{-\pi}{4L}$	$\frac{-\pi}{3.69L}$	$\frac{-\pi}{3.27L}$
$\frac{1}{2}$	$\frac{-\pi}{85.5L}$	$\frac{-\pi}{77.32L}$	$\frac{-\pi}{66.52L}$
1	0	0	0

The inverse sine of the square root of this equation for a given R is the single value of β for this case. From Eq. (23) the renormalized energy is

$$E_r=\frac{\pi}{4L}-\left(\frac{\pi}{2L}\right)(\beta^2+(1-\beta)^2). \tag{26}$$

Some values are tabulated in Table I.

3. $s=3$ ($L_2=3L_1$)

Using Eq. (19) again we find for the allowed frequencies,

$$\sin^4(\omega L_1)-\frac{3\sin^2(\omega L_1)(R+\frac{1}{3})(R+3)}{4(1+R)^2}+\frac{R}{(1+R)^2}=0. \tag{27}$$

There will be two values for β for each R. Some of the renormalized energies for $s=3$ are tabulated in Table I.

D. Casimir energies—even s

For even s we will use both Eqs. (17) and (18). We will first show that $\cos(\omega L_1)=-1$, $\omega L_1=\pi$, is a root for any even s.

From Eq. (18) we have

$$\sin(s\pi)\sin(\pi)=\left(\frac{4R}{(1-R)^2}\right)(1+\cos(\pi\langle s+1\rangle)),$$
$$1+\cos(\pi\langle s+1\rangle)=0. \tag{28}$$

So, for all even s, the polynomial has a degenerate root at $\omega L_1=\pi$.

The equation for the allowed frequencies is

$$(1-R)^2\cos(\omega L_1\langle s-1\rangle)-(1+R)^2\cos(\omega L_1\langle s+1\rangle)-4x=0,$$

with $1+\cos(\omega L_1)$ a factor. We will work out the $s=2$ case.

The allowed frequencies for $s=2$ are given in by

$$\cos^2(\omega L_1)-\cos(\omega L_1)+\frac{R}{(1+R)^2}=0 \quad \text{and} \quad \cos(\omega L_1)=-1. \tag{29}$$

Some values of the energy are tabulated in Table I.

IV. OTHER RENORMALIZATION METHODS

In the first part of the paper, the Casimir energies have been evaluated by considering the energy as a sum over possible modes of vibrations and using a limit of the Euler-MacLaurin sum formula with a cut-off function. There are several other regularization methods that could be applied to this problem.

A. Covariant point-splitting method-uniform twisted string

The result presented in Eq. (7) for the uniform twisted string can also be derived by the point-splitting method. This method is not only covariant but also cut-off independent.[21–23] To use this method the metric is assumed to be

$$ds^2=dt^2-(R_0)^2d\phi^2, \tag{30}$$

where R_0 is a constant and $\phi\epsilon[0,2\pi]$. This method, as in the previous one, begins with the possible modes of vibration. The wave equation in this metric is

$$D^{\mu}D_{\mu}\Phi(t,\phi)=0, \tag{31}$$

where D_{μ} is the covariant derivative operator for the metric (30).

As before the general solution is

$$\Phi_m(t,\phi)=Ae^{-i\omega_m t}\cos(m\phi), \quad \Phi_n(t,\phi)=Be^{-i\omega_n t}\sin(n\phi), \tag{32}$$

where A,B are constants and $\omega_m=m/R_0$, $\omega_n=n/R_0$. Now the time dependence is explicit and we use ϕ instead of x. Applying the antiperiodic boundary condition,

$$\Phi(t,\phi)=-\Phi(t,\phi+2\pi), \tag{33}$$

we obtain the eigenfunctions and eigenfrequencies, respectively, as

$$\Phi_n(t,\phi)=\frac{1}{\sqrt{\pi(2n+1)}}\exp(-i\omega_n t)\cos\left(\frac{(2n+1)\phi}{2}\right),$$
$$\omega_n=\frac{2n+1}{2R_0}, \quad n=0,1,2,3,\ldots, \tag{34}$$

and

$$\Phi_m(t,\phi)=\frac{1}{\sqrt{\pi(2n+1)}}e^{-i\omega_m t}\sin\left(\frac{(2m+1)}{2}\phi\right),$$
$$\omega_m=\frac{2m+1}{2R_0}, \quad m=0,1,2,\ldots . \tag{35}$$

The allowed frequencies are the same as in Eq. (5) with $L=2\phi R_0$. Rather than going directly to the energy as in the mode sum method, the modes are used to construct the Hadamard Green's function $G^{(1)}(x,x')$ which is written as[23]

$$G^{(1)}(x,x')=\frac{1}{2\pi}\ln\left[\frac{\cos(\Delta t/2R_0)+\cos(\delta)}{\cos(\Delta t/2R_0)-\cos(\delta)}\right], \tag{36}$$

where $\Delta t=t-t'$, and $\delta=(\phi-\phi')/2$. To renormalize this Green's function we express it as an image sum and write it as[24,25]

$$\frac{1}{2}G^{(1)}(x,x')=\frac{1}{4\pi}\sum_{n=-\infty}^{\infty}\ln\left[\frac{1}{(2n\pi+\delta)^2-(\Delta t/2R_0)^2}\right]+\frac{1}{4\pi}\ln\left[\cos\left(\frac{\Delta t}{2R_0}\right)+\cos(\delta)\right]$$
$$-\frac{1}{4\pi}\ln\left[\frac{1}{2}\right]-\frac{1}{\pi}\sum_{n=1}^{\infty}\ln\left[\frac{1}{2n\pi}\right]. \tag{37}$$

It is clear that the $n=0$ term corresponds to the infinite unbounded string result and hence the Casimir renormalization relative to the infinite string could be accomplished by dropping this term.[21] This is analogous to the energy renormalization of Eq. (9). Expressing the expectation value of the stress energy tensor as

$$\langle T_{\mu\nu}\rangle_r=\tfrac{1}{2}\operatorname*{Lim}_{x'\to x}(D_\mu D_{\nu'}-\tfrac{1}{2}g_{\mu\nu}D^\lambda D_\lambda)G_r^{(1)}(x,x'). \tag{38}$$

Using the covariant derivatives,

$$\operatorname*{Lim}_{x'\to x}\frac{1}{2}D_0D_{0'}G_r^{(1)}(x,x')=\frac{-1}{16\pi^3R_0^2}\sum_{n=1}^{\infty}\frac{1}{n^2}+\frac{1}{32\pi R_0^2},$$
$$\operatorname*{Lim}_{x'\to x}\frac{1}{2}D_\phi D_{\phi'}G_r^{(1)}(x,x')=\frac{-1}{16\pi^3}\sum_{n=1}^{\infty}\frac{1}{n^2}+\frac{1}{32\pi}, \tag{39}$$

we obtain

$$\langle T_0^0\rangle_r=\frac{1}{48\pi R_0^2},\quad \langle T_\phi^\phi\rangle_r=-\langle T_0^0\rangle_r. \tag{40}$$

The point splitting method will produce a density rather than an energy. Using this density the energy is

$$E_r=\frac{\pi}{12L}. \tag{41}$$

Equation (41) agrees with the results obtained with the sum formula and cut off, Eq. (9).

B. Regularization with the Zeta function

Another method that has been used to obtain the renormalized zero-point energies is Zeta function renormalization.[24–27] The use of Zeta function methods is interesting because the twisted string is such a simple example of the procedures. The history of Zeta function regularization applied to string loops has been reviewed by Elizalde.[27] The Zeta function method begins with a sum over an operator spectrum. We will use the Hurwitz Zeta function,[26]

$$\zeta(s^*,a)=\sum_{m=0}^{\infty}\frac{1}{(m+a)^{s^*}}, \tag{42}$$

with $\mathrm{Re}(s^*)>1$, $0<a\leq 1$. We use s^* rather than s to avoid confusion with the string length parameter.

One of the possible integral representations is

$$\zeta(s^*,a)=\frac{1}{\Gamma(s^*)}\int_0^\infty \frac{dt\, t^{(s^*-1)}e^{-at}}{1-e^{-t}}, \tag{43}$$

with $\mathrm{Re}(s^*)>1$ and $\mathrm{Re}(a)>0$. Transforming into a contour integral[26] we get

$$\zeta(s^*,a)=\frac{e^{-i\pi s^*}\Gamma(1-s^*)}{2\pi i}\oint \frac{dz\, z^{(s^*-1)}e^{-az}}{1-e^{-z}}. \tag{44}$$

This provides the analytic continuation of $\zeta(s^*,a)$ over the plane: It is regular everywhere except for a simple pole at $s^*=1$ with residue 1. In the special case where s^* is an negative integer $s^*=-m$, $m=0,1,2...$, we have

$$\zeta(-m,a)=\frac{-B_{m+1}(a)}{m+1}, \tag{45}$$

where $B_m(a)$ is the Bernoulli polynomial. The Zeta function method, just as in the mode sum method, starts with an expression for the energy as the sum over possible modes. The energy is given by Eq. (6) with $\alpha=0$, eliminating the cut off. That sum is clearly of the form (43) with $s^*=-1$. The Zeta function of interest is

$$\zeta(-1,a)=\frac{-a^2+a-\frac{1}{6}}{2}. \tag{46}$$

The Zeta function procedure regularizes the energy by assigning an analytically continued Zeta function to the energy sum.[23,27] It will be necessary to explicitly renormalize to the uniform twisted string energy at the end of the calculation. We now reconsider some of the cases considered in Sec. II using Zeta function regularization.

1. The uniform twisted string

From Eq. (5) we have $\omega_n=(2\pi/L)(n+1/2)$, $n=0,1,2,...$.
The Casimir energy is

$$E_t=2\times\frac{1}{2}\sum_{n=0}^{\infty}\frac{2\pi}{L}\left(n+\frac{1}{2}\right)=\frac{2\pi}{L}\zeta\left(-1,\frac{1}{2}\right)=\frac{\pi}{12L}, \tag{47}$$

where the factor 2 takes into account that the modes are degenerate. The simplicity of this procedure, compared to the more lengthly calculations associated with the mode sum/cut-off and point splitting methods is startling. Its very simplicity is, however, sometimes considered a drawback since the analytic continuation which removes the divergences somewhat hides the divergence behavior which could be of interest.

2. R=0

The $R=0$ case implies $T_1\to 0$ or $T_2\to\infty$.[20]
From Eq. (19) we get the allowed modes just as in the mode sum/cut-off method,

$$\omega_n=\begin{cases}\dfrac{n\pi}{L_1},\\ \dfrac{n\pi}{L_2},\end{cases}\quad n=0,1,2,\ldots\ . \tag{48}$$

The zero frequency mode is not of interest. The Casimir energy is

$$E_{1+2}=\frac{1}{2}\sum_{n=1}^{\infty}\ \frac{n\pi}{L_1}+\frac{n\pi}{L_2}. \tag{49}$$

Regularizing by the Riemann-Zeta function method we get

$$E_{1+2}=\left(\frac{\pi}{2L_1}+\frac{\pi}{2L_2}\right)\zeta(-1,1)=-\frac{\pi}{24}\left(\frac{1}{L_1}+\frac{1}{L_2}\right). \tag{50}$$

Using $s=L_2/L_1$ as before we can rewrite this equation as

$$E=\frac{-\pi}{24L}\left(s+\frac{1}{s}+2\right). \tag{51}$$

Renormalizing to the twisted string, using Eq. (23),

$$E_r=\frac{-\pi}{24L}\left(s+\frac{1}{s}+4\right). \tag{52}$$

This second renormalization must be included explicitly and is not performed by the Zeta function.

3. s an odd integer

Again, in agreement with the mode sum calculation we have from Eq. (20) the frequency spectrum

$$\omega L_1=\begin{cases}\pi(\beta+n),\\ \pi(1-\beta+n),\end{cases}$$

with $0\leqslant\beta\leqslant 1/2$, $n=0,1,2,\ldots$.

Just as in Eqs. (21) and (22) for the mode sum/cut-off method the Casimir energy for general β_i can be written as

$$E_{1+2}=\frac{\pi}{2L_1}\sum_{i=1}^{(s+1)/2}\ \zeta(-1,\beta_i)+\zeta(-1,1-\beta_i). \tag{53}$$

Using the special form for the Zeta function given in Eq. (46) we have

$$E_{1+2}=\frac{\pi(s+1)^2}{12L}-\frac{\pi(1+s)}{4L}\sum_{i=1}^{(s+1)/2}\ \beta_i^2+(1-\beta_i)^2 \tag{54}$$

or renormalizing to the uniform twisted string we have

$$E_r=E_{1+2}-E\ \text{(Uniform twisted string)},$$

$$E_r=\frac{\pi(s^2+2s)}{12L}-\frac{\pi(1+s)}{4L}\sum_{i=1}^{(s+1)/2}\beta_i^2+(1-\beta_i)^2. \tag{55}$$

V. RELATING THE TWISTED AND UNTWISTED STRING WITH $S=1$

One of the effects of once twisting the string with two segments is to compel the field to cross four string segments before returning to its initial condition. A uniform string with four segments also has this effect and the question arises of how the two cases are related.

A. The uniform string

First compare the uniform twisted string to the uniform untwisted string. Generalize the frequency conditions to allow the twisted and untwisted loops to have different radii. L_t will be the circumference of one loop of the twisted string and L_u will be the circumference of one loop of the untwisted string.

The frequency conditions are

$$\begin{aligned}&\text{twisted string: } \cos(\omega L_t)=-1,\\ &\text{untwisted string: } \cos(\omega L_u)=1.\end{aligned} \tag{56}$$

To make the strings similar one could clearly require that the path length traveled by a wave on each type of loop be the same,

$$2L_t=L_u. \tag{57}$$

Substituting into the frequency conditions one finds

$$\text{twisted string: } \cos\left(\frac{\omega L_u}{2}\right)=-1, \tag{58}$$

$$\text{untwisted string: } \cos\left(\frac{\omega L_u}{2}\right)=\pm 1. \tag{59}$$

The untwisted string contains the twisted string and the additional frequency $\omega L_u/2=2\pi,4\pi,\ldots$. For the uniform loops, there is no calculational advantage to treating one loop topology over the other but for higher numbers of segments, there is possibly a reduction in the dimensionality of the problem that needs to be solved for some of the parameter range. The next most complicated cases to compare are the two segment twisted string to the four segment untwisted string.

B. The two segment twisted string, the four segment untwisted string, $s=1$

The frequency conditions for the two segment twisted loop follows from Eq. (17b),

$$\cos\left(\frac{\omega L_u}{2}\right)=\frac{R^2-6R+1}{(1+R)^2}, \tag{60}$$

where we have made the same arguments about circumference and lengths as for the uniform string. The frequency condition for the four segment untwisted string was given in Ref. 13, Eq. (17).

$$-\frac{(1+R)^2}{8R^2}(3-10R+3R^2)+\frac{(1-R)^2}{2R^2}\cos\left(\frac{\omega L_u}{2}\right)-\frac{(1+R)^4}{8R^2}\cos(\omega L_u)=0. \tag{61}$$

The roots of this equation are

$$\cos\left(\frac{\omega L_u}{2}\right)=\frac{R^2-6R+1}{(1+R)^2} \quad \text{and} \quad +1. \tag{62}$$

Comparing (34) and (37) to (32) and (33) we see the same pattern. The untwisted string of 4 segments contains the twisted string plus a root of $+1$. Whether or not this pattern is more general is under investigation.

VI. CONCLUSIONS

We have calculated the energy of a uniform twisted loop of string and compared it to the uniform untwisted loop. We find that the untwisted loop has the lower energy for a pure antiperiodic boundary condition. More complex boundary conditions could reverse this.

The energy of a twisted two segmented loop was also calculated and, just as for the untwisted string, a non zero negative Casimir energy is observed. We found that the twisted and untwisted phases of the loop share a common point of their energy spectrum at zero tension. The double point in the energy spectrum of the twisted and untwisted loops may be important in loop dynamics. The loop tensions are part of the loop stress energy content and related to the behavior of the space time through the field equations. A process in which the loop tensions change with variations in the metric could create conditions for the loop phase transition to occur as either a one time transfer or as an oscillation between phases. A study of the behavior of the loop tension as a function of curvature is clearly an important question. It would be especially pertinent in the context of the types of radiation emitted by an oscillating loop and the question of loop stability. If loop stability is affected by the possibility of a phase transition or phase oscillation, this could have an effect on the galactic seeding process.[2,8,14]

A calculation involving loop tension and the curvature of the embedding cosmology opens up the possibility of a much more varied loop stress-energy structure. Cosmic string interiors with heat flow and vorticity,[28] and torsion[29] and spin density[30] have all been discussed in the literature. This larger array of possible stress-energy contents with both untwisted and twisted loop analogs might provide a richer loop thermodynamics with associated phases, such as spin-up/spin-down.[31] Casimir energy calculation on these more elaborate loops would be interesting. The existence of two accessible loop phases has suggested that more detailed calculations involving curvature would be valuable.

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The q-Coulomb problem in configuration space

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We formulate the q-Coulomb problem in configuration space with the aid of ladder operators for the radial wave function. The highest angular momentum state corresponding to the principal quantum number n is found to be the monomial r^{n-1} multiplied by a q-exponential. The states of lower angular momentum are q-associated Laguerre polynomials multiplied by the same q-exponential. The state functions all lie in the complex plane and may be interpreted in the standard way. The energy levels are again given by a Balmer formula with n replaced by the basic n. © *1996 American Institute of Physics.* [S0022-2488(96)03408-1]

I. INTRODUCTION

The q-Coulombic problem has been the subject of several studies which differ in the way the Coulombic symmetry is lifted.[1,2] The basic $O_3 \times O_3$ symmetry of this problem may be described in terms of the two vector integrals of the motion, $\mathbf{L}$, the angular momentum integral coming from the spherical symmetry and $\mathbf{A}$, the Lenz vector owing its existence to the k/r potential. The problem separates in spherical coordinates into an angular equation determining the eigenvalues of $\mathbf{L}^2$ and L_z and a radial equation parametrically dependent on $(L^2)'$ and determining the eigenvalues of the Hamiltonian H and $(\mathbf{A}^2)$, for which one finds

$$H' \equiv E \sim -\frac{1}{n^2},$$

$$(\mathbf{A}^2)' = m^2h^2 + 2mE((L^2)' + \hbar^2)),$$

where m is the mass. Here we discuss the q-derived problem by replacing the angular and the radial equations by their q-analogs.

II. THE ANGULAR AND RADIAL EQUATIONS (q=1)

The Hamiltonian for any spherically symmetric potential is

$$H = \frac{1}{2m}\left(\frac{1}{r}p_r^2 r + \frac{L^2}{r^2}\right) + V(r), \tag{2.1}$$

where

$$(r, p_r) = i\hbar. \tag{2.2}$$

The problem separates into an angular equation

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$$L^2\Phi_{lm}(\theta,\phi)=l(l+1)\hbar^2\Phi_{lm}(\theta,\phi) \tag{2.3}$$

and a radial equation

$$\left[\frac{1}{2m}\left(\frac{1}{r}p_r^2 r\right)+\frac{l(l+1)\hbar^2}{r^2}+V(r)\right]R(r)=ER(r). \tag{2.4}$$

The solutions of (2.3) are spherical harmonics; and, if $V(r)$ is the Coulomb potential, the solutions of (2.4) are the associated Laguerre functions.

In dimensionless form the radial equation is

$$R''+\frac{2}{x}R'+\frac{2}{x}R-\frac{l(l+1)}{x^2}R=-\lambda R. \tag{2.5}$$

Set

$$\rho=xR \tag{2.6}$$

then

$$\rho''+\frac{2}{x}\rho-\frac{l(l+1)}{x^2}\rho=-\lambda\rho. \tag{2.7}$$

The eigenvalue, λ, as determined from the asymptotic form of this equation, is

$$\lambda=-\left(\frac{\rho''}{\rho}\right)_\infty. \tag{2.7}_\infty$$

We shall discuss the radial equation with the aid of the Infeld ladder method.[3,4] This procedure sometimes permits the factorization of the Sturm–Liouville operator into the product of a raising and a lowering operator.

Equation (2.7) may be so factored in either of the following ways:

$$H_l^- H_l^+ \cdot \rho_l^\lambda=\left(\lambda+\frac{1}{l^2}\right)\rho_l^\lambda, \tag{2.8a}$$

$$H_{l+1}^+ H_{l+1}^- \cdot \rho_l^\lambda=\left(\lambda+\frac{1}{(l+1)^2}\right)\rho_l^\lambda, \tag{2.8b}$$

where

$$H_l^\pm=\frac{l}{x}-\frac{1}{l}\pm\frac{d}{dx}. \tag{2.9}$$

It follows that

$$H_l^+ H_l^-(H_l^+\rho_l^\lambda)=\left(\lambda+\frac{1}{l^2}\right)(H_l^\pm\rho_l^\lambda), \tag{2.10a}$$

$$H_{l+1}^- H_{l+1}^+(H_{l+1}^-\rho_l^\lambda)=\left(\lambda+\frac{1}{(l+1)^2}\right)(H_{l+1}^-\rho_l^\lambda). \tag{2.10b}$$

By comparing (2.8a) with (2.10b) and (2.8b) with (2.10a) we see that, up to a normalization,

$$H^{-}_{l+1}\rho^{\lambda}_{l}=\rho^{\lambda}_{l+1} \tag{2.11a}$$

and

$$H^{+}_{l}\rho^{\lambda}_{l}=\rho^{\lambda}_{l-1}. \tag{2.11b}$$

Hence H^{-}_{l+1} and H^{+}_{l} are raising and lowering operators respectively. There is a highest state given by $\rho^{\lambda}_{\bar{l}}$ where $\bar{l}=l_{\max}$ and

$$H^{-}_{\bar{l}+1}\rho^{\lambda}_{\bar{l}}=0 \tag{2.12a}$$

or

$$\left(\frac{\bar{l}+1}{x}-\frac{1}{\bar{l}+1}-\frac{d}{dx}\right)\rho^{\lambda}_{\bar{l}}=0. \tag{2.12b}$$

The solution of (2.12) is

$$\rho^{\lambda}_{\bar{l}}=x^{\bar{l}+1}e^{-x/(\bar{l}+1)}. \tag{2.13}$$

When $\rho^{\lambda}_{\bar{l}}$ is substituted in (2.8b) we find

$$\lambda=-\frac{1}{(\bar{l}+1)^2}, \tag{2.14}$$

in agreement with $(2.7)_{\infty}$.

The energy levels are usually expressed in terms of a principal quantum number n:

$$\lambda=-\frac{1}{n^2}, \tag{2.15}$$

where

$$n=\bar{l}+1. \tag{2.16}$$

Then the radial wave function with maximum l and principal quantum number n is

$$\rho^{n}_{\bar{l}}=x^{n}e^{-x/n} \tag{2.17}$$

or

$$R^{n}_{\bar{l}}=x^{n-1}e^{-x/n}. \tag{2.18}$$

To find states belonging to the same n but with lower values of l one may apply the lowering operator H^{+}_{l}. For example we find the three top states (nonrenormalized):

$l=\bar{l}$: $$\rho^{n}_{\bar{l}}\sim x^{\bar{l}+1}e^{-x/n},$$

$$l=\bar{l}-1: \qquad \rho^n_{\bar{l}-1}\sim\left[x^{\bar{l}}-\frac{1}{\bar{l}(\bar{l}+1)}x^{\bar{l}+1}\right]e^{-x/n},$$

$$l=\bar{l}-2: \qquad \rho^n_{\bar{l}-2}\sim\left[(2\bar{l}-1)x^{\bar{l}-1}-\frac{2(2\bar{l}-1)}{(\bar{l}-1)(\bar{l}+1)}x^{\bar{l}}+\frac{2}{(\bar{l}-1)(\bar{l}+1)^2}x^{\bar{l}+1}\right]e^{-x/n}, \tag{2.19}$$

where the quantum numbers of the top state are $(n,\bar{l})$. Expressed in terms of associated Laguerre polynomials, one has

$$l=\bar{l}: \qquad \rho^n_{\bar{l}}\sim x^{\bar{l}+1}L^{2\bar{l}+1}_{2\bar{l}+1}\left(\frac{2x}{n}\right)e^{-x/n},$$

$$l=\bar{l}-1: \qquad \rho^n_{\bar{l}-1}\sim x^{\bar{l}}L^{2\bar{l}-1}_{2\bar{l}}\left(\frac{2x}{n}\right)e^{-x/n}, \tag{2.20}$$

$$l=\bar{l}-2: \qquad \rho^n_{\bar{l}-2}\sim x^{\bar{l}-1}L^{2\bar{l}-3}_{2\bar{l}-1}\left(\frac{2x}{n}\right)e^{-x/n},$$

where

$$L^{2l+1}_{n+l}(x)=-((n+l)!)^2\sum_{\lambda=0}^{n-\lambda-1}\frac{(-)^\lambda x^\lambda}{\lambda!(n-l-1-\lambda)!(2l+1+\lambda)!}. \tag{2.21}$$

III. THE DEFORMATION

A. The angular equation

Replace (2.3) by

$$L^2_q\Phi^q_{lm}(\theta,\phi)=\langle l\rangle\langle l+1\rangle\Phi^q_{lm}(\theta,\phi), \tag{3.1}$$

where L^2_q is the quadratic Casimir of $SU_q(2)$ and $\langle l\rangle$ is the basic number:

$$\langle l\rangle=\frac{q^l-1}{q-1}. \tag{3.2}$$

Here we have substituted the quadratic Casimir of $SU_q(2)$ for the quadratic Casimir of $SU(2)$ and therefore replaced $l(l+1)$ by $\langle l\rangle\langle l+1\rangle$. The eigensolutions of this equation, Φ^q_{lm}, the q-spherical harmonics, have been obtained by Rideau and Winternitz.[5]

B. The radial equation

We take over (2.2) as a q-commutator:

$$(r,p_r)_q=i\hbar, \tag{3.3}$$

where the conjugate momentum p_r becomes the difference operator

$$p_r=\frac{\hbar}{i}D^q_r \tag{3.4}$$

and

$$D_r^q f(r)=\frac{f(qr)-f(r)}{(q-1)r}. \tag{3.5}$$

We shall abbreviate D_r^q as D_r.

There are various possibilities for defining the q-radial problem. Here we shall adopt the q-modified raising and lowering Eq. (2.11) in dimensionless form, as follows:

$$H^-_{\langle l+1\rangle}\rho^\lambda_{\langle l\rangle}=\rho^\lambda_{\langle l+1\rangle}, \tag{3.6}$$

$$H^+_{\langle l\rangle}\rho^\lambda_{\langle l\rangle}=\rho^\lambda_{\langle l-1\rangle}, \tag{3.7}$$

where we have replaced l by $\langle l\rangle$, d/dx by D_x, and therefore $H_l^\pm$ by

$$H^\pm_{\langle l\rangle}=\frac{\langle l\rangle}{x}-\frac{1}{\langle l\rangle}\pm D_x. \tag{3.8}$$

We define the energy by

$$\lambda=-\left(\frac{D_x^2\rho}{\rho}\right)_\infty \tag{3.9}$$

as the natural extension of (2.7).

We take the view that (3.6)–(3.9) describe the full content of the q-radial problem, since (3.6), (3.7), and (3.9) imply (2.5) and $(2.7)_\infty$ in the limit $q=1$.

Since these modified equations do not lead to an acceptable Hamiltonian, the energy is fixed not by the eigenvalues of the Hamiltonian, but by the asymptotic form of the wave function via (3.9), or equivalently by poles of the corresponding amplitude in momentum space.

The highest state $(\bar{l})$ is now given by

$$H^-_{\langle \bar{l}+1\rangle}\rho^\lambda_{\langle l\rangle}=0 \tag{3.10}$$

or

$$\left(\frac{\langle \bar{l}+1\rangle}{x}-\frac{1}{\langle \bar{l}+1\rangle}-D_x\right)\rho^\lambda_{\langle l\rangle}=0. \tag{3.11}$$

The asymptotic form of this equation is

$$D_x\rho^\lambda_{\langle \bar{l}\rangle}=-\frac{1}{\langle \bar{l}+1\rangle}\,\rho^\lambda_{\langle \bar{l}\rangle}. \tag{3.12}$$

Also

$$(D_x)^2\rho^\lambda_{\langle \bar{l}\rangle}\to\frac{1}{\langle \bar{l}+1\rangle^2}\,\rho^\lambda_{\langle \bar{l}\rangle}. \tag{3.13}$$

By (3.9) and the preceding equation we have

$$\lambda=-\frac{1}{\langle \bar{l}+1\rangle^2} \tag{3.14a}$$

or the energy is

$$E(n,\bar{l})=-\frac{1}{\langle n\rangle^2};\quad n=\bar{l}+1. \tag{3.14b}$$

The asymptotic form of $\rho^{\lambda}_{\langle\bar{l}\rangle}$ is a solution of (3.12). We see that (3.12) is satisfied by

$$\rho^{\lambda}_{\langle\bar{l}\rangle}=\mathscr{E}_q\left(\frac{-x}{\langle n\rangle}\right), \tag{3.15}$$

where $\mathscr{E}_q$ is the q-exponential

$$\mathscr{E}_q(y)=\sum\frac{y^n}{\langle n\rangle!}. \tag{3.16}$$

Let the complete solution of (3.10) be

$$\rho^{\lambda}_{\langle\bar{l}\rangle}=f(x)\mathscr{E}_q\left(-\frac{x}{\langle n\rangle}\right). \tag{3.17}$$

By the q-Leibniz rule

$$D_xP^{\lambda}_{\langle n\rangle}=f(qx)\left(-\frac{1}{\langle n\rangle}\mathscr{E}_q\left(-\frac{x}{\langle n\rangle}\right)\right)+(D_xf(x))\mathscr{E}_q\left(-\frac{x}{\langle n\rangle}\right). \tag{3.18}$$

Then (3.10) becomes

$$\left(\frac{\langle n\rangle}{x}-\frac{1}{\langle n\rangle}\right)f(x)=-\frac{1}{\langle n\rangle}f(qx)+D_xf(x) \tag{3.19}$$

or

$$\left[(q-1)\langle n\rangle-\frac{(q-1)x}{\langle n\rangle}+1\right]f(x)=\left[1-\frac{(q-1)x}{\langle n\rangle}\right]f(qx). \tag{3.20}$$

If one sets $q=1$, (3.20) is simply an identity. To discuss this difference equation first convert it to a differential equation by differentiating with respect to q and then setting $q=1$. One finds

$$\langle n\rangle_1f(x)=xf'(x). \tag{3.21}$$

Therefore

$$f(x)=x^{\langle n\rangle_1} \tag{3.22}$$

$$=x^n. \tag{3.23}$$

By (3.17) and (3.23) one would have for the highest state,

$$\rho^{n}_{\langle\bar{l}\rangle}=x^n\mathscr{E}_q\left(-\frac{x}{\langle n\rangle}\right). \tag{3.24}$$

Equation (3.24) has the correct $q=1$ limit but does not satisfy the difference equation (3.20) from which it was derived. Therefore let us return to the difference equation and rewrite it in the following form:

$$f(x)=q^{-n}\left(\frac{1+ax}{1+q^{-n}ax}\right)f(qx); \quad a=\frac{1-q}{\langle n\rangle}, \tag{3.25}$$

$$=q^{-n}R(x)f(qx), \tag{3.26}$$

where

$$R(x)=\frac{1+ax}{1+aq^{-n}x}. \tag{3.27}$$

By $N-1$ iterations

$$f(x)=q^{-nN}\prod_{s=0}^{N-1} R(q^s x)f(q^N x) \tag{3.28}$$

and

$$f(x)=\prod_{0}^{\infty} R(q^s x)\lim_{N\to\infty} q^{-nN}f(q^N x). \tag{3.29}$$

Since $|q|<1$, $q^{-nN}\to\infty$. Therefore $f(q^N x)$ must vanish in this limit as is also indicated by (3.24). Then (3.28) suggests the ansatz

$$f(x)=x^n\phi(x) \tag{3.30}$$

so that by (3.29)

$$\phi(x)=\prod_{0}^{\infty} R(q^s x)\phi(0), \tag{3.31}$$

where

$$\prod_{0}^{\infty} R(q^s x)=\prod_{0}^{\infty}\frac{1+axq^s}{1+axq^{-n+s}} \tag{3.32a}$$

$$=\frac{(-ax|q)_\infty}{(-aq^{-n}x|q)_\infty}. \tag{3.32b}$$

Here

$$(x|q)_\infty=\prod_{0}^{\infty}(1-xq^s) \tag{3.33}$$

is the displaced factorial. Set

$$\phi(0)=1. \tag{3.34}$$

Then

$$f(x)=x^n\,\frac{(-ax|q)_\infty}{(-aq^{-n}x|q)_\infty} \tag{3.35}$$

and

$$\rho^n_{\langle n\rangle}(x)=x^n\,\frac{(-ax|q)_\infty}{(-aq^{-n}x|q)_\infty}\,\mathscr{E}_q\!\left(-\frac{x}{\langle n\rangle}\right) \tag{3.36}$$

or

$$R_{n\bar{l}}(x)=x^{n-1}\,\frac{(-ax|q)_\infty}{(-aq^{-n}x|q)_\infty}\,\mathscr{E}_q\!\left(-\frac{x}{\langle n\rangle}\right). \tag{3.37}$$

But[6]

$$(-ax|q)_\infty=\frac{1}{e_q(-ax)}=\frac{1}{e_q\!\left(-(1-q)\,\dfrac{x}{\langle n\rangle}\right)}=\frac{1}{\mathscr{E}_q\!\left(-\dfrac{x}{\langle n\rangle}\right)} \tag{3.38}$$

and

$$(-aq^{-n}x|q)_\infty=\frac{1}{\mathscr{E}_q\!\left(-\dfrac{q^{-n}x}{\langle n\rangle}\right)}. \tag{3.39}$$

Therefore

$$R_{n\bar{l}}(x)=x^{n-1}\mathscr{E}_q\!\left(-\frac{q^{-n}r}{\langle n\rangle}\right). \tag{3.40}$$

The remaining states are given by (3.7). For example, the three top states are

$$l=l:\quad \rho^n_{\bar{l}}\sim x^{\bar{l}+1}\mathscr{E}_q\!\left(-\frac{q^{-n}x}{\langle n\rangle}\right), \tag{3.41}$$

$$l=\bar{l}-1:\quad \rho^n_{\bar{l}-1}\sim\left(\rho^{\bar{l}}-\frac{x^{\bar{l}+1}}{\langle\bar{l}\rangle\langle\bar{l}+1\rangle}\right)\mathscr{E}_q\!\left(-\frac{q^{-n}x}{\langle n\rangle}\right), \tag{3.42}$$

$$\begin{aligned} l=\bar{l}-2:\quad \rho^n_{\bar{l}-2}\sim\Bigg\{&[\langle\bar{l}-1\rangle+\langle\bar{l}\rangle]x^{l-1}-\left[\frac{1}{\langle\bar{l}-1\rangle}+\frac{1}{\langle\bar{l}\rangle}+\frac{\langle\bar{l}-1\rangle}{\langle\bar{l}\rangle\langle\bar{l}+1\rangle}+\frac{q^{-1}}{\langle\bar{l}+1\rangle}\right]x^{\bar{l}}\\ &+\frac{1}{\langle\bar{l}\rangle\langle\bar{l}+1\rangle}\left(\frac{1}{\langle\bar{l}-1\rangle}+\frac{1}{\langle\bar{l}+1\rangle}\right)x^{\bar{l}+1}\Bigg\}\mathscr{E}_q\!\left(-\frac{q^{-n}x}{\langle n\rangle}\right). \end{aligned} \tag{3.43}$$

These are "q-Laguerre polynomials" which approach the usual Laguerre polynomials in the limit $q=1$.

The energy levels are given by (3.14). The Coulomb degeneracy is therefore not lifted in this version of the deformation.

IV. REMARKS

As already noted, the "q-deformation" is not a unique procedure. Reference 1 makes explicit use of the full $O(4)=O(3)\times O(3)$ undeformed symmetry since the integral equation of that paper lies in the $SU(2)$ group space which is carried into itself by the left and right motions (parameter groups) described by $O(3)\times O(3)$. Reference 2 is based on the q-deformation of $O(3)$. Since the quantum groups corresponding to $SU(2)$ and $O(3)$ are different, Refs. 1 and 2 describe different deformations. Furthermore, since both solutions lie in their respective algebras, they require a rule for their physical interpretation. In Ref. 7 such a rule is provided in terms of the Hilbert space defined by the algebra itself.

The totally different procedure followed here is based on rules such as the replacement of the radial commutator by the radial q-commutator, and further described in Sec. III of this paper. These rules are similar in spirit but formally weaker than the imposition of a quantum group. On the other hand, the wave functions here obtained have the clear advantage of lying in the complex plane as well as being simply related to the $q=1$ solutions from which they are derived. There is therefore no problem of physical interpretation such as we encounter in the other deformations of the Coulomb problem.

It is still possible to make canonical transformations including transformations which exchange the roles of x and p and transform probability amplitudes between configuration and momentum space. For example, the amplitude in r-space that we have obtained here may be q-Fourier transformed to momentum space, since the momentum operator is a q-derivative.[7]

There are in addition quite different canonical transformations, namely

$$\begin{pmatrix} r \\ p_r \end{pmatrix} = T_q \begin{pmatrix} R \\ P_R \end{pmatrix} \quad T_q \epsilon SU_q(2),$$

$$\begin{pmatrix} R \\ P_R \end{pmatrix} = T_{q^{-1}} \begin{pmatrix} r \\ p_r \end{pmatrix} \quad T_{q^{-1}} \epsilon SU_{q^{-1}}(2),$$

which preserve the q-commutator

$$(r,p_r)_q=(R,P_R)_q=i\hbar.$$

In previous work[7] we have restricted canonical transformations to either $SU_q(2)$ or $SU_{q^{-1}}(2)$. Then one can posit that one set of conjugate observables lies in a q- or q^{-1}-algebra while the other does not. If the state function turns out to lie in a q-algebra, the only invariant that could naturally be associated with a numerical probability of that state would be the Woronowicz integral over the algebra.

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Cabled Wilson loops in BF theories

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A generating function for cabled Wilson loops in three-dimensional BF theories is defined, and a careful study of its behavior for vanishing cosmological constant is performed. This allows an exhaustive description of the unframed knot invariants coming from the pure BF theory based on SU(2), and, in particular, it proves a conjecture relating them to the Alexander–Conway polynomial. © *1996 American Institute of Physics.* [S0022-2488(96)00308-8]

I. INTRODUCTION

In Ref. 1, a relation was conjectured between the Alexander–Conway polynomial and the v.e.v. (*vacuum expectation value*) of a newly proposed observable for the TQFT (*topological quantum field theory*) known as BF theory[2] (or as "pure" BF theory, to distinguish it from its generalization "with a cosmological term"). The main purpose of this paper is to clarify that conjecture and to prove it in the case of SU(2), although in a slightly different form. To do so, however, we also perform a careful study of BF theories, both pure and with a cosmological term, introducing new observables that describe cabled Wilson loops.

The BF theories are interesting from both the mathematical and the physical points of view: They are TQFTs that, in principle, can be defined in any dimension (see Ref. 3 and references therein). They describe quantum gravity in three dimensions[4] and could be useful for the study of four-dimensional quantum gravity in the approach of Ref. 5. Moreover, they are related to Yang–Mills theories in the weak-coupling limit, where they could be used to describe a "topological phase"[6] (see also Ref. 7 for a related approach). Finally, hitherto only in the Abelian case, they have been used to study many-body systems.[8]

On the other side, the interest for the Alexander–Conway polynomial comes from the fact that it has always played a different role than the other knot invariants, being the only one that, hitherto, has been described by the methods of the traditional algebraic topology; yet it lacked a TQFT description (and Ref. 1 was an attempt to fill this gap).

Indeed, the Chern–Simons theory describes the knot invariants related to the q-deformation of a classical group G in terms of v.e.v.s of Wilson loops (i.e., traces of G-holonomies along the knots);[9] yet the $q=1$ case, i.e., the Alexander–Conway polynomial, does not correspond to any acceptable value of the Chern–Simons coupling constant k.

In the case of SU(2), an important improvement was given by the Melvin–Morton conjecture[10] (proved in Ref. 11), which states that the inverse of the Alexander–Conway polynomial appears in the $q-1$ expansion of the colored Jones function. Rozansky[12] was then able to prove the same result in the framework of the Chern–Simons theory; more precisely, he showed that the inverse of the Alexander–Conway polynomial is recovered by a saddle-point computation in the limit $k\to\infty$.

In Ref. 3, an equivalence between the v.e.v.s of the Chern–Simons theory and of the BF theory with cosmological constant $\kappa=1/(2k)$ was shown. The $k\to\infty$ limit (i.e., the $q=1$ case) is then simply described by removing the cosmological term, thus obtaining the pure BF theory.

In this paper we show that the trace in the fundamental representation of the pure-BF-theory observable (31), first introduced in Ref. 1, is related to the $\kappa\to 0$ limit of a newly proposed

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observable, (22), for the BF theory with a cosmological term. In the framework of the Chern–Simons theory, this observable corresponds to the "exponential" of a holonomy; so its trace is the generating function for cabled Wilson loops, and the v.e.v. of this trace is the generating function for cabled knot invariants (as suggested by the results of Ref. 13).

Since the colored Jones functions are related to the cabled knot invariants, we are able to connect the $q-1$ expansion of the former to the pure-BF-theory knot invariant. By the Melvin–Morton conjecture, we conclude that the latter is related to the Alexander–Conway polynomial, the precise relation being (49). Our proof, however, can also go the other way; i.e., should one directly prove a relation between the pure BF theory and the Alexander–Conway polynomial, then we would have a further proof of the Melvin–Morton conjecture.

Our results are not limited to the trace in the fundamental representation of a particular observable for pure BF theory. In fact, we are able to prove that, in the standard framing, this observable is the most general one can consider (see Theorem 1 and Corollary 1). Moreover, we show how to compute the higher-representation knot invariants [see (34) and (35)], and also evaluate the limit as the dimension of the representation goes to infinity [see (37) and (40)]. Thus, we have a complete description of the unframed knot invariants coming from the pure BF theory based on SU(2) (see Theorem 2). The case of links has not been considered yet.

The paper is organized as follows: In Sec. II, we describe the colored Jones functions and introduce their generating function. In Sec. III, we recall the property of the BF theory with a cosmological term and define a generating function for cabled Wilson loops. In Sec. IV, we discuss the pure BF theory and prove Theorem 1 and Corollary 1. In Sec. V, we consider the limit for vanishing cosmological constant and prove Theorem 2. We conclude our work in Sec. VI, comparing our present results with those obtained perturbatively in Ref. 1. For the sake of clarity, we have put all the cumbersome computations into some appendices, to which we shall refer in the text.

II. THE COLORED JONES FUNCTION

The colored Jones function, $J_d(C;h)$, is defined in Ref. 10 as the invariant of the knot C obtained using the irreducible $SU(2)_q$-module ($q=e^h$) of dimension d. The main properties of its expansion as a rational power series (here and in the following, the notation of Ref. 11 is used),

$$J_d(C;h)=\sum_{m=0}^{\infty}\tilde{J}_m(C;d)h^m=d\sum_{j,m=0}^{\infty}b_{jm}(C)(d-1)^j h^m, \tag{1}$$

were stated in Ref. 10:

(i) The functions $\tilde{J}_m(C;d)$ are odd in d. This means that (the analytic continuation of) $J_d(C;h)$ itself is odd:

$$J_{-d}(C;h)=-J_d(C;h). \tag{2}$$

[This of course implies that the coefficients b_{jm} in (1) are not completely independent.]

(ii) These functions are actually polynomials of degree not exceeding $2m+1$.

(iii) In the hypothesis that *the standard framing for* C *is chosen*, the degree of $\tilde{J}_m$ cannot exceed $2m-1$.

In the same hypothesis of standard framing, two conjectures were also stated in Ref. 10:

(i) The degree of $\tilde{J}_m$ cannot actually exceed $m+1$, or in other words, $b_{..}$ in (1) is an upper triangular matrix,

$$b_{jm}(C)=0, \quad \text{if } j>m. \tag{3}$$

(ii) The diagonal elements of $b_{..}$ are related to the Alexander–Conway polynomial; viz., if one defines the Melvin–Morton function as

$$JJ(C;\hbar)=\sum_{m=0}^{\infty} b_{mm}(C)\hbar^m=\lim_{d\to\infty,h\to 0,dh=\hbar}\frac{J_d(C;h)}{d} \tag{4}$$

[the limit existing because of (3)], then

$$\hbar JJ(C;\hbar)=\frac{z}{\Delta(C;z)},\quad z=e^{\hbar/2}-e^{-\hbar/2}, \tag{5}$$

where $\Delta(C;z)$ is the Alexander–Conway polynomial with the normalization $\Delta(\bigcirc;z)=1$, where $\bigcirc$ is the unknot, and skein relation

$$\Delta(C_+;z)-\Delta(C_-;z)=z\Delta(C_0;z).$$

These two conjectures have been given a functional-integral proof by Rozansky.[12] In particular he proved that the Melvin–Morton function, (4), is related to the large-k limit of the Chern–Simons theory, so it can be computed in saddle-point approximation.

Eventually, Bar-Natan and Garoufalidis[11] gave a mathematical proof of (3) and (5) on the level of weight systems.

A. The generating function for colored Jones functions

In the following sections, the generating function

$$f(C;x,h)=\sum_{d=1}^{\infty}\frac{x^d}{d!}J_d(C;h), \tag{6}$$

with $x\in\mathbb{C}$, will be needed; so it is useful to anticipate here some of its properties. These are better clarified if one introduces $\tilde{f}$ defined by

$$f(C;x,h)=xe^x\tilde{f}(C;x,h). \tag{7}$$

In fact, the expansion of $\tilde{f}$ as a rational power series,

$$\tilde{f}(C;x,h)=\sum_{j,m=0}^{\infty}\tilde{b}_{jm}(C)x^jh^m, \tag{8}$$

shares the same properties as the expansion (1) of $J_d(C;h)$ (viz., see Appendix B). One can prove that

$$b\text{..}\ \text{upper triangular}\Leftrightarrow\tilde{b}\text{..upper triangular.} \tag{9}$$

Thus, (3) implies that $\tilde{b}$.. is actually an upper triangular matrix,

$$\tilde{b}_{jm}(C)=0,\quad \text{if } j>m, \tag{10}$$

and that $\tilde{f}$ has a well-defined limit for $|x|\to\infty$, $h\to 0$, and $xh=\hbar$ kept fixed. In Appendix B, it is shown that

$$\lim_{|x|\to\infty,h\to 0,xh=\hbar}\tilde{f}(C;x,h)=JJ(C;\hbar), \tag{11}$$

and that, in general, for any $n\geqslant 0$,

$$\lim_{|x|\to\infty,h\to 0,xh=\hbar}\left(x\frac{\partial}{\partial x}\right)^n \widetilde{f}(C;x,h)=\left(\hbar\frac{d}{d\hbar}\right)^n JJ(C;\hbar). \tag{12}$$

III. THE BF THEORY WITH A COSMOLOGICAL TERM

From the field-theoretical point of view, the colored Jones function is defined as the knot invariant obtained from the v.e.v. of a suitable observable, the Wilson loop, in the Chern–Simons theory[9] (actually, the general case of a compact simple Lie group is discussed there).

For the aims of this paper, however, it is more convenient to consider the formulation given in terms of the BF theory with a cosmological term, which is equivalent[3,14] to the previous one.

We will consider here only the case of a single knot C imbedded in S^3 and study its invariants associated to the group SU(2); viz., we consider the SU(2)-principal bundle $P\to S^3$, and define the action

$$\widetilde{S_{\mathrm{BF}}}(\kappa)=\frac{1}{2\pi}\int_{S^3}\mathrm{Tr}\left(B\wedge F+\frac{\kappa^2}{3}B\wedge B\wedge B\right), \tag{13}$$

where F is the curvature two-form of the connection A, B is a form in $\Omega^1(S^3,\mathrm{ad}\,P)$, and the parameter κ is called the *cosmological constant* (this name comes from the quantum-gravity interpretation of (13)[4]).

Then, given a knot C and a base point $x_0\in C$, we consider the observable

$$\Gamma(C,x_0;\kappa):=\mathrm{Hol}_{x_0}(A+\kappa B;C)=\sum_{n=0}^{\infty}\kappa^n\gamma_n(C,x_0), \tag{14}$$

where κ is the same cosmological constant as in (13), $\mathrm{Hol}_{x_0}(A+\kappa B;C)$ denotes the holonomy of the connection $A+\kappa B$ along the knot C with base point x_0, and the γs are functionals of A and B obtained by Taylor expanding the previous holonomy.

Notice that the holonomy of a connection A along a curve C, open or closed, can be written as

$$\mathrm{Hol}(A;C)=P\,\exp\left(\int_C A\right), \tag{15}$$

where P denotes path ordering. Thus, by (14) and (15), the γs turn out to be[3,14] iterated Chen integrals of the form

$$\gamma_n(C,x_0):=\oint_{(C;x_0)}\underbrace{\hat{B}\cdots\hat{B}}_{n\text{ times}}\mathrm{Hol}_{x_0}(A;C), \tag{16}$$

where the iterated integral $\int_a^b\omega_1\cdots\omega_2\cdots\omega_n$ of n one-forms $\{\omega_i\}_{i=1,\ldots,n}$ is given by the formula $\int_{a<x_1<\cdots<x_n<b}\omega_1(x_1)\wedge\omega_2(x_2)\wedge\cdots\wedge\omega_n(x_n)$. The su(2)-valued one-form $\hat{B}$ is defined as

$$\hat{B}(x):=\mathrm{Hol}_{x_0}^{x}B(x)[\mathrm{Hol}_{x_0}^{x}]^{-1}, \tag{17}$$

with the holonomies computed along the portions of the knot C going from the base point x_0 to the running points x.

The observable Γ in (14) is invariant under a gauge transformation of the connection $A-\kappa B$, while, under the gauge transformation

$$A+\kappa B\to g(A+\kappa B)g^{-1}+gdg^{-1}, \tag{18}$$

one has

$$\Gamma(C,x_0;\kappa)\to g(x_0)\Gamma(C,x_0;\kappa)g(x_0)^{-1}. \tag{19}$$

Thus, taking the trace of Γ gives a gauge invariant observable that is, moreover, independent of x_0. The knot invariant given by the v.e.v. of this observable, wrt the (normalized) Gibbs weight $\exp[iS_{\mathrm{BF}}(\kappa)]$, can be recognized by exploiting the relation with the Chern–Simons theory,[3] viz.,

$$J_d(C;h)=\langle \mathrm{Tr}_{(d-1)/2}\Gamma(C,x_0;\kappa)\rangle_{\mathrm{BF},\kappa}, \quad h=4\pi i\kappa, \tag{20}$$

where Tr_s is the trace in the irreducible representation of spin s. In this framework, (2) is an immediate consequence of (A8).

Notice, eventually, that the observable Γ can be decomposed into its even (Γ_0) and odd ($\kappa\Gamma_1$) parts,

$$\Gamma(C,x_0;\kappa)=\Gamma_0(C,x_0;\kappa)+\kappa\Gamma_1(C,x_0;\kappa), \tag{21}$$

and that both of them are good observables for the BF theory with a cosmological term.[14]

A. The BF-theory generating function

The behavior (19) of the observable Γ under a gauge transformation of the connection $A+\kappa B$ shows that all of the traces of powers of Γ are gauge invariant; so we can consider the knot invariants given by their v.e.v.s, or as will be clear in Sec. V, their generating function,

$$E(C;x,h)=\sum_{n=0}^{\infty}\frac{x^n}{n!}\langle \mathrm{Tr}_{1/2}\Gamma(C,x_0;\kappa)^n\rangle_{\mathrm{BF},\kappa}=\langle \mathrm{Tr}_{1/2}\exp[x\Gamma(C,x_0;\kappa)]\rangle_{\mathrm{BF},\kappa},$$

$$h=4\pi i\kappa, \tag{22}$$

with $x\in\mathbb{C}$. We consider only the fundamental representation here, for the discussion in Appendix A shows that considering any other representation does not give further content of information. Notice that the rightmost term in (22) is only formal since no addition is defined in the group. However, this notation usefully reminds us that E has the formal properties of an exponential. Notice that, since Γ is a holonomy, one has

$$\Gamma(C,x_0;\kappa)^n=\Gamma(nC,x_0;\kappa), \tag{23}$$

where by nC we denote the nth cabling of the knot C; thus, $E(C;x,h)$ is the *generating function for cabled knot invariants*. In the framework of the Chern–Simons theory, Γ is replaced by the holonomy of the connection A; thus, E can also be seen as the v.e.v. of *the generating function for cabled Wilson loops*.

By using the formulas in Appendix A, one can show that there is a simple relation with the generating function for colored Jones functions defined in (6). Actually by (A6), one can express $\mathrm{Tr}_{1/2}\Gamma^n$ in terms of the traces of Γ in the representations of spin $n/2$ and $n/2-1$. By (20), it then follows that

$$E(C;x,h)=\sum_{n=0}^{\infty}\frac{x^n}{n!}[J_{n+1}(C;h)-J_{n-1}(C;h)], \tag{24}$$

where, according to (A8), $J_1=1$, $J_0=0$, $J_{-1}=-1$.

By (6) and (24), and also noting that $E(C;0,h)=2$ and $\partial_x f(C;0,h)=J_1(C;h)=1$, one obtains

$$E(C;x,h)=1+\partial_x f(C;x,h)-\int_0^x d\xi\, f(C;\xi,h). \tag{25}$$

IV. THE PURE BF THEORY

The BF theory has the nice property that its limit for vanishing cosmological constant (corresponding to the $k\to\infty$ limit in the Chern–Simons theory) is still represented by a TQFT known as pure BF theory,[2,15] whose action reads

$$S_{\mathrm{BF}}=\frac{1}{2\pi}\int_{S^3}\mathrm{Tr}(B\wedge F). \tag{26}$$

It is immediately seen that S_{BF} is invariant under gauge transformations

$$A\to gAg^{-1}+gdg^{-1},\quad B\to gBg^{-1}, \tag{27}$$

as well as under B-transformations

$$A\to A,\quad B\to B+d_A\psi. \tag{28}$$

Here g is a map from S^3 to the group, while ψ is a form in $\Omega^0(S^3,\mathrm{ad}\,P)$. The action (26) is invariant under (28) owing to the Bianchi identity.

The good observables for the pure BF theory are of course obtained by $\Gamma_0(C,x_0;\kappa)$ and $\Gamma_1(C,x_0;\kappa)$, defined in (21), in the limit $\kappa\to 0$, and are simply given by $\gamma_0(C,x_0)$ and $\gamma_1(C,x_0)$ in (16); viz.,

$$\begin{aligned}\gamma_0(C,x_0)&=\mathrm{Hol}_{x_0}(A;C),\\ \gamma_1(C,x_0)&=\oint_{x\in(C,x_0)}\mathrm{Hol}_{x_0}^{x}B(x)\mathrm{Hol}_{x}^{x_0}.\end{aligned} \tag{29}$$

Under (27) and (28), they transform as

$$\gamma_i(C,x_0)\to g(x_0)\,\gamma_i(C,x_0)g(x_0)^{-1},\quad i=0,1, \tag{30}$$

provided we fix $\psi(x_0)=0$, which can always be done.[1]

Thus, we are led to consider the v.e.v.s of $\mathrm{Tr}_d\,\gamma_0$ and $\mathrm{Tr}_d\,\gamma_1$. They, however, are rather trivial, for they correspond, respectively, to $J_d(C;0)=d$ and $(d/dh)J_d(C;0)=0$.

From a field-theoretical point of view, the reason of this triviality is the following: In perturbative BF theory (on S^3), nonvanishing v.e.v.s contain a number n_A of fields A not exceeding the number n_B of fields B.[1] Therefore, after expanding the holonomies in (29) in powers of A, one sees that only the zeroth-order term $\mathrm{Tr}_{(d-1)/2}I=d$ (where I is the group identity) survives in the v.e.v. of $\mathrm{Tr}_{(d-1)/2}\gamma_0$; while, in the v.e.v. of $\mathrm{Tr}_{(d-1)/2}\gamma_1$, only the first-order term does [the zeroth-order term vanishing because it is the trace of an element of su(2)]. However, the latter v.e.v. (of the form $\langle\oint_C A\oint_C B\rangle_{\mathrm{BF},0}$) gives the self-linking number of the knot C that, by the hypothesis of standard framing, is zero. (If one uses a more general framing, the self-linking number is the only information one gets from these v.e.v.s.)

This is the reason why in Ref. 1 one looked for composite observables that contain a higher number n_B of fields B, and are invariant under (27) and (28). In particular, the generating function of the v.e.v.s of $\mathrm{Tr}_{(d-1)/2}(\gamma_1)^n$ was taken into account,

$$W_d(C;\lambda):=\sum_{n=0}^{\infty}\frac{\lambda^n}{n!}\langle \mathrm{Tr}_{(d-1)/2}\gamma_1(C,x_0)^n\rangle_{\mathrm{BF},0}=\langle \mathrm{Tr}_{(d-1)/2}\exp[\lambda\gamma_1(C,x_0)]\rangle_{\mathrm{BF},0}, \tag{31}$$

with $\lambda\in\mathbb{C}$. Again, as in (22), the rightmost term is only formal.

In Sec. V, we shall need (31) to study the limit $\kappa\to 0$ in (22), to which (31) is apparently related. However, there is a second, perhaps more natural, generating function to be considered, viz.,

$$\widetilde{W}_d(C;\lambda):=\langle \mathrm{Tr}_{(d-1)/2}\exp[\lambda\beta(C,x_0)]\rangle_{\mathrm{BF},0}, \tag{32}$$

where

$$\beta(C,x_0):=\gamma_1(C,x_0)\cdot\gamma_0(C,x_0)^{-1}=\oint_{C,x_0}\hat{B}\in\mathrm{su}(2). \tag{33}$$

Notice that the exponential in (32) is not formal, but it actually represents the exponential map from the algebra to the group.

The generating function $\widetilde{W}$ is particularly useful because it allows us to understand the meaning of the knot invariants related to higher-dimensional representations; indeed, by using (A7), one can easily prove that

$$\widetilde{W}_{2k}(C;\lambda)=\sum_{l=1}^{k}\widetilde{W}_2(C;(2l-1)\lambda), \tag{34}$$

$$\widetilde{W}_{2k+1}(C;\lambda)=1+\sum_{l=1}^{k}\widetilde{W}_2(C;2l\lambda). \tag{35}$$

Then, a formal resummation of the geometric sums appearing in (34) and (35) gives

$$\widetilde{W}_d(C;\lambda)=\begin{cases}\left\langle \mathrm{Tr}_{1/2}\dfrac{\exp[(d+1)\lambda\beta(C,x_0)]-1}{\exp[2\lambda\beta(C,x_0)]-1}\right\rangle_{\mathrm{BF},0} & \text{if } d \text{ is even,}\\ \left\langle \mathrm{Tr}_{1/2}\dfrac{\exp[(d+1)\lambda\beta(C,x_0)]-1}{\exp[2\lambda\beta(C,x_0)]-1}\right\rangle_{\mathrm{BF},0}+1 & \text{if } d \text{ is odd.}\end{cases} \tag{36}$$

These formulas show that the limit

$$\widetilde{WW}(C;\mu):=\lim_{d\to\infty,\lambda\to 0,d\lambda=\mu}\frac{\widetilde{W}_d(C;\lambda)}{d} \tag{37}$$

is well defined, and that

$$\widetilde{WW}(C;\mu)=\left\langle \mathrm{Tr}_{1/2}\frac{\exp[\mu\beta(C,x_0)]-1}{2\mu\beta(C,x_0)}\right\rangle_{\mathrm{BF},0}=\sum_{n=0}^{\infty}\frac{1}{2(n+1)!}\langle \mathrm{Tr}_{1/2}[\mu\beta(C,x_0)]^n\rangle_{\mathrm{BF},0}. \tag{38}$$

Thus, by (32) and (38), we obtain

$$\widetilde{W}_2(C;\lambda)=2\frac{d}{d\lambda}[\lambda\widetilde{WW}(C;\lambda)], \tag{39}$$

or equivalently,

$$\widetilde{WW}(C;\mu)=\frac{1}{\mu}\int_0^{\mu/2} dx\ \widetilde{W}_2(C;2x). \tag{40}$$

Notice that (34) and (35) are actually discretizations of the Riemann integral in (40) with $x=l\lambda$.

A more rigorous proof of the above results can be obtained by expanding $\widetilde{W}_2$ in powers of λ and using (34) and (35) to get the corresponding expansion of $\widetilde{W}_d$. Then one can use the asymptotic formula

$$\sum_{l=1}^{k} l^n \overset{k\to\infty}{\sim} \frac{k^{n+1}}{n+1}$$

to get the rightmost term in (38).

So far we have considered two different generating functions, viz., (31) and (32): in general, however, there are even more choices. Indeed, because of (30), a product of powers of γ_0 and γ_1 (in any order) is still an observable whose trace is invariant under (27) and (28).

To get rid of this arbitrariness in the definition of the generating function, we need the following.

Theorem 1: In pure BF theory, the knot invariant obtained by the v.e.v. of the trace of a function of $\gamma_0(C,x_0)$ and $\gamma_1(C,x_0)$ is equal to the knot invariant obtained by replacing $\gamma_0(C,x_0)$ with the identity of the group, *provided the standard framing is chosen.*

In Ref. 14, a proof of the theorem based on an explicit study of the Feynman integrals appearing in the evaluations of the v.e.v.s was given. Here, however, we give a simpler argument, based on the formal properties of the pure BF theory.

First of all we recall that, in the explicit evaluation of the v.e.v.s in BF theory, the choice of framing is done by evaluating all the holonomies in (29) on a companion knot C' obtained by C in terms of a "small," nonvanishing normal displacement.[1] Notice that the self-linking number of C is then, by definition, the linking number of C and C'.

The proof of the theorem, then, essentially relies on the fact that, if this linking number vanishes (standard framing), one can deform C' in γ_0 in such a way that it can be completely unlinked from C and, as such, shrunk to a point; so its holonomy, γ_0, becomes the identity.

This is possible since a knot C' appearing in γ_0 (not necessarily a framing for C) "does not see itself." In fact, a small deformation of the knot C' at a certain point x amounts to introducing curvature terms in x (remember that γ_0 is a holonomy). However, in pure BF theory, the curvature vanishes everywhere but on the knot C, along which γ_1 is evaluated. (We refer to Ref. 1 for the proof that, in an observable, A acts as a source for $d_A B$, while B acts as a source for the curvature F.) Therefore, C' can be deformed freely as far as this deformation does not intersect C; self-intersections of C' are allowed, however.

When such a self-intersection occurs, one can split C' into two closed curves C'_1 and C'_2; correspondingly, the holonomy $\gamma_0(C')$ can be written as $\gamma_0(C'_1)\cdot\gamma_0(C'_2)$,

To prove the theorem, one just has to repeat this procedure until C' is replaced by a collection of circles C'_1, all of which surround one single strand of C. Then one moves the C'_1s along C, and cuts and splices them together again to form a circle C''.

Since all these deformations do not affect the linking between C and C', the linking number of C and C'' is the same as the linking number of C and C'. If this linking number vanishes (standard framing), then the circle C'' and the knot C are unlinked, and C'' can be shrunk to a point. This concludes the proof of Theorem 1.

As a consequence of Theorem 1, we have the following.

Corollary 1: $W_d(C;\lambda)$ is the most general v.e.v. one can consider in pure BF theory if the standard framing is chosen.

Moreover, we can freely switch from W_d in (31) and $\widetilde{W}_d$ in (32). Thus, by (34) and (35), the higher-representation knot invariants W_d can be related to the fundamental-representation knot invariant W_2; besides, the limit

$$WW(C;\mu):=\lim_{d\to\infty,\lambda\to 0,d\lambda=\mu}\frac{W_d(C;\lambda)}{d}, \tag{41}$$

is well defined and, by (39),

$$W_2(C;\lambda)=2\frac{d}{d\lambda}[\lambda WW(C;\lambda)]. \tag{42}$$

We conclude this section with an important remark. Pure BF theory is known to be exact in saddle-point approximation[16] as far as the partition function is concerned. This result is a simple consequence of the fact that one can arbitrarily change the "Planck constant" in front of the action by simply rescaling the field B. Since the partition function (or the v.e.v. of an observable not containing B) is not affected by this rescaling, one can send the Planck constant to zero.

This, of course, cannot be done when one computes the v.e.v. of an observable containing B, as in (31) or (32). In this case one sees that the parameter λ actually plays the role of the Planck constant, and, of course, W_d is not independent of λ.

Notice, however, that WW corresponds to the limit $\lambda\to 0$, so it should be possible to compute it by using the saddle-point approximation. Then, by (42), it is possible to recover W_2—and hence, by (34) and (35), all the W_d's—from WW.

Thus, even if pure BF theory with B-dependent observables is *not* exact in saddle-point approximation, the saddle-point approximation turns out to be all that one needs.

V. TURNING OFF THE COSMOLOGICAL CONSTANT

In this section we want to show that, in the limit of vanishing cosmological constant, the BF-theory generating function (22) is related to both the pure-BF-theory generating function (31) and the Melvin–Morton function (4).

To establish the former relation, we first observe that, in order for the significant observable γ_1 to survive in the limit $\kappa\to 0$, we have to send $|x|\to\infty$ at the same time with the prescription that $x\kappa=\lambda$ be finite. If we work with the standard framing, by Theorem 1 the observable γ_0 can be replaced by the identity of the group; so (22) diverges as e^x; thus, we are led to consider

$$\widetilde{E}(C;x,h):=e^{-x}E(C;x,h). \tag{43}$$

By using the exponential representation of (22), we can write

$$\widetilde{E}(C;x,h)=\langle \mathrm{Tr}_{1/2}\exp\{x[\kappa\gamma_1(C,x_0)+O(\kappa^2)]\}\rangle_{\mathrm{BF},\kappa}$$

and get

$$\lim_{|x|\to\infty,h\to 0,xh=\hbar}\widetilde{E}(C;x,h)=W_2(C;\lambda),\quad \hbar=4\pi i\lambda. \tag{44}$$

In Appendix C, we give a more careful proof of (44).

Notice that the limit in (44) holds irrespectively of how x is sent to infinity in the complex plane. Therefore, if one sees $\widetilde{E}$ as a meromorphic function of x and $\hbar$, this implies that the regular part in x of $\widetilde{E}$ vanishes. Thus, $\widetilde{E}$, now rewritten in terms of x and h, does not contain more powers of x than of h. In other words, if $\widetilde{E}$ is expanded as a rational power series,

$$\tilde{E}(C;x,h)=\sum_{l,m=0}^{\infty}\epsilon_{lm}(C)x^l h^m, \tag{45}$$

then $\epsilon_{\cdot\cdot}$ is an upper triangular matrix,

$$\epsilon_{jm}(C)=0, \quad \text{if } j>m. \tag{46}$$

The relation between the BF-theory generating function and the Melvin–Morton function is obtained by exploiting (25) (see Appendix D for details). We arrive to the following conclusions:

$$\epsilon_{\cdot\cdot} \text{ uppper triangular} \Leftrightarrow b_{\cdot\cdot} \text{ upper triangular}, \tag{47}$$

and

$$\epsilon_{nn}(C)=2(1+n)b_{nn}(C), \tag{48}$$

where $\epsilon_{\cdot\cdot}$ and $b_{\cdot\cdot}$ are defined, respectively, in (45) and (1). Notice that (47) and (46) give a new proof of (3).

Since E is related to W_2 and to JJ in the same limit $\kappa\to 0$, we deduce that a relation exists between W_2 and JJ. Actually, by (1), (44), (45), and (48), we obtain

$$W_2(C;\lambda)=2\frac{d}{d\hbar}[\hbar JJ(C;\hbar)], \quad \hbar=4\pi i\lambda. \tag{49}$$

In order to recognize the knot invariant given by W_2, we can now resort to (5) and obtain

$$W_2(C;\lambda)=2\left[1+\left(\frac{z}{2}\right)^2\right]^{1/2}\frac{d}{dz}\frac{z}{\Delta(C;z)}, \quad z=2i\,\sin(2\pi\lambda), \tag{50}$$

and, in particular,

$$W_2(\bigcirc;\lambda)=2\left[1+\left(\frac{z}{2}\right)^2\right]^{1/2}, \quad z=2i\,\sin(2\pi\lambda), \tag{51}$$

where $\bigcirc$ is the unknot and we have chosen the normalization $\Delta(\bigcirc;z)=1$ (cfr. Sec. II). Thus, the normalized knot invariant

$$\langle C\rangle_2(\lambda):=\frac{W_2(C;\lambda)}{W_2(\bigcirc;\lambda)}, \tag{52}$$

defined in Ref. 1, satisfies

$$\langle C\rangle_2(\lambda)=\frac{d}{dz}\frac{z}{\Delta(C;z)}, \quad z=2i\,\sin(2\pi\lambda). \tag{53}$$

In conclusion, we have shown that W_2 is related to the first derivative of the inverse of the Alexander–Conway polynomial. By (34) and (35), W_d is given by a finite sum of W_2s, evaluated at different λs. Concerning the limit $d\to\infty$, we see that (42) and (49), together with the property $WW(C;0)=JJ(C;0)=1$, imply

$$WW(C;\lambda)=JJ(C;\hbar), \quad \hbar=4\pi i\lambda, \tag{54}$$

or, because of (5),

$$4\pi i\lambda WW(C;\lambda)=\frac{z}{\Delta(C;z)},\quad z=2i\,\sin(2\pi\lambda). \tag{55}$$

The above results, together with Corollary 1, prove the following.

Theorem 2: The set of the unframed knot invariants that can be obtained from the SU(2)-BF theory coincides with the set of the coefficients of (the inverse of) the Alexander–Conway polynomial.

In Ref. 1, the authors conjectured a relation between the Alexander–Conway polynomials and the pure BF theory based on second-order calculations in the perturbative expansion. Theorem 2 supersedes this conjecture and provides the correct relation.

VI. THE PERTURBATIVE EXPANSION OF W_d

In this section we want to compare the results we have proved in Sec. V with those obtained in Ref. 1 in the framework of "perturbative" BF theory.

By "perturbative" evaluation of (31), one means an expansion of $W_d(C;\lambda)$ (or of its generalization $W_{G,R}(C;\lambda)$, where G is a compact group and R a representation) in powers of λ,

$$W_{G,R}(C;\lambda)=\sum_{n=0}^{\infty} w_n(G,R;C)\lambda^n, \tag{56}$$

where the knot invariants $w_n(G,R;C)$ (actually, they are Vassiliev invariants[17]) are computed in terms of Feynman integrals.

The first property of the expansion (56) shown in Ref. 1 is that, owing to a symmetry of the corresponding Feynman integrals, odd-order terms vanish,

$$w_{2n+1}(G,R;C)=0. \tag{57}$$

Thus, W is an even function:

$$W_{G,R}(C;-\lambda)=W_{G,R}(C;\lambda). \tag{58}$$

In the case $G=\mathrm{SU}(2)$, by using (50), (34), and (35), we see that (58) is in accordance with the fact that the Alexander-Conway polynomial $\Delta(C;z)$—for a single knot C—is an even function of z.

A further computation done in Ref. 1, for the case $G=\mathrm{SU}(N)$, showed that, up to the second order, (56) reads

$$W_{G,R}(C;\lambda)=\dim R[1+(4\pi\lambda)^2c_2(R)c_v\rho(C)+O(\lambda^4)]. \tag{59}$$

where

(i) $\dim R$ and $c_2(R)$ are, respectively, the dimension and the quadratic Casimir of the representation R;
(ii) $c_v=N$ is the quadratic Casimir of the adjoint representation; and
(iii) $\rho(C)$ is the knot invariant studied in Refs. 18 and 19 in the framework of the Chern–Simons theory.

In Refs. 18 and 19, $\rho(C)$ was proved to be related to the second coefficient of the Alexander–Conway polynomial; viz., if one writes

$$\Delta(C;z)=\sum_{n=0}^{\infty} a_n(C)z^n,\quad a_0(C)=1,\quad a_1(C)=0 \tag{60}$$

(where only a finite number of coefficients are nonvanishing), then

$$\rho(C)=2a_2(C)+\rho(\bigcirc). \tag{61}$$

Moreover, a direct computation[18] shows that

$$\rho(\bigcirc)=-\tfrac{1}{12}. \tag{62}$$

Thus, one can write (59) as

$$W_{G,R}(C;\lambda)=\dim R\left[1+(4\pi\lambda)^2 2c_2(R)c_v\left(a_2(C)-\frac{1}{24}\right)+O(\lambda^4)\right]. \tag{63}$$

If we now expand (50) as

$$W_2(C;\lambda)=2[1+\tfrac{1}{8}z^2+O(z^4)][1-3a_2(C)z^2+O(z^4)]=2[1+3z^2(\tfrac{1}{24}-a_2(C))+O(z^4)],$$

$$z=4\pi i\lambda+O(\lambda^2),$$

we get a complete agreement with (63) in the case where $G=\mathrm{SU}(2)$ and the fundamental representation, R_2, is chosen; for, in this case, $c_v=2$ and $c_2(R_2)=\frac{3}{4}$.

We can also compare the second-order expansion of (34) and (35) with (63) in the case where $G=\mathrm{SU}(2)$ and R_d is the irreducible representation of dimension d. This is done by noticing that one can compute the sums appearing in (34) and (35) as

$$\sum_{l=1}^{k}(2l-1)^2=\frac{1}{3}k(4k^2-1), \quad \sum_{l=1}^{k}l^2=\frac{2}{3}k(k+1)(2k+1).$$

Thus, one achieves complete agreement with (63) since

$$c_2(R_{2k})=\frac{(2k-1)(2k+1)}{4}, \tag{64}$$

$$c_2(R_{2k+1})=k(k+1). \tag{65}$$

By using (34) and (35), it is possible to see that—in agreement with the perturbative result of Ref. 1—the coefficients w_n in (56) are given by the product of a function depending only on the representation and a function depending only on the knot, viz.,

$$w_{2n}(\mathrm{SU}(2),R_d;C)=dg_{2n}(d)v_{2n}(C). \tag{66}$$

If we normalize $g_{2n}(2)=\frac{1}{2}$, then, by (34) and (35), we get an explicit formula for the gs:

$$g_{2n}(2k)=\frac{1}{2k}\sum_{l=1}^{k}(2l-1)^{2n}, \tag{67}$$

$$g_{2n}(2k+1)=\frac{1}{2k+1}\sum_{l=1}^{k}(2l)^{2n}. \tag{68}$$

By (64) and (65), we can also express the gs in terms of the quadratic Casimirs:

$$g_0=\tfrac{1}{2},\quad g_2=\tfrac{1}{3}c_2c_v,$$

$$g_4=\tfrac{1}{15}[6(c_2c_v)^2-c_2c_v^3],\quad g_6=\tfrac{1}{21}[12(c_2c_v)^3-6c_2^2c_v^4+c_2c_v^5], \tag{69}$$

$$\dots.$$

In general, the highest power of c_2 in g_{2n} is n.

In Ref. 1, it was conjectured that the *only* group factor to appear in g_{2n} was $(c_2c_v)^n$. From this conjecture, together with some field-theoretical arguments, it was concluded that, for some t,

$$\frac{W_{G,R}(C,\lambda)}{W_{G,R}(\bigcirc,\lambda)}=[\Delta(C;z)]^t,\quad z\propto\sqrt{c_2(R)c_v}\lambda+O(\lambda^3). \tag{70}$$

By (69), we see that the conjecture is wrong; by (49), we see that so is the conclusion (70).

It is, however, interesting to show that, if we retain only the terms $(c_2c_v)^n$ in (69), then the corresponding knot invariant is actually the (-1)-power of the Alexander–Conway polynomial. More precisely, we define the "truncated" coefficients

$$g_{2n}^{(\mathrm{tr})}(d)=[c_2(R_d)c_v]^n\gamma_{2n} \tag{71}$$

as the coefficients obtained by neglecting lower powers of $c_2(R_d)$ in (69), and the "truncated" knot invariant as

$$W_d^{(\mathrm{tr})}(C;\lambda):=\sum_{n=0}^{\infty} d\,g_{2n}^{(\mathrm{tr})}(d)v_{2n}(C)\lambda^{2n}. \tag{72}$$

Since $c_v=2$ and $c_2(R_d)\sim d^2/4$ as $d\to\infty$, the truncated coefficients $g_{2n}^{(\mathrm{tr})}(d)$ are the leading terms of the true coefficients $g_{2n}(d)$; thus, by (41) and (71),

$$WW(C;\lambda)=\sum_{n=0}^{\infty}\frac{\gamma_{2n}}{2^n}v_{2n}(C)\lambda^{2n}. \tag{73}$$

By comparing (73) with (72), we eventually get

$$W_d^{(\mathrm{tr})}(C;\lambda)=dWW(C;\sqrt{2c_2(R_d)c_v}\lambda); \tag{74}$$

thus, by (55), we see that

$$\frac{W_d^{(\mathrm{tr})}(C;\lambda)}{W_d^{(\mathrm{tr})}(\bigcirc;\lambda)}=\frac{1}{\Delta(C;z)},\quad z=2i\,\sin(2\pi\sqrt{2c_2(R_d)c_v}\lambda). \tag{75}$$

Thus, if the truncated knot invariants are used, (70) holds.

VII. CONCLUSIONS

In this paper we have discussed the unframed knot invariants coming from BF theories. Even if most of our results hold only for SU(2), we point out that Theorem 1 and Corollary 1, as well as the computation in Appendix C (with a slight abuse of notation), hold in general.

It would be interesting to generalize some of the other results to different groups and to consider links as well. However, the present case, i.e., knot observables in the theory based on SU(2), seems to be interesting enough to deserve further investigation.

Indeed, as we have noticed at the end of Sec. IV, it turns out that a saddle-point computation is enough to completely describe the pure BF theory. We defer to a forthcoming paper the related functional-integral computation.

Notice that this property of pure BF theory sets it at the boundary between TQFTs of Witten's and Schwarz's type: The former are twisted supersymmetric gauge theories (see, e.g., Ref. 20), whose main property—an effect of the twisted supersymmetry—is their independence of both the metric and the coupling constant, which makes them topological as well as exact in saddle-point approximation. The latter are topological gauge theories, as the Chern—Simons or the BF theories, whose dependence on the coupling constant is unavoidable. The pure BF theory formally belongs to the latter type, but, as the theories of the former type, is completely determined by its weak-coupling limit.

Moreover, as we have proved in Sec. V, the pure BF theory corresponds to the first diagonal in the (h,d) expansion of the colored Jones function. A description of the upper diagonals is still missing (see Ref. 21 for a first attempt); so it is natural to look for generalizations of the pure BF theory, i.e., for further variations of the Chern–Simons theory, that could correspond to these upper diagonals and, possibly, give them a better understanding (see Ref. 13 for a different approach). We are investigating along these lines.

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APPENDIX A: SOME USEFUL IDENTITIES FOR THE CHARACTERS OF SU(2)

In this section we recall some properties of the group SU(2) that are necessary for this paper. In particular, we are interested in an identity relating $\mathrm{Tr}_{1/2}\, g^n$ to the traces of g in other representations, or, in other words, we want to give $\mathrm{Tr}_{1/2}\, g^n$ an expression in primitive characters,

$$\mathrm{Tr}_{1/2} g^n = \sum_{k=0}^{\infty} \phi_{nk} \chi_{k/2}(g), \tag{A1}$$

where

$$\chi_s(g) := \mathrm{Tr}_s g, \quad 2s \in \mathbf{Z}. \tag{A2}$$

Owing to the Peter–Weil Theorem, this can be done since $\mathrm{Tr}_{1/2}\, g^n$ depends only on the conjugacy class of g and belongs to $L^2(\mathrm{SU}(2),\mathbf{C})$. By a conjugacy transformation, one can always write g as

$$g = h e^{i\alpha R_3} h^{\dagger}, \tag{A3}$$

where R_3 is the (Hermitean) generator of the Cartan subalgebra. Noticing that the spectrum of R_3 in the representation of spin l is given by $\{-2l,-2(l-1),\ldots,2(l-1),2l\}$, one obtains

$$\mathrm{Tr}_{1/2} g^n = e^{in\alpha} + e^{-in\alpha}, \tag{A4}$$

and

$$\mathrm{Tr}_l\, g = e^{2il\alpha} + e^{2i(l-1)\alpha} + \cdots + e^{-2il\alpha} = \sum_{m=-l}^{l} e^{2im\alpha}, \tag{A5}$$

where the last sum is meant to be over integers or half-integers according to the fact that l is integer or half-integer. By (A4) and (A5), it immediately follows that, for $n \geqslant 2$,

$$\mathrm{Tr}_{1/2}\, g^n = \mathrm{Tr}_{n/2} g - \mathrm{Tr}_{n/2-1} g, \quad n \in \mathbf{Z}. \tag{A6}$$

By induction one can also prove that

$$\mathrm{Tr}_s\, g = \begin{cases} \sum_{l=1}^{s+1/2} \mathrm{Tr}_{1/2} g^{2l-1} & \text{if } s \text{ is half-integer,} \\ 1 + \sum_{l=1}^{s} \mathrm{Tr}_{1/2}\, g^{2l} & \text{if } s \text{ is integer.} \end{cases} \tag{A7}$$

Moreover, by (A7) and by the fact that

$$\mathrm{Tr}_{1/2} \exp(i\mathbf{a}\cdot\mathbf{R}) = 2\cos a,$$

with $\mathbf{a} \in \mathbb{R}^3$ and $\mathbf{R} = (R^1, R^2, R^3)$ the Pauli matrices, one also obtains

$$\mathrm{Tr}_s \exp(i\mathbf{a}\cdot\mathbf{R}) = \frac{\sin(da)}{\sin(a)}, \tag{A8}$$

where $d = 2s+1$ is the dimension of the representation of spin s.

Since, for a given g, $\mathrm{Tr}_{n/2} g$ is a map defined on the positive integers, its analytic continuation over the whole complex plane is uniquely defined and is actually given by (A8).

APPENDIX B: PROPERTIES OF THE GENERATING FUNCTION FOR COLORED JONES FUNCTIONS

In this section we explore the properties of the generating function for colored Jones functions defined in (6). By (1), we can write

$$f(C;x,h) = \sum_{d=1}^{\infty} \frac{x^d}{d!}\, d \sum_{j,m=0}^{\infty} b_{jm}(C)(d-1)^j h^m = x \sum_{j,m=0}^{\infty} B_j(x) b_{jm}(C) h^m, \tag{B1}$$

where

$$B_j(x) = \sum_{d=0}^{\infty} \frac{x^d}{d!}\, d^j = \left(\frac{\partial^j}{\partial \alpha^j}\right)\Bigg|_{\alpha=\log x} \sum_{d=0}^{\infty} \frac{e^{\alpha d}}{d!} = \left(\frac{\partial^j}{\partial \alpha^j}\right)\Bigg|_{\alpha=\log x} \exp(e^{\alpha}). \tag{B2}$$

By repeatedly applying Leibniz's rule, we obtain

$$B_j(x) = e^x P_j(x) = e^x [x^j + O(x^{j-1})], \tag{B3}$$

where $P_j(x)$ is a polynomial of degree j starting with x^j, viz.,

$$P_j(x) = \sum_{l=0}^{j} x^l c_{lj}, \quad c_{jj} = 1. \tag{B4}$$

Notice that (B4) implies that $c_{..}$ is an upper triangular matrix:

$$c_{lj}(C) = 0, \quad \text{if } l > j. \tag{B5}$$

The coefficients c_{lj} can easily be computed if we consider the following generating function,

$$B(\rho,x):=\sum_{j=0}^{\infty}\frac{\rho^j}{j!}B_j(x), \tag{B6}$$

which, by (B2), can be written as

$$B(\rho,x)=\exp e^{(\alpha+\rho)}|_{\alpha=\log x}=e^x\exp[x(e^\rho-1)]. \tag{B7}$$

Thus, by (B3), we obtain

$$P(\rho,x):=\sum_{j=0}^{\infty}\frac{\rho^j}{j!}P_j(x)=\sum_{n=0}^{\infty}\frac{x^n}{n!}(e^\rho-1)^n, \tag{B8}$$

while, by (B4), we have

$$P(\rho,x)=\sum_{n,j=0}^{\infty}x^n c_{nj}\frac{\rho^j}{j!}. \tag{B9}$$

By comparing the two different expansions of P in powers of ρ given by (B8) and (B9), we obtain eventually

$$c_{nj}=\frac{(-1)^n}{n!}\sum_{l=0}^{n}\binom{n}{l}(-1)^l l^j, \tag{B10}$$

where, by convention, $0^0=1$.

We want now to compute the coefficients $\tilde{b}_{\cdot\cdot}$ defined in (8). By (7), (B1), and (B3), we can write

$$\tilde{f}(C;x,h)=\sum_{j,m=0}^{\infty}P_j(x)b_{jm}(C)h^m; \tag{B11}$$

so by (8),

$$\tilde{b}_{nm}(C)=\sum_{j=0}^{\infty}c_{nj}b_{jm}(C). \tag{B12}$$

Since the matrices $\tilde{b}_{\cdot\cdot}$ and $b_{\cdot\cdot}$ are related by the matrix $c_{\cdot\cdot}$ that, by (B5), is upper triangular, we conclude that (9) holds. Moreover, if one knows that either $\tilde{b}_{\cdot\cdot}$ or $b_{\cdot\cdot}$ is upper triangular—and by (3) we know that this is true for the latter—then one has

$$\tilde{b}_{mm}(C)=b_{mm}(C). \tag{B13}$$

This implies that, in the limit considered in (11), we can write

$$\tilde{f}(C;x,h)=\sum_{m=0}^{\infty}\tilde{b}_{mm}(C)\hbar^m+O\left(\frac{\hbar}{x}\right)=\sum_{m=0}^{\infty}b_{mm}(C)\hbar^m+O\left(\frac{\hbar}{x}\right);$$

so by (4), (11) holds. In order to prove (12), we only have to notice that the operator $(x\partial/\partial x)^n$, when applied to x^j simply produces a factor j^n; so

$$\left(x\frac{\partial}{\partial x}\right)^n\tilde{f}(C;x,h)=\sum_{m=0}^{\infty}m^n\tilde{b}_{mm}(C)\hbar^m+O\left(\frac{\hbar}{x}\right)=\sum_{m=0}^{\infty}m^n b_{mm}(C)\hbar^m+O\left(\frac{\hbar}{x}\right).$$

By comparison with the effect of the operator $(\hbar d/d\hbar)^n$ on (4), we obtain (12).

APPENDIX C: FROM E TO W_2 AS $\kappa\to 0$

In this section we want to clarify the limit in (44). By (43), (22), and (14), we have

$$\widetilde{E}(C;x,h)=e^{-x}\sum_{n=0}^{\infty}\frac{x^n}{n!}\langle \mathrm{Tr}_{1/2}[\gamma_0(C,x_0)+\kappa\gamma_1(C,x_0)+O(\kappa^2)]^n\rangle_{\mathrm{BF},\kappa}, \tag{C1}$$

where $h=4\pi i\kappa$.

In Refs. 3 and 14, it is shown that, in an observable, the field B represents a source for $F+\kappa^2 B\wedge B$, while the field A is a source only for $d_A B$. Since a variation in the framing (i.e., the companion knot along which we integrate the field A) is still given by inserting a curvature term, we can repeat the steps of the proof of Theorem 1 and show that, if the standard framing is chosen, Γ_0 can be replaced by $I+O(\kappa^2)$, where I is the group identity. As a consequence, (C1) now reads

$$\widetilde{E}(C;x,h)=e^{-x}\sum_{n=0}^{\infty}\frac{x^n}{n!}\langle \mathrm{Tr}_{1/2}[I+\kappa\gamma_1(C,x_0)+O(\kappa^2)]^n\rangle_{\mathrm{BF},\kappa} \tag{C2}$$

By using Newton's binomial formula, one can easily prove that (C2) can also be written as

$$\widetilde{E}(C;x,h)=\sum_{n=0}^{\infty}\frac{x^n}{n!}\langle \mathrm{Tr}_{1/2}[\kappa\gamma_1(C,x_0)-O(\kappa^2)]^n\rangle_{\mathrm{BF},\kappa},$$

or, setting $\lambda=x\kappa$,

$$\widetilde{E}(C;x,h)=\sum_{n=0}^{\infty}\frac{\lambda^n}{n!}\langle \mathrm{Tr}_{1/2}[\gamma_1(C,x_0)+O(\kappa)]^n\rangle_{\mathrm{BF},\kappa}. \tag{C3}$$

Now, sending $\kappa\to 0$, with λ fixed, gives (44).

APPENDIX D: FROM E TO JJ AS $h\to 0$

In this section we consider the relation between the BF-theory generating function E and the Melvin–Morton function as the expansion parameter h is sent to zero.

The starting point is relation (25), which, by (7), can be rewritten in terms of $\widetilde{f}$. Actually, the second term on the rhs of (25) is easily seen to be

$$\partial_x f(C;x,h)=e^x(x+1)\widetilde{f}(C;x,h)+e^x x\partial_x\widetilde{f}(C;x,h), \tag{D1}$$

while the computation of the last term requires more work. First of all, it is useful to introduce the following notation:

$$I_n[g](x)=\int_0^x d\xi\, e^{\xi}g^{(n)}(\xi), \tag{D2}$$

where g is a generic analytic function and $g^{(n)}$ its nth derivative. By integrating by parts, one can prove the recursion rule

$$I_n[g](x)=e^x g^{(n)}(x)-g^{(n)}(0)-I_{n+1}[g](x), \tag{D3}$$

which implies that

$$I_0[g](x)=e^x\sum_{n=0}^{\infty}(-1)^n g^{(n)}(x)-\sum_{n=0}^{\infty}(-1)^n g^{(n)}(0). \tag{D4}$$

Now we set

$$g(x)=x\tilde{f}(C;x,h) \tag{D5}$$

(where C and h are supposed to be fixed), and note that, accordingly,

$$g^{(n)}(x)=n\partial_x^{n-1}\tilde{f}(C;x,h)+x\partial_x^n\tilde{f}(C;x,h). \tag{D6}$$

Then we use (D4) to compute the last term in (25) as

$$\int_0^x d\xi f(C;\xi,h)=e^x[(x-1)\tilde{f}(C;x,h)-x\partial_x\tilde{f}(C;x,h)+R(C;x,h)]+c(C;h), \tag{D7}$$

where

$$R(C;x,h)=\sum_{n=2}^{\infty}(-1)^n[n\partial_x^{n-1}\tilde{f}(C;x,h)+x\partial_x^n\tilde{f}(C;x,h)] \tag{D8}$$

and

$$c(C;h)=\sum_{n=0}^{\infty}(-1)^n(n+1)\partial_x^n\tilde{f}(C;0,h). \tag{D9}$$

Therefore, by (43), (25), (D1), and (D7), we obtain

$$\tilde{E}(C;x,h)=2[\tilde{f}(C;x,h)+x\partial_x\tilde{f}(C;x,h)]+R(C;x,h)+e^{-x}[1-c(C;h)]. \tag{D10}$$

We defer to the end of this section the proof that $c(C;h)=1$, cf. (D23); as a consequence of this fact, (D10) actually reads

$$\tilde{E}(C;x,h)=2[\tilde{f}(C;x,h)+x\partial_x\tilde{f}(C;x,h)]+R(C;x,h). \tag{D11}$$

Now we want to reexpress (D11) as a relation between the coefficients of the power series expansions of $\tilde{E}$ and $\tilde{f}$. Indeed, by (8), the terms in square brackets in (D11) can be written as

$$\sum_{n,l=0}^{\infty}(1+l)\tilde{b}_{lm}(C)x^l h^m,$$

while

$$R(C;x,h)=\sum_{n=2}^{\infty}\sum_{l,m=0}^{\infty}(-1)^n\frac{(n+l)!}{l!}\tilde{b}_{l+n-1,m}(C)x^l h^m. \tag{D12}$$

Therefore, by (45), we get eventually

$$\epsilon_{lm}(C)=\sum_{j=0}^{\infty}n_{lj}\tilde{b}_{jm}(C), \tag{D13}$$

with

$$n_{lj}=2(1-l)\delta_{lj}+\sum_{n=2}^{\infty}(-1)^n\frac{(n+l)!}{l!}\delta_{l+n-1,j} \tag{D14}$$

($\delta_{\cdot\cdot}$ being the Kronecker delta). Since $\eta_{\cdot\cdot}$ is an upper triangular matrix, by (D13) we have that

$$\epsilon_{\cdot\cdot}\text{ upper triangular}\Leftrightarrow\tilde{b}_{\cdot\cdot}\text{ upper triangular.} \tag{D15}$$

Finally, by (9), we conclude that (47) holds. Moreover, (D14) and (B13) imply (48).

We conclude this section by showing that the function $c(C;h)$, defined in (D9), is a constant equal to one.

We start by considering the expansion of c in powers of h. By (8), we obtain

$$c(C;h)=\sum_{n,m=0}^{\infty}(-1)^n(n+1)!\tilde{b}_{nm}(C)h^m=\sum_{j,m=0}^{\infty}D_jb_{jm}(C)h^m, \tag{D16}$$

where, by (B12),

$$D_j=\sum_{n=0}^{\infty}(-1)^n(n+1)!c_{nj}. \tag{D17}$$

Notice that, by (B5), (D17) is actually a finite sum. By (B10), we can also write

$$D_j=\sum_{n=0}^{\infty}\sum_{l=0}^{n}(n+1)\binom{n}{l}(-1)^ll^j. \tag{D18}$$

Let us consider now the generating function

$$D(p):=\sum_{j=0}^{\infty}\frac{p^j}{j!}D_j. \tag{D19}$$

By (D18), it follows that

$$D(\rho)=\sum_{n=0}^{\infty}(n+1)\sum_{l=0}^{n}\binom{n}{l}(-1)^le^{\rho l}=\sum_{n=0}^{\infty}(n+1)(1-e^{\rho})^n=e^{-2\rho}. \tag{D20}$$

By comparing the expansion of D in powers of ρ in (D19) with the expansion of $e^{-2\rho}$, we conclude that

$$D_j=(-2)^j. \tag{D21}$$

Thus, (D16) reads

$$c(C;h)=\sum_{j,m=0}^{\infty}b_{jm}(C)(-2)^jh^m=-J_{-1}(C;h), \tag{D22}$$

where the last identity follows from (1). However, by (2), we have

$$J_{-1}(C;h)=-J_1(C;h)=-1.$$

Therefore, we conclude that

$$c(C;h)=1. \tag{D23}$$

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The KZ equation and the quantum-group difference equation in quantum self-dual Yang–Mills theory

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From the time-independent current $\tilde{\mathcal{J}}(\bar{y},\bar{k})$ in the quantum self-dual Yang–Mills (SDYM) theory, we construct new group-valued quantum fields $\tilde{U}(\bar{y},\bar{k})$ and $\tilde{U}^{-1}(\bar{y},\bar{k})$ which satisfy a set of exchange algebras such that fields of $\tilde{\mathcal{J}}(\bar{y},\bar{k}) \sim \tilde{U}(\bar{y},\bar{k})\partial_{\bar{y}}\tilde{U}^{-1}(\bar{y},\bar{k})$ satisfy the original time-independent current algebra. For the correlation functions of the products of the $\tilde{U}(\bar{y},\bar{k})$ and $\tilde{U}^{-1}(\bar{y},\bar{k})$ fields defined in the invariant state constructed through the current $\tilde{\mathcal{J}}(\bar{y},\bar{k})$ we can derive the Knizhnik–Zamolodchikov (KZ) equations with an additional spatial dependence on $\bar{k}$. From the $\tilde{U}(\bar{y},\bar{k})$ and $\tilde{U}^{-1}(\bar{y},\bar{k})$ fields we construct the quantum-group generators, local, global and semi-local, and their algebraic relations. For the correlation functions of the products of the $\tilde{U}$ and $\tilde{U}^{-1}$ fields defined in the invariant state constructed through the semi-local quantum-group generators we obtain the quantum-group difference equations. We give the explicit solution to the two point function. © *1996 American Institute of Physics.* [S0022-2488(96)03207-0]

I. INTRODUCTION

One of the pressing problems in particle physics is to formulate four-dimensional (4-D) quantum field theory nonperturbatively and to find nonperturbative quantum-field-theoretical solutions to the Yang–Mills equations for strong interactions, as well as to quantum gravity. The path we have taken in this pursuit of nonperturbative results has been through the integrable-system method. The main important framework the integrable-system provides is the possibility of formulating the field theory in terms of group-valued local fields. This is a nontrivial starting point for 4-D gauge theory with nonvanishing curvatures. In this formulation the self-dual Yang–Mills (SDYM) theory is the simplest, yet important prototype to work out.[1]

In Ref. 2 we succeeded in formulating the quantum SDYM field theory in terms of the group-valued local quantum field $\tilde{J}$. We obtained the interaction Hamiltonian of the $\tilde{J}$ fields, derived the exchange algebras that the $\tilde{J}$ fields satisfy, showed that the the $\tilde{J}$ fields are bimodule quantum fields and the R matrix of the exchange algebras satisfies the Yang–Baxter relations so that the products of the $\tilde{J}$ fields satisfy associativity and we developed operator-product and normal-ordering procedure for the products of fields. From the $\tilde{J}$ fields, we constructed local currents and their algebras. We found that the one-spatial-dimension integrated currents and current algebras are actually time-independent, i.e. they commute with the interaction Hamiltonian. This is a striking new feature in this 4-D quantum field theory. In this paper we develop fully the implications of these time-independent currents. (Throughout the paper we use letters with a tilde to denote quantum operator fields.)

From the time-independent current $\tilde{\mathcal{J}}(\bar{y},\bar{k})$, we construct new group-valued quantum fields $\tilde{U}(\bar{y},\bar{k})$ and $\tilde{U}^{-1}(\bar{y},\bar{k})$ that satisfy a set of exchange algebras such that fields of $\tilde{\mathcal{J}}(\bar{y},\bar{k}) \sim \tilde{U}(\bar{y},\bar{k})\partial_{\bar{y}}\tilde{U}^{-1}(\bar{y},\bar{k})$ satisfy the original time-independent current algebra. For the correlation functions of the products of the $\tilde{U}(\bar{y},\bar{k})$ and $\tilde{U}^{-1}(\bar{y},\bar{k})$ fields defined in the invariant state constructed through the current $\tilde{\mathcal{J}}(\bar{y},\bar{k})$ we can derive the Knizhnik–Zamolodchikov (KZ) equations[3] with an additional spatial dependence on $\bar{k}$. We can obtain the n-point correlation functions of the $\tilde{U}(\bar{y},\bar{k})$ and $\tilde{U}^{-1}(\bar{y},\bar{k})$ fields; they are expressible in terms of the correlation functions of the quantum WZNW theory in two-dimensions (2-D) with coefficients being unknown functions of one of the additional spatial coordinates in 4-D.

From the $\tilde{U}(\bar{y},\bar{k})$ and $\tilde{U}^{-1}(\bar{y},\bar{k})$ fields we can also construct the quantum-group generators,

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local, global and semi-local, and their algebraic relations. For the correlation functions of the products of the $\tilde{U}$ and $\tilde{U}^{-1}$ fields defined in the invariant state constructed through the semi-local quantum-group generators, using the method given by Frenkel and Reshetikhin[4] we obtain the quantum-group difference equations. We give the explicit solution to the two point function.

With these results, we have exposed probably as much as possible the quantum integrability part of this 4-D interactive theory. As expected, the 4-D interactive theory is not, and should not be, as fully integrable as integrable systems in 2-D (for example, solutions to the KZ equation have unknown functions). However it is to important to find out the quantum-field-theoretical integrability properties of the theories which have many classical integrability properties. This work on the quantum SDYM has now prepared us to investigate fuller 4-D field theories.

II. THE QUANTUM SDYM SYSTEM: HAMILTONIAN, EXCHANGE ALGEBRAS, CRITICAL EXPONENTS, OPERATOR-PRODUCT EXPANSION, NORMAL ORDERING AND CURRENT ALGEBRA

First we briefly review the quantum self-dual Yang–Mills system as formulated in our previous paper.[2] It is characterized by a quantum field Hamiltonian,

$$\tilde{H}_{\rm int}=-\alpha\int d\bar{y}(2l)^2\Sigma_k\Sigma_{\bar{k}}\Big\{\mathrm{Tr}\Big\{(\partial_k\tilde{J})(\partial_{\bar{k}}\tilde{J}^{-1})+\int_0^1 d\rho\,\mathrm{Tr}\{(\partial_\rho\tilde{J})$$
$$\times[(\partial_{\bar{k}}\tilde{J}^{-1})(\partial_k\tilde{J})-(\partial_k\tilde{J}^{-1})(\partial_{\bar{k}}\tilde{J})](\tilde{J}^{-1})\}\Big\}, \tag{1}$$

where, in the case of sl(2), $\tilde{J}=\tilde{J}(y,\bar{y},k,\bar{k})$ is a 2×2 matrix with noncommuting operator-valued entries depending on the 4-D coordinates y, $\bar{y}$, k, $\bar{k}$; and y is the time. (Here we present the theory with z and $\bar{z}$ coordinates discretized: $z=ka$, $\bar{z}=\bar{k}a$, and $a\equiv 2l/N$ is the lattice size.)

The quantum $\tilde{J}$ fields satisfy the following exchange algebras:

$$\tilde{J}_1(y,\bar{y}_1,k_1,\bar{k}_1)\tilde{J}_{II}(y,\bar{y}_2,k_2,\bar{k}_2)=1_{I,II}\tilde{J}_{II}(y,\bar{y}_2,k_2,\bar{k}_2)\tilde{J}_I(y,\bar{y}_1,k_1,\bar{k}_1)R_{I,II}(q,y_1-\bar{y}_2), \tag{2a}$$

where

$$R_{I,II}(q,\bar{y}_1-\bar{y}_2)=P_{I,II}\{[q]^{\Delta_1\epsilon(\bar{y}_1-\bar{y}_2)}\mathscr{P}^q_{j_{12}=1}-[q]^{\Delta_0\epsilon(\bar{y}_1-\bar{y}_2)}\mathscr{P}^q_{j_{12}=0}\}, \tag{2b}$$

$$\epsilon(\bar{y}_1-\bar{y}_2)=-[\ln(\bar{y}_1-\bar{y}_2+i\epsilon)-\ln(\bar{y}_2-\bar{y}_1+i\epsilon)]/\pi i \tag{2c}$$

and

$$\epsilon(\bar{y}_1-\bar{y}_2)=\pm1, \quad \text{for } \bar{y}_1\gtrless\bar{y}_2; \tag{2d}$$

$$\epsilon(\bar{y}_1-\bar{y}_2)=0, \quad \text{for } \bar{y}_1=\bar{y}_2; \tag{2e}$$

$q\equiv e^{-[i\hbar/(2\alpha a^2)]\delta_{k_1k_2}\delta_{\bar{k}_1\bar{k}_2}}$, where α is the coefficient in front of the SDYM interaction Hamiltonian, Eq. (1); $\Delta_1=-1/2$ and $\Delta_0=3/2$ are the conformal dimensions; and the $\mathscr{P}^q_{j_{12}}$'s are the q-ed projection matrices projecting the two spin 1/2 states into $j_{12}=0$ or 1, satisfying $\mathscr{P}^q_{j_{12}}\mathscr{P}^q_{j'_{12}}=\mathscr{P}^q_{j_{12}}\delta_{j_{12}j'_{12}}$. In the more explicit expressions,

$$\mathscr{P}^q_{j_{12}=1}=\mathrm{diag}\left\{1,d\begin{pmatrix}q & 1\\ 1 & q^{-1}\end{pmatrix},1\right\}, \tag{2f}$$

where $d \equiv 1/(q+q^{-1})$. The q-ed singlet projection matrix is related to the triplet one by $\mathscr{P}^q_{j_{12}=0} = 1 - \mathscr{P}^q_{j_{12}=1}$. The matrix $P_{I,II}$ interchanges matrix in space I to II and visa versa, e.g., $P_{I,II}\tilde{J}_I(y,\bar{y}_1,k_1,\bar{k}_1)\tilde{J}_{II}(y,\bar{y}_2,k_2,\bar{k}_2) = \tilde{J}_{II}(y,\bar{y}_1,k_1,\bar{k}_1)\tilde{J}_I(y,\bar{y}_2,k_2,\bar{k}_2)P_{I,II}$, and its explicit representation is $P_{I,II} = 1/2 + 1/2\sum_{a=1}^{3}\sigma_I^a\sigma_{II}^a = \mathscr{P}_{j_{12}=1} - \mathscr{P}_{j_{12}=0}$; here the $\mathscr{P}_{j_{12}}$'s are the un-q-ed ordinary projection matrices, i.e., Eq. (2b) with $q=1$. Using another fact $1_{I,II} = \mathscr{P}_{j_{12}=1} + \mathscr{P}_{j_{12}=0}$, we can easily prove that at $\bar{y}_1 = \bar{y}_2$, exchange algebra Eq. (1) gives

$$\mathscr{P}_{j_{12}}\tilde{J}_I(y,\bar{y}_1,k_1,\bar{k}_1)\tilde{J}_{II}(y,\bar{y}_1,k_1,\bar{k}_1) = \tilde{J}_I(y,\bar{y}_1,k_1,\bar{k}_1)\tilde{J}_{II}(y,\bar{y}_1,k_1,\bar{k}_1)\mathscr{P}^q_{j_{12}}, \tag{2g}$$

where $j_{12}=0,1$. Equation (2c) implies $\mathscr{P}_{j_{12}}\tilde{J}_I(y,\bar{y}_1,k_1,\bar{k}_1)\tilde{J}_{II}(y,\bar{y}_1,k_1,\bar{k}_1)\mathscr{P}^q_{j'_{12}} = 0$, for $j_{12} \neq j'_{12}$. This and the later development of the quantum-group generators rely crucially on this interpretation of the R matrix at the coincidence point, Eq. (2c). We denote $R_{I,II}(q,\bar{y}_1-\bar{y}_2) = R_{I,II}(q,+)$, for $\bar{y}_1-\bar{y}_2>0$ and $R_{I,II}(q,\bar{y}_1-\bar{y}_2) = R_{I,II}(q,-)$, for $\bar{y}_1-\bar{y}_2<0$. Note that $[R_{I,II}(q,+)]^{-1} = R_{II,I}(q,-)$ and $[R_{I,II}(q,-)]^{-1} = R_{II,I}(q,+)$.

The expression for $\epsilon(\bar{y}_1-\bar{y}_2)$, Eq. (2a), indicates that the product $\tilde{J}_I(\bar{y}_1)\tilde{J}_{II}(\bar{y}_2)$ has singularity at $\bar{y}_1-\bar{y}_2=0$, with the specific critical exponents given by

$$\begin{aligned}&\mathscr{P}_{j_{12}}\tilde{J}_I(y,\bar{y}_1,k_1,\bar{k}_1)\tilde{J}_{II}(y,\bar{y}_2,k_1,\bar{k}_1)\mathscr{P}^q_{j'_{12}}\\ &\quad = (\bar{y}_1-\bar{y}_2)^{\Delta_{j_{12}}(\ln q)/\pi i}\{:\mathscr{P}_{j_{12}}\tilde{J}_I(y,\bar{y}_1,k_1,\bar{k}_1)\tilde{J}_{II}(y,\bar{y}_2,k_1,\bar{k}_1)\mathscr{P}^q_{j'_{12}}:\}.\end{aligned} \tag{3}$$

This also defines the normal-order products to be those in the curly brackets; their Taylor expansions give the operator-product expansions.

We then defined the $\tilde{J}^{-1}$ field by the following fixed-y-time equation

$$\tilde{J}(y,\bar{y},k,\bar{k})\tilde{J}^{-1}(y,\bar{y},k,\bar{k}) = 1 = \tilde{J}^{-1}(y,\bar{y},k,\bar{k})\tilde{J}(y,\bar{y},k,\bar{k}). \tag{4}$$

From Eqs. (4) and (2a), one can easily show that the $\tilde{J}^{-1}$ field satisfies the following fixed-y-time exchange algebras:

$$\tilde{J}_I^{-1}(y,\bar{y}_1,k_1,\bar{k}_1)\tilde{J}_{II}(y,\bar{y}_2,k_2,\bar{k}_2) = \tilde{J}_{II}(y,\bar{y}_2,k_2,\bar{k}_2)R^{-1}_{I,II}(q,\bar{y}_1-\bar{y}_2)\tilde{J}_I^{-1}(y,\bar{y}_1,k_1,\bar{k}_1), \tag{5a}$$

and

$$\tilde{J}_I^{-1}(y,\bar{y}_1,k_1,\bar{k}_1)\tilde{J}_{II}^{-1}(y,\bar{y}_2,k_2,\bar{k}_2) = R^{-1}_{I,II}(q,\bar{y}_1-\bar{y}_2)\tilde{J}_{II}^{-1}(y,\bar{y}_2,k_2,\bar{k}_2)\tilde{J}_I^{-1}(y,\bar{y}_1,k_1,\bar{k}_1). \tag{5b}$$

The construction of this $\tilde{J}^{-1}$ field is crucial for us to develop of the full content of the theory in terms of the group-valued fields.

From $\hat{H}_{\text{int}}$ and the exchange algebra Eq. (2a), we can calculate the equation of motion,

$$\partial_y(\tilde{J}\partial_{\bar{y}}\tilde{J}^{-1}) = \frac{\hbar}{i}[\tilde{H},\tilde{J}\partial_{\bar{y}}\tilde{J}^{-1}] = a^{-2}\partial_k(\tilde{J}\partial_{\bar{k}}\tilde{J}^{-1}). \tag{5c}$$

From fields $\tilde{J}$ and $\tilde{J}^{-1}$, we constructed the $\widehat{\text{sl}(2)}$ current,

$$\tilde{j}(y,\bar{y},k,\bar{k}) \equiv \kappa\tilde{J}\partial_{\bar{y}}\tilde{J}^{-1}(y,\bar{y},k,\bar{k}), \tag{6}$$

where $\kappa = \pi i/\ln(q)_{k_1=k_2,\bar{k}_1=\bar{k}_2} = -2\pi\alpha a^2/\hbar$. We then showed that the following equations can be easily derived from the exchange algebras, Eqs. (2a), (5a), and (5b):

$$[\tilde{j}_I(y,\bar{y}_1,k_1,\bar{k}_1),\tilde{j}_{II}(y,\bar{y}_2,k_2,\bar{k}_2)]=[M_{I,II},\tilde{j}_{II}(y,\bar{y}_2,k_2,\bar{k}_2)]2\pi i\delta(\bar{y}_1-\bar{y}_2)\delta_{k_1k_2}\delta_{\bar{k}_1\bar{k}_2}$$
$$+\kappa M_{I,II}2\pi i\delta'(\bar{y}_1-\bar{y}_2)\delta_{k_1k_2}\delta_{\bar{k}_1\bar{k}_2}, \tag{7}$$

$$[\tilde{j}_I(y,\bar{y}_1,k_1,\bar{k}_1),\tilde{J}_{II}(y,\bar{y}_2,k_2,\bar{k}_2)]=M_{I,II}\tilde{J}_{II}(\bar{y}_2,k_2,\bar{k}_2)2\pi i\delta(\bar{y}_1-\bar{y}_2)\delta_{k_1k_2}\delta_{\bar{k}_1\bar{k}_2}, \tag{8}$$

$$[\tilde{j}_I(y,\bar{y}_1,k_1,\bar{k}_1),\tilde{J}_{II}^{-1}(y,\bar{y}_2,k_2,\bar{k}_2)]=-\tilde{J}_{II}^{-1}(\bar{y}_2,k_2,\bar{k}_2)M_{I,II}2\pi i\delta(\bar{y}_1-\bar{y}_2)\delta_{k_1k_2}\delta_{\bar{k}_1\bar{k}_2}, \tag{9}$$

where $M_{I,II}\equiv P_{I,II}-1/2=1/2\Sigma_{a=1}^{3}\sigma_I^a\sigma_{II}^a$.

Equation (7) is the current algebra of the current $\tilde{j}$. Equation (8) indicates that the left side of $\tilde{J}$ forms the fundamental representation of the current $\tilde{j}$; Eq. (9) indicates that the right side of $\tilde{J}^{-1}$ forms the fundamental representation of the current $\tilde{j}$. These are fixed time relations. Since the current $\tilde{j}$ varies with time y, i.e., $[\tilde{j},\tilde{H}]\neq 0$.

As pointed out in Ref. 2 the k-summed (one-spatial-dimension-integrated) current

$$\tilde{\mathcal{J}}(\bar{y},\bar{k})\equiv\Sigma_k\tilde{j}(\bar{y},k,\bar{k}), \tag{10}$$

is constant in time y. It can be proven by directly calculating and showing $[\tilde{\mathcal{J}},\tilde{H}_{\text{int}}]=0$, or easily seen from integrating in z the equation of motion, Eq. (5c). That is why we do not put y dependence in $\tilde{\mathcal{J}}(\bar{y},\bar{k})$. The algebras become

$$[\tilde{\mathcal{J}}_I(\bar{y}_1,\bar{k}_1),\tilde{\mathcal{J}}_{II}(\bar{y}_2,\bar{k}_2)]=[M_{I,II},\tilde{\mathcal{J}}_{II}(\bar{y}_2,\bar{k}_2)]2\pi i\delta(\bar{y}_1-\bar{y}_2)\delta_{\bar{k}_1\bar{k}_2}$$
$$+\kappa' M_{I,II}2\pi i\delta'(\bar{y}_1-\bar{y}_2)\delta_{\bar{k}_1\bar{k}_2}, \tag{11}$$

$$[\tilde{\mathcal{J}}_I(\bar{y}_1,\bar{k}_1),\tilde{J}_{II}(\bar{y}_2,k_2,\bar{k}_2)]=M_{I,II}\tilde{J}_{II}(\bar{y}_2,k_2,\bar{k}_2)2\pi i\delta(\bar{y}_1-\bar{y}_2)\delta_{\bar{k}_1\bar{k}_2}, \tag{12}$$

$$[\tilde{\mathcal{J}}_I(\bar{y}_1,k_1),\tilde{J}_{II}^{-1}(\bar{y}_2,k_2,\bar{k}_2)]=-\tilde{J}_{II}^{-1}(\bar{y}_2,k_2,\bar{k}_2)M_{I,II}2\pi i\delta(\bar{y}_1-\bar{y}_2)\delta_{\bar{k}_1\bar{k}_2}, \tag{13}$$

which can be easily obtained from Eqs. (7), (8) and (9) by k-summation and the identification $\kappa'=\kappa N=\kappa 2l/a$. Note that $\Sigma_{k_1}\delta_{k_1k_2}=1$. Taking the trace of Eq. (11) onto σ_I^a and σ_{II}^b one can easily obtain the current algebra in terms of the Lie-components of the current $[\tilde{\mathcal{J}}^a(\bar{y}_1),\tilde{\mathcal{J}}^b(\bar{y}_2)]=i\epsilon^{abc}\tilde{\mathcal{J}}^c(\bar{y}_1)2\pi i\delta(\bar{y}_1-\bar{y}_2)\delta_{\bar{k}_1\bar{k}_2}+(\kappa'/2)\delta^{ab}2\pi i\delta'(\bar{y}_1-\bar{y}_2)\delta_{\bar{k}_1\bar{k}_2}$. The corresponding continuum equations can also be easily obtained.

III. KZ EQUATIONS FOR THE CORRELATION FUNCTIONS OF THE PRODUCTS OF THE NEW GROUP-VALUED LOCAL FIELDS $\tilde{U}(\bar{y},\bar{k})$ and $\tilde{U}^{-1}(\bar{y},\bar{k})$

Next we can construct new time-independent group-valued local fields $\tilde{U}(\bar{y},\bar{k})$ and $\tilde{U}^{-1}(\bar{y},\bar{k})$ such that

$$\tilde{\mathcal{J}}_I(\bar{y}_1,\bar{k}_1)=\kappa'\tilde{U}_I\partial_{\bar{y}_1}\tilde{U}_I^{-1}(\bar{y}_1,\bar{k}_1), \tag{14}$$

and the $\tilde{U}$ and $\tilde{U}^{-1}$ fields satisfy the following exchange algebras:

$$\tilde{U}_I(\bar{y}_1,\bar{k}_1)\tilde{U}_{II}(\bar{y}_2,\bar{k}_2)=\tilde{U}_{II}(\bar{y}_2,\bar{k}_2)\tilde{U}_I(\bar{y}_1,\bar{k}_1)R_{I,II}(q',\bar{y}_1-\bar{y}_2), \tag{15}$$

$$\tilde{U}_{II}^{-1}(\bar{y}_2,\bar{k}_2)\tilde{U}_I(\bar{y}_1,\bar{k}_1)=\tilde{U}_I(\bar{y}_1,\bar{k}_1)R_{I,II}(q',\bar{y}_1-\bar{y}_2)\tilde{U}_{II}^{-1}(\bar{y}_2,\bar{k}_2), \tag{16}$$

$$\tilde{U}_I^{-1}(\bar{y}_1,\bar{k}_1)\tilde{U}_{II}^{-1}(\bar{y}_2,\bar{k}_2)=R_{I,II}(q',\bar{y}_1-\bar{y}_2)\tilde{U}_{II}^{-1}(\bar{y}_2,\bar{k}_2)\tilde{U}_I^{-1}(\bar{y}_1,\bar{k}_1), \tag{17}$$

where $q' = e^{[-i\hbar/(2\alpha 2la)]\delta_{\bar{k}_1\bar{k}_2}} = (q^{1/N})_{k_1=k_2}$ and $\kappa' = \pi i/\ln(q')_{\bar{k}_1=\bar{k}_2}$. These exchange algebras guarantee the current algebra of $\tilde{\mathscr{T}}$, Eq. (11), and also gives the following algebra:

$$[\tilde{\mathscr{T}}_I(\bar{y}_1,\bar{k}_1),\tilde{U}_{II}(\bar{y}_2,\bar{k}_2)]=M_{I,II}\tilde{U}_{II}(\bar{y}_2,\bar{k}_2)2\pi i\,\delta(\bar{y}_1-\bar{y}_2)\,\delta_{\bar{k}_1\bar{k}_2}, \tag{18}$$

$$[\tilde{\mathscr{T}}_I(\bar{y}_1,\bar{k}_1),\ \tilde{U}_{II}^{-1}(\bar{y}_2,\bar{k}_2)]=-\tilde{U}_{II}^{-1}(\bar{y}_2,\bar{k}_2)M_{I,II}2\pi i\,\delta(\bar{y}_1-\bar{y}_2)\,\delta_{\bar{k}_1\bar{k}_2}. \tag{19}$$

From $2\pi i\,\delta(\bar{y}_1-\bar{y}_2) = 1/(\bar{y}_1-\bar{y}_2-i\epsilon)-1/(\bar{y}_1-\bar{y}_2+i\epsilon)$, the commutator equations, Eqs. (7) to (9), can be written out in the commonly used operator-product-expansion forms.

Let us make the decomposition [{]

$$\tilde{\mathscr{T}}(\bar{y}_1,\bar{k}_1)=\tilde{\mathscr{T}}^{+}(\bar{y}_1,\bar{k}_1)-\tilde{\mathscr{T}}^{-}(\bar{y}_1,\bar{k}_1), \tag{20}$$

with $\tilde{\mathscr{T}}^{\pm}$ satisfying the following algebras:

$$[\tilde{\mathscr{T}}_I^{\pm}(\bar{y}_1,\bar{k}_1),\tilde{\mathscr{T}}_{II}^{\pm}(\bar{y}_2;\bar{k}_2)]=\frac{1}{\bar{y}_1-\bar{y}_2+i\epsilon}[M_{I,II},(\tilde{\mathscr{T}}_I^{\pm}(\bar{y}_1,\bar{k}_1)+\tilde{\mathscr{T}}_{II}^{\pm}(\bar{y}_2,\bar{k}_2))]\delta_{\bar{k}_1\bar{k}_2}, \tag{21}$$

$$\begin{aligned}[\tilde{\mathscr{T}}_I^{+}(\bar{y}_1,\bar{k}_1),\tilde{\mathscr{T}}_{II}^{-}(\bar{y}_2,\bar{k}_2)]=&\frac{1}{\bar{y}_1-\bar{y}_2-i\epsilon}[M_{I,II}(\tilde{\mathscr{T}}_I^{+}(\bar{y}_1,\bar{k}_1)+\tilde{\mathscr{T}}_{II}^{-}(\bar{y}_2,\bar{k}_2))]\delta_{\bar{k}_1\bar{k}_2}\\ &-\frac{1}{(\bar{y}_1-\bar{y}_2+i\epsilon)^2}\kappa' M_{I,II}\delta_{\bar{k}_1\bar{k}_2},\end{aligned} \tag{22}$$

$$[\mathscr{T}_I^{\pm}(\bar{y}_1,\bar{k}_1),\tilde{U}_{II}(\bar{y}_2,\bar{k}_2)]=\frac{-1}{\bar{y}_1-\bar{y}_2\pm i\epsilon}M_{I,II}\tilde{U}_{II}(\bar{y}_2,\bar{k}_2)\delta_{\bar{k}_1\bar{k}_2}, \tag{23}$$

so that Eqs. (11), (18), and (19) are guaranteed.

Because of the singularities in the products of fields, we must prescribe the normal-ordering procedure and make consistency checks. The goal is to express $c\partial_{\bar{y}}\tilde{U}=:\tilde{\mathscr{T}}\tilde{U}:$, where c is a constant to be determined by the normal-order procedure and consistency. Following the procedure used in Ref. 4, we define the vacuum state $|0\rangle$ to be

$$\tilde{\mathscr{T}}^{-}(\bar{y},\bar{k})|0\rangle=0 \quad \text{and} \quad \langle 0|\tilde{\mathscr{T}}^{+}(\bar{y},\bar{k})=0. \tag{24}$$

After checking the consistency with all the above algebras, we find $c=(\kappa'+2)$ and obtain

$$(\kappa'+2)\partial_{\bar{y}}\tilde{U}_I(\bar{y},\bar{k})=-:\tilde{\mathscr{T}}_I(\bar{y},\bar{k})\tilde{U}_I(\bar{y},\bar{k}):\equiv-\tilde{\mathscr{T}}_I^{+}(\bar{y},\bar{k})\tilde{U}_I(\bar{y},\bar{k})+((\tilde{U}_I(\bar{y},\bar{k}))^T(\tilde{\mathscr{T}}_I(\bar{y},\bar{k}))^T)^T. \tag{25}$$

Then following the standard procedure, we obtain the KZ equation for the $\tilde{U}$ fields,

$$\left((\kappa'+2)\partial_{\bar{y}_j}+\sum_{j\neq k}\frac{M_{J,K}}{\bar{y}_j-\bar{y}_k}\,\delta_{\bar{k}_j\bar{k}_k}\right)\langle 0|\tilde{U}_I(\bar{y}_1,\bar{k}_1)\cdots\tilde{U}_N(\bar{y}_n,\bar{k}_n)|0\rangle=0. \tag{26}$$

Notice that taking away the $\bar{k}$ dependence, we recover the KZ equation of the quantum WZNW theory, Ref. 3.

The solutions of this SDYM KZ equation are expressible in terms of those of the WZNW KZ equation, $\langle 0|g_I(\bar{y}_1)\cdots g_N(\bar{y}n)|0)$, multiplied by unknown functions in $\bar{k}$. For example,

$$\langle 0|\tilde{U}_I(\bar{y}_1,\bar{k}_1)\tilde{U}_{II}(\bar{y}_2,\bar{k}_2)|0\rangle = C_2(\bar{k}_1)\langle 0|\tilde{g}_I(\bar{y}_1)\tilde{g}_{II}(\bar{y}_2)|0\rangle_{(\kappa'+2)}\delta_{\bar{k}_1\bar{k}_2} + C_{2I}(\bar{k}_1,\bar{k}_2)\langle 0|\tilde{g}_I(\bar{y}_1)|0\rangle_{(\kappa'+2)}\langle 0|\tilde{g}_{II}(\bar{y}_2)|0\rangle_{(\kappa'+2)}(1-\delta_{\bar{k}_1\bar{k}_2}), \tag{27}$$

$$\begin{aligned}\langle 0|\tilde{U}_I(\bar{y}_1,\bar{k}_1)\tilde{U}_{II}(\bar{y}_2,\bar{k}_2)\tilde{U}_{III}(\bar{y}_3,\bar{k}_3)|0\rangle &= C_3(\bar{k}_1)\langle 0|\tilde{g}_I(\bar{y}_1)\tilde{g}_{II}(\bar{y}_2)\tilde{g}_{III}(\bar{y}_3)|0\rangle_{(\kappa'+2)}\delta_{\bar{k}_1\bar{k}_2}\delta_{\bar{k}_1\bar{k}_3} \\ &+ \sum_{j\neq k\neq l}^{1\text{ to }3} C_{3j}(\bar{k}_k,\bar{k}_j)\langle 0|\tilde{g}_J(\bar{y}_j)|0\rangle_{(\kappa'+2)}\langle 0|\tilde{g}_K(\bar{y}_k)\tilde{g}_L(\bar{y}_l)|0\rangle_{(\kappa'+2)}\delta_{\bar{k}_k\bar{k}_l}(1-\delta_{\bar{k}_k\bar{k}_j}) \\ &+ C_{34}(\bar{k}_1,\bar{k}_2,\bar{k}_3)\langle 0|\tilde{g}_I(\bar{y}_1)|0\rangle_{(\kappa'+2)}\langle 0|\tilde{g}_{II}(\bar{y}_2)|0\rangle_{(\kappa'+2)}\langle 0|\tilde{g}_{III}(\bar{y}_3)|0\rangle_{(\kappa'+2)} \\ &\times(1-\delta_{\bar{k}_1\bar{k}_2})(1-\delta_{\bar{k}_1\bar{k}_3})(1-\delta_{\bar{k}_2\bar{k}_3}),\end{aligned} \tag{28}$$

$$\begin{aligned}\langle 0|\tilde{U}_I(\bar{y}_1,\bar{k}_1)U_{II}(\bar{y}_2,\bar{k}_2)U_{III}(\bar{y}_3,\bar{k}_3)U_{IV}(\bar{y}_4,\bar{k}_4)|0\rangle &= C_4(k_1)\langle 0|\tilde{g}_I(\bar{y}_1)\tilde{g}_{II}(\bar{y}_2)\tilde{g}_{III}(\bar{y}_3)\tilde{g}_{IV}(\bar{y}_4)|0\rangle_{(\kappa'+2)}\delta_{\bar{k}_1\bar{k}_2}\delta_{\bar{k}_2\bar{k}_3}\delta_{\bar{k}_3\bar{k}_4} \\ &+ \sum_{j\neq k\neq l\neq m}^{1\text{ to }4} C_{4j}(\bar{k}_k,\bar{k}_j)\langle 0|\tilde{g}_J(\bar{y}_j)|0\rangle_{(\kappa'+2)}\langle 0|\tilde{g}_K(\bar{y}_k)\tilde{g}_L(\bar{y}_l)\tilde{g}_M(\bar{y}_m)|0\rangle_{(\kappa'+2)} \\ &\times(1-\delta_{\bar{k}_j\bar{k}_k})\delta_{\bar{k}_l\bar{k}_k}\delta_{\bar{k}_m\bar{k}_k} + \sum_{j\neq k\neq l\neq m}^{1\text{ to }4} C_{41,jklm}(\bar{k}_j,\bar{k}_l)\langle 0|\tilde{g}_J(\bar{y}_j)(\tilde{g}_K)(\bar{y}_k)|0\rangle_{(\kappa'+2)} \\ &\times\langle 0|\tilde{g}_L(\bar{y}_l)\tilde{g}_M(\bar{y}_m)|0\rangle_{(\kappa'+2)}\delta_{\bar{k}_j\bar{k}_k}\delta_{\bar{k}_l\bar{k}_m}(1-\delta_{\bar{k}_j\bar{k}_l}) + \sum_{j\neq k\neq l\neq m}^{1\text{ to }4} C_{42,jklm}(\bar{k}_j,\bar{k}_k,\bar{k}_l) \\ &\times\langle 0|\tilde{g}_J(\bar{y}_j)|0\rangle_{(\kappa'+2)}\langle 0|\tilde{g}_K(\bar{y}_k)|0\rangle_{(\kappa'+2)}\langle 0|\tilde{g}_L(\bar{y}_l)\tilde{g}_M(\bar{y}_m)|0\rangle_{(\kappa'+2)} \\ &\times(1-\delta_{\bar{k}_j\bar{k}_l})\delta_{\bar{k}_l\bar{k}_m}(1-\delta_{\bar{k}_k\bar{k}_l})(1-\delta_{\bar{k}_j\bar{k}_k}) + C_{43}(\bar{k}_1,\bar{k}_2,\bar{k}_3,\bar{k}_4)\langle 0|\tilde{g}_I(\bar{y}_1)|0\rangle_{(\kappa'+2)} \\ &\times\langle 0|\tilde{g}_{II}(\bar{y}_2)|0\rangle_{(\kappa'+2)}\langle 0|\tilde{g}_{III}(\bar{y}_3)|0\rangle_{(\kappa'+2)}\langle 0|\tilde{g}_{IV}(\bar{y}_4)|0\rangle_{(\kappa'+2)}(1-\delta_{\bar{k}_1\bar{k}_2})(1-\delta_{\bar{k}_1\bar{k}_3}) \\ &\times(1-\delta_{\bar{k}_1\bar{k}_4})(1-\delta_{\bar{k}_2\bar{k}_3})(1-\delta_{\bar{k}_2\bar{k}_4})(1-\delta_{\bar{k}_3\bar{k}_4}).\end{aligned} \tag{29}$$

These are the nonperturbative y-time independent solutions of the correlation functions of the quantum CDYM theory. As expected, the 4-D theory has more freedom which is manifested in these unknown functions.

IV. QUANTUM-GROUP CURRENT $\tilde{\mathcal{J}}^q(\bar{y},\bar{k})$ AND $\bar{y}$-GLOBAL QUANTUM-GROUP GENERATORS $\tilde{G}(\bar{k})$

Similar to the construction of the current $\tilde{\mathcal{J}}$, Eq. (14), it is natural to construct the other current,

$$\tilde{\mathcal{J}}^q(\bar{y},\bar{k}) \equiv \kappa' \tilde{U}^{-1}(\bar{y},\bar{k})\partial_{\bar{y}}\tilde{U}(\bar{y},\bar{k}), \tag{30}$$

which we shall call the quantum-group current, since it has the quantum-group index on both sides.

We can work out the algebraic relations among its matrix elements and with the fields $\tilde{U}$ and $\tilde{U}^{-1}$, like Eqs. (11) to (13) for the $\tilde{\mathcal{J}}$. All of them have nice quantum-group interpretations. However, we find that $\tilde{\mathcal{J}}^q$ is not as useful a quantity as the current $\tilde{\mathcal{J}}$ in that it can not be used to develop its vacuum states and the corresponding differential equations as the current $\tilde{\mathcal{J}}$ was used to develop the KZ equations. On the other hand we find that the following group-valued quantities,

$\tilde{G}(\bar{k})$ and $\tilde{G}^{\Delta}(\bar{y},\bar{k})$, are the appropriate quantum-group generators for further development of the theory.

The $\bar{y}$-global quantum-group generator $\tilde{G}(\bar{k})$ is derived from the quantum-group current $\tilde{\mathcal{J}}^{q}$ of Eq. (30) by a path ordered integration,

$$\tilde{G}(\bar{k})=\vec{P}\ \exp\left(\int_{-\infty}^{\infty} d\bar{y}\tilde{U}^{-1}\partial_{\bar{y}}\tilde{U}(\bar{y},\bar{k})\right)=\tilde{U}^{-1}(\bar{y}=-\infty,\bar{k})\tilde{U}(\bar{y}=+\infty,\bar{k}). \tag{31}$$

Then, from the exchange algebras of the fields $\tilde{U}$ and $\tilde{U}^{-1}$, Eqs. (15) to (17), we can derive the algebraic relations among the matrix elements of $\tilde{G}(\bar{k})$ and with the fields $\tilde{U}$ and $\tilde{U}^{-1}$,

$$\{R_{\mathrm{II,I}}(q',+)\tilde{G}_{I}(\bar{k}_1)R_{\mathrm{I,II}}(q',+)\}\tilde{G}_{\mathrm{II}}(\bar{k}_2)=\tilde{G}_{\mathrm{II}}(\bar{k}_2)\{R_{\mathrm{II,I}}(q',+)\tilde{G}_{\mathrm{I}}(\bar{k}_1)R_{\mathrm{I,II}}(q',+)\}, \tag{32}$$

$$\tilde{G}_{\mathrm{I}}(\bar{k}_1)U_{\mathrm{II}}(\bar{y}_2,\bar{k}_2)=U_{\mathrm{II}}(\bar{y}_2,\bar{k}_2)\{R_{\mathrm{II,I}}(q',+)\tilde{G}_{\mathrm{I}}(\bar{k}_1)R_{\mathrm{I,II}}(q',+)\}, \tag{33}$$

$$U_{\mathrm{II}}^{-1}(\bar{y}_2,\bar{k}_2)\tilde{G}_{\mathrm{I}}(\bar{k}_1)=\{R_{\mathrm{II,I}}(q',+)\tilde{G}_{\mathrm{I}}(\bar{k}_1)R_{\mathrm{I,II}}(q',+)\}\tilde{U}_{\mathrm{II}}^{-1}(\bar{y}_2,\bar{k}_2), \tag{34}$$

where $R_{\mathrm{I,II}}(q',+)$ is the R-matrix with $\epsilon(\bar{y}_1-\bar{y}_2)=+1$ and the curley brackets are to guide the eyes to the proper grouping of matrices and operators. These three equations are the algebraic relations parallel to those of Eqs. (11), (18) and (19). Associativity of all these fields are true because the R matrix satisfies the Yang–Baxter relations.

The basic elements of the quantum-group generators $\{\tilde{e}_i(\bar{k});\ i=3 \text{ and } \pm\}$ are related to the components of the components of the matrix $\tilde{G}(\bar{k})$ by

$$\tilde{G}(\bar{k})\equiv\begin{pmatrix}1 & 0\\ (1-q^2)\tilde{e}_{+}(\bar{k}) & 1\end{pmatrix}\begin{pmatrix}q^{-\tilde{e}_3(k)} & 0\\ 0 & q^{\tilde{e}_3(\bar{k})}\end{pmatrix}\begin{pmatrix}1 & (q^{-1}-q)\tilde{e}_{-}(\bar{k})\\ 0 & 1\end{pmatrix}, \tag{35}$$

where the $\tilde{e}_{\pm}(\bar{k})$ and $q^{-\tilde{e}_3(\bar{k})}$ satisfy local quantum-groups algebras, which generalize those given in Ref. 5.

I. THE $\bar{y}$-SEMI-LOCAL QUANTUM-GROUP GENERATOR $\tilde{G}^{\Delta}(\bar{y},\bar{k})$

Changing the integration range in Eq. (31) to a semi-local region we obtain the $\bar{y}$-semilocal quantum-group generator $\tilde{G}^{\Delta}(\bar{y},\bar{k})$ quantum group generator:

$$\tilde{G}^{\Delta}(\bar{y},\bar{k})\equiv\vec{P}\ \exp\left(\int_{\bar{y}-\Delta}^{\bar{y}+\Delta} d\bar{y}'\,\tilde{U}^{-1}(\bar{y}',\bar{k})\partial_{\bar{y}'}\tilde{U}(\bar{y}',\bar{k})\right)=\tilde{U}^{-1}(\bar{y}-\Delta,\bar{k})\tilde{U}(\bar{y}+\Delta,\bar{k}). \tag{36}$$

we can easily show that $\tilde{G}^{\Delta}$ satisfies the following algebras:

$$\begin{aligned}&\{R_{I,II}^{-1}(q',\bar{y}_1-\bar{y}_2)\tilde{G}_{I}^{\Delta}(\bar{y}_1,\bar{k}_1)R_{I,II}(q',\bar{y}_1-\bar{y}_2+2\Delta)\}\tilde{G}_{II}^{\Delta}(\bar{y}_2,\bar{k}_2)\\ &\quad=\tilde{G}_{II}^{\Delta}(\bar{y}_2,\bar{k}_2)\{R_{I,II}^{-1}(q',\bar{y}_1-\bar{y}_2-2\Delta)\tilde{G}_{I}^{\Delta}(\bar{y}_1,\bar{k}_1)R_{I,II}(q',\bar{y}_1-\bar{y}_2)\},\end{aligned} \tag{37}$$

$$\tilde{G}_{I}^{\Delta}(\bar{y}_1,\bar{k}_1)\tilde{U}_{II}(\bar{y}_2,\bar{k}_2)=\tilde{U}_{II}(\bar{y}_2,\bar{k}_2)\{R_{I,II}^{-1}(q',\bar{y}_1-\bar{y}_2-\Delta)\tilde{G}_{I}^{\Delta}(\bar{y}_1,\bar{k}_1)R_{I,II}(q',\bar{y}_1-\bar{y}_2+\Delta)\}, \tag{38}$$

$$\tilde{U}_{II}^{-1}(\bar{y}_2,\bar{k}_2)\tilde{G}_{I}^{\Delta}(\bar{y}_1,\bar{k}_1)=\{R_{I,II}^{-1}(q',\bar{y}_1-\bar{y}_2-\Delta)\tilde{G}_{I}^{\Delta}(\bar{y}_1,\bar{k}_1)R_{I,II}(q',\bar{y}_1-\bar{y}_2+\Delta)\}\tilde{U}_{II}^{-1}(\bar{y}_2,\bar{k}_2). \tag{39}$$

We next split the semi-local generator into the annihilation and creation parts following a procedure similar to that used in Ref. 4,

$$\tilde{G}_{I}^{\Delta}(\bar{y},\bar{k})\equiv[G_{I}^{\Delta^{+}}(\bar{y},\bar{k})]^{-1}G_{I}^{\Delta^{-}}(\bar{y},\bar{k}), \tag{40}$$

and $G^{\Delta\pm}(\bar{y},\bar{k})$ satisfies the following exchange algebras:

$$R_{I,II}(q',\bar{y}_1-\bar{y}_2-\Delta)G_I^{\Delta\pm}(\bar{y}_1,\bar{k}_1)G_{II}^{\Delta\pm}(\bar{y}_2,\bar{k}_2)=G_{II}^{\Delta\pm}(\bar{y}_2,\bar{k}_2)G_I^{\Delta\pm}(\bar{y}_1,\bar{k}_1)R_{I,II}(q',\bar{y}_1-\bar{y}_2-\Delta), \tag{41}$$

$$R_{I,II}(q',\bar{y}_1-\bar{y}_2)G_I^{\Delta+}(\bar{y}_1,\bar{k}_1)G_{II}^{\Delta-}(\bar{y}_2,\bar{k}_2)=G_{II}^{\Delta-}(\bar{y}_2,\bar{k}_2)G_I^{\Delta+}(\bar{y}_1,\bar{k}_1)R_{I,II}(q',\bar{y}_1-\bar{y}_2-2\Delta), \tag{42}$$

$$\tilde{U}_I(\bar{y}_1,\bar{k}_1)G_{II}^{\Delta\pm}(\bar{y}_2,\bar{k}_2)=G_{II}^{\Delta\pm}(\bar{y}_2,\bar{k}_2)\tilde{U}_I(\bar{y}_1,\bar{k}_1)R_{I,II}(q',\bar{y}_1-\bar{y}_2\pm\Delta), \tag{43}$$

such that Eqs. (37) to (39) are true.

Notice that

$$\left[\sum_n \tilde{\mathscr{T}}(\bar{y}+n\Delta,\bar{k}),G^{\Delta}(\bar{y},\bar{k})\right]=0, \tag{44}$$

which manifests what we call the $\bar{k}$-local $\mathrm{sl}^{\Delta}(n)\otimes U^{1/\Delta}q[\mathrm{sl}(n)]$ symmetry of the theory. For $\Delta\to\infty$, Eq. (44) becomes $[\tilde{\mathscr{T}}(\bar{y},\bar{k}),\tilde{G}(\bar{k})]=0$, manifesting the $\bar{k}$-local $\widehat{\mathrm{sl}(n)}\otimes Uq[\mathrm{sl}(n)]$ symmetry of the theory. For $\Delta\to 0$, Eq. (44) becomes $[\tilde{Q}(\bar{k}),\tilde{\mathscr{T}}^q(\bar{y},\bar{k})]=0$, manifesting the $\bar{k}$-local $\mathrm{sl}(n)\otimes U_q^x[\mathrm{sl}(n)]$ symmetry of the theory.

VI. QUANTUM-GROUP DIFFERENCE EQUATION OF THE CORRELATION FUNCTIONS DEFINED IN THE $|0_q\rangle$-VACUUM

Using Eq. (40), let us rewrite Eq. (36) as

$$\tilde{U}(\bar{y}+\Delta,\bar{k})=\tilde{U}(\bar{y}-\Delta,\bar{k})\tilde{G}^{\Delta}(\bar{y},\bar{k})=\tilde{U}(\bar{y}-\Delta,\bar{k})[\tilde{G}^{\Delta+}(\bar{y},\bar{k})]^{-1}G^{\Delta-}(\bar{y},\bar{k}). \tag{45}$$

Now we want to move $(G^{\Delta+}(\bar{y},\bar{k}))^{-1}$ to the left of $\tilde{U}(\bar{y}-\Delta,\bar{k})$, since we shall consider the vacuum expectation values of the $\tilde{U}$ fields by the vacuum $|0_q\rangle$ defined by

$$G^{\Delta-}(\bar{y},\bar{k})|0_q\rangle=|0_q\rangle \quad \text{and} \quad \langle 0_q|G^{\Delta+}(\bar{y},\bar{k})=\langle 0_q|. \tag{46}$$

To achieve that feat we use Eq. (43), many matrix relations and finally reach

$$\tilde{U}(\bar{y}+\Delta,\bar{k})=(((G^{\Delta+}(\bar{y},\bar{k}))^{-1})^T\Upsilon\tilde{U}^T(\bar{y}-\Delta,\bar{k}))^TG^{\Delta-}(\bar{y},\bar{k}), \tag{47}$$

where the superscript T means matrix transposition, but the order of the operator stay the same; $\Upsilon\equiv(q'+q'^{-1})/(q'^2+q'^{-2})\times\mathrm{diag}(q',q'^{-1})$, which results from

$$\Upsilon_I=(Tr)_{II}(P_{I,II}(((R_{I,II}(q',0))^{T_I})^{-1})^{T_{II}}), \tag{48}$$

where the superscripts T_I and T_{II} indicate transposition of matrices in the tensor spaces I and II, respectively.

Using Eqs. (32) and (33), we obtain the difference equation for correlation function,

$$\begin{aligned}&\langle 0_q|\tilde{U}_I(\bar{y}_1,\bar{k}_1)\cdots\tilde{U}_L(\bar{y}_l+2\Delta,\bar{k}_l)\cdots\tilde{U}_N(\bar{y}_n,\bar{k}_n)|0_q\rangle\\&\quad=\langle 0_q|\tilde{U}_I(\bar{y}_1,\bar{k}_1)\cdots\tilde{U}_L(\bar{y}_l,\bar{k}_l)\cdots\tilde{U}_N(\bar{y}_n,\bar{k}_n)|0_q\rangle R_{L,L-1}(q',\bar{y}_l-\bar{y}_{l-1})\cdots\\&\qquad\times R_{L,I}(q',\bar{y}_l-\bar{y}_1)\Upsilon_L R_{L,N}(q',\bar{y}_l-\bar{y}_n+2\Delta)\cdots R_{L,L+1}(q',\bar{y}_l-\bar{y}_{l+1}+2\Delta).\end{aligned} \tag{49}$$

For the special case of "$+2\Delta$" being at $\bar{y}_n$, Eq. (49) simplifies to the following cyclic relation:

$$\langle 0_q|\tilde{U}_I(\bar{y}_1,\bar{k}_1)\cdots\tilde{U}_N(\bar{y}_n+2\Delta,\bar{k}_n)|0_q\rangle=\langle 0_q|\tilde{U}_N(\bar{y}_n,\bar{k}_n)\tilde{U}_I(\bar{y}_1,\bar{k}_1)\cdots\tilde{U}_{N-1}(\bar{y}_{n-1},\bar{k}_{n-1})|0_q\rangle\Upsilon_N. \tag{50}$$

For the two point function, Eq. (49) becomes

$$\langle 0_q|\tilde{U}_I(\bar{y}_1,\bar{k}_1)\tilde{U}_{II}(\bar{y}_2+2\Delta,\bar{k}_2)|0_q\rangle=\langle 0_q|\tilde{U}_I(\bar{y}_1,\bar{k}_1)\tilde{U}_{II}(\bar{y}_2,\bar{k}_2)|0_q\rangle R_{II,I}(q',\bar{y}_2-\bar{y}_1)\Upsilon_{II}. \tag{51}$$

Multiplying Eq. (51) from the right by $\mathscr{P}^{q'}_{j_{12}=0}$ and using the fact $\langle 0_q|\tilde{U}_I\tilde{U}_{II}|0_q\rangle\mathscr{P}^{q'}_{j_{12}=0}=\langle 0_q|\tilde{U}_I\tilde{U}_{II}|0_q\rangle$, which can be shown using the definition of $|0_q\rangle$ given by Eq. (46), whereby Eq. (51) becomes

$$\langle 0_q|\tilde{U}_I(\bar{y}_1,\bar{k}_1)\tilde{U}_{II}(\bar{y}_2+2\Delta,\bar{k}_2)|0_q\rangle=\langle 0_q|\tilde{U}_I(\bar{y}_1,\bar{k}_1)\tilde{U}_{II}(\bar{y}_2,\bar{k}_2)|0_q\rangle q'^{-\Delta_0\epsilon(\bar{y}_1-\bar{y}_2)}\frac{q'+q'^{-1}}{q'^2+q'^{-2}}, \tag{52}$$

where the last factor on the right is from $\mathscr{P}^{q'}_{j_{12}=0}R_{I,II}(\bar{y}_1-\bar{y}_2)\Upsilon_{II}\mathscr{P}^{q'}_{j_{12}=0}=\mathscr{P}^{q'}_{j_{12}=0}q'^{-\Delta_0\epsilon(\bar{y}_1-\bar{y}_2)}\times(b/a)$ with $b/a\equiv(q'+q'^{-1})/(q'^2+q'^{-2})=([2]_{q'})^2/[4]_{q'}$ and the fact that $\mathscr{P}^{q'}_{j_{12}=0}$ multiplying the vacuum expectation value becomes unit.

Its solution can be easily found and written in the following form:

$$\begin{aligned}&\langle 0_q|\tilde{U}_I(\bar{y}_1,\bar{k}_1)\tilde{U}_{II}(\bar{y}_2,\bar{k}_2)|0_q\rangle\\&=\delta_{\bar{k}_1,\bar{k}_2}A_0(\bar{k}_1)\exp\left\{-\left(\frac{\bar{y}_1-\bar{y}_2}{2\Delta}\right)\ln\left(\frac{q'+q'^{-1}}{q'^2+q'^{-2}}\right)\right.\\&\left.+\left[\left(\frac{|\bar{y}_1-\bar{y}_2|}{2\Delta}\right)+2\sum_{n=1}^{\infty}\theta\left(-\frac{|\bar{y}_1-\bar{y}_2|}{2\Delta}-n\right)\right]\ln(q'^{\Delta_0})\right\}+(1-\delta_{\bar{k}_1\bar{k}_2})A_1(\bar{k}_1,\bar{k}_2),\end{aligned} \tag{53}$$

where A_0 and A_1 are arbitrary functions; $\theta(x)=0,\frac{1}{2},1$ for $x<0,x=0,x>0$, respectively. This expression for the solution is continuous in the $\bar{y}_1-\bar{y}_2>0$ region. For expressing the solution in a function that is continuous the $\bar{y}_1-\bar{y}_2<0$ region, we replace $\Sigma_{n=1}^{\infty}\to\Sigma_{n=0}^{\infty}$ in the square bracket of the above equations.

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Batalin–Vilkovisky formalism and integration theory on manifolds

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The correspondence between the BV formalism and integration theory on supermanifolds is established. An explicit formula for the density on a Lagrangian surface in a superspace provided with an odd symplectic structure and a volume form is proposed. © *1996 American Institute of Physics.* [S0022-2488(96)02906-4]

I. INTRODUCTION

In their outstanding works,[1] Batalin and Vilkovisky proposed the most general method for quantizing arbitrary gauge field theories.

During the years it becomes clear that this scheme is very powerful for resolving ghost problems, and moreover it contains a rich geometrical structure. In the paper[2] Witten proposed a program for the construction of String Field Theory in the framework of the Batalin–Vilkovisky formalism (BV formalism) and noted the necessity of its geometrical investigation. The BV formalism indeed uses the geometry of the superspace provided with odd symplectic structure and the volume form. The properties of this geometry and its connection to the BV formalism was investigated, for example, in Refs. 3–6. Particularly in Ref. 5, Schwarz gives the detailed geometrical analysis of the BV formalism in terms of this geometry.

However, some specific aspects of the BV formalism are not completely clarified, such as the geometrical meaning of the initial conditions of the master action; the choice of the gauge fermion and the geometrical reasons for the extending the initial space of fields with ghosts and antighost fields.

In this work we try to analyze some of these questions. For this purpose we study the analogy between the BV scheme and the corresponding constructions in differential geometry.

From the geometrical point of view to the gauge symmetries correspond the vector fields on the space of the classical fields that preserve the action. The partition function, when gauge conditions are fixed, is the integral of a nonlocal density constructed by means of these vector fields over the surface that is defined by gauge conditions. This surface is embedded in the space of the classical fields.

The gauge independence means that this density have to be closed. To make this density local in the BV formalism one have to rise the density and the gauge fixing surface on the extended space: to the gauge fixing surface corresponds the Lagrangian manifold embedded in the phase space of the "fields" and "antifields" ("fields"=classical fields, ghosts), to the closed density corresponds the volume form on this manifold (the exponent of the BV master action), which obeys the BV master equation.[1,5,6]

In the second section we briefly recall the basic formulas of the BV formalism and in the

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following[5] give the covariant explicit formula for the volume element on the Lagrangian manifold when it is given by arbitrary functions of the fields and antifields. This formula is related to the multilevel field–antifield formalism with the most general Lagrangian hypergauges.[7]

In the third section we briefly recall the basic constructions of the geometry of the superspace provided with an odd symplectic structure and volume form.[3,5,6] It is this geometry on which the BV formalism is based, and which development on the other hand was highly inspired by this formalism. In particular, we shortly describe the properties of the Δ operator arising in this geometry and the connection between the BV formalism and the Δ-operator nilpotency condition.

In the fourth section we consider the densities[8–11] (the general covariant objects that can be integrated over supersurfaces in the superspace). Following Refs. 9 and 11 we consider a special class of densities—pseudodifferential forms on which the exterior derivative can be defined correctly. Using Baranov–Schwarz (BS) transformations[9] we rise these forms to integration objects on the enlarged space and formulate the condition of closure of these forms in terms of the Δ operator.

In the fifth section, using BS transformations we study the relations between gauge symmetries in field theory and the closed pseudodifferential forms corresponding to the integrand for the partition function of the theory. We study the relations between the closure conditions and the BV master equation.

II. BV FORMALISM

In this section we recall the basic constructions of BV formalism:[1] the integral for the partition function and we rewrite this integral in the case where the Lagrangian manifold is given in a covariant way.

Let $S(\phi)$ be the action of theory with gauge symmetries $\{R^A_b(\phi)\}$:

$$R^A_b(\phi)\,\frac{\delta S(\phi)}{\delta \phi^A}=0. \tag{2.1}$$

We use de Witt condensed notations (index A runs over all the indices and the spatial coordinates of the fields ϕ). Let $\mathscr{E}$ be the space of the fields Φ^A and antifields Φ_{*A}, where $\Phi^A=(\phi^A,c^b,\nu_b,\dots)$ is the space of fields ϕ^A enlarged with the ghosts, Lagrangian multipliers for the constraints, etc., and Φ_{*A} has the parity opposite to Φ^A,

$$p(\Phi_{*A})=p(\Phi^A)+1. \tag{2.2}$$

In the space $\mathscr{E}$ one can define the symplectic structure by the odd Poisson bracket:

$$\{F,G\}=\frac{\delta F}{\delta \Phi^A}\frac{\delta G}{\delta \Phi_{*A}}+\frac{\delta F}{\delta \Phi_{*A}}\frac{\delta G}{\delta \Phi^A}\quad (\text{if } F \text{ is even}), \tag{2.3}$$

and the Δ_0 operator,

$$\Delta_0 F=\frac{\delta^2 F}{\delta \Phi_{*A}\,\delta \Phi^A}. \tag{2.4}$$

The master action $\mathscr{S}$ then can be uniquely defined by the equation

$$\Delta_0 e^{\mathscr{S}}=0\Leftrightarrow \Delta_0\mathscr{S}(\Phi^A,\Phi_{*A})+\tfrac{1}{2}\{\mathscr{S}(\Phi^A,\Phi_{*A}),\mathscr{S}(\Phi^A,\Phi_{*A})\}=0, \tag{2.5a}$$

and the initial conditions:

$$\mathscr{S}(\Phi^A,\Phi_{*A})=S(\phi)+c^b R^A_b\phi_{*A}+\cdots, \tag{2.5b}$$

where dots means terms containing ghosts and antifields of higher degrees.

If

$$[\mathbf{R}_a, \mathbf{R}_b] = t_{ab}^c \mathbf{R}_c + E_{ab}^{[AB]} \mathscr{F}_B,$$

where $\mathscr{F}_A$ are the equations of motion $[\mathscr{F}_A = \delta S(\phi)/\partial \phi^A]$, then

$$\mathscr{S}(\Phi^A, \Phi_{*A}) = S(\phi) + c^b R_b^A \phi_{*A} + \tfrac{1}{2} t_{ab}^c c^a c^b c_c^* + \tfrac{1}{2} c^a c^b E_{ab}^{CD} \phi_{*C} \phi_{*D} + \cdots . \tag{2.5c}$$

To the gauge conditions

$$f_b = 0, \tag{2.6}$$

corresponds the so-called "gauge fermion:"

$$\Psi = f_b \nu^b, \tag{2.7}$$

which defines the Lagrangian surface Λ in $\mathscr{E}$ by the equations

$$F_A(\Phi, \Phi_*) = 0, \tag{2.8}$$

where

$$F_A = \Phi_{*A} - \frac{\delta \Psi(\Phi)}{\delta \Phi^A} = 0 \tag{2.9}$$

(the surface embedded in the symplectic space is Lagrangian if it has half the dimension of space and the two-form defining the symplectic structure is equal to zero on it). The partition function Z is given by the integral of the master-action exponent over this Lagrangian surface Λ:

$$Z = \int e^{\mathscr{S}(\Phi_A, \Phi^{*A})} \delta\left(\Phi_{*A} - \frac{\delta \Psi(\Phi)}{\delta \Phi^A} \right) \mathscr{D}\Phi^* \, \mathscr{D}\Phi \tag{2.10}$$

(for details see Ref. 1).

The main statement of the BV formalism is that this integral does not depend on the choice of the Lagrangian surface Λ.

Before going into the geometrical analysis of the formula (2.10), we first rewrite it in a more covariant way if the functions F_A that define Λ by the equation (2.8) are arbitrary.

It is easy to see that the surface Λ defined by (2.8) is Lagrangian iff

$$\{F_A, F_B\}|_{F_A = 0} = 0. \tag{2.11}$$

Let us consider the integral:

$$\int e^{\mathscr{S}(\Phi_A, \Phi^{*A})} \sqrt{\mathrm{Ber} \frac{\delta(G^A, F_B)}{\delta(\Phi^A, \Phi_{*A})}} \sqrt{\mathrm{Ber}\{G^{\tilde{A}}, F_B\}} \delta(F) \mathscr{D}\Phi_* \, \mathscr{D}\Phi, \tag{2.12}$$

where G^A are arbitrary functions and $\tilde{A}$ has a parity reversed to A.

One can show that if the functions F_A define the Lagrangian manifold Λ (2.8), then this integral does not depend on the choice of the functions G^A, and it does not depend on the choice of the functions F_A defining Λ. On the other hand, in the case where the functions F_A have the form (2.9) and the functions G^A are equal to Φ^A, it evidently coincides with the BV integral (2.10) (for details see Ref. 12).

III. THE SURVEY OF BV FORMALISM GEOMETRY

The formulas (2.5)–(2.12) of the previous section have the following geometrical meaning (for details see Refs. 3,5,6 and also Ref. 13). In the superspace $E^{(n.n)}$ with the coordinates $z^A=(x^1,\ldots,x^n,\theta^1,\ldots,\theta^n)$, where x^i are even, θ^i odd coordinates one can consider the structure defined by the pair $(dv,\{,\})$, where dv is the volume form and $\{,\}$ the odd nondegenerated Poisson bracket corresponding to the odd symplectic structure. To the structure $(dv,\{,\})$ on $E^{(n.n)}$ corresponds the following geometrical constructions that constitutes the essence of BV formalism geometry.

We define a second-order differential operator on E (so-called Δ operator),

$$\Delta_{dv}f=\frac{1}{2}\operatorname{div}_{dv}\mathbf{D}_f\equiv\frac{1}{2}\frac{\mathscr{L}_{\mathbf{D}_f}dv}{dv}, \tag{3.1}$$

where $\mathbf{D}_f$ is the Hamiltonian vector field corresponding to the function f. This operator is typical for the odd symplectic geometry.[3]

Because of the Darboux theorem we can always choose (at least locally) coordinates $z^A=(x^1,\ldots,x^n,\theta^1,\ldots,\theta^n)$ (so-called Darboux coordinates) in which the symplectic structure and corresponding Poisson bracket take canonical expression:

$$\{f,g\}=\frac{\partial f}{\partial x^i}\frac{\partial g}{\partial\theta^i}+(-1)^{p(f)}\frac{\partial f}{\partial\theta^i}\frac{\partial g}{\partial x^i}. \tag{3.2}$$

If the volume form $dv=\rho(z)d^nx\,d^n\theta$ in Darboux coordinates, then

$$\Delta_{dv}f=\frac{1}{2\rho}(-1)^{p(A)}\frac{\partial}{\partial z^A}(\rho\{z^A,f\})=\frac{1}{2}\{\log\rho,f\}+\frac{\partial^2 f}{\partial x^i\,\partial\theta^i}, \tag{3.3}$$

where $p(A)$ is the parity of the coordinate z^A.

We say that the pair $(dv,\{,\})$ is canonical in the Darboux coordinates $z^A=(x^1,\ldots,x^n,\theta^1,\ldots,\theta^n)$ if $dv=1\cdot d^nx\,d^n\theta$. Then the Δ operator takes the canonical expression:

$$\Delta_0 f=\frac{\partial^2 f}{\partial x^i\,\partial\theta^i}. \tag{3.4}$$

If two Δ operators, Δ_{dv} and $\Delta_{d\tilde{v}}$, correspond to two structures with the different volume forms dv and $d\tilde{v}$ and the same symplectic structure, then it is easy to see using (3.3) that

$$\Delta_{d\tilde{v}}f=\Delta_{dv}f+\tfrac{1}{2}\{\log\lambda,f\}, \tag{3.5}$$

and

$$\Delta^2_{d\tilde{v}}f=\Delta^2_{dv}f+\{\lambda^{-1/2}\Delta_{dv}\lambda^{1/2},f\}, \tag{3.6}$$

where $d\tilde{v}=\lambda dv$.

For a given structure $(dv,\{,\})$ *the following statements are equivalent*:

(i) the operator Δ_{dv} is nilpotent,

$$\Delta^2_{dv}=0; \tag{3.7i}$$

(ii) the function $\rho(z)$ defining the volume form dv in Darboux coordinates obeys the equation

$$\Delta_0\sqrt{\rho}=0; \tag{3.7ii}$$

(iii) there exist Darboux coordinates in which the pair $(dv,\{,\})$ is canonical.

The (iii)⇒(i) is evident, the (i)⇔(ii) immediately follows from (3.6). The (i)⇒(iii) needs a more detailed analysis.

Remark: The structures $(dv,\{,\})$ for which these properties are obeyed are called SP structures.[5] One of us (O.M.K.) wants to note that in Ref. 3 where was first introduced the Δ operator related to the structure $(dv,\{,\})$ for an arbitrary volume form in superspace, the false statement was made that every $(dv,\{,\})$ structure is the SP structure.

The pair $(dv,\{,\})$ generates the invariant volume form dv_Λ on arbitrary Lagrangian manifolds Λ in E—"the square root of the volume form dv" in the following way:[5]

$$dv_\Lambda(e_1,\ldots,e_n)=\sqrt{dv(e_1,\ldots,e_n,f_1,\ldots,f_n)}, \tag{3.8}$$

where $\{e_i\}$ are the vectors tangent to Λ and $\{f_i\}$ are arbitrary vectors, such that

$$w(e_i,f_j)=\delta_{ij}$$

(w is a two-form, which defines the symplectic structure).

In these terms the BV formalism has the following geometrical meaning: We consider in the superspace $\mathcal{E}$ of the fields and antifields the pair $(dv,\{,\})$, where the volume form is defined by the master action:

$$\rho=e^{2\mathcal{S}}, \tag{3.9}$$

and $\{,\}$ is defined by (2.3). Then using (i), (ii), (iii), and comparing formulas (3.7) with formulas (2.3)–(2.5), we see that the master equation is nothing but the condition of nilpotency of the corresponding Δ operator. The partition function is nothing but the integral of the invariant volume form (3.8) on the Lagrangian surface Λ,[5] and Eq. (2.12) is the covariant expression for this volume form.

In the next section we will try to understand these statements from the point of view of integration theory on surfaces.

IV. INTEGRATION OVER SURFACES

In this section we present the basic objects of integration theory on supermanifolds: densities and dual densities.[9–11] We consider the special class of densities on which the exterior differential can be defined correctly—pseudodifferential forms.[8–11] Then we describe the Baranov–Schwarz (BS) representation of the pseudodifferential forms via the function on the superspace associated to the tangent bundle of initial space.[9] Considering the dual construction we show that the closure of the pseudodifferential form in the BS representation is formulated in terms of the Δ operator.

A. Densities

Let Ω be an arbitrary supersurface in the superspace E with coordinates z^a, given by a parametrization $z^a=z^a(\zeta^s)$. The function $L(z^a,\partial z^a/\partial\zeta^s)$ on E is called a density (covariant density), if it satisfies the condition[10]

$$L\left(z^a,\frac{\partial z^a}{\partial\zeta^{s'}}K_s^{s'}\right)=L\left(z^a,\frac{\partial z^a}{\partial\zeta^s}\right)\mathrm{Ber}\,K_s^{s'}, \tag{4.1}$$

where Ber is the superdeterminant of the matrix.

Then the following integral does not depend on the choice of the parametrization of the surface Ω:

$$\Phi_{\Omega}(L)=\int L\left(z^a(\zeta),\frac{\partial z^a(\zeta)}{\partial\zeta^s}\right)d\zeta, \tag{4.2}$$

and correctly defines the functional on the surface Ω corresponding to the density L.

In the bosonic case where there are not odd variables, one can see that if a density L is a linear function of the $\partial z^a(\zeta)/\partial\zeta^s$, then to L corresponds a differential form. The covariant density is closed if it satisfies identically the condition

$$\Phi_{\Omega+\delta\Omega}(L)=\Phi_{\Omega}(L), \tag{4.3}$$

for an arbitrary variation of an arbitrary surface Ω (up to boundary terms).

It is easy to see that

$$\Phi_{\Omega+\delta\Omega}(L)-\Phi_{\Omega}(L)=\mathcal{F}_a(z)\delta z^a, \tag{4.4}$$

where

$$\mathcal{F}_a(z)=\frac{\partial L}{\partial z^a}-(-1)^{p(a)p(s)}\frac{d}{d\zeta^s}\frac{\partial L}{\partial z^a_{,s}}, \tag{4.5}$$

are the left part of the Euler–Lagrange equations of the functional $\Phi(L)$.

B. How to define exterior derivative operator on the densities?

If d is the exterior derivative, then

$$\Phi_{\Omega+\delta\Omega}(L)-\Phi_{\Omega}(L)=\Phi_{\delta V}(dL)\ \ (\text{Stokes theorem}). \tag{4.6}$$

Equation (4.6) put strong restrictions on the class of densities on which the operator d is correctly defined.[11] Comparing (4.4), (4.5), and (4.6), we see that d is correctly defined if $\mathcal{F}_a(z)$ in (4.5) *do not contain the second derivatives of* ζ (for details see Ref. 11):

$$\frac{\partial^2 L}{\partial z^a_{,s}\,\partial z^b_{,t}}=-(-1)^{p(s)p(t)+(p(s)+p(t))p(b)}\frac{\partial^2 L}{\partial z^a_{,t}\,\partial z^b_{,s}}. \tag{4.7}$$

In this case dL defined by (4.6) does not depend on the second derivatives and

$$d^2=0. \tag{4.8}$$

The densities, which obey the conditions (4.7) are called pseudodifferential forms.

In the bosonic case from (4.7) follows that the density is a linear function of the variables $\partial z^a(\zeta)/\partial\zeta^s$, i.e. the exterior derivation can be defined only on the densities that correspond to the differential forms. In the supercase in general from (4.7) linearity conditions do not follow—the differential forms in the superspace are not in general integration objects over supersurfaces. It is the pseudodifferential forms that take their place as integration objects obeying Stokes theorem[8–11]).

To obtain the pseudodifferential forms, Baranov and Schwarz in Ref. 9 suggested the following procedure, which seems very natural in the spirit of a ghost technique:

Let STE be the superspace associated to the tangent bundle TE of the superspace E and (z^a,z^{*a}) its (local) coordinates. The coordinates z^{*a} transform from map to map like dz^a, and their parity is reversed: $p(z^{*a})=p(z^a)+1$. Then to an arbitrary function $W(z^a,z^{*a})$ on STE corresponds the density:

$$L_W = L\left(z^a, \frac{\partial z^a}{\partial \zeta^s}\right) = \int W\left(z^a, \frac{\partial z^a}{\partial \zeta^s}\,\nu^s\right) d\nu, \tag{4.9}$$

where ν^s has the reversed parity:

$$p(\nu^s) = p(\zeta^s) + 1. \tag{4.10}$$

It is easy to see using (4.10) that (4.9) obeys Eqs. (4.1) and (4.7) so that Eq. (4.9) indeed defines a density that is a pseudodifferential form. We say that the function W is the BS representation of the pseudodifferential form L_W.

A simple calculation shows that in the BS representation the exterior differentiation operator has the following expression:

$$\hat{d} = (-1)^{p(a)} z^{*a} \frac{\partial}{\partial z^a}, \quad (d(L_W) = L_{\hat{d}W}). \tag{4.11}$$

C. Dual densities

Consider now the dual constructions.

Let E be the superspace, and the volume form $dv = \rho(z)dz$ is defined on it.

Let Ω be an arbitrary supersurface in the superspace E with coordinates z^a, given not by the parametrization $z^a = z^a(\zeta^s)$ but by the equations

$$f^\alpha(z) = 0. \tag{4.12}$$

The function $\tilde{L} = \tilde{L}(z^a, \partial f^\alpha / \partial z^a)$ is called a D density (dual density) if it is satisfied to the condition

$$\tilde{L}\left(z^a, \frac{\partial f^\alpha(z)}{\partial z^a}\,\eta^\beta_\alpha\right) = \tilde{L}\left(z^a, \frac{\partial f^\alpha(z)}{\partial z^a}\right) \mathrm{Ber}\ \eta^\beta_\alpha. \tag{4.13}$$

Then the following integral does not depend on the choice of the equations (4.12) that define the surface Ω:

$$\Phi_\Omega(\tilde{L}) = \int \tilde{L}\left(z^a, \frac{\partial f^\alpha(z)}{\partial z^a}\right) \delta(f^\alpha(z)) dv, \tag{4.14}$$

and correctly defines the functional on the surface Ω corresponding to the D density $\tilde{L}$.

The D density $\tilde{L}$ corresponds to the density $L(\tilde{L} \to L)$ if for the arbitrary surface Ω the functionals (4.2) and (4.14) coincide (for details see Ref. 10).

[For example, the integrand in (2.12) is a D density that corresponds to the density (3.8).]

The D density is closed, if it satisfies the condition (4.3) (where we replace $\tilde{L} \to L$).

One can obtain the dual densities corresponding to pseudodifferential forms (such densities are called pseudointegral forms) by the procedure dual to the Baranov–Schwarz one.

Let ST^*E be the superspace associated to the cotangent bundle T^*E of the superspace E and (z^a, z^*_a) its (local) coordinates. The coordinates z^*_a transform from map to map like $\partial/\partial z^a$, and their parity is reversed: $p(z^*_a) = p(z^a) + 1$. Then to an arbitrary function $W(z^a, z^*_a)$ on ST^*E corresponds the D density—pseudointegral form:

$$\tilde{L}_W = \tilde{L}\left(z^a, \frac{\partial f^\alpha}{\partial z^a}\right) = \int W\left(z^a, \frac{\partial f^\alpha}{\partial z^a}\,\nu_\alpha\right) d\nu, \tag{4.15a}$$

where ν^α have the reversed parity like in (4.10):

$$p(\nu^\alpha)=p(f^\alpha)+1.$$

The functional (4.14) can be expressed in terms of the function W in the following way:

$$\Phi_\Omega(\widetilde{L})=\int \rho(z)W(z,z^*)\delta\left(z_a^*-\frac{\partial f^\alpha}{\partial z^a}\nu_\alpha\right)\delta(f^a)dz\ dz^*\ d\nu. \tag{4.15b}$$

A straightforward calculation shows that the operator of exterior differentiation $\widehat{\widetilde{d}}$ in the BS representation of the pseudointegral forms has the following expression:

$$\widehat{\widetilde{d}}=\frac{1}{\rho}\frac{\partial\rho}{\partial z^a}\frac{\partial}{\partial z_a^*}+\frac{\partial^2}{\partial z^a\ \partial z_a^*}. \tag{4.16}$$

(If $\widetilde{L}=\widetilde{L}_W\to L$ then $\widetilde{L}'=\widetilde{L}_{\widetilde{d}W}\to dL$.)

Comparing the equations (4.16) and (3.3), we see that on the superspace ST^*E it is natural to consider the structure $(d\hat{v},\{,\})$ (see Sec. III), where $\{,\}$ is the canonical odd symplectic structure on ST^*E generated by the relations

$$\{z^a,z_b\}=\{z^{*a},z_b^*\}=0,\quad \{z^a,z_b^*\}=(-1)^{p(a)}\delta_b^a, \tag{4.17}$$

and the volume form

$$d\hat{v}=\rho^2(z^1\cdots z^n)dz^1\cdots dz^n\ dz_1^*\cdots dz_n^*. \tag{4.18}$$

[One can note that (4.18) is in the accordance with (3.8). The space E with volume form $dv=\rho\ dz^1\cdots dz^n$ is evidently the Lagrangian surface in ST^*E with volume form (4.18)].

Comparing (4.16) and (3.3), we see that to the operator of the exterior differentiation corresponds the Δ operator:

$$\widehat{\widetilde{d}}=\Delta_{d\hat{v}} \tag{4.19a}$$

and the condition of closure of the dual density $\widetilde{L}_W$ in the BS representation is

$$\Delta_{d\hat{v}}W=0, \tag{4.19b}$$

where $d\hat{v}$ is defined by (4.18) and $\Delta_{d\hat{v}}$ by (3.3). This operator in this case is nilpotent because it corresponds to exterior differentiation operator. [Independently from (4.16) and (4.8), it follows from (4.18) and (3.7ii) or from (4.18) and (3.7iii) because $d\hat{v}$ "depends" on the half of the variables of the superspace ST^*E.]

V. THE CLOSED DENSITIES AND THE BV FORMALISM GEOMETRY

In this section we consider two examples of the previous constructions, comparing them with the constructions of Secs. II, III, IV. We check connections between the gauge symmetries of the theory, the densities that are integrand in the partition function after eliminating gauge degrees of freedom, and volume forms obeying the BV master equation.

Example 1: Let $R^a(z)(\partial/\partial z^a)$ be an even vector field on the superspace E with coordinates $(z^1,\ldots,z^n)$ and with volume form $dv=\rho(z)dz^1\cdots dz^n$. To this vector field corresponds the D density

$$\widetilde{L}=R^a(z^a)\frac{\partial f}{\partial z^a}. \tag{5.1}$$

One can define the functional on the surfaces of codimension (1.0) corresponding to the density (5.1):

$$\Phi_{\Omega}(\widetilde{L})=\int \widetilde{L}\left(z^a,\frac{\partial f(z)}{\partial z^a}\right)\delta(f(z))dv=\int R^a(z)\,\frac{\partial f(z)}{\partial z^a}\,\delta(f(z))dv, \tag{5.2}$$

where $f=0$ is the equation that defines the surface Ω (f is an even function). This functional is nothing but the well-known formula for the flux of the vector field through the surface Ω. It is evident that the density $\widetilde{L}$ in (5.1) is a pseudointegral form. To this density corresponds the function (4.15),

$$W=(-1)^{p(a)}R^a(z)z_a^*, \tag{5.3}$$

on ST^*E ($\widetilde{L}=\widetilde{L}_W$). The condition of closure of the density (5.1) is the Gauss formula:

$$\mathrm{div}_{dv}\,\mathbf{R}=\frac{1}{\rho}\,(-1)^a\,\frac{\partial(\rho R^a)}{\partial z^a}=0. \tag{5.4}$$

In BS representation it is [(4.18), (4.19)]

$$\Delta_{d\hat{v}}W=0 \quad [d\hat{v}=\rho^2(z)dz^1\cdots dz^n). \tag{5.5}$$

We can consider this example as a toy example of field theory.

Let a space E be the space of fields configurations ($z^a\to\varphi^a$) Let $R^a(z)(\partial/\partial z^a)$ be the "gauge" symmetry of the action $S(z)$ [compare with (2.1)]:

$$R^a(z)\,\frac{\partial S(z)}{\partial z^a}=0, \tag{5.6}$$

and this symmetry preserves the canonical volume form:

$$(-1)^{p(a)}\,\frac{\partial R^a}{\partial z^a}=0. \tag{5.7}$$

If we put

$$\rho=e^S, \tag{5.8}$$

then we see that the functional (5.2) corresponding to the density (5.1) constructed via the "gauge symmetry" $\mathbf{R}$ is the partition function of the theory with the action S after eliminating the "gauge" degrees of freedom corresponding to the symmetry $\mathbf{R}$. From (5.6)–(5.8) follow (5.4), (5.5); hence (5.1) is closed and (5.2) is "gauge" independent. Now we consider the more realistic example.

Example 2: Let

$$\left\{\mathbf{R}_\alpha=R^a_\alpha(z)\,\frac{\partial}{\partial z^a}\right\} \quad (\alpha=1,\ldots,m) \tag{5.9}$$

be the collection of the vector fields on the superspace E, with coordinates $(z^1,\ldots,z^n)$ and with volume form

$$dv=\rho(z)dz^1\cdots dz^n. \tag{5.10}$$

To (5.9) corresponds D density,

$$\widetilde{L}=\mathrm{Ber}\left(R^a_\alpha(z)\,\frac{\partial f^\beta}{\partial z^a}\right) \tag{5.11}$$

[the condition (4.13) is evidently satisfied]. One can consider the functional:

$$\Phi_\Omega(\widetilde{L})=\int \mathrm{Ber}\left(R^a_\alpha(z)\,\frac{\partial f^\beta}{\partial z^a}\right)\delta(f^\alpha)dv, \tag{5.12}$$

where Ω is the surface defined by the equations

$$f^\alpha=0.$$

[In the usual (not super)case, (5.12) can be considered as the flux of the polyvectorial field $\mathbf{R}_1\wedge\cdots\wedge\mathbf{R}_m$ through the surface Ω.]

One can see that $\widetilde{L}$ in (5.11) is the pseudointegral form $\widetilde{L}_W$, where W BS representation of this density can be defined by the following formal relation:

$$W=\int e^{c^\alpha R^a_\alpha(z)z^*_a}\,dc, \tag{5.13}$$

where we introduce additional variables (ghosts) c^α $[p(c^\alpha)=p(\nu^\alpha)]$. [(5.13) is correct if all the symmetries $\mathbf{R}_\alpha$ are even.]

Let the equations (5.6), (5.7) be satisfied for all $\mathbf{R}_\alpha$—these vector fields being the gauge symmetries of the theory with the action S. Again as in Example 1 we consider as volume form the exponent of the action (5.8). Is the density (5.11) closed in this case?

It is easy to see that

$$R^a(z)\,\frac{\partial S(z)}{\partial z^a}=0\Rightarrow[\mathbf{R}_\alpha,\mathbf{R}_\beta]=t^\gamma_{\alpha\beta}\mathbf{R}_c+E^{[ab]}_{\alpha\beta}\,\frac{\partial S(z)}{\partial z^b}. \tag{5.14}$$

To check the relation with the BV formalism, we consider instead superspace E the superspace E^e enlarged with the additional coordinates c^α. [The coordinates of E^e are $z^A=(z^a,c^\alpha)$.] The volume forms dv on E (5.10) and $d\hat{v}$ on ST^*E [see (4.18)] and the symplectic structure (4.17) are naturally prolongated on E^e and ST^*E^e.

Using (4.15a), (4.15b), and (5.13), we rewrite (5.12) as the integral over the space T^*SE^e:

$$\Phi_\Omega(\widetilde{L})=\int e^S e^{c^\alpha R^a_\alpha(z)z^*_a}\,dc\;\delta\left(z^*_a-\frac{\partial f^\alpha}{\partial z^a}\,\nu_\alpha\right)\delta(f^\alpha)dz\;dz^*\;dv \tag{5.15}$$

$$=\int e^S W^e(z^A,z^*_A)\,\delta\left(z^*_A-\frac{\partial f^\alpha}{\partial z^A}\,\nu_\alpha\right)\delta(f^\alpha)dz\;dz^*\;dv, \tag{5.16}$$

where

$$W^e(z^A,z^*_A)=e^{c^\alpha R^a_\alpha(z)z^*_a}, \tag{5.17}$$

is the BS representation of the pseudointegral form in ST^*E^e. Using (4.19), we can check its closure.

[(5.15), (5.16) is the partition function of the theory obtained after performing the Fadeev–Popov trick.]

Let

$$\Delta_{d\hat{v}} W^e = \Delta_{d\hat{v}} e^{c^\alpha R^a_\alpha(z) z^*_a} = 0, \tag{5.18}$$

be satisfied. The condition (5.18) means that not only the function W on ST^*E corresponds to the closed density on E [i.e., the partition function (5.15) is gauge invariant], but the function W^e on ST^*E^e corresponds to the closed density on E^e as well. In this case, from (3.6) and (3.7), it follows that the Δ operator corresponding to the volume form,

$$d\tilde{v} = (W^e)^2 \cdot d\hat{v}, \tag{5.19}$$

is nilpotent, as well as the Δ operator corresponding to the volume form (5.8). Now from (3.7) follows that the master action $\mathscr{S}$ related with $d\tilde{v}$ in the same way as S is related with dv in (5.8):

$$\mathscr{S} = S + c^\alpha R^a_\alpha z^*_a, \quad (\tilde{\rho} = e^{\mathscr{S}}), \tag{5.20}$$

obeys the master equation. So in the case where (5.18) holds, starting from gauge symmetries we constructed the closed density (5.12), (5.13), interpreting the volume form as the exponent of the action. The corresponding functional (5.12) is the partition function. Localizing this density in the space enlarged with the ghosts we came to the volume form (exponent of the master action) that obeys the master action.

In the general case the density (5.11) *is not closed* and the partition function (5.12), (5.16) is not gauge invariant.

Even in the case where the algebra of the symmetries is closed,

$$t^\gamma_{\alpha\beta} = \text{const} \quad \text{and} \quad E^{[ab]}_{\alpha\beta} \equiv 0, \tag{5.21}$$

the application of the Δ operator (4.19) to (5.17) and (5.13) give us

$$\Delta_{d\hat{v}} W^e = \Delta_{d\hat{v}} e^{c^\alpha R^a_\alpha(z) z^*_a}\, dc = \frac{1}{2}\, c^\alpha c^\beta \left(t^\gamma_{\alpha\beta} R^a_\gamma(z) + E^{[ab]}_{\alpha\beta} \frac{\partial S(z)}{\partial z^b} \right) z^*_a e^{c^\alpha R^a_\alpha(z) z^*_a}\, dc \tag{5.22}$$

and

$$\Delta_{d\hat{v}} W = \Delta_{d\hat{v}} \int e^{c^\alpha R^a_\alpha(z) z^*_a}\, dc = \int c^\alpha c^\beta \left(t^\gamma_{\alpha\beta} R^a_\gamma(z) + E^{[ab]}_{\alpha\beta} \frac{\partial S(z)}{\partial z^b} \right) z^*_a e^{c^\alpha R^a_\alpha(z) z^*_a}\, dc \tag{5.23}$$

In particular, it is easy to see from (5.22) that if the algebra of the symmetries is Abelian we come to (5.18).

If, for example, the symmetries are even and they form the closed unimodular algebra ($E^{[ab]}_{\alpha\beta} = 0$, $t^\gamma_{\alpha\beta} = \text{const}$ and $\Sigma_\alpha t^\alpha_{\alpha,\beta} = 0$), then the right-hand side of (5.23) is vanishing, so the function W corresponds to closed density in E (i.e., the partition function is gauge invariant). But the function W^e in (5.22) does not correspond to closed density in E^e. To close it in this case, one has to consider in the space ST^*E^e the function

$$W'^e(z^A, z^*_A) = e^{c^\alpha R^a_\alpha(z) z^*_a + (1/2) t^\gamma_{\alpha\beta} c^\alpha c^\beta c^*_\gamma},$$

which corresponds to a closed density in E^e. So the corresponding volume form and the master action,

$$\mathscr{S} = S + c^\alpha R^a_\alpha z^*_a + \tfrac{1}{2} t^\gamma_{\alpha\beta} c^\alpha c^\beta c^*_\gamma,$$

obey the master equation [compare with (2.5b)].

In the general case the density (5.11), (5.13) plays the role of initial conditions for constructing the closed density in enlarged space—i.e., the volume form (the exponent of the master action) obeying (3.7) (for details see Ref. 12).

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BRST quantization of gauge theory in noncommutative geometry: Matrix derivative approach

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The Becchi–Rouet–Stora–Tyutin (BRST) quantization of a gauge theory in noncommutative geometry is carried out in the "matrix derivative" approach. BRST/anti-BRST transformation rules are obtained by applying the horizontality condition, in the superconnection formalism. A BRST/anti-BRST invariant quantum action is then constructed, using an adaptation of the method devised by Baulieu and Thierry-Mieg for the Yang–Mills case. The resulting quantum action turns out to be the same as that of a gauge theory in the 't Hooft gauge with spontaneously broken symmetry. Our result shows that only the even part of the supergroup acts as a gauge symmetry, while the odd part effectively provides a global symmetry. We treat the general formalism first, then work out the SU(2/1) and SU(2/2) cases explicitly. © *1996 American Institute of Physics.* [S0022-2488(96)02907-6]

I. INTRODUCTION

The Higgs mechanism makes it possible to give masses to gauge bosons, while preserving the gauge symmetry. In this construction, some of the original scalar particle fields "mutate" into the longitudinal components of the (now massive) gauge bosons. This fact may reflect the existence of an underlying structure, in which the gauge bosons and the original scalar particles belong to the same multiplet of a larger group. It is, therefore, natural to search for such a larger symmetry group and a suitable multiplet. As a matter of fact, this idea was implemented many years ago, using the supergroup SU(2/1);[1] it was also shown that this use of a supergroup could be extended to a large class of spontaneously broken symmetries.[2] More recently, the idea has further mathematically evolved within the *superconnection* construct.[3–6]

Another recent advance in mathematical physics has consisted[7] in Connes' *noncommutative geometry*. In this formalism, the Dirac K cycle on a star algebra acting on a Hilbert space, plays an important role, with possible applications to particle physics. Connes and Lott[8] then showed in particular that the *standard model* could be obtained in noncommutative geometry, as a gauge theory with a built-in spontaneous symmetry breakdown mechanism. The base space is the product of space–time by a set of two points (L, R), i.e., two disconnected $M_L \oplus M_R$. The gauge group is in both SU(2)×U(1), with different fiber representations. The scalar connection arises when parallel transport involves moving between the two manifolds (together with a matrix derivative) acting on the combined Hilbert spaces in the associated fiber. The Connes–Lott work has been further extended to GUT (grand unified theories),[9] to gravity,[10] and to supersymmetric theories.[11]

Soon after the work of Connes and Lott, Coquereaux and other workers[12,13] showed that the Connes–Lott approach is equivalent to a theory based on the superconnection concept,[5,14] rediscovering SU(2/1) in the process. The above joint embedding of the SU(2)×U(1) representation matrices for the lepton or quark $L \oplus R$ combined Hilbert spaces precisely reproduces the SU(2/1) matrices. In the Coquereaux *et al.*'s formulation, a Z_2 graded space of matrix-valued forms is

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constructed, with a generalized derivative; 0-form and 1-form fields together represent a superconnection. The generalized derivative consists of the usual Cartan exterior differential operator, raising the form degree by one unit and thus also changing its Grassmann grading (which we denote as "w grading," i.e., **d** has odd w grading) plus a graded *discrete* operator consisting in a (graded) commutator with a constant matrix and satisfying certain algebraic conditions (including odd grading in a supergroup's generating superalgebra, "g-odd" in our nomenclature). This graded commutator (or supercommutator) with a constant matrix is the *matrix derivative*.[13] We shall denote the Coquereaux *et al.* approach as *the matrix derivative* approach.

The equivalence between the Connes–Lott and Coquereaux *et al.* approaches has been stressed by Scheck and collaborators.[15] In both approaches, the 0-form scalar field is interpreted geometrically as an object interconnecting a two-sheeted world, whereas the 1-form field plays the usual role of a gauge field. The end product is equivalent to an extension of the internal supersymmetry method in its superconnection formulation, completing, as we shall see, its geometric generation of a spontaneous symmetry breakdown mode for a local gauge symmetry.

We have recently quantized the SU(2/1) electroweak theory in the superconnection formalism.[16] In the present paper we treat the quantization of the noncommutative geometry version of this "supergauge theory," by adjoining the matrix derivative approach to the superconnection formulation. Actually, this formulation goes beyond the internal supersymmetry method in one aspect, namely the emergence of the *negative squared mass* term for the scalar (Higgs) field from the geometry; in our previous treatment, most terms in the spontaneous symmetry breakdown Lagrangian emerged geometrically, namely (aside from the usual Yang–Mills term) the "free" Higgs field Lagrangian plus its interaction with the gauge bosons—and the quartic Higgs field potential; the exception, which had to be put in "by hand" (and thus also broke the symmetry explicitly) was this negative squared mass term, which is now provided by the matrix derivative.

We obtain the Becchi–Rouet–Stora–Tyutin (BRST)/anti-BRST transformation rules of the theory, applying our *horizontality* condition, extending Thierry-Mieg's ansatz.[6,17,18] We construct the quantum action by adapting the Baulieu/Thierry-Mieg method[19] for the Yang–Mills theory.

There are two important features deriving from our result. The first is the fact that we obtain the most appropriate gauge condition for a spontaneously broken gauge theory with scalar field, the 't Hooft gauge,[20,21] simply by adapting the method of Ref. 19, which would give the Landau gauge for the unbroken Yang–Mills theory, to the noncommutative geometry framework. The other relates to the physical content of a gauge theory in the noncommutative setting. Our quantization reveals that only the even part of the supergroup indeed acts as a gauge symmetry; the odd part simply produces a global symmetry. The resulting BRST transformation rules for the fields are thus the same as those of the spontaneously broken gauge theory with a Higgs mechanism, except that the scalar field transformation rule is changed by the addition of a constant shift (a vacuum shift), due to the action of the matrix derivative, thereby implementing geometrically the triggering of the spontaneous breakdown. Other fields are not affected by the appearance of the matrix derivative.

In Sec. II, we study the BRST quantization in the matrix derivative approach for the general case. In Sec. III, we treat the SU(2/1) gauge theory, effectively an algebraically constrained standard model SU(2)×U(1) gauge theory of the electroweak interaction. In Sec. IV, we consider an SU(2/2) gauge theory, which reduces to the spontaneously broken symmetry of an SU(2) ×SU(2) σ model. Section V contains a discussion and conclusions.

II. BRST/ANTI-BRST SYMMETRY AND QUANTUM ACTION

In the matrix derivative approach of a noncommutative geometrical gauge theory, the 0-form scalar field and 1-form gauge field together form a superconnection, with w-odd forms in the g-even part and w-even forms in the g-odd part of the supergroup. We write the superconnection $\mathscr{T}$ as

$$\mathcal{J}=\mathcal{J}_{\rm ev}+\mathcal{J}_{\rm od}=\begin{pmatrix}\omega_0 & 0\\ 0 & \omega_1\end{pmatrix}+\begin{pmatrix}0 & L_{01}\\ L_{10} & 0\end{pmatrix}. \tag{1}$$

The overall Z_2 grading is given by the sum of the supermatrix grading (Z_2 "g" grading) and the differential form grading (Z_2 "w" grading). The total grading of the superconnection is therefore odd, in this Z_2 graded space.[16] Multiplication in this superspace is given by[5,12]

$$(h\otimes W)\cdot(h'\otimes W')=(-1)^{|W||h'|}(hh')\otimes(WW'), \tag{2}$$

where W, W' are differential forms of fixed Grassmannian Z_2 w gradings $|W|$, $|W'|$, and h, h' are supermatrices of fixed Z_2 g grading $|h|$, $|h'|$. With this convention, we obtain the product rule for any two elements in our total Z_2 graded space, assuming A, B, C, D to be matrix-valued differential forms, which have fixed Z_2 w gradings of 0 or 1, depending on whether they are even or odd forms, respectively,[5,12]

$$\begin{pmatrix}A & B\\ C & D\end{pmatrix}\cdot\begin{pmatrix}A' & B'\\ C' & D'\end{pmatrix}=\begin{pmatrix}A\wedge A'+(-1)^{|B|}B\wedge C' & (-1)^{|A|}A\wedge B'+B\wedge D'\\ C\wedge A'+(-1)^{|D|}D\wedge C' & (-1)^{|C|}C\wedge B'+D\wedge D'\end{pmatrix}. \tag{3}$$

Once the superconnection is given, the supercurvature $\mathcal{F}_t$ is defined in the usual manner, with the generalized derivative $\mathbf{d}_t$, consisting of the usual 1-form differential operator $\mathbf{d}$ and the *matrix derivative* $\mathbf{d}_M$:[12,13]

$$\mathcal{F}_t=\mathbf{d}_t\mathcal{J}+\mathcal{J}\cdot\mathcal{J}, \tag{4}$$

$$\mathbf{d}_t=\mathbf{d}+\mathbf{d}_M, \tag{5}$$

$$\mathbf{d}=\begin{pmatrix}d & 0\\ 0 & d\end{pmatrix},\quad \text{where } d=1\otimes dx^\mu\frac{\partial}{\partial x^\mu}. \tag{6}$$

The matrix derivative is given by

$$\mathbf{d}_M=i[\,\eta,\quad]_\pm,\quad \text{where}\quad \eta=\begin{pmatrix}0 & \zeta\\ \bar{\zeta} & 0\end{pmatrix}. \tag{7}$$

Here ζ and $\bar{\zeta}$ are constant matrices of zero forms, satisfying

$$\bar{\zeta}\zeta=\zeta\bar{\zeta}\propto 1, \tag{8}$$

so that the matrix derivative satisfies the nilpotency condition, $\mathbf{d}_M^2=0$. Note that the total grading of the matrix derivative $\mathbf{d}_M$ is odd. Thus the matrix derivative is a supercommutator, i.e., it acts as a commutator for objects of even total grading and as an anticommutator for objects of odd total grading, where by "total," we mean the product of the gradings of "g" and "w."

We now write the classical action of the gauge theory in noncommutative geometry as

$$\mathcal{S}_{\rm cl}=-\frac{1}{4}\int \mathrm{Tr}\,\mathcal{F}_t^*\cdot\mathcal{F}_t, \tag{9}$$

where * denotes taking the Hermitian conjugate for supermatrices and taking the Hodge dual for differential forms. In order to find the BRST/anti-BRST transformation rules, we use the so-called *horizontality* condition,[3,17–19] which is another description of the Maurer–Cartan equation:

$$\tilde{\mathcal{F}}_t=\mathcal{F}_t, \tag{10}$$

where $\tilde{\mathscr{F}}_t$ is the supercurvature, defined in the extended space of the *doubled* fiber bundle,[16]

$$\tilde{\mathscr{F}}_t=\tilde{\mathbf{d}}_t\tilde{\mathscr{T}}+\tilde{\mathscr{T}}\cdot\tilde{\mathscr{T}}. \tag{11}$$

"Doubling" implies the extension of the base manifold through doubling the fiber, from $\{\mathscr{G}\}$ to $\{\mathscr{G}\}\otimes\{\mathscr{G}\}$, so that we have a gauge fiber coordinate y and its dual $\bar{y}$.[6,17–19] In this extended space, the generalized derivative and superconnection are given by

$$\tilde{\mathbf{d}}_t=\mathbf{d}_t+\mathbf{s}+\bar{\mathbf{s}}, \tag{12}$$

$$\tilde{\mathscr{T}}=\mathscr{T}+\mathscr{C}+\bar{\mathscr{C}}. \tag{13}$$

Here, $\mathbf{s}$ and $\bar{\mathbf{s}}$ are 1-form differential operators acting, respectively, on the coordinates of the fiber and of its dual:

$$\begin{aligned}\mathbf{s}&=\begin{pmatrix} s & 0\\ 0 & s\end{pmatrix},\quad \text{where } s=1\otimes dy^N\frac{\partial}{\partial y^N},\\ \bar{\mathbf{s}}&=\begin{pmatrix} \bar{s} & 0\\ 0 & \bar{s}\end{pmatrix},\quad \text{where } \bar{s}=1\otimes d\bar{y}^M\frac{\partial}{\partial \bar{y}^M}.\end{aligned} \tag{14}$$

C and $\bar{C}$ are obtained from $\mathscr{T}$ by replacing dx^μ by dy^N and $d\bar{y}^M$, and represent the ghost and antighost fields, respectively:

$$\begin{aligned}\mathscr{C}&=\begin{pmatrix} c_{0N}\,dy^N & 0\\ 0 & c_{1N}\,dy^N\end{pmatrix}\equiv\begin{pmatrix} c_0 & 0\\ 0 & c_1\end{pmatrix},\\ \bar{\mathscr{C}}&=\begin{pmatrix} \bar{c}_{0M}\,d\bar{y}^M & 0\\ 0 & \bar{c}_{1M}\,d\bar{y}^M\end{pmatrix}\equiv\begin{pmatrix} \bar{c}_0 & 0\\ 0 & \bar{c}_1\end{pmatrix}.\end{aligned} \tag{15}$$

After applying the horizontality condition we obtain the BRST/anti-BRST transformation rules:

$$\begin{aligned}(dy)^1{:}\,s\mathscr{T}&=-\mathbf{d}_t\mathscr{C}-\mathscr{T}\cdot\mathscr{C}-\mathscr{C}\cdot\mathscr{T},\\ (d\bar{y})^1{:}\,\bar{s}\mathscr{T}&=-\mathbf{d}_t\bar{\mathscr{C}}-\mathscr{T}\cdot\bar{\mathscr{C}}-\bar{\mathscr{C}}\cdot\mathscr{T},\\ (dy)^2{:}\,s\mathscr{C}&=-\mathscr{C}\cdot\mathscr{C},\\ (d\bar{y})^2{:}\,\bar{s}\bar{\mathscr{C}}&=-\bar{\mathscr{C}}\cdot\bar{\mathscr{C}},\\ (dy)^1(d\bar{y})^1{:}\,s\bar{\mathscr{C}}+\bar{s}\mathscr{C}+\mathscr{C}\cdot\bar{\mathscr{C}}+\bar{\mathscr{C}}\cdot\mathscr{C}&=0.\end{aligned} \tag{16}$$

By introducing an auxiliary field $\mathscr{E}$ such that

$$s\bar{\mathscr{C}}\equiv\mathscr{E},\quad i.e.,\quad \begin{pmatrix} s\bar{c}_0 & 0\\ 0 & s\bar{c}_1\end{pmatrix}\equiv\begin{pmatrix} b_0 & 0\\ 0 & b_1\end{pmatrix}, \tag{17}$$

we can fix the remaining BRST/anti-BRST transformation rules,

$$\overline{s}\mathscr{C}=-\mathscr{B}-\mathscr{C}\cdot\overline{\mathscr{C}}-\overline{\mathscr{C}}\cdot\mathscr{C},$$

$$s\mathscr{B}=0, \tag{18}$$

$$\overline{s}\mathscr{B}=-\overline{s}(\mathscr{C}\cdot\overline{\mathscr{C}}+\overline{\mathscr{C}}\cdot\mathscr{C})=-\overline{\mathscr{C}}\cdot\mathscr{B}+\mathscr{B}\cdot\overline{\mathscr{C}}.$$

One can easily check the nilpotency property of the BRST/anti-BRST transformations, $\mathbf{s}^2=\overline{\mathbf{s}}^2=0$, for the above transformation rules (16), (17), and (18).

Decomposing $\mathscr{T}$ into $\mathscr{T}_{\rm ev}+\mathscr{T}_{\rm od}$ as in (1), we can write the even and odd parts of the first two equations in (16) separately as follows, by noting that $\mathbf{d}$, $\mathbf{s}$, and $\overline{\mathbf{s}}$ are even matrices, whose entries are one-form differential operators.

$$\begin{aligned}
\text{Even part}\ :\quad & s\mathscr{T}_{\rm ev}=-\mathbf{d}\mathscr{C}-\mathscr{T}_{\rm ev}\cdot\mathscr{C}-\mathscr{C}\cdot\mathscr{T}_{\rm ev},\\
& \overline{s}\mathscr{T}_{\rm ev}=-\mathbf{d}\overline{\mathscr{C}}-\mathscr{T}_{\rm ev}\cdot\overline{\mathscr{C}}-\overline{\mathscr{C}}\cdot\mathscr{T}_{\rm ev},\\
\text{odd part}\ :\quad & s\mathscr{T}_{\rm od}=-\mathbf{d}_M\mathscr{C}-\mathscr{T}_{\rm od}\cdot\mathscr{C}-\mathscr{C}\cdot\mathscr{T}_{\rm od},\\
& \overline{s}\mathscr{T}_{\rm od}=-\mathbf{d}_M\overline{\mathscr{C}}-\mathscr{T}_{\rm od}\cdot\overline{\mathscr{C}}-\overline{\mathscr{C}}\cdot\mathscr{T}_{\rm od}.
\end{aligned} \tag{19}$$

Note that the even parts are the usual BRST/anti-BRST transformation rules of a one-form gauge field,[19] while the odd parts are those of a matter field, plus the additional terms caused by the matrix derivative. These additional terms represent a translation of the scalar field and correspond to the vacuum shift in the usual Higgs mechanism. The difference, however, is that this is a built-in property of a gauge theory in the noncommutative geometry setting, in contradistinction to the conventional Higgs construction. The system's "ordinary" gauge symmetry is thereby broken explicitly through that geometrical setting.

Adapting the Baulieu/Thierry-Mieg method for a BRST/anti-BRST invariant quantum action, which yields the Landau gauge for the usual Yang–Mills theory,[19] we write the quantum action as

$$\mathscr{S}_Q=-\frac{1}{4}\int \mathrm{Tr}\{\mathscr{F}_t^*\cdot\mathscr{F}_t-\mathbf{s}\overline{\mathbf{s}}(\mathscr{T}^*\cdot\mathscr{T})+\alpha\mathbf{s}(\overline{\mathscr{C}}^*\cdot\mathscr{B})\}, \tag{20}$$

where α is a parameter. Using the transformation rules (16), (17), (18), and (19), we obtain

$$\mathrm{Tr}\{\mathbf{s}\overline{\mathbf{s}}(\mathscr{T}_{\rm ev}^*\cdot\mathscr{T}_{\rm ev})\}=2\,\mathrm{Tr}\{(\mathscr{T}_{\rm ev})^*\cdot(\mathbf{d}\mathscr{B})+(\mathbf{d}\overline{\mathscr{C}})^*\cdot(\mathbf{d}\mathscr{C}+\mathscr{T}_{\rm ev}\cdot\mathscr{C}+\mathscr{C}\cdot\mathscr{T}_{\rm ev})\}, \tag{21}$$

$$\mathrm{Tr}\{\mathbf{s}\overline{\mathbf{s}}(\mathscr{T}_{\rm od}^*\cdot\mathscr{T}_{\rm od})\}=2\,\mathrm{Tr}\{(\mathscr{T}_{\rm od})^*\cdot(\mathbf{d}_M\mathscr{B})+(\mathbf{d}_M\overline{\mathscr{C}})^*\cdot(\mathbf{d}_M\mathscr{C}+\mathscr{T}_{\rm od}\cdot\mathscr{C}+\mathscr{C}\cdot\mathscr{T}_{\rm od})\}, \tag{22}$$

and

$$\mathrm{Tr}\{\alpha\mathbf{s}(\overline{\mathscr{C}}^*\cdot\mathscr{B})\}=\mathrm{Tr}\{\alpha\mathscr{B}^*\cdot\mathscr{B}\}. \tag{23}$$

Thus, the quantum action $\mathscr{S}_Q$ can be written as

$$\begin{aligned}
\mathscr{S}_Q=-\frac{1}{4}\int \mathrm{TR}\{&\mathscr{F}_t^*\cdot\mathscr{F}_t+\alpha\mathscr{B}^*\cdot\mathscr{B}-2(\mathscr{T}_{\rm ev})^*\cdot(\mathbf{d}\mathscr{B})-2(\mathbf{d}\overline{\mathscr{C}})^*\cdot(\mathbf{d}\mathscr{C}+\mathscr{T}_{\rm ev}\cdot\mathscr{C}+\mathscr{C}\cdot\mathscr{T}_{\rm ev})\\
&-2(\mathscr{T}_{\rm od})^*\cdot(\mathbf{d}_M\mathscr{B})-2(\mathbf{d}_M\overline{\mathscr{C}})^*\cdot(\mathbf{d}_M\mathscr{C}+\mathscr{T}_{\rm od}\cdot\mathscr{C}+\mathscr{C}\cdot\mathscr{T}_{\rm od})\}.
\end{aligned} \tag{24}$$

One can check that this quantum action is BRST/anti-BRST invariant.

In the above quantum action (24), the terms with the auxiliary field $\mathscr{B}$ are the gauge fixing terms and give rise to the 't Hooft gauge condition[20,21] as we shall see in the next two sections.

The first term is the classical action, and the remaining terms constitute the kinetic and interaction terms of the ghost fields. In the following two sections we calculate the quantum action (24) for the SU(2/1) and SU(2/2) cases explicitly.

III. BRST QUANTIZATION OF THE SU(2/1) CASE

The generators of SU(2/1) are the same as those of SU(3), namely, the conventional λ matrices, except for t_8, which is given by

$$t_8=\frac{1}{\sqrt{3}}\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&-2\end{pmatrix}, \tag{25}$$

in order to satisfy $S\,\mathrm{Tr}(t_i)=0$. We write the SU(2/1) superconnection as

$$\begin{aligned}&\mathscr{T}=it_iJ_i \quad (i=1,2,\ldots,8)\\&=\mathscr{T}_{\mathrm{ev}}+\mathscr{T}_{\mathrm{od}}=i\begin{pmatrix}\tau_aW_a-\frac{1}{\sqrt{3}}B&0\\0&-\frac{2}{\sqrt{3}}B\end{pmatrix}+i\begin{pmatrix}0&\sqrt{2}\Phi\\\sqrt{2}\Phi^\dagger&0\end{pmatrix},\end{aligned} \tag{26}$$

where we identified the gauge and Higgs fields W_a, B, Φ, and $\Phi^\dagger$ with the components $W_a=J_a$ $(a=1,2,3)$, $B=J_8$, $\Phi=1/\sqrt{2}\binom{J_4-iJ_5}{J_6-iJ_7}$ and $\Phi^\dagger=1/\sqrt{2}\binom{J_4+iJ_5}{J_6+iJ_7}$.

We now introduce the ghost, antighost, and auxiliary fields, in the doubled-fiber bundle space,

$$\begin{aligned}&\mathscr{C}=i\begin{pmatrix}\tau_ac_a-\frac{1}{\sqrt{3}}c_8&0\\0&-\frac{2}{\sqrt{3}}c_8\end{pmatrix},\quad \bar{\mathscr{C}}=i\begin{pmatrix}\tau_a\bar{c}_a-\frac{1}{\sqrt{3}}\bar{c}_8&0\\0&-\frac{2}{\sqrt{3}}\bar{c}_8\end{pmatrix},\\&\mathscr{B}=i\begin{pmatrix}\tau_ab_a-\frac{1}{\sqrt{3}}b_8&0\\0&-\frac{2}{\sqrt{3}}b_8\end{pmatrix}\quad (a=1,2,3).\end{aligned} \tag{27}$$

In order to derive the BRST/anti-BRST transformation rules, we apply Eqs. (16)–(19) of the previous section. In calculating the SU(2/1) case, we encounter the following difficulty. With the 3×3 matrix representation, it is not possible to choose a constant matrix $\eta=\binom{0\ \ \xi}{\zeta\ \ 0}$ for the matrix derivative, satisfying the condition (8), $\bar{\zeta}\zeta=\zeta\bar{\zeta}\propto 1$, which is essential for the nilpotency of the matrix derivative. In order to resolve this difficulty, we first extend all 3×3 matrix representations of fields into 4×4 matrices, simply by adjoining a fourth row and a fourth column, with all components vanishing. We then choose the η matrix in this extended 4×4 matrix representation space, in which it does satisfy the nilpotency condition. This 4×4 η matrix, enables us to perform all calculations involving the η matrix, such as evaluating the supercurvature, etc. After this is done, we project back onto the 3×3 matrix representation space, simply discarding the fourth row and column. Note that this construction reflects the fact that the true fundamental representation of SU(2/1) is four dimensional,[3] reflecting the homomorphism with OSp(2/2) and fitting the internal

quantum numbers for quarks, i.e. $(u_R/u_L, d_L/d_R)$ where the order follows descending weak hypercharges (4/1,1/−2) [in units of (1/3)]. However, for integer charges, the upper state trivializes and disconnects (e.g., the ν_R), and we are left with the three-dimensional representation. As a matter of fact, the procedure we use here also corresponds to the *projective module* method of Connes and Lott.[8] We thus perform the actual calculation with

$$\zeta=\bar{\zeta}=\sqrt{2}k\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \quad k:\text{real},$$

and obtain the following BRST/anti-BRST transformation rules,

$$\begin{gathered}
sA_{II}=-dc_{II}-A_{II}c_{II}-c_{II}A_{II},\\
\bar{s}A_{II}=-d\bar{c}_{II}-A_{II}\bar{c}_{II}-\bar{c}_{II}A_{II},\\
sA_I=-dc_I, \quad \bar{s}A_I=-d\bar{c}_I,\\
s\Phi=-c_{II}(\Phi+\xi)-\frac{1}{\sqrt{3}}c_I(\Phi+\xi),\\
\bar{s}\Phi=-\bar{c}_{II}(\Phi+\xi)-\frac{1}{\sqrt{3}}\bar{c}_I(\Phi+\xi),\\
s\Phi^\dagger=(\Phi^\dagger+\xi^\dagger)c_{II}+\frac{1}{\sqrt{3}}(\Phi^\dagger+\xi^\dagger)c_I,\\
\bar{s}\Phi^\dagger=(\Phi^\dagger+\xi^\dagger)\bar{c}_{II}+\frac{1}{\sqrt{3}}(\Phi^\dagger+\xi^\dagger)\bar{c}_I,\\
sc_{II}=-c_{II}c_{II}, \quad \bar{s}\bar{c}_{II}=-\bar{c}_{II}\bar{c}_{II},\\
sc_I=\bar{s}\bar{c}_I=0,\\
s\bar{c}_{II}=b_{II}, \quad \bar{s}c_{II}=-b_{II}-c_{II}\bar{c}_{II}-\bar{c}_{II}c_{II},\\
sb_{II}=0, \quad \bar{s}b_{II}=-\bar{c}_{II}b_{II}+b_{II}\bar{c}_{II},\\
s\bar{c}_I=-\bar{s}c_I=b_I, \quad sb_I=\bar{s}b_I=0,
\end{gathered} \tag{28}$$

where

$$\begin{gathered}
A_{II}=i\tau_a W_a, \quad A_I=iB, \quad c_{II}=i\tau_a c_a, \quad c_I=ic_8,\\
\bar{c}_{II}=i\tau_a\bar{c}_a, \quad \bar{c}_I=i\bar{c}_8, \quad b_{II}=i\tau_a b_a \quad (a=1,2,3), \quad b_I=ib_8,\\
\xi=k\begin{pmatrix}0\\ 1\end{pmatrix}.
\end{gathered} \tag{29}$$

Note that the transformation rules of Φ and $\Phi^\dagger$ correspond to those of the Higgs fields with a shifted vacuum. For the supercurvature we obtain

$$\mathscr{F}_i=\begin{pmatrix} F_W-\frac{1}{\sqrt{3}}F_B-2(\Phi\Phi^\dagger+\xi\Phi^\dagger+\Phi\xi^\dagger) & -i\sqrt{2}\left(D\Phi+\left(i\vec{W}\cdot\vec{\tau}+\frac{i}{\sqrt{3}}B\right)\xi\right) \\ -i\sqrt{2}\left(D\Phi^\dagger-\xi^\dagger\left(i\vec{W}\cdot\vec{\tau}+\frac{i}{\sqrt{3}}B\right)\right) & -\frac{2}{\sqrt{3}}F_B-2(\Phi^\dagger\Phi+\xi^\dagger\Phi+\Phi^\dagger\xi) \end{pmatrix}, \tag{30}$$

where

$$F_W=\tfrac{1}{2}F_{W_{\mu\nu}}\,dx^\mu\wedge dx^\nu=d(i\vec{W}\cdot\vec{\tau})+(i\vec{W}\cdot\vec{\tau})(i\vec{W}\cdot\vec{\tau}),$$

$$F_B=\tfrac{1}{2}F_{B_{\mu\nu}}\,dx^\mu\wedge dx^\nu=d(iB),$$

$$\Phi=\begin{pmatrix}\phi^+\\ \phi^0\end{pmatrix}=\frac{1}{\sqrt{2}}\begin{pmatrix}\phi_3+i\phi_4\\ \phi_1+i\phi_2\end{pmatrix}=\frac{1}{\sqrt{2}}\begin{pmatrix}J_4-iJ_5\\ J_6-J_7\end{pmatrix}, \tag{31}$$

$$D\Phi=(D\Phi)_\mu\,dx^\mu=d\Phi+\left(i\vec{W}\cdot\vec{\tau}+\frac{i}{\sqrt{3}}B\right)\Phi,$$

$$D\Phi^\dagger=(D\Phi^\dagger)_\mu\,dx^\mu=d\Phi^\dagger-\Phi^\dagger\left(i\vec{W}\cdot\vec{\tau}+\frac{i}{\sqrt{3}}B\right).$$

We use $d^4x=dx^0\wedge dx^1\wedge dx^2\wedge dx^3$, $\epsilon_{0123}=1$, and adopt the convention of Ref. 22 for the dual of a differential form in n dimensions, required for (24),

$$*(dx^{i_1}\wedge dx^{i_2}\wedge\cdots\wedge dx^{i_p})=\frac{1}{(n-p)!}\,\epsilon^{i_1i_2\cdots i_p}{}_{i_{p+1}\cdots i_n}dx^{i_{p+1}}\wedge\cdots\wedge dx^{i_n}, \tag{32}$$

satisfying $**\omega_p=(-1)^{p(n-p)}\omega_p$ for a p-form ω_p.

Selecting the metric $g_{\mu\nu}=(-1,+1,+1,+1)$, the first term in (24), the classical action, is given by

$$\begin{aligned}\mathscr{L}_C=&\frac{1}{4}F_{Wa\mu\nu}F_{Wa}^{\mu\nu}+\frac{1}{4}F_{B\mu\nu}F_B^{\mu\nu}-\left(D\Phi^\dagger-\xi^\dagger\left(i\vec{W}\cdot\vec{\tau}+\frac{i}{\sqrt{3}}B\right)\right)_\mu\\ &\times\left(D\Phi+\left(i\vec{W}\cdot\vec{\tau}+\frac{i}{\sqrt{3}}B\right)\xi\right)^\mu-2((\Phi^\dagger+\xi^\dagger)(\Phi+\xi)-\xi^\dagger\xi)^2\\ =&\frac{1}{4}F_{Wa\mu\nu}F_{Wa}^{\mu\nu}+\frac{1}{4}F_{B\mu\nu}F_B^{\mu\nu}-\left(D\Phi^\dagger-ik\left(\sqrt{2}W_-,\frac{2}{\sqrt{3}}Z\right)\right)_\mu\\ &\times\left(D\Phi+ik\begin{pmatrix}\sqrt{2}W_+\\ \frac{2}{\sqrt{3}}Z\end{pmatrix}\right)^\mu-2(\Phi^\dagger\Phi+k(\phi^0-\bar{\phi}^0))^2,\end{aligned} \tag{33}$$

where $W_\pm^\mu=1/\sqrt{2}(W_1^\mu\mp iW_2^\mu)$, $Z^\mu=-(\sqrt{3}/2)W_3^\mu+(1/2)B^\mu$, $A^\mu=(1/2)W_3^\mu+(\sqrt{3}/2)B^\mu$.

In order to see the physical spectrum of the theory, we now write the above expression in the *unitary gauge*, which is given by $\Phi=\binom{0}{(1/\sqrt{2})\chi}$ with real χ.

$$\mathscr{L}_C^{UG}=\frac{1}{4}F_{Wa\mu\nu}F_{Wa}^{\mu\nu}+\frac{1}{4}F_{B\mu\nu}F_B^{\mu\nu}$$
$$\times-\left\{\frac{1}{2}\partial_\mu\chi\,\partial^\mu\chi+g^2W_{+\mu}W_-^\mu\left(\chi+\frac{\sqrt{2}k}{g}\right)^2+\frac{2}{3}g^2Z_\mu Z^\mu\left(\chi+\frac{\sqrt{2}k}{g}\right)^2\right\}$$
$$\times-\frac{1}{2}(g\chi^2+2\sqrt{2}k\chi)^2. \tag{34}$$

The coupling constant g is introduced by scaling the superconnection as $\mathscr{T}\to g\mathscr{T}$. In this unitary gauge we see that only one scalar field remains as a physical (and massive) Higgs field χ, whereas the other three scalars have been "mutated," now providing the longitudinal components of $W_\pm$ and Z. The masses of the massive particles are $M_\chi=2\sqrt{2}k$, $M_W=\sqrt{2}k$, $M_Z=(2\sqrt{2}/\sqrt{3})k$, and we see the relations $M_W^2/M_Z^2=3/4=\cos^2\theta_W$, $M_\chi=2M_W$. We shall return to the latter ratio M_χ/M_W in Sec. V, when discussing possible quantum corrections.

We now write the quantum Lagrangian of (24) as

$$\mathscr{L}_Q=\mathscr{L}_C+\mathscr{L}_1+\mathscr{L}_2, \tag{35}$$

where $\mathscr{L}_C$ is the classical Lagrangian, $\mathscr{L}_1$ stands for the ghost terms, and $\mathscr{L}_2$ for the gauge fixing terms. After some calculations, we obtain $\mathscr{L}_1$,

$$\mathscr{L}_1=\frac{1}{2}\,\mathrm{tr}\left[\partial_\mu\bar{c}_{II}\,D^\mu c_{II}+2\,\partial_\mu\bar{c}_I\,\partial^\mu c_I+\left\{\left(\bar{c}_{II}+\frac{1}{\sqrt{3}}\bar{c}_I\right)\xi(\Phi^\dagger+\xi^\dagger)\left(c_{II}+\frac{1}{\sqrt{3}}c_I\right)\right\}\right.$$
$$\left.+\left\{\xi^\dagger\left(\bar{c}_{II}+\frac{1}{\sqrt{3}}\bar{c}_I\right)\left(c_{II}+\frac{1}{\sqrt{3}}c_I\right)(\Phi+\xi)\right\}\right], \tag{36}$$

where $D^\mu c_{II}=\partial^\mu c_{II}+[A_{II}^\mu,c_{II}]$.

For $\mathscr{L}_2$, we obtain

$$\mathscr{L}_2=\frac{\alpha}{2}\left\{[(b_1)^2+(b_2)^2+(b_Z)^2+(b_A)^2]+\frac{2}{\alpha}\left[b_1(\partial_\mu W_1^\mu-\sqrt{2}k\phi_4)\right.\right.$$
$$\left.\left.+b_2(\partial_\mu W_2^\mu-\sqrt{2}k\phi_3)+b_Z\left(\partial_\mu Z^\mu-\frac{2\sqrt{2}}{\sqrt{3}}k\phi_2\right)+b_A(\partial_\mu A^\mu)\right]\right\}, \tag{37}$$

where $b_Z=-(\sqrt{3}/2)b_3+(1/2)b_8$, $b_A=(1/2)b_3+(\sqrt{3}/2)b_8$. After integrating out the auxiliary fields b_1,b_2,b_Z, and b_A, $\mathscr{L}_2$ becomes

$$\mathscr{L}_2=-\frac{1}{2\alpha}\left\{(\partial_\mu W_1^\mu-\sqrt{2}k\phi_4)^2+(\partial_\mu W_2^\mu-\sqrt{2}k\phi_3)^2+\left(\partial_\mu Z^\mu-\frac{2\sqrt{2}}{\sqrt{3}}k\phi_2\right)^2+(\partial_\mu A^\mu)^2\right\}. \tag{38}$$

This expression clearly shows that we obtain the gauge-fixed quantum Lagrangian of the 't Hooft gauge,[20,21] as we claimed in the previous section:

$$\partial_\mu W_1^\mu-M_W\phi_4=0,$$
$$\partial_\mu W_2^\mu-M_W\phi_3=0, \tag{39}$$

$$\partial_\mu Z^\mu - M_Z \phi_2 = 0,$$

$$\partial_\mu A^\mu = 0.$$

IV. BRST quantization of SU(2/2) case

We now calculate the SU(2/2) case. The generators of SU(2/2) are the same as those of SU(4), except for t_8 and t_{15}, which are replaced by

$$t_8 = \frac{1}{\sqrt{3}} \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad t_{15} = \frac{1}{\sqrt{6}} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 3 \end{pmatrix} \tag{40}$$

to conforming with the supertracelessness of the SU(2/2) generators. The superconnection for the SU(2/2) case can be written as

$$\mathcal{J} = i t_i J_i \quad (i = 1,2,\ldots,15) = \begin{pmatrix} A_L + \frac{1}{\sqrt{2}} B & i\Phi \\ i\Phi^\dagger & A_R + \frac{1}{\sqrt{2}} B \end{pmatrix}, \tag{41}$$

with one-forms in the even part and zero-forms in the odd part, given as

$$A_L = i\tau_a A_{La}, \quad A_R = i\tau_a A_{Ra}, \quad B = iIY, \quad \Phi = I\phi_0 + i\tau_a \phi_a, \tag{42}$$

where τ_a $(a=1,2,3)$ are Pauli matrices and I is 2×2 identity matrix. A_{La}, A_{Ra}, Y are real, whereas ϕ_0, ϕ_a are complex, the fields being assigned to the components of J's according to

$$A_{La} = J_a \quad (a=1,2,3), \quad A_{R_1} = J_{13}, \quad A_{R_2} = J_{14},$$

$$A_{R_3} = -\frac{1}{\sqrt{3}} (J_8 + \sqrt{2} J_{15}), \quad Y = -\frac{1}{\sqrt{3}} (\sqrt{2} J_8 - J_{15}),$$

$$\phi_0 = \frac{1}{2} [(J_4 - iJ_5) + (J_{11} - iJ_{12})], \quad \phi_1 = -\frac{i}{2} [(J_6 - iJ_7) + (J_9 - iJ_{10})],$$

$$\phi_2 = -\frac{1}{2} [(J_6 - iJ_7) - (J_9 - iJ_{10})], \quad \phi_3 = -\frac{i}{2} [(J_4 - iJ_5) - (J_{11} - iJ_{12})].$$

A_L and A_R are thus the SU(2) gauge fields, B is the U(1) gauge field, and Φ is the complex scalar field (with its four components).

We now introduce the ghost and antighost fields,

$$\mathcal{C} = \begin{pmatrix} c_L & 0 \\ 0 & c_R \end{pmatrix} + \begin{pmatrix} \frac{1}{\sqrt{2}} c_I & 0 \\ 0 & \frac{1}{\sqrt{2}} c_I \end{pmatrix}, \quad \bar{\mathcal{C}} = \begin{pmatrix} \bar{c}_L & 0 \\ 0 & \bar{c}_R \end{pmatrix} + \begin{pmatrix} \frac{1}{\sqrt{2}} \bar{c}_I & 0 \\ 0 & \frac{1}{\sqrt{2}} \bar{c}_I \end{pmatrix}. \tag{43}$$

where $c_L = i\tau_a c_{La}$, $c_R = i\tau_a c_{Ra}$ $(a=1,2,3)$, $c_I = iIc_{Ir}$, with real c_{La}, c_{Ra}, and c_{Ir} and similarly for $\bar{\mathscr{C}}$. $\{c_L, \bar{c}_L\}$ and $\{c_R, \bar{c}_R\}$ are the ghost and antighost fields for the SU(2) gauge fields A_L and A_R, respectively, and $\{c_I, \bar{c}_I\}$ are those of the U(1) gauge field B.

The BRST/anti-BRST transformation rules are obtained from (16)–(19). Choosing

$$\eta = \begin{pmatrix} 0 & \xi \\ \xi^\dagger & 0 \end{pmatrix}, \quad \text{where} \quad \xi = k\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad k;\ \text{real}, \tag{44}$$

we get

$$\begin{aligned}
sA_L &= -dc_L - A_L c_L - c_L A_L, \\
\bar{s}A_L &= -d\bar{c}_L - A_L \bar{c}_L - \bar{c}_L A_L, \\
sA_R &= -dc_R - A_R c_R - c_R A_R, \\
\bar{s}A_R &= -d\bar{c}_R - A_R \bar{c}_R - \bar{c}_R A_R, \\
sB &= -dc_I, \quad \bar{s}B = -d\bar{c}_I, \\
s\Phi &= (\Phi + \xi)c_R - c_L(\Phi + \xi), \\
\bar{s}\Phi &= (\Phi + \xi)\bar{c}_R - \bar{c}_L(\Phi + \xi), \\
s\Phi^\dagger &= (\Phi^\dagger + \xi^\dagger)c_L - c_R(\Phi^\dagger + \xi^\dagger), \\
\bar{s}\Phi^\dagger &= (\Phi^\dagger + \xi^\dagger)\bar{c}_L - \bar{c}_R(\Phi^\dagger + \xi^\dagger), \\
sc_L &= -c_L c_L, \quad \overline{sc}_L = -\bar{c}_L \bar{c}_L, \\
sc_R &= -c_R c_R, \quad \overline{sc}_R = -\bar{c}_R \bar{c}_R, \\
sc_I &= \overline{sc}_I = 0, \\
s\bar{c}_L &= b_L, \quad \bar{s}c_L = -b_L - c_L \bar{c}_L - \bar{c}_L c_L, \\
s\bar{c}_R &= b_R, \quad \bar{s}c_R = -b_R - c_R \bar{c}_R - \bar{c}_R c_R, \\
sb_L &= 0, \quad \bar{s}b_L = -\bar{c}_L + b_L + b_L \bar{c}_L, \\
sb_R &= 0, \quad \bar{s}b_R = -\bar{c}_R b_R + b_R \bar{c}_R, \\
s\bar{c}_I &= -\bar{s}c_I = b_I, \quad sb_I = \bar{s}b_I = 0.
\end{aligned} \tag{45}$$

We have introduced the auxiliary fields

$$\mathscr{B} = \begin{pmatrix} b_L & 0 \\ 0 & b_R \end{pmatrix} + \begin{pmatrix} \frac{1}{\sqrt{2}} b_I & 0 \\ 0 & \frac{1}{\sqrt{2}} b_I \end{pmatrix}$$

with $b_L=i\tau_a b_{La}$, $b_R=i\tau_a b_{Ra}$ $(a=1,2,3)$, and $b_I=iIb_{Ir}$, where b_{La}, b_{Ra}, and b_{Ir} are real. For the supercurvature, we obtain

$$\mathscr{F}_t=\begin{pmatrix} F_L+\frac{1}{\sqrt{2}}F_B-(\Phi\Phi^\dagger+\xi\Phi^\dagger+\Phi\xi^\dagger) & -i(D\Phi+A_L\xi-\xi A_R) \\ -i(D\Phi^\dagger-\xi^\dagger A_L+A_R\xi^\dagger) & F_R+\frac{1}{\sqrt{2}}F_B-(\Phi^\dagger\Phi+\xi^\dagger\Phi+\Phi^\dagger\xi) \end{pmatrix}, \tag{46}$$

where $F_L=dA_L+A_LA_L$, $F_R=dA_R+A_RA_R$, $F_B=dB$, $D\Phi=d\Phi+A_L\Phi-\Phi A_R$, $D\Phi^\dagger=d\Phi^\dagger-\Phi^\dagger A_L+A_R\Phi^\dagger$.

The classical Lagrangian, the first term in (24), is given by[23]

$$\begin{aligned}\mathscr{L}_C=\mathrm{tr}[&\tfrac{1}{4}F_{+\mu\nu}F_+^{\mu\nu}+\tfrac{1}{4}F_{-\mu\nu}F_-^{\mu\nu}+\tfrac{1}{8}F_{B\mu\nu}F_B^{\mu\nu}\\&-\tfrac{1}{2}(D\Phi^\dagger+2kA_-)_\mu(D\Phi-2kA_-)^\mu-\tfrac{1}{2}(\Phi^\dagger\Phi+k(\Phi+\Phi^\dagger))^2],\end{aligned} \tag{47}$$

where $A_\pm$ are, respectively, the vector and axial vector gauge fields, as defined by $A_\pm=(1/2)(\pm A_L+A_R)=i\tau_a A_{\pm a}$, and $F_+^{\mu\nu}=\partial^\mu A_+^\nu-\partial^\nu A_+^\mu+[A_+^\mu,A_+^\nu]+[A_-^\mu,A_-^\nu]$, $F_-^\mu=\partial^\mu A_-^\nu-\partial^\nu A_-^\mu+[A_+^\mu,A_-^\nu]+[A_-^\mu,A_+^\nu]$. The above expression tells us that the three axial vector gauge fields A_{-a} have acquired the mass $2k$, whereas the three vector gauge fields A_{+a} and the U(1) gauge field Y remain massless.

For the quantum Lagrangian $\mathscr{L}_Q$, we again write, as in (35),

$$\mathscr{L}_Q=\mathscr{L}_C+\mathscr{L}_1+\mathscr{L}_2.$$

The ghost part $\mathscr{L}_1$ is given by

$$\begin{aligned}\mathscr{L}_1=\tfrac{1}{2}\,\mathrm{tr}[&(\partial_\mu\bar{c}_L\,D^\mu c_L+\partial_\mu\bar{c}_R\,D^\mu c_R+\partial_\mu\bar{c}_L\,\partial^\mu c_I)-2k^2(\bar{c}_L-\bar{c}_R)(c_L-c_R)\\&+k(\{(\bar{c}_L-\bar{c}_R)c_R-c_L(\bar{c}_L-\bar{c}_R)\}\Phi^\dagger+\{c_R(\bar{c}_L-\bar{c}_R)-(\bar{c}_L-\bar{c}_R)c_L\}\Phi)],\end{aligned} \tag{48}$$

where $D^\mu c_L=\partial^\mu c_L+[A_L^\mu,c_L]$, $D^\mu c_R=\partial^\mu c_R+[A_R^\mu,c_R]$.

The gauge fixing part $\mathscr{L}_2$ is given by

$$\begin{aligned}\mathscr{L}_2=\alpha\Bigg\{&\left((b_{-a})^2+(b_{+a})^2+\frac{1}{2}(b_{Ir})^2\right)\\&+\frac{2}{\alpha}\left(b_{-a}(\partial_\mu A_{-a}^\mu-2k\varphi_a)+b_{+a}(\partial_\mu A_{+a}^\mu)+\frac{1}{2}b_{Ir}(\partial_\mu Y^\mu)\right)\Bigg\},\end{aligned} \tag{49}$$

where $b_\pm=(1/2)(\pm b_L+b_R)=i\tau_a b_{\pm a}$, $\varphi=(1/2)(\Phi-\Phi^\dagger)=\tau_a\varphi_a$. Integrating out the auxiliary fields $b_\pm$, $\mathscr{L}_2$ becomes

$$\mathscr{L}_2=-\frac{1}{\alpha}\left\{(\partial_\mu A_-^\mu-2k\varphi)^2+(\partial_\mu A_+^\mu)^2+\frac{1}{2}(\partial_\mu Y^\mu)^2\right\}. \tag{50}$$

This expression again displays the quantum Lagrangian in the 't Hooft gauge:

$$\partial_\mu A^\mu_{-a} - M_{A\_}\varphi_a = 0,$$

$$\partial_\mu A^\mu_{+a} = 0, \tag{51}$$

$$\partial_\mu Y^\mu = 0,$$

where $M_{A\_} = 2k$ is used. If we write Φ as $(\sigma + i\vec{\pi}\cdot\vec{\tau}) + i(\eta + \vec{\rho}\cdot\vec{\tau})$ with real $\sigma, \vec{\pi}, \eta, \vec{\rho}$ fields, then φ in $\mathcal{L}_2$ can be identified with $\vec{\pi}$. This is consistent with the fact that the $\vec{\pi}$ fields are gauged away and mutate into the longitudinal components of the axial vector fields $A\_$ in the unitary gauge. This is also related to the fact that the SU(2/2) case corresponds to the gauged SU(2)×SU(2) σ model.[23].

V. CONCLUSION

In the matrix derivative approach, derived from noncommutative geometrical gauge theory and adjoined to internal supersymmetry, in its superconnection version, the vector gauge fields and the scalar fields are combined together, constituting the superconnection. The two sets of fields are thus related as a supermultiplet from the very beginning. This provides for an elegant geometrical realization of the Higgs mechanism. The entire Lagrangian is geometrical, even including the negative mass term for the scalar field, needed to trigger the spontaneous symmetry breakdown for the (g-even) gauge subgroup. That symmetry-breaking quadratic term for the scalar field is provided by the matrix derivative, beyond the unification achieved by the supergroup by itself. Summarizing, the unification is complete, within the limitations set by the broken symmetry actual content. We return to these limitations in our last paragraph.

Another advantage of the formalism touches upon the quantum action, namely in the gauge in which it appears, as a result of the construction. This turns out to be the 't Hooft gauge, most convenient for a spontaneously broken symmetry with Higgs field and suitable for renormalization.[20,21] We obtained this action just by adapting the Baulieu/Thierry-Mieg method,[19] which would yield the Landau gauge for the unbroken Yang–Mills theory, to the matrix derivative approach.

For the calculation of the $\mathcal{F}_t^* \cdot \mathcal{F}_t$ term in the classical and some of the other parts of the quantum Lagrangian we have used the definition of (32) for the dual form. This definition gives the kinetic terms of both the vector and scalar fields automatically in their canonical form, also providing the relation $M_\chi = 2M_W$. Note that this is a classical relationship. Including a quantum correction might modify this result.[24] This mass ratio is also due to the fact that we have only one overall supergauge coupling constant g for the superconnection $\mathcal{F}$ in Sec. III, due to universality. Without the assumption of universality for the supergroup we would have independent couplings for fields corresponding to forms of different degrees—in our case the even and odd parts of the superconnection, i.e., two independent couplings. One might then obtain a different mass ratio for the Higgs and gauge bosons.[25]

Last, we note that only the even part of the supergroup is gauged in the sense of relativistic quantum field theory—even though the entire supergroup is used as a structure group for the theory and provides the geometrical framework for the quantization procedure, including the 't Hooft gauge. As a result, there is no guarantee of nonrenormalization of the theory's couplings beyond those of the g-even gauge subgroup.

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A natural extension of coherent state path integrals

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We develop the formulation of the path integrals via the coherent states based on general starting vectors. In this paper we treat the case of the ordinary canonical (Heisenberg-Weyl) coherent state. We find that an additional term appears in the action in the path integral expression. Geometric phases associated with the path integrals, including the possibilities of the experimental detection, are also discussed. © *1996 American Institute of Physics.* [S0022-2488(96)02908-8]

I. INTRODUCTION

The Feynman path integral, which is the space-time approach to quantum mechanics, provides us with the bird's-eye view by which we are able to grasp the evolution of the quantum systems globally.[1,2] Its mathematical grace and intuitive appeal have tempted quite a few to generalize the formalism to more wider cases,[2,3] such as phase space forms,[4,5] fermion systems,[5,6] spin systems[7,8] and fields (both Bose fields[5,9] and Fermi ones[5,6]).

Now let us concentrate our attention to the case of the phase space path integral, for this is not only the simplest, but also serves as a prototype in understanding the generalizations to other systems. There are two ways to obtain that path integral: in one we sum over all the histories on the phase space,[4] whereas the other performs the path integration via the states that are specified by the points on complex planes. The latter approach was pioneered by Klauder in the early sixties.[5] About that time Glauber considered the same quantum states in the context of quantum optics and called them "coherent states,"[10] whose origin dates back even to the middle of the twenties.[11]

Klauder tried to generalize such states and reached the concept of "continuous representations"[12] which gives the states that construct the paths on some manifolds. These states are called "coherent states (CS)" in a broad sense of the word. (In what follows the word "CS" is used as a plural as well as a singular.) It is by such coherent state path integrals (path integrals via CS) that the above generalizations in Refs. 3–9 are made. We can understand that the phase space manifolds on which the paths are defined are extended to the generalized ones with curvatures or even to the non-complex ones in the coherent state path integrals for other systems.

Especially the CS that Perelomov defined by the unitary irreducible representations of arbitrary Lie groups bring us a concrete and clear method to construct CS[13] and to carry out their path integration.[8] In this case the CS is determined by a point on the manifold of the coset space G/H that is related to the corresponding Lie group G and its certain isotropy subgroup H. [3,13]

As stated at the beginning, the method of path integrals is suitable for considering the problems in which the global structure of the quantum systems is important. The problem of geometric phases[14] is one of these, though it was first discussed in the formulation *à la* Schrödinger. In fact the celebrated Berry phase[15] turned out to be understood more deeply in the light of such formulation[16] and the extension to the general case[17] was also studied from the viewpoint of CS path integrals.[18]

In the present paper, following the development of the path integrals mentioned above, we try to let it take another step forward; we aim to generalize the method of coherent state path integrals by extending the canonical CS and apply it to the problems of geometric phases. The CS are

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defined following the way of Perelomov. What is different from the conventional treatment is the choice of the starting vector; we take the generic one. Next we study various aspects of the CS: overcompleteness relation, the overlap of two coherent states, typical matrix elements and uncertainty relation. These are done in Sec. II. In Sec. III the path integration is performed via the CS obtained in Sec. II. We then proceed, in Sec. IV, to consider the problems of the geometric phases associated with the CS including some applications. Discussions on future problems are given in Sec. V. In the appendices we treat some deeper arguments about the matrix elements, the CS in the light of eigenvectors and alternative derivations of the action.

II. COHERENT STATES WITH GENERAL STARTING VECTORS

This section provides us with all the equipment for Sec. III. We revisit the canonical CS *à* la Perelomov[13] as well as its properties in a somewhat different manner from what has been given.

A. Construction of the coherent states

The canonical or Heisenberg-Weyl CS are constructed from the Lie algebra satisfying the following relation:

$$[\hat{q},\hat{p}]=i\hbar\ \mathbf{1},\ \ [\hat{q},\mathbf{1}]=[\hat{p},\mathbf{1}]=0. \tag{1}$$

By transforming the basis of the algebra to

$$\hat{a}=(2\hbar)^{-1/2}(\hat{q}+i\hat{p}),\ \ \hat{a}^{+}=(2\hbar)^{-1/2}(\hat{q}-i\hat{p}), \tag{2}$$

Eq. (1) can be put into a different form,

$$[\hat{a},\hat{a}^{+}]=\mathbf{1},\ \ [\hat{a},\mathbf{1}]=[\hat{a}^{+},\mathbf{1}]=0. \tag{3}$$

We define the canonical coherent state associated with the Lie algebra (1) or (3) by operating a unitary operator,

$$\hat{D}(\alpha)=e^{\alpha\hat{a}^{+}-\alpha^{*}\hat{a}}\quad(\alpha\text{: a complex parameter}), \tag{4}$$

on a starting vector $|\psi_0\rangle$. The vector is a fixed vector in the Hilbert space which, in the present case, is identical with the Fock space for Bosons.[13] In the conventional choice, it is taken as $|0\rangle$: the ground state of the boson number operator. According to the general theory of the CS,[13] however, we have much wider possibility in choosing a starting vector; and in fact it permits any fixed vector in the Fock space, which is represented uniquely as

$$|\psi_0\rangle=\sum_{n=0}^{\infty}c_n|n\rangle,\quad\text{with}\ \sum_{n=0}^{\infty}|c_n|^2=1, \tag{5}$$

in terms of a set of vectors $\{|n\rangle\}$. Here $|n\rangle$ is the eigenstate of the number operator fullfilling $\hat{a}^{+}\hat{a}|n\rangle=n|n\rangle$ and the $\{c_n\}$ denotes the coefficients of complex numbers. Therefore our CS $|\alpha\rangle$ takes the form of

$$|\alpha\rangle=\hat{D}(\alpha)|\psi_0\rangle=\sum_{n=0}^{\infty}c_n|\alpha,n\rangle,\quad\text{with}\ |\alpha,n\rangle\equiv e^{\alpha\hat{a}^{+}-\alpha^{*}\hat{a}}|n\rangle. \tag{6}$$

Perelomov has already discussed the above point and given some formulae. But it seems that there have been no concrete arguments on the general starting vector formulation of the CS, especially on the path integration, including its relation to the recent development of the geometric phases.

Some comments may serve for our understanding of Eq. (6). A general element of the Lie algebra (3) is given by $s\mathbf{1}+i(\alpha^*\hat{a}-\alpha\hat{a}^+)$, where s is a real number. And thus its corresponding Lie group is constructed by $T(s,\alpha)\equiv e^{i(s\mathbf{1}+i(\alpha^*\hat{a}-\alpha\hat{a}^+))}=e^{is}\hat{D}(\alpha)$, which is called the Heisenberg-Weyl group W_1. Since the operators $T(s,\alpha)$ act in the Fock space and form an irreducible unitary representation of W_1, the CS for W_1 is obtained by applying the operators $T(s,\alpha)$ on $|\psi_0\rangle$. Then we find that the CS is determined by one complex number α as Eq. (6), although an element g of W_1 is specified by one real as well as one complex parameters: $g=(s,\alpha)$. This happens because the isotropy subgroup of $|\psi_0\rangle$ is $H=\{h\}$, with $h=(s,0)$, which makes no difference to CS besides changing its phase factor. So we see that the CS is determined by a point on a complex plane of the α-variable which is nothing but the coset space W_1/H.

Now, with the aid of the well-known disentangling formula: $e^{\hat{A}+\hat{B}}=e^{\hat{A}}e^{\hat{B}}e^{-(1/2)[\hat{A},\hat{B}]}$, which holds for any two operators satisfying $[\hat{A},[\hat{A},\hat{B}]]=[\hat{B},[\hat{A},\hat{B}]]=0$,[19] Eq. (6) can be put into

$$|\alpha\rangle=e^{-(1/2)|\alpha|^2}e^{\alpha\hat{a}^+}e^{-\alpha^*\hat{a}}|\psi_0\rangle=e^{(1/2)|\alpha|^2}e^{-\alpha^*\hat{a}}e^{\alpha\hat{a}^+}|\psi_0\rangle. \tag{7}$$

Our CS is, of course, represented by a linear combination of the vectors $\{|m\rangle\}$ as

$$|\alpha\rangle=\sum_{n=0}^{\infty}c_n|\alpha,n\rangle, \tag{8a}$$

with

$$\begin{aligned}|\alpha,n\rangle&=\sum_{m=0}^{\infty}\langle m|\hat{D}(\alpha)|n\rangle|m\rangle\\&=e^{-(1/2)|\alpha|^2}\left(\sum_{m=0}^{n}\left(\frac{m!}{n!}\right)^{1/2}(-\alpha^*)^{n-m}L_m^{(n-m)}(|\alpha|^2)|m\rangle\right.\\&\left.+\sum_{m=n+1}^{\infty}\left(\frac{n!}{m!}\right)^{1/2}\alpha^{m-n}L_n^{(m-n)}(|\alpha|^2)|m\rangle\right).\end{aligned} \tag{8b}$$

Here $L_k^{(l)}(x)$ is the Laguerre polynomial defined as

$$L_k^{(l)}(x)\equiv\frac{e^x x^{-l}}{k!}\frac{d^k}{dx^k}(e^{-x}x^{k+l})=\sum_{r=0}^{k}\binom{k+l}{k-r}\frac{(-x)^r}{r!}, \tag{9}$$

and we have used the expression for the matrix elements $D_{mn}(\alpha)\equiv\langle m|\hat{D}(\alpha)|n\rangle$ which has been known in quantum electrodynamics.[20] When $|\alpha\rangle$ represents the state of the photon, the absolute square of $\langle m|\alpha\rangle=\Sigma_{n=0}^{\infty}c_nD_{mn}(\alpha)$ yields the probability of finding m photons in the state $|\alpha\rangle$, as in the case of usual CS.[21] The form of Eqs. (8) is valuable for later arguments. The state $|\alpha\rangle$ may be named "extended coherent state," yet we will call it just "our CS" or "the CS" in this paper, for it has been already included in the theory of CS.[3,13]

B. Resolution of unity

The most important property that the CS enjoy is the "overcompleteness relation" or "resolution of unity" which plays a central role in performing the path integration. The relation is so closely related to the irreducibility of the representation of groups that it actually follows from the latter as a natural result.[3,13] But here we take a more concrete method, which is a natural generalization of one used for the usual CS, to obtain this relation. It is expressed as

$$\frac{1}{\pi}\int |\alpha\rangle d^2\alpha\langle\alpha| = \mathbf{1}, \tag{10}$$

where $d^2\alpha \equiv d(\mathrm{Re}\ \alpha)\ d(\mathrm{Im}\ \alpha)$.

Proof. From Eqs. (8),

$$\langle\alpha| = \sum_{\tilde{n}=0}^{\infty}\sum_{\tilde{m}=0}^{\infty} c_{\tilde{n}}^{*} D_{\tilde{m}\tilde{n}}^{*}(\alpha)\langle\tilde{m}|. \tag{11}$$

Then, by using the polar coordinate $\alpha = re^{i\theta}$ in Eqs. (8) and (11), we obtain

$$\begin{aligned}\int |\alpha\rangle d^2\alpha\langle\alpha| = \sum_{n=0}^{\infty}\sum_{\tilde{n}=0}^{\infty} c_n c_{\tilde{n}}^{*} \Bigg[\int dr d\theta\, r e^{-r^2} \\ \times\Bigg(\sum_{m=0}^{n}\sum_{\tilde{m}=0}^{\tilde{n}} \left(\frac{m!\tilde{m}!}{n!\tilde{n}!}\right)^{1/2} (-1)^{(n-m)+(\tilde{n}-\tilde{m})}\, r^{(n-m)+(\tilde{n}-\tilde{m})}\, L_m^{(n-m)}(r^2) L_{\tilde{m}}^{(\tilde{n}-\tilde{m})}(r^2) \\ + \sum_{m=0}^{n}\sum_{\tilde{m}=\tilde{n}+1}^{\infty} \left(\frac{m!\tilde{n}!}{\tilde{m}!n!}\right)^{1/2} (-1)^{n-m}\, r^{(n-m)-(\tilde{n}-\tilde{m})}\, L_m^{(n-m)}(r^2) L_{\tilde{n}}^{(\tilde{m}-\tilde{n})}(r^2) \\ + \sum_{m=n+1}^{\infty}\sum_{\tilde{m}=0}^{\tilde{n}} \left(\frac{\tilde{m}!n!}{m!\tilde{n}!}\right)^{1/2} (-1)^{\tilde{n}-\tilde{m}}\, r^{(m-n)-(\tilde{m}-\tilde{n})}\, L_n^{(m-n)}(r^2) L_{\tilde{m}}^{(\tilde{n}-\tilde{m})}(r^2) \\ + \sum_{m=n+1}^{\infty}\sum_{\tilde{m}=\tilde{n}+1}^{\infty} \left(\frac{n!\tilde{n}!}{m!\tilde{m}!}\right)^{1/2} r^{(m-n)+(\tilde{m}-\tilde{n})}\, L_n^{(m-n)}(r^2) L_{\tilde{n}}^{(\tilde{m}-\tilde{n})}(r^2) \Bigg) \\ \times |m\rangle\langle\tilde{m}|\, e^{i((m-n)-(\tilde{m}-\tilde{n}))\theta} \Bigg].\end{aligned} \tag{12}$$

Hereafter we call the integral that includes the i-th term in the big parentheses the i-th integral. Let us consider the first integral. After integrating out the θ-variable, we are left with

$$\pi\sum_{n=0}^{\infty}\sum_{\tilde{n}=0}^{\infty} c_n c_{\tilde{n}}^{*} \left[\sum_{m=0}^{n}\sum_{\tilde{m}=0}^{n} \left(\frac{m!\tilde{m}!}{n!\tilde{n}!}\right)^{1/2} |m\rangle\langle\tilde{m}| \int_0^{\infty} ds\, e^{-s}\, s^{n-m}\, L_m^{(n-m)}(s) L_{\tilde{m}}^{(n-m)}(s) \right] \delta_{m-n,\tilde{m}-\tilde{n}}, \tag{13}$$

where $s \equiv r^2$. By the use of the orthogonality relation of the Laguerre polynomials,

$$\int_0^{\infty} du\, e^{-u} u^{\eta} L_k^{(\eta)}(u) L_{k'}^{(\eta)}(u) = \begin{cases} 0, & \text{for } k \neq k', \\ \dfrac{\Gamma(\eta+k+1)}{k!}, & \text{for } k = k', \end{cases} \tag{14}$$

which is valid for $\mathrm{Re}\ \eta > -1$, the first integral yields

$$\pi\sum_{n=0}^{\infty}\sum_{\tilde{n}=0}^{\infty} c_n c_{\tilde{n}}^{*} \left(\sum_{m=0}^{n}\sum_{\tilde{m}=0}^{n} \left(\frac{m!\tilde{m}!}{n!\tilde{n}!}\right)^{1/2} \frac{n!}{m!} \delta_{m-n,\tilde{m}-\tilde{n}}\, \delta_{m,\tilde{m}}\, |m\rangle\langle\tilde{m}| \right) = \pi\sum_{n=0}^{\infty} |c_n|^2 \left(\sum_{m=0}^{n} |m\rangle\langle m| \right). \tag{15}$$

Other integrals can be calculated just in the same manner. The fourth one gives $\pi\Sigma_{n=0}^{\infty}|c_n|^2(\Sigma_{m=n+1}^{\infty}|m\rangle\langle m|)$. For the second and the third ones we can find that the condition $m-n=\tilde{m}-\tilde{n}$ comming from θ-integration does not satisfy the summation restrictions on m and $\tilde{m}$. Thus these integrals vanish. So finally the result gives

$$\int |\alpha\rangle d^2\alpha\langle\alpha| = \pi\sum_{n=0}^{\infty}|c_n|^2\left(\sum_{m=0}^{\infty}|m\rangle\langle m|\right) = \pi\sum_{n=0}^{\infty}|c_n|^2\,\mathbf{1} = \pi\,\mathbf{1}, \tag{16}$$

which completes the proof. □

C. Overlap of two coherent states

The overlap of two coherent state $|\alpha\rangle=\Sigma_{n'}^{\infty}c_{n'}|\alpha,n'\rangle$ and $|\beta\rangle=\Sigma_{n}^{\infty}c_n|\beta,n\rangle$ is one of those important quantities which we employ for various calculations in the CS. It can be derived, with the help of Eqs. (6) and (8) together with the disentangling formula, as

$$\begin{aligned}\langle\alpha|\beta\rangle &= \sum_{n=0}^{\infty}\sum_{n'=0}^{\infty}c_nc_{n'}^{*}\,\langle n'|\hat{D}^{+}(\alpha)\hat{D}(\beta)|n\rangle \\ &= e^{(1/2)(\alpha^*\beta-\alpha\beta^*)}\sum_{n=0}^{\infty}\sum_{n'=0}^{\infty}c_nc_{n'}^{*}\,D_{n'n}(\beta-\alpha) \\ &= e^{-(1/2)(|\alpha|^2+|\beta|^2-2\alpha^*\beta)}\,G(\alpha,\alpha^*,\beta,\beta^*;\{c_n\}),\end{aligned} \tag{17}$$

where

$$\begin{aligned}G(\alpha,\alpha^*,\beta,\beta^*;\{c_n\}) \equiv \sum_{n=0}^{\infty}c_n\Bigg(&\sum_{n'=0}^{n}c_{n'}^{*}\left(\frac{n'!}{n!}\right)^{1/2}(-(\beta-\alpha)^*)^{n-n'}L_{n'}^{(n-n')}(|\beta-\alpha|^2) \\ &+\sum_{n'=n+1}^{\infty}c_{n'}^{*}\left(\frac{n!}{n'!}\right)^{1/2}(\beta-\alpha)^{n'-n}\,L_{n}^{(n'-n)}(|\beta-\alpha|^2)\Bigg).\end{aligned} \tag{18}$$

Especially putting $c_0=1$ and $c_n=0$ $(n\neq 0)$ yields $G(\alpha,\alpha^*,\beta,\beta^*;\{c_n\})=1$, which, since $L_0(x)\equiv 1$ for any x, brings us back to the conventional result of the overlap. Moreover, with $L_{n'}(0)=1$, it is easy to see that any state $|\alpha\rangle$ is normalized to unity, as conforms to our construction of the CS.

D. Typical matrix elements and uncertainty relation

Our next task is to calculate typical matrix elements that we encounter in later sections. For that purpose we find it useful to employ the following identities:

$$\hat{D}^{+}(\alpha)(\hat{a})^l\hat{D}(\alpha)=(\hat{a}+\alpha)^l \quad (l\text{: positive integer}) \tag{19}$$

and

$$\hat{D}^{+}(\alpha)(\hat{a}^{+}\hat{a})\hat{D}(\alpha)=\hat{a}^{+}\hat{a}-(\alpha\hat{a}^{+}-\alpha^*\hat{a})+|\alpha|^2. \tag{20}$$

The proofs are given by the straightforward application of the formula $e^{\hat{A}}\hat{B}e^{-\hat{A}}=\hat{B}+[\hat{A},\hat{B}]+(1/2!)[\hat{A},[\hat{A},\hat{B}]]+\cdots$.[19] From these relations one can easily obtain the valuable matrix elements between the CS,

$$\langle\alpha|(\hat{a})^l|\alpha\rangle=\alpha^l+\sum_{\substack{n=0\\ \text{with } n>n'}}^{\infty}\sum_{n'=0}^{\infty}c_n c_{n'}^{*}\binom{l}{n-n'}\left(\frac{n!}{n'!}\right)^{1/2}\alpha^{l-(n-n')}, \tag{21a}$$

$$\langle\alpha|(\hat{a}^{+})^l|\alpha\rangle=(\alpha^{*})^l+\sum_{\substack{n=0\\ \text{with } n>n'}}^{\infty}\sum_{n'=0}^{\infty}c_n^{*} c_{n'}\binom{l}{n-n'}\left(\frac{n!}{n'!}\right)^{1/2}(\alpha^{*})^{l-(n-n')}, \tag{21b}$$

and

$$\langle\alpha|\hat{a}^{+}\hat{a}|\alpha\rangle=\sum_{n=1}^{\infty}(n|c_n|^2-n^{1/2}(\alpha c_n^{*}c_{n-1}-\alpha^{*}c_n c_{n-1}^{*}))+|\alpha|^2. \tag{22}$$

Putting $c_0=1$ and $c_n=0(n\neq 0)$ in Eqs. (21)–(22) yields the conventional results.

We next describe the uncertainty relation that our CS fullfills. We show the case of $|\psi_0\rangle=|n\rangle$ here, which is sufficient for us to see what the situation looks like. Then $|\alpha\rangle=|\alpha,n\rangle$. From Eqs. (2) and (21), we obtain

$$\Delta q\Delta p=\frac{\hbar}{2}(2n+1). \tag{23}$$

Thus the fluctuation is enhanced through the factor n, just like in the case of a harmonic oscillator eigenfunction. It is obvious that the usual choice of $|\psi_0\rangle=|0\rangle$ gives the minimum uncertainty.[13] It can be readily seen that $\Delta q\Delta p\simeq O(N)$ holds for more generic cases, where $N=\max n$.

III. COHERENT STATE PATH INTEGRALS

In this section we will give the explicit path integral expression of the transition amplitude by means of the CS discussed in Sec. II. We invoke a well-known prescription for the coherent state path integrals[5,9,22] and especially follow Ref. 22. What we need is the propagator $K(\alpha_f,t_f;\alpha_i,t_i)$ which starts from $|\alpha_i\rangle$ at $t=t_i$, evolves under the effect of the Hamiltonian $\hat{H}(\hat{a}^{+},\hat{a};t)$ which is assumed to be a suitably-ordered function of $\hat{a}^{+}$ and $\hat{a}$, and ends up with $|\alpha_f\rangle$ at $t=t_f$:

$$K(\alpha_f,t_f;\alpha_i,t_i)\equiv\langle\alpha_f,t_f|\alpha_i,t_i\rangle=\langle\alpha_f|T\exp[-(i/\hbar)\textstyle\int_{t_i}^{t_f}dt\hat{H}(t)]|\alpha_i\rangle; \tag{24}$$

where T denotes the time-ordered product. By dividing the time interval into infinite numbers of an infinitesimal one ϵ and the successive use of the completeness relation (10), we obtain

$$K(\alpha_f,t_f;\alpha_i,t_i)=\lim_{N\to\infty}\left(\frac{1}{\pi}\right)^N\int d^2\alpha_1\cdots\int d^2\alpha_N\,\langle\alpha_f,t_f|\alpha_N,t_N\rangle\langle\alpha_N,t_N|\alpha_{N-1},t_{N-1}\rangle\cdots$$

$$\cdots\langle\alpha_j,t_j|\alpha_{j-1},t_{j-1}\rangle\cdots\langle\alpha_1,t_1|\alpha_i,t_i\rangle, \tag{25}$$

where $\epsilon=[(1/N+1)](t_f-t_i)$ and $t_j=t_i+j\epsilon$. So we only have to consider a propagator during an infinitesimal time interval, which gives

$$\begin{aligned}\langle\alpha_j,t_j|\alpha_{j-1},t_{j-1}\rangle&=\langle\alpha_j|T\exp[-(i/\hbar)\textstyle\int_{t_{j-1}}^{t_j}dt\hat{H}(t)]|\alpha_{j-1}\rangle\\&\simeq\langle\alpha_j|\left(1-\frac{i}{\hbar}\int_{t_{j-1}}^{t_j}dt\hat{H}(\hat{a}^+,\hat{a};t)\right)|\alpha_{j-1}\rangle\\&\simeq\langle\alpha_j|\alpha_{j-1}\rangle\left(1-\frac{i}{\hbar}\epsilon H(\alpha_j,\alpha_j^*,\alpha_{j-1},\alpha_{j-1}^*;t_{j-1})\right)\\&\simeq\exp\left[-\frac{1}{2}|\alpha_j|^2-\frac{1}{2}|\alpha_{j-1}|^2+\alpha_j^*\alpha_{j-1}+\ln G(\alpha_j,\alpha_j^*,\alpha_{j-1},\alpha_{j-1}^*;\{c_n\})\right.\\&\quad\left.-\frac{i}{\hbar}\epsilon H(\alpha_j,\alpha_j^*,\alpha_{j-1},\alpha_{j-1}^*;t_{j-1})\right]\\&\simeq\exp\left[-\frac{1}{2}|\alpha_j|^2-\frac{1}{2}|\alpha_{j-1}|^2+\alpha_j^*\alpha_{j-1}+\tilde{G}(\alpha_j,\alpha_j^*,\alpha_{j-1},\alpha_{j-1}^*;\{c_n\})\right.\\&\quad\left.-\frac{i}{\hbar}\epsilon H(\alpha_j,\alpha_j^*,\alpha_{j-1},\alpha_{j-1}^*;t_{j-1})\right],\end{aligned}\tag{26}$$

in which we have employed Eqs. (17)–(18). Here

$$H(\alpha'',\alpha''^*,\alpha',\alpha'^*;t)\equiv\frac{\langle\alpha''|\hat{H}(a^+,a;t)|\alpha'\rangle}{\langle\alpha''|\alpha'\rangle}\tag{27}$$

and

$$\tilde{G}(\alpha_j,\alpha_j^*,\alpha_{j-1},\alpha_{j-1}^*;\{c_n\})\equiv\sum_{n=1}^{\infty}n^{1/2}((\alpha_j^*-\alpha_{j-1}^*)c_nc_{n-1}^*-(\alpha_j-\alpha_{j-1})c_n^*c_{n-1}).\tag{28}$$

As can be seen from Appendix A, H is a function not only of $(\alpha'')^*$ and α', but also of α'' and $(\alpha')^*$. Care should be taken that in Eq. (26), only the terms with $n-n'=0,\pm1$ in G contribute to the infinitesimal propagator within the first order of ϵ. From (25) and (26),

$$\begin{aligned}K(\alpha_f,t_f;\alpha_i,t_i)=\lim_{N\to\infty}\left(\frac{1}{\pi}\right)^N\int d^2\alpha_1\cdots\int d^2\alpha_N\\\times\exp\left[\sum_{j=1}^{N+1}\left(-\frac{1}{2}|\alpha_j|^2-\frac{1}{2}|\alpha_{j-1}|^2+\alpha_j^*\alpha_{j-1}+\tilde{G}(\alpha_j,\alpha_j^*,\alpha_{j-1},\alpha_{j-1}^*;\{c_n\})\right.\right.\\\left.\left.-\frac{i}{\hbar}\epsilon H(\alpha_j,\alpha_j^*,\alpha_{j-1},\alpha_{j-1}^*;t_{j-1})\right)\right].\end{aligned}\tag{29}$$

The exponent in Eq. (29) becomes

$$\sum_{j=1}^{N+1}\left[-\frac{1}{2}\alpha_j^*\left(\frac{\alpha_j-\alpha_{j-1}}{\epsilon}\right)+\frac{1}{2}\alpha_{j-1}\left(\frac{\alpha_j^*-\alpha_{j-1}^*}{\epsilon}\right)+\frac{\tilde{G}(\alpha_j,\alpha_j^*,\alpha_{j-1},\alpha_{j-1}^*;\{c_n\})}{\epsilon}\right.$$

$$\left.-\frac{i}{\hbar}H(\alpha_j,\alpha_j^*,\alpha_{j-1},\alpha_{j-1}^*;t_{j-1})\right]\epsilon$$

$$\to\frac{i}{\hbar}\int_{t_i}^{t_f}dt\left[\frac{i\hbar}{2}((\alpha^*\dot{\alpha}-\dot{\alpha}^*\alpha)+A(\dot{\alpha},\dot{\alpha}^*;\{c_n\}))-H(\alpha^*,\alpha,t)\right]\quad(\text{as }\epsilon\to 0),\tag{30}$$

with

$$A(\dot{\alpha},\dot{\alpha}^*;\{c_n\})\equiv-2\lim_{\epsilon\to\infty}\frac{\tilde{G}(\alpha_j,\alpha_j^*,\alpha_{j-1},\alpha_{j-1}^*;\{c_n\})}{\epsilon}=2\sum_{n=1}^{\infty}n^{1/2}(\dot{\alpha}c_n^*c_{n-1}-\dot{\alpha}^*c_nc_{n-1}^*).\tag{31}$$

Then we finally find

$$K(\alpha_f,t_f;\alpha_i,t_i)=\int\mathcal{D}[\alpha(t)]\,e^{(i/\hbar)S[\alpha(t)]},\tag{32}$$

where

$$S[\alpha(t)]\equiv\int_{t_i}^{t_f}dt\left(\frac{i\hbar}{2}((\alpha^*\dot{\alpha}-\dot{\alpha}^*\alpha)+A(\dot{\alpha},\dot{\alpha}^*;\{c_n\}))-H(\alpha^*,\alpha,t)\right)\equiv\int_{t_i}^{t_f}L\,dt,\tag{33}$$

and we symbolized

$$\mathcal{D}[\alpha(t)]\equiv\lim_{N\to\infty}\left(\frac{1}{\pi}\right)^N\prod_{j=1}^{N}d^2\alpha_j.\tag{34}$$

The result (33) is different from the usual one associated with the starting vector $|\psi_0\rangle=|0\rangle$ in that it includes the A-term depending on the starting vector $|\psi_0\rangle$. However, even if the A-term vanishes, which occurs for example no neighboring $\{c_n\}$ exists for any c_n, we have to be careful that the content of the action is different generally due to the $|\psi_0\rangle$-dependence of $H(\alpha^*,\alpha,t)$ through the first term of Eq. (22).

What information does the semi-classical limit of our CS path integral give? In the situation where $\hbar\to 0$, the principal contribution in (32) comes from the path that satisfies $\delta S=0$, which requires the Euler-Lagrange equation for $L(\alpha,\dot{\alpha},\alpha^*,\dot{\alpha}^*;t)$. Then we obtain

$$i\hbar\dot{\alpha}=\frac{\partial H}{\partial\alpha^*},\quad -i\hbar\dot{\alpha}^*=\frac{\partial H}{\partial\alpha},\tag{35}$$

which is nothing but the canonical equation as in the conventional Heisenberg-Weyl CS. We see that since the A-term is expressed as a total derivative, it does not alter the Euler-Lagrange equation. The meaning of α, however, is quite different from the usual one. In our case α indicates the displacement *from the state* $|\psi_0\rangle$. Moreover Eq. (35) depends upon $|\psi_0\rangle$ through H via Eqs. (21)-(22) as mentioned earlier.

The extension of the present framework of path integral to the field theoretic case is straightforward; thus we omit it from the present paper. It can be performed in a manner described in Refs. 3 and 9. We merely have to be careful of the definition of the field CS: we have to use the direct product state, each of which is represented by Eq. (6).

IV. GEOMETRIC PHASES

A. Theory

Consider a cyclic change of our CS, whose initial and final states are expressed $|\alpha(0)\rangle$ and $|\alpha(T)\rangle$, respectively, under the effect of a Hamiltonian $\hat{H}$ during the time interval T. In the light of the formalism developed in Sec. III, the state vector accumulates the phase $\Phi(C)$ which amounts to[18]

$$\Phi(C)=\langle\alpha(0)|\alpha(T)\rangle=\exp\left[\frac{i}{\hbar}\sum_{\substack{\text{all the cyclic}\\ \text{paths } C}}(\Gamma(C)-\Delta(C))\right], \tag{36}$$

where

$$\Gamma(C)=\int_0^T\langle\alpha|i\hbar\frac{\partial}{\partial t}|\alpha\rangle dt=\int_0^T\frac{i\hbar}{2}(\alpha^*\dot{\alpha}-\dot{\alpha}^*\alpha)dt \tag{37}$$

and

$$\Delta(C)=\int_0^T H(\alpha^*,\alpha,t)dt. \tag{38}$$

We note that the effect of the A-term disappears in the case of the cyclic change of the CS as far as no restrictions are imposed on the region of the α-plane and hence it is simply-connected. We obtain from Eq. (37),

$$\Gamma(C)=\oint_C\langle\alpha|i\hbar\nabla_{\vec{\alpha}}|\alpha\rangle\cdot d\vec{\alpha}=\oint_C p dq, \tag{39}$$

where $\vec{\alpha}\equiv(\alpha,\alpha^*)$. Equation (39) shows that $\Gamma(C)$ depends only on the curve C on the α-plane, which is the same for the original geometric phases by Berry; [15] the equation also tells us that $\Gamma(C)$ is invariant under the canonical transformations.

In the present paper we are dealing with the canonical CS, however, $\Gamma(C)$ can be defined for any coherent states.[18] It is readily seen that we can define a line integral like $\Gamma(C)$ as long as the state we consider evolves as CS. What makes the CS develop as CS is the controlling the parameters by some successive continuous measurements. Although no mention of CS was made, such a point was described in a slightly different context.[23] In Ref. 18 the path is so chosen that it satisfies the variation principle in relation to the semiclassical approximation that plays a vital role in evaluating path integrals; and some developments of the CS geometric phases[24] including the application in this direction has been done.[25–27] Yet a such restriction is not inevitable. Especially when the Hamiltonain is at most bilinear in the generators of the Lie algebras in the canonical CS case and linear in SU(2)CS or SU(1,1)CS cases, however, the CS evolves as CS under the effect of the Hamiltonian and the resulting geometric phase agrees with one obtained by the variational path. Although it may look special at first sight, the above case covers the systems which are valuable in physics. And we will also take the case for example in the following discussion, for we want to compare the result with one obtained recently[27] and investigate the effect of our CS. We will see the result that is a direct extension of Ref. 27.

B. Simple application

Now we will give a more realistic argument by taking the following system as an example in which we choose a harmonic oscillator driven by an external force. The Hamiltonian is given by

$$\hat{H}=\tfrac{1}{2}(\hat{p}^2+\omega_0{}^2\hat{q}^2)+F(t)\hat{q}, \tag{40}$$

which can be written by means of boson creation and annihilation operators as

$$\hat{H}=\hbar\omega_0\hat{a}^+\hat{a}+f(t)\hat{a}^++f^*(t)\hat{a}. \tag{41}$$

We assume that the system is described by the CS $|\alpha,n\rangle$. Then, from Eq. (29), the propagator for the Hamiltonian of Eq. (41) gives

$$\begin{aligned}K(\alpha_f,t_f;\alpha_i,t_i)=&\lim_{N\to\infty}\left(\frac{1}{\pi}\right)^N\int d^2\alpha_1\cdots\int d^2\alpha_N\\&\times\exp\left[\sum_{j=1}^{N+1}\left(-\frac{1}{2}|\alpha_j|^2-\frac{1}{2}|\alpha_{j-1}|^2+\left(1-\frac{i}{\hbar}\epsilon\omega_0\right)\alpha_j^*\alpha_{j-1}-\frac{i}{\hbar}\epsilon f_j\alpha_j^*\right.\right.\\&\left.\left.+\frac{i}{\hbar}\epsilon f_{j-1}^*\alpha_{j-1}\right)\right],\end{aligned} \tag{42}$$

where we have applied Eqs. (A3) to two nearest states with the time interval ϵ. Equation (42) is the same as that for the usual CS under the same Hamiltonian (41). As mentioned earlier the direct evaluation of the Gaussian integral shows that the transition amplitude of the path obeying the variational condition is equal to the propagator.[1,2] Therefore it is enough to consider the variational path in this case.

The type of Hamiltonian in Eqs. (40) or (41) appears in the problems of detecting gravitational radiation[28] and quantum optics.[21,29] Here we shall take up the second one for example and discuss the possibility of finding the effect of the geometric phase. Consider a single mode electric field inside a cavity driven externally by a coherent driving field. If we neglect the cavity damping, we have the Hamiltonian:[29]

$$\hat{H}=\hbar\omega_0\hat{a}^+\hat{a}+i\hbar(\hat{a}^+E(t)e^{-i\omega t}-\hat{a}E^*(t)e^{i\omega t}). \tag{43}$$

The first term denotes the cavity mode Hamiltonian, where ω_0 means the fundamental cavity resonance and the second term gives the Hamiltonian for the coherent driving field respectively. $E(t)$ is the driving field amplitude, while ω is the driving frequency. If the cavity contains the medium with unharmonicity the term having $(\hat{a}^+)^2\hat{a}^2$ is added to the Hamiltonian,[29] but we neglect such an unharmonic effect hereafter. We also assume $E(t)=Ei$, with E: a positive real constant for brevity's sake.

It may be time for us to point out the role of the variable α in relation to quantum optics. We see, from Eqs. (21) that the matrix elements of $\hat{a}$ and $\hat{a}^+$ between our CS $|\alpha,n\rangle$ are identical with those for the usual CS. Consequently α is proportional to the complex amplitude of the classical electromagnetic field obtained as the solution of Maxwell equation, which can be shown in the same manner as that for the usual CS.[21]

Now we proceed to evaluate $\Gamma(C)$. With the aid of Eqs. (21)–(22),

$$H(\alpha,\alpha^*)=\hbar[\omega_0(|\alpha|^2+n)-2Er_0], \tag{44}$$

for the Hamiltonian Eq. (43). The variation equation, Eq. (35), reads as

$$\dot{\alpha}+i\omega_0\alpha=iEe^{-i\omega t}, \tag{45}$$

which, in the polar coordinate $\alpha=re^{i\theta}$, becomes

$$\dot{r}=E\sin(\theta+\omega t),\quad r(\dot{\theta}+\omega_0)=E\cos(\theta+\omega t). \tag{46}$$

These equations give a special cyclic solution with a period $T=2\pi/\omega$:

$$r=r_0,\quad \theta=-\omega t, \tag{47}$$

where the relation

$$r_0=\frac{E}{\omega_0-\omega} \tag{48}$$

holds. Equation (48) specifies the surface in the (E,ω,ω_0) space on which the phase Γ has the same value.[25-27] In the above argument, since we consider the cyclic path with the period T, we need not bother with the asymmetry of the solution of the variation equations in the general case.[7] The geometric phase Γ is evaluated from Eq. (37) as

$$\Gamma(C)=2\pi\hbar r_0^2. \tag{49}$$

On the other hand, from Eq. (38), the dynamical phase is calculated as

$$\Delta(C)=\frac{2\pi\hbar}{\omega}(\omega_0(r_0^2+n)-2Er_0). \tag{50}$$

We next turn to the detection of the phase $\Gamma(C)$ in experiments. The strategy invokes the inteference phenomena of two beams as in the previous cases.[25-27] We use the light beam prepared in the state $|n\rangle$ which is to be split into two parts. We assume that one part is suffered under the driving field E in Eq. (43), but the other is not and that these two parts are designed to come into reunion after a time interval of T. From Eq. (48) and Eq. (50), the vanishing of $\Delta(C)$ occurs when

$$\omega=\frac{\omega_0\sqrt{E^2-n\omega_0^2}}{E+\sqrt{E^2-n\omega_0^2}}. \tag{51}$$

The inteference pattern that gives the maximum intensity yields

$$2+2\cos\left(\frac{1}{\hbar}\Gamma(C)\right)=2+2\cos\left[2\pi\left(\frac{2E^2-n\omega_0^2+2E\sqrt{E^2-n\omega_0^2}}{\omega_0^2}\right)\right]. \tag{52}$$

Then n-dependence of $\Gamma(C)$ is as follows: the larger n, the smaller the magnitude of the phase $\Gamma(C)$, which causes the change of the interference pattern even for the same Hamiltonian. Putting $n=0$ recovers the result obtained by the usual CS. Thus the present result is a natural extension of one obtained before.[27]

V. DISCUSSION

We have tried to extend the realm of CS and their path integrals with success at least mathematically in the present paper. We also see that the formalism gives a new insight into the topological problems in quantum physics. Future problems are as follows.

First, the CS will play an important role in the problems where the quantum mechanical motions are closely related to the general n-th eigenstate of the harmonic oscillator; for example the problem of an electron moving under a strong magnetic field, which is related to the lowest Landau level and once treated by the CS method,[30] can be easily extended to the case of any field strength that is related to the general Landau level.

Second, the extension of the present path integral formalism to wider CS classes may be quite intriguing from the viewpoint of mathematical physics. Some works toward the direction will be treated in subsequent papers.

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APPENDIX A: MATRIX ELEMENTS AND THE GENERATING FUNCTION

This appendix is designed for the reference of the matrix elements in Sec. IV B. Here we demonstrate the simple case of $|\alpha\rangle=|\alpha,n\rangle$, which is sufficient for Sec. IV B; more general cases are obtained just in the same manner.

Consider the following function:

$$\begin{aligned} X(\mu,\mu^*)&\equiv\langle\alpha,n|e^{\mu\hat{a}^+}e^{-\mu^*\hat{a}}|\beta,n\rangle \\ &=e^{(1/2)|\mu|^2}\langle n|\hat{D}^+(\alpha)\hat{D}(\mu)\hat{D}(\beta)|n\rangle \\ &=e^{(1/2)[|\mu|^2+(\alpha^*+\beta^*)\mu-(\alpha+\beta)\mu^*+(\alpha^*\beta-\alpha\beta^*)]}\,D_{nn}(\mu-\alpha+\beta) \qquad \text{(A1)} \\ &=e^{\alpha^*\mu-\beta\mu^*}e^{-(1/2)(|\alpha|^2+|\beta|^2-2\alpha^*\beta)}\,L_n(|\mu-\alpha+\beta|^2), \end{aligned}$$

where we used the definition of D_{nn}, i.e. Eqs. (8), and the multiplication of $\hat{D}$. Clearly, $X(\mu,\mu^*)$ is the generating function[13] for the matrix elements:

$$\langle\alpha,n|(\hat{a}_+)^u(\hat{a})^v|\beta,n\rangle=\left(\frac{\partial}{\partial\mu}\right)^u\left(-\frac{\partial}{\partial\mu^*}\right)^v X(\mu,\mu^*)\bigg|_{\mu=0}. \qquad \text{(A2)}$$

For example,

$$\langle\alpha,n|\hat{a}|\beta,n\rangle=\beta\langle\alpha,n|\beta,n\rangle-e^{-(1/2)(|\alpha|^2+|\beta|^2-2\alpha^*\beta)}\sum_{r=1}^{\infty}(-1)^r\binom{n}{r}\frac{(\beta-\alpha)^r(\beta^*-\alpha^*)^{r-1}}{(r-1)!},$$

$$\langle\alpha,n|\hat{a}^+|\beta,n\rangle=\alpha^*\langle\alpha,n|\beta,n\rangle+e^{-(1/2)(|\alpha|^2+|\beta|^2-2\alpha^*\beta)}\sum_{r=1}^{\infty}(-1)^r\binom{n}{r}\frac{(\beta-\alpha)^{r-1}(\beta^*-\alpha^*)^r}{(r-1)!},$$

$$\begin{aligned} \langle\alpha,n|\hat{a}^+\hat{a}|\beta,n\rangle&=\alpha^*\beta\langle\alpha,n|\beta,n\rangle+(|\alpha|^2+|\beta|^2-2\alpha^*\beta) \\ &\quad\times\sum_{r=1}^{\infty}(-1)^r\binom{n}{r}\frac{|\beta-\alpha|^{2(r-1)}}{(r-1)!}-\sum_{r=1}^{\infty}(-1)^r\binom{n}{r}r\frac{|\beta-\alpha|^{2(r-1)}}{(r-1)!}. \qquad \text{(A3)} \end{aligned}$$

APPENDIX B: COHERENT STATES AS EIGENVECTORS

The original definition of the canonical CS $|\alpha)$ is the state which is the eigenstate of the boson annihilation operator $\hat{a}$ with an eigenvalue α: $\hat{a}|\alpha)=\alpha|\alpha)$. A question arises: are our CS the eigenstates of any operators? If so, what are they? For simplicity let us consider the case of $|\psi_0\rangle=|n\rangle$. We have two different answers to the problem.

The first approach starts by operating $\hat{D}(\alpha)$ on the relation $\hat{a}^+\hat{a}|n\rangle=n|n\rangle$. By Eq. (20), we obtain

$$(\hat{a}^+ + \alpha^*)(\hat{a}-\alpha)|\alpha,n\rangle = n|\alpha,n\rangle, \tag{B1}$$

which clearly gives us one of the possible answers.

We can look the problem from another point of view. From the defnition of the CS,

$$\hat{D}(\alpha)\hat{a}^{n+1}\hat{D}^+(\alpha)|\alpha,n\rangle = 0, \tag{B2}$$

which, together with Eq. (19), gives

$$(\hat{a}-\alpha)^{n+1}|\alpha,n\rangle = 0. \tag{B3}$$

Therefore our CS is the generalized eigenvector belonging to the generalized eigenspace which is well-known in the theory of linear algebra for the nilpotent groups.[31] It is obvious that taking $n=0$ brings us back to the relations that the usual CS fullfill both in Eq. (B1) and in Eq. (B3).

Moreover one can see that the latter argument holds also for the case of a general starting vector $|\psi_0\rangle$; we only have to replace n with N, where $N=\max n$.

APPENDIX C: ALTERNATIVE DERIVATIONS OF THE ACTION

There are alternative derivations that lead us to Eq. (32). In (26) we can write

$$\langle\alpha_j|\alpha_{j-1}\rangle \simeq \exp\left[-\langle\alpha_j|\frac{\partial}{\partial t}|\alpha_j\rangle\epsilon\right] \quad (\text{as } \epsilon\to 0). \tag{C1}$$

With the aid of (C1), one can easily obtain the same expression as Eq. (32) for the propagator except that the action is replaced by $\tilde{S}$, where

$$\tilde{S}[\alpha(t)] \equiv \int_{t_i}^{t_f} dt\left(\langle\alpha|i\hbar\frac{\partial}{\partial t}|\alpha\rangle - H(\alpha^*,\alpha,t)\right). \tag{C2}$$

But substituting Eq. (7) into the first term in the parentheses in Eq. (C2) gives

$$\langle\alpha|i\hbar\frac{\partial}{\partial t}|\alpha\rangle = \langle\alpha|i\hbar\left(\dot{\alpha}\frac{\partial}{\partial\alpha}+\dot{\alpha}^*\frac{\partial}{\partial\alpha^*}\right)|\alpha\rangle = \frac{i\hbar}{2}((\alpha^*\dot{\alpha}-\dot{\alpha}^*\alpha)+A(\dot{\alpha},\dot{\alpha}^*;\{c_n\})), \tag{C3}$$

where the use was made of Eqs. (21). The result reveals that $\tilde{S}=S$, which completes the proof. The formula of Eq. (C2) is not restricted to the canonical CS, but works well also for the general CS, though the derivation is somewhat formal as we have seen here.

We may also calculate the term $\langle\alpha|(\partial/\partial t)|\alpha\rangle$ with the aid of Eq. (17):

$$\langle\alpha|\frac{\partial}{\partial t}|\alpha\rangle = \langle\alpha|\frac{\partial}{\partial t}|\beta\rangle\Big|_{\alpha=\beta} = \left(\dot{\beta}\frac{\partial}{\partial\beta}+\dot{\beta}^*\frac{\partial}{\partial\beta^*}\right)\langle\alpha|\beta\rangle|_{\alpha=\beta}, \tag{C4}$$

which again results in Eq. (C3), hence in Eq. (33).

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Liouville vortex and φ^4 kink solutions of the Seiberg–Witten equations

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The Seiberg–Witten equations, when dimensionally reduced to $\mathbf{R}^2$, naturally yield the Liouville equation, whose solutions are parametrized by an arbitrary analytic function $g(z)$. The magnetic flux Φ is the integral of a singular Kaehler form involving $g(z)$; for an appropriate choice of $g(z)$, N coaxial or separated vortex configurations with $\Phi=2\pi N/e$ are obtained when the integral is regularized. The regularized connection in the $\mathbf{R}^1$ case coincides with the kink solution of φ^4 theory.
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The Seiberg–Witten equations[1] do not admit nonsingular solutions unless the curvature of the four-dimensional base manifold M happens to be negative over some regions of M. In particular, if $M=\mathbf{R}^4$, the Weitzenbock formula implies that the modulus squared of the spinor field ψ must either vanish everywhere, or exhibit singularities instead of local maxima.[2] There is also a global restriction on flat-space Seiberg–Witten solutions: Integrating the Weitzenbock formula, Witten[1] showed that all nontrivial flat solutions, including dimensionally reduced ones based on $\mathbf{R}^3$, $\mathbf{R}^2$, or $\mathbf{R}^1$, are all necessarily non-L^2.

Such singular, non-L^2 solutions, while probably not useful for Donaldson theory, may nevertheless be of physical interest. For example, Freund recently recognized that a singular $U(1)$ magnetic monopole field and an accompanying spinor, found earlier by Gürsey in a different setting, solve the $\mathbf{R}^3$-reduced Seiberg–Witten equations.[3] The monopole being the characteristic topological object in $\mathbf{R}^3$, one may inquire whether there are $\mathbf{R}^2$ and $\mathbf{R}^1$ Seiberg–Witten solutions corresponding to vortices and kinks, respectively. The chief purpose of the present note is to show that such solutions indeed exist. A novel aspect of the $\mathbf{R}^n$ $(n\leqslant 2)$ case is that the three coupled Seiberg–Witten equations (we should properly count $F=dA$ as one of the three) can be reduced to a single nonlinear one. This happens to be the Liouville equation,[4] which has recently been related to $N=2$ supersymmetric Seiberg–Witten theory in another context.[5]

We follow the conventions of Akbulut[6] in the choice of the Dirac γ-matrices

$$\gamma^1=\begin{pmatrix}\mathbf{0} & \mathbf{I}\\ -\mathbf{I} & \mathbf{0}\end{pmatrix},\quad \gamma^2=\begin{pmatrix}\mathbf{0} & i\sigma_3\\ i\sigma_3 & \mathbf{0}\end{pmatrix},$$
$$\gamma^3=\begin{pmatrix}\mathbf{0} & -i\sigma_2\\ -i\sigma_2 & \mathbf{0}\end{pmatrix},\quad \gamma^4=\begin{pmatrix}\mathbf{0} & -i\sigma_1\\ -i\sigma_1 & \mathbf{0}\end{pmatrix}, \tag{1}$$

and the self-dual Σ_{ij}

$$\Sigma_{12}=\frac{1}{4}\{[\gamma^1,\gamma^2]+[\gamma^3,\gamma^4]\}=\begin{pmatrix}i\sigma_3 & \mathbf{0}\\ \mathbf{0} & \mathbf{0}\end{pmatrix},$$

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$$\Sigma_{13}=\frac{1}{4}\{[\gamma^1,\gamma^3]+[\gamma^4,\gamma^2]\}=\begin{pmatrix}-i\sigma_2 & \mathbf{0}\\ \mathbf{0} & \mathbf{0}\end{pmatrix}, \tag{2}$$

$$\Sigma_{23}=\frac{1}{4}\{[\gamma^1,\gamma^4]+[\gamma^2,\gamma^3]\}=\begin{pmatrix}-i\sigma_1 & \mathbf{0}\\ \mathbf{0} & \mathbf{0}\end{pmatrix}.$$

Taking a spinor $\psi^T=(a,b,0,0)$, a connection iA_μ, and its curvature $iF_{\mu\nu}=i(\partial_\mu A_\nu-\partial_\nu A_\mu)$, where $\mu,\nu=1,2,3,4$, the first of the Seiberg–Witten pair is nothing but the Dirac equation

$$\gamma^\mu(\partial_\mu+iA_\mu)\psi=0. \tag{3}$$

In the notation of Ref. 6, the second Seiberg–Witten equation becomes

$$\rho(iF_A^+)=\sigma(\psi), \tag{4}$$

where

$$\sigma(\psi)\equiv\begin{pmatrix}\dfrac{(|a|^2-|b|^2)}{2} & a\bar{b}\\ b\bar{a} & \dfrac{(|b|^2-|a|^2)}{2}\end{pmatrix} \tag{5}$$

and

$$\rho(iF_A^+)=\frac{i}{8}(F_{\mu\nu}+\tilde{F}_{\mu\nu})\cdot\Sigma_{\mu\nu}=\frac{i}{4}F_{\mu\nu}\Sigma_{\mu\nu}. \tag{6}$$

The vortex solutions in $\mathbf{R}^2$ follow from the *Ansatz*

$$A_\mu=(A_1,A_2,0,0), \tag{7}$$

$$\psi^T=(a,b,0,0), \tag{8}$$

where all quantities are assumed to depend only on x_1 and x_2. Putting (7) and (8) in (4), one finds two possibilities: either ($a\neq0$, $b=0$) or ($a=0$, $b\neq0$). Choosing the first, (4) reduces to

$$-F_{12}=-B_3=|a|^2, \tag{9}$$

while (3) yields

$$(-\partial_1+i\partial_2)a=(iA_1+A_2)a. \tag{10}$$

We now set

$$a=\alpha\ \exp(\omega_x+i\omega_y), \tag{11}$$

where α is a constant with the dimensions of inverse length as required by (4). This unusual dimension for the spinor field of course comes from the vacuum expectation value of the Higgs field in the twisted supersymmetric Yang–Mills theory underlying the Seiberg–Witten approach.[7] Dividing both sides of (10) by a, applying $(-\partial_1-i\partial_2)$, and separating real and imaginary parts, we find

$$(\partial_1^2+\partial_2^2)\omega_x=-B_3=\alpha^2\ \exp(2\omega_x) \tag{12}$$

and

$$(\partial_1^2+\partial_2^2)\omega_y=-(\partial_1 A_1+\partial_2 A_2). \tag{13}$$

In (12), we have also used (9). It is convenient to introduce the dimensionless coordinates $x=\alpha x_1$ and $y=\alpha x_2$ with $\alpha>0$ and to define $z(\bar{z})=x+(-)iy$. The equation (12) then becomes

$$4\partial_z\partial_{\bar{z}}\omega_x=\exp(2\omega_x). \tag{14}$$

This is, of course, the well-known Liouville equation. Using (10) and (11) we obtain

$$A_1=\alpha(\partial_y\omega_x-\partial_x\omega_y) \tag{15}$$

and

$$A_2=-\alpha(\partial_x\omega_x+\partial_y\omega_y), \tag{16}$$

which show that (13) is automatically satisfied. Equation (14) has the solution

$$\omega_x=\frac{1}{2}\ln\frac{4(dg/dz)(d\bar{g}/d\bar{z})}{(1-g\bar{g})^2}, \tag{17}$$

due to Liouville.[4] At this point, $g(z)$ is an arbitrary analytic function. Comparing (17) with (11), we see that

$$|a|=2\alpha\frac{|dg/dz|}{(1-g\bar{g})}, \tag{18}$$

which naturally suggests

$$\omega_y=\pm\arg\frac{dg}{dz}=\mp\arg\frac{d\bar{g}}{d\bar{z}}. \tag{19}$$

Note that this also makes ω_y harmonic and enforces $\nabla\cdot\mathbf{A}=0$ via (13). We finally take

$$a=2\alpha\frac{dg/dz}{(1-g\bar{g})}, \tag{20}$$

leading to

$$B_3=-\frac{4\alpha^2|dg/dz|^2}{(1-g\bar{g})^2}. \tag{21}$$

The $U(1)$ curvature is thus seen to be the Kaehler two-form

$$F=\frac{1}{e}F_{12}dx_1\wedge dx_2=\frac{i}{2e\alpha^2}F_{12}dz\wedge d\bar{z}=\frac{-2i}{e}\frac{dg\wedge d\bar{g}}{(1-g\bar{g})^2}, \tag{22}$$

where we have brought out the coupling constant e which was hidden in A_μ all along. We can also combine (15) and (16) into the one-form

$$A=\frac{i}{e}\left(\frac{\bar{g}dg}{(1-g\bar{g})}-\frac{gd\bar{g}}{(1-g\bar{g})}\right). \tag{23}$$

A number of remarks are in order:

(i) The singularity dictated by the Weitzenbock formula manifests itself in (20)–(23). The solutions are singular in the z plane along a curve defined by $g\bar{g}=1$. One can easily trace the minus in $(1-g\bar{g})$ to the relative plus sign between the two sides of the Liouville equation (14); introducing a relative minus sign in (14) changes all the $(1-g\bar{g})$ factors to $(1+g\bar{g})$ without affecting anything else.

(ii) Remarkably, (14) and (22) also arise in a twice dimensionally reduced Ansatz leading to vortexlike solutions of the self-dual Yang–Mills equations.[8] Since the $\mathbf{R}^4$ self-dual Yang–Mills (SDYM) system is conjectured to generate all integrable systems through various dimensional reductions, the appearance of (14) in both the SDYM and the Seiberg–Witten contexts may be regarded as an additional clue for similar integrability properties of the latter. Furthermore, putting $e^{w_x}=u$ in the Liouville equation (14) and performing a further dimensional reduction by demanding $u=u(|z|=r)$ results in the differential equation for the third Painlevé transcendent with $\gamma=1$, $\alpha=\beta=\delta=0$, in the notation of Ince.[9] Thus the Seiberg–Witten equations also exhibit a Painlevé property, considered an indication of integrability.[10]

(iii) In the SDYM case, passing from the $(++++)$ $\mathbf{R}^4$ to the twistor-based $(++--)$ $\mathbf{R}^{2,2}$ supplies the change in the relative sign in (14) converting the singular $(1-g\bar{g})^{-1}$ factor into $(1+g\bar{g})^{-1}$; the same obviously holds in our problem as well.

(iv) The curvature form (22) remains unchanged under $g\to 1/g$, just as it would under a gauge transformation. Indeed, this inversion of g precisely gives rise to the $U(1)$ gauge transformations

$$a\to a'=\frac{\bar{g}}{g}a \tag{24}$$

and

$$eA\to eA'=eA+id\ \ln\frac{g}{\bar{g}} \tag{25}$$

on the spinor field and the connection, respectively.

We now wish to restrict the choice of $g(z)$ by physical considerations. In Freund's case, $\int F$ gives the quantized magnetic charge; it would be natural to expect that $\int F\equiv\Phi$ is a quantized magnetic flux in $\mathbf{R}^2$ for an appropriate $g(z)$. This requires that we somehow "regularize" the singular integrand (22); happily, different approaches to making sense out of $\int F$ give the same result, as we shall see. Let us start by considering the $\mathbf{R}^{2,2}$ version of (22), which becomes the area of the Riemann sphere stereographically expressed onto the g plane:

$$\Phi=\int F=\frac{2i}{e}\int\frac{dg\wedge d\bar{g}}{(1+g\bar{g})^2}. \tag{26}$$

Note the overall sign change due to the change in the rhs of (14).

Trying $g=z^\nu$ for an axisymmetric solution centered at the origin, we find

$$\Phi=\frac{4\pi\nu}{e}\int_0^\infty\frac{(2\nu r^{2\nu-1})}{(1+r^{2\nu})^2}\,dr=\frac{4\pi\nu}{e}\int_1^\infty\frac{dw}{w^2}=\frac{4\pi\nu}{e}, \tag{27}$$

where we have put $w=1+r^{2\nu}$. We note that the gauge transformation (24) results in

$$a'=\bar{z}^\nu z^{-\nu}a=e^{-2i\nu\theta}a. \tag{28}$$

The single valuedness of a' at $\theta=2\pi$ allows the ν values

$$\nu=\tfrac{1}{2},1,\tfrac{3}{2},\ldots\ . \tag{29}$$

We need not consider $\nu\rightarrow-\nu$ as this only amounts to the gauge transformation $g\rightarrow 1/g$ mentioned earlier. Of the values in (29), it is the $\nu=\frac{1}{2}$ that corresponds to $2\pi/e$, i.e., the Nielsen–Olesen[11] unit of flux. Thus $g=z^{1/2}$ represents the basic single-vertex solution, while $g=z^{n/2}$ corresponds to a single vortex with n units of flux. It is now easy to verify that

$$g(z)=\prod_{k=1}^{n}(z-a_k)^{1/2} \tag{30}$$

describes n vortices centered at the locations $a_k=(a_{kx}+ia_{ky})$. To do this, we first switch to the compactified version of (23), which becomes

$$A=-\frac{i}{e}\left(\frac{\bar{g}dg}{(1+g\bar{g})}-\frac{gd\bar{g}}{(1+g\bar{g})}\right). \tag{31}$$

Next we use the $g(z)$ of (30) in

$$\Phi=\int_{\mathbf{R}^2}F=\int_{\partial\mathbf{R}^2}A, \tag{32}$$

where $\partial\mathbf{R}^2$ is a clockwise circle whose radius goes to infinity. Since $|g|\rightarrow|z^{n/2}|\gg 1$ on $\partial\mathbf{R}^2$, we obtain

$$\Phi=-\frac{i}{2e}\oint_{\partial\mathbf{R}^2}\left\{n\frac{dz}{z}-n\frac{d\bar{z}}{\bar{z}}\right\}=\frac{2n\pi}{e}. \tag{33}$$

The similarity of expression (30) to Weierstrassian functions suggests we might consider a doubly periodic solution on a two-dimensional lattice, with one vortex per unit lattice cell. Let us take ω_1 and ω_2 as the two basic lattice vectors, subject to the usual restriction $\mathrm{Im}(\omega_2/\omega_1)\neq 0$. For a pair of integers (n_1,n_2), $\omega=n_1\omega_1+n_2\omega_2$ is a point in the lattice. We can now choose for $g(z)$ the square root of the Weierstrassian quasi-periodic function $\sigma(z)$, i.e.,

$$g(z)=\sigma^{1/2}(z)=z^{1/2}\prod_{\omega\neq 0}\left(1-\frac{z}{\omega}\right)^{1/2}\exp\left(\frac{z^2}{4\omega^2}+\frac{z}{2\omega}\right). \tag{34}$$

The exponential factor is needed to ensure the convergence of the product.

Another method for defining the integral of the singular expression (22) is as follows. If we attempt to calculate Φ starting from (22), we obtain

$$\Phi=-\frac{4\pi\nu}{e}\int_0^\infty\frac{(2\nu r^{2\nu-1})}{(r^{2\nu}-1)^2}\,dr=-\frac{4\pi\nu}{e}\int_{-1}^\infty\frac{dw}{w^2},\quad w=r^{2\nu}-1, \tag{35}$$

instead of (27). Adopting Speer's analytic regularization,[12] we define

$$I(-1,\infty)=\int_{-1}^\infty\frac{dw}{w^2}=\left[\int_{-1}^\infty w^\lambda dw\right]_{\lambda=-2}=-1. \tag{36}$$

This is equivalent to writing $I(-1,\infty)=I(-\infty,\infty)-I(-\infty,-1)$ and throwing away the infinite "constant" $I(-\infty,\infty)$. Thus we get the same answer as in the compactified $\mathbf{R}^2$,[2] formulation.

Now let us return to Eq. (8) and ask what happens if we take $a=0$, $b\neq 0$. It is easy to check that one still ends up with the Liouville equation (14); the changes consist of $B_3\rightarrow-B_3$ and

$$b=2\alpha\frac{(d\bar{g}/d\bar{z})}{(1-g\bar{g})}. \tag{37}$$

Thus while it is not possible to change the direction of the magnetic field by $g\to 1/g$, antivortices can be obtained by $(a(g),0)\to(0,b(\bar{g}))$, $B_3\to -B_3$.

Finally, let us briefly examine the $n=1$ case. A possible *Ansatz* is

$$A_\mu=(0,0,0,A_4(x_1)) \tag{38}$$

and

$$\psi^T=(a(x_1),b(x_1),0,0). \tag{39}$$

The Seiberg–Witten equation (6) demands either $\psi^T=(a,a,0,0)$ or $\psi^T=(a,-a,0,0)$. Taking $a=\alpha\exp(\omega_x+i\omega_y)$ as before, these two cases yield

$$\partial_1(\omega_x+i\omega_y)=\pm A_4, \tag{40}$$

respectively. Thus in order for A_4 be real, ω_y can at most be a constant, which we may take to be zero. Then, using (3) we obtain

$$\partial_1^2\omega_x=\alpha^2\exp(2\omega_x). \tag{41}$$

Calling $\alpha x_1=x$ again, (41) is seen to be a y-independent version of the Liouville equation (12). While (41) may be integrated directly by elementary methods, it is simpler to read off the solution from (17) by picking a $g(z)$ such that the variable y disappears in ω_x. This happens only for $g(z)=\exp\kappa(z+x_0)$, κ and x_0 being constant real numbers [an imaginary constant added to x_0 cancels out along with the iy in (17)]. We may as well set $x_0=0$, which gives

$$\omega_x=\frac{1}{2}\ln\frac{4\kappa^2e^{2\kappa x}}{(1-e^{2\kappa x})^2}. \tag{42}$$

This results in

$$|a|=\frac{\alpha\kappa}{|\sinh\kappa x|}, \tag{43}$$

$$A_4=\pm\alpha\kappa\coth\kappa x, \tag{44}$$

and

$$E_1=\mp\frac{\alpha^2\kappa^2}{\sinh^2\kappa x}. \tag{45}$$

The expected singularity appears at $x=0$ in (42)–(45). In contrast, the nonsingular version obtained by $x_1\to ix_1$ has $(1+e^{2\kappa x})^{-2}$ in (42); in addition, cosh κx and sinh κx in (43)–(45) are now switched. Thus A_4 changes into $\pm\alpha\kappa\tanh\kappa x$, which is the well-known kink (antikink) solution of φ^4 theory.

In conclusion, we see that the dimensionally reduced Seiberg–Witten equations in $\mathbf{R}^n$ ($n=1,2,3$) yield a singular version of topological solitons characteristic of each n, the $n=3$ case being represented by Freund's monopole solution. The accompanying spinors are, of course, the new feature associated with these familiar solitons. The $n=2$ case indicates connections between integrable systems and the Seiberg–Witten equations. Finally, it should be interesting to look for

solutions of the Seiberg–Witten equations reduced to a two-dimensional manifold admitting negative local values for the scalar curvature and see how this affects the singularities.

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Transformation bracket for 2D harmonic oscillator functions and its application to few-electron quantum dots

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Transformation bracket relating 2D harmonic oscillator product states with different sets of Jacobian coordinates is derived for systems composed of an arbitrary number of particles with arbitrary masses. The numerical diagonalization of the Hamiltonian of a three-electron quantum dot is given as an example to illustrate its applications. © *1996 American Institute of Physics.* [S0022-2488(96)00606-8]

I. INTRODUCTION

In recent years, mesoscopic physics is a rapidly developing field of research. Due to the advances of microfabrication technology in semiconductors, it is now possible to confine the 2D layer of electrons gas into dots of nanometer size,[1,2] where the motion of electrons in all the three dimensions are quantized. Experimentally, the number of electrons trapped in each dot ranges from one to several hundred and can be controlled very effectively by adjusting the gate voltages applied. Therefore quantum dots should be treated as disk-like atomic systems.

So far, quantum dots have been experimentally investigated by capacitance–voltage spectroscopy,[3] vertical tunneling,[4] in-plane transport,[5] as well as far-infrared spectroscopy in quantum dot arrays.[6] The accumulated data did not vary as smoothly as those predicted by Hartree-type calculations, but showed rich structures. Understanding of the data requires that the electron–electron interaction be treated exactly. The confinement potential is, of course, shape-dependent. To most of the quantum dots, harmonic oscillator potential is a good approximation.[7] The Slater determinants composed of single harmonic oscillator functions can thus be used as basis functions to diagonalize the Hamiltonian. The drawback of this formalism is that the trivial c.m. motion has been included. To separate the c.m. motion from the relative, a set of the c.m. and relative coordinates should be introduced to describe the system. However, the (anti-) symmetrization of harmonic basis with relative coordinates as variables is automatic in the case of two electrons[8] but a nontrivial matter for systems with $N>2$. In Ref. 9, Hawlyrak has proposed a scheme to construct the antisymmetric basis functions using Schwinger's coupled Boson representation.

In this paper we presented the transformation bracket relating product states of harmonic oscillator functions with different sets of Jacobian coordinates. This bracket can have many applications: first of all, since any particle permutation just transforms one set of Jacobi coordinates into another, properly symmetrized harmonic basis functions in coordinate space can be constructed with the bracket; second, the matrix elements of any pair of particle–particle interaction can be reduced to one single integral; finally, since the Jacobian coordinates are indispensable for describing the rearrangement scattering process, the bracket also plays a powerful tool for solving the problem of single electron tunneling through quantum dot on the exact quantum mechanical basis.[10]

The following section is devoted to deriving the transformation bracket for 2D harmonic oscillators. In the third section, we present an example to show how the transformation bracket can be applied to solve the quantum dot problems.

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II. TRANSFORMATION BRACKET FOR 2D HARMONIC OSCILLATORS

Consider a system of N particles with coordinates $\mathbf{r}_i$, and masses m_i, moving independently in a 2D harmonic oscillator potential well with the frequency ω, the Hamiltonian reads

$$H=\sum_{i=1}^{N}\left(\frac{-\hbar^2}{2m_i}\nabla_{\mathbf{r}_i}^2+\frac{1}{2}m_i\omega^2 r_i^2\right). \tag{1}$$

A set of Jacobian coordinates for the system mean the components of a set of $(N-1)$ independent values $\{\boldsymbol{\xi}_j\}$ such that each vector represents the displacement of the c.m. of one subset of the N particles from the c.m. of another subset and such that no two such vectors connect with the same c.m. Associated with each Jacobian coordinate vector $\boldsymbol{\xi}_j, \mu_j$ will be the reduced mass of the pair of particle clusters the c.m. of which are joined by $\boldsymbol{\xi}_j$. Then the following relation is fulfilled

$$H=H_{cm}+H_r, \tag{2}$$

where

$$H_r=\sum_{j=1}^{N-1} h_j=\sum_{j=1}^{N-1}\left(\frac{-\hbar^2}{2\mu_j}\nabla_{\xi_j}^2+\frac{1}{2}\mu_1\omega^2\xi_j^2\right), \tag{3}$$

$$H_{cm}=\frac{-\hbar^2}{2M}\nabla_R^2+\frac{1}{2}M\omega^2R^2, \tag{4}$$

where M is the total mass, $M=\Sigma_{i=1}^{N}m_i$. $\mathbf{R}$ is the c.m. coordinate of the system, H_{cm} describes the c.m. motion, H_r describes the relative motion which we are mainly interested in. From Eqs. (2)–(4), we know that the c.m. motion is separable from the relative motion. This feature retains when particle–particle interactions are turned on. The c.m. motion is a harmonic oscillator and the relative motion is $(N-1)$ harmonic oscillators with the same frequency. Let us define a vector creator $\boldsymbol{\eta}$ by

$$\boldsymbol{\eta}=\sqrt{\frac{\mu\omega}{2\hbar}}\left(\frac{-\hbar}{\mu\omega}\nabla_{\xi}+\xi\right), \tag{5}$$

whose components η_x and η_y create quanta in the x,y oscillators, respectively. Then the Hamiltonian of an oscillator h and the angular momentum operator L_z in this representation are

$$h=\hbar\omega(\boldsymbol{\eta}\cdot\boldsymbol{\eta}^{+}+1), \tag{6}$$

$$L_z=-i\hbar\,\boldsymbol{\eta}\times\boldsymbol{\eta}^{+}, \tag{7}$$

where $\boldsymbol{\eta}^{+}$ is the Hermitian conjugation of $\boldsymbol{\eta}$. A 2D harmonic oscillator function with eigenenergy $(2n+|m|+1)\hbar m$ and angular momentum $m\hbar$ can, in the $\boldsymbol{\eta}$ representation, be written as

$$|nm\rangle=N_{nm}(\boldsymbol{\eta}\cdot\boldsymbol{\eta})^n(\eta_x+i\delta_m\eta_y)^{|m|}|0\rangle, \tag{8}$$

where $|0\rangle$ denotes the normalized ground state, N_{nm} is the normalization constant, δ_m is the sign of m given by

$$N_{nm}=\sqrt{\frac{1}{2^{2n+|m|}(|m|+n)!\cdot n!}}, \tag{9}$$

$$\delta_m=\begin{cases}+, & \text{if } m>0,\\ -, & \text{if } m\leqslant 0.\end{cases} \tag{10}$$

Thus for the relative motion of the N-particle system, we have

$$|K\rangle=\prod_{j=1}^{N-1}\{N_{n_jm_j}(\boldsymbol{\eta}_j\cdot\boldsymbol{\eta}_j)^{n_j}(\eta_{jx}+i\delta_{m_j}\eta_{jy})^{|m_j|}\}|0\rangle \tag{11}$$

and the corresponding eigenenergy $E_{[K]}$ and angular momentum $L_{z[K]}$ are given by

$$E_{[K]}=\hbar\omega\sum_{j=1}^{N-1}(2n_j+|m_j|+1), \tag{12}$$

$$L_{z[K]}=\hbar\sum_{j=1}^{N-1}m_j, \tag{13}$$

where $[K]$ denotes a set of $2(N-1)$ quantum numbers $(n_1,n_2,\ldots,n_{N-1};m_1,m_2,\ldots,m_{N-1})$.

Making use of the factorization

$$\boldsymbol{\eta}\cdot\boldsymbol{\eta}=(\eta_x-i\eta_y)(\eta_z+i\eta_y), \tag{14}$$

we can rewrite Eq. (11) into

$$|K\rangle=\prod_{j=1}^{N-1}\{N_{n_jm_j}(\eta_{jx}-\eta_{jy})^{\bar{n}_j}(\eta_{jx}+i\eta_{jy})^{\tilde{N}_j}\}|0\rangle \tag{15}$$

which will be more convenient for our following purpose, where

$$\bar{n}_j=\begin{cases}n_j, & \text{if } m_j>0,\\ n_j+|m_j|, & \text{if } m_j\leqslant 0,\end{cases}\quad \tilde{N}_j=\begin{cases}n_j+|m_j|, & \text{if } m_j>0,\\ n_j, & \text{if } m_j\leqslant 0.\end{cases} \tag{16}$$

For $N>2$ there are more than one set of Jacobian coordinates that can be assigned to the system. The different possible sets of Jacobian coordinates are related to each other by linear transformations

$$\sqrt{\mu_i^{(\alpha)}}\boldsymbol{\xi}_i^{(\alpha)}=\sum_{j=1}^{N-1}a_{ij}^{\alpha\beta}\sqrt{\mu_j^{(\beta)}}\boldsymbol{\xi}_i^{(\beta)}\quad (i=1,2,\ldots,N-1), \tag{17}$$

where all the $a_{ij}^{\alpha\beta}$ form an orthogonal matrix. Thus the Jacobian coordinates and the reduced masses and the creation-operators appearing in the above equations should be identified by superscripts $\alpha,\beta,\ldots,\gamma$, etc. Since such superscripts are absent from the terms on rhs of Eq. (1) and since they are superfluous to the c.m. quantities, Eqs. (2)–(4) imply that the following relation holds for any two sets of Jacobian coordinates for a given $N(>2)$-particle system

$$\sum_{j=1}^{N-1}\left\{\frac{-\hbar^2}{2\mu_j^{(\alpha)}}\nabla^2_{\boldsymbol{\xi}_j^{(\alpha)}}+\frac{1}{2}\mu_j^{(\alpha)}[\xi_j^{(\alpha)}]^2\right\}=\sum_{i=1}^{N-1}\left\{\frac{-\hbar^2}{2\mu_i^{(\beta)}}\nabla^2_{\boldsymbol{\xi}_i^{(\beta)}}+\frac{1}{2}\mu_i^{(\beta)}[\xi_i^{(\beta)}]^2\right\}. \tag{18}$$

Therefore an eigenstate in one set of Jacobian coordinates can be expanded by eigenstates of another set of Jacobian coordinates belonging to the same eigenvalues $E_{[K]}$ and $L_{z[K]}$

$$|K\rangle^{(\alpha)}=\sum_{[K']} B^{[K]}_{[K']}(N,\alpha\beta)|K'\rangle^{(\beta)}, \tag{19}$$

where $B^{[K]}_{[K']}(N,\alpha\beta)$ is the transformation bracket we are looking for.

With the definition of vector creator in Eq. (5), it can be easily verified that the creators associated with different sets of Jacobian coordinates are subjected to the following transformations

$$\boldsymbol{\eta}_i^{(\alpha)}=\sum_{j=1}^{N-1} a_{ij}^{\alpha\beta}\boldsymbol{\eta}_j^{(\beta)}. \tag{20}$$

Substituting Eq. (20) into Eq. (15) and expanding it in terms of the eigenstates in the β set, we obtain

$$\begin{aligned}|K\rangle^{(\alpha)}=&\sum_{\tilde{n}'_1\tilde{n}'_2\cdots\tilde{n}'_{N-1}}\ \sum_{\tilde{N}'_1\tilde{N}'_2\tilde{N}'_{N-1}}\prod_{j=1}^{N-1}\left(\frac{N_{n_jm_j}}{N_{n'_jm'_j}}\right)A^{\alpha\beta}(\tilde{n}_1,\tilde{n}_2,\ldots,\tilde{n}_{N-1};\tilde{n}'_1,\tilde{n}'_2,\ldots,\tilde{n}'_{N-1})\\&\cdot A^{\alpha\beta}(\tilde{N}_1,\tilde{N}_2,\ldots,\tilde{N}_{N-1};\tilde{N}'_1,\tilde{N}'_2,\ldots,\tilde{N}'_{N-1})\delta_{E_{[K]},E_{[K']}}\delta_{L_{z[K]},L_{z[K']}}\cdot\prod_{j=1}^{N-1}\{N_{n_jm_j}[\eta_{jx}^{(\beta)}\\&-\eta_{jy}^{(\beta)}]^{\tilde{n}'_j}[\eta_{jx}^{(\beta)}+i\eta_{jy}^{(\beta)}]^{\tilde{N}'_j}\}|0\rangle,\end{aligned} \tag{21}$$

where $A^{\alpha\beta}$ is defined by

$$\begin{aligned}A^{\alpha\beta}(\tilde{n}_1,\tilde{n}_2,\ldots,\tilde{n}_{N-1};\tilde{n}'_1,\tilde{n}'_2,\ldots,\tilde{n}'_{N-1})=&\sum_{r_1r_2\cdots r_{N-1}}\ \sum_{s_1s_2\cdots s_{N-1}}\cdots\sum_{t_1t_2\cdots t_{N-1}}\\&\cdot\prod_{i=1}^{N-1}\left\{\frac{\tilde{n}_i!(a_{i1}^{\alpha\beta})^{r_i}(a_{i2}^{\alpha\beta})^{s_i}\cdots(a_{iN-1}^{\alpha\beta})^{t_i}}{r_i!s_i!\cdots t_i!}\right\}.\end{aligned} \tag{22}$$

Summations in Eq. (22) are subjected to the conditions $\Sigma_{i=1}^{N-1}r_i=\tilde{n}'_1$, $\Sigma_{i=1}^{N-1}s_i=\tilde{n}'_2,\ldots,$ $\Sigma_{i=1}^{N-1}t_i=\tilde{n}'_{N-1}$, and $(r,s,\ldots,t)$ refers to $(N-1)$ different sets of variables.

Comparing Eq. (21) with Eqs. (15) and (19), we obtain the transformation bracket we are looking for

$$\begin{aligned}B^{[K]}_{[K']}(N,\alpha\beta)=&\prod_{j=1}^{N-1}\left\{\frac{N_{n_jm_j}}{N_{n'_jm'_j}}\right\}A^{\alpha\beta}(\tilde{n}_1,\tilde{n}_2,\ldots,\tilde{n}_{N-1};\tilde{n}'_2,\tilde{n}'_2,\ldots,\tilde{n}'_{N-1})\\&\times A^{\alpha\beta}(\tilde{N}_1,\tilde{N}_2,\ldots,\tilde{N}_{N-1};\tilde{N}'_1,\tilde{N}'_2,\ldots,\tilde{N}'_{N-1})\delta_{E_{[K]},E_{[K']}}\delta_{L_{z[K]},L_{z[K']}}.\end{aligned} \tag{23}$$

The relations between n_j, m_j and $\tilde{n}_j$, $\tilde{N}_j$ of Eq. (15) hold also for n'_j, m'_j and $\tilde{n}'_j$,$\tilde{N}'_j$.

In computing $B^{[K]}_{[K']}(N,\alpha\beta)$, it is helpful to take notice of the following properties

$$B^{[K]}_{[K']}(N,\alpha\beta)=B^{[K']}_{[K]}(N,\beta\alpha), \tag{24}$$

$$1=\sum_{[k']} B^{[K]}_{[K']}(N,\alpha\beta)\cdot B^{[K']}_{[K]}(N,\beta\alpha) \tag{25}$$

which can be derived directly from its definition.

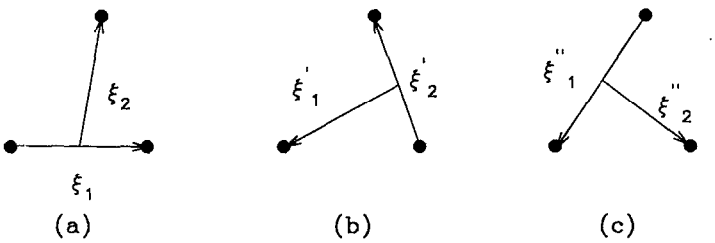

FIG. 1. Jacobian coordinates for three-body systems.

III. APPLICATIONS

Consider the motion of three electrons in a quantum dot with parabolic confinement $V(r_i)=1/2m^*\omega_0^2 r_i^2$, where m^* is the effective mass of electron. The three sets of Jacobian coordinates that can be assigned to the system are shown in Fig. 1. The linear transformation coefficients defined in Eq. (17) obviously fulfill, in this case, the following relations

$$a_{ij}^{\alpha\beta}=a_{ij}^{\beta\gamma}=a_{ij}^{\gamma\alpha} \tag{26}$$

with

$$(a_{ij}^{\alpha\beta})=\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}. \tag{27}$$

A. The Hamiltonian matrix elements between two harmonic states

The Hamiltonian describing the relative motion of three electrons can be written as

$$H_r=\frac{-\hbar^2}{2\mu_1^{(\alpha)}}\nabla^2_{\xi_1^{(\alpha)}}+\frac{-\hbar^2}{2\mu_2^{(\alpha)}}\nabla^2_{\xi_2^{(\alpha)}}+\sum_{i>j}u(r_{ij}) \tag{28}$$

with

$$u(r_{ij})=\frac{1}{6}m^*\omega_0^2 r_{ij}^2+\frac{e^2}{4\pi\epsilon r_{ij}}, \tag{29}$$

where the term proportional to r_{ij}^2 arises from the confinement. A noteworthy point is that there exists a minimum in u located at $r_{ij}=r_0\equiv(3e^2/4\pi\epsilon m^*\omega_0^2)^{1/3}$.

The Hamiltonian matrix elements $H_{[K],[K']}$ is then written as

$$\begin{aligned} H_{[K],[K']}&=\int[\phi_{n_1m_1}(\xi_1^{(\alpha)})\phi_{n_2m_2}(\xi_2^{(\alpha)})]H_r[\phi_{n_1'm_2'}(\xi_1^{(\alpha)})\phi_{n_2'm_2'}(\xi_2^{(\alpha)})]d\xi_1^{(\alpha)}d\xi_2^{(\alpha)} \\ &=H_0+H_a+H_b+H_c, \end{aligned} \tag{30}$$

where

$$H_0=(2n_1+2n_2+|m_1|+|m_2|+2)\hbar\omega\delta_{[K],[K']}, \tag{31}$$

$$H_a = U^{(m_1)}_{n_1,n_1'}\delta_{m_1,m_1'}\delta_{n_2,n_2'}\delta_{m_2,m_2'}, \tag{32}$$

$$H_b = \sum_{[K'']}\sum_{[K''']} B^{[K]}_{[K'']}(3,\alpha\beta)B^{[K']}_{[K''']}(3,\alpha\beta)U^{(m_1'')}_{n_1'',n_1'''}\delta_{m_1'',m_1'''}\delta_{n_2'',n_2'''}\delta_{m_2'',m_2'''}, \tag{33}$$

$$H_c = \sum_{[K'']}\sum_{[K''']} B^{[K]}_{[K'']}(3,\alpha\gamma)B^{[K]}_{[K''']}(3,\alpha\gamma)U^{(m_1'')}_{n_1'',n_1'''}\delta_{m_1'',m_1'''}\delta_{n_2'',n_2'''}\delta_{m_2'',m_2'''}, \tag{34}$$

$$U^{(m)}_{n,n'} = \int \phi_{nm}(\xi)u(\xi)\phi_{n'm}(\xi)d\xi. \tag{35}$$

The integrations in Eq. (35) can be carried out analytically.

B. Antisymmetrication of the basis functions

When dealing with the identical particle systems, the basis functions should have the permutation symmetry as is required. In the case of three-fermion system with total spin $S=3/2$, the antisymmetrized function $\phi_j(123)$ constructed from 2D harmonic states is of the following form

$$\begin{aligned}\phi_j(123) &= \frac{1}{6}(P_e - P_{12} - P_{13} - P_{23} + P_{123} + P_{132})[\phi_{n_1m_1}(\xi_1^{(\alpha)})\phi_{n_2m_2}(\xi_2^{(\alpha)})] \\ &= \frac{1}{3}\{[\phi_{n_1m_1}(\xi_1^{(\alpha)})\phi_{n_2m_2}(\xi_2^{(\alpha)})] + [\phi_{n_1m_1}(\xi_1^{(\beta)})\phi_{n_2m_2}(\xi_2^{(\beta)})] \\ &\quad + [\phi_{n_1m_1}(\xi_1^{(\gamma)})\phi_{n_2m_2}(\xi_2^{(\gamma)})]\} \\ &= \sum_{[K']}\frac{1}{3}\{\delta_{[K],[K']} + B^{[K]}_{[K']}(3,\beta\alpha) + B^{[K]}_{[K']}(3,\gamma\alpha)\}[\phi_{n_1'm_2'}(\xi_1^{(\alpha)})\phi_{n_2'm_2'}(\xi_2^{(\alpha)})].\end{aligned} \tag{36}$$

In the case of fermion system with $S=1/2$

$$\phi_j(123) = Q_0(123)\chi^0_{1/2} + Q_1(123)\chi^1_{1/2}, \tag{37}$$

where

$$\begin{aligned}Q_0(123) &= \frac{1}{6}(2P_e + 2P_{12} - P_{13} - P_{23} - P_{123} - P_{132})[\phi_{n_1m_1}(\xi_1^{(\alpha)})\phi_{n_2m_2}(\xi_2^{(\alpha)})] \\ &= \sum_{[K']}\frac{1}{3}[2\delta_{[K],[K']} - B^{[K]}_{[K']}(3,\beta\alpha) - B^{[K]}_{[K']}(3,\gamma\alpha)][\phi_{n_1'm_1'}(\xi_1^{(\alpha)})\phi_{n_2'm_2'}(\xi_2^{(\alpha)})],\end{aligned} \tag{38}$$

$$\begin{aligned}Q_1(123) &= \frac{\sqrt{3}}{6}(P_{13} - P_{23} + P_{123} - P_{132})[\phi_{n_1m_1}(\xi_1^{(\alpha)})\phi_{n_2m_2}(\xi_2^{(\alpha)})] \\ &= \sum_{[K']}\frac{\sqrt{3}}{3}[-B^{[K]}_{[K']}(3,\gamma\alpha) + B^{[K]}_{[K']}(3,\gamma\alpha)][\phi_{n_1'm_1'}(\xi_1^{(\alpha)})\phi_{n_2'm_2'}(\xi_2^{(\alpha)})],\end{aligned} \tag{39}$$

$$\chi^S_S = \{[\xi(1)\xi(2)]_s\xi(3)\}s. \tag{40}$$

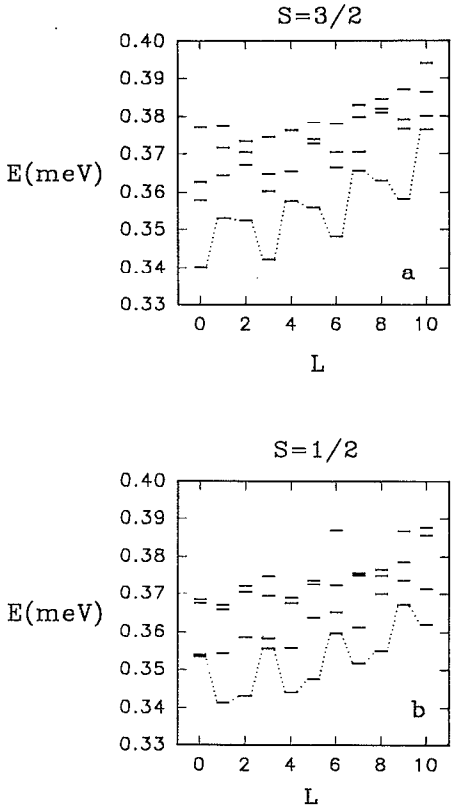

FIG. 2. Energy spectra of three electrons in a harmonic well with $\omega_0=0.01$ meV and without a magnetic field. The other parameters are taken appropriate for GaAs. The dotted lines are to guide the eyes to detect the magic numbers.

In the above equations, $\xi(i)$ is a spin state of the ith fermion, χ_S^s is the spin-part wave function with the total spin S, and with the spins of particles 1 and 2 coupled to s; Q_0 and Q_1 are the spatial parts, P_α denotes the permutation operator. A set of antisymmetrized functions $\{\phi_j(123)\}$ so obtained are, in general, linearly relevant, from which a set of orthonormalized basis functions can be constructed through the well known Schmidt procedure.

Before going to the details of the numerical results, let us discuss the implications of antisymmetrization on the geometric configurations. The minimum of total potential energy $U=\Sigma_{i>y}^3 u(r_{ij})$ is associated with an equilateral triangle (ET) with sidelength $r_{ij}=r_0$. The system should favor this configuration in order to minimize the averaged total potential energy. However, the antisymmetrization imposes restrictions on this pursuance. Let Φ_L be the spatial wave function with angular moment L and spin $S=3/2$. Since in the ET configuration a cyclic permutation of the three particles is equivalent to a rotation of $3\pi/2$, we have

$$P_{(123)}\Phi_L(ET)=R_{3\pi/2}\Phi_L(ET). \tag{41}$$

Thus we have

$$\Phi_L(ET)=e^{(i3\pi L/2)}\Phi_L(ET). \tag{42}$$

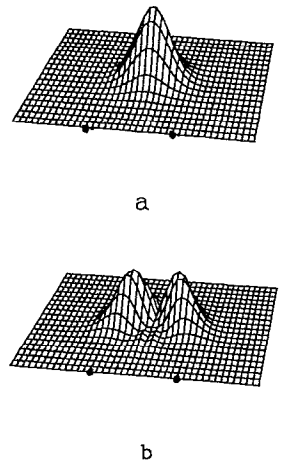

FIG. 3. Wave function distribution of the lowest state with (a) magic angular momentum; (b) non-magic angular momentum. The two dots on the front edge are positions of particles 1 and 2 with a separation r_0.

In other words, the most favorite ET component of the configurations will be completely prohibited in the $L \neq 3k$ ($k=integer$) states and this must lead to particularly high interacting energy. Similar arguments can be applied to the $S=1/2$ states. In contrast with $S=3/2$, the ET-prohibition will occur in the $L=3k$ states when $S=1/2$.

In Fig. 2, we presented the quantum spectra of three interacting electrons in a harmonic potential with a very small ω_0 ($=0.01$ meV) to emphasize the interaction. From the figure, one can see that the lowest state of a magic number of angular momentum (without ET-prohibition) is much lower than that of the adjacent non-magic numbers. In Fig. 3, we presented the wave function distributions of a magic-number state and a non-magic-number state for a comparison. In a magic-number state, the ET configuration is strongly pursued in order to minimize the potential energy while in the non-magic-number state the ET configuration is a node of the wave function demonstrating the ET-prohibition. The appearance of such a node increases both the kinetic and potential energies.

Experimentally, a vertical external magnetic field is applied. With the symmetric gauge, the Hamiltonian remains the same as Eq. (28) except for a replacement of $\omega_0 \rightarrow \sqrt{\omega_0^2+\omega_c^2/4}$ with the cyclotron frequency $\omega_c=eB/m^*$, and the additional Zeeman terms $(\omega_c L/2+g^*\mu_B B S_z)$. The Zeeman terms make states with larger L be even lower than states with smaller L when the magnetic field increases. From Fig. 2, it is easy to understand why the ground states occur only at the magic numbers of angular momentum.

Finally, we would like to emphasize that the appearance of magic numbers of angular momentum is completely due to the restrictions of geometric symmetry and permutational symmetry and has nothing to do with the details of the dynamic symmetries. With nonparabolic confinement, the c.m. motion is inseparable from the relative. For three electrons, the most favorite configuration continues to be the ET with its c.m. sitting on the minimum of the confinement and the magic numbers are of the same as discussed above.

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Multiple condensate solutions for the Chern–Simons–Higgs theory

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We study the existence of condensate solutions for the Chern-Simons-Higgs model with the choice of a potential field where both the symmetric and asymmetric vacua occur as ground states [see Hong, Kim, and Pac, Phys. Rev. Lett. **64**, 2230 (1990) and Jackiw and Weinberg, *ibid.* **64**, 2234 (1990)]. We show that if the Chern-Simons coupling parameter k is above a critical value, no such solutions can exist, while for $k>0$ below this critical value there exist at least *two* condensate solutions carrying the same quantized energy, as well as electric and magnetic charge. This multiplicity result accounts for the two vacua states present in the model. In fact, as $k\to 0^+$ it is shown that the two solutions found "bifurcate" from the asymmetric and symmetric vacuum states respectively. © *1996 American Institute of Physics.* [S0022-2488(96)03208-2]

I. INTRODUCTION

In recent years much attention has been devoted to the anyon model (see Refs. 1 and 2) and to the corresponding condensate (or multivortex) solutions which are believed relevant in several aspect of theoretical physics as, for instance, in high-temperature superconductivity. See Refs. 3–7.

Mathematically, the anyon model is a classical field theory defined on the (2+1)-Minkowski space, whose Lagrangean is characterized by the coupling of the scalar field, the Yang–Mills (or Maxwell) field and the Chern-Simons gauge field. It is the Chern-Simons term responsible for the presence of electrically and magnetically charged multivortices, known as anyons.

However in its full setting, the Euler–Lagrange equations relative to the anyon model take a complicated form, and so far a rigorous mathematical treatment of condensate solutions has been possible only for the reduced Abelian Chern–Simons–Higgs model where the Yang–Mills field is neglected. Such a reduction is justifiable at large distances and low energies where the Chern–Simons–Higgs term dominates the higher derivative Yang–Mills (or Maxwell) term.

For a special choice of the Higgs potential, where both symmetric and asymmetric vacua occur as ground states, Hong–Kim–Pac[8] and Jachiw–Weinberger[9] have observed that, in a full space settings, stationary vortex solutions for the Chern–Simons–Higgs model satisfy a set of Bogomolny-type selfdual equations similar to those obtained for the "classical" vortex theory, see Refs. 10–12

Thus, topological solutions carrying quantized electric and magnetic charge were obtained in Refs. 13 and 14, while non-topological solutions carrying fractal values of the charges were established in Refs. 15 and 16.

The same self-dual equations remain valid also under appropriate 't Hooft periodic boundary conditions, and were studied by Caffarelli and Yang in Ref. 17. They showed that, periodic multivortices (with assigned set of zeros for the Higgs scalar) exist, if and only if, the Chern-Simons coupling parameter is not too large with respect to the size of the periodic cell.

In this note, we complete the work of Caffarelli–Yang, and obtain that, to any assigned set of zeros for the Higgs scalar, there correspond (at least) two distinct solutions with the same quan-

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tized energy as well as electric and magnetic charge. This feature is in contrast with the classical vortex theory (see Refs. 10, 11, and 12) where a solution to the self-dual equation is completely characterized by the set of zeros of its Higgs scalar. However, for the Chern–Simons–Higgs model such a multiplicity property should not be surprising since it accounts for each of the vacuum state present in the potential field. In fact, we show that the solutions found can be "ordered" according to their superconducting properties; and, as the Chern-Simons coupling parameter tends to zero, the most superconducting solution tends (in a suitable norm) to the asymmetric vacuum while the other solution converges to the symmetric vacuum.

We refer to Theorem 2.1 and 2.2 of the following section for the precise statements.

II. THE CHERN–SIMONS–HIGGS MODEL, CORRESPONDING EQUATIONS AND STATEMENT OF THE MAIN RESULTS

In this section we introduce the appropriate 't Hooft periodic boundary conditions (see Ref. 18) and derive the analytical set up for the study of periodic multivortices in the Chern–Simons–Higgs model.

For this purpose, we follow[17] and show that the selfdual equations of Refs. 8 and 9 remain valid in the periodic situations.

The convention of summing repeated upper and lower indices will be observed throughout.

We consider the (2+1)-Minkowski space $R^{2,1}$ with metric tensor given by diag $(1,-1,-1)$ which we use to raise or lower indices.

According to the Abelian Higgs theory (see Ref. 10), the gauge field A defines a connection over the principle bundle $R^{2,1}\times U(1)$:

$$A=-iA_\eta dx^\eta, \quad A_\eta=A_\eta(x)\in R, \quad x=(x_0,x_1,x_2), \quad \eta=0,1,2;$$

with corresponding covariant derivative $D_A=d-iA$.

The curvature of A defines the Yang–Mills (or Maxwell) potential F_A, and it is given by

$$F_A=\frac{-i}{2}F_{\alpha,\beta}dx^\alpha\wedge dx^\beta$$

with $F_{\alpha\beta}=\partial_\alpha A_\beta-\partial_\beta A_\alpha$, $\alpha,\beta=0,1,2$.

Thus, if $\phi=\phi(x)$ is the complex valued Higgs scalar (a section over the associated bundle $R^{2,1}\times C$) and we write

$$D_A\phi=D_\eta\phi dx^\eta \text{ with } D_\eta\phi=\partial_\eta\phi-iA_\eta\phi \quad \eta=0,1,2,$$

the Chern–Simons–Higgs Lagrangean action density is defined by

$$\mathscr{L}(A,\phi)=(D_\eta\phi)(\overline{D^\eta\phi})+\tfrac{1}{4}k\epsilon^{\alpha\beta\gamma}F_{\alpha\beta}A_\gamma-V(|\phi|),$$

where $V=V(|\phi|)$ is the ($U(1)$-invariant) Higgs potential, $k>0$ is the Chern–Simons coupling parameter and the Levi–Civita tensor $\epsilon^{\alpha\beta\gamma},\alpha,\beta,\gamma=0,1,2$; is fixed by $\epsilon^{012}=1$.

The Euler–Lagrange equations corresponding to $\mathscr{L}$ are given by

$$\begin{cases} \frac{1}{2}k\epsilon^{\alpha\beta\gamma}F_{\alpha\beta}=j^\alpha=i(\phi\overline{D^\alpha\phi}-\bar{\phi}D^\alpha\phi) \\ D_\eta(D^\eta\phi)=-\dfrac{\partial V}{\partial\bar{\phi}} \end{cases}, \tag{2.1}$$

where $j^\alpha=(\rho,\mathbf{j})$ is the conserved matter current density.

We seek a static configuration of (2.1) subject to appropriate boundary condition to be specified according to the gauge invariance of $\mathscr{L}$.

For this purpose, we follow Ref. 17 and, as in Refs. 8 and 9, we obtain a reduction of (2.1) to a more convenient set of Bogomolny-type selfdual equation by the choice of the Higgs potential:

$$V(\phi)=\frac{1}{k^2}|\phi|^2(1-|\phi|^2)^2. \tag{2.2}$$

In fact, in the time independent situation, the $\alpha=0$ component of (2.1) yields to the relation:

$$kF_{1,2}=\rho=-2A_0|\phi|^2 \tag{2.3}$$

from which we derive the following form for the corresponding static energy density:

$$\mathscr{E}(A,\phi)=|D_1\phi|^2+|D_2\phi|^2+\frac{k^2}{4}\frac{F_{1,2}^2}{|\phi|^2}+\frac{1}{k^2}|\phi|^2(1-|\phi|^2)^2.$$

To specify the appropriate periodic boundary conditions, we recall the gauge invariance of $\mathscr{L}$ under the transformation:

$$\phi\to e^{i\omega}\phi, \quad A_\alpha+\partial_\alpha\omega, \quad \alpha=0,1,2,$$

with $\omega=\omega(x)$ a smooth function. In the stationary situation, the function ω depends only on (x_1,x_2) so that the gauge invariance is expressed by the transformation:

$$\phi\to e^{i\omega}\phi, \quad A_0\to A_0, \quad A_j\to A_j+\partial_j\omega; \quad j=1,2.$$

Let Ω be a basic cell in R^2 generated by the two independent vectors $\mathbf{a}^1$ and $\mathbf{a}^2$. Namely,

$$\Omega=\{x=(x_1,x_2)\in R^2: x=s_1\mathbf{a}^1+s_2\mathbf{a}^2, \quad 0<s_j<1 \quad j=1,2\}$$

with boundary,

$$\partial\Omega=\Gamma^1\cup\Gamma^2\cup\{\mathbf{a}^1+\Gamma^2\}\cup\{\mathbf{a}^2+\Gamma^1\}\cup\{\mathbf{0},\mathbf{a}^1,\mathbf{a}^2,\mathbf{a}^1+\mathbf{a}^2\}$$

where

$$\Gamma^j=\{x\in R^2: x=s_j\mathbf{a}^j 0<s_j<1\}, \quad j=1,2.$$

In view of the given gauge invariance we require the following 't Hooft boundary condition[18] to be satisfied by a solution (ϕ, A) of (2.1) in Ω:

$$\begin{cases} e^{i\xi_k(x+\mathbf{a}^k)}\phi(x+\mathbf{a}^k)=e^{i\xi_k(x)}\phi(x) \\ A_0(x+\mathbf{a}^k)=A_0(x) \\ (A_j+\partial_j\xi_k)(x+\mathbf{a}^k)=(A_j+\partial_j\xi_k)(x) \quad j=1,2, \\ \forall x\in\Gamma^1\cup\Gamma^2\backslash\Gamma^k, \quad k=1,2 \end{cases} \tag{2.4}$$

where ξ_1 and ξ_2 are smooth functions defined in a neighborhood of $\Gamma^2\cup\{\mathbf{a}^1+\Gamma^2\}$ and $\Gamma^1\cup\{\mathbf{a}^2+\Gamma^1\}$ respectively.

To simplify notation, set $\xi_k(s_1,s_2)=\xi_k(s_1\mathbf{a}^1+s_2\mathbf{a}^2)$ with $0<s_k<1$, $k=1,2$. Since ϕ is a single valued complex function, its phase change around Ω can only be a multiple of 2π and from (2.4) we are lead to the condition:

$$\xi_1(1,1^-)-\xi_1(1,0^+)+\xi_1(0,0^+)-\xi_1(0,1^-)+\xi_2(0^+,1)-\xi_2(1^-,1)+\xi_2(1^-,0)-\xi_2(0^+,0)+2\pi N=0, \tag{2.5}$$

with N a suitable integer.

As a consequence, we obtain that both, the magnetic flux Φ and the electric charge Q are quantized on the domain cell Ω. In fact, from (2.4) and (2.5) it follows:

$$\Phi=\int_\Omega F_{1,2}=\int_{\partial\Omega} A_j dx^j=2\pi N, \tag{2.6}$$

while (2.3) gives

$$Q=\int_\Omega \rho=k\Phi=2\pi kN.$$

Thus, in analogy to the classical vortex theory (see Ref. 10) the integer N (known as the vortex number or flux) defines a homotopical invariant quantity as it counts the zeros of ϕ (according to their multiplicity) inside the periodic cell Ω.

At this point, following Ref. 17, we rewrite the energy density as follows:

$$\mathcal{E}(A,\phi)=\frac{1}{4}\left[\frac{k}{|\phi|}F_{1,2}+\frac{2}{k}|\phi|(|\phi|^2-1)\right]^2+|D_1\phi+iD_2\phi|^2+F_{1,2}+\mathrm{Im}\{\partial_j\epsilon_{j,k}\bar{\phi}D_k\phi\}$$

with $\epsilon_{j,k}=-\epsilon_{k,j}$, $j,k=1,2$, and $\epsilon^{1,2}=1$.

Since, by the boundary condition (2.4), we have: $\int_\Omega \partial_j\epsilon_{j,k}\bar{\phi}D_k\phi=0$, we obtain the following form for the energy functional:

$$E(A,\phi)=\int_\Omega \mathcal{E}=\int_\Omega \frac{1}{4}\left[\frac{k}{|\phi|}F_{1,2}+\frac{2}{k}|\phi|(|\phi|^2-1)\right]^2+\int_\Omega |D_1\phi+iD_2\phi|^2+\int_\Omega F_{1,2}\geq\int_\Omega F_{1,2}.$$

Thus, the minimizer of E over the homotopically invariant constraint:

$$\int_\Omega F_{1,2}=2\pi N$$

will have to satisfy the self-dual equation:

$$\begin{cases} D_1\phi+iD_2\phi=0 \\ F_{1,2}+\dfrac{2}{k^2}|\phi|^2(|\phi|^2-1)=0 \\ kF_{1,2}+2A_0|\phi|^2=0 \end{cases} \tag{2.7}$$

together with the boundary conditions (2.4) and (2.5).

By direct inspection, it is easy to check that, for V given by (2.2), every solution (A,ϕ) for $(2.7)_k$ satisfies the full set of second order equations (2.1).

Equations $(2.7)_k$ were first derived by Refs. 8 and 9 to hold in all of R^2, provided $|\phi|$ satisfies some appropriate decay assumptions. Periodic boundary conditions were treated by Caffarelli–Yang[17] (see also Ref. 4) and here we have essentially reported their arguments.

Concerning $(2.7)_k$ subject to the boundary conditions (2.4)–(2.5) we will establish an existence and multiplicity result whenever the zeros of ϕ are prescribed together with their multiplicity.

In Theorem 2.1 we complete the existence result of Caffarelli–Yang, [17] and use it to motivate the more interesting Theorem 2.2, where we obtain a multiplicity result.

Roughly speaking, Theorems 2.1 and 2.2 assert that from the limiting value $k=0$ and each of the vacuum state $|\phi|=1$ and $|\phi|=0$ it "bifurcates" a solution to $(2.7)_k$ $k>0$, subject to the boundary conditions (2.4) and with a prescribed set of zeros for the Higgs scalar.

By taking complex conjugate of ϕ and A if necessary, we can always assume that $N\geq 0$ in (2.5) and obtain the following:

Theorem 2.1 (Existence): Let $p_1,\ldots,p_m$ be given points in Ω and $n_1,\ldots,n_m$ positive integers such that $\Sigma_{j=1}^m n_j=N$. There exists a critical value $k_c \in (0,(1/2)\sqrt{|\Omega|/\pi N})$ of the coupling parameter such that, Eq. $(2.7)_k$ subject to the boundary condition (1.4)–(1.5) admits a solution (A,ϕ) for which $p_1,\ldots,p_m$ are the zeros for ϕ with multiplicity $n_1,\ldots,n_m$, if and only if $0<k\leq k_c$.

Furthermore, when $0<k\leq k_c$ then problem $(2.7)_k$ admits a solution (A_k,ϕ_k) which, in addition to the zero set property fixed above also satisfies:

(i) The energy, magnetic flux and electric change of (A_k,ϕ_k) are respectively given by,

$$E=2\pi N, \quad \Phi=2\pi N, \quad Q=2\pi kN. \tag{2.8}$$

(ii) The solution (A_k,ϕ_k) is the most superconducting (or "maximal") in the sense that the magnitude $|\phi_k|$ takes the largest possible values among all solutions to $(2.7)_k$ with the same zero set.

(iii) The map $k\to|\phi_k|0<k\leq k_c$ is strictly monotone increasing;
$|\phi_k|<1$ in Ω;
$|\phi_k|\to 1$ as $k\to 0^+$ pointwise, a.e. in Ω and in $W^{1,q}(\Omega)$, $1<q<2$.
$F_{1,2}^{(k)}=\partial_1 A_2^{(k)}-\partial_2 A_1^{(k)}\to 2\pi\Sigma_{j=1}^N \delta_{p_j}$ in the sense of measure as $k\to 0^+$, where each Dirac distribution δ_{p_j} is repeated according to the corresponding multiplicity n_j, $j=1,\ldots,m$.

Theorem 2.2 (Multiplicity): Let $p_1,\ldots,p_m\in\Omega$, $n_1,\ldots,n_m\in N$ $\Sigma_{j=1}^m n_j=N$ and k_c be as given in Theorem 2.1.

If $0<k<k_c$, then (beside the maximal solution (A_k,ϕ_k)) Eq. $(2.7)_k$ admits a second solution $(\tilde{A}_k,\tilde{\phi}_k)$ satisfying (2.4)–(2.5) and for which $p_1,\ldots,p_m$ are the zeros of $\tilde{\phi}_k$ with multiplicity $n_1,\ldots,n_m$ respectively.

The formulas (2.8) hold respectively for the energy, magnetic flux and electric charge relative to $(\tilde{A}_k,\tilde{\phi}_k)$ and $|\tilde{\phi}_k|<|\phi_k|$ in $\Omega\setminus\{p_1,\ldots,p_m\}$. Furthermore, if $N=1$ then, for every integer $q\geq 0$ we have

$$\|\tilde{\phi}_k\|_{C^q(\Omega)}\to 0 \quad \text{as} \quad k\to 0^+.$$

We believe that the last statement in Theorem 2.2 should hold without the restriction $N=1$. However, as well shall see in Sec. III, the condition $N=1$ is essential for our method to work and a completely different approach is needed in order to treat the case $N>1$.

Theorems 2.1 and 2.2 will be proved with the help of a further reduction of Eqs. $(2.7)_k$ to a semilinear elliptic problem. This is in the spirit of the work of Taubes (cf. Refs. 12, 11, and 10) on N-vortex solutions in R^2 relative to the Ginzburg-Landau equations in superconductivity. In this situation, an analogous set of selfdual equations were first derived by Bogomolny[19] for the special value of the parameter which distinguishes between type I and II superconductors. In view of Bogomolny's equations, Taubes observed that the Higgs scalar can admit only a discrete set of zeros with integer multiplicity. Furthermore, once that such zeros (and relative multiplicity) are prescribed, the N-vortex problem reduces (in a fixed gauge) to the single unknown $u=\ln(|\phi|^2)$, which, according to the self-dual equations, will have to satisfy a semilinear elliptic equation in R^2 together with appropriate decay conditions.

In Ref. 14, Wang showed that an analogous approach is possible for the self-dual equations $(2.7)_k$ and obtained a topological N-vortex solution in R^2 for each prescribed set of zeros of the Higgs scalar. Similarly, in the periodic situation, Caffarelli–Yang[17] obtained a condensate solutions by reducing the problem to the search of a solution for a semilinear elliptic equation on the two-dimensional torus.

We will use the same approach and exploit the variational structure of the reduced elliptic problem (on the 2-torus), to obtain two solutions which define, respectively, a local minimum and a mountain-pass critical point for the associated action functional. In case $N=1$, by means of this variational characterization of the solutions, we will be able to study their behavior as $k\to 0^+$. We will see that, while (as expected) the local minimum converges, in a suitable norm, to a solution of a singular elliptic equation (involving some Dirac's measures), the mountain-pass solution yields, at the limit, to a solution of a (more surprising) mean field-type equation, whose interest has emerged already in other contests. We are referring to Eq. (3) of Sec. III, and just mention that the corresponding Dirichlet problem (3)* is amply discussed in Refs. 20–22 in connection with the study of the statistical mechanics of point vortices as a possible approach to the understanding of 2D turbulence.

We now proceed to derive our semilinear elliptic problem. To this purpose, as in Refs. 11 and 12 we observe that the first of the equations in $(2.7)_k$ may be rewritten as:

$$2\bar{\partial}\phi - i\hat{A}\phi = 0 \tag{2.9}$$

where, $\hat{A}=A_1+iA_2$ and $\bar{\partial}=\frac{1}{2}(\partial_1+i\partial_2)$.

Hence, up to a nonvanishing multiple factor, ϕ is holomorphic and therefore it admits a finite number of zeros in Ω with integer multiplicity.

Furthermore, solving for $\hat{A}$ in (1.9) we have

$$\hat{A} = -2i\bar{\partial}\ln\phi. \tag{2.10}$$

Denote by $Z(\phi)=\{p_1,\ldots,p_N\}\subset\Omega$ the zeros of ϕ each repeated according to their multiplicity.

Setting $z=x_1+ix_2$ and $u(z)=\ln|\phi(z)|^2$, we can assume that ϕ takes the form:

$$\phi(z)=\exp\left(\frac{1}{2}u(z)+i\sum_{j=1}^{N}\arg(z-p_j)\right), \tag{2.11}$$

where the somewhat arbitrary choice on the imaginary part of ϕ merely reflects the gauge invariance of the equations.

In view of (2.10), from (2.11) we may recover the A_1 and A_2 components of the connection A by the formulas:

$$A_1 = -\mathrm{Re}(2i\bar{\partial}\ln\phi) \tag{2.12}$$

$$A_2 = -\mathrm{Im}(2i\bar{\partial}\ln\phi).$$

Contrary to what might seem, a straightforward calculation shows that A_j, $j=1,2$ defines a C^∞ function on Ω.

Consequently, the curvature component $F_{1,2}=\partial_1 A_2-\partial_2 A_1$ may be computed and by the last of the equations in $(2.7)_k$ we also recover the $\alpha=0$ component of A which is given by

$$A_0 = -\frac{kF_{1,2}}{2|\phi|^2} = -\frac{k}{2|\phi|^2}(\partial_1 A_2-\partial_2 A_1). \tag{2.13}$$

Thus, problem $(2.7)_k$ is reduced to the search of a periodic function u such that,

$$u(z)=n_k \ln |z-p_k|^2 \text{ as } z\to p_k \tag{2.14}$$

(n_k is the multiplicity of p_k), and

$$\Delta u=\frac{4}{k^2} e^u(e^u-1) \text{ in } \Omega\backslash Z(\phi), \tag{2.15}$$

where (2.15) is just a restatement of the second equation in $(2.7)_k$, since away from the zeros of ϕ, the function u is smooth and by means of (2.12) we derive: $F_{1,2}=-\frac{1}{2}\Delta u$ in $\Omega\backslash Z(\phi)$.

Putting together (2.14) and (2.15) we are reduced to finding a solution u on the (flat) 2-torus for the equation:

$$\Delta u=\frac{4}{k^2} e^u(e^u-1)+4\pi\sum_{j=1}^{N} \delta_{p_j} \tag{2.16}$$

with δ_p the Dirac distribution concentrated at the point p.

This task will be taken up in the following section.

Existence of solutions for (2.16)

We identify the doubly periodic cell Ω with the two-dimensional torus, $\Omega=R^2/Z\times Z$ and let $p_1,\ldots,p_N$ be fixed points in Ω, repeated according to their multiplicity. Denote by u_0 the unique solution for:

$$\begin{cases} \Delta u_0=-\dfrac{4\pi N}{|\Omega|}+4\pi\displaystyle\sum_{j=1}^{N} \delta_{p_j} \text{ on } \Omega \\ \displaystyle\int_\Omega u_0=0 \end{cases}, \tag{2.17}$$

(see Ref. 23). As well known, $u_0\in C^\infty(\Omega\backslash\{p_1,\ldots,p_N\})$ and if n_j is the multiplicity of p_j then u_0 behaves like: $\ln(|x-p_j|^{2n_j})$ as $x\to p_j$. In particular, $u_0\in W^{1,q}(\Omega)\forall 1<q<2$. If u is a solution to (2.16), then setting $\lambda=4/k^2$ and $u=u_0+v$ we have that v is smooth and it satisfies

$$\begin{cases} \Delta v=\lambda e^{u_0+v}(e^{u_0+v}-1)+\dfrac{4\pi N}{|\Omega|}. \\ v\in H^1(\Omega) \end{cases} \tag{2.18}_\lambda$$

Conversely, every solution v of $(2.18)_{\lambda=4/k^2}$ gives rise to the solution $u=u_0+v$ of (2.16).

Thus, our effort, in this section, will be on searching for solutions $(2.18)_\lambda$.

To this purpose, we observe that $(2.18)_\lambda$ admits a variational formulation in $H^1(\Omega)$. To see this, let us fix our notation so that, $\|\ \|_p$ denotes the norm in $L^p(\Omega)p\geq 1$, and $\|u\|=(\|\nabla u\|_2^2+\|u\|_2^2)^{1/2}$ defines the norm for the Sobolev space $H^1(\Omega)$.

The Moser–Trudinger inequality (cf. Ref. 24):

$$\forall\epsilon>0 \text{ there exists a constant } C(\epsilon)>0:$$

$$\int_\Omega e^v\leq C(\epsilon)\exp\left(\left(\frac{1}{16\pi}+\epsilon\right)\|\nabla v\|_2^2\right)\forall v\in H^1(\Omega), \quad \int_\Omega v=0 \tag{2.19}$$

and the fact that $e^{u_0}\in L^\infty(\Omega)$, imply that the functional:

$$I_\lambda(v)=\frac{1}{2}\|\nabla v\|_2^2+\frac{\lambda}{2}\int_\Omega (e^{u_0+v}-1)^2+\frac{4\pi N}{|\Omega|}\int_\Omega v, \quad v\in H^1(\Omega), \tag{2.20}$$

is well defined, and $I_\lambda \in C^1(H^1(\Omega))$.

Furthermore, every critical point of I_λ in $H^1(\Omega)$ defines a (weak) solution to $(2.18)_\lambda$. By means of variational methods we shall establish the following:

Theorem 2.3: There exists a value $\lambda_c > 16\pi N/|\Omega|$ such that,

(i) if $\lambda>\lambda_c$ then $(2.18)_\lambda$ admits, at least, two solutions $v_{1,\lambda}$ and $v_{2,\lambda}$ satisfying:
$$v_{1,\lambda}<v_{2,\lambda}<-u_0 \text{ a.e. in } \Omega;$$
(ii) if $\lambda=\lambda_c$ then $(2.18)_\lambda$ admits a solution v_* satisfying: $v_*<v_{2,\lambda}, \forall \lambda>\lambda_c$;
(iii) if $\lambda<\lambda_c$ then $(2.18)_\lambda$ admits no solutions.

In order to obtain Theorem 2.3 recall the following result due to Caffarelli–Yang.

Theorem 2.4 (Caffarelli-Yang[17]): There exists a critical value $\lambda_c \geq 16\pi N/|\Omega|$ such that for every $\lambda>\lambda_c$ problem $(2.18)_\lambda$ admits a maximal solution v_λ with $u_0+v_\lambda<0$ in Ω. While for $\lambda<\lambda_c$ problem $(2.18)_\lambda$ admits no solutions.

Remark 2.1: It follows from Ref. 17 (or (3.6) below) that if $(2.18)_\lambda$ admits a solution then necessarily $\lambda>16\pi N/|\Omega|$.

Remark 2.2: Although it is not explicitly mentioned in Ref. 17, it is clear that the maximal solutions v_λ are ordered with respect to λ. Namely, if $\lambda>\eta>\lambda_c$ then $v_\lambda>v_\eta$ in Ω. To see this, notice that v_η is a strict subsolution for $(2.18)_\lambda$, $\lambda>\eta$. In fact,

$$\Delta v_\eta = \eta e^{u_0+v_\eta}(e^{u_0+v_\eta}-1)+\frac{4\pi N}{|\Omega|}=\lambda e^{u_0+v_\eta}(e^{u_0+v_\eta}-1)+(\eta-\lambda)e^{u_0+v_\eta}(e^{u_0+v_\eta}-1)+\frac{4\pi N}{|\Omega|}$$
$$>\lambda e^{u_0+v_\eta}(e^{u_0+v_\eta}-1)+\frac{4\pi N}{|\Omega|}$$

a.e. in Ω; in fact, $u_0+v_\eta<0$ in Ω and therefore $(\eta-\lambda)e^{u_0+v_\eta}(e^{u_0+v_\eta}-1)>0$ in $\Omega\backslash\{p_1,\ldots,p_N\}$.

Thus, by the sub-supersolutions method and the maximality of v_λ it must result that necessarily, $v_\eta<v_\lambda$ in Ω.

This monotonicity property allows us to obtain a solution for $(2.18)_\lambda$ at $\lambda=\lambda_c$ as given by

$$v^*(x)=\inf_{\lambda>\lambda_c} v_\lambda(x), \quad x\in\Omega. \tag{2.21}$$

Lemma 2.1: The function v_* as given in (2.21) belongs to $H^1(\Omega)$ and it defines a solution for $(2.18)_{\lambda=\lambda_c}$, in particular $\lambda_c>16\pi N/|\Omega|$.

Proof: By definition, $v_\lambda \to v_*$ pointwise a.e. in Ω. We shall prove that, in fact, $v_\lambda \to v_*$ strongly in $H^1(\Omega)$, and this will suffice to obtain the desired conclusion. To this purpose, we show that if $\lambda_n \to \lambda_c$, then after passing to a subsequence if necessary, we have $\|v_{\lambda_n}-v_*\|\to 0$ as $n\to\infty$. Set $v_n=v_{\lambda_n}$ and write: $v_n=v_n'+c_n$ with $\int_\Omega v_n'=0$ and $c_n=1/|\Omega|\int_\Omega v_n$. Since $v_n<-u_0$ in Ω it follows that,

$$c_n<-\frac{1}{|\Omega|}\int_\Omega u_0=0. \tag{2.22}$$

Furthermore, from Eq. $(2.18)_{\lambda=\lambda_n}$, we also derive

$$\|\nabla v_n'\|_2^2=\lambda_n\int_\Omega e^{u_0+v_n}v_n'-\lambda_n\int_\Omega e^{2(u_0+v_n)}v_n'\leqslant\lambda_n\int_\Omega(e^{u_0+v_n}+e^{2(u_0+v_n)})|v_n'|$$

$$\leqslant 2\lambda_n\int_\Omega|v_n'|\leqslant 2\lambda_n c\|\nabla v_n'\|_2$$

for a suitable constant $c>0$. In other words,

$$\|v_n'\|\leqslant C,\quad \forall n\in N$$

hence, passing to a subsequence if necessary, we have that $v_n'\to v_*'$ weakly in $H^1(\Omega)$, strongly in $L^p(\Omega)$, $\forall p\geqslant 1$ and pointwise almost everywhere in Ω. By the compactness of the map:

$$H^1(\Omega)\to L^1(\Omega)$$

$$u\to\int_\Omega e^{\alpha u},\quad \alpha\in R\ \text{(see Ref. 23)}$$

we may also conclude that,

$$\int_\Omega e^{u_0+v_n'}\to\int_\Omega e^{u_0+v_*'},\quad \int_\Omega e^{2(u_0+v_n')}\to\int_\Omega e^{2(u_0+v_*')} \tag{2.23}$$

as $n\to\infty$.

On the other hand, by means of the Eq. $(2.18)_{\lambda=\lambda_n}$, we also have

$$e^{2c_n}\lambda_n\int_\Omega e^{2(u_0+v_n')}-e^{c_n}\lambda_n\int_\Omega e^{u_0+v_n'}+4\pi N=0$$

and consequently,

$$e^{c_n}=\frac{\displaystyle\int_\Omega e^{u_0+v_n'}\pm\sqrt{\left(\int_\Omega e^{u_0+v_n'}\right)^2-\frac{16\pi N}{\lambda_n}\int_\Omega e^{2(u_0+v_n')}}}{\displaystyle 2\int_\Omega e^{2(u_0+v_n')}}$$

$$=\frac{8\pi N}{\lambda_n}\frac{1}{\displaystyle\int_\Omega e^{u_0+v_n'}\mp\sqrt{\left(\int_\Omega e^{u_0+v_n'}\right)^2-\frac{16\pi N}{\lambda_n}\int_\Omega e^{2(u_0+v_*')}}}$$

$$\geqslant\frac{4\pi N}{\lambda_n}\frac{1}{\int_\Omega e^{u_0+v_n'}}\longrightarrow\frac{4\pi N}{\lambda_c}\frac{1}{\int_\Omega e^{u_0+v_*'}}\ \text{as}\ n\to+\infty;\ \text{(by (2.23))}.$$

Thus c_n is also bounded from below and (by passing to a subsequence if necessary) we can assume $c_n\to c_0$ as $n\to+\infty$.

In other words, $v_n\to v_*'+c_0$ weakly in $H^1(\Omega)$, strongly in $L^p(\Omega)p\geqslant 1$ and pointwise a.e. in Ω. So necessarily,

$$v_*=v_*'+c_0\in H^1(\Omega).$$

Furthermore, as v_n, $v_*<-u_0$ in Ω, it results:

$$0<\frac{e^{u_0+v_n}-e^{u_0+v_*}}{v_n-v_*}<1 \quad \text{in } \Omega$$

and consequently

$$\left|\int_\Omega (e^{u_0+v_n}-e^{u_0+v_*})\varphi\right| \leq \int_\Omega \left(\frac{e^{u_0+v_n}-e^{u_0+v_*}}{v_n-v_*}\right)|v_n-v_*||\varphi| \leq \|v_n-v_*\|_2\|\varphi\|_2 \to 0$$

$$\text{as } n\to+\infty, \quad \forall \varphi \in H^1(\Omega). \tag{2.24}$$

Hence, $\int_\Omega e^{u_0+v_n}\varphi \to \int_\Omega e^{u_0+v_*}\varphi$ and similarly, $\int_\Omega e^{2(u_0+v_n)}\varphi \to \int_\Omega e^{2(u_0+v_*)}\varphi$ as $n\to+\infty$, $\forall \varphi \in H^1(\Omega)$.

In other words, v_* satisfies $(2.18)_{\lambda=\lambda_c}$ and by taking $\varphi=v_n-v_*$ in (2.24) we also conclude:

$$\|\nabla(v_n-v_*)\|_2^2=\lambda_n\int_\Omega (e^{u_0+v_n}-e^{u_0+v_*})(v_n-v_*)-\lambda_n\int_\Omega (e^{2(u_0+v_n)}-e^{2(u_0+v_*)})(v_n-v_*)+o(1)$$

$$\leq 2\lambda_n\|v_n-v_*\|_2^2+o(1)\to 0, \text{ as } n\to+\infty.$$

Hence $v_n\to v_*$ strongly in $H^1(\Omega)$.

Finally, it follows from Ref. 6 or (3.6) below that if $(2.18)_\lambda$ admits a solution then necessarily $\lambda>16\pi N/|\Omega|$ and consequently $\lambda_c>16\pi N/|\Omega|$.

In virtue of lemma 2.1, we are able to identify a solution for $(2.18)_\lambda$ variationally as follows.

Lemma 2.2: For every $\lambda>\lambda_c$, problem $(2.1)_\lambda$ admits a solution which defines a local minimum for I_λ in $H^1(\Omega)$.

Proof: It is clear that the solution v_* of $(2.1)_{\lambda=\lambda_c}$ (as given by lemma 2.1) defines a strict subsolution for $(2.1)_\lambda$ for every $\lambda>\lambda_c$.

Set

$$\Lambda=\{v\in H^1(\Omega): v\geq v_* \text{ a.e. in } \Omega\}.$$

From the definition of the functional I_λ, (see (2.3)) we easily see that I_λ is weakly lower semicontinuous in $H^1(\Omega)$ and it is bounded from below and coercive on Λ.

Thus, I_λ achieves its infimum in Λ, and we denote it by w_λ.

Namely,

$$I_\lambda(w_\lambda)=\inf_\Lambda I_\lambda, \quad w_\lambda\in\Lambda.$$

Since, for every $\lambda>\lambda_c$, v_* is a strict subsolution for $(2.18)_\lambda$, we may conclude that w_λ is a critical point for I_λ in $H^1(\Omega)$ (hence a solution for $(2.18)_\lambda$). Although this is a well known fact, for completeness we have included a proof in the Appendix. Furthermore, by the maximum principle, we may also conclude that $w_\lambda>v_*$ on the compact 2-torus Ω.

This says that ω_λ is a local minimum for I_λ with respect to the $C^1(\Omega)$-topology. We prove in fact that w_λ is a local minimum also in $H^1(\Omega)$-topology.

To this purpose, we follow an argument of Brezis–Nirenberg[25] and argue by contradiction. Thus we suppose that, $\forall n\in N$

$$\inf_{\|v-w_\lambda\|\leq\frac{1}{n}} I_\lambda < I_\lambda(w_\lambda). \tag{2.25}$$

As above, we see that the infimum of (2.25) is achieved at a point $v_n\in H^1(\Omega)$ which satisfies:

(1) $-\Delta v_n+\lambda e^{u_0+v_n}(e^{u_0+v_n}-1)+4\pi N/|\Omega|=\eta_n(-\Delta(v_n-w_\lambda)+v_n-w_\lambda)$;
(2) $\|v_n-w_\lambda\|\leq 1/n$.

Clearly, $\eta_n\leq 0$ and, by the Sobolev embedding, $\|v_n-w_\lambda\|_p\to 0$ as $n\to+\infty$.

Consequently,

$$-\Delta(v_n-w_\lambda)=-\frac{|\eta_n|}{1+|\eta_n|}(v_n-w_\lambda)-\frac{\lambda}{1+|\eta_n|}(e^{2(u_0+v_n)}-e^{2(u_0+w_\lambda)})+\frac{\lambda}{1+|\eta_n|}(e^{u_0+v_n}-e^{u_0+w_\lambda}):=f_n \text{ in } \Omega.$$

$f_n\in L^p(\Omega)$ $\forall p>1$ and $\|f_n\|_p\leq C\|v_n-w_\lambda\|\leq C/n$, with $C=C(p,\lambda)$ a suitable constant independent of n.

So, by elliptic estimates and the Sobolev embedding Theorem, for $p>2$ we derive that $v_n-w_\lambda\in C^{1,\alpha}(\Omega)$, $0<\alpha<1$ and $\|v_n-w_\lambda\|_{C^1(\Omega)}\to 0$ as $n\to+\infty$. But this is impossible, since w_λ is a local minimum for I_λ in the $C^1(\Omega)$ topology while $I_\lambda(v_n)=\inf_{\|v-w_\lambda\|\leq 1/n} I_\lambda<I_\lambda(w_\lambda)$.

From now on, we assume that the maximal solution v_λ (cf. Ref. 17) is the local minimum as defined by lemma 2.2 (if not, we would have already found our second solution); hence it satisfies:

$$\exists \rho_0>0: I_\lambda(v_\lambda)\leq I_\lambda(v) \quad \forall v: \|v-v_\lambda\|\leq\rho_0. \tag{2.26}$$

In order to find a second critical point, we observe that I_λ admits a "mountain-pass" structure (cf. Ref. 26). In fact, for $c>0$ we have

$$I_\lambda(v_\lambda-c)-I_\lambda(v_\lambda)=\frac{\lambda}{2}\int_\Omega[(e^{u_0+v_\lambda-c}-1)^2-(e^{u_0+v_\lambda}-1)^2]-2\pi Nc$$

$$\leq\lambda(1-e^{-c})\int_\Omega e^{u_0+v_\lambda}-2\pi Nc\to-\infty \text{ as } c\to+\infty. \tag{2.27}$$

In order to apply the minimax principle suitable to this situation we start by verifying a compactness property for I_λ as stated by the Palais–Smale (P.S.) condition.

Lemma 2.3: Every sequence $\{v_n\}\subset H^1(\Omega)$ satisfying:

(1) $I_\lambda(v_n)\to\alpha$ as $n\to+\infty$
(2) $\|I'_\lambda(v_n)\|\to 0$ as $n\to+\infty$

admits a convergent subsequence.

Proof: We have

$$\frac{1}{2}\|\nabla v_n\|_2^2+\frac{\lambda}{2}\int_\Omega(e^{u_0+v_n}-1)^2+\frac{4\pi N}{|\Omega|}\int_\Omega v_n=\alpha+o(1) \text{ as } n\to\infty \tag{2.28}$$

$$\left|\int_\Omega\nabla v_n\cdot\nabla\varphi+\lambda\int_\Omega e^{u_0+v_n}(e^{u_0+v_n}-1)\varphi+\frac{4\pi N}{|\Omega|}\int_\Omega\varphi\right|\leq\epsilon_n\|\varphi\|, \quad \epsilon_n\to 0 \tag{2.29}$$

as $n\to+\infty$, $\varphi\in H^1(\Omega)$.

By taking $\varphi=1$ in (2.29) we obtain

$$o(1)=\lambda\int_\Omega e^{u_0+v_n}(e^{u_0+v_n}-1)+4\pi N=\lambda\int_\Omega (e^{u_0+v_n}-1)^2+\lambda\int_\Omega e^{u_0+v_n}-\lambda|\Omega|+4\pi N$$

$$\geq\lambda\int_\Omega e^{u_0+v_n}-\lambda|\Omega|+4\pi N.$$

Consequently,

$$\int_\Omega e^{u_0+v_n}\leq|\Omega|-\frac{4\pi N}{\lambda}+o(1),\quad \text{as } n\to+\infty \tag{2.30}$$

and

$$\int_\Omega (e^{u_0+v_n}-1)^2\leq|\Omega|-\frac{4\pi N}{\lambda}+o(1)\ \text{ as } n\to+\infty, \tag{2.31}$$

which yields

$$\int_\Omega e^{2(u_0+v_n)}\leq 2\left(|\Omega|-\frac{4\pi N}{\lambda}\right)+o(1) \tag{2.32}$$

as $n\to+\infty$.

In particular, setting $c_n=1/|\Omega|\int_\Omega v_n$, from (2.28) and (2.31) we derive

$$\alpha+\frac{1}{2}(4\pi N-\lambda|\Omega|)+o(1)\leq\frac{\|\nabla v_n\|_2^2}{2}+4\pi N c_n\leq\alpha+o(1) \tag{2.33}$$

as $n\to+\infty$.

Decompose $v_n=v_n'+c_n$, $\int_\Omega v_n'=0$. By (2.29) with $\varphi=v_n'$ we have

$$\|\nabla v_n'\|_2^2+\lambda\int_\Omega e^{2(u_0+v_n)}v_n'-\lambda\int_\Omega e^{u_0+v_n}v_n'\leq\epsilon_n\|v_n'\|.$$

Consequently, by (2.32) and the fact that c_n is bounded above (see (2.33)) it follows:

$$\|\nabla v_n'\|_2^2+\lambda\int_\Omega e^{2(u_0+c_n)}(e^{2v_n'}-1)v_n'\leq-\lambda\int_\Omega e^{2(u_0+c_n)}v_n'+\epsilon_n\|v_n'\|+\lambda\left(\int_\Omega e^{2(u_0+v_n)}\right)^{1/2}\|v_n'\|_2$$

$$\leq C\|v_n'\|\ \text{ as } n\to+\infty, \tag{2.34}$$

for a suitable constant $C>0$.

Notice that, $(e^{2v_n'}-1)v_n'\geq 0$ a.e. in Ω, and therefore, from (2.17) we derive

$$\|v_n'\|\leq C,\quad \forall n\in N. \tag{2.35}$$

In turn, (2.35) together with (2.33) gives that $|c_n|$ is also uniformly bounded, and consequently, we have

$$\|v_n\|\leq C\quad \forall n\in N$$

for a suitable constant $C>0$.

Therefore, after passing to a subsequence (which we still denote by v_n), we may assume that,

$$v_n \rightharpoonup v \text{ weakly in } H^1(\Omega), \text{ strongly in } L^p(\Omega) p \geq 1$$

and pointwise a.e. in Ω.

In particular, $c_n \to (1/|\Omega|)\int_\Omega v = c$; and passing to the limit in (2.29) we obtain that v is a critical point for I_λ as it satisfies

$$\int_\Omega \nabla v \cdot \nabla \varphi + \lambda \int_\Omega e^{u_0+v}(e^{u_0+v}-1)\varphi + \frac{2\pi N}{|\Omega|}\int_\Omega \varphi = 0 \quad \forall \varphi \in H^1(\Omega). \tag{2.36}$$

Hence, by choosing $\varphi = v_n - v$ in (2.29) and (2.36), we conclude

$$\begin{aligned}\int_\Omega |\nabla(v_n - v)|^2 &= \lambda \int_\Omega (e^{u_0+v_n} - e^{u_0+v})(v_n - v) - \lambda \int_\Omega (e^{2(u_0+v_n)} - e^{2(u_0+v)})(v_n - v) + o(1) \\ &\leq \lambda \int_0^1 e^{tc_n+(1-t)c}\left(\int_\Omega e^{u_0+tv_n'+(1-t)v'}(v_n - v)^2 \right) dt + o(1) \\ &\leq C\|v_n - v\|_p^2 + o(1), \quad \text{as } n \to +\infty,\end{aligned}$$

for $p > 2$ and $C > 0$ a suitable constant independent of n. Therefore, $\|\nabla(v_n' - v')\| \to 0$ and in turn, $\|v_n - v\| \leq C(\|\nabla(v_n' - v')\|_2 + |c_n - c|) \to 0$ as $n \to +\infty$.

We are now ready to conclude.

The proof of Theorem 2.3: In view of lemma 2.1 and 2.2 and Caffarelli–Yang's result[17] we have that, problem $(2.18)_\lambda$ admits a solution if and only if $\lambda \geq \lambda_c > 16\pi N/|\Omega|$

Furthermore, for $\lambda > \lambda_c$, such a solution defines a local minimum for I_λ and, as already observed, it can be taken to coincide with the maximal solution v_λ for $(2.18)_\lambda$ (established by Caffarelli–Yang in Ref. 17). Therefore, (2.9) and (2.10) hold. In case v_λ is not a strict local minimum for I_λ then

$$\forall 0 < \rho < \rho_0, \quad \inf_{\|v - v_\lambda\| = \rho} I_\lambda = I_\lambda(v_\lambda) = \alpha_\lambda,$$

and, by an application of Ekeland's lemma (see Ref. 26, Corollary 1.6) we find a local minimum $v_\rho \in H^1(\Omega)$ such that $\|v_\rho - v_\lambda\| = \rho$, and $I_\lambda(v_\rho) = \alpha_\lambda$, $\forall \rho \in (0, \rho_0)$. Thus, in this situation, we obtain a one-parameter family of solutions for $(2.18)_\lambda$.

In case v_λ is a strict local minimum for I_λ (by the arguments of next section, we believe that this is always the case for $\lambda \to +\infty$) then there would exist $\rho_1 \in (0, \rho_0)$ such that

$$\inf_{\|v - v_\lambda\| = \rho_1} I_\lambda > I_\lambda(v_\lambda) = \alpha_\lambda \tag{2.37}$$

and in view of (2.27):

$$I_\lambda(v_\lambda - c_0) \leq I_\lambda(v_\lambda) - 1 < I_\lambda(v_\lambda)$$

for some $c_0 > \rho_1 > 0$ sufficiently large.

Let $\mathscr{P} = \{\gamma : [0,1] \to H^1(\Omega) \text{ continuous } \gamma(0) = v_\lambda,\ \gamma(1) = v_\lambda - c_0\}$ and set

$$\alpha = \inf_{\gamma \in \mathscr{P}} \sup_{t \in [0,1]} I_\lambda(\gamma(t)).$$

By (2.37) it results $\alpha > I_\lambda(v_\lambda) \geq \max\{I_\lambda(\gamma(0)), I_\lambda(\gamma(1))\}$ $\forall \gamma \in \mathscr{P}$. So by lemma 2.3, we see that I_λ satisfies all the hypothesis of the mountain-pass theorem of Ambrosetti–Rabinowitz[27] and we

conclude that α defines a critical value for I_λ. Since $\alpha > I_\lambda(v_\lambda)$, the corresponding critical point v yields to a second solution for $(2.18)_\lambda$. Clearly by the maximality of v_λ, it follows that $v < v_\lambda$ in Ω and the proof its completed.

III. ASYMPTOTIC BEHAVIOR FOR THE SOLUTIONS OF $(2.18)_\lambda$ AS $\lambda \to +\infty$

In this section, we would like to characterize the different nature of the solutions found in theorem 2.3, according to their behavior as $\lambda \to +\infty$.

In order to justify why a solution to $(2.18)_\lambda$ should admit a limit as $\lambda \to +\infty$, we start with the following *a priori* estimates.

Lemma 3.1: For every $q \in (1,2)$ there exists a constant $C = C(q) > 0$ (independent of λ and N) such that every solution v for $(2.18)_\lambda$ satisfies:

$$\|\nabla(u_0 + v)\|_q \leq C(4\pi N + \|\nabla u_0\|_q) \tag{3.1}$$

Proof: Let $p = q/(q-1) > 2$. Since $u_0 \in W^{1,q}(\Omega)$, the extremal problem:

$$\sup\left\{ \int_\Omega \nabla(v + u_0) \cdot \nabla \varphi, \varphi \in W^{1,p}(\Omega), \|\varphi\|_{W^{1,p}} = 1 \int_\Omega \varphi = 0 \right\} \tag{3.2}$$

achieves its supremum at some $\varphi_0 \in W^{1,p}(\Omega)$, $\int_\Omega \varphi_0 = 0$, $\|\varphi_0\|_{W^{1,p}} = 1$.

Take as test function φ in (3.2) the (normalized) unique solution for the problem:

$$\begin{cases} -\Delta \varphi = \operatorname{div}(|\nabla(v + u_0)|^{q-2} \nabla(v + u_0)) \text{ in } \Omega \\ \int_\Omega \varphi = 0 \end{cases}$$

Since $|\nabla(v + u_0)|^{q-2} \nabla(v + u_0) \in L^p(\Omega) p > 2$, by the Calderon–Zygmund inequality, we have

$$\|\nabla \varphi\|_p \leq c \|\nabla(v + u_0)\|_q^{q-1}$$

with suitable constant $c > 0$. Therefore,

$$c^{-1} \|\nabla(v + u_0)\|_q \leq \int_\Omega \nabla(v + u_0) \cdot \frac{\nabla \varphi}{\|\nabla \varphi\|_p} \leq \int_\Omega \nabla(v + u_0) \cdot \nabla \varphi_0 = -\int_\Omega \Delta v \varphi_0 + \int_\Omega \nabla u_0 \cdot \nabla \varphi_0$$

$$\leq \lambda \int_\Omega e^{u_0 + v}(1 - e^{u_0 + v}) \varphi_0 + \|\nabla u_0\|_q \|\nabla \varphi_0\|_p$$

$$\leq \|\varphi_0\|_\infty \lambda \int_\Omega e^{u_0 + v}(1 - e^{u_0 + v}) + C \|\nabla u_0\|_q ;$$

where we have used the fact that every solution of $(2.18)_\lambda$ satisfies $u_0 + v < 0$ on Ω, and therefore $1 - e^{u_0 + v} > 0$ on Ω.

On the other hand, as $p > 2$ by Sobolev embedding, we have that $\|\varphi_0\|_\infty \leq c \|\varphi_0\|_{W^{1,p}} = c$, while integrating $(2.18)_\lambda$ we have:

$$\lambda \int_\Omega e^{u_0 + v}(1 - e^{u_0 + v}) = 4\pi N. \tag{3.2'}$$

At this point, (3.1) follows immediately.

We begin by analyzing the behavior of the maximal solution v_λ as $\lambda \to +\infty$. Roughly speaking we show that v_λ "bifurcates from infinity" from the singular solution u_0.

More precisely we have the following.

Proposition 3.1: Let v_λ be the maximal solution for $(2.18)_\lambda \lambda > \lambda_c$. We have:

(i) $v_\lambda \to -u_0$ as $\lambda \to +\infty$ in $W^{1,q}(\Omega)\, 1<q<2$ and pointwise a.e. in Ω;

(ii) $\lambda e^{u_0+v_\lambda}(1-e^{u_0+v_\lambda}) \to 4\pi \Sigma_{j=1}^N \delta_{p_j}$ as $\lambda \to +\infty$, in the sense of measure.

Proof: Recall that v_λ is strictly monotone increasing in λ,

$$v_* < v_\lambda < -u_0 \text{ a.e. in } \Omega, \quad \forall \lambda > \lambda_c; \tag{3.3}$$

and

$$\int_\Omega e^{u_0+v_\lambda}(1-e^{u_0+v_\lambda}) = \frac{4\pi N}{\lambda}. \tag{3.4}$$

Set $\bar{v} = \sup_{\lambda>\lambda_c} v_\lambda(x), x \in \Omega$. We have that, $v_* < \bar{v} \leqslant -u_0$ a.e. in Ω and $v_\lambda \to \bar{v}$ pointwise a.e. in Ω, as $\lambda \to +\infty$.

By monotone (or dominated) convergence and (3.4) it follows that, as $\lambda \to +\infty$,

$$\int_\Omega e^{u_0+v_\lambda}(1-e^{u_0+v_\lambda}) \mapsto \int_\Omega e^{u_0+\bar{v}}(1-e^{u_0+\bar{v}}) = 0$$

and thus necessarily, $\bar{v} = -u_0$ a.e. in Ω.

Let $f_\lambda = \lambda e^{u_0+v_\lambda}(1-e^{u_0+v_\lambda}) \geqslant 0$. In view of (3.4) we have $\|f_\lambda\|_1 = 4\pi N$, therefore given any sequence $\lambda_n \to +\infty$, there exists a measure η on Ω such that (after passing to a subsequence if necessary) we have

$$\lambda_n e^{u_0+v_n}(1-e^{u_0+v_n}) \to \eta$$

in the sense of measure. Set $v_n = v_{\lambda_n}$, and let $\varphi \in C^\infty(\Omega)$ then:

$$\int_\Omega \lambda_n e^{u_0+v_n}(e^{u_0+v_n}-1)\varphi + \frac{4\pi N}{|\Omega|}\int_\Omega \varphi = \int_\Omega \Delta v_n \varphi = \int_\Omega v_n \Delta \varphi \overset{n\to+\infty}{\mapsto} \int_\Omega -u_0 \Delta \varphi$$

$$= -4\pi \sum_{j=1}^N \varphi(p_j) + \frac{4\pi N}{|\Omega|}\int_\Omega \varphi.$$

Consequently, $\eta = 4\pi \Sigma_{j=1}^N \delta_{p_j}$.

Since this holds for any sequence $\lambda_n \to +\infty$, we conclude, as $\lambda \to +\infty$ that,

$$\lambda e^{u_0+v_\lambda}(1-e^{u_0+v_\lambda}) \to 4\pi \sum_{j=1}^N \delta_{p_j};$$

in the sense of measure, and (ii) is established.

Next, fix $q \in (1,2)$ and let $p = q/(q-1) > 2$. For $\lambda_n \to +\infty$, and $v_n = v_{\lambda_n}$, let $\varphi_n \in W^{1,p}(\Omega)$, $\int_\Omega \varphi_n = 0$ and $\|\varphi_n\|_{W^{1,p}} = 1$ such that,

$$\int_\Omega \nabla(v_n+u_0)\cdot\nabla\varphi_n = \sup\left\{ \int_\Omega \nabla(v_n+u_0)\cdot\nabla\varphi, \int_\Omega \varphi = 0 \|\varphi\|_{W^{1,p}} = 1 \right\}.$$

As in lemma 3.1 it results,

$$c^{-1}\|\nabla(v_n+u_0)\|_q \leq \int_\Omega \nabla(v_n+u_0)\cdot\nabla\varphi_n \tag{3.5}$$

for a suitable constant $c>0$ (independent of n).

On the other hand, as $p>2$, we find a subsequence of $\{\varphi_n\}$ (which we still call φ_n) and $\varphi_0\in W^{1,p}(\Omega)$, $\int_\Omega\varphi_0=0$ such that, $\varphi_n\rightharpoonup\varphi_0$ weakly in $W^{1,p}(\Omega)$ and uniformly in Ω.

As a consequence we obtain:

$$\begin{aligned}
c^{-1}\|\nabla(v_n+u_0)\|_q &\leq \int_\Omega \nabla(v_n+u_0)\cdot\nabla\varphi_n = \int_\Omega \nabla v_n\cdot\nabla\varphi_n + \int_\Omega \nabla u_0\cdot\nabla\varphi_n \\
&= \int_\Omega \nabla v_n\cdot\nabla(\varphi_n-\varphi_0) + \int_\Omega \nabla v_n\cdot\nabla\varphi_0 + \int_\Omega \nabla u_0\cdot\nabla\varphi_n \\
&= \int_\Omega \lambda_n e^{u_0+v_n}(1-e^{u_0+v_n})(\varphi_n-\varphi_0) \\
&\quad - \frac{4\pi N}{|\Omega|}\int_\Omega(\varphi_n-\varphi_0) + \int_\Omega \lambda_n e^{u_0+v_n}(1-e^{u_0+v_n})\varphi_0 - 4\pi\sum_{j=1}^N \varphi_0(p_j)+o(1) \\
&\leq 4\pi N\|\varphi_n-\varphi_0\|_\infty + \int_\Omega \lambda_n e^{u_0+v_n}(1-e^{u_0+v_n})\varphi_0 - 4\pi\sum_{j=1}^N \varphi_0(p_j)+o(1) \\
&\to 0 \quad \text{as } n\to+\infty.
\end{aligned}$$

Since this holds for every sequence $\lambda_n\to+\infty$, we conclude that,

$$\|\nabla(u_0+v_\lambda)\|_q\to 0 \quad \text{as } \lambda\to+\infty.$$

On the other hand, by dominated convergence, we also have that $v_\lambda\to -u_0$ in $L^q(\Omega)$ and we derive the desired conclusion: $\|u_0+v_\lambda\|_{W^{1,q}}\to 0$, as $\lambda\to+\infty$.

We will exhibit a different behavior for the "mountain-pass" solution as $\lambda\to+\infty$ and $N=1$.

For this purpose we start by observing that every solution $v=v'+c$, $\int_\Omega v'=0$ for $(2.18)_\lambda$, $\lambda\geq\lambda_c$ satisfies:

$$e^{2c}\int_\Omega e^{2(u_0+v')} - e^c\int_\Omega e^{u_0+v'} + \frac{4\pi N}{\lambda} = 0,$$

hence necessarily,

$$\left(\int_\Omega e^{u_0+v'}\right)^2 - \frac{16\pi N}{\lambda}\int_\Omega e^{2(u_0+v')} \geq 0 \tag{3.6}$$

(which reaffirms the condition $\lambda_c\geq 16\pi N/|\Omega|$) and

$$e^c = \frac{\int_\Omega e^{u_0+v'} \pm \sqrt{(\int_\Omega e^{u_0+v'})^2 - (16\pi N/\lambda)\int_\Omega e^{2(u_0+v')}}}{2\int_\Omega e^{2(u_0+v')}}. \tag{3.7}$$

We show that, when $v=v_\lambda$ is the maximal solution for $(2.1)_\lambda$ and $\lambda\to+\infty$, then,

(i) the strict inequality must hold in (3.6);
(ii) the "plus" sign must be chosen in (3.7).

In fact, the monotonicity of the map: $\lambda \to v_\lambda$ guaranties that, $w_\lambda = \partial v_\lambda / \partial \lambda$ is well defined for almost every $\lambda > \lambda_c$. Furthermore $w_\lambda \geqslant 0$ a.e. in Ω and,

$$\langle I''_\lambda(v_\lambda) w_\lambda, \varphi \rangle = \int_\Omega e^{u_0+v_\lambda}(1-e^{u_0+v_\lambda})\varphi \quad \forall \varphi \in H^1(\Omega).$$

Since, $u_0 + v_\lambda < 0$ in Ω, this implies that $I''_\lambda(v_\lambda)$ is (strictly) positive definite for a.e. $\lambda > \lambda_c$. Hence, after a limiting process, we may conclude:

$$\langle I''_\lambda(v_\lambda)\varphi, \varphi \rangle \geqslant 0 \quad \forall \varphi \in H^1(\Omega). \tag{3.8}$$

Notice that (3.8) is obviously satisfied by the solution to $(2.18)_\lambda$ corresponding to the local minimum (see lemma 2.2) and therefore it should not be surprising since it is expected that the local minimum and maximal solution is one and the same.

Take $\varphi \equiv 1$ in the above inequality (3.8) to derive:

$$\lambda \int_\Omega e^{u_0+v_\lambda}(2e^{u_0+v_\lambda}-1) \geqslant 0.$$

On the other hand, by (3.7) we have:

$$\pm\lambda \sqrt{\left(\int_\Omega e^{u_0+v_\lambda}\right)^2 - \frac{16\pi N}{\lambda}\int_\Omega e^{2(u_0+v_\lambda)}} = \lambda \int_\Omega e^{u_0+v_\lambda}(2e^{u_0+v_\lambda}-1) \geqslant 0. \tag{3.9}$$

Now suppose that there exists a sequence $\lambda_n \to +\infty$ such that

$$\left(\int_\Omega e^{u_0+v'_n}\right)^2 = \frac{16\pi N}{\lambda_n}\int_\Omega e^{2(u_0+v'_n)}, \quad \forall n \in N$$

where $v_n = v_{\lambda_n} = v'_n + c_n$, $\int_\Omega v'_n = 0$. By (3.9) and Proposition 3.1 this yields the following contradiction,

$$0 = \int_\Omega (2e^{2(u_0+v_n)} - e^{u_0+v_n}) \mapsto |\Omega| \quad \text{as} \quad n \to +\infty.$$

In conclusion, there exists $\lambda_0 > 0$ such that, $\forall \lambda > \lambda_0$ (3.6) with $v = v_\lambda$ holds with a strict inequality and, in view of (3.9) the "plus" sign must be taken in (3.7).

Remark 3.1: Notice that conditions (i) and (ii) essentially characterize those solutions to $(2.18)_\lambda$ which correspond to local minima for I_λ.

Setting $v_\lambda = w'_\lambda + c_\lambda$ with $\int_\Omega w'_\lambda = 0$, we have,

$$e^{c_\lambda} = \frac{\int_\Omega e^{u_0+w'_\lambda} + \sqrt{(\int_\Omega e^{u_0+w'_\lambda})^2 - (16\pi N/\lambda)\int_\Omega e^{2(u_0+w'_\lambda)}}}{2\int_\Omega e^{2(u_0+w'_\lambda)}} > \frac{\int_\Omega e^{u_0+w'_\lambda}}{2\int_\Omega e^{2(u_0+w'_\lambda)}} \quad \text{as} \quad \lambda \to +\infty,$$

and we conclude that $c = c_\lambda$ defines a (strict) local minimum for the function

$$\psi(c) = I_\lambda(w'_\lambda + c), \quad c \in R.$$

Since v_λ is also a local minimum for I_λ with respect to all the other directions $v' \in H^1(\Omega)$, this suggests the definitions:

$$\mathcal{A}=\left\{w\in H^1(\Omega):\int_\Omega w=0,\left(\int_\Omega e^{u_0+w}\right)^2-\frac{16\pi N}{\lambda}\int_\Omega e^{2(u_0+w)}\geqslant 0\right\},$$

$$c_\pm(w)=\ln\left(\frac{\int_\Omega e^{u_0+w}\pm\sqrt{(\int_\Omega e^{u_0+w})^2-(16\pi N/\lambda)\int_\Omega e^{2(u_0+w)}}}{2\int_\Omega e^{2(u_0+w)}}\right)$$

$\forall w\in\mathcal{A}$, and alternatively characterize the local minimum for I_λ by the extremal problem:

$$\inf_{w\in\mathcal{A}}\min_{c\geqslant c_-(w)}I_\lambda(w+c)=\inf_{w\in\mathcal{A}}\left\{\int_\Omega\left[\frac{1}{2}|\nabla w|^2+\frac{\lambda}{2}(e^{u_0+w+c_+(w)}-1)^2\right]+4\pi c_+(w)\right\} \tag{3.10}$$

provided that the infimum in (3.10) is finite.

This point of view was adopted by Caffarelli–Yang in Ref. 17 where they show that, for $N=1$ and λ sufficiently large; (3.10) achieves its infimum at a solution of $(2.1)_\lambda$.

On the other hand, this approach also suggests to recast the "mountain pass" solution found above via an analogous minimax procedure which, as we shall see, turns out to be useful when studying the asymptotic behavior of such a solution for $\lambda\to+\infty$. To insure the boundedness from below of the appropriate minimization problem, as in Ref. 17, we shall treat the case $N=1$ (i.e. the vortices are periodically placed).

Proposition 3.2: Let $N=1$. There exists $\lambda_0\geqslant\lambda_c$ such that $\forall\lambda>\lambda_0$, the value

$$\beta_\lambda=\inf_{w\in\mathcal{A}}\max_{c\leqslant c_+(w)}I_\lambda(w+c)=\inf_{w\in\mathcal{A}}\left\{\int_\Omega\left[\frac{1}{2}|\nabla w|^2+\frac{\lambda}{2}(e^{u_0+w+c_-(w)}-1)^2\right]+4\pi c_-(w)\right\}$$

defines a critical value for I_λ in $H^1(\Omega)$.

Denoting with $\tilde{v}_\lambda=w_\lambda+c_\lambda\in H^1(\Omega)\int_\Omega w_\lambda=0$, the corresponding critical point we have

(1) $c_\lambda\mapsto-\infty$ as $\lambda\to+\infty$;
(2) there exists a constant $C>0$ (independent of λ) such that

$$\|w_\lambda\|\leqslant C,\quad\forall\lambda>\lambda_0.$$

Furthermore every sequence $\lambda_n\to+\infty$ admits a subsequence (still denoted by λ_n) such that, for $w_n=w_{\lambda_n}$, we have:

$$w_n\mapsto w_0\ \text{strongly in}\ H^1(\Omega),$$

and w_0 satisfies:

(3)
$$\begin{cases}-\Delta w_0=4\pi\left(\dfrac{e^{u_0+w_0}}{\int_\Omega e^{u_0+w_0}}-\dfrac{1}{|\Omega|}\right)\ \text{in}\ \Omega\\ \int_\Omega w_0=0,\quad w_0\in H^1(\Omega)\end{cases}.$$

Problem (3) is interesting in itself, and we will comment on it at the end of this section.

Proof: A direct calculation shows that,

$$\psi_\lambda(w):=\max_{c\leqslant c_+(w)}I_\lambda(w+c)=\frac{1}{2}\|\nabla w\|_2^2+\frac{\lambda}{2}\int_\Omega(e^{u_0+w+c_-(w)}-1)^2+4\pi c_-(w);\quad w\in\mathcal{A}.$$

As in Ref. 17, by means of Moser–Trudinger inequality (2.2) we show that ψ_λ is bounded from below in $\mathscr{A}$.

In fact, as $N=1$, then from the definition of $c_-(w)$, $w\in\mathscr{A}$ follows that,

$$e^{c_-(w)}=\frac{16\pi}{2\lambda}\frac{1}{\int_\Omega e^{u_0+w}+\sqrt{(\int_\Omega e^{u_0+w})^2-(16\pi/\lambda)\int_\Omega e^{2(u_0+w)}}}$$

from which we immediately derive the estimates:

$$\frac{4\pi}{\lambda}\frac{1}{\int_\Omega e^{u_0+w}}\leqslant e^{c_-(w)}\leqslant\frac{8\pi}{\lambda}\frac{1}{\int_\Omega e^{u_0+w}}, \tag{3.11}$$

and consequently,

$$\frac{\lambda}{2}\int_\Omega (e^{u_0+w+c_-(w)}-1)^2\geqslant\frac{\lambda}{2}|\Omega|-6\pi. \tag{3.12}$$

Furthermore, the first of the inequalities in (3.11) yields:

$$c_-(w)\geqslant\ln 4\pi-\ln\lambda-\ln\left(\int_\Omega e^{u_0+w}\right),$$

and, by Moser–Trudinger's inequality, for every $\epsilon>0$ and for every $q>1$, we have

$$\ln\left(\int_\Omega e^{u_0+w}\right)\leqslant\frac{1}{p}\ln\left(\int_\Omega e^{pu_0}\right)+q\left(\frac{1}{16\pi}+\epsilon\right)\|\nabla w\|_2^2+C(\epsilon) \tag{3.13}$$

with $1/p+1/q=1$ and $C(\epsilon)$ a suitable positive constant depending on $\epsilon>0$.

Consequently,

$$\psi_\lambda(w)\geqslant\left(\frac{1}{2}-\frac{q}{4}-4\pi q\epsilon\right)\|\nabla w\|_2^2+\frac{\lambda}{2}|\Omega|-4\pi\ln\lambda-C_\epsilon$$

with a suitable $C_\epsilon>0$ (independent of λ).

Therefore, for $q>1$ sufficiently close to 1 and $\epsilon>0$ sufficiently small we may conclude that the lower semicontinuous functional ψ_λ is bounded from below and coercive on $\mathscr{A}$.

Hence ψ_λ achieves its infimum on $\mathscr{A}$ and our next goal is to show that, as $\lambda\to+\infty$, such infimum lies on the interior of $\mathscr{A}$.

To this purpose, let $\lambda_0>0$ sufficiently large so that

$$\left(\int_\Omega e^{u_0}\right)^2-\frac{16\pi}{\lambda}\int_\Omega e^{2u_0}>0,\quad\forall\lambda\geqslant\lambda_0. \tag{3.14}$$

In other words, $w=0$ belongs to the interior of $\mathscr{A}$, $\forall\lambda\geqslant\lambda_0$.

Set

$$r_\lambda=\begin{cases}\inf\left\{\|\nabla w\|_2^2,\quad w\in\mathscr{A}:\left(\int_\Omega e^{u_0+w}\right)^2=\frac{16\pi}{\lambda}\int_\Omega e^{2(u_0+w)}\right\}\\ +\infty\quad\text{if }\partial\mathscr{A}\text{ is empty}\end{cases}. \tag{3.15}$$

Claim:

$$r_\lambda \to +\infty \quad \text{as} \quad \lambda \to +\infty. \tag{3.16}$$

To establish (3.16) we argue by contradiction and suppose that there exists $\lambda_n \to +\infty$, and $c > 0 : 0 \leq r_{\lambda_n} \leq c, \forall n \in N$.

For $\lambda = \lambda_n$, we have $\partial\mathcal{A}$ non-empty and the infimum in (3.15) is achieved at some $w_n \in H^1(\Omega) : \int_\Omega w_n = 0$ and $(\int_\Omega e^{u_0+w_n})^2 = (16\pi/\lambda_n)\int_\Omega e^{2(u_0+w_n)}$.

Since $\|\nabla w_n\|_2^2 \leq c \forall n \in N$, after passing to a subsequence if necessary, we can assume that $w_n \to w_0 \in H^1(\Omega)$ weakly in $H^1(\Omega)$ and $\int_\Omega e^{\alpha(u_0+w_n)} \mapsto \int_\Omega e^{\alpha(u_0+w_0)}$ with $\alpha = 1,2$. But this yields to a contradiction, since

$$0 = \left(\int_\Omega e^{u_0+w_n}\right)^2 - \frac{16\pi}{\lambda_n}\int_\Omega e^{2(u_0+w_n)} \mapsto \int_\Omega e^{u_0+w_0}$$

as $n \to +\infty$, and (3.16) is proved.

Suppose that $\partial\mathcal{A}$ is not empty and let $w \in \partial\mathcal{A}$, that is

$$\left(\int_\Omega e^{u_0+w}\right)^2 = \frac{16\pi}{\lambda}\int_\Omega e^{2(u_0+w)}. \tag{3.17}$$

In view of (3.17) we have

$$\begin{cases} c_-(w) = \ln 8\pi - \ln\lambda - \ln\int_\Omega e^{u_0+w}, \\ \int_\Omega e^{2(u_0+w+c_-(w))} = \frac{1}{2}\int_\Omega e^{u_0+w+c_-(w)} = \frac{4\pi}{\lambda}. \end{cases} \tag{3.18}$$

Thus

$$\begin{aligned} \psi_\lambda(w) &= \frac{1}{2}\|\nabla w\|_2^2 + \frac{\lambda}{2}\int_\Omega e^{2(u_0+w+c_-(w))} - \lambda\int_\Omega e^{u_0+w+c_-(w)} + \frac{\lambda}{2}|\Omega| + 4\pi c_-(w) \\ &= \frac{1}{2}\|\nabla w\|_2^2 - \frac{3\lambda}{4}e^{c_-(w)}\int_\Omega e^{u_0+w} + \frac{\lambda}{2}|\Omega| - 4\pi\ln\lambda - 4\pi\ln 8\pi - 4\pi\ln\left(\int_\Omega e^{u_0+w}\right) \\ &= \frac{1}{2}\|\nabla w\|_2^2 + \frac{\lambda}{2}|\Omega| - 4\pi\ln\lambda - 6\pi - 4\pi\ln 8\pi - 4\pi\ln\left(\int_\Omega e^{u_0+w}\right). \end{aligned}$$

By means of (3.13) with $q = 4/3$ and $\epsilon > 0$ sufficiently small, we may conclude that,

$$\psi_\lambda(w) \geq \frac{1}{8}\|\nabla w\|_2^2 + \frac{\lambda}{2}|\Omega| - 4\pi\ln\lambda - c, \quad \forall w \in \partial\mathcal{A}$$

with $c > 0$ a suitable constant independent of λ.

In other words, this proves that, if $\partial\mathcal{A}$ is non-empty, then:

$$\inf_{\partial\mathcal{A}}\psi_\lambda \geq \frac{1}{8}r_\lambda + \frac{\lambda}{2}|\Omega| - 4\pi\ln\lambda - c \tag{3.19}$$

for a suitable $c > 0$ (independent of λ).

On the other hand, if $\lambda \geq \lambda_0$, then by (3.14) we have that $w = 0$ belongs to the interior of $\mathcal{A}$. Setting $c_0 = c_-(w=0)$, and recalling,

$$\frac{4\pi}{\lambda\int_\Omega e^{u_0}} \leq e^{c_0} = \frac{\int_\Omega e^{u_0} - \sqrt{(\int_\Omega e^{u_0})^2 - (16\pi/\lambda)\int_\Omega e^{2u_0}}}{2\int_\Omega e^{2u_0}}$$

$$\leq \frac{8\pi}{\lambda\int_\Omega e^{u_0}}$$

we derive

$$\psi_\lambda(0) = \frac{\lambda}{2}\int_\Omega (e^{u_0+c_0}-1)^2 + 4\pi c_0 = \frac{\lambda}{2}\int_\Omega e^{2(u_0+c_0)} - \lambda\int_\Omega e^{u_0+c_0} + \frac{\lambda}{2}|\Omega| + 4\pi c_0$$

$$\leq -\frac{\lambda}{2}e^{c_0}\int_\Omega e^{u_0} + \frac{\lambda}{2}|\Omega| + 4\pi \ln\left(\frac{8\pi}{\int_\Omega e^{u_0}}\right) - 4\pi \ln\lambda$$

$$\leq \frac{\lambda}{2}|\Omega| - 4\pi \ln\lambda - 4\pi \ln\left(\frac{8\pi}{\int_\Omega e^{u_0}}\right) - 2\pi.$$

Thus, as $\lambda\to+\infty$ then $r_\lambda\to+\infty$ and by (3.19) we conclude

$$\inf_{\mathscr{A}}\psi_\lambda \leq \frac{\lambda}{2}|\Omega| - 4\pi \ln\lambda - 4\pi + 4\pi \ln\left(\frac{8\pi}{\int_\Omega e^{u_0}}\right) < \inf_{\partial\mathscr{A}}\psi_\lambda. \tag{3.20}$$

Therefore, for $\lambda>0$ sufficiently large, there exists $w_\lambda\in\mathscr{A}$ such that,

$$\left(\int_\Omega e^{u_0+w_\lambda}\right)^2 - \frac{16\pi}{\lambda}\int_\Omega e^{2(u_0+w_\lambda)} > 0 \tag{3.21}$$

and

$$\psi_\lambda(w_\lambda) = \inf_{\mathscr{A}}\psi_\lambda.$$

Set $\tilde{v}_\lambda = w_\lambda + c_-(w_\lambda)$, we show that it defines a critical point for I_λ and satisfies the required property (1) and (2).

To this purpose observe that from (3.21) follows that necessarily $c_-(w_\lambda) < c_+(w_\lambda)$, and therefore the property that:

$$I_\lambda(\tilde{v}_\lambda) = \max_{c\leq c_+(w_\lambda)} I_\lambda(w_\lambda + c)$$

suffices to guarantee,

$$\langle I'_\lambda(\tilde{v}_\lambda), \varphi = 1\rangle = \frac{d}{dc} I_\lambda(w_\lambda + c)|_{c=c_-(w_\lambda)} = 0. \tag{3.22}$$

On the other hand, if $\varphi\in H^1(\Omega)$ and $\int_\Omega\varphi=0$, then in view of (3.21) we can take $t>0$ sufficiently small and have that $w_\lambda + t\varphi\in\mathscr{A}$. Set $w_t = w_\lambda + t\varphi$ and let,

$$c_-(t) = \ln\left(\frac{\int_\Omega e^{u_0+w_t} - \sqrt{(\int_\Omega e^{u_0+w_t})^2 - (16\pi/\lambda)\int_\Omega e^{2(u_0+w_t)}}}{2\int_\Omega e^{2(u_0+w_t)}}\right).$$

Clearly, $c_-(t)\to c_-(w_\lambda)$ as $t\to 0^+$; and,

$$0 \leq \frac{1}{t}\left[I_\lambda(w_t + c_-(t)) - I_\lambda(w_\lambda + c_-(\lambda))\right] \leq \frac{1}{t}\left[I_\lambda(w_t + c_-(t)) - I_\lambda(w_\lambda + c_-(t))\right]$$

$$= \langle I'_\lambda(w_\lambda + c_-(t)), \varphi\rangle + o(1) \to \langle I'_\lambda(\tilde{v}_\lambda), \varphi\rangle \quad \text{as } t \to 0^+.$$

Replacing φ by $-\varphi$, we conclude $\langle I'_\lambda(\tilde{v}_\lambda), \varphi\rangle = 0$ $\forall \varphi \in H^1(\Omega)$, $\int_\Omega \varphi = 0$.

This, together with (3.22), readily implies that $\tilde{v}_\lambda$ is a critical point for I_λ, hence a solution for $(2.18)_\lambda$.

Set $c_\lambda = c_-(w_\lambda)$, from (3.11) it follows,

$$e^{c_\lambda} \leq \frac{8\pi}{\lambda} \frac{1}{\int_\Omega e^{u_0 + w_\lambda}} \leq \frac{8\pi}{\lambda |\Omega|}, \tag{3.23}$$

where we have used Jensen's inequality to obtain that $\int_\Omega e^{u_0 + w_\lambda} \geq |\Omega|$.

From (3.23) it follows immediately that $c_\lambda \to -\infty$ as $\lambda \to +\infty$, and (1) is established.

Finally, to establish (2) recall that:

$$4\pi \leq \lambda e^{c_\lambda} \int_\Omega e^{u_0 + w_\lambda} \leq 8\pi$$

(see (3.11)). Thus,

$$I_\lambda(\tilde{v}_\lambda) = \frac{1}{2}\|\nabla w_\lambda\|_2^2 + \frac{\lambda}{2}\int_\Omega e^{2(u_0 + \tilde{v}_\lambda)} - \lambda e^{c_\lambda} \int_\Omega e^{u_0 + w_\lambda} + \frac{\lambda}{2}|\Omega| + 4\pi c_\lambda$$

$$\geq \frac{1}{2}\|\nabla w_\lambda\|_2^2 - 6\pi + \frac{\lambda}{2}|\Omega| - 4\pi \ln \lambda + 4\pi \ln 4\pi - 4\pi \ln\left(\int_\Omega e^{u_0 + w_\lambda}\right).$$

So by (3.13) with $q = 4/3$ and $\epsilon > 0$ sufficiently small we may conclude:

$$\frac{1}{8}\|\nabla w_\lambda\|_2^2 + \frac{\lambda}{2}|\Omega| - 4\pi \ln \lambda - C_1 \leq I_\lambda(\tilde{v}_\lambda) \leq I_\lambda(c_-(0)) = \psi_\lambda(0) \leq + \frac{\lambda}{2}|\Omega| - 4\pi \ln \lambda + C_2$$

with C_1 and C_2 suitable positive constant independent of λ.

Consequently,

$$\|\nabla \tilde{v}_\lambda\|_2^2 = \|\nabla w_\lambda\|_2^2 \leq 8(C_1 + C_2) = C, \tag{3.24}$$

with $C > 0$ independent of λ and (ii) is proved.

Next, let $\lambda_n \to +\infty$, and set $w_n = w_{\lambda_n}$. In view of (3.24), we find a subsequence (which we still denote by w_n) and $w_0 \in H^1(\Omega)$, $\int_\Omega w_0 = 0$ such that, $w_n \to w_0$ weakly in $H^1(\Omega)$ and,

$$\int_\Omega e^{\alpha(u_0 + w_n)} \to \int_\Omega e^{\alpha(u_0 + w_0)} \quad \text{as } n \to +\infty, \quad \alpha = 1, 2.$$

Consequently, letting $c_n = c_-(w_n)$ we have

$$\lambda_n e^{c_n} = \frac{8\pi}{\int_\Omega e^{u_0 + w_n} + \sqrt{(\int_\Omega e^{u_0 + w_n})^2 - (16\pi/\lambda_n)\int_\Omega e^{2(u_0 + w_n)}}} \mapsto \frac{4\pi}{\int_\Omega e^{u_0 + w_0}}$$

as $n \to +\infty$; and

$$-\int_\Omega \nabla w_0\cdot\nabla\varphi=\lim_{n\to+\infty}\int_\Omega \nabla w_n\cdot\nabla\varphi=\lim_{n\to+\infty}\left[\lambda_n e^{c_n}\int_\Omega (e^{c_n}e^{u_0+w_n}-1)e^{u_0+w_n}\varphi+\frac{4\pi}{|\Omega|}\int_\Omega\varphi\right]$$

$$=-\frac{4\pi}{\int_\Omega e^{u_0+w_0}}\int_\Omega e^{u_0+w_0}\varphi+\frac{4\pi}{|\Omega|}\int_\Omega\varphi$$

$\forall\varphi\in H^1(\Omega)$.

So, w_0 is a solution for (3).

Finally, to show that $w_n\to w_0$ strongly in $H^1(\Omega)$ notice that,

$$\int_\Omega|\nabla(w_n-w_0)|^2=\lambda_n e^{c_n}\int_\Omega(1-e^{c_n}e^{u_0+w_n})e^{u_0+w_n}(w_n-w_0)-\frac{4\pi}{\int_\Omega e^{u_0+w_0}}\int_\Omega e^{u_0+w_0}(w_n-w_0)$$

$$=\lambda_n e^{c_n}\int_\Omega(e^{u_0+w_n}-e^{u_0+w_0})(w_n-w_0)-\lambda_n e^{2c_n}\left(\int_\Omega e^{2(u_0+w_n)}(w_n-w_0)\right)$$

$$+\left(\lambda_n e^{c_n}-\frac{4\pi}{\int_\Omega e^{u_0+w_0}}\right)\int_\Omega e^{u_0+w_0}(w_n-w_0)\mapsto 0,\quad \text{as } n\to+\infty.$$

Remark 3.2: In particular, Proposition 3.2 asserts that the limit point set Γ of $\{w_\lambda\}\subset C^\infty(\Omega)$ in the weak topology of $H^1(\Omega)$ defines the limit point set of $\{w_\lambda\}$ also in the strong topology of $H^1(\Omega)$. Since Γ is given by solution to (3), we have that $\Gamma\subset C^\infty(\Omega)$ and in fact, it defines the limit point set for $\{w_\lambda\}$ in any other relevant topology.

Corollary 3.1: Let $\tilde{v_\lambda}=w_\lambda+c_\lambda$ $\int_\Omega w_\lambda=0$ be the solution for $(2.18)_\lambda$ as given by Proposition 3.2. For every integer $k\geq 1$ there exists a constant $C=C(k)>0$ independent of λ such that,

$$\|w_\lambda\|_{C^k}\leq C. \tag{3.25}$$

Furthermore $\Gamma\subset C^\infty(\Omega)$ the limit point set of $\{w_\lambda\}$ in the weak topology of $H^1(\Omega)$ coincides with the limit point set of $\{w_\lambda\}$ in $C^k(\Omega)$ topology.

Proof: Recall that $w_\lambda\in H^1(\Omega)$ satisfies:

$$\begin{cases}-\Delta w_\lambda=\lambda e^{c_\lambda}e^{u_0+w_\lambda}(1-e^{u_0+w_\lambda+c_\lambda})-\dfrac{4\pi}{|\Omega|}:=f_\lambda & \text{on } Q\\ \int_\Omega w_\lambda=0\end{cases}$$

and

$$\lambda e^{c_\lambda}\leq\frac{8\pi}{|\Omega|}$$

(see (3.23)).

Therefore, the Moser–Trudinger inequality (2.2) together with (2) of Proposition 3.2 implies that, for every $p>1$ there exists a constant $C=C_p>0$ such that

$$\|e^{u_0+w_\lambda}\|_p\leq C\quad\forall\lambda.$$

Consequently, $\|f_\lambda\|_p\leq C_1$, $\forall\lambda$, and by elliptic L^p estimates and the Sobolev embedding, we may conclude that,

$$\|w_\lambda\|_{C^{1,\alpha}}\leq C_2$$

with $\alpha \in (0,1)$ and $C_2>0$ a suitable constant independent of λ.

Since $e^{u_0} \in C^\infty(\Gamma)$ we can iterate this procedure and by means of Schauder's estimates conclude that (3.25) holds with a suitable constant independent of λ.

Finally, if $\lambda_n \to +\infty$ and $w_n = w_{\lambda n} \rightharpoonup w_0 \in \Gamma$ weakly in $H^1(\Omega)$, then as in the proof of Proposition 3.2, we see that, $-\Delta(w_n - w_0) = h_n$ with $\|h_n\|_p \to 0$ as $n \to +\infty$ and $p>1$. Consequently, $\|w_n - w_0\|_{C^{1,\alpha}} \to 0$ as $n \to +\infty$ and $\alpha \in (0,1)$. Thus, a bootstrap argument yields $\|w_n - w_0\|_{C^{k,\alpha}} \to 0$ as $n \to +\infty$ and $k \in N$.

Final remarks

In particular. Proposition 3.2 yields the existence of a solution for problem (3). More generally, for the problem:

$$\begin{cases} -\Delta w = \eta \left(\dfrac{e^{u_0+w}}{\int_\Omega e^{u_0+w}} - \dfrac{1}{|\Omega|} \right) & \text{in } \Omega \\ \int_\Omega w = 0 \end{cases} \tag{3}_\eta$$

with $\eta \in (0,8\pi)$, this can be derived directly by minimizing the functional:

$$F(w) = \frac{1}{2} \|\nabla w\|_2^2 - \eta \ln \left(\int_\Omega e^{u_0+w} \right)$$

over the space

$$E = \left\{ w \in H^1(\Omega) : \int_\Omega w = 0 \right\}.$$

On the other hand, for $\eta \geqslant 8\pi$ it is not clear whether or not problem $(3)_\eta$ is solvable. Notice for instance that, the analogous problem, subject to Dirichlet boundary condition,

$$\begin{cases} -\Delta w = \eta \dfrac{e^w}{\int_\Omega e^w} & \text{on } \Omega \\ w = 0 & \text{on } \partial\Omega \end{cases} \tag{3}^*_\eta$$

is known to admit no solutions when Ω is a ball and $\eta \geqslant 8\pi$, see Ref. 28.

This suggest that our restriction to the case $N=1$ might be more serious than a mere technical limitation of our method, and the case $N>1$ might require a different approach all together.

Furthermore we believe that when $\eta \in (0,8\pi)$ the solution for $(3)_\eta$ is unique and $w_\lambda \to w_0$ as $\lambda \to +\infty$ (in any of the relevant norms) with w_0 the (unique!) solution to $(3)_{\eta=4\pi}$. So far however, uniqueness of $(3)_\eta$, $\eta \in (0,8\pi)$ remains an open problem supported by the fact that it has been established by Suzuki[28] for the analogous problem $(3)^*_\eta$ when $\eta \in (0,8\pi)$ and $\Omega \subset R^2$ is simply connected.

In concluding let us mention that problem $(3)^*_\eta$, has attracted much attention in view of its connection with the study of the statistical mechanics of point vortices in the mean field limit. In this contest, $(3)^*_\eta$ is commonly referred to, as the mean field equation and it has been discussed, for instance, in Refs. 20–22.

The proof of Theorems 2.1 and 2.2

At this point, Theorems 2.1 and 2.2 are easy consequence of Theorem 2.3, Propositions 3.1 and 3.2. In fact, by Theorem 2.3 the first part of Theorem 2.1 follows easily by taking $k_c = 2/\sqrt{\lambda_c} < \frac{1}{2}\sqrt{|\Omega|/\pi N}$.

Furthermore, for $0<k\leqslant k_c$, let $v_k = v_{\lambda=4/k^2}$ be the maximal solution for $(2.1)_{\lambda=4/k^2}$, then (A_k,ϕ_k) as defined by (2.11), (2.12), and (2.13) with $u=u_0+v_k$ defines a solution for $(2.7)_k$ satisfying (2.8). Since

$$|\phi_k|^2=e^{u_0+v_k}$$

we have that, ϕ_k vanishes exactly at $p_1,\ldots,p_m$ with multiplicity $n_1,\ldots,n_m$ respectively, $|\phi_k|$ satisfies the "maximality" property (ii), and the monotonicity property (iii)–*a.* of Theorem 2.1. In addition, since $v_k<-u_0$ in Ω, the estimate (iii)-*b*, also follows. Finally, by Proposition 3.1 we get that $|\phi_k|\to 1$ as $k\to 0^+$ pointwise a.e. in Ω and, by the monotone (or dominated) convergence theorem, in $L^p(\Omega)\forall p\geqslant 1$. On the other hand, for $1<q<2$, $\|\nabla|\phi_k|\|_q\leqslant\frac{1}{2}\|\nabla(u_0+v_k)\|_q\to 0$ as $k\to 0^+$, and we may conclude: $\||\phi_k|-1\|_{W^{1,q}}\to 0$ as $k\to 0$ and $1<q<2$. Finally, in virtue of (ii) of Proposition 3.1 and the second equation in $(2.7)_k$, we also derive the property (iii)—d. of Theorem 2.1.

Similarly the first part of Theorem 2.2 follows by taking $(\tilde{A}_k,\tilde{\phi}_k)$ as defined in (2.11), (2.12) and (2.13) with $u = u_0 + v_{1,\lambda=4/k^2}$ and $v_{1,\lambda}$ as given by Theorem 2.3. While for $N=1$, we may take $u = u_0 + \tilde{v}_{\lambda=4/k^2}$ for $k>0$ small and $\tilde{v}_\lambda$ as given by Proposition 3.2. In this situation,

$$|\tilde{\phi}_k|^2=e^{u_0+w_k+c_k}=Ue^{w_k+c_k}$$

with $U=e^{u_0}$ smooth, $w_k = w_{\lambda=4/k^2}$ and $c_k = c_{\lambda=4/k^2}\to -\infty$ as $k\to 0^+$. Thus, by Corollary 3.1 we conclude that, for every integer $q\geqslant 0$ there exists a positive constant $C=C(q)$ independent of k such that,

$$\|\phi_k\|_{C^q}\leqslant Ce^{c_k}\to 0 \quad \text{as } k\to 0^+.$$

We conclude by mentioning that other interesting self-dual Chern–Simons theories are discussed in Ref. 29.

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APPENDIX

In this appendix we would like to show that, the following property:

$$\int_\Omega \nabla v_*\cdot\nabla\varphi+\lambda e^{u_0+v_*}(e^{u_0+v_*}-1)\varphi+\frac{4\pi N}{|\Omega|}\varphi\leqslant 0$$

$$\forall\varphi\in H^1(\Omega),\quad \varphi\geqslant 0 \text{ a.e. in } \Omega \tag{A1}$$

implies that, if $v_0\in\Lambda=\{v\in H^1(\Omega): v\geqslant v_* \text{ a.e. in } \Omega\}$ satisfies:

$$I_\lambda(v_0)=\inf_\Lambda I_\lambda$$

then v_0 defines a critical point for I_λ in $H^1(\Omega)$.

To this purpose, let $\varphi\in H^1(\Omega)$, $t>0$ and define:

$$v_t=\max\{v_0+t\varphi,v_*\}\in\Lambda.$$

If v_+ and v_- denotes the positive and negative part of v respectively, then we may write,

$$v_t=v_0+t\varphi+w_t,\ \text{with } w_t=(v_0+t\varphi-v_*)_-\geqslant 0 \text{ a.e. in } \Omega.$$

We have

$$0 \leqslant \frac{1}{t}\,(I_\lambda(v_t)-I_\lambda(v_0)) = \frac{1}{2t}\,(\|\nabla(v_0+t\varphi+w_t)\|_2^2-\|\nabla v_0\|_2^2)+\frac{\lambda}{2t}\int_\Omega\{(e^{u_0+v_0+t\varphi+w_t}-1)^2$$

$$-(e^{u_0+v_0}-1)^2\}+\frac{4\pi N}{|\Omega|}\left(\int_\Omega\varphi+\frac{1}{t}\int_\Omega w_t\right)$$

$$=\frac{1}{2t}\,\|\nabla(t\varphi+w_t)\|_2^2+\int_\Omega\frac{\nabla v_0\cdot\nabla(t\varphi+w_t)}{t}$$

$$+\frac{\lambda}{t}\int_\Omega e^{u_0+v_0}(e^{u_0+v_0}-1)t\varphi$$

$$+\frac{\lambda}{2t}\int_\Omega\{(e^{u_0+v_t}-1)^2-(e^{u_0+v_0}-1)^2-2e^{u_0+v_0}(e^{u_0+v_0}-1)t\varphi\}$$

$$+\frac{4\pi N}{|\Omega|}\left(\int_\Omega+\frac{1}{t}\int_\Omega w_t\right).$$

Consequently,

$$\int_\Omega\nabla v_0\cdot\nabla\varphi+\lambda\int_\Omega e^{u_0+v_0}(e^{u_0+v_0}-1)\varphi+\frac{4\pi N}{|\Omega|}\int_\Omega\varphi$$

$$\geqslant-\frac{t}{2}\,\|\nabla\varphi\|_2^2-\int_\Omega\nabla\varphi\cdot\nabla w_t-\frac{1}{2t}\,\|\nabla w_t\|_2^2-\frac{1}{t}\int_\Omega\nabla v_0\cdot\nabla w_t-\frac{\lambda}{2t}\int_\Omega\{(e^{u_0+v_t}-1)^2$$

$$-(e^{u_0+v_0}-1)^2-2e^{u_0+v_0}(e^{u_0+v_0}-1)t\varphi\}-\frac{4\pi N}{|\Omega|}\frac{1}{t}\int_\Omega w_t$$

$$=O(t)+\frac{1}{t}\int_\Omega\nabla(-t\varphi-v_0+v_*)\cdot\nabla w_t-\frac{1}{t}\int_\Omega\nabla v_*\cdot\nabla w_t$$

$$+\frac{\lambda}{t}\int_\Omega e^{u_0+v_*}(e^{u_0+v_*}-1)w_t-\frac{4\pi N}{|\Omega|}\frac{1}{t}\int_\Omega w_t-\frac{1}{2t}\,\|\nabla w_t\|_2^2-\frac{\lambda}{2t}\int_\Omega\{(e^{u_0+v_0+t\varphi+w_t}-1)^2$$

$$-(e^{u_0+v_0}-1)^2-2e^{u_0+v_0}(e^{u_0+v_0}-1)(t\varphi+w_t)\}\frac{\lambda}{t}$$

$$\times\int_\Omega[e^{u_0+v_*}(e^{u_0+v_*}-1)-e^{u_0+v_0}(e^{u_0+v_0}-1)]w_t$$

$$\geqslant O(t)-\frac{\lambda}{2t}\int_0^1\left(\int_\Omega e^{u_0+v_0+s(t\varphi+w_t)}(2e^{u_0+v_0+s(t\varphi+w_t)}-1)(t\varphi+w_t)^2\right)ds$$

$$+\frac{\lambda}{t}\int_\Omega(e^{2(u_0+v_*)}-e^{2(u_0+v_0)})w_t$$

where the last inequality follows by (A1), the fact that $v_0 \geqslant v_*$ a.e. in Ω and

$$\int_\Omega \nabla(-t\varphi - v_0 + v_*)\nabla w_t = \|\nabla w_t\|_2^2.$$

Since,

$$|t\varphi + w_t| \leq t|\varphi| \quad t \in [0,1]$$

we estimate

$$\int_0^1 \int_\Omega e^{2(u_0+v_0+s(t\varphi+w_t))}(t\varphi+w_t)^2 \leq t^2 \int_\Omega e^{2(u_0+v_0+t|\varphi|)}\varphi^2 = O(t^2). \tag{A2}$$

Set,

$$\Omega_t = \{x \in \Omega : v_0(x) + t\varphi(x) - v_*(x) < 0\} \quad \text{and} \quad \Omega_0 = \{x \in \Omega : v_0(x) = v_*(x)\},$$

hence $|\Omega_t \backslash \Omega_0| \mapsto 0$ as $t \to 0^+$. Using (A2) we conclude

$$\int_\Omega \nabla v_0 \cdot \nabla\varphi + \lambda \int_\Omega e^{u_0+v_0}(e^{u_0+v_0}-1)\varphi + \frac{4\pi N}{|\Omega|}\int_\Omega \varphi$$

$$\geq O(t) + \frac{\lambda}{t}\int_{\Omega_t \backslash \Omega_0} (e^{2(u_0+v_*)} - e^{2(u_0+v_0)})(v_* - v_0 - t\varphi)$$

$$\geq -\lambda \int_{\Omega_t \backslash \Omega_0} (e^{2(u_0+v_*)} - e^{2(u_0+v_0)})\varphi + O(t) \to 0 \quad \text{as } t \to 0^+.$$

In other words, we have obtained $\langle I_\lambda'(v_0), \varphi\rangle \geq 0 \forall \varphi \in H^1(\Omega)$. Replacing φ with $-\varphi$ we obtain the reverse inequality and the desired conclusion.

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Deriving the standard model from the simplest two-point K cycle

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Basing on a differential algebra over the simplest two-point K cycle and graded Lie algebras of homomorphisms of finite projective modules, we derive the classical action of the standard model. This construction uses both the general framework of noncommutative geometry developed by Connes and ideas of the Mainz–Marseille approach to model building. We get a prediction of the Weinberg angle and constraints between the fermion masses and the masses of the W and Higgs bosons on tree level, which differ from the relations obtained by Kastler and Schücker for the quaternionic K cycle. © *1996 American Institute of Physics.*
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I. INTRODUCTION

This paper is the continuation of two earlier papers (Refs. 1, 2) by Matthes, Rudolph, and Wulkenhaar. In the first of them we presented an analysis of the structure of the differential algebra $\Lambda^*_{\mathcal{A}}$ canonically associated to the K cycle $(\mathcal{A},h,D)$ over the simplest two-point algebra $\mathcal{A}=C^\infty(X)\otimes(\mathbb{C}\oplus\mathbb{C})$. In the second one we constructed for a given finite projective right $\mathcal{A}$ module with Hermitian structure $\mathcal{E}$ the graded Lie algebra $\mathcal{H}=\mathrm{Hom}_{\mathcal{A}}(\mathcal{E},\mathcal{E}\otimes_{\mathcal{A}}\Lambda^*_{\mathcal{A}})$ with natural derivation. We showed that a certain graded Lie subalgebra $\mathcal{H}_0$ of $\mathcal{H}$ provides a rigorous mathematical link between Connes' theory and the Mainz–Marseille model building scheme.

The K cycle mentioned above together with a finite projective module $\mathcal{E}=e\mathcal{A}^2$ was used by Connes in Refs. 3 and 4 and by Connes and Lott in Ref. 5 to derive the Salam–Weinberg model in a unified form. Within this scheme the above K cycle cannot be used to obtain the full standard model. That is why Connes and Lott proposed a K cycle over the algebra $C^\infty_{\mathbb{R}}(X)\otimes(\mathbb{C}\oplus\mathbb{H})$; see Refs. 5, 3 and 6. A detailed exposition of these ideas was presented by Kastler in Refs. 7 and 8; see Ref. 9 for an earlier version, and by Kastler and Schücker in Ref. 10. One obtains a prediction of the Weinberg angle and certain tree-level constraints between the masses of the fermions and the masses of the W,Z, and Higgs bosons (Refs. 10, 11), which we review at the end of this Introduction.

Another way of obtaining the standard model by noncommutative geometry is the Mainz–Marseille model (Refs. 12–14), which uses the graded Lie algebra $\Lambda^*(X)\otimes spl(2,1)$ of matrix-valued differential forms; also see Ref. 15. We have shown in Ref. 2 that the assumptions of this approach are natural within Connes' framework. For the present paper the construction of the fermionic sector of the standard model given in Ref. 13 is of particular interest. This construction makes use of the theory of representations of the graded Lie algebra $spl(2,1)$ in a finite-dimensional vector space.[15]

Our strategy is the following: In Sec. II we give a review of some results obtained in Refs. 1 and 2. In Sec. III we construct an isomorphism $\mathbf{i}$ of graded Lie algebras from $\mathcal{H}_0$, which we constructed in Ref. 2 within Connes' theory onto its image, for which the fermionic sector in Ref. 13 serves as a guiding line. Next, in Sec. IV, we give an embedding of a subspace of $\mathbf{i}(\mathcal{H}_0)$ into the algebra of bounded operators on the Hilbert space of fermions. This allows us to construct the

fermionic action (Sec. V), the electroweak sector of the bosonic action of the standard model (Sec. VI), and the chromodynamics sector (Sec. VII). After a Wick rotation to Minkowski space and a reparametrization this action coincides with the classical action of the standard model, where some free parameters of the standard model are fixed; see Sec. VIII.

Thus, our construction rests—as the construction of Connes, Lott, and Kastler—upon a K cycle. However, we take a K cycle over the algebra $\mathcal{A}=C^\infty(X)\otimes(\mathbb{C}\oplus\mathbb{C})$, while the above authors start with a K cycle over the much bigger algebras $C^\infty_{\mathbb{R}}(X)\otimes(\mathbb{C}\oplus\mathbb{H})$ and $C^\infty_{\mathbb{R}}(X)\otimes(\mathbb{C}\oplus M_3\mathbb{C})$. To compensate this difference we use two finite projective $\mathcal{A}$ modules as an additional input: one module for the electroweak sector and the other one for the chromodynamics sector. In the construction of Connes, Lott, and Kastler the module is identical with the algebra of their K cycle, so that in their version the calculus of finite projective modules is not necessary. In both versions the differential of the differential algebras associated to the K cycles are composed of the classical exterior differential and a matrix differential, which in both versions contains fermionic mass parameters. In the construction of Connes, Lott, and Kastler the just mentioned differential algebra is of primary importance for the physical model. In our version the differential algebra plays only an auxiliary role, namely for building the graded Lie algebra $\mathcal{H}_0$. Moreover, the Hilbert space of our K cycle is also auxiliary: we have to add our physical Hilbert space by hand.

As it was shown in Ref. 2 one can derive from $\mathcal{H}_0$ the graded Lie algebra $\Lambda^*(X)\otimes spl(2,1)$, which is the starting point for the construction of the standard model in the Mainz–Marseille approach. The essential difference between $\mathcal{H}_0$ and $\Lambda^*(X)\otimes spl(2,1)$ is that $\mathcal{H}_0$ carries the fermionic mass parameters of the differential algebra associated to the K cycle. It is these fermionic mass parameters that relate the masses of the fermions to the masses of the W,Z, and Higgs bosons in the model of Connes, Lott, and Kastler, as well as in our model. Since the fermionic mass parameters are absent in $\Lambda^*(X)\otimes spl(2,1)$, there is no relation between fermion masses and boson masses in the Mainz–Marseille model.

Both in our model and in the Mainz–Marseille approach one needs certain representations of the graded Lie algebras $\mathcal{H}_0$, respectively, $\Lambda^*(X)\otimes spl(2,1)$, which are generalizations of classical $spl(2,1)$ representations.[15] The representations of $\Lambda^*(X)\otimes spl(2,1)$ generalize reducible indecomposable representations of $spl(2,1)$, which give the possibility to describe mixing between fermion generations.[13] For our model we take generalizations of the simplest irreducible representations of $spl(2,1)$, because the fermion generations are intrinsically contained in $\mathcal{H}_0$. With these representations there enters a big number of additional parameters due to not canonically determined free normalization constants of $sl(2,\mathbb{C})\oplus gl(1,\mathbb{C})$—subrepresentations of $spl(2,1)$. In the Mainz–Marseille construction these parameters are fitted to the fermion masses and the Kobayashi–Maskawa matrix. In our model there is a subtle interplay between these normalization parameters and the intrinsic fermionic mass parameters of the differential calculus. In the final Lagrangian there occur only such combinations of these parameters that for the simplest scalar product there is effectively only one additional free parameter in our model compared with the simplest version of the model of Connes, Lott, and Kastler.

From our formulation of the standard model we get tree-level predictions for the Weinberg angle θ_W and the ratios m_W/m_t, m_H/m_W, and g_3/g_2. Here, m_t, m_H, and m_W are the masses of the top quark, the Higgs boson, and the W boson and g_3, g_2 the coupling constants of the strong and weak interactions, respectively. We list our predictions (Model III, with the parameters $x>0$ and ϑ_1, ϑ_2, ϑ_3, ϑ_4) in Table I and compare them with corresponding tree-level predictions of the following noncommutative geometrical formulations of the standard model:

Model I: The construction based on a K cycle over the algebras $C^\infty_{\mathbb{R}}(X)\otimes(\mathbb{C}\oplus\mathbb{H})$ and $C^\infty_{\mathbb{R}}(X)\otimes(\mathbb{C}\oplus M_3\mathbb{C})$ as presented by Kastler and Schücker in Ref. 10. The parameters are $R>-1$, $\alpha,\beta>0$.

Model II: The Mainz–Marseille model as presented in Refs. 13 and 14, predictions for the adjoint representation of $spl(2,1)$, and a general scalar product. The parameters are $r_0, r_1, r_2>0$.

TABLE I. Comparison of tree-level predictions for general scalar products.

	Model I	Model II	Model III
$\left(\frac{m_i}{m_W}\right)^2$	$R+4>3$	...	$\frac{6+2x}{4-(1-x\sin^2\vartheta_1\cos^2\vartheta_2)}>\frac{3}{2}$
$\left(\frac{m_H}{m_W}\right)^2$	$11+3R-\frac{8+2R}{7+R}>7$	$\frac{2r_0r_2}{r_1^2}$	$\frac{8(x+3)(5\cos^2\vartheta_1+3x\cos^2\vartheta_4\sin^4\vartheta_1)\cos^4\vartheta_2}{3(4-(1-x\sin^2\vartheta_1)\cos^2\vartheta_2)^2}$
$\sin^2\theta_W$	$\frac{8+2R}{15+3R+\frac{2}{3}\alpha+2\beta}<\frac{2}{3}$	$\frac{1}{4}$	$\frac{1}{4}<\frac{3}{4}\frac{3+x}{5+3x}<\frac{9}{20}$
$\left(\frac{g_3}{g_2}\right)^2$	$\frac{R+4}{2\alpha}$	...	$\frac{3+x}{4}>\frac{3}{4}$

In Model I there is enough freedom to reproduce the experimental values for m_W/m_i, $\sin^2\theta_W$, and g_3/g_2. Then m_H is uniquely determined. Also in Model III it is possible to reproduce the experimental values for m_W/m_i, g_3/g_2, and $\sin^2\theta_W\approx 0.25$. However, then there is only an upper limit for m_H in our model; see Sec. VIII. In Model II there is no relation between fermion and boson masses and between g_3 and g_2. Moreover, this model does not give a prediction for m_H. However, in contrast to the other two models one obtains an experimentally well-confirmed relation between the Cabibbo angle and the quark masses; Ref. 16.

For the simplest scalar products given by $R=0$, $\alpha=2$, $\beta=\frac{3}{2}$ in Model I, $r_0=r_1=r_2$ in Model II and $x=1$ in Model III one gets

TABLE II. Comparison of tree-level predictions for simplest scalar products.

	Model I	Model II	Model III
m_i/m_W	2		1.41...1.63
m_H/m_W	3.14	1.41	0...2.43
$\sin^2\theta_W$	0.414	0.25	0.375
g_3/g_2	1		1

Now, m_H is fixed in Model II. In Model III there is still only an upper limit for m_H, and the relation between m_i and m_W does not fit the experimental value as well as the corresponding relation in Model I does.

II. REVIEW OF EARLIER RESULTS

In this section we give a review of some results, which were obtained in Refs. 1 and 2 and that we need for what follows. For technical reasons let for the moment X be a compact four-dimensional Riemannian spin manifold. We denote by $L^2(X,S)$ the Hilbert space of square integrable sections of the spinor bundle over X, by F a finite-dimensional Hilbert space, by C the Clifford bundle of the cotangent space over X, and by C^k the set of those sections of C whose values at each point $x\in X$ belong to the subspace spanned by products of less than or equal k elements of T_x^*X of the same parity. The simplest two-point K cycle $(\mathcal{A},h,D)$ consists of the algebra $\mathcal{A}=C^\infty(X)\otimes(\mathbb{C}\oplus\mathbb{C})$ acting on the Hilbert space $h=L^2(X,S)\otimes(F\oplus F)$ and a generalized Dirac operator $D=(D^{\rm cl}\otimes{\rm id}_{F\oplus F})\oplus(\gamma^5\otimes\mathcal{M})$. Here, $D^{\rm cl}$ is the classical Dirac operator and γ^5 the grading operator on $L^2(X,S)$. Moreover, $\mathcal{M}=\left(\begin{smallmatrix}0 & M\\ M^* & 0\end{smallmatrix}\right)$, where M is an endomorphism of F.

Now we are going to specify the parameters. We take F and M as

$$F=\mathbb{C}^3\oplus\mathbb{C}^3, \quad M=\begin{pmatrix} -m_l & 0 \\ 0 & -m_q \end{pmatrix}, \tag{1}$$

where m_l and m_q are real diagonal 3×3 matrices with non-negative entries. In principle, we could take for m_l and m_q arbitrary complex 3×3 matrices, which can be written as $u_1\delta u_2$, with u_1,u_2 unitary and δ diagonal and positive. However, the unitary matrices u_1,u_2 can be absorbed by unitary transformations of the physical fields.

One shows that the algebra $\pi(\Omega^*)$ obtained from an involutive representation π of the universal differential algebra Ω^* over $\mathcal{A}$ has the structure

$$\pi(\Omega^*)=\bigoplus_{k=0}^{\infty}\pi(\Omega^k),$$

$$\pi(\Omega^k)=\begin{bmatrix} \bigoplus_{r=0}^{m} C^{k-2r}\otimes\mathbb{C}M_1^r; & \bigoplus_{r=0}^{m} C^{k-2r-1}\gamma^5\otimes\mathbb{C}M_2^r \\ \bigoplus_{r=0}^{m} C^{k-2r-1}\gamma^5\otimes\mathbb{C}M_3^r; & \bigoplus_{r=0}^{m} C^{k-2r}\otimes\mathbb{C}M_4^r \end{bmatrix}, \tag{2}$$

where

$$M_1^r:=(MM^*)^r, \quad M_2^r:=M(M^*M)^r, \quad M_3^r:=M^*(MM^*)^r, \quad M_4^r:=(M^*M)^r. \tag{3}$$

In particular, we can identify $\mathcal{A}$ with $\pi(\Omega^0)$. We denote by $(m+1)$ the number of linear independent elements $(MM^*)^r$. In our case M and M^* commute with each other and generically we have $m=6$. We define $L^n:=C^n/C^{n-2}$, $L^*:=\oplus_{k=0}^4 L^k$, and put $L^n=\{0\}$ for $n<0$. There is a graded algebra $\Lambda^*_{\not d}$ associated with $\pi(\Omega^*)$ defined as follows:

$$\Lambda^*_{\not d}:=\bigoplus_{k=0}^{\infty}\Lambda^k_{\not d}, \quad \Lambda^k_{\not d}\equiv\sigma_k\wedge\pi(\Omega^k):=\begin{cases}\pi(\Omega^k)/\pi(\Omega^{k-2}), & \text{for } k\geq2,\\ \pi(\Omega^k), & \text{for } k=0,1,\end{cases} \tag{4}$$

with multiplication

$$\Lambda^k_{\not d}\times\Lambda^n_{\not d}\ni(\lambda^k,\tilde{\lambda}^n)\to\lambda^k\tilde{\lambda}^n:=\sigma_{k+n}(\tau^k\tilde{\tau}^n)\in\Lambda^{k+n}_{\not d}, \tag{5}$$

where $\tau^k\in\pi(\Omega^k)$, $\tilde{\tau}^n\in\pi(\Omega^n)$, such that $\sigma_k(\tau^k)=\lambda^k$, $\sigma_k(\tilde{\tau}^n)=\tilde{\lambda}^n$. One can show that elements $\lambda^k\in\Lambda^k_{\not d}$ have the form

$$\lambda^k=\begin{pmatrix} \sum_{r=0}^{m}\alpha_1^{k-2r}\otimes\mathbb{C}M_1^r; & \sum_{r=0}^{m}\alpha_2^{k-2r-1}\gamma^5\otimes\mathbb{C}M_2^r \\ \sum_{r=0}^{m}\alpha_3^{k-2r-1}\gamma^5\otimes\mathbb{C}M_3^r; & \sum_{r=0}^{m}\alpha_4^{k-2r}\otimes\mathbb{C}M_4^r \end{pmatrix}, \quad \alpha_q^n\in L^n. \tag{6}$$

Let ι_k denote the isomorphism of L^k onto $\Lambda^k(X)$, where $\Lambda^k(X)$ is the space of complex-valued k forms on X. We define the following operations:

$$[\gamma^5\otimes_{\mathscr{A}}\mathscr{M},\lambda^k]_g:=(\gamma^5\otimes_{\mathscr{A}}\mathscr{M})\cdot\lambda^k-(-1)^k\lambda^k(\gamma^5\otimes_{\mathscr{A}}\mathscr{M}),$$

$$\mathbf{d}\alpha^k:=\iota_{k+1}^{-1}\circ d\circ\iota_k(\alpha^k),\quad \mathbf{d}^*:=\gamma^5\,\mathbf{d}\gamma^5, \tag{7}$$

$$\mathbf{D}\lambda^k:=pr_{k+1}\circ((\mathbf{d}-\mathbf{d}^*)\otimes\mathrm{id}_F\otimes\mathbf{1}_{2\times 2})(\lambda^k),$$

for $\alpha^k\in L^k$, $\lambda^k\in\Lambda^k{}_{\mathscr{A}}$, where pr_{k+1} denotes the projection from $\Lambda_{\mathscr{A}}^{k+1}\oplus\Lambda_{\mathscr{A}}^{k-1}$ onto $\Lambda_{\mathscr{A}}^{k+1}$. One shows that

$$\hat{d}:=\mathbf{D}-i[\gamma^5\otimes_{\mathscr{A}}\mathscr{M},\cdot]_g \tag{8}$$

is a graded differential on $\Lambda^*{}_{\mathscr{A}}$, and one can write down explicit multiplication and differential rules for elements of $\Lambda^*{}_{\mathscr{A}}$; see Ref. 1.

In Ref. 2 we considered finite projective right $\mathscr{A}$ modules with Hermitian structure $\mathscr{E}=e\mathscr{A}^p$, where $e\in\mathrm{End}_{\mathscr{A}}(\mathscr{E})$, fulfilling $e=e^2=e^*$. Let $\mathscr{H}^k:=\mathrm{Hom}_{\mathscr{A}}(\mathscr{E},\mathscr{E}\otimes_{\mathscr{A}}\Lambda^k{}_{\mathscr{A}})$ be the set of homomorphisms of the right $\mathscr{A}$ module $\mathscr{E}$ to the right $\mathscr{A}$ module $\mathscr{E}\otimes_{\mathscr{A}}\Lambda^k{}_{\mathscr{A}}$. Elements $\varrho^k\in\mathscr{H}^k$ can be identified with $p\times p$ matrices of elements of $\Lambda^k{}_{\mathscr{A}}$, fulfilling $e\varrho^k e=\varrho^k$:

$$\varrho^k=\begin{pmatrix}\varrho^k_{11}&\cdots&\varrho^k_{1j}&\cdots&\varrho^k_{1p}\\ \vdots&\ddots&\vdots&\ddots&\vdots\\ \varrho^k_{i1}&\cdots&\varrho^k_{ij}&\cdots&\varrho^k_{ip}\\ \vdots&\ddots&\vdots&\ddots&\vdots\\ \varrho^k_{p1}&\cdots&\varrho^k_{pj}&\cdots&\varrho^k_{pp}\end{pmatrix},\quad \rho^k_{ij}\in\Lambda^k{}_{\mathscr{A}},\quad i,j=1,\ldots,p. \tag{9}$$

The space $\mathscr{H}=\oplus_{k=0}^{\infty}\mathscr{H}^k$ is an algebra with multiplication given by the tensor product of the multiplication in $\Lambda^*{}_{\mathscr{A}}$ and multiplication of $p\times p$ matrices. On $\mathscr{H}$ we have a canonical derivation $\mathscr{D}$ given by

$$\mathscr{D}\varrho=e\hat{d}(\varrho)e,\quad \varrho\in\mathscr{H}, \tag{10}$$

where $\hat{d}$ means the componentwise action on matrix elements belonging to $\Lambda^*{}_{\mathscr{A}}$. With respect to the graded commutator,

$$[\varrho^k,\tilde{\varrho}^n]_g:=\varrho^k\cdot\tilde{\varrho}^n-(-1)^{kn}\tilde{\varrho}^n\varrho^k,\quad \varrho^k\in\mathscr{H}^k,\quad \tilde{\varrho}^n\in\mathscr{H}^n, \tag{11}$$

$\mathscr{H}$ is a graded Lie algebra with graded derivation $\mathscr{D}$.

We define on $\Lambda^*{}_{\mathscr{A}}$, see (6), a linear map $T_\Lambda:\Lambda^*{}_{\mathscr{A}}\to L^*$ by

$$T_\Lambda\left(\begin{pmatrix}\sum_{t=0}^{m}\alpha_1^{k-2t}\otimes M_1^t; & \sum_{t=0}^{m}\alpha_2^{k-2t-1}\gamma^5\otimes M_2^t\\ \sum_{t=0}^{m}\alpha_3^{k-2t-l}\gamma^5\otimes M_3^t; & \sum_{t=0}^{m}\alpha_4^{k-2t}\otimes M_4^t\end{pmatrix}\right):=\sum_{t=0}^{m}(\alpha_1^{k-2t}-\alpha_4^{k-2t}), \tag{12}$$

which can be interpreted as a generalized trace. We have proved in Ref. 2 that there exists a graded Lie subalgebra $\mathscr{H}_0$ of $\mathscr{H}$ defined by

$$\mathscr{H}_0=\bigotimes_{k=0}^{\infty}\mathscr{H}_0^k,\quad \mathscr{H}_0^k=\left\{\varrho^k\in\mathscr{H}^k,\sum_{i=1}^{p}T_\Lambda(\varrho_n^k)=0\right\} \tag{13}$$

[in the notation of (9)]. Moreover, $\mathscr{D}$ is a graded derivation on $\mathscr{H}_0$.

Any connection ∇ on $\mathscr{E}$ has the form

$$\nabla = e\hat{d} + \rho, \quad \rho = -\rho^* \in \mathscr{H}^1. \tag{14}$$

The situation found in physics suggests to consider special connections, namely such that $\rho \in \mathscr{H}^1_0$. This implies that the gauge group is restricted to

$$\mathscr{U} = \{u \in \mathrm{Aut}_{\mathscr{A}}(\mathscr{E}), \quad uu^* = u^*u = e, \quad u\,\mathbf{d}u^* \in \mathscr{H}^1_0\}, \tag{15}$$

see Ref. 2, where $\mathbf{d}u^*$ means the action of the differential $\mathbf{d}$ on the L^* component of $u^* \in \mathscr{U}$. Gauge transformations of the connection ∇ are given by $u\,\nabla u^*$.

III. AN ISOMORPHISM OF GRADED LIE ALGEBRAS

Here we fix the module $\mathscr{E}$ by taking $p=2$ and for the projector $e = \left(\begin{smallmatrix} e' & 0 \\ 0 & 1_{\mathscr{A}} \end{smallmatrix}\right)$, where $1_{\mathscr{A}} = \left(\begin{smallmatrix} 1\otimes \mathrm{id}_F & 0 \\ 0 & 1\otimes \mathrm{id}_F \end{smallmatrix}\right) \in \mathscr{A}$ is the identity of $\mathscr{A}$ and $e' = \left(\begin{smallmatrix} 1\otimes \mathrm{id}_F & 0 \\ 0 & 0 \end{smallmatrix}\right) \in \mathscr{A}$. Then from (6), (9), (12), (13) and the discussion in Ref. 2 we get that elements $\varrho^k \in \mathscr{H}^k_0$ have the form

$$\varrho^k = \sum_{r=0}^{m} \begin{pmatrix} \frac{1}{2}(\alpha_0^{k-2r} + \alpha_3^{k-2r}) \otimes M_1^r & 0 & \alpha_-^{k-2r} \otimes M_1^r & \alpha_4^{k-2r-1}\gamma^5 \otimes M_2^r \\ 0 & 0 & 0 & 0 \\ \alpha_+^{k-2r} \otimes M_1^r & 0 & \frac{1}{2}(\alpha_0^{k-2r} - \alpha_3^{k-2r}) \otimes M_1^r & \alpha_5^{k-2r-1}\gamma^5 \otimes M_2^r \\ \alpha_6^{k-2r-1}\gamma^5 \otimes M_3^r & 0 & \alpha_7^{k-2r-1}\gamma^5 \otimes M_3^r & \alpha_0^{k-2r} \otimes M_4^r \end{pmatrix} \tag{16}$$

where $\alpha_f^n \in L^n$, $f = 0,+,-,3,4,5,6,7$. Due to (1) and (3) we have $M_s^r \in M_3\mathbb{C} \otimes M_2\mathbb{C}$, which means $\varrho^k \in L^* \otimes M_4\mathbb{C} \otimes M_3\mathbb{C} \otimes M_2\mathbb{C}$. In (16) we considered ϱ^k as a 4×4 matrix with $L^* \otimes M_3\mathbb{C} \otimes M_2\mathbb{C}$-valued entries. Of course, ϱ^k can also be treated as a 2×2 matrix with $L^* \otimes M_4\mathbb{C} \otimes M_3\mathbb{C}$-valued entries. With regard to this view, ϱ^k has the form

$$\varrho^k = \begin{pmatrix} \varrho_l^k & 0 \\ 0 & \varrho_q^k \end{pmatrix},$$

$$\varrho_l^k = \sum_{r=0}^{m} \begin{pmatrix} \frac{1}{2}(\alpha_0^{k-2r} + \alpha_3^{k-2r}) \otimes l_1^r & 0 & \alpha_-^{k-2r} \otimes l_1^r & \alpha_4^{k-2r-1}\gamma^5 \otimes l_2^r \\ 0 & 0 & 0 & 0 \\ \alpha_+^{k-2r} \otimes l_1^r & 0 & \frac{1}{2}(\alpha_0^{k-2r} - \alpha_3^{k-2r}) \otimes l_1^r & \alpha_5^{k-2r-1}\gamma^5 \otimes l_2^r \\ \alpha_6^{k-2r-1}\gamma^5 \otimes l_3^r & 0 & \alpha_7^{k-2r-1}\gamma^5 \otimes l_3^r & \alpha_0^{k-2r} \otimes l_4^r \end{pmatrix},$$

$$\varrho_q^k = \sum_{r=0}^{m} \begin{pmatrix} \frac{1}{2}(\alpha_0^{k-2r} + \alpha_3^{k-2r}) \otimes q_1^r & 0 & \alpha_-^{k-2r} \otimes q_1^r & \alpha_4^{k-2r-1}\gamma^5 \otimes q_2^r \\ 0 & 0 & 0 & 0 \\ \alpha_4^{k-2r} \otimes q_1^r & 0 & \frac{1}{2}(\alpha_0^{k-2r} - \alpha_3^{k-2r}) \otimes q_1^r & \alpha_5^{k-2r-1}\gamma^5 \otimes q_2^r \\ \alpha_6^{k-2r-1}\gamma^5 \otimes q_3^r & 0 & \alpha_7^{k-2r-1}\gamma^5 \otimes q_3^r & \alpha_0^{k-2r} \otimes q_4^r \end{pmatrix}, \tag{17}$$

where

$$\begin{aligned} &l_1^r = (m_l m_l^*)^r, \quad l_2^r = -m_l(m_l^* m_l)^r, \quad l_3^r = -m_l^*(m_l m_l^*)^r, \quad l_4^r = (m_l^* m_l)^r, \\ &q_1^r = (m_q m_q^*)^r, \quad q_2^r = -m_q(m_q^* m_q)^r, \quad q_3^r = -m_q^*(m_q m_q^*)^r, \quad q_4^r = (m_q^* m_q)^r. \end{aligned} \tag{18}$$

We introduce an isomorphism $\mathbf{i}$ of graded Lie algebras, which generalizes certain representations Refs. 15, 13 of the graded Lie algebra $spl(2,1)$ to the graded Lie algebra $\mathscr{H}_0$:

$$\mathbf{i}(\varrho^k)=\begin{pmatrix}\mathbf{i}_l(\varrho_l^k) & 0\\ 0 & \mathbf{i}_q(\varrho_q^k)\otimes\mathbb{1}_{3\times3}\end{pmatrix}, \tag{19}$$

$$\mathbf{i}_l(\varrho_l^k)=\sum_{r=0}^{m}\begin{pmatrix}\frac{1}{2}(\alpha_0^{k-2}+\alpha_3^{k-2r})\otimes l_1^r & \alpha_-^{k-2r}\otimes l_1^r & \alpha_4^{k-2r-1}\gamma^5\otimes\epsilon l_2^r\\ \alpha_+^{k-2r}\otimes l_1^r & \frac{1}{2}(\alpha_0^{k-2r}-\alpha_3^{k-2r})\otimes l_1^r & \alpha_5^{k-2r-1}\gamma^5\otimes\epsilon l_2^r\\ \alpha_6^{k-2r-1}\gamma^5\otimes\epsilon^{-1}l_3^r & \alpha_7^{k-2r-1}\gamma^5\otimes\epsilon^{-1}l_3^r & \alpha_0^{k-2r}\otimes l_4^r\end{pmatrix}, \tag{20}$$

$$\mathbf{i}_q(\varrho_q^k)=\sum_{r=0}^{m}\begin{pmatrix}(\frac{1}{2}\alpha_3^{k-2r}-\frac{1}{6}\alpha_0^{k-2r})\otimes q_1^r & \alpha_-^{k-2r}\otimes q_1^r & \alpha_7^{k-2r-1}\gamma^5\otimes\beta\sqrt{\frac{2}{3}}\,q_2^r & \alpha_4^{k-2r-1}\gamma^5\otimes\sqrt{\frac{1}{3}}\,q_2^r\chi\gamma\\ \alpha_+^{k-2r}\otimes q_1^r & (-\frac{1}{2}\alpha_3^{k-2r}-\frac{1}{6}\alpha_0^{k-2r})\otimes q_1^r & -\alpha_6^{k-2r-1}\gamma^5\otimes\beta\sqrt{\frac{2}{3}}\,q_2^r & \alpha_5^{k-2r-1}\gamma^5\otimes\sqrt{\frac{1}{3}}\,q_2^r\chi\gamma\\ -\alpha_5^{k-2r-1}\gamma^5\otimes\beta^{-1}\sqrt{\frac{2}{3}}\,q_3^r & \alpha_4^{k-2r-1}\gamma^5\otimes\beta^{-1}\sqrt{\frac{2}{3}}\,q_3^r & -\frac{2}{3}\alpha_0^{k-2r}\otimes q_4^r & 0\\ \alpha_6^{k-2r-1}\gamma^5\otimes(\chi\gamma)^{-1}\sqrt{\frac{1}{3}}\,q_3^r & \alpha_7^{k-2r-1}\gamma^5\otimes(\chi\gamma)^{-1}\sqrt{\frac{1}{3}}\,q_3^r & 0 & \frac{1}{3}\alpha_0^{k-2r}\otimes\chi^{-1}q_4^r\chi\end{pmatrix}. \tag{21}$$

The isomorphism $\mathbf{i}$ fulfills $\mathbf{i}([\varrho^k,\tilde{\varrho}^n]_g)=\mathbf{i}(\varrho^k)\mathbf{i}(\tilde{\varrho}^n)-(-)^{kn}\mathbf{i}(\tilde{\varrho}^n)\mathbf{i}(\varrho^k)$, for $\varrho^k\in\mathscr{H}_0^k$ and $\tilde{\varrho}^n\in\mathscr{H}_0^n$, where the multiplication $\mathbf{i}(\varrho^k)\mathbf{i}(\tilde{\varrho}^n)$ is the natural combination of the multiplication $\wedge$ in L^* and matrix multiplication.

In the above formulas ϵ and β are invertible diagonal 3×3 matrices, which, therefore, commute with m_l, m_l^*, m_q, m_q^*. For the invertible 3×3 matrices γ and χ we have to demand $(\chi\gamma)^{-1}m_q^*m_q\chi\gamma=\chi^{-1}m_q^*m_q\chi$, which is achieved by taking $\chi\gamma\chi^{-1}$ diagonal. The matrix χ need not be unitary. In principle, we could in an analogous way introduce matrices such as χ in the third row and column in (20) and (21), too. However, this can be reabsorbed by unitary transformations of the physical fields. Thus, the freedom in the choice of the isomorphism $\mathbf{i}$, modulo unitary transformations, introduced a lot of additional free parameters in (20) and (21). But, we shall see at the end of Sec. V that all these parameters are (not uniquely) fixed by the physical model. The genuine free parameters are the six eigenvalues of M; see (1).

The motivation to consider just the isomorphism (20), (21) comes from our paper,[2] where we constructed a partial homomorphism of $\mathscr{H}_0$ onto $\Lambda^*(X)\otimes spl(2,1)$, and the paper,[13] where similar looking representations of $spl(2,1)$ were used to write down a fermionic Lagrangian for the standard model.

IV. BOUNDED OPERATORS ON THE HILBERT SPACE OF FERMIONS

Here we are going to associate to each $\mathbf{i}(\rho^k)\in\mathbf{i}(\mathscr{H}_0^k)$, $k=0,1,2$, a bounded operator on the Hilbert space,

$$H=H_l\oplus H_q,$$

$$H_l=L^2(X,S)\otimes\mathbb{C}^3\otimes\mathbb{C}^3,\quad H_q=L^2(X,S)\otimes(\mathbb{C}^4\oplus\mathbb{C}^4\oplus\mathbb{C}^4)\otimes\mathbb{C}^3. \tag{22}$$

First, because of $L^0 \equiv C^0$ and $L^1 \equiv C^1$ we can regard elements of $\mathbf{i}(\mathscr{H}_0^0)$ and $\mathbf{i}(\mathscr{H}_0^1)$ in a natural way as bounded operators on H, see (20) and (21), where the matrices l_s^r and q_s^r act on the last $\mathbb{C}^3$ components. Next, we associate to the local basis $[\gamma^\mu] \wedge [\gamma^\nu]$ in L^2 the operator $\mathbf{c}([\gamma^\mu] \wedge [\gamma^\nu]) := \gamma^\mu \cdot \gamma^\nu \in B(L^2(X,S))$, for $1 \leq \mu < \nu \leq 4$. By linear extension we obtain a vector space isomorphism $\mathbf{c}$ of L^2 onto its image. The isomorphism $\mathbf{c}$ induces the vector space isomorphism $\tilde{\mathbf{c}}\mathbf{i}(\mathscr{H}_0^2) \to \tilde{\mathbf{c}} \circ \mathbf{i}(\mathscr{H}_0^2)$, $\tilde{\mathbf{c}} \circ \mathbf{i}(\mathscr{H}_0^2) \subset B(H)$:

$$\tilde{\mathbf{c}} \circ \mathbf{i}(\varrho^2) := \begin{pmatrix} (\mathbf{c} \otimes \mathrm{id}_{\mathbb{C}^3 \otimes \mathbb{C}^3})(\mathbf{i}_l(\varrho_l^2)) & 0 \\ 0 & \{(\mathbf{c} \otimes \mathrm{id}_{\mathbb{C}^3 \otimes \mathbb{C}^3})(\mathbf{i}_q(\varrho_q^2))\} \otimes \mathbf{1}_{3\times 3} \end{pmatrix}. \tag{23}$$

for $\varrho^2 \in \mathscr{H}_0^2$. Next, we define a vector subspace $\tilde{\mathscr{T}}^2 \subset B(H)$ as

$$\tilde{\mathscr{T}}^2 = \Big\{ \sum_\alpha (\mathbf{i}(\varrho_\alpha^l) \cdot \mathbf{i}(\tilde{\varrho}^1{}_\alpha) + \mathbf{i}(\tilde{\varrho}^1{}_\alpha) \cdot \mathbf{i}(\varrho_\alpha^1)), \quad \varrho_\alpha^1, \tilde{\varrho}^1{}_\alpha \in \mathscr{H}_0^1, \text{ finite sum} \Big\}. \tag{24}$$

where $\cdot$ denotes the multiplication in $B(H)$, and put

$$\mathscr{T}^2 = \tilde{\mathbf{c}} \circ \mathbf{i}(\mathscr{H}_0^2) + \tilde{\mathscr{T}}^2. \tag{25}$$

One easily convinces oneself that another characterization of this space is

$$\mathscr{T}^2 = \tilde{\mathbf{c}} \circ \mathbf{i}(\mathscr{H}_0^2) \oplus \mathbf{i}(\mathscr{H}_0^0) \oplus \Delta,$$

$$\Delta = \{\mathbf{i}(\mathrm{diag}(\alpha_3^0, 0, -\alpha_3^0, 0) \otimes \mathrm{id}_F) \ \mathbf{i}(\mathrm{diag}(\tilde{\alpha}^0{}_3, 0, -\tilde{\alpha}^0{}_3, 0) \otimes \mathrm{id}_F) + \mathbf{i}(\mathrm{diag}(\alpha_0^0, 0, \alpha_0^0, 2\alpha_0^0) \otimes \mathrm{id}_F) \ \mathbf{i}(\mathrm{diag}(\tilde{\alpha}^0{}_0, 0, \tilde{\alpha}^0{}_0, 2\tilde{\alpha}^0{}_0) \otimes \mathrm{id}_F), \quad \alpha_3^0, \tilde{\alpha}^0{}_3, \alpha_0^0, \tilde{\alpha}^0{}_0 \in C^0\}. \tag{26}$$

Let $\mathbf{p}_2$ be the projection of $\mathscr{T}^2 = \tilde{\mathbf{c}} \circ \mathbf{i}(\mathscr{H}_0^2) \oplus \mathbf{i}(\mathscr{H}_0^0) \oplus \Delta$ onto its first component $\tilde{\mathbf{c}} \circ \mathbf{i}(\mathscr{H}_0^2)$. Then we have

$$\tilde{\mathbf{c}}^{-1} \circ \mathbf{p}_2(\mathbf{i}(\varrho^1) \cdot \mathbf{i}(\tilde{\varrho}^1) + \mathbf{i}(\tilde{\varrho}^1) \cdot \mathbf{i}(\tilde{\varrho}^1)) = \mathbf{i}([\varrho^1, \tilde{\varrho}^1]_g), \tag{27}$$

which is in some sense an analogy to (5).

On $B(H)$ there is a natural scalar product given by the Dixmier trace Tr_ω:

$$\langle b, \tilde{b} \rangle_{B(H)} = \mathrm{Tr}_\omega(b^* \tilde{b} |D|^{-4}), \quad b, \tilde{b} \in B(H), \tag{28}$$

where D is the generalized Dirac operator of the K cycle and * denotes the involution in $B(H)$. In the case considered here the Dixmier trace can be expressed by a combination of the usual trace over the matrix structure, including the trace in the Clifford algebra and integration over the manifold X:

$$\langle b, \tilde{b} \rangle_{B(H)} = \frac{1}{32\pi^2} \int_X v_g \ \mathrm{tr}(b^* \tilde{b}), \tag{29}$$

where v_g is the canonical volume form on X and the factor $1/32\pi^2$ is taken from Ref. 6. By restriction of the scalar product (28) to $\mathscr{T}^2 \subset B(H)$ we get a natural scalar product on $\mathscr{T}^2$. However, since elements of $\mathscr{T}^2$ are diagonal with respect to the splitting $H = H_l \oplus H_q$ in (22), we can take as a scalar product $\langle \ , \ \rangle_{\mathscr{T}^2}$ on $\mathscr{T}^2$ a convex linear combination of the partial traces in $B(H_l)$ and $B(H_q)$, in the same way as in Ref. 11:

$$\langle b, \tilde{b} \rangle_{\mathscr{T}^2} = \langle zb, \tilde{b} \rangle_{B(H)}, \quad z = \begin{pmatrix} x\mathbf{1}_{9\times 9} & 0 \\ 0 & \mathbf{1}_{36\times 36} \end{pmatrix}, \tag{30}$$

for $b,\tilde{b}\in\mathscr{T}^2$ and $0<x<\infty$.

The direct sum decomposition $\mathscr{T}^2=\tilde{\mathbf{c}}\circ\mathbf{i}(\mathscr{H}_0^2)\oplus\ker\mathbf{p}_2$ is not an orthogonal decomposition with respect to $\langle\ ,\ \rangle_{\mathscr{T}^2}$. Let $\mathbf{s}_2$ be the orthogonal projection from $\mathscr{T}^2$ onto the orthogonal complement of the subspace $\ker\mathbf{p}_2$ (after a completion with respect to the scalar product). Then we define the canonical embedding $\mathbf{e}:\mathscr{H}_0^2\to B(H)$ by

$$\mathbf{e}(\varrho^2)=\mathbf{s}_2\circ\tilde{\mathbf{c}}\circ\mathbf{i}(\varrho^2),\quad \varrho^2\in\mathscr{H}_0^2. \tag{31}$$

In the same way as in Ref. 1 one can show that $\mathbf{e}(\varrho^2)$ is given by (20) and (21) if we replace

$$\alpha_f^2\mapsto\mathbf{c}(\alpha_f^2),\quad f=0,+,-,3, \tag{32}$$

$$l_s^2\mapsto\tilde{l}_s^2:=l_s^2-\frac{\operatorname{tr} l_s^2}{3}\,1_{3\times3},\quad q_s^2\mapsto\tilde{q}_s^2:=q_s^2-\frac{\operatorname{tr} q_s^2}{3}\,1_{3\times3},\quad s=1,4. \tag{33}$$

Thus, the operators on H associated to $\mathbf{i}(\varrho^k)\in\mathbf{i}(\mathscr{H}_0^k)$, $k=0,1,2$, are $\mathbf{i}(\varrho^k)$ themselves for $k=0,1$ and $\mathbf{e}(\varrho^k)$ for $k=2$. Of course, this construction can be extended to $\mathbf{i}(\mathscr{H}_0^k)$, $k>2$, but we do not need this for model building.

V. THE FERMIONIC ACTION

The connection form ρ is a skew-adjoint element of $\mathscr{H}_0^1$; see. (14). Therefore, we have

$$\rho=\begin{pmatrix} (\frac{1}{2}A^3+\frac{1}{2}A^0)\otimes\mathrm{id}_F & 0 & A^-\otimes\mathrm{id}_F & -i\Phi^1\gamma^5\otimes M \\ 0 & 0 & 0 & 0 \\ A^+\otimes\mathrm{id}_F & 0 & (-\frac{1}{2}A^3+\frac{1}{2}A^0)\otimes\mathrm{id}_F & -i\Phi^2\gamma^5\otimes M \\ -i\bar{\Phi}^1\gamma^5\otimes M^* & 0 & -i\bar{\Phi}^2\gamma^5\otimes M^* & A^0\otimes\mathrm{id}_F \end{pmatrix}, \tag{34}$$

where $A^0=-(A^0)^*$, $A^3=-(A^3)^*$, $A^+=-(A^-)^*\in L^1$, and $\Phi^1,\Phi^2\in L^0$. Applying the isomorphism $\mathbf{i}$ and abbreviating $\mathbf{1}=1_{3\times3}$, we get from (18), (20), and (21),

$$\mathbf{i}_l(\rho_l)=\begin{pmatrix} (\frac{1}{2}A^3+\frac{1}{2}A^0)\otimes\mathbf{1} & A^-\otimes\mathbf{1} & i\Phi^1\gamma^5\otimes\epsilon m_l \\ A^+\otimes\mathbf{1} & (-\frac{1}{2}A^3+\frac{1}{2}A^0)\otimes\mathbf{1} & i\Phi^2\gamma^5\otimes\epsilon m_l \\ i\bar{\Phi}^1\gamma^5\otimes\epsilon^{-1}m_l^* & i\bar{\Phi}^2\gamma^5\otimes\epsilon^{-1}m_l^* & A^0\otimes\mathbf{1} \end{pmatrix}, \tag{35}$$

$$\mathbf{i}_q(\rho_q)=\begin{pmatrix} (\frac{1}{2}A^3-\frac{1}{6}A^0)\otimes\mathbf{1} & A^-\otimes\mathbf{1} & i\bar{\Phi}^2\gamma^5\otimes\sqrt{\frac{2}{3}}\beta m_q & i\Phi^1\gamma^5\otimes\sqrt{\frac{1}{3}}m_q\chi\gamma \\ A^+\otimes\mathbf{1} & (-\frac{1}{2}A^3-\frac{1}{6}A^{(0)})\otimes\mathbf{1} & -i\bar{\Phi}^1\gamma^5\otimes\sqrt{\frac{2}{3}}\beta m_4 & i\Phi^2\gamma^5\otimes\sqrt{\frac{1}{3}}m_q\chi\gamma \\ -i\Phi^2\gamma^5\otimes\sqrt{\frac{2}{3}}\beta^{-1}m_q^* & i\Phi^1\gamma^5\otimes\sqrt{\frac{2}{3}}\beta^{-1}m_q^* & -\frac{2}{3}A^0\otimes\mathbf{1} & 0 \\ i\bar{\Phi}^1\gamma^5\otimes\sqrt{\frac{1}{3}}(\chi\gamma)^{-1}m_q^* & i\bar{\Phi}^2\gamma^5\otimes\sqrt{\frac{1}{3}}(\chi\gamma)^{-1}m_q^* & 0 & \frac{1}{3}A^0\otimes\mathbf{1} \end{pmatrix}. \tag{36}$$

The connection ∇ can be extended to an operator $\nabla:\mathscr{E}\otimes_{\mathscr{A}}h\to\mathscr{E}\otimes_{\mathscr{A}}h$,

$$\begin{aligned}\nabla(\xi\otimes_{\mathcal{A}}\psi)&=(i\,\nabla\xi)\otimes_{\mathcal{A}}\psi+\xi\otimes_{\mathcal{A}}D\psi=e\{((D\otimes\mathbb{1}_{2\times2})\xi-\xi D)+i\rho\xi\}\otimes_{\mathcal{A}}\psi+\xi\otimes_{\mathcal{A}}D\psi\\&=(e(D\otimes\mathbb{1}_{2\times2})e+i\rho)(\xi\otimes_{\mathcal{A}}\psi)\\&=(D^{\mathrm{cl}}+\mu+i\rho)(\xi\otimes_{\mathcal{A}}\psi),\\ \mu&=e(\gamma^5\otimes\mathcal{M}\otimes\mathbb{1}_{2\times2})e,\end{aligned}\tag{37}$$

for $\xi\in\mathcal{E}$, $\psi\in h$; see Ref. 5. We have used $\hat{d}a=-i[D,a]$ for $a\in\mathcal{A}$, see Ref. 1, and $L^n\equiv C^n$ for $n=0,1$. We have $\mu\in\mathcal{M}_0^1$, hence we can apply the isomorphism $\mathbf{i}$, and we find

$$\mathbf{i}_l(\mu_l)=\begin{pmatrix}0&0&0\\0&0&-\gamma^5\otimes\epsilon m_l\\0&-\gamma^5\otimes\epsilon^{-1}m_l^*&0\end{pmatrix},$$

$$\mathbf{i}_q(\mu_q)=\begin{pmatrix}0&0&-\gamma^5\otimes\sqrt{\frac{2}{3}}\,\beta m_q&0\\0&0&0&-\gamma^5\otimes\sqrt{\frac{1}{3}}\,m_q\chi\gamma\\\gamma^5\otimes\sqrt{\frac{2}{3}}\beta^{-1}m_q^*&0&0&0\\0&-\gamma^5\otimes\sqrt{\frac{1}{3}}\,(\chi\gamma)^{-1}m_q^*&0&0\end{pmatrix}.\tag{38}$$

The situation found in nature demands to use a pseudo-Riemannian manifold X_M instead of the Riemannian manifold X. We are interested in the case that X_M is the Minkowski space. We convert the results obtained so far for the Euclidian manifold X by a Wick rotation to Minkowski space. If we denote by $L^2(X_M,S)$ the space of square integrable sections of the spinor bundle over X_M then instead of H, see (22), we have to take the space

$$H_M=\{L^2(X_M,S)\otimes\mathbb{C}^3\oplus\mathbb{C}^3\}\oplus\{L^2(X_M,S)\otimes(\mathbb{C}^4\oplus\mathbb{C}^4\oplus\mathbb{C}^4)\otimes\mathbb{C}^3\}.\tag{39}$$

On H_M we have the invariant product

$$\langle\Psi,\widetilde{\Psi}\rangle_{H_M}:=\int_{X_M}\upsilon_M\Psi^*\gamma^0\widetilde{\Psi},\quad\Psi,\widetilde{\Psi}\in H_M,\tag{40}$$

where υ_M is the canonical volume form on X_M. Due to (37) the natural fermionic action is

$$S_F=\tfrac{1}{2}\langle\Psi,(D^{\mathrm{cl}}+i(\mu+i\rho_M))\Psi\rangle_{H_M}+\mathrm{H.c.},\quad\Psi\in H_M,\tag{41}$$

where ρ_M is the connection form ρ rotated to Minkowski space and H.c. denotes the Hermitian conjugate of the preceding term. We take

$$\Psi=(\Psi_l,\Psi_q)^T,\quad\Psi_l=(\nu_L,e_L,e_R)^T,\quad\Psi_q=(u_L,d_L,u_R,d_R)^T,\tag{42}$$

where $e_L,\nu_L,e_R\in L^2(X_M,S)\otimes\mathbb{C}^3$ and $u_L,d_L,u_R,d_R\in L^2(X,S)\otimes\mathbb{C}^3\otimes\mathbb{C}^3$, with

$$(\gamma^5\otimes\mathrm{id})f_L=-f_L,\quad(\gamma^5\otimes\mathrm{id})f_R=f_R,\quad f=e,\upsilon,u,d.\tag{43}$$

We obtain, denoting the Wick rotated fields $A^{0,+,-,3}$ and $\Phi^{1,2}$ by the same symbols,

$$S_F=\int_{X_M}\upsilon_M(\mathcal{L}_l+\mathcal{L}_l'+\mathcal{L}_q+\mathcal{L}_q'),\tag{44}$$

$$\mathscr{L}_l=(\nu_L^*,e_L^*)\left\{\gamma^0\begin{pmatrix} D^{\rm cl}+i(\frac{1}{2}A^3+\frac{1}{2}A^0) & iA^- \\ iA^+ & D^{\rm cl}+i(-\frac{1}{2}A^3+\frac{1}{2}A^0)\end{pmatrix}\otimes\mathbb{1}\right\}\begin{pmatrix}\nu_L\\ e_L\end{pmatrix}$$
$$+e_R^*\{\gamma^0(D^{\rm cl}+iA^0)\otimes\mathbb{1}\}\epsilon_R,$$

$$\mathscr{L}_l'=-\left\{e_R^*\{\gamma^0(\bar\Phi^1;\bar\Phi^2+1)\otimes\tfrac{1}{2}(\epsilon^*-\epsilon^{-1})m_l^*\}\begin{pmatrix}\nu_L\\ e_L\end{pmatrix}+\text{H.c.}\right\},$$

$$\mathscr{L}_q=(u_L^*,d_L^*)\left\{\gamma^0\begin{pmatrix} D^{\rm cl}+i(\frac{1}{2}A^3-\frac{1}{6}A^0) & iA^- \\ iA^+ & D^{\rm cl}+i(-\frac{1}{2}A^3-\frac{1}{6}A^0)\end{pmatrix}\otimes\mathbb{1}_c\otimes\mathbb{1}\right\}\begin{pmatrix}u_L\\ d_L\end{pmatrix}$$
$$+u_R^*\{\gamma^0(D^{\rm cl}-\tfrac{2}{3}iA^0)\otimes\mathbb{1}_c\otimes\mathbb{1}\}u_R+d_R^*\{\gamma^0(D^{\rm cl}+\tfrac{1}{3}iA^0)\otimes\mathbb{1}_c\otimes\mathbb{1}\}d_R,$$

$$\mathscr{L}_q'=-\left\{u_R^*\{\gamma^0(\Phi^2+1;-\Phi^1)\otimes\mathbb{1}_c\otimes\tfrac{1}{2}\sqrt{\tfrac{2}{3}}(\beta^*+\beta^{-1})m_q^*\}\begin{pmatrix}u_L\\ d_L\end{pmatrix}+\text{H.c.}\right\}$$
$$-\left\{d_R^*\{\gamma^0(\bar\Phi^1;\bar\Phi^2+1)\otimes\mathbb{1}_c\otimes\tfrac{1}{2}\sqrt{\tfrac{1}{3}}(\chi\gamma)^*-(\chi\gamma)^{-1}m_q^*\}\begin{pmatrix}u_L\\ d_L\end{pmatrix}+\text{H.c.}\right\},$$

where $\mathbb{1}_c=\mathbb{1}_{3\times3}$ is the identity acting on the colour space of the quarks; see Sec. VII. Comparing this with the classical fermionic action,[17] we read off the mass matrices of the fermions,

$$m_e=\tfrac{1}{2}(\epsilon^*-\epsilon^{-1})m_l^*,\quad m_u=\tfrac{1}{2}\sqrt{\tfrac{2}{3}}(\beta^*+\beta^{-1})m_q^*,\quad m_d'=\tfrac{1}{2}\sqrt{\tfrac{1}{3}}((\chi\gamma)^*-(\chi\gamma)^{-1})m_q^*. \tag{45}$$

where $e\equiv(e,\mu,\tau)^T$, $u\equiv(u,c,t)^T$, $d\equiv(d,s,b)^T$. The matrices m_e,m_u are diagonal. We can assume that their diagonal matrix elements are positive, otherwise this is achieved by unitary transformations $e_R\mapsto u_e e_R$, $u_R\mapsto u_u u_R$ with diagonal unitary matrices u_e,u_u. However, the matrix m_d' is—in general—an arbitrary nondiagonal 3×3 matrix. There exist unitary matrices u_1,u_2, so that $m_d'=u_1 m_d u_2^*$ for a diagonal matrix m_d with positive diagonal matrix elements. The matrix u_1 can be absorbed by means of a unitary transformation $d_R\mapsto u_1 d_R$. But the matrix u_2^* cannot be absorbed by a unitary transformation $\binom{u_L}{d_L}\mapsto\left(\begin{smallmatrix}u_2 & 0\\ 0 & u_2\end{smallmatrix}\right)\binom{u_L}{d_L}$, because this would make the matrix m_u nondiagonal. All we can do are transformations $\binom{u_L}{d_L}\mapsto\left(\begin{smallmatrix}\delta_1 & 0\\ 0 & \delta_1\end{smallmatrix}\right)\binom{u_L}{d_L}$, $u_R\mapsto\delta_1 u_R$ and $d_R\mapsto\delta_2 d_R$ by diagonal unitary matrices δ_1,δ_2, so that m_u remains invariant and $u_2^*\mapsto\delta_1^* u_2^*\delta_2=:V$. The matrix V is the famous Kobayashi–Maskawa matrix, which for an appropriate choice of δ_1,δ_2 can be brought into the standard form parametrized by three rotation angles and one phase. Thus, we can rewrite $\mathscr{L}_l'$ and $\mathscr{L}_q'$ as

$$\mathscr{L}_l'=-\left\{e_R^*\{\gamma^0(\bar\Phi^1;\bar\Phi^2+1)\otimes m_e\}\begin{pmatrix}\nu_L\\ e_L\end{pmatrix}+\text{H.c.}\right\},$$

$$\mathscr{L}_q'=-\left\{u_R^*\{\gamma^0(\Phi^2+1;-\Phi^1)\otimes m_\mu\otimes\mathbb{1}_c\}\begin{pmatrix}u_L\\ d_L\end{pmatrix}+\text{H.c.}\right\}$$
$$-\left\{d_R^*\{\gamma^0(\bar\Phi^1;\bar\Phi^2+1)\otimes m_d V\otimes\mathbb{1}_c\}\begin{pmatrix}u_L\\ d_L\end{pmatrix}+\text{H.c.}\right\}. \tag{46}$$

Now we count the free parameters on which the physical masses in our model depend. We can regard (45) as equations for computing the fermion masses and the Kobayashi–Maskawa matrix for given 3×3 matrices $\beta,\gamma,\epsilon,\chi,m_l,m_q$. But if we take the point of view that the fermion masses

and the Kobayashi–Maskawa matrix (13 parameters) are given by experiment, and if we keep the diagonal positive matrices m_l and m_q as additional free parameters, then (45), with $m'_d = m_d V$, are equations to determine $\beta,\gamma,\epsilon,\chi$. This gives a system of quadratic equations for the matrix elements of $\beta,\gamma,\epsilon,\chi$. We take any of the (possibly complex) solutions of this system to fix the matrices $\beta,\gamma,\epsilon,\chi$. Then, there remain only the six free parameters in the diagonal of m_l and m_q.

We remark that the presented construction of the fermionic action of the standard model yields immediately the correct hypercharges of the fermions—namely the coefficients in front of $-\frac{1}{2}A^0$ in (35) and (36). This is possible because we use the isomorphism $\mathbf{i}$ of graded Lie algebras, which allows embeddings into the space of bounded operators on the fermionic Hilbert space different from the fundamental embedding. For matrix algebras there exist—besides the trivial representation—only the fundamental representation and, hence, only the fundamental embedding. Therefore, in the derivation of the standard model elaborated on by Kastler,[7] one must additionally consider the chromodynamics algebra and impose a generalized Poincaré duality condition (Refs. 3, 7) in order to obtain the correct hypercharges.

VI. THE BOSONIC ACTION

We recall[2] that the curvature θ of the connection ∇ is given by

$$\theta = \mathscr{D}\rho + \tfrac{1}{2}\{\rho,\rho\}_g + \theta_0 = \mathbf{D}\rho - i[\mu,\rho]_g + \tfrac{1}{2}[\rho,\rho]_g + \theta_0, \tag{47}$$

where

$$\theta_0 = e\hat{d}(e)\hat{d}(e)e = \mathrm{diag}(MM^*,0,0,0). \tag{48}$$

The problem is that $\theta_0 \notin \mathscr{H}_0$, so that it is not possible to apply the isomorphism $\mathbf{i}$. We propose to replace here the isomorphism $\mathbf{i}$ by a linear mapping $\mathbf{i}'$ defined as follows. Looking at (16) we see that θ_0 is given by putting $\alpha_3^0 = \alpha_0^0 = 1$ and all other $\alpha_f^{0,1,2} = 0$, and then projecting away the last row and column. Thus, to the element $\widetilde{\theta}_0 \in \mathscr{H}_0^2$ given by $\alpha_3^0 = \alpha_0^0 = 1$ we apply the isomorphism $\mathbf{i}$, giving $\mathbf{i}_l(\widetilde{\theta}_{0,l}) = \mathrm{diag}(1_1^1,0,1_4^1)$ and $\mathbf{i}_q(\widetilde{\theta}_{0,q}) = \mathrm{diag}(\frac{1}{3}q_1^1, -\frac{2}{3}q_4^1, -\frac{2}{3}q_4^1, \frac{1}{3}q_4^1)$; see (20) and (21). Now we apply a reasonable projection:

$$\mathbf{i}'_l(\theta_{0,l}) := \mathrm{diag}(1_1^1,0,0), \quad \mathbf{i}'_q(\theta_{0,q}) := \mathrm{diag}(\tfrac{1}{3}q_1^1, -\tfrac{2}{3}q_1^1, -\tfrac{2}{3}q_4^1, 0). \tag{49}$$

The choice $\mathbf{i}'_f(\theta_{0,l})$ is plausible, but I have no deeper explanation for $\mathbf{i}'_q(\theta_{0,q})$, except that we need this below. We recall that $l_1^1 = l_4^1 = m_l m_l^* \equiv |m_l|^2$ and $q_1^1 = q_4^1 = m_q m_q^* \equiv |m_q|^2$. Then, using (35), (36), and (38), the transported curvature is given by ($f \in \{l,q\}$)

$$\mathbf{i}_f(\theta_f) = \mathbf{D}(\mathbf{i}_f(\rho_f)) - i[\mathbf{i}_f(\mu_f),\mathbf{i}_f(\rho_f)]_g + \tfrac{1}{2}[\mathbf{i}_f(\rho_f),\mathbf{i}_f(\rho_f)]_g + \mathbf{i}'_f(\theta_{0,f}), \tag{50}$$

$$\mathbf{i}_l(\theta_l) = \begin{pmatrix} (\frac{1}{2}\,\mathbf{d}(A^3+A^0)+A^-\wedge A^+) & (\mathbf{d}A^- + A^3\wedge A^-)\otimes \mathbb{1} & i(\mathbf{d}\Phi^1 + \frac{1}{2}(A^3-A^0)\Phi^1 \\ \otimes \mathbb{1} - (|\Phi^1|^2-1)\otimes|m_l|^2 & -\Phi^1(\bar{\Phi}^2+1)\otimes|m_l|^2 & +A^-(\Phi^2+1))\gamma^5\otimes\epsilon m_l \\ (\mathbf{d}A^+ + A^+\wedge A^3)\otimes\mathbb{1} & (\mathbf{d}(A^0-A^3)+A^+\wedge A^-) & i(-\frac{1}{2}(A^3+A^0)(\Phi^2+1) \\ -(\Phi^2+1)\bar{\Phi}^1\otimes|m_l|^2 & \otimes\mathbb{1} - (|\Phi^2+1|^2-1)\otimes|m_l|^2 & +\mathbf{d}\Phi^2 + A^+\Phi^1)\gamma^5\otimes\epsilon m_l \\ i(\mathbf{d}\bar{\Phi}^1 - \frac{1}{2}\bar{\Phi}^1(A^3-A^0) & i(\frac{1}{2}(\bar{\Phi}^2+1)(A^3+A^0) & \mathbf{d}A^0\otimes\mathbb{1} - (|\Phi^1|^2 \\ -(\bar{\Phi}^2+1)A^+)\gamma^5\otimes\epsilon^{-1}m_l^* & +\mathbf{d}\bar{\Phi}^2 - \bar{\Phi}^1 A^-)\gamma^5\otimes\epsilon^{-1}m_l^* & +|\Phi^2+1|^2 - 1\otimes|m_l|^2 \end{pmatrix}.$$

$$i_q(\theta_q)=\begin{pmatrix}
\begin{array}{l}(\mathrm{d}(\frac{1}{2}A^3-\frac{1}{6}A^0)\\ +A^-\wedge A^+)\otimes 1\\ +(\frac{2}{3}|\Phi^2+1|^2-\frac{1}{3}\\ -\frac{1}{3}|\Phi^1|^2)\otimes|m_q|^2\end{array} & \begin{array}{l}(\mathrm{d}A^-+A^3\wedge A^-)\otimes 1\\ -\Phi^1(\bar\Phi^2+1)\\ \otimes|m_q|^2\end{array} & \begin{array}{l}i(d\bar\Phi^2-\bar\Phi^1A^-\\ +\frac{1}{2}(\bar\Phi^2+1)\\ \times(A^3+A^0))\gamma^5\\ \otimes\sqrt{\frac{2}{3}}\,\beta m_q\end{array} & \begin{array}{l}i(\mathrm{d}\Phi^1+\\ \frac{1}{2}(A^3-A^0)\Phi^1+\\ +A^-(\Phi^2+1))\gamma^5\\ \otimes\sqrt{\frac{1}{3}}\,m_q\chi\gamma\end{array} \\
\begin{array}{l}(\mathrm{d}A^++A^+\wedge A^3)\\ \otimes 1\\ -(\Phi^2+1)\bar\Phi^1\otimes|m_q|^2\end{array} & \begin{array}{l}(\mathrm{d}(-\frac{1}{2}A^3-\frac{1}{6}A^0)\\ +A^+\wedge A^-)\otimes 1\\ -(\frac{1}{3}|\Phi^2+1|^2+\frac{1}{3}\\ -\frac{2}{3}|\Phi^1|^2\otimes|m_q|^2\end{array} & \begin{array}{l}-i(\mathrm{d}\bar\Phi^1\\ -(\bar\Phi^2+1)A^+\\ -\frac{1}{2}\bar\Phi^1(A^3-A^0))\gamma^5\\ \otimes\sqrt{\frac{2}{3}}\,\beta m_q\end{array} & \begin{array}{l}i(\mathrm{d}\Phi^2+A^+\Phi^1\\ -\frac{1}{2}(A^3+A^0)\\ \times(\Phi^2+1))\gamma^5\\ \otimes\sqrt{\frac{1}{3}}\,m_q\chi\gamma\end{array} \\
\begin{array}{l}-i(\mathrm{d}\Phi^2+A^+\Phi^1\\ -\frac{1}{2}(A^3+A^0)\\ \times(\Phi^2+1))\gamma^5\\ \otimes\sqrt{\frac{2}{3}}\,\beta^{-1}m_q^*\end{array} & \begin{array}{l}i(\mathrm{d}\Phi^1\\ +A^-(\Phi^2+1)\\ +\frac{1}{2}(A^3-A^0)\Phi^1)\gamma^5\\ \otimes\sqrt{\frac{2}{3}}\,\beta^{-1}m_q^*\end{array} & \begin{array}{l}-\frac{2}{3}\,\mathrm{d}A^0\otimes 1\\ +\frac{2}{3}(|\Phi^1|^2\\ +|\Phi^2+1|^2-2)\\ \otimes|m_q|^2\end{array} & 0 \\
\begin{array}{l}i(\mathrm{d}\bar\Phi^1\\ -(\bar\Phi^2+1)A^+\\ -\frac{1}{2}\bar\Phi^1(A^3-A^0))\gamma^5\\ \otimes\sqrt{\frac{1}{3}}\,(\chi\gamma)^{-1}m_q^*\end{array} & \begin{array}{l}i(\mathrm{d}\bar\Phi^2-\bar\Phi^1A^-\\ +\frac{1}{2}(\bar\Phi^2+1)\\ \times(A^3+A^0))\gamma^5\\ \otimes\sqrt{\frac{1}{3}}\,(\chi\gamma)^{-1}m_q^*\end{array} & 0 & \begin{array}{l}\frac{1}{3}\,\mathrm{d}A^0\otimes 1\\ -\frac{1}{3}(|\Phi^1|^2\\ +|\Phi^2+1|^2-1)\\ \otimes\chi^{-1}|m_q|^2\chi\end{array}
\end{pmatrix}.$$

Now we take the embedding $\mathbf{e}$ of θ into $B(H)$, which means to perform the replacements (32) and (33) in the above matrices, see Sec. IV. We introduce the abbreviations $|m|^2=mm^*$, $|m|^4:=(mm^*)^2$, and $|m|^{-2}:=(mm^*)^{-1}$, for a 3×3 matrix m. Thus, we get the Euclidean bosonic action—for an appropriate choice of the constants—as

$$S_B=\frac{8\pi^2}{3(x+3)g_2^2}\,\mathrm{Tr}_\omega\{(z\mathbf{e}(\theta))^*\mathbf{e}(\theta)\}=\frac{1}{12(x+3)g_2^2}\int_X v_g\,\mathrm{tr}\{z(\mathbf{e}(\theta))^*\mathbf{e}(\theta)\}$$

$$=\int_X v_g(\mathscr{L}_2+\mathscr{L}_1+\mathscr{L}_0),$$

$$\mathscr{L}_2=-\frac{1}{2g_2^2}\,\delta^{\mu\kappa}\delta^{\nu\lambda}\left\{\mathrm{tr}(F_{\mu\nu}F_{\kappa\lambda})+\frac{9x+11}{6x+18}\,F'_{\mu\nu}F'_{\kappa\lambda}\right\},$$

$$F_{\mu\nu}=\begin{pmatrix}\frac{1}{2}\,\partial_{[\mu}A^3_{\nu]}+A^-_{[\mu}A^+_{\nu]} & \partial_{[\mu}A^-_{\nu]}+A^3_{[\mu}A^-_{\nu]}\\ \partial_{[\mu}A^+_{\nu]}+A^+_{[\mu}A^3_{\nu]} & -\frac{1}{2}\,\partial_{[\mu}A^3_{\nu]}-A^-_{[\mu}A^+_{\nu]}\end{pmatrix},\quad F'_{\mu\nu}=\partial_{[\mu}A_{\nu]},$$

$$\mathscr{L}_1=\frac{1}{3(x+3)g_2^2}\,\delta^{\mu\nu}\overline{(D_\mu\Phi^1)}D_\nu\Phi^1+\overline{(D_\mu(\Phi^2+1)}D_\nu(\Phi^2+1))$$

$$\times\mathrm{tr}\{\chi(|\epsilon|^2+|\epsilon|^{-2})|m_l|^2+(2|\beta|^2+2|\beta|^{-2}+|\chi\gamma|^2+|\chi\gamma|^{-2})|m_q|^2\},$$

$$\begin{pmatrix} D_\mu\Phi^1 \\ D_\mu(\Phi^2+1) \end{pmatrix} = \begin{pmatrix} \partial_\mu\Phi^1 \\ \partial_\mu\Phi^2 \end{pmatrix} + \begin{pmatrix} \frac{1}{2}(A^3_\mu - A^0_\mu) & A^-_\mu \\ A^+_\mu & -\frac{1}{2}(A^3_\mu + A^0_\mu) \end{pmatrix} \begin{pmatrix} \Phi^1 \\ \Phi^2+1 \end{pmatrix},$$

$$\mathscr{L}_0 = \frac{2}{3(x+3)g_2^2}(|\Phi^1|^2+|\Phi^2+1|^2-1)^2\left(x|\widetilde{m}_l|^4+\frac{5}{3}|\widetilde{m}_q|^4\right)+\frac{1}{(x+3)g_2^2}\,\mathrm{tr}\left(\frac{1}{3}x|\widetilde{m}_l|^4+|\widetilde{m}_q|^4\right), \tag{51}$$

with $X_{[\mu}Y_{\nu]} \equiv X_\mu Y_\nu - X_\nu Y_\mu$. We have used $\mathrm{tr}_C(1)=4$, $\mathrm{tr}_C(\gamma^{\mu'}\cdot\gamma^{\nu'})=4\delta^{\mu'\nu'}$ and $\mathrm{tr}_C(\gamma^\mu\cdot\gamma^\nu\cdot\gamma^\kappa\cdot\gamma^\lambda)=4(\delta^{\nu\kappa}\delta^{\mu\lambda}-\delta^{\mu\kappa}\delta^{\nu\lambda})$ for $\mu\neq\nu,\kappa\neq\lambda$, where tr_C denotes the trace in the space of sections of the Clifford bundle C. We remark that the part $\mathscr{L}_0$ of the Lagrangian would vanish if there was only one generation of fermions, because in this case a formula corresponding to (33) would give zero for $\widetilde{m}_l$ and $\widetilde{m}_q$. But manifestly there are three fermionic generations in nature. Next, we perform some reparametrizations. We put

$$A^3_\mu = ig_2W^3_\mu, \quad A^-_\mu = \frac{i}{2}g_2(W^1_\mu - iW^2_\mu), \quad A^+_\mu = \frac{i}{2}g_2(W^1_\mu + iW^2_\mu),$$

$$A^0_\mu = -\sqrt{\frac{3x+9}{9x+11}}\,ig_2W^0_\mu, \tag{52}$$

$$\Phi^{1,2} = \sqrt{\frac{3(x+3)g_2^2}{2\,\mathrm{tr}\{x(|\epsilon|^2+|\epsilon|^{-2})|m_l|^2+(2|\beta|^2+2|\beta|^{-2}+|\chi\gamma|^2+|\chi\gamma|^{-2})|m_q|^2\}}}\,\phi_{1,2}.$$

This gives (I.T.≡interaction terms, C.C.≡cosmological constant)

$$\mathscr{L}_2 = \frac{1}{4}\delta^{\mu\kappa}\delta^{\nu\lambda}\left\{\sum_{a=1}^{3}F^a_{\mu\nu}F^a_{\kappa\lambda}+F^0_{\mu\nu}F^a_{\kappa\lambda}\right\}, \tag{53}$$

$$\mathscr{L}_1 = \frac{1}{2}\delta^{\mu\nu}\left\{\sum_{j=1}^{2}(\partial_\mu\phi_j)(\partial_\nu\phi_j)+m_W^2(W^1_\mu W^1_\nu+W^2_\mu W^2_\nu)+m_Z^2Z_\mu Z_\nu\right\}+\text{I.T.}, \tag{54}$$

$$\mathscr{L}_0 = \tfrac{1}{2}m_H^2(\mathrm{Re}\ \phi_2)^2+\text{I.T.}+\text{C.C.}, \tag{55}$$

where

$$F^a_{\mu\nu} = \partial_{[\mu}W^a_{\nu]} - g_2\sum_{b,c=1}^{3}\epsilon^a_{bc}W^b_\mu W^c_\nu, \quad F^0_{\mu\nu} = \partial_{[\mu}W^0_{\nu]},$$

$$Z = \cos\,\theta_W W^3 - \sin\,\theta_W W^0,$$

$$P = \sin\,\theta_W W^3 + \cos\,\theta_W W^0,$$

$$\sin^2\,\theta_W = \frac{3}{4}\frac{3+x}{5+3x}, \tag{56}$$

$$m_W = \sqrt{\frac{1}{6(x+3)}}\{\chi(|\epsilon|^2+|\epsilon|^{-2})|m_l|^2+(2|\beta|^2+2|\beta|^{-2}+|\chi\gamma|^2+|\chi\gamma|^{-2})|m_q|^2\}, \tag{57}$$

$$m_z = m_W/\cos\,\theta_W,$$

$$m_H=\frac{2}{3m_W}\sqrt{\frac{1}{x+3}(3x|\tilde{m}_l|^4+5|\tilde{m}_q|^4)}. \tag{58}$$

We can transform this action to Minkowski space by a Wick rotation of the physical fields, replacing $\delta^{\mu\nu}\mapsto -g^{\mu\nu}$ and introducing a global minus sign in the action. Then this action coincides with the electroweak sector of the classical bosonic action of the standard model,[17] where the Weinberg angle θ_W and the masses m_W of the W boson and m_H of the Higgs boson are fixed; see (56), (57), and (58). Inserting the reparameterizations (52) into (44), we get precisely the electroweak sector of the fermionic action of the standard model.[17] According to Ref. 2, the gauge group associated to the module $\mathscr{E}$ discussed in the beginning of Sec. III is isomorphic to $C^\infty_{\mathrm{R}}(X_M)\otimes(SU(2)\times U(1))$, where $C^\infty_{\mathrm{R}}(X_M)$ denotes the algebra of real smooth functions on the Minkowski space. The action is by construction invariant under gauge transformations.

VII. THE CHROMODYNAMICS SECTOR

The chromodynamics sector can be obtained from the module $\mathscr{E}_c=e_c\mathscr{A}^3$, with $e_c=\mathrm{diag}(e',e',e')$. The analysis of this case[2] shows that

$$\mathscr{H}^k_{0,c}=\bigoplus_{i=0}^{m} L^{k-2r}\otimes sl(3,\mathbb{C})\otimes M^r_l, \tag{59}$$

after omitting the rows and columns consisting of zeros only. Thus, elements $\varrho^k\in\mathscr{H}^k_{0,c}$ are of the form $\varrho^k=\Sigma_{r=0}^m G^{k-2r}\otimes M^r_4$, where $G^{k-2r}\in L^{k-2r}\otimes sl(3,\mathbb{C})$. We split $\mathscr{H}^k_{0,c}$ into its l^r_1- and q^r_l part, we take the trivial representation $\mathbf{i}_{c,l}(\varrho^k_l)\equiv 0$ of the l^r_l part, and the fundamental representation (tensorized with $1_{4\times 4}$) of the q^r_l part:

$$\mathbf{i}_{c,q}(\varrho^k_q)=\sum_{r=0}^{m}\mathrm{diag}(G^{k-2r},G^{k-2r},G^{k-2r},G^{k-2r})\otimes q^r_l. \tag{60}$$

Obviously, elements $\mathbf{i}_c(\varrho^k)$ are bounded operators on H for $k=0,1$. In analogy to the procedure in Sec. IV we construct the space $\mathscr{T}^2_c\subset B(H)$, which turns out to be

$$\mathscr{T}^2_c=\tilde{\mathbf{c}}_c\circ\mathbf{i}_c(\mathscr{H}^2_{0,c})+\mathbf{i}_c(C^0\otimes gl(3,\mathbb{C})\otimes\mathrm{id}_F), \tag{61}$$

where $\tilde{\mathbf{c}}_c$ is defined in analogy to (23) and where we extended $\mathbf{i}_c|_{\mathscr{H}^0_{0,c}}$ naturally to $C^0\otimes gl(3,\mathbb{C})\otimes\mathrm{id}_F$.

From (59) we find for the chromodynamics connection form $\varrho_c=G\otimes\mathrm{id}_F$, $G=-G^*\in L^1\otimes su(3)$. After rotating to Minkowski space ($G\mapsto G_M$) we obtain the following contribution to the fermionic action:

$$\mathscr{L}_s=(u^*_L;d^*_L;u^*_R;d^*_R)\left\{\gamma^0\begin{pmatrix} iG_M & 0 & 0 & 0\\ 0 & iG_M & 0 & 0\\ 0 & 0 & iG_M & 0\\ 0 & 0 & 0 & iG_M\end{pmatrix}\otimes 1\right\}\begin{pmatrix} u_L\\ d_L\\ u_R\\ d_R\end{pmatrix}. \tag{62}$$

The curvature θ_c of the chromodynamics connection ∇_c is given by

$$\theta=\mathbf{d}\rho_c+\tfrac{1}{2}[\rho_c,\rho_c]_g+\theta_{0,c},\quad \theta_{0,c}=1_c\otimes M^1_1. \tag{63}$$

These equations follow from the discussion in Ref. 2. We put in local bases

$$G=\frac{i}{2}\,g_3 G^a_\mu \gamma^\mu\otimes\lambda_a\,, \tag{64}$$

where λ_a, $a=1,...,8$, are the Gell–Mann matrices, fulfilling $[\lambda_b,\lambda_c]=\Sigma_{a=1}^{8}2if^a_{bc}\lambda_a$, $f^a_{bc}\in\mathbb{R}$, and $\mathrm{tr}(\lambda_a\lambda_b)=2\delta_{ab}$. Denoting by $\mathbf{e}_c(\theta_c)$ the embedding of θ_c into $B(H)$, we obtain for the Euclidian bosonic action of the chromodynamics sector

$$S^0_B=\frac{8\pi^2}{3(3+x)g_2^2}\,\mathrm{Tr}_\omega\{z(\mathbf{e}_c(\theta_c))^*\mathbf{e}_c(\theta_c)\}=\int_X v_g\mathscr{L}_c\,,$$
$$\mathscr{L}_c=\frac{1}{4}\sum_{a=1}^{8}\delta^{\mu\kappa}\delta^{\nu\lambda}F^a_{c,\mu\nu}F^a_{c,\kappa\lambda}+\frac{1}{g_3^2}\,(|\widetilde{m}_q|^4), \tag{65}$$

$$F^a_{c,\mu\nu}=\partial_{[\mu}G^a_{\nu]}-g_3\sum_{b,c=1}^{8}f^a_{bc}G^b_\mu G^c_\nu\,,$$
$$(g_3/g_2)^2=(3+x)/4. \tag{66}$$

Rotation to Minkowski space ($G\mapsto G_M$, $\delta^{\mu\nu}\to-g^{\mu\nu}$, $v_g\to v_M$, and global minus sign) transforms the first term in $\mathscr{L}_c$ into the bosonic action of chromodynamics,[17] the second term in $\mathscr{L}_c$ contributes to the "cosmological constant." The relation (66) between the coupling constants g_3 and g_2 of the strong and weak interactions, respectively, should not be taken too seriously, because it can easily be changed by a different normalization of the chromodynamics action. But if we take everywhere the simplest scalar product given by $x=1$ then we get $g_3=g_2$ from this model (just as in Refs. 11 and 10 for the simplest scalar product). According to Ref. 2, the gauge group associated to the module $\mathscr{E}_c$ is isomorphic to $C^\infty_{\mathbb{R}}(X_M)\otimes SU(3)$.

VIII. REMARKS ON MASS RELATIONS

In this section we are going to discuss the mass relations (57) and (58). This will be done only for $\mathrm{tr}(|m_l|^2)\leqslant\mathrm{tr}(|m_q|^2)$, because lepton masses are small compared with the quark masses of the same generation so that the case $\mathrm{tr}(|m_l|^2)\leqslant\mathrm{tr}(|m_q|^2)$ is more natural than the case $\mathrm{tr}(|m_l|^2)>\mathrm{tr}(|m_q|^2)$; see (45). Hence, we put

$$\mathrm{tr}(|m_l|^2)=\sin^2\vartheta_1\;\mathrm{tr}(|m_q|^2).$$

From the second equation of (45) we obtain $\mathrm{tr}(|m_u|^2)\geqslant\frac{2}{3}\mathrm{tr}(|m_q|^2)$, so that we put

$$\mathrm{tr}(|m_q|^2)=\tfrac{3}{2}\cos^2\vartheta_2\;\mathrm{tr}(|m_u|^2)=\tfrac{3}{2}m_t^2\cos^2\vartheta_2\,.$$

Here and in the sequel we neglect the other fermion masses against the mass m_t of the top quark. Then we get for (57),

$$m_W=\sqrt{(2/(3+x))\;\mathrm{tr}\{x(\tfrac{1}{3}|m_e|^2+\tfrac{1}{6}|m_l|^2)+(|m_u|^2+|m_d|^2-\tfrac{1}{6}|m_q|^2)\}}$$
$$=\sqrt{(2/(3+x))\;(1-\tfrac{1}{4}(1-x\sin^2\vartheta_1)\cos^2\vartheta_2)}m_t<\sqrt{\tfrac{2}{3}}\,m_t\,. \tag{67}$$

For $m\in M_3\mathbb{C}$ we have $\mathrm{tr}(|\widetilde{m}|^4)\equiv\mathrm{tr}\{(|m|^2-\frac{1}{3}(\mathrm{tr}(|m|^2))1)^2\}\leqslant\frac{2}{3}(\mathrm{tr}(|m|^2))^2$: see (33). Therefore, we put

$$\mathrm{tr}(|\tilde{m}_q|^4)=\tfrac{2}{3}\cos^2\vartheta_3(\mathrm{tr}(|m_q|^2))^2=\tfrac{3}{2}m_l^4\cos^2\vartheta_3\cos^4\vartheta_2,$$

$$\mathrm{tr}(|\tilde{m}_t|^4)=\tfrac{2}{3}\cos^2\vartheta_4(\mathrm{tr}(|m_t|^2))^2=\tfrac{3}{2}m_l^4\cos^2\vartheta_4\cos^4\vartheta_2\sin^4\vartheta_1.$$

Now we find for (58),

$$m_H=\sqrt{\frac{20\cos^2\vartheta_3+12x\cos^2\vartheta_4\sin^4\vartheta_1}{12-3(1-x\sin^2\vartheta_1)\cos^2\vartheta_2}}\,m_t\cos^2\vartheta_2<2m_t. \tag{68}$$

The experimental values $m_W=80$ GeV and $m_t=174$ GeV can be reproduced in the case $x\sin^2\vartheta_1\ll 1$ by $x=6.5...9.6$, depending on ϑ_2'; see (67). Then, by choosing ϑ_2 and ϑ_3, we can adjust m_H to any value smaller than $\sqrt{\frac{20}{9}}m_t=259$ GeV; see (68). Moreover, we find for the Weinberg angle $\sin^2\theta_W=0.27...0.29$, see (56), and for the ratio of the coupling constants of the strong and weak interactions $(g_3/g_2)^2=2.3...3.9$; see (66). In the case $x\sin^2\vartheta_1\gg 4$ we can reproduce the m_W/m_t ratio for $\sin^2\vartheta\approx 1$ and $\cos^2\vartheta_2\approx 1$. By choosing ϑ_4 we can adjust m_H to any value smaller than $2m_t=346$ GeV. Moreover, in this case we have $\sin^2\theta_W=0.25$ and $g_3\gg g_2$. Hence, we have enough freedom to bring the tree-level predictions (67), (68), (56), and (66) of our model into agreement with experimental data. However, these "predictions" have only a heuristic value, because they do not survive the classical quantization procedure. But there seems to be only a weak scale dependence.[18]

The simplest scalar product is given by $x=1$. In this case we get

$$m_W=\sqrt{\tfrac{1}{2}(1-\tfrac{1}{4}\cos^2\vartheta_1\cos^2\vartheta_2)}m_t,\quad \sqrt{\tfrac{1}{2}}m_t<m_W<\sqrt{\tfrac{3}{8}}m_t,$$

$$m_H=\sqrt{\frac{20\cos^2\vartheta_1+12\cos^2\vartheta_4\sin^4\vartheta_1}{12-3\cos^2\vartheta_1\cos^2\vartheta_2}}\,m_t\cos^2\vartheta_2<\sqrt{\tfrac{8}{3}}\,m_t,$$

$$\sin^2\theta_W=\tfrac{3}{8},\quad g_3=g_2. \tag{69}$$

These mass relations differ from the relations $m_t=2m_W$ and $m_H=3.14m_W$ obtained by Kastler and Schücker in Refs. 11 and 10 for the quaternionic K cycle, together with the simplest scalar product. While the m_W/m_t ratio is approximately stable, we get for the m_H/m_t ratio only an upper limit. Thus, we see that in comparison to the simplest model by Connes, Lott, and Kastler we get within our simplest model effectively one additional parameter determining the m_H/m_t ratio.

This means that although we introduced plenty of free parameters during the construction, these parameters occur in the final Lagrangians in the case of the simplest scalar product only in such combinations that we end up with nine parameters for the fermion masses, four parameters of the Kobayashi–Maskawa matrix, one undetermined coupling constant, and one additional parameter, which determines the ratio between the masses of the Higgs boson and the top quark. For this last parameter we have only an upper limit. Therefore, our model is less predictive than the model by Connes, Lott, and Kastler.

To summarize, the purpose of this paper was to present a different construction of the classical action of the standard model, which uses the simplest possible (nonclassical) algebra and puts the complexity into the module. In noncommutative geometry a K cycle replaces the notion of a manifold and a finite projective module over the algebra of this K cycle the notion of a vector bundle over this manifold. Therefore, our approach (a K cycle together with two associated modules—one for the electroweak sector and the other one for the chromodynamics sector) corresponds to a classical manifold with two associated fiber bundles over that manifold—a principal fiber bundle with structure group $SU(2)\times U(1)$ for the electroweak sector and a principal fiber bundle with structure group $SU(3)$ for the chromodynamics sector.

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Discrete Weyl–Heisenberg transforms

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The concepts of von Neumann lattices and tight frames are used for defining discrete quantum mechanical transforms in the phase plane. These transforms are obtained by finite shifts la and mb in the coordinate x and momentum p, respectively, of the Weyl–Heisenberg group, and they are called the discrete Weyl–Heisenberg transforms $\psi(la,mb)$. Here $ab=h/N$ with h the Planck constant, l and m integers, and N a positive integer. A construction is carried out of $\psi(la,mb)$ for a general Weyl–Heisenberg set by using the kq-representation, in which a useful formula is established for the frame operator. The construction is illustrated on an example of the ground state of a harmonic oscillator. It is shown that any physical quantity can be described by the discrete Weyl–Heisenberg transform. Connections are established between $\psi(la,mb)$, the Bargmann representation, and the Husimi distribution function. © *1996 American Institute of Physics.*
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In the early 1930s von Neumann[1] introduced a complete set of coherent states on a lattice in the phase plane with a unit cell of area h, the Planck constant. These states, in addition to forming a complete set, have also the attractive property of being well localized both in coordinate x and momentum p around each point la,mb on the lattice where a and b are constants with $ab=h$, and $l,m=0,\pm1,\pm2,...$, on the lattice. In 1946 Gabor[2] defined a similar set of states in the plane of time t and frequency ν with a unit cell of area 1. It has the same localization property for t and ν as the von Neumann set has with respect to x and p. This is, in principle, the same set of states which can therefore be called the von-Neumann–Gabor set.

The completeness of the von-Neumann–Gabor set (VNG set) was proven only in the 1970s.[3–5] It has, however, turned out[3,5] that the VNG set is over-complete by exactly one state: It remains complete if one state is removed, but ceases to be complete when more than one state is removed. This is a very unusual peculiarity which is characteristic to the VNG sets. It turns out that because of this peculiarity, expansions in such sets do not have good convergence properties.[6] In recent years an important contribution was made by Daubechies, Grossmann, and Meyer[7] who introduced the concept of frames for discrete sets in phase plane with $ab\leqslant h$. These latter sets are called the Weyl–Heisenberg sets (WH set), while the name VNG set is reserved here for the case when $ab=h$. It was shown in Ref. 7 that expansions in frames have good convergence properties and, as a consequence of this, frames have recently acquired much interest in signal processing.[8] The interest in the WH states stems from the fact that they carry simultaneous information about the coordinate and momentum (or time and frequency). As is well known one cannot construct in quantum mechanics wavefunctions $\psi(x,p)$ that depend on both the coordinate x and the momentum p, because this would be in violation of the uncertainty principle. In view of this restriction on the wavefunction, the approach of phase space distributions depending on x and p has developed in quantum mechanics, the most famous among them being the Wigner function.[9] These distributions are quadratic in the wavefunction and they carry some information on the simultaneous probability density for x and p. It should also, in principle, be possible to construct wavefunctions that depend on partial information about both x and p. An example of such a possibility is the kq-representation[10] in which the information about x is carried by the quasicoordinate q and the information about p by the quasimomentum $\hbar k$. Here q and k in the wavefunction $C(k,q)$ vary in a unit cell of the VNG lattice with area 2π, and they tell us where inside this cell x and $p/\hbar$ are,

but do not say anything about the number of cell (l,m). An alternative possibility would result if the wavefunction depended on l and m, $\psi(l,m)$, telling us in which unit cell x and p are, but saying nothing about their location inside the cell. Such a wavefunction $\psi(l,m)$ should then be in some sense a Fourier transform of the kq-wave function $C(k,q)$. To our knowledge no such wavefunction $\psi(l,m)$ has as yet been constructed, and one can even wonder whether such a wavefunction exists.

In this paper we use the concept of frames in signal processing[7] in order to construct what we call the discrete Weyl–Heisenberg transform $\psi(la,mb)$. The points (la,mb) are on the WH-lattice with $l,m=0,\pm1,\pm2,\ldots$. It is shown that for some special sets this discrete representation is closely related to a discrete subset of the Senitsky–Glauber coherent states[11] $|\alpha\rangle$. In constructing $\psi(la,mb)$ much use will be made of the elegant and powerful notion of tight frames.[7] The latter are defined in the following way. One first defines a frame: the WH-set is a frame if the frame operator F,

$$A \leqslant F \equiv \sum_{l,m=-\infty}^{\infty} |g_{lm}\rangle\langle g_{lm}| \leqslant B, \tag{1}$$

is bounded by two positive constants A and B, $A \leqslant F \leqslant B$; A and B are called the frame bounds. Here $|g_{lm}\rangle$ is a state of the set assigned to the cell (la,mb) of the lattice and in what follows it will be assumed that $ab=h/N$ with $N=1,2,\ldots$. One obtains a tight frame when the frame operator F in Eq. (1) is a multiple of the unit operator:

$$F=\sum_{l,m} |g_{lm}\rangle\langle g_{lm}| = AI. \tag{2}$$

Here A is a positive constant. An explicit construction is presented in this paper for WH tight frames with $A=1$:

$$\sum_{l,m} |g_{lm}\rangle\langle g_{lm}| = I. \tag{3}$$

Frames that satisfy this equation are called tight frames with bound 1. In quantum mechanics an equation of the type of Eq. (3) is usually obtained for an orthonormal basis. In Eq. (3), however, the states $|g_{lm}\rangle$ are not orthogonal, and as is known for them to satisfy Eq. (3), they cannot be normalized to one.[7] A full quantum mechanical framework is derived in this paper for these WH sets $|g_{lm}\rangle$ by using Eq. (3). This includes expressions for any operators, for their expectation values, etc. In other words, we construct in this paper what we call the discrete Weyl–Heisenberg transform $\psi(la,mb)$. It should be pointed out that originally the VNG set was built on coherent states.[1,11] This was later extended to cover any state in the Hilbert space and, correspondingly, it was called the Weyl–Heisenberg set.[12] In this paper a definition is presented of a quantum mechanical transform for a general WH tight frame and as a particular example the set of coherent states is considered.

Given a state $|g\rangle$ in Hilbert space, a Weyl–Heisenberg discrete set is defined in the following way. One uses the destruction a and creation a^+ operators and the constants α and α^*,

$$a=\frac{1}{\lambda\sqrt{2}}\left(x+i\frac{\lambda^2}{\hbar}p\right),\quad a^+=\frac{1}{\lambda\sqrt{2}}\left(x-i\frac{\lambda^2}{\hbar}p\right),$$
$$\alpha=\frac{1}{\lambda\sqrt{2}}\left(\bar{x}+i\frac{\lambda^2}{\hbar}\bar{p}\right),\quad \alpha^*=\frac{1}{\lambda\sqrt{2}}\left(\bar{x}-i\frac{\lambda^2}{\hbar}\bar{p}\right), \tag{4}$$

for defining the shift operator,

$$D(\alpha)=\exp(\alpha a^+-\alpha^* a), \tag{5}$$

and correspondingly the WH set,

$$|g_{la,mb}\rangle=D[\alpha(la,mb)]|g\rangle. \tag{6}$$

The following notations are used in Eqs. (4)–(6): λ, $\bar{x}$, and $\bar{p}$ are arbitrary constants,

$$\alpha(la,mb)=\frac{1}{\lambda\sqrt{2}}\left(la+i\frac{\lambda^2}{\hbar}mb\right), \tag{7}$$

while the constants a and b satisfy the relation

$$ab=\frac{h}{N},\quad N=1,2,3,\ldots, \tag{8}$$

where $l,m=0,\pm1,\pm2,\ldots$. When $N=1$, the set in Eq. (6) is the VNG set. It was proven in Ref. 7 that the set in Eq. (6) is a frame for $N\geqslant 2$. It is also known[13] that if $|g_{la,mb}\rangle$ is a frame [see Eqs. (1) and (6)], then

$$\frac{1}{F^{1/2}}|g_{la,mb}\rangle \tag{9}$$

is a tight frame with bound 1, where F is the frame operator [see Eq. (1)]. We are now going to present an explicit construction of the tight frame as given in Eq. (9) by using the kq-representation.[10] The wavefunctions $\psi(x)$ and $C(k,q)$ in the x and in the kq-representations, respectively, are related in the following way:

$$C^{(d)}(k,q)=\left(\frac{d}{2\pi}\right)^{1/2}\sum_n \exp(iknd)\psi(q-nd),\quad \psi(x)=\left(\frac{d}{2\pi}\right)^{1/2}\int_{-\pi/d}^{\pi/d}C^{(d)}(x,k)dk, \tag{10}$$

where d is an arbitrary constant. The basic operators x and p in this representation are[10]

$$x=i\frac{\partial}{\partial k}+q,\quad p=-i\hbar\frac{\partial}{\partial q}. \tag{11}$$

The kq-wave function $C^{(d)}(k,q)$ satisfies the following boundary conditions:

$$\exp(-ikd)C^{(d)}(k,q+d)=C^{(d)}\left(k+\frac{2\pi}{d},q\right)=C^{(d)}(k,q). \tag{12}$$

In signal processing $C(k,q)$ is called the Zak transform.[14] Bearing in mind the boundary condition (12) it will be convenient to write the shift operator $D[\alpha(la,mb)]$ as a product of two shift operators by splitting $\alpha(la,mb)$ in the following way:

$$\alpha(la,mb)=\alpha\left(l_1 d,m_1\frac{2\pi}{d}\hbar\right)+\alpha\left(l_2\frac{d}{L},m_2\frac{2\pi}{MD}\hbar\right), \tag{13}$$

where the αs are defined in Eq. (7), and where the integers are as follows

$$l=l_1L+l_2,\quad m=m_1M+m_2,\quad LM=N,\quad d=La. \tag{14}$$

Here $l_1,m_1=0,\pm1,\pm2,\ldots$, $l_2=0,1,\ldots L-1$, and $m_2=0,1,\ldots M-1$.

The frame operator F [Eq. (1)] in the kq-representation for the Weyl–Heisenberg set is[7,15]

$$\begin{aligned}\langle k,q|F|k',q'\rangle=&\sum_{l_1,m_1;l_{2,2}}\exp\left[-il_1(k-k')d+im_1(q-q')\frac{2\pi}{d}\right]\\&\times\left[D\left[\alpha\left(l_2\frac{d}{L},m_2\frac{2\pi}{Md}\hbar\right)\right]g^{(d)}(k,q)\right]^{*}D\left[\alpha\left(l_2\frac{d}{L},m_2\frac{2\pi}{Md}\hbar\right)\right]g^{(d)}(k',q')\\=&2\pi\sum_{l_2m_2}\left|g^{(d)}\left(k-\frac{2\pi}{Md}m_2,q-\frac{d}{L}l_2\right)\right|^2\\&\times\sum_{l_1}\delta\left(k-k'-\frac{2\pi}{d}l_1\right)\sum_{m_1}\delta(q-q'-dm_1),\end{aligned} \tag{15}$$

where we used the Poisson summation formula for distributions:[16]

$$\sum_l\exp(ildk)=\frac{2\pi}{d}\sum_l\delta\left(k-\frac{2\pi}{d}l\right). \tag{16}$$

What Eq. (15) actually means is that in the kq-representation the frame operator $F(k,q)$ is just the multiplication operator[13,17]

$$F(k,q)=2\pi\sum_{m_2=1}^{M}\sum_{l_2=1}^{L}\left|g^{(d)}\left(k-\frac{2\pi}{Md}m_2,q-\frac{d}{L}l_2\right)\right|^2. \tag{17}$$

When the WH set $|g_{la,mb}\rangle$ is a frame, one can use Eqs. (9) and (17) for constructing a tight frame. This can be done in the following way. According to Eq. (9) we define a new window function

$$\phi^{(d)}(k,q)=\frac{g^{(d)}(k,q)}{F^{1/2}(k,q)}. \tag{18}$$

We then have

$$\phi^{(d)}_{la,mb}(k,q)=D[\alpha(la,mb)]\phi^{(d)}(k,q)=\frac{g^{(d)}_{la,mb}(k,q)}{F^{1/2}(k,q)}, \tag{19}$$

where $F(k,q)$ is given by Eq. (17). For the case $N=2$ and when $g^{(d)}(k,q)$ is the ground state of a harmonic oscillator, this construction was explicitly carried out by Daubechies, Jaffard, and Journe.[18]

Having defined a WH tight frame $|\phi_{la,mb}\rangle$ we use it for a convenient decomposition of the unit operator I:

$$\sum_{l,m}^{\cdot} |\phi_{la,mb}\rangle\langle\phi_{la,mb}| = I. \tag{20}$$

From here any state $|\psi\rangle$ can be expanded in the following way:

$$|\psi\rangle = \sum_{l,m} \langle\phi_{la,mb}|\psi\rangle|\phi_{la,mb}\rangle. \tag{21}$$

Equations (20) and (21) look very much the same as in the case when $|\phi_{la,mb}\rangle$ is an orthonormal basis. However, the WH set $|\phi_{la,mb}\rangle$ is highly overcomplete (for $N\geq 2$) and not orthogonal. As a consequence of the overcompleteness the expansion in the set $|\phi_{la,mb}\rangle$ can be carried out with many other collections of coefficients c_{lm}:

$$|\psi\rangle = \sum_{l,m} c_{lm}|\phi_{la,mb}\rangle. \tag{22}$$

There is, however, a very special feature that the expansion coefficients $\langle\phi_{la,mb}|\psi\rangle$ in Eq. (21) possess. From the identity resolution [Eq. (20)] it follows that

$$\langle\psi|\psi\rangle = \sum_{l,m} |\langle\phi_{la,mb}|\psi\rangle|^2. \tag{23}$$

The special feature of $\langle\phi_{la,mb}|\psi\rangle$ is that among all the collections of c_{lm} in Eq. (22) for a given $|\psi\rangle$, the $\langle\phi_{la,mb}|\psi\rangle$ lead to a "minimal solution" [8,15]

$$\langle\psi|\psi\rangle = \sum_{l,m} |\langle\phi_{la,mb}|\psi\rangle|^2 \leq \sum_{l,m} |c_{lm}|^2. \tag{24}$$

The equality sign is reached only when $c_{lm} = \langle\phi_{la,mb}|\psi\rangle|$.

Based on this special feature of the expansion coefficients $\langle\phi_{la,mb}|\psi\rangle|$ in Eq. (21) we define the quantum mechanical discrete Weyl–Heisenberg transform $\psi^{(\phi)}(la,mb)$ for the function ϕ [see Eq. (18)] in the following way:

$$\psi^{(\phi)}(la,mb) \equiv \langle\phi_{la,mb}|\psi\rangle|. \tag{25}$$

Here $\psi^{(\phi)}(la,mb)$ contains partial information about x (via la) and partial information about p (via mb) with the pair (la,mb) specifying the cell in the phase plane around which ϕ_{lm} is localized [Eq. (19)]. What is very satisfying about this definition of $\psi^{(\phi)}(la,mb)$ is that for a normalized state, $\langle\psi|\psi\rangle = 1$,

$$P(la,mb) = |\psi(la,mb)|^2 \tag{26}$$

can be interpreted as giving the probability to find x and p in the cell (l,m) in phase plane. This is so because from Eqs. (23) and (25) it follows that

$$\sum_{l,m} P(la,mb) = \sum_{l,m} |\psi(la,mb)|^2 = 1 \tag{27}$$

as is required from a probability distribution.

It is to be pointed out that despite satisfying the probability requirement in Eq. (27), the discrete Weyl–Heisenberg transform $\psi(la,mb)$ cannot be given the interpretation of a wavefunction in quantum mechanics. The main reason for this is that la and mb are not eigenvalues of

some commuting physical observables. The situation is very much like that with coherent states $|\alpha\rangle$, when $\langle\alpha|\psi\rangle$ gives some probability information of the distribution of x and p in the state $|\psi\rangle$, but it can nevertheless not be interpreted as a wavefunction.

Before showing how the transform $\psi(la,mb)$ can be used for representing operators and expectation values, let us first work out an example. As an important illustration of $\psi(la,mb)$ we give in what follows an explicit construction of it for the case when $|g\rangle$ is the ground state of a Harmonic oscillator:

$$\langle x|g_0\rangle=\left(\frac{1}{\pi\lambda^2}\right)^{1/4}\exp\left(-\frac{x^2}{2\lambda^2}\right). \tag{28}$$

In the kq-representation this function is[6] [see Eq. (10) above]

$$g_0^{(d)}(k,q)=\left(\frac{d}{2\pi^{3/2}\lambda}\right)^{1/2}\exp\left(-\frac{q^2}{2\lambda^2}\right)\theta_3\left(\frac{kd}{2}-i\,\frac{qd}{2\lambda^2}\,\middle|\,i\,\frac{d^2}{2\pi\lambda^2}\right), \tag{29}$$

where θ_3 is the Jacobi Theta function[19]

$$\theta_3(z|\tau)=\sum_n e^{2izn+i\pi\tau n^2}. \tag{30}$$

For constructing the tight WH frame [Eq. (19)] we have to find the frame operator $F(k,q)$ [Eq. (17)]. For this purpose one can use the known formulas from VNG lattices[20] for any kq-function $g^{(d)}(k,q)$:

$$2\pi|g^{(d)}(k,q)|^2=\sum_{m,n}(-1)^{mn}\langle q_{md,\hbar(2\pi/d)n}|g\rangle\exp\left(i\,\frac{2\pi}{d}\,qm-idkm\right). \tag{31}$$

By using this formula, the summation on l_2,m_2 in Eq. (17) gives the following result for the frame operator $F(k,q)$:

$$F(k,q)=N\sum_{m,n}(-1)^{mnN}\langle g_{mLd,nM(2\pi/d)\hbar}|g\rangle\exp\left(i\,\frac{2\pi}{d}\,qmL-ikdnM\right), \tag{32}$$

where $N=LM$ [Eq. (14)]. This is a useful expression for the frame operator $F(k,q)$ in the kq-representation for any $g^{(d)}(k,q)$. For the ground state of the harmonic oscillator [Eqs. (28) and (29)], the operator $F(k,q)$ becomes[20]

$$F_0(k,q)=N\sum_{m,n}(-1)^{mnN}\exp\left\{-\frac{d^2}{4\lambda^2}\left[(nM)^2+\left(\frac{2\pi\lambda^2}{d^2}\right)^2(mL)^2\right]\right\}\exp\left(i\,\frac{2\pi}{d}\,qmL-ikdnM\right). \tag{33}$$

This is a very simple formula which becomes even simpler for the symmetric case of

$$N=L^2=M^2\equiv S^2 \quad\text{and}\quad \frac{2\pi\lambda^2}{d^2}=1. \tag{34}$$

We then have

$$F_0^{(N)}(k,q)=N\sum_{m,n}(-1)^{mnN}\exp\left[-\frac{N\pi}{2}(m^2+n^2)\right]\exp\left(i\,\frac{2\pi}{d}\,qmS-ikdnS\right). \tag{35}$$

Thus, for $N=4$, $F_0^{(4)}(k,q)$ becomes [see Eq. (30)]

$$F_0^{(4)}(k,q)=4\theta_3\left(2\pi\frac{q}{d}\middle|2i\right)\theta_3(kd|2i). \tag{36}$$

The frame operators in Eqs. (35) and (36) are very smooth functions of the k and q variables and they have the very good feature that their bounds [see Eq. (1)] A and B are close to one another. Thus, already for $N=4$ [Eq. (36)] one can check by using numerical values for θ_3-functions[19] that

$$A=3.970, \quad B=4.030, \quad \frac{B-A}{B+A}=0.0074. \tag{37}$$

This ratio goes rapidly down for $N>4$. One can therefore assume to a good approximation that the frame operator $F_0^{(N)}(k,q)\approx N$ for $N\geq 4$. It follows that for the symmetric case [Eq. (34)] the tight frame $(\phi_0^{(d)})_{la,mb}(k,q)$ for the ground state of a harmonic oscillator differs from the frame $(g_0^{(d)})_{la,mb}(k,q)$ only by the constant factor $S(N=S^2)$,

$$(\phi_0^{(d)})_{la,mb}(k,q)=\frac{1}{S}(g_0^d)_{la,mb}(k,q), \tag{38}$$

where a and b are defined in Eqs. (7) and (8). Also in this approximation the frame operator $F_0^{(N)}\approx N$ gives the number of the WH set states in a unit cell of the VNG lattice. For the ground state of the harmonic oscillator, we actually return to the original von Neumann coherent states[1,11] and correspondingly we can use the notation [see Eq. (38)]

$$(\phi_0^{(d)})_{la,mb}(k,q)\approx\frac{1}{S}\langle k,q|\alpha(la,mb)\rangle, \tag{39}$$

where $|\alpha(la,mb)\rangle$ is a coherent state[11] with $\alpha(la,mb)\rangle$ given in Eq. (7). What should, however, be pointed out is that the WH set $|\alpha(la,mb)\rangle$ is a frame, while $(\phi_0^{(d)})_{la,mb}$ is, to a "good approximation," a tight frame.

Having the result in Eq. (39), it is easy to write down the discrete Weyl–Heisenberg transform $\psi^{(g_0)}(la,mb)$ for any state $|\psi\rangle$. The superscript g_0 indicates that the ground state of the harmonic oscillator was used [see Eq. (28)] for constructing the Weyl–Heisenberg set. We have

$$\psi^{(g_0)}(la,mb)\approx\frac{1}{S}\langle\alpha(la,mb)|\psi\rangle. \tag{40}$$

As is well know the bracket on the right-hand side of Eq. (40) can be written as follows:

$$\langle\alpha(la,mb)|\psi\rangle=\exp(-\tfrac{1}{2}|\alpha(la,mb)|^2)\psi[\alpha^*(la,mb)], \tag{41}$$

where $\psi(\alpha^*)$ for continuous α is an analytic function of α^* and it is known as the Bargmann representation[21] of $|\psi\rangle$. Thus for the nth harmonic oscillator state $|\psi_n\rangle$, Eq. (40) becomes

$$\psi_{(n)}^{(g_0)}(la,mb)\approx\frac{1}{S}\exp\left(-\frac{1}{2}|\alpha(la,mb)|^2\right)\frac{\alpha^{*n}(la,mb)}{\sqrt{n!}}. \tag{42}$$

The probability distribution for this state will correspondingly be [see Eq. (26)]

$$P_n^{(g_0)}(la,mb)=|\psi_n^{(g_0)}(la,mb)|^2\approx\frac{1}{N}\exp(-|\alpha(la,mb)|^2)\frac{|\alpha(la,mb)|^{2n}}{n!}$$
$$=\frac{1}{N}\exp\left[-\pi\left(\frac{l^2}{L^2}+\frac{m^2}{M^2}\right)\right]\frac{\pi^n(l^2/L^2+m^2/M^2)^n}{n!}, \tag{43}$$

where Eqs. (7), (8), and (34) were used. This is a simple function which can be interpreted as giving the probability of finding x and p in the cell $la,mb(ab=h/N)$ in the state $|\psi_n\rangle$.

Equation (40) gives an approximate relation between the discrete Weyl–Heisenberg transform $\psi(la,mb)$ and the Bargmann representation $\langle\alpha(la,mb)|\psi\rangle$ of the state $|\psi\rangle$.

In the case of coherent states, the continuous transform $\langle\alpha|\psi\rangle$ [Eq. (41)] was used by Husimi[22] to define a phase space distribution function $P_H(x,p)$ which carries his name and which is connected to the Wigner function in the following way:[22]

$$P_H(x,p)=\frac{1}{2\pi\hbar}\langle\alpha|\psi\rangle|^2=\int W_{g_0}(x-x',p-p')W_\psi(x',p'),dx'dp', \tag{44}$$

where g_0 is given in Eq. (28) and where the Wigner function for any $\psi(x)$ is[9]

$$W(x,p)=\frac{1}{2\pi\hbar}\int\exp\left(-\frac{i}{\hbar}pz\right)\psi^*\left(x-\frac{1}{2}z\right)\psi\left(x+\frac{1}{2}z\right)dz. \tag{45}$$

Following the definition in Eq. (44), one can consider $P(la,mb)$ in Eq. (26) as being an extension of the Husimi distribution to any WH tight frame with the window function of ϕ. In the particular case when ϕ corresponds to the ground state of a harmonic oscillator [Eq. (39)], the discrete Husimi distribution becomes [see Eqs. (40) and (44)]

$$P^{(g_0)}(la,mb)\approx\frac{1}{N}|\langle\alpha(la,mb)|\psi\rangle|^2=\frac{2\pi\hbar}{N}\int W_{g_0}(la-x',mb-p')W_\psi(x',p')dx'dp'. \tag{46}$$

When $|\psi\rangle$ is the nth harmonic oscillator state $|\psi_n\rangle$, the discrete Husimi distribution is given by Eq. (43). This completes the description of the illustrative example for the Weyl–Heisenberg tight frame built on the ground state of a harmonic oscillator. In summing up this example it should be pointed out that the discrete Weyl–Heisenberg transform $\psi^{(g_0)}(la,mb)$ can be easily used in view of its relation to the coherent state amplitude $\langle\alpha(la,mb)|\psi\rangle$ as given by Eq. (40).

We now show how the WH transform $\psi(la,mb)$ can be used in the general framework of quantum mechanics. For this we show how to represent any operator $\hat{O}$ by using this transform. Given a matrix element $\langle\psi_i|\hat{O}|\psi_j\rangle$ of the operator $\hat{O}$ between the states $|\psi_i\rangle$ and $|\psi_j\rangle$ one can use the unit operator decomposition formula [Eq. (20)] to find

$$\langle\psi_i|\hat{O}|\psi_j\rangle=\sum_{l,m,l',m'}\langle\psi_i||\phi_{la,mb}\rangle\langle\phi_{la,mb}|\hat{O}|\phi_{l'a,m'b}\rangle\langle\phi_{l'a,m'b}|\psi_j\rangle$$
$$=\sum_{l,m,l',m'}\psi_i^{(\phi)*}(la,mb)\langle\phi_{la,mb}|\hat{O}|\phi_{l'a,m'b}\rangle\psi_j^{(\phi)*}(l'a,m'b). \tag{47}$$

When $i=j$, this formula gives the expectation value of $\hat{O}$ in the state $|\psi_i\rangle$ expressed via the discrete Weyl–Heisenberg transform $\psi_i^{(\phi)}(la,mb)$ and the matrix elements $\langle\phi_{la,mb}|\hat{O}|\phi_{l'a,m'b}\rangle$. In the case when the WH tight frame is built on the ground state of the harmonic oscillator, one can use Eq. (39) and (40) in order to simplify the general expression in Eq. (47). We see therefore that any quantity in quantum mechanics is expressible via the discrete WH transform $\psi(la,mb)$.

In conclusion, in this paper a quantum mechanical transform is defined, called the discrete Weyl–Heisenberg transform, which carries simultaneous information of the coordinate and momentum in a given state $|\psi\rangle$. This information is extracted by forming a scalar product of $|\psi\rangle$ with a discrete Weyl–Heisenberg set $|\phi_{la,mb}\rangle$ in the phase plane, where la and mb give the coordinate x and the momentum p, respectively (l and m being integers). When $|\phi_{la,mb}\rangle$ is chosen to be a tight frame with bound 1, the $\psi(la,mb)=\langle\phi_{la,mb}|\psi\rangle$ is then the discrete Weyl–Heisenberg transform. The $\psi(la,mb)$ is reminiscent of the Bargmann representation in quantum mechanics[22] and the windowed Fourier transform in signal processing.[23] In the latter case the simultaneous information is about time and frequency.

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On the Green-functions technique and phase velocity approximation of axially symmetric fields in stratified media

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In this paper a numerical method is developed to solve a one-dimensional inverse scattering problem associated with a pair of two coupled partial differential equations. These equations are for the Green functions that can be used for the optimization of electromagnetic energy within selected regions of a medium in which the propagation is taking place. The method is based upon constructing the Nth degree interpolation polynomial to approximate the Green functions and the phase velocity function using Legendre–Gauss–Lobatto collocation points. An example is given to demonstrate the accuracy of the developed method. © *1996 American Institute of Physics.* [S0022-2488(96)01907-X]

I. INTRODUCTION

Decomposition of the total electromagnetic field which is propagating through an inhomogeneous medium into two components traveling in opposite directions is referred to as wave splitting technique. This technique along with the invariant technique is applied to the solution of inverse problems. Wave splitting and invariant imbedding techniques are presented in Refs. 1–4. Two related methods of the Green functions based upon wave splitting are introduced in Refs. 5 and 6. In general, they are formulated in the form of an inverse problem and described by a set of linear coupled partial differential equations. This problem is also addressed in Refs. 7 and 8. It has been shown in Ref. 9 that the wave-splitting Green function approach to the one-dimensional electromagnetic inverse problem is a well-posed inverse problem.

In Ref. 5 an electromagnetic plane wave impinging normally on a one-dimensional dissipative medium is characterized by spatially varying permittivity and conductivity profiles. Furthermore, a technique that maximizes the electromagnetic energy within a specified region of the medium is introduced. This is accomplished through the application of the Green functions technique. This technique is distinctively different by contrast from the invariant imbedding method. It yields the fields inside the inhomogeneous medium where the boundary values of the Green functions are the scattering kernels for the physical scattering geometry. This connection provides an alternative and efficient approach to obtain the scattering kernels. It is utilized in Refs. 10 and 11 to produce such kernels and the Green functions for an oblique incidence on a plasma and a point source excitation of a half-space, respectively. The Green functions are used to represent a time-averaged electromagnetic energy in regions within a medium by a weakly continuous functional for the purpose of optimization of the electromagnetic energy as suggested in Ref. 12. A higher dimension of this Green functions technique is suggested in Ref. 6 for the application to the treatment of cancer cells in the human body without the destruction of the surrounding healthy tissue. A time domain inverse scattering problem is regarded in Ref. 6 for axially symmetric electromagnetic fields in a stratified slab. The axial symmetry of the field is promoted through a Hankel transform

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which results in a one-dimensional wave equation to which wave splitting is applied. The inverse scattering problem is formulated in the form of a pair of two coupled partial differential equations in which the Green functions are present where they are functions of time and displacement. In this paper the one-dimensional inverse problem for the case of nonconductive and dielectric stratified medium is considered. We are solving this inverse problem and generating the Green functions and the phase velocity from the knowledge of the reflection kernels. Our approach is based on a spectral collocation method (pseudospectral method[13]) in which we construct the Nth degree interpolating polynomials to approximate the Green functions and the phase velocity of the medium. These polynomials are defined through the use of Legendre–Gauss–Lobatto points as collocation points and Lagrange polynomials as trial functions.

The paper is organized as follows: In Sec. II we describe the basic formulation of the pseudospectral Legendre method required for our subsequent development. Section III is devoted to the formulation of the inverse scattering problem. In Sec. IV, the proposed method is used to approximate the Green functions and the phase velocity function. In Sec. V, we report our numerical finding and demonstrate the efficiency and the accuracy of the proposed numerical scheme.

II. PSEUDOSPECTRAL LEGENDRE METHOD

Let $L_N(t)$, $-1\leqslant t\leqslant 1$ denote the Legendre polynomial of order N, then the Legendre–Gauss–Lobatto nodes are defined in Ref. 13 by

$$t_0=-1, \quad t_N=1, \quad t_m \text{ are the zeros of } L'_N(t),$$
$$1\leqslant m\leqslant N-1, \tag{1}$$

where $L'_N(t)$ denotes the first derivative of $L_N(t)$. No explicit formula of the nodes in Eq. (1) is known, however, they can be computed numerically. Define the polynomial approximation of $F(t)$ by

$$F^N(t)=\sum_{l=0}^{N} b_l\phi_l(t), \tag{2}$$

where

$$\phi_h(t)=\frac{1}{N(N+1)L_N(t_h)}\cdot\frac{(t^2-1)L'_N}{(t-t_h)}, \quad h=0,1,\ldots,N, \tag{3}$$

are Lagrange polynomials of order h, with the property

$$\phi_h(t_j)=\delta_{hj}=\begin{cases}0 & \text{if } h\neq j\\ 1 & \text{if } h=j\end{cases} \tag{4}$$

therefore $F^N(t_h)=b_h$. For the accuracy of pseudospectral Legendre approximation and error at the collocation points refer to Ref. 13.

III. PROBLEM FORMULATION

The inverse scattering problem is formulated in Ref. 6 as a pair of two coupled partial differential equations as

$$\frac{\partial}{\partial z}\begin{bmatrix}G_{11}\\ G_{21}\end{bmatrix}=\frac{2}{c}\frac{\partial}{\partial t}\begin{bmatrix}0\\ G_{21}\end{bmatrix}+a^+(0,z)\begin{bmatrix}-(A+B)\\ B\end{bmatrix}$$

$$+\begin{bmatrix} -\frac{1}{2}(bc-c_z/c)-(A+B)* & -c_z/2c+B* \\ -c_z/2c+B* & \frac{1}{2}(bc+c_z/c)+(A-B)* \end{bmatrix}\cdot\begin{bmatrix} G_{11} \\ G_{21} \end{bmatrix}, \tag{5}$$

$$\frac{\partial}{\partial z}\begin{bmatrix} G_{22} \\ G_{12} \end{bmatrix}=-\frac{2}{c}\frac{\partial}{\partial t}\begin{bmatrix} 0 \\ G_{12} \end{bmatrix}+a^{-}(z,L)\begin{bmatrix} (A-B) \\ B \end{bmatrix}$$

$$+\begin{bmatrix} \frac{1}{2}(bc+c_z/c)+(A-B)* & -c_z/2c+B* \\ -c_z/2c+B* & -\frac{1}{2}(bc-c_z/c)-(A+B)* \end{bmatrix}\cdot\begin{bmatrix} G_{22} \\ G_{12} \end{bmatrix}. \tag{6}$$

z represents depth in the medium, t represents time, $G_{ij}(i,j=1,2)$ are the Green functions and the asterisk represents a convolution in time. The convolution in time of two functions $r(z,t)$ and $s(z,t)$ is

$$r(z,t)*s(z,t)=\int_0^t r(z,x)s(z,t-x)dx.$$

c is the phase velocity of the electromagnetic field in the medium and the function $b(z)$ is related to the conductivity of the medium, $\sigma(z)$, through the equation

$$b(z)=\sigma(z)\mu_0, \tag{7}$$

where μ_0 is the permeability in vacuum. Since we are considering the nonconductive case, the function $b(z)$ is zero. It is given in Ref. 6 that

$$A(z,t)=(a_1/c)\left[J_1(a_1t)\frac{e^{-b_1t}}{t}\right], \tag{8}$$

$$D(z,t)=c^2e^{-b_1t}\cos(a_1t), \tag{10}$$

$$C(z,t)=(c^2/a_1)\sin(a_1t)e^{-b_1t}. \tag{11}$$

$J_1(x)$ is the Bessel function of the first kind of order one and κ is the Hankel transform parameter

$$B(z,t)=(c_z/2c)\kappa^2C(z,t)+\tfrac{1}{2}c_1[D(z,t)-b_1C(z,t)]. \tag{9}$$

This medium is inhomogeneous, of a known thickness and bounded with two known homogeneous media. The parameters $b_1,a_1,c_1,a^{+}(0,z),a^{-}(z,L)$ are functions of the electromagnetic properties of the medium, they are given in Ref. 6. For the case considered in this paper $b_1=c_1=0$ and

$$a_1=c\kappa, \tag{12}$$

$$a^{+}(0,z)=\sqrt{c(z)/c(0)}, \tag{13}$$

$$a^{-}(z,L)=\sqrt{c(z)/c(L)}. \tag{14}$$

L is the thickness of the medium. Thus the region $0\leqslant z\leqslant L$ is inhomogeneous and the regions $z<0$ and $z>L$ are homogeneous. Initial and boundary conditions on the Green functions are

$$G_{12}(z,0)=-\tfrac{1}{4}a^{-}(z,L)c_z, \tag{15}$$

$$G_{21}(z,0)=\tfrac{1}{4}a^{+}(0,z)c_z, \tag{16}$$

$$G_{11}(0,t)=0, \tag{17}$$

$$G_{21}(L,t)=0, \quad t>0, \tag{18}$$

$$G_{22}(L,t)=0, \quad t>0, \tag{19}$$

$$G_{12}(0,t)=0, \quad t>0. \tag{20}$$

IV. APPLICATION OF LEGENDRE–GAUSS–LOBATTO METHOD TO APPROXIMATE THE GREEN-FUNCTIONS AND THE PHASE VELOCITY FUNCTION

In order to apply Legendre–Gauss–Lobatto nodes and solve the inverse scattering problem we introduce the following transformations:

$$z=\frac{L}{2}(1+\alpha), \tag{21}$$

$$t=\frac{T}{2}(1+\beta). \tag{22}$$

The values of α and β are in the interval $[-1,1]$. T is the duration of the reflection scattering kernels $R^{\pm}(0,L,t)$. These two kernels are related to the phase velocity and the Green functions as[6]

$$R^{+}(z,L,t)_{\substack{|z=0\\ t=0}}=\tfrac{1}{4}c_z|_{z=0}. \tag{23}$$

$$G_{21}(0,t)=R^{+}(0,L,t), \tag{24}$$

$$R^{-}(z,L,t)_{\substack{|z=0\\ t=0}}=-\tfrac{1}{4}c_z|_{z=L}, \tag{25}$$

$$G_{12}(L,t)=R^{-}(0,L,t). \tag{26}$$

In general, the inputs to this method are the reflection kernels $R^{\pm}(0,L,t)$ and no information on the transmission kernels $T^{\pm}(z,L,t)$ is required. However, for the case considered in this paper the input is $R^{+}(0,L,t)$. Define the approximation of the function $A(z,t)$ as

$$A^{N}(\alpha,\beta)=\sum_{i=0}^{N}\sum_{j=0}^{N}a_{ij}\phi_i(\alpha)\phi_j(\beta), \tag{27}$$

where the a's are the coefficients and the functions ϕ_i are given in Eq. (3). Similar definitions for the function $B(z,t)$ and the Green functions $G_{11}(z,t)$, $G_{21}(z,t)$, $G_{22}(z,t)$, and $G_{12}(z,t)$ are formulated with the coefficients b, γ, θ, ζ, and η, respectively. The phase velocity function, $c(z)$, is assumed continuously differentiable within the medium. We define its approximation as

$$c^{N}(\alpha)=\sum_{i=0}^{N}\lambda_i\phi_i(\alpha). \tag{28}$$

The differentiations of $G^{N}{}_{11}(\alpha,\beta)$ with respect to α and β are

$$G_{11}{}^{N}(\alpha,\beta)_{\alpha}=\sum_{i=0}^{N}\sum_{j=0}^{N}\gamma_{ij}\phi'_i(\alpha)\phi_j(\beta), \tag{29}$$

$$G_{11}{}^{N}(\alpha,\beta)_{\beta}=\sum_{i=0}^{N}\sum_{j=0}^{N}\gamma_{ij}\phi_i(\alpha)\phi'_j(\beta). \tag{30}$$

Equations similar to Eqs. (29) and (30) can be generated for the other Green functions. Considering the nonconductive case and applying the approximations of the functions A, B, c, G_{11}, G_{21} and the corresponding derivatives of the last two functions to the coupled partial differential equations in Eq. (5) we get

$$\begin{aligned}
&\frac{2}{L}\sum_{i=0}^{N}\sum_{j=0}^{N}\gamma_{ij}\phi'_i(\alpha)\phi_j(\beta)\\
&\quad=-\sqrt{\frac{\Sigma_{i=0}^{N}\lambda_i\phi_i(\alpha)}{\lambda_0}}\cdot\left\{\sum_{i=0}^{N}\sum_{j=0}^{N}a_{ij}\phi_i(\alpha)\phi_j(\beta)+\sum_{i=0}^{N}\sum_{j=0}^{N}b_{ij}\phi_i(\alpha)\phi_i(\beta)\right\}\\
&\qquad+\frac{1}{2}\frac{\Sigma_{i=0}^{N}\lambda_i\phi'_i(\alpha)}{\Sigma_{i=0}^{N}\lambda_i\phi_i(\alpha)}\cdot\sum_{i=0}^{N}\sum_{j=0}^{N}\gamma_{ij}\phi_i(\alpha)\phi_j(\beta)\\
&\qquad-\left\{\sum_{i=0}^{N}\sum_{j=0}^{N}a_{ij}\phi_i(\alpha)\phi_j(\beta)+\sum_{i=0}^{N}\sum_{j=0}^{N}b_{ij}\phi_i(\alpha)\phi_i(\beta)\right\}*\sum_{i=0}^{N}\sum_{j=0}^{N}\gamma_{ij}\phi_i(\alpha)\phi_j(\beta)\\
&\qquad-\frac{1}{2}\frac{\Sigma_{i=0}^{N}\lambda_i\phi'_i(\alpha)}{\Sigma_{i=0}^{N}\lambda_i\phi_i(\alpha)}\cdot\left[\sum_{i=0}^{N}\sum_{j=0}^{N}\theta_{ij}\phi_i(\alpha)\phi_j(\beta)\right]\\
&\qquad+\left\{\sum_{i=0}^{N}\sum_{j=0}^{N}b_{ij}\phi_i(\alpha)\phi_i(\beta)\right\}*\left[\sum_{i=0}^{N}\sum_{j=0}^{N}\theta_{ij}\phi_i(\alpha)\phi_j(\beta)\right]
\end{aligned} \tag{31}$$

and

$$\begin{aligned}
&\frac{2}{L}\sum_{i=0}^{N}\sum_{j=0}^{N}\theta_{ij}\phi'_i(\alpha)\phi_j(\beta)\\
&\quad=\frac{4}{T\cdot\Sigma_{i=0}^{N}\lambda_i\phi_i(\alpha)}\cdot\sum_{i=0}^{N}\sum_{j=0}^{N}\theta_{ij}\phi_i(\alpha)\phi'_j(\beta)+\sqrt{\frac{\Sigma_{i=0}^{N}\lambda_i\phi_i(\alpha)}{\lambda_0}}\\
&\qquad\times\sum_{i=0}^{N}\sum_{j=0}^{N}b_{ij}\phi_i(\alpha)\phi_i(\beta)-\frac{1}{2}\frac{\Sigma_{i=0}^{N}\lambda\ \ _i\phi'_i(\alpha)}{\Sigma_{i=0}^{N}\lambda_i\phi_i(\alpha)}\cdot\sum_{i=0}^{N}\sum_{j=0}^{N}\gamma_{ij}\phi_i(\alpha)\phi_j(\beta)\\
&\qquad+\sum_{i=0}^{N}\sum_{j=0}^{N}b_{ij}\phi_i(\alpha)\phi_i(\beta)*\sum_{i=0}^{N}\sum_{j=0}^{N}\gamma_{ij}\phi_i(\alpha)\phi_j(\beta)\\
&\qquad+\frac{1}{2}\frac{\Sigma_{i=0}^{N}\lambda_i\phi'_i(\alpha)}{\Sigma_{i=0}^{N}\lambda_i\phi_i(\alpha)}\sum_{i=0}^{N}\sum_{j=0}^{N}\theta_{ij}\phi_i(\alpha)\phi_j(\beta)+\left\{\sum_{i=0}^{N}\sum_{j=0}^{N}a_{ij}\phi_i(\alpha)\phi_i(\beta)\right.\\
&\qquad\left.-\sum_{i=0}^{N}\sum_{j=0}^{N}b_{ij}\phi_i(\alpha)\phi_i(\beta)\right\}*\left[\sum_{i=0}^{N}\sum_{j=0}^{N}\theta_{ij}\phi_i(\alpha)\phi_j(\beta)\right].
\end{aligned} \tag{32}$$

At the Legendre–Gauss–Lobatto nodes $\alpha=\alpha_n$ and $\beta=\beta_m$ Eqs. (31) and (32) reduce to

$$\frac{2}{L}\sum_{i=0}^{N}\gamma_{im}\phi'_i(\alpha_n)$$

$$=-\sqrt{\frac{\lambda_n}{\lambda_0}}\cdot\{a_{nm}+b_{nm}\}+\frac{1}{2}\frac{\Sigma_{i=0}^{N}\lambda_i\phi'_i(\alpha_n)}{\lambda_n}\cdot\gamma_{nm}-\frac{T}{2}(1+\beta_m)$$
$$\times\sum_{j=0}^{N}a_{nj}\sum_{q=0}^{N}\gamma_{nq}\int_{-1}^{1}\phi_j(u)\phi_q(u)du-\frac{T}{2}(1+\beta_m)$$
$$\times\sum_{j=0}^{N}b_{nj}\sum_{q=0}^{N}\gamma_{nq}\int_{-1}^{1}\phi_j(u)\phi_q(u)du-\frac{1}{2}\frac{\Sigma_{i=0}^{N}\lambda_i\phi'_i(\alpha_n)}{\lambda_n}\cdot\theta_{nm}+\frac{T}{2}(1+\beta_m)$$
$$\times\sum_{j=0}^{N}b_{nj}\sum_{q=0}^{N}\theta_{nq}\int_{-1}^{1}\phi_j(u)\phi_q(u)du, \tag{33}$$

and

$$\frac{2}{L}\sum_{i=0}^{N}\theta_{im}\phi'_i(\alpha_n)$$

$$=\frac{4}{T\cdot\lambda_n}\cdot\sum_{j=0}^{N}\theta_{nj}\phi'_j(\beta_m)+\sqrt{\frac{\lambda_n}{\lambda_0}}\cdot b_{nm}-\frac{1}{2}\frac{\Sigma_{i=0}^{N}\lambda_i\phi'_i(\alpha_n)}{\lambda_n}\cdot\gamma_{nm}+\frac{T}{2}(1+\beta_m)$$
$$\times\sum_{j=0}^{N}b_{nj}\sum_{q=0}^{N}\gamma_{nq}\int_{-1}^{1}\phi_j(u)\phi_q(u)du+\frac{1}{2}\frac{\Sigma_{i=0}^{N}\lambda_i\phi'_i(\alpha_n)}{\lambda_n}\cdot\theta_{nm}+\frac{T}{2}(1+\beta_m)$$
$$\times\sum_{j=0}^{N}a_{nj}\sum_{q=0}^{N}\theta_{nq}\int_{-1}^{1}\phi_j(u)\phi_q(u)du-\frac{T}{2}(1+\beta_m)$$
$$\times\sum_{j=0}^{N}b_{nj}\sum_{q=0}^{N}\theta_{nq}\int_{-1}^{1}\phi_j(u)\phi_q(u)du, \tag{34}$$

where

$$a_{hg}=\frac{\kappa}{\frac{T}{2}(1+\beta_g)}\cdot J_1\left[\lambda_h\kappa\frac{T}{2}(1+\beta_g)\right], \tag{35}$$

$$b_{hg}=\frac{\kappa}{\lambda_h}\sum_{i=0}^{N}\lambda_i\phi'_i(\alpha_h)\cdot\sin\left[\lambda_h\kappa\frac{T}{2}(1+\beta_g)\right]. \tag{36}$$

Applying Eqs. (16)–(18) and (23)–(25) along with

$$4R^{+}(-1,1,-1)=\sum_{i=0}^{N}\lambda_i\phi'_i(-1) \tag{37}$$

to Eqs. (33) and (34) a set of algebraic equations is generated. In this case the inverse scattering problem is solved where the number of the unknown coefficients λ_{ij}, θ_{ij}, and γ_{ij} is equal to that of the algebraic equations which is $2N^2+N+1$. The coupled partial differential equations given in

TABLE I. Approximate and exact values of the phase velocity function.

α_n $0\leq n\leq 9$	Approximate (no noise) $c^9(\alpha_n)$	Approximate (with noise) $c^9(\alpha_n)$	Exact $c(\alpha_n)$
−1.000 000	282.094 72	282.101 22	282.094 79
−0.919 534	276.559 67	277.435 01	276.559 60
−0.738 774	265.288 24	264.377 63	265.288 21
−0.477 925	251.535 41	251.533 12	251.535 44
−0.165 290	238.362 25	238.361 06	238.362 20
0.165 290	227.704 25	227.703 83	227.704 26
0.477 925	220.236 72	220.235 88	220.236 76
0.738 774	215.709 06	215.689 63	215.709 04
0.919 534	213.403 41	213.325 87	213.403 45
1.000 000	212.585 93	212.422 63	212.585 91

Eq. (6) are discretized in the same fashion, however, this time the components of the phase velocity at the collocation points are already known from the solution of Eq. (5). Consequently, the direct problem is solved and the remaining coefficients ζ_{ij} and η_{ij} are generated. As a result the Green functions along with components of the phase velocity function are available at the collocation points.

V. AN ILLUSTRATIVE EXAMPLE

We selected an inhomogeneous medium of a known permittivity profile. The medium was of thickness $L=0.1$ m and conductivity $\sigma(z)=0$, where z represents depth in the medium. Then we assumed that a known one sided, down-going electromagnetic wave was incident on the medium from the top. The reflected electromagnetic data at the interface $z=0$ was assumed to be of a finite period of time $T=0.1$ s. Using a specific value of the Hankel transform parameter $\kappa=0.1$ m^{-1} and the pseudospectral Legendre approach, we solved the direct problem which is in the form of partial differential equations in Ref. 6 for the reflection kernel $R^+(0,0.1,t;0.1)$. This reflection kernel was used as an input to the method presented in this paper to solve the inverse problem. Values of the Green functions and the phase velocity function at the collocation points with $N=9$ were generated. Approximate and exact values of the phase velocity at the collocation points are listed in Table I. To illustrate how the method reconstructs the phase velocity profile with noisy data, Gaussian noise with STD=0.05 was added to the reflection kernel $R^+(0,0.1,t;0.1)$. This corresponds to a signal to noise ratio of 5.4 as suggested in Ref. 14. The Green functions $G_{11}(z,t)$ and $G_{21}(z,t)$ that corresponds to the data with no noise are given in Figs. 1 and 2, respectively. Using the same value of the Hankel transform parameter $\kappa=0.1$ m^{-1}, we applied the pseudospec-

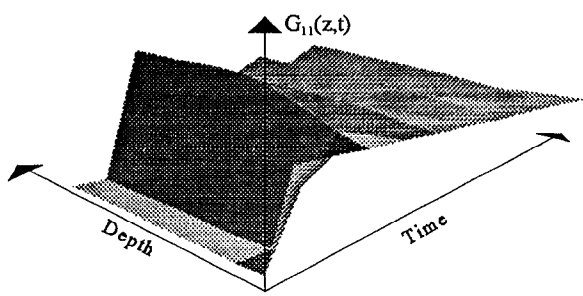

FIG. 1. The Green function $G_{11}(z,t)$.

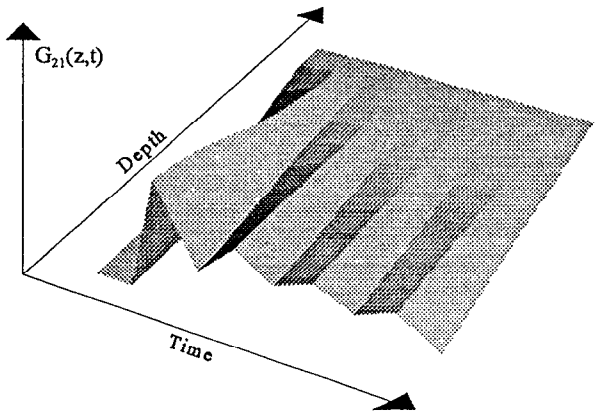

FIG. 2. The Green function $G_{21}(z,t)$.

tral Legendre approach and solved the partial differential equations given in Ref. 6 for the transmission kernels $T^{\pm}(z,L,t;\kappa)$ and then solved the set of equations of the Green functions which are also given in Ref. 6. These equations are relations between the Green functions, reflection kernels and the transmission kernels. The values of the Green functions generated by the method of this paper and those generated through the method of Ref. 6 were in close agreement. As a demonstration, the values of the function $G^9{}_{11}(\alpha,\beta)$ generated through both methods at the collocation points $\beta=-1$ and $\beta=0.165\ 28$ are given in Table II. These collocation points correspond to $t=0$ s and $t=0.058\ 26$ s, respectively. The CPU execution time in this example was 2 s on a Sun-Sparc Station II.

VI. CONCLUSION

An alternative scheme for solving a one-dimensional inverse problem for inhomogeneous nonconductive media is proposed in this paper. The method is based upon constructing the Nth degree interpolation polynomial to approximate the Green functions and the phase velocity function using Legendre–Gauss–Lobatto collocation points. The input to the scheme is the reflection kernel. From this input data, the scheme generates values of the Green functions and the phase velocity function at the collocation points through the solution of a set of algebraic equations. The rapid rate of convergence of pseudospectral Legendre approximations, see Ref. 13, and the Kronecker property that is presented in Eq. (4) makes the scheme very attractive.

TABLE II. Values of the Green function $G^9_{11}(\alpha,\beta)$ at $\beta=-1$ and $\beta=0.165\ 28$.

α_n $0\leq n\leq 9$	$G^9_{11}(\alpha_n,-1)$ This method	$G^9_{11}(\alpha_n,-1)$ Method of Ref. 6	$G^9_{11}(\alpha_n,.16\ 528)$ This method	$G^9_{11}(\alpha_n,.16\ 528)$ Method of Ref. 6
−1.000 000	0.000 00	0.000 00	0.000 00	0.000 00
−0.919 534	−19.988 80	−19.988 66	−0.006 65	−0.006 61
−0.738 774	−59.629 04	−59.629 13	−0.019 32	−0.019 37
−0.477 925	−106.252 42	−106.252 25	−0.033 21	−0.033 23
−0.165 290	−150.036 06	−150.036 24	−0.045 07	−0.045 02
0.165 290	−186.690 01	−186.690 21	−0.054 07	−0.054 04
0.477 925	−215.513 49	−215.513 61	−0.060 72	−0.060 73
0.738 774	−236.990 88	−236.990 67	−0.065 62	−0.065 65
0.919 534	−251.100 06	−251.100 11	−0.068 91	−0.068 93
1.000 000	−257.238 20	−257.238 31	−0.070 38	−0.070 36

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Self-dual Maxwell fields on curved space–times

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We present a manifestly conformally invariant formulation of Maxwell equations on asymptotically flat space–times. It is shown how to construct regular self-dual and antiself-dual fields from suitable radiation data, and the general solution as a sum of fields with both types of duality. The basic variable in this formalism is a scalar field F defined as the phase of the parallel propagator (associated with the Maxwell potential) from interior points to future null infinity along null geodesics. Field equations equivalent to the source free Maxwell's equations are derived for F. A perturbative solution based on Huygens' principle is proposed. Exact solutions are found for H-spaces. The use of these results on gravitational lensing is discussed. © *1996 American Institute of Physics.* [S0022-2488(96)00507-5]

I. INTRODUCTION

The global behavior of electromagnetic radiation on curved space–times is used in astrophysics to study several interesting phenomena. In gravitational lensing one studies the global behavior of null geodesics in a gravitational field produced by sources with compact support. Several authors have also used parallel propagation of vectors on null geodesics to study the behavior of polarized light. Recently, a non-local formalism for general relativity (GR) was presented[1,2] where the fundamental variable contains all the information of the null geodesics of the given space–time, thus providing a useful tool to study electromagnetic radiation in the geometrical optics limit.

It has also been emphasized that when the wavelength of the radiation is of the same order of magnitude of the gravitational radius of an intervening compact object, diffraction effects have to be taken into account. That is, in this case one needs wave optics on a curved background. However, it is difficult to find global solutions of Maxwell's equations on a general space–time since a Green function for this problem is generally not available. In practice, one either tries to find a Green function perturbatively, or assumes a flat background except on a small region of interest, or considers space–times with high degrees of symmetry.

We present here a new formulation of Maxwell theory where the basic variable,

$$F \equiv \int_{\gamma} A_a dx^a, \tag{I.1}$$

a line integral of the Maxwell potential along a specific path γ, is a non-local object and where regularity of this variable is equivalent to regularity of the Maxwell field on a global scale. We derive field equations for this variable whose regular solutions automatically yield global solutions of the Maxwell's equations. Even the perturbed solutions of these non-local equations are, by construction, regular fields on a global scale. The formalism has another interesting feature, namely, the background geometry enters the field equations only through its conformal structure.[1,2] Thus, this non-local formulation of Maxwell theory is manifestly conformally invariant. It is also well adapted to discuss different global problems concerning electromagnetic radia-

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tion. In the geometrical optics limit one recovers the description of the null geodesics via the non-local formulation of GR. In the full theory the formalism defines in a precise way Huygens or non-Huygens propagation of electromagnetic radiation on a curved background.

Before presenting technical details we briefly review some results already obtained using the basic variable in our formalism. In recent years this variable has received considerable attention not only for Maxwell Theory, but also for Yang–Mills Theory and General Relativity.[3–6] In 1975 Wu and Yang[7] suggested that the parallel propagator of a Maxwell potential A_a along a path γ,

$$\exp\left(-i\int_\gamma A_a dx^a\right)=\exp(-iF), \tag{I.2}$$

was better suited than the Maxwell field or potential to describe electromagnetism. [Note that our variable F is the phase of the propagator introduced in (I.2).]

In 1980 Sparling[8,9] obtained the field equations for the phase of the parallel propagator associated with a self-dual Maxwell field along null geodesics in Minkowski space. A brief description of his method follows.

Denoting by x points in the space–time, $(u,\zeta,\bar{\zeta})$ points in the future null boundary $\mathscr{I}^+$, the Sparling equation has the simple form

$$\eth F=-A_R(x,\zeta,\bar{\zeta}), \tag{I.3}$$

where F, the phase of the parallel propagator (I.2), is the line integral of the Maxwell potential along a null geodesic that begins at a point x and ends at null infinity intersecting the generator $(\zeta,\bar{\zeta})$ of $\mathscr{I}^+$; the "eth operator" $\eth$ is essentially $\partial/\partial\zeta$, and A_R, the "restricted" free data at $\mathscr{I}^+$, is obtained by evaluating the data $A(u,\zeta,\bar{\zeta})$ at the intersection of the future light cone of x with $\mathscr{I}^+$, the "light cone cut". In a general, asymptotically flat (in future null directions) space–time, the light cone cuts are 2-surfaces embedded in $\mathscr{I}^+$, described parametrically as

$$u=Z(x,\zeta,\bar{\zeta}). \tag{I.4}$$

In Minkowski space–time the Z function has a simple form in standard Lorentz coordinates x^a,

$$Z(x,\zeta,\bar{\zeta})=x^a l_a(\zeta,\bar{\zeta}), \tag{I.5}$$

where $l_a(\zeta,\bar{\zeta})$ spans the sphere of null covectors at x. Its explicit form in Minkowski coordinates is given in Appendix B.

Using the Green function of the eth operator one obtains the regular solution of (I.3) which, after a reconstruction procedure, yields the general solution of the self-dual Maxwell equations in Minkowski space.

Notice that in a similar way [starting from the complex conjugate of (I.3)] one obtains the field equations for the antiself-dual case. Furthermore, adding both solutions yields a general real Maxwell field satisfying the source free equations. Thus (I.3), a single equation for a scalar field, is equivalent to the full set of Maxwell equations on Minkowski space.

Is it possible to generalize the Sparling equation to curved space–times? Since one knows that, due to the linearity of the theory, self-dual data must produce a self-dual field, in principle it is possible to find a suitable generalization of Sparling's formalism for a "self-dual" parallel propagator on a curved space–time.

In this paper we present this generalization. We introduce the phase of the parallel propagator for a self-dual field associated with a special set of open curves, i.e., null geodesics that start at an interior point of the space–time and end at $\mathscr{I}^+$. We obtain the field equation for this propagator equivalent to the self-dual Maxwell's equations on curved space–times. This is a single equation on a complex non-local function where the free data enters as a source term.

The cut function Z (I.4) that describes the light cone cuts of $\mathscr{I}^+$ plays a fundamental role in our approach. As shown in Refs. 1 and 2, all the information about the conformal geometry of space–time is encoded in Z. Since Maxwell's equations are conformally invariant, the function Z contains precisely the needed information of the background space–time geometry. As a result we obtain a manifestly conformally invariant formulation of regular Maxwell's fields on space–times which are asymptotically flat at future null infinity.

In section II we review the geometrical meaning of Z, show its relationship to the underlying conformal metric and obtain some results that are used in the derivation of the field equation for our variable. In section III, we present the non-local variable F and give its kinematical relation with the Maxwell field. We derive field equations for F equivalent to the self-dual and antiself-dual Maxwell's equations and show how to recover a general Maxwell field from knowledge of F. A perturbative method for solving the field equation is presented and then used to show the non-Huygens nature of Maxwell fields propagating on curved space–times. A variation of this method to study fields on space–times which are small deviations from Minkowski space is suggested. In section IV the formalism is applied to obtain exact solutions in H spaces. The zeroth and first order solution to the field equation on small deviations from Minkowski space are also calculated. Section V contains a summary of the results and a brief discussion on the use of this formalism to approach the problems of scattering and gravitational lensing. In Appendix A we derive the equation for F in the general case (i.e., complex Maxwell fields without a definite duality), show the equivalence with the self-dual formulation and show how to recover the field strength and potential from F. Appendix B contains some review material on differential equations involving the eth operator and their Green functions, necessary for the article to be self-contained. Appendices C and D contain auxiliary calculations.

II. GEOMETRICAL PRELIMINARIES

A. The notion of duality

On the space–time (M, g_{ab}) a volume form ϵ_{abcd} is chosen satisfying the normalization condition

$$\epsilon_{abcd}\epsilon^{abcd} = -4!, \tag{II.1}$$

where, as usual, indices are raised using the inverse of the metric. Up to a sign (i.e., a choice of orientation), (II.1) singles out a unique volume form, which, together with the inverse of the metric, is used to construct the dual operator, a conformally invariant linear operator acting on 2-forms as

$$W_{ab} \to {}^*W_{ab} \equiv \tfrac{1}{2}\,\epsilon_{abcd} g^{ce} g^{df} W_{ef}. \tag{II.2}$$

From (II.1) and (II.2) it follows that ${}^{**}W_{ab} = -W_{ab}$, and so the possible eigenvalues of the dual operator are $\pm i$. A 2-form is called self-dual (SD) [antiself-dual (ASD)] if it is an eigenvector corresponding to the eigenvalue $i[-i]$. Under the inner product $g^{ac} g^{bd} W_{ab} Q_{cd}$ SD and ASD 2-forms are orthogonal to each other. It is important to note that every 2-form can be written as a sum of eigenvectors of the dual operator:

$$W_{ab} = W^+_{ab} + W^-_{ab}, \quad W^{\pm} \equiv \tfrac{1}{2}\,[W_{ab} \mp i {}^*W_{ab}]. \tag{II.3}$$

$W^+_{ab}[W^-_{ab}]$ is commonly referred to as "the SD [ASD] part of W_{ab}." This decomposition allows a compact form for (source free) Maxwell's equations, explicitly exhibiting their conformal invariance,

$$\partial_{[a} F^+_{bc]} = 0, \quad \partial_{[a} F^-_{bc]} = 0. \tag{II.4}$$

For real fields, the second equation is the complex conjugate of the first one, and Maxwell's equations reduce to a first order equation on a complex potential A_b^+,

$$\tfrac{1}{2}\,\epsilon_{ab}{}^{cd}\partial_{[c}A^+_{d]}=i\,\partial_{[a}A^+_{b]}, \tag{II.5}$$

instead of the usual second order equation on a real potential. It is clear from (II.4) and (II.3) that SD [ASD] closed 2-forms satisfy Maxwell's source free equations, and also that any solution of these equations is the sum of a SD closed 2-form and an ASD one. It follows that the problem of solving Maxwell's equations on (M,g_{ab}) amounts to finding SD and ASD closed 2-forms satisfying appropriate "initial conditions". The first step is to construct the dual operator (II.2), which, being conformally invariant, can be readily obtained from the Z function, as it is shown in the following subsection.

B. A non-local description of space–time

The theory of light cone cuts of null infinity[1,2] offers a completely different approach to general relativity. Instead of using a local field, the metric g_{ab}, to describe the geometry of the space–time, one introduces a non-local function that plays an equally important role, as it contains all the information of the conformal structure of space–time. In particular, it yields the null geodesics. A brief description of the kinematical features of this theory follows. The dynamics as well as other properties of this non-local variable are not presented here (in our formulation of Maxwell theory the background geometry is assumed fixed) but they can be found in (Refs. 1 and 2) and references therein.

Assume the space–time (M,g_{ab}) is asymptotically flat at future null infinity, $\mathscr{I}^+$. The intersection of the future null cone from $x^a\in M$ with $\mathscr{I}^+$ is a 2-surface called a light cone cut of null infinity. Introducing on $\mathscr{I}^+$ Bondi coordinates $(u,\zeta,\bar\zeta)$ this cut can be locally described as

$$u=Z(x^a,\zeta,\bar\zeta). \tag{II.6}$$

Assuming the smooth function Z is given, we introduce the following scalars:

$$u=Z(x^a,\zeta,\bar\zeta)\quad \omega=\eth\dot Z,\quad \bar\omega=\eth Z,\quad r=\eth\bar\eth Z, \tag{II.7}$$

where the $\eth$ (eth) and $\bar\eth$ (eth-bar) operators, defined in (B1) and (B2), are essentially partial derivatives with respect to ζ and $\bar\zeta$ respectively. For each $(\zeta,\bar\zeta)\in S^2$ the scalars (II.7) define a coordinate system. An alternative notation found in the literature is

$$(u,\omega,\bar\omega,r)=(\theta^0,\theta^+,\theta^-,\theta^1)=\theta^i,$$

with its gradient and dual vector basis denoted by $\theta^i{}_{,a}$, and θ^a_i, respectively. In past references, however, the following associated vector basis has been used:

$$\hat L^a=\theta^a_1,\quad \hat M^a=-\theta^a_{-1},\quad \hat{\bar M}^a=-\theta^a_+,\quad \hat N^a=\theta^a_0, \tag{II.8}$$

and we will keep the above convention in this work.

The coordinates (II.7) have an interesting geometrical interpretation: the points x^a satisfying $u=Z(x^a,\zeta,\bar\zeta)=$const. form the past light cone of $(u,\zeta,\bar\zeta)$ at $\mathscr{I}^+$, ω and $\bar\omega$ determine the direction angle of a geodesic on that cone and τ uniquely locates a point on that geodesic.[10,11] It follows that any null geodesic is characterized by the parameters $(u,\omega,\bar\omega,\zeta,\bar\zeta)$, and that the tangent at x to the affinely parametrized geodesic $[u=Z(x,\zeta,\bar\zeta),\ \omega=\eth Z(x,\zeta,\bar\zeta),\ \bar\omega=\bar\eth Z(x,\zeta,\bar\zeta);\zeta,\bar\zeta]$ is the null vector

$$Z^a(x,\zeta,\bar\zeta)\equiv g^{ab}Z_{,b}(x,\zeta,\bar\zeta). \tag{II.9}$$

By letting $(\zeta,\bar{\zeta})$ range over the sphere, this vector ranges over the -future- cone of null directions at x^a. Thus, the function Z determines the conformal structure of the space–time. As done in Ref. 1, we exploit the fact that Z depends smoothly on $(\zeta,\bar{\zeta})$ to obtain the components $g^{ij}(x,\zeta,\bar{\zeta})\equiv g^{ab}\theta^i_{,a}\theta^j_{,b}$ of the metric in the coordinate systems (II.7). The starting point is the fact that (II.9) is null, which immediately implies that

$$g^{00}=g^{ab}(x)\,\theta^0_{,a}\theta^0_{,b}=0. \tag{II.10}$$

Note that this result is true for any value of $(\zeta,\bar{\zeta})$. Thus, $\eth$ and $\bar{\eth}$ of (II.10) are also equal to zero. However, explicitly taking $\eth$ and $\bar{\eth}$ of (II.10) plus the fact that the metric does not depends on $(\zeta,\bar{\zeta})$ yields

$$\eth^{00}_g=2g^{ab}(x)\,\theta^0_{,a}\eth\theta^0_{,b}=2g^{0+}=0,\quad \bar{\eth}g^{00}=2g^{0-}=0. \tag{II.11}$$

Thus, we have obtained three (trivial) components of the conformal metric. As the above equations suggest, the metric components in this coordinate system are obtained by taking a sufficient number of $\eth$ and $\bar{\eth}$ derivatives of (II.10).

Taking $\eth\bar{\eth}$ of (II.10) we obtain

$$g^{-+}=-g^{01}. \tag{II.12}$$

Taking $\eth^2$ of (II.10) we get

$$g^{++}+g^{ab}Z_{,a}\Lambda_{,b}=0,$$

where $\Lambda\equiv\eth^2Z$. Assuming Λ is expressed in the θ^i coordinates as $\Lambda(\theta^i,\zeta,\bar{\zeta})$ one has $\Lambda_{,b}=\Lambda_{,i}\theta^i_{,b}$. Using the previous results we immediately obtain

$$g^{++}=-g^{01}\Lambda_{,r}. \tag{II.13}$$

We can continue this procedure until all the components (up to a choice of g^{01}) are obtained [1]. It is worth mentioning that knowledge of Λ determines all the non-trivial $g^{ij}(\theta^i,\zeta,\bar{\zeta})$. The final form of the metric is given by

$$g^{01}\begin{pmatrix} 0 & 0 & 0 & 1\\ 0 & -\Lambda_{,r} & -1 & h^{1+}\\ 0 & -1 & -\bar{\Lambda}_{,r} & h^{1-}\\ 1 & h^{1+} & h^{1-} & h^{11}\end{pmatrix}, \tag{II.14}$$

where the h^{1j} depend explicitly on Λ [1]. (In the derivation of our field equations, however, they will not be needed since we are only looking for the projection of the metric on the null surfaces $Z=$const).

Thus, in this approach the function Z serves a dual purpose: $\eth^2Z\equiv\Lambda$ determines the conformal metric and (II.7) are natural coordinates that allow simple expressions for many relevant tensor fields, as the metric itself. In the particular case $\Lambda=0$ we obtain conformal Minkowski space and, for each $(\zeta,\bar{\zeta})$, (II.7) becomes a null coordinate system (Appendix B). In general, θ^0 is a null coordinate, and simple expressions for both the null cone congruence from a point x^a and the geodesic deviation vectors of this congruence are obtained using the θ^i coordinates. Since these results will be used in following sections, we present them now. The detailed calculations can be found in Appendix C.

If we denote by $x^a(x_0^b,\zeta,\bar{\zeta},r)$ the parametric form of the null cone with apex at a point $x_0^b \in M$, $r = \eth\bar{\eth}Z(x^a,\zeta,\bar{\zeta}) - \eth\bar{\eth}Z(x_0^a,\zeta,\bar{\zeta})$ [refer to (C.1)–(C.3)], then a null geodesic on this cone is characterized by a fixed value of $(\zeta,\bar{\zeta})$ (a generator of $\mathscr{I}^+$). Neighboring rays around this fixed null geodesic, corresponding to different values of ζ, are described by the geodesic deviation vector $M^a \equiv \partial x^a$. As shown in Appendix C [see (C.6)], M^a can be written as

$$M^a \equiv (1+\zeta\bar{\zeta})\frac{\partial x^a(x_0,\zeta,\bar{\zeta},r)}{\partial\zeta} = (r-r_0)\hat{M}^a + (\Lambda-\Lambda_0)\hat{\bar{M}}^a - \eth(r-r_0)\hat{L}^a, \tag{II.15}$$

where the subindex 0 means that the corresponding scalar is evaluated at the apex x_0.

Finally, we present the explicit form of the dual of the light cone 2-surface element $\hat{L}_{[a}M_{b]}$ in our basis since this result is later used in the derivation of the field equations. We start by noting from (II.9), (II.14) and (II.8) that

$$\begin{aligned} Z^a &= g^{ab}u_{,b} = g^{01}\hat{L}^a, \\ g^{ab}\omega_{,b} &= g^{1+}\hat{L}^a + g^{01}\Lambda_{,r}\hat{\bar{M}}^a + g^{01}\hat{M}^a. \end{aligned} \tag{II.16}$$

The determinant of (II.14) yields the volume form

$$\epsilon = \frac{-i}{\sqrt{p}(g^{01})^2}\, du\wedge d\omega\wedge d\bar{\omega}\wedge dr, \quad p = 1-\Lambda_{,r}\bar{\Lambda}_{,r}, \tag{II.17}$$

which, together with (II.8), (II.2) and (II.16), gives

$$*\hat{L}_{[a}\hat{M}_{b]} = \frac{-i}{\sqrt{p}(g^{01})^2}\, u_{[,a}\omega_{,b]} = \frac{-i}{\sqrt{p}}[\hat{L}_{[a}\hat{M}_{b]} + \Lambda_{,r}\hat{L}_{[a}\hat{\bar{M}}_{b]}]. \tag{II.18}$$

(II.15) and (II.18) yield

$$*\hat{L}_{[a}M_{b]} = -i[\hat{L}_{[a}M_{b]} + 2\bar{f}\hat{L}_{[a}\hat{M}_{b]} + 2g\hat{L}_{[a}\hat{\bar{M}}_{b]}], \tag{II.19}$$

where

$$\begin{aligned} f &= \tfrac{1}{2}[(r-r_0)h - (1+h)(\bar{\Lambda}-\bar{L}_0)\Lambda_{,r}], \\ g &= \tfrac{1}{2}[(1+h)(r-r_0)\Lambda_{,r} - (2+h)(\Lambda-\Lambda_0)], \end{aligned} \tag{II.20}$$

and $h \equiv 1/\sqrt{p} - 1$. Alternatively, using (II.3),

$$\hat{L}_{[a}M^+_{b]} = -[\bar{f}\hat{L}_{[a}\hat{M}_{b]} + g\hat{L}_{[a}\hat{\bar{M}}_{b]}]. \tag{II.21}$$

Note that in the $\Lambda=0$ limit $\hat{L}_{[a}M_{b]}$ is ASD. Thus f and g represent the departure of $\hat{L}_{[a}M_{b]}$ from being an ASD 2-form.

III. A NON-LOCAL VARIABLE FOR MAXWELL FIELDS

A. Definitions and kinematical relations

Let A_a be a Maxwell potential whose projection to $\mathscr{I}^+$ has vanishing contraction with vectors tangent to the generators, $F_{ab} = 2\nabla_{[a}A_{b]}$ be its field strength. We define our basic variable F as

$$F(x,\zeta,\bar{\zeta})=-\int_x^\infty A_a Z^a ds=-\int_x^\infty A_a \hat{L}^a dr, \tag{III.1}$$

where the integral is taken along the null geodesic $l_x(\zeta,\bar{\zeta})$ that connects the point x with the generator $(\zeta,\bar{\zeta})$ of $\mathscr{I}^+$, s is an affine length and the second equality follows directly from (II.16). F is a non-local function on the space of null directions of space–time with a simple geometrical meaning: $G\equiv e^{iF}$ gives the parallel transport along $l_x(\zeta,\bar{\zeta})$ between x and the point at which $l_x(\zeta,\bar{\zeta})$ intersects $\mathscr{I}^+$. As A_a is a regular potential with a smooth extension to $\mathscr{I}^+$, the integrand of (III.1) behaves as s^{-2} when $s\to\infty$, thus giving a finite F. Conversely, if F is assumed to be regular, then the integrand "peels" appropriately.

We consider now the problem of obtaining A_a from a given regular F, i.e., inverting (III.1). This will be particularly important when we impose field equations on F since the potential A_a will then be a derived object. It follows from (III.1) and (II.9) that F satisfies

$$Z_{,a}(\nabla^a F-A^a(x))=0. \tag{III.2}$$

Taking a sufficient number of $\eth$ and $\bar{\eth}$ derivatives of (III.2) we obtain the components of $A^a(x)$ in the θ_i^a basis:

$$\begin{aligned} Z_{,b}(A^b-\nabla^b F)&=0,\\ \eth Z_{,b}(A^b-\nabla^b F)&=Z_{,b}\nabla^b \eth F,\\ \bar{\eth} Z_{,b}(A^b-\nabla^b F)&=Z_{,b}\nabla^b \bar{\eth} F,\\ \eth\bar{\eth} Z_{,b}(A^b-\nabla^b F)&=\bar{\eth} Z_{,b}\nabla^b \eth F+\eth Z_{,b}\nabla^b \bar{\eth} F+Z_{,b}\nabla^b \eth\bar{\eth} F, \end{aligned} \tag{III.3}$$

from where

$$A^a=\nabla^a F+(\theta_-^a \theta_{,b}^0+\theta_1^a\theta_{,b}^+)\nabla^b\bar{\eth}F+(\theta_+^a\theta_{,b}^0+\theta_1^a\theta_{,b}^-)\nabla^b\eth F+\theta_1^a\theta_{,b}^0\nabla^b\eth\bar{\eth}F. \tag{III.4}$$

Note that (III.4) naturally induces a gauge transformation giving a new potential,

$$A'_b=A_b-\nabla_b F.$$

Consider now the 2-surface $\Delta_x(\zeta,\bar{\zeta})$ swept by $l_x(\zeta,\bar{\zeta})$ as ζ moves in $[\zeta,\zeta+d\zeta]$ with $\bar{\zeta}$ fixed, denote by $\partial\Delta_x(\zeta,\bar{\zeta})$ its closed boundary constructed from two neighboring null geodesics $l_x(\zeta,\bar{\zeta})$ and $l_x(\zeta+d\zeta,\bar{\zeta})$, closed at $\mathscr{I}^+$ by the connecting vector $M^a d\zeta/P$. Using the phase of the holonomy operator,

$$\mathscr{H}=\int_{\partial\Delta_x(\zeta,\bar{\zeta})} A_a dx^a=\int_{\Delta_x(\zeta,\bar{\zeta})} F_{ab}dx^a dx^b, \tag{III.5}$$

one can find a useful relationship between F, the field strength F_{ab} and the free Maxwell data at $\mathscr{I}^+$.

We recall that source free Maxwell fields are uniquely determined by the data $(A(u,\zeta,\bar{\zeta}),\bar{A}(u,\zeta,\bar{\zeta}))$ on the "initial value" surface $\mathscr{I}^+$ [12]. These functions are defined by the following equations:

$$A(u,\zeta,\bar{\zeta})\equiv\lim_{\mathscr{I}^+} A_a M^a,\quad \bar{A}(u,\zeta,\bar{\zeta})\equiv\lim_{\mathscr{I}^+} A_a\bar{M}^a, \tag{III.6}$$

where the limit is taken along $l_x(\zeta,\bar{\zeta})$, x is any point satisfying $Z(x,\zeta,\bar{\zeta})=u$, and M^a and $\bar{M}^a$, given in (C.6) and c.c., are geodesic deviation vectors of the future null cone of x (see Appendix C). A and $\bar{A}$ are, respectively, associated to the SD and ASD parts of the field by the following equations (obtained from Ref. 13):

$$\lim_{\mathscr{I}^+} F^-_{ab}M^a\bar{M}^b=\eth\bar{A}, \quad \lim_{\mathscr{I}^+} F^+_{ab}M^a\bar{M}^b=-\bar{\eth}A. \tag{III.7}$$

Thus, $\bar{A}=0$ [$A=0$] for SD [ASD] fields. For real fields, $\bar{A}$ is the complex conjugate of A, the two degrees of freedom of the radiation fields are contained in a single complex function.

Defining the differential holonomy as

$$H(x,\zeta,\bar{\zeta})\equiv\int_x^\infty F_{ab}\hat{L}^aM^b dr, \tag{III.8}$$

i.e. $\mathscr{H}=Hd\zeta/P$, it follows directly from (III.5) and (III.6) that

$$\eth F(x,\zeta,\bar{\zeta})+A_R(x,\zeta,\bar{\zeta})=H(x,\zeta,\bar{\zeta}), \tag{III.9}$$

where the complex scalar $A_R(x,\zeta,\bar{\zeta})$ is the restriction of the free data $A(u,\zeta,\bar{\zeta})$ at $\mathscr{I}^+$ to the cut $u=Z(x,\zeta,\bar{\zeta})$, i.e.,

$$A_R(x,\zeta,\bar{\zeta})\equiv A(u=Z_1\zeta,\bar{\zeta}). \tag{III.10}$$

In an analogous way, using the holonomy phase $\bar{\mathscr{H}}$ around the loop $\partial\bar{\Delta}_x(\zeta,\bar{\zeta})$[$\Delta_x(\zeta,\bar{\zeta})$ being the 2-surface swept by $l_x(\zeta,\bar{\zeta})$ as $\bar{\zeta}$ moves in $[\bar{\zeta},\bar{\zeta}+d\bar{\zeta}]$ with ζ fixed] and defining

$$\bar{H}(x,\zeta,\bar{\zeta})\equiv\int_x^\infty F_{ab}\hat{L}^a\hat{M}^b dr, \tag{III.11}$$

one obtains

$$\bar{\eth}F(x,\zeta,\bar{\zeta})+\bar{A}_R(x,\zeta,\bar{\zeta})=\bar{H}(x,\zeta,\bar{\zeta}), \tag{III.12}$$

with $\bar{A}_R(x,\zeta,\bar{\zeta})$ the restriction of $\bar{A}(u,\zeta,\bar{\zeta})$ to the cut

$$\bar{A}_R(x,\zeta,\bar{\zeta})=\bar{A}(u=Z,\zeta,\bar{\zeta}) \tag{III.13}$$

(we will omit the subindex R from now on).

Equations (III.8) and (III.9) give $\eth F$ as a functional of the field strength F_{ab} and the free data $A(u,\zeta,\bar{\zeta})$. One can invert (III.8), using (III.9), to obtain F_{ab} in terms of $\eth F$ and c.c. This is done in Appendix A. The desired relationship is

$$\hat{\phi}\equiv F_{ab}(x)\hat{L}^a\hat{M}^b=\left[\frac{(\eth F)_{,r}-\Lambda_{,r}(\bar{\eth}F)_{,r}}{1-\Lambda_{,r}\bar{\Lambda}_{,r}}\right]_{,r}\equiv\hat{\Phi}[F] \quad \text{and c.c.} \tag{III.14}$$

Note that F_{ab} does not depend on $(\zeta,\bar{\zeta})$, whereas $\hat{L}^a\hat{M}^b$ does. Thus, evaluating (III.14) for different values of $(\zeta,\bar{\zeta})$ yields different components of $F_{ab}(x)$. Alternatively, we can take a sufficient number of $\eth$ and $\bar{\eth}$ derivatives of (III.14) [as was done in (III.3)] to obtain the components of F_{ab} in the $\theta^i_{,a}$ basis.

B. The field equations for F

We now want to find the equation satisfied by F when the field strength F_{ab} is a (closed) SD 2-form. The fact that F_{ab} is closed was already used in the definition of F and in eq. (III.9) as an application of the Stokes theorem.

A SD field satisfies

$$F_{ab}=F^{+}_{ab}. \tag{III.15}$$

Thus, integrating (III.15) on $\Delta_x(\zeta,\bar{\zeta})$ yields

$$H=\int_x^\infty F_{ab}\hat{L}^{[a}M^{b]}dr=\int_x^\infty F^{+}_{ab}(\hat{L}^{[a}M^{b]})dr=\int_x^\infty F^{ab}(\hat{L}_{[a}M_{b]})^{+}dr, \tag{III.16}$$

where the last equality follows from the vanishing contraction between SD and ASD 2-forms. Inserting (II.21) in (III.16) and using (III.9) and (III.14) yields the following integro-differential equation for F in the SD case (the + sign is used to indicate that the associated field is SD),

$$\eth F^{+}+A+\int_x^{My}(\bar{f}\hat{\Phi}[F^{+}]+g\hat{\bar{\Phi}}[F^{+}])dr=0. \tag{III.17}$$

Equation (III.17) is the desired generalization of the Sparling equation[8,9] to curved space-times.

A similar calculation yields the equation for F in the ASD case,

$$\bar{\eth}F^{-}+\bar{A}+\int_x^\infty(f\hat{\bar{\Phi}}[F^{-}]+\bar{g}\hat{\Phi}[F^{-}])dr=0. \tag{III.18}$$

A few remarks follow.

1. The kernel of the eth operator-acting on spin weight 0 functions- is the set of constant functions on the sphere (Appendix B). It then follows from (III.17) and (III.14) that the solutions of eq. (III.17) have the ambiguity of an arbitrary additive function $h(x)$. The origin of this term can be traced back to the definition of F.[14] If we integrate (III.17) using the Green function $G_{0,1'}(\zeta,\bar{\zeta};\zeta',\bar{\zeta}')$ for $\eth$ given in (B.8) (subindices indicate the spin weight for each variable), we obtain the following compact form for (III.17):

$$F-\mathscr{G}[F]=\mathscr{F}, \tag{III.19}$$

where

$$\mathscr{F}\equiv-\int_{S^2}G_{0,-1'}(\zeta,\bar{\zeta};\zeta',\bar{\zeta}')A_R(x,\zeta',\bar{\zeta}')dS' \tag{III.20}$$

and

$$\mathscr{G}[\cdot]\equiv-\int_{S^2}G_{0,-1'}(\zeta,\bar{\zeta};\zeta',\bar{\zeta}')\left(\int(\bar{f}\hat{\Phi}[\cdot]+g\hat{\bar{\Phi}}[\cdot])dr'\right)dS'. \tag{III.21}$$

In (III.21), the line integral is along $l_x(\zeta',\bar{\zeta}')$, and extends from x to $\mathscr{I}^+$. By omitting the term $h(x)$ on the r.h.s. of (III.19) we have selected the particular solution (i.e., chosen the gauge[14]) satisfying the condition $\int_{S^2}F(x,\zeta,\bar{\zeta})dS=0$. This follows from the fact that $\int_{S^2}G_{0,1'}(\zeta,\bar{\zeta};\zeta',\bar{\zeta}')dS=0$.[15] Analogous comments to this and the following remarks apply to the ASD case.

2. We know that there is a one to one correspondence between the free data $A(u,\zeta,\bar{\zeta})$ and the solution of the source free Maxwell's equations. Therefore it is appropriate to ask if the regular solutions to (III.19) uniquely correspond to a given $A(u,\zeta,\bar{\zeta})$. Although this issue is very involved due to the non-local nature of the equation, in those cases where a norm $\|\cdot\|$ can be defined on the linear space V of admissible functions $F(x,\zeta,\bar{\zeta})$, such that the linear operator $\mathcal{G}$ is continuous and has a norm less than 1 (meaning $\sup_V \|\mathcal{G}[F]\|/\|F\|<1$), the uniqueness of the solution of (III.19) is easily proved. In this case the operator $I-\mathcal{G}$ is known to be invertible, with its inverse given by the -convergent- power series,

$$[I-\mathcal{G}]^{-1}=I+\mathcal{G}+\mathcal{G}^2+\mathcal{G}^3+\dots . \tag{III.22}$$

The definition of $(V,\|\cdot\|)$ is a technically involved problem we defer for future work. Note however that, as $\mathcal{G}=0$ when $\Lambda=0$, any natural norm will satisfy the condition $\|\mathcal{G}\|<1$ when $\Lambda\simeq 0$ [this limit corresponds to a small deviation from -conformal- Minkowski space (Appendix B)].

From now on, we will assume that the linear operator $\mathcal{G}$ is such that (III.19) has a unique solution.

3. Although we have only proved that SD Maxwell's equations imply (III.19), the converse is also true. The equivalence of both sets of equations follows from the uniqueness of the solution of (III.19). A is the data for a unique SD Maxwell field F_{ab}. If B_a is the potential satisfying the conditions in Ref. 14 and

$$\int_{S^2}\left[\int_x^\infty B_a Z^a ds\right] dS=0,$$

then (III.1) constructed from B_a is a solution of (III.19) (remark 1). Now, F constructed in this way is *the only* solution of (III.19). It follows from remark 1 that, when applied to a solution of (III.17), (III.4) yields a potential $A_a(x)=B_a(x)+\nabla_a h(x)$ for the SD field $F_{ab}(x)$.

4. The equation satisfied by F in the general case is derived in Appendix A. It is shown that we can first solve for the SD and ASD parts and then add them up, i.e., if

$$F\equiv F^+ + F^-, \tag{III.23}$$

where F^+ and F^- are solutions of (III.17) and (III.18), respectively, then F yields -via (III.4) or (III.14)- a regular solution of the full source free-Maxwell's equations with "initial data" $(A,\bar{A})$ on the characteristic surface $\mathcal{I}^+$.

5. The function Z plays two distinct roles in the field equations (III.17), (III.18). It determines the restriction of the free data $A(\bar{A})$ to the cut $u=Z$ and it also enters the integral term via (II.20) and (III.14).

Two different perturbative methods to solve (III.17) may be suggested based on the information we have about Z:

(a) If the conformal geometry of the space–time is fully known (Z is given) we can construct the linear operator (III.21), and then apply (III.22) to solve (III.19),

$$F=[1-\mathcal{G}]^{-1}\mathcal{F}=[1+\mathcal{G}+\mathcal{G}^2+\mathcal{G}^3+\dots]\mathcal{F}. \tag{III.24}$$

Note that if F_n is the sum of the first n terms in (III.24) then

$$F=\lim_{n\to\infty} F_n, \quad F_{n+1}=\mathcal{G}[F_n]+\mathcal{F}, \tag{III.25}$$

an iterative process that could have been suggested directly from (III.19).

(b) If the space–time is a small deviation from -conformal- Minkowski space, then $\Lambda\simeq 0$ (Appendix B) and we can expand F around $\Lambda=0$. The expansion is obtained by rearranging

(III.24) guided by the observation that f only contains terms Λ^n with $n\geqslant 2$, g contains terms with $n\geqslant 1$ (II.20) and $\mathscr{G}$ contains terms $n\geqslant 1$ (III.21). Slightly modifying (III.25) by keeping track of the different powers of Λ we generate an iterative method to solve (III.17) in nearly Minkowskian backgrounds. The first two terms are explicitly calculated in part B of the following section.

6. The leading order term $\mathscr{F}(x,\zeta,\bar{\zeta})$ in the expansion series (III.24) represents the Huygens' part of the field, i.e., the contribution of A_R (the restriction of the data A to the light cone cut of x). It is clear that the other terms are non-Huygens. As an example, to calculate $\mathscr{G}\mathscr{F}$ at x we need to know $\mathscr{F}$ in the future cone of x [this follows from (III.21) and (III.14)]. From (III.20), the restriction of the data to the whole region of $\mathscr{I}^+$ enclosed by the light cone cut of x is needed, not only its value at the cut. A similar reasoning shows that to calculate all the other terms in (III.24) we only need the data in this region, as expected from general principles (the field at x can not affect its value out of the cut on $\mathscr{I}^+$). This shows that, on a general background, Maxwell fields do not obey the Huygens' principle. In the perturbation scheme (III.24) one assumes that the background geometry is such that the Huygens' part is dominant. The (finite) perturbation series will therefore be a good approximation to the solution whenever the support of the Green function for Maxwell's equations lies mainly on the characteristic surfaces.

IV. APPLICATIONS

A. Propagation of Maxwell fields on self-dual space–times

It is well known that SD and ASD Maxwell fields have zero stress-energy tensor and thus are solutions of the Einstein–Maxwell equations on a vacuum space–time. If the vacuum space–time is self-dual these solutions represent the (classical) interaction of photons with non-linear gravitatons.[16] Before proceeding further with our formalism, we present a brief review of the geometry of asymptotically flat self-dual space–times, the so called H-spaces. For a detailed account the reader is referred to Ref. 16.

Given an arbitrary null hypersurface whose intersection with $\mathscr{I}^+$ is described by the "cut" $u=Z(\zeta,\bar{\zeta})$, the condition for it to have asymptotically vanishing shear is that it satisfies the so called "good cut equation":[16]

$$\eth^2 Z=\sigma_B(Z,\zeta,\bar{\zeta}), \tag{IV.1}$$

where $\sigma_B(u,\zeta,\bar{\zeta})$ is the asymptotic shear associated with the Bondi cut $u=$constant. Note that (IV.1) is a non-linear second order p.d.e for a function Z on the sphere. Since σ_B is complex and Z real, in general eq. (IV.1) has no real solutions.

However, if we allow Z to be complex and if $\sigma_B(u,\zeta,\bar{\zeta})$ can be extended to a holomorphic function of *three independent complex variables* $(u,\zeta,\bar{\zeta})$, one can show that the good cut equation (IV.1) has a four-parameter family of (complex) solutions $Z(x,\zeta,\bar{\zeta})$. The space of solutions $\{Z(x,\zeta,\bar{\zeta}),x\in C^4\}$ is called H-space and can be given the structure of a complex manifold. One can also show that the function Z induces a holomorphic metric g_{ab} on H that satisfies the vacuum equations and has a self-dual Weyl tensor.[16]

Since σ_B represents (from the standard formulation of GR) outgoing gravitational waves, one has available a natural linear structure of superposition of incoming waves that yields a non-linear superposition of self-dual metrics [eq. (IV.1) is intrinsically non-linear]. Moreover, despite all the non-linearity of the theory, the scattering of self-dual gravitational waves is trivial. The solutions of (IV.1) are usually called "non-linear gravitons." Although self-dual solutions of Einstein's equations seem to be a mathematical device with no physical interest, they play a key role in the canonical approach to quantum gravity.[5]

To obtain the general solution of Maxwell's equations on H-spaces we will assume the Z function, which is obtained by solving (IV.1), is given and repeat the steps leading to (II.14). However, in this case the conformal factor is chosen as $g^{01}=1$.[16] From this condition and the fact that $\nabla_a\Lambda=(d\sigma/du)Z_a\equiv\sigma_B Z_a$ [see (IV.1)], we can readily write down the metric components g^{ij},

$$g^{ij}(x,\zeta,\bar{\zeta})=\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & -\bar{\Lambda}_{,r} & g^{1-} \\ 1 & 0 & g^{1-} & g^{11} \end{pmatrix}, \tag{IV.2}$$

with

$$g^{1-}=-\tfrac{1}{2}\,\eth\bar{\Lambda}_{,r} \quad g^{11}=-2+\bar{\Lambda}_{,r}\dot{\sigma}-\tfrac{1}{2}\,\eth^2\bar{\Lambda}_{,r}. \tag{IV.3}$$

We also observe from (II.20) and (IV.1) that, for H-spaces,

$$f=\bar{f}=g=0, \quad \bar{g}=\tfrac{1}{2}\,[(r-r_0)\bar{\Lambda}_{,r}-2(\bar{\Lambda}-\bar{\Lambda}_0)], \tag{IV.4}$$

i.e., in H-spaces the SD part of $\hat{L}_{[a}M_{b]}$ vanishes. Therefore, for self-dual space–times (III.17) adopts the simple form

$$\eth F=-A(Z(x,\bar{\zeta},\bar{\zeta}),\zeta,\bar{\zeta}). \tag{IV.5}$$

The solution of eq. (IV.5) is

$$F(x,\zeta,\bar{\zeta})=-\int_{S^2}G_{0,-1'}(\zeta,\bar{\zeta};\zeta',\bar{\zeta}')A(Z(x,\zeta',\bar{\zeta}'),\zeta',\bar{\zeta}')dS'. \tag{IV.6}$$

Note from (IV.5) that two terms on the r.h.s. of (III.4) vanish. The remaining term is simplified by the explicit form of the metric, eq. (IV.2), giving

$$A_a(x)=2(\nabla^b\eth F)Z_{[a}\eth Z_{b]}+\nabla_a F. \tag{IV.7}$$

Introducing the normalized null tetrad $\{\mathscr{L}^a,\mathscr{M}^a,\bar{\mathscr{M}}^a,\mathscr{N}^a\}$, where

$$\begin{aligned} &\mathscr{L}_a=\nabla_a u, \quad \mathscr{M}_a=\nabla_a\omega, \quad \bar{\mathscr{M}}_a=\nabla_a\bar{\omega}+\tfrac{1}{4}\,(\eth\bar{\Lambda}_{,r})\nabla_a u-\tfrac{1}{2}\,\bar{\Lambda}_{,r}\nabla_a\omega, \\ &\mathscr{N}_a=\nabla_a u+\nabla_a r+(\tfrac{1}{4}\,\eth^2\bar{\Lambda}_{,r}-\tfrac{1}{2}\,\bar{\Lambda}_{,r}\dot{\sigma})\nabla_a u-\tfrac{1}{4}\,(\eth\bar{\Lambda}_{,r})\nabla_a\omega, \end{aligned} \tag{IV.8}$$

and performing the natural gauge transformation $A_a\to A_a-\nabla_a F$, we can rewrite (IV.7) in a more convenient form. The details are given in Appendix D. The final result is

$$A_a(x)=\frac{1}{4\pi}\int_{S^2}dS\dot{A}(Z(x,\zeta,\bar{\zeta}),\zeta,\bar{\zeta})\bar{\mathscr{M}}_a(x,\zeta,\bar{\zeta}), \tag{IV.9}$$

$$F_{ab}(x)=\frac{1}{2\pi}\int_{s^2}dS[\ddot{A}\mathscr{L}_{[a}\bar{\mathscr{M}}_{b]}+\dot{A}\nabla_{[a}\bar{\mathscr{M}}_{b]}], \tag{IV.10}$$

where $\dot{A}\equiv(\partial/\partial u)A$.

To check that F_{ab} satisfies the field equations, we only have to prove that it is a SD field. Since $\mathscr{L}_{[a}\bar{\mathscr{M}}_{b]}$ is, by construction, SD (IV.8), we should only show that $\nabla_{[a}\bar{\mathscr{M}}_{b]}$ is SD, that is, it has vanishing contraction with any ASD 2-form. In particular, if we introduce the ASD 2-form basis,

$$\mathscr{L}_{[a}\mathscr{M}_{b]}, \quad \mathscr{L}_{[a}\mathscr{N}_{b]}+\bar{\mathscr{M}}_{[a}\mathscr{M}_{b]}, \quad \bar{\mathscr{M}}_{[a}\mathscr{N}_{b]},$$

we should check that

$$\mathscr{L}^a \mathscr{M}^b \nabla_{[a} \bar{\mathscr{M}}_{b]} = (\mathscr{L}^a \mathscr{N}^b + \bar{\mathscr{M}}^a \mathscr{M}^b) \nabla_{[a} \bar{\mathscr{M}}_{b]} = \bar{\mathscr{M}}^a \mathscr{N}^b \nabla_{[a} \bar{\mathscr{M}}_{b]} = 0,$$

where

$$\nabla_{[a} \bar{\mathscr{M}}_{b]} = \mathscr{M}_{[a} \nabla_{b]} (\bar{\Lambda} \bar{\Lambda}_{,r}).$$

The first equality is immediate, whereas the second and third follow from the following relationships in H-space,[17]

$$\bar{\Lambda}_{,\bar{\omega}} = -\tfrac{1}{2} \eth \bar{\Lambda}_{,r}, \quad \bar{\Lambda}_{,\omega} = \tfrac{1}{2} \bar{\eth} \bar{\Lambda}_{,r},$$
$$\bar{\Lambda}_{,u} = \tfrac{1}{2} \bar{\Lambda}_{,r} - \tfrac{1}{4} \bar{\Lambda}_{,r}^2 \dot{\sigma}_B - \tfrac{1}{4} \bar{\eth} \eth \bar{\Lambda}_{,r} + \tfrac{1}{8} \bar{\Lambda}_{,r} \eth^2 \bar{\Lambda}_{,r} - \tfrac{1}{16} (\eth \bar{\Lambda}_{,r})^2. \tag{IV.11}$$

The solution to the ASD field equation (III.18) can be obtained following a similar approach to the one outlined above. In this case, however, the equations are more involved since the integral term in (III.18) is not trivial. (Note that the ASD fields are not just the complex conjugate of SD fields, as the underlying manifold is complex in this case.) There is an alternative approach based on the observation from (IV.8) that for each $(\zeta, \bar{\zeta}) \in S^2$, the 2-form,

$$\mathscr{L}_{[a} \bar{\mathscr{M}}_{b]} = \nabla_{[a} u \nabla_{b]} \omega \tag{IV.12}$$

is closed and ASD and thus, it is a particular solution of Maxwell equations.

If we multiply (IV.12) with *any* complex scalar function of $(u, \zeta, \bar{\zeta})$ and then integrate on the sphere we should obtain the general ASD field. Taking eqs. (IV.9) and (IV.10) as a reference, we make the following ansatz for the general solution of the ASD field equations:

$$A_a(x) = \frac{1}{4\pi} \int_{S^2} dS \dot{\bar{A}}(Z(x, \zeta, \bar{\zeta}), \zeta, \bar{\zeta}) \bar{\mathscr{M}}_a(x, \zeta, \bar{\zeta}), \tag{IV.13}$$

$$F_{ab}(x) = \frac{1}{2\pi} \int_{s^2} dS \ddot{\bar{A}} \mathscr{L}_{[a} \bar{\mathscr{M}}_{b]}. \tag{IV.14}$$

It only remains to check that $\bar{A}$ in (IV.13) is in fact the asymptotic value of the Maxwell connection, as had previously been defined. This is done in Appendix D.

As pointed out in Appendix B, the function (B.5) $Z^{(0)}(x, \zeta, \bar{\zeta})$ with $x \in C^4$ is the general regular solution of the good cut equation (IV.1) when $\sigma_B = 0$. This function describes the light cone cuts of complex Minkowski space–time. Complex Minkowski space–time is therefore a particular case of H space where (IV.10) and (IV.14) reduce to D'Adamard [18] solutions of Maxwell equations. Thus, (IV.10) and (IV.14) are the generalizations of D'Adamard formula to H spaces.

B. Small deviations from Minkowski space

When discussing the propagation of light on vacuum space–times, it is often a good approximation to consider the background geometry as a small deviation from Minkowski space. In those cases we can replace F by the first terms in the expansion $F = \Sigma_n F^{(n)}$ in powers of Λ, as Minkowski space is characterized by the equation $\Lambda = 0$. We will apply method b of remark 5 in section III to calculate the first two terms of this perturbative solution. This method is based on the facts that $\mathscr{S}$ in (III.24) contains no $\mathscr{O}(\Lambda^0)$ term and that Z is a linear functional of Λ,

$$Z=Z^{(0)}+\int_{S^2}G_{0,-2'}\Lambda dS'\equiv Z^{(0)}+Z^{(1)}. \tag{IV.15}$$

In (IV.15) $G_{0,-2'}$ is the Green function (B.9) for $\eth^2$ and $Z^{(0)}$ the general solution of the equation $\eth^2 Z=0$, given in inertial coordinates in (B.5).

Order 0

At $\mathcal{O}(\Lambda^0)$, $Z=Z^{(0)}$ (IV.15), $f=g=0$ (II.20) and (III.17) reduces to the Sparling equation (I.3), as expected. The solution is given by the first term in (III.24), with $\mathcal{F}$ calculated using $Z^{(0)}$. We can readily write down the field strength from (IV.10) and (B.7). This is just the D'Adamard formula,

$$F^{(0)}_{ab}(x)=\frac{1}{2\pi}\sum_{S^2}\ddot{A}(x^c l'_c,\zeta',\bar{\zeta}')l_{[a}(\zeta',\bar{\zeta}')\bar{m}_{b]}(\zeta',\bar{\zeta}')dS'. \tag{IV.16}$$

Order 1

As pointed out above, $\mathcal{G}$ in (III.24) contains no order zero term. Therefore, the first order expansion of F agrees with that of $(1+\mathcal{G})\mathcal{F}$. From (II.20) we obtain the first order approximations for f and g,

$$f=0,\quad g=\tfrac{1}{2}[(r-r_0)\Lambda_{,r}-2(\Lambda-\Lambda_0)]. \tag{IV.17}$$

Thus, the linear expansion of F is

$$F^{(0)}+F^{(1)}=-\int_{S^2}G_{0,-1'}\left[A(Z^{(0)},\zeta',\bar{\zeta}')+\dot{A}(Z^{(0)},\zeta',\bar{\zeta}')Z^{(1)}+\int_x^\infty g\hat{\phi}^{(0)}dr'\right]dS', \tag{IV.18}$$

with $\hat{\phi}^0=F^{(0)}_{ab}l^a\bar{m}^b$ and g in (IV.17).

Although in principle the Z function is assumed to be given, the background geometry is usually described in terms of the metric and its associated tensors. In those cases, the process of obtaining Z or Λ is involved (one must solve the geodesic deviation). However, it can be shown[2] that in the linear gravity approximation

$$\Lambda\simeq\sigma_B(Z^{(0)},\zeta,\bar{\zeta})-\int_r^\infty(r'-r)\Psi_0(Z^{(0)},\eth Z^{(0)},\bar{\eth}Z^{(0)},r',\zeta,\bar{\zeta})dr'. \tag{IV.19}$$

If the space–time is a small deviation from Minkowski space and if the Weyl tensor, rather than Z or Λ, is given, one can then use (IV.19) in (IV.15) and (IV.18) to obtain the linear gravity approximations of Z and F.

V. SUMMARY AND CONCLUSIONS

We have presented a manifestly conformally invariant formulation of Maxwell theory on asymptotically flat space–times. The field equations for our basic variable, the phase of the parallel propagator associated with self-dual (or antiself-dual) Maxwell fields, contain the free data $A(u,\zeta,\bar{\zeta})$ (or $\bar{A}$) at $\mathcal{I}^+$ as a source term and the solution of those equations is the generalization of D'Adamard's formula to curved space–times. A method to reconstruct the Maxwell field was given. In particular, adding a solution of (III.17) and its complex conjugate yields a real field that satisfies the source free Maxwell's equations. Since the free data has a well defined physical interpretation, namely, it represents incoming radiation, the solutions to the field equations represent the scattering of light due to the background curvature.

Exact solutions of the field equations were obtained when the background geometry was self-dual. A Huygens perturbation series was presented. The terms in the series can be given a physical interpretation. The zeroth order term represents a Huygens propagation on curved spaces. The first and higher order term yield the tails of the electromagnetic wave produced by the scattering of the field in the non-trivial geometry.

Since this formalism is specially adapted to discuss the evolution of electromagnetic radiation on a curved space–time we now address a few questions that can be answered without involved calculations or too many technical details.

We start with a question that was partially answered in Ref. 19; do SD or ASD Maxwell fields have trivial scattering in self-dual space–times? Since for H spaces σ_B is the same at $\mathscr{I}^+$ and $\mathscr{I}^-$, it follows from (IV.1) that cuts Z at $\mathscr{I}^+$ or at $\mathscr{I}^-$ are the same. Inserting this condition in (IV.10) and (IV.14) implies that the free data A at $\mathscr{I}^+$ or $\mathscr{I}^-$ are also the same. Thus, we conclude that electromagnetic radiation does not interact with self-dual gravitational waves.

A question that arises in the context of gravitational lensing is: does the curvature of space-time rotate the polarization vector of an electromagnetic wave? The difficulty with this question is that one should assign a meaning to the word "rotate" since it implies a comparison of vectors at different locations. An analogous, question is: can the curvature of space–time change the helicity on an electromagnetic wave?

To answer this question we first discuss the notion of helicity in our formalism. In Minkowski space one can show that self-dual Maxwell fields yield positive and negative helicity states via the positive or negative frequency decomposition of the free data $A(u,\zeta,\bar{\zeta})$ at $\mathscr{I}^+$.[20] Since asymptotically flat space–times share the same null boundary with Minkowski space, it is possible to define the notion of asymptotic helicity for the electromagnetic radiation. The Fourier transform of the data, $A(\omega,\zeta,\bar{\zeta})$, defines, for positive or negative frequencies ω, the corresponding asymptotic helicity states for the incoming radiation. The scattering of Maxwell fields is then studied by giving the initial data $A_{\mathscr{I}^-}$ at $\mathscr{I}^-$, solving the field equations in an entirely analogous way to what was done in section III, and then projecting the field to $\mathscr{I}^+$ as in (III.7) to obtain $A_{\mathscr{I}^+}$. By analyzing the frequency content of $A_{\mathscr{I}^+}$ we can determine whether or not helicity has been conserved. Our equations clearly suggest that helicity is not conserved.

The problem of scattering and its applications to gravitational lensing is currently being studied. A thorough discussion using this formalism will be presented in a following work.

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APPENDIX A: THE FIELD EQUATION FOR THE F FUNCTION

We derive here an equation for F equivalent to the full set of source free Maxwell's equations. To do this consider the 3-volume V limited by (i) $\Delta_x(\zeta,\bar{\zeta})$, (ii) $\Delta_x(\zeta,\bar{\zeta}+d\bar{\zeta})$, (iii) $\bar{\Delta}_x(\zeta,\bar{\zeta})$, (iv) $\bar{\Delta}_x(\zeta+d\zeta,\bar{\zeta})$ and (v) the cap on $\mathscr{I}^+$; the corresponding surface elements being $\hat{L}^{[a}M^{b]}(x,\zeta,\bar{\zeta})(d\zeta dr/P)$, etc.[21] If the source free Maxwell's equations,

$$\partial^*_{[a}F_{bc]}=0,$$

are integrated in V we obtain (the i factor is put for later convenience)

$$0=\int_V i3!\partial^*_{[a}F_{bc]}dx^a dx^b dx^c=\int_{\partial V} i^*F_{bc}dx^b dx^c. \tag{A1}$$

The surface term is the sum of five integrals. As an example we calculate the surface integral over regions (i) and (ii):

$$\int_{(i)+(ii)} i^*F_{ab}dx^a dx^b = \frac{C(x,\zeta,\bar{\zeta})}{P(\zeta,\bar{\zeta})}\,d\zeta' - \frac{C(x,\zeta,\bar{\zeta}+d\bar{\zeta})}{P(\zeta,\bar{\zeta}+d\bar{\zeta})}\,d\zeta = -\bar{\delta}C\,\frac{d\zeta d\bar{\zeta}}{P^2}, \tag{A2}$$

where

$$C \equiv \int i^*F_{ab}\hat{L}^{[a}M^{b]}dr = \int F^{ab}i^*\hat{L}_{[a}M_{b]}ds. \tag{A3}$$

Analogously

$$\int_{(iii)+(iv)} i^*F_{ab} = -\delta\bar{C}\,\frac{d\zeta d\bar{\zeta}}{P^2}. \tag{A4}$$

Using (II.19), (A3) takes the following form:

$$C = H + 2\int (\bar{f}\hat{\phi} + g\hat{\bar{\phi}})dr \tag{A5}$$

From (A1), (A2) and (A4) we get

$$\bar{\delta}C + \delta\bar{C} + (i^*F_{ab}M^a\bar{M}^b)_{,\mathcal{I}^+} = 0. \tag{A6}$$

Using (A5), (III.7), (III.9) and (III.12), we can rewrite (A6) as

$$\delta\bar{\delta}F + \delta\bar{A} + \bar{\delta}A + \delta\int_{r_0}^{\infty}(f\hat{\bar{\phi}} + \bar{g}\hat{\phi})dr + \bar{\delta}\int_{r_0}^{\infty}(\bar{f}\hat{\phi} + g\hat{\bar{\phi}})dr = 0. \tag{A7}$$

Note that for SD [ASD] fields (A7) reduces to (III.17) [(III.18)].

We now show how to recover the Maxwell field F_{ab} from $F(x,\zeta,\bar{\zeta})$. Using eq. (C6) we can rewrite (III.3) as

$$H(x,\zeta,\bar{\zeta}) = \int_r^{\infty} F_{ab}(r')\hat{L}^a(r',\zeta,\bar{\zeta})[(r'-r)\hat{M}^b(r',\zeta,\bar{\zeta}) + (\Lambda(r',\zeta,\bar{\zeta}) - \Lambda(r,\zeta,\bar{\zeta}))\hat{\bar{M}}^b(r',\zeta,\bar{\zeta})]dr'. \tag{A8}$$

The integral is along $l_x(\zeta,\bar{\zeta})$, parametrized as in Appendix C, i.e., a point x' in the geodesic is given by $x' = x'(u,\omega,\bar{\omega},r';\zeta,\bar{\zeta})$. From (A8)

$$\hat{L}^a\nabla_a H = H_{,r} = -\int_r^{\infty}\hat{\phi}(r',\zeta,\bar{\zeta})dr' - \Lambda_{,r}\int_r^{\infty}\hat{\bar{\Phi}}(r',\zeta,\bar{\zeta})dr'.$$

Using this equation and its complex conjugate one can algebraically solve for $\int_r^{\infty}\hat{\phi}(r',\zeta,\bar{\zeta})dr'$. Taking one more radial derivative yields

$$\hat{\phi} = \left[\frac{(\delta F)_{,r} - \Lambda_{,r}(\bar{\delta}F)_{,r}}{1 - \Lambda_{,r}\bar{\Lambda}_{,r}}\right]_{,r} \equiv \hat{\Phi}[F] \quad \text{and c.c.}, \tag{A9}$$

i.e., eq. (III.14).

Putting together (A7) and (A9) we obtain the following integro-differential equation for F:

$$\eth\bar{\eth}F+\eth\left[\bar{A}+\int_{r_0}^{\infty}(f\hat{\Phi}[F]+\bar{g}\hat{\Phi}[F])dr\right]+\bar{\eth}\left[A+\int_{r_0}^{\infty}(\bar{f}\hat{\Phi}[F]+g\hat{\phi}[F])dr\right]=0. \tag{A10}$$

(A10) is our version of the source free Maxwell equations on curved spaces. It is not hard to see from (A10) that F is linear in the data $(A,\bar{A})$, from where it follows that we can first solve for the SD part of the field (by setting $\bar{A}=0$), and then add the solution for the ASD part ($A=0$), as in (III.23).

APPENDIX B: GREEN FUNCTIONS FOR THE ETH OPERATOR

The action of the eth operator on a spin weight s function f_s is given by[15]

$$g_{s+1}=\eth f_s\equiv P^{1-s}\frac{\partial}{\partial\zeta}(P^s f_s),\quad P\equiv 1+\zeta\bar{\zeta}. \tag{B1}$$

Similarly, the action of the eth-bar operator is

$$h_{s-1}=\bar{\eth}f_s\equiv P^{1+s}\frac{\partial}{\partial\bar{\zeta}}(P^{-s}f_s), \tag{B2}$$

therefore the commutator is

$$\bar{\eth}\eth-\eth\bar{\eth})f_s=2sf_s. \tag{B3}$$

From (B1), it follows that the only *regular* solution of the equation $\partial f_0=0$ is a constant. As the linear operator $\hat{\Phi}[\cdot]$ (III.14) acting on an S^2 constant gives zero, the solution F to the field equation (III.17) has the indeterminacy of an additive function of the space–time coordinates $f(x)$. As explained in remark 2 of Section III and in Ref. 14 this is a gauge term. Also from (B1), the general (regular) solution $Z^{(0)}$ of the "good cut equation" (IV.1) with $\sigma_B=0$,

$$\Lambda=\eth^2Z^{(0)}=0, \tag{B4}$$

is found to be a linear combination of 1, ζ/P, $\bar{\zeta}/P$ and $\zeta\bar{\zeta}/P$.[16] The choice of parametrization of the solution space gives a coordinate system for this H space (section IV). In particular, by choosing

$$Z^{(0)}(x,\zeta,\bar{\zeta})=x^a l_a(\zeta,\bar{\zeta}), \tag{B5}$$

$$l_a(\zeta,\bar{\zeta})=\frac{1}{\sqrt{2}P}(-1-\zeta\bar{\zeta},\zeta+\bar{\zeta},i(\bar{\zeta}-\zeta),-1+\zeta\bar{\zeta}), \tag{B6}$$

it is easily shown that this H space is (complex) Minkowski space–time (equivalently, $Z^{(0)}$ gives the family of space–times conformal to Minkowski space), and that x are inertial coordinates. This is proven by first obtaining the metric tensor (IV.2) and then transforming to the x coordinates using (II.7) and (B5). The result is $g^{ab}=\mathrm{diag}(-1,1,1,1,)$. Furthermore, the null tetrad (IV.8) is covariantly constant. In the x^a coordinates,

$$\mathscr{L}^a(x,\zeta,\bar{\zeta})=l^a(\zeta,\bar{\zeta})=g^{ab}l_a(\zeta,\bar{\zeta}),\quad \mathscr{M}^a(x,\zeta,\bar{\zeta})=\eth l^a(\zeta,\bar{\zeta})\equiv m^a(\zeta,\bar{\zeta}),$$

$$\bar{\mathscr{M}}^a(x,\zeta,\bar{\zeta})=\bar{\eth}l^a(\zeta,\bar{\zeta})\equiv\bar{m}^a(\zeta,\bar{\zeta}),\quad \mathscr{N}^a(x,\zeta,\bar{\zeta})=(1+\eth\bar{\eth})l^a(\zeta,\bar{\zeta})\equiv n^a(\zeta,\bar{\zeta}), \tag{B7}$$

where the usual notation for this tetrad in Minkowski space was introduced.

In a guide to construct Green functions for arbitrary combinations of ð and ð in terms of contractions of the tetrad (B7) is given. In particular, it is easy to verify from the information given there that

$$G_{0,-1'}(\zeta,\bar{\zeta};\zeta',\bar{\zeta},)\equiv\frac{1}{4\pi}\frac{l(\zeta,\bar{\zeta})\cdot\bar{m}(\zeta',\bar{\zeta}')}{l(\zeta,\bar{\zeta})\cdot l(\zeta',\bar{\zeta}')} \tag{B8}$$

is the Green function for the ð operator acting on spin-weight 0 functions. This function is used in the definition of $\mathscr{S}$ in the solution of the field equation (III.17)

Similarly, the Green function of $ð^2$ acting on spin-weight zero functions is

$$G_{0,-2'}(\zeta,\bar{\zeta};\zeta',\bar{\zeta},)\equiv\frac{1}{4\pi}\frac{(l\cdot\bar{m}')^2}{l\cdot l'}. \tag{B9}$$

This is used in (IV.15) to obtain $Z^{(1)}$.

APPENDIX C: GEODESIC DEVIATION VECTOR

Inverting (II.7) with $(\zeta,\bar{\zeta})$ fixed we get

$$x^a=x^a(u,\omega,\bar{\omega},r;\zeta,\bar{\zeta}). \tag{C1}$$

If $x\in l_{x_0}(\zeta,\bar{\zeta})$, the null geodesic with end points at x_0 and the $(\zeta,\bar{\zeta})$ generator of $\mathscr{I}^+$, then

$$u(x;\zeta,\bar{\zeta})=u(x_0,\zeta,\bar{\zeta}),\quad \omega(x,\zeta,\bar{\zeta})=\omega(x_0;\zeta,\bar{\zeta}),\quad \bar{\omega}(x,\zeta,\bar{\zeta})=\bar{\omega}(x_0;\zeta,\bar{\zeta}), \tag{C2}$$

as can be easily seen from (II.9), (II.10), (II.11) and the fact that $Z^a(x,\zeta,\bar{\zeta})$ is tangent to the geodesic at x. Thus, for $x\in C_{x_0}$, the future null cone of x_0, it follows from (C1) and (C2) that

$$x^a=x^a(u=Z(x_0;\zeta,\bar{\zeta}),\quad \omega=ðZ(x_0,\zeta,\bar{\zeta}),\quad \bar{\omega}=\bar{ð}Z(x_0;\zeta,\bar{\zeta}),\quad r+ðð Z(x_0,\zeta,\bar{\zeta});\zeta,\bar{\zeta}. \tag{C3}$$

In (C3), r has been redefined in order to obtain a coordinate system $(r,\zeta,\bar{\zeta})$ for C_{x_0}. The geodesic deviation vector $M^a\equiv ðx^a$ can be obtained from (C3) using (B1) and (B2),

$$P\frac{d}{d\zeta}x^a=\hat{N}^a\omega(x_0^b,\zeta,\bar{\zeta})-\hat{\bar{M}}^a[\Lambda(x_0^b,\zeta,\bar{\zeta})-\bar{\zeta}\omega]$$

$$-\hat{M}^a[r(x_0^b,\zeta,\bar{\zeta})+\bar{\zeta}\bar{\omega}]+\hat{L}^a ðr(x_0,\zeta,\bar{\zeta})+P\frac{\partial x^a}{\partial\zeta}. \tag{C4}$$

The last term in (C4) is the partial derivative of (C1) with respect to ζ. To calculate this derivative, we note from (II.7), (B1) and (B2) that, if x and $(\zeta,\bar{\zeta})$ moves in such a way that $u,\omega,\bar{\omega},r$ remain fixed, then

$$0=\delta u=\delta x^a\nabla_a u+\frac{\delta\zeta}{P}\omega,\quad 0=\delta\omega=\delta x^a\nabla_a\omega+\frac{\delta\zeta}{P}[\Lambda-\bar{\zeta}\omega],$$

$$0=\delta\bar{\omega}=\delta x^a\nabla_a\bar{\omega}+\frac{\delta\zeta}{P}[r+\bar{\zeta}\bar{\omega}],\quad 0=\delta r=\delta x^a\nabla_a r+\frac{\delta\zeta}{P}\bar{ð}r.$$

Using (B3) and the fact that $\nabla_a u,\nabla_a r,\nabla_a\omega,\nabla_a\bar{\omega}$ is the dual of the basis $\hat{N}^a,\hat{L}^a,-\hat{\bar{M}}^a,-\hat{M}^a$ we get

$$P\frac{\partial}{\partial\zeta}x^a=P\frac{\delta x^a}{\delta\zeta}=-\hat{L}^a\eth r+\hat{\bar{M}}^a[\Lambda-\bar{\zeta}\omega]+\hat{M}^a[r+\bar{\zeta}\bar{\omega}]-\omega\hat{N}^a. \tag{C5}$$

From (C4) and (C5) we obtain the following formula for the geodesic deviation vector:

$$M^a=P\frac{dx^a}{d\zeta}=(\Lambda-\Lambda_0)\hat{\bar{M}}^a(r-r_0)\hat{M}^a-\hat{L}^a\partial(r-r_0). \tag{C6}$$

APPENDIX D:

In this Appendix we complete the steps that lead to Eq. (IV.10) and we prove that in the ASD solution (IV.14), $\bar{A}$ is the data at $\mathscr{I}^+$ as had previously been defined.

Since the r.h.s of (IV.7) does not depend on $(\zeta,\bar{\zeta})$ one can perform an integration on the sphere without changing the result. Thus,

$$A_a(x)=2\frac{1}{4\pi}\int_{S^2}[(\nabla^b\bar{\eth}F)Z_{[a}\eth Z_{b]}]dS+\nabla_a\frac{1}{4\pi}\int_{S^2}F(x,\zeta,\bar{\zeta})dS. \tag{D1}$$

The last integral on the right vanishes if the -c.c. of-the solution (III.24) of (III.17) is chosen (see remark 1 in Section III). If not, it merely reduces to an unimportant gauge term that we will omit. Using (IV6) we can rewrite the above expression as

$$\begin{aligned}A_a(x)=-2\frac{1}{4\pi}\int_{S^2\times S^2}&dSdS'Z_{[a}(x,\zeta,\bar{\zeta})\eth Z_{b]}(x,\zeta,\bar{\zeta})\bar{\eth}G_{0,-1'}\\&\times(\zeta,\bar{\zeta};\zeta',\bar{\zeta}')\dot{A}(Z',\zeta',\bar{\zeta}')Z'^b,\end{aligned} \tag{D2}$$

where $\dot{A}(u,\zeta,\bar{\zeta})\equiv(\partial/\partial u)A(u,\zeta,\bar{\zeta})$. (B3) and $\eth(Z_{[a}\eth Z_{b]})=0$ [which follows from (IV.1)] yield

$$\eth\bar{\eth}(Z_{[a}\bar{\eth}Z_{b]})=\bar{\eth}\bar{\eth}(Z_{[a}\bar{\eth}Z_{b]})-2(Z_{[a}\eth Z_{b]})=-2Z_{[a}\eth Z_{b]},$$

which allows us to rewrite the dS integral in (D2) as

$$\begin{aligned}-2\int_{s^2}(\bar{\eth}G)Z_{[a}\bar{\eth}Z_{b]}dS&=\int_{S^2}(\bar{\eth}G_{0,-1'})\eth\bar{\eth}(Z_{[a}\eth Z_{b]})dS\\&=\int_{S^2}(\eth G_{0,-1'})\bar{\eth}^2(Z_{[a}\eth Z_{b]})dS\\&=\bar{\eth}'^2(Z'_{[a}\eth Z'_{b]}),\end{aligned} \tag{D3}$$

where we have used the fact that $G_{0,-1'}$ is the Green function of the $\eth$ operator. Inserting this result in (D2) gives

$$A_a(x)=\frac{1}{4\pi}\int_{S^2}dS'\dot{A}(Z',\zeta',\bar{\zeta}')Z'^b\bar{\eth}'^2(Z'_{[a}\eth' Z'_{b]}). \tag{D4}$$

Using (IV.2) the contraction can be calculated giving (IV.9).

We now show that the free data in (IV.13) is the asymptotic value of the connection at $\mathscr{I}^+$. From (III.18), the (restricted) free data is given by the following limit, taken along $l_{x_0}(\zeta,\bar{\zeta})$:

$$\bar{A}(x_0,\zeta,\bar{\zeta})=-\lim_{x\to\mathscr{I}^+}\bar{\eth}F(x,\zeta,\bar{\zeta}). \tag{D5}$$

If (III.1) is calculated using (IV.13) then

$$F(x,\zeta,\bar{\zeta})=\frac{1}{4\pi}\int_{S^2}dS'\int_{r(x,\zeta,\bar{\zeta})}^{\infty}dr'\mathring{A}(Z'(x'),\zeta',\bar{\zeta}')Z^b(x')\eth Z'_b(x'), \tag{D6}$$

where again the natural coordinates of section II are used and

$$x'=x'(u,\omega,\bar{\omega},r';\zeta,\bar{\zeta}),\quad u=Z(x;\zeta,\bar{\zeta}),\quad \omega=\eth Z(x;\zeta,\bar{\zeta}),\quad \bar{\omega}=\bar{\eth}Z(x;\zeta,\bar{\zeta}). \tag{D7}$$

Let us change coordinates and view a point x' in $l_x(\zeta,\bar{\zeta})$ as the intersection of $l_x(\zeta,\bar{\zeta})$ with the past cone of $(u,\zeta',\bar{\zeta}')$ at $\mathscr{I}^+$ [i.e., $(u,\zeta',\bar{\zeta}')$ is the point at which $l_{x'}(\zeta',\bar{\zeta}')$ intersects $\mathscr{I}^+$]. Keeping $(\zeta',\bar{\zeta}')$ fixed, u parametrizes $l_x(\zeta,\bar{\zeta})$, thus

$$x'=x'(x,\zeta,\bar{\zeta};u,\zeta',\bar{\zeta}'),\quad \frac{du}{dr'}=Z^c(x')Z'_c(x') \tag{D8}$$

and

$$\bar{\eth}F=\frac{1}{4\pi}\int_{S^2}dS'\int_{Z(x,\zeta',\bar{\zeta})}^{\infty}du\mathring{A}(u,\zeta',\bar{\zeta}')\bar{\eth}\left[\frac{Z^b(x')\eth' Z'_b(x')}{Z^c(x')Z'_c(x')}\right], \tag{D9}$$

where $\eth'$ is calculated without taking into account the $(\zeta',\bar{\zeta}')$ dependence of x' in (D7). Note that[22]

$$\bar{\eth}\left[\frac{Z^b(x')\bar{\partial}' Z'_b(x')}{Z^c(x')Z'_c(x')}\right]=\frac{\mathscr{L}^a(x')\,\bar{\mathscr{M}}^b(x')\mathscr{L}'_{[a}(x')\mathscr{M}'_{b]}(x')+\mathscr{O}(\bar{\Lambda},r)}{(\mathscr{L}^c(x')\mathscr{L}'_c(x'))^2}. \tag{D10}$$

Being $\mathscr{L}'_{[a}\mathscr{M}'_{b]}$ ASD and $\mathscr{L}_{[a}\bar{\mathscr{M}}_{b]}$ SD, their contraction is zero, so it is clear that in the $x\to\mathscr{I}^+$ limit (D10) will be zero in the $\zeta\neq\zeta'$ case, and a 0/0 indeterminacy if $\zeta=\zeta'$. Note that, if the H space is asymptotically flat, then $\lim_{\mathscr{I}^+}\bar{\Lambda}_{,r}(x,\zeta,\bar{\zeta})=0$, the limit taken along $l_x(\zeta,\bar{\zeta})$. To study the $\zeta\simeq\zeta'$ case, we express Z'_c as a second order Taylor expansion of Z_c around $(\zeta,\bar{\zeta})$. To do this, we obtain from (B.1) and (B.2) the relationship between $\eth Z_c,\bar{\eth}Z_c,\eth\bar{\eth}Z_c,\eth^2Z_c,\bar{\eth}^2Z_c$ and the first and second partial derivatives of Z_c, and then use (IV.1) and (IV.2). The result is

$$\begin{aligned}Z^cZ'_c&=\left[(\zeta-\zeta')(\bar{\zeta}-\bar{\zeta}')+\frac{1}{2}(\bar{\zeta}-\bar{\zeta}')^2\bar{\Lambda}_{,r}\right]/P^2+\mathscr{O}((\zeta-\zeta')^3)\\&=\left[(\zeta-\zeta')(\bar{\zeta}-\bar{\zeta}')+\frac{1}{2}(\bar{\zeta}-\bar{\zeta}')^2\bar{\Lambda}_{,r}\right]/[PP']+\mathscr{O}((\zeta-\zeta')^3)\\&=l\cdot l'+\frac{(\bar{\zeta}'-\bar{\zeta})^2}{2PP'}\bar{\Lambda}_{,r}+\mathscr{O}((\zeta-\zeta')^3),\end{aligned} \tag{D11}$$

where the notation of Appendix B has been used. In the $x\to\mathscr{I}^+$ limit, $\bar{\Lambda}_{,r}\to 0$. From (D11) and (B8),

$$-\lim_{x\to\mathscr{I}^+}\frac{1}{4\pi}\bar{\eth}\left[\frac{Z^b(x')\bar{\eth}' Z'_b(x')}{Z^c(x')Z'_c(x')}\right]=-\frac{1}{4\pi}\bar{\eth}\eth'\ln(l\cdot l')=\delta_{-1,1}(\zeta,\bar{\zeta};\zeta',\bar{\zeta}'). \tag{D12}$$

From (D9) and (D12),

$$-\lim_{x\to\mathscr{I}^+}\eth F(x,\zeta,\bar{\zeta})=-\int_{Z(x,\zeta,\bar{\zeta})}^{\infty}du\dot{\bar{A}}(u,\zeta,\bar{\zeta})=\bar{A}(Z(x_0,\zeta,\bar{\zeta}),\zeta,\bar{\zeta}), \tag{D13}$$

and so $\bar{A}$ in (IV.13) is the (restricted) free data, as we wanted to show.

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An invariant imbedding analysis of general wave scattering problems

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The invariant imbedding technique, via the solution of a Riccati-type equation, is modified to calculate the wave fields inside and scattered from a strongly (laterally and vertically) heterogenous, anisotropic inclusion, which may be large but remains compact. The factorization underlying this approach is carried out with respect to direction of average power flow rather than the more conventional factorization with respect to local direction of propagation. The solution of the operator Riccati equation is related to the Dirichlet-to-Neumann map. The formulation is robust in the sense that it can handle a rather extreme range of modal wave speeds, and allows continuous as well as discontinuous medium variations on different (wave) length scales. It also, inherently, takes care of critical-angle phenomena. The algorithm, based on the invariant imbedding approach, yields the internal fields for a full survey of sources and receivers simultaneously. The wave field solution in the inclusion is coupled to the external field via a boundary element approach.
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I. INTRODUCTION

In this article, we discuss a generalization of the invariant imbedding approach[1–4] to calculate the transmitted and backscattered wave fields from a strongly (laterally and vertically) heterogeneous, anisotropic inclusion. The inclusion, typically the size of a couple of wavelengths, defines a compact domain in which the system of coordinates is allowed to be curvilinear to accommodate for sharp as well as anomalous boundary conditions on hypersurfaces and interfaces in the configuration.

A directional decomposition of the wave field underlies the method of invariant imbedding. In the approach proposed in this article, the directional decomposition is carried out with respect to the direction of power flow averaged over a level hypersurface and a period in time, and as such differs from the one carried out with respect to the local propagation direction (Weston[5,6]). The separation into "up" and "down" no longer permits a separation into "left" and "right", here up/down is defined with respect to the local vertical direction, the direction of preference, normal to the hypersurfaces.

As in the standard invariant imbedding approach, we arrive at a Riccati-type equation, but here the standard "slab" has been deformed into a compact manifold. Our Riccati equation is an operator equation rather than an ordinary differential equation. Its solution has the interpretation of admittance operator, and bears close resemblance with the established Dirichlet-to-Neumann map in boundary value problems.[7–9] The internal field in the inclusion is decomposed into two families of "one-way" fundamental solutions.

The Dirichlet-to-Neumann map has been used in the analysis of several physical phenomena. These phenomena dominantly comprised elliptic equations, such as in electric conductivity and static elasticity. The Dirichlet-to-Neumann map appears to be particularly useful in inverse problems. Amongst the extensive literature on this subject is the work of Lee and Uhlmann,[7] who

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derived a reconstruction procedure for anisotropic conductivities by boundary measurements; Nakamura and Uhlmann[8] established uniqueness for the inverse boundary value problems in static elasticity. Our aim is to employ the Dirichlet-to-Neumann map in hyperbolic, wave scattering problems. The feasibility of this has been established by Weston[6] and Fishman,[10] and earlier by Burridge[11] in crack propagation and wave diffraction, and has been further exploited in earthquake seismology.[12,13] The idea of introducing an operator that accounts for the most complicated part of the scattering process is much in the spirit of the T-matrix approach, be it that our approach decomposes the wave field rather than the medium into two constituents (see, e.g., Varadan and Varadan[14]).

The multidimensional invariant imbedding approach proposed in this article has certain advantages for the simulation of waves in complex media, since

(1) the medium can contain sharp and strong discontinuities over potentially many, closely spaced, curved interfaces,

(2) the medium can have a wide range of modal wave speeds,

(3) the medium can be generally anisotropic,

(4) it handles critical-angle phenomena and diffraction without any precaution.

The aim of the approach is to reach a generic accuracy similar to the one of the layer-matrix approach for the computation of the wave field in stratified media (see Kennett[15,16]). Further, invariant imbedding formulations are of theoretical importance to the method of stochastic averaging of wave fields propagating through media with strong small-scale (subwave length) fluctuations. Established proofs of pulse stabilization in the transmitted and backscattered fields in stratified media of such type rely on the structure and properties of the Riccati equation.[17]

The article is organized as follows. In Sec. II, the hyperbolic system on a compact manifold is introduced; Sec. III contains the associated representation theorems. In Sec. IV, the directional decomposition and the subsequent invariant imbedding formulation of the scattering problem to evaluate the internal field are discussed. To this end, an admittance operator is introduced. The existence of the continuation proposed depends on an up/down decomposition of the wave field representation with respect to direction of average power flow. The admittance satisfies a pseudo-differential operator Riccati equation. In Sec. V, the boundary-element method is employed to couple the solution inside the compact domain to the outside world, to evaluate the backscattered and transmitted fields. This hybrid approach is followed since the embedding (the outside world) is typically homogeneous or stratified and thus the embedding's wave field solution can be evaluated with simple methods. In Sec. VI, periodic boundary conditions in the directions transverse to the direction of preference are applied; the numerical aspects of solving the Riccati/one-way system of equations making use of pseudospectral techniques are discussed. To this end, the operator Riccati equation is transformed into an equation for the co-kernel of the admittance operator. Finally, the stability of the continuation is discussed.

II. THE BASIC EQUATIONS

In this section the symmetric hyperbolic system on a compact manifold is introduced. The system applies to wave motion in anisotropic fluid, and elastic and poroelastic media. The observable quantities will be represented by a general $2p\times 1$ field matrix $\mathbf{F}$, which is built from the components of vectors, v say, and tensors, σ say. We will apply the summation convention.

A. Fourier transformation and time averaging

Let t denote time and ω denote angular frequency. The one-sided Fourier transformation is employed to make use of the causality imposed on the wave motion. To show the notation, consider the contravariant vector v^i for which

$$v^i(x_m,\omega)=\int_{t\in\mathbb{R}_{\geqslant 0}} v^i(x_m,t)\exp(-i\omega t)dt. \tag{II.1}$$

Then

$$v^i(x_m,t)=\frac{1}{2\pi}\int_{\omega\in\mathbb{R}-i0} v^i(x_m,\omega)\exp(i\omega t)d\omega. \tag{II.2}$$

A "steady state" constituent is then represented by

$$\mathrm{Re}\{v^i(x_m,\omega)\exp(i\omega t)\}.$$

Let $\sigma_i{}^j$ be a mixed covariant/contravariant tensor, then

$$\mathrm{Re}\{v^i\exp(i\omega t)\}\mathrm{Re}\{\sigma_i{}^k\exp(i\omega t)\}=\tfrac{1}{4}[\bar{v}^i\sigma_i{}^k+v_i\bar{\sigma}_i{}^k]+\tfrac{1}{4}[v^i\sigma_i{}^k\exp(2i\omega t)+\bar{v}^i\bar{\sigma}_i{}^k\exp(-2i\omega t)]. \tag{II.3}$$

Taking the time average $\langle\cdots\rangle_T$ over a period, $T=2\pi/\omega$, of the latter expression then amounts to

$$-\langle\mathrm{Re}\{v^i\exp(i\omega t)\}\mathrm{Re}\{\sigma_i{}^k\exp(i\omega t)\}\rangle_T=-\tfrac{1}{2}\mathrm{Re}\{\bar{v}^i\sigma_i{}^k\}, \tag{II.4}$$

which upon identifying v^i with the (contravariant) particle velocity and $\sigma_i{}^k$ with the (covariant/contravariant) stress corresponds to the k component of the time-averaged (contravariant) elastodynamic Poynting vector. [In this framework, the strain tensor $\epsilon^i{}_j$ becomes mixed contravariant/covariant.]

B. Coordinate transformations and forms, and direction of preference

Let x_j denote global Cartesian coordinates in three-dimensional space. We employ curvilinear coordinates ξ_j on a manifold, standardly taken as contravariant, according to the transformation

$$x_j\rightarrow\xi_j, \tag{II.5}$$

with

$$x_\nu=\xi_\nu,\quad \nu=1,2\qquad \text{and } x_3=\mathrm{f}(\xi_\nu,\xi_3). \tag{II.6}$$

These coordinates parametrize curved hypersurfaces according to $\xi_3=$const. The function f is assumed to be single-valued and continuous; $\xi_3(x_1,x_2,x_3)$ is obtained via the implicit function theorem. Implicitly, a direction of preference has been introduced, viz., locally along the ξ_3-axis.

The spatial derivatives and forms transform as

$$\partial_{x_i}=\mathrm{u}_{ij}^{-1}\partial_{\xi_j},\quad dx_i=\mathrm{u}_{ji}d\xi_j, \tag{II.7}$$

employing the summation convention, in which the transformation matrices,

$$\mathrm{u}_{ij}=\frac{\partial x_j}{\partial\xi_i},\quad \mathrm{u}_{ij}^{-1}=\frac{\partial\xi_j}{\partial x_i},$$

are given by

$$\mathsf{u}=\begin{pmatrix} 1 & 0 & (\partial_{\xi_1}\mathsf{f}) \\ 0 & 1 & (\partial_{\xi_2}\mathsf{f}) \\ 0 & 0 & (\partial_{\xi_3}\mathsf{f}) \end{pmatrix}, \quad \mathsf{u}^{-1}=\begin{pmatrix} 1 & 0 & -\left(\dfrac{\partial_{\xi_1}\mathsf{f}}{\partial_{\xi_3}\mathsf{f}}\right) \\ 0 & 1 & -\left(\dfrac{\partial_{\xi_2}\mathsf{f}}{\partial_{\xi_3}\mathsf{f}}\right) \\ 0 & 0 & \left(\dfrac{1}{\partial_{\xi_3}\mathsf{f}}\right) \end{pmatrix}. \tag{II.8}$$

We have $\det(\mathsf{u}) = (\partial_{\xi_3}\mathsf{f})$, and assume that the Jacobian is regular. This condition can be somewhat relaxed, which will be discussed below. In curved space

$$D_\nu=\frac{i}{\omega}\,\partial_{\xi_\nu}, \quad \nu=1,2 \tag{II.9}$$

are referred to as the *local horizontal slowness operators.*

The metric tensor g_{ij}, associated with the coordinate transformation introduced above, is given by

$$\mathsf{g}_{ij}=\mathsf{u}_{ik}\mathsf{u}_{jl}\delta_{kl}, \quad \mathsf{g}^{ij}=\mathsf{g}_{ij}^{-1}=\mathsf{u}_{ki}^{-1}\mathsf{u}_{lj}^{-1}\delta^{kl};$$

thus

$$(\mathsf{g}_{ij})=\begin{pmatrix} 1+(\partial_{\xi_1}\mathsf{f})^2 & (\partial_{\xi_1}\mathsf{f})(\partial_{\xi_2}\mathsf{f}) & (\partial_{\xi_1}\mathsf{f})(\partial_{\xi_3}\mathsf{f}) \\ (\partial_{\xi_2}\mathsf{f})(\partial_{\xi_1}\mathsf{f}) & 1+(\partial_{\xi_2}\mathsf{f})^2 & (\partial_{\xi_2}\mathsf{f})(\partial_{\xi_3}\mathsf{f}) \\ (\partial_{\xi_3}\mathsf{f})(\partial_{\xi_1}\mathsf{f}) & (\partial_{\xi_3}\mathsf{f})(\partial_{\xi_2}\mathsf{f}) & (\partial_{\xi_3}\mathsf{f})^2 \end{pmatrix} \tag{II.10}$$

and

$$\mathsf{g}^{ij}=\begin{pmatrix} 1 & 0 & -\dfrac{\partial_{\xi_1}\mathsf{f}}{\partial_{\xi_3}\mathsf{f}} \\ 0 & 1 & -\left(\dfrac{\partial_{\xi_2}\mathsf{f}}{\partial_{\xi_3}\mathsf{f}}\right) \\ -\left(\dfrac{\partial_{\xi_1}\mathsf{f}}{\partial_{\xi_3}\mathsf{f}}\right) & -\left(\dfrac{\partial_{\xi_2}\mathsf{f}}{\partial_{\xi_3}\mathsf{f}}\right) & \dfrac{1+(\partial_{\xi_1}\mathsf{f})^2+(\partial_{\xi_2}\mathsf{f})^2}{(\partial_{\xi_3}\mathsf{f})^2} \end{pmatrix}. \tag{II.11}$$

The invariant volume form is then given by

$$dx_1dx_2dx_3=\sqrt{\det(\mathsf{g})}\;d\xi_1d\xi_2d\xi_3.$$

with

$$\det(\mathsf{g})=(\partial_{\xi_3}\mathsf{f})^2. \tag{II.12}$$

To identify the local vertical direction, we employ the vector n_i, normal to the surface ξ_3=const, given by

$$n_i=\sqrt{\mathsf{g}_{33}}\mathsf{u}_{i3}^{-1}=(\partial_{\xi_3}\mathsf{f})\mathsf{u}_{i3}^{-1}$$

or [from the gradient of $(x_3-\mathrm{f})$]

$$n_\nu=-\partial_{\xi_\nu}\mathrm{f},\quad n_3=1 \tag{II.13}$$

with

$$\|\mathbf{n}\|=\det(\mathsf{u})\|\mathsf{u}_{.3}^{-1}\|=[(\partial_{\xi_1}\mathrm{f})^2+(\partial_{\xi_2}\mathrm{f})^2+1]^{1/2}.$$

From Eqs. (II.8) and (II.13) it follows that Eq. (II.7) can be written explicitly in the form

$$\partial_{x_i}=\partial_{\xi_i}-\delta_{i3}\partial_{\xi_3}+\frac{1}{(\partial_{\xi_3}\mathrm{f})}\,n_i\partial_{\xi_3}. \tag{II.14}$$

A surface element $dA(\xi)$, locally normal to n_i and in a level surface of ξ_3, follows from the transformation

$$\frac{n_j\delta_{j3}}{\|\mathbf{n}\|}\,dA(\xi)=d\xi_1 d\xi_2=dx_1dx_2,$$

hence

$$dA(\xi)=\|\mathbf{n}\|d\xi_1d\xi_2. \tag{II.15}$$

A *stretched* normal component of a tensor is typically given by $\sigma_i{}^n=\sigma_i{}^k n_k$, the superscript n is reserved for this particular contraction. A factor $\|\mathbf{n}\|$ is thus absorbed in the normal vector and tensor components.

C. Transformation of field quantities

We will follow a covariant formulation of elasticity; see Fung.[18] For scalar quantities we apply the standard transformation rule

$$\rho'(\xi_m,\omega)=\rho(x_m,\omega). \tag{II.16}$$

For contravariant and covariant vectors v, and mixed co- and contravariant tensors σ, the transformations yield

$$v'_i(\xi_m,\omega)=\mathsf{u}_{ik}v_k(x_m,\omega),\qquad v_i(x_m,\omega)=\mathsf{u}^{-1}_{ik}v'_k(\xi_m,\omega),$$

$$v'^i(\xi_m,\omega)=\mathsf{u}^{-1}_{ki}v^k(x_m,\omega),\qquad v^i(x_m,\omega)=\mathsf{u}_{ki}v'^k(\xi_m,\omega),$$

$$\sigma'_i{}^j(\xi_m,\omega)=\mathsf{u}_{ik}\mathsf{u}^{-1}_{lj}\sigma_k{}^l(x_m,\omega),\quad \sigma_i{}^j(x_m,\omega)=\mathsf{u}^{-1}_{ik}\mathsf{u}_{lj}\sigma'_k{}^l(\xi_m,\omega),$$

where $v^k=v_k$, $v'^i=v'_k\mathsf{g}^{ki}$ and $\sigma'_i{}^j=\sigma'^{kj}\mathsf{g}_{ki}$. [The physical tensor components are given by $v'^i\sqrt{\mathsf{g}_{ii}}$ and $v'_i\sqrt{\mathsf{g}^{ii}}$, $\sigma'_i{}^j\sqrt{\mathsf{g}^{jj}/\mathsf{g}^{ii}}$ (no sums).] Note that $v^n=v^kn_k=\sqrt{\mathsf{g}_{33}}v'^3$. The covariant derivative D_j of a covariant vector follows as

$$\mathsf{D}_jv'_i=\partial_{\xi_j}v'_i-\Gamma^k_{ij}v'_k,\quad \partial_{x_j}v^i=\mathsf{u}^{-1}_{jl}\mathsf{u}^{-1}_{ip}\mathsf{D}_lv'_p; \tag{II.17}$$

the covariant derivative D_j of a contravariant vector follows as

$$\mathsf{D}_jv'^i=\partial_{\xi_j}v'^i+\Gamma^i_{jk}v'^k,\quad \partial_{x_j}v^i=\mathsf{u}^{-1}_{jl}\mathsf{u}_{pi}\mathsf{D}_lv'^p; \tag{II.18}$$

the covariant derivative of a mixed co- and contravariant tensor follows as

$$\mathsf{D}_k\sigma'_i{}^j=\partial_{\xi_k}\sigma'_i{}^j+\Gamma^j_{kl}\sigma'_i{}^l-\Gamma^l_{ik}\sigma'_l{}^j,\quad \partial_{x_k}\sigma_i{}^j=\mathsf{u}^{-1}_{kl}\mathsf{u}^{-1}_{ip}\mathsf{u}_{qj}\mathsf{D}_l\sigma'_p{}^q. \tag{II.19}$$

In our notation the Christoffel symbols are given by

$$\Gamma^i_{jk}=\mathsf{u}^{-1}_{li}\partial_{\xi_j}\mathsf{u}_{kl}=\tfrac{1}{2}\mathsf{g}^{il}[\partial_{\xi_j}\mathsf{g}_{kl}+\partial_{\xi_k}\mathsf{g}_{lj}-\partial_{\xi_l}\mathsf{g}_{jk}].$$

The physical equations of motion and the constitutive relations are obtained from their Cartesian form by replacing the vectors and tensors appropriately, and replacing the partial derivatives by their covariant counterparts.

If we want to allow kinks in the level surfaces, however, we should not differentiate factors $\partial_{\xi_\mu}\mathsf{f}$ with respect to ξ_ν any further. Then, we deviate from the covariant transformation rule, viz., by applying a straightforward change of coordinates,

$$\begin{aligned} v'^i(\xi_m,\omega)&=v^i(x_m,\omega),\\ \sigma'^{ij}(\xi_m,\omega)&=\sigma^{ij}(x_m,\omega), \end{aligned} \tag{II.20}$$

avoiding the introduction of the Christoffel symbols in the equations.

D. The hyperbolic system

We consider a generic symmetric hyperbolic system reduced to the form

$$\partial_{\xi_3}\mathbf{F}+i\omega\mathbf{A}(D_\nu,\partial_{\xi_k}\mathsf{f})\mathbf{F}=\mathbf{N}. \tag{II.21}$$

Here, $\mathbf{F}$ denotes the field matrix of physically observable quantities [e.g., $\mathbf{F}=(-p',v'^n)^T$ for fluid, $\mathbf{F}=(\sigma'^{in},v'^j)^T$ for solid, and $\mathbf{F}=(\sigma'^{in},-p,v'^j,w'^n)^T$ for poroelastic media where p denotes pressure and w infiltration velocity], $\mathbf{A}$ is a matrix of partial differential operators elliptic with parameters (yet to be determined) in (ξ_1,ξ_2)-space, and $\mathbf{N}$ is the matrix of notional sources. The dimension of $\mathbf{F}$ is $2p$ and can be smaller or greater than the dimension of the underlying manifold, 3 in our case. Using this, we introduce a generic *partitioning* of field quantities

$$\mathbf{F}=\begin{pmatrix}\mathbf{F}_1\\ \mathbf{F}_2\end{pmatrix},$$

such that the number of components of $\mathbf{F}_1$ and $\mathbf{F}_2$ are equal to p.

With respect to any partitioning, the system's matrix $\mathbf{A}$ satisfies the symplectic property

$$\mathbf{A}^T\mathbf{J}=-\mathbf{J}\mathbf{A}, \tag{II.22}$$

where a superscript T denotes the adjoint with respect to the real inner product in $[L^2(\mathbb{R}^2)]^{2p}$, and

$$\mathbf{J}=\begin{pmatrix}0 & \boldsymbol{I}\\ -\boldsymbol{I} & 0\end{pmatrix},\quad \text{but also set}\quad \mathbf{K}=\begin{pmatrix}0 & \boldsymbol{I}\\ \boldsymbol{I} & 0\end{pmatrix}$$

for the later analysis. Apart from the horizontal slowness operators, the system's matrix will contain the medium parameters, the normal $\mathbf{n}$ through tensor contractions, and the Jacobian $\det(\mathsf{u})$. An example is derived in App. A.

We are now in the position to formulate our scattering problem. We consider a compact inclusion in an infinite imbedding. The inclusion is irradiated by a point source located in the imbedding; the scattered field is observed in the embedding as well. The field inside the inclusion will be analyzed with an invariant imbedding approach.

III. REPRESENTATION THEOREMS

For the later analysis, we need the representation theorems for the solution of the hyperbolic system. We summarize these theorems in our coordinate system.

A. Reciprocity

Consider two physical states $(\mathbf{N}^a, \mathbf{F}^a)$ and $(\mathbf{N}^b, \mathbf{F}^b)$ in the same medium that both satisfy the system of equations (II.21), i.e.,

$$\partial_{\xi_3}\mathbf{F}^{a,b}+i\omega\mathbf{A}\mathbf{F}^{a,b}=\mathbf{N}^{a,b}.$$

Consider the interaction quantity (note that a factor $\|\mathbf{n}\|$ has been absorbed in $\mathbf{F}_1^{a,b}$)

$$\int_{\xi_\mu\in\mathbb{R}}(\mathbf{F}^a)^T(\xi_\mu,\xi_3)\mathbf{J}\mathbf{F}^b(\xi_\mu,\xi_3)d\xi_1d\xi_2,$$

in which the integral splits into real inner products in $[L^2(\mathbb{R}^2)]^p$. In the previous section, with respect to the full inner product, we have defined the adjoint of $\mathbf{A}$. Employ Eq. (II.21) to obtain

$$\begin{aligned}&\partial_{\xi_3}\int_{\xi_\mu\in\mathbb{R}}(\mathbf{F}^a)^T(\xi_\mu,\xi_3)\mathbf{J}\mathbf{F}^b(\xi_\mu,\xi_3)d\xi_1d\xi_2\\&\quad=-i\omega\int_{\xi_\mu\in\mathbb{R}}(\mathbf{F}^a)^T(\xi_\mu,\xi_3)[\mathbf{A}^T\mathbf{J}+\mathbf{J}\mathbf{A}]\mathbf{F}^b(\xi_\mu,\xi_3)d\xi_1d\xi_2\\&\qquad+\int_{\xi_\mu\in\mathbb{R}}[(\mathbf{N}^a)^T(\xi_\mu,\xi_3)\mathbf{J}\mathbf{F}^b(\xi_\mu,\xi_3)+(\mathbf{F}^a)^T(\xi_\mu,\xi_3)\mathbf{J}\mathbf{N}^b(\xi_\mu,\xi_3)]d\xi_1d\xi_2,\end{aligned}$$

which, given the symmetries (II.22), reduces to a reciprocity relation of the time-convolution type,

$$\begin{aligned}&\int_{\xi_3=\xi_3^0}^{\xi_3^1}\int_{\xi_\mu\in\mathbb{R}}[(\mathbf{N}^a)^T(\xi_\mu,\xi_3)\mathbf{J}\mathbf{F}^b(\xi_\mu,\xi_3)+(\mathbf{F}^a)^T(\xi_\mu,\xi_3)\mathbf{J}\mathbf{N}^b(\xi_\mu,\xi_3)]d\xi_1d\xi_2d\xi_3\\&\quad=\int_{\xi_\mu\in\mathbb{R}}(\mathbf{F}^a)^T(\xi_\mu,\xi_3^1)\mathbf{J}\mathbf{F}^b(\xi_\mu,\xi_3^1)d\xi_1d\xi_2-\int_{\xi_\mu\in\mathbb{R}}(\mathbf{F}^a)^T(\xi_\mu,\xi_3^0)\mathbf{J}\mathbf{F}^b(\xi_\mu,\xi_3^0)d\xi_1d\xi_2.\end{aligned}\tag{III.1}$$

Repeating the steps above for the interaction quantity

$$\int_{\xi_\mu\in\mathbb{R}}\overline{(\mathbf{F}^a)^T}(\xi_\mu,\xi_3)\mathbf{K}\mathbf{F}^b(\xi_\mu,\xi_3)d\xi_1d\xi_2,$$

where the overbar denotes complex conjugation, yields

$$\begin{aligned}&\partial_{\xi_3}\int_{\xi_\mu\in\mathbb{R}}\overline{(\mathbf{F}^a)^T}(\xi_\mu,\xi_3)\mathbf{K}\mathbf{F}^b(\xi_\mu,\xi_3)d\xi_1d\xi_2\\&\quad=-i\omega\int_{\xi_\mu\in\mathbb{R}}\overline{(\mathbf{F}^a)^T}(\xi_\mu,\xi_3)[-\overline{\mathbf{A}^T}\mathbf{K}+\mathbf{K}\mathbf{A}]\mathbf{F}^b(\xi_\mu,\xi_3)d\xi_1d\xi_2\\&\qquad+\int_{\xi_\mu\in\mathbb{R}}[\overline{(\mathbf{N}^a)^T}(\xi_\mu,\xi_3)\mathbf{K}\mathbf{F}^b(\xi_\mu,\xi_3)+\overline{(\mathbf{F}^a)^T}(\xi_\mu,\xi_3)\mathbf{K}\mathbf{N}^b(\xi_\mu,\xi_3)]d\xi_1d\xi_2,\end{aligned}$$

and a reciprocity relation of the time-correlation type follows as

$$\int_{\xi_3=\xi_3^0}^{\xi_3^1}\int_{\xi_\mu\in\mathbb{R}}[\overline{(\mathbf{N}^a)^T}(\xi_\mu,\xi_3)\mathbf{K}\mathbf{F}^b(\xi_\mu,\xi_3)+\overline{(\mathbf{F}^a)^T}(\xi_\mu,\xi_3)\mathbf{K}\mathbf{N}^b(\xi_\mu,\xi_3)]d\xi_1 d\xi_2 d\xi_3$$
$$=i\omega\int_{\xi_3=\xi_3^0}^{\xi_3^1}\int_{\xi_\mu\in\mathbb{R}}\overline{(\mathbf{F}^a)^T}(\xi_\mu,\xi_3)[\overline{\mathbf{A}^T}\mathbf{K}-\mathbf{K}\mathbf{A}]\mathbf{F}^b(\xi_\mu,\xi_3)d\xi_1 d\xi_2 d\xi_3$$
$$+\int_{\xi_\mu\in\mathbb{R}}\overline{(\mathbf{F}^a)^T}(\xi_\mu,\xi_3^1)\mathbf{K}\mathbf{F}^b(\xi_\mu,\xi_3^1)d\xi_1 d\xi_2-\int_{\xi_\mu\in\mathbb{R}}\overline{(\mathbf{F}^a)^T}(\xi_\mu,\xi_3^0)\mathbf{K}\mathbf{F}^b(\xi_\mu,\xi_3^0)d\xi_1 d\xi_2. \tag{III.2}$$

In nondissipative media, we have

$$\overline{\mathbf{A}^T}\mathbf{K}-\mathbf{K}\mathbf{A}=0.$$

B. The dissipative part of the complex energy balance

To derive the dissipative part of the complex energy balance associated with the hyperbolic system, set $b=a$ in Eq. (III.2); omit the state's superscript. Set $\overline{\cdot^T}=\cdot^\dagger$, then

$$-\int_{\xi_\mu\in\mathbb{R}}\mathbf{F}^\dagger(\xi_\mu,\xi_3^1)\mathbf{K}\mathbf{F}(\xi_\mu,\xi_3^1)d\xi_1 d\xi_2+\int_{\xi_\mu\in\mathbb{R}}\mathbf{F}^\dagger(\xi_\mu,\xi_3^0)\mathbf{K}\mathbf{F}(\xi_\mu,\xi_3^0)d\xi_1 d\xi_2$$
$$=i\omega\int_{\xi_3=\xi_3^0}^{\xi_3^1}\int_{\xi_\mu\in\mathbb{R}}\mathbf{F}^\dagger(\xi_\mu,\xi_3)[\mathbf{A}^\dagger\mathbf{K}-\mathbf{K}\mathbf{A}]\mathbf{F}(\xi_\mu,\xi_3)d\xi_1 d\xi_2 d\xi_3$$
$$-\int_{\xi_3=\xi_3^0}^{\xi_3^1}\int_{\xi_\mu\in\mathbb{R}}[\mathbf{N}^\dagger(\xi_\mu,\xi_3)\mathbf{K}\mathbf{F}(\xi_\mu,\xi_3)+\mathbf{F}^\dagger(\xi_\mu,\xi_3)\mathbf{K}\mathbf{N}(\xi_\mu,\xi_3)]d\xi_1 d\xi_2 d\xi_3. \tag{III.3}$$

This equation is completely real-valued. From its left-hand side we obtain the time-averaged normal component of the Poynting vector [cf. Eq. (II.4)]

$$4\langle S_n\rangle_T=-\mathbf{F}^\dagger\mathbf{K}\mathbf{F}=-2\,\mathrm{Re}\{\mathbf{F}_1^\dagger\mathbf{F}_2\}. \tag{III.4}$$

The time-averaged volumetric rate of energy input by external forces is given by

$$4\langle C_{src}\rangle_T=-[\mathbf{N}^\dagger\mathbf{K}\mathbf{F}+\mathbf{F}^\dagger\mathbf{K}\mathbf{N}]=-2\,\mathrm{Re}\{\mathbf{N}^\dagger\mathbf{K}\mathbf{F}\}. \tag{III.5}$$

The remaining term is interpreted as the dissipation potential,

$$4\langle D\rangle_T=-i\omega\mathbf{F}^\dagger[\mathbf{A}^\dagger\mathbf{K}-\mathbf{K}\mathbf{A}]\mathbf{F}=2\omega\,\mathrm{Im}\{\mathbf{F}^\dagger\mathbf{A}^\dagger\mathbf{K}\mathbf{F}\}. \tag{III.6}$$

For passive systems the operator $i\omega[\mathbf{K}\mathbf{A}-\mathbf{A}^\dagger\mathbf{K}]$ is positive. Note that the full complex energy balance follows upon considering the quantity

$$\int_{\xi_\mu\in\mathbb{R}}\mathbf{F}_1^\dagger(\xi_\mu,\xi_3)\mathbf{F}_2(\xi_\mu,\xi_3)d\xi_1 d\xi_2$$

and following the derivation of the reciprocity relation of the time-correlation type.

C. Representation theorem

Finally, we employ the reciprocity relation of the time-convolution type to derive a particular representation theorem, which will be of use for the field inside the inclusion. Define a Green's tensor $\mathbf{G}^I(\xi_\mu,\xi_3;\xi'_\nu,\xi'_3)$ through its notional sources,

$$\mathbf{N}^I=\begin{pmatrix} 0 \\ \boldsymbol{I}\delta(\xi_\mu-\xi'_\mu)\,\delta(\xi_3-\xi'_3)\end{pmatrix}.$$

Substituting this Green's tensor into Eq. (III.1) for state b yields the representation

$$\mathbf{F}_1^T(\xi'_\nu,\xi'_3)=-\int_{\xi_3=\xi_3^0}^{\xi_3^1}\int_{\xi_\mu\in\mathbb{R}}\mathbf{N}^T(\xi_\mu,\xi_3)\mathbf{J}\mathbf{G}^I(\xi_\mu,\xi_3)d\xi_1 d\xi_2 d\xi_3$$
$$+\int_{\xi_\mu\in\mathbb{R}}\mathbf{F}^T(\xi_\mu,\xi_3^1)\mathbf{J}\mathbf{G}^I(\xi_\mu,\xi_3^1)d\xi_1 d\xi_2-\int_{\xi_\mu\in\mathbb{R}}\mathbf{F}^T(\xi_\mu,\xi_3^0)\mathbf{J}\mathbf{G}^I(\xi_\mu,\xi_3^0)d\xi_1 d\xi_2 \tag{III.7}$$

if $\xi'_3\in(\xi_0^3,\xi_3^1)$. For the time being, we leave the boundary conditions for $\mathbf{G}^I$ free. If the system is dissipative, or the heterogenous domain is not compact (is extended to infinity through thin slabs centered on the level surface $x_3=0$), nonradiating boundary conditions of the "rigid" ($\mathbf{G}_2^I|_{\partial\mathscr{L}}=0$) or "normal-traction free" ($\mathbf{G}_1^I|_{\partial\mathscr{L}}=0$) types can be applied to arrive at Rayleigh-type integral representations.[19]

IV. INVARIANT IMBEDDING FORMULATION

In this section, we analyze the internal fields of the scattering problem. The configuration consists of a heterogeneous, compact domain $\mathscr{L}$, in which we have curvilinear coordinates (ξ_μ,ξ_3), imbedded in a homogeneous medium. Outside $\mathscr{L}$ the curvilinear coordinates transfer into the Cartesian coordinates (x_μ,x_3). The level surfaces $\xi_3=\xi_3^0,\xi_3^1$ bounding the heterogeneous domain, and the ones in between, are smoothly connected to the level surface $x_3=0$ outside this domain. Let the level surface $\xi_3=\xi_3^0$ represent the upper boundary $\partial\mathscr{L}^+$ of the heterogeneous domain, and let the level surface $\xi_3=\xi_3^1$ represent the lower boundary $\partial\mathscr{L}^-$; $\partial\mathscr{L}=\partial\mathscr{L}^+\cup\partial\mathscr{L}^-$. Inside $\mathscr{L}$ we assume that there are no sources, i.e., $\mathbf{N}=\mathbf{0}$.

A. Normalization

Given the partitioned wave field, we introduce a scaling matrix (multiplication) $\mathbf{Y}_0$ to be applied to the state vector $\mathbf{F}$, for two purposes:

(1) to balance the values of $\mathbf{F}_1$ and $\mathbf{F}_2$;
(2) to ensure that $\mathbf{A}$ becomes an elliptic operator with parameters which has a proper polyhomogeneous expansion of its symbol (de Hoop and de Hoop[20]); this expansion, as well as the one for the resolvent of $\mathbf{A}$, consists of increasingly smooth operators. We will not explicitly employ it in the further analysis.

The second issue is a condition necessary to ensure that the Dirichlet-to-Neumann map can be represented as a pseudo-differential operator. Thus, set

$$\mathbf{F}'=\mathbf{Y}_0\mathbf{F},\quad \mathbf{Y}_0=\begin{pmatrix} Y_0 & 0 \\ 0 & \boldsymbol{I}\end{pmatrix},\quad Y_0^T=Y_0. \tag{IV.1}$$

Then

$$\partial_3\mathbf{F}'+\omega\mathbf{A}'\mathbf{F}'=-\mathbf{X}\mathbf{F}'+\mathbf{N}' \tag{IV.2}$$

with

$$\mathbf{A}'=\mathbf{Y}_0\mathbf{A}\mathbf{Y}_0^{-1},\quad \mathbf{X}=\mathbf{Y}_0(\partial_3\mathbf{Y}_0^{-1}),\quad \mathbf{N}'=\mathbf{Y}_0\mathbf{N}. \tag{IV.3}$$

The parameters, η_0 say, are introduced in the operator $\mathbf{A}'$ upon replacing $(Y_0)_{ij}$ by $(\eta_0)_i(Y_0)_{ij}$ (no sums). The symplectic matrix in this normalization becomes

$$\mathbf{J}' = \mathbf{Y}_0^{-1}\mathbf{J}\mathbf{Y}_0^{-1} = \begin{pmatrix} 0 & Y_0^{-1} \\ -Y_0^{-1} & 0 \end{pmatrix}$$

so that

$$(\mathbf{A}')^T\mathbf{J}' = -\mathbf{J}'\mathbf{A}'. \tag{IV.4}$$

We will omit the primes in the further analysis.

B. Wave field decomposition

At any level surface in the inclusion, we seek a directional decomposition

$$\mathbf{F}_1 = \mathbf{F}_1^+ + \mathbf{F}_1^-, \tag{IV.5}$$

$$\mathbf{F}_2 = \mathbf{F}_2^+ + \mathbf{F}_2^- \quad \text{such that} \quad \mathbf{F}_2^\pm = \boldsymbol{Y}^\pm \mathbf{F}_1^\pm, \tag{IV.6}$$

and that the decomposed constituents satisfy Eq. (II.21) individually

$$\partial_3 \mathbf{F}_1^+ + i\omega(\mathbf{A}_{1,1} + \mathbf{A}_{1,2}\boldsymbol{Y}^+)\mathbf{F}_1^+ = 0, \tag{IV.7}$$

$$\partial_3 \mathbf{F}_1^- + i\omega(\mathbf{A}_{1,1} + \mathbf{A}_{1,2}\boldsymbol{Y}^-)\mathbf{F}_1^- = 0 \quad \text{in } \mathscr{D}. \tag{IV.8}$$

Here, $\boldsymbol{Y}^+$ and $\boldsymbol{Y}^-$ have the interpretation of *admittance operators* and are yet to be constructed; they will appear to be pseudodifferential operators of order 1. The admittance operator on a level surface defines a 2-form according to

$$\mathbf{F}_1^\pm \rightarrow \boldsymbol{Y}^\pm \mathbf{F}_1^\pm|_{\xi_3 = \text{const}}\, d\xi_1 d\xi_2,$$

which can be identified as the Dirichlet-to-Neumann map.[7] In the context of the "parameters," note that the transformation

$$\boldsymbol{Y}^\pm = (\boldsymbol{Y}^\pm)' Y_0$$

takes care of the normalization. It is important to note that $\mathbf{F}_1$ and $\boldsymbol{Y}$ are both continuous even at level surfaces across which the coefficients of the hyperbolic system jump by finite amounts.

We will now discuss the condition for such a wave field decomposition to exist. Apply the operator $\boldsymbol{Y}^-$ to both sides of Eq. (IV.5) and subtract the resulting equation from Eq. (IV.6). Then we obtain

$$\mathbf{F}_2 - \boldsymbol{Y}^-\mathbf{F}_1 = (\boldsymbol{Y}^+ - \boldsymbol{Y}^-)\mathbf{F}_1^+. \tag{IV.9}$$

Likewise, applying the operator $\boldsymbol{Y}^+$ to both sides of Eq. (IV.5) and subtracting Eq. (IV.6) from the resulting equation, leads to

$$\boldsymbol{Y}^+\mathbf{F}_1 - \mathbf{F}_2 = (\boldsymbol{Y}^+ - \boldsymbol{Y}^-)\mathbf{F}_1^-. \tag{IV.10}$$

If $(\boldsymbol{Y}^+ - \boldsymbol{Y}^-)$ would be invertible, Eqs. (IV.9) and (IV.10) would imply

$$\mathbf{F}_1^+ = (\boldsymbol{Y}^+ - \boldsymbol{Y}^-)^{-1}(\mathbf{F}_2 - \boldsymbol{Y}^-\mathbf{F}_1), \tag{IV.11}$$

$$\mathbf{F}_1^- = (\boldsymbol{Y}^+ - \boldsymbol{Y}^-)^{-1}(\boldsymbol{Y}^+\mathbf{F}_1 - \mathbf{F}_2). \tag{IV.12}$$

A sufficient condition for the inverse of $(\boldsymbol{Y}^+ - \boldsymbol{Y}^-)$ to exist is

$$(\boldsymbol{Y}^+ - \boldsymbol{Y}^-) + (\boldsymbol{Y}^+ - \boldsymbol{Y}^-)^\dagger \text{ is negative or positive}$$

implying that the spectrum of the operator $(\boldsymbol{Y}^+ - \boldsymbol{Y}^-)$ is bounded away from zero. This condition can be separated into two, physical, sufficient conditions, viz. the ones

$$\left.\begin{array}{ll} \boldsymbol{Y}^- + (\boldsymbol{Y}^+)^\dagger & \text{is a negative} \\ \boldsymbol{Y}^- + (\boldsymbol{Y}^-)^\dagger & \text{is a positive} \end{array}\right\} \text{ operator in each level surface.} \tag{IV.13}$$

This means that the Hermitean parts of the operators $\boldsymbol{Y}^\pm$ must be positive/negative. In the time-Laplace domain (see the next subsection), these conditions entail that the Hermitean parts are elliptic. We will loosely refer to them as ellipticity conditions, even in the frequency (ω) domain.

Let us continue with the latter existence conditions. They have the following interpretation. The power flow in the local $+\xi_3$-direction averaged over any level surface and a period [cf. Eq. (III.4)] is proportional to

$$-\int_{\xi_\mu \in \mathrm{R}} \mathbf{F}^\dagger \mathbf{K} \mathbf{F} d\xi_1 d\xi_2 = -2\int_{\xi_\mu \in \mathrm{R}} \mathrm{Re}\{\mathbf{F}_1^\dagger \mathbf{F}_2\} d\xi_1 d\xi_2 = -\int_{\xi_\mu \in \mathrm{R}} \mathbf{F}_1^\dagger (\boldsymbol{Y} + \boldsymbol{Y}^\dagger)\mathbf{F}_1 d\xi_1 d\xi_2,$$

for the $+$ and $-$ solutions. Hence, the sign of $(\boldsymbol{Y}+\boldsymbol{Y}^\dagger)$ determines the direction of average power flow: for the $\pm$-sign in the $\mp\xi_3$-direction. The ellipticity condition implies that there must be transport of energy through the domain under consideration. A somewhat paradoxal case arises if the wave constituent is (locally) propagating in one section of a level surface but (locally) evanescent in another section of the same level surface. However, since the sense of propagation is defined globally in each level surface, localized departures from the sense of propagation are possible. A more extreme possibility is the one where energy flow in one section of the level surface is opposite in direction to the overall flow. We find that the existence conditions enforce the directional decomposition.

In summary, the existence of our wave field decomposition depends on the existence of admittance operators with globally elliptic Hermitean parts, the signs of which are associated with the direction of average power flow. The energy balance provides the tool to reduce the conditions of global ellipticity to similar conditions on the bounding level surfaces $\partial\mathscr{D}$ of the heterogeneous, compact domain $\mathscr{D}$.

Upon integrating the dissipative part of the complex energy balance over a volume $\mathscr{D}_{[\xi_3^a,\xi_3^b]}$ that is bounded by two arbitrary level surfaces $\{\xi_3=\xi_3^a\}$ and $\{\xi_3=\xi_3^b\}$ $(\xi_3^b > \xi_3^a)$, we obtain

$$\int_{\xi_\mu \in \mathrm{R}} \langle \boldsymbol{S}_n \rangle_T|_{\xi_3=\xi_3^a} d\xi_1 d\xi_2 = \int_{\xi_\mu \in \mathrm{R}} \langle \boldsymbol{S}_n \rangle_T|_{\xi_3=\xi_3^b} d\xi_1 d\xi_2 + \int_{\xi_3=\xi_3^a}^{\xi_3^b} \int_{\xi_\mu \in \mathrm{R}} \langle \boldsymbol{D} \rangle_T d\xi_1 d\xi_2 d\xi_3,$$

having excluded the presence of external sources in the volume. For the sign of the component of the averaged Poynting vector normal to the level surface at $\xi_3=\xi_3^b$ to be positive, it is necessary that the sign of the latter component be positive at $\xi_3=\xi_3^a$. This observation holds if the $+\xi_3$-direction coincides with the direction of average power flow. Thus, imposing the condition of ellipticity with the negative sign at $\xi_3=\xi_3^1$ on $\boldsymbol{Y}^+$ guarantees its global proper behavior; similarly, for $\boldsymbol{Y}^-$ imposing the condition of ellipticity with the positive sign at $\xi_3=\xi_3^0$ guarantees that for $\xi_3 \geqslant \xi_3^0$ the $-\xi_3$-direction coincides with the direction of average power flow. The existence conditions obtain the form of constraints on the initial conditions and in fact correspond with radiation conditions.

C. The admittance operator

The admittance operator is a pseudodifferential operator of order 1. (For an overview of such operators, see Hörmander.[21]) In terms of an integral representation with Schwartz kernel $\mathscr{Y}$, we have

$$(\boldsymbol{Y}\mathbf{F}_1)(\xi_\mu,\xi_3)=\int_{\xi'_\nu\in\mathbb{R}}\mathscr{Y}(\xi_\mu,\xi'_\nu;\xi_3)\mathbf{F}_1(\xi'_\nu,\xi_3)d\xi'_1d\xi'_2. \tag{IV.14}$$

Given the plane-wave representation of the field quantities

$$\widetilde{\mathbf{F}}_1(\alpha_\nu,\xi_3)=\int_{\xi_\nu\in\mathbb{R}}\mathbf{F}_1(\xi_\nu,\xi_3)\exp(i\omega\alpha_\nu\xi_\nu)d\xi_1d\xi_2, \tag{IV.15}$$

we can relate the Schwartz kernel of the admittance operator to its left symbol, viz.,

$$\mathscr{Y}(\xi_\mu,\xi'_\nu;\xi_3)=\left(\frac{\omega}{2\pi}\right)^2\int_{\alpha_\nu\in\mathbb{R}}y(\xi_\mu,\alpha_\nu;\xi_3)\exp[i\omega\alpha_\nu(\xi'_\nu-\xi_\nu)]d\alpha_1d\alpha_2, \tag{IV.16}$$

which means that, schematically,

$$\boldsymbol{Y}\exp(-i\omega\alpha_\nu\xi_\nu)=y(\xi_\mu,\alpha_\nu;\xi_3)\exp(-i\omega\alpha_\nu\xi_\nu). \tag{IV.17}$$

In the horizontal Fourier domain, Eq. (IV.14) becomes

$$(\widetilde{\boldsymbol{Y}}\,\widetilde{\mathbf{F}}_1)(\alpha_\mu,\xi_3)=\left(\frac{\omega}{2\pi}\right)^2\int_{\alpha'_\nu\in\mathbb{R}}\tilde{y}(\alpha_\mu-\alpha'_\mu,\alpha'_\nu;\xi_3)\widetilde{\mathbf{F}}_1(\alpha'_\nu,\xi_3)d\alpha'_1d\alpha'_2, \tag{IV.18}$$

where the co-kernel $\tilde{y}$ is given by

$$\tilde{y}(\alpha_\mu,\alpha'_\nu;\xi_3)=\int_{\xi_\mu\in\mathbb{R}}y(\xi_\mu,\alpha'_\nu;\xi_3)\exp(i\omega\alpha_\mu\xi_\mu)d\xi_1d\xi_2. \tag{IV.19}$$

Co-kernels compose according to

$$\widetilde{ya}(\alpha_\mu,\alpha'_\nu;\xi_3)=\left(\frac{\omega}{2\pi}\right)^2\int_{\alpha''_\nu\in\mathbb{R}}\tilde{y}(\alpha_\mu-\alpha''_\mu,\alpha'_\nu+\alpha''_\nu;\xi_3)\tilde{a}(\alpha''_\mu,\alpha'_\nu;\xi_3)d\alpha''_1d\alpha''_2. \tag{IV.20}$$

Note that the locally vertical power flow averaged over a period in time and integrated over a level surface can be expressed in the co-kernel according to

$$-\tfrac{1}{2}\mathrm{Re}\int_{\alpha_\mu\in\mathbb{R}}\int_{\alpha'_\nu\in\mathbb{R}}\widetilde{\mathbf{F}}_1^\dagger(\alpha_\mu,\xi_3)\tilde{y}(\alpha_\mu-\alpha'_\mu,\alpha'_\nu;\xi_3)\widetilde{\mathbf{F}}_1(\alpha'_\nu,\xi_3)d\alpha'_1d\alpha'_2d\alpha_1d\alpha_2,$$

which can be written as a complex inner product. For the numerical representation a pseudospectral approach will be followed based on the horizontal Fourier and co-kernel representations.

The time-Laplace (s-) domain formulation follows from the analysis above upon substituting $s=i\omega$ and $\alpha^s_\nu=-i\alpha_\nu$; then $is\alpha^s_\nu\xi_\nu=i\omega\alpha_\nu\xi_\nu$.

D. The operator Riccati equation

Finally, we will derive the equation that $\boldsymbol{Y}^\pm$ must satisfy. To ensure that the decomposed constituents satisfy Eqs. (IV.7) and (IV.8), we will substitute Eq. (IV.11) into Eq. (IV.7). Note that

$$\partial_3[(\boldsymbol{Y}^+-\boldsymbol{Y}^-)^{-1}]=-(\boldsymbol{Y}^+-\boldsymbol{Y}^-)^{-1}[\partial_3(\boldsymbol{Y}^+-\boldsymbol{Y}^-)](\boldsymbol{Y}^+-\boldsymbol{Y}^-)^{-1}.$$

Upon differentiating Eq. (IV.11), we obtain

$$\partial_3\mathbf{F}_1^+=-(\boldsymbol{Y}^+-\boldsymbol{Y}^-)^{-1}\{[\partial_3(\boldsymbol{Y}^+-\boldsymbol{Y}^-)]\mathbf{F}_1^+-\partial_3\mathbf{F}_2+(\partial_3\boldsymbol{Y}^-)\mathbf{F}_1+\boldsymbol{Y}^-\partial_3\mathbf{F}_1\}. \tag{IV.21}$$

Substitute Eq. (II.21) into Eq. (IV.21) to arrive at

$$\begin{aligned}\partial_3\mathbf{F}_1^+=&-(\boldsymbol{Y}^+-\boldsymbol{Y}^-)^{-1}\{[\partial_3(\boldsymbol{Y}^+-\boldsymbol{Y}^-)]\mathbf{F}_1^+ +i\omega(\mathbf{A}_{2,1}\mathbf{F}_1+\mathbf{A}_{2,2}\mathbf{F}_2)\\ &+(\partial_3\boldsymbol{Y}^-)\mathbf{F}_1-i\omega\boldsymbol{Y}^-(\mathbf{A}_{1,1}\mathbf{F}_1+\mathbf{A}_{1,2}\mathbf{F}_2)\}.\end{aligned} \tag{IV.22}$$

At this point, substitute Eqs. (IV.5)–(IV.6) into Eq. (IV.22) and collect terms with $\mathbf{F}_1^+$ and $\mathbf{F}_1^-$. We obtain

$$\begin{aligned}\partial_3\mathbf{F}_1^+=&-(\boldsymbol{Y}^+-\boldsymbol{Y}^-)^{-1}\{[\partial_3\boldsymbol{Y}^+-i\omega\boldsymbol{Y}^+(\mathbf{A}_{1,1}+\mathbf{A}_{1,2}\boldsymbol{Y}^+)+i\omega(\boldsymbol{A}_{2,1}+\boldsymbol{A}_{2,2}\boldsymbol{Y}^+)]\boldsymbol{F}_1^+ +i\omega(\boldsymbol{Y}^+-\boldsymbol{Y}^-)\\ &(\mathbf{A}_{1,1}+\mathbf{A}_{1,2}\boldsymbol{Y}^+)\mathbf{F}_1^+ +[\partial_3\boldsymbol{Y}^--i\omega\boldsymbol{Y}^-(\mathbf{A}_{1,1}+\mathbf{A}_{1,2}\boldsymbol{Y}^-)+i\omega(\mathbf{A}_{2,1}+\mathbf{A}_{2,2}\boldsymbol{Y}^-)]\mathbf{F}_1^-\}.\end{aligned}$$

Thus, if $\boldsymbol{Y}^{\pm}$ satisfy the pseudodifferential operator equation

$$\partial_3\boldsymbol{Y}-i\omega\boldsymbol{Y}(\mathbf{A}_{1,1}+\mathbf{A}_{1,2}\boldsymbol{Y})+i\omega(\mathbf{A}_{2,1}+\mathbf{A}_{2,2}\boldsymbol{Y})=0, \tag{IV.23}$$

Eq. (IV.7) is satisfied. A similar reasoning holds for $\mathbf{F}_1^-$. Equation (IV.23) can be written in the form of a nonlinear Riccati equation

$$\partial_3\boldsymbol{Y}-i\omega(\boldsymbol{Y}\ \ -\boldsymbol{I})\mathbf{A}\begin{pmatrix}\boldsymbol{I}\\ \boldsymbol{Y}\end{pmatrix}=0. \tag{IV.24}$$

Supplemented by the linear one-way equation for $\mathbf{F}_1$,

$$\partial_3\mathbf{F}_1+i\omega(\mathbf{A}_{1,1}+\mathbf{A}_{1,2}\boldsymbol{Y})\mathbf{F}_1=0, \tag{IV.25}$$

the solution yields the + and − constituents, provided that the existence conditions at the boundary are satisfied. (In view of the symmetry properties of $\mathbf{A}$, $\boldsymbol{Y}^T$ satisfies the same equation as $\boldsymbol{Y}$.) The system of equations involves observable that are, in principle, continuous across surfaces with sharp discontinuities. It requires a solution via an evolution operator acting in the flow direction of the one-way equation coupled to a solution via an evolution operator of the Riccati equation acting in the opposite direction.

The system (IV.23)–(IV.25) reduces significantly if the underlying medium is locally up/down symmetric. Then the partitioning, in the covariant formulation, can be carried out in such a way that $\mathbf{A}_{1,1}=\mathbf{A}_{2,2}=0$. Equation (IV.25) reduces to the conventional one-way wave equation,

$$\partial_3\mathbf{F}_1+i\omega\mathbf{A}_{1,2}\boldsymbol{Y}\mathbf{F}_1=0,$$

while Eq. (IV.23) reduces to the form

$$\frac{i}{\omega}\,\partial_3\boldsymbol{Y}+\boldsymbol{Y}\mathbf{A}_{1,2}\boldsymbol{Y}-\mathbf{A}_{2,1}=0,$$

which is associated with the composition equation for the vertical slowness operators Γ identified as $\Gamma^{\pm}=\mathbf{A}_{1,2}\boldsymbol{Y}^{\pm}$; see de Hoop.[22] The vertical slowness operators are the generalized eigenvalues of the system matrix operator $\mathbf{A}$; we denote their left symbols as $\gamma^{\pm}$.

E. Fundamental solutions

To solve the system of equations (IV.23)–(IV.25) inside the heterogeneous, compact domain, we will follow a fundamental solutions approach (see, e.g., Krueger and Ochs).[23] In the process of constructing fundamental solutions, we will enforce the decomposition's existence conditions at the boundaries. The fundamental solutions are derived from the Green's tensors of the one-way equations, associated with point sources on one of the bounding level surfaces. The solution $(\boldsymbol{Y}^+,\mathbf{G}_1^+)$ yields downward directed energy flow ($\boldsymbol{Y}$ must be solved upward and $\mathbf{G}_1$ is solved downward) and the solution $(\boldsymbol{Y}^-,\mathbf{G}_1^-)$ yields upward directed energy flow ($\boldsymbol{Y}$ must be solved downward and $\mathbf{G}_1$ is solved upward). Here, $\mathbf{G}_1^+ = \mathbf{G}_1^+(\xi_\mu,\xi_3;\xi'_\nu,\xi_3^0)$ and $\mathbf{G}_1^- = \mathbf{G}_1^-(\xi_\mu,\xi_3;\xi'_\nu,\xi_3^1)$. Thus

$$\partial_3\mathbf{G}_1^+ + i\omega(\mathbf{A}_{1,1}+\mathbf{A}_{1,2}\boldsymbol{Y}^+)\mathbf{G}_1^+ = 0 \quad \text{for } \xi_3\in(\xi_3^0,\xi_3^1],$$
$$\mathbf{G}_1^+(\xi_\mu,\xi_3^0;\xi'_\nu,\xi_3^0) = \boldsymbol{I}\delta(\xi_\mu-\xi'_\mu) \quad \text{and} \quad \boldsymbol{Y}^+|_{\xi_3=\xi_3^1} = \boldsymbol{Y}^1; \tag{IV.26}$$

$$\partial_3\mathbf{G}_1^- + i\omega(\mathbf{A}_{1,1}+\mathbf{A}_{1,2}\boldsymbol{Y}^-)\mathbf{G}_1^- = 0 \quad \text{for } \xi_3\in[\xi_3^0,\xi_3^1),$$
$$\mathbf{G}_1^-(\xi_\mu,\xi_3^1;\xi'_\nu,\xi_3^1) = \boldsymbol{I}\delta(\xi_\mu-\xi'_\mu) \quad \text{and} \quad \boldsymbol{Y}^-|_{\xi_3=\xi_3^0} = \boldsymbol{Y}^0. \tag{IV.27}$$

To generate the fundamental solutions, we assume "appropriate" initial conditions $\boldsymbol{Y}^0$ for $\boldsymbol{Y}^-$ at the upper boundary and $\boldsymbol{Y}^1$ for $\boldsymbol{Y}^+$ at the lower boundary. Note that there is no unique choice of appropriate initial conditions, and hence a whole family of decompositions exists. However, the natural choice are the "radiation" conditions for the admittance symbols

$$y^1(\xi_\mu,\alpha_\nu) = ((a_{1,2})^{-1}\gamma^+)(\xi_\mu,\alpha_\nu), \quad y^0(\xi_\mu,\alpha_\nu) = ((a_{1,2})^{-1}\gamma^-)(\xi_\mu,\alpha_\nu), \tag{IV.28}$$

where $\gamma^\pm$ are the down/up local (principal) vertical slowness symbols in the embedding at the boundary $\partial\mathscr{D}$ of $\mathscr{D}$. This choice guarantees that the ellipticity conditions are satisfied, provided that the embedding is (slightly) dissipative; then purely evanescent modes do not occur.

However, in practice, simpler choices can be used, for example the vertically traveling components,

$$y^1(\xi_\mu,\alpha_\nu) = y^\downarrow(\xi_\mu) \equiv ((a_{1,2})^{-1}\gamma^+)(\xi_\mu,0),$$
$$y^0(\xi_\mu,\alpha_\nu) = y^\uparrow(\xi_\mu) \equiv ((a_{1,2})^{-1}\gamma^-)(\xi_\mu,0).$$

The implied initial values for $\mathbf{G}_2^\pm$ are essentially nonlocal in view of the definite power flow directions of the fundamental solutions:

$$\mathbf{G}_2^+(\xi_\mu,\xi_3;\xi'_\nu,\xi_3^0) = \mathscr{G}^+(\xi_\mu,\xi'_\nu;\xi_3) \quad \text{at } \xi_3=\xi_3^0$$

and

$$\mathbf{G}_2^-(\xi_\mu,\xi_3;\xi'_\nu,\xi_3^1) = \mathscr{G}^-(\xi_\mu,\xi'_\nu;\xi_3) \quad \text{at } \xi_3=\xi_3^1.$$

The internal field, i.e., the field inside the heterogeneous, compact inclusion, is finally written as

$$\mathbf{F}_1^{\text{int}} = \mathbf{F}_1^+ + \mathbf{F}_1^-,$$

$$\mathbf{F}_1^+(\xi_\mu,\xi_3) = \int_{\xi'_\nu\in\mathbb{R}} \mathbf{G}_1^+(\xi_\mu,\xi_3;\xi'_\nu,\xi_3^0)\boldsymbol{\alpha}^+(\xi'_\nu)d\xi'_1 d\xi'_2,$$

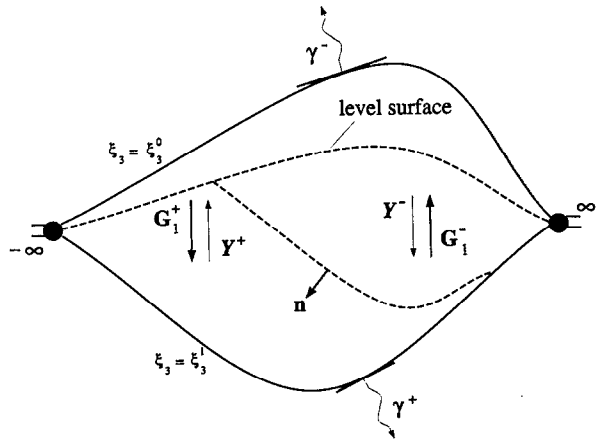

FIG. 1. The inclusion configuration.

$$\mathbf{F}_1^-(\xi_\mu,\xi_3)=\int_{\xi'_\nu\in\mathrm{R}}\mathbf{G}_1^-(\xi_\mu,\xi_3;\xi'_\nu,\xi_3^1)\boldsymbol{\alpha}^-(\xi'_\nu)d\xi'_1d\xi'_2, \tag{IV.29}$$

in which $\boldsymbol{\alpha}^+$ and $\boldsymbol{\alpha}^-$ are p-dimensional vectors in the bounding level surfaces. They equal the boundary values of the down- and upgoing constituents, viz.,

$$\boldsymbol{\alpha}^+(\xi_\mu)=\mathbf{F}_1^+(\xi_\mu,\xi_3^0) \quad \text{and} \quad \boldsymbol{\alpha}^-(\xi_\mu)=\mathbf{F}_1^-(\xi_\mu,\xi_3^1).$$

The respective 2-components of the two constituents on the boundary follow upon applying the Dirichlet-to-Neumann map with Schwartz kernel $\mathscr{Y}^+(\xi_\mu,\xi'_\nu;\xi_3^0)$ to $\mathbf{F}_1^+(\xi_\mu,\xi_3^0)$ to construct $\mathbf{F}_2^+(\xi_\mu,\xi_3^0)$ and applying the Dirichlet-to-Neumann map with Schwartz kernel $\mathscr{Y}^-(\xi_\mu,\xi'_\nu;\xi_3^1)$ to $\mathbf{F}_1^-(\xi_\mu,\xi_3^1)$ to construct $\mathbf{F}_2^-(\xi'_\nu,\xi_3^1)$. The entire construction is illustrated in Fig. 1. An alternative way of deriving a representation of the type Eq. (IV.29) is given in App. B.

The vectors $\boldsymbol{\alpha}^+$ and $\boldsymbol{\alpha}^-$ are determined by the values of the 1-component of the total field on the boundary $\partial\mathscr{D}^+\cup\partial\mathscr{D}^-$. The solvability of the resulting system of boundary integral equations determines whether the radiation conditions earlier employed are actually justified. To set up the latter system, one has to evaluate $\mathbf{G}_1^\pm$ for all values of $\xi'_j\in\partial\mathscr{D}^\pm$.

V. BACKSCATTERED AND TRANSMITTED FIELDS

In this section, the internal field solution is coupled to the external field solution to accomplish a representation for the backscattered ($x_3<0$) and transmitted ($x_3>0$) fields. To this end, the boundary-element method in accordance with Kupradze's Ansatz approach[24,25] is applied. First, we introduce the Green's tensor $\mathbf{H}$ in the imbedding, satisfying

$$\partial_{x_3}\mathbf{H}+i\omega\mathbf{A}(D_\nu)\mathbf{H}=\mathbf{N}^H \qquad \text{for} \quad x_j\in(\mathbb{R}^3\backslash\mathscr{D})\cup\partial\mathscr{D}, \tag{V.1}$$

with (unit body force) notional source

$$\mathbf{N}^H=\begin{pmatrix}I\delta(\xi_\mu-\xi'_\mu)\delta(\xi_3-\xi'_3)\\0\end{pmatrix}. \tag{V.2}$$

The medium of the embedding is assumed to be simple, i.e., typically homogeneous or planarly layered. Then a decomposition into "up" and "down" propagating constituents is readily carried out. Thus set

$$\mathbf{H}=\mathbf{H}^{+}+\mathbf{H}^{-},$$

$$\mathbf{H}^{+}\equiv 0 \quad \text{if } x_3<0 \quad \text{or } \xi_3<\xi_3^1,$$

$$\mathbf{H}^{-}\equiv 0 \quad \text{if } x_3>0 \quad \text{or } \xi_3>\xi_3^0. \tag{V.3}$$

The superscript + refers to the causal solution traveling in the positive x_3-direction and the superscript − refers to the causal solution traveling in the negative x_3-direction. Further, $\mathbf{H}_1$ denotes the "traction" Green's tensor due to a unit "body force," and $\mathbf{H}_2$ denotes the "particle velocity" Green's tensor due to a unit "body force."

Let $\partial\mathscr{S}_\infty^+$ denote the upper hemisphere at infinity in $\mathbb{R}^3$, and let $\partial\mathscr{S}_\infty^-$ denote the lower hemisphere at infinity. The section of the plane $\{x_3=0\}$ interconnecting $\partial\mathscr{D}$ with $\partial\mathscr{S}_\infty$ is denoted as $\partial\Xi$. Let the domains $\mathscr{V}^{\mp}$ be the ones bounded by $\partial\mathscr{V}^{\mp}=\partial\mathscr{D}^{\pm}\cup\partial\Xi\cup\partial\mathscr{S}_\infty^{\mp}$.

A. The boundary-element method

Write the external field in the form

$$\mathbf{F}^{\text{ext}}=\mathbf{F}^{\text{inc}}+\mathbf{F}^{\text{sc}}, \tag{V.4}$$

where $\mathbf{F}^{\text{inc}}$ denotes the irradiating or incident field which is typically excited by a source in the embedding, and $\mathbf{F}^{\text{sc}}$ denotes the scattered field; the scattered field satisfies the source-free hyperbolic system. The secondary sources associated with $\mathbf{F}^{\text{sc}}$ and the incident field in our scattering problem will be specified at the boundary $\partial\mathscr{D}$ of the compact domain, i.e., at $\xi_3=\xi_3^0$ and ξ_3^1 as well as at $\partial\Xi$ in the plane $\{x_3=0\}$ outside the domain. Then the external field is matched with the internal field on the boundary.

Any physical solution can be represented as a Kirchhoff boundary integral with kernel $\mathbf{H}_1^{\pm}$ outside the heterogeneous domain,

$$\mathbf{F}_1^{\text{sc}}=\mathbf{F}_1^{\text{sc},+}+\mathbf{F}_1^{\text{sc},-},$$

$$\mathbf{F}_1^{\text{sc},+}(\xi_\mu,\xi_3)=\int_{\xi'_\nu\in\mathbf{R}}\mathbf{H}_1^{+}(\xi_\mu,\xi_3;\xi'_\nu,\xi_3^1)\boldsymbol{\beta}^{+}(\xi'_\nu)d\xi'_1d\xi'_2 \quad \text{for } \xi\in\mathscr{V}^{+},$$

$$\mathbf{F}_1^{\text{sc},-}(\xi_\mu,\xi_3)=\int_{\xi'_\nu\in\mathbf{R}}\mathbf{H}_1^{-}(\xi_\mu,\xi_3;\xi'_\nu,\xi_3^0)\boldsymbol{\beta}^{-}(\xi'_\nu)d\xi'_1d\xi'_2 \quad \text{for } \xi\in\mathscr{V}^{-}, \tag{V.5}$$

where, according to Kupradze's Ansatz approach, $\boldsymbol{\beta}^{+}$ and $\boldsymbol{\beta}^{-}$ represent surface densities of force (dipoles). To remove the singularities arising from the kernels $\mathbf{H}_1^{+}$, the densities are shifted infinitesimally away from the bounding level surfaces; see Fig. 2. The representation for $\mathbf{F}_1^{\text{sc},\pm}$ follows upon applying the reciprocity theorem of the time-convolution type in the volume $\mathscr{V}^{\pm}$; see Fig. 2. The 2-components of the scattered field follow from the constitutive part of the hyperbolic equations as[24]

$$\mathbf{F}_2^{\text{sc},+}(\xi_\mu,\xi_3)=\tfrac{1}{2}\chi_{\partial\mathscr{V}^{-}}(\xi_3)\boldsymbol{\beta}^{+}(\xi_\mu)+\int_{\xi'_\nu\in\mathbf{R}}\mathbf{H}_2^{+}(\xi_\mu,\xi_3;\xi'_\nu,\xi_3^1)\boldsymbol{\beta}^{+}(\xi'_\nu)d\xi'_1d\xi'_2,$$

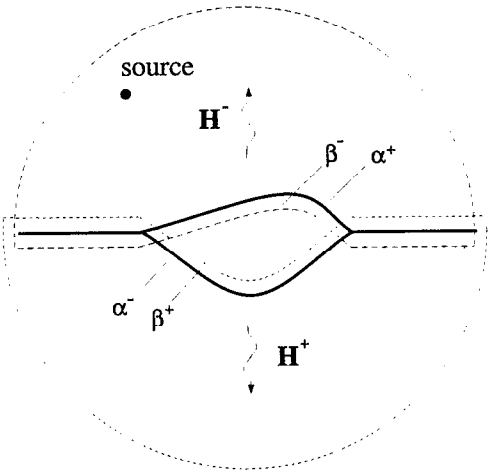

FIG. 2. The integral boundaries, limiting procedure.

$$\mathbf{F}_2^{\mathrm{sc},-}(\xi_\mu,\xi_3)=\tfrac{1}{2}\chi_{\partial\mathscr{L}^+}(\xi_3)\boldsymbol{\beta}^-(\xi_\mu)+\int_{\xi'_\nu\in\mathbb{R}}\mathbf{H}_2^-(\xi_\mu,\xi_3;\xi'_\nu,\xi_3^0)\boldsymbol{\beta}^-(\xi'_\nu)d\xi'_1d\xi'_2. \tag{V.6}$$

We have four unknown vector quantities and hence we need a system of four equations to solve the scattering problem. Expanding both components of the internal and external fields on the boundary, $\partial\mathscr{L}^+$ and $\partial\mathscr{L}^-$, yields the system of equations

$$\boldsymbol{\alpha}^+ + \int_{\xi'_\nu\in\mathbb{R}}\mathbf{G}_1^-(\cdot;\xi'_\nu,\xi_3^1)\boldsymbol{\alpha}^-(\xi'_\nu)d\xi'_1d\xi'_2\Big|_{\xi_3=\xi_3^0}$$

$$=\left[\mathbf{F}_1^{\mathrm{inc}}+\int_{\xi'_\nu\in\mathbb{R}}\mathbf{H}_1^-(\cdot;\xi'_\nu,\xi_3^0)\boldsymbol{\beta}^-(\xi'_\nu)d\xi'_1d\xi'_2\right]\Big|_{\xi_3=\xi_3^0}, \tag{V.7}$$

$$\int_{\xi'_\nu\in\mathbb{R}}\mathbf{G}_1^+(\cdot;\xi'_\nu,\xi_3^0)\boldsymbol{\alpha}^+(\xi'_\nu)d\xi'_1d\xi'_2\Big|_{\xi_3=\xi_3^1}+\boldsymbol{\alpha}^-$$

$$=\left[\mathbf{F}_1^{\mathrm{inc}}+\int_{\xi'_\nu\in\mathbb{R}}\mathbf{H}_1^+(\cdot;\xi'_\nu,\xi_3^1)\boldsymbol{\beta}^+(\xi'_\nu)d\xi'_1d\xi'_2\right]\Big|_{\xi_3=\xi_3^1}, \tag{V.8}$$

while

$$\mathbf{Y}^+\Big|_{\xi_3=\xi_3^0}\boldsymbol{\alpha}^+ + \mathbf{Y}^0\int_{\xi'_\nu\in\mathbb{R}}\mathbf{G}_1^-(\cdot;\xi'_\nu,\xi_3^1)\boldsymbol{\alpha}^-(\xi'_\nu)d\xi'_1d\xi'_2\Big|_{\xi_3=\xi_3^0}$$

$$=\tfrac{1}{2}\boldsymbol{\beta}^-+\left[\mathbf{F}_2^{\mathrm{inc}}+\int_{\xi'_\nu\in\mathbb{R}}\mathbf{H}_2^-(\cdot;\xi'_\nu,\xi_3^0)\boldsymbol{\beta}^-(\xi'_\nu)d\xi'_1d\xi'_2\right]\Big|_{\xi_3=\xi_3^0}, \tag{V.9}$$

$$\boldsymbol{Y}^1 \int_{\xi'_\nu \in \mathbb{R}} \mathbf{G}_1^+(\cdot;\xi'_\nu,\xi_3^0)\boldsymbol{\alpha}^+(\xi'_\nu)d\xi'_1 d\xi'_2 \Big|_{-\xi_3=\xi_3^1} + \boldsymbol{Y}^- \Big|_{\xi_3=\xi_3^1} \boldsymbol{\alpha}^-$$

$$= \tfrac{1}{2}\boldsymbol{\beta}^+ + \left[\mathbf{F}_2^{\mathrm{inc}} + \int_{\xi'_\nu \in \mathbb{R}} \mathbf{H}_2^+(\cdot;\xi'_\nu,\xi_3^1)\boldsymbol{\beta}^+(\xi'_\nu)d\xi'_1 d\xi'_2\right]\Big|_{\xi_3=\xi_3^1}; \tag{V.10}$$

in addition, on $\partial\Xi$ we get the boundary condition

$$0 = \int_{\xi'_\nu \in \mathbb{R}} \mathbf{H}_1^+(\cdot;\xi'_\nu,\xi_3^1)\boldsymbol{\beta}^+(\xi'_\nu)d\xi'_1 d\xi'_2 + \int_{\xi'_\nu \in \mathbb{R}} \mathbf{H}_1^-(\cdot;\xi'_\nu,\xi_3^0)\boldsymbol{\beta}^-(\xi'_\nu)d\xi'_1 d\xi'_2. \tag{V.11}$$

For all practical purposes, these boundary conditions are solved in the least-squares sense, in the horizontal Fourier domain. Note that the (constrained) freedom in the choice of $\boldsymbol{Y}^0$ and $\boldsymbol{Y}^1$ is explicit as well as implicitly present in $\mathbf{G}_1^-$ and $\mathbf{G}_1^+$.

VI. NUMERICAL ISSUES

The system of equations (IV.23)–(IV.25) can be solved along the lines of a pseudospectral/finite-difference scheme. In this section the most important details of such an approach will be discussed.

Double periodic boundary conditions are applied in the ξ-domain, along the level surfaces of ξ_3. This is preferably done on a hexagonal grid rather than our orthogonal one. The period in the ξ_ν-direction is denoted as Ξ_ν. Further, periodic boundary conditions are applied in t. A standard fast Fourier transform (FFT) representation is employed to obtain the wave field representation in time-frequency domain. A Fourier series is employed to represent the wave field as a function of the curvilinear transverse coordinates. The relevant sampling intervals in time and space are denoted as Δt, $\Delta\xi_\nu$, and $\Delta\xi_3 \equiv h$.

A. The periodic case, and discretization in the transverse directions

Consider the (ξ_ν, ξ_3) coordinate system. To reduce the stretch of the transient wave with the medium's wave speed along the horizontal or transverse directions, we apply a horizontal distance to travel-time transformation

$$\xi_1 \to \tau_1: \quad \tau_1(\xi_1) + \frac{T_1}{2} = \int_{\xi=-\Xi_1/2}^{\xi_1} V_{o,1}^{-1}(\xi)d\xi, \tag{VI.1}$$

where

$$V_{o,1}(\xi) \equiv \min_{\{\xi_2,\xi_3\}} \min_{\text{modes}} \min_{\text{directions}} V(\xi,\xi_2,\xi_3) \tag{VI.2}$$

with V denoting the modal phase velocity, being dependent on direction of propagation, and

$$T_1 \equiv \int_{\xi=-\Xi_1/2}^{\Xi_1/2} V_{o,1}^{-1}(\xi)d\xi. \tag{VI.3}$$

Then, $\tau_1(-\Xi_1/2) = -T_1/2$ and $\tau_1(\Xi_1/2) = T_1/2$. We have

$$\partial_{\xi_1} = V_{o,1}^{-1}(\xi_1)\partial_{\tau_1}. \tag{VI.4}$$

A similar transformation is carried out for ξ_2.

Consider the solution on the region $[-\Xi_1/2, \Xi_1/2]\times[-\Xi_2/2, \Xi_2/2]$ in a level surface of ξ_3 coordinated by $\{\xi_1,\xi_2\}$. Let us focus on the ξ_1-coordinate. We introduce the Fourier series basis functions

$$\psi_{k_1}(\tau_1)=\exp[-(2\pi i/T_1)k_1\tau_1], \tag{VI.5}$$

which define the wave number $\omega_1' = k_1(2\pi/T_1)$ [compare with $\omega\alpha_1$ in Eq. (IV.15)]. Then, for a general quantity f, we have

$$\tilde{f}_{k_1}=\langle f,\psi_{k_1}\rangle\equiv\frac{1}{T_1}\int_{\tau_1=-T_1/2}^{T_1/2} f(\tau_1)\overline{\psi_{k_1}(\tau_1)}d\tau_1, \tag{VI.6}$$

which is an integral over the one-dimensional torus $\mathscr{T}^1$, if

$$f(\tau_1)=\sum_{k_1=-\infty}^{\infty}\tilde{f}_{k_1}\psi_{k_1}(\tau_1). \tag{VI.7}$$

Note that the $\tilde{f}_{k_1}$ are implicitly functions of (τ_2,ξ_3), and satisfy $\Sigma_{k_1=-\infty}^{\infty}|\tilde{f}_{k_1}|^2(1+|k_1|^2)^r<\infty$ when f is restricted to the Sobolev space $H^r(\mathscr{T}^1)$. Note that the pseudo-differential operators, like the admittance operator, are continuous between appropriate Sobolev spaces.

Upon discretizing the integral in Eq. (VI.6), and truncating the summation in Eq. (VI.7), we arrive at the transform pair

$$\tilde{f}_{k_1}\simeq\frac{1}{N_1\Delta\tau_1}\sum_{l_1=-N_1/2}^{N_1/2-1} f(l_1\Delta\tau_1)\overline{\psi_{k_1}(l_1\Delta\tau_1)}\Delta\tau_1, \tag{VI.8}$$

$$f(l_1\Delta\tau_1)\simeq\sum_{k_1=-(M_1-1)/2}^{(M_1-1)/2}\tilde{f}_{k_1}\psi_{k_1}(l_1\Delta\tau_1) \tag{VI.9}$$

with

$$N_1\Delta\tau_1=T_1, \quad \text{hence} \quad \Delta\omega_1'\Delta\tau_1=\frac{2\pi}{N_1}. \tag{VI.10}$$

Note that for $M_1=N_1+1$ we obtain the well-known discrete Fourier transform (DFT) pair. However, here the values of N_1 and M_1 are left uncoupled, but assuming that N_1 is even and M_1 is odd. Due to the discretization Eq. (VI.8) of the integral in Eq. (VI.6), the field becomes also periodic in the k_1-domain with period N_1 and associated Nyquist horizontal wave number $\omega_{1,\mathrm{Nyq}}' = \pi/\Delta\tau_1$. In general, the horizontal wave number content (band width) of the wave field solution will be much less than this Nyquist value, which allows us to use $M_1\ll N_1$.

The co-kernel $\tilde{a}$ of the matrix operator $\mathbf{A}$ is of the form

$$\tilde{a}_{k_1-l_1,l_1}=\langle\psi_{k_1},\mathbf{A}\psi_{l_1}\rangle; \tag{VI.11}$$

for an element of the system's matrix of partial differential operators, we typically get

$$\begin{aligned}\langle\psi_{k_1},\partial_{\tau_1}(\rho(\tau_1,\xi_3)\partial_{\tau_1}\cdot)\psi_{l_1}\rangle&=(\widetilde{\partial_{\tau_1}\rho})_{k_1-l_i}(-il_1\Delta\omega_1')-\tilde{\rho}_{k_1-l_1}(-il_1\Delta\omega_1')^2\\&=(-ik_1\Delta\omega_1')(-il_1\Delta\omega_1')\tilde{\rho}_{k_1-l_1}.\end{aligned} \tag{VI.12}$$

Observe that upon imposing the periodic boundary conditions, the operators involved in the scattering problem will become compact.

Equations (IV.23)–(IV.25) are thus obtained in the discrete horizontal wave number domain; in fact, they have the form of a system of ordinary differential equations.

B. Discretization in the normal direction

For the discretization of the evolution equations we employ the fourth-order Runge–Kutta scheme. [We could have proposed any locally stable finite difference scheme.] We write Eqs. (IV.23)–(IV.25) in the generic co-kernel form

$$\partial_3 y + i\omega F(\xi_3, y) = 0, \tag{VI.13}$$

where we have suppressed the ξ_ν and ω dependence of F. The explicit fourth-order Runge–Kutta scheme is given by

$$y(\xi_3+h) = y(\xi_3) + \tfrac{1}{6}y_0 + \tfrac{1}{3}y_1 + \tfrac{1}{3}y_2 + \tfrac{1}{6}y_3 + O(h^5), \tag{VI.14}$$

where

$$y_0 = -i\omega h F(\xi_3, y(\xi_3)), \tag{VI.15}$$

$$y_1 = -i\omega h F(\xi_3 + \tfrac{1}{2}h, y(\xi_3) + \tfrac{1}{2}y_0), \tag{VI.16}$$

$$y_2 = -i\omega h F(\xi_3 + \tfrac{1}{2}h, y(\xi_3) + \tfrac{1}{2}y_1), \tag{VI.17}$$

$$y_3 = -i\omega h F(\xi_3, y(\xi_3) + y_2). \tag{VI.18}$$

To make this scheme quasi stable, the stepsize h is adapted in accordance with an eigenvalue analysis of $(\partial_y F)(\xi_3, y(\xi_3))$ over each range $\{\xi_3, \xi_3+h\}$ as it arises in the linearization of Eq. (VI.13).

To be more specific, consider a range $\{\xi_3^c, \xi_3^c + h\}$, say. Equation (IV.25) for $\mathbf{F}_1$is linear, hence

$$(\partial_y F)(\xi_3, y(\xi_3)) \to \mathbf{D} \equiv \mathbf{A}_{1,1} + \mathbf{A}_{1,2}\boldsymbol{Y}; \quad \mathbf{D}_c = \mathbf{D}|_{\xi_3 = \xi_3^c}. \tag{VI.19}$$

The linearization of Eq. (IV.23) follows from substituting

$$\boldsymbol{Y} = \boldsymbol{Y}_c + \boldsymbol{E} \quad \text{with} \quad \boldsymbol{Y}_c = \boldsymbol{Y}|_{\xi_3 = \xi_3^c};$$

omitting terms $O(\boldsymbol{E}^2)$ and using the symmetry properties of $\mathbf{A}$ then leads to the equation

$$\partial_3 \boldsymbol{E} - i\omega \{\boldsymbol{E}\mathbf{D}_c + \mathbf{D}_c^T \boldsymbol{E}\} \simeq (\partial_3 \boldsymbol{Y})_c, \tag{VI.20}$$

where

$$(\partial_3 \boldsymbol{Y})_c = i\omega \{\boldsymbol{Y}_c(\mathbf{A}_{1,1} + \mathbf{A}_{1,2}\boldsymbol{Y}_c) - (\mathbf{A}_{2,1} + \mathbf{A}_{2,2}\boldsymbol{Y}_c)\};$$

hence

$$(\partial_y F)(\xi_3, y(\xi_3))y \to -\{\boldsymbol{E}\mathbf{D} + \mathbf{D}^T\boldsymbol{E}\}. \tag{VI.21}$$

From the latter equation, in view of the equivalence in spectral properties of $\mathbf{D}$ and $\mathbf{D}^T$, it follows that the stability bound on h from the linearized Riccati equation for the admittance operator must be half the bound on h from the field equation based on Eq. (VI.19). However, since the equation

for the admittance operator must be solved prior to the one for the relevant field quantities, the Runge–Kutta scheme requires the sampling in ξ_3 of the admittance to be twice as dense as the one of the field anyway. [The material properties, in turn, have to be sampled four times as densely as the field.]

We will analyze the upper bound for h following from the field equation in more detail. Within the interval $\{\xi_3^c, \xi_3^c + h\}$, we assume the operator $\mathbf{A}$ to be slowly varying. Then, within this interval, we have [cf. Eq. (VI.19)]

$$\mathbf{D} = \mathbf{D}_c + \mathbf{A}_{1,2}\boldsymbol{E}. \tag{VI.22}$$

Using Eq. (VI.22), the norm of $\mathbf{D}$ can be estimated as

$$\|\mathbf{D}\| \leqslant \|\mathbf{D}_c\| + \|\mathbf{A}_{1,2}\boldsymbol{E}\|. \tag{VI.23}$$

The second norm on the right-hand side of Eq. (VI.23) can be estimated as

$$\|\mathbf{A}_{1,2}\boldsymbol{E}\| \leqslant h \, \|\delta_3 \boldsymbol{D}\|_{\max} \quad \text{with} \quad \|\delta_3 \mathbf{D}\|_{\max} \equiv \max_{\{\xi_3^c, \xi_3^c + h\}} \|\delta_3 \mathbf{D}\|$$

in which

$$\|\delta_3 \mathbf{D}\|_{\max} \sim \|(\partial_3 \mathbf{D})_c\| \simeq \|\mathbf{A}_{1,2}(\partial_3 \boldsymbol{E})_c\| \simeq \|\mathbf{A}_{1,2}(\partial_3 \boldsymbol{Y})_c\|$$

using Eq. (VI.20); here, δ_3 denotes the two-point difference operator. Substituting this result in Eq. (VI.23), we obtain

$$\|\mathbf{D}\| \leqslant \|\mathbf{D}_c\| + h \|\delta_3 \mathbf{D}\|_{\max}. \tag{VI.24}$$

Now, suppose we have the estimate

$$h\omega \, \|\mathbf{D}\| \leqslant \theta \tag{VI.25}$$

for some value of θ. Then the explicit Runge–Kutta scheme Eq. (VI.14) implies an upper bound δ for the amplication factor with

$$\delta = \frac{1}{720} \, \theta^5.$$

By choosing θ appropriately, the amplification can be reduced to any desired level. To arrive at an explicit bound, use Eq. (VI.24) in Eq. (VI.25)

$$h\omega \, (\|\mathbf{D}_c\| + h \|\delta_3 \mathbf{D}\|_{\max}) \leqslant \theta$$

to guarantee Eq. (VI.25). Upon analyzing the left-hand side of the latter inequality quadratic in $h\omega$, it is found that

$$h\omega \leqslant \frac{2\theta}{\|\mathbf{D}_c\| + \sqrt{\|\mathbf{D}_c\|^2 + 4\omega^{-1}\theta \|\delta_3 \mathbf{D}\|_{\max}}}. \tag{VI.26}$$

For practical purposes, we introduce a more conservative upper bound through

$$\sqrt{\|\mathbf{D}_c\|^2 + 4\omega^{-1}\theta \|\delta_3 \mathbf{D}\|_{\max}} \leqslant \|\mathbf{D}_c\| + 2\sqrt{\omega^{-1}\theta \|\delta_3 \mathbf{D}\|_{\max}},$$

which yields the approximation of Eq. (VI.26)

$$h\omega \leqslant \frac{\theta}{\|\mathbf{D}_c\| + \sqrt{\omega^{-1}\theta}\|\delta_3\mathbf{D}\|_{\max}}. \tag{VI.27}$$

Naturally, our sampling rate must be dependent on the frequency. The norms of the operators occurring in Eq. (VI.27) follow from (estimates of) the maximum eigenvalues of their respective co-kernel matrix representations.

A summary of the necessary steps in the numerical scheme is given in Appendix C.

VII. DISCUSSION

We have considered the Dirichlet-to-Neumann map or admittance operator at the boundary of a large inclusion, and analyzed the equations governing the continuation of this operator away from the boundary. Such a continuation required a directional decomposition of the (internal) wave field, viz., with respect to power flow averaged over a period in time and a level hypersurface in space, and the introduction of pseudodifferential operators. The continuation, essentially, followed from an invariant imbedding approach extended to higher dimensions. In the double periodic case, the latter approach reduced the continuation problem to solving a large system of ordinary differential equations; an explicit construction, based on the latter system, has been derived and its stability properties have been analyzed.

We envisage as a key application the analysis and computation of time-domain transient wave phenomena. This implied that we did not have to consider general frequencies, but only the ones relevant to carry out a proper inverse Fourier transform back to the time domain. In this respect, special care had to be taken to avoid possible resonances in the configuration.

The continuation of the admittance operator leads, in case the medium exhibits a local direction of preference, to an accurate method for the numerical simulation of waves. It suffers from only few limitations as far as the coefficients of the original hyperbolic system are concerned. Apart from conditions on proper sampling, it was assumed that the coefficients can only jump across hypersurfaces. Such surfaces, or interfaces, then determined the coordinates on the manifold as well as the local (normal) direction of preference. With those restrictions, general symmetric hyperbolic systems can be solved this way; the occurrence of anisotropy does not require special care.

The framework of continuation of the admittance operator has been designed to fill the gap between long wavelength and short wavelength theories, i.e., that scale where multiple scattering and mode interactions are the dominant phenomena of interest. In a scattering configuration as a whole, different scales may enter the direct problem; then the theory should only be applied locally. Since the admittance operator defines the Dirichlet-to-Neumann map, the framework discussed in this article opens the way for developing an inverse scattering theory from local boundary measurements.

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APPENDIX A: AN EXAMPLE—THE ANISOTROPIC FLUID

1. Covariant formulation

In the case of an anisotropic fluid, the hyperbolic system is given by

$$\mathrm{D}_k v^k = -i\omega\kappa^{-1}p \quad \text{with} \quad \mathrm{D}_k v^k = (\partial_{\xi_k} + \Gamma^j_{jk})v^k, \tag{A1}$$

$$-\mathsf{D}_{ip}=i\omega\rho_{ij}v^j \quad \text{with} \quad \mathsf{D}_{ip}=\partial_{\xi_i}p. \tag{A2}$$

We extract the locally normal component of the particle velocity,

$$v^n=n_jv^j, \tag{A3}$$

so that

$$v^i=V^i+v^n\frac{n^i}{\|\mathbf{n}\|^2} \quad \text{with} \quad V^i=\left(\delta^i{}_j-\frac{n^in_j}{\|\mathbf{n}\|^2}\right)v^j. \tag{A4}$$

Indeed, $V^n=0$. From Eq. (A2) we find that

$$-(\rho^{-1})^{jk}\mathsf{D}_kp=i\omega v^j. \tag{A5}$$

Set

$$\Sigma^{ij}\equiv(\rho^{-1})^{ij}, \quad \Sigma^j\equiv n_i(\rho^{-1})^{ij}.$$

Contracting Eq. (A5) with n_j yields

$$-\Sigma^k\mathsf{D}_kp=i\omega v^n,$$

hence

$$-\Sigma^\nu\mathsf{D}_\nu p-\Sigma^3\mathsf{D}_3p=i\omega v^n. \tag{A6}$$

On the other hand, contracting Eq. (A5) with $(\delta^i{}_j-n^in_j\|\mathbf{n}\|^{-2})$ yields

$$i\omega V^i=-\left(\delta^i{}_j-\frac{n^in_j}{\|\mathbf{n}\|^2}\right)(\rho^{-1})^{jk}\mathsf{D}_kp,$$

hence, upon substituting Eq. (A6),

$$i\omega\left(V^k+v^n\frac{n^k}{\|\mathbf{n}\|^2}\right)=(-\Sigma^{k\nu}+\Sigma^{k3}(\Sigma^3)^{-1}\Sigma^\nu)\mathsf{D}_\nu p+i\omega(\Sigma^3)^{-1}\Sigma^{k3}v^n. \tag{A7}$$

Now, substituting Eq. (A4) into Eq. (A1) yields

$$\mathsf{D}_3\left(V^3+v^n\frac{n^3}{\|\mathbf{n}\|^2}\right)+\mathsf{D}_\mu\left(V^\mu+v^n\frac{n^\mu}{\|\mathbf{n}\|^2}\right)=-i\omega\kappa^{-1}p.$$

In the covariant formulation, it follows that $\mathbf{n}$ must coincide with the unit vector in the ξ_3-direction. This implies that $v^n=v^3$, $V^3=0$, and $\Sigma^j=\Sigma^{3j}$. Eliminating V^μ with the aid of Eq. (A7) then amounts to

$$\mathsf{D}_\mu[(\Sigma^{33})^{-1}\Sigma^{\mu3}v^3]+\mathsf{D}_3v^3=\mathsf{D}_\mu\left[[-\Sigma^{\mu\nu}+\Sigma^{\mu3}(\Sigma^{33})^{-1}\Sigma^{3\nu}]\frac{i}{\omega}\mathsf{D}_\nu p\right]-i\omega\kappa^{-1}p. \tag{A8}$$

Hence, combining Eqs. (A6) and (A8) implies the covariant system's matrix operator

$$\mathbf{A}_C=\begin{pmatrix} -(\Sigma^{33})^{-1}\Sigma^{3\nu}\,\dfrac{i}{\omega}\,\partial_{\xi_\nu} & -(\Sigma^{33})^{-1} \\ \dfrac{i}{\omega}\,\mathsf{D}_\mu\left[(-\Sigma^{\mu\nu}+\Sigma^{\mu 3}(\Sigma^{33})^{-1}\Sigma^{3\nu})\,\dfrac{i}{\omega}\,\partial_{\xi_\nu}\cdot\right]-\kappa^{-1} & -\dfrac{i}{\omega}\,\mathsf{D}_\mu[\Sigma^{\mu 3}(\Sigma^{33})^{-1}\cdot] \end{pmatrix}; \tag{A9}$$

the Christoffel symbols appear in $\mathsf{D}_\mu = \partial_{\xi_\mu} + \Gamma^j_{j\mu}$. To arrive at the reduced system of the type (II.21), we have to add

$$\mathbf{A}_\Gamma=\begin{pmatrix} 0 & 0 \\ 0 & -\dfrac{i}{\omega}\,\Gamma^j_{j3} \end{pmatrix} \tag{A10}$$

to $\mathbf{A}_C$: $\mathbf{A}=\mathbf{A}_C+\mathbf{A}_\Gamma$. Note that monoclynic symmetry implies that $\Sigma^{3\nu}=\Sigma^{\mu 3}=0$; then $\mathbf{A}_C$ becomes a purely off-diagonal matrix operator.

2. Quasiscalar formulation

Consider Eq. (A2), but now in a Cartesian frame. Substituting Eq. (II.14) then leads to

$$-(\rho^{-1})_{jk}\left[\partial_{\xi_k}-\delta_{k3}\partial_{\xi_3}+\frac{1}{\sqrt{g_{33}}}\,n_k\partial_{\xi_3}\right]p=i\omega v_j, \tag{A11}$$

hence

$$-\left[(\rho^{-1})_{i\nu}\partial_{\xi_\nu}+\frac{(\rho^{-1})_{ij}n_j}{\sqrt{g_{33}}}\,\partial_{\xi_3}\right]p=i\omega v_i. \tag{A12}$$

Contract Eq. (A12) with n_i and set

$$\Sigma_{ij}\equiv(\rho^{-1})_{ij},\quad \Sigma_{n\nu}\equiv n_i(\rho^{-1})_{i\nu},\quad \Sigma_{in}\equiv(\rho^{-1})_{ij}n_j,\quad \Sigma_{nn}\equiv n_i(\rho^{-1})_{ij}n_j$$

then

$$-\Sigma_{n\nu}\partial_{\xi_\nu}p-\frac{\Sigma_{nn}}{\sqrt{g_{33}}}\,\partial_{\xi_3}p=i\omega v_n. \tag{A13}$$

Contract Eq. (A12) with $(\delta_{ki}-n_kn_i\|\mathbf{n}\|^{-2})$ to get

$$i\omega\left(V_k+v_n\frac{n_k}{\|\mathbf{n}\|^2}\right)=(-\Sigma_{k\nu}+\Sigma_{kn}\Sigma_{nn}^{-1}\Sigma_{n\nu})\partial_{\xi_\nu}p+i\omega\Sigma_{nn}^{-1}\Sigma_{kn}v_n. \tag{A14}$$

In the quasiscalar formulation, $\mathbf{n}$ is given by Eq. (II.13). Substituting Eqs. (II.14) and (A4) into Eq. (A1) now leads to ($n_3\equiv 1$)

$$\frac{1}{\sqrt{g_{33}}}\,\partial_{\xi_3}v_n+\left[\partial_{\xi_\mu}-\frac{1}{\sqrt{g_{33}}}\,(\partial_{\xi_3}n_\mu)\right]\left(V_\mu+v_n\frac{n_\mu}{\|\mathbf{n}\|^2}\right)=-i\omega\kappa^{-1}p.$$

Substituting Eq. (A13) into the latter equation yields

$$\sqrt{g_{33}}\partial_{\xi_\mu}-(\partial_{\xi_3}n_\mu)](\Sigma_{nn}^{-1}\Sigma_{\mu n}v_n)+\partial_{\xi_3}v_n$$

$$=[\sqrt{g_{33}}\partial_{\xi_\mu}-(\partial_{\xi_3}n_\mu)]\left[(-\Sigma_{\mu\nu}+\Sigma_{\mu n}\Sigma_{nn}^{-1}\Sigma_{n\nu})\frac{i}{\omega}\mu_{\xi_\nu}p\right]-i\omega\sqrt{g_{33}}\kappa^{-1}p. \tag{A15}$$

Using Eq. (II.13), we find that

$$[\sqrt{g_{33}}\partial_{\xi_\mu}-(\partial_{\xi_3}n_\mu)]\cdot=\partial_{\xi_\mu}[(\partial_{\xi_3}\mathrm{f})\cdot]=\partial_{\xi_\mu}[\sqrt{g_{33}}\cdot]. \tag{A16}$$

Then, combining Eqs. (A13) and (A15), the system's matrix operator follows as

$$\mathbf{A}=-\begin{pmatrix} \sqrt{g_{33}}\Sigma_{nn}^{-1}\Sigma_{n\nu}\frac{i}{\omega}\partial_{\xi_\nu} & \sqrt{g_{33}}\Sigma_{nn}^{-1} \\ \frac{i}{\omega}\partial_{\xi_\mu}\left[\sqrt{g_{33}}\widehat{\Sigma_{\mu\nu}}\frac{i}{\omega}\partial_{\xi_\nu}\cdot\right]+\sqrt{g_{33}}\kappa^{-1} & \frac{i}{\omega}\partial_{\xi_\mu}(\sqrt{g_{33}}\Sigma_{\mu n}\Sigma_{nn}^{-1}\cdot) \end{pmatrix}. \tag{A17}$$

with

$$\widehat{\Sigma_{\mu\nu}}\equiv\Sigma_{\mu\nu}-\Sigma_{\mu n}\Sigma_{nn}^{-1}\Sigma_{n\nu}. \tag{A18}$$

Note that, in general, the system's matrix is dense, even in the isotropic medium case; then we have

$$\Sigma_{ij}=\rho^{-1}\delta_{ij},\quad \Sigma_{n\nu}=\rho^{-1}n_\nu,\quad \Sigma_{in}=\rho^{-1}n_i,\quad \Sigma_{nn}=\rho^{-1}\|\mathbf{n}\|^2,$$

while

$$\widehat{\Sigma_{\mu\nu}}=\frac{1}{\rho}\left(\delta_{\mu\nu}-\frac{n_\mu n_\nu}{\|\mathbf{n}\|^2}\right).$$

APPENDIX B: EVOLUTION OF THE ADMITTANCE OPERATOR IN TERMS OF A GREEN'S TENSOR

1. Representation theorem

The starting point of this appendix is a representation theorem for $\mathbf{F}_2$ that follows from Eq. (III.1) upon substituting the Green's tensor $\mathbf{G}^{II}(\xi_\mu\xi_3,\xi'_\nu,\xi'_3)$ with notional sources

$$\mathbf{N}^{II}=\begin{pmatrix} I\delta(\xi_\mu-\xi'_\mu)\delta(\xi_3-\xi'_3) \\ 0 \end{pmatrix}.$$

Substituting this Green's tensor into Eq. (III.1) for state a yields the representation

$$\mathbf{F}_2(\xi'_\nu,\xi'_3)=-\int_{\xi_3=\xi_3^0}^{\xi_3^1}\int_{\xi_\mu\in\mathbb{R}}(\mathbf{G}^{II})^T(\xi_\mu,\xi_3)\mathbf{J}\mathbf{N}(\xi_\mu,\xi_3)d\xi_1d\xi_2d\xi_3$$

$$+\int_{\xi_\mu\in\mathbb{R}}(\mathbf{G}^{II})^T(\xi_\mu,\xi_3^1)\mathbf{J}\mathbf{F}(\xi_\mu,\xi_3^1)d\xi_1d\xi_2-\int_{\xi_\mu\in\mathbb{R}}(\mathbf{G}^{II})^T(\xi_\mu,\xi_3^0)\mathbf{J}\mathbf{F}(\xi_\mu,\xi_3^0)d\xi_1d\xi_2 \tag{B1}$$

if $\xi'_3\in(\xi_3^0,\xi_3^1)$. We will impose specific boundary conditions for the Green's tensor, viz., of the "normal-traction free" type,

$$\mathbf{G}_1^{II}|_{\partial\mathscr{V}}=0.$$

This boundary condition is nonradiating, implying that in the case of a nondissipative compact domain $\mathscr{D}$ the Green's tensor exists at the configuration's resonance frequencies only. By opening up the compact domain in $\mathbb{R}^3$ towards infinity along thin slabs centered on $x_3=0$, the configuration deforms into an open resonator; then $\mathbf{G}^{II}$ exists away from the resonance frequencies.

One of the reciprocity relations for such a Green's tensor follows as

$$(\mathbf{G}_2^{II})^T(\xi_\mu,\xi_3;\xi'_\nu,\xi'_3)=\mathbf{G}_2^{II}(\xi'_\nu,\xi'_3;\xi_\mu,\xi_3).$$

Using this relation and the nonradiating boundary condition in Eq. (B1) yields

$$\begin{aligned}\mathbf{F}_2(\xi'_\nu,\xi'_3)=&-\int_{\xi'_3=\xi_3^0}^{\xi_3^1}\int_{\xi_\mu\in\mathbb{R}}(\mathbf{G}^{II})^T(\xi_\mu,\xi_3;\xi'_\nu,\xi'_3)\mathbf{JN}(\xi_\mu,\xi_3)d\xi_1d\xi_2d\xi_3\\&-\int_{\xi_\mu\in\mathbb{R}}\mathbf{G}_2^{II}(\xi'_\nu,\xi'_3;\xi_\mu,\xi_3^1)\mathbf{F}_1(\xi_\mu,\xi_3^1)d\xi_1d\xi_2\\&+\int_{\xi_\mu\in\mathbb{R}}\mathbf{G}_2^{II}(\xi'_\nu,\xi'_3;\xi_\mu,\xi_3^0)\mathbf{F}_1(\xi_\mu,\xi_3^0)d\xi_1d\xi_2.\end{aligned}\tag{B2}$$

2. The evolution equations

Assume that $\mathbf{N}=\mathbf{0}$ in $\mathscr{D}_{[\xi_3^0,\xi_3^1]}$; then the volume integral on the right-hand side of Eq. (B2) vanishes and

$$\begin{aligned}\mathbf{F}_2(\xi'_\nu,\xi'_3)&=\mathbf{F}_2^0(\xi'_\nu,\xi'_3)+\mathbf{F}_2^1(\xi'_\nu,\xi'_3),\\\mathbf{F}_2^1(\xi'_\nu,\xi'_3)&=-\int_{\xi_\mu\in\mathbb{R}}\mathbf{G}_2^{II}(\xi'_\nu,\xi'_3;\xi_\mu,\xi_3^1)\mathbf{F}_1(\xi_\mu,\xi_3^1)d\xi_1d\xi_2,\\\mathbf{F}_2^0(\xi'_\nu,\xi'_3)&=\int_{\xi_\mu\in\mathbb{R}}\mathbf{G}_2^{II}(\xi'_\nu,\xi'_3;\xi_\mu,\xi_3^0)\mathbf{F}_1(\xi_\mu,\xi_3^0)d\xi_1d\xi_2,\end{aligned}\tag{B3}$$

for $\xi'_3\in(\xi_3^0,\xi_3^1)$. Apply representation (B3) in $\xi'_3=\xi_3^0$ and in $\xi'_3=\xi_3^0$. Set

$$\begin{aligned}(\mathbf{g}_2^{01}\mathbf{F}_1(.,\xi_3^1))(\xi'_\nu,\xi_3^0)&=\int_{\xi_\mu\in\mathbb{R}}\mathbf{G}_2^{II}(\xi'_\nu,\xi_3^0;\xi_\mu,\xi_3^1)\mathbf{F}_1(\xi_\mu,\xi_3^1)d\xi_1d\xi_2,\\(\mathbf{g}_2^{00}\mathbf{F}_1(\cdot,\xi_3^0))(\xi'_\nu,\xi_3^0)&=\int_{\xi_\mu\in\mathbb{R}}\mathbf{G}_2^{II}(\xi'_\nu,\xi_3^0;\xi_\mu,\xi_3^0)\mathbf{F}_1(\xi_\mu,\xi_3^0)d\xi_1d\xi_2,\\(\mathbf{g}_2^{11}\mathbf{F}_1(\cdot,\xi_3^1))(\xi'_\nu,\xi_3^1)&=\int_{\xi_\mu\in\mathbb{R}}\mathbf{G}_2^{II}(\xi'_\nu,\xi_3^1;\xi_\mu;\xi_3^1)\mathbf{F}_1(\xi_\mu,\xi_3^1)d\xi_1d\xi_2,\\(\mathbf{g}_2^{10}\mathbf{F}_1(\cdot,\xi_3^0))(\xi'_\nu,\xi_3^1)&=\int_{\xi_\mu\in\mathbb{R}}\mathbf{G}_2^{II}(\xi'_\nu,\xi_3^1;\xi_\mu,\xi_3^0)\mathbf{F}_1(\xi_\mu,\xi_3^0)d\xi_1d\xi_2.\end{aligned}\tag{B4}$$

Then

$$\begin{pmatrix}\mathbf{F}_2(\cdot,\xi_3^0)\\\mathbf{F}_2(\cdot,\xi_3^1)\end{pmatrix}=\begin{pmatrix}\mathbf{g}_2^{00}&-\mathbf{g}_2^{01}\\-\mathbf{g}_2^{10}&\mathbf{g}_2^{11}\end{pmatrix}\begin{pmatrix}\mathbf{F}_1(\cdot,\xi_3^0)\\\mathbf{F}_1(\cdot,\xi_3^1)\end{pmatrix}.\tag{B5}$$

Let the admittance operator be known at level surface $\xi_3=\xi_3^1$, i.e.,

$$\mathbf{F}_2(\cdot,\xi_3^1)=\boldsymbol{Y}^1\mathbf{F}_1(\cdot,\xi_3^1), \tag{B6}$$

where $\boldsymbol{Y}^1=\boldsymbol{Y}|_{\xi_3=\xi_3^1}$ as in the main text. Substituting Eq. (B6) into Eq. (B5) and solving the resulting operator equation yields the (forward) evolution equation for $\mathbf{F}_1$,

$$\mathbf{F}_1(\cdot,\xi_3^1)=-(\boldsymbol{Y}^1-\mathbf{g}_2^{11})^{-1}\mathbf{g}_2^{10}\mathbf{F}_1(\cdot,\xi_3^0), \tag{B7}$$

and the (backward) evolution equation for $\boldsymbol{Y}$

$$\boldsymbol{Y}^0=\mathbf{g}_2^{00}-\mathbf{g}_2^{01}(\boldsymbol{Y}^1-\mathbf{g}_2^{11})^{-1}\mathbf{g}_2^{10} \tag{B8}$$

upon identifying $\mathbf{F}_2(\cdot,\xi_3^0)=\boldsymbol{Y}^0\mathbf{F}_1(\cdot,\xi_3^0)$.

The existence of $(\boldsymbol{Y}^1-\mathbf{g}_2^{11})^{-1}$ needs to be further investigated. As in the main text, we will use a power flow argument. First, supplement representation (B3) with the 1-components

$$\begin{aligned}\mathbf{F}_1^1(\xi_\nu',\xi_3')&=-\int_{\xi_\mu\in\mathbb{R}}\mathbf{G}_1^{II}(\xi_\nu',\xi_3';\xi_\mu,\xi_3^1)\mathbf{F}_1(\xi_\mu,\xi_3^1)d\xi_1d\xi_2,\\ \mathbf{F}_1^0(\xi_\nu',\xi_3')&=\int_{\xi_\mu\in\mathbb{R}}\mathbf{G}_1^{II}(\xi_\nu',\xi_3';\xi_\mu,\xi_3^0)\mathbf{F}_1(\xi_\mu,\xi_3^0)d\xi_1d\xi_2.\end{aligned} \tag{B9}$$

Note that $\mathbf{F}^1$ and $\mathbf{F}^2$ independently satisfy the homogeneous hyperbolic system in $\mathscr{D}\backslash\partial\mathscr{D}$, with boundary values

$$\mathbf{F}_1^1(\cdot,\xi_3^0)=0,\quad \mathbf{F}_1^0(\cdot,\xi_3^0)=\mathbf{F}_1(\cdot,\xi_3^0), \tag{B10}$$

$$\mathbf{F}_1^1(\cdot,\xi_3^1)=\mathbf{F}_1(\cdot,\xi_3^1),\quad \mathbf{F}_1^0(\cdot,\xi_3^1)=0. \tag{B11}$$

From the fact that $\mathbf{F}_1^1(\cdot,\xi_3^0)=0$ it follows that the solution $\mathbf{F}^1$ does not allow any energy transport across the bounding level surface $\xi_3=\xi_3^0$. Then the physics constrains the averaged locally vertical component of the Poynting vector according to

$$0\geqslant-\int_{\xi_\mu\in\mathbb{R}}\tfrac{1}{2}\,\mathrm{Re}\{(\mathbf{F}_1^1)^\dagger\mathbf{F}_2^1\}(\xi_\mu,\xi_3^1)d\xi_1d\xi_2=-\tfrac{1}{2}\int_{\xi_\mu\in\mathbb{R}}(\mathbf{F}_1^1)^\dagger[\mathbf{g}_2^{11}+(\mathbf{g}_2^{11})^\dagger]\mathbf{F}_1^1(\xi_\mu,\xi_3^1)d\xi_1d\xi_2. \tag{B12}$$

Thus the Hermitian part of $\mathbf{g}_2^{11}$ is a negative or vanishing operator.

From the fact that $\mathbf{F}_1^0(\cdot,\xi_3^1)=0$ it follows that the solution $\mathbf{F}^0$ does not allow any energy transport across the bounding level surface $\xi_3=\xi_3^1$. Then the physics constrains the averaged locally vertical component of the Poynting vector according to

$$0\leqslant-\int_{\xi_\mu\in\mathbb{R}}\tfrac{1}{2}\,\mathrm{Re}\{(\mathbf{F}_1^0)^\dagger\mathbf{F}_2^0\}(\xi_\mu,\xi_3^0)d\xi_1d\xi_2=-\tfrac{1}{2}\int_{\xi_\mu\in\mathbb{R}}(\mathbf{F}_1^0)^\dagger[\mathbf{g}_2^{00}+(\mathbf{g}_2^{00})^\dagger]\mathbf{F}_1^0(\xi_\mu,\xi_3^0)d\xi_1d\xi_2. \tag{B13}$$

Thus the Hermitian part of $\mathbf{g}_2^{00}$ is a positive or vanishing operator.

In conclusion, $\boldsymbol{Y}^1$ is positive and $\mathbf{g}^{11}$ is negative or vanishing, which guarantees the existence of $(\boldsymbol{Y}^1-\mathbf{g}_2^{11})^{-1}$.

APPENDIX C: THE NUMERICAL SCHEME

For all frequencies calculate the fundamental solutions in inclusion: apply the radiation boundary conditions (IV.28), solve the Riccati equation for positive and negative directions (IV.23), reverse the order of both Riccati equation solutions, apply the point source boundary conditions (IV.26) and (IV.27), solve the one-way equation for negative and positive directions (IV.25) and save the fundamental solutions in the transverse wave number domain.

Calculate the boundary mapping: compose the wave number constituents of the fundamental solutions to give the fundamental solutions in the space domain (VI.7), combine the fundamental solutions with BEM for scattered fields in the embedding (IV.29), match the boundary conditions to calculate the kernel "matrices" mapping the incident field to the boundary source distribution and the weights of the fundamental solutions (IV.7)–(IV.10), and save these matrices.

Given the incident field: for all receivers in the inclusion obtain the weights of the fundamental solutions, for all receivers in the embedding obtain the boundary source distribution.

Evaluate the scattered field according to Eqs. (IV.29) and (V.6), which ends the frequency loop.

Multiply the total field with the source signature spectrum and inverse Fourier transform the result (II.2).

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The construction of spinor fields on manifolds with smooth degenerate metrics

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We examine some of the subtleties inherent in formulating a theory of spinors on a manifold with a smooth degenerate metric. We concentrate on the case where the metric is singular on a hypersurface that partitions the manifold into Lorentzian and Euclidean domains. We introduce the notion of a complex spinor fibration to make precise the meaning of continuity of a spinor field and give an expression for the components of a local spinor connection that is valid in the absence of a frame of local orthonormal vectors. These considerations enable one to construct a Dirac equation for the discussion of the behavior of spinors in the vicinity of the metric degeneracy. We conclude that the theory contains more freedom than the spacetime Dirac theory and we discuss some of the implications of this for the continuity of conserved currents. © *1996 American Institute of Physics.* [S0022-2488(96)01707-0]

I. INTRODUCTION

The interest in the influence of topology on physics is an old one. In recent times there has also been considerable debate on the influence of the geometrical structure of spacetime that may accompany a change in its overall topology. This has been partly motivated by the implications of the semi-classical theory of quantum gravity and partly by the interest in field theories on background spacetimes with interesting topologies. Further motivation arises from string theories in which string interactions arise from the topology of world sheets. In all these approaches fundamental assumptions about the signature of the spacetime metric are required. Such assumptions dictate the detailed behavior of both the causal structure of the theory and the selection rules for topology change. In the context of classical theory there are powerful constraints on the nature of such changes on manifolds with a global Lorentzian signature and a spinor structure.[1] To escape such constraints a number of authors have contemplated geometries in which the metric is allowed to become degenerate, particularly on hypersurfaces that partition the manifold into Lorentzian and Euclidean regions. Despite the obvious implications for causality there have been serious attempts to follow the consequences for physics associated with signature changing metrics. Despite the absence of a rigorous theory of second quantized fields on such a background, in Ref. 2 it was suggested that a quantized scalar field could exhibit spontaneous particle production even in the absence of gravitational curvature. This result relied on certain natural linear boundary conditions that were imposed on the scalar field at the hypersurface of signature change. Since there

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is no continuous orthonormal coframe in the presence of metric degeneracy and the field equations are themselves dependent on the metric one must rely on a prescribed differential structure in order to define the necessary limits of the gradients of the scalar field in the vicinity of the metric degeneracy. In practice this means one can always rely on a local coordinate coframe to effect one's calculations. Furthermore the differentiability class of all tensor fields is defined with respect to the differentiability of their components in an arbitrary coordinate (co-)frame independent of any metric structure.

Since matter in flat Lorentzian spacetime is also described in terms of various representations of the Lorentzian SPIN group it is natural to try and extend these considerations to the behavior of spinor fields on manifolds with a degenerate metric. In particular one may wish to formulate a dynamical theory of spinor fields and deduce from their field equations a class of natural boundary conditions at the hypersurface of signature change. However a number of interesting problems then arise that have no counterpart in the theory of tensor fields. The most obvious is that the dimensionality of the real irreducible SPIN representations is signature dependent so that it becomes meaningless to try and match spinor fields belonging to representations with different dimensions. If one persists with the search for matching conditions one must in general consider complex representations.

In a smooth local basis of spinor fields one can define the differentiability class of the components of a spinor field. Such a basis is a basis for a module carrying representations of the SPIN group, which is a double cover of the $SO(p,q)$ group associated with the signature of the underlying metric on the manifold. Clearly this procedure will fail at the hypersurface where the signature changes, since the SPIN groups differ across the hypersurface. In order to define continuous spinor fields on a neighborhood crossing the hypersurface, alternatives to the traditional reliance on lifting orthonormal frames to spinor frames must be pursued. Of necessity one must expect some arbitrariness in defining the notion of a continuous spinor field in the presence of signature change.

It is natural to subject local spinor fields to the appropriate Dirac equation in regions where the metric is non-degenerate. In such regions the conventional Dirac operator can be defined in terms of a spinor covariant derivative that is designed to satisfy the natural Leibniz rules on products of tensors and spinors. In this manner it can be made compatible with the natural linear connection on tensors. A unique Levi-Civita tensor covariant derivative is determined completely by the metric tensor. When this metric is non-degenerate one can exploit the existence of local orthonormal frames to uniquely fix the spinor connection that determines the spinor covariant derivative. It is important to stress that it is only the *existence* of a class of orthonormal frames that is necessary to effect this determination, since it provides a reference frame for normalization. The SPIN connection so defined is then compatible with a SPIN invariant inner product on spinors. If one attempts to define a spinor connection in the absence of a class of orthonormal frames then one must recognize the inherent arbitrariness that cannot be removed by normalization. Since we are interested in subjecting our spinor fields to the appropriate Dirac equation in regions where the metric is regular we must accommodate this freedom in the spinor connection if we wish to discuss the matching of spinor solutions at the hypersurface of degeneracy.

Little attention has been devoted to the formulation of spinor fields on spaces with degenerate metrics. Romano[3] recognized that the choice of spinor equation was not straightforward. His analysis was restricted to the case of a discontinuous change of signature, whereas in this article we restrict ourselves instead to the case of continuous degenerate metrics. It is our purpose to examine the essential arbitrariness inherent in a formulation of spinor theory on manifolds with such metrics.

In section II we offer a definition of complex spinors in terms of a *spinor fibration* over a manifold. Although our construction relies on the representation theory of Clifford algebras, we have translated our arguments into the traditional language of γ matrices. The essential novelty is that these are matrix representations of a set of coordinate vector fields that constitute a frame in

the vicinity of the metric degeneracy. The representation structure is explicitly presented in terms of degenerate metrics in two and four dimensions.

Having defined the notion of spinor continuity in terms of a spinor fibration, we turn to the notion of the spinor covariant derivative in section III. We show how this can be determined to be both compatible with a SPIN invariant inner product and to commute with the complex structure ("charge conjugation"). In section IV we write down and solve the two dimensional Dirac equation written in terms of this spin connection, making explicit the dependence of the singularity structure of these solutions on both the spin metric and the metric on the underlying manifold. We conclude with a brief discussion of the $U(1)$ currents associated with these solutions and offer some speculations on alternative approaches.

II. SPINORS

In $n=2m$ dimensions we consider the manifold $M=\mathbb{R}^{2m}$ with metric

$$g=h(t)dt\otimes dt+\hat{g}_{ij}(\vec{x})dx^i\otimes dx^j \tag{1}$$

in a chart $(t,x^i)=(x^\mu)$, $i=1,\ \ldots,n-1$, where $\hat{g}$ is assumed to be positive definite. h is a smooth function which may have zeroes (at most countably many that are nowhere dense). However, we require that h changes sign at zeroes of h. None of the crucial steps of the development below rely on the topological triviality of this particular manifold. Although the discussion applies to complex spinors on any even dimensional manifold with signature change, we will pay particular attention to the cases $n=4$ and $n=2$.

Kossowski and Kriele have shown[4] under fairly general conditions that, at any zero of h where $\dot{h}\neq 0$, one can switch to coordinates (t',x^i) in a neighborhood of the zero such that $h(t)dt^2=t'dt'^2$. However, the precise nature of the signature change is not of importance within the scope of this article.

To define Dirac spinors on a manifold M of constant signature one usually[5] considers local irreducible representations $\boldsymbol{\gamma}$ of the complex Clifford algebra bundle

$$\mathcal{Cl}(M)=\cup_{p\in M}\mathcal{Cl}(T_pM,g_p), \tag{2}$$

i.e, $\boldsymbol{\gamma}$ is a fiber preserving homomorphism,

$$\boldsymbol{\gamma}:\pi^{-1}(U)\subset\mathcal{Cl}(M)\rightarrow M_k(\mathbb{C})\times U, \tag{3}$$

where $\pi:\mathcal{Cl}(M)\rightarrow M$ is the bundle projection, U is an open subset of M, and $M_k(\mathbb{C})$ is the set of complex $k\times k$ matrices ($k=2^m$). We will assume for now that $\boldsymbol{\gamma}$ is at least continuous. If the representation $\boldsymbol{\gamma}$ is also faithful, which is the case for even dimension of M, then $\boldsymbol{\gamma}$ is just a local trivialization of $\mathcal{Cl}(M)$. In particular, for vector fields X and Y, $\boldsymbol{\gamma}$ satisfies

$$\{\boldsymbol{\gamma}(X),\boldsymbol{\gamma}(Y)\}=2\,g(X,Y)\mathbf{1}. \tag{4}$$

With respect to a local coordinate chart $\boldsymbol{\gamma}$ is given by its components

$$\gamma_\mu:=\boldsymbol{\gamma}(\partial_\mu). \tag{5}$$

(Note that we use bold-faced $\boldsymbol{\gamma}$ for the representation map, and light-faced symbols for particular images under a representation. Both kinds of symbols may appear in a single expression, in which case a map defined by pointwise multiplication is described as in $[\gamma_\mu\boldsymbol{\gamma}](a)=\gamma_\mu[\boldsymbol{\gamma}(a)]$, $a\in\mathcal{Cl}(M)$.) With this definition we obtain the familiar relationship

$$\{\gamma_\mu,\gamma_\nu\}=2\,g_{\mu\nu}\mathbf{1}. \tag{6}$$

The Dirac spinor bundle $S(M)$ is a vector bundle carrying such a representation γ, i.e., there is a chart for $S(M)$ such that the Clifford action of $\mathcal{C}l(M)$ on $S(M)$ is given by multiplication of the γ-matrices with column spinors. If $\mathcal{C}l(M)$ transforms under a product of tensor representations of the orthogonal group and the Clifford action is covariant under this transformation, then $S(M)$ transforms under a spin representation of the orthogonal group.

Except for regions that contain zeroes of h it is straightforward to generalize these ideas to our signature changing spacetime M. The crucial question is how to link the spinor bundles across hypersurfaces of signature change. In the following exposition we will use the fact that the Clifford bundles are linked and lift this link to the spinor bundles. Specifically we will consider an algebra fibration which coincides with the Clifford bundles where the metric is non-degenerate and representations of this fibration which are continuous across a hypersurface of signature change. A detailed study of such representations suggests certain additional conditions which are sufficient to ensure the invariance of the resulting structure under appropriate changes of representations and/or coordinates. Since the group of transition functions is different for different signature we will adopt the term "fibration" for $\mathcal{C}l(M)$ and $S(M)$ instead of "bundle," but we will still refer to this object as the "Clifford" and "spinor" fibration, although we use these expressions in a non-traditional context.

The following example will illustrate some of the key issues we have to face.

A. An example in two dimensions

In $n=2$ dimensions we consider $M=\mathbb{R}^2$ with coordinates (t,x) and metric

$$g=h(t)dt\otimes dt+dx\otimes dx, \tag{7}$$

i.e., $\hat{g}=1$. Then the following γ-matrices:

$$\gamma_x=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix},\gamma_t=\begin{pmatrix}0 & 1\\ h(t) & 0\end{pmatrix}, \tag{8}$$

define a continuous representation γ on all of M which is faithful and irreducible for $h(t)\neq 0$. Note that γ_t is necessarily degenerate at zeroes of h, where the matrix algebra generated by these matrices actually reduces to upper-triangular matrices. Therefore, this representation is neither faithful nor irreducible at metric degeneracies. This behavior is generic because of an incompatibility of representations of degenerate and non-degenerate Clifford algebras: Since the Clifford algebra is no longer semi-simple for $h=0$, the dimension of an irreducible representation is smaller by a factor of two. The irreducible representation of the degenerate algebra is in fact just an irreducible representation of its non-degenerate "spatial" part, i.e., the part corresponding to the "spatial" γ_x. For the representation to remain faithful it would have to double its dimension in order to accommodate the whole nilpotent ideal generated by the degenerate direction. (Note that half of the algebra, namely the ideal generated by γ_t, is nilpotent of order 2 at the degeneracy.)

B. The general case

For a precise description of the behavior of a representation around a metric degeneracy we examine the behavior of $\gamma(\partial_\mu)|_p$ as p approaches a hypersurface $H=\{t=t_0\}$, where $h(t_0)=0$.

Observation 1: *If a continuous local representation γ satisfies Eq. (4) on an open set $U\subset M$ intersecting H and is faithful and irreducible on $U\backslash H$, then γ is a faithful representation of the "spatial subalgebra" $\mathcal{C}l^{sp}(M)$ generated by $\{\partial_i\}_{i=1,\ldots,n-1}$ on all of U. Furthermore, $\mathcal{C}l^{sp}(M)$ contains central orthogonal idempotents $P_\pm$ which effect a Pierce decomposition of $\mathcal{C}l(M)$ and a corresponding decomposition of γ. Given a particular form of $\gamma(P_\pm)$, this decomposition is reflected in a block structure of the matrix representation.*

From the previous example we infer that $\gamma(\partial_t)|_p$ becomes degenerate as $p \to H$. For the other coordinate vector fields this is not the case, since $\gamma(\partial_i)^2 = \mathbf{1}$ everywhere in U. This corresponds to the fact that the algebra generated by $\{\partial_i\}_{i=1,\ldots,n-1}$, which we call the "spatial subalgebra" $\mathcal{C}\ell^{sp}(M)$ remains non-degenerate on H, whence γ restricted to $\mathcal{C}\ell^{sp}(M)$ remains a faithful representation. Therefore, this spatial subalgebra does not "notice" the metric degeneracy and will provide the link that constrains the behavior of γ_t as we pass through H. $\mathcal{C}\ell^{sp}(M)$ contains central orthogonal idempotents,

$$P_\pm := \frac{1}{2}(1 \pm z), \tag{9}$$

where z is the normalized dual of the volume element of H, whence $z^2 = 1$, $P_\pm^2 = P_\pm$, and $P_\pm P_\mp = 0$. For example, $z = \partial_x$ for the metric given by Eq. (7), whereas $z = i\det\hat{g}^{-1/2}\partial_1 \wedge \partial_2 \wedge \partial_3$ in four dimensions with metric given by Eq. (1). The idempotents or projectors $P_\pm$ split $\mathcal{C}\ell^{sp}(M)$ into a direct sum of simple components,

$$\mathcal{C}\ell^{sp}(M) = \mathcal{C}\ell_+(M) \oplus \mathcal{C}\ell_-(M), \tag{10}$$

where

$$\mathcal{C}\ell_\pm(M) := P_\pm \mathcal{C}\ell(M) P_\pm . \tag{11}$$

Therefore γ induces inequivalent representations

$$\gamma_\pm := \gamma_\pm \gamma \gamma_\pm \tag{12}$$

of $\mathcal{C}\ell^{sp}(M)$, where

$$\gamma_\pm := \gamma(P_\pm). \tag{13}$$

So we get the following Pierce decomposition with respect to the idempotents $P_\pm$:

$$\begin{aligned}\mathcal{C}\ell(M) &= (P_+ + P_-)\mathcal{C}\ell(M)(P_+ + P_-) \\ &= P_+\mathcal{C}\ell(M)P_+ \oplus P_+\mathcal{C}\ell(M)P_- \oplus P_-\mathcal{C}\ell(M)P_+ \oplus P_-\mathcal{C}\ell(M)P_- \\ &= \mathcal{C}\ell_+(M) \oplus P_+\mathcal{C}\ell(M)P_- \oplus P_-\mathcal{C}\ell(M)P_+ \oplus \mathcal{C}\ell_-(M),\end{aligned} \tag{14}$$

which translates into representations

$$\gamma = \gamma_+\gamma\gamma_+ + \gamma_+\gamma\gamma_- + \gamma_-\gamma\gamma_+ + \gamma_-\gamma\gamma_- = \gamma_+ + \gamma_+\gamma\gamma_- + \gamma_-\gamma\gamma_+ + \gamma_- . \tag{15}$$

Since $\mathcal{C}\ell^{sp}(M)$ commutes with $P_\pm$ and

$$\mathcal{C}\ell(M) = \mathcal{C}\ell^{sp}(M) \oplus \mathcal{C}\ell^{sp}(M)\partial_t = \mathcal{C}\ell^{sp}(M) \oplus \partial_t\mathcal{C}\ell^{sp}(M), \tag{16}$$

the cross terms in Eq. (14) come from ∂_t:

$$P_\pm \mathcal{C}\ell(M) P_\mp = P_\pm(\mathcal{C}\ell^{sp}(M)\partial_t)P_\mp = \mathcal{C}\ell_\pm(M)\partial_t = P_\pm(\partial_t\mathcal{C}\ell^{sp}(M))P_\mp = \partial_t\mathcal{C}\ell_\mp(M). \tag{17}$$

[Note that $P_\pm\partial_t = \partial_t P_\mp$ and $P_\pm\mathcal{C}\ell^{sp}(M)P_\mp = 0$.] This can also be seen from the decomposition of γ_t:

$$\gamma_t = \gamma_+\gamma_t\gamma_- + \gamma_-\gamma_t\gamma_+ . \tag{18}$$

If $\gamma_\pm$ takes the form

$$\gamma_+=\begin{pmatrix}\mathbf{1} & \mathbf{0}\\ \mathbf{0} & \mathbf{0}\end{pmatrix},\quad \gamma_-=\begin{pmatrix}\mathbf{0} & \mathbf{0}\\ \mathbf{0} & \mathbf{1}\end{pmatrix}, \tag{19}$$

in terms of $2^{m-1}\times 2^{m-1}$ unit and zero matrices, which can always be achieved by an equivalence transformation pointwise on U (even on H), then the Pierce decomposition is reflected in a block structure of the matrix representation $\gamma(\mathcal{C}\ell(M))$. In particular, the induced representations $\gamma_\pm$ only have one non-zero block, namely in the upper left (lower right) corner. Denoting the non-zero blocks of the corresponding matrices by overlined symbols, for example,

$$\gamma_+(\mathcal{C}\ell_+(M))=\begin{pmatrix}\overline{\gamma_+(\mathcal{C}\ell_+(M))} & \mathbf{0}\\ \mathbf{0} & \mathbf{0}\end{pmatrix}, \tag{20}$$

we have the following block structure of $\gamma(\mathcal{C}\ell(M))$:

$$\begin{aligned}\gamma(\mathcal{C}\ell(M))&=\begin{pmatrix}\overline{\gamma_+(\mathcal{C}\ell_+(M))} & \overline{\gamma_+\gamma_t\gamma_-(\mathcal{C}\ell_-(M))}\\ \overline{\gamma_-\gamma_t\gamma_+(\mathcal{C}\ell_+(M))} & \overline{\gamma_-(\mathcal{C}\ell_-(M))}\end{pmatrix}\\ &=\begin{pmatrix}\overline{\gamma_+(\mathcal{C}\ell_+(M))} & \overline{\gamma_+(\mathcal{C}\ell_+(M))\gamma_t\gamma_-}\\ \overline{\gamma_-(\mathcal{C}\ell_-(M))\gamma_t\gamma_+} & \overline{\gamma_-(\mathcal{C}\ell_-(M))}\end{pmatrix}.\end{aligned} \tag{21}$$

[To arrive at this equation apply γ to Eq. (14) using Eqs. (12), (17), (19) and inserting projectors $P_\pm$ when appropriate.] This block structure helps us to understand what happens to a representation when we cross H. The blocks on the diagonal make up the spatial subalgebra and do not contain γ_t. Therefore, these blocks remain non-degenerate throughout U. The off-diagonal blocks show that γ_t intertwines γ_+ and γ_-.

Observation 2: *The inequivalent faithful representations $\gamma_\pm$ of $\mathcal{C}\ell^{sp}(M)$ have equivalent restrictions $\gamma_\pm^+$ to the even subalgebra $\mathcal{C}\ell^+(M)\subset\mathcal{C}\ell^{sp}(M)$. Furthermore, the restrictions $\gamma_\pm^+$ are intertwined by γ_t, which implies that for any $p\in H$, one of the off-diagonal blocks of $\gamma_t|_p$ in the previously discussed block structure vanishes and the other either vanishes or is regular. (The diagonal blocks are trivially zero.)*

Even though the representations $\gamma_\pm$ vanish on one of the simple components, $\gamma_\pm(\mathcal{C}\ell_\mp(M))=0$, they are equivalent when restricted to the even part $\mathcal{C}\ell^+(M)$ of $\mathcal{C}\ell^{sp}(M)$, which is a simple algebra isomorphic to $\mathcal{C}\ell_\pm(M)$. Applying $\gamma_i\gamma_t=-\gamma_t\gamma_i$ twice, we have $\gamma_i\gamma_j\gamma_t=+\gamma_t\gamma_i\gamma_j$, which implies that the restrictions $\gamma_\pm^+$ of $\gamma_\pm$ to $\mathcal{C}\ell^+(M)$ are intertwined by γ_t:

$$\gamma_\pm^+\gamma_t=\gamma_t\gamma_\mp^+. \tag{22}$$

In the block structure (21) the non-zero blocks $\overline{\gamma_\pm^+(\mathcal{C}\ell^+(M))}$ induce irreducible representations $\overline{\gamma_\pm^+}:\pi^{-1}(U)\cap\mathcal{C}\ell^+(M)\to M_{k/2}(\mathbb{C})\times U$. Since an intertwiner of two irreducible representations is determined up to a scale, with the intertwiner being non-singular unless the scale is zero, we see from the non-zero blocks associated with Eq. (22) that the two blocks of $\gamma_t=\gamma_+\gamma_t\gamma_-+\gamma_-\gamma_t\gamma_+$ are determined by Eq. (22) up to a scale. Since $(\gamma_\pm\gamma_t\gamma_\mp)\times(\gamma_\mp\gamma_t\gamma_\pm)=h(t)\gamma_\pm$, in fact, only a relative scale remains undetermined. Therefore at least one entire block of γ_t has to vanish for $h(t)\to 0$, so that we are left with a block triangular or block diagonal matrix algebra on H.

Even though we may not be able to achieve this block structure on all of U at the same time, this argument still shows that γ_t is determined up to a relative scale between $\gamma_+\gamma_t\gamma_-$ and $\gamma_-\gamma_t\gamma_+$ and that $\gamma(\mathcal{C}\ell(M))$ is isomorphic to a block triangular or block diagonal matrix algebra at each point of H.

Observation 3: *Two continuous local representations* $\gamma_{(r)}$, $r=1, 2$, *satisfying Eq. (4) on an open set* $U \subset M$ *intersecting* H *and faithful irreducible on* $U \backslash H$, *are equivalent if and only if the block structures of* $\gamma_{(r)}(\partial_t)|_H$ *agree. Furthermore, the intertwiner is guaranteed to be continuous across* H *if one block of* $\gamma_{(r)}(\partial_t)$ *stays regular.*

Given two overlapping local representations, we can use the same decomposition to show that it is a necessary condition that γ_t has the same behavior on H for both representations if they are related by a non-singular intertwiner. Conversely, if the behavior of γ_t is different for two local representations, the intertwiner necessarily becomes singular on H. Not only the agreement in block structure but its particular form on H is of importance. If both blocks of γ_t vanish, i.e., γ_t vanishes entirely for both overlapping local representations, their intertwiner may be discontinuous. If on the other hand only one block of γ_t vanishes then the intertwiner inherits the smoothness properties of the local representations, in particular it is at least continuous. In this case the non-zero block of γ_t serves as a link across H and no additional requirement of continuity of the intertwiner is needed to ensure that the gluing together of local representations is well-defined. Of course, the transition functions can be restricted to lie in the appropriate spin groups away from H, which requires the transition functions on H to continuously connect both spin groups.

C. Criteria for a spinor fibration

It can be shown that if γ is assumed to be not only C^1 away from H (this is required in order to define a spin connection as we will see in section IIIC) but also to have bounded partial derivatives on any bounded set, then exactly one of $\gamma_\pm \gamma_t \gamma_\mp$ vanishes on all of H and the other one does not. Therefore, a simple smoothness assumption gains the desired control over the block structure. Since the minor technical difference between requiring bounded partial derivatives on bounded sets and C^1, namely that the partial derivatives have limits on H, does not affect the continuity structure of the spinor fibration in question, we will use the more intuitive condition of continuous differentiability. Allowing the partial derivatives of γ to be locally unbounded relinquishes any control over the block structure, e.g., in the two dimensional example:

$$\gamma_x = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \gamma_t = \begin{cases} \begin{pmatrix} 0 & |h(t)|^{1/2}+x^2 \\ h(t)[|h(t)|^{1/2}+x^2]^{-1} & 0 \end{pmatrix}, & \text{for } x>0. \\ \begin{pmatrix} 0 & |h(t)|^{1/2} \\ h(t)|h(t)|^{-1/2} & 0 \end{pmatrix}, & \text{for } x \leqslant 0. \end{cases} \tag{23}$$

Piecing γ's like this one together we can get any behavior of γ_t on H we (do not) like.

These observations lead us to a set of criteria for local representations which ensure that they are related by C^1 equivalence transformations:

(i) γ is C^1 satisfying Eq. (4).

(ii) γ is faithful irreducible for $h(t) \neq 0$.

(iii) $\gamma_- \gamma_t \to 0$ for $h(t) \to 0$.

[Of course, the γ-matrices given by Eq. (8) satisfy these criteria.] Condition (iii) singles out one class of representations with a certain behavior for $h(t) \to 0$. Equally well, one could require

(iii′) $\gamma_+ \gamma_t \to 0$ for $h(t) \to 0$,

or even a mixture of both, fixing the behavior of the representation for each hypersurface of metric degeneracy separately. In this paper we focus on the issues arising from just one zero of h. In this case (iii′) is obtained from (iii) under a spatial inversion.

D. A possible generalization

We can relax the assumption of a metric of the form Eq. (1) if we assume the existence of a local frame of non-zero vector fields $\{X_\mu\}$ on any open set intersecting a hypersurface H of

signature change, such that $X_i \in T(H)$ satisfies $g(X_i,X_j)|_H=\delta_{ij}$ and $g(X_0,X_\mu)|_H=0$ and construct $\gamma(X_\mu)$ instead of $\gamma(\partial_\mu)$. The spatial subalgebra $\mathcal{Cl}^{sp}(M)$ of $\mathcal{Cl}(M)$ generated by $\{X_i\}$ coincides with the appropriate extension of $\mathcal{Cl}(H)=\cup_{p\in H}\mathcal{Cl}(T_pH,H^*g_p)$, which is really the only intrinsic structure in the vicinity of H. It is essential that the pullback metric H^*g_p be non-degenerate. It is then straightforward to retrace the steps we followed above and come to the same conclusions. Of course, the existence of a global fibration $S(M)$ will depend on the topology of M and possibly on the topology of hypersurfaces of metric degeneracy.

III. THE SPINOR COVARIANT DERIVATIVE

Having defined a spinor fibration $S(M)$ we have a notion of continuity of a spinor field. Namely, a spinor field is continuous if its component sections are continuous with respect to a bundle chart. In other words, given a set of γ-matrices satisfying appropriate conditions, a continuous spinor field is given by a column of continuous functions on which these γ-matrices act.

In order to write down a Dirac equation on M, we need a notion of covariant differentiation of a spinor field. However, given a linear connection on M, the spinor connection is not uniquely determined unless it is also required to be compatible with both a choice of spinor metric and a notion of charge conjugation. Furthermore, the traditional construction of a spinor connection relies on the existence of a non-degenerate metric. In the following we discuss these separate aspects in regions where the metric is manifestly non-degenerate. In section IV the interrelation between these different aspects will be examined in the vicinity of a hypersurface of signature change.

Authors of other literature on this subject usually work in orthonormal frames (see for example Ref. 6) with the notable exception of an early review[7] which also contains references to most of the original work and notes the scaling freedom in the spinor metric discussed below.

A. The spinor metric

In order to discuss the Dirac equation below we introduce the notion of a spinor metric. In particular, we adopt a Hermitian symmetric spin invariant bilinear form on Dirac spinors,

$$S(M)\times S(M)\to\mathfrak{F}(M),$$

$$\Psi,\Xi\mapsto(\Psi,\Xi)=\Psi^\dagger C\Xi, \tag{24}$$

where $\mathfrak{F}(M)$ denotes the space of functions on M and C is chosen to satisfy

$$C=C^\dagger, \tag{25}$$

$$C\gamma_\mu=-\gamma_\mu^\dagger C, \tag{26}$$

on M. The familiar Dirac adjoint is then given by

$$\bar{\Psi}=\Psi^\dagger C. \tag{27}$$

For our example, Eq. (8),

$$C_1=\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}, \tag{28}$$

satisfies Eqs. (25) and (26). However, the spinor metric C is only determined up to a real scalar at each point of the manifold. Therefore $C_f=fC_1$ could equally well be chosen as a spinor metric, where $f=f^*\in\mathfrak{F}(M)$. Usually the spinor metric is required to be smooth and non-degenerate, which restricts f to be smooth and non-zero. This is one of the reasons why the choice of spinor metric does not usually appear in the standard discussion of the Dirac equation. The scaling function f is normalized to make the equation simple, i.e., C is chosen to be constant for constant

γ-matrices. (Note that the γ-matrices cannot be constant across a hypersurface of signature change.) The behavior of f where the spacetime metric is degenerate must be postulated separately, and it can not *a priori* be ruled out that f may be zero or singular there.

B. Charge conjugation

Charge conjugation can be defined as a map,

$$S(M)\to S(M),$$

$$\Psi\mapsto\Psi^c:=B^*\Psi^*, \tag{29}$$

where B satisfies

$$B\gamma_\mu=\gamma_\mu^* B, \tag{30}$$

$$B^*B=\pm\mathbf{1}=\beta\mathbf{1}. \tag{31}$$

These conditions determine B up to a phase which may vary over M. The sign in the second condition depends on the signature. $\beta=+1$ if there exists a real representation $\beta=-1$ otherwise. Defining the index ν of a metric to be the (signed) difference of the number of positive and negative eigenvalues of the metric, we note that

$$\beta=\begin{cases}+1, & \text{for } \nu\equiv 0,\ 2 \bmod 8,\\ -1, & \text{for } \nu\equiv 4,\ 6 \bmod 8.\end{cases} \tag{32}$$

Therefore, β changes sign and B is necessarily discontinuous if the signature changes from $(-+++)$, i.e., $\nu=2$, to $(++++)$, i.e., $\nu=4$, in four dimensions, while for the change of signature $(-+)\to(++)$ in two dimensions $\beta=1$ in both regions. Since β also determines the periodicity of the charge conjugation operation, namely

$$(\Psi^c)^c=\beta\Psi, \tag{33}$$

continuity of a spinor is only compatible with continuity of its charge conjugate if β is the same in Euclidean and Lorentzian regions. [This observation warrants an investigation of alternative spinor metrics and notions of charge conjugation for the opposite metrics, i.e., signature changing from $(+---)$ to $(----)$, in four dimensions. The reader is invited to pursue these technical aspects which lie outside the main thrust of this article. Note that the standard definitions for opposite Lorentzian metrics differ by signs in Eqs. (26) and (30). For completeness, one may also consider the inclusion of spinors with Grassmann-valued components or even non-standard versions of Eqs. (26) and (30).]

For our 2 dimensional example, we may take

$$B=e^{i\theta}\mathbf{1}, \tag{34}$$

where $\theta=\theta^*\in\mathfrak{F}(M)$.

C. The spinor connection

Given a spinor metric the spinor covariant derivative S_μ with respect to a vectorfield ∂_μ is given by

$$S_\mu=\partial_\mu+\Sigma_\mu, \tag{35}$$

where the spinor connection Σ_μ has to be determined such that the axioms for a spinor covariant derivative are satisfied:

$$S_\mu(a^\nu\gamma_\nu\Psi)=(\nabla_\mu a^\nu)\gamma_\nu\Psi+a^\nu\gamma_\nu(S_\mu\Psi), \tag{36}$$

$$\partial_\mu(\Psi,\Xi)=(S_\mu\Psi,\Xi)+(\Psi,S_\mu\Xi), \tag{37}$$

$$S_\mu(\Psi^c)=(S_\mu\Psi)^c. \tag{38}$$

$\nabla_\mu a^\nu:=a^\nu{}_{;\mu}:=\partial_\mu a^\nu+\Gamma^\nu{}_{\mu\rho}a^\rho$ denotes the components of the covariant derivative of the vector field given by a^ν, where $\Gamma_{\rho\mu\nu}$ are the spacetime connection coefficients, i.e., for the Levi-Civita connection $\Gamma_{\rho\mu\nu}=\frac{1}{2}(\partial_\mu g_{\nu\rho}+\partial_\nu g_{\mu\rho}-\partial_\rho g_{\mu\nu})$. These axioms ensure compatibility of covariant differentiation of tensors and spinors, Eq. (36), and compatibility of the spinor covariant derivative with the spinor metric and charge conjugation, Eqs. (37) and (38). Using the defining properties, Eqs. (35), (25), (26), (30), and (31), in Eqs. (36)–(38) we get the following conditions:

$$\partial_\mu\gamma_\nu-\Gamma^\rho{}_{\mu\nu}\gamma_\rho=[\gamma_\nu,\Sigma_\mu]=\gamma_\nu\Sigma_\mu-\Sigma_\mu\gamma_\nu, \tag{39}$$

$$C^{-1}\partial_\mu C=\Sigma_\mu+C^{-1}\Sigma_\mu^\dagger C, \tag{40}$$

$$B^{-1}\partial_\mu B=\Sigma_\mu-B^{-1}\Sigma_\mu^* B. \tag{41}$$

In order to give an explicit expression for Σ_μ we expand it in a basis of the Clifford algebra:

$$\Sigma_\mu=\sum_I \sigma_{\mu I}\gamma^I, \tag{42}$$

where the sum is taken over the set of ordered indices $\{(i_1,\ldots,i_p):1\leqslant i_1<\cdots<i_p\leqslant n,\ 0\leqslant p\leqslant n-1\}$, with $n=\dim M$, where also $\gamma^{(i_1\cdots i_p)}=\gamma^{i_1}\ldots\gamma^{i_p}$ and $\gamma^\emptyset=\mathbf{1}$ are understood. (Note that the superscript is the empty set $\emptyset$ *not* 0 in the last equation.) In particular $\{\gamma^I\}$ is a basis for the Clifford algebra in the representation γ.

We first solve for the components of Σ_μ using Eq. (39):

$$[\gamma_\nu,\Sigma_\mu]=\left[\gamma_\nu,\sum_I \sigma_{\mu I}\gamma^I\right]=2\sum_{\substack{\nu\notin I\\ |I|\text{odd}}}\sigma_{\mu I}\gamma_\nu\gamma^I+2\sum_{\substack{\nu\in I\\ |I|\text{even}}}\sigma_{\mu I}\gamma_\nu\gamma^I, \tag{43}$$

where $|I|$ denotes the length of the multi index. Thus all but the scalar part of Σ_μ is determined:

$$\sigma_{\mu I}=\frac{1}{2^{N+1}}\mathrm{tr}[\gamma_{I^r}\gamma^\nu(\partial_\mu\gamma_\nu-\Gamma^\rho{}_{\mu\nu}\gamma_\rho)]\quad(\text{no sum over }\nu), \tag{44}$$

where for given I one may choose any ν such that for $|I|$ even $\nu\in I$ while for $|I|$ odd $\nu\notin I$. (I^r denotes indices in reversed order, $N=2^{n/2}$.) For example, to calculate $\sigma_{\mu(0,1,2,3)}$ in four dimensions we may take any $\nu\in\{0,1,2,3\}$, the result is guaranteed to be the same.

We solve for the scalar part of Σ_μ using Eqs. (40) and (41):

$$\sigma_{\mu\emptyset}=\frac{1}{2^{N+1}}\mathrm{tr}(C^{-1}\partial_\mu C+B^{-1}\partial_\mu B). \tag{45}$$

Thus Σ_μ is completely determined. Eq. (45) is derived from the general conditions arising from Eqs. (40) and (41):

$$\mathrm{Re}\ \sigma_{\mu I}=\frac{1}{2^{N+1}}\mathrm{tr}(\gamma_{I^r}C^{-1}\partial_\mu C)\quad(|I|\ \text{even}), \tag{46}$$

$$\text{Im}\ \sigma_{\mu I}=\frac{1}{2^{N+1}i}\ \text{tr}(\gamma_{I'}B^{-1}\partial_\mu B). \tag{47}$$

Again these expressions are guaranteed to be real and compatible with Eq. (44). In some instances it may actually be more convenient to use these latter relationships to solve for various components of Σ_μ.

Applying Eqs. (44) and (45) to Eqs. (8), (25), (26), (30), and (31), we obtain for the spinor connection for our 2 dimensional example,

$$\Sigma_x=\frac{1}{2}f^{-1}\partial_x f+\frac{1}{2}i\partial_x\theta,$$

$$\Sigma_t=\frac{1}{2}f^{-1}\partial_t f+\frac{1}{2}i\partial_t\theta+\frac{1}{4}h^{-1}\partial_t h\,\gamma_x. \tag{48}$$

In the case of a local orthonormal frame $\{X_a\}$ with constant γ-matrices and constant matrices C and B, the familiar solution for Σ_a is purely a bivector

$$\Sigma_a=\frac{1}{4}\omega_{abc}\gamma^b\gamma^c, \tag{49}$$

where $\omega_{abc}=g(X_b,\nabla_{X_a}X_c)$ are the connection coefficients. (Note that the metric compatibility of the connection implies $\omega_{abc}=-\omega_{acb}$.)

IV. THE MASSLESS DIRAC EQUATION IN TWO DIMENSIONS

With the definition (35) of the spinor covariant derivative the massless Dirac equation in arbitrary dimensions takes the form

$$\not{S}\Psi\equiv\gamma^\mu S_\mu\Psi=0. \tag{50}$$

In two dimensions for the spinor connection (48) we obtain a family of equations depending on the two real functions f and θ:

$$\left[\gamma^\mu\left(\partial_\mu+\frac{1}{2}f^{-1}\partial_\mu f+\frac{1}{2}i\partial_\mu\theta\right)+\gamma^t\frac{1}{4}h^{-1}\partial_t h\,\gamma_x\right]\Psi=0. \tag{51}$$

A. Solution for the massless Dirac equation in two dimensions

We solve this equation for regions where it is regular. It is easy to check that Eq. (51) is equivalent to

$$\gamma^\mu[(f^{-1/2}e^{-1/2i\theta}D^{-1})\partial_\mu(f^{1/2}e^{1/2i\theta}D)]\Psi=0, \tag{52}$$

where the matrix D must satisfy

$$\partial_t D=D\frac{1}{4}h^{-1}\partial_t h\,\gamma_x, \tag{53}$$

$$\partial_x D=0. \tag{54}$$

Thus, up to an unimportant constant factor,

$$D=\frac{1}{2}[|h|^{1/4}(1+\gamma_x)+|h|^{-1/4}(1-\gamma_x)]=\begin{pmatrix}|h|^{1/4} & 0\\ 0 & |h|^{-1/4}\end{pmatrix}, \tag{55}$$

with

$$D^{-1}=\frac{1}{2}[|h|^{-1/4}(1+\gamma_x)+|h|^{1/4}(1-\gamma_x)]=\begin{pmatrix}|h|^{-1/4} & 0\\ 0 & |h|^{1/4}\end{pmatrix}. \tag{56}$$

The plane wave ansatz,

$$\Psi=(f^{-1/2}e^{-1/2i\theta}D^{-1})\psi_0 e^{-i(k_\tau\tau-k_x x)}, \tag{57}$$

where $\tau=\int\sqrt{|h(t)|}dt$, leads to

$$(-\gamma^t\sqrt{|h|}k_\tau+\gamma^x k_x)D^{-1}\psi_0=0. \tag{58}$$

For non-trivial solutions we need

$$\det(-\gamma^t\sqrt{|h|}k_\tau+\gamma^x k_x)=-k_x^2-h^{-1}|h|k_\tau^2=0, \tag{59}$$

which gives the dispersion relation

$$k_\tau=\begin{cases}\pm k_x, & \text{for } h<0,\\ \pm ik_x, & \text{for } h>0,\end{cases} \tag{60}$$

and corresponding solutions for ψ_0,

$$\psi_0=\begin{pmatrix}1\\ \mp 1\end{pmatrix}, \quad \text{for } h<0,\ k_\tau=\pm k_x, \tag{61}$$

$$\psi_0=\begin{pmatrix}1\\ \mp i\end{pmatrix}, \quad \text{for } h>0,\ k_\tau=\pm ik_x. \tag{62}$$

Thus the general solutions for regions where $h\neq 0$ and $f\neq 0$ are

$$\Psi_L=(f^{-1/2}e^{-(1/2)i\theta}D^{-1})\sum_{k>0}\left[\left(a_k^+e^{ikx}\begin{pmatrix}1\\ -1\end{pmatrix}+a_k^-e^{-ikx}\begin{pmatrix}1\\ 1\end{pmatrix}\right)e^{-ik\tau}\right.$$
$$\left.+\left(b_k^+e^{ikx}\begin{pmatrix}1\\ 1\end{pmatrix}+b_k^-e^{-ikx}\begin{pmatrix}1\\ -1\end{pmatrix}\right)e^{ik\tau}\right] \quad (h<0). \tag{63}$$

$$\Psi_E=|(f^{-1/2}e^{-(1/2)i\theta}D^{-1})\sum_{k>0}\left[\left(c_k^+e^{ikx}\begin{pmatrix}1\\ -i\end{pmatrix}+c_k^-e^{-ikx}\begin{pmatrix}1\\ i\end{pmatrix}\right)e^{k\tau}\right.$$
$$\left.+\left(d_k^+e^{ikx}\begin{pmatrix}1\\ i\end{pmatrix}+d_k^-e^{-ikx}\begin{pmatrix}1\\ -i\end{pmatrix}\right)e^{-k\tau}\right] \quad (h>0), \tag{64}$$

where $a_k^\pm$, $b_k^\pm$, $c_k^\pm$, and $d_k^\pm$ are arbitrary complex constants. (We omit the zero frequency solution.)

B. Asymptotic behavior and continuity of solutions

Assuming the Fourier sums above are convergent then the singularity structure of these solutions in the vicinity of the degeneracy is determined by $f^{-1/2}D^{-1}$:

$$\Psi_{L/E} \simeq \begin{pmatrix} O(f^{-1/2}|h|^{-1/4}) \\ O(f^{-1/2}|h|^{1/4}) \end{pmatrix}. \tag{65}$$

In particular, solutions are bounded if $f \simeq O(|h|^{-1/2})$. Thus one cannot have both bounded solutions and a bounded spinor metric at the degeneracy hypersurface. One possible choice is $f=|h|^{-1/2}$, in which case a continuous match of a Lorentzian and Euclidean solution would imply

$$a_k^+ + b_k^+ = c_k^+ + d_k^+ , \quad a_k^- + b_k^- = c_k^- + d_k^- , \tag{66}$$

where $\tau(t_0)=0$ is assumed. With this choice, requiring continuity does not induce a bijective map between Lorentzian and Euclidean solutions.

V. CURRENTS

There are two important currents that are locally conserved for solutions to the massless Dirac equation above. In regular domains the current

$$j_D^\mu[\Psi,\Xi] = \mathrm{Im}(\Psi, \gamma^\mu \Xi) \tag{67}$$

is conserved for solutions Ψ,Ξ:

$$\begin{aligned} \nabla_\mu(\Psi,\gamma^\mu\Xi) &= \partial_\mu(\Psi,\gamma^\mu\Xi) + \Gamma^\mu{}_{\mu\rho}(\Psi,\gamma^\rho\Xi) \\ &= (S_\mu\Psi,\gamma^\mu\Xi) + (\Psi, S_\mu(\gamma^\mu\Xi)) + \Gamma^\mu{}_{\mu\rho}(\Psi,\gamma^\rho\Xi) \\ &= -(\gamma^\mu S_\mu\Psi,\Xi) + (\Psi,\gamma^\mu S_\mu\Xi), \end{aligned} \tag{68}$$

using $[S_\mu,\gamma^\nu] = -\Gamma^\nu{}_{\mu\rho}\gamma^\rho$ and $(\Psi,\gamma^\mu\Xi) = -(\gamma^\mu\Psi,\Xi)$ which follow from the definitions and properties of the spinor covariant derivative and spinor metric (see section III). For a massless theory the axial vector current is also conserved,

$$j_A^\mu[\Psi,\Xi] = \mathrm{Re}(\Psi, \mathfrak{z}\gamma^\mu\Xi), \tag{69}$$

where $\mathfrak{z} = \sqrt{|h|}\gamma^t\gamma^x$, since

$$\nabla_\mu(\Psi,\mathfrak{z}\gamma^\mu\Xi) = (\gamma^\mu S_\mu\Psi,\mathfrak{z}\Xi) + (\Psi,\mathfrak{z}\gamma^\mu S_\mu\Xi). \tag{70}$$

Note that $\nabla\mathfrak{z}=0$, since the connection is metric compatible and $\mathfrak{z}$ is the metric dual of the metric volume element.

Given

$$\Psi = (f^{-1/2}e^{-1/2i\theta}D^{-1})\psi, \quad \Xi = (f^{-1/2}e^{-(1/2)i\theta}D^{-1})\xi, \tag{71}$$

which are defined piecewise on the non-degenerate parts of M, where they satisfy the massless Dirac equation, we obtain for the components of the Dirac current,

$$j_D^t[\Psi,\Xi] = -|h|^{-1/2}\mathrm{Re}\ \psi^\dagger \begin{pmatrix} 1 & 0 \\ 0 & -\mathrm{sgn}\ h \end{pmatrix}\xi, \quad j_D^x[\Psi,\Xi] = \mathrm{Re}\psi^\dagger \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\xi, \tag{72}$$

and for the components of the axial current

$$j^t_A[\Psi,\Xi]=h^{-1}|h|^{1/2}\mathrm{Im}\ \psi^\dagger\begin{pmatrix}0&1\\1&0\end{pmatrix}\xi,\ j^x_A[\Psi,\Xi]=\mathrm{Im}\ \psi^\dagger\begin{pmatrix}1&0\\0&-\mathrm{sgn}\ h\end{pmatrix}\xi. \tag{73}$$

The continuity of these currents depends on the assumptions made for the continuity of the spinor components. From our discussion above it is clear that this requires some assumptions about the behavior of the spinor metric in the vicinity of the signature change.

However some purely signature dependent effects can be seen by considering the coordinate independent contractions,

$$g_{\mu\nu}j^\mu_{D/A}[\Psi,\Xi]j^\nu_{D/A}[\Psi,\Xi]\simeq O(1), \tag{74}$$

which stay bounded near the hypersurface of signature change but contain terms which depend on sgn h. [Note that $\psi\simeq O(1)\simeq\xi$.] Thus the currents do not exhibit any divergences which depend on the choice of spinor metric or on h, although they can be seen to be discontinuous in general for any linear prescription relating spinor data across the hypersurface of signature change.

VI. CONCLUSION

We have drawn attention to some of the subtleties involved in discussing spinor fields in the presence of a smooth metric degeneracy. By insisting on interpolating smoothly (C^1) between the representations on either side of the degeneracy, we have been able to derive a number of interesting results. In particular, we have introduced the notion of a spinor fibration and used this to give a natural interpolation between the notions of a spinor on the two sides of the degeneracy. This enables one to discuss the concept of continuity of a spinor field in this context. Despite the absence of a continuous field of local orthonormal frames we have shown how a local massless Dirac equation can be constructed, albeit in terms of a class of spinor metrics equivalent up to local scalings and a phase freedom associated with charge conjugation. We have shown that the singularity structure of the solutions at metric degeneracies depends on the choice of spinor metric. An important conclusion of our work is that it is impossible to have both a continuous spinor metric and continuous solutions to the Dirac equation. Researchers studying spinor fields on manifolds with smooth degenerate metrics will be forced to make a choice. Furthermore, our formalism allows one to determine explicitly how various assumptions regarding the continuity of the spinor components affect the continuity of the Dirac current.

A dynamic theory of spinors on a degenerate background geometry may require a dynamical prescription to remove the freedom inherent in the construction of the spinor connection. One way to implement this idea would be to promote the scaling degree of freedom in the spinor metric to an independent scalar field and include this in the dynamical theory. A less radical suggestion might be to relinquish completely the irreducible spinor representations for matter by embedding a multiplet of spinor fields into a single Kähler field. The natural dynamics of such a multicomponent tensor field depends only on the metric structure of the manifold which is no longer required to sustain a spinor structure.

Relinquishing the assumption of a smooth interpolation of representations on either side of the metric degeneracy may lead to an alternative construction of a spinor fibration. However, it is unlikely to circumvent the discontinuity of the currents which was found to be purely an algebraic effect of the signature change.

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Master equation based formulation of nonequilibrium statistical mechanics

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For a nonequilibrium system characterized by its state space, by a dynamics defined by a transfer matrix and by a reference equilibrium dynamics given by a detailed-balance transfer matrix, we define various nonequilibrium concepts: relative entropy, dissipation during the relaxation to the stationary state, path entropy, cost for maintaining the system in a nonequilibrium state, fluctuation-dissipation theory, and finally a tree integral formula for the stationary state. © *1996 American Institute of Physics.* [S0022-2488(96)02808-3]

I. INTRODUCTION

For systems that are not in equilibrium, much of the general power of thermodynamics and statistical mechanics is lost. For chemical reactions, for fluids, for dynamic critical phenomena, or metastable states, and for many, many natural, social, and economic systems, specific methods have been developed to deal with time-dependent collective phenomena (see among many possible references [1–9]). The absence of overriding laws, such as the entropy-related variational principles of equilibrium statistical mechanics, has long been lamented, although there have been many attempts, for example to define generalizations of thermodynamic functions (see Refs. 1, 2, 6, and 10–12 for recent definitions). In the present paper we use a dynamical framework broad enough to cover most of the phenomena of interest and find that there *are* general statements that can be made. Of course, there is a kind of complementarity principle. The vast range of nonequilibrium phenomena in open systems precludes certain kinds of specific predictions and forces on us a level of abstraction that may limit usefulness.

The framework is the master equation. A state space and transition probabilities between states are given. This will not describe situations where quantum interference is important, but is nevertheless rather comprehensive—even finite memory effects can be included by enlarging the state space. In its various forms, for example, the Fokker–Planck equation, the master equation has already been used in many contexts. Our goal will be to seek general versions of the broadest kind of equilibrium information, things analogous to entropy inequalities, fluctuation-dissipation theorems, and the characterization of the steady state, when there is one.

Label the states x, $y \in X$ and the transition probabilities R_{xy}, defined as the (conditional) probability that the state of the system at time $t+\Delta t$ is x, given that it was y at time t. For most of the present paper, we take X and Δt finite. The stochastic matrix R is *not* assumed to satisfy detailed balance (for any vector) and indeed *it is this feature that is of greatest interest.* To avoid irrelevant mathematical complications, R is assumed to be irreducible.

For some of our results it would be easy to take continuum limits. Indeed in previous works (Refs. 13–15) we used the master equation approach advocated here to define a metastable state and in Ref. 16 to establish "self-organized criticality" (see Refs. 17 and 18) in a model system. These results were based on showing the disappearance of an energy gap, clearly going beyond the finite state context. Similarly, in Ref. 19 various critical properties in directed percolation derive

from the spectrum and eigenfunctions of the matrix R, in particular, its infinite size limit.

Within this framework there emerges the important general concept of *current*. By this we mean the flow of probability that can exist, even in the stationary state: $J_{xy}=R_{xy}\tilde{p}_y-R_{yx}\tilde{p}_x$, where $R\tilde{p}=\tilde{p}$. Currents, in particular current loops, which do not exist at equilibrium, are essential to anything one would consider *complex* as a dynamical system (see, e.g., Ref. 20 for different perspectives and Ref. 21 for other opinions). One must be careful here to distinguish currents in X from currents in an underlying physical coordinate space. For example, in this terminology, heat conduction with detailed balance is not complex, even though it is not in equilibrium. We shall discuss these matters in another publication.

The present paper is intended as an exposition of our general framework. In developing this framework we have had a number of examples in mind and in future publications we intend to exhibit these applications. However, because the present exposition is already rather lengthy, we will give only minimal indications of these examples. It is also clear that the wealth of potential applications will require tweaking of our framework. For example, directed percolation on finite systems generally has a trivial (absorbing) stationary state. By minor modification of the dynamics the interesting behavior of such systems can be studied with the present techniques (see, for example Ref. 22). However, in the present paper we do not focus on those issues.

Summary of results. A natural construct is the relative entropy $S(p|q)=-\Sigma_x p_x \log(p_x/q_x)$ of two distributions. For equilibrium theory this is already important [e.g., if q is the Gibbs state, $S(p|q)$ is essentially a thermodynamic potential] and it is also used extensively in information theory. It is easy to show (and well known) that

$$S(p|q)\leqslant S(Rp|Rp)\leqslant 0.$$

Much of this work focuses on the invariant state of R, which is called $\tilde{p}$. Thus $\tilde{p}=R\tilde{p}$. The analog of the entropy increase in equilibrium systems is the fact that $S(p|\tilde{p})$ can only increase as R is successively applied to p. In fact, we have a stronger statement: If δ is small and $p_\delta(x)\equiv\tilde{p}(x)\exp(\delta\varphi_1(x))$, then $S(p_\delta|\tilde{p})\sim-\delta^2\langle\varphi_1^2\rangle_{\tilde{p}}/2$. This allows bounds on the rate of approach to stationarity (i.e., $\tilde{p}$). Let ${}^tR$ be the transpose of R and $({}^tR)^*$ be its adjoint with respect to the inner product using $\tilde{p}$ as a weight. Let φ_1 be the eigenvector of ${}^tR({}^tR)^*$ with maximum eigenvalue $\mu_{\max}$, different from 1, then

$$S(Rp|\tilde{p})-S(p|\tilde{p})\geqslant\tfrac{1}{2}\langle\delta^2\varphi_1^2\rangle(1-\mu_{\max}).$$

This is a statement about dissipation and fluctuations, although in a moment we shall get to the usual form. In this context we are also able to get results on "excess work," a concept that has been used in the chemical literature.[10]

One question of great interest is, what does it "cost" to keep the system out of equilibrium? The matrix R can describe a system with temperature gradients, with sunlight, with wind, with currency exchange rate shifts. How can one associate a general cost? Given the broad nature of our goals, we preferred not to model the reservoirs that maintain R's imbalances. Rather, we assume that R is to be compared with a fiducial W, which is a transition matrix with an equilibrium state and detailed balance $[W_{xy}p_{\rm eq}(y)=W_{yx}p_{\rm eq}(x)]$. For example, if R describes Rayleigh–Benard flow, then W could represent a world uniformly at the temperature of the upper (or the colder) plate. The cost should then be what it takes to heat the lower plate. The choice of W is made by the observer and is partly conventional, depending on what the observer or designer intends to do with the R matrix. For example, in a Carnot cycle completed by a necessarily out-of-equilibrium engine, depending on whether the cycle is used to move a car or function as a refrigerator, W would be the thermal state at low or high temperature, respectively. However, within our general framework one is not committed to such a detailed point of view.

By considering a path entropy, we find it appropriate to define

$$\Delta_1\mathscr{I}(R,\tilde{p},W)=-\sum_{x,y} R_{xy}\tilde{p}(y)\log\left(\frac{R_{xy}}{W_{xy}}\right),$$

to be the dissipation per time step required to maintain the state $\tilde{p}$, against a tendency to relax to equilibrium. The following remarkable inequality emerges:

$$S(W\tilde{p}|p_{\rm eq})-S(\tilde{p}|p_{\rm eq})\leqslant 4\,\Delta_1\mathscr{I}(R,\tilde{p},W).$$

This inequality is proved for $\tilde{p}$ near equilibrium. It means that if we start with a certain stationary state and switch off the reservoirs defining R, so that $\tilde{p}$ starts to relax to the equilibrium $p_{\rm eq}$ by the W evolution, the dissipation per unit time is always less than four times the cost to maintain $\tilde{p}$, as defined by the path entropy.

To state a nonequilibrium fluctuation-dissipation theorem in a form similar to its usual equilibrium formulation, it is necessary to climb down from the grand generality adopted until this point. A distinction must be drawn between fast and slow variables—the motion of one dissipates while the others fluctuate. In the context of our master equation model we achieve this result. In fact, what we get is stronger than what is known in the equilibrium case. In particular, we have independent expressions for fluctuation and dissipation and the comparison of these expressions gives the fluctuation-dissipation statement, while traditional derivations do not give separate expressions for fluctuation and dissipation. Note that the state around which this generalized fluctuation dissipation theorem holds is *not* equilibrium but is the stationary state $\tilde{p}$. More precisely, let A be a slow variable of the system that is chosen to be a left eigenvector of the transfer matrix R whose eigenvalue is close to 1, and let p_α be a perturbation of the stationary state, such that $\langle A(0)\rangle_{p_\alpha}$ (average of A at time 0 in the state p_α) is given, then the dissipation is

$$\langle A(\Delta t)-A(0)\rangle\sim\langle A(0)\rangle_{p_\alpha}(\lambda-1),$$

while the fluctuation is

$$\langle(A(\Delta t)-A(0))\rangle\sim(\lambda-1)(-2\langle A^2\rangle_{p_\alpha})+O(\alpha).$$

The elimination of $\lambda-1$ then provides the analog of the fluctuation-dissipation relation in a nonequilibrium stationary state.

Finally, we state a generalization of the Onsager reciprocity relations for a general nonequilibrium system. The Onsager coefficients L_{kj} are not, in general, symmetric, but they are symmetric in the case of detailed balance dynamics.

In general, most of our statements (with the exception of the statements of Secs. II A and II B), hold for states near the stationary state, or for stationary states near an equilibrium state of reference (and an R matrix near a detailed balance matrix W). In our general framework, it is difficult to estimate how "near" one must be so that our statements remain valid. In particular, we do not discuss criticality (although everything we say is valid in this context too). Finally, we present a general expression for the stationary state of any stochastic matrix R. This is potentially important: for equilibrium theory, merely writing down the Gibbs state, $\exp(-\beta H)$, is a major step toward calculating various quantities. Our expression for the state is in terms of a sum over spanning trees built out of R and is reminiscent of a path integral formula; actually it is a "tree-integral formula." At the computational level this may turn out to be difficult to work with. (An Ising model with 5 spins has a 32×32 transition matrix. The number of spanning trees on 32 objects is about 10^{45}.) However, for formal manipulations it should be useful; for example, it could lead to an abstract definition of nonequilibrium phase transition.

II. DISSIPATION DURING THE RELAXATION TO THE STATIONARY STATE

In the following, X denotes a discrete space with points $x,y,\ldots$. We start by recalling elementary facts about probability distributions and their entropy on X.

A. Relative entropy of two probability distributions

Let p and q be two probability distributions on X. The relative entropy is defined to be

$$S(p|q)=-\sum_{x\in X} p(x)\log\frac{p(x)}{q(x)}.$$

By convention, $0\log 0=0$. It follows that

$$S(p|q)\leqslant 0. \tag{2.1}$$

The proof is immediate. We have

$$S(p|q)=-\sum p(x)\log\frac{p(x)}{q(x)}=-\sum q(x)L\left(\frac{p(x)}{q(x)}\right),$$

where $L(\xi)\equiv\xi\log\xi$. But $L'(\xi)=1+\log\xi$ and $L''\xi)=(1/\xi)\geqslant 0$, so L is convex. As a consequence, $L(\Sigma_x q(x)\alpha(x))\leqslant\Sigma q(x)L(\alpha(x))$, provided $\Sigma_x q(x)=1$. So

$$S(p|q)\leqslant -L\left(\sum_x q(x)\frac{p(x)}{q(x)}\right)=-L(1)=0.$$

Remark: If $\tilde{p}$ is an equilibrium distribution of the form $\tilde{p}(x)=\exp(-\beta E_x)/\mathcal{Z}$, the quantity S is (up to a sign) the corresponding thermodynamic potential. Specifically, $S(q|p)=\beta[\tilde{F}-F_q]$, where $\tilde{F}=-T\log\mathcal{Z}$ (the usual free energy) and $F_q=\langle E\rangle_q-T(-\Sigma q\log q)$.

B. Increase of the relative entropy

The result below, Eq. (2.2), is derived as in Ref. 23 but adapted to our notation.

We consider two distributions p_0,q_0 and a Markov chain on X, with transition matrix R_{xy} ($R_{xy}\equiv R_{x\leftarrow y}$ is the probability that starting from y, one has a transition $y\to x$ in unit time step). We call p_1, q_1 the probability distributions at time 1,

$$p_1(x)=\sum R_{xy}p_0(y),\quad q_1(x)=\sum R_{xy}q_0(y).$$

Then

$$S(p_0|q_0)\leqslant S(p_1|q_1). \tag{2.2}$$

Proof: Consider the states of the Markov chain at times 0 and 1, namely $\{x_0,x_1\}$. If the initial probability distribution is p_0, the joint law of $\{x_0,x_1\}$ is $P(x_0,x_1)=R_{x_1x_0}p_0(x_0)$, and if the initial probability distribution is q_0, the joint law of $\{x_0,x_1\}$ is $Q(x_0,x_1)=R_{x_1x_0}q_0(x_0)$. Then

$$S(P|Q)=-\sum_{x_0,x_1}P(x_0,x_1)\log\frac{P(x_0,x_1)}{Q(x_0,x_1)}=-\sum_{x_0,x_1}R_{x_1x_0}p_0(x_0)\log\frac{p_0(x_0)}{q_0(x_0)}=S(p_0|q_0).$$

Now, we compute $S(P|Q)$ in a different way. We can write P and Q by conditioning the past x_0 knowing the future x_1 in the following way:

$$P(x_0,x_1)=p_1(x_1)r_{x_1x_0}, \quad Q(x_0,x_1)=q_1(x_1)s_{x_1x_0},$$

where $p_1(x_1)$ [resp., $q_1(x_1)$] are the distribution probabilities of x_1, the initial distribution of x_0 being $p_0(x_0)$ [resp., $q_0(x_0)$], and where $r_{x_1x_0}$ is the distribution probability of x_0, knowing that the position at time 1 of the chain is x_1 [given the fact that the distribution of x_1 is $p_1(x_1)$], and, in the same manner, $s_{x_1x_0}$ is the distribution probability of x_0 knowing that at time 1 the position of the chain is x_1 [given the fact that the distribution of x_1 is $q_1(x_1)$].

Then the same computation proves that

$$S(P|Q)=S(p_1|q_1)+\sum_{x_1} p_1(x_1)S(r_{x_1,*}|s_{x_1,*}),$$

where

$$S(r_{x_1,*}|s_{x_1,*})=-\sum_{x_0} r_{x_1x_0}\log\frac{r_{x_1x_0}}{s_{x_1x_0}}\leqslant 0.$$

So we have

$$S(p_0|q_0)=S(P|Q)\leqslant S(p_1|q_1).$$

Remark: For $\tilde{p}=\exp(-\beta E_x)/\mathcal{Z}$, this shows that $F_q=\Sigma E_x q(x)-TS(q|1)$ can only decrease. (This F_q is the same as defined in our remark at the end of the previous section.)

C. Computation near the stationary state

Although Eq. (2.2) is known in the information theory context, the matter we now discuss appears more relevant to physical and chemical systems as such. To the extent that similar or weaker results are known, they arise in the statistical mechanics literature. As we proceed, we shall give references wherever appropriate. In any case the results we now derive are not contained in Ref. 23. We shall see that they are completely general and do not refer to any special feature of the physical or chemical systems we consider.

As above, our system is described by a state space X and its evolution can be represented by a stochastic matrix R_{xy} (which is the probability of a transition $y\to x$ in a unit time step Δt). We assume that R has a unique stationary state $\tilde{p}(x)$ satisfying

$$\tilde{p}(x)=\sum_y R_{xy}\tilde{p}(y). \tag{2.3}$$

Remark: Note that by virtue of (2.2), for any q,

$$S(Rq|\tilde{p})\geqslant S(q|\tilde{p}). \tag{2.4}$$

We consider a neighboring state $p_\delta(x)$, where δ is a small parameter, namely

$$p_\delta(x)\equiv\tilde{p}(x)\exp(\varphi(x,\delta)),$$

where

$$\varphi(x,\delta)\equiv\delta\varphi_1(x)+\delta^2\varphi_2(x)+\cdots.$$

Then, for small δ, it follows that

$$S(p_\delta|\tilde{p}) \sim -\frac{\delta^2}{2}\langle\varphi_1^2\rangle_{\tilde{p}}, \tag{2.5}$$

where $\langle\varphi_1^2\rangle_{\tilde{p}}$ is the mean square average of φ_1 in the state $\tilde{p}$,

$$\langle\varphi_1^2\rangle_{\tilde{p}} = \sum_x \tilde{p}(x)\varphi_1^2(x).$$

Proof: We start from the definition

$$S(p_\delta|\tilde{p}) = \sum p_\delta(x)\log\frac{p_\delta(x)}{\tilde{p}(x)}.$$

Then

$$\frac{\partial S}{\partial\delta} = -\sum \frac{\partial p_\delta(x)}{\partial\delta}\left(1+\log\frac{p_\delta(x)}{\tilde{p}(x)}\right),$$

$$\frac{\partial^2 S}{\partial\delta^2} = -\sum \frac{\partial^2 p_\delta(x)}{\partial\delta^2}\left(1+\log\frac{p_\delta(x)}{\tilde{p}(x)}\right) - \sum \frac{1}{p_\delta(x)}\left(\frac{\partial p_\delta(x)}{\partial\delta}\right)^2.$$

Now we have $\Sigma p_\delta(x)=1$. Therefore $\Sigma\partial p_\delta(x)/\partial\delta=0$ and $\Sigma\partial^2 p_\delta(x)/\partial\delta^2=0$. It follows that

$$S(p_\delta|\tilde{p}) \sim -\frac{\delta^2}{2}\sum_x \frac{1}{p_\delta(x)}\left(\frac{\partial p_\delta(x)}{\partial\delta}\right)^2\Bigg|_{\delta=0}.$$

But

$$\left.\frac{\partial p_\delta(x)}{\partial\delta}\right|_{\delta=0} = p_\delta(x)\varphi_1(x).$$

D. Variation of entropy near the stationary state

We again consider a state $p_\delta(x)$ near the stationary state, and for simplicity we drop the δ index. We note that

$$p(x) = \tilde{p}(x)\exp(\delta\varphi_1(x)+\delta^2\varphi_2(x)+\cdots).$$

We consider at time step Δt (one time step) the evolution of p, namely

$$p(x,\Delta t) = \sum_y R_{xy}p(y).$$

We know by Eq. (2.2) of Sec. II B that

$$S(p|\tilde{p}) \leqslant S(p(\cdot,\Delta t)|\tilde{p}),$$

but here we shall find the difference between these two entropies. We can write

$$p(x,\Delta t) = \tilde{p}(x)\exp(\delta\psi_1(x)+\delta^2\psi_2(x)+\cdots).$$

Now

$$\tilde{p}(x)\exp(\delta\psi_1(x)+\delta^2\psi_2(x)+\cdots)=\sum_y R_{xy}\tilde{p}(y)\exp(\delta\varphi_1(y)+\delta^2\varphi_2(y)+\cdots).$$

Comparing the terms of order δ, we find

$$\psi_1(x)=\frac{1}{\tilde{p}(x)}\sum_y R_{xy}\tilde{p}(y)\varphi_1(y), \tag{2.6}$$

or in vector notation,

$$\psi_1=\left(\operatorname{diag}\frac{1}{\tilde{p}}\right)R(\operatorname{diag}\tilde{p})\varphi_1. \tag{2.6'}$$

Then, in our context, we have

$$S(p(\cdot,\Delta t)|\tilde{p})-S(p|\tilde{p})\sim-\frac{1}{2}\left[\left\langle\left(\frac{1}{\operatorname{diag}\tilde{p}}R\ \operatorname{diag}\tilde{p}\ \delta\varphi_1\right)^2\right\rangle_{\tilde{p}}-\langle(\delta\varphi_1)^2\rangle_{\tilde{p}}\right]. \tag{2.7}$$

We shall study a lower bound for this quantity. To do this, we maximize the quantity

$$\max\left\langle\left(\frac{1}{\operatorname{diag}\tilde{p}}R\ \operatorname{diag}\tilde{p}\varphi_1\right)^2\right\rangle_{\tilde{p}},$$

subject to the conditions $\langle\varphi_1^2\rangle_{\tilde{p}}=1$ and $\langle\varphi_1\rangle_{\tilde{p}}=0$. [The last condition is a consequence of $\Sigma_x p_\delta(x)=1$, so that $\Sigma\varphi_1(x)\tilde{p}(x)=0$.]

To find this maximum, we introduce a Lagrange multiplier μ for the constraint $\langle\varphi_1^2\rangle_{\tilde{p}}=1$ and we assume that φ_1 has been found. Then, for any variation $\varphi_1+\epsilon_1$, we must have

$$\sum_x\tilde{p}(x)\left(\frac{1}{\operatorname{diag}\tilde{p}}R\ \operatorname{diag}\tilde{p}\varphi_1\right)_x\left(\frac{1}{\operatorname{diag}\tilde{p}}R\ \operatorname{diag}\tilde{p}\epsilon_1\right)_x-\mu\sum\tilde{p}(x)\epsilon_1(x)=0.$$

Rearranging, the factor of $\epsilon_1(x)$ must vanish identically, so that

$${}^tR\ \operatorname{diag}\left(\frac{1}{\tilde{p}}\right)R(\operatorname{diag}\tilde{p})\varphi_1=\mu\varphi_1. \tag{2.8}$$

Denote $M={}^tR$ (so $M_{xy}=R_{yx}$). We notice that the adjoint M^* of M for the scalar product,

$$(v|w)_{\tilde{p}}=\sum\tilde{p}(x)v(x)^*w(x), \tag{2.9}$$

is just

$$M^*=\operatorname{diag}\left(\frac{1}{\tilde{p}}\right)R\ \operatorname{diag}\tilde{p}, \tag{2.10}$$

and so Eq. (2.8) can be rewritten as

$$MM^*\varphi_1=\mu\varphi_1. \tag{2.11}$$

MM* is self-adjoint with respect to the scalar product $(\ |\ )_{\tilde{p}}$. Moreover, all its eigenvalues are obviously positive. Call $N=MM^*$. We show that all eigenvalues of N are less than 1. Let φ be eigenvector of eigenvalue μ,

$$\max_{y\in X}|N\varphi(y)|\leqslant\sum R_{xy}\frac{1}{\tilde{p}(x)}R_{xy}\tilde{p}(z)|\varphi(z)|\leqslant\max_{z}|\varphi(z)|\left(\sum_{x}R_{xy}\frac{1}{\tilde{p}(x)}\sum_{z}R_{xy}\tilde{p}(z)\right)$$

$$\leqslant\max|\varphi(z)|\left(\sum_{x}R_{xy}\frac{1}{\tilde{p}(x)}\tilde{p}(x)\right)=\max|\varphi(z)|,$$

but because of Eq. (2.11), $N\varphi=\mu\varphi$. We see that if $\varphi\not\equiv 0$, $\mu\leqslant 1$.

Obviously the matrix $N=MM^*$ has the eigenvalue 1 with trivial eigenvector $\{1\}$ because

$$\sum_{x,z}R_{xy}\frac{1}{\tilde{p}(x)}R_{xz}\tilde{p}(z)=1,\quad\text{for all } y.$$

Now in the variational problem above, we considered an eigenvector φ_1 that is orthogonal to the trivial eigenvector $\{1\}$ (because we imposed $\langle\varphi_1\rangle_{\tilde{p}}=0$). So, *we have proved that*

$$S(p(\cdot,\Delta t)|\tilde{p})-S(p|\tilde{p})\geqslant\tfrac{1}{2}\langle\delta^2\varphi_1^2\rangle_{\tilde{p}}(1-\mu_{\max}),\tag{2.12}$$

where $\mu_{\max}$ is the maximal eigenvalue of MM^* corresponding to an eigenvector φ_1 orthogonal to the trivial eigenvector $\{1\}$.

It remains to prove that $\mu_{\max}<1$. Suppose that $v(x)$ is an eigenvector of eigenvalue 1 but different from the trivial eigenvector $\{1\}$; thus $v(x)$ is orthogonal to $\{1\}$ for the scalar product $(\ |\ )_{\tilde{p}}$,

$$\sum\tilde{p}(x)v(x)=0.$$

We have

$$v(x)=\sum_{y,z}R_{yx}\frac{1}{\tilde{p}(y)}R_{yz}\tilde{p}v(z).$$

But $\tilde{p}(x)\neq 0$ for all x, so that at least one $v(x)$ must be negative. As a consequence, we obtain from the preceding inequality a strict inequality,

$$|v(x)|<\sum_{y,z}R_{yx}\frac{1}{\tilde{p}(y)}R_{yz}\tilde{p}(z)|v(z)|,$$

or finally

$$\max_{x\in X}|v(x)|<\max_{z\in X}|v(z)|,$$

which is a contradiction

Remark 1: All this assumes that $\tilde{p}(x)\neq 0$ for all x because we need to define $1/\tilde{p}(x)$ for all x. This is the case if R is irreducible. If R is reducible, one can sometimes introduce small matrix elements to make it irreducible while preserving its essential features, as in Ref. 22.

Remark 2: This "universal" inequality,

$$S(p(\cdot,\Delta(\cdot)|\tilde{p})-S(p(\cdot)|\tilde{p})\geq\tfrac{1}{2}\langle\delta^2\varphi_1^2\rangle_{\tilde{p}}(1-\mu_{\max})$$

is a kind of *fluctuation dissipation inequality* for nearby states, p, because the left side is the dissipation (in one time step) and the right side involves a fluctuation $\langle\delta^2\varphi_1^2\rangle$ of the relative free energy of p with respect to $\tilde{p}$ (and a factor that is $1-\mu_{\max}$).

Remark 3: If R satisfies detailed balance, then

$$M^*={}^tR$$

and

$$MM^*=({}^tR)^2.$$

In general, we see that the relevant operator is MM^* and not $M^2=({}^tR)^2$.

E. The notion of excess work

The notion of excess work has been introduced by Ross, Hunt, and Hunt[10] and we can give a meaning to it in our abstract setting.

We start from a stationary state $\tilde{p}(x)$ (and as usual the stochastic matrix, R). We can do two things.

(i) We force a variation of the state $\tilde{p}$ (by an external process) so that we have a displaced state $p(x)$,

$$p(x)=\tilde{p}(x)\exp(\delta\varphi_1(x)+\delta^2\varphi_2(x)+\cdots).$$

The relative cost in entropy for doing this is

$$S(p|\tilde{p})\sim-\frac{\delta^2}{2}\langle\varphi_1^2(x)\rangle_{\tilde{p}},$$

as we know from Eq. (2.5).

(ii) We start from a certain state q,

$$q(x)=\tilde{p}(x)\exp(\delta\psi_1(x)+\delta^2\psi_2(x)+\cdots),$$

and let it evolve in one time step Δt in such a way that the variation of free energy is exactly $\delta\varphi_1(x)$ (up to δ^2), so that we *want*

$$q(x,\Delta t)=\tilde{p}(x)\exp(\delta\psi_1(x)+\delta\varphi_1(x)+\cdots).$$

This implies

$$\tilde{p}(x)[\varphi_1(x)+\psi_1(x)]=\sum_y R_{xy}\tilde{p}(y)\psi_1(y). \tag{2.13}$$

The variation of entropy is then easily seen to be

$$S(q(\cdot,\Delta t)|\tilde{p})-S(q(\cdot)|\tilde{p})=-\frac{\delta^2}{2}(\langle\varphi_1^2\rangle_{\tilde{p}}+2(\psi_1|\varphi_1)_{\tilde{p}}),$$

with ψ_1 fixed by Eq. (2.13), or

$$\left[I-\operatorname{diag}\left(\frac{1}{\tilde{p}}\right)R\ \operatorname{diag}\tilde{p}\right]\psi_1\equiv-\varphi_1.$$

Alternatively,

$$\operatorname{diag}\tilde{p}(\varphi_1+\varphi_1)=R(\operatorname{diag}\tilde{p})\psi_1=-R(\operatorname{diag}\tilde{p})\left[I-\operatorname{diag}\left(\frac{1}{\tilde{p}}\right)R\ \operatorname{diag}\tilde{p}\right]^{-1}\varphi_1.$$

The excess work W_{exc} is given by (see Ref. 10)

$$\begin{aligned}
W_{\mathrm{exc}}&=S(q(\cdot,\Delta t)|\tilde{p})-S(q(\cdot)|\tilde{p})+S(p|\tilde{p})\\
&=-\delta^2\sum_x\tilde{p}(x)\varphi_1(x)(\varphi_1(x)+\psi_1(x))\\
&=-\delta^2\sum\varphi_1(x)(R(\operatorname{diag}\tilde{p})\psi_1)(x)\\
&=\delta^2\sum_x\left(\left[I-\left(\operatorname{diag}\frac{1}{\tilde{p}}\right)R(\operatorname{diag}\tilde{p})\right]\psi_1\right)_x((R\ \operatorname{diag}\tilde{p})\psi_1)_x\\
&=\delta^2\sum_x\tilde{p}(x)\psi_1(x)\left[({}^tR\psi_1)_x-\left({}^tR\ \operatorname{diag}\frac{1}{\tilde{p}}R\ \operatorname{diag}\tilde{p}\psi_1\right)_x\right]\\
&=\delta^2[(\psi_1|M\psi_1)-(\psi_1|MM^*\psi_1)],
\end{aligned}$$

where $M={}^tR$, $M^*=\operatorname{diag}(1/\tilde{p})R(\operatorname{diag}\tilde{p})$, and the scalar product has the weight $\tilde{p}$ as usual. One can rewrite this as

$$W_{\mathrm{exc}}=\delta^2\left[\left(\psi_1\left|\frac{M+M^*}{2}\psi_1\right.\right)-(\psi_1|MM^*\psi_1)\right]. \tag{2.14}$$

Notice that if R *satisfies detailed balance*, we have seen that

$$M^*=M={}^tR,$$

and so, because ${}^tR-({}^tR)^2\geqslant 0$, because ${}^tR$ has eigenvalue less than or equal to 1, we have

$$W_{\mathrm{exc}}=\delta^2[(\psi_1|({}^tR-({}^tR)^2)\psi_1)]\geqslant 0,$$

which is exactly Ross' result in our abstract context.

Remark: Ross *et al.* derive this result for the stochastic matrix corresponding to a master equation of a linear chemical system, in which case it is known that the master equation satisfies detailed balance. This is not the case for nonlinear chemical reactions. But we still have an expression for the excess work, in general.

Remark: For a stochastic matrix S that is self-adjoint with respect to a scalar product, it is clear that

$$(\psi|S\psi)\geqslant(\psi|S^2\psi).$$

Moreover, to prove that the excess work is positive, we would have to prove that $M+M^*-2MM^*$ is a positive matrix self-adjoint with respect to the scalar product $(\ |\ )_{\bar{p}}$.

III. PATH ENTROPIES AND DISSIPATION TO MAINTAIN THE STATIONARY STATE

To maintain a system in a nonequilibrium state against an equilibrated environment, it is necessary to dissipate energy. We introduce measures for the rate of dissipation of free energy.

A. Absolute path entropy

(a) Measure on a space of paths. Let X be our usual state space. A path up to time $T(T=n\ \Delta t)$ is a sequence $\gamma=\{x_0,x_1,\ldots,x_T\}$ of points in X. A path is then a sequence of transformations. For example, a Carnot cycle or a biochemical cycle will be realized by closed paths.

If p is an initial distribution, we define a probability measure $\mu^{(R,p)}(\gamma)$ on the space of paths by the formula

$$\mu^{(R,p)}(\gamma)=R_{x_Tx_{T-1}}R_{x_{T-1}x_{T-2}}\cdots R_{x_1x_0}p(x_0). \tag{3.1}$$

(b) We define an absolute entropy as

$$\sigma(T|R,p)=-\sum_{\gamma=\text{path up to } T}\mu^{(R,p)}(\gamma)\log\,\mu^{(R,p)}(\gamma)$$

$$=-\sum_{\gamma}\mu^{(R,p)}(\gamma)\left[\sum_{n=0}^{T-1}\log R_{x_{n+1}x_n}+\log p(x_0)\right].$$

As usual, we define recursively

$$(R^kp)(x)=\sum_y R_{xy}(R^{k-1}p)(y).$$

Then

$$\sum_{\gamma}\mu^{(R,p)}(\gamma)\log R_{x_{n+1}x_n}=\sum R_{x_Tx_{T-1}}\cdots R_{x_{n+1}x_n}\log R_{x_{n+1}x_n}(R^np)(x_n)$$

$$=\sum_{x_{n+1},x_n}R_{x_{n+1}x_n}\log R_{x_{n+1}x_n}(R^np)(x_n).$$

But

$$\sum_{x_{n+1}}R_{x_{n+1}x_n}(R^np)(x_n)=1.$$

Because $L(\xi)=\xi\log\xi$ is convex, we have

$$\sum_{x_{n+1},x_n} R_{x_{n+1}x_n}(R^n p)(x_n)\log R_{x_{n+1}x_n}$$

$$\geqslant \sum_{x_{n+1}} \left(\sum_{x_n} R_{x_{n+1}x_n}(R^n p)(x_n)\right)\log\left(\sum_{x_n} R_{x_{n+1}x_n}(R^n p)(x_n)\right)$$

$$= \sum_{x_{n+1}} (R^{n+1}p)(x_{n+1})\log(R^{n+1}p)(x_{n+1})$$

$$\equiv -S(R^{n+1}p) \quad \text{(absolute entropy of } R^{n+1}p\text{)}.$$

Finally,

$$\sigma(T|R,p)\leqslant \sum_{n=0}^{T} S(R^n p).$$

In particular, if $p=\tilde{p}$,

$$\sigma(T|R,\tilde{p})\leqslant (T+1)S(\tilde{p}).$$

B. Relative entropy on paths

The preceding concept involved the transition matrix R alone and, as such, did not measure the cost of the process R itself. Now, to quantify the extra dissipation needed to maintain a nonequilibrium state in a larger environment, we represent the action of this environment on our system by a stochastic matrix W satisfying the detailed balance. Namely, under the influence of W, the system X relaxes to an equilibrium state p_{eq} and we assume that for all x,y,

$$W_{yx}p_{\text{eq}}(x)=W_{xy}p_{\text{eq}}(y).$$

On the path space of X, we can consider the measure $\mu^{(R,p)}$, as well as the measures $\mu^{(W,q)}$, $\mu^{(W,p_{\text{eq}})}$.

The extra dissipation needed to maintain the R-dynamics in the larger equilibrium environment where action on the system is given by W is represented by the relative path entropy:

$$\mathscr{S}(T|(R,p),(W,q))=-\sum_{\text{path to } T} \mu^{(R,p)}(\gamma)\log\frac{\mu^{(R,p)}(\gamma)}{\mu^{(W,q)}(\gamma)}. \tag{3.2}$$

This can be rewritten using our basic quantity, $S(p|q)$, the relative entropy of Eq. (2.1),

$$\mathscr{S}(T|(R,p),(W,q))=S(p|q)-\sum_{\gamma=\text{path to } T} \mu^{(R,p)}(\gamma)\log\frac{R_{x_T x_{T-1}}\cdots R_{x_1 x_0}}{W_{x_T x_{T-1}}\cdots W_{x_1 x_0}}.$$

Analysis of $\mathscr{S}$. In the preceding equation, the second term is

$$\sum_{\gamma}\sum_{n=0}^{T-1} \mu^{(R,p)}(\gamma)\log\frac{R_{x_{n+1}x_n}}{W_{x_{n+1}x_n}}.$$

Now consider

$$\sum_{\gamma} \mu^{(R,p)}(\gamma)\log\frac{R_{x_{n+1}x_n}}{W_{x_{n+1}x_n}} = \sum_{x_{n+1},x_n} (R^n p)(x_n) R_{x_{n+1}x_n} \log\frac{R_{x_{n+1}x_n}}{W_{x_{n+1}x_n}}$$

$$= \sum_{x_n} (R^n p)(x_n) \sum_{x_{n+1}} W_{x_{n+1}x_n} \frac{R_{x_{n+1}x_n}}{W_{x_{n+1}x_n}} \log\frac{R_{x_{n+1}x_n}}{W_{x_{n+1}x_n}}. \tag{3.3}$$

Using the convexity of $\xi\log\xi$, this is

$$\geqslant \sum_{x_n} (R^n p)(x_n) \left(\sum_{x_{n+1}} W_{x_{n+1}x_n} \frac{R_{x_{n+1}x_n}}{W_{x_{n+1}x_n}} \right) \left(\log\left(\sum_{x_{n+1}} W_{x_{n+1}x_n} \frac{R_{x_{n+1}x_n}}{W_{x_{n+1}x_n}} \right) \right),$$

and so, this is positive or zero because $\Sigma_{x_{n+1}} R_{x_{n+1}x_n} = 1$. Let us define

$$\Delta_1 \mathcal{S}(R,q,W) = -\sum_{x,y} R_{xy} q(y) \log\frac{R_{xy}}{W_{x,y}}. \tag{3.4}$$

Then, from Eq. (3.3),

$$\mathcal{S}(T|(R,p),(W,q)) = S(p|q) + \sum_{t=0}^{T-1} \Delta_1 \mathcal{S}(R,R^t p,W), \tag{3.5}$$

and we have proved above that

$$\Delta_1 \mathcal{S}(R,q,W) \leqslant 0. \tag{3.6}$$

In particular,

$$\mathcal{S}(T|(R,p),(W,q)) \leqslant 0. \tag{3.7}$$

Note that *this is also decreasing with T*, i.e., *each increment* $\Delta_1 \mathcal{S}(R,R^t p,W) \leqslant 0$.

A Particular case: Take $p = \tilde{p}$, the stationary state, so that $R^t \tilde{p} = \tilde{p}$ for all t. Then $S(T|(R,\tilde{p}),(W,q)) = S(\tilde{p}|q) + T\,\Delta_1 S(R,\tilde{p},W)$. In this case, the fundamental quantity,

$$\Delta_1 \mathcal{S}(R,\tilde{p},W) = -\sum_{xy} R_{xy} \tilde{p}(y) \log\frac{R_{xy}}{W_{xy}} \tag{3.8}$$

is the *rate of dissipation per unit time step to maintain the stationary state* $\tilde{p}$ *(in the R-dynamics) against the W dynamics.*

We introduce

$$R_{xy} = W_{xy} e^{f_{xy}}. \tag{3.9}$$

Then

$$\Delta_1 \mathcal{S}(R,\tilde{p},W) = -\sum_{xy} R_{xy} \tilde{p}(y) f_{xy}. \tag{3.10}$$

Remark: If $f_{xy} = \varphi_x - \varphi_y$ then it is immediate that $\Delta_1 S(R,\tilde{p},W) = 0$. But in this case we would have

$$W_{xy} e^{\varphi_y} \tilde{p}(y) = \tilde{p}(x),$$

so that $e^{\varphi_y}\tilde{p}(y)$ would be the equilibrium state $p_{\rm eq}$ of W. But also $\Sigma_x R_{xy}=1$, so that $\Sigma_x W_{xy}e^{-\varphi_x} = e^{-\varphi_y}$. This implies that $\{e^{-\varphi_x}\}$ would be the left eigenvector of eigenvalue 1 of W and (in the absence of degeneracy) this would be a constant. Then $\tilde{p}$ would just be the equilibrium $p_{\rm eq}$ and $R=W$.

C. The minimal rate of dissipation of a given state

In this section, we start with a given $\tilde{p}$ (in a detailed balance dynamics W) and we want to build an R-dynamics for which $\tilde{p}$ is stationary but that minimizes the dissipation of energy with respect to an underlying detailed balance dynamics W. The rate of dissipation is $\Delta_1\mathscr{S}(R,\tilde{p},W)$. We define, as in Eq. (3.9),

$$R_{xy}=W_{xy}e^{f_{xy}},$$

and we want to minimize

$$|\Delta_1\mathscr{S}(R,\tilde{p},W)|=\sum_{xy} W_{xy}e^{f_{xy}}\tilde{p}(y)f_{xy},$$

subject to the conditions

(i) $\Sigma_x W_{xy}e^{f_{xy}} = 1$, for all y;

(ii) R preserves the stationary state $\tilde{p}$, or $\Sigma_y W_{xy}e^{f_{xy}}\tilde{p}(y) = \tilde{p}(x)$ for all x. We examine the effect of a variation δf_{xy} on $|\Delta_1\mathscr{S}(R,\tilde{p},W)|$,

$$\delta|\Delta_1\mathscr{S}(R,\tilde{p},W)|=\sum_{yx} W_{yx}\tilde{p}(x)\exp(f_{yx})(1+f_{yx})\,\delta f_{yx}. \tag{3.11}$$

The variations of the two constraints are

$$\delta\left(\sum_y W_{yx}\exp(f_{yx})-1\right)=\sum_y W_{yx}\exp(f_{yx})\,\delta f_{yx}, \tag{3.12}$$

$$\delta\left(\sum_y W_{yx}\exp(f_{yx})\tilde{p}(y)\right)=\sum_x W_{yx}\exp(f_{yx})\tilde{p}(x)\,\delta f_{yx}. \tag{3.13}$$

As usual, we introduce two Lagrange multipliers, λ_x for the constraints (3.12) and μ_y for the constraints (3.13), and write

$$0=\delta|\Delta_1\mathscr{S}(R,\tilde{p},W)|+\sum_x \lambda_x\delta\left(\sum_y W_{yx}\exp(f_{yx})-1\right)$$
$$+\sum_y \mu_y\delta\left(\sum_x W_{yx}\exp(f_{yx})\tilde{p}(x)-\tilde{p}(y)\right).$$

After rearrangement, this gives

$$0=\sum_{yx}\delta f_{yx}\exp(f_{yx})W_{yx}[\tilde{p}(x)(1+f_{yx})+\lambda_x+\mu_y\tilde{p}(x)].$$

If $W_{yx}=0$, we have no condition. But, if $W_{yx}\neq 0$ we obtain

$$f_{yx}=-\frac{\lambda_x}{\tilde{p}(x)}-\mu_y-1,$$

and then λ_x and μ_y are determined using the two constraints:

$$1=\sum_y W_{yx}\exp\left(-\frac{\lambda_x}{\tilde{p}(x)}\right)\exp(-\mu_y-1),$$

$$\tilde{p}(y)=\sum_x W_{yx}\exp\left(-\frac{\lambda_x}{\tilde{p}(x)}\right)\exp(-\mu_y-1)\tilde{p}(x).$$

Then, we see that $R_{yx}=0$ when $W_{yx}=0$ (this is our ansatz anyway), and

$$R_{yx}=W_{yx}\exp(\rho_y-\sigma_x), \tag{3.14}$$

when $W_{yx}\neq 0$, so that we can always use Eq. (3.14). Using (3.14), we can compute the rate of dissipation

$$|\Delta_1\mathcal{S}(R,\tilde{p},W)|=\sum_{y,x} W_{yx}\exp(f_{yx})f_{yx}\tilde{p}(x).$$

But

$$\sum_x W_{yx}e^{-\sigma_x}\tilde{p}(x)=e^{-\rho_y}\tilde{p}(y),\quad \sum_y W_{yx}e^{\rho_y}=e^{\sigma_x},$$

so that finally the minimal rate of dissipation is

$$|\Delta_1\mathcal{S}(R,\tilde{p},W)|=\sum_x \tilde{p}(x)(\rho_x-\sigma_x). \tag{3.15}$$

D. Analysis near equilibrium

In this section, we consider an equilibrium state p_{eq} with its detailed balance dynamics given by the matrix W. We further consider a nonequilibrium state $\tilde{p}$, which is close to p_{eq}, whose dynamics are given by a (non-detailed-balance) stochastic matrix R, close to W. We fix the notation as follows:

$$\tilde{p}(x)=p_{\mathrm{eq}}(x)\exp(\varphi(x,\delta))\equiv p_{\mathrm{eq}}(x)\exp(\delta\varphi_1(x)+\delta^2\varphi_2(x)+\cdots), \tag{3.16}$$

$$R_{xy}=W_{xy}\exp(f(x,y,\delta))\equiv W_{xy}\exp(\delta f_{xy}^{(1)}+\delta^2 f_{xy}^{(2)}+\cdots). \tag{3.17}$$

1. Identities satisfied by $f^{(1)}$ and φ_1

We differentiate the relation $\Sigma_y R_{yx}=1$ with respect to δ at $\delta=0$. This gives

$$\sum_y W_{yx}f_{yx}^{(1)}=0. \tag{3.18}$$

Similarly, the relation $\tilde{p}(x)=\Sigma_y R_{xy}\tilde{p}(y)$ is differentiated with respect to δ at $\delta=0$. This implies

$$p_{\mathrm{eq}}(x)\varphi_1(x)=\sum_y W_{xy}f_{yx}^{(1)}p_{\mathrm{eq}}(y)+\sum_y W_{xy}\varphi_1(y)p_{\mathrm{eq}}(y), \tag{3.19}$$

or using detailed balance,

$$W_{xy}p_{\rm eq}(y)=W_{yx}p_{\rm eq}(x),$$

$$\varphi_1(x)=\sum_y W_{yx}f^{(1)}_{yx}+\sum_y W_{yz}\varphi_1(y). \tag{3.20}$$

2. Variation of the entropy near the equilibrium state

Suppose that we start from the stationary state $\tilde{p}(x)$ and let it evolve spontaneously using the detailed balance dynamics W. We can compute in one time step Δt, the variation of relative entropy as in Sec. II D, except now $\tilde{p}\to p_{\rm eq}$ and $R\to W$. We obtain

$$S(\tilde{p}(\cdot,\Delta t)|p_{\rm eq})-S(\tilde{p}|p_{\rm eq})=\frac{\delta^2}{2}\left[\langle\varphi_1^2\rangle_{p_{\rm eq}}-\left\langle\left(\frac{1}{\text{diag } p_{\rm eq}}W\ \text{diag}\ p_{\rm eq}\varphi_1\right)^2\right\rangle_{p_{\rm eq}}\right].$$

But for detailed balance we have $((1/\text{diag}\, p_{\rm eq})W\ \text{diag}\, p_{\rm eq})_{xy}=(1/p_{\rm eq}(x))W_{xy}p_{\rm eq}(y)=W_{yx}$. Thus

$$S(\tilde{p}(\cdot,\Delta t)|p_{\rm eq})-S(\tilde{p}(\cdot)\cdot|p_{\rm eq})=\frac{\delta^2}{2}\left[\langle\varphi_1^2\rangle_{p_{\rm eq}}-\langle({}^tW\varphi_1)^2\rangle_{p_{\rm eq}}\right]. \tag{3.21}$$

3. Rate of dissipation

We now compute the rate of dissipation $|\Delta_1\mathscr{I}(\mathrm{R},\tilde{\mathrm{p}},\mathrm{W})|$. In Sec. III C, we obtained

$$|\Delta_1\mathscr{I}(R,\tilde{p},W)|=\sum_{xy}\ \exp(f(x,y,\delta))\tilde{p}(y)f(x,y,\delta),$$

which is evidently 0 for $\delta=0$ because $f(x,y,0)=0$. We expand this quantity in powers of δ up to second order. We write

$$\tilde{p}(x)=p_{\rm eq}(x)+\delta p_1(x)+O(\delta^2).$$

(We will not need the second order term in $\tilde{p}$.)

$$|\Delta_1\mathscr{I}(R,\tilde{p},W)|=\sum_{xy}W_{xy}\left\{1+\delta f^{(1)}_{xy}+\delta^2 f^{(2)}_{xy}+\frac{\delta^2}{2}(f^{(1)}_{xy})^2\right\}$$
$$\times\{p_{\rm eq}(y)+\delta p_1(y)\}\{\delta f^{(1)}_{xy}+\delta^2 f^2_{xy}\}+O(\delta^3).$$

The first-order term in δ is

$$\sum_y p_{\rm eq}(y)\sum_x W_{xy}f^{(1)}_{xy}.$$

But this is 0 because of relation (3.15) above,

$$\sum_x W_{xy}f^{(1)}_{xy}=0.$$

So we compute the second-order terms in δ; these are

$$\sum_{x,y} W_{xy} p_{\mathrm{eq}}(y)(f_{xy}^{(2)}+(f_{xy}^{(1)})^2)+\sum_{x,y} W_{xy} f_{xy}^{(1)} p_1(y).$$

But expanding $\Sigma_x R_{xy}=1$ up to second order gives

$$\sum_{x} W_{xy} f_{xy}^{(1)}=0 \quad \text{[relation (3.18) above]},$$

$$\sum_{x} W_{xy}\left(f_{xy}^{(2)}+\frac{1}{2}(f_{xy}^{(1)})^2\right)=0.$$

There remains only a single term, so that

$$|\Delta_1 \mathscr{S}(R,\tilde{p},W)|=\frac{\delta^2}{2}\sum_{x,y} W_{xy} p_{\mathrm{eq}}(y)(f_{xy}^{(1)})^2. \tag{3.22}$$

4. Minimal rate of dissipation

Starting from this last equation let us compute the minimal rate of dissipation, given $\tilde{p}$ and W. We thus have to minimize $|\Delta_1 \mathscr{S}(R,\tilde{p},W)|$ with respect to $f_{xy}^{(1)}$ under the conditions (3.18) and (3.20).

Introducing Lagrange multipliers λ_x, μ_y for (3.18) and (3.20), we see that

$$\sum_{x,y} W_{xy} p_{\mathrm{eq}}(y) f_{xy}^{(1)}\,(\delta f_{xy}^{(1)})+\sum_{x}\lambda_x\sum_{y} W_{yx}\,\delta f_{yx}^{(1)}+\sum_{x}\mu_x\sum_{y} W_{yx}\,\delta f_{xy}^{(1)}=0.$$

This implies that

$$W_{xy} p_{\mathrm{eq}}(y) f_{xy}^{(1)}+W_{xy}\lambda_y+\mu_x W_{yx}=0.$$

Using detailed balance, $W_{yx}=W_{xy}p_{\mathrm{eq}}(y)/p_{\mathrm{eq}}(x)$, we see that either

$$(1)\quad W_{xy}=0, \quad \text{or}$$

$$(2)\quad f_{xy}^{(1)}+\frac{\lambda_y}{p_{\mathrm{eq}}(y)}+\frac{\mu_x}{p_{\mathrm{eq}}(x)}=0,$$

which is exactly what we obtained above in a more general setting, namely

$$f_{xy}^{(1)}=\rho(x)-\sigma(y).$$

Let us assume that $f_{xy}^{(1)}$ has this form and determine σ and ρ using the constraints (3.18) and (3.20) above. This gives the following.

(1) For the constraint (3.18), $\Sigma_x W_{xy} f_{xy}^{(1)}=0$,

$$\sigma(x)=\sum_{y}\rho(y)W_{yx} \quad \text{or} \quad \sigma=\rho^t W. \tag{3.23}$$

(2) For the constraint (3.20), $\sigma_1(x)=\Sigma_y W_{yx} f_{xy}^{(1)}+\Sigma_y W_{yx}\varphi_1(y)$,

$$\varphi_1(x)=\sum_y W_{yx}(\rho(x)-\sigma(y))+\sum_y W_{yx}\varphi_1(y)$$

$$=\rho(x)-\sum_y \sigma(y)W_{yx}+\sum_y W_{yx}\varphi_1(y)$$

$$=(\rho(I-{}^tW)(I+{}^tW))_x+\sum_y W_{yx}\varphi_1(y).$$

This can be solved as

$$\varphi_1(I-{}^tW)=\rho(I+{}^tW)(I-{}^tW)$$

or

$$\varphi_1=\rho(I+{}^tW). \tag{3.24}$$

Now we can compute the minimal rate of dissipation (to maintain $\tilde{p}$ against the thermal detailed balance dynamics given by W),

$$|\Delta_1\mathscr{A}(R,\tilde{p},W)|=\frac{\delta^2}{2}\sum_{x,y} W_{xy}p_{\mathrm{eq}}(y)(f_{xy}^{(1)})^2=\frac{\delta^2}{2}\sum_{x,y} W_{xy}p_{\mathrm{eq}}(y)(\rho(x)-\sigma(y))^2.$$

Let us expand, using (3.23), $\sigma=\rho^tW$,

$$\sum_{x,y} W_{xy}(y)(\rho(x)-\sigma(y))^2$$

$$=\sum_{x,y} W_{xy}p_{\mathrm{eq}}(y)\rho(x)^2-2\sum_{x,yp} p_{\mathrm{eq}}(y)\rho(x)\sigma(y)+\sum_{x,y} W_{xy}p_{\mathrm{eq}}(y)\sigma(y)^2.$$

We consider the three terms above,

$$\sum_{x,y} W_{xy}p_{\mathrm{eq}}(y)\rho(x)^2=\sum_x p_{\mathrm{eq}}(x)\rho(x)^2-2\sum_{x,y} W_{xy}p_{\mathrm{eq}}(y)\rho(x)\sigma(y)$$

$$=-2\sum_y (\rho^tW)_y p_{\mathrm{eq}}(y)(\rho^tW)_y,$$

$$\sum_{x,y} W_{xy}p_{\mathrm{eq}}(y)\sigma(y)^2=\sum_y p_{\mathrm{eq}}(y)\sigma(y)^2=\sum_y p_{\mathrm{eq}}(y)((\rho^tW)_y),$$

so that

$$|\Delta_1\mathscr{A}(R,\tilde{p},W)|=\frac{\delta^2}{2}(\|\rho\|_{p_{\mathrm{eq}}}^2-\|\rho^tW\|_{p_{\mathrm{eq}}}^2). \tag{3.25}$$

5. Comparison of the rate of dissipation and the variation of S

We come back to relation (3.21), namely

$$S(\tilde{p}(\cdot,\Delta t)|p_{\mathrm{eq}})-S(\tilde{p}|p_{\mathrm{eq}})=\frac{\delta^2}{2}[\|\varphi_1\|_{p_{\mathrm{eq}}}^2-\|\varphi_1{}^tW\|_{p_{\mathrm{eq}}}^2]. \tag{3.26}$$

We see that this is similar to the relation (3.25) for the minimal rate of dissipation in the R-dynamics, except for the fact that $\varphi_1=\rho(I+{}^tW)$. [See the relation (3.24).]

We know that $\Sigma p_{\rm eq}(x)\varphi_1(x)=0$ so that φ_1 can be expanded in terms of the left eigenvectors of W with eigenvalues different from 1. Because of the (3.24), the same expansion is possible for ρ, and we therefore write

$$\rho=\sum c_n\theta_n^{(L)},$$

where $\theta_n^{(L)}$ are the left eigenvectors of W of eigenvalue less than 1.

Moreover, $\{\theta_n^{(L)}\}$ form an orthonormal basis for the equilibrium scalar product $p_{\rm eq}$ (because ${}^tW$ is self-adjoint for this scalar product due to detailed balance). It follows that

$$S(\tilde{p}(\cdot,\Delta t)|p_{\rm eq})-S(\tilde{p}(\cdot)|p_{\rm eq})=\frac{\delta^2}{2}\sum_n |c_n|^2|(1+\lambda_n)|^2(1-|\lambda_n^2|)$$

and

$$|\Delta_1\mathscr{S}(R,\tilde{p},W)|=\frac{\delta^2}{2}\sum_x |c_n|^2(1-|\lambda_n^2|).$$

Because $0\leqslant|\lambda_n|\leqslant 1$, we see that we always have

$$\tfrac{1}{4}[S(\tilde{p}(\cdot,\Delta t)|p_{\rm eq})-S(\tilde{p}(\cdot)|p_{\rm eq})]\leqslant|\Delta_1\mathscr{S}(R,\tilde{p},W)|. \tag{3.27}$$

The interpretation of this inequality is clear. If we start with the stationary state $\tilde{p}$ and switch off the R dynamics (so that $\tilde{p}$ starts to evolve by the detailed balance dynamics toward $p_{\rm eq}$), the dissipation is less than four times the cost to maintain $\tilde{p}$ using the dynamics in the larger environment (acting with W) on the system.

IV. FLUCTUATION AND DISSIPATION FOR SLOW VARIABLES

A. The macroscopic entropy

1. Fast and slow variables

Usually, a system with state space X is characterized by a small number of "slow" variables and by other "fast" variables. Such variables can be distinguished in terms of the eigenvalues of the master equation, i.e., in our case, in terms of the eigenvalues of the stochastic matrix R. Essentially, the slow variables are functions f on X, such that their set of values $\{f_x\}$ $(x\in X)$ can be decomposed on left eigenvectors of the matrix R associated with eigenvalues of R very close to 1 (but not equal to 1).

In this section, we shall assume that the system is characterized by only one slow variable $A_x(x\in X)$ taking values $a,a',\ldots$. We shall denote by u the other coordinates, so that a point x in X is identified with a couple (a,u), with $a=A(x)$.

2. Reduced description

At this point, it is customary to describe the system by the variable A alone. This is the reduced or macroscopic description, which is a coarse grained description of the full description by (a,u). We also must change the time scale, because in the time scale Δt (of the R dynamics), A does not evolve in an appreciable manner. So the relevant time scale becomes much longer, and the general idea is that, relative to this longer time scale, A varies but u readjusts itself instantaneously to its relative stationary distribution. This is the idea of all macroscopic descriptions (see Refs. 1, 6, and 7, among many references).

In our context, we can make this precise in the following way. We start as usual from a stationary state $\tilde{p}(x)$ and we define a reduced (or macroscopic) state $\tilde{P}$ by

$$\tilde{P}(x)=\sum_{\{x\in X|A(x)=a\}}\tilde{p}(x)=\sum_{u}\tilde{p}(x,u). \tag{4.1}$$

Following customary practice, we define a function $\Sigma(a)$ by the formula

$$\tilde{P}(a)=\exp(-\Sigma(a)) \tag{4.2}$$

(see, for example, Ref. 1, in the context of an equilibrium situation, and Refs. 2, 6, 10, and 24 for generalizations to nonequilibrium situations). Here $\Sigma(a)$ is a Lyapunov function for the reduced evolution of the A variable, as we shall see below.

In the case of equilibrium, $\Sigma(a)$ is the Einstein entropy. We shall assume now that the average of A in the stationary state is 0.

$$\langle A\rangle_{\tilde{p}}\equiv\sum A(x)\tilde{p}(x)=0. \tag{4.3}$$

3. Relation to the relative entropy

Let us assume that we have prepared the system in the state $\tilde{p}(x)$ (the stationary state for the R-dynamics), but that we observe in a particular sample of the system a certain fluctuation of A, so that A takes a value $a\neq 0$. Then, the probability distribution of the fast variables u, given the fact one observes the fluctuation a of A, is the conditional stationary probability distribution

$$\tilde{\pi}_a(u)=\frac{\tilde{p}(a,u)}{\tilde{P}(a)}, \tag{4.4}$$

and the quasistationary state is thus a state q_a,

$$q_a(x)\equiv\tilde{\pi}_a(u)\,\delta(A(x)-a). \tag{4.5}$$

It follows immediately that the relative entropy of q_a with respect to $\tilde{p}$, namely $S(q_a|\tilde{p})$ [see Eq. (1.1)], is in fact, $-\Sigma(a)$,

$$S(q_a|\tilde{p})=-\Sigma(a), \tag{4.6}$$

where $\Sigma(a)$ is defined as in Eq. (4.2). We calculate this as follows.

$$S(q_a|\tilde{p})=-\sum_{a}\tilde{\pi}_a(u)\,\delta(A(x)-a)\log\frac{\tilde{\pi}_a(u)}{\tilde{p}(a,u)}=-\log\frac{1}{\tilde{P}(a)}=-\Sigma(a).$$

This explains why $\Sigma(a)$ could be taken as a Lyapunov function for the evolution of a. If we wait an appropriate time, a would vary by a small quantity δa, while the fast u variables would recover their conditional stationary distribution. Our earlier assumption on time scales is precisely the assumption that such an appropriate time exists. Then the state q_a would become $q_{a+\delta a}$ by the R evolution, the variables u keeping their conditional stationary distribution. Under this circumstance,

$$S(q_{a+\delta a}|\tilde{p})-S(q_a|\tilde{p})\geq 0,$$

since $q_{a+\delta a}\approx Rq_a$ [cf. Eq. (2.4)]. This implies

$$\Sigma(a+\delta a)\leqslant\Sigma(a).$$

B. Fluctuation dissipation, in general

The usual near-equilibrium fluctuation dissipation theory is a formal consequence of the fact that a certain state p_{eq} is a stationary state of the W evolution: Writing the stationarity of the equilibrium state explicitly leads to an identity that can then be reinterpreted as a physical relation between fluctuation and dissipation (see Refs. 1, 6, 12, and 25 among many references). In the language of the previous section, if we are in a stationary state, and if we observe an actual fluctuation of A equal to a [this fluctuation has a probability $\widetilde{P}(a)$], then the dissipation induced by the reduction to 0 of this fluctuation is related in a natural way to this fluctuation (in a linear way), the proportionality coefficient being some given "transport" characteristic of the system (see Ref. 23).

We will show that it is possible to derive the fluctuation-dissipation theory in our context using the formalism of Sec. IV A. Moreover, our demonstration is not limited to near-equilibrium situations (and gives, in fact, a correction to it, as well as a finite-size effect correction).

There are various ways to derive fluctuation-dissipation theorems, each of which provides, in general, extra information, in particular about the transport or relaxation coefficients. Here we shall relate the "transport" coefficient to the eigenvalues of R. In our abstract context, we shall choose an analog of linear response theory (as presented, for example, in Ref. 25). We produce the fluctuation of the macroscopic variable A using an external force that modifies the stationary state $\widetilde{p}$.

C. Linear response theory: General computation

The general situation is as in Sec. IV A: we distinguish a variable $A(x)$ $(x\in X)$ and other variables u, so that $x=(a,u)$, where $a=A(x)$. Moreover, we have the stationary state $\widetilde{p}(x)$ with respect to the R dynamics as usual. We finally assume that A has average 0 in the stationary state [Eq. (4.3)].

1. The displaced state

We define, in analogy with the analysis of Sec. II B, a displaced state,

$$p_\alpha(x)=\frac{1}{Z_\alpha}\widetilde{p}(x)\exp(\alpha A(x)+\cdots), \tag{4.7}$$

where α is a small parameter and the ellipses represents higher-order terms in α. Then α can be viewed as a "conjugate field," αA being an extra energy (this field is imposed by an external source or observer on which the system does not react).

We have, because (by assumption) $\langle A(\,\cdot\,)\rangle_{\widetilde{p}}=0$,

$$Z_\alpha=\sum_x \widetilde{p}(x)\exp(\alpha A(x)+\cdots)=1+\frac{\alpha^2}{2}\langle A(x)^2\rangle_{\widetilde{p}}+\cdots,$$

so that one can suppress Z_α as being higher order in α, and write simply

$$p_\alpha(x)=\widetilde{p}(x)\exp(\alpha A(x)+\cdots). \tag{4.8}$$

Now, we have

$$\langle A\rangle_{p_\alpha}=\langle A\rangle_{\widetilde{p}}+\alpha\langle A^2\rangle_{\widetilde{p}}+\cdots,$$

so that for small α,

$$\langle A\rangle_{p_\alpha}=\alpha\langle A^2\rangle_{\tilde{p}}, \tag{4.9}$$

and $\langle A^2\rangle_{\tilde{p}}$ appears as usual to be the susceptibility for A.

2. Variation of the mean value

We start at time $t=0$ from the state $p_\alpha(x)$ given by (4.1). In one time step, the state becomes

$$p_\alpha(x,\Delta t)=\sum_y R_{xy}p_\alpha(y)=\sum_y R_{xy}\tilde{p}(y)\exp(\alpha A(y)),$$

and at time Δt,

$$\langle A(\Delta t)\rangle_{p_\alpha}=\sum_x A(x)p_\alpha(x,\Delta t).$$

Expanding

$$\langle A(\Delta t)\rangle_{p_\alpha}=\sum_{x,y} A(x)R_{xy}\tilde{p}(y)+\alpha\sum_{x,y} A(x)R_{xy}\tilde{p}(y)A(y)+\cdots .$$

The first term is 0 because this is $\Sigma_x A(x)\tilde{p}(x)$. Finally, we have, modulo terms of order α^2,

$$\langle A(\Delta t)-A(0)\rangle_{p_\alpha}=\alpha\sum_{x,y} A(x)(R_{xy}-\delta_{xy})A(y)\tilde{p}(y). \tag{4.10}$$

We can also eliminate α using Eq. (4.9) and get

$$\langle A(\Delta t)-A(0)\rangle_{p_\alpha}=\frac{\langle A\rangle_{p_\alpha}}{\langle A^2\rangle_{\tilde{p}}}\sum_{x,y} A(x)(R_{xy}-\delta_{xy})A(y)\tilde{p}(y). \tag{4.11}$$

3. Second moment

We now want to compute $\langle (A(\Delta t)-A(0))^2\rangle_{p_\alpha}$

(a) Computation of $\langle A(\Delta t)^2\rangle_{p_\alpha}$. This is, modulo terms in α^2,

$$\langle A(\Delta t)^2\rangle_{p_\alpha}=\sum_{x,y} A(x)^2R_{xy}\tilde{p}(y)\exp(\alpha A(y))=\langle A^2\rangle_{\tilde{p}}+\alpha\sum_{x,y} A(x)^2R_{xy}\tilde{p}(y)A(y). \tag{4.12}$$

(b) Computation of $\langle A^2\rangle_{p_\alpha}$. Again up to order α^2,

$$\langle A(0)^2\rangle_{p_\alpha}=\langle A^2\rangle_{\tilde{p}}+\alpha\langle A^3\rangle_{\tilde{p}}. \tag{4.13}$$

(c) Computation of $\langle A(\Delta t)A(0)\rangle_{p_\alpha}$

$$\begin{aligned}\langle A(\Delta t)A(0)\rangle_{p_\alpha}&=\sum_{x,y} A(x)R_{xy}A(y)\tilde{p}(y)\exp(\alpha A(y))\\&=\sum_{x,y} A(x)R_{xy}A(y)\tilde{p}(y)+\alpha\sum_{x,y} A(x)R_{xy}A(y)^2\tilde{p}(y).\end{aligned} \tag{4.14}$$

(d) Computation of $\langle (A(\Delta t)-A(0))^2\rangle_{p_\alpha}$ From Eqs. (4.12)–(4.14) we obtain, after rearrangement,

$$\langle (A(\Delta t)-A(0))^2\rangle_{p_\alpha}=-2\sum_{x,y} A(x)(R_{xy}-\delta_{xy})A(y)\tilde{p}(y)+\alpha\sum_{x,y}[A(x)^2A(y)(R_{xy}\tilde{p}(y) -R_{yx}\tilde{p}(x))-\tilde{p}(y)A(x)A(y)^2(R_{xy}-\delta_{xy})]. \tag{4.15}$$

We see that this term is again of order Δt because $R_{xy}-\delta_{xy}$ is of order Δt and because we can rewrite

$$R_{xy}\tilde{p}(y)-R_{yx}\tilde{p}(x)=(R_{xy}-\delta_{xy})\tilde{p}(y)-(R_{yx}-\delta_{yx})\tilde{p}(x).$$

D. The case of a left eigenvector of *R*

We shall now take for A a slow variable of the system, i.e., a variable that decays in one of the slowest possible modes. One way to do this is to choose for A a left eigenvector of the transfer matrix R with eigenvalue λ near 1 (but not exactly 1). (In fact, for our purposes the essential point is that the eigenvalue associated with A satisfy $1>\lambda\gg|\lambda'|$ for all other eigenvalues λ'. The closeness of λ to 1 is not used significantly.)

1. First moment

We assume for all $y\in X$, that

$$\lambda A_y=\sum_x A_x R_{xy}.$$

From Eq. (4.11) we obtain to first order in α,

$$\langle A(\Delta t)-A(0)\rangle_{p_\alpha}=\langle \dot{A}(0)\rangle_{p_\alpha}(\lambda-1). \tag{4.16}$$

2. Second moment

We obtain from Eq. (4.15),

$$\langle (A(\Delta t)-A(0))^2\rangle_{p_\alpha}=(\lambda-1)[-2\langle A^2\rangle_{\tilde{p}}-\alpha\langle A^3\rangle_{\tilde{p}}]+\alpha\sum_{x,y} A(x)^2A(y)(R_{xy}\tilde{p}(y)-R_{yx}\tilde{p}(x)). \tag{4.17}$$

3. The case of detailed balance

When R satisfies detailed balance, the second term on the right-hand side of Eq. (4.17) above vanishes identically and

$$\langle (A(\Delta t)-A(0))^2\rangle_{p_\alpha}=(1-\lambda)[-2\langle A^2\rangle_{\tilde{p}}+\alpha\langle A^3\rangle_{\tilde{p}}]. \tag{4.18}$$

Moreover, in this case, we can compute the rate of dissipation in one unit time step Δt starting from the state p_α and using the R dynamics. This is

$$S(p_\alpha(\cdot,\Delta t)|\tilde{p})-S(p_\alpha|\tilde{p})=\frac{\alpha^2}{2}\langle A^2\rangle_{\tilde{p}}(1-\lambda)(1+\lambda). \tag{4.19}$$

We saw the same result in Sec. II. To see the correspondence, take $\varphi_1=A$ and notice that $M=M^*={}^tR$, so that the μ eigenvalue of MM^* corresponding to $\varphi_1=A$ is $\mu=\lambda^2$.

4. Fluctuation dissipation

We return to the general (non-detailed-balance) case. If A is decaying slowly, $\lambda \approx 1$, and

$$S(p_\alpha(\cdot,\Delta t)|\bar{p}) - S(p_\alpha|\bar{p}) \sim \langle A^2\rangle_{\bar{p}}(1-\lambda). \tag{4.20}$$

Moreover, let us compare Eqs. (4.16) and (4.17) and let us assume that $\alpha\langle A^3\rangle_{\bar{p}} \approx 0$. Then eliminating $\lambda - 1$ from both equations, we obtain

$$\langle (A(\Delta t) - A(0))^2\rangle_{p_\alpha} = 2\langle A^2\rangle_{\bar{p}} \left| \frac{\langle A(\Delta t) - A(0)\rangle_{p_\alpha}}{\langle A(0)\rangle_{p_\alpha}} \right|. \tag{4.21}$$

This relation is, in our context, the analog of the standard fluctuation-dissipation theorem.

Example: The prototype of fluctuation-dissipation theory is obtained for a Langevin particle (of mass $m=1$) with the equation of motion

$$dx = v\ dt, \quad dv = -fv\ dt + dB(t),$$

where $dB(t)$ is the white noise force,

$$\langle dB(t)dB(s)\rangle = 2D\,\delta(t-s).$$

In the sense of our development, the "fast variables" are the sources of the noise. The variables x and v are "macroscopic" and "slow." The Fokker Planck equation is

$$L = \frac{\partial}{\partial v}\left(D\,\frac{\partial}{\partial v} + fv \right) - v\,\frac{\partial}{\partial x}.$$

This corresponds to a reduced operator (projected onto the slow variables) description of $I-R$ for the discrete time case. The space X consists of the configuration space (x,v) of the Langevin particle as well as the degrees of freedom that give rise to the white noise (that the Fokker–Planck equation absorbs into the diffusion coefficient). Take for A the function v. Then

$$L^* v = \left(D\,\frac{\partial^2}{\partial v^2} - fv\,\frac{\partial}{\partial v} + v\,\frac{\partial}{\partial x} \right) v = -fv,$$

and v is an eigenfunction of L^* with eigenvalue $-f$ (but not necessarily of the full operator that includes the sources of the noise). Now let us consider, instead of a state p_α, a state $\delta(v-v_0)$. Then

$$\langle v(\Delta t) - v_0\rangle_{\delta(v-v_0)} = \int (v-v_0)p(\Delta t, v|v_0)dv.$$

But

$$\begin{aligned} \lim_{\Delta t\to 0} \frac{\partial}{\partial \Delta t}\langle v(\Delta t) - v_0\rangle_{\delta(v-v_0)} &= \lim_{\Delta t\to 0} \int (v-v_0)L_v p(\Delta t, v|v_0)dv \\ &= \int L_v^*(v-v_0)\,\delta(v-v_0)dv \\ &= -fv_0. \end{aligned}$$

In the same way,

$$\lim_{\Delta t\to 0}\frac{\partial}{\partial \Delta t}\langle (v(\Delta t)-v(0))^2\rangle_{\delta(v-v_0)}=\int L_v^*(v-v_0)^2\delta(v-v_0)dv_0=2D.$$

Then our statement of the fluctuation-dissipation theorem [Eq. (4.21)] becomes

$$\lim_{\Delta t\to 0}\frac{\partial}{\partial \Delta t}\langle (v(\Delta t)-v(0))^2\rangle_{\delta(v-v_0)}$$

$$=2\langle v^2\rangle_{p_{\rm eq}}\left|\lim_{\Delta t\to 0} v\left(\frac{(\partial/\partial\Delta t)\langle v(\Delta t)-v_0\rangle_{\delta(v-v_0)}}{\langle v\rangle_{\delta(v-v_0)}}\right)\right|,$$

or

$$2D=2k_{\rm B}Tf,$$

which is the usual Einstein relation for $m=1$. So the relation (4.21) is the generalization of the standard fluctuation-dissipation theory in our context.

Remark: For initial conditions far from the stationary state, dissipation may be dominated by the friction coefficients, "f," irrespective of the fluctuations. As such, this way of calculating heat production, etc., will not involve the fluctuations. However, the validity of these mean field calculations (and use of f to derive heat production) does not contradict the fluctuation-dissipation theorem because it is a far from stationary-state situation.

5. The general case

In fact, Eqs. (4.16) and (4.17), even in the detailed balance case, are more precise than the fluctuation-dissipation theorem, because the fluctuation-dissipation theorem (in its usual statement) is the relation (4.21), relating these two quantities. In our case, we have separately derived each of the moments $\langle A(\Delta t)-A(0)\rangle_{p_\alpha}$ (the dissipation) and $\langle (A(\Delta t)-A(0))^2\rangle_{p_\alpha}$ (the fluctuation) *separately*, and related them to the spectrum of the transfer matrix.

Equation (4.16) [for $\langle A(\Delta t)-A(0)\rangle_{p_\alpha}$] is straightforward.

Equation (4.17) [for $\langle (A(\Delta t)-A(0))\rangle_{p_\alpha}$)] contains a correction Γ of cubic order in A and first order in α,

$$\Gamma\equiv\alpha\sum_{x,y}A(x)^2A(y)(R_{xy}\tilde{p}(y)-R_{yx}\tilde{p}(x)).$$

Notice, also, that if we are away from criticality, both Γ and $\langle A^3\rangle_{\tilde{p}}$ would be close to 0.

E. Summary

In a sense, the standard fluctuation-dissipation theorem is a tautology; namely, the assertion that the stationary state is a solution of the stationary equation (see Ref. 12). In our situation, we say more because we compute separately the fluctuation *and* the dissipation in terms of the spectrum of the transfer matrix and then deduce the relation between the fluctuation and dissipation by eliminating the eigenvalue of the transfer matrix. Still, at our level of abstraction, all these identities can only be tautological. (The physics enters in judging the suitability of the stochastic description and the time scale separation.)

We now summarize our results concerning the fluctuation-dissipation theorem. Let A be a slow variable of the system, so $AR=\lambda R$ for a λ close to 1; it follows that $\langle A\rangle_{\tilde{p}}=0$. Let

$$p_\alpha(x)=\tilde{p}(x)\exp(\alpha A(x)+O(\alpha^2)), \tag{4.22}$$

be a neighboring state of the stationary state $\tilde{p}$, so that

$$\langle A\rangle_{p_\alpha}=\alpha\langle A^2\rangle_{\tilde{p}}+O(\alpha^2). \tag{4.23}$$

Then we have the two relations [see Eqs. (4.16) and (4.17)]:
dissipation,

$$\langle A(\Delta t)-A(0)\rangle_{p_\alpha}=\langle A\rangle_{p_\alpha}(\lambda-1); \tag{4.24}$$

fluctuation,

$$\langle (A(\Delta t)-A(0))^2\rangle_{p_\alpha}=-2(\lambda-1)\langle A^2\rangle_{\tilde{p}}+O(\alpha A^3). \tag{4.25}$$

We thus obtain
fluctuation dissipation:

$$\langle (A(\Delta t)-A(0))^2\rangle_{p_\alpha}=\frac{2\langle A^2\rangle_{\tilde{p}}}{\langle A\rangle_{p_\alpha}}\langle A(\Delta t)-A(0)\rangle_{p_\alpha}. \tag{4.26}$$

In this form we have a statement relating changes in a variable as it returns to the steady state ("dissipation") to its spontaneous fluctuations in that steady state. The term "dissipation," suggesting energy flow, may not apply in all applications of this theorem. There will nonetheless be inequalities relating this "dissipation" to changes in the relative entropy that we have defined.

Another (inequivalent) statement is that if

$$p(x)=\tilde{p}(x)\exp(\delta\varphi_1(x)+\cdots),$$

then

$$S(p(\cdot,\Delta t)|\tilde{p})-S(p|\tilde{p})\geqslant\tfrac{1}{2}\langle\delta^2\varphi_1^2\rangle_{\tilde{p}}(1-\mu_{\max}), \tag{4.27}$$

where $\mu_{\max}$ is the maximal (non-1) eigenvalue of the matrix ${}^tR(1/\tilde{p})\,R$ diag $(\tilde{p})$ [see Eqs. (1.11)–(1.12)].

F. Generalization to the case of *n* slow variables

1. Entropy

Let us now assume that one can find n slow variables $A_1,\ldots,A_n$ for the R dynamics. Take these such that

$$\langle A_j\rangle_{\tilde{p}}=0, \quad \text{for all } j.$$

For given values $a_1,\ldots,a_n$, we define

$$\tilde{P}(a_1,\ldots,a_n)=\sum_{\{x\in X|A_j(x)=a_j \text{ for all } j\}}\tilde{p}(x),$$

and we define a function

$$\Sigma(a_1,\ldots,a_n)=-\log\tilde{P}(a_1,\ldots,a_n).$$

As before (Sec. IV A), we have

$$\Sigma(a_1,\ldots,a_n)=-S(q_a|\tilde{p}),$$

where

$$q_a(x)=\frac{\tilde{p}(a,u)}{\tilde{P}(a)}\prod_j \delta(A_j(x)-a_j),$$

and Σ will be a Lyapunov function for the evolution of $a_1,...,a_n$.

2. General linear response theory

We generalize the results of Secs. IV C and IV D. Call $\alpha\equiv(\alpha_1,...,\alpha_n)$, where α_j is a conjugate variable for A_j and define as in Sec. IV C,

$$p_\alpha(x)=\frac{1}{Z_\alpha}\tilde{p}(x)\exp\left(\sum_{i=1}^{n}\alpha_i A_i+O(\alpha^2)\right).$$

It is immediate that

$$\langle A_i\rangle_{p_\alpha}=\sum_{j=1}^{n}\alpha_j\langle A_iA_j\rangle_{\tilde{p}}+O(\alpha^2).$$

One also proves

$$\langle A_i(\Delta t)-A_i(0)\rangle_{p_\alpha}=\sum_{j=1}^{n}\alpha_j\sum_{x,y}A_i(x)(R_{xy}-\delta_{xy})\tilde{p}(y)A_j(y)+O(\alpha^2)$$

and

$$\begin{aligned}\langle (A_i(\Delta t)-A_i(0))(A_j(\Delta t)-A_j(0))\rangle_{p_\alpha}&\\ =-\sum_{x,y}A_i(x)((R_{xy}-\delta_{xy})\tilde{p}(y)+(R_{yx}-\delta_{yx})\tilde{p}(x))A_j(y)+\sum_{k=1}^{n}\alpha_k\sum_{x,y}[-\tfrac{1}{2}A_i(x)((R_{xy}&\\ -\delta_{xy})\tilde{p}(y)A_k(y)+(R_{yx}-\delta_{yx})\tilde{p}(x)A_k(x))A_j(y)+\tfrac{1}{2}A_i(x)(A_j(x)R_{xy}\tilde{p}(y)A_k(y)&\\ -A_j(y)R_{yx}\tilde{p}(x)A_k(x))+\tfrac{1}{2}A_j(x)(A_i(x)R_{xy}\tilde{p}(y)A_k(y)-A_i(y)R_{yx}\tilde{p}(x)A_k(x))]+O(\alpha^2).&\end{aligned}$$

3. Choice of A_i as eigenvectors

We now choose the A_i to be left eigenvectors of R,

$$\sum A_i(x)R_{xy}=\lambda_iA_i(y).$$

Then, modulo $O(\alpha^2)$,

$$\langle A_i(\Delta t)-A_i(0)\rangle_{p_\alpha}=(\lambda_i-1)\sum_k\alpha_k\langle A_iA_k\rangle_{\tilde{p}}=(\lambda_i-1)\langle A_i(0)\rangle_{p_\alpha},$$

and modulo $O(\alpha A^3)$ terms,

$$\langle (A_i(\Delta t)-A_i(0))(A_j(\Delta t)-A_j(0))\rangle_{p_\alpha}=-\langle A_iA_j\rangle_{\tilde{p}}(\lambda_i+\lambda_j-2).$$

We can eliminate the eigenvalues $\lambda_i - 1$ and obtain modulo $O(\alpha A^3)$ terms,

$$\langle (A_i(\Delta t) - A_i(0))(A_j(\Delta t) - A_j(0)) \rangle_{p_\alpha}$$
$$= -\langle A_i A_j \rangle_{\tilde{p}} \left(\frac{\langle A_i(\Delta t) - A_i(0) \rangle_{p_\alpha}}{\langle A_i(0) \rangle_{p_\alpha}} + \frac{\langle A_j(\Delta t) - A_j(0) \rangle_{p_\alpha}}{\langle A_j(0) \rangle_{p_\alpha}} \right),$$

which is the fluctuation-dissipation statement in our general context.

Remark: If $(R, \tilde{p})$ satisfies detailed balance, $\tilde{p}$ vanishes nowhere and A is a left eigenvector of R with eigenvalue λ, then $\tilde{p}(x)A(x)$ is a right eigenvector of R with eigenvalue λ. When applied to the above equations and use is made of the orthogonality of the left and right eigenvectors of R, this implies a diagonal susceptibility matrix. In effect this says that choosing left eigenvectors of R as the slow variables chooses the macroscopic variables to be in a form diagonalizing the susceptibility.

G. Onsager reciprocity relations for nonequilibrium states

We consider a stationary state $\tilde{p}$ for a stochastic matrix R, and we consider the observables $A_1, \ldots, A_n$ with

$$\langle A_i \rangle_{\tilde{p}} = 0.$$

As usual, we define $p_\alpha = \tilde{p} \exp(\Sigma \alpha_i A_i + \cdots)$, and it follows that

$$\langle A_i \rangle_{\tilde{p}} = \sum_j \langle A_i A_j \rangle_{\tilde{p}} \alpha_j \tag{4.28}$$

(up to powers of α^2). We have seen that the relative entropy is

$$S(p_\alpha | \tilde{p}) = -\sum_{k,l} \langle A_k A_l \rangle_p^{-1} \langle A_k \rangle_{p_\alpha} \langle A_l \rangle_{p_\alpha}, \tag{4.29}$$

so that the corresponding forces F_k are given by

$$F_k \equiv -\frac{\partial S(p_\alpha | \tilde{p})}{\partial \langle A_k \rangle_{p_\alpha}} = \sum_l \langle A_k A_l \rangle_p^{-1} \langle A_l \rangle_{p_\alpha} = \alpha_k. \tag{4.30}$$

Moreover, the current (in one time step Δt) for A_k is given by

$$J_k \equiv \langle A_k(\Delta t) - A_k(0) \rangle_{p_\alpha} = \sum_j \alpha_j \sum_{xy} A_k(x)(R_{xy} - \delta_{xy}) \tilde{p}(y) A_j(y). \tag{4.31}$$

We can then write

$$J_k = \sum_j L_{kj} \alpha_j = \sum_j L_{kj} F_j, \tag{4.32}$$

where

$$L_{kj} = \sum_{xy} A_k(x)(R_{xy} - \delta_{xy}) \tilde{p}(y) A_j(y). \tag{4.33}$$

In general, the matrix L_{kj} is not symmetric. However, when $(R,\tilde{p})$ satisfies detailed balance, $R_{xy}\tilde{p}(y)=R_{yx}\tilde{p}(x)$, one can immediately see that $L_{kj}=L_{jk}$. Thus, an *absence* of detailed balance in R is manifested at the macroscopic level.

V. A PATH SUMMATION FORMULA FOR THE STATIONARY STATE

A. Expression of the stationary state in term of determinants

We consider a general $N\times N$ matrix A. Let us suppose that λ_0 is a nondegenerate eigenvalue of A and consider the right eigenvector u and the left eigenvector v of A of eigenvalue λ_0, so that

$$Au=\lambda_0 u, \quad vA=\lambda_0 v.$$

We normalize u,v so that

$$\sum_{i=1}^{N} u_i v_i=1. \tag{5.1}$$

Moreover, call $M(\lambda)_{ij}$ the minor of the element (i,j) in the matrix $\lambda I-A$ and $C(\lambda)$ the characteristic polynomial of A. Then one has the following identity:

$$u_i v_j=\frac{(-1)^{i+j}M_{ji}(\lambda_0)}{dC(\lambda_0)/d\lambda}. \tag{5.2}$$

This identity is derived in Appendix A, but can also be found in Ref. 26.

We apply this formula to a stochastic matrix R and to its eigenvalue 1, which we assume nondegenerate. The right eigenvector is the stationary state $\tilde{p}_j$ and the left eigenvector is $v_i=1$ for all i. The normalization condition of Eq. (5.1) is the normalization of the stationary state. Then Eq. (5.2) reduces to

$$\tilde{p}_i=\frac{(-1)^{i+j}M_{ji}(1)}{dC(1)/d\lambda}. \tag{5.3}$$

In particular, it is convenient to set $i=j$ and arrive at

$$\tilde{p}_i=\frac{M_{ii}(1)}{dC(1)/d\lambda}.$$

Using the normalization condition, we deduce the following identity:

$$\frac{dC(1)}{d\lambda}=\sum_{i=1}^{N} M_{ii}(1) \tag{5.4}$$

(this is a kind of partition function formula) and

$$\tilde{p}_i=\frac{M_{ii}(1)}{\Sigma_{j=1}^{N}M_{jj}(1)}. \tag{5.5}$$

B. Tree summation formula for the stationary state

We shall now state and derive a "tree integral" formula for the stationary state from Eq. (5.5). This result has been independently discovered on several occasions (including by us); we will

include our derivation, since the result is not known in the physics literature and is of interest for our statistical mechanics application. See Refs. 27–29, which may also be consulted for some of our tree-theory terminology.

We consider a stochastic matrix R of size N. Consider also the set of states $\{1,\ldots,N\}$ and among these points, we mark one point, say j_0, which we call the root. We can define a spanning tree of root j_0 as an oriented tree of root j_0 (the orientation going from the leaves to the root), such that any state $1 \leqslant k \leqslant N$ is a vertex of the tree.

We call T_j such a tree. Now, any edge (k,l) of T_j such that (k,l) is oriented from k to l is labeled by R_{lk}. The weight of the tree T_j is defined by

$$W(T_j)=\prod_{(k,l)\in T_j} R_{lk}. \tag{5.6}$$

We have the following result:
The minor M_{ij} of $-1+R_{jj}$ in $-I+R$ (for an $N\times N$ stochastic matrix R) is given by

$$M_{jj}=(-1)^{N-1}\sum_{T_j} W(T_j), \tag{5.7}$$

where the sum is taken over all spanning trees T_j with root j, as defined above. We shall prove this result in Sec. V D, but we can immediately make a number of comments: (i) Apart from the overall $(-1)^{N-1}$, M_{jj} is given by a sum of positive terms. (ii) M_{jj} is homogeneous of degree $N-1$ with respect to the $\{R_{kl}\}$ (for $k\neq l$). (iii) In a given term, $W(T_j)$, for a fixed T_j, a given R_{kl} does not appear twice. Moreover, one cannot have within a particular $W(T_j)$ a product of the type $R_{ik}R_{lk}$, but one can have terms like $R_{ki}R_{kl}$. Finally, one cannot have closed loops like $R_{i_1i_2}R_{i_2i_1}$.

The proofs of these statements are a direct consequence of the definition of a tree and of the weight W associated with it.

(i) Is obvious.

(ii) Is a consequence of the fact that a spanning tree for a set of N points has $N-1$ edges.

(iii) It is obvious that a given R_{kl} appears at most once in a $W(T_j)$. Moreover, since $W(T_j)$ is constructed by taking the product of the R_{lk}, starting from the leaves and following the edges up to the root j, it is clear that one cannot have a term $R_{ik}R_{lk}$ (this would mean that the vertex k has two fathers in the tree), but one can have $R_{ni}R_{nl}$ (when i and l are sons of the same father n).

Finally, we see that Eq. (5.5) has a natural meaning when we use the calculation of M_{jj} given in Eq. (5.7). The stationary probability of the state j is obtained by summing over all oriented paths leading from various points of the state space to the point j, quantities that are, for each path, the product of the elements R_{nl} that one encounters along the oriented path. Moreover, these paths may have several irreducible components leading to j, and they contain no loop. This is why such an oriented reducible path leading to j, is, in fact, a tree with root j.

C. The case of detailed balance

Detailed balance means that for all i,j,

$$\frac{R_{ij}}{R_{ji}}=\frac{\tilde{p}_i}{\tilde{p}_j}. \tag{5.8}$$

In particular, this implies that for any closed cycle $c=(x_1,x_2,x_3,\ldots,x_k,x_1)$ we have

$$\frac{R_{x_1x_k}R_{x_kx_{k-1}}\cdots R_{x_2x_1}}{R_{x_1x_2}R_{x_2x_3}\cdots R_{x_kx_1}}=1, \tag{5.9}$$

or with obvious notation,

$$\frac{\Pi_C R}{\Pi_{C^{-1}}R}=1,$$

where C^{-1} denotes the reverse cycle. On the other hand, we have proved above

$$\frac{\tilde{p}_i}{\tilde{p}_j}=\frac{M_{ii}}{M_{jj}},$$

in the general case.

Let us now assume that Eq. (5.9) holds for any closed cycle and prove that detailed balance holds. To fix everything, take $i=1$, $j=2$ and consider a tree of the type T_1. In this tree, there is a certain (unique) oriented path $\gamma(T_1)$ leading from 2 to 1, and this path has a certain length, $|\gamma(T_1)|$. Then

$$W(T_1)=\left[\prod_{\gamma(T_1)} R\right]W(T_1|\gamma(T_1)),$$

where $W(T_1|\gamma(T_1))$ is the product of all the elements of R along the edges of T_1 that are not on $\gamma(T_1)$.

Now, the edges of T_1 that are not on $\gamma(T_1)$ form a collection of $N-1-|\gamma(T_1)|$ edges [because $W(T_1)$ has $N-1$ edges, as we have seen]. These edges form a disjoint union of oriented trees with roots on the path $\gamma(T_1)$ and with their other vertices outside $\gamma(T_1)$ (this union of disjoint trees is a "forest").

Conversely, given a directed path γ leading from 2 to 1, and a forest F of trees having their roots in γ and their other vertices outside γ and with a total number of edges $N-1-|\gamma|$, the union of γ and F is a spanning oriented tree with root 1. This means that one can write

$$M_{11}=\sum_{\gamma \text{ from 2 to 1}}\left(\prod_{\gamma} R\right)\Phi(\gamma), \tag{5.10}$$

where $\Phi(\gamma)$ is defined to be

$$\Phi(\gamma)=\sum_{F} W(F), \tag{5.11}$$

where the sum is taken over all the oriented forests F having $N-1-|\gamma|$ edges, their roots on γ, and their other vertices outside γ, and $W(F)$ is the product of the R on all edges of F. In the same way,

$$M_{22}=\sum_{\gamma' \text{ leading from 1 to 2}}\left(\prod_{\gamma'} R\right)\Phi(\gamma'). \tag{5.12}$$

Now, for any path from 2 to 1, γ, one can find the inverse path γ^{-1} from 1 to 2 so that Eq. (5.12) can be rewritten,

$$M_{22}=\sum_{\gamma \text{ leading from 2 to 1}}\left(\prod_{\gamma^{-1}} R\right)\Phi(\gamma^{-1}).$$

But it is clear that

$$\Phi(\gamma)=\Phi(\gamma^{-1}),$$

and moreover, because of Eq. (5.9),

$$\frac{\Pi_\gamma R}{\Pi_{\gamma^{-1}} R}=\frac{R_{12}}{R_{21}},$$

so that

$$M_{11}=M_{22}\frac{R_{12}}{R_{21}},$$

from which we deduce Eq. (5.8).

D. Proof of Eq. (5.7)

We shall prove something slightly more general. In the following, Latin indices run from 1 to N and Greek indices run from $\underline{1}$ to $\underline{p}$. We consider $b_{\alpha i}$ and a_{ij} $(i\neq j)$ to be positive numbers. (For emphasis, numerical values taken by Greek indices are underlined. We make this distinction because at a later stage we will need to deal with switches between one sort of index and the other.)

We define the following determinant:

$$D_N(b,a)=\det\begin{vmatrix} -\sum_{\alpha=1}^{p} b_{\alpha 1}-\sum_{i=2}^{N} a_{i1} & a_{12} & \cdots & a_{1N} \\ a_{21} & -\sum_{\alpha=1}^{p} b_{\alpha 2}-\sum_{\substack{i=1\\ i\neq 2}}^{N} a_{i2} & \cdots & a_{2N} \\ \vdots & & \vdots & \vdots \\ \vdots & & \vdots & \vdots \\ a_{N1} & a_{N2} & \cdots & -\sum_{\alpha=1}^{p} b_{\alpha N}-\sum_{i\neq N} a_{iN} \end{vmatrix}.$$

It is obvious that if all bs are zero, this determinant is zero because the sum of all lines is zero.

Moreover, $D_N(b,a)$ is a homogeneous function of degree N of the bs and the as. We now consider the set $\{\underline{1},...,\underline{p}\}\cup\{1,...,N\}$, and for each α we consider an oriented tree T_α with root α and with other vertices in $\{1,...,N\}$. To any oriented edge (k,l) or (n,α) of T_α, we associate the label a_{lk} or $b_{\alpha n}$. We define

$$W(T_\alpha)=\left(\prod_{(k,l)\in T_\alpha} a_{lk}\right)\left(\prod_{(n,\alpha)\in T_\alpha} b_{\alpha n}\right). \tag{5.14}$$

We call a spanning forest a union of disjoint trees $\{T_\alpha\}$ for $\alpha=\underline{1},...,\underline{p}$ as before, such that all other vertices $1\leq i\leq N$ belong to a tree T_α of the forest (and then to a unique one),

$$W(F)=\prod_{F=\{T_\alpha\}} W(T_\alpha), \tag{5.15}$$

with the convention that, if T_α contains no edge, $W(T_\alpha)=1$. In particular, a spanning forest has N edges.

The main result of this section is that

$$D_N(b,a)=(-1)^N\sum_F W(F), \tag{5.16}$$

where the sum is taken on all spanning forests, as defined before. The proof of this statement is by induction on N.

First, for $N=2$ we have

$$D_2(b,a)=\det\begin{vmatrix} -\sum_{\alpha=\underline{1}}^{p} b_{\alpha 1}-a_{21} & a_{12} \\ a_{21} & -\sum_{\alpha=\underline{1}}^{p} b_{\alpha 2}-a_{12} \end{vmatrix} = \sum_{\alpha,\beta=\underline{1}}^{p} b_{\alpha 1}b_{\beta 2}+\sum_{\alpha=\underline{1}}^{p} b_{a1}a_{12}+\sum_{\alpha=\underline{1}}^{p} b_{\alpha 2}a_{21},$$

which obviously has the structure of Eq. (5.16).

We now assume that the statement is true for all determinants of size less than N, and we consider D_N as defined by Eq. (5.13). It is clear that D_N is symmetric by permutation of the Latin indices. As we have seen, it is a polynomial in the $b_{\alpha j}$ of degree $\leqslant N$ without a constant term [because $D_N(0,a)=0$]. Moreover, it is clear that in a given monomial, one cannot have products $b_{\alpha j}b_{\beta j}$, $a_{ik}a_{jk}$, because they correspond to terms in the same column of $D_N(b,a)$.

By symmetry, we can consider only the terms containing $b_{\underline{1}1}$ as a factor. Such a term is obviously

$$-b_{\underline{1}1}\det\begin{vmatrix} -\sum_{\alpha=\underline{1}}^{p} b_{\alpha 2}-\sum_{\substack{i=1\\ i\neq 2}}^{N} a_{i2} & a_{23} & \cdots & a_{2N} \\ a_{32} & -\sum_{\alpha=\underline{1}}^{p} b_{\alpha 3}-\sum_{\substack{i=1\\ i\neq 3}}^{N} a_{i3} & \cdots & a_{3N} \\ \vdots & & \vdots & \vdots \\ \vdots & & \vdots & \vdots \\ a_{N2} & a_{N3} & \cdots & -\sum_{\alpha=\underline{1}}^{p} b_{\alpha N}-\sum_{i\neq N} a_{iN} \end{vmatrix}.$$

But the determinant multiplying $-b_{\underline{1}1}$ is a determinant of the type $D_{N-1}(b',a')$, where now the new greek indices vary in the new set:

$$\{\underline{1},\ldots,\underline{p},\underline{p+1}\}\equiv\{\underline{1},\ldots,\underline{p},1\}$$

(i.e., $\underline{p+1}$ is the old latin index 1), and the set $\{1,\ldots,N\}$ has been replaced by $\{2,\ldots,N\}$ and with the identifications

$$b'_{\alpha i}=b_{\alpha i},\quad \underline{1}\leqslant\alpha\leqslant\underline{p},\quad 2\leqslant i\leqslant N,$$

$$b'_{\underline{p+1},i}=a_{1,i},\quad 2\leqslant i\leqslant N,$$

$$a'_{ij}=a_{ij},\quad 2\leqslant i\neq j\leqslant N.$$

But now, $D_{N-1}(b',a')$ is a sum over all spanning forests F' (with $N-1$ edges) of the weight of these forests. Each forest F' is a union of trees $\{T'_\alpha\}$ with roots in $\{\underline{1},...,\underline{p},1\}$ and with other vertices in $\{2,...,N\}$ and

$$W(F')=\left[\prod_{\alpha=\underline{1}}^{\underline{p}} W(T'_\alpha)\right]W(T'_1).$$

It may happen that some trees have no edge. Then we rewrite

$$b_{\underline{1}1}W(F')=(b_{\underline{1}1}W(T'_1)W(T'_{\underline{1}}))\prod_{\alpha=\underline{2}}^{\underline{p}} W(T'_\alpha).$$

But this is exactly

$$b_{\underline{1}1}W(F')=\prod_{\alpha=\underline{1}}^{\underline{p}} W(T_\alpha),$$

with

$$\begin{aligned} T_\alpha &= T'_\alpha, \quad \text{for } \alpha=\underline{2},...,\underline{p}, \\ T_{\underline{1}} &= T'_{\underline{1}}\cup((1\underline{1})\cup T'_1), \end{aligned} \tag{5.17}$$

where $((\underline{1}1)\cup T_1)$ denotes a tree having as the root the point $\underline{1}$ and obtained by taking the edge $(1\underline{1})$ from 1 to $\underline{1}$ and attaching to it the tree T'_1 of root 1 (if it has some edge). Then

$$b_{\underline{1}1}W(F')=W(F),$$

where

$$F=\{T_{\underline{1}},T_{\underline{2}},...,T_{\underline{p}}\}.$$

Conversely, any spanning forest F that contains the oriented edge, $(1\underline{1})$, is obviously a union of disjoint trees $T_{\underline{1}},...,T_{\underline{p}}$ with $T_{\underline{1}}$ given as in Eq. (5.17), namely

$$T_{\underline{1}}=T'_{\underline{1}}\cup((1\underline{1})\cup T'_1),$$

with $T'_{\underline{1}}$ having its root in $\underline{1}$ and vertices in $\{2,...,N\}$ and T'_1 having its root in 1 and its vertices in $\{2,...,N\}$.

Thus, in $D_N(b,a)$ the terms containing $b_{\underline{1}1}$ are of the type $(-1)^N\Sigma_{1\underline{1}\in F}W(F)$. This proves Eq. (5.16).

Proof of Eq. (5.7) for M_{jj}: Eq. (5.7) is a particular case of Eq. (5.16). In this case, $p=1=j$, the $N-2$ indices $l\neq j$ correspond to the Latin indices, and the Greek index α can take only the value j. Finally $b_{\alpha l}=a_{jl}$ and for $l,k\neq j$, $a_{lk}=R_{lk}$.

In this case a spanning forest for $\{\underline{1}\}\cup\{1,...,N-2\}$ having its root at j and other indices at points $k\neq j$ is exactly a spanning tree with root at j.

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APPENDIX: MATRIX FORMULAS

In this appendix, we derive the formulas of Sec. V A. We consider a matrix A and an eigenvalue λ_j of A. Call $\lambda_1,...,\lambda_p$ the other distinct eigenvalues. Then the matrix A can be decomposed in the Jordan normal form and we call E_{λ_j} the subspace associated with the eigenvalue λ_j in this decomposition. We call P_{λ_j} the projector on E_{λ_j} defined by

$$P_{\lambda_j}|_{E_{\lambda_j}}=I,$$
$$P_{\lambda_j}|_{E_{\lambda_l}}=0, \quad j\neq l. \tag{A1}$$

Take a contour γ_j in the complex plane surrounding λ_j once, but no λ_l for $l\neq j$. Then

$$P_{\lambda_j}=\frac{1}{2i\pi}\int_{\gamma_j}(z-A)^{-1}\,dz. \tag{A2}$$

Formula (A2) is obvious: take a vector u in the space E_{λ_l} for $l\neq j$. Then $(z-A)^{-1}u$ is holomorphic in a neighborhood of λ_j and

$$\int_{\gamma_j}(z-A)^{-1}u\,dz=0.$$

Now, if u is in the space E_{λ_j}, we can write on E_{λ_j},

$$A|_{E_{\lambda_j}}=(\text{diag}\,\lambda_j)+T,$$

where T is an upper triangular matrix. Then

$$(z-A)^{-1}|_{E_{\lambda_j}}=\text{diag}(z-\lambda_j)^{-1}+T',$$

where T' is another upper triangular matrix (depending holomorphically on z in a neighborhood of λ_j). Then

$$\frac{1}{2i\pi}\int_{\gamma_j}(z-A)^{-1}u\,dz=u,$$

so that the Cauchy integral on the right-hand side of (A2) is given exactly by (A1). In particular, since $(z-A)^{-1}_{nl}=(-1)^{n+l}[M_{ln}(z)/C(z)]$, we have, from (A2),

$$(P_{\lambda_j})_{nl}=(-1)^{n+l}\,\text{Residue}_{\lambda_j}\left(\frac{M_{ln}(z)}{C(z)}\right).$$

If λ_j is a simple eigenvalue, then E_{λ_j} is generated by the right eigenvector u and the projector is simply given by

$$(P_{\lambda_j})_{nl}=u_n^* v_l,$$

with the normalization condition of Eq. (5.1).

In the case of a stochastic matrix R, if we take, say M_{11}, it is easy to see that $M_{11}=(-1)^{l+1}M_{l1}$ directly (write down M_{11} explicitly, then replace row number l by the sum of all rows of M_{11} and use the stochastic property $\Sigma_{l=1}^{N}R_{ln}=1$). In general,

$$M_{nn}=(-1)^{n+l}M_{ln}.$$

But because $\det(I-R)=0$, we have

$$\sum_{j=1}^{N}(\delta_{lj}-R_{lj})(-1)^{j}M_{lj}=0, \quad l=1,\ldots,N,$$

which implies that the vector with components M_{jj} is an eigenvector of eigenvalue 1 of R.

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Scattering matrix in external field problems

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We discuss several aspects of second quantized scattering operators $\hat{S}$ for fermions in external time-dependent fields. We derive our results on a general, abstract level having in mind as a main application potentials of the Yang-Mills type and in various dimensions. We present a new and powerful method for proving the existence of $\hat{S}$ which is also applicable to other situations like external gravitational fields. We also give two complementary derivations of the change of phase of the scattering matrix under generalized gauge transformations which can be used whenever our method of proving the existence of $\hat{S}$ applies. The first is based on a causality argument, i.e., $\hat{S}$ (including phase) is determined from a time evolution, and the second exploits the geometry of certain infinite-dimensional group extensions associated with the second quantization of one-particle operators. As a special case we obtain a Hamiltonian derivation of the axial fermion-Yang-Mills anomaly and the Schwinger terms related to it via the descent equations, which is on the same footing and traces them back to a common root. © *1996 American Institute of Physics.* [S0022-2488(96)03107-6]

I. INTRODUCTION

The main difficulty when quantizing fermions in higher than two space-time dimensions in background (gauge) fields is that the interaction term generically is too large to allow a naive application of the standard methods of canonical quantization. More precisely, if ϵ is the sign of the "free" Hamiltonian, then only those one-particle operators A are well-defined in the free Fock space which satisfy the condition that $[\epsilon, A]$ is of Hilbert-Schmidt type. For example, the minimal gauge interaction operator does not satisfy this condition when the space-time dimension is higher than 2. The same holds for gauge transformation operators which makes the implementation of these operators somewhat tricky.[1]

The one-particle time evolution operator can be constructed for example by the Dyson expansion provided that the potential is smooth and appropriate boundary conditions are satisfied. However, the time evolution cannot be quantized because of the remarks above. The asymptotic scattering operator S is better behaving. One can show that it satisfies the Hilbert-Schmidt condition. The existing proofs are rather involved.[2,3] In this article we give a conceptually simpler proof using the methods introduced earlier for the construction of the quantum gauge transformations and computation of commutator anomalies.[1] The method is based on the observation that the interaction Hamiltonians can be conjugated by unitary operators such that the resulting equivalent Hamiltonians satisfy the Hilbert-Schmidt condition with respect to fixed free Hamiltonian. Moreover, we give an effective method for an actual construction of such unitary conjugations, as a function of (time-dependent) background fields. This method is very general and does not use the specific properties of gauge interactions. In general, it applies to any bounded interactions such that its commutator with the absolute value of the free Hamiltonian does not have worse fall-off properties in the momentum space than the original operator. Gravitational background fields can be also treated using a somewhat modified form of the conjugation (Appendix A).

In sections III and IV we discuss the determination of the phase of the quantum scattering operator. It is shown that the phase is uniquely determined by causality (section III), or, alternatively, by the geometric structure of the central extension of the group of one-particle (renormalized) time evolution operators (section IV). Our treatment relies heavily on the theory of infinite-

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dimensional linear groups. Some of the basic aspects of the theory of these groups in quantum field theory are recalled on the way; for further reading we recommend Refs. 4 and 5.

II. EXISTENCE OF QUANTUM SCATTERING OPERATORS

Consider a family of Hamiltonians of the form $H_A(t)=D_0+A(t)$ acting in a one-particle Hilbert space H where $t\mapsto A(t)$ is smooth and compactly supported ($t,t'\in\mathbb{R}$ here and in the following). We assume that D_0 is a self-adjoint operator and the $A(t)$ are bounded self-adjoint operators [so that the $D_0+A(t)$ are all self-adjoint for all t (Ref. 6)]. We study the time evolution equation

$$i\partial_t U_A(t,t')=H_A(t)U_A(t,t'),\quad U_A(t,t)=1. \tag{2.1}$$

Writing $V_A(t,t') = e^{itD_0}U_A(t,t')e^{-it'D_0}$ we obtain an equivalent equation

$$i\partial_t V_A(t,t')=h_A(t)V_A(t,t'),\quad V_A(t,t)=1 \tag{2.2}$$

where $h_A(t) = e^{itD_0}A(t)e^{-itD_0}$. Since $h_A(t)$ is bounded, this equation has a solution for all finite times given by the Dyson expansion

$$V_A(t,t')=\sum_{n=0}^{\infty} V_n(t,t'),\quad V_0(t,t')=1,\quad V_{n+1}(t,t')=-i\int_{t'}^{t} ds h_A(s)V_n(s,t') \tag{2.3}$$

[it is easy to see that this series converges absolutely in the operator norm $\|\cdot\|$ if one assumes $\int_{\mathbb{R}}dt\|A(t)\|<\infty$; see Appendix B 1].

Let $\epsilon=D_0/|D_0|$. (This is well-defined even if zero is in the spectrum of D_0 if we set $x/|x|=1$ and -1 for $x\geq 0$ and $x<0$, respectively, and use the spectral theorem of self-adjoint operators.[6])

The spectral decomposition $H=H_+\oplus H_-$ corresponding to the splitting of the spectrum of D_0 to positive and negative parts fixes an irreducible representation of the canonical anticommutation relations (CAR), uniquely defined up to unitary equivalence, in a Fock space $\mathcal{F}$ with a vacuum $|0\rangle$ which is annihilated by the elements $a^*(v_-)$ and $a(v_+)$, $v_\pm\in H_\pm$, of the CAR algebra

$$a^*(v)a(v')+a(v')a^*(v)=(v,v'), \tag{2.4}$$

and all the other anticommutators are equal to zero. Let $\{e_n\}_{n\in\mathbb{Z}}$ be an orthonormal basis in H such that $\{e_n\}_{n\geq 0}$ span H_+ and $\{e_n\}_{n<0}$ span H_-. Set $a_n=a(e_n)$ and $a_n^*=a^*(e_n)$. Fix the usual normal ordering for the products of creation and annihilation operators by: $a_n^*a_n:=-a_ma_n^*$ if $n=m<0$ and all the other products remain unchanged.

It is known that a bounded one-particle operator $X=(X_{nm})$ can be canonically quantized as

$$d\Gamma(X)=\sum X_{nm}:a_n^*a_m: \tag{2.5}$$

iff $[\epsilon,X]$ is of Hilbert-Schmidt type.[7,4] This quantization is such that $[d\Gamma(X),a^*(v)]=a^*(Xv)$ for all $v\in H$, and preserves the commutation relations of the Lie algebra of linear operators on H except for a complex valued cocycle ("Schwinger term"); see section III. Similarly, a unitary operator U on H can be second quantized to an operator $\Gamma(U)$ obeying $\Gamma(U)a^*(v)\Gamma(U)^{-1}=a^*(Uv)$ if and only if $[\epsilon,U]$ is of Hilbert-Schmidt type.[8,9]

If we have a time evolution with Hilbert-Schmidt $[\epsilon,A(t)]$ for all t, then it is easy to see that $[\epsilon,V_A(t,t')]$ is always of Hilbert-Schmidt type (if one assumes $\int_{\mathbb{R}}dt\|[\epsilon,A(t)]\|_2<\infty$ where $\|\cdot\|_2$ is the Hilbert-Schmidt norm; see Appendix B 1), and this trivially implies that the scattering operator

$$S_A = \lim_{t_f \to \infty} \lim_{t_i \to -\infty} V_A(t_f, t_i) \tag{2.6}$$

can be second quantized [note that due to our compactness assumption, $S_A = V_A(T, -T)$ for some $T < \infty$].

In many interesting situations $[\epsilon, A(t)]$ is not of Hilbert-Schmidt type, and $[\epsilon, V_A(t,t')]$ is not of Hilbert-Schmidt type either, and the canonical quantum operator $\Gamma(V_A(t,t'))$ does therefore not exist. Nevertheless the scattering operator can be still second quantized in many such cases. We will give proof below of a general, abstract result for this. As a motivation for our abstract setting, we first discuss a special case. We shall use some basic facts about pseudodifferential operators (PSDO):[10] see Appendix C for notation.

We assume that space-time is $M^n \times \mathbb{R}$ where M^n is a n-dimensional compact manifold with spin structure and $H = L^2(M^n) \oplus V$ where V is a vector space carrying the spin and color indices of the fermions. The following discussion applies also to noncompact situations like $M = \mathbb{R}^n$ but then one has to assume suitable fall-off properties of the interaction as $x \to \infty$. For example, in the case of a gauge interaction the requirement that the vector potential and all its derivatives fall off faster than $|x|^{-n/2}$ as $|x| \to \infty$ would be sufficient. Moreover, we assume that the free hamiltonian D_0 is a self-adjoint PSDO of order $\geqslant 1$.

We denote as B_2 the ideal of Hilbert-Schmidt operators in the algebra of bounded operators on H. In case D_0 has no mass gap in the spectrum around zero we interpret D_0^{-1} as $D_0(D_0^2 + \lambda)^{-1}$ for some $\lambda > 0$, and similarly for $|D_0|^{-1}$. We use this simplified notation since the precise value of λ is irrelevant (the essential regularizations concern the ultraviolet and λ is a harmless infrared regulator—if not evident to the reader, this will become clear in the following). Thus D_0^{-1} is always a bounded self-adjoint operator (its operator norm is $\leqslant 1/\sqrt{\lambda}$).

Denote as O_{-k} the PSDO's of order $\leqslant -k$ on a compact manifold M or in $\mathbb{R}^n$ with the asymptotic conditions discussed above, especially O_0 are bounded PSDO's. We assume that D_0 is a Dirac operator. We state the basic properties of these bounded PSDO's which we shall need in the proof of the main theorem (see Appendix C):

$$\begin{aligned} &\text{(i)} \quad O_0 \text{ is an algebra of bounded operators} \\ &\text{(ii)} \quad a \in O_0 \Rightarrow [|D_0|, a] \in O_0 \\ &\text{(iii)} \quad \exists p < \infty\colon \ |D_0|^{-p} a \in B_2 \quad \forall a \in O_0 . \end{aligned} \tag{2.7}$$

Since this is all we need in our proof, our result below applies to the set of all bounded operators $O_0^{(p)}$ with the properties (2.7): we regard $O_0^{(p)}$ as the abstract generalization of the PSDO's O_0. It can be defined as follows: $O_0^{(p)}$ is the algebra of all bounded operators a such that $a_{(n)} \equiv [|D_0|, a_{(n-1)}]$ $(a_{(0)} = a)$ is bounded and $|D_0|^{-p} a_{(n)}$ is of Hilbert-Schmidt type for all $n = 1, 2, \ldots$.

We shall show that S_A can be quantized whenever $A \in O_0^{(p)}$. The idea is to construct a time-dependent family of operators $T(A) = T_t(A)$ for a regularization on the one particle level,[1] i.e., consider the modified time evolution $T_t(A) U_A(t,t') T_{t'}(A)^{-1}$ which can be second quantized even if $U_A(t,t')$ cannot. It is easy to see that the latter is generated by the Hamiltonian $H'_A(t) = T_t(A) H_A(t) T_t(A)^{-1} - i[\partial_t T_t(A)] T_t(A)^{-1} = D_0 + A'(t)$ where

$$A'(t) = i[\partial_t T_t(A)] T_t(A)^{-1} - [D_0, T_t(A)] T_t(A)^{-1} + T_t(A) A(t) T_t(A)^{-1}. \tag{2.8}$$

Our strategy thus is to choose $T(A)$ in such a way that A' is better behaved than the original interaction A, i.e., that $[\epsilon, A'] \in B_2$. It is important to note that a conjugation $T_t(A)$, which becomes the identity as $|t| \to \infty$, does not alter the scattering matrix, $S_{A'} = S_A$.

All differentiations of operators etc., in the following are meant with respect to the operator norm.

Definition 2.9: Let D_0 be a self-adjoint operator and $O_0^{(p)}$ as above. We call an interaction A regular (*with respect* to D_0) if $A(t)$ and the derivatives $(\partial_t)^k A(t)$, $k=1,\ldots,p$, are in $O_0^{(p)}$ for all $t\in\mathbb{R}$ and some $p<\infty$. We denote the set of all such interactions (for fixed p) as $\mathscr{A}_p$.

Theorem 2.10: For all $p<\infty$ and interactions $A(t)\in\mathscr{A}_p$, there is a family of unitary operators $T_t(A)$ differentiable in t and such that the transformed time evolution $V_{A'}(t,t')$, A' Eq. (2.8), can be second quantized, $[\epsilon,V_{A'}(t,t')]\in B_2$ for all $t,t'\in\mathbb{R}$. Moreover $T(A)$ can be chosen local in time, i.e., $T_t(A)=1$ if $A(t)=0$ and $(\partial_t)^k A(t)=0$ for $k=1,\ldots,p$.

Corollary 2.11: For all regular interactions $A(t)$ compactly supported in t, the scattering operator S_A exists and can be second quantized, $[\epsilon,S_A]\in B_2$.

Proof of theorem: In this proof we write O_0 short for $O_0^{(p)}$, and we define

$$O_{-k}=\{a\in O_0\,|\,|D_0|^k a\in O_0\}.$$

Note that if $a\in O_{-k}$ then $|D_0|^{k'-l}a|D_0|^l\in O_0$ for all integers l and $k'=0,1,\ldots,k$. Below we consider maps $A:\mathbb{R}\to O_0$, $t\mapsto A(t)$ such that $[\epsilon,A]$ maps $\mathbb{R}$ to O_{-k}. We say that such a map is C^r if it is times differentiable with all derivatives $\partial_t^l A$ and $\partial_t^l[\epsilon,A]$ continuous maps $\mathbb{R}\to O_0$ and $\mathbb{R}\to O_{-k}$, respectively for $l=1,2,\ldots,r$.

We first prove the following key lemma providing the recipe for constructing $T(A)$.

Lemma 2.12: Let $A:\mathbb{R}\to O_0$ such that $[\epsilon,A]:\mathbb{R}\to O_{-k}$ be C^r with $r\geq 1$. Then $A'(t)$, defined by (2.8), with the unitary operator

$$T_t(A)=e^{\alpha(t)},\quad \alpha(t)=-\frac{1}{8}\left(|D_0|^{-1}[\epsilon,A(t)]+[\epsilon,A(t)]|D_0|^{-1}\right), \tag{2.13}$$

defines a map $A':\mathbb{R}\to O_0$ such that $[\epsilon,A']$ maps $\mathbb{R}$ into O_{-k-1} and is C^{r-1}.

Proof of lemma: We write $A'(t)=A_1'(t)+A_2'(t)$ where

$$A_1'=A+[D_0,\alpha]$$

are the leading terms in an expansion in powers of $|D_0|$, and

$$A_2'=-iT(A)^{-1}\partial_t(T(A)-1)+T(A)^{-1}[D_0,T(A)-\alpha-1]+T(A)^{-1}[A,T(A)-1]$$

is the rest. In the following we refer to maps $a:\mathbb{R}\to O_{-k}$ also as $a\in O_{-k}$, etc.

We first consider A_2'. We observe that

$$T(A)-1=\alpha T_1=T_1\alpha,\quad T(A)-1-\alpha=\alpha^2 T_2=T_2\alpha^2$$

where the operators $a=T(A)^{-1}$, $T_{1,2}$ and $\partial_t(T_1)$ all are bounded, and all these latter operators a are such that $ab,ba\in O_{-l}$, whenever $b\in O_{-l}$ for all $l=0,1,\ldots$. (intuitively this is quite obvious; the precise argument is somewhat technical and therefore deferred to Appendix B 2). Moreover, by assumption α and $\partial_t(\alpha)$ are in O_{-k-1}, and (2.7) and the definition of O_{-k} imply that αD_0 and $D_0\alpha$ are in O_{-k}; also for $A\in O_0$, $A\alpha$ and αA are in O_{-k-1}. We conclude that A_2' is in O_{-k-1}. By definition this implies $A_2'\in O_0$ and $[\epsilon,A_2']\in O_{-k-1}$.

$A_1'\in O_0$ follows from $\alpha\in O_{-k-1}$ as discussed above. The nontrivial part left to show is that $[\epsilon,A_1']\in O_{-k-1}$. This can be seen by the following calculation,

$$[\epsilon,A_1']=[\epsilon,A]-\frac{1}{8}[\epsilon,[D_0,|D_0|^{-1}[\epsilon,A(t)]+[\epsilon,A]|D_0|^{-1}]]$$

$$=\frac{1}{8}(8[\epsilon,A]-[\epsilon,\epsilon[\epsilon,A]-|D_0|^{-1}[\epsilon,A(t)]|D_0|\epsilon+\epsilon|D_0|[\epsilon,A(t)]|D_0|^{-1}-[\epsilon,A(T)]\epsilon])$$

$$=\frac{1}{8}(8[\epsilon,A]-4[\epsilon,A]-2|D_0|[\epsilon,A]|D_0|^{-1}-2|D_0|^{-1}[\epsilon,A]|D_0|)$$

$$=\frac{1}{4}(|D_0|^{-1}[|D_0|,[\epsilon,A]]-[|D_0|,[\epsilon,A]]|D_0|^{-1})$$

where we used $[\epsilon,A]=-\epsilon[\epsilon,A]\epsilon$ and $\epsilon D_0^{\pm 1}=D_0^{\pm 1}\epsilon=|D_0^{\pm 1}|$. Thus

$$[\epsilon,A_1']=\frac{1}{4}[|D_0|^{-1},[|D_0|,[\epsilon,A]]]$$

which is in O_{-k-1} by definition.

We gave the details of this calculation using D_0^{-1} for simplicity. If we replace D_0^{-1} by $D_0(D_0^2+\lambda)^{-1}$ a similar calculation leads to the same conclusion,

$$[\epsilon,A_1']=\frac{1}{4}[|D_0|(D_0^2+\lambda)^{-1},[|D_0|,[\epsilon,A]]]+\frac{1}{2}\lambda((D_0^2+\lambda)^{-1}[\epsilon,A]+[\epsilon,A](D_0^2+\lambda)^{-1}).$$

This proves our lemma.

We can apply this method successively: Starting from some interaction $A_0=A$ such that $[\epsilon,A]\in O_0$ we get a new interaction $A_1=A'$ using the conjugation $T(A)$, with $[\epsilon,A_1]\in O_{-1}$. We can then insert A_1 as an argument to $T(\cdot)$ and obtain a unitary operator $T(A_1)$. This defines again a new interaction $A_2=A_1'$ such that $[\epsilon,A_2]\in O_{-2}$. Continuing this way we obtain, after p steps, a unitary operator $T^{(p)}(A)=T(A_{p-1})\ldots T(A_0)$ such that the time evolution for the operator $T_t^{(p)}(A)U(t,t')T_{t'}^{(p)}(A)^{-1}$ is determined by an interaction A_p such that $[\epsilon,A_p(t)]\in O_{-p}$ for all t. For sufficiently big p the new interaction satisfies the Hilbert-Schmidt condition, and thus the corresponding scattering operator can be second quantized. Since $T_t^{(p)}(A)$ by construction is equal to the identity for times t where $A(t)$ and all its t-derivatives vanish, the latter scattering operator is equal to S_A. This implies Theorem 2.10.

Remark 1: As a particular case, our result gives the existence of the scattering operators for Dirac (or Weyl) fermions in external Yang-Mills fields, on a compact space manifold M^n or on $\mathbb{R}^n$ with sufficient fall-off properties for the vector potential as $|x|\to\infty$. Here our discussion above implies $p>n/2$, but for n odd one can show that actually $p=(n-1)/2$ is already sufficient, provided that $A(t)$ is $(n+1)/2$ differentiable in t (e.g., for $n=1$ no regularization is necessary). The latter follows from the following fact: if $A:\mathbb{R}\to O_0$ with $[\epsilon,A]:\mathbb{R}\to O_{-k}$ is C^1, then $[\epsilon,V(t,t')]\in O_{-k-1}$ for all t,t'.

To see this, consider $B(t)\equiv[\epsilon,h(t)]=[\epsilon,\epsilon^{iD_0t}A(t)\epsilon^{-iD_0t}]$ and observe that

$$\frac{d}{dt}B(t)=[\epsilon,[iD_0,h(t)]]+[\epsilon,\epsilon^{iD_0t}\dot{A}(t)\epsilon^{-iD_0t}]=2iD_0B(t)+i\epsilon[B,|D_0|]+\epsilon^{iD_0t}[\epsilon,\dot{A}(t)]\epsilon^{-iD_0t}$$

with $\dot{A}(t)=dA(t)/dt$, i.e.

$$B(t)\sim-\frac{i}{2}\frac{d}{dt}D_0^{-1}B(t)$$

where $\sim$ means "equal up to terms which obviously are in O_{-k-1}." [Note that at this point we require that $A(t)$ is C^1.] Inserting this in

$$[\epsilon, V_{n+1}(t,t')] = -i\int_{t'}^{t} ds\{B(s)V_n(s,t') + h(s)[\epsilon, V_n(s,t')]\}$$

following from Eq. (2.3), we obtain by induction (i.e., assuming $[\epsilon, V_{m\leqslant n}]\sim 0$: we use partial integration and (2.3)),

$$[\epsilon, V_{n+1}(t,t')]\sim -\frac{1}{2} D_0^{-1}B(s)V_n(s,t')\Big|_{s=t'}^{t} - i\int_{t'}^{t} ds\,\frac{1}{2} D_0^{-1}B(s)h(s)V_{n-1}(s,t')\sim 0$$

(since $B\in O_{-k}$, $V_n\in O_0$, and $D_0^{-1}a\sim 0$ for $a\in O_{-k}$).

Remark 2: We stress the Hilbert-Schmidt property of the scattering operator since only this is of primary interest for quantum field theory. However, our argument above shows that usually $[\epsilon, S_A]$ is much better behaved: e.g., in the fermion-Yang-Mills case it is in all Schatten classes B_q for $q>0$. (This follows from $O_{-k}\subset B_{(n+1)/k}$ in the case of PSDO and the possibility of choosing number p of regularization above arbitrarily large.)

Remark 3: Going through the proof above one can check that Theorem 2.10 can be slightly generalized: one can include in $O_0^{(p)}$ all bounded operators a such that $a_{(n)}$ is bounded and $|D_0|^{-p}a_{(n)}\in B_2$ for $n=1,2,\ldots,p$ (but not necessarily $n>p$).

III. PHASE OF QUANTUM SCATTERING OPERATOR: CAUSAL APPROACH

In the previous section we have shown that the one-particle scattering operator S satisfies the Hilbert-Schmidt condition for $[\epsilon, S]$ and therefore it can be promoted to a unitary operator $\hat{S}=\Gamma(S)$ in the Fock space $\mathscr{F}$. However, by this the operator $\hat{S}$ is uniquely defined only up to a phase. In this section we show that the regularization for the time evolution operators in the previous section fixes the phase in a natural causal manner.

We denote the group of unitary operators U on H with Hilbert-Schmidt $[\epsilon, U]$ as U_1. All $U\in U_1$ can be second quantized, and the second quantization $\Gamma(U)=\Gamma(U^{-1})^{-1}$ of $U\in U_1$ is unique up to a phase [=element in $U(1)$] which implies that for some local (near the unit element in U_1, e.g.) choice of of phases

$$\Gamma(U)\Gamma(V)=\chi(U,V)\Gamma(UV)\quad \forall U,V\in U_1, \tag{3.1}$$

where $\chi: U_1\times U_1\to U(1)$ is only defined locally (a derivation of an explicit, locally valid formula of χ is given in Ref. 11: in the second quantization setting see also Ref. 12). The latter is a nontrivial local 2-cocycle providing a central extension $\hat{U}_1$ of U_1 by $U(1)$. Similarly the (complexification of the) Lie algebra u_1 of U_1 contains all bounded operators X on H with Hilbert-Schmidt $[\epsilon, X]$ and its second quantization $u_1\ni X\to d\Gamma(X)=d\Gamma(X^*)^*$ gives a representation of a central extension $\hat{u}_1=u_1\oplus \mathbb{C}$ of u_1,

$$[d\Gamma(X), d\Gamma(Y)] = d\Gamma_1([X,Y]) + c_L(X,Y), \tag{3.2}$$

with a Lie algebra 2-cocycle[13]

$$c_L(X,Y)=\frac{1}{4}\,\mathrm{Tr}\,\epsilon[\epsilon,X][\epsilon,Y] \tag{3.3}$$

which is the infinitesimal version of the Lie group 2-cocycle χ above (Tr is the Hilbert space trace throughout the paper). It is possible to choose phases such that

$$\Gamma(e^{iX})=e^{id\Gamma(X)} \quad \forall X=X^* \text{ close to } 0\in u_1 \tag{3.4}$$

[the existence of the $e^{id\Gamma(X)}$ as a unitary operator follows from Stone's theorem[6] since $d\Gamma(X)$ is self-adjoint[4]]. This equation actually is true for all $X\in u_1$, but it fixes the phase of $\Gamma(U)$ for only $U\in U_1$ sufficiently close to the identity where local bijectivity of the exponential mapping is guaranteed. We will assume this phase convention in the following. Then (3.2) implies

$$\Gamma(e^{-i\delta sX}e^{-i\delta tY}e^{i\delta sX})=e^{\delta s\,\delta t c_L(X,Y)}\Gamma(e^{-i\delta sX})\Gamma(e^{-i\delta tY})\Gamma(e^{i\delta sX})+\mathcal{O}(\delta s^2,\delta t^2) \tag{3.5}$$

for all $X,Y\in u_1$ and sufficiently small $\delta s,\delta t\in\mathbb{R}$ [to see this, use (3.4) and expand both sides of this equation in powers of δs and δt].

We now consider a time evolution $V_A(t,t')=V(t,t')$ defined in eq. (2.2) with $h_A=h$: $\mathbb{R}\to u_1$ smooth and compactly supported. We first consider the simple case where $h(t)\in u_1$ so that $V(t,t')\in U_1$ for all $t,t'\in\mathbb{R}$. As shown in the last section, many interesting cases can be brought to this simplest situation using the conjugation by a family of operators $T(A)$ (we will discuss this in more detail further below).

We first note the essential group property of the time evolution.

$$V(t,t')V(t',t'')=V(t,t'') \quad \forall t,t',t''\in\mathbb{R}, \tag{3.6}$$

which follows from (2.2): it is this what we mean by causality. Somewhat parallel to our discussion, the use of the causality condition in the renormalization of a quantum field theory has been stressed by Scharf and his coworkers.[14]

To construct the second quantization of the scattering operator $S=S_A$ (2.6) including the phase, we first second quantize the time evolution. The naive guess $\Gamma(V(t,t'))$ for this is not right since this is not a time evolution: it does not obey an equation similar to (3.6) due to the Schwinger term χ in (3.1) which gives nontrivial contributions in general. One can, however, define $\hat{V}(t,t')=\lim_{N\to\infty}\hat{V}^{(N)}(t,t')$ with

$$\hat{V}^{(N)}(t,t')=\prod_{N\geq\nu\geq 1}\Gamma(V(t_\nu,t_{\nu-1})), \quad t_\nu=t'+\frac{(t-t')\nu}{N} \tag{3.7}$$

where $\Pi_{N\geq\nu\geq 1}F(t_\nu,t_{\nu-1})$ is the ordered product $F(t_N,t_{N-1})F(t_{N-1},t_{N-2})\ldots F(t_2,t_1)$ for any operator valued function F on $\mathbb{R}\times\mathbb{R}$. This is a time evolution by construction, and with (3.1)

$$\hat{V}(t,t')=\eta(t,t')\Gamma(V(t,t')), \tag{3.8a}$$

where η is a phase valued function on $\mathbb{R}\times\mathbb{R}$ which can be explicitly computed in terms of χ [for $V(t,t')$ in some neighborhood of the identity].[12] This allows us to calculate the scattering operator $\hat{S}=\hat{V}(T,-T)$ including phase as follows [here and in the following we assume that T is big enough so that $h(t)$ vanishes for $|t|>T/2$, say]: choose some partition $t_0=-T<t_1<\ldots<t_n=T$ of the time interval $[-T,T]$ such that all $V(t_i,t_{i-1})$ are in the neighborhood of the identity for which $\eta(t,t')$ is defined. Then

$$\hat{S}=\prod_{n\geq i\geq 1}\eta(t_i,t_{i-1})\Gamma(V(t_i,t_{i-1})) \tag{3.8b}$$

can be shown to be independent of which particular partition is chosen.

Remark 1: We note our formulas (3.8a) and (3.8b) still do not fix the phase of $\hat{S}$ completely since the function $\eta(t,t')$ is unique only up to

$$\eta(t,t')\mapsto\exp\left(-i\int_{t'}^{t}d\bar{t}E(\bar{t})\right)\eta(t,t') \tag{3.9}$$

with E a smooth real-valued function on $\mathbb{R}$. This is due to the ambiguity of the second quantization map $u_1 \ni X \to d\Gamma(X)$ which can be changed by smooth, linear functions $b: u_1 \mapsto \mathbb{C}$ with $b(X^*) = b(X)^*$. A shift $d\Gamma(X) \to d\Gamma(X) + b(X)$ changes (3.3) by a trivial 2-cocycle, $c_L(X,Y) \to c_L(X,Y) - b([X,Y])$, and this implies (3.9) with $E(t) = b(h(t))$.

Remark 2: Since $h(t) \in u_1$ for all t, the second quantized Hamiltonian $\hat{h}(t) = d\Gamma(h(t))$ (in the interaction picture) always exists, and it should be the generator of the second quantized time evolution $\hat{V}(t,t')$. Moreover, the ambiguity (3.9) of the phase of $\hat{V}(t,t')$ corresponds to a shift $\hat{h}(t) \to \hat{h}(t) + E(t)$ which physically amounts to a change of the zero-point energy. It would be difficult to construct $\hat{V}(t,t')$ directly from $\hat{h}(t)$ since the latter is unbounded which makes the existence of a Dyson series nontrivial. This technical problem is avoided in our approach above.

In the following we are interested in the change of the second quantized time evolution operator under transformations

$$V(t,t') \mapsto (g \cdot V)(t,t') \equiv g(t) V(t,t') g(t')^{-1}, \tag{3.10}$$

where g: $\mathbb{R} \mapsto U_1$, where $g(t)$ is assumed to be sufficiently smooth and such that $g(t) = 1$ for $|t| > T/2$. We will derive an explicit formula for the gauge anomaly of the time evolution,

$$\lambda(t,g) \equiv \Gamma(g(t))^{-1} \widehat{(g \cdot V)}(t,-T) \hat{V}(-T,t), \tag{3.11}$$

which is a phase factor according to our discussion above [since the r.h.s. is the second quantization of $g(t)^{-1}(g \cdot V)(t,-T) V(-T,t)$ equal to the identity]. In particular, $\lambda(g) \equiv \lambda(T,g)$ is the change of the quantum scattering operator $\hat{S}$ under the transformation g.

We first consider only infinitesimal gauge transformations $g(t) = e^{-i\delta s X(t)}$ for $\delta s \to 0$. We calculate $\lambda(t,g)$ as $\lim_{N\to\infty} \lambda^{(N)}$ where

$$\lambda^{(N)} = \Gamma(g(t))^{-1} \left\{ \prod_{N \geq \nu \geq 1} \Gamma(g(t_\nu) V(t_\nu, t_{\nu-1}) g(t_{\nu-1})^{-1}) \right\} \left\{ \prod_{1 \leq \nu \leq N} \Gamma(V(t_{\nu-1}, t_\nu)) \right\}$$

with $t_\nu = -T + (t+T)\nu/N$. Now (3.1) implies

$$\Gamma(g(t+\delta t) V(t+\delta t, t) g(t)^{-1}) = \lambda^{(t+\delta t, t)}(g) \Gamma(g(t+\delta t)) \Gamma(V(t+\delta t, t)) \Gamma(g(t))^{-1}$$

for some phase factors $\lambda^{(t+\delta t,t)}$, and we explicitly see that the various factors $\Gamma(g(t_\nu))$ and $\Gamma(g(t_{\nu-1}))^{-1}$ cancel each other leaving only phase factors. Using $V(t+\delta t, t) \simeq e^{-i\delta t h(t)}$, $g(t+\delta t) \simeq e^{-i\delta s X(t)}$ and (3.5), we get $\lambda^{(t+\delta t,t)}(g) \simeq e^{\delta s\, \delta t c_L(X(t), h(t))}$ ($\simeq$ means "equal up to irrelevant higher order terms in δs and δt"). Thus $\lambda^{(N)}$ is just the exponent of a Riemann sum, and in the limit $N \to \infty$.

$$\lambda(t, e^{-i\delta s X}) = \exp\left(\delta s \int_{-T}^{t} d\bar{t}\, c_L(X(\bar{t}), h(\bar{t})) \right) + \mathcal{O}(\delta s^2).$$

We now consider the case of finite gauge transformations $g(t)$ and introduce a homotopy $g_s(t)$, $0 \leq s \leq 1$, smoothly deforming it to the identity

$$g_1(t) = g(t) \quad \text{and} \quad g_0(t) = 1 \quad \forall t, \quad g_s(t) = 1 \quad \text{for } |t| > T/2. \tag{3.12}$$

To be specific, we first restrict ourselves to gauge transformations $g(t) = e^{-iX(t)}$ with $X(t) \in u_1$ for all t, and $g_s(t) = g(t) = e^{-isX(t)}$. We define $V_s(t,t') \equiv (g_s \cdot V)(t,t')$ and

$$\lambda_{s,s'} \equiv \Gamma(g_s(t))^{-1} \hat{V}_s(t,-T) \hat{V}_{s'}(-T,t) \Gamma(g_{s'}(t))$$

so that $\lambda(g)=\lambda_{1,0}$. We observe that these phases have the group property $\lambda_{s,s'}\lambda_{s',s''}=\lambda_{s,s''}$ for all $0\leq s,s',s''\leq 1$; thus we can evaluate $\lambda(g)$ as $\lim_{M\to\infty}\lambda_M$ where

$$\lambda_M=\prod_{M\geq\mu\geq 1}\lambda_{s_\mu,s_{\mu-1}},\quad s_\mu=\frac{\mu}{M}.$$

Now $\lambda_{s+\delta s,s}$ is the change of phase of $\hat{V}_s(T,-T)$ under an infinitesimal gauge transformation $g_{s+\delta s}(t)g_s(t)^{-1}\simeq e^{-i\delta s X_s(t)}$ and thus equal to $\exp[\delta s\int_{-T}^{t}d\bar{t}c_L(X_s(\bar{t}),h_s(\bar{t}))]$ with

$$h_s(t)=i\{\partial_t V_s(t)\}V_s(t)^{-1},\quad X_s(t)=i\{\partial_s V_s(t)\}V_s(t)^{-1},\quad V_s(t)=g_s(t)V(t,-T)\tag{3.13}$$

[we used $g_s(-T)=1$)]. Again λ_M becomes the exponential of a Riemann sum, and in the limit $M\to\infty$ we obtain

Theorem 3.14:

$$\lambda(t,g)=\exp\left(\int_0^1 ds\int_{-T}^{t}d\bar{t}c_L(X_s(\bar{t}),h_s(\bar{t}))\right).$$

Note that this result was derived for the special homotopy $g_s(t)=e^{-isX(t)}$, but our derivation can be immediately generalized to arbitrary gauge transformations $g(t)$ and homotopies $g_s(t)$ (sufficiently smooth in s and t) obeying (3.12). For $t\geq T$, $\lambda(t,g)=\lambda(g)$ (3.14) is then actually independent of the homotopy chosen [this follows from its definition (3.11) which does not depend on the homotopy]. For intermediate times $-T<t<T$ this is not true. The reason is that then the phase of the implementors $\Gamma(g(t))$ in (3.11) depends on the homotopy: our derivation above implies that this phase has to be chosen such that

$$\Gamma(g(t))=\lim_{M\to\infty}\prod_{M\geq\mu\geq 1}\Gamma(g_{s_\mu}(t)g_{s_{\mu-1}}(t)^{-1}),\quad s_\mu=\frac{\mu}{M},$$

and this coincides with our phase convention (3.4) only for homotopies $s\mapsto g_s(t)=e^{-isX(t)}$.

Remark 3: Our derivation of (3.14) above was given for one-parameter groups in U_1 for simplicity, but the result immediately generalizes to GL_1 which is the group of all (not only unitary) invertible operators U on H with Hilbert-Schmidt $[\epsilon,U]$: Eq. (3.14) remains true for $h(t)\in u_1$ not self-adjoint and $g(t)\in GL_1$. The technical problem for proving this more general result by the method above is that $\epsilon^{-i\delta t d\Gamma(X)}$ is unbounded if $d\Gamma(X)$ is not self-adjoint; thus one has to be careful with the domains of operators (the latter could, however, be handled by methods described in Ref. 15). Our alternative derivation of (3.14) in the next section is for GL_1 and bypasses such domain questions.

We consider now time evolutions generated by Hamiltonians $H_A(t)=D_0+A(t)$ with $A(t)\in\mathscr{A}$ [cf. definition (2.9)] and generalized gauge transformations

$$A(t)\to g\cdot A(t)=i(\partial_t g(t))g(t)^{-1}-[D_0,g(t)]g(t)^{-1}+g(t)A(t)g(t)^{-1}\tag{3.15}$$

so that $U_{g\cdot A}(t,t')=g(t)U_A(t,t')g(t')^{-1}$. We denote the group of all $g(t)$ which leave $\mathscr{A}$ invariant as $\mathscr{G}$. Note that $\mathscr{G}$ contains all $g(t)$ sufficiently smooth in t (i.e., C^{p+1}), which are unitary operators in O_0 for all t. We also introduce the Lie algebra $\mathrm{Lie}\mathscr{G}$ of $\mathscr{G}$. In the following, all A are in $\mathscr{A}$, all g,g',g'' in $\mathscr{G}$ and all $X,Y,Z\in\mathrm{Lie}\mathscr{G}$, except when stated otherwise. As before, we assume all these functions are trivial for $|t|>T/2$.

By Theorem 2.10, there exist appropriate regularization operators $T(A)$ and $T(g\cdot A)$ such that A' and $(g\cdot A)'$, defined in (2.8), all lead to time evolutions which can be second quantized, i.e., they are always in u_1. This also implies that the operators $T_t(g\cdot A)g(t)T_t(A)^{-1}=U_{g\cdot A}(t,-T)U_A(-T,t)$ all are in U_1, and thus

$$\Gamma_t(g;A)\equiv\Gamma(g'_A(t)),\quad g'_A(t)\equiv e^{itD_0}T_t(g\cdot A)g(t)T_t(A)^{-1}e^{-itD_0} \tag{3.16}$$

always exist. These unitary operators have the natural interpretation as implementors of the generalized gauge transformations g at fixed time t. They are local in time, i.e., only depend on g, A and t-derivatives thereof, at time t. We observe that they obey the relations

$$\Gamma(g';g\cdot A)\Gamma(g;A)=\chi(g',g;A)\Gamma(g'g;A), \tag{3.17a}$$

where we have dropped the common time argument t, with

$$\chi_t(g',g;A)=\chi((g')'_{g\cdot A}(t),g'_A(t)) \tag{3.17b}$$

defined locally [this follows from (3.1)]. Note that (3.17a) and associativity of the operator product imply the 2-cocycle relation

$$\chi(g'',g'g;A)\chi(g',g;A)=\chi(g'',g';g\cdot A)\chi(g''g',g;A). \tag{3.18}$$

Our construction above can now be used to calculate

$$\lambda(t,g;A)\equiv\Gamma_t(g;A)^{-1}\widehat{V_{(g,A)'}}(t,-T)\widehat{V_{A'}}(-T,t), \tag{3.19}$$

which we define as the change of the quantum time evolution $\widehat{V_{A'}}$ under the generalized gauge transformation g. We immediately get the formula

$$\lambda(t,g;A)=\exp\left(\int_0^1 ds\int_{-T}^{t}d\bar{t}\,c_L(\{\partial_s V_s(\bar{t})\}V_s(\bar{t})^{-1},\{\partial_t V_s(\bar{t})\}V_s(\bar{t})^{-1})\right) \tag{3.20a}$$

with

$$V_s(t)=e^{itD_0}T_t(g_s\cdot A)g_s(t)U_A(t,-T)e^{iTD_0} \tag{3.20b}$$

and $g_s(t)\in\mathcal{G}$ a homotopy interpolating between 1 and $g(t)$. Similarly as discussed above after Theorem 3.11, for $t\geq T$ (but in general not for intermediate times $-T<t<T$) this formula is independent of the homotopy $s\mapsto g_s(t)$ chosen.

We observe that these phases are connected with the Schwinger terms in (3.17b) via the relation

$$\lambda(t,g';g\cdot A)\lambda(t,g;A)\chi_t(g',g;A)=\lambda(t,g'g;A). \tag{3.21}$$

This follows from a simple calculation using the definition (3.19) and $(g'g)\cdot A=g'\cdot(g\cdot A)$,

$$\Gamma_t(g';g\cdot A)\lambda(t,g';g\cdot A)\Gamma_t(g;A)\lambda(t,g;A)$$

$$=\widehat{V_{(g'g\cdot A)'}}(t,-T)\widehat{V_{(g\cdot A)'}}(-T,t)\widehat{V_{(g\cdot A)'}}(t,-T)\widehat{V_{A'}}(-T,t)=\Gamma_t(g'g;A)\lambda(t,g'g;A),$$

and inserting (3.17a). According to our derivation, this equation is valid only locally [i.e., $g(t)$ and $g'(t)$ close to identity].

Especially for $t=T$, $\lambda(g;A)\equiv\lambda(T,g:A)$ is equal to the change of the quantum scattering matrix $\hat{S}_A$ under the transformation g, and Eq. (3.21) reduces to the 1-cocycle relation, $\lambda(g';g\cdot A)\lambda(g;A)=\lambda(g'g;A)$ [since $\chi(1,1;0)=1$]. The physical meaning of $\lambda(g;A)$ is as follows. We recall that the log of the vacuum expectation value of $\hat{S}_A$ is equal to the Minkowskian action of the fermions in the time dependent external field A, thus $\log\lambda(g;A)$ is the change of the

latter by the generalized time dependent gauge transformation $g(t)$. Especially for infinitesimal transformations $g(t)=1-i\delta s X(t)+\ldots$ it gives the generalized gauge anomaly $\mathrm{Anom}(X;A)=d/ds\ \log\lambda(e^{-isX};A)|_{s=0}$. We obtain

$$\mathrm{Anom}(X;A)=\int_{-T}^{T}dt\,\bar{\omega}^1(X(t),A(t)),\quad \bar{\omega}^1(X(t),A(t))=c_L(X'_A(t),h_{A'}(t)),\tag{3.22}$$

where $h_{A'}(t)=e^{itD_0}A'(t)e^{-itD_0}$ with A' given in Eq. (2.8), and

$$X'_A(t)\equiv e^{itD_0}[\{\mathscr{L}_X T_t(A)\}T_t(A)^{-1}-T_t(A)X(t)T_t(A)^{-1}]e^{-itD_0}\tag{3.23}$$

is in u_1 for all $A\in\mathscr{A}$ and $X\in\mathrm{Lie}\mathscr{G}$; we introduced the Lie derivative acting on functionals f on $\mathscr{A}$ as

$$\mathscr{L}_X f(A)=i\frac{d}{ds}f(e^{-isX}A)\bigg|_{s=0}.$$

Similarly, the infinitesimal version of (3.17a) and (3.17b) is[1]

$$[G(X;A),G(Y;A)]=G([X,Y];A)+S(X,Y;A)\tag{3.24a}$$

where $G(X;A)=\mathscr{L}_X+d\Gamma(X'_A)$ are implementors of infinitesimal gauge transformations and

$$S_t(X,Y;A)=c_L(X'_A(t),Y'_A(t)),\tag{3.24b}$$

a Schwinger term satisfying the 2-cocycle relation $\mathscr{L}_X S(Y,Z;A)+S(X,[Y,Z];A)+\mathrm{cycl.}=0$ [the latter is the infinitesimal version of (3.18) and also follows from the Jacobi identity].

Especially, if we consider the Yang-Mills case and infinitesimal chiral gauge transformations, $\mathrm{Anom}(X;A)$ is just the axial gauge anomaly and $S(X,Y;A)$ the Schwinger term appearing in the commutators of the chiral Gauss' law generators $G(X;A)$. We thus have obtained a Hamiltonian derivation of these two different manifestations of the gauge anomaly in a Hamiltonian framework which traces them back to a common root, i.e., the 2-cocycle c_L in (3.2).

It is interesting to consider also the infinitesimal version of Eq. (3.21) which can be written as

$$\delta\bar{\omega}^1+\partial_t S=0\tag{3.25}$$

where

$$(\delta\omega^1)(X,Y;A)=\mathscr{L}_X\omega^1(Y;A)-\mathscr{L}_Y\omega^1(X;A)-\omega^1([X;Y];A)$$

is defined on functions ω^1 on Lie $\mathscr{G}\times\mathscr{A}$. To interpret this equation, we recall that the above mentioned fermion-Yang-Mills anomalies are connected by descent equations:[16] the axial anomaly on a $n+1$ (even)-dimensional space-time manifold M^{n+1} is the integral of a $(n+1)$-(de Rham) form $\omega^1_{n+1}(X;A)$ over M^{n+1}; it depends on one infinitesimal gauge transformations X and the Yang-Mills field A. The corresponding Schwinger term is on n-dimensional space M^n and an integral of a n-form $\omega^1_n(X,Y;A)$ over M^n depending on two infinitesimal gauge transformations X, Y, and A. Embedding M^n in M^{n+1}, the descent equations are $\delta\omega^1_{n+1}+d\omega^2_n=0$ where δ is defined as above and d is the usual exterior differentiation of de Rham forms. Setting $M^{n+1}=M^n\times\mathbb{R}$ and $\bar{\omega}^1=\int_{M^n}\omega^1_{n+1}$ and $S=\int_{M^n}\omega^2_n$, one exactly obtains our Eq. (3.25). We thus have obtained an explicit field theory derivation of this descent equation for all odd dimensions n the Hamiltonian framework. We stress, however, that our equation (3.25) is not restricted to the Yang-Mills case but in fact is more general.

Remark 4: As just mentioned, fermion-Yang-Mills anomalies are local de Rham forms, whereas our formulas (3.22) for the axial anomaly and (3.24b) for the Schwinger term are not explicitly local in space. In the Yang-Mills case one can prove, however, that they cohomologous to local de Rham forms. General arguments and mathematical techniques for showing this by explicit calculations have been given recently.[1,17,18] Nevertheless it would be interesting to explicitly do this latter calculation for all dimensions. In this article we will only sketch the simplest case $n=1$ (end of next section).

In the next section we will give a different, more geometric approach to the phase of the scattering operator where the path independence of the anomaly becomes evident. Another important benefit in the geometric approach is that we can easily compute the cohomology class of the anomaly without going to the details of the renormalization $T(A)$.

IV. THE QUANTUM PHASE AND PARALLEL TRANSPORT

Let $\hat{G}$ be a central extension of a Lie group G by $\mathbb{C}^\times$. The Lie algebra $\hat{g}$ of $\hat{G}$ is a vector space direct sum $g\oplus\mathbb{C}$. Let π be the projection on the second summand and let $\theta=\mathbf{g}^{-1}d\mathbf{g}$ be the left Maurer-Cartan one-form. We can then define a complex valued one-form ϕ on $\hat{G}$ by $\phi=\pi(\theta)$. This is a connection form in the principal $\mathbb{C}^\times$ bundle $\hat{G}\to G$. Its curvature is a left invariant two-form on G given by $\omega(X,Y)=c(X,Y)$, where left invariant vector fields X,Y on G are identified as elements of the Lie algebra and c is the 2-cocycle on g defining the central extension

$$[(X,\lambda),(Y,\mu)]=([X,Y],c(X,Y)). \tag{4.1}$$

Recall that GL_1 is the group of invertible linear transformations $\mathbf{g}:H\to H$ such that $[\epsilon,\mathbf{g}]$ is of Hilbert-Schmidt type and U_1 its unitary subgroup. Let us apply the above remarks to $G=U_1$, and to the Lie algebra cocycle c_L (3.3) arising when promoting the one-particle operators to operators (2.5) in the fermionic Fock space, as discussed in the last section.

The central extension $\widehat{GL}_1$ is a nontrivial $\mathbb{C}^\times$ bundle over the base GL_1.[11] The elements of the group $\widehat{GL}_1$ (containing the unitary subgroup $\hat{U}_1$) can be thought of equivalence classes of pairs $(\mathbf{g},q)$, where $\mathbf{g}\in GL_1$ and $q:H_+\to H_+$ is an invertible operator such that $a-q$ is a trace-class operator,

$$\mathbf{g}=\begin{pmatrix} a & b \\ c & d \end{pmatrix}. \tag{4.2}$$

We have assumed that $\operatorname{ind} a=0$. If this is not the case, the subspace H_+ must be either enlarged or made smaller by a suitable finite-dimensional subspace in order to achieve $\operatorname{ind} a=0$. The equivalence relation is determined by $(\mathbf{g},q)\sim(\mathbf{g}',q')$ if $\mathbf{g}=\mathbf{g}'$ and $\det(q'q^{-1})=1$. Thus the fiber of the extension is $\mathbb{C}^\times$ and it is parameterized by (the nonexisting) determinant of q.

The product is defined simply $(\mathbf{g},q)(\mathbf{g}',q')=(\mathbf{g}\mathbf{g}',qq')$. Near the unit element in G we can define a local section $\mathbf{g}\mapsto(\mathbf{g},a)$.[11] Denoting

$$\mathbf{g}^{-1}=\begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}$$

we can write the connection form as

$$\phi=\operatorname{Tr}[(\mathbf{g}^{-1}d\mathbf{g})a-q^{-1}dq]=\operatorname{Tr}[\alpha da+\beta dc-q^{-1}dq]. \tag{4.3}$$

The curvature of this connection at $\mathbf{g}=1$ is

$$\omega=-\operatorname{Tr}(d\beta d\gamma) \tag{4.4}$$

and is easily checked to agree with c_L in (3.3).

We compute the parallel transport determined by the connection in the range of the local section. Let $\mathbf{g}(t)$ be a path in GL_1, $-T\leqslant t\leqslant T$, with $\mathbf{g}(-T)=1$. The lift $(\mathbf{g}(t),q(t))$ is parallel if

$$0=\phi(g(t),q(t))(dg,dq)=\mathrm{Tr}[\alpha(t)a'(t)+\beta(t)c'(t)-q(t)^{-1}q'(t)].$$

Thus the parallel transport, relative to the trivialization $\mathbf{g}\mapsto(\mathbf{g},a)$, along the path $\mathbf{g}(t)$ in the base is accompanied with the multiplication by the complex number

$$\exp\left(-\int_{-T}^{T}\mathrm{Tr}[\{\alpha(t)-a(t)^{-1}\}a'(t)+\beta(t)c'(t)]dt\right) \tag{4.5}$$

in the fiber C.

Formally,

$$\mathrm{Tr}\, q^{-1}q'=\mathrm{Tr}[\alpha a'+\beta c']$$

and so

$$\det q(T)=\exp\int_{-T}^{T}\mathrm{Tr}\,[\alpha(t)a'(t)+\beta(t)c'(t)]dt$$

and also

$$\det a(T)=\exp\int_{-T}^{T}\mathrm{Tr}\, a(t)^{-1}a'(t)dt.$$

Individually, the traces in these two expressions do not converge, but put together the trace converges and gives

$$\det[a(T)q(T)^{-1}]=\exp\left\{\int_{-T}^{T}\mathrm{Tr}\,[(\alpha-a^{-1})a'+\beta c']dt\right\}. \tag{4.6}$$

Note that the exponent diverges outside of the domain of the local section, reflecting the fact that $\det a(T)=0$ outside of the domain.

We can now apply the above results to the "renormalized" one-particle time evolution operators $\mathbf{g}(t)=V_{A'}(t)=e^{itD_0}T_1(A)U_A(t,-T)e^{iTD_0}$. For all times t, these are elements of the group U_1. On the other hand, in the Fock representation of $\widehat{GL}_1$ these correspond to elements $\widehat{V_{A'}(t)}$ in the central extension $\hat{U}_1$. The phase of the quantum time evolution operator is then uniquely given by the parallel transport described above.

The Minkowskian effective action is by definition the vacuum expectation value of the quantum scattering operator $\hat{S}_A$. The vacuum is invariant under the free time evolution $\exp(itD_0)$ and taking into account the assumption that the interaction has essentially compact support in time, we can write

$$Z(A)=\langle 0|(V_{A'}(T),q(T))|0\rangle. \tag{4.7}$$

The vacuum expectation value is given by a simple formula,[11,19]

$$\langle 0|(\mathbf{g},q)|0\rangle=\det(aq^{-1}) \tag{4.8}$$

and therefore the parallel transport (4.5) (with respect to the given local trivialization) is equal the effective action $Z(A)$.

The above formalism can be applied for computing the gauge anomaly in the space-time formalism starting from the commutator anomaly (3.3). Let $g(t)\in\mathcal{G}$ be a time-dependent gauge transformation such that at $t=\pm T$ it is equal to the identity. The change in the phase of the effective action is now

$$\lambda(g;A)=\exp\left(\int_\gamma \phi\right)$$

where γ is the closed loop in U_1 obtained by first following backwards in time from T to $-T$ the time evolution $U_{A'}(t)$, following then the gauge transformed time evolution operators $g(t)U_{A'}(t)$ back from $-T$ to T. The parallel transport around a closed loop can be written as an integral of the curvature ω over a surface S enclosed by the loop γ. By construction, the gauge anomaly λ satisfies the 1-cocycle condition $\lambda(gg';A)=\lambda(g;g'.A)\lambda(g';A)$.

Joining $g(t)$ to the identity by a homotopy $g_s(t)$, $0\leqslant s\leqslant 1$, and writing $V_s(t)=g_s(t)U_{A'}(t)$ we get

$$\log\lambda(g;A)=\int_S dtdsc_L(\partial_s VV^{-1},\partial_s VV^{-1})=\frac{1}{4}\int dtds\,\mathrm{Tr}\,\epsilon[\epsilon,\partial_t,VV^{-1}][\epsilon,\partial_s VV^{-1}]. \quad (4.9)$$

This result agrees with (3.14). For infinitesimal gauge transformations $g_s(t)=1-isX(t)+\cdots$ we get axial anomaly (3.22) as discussed in the last section.

Let us complete the calculation for $1+1$ space-time dimensions in the case of chiral fermions in external Yang-Mills field. Now the chiral Hamiltonian on the circle S^1 acting on one-component spinors is $H(t)=-i\partial/\partial x-A_+$, where $A_+=A_0+A_1$ (0 and 1 are space–time indices). We now use that for $n=1$ one can choose $T_t(A)=1$ independent of A (see our remark 1 at the end of section II). Thus, applying (3.22) derived either from (3.20) or (4.9), we get

$$\mathrm{Anom}(X;A)=\frac{1}{4}\int_{-T}^{T}dt\,\mathrm{Tr}\,\epsilon[\epsilon,A_+][\epsilon,X(t)]=\frac{1}{2\pi i}\int_{-T}^{T}dt\int_{S^1}dx\ \mathrm{tr}\,A_+(t,x)\frac{\partial}{\partial x}X(t,x).$$

Here we have used the general formula

$$\frac{1}{4}\mathrm{Tr}\epsilon[\epsilon,X][\epsilon,Y]=\frac{1}{2}\mathrm{Tr}_C X[\epsilon,Y]=\frac{1}{2\pi i}\int_{S^1}dx\ \mathrm{tr}\,X\partial_x Y \quad (4.10)$$

valid for smooth multiplication operators X,Y on the unit circle; here we introduced the notation $\mathrm{Tr}_C(a)\equiv\frac{1}{2}\mathrm{Tr}(a+\epsilon a\epsilon)$ (conditional trace) which will be useful below. Up to a coboundary ($=a$ gauge variation of the local functional $\propto\int\mathrm{tr}\,A_+A_1$) this form of the anomaly is equal to the standard form of the two-dimensional chiral anomaly

$$\mathrm{Anom}(X;A)=\frac{1}{4\pi i}\int_{S^1\times\mathbb{R}}\mathrm{tr}\,A dX. \quad (4.11)$$

We finally note that this same equation also allows to calculate the Schwinger term (3.24b).

$$S(X,Y;A)=\frac{1}{2\pi i}\int_{S^1}\mathrm{tr}\,X dY \quad (4.12)$$

which actually is independent of A. This is the Kac-Moody cocycle and also the Schwinger term related to the axial anomaly (4.11) via the descent equations, as discussed at the end of the last section.

The cohomology class of the anomaly in dimensions $n+1>2$

The group GL_p consists of all bounded invertible operators (4.2) in $H=H_+\oplus H_-$ such that the off-diagonal blocks b,c are in the Schatten ideal B_{2p}. For any $p\geqslant 1$ the group GL_p contracts to the subgroup GL_1.[20] On the other hand, in GL_1 one can produce cohomologically equivalent cocycles $c_p\sim c_L$ such that c_p extends from GL_1 to GL_p. These are relevant for understanding the gauge group action in space-time dimension $n+1>2$. The static gauge transformations are elements of GL_p for $p>n/2$. For example, when $n=3$ the gauge group $\mathscr{G}_n=\mathrm{Map}\,(M^n,G)\subset GL_2$ and one has[21]

$$c_2(X,Y;f)=\frac{1}{8}\,\mathrm{Tr}_C[\epsilon,f]f^{-1}[[\epsilon,X],[\epsilon,Y]], \tag{4.13}$$

where $c_2(X,Y;f)$ is the value of a two-form on GL_2 at a point f to the directions of the left invariant vector fields (=Lie algebra elements) X,Y. This formula has been generalized for arbitrary p.[22,23]

In order to fix the cohomology class of the 1-cocycle $\lambda(g;A)$ it is sufficient to look how λ winds around the circle when a family $f(t,s)$ of time-dependent gauge transformations wraps around a closed surface S (parameterized by s,t) in the group $\mathscr{G}_n$ of static gauge transformations. This follows from the fact that the cohomology class of any two-form is determined by giving its integral over all closed 2-cycles. The winding number is given by the integral of the curvature c_L around the surface S in GL_1 defined by the family of gauge transformed renormalized evolution operators.

For any fixed potential A and a homotopy $f(t,s)$ of time-dependent gauge transformations we have a map $S=[-T,T]\times[0,1]\to GL_p$ given by $(t,s)\mapsto f(t,s)U(t)$, where $U(t)$ is the nonrenormalized time evolution operator determined by A. The renormalization $T(A)$ does not change the homology class of the surface S in $GL_1\subset GL_p$ since $T(A)$ is defined over a contractible parameter space. It follows that the integral over a closed surface S of the curvature on GL_1 is given by the integral of c_p of the nonrenormalized operators $f(t,s)U(t)$. Furthermore, the surface $(t,s)\mapsto f(t,s)U(t)$ contracts to $(t,s)\mapsto f(t,s)$. This follows from the fact that each component of U_p is simply connected and so $(t,s)\mapsto U(t)$ is contractible. Therefore, the final result for the anomaly around a closed surface is

$$\int_{f(t,s)} c_p=\int_{-T}^{T}dt\int_0^1 ds\,c_p(i(\partial_t f)f^{-1},i(\partial_t f)f^{-1}). \tag{4.14}$$

In the case $M=S^1$ $(p=1)$ this gives

$$\begin{aligned}-\frac{1}{2}\int_S dtds\ \mathrm{Tr}_C(\partial_t f)f^{-1}[\epsilon,(\partial_s f)f^{-1}]&=-\frac{1}{2\pi i}\int_{S\times S^1}dtdsdx\ \mathrm{tr}(\partial_t f)f^{-1}\partial_x((\partial_s f)f^{-1})\\&=\frac{1}{12\pi i}\int_{S\times S^1}\mathrm{tr}(f^{-1}df)^3,\end{aligned} \tag{4.15}$$

where we have used (4.10) in the first step and $\partial_x f^{-1}=-f^{-1}\partial_x(f)f^{-1}$ in the second step (the factor $1/6=1/3!$ is from antisymmetrization in the variables t,s,x which amounts to partial integrations).

In dimension $n=3$ $(p=2)$ a similar calculation gives

$$-\frac{1}{8}\int_S dtds\,\mathrm{Tr}_C[\epsilon,f]f^{-1}[[\epsilon,(\partial_t f)f^{-1}],[\epsilon,(\partial_s f)f^{-1}]]$$

$$=\frac{1}{24\pi^2}\int_S dtds\int_{\mathbb{R}^3} d^3x\,\epsilon^{ijk}\,\mathrm{tr}(\partial_i f)f^{-1}[(\partial_j(\partial_t f)f^{-1}),(\partial_k(\partial_s f)f^{-1})]$$

$$=\frac{1}{240\pi^2}\int_{S\times\mathbb{R}^3}\mathrm{tr}(f^{-1}df)^5 \tag{4.16}$$

where $\partial_i = \partial/\partial x_i$, ϵ^{ijk} is the antisymmetric tensor with $\epsilon^{123}=1$, and in the second step we again antisymmetrize in the variables t,s,x_1,x_2,x_3 which gives the combinatorial factor $1/10=3!2!/5!$. In the first step we used the three-dimensional analog of Eq. (4.10),[24]

$$\mathrm{Tr}_C(X_0[\epsilon,X_1][\epsilon,X_2][\epsilon,X_3])=-\frac{1}{3\pi^2}\int_{\mathbb{R}^3}\mathrm{tr}\,X_0dX_1dX_2dX_3\,. \tag{4.17}$$

Similar results can be derived for all $p>0$ using the results from Refs. 24 and 23. We note that $\int_{f(t,s)}c_p$ agrees with the integral of the two form over S in a gauge orbit obtained by the descent equations.[16] For example, in three space dimensions ($p=2$) this form is

$$\frac{i}{24\pi^2}\int_{\mathbb{R}^3}\mathrm{tr}\,A[dX,dY] \tag{4.18}$$

which is the commutator anomaly in three space dimensions[25,26] [by a similar calculation as above it is easy to see that replacing A, X, and Y by $i(df)f^{-1}$, $i(\partial_t f)f^{-1}$, and $i(\partial_s f)f^{-1}$ and integrating over S^2 also leads to Eq. (4.16)]. We finally note that these results can be understood on a more fundamental level using a generalization of the descent equations to noncommutative geometry[23] and the fact that the conditional trace Tr_C is indeed a generalization of integration of de Rham forms (which is the natural interpretation of Eqs. (4.10) and (4.17)[17,24]).

V. CONCLUSIONS

In section II we gave a new proof for the existence of the second quantized fermionic scattering operator in external Yang-Mills fields. The proof is valid also in a more abstract setting of generalized gauge interactions in the spirit of Connes's noncommutative geometry. In section III we derived a formula for the phase of the scattering operator and its gauge variation from the concept of causality by using the local 2-cocycle on the group GL_1. In section IV we gave an alternative geometric derivation using a connection on the global group extension $\widehat{GL}_1$. A constructive interpretation for the descent equations was given in the Hamiltonian framework, linking the anomaly of the Minkowskian effective action to the Schwinger terms. This is complementary to the standard approach which starts from the euclidean functional determinant.

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APPENDIX A: THE CASE OF AN EXTERNAL METRIC

Let $g=(g_{ij}(x,t))$ be a time-dependent metric tensor in $\mathbb{R}^n$. We assume that space and time has been foliated by a choice of the time coordinate such that the space coordinates $x_1,\ldots,x_n$ are orthogonal with respect to the time t, i.e., $g_{0i}=g_{i0}=0$ for $1\leqslant i\leqslant n$. The Weyl equation is written as

$$ig_{00}\partial_t\psi=\gamma^k h_{kj}(i\partial_j+\Gamma_j)\psi\simeq g_{00}D_h\psi \tag{A1}$$

where $h_{kj}(x)$ are the components of an oriented orthonormal basis in $(\mathbb{R}^n,g)$.

$$h_{kj}h_{mj}=g_{km}. \tag{A2}$$

The matrices Γ_j, are the components of the spin connection (defined by the Levi-Civita connection of g), taking values in the Lie algebra of the spin group Spin (n).

We assume that the deviation of the metric g from the euclidean metric has only compact support in space and time. Furthermore, $g(x,t)$ is assumed to be smooth. If the dimension $n=2N+1$ then the γ's are $2^N\times 2^N$ complex matrices with the property

$$\gamma^i\gamma^j+\gamma^j\gamma^i=2\delta_{ij}. \tag{A3}$$

The Lie algebra of Spin(n) is spanned by the commutators $[\gamma_i,\gamma_j]$. If $n=3$ the γ-matrices are just the 2×2 Pauli matrices which are also the generators of the spin group Spin(3)=SU(2).

The principal symbol of the Dirac Hamiltonian is $\gamma^k h_{kj}p_j$. The complete symbol is the sum of the principal symbol and of a symbol of order zero in the momenta.

Because for any given pair q,p of nonzero vectors there is a rotation R such that $q=Rp$, there exists an element $B(p,x)\in\mathrm{Spin}(n)$ such that

$$B\gamma^k p_k B^*=\lambda(x,p)\gamma^k h_{kj}p_j. \tag{A4}$$

Here the product is a matrix product, no momentum space differentiation is involved, and the scale factor λ is the ratio of the euclidean lengths of the vectors $p=\gamma^k p_k$ and $q=\gamma^k h_{kj}p_j$. Both λ and B are homogeneous functions of order zero in momenta.

At the first sight it appears that it is not possible to construct B as a continuous function of the h field, the apparent obstruction being the hairy ball theorem: For a given direction q one can always choose a rotation R_q such that $R_q\cdot p=q$, but R_q is not a continuous function of q when n is odd and at least equal to 3. However, here we can profit from the information encoded in the matrix h.

The set of all orthogonal transformations which takes p to $q=h\cdot p$ (up to a scale) form a fiber $P_{p,q}$ in a principal bundle P with base $X=GL_+(n,\mathbb{R})\times S^{n-1}$, consisting of the pairs $(h,p/|p|)$, and the fiber is isomorphic with $\mathrm{SO}(n-1)$; the '+' refers to matrices with positive determinant. The base contracts to $X'=\mathrm{SO}(n)\times S^{n-1}$ (by the Cartan decomposition). On the other hand, over X' the bundle P is trivial, the trivialization being given by $(h,p)\mapsto h$. Thus P is trivial. We choose a trivialization $(h,p)\mapsto R(h,p)$. We choose $B(h,p)\in\mathrm{Spin}(n)$ which projects down to $R\in\mathrm{SO}(n)$. There is a $\mathbb{Z}_2$ ambiguity in the choice which does not bother us since the transformation law for the Dirac operator is quadratic in B.

If we compute the left-hand side in (A4) with the complete star product instead of the matrix product, we generate symbols of order less than or equal to zero. Thus we have proven the following lemma:

Lemma. There is a function $B(h)$ of the basis h taking values in the group of invertible PSDO's of order zero such that $B^*\gamma^k h_{kj}p_j B$ differs from $\lambda(x,p)^{-1}\gamma^k p_k$ by an operator of order zero.

The unitarily equivalent Hamiltonian $B'=B^*D_hB$ has then the property that $[\epsilon,B^*D_hB]$ is a PSDO of order zero. One can now apply the recursive method in section 2 to obtain the renormalization operator $T=T(A)$ where now $A=B'-D_0$ and $D_0=\gamma^k p_k$. [The crucial step is the first application of Lemma 2.12: even though $A\in O_1$ (*i.e.*, $|D_0|^{-1}A\in O_0$) is unbounded, α Eq. (2.13) is O_{-1} and thus A' Eq. (2.8) is in O_0 (bounded). We also note that in this argument one never

considers the (ill defined) time evolution (Dyson series) Eq. (2.3) with the unbounded potential $A(t)$ but only the regularized one with a bounded potential.] This method applies as well to the case of combined background gauge and gravitational interactions.

APPENDIX B: ESTIMATES

(1) We consider here the Dyson series (2.3) solving the time evolution equation (2.2) with $h_A(t) = e^{itD_0}A(t)e^{-itD_0}$. If $A(t)$ is bounded for all t, one can easily prove by induction that

$$\|V_n(t,t')\| \leq \frac{1}{n!}\left(\int_{t'}^{t} dr\|A(r)\|\right)^n$$

which shows that (2.3) converges in the operator norm $\|\cdot\|$ for all $t,t' \in \mathbb{R}$.

Similarly, if $[\epsilon,A(t)]$ is of Hilbert-Schmidt type for all t, then the Hilbert-Schmidt norm of V_n can be estimated as

$$\|[\epsilon,V_n(t,t')]\|_2 \leq \int_{t'}^{t} dr\|[\epsilon,A(r)]\|_2 \frac{1}{(n-1)!}\left(\int_{t'}^{t} dr\|A(r)\|\right)^{n-1}$$

showing that $[\epsilon,V(t,t')]$ is also of Hilbert-Schmidt type.

(2) Here we prove the following result which was used in the proof of Lemma 2.12 in the main text (for notation see there): Let

$$f(x)=e^{-x}, \quad x^{-1}(e^x-1), \quad x^{-2}(e^x-1-x)$$

($x \in \mathbb{R}$). Then for all $\alpha=\alpha(t) \in O_0$ with $\alpha'=d\alpha/dt \in O_0$, the operators

$$a=f(\alpha), \quad \frac{d}{dt}f(\alpha)$$

all exist and

$$a_{(n)}=[|D_0|,a_{(n-1)}], \quad a_0=a$$

for $n=0,1,2,...$ all are bounded. Especially ab and ba are in O_{-l} for all $b \in O_{-l}$, $l=0,1,...$.

Proof: The functions $f(x)$ above all are analytic and have Taylor series with infinite radius of convergence,

$$f(x)=\sum_{\nu=0}^{\infty} c_\nu x^\nu, \quad \sum_{\nu=0}^{\infty} |c_\nu| x^\nu \equiv \tilde{f}(x),$$

thus

$$\|f(\alpha)_{(1)}\| = \|\sum_\nu c_\nu[|D_0|,\alpha^\nu]\| \leq \sum |c_\nu|\nu\|\alpha\|^{\nu-1}\|\alpha_{(1)}\| = \tilde{f}'(\|\alpha\|)\|\alpha_{(1)}\|,$$

and this argument can be easily extended to upper bound all $\|f(\alpha)_{(n)}\|$ by polynomials in $\tilde{f}^{(1\leq\nu\leq n)}(\|\alpha\|)$ (ν-th derivative) and $\|\alpha_{1\leq m\leq n}\|$. An efficient way to obtain these bounds is to use the generating functional for these repeated commutators,

$$e^{is|D_0|}\alpha e^{-is|D_0|} = \sum_{n=0}^{\infty} \frac{(is)^n}{n!}\alpha_{(n)},$$

i.e.

$$\|f(\alpha)_{(n)}\| = \left\| \frac{d^n}{d(is)^n} \epsilon^{is|D_0|} f(\alpha) \epsilon^{-is|D_0|} \right\|_{s=0}$$

$$= \left\| \frac{d^n}{d(is)^n} f(e^{is|D_0|} \alpha e^{-is|D_0|}) \right\|_{s=0} \leqslant \frac{d^n}{ds^n} \tilde{f}\left(\sum_{m=1}^{n} \frac{\|\alpha_{(m)}\| s^m}{m!} \right) \Bigg|_{s=0}.$$

Similarly,

$$F(\alpha,\alpha') \equiv \frac{d}{dt} f(\alpha) = \sum_{\nu=0}^{\infty} c_\nu \sum_{\mu=0}^{\nu-1} \alpha^{\nu-1-\mu} \alpha' \alpha^{\mu}$$

and

$$\|F(\alpha,\alpha')_{(n)}\| = \left\| \frac{d^n}{d(is)^n} F(e^{is|D_0|} \alpha e^{-is|D_0|}, e^{is|D_0|} \alpha' e^{-is|D_0|}) \right\|_{s=0}$$

$$\leqslant \frac{d^n}{ds^n} \tilde{f}'\left(\sum_{m=1}^{n} \frac{\alpha_{(m)}\| s^m}{m!} \right)\left(\sum_{m'=1}^{n} \frac{\|\alpha'_{(m')}\| s^{m'}}{m'!} \right) \Bigg|_{s=0}$$

which also is always finite by our assumption $\alpha,\alpha' \in O_0$.

If all repeated commutators $a_{(n)}$ of a with $|D_0|$ are bounded and $b \in O_{-l}$, then $ab, ba \in O_{-l}$ follows from the definition of O_{-l} and the ideal property of B_2.

APPENDIX C: PSEUDODIFFERTIAL OPERATORS (PSDO's)

To fix our notation we summarize here the basic definitions and facts about PSDO's.[10] A PSDO A on the Hilbert space $L^2(M^n) \oplus V$, with M^n a smooth manifold and V a finite-dimensional vector space, is given locally by its symbol $a(x,p) = \sigma(A)(x,p)$ which is a smooth matrix-$[gl(V,V)$-$]$ valued function of the local coordinates $x \in U \subset \mathbb{R}^n$ and momenta $p \in \mathbb{R}^n$.[10] The action of A on a section ψ with support in U is given as

$$(A\psi)(x) = \frac{1}{(2\pi)^{n/2}} \int a(x,p) \hat{\psi}(p) e^{-ip\cdot x} dp, \tag{C1}$$

where $\hat{\psi}$ is the Fourier transform of the function $\psi: U \to V$,

$$\hat{\psi}(p) = \frac{1}{(2\pi)^{n/2}} \int e^{ix\cdot p} \psi(x) dx. \tag{C2}$$

We shall consider the restricted class of PSDO's which admit an asymptotic expansion of the symbol as

$$a(x,p) \sim a_k(x,p) + a_{k-1}(x,p) + a_{k-2}(x,p) + \cdots,$$

where k is an integer and each a_j is a homogeneous matrix-valued function of the momenta, of order j, with $|a_j| \sim |p|^j$ as $\sqrt{p_1^2 + \ldots + p_n^2} = |p| \to \infty$. The order of such a PSDO is ord $a = k$.

The asymptotic expansion for the product of two PSDO's is given by the formula

$$a * b \sim \sum \frac{(-i)^{|m|}}{m!} [(\partial_p)^m a(x,p)][(\partial_x)^m b(x,p)], \tag{C3}$$

where the sum is over all sets of nonnegative integers $m=(m_1,\ldots,m_n)$, $|m|=m_1+\cdots+m_n$, $\partial_x^m = (\partial/\partial x_1)^{m_n}\cdots(\partial/\partial x_n)^{m_n}$, etc., and $m!=m_1!\cdots m_n!$.

The order of $a*b$ is equal to the sum of ord a+ord b since the leading term in $a*b$ is just the matrix product ab of the symbols.

The symbol of a massless Dirac operator D_A in an external vector potential A is $\gamma^k(p_k+A_k)$ where $\gamma_i\gamma_j+\gamma_j\gamma_i=g_{ij}$ are the Dirac gamma matrices and $g=(g_{ij})$ is the metric tensor. The symbol for the square D_A^2 is p^2+ lower order terms in p and therefore the symbol of $|D_A|$ is $|p|+$lower order terms. From this follows, using (C3), that the symbol of $[|D_A|,B]$ is $|p_k/|p|\partial/\partial x_k b(x,p)+$terms of order ord B for any PSDO B with symbol b. In particular, the order of $[|D_A|,B]$ is at most equal to the order of B.

On a compact manifold of dimension n a PSDO is of the trace class if its order is strictly less than $-n$ and it is of Hilbert-Schmidt type if the order is $<-n/2$. In $\mathbb{R}^n$ one has to assume in addition that the symbol is either compactly supported in x or at least the asymptotic behavior of the symbol and its derivatives at $|x|\to\infty$ is as $|x|^{-k}$, where $k>n$ in case of trace class operators and $k>n/2$ for Hilbert-Schmidt operators. In $\mathbb{R}^n$ the trace (when it exists) of a PSDO is simply given as

$$\mathrm{Tr}\, A=\frac{1}{(2\pi)^n}\int \mathrm{tr}\, a(x,p)dpdx. \tag{C4}$$

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Quasi-exactly solvable potentials on the line and orthogonal polynomials

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In this paper we show that a quasi-exactly solvable (normalizable or periodic) one-dimensional Hamiltonian satisfying very mild conditions defines a family of weakly orthogonal polynomials which obey a three-term recursion relation. In particular, we prove that (normalizable) exactly solvable one-dimensional systems are characterized by the fact that their associated polynomials satisfy a two-term recursion relation. We study the properties of the family of weakly orthogonal polynomials defined by an arbitrary one-dimensional quasi-exactly solvable Hamiltonian, showing in particular that its associated Stieltjes measure is supported on a finite set. From this we deduce that the corresponding moment problem is determined, and that the kth moment grows like the kth power of a constant as k tends to infinity. We also show that the moments satisfy a constant coefficient linear difference equation, and that this property actually characterizes weakly orthogonal polynomial systems. © *1996 American Institute of Physics.* [S0022-2488(96)03108-8]

I. INTRODUCTION

In a recent paper,[1] Bender and Dunne introduced a remarkable family of orthogonal polynomials associated to the one-dimensional Hamiltonian

$$H=-\partial_x^2+\frac{(4s-1)(4s-3)}{4x^2}-(4s+4J-2)x^2+x^6, \tag{1}$$

where J is a positive integer and s is a real parameter. If $\psi_E(x)$ denotes an eigenfunction of H with energy E, the polynomials $P_k(E)$ in question are proportional to the coefficients in the expansion of $e^{x^4/4}x^{1/2-2s}\psi_E(x)$ in powers of x^2, namely

$$\psi_E(x)=e^{-x^4/4}x^{2s-1/2}\sum_{k=0}^{\infty}\frac{(-1)^k}{k!}\frac{P_k(E)}{\Gamma(k+2s)}\left(\frac{x^2}{4}\right)^k.$$

These polynomials are easily shown to satisfy a three-term recursion relation, from which it follows[2] that they are orthogonal with respect to a certain Stieltjes measure $d\omega(E)$ (ω being a function of bounded variation):

$$\int P_k(E)P_l(E)d\omega(E)=0, \quad k\neq l. \tag{2}$$

The form of the coefficients of the recursion relation satisfied by the polynomial system $\{P_k(E)\}_{k=0}^{\infty}$ implies that this system has several remarkable properties. First of all, the norm of the polynomials P_k with $k\geqslant J$ vanishes. Thus the polynomials P_k form what is called a *weakly orthogonal* polynomial system.[2] To be precise, we shall use from now on the term *orthogonal polynomial system* for a family of orthogonal polynomials $\{P_k(E)\}_{k=0}^{\infty}$ with $\deg P_k=k$ for all k, and such that the norm of P_k does not vanish for any k.

Second, each P_k with $k\geqslant J$ factors into the product of P_J and another polynomial, i.e.,

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$$P_{J+m}=P_J Q_m, \quad m\geq 0,$$

where Q_m has degree m. Finally, the J simple real zeros of P_J are eigenvalues of H whose corresponding eigenfunctions, being the product of the factor

$$\mu(x)=e^{-x^4/4}x^{2s-1/2}$$

times a polynomial in x^2, are square integrable. The existence of these exactly computable eigenfunctions and eigenvalues of H had been deduced before[3,4] from the fact that H is *quasi-exactly solvable*, meaning that it is an element of the enveloping algebra of a certain realization of $\mathfrak{sl}(2,\mathbb{R})$ in terms of first-order differential operators acting on a finite-dimensional subspace of the space of C^∞ functions (see the next section for more details). The above results strongly suggest[5] that there is a connection between quasi-exactly solvable Hamiltonians and certain families of weakly orthogonal polynomials. In this paper, we show in detail that this is indeed the case for all one-dimensional quasi-exactly solvable Hamiltonians, both normalizable and periodic, satisfying very general conditions.

The paper is organized as follows. Using the results on quasi-exact solvability reviewed in Sec. II, we explain in Sec. III how to construct the weakly orthogonal polynomial system associated to each of the normal forms of a one-dimensional quasi-exactly solvable Hamiltonian listed in Refs. 4 and 6. Like the polynomial system introduced in Ref. 1, this system always satisfies a three-term recursion relation, whose coefficients we explicitly compute. This allows us to prove that one-dimensional (normalizable) exactly solvable Hamiltonians are characterized by the fact that their associated polynomials satisfy a two-term recursion relation. In Sec. IV we show that the polynomials associated to an arbitrary one-dimensional quasi-exactly solvable Hamiltonian enjoy properties completely akin to those listed above for the Hamiltonian (1). We also study in this section the properties of the moment functional defined by the family of weakly orthogonal polynomials of a quasi-exactly solvable Hamiltonian, giving a rigorous proof of the fact that its associated Stieltjes measure is supported on a finite set,[5] so that the integral (2) reduces to a finite sum. From this we deduce that the associated (Hamburger or Stieltjes) moment problem is determined, and that the kth moment behaves like the kth power of a constant for large k, illustrating this statement with an explicit example for the Hamiltonian (1). We also show that the moments satisfy a constant coefficient linear difference equation, a property which in fact characterizes weakly orthogonal polynomial systems. The paper ends (Sec. V) with a brief review of these results, stressing the role played by weak orthogonality—as opposed to true orthogonality—in their derivation.

II. QUASI-EXACTLY SOLVABLE POTENTIALS

For the reader's convenience, we present in this section a summary of the major results in the theory of quasi-exactly solvable systems that we shall need in the sequel. A one-dimensional Schrödinger operator (or Hamiltonian) $H=-\partial_x^2+V(x)$ is *quasi-exactly solvable* if there exists a finite-dimensional Lie algebra of first-order differential operators

$$\mathfrak{g}=\mathrm{Span}\{\xi_a(x)\partial_x+\eta_a(x)\,|\,1\leq a\leq r\}\equiv\mathrm{Span}\{T_a(x)\,|\,1\leq a\leq r\}$$

such that

(i) $\mathfrak{g}$ leaves invariant a finite-dimensional module of smooth functions $\mathfrak{N}\subset C^\infty(\mathbb{R})$, i.e., $X\cdot f\in\mathfrak{N}$ for all $f\in\mathfrak{N}$ and all $X\in\mathfrak{g}$. In other words, $\mathfrak{g}$ admits a finite-dimensional representation in terms of smooth functions.

(ii) H is in the universal enveloping algebra of $\mathfrak{g}$, i.e., H can be expressed as a polynomial in the generators T_a, $1\leq a\leq r$, of $\mathfrak{g}$.

A Lie algebra of first-order differential operators satisfying (i) is called *quasi-exactly solvable*. A Hamiltonian H satisfying condition (ii) above for an arbitrary (not necessarily quasi-exactly solvable) Lie algebra $\mathfrak{g}$ is said to be *Lie algebraic*.

If H is quasi-exactly solvable, it follows that the restriction of H to $\mathfrak{N}$ is a finite-dimensional linear operator $\mathfrak{N}\to\mathfrak{N}$, and therefore the eigenfunctions of H lying in $\mathfrak{N}$ and their corresponding eigenvalues can be exactly computed by purely algebraic methods (diagonalizing a square matrix of order $\dim \mathfrak{N}$). We shall refer to these eigenfunctions of H lying in $\mathfrak{N}$ as its *algebraic eigenfunctions* (although, of course, they need not be algebraic functions in the technical sense of the word). The functions in $\mathfrak{N}$ need not *a priori* satisfy any boundary conditions (like square-integrability, periodicity, vanishing at the end points, etc.) coming from the physics of the problem, whose mathematical purpose is to guarantee that H is a self-adjoint operator. If they do, then the restriction of H to $\mathfrak{N}$ is self-adjoint, and therefore H has exactly $\dim \mathfrak{N}$ linearly independent algebraic eigenfunctions, whose corresponding $\dim \mathfrak{N}$ *real* eigenvalues (counting multiplicities) are exactly (i.e., algebraically) computable. We shall say in this case that the quasi-exactly solvable potential H (or the potential V) is *fully algebraic*. See Refs. 4 and 6 for an in-depth discussion of fully algebraic potentials under the boundary condition of square integrability on $\mathbb{R}$.

It can be shown (cf. Ref. 7) that a quasi-exactly solvable Schrödinger operator H can be expressed as a polynomial of degree at most two in the generators T_a, $1\leqslant a\leqslant r$, of $\mathfrak{g}$. Moreover, a well known theorem[3,8,7] asserts that every quasi-exactly solvable Lie algebra of first-order differential operators $\mathfrak{g}$ is related by a (local) change of variable

$$z=\zeta(x) \tag{3}$$

and a *gauge transformation* with gauge factor $\mu(z)>0$ to (a subalgebra of) one of the Lie algebras $\mathfrak{g}^n=\mathfrak{h}^n\oplus\mathbb{R}$, where $\mathfrak{h}^n=\mathrm{Span}\{J^n_-,J^n_0,J^n_+\}\approx\mathfrak{sl}(2,\mathbb{R})$,

$$J^n_-=\partial_z,\quad J^n_0=z\partial_z-\frac{n}{2},\quad J^n_+=z^2\partial_z-nz, \tag{4}$$

and n is a nonnegative integer. In other words, every element $X(x)\in\mathfrak{g}$ is of the form

$$X(x)=\mu(z)\cdot J(z)\cdot\left.\frac{1}{\mu(z)}\right|_{z=\zeta(x)},\quad J(z)\in\mathfrak{g}^n,$$

for some fixed n. This implies that the *gauge Hamiltonian*

$$H_{\text{gauge}}(z)=\left.\frac{1}{\mu(z)}\cdot H(x)\cdot\mu(z)\right|_{x=\zeta^{-1}(z)} \tag{5}$$

is also a polynomial of degree at most two in the generators J^n_ϵ, i.e., (dropping the explicit n dependence in the generators J^n_ϵ)

$$-H_{\text{gauge}}=\sum_{a,b}c_{ab}J_aJ_b+\sum_a c_aJ_a+c_*, \tag{6}$$

for some real constants c_*, c_a, and $c_{ab}=c_{ba}$ (the minus sign is for later convenience). The spectral problems of H and H_{gauge} are related in an obvious way: indeed, from (5) it follows that if $\chi(z)$ is an eigenfunction of H_{gauge} with eigenvalue E then

$$\psi(x)=\mu(z)\chi(z)|_{z=\zeta(x)} \tag{7}$$

will be an eigenfunction of H with the same eigenvalue (not taking into account the boundary conditions). Since the Lie algebra $\mathfrak{g}^n$ admits as invariant module the space $\mathscr{P}_n$ of real polynomials of degree at most n in z, if H is fully algebraic then H_{gauge} has $n+1$ linearly independent algebraic eigenfunctions lying in $\mathscr{P}_n$. Hence H has $n+1$ linearly independent algebraic eigenfunctions of the form (7), with $\chi \in \mathscr{P}_n$ a polynomial of degree at most n.

From (4) and (6) it follows[4] that the gauge Hamiltonian is of the form

$$-H_{\text{gauge}} = P(z)\partial_z^2 + \left\{ Q(z) - \frac{n-1}{2} P'(z) \right\} \partial_z + \left\{ R - \frac{n}{2} Q'(z) + \frac{n(n-1)}{12} P''(z) \right\}, \tag{8}$$

where P, Q, and R are polynomials of degrees 4, 2, and 0, respectively, given by

$$P(z) = c_{++}z^4 + 2c_{+0}z^3 + c_{00}z^2 + 2c_{0-}z + c_{--}, \tag{9}$$

$$Q(z) = c_+ z^2 + c_0 z + c_-, \tag{10}$$

$$R = \frac{n(n+2)}{12} c_{00} + c_*. \tag{11}$$

Note that, due to the Casimir relation

$$J_0^2 - \frac{1}{2}(J_+J_- + J_-J_+) = \frac{n}{4}(n+2),$$

we have set, without loss of generality, $c_{+-}=0$. There are also explicit formulas for the change of variables (3) and gauge factor $\mu(z)$ needed to put the differential operator (8) in Schrödinger form, cf. Ref. 4. Indeed, assuming that $P(z)>0$ on an interval I then for $z \in I$ we have

$$x = \zeta^{-1}(z) = \int^z \frac{dy}{\sqrt{P(y)}}, \quad \mu(z) = P(z)^{-n/4} \exp\left\{ \int^z \frac{Q(y)}{2P(y)}\, dy \right\} \tag{12}$$

and

$$V(x) = -R + \left. \frac{-n(n+2)(PP'' - \frac{3}{4}P'^2) - 3(n+1)(QP' - 2PQ') + 3Q^2}{12P} \right|_{z=\zeta(x)}, \tag{13}$$

where the primes denote derivatives with respect to z.

The canonical form (8) of the quasi-exactly solvable Hamiltonian H is not unique, since there is a residual symmetry group preserving the Lie algebra $\mathfrak{h}^n$, given by the adjoint action on $\mathfrak{h}^n$ of the Lie group of transformations generated by $\mathfrak{g}^n = \mathfrak{h}^n \oplus \mathbb{R}$. More precisely, the elements of $\mathfrak{g}^n$ are the infinitesimal generators of the standard GL(2,$\mathbb{R}$) action on the space $\mathscr{P}_n$, given by

$$p(z) \in \mathscr{P}_n \mapsto \hat{p}(w) = (\gamma w + \delta)^n p\left(\frac{\alpha w + \beta}{\gamma w + \delta} \right), \quad \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \in GL(2,\mathbb{R}). \tag{14}$$

We shall denote, as is customary, by ρ_n this (irreducible) multiplier representation of GL(2,$\mathbb{R}$) on $\mathscr{P}_n$. Note that the action (14) is just the composition of the projective transformation

$$z = \frac{\alpha w + \beta}{\gamma w + \delta}$$

and the gauge transformation with gauge factor $\mu(w)=(\gamma w+\delta)^n$. The adjoint action of $\mathrm{GL}(2,\mathbb{R})$ on $\mathfrak{h}^n$ induced by (14) is given by

$$J(z)\mapsto\hat{J}(w)=(\gamma w+\delta)^n\cdot J\left(\frac{\alpha w+\beta}{\gamma w+\delta}\right)\cdot(\gamma w+\delta)^{-n}. \tag{15}$$

A straightforward calculation[4] shows that the generators of $\mathfrak{h}^n$ transform under the representation $\rho_{2,-1}$—where $\rho_{n,i}=\rho_n\otimes\det^i$, $\det{:}A\mapsto\det A$ being the standard determinantal representation—independently of n. As a consequence of all this, the transformed differential operator

$$\hat{H}_{\text{gauge}}=(\gamma w+\delta)^n\cdot H_{\text{gauge}}\left(\frac{\alpha w+\beta}{\gamma w+\delta}\right)\cdot(\gamma w+\delta)^{-n} \tag{16}$$

is still of the form (8), with P, Q, and R replaced by appropriate polynomials $\hat{P}$, $\hat{Q}$, and $\hat{R}$ of respective degrees 4, 2, and 0. It can be shown, cf. Ref. 4, that $\hat{R}=R$ and

$$\hat{P}(w)=\frac{(\gamma w+\delta)^4}{\Delta^2}P\left(\frac{\alpha w+\beta}{\gamma w+\delta}\right),\quad \hat{Q}(w)=\frac{(\gamma w+\delta)^2}{\Delta}Q\left(\frac{\alpha w+\beta}{\gamma w+\delta}\right), \tag{17}$$

with

$$\Delta=\det\begin{pmatrix}\alpha & \beta\\ \gamma & \delta\end{pmatrix}.$$

Hence the polynomials P, Q, and R determining the differential operator H_{gauge} transform under the representations $\rho_{4,-2}$, $\rho_{2,-1}$, and ρ_0 of $\mathrm{GL}(2,\mathbb{R})$. Furthermore, the algebraic eigenfunctions of H_{gauge} clearly transform under the representation ρ_n; indeed, if $\chi(z)$ is an eigenfunction of H_{gauge} with eigenvalue E then it follows from (16) that

$$\hat{\chi}(w)=(\gamma w+\delta)^n\cdot\chi\left(\frac{\alpha w+\beta}{\gamma w+\delta}\right) \tag{18}$$

is an eigenfunction of $\hat{H}_{\text{gauge}}$ with the same eigenvalue.

In Refs. 6 and 4, the form invariance of the differential operator H_{gauge} under the $\mathrm{GL}(2,\mathbb{R})$ action (16) described above was exploited to place H_{gauge} in canonical form. Indeed, it can be shown that there are ten inequivalent real normal forms for a (nonzero) fourth-degree polynomial P (Ref. 9) transforming under the representation $\rho_{4,-2}$ of $\mathrm{GL}(2,\mathbb{R})$, each of which leads to a canonical form for H_{gauge}. Of these ten canonical forms, five correspond to *normalizable* Hamiltonians, whose algebraic eigenfunctions are square integrable (provided the coefficients c_{ab} and c_a satisfy certain inequalities), and the remaining are associated to Hamiltonians with periodic potentials. The five normal forms associated to normalizable Hamiltonians, which are characterized by the fact that P has at least one multiple root on the real projective line $\mathbb{RP}$, are given by

$$\begin{aligned}&1.\ \nu(z^2+1),\\ &2.\ \nu(z^2-1),\\ &3.\ \nu z^2,\\ &4.\ z,\\ &5.\ 1,\end{aligned} \tag{19}$$

where $\nu>0$ is a real parameter. For example, the quasi-exactly solvable potential discussed in Ref. 1 corresponds to the fourth normalizable canonical form $P(z)=z$. The remaining normal forms, corresponding to periodic potentials, are

$$\begin{aligned} &6.\ \nu(1-z^2)(1-\kappa^2 z^2),\\ &7.\ \nu(1-z^2)(1-\kappa^2(1-z^2)),\\ &8.\ \nu(1+z^2)(1+(1-\kappa^2)z^2),\\ &9.\ \nu(1+z^2)^2,\\ &10.\ \nu(1-z^2), \end{aligned} \tag{20}$$

where $\nu>0$, $0<\kappa<1$.

III. THE RECURSION RELATION

Let $H=-\partial_x^2+V(x)$ be a quasi-exactly solvable Hamiltonian. From the previous section, we know that there is a change of variable (3) and gauge factor $\mu(z)>0$ such that $H(x)=\mu(z)\cdot H_{\text{gauge}}(z)\cdot[1/\mu(z)]\big|_{z=\zeta(x)}$, with H_{gauge} given by (6) (and $c_{+-}=0$). Furthermore, if H is fully algebraic then it has $n+1$ algebraic eigenfunctions of the form (7), with $\chi(z)\in\mathscr{P}_n$ an eigenfunction of H_{gauge}. Let $\chi_E(z)$ be an eigenfunction of H_{gauge} with eigenvalue E (not necessarily a polynomial in z). Writing

$$\chi_E(z)=\sum_{k=0}^{\infty} P_k(E)\chi_k(z), \tag{21}$$

where

$$\chi_k(z)=\frac{z^k}{k!},\quad k\geq 0,$$

and taking into account that

$$J_-\cdot\chi_k=\chi_{k-1},\quad J_0\cdot\chi_k=\left(k-\frac{n}{2}\right)\chi_k,\quad J_+\cdot\chi_k=(k-n)(k+1)\chi_{k+1}, \tag{22}$$

cf. (4), we easily find that the coefficients $P_k(E)$ satisfy the following five-term recursion relation:

$$\begin{aligned} -c_{--}P_{k+2}=&[(2k-n+1)c_{0-}+c_-]P_{k+1}+\left[E+c_*+c_0\left(k-\frac{n}{2}\right)+c_{00}\left(k-\frac{n}{2}\right)^2\right]P_k+k(k-1-n)\\ &\times[(2k-n-1)c_{+0}+c_+]P_{k-1}+k(k-1)(k-1-n)(k-2-n)c_{++}P_{k-2},\quad k\geq 0. \end{aligned} \tag{23}$$

If $c_{--}\neq 0$, the general solution of the recursion relation (23) depends on the two arbitrary functions $P_0(E)$ and $P_1(E)$. This simply reflects the fact that when $c_{--}\neq 0$ the leading coefficient $P(z)$ of H_{gauge} does not vanish at $z=0$ [cf. (9)]; thus, the differential equation $(H_{\text{gauge}}-E)\chi_E=0$ has a regular point at the origin, and therefore it admits two linearly independent solutions (21) analytic at 0. If $P_0(E)$ and $P_1(E)$ are chosen to be polynomials in E, then (23) implies that all the coefficients $P_k(E)$ are polynomials in E. However, the general recursion relation (23) suffers from two major drawbacks. In the first place, even if we choose $P_0(E)$ and $P_1(E)$ as polynomials of

degree 0 and 1 in E, respectively, (23) is incompatible with the desirable property that $P_k(E)$ be of degree k in E for all k, unless $c_{--}=0$. Second, even in this case (23) will be in general a four-term recursion relation, implying that the polynomials $P_k(E)$ may not be orthogonal with respect to any (nonzero) Stieltjes measure $d\omega(E)$. Indeed, it is well known,[2,10] that a necessary and sufficient condition for a family of polynomials $\{P_k\}_{k=0}^{\infty}$ (with deg $P_k=k$) to form an orthogonal polynomial system is that $P_k(E)$ satisfies a *three*-term recursion relation of the form

$$P_k=(A_kE+B_k)P_{k-1}+C_kP_{k-2}, \quad k\geq 1, \tag{24}$$

where the coefficients A_k, B_k, C_k are *independent* of E, $A_k\neq 0$, $C_1=0$, and $C_k\neq 0$ for $k>1$. If the coefficient C_k in (24) vanishes for some positive integer k, then this recursion relation only defines a *weakly* orthogonal polynomial system.[11] It is one of the main goals of this paper to show that both difficulties described above can always be overcome, provided (roughly speaking) that we expand the eigenfunction χ_E with respect to an appropriate variable. This will be achieved by using the nonuniqueness of H_{gauge}, due to the GL(2) symmetry described in the previous section, to place H_{gauge} in a suitable canonical form.

From the form of the recursion relation (23), it follows that both difficulties described above disappear if

$$c_{--}=c_{++}=0. \tag{25}$$

Indeed, if (25) holds then (23) reduces to the three-term recursion relation

$$-[(2k-n-1)c_{0-}+c_-]P_k=\left[E+c_*+c_0\left(k-\frac{n}{2}-1\right)+c_{00}\left(k-\frac{n}{2}-1\right)^2\right]P_{k-1}+(k-1)\times(k-2-n)[(2k-n-3)c_{+0}+c_+]P_{k-2}, \quad k\geq 1, \tag{26}$$

which uniquely determines all the functions $P_k(E)$ in terms of $P_0(E)$ provided that, for all positive integer values of k, the coefficient of the left-hand side of (26) does not vanish. If $P_0(E)$ is taken as a constant, for instance if $P_0(E)=1$, then (26) implies that $P_k(E)$ is a polynomial of degree k in E for all $k\geq 0$.

Let us see now that we can always arrange for (25) to be satisfied, by using the action (17) to transform $P(z)$ into a normal form $\hat{P}(w)$ for which (25) holds. Indeed, (25) simply states that the polynomial $P(z)$ vanishes at $z=0$ and $z=\infty$, when z is allowed to vary over the complex projective line $\mathbb{CP}$. Note that we need z to belong to the *complex* projective line at this stage so that P is guaranteed to have a root, which is essential for the argument that follows. Consequently, the GL(2,$\mathbb{R}$) action described in the previous section will be replaced in what follows by a GL(2,$\mathbb{C}$) action.

We can assume, first of all, that $P(z)$ is one of the normal forms listed in Eqs. (19) and (20). We must distinguish three cases, characterized by the position of the roots of P in the complex projective line. Indeed, either P has two different roots $z_1\neq z_2$ in $\mathbb{CP}$, or it has four coincident roots. In the first case, either one of the roots is at infinity, or both roots are finite.

A. Case 1: P has two different roots $z_1\neq z_2=\infty$

This case occurs when P is one of the first four normalizable canonical forms (19), or the fifth periodic canonical form (20). In this case, the translation $w=z-z_1$ transforms $P(z)$ into a polynomial $\hat{P}(w)$ vanishing at zero and infinity. In the original z coordinate, by (18) this amounts to replacing (21) by

$$\chi_E(z)=\sum_{k=0}^{\infty}P_k(E)\frac{(z-z_1)^k}{k!}. \tag{27}$$

In other words, we expand $\chi_E(z)$ as a power series around the point $z=z_1$, which is a singular point of the linear differential equation $(H_{\text{gauge}}-E)\chi_E=0$ (if z_1 is a simple root of P, z_1 is actually a regular singular point, whose indicial equation is easily seen to have 0 as a root). By (7), in the "physical" coordinate x (27) becomes

$$\psi_E(x)=\mu(\zeta(x))\sum_{k=0}^{\infty} P_k(E)\,\frac{(\zeta(x)-z_1)^k}{k!} \tag{28}$$

B. Case 2: P has two different finite roots $z_1 \neq z_2$

This is the case when P is one of the first four periodic normal forms (20). The projective transformation $w=(z-z_1)/(z-z_2)$ will again transform $P(z)$ into a polynomial $\hat{P}(w)$ vanishing at $w=0, \infty$. Going back to the original z coordinate, by (18) we just have to replace (21) by

$$\chi_E(z)=(z-z_2)^n\sum_{k=0}^{\infty}\frac{1}{k!}P_k(E)\left(\frac{z-z_1}{z-z_2}\right)^k, \tag{29}$$

apart from an inessential overall factor. In terms of the physical coordinate x, (29) can be written as

$$\psi_E(x)=\mu(\zeta(x))(\zeta(x)-z_2)^n\sum_{k=0}^{\infty}\frac{1}{k!}P_k(E)\left(\frac{\zeta(x)-z_1}{\zeta(x)-z_2}\right)^k. \tag{30}$$

C. Case 3: P has a quadruple root

This corresponds to the fifth normalizable canonical form, $P=1$, which has a quadruple root at infinity. Note that $P=1$ implies that the physical coordinate x can be taken as the canonical coordinate z. By (9), we have

$$c_{++}=c_{+0}=c_{00}=c_{0-}=0, \quad c_{--}=1.$$

Performing an additional translation, if necessary, we can also take without loss of generality $c_-=Q(0)=0$ (notice that P is constant, and therefore does not change under translations). Thus Eq. (23) reduces in this case to

$$-P_{k+2}=\left[E+c_*+c_0\left(k-\frac{n}{2}\right)\right]P_k+k(k-1-n)c_+P_{k-1}, \quad k\geq 0. \tag{31}$$

Since $P=1$ is the fifth normalizable case of Refs. 4 and 6, c_+ must vanish if we want H to be *normalizable*, i.e., the algebraic eigenfunctions of H to be square integrable. Therefore, in this case (31) reduces to

$$-P_{k+2}=\left[E+c_*+c_0\left(k-\frac{n}{2}\right)\right]P_k, \quad k\geq 0,$$

which is equivalent to two two-term recursion relations for the even and odd coefficients $P_j^0=P_{2j}$ and $P_j^1=P_{2j+1}$, namely

$$-P_{j+1}^{\epsilon}=\left[E+c_*+c_0\left(2j+\epsilon-\frac{n}{2}\right)\right]P_j^{\epsilon}, \quad j\geq 0; \quad \epsilon=0,1. \tag{32}$$

Note that in this case the potential is $V(x)=1/4c_0^2x^2-c_*$ (with $c_0<0$), cf. Ref. 4.

To complete the discussion of cases 1 and 2, we still have to deal with an important technical issue; namely, we must find under what conditions the coefficient of P_k in (26) never vanishes for positive integer values of k. Let $\hat{P}$ and $\hat{Q}$ be the transforms of P and Q under the projective transformation $z \mapsto w$ defined in the foregoing discussion of cases 1 and 2; note that, by construction, $\hat{P}(w)$ vanishes at $w=0, \infty$. The coefficient of interest can be expressed as

$$(2k-n-1)\hat{c}_{0-}+\hat{c}_{-}, \quad k \geq 1, \tag{33}$$

where

$$\hat{c}_{0-}=\tfrac{1}{2}\hat{P}'(0), \quad \hat{c}_{-}=\hat{Q}(0).$$

From (17) it easily follows that

$$\hat{c}_{0-}=\tfrac{1}{2}P'(z_1), \quad \hat{c}_{-}=Q(z_1), \tag{34}$$

for case 1 ($w=z-z_1$), and

$$\hat{c}_{0-}=\frac{P'(z_1)}{2(z_1-z_2)}, \quad \hat{c}_{-}=\frac{Q(z_1)}{z_1-z_2}, \tag{35}$$

for case 2 ($w=(z-z_1)/(z-z_2)$). We shall now distinguish three subcases:

1. Case i. z_1 is a simple real root of P

This case occurs when P is one of the canonical forms 2, 4, 6, 7, or 10. Note that in this case the mapping $z \mapsto w$ is real, and so are the coefficients $\hat{c}_{0-}$, $\hat{c}_{-}$. From (12) and (34)–(35) it is immediate to deduce the asymptotic formulas

$$x \underset{z \to z_1}{\sim} |z-z_1|^{1/2}, \quad \mu(z) \underset{z \to z_1}{\sim} |z-z_1|^{1/4(\hat{c}_{-}/c_{0-}-n)},$$

where we have dropped unessential constant multiplicative factors from the right-hand side, and have taken for convenience z_1 as the lower limit of the integral giving x in terms of z. We saw in the previous section that when H is fully algebraic it has $n+1$ linearly independent algebraic eigenfunctions of the form (7), where $\chi \in \mathscr{P}_n$. It follows that the polynomial factor $\chi(z)$ cannot vanish at the origin for all the algebraic eigenfunctions of H. Hence there is at least one algebraic eigenfunction of H whose asymptotic behavior at $x=0$ is given by

$$\psi(x) \underset{x \to 0}{\sim} |x|^{1/2(\hat{c}_{-}/\hat{c}_{0-}-n)}.$$

If *all* the algebraic eigenfunctions of H are regular at $x=0$, then we must have

$$\hat{c}_{-}/\hat{c}_{0-}-n \geq 0. \tag{36}$$

Since (33) can be written as

$$2\hat{c}_{0-}\left[\frac{1}{2}\left(\frac{\hat{c}_{-}}{\hat{c}_{0-}}-n\right)+\left(k-\frac{1}{2}\right)\right],$$

it follows from (36) that the coefficient (33) cannot vanish in this case.

2. Case ii. z_1 is a simple complex root of P

In this case P is either the first or the eighth canonical form. Since z_1 is not real, the mapping $z \mapsto w$ is not real either, and the above asymptotic argument is not valid (the eigenfunctions of H need not be regular outside the real axis). For the first canonical form (19), we can take $w=z-i$ and therefore

$$\hat{c}_{0-}=i\nu, \quad \hat{c}_{-}=c_{-}-c_{+}+ic_0$$

from (34). Hence the coefficient (33) does not vanish in this case provided that the following conditions are satisfied:

$$c_{-}\neq c_{+} \quad \text{or} \quad \frac{1}{2}\left(n+1-\frac{c_0}{\nu}\right)\neq 1,2,\ldots . \tag{37}$$

It is easily checked that the choice $w=z+i$ leads exactly to the same conditions. For the eighth canonical form, we can take $w=(z-i)/(z+i)$, and therefore, from (35),

$$\hat{c}_{0-}=\frac{1}{2}\nu\kappa^2, \quad \hat{c}_{-}=\frac{c_0}{2}+\frac{i}{2}(c_{+}-c_{-}).$$

Hence in this case the conditions for the coefficient (33) not to vanish are

$$c_{-}\neq c_{+} \quad \text{or} \quad \frac{1}{2}\left(n+1-\frac{c_0}{\nu\kappa^2}\right)\neq 1,2,\ldots . \tag{38}$$

It is straightforward to check that the choice $w=(z+i)/(z-i)$ yields the same conditions, while the other natural choice $w=(\sqrt{1-\kappa^2}z\mp i)/(\sqrt{1-\kappa^2}z\pm i)$ only has the effect of replacing the first condition (38) by $c_{+}\neq(1-\kappa^2)c_{-}$.

3. Case iii. z_1 is a multiple root of P

This case takes place when P is either the third or the ninth canonical form, and in both cases (33) reduces to $\hat{c}_{-}$. For the third canonical form (19), if $c_{-}\neq 0$ then we take $w=z$, and therefore $\hat{c}_{-}=c_{-}\neq 0$. If $c_{-}=0$, then $c_{+}\neq 0$ if all the algebraic eigenfunctions of H are square integrable (see Ref. 4). Hence, taking $w=1/z$, we get $\hat{P}(w)=\nu w^2$ and $\hat{Q}=-(c_{+}+c_0 w)$, so that $\hat{c}_{0-}=0$ and $\hat{c}_{-}=-c_{+}\neq 0$. Hence the coefficient (33) cannot vanish in this case. Finally, if P is the ninth canonical form (20) then $w=(z-i)/(z+i)$ and

$$\hat{c}_{-}=\frac{c_0}{2}+\frac{i}{2}(c_{+}-c_{-}).$$

Hence (33) will not vanish if

$$c_{+}\neq c_{-} \quad \text{or} \quad c_0\neq 0. \tag{39}$$

Note that when (39) does not hold V reduces to a constant potential:

$$V=\frac{c_{-}^2}{4\nu}-\frac{5}{12}n(n+2)-c_{*}.$$

In summary, the previous analysis shows that the critical coefficient (33) cannot vanish for any positive integer k provided that V is fully algebraic, that all its algebraic eigenfunctions are

regular [or square integrable, for the third normalizable canonical form (19)], and that conditions (37), (38), and (39) are satisfied when P is one of the normal forms 1, 8, or 9, respectively. If (33) does not vanish, defining new polynomials $\hat{P}_k$ by

$$P_k=\begin{cases}\dfrac{(-1)^k}{(2\hat{c}_{0-})^k}\dfrac{\hat{P}_k}{\Gamma\left(\dfrac{\hat{c}_-}{2\hat{c}_{0-}}+k-\dfrac{n}{2}+\dfrac{1}{2}\right)}, & \text{if } \hat{c}_{0-}\neq 0;\\ \dfrac{(-1)^k}{\hat{c}_-^k}\hat{P}_k, & \text{if } \hat{c}_{0-}=0\end{cases} \tag{40}$$

the recursion relation (26) can be written in the more standard form

$$\hat{P}_{k+1}=\left[E+c_*+\hat{c}_0\left(k-\frac{n}{2}\right)+\hat{c}_{00}\left(k-\frac{n}{2}\right)^2\right]\hat{P}_k-k(k-n-1)[\hat{c}_{+0}(2k-n-1)+\hat{c}_+]$$
$$\times[\hat{c}_{0-}(2k-n-1)+\hat{c}_-]\hat{P}_{k-1},\quad k\geq 0. \tag{41}$$

We have thus proved the main theorem in this section.

Theorem 1: Let V be a fully algebraic one-dimensional quasi-exactly solvable potential whose algebraic eigenfunctions are all regular [or normalizable, if V corresponds to the third or fifth canonical forms in (19)]. Assume, furthermore, that conditions (37), (38), or (39) are satisfied, if V is obtained from the first, eighth, or ninth canonical forms (19)–(20), respectively. Then V defines a family of weakly orthogonal polynomials $\{\hat{P}_k\}_{k=0}^{\infty}$ satisfying a three-term recursion relation (41) [or (32), if V corresponds to the fifth canonical form]. The polynomials $\hat{P}_k$ are defined by (40) and (28), if V is associated to one of the canonical forms 1–4 or 10, or by (40) and (30), if V corresponds to one of the normal forms 6–9. Finally, the potential V associated to the fifth canonical form defines two families of weakly orthogonal polynomials $P_j^0=P_{2j}$ and $P_j^1=P_{2j+1}$ through (28).

We shall say that a quasi-exactly solvable potential V is *exactly solvable* if it is independent of the "spin" parameter n. This implies that V has n algebraic eigenvalues and eigenfunctions for arbitrary $n\in\mathbb{N}$, so that we can algebraically compute an infinite number of eigenvalues of V (leaving aside the boundary conditions). All exactly solvable normalizable one-dimensional potentials have been classified; see Ref. 4 for a complete list. The quintessential example of exactly solvable one-dimensional potential is the harmonic oscillator potential, which corresponds to the fifth canonical form (19). We have seen in the previous section that in this case there are two families of orthogonal polynomials [the odd and even coefficients in (28)], each of which satisfies a two-term recursion relation (32). We shall now show that, as conjectured in Ref. 1, the latter property actually characterizes exactly solvable normalizable potentials:

Theorem 2: The weakly orthogonal polynomial system associated to an exactly solvable normalizable potential satisfies a two-term recursion relation.

Proof: The proof is a simple case-by-case analysis using the classification of exactly solvable normalizable potentials given in Ref. 4. Indeed, for the first normalizable canonical form $P(z)=\nu(z^2+1)$ we have $w=z\mp i$, and therefore $\hat{P}(w)=P(w\pm i)=\nu w(w\pm 2i)$, so that $\hat{c}_{+0}=0$. Since $\hat{Q}(w)=Q(w\pm i)$, we also have $\hat{c}_+=\hat{Q}''(0)/2=Q''(\pm i)/2=c_+$. But the exactly solvable potentials associated to this normal form are characterized by the vanishing of c_+, Ref. 4, so that $\hat{c}_+=\hat{c}_{+0}=0$, and (41) is a two-term recursion relation. Similarly, for the second normalizable canonical form, $P(z)=\nu(z^2-1)$ and, for instance, $w=z\mp 1$. Proceeding as before we obtain that $\hat{c}_{+0}=0$ and $\hat{c}_+=c_+$. Since exactly solvable potentials are again those satisfying the condition $c_+=0$, (41) reduces to a two-term recursion relation.

The third normalizable canonical form has $P(z)=\nu z^2$, and therefore $c_{+0}=c_{0-}=0$. The exactly solvable potentials are characterized by the vanishing of the coefficients c_+ or c_-, but not

both simultaneously. In the former case we can take $w=z$, while in the latter w is proportional to $1/z$ [see the foregoing discussion on the vanishing of the critical coefficient (33)]. In either case, the coefficient of P_{k-1} in (41) vanishes identically.

The fourth normalizable canonical form is given by $P(z)=z$, so that $w=z$ and $\hat{c}_{+0}=c_{+0}=0$, and its exactly solvable potentials are defined by the vanishing of the coefficient $c_+=\hat{c}_+=0$, so that (41) is two term. Finally, for the fifth normalizable canonical form $P(z)=1$ all normalizable potentials are automatically exactly solvable (they are translates of the harmonic oscillator), and we have already seen that its associated orthogonal polynomials satisfy the two-term recursion relations (32). Q.E.D.

IV. THE ORTHOGONAL POLYNOMIALS

We shall study in this section the properties of the family of weakly orthogonal polynomials associated to a quasi-exactly solvable one-dimensional Hamiltonian in the manner described in the previous section. Since, as we shall see, these properties can be established directly from the recursion relation (41) or (32), these polynomials have basically the same properties as those studied by Bender and Dunne in Ref. 1.

We have seen in the previous section that the polynomials $\hat{P}(E)$ defined by a quasi-exactly solvable one-dimensional Hamiltonian satisfy a three-term recursion relation of the form

$$\hat{P}_{k+1}=(E-b_k)\hat{P}_k-a_k\hat{P}_{k-1}, \quad k\geq 0, \tag{42}$$

with $a_0=0$ and

$$a_{n+1}=0. \tag{43}$$

For the fifth canonical form, the polynomials $(-1)^k P_k^0$ and $(-1)^k P_k^1$ also satisfy a recursion relation of the form (42), with $a_k=0$ for all $k\geq 0$. Note that the coefficients a_k, b_k in (42) are guaranteed to be real only for the canonical forms 2–7 and 10 (for which P has a real root). As remarked in the previous section, the vanishing of a_k for a positive integer value of k means that the polynomials $\hat{P}_k$ are only weakly orthogonal. In particular, many classical results, based on the fact that $a_k>0$ (or sometimes $a_k\geq 0$) for $k\geq 1$ cannot be applied in our case.

By Favard's theorem, Ref. 2, there is a *moment functional*, that is a linear functional $\mathscr{L}$ acting in the space $\mathbb{C}[E]$ of (complex) univariate polynomials, such that the polynomials $\hat{P}_k$ are orthogonal under $\mathscr{L}$:

$$\mathscr{L}(\hat{P}_k\hat{P}_l)=\gamma_k\delta_{kl}, \quad k,l\in\mathbb{N}. \tag{44}$$

The functional $\mathscr{L}$ is unique if we impose the normalization condition $\mathscr{L}(\hat{P}_0)=\mathscr{L}(1)=1$. It is also known (Boas's theorem[2]) that there is a (not necessarily unique) function of bounded variation ω such that

$$\mathscr{L}(p)=\int_{-\infty}^{\infty} p(E)\,d\omega(E) \tag{45}$$

for an arbitrary polynomial p. The coefficient $\gamma_k=\mathscr{L}(\hat{P}_k^2)$, which therefore plays the role of the square of the norm of $\hat{P}_k$, can be computed by multiplying (42) by $\hat{P}_{k-1}$ and taking $\mathscr{L}$ of both sides, obtaining

$$0=\gamma_k-a_k\gamma_{k-1}, \quad k\geq 1.$$

Taking into account that $\gamma_0=\mathscr{L}(1)=1$ we get

$$\gamma_k=\prod_{j=1}^{k} a_j, \quad k\geq 1. \tag{46}$$

In particular, from this formula follows one of the key properties of the weakly orthogonal polynomial system associated to a one-dimensional quasi-exactly solvable Hamiltonian. Namely, from (43) we have

$$\gamma_k=0, \quad k\geq n+1,$$

so that *all the polynomials* $\hat{P}_k$ *with* $k\geq n+1$ *have zero norm.* From this formula it also follows that the "squared norms" γ_k will be positive for $k\leq n$ if and only if $a_k>0$ for $1\leq k\leq n$. It can be shown by a straightforward computation that this is always the case when P is one of canonical forms 2–4 in (19), assuming that all the eigenfunctions of H are square integrable and that H is *not* exactly solvable. Note also that when H is normalizable [canonical forms 1–5 in (19)] and exactly solvable then $a_k=0$ for all $k\geq 0$. Hence the square norms of all the polynomials $\hat{P}_k$ vanish, from which it easily follows from (42) that $\mathscr{L}=\delta(E-b_0)$.

Other important properties of the polynomials $\hat{P}_k$ concern their zeros. Classically,[2] it can be shown that if $a_k>0$ for all $k\in\mathbb{N}$ then the zeros of the polynomials $\hat{P}_k$ satisfying a three-term recursion relation (42) are real and simple. In our case the condition $a_k>0$ for all $k\in\mathbb{N}$ can never hold on account of (43). However, if H is fully algebraic it can still be proved that all the zeros of $\hat{P}_{n+1}$ are real and simple. Indeed, by hypothesis H is self-adjoint on the space $\mathfrak{N}$ of functions of the form (7), with $\chi\in\mathscr{P}_n$. Hence H has $n+1$ linearly independent algebraic eigenfunctions lying in $\mathfrak{N}$, whose corresponding eigenvalues are real (by self-adjointness) and distinct (H being a one-dimensional Sturm–Liouville operator). Let us denote by $E_0<E_1<\ldots<E_n$ these $n+1$ real eigenvalues of H on $\mathfrak{N}$, and by $\psi_l(x)\equiv\psi_{E_l}(x)$ the eigenfunction corresponding to the eigenvalue E_l. Then (7) and either (28) or (30) imply that $P_k(E_l)=0$, or equivalently $\hat{P}_k(E_l)=0$, for $k\geq n+1$ and $0\leq l\leq n$. In particular, since $\hat{P}_{n+1}$ is of degree $n+1$ and all the eigenvalues E_l are different, it follows that

$$\hat{P}_{n+1}(E)=\prod_{l=0}^{n}(E-E_l), \tag{47}$$

where we have used (42) and the fact that $\hat{P}_0=1$. In other words, $\hat{P}_{n+1}$ *has* $n+1$ *simple real zeros at the* $n+1$ *algebraic eigenvalues of* H. Furthermore, from the fact that $\hat{P}_k$ vanishes at E_l for $k\geq n+1$ we conclude that there exist monic polynomials Q_k of degree k such that

$$\hat{P}_{k+n+1}=Q_k\hat{P}_{n+1}, \quad k\geq 0. \tag{48}$$

This is the so called *factorization property* of the polynomial system $\{\hat{P}_k\}_{k\in\mathbb{N}}$, cf. Ref. 1. Note that the vanishing of $\hat{P}_k(E_l)$ for all $k\geq n+1$ is consistent with the recursion relation on account of (43). In fact, when a_k is positive for $k\geq 1$ and b_k is real for $k\geq 0$, (47) follows directly from the recursion relation by Lemma 3, without using the fact that the polynomials $\hat{P}_k$ are associated to a fully algebraic quasi-exactly solvable one-dimensional Hamiltonian. The vanishing of $\hat{P}_k(E_l)$ for $k>n+1$ is then an immediate consequence of $\hat{P}_{n+1}(E_l)=0$, the recursion relation (42) and (43).

From the previous equation and (42) it follows that the polynomials Q_k also satisfy a three-term recursion, namely

$$Q_{k+1}=(E-b_{k+n+1})Q_k-a_{k+n+1}Q_{k-1}, \quad k\geq 0,$$

and are therefore orthogonal with respect to an appropriate moment functional $\mathscr{L}_Q$ (in general different from $\mathscr{L}$).

It was heuristically argued in Ref. 5 that

$$\mathscr{L}=\sum_{j=0}^{n}\omega_j\delta(E-E_j) \tag{49}$$

on $\mathbb{C}[E]$, where the coefficients ω_j are defined by

$$\sum_{l=0}^{n}\hat{P}_k(E_l)\omega_l=\delta_{k0},\quad k=0,1,\ldots,n. \tag{50}$$

Equivalently, the discrete Stieltjes measure $d\hat{\omega}(E)$ defined by the function

$$\hat{\omega}(E)=\sum_{j=0}^{n}\omega_j\theta(E-E_j), \tag{51}$$

where $\theta(t)$ is Heaviside's step function, satisfies (45). Note that the linear system (50) uniquely defines the $n+1$ constants ω_j, since by (27) or (29) its coefficient matrix is the matrix of the change of basis $\{c_k(z-z_1)^k/k!\}_{k=0}^n$ or $\{c_k(z-z_1)^k(z-z_2)^{n-k}/k!\}_{k=0}^n$ to $\{\chi_{E_l}\}_{l=0}^n$ in $\mathbb{C}\otimes\mathscr{P}_n$, c_k being the coefficient of $\hat{P}_k$ in (40). It is not difficult to show rigorously that (44) is satisfied. Indeed, by the uniqueness of $\mathscr{L}$ this is equivalent to showing that if $\mathscr{L}_0=\Sigma_{j=0}^n\omega_j\delta(E-E_j)$ then

$$\mathscr{L}_0(\hat{P}_k\hat{P}_l)=0,\quad k\neq l, \tag{52}$$

and that

$$\mathscr{L}_0(\hat{P}_0)=\mathscr{L}_0(1)=1,$$

since $\mathscr{L}(\hat{P}_k^2)$ and $\mathscr{L}_0(\hat{P}_k^2)$ must coincide if (52) holds due to the recursion relation (42) and (46). From the definition of ω_j we deduce that the last equation, together with (52) for $k=0$ and $l=1,\ldots,n$, are satisfied. Suppose now that (52) holds for $k=0,1,\ldots,K$ $(K\leqslant n-1)$ and $k<l\leqslant n$. Multiplying (42) by $\hat{P}_l$ and taking $\mathscr{L}_0$ of both sides we obtain

$$\mathscr{L}_0(\hat{P}_{K+1}\hat{P}_l)=\mathscr{L}_0((E-b_K)\hat{P}_K\hat{P}_l)-a_K\mathscr{L}_0(\hat{P}_{K-1}\hat{P}_l)=\mathscr{L}_0(E\hat{P}_K\hat{P}_l)$$

if $K+1<l\leqslant n$, by the induction hypothesis. But, using again (42),

$$\mathscr{L}_0(E\hat{P}_K\hat{P}_l)=\mathscr{L}_0(\hat{P}_K\cdot E\hat{P}_l)=\mathscr{L}_0(\hat{P}_K\hat{P}_{l+1})+b_l\mathscr{L}_0(\hat{P}_K\hat{P}_l)+a_l\mathscr{L}_0(\hat{P}_K\hat{P}_{l-1})=0,$$

by the induction hypothesis (since $l>K+1$ implies $l-1>K$). Hence (52) is true for $0\leqslant k,l\leqslant n$. Finally, (52) is trivially true when k or l are greater than n by the factorization property (48) and (47).

We shall next show that all the coefficients ω_j are positive if b_k is real for all $0\leqslant k\leqslant n$ and $a_k>0$ for $1\leqslant k\leqslant n$. [Several instances of this result were checked numerically in Ref. 5 for the orthogonal polynomials associated to the Hamiltonian (1).] The proof is based on the following simple lemma:

Lemma 3: If $a_k>0$ for $k=1,2,\ldots,n$ and b_k is real for $k=0,1,\ldots,n$ then $\mathscr{L}$ is positive-definite on $\mathscr{P}_{2n}$. In other words, if $p\in\mathscr{P}_{2n}$ is a real polynomial of degree at most $2n$, $p\neq 0$ and $p(E)\geqslant 0$ for all $E\in\mathbb{R}$ then $\mathscr{L}(p)>0$.

Proof: A polynomial $p\in\mathscr{P}_{2n}$ which is non-negative for all real values of E must be of the form q^2+r^2, where $q,r\in\mathscr{P}_n$ are real polynomials. Write $q=\Sigma_{k=0}^n q_k\hat{P}_k$; then all the coefficients q_k are real, since $\hat{P}_k$ is a real polynomial for $0\leqslant k\leqslant n$ by the hypotheses. Using the orthogonality of the polynomials $\hat{P}_k$ we obtain $\mathscr{L}(q^2)=\Sigma_{k=0}^n q_k^2\gamma_k$. Similarly, if $r=\Sigma_{k=0}^n p_k\hat{P}_k$ then $\mathscr{L}(r)=\Sigma_{k=0}^n r_k^2\gamma_k$, and $\mathscr{L}(p)=\Sigma_{k=0}^n(q_k^2+r_k^2)\gamma_k$. Since $\gamma_k>0$ for $k=0,1,\ldots,n$ by (46) and the

hypothesis on the coefficients a_k, it follows that $\mathscr{L}(p)\geq 0$, and $\mathscr{L}(p)=0$ if and only if $q_k=r_k=0$ for $k=0,1,\ldots,n$, that is if and only if $p=0$. Q.E.D.

Proposition 4: If $a_k>0$ for $k=1,2,\ldots,n$ and b_k is real for $k=0,1,\ldots,n$ then $\omega_k>0$ for all $k=0,1,\ldots n$.

Proof: Apply the previous lemma to the polynomials $\Pi_{0\leq j\neq k\leq n}(E-E_j)^2\in\mathscr{P}_{2n}$ for $k=0,1,\ldots n$. Q.E.D.

Note that the hypotheses of the previous proposition are satisfied when P is one of the canonical forms 2, 3, or 4, provided that all the eigenfunctions of H are square-integrable and that H is *not* exactly solvable. In particular, it is satisfied by the Hamiltonian (1).

The (Hamburger) *moment problem* for the moment functional (49) associated to the weakly orthogonal polynomials defined by a quasi-exactly solvable one-dimensional Hamiltonian consists in determining whether there is a *distribution function* (i.e., a nondecreasing function of bounded variation) ω such that $\mathscr{L}$ can be represented by (45) for an arbitrary polynomial p. We have already shown that this problem has a solution (51), since (51) is clearly nondecreasing and of bounded variation. We shall next show that this solution is unique (up to an additive constant), so that the moment problem associated to the weakly orthogonal polynomial system $\{\hat{P}_k\}_{k\in\mathbb{N}}$ is always determined.[12] Essentially, this is due to the fact that the *spectrum*

$$\sigma(\hat{\omega})=\{E\in\mathbb{R}:\hat{\omega}(E+\delta)-\hat{\omega}(E-\delta)>0,\forall\,\delta>0\}$$

of the distribution function (51) is the finite set $\{E_l\}_{l=0}^{n}$.[13] According to a well known result in the classical theory of orthogonal polynomials,[2] a distribution function ω defines a positive-definite functional on $\mathbb{C}[E]$ through integration with respect to the Stieltjes measure $d\omega(E)$ if and only if the spectrum of ω is infinite. Since $\mathscr{L}$ is not positive-definite ($\mathscr{L}(\hat{P}_{n+1}^2)=\gamma_{n+1}=0$), any solution ω of (45) must have a finite spectrum, and will thus be of the form

$$\omega(E)=\sum_{k=0}^{\tilde{n}}\tilde{\omega}_k\theta(E-\tilde{E}_k)+C$$

for some constant C, up to an immaterial redefinition of ω in $\sigma(\omega)$. If I is a compact interval containing $\sigma(\hat{\omega})\cup\sigma(\omega)$, then

$$\mathscr{L}(p)=\int_I p(E)d\hat{\omega}(E)=\int_I p(E)d\omega(E),\quad \forall p\in\mathbb{C}[E].$$

Since I is compact, a well known theorem (cf. Ref. 2) shows that $\hat{\omega}$ and ω differ by a constant at all points in which both $\hat{\omega}$ and ω are continuous. But this easily implies that $E_k=\tilde{E}_k$ and $\omega_k=\tilde{\omega}_k$ for $k=0,1,\ldots,n=\tilde{n}$, whence $\omega=\hat{\omega}+C$, as stated. Note that the same argument shows that the moment problem in any interval containing $[E_0,E_n]$ is determined; in particular, the (Stieltjes) moment problem in $[E_0,\infty)$ is also determined. In this respect, the weakly orthogonal polynomials associated to a quasi-exactly solvable one-dimensional Hamiltonian behave in exactly the same way as the classical orthogonal polynomials, whose moment problem is also determined.[2]

The *moments* of the moment functional $\mathscr{L}$ are by definition the numbers

$$\mu_k=\mathscr{L}(E^k)=\int_{-\infty}^{\infty}E^k\,d\hat{\omega}(E)=\sum_{l=0}^{n}\omega_l E_l^k,\quad k\in\mathbb{N}. \tag{53}$$

If the hypotheses of Proposition 4 hold, all the moments are real. From (53) we see that the module of the kth moment μ_k does not grow factorially as k tends to infinity, as argued in Ref. 1, but instead it diverges like the kth power of a constant.[14]

We shall next show that if the coefficient a_k satisfies the condition

$$a_k \neq 0, \quad 1 \leqslant k \leqslant n, \tag{54}$$

which guarantees that the polynomials $\hat{P}_k$ have nonzero norm for $k \leqslant n$, then *the moments* μ_k *with* $k \geqslant n+1$ *satisfy a constant coefficient difference equation of order* $n+1$. To this end, recall first of all that the bilinear form $\langle p,q\rangle = \mathscr{L}(pq)$ defined by $\mathscr{L}$ in $\mathbb{C}[E]$, when restricted to the subspace $\mathbb{C}\otimes\mathscr{P}_l$, is represented in the basis $\{E^k\}_{0\leqslant k\leqslant l}$ by the symmetric matrix $(\mu_{i+j})_{0\leqslant i,j\leqslant l}$, whose determinant we shall denote by Δ_l. On the other hand, the matrix of the bilinear form $\langle\cdot,\cdot\rangle$ in the basis $\{\hat{P}_k\}_{0\leqslant k\leqslant l}$ is clearly $\mathrm{diag}(1,\gamma_1,\ldots,\gamma_l)$; therefore, by (46) and the hypothesis on the coefficients a_k, we conclude that $\Delta_n \neq 0$ and

$$\Delta_k = 0, \quad k \geqslant n+1. \tag{55}$$

In particular, since $\Delta_n \neq 0$ but $\Delta_{n+1} = 0$, the last column of Δ_{n+1} must be a linear combination of the remaining columns, so that

$$\mu_k = \sum_{i=1}^{n+1} c_i \mu_{k-i}, \quad n+1 \leqslant k \leqslant 2(n+1), \tag{56}$$

for some (in general complex) constants $c_1,\ldots,c_{n+1}$. An easy induction argument using (55) then shows that the above relation is actually valid with the *same* constant coefficients c_i for all $k \geqslant n+1$, as claimed. In fact, it is not hard to see that c_i in (56) is minus the coefficient of E^{n+1-i} in $\hat{P}_{n+1}$. Indeed, write $\hat{P}_{n+1} = E^{n+1} - p_n$, with

$$p_n = \sum_{i=1}^{n+1} \tilde{c}_i E^{n+1-i},$$

and let $Q_k = E^k - q_{k-1}$, so that $q_{-1} = 0$ and $\deg q_{k-1} \leqslant k-1$ for $k \geqslant 1$. From (48) it follows that

$$\hat{P}_k = E^k - E^{k-n-1} p_n - q_{k-n-2} \hat{P}_{n+1}, \quad k \geqslant n+1,$$

which by (44) implies that

$$\mu_k = \mathscr{L}(E^k) = \mathscr{L}(E^{k-n-1} p_n) = \sum_{i=1}^{n+1} \tilde{c}_i \mu_{k-i}, \quad n+1 \leqslant k \leqslant 2(n+1).$$

Comparing with (56) and taking into account the linear independence of the columns of Δ_n we immediately obtain that $\tilde{c}_i = c_i$ for $i = 1,2,\ldots,n+1$, as stated.

Note that the fact that the moments satisfy a constant coefficient recursion relation (56) (with $k \geqslant n+1$) actually characterizes weakly orthogonal polynomial systems. Indeed, (56) simply expresses the fact that the $(n+2)$th column of Δ_l for $l \geqslant n+1$ is a linear combination of the first $n+1$ columns. Hence (56) implies (55), and since $\Delta_{n+1} = \prod_{j=1}^{n+1} \gamma_j$ this means that $\gamma_k = 0$ for some $k \leqslant n+1$, so that $a_k = 0$ for some $k \leqslant n+1$ by (46).

Consider, for example, the Hamiltonian (1) studied in Ref. 1, which corresponds to the fourth canonical form with

$$n = J-1, \quad c_+ = -16, \quad c_0 = c_* = 0, \quad c_- = 2s + \tfrac{1}{2}(n-1). \tag{57}$$

The coefficients of the corresponding recursion relation (42) are easily found to be

$$b_k = 0, \quad a_k = 16k(J-k)(k+2s-1), \quad k \geqslant 0. \tag{58}$$

Since we can take $s \geqslant 1/2$ without loss of generality, we see that $a_k > 0$ for $1 \leqslant k \leqslant n$, so that (54) is satisfied. Furthermore, since b_k vanishes for all $k \geqslant 0$ the polynomials $\hat{P}_k$ have parity $(-1)^k$, and

therefore all the odd moments vanish (the corresponding moment functional is said to be *symmetric*). For $J=3$ (that is, $n=2$), according to the foregoing observations we know that the moments satisfy a third-order recursion relation of the form (56), whose coefficients are minus the coefficients of E^2, E, and 1 in $\hat{P}_3$. From (42) (with $\hat{P}_0=1$) we obtain

$$\hat{P}_1=E, \quad \hat{P}_2=E^2-64s, \quad \hat{P}_3(E)=E^3-32(4s+1)E, \tag{59}$$

so that $c_1=c_3=0$—as expected, since the moment functional is symmetric—and $c_2=32(4s+1)$. Therefore the even moments satisfy the first-order recursion relation

$$\mu_{2j}=32(4s+1)\mu_{2j-2}, \quad j\geq 2, \tag{60}$$

and since $\mu_2=\gamma_1=a_1=64s$, from (60) we obtain

$$\mu_{2j}=32^{j-1}(4s+1)^{j-1}\cdot 64s, \quad j\geq 1. \tag{61}$$

Thus, in this case μ_{2j} has a pure power growth. The same result can be obtained using (53). Indeed, from (59) we have

$$E_0=-\lambda\equiv-\sqrt{32(4s+1)}, \quad E_1=0, \quad E_2=\lambda,$$

and therefore

$$\omega_0=\frac{s}{4s+1}, \quad \omega_1=\frac{2s+1}{4s+1}, \quad \omega_2=\omega_0$$

from (50) and (59). Thus

$$\mu_k=\frac{s}{4s+1}[(-\lambda)^k+\lambda^k],$$

which yields $\mu_{2j+1}=0$ for $j\geq 0$ and (61).

V. CONCLUSIONS

We have shown in this paper how every quasi-exactly solvable one-dimensional Hamiltonian satisfying conditions (37)–(39) defines a weakly orthogonal polynomial system $\{\hat{P}_k\}_{k=0}^{\infty}$ through the three-term recursion relation (41) (with initial condition $\hat{P}_0=1$). It is important, in this context, to emphasize the *weak* orthogonality of the polynomials $\hat{P}_k$, i.e., the fact that the norm of $\hat{P}_k$ may vanish—and in fact *does* vanish for $k\geq n+1$, n being the "spin" parameter present in the Hamiltonian. As explained in Sec. IV, this is an inevitable consequence of the vanishing of the coefficient of $\hat{P}_{k-1}$ in the recursion relation (41) for $k=n+1$, which is made possible by the fact that the parameter n is a non-negative integer. The latter fact, however, is an intrinsic property of one-dimensional quasi-exactly solvable (as opposed to merely Lie-algebraic) Hamiltonians; indeed, it is a key factor in the explanation of the partial integrability of a quasi-exactly solvable Hamiltonian outlined in Sec. II. To better illustrate this point, consider the Hamiltonian (1), which is Lie-algebraic for all real values of the parameter J. Indeed, H can be written in the form (5)–(6), with $\zeta(x)=x^2/4$, $\mu(z)=e^{-4z^2}z^{s-1/4}$, $c_{++}=c_{+0}=c_{00}=c_{+-}=c_{--}=0$, $c_{0-}=1/2$, and the remaining coefficients given by (57), where now n is to be regarded as an arbitrary real parameter. When n is not a non-negative integer, the generators (4) do not leave invariant any finite-dimensional polynomial module $\mathcal{P}_n$, so that H is in general nonintegrable—there is no special reason for H to have algebraically computable eigenfunctions of the form (7), with χ a polynomial. However, even when n is not a non-negative integer, the Lie-algebraic nature of H and

conditions (25) imply that the polynomials $\hat{P}_k$ defined by (7), (21), and (40) still satisfy a three-term recursion relation (42), with the coefficients given by (58). In other words, what makes H quasi-exactly solvable is not merely the fact that its associated polynomials satisfy a three-term recursion relation (42) (which implies their orthogonality with respect to some Stieltjes measure), but the fact that the coefficient a_k in this recursion relation vanishes for some positive integer value of k, so that the associated polynomials $\hat{P}_k$ can only be weakly orthogonal.

As we saw in Sec. IV, the Stieltjes measure with respect to which the polynomials $\hat{P}_k$ associated to a quasi-exactly solvable Hamiltonian H are orthogonal is supported in the set of algebraic eigenvalues of H, which is a finite set. For this reason, the polynomials $\hat{P}_k$ are *discrete polynomials*. Although the classical (Hermite, Legendre, Laguerre, Tchebycheff, etc.) polynomials of Mathematical Physics are orthogonal with respect to a continuous measure, discrete (Charlier, Hahn, Krawtchouk, Meixner, Tchebycheff, etc.) polynomials have also been studied in the mathematical literature of orthogonal polynomials, cf. Ref. 2. Note that a discrete polynomial system is truly—as opposed to weakly—orthogonal if and only if the supporting set of its Stieltjes measure is infinite. Some of the discrete polynomials cited above, like the Hahn, Krawtchouk, or discrete Tchebycheff polynomials, are in fact weakly orthogonal. In general, weakly orthogonal polynomials arise naturally, for instance, in the theory of approximate polynomial curve fitting.[15] More recently,[16] the study of second-order finite difference eigenvalue equations with infinitely many polynomial solutions has led to an interesting connection between a nonstandard finite-dimensional representation of $\mathfrak{sl}(2)$ and certain families of weakly orthogonal discrete polynomials (Hahn polynomials and analytically continued Hahn polynomials).

Let us stress, in closing, that the present paper deals only with one-dimensional quasi-exactly solvable Hamiltonians. It is an interesting open problem to generalize these results to quasi-exactly solvable multi-dimensional systems, a possibility already considered in Ref. 5, where a heuristic (but inconclusive, in our opinion) argument was advanced suggesting that all quasi-exactly solvable systems give rise to weakly orthogonal polynomials. In the two-dimensional case, at least, the classification of quasi-exactly solvable Lie algebras of first-order differential operators in two variables presented in Refs. 7 and 17 could be used as a starting point for an analysis along the present lines.

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[13] A classical theorem, Ref. 2, asserts that the moment problem of a positive-definite moment functional with bounded spectrum is determined; this theorem is not directly applicable in our case, however, since $\mathscr{L}$ is not positive-definite.

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Constructive building of the Lax pair in the non-linear sigma model

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A derivation of the Lax pair for the $(1+1)$-dimensional non-linear σ-model is described. Its main benefit is to have a clearer physical origin and to allow the study of a generalization to higher dimensions. © *1996 American Institute of Physics.* [S0022-2488(96)01007-9]

I. INTRODUCTION

It has been known for several years that the non-linear σ-model, in a two dimensional space–time, has a non-local conservation law[1] that can be cast as a non-local symmetry transformation.[2,3] This is usually shown to be true on the basis of the existence of a "Lax pair," a pair of linear differential equations depending on a spectral parameter, whose compatibility condition is exactly the field equation of the model. Exact integrability of the system follows, via the inverse scattering procedure.[4]

An infinite set of non-local conserved charges can be directly obtained from this Lax system, as in Ref. 1, or as in Ref. 2. In the former reference the authors prove that, with a careful selection of the boundary conditions, the variable of the Lax pair is time independent for spatial coordinate $x^1=+\infty$, given initial conditions at $x^1=-\infty$. Thus a Taylor expansion in the spectral parameter gives a series of non-local conserved charges. In the latter paper, the authors apply the transformation to the global (left, for instance) conserved current. This gives them a spectral parameter dependent conserved current, which upon Taylor expansion generates an infinite set of non-local currents, all of them conserved.

Although very well known and studied, in general and applied to this particular model, the Lax pair has a somewhat obscure physical origin. Also, there is no systematic way to find it in a given system. We hope to contribute a small step to solve these problems. We show here a way to get the Lax equation for the two dimensional σ-model, which somewhat clarifies its physical meaning. This way of proceeding also enables the study of a possible generalization to more dimensions.

We should stress here that a higher dimensional version of the non-local symmetry of this model is sensible. Actually the (4D Euclidean) self-dual gauge theory has this kind of symmetry transformation,[5] which is also related to several $(2+1)$ dimensional integrable systems.[6] Moreover, this symmetry and its associated Lax pair is also present in (at least) a subspace of the solution's manifold of a large class of models based on vacuum general relativity.[7,8]

Aside from its own interest, the non-local symmetry of this system is relevant in the Gribov problem. We must only realize that (classically) the vacuum sector of the Yang–Mills theory is exactly the n dimensional σ-model if we choose the Lorentz $(\partial\cdot A=0)$ gauge. So the existence of a continuous 1-parameter family of solutions of the non-linear σ-model tells us of a continuum of vacua in the non-Abelian gauge theories in the Lorentz gauge.

II. CONSTRUCTING THE LAX PAIR

Only to fix our notation, we enumerate first some standard results about this model. We write for the action

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$$S=\int \mathrm{d}^d x \mathrm{Tr}[\partial_\mu(g^{-1})\partial^\mu g],$$

where g is a (G) group valued field over Minkowsky space–time M^d. We will consider here only a principal chiral field (group valued field), the symmetric space case will be addressed in Appendix **B**. This action has two global symmetries,

$$g(x)\mapsto Lg(x),$$

$$g(x)\mapsto g(x)R, \text{ with } L,R\in G \text{ and independent of } x\in M^d,$$

that tell us of the conservation of the (Noether) currents,

$$L_\mu \equiv g\partial_\mu g^{-1} \quad \text{and} \quad R_\mu \equiv g^{-1}\partial_\mu g,$$

which are related by $R_\mu = -g^{-1}L_\mu g$.

The equations of motion of this model can be written as[9]

$$\Box g+(\partial_\mu g\partial^\mu g^{-1})g\doteq 0, \tag{1}$$

or as

$$\partial\cdot L\doteq 0, \tag{2}$$

in terms of the left current, or equivalently $\partial\cdot R\doteq 0$ in terms of the right one. These currents obviously satisfy a "zero-curvature" condition,

$$\begin{aligned} F_{\mu\nu}(L)&\equiv\partial_\mu L_\nu-\partial_\nu L_\mu+[L_\mu,L_\nu]=0,\\ F_{\mu\nu}(R)&\equiv\partial_\mu R_\nu-\partial_\nu R_\mu+[R_\mu,R_\nu]=0. \end{aligned} \tag{3}$$

With this notation, the linear (when left-multiplied by U) equations,

$$U^{-1}\partial_\mu U=\frac{1}{2}[(1-\cosh(\lambda))L_\mu-\sinh(\lambda)\epsilon_{\mu\nu}L^\nu], \tag{4}$$

are called the Lax pair. λ is the spectral parameter and ϵ is the Levi-Civita tensor. The group valued field U should here be taken as the variable, for each given L. It is straightforward to verify that the compatibility condition $[\partial_\mu,\partial_\nu]U=0$ is satisfied for pure gauge L's with zero divergence. In this case a formal solution to Eq. (4) is given by

$$U(x)=U_o\mathrm{Pexp}\int \frac{1}{2}[(1-\cosh(\lambda))L_\mu-\sinh(\lambda)\epsilon_{\mu\nu}L^\nu]\mathrm{d}x^\mu,$$

where P is the path ordering operator (ordering from left to right), along a path from a fixed point to x. A completely analogous Lax pair can be constructed with the right current,

$$V^{-1}\partial_\mu V=\frac{1}{2}[(1-\cosh(\lambda))R_\mu-\sinh(\lambda)\epsilon_{\mu\nu}R^\nu]. \tag{5}$$

Bäklund transformations are at this point usually introduced.

We can in a sense reverse this argument, starting from a transformation $g\mapsto g'$ with

$$g'(x)=U(x)g(x)V^{-1}(x), \tag{6}$$

where U and V are some group valued fields. This is a pretty general form, but looking at the action we realize we can make it *a-priori* invariant asking for (6) to fulfill

$$\partial_\mu g' = \partial_\mu (U g V^{-1}) = U \Lambda_{\mu\nu} \partial^\nu g V^{-1}. \tag{7}$$

Here Λ is an undetermined Lorentz transformation,[10] $\Lambda_{\mu\nu}\Lambda^{\mu\sigma} = \delta^\sigma_\nu$. This obviously makes the action invariant, but what is not so trivial to fulfill is the consistency of condition (7), that is U and V such that this equation holds may not exist. Indeed in the $(1+1)$ dimensional case this condition is only solvable over the field equation solutions. Equation (7) can also be written as

$$U^{-1}\partial_\mu U - g V^{-1} \partial_\mu V g^{-1} = L_\mu - \Lambda_{\mu\nu} L^\nu, \tag{8}$$

and implies for L the transformation law

$$L'_\mu = U \Lambda_{\mu\nu} L^\nu U^{-1}. \tag{9}$$

We see that the Lax pairs (4) and (5) satisfy Eq. (8) in the $(1+1)$ dimensional case, because in this case any Lorentz transformation can be written as $\Lambda_{\mu\nu} = \cosh(\lambda)\eta_{\mu\nu} + \sinh(\lambda)\epsilon_{\mu\nu}$, η being the Minkowski metric. Anyway, Eq. (6) and Eq. (8) enable a testable path to generalization to higher dimensions.

We can obtain the Lax pair doing a series of infinitesimal transformations, with

$$\Lambda_{\mu\nu} = \eta_{\mu\nu} + \omega_{\mu\nu}, \quad |\omega_{\mu\nu}| \ll 1,$$

where $\omega_{\mu\nu}$ is an antisymmetric tensor. For just one transformation, we have

$$U = 1 + u + \mathcal{O}(\omega^2_{\mu\nu}), \quad V = 1 + v + \mathcal{O}(\omega^2_{\mu\nu}),$$

$$U^{-1}\partial_\mu U \simeq \partial_\mu u, \quad V^{-1}\partial_\mu V \simeq \partial_\mu v, \tag{10}$$

where we have taken U and V so as to preserve boundary conditions for g. That is, for the identity transformation we should have $g' = g$ so $U(\omega_{\mu\nu} = 0) = V(\omega_{\mu\nu} = 0) = 1$.

Therefore we have

$$\begin{aligned} L'_\mu &= g' \partial_\mu [g'^{-1}] = (1+u) g (1-v) \partial_\mu [(1+v) g^{-1} (1-u)] \\ &= L_\mu - \partial_\mu u + [u, L_\mu] + g \partial_\mu v g^{-1}. \end{aligned} \tag{11}$$

But Eq. (8) gives

$$\partial_\mu u = g \partial_\mu v g^{-1} - \omega_{\mu\nu} L^\nu, \tag{12}$$

up to first order in ω, so we get

$$L'_\mu = L_\mu + [u, L_\mu] + \omega_{\mu\nu} L^\nu + \mathcal{O}(\omega^2). \tag{13}$$

Calculating now the divergence of Eq. (13),

$$\begin{aligned} \partial \cdot L' &\doteq [\partial_\mu u, L^\mu] + \partial^\mu (\omega_{\mu\nu} L^\nu) \\ &= \left[\partial_\mu u + \frac{1}{2} \omega_{\mu\nu} L^\nu, L^\mu \right], \end{aligned} \tag{14}$$

where constancy of $\omega_{\mu\nu}$ was assumed and Eq. (3) was employed. If we impose $\partial \cdot L'$ to be zero [weakly, for all L verifying Eq. (2) and Eq. (3)], it is enough to take

$$\partial_\mu u + \frac{1}{2}\omega_{\mu\nu}L^\nu = \alpha L_\mu . \tag{15}$$

But for this equation to be consistent it should verify the condition[11]

$$[\partial_\mu, \partial_\nu]u = 0, \tag{16}$$

that is

$$\frac{1}{2}\omega_{\mu\sigma}\partial_\nu L^\sigma - \frac{1}{2}\omega_{\nu\sigma}\partial_\mu L^\sigma + \alpha(\partial_\mu L_\nu - \partial_\nu L_\mu) = 0. \tag{17}$$

If we now restrict ourselves to work in $1+1$ dimensions we can write $\omega_{\mu\nu} = \gamma\epsilon_{\mu\nu}$. So we obtain from Eq. (17)

$$\alpha(\partial_\mu L_\nu - \partial_\nu L_\mu) = 0, \tag{18}$$

because for $\mu \neq \nu$ it is $\epsilon_{\nu\sigma}\partial_\mu L^\sigma - \epsilon_{\mu\sigma}\partial_\nu L^\sigma = -\epsilon_{\mu\nu}\partial\cdot L \doteq 0$. We can then choose $\alpha = 0$, so

$$\partial_\mu u = -\frac{1}{2}\gamma\epsilon_{\mu\nu}L^\nu, \tag{19}$$

up to order γ. Renaming γ as γ_0, we can now iterate this procedure (obviously we must check consistency) doing a transformation of parameter γ_1 to obtain $g_{(2)}$, $L^\mu_{(2)}$ starting from $g_{(1)}$, $L^\mu_{(1)}$, etc. This can be summarized as shown below:

$$g, L \xrightarrow{\gamma_0, u_{(0)}} g_{(1)}, L_{(1)} \xrightarrow{\gamma_1, u_{(1)}} g_{(2)}, L_{(2)} \longrightarrow \cdots$$

Up to this point we have

$$\partial_\mu u_{(0)} = -\frac{1}{2}\gamma_0\epsilon_{\mu\nu}L^\nu_{(0)}, \tag{20a}$$

$$L^\mu_{(1)} = L^\mu_{(0)} + [u_{(0)}, L^\mu_{(0)}] + \gamma_0\epsilon^\mu{}_\nu L^\nu_{(0)} + \mathcal{O}(\gamma_0^2), \tag{20b}$$

and $v_{(0)}$ can be found from $\partial_\mu u_{(0)} = g_{(0)}\partial_\mu v_{(0)}[g_{(0)}]^{-1} - \gamma_0\epsilon_{\mu\nu}L^\nu_{(0)}$. We want to show first that this procedure can be iterated as many times as we want, and then we will show that this iteration leads us to a non-infinitesimal transformation, giving the usual Lax pair.

We started from a $L_{(0)}$ configuration with zero divergence and curvature and, because of integrability of Eq. (20a), $L_{(1)}$ given by Eq. (20b) is well defined. To restart the process $L_{(1)}$ should also have zero divergence and curvature. But, by construction $L_{(1)}$ has zero curvature up to leading order in γ_0, as it has been defined as $L^\mu_{(1)} = g_{(1)}\partial^\mu g^{-1}_{(1)}$, neglecting higher order terms. $L_{(1)}$ has also zero divergence, as $u_{(0)}$ was chosen for this purpose. Taking into account the discussion in Appendix **A** a well defined procedure for integrating the analog of Eq. (20a) for the second iteration can be given.

With exactly the same reasoning we see that for any n

$$\partial_\mu u_{(n)} = -\frac{1}{2}\gamma_n\epsilon_{\mu\nu}L^\nu_{(n)}, \tag{21a}$$

$$L^\mu_{(n+1)} = L^\mu_{(n)} + [u_{(n)}, L^\mu_{(n)}] + \gamma_n\epsilon^\mu{}_\nu L^\nu_{(n)}, \tag{21b}$$

provide us with

(I) a well defined $L^{\mu}_{(n+1)}$, because $[\partial_\mu,\partial_\nu]u_{(n)}=\frac{1}{2}\gamma_n\epsilon_{\mu\nu}\partial\cdot L_{(n)}$

(II) a zero divergence $L^{\mu}_{(n+1)}$, up to order γ_{n-1}

(III) a zero curvature $L^{\mu}_{(n+1)}$, up to order γ_n.

This can also be verified inductively. This way it is easier to see that

$$-[\partial_\mu,\partial_\nu]u_{(n)}=\frac{1}{2}\gamma_n\epsilon_{\mu\nu}\partial\cdot L_{(n)}=\gamma_n\mathcal{O}(\gamma_{n-2}^2,\ldots,\gamma_0^2),$$

$$-\partial\cdot L_{(n+1)}=\partial\cdot L_{(n)}+[u_{(n)},\partial\cdot L_{(n)}]-\gamma_n F_{01}(L_{(n)})=\mathcal{O}(\gamma_{n-1}^2,\ldots,\gamma_0^2),$$

$$\begin{aligned}-F_{\mu\nu}(L_{(n+1)})&=F_{\mu\nu}(L_{(n)})-\gamma_n\epsilon_{\mu\nu}\partial\cdot L_{(n)}+[u_{(n)},F_{\mu\nu}(L_{(n)})]\\&\quad+[\text{terms with }\gamma_n u_{(n)},\ \gamma_n^2,\ u_{(n)}^2,\text{ all are }\mathcal{O}(\gamma_n^2)]\\&=\mathcal{O}(\gamma_n^2,\ldots,\gamma_0^2).\end{aligned}$$

We now want to find $L^{\mu}_{(n)}$ and $g_{(n)}$ explicitly in terms of $L^{\mu}\equiv L^{\mu}_{(0)}$ and $g\equiv g_{(0)}$. Following Eq. (6) and Eq. (10), $g_{(n)}$ is given by

$$\begin{aligned}g_{(n+1)}&=(1+u_{(n)})g_{(n)}(1-v_{(n)})\\&=(1+u_{(n)})(1+u_{(n-1)})\ldots(1+u_{(0)})g_{(0)}(1-v_{(0)})\ldots(1-v_{(n)}).\end{aligned}$$

What we need is $U=$ (Limit of) $(1+u_{(n)})\ldots(1+u_{(0)})$, or considering the Lax pair we want to find, the equation satisfied by U: $U^{-1}\partial_\mu U=$ (something). For $n=0$ we have

$$\begin{aligned}U_0^{-1}\partial_\mu U_0&=(1-u_{(0)})\partial_\mu(1+u_{(0)})\\&=\partial_\mu u_{(0)}+\mathcal{O}(\gamma_0^2)=-\frac{1}{2}\gamma_0\epsilon_{\mu\nu}L^{\nu}_{(0)}.\end{aligned}$$

Writing $\Pi_{i=0}^{n}a_i$ for $a_0\ldots a_n$, and $\Pi_{i=n}^{0}a_i$ for $a_n\ldots a_0$ we get for an arbitrary n

$$\begin{aligned}U_n^{-1}\partial_\mu U_n&=\prod_{i=0}^{n}(1-u_{(i)})\partial_\mu\prod_{i=n}^{0}(1+u_{(i)})\\&=\sum_{j=0}^{n}\left[\prod_{i=0}^{j-1}(1-u_{(i)})\partial_\mu u_{(j)}\prod_{i=j-1}^{0}(1+u_{(i)})+\mathcal{O}(\gamma_n^2,\ldots,\gamma_j^2)\right].\end{aligned}$$

Here products $(1-u_{(i)})(1+u_{(i)})$, coming from the terms in U^{-1} and $\partial_\mu U$ respectively, cancel to first order in the parameter. If we now rewrite Eq. (21b) as

$$\begin{aligned}L^{\mu}_{(i)}&=L^{\mu}_{(i-1)}+[u_{(i-1)},L^{\mu}_{(i-1)}]+\gamma_{i-1}\epsilon^{\mu}{}_{\nu}L^{\nu}_{(i-1)}\\&=(1+u_{(i-1)})(\eta^{\mu}{}_{\nu}+\gamma_{i-1}\epsilon^{\mu}{}_{\nu})L^{\nu}_{(i-1)}(1-u_{(i-1)}),\end{aligned}\tag{22}$$

up to higher order terms, and we use Eq. (21a), we get

$$U_n^{-1}\partial_\mu U_n=\sum_{j=0}^{n}-\frac{1}{2}\gamma_j\epsilon_{\mu\nu_j}\left[\prod_{i=0}^{j-2}(1-u_{(i)})(\eta^{\nu_j}{}_{\nu_{j-1}}+\gamma_{j-1}\epsilon^{\nu_j}{}_{\nu_{j-1}})L_{(j-1)}^{\nu_{j-1}}\prod_{i=j-2}^{0}(1+u_{(i)})\right]$$
$$+\mathcal{O}(\gamma_n^2,\ldots,\gamma_0^2).$$

In this last equation factors $(1-u_{(j-1)})$ and $(1+u_{(j-1)})$ cancel at each side of the $L_{(j-1)}$. It is now easy to see that after employing Eq. (22) $(j-1)$ times more we obtain

$$U_n^{-1}\partial_\mu U_n=\sum_{j=0}^{n}-\frac{1}{2}\gamma_j\epsilon_{\mu\nu_j}(\eta^{\nu_j}{}_{\nu_{j-1}}+\gamma_{j-1}\epsilon^{\nu_j}{}_{\nu_{j-1}})\ldots(\eta^{\nu_1}{}_{\nu_0}+\gamma_0\epsilon^{\nu_1}{}_{\nu_0})L_{(0)}^{\nu_0}.$$

Expanding the sums and products, the final expression for this is

$$U_n^{-1}\partial^\mu U_n=-\frac{1}{2}\left(\sum\gamma+\sum_{\neq}\gamma\gamma\gamma+\ldots\right)\epsilon^\mu{}_\nu L_{(0)}^\nu-\frac{1}{2}\left(\sum_{\neq}\gamma\gamma+\ldots\right)L_{(0)}^\mu,$$

where all sums are with indices ranging from 0 to n, all indices are different within the sums and each term is included only once, i.e., $(\Sigma_{\neq}\gamma\gamma)$ means $(\Sigma_{i_1=0}^{n}\Sigma_{i_2>i_1}^{n}\gamma_{i_1}\gamma_{i_2})$, etc.

If we now fix all parameters γ_i to be equal, and define them as $\lambda/(n+1)$, we obtain

$$\sum\gamma=\sum_{i=0}^{n}\gamma_i=\lambda,$$

$$\sum_{\neq}\gamma\gamma=\sum_{i=0}^{n}\sum_{j>i}^{n}\gamma_i\gamma_j=\frac{\lambda^2}{(n+1)^2}\binom{N+1}{2}=\frac{\lambda^2}{2!}+\mathcal{O}\left(\frac{1}{n}\right),$$

$$\sum_{\neq}\gamma\gamma\gamma=\frac{1}{3!}\lambda^3+\mathcal{O}\left(\frac{1}{n}\right),$$

etc.,

whenever the order of the term is much lower than n. Therefore we get, in the large n limit, a Taylor series. Obviously this series adds up to

$$U^{-1}\partial^\mu U=\frac{1}{2}[(1-\cosh(\lambda))L^\mu-\sinh(\lambda)\epsilon^{\mu\nu}L_\nu],\tag{23}$$

that is what we had in Eq. (4).

III. DISCUSSION AND CONCLUSIONS

We have obtained the Lax pair for the non-linear σ-model in a mainly constructive way. It can now be given a physical significance, because it is the compatibility condition for the existence of a family of (non-linear/non-local) weak symmetry transformations for the model. The spectral parameter of such a family appears here as the parameter of a Lorentz transformation involved in the invariance of the action under the symmetry transformation. Built this way, it seems more realistic to think about its possible generalization to higher dimensions. Anyway, it is not an easy thing: for a $(2+1)$-dimensional space-time the construction breaks down at Eq. (18) because the first two terms of Eq. (17) do not cancel anymore, so α can not be chosen as zero to make Eq. (16) hold. One can try to restrict the symmetry to only a subset of the solutions' space, considering for instance only those fields g that are axially symmetric. Since we want to iterate the transformation

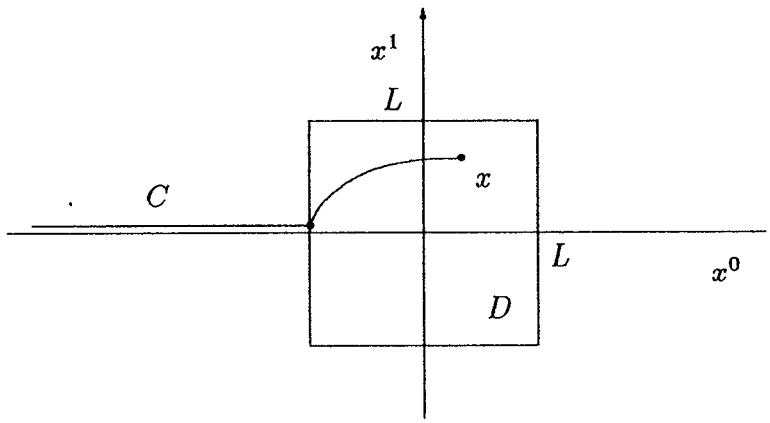

FIG. 1. Setup for integration of Eq. (21a).

in such a way that the new solution also has axial symmetry, the problem is that for physical consistency the $\omega_{\mu\nu}$ tensor of parameters should also be axially symmetric. This means that the (Cartesian) components $\omega_{\mu\nu}$ are position dependent. Therefore, if we want a non-trivial transformation, the second part of Eq. (14) must be modified with the addition of a term $L^\nu \partial^\mu \omega_{\mu\nu}$.

IV. ACKNOWLEDGMENT

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APPENDIX A: PATH INDEPENDENCE

Note that being $[\partial_\mu, \partial_\nu] u_{(n)} = 0 + \mathcal{O}(\gamma_i^2)$ (i.e., not exactly zero in general) we still have a "small" path dependency in $u_{(n)}$. How can we deal with it?

We aim at obtaining a ("true") function $g'(x)$, starting from $g(x)$, making N steps of parameters $\gamma_0, \ldots, \gamma_{N-1}$, and finally taking the limit $N \to \infty$, with (for all i) $N\gamma_i = \lambda$, a non-infinitesimal quantity. However, before the limit procedure, the N-times iterated "function" $g_{(N)}(x)$ may be defined only on a bounded domain D_N of M^2. We can choose, for instance, a square region $|x^\mu| < L$, with $L^2 \sim 1/\max(\gamma_i)$. So for $x \in D_N$ we can find $u_{(i)}(x)$ from Eq. (21a) integrating over a path C, consisting of a fixed piece from $-\infty$ to some point on the boundary of D_N, and an arbitrary piece *inside* D_N to x (as shown in Fig. 1). Therefore, integrating over two different paths we get two different u's, with

$$|\Delta u_{(i)}| \sim |[\partial_0, \partial_1] u_{(i)}|\,|\text{ Area between paths}|$$

$$\leq |\gamma_i|\,|\partial \cdot L_{(i)}| L^2 \leq \frac{\gamma_i}{\max(\gamma_j)} \gamma_{i-2}^2,$$

and we obtain a "fixed" error for $g_{(N)}(x)$ whenever x is inside D_N, with a given $\lambda = N\gamma_i$.

APPENDIX B: SYMMETRIC SPACE CASE

Keeping the same action as in Section II but allowing the field g to vary only on a symmetric space we get what is called a symmetric space sigma model.

A symmetric space[12] is a homogeneous group G/H together with an involution i in G ($i^2 = 1$), where G is a connected Lie group and H is a closed subgroup of G consisting of (at least the unit component of) the set of fixed points of i. This involution selects in a natural way a

subalgebra $\mathfrak{h}$ and a subspace $\mathfrak{m}$ of the Lie algebra $\mathfrak{g}$ of G. These are the eigenspaces corresponding to eigenvalues ± 1 of the involution induced by i on the algebra $\mathfrak{g}$. Moreover, $\mathfrak{h}$ is exactly the Lie algebra of H, and together with $\mathfrak{m}$ they span $\mathfrak{g}$. It is easy to see that

$$[\mathfrak{h},\mathfrak{m}]\subset\mathfrak{m},$$

$$[\mathfrak{m},\mathfrak{m}]\subset\mathfrak{h},$$

and, $\mathfrak{h}$ being an algebra, $[\mathfrak{h},\mathfrak{h}]\subset\mathfrak{h}$. Let us call π the projector from $\mathfrak{g}$ onto $\mathfrak{h}$, having kernel $\mathfrak{m}$. This projector can be extended naturally to one acting over the whole tangent space of G, as

$$\pi(\partial g)=g\,\pi(g^{-1}\partial g).$$

We must also require this space to be a Riemannian symmetric space, i.e., the group $\mathrm{Ad}_g(H)$ of adjoint transformations on $\mathfrak{g}$ should be compact, for in this case we have an H-invariant scalar product $\langle\cdot,\cdot\rangle$ needed for defining the action.

This symmetric space model is equivalent[2] to a (G) group valued σ-model but with a modified action,

$$S=\int \mathrm{d}^dx\langle D_\mu g, D^\mu g\rangle,$$

where normal derivatives are replaced by covariant ones with a g dependent connection A_μ. Explicitly, we must take

$$\begin{aligned} D_\mu g &= \partial_\mu g - g\,\pi(g^{-1}\partial_\mu g)\\ &= (1-\pi)\partial_\mu g. \end{aligned}$$

We have now a left *G-global* and a right *H-gauge* symmetries. Currents are $L_\mu \equiv -D_\mu g g^{-1}$ and $R_\mu \equiv g^{-1}D_\mu g$, which are related by $R_\mu = -g^{-1}L_\mu g$ as before. L is conserved ($\partial\cdot L \doteq 0$) and R is covariantly conserved. Using that $[\mathfrak{m},\mathfrak{m}]\subset\mathfrak{h}$, one can check that these currents have zero curvature,

$$F_{\mu\nu}(L)\equiv\partial_\mu L_\nu-\partial_\nu L_\mu+f[L_\mu,L_\nu]=0,$$

$$F_{\mu\nu}(R)\equiv\partial_\mu R_\nu-\partial_\nu R_\mu+f[R_\mu,R_\nu]=0.$$

Here $f=2$, and it is kept explicitly to show the difference with the already treated $f=1$ case.

In this case we can generalize the Lax pair construction retaining Eq. (6), but replacing normal by covariant derivatives in Eq. (7):

$$D_\mu g' = D_\mu(UgV^{-1}) = U\Lambda_{\mu\nu}D^\nu g V^{-1}$$

(remember $D_\mu g'$ means employing g' also in the corresponding connection). This implies that Eq. (9) and its infinitesimal expression, Eq. (12), are unchanged. Eq. (8) should now be replaced by

$$\begin{aligned} V(\Lambda_{\mu\nu}R^\nu - R_\mu)V^{-1} = &-\pi(VR_\mu V^{-1})\\ &+(1-\pi)[VA_\mu V^{-1}-\partial_\mu VV^{-1}+Vg^{-1}U^{-1}\partial_\mu UgV^{-1}], \end{aligned}$$

which reduces to (8) in the $H=1$ case. This can be decomposed in two more useful equations, projecting over $\mathfrak{h}$ and $\mathfrak{m}$ with π and $(1-\pi)$, respectively. Doing so, we get

$$V\Lambda_{\mu\nu}R^{\nu}V^{-1}=(\text{ vertical}), \tag{24a}$$

$$A_{\mu}-V^{-1}\partial_{\mu}V+g^{-1}U^{-1}\partial_{\mu}Ug+(R_{\mu}-\Lambda_{\mu\nu}R^{\nu})=V^{-1}(\text{ horizontal})V. \tag{24b}$$

Instead of Eq. (14) we get

$$\partial\cdot L'=\left[\partial_{\mu}u+\frac{f}{2}\omega_{\mu\nu}L^{\nu},L^{\mu}\right],$$

with a constant $\omega_{\mu\nu}$. From now on we only have to take into account the coefficient f. This results in changing the 1/2 factor by $f/2$ in Eq. (19) and all subsequent formulas. As it should, in the symmetric space case the Lax pair for U loses the 1/2 factor, $U^{-1}\partial_{\mu}U=(1-\cosh(\lambda))L_{\mu}-\sinh(\lambda)\epsilon_{\mu\nu}L^{\nu}$, and the one for V becomes zero, or a purely horizontal contribution $((1-\pi)(V^{-1}\partial V)=0)$ that corresponds anyway to a gauge transformation. This can be seen from Eq. (24a) because being $\pi(R_{\mu})=0$ (vertical), V must be generated by a horizontal element of $\mathfrak{g}$.

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Integrable discretizations of the Bogoyavlensky lattices

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Discretizations of the Bogoyavlensky lattices are introduced, belonging to the same hierarchies as the continuous-time systems. The construction exemplifies the general scheme for integrable discretization of systems on Lie algebras with r-matrix Poisson brackets. An initial value problem for the difference equations is solved in terms of a factorization problem in a group. Interpolating Hamiltonian flows are found. © *1996 American Institute of Physics.* [S0022-2488(96)00908-5]

I. INTRODUCTION

The subject of integrable symplectic maps has received, in recent years, considerable attention. Given an integrable system of ordinary differential equations with such attributes as Lax pair, r-matrix, and so on, one would like to construct its difference approximation, desirably also with a (discrete-time analog of) Lax pair, r-matrix, etc. Recent years brought us several successful examples of such a construction.[1–10]

Recently, stimulated by the results of Refs. 6 and 7, there was formulated a general recipe for producing discretizations sharing the Lax matrix with the continuous-time system, so that the discrete-time system belongs to the *same* integrable hierarchy as the underlying continuous-time one.[8–10]

In the present paper we want to describe a new application of this scheme, to a class of integrable systems known as Bogoyavlensky lattices[11] (although some special cases were discovered earlier in Refs. 12 and 13). An r-matrix interpretation of these systems was given in Ref. 14. Some of the discrete time equations studied in the present paper appeared previously in the literature,[15] as certain reductions of the discrete KP equation in the bilinear form. They were derived also in Ref. 16 from an *ad hoc* ansatz for the Lax pair. Our approach is quite different and enables us to get these equations systematically, and, moreover, provides automatically the Hamiltonian formulation along with the interpolating Hamiltonian flows, as well as the solution in terms of matrix factorizations.

II. CONTINUOUS-TIME BOGOYAVLENSKY LATTICES

The Bogoyavlensky lattices were introduced in Ref. 11 as three families of integrable lattice systems depending on integer parameter $m \geqslant 1$ ($m>1$ for the third one):

$$\dot{a}_k = a_k\left(\sum_{j=1}^{m} a_{k+j} - \sum_{j=1}^{m} a_{k-j}\right), \tag{2.1}$$

$$\dot{a}_k = a_k\left(\prod_{j=1}^{m} a_{k+j} - \prod_{j=1}^{m} a_{k-j}\right), \tag{2.2}$$

$$\dot{a}_k = a_k\left(\prod_{j=0}^{m} a_{k+j}^{-1} - \prod_{j=0}^{m} a_{k-j}^{-1}\right) = \prod_{j=1}^{m} a_{k+j}^{-1} - \prod_{j=1}^{m} a_{k-j}^{-1}. \tag{2.3}$$

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We shall call these systems lattice 1, lattice 2, and lattice 3, respectively.

The lattices 1 and 2 serve as generalizations of the famous Volterra lattice,

$$\dot{a}_k=a_k(a_{k+1}-a_{k-1}), \tag{2.4}$$

which is $m=1$ special case of both the systems (2.1) and (2.2). Certain generalizations of the Volterra lattice, including also lattice 1, were introduced independently (and earlier) by Narita;[12] some special case of the lattice 1 was found also by Itoh.[13]

The lattice 3 after the change of variables $a_k \mapsto a_k^{-1}$ and $t \mapsto -t$ turns into

$$\dot{a}_k=a_k^2\left(\prod_{j=1}^{m} a_{k+j}-\prod_{j=1}^{m} a_{k-j}\right), \tag{2.5}$$

which serves as a generalization of the so-called modified Volterra lattice, the $m=1$ particular case of (2.5):

$$\dot{a}_k=a_k^2(a_{k+1}-a_{k-1}). \tag{2.6}$$

All these systems may be considered on an infinite lattice (all the subscripts belong to $\mathbb{Z}$), and admit also periodic finite-dimensional reductions (all the subscripts belong to $\mathbb{Z}/N\mathbb{Z}$, where N is the number of particles). The lattices 1 and 2 admit also finite-dimensional versions with boundary conditions of the open-end type:

$$\text{for system (2.1):} \quad a_k=0 \quad \text{for } k\leqslant 0, \quad k\geqslant N-m+1;$$

$$\text{for system (2.2):} \quad a_k=0 \quad \text{for } k\leqslant 0, \quad k\geqslant N.$$

Bogoyavlensky has found also the Lax representations for these systems of the form

$$\dot{T}=[T, B], \tag{2.7}$$

where for the system (2.1)

$$T(a,\lambda)=\lambda^{-m}\sum a_k E_{k,k+m}+\lambda\sum E_{k+1,k}, \tag{2.8}$$

$$B(a,\lambda)=\sum (a_k+a_{k-1}+\cdots+a_{k-m})E_{k,k}+\lambda^{m+1}\sum E_{k+m+1,k}, \tag{2.9}$$

for the system (2.2)

$$T(a,\lambda)=\lambda^{-1}\sum a_k E_{k,k+1}+\lambda^{m}\sum E_{k+m,k}, \tag{2.10}$$

$$B(a,\lambda)=-\lambda^{-m-1}\sum a_k a_{k+1}\cdots a_{k+m}E_{k,k+m+1}, \tag{2.11}$$

and for the system (2.3)

$$T(a,\lambda)=\lambda^{-1}\sum a_k E_{k,k+1}+\lambda^{-m-1}\sum E_{k,k+m+1}, \tag{2.12}$$

$$B(a,\lambda)=\lambda^m\sum a_k^{-1}a_{k+1}^{-1}\cdots a_{k+m-1}^{-1}E_{k+m,k}, \tag{2.13}$$

Here for the infinite lattices all the subscripts belong to $\mathbb{Z}$, for the periodic case all the subscripts belong to $\mathbb{Z}/N\mathbb{Z}$, and for the open-end case all the subscripts belong to $1,\ldots,N$. Moreover, in the infinite-dimensional and open-end cases the dependence on the spectral parameter λ becomes inessential and may be suppressed by setting $\lambda=1$. Below we consider only finite lattices.

All the Bogoyavlensky lattices are Hamiltonian systems. More precisely, each system (2.1), (2.2), and (2.3) is Hamiltonian with respect to a certain quadratic Poisson bracket

$$\{a_k,a_j\}=\pi_{kj}a_ka_j, \tag{2.14}$$

with a skew-symmetric matrix (π_{kj}). The corresponding Hamiltonians are

$$H(a)=\frac{1}{(m+1)}\operatorname{tr}(T^{m+1})=\sum a_k \quad \text{for the systems (2.1)},$$

$$H(a)=\frac{1}{(m+1)}\operatorname{tr}(T^{m+1})=\sum a_ka_{k+1}\cdots a_{k+m-1} \quad \text{for the systems (2.2)},$$

$$H(a)=\frac{-1}{m}\operatorname{tr}(T^{-m})=\sum a_k^{-1}a_{k+1}^{-1}\cdots a_{k+m}^{-1} \quad \text{for the system (2.3)}.$$

The Poisson brackets (2.14), i.e., the matrices (π_{kj}), in the context of infinite systems were found for the lattice 1 in the original papers by Bogoyavlensky,[11] and for the lattices 2 and 3 in Ref. 17. For the finite lattices, where some subtleties come out, this was done systematically in Ref. 14.

III. DISCRETE TIME BOGOYAVLENSKY LATTICES

We present now equations of motion of some difference equations which can be considered as analogs and approximations to the Bogoyavlensky lattices for the case of the discrete time. The "Proposition k" ($k=1,2,3$) deals with the "discrete time Bogoyavlensky lattice k." We use tilde to denote the time shift, so that, for example, $\tilde{v}_k=v_k(t+h)$, if $v_k=v_k(t)$.

Proposition 1: The system of difference equations

$$\tilde{v}_k\prod_{j=1}^{m}(1+h\tilde{v}_{k-j})=v_k\prod_{j=1}^{m}(1+hv_{k+j}) \tag{3.1}$$

admits a Lax representation

$$\tilde{T}=L^{-1}TL$$

with the matrices

$$T(v,\lambda)=\lambda^{-m}\sum \alpha_kE_{k,k+m}+\lambda\sum E_{k+1,k}, \tag{3.2}$$

$$L(v,\lambda)=\sum \beta_kE_{k,k}+h\lambda^{m+1}\sum E_{k+m+1,k}, \tag{3.3}$$

where

$$a_k=v_k\prod_{j=1}^{m}(1+hv_{k-j}),\quad \beta_k=\prod_{j=0}^{m}(1+hv_{k-j}). \tag{3.4}$$

Proposition 2: The system of difference equations

$$\tilde{v}_k\left(1+h\prod_{j=1}^{m}\tilde{v}_{k-j}\right)=v_k\left(1+h\prod_{j=1}^{m}v_{k+j}\right) \tag{3.5}$$

admits a Lax representation

$$\tilde{T}=UTU^{-1}$$

with the matrices

$$T(v,\lambda)=\lambda^{-1}\sum a_kE_{k,k+1}+\lambda^m\sum E_{k+m,k}, \tag{3.6}$$

$$U(v,\lambda)=I+h\lambda^{-m-1}\sum \gamma_kE_{k,k+m+1}, \tag{3.7}$$

where

$$a_k=v_k\left(1+h\prod_{j=1}^{m}v_{k-j}\right),\quad \gamma_k=\prod_{j=0}^{m}v_{k+j}. \tag{3.8}$$

Proposition 3: The system of difference equations

$$\tilde{v}_k\left(1+h\prod_{j=0}^{m}\tilde{v}^{-1}_{k-j}\right)=v_k\left(1+h\prod_{j=0}^{m}v^{-1}_{k+j}\right) \tag{3.9}$$

admits a Lax representation

$$\tilde{T}=L^{-1}TL$$

with the Lax matrices

$$T(v,\lambda)=\lambda^{-1}\sum a_kE_{k,k+1}+\lambda^{-m-1}\sum E_{k,k+m+1}, \tag{3.10}$$

$$L(v,\lambda)=1+h\lambda^m\sum \alpha_kE_{k+m,k}, \tag{3.11}$$

where

$$a_k=v_k\left(1+h\prod_{j=0}^{m}v^{-1}_{k-j}\right),\quad \alpha_k=\prod_{j=0}^{m-1}v^{-1}_{k+j}. \tag{3.12}$$

Remark 1: Upon change of variables $v_k\mapsto v_k^{-1}$ and $h\mapsto -h$ the system (3.9) turns into

$$\tilde{v}_k\left(1-h\prod_{j=0}^{m}\tilde{v}_{k-j}\right)^{-1}=v_k\left(1-h\prod_{j=0}^{m}v_{k+j}\right)^{-1}, \tag{3.13}$$

which may be considered as a discrete time analog and approximation to (2.5).

Remark 2: The equation (3.1) was found in Ref. 15 as a certain reduction of the discrete KP equation in the bilinear form. The equations (3.1) and (3.5) for $m=1$ coincide, as they should (Volterra lattice). The Lax representation for this case with the matrices (3.6) and (3.7) was also given in Ref. 15, but without any hint on how it was obtained. After the present paper was submitted for publication, I became aware of Ref. 16, where equations (3.1), (3.5), and (3.9) are derived from an *ad hoc* ansatz for the Lax pair. (I thank V. Papageorgiou and F. W. Nijhoff for sending me their paper prior to publication.) However, our point of view and results concerning these equations are very different from those of Ref. 16.

In the above formulation the Propositions 1–3 may be easily checked by a direct computation, but their origin remains hidden. In the following sections we shall give a way to *derive* them systematically, which, as a by-product, will unvail an underlying invariant Poisson structure of these discrete systems, as well as a role of the auxiliary matrices L, U. This, in turn, will enable us to solve the initial value problems for our systems in terms of matrix factorizations and to find interpolating Hamiltonian flows. Our construction is just a particular case of a general one, applicable, in principle, to every system admitting an r-matrix interpretation. The key observation is that the Lax matrices (3.2), (3.6), and (3.10) of the discrete time systems formally coincide with the corresponding Lax matrices (2.8), (2.10), and (2.12) of the continuous time ones.

IV. ALGEBRAIC STRUCTURE OF BOGOYAVLENSKY LATTICES

In Ref. 14 we gave an r-matrix interpretation of the Bogoyavlensky lattices as simplest representatives of integrable hierarchies on associative algebras. The main results of Ref. 14 may be summarized as follows.

(1) For the *open-end case* (applies only to the lattices 1 and 2) we set $\mathbf{g}=\mathrm{gl}(N)$. To this algebra there corresponds a group $\mathbf{G}=\mathrm{GL}(N)$. As a linear space, $\mathbf{g}$ may be represented as a direct sum of two subspaces, which serve also as subalgebras: $\mathbf{g}=\mathbf{g}_+\oplus\mathbf{g}_-$. Here $\mathbf{g}_+$ ($\mathbf{g}_-$) is a space of all lower triangular (resp. strictly upper triangular) N by N matrices. The corresponding subgroups: $\mathbf{G}_+$ ($\mathbf{G}_-$) is a group of all nondegenerate lower triangular N by N matrices (resp. upper triangular N by N matrices with unities on the diagonal).

(2) For the *periodic case* (of all lattices 1, 2, and 3) $\mathbf{g}$ is a certain twisted loop algebra over $\mathrm{gl}(N)$, namely the algebra of formal semi-infinite Laurent series $T(\lambda)$ over $\mathrm{gl}(N)$, satisfying $\Omega T(\lambda)\Omega^{-1}=T(\omega\lambda)$, where $\Omega=\mathrm{diag}(1,\omega,\ldots,\omega^{N-1})$ and $\omega=\exp(2\pi i/N)$. The corresponding group is the twisted loop group $\mathbf{G}$ consisting of $\mathrm{GL}(N)$-valued functions $T(\lambda)$ of the complex parameter λ, regular in $\mathbb{C}P^1\{0,\infty\}$ and satisfying $\Omega T(\lambda)\Omega^{-1}=T(\omega\lambda)$. Again, as a linear space $\mathbf{g}=\mathbf{g}_+\oplus\mathbf{g}_-$, where for the lattices 1 and 2, $\mathbf{g}_+$ ($\mathbf{g}_-$) is a subspace and subalgebra consisting of $T(\lambda)$ containing only non-negative (resp. only negative) powers of λ, and the case of the lattice 3 differs in that, to which subalgebra do diagonal matrices belong: $\mathbf{g}_+$ contains only positive, and $\mathbf{g}_-$ only nonpositive powers of λ. For the lattices 1 and 2 the corresponding subgroups $\mathbf{G}_+$ and $\mathbf{G}_-$ consist of $T(\lambda)$ regular in the neighborhood of $\lambda=0$ (resp. regular in the neighborhood of $\lambda=\infty$ and taking the value I in $\lambda=\infty$). For the lattice 3 $\mathbf{G}_+$ is formed by $T(\lambda)$ regular in the neighborhood of $\lambda=0$ with $T(0)=I$, and $\mathbf{G}_-$ is formed by $T(\lambda)$ regular in the neighborhood of $\lambda=\infty$.

We shall need a notion of the gradient $\nabla\varphi(T)\in\mathbf{g}$ of a function $\varphi:\mathbf{g}\to\mathbb{C}$, defined in the open-end case by the relation

$$\mathrm{tr}(\nabla\varphi(T)X)=\frac{d}{d\varepsilon}\,\varphi(T+\varepsilon X)\bigg|_{\varepsilon=0}\qquad\forall X\in\mathbf{g};$$

in the periodic case "tr" should be replaced by "tr_0", the free term in the Laurent series for the trace.

For both the open-end and periodic cases every $T \in \mathbf{g}$ admits a unique decomposition $T = l(T) + u(T)$, where $l(T) \in \mathbf{g}_+$ and $u(T) \in \mathbf{g}_-$. Analogously, for both cases every $T \in \mathbf{G}$ from some neighborhood of the group unity admits a unique factorization $T = \mathscr{L}(T)\mathscr{U}(T)$, where $\mathscr{L}(T) \in \mathbf{G}_+$ and $\mathscr{U}(T) \in \mathbf{G}_-$.

There hold the following statements.

(a) For each system (2.1), (2.2), and (2.3) there exists a quadratic r-matrix Poisson bracket on $\mathbf{g}$ whose Dirac reduction to the corresponding set of matrices $\mathscr{P} = \{T(a,\lambda)\}$ from (2.8), (2.10), or (2.12), respectively, is given by (2.14).

(b) Let $\varphi: \mathbf{g} \to \mathbf{C}$ be an invariant function, so that $d\varphi(T) = T\nabla\varphi(T) = \nabla\varphi(T)T$ is covariant under conjugation. Then the Hamiltonian flow on $\mathbf{g}$ with the Hamiltonian function $\varphi(T^p)/p$ (here and below $p = m+1$ for the lattices 1 and 2, and $p = m$ for the lattice 3) is tangent to $\mathscr{P}$ and has the Lax form

$$\dot{T} = [T,\ l(d\varphi(T^p))] = -[T,\ u(d\varphi(T^p))]. \tag{4.1}$$

This flow admits the following solution in terms of the factorization problem

$$e^{td\varphi(T^p(0))} = \mathscr{L}(t)\mathscr{U}(t), \quad \mathscr{L}(t) \in \mathbf{G}_+, \quad \mathscr{U}(t) \in \mathbf{G}_-$$

(this problem has solutions at least for sufficiently small t):

$$T(t) = \mathscr{L}^{-1}(t)T(0)\mathscr{L}(t) = \mathscr{U}(t)T(0)\mathscr{U}^{-1}(t).$$

(c) Let $f: \mathbf{g} \to \mathbf{G}$ be a conjugation covariant function on $\mathbf{g}$. Then the difference equation

$$\tilde{T} = \mathscr{L}^{-1}(f(T^p))T\mathscr{L}(f(T^p)) = \mathscr{U}(f(T^p))T\mathscr{U}^{-1}(f(T^p)) \tag{4.2}$$

defines a Poisson map $\mathbf{g} \to \mathbf{g}$ which leaves $\mathscr{P}$ invariant, the restriction of this map on $\mathscr{P}$ being Poisson with respect to the reduced bracket (2.14). This difference equation admits the following solution in terms of the factorization problem

$$f^n(T^p(0)) = \mathscr{L}(nh)\mathscr{U}(nh), \quad \mathscr{L}(nh) \in \mathbf{G}_+, \quad \mathscr{U}(nh) \in \mathbf{G}_-$$

[this problem has solutions for a given n at least if $f(T(0))$ is sufficiently close to the group unity I]:

$$T(nh) = \mathscr{L}^{-1}(nh)T(0)\mathscr{L}(nh) = \mathscr{U}(nh)T(0)\mathscr{U}^{-1}(nh).$$

(d) The solutions of the difference equation (4.2) are interpolated by the flow (4.1) with the Hamiltonian function $\varphi(T^p)/p$, where $\varphi(T)$ is defined by

$$d\varphi(T) = h^{-1}\log(f(T)). \tag{4.3}$$

The statements (a) and (b) explain the Lax equation (2.7) with the matrices (2.8)–(2.13); as for the system (2.1) we have $B(a,\lambda) = l(T^{m+1}(a,\lambda))$, for the system (2.2) we have $B(a,\lambda) = -u(T^{m+1}(a,\lambda))$, and for the system (2.3) we have $B(a,\lambda) = l(T^{-m}(a,\lambda))$.

V. A DISCRETIZATION OF THE BOGOYAVLENSKY LATTICE 1

We get a correct perspective for the interpretation of the system (3.1) [as well as the systems (3.5) and (3.9)] if we take an "inverse" view-point. We consider the first equation in (3.4) as an implicit definition of the functions $v_k = v_k(a)$, rather then the expressions of a_k through v_j. In the open-end case the sequence of v_k's can be computed even explicitly, term by term, starting with

$v_k=a_k/(1+h\Sigma_{j=1}^{k-1}a_j)$ for $1\leqslant k\leqslant m+1$. In particular, for $m=1$, one has $v_k=a_k/(1+hv_{k-1})$, which implies a nice representation in form of a finite continued fraction:

$$v_k=\cfrac{a_k}{1+\cfrac{ha_{k-1}}{1+\ddots+\cfrac{ha_2}{1+ha_1}}}. \tag{5.1}$$

In the periodic case the existence of the functions $v_k=v_k(a)$, at least for h small enough, follows from the implicit functions theorem. Again, for $m=1$ we get an expression in the form of an infinite N-periodic continued fraction of the type (5.1).

The second equation in (3.4) may be rewritten as a recurrent relation for $\beta_k=\beta_k(a)$. In fact, we have $\beta_k-ha_k=\Pi_{j=1}^{m}(1+hv_{k-j})$, so that $a_k/(\beta_k-ha_k)=v_k$, and finally

$$\beta_k-ha_k=\prod_{j=1}^{m}\left(1+\frac{ha_{k-j}}{\beta_{k-j}-ha_{k-j}}\right). \tag{5.2}$$

Conversely, the last formula implies (3.4), if one sets $v_k=a_k/(\beta_k-ha_k)$.

The formula (5.2) may also serve for a successive computation of β_ks in the open-end case, and in the periodic case it uniquely defines a set of β_k-ha_k, $1\leqslant k\leqslant N$, via the implicit functions theorem. In both cases it is easy to see that

$$\beta_k=1+h\sum_{j=0}^{m}a_{k-j}+O(h^2). \tag{5.3}$$

Theorem 1: The quantities β_k defined by (5.2) serve as coefficients of the matrix

$$L=\mathscr{Z}(I+hT^{m+1})=\sum_k \beta_k E_{k,k}+h\lambda^{m+1}\sum_k E_{k+m+1,k}. \tag{5.4}$$

The discrete time Lax equation

$$\widetilde{T}=L^{-1}TL=\mathscr{Z}^{-1}(I+hT^{m+1})T\mathscr{Z}(I+hT^{m+1}). \tag{5.5}$$

with the Lax matrix (2.8) generates the following map on $\mathbb{R}^N\{a\}$, equivalent to (3.1):

$$\widetilde{a}_k=\frac{\beta_{k+m}}{\beta_k}a_k. \tag{5.6}$$

This map is Poisson with respect to the Poisson bracket (2.14) corresponding to the lattice 1, and is interpolated by the flow with the Hamiltonian function

$$\frac{1}{m+1}\operatorname{tr}\Phi(T^{m+1}),\quad \text{where}\quad \Phi(\xi)=h^{-1}\int_0^{\xi}\log(1+h\eta)\,\frac{d\eta}{\eta}. \tag{5.7}$$

Proof: The last two statements follow from the results formulated in the previous section, provided the first two statements are proved. Suppose for a moment that the $\mathscr{Z}$-factor of $I+hT^{m+1}$ has the form (5.4). Then the evolution equation (5.5), i.e., $L\widetilde{T}=TL$, is equivalent to

$$\beta_k\bar{a}_k=a_k\beta_{k+m},\quad h\tilde{a}_k+\beta_{k+m+1}=ha_{k+m+1}+\beta_{k+m}. \tag{5.8}$$

This in turn is equivalent to a combination of an evolution equation (5.6) with the condition of compatibility of two equations in (5.8):

$$\beta_k-ha_k=\frac{\beta_k}{\beta_{k+m}}(\beta_{k+m+1}-ha_{k+m+1}). \tag{5.9}$$

The last equation is equivalent to the fact that

$$\frac{\prod_{j=0}^{m}(\beta_{k+j}-ha_{k+j})}{\prod_{j=0}^{m-1}\beta_{k+j}}=\text{const}, \tag{5.10}$$

i.e., does not depend on k. We shall prove that the actual value of this constant is equal to 1, which is just equivalent to (5.2).

The inspection of the structure of the matrix T^{m+1} for T from (2.8) convinces us that the $\mathscr{L}$-factor of $I+hT^{m+1}$ has in fact the form (5.4), while the $\mathscr{U}$-factor has the form

$$U=\mathscr{U}(I+hT^{m+1})=I+h\sum_{j=1}^{m}\lambda^{-j(m+1)}\sum_k\gamma_k^{(j)}E_{k,k+j(m+1)}.$$

The quantities $\beta_k,\gamma_k^{(j)}$ are completely defined by the set of recurrent relations following from the definitions:

$$\beta_k+h^2\gamma_{k-m-1}^{(1)}=1+h\sum_{j=0}^{m}a_{k-j}, \tag{5.11}$$

$$\beta_k\gamma_k^{(j)}+h\gamma_{k-m-1}^{(j+1)}=\text{coef. by }\lambda^{-j(m+1)}E_{k,k+j(m+1)}\text{ in }T^{m+1},\quad 1\leq j\leq m-1;$$

$$\beta_k\gamma_k^{(m)}=\prod_{j=0}^{m}a_{k+jm}.$$

Now we are in a position to prove that the constant in (5.10) is equal to 1.

Indeed, in the open-end case it is enough to compute from (5.11) the first $m+1$ values of β_k, namely $\beta_k=1+h\Sigma_{j=1}^{k}a_j$, $1\leq k\leq m+1$, which implies $\Pi_{j=1}^{m+1}(\beta_j-ha_j)/\Pi_{j=1}^{m}\beta_j=1$.

In the periodic case we have found only a combinatoric proof based on tedious computations. For the sake of simplicity and in order to avoid complicated notations we present the corresponding argument only in the simplest cases $m=1,2$.

In the case $m=1$ the defining recurrent relations take the form

$$\beta_k+h^2\gamma_{k-2}^{(1)}=1+ha_k+ha_{k-1},\quad \beta_k\gamma_k^{(1)}=a_ka_{k+1}.$$

Excluding $\gamma_k^{(1)}$ from these relations, we obtain

$$1=\beta_{k+2}-ha_{k+2}-ha_{k+1}\frac{\beta_k-ha_k}{\beta_k}.$$

Replacing the fraction on the right-hand side through its expression following from (5.9) for $m=1$, we obtain

$$1=\frac{(\beta_{k+2}-ha_{k+2})(\beta_{k+1}-ha_{k+1})}{\beta_{k+1}},$$

which proves the theorem in the case $m=1$.

For $m=2$, the defining recurrent relations take the form

$$\beta_k+h^2\gamma^{(1)}_{k-3}=1+ha_k+ha_{k-1}+ha_{k-2},$$

$$\beta_k\gamma^{(1)}_k+h\gamma^{(2)}_{k-3}=a_ka_{k+2}+a_ka_{k+1}+a_{k-1}a_{k+1},\quad \beta_k\gamma^{(2)}_k=a_ka_{k+2}a_{k+4}.$$

Excluding from these relations $\gamma^{(j)}_k$, we obtain

$$1=\beta_{k+3}-ha_{k+3}-h(a_{k+2}+a_{k+1})\frac{\beta_k-ha_k}{\beta_k}+h^2a_{k+1}a_{k-1}\frac{\beta_{k-3}-ha_{k-3}}{\beta_k\beta_{k-3}}.$$

According to (5.9) for $m=2$, this is equivalent to

$$\begin{aligned}1&=\beta_{k+3}-ha_{k+3}-h(a_{k+2}+a_{k+1})\frac{\beta_{k+3}-ha_{k+3}}{\beta_{k+2}}+h^2a_{k+1}a_{k-1}\frac{\beta_{k+3}-ha_{k+3}}{\beta_{k+2}\beta_{k-1}}\\&=\frac{(\beta_{k+3}-ha_{k+3})(\beta_{k+2}-ha_{k+2})}{\beta_{k+2}}-ha_{k+1}\frac{(\beta_{k+3}-ha_{k+3})(\beta_{k-1}-ha_{k-1})}{\beta_{k+2}\beta_{k-1}}.\end{aligned}$$

Using in the last term once more (5.9) for $m=2$, we obtain

$$1=\frac{(\beta_{k+3}-ha_{k+3})(\beta_{k+2}-ha_{k+2})(\beta_{k+1}-ha_{k+1})}{\beta_{k+2}\beta_{k+1}},$$

which proves the theorem for $m=2$. The pattern of the proof for a general m may be seen from these two particular cases.

VI. A DISCRETIZATION OF THE BOGOYAVLENSKY LATTICE 2

For the lattice 2 we again consider the first equation in (3.8) as a definition of the functions $v_k=v_k(a)$. In the open-end case we can compute these functions successively, starting with $v_k=a_k(1+h\Sigma_{j=1}^{k-2}\Pi_{l=1}^{j}a_l)/(1+h\Sigma_{j=1}^{k-1}\Pi_{l=1}^{j}a_l)$ for $1\leqslant k\leqslant m+1$. In the periodic case the implicit functions theorem has to be invoked. In particular, for the case $m=1$ we obtain the same continued fractions expressions as in the previous section.

The second equation in (3.8) may be represented as a recurrent relation for $\gamma_k=\gamma_k(a)$. Indeed, we have $a_k-h\gamma_{k-m}=v_k$, so that

$$a_k-h\gamma_{k-m}=\frac{a_k}{1+h\prod_{j=1}^{m}(a_{k-j}-h\gamma_{k-m-j})}. \tag{6.1}$$

Conversely, the last formula implies (3.8), if one sets $v_k=a_k-h\gamma_{k-m}$.

In the open-end case the formula (6.1) serves as a basis for successive computation of γ_ks, and in the periodic case it uniquely defines, by the implicit function theorem, the quantities $a_{k+m}-h\gamma_k$, $1\leqslant k\leqslant N$. In both cases there holds the following asymptotic relation:

$$\gamma_k=\prod_{j=0}^{m}a_{k+j}(1+O(h)). \tag{6.2}$$

Theorem 2: The quantities γ_k defined by (6.1) serve as coefficients of the matrix

$$U=\mathscr{U}(I+hT^{m+1})=I+h\lambda^{-(m+1)}\sum_k \gamma_k E_{k,k+m+1}, \tag{6.3}$$

The discrete time Lax equation

$$\widetilde{T}=UTU^{-1}=\mathscr{U}(I+hT^{m+1})T\mathscr{U}^{-1}(I+hT^{m+1}) \tag{6.4}$$

with the Lax matrix (2.10) generates the following map on $\mathbb{R}^N\{a\}$, equivalent to (3.5):

$$\widetilde{a}_k=\frac{a_k-h\gamma_{k-m}}{a_{k+m+1}-h\gamma_{k+1}}a_{k+m+1}. \tag{6.5}$$

This map is Poisson with respect to the Poisson bracket (2.14) corresponding to the lattice 2, and is interpolated by the flow with the Hamiltonian function (5.7).

Proof: Again, it suffices to prove the first two statements. Assuming for a moment that the $\mathscr{U}$-factor of the the matrix $I+hT^{m+1}$ for T from (2.10) has the form (6.3), we see that the evolution equation (6.4), i.e., $\widetilde{T}U=UT$, is equivalent to

$$\widetilde{a}_k\gamma_{k+1}=\gamma_k a_{k+m+1}, \quad \widetilde{a}_k+h\gamma_{k-m}=a_k+h\gamma_k. \tag{6.6}$$

This in turn is equivalent to a combination of an evolution equation (6.5) with the condition of compatibility of two equations in (6.6):

$$a_k-h\gamma_{k-m}=\frac{\gamma_k}{\gamma_{k+1}}(a_{k+m+1}-h\gamma_{k+1}). \tag{6.7}$$

The last equation is equivalent to the fact that

$$\frac{1}{\gamma_k}\prod_{j=0}^{m}(a_{k+m-j}-h\gamma_{k-j})=\text{const}, \tag{6.8}$$

i.e., does not depend on k. We shall prove that the actual value of this constant is equal to 1, which is equivalent to (6.1).

This time the inspection convinces us that the $\mathscr{U}$-factor of the matrix $I+hT^{m+1}$ for T from (2.10) must indeed have the form (6.3), while the $\mathscr{L}$-factor must have the form

$$L=\mathscr{L}(I+hT^{m+1})=\sum_k \beta_k^{(0)}E_{k,k}+h\sum_{j=1}^{m}\lambda^{j(m+1)}\sum_k \beta_k^{(j)}E_{k+j(m+1),k},$$

where $\beta_k^{(m)}=1$, and other quantities $\gamma_k,\beta_k^{(j)}$ are completely defined by the recurrent relations following from the definitions:

$$\beta_k^{(0)}\gamma_k=\prod_{j=0}^{m}a_{k+j}, \tag{6.9}$$

$$\beta_k^{(0)}+h^2\beta_{k-m-1}^{(1)}\gamma_{k-m-1}=1+h\sum_{l=k-m}^{k}\prod_{j=0}^{m-1}a_{l+j}, \tag{6.10}$$

$\beta_k^{(j)}+h\beta_{k-m-1}^{(j+t)}\gamma_{k-m-1}=$coef. by $\lambda^{j(m+1)}E_{k+j(m+1),k}$ in T^{m+1}, $1\leqslant j\leqslant m-1$.

To prove that the constant in (6.8) is equal to 1, in the open-end case it is enough to compute from (6.9) and (6.10) the first $m+1$ values of γ_k, namely $\gamma_k=\Pi_{j=0}^{m}a_{k+j}/(1+h\Sigma_{l=1}^{k}\Pi a_{l+j})$, $1\leqslant k\leqslant m+1$, which implies $\Pi_{j=1}^{m+1}(a_{j+m}-h\gamma_j)/\gamma_{m+1}=1$.

In the periodic case we shall again give the proof only for $m=1,2$, leaving the tedious calculations for the general case to the reader. For $m=1$ the defining recurrences (6.9) and (6.10) take the form

$$\beta_k^{(0)}\gamma_k=a_ka_{k+1},\quad \beta_k^{(0)}+h^2\gamma_{k-2}=1+ha_k+ha_{k-1}.$$

Excluding from these relations $\beta_k^{(0)}$, we obtain

$$1=\frac{a_k}{\gamma_k}(a_{k+1}-h\gamma_k)-h(a_{k-1}-h\gamma_{k-2}).$$

Replacing the last term on the right-hand side through its expression following from (6.7) for $m=1$, we obtain

$$1=\frac{(a_{k+1}-h\gamma_k)(a_k-h\gamma_{k-1})}{\gamma_k},$$

which proves the theorem for $m=1$.

In the case $m=2$ the recurrent relations (6.9) and (6.10) take the form

$$\beta_k^{(0)}\gamma_k=a_ka_{k+1}a_{k+2},\quad \beta_k^{(0)}+h^2\beta_{k-3}^{(1)}\gamma_{k-3}=1+h(a_{k-2}a_{k-1}+a_{k-1}a_k+a_ka_{k+1}),$$

$$\beta_k^{(1)}+h\gamma_{k-3}=a_{k-1}+a_{k+1}+a_{k+3}.$$

Excluding $\beta_k^{(j)}$ from these relations, we obtain

$$1=\frac{a_ka_{k+1}}{\gamma_k}(a_{k+2}-h\gamma_k)-h(a_{k-2}+a_k)(a_{k-1}-h\gamma_{k-3})+h^2\gamma_{k-3}(a_{k-4}-h\gamma_{k-6}).$$

Using on the right-hand side repeatedly (6.7) for $m=2$, we can rewrite it as

$$1=\frac{a_ka_{k+1}}{\gamma_k}(a_{k+2}-h\gamma_k)-\frac{h(a_{k-2}+a_k)\gamma_{k-1}}{\gamma_k}(a_{k+2}-h\gamma_k)+\frac{h^2\gamma_{k-4}\gamma_{k-1}}{\gamma_k}(a_{k+2}-h\gamma_k)$$

$$=\frac{a_k}{\gamma_k}(a_{k+2}-h\gamma_k)(a_{k+1}-h\gamma_{k-1})-\frac{h\gamma_{k-1}}{\gamma_k}(a_{k+2}-h\gamma_k)(a_{k-2}-h\gamma_{k-4}).$$

Using in the last term once more (6.7) for $m=2$, we obtain

$$1=\frac{1}{\gamma_k}(a_{k+2}-h\gamma_k)(a_{k+1}-h\gamma_{k-1})(a_k-h\gamma_{k-2}),$$

which finishes the proof for $m=2$.

VII. A DISCRETIZATION OF THE BOGOYAVLENSKY LATTICE 3

For the lattice 3 we again define the functions $v_k=v_k(a)$ by means of the first equation in (3.12), which is justified by the implicit function theorem (as opposed to the lattices 1,2, this time an open-end reduction is not admissible, so that only the periodic case needs to be considered). In particular, for $m=1$ we have $v_k=a_k-h/v_{k-1}$, which leads to the expression in terms of an infinite N-periodic continued fraction:

$$v_k=a_k-\cfrac{h}{a_{k-1}-\ddots-\cfrac{h}{a_{k-N+1}-\cfrac{h}{v_k}}}.$$

The second equation in (3.8) implies $a_k-h\alpha_{k-m}=v_k$, and hence

$$\alpha_k=\prod_{j=0}^{m-1}\frac{1}{a_{k+j}-h\alpha_{k+j-m}}. \tag{7.1}$$

Conversely, the last formula implies (3.12), if one defines $v_k=a_k-h\alpha_{k-m}$.

The formula (7.1) defines, by the implicit function theorem, the set of quantities $\alpha_k, 1\leqslant k\leqslant N$, satisfying

$$\alpha_k=\prod_{j=0}^{m-1}a_{k+j}^{-1}(1+O(h)). \tag{7.2}$$

Theorem 3: The quantities α_k defined by (7.1) serve as coefficients of the matrix

$$L=\mathscr{L}(I+hT^{-m})=I+h\lambda^m\sum_k \alpha_k E_{k+m,k}. \tag{7.3}$$

The discrete time Lax equation

$$\widetilde{T}=L^{-1}TL=\mathscr{L}^{-1}(I+hT^{-m})T\mathscr{L}(I+hT^{-m}) \tag{7.4}$$

with the Lax matrix (2.12) generates the following map on $\mathbb{R}^N\{a\}$, equivalent to (3.9):

$$\widetilde{a}_k=\frac{a_k-h\alpha_{k-m}}{a_{k+m}-h\alpha_k}a_{k+m}. \tag{7.5}$$

This map is Poisson with respect to the Poisson bracket (2.14) corresponding to the lattice 3, and is interpolated by the flow with the Hamiltonian function

$$-\frac{1}{m}\operatorname{tr}\Phi(T^{-m}),\quad \text{where}\quad \Phi(\xi)=h^{-1}\int_0^{\xi}\log(1+h\eta)\frac{d\eta}{\eta}.$$

Proof: Again, it suffices to prove the first two statements. Assuming for a moment that the $\mathscr{L}$-factor of the matrix $I+hT^{-m}$ for T from (2.12) has the form (7.3), we see that the evolution equation (7.4), i.e., $L\widetilde{T}=TL$, is equivalent to

$$\alpha_k\widetilde{a}_k=a_{k+m}\alpha_{k+1},\quad \widetilde{a}_k+h\alpha_{k-m}=a_k+h\alpha_{k+1}. \tag{7.6}$$

This in turn is equivalent to a combination of an evolution equation (7.5) with the condition of compatibility of two equations in (7.6):

$$a_k-h\alpha_{k-m}=\frac{\alpha_{k+1}}{\alpha_k}(a_{k+m}-h\alpha_k). \tag{7.7}$$

The last equation is equivalent to the fact that

$$\alpha_k \prod_{j=0}^{m-1} (a_{k+j} - h\alpha_{k+k-m}) = \text{const}, \tag{7.8}$$

i.e., does not depend on k. We shall prove that the actual value of this constant is equal to 1, which is equivalent to (7.1).

To compute the $\mathscr{L}$-factor of the matrix $I+hT^{-m}$ for T from (2.12), we notice, first, that $T^{-1}=CD^{-1}$, where

$$C=\lambda\sum_k a_k^{-1}E_{k+1,k}, \quad D=I+\lambda^{-m}\sum_k a_{k+m}^{-1}E_{k,k+m}.$$

Further, notice that the $\mathscr{L}$-factor of any matrix is not changed under the right multiplication by the factor from $\mathbf{G}_-$. We multiply the matrix $I+hT^{-m}=I+(CD^{-1})^m$ from the right by $(DC^{-1})^m C^m$. To see that this matrix belongs to G_-, notice that it is equal to $DD_1\cdots D_{m-1}$, where $D_j=C^{-j}DC^j=I+\lambda^{-m}\Sigma d_k^{(j)}E_{k,k+m}\in\mathbf{G}_-$. For the further reference we give here an explicit formula

$$d_k^{(j)}=\prod_{l=0}^{j-1} a_{k+1}\prod_{l=0}^{j} a_{k+m+l}^{-1}.$$

So we obtain

$$\mathscr{L}(I+hT^{-m})=\mathscr{L}(DD_1\cdots D_{m-1}+hC^m),$$

and an inspection of this formula convinces us that this factor must indeed be of the form (7.3), while

$$\mathscr{U}(DD_1\cdots D_{m-1}+hC^m)=\sum_{j=0}^{m}\lambda^{-jm}\sum_k \beta_k^{(j)}E_{k,k+jm}.$$

Here the quantities $\alpha_k,\beta_k^{(j)}$ are completely defined by the recurrent relations following from the definitions:

$$\alpha_k\beta_k^{(0)}=\prod_{j=0}^{m-1} a_{k+j}^{-1}, \tag{7.9}$$

$$\beta_k^{(0)}+h\alpha_{k-m}\beta_{k-m}^{(1)}=1, \tag{7.10}$$

$\beta_k^{(j)}+h\alpha_{k-m}\beta_{k-m}^{(j+1)}=$coef. by $\lambda^{-jm}E_{k,k+jm}$ in $DD_1\cdots D_{m-1}$, $1\leq j\leq m$. (In the last equation for $j=m$ one must set $\beta_k^{(m+1)}=0$, which leads to $\beta_k^{(m)}=\Pi_{l=0}^{m-1}a_{k+m^2+l}^{-1}$.)

Again, we shall prove that the constant in (7.8) is equal to 1, only for the two simplest cases $m=1,2$, leaving the calculations for the general case to the reader.

For $m=1$ the defining recurrences (7.9) and (7.10) read

$$\alpha_k\beta_k^{(0)}=a_k^{-1}, \quad \beta_k^{(0)}+h\alpha_{k-1}\beta_{k-1}^{(1)}=1, \quad \beta_k^{(1)}=a_{k+1}^{-1}.$$

Excluding from these relations $\beta_k^{(0)},\beta_k^{(1)}$, we obtain

$$\frac{a_k^{-1}}{\alpha_k}=1-ha_k^{-1}\alpha_{k-1} \quad \text{or} \quad \frac{1}{\alpha_k}=a_k-h\alpha_{k-1},$$

which proves the theorem for $m=1$.

In the case $m=2$ the recurrent relations (7.9) and (7.10) take the form

$$\alpha_k\beta_k^{(0)}=a_k^{-1}a_{k+1}^{-1} \quad \beta_k^{(0)}+h\alpha_{k-2}\beta_{k-2}^{(1)}=1,$$

$$\beta_k^{(1)}+h\alpha_{k-2}\beta_{k-2}^{(2)}=a_{k+2}^{-1}+a_ka_{k+2}^{-1}a_{k+3}^{-1}, \quad \beta_k^{(2)}=a_{k+4}^{-1}a_{k+5}^{-1}.$$

Excluding $\beta_k^{(j)}$ from these relations, we obtain

$$\frac{a_k^{-1}a_{k+1}^{-1}}{\alpha_k}=1-h\alpha_{k-2}(a_k^{-1}+a_{k-2}a_k^{-1}a_{k+1}^{-1}-h\alpha_{k-4}a_k^{-1}a_{k+1}^{-1}),$$

or

$$\frac{1}{\alpha_k}=a_{k+1}(a_k-h\alpha_{k-2})-h\alpha_{k-2}(a_{k-2}-h\alpha_{k-4}).$$

Using in the last term on the right-hand side (7.7) for $m=2$, we can rewrite the last expression as

$$\frac{1}{\alpha_k}=a_{k+1}(a_k-h\alpha_{k-2})-h\alpha_{k-1}(a_k-h\alpha_{k-2})=(a_{k+1}-h\alpha_{k-1})(a_k-h\alpha_{k-2}).$$

This finishes the proof for $m=2$. Again, we hope that the pattern of the general proof is clear from these two simple cases. It would be highly desirable to find a less computational proof for the periodic case of all three lattices.

VIII. CONCLUSION

A new application of a general scheme for producing integrable discretizations for integrable Hamiltonian flows is described in the present paper. Advantages of this approach are rather obvious: it is, in principle, applicable in a standardized way to every system admitting an r-matrix formulation, at least with a constant r-matrix satisfying the modified Yang–Baxter equation. We shall demonstrate elsewhere that the discrete time systems from Refs. 6 and 7 with dynamical r-matrices may be also included into this framework. We hope also to report on numerous further applications of this approach in the future.

The drawback of this scheme is also obvious to any expert in this field. Namely, some of the most beautiful discretizations do not live on the same r-matrix orbits as their continuous time counterparts,[1,3–5] and there seems to exist no way of *a priori* identifying the correct orbit for nice discretizations. However, we hope that continuing to collect examples will someday bring some light to this intriguing problem.

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On the ionization of a Keplerian binary system by periodic gravitational radiation

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The gravitational ionization of a Keplerian binary system via normally incident periodic gravitational radiation of definite helicity is discussed. The periodic orbits of the planar tidal equation are investigated on the basis of degenerate continuation theory. The relevance of the Kolmogorov-Arnold-Moser theory to the question of gravitational ionization is elucidated, and it is conjectured that the process of ionization is closely related to the Arnold diffusion of the perturbed system. © *1996 American Institute of Physics.* [S0022-2488(96)02208-6]

I. INTRODUCTION

In a recent paper,[1] we considered the long-term nonlinear perturbations of Keplerian orbits by incident gravitational waves of wavelengths much larger than the size of the system. In particular, we studied the periodic orbits of the perturbed system using the methods developed in Ref. 2. The existence of periodic orbits indicates the possibility of balance in the exchange of energy between the binary and the external radiation field. Thus gravitational ionization does not occur for such orbits. The issue of gravitational ionization is interesting as it involves the transport of energy by gravitational radiation and is analogous to the corresponding phenomenon that is well known in the electromagnetic context.

The theoretical investigation of the interaction of a binary system with the gravitational radiation field reveals subtle phenomena that are further studied in this paper. In particular, the absorption of gravitational radiation energy by the binary is not unidirectional in general. That is, the orbital energy of a binary immersed in a gravitational radiation field does not in general increase monotonically with time. On the other hand, the emission of gravitational radiation by the binary is expected to be accompanied by the monotonic decrease of the orbital energy of the system. In absorption, however, the incident wave can deposit energy into the orbit during one time interval and remove energy from the orbit during another time interval. A periodic orbit would result—even when the emission of the radiation by the binary is ignored—if after a certain time the net flow of energy between the incident wave and the binary is zero.

Let us imagine, for the sake of simplicity, that gravitational radiation is incident on a Newtonian binary system consisting of a massive body of mass M_0 at the origin of inertial coordinates and a particle of test mass $m_0 \ll M_0$ that revolves around it in the (x,y)-plane. The dynamical equation in this case is of the general form[3,4]

$$\frac{d^2x^i}{dt^2}+\frac{kx^i}{r^3}+\epsilon\mathscr{K}_{ij}(t)x^j=0, \tag{1}$$

where $k=G_0(M_0+m_0)$, ϵ, $0<\epsilon\ll 1$, is the perturbation parameter and $\epsilon\mathscr{K}_{ij}$ is the tidal matrix associated with the incident gravitational waves. Here $\mathscr{K}$ is symmetric and traceless, and is related to the gravitational perturbation of the Minkowski space-time by

$$\mathscr{K}_{ij}(t) = -\frac{1}{2}\frac{\partial^2 \chi_{ij}}{\partial t^2}(t,\mathbf{0}), \tag{2}$$

where $g_{\mu\nu} = \eta_{\mu\nu} + \epsilon\chi_{\mu\nu}$. Here we employ the transverse-traceless gauge for gravitational radiation, i.e. $\chi_{0\mu} = 0$, χ_{ij} is traceless and $\partial_j \chi_{ij} = 0$; moreover, χ_{ij} is a solution of the wave equation $\Box \chi_{ij} = 0$. Thus the gravitational radiation field can be expressed as a Fourier sum of monochromatic waves of frequency $\Omega_\star$ and wave vector $\mathbf{K}_\star$, $c|\mathbf{K}_\star| = \Omega_\star$,

$$\chi_{ij}(t,\mathbf{x}) = \mathrm{Re}\sum_{\mathbf{K}_\star} \hat{\chi}_{ij}(\mathbf{K}_\star)\exp(i\mathbf{K}_\star \cdot \mathbf{x} - i\Omega_\star t), \tag{3}$$

where $\hat{\chi}_{ij}$ is symmetric, traceless and $\hat{\chi}_{ij}K_\star^j = 0$. The summation in (3) extends over all waves with $2\pi c/\Omega_\star$ much larger than the average orbital radius. Equation (1) contains only the essential physics of the interaction of long-wavelength gravitational radiation with a Newtonian binary system; in fact, relativistic (i.e., post-Keplerian) effects in the binary are totally neglected. In particular, the emission of gravitational waves is ignored. The motivation for our treatment as well as its limitations is presented in detail in our recent work.[1]

The incident wave exchanges energy and angular momentum with the binary orbit but not linear momentum in the *quadrupole* approximation under consideration here.[1] This is in exact analogy with the electromagnetic problem of the interaction of an electromagnetic wave with an atom in the *dipole* approximation.

A simple linear perturbation treatment of (1) has revealed the possibility of the existence of resonances at $\Omega_\star = m\omega$, $m = 1,2,3, \ldots$, where ω is the Keplerian frequency of the unperturbed elliptical orbit. Moreover, in this analysis secular terms appear that lead to the breakdown of the linear theory over time.[4] Thus linear perturbation theory is inappropriate for the investigation of periodic orbits of the perturbed system, since a periodic orbit is expected to persist forever beyond a certain point in time.

In the first treatment of the nonlinear case,[1] we considered a single monochromatic plane wave of frequency $\Omega_\star$ that was normally incident on a Keplerian orbit of frequency ω. We found that in the generic case, certain orbits satisfying the resonance condition $\Omega_\star = m\omega$, $m = 1,2,3,\ldots$, could be continued to periodic orbits of the nonlinear system. The existence of periodic solutions of (1) demonstrates that ionization does not always occur; in fact, in a periodic orbit the energy exchange with the radiation field must be steady without any net flow. In addition, we found that for incident circularly polarized radiation of definite helicity the rotation of the inertial coordinates by frequency $\Omega_\star/2$ rendered the dynamical equations autonomous. The invariance of this autonomous system under time translation implies the existence of an energy integral in the rotating frame. In this case, the Kolmogorov-Arnold-Moser (KAM) theory implies that for sufficiently small ϵ ionization can never occur in this system regardless of the magnitude of $\Omega_\star/\omega$. To understand intuitively how this could come about, it should be pointed out that a binary system can gain or lose energy as it interacts with an incident gravitational wave. The situation in absorption is in contrast to the emission of gravitational waves by a binary. In the latter situation, the binary is expected to lose energy monotonically; in fact, this is consistent with the observed rate of inward spiraling of the Hulse-Taylor binary pulsar.[5,6] It follows that the reciprocity between emission and absorption of gravitational waves does not hold in general. This notion of reciprocity is valid in some other situations, however. For instance, a Keplerian ellipse of frequency ω emits gravitational radiation of frequency $m\omega$, $m = 1,2,3, \ldots$, which corresponds to the resonance condition for absorption.

Let us now consider a *general* periodic gravitational wave of period $2\pi/\Omega_\star$ that is normally incident on the binary system. The existence of certain periodic solutions of the perturbed system may be expected on general grounds. It would therefore be more interesting to investigate the interaction of circularly polarized gravitational radiation with the binary system and to determine

the stability of the resulting autonomous system under periodic perturbations. That is, a periodic wave may be expressed as a Fourier sum of components with frequencies $n\Omega_\star$, $n=1,2,3,\ldots$. For a single component of definite helicity, the transformation to the corresponding rotating frame would essentially remove the dependence of this perturbation upon time and for ϵ below a certain limit the orbit would remain forever bounded even though there is a steady flow of incident gravitational radiation energy in the inertial frame. However, the time-dependence of the other Fourier components would not disappear in the rotating frame, and we would like to study the influence of these components on the ionization of the system. Though we develop methods that are applicable to a general periodic perturbation, we restrict our attention to a tractable problem for the sake of simplicity.

In this paper, we consider a superposition of several harmonics in the perturbing function; clearly, the response of the system is not a superposition of the individual responses as a consequence of the intrinsic nonlinearity of the problem under consideration here. Specifically, we showed in Ref. 1 that for a normally incident circularly polarized monochromatic plane wave the motion is restricted to the (x,y)-plane and that a transformation to the uniformly rotating coordinate system in this plane with half the wave's frequency would result in an autonomous system for the equation of motion to which the KAM theory can be applied. It follows from the KAM theory that for sufficiently small ϵ the motion is confined and ionization does not occur. We wish to explore the sensitivity of this interesting result to the particular form of the incident wave. Therefore, we consider here a principal right circularly polarized wave of frequency $\Omega_\star=2\Omega$ that is slightly modified by the presence of similar components of frequencies Ω and 3Ω as follows:

$$\begin{aligned}\chi_{11}(t,\mathbf{0}) &= \cos 2\Omega t+2\delta[(\alpha-\beta)\cos\Omega t+\tfrac{1}{9}(\alpha+\beta)\cos 3\Omega t],\\ \chi_{12}(t,\mathbf{0}) &= \sin 2\Omega t+2\delta[(\alpha-\beta)\sin\Omega t+\tfrac{1}{9}(\alpha+\beta)\sin 3\Omega t],\end{aligned} \tag{4}$$

$\chi_{13}=\chi_{23}=\chi_{33}=0$. The other components of χ follow from the fact that χ is a symmetric traceless matrix. Here δ, $0<\delta\ll 1$, is a new perturbation parameter that determines the relative strength of the extra secondary components compared to the primary Fourier component of the normally incident radiation. Moreover, α and β are constant amplitudes of the order of unity, and the other numerical coefficients have been introduced for the sake of simplicity.

The plan of this paper is as follows: In Section II, we present the basic equations for a Hamiltonian description of the perturbed orbit in terms of Delaunay variables. Sections III–V are devoted to a development of degenerate continuation theory that is necessary for the identification of periodic orbits of the nonlinear problem via the methods and ideas that are originally due to Poincaré. The existence of periodic orbits, described in Section V, demonstrates that a state of equilibrium can be established between the wave and the binary such that ionization does not occur; in fact, the net flow of energy vanishes in this case. To apply the KAM theory to our problem, it is best to transform (1) to a uniformly rotating frame as in Section VI. It follows from the description of the nonlinear system in this reference frame that Arnold diffusion is expected for $\delta>0$, even for sufficiently small ϵ. Numerical experiments described in Section VII tend to corroborate the conjecture that gravitational ionization is tantamount to Arnold diffusion in this system. For background material, this paper relies heavily on our previous detailed treatment of the nonlinear problem for the case where the incident wave is essentially a simple monochromatic Fourier component;[1] however, we have attempted to present sufficient detail here in order to render the present paper essentially self-contained.

II. HAMILTONIAN DESCRIPTION IN DELAUNAY ELEMENTS

Using (1), (2) and (4), we can write the associated Hamiltonian for this system as the sum of the Kepler Hamiltonian and the quadrupole perturbation given by $\frac{1}{2}\epsilon\mathscr{K}_{ij}\,x^ix^j$. The motion is taken

to be in the (x,y)-plane, since the radiation is transverse and normally incident on the orbital plane; therefore, polar coordinates are convenient. Defining $\phi(t)$ and $\psi(t)$ as

$$\begin{aligned}\phi(t)&=\Omega^2\left\{\cos 2\Omega t+\frac{\delta}{2}[(\alpha-\beta)\cos\Omega t+(\alpha+\beta)\cos 3\Omega t]\right\},\\ \psi(t)&=\Omega^2\left\{\sin 2\Omega t+\frac{\delta}{2}[(\alpha-\beta)\sin\Omega t+(\alpha+\beta)\sin 3\Omega t]\right\},\end{aligned}\tag{5}$$

the Hamiltonian in polar coordinates may be written as

$$\mathscr{H}=\frac{1}{2}\left(p_r^2+\frac{p_\theta^2}{r^2}\right)-\frac{k}{r}+\epsilon r^2[\phi(t)\cos 2\theta+\psi(t)\sin 2\theta].\tag{6}$$

To express the Hamiltonian in a form particularly suitable for the analysis of orbital dynamics, we transform to the Delaunay elements (L,G,ℓ,g). To this end, consider the bounded motion of the test particle according to the Hamiltonian (6). At each instant of time, the particle can be described as belonging to an osculating Keplerian ellipse; that is, the perturbed motion passes through an infinite sequence of osculating ellipses in the course of time. Each such ellipse is described by the unperturbed Hamiltonian

$$H=\frac{1}{2}\left(p_r^2+\frac{p_\theta^2}{r^2}\right)-\frac{k}{r},$$

where we consider only bounded motions with $E=H(p_r,p_\theta,r,\theta)<0$. Let us now consider the canonical transformation from (p_r,p_θ,r,θ) to variables intrinsic to the ellipse. Thus we define action variables

$$L:=\left(\frac{-k^2}{2E}\right)^{1/2},\quad\text{and}\quad G:=p_\theta,$$

which correspond to an osculating Keplerian ellipse with semimajor axis a, $a=L^2/k$, and eccentricity e,

$$e=\left(1-\frac{G^2}{L^2}\right)^{1/2},$$

such that $0\leq e<1$. The equation of this ellipse is given by

$$r=a(1-e\cos\hat{u}),\quad\text{or}\quad r=a\frac{1-e^2}{1+e\cos\hat{v}},$$

where $\hat{u}$ is the eccentric anomaly and $\hat{v}$ is the true anomaly. The new canonical angle variables ℓ and g are then given by

$$\ell=\hat{u}-e\sin\hat{u},\quad g=\theta-\hat{v}.$$

In the following, we exclude $e=0$ and focus attention instead on noncircular elliptical orbits. The resulting Hamiltonian of the perturbed system in Delaunay variables is

$$\mathscr{H}=-\frac{k^2}{2L^2}+\epsilon[\mathscr{C}(L,G,\ell,g)\phi(t)+\mathscr{S}(L,G,\ell,g)\psi(t)],\tag{7}$$

where, in polar coordinates, $\mathscr{C}=r^2\cos 2\theta$ and $\mathscr{S}=r^2\sin 2\theta$. In Delaunay elements, $\mathscr{C}(L,G,\ell,g)$ and $\mathscr{S}(L,G,\ell,g)$ are given by

$$\begin{aligned}\mathscr{C}(L,G,\ell,g)&=\frac{5}{2}a^2e^2\cos 2g+a^2\sum_{\nu=1}^{\infty}\left(A_\nu(e)\cos 2g\cos\nu\ell-B_\nu(e)\sin 2g\sin\nu\ell\right),\\ \mathscr{S}(L,G,\ell,g)&=\frac{5}{2}a^2e^2\sin 2g+a^2\sum_{\nu=1}^{\infty}\left(A_\nu(e)\sin 2g\cos\nu\ell+B_\nu(e)\cos 2g\sin\nu\ell\right),\end{aligned}\tag{8}$$

where

$$\begin{aligned}A_\nu(e)&=\frac{4}{\nu^2e^2}\left(2\nu e(1-e^2)J_\nu'(\nu e)-(2-e^2)J_\nu(\nu e)\right),\\ B_\nu(e)&=-\frac{8}{\nu^2e^2}\sqrt{1-e^2}\left(eJ_\nu'(\nu e)-\nu(1-e^2)J_\nu(\nu e)\right).\end{aligned}\tag{9}$$

Here J_ν is the Bessel function of order ν, and a prime indicates the derivative of the function with respect to its argument. The dynamical equations are derived in the usual way from the Hamiltonian (7). Moreover, these equations are given in Delaunay elements by

$$\begin{aligned}\dot L&=-\epsilon\left(\frac{\partial\mathscr{C}(L,G,\ell,g)}{\partial\ell}\phi(t)+\frac{\partial\mathscr{S}(L,G,\ell,g)}{\partial\ell}\psi(t)\right),\\ \dot G&=-\epsilon\left(\frac{\partial\mathscr{C}(L,G,\ell,g)}{\partial g}\phi(t)+\frac{\partial\mathscr{S}(L,G,\ell,g)}{\partial g}\psi(t)\right),\\ \dot\ell&=\omega+\epsilon\left(\frac{\partial\mathscr{C}(L,G,\ell,g)}{\partial L}\phi(t)+\frac{\partial\mathscr{S}(L,G,\ell,g)}{\partial L}\psi(t)\right),\\ \dot g&=\epsilon\left(\frac{\partial\mathscr{C}(L,G,\ell,g)}{\partial G}\phi(t)+\frac{\partial\mathscr{S}(L,G,\ell,g)}{\partial G}\psi(t)\right),\end{aligned}\tag{10}$$

where ω is the Keplerian frequency of the binary given by $\omega^2=k/a^3$.

III. BIFURCATION FUNCTION

To establish the continuation (persistence) of periodic orbits of the Kepler problem to the system (10), we employ a method proposed in Ref. 2 and used in Ref. 1; we only state the main ideas here and the reader is referred to these references for details.

System (10) has the abstract form

$$\dot u=F(u)+\epsilon h(u,t),\tag{11}$$

where u is a coordinate on a manifold M that consists of a cross product of Euclidean spaces and tori, and the function h is periodic with period $2\pi/\Omega$ in its second argument. We consider solutions $t\mapsto u(t,\xi,\epsilon)$ of (11) with initial condition $u(0,\xi,\epsilon)=\xi$, $\xi\in M$, and define the mth order Poincaré map by $\mathscr{P}^m(\xi,\epsilon)=u(2\pi m/\Omega,\xi,\epsilon)$. Fixed points of this mth order Poincaré map correspond to periodic solutions of (11). Consider the unperturbed periodic solutions of (11) with $\epsilon=0$. These correspond to fixed points of the unperturbed mth order Poincaré map defined by $p^m(\xi)=\mathscr{P}^m(\xi,0)$. Let us now suppose that there is a submanifold $\mathscr{Z}\subset M$ that consists of fixed points of p^m, and $\zeta\in\mathscr{Z}$. If there is a continuous curve $\epsilon\mapsto\kappa(\epsilon)$ in M such that $\kappa(0)=\zeta$ and

$\mathcal{P}^m[\kappa(\epsilon),\epsilon]\equiv\kappa(\epsilon)$, i.e. for each fixed value of ϵ, $\kappa(\epsilon)$ is a fixed point of the mth order Poincaré map, then the unperturbed periodic orbit is continuable. The continuation is established by the method of Lyapunov-Schmidt reduction to the Implicit Function Theorem and requires that every vector in $T_\zeta M$ that is tangent to the submanifold $\mathcal{Z}$ be in the kernel of the infinitesimal displacement $\mathcal{D}(\zeta)=Dp^m(\zeta)-I$. This is equivalent to the requirement that for each $\zeta\in\mathcal{Z}$, the dimension of the kernel of the infinitesimal displacement at ζ be equal to the dimension of the manifold $\mathcal{Z}$. The manifold $\mathcal{Z}$ is called normally nondegenerate if it satisfies this condition.

Let $\mathcal{Z}$ be a normally nondegenerate submanifold of M with dimension q; then, the range of the infinitesimal displacement at each point of $\mathcal{Z}$ has codimension q. For each $\zeta\in\mathcal{Z}$, there is a vector complement $\hat{\mathcal{S}}(\zeta)$ to the range of the infinitesimal displacement of dimension q. We denote the projection of $T_\zeta M$ to $\hat{\mathcal{S}}(\zeta)$ by $\hat{s}(\zeta)$.

Let $\zeta\in\mathcal{Z}$ and consider the curve in the manifold M defined by $\epsilon\mapsto\mathcal{P}^m(\zeta,\epsilon)$; it passes through ζ at $\epsilon=0$ and its tangent vector at $\epsilon=0$ is in $T_\zeta M$. This tangent vector can be identified with the partial derivative $\mathcal{P}^m_\epsilon(\zeta,0)$. The bifurcation function $\mathcal{B}$ is defined to be the map from $\mathcal{Z}$ to the complement $\hat{\mathcal{S}}$ of the range of the infinitesimal displacement,

$$\mathcal{B}(\zeta)=\hat{s}(\zeta)\mathcal{P}^m_\epsilon(\zeta,0),$$

so that in local coordinates $\mathcal{B}:\mathbb{R}^q\to\mathbb{R}^q$. We define $\zeta\in\mathcal{Z}$ to be a simple zero of the bifurcation function if $\mathcal{B}(\zeta)=0$ and the derivative $D\mathcal{B}(\zeta)$ is invertible. The following continuation theorem is proved in Ref. 2.

Theorem: III.1: *Let $\mathcal{Z}$ denote a normally nondegenerate fixed point submanifold of M for the system (11). If $\zeta\in\mathcal{Z}$ is a simple zero of the corresponding bifurcation function, then the unperturbed periodic orbit of (11) with initial point ζ is continuable.*

To apply Theorem III.1 to the perturbed Kepler problem, we must compute the partial derivative $\mathcal{P}^m_\epsilon(\zeta,0)$ of the corresponding Poincaré map. For the system (10), the manifold M is the four dimensional Delaunay coordinate space and the Poincaré map is defined as the strobe with period $2\pi m/\Omega$ where Ω is the frequency of the perturbation. The partial derivative is obtained from the solution $t\mapsto W(t)$ of the second variational initial value problem

$$\dot{W}=DF(u(t,\zeta,0))W+h(u(t,\zeta,0),t),\quad W(0)=0.$$

In fact, we have $W(t)=u_\epsilon(t,\zeta,0)$ and

$$\mathcal{P}^m_\epsilon(\zeta,0)=W(2\pi m/\Omega).$$

We use Theorem III.1 to establish the existence of periodic orbits for the system (10). Of course, this will establish the existence of periodic orbits for our model system (1), which describes the perturbation of a Keplerian binary system by a multi-frequency periodic gravitational wave. We begin by identifying the normally nondegenerate fixed point submanifold of M mentioned in Theorem III.1. Recall that the frequency of the unperturbed periodic Keplerian orbit is $\omega=k^2/L^3$. The three-dimensional manifold

$$\mathcal{Z}^L:=\{(L,G,\ell,g):m\omega=n\Omega\},$$

where m and n are relatively prime positive integers, is a normally nondegenerate submanifold of M (cf. Ref. 1). Furthermore, the range of the infinitesimal displacement is complemented by the span of the vectors

$$\begin{pmatrix}1\\0\\0\\0\end{pmatrix},\begin{pmatrix}0\\1\\0\\0\end{pmatrix},\begin{pmatrix}0\\0\\0\\1\end{pmatrix}.$$

The bifurcation function associated with (10) is the projection of the partial derivative $\mathscr{P}^m_\epsilon(L,G,\ell,g,0)$ on the manifold $\mathscr{Z}^L$ onto the complement of the range of the infinitesimal displacement. To determine the bifurcation function, we solve the variational initial value problem

$$\dot{L}_\epsilon=-\frac{\partial\mathscr{C}}{\partial\ell}(L,G,\ell+\omega t,g)\phi(t)-\frac{\partial\mathscr{S}}{\partial\ell}(L,G,\ell+\omega t,g)\psi(t),$$

$$\dot{G}_\epsilon=-\frac{\partial\mathscr{C}}{\partial g}(L,G,\ell+\omega t,g)\phi(t)-\frac{\partial\mathscr{S}}{\partial g}(L,G,\ell+\omega t,g)\psi(t),$$

$$\dot{\ell}_\epsilon=-\frac{3k^2}{L^4}L_\epsilon+\frac{\partial\mathscr{C}}{\partial L}(L,G,\ell+\omega t,g)\phi(t)+\frac{\partial\mathscr{S}}{\partial L}(L,G,\ell+\omega t,g)\psi(t),$$

$$\dot{g}_\epsilon=\frac{\partial\mathscr{C}}{\partial G}(L,G,\ell+\omega t,g)\phi(t)+\frac{\partial\mathscr{S}}{\partial G}(L,G,\ell+\omega t,g)\psi(t),$$

with zero initial values; then, the solution evaluated at $t=m(2\pi/\Omega)$ is projected to the complement of the range of the infinitesimal displacement. It follows from a detailed analysis that one can set the initial value of time equal to zero, as we have done, with no loss in generality. The bifurcation function is thus given by

$$\mathscr{B}(G,\ell,g)=(B^L(G,\ell,g),B^G(G,\ell,g),B^g(G,\ell,g)),$$

where

$$B^L(G,\ell,g):=-\frac{\partial\mathscr{T}}{\partial\ell},\quad B^G(G,\ell,g):=-\frac{\partial\mathscr{T}}{\partial g},\quad B^g(G,\ell,g):=\frac{\partial\mathscr{T}}{\partial G},\tag{12}$$

and

$$\mathscr{T}:=\int_0^{2\pi m/\Omega}[\mathscr{C}(L,G,\ell+\omega t,g)\phi(t)+\mathscr{S}(L,G,\ell+\omega t,g)\psi(t)]dt.$$

To evaluate $\mathscr{T}$, we use the resonance relation $n\Omega=m\omega$ to change the variable of integration from t to $\hat{\sigma}=\Omega t/m+\ell/n$, then observe that the integrand of $\mathscr{T}$ is periodic with period 2π and substitute the Fourier series expansions for $\mathscr{C}$ and $\mathscr{S}$. After performing these steps, we obtain the following expression for $\mathscr{T}$ in case $n=1$:

$$\mathscr{T}=\pi ma^2\Omega\Big\{U_{2m}(e)\cos(2g+2m\ell)+\frac{\delta}{2}[(\alpha-\beta)U_m(e)\cos(2g+m\ell)$$
$$+(\alpha+\beta)U_{3m}(e)\cos(2g+3m\ell)]\Big\},\tag{13}$$

where

$$U_\nu(e)=A_\nu(e)+B_\nu(e).$$

If $n=2$ and m is odd, then

$$\mathcal{J}=\pi m a^2\Omega U_m(e)\cos(2g+m\ell);$$

while for $n=3$, if m is prime relative to 3, then

$$\mathcal{J}=\tfrac{1}{2}\pi m a^2\Omega\,\delta(\alpha+\beta)U_m(e)\cos(2g+m\ell).$$

It turns out that $\mathcal{J}=0$ for $n>3$, as expected.

We show in Ref. 1 that the bifurcation function does not have a simple zero for an incident monochromatic gravitational wave of definite helicity. The role of the secondary components of the wave is to resolve this issue for the bifurcation problem under consideration here. This is indeed the case for $n=1$ as demonstrated in the next section. However, for $n=2$ and $n=3$ simple zeros do not exist, and the consideration of these cases would require the calculation of the solutions of higher order variational initial value problems. On the other hand, higher order perturbing functions of order ϵ^2, etc., are neglected in the formulation of equation (1), which is the starting point of our analysis. It follows from this remark that the treatment of the cases $n=2$ and $n=3$ is beyond the scope of this work. Thus, we assume $n=1$ in the remainder of this section.

Substituting (13) into (12), we obtain the following explicit form for the bifurcation function $(n=1)$:

$$B^L(G,\ell,g)=2\pi m^2a^2\Omega\Big\{U_{2m}(e)\sin(2g+2m\ell)+\frac{\delta}{4}[(\alpha-\beta)U_m(e)\sin(2g+m\ell)$$
$$+3(\alpha+\beta)U_{3m}(e)\sin(2g+3m\ell)]\Big\},$$

$$B^G(G,\ell,g)=2\pi ma^2\Omega\Big\{U_{2m}(e)\sin(2g+2m\ell)+\frac{\delta}{2}[(\alpha-\beta)U_m(e)\sin(2g+m\ell)$$
$$+(\alpha+\beta)U_{3m}(e)\sin(2g+3m\ell)]\Big\},$$

$$B^g(G,\ell,g)=-\pi ma^2\Omega\left(\frac{G}{eL^2}\right)\Big\{U'_{2m}(e)\cos(2g+2m\ell)+\frac{\delta}{2}[(\alpha-\beta)U'_m(e)\cos(2g+m\ell)$$
$$+(\alpha+\beta)U'_{3m}(e)\cos(2g+3m\ell)]\Big\}, \tag{14}$$

where in the expression for B^g we have used the fact that the eccentricity e and the Delaunay element G are related by $G=\pm L\sqrt{1-e^2}$. We therefore make a change of variable from G to e and observe that the zeros and their multiplicities for the bifurcation function $\mathcal{B}$ are identical to those of the function

$$\mathcal{F}(e,\ell,g)=(F^L(e,\ell,g),F^G(e,\ell,g),F^g(e,\ell,g)),$$

where

FL(e,ℓ,g) = U2m(e)sin(2g+2mℓ) + δ4 [($\alpha-\beta$)Um(e)sin(2g+mℓ)

$$+3(\alpha+\beta)U_{3m}(e)\sin(2g+3m\ell)],$$

$$F^G(e,\ell,g)=U_{2m}(e)\sin(2g+2m\ell)+\frac{\delta}{2}[(\alpha-\beta)U_m(e)\sin(2g+m\ell)$$

$$+(\alpha+\beta)U_{3m}(e)\sin(2g+3m\ell)], \tag{15}$$

$$F^g(e,\ell,g)=U'_{2m}(e)\cos(2g+2m\ell)+\frac{\delta}{2}[(\alpha-\beta)U'_m(e)\cos(2g+m\ell)$$

$$+(\alpha+\beta)U'_{3m}(e)\cos(2g+3m\ell)].$$

To apply Theorem III.1, we must determine the simple zeros of the bifurcation function (14) or, equivalently, (15). We will show that simple zeros exist by a perturbation argument which is presented in the next section.

IV. ZEROS OF A DEGENERATE BIFURCATION FUNCTION

The bifurcation function (15) has the following abstract form:

$$\Delta(\mu,\hat{\epsilon})=\tau(\mu)+\hat{\epsilon}\varphi(\mu)=0, \quad \mu\in\mathbb{R}^3, \tag{16}$$

where the functions $\Delta:\mathbb{R}^3\times\mathbb{R}\mapsto\mathbb{R}^3$ and $\tau,\varphi:\mathbb{R}^3\mapsto\mathbb{R}^3$ are given in components by

$$\tau(\mu)=\begin{pmatrix}\tau_1(\mu)\\ \tau_2(\mu)\\ \tau_3(\mu)\end{pmatrix}, \quad \varphi(\mu)=\begin{pmatrix}\varphi_1(\mu)\\ \varphi_2(\mu)\\ \varphi_3(\mu)\end{pmatrix},$$

and where the first two components of τ are equal. In fact, we define $\hat{\tau}=\tau_1=\tau_2$.

Remark IV.1: *The fact that the bifurcation function has the abstract form (16) is not accidental. Every normally incident gravitational plane wave whose Fourier representation has as its dominant term a purely circularly polarized wave will result in a bifurcation function of the form (16) at resonance.*

We will determine the zero set for Δ in case $\hat{\epsilon}$ is sufficiently small.

Lemma IV.2: *Suppose Δ is defined by (16). If $\eta\in\mathbb{R}^3$ is such that $\tau(\eta)=0$ while the vectors* $\operatorname{grad}\hat{\tau}(\eta)$ *and* $\operatorname{grad}\tau_3(\eta)$ *are linearly independent, then there is a curve $s\mapsto\Gamma(s)$ in $\mathbb{R}^3$ such that $\Gamma(0)=\eta$, $\Gamma'(0)\neq 0$, and $\Delta(\Gamma(s),0)\equiv 0$. If such a curve exists and $s=0$ is a simple zero of the real-valued function $s\mapsto\varphi_2(\Gamma(s))-\varphi_1(\Gamma(s))$, then there is a curve $\hat{\epsilon}\mapsto\Upsilon(\hat{\epsilon})$ in $\mathbb{R}^3$ such that $\Upsilon(0)=\eta$ and $\Delta(\Upsilon(\hat{\epsilon}),\hat{\epsilon})\equiv 0$. Moreover, for each sufficiently small $\hat{\epsilon}\neq 0$, the point $\Upsilon(\hat{\epsilon})\in\mathbb{R}^3$ is a simple zero of the function $\mu\mapsto\Delta(\mu,\hat{\epsilon})$.*

Proof: The linearly independent vectors grad $\hat{\tau}(\eta)$ and grad $\tau_3(\eta)$ span a plane Q in $\mathbb{R}^3$. Let S denote one of the two possible rotation operators in space that preserves Q and rotates each vector in Q through $\pi/2$ radians. We note that S grad $\hat{\tau}(\eta)$ and S grad $\tau_3(\eta)$ are linearly independent vectors in Q. Also, we let v denote a vector in space such that the set $\{S \text{ grad } \hat{\tau}(\eta), S \text{ grad } \tau_3(\eta), v\}$ is linearly independent. This requirement is satisfied, for instance, if we choose v to be equal to the cross product of S $\operatorname{grad}\hat{\tau}(\eta)$ and S $\operatorname{grad}\tau_3(\eta)$.

The function $w:\mathbb{R}^3\mapsto\mathbb{R}^3$ defined by

$$(\mu_1,\mu_2,\mu_3)\mapsto\mu_1 S \text{ grad } \tau_3(\eta)+\mu_2 S \text{ grad } \hat{\tau}(\eta)+\mu_3 v+\eta$$

is invertible. We use it to define $\Theta:\mathbb{R}^3\to\mathbb{R}^2$ given by

$$\Theta(\mu_1,\mu_2,\mu_3)=(\hat{\tau}(w(\mu_1,\mu_2,\mu_3)),\tau_3(w(\mu_1,\mu_2,\mu_3)).$$

It follows that $\Theta(0)=0$. Moreover, the derivative of the transformation

$$(\mu_1,\mu_2)\mapsto(\hat{\tau}(w(\mu_1,\mu_2,0)),\tau_3(w(\mu_1,\mu_2,0))$$

at $(\mu_1,\mu_2)=(0,0)$ is given by the matrix

$$\begin{pmatrix} \text{grad } \hat{\tau}(\eta)\cdot S \text{ grad } \tau_3(\eta) & 0 \\ 0 & \text{grad } \tau_3(\eta)\cdot S \text{ grad } \hat{\tau}(\eta) \end{pmatrix} \tag{17}$$

that represents the partial derivative of Θ with respect to its first two arguments at the origin.

Using the linear independence of grad $\hat{\tau}(\eta)$ and grad $\tau_3(\eta)$, it is easy to see that the diagonal elements of the matrix (17) are both nonzero. Thus, by the Implicit Function Theorem, there is a unique curve $s\mapsto\sigma(s)$ in the (μ_1,μ_2)-plane such that $\sigma(0)=(0,0)$ and $\Theta(\sigma(s),s)\equiv 0$. The curve $\Gamma(s):=w(\sigma(s),s)$ is such that $\Gamma(0)=\eta$ and $\Delta(\Gamma(s),0)\equiv 0$. Moreover,

$$\Gamma'(0)=Dw(0)\begin{pmatrix}\sigma'(0)\\ 1\end{pmatrix}.$$

Since $Dw(0)$ is invertible and the vector $(\sigma'(0),1)\neq 0$, we have that $\Gamma'(0)\neq 0$. This proves the first assertion of the theorem.

Under the assumption that $s=0$ is a simple zero of the function $s\mapsto\varphi_2(\Gamma(s))-\varphi_1(\Gamma(s))$, we will use the Lyapunov-Schmidt reduction procedure to show that the corresponding point $\eta=\Gamma(0)$ in $\mathbb{R}^3$ is continuable as a zero of Δ. As $\Gamma'(0)\neq 0$, the image $\hat{\mathcal{Z}}$ of Γ is locally a one dimensional submanifold of $\mathbb{R}^3$. Moreover, $\hat{\mathcal{Z}}$ is normally nondegenerate in the sense that at each point $\hat{z}\in\hat{\mathcal{Z}}$ sufficiently close to η, the kernel $\hat{K}$ of $D\tau(\hat{z})$ is exactly the one dimensional tangent space of $\hat{\mathcal{Z}}$. In fact, since this tangent space is clearly in $\hat{K}$, it suffices to show that $\hat{K}$ is one dimensional. The derivative of τ is expressed in the standard vector notation by

$$D\tau(\hat{z})=\begin{pmatrix}\text{grad } \hat{\tau}(\hat{z})\\ \text{grad } \hat{\tau}(\hat{z})\\ \text{grad } \tau_3(\hat{z})\end{pmatrix}.$$

Since the vectors grad $\hat{\tau}(\hat{z})$ and grad $\tau_3(\hat{z})$ are linearly independent at $\hat{z}=\eta$, they will, by continuity, remain linearly independent in an open neighborhood of η. Thus, their span is two dimensional at each point of this neighborhood. In particular, for $\hat{z}$ in this neighborhood, it is clear (by matrix multiplication) that grad $\hat{\tau}(\hat{z})$ and grad $\tau_3(\hat{z})$ are not both in $\hat{K}$. This proves that $\hat{K}$ is one dimensional. It follows from the same Lyapunov-Schmidt reduction procedure that is used to prove Theorem III.1 (see Ref. 2) that if $\Pi(\hat{z})$ denotes a projection to the complement $\hat{\mathcal{Y}}$ of the range of $D\tau(\hat{z})$, then simple zeros of the map from $\hat{\mathcal{Z}}$ to $\mathbb{R}$ given by $\hat{z}\mapsto\Pi(\hat{z})\Delta_{\hat{\epsilon}}(\hat{z},0)$ are continuable. Thus, if η is such a simple zero, there is a curve $\hat{\epsilon}\mapsto\Upsilon(\hat{\epsilon})$ such that $\Upsilon(0)=\eta$ and $\Delta(\Upsilon(\hat{\epsilon}),\hat{\epsilon})\equiv 0$ as required in the lemma.

To construct such a projection into $\hat{\mathcal{Y}}$, it can be shown that, in fact, the range of $D\tau(\hat{z})$ is spanned by the transpositions of the vectors $(1,1,0)$ and $(0,0,1)$. To see this, it is sufficient to note that $D\tau(\hat{z})S$ grad $\hat{\tau}(\hat{z})$ is the transpose of a scalar multiple of $(0,0,1)$ while $D\tau(\hat{z})S$ grad $\tau_3(\hat{z})$ is a scalar multiple of the transpose of $(1,1,0)$. The transpose of the vector $(0,1,0)$ clearly spans a complement to the range that we will denote by $\hat{\mathcal{Y}}$. Thus, if $(\rho_1,\rho_2,\rho_3)\in\mathbb{R}^3$, the projection Π is easily computed and is given by $\Pi(\rho_1,\rho_2,\rho_3)=\rho_2-\rho_1$. Note that Π does not depend on the base point $\hat{z}\in\hat{\mathcal{Z}}$.

Using the projection Π and the definition of Δ, the Lyapunov-Schmidt reduced function $\hat{z}\mapsto\Pi(\hat{z})\Delta_{\hat{\epsilon}}(\hat{z},0)$ is given by $\hat{z}\mapsto\varphi_2(\hat{z})-\varphi_1(\hat{z})$ for $\hat{z}\in\hat{\mathcal{Z}}$. Thus, if, in the coordinates of $\hat{\mathcal{Z}}$, $s=0$ is a simple zero of $s\mapsto\varphi_2(\Gamma(s))-\varphi_1(\Gamma(s))$, then $\eta=\Gamma(0)$ is a continuable zero of Δ given by a curve Υ, as required in the statement of the lemma.

It remains to show that $\Upsilon(\hat{\epsilon})$, for sufficiently small $\hat{\epsilon}\neq 0$, is in fact a *simple* zero of the function $\mu\mapsto\Delta(\mu,\hat{\epsilon})$. To this end, it suffices to show that the matrix $D\Delta(\Upsilon(\hat{\epsilon}),\hat{\epsilon})$ does not have a zero eigenvalue. But, under the hypotheses of the lemma, the matrix $D\Delta(\eta,0)$ has a one dimensional kernel, namely the tangent space of $\hat{\mathcal{Z}}$. This means that $D\Delta(\eta,0)$ has exactly one zero eigenvalue. By the continuity of eigenvalues of matrices, there is a smooth family of eigenvalues $\lambda(\hat{\epsilon})$ such that $\lambda(0)=0$ and a corresponding smooth family of eigenvectors $V(\hat{\epsilon})$ such that $V(0)$ is a nonzero vector tangent to $\hat{\mathcal{Z}}$ with

$$D\Delta(\Upsilon(\hat{\epsilon}),\hat{\epsilon})V(\hat{\epsilon})=\lambda(\hat{\epsilon})V(\hat{\epsilon}).$$

It suffices to show that if $\hat{\epsilon}$ is positive and sufficiently small, then $\lambda(\hat{\epsilon})\neq 0$. By continuity, the remaining two eigenvalues of the matrix will be nonzero as well. The desired result follows as soon as we show that the derivative $\lambda'(0)\neq 0$. For this we have

$$D^2\Delta(\eta,0)(\Upsilon'(0),V(0))+D\Delta_{\hat{\epsilon}}(\eta,0)V(0)+D\Delta(\eta,0)V'(0)=\lambda'(0)V(0),$$

where D denotes differentiation with respect to the space variable $\mu\in\mathbb{R}^3$. After projection by Π into the complement of the range of $D\Delta(\eta,0)$,

$$\Pi D^2\Delta(\eta,0)(\Upsilon'(0),V(0))+\Pi D\Delta_{\hat{\epsilon}}(\eta,0)V(0)=\lambda'(0)\Pi V(0).$$

We claim that $\Pi D^2\Delta(\eta,0)(\Upsilon'(0),V(0))=0$. Once this claim is proved, the fact that $\lambda'(0)\neq 0$ would follow provided $\Pi D\Delta_{\hat{\epsilon}}(\eta,0)V(0)\neq 0$. The key point to note is that the projection operator, Π, is independent of the base point, i.e. the range of the projection operator is spanned by a constant basis vector independent of the base point. Thus since $\Delta_{\hat{\epsilon}}(\Gamma(s),0)=\varphi(\Gamma(s))$, we have

$$\frac{d}{ds}\Pi\varphi(\Gamma(s))|_{s=0}=\Pi D\varphi(\eta)\Gamma'(0)=\Pi D\Delta_{\hat{\epsilon}}(\eta,0)\Gamma'(0).$$

Since $\hat{\mathcal{Z}}$ is one dimensional, $\Gamma'(0)$ is just a scalar multiple of $V(0)$ and therefore if $\Pi D\varphi(\eta)\Gamma'(0)\neq 0$, then $\Pi D\Delta_{\hat{\epsilon}}(\eta,0)V(0)\neq 0$. By the definition of the components of φ and of the projection Π, we have

$$\frac{d}{ds}\Pi\varphi(\Gamma(s))|_{s=0}=\frac{d}{ds}[\varphi_2(\Gamma(s))-\varphi_1(\Gamma(s))]|_{s=0}.$$

Thus, if $s=0$ is a simple zero of $s\mapsto\varphi_2(\Gamma(s))-\varphi_1(\Gamma(s))$, then

$$\Pi D\Delta_{\hat{\epsilon}}(\eta,0)V(0)\neq 0,$$

as required.

To verify the claim, note that since Π projects to the complement of the range of $D\Delta(\eta,0)$ and since Π does not depend on the base point on $\hat{\mathcal{Z}}$, we have $\Pi D\Delta(\Gamma(\vartheta),0)\Upsilon'(\vartheta)\equiv 0$ for the real variable ϑ in the common domain of Γ and Υ. This implies that

$$0=\mathrm{d}\mathrm{d}\vartheta[\Pi D\Delta(\Gamma(\vartheta),0)\Upsilon\prime(\vartheta)]|\vartheta=0=\Pi D2\Delta(\eta,0)(\Gamma\prime(0),\Upsilon\prime(0))+\Pi D\Delta(\eta,0)\Upsilon\prime\prime(0)$$

$$= \hat{c}\Pi D^2\Delta(\eta,0)(V(0),\Upsilon'(0)),$$

where $\hat{c}V(0)=\Gamma'(0)$. Since $\hat{c}\neq 0$, the lemma is proved.

V. PERIODIC ORBITS

We now use Lemma IV.2 to prove that some of the zeros of the bifurcation function (15) are simple. We note that once this result is established, it will follow from Theorem III.1 that the corresponding bounded orbits of the Keplerian two-body system are continuable under perturbation by periodic gravitational waves.

If $\delta=0$, then the zeros of (15) are the union of the following one dimensional sets:

$$\begin{aligned}
\mathcal{Z}_1^+ &= \{(e,\ell,g): 2g+2m\ell=0, \quad U'_{2m}(e)=0\},\\
\mathcal{Z}_1^- &= \{(e,\ell,g): 2g+2m\ell=\pi, \quad U'_{2m}(e)=0\},\\
\mathcal{Z}_2^+ &= \left\{(e,\ell,g): 2g+2m\ell=\frac{\pi}{2}, \quad U_{2m}(e)=0\right\},\\
\mathcal{Z}_2^- &= \left\{(e,\ell,g): 2g+2m\ell=\frac{3\pi}{2}, \quad U_{2m}(e)=0\right\}.
\end{aligned} \tag{18}$$

We will show that the zeros in the sets $\mathcal{Z}_1^{\pm}$ and $\mathcal{Z}_2^{\pm}$ continue to simple zeros of the bifurcation function for sufficiently small $\delta\neq 0$. To conform with Lemma IV.2, we use (15) to identify the components of Δ as they appear in the lemma as follows:

$$\hat{\tau}(e,\ell,g) = U_{2m}(e)\sin(2g+2m\ell),$$

$$\tau_3(e,\ell,g) = U'_{2m}(e)\cos(2g+2m\ell),$$

$$\begin{aligned}
\varphi_1(e,\ell,g) = \tfrac{1}{4}[&(\alpha-\beta)U_m(e)\sin(2g+m\ell)\\
&+3(\alpha+\beta)U_{3m}(e)\sin(2g+3m\ell)],
\end{aligned}$$

$$\begin{aligned}
\varphi_2(e,\ell,g) = \tfrac{1}{2}[&(\alpha-\beta)U_m(e)\sin(2g+m\ell)\\
&+(\alpha+\beta)U_{3m}(e)\sin(2g+3m\ell)],
\end{aligned}$$

$$\begin{aligned}
\varphi_3(e,\ell,g) = \tfrac{1}{2}[&(\alpha-\beta)U'_m(e)\cos(2g+m\ell)\\
&+(\alpha+\beta)U'_{3m}(e)\cos(2g+3m\ell)].
\end{aligned}$$

Also, we note that δ in (15) plays the role of $\hat{\epsilon}$ in the lemma.

There are four cases to consider corresponding to the zero sets (18) of the unperturbed bifurcation function (14). We will consider the zero set $\mathcal{Z}_1^+$ for illustrative purposes, as the computational procedure is identical in all four cases. The set $\mathcal{Z}_1^+$ is just a line in $\mathbb{R}^3$, so here the curve Γ in the lemma can be taken to be a parametrization of this line starting at an appropriate point. By a direct calculation, the function $\varphi_2-\varphi_1$ on $\mathcal{Z}_1^+$ is given by

$$\tfrac{1}{4}[(\alpha-\beta)U_m(e)+(\alpha+\beta)U_{3m}(e)]\sin g.$$

The zeros of this function along $\mathscr{Z}_1^+$ are clearly simple provided the coefficient of $\sin g$ does not vanish at the value of the eccentricity determined by membership in $\mathscr{Z}_1^+$. The main result of this section is the following theorem.

Theorem V.1: *Consider the system (10) and suppose that (L,G,ℓ,g) is on an unperturbed $(m:n)$ resonant periodic solution with $n=1$, that is, $L^3=mk^2/\Omega$. If (e,ℓ,g) is in $\mathscr{Z}_1^+$ or $\mathscr{Z}_1^-$, respectively, (e,ℓ,g) is in $\mathscr{Z}_2^+$ or $\mathscr{Z}_2^-$, where e is the eccentricity of the corresponding Keplerian ellipse $(e^2=1-G^2/L^2)$ and if*

$$(\alpha-\beta)U_m(e)+(\alpha+\beta)U_{3m}(e)\neq 0,$$

respectively,

$$(\alpha-\beta)U_m(e)-(\alpha+\beta)U_{3m}(e)\neq 0,$$

then the Keplerian ellipse continues to a periodic orbit under the perturbation.

It remains to show that the sets $\{\mathscr{Z}_i^{\pm}\}$, $i=1,2$, are not empty. This fact will follow as soon as we show that both of the functions U_{2m} and U'_{2m} have zeros on the interval $0<e<1$.

Recall that $U_{2m}(e)=A_{2m}(e)+B_{2m}(e)$ and note that both A_{2m} and B_{2m} have removable singularities at $e=0$. Moreover, both have Taylor series at $e=0$ with leading terms given by

$$2(2m-1)\frac{m^{2m-2}}{(2m)!}e^{2(m-1)}.$$

In particular, if $m=1$, then $\lim_{e\to 0^+} U_2(e)=2$ and for $m>1$, the limit is zero, but $U_{2m}(e)>0$ for sufficiently small eccentricity. Also, $\lim_{e\to 1^-} U_{2m}=-J_{2m}(2m)/m^2$. By a standard property of the Bessel functions, $J_\nu(\nu)>0$; hence, $U_{2m}(1)<0$. This proves U_{2m} has at least one zero on the interval $0<e<1$. Numerical calculations suggest that this zero is unique.

A simple argument can be given to prove the existence of a zero in the case $m=1$ for the function U'_{2m}. In this case, the series expansion of U'_2 at $e=0$ is $-10e+O(e^2)$. Thus, $U'_2(e)<0$ for a small but positive eccentricity. The limit as $e\to 1^-$ is the same as

$$\lim_{e\to 1^-}\frac{2}{\sqrt{1-e^2}}J'_2(2).$$

By standard properties of the Bessel functions, $J_2(0)=0$ and $J_2>0$ on the interval $(0,\ j'_{2,1})$, where $j'_{2,1}$ is the first zero of J'_2. Hence, $J'_2>0$ on $(0,\ j'_{2,1})$. But, we also have $2<j'_{2,1}$. Thus, $J'_2(2)>0$ and $U'_2(e)\to\infty$ as $e\to 1^-$. This proves that $U'_2(e)$ has at least one zero on the interval $0<e<1$; moreover, numerical computations suggest that this zero is unique.

For $m\geq 2$, we will outline a proof that shows the function U'_{2m} has at least two zeros on the interval $0<e<1$. An asymptotic analysis shows that the function U'_{2m} is positive near the end points of the interval. The proof is completed by showing that U'_{2m} has a negative value within the interval. To this end, note that the function U'_{2m} has the form

$$U'_{2m}(e)=\gamma_1(m,e)J_{2m}(2me)+\gamma_2(m,e)J'_{2m}(2me),$$

where γ_1 and γ_2 are computed using (9). Moreover, by standard properties of the Bessel functions, both of the functions $e\mapsto J_{2m}(2me)$ and $e\mapsto J'_{2m}(2me)$ are positive for $0<e<1$. Let us define $\hat{e}:=(1-1/(4m^2))^{1/2}$, and observe that $0<\hat{e}<1$. A simple computation shows that

$$\gamma_1(m,\hat{e})<0,\quad \gamma_2(m,\hat{e})<0.$$

Hence, we have $U'_{2m}(\hat{e})<0$, as desired. Numerical computations suggest that the function U'_{2m} has exactly two zeros on the interval $0<e<1$.

It follows from these results that the resonant interaction of the incident multi-frequency gravitational wave of definite helicity with a Keplerian binary can result in orbits that are periodic with period $2\pi/\Omega$, where $\Omega=m\omega$, $m=1,2,3,\ldots$. It is conceivable that other periodic orbits may exist; however, our method can identify only those periodic orbits that are continuations of resonant Keplerian orbits of the unperturbed system.

VI. ROTATING FRAME

In a manner similar to that used by Hill in his treatment of the lunar theory,[7–9] we can view the dynamical system described by (6) in Cartesian coordinates rotating at half the principal frequency of the incident gravitational wave ($\Omega_*=2\Omega$). These coordinates—that we again represent by (x,y)—rotate with frequency $\frac{1}{2}\Omega_*=\Omega$ with respect to inertial coordinates; therefore, the equations of motion in these coordinates are given by

$$\begin{aligned}&\frac{d^2x}{dt^2}-2\Omega\frac{dy}{dt}-\Omega^2x+\frac{kx}{r^3}+2\epsilon\Omega^2[(1+\delta\alpha\cos\Omega t)x+(\delta\beta\sin\Omega t)y]=0,\\&\frac{d^2y}{dt^2}+2\Omega\frac{dx}{dt}-\Omega^2y+\frac{ky}{r^3}+2\epsilon\Omega^2[(\delta\beta\sin\Omega t)x-(1+\delta\alpha\cos\Omega t)y]=0.\end{aligned}\tag{19}$$

Let $X:=\dot{x}-\Omega y$ and $Y:=\dot{y}+\Omega x$ be the canonical momenta conjugate to x and y, respectively. Then (19) is equivalent to a Hamiltonian system with Hamiltonian

$$\begin{aligned}\mathscr{H}_R=&\frac{1}{2}(X^2+Y^2)+\Omega(yX-xY)-\frac{k}{r}\\&+\epsilon\Omega^2[(1+\delta\alpha\cos\Omega t)(x^2-y^2)+2(\delta\beta\sin\Omega t)xy].\end{aligned}\tag{20}$$

By identifying the momenta in polar rotating coordinates as $p_r=(xX+yY)/r$ and $p_\theta=xY-yX$, (20) in polar coordinates is given by

$$\begin{aligned}\mathscr{H}_R=&\frac{1}{2}\left(p_r^2+\frac{p_\theta^2}{r^2}\right)-\frac{k}{r}-\Omega p_\theta+\epsilon\Omega^2r^2[\cos 2\theta\\&+\delta(\alpha\cos 2\theta\cos\Omega t+\beta\sin 2\theta\sin\Omega t)],\end{aligned}\tag{21}$$

which in the corresponding Delaunay elements becomes

$$\begin{aligned}\mathscr{H}_R=&-\frac{k^2}{2L^2}-\Omega G+\epsilon\Omega^2\{\mathscr{C}(L,G,\ell,g)+\delta[\alpha\mathscr{C}(L,G,\ell,g)\cos\Omega t\\&+\beta\mathscr{S}(L,G,\ell,g)\sin\Omega t]\}.\end{aligned}\tag{22}$$

The Hamiltonian system given by (22) has periodic orbits with period $2\pi/\Omega$, where $\Omega=m\omega$, $m=1,2,\ldots$; this assertion can be demonstrated using results that have already been obtained in this paper. In fact, using the resonance assumption, periodic orbits exist in the inertial frame with period $2\pi/\Omega$ as shown in Section V. An orbit in the inertial frame, $t\mapsto(x_I(t),y_I(t))$, is represented in the rotating frame by

$$\begin{aligned}x_R(t)&=x_I(t)\cos\Omega t+y_I(t)\sin\Omega t,\\y_R(t)&=-x_I(t)\sin\Omega t+y_I(t)\cos\Omega t.\end{aligned}$$

It follows from these relations that if $x_I(t)$ and $y_I(t)$ are periodic with period $2\pi/\Omega$, then so are $x_R(t)$ and $y_R(t)$. Therefore, the orbits that are periodic in the inertial frame with period $2\pi/\Omega$ are observed to be periodic with period $2\pi/\Omega$ in the rotating frame. It is also possible to arrive at this conclusion by direct application of the methods developed in the previous sections.

To understand the physical structure of Hamiltonian (22), imagine right circularly polarized gravitational radiation of frequency 2Ω that is normally incident on the orbital plane. It follows from our previous work,[I] as well as equation (19), that in a reference frame rotating with frequency Ω the wave stands still. That is, observers at rest in the rotating frame do not perceive the variability associated with a wave so that in the absence of secondaries ($\delta=0$) the dynamical system (19) is autonomous. That an observer—by merely rotating about the propagation axis of the circularly polarized wave—could make the wave stand completely still would be a remarkable physical effect and deserves further discussion.

It is a fundamental consequence of Lorentz invariance that all basic radiation fields travel with speed c with respect to all *inertial* observers. This may be illustrated by an example: Let an inertial observer move with speed v_0 along the propagation axis of a monochromatic plane gravitational wave of frequency $\Omega_\star$. The frequency and the wave vector of the radiation as perceived by the moving observer are smaller than those measured by static inertial observers by a common Doppler factor of

$$\left(\frac{c-v_0}{c+v_0}\right)^{1/2}.$$

Mathematically, as $v_0\to c$ this ratio goes to zero and hence the frequency and wave vector of the radiation vanish so that the wave might appear to stand still. This limit is not physically allowed, however. No observer can move at the speed of light, although—theoretically—one can get arbitrarily close. Therefore, the wave can never stand still for an inertial observer. It has been shown[10] that according to the standard Einstein theory this is not the case for accelerated observers, i.e. an accelerated observer can indeed stand still with respect to a gravitational wave. The autonomous nature of the system (19) for $\delta=0$ provides an interesting illustration of this fact. That is, consider an observer at the center of a system of coordinates rotating with frequency Ω. The observer does not move, but the fact that it refers its observations to the axes that rotate with frequency Ω with respect to the inertial axes makes it a noninertial observer. Radiation of frequency $\Omega_\star$ is incident in the inertial frame along the axis of rotation. According to the noninertial observer, the frequency of the gravitational wave is $\Omega_\star'=\Omega_\star\mp 2\Omega$, where the upper sign refers to right circularly polarized (RCP) gravitational radiation and the lower sign refers to left circularly polarized (LCP) gravitational radiation. The first (second) case has helicity $+2$ (-2), so that $\Omega_\star'=\Omega_\star-\mathbf{h}\cdot\mathbf{\Omega}$, where $\mathbf{h}$ is the helicity of the gravitational radiation field; this is an example of the general phenomenon of helicity-rotation coupling. Now if $\Omega=\frac{1}{2}\Omega_\star$ for RCP gravitational waves or $\Omega=-\frac{1}{2}\Omega_\star$ for LCP gravitational waves, we find that $\Omega_\star'$ vanishes according to the noninertial observer (as well as any other observer at rest in the rotating frame anywhere along the z-axis) and the radiation field stands still. It has been shown in Ref. 1 that for a monochromatic gravitational wave with definite helicity and sufficiently small amplitude this observation concerning a rotating observer leads to the conclusion that a Keplerian system in the presence of this radiation can never ionize. *In principle, this absence of ionization could be considered an observable consequence of the physical possibility that a gravitational wave could stand completely still.*

Let us now consider the possibility of ionization of the binary system as a function of the parameter δ. The transformation to the rotating frame leaves the orbital radius unchanged; therefore, the ionization problem can be discussed equally well in the rotating frame. In fact, the problem becomes simpler since the principal component of the incident radiation field loses its time-dependence as in (22). Thus if $\delta=0$, the KAM theorem implies that for sufficiently small ϵ the perturbed trajectory is bounded since it is trapped between two dimensional invariant tori in

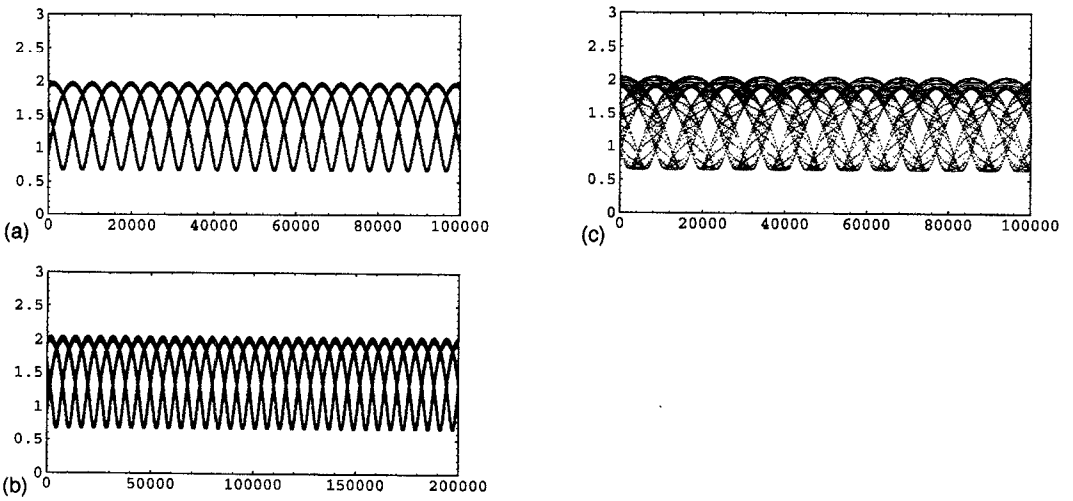

FIG. 1. Orbital radius versus time plots for the dynamical system given by Hamiltonian (6) with initial conditions $(p_r, p_\theta, r, \theta)$ equal to (0.5,1,1,0) and parameter values $\epsilon=0.001$, $\delta=0$, $\alpha=2.5$, $\beta=2$, $k=1$ and, from (a) to (c), $\Omega=2$, $\Omega=9\sqrt{3}/8$, $\Omega=1$.

the three dimensional energy surfaces. When $\delta\neq 0$, however, the two secondary components in the inertial frame both reduce to a perturbation of frequency Ω in the rotating frame; that is, the three Fourier components of the radiation field in the inertial frame are RCP waves with frequencies $\Omega_*=\Omega,2\Omega$ and 3Ω, while the tidal matrix in the rotating frame has frequencies given by $\Omega'_*=\Omega_*-2\Omega$, i.e. $-\Omega,0$ and Ω for the three components, respectively. The perturbation of frequency Ω in the rotating frame is expected to lead to Arnold diffusion[11,12] and hence ionization of the system. However, it has not been possible thus far to prove ionization for the system (22); therefore, we resort to numerical work in the following section.

VII. NUMERICAL EXPERIMENTS

In this section we illustrate—by means of numerical experiments—the conjecture that gravitational ionization and Arnold diffusion are closely related. The interpretation of the numerical results is simplified if we take the viewpoint of inertial observers and consider the perturbed motion given by Hamiltonian (6).

We have performed several numerical experiments to test the diffusion and ionization properties of the dynamical system that is represented by the Hamiltonian (6). The physical meaning of these numerical experiments is essentially the same as in our previous paper (cf. Figure 2 in Ref. 1): Let us choose two scales for the measurement of time and length that are arbitrary except that they are connected here by our choice of $k=1$. In these otherwise unspecified units, we have chosen an unperturbed ellipse of semimajor axis $a=4/3$ and eccentricity $e=1/2$ such that $g=-\pi/2$ and the Keplerian frequency is $\omega=3\sqrt{3}/8$. The ellipse is perturbed by the presence of periodic gravitational radiation and the orbital radius of the osculating ellipse is then plotted versus time in these units in Figures 1–4. These figures represent the results of our numerical experiments in which we have set the parameters of the external perturbation as follows:

$$\epsilon=0.001, \quad \alpha=2.5, \quad \beta=2,$$

and have changed δ in the range $0\leqslant\delta\leqslant 1$ and Ω in the range $1\leqslant\Omega\leqslant 2$. In each run, we set the initial conditions to be

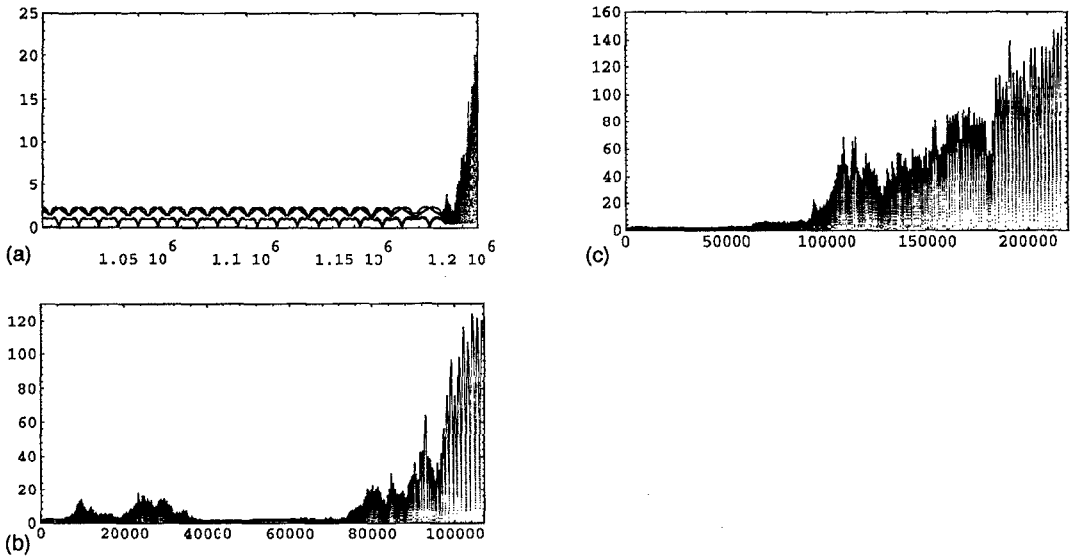

FIG. 2. Orbital radius versus time plots for the dynamical system given by the Hamiltonian (6) with initial conditions $(p_r, p_\theta, r, \theta)$ equal to (0.5,1,1,0) and parameter values $\epsilon = 0.001$, $\delta = 0.5$, $\alpha = 2.5$, $\beta = 2$, $k = 1$ and, from (a) to (c), $\Omega = 2$, $\Omega = 9\sqrt{3}/8$, $\Omega = 1$.

$$(p_r, p_\theta, r, \theta) = (0.5,1,1,0),$$

which correspond to the unperturbed ellipse described above. After integration over each time interval corresponding to one cycle of the perturbation, i.e. $2\pi/\Omega$, the corresponding elapsed time t and orbital radius are plotted. Clearly, for each value of t (abscissa) there is only one value of orbital radius r (ordinate); however, this is not discernible in some of the figures due to the way in which the plots have been prepared. The KAM theorem is illustrated in Figure 1, where the

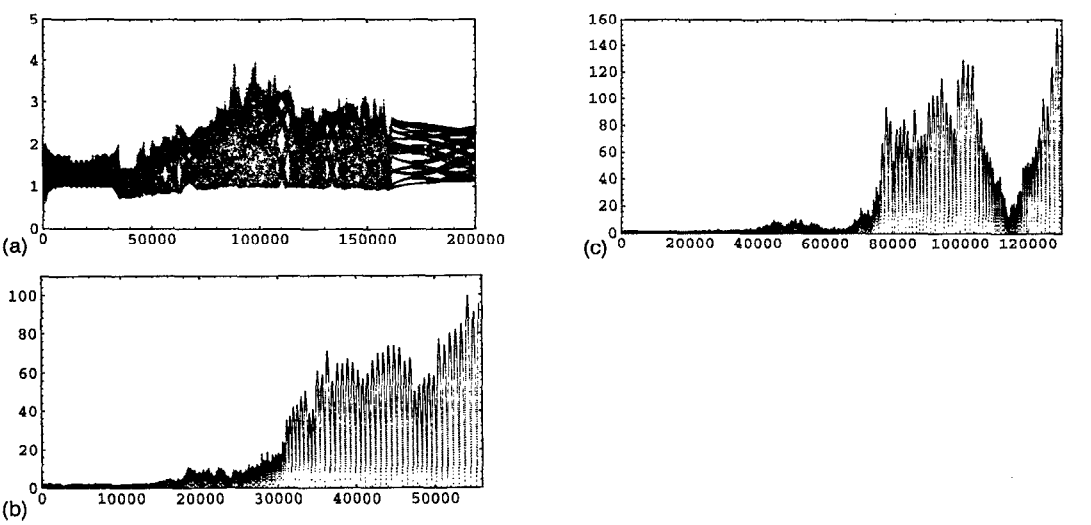

FIG. 3. Orbital radius versus time plots for the dynamical system given by the Hamiltonian (6) with initial conditions $(p_r, p_\theta, r, \theta)$ equal to (0.5,1,1,0) and parameter values $\epsilon = 0.001$, $\delta = 1$, $\alpha = 2.5$, $\beta = 2$, $k = 1$ and, from (a) to (c), $\Omega = 2$, $\Omega = 9\sqrt{3}/8$, $\Omega = 1$.

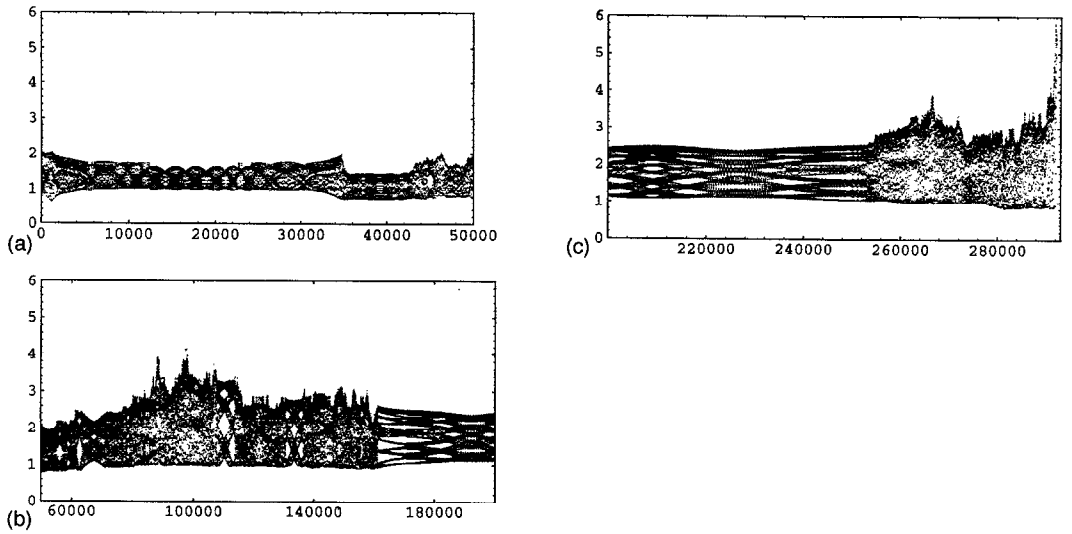

FIG. 4. Orbital radius versus time plots for the dynamical system given by the Hamiltonian (6) with initial conditions $(p_r, p_\theta, r, \theta)$ equal to (0.5,1,1,0) and parameter values $\epsilon=0.001$, $\delta=0.5$, $\alpha=2.5$, $\beta=2$, $k=1$, $\Omega=2$. This is an extended form of the plot presented in panel (a) of Figure 3.

value of r appears to oscillate between $\simeq a(1-e)=2/3$ and $\simeq a(1+e)=2$, thus indicating the complete absence of ionization. The possibility of ionization of the system is illustrated in Figures 2 and 3 for $\delta>0$, where the initial ellipse is near resonance in the first panel, on resonance in the middle panel and off resonance in the last panel. More precisely, the middle panel in either Figure 2 or Figure 3 corresponds to an exact third order resonance since $\Omega/\omega=3$, while the first panel illustrates the response of the ellipse to the external perturbation near resonance $\Omega/\omega\approx 3.08$; the last panel is off resonance with $\Omega/\omega\approx 1.54$. Additional calculations extending the integration time for the system depicted in the first panel of Figure 3 have been performed. These results suggest that a bursting behavior occurs in which the near resonance condition shown at the right end of this panel is followed by chaotic motion similar to that shown in the middle of this panel that in turn is followed by a period of near resonance. This recurrence of chaotic and near resonance behavior appears to continue for the extended interval of time studied as illustrated in Figure 4. Thus, this behavior is consistent with a type of chaotic behavior, called intermittent chaos, that has been studied for dissipative systems.[12] If the behavior suggested by these simulations is indeed present in the Hamiltonian system (6), then our result would be an example of *Hamiltonian intermittency*.

Imagine, for the sake of concreteness, a binary system consisting of an artificial satellite in an eccentric orbit about the Earth. Let the scales of length and time be R_0 and T_0, respectively; then, $R_0^3=kT_0^2$. Thus, if we take $R_0=10^9$ cm for the problem under consideration, it turns out that $T_0\approx 1.6\times 10^3$ s. The gravitational wave in our numerical experiments would then have a frequency of the order of $\Omega\approx 10^{-3}$ rad s^{-1}, corresponding approximately to 1.5×10^{-4} Hz as well as to a wavelength of 2×10^{14} cm, and an amplitude of the order of $\epsilon=10^{-3}$. Gravitational waves have not yet been directly observed; however, in a realistic situation the amplitude of the wave would be expected to be of the order of 10^{-20}.

Our numerical experiments are consistent with the expected behavior for a $2\frac{1}{2}$-degree of freedom Hamiltonian system. In fact, by introducing a fictitious action variable (cf. Sec. 6 in Ref. 1), our system is equivalent to an *autonomous* Hamiltonian system with *three* degrees of freedom. Each orbit of this new system is constrained to an energy manifold. However, whereas the two

dimensional KAM tori (if they exist for our choice of parameter values) separate each three dimensional energy manifold for the corresponding two-degree of freedom Hamiltonian system that we obtain with $\delta=0$, the three dimensional KAM tori, that may exist for the three-degree of freedom Hamiltonian system that we obtain with $\delta\neq 0$, do not separate space within the five dimensional energy manifolds. Of course, for sufficiently small choices of δ, there are orbits of the three-degree of freedom Hamiltonian system that remain bounded for all time; for example, the periodic orbits of Section V and the orbits confined to KAM tori. While the totality of bounded orbits in an energy manifold may be a set of positive measure, we expect that every open set of the five dimensional energy manifold contains an initial condition for a trajectory that will diffuse throughout the energy manifold. In fact, we expect this behavior for all $\delta>0$. On the other hand, as δ decreases toward zero, the time required to leave the vicinity of a KAM torus is expected to grow at an exponential rate. Figures 1–4 illustrate dynamical behavior that is characteristic of Arnold diffusion.[12]

APPENDIX: LATERALLY INCIDENT RADIATION

The purpose of this appendix is to point out that the main results of this paper still hold for a more general incident gravitational wave than that considered in (4).

In the general case of incident gravitational radiation on a binary system, the motion of the system away from the initial orbital plane (i.e., along the z-direction) also needs to be taken into account. It is necessary to mention here that *initial conditions* are generally ignored in our theoretical approach, which relies on the properties of the perturbed system once transients have died away and a "steady state" situation has been established. In this paper, we have limited our considerations to normally incident waves; in fact, the transversality of gravitational radiation makes it possible to set $z=0$ for normally incident waves. We wish to note here that essentially the same results can be obtained for a more general incident radiation field.

Consider, for instance, the superposition of a left circularly polarized (LCP) wave of frequency Ω traveling along the z-axis with a linearly polarized wave of frequency Ω traveling along the x-axis. Specifically, let χ_{ij} be of the form

$$\chi(t,\mathbf{0})=\begin{pmatrix} \cos\Omega t & -\sin\Omega t & 0 \\ -\sin\Omega t & 3\cos\Omega t & 0 \\ 0 & 0 & -4\cos\Omega t \end{pmatrix}, \tag{23}$$

up to a constant factor. It follows from (2) that the corresponding $\mathscr{K}$ is of the form

$$\mathscr{K}=\tfrac{1}{2}\Omega^2\chi(t,\mathbf{0}), \tag{24}$$

so that the equation of motion (1) along the z-direction is given by

$$\frac{d^2z}{dt^2}+\frac{kz}{r^3}-2\epsilon\Omega^2 z\cos\Omega t=0. \tag{25}$$

This equation is satisfied by $z=0$, which is consistent with the fact that the orbit is always in the (x,y)-plane. Therefore, to the incident radiation field in (4) one could add radiation fields of the type given by (23). Moreover, upon transformation to the rotating frame,

$$\mathscr{K}'=R^{-1}\mathscr{K}R=\frac{1}{2}\Omega^2\begin{pmatrix} \cos\Omega t & \sin\Omega t & 0 \\ \sin\Omega t & 3\cos\Omega t & 0 \\ 0 & 0 & -4\cos\Omega t \end{pmatrix}, \tag{26}$$

where

$$R=\begin{pmatrix} \cos \Omega t & -\sin \Omega t & 0 \\ \sin \Omega t & \cos \Omega t & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{27}$$

is the rotation matrix used in Section VII. It is remarkable that the tidal matrix $\mathscr{K}'$ in the rotating frame has the same frequency Ω as in the inertial frame; in fact, $\mathscr{K}'$ can be obtained from $\mathscr{K}$ simply by letting $\Omega \to -\Omega$.

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A Riemannian generalization of a result of DeWitt concerning Ricci-flat Lorentz metrics

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For any given nonzero real number, α, and any curve from some open interval, I, into the space $\mathcal{M}$, of Riemannian metrics on a compact manifold M, a metric, $\tilde{g}$, on the manifold $I\times M$ can be constructed in a natural way; the metric is Riemannian for α positive and Lorentzian for α negative. The aim of this paper is to show that $\tilde{g}$ is an Einstein metric, with constant λ, if and only if the curve of metrics is a solution of a certain Lagrangian on $\mathcal{M}$ defined in terms of the DeWitt metric on $\mathcal{M}$, the total scalar curvature functional and the values α and λ. This result was obtained by DeWitt [Phys. Rev. **160**, 1113 (1967)], for the case where the dimension of M is three, α is negative and $\lambda=0$, in the context of a formulation of Einstein equations of evolution as a dynamical system. DeWitt metric is a member of a one parameter family of pseudometrics on $\mathcal{M}$; it is shown here that, no other such a metric can be used to describe the relationship of the $(n+1)$ geometry of $I\times M$ with the dynamics on $\mathcal{M}$, so a characterization of the DeWitt metric is obtained. © *1996 American Institute of Physics.* [S0022-2488(96)01207-8]

I. INTRODUCTION

Let $(N,\tilde{g})$ be a four-dimensional Lorentz manifold and let M be three-dimensional spacelike submanifold of N such that $\tilde{g}$ defines on M a one parameter family of Riemannian metrics, g_t. It is known that Einstein field equations in N, that is those describing the vanishing of the Ricci tensor of $\tilde{g}$, can be written as time evolution equations for the curve $t\to g_t$ in the manifold $\mathcal{M}$ of all Riemannian metrics on M. In Ref. 1, these equations are described as geodesic equations in $\mathcal{M}$, considered with a metric, which is now usually known as the DeWitt metric, and modified by a term due to the gravitational potential. More precisely, one of the results in Ref. 1, stated as in Ref. 2, reads as follows:

Theorem 1.1: *Let M be a compact, 3-dimensional manifold and let g_t, $t\in I=(-\varepsilon,\varepsilon)$, be a curve in the manifold of metrics $\mathcal{M}$. Let $(N,\tilde{g})$ be the Lorentz 4-manifold, where $N=I\times M$ and $\tilde{g}$ is defined in such a way that in an adapted coordinate system,*

$$\tilde{g}_{ij}(t,p)=(g_t)_{ij}(p);\quad \tilde{g}_{i0}\equiv 0;\quad \tilde{g}_{00}\equiv -1,$$

for each $i,j=1,2,3$. Then, $\tilde{g}$ is Ricci flat if and only if the curve g_t satisfies the second order differential equation,

$$g''=g'g^{-1}g'-\frac{1}{2}\mathrm{tr}(g^{-1}g')g'-\frac{1}{8}\langle g',g'\rangle_g^- g-2\rho_0(g)-\frac{1}{12}\tau(g)g,$$

together with the constraints $\delta_g(g'-\mathrm{tr}(g^{-1}g')g)=0$ and $\mathcal{H}(g,g'):=\frac{1}{2}\langle g',g'\rangle_g^- -2\tau(g)=0$. Here, $\rho_0(g)$, $\tau(g)$ and δ_g, represent the traceless part of the Ricci tensor, the scalar curvature and the divergence operator of the metric g and, $\langle,\rangle_g^-$ is the pointwise product that gives, by integration over M, the DeWitt metric G_g^-.

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The second order equation is equivalent to the curve being a solution of the Lagrangian $L(g)=\frac{1}{2}G_g^-(g,g)+2S(g)$ and can be written as $g''=\Gamma^-(g,g')+2\mathrm{grad}^- S(g)$, where S is the total scalar curvature functional and Γ^- represents the Riemannian spray.

The purpose of this article is to give some generalizations of Theorem 1.1; namely we will prove that the assumption on the dimension of the manifold M is not necessary and also, that the conclusion is independent of the metric $\tilde{g}$ being Lorentzian. On the contrary, we will show that the DeWitt metric is the only metric, among those of a natural one parameter family of pseudometrics on $\mathcal{M}$, for which Einstein equations can be written in terms of its spray, gradients and divergences.

A Ricci flat metric is, in particular, an Einstein metric. Our last result is a generalization of Theorem 1.1 to this situation. We give the proof of the above mentioned results in Section IV.

Section II is concerned with the manifold of Riemannian metrics on a compact manifold and with the total scalar curvature functional, also known as gravitational potential. Although this material is fairly standard, we have included here a survey in order to establish the notation and to write the known results in the form in which they are going to be used in the sequel.

In Section III, we describe a one parameter family of weak pseudometrics, G^c, on the manifold $\mathcal{M}$; the usual L^2 metric and the DeWitt metric are among them. We use some results of Ref. 3 to obtain the explicit formulae for the Riemannian spray, gradients and divergences corresponding to each G^c.

II. PRELIMINARIES

Several topologies can be defined on sets of differentiable maps between manifolds, by using the adequate jet space; in this paper we will consider the C^∞-compact topology. With this topology, the space of smooth sections of a vector bundle over a manifold is a locally convex topological vector space; more precisely, it is a Fréchet space. Thus, it is possible to define manifolds modeled on these spaces of sections; the spaces themselves are manifolds with a single chart.

Many geometric structures on a manifold are defined to be one, or several, tensor fields satisfying certain conditions; so, each class of structures determines a subset of some space of tensor fields and, frequently, these subsets admit a structure of manifold modeled on spaces of sections.

Let M be a finite-dimensional, smooth manifold and for each nonnegative integers (r,s), let $\Gamma^\infty(T_{(r,s)}(M))$ be the space of r-times contravariant, s-times covariant, tensor fields on M. The C^∞-compact topology on it can be described in terms of a Riemannian metric on M, in a manner completely analogous to that used to define the same topology, on the space of smooth functions from an open domain of Euclidean space. It is only necessary to change the Euclidean norm, by the norm determined by the metric, and ordinary partial derivatives, by covariant derivatives with respect to its Levi-Civita connection. A detailed description can be seen in Ref. 4.

With exactly the same procedure, any other topology, of those usually defined on spaces of functions of Euclidean domains, can be extended to spaces of tensor fields. Among them, we can find the topologies associated either to Lebesgue or to Sobolev norms, which are obtained by integration of different powers of the norms of the tensor field or of its covariant derivatives. Nevertheless, if the manifold is not compact, the topology so defined depends upon the metric used for the definition and this fact has also a negative influence on the C^∞-compact topology; in fact, only for a compact manifold, spaces of sections, endowed with the C^∞-compact topology, are inverse limits of Hilbert spaces.

In what follows, we will assume that M is a compact manifold without boundary.

Let us denote by $S^2(M)$ the subspace of the symmetric elements of $\Gamma^\infty(T_{(0,2)}(M))$; it is easy to see that it is closed in the C^∞-compact topology and therefore it is a Fréchet space. Under the compactness assumption, the subset $\mathcal{M}\subset S^2(M)$, of positive definite elements, is open and then, it admits a Fréchet manifold structure modeled on $S^2(M)$. $\mathcal{M}$ is the manifolds of the metrics and it is a convex cone.

The diffeomorphism group of the manifold M, denoted by $\mathscr{D}$, is also a Fréchet manifold; its model is the space of vector fields on $\mathscr{M}$. $\mathscr{D}$ acts on each space of covariant tensor fields by pull-back.

For given $\varphi \in \mathscr{D}$, the map $\varphi:(M,\varphi^*g)\to(M,g)$ is, by definition, an isometry and so, any map of geometrical meaning, from $\mathscr{M}$ to a tensor field space, should be invariant by the action of $\mathscr{D}$. Examples of such maps, that we will use here, are the following.

– The Riemann curvature $R:\mathscr{M}\to\Gamma^\infty(T_{(0,4)}(M))$; it is given by $R(g)(X,Y,Z,W)=g(R_g(X,Y,Z),W)$ where $R_g(X,Y,Z)=-\nabla^g_X\nabla^g_Y Z+\nabla^g_Y\nabla^g_X Z+\nabla^g_{[X,Y]}Z$.

– The Ricci tensor $\rho:\mathscr{M}\to S^2(M)$; it is defined by $\rho(g)(X,Y)=\mathrm{tr}A^g_{X,Y}$ where $A^g_{X,Y}$ represents the (1,1)-tensor field given by $A^g_{X,Y}(Z)=R_g(X,Z,Y)$.

– The scalar curvature $\tau:\mathscr{M}\to C^\infty(M)$ given by $\tau(g)=\mathrm{tr}(g^{-1}\rho)$.

– The volume form $\mathrm{vol}:\mathscr{M}\to\Lambda^n(M)$, if $\mathscr{M}$ is oriented.

The scalar curvature is a particular case of what is called a natural Lagrangian; that is, a map $L:\mathscr{M}\to C^\infty(M)$ which is $\mathscr{D}$-invariant and that only depends on some k-th order jet of the metric.

Definition 2.1: A differentiable map $F:\mathscr{M}\to\mathbb{R}$ is said to be a Riemannian functional if and only if $F(\varphi^*g)=F(g)$ for all $(\varphi,g)\in\mathscr{D}\times\mathscr{M}$.

The condition on F defined above is equivalent to the map being constant on the $\mathscr{D}$-orbits.

Definition 2.2: Let $F:\mathscr{M}\to\mathbb{R}$ be a Riemannian functional; for a given $g\in\mathscr{M}$ let us denote by $T_gF:T_g\mathscr{M}\to\mathbb{R}$ the tangent map to F at g. A metric, g, is a critical point of F if and only if $\mathrm{Ker}(T_gF)=T_g\mathscr{M}$.

Definition 2.3: Let $L:\mathscr{M}\to C^\infty(M)$ be a, $\mathscr{D}$-invariant, smooth map. The Riemannian functional associated to L is defined as $F_L(g)=\int_M L(g)\mathrm{vol}(g)$ where $\mathrm{vol}(g)$ represents the volume element of g (a density on M unless M is oriented). In particular, F_τ is the total scalar curvature and will be denoted by S; if L is given by $L(g)\equiv 1$, then F_L is the volume functional.

The computations necessary to obtain the differential of maps related with the curvature operator have been done usually in local coordinates, and they are well known from a long time ago; in particular, those concerning total scalar curvature go back to Hilbert[5]. A good review of the known results is included in the corresponding chapter of Besse.[6]

The next statement contains several known results concerning the differential of the scalar curvature map. They are written in the form in which we are going to use them later.

Proposition 2.4

(1) $(T_g\mathrm{vol})(h)=\frac{1}{2}\mathrm{tr}(g^{-1}h)\mathrm{vol}(g)$,

(2) $(T_gF_L)(h)=\int_M((T_gL)(h)+\frac{1}{2}\langle L(g)g,h\rangle_g)\mathrm{vol}(g)$,

(3) $(T_g\tau)(h)=-\langle\rho(g),h\rangle_g+\Delta^g(\mathrm{tr}(g^{-1}h))+\delta_g\delta_g h$,

(4) $(T_gS)(h)=\int_M\langle-\rho(g)+\frac{1}{2}\tau(g)g,h\rangle_g\mathrm{vol}(g)$,

where δ_g is the divergence operator of the metric g, given by $\delta_g T=-\mathrm{tr}(g^{-1}\nabla^g T)$, and Δ^g is the Laplace operator, $\Delta^g T=-\mathrm{tr}(g^{-1}(\nabla^g)^2T)$. Here, $\langle,\rangle_g$ represents the usual pointwise product of tensor fields given by the metric which, for 2-covariant symmetric tensor fields, has the form $\langle k,h\rangle_g=\mathrm{tr}(g^{-1}kg^{-1}h)$.

The L^2 inner product on $S^2(M)$, obtained by integration of the usual pointwise product, gives rise to a Riemannian metric, G, on $\mathscr{M}$ by the formula

$$G_g(h,k)=\int_M\langle h,k\rangle_g\mathrm{vol}(g).$$

G is a symmetric, $\mathscr{D}$-invariant, bilinear form but it is a weak metric; in fact, the map, from $T_g\mathscr{M}$ into its dual, induced by G, is only injective and the topology, in $T_g\mathscr{M}$, defined by the G_g-norm is not the one obtained from the differentiable structure considered in $\mathscr{M}$.

Definition 2.5: Let $F:\mathscr{M}\to\mathbb{R}$ be a Riemannian functional. If there is a map $\mathrm{grad}F:\mathscr{M}\to S^2(M)$ *such that $G_g(\mathrm{grad}F(g),h)=(T_gF)(h)$, for each $g\in\mathscr{M}$ and each $h\in T_g\mathscr{M}$, this map is said to be the G-gradient of F.*

If F is such that its G-gradient exits then, a metric g is a critical point of F if and only if $\mathrm{grad}F(g)=0$.

From (4) of Proposition 2.4, the total scalar curvature admits a G-gradient, namely $\mathrm{grad}S(g)=-\rho(g)+\frac{1}{2}\tau(g)g$. For a manifold, of dimension $n\neq 2$, a metric is a critical point of S if and only if it is Ricci flat.

The next property, usually known as conservation laws, follows directly from the fact that, due to the $\mathscr{D}$-invariance of a Riemannian functional, its G-gradient must be, at each metric g, G_g-orthogonal to the orbit. The tangent space, at g, to the $\mathscr{D}$-orbit is the image of the elliptic differential operator $\delta_g^*:\Lambda^1(M)\to S^2(M)$ given by $\delta_g^*(\omega)=\mathrm{symm}(\nabla\omega)$; its formal G_g-adjoint is the divergence operator of g and then, the elements of $S^2(M)$ which are G_g-orthogonal to the orbit are just those of $\mathrm{Ker}\delta_g$.

Proposition 2.6: Let grad F *be the G-gradient of a Riemannian functional F; then, for each $g\in\mathscr{M}$ the tensor field* $\mathrm{grad}F(g)$ *has vanishing g-divergence.*

III. THE ONE PARAMETER FAMILY OF PSEUDOMETRICS, G^c ON $\mathscr{M}$

Each metric, g, determines an algebraic decomposition of the tangent space $T_g\mathscr{M}=S^2(M)$ as follows: $T_g\mathscr{M}=V_0(g)\oplus V_1(g)$ where, $V_0(g)=\{h\in T_g\mathscr{M};\mathrm{tr}(g^{-1}h)=0\}$ and $V_1(g)=C^\infty(M)g$; for an element $h\in S^2(M)$ we will represent by h_0 its traceless part, that is $h_0=h-(1/n)\ \mathrm{tr}(g^{-1}h)g$.

For each $c\in\mathbb{R}$, $c\neq 0$, a pointwise product is defined by the expression $\langle k,h\rangle_g^c=\mathrm{tr}(g^{-1}k_0g^{-1}h_0)+c\,\mathrm{tr}(g^{-1}k)\mathrm{tr}(g^{-1}h)$. We recover the usual pointwise product for $c=1/n$. By integration of the corresponding pointwise product, a weak pseudometric, G^c, is defined on $\mathscr{M}$; for $c>0$ it is in fact a metric.

In Ref. 7, Killing vector fields with respect to these pseudometrics have been studied. In Ref. 3 the pseudometrics G^c are extended to the space $\mathscr{B}$, of nondegenerate 2-times covariant tensor fields, and their Levi-Civita connection, geodesics, exponential mapping and curvature are calculated.

Proposition 3.1: Let $t\mapsto g(t)$ be a smooth curve in $\mathscr{M}$. It is a geodesic of the manifold $(\mathscr{M},G^c)$ if and only if

$$g''=g'g^{-1}g'-\frac{1}{2}\mathrm{tr}(g^{-1}g')g'+\frac{1}{4cn}\mathrm{tr}(g^{-1}g'g^{-1}g')g+\frac{cn-1}{4cn^2}\mathrm{tr}(g^{-1}g')^2g.$$

Therefore, the geodesic spray of G^c is given by

$$\Gamma^c(g,h)=hg^{-1}h-\frac{1}{2}\mathrm{tr}(g^{-1}h)h+\frac{1}{4cn}\langle h,h\rangle_g^c g.$$

Here g', g'', represent $(\partial/\partial t)g$ and $(\partial^2/\partial t^2)g$.

Proof: In Ref. 3 (Theorem 3.2) it is shown that the submanifold $\mathscr{M}$ of $\mathscr{B}$ is geodesically closed and then the geodesic equation is just the one appearing in 2.3 of Ref. 3. For the second assertion we have only to use the fact that $\Gamma^c(g,h)$ is the geodesic spray if and only if the geodesic equation is $g''=\Gamma^c(g,g')$, and the definition of $\langle,\rangle_g^c$. ■

Lemma 3.2: Let $F:\mathscr{M}\to\mathbb{R}$ be a Riemannian functional. Then, F admits G^c-gradient if and only if it admits G-gradient and both vector fields are related by

$$\mathrm{grad}^cF(g)=\mathrm{grad}F(g)-\frac{cn-1}{cn^2}\mathrm{tr}(g^{-1}\mathrm{grad}F(g))g.$$

Proof: By definition of the gradient,

$$G_g^c(\mathrm{grad}^c F(g),h)=(T_gF)(h)=G_g(\mathrm{grad}F(g),h).$$

Now, it is easy to see (Lemma 1.4 in Ref. 3) that the last member is equal to $G_g^c(\mathrm{grad}F(g)-[(cn-1)/cn^2](g^{-1}\mathrm{grad}F(g))g,h)$ from where the expression holds. ■

In the particular cases of the volume and total scalar curvature functionals, combining the above Lemma and formulae in Proposition 2.4 we obtain the following

Lemma 3.3:

(1) $\mathrm{grad}^c V(g)=(1/2cn)g$.

(2) $\mathrm{grad}^c S(g)=-\rho_0(g)+[(n-2)/2cn^2]\tau(g)g$.

For the G^c-gradient of a Riemannian functional, the same arguments used in 2.6 allow us to conclude that if δ_g^c represents the formal G^c-adjoint of the operator δ_g^* then, for every Riemannian functional F, we have $\delta_g^c(\mathrm{grad}^c F(g))=0$.

It is easy to see that the operator δ_g^c is given by $\delta_g^c(h)=\delta_g(h_0)-cd(\mathrm{tr}(g^{-1}h))$; in fact, using Lemma 1.4 of Ref. 3, we have

$$G_g^c(\delta_g^*(\omega),h)=G_g\left(\delta_g^*(\omega),h+\frac{cn-1}{n}\mathrm{tr}(g^{-1}h)g\right)=\left\langle \omega,\delta_g\left(h+\frac{cn-1}{n}\mathrm{tr}(g^{-1}h)g\right)\right\rangle_g,$$

for all $\omega\in\Lambda^1(M)$. Therefore $\delta_g^c(h)=\delta_g(h_0+c\,\mathrm{tr}(g^{-1}h)g)=\delta_g(h_0)-cd(\mathrm{tr}(g^{-1}h))$ and we have shown the following

Proposition 3.4: Let $\mathrm{grad}^c F$ *be the* G^c*-gradient of a Riemannian functional* F*; then, for each* $g\in\mathscr{M}$ *the tensor field* $(\mathrm{grad}^c F(g))_0+c\,\mathrm{tr}(g^{-1}(\mathrm{grad}^c F(g)))g$ *has vanishing* g*-divergence.*

Apart from the case $c=1/n$, the other distinguished member of the family of pseudometrics is the one corresponding to $c=(1-n)/n$; we will denote it by G^-. It is known as the DeWitt metric because it has been defined in Ref. 1, for the particular case $n=3$ and $c=-2/3$; for this case, the expression of the geodesic spray can be found there.

IV. RELATIONSHIP WITH THE $(n+1)$ GEOMETRY

In this section we study some generalizations of Theorem 1.1; let us start with a technical Lemma.

Lemma 4.1: Let g_t, $t\in I=(-\varepsilon,\varepsilon)$, *be a curve in the manifold* $\mathscr{M}$, *of metrics on* M, *and let* α *be a real number, different from* 0. *On the manifold* $N=I\times M$, *let us consider the pseudometric,* $\tilde{g}$, *defined in such a way that, in an adapted coordinate system, is given by*

$$\tilde{g}_{ij}(t,p)=(g_t)_{ij}(p);\quad \tilde{g}_{i0}\equiv 0;\quad \tilde{g}_{00}\equiv\alpha,$$

for each $i,j=1,\ldots,n$. *Then, Christoffel symbols of* $\tilde{g}$ *are given by*

$$\tilde{\Gamma}_{ij}^k(t,p)=(\Gamma^t)_{ij}^k(p),\quad \tilde{\Gamma}_{ij}^0(t,p)=\frac{-1}{2\alpha}(g_t')_{ij}(p),\quad \tilde{\Gamma}_{0j}^k(t,p)=\frac{1}{2}(g_t^{-1}g_t')_j^k(p),$$

$$\tilde{\Gamma}_{0j}^0(t,p)=\tilde{\Gamma}_{00}^k(t,p)=\tilde{\Gamma}_{00}^0(t,p)=0.$$

The components of the Ricci tensor are

$$\tilde{\rho}_{i0}(t,p)=\frac{-1}{2}\{(d\,\mathrm{tr}(g_t^{-1}g_t'))_i(p)+(\delta_t g_t')_i(p)\},$$

$$\tilde{\rho}_{00}(t,p)=\frac{-1}{2}\mathrm{tr}(g_t^{-1}g_t'')+\frac{1}{4}\mathrm{tr}(g_t^{-1}g_t'g_t^{-1}g_t'),$$

$$\widetilde{\rho}_{ij}(t,p)=\frac{-1}{2\alpha}(g_t'')_{ij}(p)+\frac{1}{2\alpha}(g_t'g_t^{-1}g_t')_{ij}(p)-\frac{1}{4\alpha}\mathrm{tr}(g_t^{-1}g_t')(g_t')_{ij}(p)+\rho_{ij}^t(p),$$

where, for simplicity, we have represented by $(\Gamma^t)_{ij}^k$, ρ_{ij}^t, δ_t, *the Christoffel symbols, the Ricci tensor and the divergence of* g_t, *respectively.*

Proof: Christoffel symbols are obtained by straightforward computation. Now, the components of Ricci tensor are given by

$$\widetilde{\rho}_{AB}=\sum_{C=0}^{n}\widetilde{R}_{ABC}^{C},$$

with

$$\widetilde{R}_{ABC}^{E}=(\widetilde{R}(\partial_B,\partial_C)\partial_A)^E=-\partial_B(\widetilde{\Gamma}_{CA}^E)+\partial_C(\widetilde{\Gamma}_{BA}^E)-\sum_{D=0}^{n}\widetilde{\Gamma}_{BD}^E\widetilde{\Gamma}_{CA}^D+\sum_{D=0}^{n}\widetilde{\Gamma}_{CD}^E\widetilde{\Gamma}_{BA}^D,$$

where $A,B,C,E\in\{0,1,\ldots,n\}$; see Ref. 8, p. 87.

The values of $\widetilde{\rho}_{ij}$ and $\widetilde{\rho}_{00}$ are obtained directly from the expressions above. It is easy to see that $\widetilde{R}_{i00}^0=0$ and then

$$\widetilde{\rho}_{i0}=\sum_{k=1}^{n}\widetilde{R}_{i0k}^{k}.$$

Therefore

$$\widetilde{\rho}_{i0}(t,p)=\frac{-1}{2}(d\mathrm{tr}(g_t^{-1}g_t'))_i(p)$$
$$+\frac{1}{2}\sum_k\left\{\partial_k(g_t^{-1}g_t')_i^k(p)-\sum_l(g_t^{-1}g_t')_k^l(\Gamma^t)_{il}^k(p)+\sum_l(g_t^{-1}g_t')_i^l(\Gamma^t)_{kl}^k(p)\right\}.$$

In order to finish the proof, we only need to show that for each metric g and each $h\in S^2(M)$,

$$\sum_k\left\{\partial_k(g^{-1}h)_i^k-\sum_l(g^{-1}h)_k^l\Gamma_{il}^k+\sum_l(g^{-1}h)_i^l\Gamma_{kl}^k\right\}=-(\delta_g(h))_i.$$

In fact

$$\sum_k\partial_k(g^{-1}h)_i^k=\sum_{k,l}g^{kl}\partial_k(h_{li})-\sum_{k,l,r,j}g^{kl}\partial_k(g_{lj})g^{jr}h_{ri},$$

and

$$\sum_{k,l}(g^{-1}h)_i^l\Gamma_{kl}^k=\frac{1}{2}\sum_{k,l,r,j}g^{lr}h_{ri}g^{kj}\partial_l(g_{jk}).$$

By adding the right-hand terms of both equalities we obtain

$$\sum_{k,l}g^{kl}\partial_k(h_{li})-\sum_{k,l,r}g^{kl}\Gamma_{lk}^r h_{ri},$$

and the result follows from the definition of the divergence. ■

Proposition 4.2: Let g_t, $\tilde{g}$, be as described in the previous Lemma. The first and second variations of the curve of metrics and the Ricci tensor of $\tilde{g}$ are related by

(1) $\tilde{\rho}_{i0}=-\frac{1}{2}(\delta_g^- g')_i$,

(2) $\tilde{\rho}_{00}=\alpha\mathrm{tr}(g^{-1}\tilde{\rho})-\alpha\tau-\frac{1}{4}\langle g',g'\rangle_g^c+\frac{n-1+cn}{4n}\mathrm{tr}(g^{-1}g')^2$,

(3) $$g''=-2\alpha\tilde{\rho}+\frac{n-2+2cn}{cn^2}(\alpha\mathrm{tr}(g^{-1}\tilde{\rho})-\tilde{\rho}_{00})g+\Gamma^c(g,g')-2\alpha\mathrm{grad}^c S(g)$$
$$-\frac{n-1+cn}{2cn^2}\left(\langle g',g'\rangle_g^c-\frac{n-2+2cn}{2}\mathrm{tr}(g^{-1}g')^2\right)g.$$

Proof: First equality is just the corresponding equality in Lemma 4.1, written in terms of the gradient operator associated to the DeWitt metric. For the second one we take the trace of g'' and then, we use the definition of $\langle,\rangle_g^c$.

Finally, the last equality can be obtained as follows: using Proposition 3.1, Lemma 3.3 and Lemma 4.1, it is easy to see that

$$g''=-2\alpha\tilde{\rho}+\Gamma^c(g,g')-2\alpha\mathrm{grad}^c S(g)+\left(\frac{n-2+2cn}{cn^2}\alpha\tau-\frac{1}{4cn}\langle g',g'\rangle_g^c\right)g.$$

To obtain the result we only need to change $\alpha\tau$ by its value obtained from (2). ■

Proposition 4.3: Let M be a compact, n-dimensional manifold and let g_t, $t\in I=(-\varepsilon,\varepsilon)$, be a curve in the manifold of metrics $\mathcal{M}$. Let $(N,\tilde{g})$ be the pseudoRiemannian $(n+1)$-manifold, where $N=I\times M$ and $\tilde{g}$ is defined in such a way that in an adapted chart,

$$\tilde{g}_{ij}(t,p)=(g_t)_{ij}(p);\quad \tilde{g}_{i0}\equiv 0;\quad \tilde{g}_{00}\equiv\alpha,$$

for each $i,j=1,\ldots,n$. Then $\tilde{g}$ is Ricci flat if and only if the curve satisfies the second order differential equation $g''=\Gamma^-(g,g')-2\alpha\mathrm{grad}^- S(g)$ together with the constraints $\delta_g^- g'=0$ and $\mathcal{H}(g,g'):=\frac{1}{2}\langle g',g'\rangle_g^- +2\alpha\tau(g)=0$.

Proof: Let us assume first that $\tilde{g}$ is Ricci flat. By (1) of 4.2, $\delta_g^- g'=0$ and if we take $c=[(1-n)/n]$ in (2), we also have the second constraint. The differential equation that the curve should satisfy comes from (3). The converse follows also immediately from the Proposition above. ■

Proposition 4.4: The DeWitt metric is the only metric, among those belonging to the one parameter family G^c, for which the above result holds. In fact if g_t, $t\in I=(-\varepsilon,\varepsilon)$, is a curve, in the manifold of metrics of a compact manifold, such that $\tilde{g}$ is Ricci flat and g_t satisfies

(1) $g''=\Gamma^c(g,g')-2\alpha\mathrm{grad}^c S(g)$ *and*

(2) $\frac{1}{2}\langle g',g'\rangle_g^c+2\alpha\tau(g)=0$,

for some $c\neq(1-n)/n$, then, $g_t=g_0$, for all t, and g_0 is Ricci flat.

Proof: Under the assumptions, equalities (2) and (3) of Proposition 4.2 become, respectively, $\mathrm{tr}(g^{-1}g')=0$ and $\langle g',g'\rangle_g^c-[(n-2+2cn)/2]\mathrm{tr}(g^{-1}g')^2=0$; so, $\mathrm{tr}(g^{-1}(g')_0 g^{-1}(g')_0)=0$ from where g' should vanish and the curve of metrics is constant to the initial value g_0. Now, from (1), the metric g_0 is a critical point of S and then it should be Ricci flat, provided the dimension of M is not 2. For a 2-dimensional manifold, a critical point of S has only $\rho_0=0$ and we have to use also (2) in order to conclude. ■

Proposition 4.5: Let g_t and $\tilde{g}$ be as described in Proposition 4.3. Then, the metric $\tilde{g}$ is Einstein with constant λ (i.e., $\tilde{\rho}=\lambda\tilde{g}$) if and only if the curve satisfies the second order differential

equation $g''=\Gamma^-(g,g')-2\alpha\operatorname{grad}^- S_\lambda(g)$ *together with the constraints* $\delta_g^- g'=0$ *and* $\mathscr{H}_\lambda(g,g'):=\frac{1}{2}\langle g',g'\rangle_g^- +2\alpha\tau^\lambda(g)=0$, where $\tau^\lambda(g)=\tau-\lambda(n-1)$ and $S_\lambda(g)=\int_M \tau^\lambda(g)\operatorname{vol}(g)$.

Proof: Let us assume first that $\tilde{\rho}=\lambda\tilde{g}$. By (1) of Proposition 4.2, $\delta_g^- g'=0$. If we take $c=(1-n)/n$ in (2), we have

$$\lambda\alpha=\lambda\alpha n-\alpha\tau-\frac{1}{4}\langle g',g'\rangle_g^-,$$

and so the second constraint. Now, equality (3) of Proposition 4.2 gives

$$g''=-\alpha\lambda g+\Gamma^-(g',g')-2\alpha\operatorname{grad}^- S(g);$$

the result follows from (1) of Lemma 3.3.

For the converse, equalities above imply that the components of the Ricci tensor of $\tilde{g}$ satisfy the following:

$$\tilde{\rho}_{00}=\alpha\operatorname{tr}(g^{-1}\tilde{\rho})-\lambda\alpha(n-1)$$

and

$$2\alpha\tilde{\rho}=\lambda\alpha g+\frac{1}{n-1}(\alpha\operatorname{tr}(g^{-1}\tilde{\rho})-\tilde{\rho}_{00})g.$$

As a consequence, $\tilde{\rho}=\lambda\tilde{g}$. ■

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Conditions on the stability of the external space solutions in a higher-dimensional quadratic theory of gravity

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By using Lyapounov's direct method we examine the conditions under which stable solutions to the field equations for the scale function of the external space may be derived in the context of a five-dimensional quadratic theory of gravity. We show that the time evolution of the distance, in a diagram $t-R$, between our solution to the field equations and a neighbouring one is determined, in the linear approximation, in terms of a second-order linear differential equation. Asking for bounded solutions of this equation we arrive at a stability criterion for the external scale function solutions, indicating that there exist three types of cosmological evolution of the visible universe which are linearly stable at all times. These are (i) the Milne model, (ii) the spatially flat Friedmann radiation solution, and (iii) the De Sitter inflationary solution. © *1996 American Institute of Physics.*
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I. INTRODUCTION

The idea that the space–time may have more than four dimensions has been extensively studied, as an attractive way to unify all gauge interactions with gravity, in a *supergravity* scenario[1–3] and in *superstring* theories.[4] In a realistic higher-dimensional theory the extra dimensions are assumed to form, at present, a compact manifold (*internal space*) of very small size compared to that of the visible universe (*external space*),[5–8] leading to the problem of *compactification*.[8] It has been suggested that compactification of the extra space may be achieved in a natural way by adding a square curvature term, $\mathrm{R}_{\mu\nu\kappa\lambda}\mathrm{R}^{\mu\nu\kappa\lambda}$, in the action for the gravitational field.[9,10]

Gravitational Lagrangians containing quadratic terms of the curvature tensor have been studied classically in the search of inflationary solutions[11,12] and solutions free from cosmological singularities.[13–17] However, they attracted the interest of cosmologists only after it became clear that when gravity is extracted by the low energy approximation of superstrings, an additional $\mathrm{R}_{\mu\nu\kappa\lambda}\mathrm{R}^{\mu\nu\kappa\lambda}$ term arises in the gravitational action.[18,19]

The introduction of a quadratic combination into the gravitational action leads to differential equations of the fourth order with respect to the metric.[20,21] There is one particular combination of the quadratic curvature terms[22,23] which, in connection to the linear Einstein–Hilbert (EH) term, yields second-order differential equations. We refer to it as the Gauss–Bonnett (GB) combination, since in four dimensions it satisfies the relation

$$\frac{\delta}{\delta g_{\mu\nu}}\int(\mathrm{R}^2-4\mathrm{R}_{\mu\nu}\mathrm{R}^{\mu\nu}+\mathrm{R}_{\mu\nu\kappa\lambda}\mathrm{R}^{\mu\nu\kappa\lambda})\sqrt{-g}\,d^4x=0 \tag{1.1}$$

corresponding to the GB theorem.[24] Equation (1.1) implies that the addition of the GB combination to the EH Largangian will not affect the four-dimensional field equations. Therefore, the resulting theory differs from general relativity (GR) only if the space–time has more than four dimensions and, probably, yields a natural generalization of GR in higher-dimensional space–times.

In the present paper we examine the conditions under which stable solutions to the field equations for the scale function of the external space may be obtained, in the context of a five-dimensional GB cosmology. We use Lyapounov's method[25] to determine the stability conditions in terms of an *isochronous correspondence*[26] between the curve $R_0(t)$, obtained from our solution to the field equations, and another one, $R(t)$, corresponding to a neighboring set of initial conditions. The distance between these two curves, $\chi(t)$, at each time, is given by

$$\chi(t)=R(t)-R_0(t). \tag{1.2}$$

In Sec. II we derive the explicit form of the field equations for a quadratic theory in five dimensions. In Sec. III we consider the case of a pressureless internal space. Then the field equations *decouple* and the solution for the external scale function (representing the evolution of the ordinary universe) can be found independently of the corresponding internal one. We express the cosmological field equation for $R(t)$ in terms of $\chi(t)$ and show that, in the linear approximation, its evolution is determined by a second-order linear differential equation with time-dependent coefficients. In this case, we examine the conditions under which the origin $\chi=0$ is stable. By Eq. (1.2), the stability properties of $R_0(t)$ are the same as those of the zero solution.[27] On general grounds concerning the stability of linear systems[25–27] the solution $\chi=0$ is stable, provided that every solution of the linear equation for $\chi(t)$ is bounded. Accordingly we arrive at a criterion which guarantees the boundness of the solutions $\chi(t)$ and, therefore, the stability of the zero solution $\chi=0$ as well. Some cosmological implications of these results are finally discussed in Sec. IV.

II. THE FIELD EQUATIONS

In a recent paper[28] we have considered a five-dimensional model with a homogeneous and isotropic, three-dimensional external space and a bounded one-dimensional internal space. The space–time metric is of the form

$$ds^2=-dt^2+R^2(t)\left[\frac{dr^2}{1-kr^2}+r^2(d\theta^2+\sin^2\theta\, d\phi^2)\right]+S^2(t)(dx^5)^2, \tag{2.1}$$

where $\hbar=1=c$, $R(t)$ and $S(t)$ are the cosmic scale functions of the external and the internal spaces, respectively, and $k=-1, 0, +1$ is the curvature parameter of the external space. This model may be obtained through Hamilton's principle, where the gravitational part of the action is of the form

$$I_{GR}=\frac{1}{L_5}\int\sqrt{-g}\left[\frac{1}{2\kappa}\mathbb{R}+\alpha(\mathbb{R}^2-4\mathbb{R}_{\mu\nu}\mathbb{R}^{\mu\nu}+\mathbb{R}_{\mu\nu\kappa\lambda}\mathbb{R}^{\mu\nu\kappa\lambda})\right]d^5x. \tag{2.2}$$

In Eq. (2.2) Greek indices refer to the five-dimensional space–time, $\kappa=8\pi G$, α is a dimensionless constant and $L_5=2\pi R_5$ is a normalization constant,[29] corresponding to the *physical size* of the internal space, once it can be considered static.[20] As far as the matter content is concerned, we have considered an anisotropic perfect fluid source, having an energy-momentum tensor of the form $T_{\mu\nu}=\mathrm{diag}(\varrho, -p_3, -p_3, -p_3, -p_5)$, where p_3 and p_5 are the pressures of the fluid for the external and the internal space, respectively, and ϱ is the total mass energy density. The corresponding field equations, in connection to the conservation law $T^{\mu\nu}{}_{;\nu}=0$, are decomposed into three independent equations[28] involving $R(t)$, $S(t)$, ϱ, p_3, and p_5:

$$3\frac{\dot R}{R}\frac{\dot S}{S}+3\left[\left(\frac{\dot R}{R}\right)^2+\frac{k}{R^2}\right]+12\eta\left[\left(\frac{\dot R}{R}\right)^2+\frac{k}{R^2}\right]\frac{\dot R}{R}\frac{\dot S}{S}=8\pi G_5\varrho, \tag{2.3a}$$

$$3\frac{\ddot{R}}{R}+3\left[\left(\frac{\dot{R}}{R}\right)^2+\frac{k}{R^2}\right]+12\eta\left[\left(\frac{\dot{R}}{R}\right)^2+\frac{k}{R^2}\right]\frac{\ddot{R}}{R}=-8\pi G_5 p_5, \tag{2.3b}$$

$$\frac{d\varrho}{dt}+3\frac{\dot{R}}{R}p_3+\frac{\dot{S}}{S}p_5+\left(3\frac{\dot{R}}{R}+\frac{\dot{S}}{S}\right)\varrho=0, \tag{2.3c}$$

where an overdot denotes derivative with respect to time, $\eta=16\pi G\alpha$ is a constant of dimensions T^2, and $G_5=GL_5$ is the five-dimensional gravitational constant.[30] The system of Eqs. (2.3), together with the two equations of state for the matter content (one for each subspace[31]), determine completely the evolution of the five-dimensional cosmological model. Its solution will give us the unknown scale functions of the two subspaces, $R(t)$ and $S(t)$, as well as the time evolution of the matter-energy density, $\varrho(t)$. It corresponds to a Cauchy problem which has solution only if $R\neq 0$ and $S\neq 0$, $\forall t$. Cauchy's criterion[32] implies that, for a given set of initial conditions, the solution is unique, provided

$$1+4\eta W\neq 0, \quad \forall t, \tag{2.4}$$

where W stands for the combination[28]

$$W=\left(\frac{\dot{R}}{R}\right)^2+\frac{k}{R^2}=-\frac{1}{4\eta}\left[1\mp\sqrt{1-\left(\frac{R_m}{R}\right)^4}\right]. \tag{2.5}$$

In Eq. (2.5) R_m is the lowest bound of $R(t)$ for which we obtain physically acceptable solutions within the context of the quadratic theory under consideration.[28] Then, combination of Eqs. (2.4) and (2.5) indicates that $R(t)>R_m$, $\forall t$. For a monotonicaly increasing function $R(t)$, we have $R(t)>R_m$ when $t>t_m(t_m>0)$.

As in Ref. 28, we consider models of an already compactified internal space.[28,31,33] Compactification is a topological process of quantum origin, leading to the separation of the extra dimensions from the ordinary ones.[30] Therefore, we study only the process of contraction of the internal space, which may be understood by the classical equations of motion. Clearly, the contraction of the internal space presupposes the separation of the extra dimensions from the ordinary ones and starts immediately after compactification.

III. CONDITIONS ON THE STABILITY OF THE EXTERNAL SPACE SOLUTIONS

When the equations of state for the matter content in the two subspaces are determined, Eq. (2.3c) may be readily solved to give $\varrho(t)$ in terms of $R(t)$ and $S(t)$. Then, in order to determine the evolution of the five-dimensional model, one has to solve the self-consistent system of coupled Eqs. (2.3a) and (2.3b). As equation of state in the internal space, we choose $p_5=0$. It corresponds to an internal matter content in the form of dust, indicating the absence of motion along the extra dimension. This equation of state may represent successfully the later stages of the cosmological evolution in a five-dimensional theory of gravity, where the physical size of the internal space is very small.[33–35]

Now, the field equations (2.3a) and (2.3b) *decouple*. Each of them corresponds to a differential equation of only one scale function. Indeed, in this case Eq. (2.3b) has the first integral[28]

$$R^4\left[\left(\frac{\dot{R}}{R}\right)^2+\frac{k}{R^2}\right]+2\eta R^4\left[\left(\frac{\dot{R}}{R}\right)^2+\frac{k}{R^2}\right]^2=\text{const.} \tag{3.1}$$

Its solution will give the explicit time dependence of $R(t)$. Accordingly, Eq. (2.3a) becomes a differential equation of $S(t)$ with time-dependent coefficients, resulting in this form through the solution of Eq. (3.1).[32] Therefore, we end up with a problem involving the description of two

subspaces, where the evolution of each space obeys an ordinary differential field equation of time only. In this sense, the expansion of the visible universe, through Eq. (2.3b), does not depend on the evolution of the internal space. This result has a clear physical meaning:[28] The two subspaces are completely disjoint. This is not unexpected, since we have considered a cosmological model *after* the compactification process, which implies the separation of the extra dimensions from the ordinary ones. The external space will evolve according to Eq. (2.3b) independently on the time behavior of the internal one.

In this case, we examine the *stability* of the solutions of the self-consistent equation (2.3b) by using Lyapounov's direct method.[25] The solutions represent the time evolution of the visible universe and we would like to know under which conditions a stable solution at all times may be obtained, within the context of the quadratic theory under consideration. The question that arises now is, which solutions are considered stable at all times.

Let us denote by $R_0(t)$ the solution to Eq. (2.3b), whose stability is under consideration, and by $R(t)$ any other solution of it. Equation (2.3b), with the aid of Eq. (2.5), may be expressed in the form

$$\ddot{R}=-\frac{R}{4\eta}\left[1\mp\frac{1}{\sqrt{1-z}}\right], \tag{3.2}$$

where we have set $z=(R_m/R)$.[4] Clearly, by virtue of Eqs. (2.4) and (2.5), $z<1\forall t$. The distance, at each time, between the two corresponding curves $R(t)$ and $R_0(t)$ in a diagram $t-R$ is given by Eq. (1.2). We write Eq. (3.2) in terms of $\chi(t)$ and study its evolution in time. In this case, $\chi(t)$ actually represents a perturbation of the original solution, $R_0(t)$. We will examine the evolution of a small $\chi(t)$, since the question of stability is whether such small disturbances grow or not.[25–27]

We consider the linear stability of the resulting equation around the origin $\chi=0$, which corresponds to $R(t)=R_0(t),\forall t$.[25,27] If the zero solution $\chi=0$ is linearly stable, so is the evolution of the external space, since $R(t)$ remains *near* $R_0(t)$ at all times.[25,27,36] This is true only for smooth functions of time, i.e., functions for which $|\dot{R}(t)|<\infty,\forall t$. Equation (3.2), in linear terms of χ, may be written in the form[37]

$$\ddot{\chi}=-\frac{1}{4\eta}\chi\left[1\mp\frac{1-3z_0}{(1-z_0)^{3/2}}\right], \tag{3.3}$$

where $z_0=(R_m/R_0)$.[4] Since $R_0(t)$ is assumed known, Eq. (3.3) is a linear second-order differential equation for $\chi(t)$, with time-dependent coefficients. It is more convenient to write the function in the square brackets on the rhs of Eq. (3.3) in terms of a hypergeometric series, thus obtaining[38,39]

$$\ddot{\chi}=-\frac{1}{4\eta}\chi[1\mp{}_2F_1(\tfrac{1}{2},\tfrac{3}{4};-\tfrac{1}{4};z_0)]. \tag{3.4}$$

This is a choice to be justified by the subsequent analysis. We consider the case where η is positive ($\eta>0$) and we substitute $\xi=at$, where $a^2=(2\eta)^{-1}$. Then Eq. (3.4) can be cast into the form

$$\frac{d^2}{d\xi^2}\chi(\xi)+[1-\epsilon(\xi)]\chi(\xi)=0, \tag{3.5}$$

where

$$\epsilon(\xi)=\tfrac{1}{2}[1\pm{}_2F_1(\tfrac{1}{2},\tfrac{3}{4};-\tfrac{1}{4};z_0)]. \tag{3.6}$$

According to a general theorem on the stability property of linear systems,[25–27] the zero solution of Eq. (3.5) is stable for $\xi \geqslant \xi_{in}$ provided that every solution of this equation is *bounded*.[27] The constant value $\xi_{in}=at_{in}$ corresponds to the initial time, which, for every monotonically expanding solution $R_0(t)$, satisfies the condition[28] $t_{in}>t_m$.

By Eq. (1.2), the stability properties of $R_0(t)$ are the same as those of the zero solution of Eq. (3.5). Therefore, in order to determine the conditions under which a particular solution $R_0(t)$ is linearly stable at all times $t \geqslant t_{in}$, we have to investigate under which conditions Eq. (3.5) possesses bounded solutions inside the interval $[\xi_{in},\infty)$. Solutions of Eq. (3.5) exist[36,40] and can be put in the formal form[36]

$$\chi(\xi)=e^{i\xi}[1+h(\xi)]. \tag{3.7}$$

To guarantee the boundness of $\chi(\xi)$ we have to determine only the conditions under which $h(\xi)$ is finite, since the first term on the rhs of Eq. (3.7) is bounded for every $\xi \geqslant \xi_{in}$. Thus, the problem of determining the stability conditions of the external space solutions has now been reduced to the determination of the conditions under which the function $h(\xi)$ is bounded. To derive the functional form of $h(\xi)$, we combine Eqs. (3.5) and (3.7), obtaining

$$h''(\xi)+2ih'(\xi)-\varepsilon(\xi)h(\xi)=\varepsilon(\xi), \tag{3.8}$$

where a prime denotes differentiation with respect to ξ. Now, to solve this inhomogeneous differential equation for $h(\xi)$, we apply the method of *variation of parameters*.[36,38] The result may be written as an integral equation of Volterra's type[41]

$$h(\xi)=\frac{1}{2i}\int_{\xi_{in}}^{\xi}(1-e^{2i(\zeta-\xi)})\varepsilon(\zeta)[1+h(\zeta)]d\zeta. \tag{3.9}$$

Conversely, it can be verified by differentiation that any twice-differentiable solution of Eq. (3.9) satisfies Eq. (3.8). The general solution of Eq. (3.9) may be obtained in the form of a uniformly convergent series.[36] Accordingly, we define a sequence $h_s(\xi)$ $(s=0,1,2,...)$, with $h_0(\xi)=0$ and

$$h_s(\xi)=\frac{1}{2i}\int_{\xi_{in}}^{\xi}(1-e^{2i(\zeta-\xi)})\varepsilon(\zeta)[1+h_{s-1}(\zeta)]d\zeta \quad (s\geqslant 1), \tag{3.10}$$

where, in particular,

$$h_1(\xi)=\frac{1}{2i}\int_{\xi_{in}}^{\xi}(1-e^{2i(\zeta-\xi)})\varepsilon(\zeta)d\zeta. \tag{3.11}$$

Since $|1-e^{2i(\zeta-\xi)}|\leqslant 2$ we obtain $|h_1(\xi)|\leqslant\Psi(\xi)$, where

$$\Psi(\xi)=\int_{\xi_{in}}^{\xi}|\varepsilon(\zeta)|d\zeta \tag{3.12}$$

and the equality in Eq. (3.12) occurs when $\xi=\xi_{in}$. Then, by induction we find that the relation

$$|h_s(\xi)-h_{s-1}(\xi)|\leqslant\frac{\Psi^s(\xi)}{s!} \tag{3.13}$$

holds, for all s. Now, as long as $\Psi(\xi)$ is bounded, the series

$$h(\xi)=\sum_{s=0}^{\infty}[h_{s+1}(\xi)-h_s(\xi)] \tag{3.14}$$

satisfies the Weierstrass criterion and converges absolutely and uniformly.[36,39] Then, by summation of Eq. (3.14) and use of Eqs. (3.10) and (3.11), we verify that $h(\xi)$ satisfies the integral equation (3.9).

Therefore, Eq. (3.9) [and hence Eq. (3.8) also] admits bounded solutions, $h(\xi)$, such that

$$|h(\xi)|\leqslant e^{\Psi(\xi)}-1 \tag{3.15}$$

as results with the aid of Eq. (3.13). In this case, from Eq. (3.7) we obtain

$$|\chi(\xi)|\leqslant e^{\Psi(\xi)}. \tag{3.16}$$

Equation (3.16) indicates that a *bounded* function $\chi(\xi)$ exists for every $\xi\geqslant\xi_{in}$ if the integral $\Psi(\xi)$ converges in the corresponding time interval. Then, the origin $\chi=0$ is stable. The result guarantees the linear stability of the external space solutions, $R_0(t)$. To determine their stability properties at all times $t\geqslant t_{in}$, we need to investigate the conditions under which $\Psi(\xi)$ converges as $\xi\to\infty$:

$$\Psi=\int_{\xi_{in}}^{\infty}|\varepsilon(\xi)|d\xi<\infty. \tag{3.17}$$

According to the preceding analysis, Eq. (3.17) provides a criterion for the linear stability of the cosmological solutions $R_0(t)$ at all times, once the equation for the perturbation $\chi(t)$ is written in the form (3.5). The question that arises now is, under which conditions this criterion may be applied in our case, where Eq. (3.17) has the form

$$\Psi=\frac{1}{2}\int_{\xi_{in}}^{\infty}\left|1\pm{}_2F_1\left(\frac{1}{2},\frac{3}{4};-\frac{1}{4};z_0\right)\right|d\xi. \tag{3.18}$$

Having the minus sign on the rhs of Eq. (3.18), we obtain

$$\Psi=\frac{1}{2}\int_{\xi_{in}}^{\infty}\left[1-{}_2F_1\left(\frac{1}{2},\frac{3}{4};-\frac{1}{4};z_0\right)\right]d\xi \tag{3.19}$$

since the integrant in Eq. (3.19) is positive.[38,42] We normalize $R_0(\xi)$ as $R_N(\xi)=R_0(\xi)/R_m$ to obtain $z_0=1/R_N^4(\xi)$, where $R_N(\xi)$ simply measures $R_0(\xi)$ in units of R_m. Now, we expand the hypergeometric series involved, in terms of $R_N(\xi)$, to obtain

$$\Psi=\frac{2}{\sqrt{\pi}}\sum_{n=1}^{\infty}\left(n-\frac{1}{4}\right)\frac{\Gamma(n+\frac{1}{2})}{\Gamma(n+1)}\int_{\xi_{in}}^{\infty}\frac{1}{R_N^{4n}(\xi)}\,d\xi. \tag{3.20}$$

We will examine the stability of the monotonically increasing solutions for the external space, in connection to the cosmological observations at the present epoch. For this kind of cosmological evolution we have $\xi_{in}>\xi_m$ within the context of the quadratic theory under consideration.[28] In particular, we consider two different types of evolution.

(i) Power law solutions of the form

$$R_N(\xi)\sim\left(\frac{\xi}{\xi_m}\right)^{\lambda}. \tag{3.21}$$

Cosmological models of this form have been widely obtained in the context of the GB cosmology, either as exact solutions or as approximate ones.[16,20,28,33] Inserting Eq. (3.21) into (3.20), for $\lambda \neq \frac{1}{4}$, we obtain

$$\Psi = -\frac{2}{\sqrt{\pi}} \sum_{n=1}^{\infty} \frac{(4n-1)}{(4n\lambda-1)} \frac{\Gamma(n+\frac{1}{2})}{\Gamma(n+1)} \left(\frac{\xi_m}{\xi}\right)^{4n\lambda-1} \Bigg|_{\xi_{in}}^{\infty}. \tag{3.22}$$

As long as $\lambda > \frac{1}{4}$, the rhs of Eq. (3.22) is finite and positive. Indeed, in this case, Eq. (3.22) results in the infinite series form

$$\Psi = \frac{2}{\sqrt{\pi}} \sum_{n=1}^{\infty} \frac{(4n-1)}{(4n\lambda-1)} \frac{\Gamma(n+\frac{1}{2})}{\Gamma(n+1)} \left(\frac{\xi_m}{\xi_{in}}\right)^{4n\lambda-1}, \tag{3.23}$$

which, since $\xi_{in} > \xi_m$ converges absolutely. Therefore, the external space solutions of the form (3.21) with $\lambda > \frac{1}{4}$ satisfy the stability criterion (3.17) and, hence, they may be characterized as linearly stable at all times.

Some models of the form (3.21) have been obtained as solutions of Eq. (2.3b) for the external space, in the context of the five-dimensional GB cosmology under consideration.[28] These are (a) the Milne model ($\lambda=1$) in the zeroth-order approximation, for $k=-1$ and (b) the Friedmann radiation model ($\lambda=\frac{1}{2}$) in the first-order approximation for $k=0$. Both models have been obtained also as solutions in the EH cosmology. The fact that they result as solutions of the quadratic theory, as well, is very important, since, in this way, their linear stability is guaranteed through the criterion (3.17).

(ii) Exponential solutions of the form

$$R_N(\xi) \sim e^{\alpha\xi} \quad (\alpha > 0). \tag{3.24}$$

The models are linearly stable at all times, even after relaxing the condition $\xi_{in} > \xi_m$. Indeed, for every $\xi > 0$, integration of Eq. (3.20) gives

$$\Psi = \frac{2}{\sqrt{\pi}} \sum_{n=1}^{\infty} \frac{(4n-1)}{4n} \frac{\Gamma(n+\frac{1}{2})}{\Gamma(n+1)} e^{-4\alpha n \xi_{in}}, \tag{3.25}$$

which, since α, $\xi_{in} > 0$, converges absolutely. These models are obtained as solutions of the quadratic theory under consideration in the zeroth-order approximation,[28] for $k=0$. The result that they are linearly stable is in complete agreement with the fact that the De Sitter universe is an "*attractor*" of the GB cosmology.[11,12,30,43–46]

IV. DISCUSSION AND CONCLUSIONS

In the present paper we have examined under which conditions a stable solution for the external space (representing the evolution of the visible universe) may be obtained, in the context of a five-dimensional GB cosmology. We have considered $p_5=0$ in connection to cosmological models of an already compactified internal space; that is, we have studied only the process of contraction of the internal space, which may be understood by the classical equations of motion and starts immediately after compactification. In this case, the two subspaces are completely disjoint and the field equations decouple.

Since the two subspaces are disjoint, we have used Lyapounov's direct method[25–27] to find a criterion which guarantees the linear stability of the external space solutions. Investigation of the stability properties of the external space is very important, since it could lead to the determination of preferable solutions for the visible universe.

According to the theory of cosmological perturbations,[47] instabilities in the energy density may arise due to quantum phenomena at the Planck energy scale. These instabilities could affect the set of the initial conditions of a classical space-time, which emerges out of the Planck epoch, modifying its time evolution. In this case, we would like to know if the perturbed behavior of the visible universe differs from the unperturbed one by an acceptably small amount. If there exists a particular solution for which this is true, then every other physically acceptable solution, which may arise due to changes in the set of the initial conditions, will remain close to this particular one at all times. The changes in the initial conditions, it does not matter how, may be arbitrary and hence a stable model acts as an "*attractor.*" Now, if some special solution is the attractor for a wide range of initial conditions, such a solution is naturally realized asymptotically.[33]

Therefore, we have perturbed our original solution $R_0(t)$ by a small amount $\chi(t)$ and we have examined whether this perturbation grows in time or not. In linear terms, its time evolution is determined by the second-order linear differential equation (3.3). Now, if the zero solution, $\chi=0$, of this equation is stable, then every solution $R(t)$ remains "*near*" $R_0(t)$ at all times. The solution $\chi=0$ is stable, provided that every solution of Eq. (3.3) is bounded. It has been verified that the boundness of the solutions, at all times, is guaranteed by the convergence of the integral (3.17) as $t\to\infty$. Accordingly, Eq. (3.17) may be considered as a criterion which determines under which conditions stable solutions for the external space are possible or not.

Under some restrictions on the free parameters involved, this criterion is satisfied by three types of cosmological evolution obtained in the context of the quadratic theory under consideration: (i) the Milne universe, (ii) the Friedmann radiation model with $k=0$, and (iii) the inflationary De Sitter solution. Each of these models may arise as a natural candidate to describe the evolution of the visible space. Indeed, it has been found numerically that the De Sitter solution corresponds to an *attractor* of the GB cosmology,[43,46] while a similar result seems to hold also for the spatially flat Friedmann radiation solution.[48]

It is probable that, if one of these models determines the evolution of the ordinary space in a quadratic theory with $\eta>0$, every unpredictable instability[47] will affect only the dynamics of the one-dimensional internal space, leaving the external one unaltered. Consequently, to consider a quadratic higher-dimensional theory of gravity may be of great use in the theoretical establishment of the stability properties for the visible space and its observational characteristics, at least as regards some particular solutions.

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Inhomogeneous Kasner-type cylindrically symmetric models in Kaluza–Klein space–time

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We consider a cylindrically symmetric metric separable in space and time variables having Kasnerian time dependence in the Kaluza–Klein space–time. We obtain perfect fluid models that admit the dimensional reduction yielding the usual four-dimensional space–time as the universe expands. The models are inhomogeneous and they have the Kasnerian vacuum solution as their matter-free limit. The five-dimensional Kasnerian vacuum solution goes over on dimensional reduction to the radiation Friedman–Robertson–Walker flat model. © *1996 American Institute of Physics.* [S0022-2488(96)00707-4]

I. INTRODUCTION

The consideration of cosmological models in higher dimensions has recently attracted the attention of many workers. The main motivation for this has been the early universe physics and cosmology. The extra dimensions are supposed to be relevant only at the scale of Planck length and as the universe expands the extra dimensions contract, leaving behind the observable four-dimensional (4–d) space–time. The work was initiated in this direction in the late 1980s.[1,2] To begin with, 5-d Kasnerian vacuum solutions were obtained[2] in which the extra fifth dimension shrank as the universe expanded.

In the early stages of evolution, it is expected that the universe will be inhomogeneous to allow for generic initial conditions and formation of large scale structures in the universe. This is why inhomogeneous solutions of Einstein equations have been considered by several authors.[3–10] Amongst them there exists a very interesting family of nonsingular cosmological models satisfying the strong energy condition $\rho+3p\geqslant 0$ with physically acceptable equations of state $\rho=3p$ and $\rho=p$.[8,9] Inhomogeneous cosmological models have also been considered in the 5-d Kaluza–Klein space–time.[11–15] Very recently Banerjee *et al.*[15] obtained the 5-d nonsingular solutions for stiff fluid and vacuum obtained by Dadhich *et al.*[9]

In this paper we wish to study the 5-d cylindrically symmetric cosmological models that have the Kasnerian time dependence[16] which reduce to the usual 4-d universe as the expansion proceeds. The time dependence in the metric will be given by powers of the cosmic time t and space dependence by powers of $(1+r^2)$. In the nonsingular metric,[8,9] the space dependence is given by $\cosh r$, which is equivalent to $(1+r^2)$. We shall thus obtain the 5-d Davidson-type[3] inhomogeneous cylindrical models.

In Sec. II we list the Ricci tensor for the general cylindrically symmetric metric and set up the field equations. The exact solutions of the equations with the above prescription for the metric are discussed in Secs. III and IV, followed by discussion.

II. THE METRIC AND THE FIELD EQUATIONS

We consider the five-dimensional cylindrically symmetric space–time given by the line element

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$$ds^2=D^2dt^2-A^2dr^2-B^2dz^2-C^2d\varphi^2-E^2d\psi^2, \tag{2.1}$$

where A, B, C, D, and E are functions of the radial coordinate r and the time t. Here ψ is the extra dimension.

Introducing the pentad

$$\theta^1=Adr, \quad \theta^2=Bdz, \quad \theta^3=Cd\varphi, \quad \theta^4=Ed\psi, \quad \theta^5=Ddt, \tag{2.2}$$

we can express the metric (2.1) in the form

$$ds^2=(\theta^5)^2-(\theta^1)^2-(\theta^2)^2-(\theta^3)^2-(\theta^4)^2=g_{(ab)}\theta^a\theta^b. \tag{2.3}$$

Here and in what follows the bracketed indices denote pentad components. The surviving $R_{(ab)}$ for the metric (2.1) are listed below for ready reference:

$$R_{(15)}=\frac{1}{AD}\left[\frac{\dot{B}'}{B}+\frac{\dot{C}'}{C}+\frac{\dot{E}'}{E}-\frac{\dot{A}}{A}\left(\frac{B'}{B}+\frac{C'}{C}+\frac{E'}{E}\right)-\frac{D'}{D}\left(\frac{\dot{B}}{B}+\frac{\dot{C}}{C}+\frac{\dot{E}}{E}\right)\right], \tag{2.4}$$

$$R_{(11)}=\frac{1}{A^2}\left[\frac{B''}{B}+\frac{C''}{C}+\frac{D''}{D}+\frac{E''}{E}-\frac{A'}{A}\left(\frac{B'}{B}+\frac{C'}{C}+\frac{D'}{D}+\frac{E'}{E}\right)\right]$$
$$-\frac{1}{D^2}\left[\frac{\ddot{A}}{A}+\frac{\dot{A}}{A}\left(\frac{\dot{B}}{B}+\frac{\dot{C}}{C}+\frac{\dot{E}}{E}-\frac{\dot{D}}{D}\right)\right], \tag{2.5}$$

$$R_{(22)}=\frac{1}{A^2}\left[\frac{B''}{B}+\frac{B'}{B}\left(\frac{C'}{C}+\frac{D'}{D}+\frac{E'}{E}-\frac{A'}{A}\right)\right]-\frac{1}{D^2}\left[\frac{\ddot{B}}{B}+\frac{\dot{B}}{B}\left(\frac{\dot{A}}{A}+\frac{\dot{C}}{C}+\frac{\dot{E}}{E}-\frac{\dot{D}}{D}\right)\right], \tag{2.6}$$

$$R_{(33)}=\frac{1}{A^2}\left[\frac{C''}{C}+\frac{C'}{C}\left(\frac{B'}{B}+\frac{D'}{D}+\frac{E'}{E}-\frac{A'}{A}\right)\right]-\frac{1}{D^2}\left[\frac{\ddot{C}}{C}+\frac{\dot{C}}{C}\left(\frac{\dot{A}}{A}+\frac{\dot{B}}{B}+\frac{\dot{E}}{E}-\frac{\dot{D}}{D}\right)\right], \tag{2.7}$$

$$R_{(44)}=\frac{1}{A^2}\left[\frac{E''}{E}+\frac{E'}{E}\left(\frac{B'}{B}+\frac{D'}{D}+\frac{C'}{C}-\frac{A'}{A}\right)\right]-\frac{1}{D^2}\left[\frac{\ddot{E}}{E}+\frac{\dot{E}}{E}\left(\frac{\dot{A}}{A}+\frac{\dot{B}}{B}+\frac{\dot{C}}{C}-\frac{\dot{D}}{D}\right)\right], \tag{2.8}$$

$$R_{(55)}=\frac{1}{D^2}\left[\frac{\ddot{A}}{A}+\frac{\ddot{B}}{B}+\frac{\ddot{C}}{C}+\frac{\ddot{E}}{E}-\frac{\dot{D}}{D}\left(\frac{\dot{A}}{A}+\frac{\dot{B}}{B}+\frac{\dot{C}}{C}+\frac{\dot{E}}{E}\right)\right]-\frac{1}{A^2}\left[\frac{D''}{D}+\frac{D'}{D}\left(\frac{B'}{B}+\frac{C'}{C}+\frac{E'}{E}-\frac{A'}{A}\right)\right]. \tag{2.9}$$

Here and in what follows an overhead dash and a dot indicate differentiation with respect to r and t, respectively. Here ψ is taken in the form of a Kaluza–Klein (KK) parameter such that $0\leqslant\psi\leqslant 2\pi R_5$, where R_5 is the radius of KK circle.

We assume that the space–time is filled with a perfect fluid distribution described by

$$T_{ik}=(p+\rho)v_iv_k-pg_{ik}, \quad v_iv^i=1, \tag{2.10}$$

where ρ, p, and v^i stand for the energy density, the pressure, and the unit timelike flow vector, respectively.

The Einstein field equations are

$$R_{ik}-\tfrac{1}{2}Rg_{ik}=-8\pi T_{ik}, \tag{2.11}$$

and hence we write

$$R_{(ab)}=-8\pi[(p+\rho)v_{(a)}v_{(b)}-\tfrac{1}{3}(\rho-p)g_{(ab)}]. \tag{2.12}$$

We use comoving coordinates. Therefore we have

$$v_{(a)}=(0,0,0,0,1). \tag{2.13}$$

In view of (2.13), the field equations (2.12) give rise to the following relations:

$$R_{(15)}=0, \tag{2.14}$$

$$R_{(11)}=R_{(22)}=R_{(33)}=R_{(44)}, \tag{2.15}$$

$$8\pi\rho=-\tfrac{1}{2}[R_{(55)}+4R_{(22)}], \tag{2.16}$$

$$8\pi p=\tfrac{1}{2}[2R_{(22)}-R_{(55)}]. \tag{2.17}$$

III. PERFECT FLUID MODELS

As stated in the Introduction, we write for A, B, C, D, and E:

$$A=t^{\alpha}(1+r^2)^a,\quad B=t^{\beta}(1+r^2)^b,\quad C=rt^{\gamma}(1+r^2)^c,\quad D=(1+r^2)^d,\quad E=t^{\delta}(1+r^2)^e, \tag{3.1}$$

where a, b, c, d, e, α, β, γ, and δ are real constants. Time dependence in the function D is not included because such a dependence can always be removed by redefining the time coordinate.

Let us first consider the equation (2.14). Using (3.1) and (2.14) we obtain

$$\alpha=\gamma \tag{3.2}$$

and

$$\beta(b-d)+\delta(e-d)-\alpha(b+e+d)=0. \tag{3.3}$$

The equation $R_{(22)}=R_{(44)}$ of (2.15) implies

$$b=e \tag{3.4}$$

and

$$2\alpha+\beta+\delta=1. \tag{3.5}$$

On the other hand, $R_{(22)}=R_{(11)}$ of (2.15) leads to

$$a=3c+d \tag{3.6}$$

and

$$b+c+d+2c^2+4cd+4bc+2bd=0. \tag{3.7}$$

Lastly, the remaining equation $R_{(22)}=R_{(33)}$ of (2.15) leads to one more restriction,

$$(b-c)[2(b-c)-1]=0. \tag{3.8}$$

In view of (3.1), (2.16) and (2.17) determine ρ and p as

$$16\pi\rho=\frac{1}{D^2t^2}\left[1-(2\alpha^2+\beta^2+\delta^2)\right]-\frac{4(4b-d)}{A^2(1+r^2)^2}\left[1+2r^2(b-c)\right] \tag{3.9}$$

and

$$16\pi p=\frac{1}{D^2t^2}\left[1-(2\alpha^2+\beta^2+\delta^2)\right]+\frac{4(2b+d)}{A^2(1+r^2)^2}\left[1+2r^2(b-c)\right], \tag{3.10}$$

where A and D are given by (3.1).

The equation (3.8) gives rise to two separate cases: *case (i):* $b=c$ and *case (ii):* $b=c+\frac{1}{2}$. We now discuss them separately.

Case (i): $b=c$. In this case the constants a, c, d, e, and α can be expressed in terms of b. Using (3.2)–(3.7) we have

$$a=\frac{b(1+12b)}{1+6b},\quad c=b,\quad d=-\frac{2b(1+3b)}{(1+6b)},\quad e=b,\quad \alpha=\gamma=\frac{(1+4b)}{2(1+5b)}, \tag{3.11}$$

and

$$\beta+\delta+\frac{(1+4b)}{(1+5b)}=1. \tag{3.12}$$

The density ρ and the pressure p for this case are given by

$$16\pi\rho=\frac{1}{D^2t^2}\left\{1-(2\alpha^2+\beta^2+\delta^2)\right\}-\frac{24b(1+5b)}{(1+6b)A^2(1+r^2)^2} \tag{3.13}$$

and

$$16\pi p=\frac{1}{D^2t^2}\left\{1-(2\alpha^2+\beta^2+\delta^2)\right\}+\frac{24b^2}{(1+6b)A^2(1+r^2)^2}, \tag{3.14}$$

where

$$D=(1+r^2)^{-2b(1+3b)/(1+6b)},\quad A=t^{(1+4b)/2(1+5b)}(1+r^2)^{b(1+12b)/(1+6b)}. \tag{3.15}$$

The physical requirements $\rho\geq 0$ and $p\geq 0$ are satisfied if

$$-\frac{1}{6}<b\leq 0,\quad 2\alpha^2+\beta^2+\delta^2\leq 1. \tag{3.16}$$

Here ρ and p are decreasing functions of r and t and they tend to zero as r and/or t tend to infinity. The geometry of the five-dimensional cylindrical universe is described by the line element

$$\begin{aligned} ds^2=&(1+r^2)^{-4b(1+3b)/(1+6b)}dt^2-(1+r^2)^{2b(1+12b)/(1+6b)}t^{(1+4b)/(1+5b)}dr^2\\ &-(1+r^2)^{2b}[t^{2\beta}dz^2+r^2t^{(1+4b)/(1+5b)}d\varphi^2+t^{2\delta}d\psi^2], \end{aligned} \tag{3.17}$$

where β and δ are related by (3.12).

Case (ii): $b=c+\frac{1}{2}$. For this case we have

$$a=\frac{20b-24b^2-3}{2(1-6b)},\quad c=b-\frac{1}{2},\quad d=\frac{2b(3b-1)}{(1-6b)},\quad e=b,\quad \gamma=\alpha=\frac{(1-4b)}{2(1-5b)}, \tag{3.18}$$

$$\beta+\delta+\frac{(1-4b)}{(1-5b)}=1, \tag{3.19}$$

$$16\pi\rho=\frac{1}{D^2t^2}\{1-(2\alpha^2+\beta^2+\delta^2)\}-\frac{24b(1-5b)}{(1-6b)A^2(1+r^2)}, \tag{3.20}$$

and

$$16\pi p=\frac{1}{D^2t^2}\{1-(2\alpha^2+\beta^2+\delta^2)\}-\frac{24b^2}{(1-6b)A^2(1+r^2)}, \tag{3.21}$$

where

$$D=(1+r^2)^{2b(3b-1)/(1-6b)}, \quad A=(1+r^2)^{(20b-24b^2-3)/2(1-6b)}t^{(1-4b)/2(1-5b)}. \tag{3.22}$$

The physical requirements $\rho\geqslant 0$ and $p\geqslant 0$ give rise to the inequalities

$$0\leqslant b<\tfrac{1}{5}, \quad 2\alpha^2+\beta^2+\delta^2\leqslant 1. \tag{3.23}$$

The metric is given by

$$ds^2=(1+r^2)^{4b(3b-1)/(1-6b)}dt^2-(1+r^2)^{(20b-24b^2-3)/(1-6b)}t^{(1-4b)/(1-5b)}dr^2$$
$$-(1+r^2)^{2b}\left[t^{2\beta}dz^2+\frac{r^2}{(1+r^2)}t^{(1-4b)/(1-5b)}d\varphi^2+t^{2\delta}d\psi^2\right], \tag{3.24}$$

where β and δ are related by (3.19).

Note that one of the Kasnerian constraints $\alpha+\beta+\gamma+\delta=1$ is always satisfied in both the cases considered above. We, however, have two-parameter arbitrariness in choosing b and one of β and δ. This is quite interesting. For dimensional reduction $\delta<0$, which can always be so chosen. That is, all the models described by (3.1) will always permit the dimensional reduction.

IV. PARTICULAR CASES

Both the cases admit stiff fluid model for $b=0$. Then both the metrics (3.17) and (3.24) reduce to the same metric given by

$$ds^2=dt^2-tdr^2-t^{-2\delta}dz^2-r^2td\varphi^2-t^{2\delta}d\psi^2 \tag{4.1}$$

with

$$16\pi\rho=16\pi p=\frac{1}{2t^2}(1-4\delta^2)\geqslant o \quad \text{for } \frac{1}{4}\geqslant\delta^2. \tag{4.2}$$

The equality will give the Kasnerian vacuum solution. Here δ can be negative to permit the dimensional reduction.

It may be noted that the parameter b is the measure of inhomogeneity; whenever it vanishes then the model becomes homogeneous. Hence stiff fluid condition forces homogeneity.

Let us now consider the equation of state $\rho=kp$, $k>1$, for the perfect fluid.

First of all we must, in addition to $\alpha+\beta+\gamma+\delta=1$, have

$$\alpha^2+\beta^2+\gamma^2+\delta^2=1. \tag{4.3}$$

This means we have the exact Kasnerian time evolution. Equations (3.13) and (3.14) of the case (i) of Sec. III imply

$$b=-\frac{1}{k+5}, \tag{4.4}$$

where $k>1$. For the radiation universe $k=3$ and we shall have

$$e=c=b=-\tfrac{1}{8}, \quad a=\tfrac{1}{4}, \quad d=\tfrac{5}{8}, \quad \alpha=\gamma=\tfrac{2}{3}, \quad \beta=0, \quad \delta=-\tfrac{1}{3},$$

where values of β and δ can be interchanged. The density is given by

$$16\pi\rho=\tfrac{9}{2}(1+r^2)^{-5/2}t^{-4/3}, \tag{4.5}$$

which remains always positive and decreases with r and t. Since one of β and δ is always negative, the dimensional reduction is permitted.

In the case (ii) of Sec. III, the same considerations lead to $1>k>0$ and hence it is not physically admissible.

V. DISCUSSION

It can be easily verified that $R_{ik}v^iv^k=-(16\pi/3)(\rho+2p)\leq 0$, and hence the strong energy condition is always satisfied in our models. The expansion of the universe is $\theta=(tD)^{-1}$, which will tend to zero as $t\to\infty$. All the models admit the dimensional reduction as either δ or β is always negative. Note that our models are inhomogeneous.

The matter-free limit of the models, except the radiation model, yields the Kasnerian vacuum solution[2] given by

$$ds^2=dt^2-t(dr^2+r^2d\varphi^2+dz^2)-\frac{1}{t}\,d\psi^2, \tag{5.1}$$

which under dimensional reduction for large t reduces to the 4-d metric

$$ds^2=dt^2-t(dr^2+r^2d\varphi^2+dz^2). \tag{5.2}$$

This is the Friedman–Robertson–Walker (FRW) flat radiation universe with $\rho=3p$,

$$8\pi\rho=\frac{3}{4t^2}. \tag{5.3}$$

This is quite interesting that the 5-d vacuum solution goes over to the FRW radiation universe. It has been argued that 5-d vacuum solutions can on dimensional reduction represent matter field in four dimensions.[17]

It may also be noted that the stiff fluid condition requires $b=0$, which makes the model homogeneous. Hence the parameter b can be regarded as the measure of inhomogeneity.

There is one interesting static particular case of the general metric (2.1) which is the analog of the 4-d Levi–Civita vacuum solution. In here we have

$$A=B=r^a, \quad C=r^c, \quad D=r^d, \quad E=r^e, \tag{5.4}$$

where the constants a,c,d,e are constrained by

$$c+d+e=1, \quad c^2+d^2+e^2=1+2a. \tag{5.5}$$

The 5-d vacuum metric is given by

$$ds^2 = r^{2d}dt^2 - r^{2(d^2+e^2+de-d-e)}(dr^2+dz^2) - r^{2(1-d-e)}d\varphi^2 - r^{2e}d\psi^2, \tag{5.6}$$

where d and e are arbitrary constants. It will reduce to the Levi–Civita vacuum solution when ψ=constant and $e=0$. It can serve as the exterior vacuum solution for 5-d cylindrically symmetric static distributions.

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Non-covariance of the generalized holonomies: Examples

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A key aspect of a recent proposal for a *generalized loop representation* of quantum Yang–Mills theory and gravity is considered. Such a representation of the quantum theory has been expected to arise via consideration of a particular algebra of observables – given by the traces of the holonomies of *generalized loops*. We notice, however, a technical subtlety, which prevents us from reaching the conclusion that the generalized holonomies are covariant with respect to small gauge transformations. Further analysis is given which shows that they are *not* covariant with respect to small gauge transformations; their traces are *not* observables of the gauge theory. This result indicates what may be a serious complication to the use of generalized loops in physics, but does not affect the ordinary loop representation. © *1996 American Institute of Physics.* [S0022-2488(96)03607-9]

I. INTRODUCTION

There has recently been a variety of attempts to formulate gauge theories in terms of loops.[1,2] One of the key technical developments which suggests such a formulation of gauge theory is Giles' result[3] that, for $SU(N)$ theories, the information contained in the Wilson loops (i.e., the traces of all holonomies around closed curves) is sufficient for the reconstruction of the connection up to local gauge transformations. That is, the Wilson loops contain all of the gauge-invariant information about the connection. Since the Wilson loops separate points of the space of connections modulo gauge transformations, there is a sense in which any gauge-invariant function on the relevant space of connections (and hence any configuration observable of the gauge theory) may be expressed in terms of the Wilson loops. The (over-)completeness of these observables suggests that they be taken as the basic configuration observables in the quantization scheme.

This idea, along with Ashtekar's connection-dynamic formulation[4] of general relativity, provides the foundation of the Ashtekar–Rovelli–Smolin approach to quantum gravity. The duality between connections and loops[5] suggests the possibility of representing states by functions of loops. The idea of the loop representation was first introduced to gravity by Rovelli and Smolin,[6] and has resulted in a formalism with several attractive features. Most notable are the relationship between diffeomorphism invariance and knot theory, the combinatorial aspect of the formalism, and a sense in which discreteness emerges. For details of this approach to quantum gravity see Refs. 7 and 8.

Despite the merits of the loop-representation, subtle alternatives are also being explored. The problem of regularization of the Wilson loop operators suggests that one introduce a thickening, or framing, of the loops. A novel suggestion is presented by recent results of Di Bartolo, Gambini, and Griego.[9,10] The space of loops based at a fixed point forms a group,[11] but not a Lie group. In an attempt to "coordinatize" the group of based loops, the authors of Ref. 9 came upon a generalization of the notion of a loop. The result is an infinite-dimensional Lie group, which contains the group of (based) loops as a subgroup. The elements of this *extended loop group*[12] are (sequences of) distributional quantities, ordinary loops being the "most distributional" elements. There are also elements, however, which are "less distributional" than loops, objects that we may

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think of as "smoothened loops." With regularization issues in mind, the existence of the smoothened loops is of obvious interest. An anticipated benefit of the use of generalized loops is the ability to apply familiar functional methods to the study of the (generalized) loop representation. Further, we will see that the extended loop group has the global structure of a vector space. Hence, integration on the generalized loop space is a fairly straight-forward matter. Integration techniques may supply a form of the inner-product which is inherent to the loop space.

For these reasons, one is motivated to examine the role of generalized loops in gauge theory. Recall that the idea of the loop representation is based on the Wilson loops. Since, as we will see, the generalized loops are defined via inspection of the functional form of the holonomies of ordinary loops, the holonomy formally extends to the extended loop group. It is through this extension of the holonomy that one can imagine the construction of a generalized loop representation. For such a formulation of quantum Yang–Mills theory or gravity to make sense, the generalized holonomies must be gauge-covariant with respect to (small) gauge transformations. At the very least, the traced holonomies should be gauge-invariant. The main result presented here is the fact that *the generalized holonomies are not covariant with respect to small gauge transformations*. Despite the beauty of the extended loop group, its use in gauge theory may therefore be limited.

In Sec. II, we review the construction of the extended loop group and discuss some useful properties of its elements. In Sec. III we focus on the generalized holonomies, with particular attention given to their transformation properties. Consideration of the Abelian case will suggest simple examples of non-covariance of the generalized $SU(2)$ holonomies. Two such examples are presented in Sec. IV. Finally, in Sec. V, we conclude with generalizations of the results and remarks concerning their relevance in physics.

II. GENERALIZED LOOPS

The purpose of this section is to recall the basic ideas regarding generalized loops (for details, see the original work[9]). After introducing the group of loops on an arbitrary connected manifold, consideration of the holonomies will suggest a generalization of the notion of loops. The set of these generalized loops—the extended loop group—forms an infinite-dimensional Lie group.

Fix a point p on an arbitrary connected manifold $\mathcal{M}$ and consider the space $\mathcal{C}_p$ of closed curves based at p. Elements of $\mathcal{C}_p$ are piecewise-smooth maps $C:I\to\mathcal{M}$ such that $C(0)=p=C(1)$, where I is the unit interval. Now, our main motivation for considering the space $\mathcal{C}_p$ is that the trace of the holonomy of a physical gauge field around any closed curve is gauge-invariant, i.e., an observable of the classical field theory. Since we are primarily concerned with the observables, we are not interested in the space $\mathcal{C}_p$ itself, but in a space of equivalence classes of elements of $\mathcal{C}_p$. For example, two closed curves which differ merely by reparametrization yield the same holonomies for an arbitrary smooth connection over $\mathcal{M}$. Gambini and Trias[11] provide an appropriate identification of elements of $\mathcal{C}_p$: Two closed curves $C,C'\in\mathcal{C}_p$ are deemed equivalent if $C\circ\bar{C}'$ is contractible *within itself* to the trivial curve $\iota(s)\equiv p$, where $\bar{C}'$ is the reversed path $\bar{C}'(s)=C'(1-s)$. With this equivalence relation on $\mathcal{C}_p$, it is easy to see that two closed curves which are equivalent give the same holonomies for any smooth connection over $\mathcal{M}$. Denote by $\mathcal{L}_p$ the space obtained by dividing $\mathcal{C}_p$ by this equivalence relation. The obvious composition of paths induces a *group operation* on the set $\mathcal{L}_p$, which we will call the *group of loops* based at p.

Next, consider a connection $\mathbf{A}$ on a principal bundle $P(\mathcal{M},G)$, where G is a compact, connected Lie group. For the sake of simplicity, we shall assume that P is trivial and view connections as Lie algebra-valued one-forms on $\mathcal{M}$. [Below, we will restrict attention to the case $G=SU(2)$, for which every bundle is trivial.] To an element $\gamma\in\mathcal{L}_p$ we may associate the holonomy, $U_A[\gamma]$, around any path C in the equivalence class defining γ. Expressed in terms of the fundamental representations of the gauge group G and its Lie algebra, the holonomy takes the form of the path-ordered exponential, which may be written explicitly as

$$U_A[\gamma]=P\exp\oint_C \mathbf{A}=\sum_{n=0}^{\infty}\int\cdots\int X_\gamma^{a_1\cdots a_n}(x_1,\ldots,x_n)\mathbf{A}_{a_1}(x_1)\cdots\mathbf{A}_{a_n}(x_n), \tag{1}$$

where

$$X_\gamma^{a_1\cdots a_n}(x_1,\ldots,x_n):=\oint_C dy^{a_1}\int_{y_1}^1 dy^{a_2}\cdots\int_{y_{n-1}}^1 dy^{a_n}\delta(x_1,y_1)\cdots\delta(x_n,y_n), \tag{2}$$

and the zeroth term in Eq. (1) is taken to be the identity. In Eq. (2) the index a_k is "attached" to the point x_k, and for each n, $X_\gamma^{a_1\cdots a_n}(x_1,\ldots,x_n)$ is an n-point distributional vector density of weight one in each argument x_k. As suggested by the subscript on the X's, these n-point distributions are independent of the particular path C chosen from the equivalence class determined by $\gamma\in\mathscr{L}_p$. It will be convenient to employ the notation

$$X_\gamma^{\mu_1\cdots\mu_n}:=X_\gamma^{a_1\cdots a_n}(x_1,\ldots,x_n), \tag{3}$$

where the index μ_k now represents the pair (a_k,x_k), and contraction of greek indices represents both contraction of the latin index and the integration over $\mathscr{M}$.

Thus, to every element $\gamma\in\mathscr{L}_p$ is associated a string,

$$X_\gamma:=(1,\ X_\gamma^{\mu_1},\ \ldots,\ X_\gamma^{\mu_1\cdots\mu_n},\ \ldots),$$

of multi-vector densities. As is observed in Ref. 9, if $\gamma,\eta\in\mathscr{L}_p$, the multi-densities corresponding to their product may be expressed as

$$X_{\gamma\circ\eta}^{\mu_1\cdots\mu_n}=\sum_{k=0}^{n} X_\gamma^{\mu_1\cdots\mu_k}X_\eta^{\mu_{k+1}\cdots\mu_n}, \tag{4}$$

with the convention that

$$X^{\mu_1\cdots\mu_0}:=1.$$

These strings of multi-densities satisfy two useful identities. Denote by X the string corresponding to an arbitrary loop in $\mathscr{L}_p$. The first identity reflects the ordering of points on the image of the loop;

$$X^{\underline{\mu_1\cdots\mu_k}\mu_{k+1}\cdots\mu_n}=X^{\mu_1\cdots\mu_k}X^{\mu_{k+1}\cdots\mu_n}, \tag{5}$$

where the left side is obtained by summing over all permutations of the μ_i which preserve the relative ordering of the first k indices and also the relative ordering of remaining $n-k$. For example,

$$X^{\underline{\mu_1\mu_2}\mu_3\mu_4}=X^{\mu_1\mu_2\mu_3\mu_4}+X^{\mu_1\mu_3\mu_2\mu_4}+X^{\mu_1\mu_3\mu_4\mu_2}+X^{\mu_3\mu_1\mu_2\mu_4}+X^{\mu_3\mu_1\mu_4\mu_2}+X^{\mu_3\mu_4\mu_1\mu_2}.$$

Next, since taking the divergence of a vector density requires no additional structure (e.g., a metric or derivative operator) on $\mathscr{M}$, it is natural to ask whether the divergence of an entry of X satisfies any useful property. The answer is in the affirmative;

$$\frac{\partial}{\partial x^{a_k}}X^{\mu_1\cdots\mu_n}=[\delta(x_k,x_{k-1})-\delta(x_k,x_{k+1})]X^{\mu_1\cdots\hat{\mu}_k\cdots\mu_n}, \tag{6}$$

where the caret over the μ_k is intended to indicate its absence, and the mixed notation on the left side should be transparent. By definition, x_0 and x_{n+1} are taken to be the base point, p. Thus the divergence of the rank-n entry of X is directly related to the rank-(n-1) entry.

The basic idea of Di Bartolo, Gambini, and Griego[9] is to consider the space of *all* objects satisfying these relations. To be precise, let $\mathscr{E}$ be the space of all sequences $(E^0, E^{\mu_1}, \ldots, E^{\mu_1\cdots\mu_n}, \ldots)$, where E^0 is a real number and $E^{\mu_1\cdots\mu_n}$ is a *distributional* vector-density in each index. $\mathscr{E}$ becomes an associative algebra when equipped with the product motivated by Eq. (4); given $E_1, E_2 \in \mathscr{E}$, we define

$$(E_1 \times E_2)^{\mu_1\cdots\mu_n} := \sum_{k=0}^{n} E_1^{\mu_1\cdots\mu_k} E_2^{\mu_{k+1}\cdots\mu_n}, \tag{7}$$

where $E^{\mu_1\cdots\mu_0} := E^0 \in \mathbb{R}$. The extended loop group (based at $p \in \mathscr{M}$) is defined to consist of those elements of $\mathscr{E}$ which satisfy the algebraic relation (5) and the differential relation (6) and for which the rank-zero entry is unity. This set, denoted by $\mathscr{X}_p$, is closed under the product defined above and every element is seen to have an inverse with respect to the identity element, $I := (1,0,0\ldots)$. $\mathscr{X}_p$ is then a group which contains $\mathscr{L}_p$ as a subgroup.

Next, $\mathscr{X}_p$ is an infinite-dimensional Lie group in the following sense. For any element $X \in \mathscr{X}_p$, the logarithm

$$\ln(X) := \sum_{m=1}^{\infty} \frac{(-)^{m+1}}{m} (X-I)^m$$

is a well-defined element of $\mathscr{E}$ (with vanishing rank-zero entry) which satisfies the differential relation given by Eq. (6) and the *homogeneous algebraic relation*

$$\ln(X)^{\underline{\mu_1\cdots\mu_k}\mu_{k+1}\cdots\mu_n} = 0, \quad \forall \quad 0 < k < n. \tag{8}$$

Let $\mathscr{F}_p$ consist of all elements of $\mathscr{E}$ which satisfy these two conditions and with vanishing rank-zero entry. One can show that if $F \in \mathscr{F}_p$ then $\exp(F) := \Sigma_{k=0}^{\infty} (1/k!)\, F^k$ is a well-defined element of $\mathscr{X}_p$. Further, for any element $X \in \mathscr{X}_p$ the logarithm $F = \ln X$ is the unique element of $\mathscr{F}_p$ for which $X = \exp(F)$. $\mathscr{F}_p$ is closed under the Lie bracket given by the commutator with respect to the associative product (7), defined on $\mathscr{E}$; this is the Lie bracket relevant to the group operation on $\mathscr{X}_p$. Thus, $\mathscr{F}_p$ is simply the Lie algebra corresponding to $\mathscr{X}_p$. Note also that $\mathscr{X}_p$ has the global structure of an infinite-dimensional vector space since there is a one-one correspondence between its elements and elements of its Lie algebra. In particular, we may unambiguously take the real power of any element in $\mathscr{X}_p$; $X^t := \exp(t \ln X)$.

One may then think of $\mathscr{X}_p$ as a "completion" of the group $\mathscr{L}_p$. Any generalized loop $X \in \mathscr{X}_p$ defines the one-parameter subgroup of $\mathscr{X}_p$, consisting of all real powers of X. Since generic elements of $\mathscr{X}_p$ are not easily described in terms of the geometry of the underlying manifold $\mathscr{M}$, it is most instructive to think of X^t in the group-theoretic sense.

Given a G-connection, one may consider the formal expression for the holonomy around an arbitrary extended loop,

$$U_A[X] := \sum_{n=0}^{\infty} X^{\mu_1\cdots\mu_n} \mathbf{A}_{\mu_1} \cdots \mathbf{A}_{\mu_n}. \tag{9}$$

There is no claim that the extended holonomies take values in the gauge group, or even that they converge. However, in Ref. 9 it is formally shown that $U_A[X_1 \times X_2] = U_A[X_1] U_A[X_2]$, where the right side is given by matrix multiplication in the fundamental representation. At least at the formal level, the holonomy extends to a homomorphism on $\mathscr{X}_p$. It is worth noticing one particular

situation in which the extended holonomies converge to elements of the gauge group. Suppose that $\mathbf{A}$ is an *Abelian* connection; i.e., $[\mathbf{A}(x),\mathbf{A}(y)]=0$. Then, using the algebraic relation (5), it is a simple matter to show that for any $X \in \mathscr{X}_p$,

$$U_A^{(n)}[X] := X^{\mu_1 \cdots \mu_n} \mathbf{A}_{\mu_1} \cdots \mathbf{A}_{\mu_n} = \frac{1}{n!}(X^\mu \mathbf{A}_\mu)^n. \tag{10}$$

So the extended holonomy corresponding to any Abelian connection is just given by the exponential of $X^\mu \mathbf{A}_\mu$. (This result depends only on the fact that the restriction of $\mathbf{A}$ to the support of X is Abelian.) If, for example, the support of $\mathbf{A}$ is also of compact closure, the holonomy is convergent and group-valued on all of $\mathscr{X}_p$. This result will be used extensively in what follows.

III. THE GENERALIZED HOLONOMIES

The construction of the extended loop group is elegant and of considerable interest from a purely mathematical point of view. However, the intention extends to physics as well. The idea is simply to generalize the formalism used in the ordinary loop representations of gauge theories, i.e., to consider the traces of the extended holonomies as observables for Yang-Mills theory and, perhaps more importantly, general relativity. In particular, an extended loop representation for quantum general relativity may be an especially useful setting for consideration of an inverse loop transform and the framing problem of knot invariants.[10,13]

With the intended application of the generalized loops in mind, it is natural to examine the behavior of the extended holonomies under gauge transformations. One often distinguishes between two types of gauge freedom. The gauge which is generated by the (first-class) constraints is *physical* gauge freedom, while that which is not is *symmetry*. The physical gauge freedom then corresponds to that generated by the infinitesimal gauge transformations. Thus, in order for the traces of the extended holonomies to give observables, it is necessary that they be invariant under small gauge transformations. This issue was considered in Ref. 9, but as is usual in pioneering work, a detailed analysis was sacrificed for the sake of progress in other directions.

Such an analysis is the purpose of this section. We will find that there is a technical subtlety which prevents us from accepting the naive conclusion that the extended holonomies are (formally) gauge covariant with respect to infinitesimal gauge transformations. In order to gain some insight about the transformations properties of the holonomies, we will then consider the Abelian case. In all that follows, we will restrict attention to the manifold $\mathscr{M} \approx \mathbb{R}^3$.

Recall that an infinitesimal gauge transformation is given by a map $\Lambda: \mathscr{M} \to \mathscr{L}G$, where $\mathscr{L}G$ is the Lie algebra of G. To first order in Λ, the gauge-transformed connection is given by

$$\mathbf{A}^\Lambda = \mathbf{A} + d\Lambda + [\mathbf{A},\Lambda].$$

Set

$$U_A^{(n)}[X] := X^{\mu_1 \cdots \mu_n} \mathbf{A}_{\mu_1} \cdots \mathbf{A}_{\mu_n},$$

as in Eq. (10), so that

$$U_A[X] = \sum_{n=0}^{\infty} U_A^{(n)}[X].$$

Using the differential relation (6) satisfied by the generalized loops, one may obtain the holonomy corresponding to the gauge-transformed connection;

$$U_{A^\Lambda}^{(n)}[X] = U_A^{(n)}[X] + [U_A^{(n-1)}[X],\Lambda(p)] + f_{(A,\Lambda)}^{(n)}[X] - f_{(A,\Lambda)}^{(n-1)}[X], \tag{11}$$

where

$$f^{(n)}_{(A,\Lambda)}[X]:=\sum_{k=1}^{n} X^{\mu_1\cdots\mu_n}\mathbf{A}_{\mu_1}\cdots\mathbf{A}_{\mu_{k-1}}[\mathbf{A},\Lambda]_{\mu_k}\mathbf{A}_{\mu_{k+1}}\cdots\mathbf{A}_{\mu_n}. \tag{12}$$

One is tempted to conclude from Eq. (11) that, since the $f^{(n)}$ cancel upon summation of the series for the transformed holonomy, all extended holonomies are formally gauge-covariant. However, let us proceed more carefully. Consider the partial sum,

$$\sum_{n=0}^{N} U^{(n)}_{A^\Lambda}[X]=\sum_{n=0}^{N} U^{(n)}_{A}[X]+\left[\sum_{n=0}^{N} U^{(n)}_{A}[X],\Lambda(p)\right]-[U^{(N)}_{A}[X],\Lambda(p)]+f^{(N)}_{(A,\Lambda)}[X]. \tag{13}$$

If we suppose that $U_A[X]$ converges, then $U^{(N)}_A[X]\to 0$ as $N\to\infty$ and the extended holonomy is covariant under infinitesimal gauge-transformations only if

$$f^{(N)}_{(A,\Lambda)}[X]\to 0, \quad \text{as} \quad N\to\infty. \tag{14}$$

Thus, gauge-covariance of the extended holonomies does not follow trivially from Eq. (11).

We are now faced with the problem of whether the notion of holonomy generalizes to the extended loop group. Although, by inspection of Eq. (12), the Abelian case is trivial, an example will lead the way to an understanding of the non-Abelian case. Therefore, let us consider $G=U(1)$. Let γ be the loop determined by the curve

$$C(s)=(\cos(2\pi s),\sin(2\pi s),0).$$

This loop determines an element $X_\gamma\in\mathscr{X}_p$, where the base point has been fixed as $p=(1,0,0)$. We will focus on the generalized holonomies of an arbitrary real power, X^t_γ, of this particular loop.

The generic $U(1)$-connection is of the form

$$\mathbf{A}(x)=-i\omega(x),$$

where ω is a real one-form on $\mathscr{M}$. To compute the holonomy of $\mathbf{A}$ around X^t_γ, we need only know the rank-1 entry of X^t_γ,

$$(X^t_\gamma)^\mu=tX^\mu_\gamma,$$

and that, with respect to the cylindrical coordinates z,r,θ,

$$X^\mu_\gamma=\frac{1}{r}\delta^1(r,1)\delta^1(z,0)\left(\frac{\partial}{\partial\theta}\right)^\mu.$$

By Eq. (10), the holonomy is then given by

$$U_A[X^t_\gamma]=\exp(tX^\mu\mathbf{A}_\mu)=\exp\left(-it\oint_\Gamma\omega\right), \tag{15}$$

where Γ is the unit circle in the x-y plane (the image of C). The holonomy of the gauge-transformed connection $\mathbf{A}^g=\mathbf{A}+g^{-1}\mathbf{d}g$ is

$$U_{Ag}[X^t_\gamma]=U_A[X^t_\gamma]\cdot\exp(-2\pi i t w_\gamma[g]), \tag{16}$$

where

$$w_\gamma[g] := \frac{i}{2\pi} \oint_\Gamma g^{-1} dg \in \mathbb{Z}. \tag{17}$$

Note that the pull-back of g to Γ is a map from the circle into $U(1)$ and that $w_\gamma[g]$ is simply the winding number of this map, i.e., the number of times g wraps $U(1)$ around Γ. Suppose g is a small gauge transformation. Then, by definition, there exists a homotopy g_λ (a smooth one-parameter family of gauge transformations, $\lambda \in [0,1]$) connecting $g = g_1$ to the trivial map $g_0 \equiv \mathbf{1}$. By pulling the homotopy back to Γ, one then obtains a one-parameter family of maps from the circle into $U(1)$. Since the winding number is integral, it must be the same for each g_λ. Hence, $w_\gamma[g] = w_\gamma[g_1] = w_\gamma[g_0] = 0$. We then see that the holonomy (15) is covariant with respect to small gauge transformations. Note that this was not a general proof of covariance of the $U(1)$-holonomies (the general proof is much simpler than what we have done above!). The above reasoning applies only to the arbitrary real power of the particular loop γ. The utility of our result, however, lies not in the conclusion, but in the methodology. The above ansatz, when applied to the case $G = SU(2)$, will suggest simple examples which show that the non-Abelian holonomies are *not* covariant with respect to small gauge.

IV. NON-COVARIANCE OF THE GENERALIZED HOLONOMIES

We can study the non-Abelian case, by "embedding" the above result into $SU(2)$. The idea in mind is to replace $U(1)$ by an Abelian subgroup of $SU(2)$. After making this idea more precise, natural examples of non-covariance will be presented. The first is, perhaps, the most natural; it involves the holonomy of the real power of an ordinary loop. For the second example, we will consider the holonomies of generalized loops which are "least distributional," in a sense to be explained below.

Let us consider an arbitrary Abelian subgroup of $SU(2)$. This subgroup is generated by an element, $\mathbf{T}$, of the Lie algebra, $\mathcal{L}SU(2)$. We may assume, without loss of generality, that $\mathbf{T}$ is normalized as

$$\mathrm{tr}(\mathbf{T}^2) = -2,$$

so that, for example,

$$\exp[r\mathbf{T}] = \exp[(r + 2\pi n)\mathbf{T}], \quad \forall \quad n \in \mathbb{Z}, \quad r \in \mathbb{R}. \tag{18}$$

Now suppose $\mathbf{A}$ is an $SU(2)$-connection which is proportional to $\mathbf{T}$; i.e.,

$$\mathbf{A} = \omega \mathbf{T}, \tag{19}$$

for some one-form ω. Suppose further that $g: \mathbb{R}^3 \to SU(2)$ is an $SU(2)$ gauge transformation whose restriction to Γ is contained in the $U(1)$-subgroup generated by $\mathbf{T}$. We can now mimic the discussion leading to Eq. (16) by making the replacement $-i \mapsto \mathbf{T}$. We obtain

$$U_{Ag}[X^t_\gamma] = U_A[X^t_\gamma] \cdot \exp(2\pi t v_\gamma[g]\mathbf{T}), \tag{20}$$

where v_γ is defined as

$$v_\gamma[g]\mathbf{T} := \frac{1}{2\pi} \oint_\Gamma g^{-1} \mathbf{d} g. \tag{21}$$

The meaning of v_γ is analogous to that of w_γ; it is simply the number of times g winds the $U(1)$-subgroup generated by $\mathbf{T}$ around the circle Γ. Of course, v_γ is only defined for such an Abelian gauge transformation.

For integral t, X_γ^t corresponds to an ordinary loop and the holonomy is covariant under all gauge transformations. But for the above holonomy to transform covariantly for all *real* t, $v_\gamma[g]$ must be trivial. Recall that in Sec. III it was the non-simple connectivity of $U(1)$ that prevented us from finding small gauge transformations with non-trivial winding number around Γ. $SU(2)$ is, of course, simply connected; hence, one may wonder whether there exist small gauge transformations with non-trivial v_γ. In fact, there do exist such gauge transformations. The task at hand is to produce an explicit expression for a small gauge transformation whose restriction to Γ lies is an Abelian subgroup of $SU(2)$, and which winds Γ non-trivially around this Abelian subgroup. Since the exponential factor in Eq. (21) is independent of the connection, we will then have shown that the generalized holonomies are not gauge covariant.

To this end, let us first focus on a convenient description of the manifold structure of $SU(2)$. The Lie algebra, $\mathcal{L}SU(2)$, of $SU(2)$ is a real, three-dimensional vector space with a natural (Killing–Cartan) inner-product, which, in the fundamental representation, takes the form[14]

$$(\mathbf{T}_1,\mathbf{T}_2) := -2\ \mathrm{tr}(\mathbf{T}_1\mathbf{T}_2). \tag{22}$$

Fix a basis $\{\tau_1,\tau_2,\tau_3\}$ for the Lie algebra, which is ortho-normal with respect to this inner-product. For any element $\mathbf{L} \in \mathcal{L}SU(2)$, $\exp \mathbf{L}$ may be uniquely written as[15]

$$\exp(\mathbf{L}) = a_0\mathbf{1} + 2[a_1\tau_1 + a_2\tau_2 + a_3\tau_3], \tag{23}$$

where $a_0^2+a_1^2+a_2^2+a_3^2=1$. While $a_0,\ldots,a_3$ may be written in terms of $\mathbf{L}$, we will not find their explicit form useful. Having chosen a basis $\{\tau_1,\tau_2,\tau_3\}$ for the Lie algebra, we then obtain an isomorphism of $SU(2)$ with the unit 3-sphere in $\mathbb{R}^4$. Of course, the identity $\mathbf{1}$ is represented by the point $(1,0,0,0)$. We will abuse notation and write $\exp(\mathbf{L}) = (a_0,a_1,a_2,a_3) = a_i\vec{e}_i$, where the a_i are those appearing in Eq. (23), and $\vec{e}_i$ form the obvious ortho-normal basis of $\mathbb{R}^4$. The algebra $\mathcal{L}SU(2)$ may be viewed as the tangent space to $SU(2)$ at the identity, and with the Lie algebra element, $\mathbf{L} = L^1\tau_1 + L^2\tau_2 + L^3\tau_3$, we may identify the vector $(0,L^1,L^2,L^3) \in \mathbb{R}^4$. The $U(1)$-subgroup generated by $\mathbf{L}$ is now simply represented by the great circle (through $\mathbf{1}$) whose tangent at the identity is proportional to $\mathbf{L}$. For example, $\exp(\alpha\tau_1) = (\cos(\alpha/2),\sin(\alpha/2),0,0)$.

We may now view a gauge transformation as a smooth map $g:\mathbb{R}^3 \to \mathbb{R}^4$ whose image is contained in the unit 3-sphere. Choose the basis $\{\tau_1,\tau_2,\tau_3\}$ so that the (arbitrary) algebra element considered above is given by $\mathbf{T} = 2\tau_1$ and let us look for a small gauge transformation g for which $g(\cos\theta,\sin\theta,0) = \exp(\theta\mathbf{T}) = (\cos\theta,\sin\theta,0,0)$. We will then have $v_\gamma[g] = 1$, and our goal will have been accomplished.

At this point, a brief digression will be quite instructive. Let us display a particular homotopy connecting the curve $h(\theta) = \exp(\theta\mathbf{T})$ to the trivial curve $\iota(\theta) \equiv \mathbf{1}$. This can be done geometrically, as follows. Consider the intersection of $SU(2)$ (the 3-sphere in $\mathbb{R}^4$) and the hyperplane $P^3 = \{\vec{a} \in \mathbb{R}^4 | a_3 = 0\}$. This is a 2-sphere in $\mathbb{R}^4$, which we will denote as S. Let $P^2(\alpha)$ be the 2-plane in P^3 consisting of points of the form $\vec{e}_0 + \vec{v}$ such that $\vec{v}\cdot\vec{n}(\alpha) = 0$, where $\vec{n}(\alpha) = \vec{e}_2\cos\alpha + \vec{e}_0\sin\alpha$. The intersection of S with $P^2(\alpha)$ is a circle of radius $r(\alpha) = \sin\alpha$, which may be parameterized as

$$h_\alpha(\theta) = \begin{pmatrix} 1-(1-\cos\theta)\sin^2\alpha \\ \sin\theta\sin\alpha \\ (1-\cos\theta)\sin\alpha\cos\alpha \\ 0 \end{pmatrix}, \tag{24}$$

for $\theta \in [0,2\pi]$. As α varies from 0 to π, these circles "foliate" the sphere S. Notice, in particular, that $h_0(\theta) \equiv \mathbf{1}$ and $h_{\pi/2}(\theta) = (\cos\theta,\sin\theta,0,0) = \exp(\theta\mathbf{T})$. Therefore, h_α provides the desired homotopy (see Fig. 1). This homotopy will play a very important role in the examples that follow.

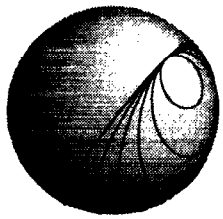

FIG. 1. A convenient homotopy connecting the trivial curve to the curve winding once around the $U(1)$-subgroup generated by $\mathbf{T}$. For each $0 \leq \alpha \leq \pi/2$, the image of h_α is a circle on the 2-sphere S, as shown for various values of the parameter α. As α decreases from $\pi/2$ to 0, h_α shrinks to a point (the identity element).

A. Example 1

We can now suggest the form of a gauge transformation $g:\mathbb{R}^3 \to SU(2)$ which is demonstrably small, whose restriction to the unit circle in the x-y plane lies in the Abelian subgroup generated by $\mathbf{T}$, and which winds this subgroup non-trivially around the unit circle. In order to satisfy generic boundary conditions at infinity, we will also demand that g be trivial outside of a compact region.

The desired gauge transformation may be obtained from a smooth assignment of the angle α to each pair of cylindrical coordinates r,z; i.e., we try

$$g(r\cos\theta, r\sin\theta, z) := h_{\alpha(r,z)}(\theta), \tag{25}$$

such that $\alpha(1,0) = \pi/2$. Any such gauge transformation is obviously small since the one-parameter family of gauge transformations,

$$g_\lambda(r\cos\theta, r\sin\theta, z) := h_{\lambda\alpha(r,z)}(\theta), \quad \lambda \in [0,1] \tag{26}$$

provides a homotopy connecting g to the trivial map.

It remains only to produce the assignment $\alpha(r,z)$. This may be accomplished by use of the smearing function,

$$\sigma_\Delta(x) := \begin{cases} e\cdot\exp\left(\dfrac{-\Delta^2}{\Delta^2 - x^2}\right) & : |x| \leq \Delta, \\ 0 & : |x| \geq \Delta. \end{cases} \tag{27}$$

σ_Δ is symmetric about $x=0$, at which it attains its maximum value $\sigma_\Delta(0)=1$. Most important, σ_Δ is an infinitely differentiable function, the support of which is compact. Putting $\alpha(r,z) := (\pi/2)\,\sigma_{1/2}(z)\sigma_{1/2}(r-1)$, we obtain

$$g(r\cos\theta, r\sin\theta, z) := h_{\pi/2\,\sigma_{1/2}(z)\sigma_{1/2}(r-1)}(\theta)$$

$$= \begin{pmatrix} 1-(1-\cos\theta)\sin^2\left[\dfrac{\pi}{2}\sigma_{1/2}(z)\sigma_{1/2}(r-1)\right] \\ \sin\theta\,\sin\left[\dfrac{\pi}{2}\sigma_{1/2}(z)\sigma_{1/2}(r-1)\right] \\ (1-\cos\theta)\sin\left[\dfrac{\pi}{2}\sigma_{1/2}(z)\sigma_{1/2}(r-1)\right]\cos\left[\dfrac{\pi}{2}\sigma_{1/2}(z)\sigma_{1/2}(r-1)\right] \\ 0 \end{pmatrix}. \tag{28}$$

Note that g is infinitely differentiable and is trivial outside a compact region. Further, since $\alpha_{1/2}(r=1,z=0)=\pi/2$, its restriction to the circle Γ is given by $g(\cos\theta,\sin\theta,0)=\exp(\theta\mathbf{T})$, as desired.

The purpose of this sub-section was the construction of this gauge-transformation. For any connection of the form written in Eq. (19), the holonomy "around" X^t_γ is *non-covariant*, according to Eq. (20). For example, choose

$$\mathbf{A}(r\cos\theta,r\sin\theta,z):=A\sigma_{1/2}(z)\sigma_{1/2}(r-1)\mathbf{T}d\theta,\quad A\in\mathbb{R} \tag{29}$$

(which also vanishes outside of a compact region). We then have

$$U_A[X^t_\gamma]=\exp[2\pi At\mathbf{T}], \tag{30}$$

and

$$U_{As}[X^t_\gamma]=\exp[2\pi At\mathbf{T}]\cdot\exp[2\pi t\mathbf{T}]. \tag{31}$$

This completes the first example.

B. Example 2

The above example involved what may be, from the Lie algebraic point of view, the most notable element of the extended loop group – the real power of an ordinary loop. The extended loop group also contains elements which seem radically different than ordinary loops, but which may be quite useful. These elements are, in a sense, "less distributional" than the ordinary loops. The differential relation (6) does not allow the existence of smooth extended loops, i.e., those for which all entries are smooth; they must be genuinely distributional. However, it is a trivial application of the results of Ref. 9 to show that given an arbitrary multi-vector density $Y^{\mu_1\cdots\mu_m}$ which is divergence-free in each index and satisfies the *homogeneous* algebraic relation (8), there exists an element $X\in\mathscr{X}_p$ such that $X^{\mu_1\cdots\mu_k}=0$, $\forall\, k<m$ and $X^{\mu_1\cdots\mu_m}=Y^{\mu_1\cdots\mu_m}$. In particular, we may choose $Y^{\mu_1\cdots\mu_m}$ to be *smooth*. The set of all extended loops whose first non-vanishing entry is smooth is a sub-Lie group of $\mathscr{X}_p$. One might think of these elements as "smoothened loops."

As was mentioned in the Introduction, the existence of the smoothened loops is a nice feature of $\mathscr{X}_p$. If X is as described above, then due to Eq. (6), $X^{\mu_1\cdots\mu_n}$ must be a genuine distribution for each $n>m$. Therefore, the hope of obtaining a gauge-invariant smearing of the connection by *smooth* functions is not borne out. Nonetheless, one might hope[10] that some light may be shed on the problem of regularization of the Wilson loop variables. Could it be that, by some mathematical miracle, the holonomies of smoothened loops do not suffer from the problem of non-covariance illustrated above? By "smearing out" the previous example, we will see that the answer to this question is, unfortunately, negative.

Recall that for Abelian connections, it is only the rank-one entry of X on which the holonomy $U_A[X]$ depends. Choose an element $X\in\mathscr{X}_p$ for which

$$X^\mu=\left(\frac{\partial}{\partial\theta}\right)^\mu\sigma_{1/2}(z)\sigma_{1/2}(r-1). \tag{32}$$

X^μ is a smooth vector density of compact support, which may be viewed as a smoothened version of the X^μ_γ considered above. Let $\mathbf{A}$ be as in the definition (29). A short calculation yields the holonomy

$$U_A[X]=\exp(X^\mu A_\mu)=\exp(2\pi A\, e^6\mathbf{T}). \tag{33}$$

In the spirit of the previous example, we construct a gauge transformation $\tilde{g}$ which commutes with **A**. The restriction of $\tilde{g}$ to the support of **A** must then take values in the Abelian subgroup generated by **T**. The idea is simply to replace the smearing function σ in Eq. (28). The function

$$t_\Delta(x) := \frac{2}{\Delta\, e^3}\int_{-\infty}^{x} dx'\,\sigma_\Delta(x') \tag{34}$$

is a smoothened step function. It vanishes for all $x \leqslant -\Delta$ and is unity for all $x \geqslant \Delta$. Of course, t_Δ is infinitely differentiable everywhere. Define

$$s_\Delta(x) := \begin{cases} t_\Delta(x+3\Delta) & : \quad x \leqslant 0, \\ 1 - t_\Delta(x-3\Delta) & : \quad x \geqslant 0. \end{cases} \tag{35}$$

This function is non-vanishing only for $|x| \leqslant 4\Delta$ and is constant on the interval $|x| \leqslant 2\Delta$, on which it assumes the value 1. Using $s_{1/4}$ in place of $\sigma_{1/2}$ in Eq. (28), one obtains the desired gauge transformation; put

$$\tilde{g}(r\cos\theta, r\sin\theta, z) := h_{\pi/2\, s_{1/4}(z) s_{1/4}(r-1)}(\theta)$$

$$= \begin{pmatrix} 1-(1-\cos\theta)\sin^2\left[\frac{\pi}{2} s_{1/4}(z) s_{1/4}(r-1)\right] \\ \sin\theta\,\sin\left[\frac{\pi}{2} s_{1/4}(z) s_{1/4}(r-1)\right] \\ \sin\left[\frac{\pi}{2} s_{1/4}(z) s_{1/4}(r-1)\right](1-\cos\theta)\cos\left[\frac{\pi}{2} s_{1/4}(z) s_{1/4}(r-1)\right] \\ 0 \end{pmatrix}. \tag{36}$$

On the support of X^μ, $\tilde{g}$ takes a very simple form; for $|z| \leqslant \frac{1}{2}$ and $|r-1| \leqslant \frac{1}{2}$, $\tilde{g}(r\cos\theta, r\sin\theta, z) = (\cos\theta, \sin\theta, 0, 0) = \exp(\theta \mathbf{T})$. One may then obtain

$$\int X^a \tilde{g}^{-1}(\mathbf{d}\tilde{g})_a = \frac{\pi\, e^3}{8}\mathbf{T}. \tag{37}$$

Finally,

$$U_{A\tilde{g}}[X] = U_A[X]\cdot\exp\left(\frac{\pi\, e^3}{8}\mathbf{T}\right). \tag{38}$$

The extended "holonomies" of the smoothened loops are not covariant with respect to small gauge transformations.

V. GENERALIZATIONS AND CONCLUSIONS

The extended loop group is a well-defined mathematical object. It is an infinite-dimensional group which encompasses the group of based loops on an arbitrary connected manifold, $\mathcal{M}$. (Note that we have used the term "Lie group" fairly loosely. For the sake of rigor, it should be shown that $\mathcal{X}_p$ admits a manifold structure with respect to which the group operations are continuous.) For applications to physics, however, one would also like to extend the concept of holonomy. In fact, the construction of the extended loop group was based on the functional form of the holonomy of ordinary loops. There is then the obvious candidate for a generalized holonomy. We

have found, however, that for the case $\mathcal{M} \approx \mathbb{R}^3$ this generalized holonomy is not covariant with respect to small gauge transformations. Its trace does not provide gauge-invariant functionals on the space of connections for an $SU(2)$ gauge theory on Minkowski space, for example.

In fact, the result is of a very general validity. Since any simple Lie group contains an $SU(2)$ subgroup, it extends to the non-Abelian case with such gauge groups – those which are typically relevant in physics. The result also applies to the case of gravity in terms of the Ashtekar variables. Further, although we restricted our attention to $\mathcal{M} \approx \mathbb{R}^3$, all of the mappings used in the first example are of compact support. We may then extend the result to an arbitrary manifold. (Note, however, that since the topology of $\mathbb{R}^3$ was used in a critical way in defining the smoothened loop group, the second example does not extend to manifolds of arbitrary topology; i.e., it is not clear that one can even define the smoothened loop group for the arbitrary case.)

From our point of view, the potential power of the extended loop group involves the use of the traced holonomies as a large class of observables for gauge theories. Our results then suggest a re-evaluation of the extended loop group as an arena for quantum gravity and Yang–Mills theory.

There are three alternatives worth consideration. First, the following question arises: What characterizes those generalized loops for which the holonomies are covariant? Perhaps consideration of this question would shed some light on the appropriate extension of the loop representation. Note however, that by Example 1, one will not have the continuous structure of a Lie group at one's disposal. Thus, techniques involving functional differentiation are not likely to be straight-forward in such a formulation. A second alternative, suggested by Di Bartolo, *et al.*, is to design a different extension of the holonomy which is covariant.[16] Alternatively, since observables of the theory are our primary concern, it may be most productive to focus on an extension of the concept of the Wilson loops. It may be the case, for example, that such an extension exists which does not manifest itself as the trace of a holonomy. Last, if some generalization of the ordinary loop representation is needed, it may turn out that the appropriate generalization is altogether different than that suggested by the existence of the extended loop group.

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Perturbations of solutions of the Einstein–Maxwell equations with a null background electromagnetic field

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Expressions for the complete metric and vector potential perturbations of solutions of the Einstein–Maxwell equations with a null background electromagnetic field in terms of two complex scalar potentials are derived using Wald's method of adjoint operators. The perturbations of the Bell–Szekeres solution, in the regions prior to the collision of the plane-fronted waves, are obtained by this approach. We find that there exist nontrivial u-independent perturbations (where ∂_u defines the direction of propagation of the colliding wave) which, when the electromagnetic perturbation vanishes, are exact solutions of the Einstein–Maxwell equations. © *1996 American Institute of Physics.* [S0022-2488(96)00207-1]

I. INTRODUCTION

In the study of the perturbations of solutions of the Einstein equations by massless fields it is convenient to have expressions for the complete perturbations in terms of some few potentials, since this reduces the number of differential equations to solve and automatically gives the correct relative normalization for all the components of the perturbation. In the case of the algebraically special solutions of the Einstein vacuum field equations, the perturbations by massless fields of spin $\frac{1}{2}$ (neutrinos), 1 (electromagnetic field), $\frac{3}{2}$ (gravitinos), and 2 (gravitational perturbations) can be expressed in terms of a single scalar potential which obeys a second-order linear partial differential equation.[1–8]

When there is a background electromagnetic field, the electromagnetic perturbations are coupled to the gravitational perturbations. If the background electromagnetic field is non-null (algebraically general) and one of its principal null directions is geodetic and shearfree, the metric and vector potential perturbations can be expressed in terms of four scalar potentials that satisfy a system of four first-order partial differential equations.[9–12] While if the background electromagnetic field is null (algebraically special), the electromagnetic and gravitational perturbations can be expressed in terms of two scalar potentials that obey a system of two second-order partial differential equations.[13]

There are two systematic procedures to obtain the expressions of the perturbations in terms of potentials. One of them is based on the use of coordinates adapted to the totally null foliation of the space–times considered.[5,6,8,10,11,13,14] A second procedure, which is more elementary and involves shorter derivations, is Wald's method of adjoint operators, which is applicable when one can obtain decoupled equations from the perturbation equations.[3,4,7,9,12]

The aim of this paper is to give a derivation of the expressions for the complete perturbations of the solutions of the Einstein–Maxwell equations with a null background electromagnetic field in terms of two complex scalar potentials using Wald's method and the Newman–Penrose notation. The final expressions are equivalent to those obtained in Ref. 13, making use of the complex extension of the space–time and the spinor formalism. The usefulness of the formulas derived here is illustrated by considering the coupled perturbations of the Bell–Szekeres solution, which represents the collision of two plane electromagnetic waves, in the regions that contain the approaching waves (the electromagnetic field in the interaction region subsequent to the collision is algebraically general). These perturbations have been studied previously by Chandrasekhar and Xanthopoulos,[15] who solved directly the perturbation equations written in the Newman–Penrose

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notation. Our results differ from those of Ref. 15 in several aspects and we point out the origin of the discrepancies.

In Sec. II we obtain a decoupled system of two equations from the perturbation equations of a solution of the Einstein–Maxwell equations with a null background electromagnetic field which leads, making use of Wald's method, to the expressions for the complete metric and vector potential perturbations in terms of scalar potentials. In Sec. III, we find the perturbations of the Bell–Szekeres solution in those regions where the background electromagnetic field is null. Even though there is no proof that all perturbations of the solutions under consideration can be generated by the two scalar potentials employed here (see, however, Ref. 9), it has been shown,[5,6,16] by direct integration, that the general solution of the massless field equations of spin $\frac{1}{2}$, 1, and $\frac{3}{2}$ in an algebraically special space–time that admits a geodetic and shearfree null congruence can be expressed in terms of a single complex scalar potential that satisfies a second-order partial differential equation; hence, in the present case one expects that all the gravitational and electromagnetic perturbations can be expressed in terms of two complex potentials obeying a system of two second-order equations.

II. DECOUPLED EQUATIONS AND SCALAR POTENTIALS

Wald's method allows us to express the solution of a system of linear partial differential equations in terms of potentials. If $f_{\mu\nu\ldots}$ is an m-index tensor field that obeys a system of linear partial differential equations of the form

$$[\mathscr{E}(f_{\mu\nu\ldots})]_{\rho\sigma\ldots}=0, \tag{1}$$

where $\mathscr{E}$ is a linear differential operator that takes m-index tensor fields into n-index tensor fields, and if, by combining the equations in (1) and their derivatives, one is able to obtain a decoupled equation of the form

$$\mathscr{C}(\chi)=0, \tag{2}$$

where $\mathscr{C}$ is a linear differential operator that maps scalar fields into scalar fields and χ is a function made out (linearly) of $f_{\mu\nu\ldots}$ and its derivatives, then there exists a linear operator $\mathscr{T}$ such that $\chi=\mathscr{T}(f_{\mu\nu\ldots})$ and

$$\mathscr{C}\mathscr{T}=\mathscr{S}\mathscr{E}, \tag{3}$$

for some linear operator $\mathscr{S}$ which takes n-index tensor fields into scalar fields. By defining the adjoint, $\mathscr{E}^\dagger$, of $\mathscr{E}$ as that linear partial differential operator taking n-index tensor fields into m-index tensor fields such that

$$g^{\rho\sigma\cdots}[\mathscr{E}(f_{\mu\nu\ldots})]_{\rho\sigma\ldots}-[\mathscr{E}^\dagger(g^{\rho\sigma\cdots})]^{\mu\nu\cdots}f_{\mu\nu\ldots}=\nabla_\mu s^\mu, \tag{4}$$

where s^μ is some vector field, and similarly for the other operators, from Eq. (3) it follows that

$$\mathscr{E}^\dagger\mathscr{S}^\dagger=\mathscr{T}^\dagger\mathscr{C}^\dagger. \tag{5}$$

Therefore, if ψ is a scalar function satisfying $\mathscr{C}^\dagger(\psi)=0$, Eq.(5) implies that $t_{\mu\nu\ldots}=[\mathscr{S}^\dagger(\psi)]_{\mu\nu\ldots}$ satisfies the system of equations $\mathscr{E}^\dagger(t_{\mu\nu\ldots})=0$. Thus, if $\mathscr{E}$ is self-adjoint, $\mathscr{E}^\dagger=\mathscr{E}$ (as in the case of the source-free Maxwell equations for the vector potential and of the linearized Einstein vacuum field equations),[3] $\mathscr{S}^\dagger(\psi)$ is a solution of the original system, provided that the scalar potential ψ satisfies $\mathscr{C}^\dagger(\psi)=0$.

The linearized Einstein–Maxwell equations for the metric perturbations, $h_{\mu\nu}$, and the vector potential perturbations, b_μ, can be expressed in the form

$$\begin{bmatrix} \mathscr{E}_G & \mathscr{E}_{GE} \\ \mathscr{E}_{EG} & \mathscr{E}_E \end{bmatrix} \begin{bmatrix} (h_{\mu\nu}) \\ (b_\mu) \end{bmatrix} = 0, \tag{6}$$

where $\mathscr{E}_G$, $\mathscr{E}_{GE}$, $\mathscr{E}_{EG}$, and $\mathscr{E}_E$ are linear operators, and, when the background electromagnetic field is null, there exists a decoupled set of equations that follows from Eq. (6) which can also be written in matrix form [see Eqs. (21) below]. If the adjoint of an operator of the form

$$\begin{bmatrix} \mathscr{A}_{11} & \cdots & \mathscr{A}_{1s} \\ \vdots & & \\ \mathscr{A}_{r1} & \cdots & \mathscr{A}_{rs} \end{bmatrix},$$

where the $\mathscr{A}_{ij}$ are linear differential operators, is given by[12]

$$\begin{bmatrix} \mathscr{A}_{11} & \cdots & \mathscr{A}_{1s} \\ \vdots & & \\ \mathscr{A}_{r1} & \cdots & \mathscr{A}_{rs} \end{bmatrix}^\dagger = \begin{bmatrix} \mathscr{A}_{11}^\dagger & \cdots & \mathscr{A}_{r1}^\dagger \\ \vdots & & \\ \mathscr{A}_{1s}^\dagger & \cdots & \mathscr{A}_{rs}^\dagger \end{bmatrix}, \tag{7}$$

then, by multiplying one of the rows of Eq. (6) by an appropriate factor, the operator appearing in Eq. (6) is self-adjoint[9] and the conclusions of the preceding paragraph apply with χ and ψ being columns with several components. The adjoint operators can be readily obtained making use of Eq. (7), the properties $(\mathscr{A}\mathscr{B})^\dagger = \mathscr{B}^\dagger\mathscr{A}^\dagger$, $(\mathscr{A}+\mathscr{B})^\dagger = \mathscr{A}^\dagger + \mathscr{B}^\dagger$, and

$$\begin{aligned} &D^\dagger = -D - \varepsilon - \bar{\varepsilon} + \rho + \bar{\rho}, \quad \Delta^\dagger = -\Delta + \gamma + \bar{\gamma} - \mu - \bar{\mu}, \\ &\delta^\dagger = -\delta - \beta + \bar{\alpha} + \tau - \bar{\pi}, \quad \bar{\delta}^\dagger = -\bar{\delta} + \alpha - \bar{\beta} - \pi + \bar{\tau}. \end{aligned} \tag{8}$$

We shall consider a solution of the Einstein–Maxwell equations with a null background electromagnetic field and a possibly nonzero cosmological constant. Taking the tetrad vector l^μ along the (double) principal null direction of the background electromagnetic field, we have $\varphi_0 = 0 = \varphi_1$ and from the Maxwell equations it follows that $\kappa = 0 = \sigma$ (Mariot–Robinson theorem). Then, from the Goldberg–Sachs theorem one finds that $\Psi_0 = 0 = \Psi_1$. Denoting with a superscript B the first-order perturbed values of the corresponding quantities, from the Maxwell equations one obtains

$$(\bar{\delta} - 2\alpha + \pi)\varphi_0^B - (D - 2\rho)\varphi_1^B - \kappa^B \varphi_2 = 2\pi l^\mu j_\mu, \tag{9}$$

$$(\Delta - 2\gamma + \mu)\varphi_0^B - (\delta - 2\tau)\varphi_1^B - \sigma^B \varphi_2 = 2\pi m^\mu j_\mu, \tag{10}$$

where we have included a source for the electromagnetic perturbations, j_μ, in order to find an operator identity of the form (3) (cf. also Refs. 3, 7, 9, and 12).

Applying $(\delta - \beta - \bar{\alpha} - 2\tau + \bar{\pi})$ to Eq. (9) and $(D - \varepsilon + \bar{\varepsilon} - 2\rho - \bar{\rho})$ to Eq. (10) and subtracting, the terms with ψ_1^B cancel by virtue of the identity[17]

$$[D + (p-1)\varepsilon + \bar{\varepsilon} + q\rho - \bar{\rho}](\delta + p\beta + q\tau) = [\delta + (p-1)\beta - \bar{\alpha} + q\tau + \bar{\pi}](D + p\varepsilon + q\rho), \tag{11}$$

where p and q are arbitrary constants, which is a consequence of $\kappa = \sigma = \Psi_1 = 0$. Making use of the Maxwell equations

$$(D + 2\varepsilon - \rho)\varphi_2 = 0 = (\delta + 2\beta - \tau)\varphi_2 \tag{12}$$

and of the Ricci identity

$$(D-3\varepsilon+\bar{\varepsilon}-\rho-\bar{\rho})\sigma^B-(\delta-3\beta-\bar{\alpha}-\tau+\bar{\pi})\kappa^B=\Psi_0^B, \tag{13}$$

one finds that

$$\mathscr{O}_E(\varphi_0^B)-\varphi_2\Psi_0^B=2\pi[(D-\varepsilon+\bar{\varepsilon}-2\rho-\bar{\rho})(m^\mu j_\mu)-(\delta-\beta-\bar{\alpha}-2\tau+\bar{\pi})(l^\mu j_\mu)], \tag{14}$$

where

$$\mathscr{O}_E\equiv(D-\varepsilon+\bar{\varepsilon}-2\rho-\bar{\rho})(\Delta-2\gamma+\mu)-(\delta-\beta-\bar{\alpha}-2\tau+\bar{\pi})(\bar{\delta}-2\alpha+\pi). \tag{15}$$

Similarly, from the Bianchi identities one obtains

$$\begin{aligned}(\bar{\delta}-4\alpha+\pi)\Psi_0^B-(D-2\varepsilon-4\rho)\Psi_1^B-3\kappa^B\Psi_2\\ =4\pi[(\delta-2\beta-2\bar{\alpha}+\bar{\pi})l^\mu l^\nu T_{\mu\nu}-(D-2\varepsilon-2\bar{\rho})l^\mu m^\nu T_{\mu\nu}],\end{aligned} \tag{16}$$

$$\begin{aligned}(\Delta-4\gamma+\mu)\Psi_0^B-(\delta-2\beta-4\tau)\Psi_1^B-3\sigma^B\Psi_2+2(D-2\varepsilon+2\bar{\varepsilon}-\bar{\rho})\overline{\varphi_2}\varphi_0^B\\ =4\pi[(\delta-2\beta+2\bar{\pi})l^\mu m^\nu T_{\mu\nu}-\bar{\lambda}l^\mu l^\nu T_{\mu\nu}-(D-2\varepsilon+2\bar{\varepsilon}-\bar{\rho})m^\mu m^\nu T_{\mu\nu}],\end{aligned} \tag{17}$$

where we have included a source for the gravitational perturbations, $T_{\mu\nu}$ (in addition to the contribution coming from the electromagnetic perturbations), which will allow us to identify the operator $\mathscr{T}$, and we have made use of the Einstein field equations. Applying $(\delta-3\beta-\bar{\alpha}-4\tau+\bar{\pi})$ to Eq. (16) and $(D-3\varepsilon+\bar{\varepsilon}-4\rho-\bar{\rho})$ to Eq. (17), subtracting and using Eqs. (11)–(13) and the Bianchi identities $(D-3\rho)\Psi_2=0=(\delta-3\tau)\Psi_2$, it follows that

$$\begin{aligned}&\mathscr{O}_G(\Psi_0^B)+2\overline{\varphi_2}(D-3\varepsilon-\bar{\varepsilon}-4\rho)(D-2\varepsilon)\varphi_0^B\\ &=4\pi\{(D-3\varepsilon+\bar{\varepsilon}-4\rho-\bar{\rho})[(\delta-2\beta+2\bar{\pi})l^\mu m^\nu T_{\mu\nu}-(D-2\varepsilon+2\bar{\varepsilon}-\bar{\rho})\\ &\quad\times m^\mu m^\nu T_{\mu\nu}-\bar{\lambda}l^\mu l^\nu T_{\mu\nu}]+(\delta-3\beta-\bar{\alpha}-4\tau+\bar{\pi})\\ &\quad\times[(D-2\varepsilon-2\bar{\rho})l^\mu m^\nu T_{\mu\nu}-(\delta-2\beta-2\bar{\alpha}+\bar{\pi})l^\mu l^\nu T_{\mu\nu}]\},\end{aligned} \tag{18}$$

where

$$\mathscr{O}_G\equiv(D-3\varepsilon+\bar{\varepsilon}-4\rho-\bar{\rho})(\Delta-4\gamma+\mu)-(\delta-3\beta-\bar{\alpha}-4\tau+\bar{\pi})(\bar{\delta}-4\alpha+\pi)-3\Psi_2. \tag{19}$$

Thus, setting $j_\mu=0$, $T_{\mu\nu}=0$ in Eqs. (14) and (18), we find that the perturbation equations imply that φ_0^B and Ψ_0^B satisfy the equations

$$\begin{aligned}\mathscr{O}_E(\varphi_0^B)-\varphi_2\Psi_0^B=0,\\ \mathscr{O}_G(\Psi_0^B)+2\overline{\varphi_2}(D-3\varepsilon-\bar{\varepsilon}-4\rho)(D-2\varepsilon)\varphi_0^B=0.\end{aligned} \tag{20}$$

On the other hand, Eqs. (14) and (18) can be expressed in the form

$$\begin{bmatrix} \mathcal{O}_G & 2\overline{\varphi_2}(D-3\varepsilon-\bar{\varepsilon}-4\rho)(D-2\varepsilon) \\ -\varphi_2 & \mathcal{O}_E \end{bmatrix} \begin{bmatrix} \Psi_0^B \\ \varphi_0^B \end{bmatrix}$$

$$= 4\pi \begin{bmatrix} (D-3\varepsilon+\bar{\varepsilon}-4\rho-\bar{\rho})[(\delta-2\beta+2\bar{\pi})l^\mu m^\nu T_{\mu\nu}-(D-2\varepsilon+2\bar{\varepsilon}-\bar{\rho})m^\mu m^\nu T_{\mu\nu} \\ -\bar{\lambda}l^\mu l^\nu T_{\mu\nu}]+(\delta-3\beta-\bar{\alpha}-4\tau+\bar{\pi})[(D-2\varepsilon-2\bar{\rho})l^\mu m^\nu T_{\mu\nu} \\ -(\delta-2\beta-2\bar{\alpha}+\bar{\pi})l^\mu l^\nu T_{\mu\nu}] \\ \\ \frac{1}{2}[(D-\varepsilon+\bar{\varepsilon}-2\rho-\bar{\rho})m^\mu-(\delta-\beta-\bar{\alpha}-2\tau+\bar{\pi})l^\mu]j_\mu \end{bmatrix}, \quad (21)$$

which is an equation of the form (3), where the 2×2 matrix on the left-hand side corresponds to the operator $\mathcal{O}$,

$$\begin{bmatrix} \Psi_0^B \\ \varphi_0^B \end{bmatrix} = \mathcal{I} \begin{bmatrix} (h_{\mu\nu}) \\ (b_\mu) \end{bmatrix},$$

and the column on the right-hand side is, essentially,

$$\mathcal{S} \begin{bmatrix} (T_{\mu\nu}) \\ (j_\mu) \end{bmatrix}.$$

Making use of Eqs. (7), (8), and (12) one readily finds that

$$\mathcal{O}^\dagger = \begin{bmatrix} \mathcal{O}_G^\dagger & -\varphi_2 \\ 2\overline{\varphi_2}(D+3\varepsilon-\bar{\varepsilon}-\rho)(D+4\varepsilon+3\rho) & \mathcal{O}_E^\dagger \end{bmatrix},$$

where

$$\begin{aligned} \mathcal{O}_G^\dagger &\equiv (\Delta+3\gamma-\bar{\gamma}+\bar{\mu})(D+4\varepsilon+3\rho)-(\bar{\delta}+3\alpha+\bar{\beta}-\bar{\tau})(\delta+4\beta+3\tau)-3\Psi_2, \\ \mathcal{O}_E^\dagger &\equiv (\Delta+\gamma-\bar{\gamma}+\bar{\mu})(D+2\varepsilon+\rho)-(\bar{\delta}+\alpha+\bar{\beta}-\bar{\tau})(\delta+2\beta+\tau), \end{aligned} \quad (22)$$

and that the adjoints of the operators acting on $T_{\mu\nu}$ and j_μ on the right-hand side of Eq. (21) are (excluding the constant factor 4π)

$$\begin{aligned} &-l^\mu l^\nu[(\delta+3\beta+\bar{\alpha}-\tau)(\delta+4\beta+3\tau)-\bar{\lambda}(D+4\varepsilon+3\rho)]-m^\mu m^\nu(D+3\varepsilon-\bar{\varepsilon}-\rho)(D+4\varepsilon+3\rho) \\ &+l^{(\mu}m^{\nu)}[(D+3\varepsilon+\bar{\varepsilon}-\rho+\bar{\rho})(\delta+4\beta+3\tau)+(\delta+3\beta-\bar{\alpha}-\tau-\bar{\pi})(D+4\varepsilon+3\rho)], \\ &\frac{1}{2}[l^\mu(\delta+2\beta+\tau)-m^\mu(D+2\varepsilon+\rho)]. \end{aligned} \quad (23)$$

Hence, if the scalar potentials, ψ_G, ψ_E, satisfy the equation $\mathcal{O}^\dagger\begin{bmatrix}\psi_G \\ \psi_E\end{bmatrix} = 0$ i.e.,

$$\begin{aligned} &\mathcal{O}_G^\dagger(\psi_G)-\varphi_2\psi_E=0, \\ &2\overline{\varphi_2}(D+3\varepsilon-\bar{\varepsilon}-\rho)(D+4\varepsilon+3\rho)\psi_G+\mathcal{O}_E^\dagger(\psi_E)=0, \end{aligned} \quad (24)$$

then the metric and vector potential perturbations are obtained by applying the operators (23) on the two-component column formed by ψ_G and ψ_E. In order to find the correct relative normalization one can use the fact that the perturbations Ψ_0^B and φ_0^B generated by ψ_G and ψ_E must satisfy Eqs. (20) [see Eqs. (27) and (29) below]. Thus, we find for the *real* perturbations

$$h_{\mu\nu}=-2\{l_\mu l_\nu[(\delta+3\beta+\bar{\alpha}-\tau)(\delta+4\beta+3\tau)-\bar{\lambda}(D+4\varepsilon+3\rho)]$$
$$+m_\mu m_\nu(D+3\varepsilon-\bar{\varepsilon}-\rho)(D+4\varepsilon+3\rho)-l_{(\mu}m_{\nu)}[(D+3\varepsilon+\bar{\varepsilon}-\rho+\bar{\rho})(\delta+4\beta+3\tau)$$
$$+(\delta+3\beta-\bar{\alpha}-\tau-\bar{\pi})(D+4\varepsilon+3\rho)]\}\psi_G+\text{c.c.}, \tag{25}$$

$$b_\mu=\tfrac{1}{2}[l_\mu(\delta+2\beta+\tau)-m_\mu(D+2\varepsilon+\rho)]\psi_E+\text{c.c.} \tag{26}$$

Then, the components of the perturbed electromagnetic field are given by

$$\overline{\varphi_0^B}=\tfrac{1}{2}(D+\varepsilon-\bar{\varepsilon}-\rho)(D+2\varepsilon+\rho)\psi_E,$$

$$\overline{\varphi_1^B}=\tfrac{1}{4}[(D+\varepsilon+\bar{\varepsilon}-\rho+\bar{\rho})(\delta+2\beta+\tau)+(\delta+\beta-\bar{\alpha}-\tau-\bar{\pi})(D+2\varepsilon+\rho)]\psi_E,$$

$$\overline{\varphi_2^B}=\tfrac{1}{2}[(\delta+\beta+\bar{\alpha}-\tau)(\delta+2\beta+\tau)-\bar{\lambda}(D+2\varepsilon+\rho)]\psi_E+\varphi_2(D-\varepsilon+3\bar{\varepsilon}-\bar{\rho})(D+4\bar{\varepsilon}+3\bar{\rho})\overline{\psi_G}, \tag{27}$$

where we have made use of Eq. (24). The components of the perturbed Weyl spinor can be obtained from Eq. (25), making use of the formula

$$\Psi^B_{ACDE}=\tfrac{1}{2}\nabla^{R'}{}_{(A}\nabla^{S'}{}_{C}h_{DE)R'S'}. \tag{28}$$

In this manner, we find that

$$\overline{\Psi_0^B}=-(D+\varepsilon-3\bar{\varepsilon}-\rho)(D+2\varepsilon-2\bar{\varepsilon}-\rho)(D+3\varepsilon-\bar{\varepsilon}-\rho)(D+4\varepsilon+3\rho)\psi_G, \tag{29}$$

$$\overline{\Psi_4^B}=-[(\delta+\beta+3\bar{\alpha}-\tau)(\delta+2\beta+2\bar{\alpha}-\tau)-\bar{\lambda}(D+2\varepsilon+2\bar{\varepsilon}-\rho+2\bar{\rho})]$$
$$\times\{[(\delta+3\beta+\bar{\alpha}-\tau)(\delta+4\beta+3\tau)-\bar{\lambda}(D+4\varepsilon+3\rho)]\psi_G$$
$$+[(\bar{\delta}+\alpha+3\bar{\beta}-\bar{\tau})(\bar{\delta}+4\bar{\beta}+3\bar{\tau})-\lambda(D+4\bar{\varepsilon}+3\bar{\rho})]\overline{\Psi_G}\}$$
$$-[(\Delta-\gamma+3\bar{\gamma}+\mu)(\Delta-2\gamma+2\bar{\gamma}+\mu)+\nu(\delta-2\beta+2\bar{\alpha})$$
$$-\bar{\nu}(\bar{\delta}-2\alpha+2\bar{\beta}+\pi+2\bar{\tau})+((\delta+3\beta+\bar{\alpha}-\tau)\nu-\lambda\bar{\lambda})]$$
$$\times(D-\varepsilon+3\bar{\varepsilon}-\bar{\rho})(D+4\bar{\varepsilon}+3\bar{\rho})\overline{\psi_G}$$
$$+\tfrac{1}{2}[(\Delta-\gamma+3\bar{\gamma}+\mu)(\delta+2\bar{\alpha}-2\tau)+(\delta+\beta+3\bar{\alpha}-\tau)(\Delta+2\bar{\gamma}+2\mu)$$
$$-\bar{\nu}(D+2\bar{\varepsilon}-2\rho+2\bar{\rho})-\bar{\lambda}(\bar{\delta}+2\bar{\beta}+2\pi+2\bar{\tau})]$$
$$\times[(D+\varepsilon+3\bar{\varepsilon}+\rho-\bar{\rho})(\bar{\delta}+4\bar{\beta}+3\bar{\tau})+(\bar{\delta}-\alpha+3\bar{\beta}-\pi-\bar{\tau})(D+4\bar{\varepsilon}+3\bar{\rho})]\overline{\psi_G}$$
$$+[(\delta-\beta+3\bar{\alpha}-\bar{\pi})\bar{\lambda}][(D+3\varepsilon+\bar{\varepsilon}-\rho+\bar{\rho})(\delta+4\beta+3\tau)$$
$$+(\delta+3\beta-\bar{\alpha}-\tau-\bar{\pi})(D+4\varepsilon+3\rho)]\psi_G$$
$$-2\overline{\lambda\lambda}(D+3\varepsilon-\bar{\varepsilon}-\rho)(D+4\varepsilon+3\rho)\psi_G.$$

III. PERTURBATIONS OF THE BELL–SZEKERES SOLUTION

As shown in Ref. 15, the metric in each of the regions prior to the collision of the plane-fronted waves in the Bell–Szekeres solution can be specified by the null tetrad

$$D=-\frac{1}{\sqrt{2}}\,\partial_u,\quad \Delta=-\frac{1}{\sqrt{2}}\,(1-v^2)^{1/2}\partial_v,$$

$$\delta=\frac{1}{\sqrt{2}}\,(1-v^2)^{-1/2}(\partial_{x^1}-i\partial_{x^2}),\quad \bar{\delta}=\frac{1}{\sqrt{2}}\,(1-v^2)^{-1/2}(\partial_{x^1}+i\partial_{x^2}), \tag{30}$$

where u,v,x^1,x^2 are real coordinates. The only nonvanishing spin-coefficient is given by

$$\mu=\Delta\,\ln(1-v^2)^{1/2}, \tag{31}$$

the only nonvanishing component of the curvature is

$$\Phi_{22}=\tfrac{1}{2}, \tag{32}$$

and the electromagnetic field is given by

$$\varphi_0=0=\varphi_1,\quad \varphi_2=\tfrac{1}{2}. \tag{33}$$

Hence, the results of the preceding section can be applied to this solution with the null tetrad (30). Since u, x^1, and x^2 are ignorable coordinates, we seek solutions of Eqs. (24) of the form

$$\psi_E=f(v)e^{i(k_1x^1+k_2x^2+k_3u)},\quad \psi_G=g(v)e^{i(k_1x^1+k_2x^2+k_3u)}, \tag{34}$$

where k_1, k_2, and k_3 are constants. Substituting Eqs. (30), (31), (33), and (34) into Eqs. (24) one obtains the linear ordinary differential equations

$$ik_3\frac{d}{dv}\,[(1-v^2)^{1/2}g]+\frac{k_1^2+k_2^2}{1-v^2}\,g=f,$$

$$ik_3\frac{d}{dv}\,[(1-v^2)^{1/2}f]+\frac{k_1^2+k_2^2}{1-v^2}\,f=k_3^2g. \tag{35}$$

It can be easily verified that, if $k_3\neq0$, the most general solution of Eqs. (35) is given by[15]

$$f=(C_1v(1-v^2)^{-1/2}+C_2)\exp\left[i\,\frac{(k_1^2+k_2^2)}{k_3}\,v(1-v^2)^{-1/2}\right],$$

$$g=ik_3^{-1}(-C_2v(1-v^2)^{-1/2}+C_1)\exp\left[i\,\frac{(k_1^2+k_2^2)}{k_3}\,v(1-v^2)^{-1/2}\right], \tag{36}$$

where C_1 and C_2 are arbitrary constants (the case where k_3 vanishes will be treated below).

From Eqs. (27)–(31), (33), and (34) one obtains

$$\overline{\varphi_0^B}=-\tfrac{1}{4}k_3^2f(v)e^{i(k_1x^1+k_2x^2+k_3u)},\quad \overline{\varphi_1^B}=\frac{i(k_2+ik_1)}{k_3\sqrt{1-v^2}}\,\overline{\varphi_0^B},$$

$$\overline{\varphi_2^B}=-\frac{(k_2+ik_1)^2}{k_3^2(1-v^2)}\,\overline{\varphi_0^B}-\tfrac{1}{4}\overline{k_3^2g(v)e^{i(k_1x^1+k_2x^2+k_3u)}},$$

$$\overline{\Psi_0^B}=-\tfrac{1}{4}k_3^4 g(v)e^{i(k_1x^1+k_2x^2+k_3u)},\quad \overline{\Psi_1^B}=i\,\frac{(k_2+ik_1)}{k_3\sqrt{1-v^2}}\,\overline{\Psi_0^B},$$

$$\overline{\Psi_2^B}=-\frac{(k_2+ik_1)^2}{k_3^2(1-v^2)}\,\overline{\Psi_0^B},\quad \overline{\Psi_3^B}=-i\,\frac{(k_2+ik_1)^3}{k_3^3(1-v^2)^{3/2}}\,\overline{\Psi_0^B},\tag{37}$$

$$\overline{\Psi_4^B}=\frac{(k_2+ik_1)^4}{k_3^4(1-v^2)^2}\,\overline{\Psi_0^B}-\overline{\tfrac{1}{4}k_3^2 g(v)e^{i(k_1x^1+k_2x^2+k_3u)}},$$

where in the last equality we have made use of the fact that, in the present case, the terms containing $\overline{\psi_G}$ in Eq. (29) reduce to

$$\tfrac{1}{2}D^2\overline{\psi_G}\tag{38}$$

as a consequence of Eqs. (24).

The expressions for φ_2^B and Ψ_4^B given in Eqs. (37) (which are the only ones that contain $e^{i(k_1x^1+k_2x^2+k_3u)}$ and its complex conjugate) do not agree with the corresponding expressions obtained by Chandrasekhar and Xanthopoulos.[15] The error in Ref. 15 comes from the assumption that *all* the perturbed quantities have a dependence on x^1, x^2, and u of the form

$$e^{i(k_1x^1+k_2x^2+k_3u)}\tag{39}$$

even though some of the equations considered in that paper contain the perturbations of the electromagnetic field and of the conformal curvature and their complex conjugates [see, e.g., Eqs. (164) and (167) of Ref. 15].

It may be noticed that, in the approach followed here, the simultaneous presence of a factor (39) and its complex conjugate in some of the perturbed quantities arises naturally as a consequence of considering real metric and vector potential perturbations, despite the fact that the potentials ψ_E and ψ_G have a dependence on the ignorable coordinates of the form (39). [As pointed out in Ref. 18, the presence of the factor (39) and its complex conjugate in φ_2^B and Ψ_4^B means that there is a change in the polarization of the perturbations produced by their scattering from the background solution.] As noted in Ref. 15, the perturbations (37) diverge at $v=1$.

Now we shall consider the u-independent perturbations (which correspond to the case $k_3=0$). It is convenient to use in place of the real coordinates x^1 and x^2, the complex variable

$$z\equiv\frac{x^1+ix^2}{\sqrt{2}}\tag{40}$$

and its complex conjugate. Then, $\delta=(1-v^2)^{-1/2}\partial_z$ and $\overline{\delta}=(1-v^2)^{-1/2}\partial_{\bar{z}}$.

Assuming that the potentials ψ_G and ψ_E do not depend on u from Eqs. (24) it follows that

$$\psi_G=(1-v^2)^2[\bar{z}F(v,z)+G(v,z)],$$

$$\psi_E=-2(1-v^2)\partial_z F(v,z),\tag{41}$$

where $F(v,z)$ and $G(v,z)$ are arbitrary functions and the factors $(1-v^2)$ are introduced for convenience. {In these expressions for ψ_G and ψ_E we have excluded terms of the form $(1-v^2)^2[z\tilde{F}(v,\bar{z})+\tilde{G}(v,\bar{z})]$ and $-2(1-v^2)\partial_{\bar{z}}\tilde{F}(v,\bar{z})$, respectively, which yield trivial perturbations [see Eqs. (25) and (26)].} The metric and vector potential perturbations generated by (41) are

$$h_{\mu\nu}=-2(1-v^2)\{\bar{z}\partial_z^2F(v,z)+\partial_z^2G(v,z)+z\overline{\partial_z^2F(v,z)}+\overline{\partial_z^2G(v,z)}\}l_\mu l_\nu,$$
$$b_\mu=-\sqrt{1-v^2}[\partial_z^2F(v,z)+\overline{\partial_z^2F(v,z)}]l_\mu. \tag{42}$$

with $l_\mu dx^\mu=-\sqrt{2}(1-v^2)^{-1/2}\,dv$. And, according to Eqs. (27)–(29), the only nonvanishing components of the perturbed electromagnetic field and of the perturbed Weyl spinor are

$$\overline{\varphi_2^B}=-\partial_z^3F(v,z),\quad \overline{\Psi_4^B}=-\bar{z}\partial_z^4F(v,z)-\partial_z^4G(v,z). \tag{43}$$

Thus, contrary to the claim made in Ref. 15, there exist nontrivial u-independent perturbations which, moreover, need not diverge at $v=1$. Furthermore, if $\partial_z^3F=0$ (i.e., when the electromagnetic perturbations vanish), the metric perturbation (42) is not only a solution of the linearized Einstein–Maxwell equations, but it also corresponds to an *exact* solution of the Einstein–Maxwell equations. This result is analogous to Xanthopoulos theorem,[19] except that in the present case the background solution possesses an electromagnetic field (see also Ref. 20).

IV. CONCLUDING REMARKS

One of the advantages of finding the perturbations in terms of potentials is that one only has to find a consistent solution of the differential equations for the potentials, since the metric and vector potential perturbations are obtained by differentiating the potentials. It may be noticed, for instance, that in the study of the perturbations of the solution (31)–(33) presented in Ref. 15, after imposing some gauge conditions, at least 27 equations had to be considered.

Since we have found that there exist well-behaved perturbations in the region of the Bell–Szekeres solution that contain the approaching waves, it is interesting to find out whether these perturbations can be matched continuously with perturbations in the interaction region of the colliding waves (cf. Ref. 15).

Note added in proof: The term $\frac{1}{2}\Phi_{(AC'R'S'}h_{DE)R'S'}$ is missing in the right-hand side of Eq. (28), which only contributes to Ψ_4^B and cancels the second term in the right-hand side of the last equality in Eqs. (37).

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Three-dimensional Riemannian manifolds with constant principal Ricci curvatures $\rho_1=\rho_2\neq\rho_3$

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The main aim of this paper is the study of (nonhomogeneous) three-dimensional Riemannian manifolds with constant principal Ricci curvatures $\rho_1=\rho_2\neq\rho_3$. An error in a recent paper by McManus is pointed out and corrected, and it is shown that the techniques introduced by McManus provide a very simple method to obtain the complete local classification of these manifolds, which was first given by Kowalski.
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I. INTRODUCTION

A (pseudo-)Riemannian manifold (M,g) is said to be *curvature homogeneous*[1] if, for every pair of points $p,q\in M$, there exists a linear isometry $\varphi:T_pM\to T_qM$, such that, for all $X,Y,Z\in T_pM$,

$$\varphi R_{XY}Z=R_{\varphi X\varphi Y}\varphi Z,$$

where R denotes the Riemann curvature tensor of (M,g). It is easily seen that any (locally) homogeneous manifold is automatically curvature homogeneous, and in Ref. 1. Singer states the problem of constructing examples of nonhomogeneous curvature homogeneous spaces. This problem was studied extensively in both the Riemannian and Lorentzian case (see, e.g., Refs. 2–10), leading to the construction of a large number of explicit examples. For more information on the subject of curvature homogeneity and for a survey of known results, we refer to Refs. 11–14.

It is well known that the Riemann curvature tensor of a three-dimensional Riemannian manifold (M,g) is completely determined by its Ricci tensor and, as a consequence, a three-dimensional Riemannian manifold is curvature homogeneous if and only if it has constant *principal Ricci curvatures*, i.e., its Ricci tensor has constant eigenvalues. If all principal Ricci curvatures are equal (and constant), the manifold (M,g) is of constant curvature and hence locally homogeneous. In a number of recent papers (Refs. 5, 6, 15, and 16), the authors studied the problem of three-dimensional Riemannian manifolds with constant principal Ricci curvatures $\rho_1=\rho_2\neq\rho_3$. In Refs. 5 and 6, explicit examples of nonhomogeneous curvature homogeneous spaces with principal Ricci curvatures

$$\rho_1=\rho_2\neq\rho_3=0$$

were obtained by generalizing a construction of Sekigawa,[2] and it was later shown in Ref. 15 (see also Ref. 13) that these are the only examples of such manifolds. In Ref. 16, Kowalski gives a complete (local) classification of all three-dimensional Riemannian manifolds with constant principal Ricci curvatures $\rho_1=\rho_2\neq\rho_3(\neq0)$. He proves that, for any choice of constants $0\neq\alpha\neq\beta$, there exists a family of nonhomogeneous curvature homogeneous Riemannian manifolds (depending on two functions of one variable) whose associated principal Ricci curvatures are given by

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$$\rho_1=\rho_2=\beta, \quad \rho_3=\alpha, \tag{1}$$

and he constructs some explicit examples of such metrics. However, we remark that the techniques used in this paper are quite complicated, (e.g., the introduction of asymptotic foliations), and the computations involved in the proofs are of a rather complex nature.

In their study of space-times admitting shear-free, irrotational, geodesic time-like congruences, Coley and McManus (Refs. 17 and 18) were led to consider three-dimensional Riemannian manifolds with constant principal Ricci curvatures satisfying (1). Further, in Refs. 19 and 20, Bona and Coll studied the isometry groups of three-dimensional Riemannian metrics using the eigenvalues and eigenvectors of their Ricci tensor. In particular, they made a study of three-dimensional Riemannian manifolds satisfying (1) and admitting a three-dimensional or four-dimensional isometry group, which acts transitively. Motivated by these results, McManus[21] addresses, independently of the work of Kowalski, the problem of completely classifying these manifolds in the homogeneous and nonhomogeneous cases. Unfortunately, one of the main results (Theorem 2) stated in Ref. 21 (as well as Theorem 2 in Ref. 18) claims that a three-dimensional Riemannian manifold with constant principal Ricci curvatures $\rho_1=\rho_2\neq\rho_3$ is nonhomogeneous if and only if the simple principal Ricci curvature is zero and the shear of its principal Ricci direction is nonzero, leading to an obvious contradiction with the results of Ref. 16.

The first aim of this paper is to point out and correct the error made in Ref. 21. We will show that the techniques introduced by McManus can be applied to prove the (local) existence of a family of nonhomogeneous three-dimensional Riemannian manifolds with constant principal Ricci curvatures given by (1). We will then determine which of the metrics obtained in this way are isometric, thereby giving an alternative proof of the classification result from Ref. 16. It will turn out that the computations needed in this approach are much simpler than those used by Kowalski,[16] leading to a considerable simplification of the classification result, although up to this moment we were unable to find new examples of such spaces.

The paper is organized as follows. In Sec. II, we derive the differential equations that have to be satisfied by a Riemannian manifold with constant principal Ricci curvatures given by (1). We remark that many of the equations in this section have already been obtained in Refs. 19–21, but are collected here for easy reference. In Sec. III, we then investigate which of these manifolds are locally homogeneous. In Sec. IV we study the differential equations of Sec. II in more detail. Correcting the mistake in Ref. 21, we prove the (local) existence of nonhomogeneous Riemannian manifolds whose principal Ricci curvatures satisfy (1) for arbitrary constants α and β. Finally, in Sec. V we investigate the problem of determining which of these manifolds are isometric, thereby obtaining a new (and simpler) proof of the classification result in Ref. 16.

We end this section by remarking that the techniques used in the present paper can be adapted easily to the case where M is a three-dimensional Lorentzian manifold, leading to a similar classification of Lorentzian manifolds with constant principal Ricci curvatures given by (1). Again, this problem was studied before by McManus,[22] but, unfortunately, a similar mistake was made in this paper. In a forthcoming publication,[23] we will correct this error (as well as another one appearing in Ref. 22), and we will prove a classification result similar to the one given in the present paper.

II. THE BASIC DIFFERENTIAL EQUATIONS

We start this section by fixing some notations. In what follows, we denote by (M,g) a (smooth) three-dimensional Riemannian manifold and by ∇ the *Levi Civita connection* associated to g. Further, we define the *Riemann curvature tensor* R of (M,g) as the (1,3)-tensor field,

$$R_{XY}Z=\nabla_{[X,Y]}Z-\nabla_X\nabla_Y Z+\nabla_Y\nabla_X Z, \tag{2}$$

for all vector fields $X,Y,Z\in\mathfrak{X}(M)$. The *Ricci curvature tensor* ρ is defined (at the point $p\in M$) as the trace

$$\rho(X,Y)(p)=\sum_{i=1}^{3} g(R_{XE_i}Y,E_i)(p), \tag{3}$$

where $X,Y\in T_pM$ and $\{E_1,E_2,E_3\}$ is an orthonormal basis for T_pM, and the trace

$$\tau(p)=\sum_{i=1}^{3} \rho(E_i,E_i)(p),$$

is called the *scalar curvature* of (M,g) at p.

Let $\xi\in\mathfrak{X}(M)$ be a vector field of unit length, denote by η the metric dual of ξ, i.e., the one-form given, for all $X\in\mathfrak{X}(M)$, by

$$\eta(X)=g(X,\xi),$$

and by $h=g-\eta\otimes\eta$ the *projection tensor* associated to ξ. Then it is well known that there exists a *unique* decomposition

$$g(\nabla_X\xi,Y)=\sigma(X,Y)+\omega(X,Y)+\tfrac{1}{2}\theta h(X,Y)+g(\nabla_\xi\xi,Y)g(\xi,X), \tag{4}$$

where σ is a trace-free, symmetric (0,2)-tensor field and ω is an antisymmetric (0,2)-tensor field, such that, for all $X\in\mathfrak{X}(M)$,

$$\omega(X,\xi)=\sigma(X,\xi)=0.$$

The function

$$\theta=\sum_{i=1}^{3} g(\nabla_{E_i}\xi,E_i),$$

is said to be the *expansion* of ξ, and the (0,2)-tensor field σ (resp., ω) is called the *shear tensor* (resp., *twist tensor*) of ξ.

Now, let us suppose that (M,g) is a three-dimensional Riemannian manifold whose constant principal Ricci curvatures are given by (1). Then, locally, we can construct an orthonormal frame field $\{E_1,E_2,E_3\}$ consisting of principal Ricci directions, i.e., such that

$$\rho(E_1,E_1)=\rho(E_2,E_2)=\beta,\quad \rho(E_3,E_3)=\alpha,\quad \rho(E_i,E_j)=0,\quad \text{if } i\neq j. \tag{5}$$

Twice contracting the second Bianchi identity,

$$\nabla_{E_i}R_{E_jE_k}E_l+\nabla_{E_j}R_{E_kE_i}E_l+\nabla_{E_k}R_{E_iE_j}E_l=0,$$

we obtain the so-called three-dimensional second Bianchi identity,

$$E_i(\tau)-2\sum_{j=1}^{3}\nabla_{E_j}\rho(E_i,E_j)=0,\quad i\in\{1,2,3\}, \tag{6}$$

and taking into account that $\tau=2\beta+\alpha$ is constant along M, (6) is equivalent to

$$\sum_{j=1}^{3} g(\nabla_{E_j}E_i,E_j)\rho(E_j,E_j)+g(\nabla_{E_j}E_j,E_i)\rho(E_i,E_i)=0, \tag{7}$$

for all $i\in\{1,2,3\}$. Using the fact that $\alpha\neq\beta$, (7) yields that

$$g(\nabla_{E_3}E_3,E_1)=0,\quad g(\nabla_{E_3}E_3,E_2)=0,$$
$$g(\nabla_{E_1}E_3,E_1)+g(\nabla_{E_2}E_3,E_2)=0, \tag{8}$$

i.e., the simple principal Ricci direction E_3 is *geodesic* and *expansion-free*.[19–21]

At each point $p\in M$, the linear operator $\bar{\sigma}(p):T_pM\to T_pM$ associated to the shear tensor of E_3 is self-adjoint and trace-free, and $\bar{\sigma}E_3=0$. Hence, diagonalizing the operator $\bar{\sigma}$ at all points $p\in M$, we obtain a (local) orthonormal frame field $\{E_1,E_2,E_3\}$, consisting of principal Ricci directions [as in (5)] and such that the shear tensor of E_3 takes the form

$$\sigma(E_1,E_1)=-\sigma(E_2,E_2)=\sigma,\quad \sigma(E_1,E_2)=0,\quad \sigma(E_3,E_i)=0,\quad i\in\{1,2,3\}. \tag{9}$$

It follows from (4), (8), and (9) that, with respect to this local orthonormal frame field, the components of the Levi Civita connection of (M,g) are given by

$$\nabla_{E_1}E_1=-\theta_2E_2-\sigma E_3,\quad \nabla_{E_2}E_1=\theta_1E_2+\omega E_3,\quad \nabla_{E_3}E_1=kE_2,$$
$$\nabla_{E_1}E_2=\theta_2E_1-\omega E_3,\quad \nabla_{E_2}E_2=-\theta_1E_1+\sigma E_3,\quad \nabla_{E_3}E_2=-kE_1, \tag{10}$$
$$\nabla_{E_1}E_3=\sigma E_1+\omega E_2,\quad \nabla_{E_2}E_3=-\omega E_1-\sigma E_2,\quad \nabla_{E_3}E_3=0,$$

where we have denoted by $\omega=\omega(E_1,E_2)$ the only nonvanishing component of the twist tensor of E_3, and by $\theta_1=g(\nabla_{E_2}E_1,E_2)$ and $\theta_2=g(\nabla_{E_1}E_2,E_1)$ the expansions of E_1 and E_2. A straightforward computation using (2), (3), and (10) [or, alternatively, expressing the fact that, for all $X,Y\in\mathfrak{X}(M)$, $\rho(X,Y)=-[\nabla_X,\delta]Y-\operatorname{tr}\nabla Y\circ\nabla X$, where δ denotes the divergence operator] then yields that

$$\rho(E_1,E_1)=-\theta_2^2-\theta_1^2-2k\omega-E_1(\theta_1)-E_2(\theta_2)-E_3(\sigma),$$
$$\rho(E_2,E_2)=-\theta_2^2-\theta_1^2-2k\omega-E_1(\theta_1)-E_2(\theta_2)+E_3(\sigma),$$
$$\rho(E_3,E_3)=2(\omega^2-\sigma^2),$$
$$\rho(E_1,E_2)=-2k\sigma-E_3(\omega)=-2k\sigma+E_3(\omega), \tag{11}$$
$$\rho(E_1,E_3)=2\theta_1\sigma+E_1(\sigma)+E_2(\omega)=-(\omega-k)\theta_2+\sigma\theta_1+E_2(k)-E_3(\theta_1),$$
$$\rho(E_2,E_3)=-2\theta_2\sigma-E_1(\omega)-E_2(\sigma)=(\omega-k)\theta_1-\sigma\theta_2-E_1(k)-E_3(\theta_2).$$

From (11) and the fact that $\rho(E_1,E_2)=0$, it follows immediately that

$$k\sigma=0. \tag{12}$$

Let us suppose that $k\neq0$ at a point $p\in M$. Then there exists an open neighborhood U around p such that $k\neq0$ on U, and (12) implies that $\sigma=0$ on U. Consequently, the frame field $\{E_1,E_2,E_3\}$ is only determined up to a rotation of the vectors E_1 and E_2, i.e., we can replace it by a new frame field,

$$E_1'=\sin\varphi E_1+\cos\varphi E_2,\quad E_2'=-\cos\varphi E_1+\sin\varphi E_2,\quad E_3'=E_3.$$

In this new frame field, we have

$$\nabla_{E_3'}E_1' = -(E_3(\varphi)-k)E_2' = k'E_2',$$

and choosing the function $\varphi \in C^\infty(M)$ to be a solution of the differential equation

$$E_3(\varphi) = k,$$

we see that $k'=0$. As a consequence, we can always specify the (local) orthonormal frame field $\{E_1,E_2,E_3\}$ in such a way that $k=0$.

Expressing (5) using (11), we then obtain the equations

$$2(\omega^2-\sigma^2)=\alpha, \tag{13}$$

$$E_3(\omega)=E_3(\sigma)=0, \tag{14}$$

$$E_3(\theta_1)-\sigma\theta_1+\omega\theta_2=0, \tag{15}$$

$$E_3(\theta_2)-\omega\theta_1+\sigma\theta_2=0, \tag{16}$$

$$E_1(\sigma)+E_2(\omega)+2\theta_1\sigma=0, \tag{17}$$

$$E_1(\omega)+E_2(\sigma)+2\theta_2\sigma=0, \tag{18}$$

$$E_1(\theta_1)+E_2(\theta_2)+\theta_1^2+\theta_2^2+\beta=0. \tag{19}$$

It is easily seen from (10) that the Lie brackets of the orthonormal vectors E_1,E_2,E_3 are given by

$$[E_1,E_2]=\theta_2E_1-\theta_1E_2-2\omega E_3, \tag{20}$$

$$[E_1,E_3]=\sigma E_1+\omega E_2, \tag{21}$$

$$[E_2,E_3]=-\omega E_1-\sigma E_2. \tag{22}$$

Conversely, the Koszul formula,[24]

$$2g(\nabla_X Y,Z)=X(g(Y,Z))+Y(g(Z,X))-Z(g(X,Y))-g(X,[Y,Z])+g(Y,[Z,X])+g(Z,[X,Y]),$$

for all $X,Y,Z\in\mathfrak{X}(M)$, immediately shows that (20)–(22) imply (10).

Summarizing, we obtain the following.

Theorem 1: A three-dimensional Riemannian manifold (M,g) has constant principal Ricci curvatures given by (1) if and only if, in the neighborhood of each point $p\in M$, there exists an orthonormal frame field $\{E_1,E_2,E_3\}$ and functions ω, σ, θ_1, and θ_2, such that (13)–(22) hold.

Remark 1: It is easily seen that, replacing E_1 by $-E_1$ and E_3 by $-E_3$ if necessary, we can always choose the orthonormal frame field $\{E_1,E_2,E_3\}$ in such a way that $\sigma\geqslant 0$ and $\omega\geqslant 0$.

III. CURVATURE INVARIANTS AND HOMOGENEITY

As we have already mentioned in Sec. I, one of the main topics in the study of curvature homogeneous manifolds is the investigation of the existence of nonhomogeneous curvature homogeneous manifolds. It is therefore important to have a simple criterion to decide if a given curvature homogeneous manifold is locally homogeneous or not, and the aim of this section is to prove such a criterion for the case of three-dimensional Riemannian manifolds with constant principal Ricci curvatures $\rho_1=\rho_2\neq\rho_3$. To this purpose, let us assume that (M,g) is such a mani-

fold, and that the orthonormal frame field $\{E_1,E_2,E_3\}$ and the functions σ, ω, θ_1, and θ_2 are constructed as in Sec. II, i.e., they satisfy Eqs. (13)–(22). We are then able to prove the following.

Theorem 2: The curvature homogeneous Riemannian manifold (M,g) determined by (13)–(22) is (locally) homogeneous if and only if σ and ω are constant along M. Moreover, all locally homogeneous manifolds corresponding to given constants $\sigma,\omega,\alpha=2(\omega^2-\sigma^2)$ and β are locally isometric.

Proof: It was shown in Ref. 25 that a three-dimensional Riemannian manifold (M,g) with constant principal Ricci curvatures,

$$\rho_1=\rho_2=\beta\neq\alpha=\rho_3,$$

is locally homogeneous if and only if $\|\nabla\rho\|^2=\Sigma_{i,j,k=1}^{3}(\nabla_{E_i}\rho(E_j,E_k))^2$ is constant along M, and that the constants α, β, and $\|\nabla\rho\|^2$ give complete isometry invariants for (the universal covering manifold of) this manifold. From (5) and (10) we can easily compute that

$$\|\nabla\rho\|^2=4(\alpha-\beta)^2(\sigma^2+\omega^2),$$

which, together with (13), implies the required result. ■

IV. NONHOMOGENEOUS SOLUTIONS

We have shown in Theorem 1 that the necessary and sufficient condition for a three-dimensional Riemannian manifold to have constant principal Ricci curvatures as in (1) is the existence of a (local) orthonormal frame field $\{E_1,E_2,E_3\}$ and functions σ, ω, θ_1, and θ_2 satisfying (13)–(22). Moreover, we have seen in Sec. III that such a manifold is nonhomogeneous if and only if σ (and hence ω) is nonconstant along M. The aim of this section is to investigate the (local) existence of such nonhomogeneous manifolds. In Ref. 21, McManus claims that, if $\alpha\neq0$, the only solutions of the differential equations (13)–(22) are given by $\theta_1=\theta_2=\beta=0$, yielding that ω is constant along M and implying that no nonhomogeneous solutions exist. We will show that, if $\alpha\neq0$, the complete solution of the system of differential equations (13)–(22) is determined by (the solutions of) a system of two (partial) differential equations of second order, and we will prove the existence of solutions to these differential equations (for any choice of $\alpha\neq0$ and β), thereby pointing out and correcting the mistake made in Ref. 21. In the case where $\alpha=0$, we will determine the complete solution of the system of differential equations (13)–(22). It should be pointed out that a number of the expressions in this section were already obtained by McManus in Ref. 21, but are inserted here for easy reference.

We remark that, as M is supposed to be a nonhomogeneous manifold, the functions σ and ω are nonconstant and hence σ and ω are nonzero almost everywhere on M. For the sake of simplicity we will therefore, in what follows, restrict our attention to the generic points in M, i.e., the points p such that ω and σ are nonzero at p (and hence in a neighborhood U of p).

We start our computation by choosing a coordinate system (x,y',z') on a (possibly smaller) neighborhood U in M such that, for all points $p\in U$,

$$\frac{\partial}{\partial x}(p)=E_3(p),$$

and we write

$$E_1=a\frac{\partial}{\partial x}+b\frac{\partial}{\partial y'}+c\frac{\partial}{\partial z'},\quad E_2=d\frac{\partial}{\partial x}+e\frac{\partial}{\partial y'}+f\frac{\partial}{\partial z'}. \tag{23}$$

With respect to such a coordinate system, (14) implies that

$$\frac{\partial \sigma}{\partial x}=\frac{\partial \omega}{\partial x}=0, \tag{24}$$

while (15) and (16) take the form

$$\frac{\partial \theta_1}{\partial x}=\sigma\theta_1-\omega\theta_2, \quad \frac{\partial \theta_2}{\partial x}=\omega\theta_1-\sigma\theta_2, \tag{25}$$

and (21) and (22) yield that

$$\begin{aligned} &\frac{\partial a}{\partial x}=-\sigma a-\omega d, \quad \frac{\partial b}{\partial x}=-\sigma b-\omega e, \quad \frac{\partial c}{\partial x}=-\sigma c-\omega f, \\ &\frac{\partial d}{\partial x}=\omega a+\sigma d, \quad \frac{\partial e}{\partial x}=\omega b+\sigma e, \quad \frac{\partial f}{\partial x}=\omega c+\sigma f. \end{aligned} \tag{26}$$

Differentiating (25) with respect to x and using (13), (24), and (25), we see that

$$\frac{\partial^2 \theta_1}{\partial x^2}=-\frac{\alpha}{2}\theta_1.$$

Hence, the solution of the differential equations (25) depends on the sign of α, and in what follows we will therefore consider the cases $\alpha>0$, $\alpha<0$, and $\alpha=0$ separately.

Case I: $\alpha<0$.

In this case, putting $\lambda=\sqrt{-\alpha/2}$, (25) yields

$$\begin{aligned} \theta_1&=A(y',z')e^{\lambda x}+B(y',z')e^{-\lambda x}, \\ \theta_2&=-\frac{\lambda-\sigma}{\omega}Ae^{\lambda x}+\frac{\lambda+\sigma}{\omega}Be^{-\lambda x}, \end{aligned} \tag{27}$$

while (26) implies that

$$\begin{aligned} a&=a_1(y',z')e^{\lambda x}+a_2(y',z')e^{-\lambda x}, \\ b&=b_1(y',z')e^{\lambda x}+b_2(y',z')e^{-\lambda x}, \\ c&=c_1(y',z')e^{\lambda x}+c_2(y',z')e^{-\lambda x}, \\ d&=-\frac{\lambda+\sigma}{\omega}a_1e^{\lambda x}+\frac{\lambda-\sigma}{\omega}a_2e^{-\lambda x}, \\ e&=-\frac{\lambda+\sigma}{\omega}b_1e^{\lambda x}+\frac{\lambda-\sigma}{\omega}b_2e^{-\lambda x}, \\ f&=-\frac{\lambda+\sigma}{\omega}c_1e^{\lambda x}+\frac{\lambda-\sigma}{\omega}c_2e^{-\lambda x}. \end{aligned} \tag{28}$$

Now, let us suppose that (x,y,z) is a new coordinate system on U, such that

$$y=F(y',z'), \quad z=G(y',z').$$

With respect to this new coordinate system, the frame field $\{E_1,E_2,E_3\}$ can be written in the form

$$E_1=a\frac{\partial}{\partial x}+\left(b\frac{\partial F}{\partial y'}+c\frac{\partial F}{\partial z'}\right)\frac{\partial}{\partial y}+\left(b\frac{\partial G}{\partial y'}+c\frac{\partial G}{\partial z'}\right)\frac{\partial}{\partial z},$$

$$E_2=d\frac{\partial}{\partial x}+\left(e\frac{\partial F}{\partial y'}+f\frac{\partial F}{\partial z'}\right)\frac{\partial}{\partial y}+\left(e\frac{\partial G}{\partial y'}+f\frac{\partial G}{\partial z'}\right)\frac{\partial}{\partial z},$$

$$E_3=\frac{\partial}{\partial x},$$

and using (28) it is then easily seen that the functions F and G can be chosen in such a way that

$$b_2(y,z)=c_1(y,z)=0,\quad b_1(y,z)c_2(y,z)\neq 0.$$

Using (27) and (28) in (17), we find that

$$A=\frac{\lambda b_1}{2\sigma(\sigma-\lambda)}\frac{\partial\sigma}{\partial y},\quad B=-\frac{\lambda c_2}{2\sigma(\sigma+\lambda)}\frac{\partial\sigma}{\partial z},\tag{29}$$

and (18) is an immediate consequence of (29). A straightforward computation using (27), (28), and (29) then shows that (20) is equivalent to

$$-2\lambda^2a_2b_1+\lambda c_2b_1\frac{2\sigma-\lambda}{\sigma(\sigma-\lambda)}\frac{\partial\sigma}{\partial z}-2\lambda c_2\frac{\partial b_1}{\partial z}=0,\tag{30}$$

$$-2\lambda^2a_1c_2-\lambda c_2b_1\frac{2\sigma+\lambda}{\sigma(\sigma+\lambda)}\frac{\partial\sigma}{\partial y}+2\lambda b_1\frac{\partial c_2}{\partial y}=0,\tag{31}$$

$$b_1\frac{\partial a_2}{\partial y}-c_2\frac{\partial a_1}{\partial z}+\frac{c_2a_1}{b_1}\frac{\partial b_1}{\partial z}-\frac{a_2b_1}{c_2}\frac{\partial c_2}{\partial y}+\frac{\omega^2}{\lambda}=0.\tag{32}$$

Finally, solving a_1 and a_2 from (31) and (30) and substituting in (32) and (19), we obtain two partial differential equations of second order in σ and $\varphi=b_1c_2$:

$$\varphi\frac{\partial^2}{\partial y\,\partial z}\left(\ln\left(\frac{\sigma^2(\sigma^2-\lambda^2)}{\varphi^2}\right)\right)+2(\sigma^2-\lambda^2)=0,$$

$$-2\lambda^2\frac{\varphi}{\sigma}\frac{\partial^2\sigma}{\partial y\,\partial z}+2\lambda^2\varphi\frac{2\sigma^2-\lambda^2}{\sigma^2(\sigma^2-\lambda^2)}\frac{\partial\sigma}{\partial y}\frac{\partial\sigma}{\partial z}-\beta(\sigma^2-\lambda^2)=0.$$

A straightforward application of the Cauchy-Kowalewski theorem yields that, at least in the analytic case, there exists a family of solutions for Eqs. (13)–(22), depending on four functions of one variable (the initial conditions for the functions φ and σ), and one function of two variables (as $\varphi=b_1c_2$).

Case II: $\alpha>0$.

The computations in this case are very similar to those of Case I, although they turn out to be more complicated. We start by putting $\lambda=\sqrt{\alpha/2}$. Then (15) and (16) yield that

$$\theta_1=A(y,z)\cos\lambda x+B(y,z)\sin\lambda x,$$

$$\theta_2=\frac{\sigma A-\lambda B}{\omega}\cos\lambda x+\frac{\lambda A+\sigma B}{\omega}\sin\lambda x,$$

while (21) and (22) imply that

$$\begin{aligned}
a&=a_1(y,z)\cos\lambda x+a_2(y,z)\sin\lambda x,\\
b&=b_1(y,z)\cos\lambda x+b_2(y,z)\sin\lambda x,\\
c&=c_1(y,z)\cos\lambda x+c_2(y,z)\sin\lambda x,\\
d&=-\frac{\sigma a_1+\lambda a_2}{\omega}\cos\lambda x+\frac{\lambda a_1-\sigma a_2}{\omega}\sin\lambda x,\\
e&=-\frac{\sigma b_1+\lambda b_2}{\omega}\cos\lambda x+\frac{\lambda b_1-\sigma b_2}{\omega}\sin\lambda x,\\
f&=-\frac{\sigma c_1+\lambda c_2}{\omega}\cos\lambda x+\frac{\lambda c_1-\sigma c_2}{\omega}\sin\lambda x.
\end{aligned}\tag{33}$$

As in the previous case, we can choose a new coordinate system,

$$x,\quad y=F(y',z'),\quad z=G(y',z'),$$

such that

$$b_2(y,z)=c_1(y,z)=0,\quad b_1(y,z)c_2(y,z)\neq 0,$$

and Eq. (17) now yields that

$$A(y,z)=\frac{1}{2\omega\sigma}\left(b_1\sigma\frac{\partial\omega}{\partial y}-b_1\omega\frac{\partial\sigma}{\partial y}+c_2\lambda\frac{\partial\omega}{\partial z}\right),\tag{34}$$

$$B(y,z)=\frac{1}{2\omega\sigma}\left(c_2\sigma\frac{\partial\omega}{\partial z}-c_2\omega\frac{\partial\sigma}{\partial z}-b_1\lambda\frac{\partial\omega}{\partial y}\right),\tag{35}$$

while (18) is again an immediate consequence of (34) and (35).

As before, substituting these expressions in (20) yields that

$$-b_1c_2\frac{\partial(\sigma\omega)}{\partial z}-\lambda b_1^2\frac{\partial\omega}{\partial y}+2a_1b_1\lambda\omega\sigma+2\omega\sigma c_2\frac{\partial b_1}{\partial z}=0,$$

$$b_1c_2\frac{\partial(\sigma\omega)}{\partial y}-\lambda c_2^2\frac{\partial\omega}{\partial z}+2a_2c_2\lambda\omega\sigma-2\omega\sigma b_1\frac{\partial c_2}{\partial y}=0.$$

These equations can be solved for a_1 and a_2, and from (19) and (20) we obtain two partial differential equations of second order in σ and b_1 (depending on a free parameter c_2), which are of a rather complicated nature and will therefore be omitted. An argument similar to that in Case I then shows that, at least in the analytic case, there exists a family of solutions that depends on four functions of one variable (the initial conditions for the functions σ and b_1) and one function of two variables (namely c_2).

Case III: $\alpha=0$.

In this case, our choice of the vector fields E_1 and E_2 (see Remark 1) implies that $\sigma=\omega$. From (17), (18), and the fact that $\sigma\neq 0$, we then obtain that

$$\theta_1=\theta_2=\theta,$$

and denoting by $\{E_1',E_2',E_3'\}$ the new frame field (again consisting of principal Ricci directions) given by

$$E_1'=\frac{\sqrt{2}}{2}(E_1-E_2),\quad E_2'=\frac{\sqrt{2}}{2}(E_1+E_2),\quad E_3'=E_3,$$

Eqs. (13)–(22) can be written as

$$E_3'(\sigma)=E_3'(\theta)=0, \tag{36}$$

$$E_2'(\sigma)+\sqrt{2}\,\theta\sigma=0, \tag{37}$$

$$\sqrt{2}E_2'(\theta)+2\theta^2+\beta=0, \tag{38}$$

$$[E_1',E_2']=\sqrt{2}\,\theta E_1'-2\sigma E_3', \tag{39}$$

$$[E_1',E_3']=2\sigma E_2', \tag{40}$$

$$[E_2',E_3']=0. \tag{41}$$

From (41) we see that we can choose a coordinate system (x,y,z), such that

$$E_1'=a\frac{\partial}{\partial x}+b\frac{\partial}{\partial y}+c\frac{\partial}{\partial z},\quad E_2'=\frac{\partial}{\partial y},\quad E_3'=\frac{\partial}{\partial x}. \tag{42}$$

With respect to such a coordinate system, (36) implies that

$$\frac{\partial\sigma}{\partial x}=\frac{\partial\theta}{\partial x}=0,$$

while we obtain from (37) and (38) that

$$\sqrt{2}\frac{\partial\theta}{\partial y}+2\theta^2+\beta=0, \tag{43}$$

$$\frac{\partial\sigma}{\partial y}+\sqrt{2}\,\theta\sigma=0, \tag{44}$$

and (39) and (40) take the form

$$\begin{gathered}\frac{\partial a}{\partial x}=0,\quad \frac{\partial b}{\partial x}=-2\sigma,\quad \frac{\partial c}{\partial x}=0,\\ \frac{\partial a}{\partial y}=-\sqrt{2}\,\theta a+2\sigma,\quad \frac{\partial b}{\partial y}=-\sqrt{2}\,\theta b,\quad \frac{\partial c}{\partial y}=-\sqrt{2}\,\theta c.\end{gathered} \tag{45}$$

(1) $\beta>0$. In this case, the complete solution of (43) is given by

$$\theta=\sqrt{\frac{\beta}{2}}\tan(-\sqrt{\beta}y+f_1(z)).$$

Substituting this expression in (44), we then obtain that

$$\sigma=\frac{f_2(z)}{\cos(-\sqrt{\beta}y+f_1(z))},$$

and it follows from (45) that

$$a=\frac{2f_2(z)y+f_3(z)}{\cos(-\sqrt{\beta}y+f_1(z))},\quad b=\frac{-2f_2(z)x+f_4(z)}{\cos(-\sqrt{\beta}y+f_1(z))},\quad c=\frac{f_5(z)}{\cos(-\sqrt{\beta}y+f_1(z))},\tag{46}$$

completing the integration of (13)–(22).

(2) $\beta<0$. The complete solution of (43) is now given by

$$\theta=\sqrt{-\frac{\beta}{2}}\tanh(\sqrt{-\beta}y+f_1(z)).$$

Again substituting this expression in (44), we then obtain that

$$\sigma=\frac{f_2(z)}{\cosh(\sqrt{-\beta}y+f_1(z))},$$

and it follows from (45) that

$$a=\frac{2f_2(z)y+f_3(z)}{\cosh(\sqrt{-\beta}y+f_1(z))},\quad b=\frac{-2f_2(z)x+f_4(z)}{\cosh(\sqrt{-\beta}y+f_1(z))},\quad c=\frac{f_5(z)}{\cosh(\sqrt{-\beta}y+f_1(z))},\tag{47}$$

which concludes the integration of (13)–(22) in this case.

V. ISOMETRIC NONHOMOGENEOUS SOLUTIONS

In the previous section we have determined, for each choice of two constants $\alpha\neq\beta$, a family of nonhomogeneous Riemannian metrics whose principal Ricci curvatures are given by (1). This family of metrics depends (at least in the analytic case) on four functions of one variable and one function of two variables (if $\alpha\neq0$) or on five functions of one variable (if $\alpha=0$). In this section, we will investigate which of these metrics are locally isometric, thereby giving a new proof of the main results of Ref. 16.

Let (M,g) and (M',g') be (nonhomogeneous) three-dimensional Riemannian manifolds with constant principal Ricci curvatures $\alpha\neq\beta$, and let $\{E_1,E_2,E_3\}$ (resp., $\{E_1',E_2',E_3'\}$) be the (local) frame field along M (resp., M') consisting of principal Ricci directions constructed as in Sec. II. Then we have the following.

Theorem 3: The differentiable mapping $F:M\to M'$ is a (local) isometry if and only if

$$F_*E_1=\epsilon E_1',\quad F_*E_2=\epsilon E_2',\quad F_*E_3=E_3',$$

or

$$F_*E_1=\epsilon E_2',\quad F_*E_2=\epsilon E_1',\quad F_*E_3=-E_3',\quad \epsilon=\pm1.\tag{48}$$

Proof: First, if F is a local isometry of (M,g) and (M',g'), then it preserves (up to the sign) the simple principal Ricci direction E_3. As F also preserves the Levi Civita connection, it then preserves the shear tensor of E_3 and hence its eigendirections E_1 and E_2, and (48) follows from our choice of sign for σ and ω.

Conversely, if F satisfies (48), it maps a local orthonormal frame field along M into a local orthonormal frame field along M', proving that F is a local isometry. ■

Now, let us first assume that $\alpha<0$ and that the frame field $\{E_1,E_2,E_3\}$ is determined by (23) and (28). Then it is easily seen that the differentiable mapping $F:M\to M'$, given by

$$x'=x'(x,y,z), \quad y'=y'(x,y,z), \quad z'=z'(x,y,z),$$

satisfies (48) if and only if

$$x'=\pm x+f_1(y,z), \quad y'=f_2(y), \quad z'=f_3(z),$$

or

$$x'=\pm x+f_1(y,z), \quad y'=f_2(z), \quad z'=f_3(y).$$

Using a similar (but more complicated) argument in the case $\alpha>0$, we conclude that, in the case $\alpha\neq 0$, there is a family of isometries depending on two functions of one variable and one function of two variables.

In the case where $\alpha=0$, let us assume that the frame field is given by (42) and (46) [or (47)]. An argument similar to the one above then shows that the differentiable mapping $F:M\to M'$ satisfies (48) if and only if

$$x'=x+f_1(z), \quad y'=y+f_2(z), \quad z'=f_3(z)$$

(or a similar form for the other cases), and we conclude that, in this case, the family of isometries depends on three functions of one variable.

Comparing the family of solutions of the Eqs. (13)–(22) discovered in Sec. IV with the number of isometries for these metrics found in Sec. V, we obtain the following result from Ref. 16.

Theorem 4: Let $\alpha\neq\beta$ be constants. Then there exists a family of local nonhomogeneous Riemannian metrics, which are not (locally) isometric and whose constant principal Ricci curvatures satisfy (1), and this family depends on two arbitrary functions of one variable.

Remark 2: In the case $\alpha=0$, we know that the Riemannian metric g is completely determined by the orthonormal frame field $\{E_1,E_2,E_3\}$ given by (42) and (46) [or (47)]. Applying a suitable local isometry F of the form

$$x'=x+F_1(z), \quad y'=y+F_2(z), \quad z'=F_3(z),$$

we can map the frame field $\{E_1,E_2,E_3\}$ into the frame field

$$E_1'=a'\frac{\partial}{\partial x'}+b'\frac{\partial}{\partial y'}+c'\frac{\partial}{\partial z'}, \quad E_2'=\frac{\partial}{\partial y'}, \quad E_3'=\frac{\partial}{\partial x'},$$

where

$$a'=\frac{y'\varphi_2(z')}{\cos(-\sqrt{\beta}y'+\varphi_1(z'))},$$

$$b'=\frac{-x'\varphi_2(z')}{\cos(-\sqrt{\beta}y'+\varphi_1(z'))},$$

$$c' = \frac{\varphi_2(z')}{\cos(-\sqrt{\beta}y' + \varphi_1(z'))},$$

resp.,

$$a' = \frac{y'\varphi_2(z')}{\cosh(\sqrt{-\beta}y' + \varphi_1(z'))},$$

$$b' = \frac{-x'\varphi_2(z')}{\cosh(\sqrt{-\beta}y' + \varphi_1(z'))},$$

$$c' = \frac{\varphi_2(z')}{\cosh(\sqrt{-\beta}y' + \varphi_1(z'))},$$

showing that all these metrics are locally isometric to the Riemannian metrics of the form

$$g = \omega_1^2 + \omega_2^2 + \omega_3^2,$$

with

$$\omega_1 = (\mu_1(z')\cos(-\sqrt{\beta}y') + \mu_2(z')\sin(-\sqrt{\beta}y'))dz',$$

$$\omega_2 = dy' + x'dz', \quad \omega_3 = dx' - y'dz',$$

resp.,

$$\omega_1 = (\mu_1(z')\cosh(\sqrt{-\beta}y') + \mu_2(z')\sinh(\sqrt{-\beta}y'))dz',$$

$$\omega_2 = dy' + x'dz', \quad \omega_3 = dx' - y'dz',$$

which are exactly the metrics constructed in Ref. 6, the functions μ_1 and μ_2 being the two functions of one variable given by Theorem 4.

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Summation of power series by continued exponentials

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It is proposed that a power series may be summed (analytically continued outside its radius of convergence) by converting it to a continued exponential, which is a structure of the form $a_0 \exp(a_1 z \exp(a_2 z \exp(a_3 z \exp(a_4 z \ldots))))$. The continued-exponential coefficients $\{a_i\}$ for a given function $f(z)$ are determined by equating the Taylor coefficients of the continued exponential with those of $f(z)$. (The coefficients $\{a_i\}$ have a combinatoric interpretation; the nth Taylor coefficient enumerates all $n+1$-vertex tree graphs whose vertex amplitudes are $\{a_i\}$.) Continued exponentials have remarkable convergence properties. When a power series has a nonzero radius of convergence, the corresponding continued exponential often converges in a heart-shaped region Ω, whose cusp is determined by the nearest zero or singularity of the function being approximated. The convergence region Ω contains and is much larger than the circle of convergence of the power series. Outside Ω, the complex plane is divided up into an elaborate patchwork of regions in which the continued exponential may either diverge or else approach an N-cycle, $N=2,3,4,\ldots$.
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I. INTRODUCTION

A variety of mathematical techniques have been invented to accelerate the rate of convergence of a slowly convergent series and to assign a finite value to the sum of a divergent series. Such techniques are generally referred to as *summation methods*.[1] Summation methods are extremely useful to theoretical and mathematical physicists. The most powerful analytic tool for solving hard problems in theoretical physics is perturbation theory. However, perturbation series are notoriously badly behaved; they are either slowly convergent or, very often, they are divergent. Summation methods are crucial because they provide a way to recover useful physical information from perturbative calculations.

Consider a perturbation series in the form of a power series

$$\sum_{n=0}^{\infty} c_n z^n. \tag{1.1}$$

Here z is called the perturbation parameter and $\{c_n\}$ are the perturbation coefficients. One technique commonly used to improve the rate of convergence of such a series and/or to assign a meaningful sum to the series is called Padé summation.[2] To sum a formal power series using Padé summation one converts the series to a continued fraction. Continued-fraction coefficients are obtained by expanding the continued fraction as a power series, which is then identified term by term with the formal power series to be summed. A truncated continued fraction is a rational function; the rational functions obtained by successive truncation are called Padé approximants. Even if the perturbation series diverges, the Padé approximants often form a rapidly convergent sequence whose limiting value is physically meaningful.[3]

Recall that when a power series converges, its region of convergence is a disc in the complex plane. Generally, a summation method enlarges this region of convergence. For example, when one converts a power series representing a Stieltjes function [such as $\log(1+z)$] to a continued fraction, the sequence of Padé approximants converges in a cut plane that contains the disc.

In this paper we propose a new method for summing power series. The idea is to convert the series to a *continued exponential*, an infinite tower of exponentials of the form

$$a_0 \exp(a_1 z \exp(a_2 z \exp(a_3 z \exp(a_4 z \ldots)))). \tag{1.2}$$

This continued exponential is said to converge for a particular value of z if the sequence $E_0 \equiv a_0$, $E_1 \equiv a_0 \exp(a_1 z)$, $E_2 \equiv a_0 \exp(a_1 z \exp(a_2 z))$, ... converges.[4] We will see that continued exponentials often converge in a larger region than their associated Taylor series. When a continued exponential does not converge, the sequence $\{E_n\}$ may either grow out of bounds or it may approach a limit cycle. This limit cycle may be of finite length or it may even be infinite. [Later in this section we generalize the form of the continued exponential in Eq. (1.2) by replacing the structure $a_n z$ by $a_n z^{b_n}$. For example, to expand $\cos z$ as a continued exponential we take $b_n = 2$ for all $n \geq 1$.]

Having defined a continued exponential, we next consider some elementary operations that may be performed. For example, multiplying a continued exponential by a constant, or raising a continued exponential to a power are trivial. Unfortunately, most arithmetical operations, such as adding or multiplying two continued exponentials, are impossible.

It is straightforward to expand a continued exponential of the form $a_0 e^{a_1 z e^{a_2 z \cdots}}$ as a Taylor series. The first n terms of this Taylor series are obtained by truncating the continued exponential after the first n coefficients, expanding the finite tower as a Taylor series, and then retaining the first n terms of this Taylor series. The z^n term ($n>0$) of the Taylor series has 2^{n-1} contributions of the form $a_0 a_1^{j_1} \ldots a_k^{j_k}$ with $j_1 + \ldots + j_k = n$, where $j_i > 0$ for all i. Explicitly, the Taylor series is

$$a_0 + \sum_{n=1}^{\infty} \sum_{j_1 + \ldots + j_k = n} \frac{j_1^{j_2} j_2^{j_3} \cdots j_{k-1}^{j_k}}{j_1! j_2! j_3! \cdots j_k!} a_0 a_1^{j_1} \ldots a_k^{j_k} z^n. \tag{1.3}$$

To convert the power series in Eq. (1.1) to the continued exponential in Eq. (1.2) we expand the continued exponential as a Taylor series and set this series equal to the original power series. This gives an infinite sequence of equations that relate the Taylor coefficients $\{c_i\}$ to the continued-exponential coefficients $\{a_i\}$:

$$\begin{aligned}
c_0 &= a_0, \\
c_1 &= a_1 a_0, \\
c_2 &= a_0 a_1 a_2 + \tfrac{1}{2} a_0 a_1^2, \\
c_3 &= a_0 a_1 a_2 a_3 + \tfrac{1}{2} a_0 a_1 a_2^2 + a_0 a_1^2 a_2 + \tfrac{1}{6} a_0 a_1^3, \\
c_4 &= a_0 a_1 a_2 a_3 a_4 + \tfrac{1}{2} a_0 a_1 a_2 a_3^2 + a_0 a_1 a_2^2 a_3 + a_0 a_1^2 a_2 a_3 \\
&\quad + \tfrac{1}{6} a_0 a_1 a_2^3 + a_0 a_1^2 a_2^2 + \tfrac{1}{2} a_0 a_1^3 a_2 + \tfrac{1}{24} a_0 a_1^4,
\end{aligned} \tag{1.4}$$

and so on. These equations may be solved sequentially for the continued exponential coefficients:

$$a_0=c_0,$$

$$a_1=c_1/c_0,$$

$$a_2=\frac{2c_0c_2-c_1^2}{2c_0c_1}, \tag{1.5}$$

$$a_3=\frac{24c_0^2c_1c_3-12c_0^2c_2^2-12c_0c_1^2c_2+5c_1^4}{24c_0^2c_1c_2-12c_0c_1^3},$$

$$\begin{aligned}a_4=&(1152c_0^4c_1^2c_2c_4-576c_0^3c_1^4c_4-576c_0^4c_1^2c_3^2-576c_0^4c_1c_2^2c_3+576c_0^3c_1^3c_2c_3+48c_0^2c_1^5c_3\\&+240c_0^4c_2^4-480c_0^3c_1^2c_2^3+456c_0^2c_1^4c_2^2-264c_0c_1^6c_2+47c_1^8)/(1152c_0^4c_1^2c_2c_3-576c_0^3c_1^4c_3\\&-576c_0^4c_1c_2^3-288c_0^3c_1^3c_2^2+528c_0^2c_1^5c_2-120c_0c_1^7),\end{aligned}$$

and so on.

There is an *efficient* computational procedure for converting a formal power series to a continued exponential. This iterative procedure relies on taking logarithms and uses the first N terms of the power series as input. At each step we identify the leading term in the power series as the next term in the continued exponential. Then we normalize the power series by dividing by the first term and take its logarithm according to the formula

$$\log(1+x)=x-\tfrac{1}{2}x^2+\tfrac{1}{3}x^3-\ldots.$$

The result of this process is a continued exponential of a more general form: $a_0z^{b_0}e^{a_1z^{b_1}e^{a_2z^{b_2}\cdots}}$. In this representation the monomial $a_0z^{b_0}$ is the leading term of the power series. Note that the first N coefficients of the generalized continued exponential can be calculated (using MAPLE, Mathematica, or MACSYMA) in $O(N^4)$ time.[5]

There is only one example for which both the continued exponential coefficients and the Taylor series coefficients are known in closed form:

$$e^{ze^{ze^{ze^{z\cdots}}}}=\sum_{n=0}^{\infty}\frac{(n+1)^{n-1}}{n!}z^n. \tag{1.6}$$

For this example one can verify that $a_n=1$ and $c_n=(n+1)^{n-1}/n!$ satisfy Eqs. (1.4) and (1.5) and that the right side of Eq. (1.6) has the form in Eq. (1.3). The Taylor series on the right side of Eq. (1.6) converges in a disc of radius $1/e$ about the origin. However, as we will see, the continued exponential converges in a larger region whose shape is similar to that of a cardioid. The boundary of this heart-shaped region is given by the parametric equations $r=e^{-\cos t}$ and $\theta=t-\sin t$, where $0\leq\theta<2\pi$.

If the continued exponential coefficients a_n approach a constant, then the region of convergence is the heart-shaped region above, scaled by an appropriate factor. For example, when the Taylor series for $1/(1-z)$ about $z=0$ is converted to a continued exponential, the resulting coefficients satisfy $\lim_{n\to\infty}a_n=1/e$. In this case, the region of convergence is a cardioid with the cusp at $z=1$. This cardioid is larger than the region of convergence of the Taylor series, which is the unit disk.

In general, the boundary of the region of convergence of a continued exponential is determined by the zeros and the singularities of the function being represented. For example, the continued exponential representations for the functions $1-z$ and $1/(1-z)$ have the same region of convergence; in the former case the function has a zero at $z=1$ and in the latter case the function

has a pole at $z=1$. In either case the cusp of the cardioid is located at $z=1$. The function $\cos z$ vanishes at $z=\pm\pi/2$. The continued exponential representation of this function converges in a double cardioid with cusps at $z=\pm\pi/2$. The function $1/\cos/tz$ converges in the same double cardioid.

The most remarkable aspects of continued exponentials become apparent when they do *not* converge. Outside this region of convergence the continued exponential sequence E_0, E_1, $E_2, \ldots$ may either grow out of bounds (like the partial sums of a Taylor series outside the disc of convergence) or it may converge to a cycle of length N, $N=2, 3, 4, \ldots$, or even an infinite limit cycle. (By an *infinite limit cycle* we mean an infinite bounded sequence that does not approach a finite limit cycle.) The boundary of the region in which the sequence $\{E_n\}$ is unbounded appears fractal.

In comparison, the convergence properties of Taylor series are much simpler. A Taylor series converges (geometrically) inside its circle of convergence and diverges outside the circle of convergence. The only portion of the complex plane where a Taylor series may exhibit interesting convergence behavior, such as the nonuniform convergence typical of Fourier series, is *on* the circle of convergence. However, the circle of convergence is a one-dimensional object, a set of measure zero in the complex plane. Continued exponentials are thus much more elaborate than Taylor series.

This paper is organized as follows. In Sec. II we show that continued exponentials have a combinatoric interpretation; the coefficient of z^n in the Taylor series of $a_0 e^{a_1 z e^{a_2 z \cdots}}$ represents the sum of the amplitudes of tree graphs having $n+1$ vertices. In Sec. III we present a detailed discussion of the continued exponential Eq. (1.6), whose coefficients are all unity. We compare the convergence of this continued exponential with that of the continued fraction and Taylor series representations of this function. Section IV considers the continued exponential expansions of the polynomial $1-z$, the trigonometric functions $\sin z$ and $\cos z$, an Airy function, and the Stieltjes function whose formal power series is $\Sigma_{n=0}^{\infty}(-1)^n n! z^n$. Section V examines the continued exponential expansions of quadratic polynomials. Some concluding remarks are given in Sec. VI.

II. CONTINUED EXPONENTIALS AND TREE GRAPHS

Continued exponentials have a strong connection with combinatorics.[6] When a continued exponential is expanded as a Taylor series as in Eq. (1.3) the coefficient of z^n in this series counts all rooted tree graphs having $n+1$ vertices.

A tree graph is a graph having no closed loops. A rooted tree graph begins at a particular vertex called the root, with which we associate the weight a_0. Every other vertex is connected by a unique path to the root. If the length of this path is k we assign the weight a_k to the vertex: vertices connected to the root by one edge are weighted a_1, and so on. Each tree graph is assigned a symmetry number, which is defined as the reciprocal of the size of the automorphism group of the graph. The coefficient

$$\frac{j_1^{j_2} j_2^{j_3} \cdots j_{k-1}^{j_k}}{j_1! j_2! \cdots j_k!} a_0 a_1^{j_1} \cdots a_k^{j_k} \tag{2.1}$$

is the sum of the symmetry numbers of all rooted tree graphs having j_i vertices at a distance i from the root.

Because Eq. (2.1) is the summand in Eq. (1.3) continued exponentials enumerate tree graphs. The z^n term enumerates *all* rooted tree graphs with n+1 vertices, accounting for symmetry. To illustrate this graph counting, consider the z^5 term of the continued exponential $a_0 e^{a_1 z e^{a_2 z \cdots}}$:

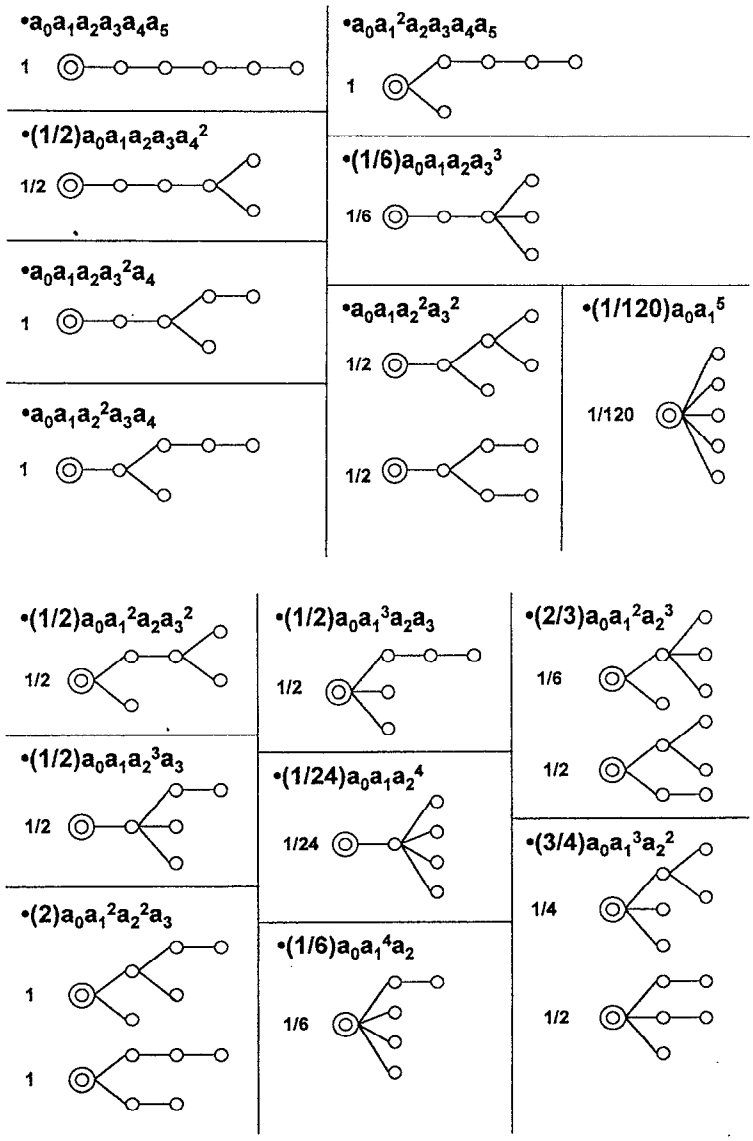

FIG. 1. Graphical representation of Eq. (2.2). Shown are all rooted tree graphs with six vertices a_i. Each vertex, indicated by a circle, lies at a distance i from the root, which is indicated by a double nested circle. The number adjacent to each graph is the symmetry number of that graph.

$$a_0a_1a_2a_3a_4a_5+\tfrac{1}{2}a_0a_1a_2a_3a_4^2+a_0a_1a_2a_3^2a_4+a_0a_1a_2^2a_3a_4+a_0a_1^2a_2a_3a_4+\tfrac{1}{6}a_0a_1a_2a_3^3$$
$$+a_0a_1a_2^2a_3^2+\tfrac{1}{2}a_0a_1^2a_2a_3^2+\tfrac{1}{2}a_0a_1^3a_2a_3+2a_0a_1^2a_2^2a_3+\tfrac{1}{2}a_0a1^3a_2a_3+\tfrac{1}{24}a_0a_1a_2^4+\tfrac{2}{3}a_0a_1^2a_2^3$$
$$+\tfrac{3}{4}a_0a_1^3a_2^2+\tfrac{1}{6}a_0a_1^4a_2+\tfrac{1}{120}a_0a_1^5. \tag{2.2}$$

This expression, which is the next in the sequence of coefficients given in Eq. (1.4), is a sum of terms of the form $a_0a_1^{j_1}\ldots a_k^{j_k}$ with $j_1+\ldots+j_k=5$, $j_i>0$. This term enumerates, according to symmetry number, all six-vertex rooted tree graphs with vertices a_j at a distance j from the root

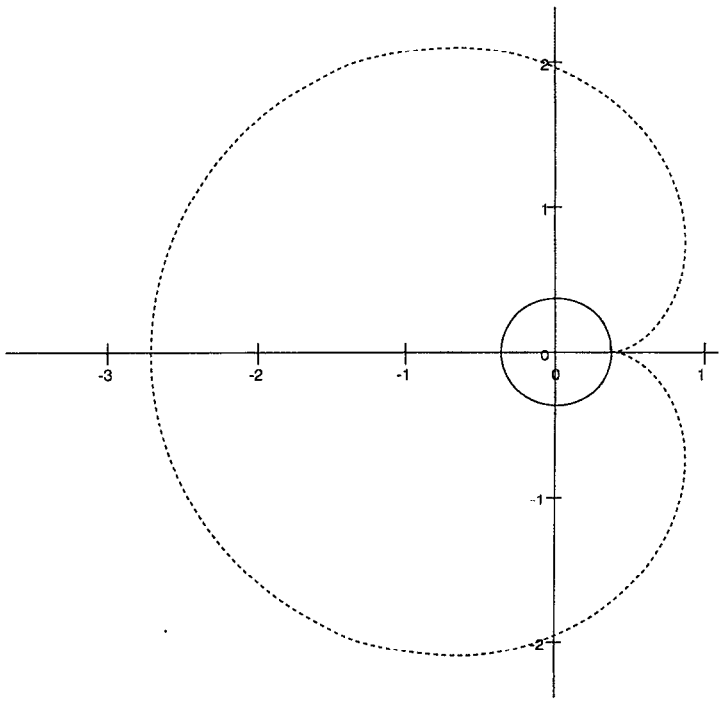

FIG. 2. The boundary (dashed line) of the region of convergence of the continued exponential whose coefficients are $a_n=1$. The shape of the boundary resembles that of a cardioid with a cusp located at $(1/e,0)$. We refer to this heart-shaped region as Ω. The boundary of Ω is given in implicit parametric form in Eq. (3.2). The solid line is the circle of convergence of the Taylor series representation of the same function.

of the tree (see Fig. 1). For example, the term $\frac{3}{4}a_0a_1^3a_2^2$ enumerates tree graphs with a root, three vertices at a distance 1 from the root, and 2 vertices at a distance 2 from the root. Up to isomorphism, there are two such graph trees. The first has 4 automorphisms, so its symmetry number is 1/4. The second tree has two automorphisms, so its symmetry number is 1/2. The sum of the symmetry numbers is $1/4+1/2=3/4$, the coefficient in the continued exponential expansion.

One can give another combinatoric interpretation of Eq. (1.3) as a composition theorem for the enumeration of certain subsets of symmetric semigroups and the corresponding sets of labeled functional digraphs.[7]

III. ILLUSTRATIVE EXAMPLE

Consider the differential equation initial-value problem

$$y'(z)=\frac{y^2}{1-zy},\quad y(0)=1. \tag{3.1}$$

The unique solution to this equation can be written in implicit form as $y=e^{zy}$. The solution to this functional equation that is analytic at $z=0$ has the Taylor series $\sum_{n=0}^{\infty}(n+1)^{n-1}z^n/n!$. The functional equation is also satisfied by the continued exponential $e^{ze^{ze^{z\cdots}}}$ in its region of convergence. For those values of z for which both the Taylor series and the continued exponential converge, they are equal. This equality is expressed formally by Eq. (1.6).

TABLE I. Comparison of convergence rates for the continued exponential, the continued fraction (Padé), and the Taylor series for the function $f(z)$, whose Taylor series is given in (3.1). Here we take $z=-0.2$, which lies inside the radius of convergence of the Taylor series. In the first column, the integer n represents the order of the approximation. Observe that while all three approximation schemes converge, the absolute errors (in parentheses) are significantly smaller for the continued fraction and the continued exponential. The exact value is $f(-0.2)=0.84457986749555\ldots$.

Order n	Continued Exponential	Continued Fraction	Taylor Series
0	1.0 (0.16)	1.0 (0.16)	1.0 (0.16)
1	0.8187307530780 (0.026)	0.83333333333333 (0.011)	0.8 (0.045)
2	0.8489575018686 (0.0044)	0.84615384615385 (0.0016)	0.86 (0.015)
3	0.8438407387346 (0.00074)	0.84444444444444 (0.00014)	0.83866667 (0.0059)
4	0.8447047273782 (0.00013)	0.84459732901659 (0.000018)	0.847 (0.0024)
5	0.84455877693024 (0.000021)	0.84457826304384 (1.6×10^{-6})	0.84354400 (0.0010)
6	0.8445834300364 (3.6×10^{-6})	0.84458006597567 (2.0×10^{-7})	0.84503796 (0.00046)
7	0.8445792657257 (6.0×10^{-7})	0.84457984859380 (1.9×10^{-8})	0.84437219 (0.00021)
8	0.8445799691441 (1.0×10^{-7})	0.84457986977521 (2.3×10^{-9})	0.84467587 (0.000096)
9	0.8445798503255 (1.7×10^{-8})	0.84457986727347 (2.2×10^{-10})	0.84453478 (0.000045)
10	0.8445798703959 (2.9×10^{-9})	0.84457986752187 (2.6×10^{-11})	0.84460132 (0.000022)
11	0.8445798670056 (4.9×10^{-10})	0.84457986749294 (2.6×10^{-12})	0.84456955 (0.000010)
12	0.8445798675783 (8.3×10^{-11})	0.84457986749585 (3.1×10^{-13})	0.84458488 (5.0×10^{-6})
∞	0.84457986749555	0.84457986749555	0.84457986749555

The Taylor series on the right side of Eq. (1.6) converges in a disc of radius $1/e$ about the origin. The convergence of the continued exponential is more complicated and has been investigated by Creutz and Sternheimer,[8–10] Baker and Rippon,[11–17] and others.[18–21] This continued exponential converges in a much larger region that contains the circle of convergence of the Taylor series. The boundary of the region of convergence of the continued exponential is similar in shape to that of a cardioid with a cusp located at $(1/e,0)$ (see Fig. 2). We will refer to this heart-shaped region as Ω. The boundary of Ω is given in implicit parametric form by

$$r=e^{-\cos t},$$
$$\theta=t-\sin t \quad (0\leqslant\theta<2\pi). \tag{3.2}$$

To derive Eq. (3.2) we argue as follows. In the complex plane, the continued exponential $e^{ze^{ze^{z\cdots}}}$ converges when the sequence $1, e^z, e^{ze^z}, \ldots$ converges. If it exists, the limit y_0 will be an attractive fixed point of the equation $y=e^{yz}$. Let $z=we^{-w}$. Then the fixed point y_0 is e^w. The multiplier of this fixed point (which determines whether it is attractive or repulsive) is w. Thus, the fixed point is attractive if and only if $|w|<1$. The region of convergence Ω is given by we^{-w} where $|w|<1$ and the boundary of Ω is given by $|w|=1$, which is equivalent to Eq. (3.2). The above argument shows that the rate of convergence at a point inside the cardioid is exponential.

It is instructive to compare numerically the convergence rates of the Taylor series and continued exponential in Eq. (1.6) and the continued fraction (Padé sequence) generated by the Taylor series. Tables I, II, and III list the first 12 terms in the continued exponential and continued fraction sequences and the first 12 partial sums of the Taylor series for three values of z: $z=-0.2$, $z=\frac{1}{2}i$, and $z=-1.5$. The point $z=-0.2$ lies inside the radius of convergence of the Taylor series. Observe that at this point the continued fraction and continued exponential converge far more rapidly than the Taylor series. The other two points lie inside the convergence region Ω but outside the radius of convergence of the Taylor series. For these two points the Padé converges more rapidly than the continued exponential but both the Padé and continued exponential provide a means of summing the Taylor series outside of its radius of convergence.

TABLE II. Same as in Table I, except that here we take $z=0.5i$, which lies outside the radius of convergence of the Taylor series. The continued exponential and continued fraction converge but the Taylor series diverges as n, the order of the approximation, increases. The exact value is $f(0.5i)=0.7852571487+0.3251992959i$.

Order n	Continued Exponential	Continued Fraction	Taylor Series
0	1	1.0	1.0
1	0.87758256+0.47942554 i	0.8+0.4 i	1.0+0.5 i
2	0.71231190+0.33429136 i	0.76+0.32 i	0.625+0.5 i
3	0.79298003+0.29500483 i	0.7895196507+0.3213973799 i	0.625+0.167 i
4	0.79592152+0.33322204 i	0.7857646430+0.3269503294 i	0.951+0.167 i
5	0.78037531+0.32806317 i	0.7848536055+0.3250627960 i	0.951+0.504 i
6	0.78492383+0.32281899 i	0.7853504057+0.3251072592 i	0.586+0.504 i
7	0.78624653+0.32545553 i	0.7852630595+0.3252303705 i	0.586+0.098 i
8	0.78499560+0.32554601 i	0.7852480399+0.3251965763 i	1.049+0.098 i
9	0.78516355+0.32504025 i	0.7852589388+0.3251977857 i	1.049+0.636 i
10	0.78533482+0.32518840 i	0.7852572953+0.3251999736 i	0.415+0.636 i
11	0.78524880+0.32523156 i	0.7852569857+0.3251992357 i	0.415-0.121 i
12	0.78524584+0.32519077 i	0.7852571861+0.3251992630 i	1.328-0.121 i
∞	0.78525715+0.32519930 i	0.7852571487+0.3251992959 i	∞

Outside the convergence region Ω, the continued exponential sequence $E_0, E_1, E_2, \ldots$ behaves in a remarkable fashion. This sequence may either diverge (like the partial sums of a Taylor series outside the circle of convergence) or may it converge to a cycle of length N, $N=2, 3, 4, \ldots$. For example, the continued exponential $e^{ze^{ze^{z\cdots}}}$ converges to a two-cycle when $z=-9$. The first few terms in the sequence are 1, $e^{-9}=0.0001234$, $e^{-9e^{-9}}=0.99889$, $e^{-9e^{-9e^{-9}}}=0.0001246$, ...

Cycles of every integer length can be found outside the region of convergence. In Fig. 3 we display the regions in the complex-z plane for which the continued exponential sequence converges to an N-cycle. The boundary of the region in which the sequence $\{E_n\}$ is unbounded appears fractal.

Baker and Rippon have made other observations. The regions of convergence to a cycle are actually strips in the complex plane which extend infinitely far in the positive real direction. The

TABLE III. Same as in Table I, except that here we take $z=-1.5$, which lies outside the radius of convergence of the Taylor series. The continued exponential and continued fraction converge but the Taylor series diverges as n, the order of the approximation, increases.

Order n	Continued Exponential	Continued Fraction	Taylor Series
0	1.0 (0.516)	1.0 (0.516)	1.0 (0.516)
1	0.2231302 (0.261)	0.4000000 (0.0839)	-0.5 (0.984)
2	0.7155561 (0.232)	0.5384615 (0.0546)	2.875 (2.39)
3	0.3418668 (0.142)	0.4705882 (0.0133)	-6.125 (6.61)
4	0.5988165 (0.115)	0.4911081 (0.00720)	20.24219 (19.8)
5	0.4072921 (0.0766)	0.4818707 (0.00204)	-61.77031 (62.2)
6	0.5428414 (0.0589)	0.4849169 (0.00101)	204.1217 (204)
7	0.4429661 (0.0409)	0.4836004 (0.000307)	-684.5640 (685)
8	0.5145569 (0.0306)	0.4840524 (0.000145)	2355.671 (2355)
9	0.4621641 (0.0217)	0.4838615 (0.0000459)	-8238.2897 (8239)
10	0.4999506 (0.0160)	0.4839286 (0.0000212)	29231.71 (29231)
11	0.4724016 (0.0115)	0.4839006 (0.673×10^{-5})	-104939.9 (104940)
12	0.4923318 (0.00842)	0.4839106 (0.322×10^{-5})	380499.5 (380499)
∞	0.4839074 (exact)	0.4839074 (exact)	∞

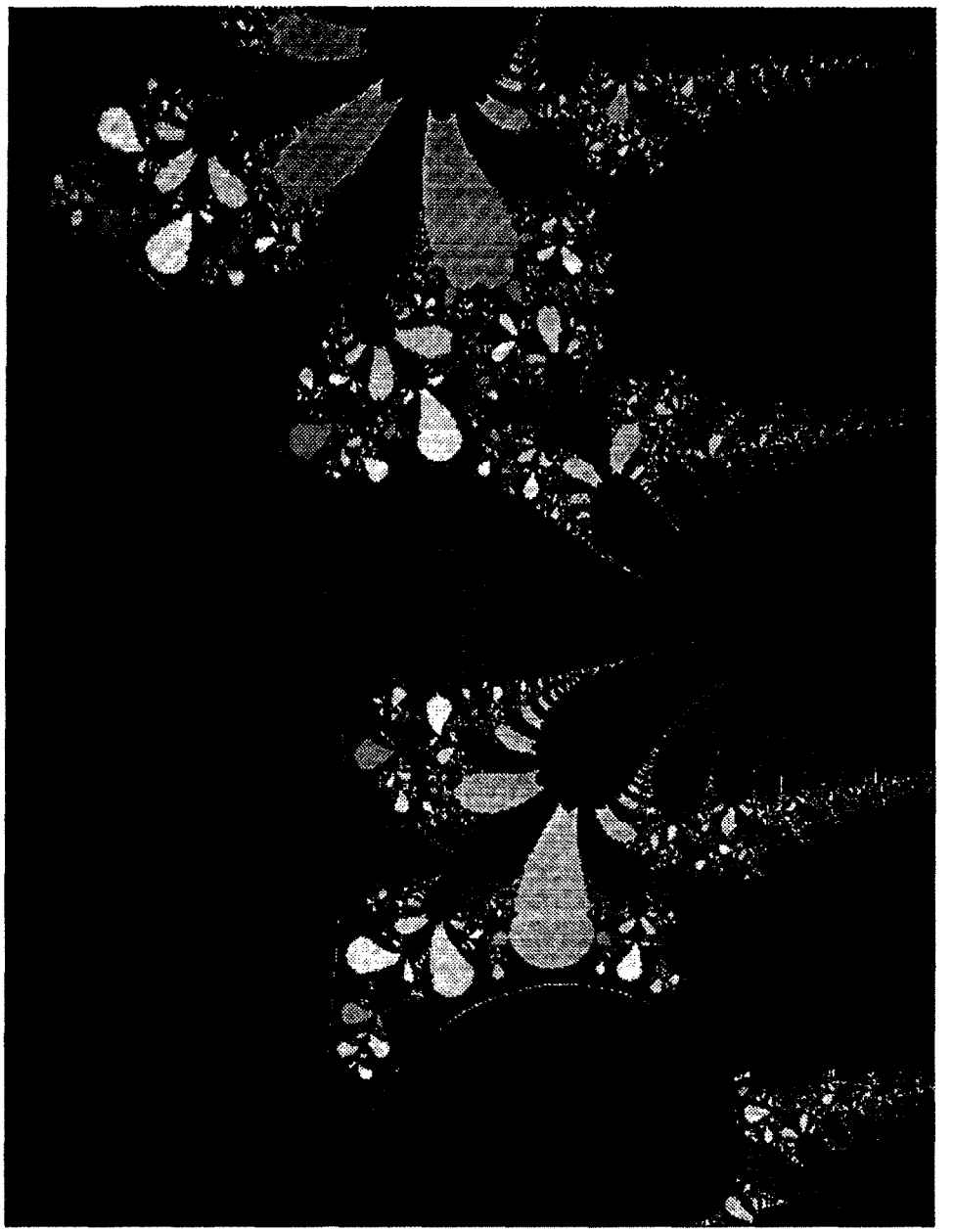

FIG. 3. Regions in the upper complex-z plane for which the continued exponential, whose coefficients are all 1, converges to an N-cycle. The regions in the lower-half plane are mirror images of those in the upper-half plane. Cycles of every integer length can be found outside the cardioid-shaped region of convergence Ω (purple). The boundary of the region (black) in which the sequence $\{E_n\}$ is unbounded appears fractal. Note that each region [except for Ω and the region of two-cycle (red)] is actually an infinitely long strip that becomes infinitely thin as it extends to $\mathrm{Re}(z)=\infty$. Each strip is artificially truncated by a crescent. The regions of three-cycles are magenta, four-cycles are green, five-cycles are yellow, six-cycles are blue, seven- through thirteen-cycles are various shades of pink.

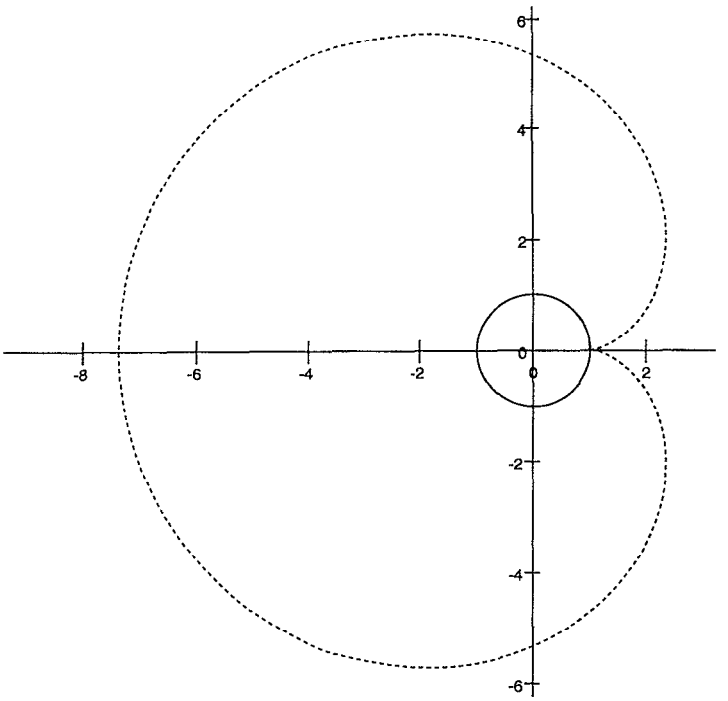

FIG. 4. Region of convergence (dashed line) of the continued exponential for the function $1/(1-z)$. The singularity at $z=1$ determines the location of the cusp. The solid line is the circle of convergence of the Taylor series for $1/(1-z)$.

ordering of these strips is well defined, and has interesting properties. For example, between every pair of adjacent n-strips is an infinite number of $(n+1)$-strips for $n>2$. Also, Baker and Rippon conjecture that the regions of convergence to a cycle are dense in the complex plane.

IV. ADDITIONAL EXAMPLES

In this section we consider a number of additional examples of continued exponentials.

A. The function $1/(1-z)$

Since the first finitely many coefficients a_i do not affect the convergence of a continued exponential, it is reasonable to suppose that if the coefficients a_i of the continued exponential $a_0 e^{a_1 z e^{a_2 z e^{a_3 z \cdots}}}$ approach a constant, then the region of convergence is the cardioid Ω scaled by an appropriate factor. An elementary example of a function for which the continued exponential coefficients approach a constant is $1/(1-z)$, whose Taylor series is $\Sigma_0^\infty z^n$. This Taylor series converges in a disc of radius 1. Its continued exponential coefficients are $a_0=1$, $a_1=1$, $a_2=\frac{1}{2}$, $a_3=\frac{5}{12}$, $a_4=\frac{47}{120}$, $a_5=\frac{12917}{33840}$, $a_6=\frac{329458703}{874222560}$, and so on. The coefficients a_i approach the limit $1/e\approx 0.36788$ monotonically. We have confirmed empirically that the region of convergence is $e\Omega$ (that is, the region Ω dilated by the factor e) (see Fig. 4). The cusp now lies at (1,0). This region is much larger than the region of convergence of the Taylor series. Note that the singularity at $z=1$ determines the location of the cusp of the cardioid.

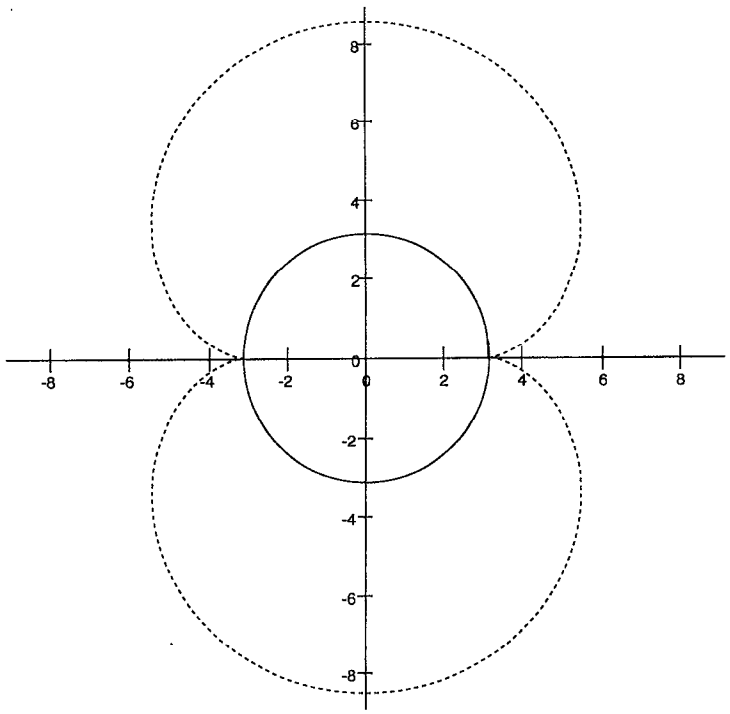

FIG. 5. Region of convergence (dashed line) of the continued exponential representing the function $z/\sin z$. Note that the region of convergence resembles a double cardioid. The cusps lie at $\pm\pi$, the nearest poles of the function. The solid line is the circle of convergence of the Taylor series for $z/\sin z$.

B. The function $z/(\sin z)$

Consider the function $z/(\sin z)$. Its Taylor series has a radius of convergence of π. By iteratively taking the logarithm of this Taylor series we find that its continued exponential is $a_0 e^{a_1 z^2 e^{a_2 z^2 e^{a_3 z^2 \cdots}}}$, where $a_0=1$, $a_1=\frac{1}{6}$, $a_2=\frac{1}{30}$, $a_3=\frac{59}{1260}$, $a_4=\frac{1219}{29736}$, $a_5=\frac{2300350279}{59809503600}$, and $\lim_{n\to\infty} a_n = 1/\pi^2 e \approx (0.037274)$. The sequence of continued exponential coefficients is monotone decreasing beginning with a_3. As in the previous example, the continued exponential converges when $z^2/\pi^2 e$ is inside the cardioid Ω, or equivalently, when z is in the double cardioid $\sqrt{\pi^2 e\Omega}$ shown in Fig. 5. This cardioid has cusps at $z=\pm\pi$, the location of the singularities of the function $z/(\sin z)$. The continued exponential converges in a much larger region than the Taylor series.

The continued exponential representation for the function $\sin z$ may be derived from that of $z/\sin z$:

$$\sin z = \frac{1}{a_0} z e^{-a_1 z^2 e^{a_2 z^2 e^{a_3 z^2 \cdots}}}.$$

Note that only the first two terms of this continued exponential differ from that of $z/(\sin z)$. The region of convergence of the continued exponential for the function $\sin z$ is the same double cardioid as that for the function $z/(\sin z)$. However, the Taylor series for the function $\sin z$ has an infinite radius of convergence. For the function $\sin z$ it is the zeros at $z=\pm\pi$ that determine the cusps of the cardioid.

Similarly, the continued exponentials for the functions $\cos z$ and $1/\cos z$ are identical except for the sign of a_1. Both continued exponentials have the same region of convergence, a double cardioid with cusps at $z=\pm\frac{1}{2}\pi$. These continued exponentials have the form

$$\cos z = a_0 e^{a_1 z^2 e^{a_2 z^2 e^{a_3 z^2 \cdots}}}$$

and

$$\frac{1}{\cos z} = \frac{1}{a_0} e^{-a_1 z^2 e^{a_2 z^2 e^{a_3 z^2 \cdots}}},$$

where $a_0=1$, $a_1=-\frac{1}{2}$, $a_2=\frac{1}{6}$, $a_3=\frac{11}{60}$, $a_4=\frac{4379}{27720}$, $a_5=\frac{7462435}{48554352}$, and so on. This sequence is monotone decreasing beginning with a_3 and it converges to the value $4/\pi^2 e$. Again, it is the zeros and/or singularities that determine the region of convergence of the continued exponential.

C. Continued exponential representation of an Airy function

The solution to the initial-value problem

$$y''(z)=zy(z), \quad y(0)=1, \; y'(0)=0,$$

can be expressed in terms of Airy functions $\mathrm{Ai}(x)$ and $\mathrm{Bi}(x)$:

$$y(z)=\pi[\mathrm{Bi}'(0)\mathrm{Ai}(z)-\mathrm{Ai}'(0)\mathrm{Bi}(z)].$$

This function has the Taylor series form

$$y(z)=\sum_{n=0}^{\infty}\frac{3^n\Gamma(n+1/3)}{(3n)!\Gamma(1/3)}z^{3n}.$$

If we convert this Taylor series to a continued exponential we obtain

$$y(z)=a_0 e^{a_1 z^3 e^{a_2 z^3 e^{a_3 z^3 \cdots}}},$$

where $a_0=1$, $a_1=\frac{1}{6}$, $a_2=-\frac{1}{20}$, $a_3=-\frac{7}{120}$, $a_4=-\frac{185}{3696}$, $a_5=-\frac{133817}{2772000}$, and so on.

To determine the region of convergence of the continued exponential we first observe that the continued exponential is a function of z^3. Thus, we expect the region of convergence to be a triple cardioid having three cusps. We find the location of the cusps by calculating that $\lim_{n\to\infty}a_n\approx -0.046939$; thus, the region of convergence consists of all z satisfying

$$-0.046939z^3\in\Omega.$$

This region of convergence is shown in Fig. 6. The cusps occur at the three zeros of $y(z)$ that are nearest to the origin. The locations of these zeros are given by the formula

$$z=-\left(\frac{1}{0.046939e}\right)^{1/3}\omega=-1.98635\omega,$$

where ω is a cube root of 1.

This example clearly demonstrates how the continued exponential accelerates the convergence of the Taylor series. Even though the radius of convergence of the Taylor series is infinite, the continued exponential converges faster than the Taylor series so long as z lies well inside the triple

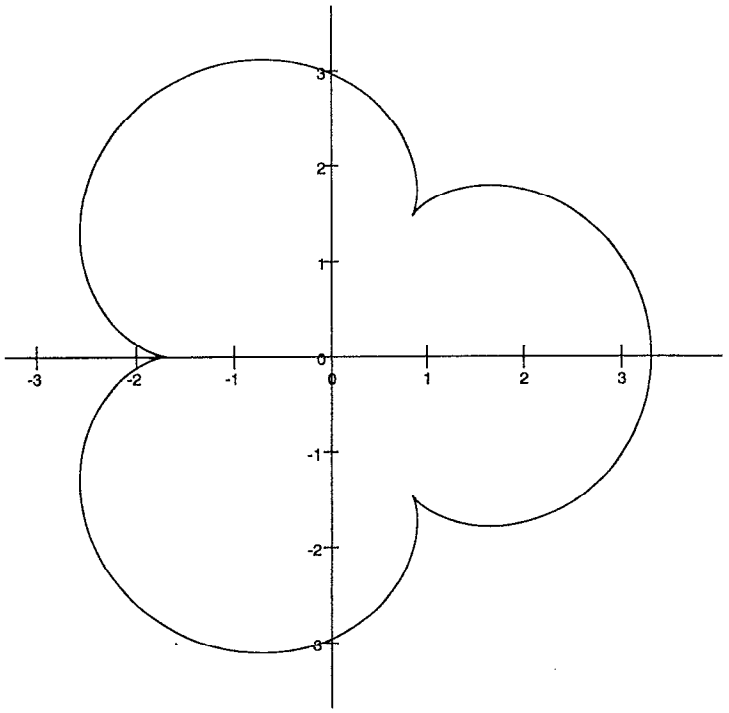

FIG. 6. Region of convergence of the continued exponential representing the Airy function $y(z)$ discussed in Sec. IV C. This triple cardioid has cusps at -1.98635ω, where ω is a cube root of 1. The cusps are located at the zeros of $y(z)$ that are nearest to the origin.

cardioid. For example, at $z=1$ a ten-term partial sum of Taylor series differs from the exact answer by a relative error of order 10^{-6} while a tenth-order continued exponential (constructed from the first ten terms in the Taylor series) has a relative error of order 10^{-14}. For a 15-term Taylor series, the relative error drops to 10^{-11} while that for a continued exponential drops to 10^{-21}.

D. Continued exponential representation of a Stieltjes function

Consider the Stieltjes function

$$f(z)=\int_0^\infty dt\frac{e^{-t}}{1+zt}. \tag{4.1}$$

The power series representation for this well known function is

$$f(z)\sim\sum_0^\infty (-1)^n n!z^n(|z|\to 0,\ \arg z<\pi).$$

This power series is divergent (it has a zero radius of convergence) but it is asymptotic to the function $f(z)$ as $z\to 0$ in the z plane cut along the negative real axis.

It is well known that the Padé sequence for this function converges for all z in the cut plane. What happens if we attempt to sum this series using a continued exponential? Converting Eq. (4.1) to a continued exponential gives

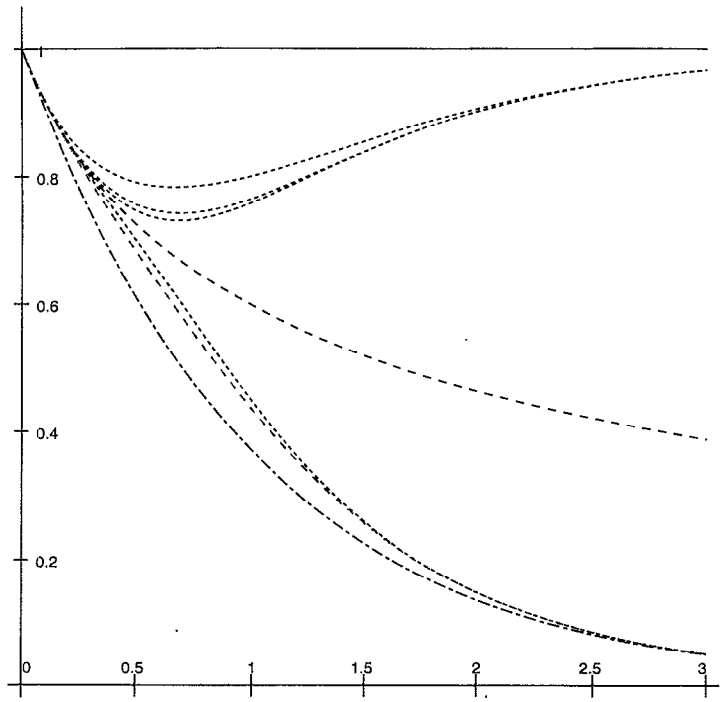

FIG. 7. Continued exponential approximants for the Stieltjes function $f(z)$ (solid line) discussed in Sec. IV D. When z is positive the continued exponential sequence (dashed lines) oscillates above and below $f(z)$ and converges to a cycle of length 2. For small values of z, this cycle is close to the exact value of $f(z)$. However, the continued exponential does *not* converge to $f(z)$.

$$f(z)=a_0 e^{a_1 z e^{a_2 z e^{a_3 z \cdots}}},$$

where $a_0=1$, $a_1=-1$, $a_2=-\frac{3}{2}$, $a_3=-\frac{77}{36}$, $a_4=-\frac{1405}{504}$, and so on. This continued exponential is different from those examined previously because the continued exponential coefficients grow with n rather than approaching a limit. In fact, $a_n \sim Cn$ as $n\to\infty$, where $C\approx -0.632$.

When z is positive the continued exponential sequence approaches a cycle of length 2 (see Fig. 7). For small values of z, this cycle is close to the exact value of $f(z)$ and oscillates above and below $f(z)$. However, the continued exponential does *not* converge to $f(z)$ and thus for this function it is not as useful as the Padé sequence. We do not know if it is possible to recover the exact value of $f(z)$ from the elements of the two-cycle; a calculational procedure, if one exists, would be more elaborate than an ordinary average or a geometric mean.

V. APPEARANCE OF CHAOTIC STRUCTURES

We have seen in Sec. IV that the cusp of the cardioid-shaped region of convergence of a continued exponential is located at the nearest zero or singularity of the function being represented. (We have also examined functions of the form $f(z^n)$, whose nearest zeros are arranged symmetrically around the origin at angles $2\pi/n$, where n is an integer. The convergence regions of such functions have n cusps.) In this section we briefly examine the extremely difficult problem of what happens when there is not just one but two nearest zeros (or singularities), which are not symmetrically arranged about the origin. An elementary function having this property is a quadratic polynomial of the form $(z-b+i)(z-b-i)$, where $b>0$.

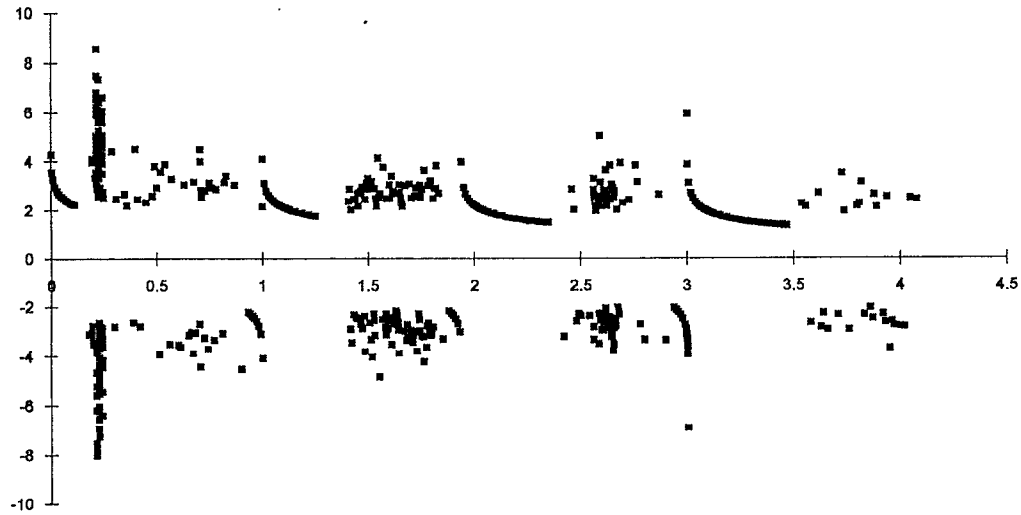

FIG. 8. A plot of the function $\mathrm{sgn}[f(b)][2+\log|f(b)|]$, $0 \leq b \leq 4.2$, where $f(b)$ is defined in Eq. (5.1). Observe that on the real line there are intervals where $f(b)$ appears meromorphic; that is, $f(b)$ is continuous except for simple poles. (One such interval is $2.9 \leq b \leq 3.5$.) These intervals are dispersed chaotically on the real line. Between pairs of intervals the function $f(b)$ appears noisy; however, on a finer scale we see that this noise is actually resolved into smaller subintervals where $f(b)$ is again meromorphic (see Fig. 9).

From our numerical studies (to order 100) of the function $(z-b+i)(z-b-i)$ it appears that the terms of the continued exponential representation often approach a constant, whose value depends on the parameter b. The continued exponential coefficients sometimes approach a limit monotonically, and sometimes sinusoidally. It is difficult to study this convergence because it tends to be very slow; we also find instances where the coefficients appear to converge slowly but then diverge.

Assuming that the coefficients a_n of the continued exponential converge for some values of b, the limit,

$$f(b) = \lim_{n \to \infty} a_n, \tag{5.1}$$

when it exists, is a function of the parameter b. The limiting function $f(b)$ depends chaotically upon b. We find that on the real line there are intervals where $f(b)$ is meromorphic; that is, $f(b)$ is continuous on the interval except for simple poles. These intervals are dispersed chaotically on the real line (see Figs. 8 and 9).

For each interval, the number of the coefficient following the last sign change is constant and will be called the convergence parameter of the interval. There may be several intervals with the same convergence parameter. We find that the length of an interval is roughly inversely related to the convergence parameter.

VI. CONCLUSIONS

We conclude this paper with several brief observations. First, it is clear from the examples we have presented that continued exponentials are a powerful and broadly applicable method for accelerating the convergence of a Taylor series inside its circle of convergence. Second, continued exponentials provide a means of analytically continuing a Taylor series to a much larger region

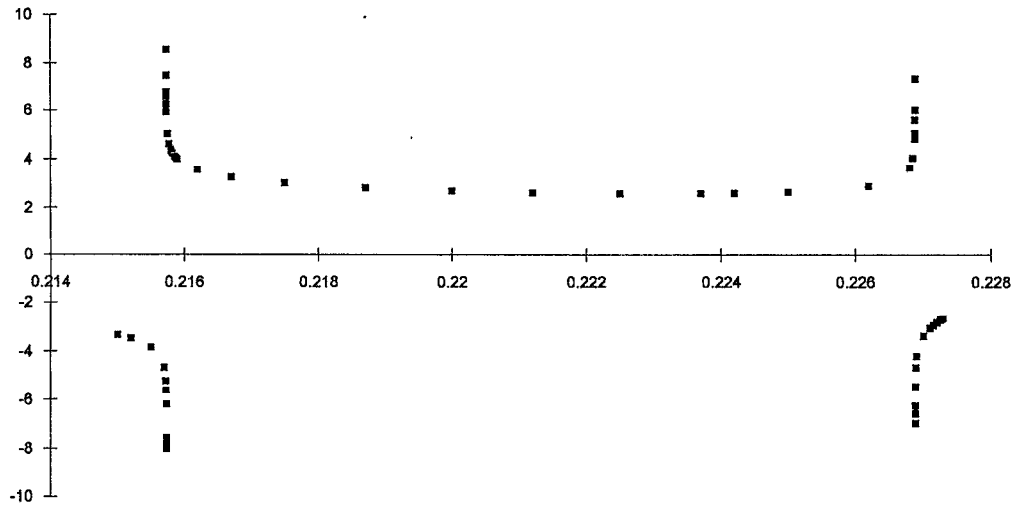

FIG. 9. Same as in Fig. 8 except that the domain is restricted to $0.215 \leq b \leq 0.228$.

than its circle of convergence so long as the function is zero free inside and near its circle of convergence. However, we do not yet know how to use continued exponentials to sum power series having a zero radius of convergence.

As we can see from the examples considered in this paper, the region of convergence of a continued exponential is determined by the zeros as well as by the singularities of the function being represented. This is true because a continued exponential approximates both a function and its reciprocal simultaneously. The function being approximated is zero-free in the region of convergence (except possibly for a zero at the origin). This observation may have some application in the study of complex variables; while it is often easy to locate the singularities of an analytic function it may be difficult to find the zeros. For example, finding the locations of the zeros of the Riemann zeta function is a well known, unsolved problem. Excluding the zeros away from $\mathrm{Re}(z)=1$ would be major progress in understanding the distribution of primes.

Finally, we remark that the theory of continued exponentials is intimately tied to the theory of chaos because it deals with iterated functions. We see chaotic structures emerge when we look at the cyclical convergence properties of a continued exponential outside the cardioid of convergence (see Fig. 3). Furthermore, we see chaotic behavior in such functions as $(z-b+i)(z-b-i)$ (Sec. V). The connection between chaos and continued exponentials deserves further study.

ACKNOWLEDGMENTS

We are indebted to D. Bessis and R. Stanley for many instructive discussions. We thank the U.S. Department of Energy for financial support. One of us (J.P.V.) thanks the Luthra foundation for partial financial support in the form of a travel grant.

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multiple values, depending on which value of $\log(i)$ is chosen. We avoid the ambiguity associated with evaluating $\beta_0^{\beta_1^{\beta_2 \cdots}}$ by considering instead continued exponentials of the form $\alpha_0 e^{\alpha_1 e^{\alpha_2 \cdots}}$.

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On the structure of symmetric self-dual Lie algebras

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A finite-dimensional Lie algebra is called (symmetric) self-dual, if it possesses an invariant nondegenerate (symmetric) bilinear form. Symmetric self-dual Lie algebras have been studied by Medina and Revoy, who have proven a very useful theorem about their structure. In this paper we prove a refinement of their theorem that has wide applicability in conformal field theory, where symmetric self-dual Lie algebras start to play an important role due to the fact that they are precisely the Lie algebras that admit a Sugawara construction. We also prove a few corollaries that are important in conformal field theory. © *1996 American Institute of Physics.* [S0022-2488(96)03307-5]

I. INTRODUCTION AND MOTIVATION

For most physical applications, reductive Lie algebras are the most natural Lie algebras to consider. This is because they are the Lie algebras of the compact Lie groups, which have played a privileged role in physical theories. Reductive Lie algebras are completely classified, since they are direct products of Abelian and semisimple Lie algebras, and essentially everything is known about them and their representations, at least the finite-dimensional ones. However by any reasonable measure, reductive Lie algebras are rare; and comparatively little is known about their nonreductive counterparts. The Levi–Malcev theorem reduces the classification problem for general Lie algebras to that of semidirect products (i.e., split extensions) of semisimple and solvable Lie algebras; but already classifying solvable Lie algebras seems to be as hard as classifying Lie algebras in general: by brute force one can classify all Lie algebras of dimension $\leqslant 5$, and restricting oneself to solvable Lie algebras does not get one any further (although all nilpotent six-dimensional Lie algebras are known). Therefore in order to probe the space of Lie algebras one could hope to benefit by restricting oneself to a class of Lie algebras including the reductive Lie algebras but that are still special enough to allow for a classification. One property shared by all reductive Lie algebras is the existence of an invariant metric; that is, an invariant nondegenerate symmetric bilinear form. We will call Lie algebras possessing an invariant metric *symmetric self-dual* Lie algebras, and they compromise a nontrivial generalization of reductive Lie algebras. Although no classification exists to this date, there exists a structure theorem[1] that tells us in principle how to construct Lie algebras with an invariant metric starting from the reductive Lie algebras. In fact, reductive Lie algebras can be obtained from simple Lie algebras and the one-dimensional Lie algebra by the operation of direct sum. What Medina and Revoy found Ref. 1 is that all Lie algebras with an invariant metric can be obtained from the same ingredients provided that we introduce a new operation—the *double extension*—which generalizes the semidirect product in a nontrivial way.

The importance of symmetric self-dual Lie algebras in conformal field theory (and via CFT in

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string theory) has to do with the following curious fact.[2,3] symmetric self-dual Lie algebras are precisely the Lie algebras for which a Sugawara construction exists. This fact may not appear so surprising if one assumes that the relation between the Sugawara construction and the WZW model persists in the nonreductive case: a WZW model needs for its definition a Lie group possessing a bi-invariant metric and this condition translates, at the level of the Lie algebra, into the statement that its Lie algebra should possess an invariant metric. Interestingly enough, the relation between the WZW model and the Sugawara construction does persist in the nonreductive case,[4] but the proof of this statement is not immediate and happens to necessitate detailed knowledge of the structure of symmetric self-dual Lie algebras, and, in particular, some refinements of the structure theorem in Ref. 1. The purpose of this paper is to collect those results on the structure of symmetric self-dual Lie algebras that were used in Ref. 4. Of necessity, those results are of a less physical nature than their applications, and we felt it inappropriate to include them together; hence the present paper.

This paper is organized as follows. In Sec. II we assemble some basic properties of symmetric self-dual Lie algebras and some properties of their ideals, which will be needed when we review the structure theorem of Medina and Revoy in Sec. III. In Sec. IV we define the double extension of a symmetric self-dual Lie algebra by a second Lie algebra and we work out some explicit formulas that we will need later. In Sec. V we discuss some examples of nonreductive self-dual Lie algebras. In Secs. VI and VII we prove some useful refinements and corollaries of the structure theorem. In Sec. VIII we comment briefly on the applications of this formalism to conformal field theory and string theory; and finally, in Sec. IV we mention some possible extensions and open problems. The paper also includes an appendix of a result on splittings of exact sequences involving Lie algebras. This result is used by Medina and Revoy, but we have not found a reference for it anywhere and we were forced to rederive it ourselves. We include it here for completeness.

II. BASIC PROPERTIES OF SYMMETRIC SELF-DUAL LIE ALGEBRAS

In this section we set up the notation and we introduce the necessary concepts about symmetric self-dual Lie algebras that we will need in the sequel.

Definition 2.1: Let $\mathscr{E}$ denote the class of pairs $(\mathfrak{g},\langle -,-\rangle)$, where $\mathfrak{g}$ is a finite-dimensional Lie algebra and $\langle -,-\rangle$ is a nondegenerate ad-invariant symmetric bilinear form on $\mathfrak{g}$. We shall call such a bilinear form simply an *invariant metric*, and we shall (tentatively) call an element of $\mathscr{E}$ a *symmetric self-dual* Lie algebra.

Remark 2.2: We should hasten to add that the nomenclature is by no means standard. French authors call these Lie algebras "orthogonal," whereas others call them "self-dual." The name "self-dual" presumably comes from the fact that the adjoint representation is equivalent to the coadjoint representation. But clearly for this to be the case, all that one requires is a nondegenerate invariant bilinear form on $\mathfrak{g}$, but not one that need be symmetric. After consulting with G. Zuckerman, who seems to have inspired "self-dual" in Ref. 5, we have chosen the compromise "symmetric self-dual," since it causes no confusion with the Lie algebras of the orthogonal Lie groups and does not preempt the term self-dual for their more general cousins. Nevertheless, since only symmetric self-dual Lie algebras will play a role in this paper, *we will use the term "self-dual" from now on to mean "symmetric self-dual" unless otherwise stated.*

Let us first mention some minor matters of notation. If a Lie algebra $\mathfrak{g}$ should decompose as a direct sum of *subspaces* A and B we will write $\mathfrak{g}=A\oplus B$. If moreover, the subspaces are *ideals*, so that the decomposition is one of Lie algebras, then we will write $\mathfrak{g}=A\times B$. It will prove convenient to introduce some nomenclature for particular subspaces of a self-dual Lie algebra depending on how the metric behaves on them.

Definition 2.3: Let $(\mathfrak{g},\langle -,-\rangle)$ be a self-dual Lie algebra. For any subspace $V\subset\mathfrak{g}$, let $V^{\perp}=\{w\in\mathfrak{g}|\langle w,v\rangle=0 \text{ for all } v\in V\}$. Notice that the operation $V\to V^{\perp}$ is involutive, so that $(V^{\perp})^{\perp}=V$. We say that

$$V \text{ is } \textit{isotropic} \Leftrightarrow V \subset V^{\perp},$$

$$V \text{ is } \textit{coisotropic} \Leftrightarrow V \supset V^{\perp},$$

$$V \text{ is } \textit{Lagrangian} \Leftrightarrow V = V^{\perp},$$

$$V \text{ is } \textit{degenerate} \Leftrightarrow V \cap V^{\perp} \neq 0,$$

$$V \text{ is } \textit{nondegenerate} \Leftrightarrow V \cap V^{\perp} = 0.$$

Let $(\mathfrak{g},\langle -,-\rangle)$ be a self-dual Lie algebra. We define the centralizer $Z_{\mathfrak{g}}(V)$ of a subspace $V \subset \mathfrak{g}$ as all those elements in the Lie algebra that commute with all elements of the subspace; that is $Z_{\mathfrak{g}}(V) \cong \{w \in \mathfrak{g} | [w,v]=0 \text{ for all } v \in V\}$. For a self-dual Lie algebra, centralizers and ideals are intimately linked, as the following lemma suggests.

Lemma 2.4: $I \subset \mathfrak{g}$ is an ideal if and only if $I^{\perp} \subset Z_{\mathfrak{g}}(I)$.

Proof: This follows immediately by the invariance of the metric. Indeed, $\langle [\mathfrak{g},I],I^{\perp}\rangle = \langle \mathfrak{g},[I,I^{\perp}]\rangle$, from where it follows that $[\mathfrak{g},I] \subset I^{\perp\perp} = I$ if and only if $[I,I^{\perp}]=0$.

The center of a self-dual Lie algebra can be also characterized very easily. In fact, the following occurs.

Lemma 2.5: Let $[\mathfrak{g},\mathfrak{g}]$ denote the first derived ideal and $Z(\mathfrak{g})$ be the center. Then $[\mathfrak{g},\mathfrak{g}]^{\perp} = Z(\mathfrak{g})$.

Proof: $x \in Z(\mathfrak{g}) \Leftrightarrow [x,y]=0, \forall y \Leftrightarrow \langle [x,y],z\rangle = 0, \forall y,z \Leftrightarrow \langle x,[y,z]\rangle = 0 \forall y,z \Leftrightarrow x \in |\mathfrak{g},\mathfrak{g}|^{\perp}$.

First of all, notice that if $I \subset \mathfrak{g}$ is an ideal, so is $I^{\perp}$. Recall that an ideal $I \subset \mathfrak{g}$ is minimal if it does not properly contain another nontrivial ideal $J \subset \mathfrak{g}$. In other words, if $I \subset \mathfrak{g}$ is a minimal ideal and if $J \subset \mathfrak{g}$ is another ideal with $J \subset I$, then either $J=0$ or $J=1$. Below we list some properties of minimal ideals that we shall need in the proof of the structure theorem or its refinements.

Proposition 2.6: Let $(\mathfrak{g},\langle -,-\rangle)$ be self-dual, and let $I \subset \mathfrak{g}$ be a minimal ideal. Then (1) If I is nondegenerate, then it is a factor, and hence simple or one dimensional; (2) if I is degenerate, then it is isotropic and Abelian; and (3) $I^{\perp}$ is a maximal ideal.

Proof: Let $I \in \mathfrak{g}$ be any ideal. Then so are $I^{\perp}$ and $I \cap I^{\perp} \subset I$, since the intersection of two ideals is an ideal. Since I is minimal, $I \cap I^{\perp}$ is either 0 or I.

(1) Let us take the first possibility: $I \cap I^{\perp}=0$. Definition 2.3 tells us that I is nondegenerate. Since both I and $I^{\perp}$ are ideals, $[I,I^{\perp}] \subset I$ and $[I,I^{\perp}] \subset I^{\perp}$; hence $[I,I^{\perp}] \subset I \cap I^{\perp}=0$. This means that $[I,I^{\perp}]=0$ and $\mathfrak{g}=I \times I^{\perp}$. Since I is a factor, any ideal of I is automatically an ideal of $\mathfrak{g}$. But by minimality, I cannot have any proper ideals, hence I is either simple or one-dimensional.

(2) The other possibility is that $I \cap I^{\perp}=I$, which means that I is degenerate. In fact, Definition 2.3 tells us that $I \subset I^{\perp}$ is isotropic. And by Lemma 2.4, $I \subsetneq I^{\perp} Z_{\mathfrak{g}}(I)$, whence it is Abelian.

(3) Finally, suppose that there exists a proper ideal J such that $I^{\perp} \subsetneq J$. Taking $^{\perp}$, we find $J^{\perp} \subsetneq I^{\perp\perp} = I$, which violates minimality. Hence $I^{\perp}$ is maximal. □

III. THE STRUCTURE THEOREM OF MEDINA AND REVOY

The class $\mathscr{C}$ of self-dual Lie algebras is closed under the operation of an orthogonal direct product; indeed, if $(\mathfrak{g}_1,\langle -,-\rangle_1)$ and $(\mathfrak{g}_2,\langle -,-\rangle_2)$ are two self-dual Lie algebras, so is $(\mathfrak{g}_1 \times \mathfrak{g}_2, \langle -,-\rangle_1 \oplus \langle -,-\rangle_2)$. We call a self-dual Lie algebra $(\mathfrak{g},\langle -,-\rangle)$ *indecomposable* if it cannot be written as such a direct product; and *decomposable* if it can. The following preliminary result on the structure of self-dual Lie algebras follows immediately from Proposition 2.6.

Corollary 3.1: Let $(\mathfrak{g},\langle -,-\rangle)$ be an indecomposable Lie algebra. Then exactly one of the following cases hold: (1) $\mathfrak{g}$ is simple (2); $\mathfrak{g}$ is one-dimensional; or (3) $\mathfrak{g}$ is not simple, $\dim \mathfrak{g}>1$, and every proper idal of $\mathfrak{g}$ is degenerate. □

It is clear that every self-dual Lie algebra is a product of objects of the types described above. Objects of types (1) and (2) are well known: they correspond to the direct product of a semisimple Lie algebra and an Abelian Lie algebra; that is, they are reductive. The class of objects of type (3) is more exotic. The following is the smallest such Lie algebra.

Example 3.2: Let $\mathfrak{g}$ be the four-dimensional Lie algebra with basis $\{h,e_\pm,g\}$ and Lie brackets

$$[h,e_\pm]=\pm e_\pm \quad \text{and} \quad [e_+,e_-]=g.$$

This Lie algebra is solvable but not nilpotent. For any scalars $\alpha\neq 0$ and β, the bilinear form

$$\langle e_+,e_-\rangle=\alpha, \quad \langle h,h\rangle=\beta, \quad \text{and} \quad \langle h,g\rangle=\alpha,$$

is invariant and nondegenerate. Hence it is a nonreductive self-dual Lie algebra. As shown in Ref. 6 the WZW model associated with this Lie algebra is an exact string background describing a gravitational wave. More nonreductive examples will be given in Sec. V.

In this section we will see that indecomposable self-dual Lie algebras of type (3) are easy to characterize. We shall do so in steps.

Let $(\mathfrak{d},\langle -,-\rangle)\in\mathscr{E}$ be indecomposable with $\mathfrak{d}$ not simple and with $\dim\mathfrak{d}>1$. We fix a proper minimal ideal $I\subset\mathfrak{d}$. By Corollary 3.1, it is degenerate and by Proposition 2.6 (2) it is isotropic and Abelian. By Lemma 2.4, I is a central ideal of $I^\perp$; whence $\mathfrak{g}=I^\perp/I$ is a Lie algebra. Moreover, since $I=I^{\perp\perp}$, $\mathfrak{g}$ inherits an invariant metric $\langle -,-\rangle_\mathfrak{g}$. In other words, we have proven the following lemma.

Lemma 3.3: We have an exact sequence

$$0\to I\to I^\perp\to\mathfrak{g}\to 0, \tag{3.4}$$

with $(\mathfrak{g},\langle -,-\rangle_\mathfrak{g})$ an object in $\mathscr{E}$.

It may seem overkill to use the language of exact sequences, but it turns out that it will be very useful and it will save us some time in the end. For the reader not familiar with this language, we simply recall that a sequence is exact whenever the kernel of any arrow is the image of the preceding one. In particular, the exactness of the above sequence simply says that $I\subset I^\perp$ is a Lie subalgebra (and an ideal since it is the kernel of a homomorphism) and that $\mathfrak{g}\cong I^\perp/I$ as Lie algebras. Moreover, since we are quotienting $I^\perp$ by its $^\perp$, the resulting quotient inherits a nondegenerate metric.

Before continuing, let us make the following notational remark. Below we will find it necessary to distinguish the Lie bracket and the inner product of the same pair of vectors when thought of as elements of different Lie algebraic structures on the same vector space. We will assume that when nothing is specified, the Lie bracket and the metric correspond to those in $\mathfrak{d}$.

Continuing with the argument, by Proposition 2.6 (3), $I^\perp$ is a maximal ideal of $\mathfrak{d}$; whence $\mathfrak{h}=\mathfrak{d}/I^\perp$ is a Lie algebra without proper ideals; that is, either $\mathfrak{h}$ is simple or one dimensional. It now follows that we can actually identify $\mathfrak{h}$ with a *subalgebra* of $\mathfrak{d}$. The proof of this lemma is much more technical than the proof of the structure theorem, and so we leave it to the Appendix. It is worth pointing out, however, that it is precisely this lemma that prevents the straightforward extension of the structure theorem to self-dual Lie superalgebras.

Lemma 3.5: The exact sequence

$$0\to I^\perp\to\mathfrak{d}\to\mathfrak{h}\to 0, \tag{3.6}$$

splits whenever $\mathfrak{h}$ is simple or one dimensional; that is, for such $\mathfrak{h}$, $\mathfrak{d}\cong\mathfrak{h}\ltimes I^\perp$.

In particular, $\mathfrak{d}=\mathfrak{h}\oplus I^\perp$, whence $V\equiv\mathfrak{h}\oplus I\subset\mathfrak{d}$ is a nondegenerate subspace of $\mathfrak{d}$. This implies that as vector spaces $\mathfrak{d}=V\oplus V^\perp$, and $I^\perp=V^\perp\oplus I$. The map $I^\perp\to\mathfrak{g}$ in (3.4) defines a vector space

isomorphism $\mathfrak{g}\cong V^\perp$. With some abuse of notation we will identify $\mathfrak{g}$ with $V^\perp\subset\mathfrak{0}$. In general, though, $V^\perp$ will fail to be a subalgebra. But all that happens is that it acquires a central extension. In fact, if $x,y,\in V^\perp$, then

$$[x,y]=[x,y]_{\mathfrak{g}}+\beta(x,y),$$

for some 2-cocycle $\beta:\wedge^2\mathfrak{g}\to I$, where, since $I\subset I^\perp$ is central, it becomes a trivial $\mathfrak{g}$ module. The cohomology class of this cocycle is the one defining the central extension (3.4).

Definition 3.7: Let $\mathfrak{g}$ be a self-dual Lie algebra. A linear map $D:\mathfrak{g}\to\mathfrak{g}$ is an *antisymmetric derivation* if D preserves both the Lie bracket and the invariant metric; that is, if

$$D([x,y])=[Dx,y]+[x,Dy] \quad \text{and} \quad \langle Dx,y\rangle=-\langle x,Dy\rangle.$$

Lemma 3.8: $\mathfrak{h}$ acts on $\mathfrak{g}$ via antisymmetric derivations.

Proof: We can define an action of $\mathfrak{h}$ on $\mathfrak{g}$ as follows. Take $x\in\mathfrak{g}$ and lift it to $V^\perp\subset\mathfrak{d}$. If $h\in\mathfrak{h}$, then we can define $h\cdot x=[h,x]$. *A priori*, this bracket is in $I^\perp=V^\perp\oplus I$. But we show that it is in fact in $V^\perp$. Indeed, let $h'\in\mathfrak{h}$ and compute $\langle h',[h,x]\rangle=\langle[h',h],x\rangle$. Since $[h',h]\in\mathfrak{h}\subset V$, the rhs is zero for all h'. Therefore $[h,x]\in\mathfrak{h}^\perp$. But nondegenary of V implies that $I\cap\mathfrak{h}^\perp=0$, whence $[h,x]\in V^\perp$. Since the bracket and metric of $\mathfrak{g}$ are induced from those of $\mathfrak{d}$, and $\mathfrak{h}\in\mathfrak{d}$ acts via (inner) antisymmetric derivations, it also acts on $\mathfrak{g}$ as antisymmetric derivations.

The action of $\mathfrak{h}$ on $\mathfrak{g}$ is intimately linked to the cocycle β characterizing the central extension (3.4). In fact, let $h\in\mathfrak{h}$ and $x,y\in\mathfrak{g}$. Lifting x and y back to $V^\perp\subset\mathfrak{d}$ we compute $\langle h\cdot x,y\rangle_{\mathfrak{g}}=\langle[h,x],y\rangle=\langle h,[x,y]\rangle=\langle h,[x,y]_{\mathfrak{g}}+\beta(x,y)\rangle$. But since $\mathfrak{h}$ is orthogonal to $V^\perp$, we find that

$$\langle h\cdot x,y\rangle_{\mathfrak{g}}=\langle h,\beta(x,y)\rangle. \tag{3.9}$$

Lemma 3.10: As $\mathfrak{h}$ modules, $I\cong\mathfrak{h}^*$.

Proof: Let $h\in\mathfrak{h}$ and $x\in I$. Since I is an ideal, $[h,x]\in I$, whence it is an $\mathfrak{h}$ module. Because $V=\mathfrak{h}\oplus I$ is nondegenerate and I is isotropic, we can identify I with $\mathfrak{h}^*$ as vector spaces: the isomorphism given by $I\ni x\to\langle x,-\rangle$ restricted to $\mathfrak{h}$. Now notice that for all $h'\in\mathfrak{h}$, $\langle[h,x],h'\rangle=-\langle x,[h,h']\rangle$, whence $I\cong\mathfrak{h}^*$ as $\mathfrak{h}$ modules. □

In summary, we have proven the following structure theorem.

Theorem 3.11: (Medina–Revoy[1]) Let$(\mathfrak{d},\langle-,-\rangle)$ be an indecomposable object in $\mathscr{C}$ such that $\mathfrak{d}$ is not simple nor one dimensional. Then $\mathfrak{d}$ is isomorphic to the Lie algebra with underlying vector space $\mathfrak{g}\oplus\mathfrak{h}\oplus\mathfrak{h}^*$, where (1) $\mathfrak{g}$ is the Lie algebra defined (3.4) and which inherits an invariant metric $\langle-,-\rangle_{\mathfrak{g}}$ by restricting $\langle-,-\rangle$; (2) $\mathfrak{h}$ is the Lie algebra defined by (3.6), which is either one dimensional or simple; (3) $\mathfrak{h}$ acts on $\mathfrak{g}$ via antisymmetric derivations: $(h,x)\to h\cdot x$ for $h\in\mathfrak{h}$ and $x\in\mathfrak{g}$; and (4) the Lie brackets are given for $x,x'\in\mathfrak{g}$, $h,h'\in\mathfrak{h}$ and $\alpha,\alpha'\in\mathfrak{h}^*$ by

$$[(x,h,\alpha),(x',h',\alpha')]=([x,x']_{\mathfrak{g}}+h\cdot x'-h'\cdot x,[h,h']_{\mathfrak{h}},\beta(x,x')+\mathrm{ad}_h^*\cdot\alpha'-\mathrm{ad}_h^*\cdot\alpha), \tag{3.12}$$

where $\beta:\wedge^2\mathfrak{g}\to\mathfrak{h}^*$ is given by (3.9). □

IV. DOUBLE EXTENSIONS

In this section we review the definition of a double extension, formalizing the results in the previous section on the structure of nonreductive indecomposable self-dual Lie algebras.

Definition 4.1: Given $(\mathfrak{g},\langle-,-\rangle_{\mathfrak{g}})\in\mathscr{C}$ and $\mathfrak{h}$ a Lie Algebra acting on $\mathfrak{g}$ via antisymmetric derivations, the Lie algebra $\mathfrak{d}$ defined on the vector space as $\mathfrak{g}\oplus\mathfrak{h}\oplus\mathfrak{h}^*$ by (3.12) and (3.9) is called the *double extension* of $\mathfrak{g}$ *by* $\mathfrak{h}$ and we denote it by $D(\mathfrak{g},\mathfrak{h})$.

Remark 4.2: Notice that the notation $D(\mathfrak{g},\mathfrak{h})$ is ambiguous on two counts. First of all, the data is not just $\mathfrak{g}$ but $(\mathfrak{g},\langle-,-\rangle_{\mathfrak{g}})$; and also not just $\mathfrak{h}$ but $\mathfrak{h}$ together with the action of $\mathfrak{h}$ on $\mathfrak{g}$ via antisymmetric derivations. Nevertheless, for the purposes of this paper, any ambiguity that might arise will be resolved contextually.

Provided that $\mathfrak{g}$ be self-dual, the double extension of $\mathfrak{g}$ by $\mathfrak{h}$ always carries an invariant metric. Indeed, if $\langle-,-\rangle_{\mathfrak{h}}$ is any invariant bilinear form on $\mathfrak{h}$, we define

$$\langle(x,h,\alpha),(x',h',\alpha')\rangle=\langle x,x'\rangle_{\mathfrak{g}}+\langle h,h'\rangle_{\mathfrak{h}}+\alpha(h')+\alpha'(h), \tag{4.3}$$

for all $x,x'\in\mathfrak{g},h,h'\in\mathfrak{h}$, and $\alpha,\alpha'\in\mathfrak{h}^*$. A routine calculation shows that this metric is invariant, whence $(\mathfrak{g},\langle-,-\rangle)$ is a self-dual Lie algebra.

Remark 4.4: It is worth pointing out that if the action of $\mathfrak{h}$ on $\mathfrak{g}$ is trivial, then the double extension is decomposable and isomorphic to $\mathfrak{g}\times(\mathfrak{h}\ltimes\mathfrak{h}^*)$. In particular, if $\mathfrak{g}=0$, then the double extension is $(\mathfrak{h}\ltimes\mathfrak{h}^*)$, which is the classical double of $\mathfrak{h}$ given the trivial bialgebra structure.[7]

It will be convenient later on to work with the explicit expression for the Lie brackets and for the invariant metric of a double extension. Hence we will now work out these expressions in a basis. We let $(\mathfrak{g},\langle-,-\rangle_{\mathfrak{g}})$ be a self-dual Lie algebra. Let the invariant metric have components $\Omega^{\mathfrak{g}}_{ij}$ relative to a fixed basis $\{G_i\}$. Also relative to this basis, we will let the Lie bracket in $\mathfrak{g}$ be given by $[G_i,G_j]_{\mathfrak{g}}=f_{ij}{}^kG_k$. We consider also a Lie bracket $\mathfrak{h}$, with basis $\{H_\alpha\}$, acting on $\mathfrak{g}$ via antisymmetric derivations,

$$H_\alpha\cdot G_i=f^j_{\alpha i}G_j,$$

and with Lie brackets given by $[H_\alpha,H_\beta]_{\mathfrak{h}}=f^\gamma_{\alpha\beta}H_\gamma$. Its dual $\mathfrak{h}^*$ has a canonical dual basis given by $\{H^\alpha\}$.

The double extension $\mathfrak{g}=D(\mathfrak{g},\mathfrak{h})$ will be then defined on the vector space $\mathfrak{g}\oplus\mathfrak{h}\oplus\mathfrak{h}^*$ by the following Lie brackets:

$$[G_i,G_j]=f^k_{ij}G_k+f_{ij\alpha}H^\alpha,\quad [H_\alpha,G_i]=f^j_{\alpha i}G_j,$$

$$[H_\alpha,H_\beta]=f^\gamma_{\alpha\beta}H_\gamma,\quad [H_\alpha,H^\beta]=-f^\beta_{\alpha\gamma}H^\gamma,$$

$$[H^\alpha,G_i]=[H^\alpha,H^\beta]=0,$$

where $f_{ij\alpha}=f^k_{\alpha i}\Omega^{\mathfrak{g}}_{kj}$. The above explicit expression makes manifest the fact mentioned in Remark 4.2 that $D(\mathfrak{g},\mathfrak{h})$ does not depend on $\mathfrak{g}$ and $\mathfrak{h}$ only through their Lie algebra structures, as the notation would suggest, but also on the action of $\mathfrak{h}$ and $\mathfrak{g}$ and on the metric of $\mathfrak{g}$.

The invariant metric on $D(\mathfrak{g},\mathfrak{h})$ is given by

$$\Omega^{\mathfrak{g}}_{ab}=H_a\begin{array}{c}\\ G_i\\ H_\alpha\\ H^\alpha\end{array}\begin{array}{c}\begin{array}{ccc}G_j & H_\beta & H^\beta\end{array}\\ \begin{pmatrix}\varphi^{\mathfrak{g}}_{ij} & 0 & 0\\ 0 & h_{\alpha\beta} & \delta_{\alpha\beta}\\ 0 & \delta^\alpha_\beta & 0\end{pmatrix}\end{array},$$

where $(h_{\alpha\beta})$ is an arbitrary (possibly degenerate) invariant bilinear from in $\mathfrak{h}$. We also record for future use the Killing form of the above double extension $\kappa^{\mathfrak{d}}$. This form will of course be degenerate, having the form

$$\begin{array}{r} \\ G_i \\ \kappa^{\mathfrak{d}}_{ab}=H_a \\ H^a \end{array} \begin{array}{c} \begin{array}{ccc} G_j & H_\beta & H^\beta \end{array} \\ \begin{pmatrix} \kappa^{\mathfrak{g}}_{ij} & \kappa^{\mathfrak{g}}_{i\beta} & 0 \\ \kappa^{\mathfrak{d}}_{\alpha j} & \kappa^{\mathfrak{d}}_{\alpha\beta} & 0 \\ 0 & 0 & 0 \end{pmatrix} \end{array},$$

where $\kappa^{\mathfrak{g}}$ is the Killing form of $\mathfrak{g}$ and where

$$\kappa^{\mathfrak{d}}_{i\alpha}=f^k_{ij}f^j_{\alpha k} \qquad \text{and} \qquad \kappa^{\mathfrak{d}}_{\alpha\beta}=f^j_{\alpha i}f^i_{\beta j}+2\kappa^{\mathfrak{h}}_{\alpha\beta}.$$

V. SOME NONREDUCTIVE EXAMPLES

Before going on to the main results of this paper, refining and extending the results described in the previous sections, let us pause to exhibit some examples of nonreductive indecomposable self-dual Lie algebras.

In Example 3.2 we saw the simplest such algebra: a four-dimensional solvable (but not nilpotent) Lie algebra. Over the complex numbers, it is the only such example in four dimensions. Viewed as a double extension, the algebra in Example 3.2 can be understood as $\mathfrak{D}(\mathfrak{b},\mathfrak{a})$, where $\mathfrak{a}$ is the one-dimensional Lie algebra and $\mathfrak{b}$ is a two-dimensional Abelian Lie algebra. Because $\mathfrak{b}$ is Abelian, all metrics are invariant, and over the complex numbers all metrics are equivalent, meaning that they can be transformed into one another by an automorphism of $\mathfrak{b}$. Over the reals, however, the signature of the metric is an invariant and we have two classes of metrics: the Euclidean and the Lorentzian.

We let $\mathfrak{a}_2$ denote the real self-dual Abelian Lie algebra with basis $\{e_1,e_2\}$ and with Euclidean metric $\langle e_i,e_j\rangle=\delta_{ij}$. Similarly, let $\mathfrak{a}_{1,1}$ denote the Lorentzian real form of the complex Lie algebra $\mathfrak{b}$. It has basis $\{e_1,e_2\}$ and Lorentzian metric $\langle e_1,e_1\rangle=-\langle e_2,e_2\rangle=1$. Since these Lie algebras are Abelian, any endomorphism is a derivation. The choice of metric dictates which are antisymmetric. For $\mathfrak{a}_2$ the Lie algebra of antisymmetric derivations is $so(2)$, whereas for $\mathfrak{a}_{1,1}$ it is $so(1,1)$. They are one-dimensional Abelian Lie algebras. We can now form the double extensions $\mathfrak{D}(\mathfrak{a}_2, so(2))$, and $\mathfrak{D}(\mathfrak{a}_{1,1}, so(1,1))$. These Lie algebras are self-dual, indecomposable, and nonreductive: in fact, they are solvable and not nilpotent. They are different real forms of the complex Lie algebra discussed in Example 3.2.

This interpretation allows us to generalize this example as follows[6,3]. Let $\mathbb{E}_{p,q}$ be the $(p+q)$-dimensional pseudo-Euclidean space with signature (p,q), and let $\mathfrak{a}_{p,q}$ denote the resulting self-dual Abelian Lie algebra. The Lie algebra of antisymmetric derivations is isomorphic to $so(p,q)$. We can form the double extension $\mathfrak{D}(\mathfrak{a}_{p,q}, so(p,q))$. This Lie algebra is self-dual, indecomposable, and nonreductive. It is not necessary to extend by the full Lie algebra of antisymmetric derivations to obtain an indecomposable double extension. Given a subalgebra $\mathfrak{h}\subset so(p,q)$ which acts effectively on $\mathbb{E}_{p,q}$, we can form $\mathfrak{D}(\mathfrak{a}_{p,q}, \mathfrak{h})$.

Other examples are known. In Ref. 9 some examples were obtained by Wigner contractions of semisimple Lie algebras, and this was further generalized in Ref. 3. Let $\mathfrak{g}$ be a semisimple Lie algebra and $\mathfrak{h}$ a subalgebra reductive in $\mathfrak{g}$ and such that there exists an $\mathfrak{h}$-invariant metric in $\mathfrak{g}$ relative to that $\mathfrak{g}$ splits as $\mathfrak{g}=\mathfrak{h}\oplus\mathfrak{h}^\perp$. This is true, for example, if $\mathfrak{g}$ is the Lie algebra of a compact Lie group and $\mathfrak{h}$ the Lie algebra of a (compact) Lie subgroup as in Ref. 9, or if both $\mathfrak{g}$ and $\mathfrak{h}$ are semisimple, among other cases. The models of Ref. 9 will be obtained as Wigner contractions of $\mathfrak{g}\times\mathfrak{h}$. Let $\mathfrak{e}=\mathfrak{h}^\perp$ denote the orthogonal complement of $\mathfrak{h}$ in $\mathfrak{g}$ relative to any $\mathfrak{h}$-invariant metric. Let us define subspaces $\mathfrak{h}_\pm\subset\mathfrak{h}\times\mathfrak{h}$ by $\mathfrak{h}_\pm=\{(h,\pm h)\in\mathfrak{h}\times\mathfrak{h}\}$. Choose bases $\{H^{(1)}_a\}$ and $\{H^{(2)}_a\}$ for the two copies of $\mathfrak{h}$, respectively, and $\{K_i\}$ for $\mathfrak{e}$. Then $\{H^\pm_a=H^{(1)}_a\pm H^{(2)}_a\}$ are bases for $\mathfrak{h}_\pm$, and the nonzero brackets of $\mathfrak{g}\times\mathfrak{h}$ are in this basis given by

$$[K_i,K_j]=f^k_{ij}K_k+\frac{1}{2}f^a_{ij}(H^+_\alpha+H^-_a), \quad [H^\pm_a,H^\pm_b]=f^c_{ab}H^+_c, \tag{5.1}$$

$$[H_a^{\pm},K_i]=f_{ai}^{j}K_j, \quad [H_a^{+},H_b^{-}]=f_{ab}^{c}H_c^{-},$$

where the f's are the structure constants of g in the chosen basis. To recover the structure of a double extension [compare with (3.12)], we would like that $[K_i,K_j]$ would not to close into H_a^{+}, and that $[H_a^{-},H_b^{-}]$ and $[H_a^{-},K_i]$ would vanish. The way out is to perform a contraction. To this effect, we define the following rescaled generators: $H_a^{+}(\epsilon)=\epsilon^{\Delta\pm}H_a^{+}$, and $K_i(\epsilon)=\epsilon^{\Delta}K_i$. Rewriting (5.1) in terms of the rescaled generators, we notice that we can get rid of the unwanted terms in the limit $\epsilon\to 0$ provided that we choose $\Delta_{+}=0$ and $\Delta_{-}=2\Delta>0$. Let us then choose these scaling dimensions, take the limit $\epsilon\to 0$, and introduce generators $X_i=K_i(0)$, $H_a=H_a^{+}(0)$, and $H^a=\frac{1}{2}g^{ab}H_b^{-}(0)$, where g^{ab} is the inverse of the $\mathfrak{h}$-invariant metric on $\mathfrak{h}$. With this notation and using the invariance of the metric, we find that the algebra becomes precisely (3.12), but with $f_{ij}^{k}=0$.

Notice that if we take $\mathfrak{g}$ to be any one of the de Sitter algebras for a space-time of signature (p,q)—that is, $\mathfrak{g}=so(p+1,q)$ or $\mathfrak{g}=so(p,q+1)$— and $\mathfrak{h}=so(p,q)$, then we recover precisely the examples described above.

All these examples share one property in common: they are double extensions $\mathfrak{D}(\mathfrak{a},\mathfrak{b})$, where $\mathfrak{a}$ is Abelian. Only one example is known of an indecomposable nonreductive self-dual Lie algebra that is the double extension of a non-Abelian Lie algebra. We refer the reader Ref. 10 for the details.

VI. SOME USEFUL REFINEMENTS

In this section we prove some refinements of Theorem 3.11 that have proven instrumental in the applications to Conformal Field Theory. We start by listing some conditions on $\mathfrak{g}$ under which any double extension $D(\mathfrak{g},\mathfrak{h})$ will fail to be indecomposable.

Remark 4.4 tells us that a double extension need not be indecomposable even if $\mathfrak{h}$ is taken to be simple or one dimensional; and one such example is when $\mathfrak{h}$ acts on $\mathfrak{g}$ via inner derivations, as we now see.

Proposition 6.1: If $\mathfrak{h}$ acts on $(\mathfrak{g},\langle-,-\rangle)\in\mathscr{E}$ via inner derivations, then $D(\mathfrak{g},\mathfrak{h})\cong\mathfrak{g}\times(\mathfrak{h}\ltimes\mathfrak{h}^{*})$.

Proof: Let $\varphi:\mathfrak{h}\to\mathfrak{g}$ be the homomorphism defining the action of $\mathfrak{h}$ on $\mathfrak{g}$. In other words, for $h\in\mathfrak{h}$ and $x\in\mathfrak{g}$, $h\cdot x=[\varphi(h),x]_{\mathfrak{g}}$. Let $\varphi^{\flat}:\mathfrak{h}\to\mathfrak{g}^{*}$ be the map sending $h\mapsto\langle\varphi(h),-\rangle_{\mathfrak{g}}$, and let $\varphi^{\sharp}:\mathfrak{g}\to\mathfrak{h}^{*}$ denote its transpose. Notice that because the metric of $\mathfrak{g}$ is $\mathfrak{h}$ invariant, these maps are actually intertwiners of the action of $\mathfrak{h}$; in particular, for $h\in\mathfrak{h}$ and $x\in\mathfrak{g}$, we have that

$$[h,\varphi^{\sharp}(x)]=\varphi^{\sharp}([\varphi(h),x]_{\mathfrak{g}}). \tag{6.2}$$

We can now define the following vector space automorphism Ψ of $\mathfrak{g}\oplus\mathfrak{h}\oplus\mathfrak{h}^{*}$:

$$\Psi(x,h,\alpha)=(x-\varphi^{\sharp}(x),h+\varphi(h),\alpha).$$

We claim that Ψ is a Lie algebra isomorphism $D(\mathfrak{g},\mathfrak{h})\xrightarrow{\cong}\mathfrak{g}\times(\mathfrak{h}\ltimes\mathfrak{h}^{*})$. Indeed, for $x,y\in\mathfrak{g}$, $\Psi([x,y])=\Psi([x,y]_{\mathfrak{g}}+\beta(x,y))=[x,y]_{\mathfrak{g}}-\varphi^{\sharp}([x,y]_{\mathfrak{g}})+\beta(x,y)$. But from (3.9) we have that $\beta(x,y)=\varphi^{\sharp}([x,y]_{\mathfrak{g}})$, whence $\Psi([x,y])=[\Psi(x),\Psi(y)]$. Second, we have that, on the one hand, for $h\in\mathfrak{h}$, $\Psi([h,x])=\Psi([\varphi(h),x]_{\mathfrak{g}})=[\varphi(h),x]_{\mathfrak{g}}-\varphi^{\sharp}([\varphi(h),x]_{\mathfrak{g}})$ and $[\Psi(h),\Psi(x)]=[h+\varphi(h),x-\varphi^{\sharp}(x)]=[\varphi(h),x]_{\mathfrak{g}}-[h,\varphi^{\sharp}(x)]$, on the other. But both of these expressions agree by virtue of (6.2). Similarly, $\Psi([h,h'])=[h,h']+\varphi([h,h'])$ agrees with $[\Psi(h),\Psi(h')]=[h+\varphi(h),h'+\varphi(h')]=[h,h']+[\varphi(h),\varphi(h')]$ for all $h'\in\mathfrak{h}$, since φ is a homomorphism of Lie algebras. The rest of the brackets are verified in a similar fashion. □

Remark 6.3: The invariant metric in $(\mathfrak{h}\ltimes\mathfrak{h}^{*})$ is now given by

$$\langle(h,\alpha),(h',\alpha')\rangle=\langle h,h'\rangle_{\mathfrak{h}}+\langle\varphi(h),\varphi(h')\rangle_{\mathfrak{g}}+\alpha(h')+\alpha'(h).$$

In other words, $\langle -,- \rangle_{\mathfrak{h}}$ receives a correction coming from the pull-back by φ to $\mathfrak{h}$ of the invariant metric in $\mathfrak{g}$; that is, $\langle -,- \rangle_{\mathfrak{h}} + \varphi^* \langle -,- \rangle$.

In particular, if all the antisymmetric derivations of $\mathfrak{g}$ are inner, then $\mathfrak{g}$ factors out of the double extension. This idea can be pursued further, but first a definition. Recall a (real) Lie algebra $\mathfrak{g}$ is *perfect* if $[\mathfrak{g},\mathfrak{g}]=\mathfrak{g}$ or, equivalently, if $H^1(\mathfrak{g};\mathbb{R})=0$. By analogy let us define the following.

Definition 6.4: We say that a (real) Lie algebra $\mathfrak{p}$ is *pluperfect* whenever $H^1(\mathfrak{p};\mathbb{R}) = H^2(\mathfrak{p};\mathbb{R})=0$. Notice that semisimple Lie algebras are pluperfect.

Theorem 6.5: The Lie algebra $\mathfrak{g}$ in Theorem 3.11 cannot have a pluperfect factor.

Proof: We will prove that if $\mathfrak{g}$ has a pluperfect factor, then its double extension is decomposable, in contradiction to the hypothesis of Theorem 3.11. Thus let $(\mathfrak{g},\langle -,- \rangle_{\mathfrak{g}})$ be an object in $\mathscr{C}$ such that $\mathfrak{g}=\mathfrak{p}\times\mathfrak{a}$ with $\mathfrak{p}$ pluperfect and $\mathfrak{a}$ arbitrary without pluperfect factors.

(1) $\mathfrak{p}$ and $\mathfrak{a}$ are orthogonal.

$\mathfrak{p}$ is, in particular, perfect, which together with the invariance of the metric implies that $\langle \mathfrak{p},\mathfrak{a} \rangle = \langle [\mathfrak{p},\mathfrak{p}],\mathfrak{a} \rangle = \langle \mathfrak{p},[\mathfrak{p},\mathfrak{a}] \rangle = 0$.

(2) Let $\mathrm{Der}_{\mathfrak{a}}$ stand for the antisymmetric derivations. Then $\mathrm{Der}_{\mathfrak{a}}\mathfrak{g}=\mathfrak{p}\times\mathrm{Der}_{\mathfrak{a}}\mathfrak{a}$.

Let $d \in \mathrm{Der}_{\mathfrak{a}}\mathfrak{g}$ be an antisymmetric derivation. If $x \in \mathfrak{g}$ we write $d(x)=d_1(x)+d_2(x)$, where $d_1(x) \in \mathfrak{p}$ and $d_2(x) \in \mathfrak{a}$. Let $s,s' \in \mathfrak{p}$. Since d is a derivation, we have $[d(s),s'] + [s,d(s')] = d([s,s'])$. Breaking it up into its components, we find that $[d_1(s),s'] + [s,d_1(s')] = d_2([s,s'])$ and that $d_2([s,s'])=0$. The former equation says that $d_1 \in \mathrm{Der}\,\mathfrak{p}$, whereas the latter says that d_2 annihilates $[\mathfrak{p},\mathfrak{p}]=\mathfrak{p}$. If $a \in \mathfrak{a}$ we have $[s,d(a)] + [d(s),a] = 0$. Breaking it up into components we find $[s,d_1(a)]=0$, which says the $d_1(a)$ is central in $\mathfrak{p}$. But since $[\mathfrak{p},\mathfrak{p}]=\mathfrak{p}$, Lemma 2.5 says that the center is trivial, whence $d_1(a)$ must vanish. If $a' \in \mathfrak{a}$, then $[d(a),a'] + [a,d(a')] = d([a,a'])$, which breaks up as $[d_2(a),a'] + [a,d_2(a')] = d_2([a,a'])$. This means that $d_2 \in \mathrm{Der}\,\mathfrak{a}$. Finally, the antisymmetry condition says that $d_2 \in \mathrm{Der}_{\mathfrak{a}}\mathfrak{a}$, whereas from $H^2(\mathfrak{p};\mathbb{R})=0$ it follows that all antisymmetric derivations of $\mathfrak{p}$ are inner: every antisymmetric derivation $D \in \mathrm{Der}_{\mathfrak{a}}\mathfrak{p}$ defines, a 2-cocycle by $\gamma(s,s')=\langle d(s),s' \rangle$, which is a coboundary $\gamma(s,s') = -\eta([s,s'])$ for some $\eta \in \mathfrak{p}^*$. But this means that there exists $s'' \in \mathfrak{p}$ such that $-\eta([s,s']) = \langle s'',[s,s'] \rangle = \langle [s'',s],s' \rangle$, whence $d(s)=[s'',s]$ is inner. Conversely, all inner derivations are antisymmetric, so that $d_1 \in ad\,\mathfrak{p}$.

In particular, since $\mathfrak{h}$ acts $\mathfrak{g}$ via inner derivations, there exists a Lie algebra (hence $\mathfrak{h}$ module) morphism $\varphi:\mathfrak{h}\to\mathfrak{p}$ such that for $h \in \mathfrak{h}$ and $s \in \mathfrak{p}$, $h \cdot s = [\varphi(h),s]_{\mathfrak{p}}$. Then the proof of Proposition 6.1 implies, *mutatis mutandis*, that $\mathfrak{p}$ factors out of the double extension.

In other words, the vector space automorphism Ψ of $\mathfrak{p}\oplus\mathfrak{a}\oplus\mathfrak{h}\oplus\mathfrak{h}^*$:

$$\Psi(s,a,h,\alpha) = (s-\varphi^\sharp(s),a,h+\varphi(h),\alpha)$$

defines a Lie algebra isomorphism $D(\mathfrak{p}\times\mathfrak{a},\mathfrak{h}) \xrightarrow{\simeq} \mathfrak{p}\times D(\mathfrak{a},\mathfrak{h})$. Furthermore, the invariant metric in $D(\mathfrak{a},\mathfrak{h})$ is now given by

$$\langle (a,h,\alpha),(a',h',\alpha') \rangle = \langle a,a' \rangle_{\mathfrak{a}} + \langle h,h' \rangle_{\mathfrak{h}} + \langle \varphi(h),\varphi(h') \rangle_{\mathfrak{p}} + \alpha(h') + \alpha'(h).$$

This concludes the proof of Theorem 6.5. □

As a corollary of Theorem 3.11 and Theorem 6.5 we have the following characterization of the class $\mathscr{C}$.

Corollary 6.6: The class $\mathscr{C}$ breaks up as $\mathscr{C}_S \times \mathscr{C}_N$, where $\mathscr{C}_S$ is the subclass of semisimple Lie algebras and $\mathscr{C}_N$ is the smallest class of real finite-dimensional Lie algebras containing the one-dimensional Lie algebra and closed under the operations of direct product and double extension by a simple or one-dimensional algebra. In particular, all objects in $\mathscr{C}_N$ are nonsemisimple. Moreover, the subclass $\mathscr{C}'_S \subset \mathscr{C}_N$ of solvable Lie algebras is the class generated by the one dimensional Lie algebra under the operations of direct product and double extension by the one-dimensional Lie algebra. □

VII. DEFORMING THE INVARIANT METRIC

Let $(\mathfrak{d},\Omega)$ be a self-dual Lie algebra. We would like to ask whether one can deform the metric Ω while retaining nondegeneracy. Rather than analyze this problem in its full generality, we will limit ourselves to the case of interest in Conformal Field Theory. Namely, we will deform Ω by a scalar multiple of the Killing form κ. Such shifts are the typical effect of quantum renormalization. Let t be a scalar (a real or complex number) and let g_t denote the bilinear form $g_t=\Omega-t\kappa$. Fix t once and for all and define $\mathfrak{d}^\perp$ to be the radical of g_t; that is, $\mathfrak{d}^\perp=\{v\in\mathfrak{d}|g_t(v,w)=0\forall w\in\mathfrak{d}\}$. Notice that $\mathfrak{d}^\perp\subset\mathfrak{d}$ is an ideal, since the bilinear form g_t is invariant. In particular, $\mathfrak{d}^\perp$ is a Lie algebra. We will prove the following result.

Theorem 7.1: If $(\mathfrak{d},\Omega)$ is an indecomposable self-dual Lie algebra, then $\mathfrak{d}^\perp=0$ unless $\mathfrak{d}$ is simple and $\Delta=t\kappa$, in which case $g_t=0$ and $\mathfrak{d}^\perp=\mathfrak{d}$.

Proof: Since $(\mathfrak{d},\Omega)$ is indecomposable, then by Theorem 3.11 it is either simple, one dimensional, or a double extension $D(\mathfrak{g},\mathfrak{h})$, where $\mathfrak{h}$ is simple or one dimensional. The theorem is clear for the first two cases, as we now show. If $\mathfrak{d}$ is one dimensional, then $\kappa=0$ and $\mathfrak{d}^\perp=0$; and similarly if $\mathfrak{d}$ is simple, then $\mathfrak{d}^\perp$, being an ideal, must be either 0 or $\mathfrak{d}$; the latter case corresponding to the case $g_t=0$, or equivalently $\Omega=t\kappa$. Therefore all we have left to tackle is the case where $\mathfrak{d}=D(\mathfrak{g},\mathfrak{h})$ is a double extension. The theorem will follow if we can prove that $\mathfrak{d}^\perp=0$ in this case.

We proceed by induction on the dimension of the Lie algebra. Suppose that the theorem is true for all indecomposable self-dual Lie algebras of dimension $\leqslant N$—the case $N=1$ being trivially satisfied—and let $\mathfrak{d}=D(\mathfrak{g},\mathfrak{h})$ be an indecomposable double extension of dimension $N+1$. [Actually we have not shown that there is no indecomposable self-dual Lie algebra in every dimension. So if there is no indecomposable $\mathfrak{d}=D(\mathfrak{g},\mathfrak{h})$ in dimenson $N+1$ then take one of the smallest dimension $>N$.] The theorem follows if we can prove that $\mathfrak{d}^\perp=0$. We now have the following lemma, whose proof we give below.

Lemma 7.2: Let $\mathfrak{d}=D(\mathfrak{g},\mathfrak{h})$ be a double extension, with $\mathfrak{g}$ and $\mathfrak{h}$ arbitrary. Then there is a Lie algebra isomorphism:

$$\mathfrak{d}^\perp=D(\mathfrak{g},\mathfrak{h})^\perp\cong\mathfrak{g}^\perp.$$

□

Using Lemma 7.2, we have that $\mathfrak{d}^\perp\cong\mathfrak{g}^\perp$. In general, $\mathfrak{g}$ need not be indecomposable, so write it as $\mathfrak{g}=\mathfrak{g}_1\times\cdots\times\mathfrak{g}_\kappa$, where each $\mathfrak{g}_i$ is indecomposable. Clearly, $\mathfrak{g}^\perp\cong\mathfrak{g}_1^\perp\times\cdots\times\mathfrak{g}_\kappa^\perp$. Since $\dim\mathfrak{g}_i<\dim\mathfrak{d}$ for each i, we can apply the induction hypothesis to deduce that $\mathfrak{g}_i^\perp$ will only be nonzero when $\mathfrak{g}_i$ is simple. But if $\mathfrak{g}$ would have a simple factor, Theorem 6.5 would imply that $\mathfrak{d}$ is decomposable, violating the hypothesis. Therefore $\mathfrak{g}^\perp=0$ and we can extend the induction hypothesis. □

Corollary 7.3: Let $(\mathfrak{d},\Omega)$ be any self-dual Lie algebra. Then (1) $\mathfrak{d}^\perp$ is semisimple; (2) $\mathfrak{d}$ decomposes into an orthogonal direct sum $\mathfrak{d}=\mathfrak{d}^\perp\times\mathfrak{d}_1$, where $\mathfrak{d}^\perp$ is semisimple, and $\mathfrak{d}_1^\perp=0$.

Proof: (1) is an immediate corollary. Since $\mathfrak{d}^\perp$ is a semisimple ideal, it is a factor; hence (2). Finally we prove the lemma. □

Proof (of Lemma 7.2): In the explicit basis introduced in Sec. IV, we let $v=v^jG_j+v^\alpha H_\alpha+v_\alpha H^\alpha$ belong to $\mathfrak{d}^\perp$ and let us see what this implies. The bilinear form defining $^\perp$ is $\Omega^{\mathfrak{d}}_{ab}-t\kappa^{\mathfrak{d}}_{ab}$, whose matrix is given by

$$\begin{array}{c} \\ G_i \\ H_\alpha \\ H^\alpha \end{array}\begin{array}{c} \begin{array}{ccc} G_j & H_\beta & H^\beta \end{array} \\ \begin{pmatrix} \Omega^{\mathfrak{g}}_{ij}-t\kappa^{\mathfrak{g}}_{ij} & -t\kappa^{\mathfrak{d}}_{i\beta} & 0 \\ -t\kappa^{\mathfrak{d}}_{\alpha j} & h_{\alpha\beta}-t\kappa^{\mathfrak{d}}_{\alpha\beta} & \delta_\alpha{}^\beta \\ 0 & \delta^\alpha{}_\beta & 0 \end{pmatrix} \end{array}.$$

Therefore, $v\in\mathfrak{d}^\perp$ implies that

$$(\Omega^{\mathfrak{d}}_{ab}-t\kappa^{\mathfrak{d}}_{ab})\begin{pmatrix} v^j \\ v^\beta \\ v_\beta \end{pmatrix}=\begin{pmatrix} (\Omega^{\mathfrak{g}}_{ij}-t\kappa^{\mathfrak{g}}_{ij})v^j-t\kappa^{\mathfrak{d}}_{i\beta}v^\beta \\ -t\kappa^{\mathfrak{d}}_{\alpha j}v^j+(h_{\alpha\beta}-t\kappa^{\mathfrak{d}}_{\alpha\beta})v^\beta+v_\alpha \\ v^\alpha \end{pmatrix}=0.$$

This in turn yields the equations $v^\alpha=0$, $v_\alpha = t\kappa^{\mathfrak{d}}_{\alpha j}v^j$, and

$$(\Omega^{\mathfrak{g}}_{ij}-t\kappa^{\mathfrak{g}}_{ij})v^j=0,$$

whence v^jG_j belongs to $\mathfrak{g}^\perp$. Conversely, any $v^jG_j\in\mathfrak{g}^\perp$ extends to a vector $v^jG_j + tv^j\kappa^{\mathfrak{d}}_{\alpha j}H^\alpha$, which by the above computation belongs to $\mathfrak{d}^\perp$. In summary, we have a vector space isomorphism $s:\mathfrak{g}^\perp\to\mathfrak{d}^\perp$, defined by $s(v^jG_j) = v^jG'_j$ where $G'_j = G_j + t\kappa^{\mathfrak{d}}_{\alpha j}H^\alpha$. We will not show that this is also an isomorphism of Lie algebras. Computing the brackets in $\mathfrak{d}$, we obtain

$$[s(G_i),s(G_j)]_{\mathfrak{d}}=[G'_i,G'_j]_{\mathfrak{d}}=f^k_{ij}G_k+f_{ij\alpha}H^\alpha=f^k_{ij}G^j_k+(f_{ij\alpha}-tf^k_{ij}\kappa^{\mathfrak{d}}_{k\alpha})H^\alpha. \tag{7.4}$$

Now notice that $f_{ija} = f^a_j\Omega^{\mathfrak{d}}_{a\alpha}$, that $f^k_{ij}\kappa^{\mathfrak{d}}_{k\alpha} = f^a_{ij}\kappa^{\mathfrak{d}}_{a\alpha}$; so that we rewrite (7.4) as

$$[G'_i,G'_j]_{\mathfrak{d}}=f^k_{ij}G'_k+f^a_{ij}(g^{\mathfrak{d}}_i)_{a\alpha}H^\alpha.$$

Using that $g^{\mathfrak{d}}_i$ is an invariant bilinear form, we arrive at

$$[G'_i,G'_j]_{\mathfrak{d}}=f^k_{ij}G'_k-f^a_{i\alpha}(g^{\mathfrak{d}}_t)_{aj}H^\alpha.$$

Finally, we notice that $f^a_{i\alpha}(g^{\mathfrak{d}}_t)_{aj} = f_{i\alpha}{}^k(g^{\mathfrak{d}}_t)_{kj}$ and that the restriction of $g^{\mathfrak{d}}_t$ to $\mathfrak{g}$ coincides with $g^{\mathfrak{g}}_t$, so that we end up with

$$[G'_i,G'_j]_{\mathfrak{d}}=f^k_{ij}G'_k-f_{i\alpha}{}^k(g^{\mathfrak{d}}_t)_{jk}H^\alpha,$$

which shows explicitly that if v^iG_i and w^jG_j are in $\mathfrak{g}^\perp$ then

$$[s(v^iG_i),s(w^jG_j)]_{\mathfrak{d}}=s([v^iG_i,w^jG_j]_{\mathfrak{g}},$$

so that s is a homomorphism. □

VIII. APPLICATIONS IN CONFORMAL FIELD THEORY

To conclude we would like to mention very briefly some of the applications of self-dual Lie algebras, and, in particular, of the results in this paper in conformal field theory. We will be brief and will limit ourselves mostly to directing the attention of the reader to the relevant literature.

Any conformally invariant two-dimensional σ model (of the right central charge) is a possible (bosonic) string background. Any such σ model is classically conformally invariant, but demanding that this persists upon quantitation imposes equations on the metric that need to be satisfied. Therefore in the process of satisfying these equations, the classical form of the metric gets "renormalized" and it is seldom the case that one can write down a nontrivial metric that exactly solves the equations—that is, an exact string background. In Ref. 6 Nappi and Witten constructed one such exact string background out of a WZW model with target space a four-dimensional solvable Lie group. The nonperturbative proof of the conformal invariance of the theory made use of a Sugawara construction built out of a nondegenerate metric on the Lie algebra. This fact prompted Mohammedi[2] to investigate the existence of a Sugawara construction on a given Lie algebra $\mathfrak{g}$. The conclusion of his analysis (see also Ref. 3) is that a Sugawara construction exists if and only if $\mathfrak{g}$ is self-dual. Self-dual Sugawara constructions have appeared also in the work of Lian[5] on finitely generated simple vertex operator algebras.

In Ref. 3 we analyzed the Sugawara constructions arising out of self-dual Lie algebras, with the motivation of answering the following question. All examples of nonsemisimple Sugawara constructions known at the time shared the property that the central charge was equal to the dimension of the Lie algebra. *Was this inevitable or could one construct CFTs with nonintegral values of the central charge?* The answer turns out to be negative—a fact we established in Ref. 3. More precisely, we used Corollary 6.6 (derived from a weaker version of Theorem 6.5) to deduce that the Sugawara central charge associated with any self-dual Lie algebra in the class $\mathscr{C}_N$ is integral and equal to the dimension of the Lie algebra. Hence any other value for the central charge has its origins in a Sugawara construction in the class $\mathscr{C}_S$. A detailed analysis of the self-dual Lie algebras in low dimension has been made by Kehagias, who classified the WZW models in (target) dimension $\leqslant 5$ and, in addition, all those six dimensional ones with nilpotent target group.[11] These limits are dictated by the present classification of arbitrary Lie algebras. More recently, we have studied the coset constructions arising out of self-dual Lie algebras[4] as well as settled some issues concerning the relation between the WZW model and the Sugawara construction, for which Theorem 7.1 proved instrumental. In Ref. 4 the reader may also find more references on nonreductive Sugawara constructions and (gauged) WZW models.

We conclude this brief survey of applications with a word on supersymmetry. It was proven Ref. 2 that the condition for the existence of an $N=1$ supersymmetric Sugawara construction on the $N=1$ affine Lie algebra $\hat{\mathfrak{g}}_{N=1}$ is also that $\mathfrak{g}$ be self-dual. This opens possibility of studying for which self-dual Lie algebras $\mathfrak{g}$, does the $N=1$ Sugawara construction $\hat{\mathfrak{g}}_{N=1}$ admit an $N=2$ extension. The conditions were found in Ref. 12 and reinterpreted in Ref. 13 in order to classify all those solvable six dimensional—that is, those with central charge $c=9$—self-dual Lie algebras admitting an $N=2$ construction. The conditions under which a pair of self-dual Lie algebras $(\mathfrak{h},\mathfrak{g})$ admits an $N=1$ and an $N=2$ coset construction have found Ref. 14, which can be thought of as a continuation of Ref. 4 and where further use is made of the results described in this paper.

IX. SOME OPEN PROBLEMS

We have seen that the results of Medina and Revoy, suitably refined and augmented, have a wide applicability in Conformal Field Theory. Certainly there still remains a lot to be learned from self-dual Lie algebras and, if we compare them with semisimple Lie algebras, very little is known about them indeed. At this stage a complete classification is hard to envision, but some more modest results would be welcome; for instance, the classification of all six-dimensional self-dual Lie algebras. An interesting open problem is the extension of these results to self-dual Lie superalgebras. As shown in Ref. 15 and in Ref. 4, self-dual Lie superalgebras also lead to Sugawara constructions. Motivated by this fact, one would like to have a structure theorem for such Lie superalgebras. If we study closely the results outlined in this paper, one sees that one can substitute Lie algebra for Lie superalgebra in many of the results and the statements and proofs still hold *mutatis mutandis*. (Statements like Corollary 6.6 would, of course, have to be modified, since not all simple Lie superalgebras are self-dual.) The only exception is Lemma 3.5, for which we have not been able to find a proof nor a counterexample. The notion of a double extension still works and allows one to construct self-dual Lie superalgebras, but without a superanalog of Lemma 3.5, nothing guarantees that this is the way to obtain them all.

Notice that although the results described in this paper hold for symmetric self-dual Lie algebras, one could have used an antisymmetric form for much of the discussion in this paper and many of the results would have remained unchanged. However, had we dropped any symmetry requirements whatsoever, the results would need severe modification. The determination of a structure theorem for these more general self-dual Lie algebras is an open problem—one we find intriguing and to which we may return elsewhere.

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APPENDIX A: SPLIT EXTENSIONS OF SOME LIE ALGEBRAS

We now prove Lemma 3.5. More precisely we prove the following result, which implies Lemma 3.5.

Proposition A.1: If c is simple or one dimensional, every Lie algebra extension,

$$0\to\mathfrak{a}\to\mathfrak{b}\to\mathfrak{c}\to 0, \tag{A1}$$

splits.

Remark A.3: Before we proceed to the proof we mention that if $\mathfrak{a}$ were Abelian the result would follow immediately as a consequence of the second Whitehead lemma: $H^2(\mathfrak{c};\mathfrak{a})=0$. Similarly, if $\mathfrak{a}$ were solvable one could proceed by induction on the derived length of $\mathfrak{a}$. If, on the other hand, $\mathfrak{a}$ were semisimple, then $\mathfrak{b}$ would decompose as a direct product $\mathfrak{a}\times\mathfrak{c}$. However, we are interested in general $\mathfrak{a}$. This result should be standard but we have not found it in the literature.

Proof (of Proposition A.1): Let $0\to\mathfrak{r}\to\mathfrak{a}\to\mathfrak{l}\to 0$ be a Levi decomposition for $\mathfrak{a}$ with $\mathfrak{r}$ the radical and $\mathfrak{l}$ semisimple. Since $\mathfrak{r}$ is a characteristic ideal of $\mathfrak{a}$ and $\mathfrak{a}$ is an ideal of $\mathfrak{b}$, $\mathfrak{r}$ is an ideal of $\mathfrak{b}$. Let $\mathfrak{g}\equiv\mathfrak{b}/\mathfrak{r}$. Since $\mathfrak{l}\subset\mathfrak{a}$ is a subalgebra we have a map $\mathfrak{l}\to\mathfrak{g}$ induced by the composition of $\mathfrak{a}\to\mathfrak{b}\to\mathfrak{g}$. It is clear that this map is one to one and the image of $\mathfrak{l}$ in $\mathfrak{g}$ is an ideal. Define then $\mathfrak{h}\equiv\mathfrak{g}/\mathfrak{l}$. Since $\mathfrak{l}$ is semisimple, the sequence $0\to\mathfrak{l}\to\mathfrak{g}\to\mathfrak{h}\to 0$ splits, and we can identify $\mathfrak{h}$ with an ideal of $\mathfrak{g}$, so that $\mathfrak{g}=\mathfrak{h}\times\mathfrak{l}$. Indeed, notice that $\mathfrak{l}\cong\mathfrak{a}/\mathfrak{r}$ and that $\mathfrak{g}\cong\mathfrak{b}/\mathfrak{r}$, and this implies that $\mathfrak{h}\cong\mathfrak{g}/\mathfrak{l}=(\mathfrak{b}/\mathfrak{r})/(\mathfrak{a}/\mathfrak{r})\cong\mathfrak{b}/\mathfrak{a}\cong\mathfrak{c}$, whence $\mathfrak{g}=\mathfrak{l}\times\mathfrak{c}$.

The key observation is that the obstruction is now a linear map $\beta:\Lambda^2\mathfrak{c}\to\mathfrak{a}\cong\mathfrak{r}\oplus\mathfrak{l}$.

(1) Case: $\mathfrak{c}$ simple

If $\mathfrak{c}$ is simple, $\mathfrak{g}$ is semisimple, which imp,lies that $\mathfrak{r}$ is the radial of $\mathfrak{b}$. The splitting of (A1) then follows from the Levi–Malcev theorem.

(2) Case: $\mathfrak{c}$ one dimensional

The splitting of (A1) is equivalent to the splitting of

$$0\to\mathfrak{r}\to\mathfrak{b}\to\mathfrak{l}\times\mathfrak{c}\to 0. \tag{A2}$$

Since $\mathfrak{r}$ is solvable, we will prove this by induction on its derived length. If $\mathfrak{r}$ is Abelian, then the split follows as a result of the fact that

$$H^2(\mathfrak{l}\times\mathfrak{c},\mathfrak{r})=\bigoplus_{i=0}^{2}H^i(\mathfrak{l};\mathbb{R})\otimes H^{2-i}(\mathfrak{c};\mathfrak{r})=0.$$

We take as our induction hypothesis that the above sequence splits for every solvable algebra of derived length $<n$. We let $\mathfrak{r}$ have derived length n and consider the exact sequence

$$0\to\mathfrak{r}/[\mathfrak{r},\mathfrak{r}]\to\mathfrak{b}/[\mathfrak{r},\mathfrak{r}]\to\mathfrak{l}\times\mathfrak{c}\to 0.$$

It splits by the induction hypothesis since $\mathfrak{r}/[\mathfrak{r},\mathfrak{r}]$ is Abelian and has derived length zero. Let $s:\mathfrak{l}\times\mathfrak{c}\to\mathfrak{b}/[\mathfrak{r},\mathfrak{r}]$ denote the splitting map and let $s(\mathfrak{l}\times\mathfrak{c})=\mathfrak{p}/[\mathfrak{r},\mathfrak{r}]$, where the subalgebra $\mathfrak{p}\subset\mathfrak{b}$ is the preimage of $\mathfrak{l}\times\mathfrak{r}$. Now, the exact sequence,

$$0\to[\mathfrak{r},\mathfrak{r}]\to\mathfrak{p}\to\mathfrak{p}/[\mathfrak{r},\mathfrak{r}]\to 0,$$

splits by the induction hypothesis since the derived length of $[\mathfrak{r},\mathfrak{r}]$ is $n-1$. Let $z:\mathfrak{l}\times\mathfrak{c}\to\mathfrak{p}$ denote the splitting map. Then the composition $s\circ z:\mathfrak{l}\times\mathfrak{c}\to\mathfrak{p}/[\mathfrak{r},\mathfrak{r}]\to\mathfrak{p}\subset\mathfrak{b}$ is the desired splitting of (A2). □

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A q-deformed $e(4)$ and continuous q-Jacobi polynomials

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We present an algebraic interpretation of the continuous q-Jacobi polynomials. They are shown to realize a basis for a representation space of a q deformation of the four-dimensional Euclidean algebra $e(4)$. A q analog of the expansion of an exponential in Jacobi polynomials is naturally obtained from this model. © *1996 American Institute of Physics.* [S0022-2488(96)03407-X]

I. INTRODUCTION

Most special functions of mathematical physics admit q analogs, namely deformations involving a parameter q. These q-special functions,[1,2] which share many common properties with their undeformed counterparts, have become a subject of very intense research since quantum groups and algebras were introduced. Most remarkably, just as Lie algebras provide a unifying framework for discussing special functions, quantum algebras furnish an equivalent setting for studying q-special functions. Indeed, q-orthogonal polynomials and q-special functions arise as basis vectors of quantum algebra representations or as matrix elements of q exponentials of generators in such representations (e.g. Refs. 3–12). Moreover, the algebraic interpretation leads naturally to generating relations, orthogonality properties, and additional formulas for these functions.

Most of the q polynomials encountered in these investigations were orthogonal with respect to a discrete measure. Still, many q polynomials are known to be orthogonal with respect to continuous measures,[1,2] and it is natural to look for their algebraic interpretation. These polynomials are all encompassed as special cases of the four-parameter family of Askey–Wilson polynomials $p_n(x;a,b,c,d,|q)$. It might thus seem more economical, at first sight, to obtain directly the algebraic interpretation of the Askey–Wilson polynomials and to extract therefrom the interpretation of the various polynomials as special cases. This, however, would be an extremely arduous undertaking, since the complexity of the quantum algebra associated with a family of q polynomials increases rapidly with their number of parameters. It is therefore more advisable to start from the bottom of the Askey–Wilson hierarchy, and to consider systematically cases of increasing complexity. Thus, after an initial study[13] dealing with Roger's continuous q-Hermite and continuous q-ultraspherical polynomials, which involve zero and one parameter, respectively, we tackled the one-parameter class of continuous big q-Hermite polynomials,[14] and showed how the q-oscillator algebra can be used to obtain relations between q-Hermite, big q-Hermite, Wall, and q-Laguerre polynomials.[15]

We pursue this approach here by showing that a q deformation of the four-dimensional Euclidean algebra $e(4)$ provides an algebraic interpretation of the two-parameter family of q-Jacobi polynomials $P_n^{(\alpha,\beta)}(x|q)$. The latter are defined in Sec. II, where certain preliminary results are also presented, while the realization of a q deformation of $e(4)$ is given in Sec. III. As illustration of the usefulness of the algebraic approach, we derive in Sec. IV a q analog[16] of the formula for the expansion of an exponential in Jacobi polynomials:

(1)

$$e^{irx}=e^{-ir}\sum_{n=0}^{\infty}\frac{(\alpha+\beta+1)_n}{(\alpha+\beta+1)_{2n}}(2ir)^n{}_1F_1\left(\begin{matrix}n+\beta+1\\2n+\alpha+\beta+2\end{matrix}\middle|2ir\right)P_n^{(\alpha,\beta)}(x),$$

$$-1<x<1. \tag{1.1}$$

We have not been able to find in the literature an algebraic derivation of (1.1). It will be briefly discussed in the Appendix; it essentially amounts to the $q\to 1^-$ limit of the construction given in the body of the paper.

II. DEFINITIONS AND PRELIMINARY RESULTS

We shall use standard notation for the q-shifted factorials $(a;q)_\alpha$,

$$(a;q)_\alpha=\frac{(a;q)_\infty}{(aq^\alpha;q)_\infty}, \tag{2.1a}$$

$$(a;q)_\infty=\prod_{k=0}^{\infty}(1-aq^k),\quad |q|<1, \tag{2.1b}$$

$$(a_1,a_2,\ldots,a_k;q)_\alpha=(a_1;q)_\alpha(a_2;q)_\alpha\cdots(a_k;q)_\alpha, \tag{2.1c}$$

as well as for the q-hypergeometric series ${}_r\phi_s$,

$$\begin{aligned}&{}_r\phi_s(a_1,a_2,\ldots,a_r;b_1,\ldots,b_s;q,z)\\&\quad={}_r\phi_s\left(\begin{matrix}a_1,a_2,\ldots,a_r\\b_1,\ldots,b_s\end{matrix}\middle|q;z\right)\\&\quad=\sum_{n=0}^{\infty}\frac{(a_1,\ldots,a_r;q)_n}{(q,b_1,\ldots,b_s;q)_n}[(-1)^nq^{n(n-1)/2}]^{1+s-r}z^n.\end{aligned} \tag{2.2}$$

Defining the Askey–Wilson polynomials,[1,2,17]

$$p_n(x;a,b,c,d|q)=(ab,ac,ad;q)_n a^{-n}\times{}_4\phi_3\left(\begin{matrix}q^{-n},abcdq^{n-1},ae^{i\theta},ae^{-i\theta}\\ab,ac,ad\end{matrix}\middle|q;q\right), \tag{2.3}$$

with

$$x=\cos\,\theta, \tag{2.4}$$

we can express the continuous q-Jacobi polynomials $P_n{}^{(\alpha,\beta)}(x|q)$ in the following manner:[1,2]

$$\begin{aligned}P_n^{(\alpha,\beta)}(x|q)=&\frac{q^{n(2\alpha+1)/4}}{(q,-q^{(\alpha+\beta+1)/2},-q^{(\alpha+\beta+2)/2};q)_n}\\&\times p_n(x;q^{(2\alpha+1)/4},q^{(2\alpha+3)/4},-q^{(2\beta+1)/4},-q^{(2\beta+3)/4}|q),\end{aligned} \tag{2.5}$$

This definition corresponds to the original normalization of Ref. 17. One also finds in the literature q-Jacobi polynomials $P_n{}^{(\alpha,\beta)}(x;q)$ with a different normalization, introduced in Ref. 18. These two types of q-Jacobi polynomials are connected by the quadratic transformation

$$P_n^{(\alpha,\beta)}(x;q)=\frac{(-q^{\alpha+\beta+1};q)_n}{(-q;q)_n}q^{-\alpha n}P_n^{(\alpha,\beta)}(x|q^2). \tag{2.6}$$

It is well known that the following two q analogs of the exponential function:[1]

$$e_q(z)=\sum_{n=0}^{\infty}\frac{1}{(q;q)_n}z^n=\frac{1}{(z;q)_\infty},$$
$$E_q(z)=\sum_{n=0}^{\infty}\frac{q^{n(n-1)/2}}{(q;q)_n}z^n=(-z;q)_\infty, \tag{2.7}$$

are eigenfunctions of the q-derivative operators D_z^+ and D_z^-, respectively, which are defined by

$$D_z^{\pm}=\frac{1}{z}(1-T_z^{\pm 1}). \tag{2.8}$$

The operator T_z is the q-shift operator, the powers of which act as follows on any function of z:

$$T_z^{\alpha}f(z)=f(q^{\alpha}z), \quad \alpha\in\mathbb{R}. \tag{2.9}$$

The q-derivative operators $D_z^{\pm}$, however, are not the appropriate ones for the study of the continuous q-orthogonal polynomials. Rather, one uses the divided difference operator[17,19]

$$\tau=\frac{1}{z-z^{-1}}(T_z^{1/2}-T_z^{-1/2}), \tag{2.10}$$

the eigenfunctions of which are a third q analog of the exponential function,[20]

$$\mathscr{E}_q(x;a,b)=\sum_{n=0}^{\infty}\frac{q^{n^2/4}}{(q;q)_n}(aq^{(1-n)/2}e^{i\theta};q)_n(aq^{(1-n)/2}e^{-i\theta};q)_n b^n. \tag{2.11}$$

One has, indeed,

$$\tau\mathscr{E}_q(x;a,b)=abq^{-1/4}\mathscr{E}_q(x;a,b). \tag{2.12}$$

In the following, we shall need not only the action of the divided difference operator τ on the q exponential $\mathscr{E}_q(x;-i,r)$, but also that of the operators,

$$\tilde{\tau}_q^*=q^{-1/2}\frac{1}{z-z^{-1}}\left(\frac{1}{z^2}T_z^{1/2}-z^2T_z^{-1/2}\right), \tag{2.13}$$

$$\tilde{\mu}_q=\frac{1}{z-z^{-1}}\left(-\frac{1}{z}T_z^{1/2}+zT_z^{-1/2}\right), \tag{2.14}$$

$\tilde{\tau}^*_{1/q}$ and $\tilde{\mu}_{1/q}$. The operators (2.13) and (2.14) are those to which the ladder operators τ^* and μ of Ref. 19 reduce when the four parameters in the Askey–Wilson polynomials vanish. We can express the action of these operators on $\mathscr{E}_q(x;-i,r)$ in the following manner:

$$\tilde{\tau}_q^*\mathscr{E}_q(x;-i,r)=i\frac{q^{1/4}}{r}\left[\left(1+\frac{r^2}{q^2}\right)T_r^{-1}-1\right]\mathscr{E}_q(x;-i,r), \tag{2.15a}$$

$$\tilde{\mu}_q\mathscr{E}_q(x;-i,r)=\frac{(-r^2/q;q^2)_\infty}{(-r^2;q^2)_\infty}T_r^{-1/2}\mathscr{E}_q(x;-i,r), \tag{2.15b}$$

$$\tilde{\tau}^{*}_{1/q}\mathscr{E}_q(x;-i,r)=-i\,\frac{q^{1/4}}{r}\,[(1+r^2q)T_r-1]\mathscr{E}_q(x;-i,r), \tag{2.15c}$$

and

$$\tilde{\mu}_{1/q}\mathscr{E}_q(x;-i,r)=\frac{(-r^2q;q^2)_\infty}{(-r^2q^2,q^2)_\infty}\,T_r^{1/2}\mathscr{E}_q(x;-i,r). \tag{2.15d}$$

The first two of these equations are most readily proved by expanding $\mathscr{E}_q(x;-i,r)$ on a basis of continuous q-Hermite polynomials $H_k(x|q)$,[13]

$$(-r^2;q^2)_\infty\mathscr{E}_q(x;-i,r)=\sum_{k=0}^{\infty}\frac{q^{k^2/4}}{(q;q)_k}\,(ir)^kH_k(x|q), \tag{2.16}$$

and exploiting the known action of $\tilde{\tau}^{*}_q$ and $\tilde{\mu}_q$ on the latter,[14]

$$\tilde{\tau}^{*}_qH_k(x|q)=-q^{-(k+1)/2}H_{k+1}(x|q),\quad \tilde{\mu}_qH_k(x|q)=q^{-k/2}H_k(x|q). \tag{2.17}$$

The last two equations are then a consequence of the following properties of the q exponentials:

$$E_q(x)=e_{1/q}(-x/q),\quad E_{1/q}(x)=e_q(-qx), \tag{2.18}$$

$$\mathscr{E}_{1/q}(x;a,b)=\mathscr{E}_q(x;1/a,-q^{1/2}a^2b). \tag{2.19}$$

III. A MODEL FOR q-DEFORMED $e(4)$

We will now construct a model for a q deformation of the Lie algebra $e(4)$, involving operators acting on functions of the three variables $x=(z+z^{-1})/2$, s, and t. The generators of the q-deformed algebra will involve four operators that are, essentially, the ladder operators introduced in Ref. 19, namely the divided difference operator τ, already defined in (2.10), as well as

$$\begin{aligned}\tau^{*}=\frac{q^{-1/2}}{z-z^{-1}}\Bigg[&\frac{1}{z^2}\,(1-q^{-1/4}zT_s^{1/2}T_t^{-1/2})(1-q^{1/4}zT_s^{1/2}T_t^{-1/2})(1+q^{-1/4}zT_s^{1/2}T_t^{1/2})\\&\times(1+q^{1/4}zT_s^{1/2}T_t^{1/2})T_z^{1/2}-z^2\left(1-\frac{q^{-1/4}}{z}\,T_s^{1/2}T_t^{-1/2}\right)\left(1-\frac{q^{1/4}}{z}\,T_s^{1/2}T_t^{-1/2}\right)\\&\times\left(1+\frac{q^{-1/4}}{z}\,T_s^{1/2}T_t^{1/2}\right)\left(1+\frac{q^{1/4}}{z}\,T_s^{1/2}T_t^{1/2}\right)T_z^{-1/2}\Bigg],\end{aligned} \tag{3.1}$$

$$\begin{aligned}\mu=\frac{1}{z-z^{-1}}\Bigg[&-\frac{1}{z}\,(1-q^{-1/4}zT_s^{1/2}T_t^{-1/2})(1-q^{1/4}zT_s^{1/2}T_t^{-1/2})T_z^{1/2}\\&+z\left(1-\frac{q^{-1/4}}{z}\,T_s^{1/2}T_t^{-1/2}\right)\left(1-\frac{q^{1/4}}{z}\,T_s^{1/2}T_t^{-1/2}\right)T_z^{-1/2}\Bigg],\end{aligned} \tag{3.2}$$

and

$$\begin{aligned}\mu^{*}=\frac{1}{z-z^{-1}}\Bigg[&-\frac{1}{z}\,(1+q^{-1/4}zT_s^{1/2}T_t^{1/2})(1+q^{1/4}zT_s^{1/2}T_t^{1/2})T_z^{1/2}\\&+z\left(1+\frac{q^{-1/4}}{z}\,T_s^{1/2}T_t^{1/2}\right)\left(1+\frac{q^{1/4}}{z}\,T_s^{1/2}T_t^{1/2}\right)T_z^{-1/2}\Bigg].\end{aligned} \tag{3.3}$$

Let us now define the following ten generators:

$$L_+ = \frac{1}{1-q}\, s\tau, \tag{3.4a}$$

$$L_- = \frac{1}{1-q}\,\frac{1}{s}\,\tau^*, \tag{3.4b}$$

$$L_0 = \frac{1}{1-q}\,(1-T_s^2), \tag{3.4c}$$

$$J_+ = \frac{q^{1/2}}{1-q}\, t\mu T_s^{-1/2}, \tag{3.4d}$$

$$J_- = \frac{1}{1-q}\,\frac{1}{t}\,\mu^* T_s^{-1/2}, \tag{3.4e}$$

$$K = T_t, \tag{3.4f}$$

$$P_+ = s^{1/2} t^{1/2}, \tag{3.4g}$$

$$P_- = \frac{q^{-1/2}}{s^{1/2} t^{1/2}}\,(1+q^{-1/4} z T_s^{1/2} T_t^{1/2})\left(1+\frac{q^{-1/4}}{z}\,T_s^{1/2} T_t^{1/2}\right) T_t^{1/2}, \tag{3.4h}$$

$$Q_+ = q^{-1/4}\,\frac{s^{1/2}}{t^{1/2}}\,\frac{1}{z-z^{-1}}\left[\left(1+\frac{q^{1/4}}{z}\,T_s^{1/2} T_t^{1/2}\right) T_z^{-1/2} - (1+q^{1/4} z T_s^{1/2} T_t^{1/2}) T_z^{1/2}\right] T_t^{1/2}, \tag{3.4i}$$

$$\begin{aligned} Q_- = -q^{-1/2}\,\frac{t^{1/2}}{s^{1/2}}\,\frac{1}{z-z^{-1}}\Bigg[&\frac{1}{z^2}\,(1-q^{-1/4} z T_s^{1/2} T_t^{-1/2})(1-q^{1/4} z T_s^{1/2} T_t^{-1/2})(1+q^{1/4} z T_s^{1/2} T_t^{1/2}) \\ &\times T_z^{1/2} - z^2\left(1-\frac{q^{-1/4}}{z}\,T_s^{1/2} T_t^{-1/2}\right)\left(1-\frac{q^{1/4}}{z}\,T_s^{1/2} T_t^{-1/2}\right)\left(1+\frac{q^{1/4}}{z}\,T_s^{1/2} T_t^{1/2}\right) T_z^{-1/2}\Bigg]. \end{aligned} \tag{3.4j}$$

To these we will add the operator

$$H = T_s, \tag{3.5}$$

which proves more convenient to use, occasionally, than L_0.

The ten operators we have just introduced can be shown to realize the q-algebra characterized by the following commutation relations:

$$\begin{aligned} &qL_+L_- - L_-L_+ = L_0, && [J_+, J_-] = \frac{K-K^{-1}}{q^{1/2}-q^{-1/2}}, \\ &q^{\mp 1} L_0 L_\pm - q^{\pm 1} L_\pm L_0 = \pm\frac{1+q}{q}\,L_\pm, && KJ_\pm = q^{\pm 1} J_\pm K, \\ &L_0 P_+ - qP_+ L_0 = P_+, && KP_+ = q^{1/2} P_+ K, \\ &[L_+, P_+] = 0, && q^{1/4} J_+ P_+ = P_+ J_+, \end{aligned}$$

$$
\begin{aligned}
&qP_+L_- - L_-P_+ = Q_-, && P_+J_- - q^{1/4}J_-P_+ = Q_+,\\
&P_-L_0 - qL_0P_- = P_-, && KP_- = q^{-1/2}P_-K,\\
&qL_+P_- - P_-L_+ = q^{-1/4}Q_+, && J_+P_- - q^{-1/4}P_-J_+ = Q_-K,\\
&[L_-, P_-] = 0, && q^{3/4}P_-J_- = J_-P_-,\\
&L_0Q_+ - qQ_+L_0 = Q_+, && KQ_+ = q^{-1/2}Q_+K,\\
&[L_+, Q_+] = 0, && Q_+J_+ - q^{1/4}J_+Q_+ = KP_+,\\
&L_-Q_+ - qQ_+L_- = q^{1/4}P_-, && J_-Q_+ = q^{3/4}Q_+J_-,\\
&Q_-L_0 - qL_0Q_- = Q_-, && KQ_- = q^{1/2}Q_-K,\\
&Q_-L_+ - qL_+Q_- = P_+, && q^{1/4}J_+Q_- = Q_-J_+,\\
&[L_-, Q_-] = 0, && J_-Q_- - q^{-1/4}Q_-J_- = P_-,
\end{aligned}
\tag{3.6}
$$

$$qP_+P_- - q^{1/4}P_-P_+ = -(1-q^{1/2})(1-KH)K^{1/2},$$

$$q^{3/4}P_+Q_+ - Q_+P_+ = (1-q)(1-q^{1/2})K^{1/2}L_+,$$

$$[P_+, Q_-] = q^{-3/4}(1-q)(1-q^{1/2})J_+HK^{1/2},$$

$$[Q_+, P_-] = q^{-7/4}(1-q)(1-q^{1/2})J_-HK^{3/2},$$

$$Q_-P_- - q^{-3/4}P_-Q_- = q^{-1}(1-q)(1-q^{1/2})L_-K^{1/2},$$

$$Q_+Q_- - q^{-1/4}Q_-Q_+ + qP_+P_- - q^{-3/4}P_-P_+$$

$$= (1-q)(1-q^{1/2})(q^{-1}L_-L_+ - qL_+L_-)K^{1/2}.$$

Moreover, the operators of the set $\{L_\pm, L_0\}$ commute with those of the set $\{J_\pm, K\}$. As will be shown in the Appendix, this q-deformed algebra reduces, in the $q \to 1^-$ limit, to the Lie algebra $e(4)$ of the Euclidean group in four dimensions $E(4)$. Thus, the ten operators (3.6) provide a model for a q deformation of the latter. Interestingly enough, the two sets $\{L_\pm, L_0\}$ and $\{J_\pm, K\}$ realize two different q deformations of the two $sl(2)$ subalgebras of $e(4)$.

The module associated with our model has the basis vectors

$$F_n^{(\alpha,\beta)}(x,s,t) = s^{(\alpha+\beta)/2}P_n^{(\alpha,\beta)}(x|q)t^{(\beta-\alpha)/2}. \tag{3.7}$$

The action of the ten operators (3.6) on the latter can be shown to be the following:

$$L_+F_n^{(\alpha,\beta)} = -\frac{q^{-n+\alpha/2+3/4}(1-q^{n+\alpha+\beta+1})}{(1-q)(1+q^{(\alpha+\beta+1)/2})(1+q^{(\alpha+\beta+2)/2})}F_{n-1}^{(\alpha+1,\beta+1)}, \tag{3.8a}$$

$$L_-F_n^{(\alpha,\beta)} = -\frac{1}{q^{\alpha/2+1/4}}\frac{1-q^{n+1}}{1-q}(1+q^{(\alpha+\beta-1)/2})(1+q^{(\alpha+\beta)/2})F_{n+1}^{(\alpha-1,\beta-1)}, \tag{3.8b}$$

$$L_0 F_n^{(\alpha,\beta)} = \frac{1-q^{\alpha+\beta}}{1-q} F_n^{(\alpha,\beta)}, \tag{3.8c}$$

$$J_+ F_n^{(\alpha,\beta)} = \frac{q^{-(\alpha+\beta-2)/4}}{1-q} (1-q^{n+\alpha}) F_n^{(\alpha-1,\beta+1)}, \tag{3.8d}$$

$$J_- F_n^{(\alpha,\beta)} = \frac{q^{-n-(\alpha+\beta)/4}}{1-q} (1-q^{n+\beta}) F_n^{(\alpha+1,\beta-1)}, \tag{3.8e}$$

$$K F_n^{(\alpha,\beta)} = q^{(\beta-\alpha)/2} F_n^{(\alpha,\beta)}, \tag{3.8f}$$

$$P_+ F_n^{(\alpha,\beta)} = \frac{1}{(1+q^{(\alpha+\beta+1)/2})(1-q^{(2n+\alpha+\beta+1)/2})} \times [(1-q^{n+\alpha+\beta+1}) F_n^{(\alpha,\beta+1)} + q^{(\alpha+\beta+1)/2}(1-q^{n+\alpha}) F_{n-1}^{(\alpha,\beta+1)}], \tag{3.8g}$$

$$P_- F_n^{(\alpha,\beta)} = q^{-(\alpha+\beta)/4} \frac{1+q^{(\alpha+\beta)/2}}{q^{\alpha/2+1}} \frac{1}{(1-q^{(2n+\alpha+\beta+1)/2})} \times [q^{\beta}(1-q^{n+1}) F_{n+1}^{(\alpha,\beta-1)} + q^{(\alpha+\beta+1)/2}(1-q^{n+\beta}) F_n^{(\alpha,\beta-1)}], \tag{3.8h}$$

$$Q_+ F_n^{(\alpha,\beta)} = -\frac{q^{-(\alpha+\beta)/4}}{(1+q^{(\alpha+\beta+1)/2})(1-q^{(2n+\alpha+\beta+1)/2})} \times [q^{\beta}(1-q^{n+\alpha+\beta+1}) F_n^{(\alpha+1,\beta)} - q^{-n+(\alpha+\beta+1)/2}(1-q^{n+\beta}) F_{n-1}^{(\alpha+1,\beta)}], \tag{3.8i}$$

$$Q_- F_n^{(\alpha,\beta)} = \frac{1+q^{(\alpha+\beta)/2}}{q^{\alpha/2+1/4}} \frac{1}{(1-q^{(2n+\alpha+\beta+1)/2})} \times [(1-q^{n+1}) F_{n+1}^{(\alpha-1,\beta)} - q^{n+(\alpha+\beta+1)/2}(1-q^{n+\alpha}) F_n^{(\alpha-1,\beta)}]. \tag{3.8j}$$

IV. THE q-ANALOG OF THE EXPANSION OF A PLANE WAVE IN TERMS OF JACOBI POLYNOMIALS

In order to illustrate how some of the previous results may be applied to the theory of q-special functions, we will now derive algebraically a q analog of the expansion (1.1) of a plane wave in terms of Jacobi polynomials. As a starting point, we will let $\mathscr{E}_q(x;-i,r)$ act on the function $F_0^{(\alpha,\beta)}(x,s,t)$ and expand the result on the complete basis (3.7):

$$\mathscr{E}_q(x;-i,r) F_0^{(\alpha,\beta)}(x,s,t) = \sum_{n=0}^{\infty} W_n^{(\alpha,\beta)}(r) F_n^{(\alpha,\beta)}(x,s,t). \tag{4.1}$$

This expansion involves no summation over α and β, because the left-hand side is an eigenfunction of L_0 and K, which both commute with the q exponential. Therefore, the right-hand side also must be an eigenstate of these operators, with the same eigenvalues. We will extract from (4.1) the expansion we are looking for by exploiting the properties of the model we have built for q-deformed $e(4)$ in the previous section. Acting successively with L_+, L_-, and P_+ on both members of (4.1) will yield enough conditions on the coefficients $W_n^{(\alpha,\beta)}$ to make their complete determination possible.

The action of the operator L_+ on the left-hand side of (4.1) follows directly from its definition (3.4a), the definition (3.7) of $F_0^{(\alpha,\beta)}$ and Eq. (2.12),

$$L_+ \mathscr{E}_q(x;-i,r)F_0^{(\alpha,\beta)} = -\frac{irq^{-1/4}}{1-q}\,\mathscr{E}_q(x;-i,r)F_0^{(\alpha+1,\beta+1)}$$
$$= -\frac{irq^{-1/4}}{1-q}\sum_{n=0}^{\infty} W_n^{(\alpha+1,\beta+1)}F_n^{(\alpha+1,\beta+1)}, \tag{4.2}$$

while its action on the right-hand side is an immediate consequence of (3.8a),

$$L_+\sum_{n=0}^{\infty} W_n^{(\alpha,\beta)}F_n^{(\alpha,\beta)} = -\sum_{n=0}^{\infty}\frac{q^{-n+\alpha/2+3/4}(1-q^{n+\alpha+\beta+1})}{(1-q)(1+q^{(\alpha+\beta+1)/2})(1+q^{(\alpha+\beta+2)/2})}\,W_n^{(\alpha,\beta)}F_{n-1}^{(\alpha+1,\beta+1)}. \tag{4.3}$$

Comparing (4.2) and (4.3), we obtain a first condition on the coefficients $W_n^{(\alpha,\beta)}$;

$$W_{n-1}^{(\alpha+1,\beta+1)}(r) = -\frac{i}{r}\frac{q^{-n+\alpha/2+1}(1-q^{n+\alpha+\beta+1})}{(1+q^{(\alpha+\beta+1)/2})(1+q^{(\alpha+\beta+2)/2})}\,W_n^{(\alpha,\beta)}(r). \tag{4.4}$$

The action of L_- on the left-hand side of (4.1) is a less straightforward operation, since one must first know the result of acting with τ^* on $\mathscr{E}_q(x;-i;r)F_0^{(\alpha,\beta)}$. This can be determined by expressing τ^* in terms of the operators defined in (2.10), (2.13), and (2.14),

$$\tau^* F_n^{(\alpha,\beta)} = [\tilde{\tau}_q^* + q^{-3/4}(1+q^{1/2})(q^{\alpha/2}-q^{\beta/2})\tilde{\mu}_q + q^{-1/2}[q^\alpha + q^\beta - q^{(\alpha+\beta-1)/2}(1+q^{1/2})^2]\tau$$
$$+ q^{-3/4}(1+q^{1/2})q^{(\alpha+\beta)/2}(q^{\alpha/2}-q^{\beta/2})\tilde{\mu}_{1/q} - q^{\alpha+\beta-1}\tilde{\tau}_{1/q}^*]F_n^{(\alpha,\beta)}. \tag{4.5}$$

Using the relations (2.12) and (2.15), one then obtains

$$\tau^*\mathscr{E}_q(x;-i,r)F_0^{(\alpha,\beta)} = \tau_r^*(\alpha,\beta)\mathscr{E}_q(x;-i,r)F_0^{(\alpha,\beta)}, \tag{4.6}$$

where $\tau_r^*(\alpha,\beta)$ is an operator acting on the variable r instead of x:

$$\tau_r^*(\alpha,\beta) \equiv \left\{ i\frac{q^{1/4}}{r}\left[\left(1+\frac{r^2}{q^2}\right)T_r^{-1}-1\right] + q^{-3/4}(1+q^{1/2})(q^{\alpha/2}-q^{\beta/2})\frac{(-r^2/q;q^2)_\infty}{(-r^2;q^2)_\infty}\,T_r^{-1/2}\right.$$
$$- irq^{-3/4}[q^\alpha + q^\beta - q^{(\alpha+\beta-1)/2}(1+q^{1/2})^2] + q^{-3/4}(1+q^{1/2})q^{(\alpha+\beta)/2}$$
$$\left.\times(q^{\alpha/2}-q^{\beta/2})\frac{(-r^2q;q^2)_\infty}{(-r^2q^2;q^2)_\infty}\,T_r^{1/2} + i\frac{q^{1/4}}{r}\,q^{\alpha+\beta-1}[(1+r^2q)T_r - 1]\right\}. \tag{4.7}$$

Steps analogous to those leading to (4.2) and (4.3) finally yield, for the action of L_- on both members of (4.1),

$$\tau_r^*(\alpha,\beta)\sum_{n=0}^{\infty} W_n^{(\alpha-1,\beta-1)}(r)F_n^{(\alpha-1,\beta-1)}(x,s,t)$$
$$= -\frac{(1+q^{(\alpha+\beta-1)/2})(1+q^{(\alpha+\beta)/2})}{q^{\alpha/2+1/4}}\sum_{n=0}^{\infty}(1-q^{n+1})W_n^{(\alpha,\beta)}(r)$$
$$\times F_{n+1}^{(\alpha-1,\beta-1)}(x,s,t), \tag{4.8}$$

which entails the following conditions on the coefficients $W_n^{(\alpha,\beta)}$:

$$\tau_r^*(\alpha,\beta)W_0^{(\alpha-1,\beta-1)}(r)=0, \tag{4.9a}$$

$$\tau_r^*(\alpha,\beta)W_{n+1}^{(\alpha-1,\beta-1)}(r)=-\frac{(1-q^{n+1})}{q^{\alpha/2+1/4}}(1+q^{(\alpha+\beta-1)/2})(1+q^{(\alpha+\beta)/2})W_n^{(\alpha,\beta)}(r),$$

$$n\geqslant 0. \tag{4.9b}$$

Using (4.4), one can express $W_n^{(\alpha,\beta)}$ in terms of the $W_{n+1}^{(\alpha-1,\beta-1)}$, so that (4.9) can be rewritten as

$$\tau_r^*(\alpha+1,\beta+1)W_n^{(\alpha,\beta)}(r)=\frac{i}{r}q^{-n+1/4}(1-q^{n+\alpha+\beta+1})(1-q^n)W_n^{(\alpha,\beta)}(r). \tag{4.10}$$

Notice that this condition includes (4.9a), since the right-hand side vanishes for $n=0$. In terms of the variable $y=ir$, it becomes

$$\begin{aligned}\Bigg\{\Bigg[\left(1-\frac{y^2}{q^2}\right)T_y^{-1}-1\Bigg]&-y(1+q^{-1/2})(q^{\alpha/2}-q^{\beta/2})\frac{(y^2/q;q^2)_\infty}{(y^2;q^2)_\infty}T_y^{-1/2}\\&+y^2[q^\alpha+q^\beta-q^{(\alpha+\beta-1)/2}(1+q^{1/2})^2]+(1-q^{-n})(1-q^{n+\alpha+\beta+1})\\&-y(1+q^{1/2})q^{(\alpha+\beta+1)/2}(q^{\alpha/2}-q^{\beta/2})\frac{(y^2q;q^2)_\infty}{(y^2q^2;q^2)_\infty}T_y^{1/2}\\&+q^{\alpha+\beta+1}[(1-y^2q)T_y-1]\Bigg\}W_n^{(\alpha,\beta)}(y)=0.\end{aligned} \tag{4.11}$$

This q-difference equation determines the function $W_n^{(\alpha,\beta)}(y)$ up to a multiplicative constant. The first problem one meets when trying to solve it comes from the two terms involving ratios of infinite q-shifted factorials (which, incidentally, happen to disappear in the special case $\alpha=\beta$, where the continuous q-Jacobi polynomials reduce to continuous q-ultraspherical polynomials). Hopefully, one can eliminate these unwieldy ratios by assuming that $W_n^{(\alpha,\beta)}(y)$ itself contains a similar ratio such that it is reconstituted up to a simple multiplicative factor when acted upon by the operators involved in the various terms of the equation. Then, the common ratio of infinite q-shifted factorials can be factored out. Assuming that $W_n^{(\alpha,\beta)}(y)$ is of the form

$$W_n^{(\alpha,\beta)}(y)=C_n^{(\alpha,\beta)}\frac{(\sigma y^k q^l;q^m)_\infty}{(\rho y^\kappa q^\lambda;q^\mu)_\infty}w_n(y), \tag{4.12}$$

where $C_n^{(\alpha,\beta)}$ is a constant, one checks easily that this condition is realized only if the parameters of the ratio take the values $\sigma=\pm 1$, $\rho=-\sigma$, $k=\kappa=m=\mu=1$, $l=1/2$, and $\lambda=0$. Indeed,

$$\frac{(y^2/q;q^2)_\infty}{(y^2;q^2)_\infty}T_y^{-1/2}\frac{(\sigma y q^{1/2};q)_\infty}{(-\sigma y;q)_\infty}=(1-\sigma q^{-1/2}y)\frac{(\sigma y q^{1/2};q)_\infty}{(-\sigma y;q)_\infty}, \tag{4.13a}$$

$$\frac{(y^2q;q^2)_\infty}{(y^2q^2;q^2)_\infty}T_y^{1/2}\frac{(\sigma y q^{1/2};q)_\infty}{(-\sigma y;q)_\infty}=(1+\sigma y)\frac{(\sigma y q^{1/2};q)_\infty}{(-\sigma y;q)_\infty}, \tag{4.13b}$$

and the simpler operators T_y and T_y^{-1} act in an analogous fashion.

Equation (4.11) can be further simplified by making the substitution $q^{1/2}\to q$, to eliminate fractional powers of T_y, and, finally, by writing $w_n(y)=y^n\phi_n(y)$, so that

$$W_n^{(\alpha,\beta)}(y)=C_n^{(\alpha,\beta)}\frac{(\sigma y q^{1/2};q)_\infty}{(-\sigma y;q)_\infty}\,y^n\phi_n(y). \tag{4.14}$$

It then reduces to

$$\begin{aligned}&\{q^2(1-\sigma q^{-2}y)(1-\sigma q^{-1}y)T_y^{-2}-(1+q)(a-b)y(1-\sigma q^{-1}y)T_y^{-1}\\&+[(a-b)^2-abq^{-1}(1+q^2)]y^2-(1+q)ab(a-b)y(1+\sigma y)T_y\\&+a^2b^2(1+\sigma qy)(1+\sigma y)T_y^2-q^2-a^2b^2\}\phi_n(y)=0,\end{aligned} \tag{4.15}$$

with the notation

$$a=q^{n+\alpha+1},\quad b=q^{n+\beta+1}. \tag{4.16}$$

Amazingly enough, this equation can be factorized in the following manner:

$$\begin{aligned}&[ab(1+\sigma y)T_y-(a-b)y+q+ab+q(1-\sigma q^{-1}y)T_y^{-1}]\\&\times[ab(1+\sigma y)T_y-(a-b)y-q-ab+q(1-\sigma q^{-1}y)T_y^{-1}]\phi_n(y)=0.\end{aligned} \tag{4.17}$$

For $\sigma=1$, one recognizes in the second factor of (4.17), the equation

$$[(1-bT_y)(1+aT_y)-(1-abT_y)D_y^+]\phi(y)=0, \tag{4.18}$$

when multiplied from the left by $-yT_y^{-1}$. Thus, in order to find a solution of (4.17) in that case, it is enough to solve the much simpler equation (4.18). Solutions of the latter are known:[21] the regular one is the basic hypergeometric series ${}_2\phi_1(b,-a;ab;q,y)$. Therefore, up to a multiplicative constant, the solution of Eq. (4.11) is

$$W_n^{(\alpha,\beta)}(y)=C_n^{(\alpha,\beta)}\frac{(\sigma y q^{1/2};q)_\infty}{(-\sigma y;q)_\infty}\,y^n\,{}_2\phi_1\left(\begin{matrix}q^{(n+\beta+1)/2},-q^{(n+\alpha+1)/2}\\ q^{(2n+\alpha+\beta+2)/2}\end{matrix}\middle|\,q^{1/2};y\right), \tag{4.19}$$

for $\sigma=1$. When $\sigma=-1$, one falls back on the previous case by doing $y\to -y$ and $a\leftrightarrow b$ in (4.17). Using Heines's q analog of Euler's transformation formula,[1] one easily shows that performing these substitutions in (4.19) yields no new solution.

All that remains to be done, now, is to determine the multiplicative constants $C_n^{(\alpha,\beta)}$. A two-term recurrence relation for these quantities can be obtained by acting on both members of (4.1) with the operator P_+. Proceeding in the usual manner, one obtains a condition on the coefficients $W_n^{(\alpha,\beta)}$, which, once expressed in terms of the $C_n^{(\alpha,\beta)}$ through (4.19), reads

$$\begin{aligned}&C_n^{(\alpha,\beta+1)}\,{}_2\phi_1((qb)^{1/2},-a^{1/2};(qab)^{1/2};q^{1/2},y)\\&=\frac{1}{1+q^{(\alpha+\beta+1)/2}}\left\{\frac{1-q^{n+\alpha+\beta+1}}{1-q^{(2n+\alpha+\beta+1)/2}}\,C_n^{(\alpha,\beta)}\,{}_2\phi_1(b^{1/2},-a^{1/2};(ab)^{1/2};q^{1/2},y)\right.\\&\left.+\frac{q^{(\alpha+\beta+1)/2}(1-q^{n+\alpha+1})}{1-q^{(2n+\alpha+\beta+3)/2}}\,C_{n+1}^{(\alpha,\beta)}y\,{}_2\phi_1((qb)^{1/2},-(qa)^{1/2};q(ab)^{1/2};q^{1/2},y)\right\}.\end{aligned} \tag{4.20}$$

Now, it is a simple matter to prove the following three-term recurrence relation:

$$ {}_2\phi_1(bq,-a;abq;q,y)={}_2\phi_1(b,-a;ab;q,y)+\frac{b(1-a^2)}{(1-ab)(1-abq)}\,y\,{}_2\phi_1(bq,-aq;abq^2;q,y). \tag{4.21} $$

When used on the left-hand side of (4.20), the latter leads to a relation between two linearly independent functions ${}_2\phi_1$, which yields the following two conditions on the multiplicative coefficients $C_n^{(\alpha,\beta)}$:

$$ C_n^{(\alpha,\beta+1)}=\frac{1-q^{n+\alpha+\beta+1}}{(1+q^{(\alpha+\beta+1)/2})(1-q^{(2n+\alpha+\beta+1)/2})}\,C_n^{(\alpha,\beta)}, \tag{4.22a} $$

$$ \frac{q^{n/2}}{1-q^{(2n+\alpha+\beta+2)/2}}\,C_n^{(\alpha,\beta+1)}=\frac{q^{\alpha/2}}{1+q^{(\alpha+\beta+1)/2}}\,C_{n+1}^{(\alpha,\beta)}. \tag{4.22b} $$

Eliminating $C_n^{(\alpha,\beta+1)}$ from these equations, one obtains a two-term recurrence relation,

$$ C_{n+1}^{(\alpha,\beta)}=\frac{q^{(n-\alpha)/2}(1-q^{n+\alpha+\beta+1})}{(1-q^{(2n+\alpha+\beta+1)/2})(1-q^{(2n+\alpha+\beta+2)/2})}\,C_n^{(\alpha,\beta)}, \tag{4.23} $$

which is easily solved by iteration and determines $C_n^{(\alpha,\beta)}$ up to a multiplicative function of α and β, $C_0^{(\alpha,\beta)}$,

$$ C_n^{(\alpha,\beta)}=\frac{q^{n(n-2\alpha-1)/4}(q^{\alpha+\beta+1};q)_n}{(q^{(\alpha+\beta+1)/2},q^{(\alpha+\beta+2)/2};q)_n}\,C_0^{(\alpha,\beta)}. \tag{4.24} $$

It turns out that $C_0^{(\alpha,\beta)}$ is a constant independent of α and β. Indeed, for $n=0$ Eq. (4.22a) becomes

$$ C_0^{(\alpha,\beta+1)}=C_0^{(\alpha,\beta)}. \tag{4.25} $$

Besides, using Eq. (4.19), we can rewrite (4.4) in the following manner:

$$ C_{n+1}^{(\alpha,\beta)}=\frac{(1+q^{(\alpha+\beta+1)/2})(1+q^{(\alpha+\beta+2)/2})}{q^{-n+\alpha/2}(1-q^{n+\alpha+\beta+2})}\,C_n^{(\alpha+1,\beta+1)}. \tag{4.26} $$

Equating the right-hand sides of (4.23) and (4.26), and setting $n=0$, we obtain

$$ C_0^{(\alpha+1,\beta+1)}=C_0^{(\alpha,\beta)}. \tag{4.27} $$

The fact that $C_0^{(\alpha,\beta)}$ is a constant follows immediately from (4.25) and (4.27). Its value can be determined to be $C_0^{(\alpha,\beta)}=1$ by setting $r=0$ in (4.1) and (4.19).

Finally, setting $s=t=1$ in (4.1), we obtain the expansion of the q exponential in terms of continuous q-Jacobi polynomials,

$$ \mathscr{E}_q(x;-i,r)=\sum_{n=0}^{\infty} W_n^{(\alpha,\beta)}(r)P_n^{(\alpha,\beta)}(x|q), \tag{4.28a} $$

with

$$W_n^{(\alpha,\beta)}(r)=q^{n(n-2\alpha-1)/4}\frac{(q^{\alpha+\beta+1};q)_n}{(q^{(\alpha+\beta+1)/2},q^{(\alpha+\beta+2)/2};q)_n}(ir)^n\frac{(irq^{1/2};q)_\infty}{(-ir;q)_\infty}$$
$$\times{}_2\phi_1\left(\begin{matrix}q^{(n+\beta+1)/2},-q^{(n+\alpha+1)/2},\\ q^{(2n+\alpha+\beta+2)/2}\end{matrix}\middle|q^{1/2};ir\right). \tag{4.28b}$$

This q analog of the expansion (1.1) was first obtained in Ref. 16. We have derived it here in a purely algebraic manner.

In the special case $\alpha=\beta$, the continuous q-Jacobi polynomials $P_n^{(\alpha,\beta)}(x|q)$ reduce to continuous q-ultraspherical polynomials $C_n(x;q^m|q)$,[2]

$$P_n^{(\alpha,\alpha)}(x|q)=q^{n(2\alpha+1)/4}\frac{(q^{\alpha+1};q)_n}{(q^{2\alpha+1};q)_n}C_n(x;q^{\alpha+1/2}|q). \tag{4.29}$$

Setting $\alpha=\beta$ in Eqs. (4.28), defining $l=\alpha+1/2$, and using (4.29) as well as the relation[1]

$${}_2\phi_1\left(\begin{matrix}q^{(n+l+1/2)/2},-q^{(n+l+1/2)/2}\\ q^{n+l+1/2}\end{matrix}\middle|q^{1/2};ir\right)=(q;q)_{n+l}\frac{r^{-(n+l)}}{(ir;q^{1/2})_\infty}J_{n+l}^{(2)}(2r;q), \tag{4.30}$$

one obtains readily the q analog of the Fourier–Gegenbauer expansion,[13,20]

$$\mathscr{E}_q(x;-i,r)=\frac{r^{-l}}{(-r^2;q^2)_\infty}(q;q)_{l-1}\sum_{n=0}^{\infty}i^n q^{n^2/4}(1-q^{n+l})J_{n+l}^{(2)}(2r;q)C_n(x;q^l|q), \tag{4.31}$$

as a special case of the expansion (4.28).

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APPENDIX: THE $q\to 1^-$ LIMIT

Before considering the $q\to 1^-$ limit of the model given in Sec. III, let us first recall the structure of the Lie algebra of Euclidean transformations in a four-dimensional space. The six rotation operators m_{ij} and the four translation operators p_i have the following commutation relations:

$$[m_{ij},m_{kl}]=\delta_{jk}m_{il}-\delta_{jl}m_{ik}-\delta_{ik}m_{jl}+\delta_{il}m_{jk}, \tag{A1}$$

$$[m_{ij},p_k]=\delta_{jk}p_i-\delta_{ik}p_j, \tag{A2}$$

$$[p_i,p_j]=0. \tag{A3}$$

In order to investigate the structure of this algebra, it proves useful to define the following linear combinations of the six m_{ij}'s:

$$l_1=\frac{i}{2}(m_{32}+m_{41}),\quad l_2=\frac{i}{2}(m_{13}+m_{42}),\quad l_3=\frac{i}{2}(m_{21}+m_{43}),$$
$$j_1=\frac{i}{2}(m_{32}-m_{41}),\quad j_2=\frac{i}{2}(m_{13}-m_{42}),\quad j_3=\frac{i}{2}(m_{21}-m_{43}). \tag{A4}$$

As a consequence of (A3), they obey the commutation relations

$$[l_\lambda, l_\mu] = \epsilon_{\lambda\mu\nu} l_\nu, \quad [j_\lambda, j_\mu] = \epsilon_{\lambda\mu\nu} j_\nu, \quad [l_\mu, j_\nu] = 0, \tag{A5}$$

where Greek indices take values from 1 to 3 only. This makes explicit that the $so(4)$ subalgebra of $e(4)$ is isomorphic to $so(3) \oplus so(3)$.

Finally, introducing the further definitions

$$\begin{aligned} l_\pm &= l_1 \pm i l_2, & l_0 &= 2 l_3, \\ j_\pm &= j_1 \pm i j_2, & j_0 &= 2 j_3, \\ p_\pm &= p_2 \pm i p_3, & q_\pm &= p_1 \pm i p_4, \end{aligned} \tag{A6}$$

we can write the Lie algebra of Euclidean transformations in a four-dimensional space in the following manner:

$$\begin{aligned} [l_+, l_-] &= l_0, & [j_+, j_-] &= j_0, \\ [l_0, l_\pm] &= \pm 2 l_\pm, & [j_0, j_\pm] &= \pm 2 j_\pm, \\ [l_0, p_\pm] &= \pm p_\pm, & [j_0, p_\pm] &= \pm p_\pm, \\ [l_\pm, p_\pm] &= 0, & [j_\pm, p_\pm] &= 0, \\ [l_\pm, p_\mp] &= \pm q_\pm, & [j_\pm, p_\mp] &= \pm q_\mp, \\ [l_0, q_\pm] &= \pm q_\pm, & [j_0, q_\pm] &= \mp q_\pm, \\ [l_\pm, q_\pm] &= 0, & [j_\pm, q_\mp] &= 0, \\ [l_\pm, q_\mp] &= \mp p_\pm, & [j_\pm, q_\pm] &= \mp p_\pm. \end{aligned} \tag{A7}$$

Moreover, the four translation operators $\{p_+, p_-, q_+, q_-\}$ all commute with each other.

Now, defining the operator J_0 through

$$K = q^{J_0/2}, \tag{A8}$$

one sees readily that the q-deformed algebra (3.6) reduces to the Lie algebra we have just written, when $q \to 1^-$, with

$$\lim_{q \to 1^-} L_\pm = l_\pm, \tag{A9}$$

and so on. Explicitly, the operators defined in (3.4), (A8) and (A9) then become

$$\begin{aligned} l_0 &= 2s \frac{\partial}{\partial s}, & j_0 &= 2t \frac{\partial}{\partial t}, \\ l_+ &= -\frac{s}{2} \frac{\partial}{\partial x}, & j_+ &= t\left[(x-1)\frac{\partial}{\partial x} + s\frac{\partial}{\partial s} - t\frac{\partial}{\partial t}\right], \\ l_- &= \frac{2}{s}\left[(1-x^2)\frac{\partial}{\partial x} - 2xs\frac{\partial}{\partial s} + 2t\frac{\partial}{\partial t}\right], & j_- &= \frac{1}{t}\left[(x+1)\frac{\partial}{\partial x} + s\frac{\partial}{\partial s} + t\frac{\partial}{\partial t}\right], \\ p_+ &= s^{1/2} t^{1/2}, & p_- &= 2 s^{-1/2} (x+1) t^{-1/2}, \end{aligned} \tag{A10}$$

$$q_+ = -s^{1/2}t^{-1/2}, \quad q_- = 2s^{-1/2}(x-1)t^{1/2},$$

while the basis vectors are now expressed[2] in terms of classical Jacobi polynomials,

$$f_n^{(\alpha,\beta)}(x,s,t) = \lim_{q\to 1^-} F_n^{(\alpha,\beta)}(x,s,t) = s^{(\alpha+\beta)/2} P_n^{(\alpha,\beta)}(x) t^{(\beta-\alpha)/2}. \tag{A11}$$

In this realization, the action of the generators on the basis vectors is the following:

$$\begin{aligned}
l_+ f_n^{(\alpha,\beta)} &= -\frac{n+\alpha+\beta+1}{4} f_{n-1}^{(\alpha+1,\beta+1)}, \quad j_+ f_n^{(\alpha,\beta)} = (n+\alpha) f_n^{(\alpha-1,\beta+1)}, \\
l_- f_n^{(\alpha,\beta)} &= -4(n+1) f_{n+1}^{(\alpha-1,\beta-1)}, \quad j_- f_n^{(\alpha,\beta)} = (n+\beta) f_n^{(\alpha+1,\beta-1)}, \\
l_0 f_n^{(\alpha,\beta)} &= (\alpha+\beta) f_n^{(\alpha,\beta)}, \quad j_0 f_n^{(\alpha,\beta)} = (\beta-\alpha) f_n^{(\alpha,\beta)}, \\
p_+ f_n^{(\alpha,\beta)} &= \frac{1}{2n+\alpha+\beta+1}\left[(n+\alpha+\beta+1) f_n^{(\alpha,\beta+1)} + (n+\alpha) f_{n-1}^{(\alpha,\beta+1)}\right], \\
q_+ f_n^{(\alpha,\beta)} &= -\frac{1}{2n+\alpha+\beta+1}\left[(n+\alpha+\beta+1) f_n^{(\alpha+1,\beta)} - (n+\beta) f_{n-1}^{(\alpha+1,\beta)}\right], \\
p_- f_n^{(\alpha,\beta)} &= \frac{4}{2n+\alpha+\beta+1}\left[(n+1) f_{n+1}^{(\alpha,\beta-1)} + (n+\beta) f_n^{(\alpha,\beta-1)}\right], \\
q_- f_n^{(\alpha,\beta)} &= \frac{4}{2n+\alpha+\beta+1}\left[(n+1) f_{n+1}^{(\alpha-1,\beta)} - (n+\alpha) f_n^{(\alpha-1,\beta)}\right],
\end{aligned} \tag{A12}$$

as can be seen by taking the limit $q\to 1^-$ in (3.8), or by applying directly the operators (A10) to the basis functions $f_n^{(\alpha,\beta)}(x,s,t)$.

The algebraic derivation of the expansion of an exponential in terms of Jacobi polynomials, Eq. (1.1), is also the $q\to 1^-$ limit of the derivation given in Sec. IV for the q analog of this expansion. Writing

$$e^{irx} f_0^{(\alpha,\beta)} = \sum_{n=0}^{\infty} w_n^{(\alpha,\beta)}(r) f_n^{(\alpha,\beta)}(x,s,t), \tag{A13}$$

one determines the coefficients $w_n^{(\alpha,\beta)}(r)$ by acting on (A12) with the generators l_+, l_-, and p_+. This yields, respectively, the following three relations:

$$w_{n-1}^{(\alpha+1,\beta+1)}(r) = -\frac{i}{r}\frac{n+\alpha+\beta+1}{2} w_n^{(\alpha,\beta)}(r), \tag{A14}$$

$$\left\{ ir\left(1+\frac{\partial^2}{\partial r^2}\right) + (\alpha+\beta) i \frac{\partial}{\partial r} + \beta - \alpha \right\} w_{n+1}^{(\alpha-1,\beta-1)}(r) = -2(n+1) w_n^{(\alpha,\beta)}(r), \tag{A15}$$

and

$$w_n^{(\alpha,\beta+1)}(r) = \frac{n+\alpha+\beta+1}{2n+\alpha+\beta+1} w_n^{(\alpha,\beta)}(r) + \frac{n+\alpha+1}{2n+\alpha+\beta+3} w_{n+1}^{(\alpha,\beta)}(r). \tag{A16}$$

The first two relations give

$$\left\{ir\left(1+\frac{\partial^2}{\partial r^2}\right)+(\alpha+\beta+2)i\,\frac{\partial}{\partial r}+\beta-\alpha\right\}w_n^{(\alpha,\beta)}(r)=\frac{i}{r}\,n(n+\alpha+\beta+1)w_n^{(\alpha,\beta)}(r), \quad \text{(A17)}$$

which is easily seen to have the solution

$$w_n^{(\alpha,\beta)}(r)=c_n^{(\alpha,\beta)}e^{-ir}(2ir)^n{}_1F_1\left(\begin{matrix}n+\beta+1\\2n+\alpha+\beta+2\end{matrix}\middle|2ir\right). \quad \text{(A18)}$$

Proceeding as in the previous section, one finds that, as a consequence of (A16), the multiplicative constant is

$$c_n^{(\alpha,\beta)}=\frac{(\alpha+\beta+1)_n}{(\alpha+\beta+1)_{2n}}. \quad \text{(A19)}$$

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Some trigonometric identities. II

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Some trigonometric sums arising in the perturbative study of integrable chiral Z_n quantum chains are directly evaluated. © *1996 American Institute of Physics.* [S0022-2488(96)01006-7]

I. INTRODUCTION AND RESULTS

In the study of chiral Potts model[1] and of the integrable chiral Z_n quantum chains,[2] the high- and low-temperature expansions of the free energy serve as generating functions for some classes of trigonometric sums. In a previous paper[3] we gave a method of evaluating directly trigonometric sums of the form

$$T_k(p)=\sum_{j=1}^{n-1}\frac{\sin^2(\pi jp/n)}{\sin^{2k+2}(\pi j/n)}, \tag{1.1}$$

$$U_k(p)=\sum_{j=1}^{n-1}\sum_{l=1}^{n-1}\frac{2(1-\omega^{jp})+2(1-\omega^{lp})-(1-\omega^{(j-l)p})}{(\sin(\pi j/n)\sin(\pi l/n))^{2k}}, \tag{1.2}$$

$$V_k(p)=\sum_{j=1}^{n-1}\sin^2\left(\frac{\pi jp}{n}\right)\sum_{l=1,l\neq j}^{n-1}\sum_{m=1,m\neq j}^{n-1}\left[\sin\left(\frac{\pi l}{n}\right)\sin\left(\frac{\pi(j-l)}{n}\right)\sin\left(\frac{\pi m}{n}\right)\sin\left(\frac{\pi(j-m)}{n}\right)\right]^{-k}, \tag{1.3}$$

$$W_k(p)=\sum_{j=1}^{n-1}\sin^2\left(\frac{\pi jp}{n}\right)\sum_{l=1,l\neq j}^{n-1}\sum_{m=1,m\neq l}^{n-1}\left[\sin\left(\frac{\pi j}{n}\right)\sin\left(\frac{\pi(j-l)}{n}\right)\sin\left(\frac{\pi(l-m)}{n}\right)\sin\left(\frac{\pi m}{n}\right)\right]^{-k}, \tag{1.4}$$

where n,k,p are all integers and the dependence on n is implicit in the definitions (1.1)–(1.4); we have set

$$\omega=\exp(2\pi i/n). \tag{1.5}$$

For this we needed the classical properties of polynomials and rational functions (the Appendix summarizes the results). This time we give a method of evaluating sums of the form

$$I(k,p)=\sum_{\substack{j_1,\ldots,j_k=1\\ j_r\neq j_{r+1}}}^{n-1}\left\{\sin\left(\frac{\pi j_1}{n}\right)\sin\frac{\pi}{n}(j_1-j_2)\cdots\sin\frac{\pi}{n}(j_{k-1}-j_k)\sin\left(\frac{\pi j_k}{n}\right)\right\}^{-p}, \tag{1.6}$$

or alternately sums

$$\bar{I}(k,p)=-(2i)^{(k+1)p}I(k,p), \tag{1.7}$$

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which may eventually be written as

$$\bar{I}(k,p)=\sum_{\substack{j_1,\ldots,j_k=1\\ j_r\neq j_{r+1}}}^{n-1}\left\{\frac{1}{1-\omega^{j_1}}\,\omega^{j_1}\,\frac{1}{\omega^{j_1}-\omega^{j_2}}\,\omega^{j_2}\cdots\frac{1}{\omega^{j_{k-1}}-\omega^{j_k}}\,\omega^{j_k}\,\frac{1}{\omega^{j_k}-1}\right\}^p. \tag{1.8}$$

Changing the summation indices j_r to $n-j_r$, one sees that $I(k,p)=0$ if $(k+1)p$ is odd; $\bar{I}(k,p)$ [or $I(k,p)$] will be expressed as a combination of sums of powers of a certain function $F(j,p)$:

$$\bar{I}(k,p)=\sum_{r=1}^{k+1}(-1)^{r+1}\sum_{\substack{l_1,\ldots,l_r;l_i\geqslant 2\\ l_1+\cdots+l_r=k+1}} G_{l_1}\cdots G_{l_r}, \tag{1.9}$$

$$G_l=\frac{1}{n}\sum_{j=0}^{n-1}[F(j,p)]^l. \tag{1.10}$$

Here $F(j,p)$ is a polynomial in j and n of degree p:

$$F(j,p)=(-1)^p\left[n\binom{j+p-1}{p-1}-\binom{j+p}{p}+\sum_{l=1}^{p}\binom{j+p}{p-l}t_l\right] \tag{1.11}$$

with

$$t_l=\sum_{q=1}^{n-1}(\omega^q-1)^{-l}, \tag{1.12}$$

a polynomial in n. The t_l can be calculated successively from the recurrence equation

$$t_l=c_1t_{l-1}-c_2t_{l-2}+\cdots+(-1)^lc_{l-1}t_1+(-1)^{l+1}lc_l, \tag{1.13}$$

with

$$c_j=(-1)^j\frac{1}{j+1}\binom{n-1}{j}. \tag{1.14}$$

II. $\bar{I}(k,p)$ AS A COMBINATION OF TRACES OF POWERS OF AN $n\times n$ MATRIX

Let us define the $n\times n$ matrix M_{ij}, $i,j=0,1,\ldots,n-1$, as

$$M_{ij}=\omega^{ip/2}(\omega^i-\omega^j)^{-p}\omega^{jp/2}=\frac{\omega^{(i-j)p/2}}{(\omega^{i-j}-1)^p},\quad \text{if } i\neq j, \tag{2.1}$$

$$M_{ii}=0. \tag{2.2}$$

This matrix is symmetric or antisymmetric according to whether p is even or odd. Then

$$\bar{I}(k,p)=\sum_{\substack{j_1,\ldots,j_k=1\\ j_r\neq j_{r+1}}}^{n-1}M_{0j_1}M_{j_1j_2}\cdots M_{j_{k-1}j_k}M_{j_k0}. \tag{2.3}$$

To put the index 0 on the same level as the other indices $1,2,\ldots,n-1$, we write Eq. (2.3) as

$$\bar{I}(k,p)=[M(I-P)M(I-P)M\cdots M(I-P)M]_{00}, \tag{2.4}$$

where I is the $n\times n$ unit matrix and the projector P is the $n\times n$ matrix all of whose elements are zero except the (1,1) element which is 1:

$$I=\begin{bmatrix}1&0&\cdots&0\\0&1&\cdots&0\\.&.&\cdots&.\\0&0&\cdots&1\end{bmatrix},\quad P=\begin{bmatrix}1&0&\cdots&0\\0&0&\cdots&0\\.&.&\cdots&.\\0&0&\cdots&0\end{bmatrix}. \tag{2.5}$$

Thus

$$\bar{I}(k,p)=\sum_{r=1}^{k+1}(-1)^{r+1}\prod_{l_1,\ldots,l_r}(M^{l_i})_{00},\quad l_1+\cdots+l_r=k+1, \tag{2.6}$$

where $(M^l)_{00}$ has the same structure as $\bar{I}(k,l)$ except that the summation over the intermediate indices now runs from 0 to $n-1$. As M_{ij} and hence $(M^k)_{ij}$ depend only on $i-j \bmod n$,

$$(M^l)_{00}=(M^l)_{jj},\quad j=1,2,\ldots,n-1. \tag{2.7}$$

Then we rewrite Eq. (2.6) as

$$\bar{I}(k,p)=\sum_{r=1}^{k+1}(-1)^{r+1}\prod_{l_1,\ldots,l_r}\left(\frac{1}{n}\operatorname{tr} M^{l_i}\right),\quad l_1+\cdots+l_r=k+1. \tag{2.8}$$

Setting

$$G_l=\frac{1}{n}\operatorname{tr} M^l, \tag{2.9}$$

one has, for example,

$$\bar{I}(1,p)=G_2, \tag{2.10}$$

$$\bar{I}(2,p)=G_3, \tag{2.11}$$

$$\bar{I}(3,p)=G_4-G_2^2, \tag{2.12}$$

$$\bar{I}(4,p)=G_5-2G_3G_2, \tag{2.13}$$

$$\bar{I}(5,p)=G_6-2G_4G_2-G_3^2+G_2^3, \tag{2.14}$$

etc.

III. DIAGONALIZATION OF *M*

Fortunately, the matrix M may be easily diagonalized with the obviously unitary matrix B:

$$B_{ij}=\frac{1}{\sqrt{n}}\omega^{i(j+p/2)},\quad i,j=0,1,\ldots,n-1. \tag{3.1}$$

We have

$$(B^{\dagger}MB)_{ij}=\frac{1}{n}\sum_{l,m=0}^{n-1}\omega^{-l(i+p/2)}\frac{\omega^{(l-m)p/2}}{(\omega^{l-m}-1)^{p}}\omega^{m(j+p/2)}(1-\delta_{lm}). \tag{3.2}$$

Setting $l-m=q$ as a new summation index, one has

$$(B^{\dagger}MB)_{ij}=\frac{1}{n}\sum_{m=0}^{n-1}\omega^{m(j-1)}\sum_{q=1}^{n-1}\frac{\omega^{-iq}}{(\omega^{q}-1)^{p}}=\delta_{ij}F(j,p), \tag{3.3}$$

where the quantities

$$\begin{aligned}F(j,p)&=\sum_{q=1}^{n-1}\frac{\omega^{-jq}}{(\omega^{q}-1)^{p}},\\&=\sum_{q=1}^{n-1}\frac{\omega^{q(j+p)}}{(1-\omega^{q})^{p}},\quad j=0,1,\ldots,n-1,\end{aligned} \tag{3.4}$$

are the eigenvalues of M. To get the second form in Eq. (3.4) one changes, for example, the summation index q to $n-q$. Note that

$$F(j,p)=(-1)^{p}F(n-p-j,p). \tag{3.5}$$

IV. CALCULATION OF THE EIGENVALUES

To compute $F(j,p)$, we use partial fractions

$$\frac{x^{j+p}}{(x-1)^{p}}=A(x)+\sum_{l=1}^{p}\frac{a_l}{(x-1)^{l}}, \tag{4.1}$$

where $A(x)$ is a polynomial of degree j and $a_1,\ldots,a_p$ are constants. Clearing the denominators, one has

$$x^{j+p}=(x-1)^{p}A(x)+\sum_{l=1}^{p}a_l(x-1)^{p-l}, \tag{4.2}$$

and a simple limiting procedure gives

$$a_l=\binom{j+p}{p-l},\quad l=1,2,\ldots,p, \tag{4.3}$$

$$A(1)=\binom{j+p}{p}. \tag{4.4}$$

We shall also need

$$A(0)=a_1-a_2+a_3-a_4+\cdots+(-1)^{p+1}a_p=\sum_{l=1}^{p}(-1)^{l+1}\binom{j+p}{p-l}=\binom{j+p-1}{p-1}. \tag{4.5}$$

The summation over the index q of the polynomial part of (4.1) is easily performed using a trick similar to that in Ref. 3: setting $A(x)=\Sigma_{s=0}^{j}\lambda_s x^{s}$, we have

$$\sum_{q=1}^{n-1} A(\omega^q)=\sum_{s=0}^{j}\lambda_s\sum_{q=1}^{n-1}\omega^{qs}=\sum_{s=0}^{j}\lambda_s(-1+n\delta_{s,0})=nA(0)-A(1). \tag{4.6}$$

As to the remaining polar part, it is rewritten as $\Sigma_{l=1}^{p}a_l t^l$ with

$$t_l=\sum_{q=1}^{n-1}(\omega^q-1)^{-l}. \tag{4.7}$$

Therefore,

$$F(j,p)=(-1)^p\left\{nA(0)-A(1)+\sum_{l=1}^{p}a_l t_l\right\}. \tag{4.8}$$

The $A(0)$, $A(1)$, and a_l are given by Eqs. (4.5), (4.4), and (4.3). The t_l are the power sums of the roots of the algebraic equation

$$(y+1)^n-y^n=0 \tag{4.9}$$

and can be computed readily (see Ref. 3). In particular, the t_l can be determined successively from the recurrence equation

$$t_l=c_1t_{l-1}-c_2t_{l-2}+c_3t_{l-3}-\cdots+(-1)^l c_{l-1}t_1+(-1)^{l+1}lc_l \tag{4.10}$$

with the elementary symmetric functions

$$c_j=(-1)^j\frac{1}{n}\binom{n}{j+1}=(-1)^j\frac{1}{j+1}\binom{n-1}{j}. \tag{4.11}$$

Thus

$$t_1=-\tfrac{1}{2}(n-1),$$

$$t_2=-\tfrac{1}{12}(n-1)(n-5),$$

$$t_3=\tfrac{1}{8}(n-1)(n-3),$$

$$t_4=\tfrac{1}{720}(n-1)(n^3+n^2-109n+251),$$

$$t_5=-\tfrac{1}{288}(n-1)(n^3+n^2-49n+95),$$

etc. We finally have

$$\frac{1}{n}\operatorname{tr} M^k=\frac{1}{n}\sum_{j=0}^{n-1}[F(j,p)]^k, \tag{4.12}$$

$$F(j,p)=(-1)^p\left[n\binom{j+p-1}{p-1}-\binom{j+p}{p}+\sum_{l=1}^{p}\binom{j+p}{p-l}t_l\right], \tag{4.13}$$

and t_l are given by Eqs. (4.10) and (4.11). For example,

$$F(j,1)=j-\tfrac{1}{2}(n-1), \tag{4.14}$$

$$F(j,2)=-\frac{1}{2}\left[\left(j-\frac{n-2}{2}\right)^2-\frac{1}{12}(n^2+2)\right], \tag{4.15}$$

$$F(j,3)=\frac{1}{6}\left(j-\frac{n-3}{2}\right)^3-\frac{1}{24}(n^2+3)\left(j-\frac{n-3}{2}\right), \tag{4.16}$$

$$F(j,4)=-\frac{1}{24}\left(j-\frac{n-4}{2}\right)^4+\frac{1}{48}(n^2+4)\left(j-\frac{n-4}{2}\right)^2-\frac{1}{5760}(7n^4+40n^2+88), \tag{4.17}$$

etc. Here $F(j,p)$ is a polynomial in $j-\frac{1}{2}(n-p)$ having the same parity as p, a simple consequence of the symmetry equation (3.5), and from the above expressions (4.14)–(4.17) it seems that the coefficients are even functions of n.

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APPENDIX: SUMMARY OF TRIGONOMETRIC SUMS

Summary of the trigonometric sums (1.1)–(1.4):

$$T_k(p)=p^2T_k-4\sum_{l=1}^{p}(p-l)T_{k-1}(l),$$

$$T_0(p)=p(n-p),$$

$$T_k\equiv T_k(1) \quad \text{are determined separately}$$

(see Ref. 3).

$$U_k(p)=(-1)^{k-1}2^{2k}T_{k-1}(p)T_k+2^{4k-2}T_{k-1}^2(p),$$

$$V_k(p)=4^k\sum_{l=0}^{k}(-1)^l\binom{k}{l}T_{2k-l-1}(p),$$

$$W_k(p)=-4^k\sum_{j=1}^{n-1}\frac{\sin^2(\pi jp/n)}{\sin^{2k}(\pi j/n)}\left\{2^kT_k+\left(1-\frac{3}{2\sin^2(\pi j/n)}\right)^k\right\}.$$

Thus $T_k(p)$ can be successively evaluated knowing T_k and then $U_k(p)$, $V_k(p)$, $W_k(p)$ can be evaluated successively.

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Continuous wavelet transforms on the sphere

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In this very short paper we shall construct a continuous wavelet analysis based on dilations translations and rotations on the sphere. It is the analog of the construction proposed by Murenzi [in his thesis, 1990], on $\mathbb{R}^2$. At small scale we shall recover the Euclidian structure of the sphere. At large scale we obtain that the wavelet transform decays rapidly because the sphere is compact. © *1996 American Institute of Physics.* [S0022-2488(96)01408-9]

I. INTRODUCTION

Recently the construction of wavelets on the sphere has attracted attention in particular in view of applications to geophysical situations.[1] Some recent constructions of decompositions of unity on the sphere are Refs. 2–5. The first construction is based on group representations in the tangent bundle of the sphere. The second construction is mainly based on the Poisson or Heat semi-group. It also focuses on rotation invariant wavelets. The third construction is more of Weyl–Heisenberg type. The fourth construction is based on the Calderón reproducing formula. The construction we propose in this paper is different in that it constructs a family of wavelets in a more *ad hoc* way. At small scale we shall see that the sphere is flat and asymptotically our wavelet analysis tends to the usual wavelet analysis of functions on $\mathbb{R}^2$ based on dilations and rotations. A discretized version of continuous wavelet analysis on the sphere can, e.g., be found in Refs. 6 and 7.

II. THE ROTATION GROUP

We now want to decompose the Hilbert space $L^2(S^2)=L^2(S^2,d\Omega)$ of square integrable functions over the unit sphere S^2; that is, S^2 is the subset of all points x in three-dimensional Euclidean space with $|x|=1$. Here $d\Omega$ is the surface measure of the sphere. We sometimes use spherical coordinates (θ,ϕ), where θ are the latitudes and ϕ the longitudes. Thus $\theta=0$ corresponds to the north pole, that we occasionally denote by N. The south pole S corresponds to $\theta=\pi$. We denote by $\mathrm{SO}(n)$ the group of rotations of n-dimensional space. Then the two-sphere may be identified with the homogeneous space $\mathrm{SO}(3)/\mathrm{SO}(2)$. We therefore have natural left action $x\mapsto\xi\cdot x$ of $\xi\in\mathrm{SO}(3)$ on $x\in S^2$. It is given by the rotations of the sphere. We thus have an obvious unitary representations of $\mathrm{SO}(3)$ in $L^2(S^2)$ by means of

$$(U(\xi)s)(x)=s(x\cdot\xi^{-1}),\quad U(\xi)U(\xi')=U(\xi\xi').$$

A. Spherical harmonics

As is well known, the representation U is reducible. It splits into irreducible components

$$L^2(S^2)=\oplus W_l.$$

Each W_l is $2l+1$-dimensional. Consider the spherical harmonics Y_l^n, with $l=1,1,\ldots$, $n=-l,-l+1,\ldots,l$. The collection $\{Y_l^m|\ |m|\leqslant l\}$ is an ortho-normal basis of W_l. Thus they are an ortho-normal basis of $L^2(S^2)\ominus\mathbb{C}$. The complete collection $\{Y_l^m\}$ is an ortho-normal basis of $L^2(S^2)$.

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In terms of the Y_l^m the representation U of SO(3) reads

$$\langle Y_l^m | U(\xi) | Y_{l'}^n \rangle = \delta_{l,l'} D_l^{m,n}(\xi),$$

where the $D^{m,n}$ are the Wiegner functions. For $n=0$ we explicitly have

$$\xi = x\phi \Rightarrow D_l^{m,0}(\xi) = Y_l^n(x). \tag{1}$$

That means $D^{m,0}(\xi)$ depends only on the coset $\xi/\mathrm{SO}(2)$ which can identify with a point in S^2.

It is natural to introduce the Fourier coefficients of $s \in L^2(S^2)$ via

$$\hat{s}(l,n) = \langle Y_l^n | s \rangle.$$

Then Plancherel's formula takes on the following form:

$$\int_{S^2} d\Omega(x) \overline{s}(x) r(x) = \sum_{l=0}^{\infty} \sum_{|m| \le l} \overline{\hat{s}(l,m)} \hat{r}(l,m).$$

III. MURENZI WAVELETS ON THE SPHERE

We now present the construction of directional wavelets over the sphere. The problem is that there is no "good" dilation operator on the sphere. This is intuitively clear, since, e.g., dilations along a geodesic around the north pole would create more and more singular functions at the south pole. We therefore will introduce the different scales in a more or less *ad hoc* way.

Let $g_a \in L^2(S^2, d\Omega)$ be a family of functions indexed by a parameter $a>0$. We usually suppose that $a \to g_a$ is Bochner integrable, but for all practical purposes one might suppose-at-least continuity $(a \mapsto g_a) \in C^0(\mathbf{R}_+, L^2(S^2))$.

We then define a wavelet transform of $s \in L^2(S^2, d\Omega)$ with respect to this family of functions as the following set of scalar products:

$$\mathscr{W}[\{g_a\}, s](\xi, a) = \langle U(\xi) g_a | s \rangle, \quad \xi \in \mathrm{SO}(3), \quad a \in \mathbf{R}_+ .$$

We sometimes also write $\mathscr{W}_{\{g_a\}} s$ and if no confusion is possible we simple write $\mathscr{W}_g s$. It is a function over the parameter half-space

$$\mathrm{H} = \mathrm{SO}(3) \times \mathbf{R}_+ .$$

Since the group SO(3) is compact, it is unimodular and hence it has an essentially unique invariant measure denoted by $d\Sigma$. We normalize it such that

$$\int_{\mathrm{SO}(3)} d\Sigma = 4\pi^2,$$

which is possible since SO(3) is compact.

The formal wavelet synthesis with respect to a family $h_a \in L^2(S^2, d\Omega)$ reads now

$$\mathscr{M}[\{h_a\}, T](x) = \int_0^{\infty} \frac{da}{a} \int_{\mathrm{SO}(3)} d\Sigma(\xi) T(\xi, a) (U(\xi) h_a)(x)$$

Again we simply write $\mathscr{M}_{\{h_a\}} r$ or simply $\mathscr{M}_h s$ if no confusion is possible.

Definition III.1: We say a family of functions $g_a \in C^{\infty}(S^2)$ is admissible if the following three conditions are met.

Condition 1 (energy conservation): There is a finite constant c_g, $0<|c_g|<\infty$, such that for all $s\in L^2(S^2)$ with $\int_{S^2} s = 0$ we have

$$\int_{\mathrm{H}} \frac{d\Sigma(\xi)\wedge da}{a} |\mathscr{W}[\{g_a\}, s](\xi,a)|^2 = c_g \int_{S^2} d\Omega(x)|s(x)|^2.$$

Condition 2 (large scale decay): For all $\alpha>0$, there is a finite constant c_α such that for $a>1$ we have

$$|\mathscr{W}[\{g_a\}, s](\xi,a)| \leq c_\alpha a^{-\alpha}.$$

Condition 3 (Euclidian limit): There is a function $g\in L^2(\mathbb{R}^2)$ such that the following limit holds pointwise almost everywhere:

$$\lim_{a\to 0} a^2 g_a(\Phi^{-1}(ax)) = g(x),$$

where $\Phi: S^2\setminus\{0,0-1\}\to\mathbb{R}^2$ is the stereographic projection of the sphere with the south pole removed onto the open two-dimensional plane.

Some comments are in order. Condition 1 says that the wavelet transform is a partial isometry. Condition 2 and 3 allow us to interpret a as a scale parameter: condition 2 says that there are now features at large scale. This is natural since the functions on the sphere live on a compact space. This also is similar to what can be observed on the circle (e.g., Ref. 8). Condition 3 finally tells us that at small scales, the earth is flat; that is, asymptotically a behaves like a dilation parameter as $a\to 0$. Clearly one might be interested in stronger convergence properties depending on the application. The reason why we still want to have at least at small scale a dilation-like behavior is simply the fact that local regularity analysis (e.g., pointwise Hölder continuity) is based on dilations being incorporated into wavelet analysis (e.g., Refs. 9 and 10).

In analogy with the case of wavelet analysis over $\mathbb{R}^2$ we also consider admissible pairs.

Definition III.2: We say that $\{g_a\}$ and $\{h_a\}$ are an admissible analysis reconstruction pair if they satisfy Condition 2 and Condition 3 and if, in addition, Condition 1 is replaced by the following.

Condition 4 (boundedness of wavelet transform): There is a constant c_g such that

$$\int_{\mathrm{H}} \frac{d\Sigma(\xi)\wedge da}{a} |\mathscr{W}[\{g_a\}, s](\xi,a)|^2 \leq c_g \int_{S^2} d\Omega(x)|s(x)|^2.$$

Condition 5 (boundedness of wavelet synthesis): There is a constant c_h such that

$$\int_{S^2} d\Omega(x)|\mathscr{M}_{\{h_a\}}T(x)|^2 \leq c_h \int_{\mathrm{H}} \frac{d\Sigma(\xi)\wedge da}{a} |T(\xi,a)|^2.$$

Condition 6 (inversion formula):

$$\mathscr{M}_{\{h_a\}}\mathscr{W}_{\{g_a\}} = \mathbb{1}.$$

We always have that $\mathscr{M}_{\{g_a\}}$ is the adjoint of $\mathscr{W}_{\{g_a\}}$ as can be formally seen by exchanging the integrals

$$\int_{S^2} d\Omega(x)\overline{(\mathscr{M}_{\{g_a\}})r(x)}s(x) = \int_{\mathrm{H}} \frac{d\Sigma(\xi)\wedge da}{a} r(\xi,a)\mathscr{W}_{\{g_a\}}s(\xi,a).$$

We now want to give sufficient conditions on g_a that ensure that $\{g_a\}$ is admissible.

Theorem III.1: Condition 1 (energy conservation) holds iff $\widehat{g_a}(l,m) = \langle Y_l^m | g_a \rangle_{L^2(S^2,d\Omega)}$ satisfies

$$c_g(l) = \frac{8\pi}{2l+1} \int_0^\infty \frac{da}{a} \sum_{|m|\leq l} |\widehat{g_a}(l,m)|^2 = c_g$$

with some c_g independent of l.

Proof: The proof is essentially the same as for standard wavelet analysis if we restrict ourselves to the invariant subspaces W_l. The general case follows by decomposition into irreducible components.

We come to the details. For fixed $r \in L^2(S^2,d\Omega)$ consider the operator

$$B[r]:s \mapsto \int_{SO(3)} d\Sigma(\xi) \langle U(\xi) r | s \rangle U(\xi) r.$$

It is a bounded operator from $L^2(S^2,d\Omega)$ into itself. In addition, since $d\Sigma$ is invariant under the group translations, it is easy to verify that

$$B[r]U(\xi) = U(\xi)B[r]$$

for all ξ. Thus we have have Schur's lemma, applied to each irreducible subspace W_l,

$$B[r] = \sum_{l=0}^{\infty} c_r(l) \Pi_l,$$

where the Π_l are the projectors on the invariant spaces W_l, and $c_r(l)$ are some constants. To compute the constants we note that the Wiegner functions $D_l^{m,m'}$ are known to satisfy at

$$\int_{SO(3)} d\Sigma(\xi) D_{l_1}^{m_1,m_1'}(\xi)^* D_{l_2}^{m_2,m_2'}(\xi) = \frac{8\pi}{2l_1+1} \delta_{l_1,l_2} \delta_{m_1,m_2} \delta_{m_1',m_2'}.$$

We may take $s = Y_l^0$ and hence

$$c_r(l) = \frac{8\pi}{2l+1} \sum_{|m|\leq l} |\hat{r}(l,m)|^2.$$

Now we have

$$\|\mathscr{W}_{\{g_a\}} s\|^2_{L^2(S^2,d\Omega)} = \int_0^\infty \frac{da}{a} \langle s | B[g_a] s \rangle.$$

Therefore, we have by the previous result

$$\|\mathscr{W}_{\{g_a\}} s\|^2_{L^2(S^2,d\Omega)} = \int_0^\infty \frac{da}{a} \sum_{l=1}^{\infty} c_{g_a}(l) \|\Pi_l s\|^2_{L^2(S^2,d\Omega)}.$$

Therefore conservation of energy holds for all s iff

$$\int_0^\infty \frac{da}{a} c_{g_a}(l) = c_g,$$

independent of l, which is precisely the statement of the theorem. □

Corollary III.1: Condition 4 (boundedness of transform) holds iff there is a constant $c<\infty$ such that $c_g(l)\leq c$. Condition 5 holds iff $c_h(l)\leq c$. Finally Condition 6 holds iff

$$\frac{8\pi}{2l+1}\int_0^\infty \frac{da}{a}\sum_{|m|\leq l}\overline{\widehat{g_a}(l,m)}\widehat{h_a}(l,m)=1.$$

Proof: The first statement is obvious. For the second we note that the wavelet synthesis is the adjoint of the wavelet analysis. Hence it has the same norm. For the last statement it is enough to consider the operator

$$B:s\mapsto\int_{SO(3)}d\Sigma(\xi)\langle U(\xi)g_a|s\rangle U(\xi)h_a$$

and to integrate over a as before. □

Corollary III.2: If g_a and h_a are an admissible analysis-reconstruction pair, then we have the following identity valid for s, $r\in L^2(S^2,d\Omega)$ and $\int s=\int r=0$:

$$\int_0^\infty\frac{da}{a}\int_{SO(3)}d\Sigma(\xi)\overline{\mathscr{W}[\{g_a\},s](\xi,a)}\mathscr{W}[\{h_a\},r](\xi,a)=c_{g,h}\int_{S^2}d\Omega(x)\overline{s(x)}r(x).$$

Proof: Indeed, we may write

$$\langle\mathscr{W}_{\{h_a\}}s|\mathscr{W}_{\{g_a\}}r\rangle_{L^2(SO(3)\times R_+)}=\langle s|\mathscr{M}_{\{h_a\}}\mathscr{W}_{\{g_a\}}r\rangle_{L^2(SO(3)\times R_+)}=\langle s|r\rangle_{L^2(S^2)}.$$

□

Condition 2, the large scale decay, is easy to meet.

Theorem III.2: Condition 2 (large scale decay) holds iff

$$\sum_{l=0}^\infty\sum_{|m|\leq l}|\widehat{g_a}(l,m)|^2\leq O(a^{-\infty}),\quad a\to\infty.$$

Proof: Use Parsevals equation on the sphere. □

As usual, the image is characterized by a reproducing kernel equation

Theorem III.3: Let $g_a,h_a\in L^2(S^2,d\Omega)$ be an analysis-reconstruction pair. Then $T\in$ immag $\mathscr{W}_{\{g_a\}}$ if and only if

$$T(\xi,a)=\int_H\frac{d\Sigma(\rho)\wedge da'}{a'}\Pi_{g,h}(\xi\cdot\rho^{-1},a,a')T(\rho,a'),$$

where

$$\Pi_{g_a,h_a}(\xi,a,a')=\mathscr{W}_{\{g_a\}}h_{a'}(\xi,a).$$

For arbitrary T the right-hand side defines a projector onto immag $\mathscr{W}_g$. In the case $g=h$, this projector is orthogonal.

Proof: This is a standard argument for partial isometries. We may suppose $c_{g,h}=1$. Consider $\Pi=\mathscr{W}_g\mathscr{M}_h$. We have

$$\Pi^2=\mathscr{W}_g(\mathscr{M}_h\mathscr{W}_g)\mathscr{M}_h=\mathscr{W}_g\mathscr{M}_h=\Pi.$$

Thus Π is a projector. Its range lies obviously in immag $\mathscr{W}_g$ and, since $T=\mathscr{W}_g s$ implies

$$\Pi T = \mathscr{W}_g(\mathscr{M}_h \mathscr{W}_g)s = \mathscr{W}_g s = T,$$

the other inclusion holds as well. In the case $g=h$, the operator is self-adjoint. The reproducing formula above follows now by exchanging the integrals in

$$T(\xi,a) = \int_{S^2} d\Omega(x) \int_{\mathrm{H}} \frac{d\Sigma(\rho)\wedge da'}{a'} \overline{U(\xi)g_a(x)} T(\rho,a') U(\rho) h_{a'}(x)$$

$$= \int_{\mathrm{H}} \frac{d\Sigma(\rho)\wedge da'}{a'} T(\rho,a') \langle U(\xi)g_a(x) | U(\rho)h_{a'}(x)\rangle_{L^2(S^2,d\Omega)}.$$

But now

$$\langle U(\xi)g_a(x) | U(\rho)h_a(x)\rangle = \langle U(\rho^{-1}\xi)g_a(x) | h_{a'}(x)\rangle = \mathscr{W}_g h_{a'}(\rho^{-1}\xi, a),$$

and the theorem is proved. □

IV. THE EUCLIDEAN LIMIT

The Euclidean limit is the most interesting constraint. Here we proceed as follows. Let $S_0(\mathbb{R}^2)$ be the subspace of the class of Schwartz of functions g for which all moments vanish ($\alpha \in \mathbb{N}^2$):

$$\int_{\mathbb{R}^2} d^2x\, x^\alpha g(x) = 0 \Leftrightarrow \hat{g}(k) = O(k^\infty) \quad (k \to 0).$$

We choose this context for convenience only. As the proofs will show, larger function spaces are possible. We now want to find an admissible family $g_a \in S_0(\mathbb{R}^2)$ that satisfies the Eucledian limit in the sense that we have pointwise

$$\lim_{a\to 0} a^2 g_a(a\theta,\phi) = g(\theta,\phi).$$

On the left-hand side we have local spherical coordinates, whereas on the right-hand side we have polar coordinates. That is we have written g as $g=g(r,\phi)$ with $r>0$ and $\phi \in [0, 2\pi)$. Note that for the case of pointwise convergence, any local coordinate system will produce equivalent results provided it agrees in first order at the north pole with the coordinate system given through stereographic projection. However, if one wants to consider topologies involving estimates of derivatives, the order of contact must be higher than first order. For the sake of simplicity we will only work out the case of pointwise convergence.

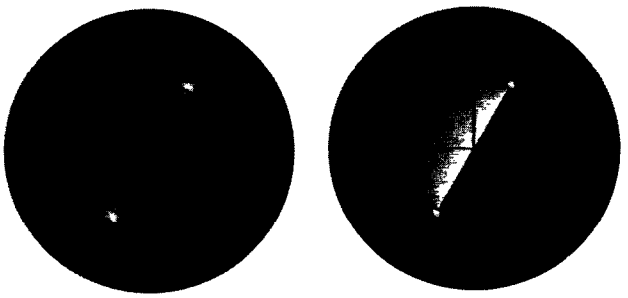

FIG. 1. The modulus and the phase at scale $a=4$.

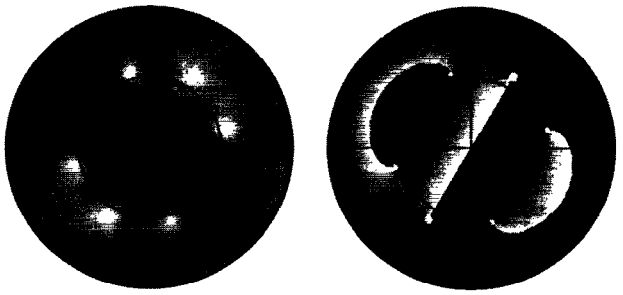

FIG. 2. The modulus and the phase at scale $a=2$.

We now come to the construction. Take the two-dimensional Fourier transform of g and write it in polar coordinates, $\hat{g}=\hat{g}(k,\phi)$. Decompose for each k into a Fourier series

$$\hat{g}(k,\varphi)=\frac{1}{2\pi}\sum_{n\in Z}\hat{\gamma}(k,n)e^{in\varphi},\quad \hat{\gamma}(r,n)=\int_0^{2\pi}d\varphi\ \hat{g}(k,\varphi)e^{-in\varphi}.$$

We first shall prove that the Euclidean limit holds for the following family of functions:

$$g_a=\sum_{l=0}^{\infty}\sum_{|m|\leqslant l}\widehat{g_a}(l,m)Y_l^m,\quad \widehat{g_a}(l,m)=\sqrt{l}\,\hat{\gamma}(al,m).$$

Later we modify this family slightly to make it admissible.

That the Euclidean limit holds can be observed numerically by looking at Figs. 1–5, where the scale of the Morlet wavelet changes from $a=2$ to $a=\frac{1}{4}$. The thick outermost circle corresponds to the south pole. The inner circle is the equator. The center of the picture is the north pole. In all figures we have fixed the rotation around the north pole to $2\pi/3$.

We come to the details. As we did before let us also write g in polar coordinates, $g=g(r,\phi)$, $r>0$, $\phi\in[0,2\pi)$, and let us introduce the Fourier coefficients with respect to ϕ:

$$g(r,\phi)=\frac{1}{2\pi}\sum_{n\in Z}\gamma(r,n)e^{in\phi},\quad \gamma(r,n)=\int_0^{2\pi}d\phi\ \hat{g}(r,\phi)e^{-in\phi}.$$

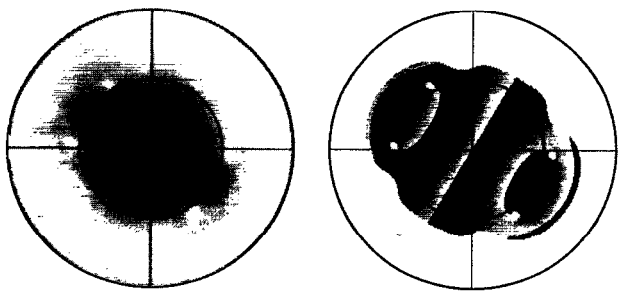

FIG. 3. The modulus and the phase at scale $a=1$.

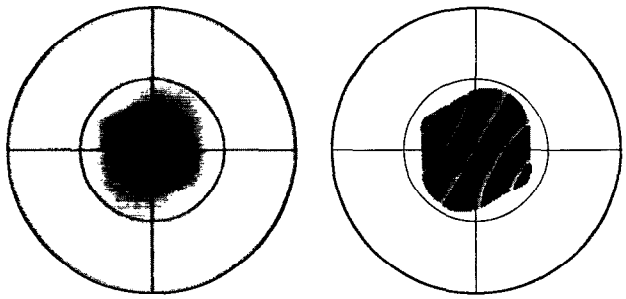

FIG. 4. The modulus and the phase at scale $a=\frac{1}{2}$.

Lemma IV.1: The following relation holds,

$$\hat{\gamma}(k,n)=\int_0^\infty r\,dr\;\gamma(r,n)J_n(kr).$$

where J_n is the nth-order Bessel function.

Proof: The Fourier transform of g reads in spherical coordinates $k>0$, $\phi\in[0,2\pi)$,

$$\begin{aligned}\hat{g}(k,\phi)&=\int_0^\infty r\,dr\int_0^{2\pi}d\varphi\;g(r,\varphi)e^{-ikr\cos(\phi-\varphi)}\\&=\frac{1}{2\pi}\sum_{n\in Z}\int_0^\infty r\,dr\int_0^{2\pi}d\varphi\;\gamma(r,n)e^{-i(kr\cos(\phi-\varphi)+n\varphi)}\\&=\frac{1}{2\pi}\sum_{n\in Z}e^{in\phi}\int_0^\infty r\,dr\int_0^{2\pi}d\varphi\;\gamma(r,n)e^{-i(kr\cos(\varphi)+n\varphi)}\\&=\frac{1}{2\pi}\sum_{n\in Z}\int_0^\infty r\,dr\;\gamma(r,n)J_n(kr)e^{in\phi}.\end{aligned}$$

Upon identifying the terms of both expressions, the expansion coefficients γ and $\hat{\gamma}$ are related as stated in the lemma.

Now the following limit is known to hold uniformly for $\theta\in I$, compact (see, e.g., Ref. 11):

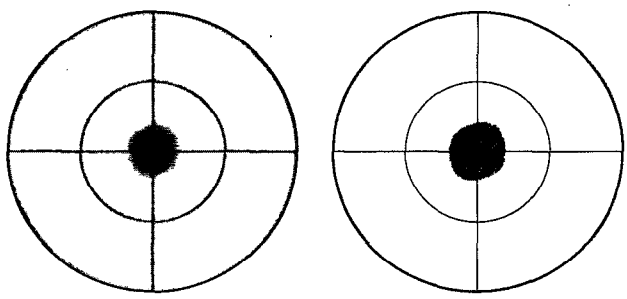

FIG. 5. The modulus and the phase at scale $a=\frac{1}{4}$.

$$\lim_{l\to\infty}\sqrt{\frac{2\pi}{l}}\,Y_l^m(\theta/l,\phi)=J_m(\theta)e^{im\phi}.$$

We now propose to look at the limit $a\to 0$ in

$$a^2\sum_{l=0}^{\infty}\sum_{|m|\le l}\hat{\gamma}(al,m)l^{-1/2}Y_l^m(a\theta,\phi).$$

Note that

$$\sum_{|m|\le l}|Y_l^m|^2=\frac{2l+1}{4\pi}.$$

Therefore, by Schwarz's inequality, discarding a term smaller than $a^2\epsilon$, we may suppose that g such that $\hat{g}$ is supported by a corona $c_1\le|k|\le c_2$. Now as a gets small, the l that contribute to the sum get large since al stays in $[c_1, c_2]$. We thus can use the above asymptotic for Y_l^m without changing the limit, and we obtain

$$a\sum_{l=0}^{\infty}\sum_{|m|\le l}(al)\hat{\gamma}(al,m)J_m(al\theta)e^{im\phi}.$$

As $a\to 0$, the sum over l may be replaced by a Riemann integral and we obtain as limit $(al\to r, a\to dr)$

$$\frac{1}{2\pi}\sum_{m\in\mathbb{Z}}\int_0^{\infty}r\,dr\,\hat{\gamma}(r,m)J_m(r\theta)e^{im\phi}.$$

By the Fourier inversion formula (Lemma IV.1) this equals $g(\theta,\phi)$ in polar coordinates.

V. AN ADMISSIBLE FAMILY

We now modify the family slightly to make it admissible. Consider again a function $g\in S_0(\mathbb{R}^2)$. Then let as before

$$\hat{\gamma}(k,m)=\int_0^{2\pi}d\phi\;\hat{g}(k,\phi)e^{-im\phi}$$

Now set

$$g_a=\sum_{l=0}^{\infty}\sum_{|m|\le l}\widehat{g_a}(k,m)Y_l^m$$

with

$$\widehat{g_a}(k,m)=\frac{\hat{\gamma}(al,m)}{\sqrt{\dfrac{8\pi^2}{2l+1}\displaystyle\int_0^{\infty}\frac{da'}{a'}\sum_{|m|\le l}|\hat{\gamma}(a',m)|^2}}.$$

Theorem V.1: The $\{g_a\}$ is an admissible family.

Proof: Clearly Conditions 1 and 2 are satisfied. To show that the Euclidian limit holds we note that by Parsevals equation we have for $l\to\infty$

$$\int_0^\infty \frac{da}{a} \sum_{|m|\leq l} \to \int_0^\infty \frac{da'}{a'} \int_0^{2\pi} |\hat{g}(a',\phi)|^2 = \int_{\mathbb{R}^2} \frac{d^2k}{|k|^2} |\hat{g}(k)|^2.$$

Note that the integral on the right-hand side is the admissibility condition of Murenzi.[1] It therefore follows that

$$\sqrt{l}\,\hat{\gamma}(al,m) \to \widehat{g_a}(l,m),$$

as it should.

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Quantization of differential calculi on universal enveloping algebras

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A method to construct differential calculi on quantized universal enveloping algebras is discussed. These differential calculi are obtained by quantizing calculi on "classical" enveloping algebras provided with appropriate co-Poisson structures. The procedure is demonstrated by applying it to the standard quantizations of the Heisenberg algebra and the algebra $gl(2)$. © *1996 American Institute of Physics.* [S0022-2488(96)04206-5]

I. INTRODUCTION

Noncommutative differential geometry, currently a field of active research, deals with differential calculus on algebras which are generally noncommutative. There are a few basic principles to construct such a noncommutative theory. One can replace the commutative function algebra on a space by some noncommutative algebra and try to generalize the basic concepts of the traditional case to this more abstract situation. Then there is the approach, already standard in algebraic geometry, to encode the structure of the underlying space into the function algebra defined on the space, which in turn is deformed. This is the approach customary in quantum group theory. These ideas led Connes (see, e.g., Ref. 1) and his collaborators to create "noncommutative geometry." Here, the commutative function algebra is replaced by some noncommutative C^*-algebra.

In quantum group theory it was Woronowicz,[2] who first developed the theory of differential calculus on quantum groups, giving a very interesting example of noncommutative differential geometry. This rather abstract theory has been reformulated in more concrete terms by Wess and Zumino.[3] A substantial number of very interesting papers, proposing other approaches, elucidating various aspects, studying concrete examples or dealing with applications have been written since. See, e.g., Refs. 4–7.

In this paper we discuss a method to construct a differential calculus on a quantized universal enveloping algebra $U_h(\mathfrak{g})$ of a Lie algebra $\mathfrak{g}$. We follow the idea of Faddeev and his school[8] that all objects of a quantized theory should appear naturally as a result of quantization of appropriate Poisson structures. Accordingly, our starting point should be a differential calculus on $U(\mathfrak{g})$. These differential calculi are provided and studied in Ref. 9. Moreover, they turn out to be Hopf algebras and actually such a differential calculus turns out to be the universal enveloping algebra of a color Lie superalgebra, see Ref. 10. Consequently, our starting point is this enveloping algebra $U(L)$ equipped with an appropriate co-Poisson bracket δ. Its restriction to L, notation δ_L, defines a color Lie bisuperalgebra structure which may be obtained by extending the cocommutator $\delta_{\mathfrak{g}}$ of $\mathfrak{g}$.

The procedure is illustrated by two examples. We apply it to the standard quantizations of the enveloping algebra of the Heisenberg algebra and the algebra $gl(2)$.

Matrix quantum groups can be embedded as Hopf algebra in a quantization of the enveloping algebra of the dual Lie algebra, see Ref. 11. This indicates that our construction can be used to obtain differential calculi on quantum groups. Work on this is in progress; we will report on this in the near future.

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II. THE QUANTIZATION METHOD

Let $\mathfrak{g}$ be a finite dimensional Lie algebra over the field of complex numbers C. We present a procedure to construct differential calculi on quantized universal enveloping algebras of $\mathfrak{g}$ by quantizing differential calculi on the classical universal enveloping algebra $U(\mathfrak{g})$. This method connects the following two concepts related to $U(\mathfrak{g})$: quantization and differential calculus. In the classical limit the inter-relation between these concepts is expressed by a compatibility condition between the cocommutator that determines the Lie bialgebra structure on $\mathfrak{g}$ and the differential d. In order to explain the origin of this compatibility condition we shortly recall some notions related to differential calculi and quantization.

A quantization of the Lie algebra $\mathfrak{g}$ is a Hopf algebra deformation $U_h(\mathfrak{g})$ of $U(\mathfrak{g})$. Usually, $U_h(\mathfrak{g})$ is called a quantized universal enveloping algebra. The map δ defined by

$$\delta(x)=\frac{\Delta_h(x)-\Delta_h^{\mathrm{op}}(x)}{h} \bmod h \qquad \delta: U(\mathfrak{g})\mapsto U(\mathfrak{g})\otimes U(\mathfrak{g}) \tag{2.1}$$

is a co-Poisson bracket on $U(\mathfrak{g})$. In this formula Δ_h represents the comultiplication of $U_h(\mathfrak{g})$ and Δ_h^{op} the opposite comultiplication given by $\Delta_h^{\mathrm{op}}=\sigma\circ\Delta_h$, where σ is the ordinary flip operator on the tensor product. The restriction of δ to $\mathfrak{g}$, which will be denoted by $\delta_{\mathfrak{g}}$, defines a Lie bialgebra $(\mathfrak{g},\delta_{\mathfrak{g}})$. This means that $\delta_{\mathfrak{g}}:\mathfrak{g}\mapsto\mathfrak{g}\otimes\mathfrak{g}$ is a 1-cocycle and $\delta_{\mathfrak{g}}^*:\mathfrak{g}^*\mapsto\mathfrak{g}^*\otimes\mathfrak{g}^*$ is a Lie bracket on $\mathfrak{g}^*$. The Lie bialgebra $(\mathfrak{g},\delta_{\mathfrak{g}})$ is called the classical limit of the quantization $U_h(\mathfrak{g})$ and $\delta_{\mathfrak{g}}$ is called the cocommutator. For more details on this we refer to Ref. 12.

A differential Hopf algebra (see, e.g., Ref. 13) is an N-graded Hopf algebra $\Omega=\Sigma_{p=0}^{\infty}\Omega^p$ equipped with a differential d. This operator d is a graded derivation of degree $+1$ with the property $d^2=0$. Furthermore it satisfies $(d\otimes id+\tau\otimes d)\circ\Delta=\Delta\circ d$ and $\epsilon\circ d=0$, where Δ denotes the comultiplication and ϵ the counit of Ω. The linear map $\tau:\Omega\to\Omega$ has degree zero and satisfies $\tau(a)=(-1)^p a$ for all $a\in\Omega^p$. A differential calculus on $U(g)$ is a differential Hopf algebra Ω with the additional properties $\Omega^0=U(\mathfrak{g})$ and Ω is generated by $\Omega^0\cup d(\Omega^0)$.

In Ref. 10 we showed that a differential calculus on $U(\mathfrak{g})$ of Poincaré–Birkhoff–Witt-type can be described as the universal enveloping algebra of a color Lie superalgebra L which is a natural extension of the Lie algebra $\mathfrak{g}$. For the sake of clarity, we recall the definition of color Lie superalgebra (see Ref. 14). Let G be an abelian semigroup and α a 2-cocycle on G with values in C*. An (α)-color Lie superalgebra is a G-graded algebra L with product $[,]$ satisfying

$$[x,y]=-\alpha(p,q)[y,x] \quad \text{and} \quad \alpha(p,r)[[x,y],z]+\alpha(q,p)[[y,z],x]+\alpha(r,q)[[z,x],y]=0$$

for all $x\in L^p, y\in L^q, z\in L^r$. As in the case of ordinary Lie algebras, one can define the universal enveloping algebra of a color Lie superalgebra and a corresponding Hopf algebraic structure on it. The structure of the above mentioned color Lie superalgebra L, which represents the differential calculus on $U(\mathfrak{g})$, is as follows. L is the N-graded algebra $L=\oplus_{p\in\mathrm{N}}L^p$, where $L^0=\mathfrak{g}=\langle x^1,x^2,\ldots,x^n\rangle$, $L^1=\langle\hat{x}^1,\hat{x}^2,..,\hat{x}^n\rangle$, and $L^p=0$ for all $p\geq 2$. The corresponding 2-cocycle α is given by

$$\alpha:\mathrm{N}\times\mathrm{N}\to\mathrm{C}^* \qquad \alpha(p,q)=(-1)^{pq}.$$

The Lie bracket of L is such that its restriction to L^0 is simply the Lie bracket of $\mathfrak{g}$ and the linear map $d:L\mapsto L$ given by $d(x_i)=\hat{x}_i$ and $d(\hat{x}_i)=0$ for all $1\leq i\leq n=\dim(\mathfrak{g})$ is a graded derivation of degree $+1$ on L. So the bracket of L is of the following form:

$$[x_i,x_j]=c_{ij}^k x_k; \quad [x_i,\hat{x}_j]=a_{ij}^k\hat{x}_k; \quad [\hat{x}_i,\hat{x}_j]=0.$$

We use the notation $\hat{x}_i$ to emphasize the fact that these elements have been formally introduced to represent the differentials of the elements x_i. The differential d on $\Omega=U(L)$ is defined as the unique graded derivation extending the operator d on L.

We come to the introduction of a differential calculus on $U_h(\mathfrak{g})$. According to the foregoing, a differential calculus on $U_h(\mathfrak{g})$ is a differential Hopf algebra Ω_h, with differential denoted by d_h, which is generated by $\Omega_h^0 \cup d_h(\Omega_h^0)$, where $\Omega_h^0=U_h(\mathfrak{g})$. On the other hand, as analog to the quantization procedure, it is natural that, by putting h equal to zero, Ω_h reduces to $U(L)$, where L is a color Lie superalgebra extension of $\mathfrak{g}$ of the form described above, and d_h reduces to the differential d of $U(L)$. This implies that (Ω_h, d_h) is a differential Hopf algebra deformation of $(U(L),d)$. We demand this deformation to be homogeneous of degree zero such that the N-grading of $U(L)$ induces the N-grading on $U_h(L)$. In particular $\Omega_h=U_h(L)$ is a Hopf algebra deformation of $U(L)$, or in other words a quantization of the color Lie superalgebra L. The classical limit of this quantization is a color Lie bisuperalgebra (L,δ_L) extending the Lie bialgebra $(\mathfrak{g},\delta_{\mathfrak{g}})$, which is the classical limit of $U_h(\mathfrak{g})$. This gives rise to the following commutative diagram:

$$\begin{array}{ccc} U_h(\mathfrak{g}) & \rightarrow & U_h(L) \\ \downarrow & & \downarrow \\ (g,\delta_{\mathfrak{g}}) & \rightarrow & (L,\delta_L) \end{array}$$

The vertical arrows denote the classical limit and the horizontal ones denote the canonical embeddings of (N-graded) Hopf algebras and color Lie bisuperalgebras.

We denote the comultiplication of $U_h(L)$ by Δ_h. From the definition of a differential Hopf algebra we know that $\Delta_h \circ d_h=(d_h)_{\otimes}\circ\Delta_h$ with $(d_h)_{\otimes}=d_h\otimes id+\tau\otimes d_h$. The co-Poisson bracket $\delta: U(L)\mapsto U(L)\otimes U(L)$ is defined as in the classical case described in formula (2.1), with the exception that, in the definition of Δ_h^{op} the operator σ denotes the graded flip operator, which is defined by

$$\sigma(x\otimes y)=(-1)^{pq}y\otimes x \quad \text{for all} \quad x\in U_h(L)^p, y\in U_h(L)^q.$$

One can easily verify that d_h has the property $\sigma\circ(d_h)_{\otimes}=(d_h)_{\otimes}\circ\sigma$. From this it follows that

$$\frac{\Delta_h-\Delta_h^{\mathrm{op}}}{h}\circ d_h=(d_h)_{\otimes}\circ\frac{\Delta_h-\Delta_h^{\mathrm{op}}}{h}$$

and for h equal to zero this reduces to

$$\delta\circ d=d_{\otimes}\circ\delta,$$

so the differential operator should commute with the co-Poisson bracket δ on $U(L)$. The restriction to L yields the following condition for the cocommutator δ_L:

$$\delta_L\circ d=d_{\otimes}\circ\delta_L. \tag{2.2}$$

To understand the meaning of this condition, let us assume we have a color Lie superalgebra L equipped with an operator d representing a differential calculus on $U(\mathfrak{g})$. Any Lie bialgebra $(\mathfrak{g},\delta_{\mathfrak{g}})$ gives rise to a unique extension $\delta_L: L\mapsto L\otimes L$ satisfying condition (2.2). We call the differential calculus on $U(\mathfrak{g})$ and the Lie bialgebra $(\mathfrak{g},\delta_{\mathfrak{g}})$ compatible if and only if (L,δ_L) is a color Lie bisuperalgebra. From the preceding reasoning we learn that this is a necessary condition in order to obtain a differential calculus on $U_h(\mathfrak{g})$ starting from the differential calculus on $U(\mathfrak{g})$ given by L. The examples we have studied so far seem to indicate that the condition is also sufficient.

Thus from the discussion above we can subtract the following procedure to construct a differential calculus on a quantized universal enveloping algebra.

(1) Construct a differential calculus on $U(\mathfrak{g})$.
(2) Compute a Lie bialgebra $(\mathfrak{g},\delta_{\mathfrak{g}})$ which is compatible with the constructed differential calculus.
(3) Quantize $(\mathfrak{g},\delta_{\mathfrak{g}})$, i.e., construct a quantized universal enveloping algebra $U_h(\mathfrak{g})$ with classical limit $(\mathfrak{g},\delta_{\mathfrak{g}})$.
(4) Quantize (L,δ_L) where δ_L is the unique extension of $\delta_{\mathfrak{g}}$ given by formula (2.2).

Note that in the last step one can fruitfully use that $U_h(L)$ is an extension of $U_h(\mathfrak{g})$ and that the differential d_h should respect the defining relations of $U_h(L)$. We will illustrate this in more detail in the examples.

Finally, we mention that there is a nice algebraic interpretation for the compatibility condition (2.2). The linear operator d on L is a graded derivation, this means that

$$d([x,y])=[d(x),y)]+(-1)^p[x,d(y)] \quad \text{for } x\in L^p, y\in L,$$

or equivalently $[,]\circ d_{\otimes}=d\circ[,]$, where $[,]$ denotes the Lie bracket of L. Analogously, the linear operator d^* is a graded derivation on L^* with Lie bracket δ_L^* if it satisfies $\delta_L^*\circ(d^*)_{\otimes}=d^*\circ\delta_L^*$. But this is equivalent to Eq. (2.2). So we can express the compatibility condition appropriately by saying that d should be a color Lie bisuperalgebra derivation on (L,δ_L).

III. THE HEISENBERG ALGEBRA

As first example, we will consider the Heisenberg algebra H. A basis of H is given by $\{p,q,c\}$ and the Lie product is given by

$$[p,q]=c; \quad [p,c]=0; \quad [q,c]=0.$$

A. The differential calculus on $U(H)$

In Ref. 9 we constructed all differential calculi $\Omega=\Sigma_{p=0}^{\infty}\Omega^p$ of Poincaré–Birkhoff–Witt-type on H. Here, $\Omega^0=U(H)$ and Ω^p denotes the space of p-forms; in particular $\Omega^1=d(\Omega^0)$. As we described in Sec. II, Ω is isomorphic to $U(L)$, where L is a color Lie superalgebra such that $L^0=H$ and $L^1=\hat{H}$. In particular, the differential calculus is completely determined by the map $\rho:H\to gl(\hat{H})$, which is in fact the commutator in L of elements from L_0 and L_1. (L_1 is a representation of L_0 using the commutator). As basis of $\hat{H}$ we will use $\{\hat{p},\hat{q},\hat{c}\}$, where $d(x)$ denotes the element $\hat{x}$. It turns out that the simplest and most elegant solution is described by

$$\rho(p)(q)=[p,\hat{q}]=\tfrac{1}{2}\hat{c}, \quad \rho(q)(p)=[q,\hat{p}]=-\tfrac{1}{2}\hat{c},$$

and all others equal to zero.

Summarizing we start with the quotient of the free N-graded associative algebra on the alphabet $\{p,q,c,\hat{p},\hat{q},\hat{c}\}$, where $\{p,q,c\}$ are homogeneous of degree 0 and $\{\hat{p},\hat{q},\hat{c}\}$ are homogeneous of degree 1, divided by the ideal I which is generated by the following homogeneous relations:

$$pq-qp=c; \quad pc-cp=0; \quad qc-cq=0$$

$$p\hat{p}=\hat{p}p; \quad p\hat{q}=\hat{q}p+\tfrac{1}{2}\hat{c}; \quad p\hat{c}=\hat{c}p$$

$$q\hat{p}=\hat{p}q-\tfrac{1}{2}\hat{c}; \quad q\hat{q}=\hat{q}q; \quad q\hat{c}=\hat{c}q$$

$$c\hat{p}=\hat{p}c; \quad c\hat{q}=\hat{q}c; \quad c\hat{c}=\hat{c}c$$

$$\hat{p}\hat{q}=-\hat{q}\hat{p}; \quad \hat{p}\hat{c}=-\hat{c}\hat{p}; \quad \hat{q}\hat{c}=-\hat{c}\hat{q}$$

$$\hat{p}\hat{p}=0; \quad \hat{q}\hat{q}=0; \quad \hat{c}\hat{c}=0.$$

The differential d is the unique graded derivation of degree $+1$ satisfying $d(p)=\hat{p}$, $d(q)=\hat{q}$, $d(c)=\hat{c}$ and $d(\hat{p})=0$, $d(\hat{q})=0$, $d(\hat{c})=0$.

B. The compatible cocommutator on H

Next we have to construct a Lie bialgebra structure on H, which is compatible with d. This is a matter of straight computation, which we performed using computer algebra. There is a unique solution, given by

$$\delta(c)=0; \quad \delta(p)=p\wedge c; \quad \delta(q)=q\wedge c;$$

and consequently the continuation to $\hat{H}=d(H)$, which is prescribed by $\delta(\hat{x})=(d\otimes id+\tau\otimes d)\circ\delta(x)$, yields

$$\delta(\hat{c})=0; \quad \delta(\hat{p})=\hat{p}\wedge c+p\wedge\hat{c}; \quad \delta(\hat{q})=\hat{q}\wedge c+q\wedge\hat{c}.$$

Note that the restriction of δ to H is a cocommutator of coboundary type with corresponding R-matrix

$$R=p\wedge q. \tag{3.1}$$

One can easily verify that δ itself is not of coboundary type.

C. Quantization of (H,δ)

In order to quantize the situation above, we note that the R-matrix (3.1) is the standard one. This suggests that we can take for $U_h(H)$ the standard quantization

$$\Delta_h(p)=p\otimes e^{hc}+1\otimes p; \quad \Delta_h(q)=q\otimes 1+e^{-hc}\otimes q; \quad \Delta_h(c)=c\otimes 1+1\otimes c$$

and the only relation in $U_h(H)$ that differs from the relations in $U(H)$ is

$$[p,q]=\frac{\sinh(hc)}{\sinh(h)}.$$

The unit and counit are unchanged. The antipode is rather easy to compute, from Ref. 12 we know that it exists. For example to calculate $S_h(p)$, we consider

$$0=\mu_h\circ(S_h\otimes id)\circ\Delta_h(p)=S_h(p)e^{hc}+p.$$

Hence we find

$$S_h(p)=-pe^{-hc}$$

and similarly

$$S_h(q)=-qe^{hc}; \quad S_h(c)=-c.$$

Although $U_h(H)$ is clearly not cocommutative, one can easily verify that the antipode still satisfies $S_h^2=Id$.

D. Quantization of (L,δ)

From here on we will use $\hat{x}$ to denote the element $d_h(x)$. Due to $\Delta_h\circ d_h=(d_h)_\otimes\circ\Delta_h$, we have $\Delta_h(\hat{c})=\hat{c}\otimes 1+1\otimes\hat{c}$ and

$$\Delta_h(\hat{p})=\hat{p}\otimes e^{hc}+p\otimes h\hat{c}e^{hc}+1\otimes\hat{p};\quad \Delta_h(\hat{q})=\hat{q}\otimes 1+e^{-hc}\otimes\hat{q}-h\hat{c}e^{-hc}\otimes q.$$

It remains to determine the new relations in Ω_h; since $\Delta_h(c)$ and $\Delta_h(\hat{c})$ are unchanged it is natural to require that only the relations $[p,\hat{q}]$, $[\hat{p},q]$, and $[\hat{p},\hat{q}]$ will change.

So, let us assume that $[p,\hat{q}]=\alpha_1$ and $[\hat{p},q]=\alpha_2$. From $[p,q]=[\sinh(hc)]/[\sinh(h)]$ it follows that

$$\alpha_1+\alpha_2=[p,\hat{q}]+[\hat{p},q]=d_h([p,q])=h\hat{c}\,\frac{\cosh(hc)}{\sinh(h)}. \tag{3.2}$$

Further we have

$$\Delta_h(\alpha_1)=\Delta_h(p\hat{q}-\hat{q}p)=(p\otimes e^{hc}+1\otimes p)(\hat{q}\otimes 1-h\hat{c}e^{-hc}\otimes q+e^{-hc}\otimes\hat{q})-(\hat{q}\otimes 1-h\hat{c}e^{-hc}\otimes q$$
$$+e^{-hc}\otimes\hat{q})(p\otimes e^{hc}+1\otimes p)=[p,\hat{q}]\otimes e^{hc}-h\hat{c}e^{-hc}\otimes[p,q]+e^{-hc}\otimes[p,\hat{q}]$$

so,

$$\Delta_h(\alpha_1)=\alpha_1\otimes e^{hc}-h\hat{c}e^{-hc}\otimes\frac{\sinh(hc)}{\sinh(h)}+e^{-hc}\otimes\alpha_1. \tag{3.3}$$

In the same way we find for α_2

$$\Delta_h(\alpha_2)=\alpha_2\otimes e^{hc}+\frac{\sinh(hc)}{\sinh(h)}\otimes h\hat{c}e^{-hc}+e^{-hc}\otimes\alpha_2. \tag{3.4}$$

Equations (3.2), (3.3), and (3.4) suggest to take

$$\alpha_i=\frac{\lambda_i e^{hc}+\mu_i e^{-hc}}{\sinh(h)}\,h\hat{c};\quad (i=1,2).$$

Substitution yields a unique solution

$$[p,\hat{q}]=h\hat{c}\,\frac{e^{-hc}}{2\sinh(h)};\quad [\hat{p},q]=h\hat{c}\,\frac{e^{hc}}{2\sinh(h)}. \tag{3.5}$$

This also dictates the relation between $\hat{p}$ and $\hat{q}$ by differentiation of Eq. (3.5)

$$\hat{p}\hat{q}=-\hat{q}\hat{p}.$$

Finally, from $S_h\circ d_h=d_h\circ S_h$ it follows that the extension of the antipode is given by

$$S_h(\hat{p})=-(\hat{p}-hp\hat{c})e^{-hc};\quad S_h(\hat{q})=-(\hat{q}+hq\hat{c})e^{hc};\quad S_h(\hat{c})=-\hat{c}.$$

It still satisfies $S_h^2=Id$. In order to compute the action of S_h on an arbitrary element of Ω_h, one can use linearity and the antialgebra-morphism property

$$S_h(ab)=(-1)^{rs}S_h(b)S_h(a);\quad (a\in\Omega^r,b\in\Omega^s).$$

E. Summary of results for *H*

For clearness' sake, we summarize the results of this section in the following theorem.

Theorem 1: *The standard quantization of the Heisenberg algebra H, given by*

$$[p,q]=\frac{\sinh(hc)}{\sinh(h)};\quad [p,c]=0;\quad [q,c]=0$$

and

$$\Delta_h(p)=p\otimes e^{hc}+1\otimes p;\quad \Delta_h(q)=q\otimes 1+e^{-hc}\otimes q;\quad \Delta_h(c)=c\otimes 1+1\otimes c$$
$$S_h(p)=-pe^{-hc};\quad S_h(q)=-qe^{hc};\quad S_h(c)=-c$$

admits a differential calculus d_h. If we denote $d_h(x)$ by $\hat{x}$ for all elements x in H, then $\hat{c}$ is primitive and

$$\Delta_h(\hat{p})=\hat{p}\otimes e^{hc}+p\otimes h\hat{c}e^{hc}+1\otimes\hat{p};\quad \Delta_h(\hat{q})=\hat{q}\otimes 1+e^{-hc}\otimes\hat{q}-h\hat{c}e^{-hc}\otimes q$$
$$S_h(\hat{p})=-(\hat{p}-hp\hat{c})e^{-hc};\quad S_h(\hat{q})=-(\hat{q}+hq\hat{c})e^{hc}.$$

The commutation between functions and forms is described by

$$[p,\hat{q}]=h\hat{c}\,\frac{e^{-hc}}{2\sinh(h)};\quad [q,\hat{p}]=-h\hat{c}\,\frac{e^{hc}}{2\sinh(h)}$$

and $[x,\hat{y}]=0$ for all other choices of elements x and y from $\{p,q,c\}$. Finally, the commutation of forms is determined by the relation $\hat{x}\hat{y}=-\hat{y}\hat{x}$ for all $x,y\in H$.

Finally, we remark that by an obvious and small modification the same result is obtained for the general $2n+1$-dimensional Heisenberg algebra with basis $\{p_i,q_i,c\}_{1\leqslant i\leqslant n}$ and Lie product given by

$$[p_i,q_j]=\delta_j^i c;\quad [p_i,c]=0;\quad [q_i,c]=0;\quad [p_i,p_j]=0;\quad [q_i,q_j]=0.$$

IV. THE ALGEBRA *gl*(2)

The next example that we consider is $gl(2)$. We will denote

$$E_+=E_{12};\quad E_-=E_{21};\quad H_+=E_{11};\quad H_-=E_{22}.$$

Hence in the enveloping algebra $U(gl(2))$, we have the following relations:

$$[H_+,H_-]=0;\quad [H_+,E_\pm]=\pm E_\pm;\quad [H_-,E_\pm]=\mp E_\pm;\quad [E_+,E_-]=H_+-H_-.$$

A. The differential calculus on *U*(*gl*(2))

On $U(gl(2))$ we can construct differential calculi of Poincaré–Birkhoff–Witt type; as said in the previous sections, these calculi are completely determined by an appropriate representation $\rho: gl(2)\to\widehat{gl(2)}$. For $gl(n)$ there is a natural solution, namely,

$$\rho(x)\hat{y}=\widehat{xy},$$

where xy denotes the product of x and y as $n\times n$ matrices. We will use this ρ in the sequel. Hence we can determine the differential calculus Ω. Apart from the relations above, it satisfies the following relations ($\hat{x}=d(x);\ x\in gl(2)$):

$$[H_\pm,\hat{E}_\pm]=\hat{E}_\pm;\quad [H_\pm,\hat{E}_\mp]=0;\quad [H_\pm,\hat{H}_\pm]=\hat{H}_\pm;\quad [H_\pm,\hat{H}_\mp]=0$$
$$[E_\pm,\hat{E}_\pm]=0;\quad [E_\pm,\hat{E}_\mp]=\hat{H}_\pm;\quad [E_\pm,\hat{H}_\pm]=0;\quad [E_\pm,\hat{H}_\mp]=\hat{E}_\pm.$$

Note the similar roles that H_+ and H_- play; hence the basis chosen (instead of H_+-H_- and H_++H_-) is very natural. One can note that the representation ρ is the direct sum of two 2-dimensional $gl(2)$-representations V_1 and V_2, where $V_1=\langle\hat{E}_+,\hat{H}_-\rangle$ and $V_2=\langle\hat{E}_-,\hat{H}_+\rangle$.

B. The compatible cocommutator on $gl(2)$

Again compatible Lie bialgebra structures can be computed. There is a unique solution if we demand the solution to be homogeneous of degree zero with respect to the natural grading on $gl(2)$ defined by $|H_\pm|=0$, $|E_\pm|=\pm 1$. This solution is given by

$$\delta(H_\pm)=0;\quad \delta(E_+)=E_+\wedge H_-;\quad \delta(E_-)=H_+\wedge E_-$$

which extends to L as

$$\delta(\hat{H}_\pm)=0;\quad \delta(\hat{E}_+)=\hat{E}_+\wedge H_-+E_+\wedge\hat{H}_-;\quad \delta(\hat{E}_-)=\hat{H}_+\wedge E_-+H_+\wedge\hat{E}_-.$$

As in the case of the Heisenberg algebra, δ itself is not of coboundary type. Its restriction to $gl(2)$ is coboundary, the corresponding R-matrix is given by $R=\frac{1}{2}(E_+\wedge E_-+H_+\wedge H_-)$.

C. Quantization of $(gl(2),\delta)$

The way of quantizing is similar as in the case of the Heisenberg algebra. Again $\delta(H_\pm)=0$ suggests to take

$$\Delta_h(H_\pm)=H_\pm\otimes 1+1\otimes H_\pm.$$

Similarly $\delta(E_+)=E_+\wedge H_-$ and $\delta(E_-)=H_+\wedge E_-$ suggest

$$\Delta_h(E_+)=E_+\otimes e^{hH_-}+1\otimes E_+;\quad \Delta_h(E_-)=E_-\otimes 1+e^{hH_+}\otimes E_-.$$

From this it follows that the antipode is given by

$$S_h(H_\pm)=-H_\pm;\quad S_h(E_+)=-E_+e^{-hH_-};\quad S_h(E_-)=-e^{-hH_+}E_-.$$

The commutation relation between E_+ and E_- has to be changed, all others in $gl(2)$ remain the same

$$[E_+,E_-]=\frac{e^{hH_+}-e^{hH_-}}{2\sinh(h)}.$$

D. Quantization of (L,δ)

Extending Δ_h to $\widehat{gl(2)}$ is straightforward, the only complication is that $[H_\pm,\hat{H}_\pm]=\hat{H}_\pm$. Due to this, we have

$$d_h(e^{hH_\pm})=\hat{H}_\pm e^{hH_\pm}(e^h-1).$$

So we find

$$\Delta_h(\hat{H}_\pm)=\hat{H}_\pm\otimes 1+1\otimes\hat{H}_\pm$$

and

$$\Delta_h(\hat{E}_+)=\hat{E}_+\otimes e^{hH_-}+E_+\otimes\hat{H}_-e^{hH_-}(e^h-1)+1\otimes\hat{E}_+;$$

$$\Delta_h(\hat{E}_-)=\hat{E}_-\otimes 1+\hat{H}_+e^{hH_+}(e^h-1)\otimes E_-+1\otimes\hat{E}_-.$$

Now we have to adjust the relations between $gl(2)$ and $\widehat{gl(2)}$, so that Δ_h becomes an algebra-morphism. One can check by direct calculation that we can take all commutators involving either $H_\pm$ or $\hat{H}_\pm$ unchanged. We will require that $[\hat{x},\hat{y}]=0$ remains unchanged for all $x,y\in gl(2)$. Hence our problem is to adjust the commutators $[E_\pm,\hat{E}_\pm]$ and $[E_\pm,\hat{E}_\mp]$.

Let us first consider $[E_+,\hat{E}_+]$. For this we consider $[\hat{E}_+,\hat{E}_+]=0$, so that $\hat{E}_+\hat{E}_+=0$. Applying Δ_h, we find

$$\Delta_h(\hat{E}_+)\Delta_h(\hat{E}_+)=\cdots=(-E_+\hat{E}_++e^h\hat{E}_+E_+)\otimes\hat{H}_-e^{2hH_-}(e^h-1)=0.$$

Here, we used that $e^{hH_-}\hat{H}_- = \hat{H}_-e^{hH_-}e^h$, since $[H_-,\hat{H}_-]=\hat{H}_-$. So this forces

$$E_+\hat{E}_+-e^h\hat{E}_+E_+=0.$$

Similarly we find

$$E_-\hat{E}_--e^h\hat{E}_-E_-=0.$$

One must check that these relations are compatible with Δ_h, i.e., that $\Delta_h(E_+\hat{E}_+-e^h\hat{E}_+E_+)=0$. This is indeed the case.

Finally, it remains to obtain $[E_\pm,\hat{E}_\mp]$. A tedious calculation shows that we can choose

$$[E_\pm,\hat{E}_\mp]=\frac{e^h-1}{2\sinh(h)}\hat{H}_\pm e^{hH_\pm}.$$

Finally, the antipode is not difficult to calculate. In fact we have $S_h(\hat{H}_\pm)=-\hat{H}_\pm$ and

$$S_h(\hat{E}_+)=-(\hat{E}_++E_+\hat{H}_-(e^{-h}-1))e^{-hH_-};$$

$$S_h(\hat{E}_-)=-e^{-hH_+}\hat{E}_--\hat{H}_+(e^{-h}-1)e^{-hH_+}E_-$$

as follows from the formula $S_h\circ d_h=d_h\circ S_h$. We remark that the square of the antipode on $U_h(gl(2))$ is given by

$$S_h^2(H_\pm)=H_\pm;\quad S_h^2(E_+)=e^{hH_-}E_+e^{-hH_-}=e^{-h}E_+\quad S_h^2(E_-)=e^{-hH_+}E_-e^{hH_+}=e^hE_-$$

and again due to the commutation of S_h and d_h also

$$S_h^2(\hat{H}_\pm)=\hat{H}_\pm;\quad S_h^2(\hat{E}_\pm)=e^{\mp h}\hat{E}_\pm.$$

Concluding we can say that we completed the quantization. The choice of Δ_h was quite natural, and led to deforming the commutation relations involving only $E_\pm$ and $\hat{E}_\pm$.

E. Summary of results for *gl*(2)

For clearness' sake, we summarize the results of this section in the following theorem.

Theorem 2: *The quantization of the algebra* $gl(2)$, *given by*

$$[H_+,H_-]=0;\quad [H_+,E_\pm]=\pm E_\pm;\quad [H_-,E_\pm]=\mp E_\pm;\quad [E_+,E_-]=\frac{e^{hH_+}-e^{hH_-}}{2\sinh(h)}$$

and

$$\Delta_h(H_\pm)=H_\pm\otimes 1+1\otimes H_\pm;$$

$$\Delta_h(E_+)=E_+\otimes e^{hH_-}+1\otimes E_+;\quad \Delta_h(E_-)=E_-\otimes 1+e^{hH_+}\otimes E_-$$

with corresponding antipode given by

$$S_h(H_\pm)=-H_\pm;\quad S_h(E_+)=-E_+e^{-hH_-};\quad S_h(E_-)=-e^{-hH_+}E_-$$

admits a differential calculus d_h. If we denote $d_h(x)$ by $\hat{x}$ for all elements x in $gl(2)$, then $\hat{H}_\pm$ is primitive and

$$\Delta_h(\hat{E}_+)=\hat{E}_+\otimes e^{hH_-}+E_+\otimes\hat{H}_-e^{hH_-}(e^h-1)+1\otimes\hat{E}_+;$$

$$\Delta_h(\hat{E}_-)=\hat{E}_-\otimes 1+\hat{H}_+e^{hH_+}(e^h-1)\otimes E_-+1\otimes\hat{E}_-;$$

$$S_h(\hat{E}_+)=-(\hat{E}_++E_+\hat{H}_-(e^{-h}-1))e^{-hH_-},\quad S_h(\hat{E}_-)=-e^{-hH_+}\hat{E}_--\hat{H}_+(e^{-h}-1)e^{-hH_+}E_-.$$

The commutation between functions and forms is described by

$$[H_\pm,\hat{E}_\pm]=\hat{E}_\pm;\quad [H_\pm,\hat{E}_\mp]=0;\quad [H_\pm,\hat{H}_\pm]=\hat{H}_\pm;\quad [H_\pm,\hat{H}_\mp]=0,$$

$$E_\pm\hat{E}_\pm-e^h\hat{E}_\pm E_\pm=0;\quad [E_\pm,\hat{E}_\mp]=\frac{e^h-1}{2\sinh(h)}\hat{H}_\pm e^{hH_\pm};\quad [E_\pm,\hat{H}_\pm]=0;\quad [E_\pm,\hat{H}_\mp]=\hat{E}_\pm.$$

Finally, the commutation of forms is determined by the relation $\hat{x}\hat{y}=-\hat{y}\hat{x}$ for all $x,y\in gl(2)$.

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On the Lie superalgebra embedding $C(n+1) \supset B(0,n)$ and dimension formulas

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It is shown that the orthosymplectic Lie superalgebras osp $(m/2n)$ have a nonregular subalgebra osp$(1/2n)$. This implies that paraboson operators can be realized as elements of osp$(m/2n)$. The embedding osp$(2/2n) \supset$ osp$(1/2n)$, or, in a different notation, $C(n+1) \supset B(0,n)$, is studied in more detail. In particular, branching rules are determined for all typical and atypical irreducible representations of osp$(2/2n)$ with respect to the subalgebra osp$(1/2n)$. Finally, dimension and superdimension formulas are given for the Lie superalgebras under consideration. © *1996 American Institute of Physics.* [S0022-2488(96)01108-5]

I. INTRODUCTION

Lie superalgebras and their irreducible representations (simple modules) have been the subject of much attention in both the mathematical[1–4] and the physics[5–9] literature. However, even for the simplest family of basic classical Lie superalgebras, namely sl(m/n), a number of open problems remain with respect to understanding all finite-dimensional simple modules. The main reason is the existence of so-called *atypical* modules,[2,3] besides the *typical* modules which are well understood. For singly atypical modules (for which the highest weight Λ is atypical with respect to only one single odd root) of sl(m/n), a character formula has been constructed[10] and also the dimensions can be obtained.[11] For the remaining atypical modules, a number of conjectures have been formulated.[12–14]

The Lie superalgebras considered in this paper are the orthosymplectic superalgebras osp$(m/2n)$, and in particular those with $m=1$ and $m=2$. For osp$(1/2n)$, or $B(0,n)$ in Kac's notation, all representations are typical and thus a character formula is known for all of its finite-dimensional simple modules. An interesting feature of osp$(1/2n)$ is its relation with the so-called paraboson algebra, established by Palev.[15] We shall use this relation here in order to identify a nonregular osp$(1/2n)$ subalgebra in osp$(m/2n)$. The Lie superalgebra osp$(2/2n)$, or $C(n+1)$ in Kac's notation, does have both typical and atypical representations. However, the atypical modules are only singly atypical, and thus the techniques of Ref. 12 could be used to construct their characters.[16] Thus, also here a character formula is available for all finite-dimensional simple modules.

Little work has been done on branching rules for Lie superalgebras. The reason is quite obvious: all simple Lie superalgebras except for $B(0,n)$ have finite-dimensional indecomposable representations. Thus for a subalgebra pair of Lie superalgebras $G_1 \supset G_2$, the decomposition of a simple G_1 module with respect to G_2 is, in general, not completely reducible. The branching considered in this paper, $C(n+1) \supset B(0,n)$, does not have this disadvantage. Moreover, since the characters of all simple modules (both typical and atypical) of $C(n+1)$ are known, we can give a complete set of branching rules (Proposition 2). In particular, the branching rules shed some further light on the structure of atypical representations of $C(n+1)$.

The structure of the paper is as follows. In Sec. II we give the main definitions for osp$(m/2n)$.

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In Sec. III we consider the nonregular embedding $\mathrm{osp}(m/2n)\supset\mathrm{osp}(1/2n)$, and as a byproduct gives a realization of n paraboson operators in $\mathrm{osp}(m/2n)$. In Sec. IV, the representation theory of $\mathrm{osp}(2/2n)=C(n+1)$ is recalled, and this is used in Sec. V to find the decomposition of simple $\mathrm{osp}(2/2n)$ modules with respect to its subalgebra $\mathrm{osp}(1/2n)$. Examples are given, and can be checked by counting dimensions and superdimensions. In a final section, (super)dimension formulas are given for $\mathrm{sp}(2n)$, $\mathrm{osp}(1/2n)$, and $\mathrm{osp}(2/2n)$. Some of these formulas are not new, but were never given in the partition notation for the highest weight. The dimension formula for atypical representations of $\mathrm{osp}(2/2n)$, however, is new; an alternative expression for this formula is constructed in the Appendix.

II. THE LIE SUPERALGEBRAS osp($m/2n$)

The general linear Lie superalgebra $G=\mathrm{gl}(m/n)$ with $m,n\in\mathbb{N}$ is defined[2,4] by

$$\mathrm{gl}(m/n)=\left\{x=\begin{pmatrix}A & B\\ C & D\end{pmatrix}\middle|\,A\in M_{m\times m},B\in M_{m\times n},C\in M_{n\times m},D\in M_{n\times n}\right\},\tag{1}$$

where $M_{p\times q}$ is the space of all $p\times q$ complex matrices. The even subspace $\mathrm{gl}(m/n)_{\bar{0}}$ has $B=0$ and $C=0$; the odd subspace $\mathrm{gl}(m/n)_{\bar{1}}$ has $A=0$ and $D=0$. The Lie superalgebra bracket is determined by

$$[a,b]=ab-(-1)^{\alpha\beta}ba,\quad \forall a\in G_\alpha \text{ and } \forall b\in G_\beta\quad(\alpha,\beta\in\{\bar{0},\bar{1}\}).\tag{2}$$

One defines the *supertrace* $\mathrm{str}(x)$ of $x=\left(\begin{smallmatrix}A & B\\ C & D\end{smallmatrix}\right)$ as[2,4] $\mathrm{str}(x)=\mathrm{tr}(A)-\mathrm{tr}(D)$, where tr is the ordinary trace. The *special linear Lie superalgebra* $\mathrm{sl}(m/n)$ is

$$\mathrm{sl}(m/n)=\{x\in\mathrm{gl}(m/n)\,|\,\mathrm{str}(x)=0\}.\tag{3}$$

Using the definition of *supertranspose* of $x=\left(\begin{smallmatrix}A & B\\ C & D\end{smallmatrix}\right)$,

$$x^T=\begin{pmatrix}A^t & -C^t\\ B^t & D^t\end{pmatrix},\tag{4}$$

with A^t the ordinary transpose of A, the orthosymplectic subalgebra $\mathrm{osp}(m/2n)$ of $\mathrm{sl}(m/2n)$ is defined[2,4] as

$$\mathrm{osp}(m/2n)=\left\{x=\begin{pmatrix}A & B\\ C & D\end{pmatrix}\in\mathrm{sl}(m/2n)\middle|\,x_\alpha^TJ+(-1)^\alpha Jx_\alpha=0,\quad\forall x_\alpha\in\mathrm{sl}(m/2n)_\alpha\ (\alpha=\bar{0},\bar{1})\right\},\tag{5}$$

where

$$J=\begin{pmatrix}I_m & & \\ & 0 & I_n\\ & -I_n & 0\end{pmatrix}\tag{6}$$

and I_q is the $q\times q$ identity matrix. In the notation of Kac,[2] $B(m,n)=\mathrm{osp}(2m+1/2n)$, $D(m,n)=\mathrm{osp}(2m/2n)$ for $m\neq1$ and $C(n+1)=\mathrm{osp}(2/2n)$.

III. THE NONREGULAR EMBEDDING osp($m/2n$)$\supset$osp(1/2n)

In this section the embedding osp$(m/2n)\supset$osp$(1/2n)$ $(m>1)$ will be established. This is a nonregular embedding, in the sense that the root vectors of osp$(1/2n)$ are not root vectors of osp$(m/2n)$ (see Ref. 2, or the following section, for the set of roots).

Let $E_{i,j}\in$gl$(m/2n)$ denote the matrix with entry 1 at position (i,j) and 0 elsewhere. The following matrices are odd elements of osp$(m/2n)$:

$$b_k^+=\sqrt{\frac{2}{m}}\sum_{i=1}^{m}(E_{i,m+n+k}+E_{m+k,i}), \tag{7}$$

$$b_k^-=\sqrt{\frac{2}{m}}\sum_{i=1}^{m}(E_{i,m+k}-E_{m+n+k,i}), \quad k=1,2,\ldots,n. \tag{8}$$

Proposition 1: The elements b_k^ξ satisfy the following relation:

$$[[b_i^\xi,b_j^\eta],b_k^\theta]=2\theta\delta_{j,k}\delta_{\theta,-\eta}b_i^\xi+2\theta\delta_{i,k}\delta_{\theta,-\xi}b_j^\eta \quad (i,j,k=1,2,\ldots,n;\xi,\eta,\theta=\pm). \tag{9}$$

Note that in (9) the inner bracket stands for an anticommutator, and the outer bracket for a commutator. Relation (9) is the defining equation for paraboson operators.[15,17,18] Thus the proposition claims that a set of n paraboson operators have a realization in osp$(m/2n)$.

The proof of (9) is by straightforward computation: for $(\xi,\eta,\theta)=(+,+,+)$ or $(-,-,-)$ the calculation is trivial; due to symmetry of the anticommutator the remaining cases to be checked are $(+,+,-)$, $(+,-,+)$, $(+,-,-)$, and $(-,-,+)$.

Next, a theorem of Palev[15] is used: the Lie superalgebra generated by $2n$ odd elements b_k^ξ satisfying the relations (9) is osp$(1/2n)$. Therefore it follows that osp$(m/2n)$ contains osp$(1/2n)$ as a (nonregular) subalgebra (algebra–subalgebra in the sense of Lie superalgebras).

IV. THE LIE SUPERALGEBRA $C(n+1)$=osp(2/2n) AND ITS REPRESENTATIONS

In this section, $G=C(n+1)=$osp$(2/2n)$. The Lie superalgebra G has a Cartan subalgebra H spanned by the diagonal matrices in (5) with $m=2$. The dual space H^* is described in the basis of forms ϵ and δ_j $(j=1,\ldots,n)$, where $\epsilon:x\to A_{1,1}$ and $\delta_j:x\to D_{jj}$ for $x=\left(\begin{smallmatrix}A&B\\C&D\end{smallmatrix}\right)$. Denote by Δ the set of all roots of G, by Δ_0 the set of even roots, and by Δ_1 the set of odd roots. We have[2,16]

$$\Delta_0=\{\delta_j-\delta_k(j\neq k),\pm(\delta_j+\delta_k),(1\leqslant j,k\leqslant n)\}, \tag{10}$$

$$\Delta_1=\{\epsilon\pm\delta_k,-\epsilon\pm\delta_k,(1\leqslant k\leqslant n)\}, \tag{11}$$

$$\Delta=\Delta_0\cup\Delta_1. \tag{12}$$

A set of simple roots $\{\alpha_0,\alpha_1,\ldots,\alpha_n\}$ of Δ may be chosen as follows:[2] $\alpha_0=\epsilon-\delta_1$, $\alpha_j=\delta_j-\delta_{j+1}(1\leqslant j\leqslant n-1)$, and $\alpha_n=2\delta_n$. This choice corresponds to the "distinguished basis."[3] The even and odd *positive* roots of G are then given by

$$\Delta_0^+=\{\delta_j-\delta_k(j<k),\delta_j+\delta_k\}, \quad \Delta_1^+=\{\epsilon\pm\delta_k\}. \tag{13}$$

The nondegenerate bilinear form $\langle|\rangle$ on H^* is determined by[16]

$$\langle\epsilon|\epsilon\rangle=1, \quad \langle\epsilon|\delta_j\rangle=0, \quad \text{and} \quad \langle\delta_j|\delta_k\rangle=-\delta_{jk}. \tag{14}$$

An element $\Lambda\in H^*$ with $\Lambda=\lambda_0\epsilon+\Sigma_{j=1}^n\lambda_j\delta_j$ can be written as $\Lambda=(\lambda_0;\lambda_1,\ldots,\lambda_n)$ in terms of its *components* in the $\epsilon\delta$-basis, or in terms of its *Dynkin labels* $\Lambda=[a_0;a_1,\ldots,a_n]$,

where

$$a_0=\lambda_0+\lambda_1, \quad a_k=\lambda_k-\lambda_{k+1} \quad (1\leqslant k\leqslant n-1), \quad \text{and } a_n=\lambda_n. \tag{15}$$

A weight $\Lambda\in H^*$ is *integral dominant* if all $a_i\in\mathbb{N}$ for $i=1,\ldots,n$. This implies that $\lambda_1\geqslant\lambda_2\geqslant\cdots$. Thus in terms of its components, an integral dominant weight is characterized by a complex number λ_0 and a *partition* $\lambda=(\lambda_1,\ldots,\lambda_n)$ consisting of at most n parts.

Kac[3] showed that every integral dominant weight Λ uniquely determines a simple finite-dimensional highest weight module $V(\Lambda)$, and vice versa that every simple finite-dimensional G-module is uniquely characterized by its integral dominant highest weight Λ. In order to describe the structure of such a simple module $V(\Lambda)$ by means of its character, we need to introduce a few more objects. The *Weyl group* W of G is defined to be the Weyl group of $G_{\bar{0}}$, so in this case it is just the Weyl group of the symplectic Lie algebra $\mathrm{sp}(2n)$. As usual, $\varepsilon(w)$ denotes the signature of $\omega\in W$. Further on, we denote $\rho=\rho_0-\rho_1$ with

$$\rho_0=\frac{1}{2}\sum_{\alpha\in\Delta_0^+}\alpha, \quad \rho_1=\frac{1}{2}\sum_{\beta\in\Delta_1^+}\beta, \tag{16}$$

or explicitly, $\rho_0=\Sigma_{k=1}^n(n+1-k)\delta_k$ and $\rho_1=n\epsilon$.

Kac[3] distinguished between *typical* and *atypical* modules: $V(\Lambda)$ and Λ are said to be typical if and only if $\langle\Lambda+\rho|\beta\rangle\neq 0$ for all $\beta\in\Delta_1^+$. Otherwise, $V(\Lambda)$ and Λ are said to be atypical. Explicitly, an integral dominant weight $\Lambda=(\lambda_0;\lambda)$ is typical if

$$\lambda_0\neq n\pm(\lambda_k+n+1-k) \quad (k=1,2,\ldots,n). \tag{17}$$

For a typical module $V(\Lambda)$, Kac proved the following character formula:[3]

$$\mathrm{ch}\ V(\Lambda)=L_0^{-1}\sum_{w\in W}\varepsilon(w)w\left(e^{\Lambda+\rho_0}\sum_{\beta\in\Delta_1^+}(1+e^{-\beta})\right), \tag{18}$$

where $L_0=\Pi_{\alpha\in\Delta_0^+}(e^{\alpha/2}-e^{-\alpha/2})$ and $e^\lambda(\lambda\in H^*)$ is the *formal exponential*.

For atypical modules of $C(n+1)$, the characters were determined in Ref. 16, where two alternative expressions were given. The one we shall use here is

$$\mathrm{ch}\ V(\Lambda)=L_0^{-1}\sum_{w\in W}\varepsilon(w)w\left(e^{\Lambda+\rho_0}\prod_{\substack{\beta\in\Delta_1^+\\ \langle\Lambda+\rho|\beta\rangle\neq 0}}(1+e^{-\beta})\right). \tag{19}$$

These character formulas contain all the information on the weight structure of the simple modules. Hence, to determine the decomposition of a G module with respect to a subalgebra of G, the character is in principle all that is needed.

V. THE BRANCHING $C(n+1)=\mathrm{osp}(2/2n)\supset\mathrm{osp}(1/2n)=B(0,n)$

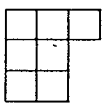
The embedding $\mathrm{osp}(2/2n)\supset\mathrm{osp}(1/2n)$ was described in Sec. III. The two Lie superalgebras have almost the same even subalgebra: $\mathrm{osp}(2/2n)_{\bar{0}}=\mathbb{C}\oplus\mathrm{sp}(2n)$ and $\mathrm{osp}(1/2n)_{\bar{0}}=\mathrm{sp}(2n)$. They have the same Weyl group W, namely the Weyl group of $\mathrm{sp}(2n)$. And the weight space of $\mathrm{osp}(1/2n)$ can be identified with the subspace of H^* spanned by the δ_ks only. Thus for an $\mathrm{osp}(2/2n)$ module $V(\Lambda)$ reduced to $\mathrm{osp}(1/2n)$, the $\mathrm{osp}(1/2n)$ weights are determined by projecting the $\mathrm{osp}(2/2n)$ weights on this subspace, i.e., by putting the ϵ-component equal to 0. Since all finite-dimensional modules of $\mathrm{osp}(1/2n)$ are completely reducible [cf. Kac;[3] note that $\mathrm{osp}(1/2n)$ is

the only simple Lie superalgebra with this property], one simply has to decompose the character of this osp(1/2n) module into simple osp(1/2n) characters in order to obtain the decomposition of $V(\Lambda)$ into simple osp(1/2n) modules.

A simple osp(1/2n) module $V=V(\mu)$ is uniquely characterized by its highest weight $\mu=\Sigma_{j=1}^{n}\mu_j\delta_j=(\mu_1,\ldots,\mu_n)$, which is integral dominant, i.e., μ forms a partition. All $V(\mu)$ are typical, with their character given by

$$\text{ch } V(\mu)=L_0^{-1}\sum_{w\in W}\varepsilon(w)w\left(e^{\mu+\rho_0}\prod_{j=1}^{n}(1+e^{-\delta_j})\right); \tag{20}$$

herein, L_0, W, and ρ_0 are the same as in (18). The procedure to determine the decomposition of a simple osp(2/2n) module $V(\Lambda)$ into simple osp(1/2n) modules $V(\mu)$ is thus as follows: consider the character ch $V(\Lambda)$, substitute herein $\epsilon=0$, and rewrite the result as a sum of characters ch $V(\mu)$ of the type (20). This procedure can formally be executed for both typical and atypical representations of osp(2/2n). Without going into the details of the computation, we give the main result in Proposition 2. Before formulating this result, recall that a partition $\lambda=(\lambda_1,\lambda_2,\ldots)$ is conveniently represented[19] by its Young diagram F^λ consisting of left-adjusted rows of boxes of length λ_i. A diagram F^σ obtained from F^λ by adding or removing certain boxes is called *standard* if it still corresponds to a partition, i.e., if $\sigma_1\geqslant\sigma_2\geqslant\cdots$. For example, let

$F^{(3,2,2)}=$  . (21)

Adding one box in the second row yields a standard diagram; adding one box in the third row yields a nonstandard diagram.

Proposition 2: Let $\Lambda=(\lambda_0;\lambda)=(\lambda_0;\lambda_1,\lambda_2,\ldots,\lambda_n)\in H^*$ be integral dominant and $V(\Lambda)$ the simple osp(2/2n) module with highest weight Λ. Then the set of μs determining the decomposition of $V(\Lambda)$ into simple osp(1/2n) modules $V(\mu)$ is found as follows.

(a) If Λ is typical construct all standard diagrams F^μ obtained from F^λ by adding either no or else one box into each row of F^λ.

(b) If Λ is atypical with respect to $\epsilon-\delta_k$, i.e., $\lambda_0=-\lambda_k+k-1$, then construct all standard diagrams F^μ obtained from F^λ by adding no box in row k and by adding either no or else one box into each row different from k.

(c) If Λ is atypical with respect to $\epsilon+\delta_k$, i.e., $\lambda_0=\lambda_k-k+2n+1$, then construct all standard diagrams F^μ obtained from F^λ by adding one box in row k and by adding either no or else one box into each row different from k.

The proposition makes the distinction between typical and atypical modules very clear. To illustrate this, consider osp(2/6)$\supset$osp(1/6) for $V(\Lambda)$ with $\Lambda=(\lambda_0;3,2,2)$. For $\lambda_0\notin\{-3,-1,0,6,7,9\}$, $V(\Lambda)$ is typical and the decomposition is given by

$$\begin{aligned}(\lambda_0;3,2,2)&\rightarrow(3,2,2)\oplus(4,2,2)\oplus(3,3,2)\oplus(4,3,2)\oplus(3,3,3)\oplus(4,3,3),\\ 24192 &= 1386+4095+2310+9009+1386+6006,\\ 0 &= 54-135-70+231+30-110.\end{aligned}$$

If $\lambda_0=-1$, Λ is atypical with respect to $\epsilon-\delta_2$ and in this case the decomposition is

$$\begin{aligned}(-1;3,2,2)&\rightarrow(3,2,2)\oplus(4,2,2),\\ 5481 &= 1386+4095,\\ 81 &= -54+135.\end{aligned} \tag{22}$$

If $\lambda_0=6$, Λ is atypical with respect to $\epsilon+\delta_3$ and then the decomposition is given by

$$\begin{aligned}(6;3,2,2)&\rightarrow(3,3,3)\oplus(4,3,3),\\ 7392 &= 1386 + 6006,\\ 80 &= -30 + 110.\end{aligned}\tag{23}$$

Below the representation labels are given the dimensions ($\dim V = \dim V_{\bar{0}} + \dim V_{\bar{1}}$) and so-called superdimensions ($\mathrm{sdim}\, V = \dim V_{\bar{0}} - \dim V_{\bar{1}}$). Some but not all of these dimensions can be found in the tables of Thierry-Mieg.[20] In Sec. VI, we shall list the known dimension formulas for osp($m/2n$) ($m=0,1,2$) and give some new expressions.

VI. DIMENSION FORMULAS

Below we summarize the dimension and superdimension formulas for the simple modules of the Lie superalgebras treated in this paper, in an obvious notation. First we recall the dimension formula of the simple module with highest weight $\lambda=\sum_{i=1}^{n}\lambda_i\delta_i$ for the Lie algebra sp($2n$), taken from Ref. 21. Next are given the superdimension and dimension formula for osp($1/2n$); these can be deduced from Ref. 3 (up to some printing errors). From the same reference follow the dimension and superdimension of *typical* representations of osp($2/2n$) [here, the highest weight of the module is $\Lambda=(\lambda_0;\lambda)$, but λ_0 does not appear in the dimension formulas]:

$$\dim_{\mathrm{sp}(2n)}(\lambda)=\prod_{i=1}^{n}\frac{\lambda_i+n+1-i}{n+1-i}\prod_{1\leq i<j\leq n}\frac{(\lambda_i-\lambda_j+j-i)(\lambda_i+\lambda_j+2n+2-i-j)}{(j-i)(2n+2-i-j)};\tag{24}$$

$$\mathrm{sdim}_{\mathrm{osp}(1/2n)}(\lambda)=\prod_{1\leq i<j\leq n}\frac{(\lambda_i-\lambda_j+j-i)(\lambda_i+\lambda_j+2n+1-i-j)}{(j-i)(2n+1-i-j)};\tag{25}$$

$$\dim_{\mathrm{osp}(1/2n)}(\lambda)=\prod_{i=1}^{n}\frac{\lambda_i+n-i+\frac{1}{2}}{n-i+\frac{1}{2}}\,\mathrm{sdim}_{\mathrm{osp}(1/2n)}(\lambda);\tag{26}$$

$$\mathrm{sdim}^{\mathrm{typ}}_{\mathrm{osp}(2/2n)}(\lambda_0;\lambda)=0;\tag{27}$$

$$\dim{}^{\mathrm{typ}}_{\mathrm{osp}(2/2n)}(\lambda_0;\lambda)=2^{2n}\dim_{\mathrm{sp}(2n)}(\lambda).\tag{28}$$

What remains to be determined are formulas for the dimensions and superdimensions of *atypical* irreducible representations of osp($2/2n$). For the superdimension, a formula can be derived from equation (6.21) of Ref. 16:

$$\mathrm{sdim}^{\mathrm{atyp}:\epsilon\pm\delta_k}_{\mathrm{osp}(2/2n)}(\lambda_0;\lambda)=\dim_{\mathrm{sp}(2n-2)}(\lambda_1+1,\lambda_2+1,\ldots,\lambda_{k-1}+1,\lambda_{k+1},\lambda_{k+2},\ldots,\lambda_n).\tag{29}$$

Again, the notation should be obvious: $\mathrm{sdim}^{\mathrm{atyp}:\beta}_{\mathrm{osp}(2/2n)}(\lambda_0;\lambda)$ stands for the superdimension of a simple module with highest weight $\Lambda=(\lambda_0;\lambda)$ atypical with respect to a positive odd root β. The dimension formula for an atypical osp($2/2n$) module is more difficult to obtain. In fact, contrary to the dimension formulas given so far, it is not completely but only partially factorizable into monomials in the λ_i. A technique to obtain a dimension formula from a character formula of the type (19) was given by Kac and Wakimoto.[22] Following this technique leads in the present case to the following formulas:

$$\dim^{\text{atyp};\epsilon+\delta_k}_{\text{osp}(2/2n)}(\lambda_0;\lambda)=\frac{2^{2n-1}}{n!}\left(\prod_{i=1}^{n}\frac{(2i)!}{(n-i)!(n+i)!}\right)\prod_{\substack{i=1\\ i\neq k}}^{n}x_i\prod_{\substack{1\leq i<j\leq n\\ i,j\neq k}}(x_i-x_j)(x_i+x_j)$$
$$\times(-1)^{k-1}\sum_{j=0}^{2n-1}\sum_{l=0}^{j}(-1)^l 2^{-j}\binom{j}{l}(x_k-l)\prod_{\substack{i=1\\ i\neq k}}^{n}(x_k-l-x_i)(x_k-l+x_i), \tag{30}$$

where $x_i=\lambda_i+n+1-i$;

$$\dim^{\text{atyp};\epsilon-\delta_k}_{\text{osp}(2/2n)}(\lambda_0;\lambda)=\frac{2^{2n-1}}{n!}\left(\prod_{i=1}^{n}\frac{(2i)!}{(n-i)!(n+i)!}\right)\prod_{\substack{i=1\\ i\neq k}}^{n}x_i\prod_{\substack{1\leq i<j\leq n\\ i,j\neq k}}(x_i-x_j)(x_i+x_j)$$
$$\times(-1)^{k-1}\sum_{j=0}^{2n-1}\sum_{l=0}^{j}(-1)^l 2^{-j}\binom{j}{l}(x_k-l)\prod_{\substack{i=1\\ i\neq k}}^{n}(x_k-l-x_i)(x_k-l+x_i), \tag{31}$$

where $x_i=\lambda_i+n+1-i(i\neq k)$ and $x_k=\lambda_k+n-k$.

For example, consider osp(2/6) and representations that are atypical with respect to $\epsilon+\delta_3$; then (30) yields

$$\begin{aligned}\dim^{\text{atyp};\epsilon+\delta_3}_{\text{osp}(2/6)}(\lambda_0=\lambda_3+4;\lambda_1,\lambda_2,\lambda_3)=&\tfrac{1}{90}(\lambda_1+3)(\lambda_2+2)(\lambda_1-\lambda_2+1)(\lambda_1+\lambda_2+5)(2\lambda_3+3)\\ &\times(2\lambda_1^2\lambda_2^2-2\lambda_1^2\lambda_3^2-2\lambda_2^2\lambda_3^2+2\lambda_3^4+8\lambda_1^2\lambda_2+12\lambda_1\lambda_2^2\\ &-6\lambda_1^2\lambda_3-6\lambda_2^2\lambda_3-12\lambda_1\lambda_3^2-8\lambda_2\lambda_3^2+12\lambda_3^3+5\lambda_1^2\\ &+48\lambda_1\lambda_2+15\lambda_2^2-36\lambda_1\lambda_3-24\lambda_2\lambda_3-4\lambda_3^2\\ &+30\lambda_1+60\lambda_2-66\lambda_3+35).\end{aligned} \tag{32}$$

Using this formula, the dimension in (23) can be calculated. Note in (32) that the polynomial obtained from the sum over j and l part in (30), with the proper arguments, gives rise to one more factor, namely $(2\lambda_3+3)=(2x_3+1)$. All other examples we have worked through confirm this extra factor. This comes as no surprise. Indeed, the branching rule for an atypical representation (of type $\epsilon+\delta_k$, for example) determined in the previous section implies that all osp(1/2n) components of this representation have $(x_k+\frac{1}{2})$ as a factor for their dimensions, thus also the total osp(2/2n) dimension should have this factor. This means that the polynomial part (i.e., sum over j and l) in (30) or (31) can be rewritten in another form, giving this extra factor explicitly. Identifying this polynomial in (30) as $P_{n-1}(x_k;x_1,x_2,\ldots,x_{k-1},x_{k+1},\ldots,x_n)$, it is of the type

$$P_N(z;z_1,\ldots,z_N)=\sum_{j=0}^{2N+1}\sum_{l=0}^{j}(-1)^l\binom{j}{l}2^{-j}(z-l)\prod_{i=1}^{N}(z-l-z_i)(z-l+z_i), \tag{33}$$

and the presently obtained branching rule implies that this polynomial has a factor $(2z+1)$. After various combinatorial manipulations, the details of which are presented in the Appendix, we arrived indeed at the following expression:

$$P_N(z;z_1,\ldots,z_N)=(2z+1)\sum_{p=0}^{N}\left(\sum_{m=0}^{p}\alpha_{p,m}\prod_{q=2}^{m+1}(2z+q)\right)e_{N-p}. \tag{34}$$

Herein, e_r is the rth elementary symmetric function[19] in the variables $z^2-z_1^2,\ldots,z^2-z_N^2$, and an expression for the coefficient $\alpha_{p,m}$ is given by

$$\alpha_{p,m}=\sum_{j=0}^{2p+1}\sum_{a=0}^{j}\sum_{b=0}^{m}2^{-j-1}(-1)^{a+b}\frac{1}{(m+1)!}\binom{j}{a}\binom{m+1}{b+1}a^p(a+b+2)^p(2a+b+2). \tag{35}$$

In the last formula, 0^0 should be interpreted as 1.

APPENDIX: PROOF OF (34)

First, we prove two short lemmas.

Lemma 1: Let $f(z)$ and $g(z)$ be real polynomials in z with $g(z-\frac{1}{2})+g(z+\frac{1}{2})=f(z)$. If $f(-z)=-f(z)$, then also $g(-z)=-g(z)$.

Proof: Putting $z=0$, and using $f(0)=0$, yields $g(-1/2)=-g(1/2)$. Assume now $g(-k/2)=-g(k/2)$ for k an odd positive integer. Then,

$$g\left(\frac{k}{2}\right)+g\left(\frac{k}{2}+1\right)=f\left(\frac{k+1}{2}\right)=-f\left(-\frac{k+1}{2}\right)=-g\left(-\frac{k}{2}\right)-g\left(-\frac{k}{2}-1\right),$$

thus also $g(-k/2-1)=-g(k/2+1)$. By induction $g(-k/2)=-g(k/2)$ for all odd positive integers k. Since $g(z)$ is a polynomial, this can only happen when $g(-z)=-g(z)$.

The second lemma follows from numerical analysis results, and uses the translation operator $Ef(z)=f(z+1)$ and the forward difference operator $\Delta f(z)=f(z+1)-f(z)$; thus $\Delta=E-1$.

Lemma 2: Let $f(z)$ be a polynomial in z of degree n. Then

$$\sum_{k=0}^{j}(-1)^k\binom{j}{k}f(z+k)=0 \quad \text{for } j>n.$$

Proof: The sum can be written as

$$\sum_{k=0}^{j}(-1)^k\binom{j}{k}f(z+k)=\sum_{k=0}^{j}(-1)^k\binom{j}{k}E^kf(z)=(1-E)^jf(z)=(-\Delta)^jf(z),$$

and this is zero, since it is a classical result that $\Delta^j f(z)=0$ for $f(z)$ a polynomial with degree $n<j$.

Consider now (33); using

$$\prod_{i=1}^{N}(z-l-z_i)(z-l+z_i)=\prod_{i=1}^{n}(l^2-2zl+(z^2-z_i^2)),$$

and

$$\prod_{i=1}^{N}(x+x_i)=\sum_{n=0}^{N}x^n e_{N-n}(x_1,\ldots,x_N),$$

with e_r the rth elementary symmetric function, we see that

$$P_N(z;z_1,\ldots,z_N)=\sum_{n=0}^{N}p_n(z)e_{N-n}(z^2-z_1^2,\ldots,z^2-z_N^2),$$

with

$$p_n(z)=\sum_j \sum_l (-1)^l \binom{j}{l} 2^{-j}(z-l)l^n(l-2z)^n.$$

By Lemma 2, the sum over j runs from 0 to $2n+1$; the sum over l is restricted by the binomial coefficient. Next, we use

$$\begin{aligned}(z-l)l^n(l-2z)^n &= \sum_i \binom{n}{i} l^{2n-i}(-2z)^i(z-l)\\ &= -\frac{1}{2}\sum_i \binom{n}{i} l^{2n-i}(-2z)^{i+1} - \sum_i \binom{n}{i} l^{2n+1-i}(-2z)^i\\ &= -\frac{1}{2}\sum_i \binom{n}{i-1} l^{2n+1-i}(-2z)^i - \sum_i \binom{n}{i} l^{2n+1-i}(-2z)^i\\ &= -\frac{1}{2}\sum_i l^{2n+1-i}(-2z)^i\left\{\binom{n}{i-1}+2\binom{n}{i}\right\}\\ &= -\frac{1}{2}\sum_i l^{2n+1-i}(-2z)^i\left\{\binom{n}{i}+\binom{n+1}{i}\right\},\end{aligned}$$

so

$$p_n(z)=\sum_{i,j,l} (-1)^{l+1}\binom{j}{l}2^{-j-1}\left\{\binom{n}{i}+\binom{n+1}{i}\right\} l^{2n+1-i}(-2z)^i. \tag{A1}$$

In order to see that $p_n(z)$ has $2z+1$ as a divisor, and to rewrite the quotient in an appropriate form, we shall express all quantities in terms of the functions $w_m(z)$, where $w_0(z)=1$ and

$$w_m(z)=\prod_{q=1}^{m}(-2z-q).$$

Using the following formula from combinatorial analysis,

$$x^r=\sum_{m,k}\frac{(-1)^{m-k}}{m!}\binom{m}{k}k^r x(x-1)\cdots(x-m+1),$$

on $(-2z)^i=\Sigma_r\binom{i}{r}(-2z-1)^r$, yields

$$(-2z)^i=\sum_r\binom{i}{r}\sum_{m,k}\frac{(-1)^{m-k}}{m!}\binom{m}{k}k^r w_m(z)=\sum_{m,k}\frac{(-1)^{m-k}}{m!}\binom{m}{k}(k+1)^i w_m(z).$$

Putting this back in (A1) gives

$$p_n(z)=\sum_{m=0}^{2n+1}\beta_{n,m}w_m(z),$$

with

$$\beta_{n,m}=\sum_{i,j,l,k}(-1)^{l+1}\binom{j}{l}2^{-j-1}\left\{\binom{n}{i}+\binom{n+1}{i}\right\}l^{2n+1-i}\frac{(-1)^{m-k}}{m!}\binom{m}{k}(k+1)^i$$

$$=\sum_{j,l,k}\frac{(-1)^{l+m+k+1}}{m!}\binom{j}{l}\binom{m}{k}2^{-j-1}\sum_i\left\{\binom{n}{i}+\binom{n+1}{i}\right\}l^{2n+1-i}(k+1)^i$$

$$=\sum_{j,l,k}\frac{(-1)^{l+m+k+1}}{m!}\binom{j}{l}\binom{m}{k}2^{-j-1}\{l^n(l+k+1)^{n+1}+l^{n+1}(l+k+1)^n\}$$

$$=\sum_{j,l,k}\frac{(-1)^{l+m+k+1}}{m!}\binom{j}{l}\binom{m}{k}2^{-j-1}l^n(l+k+1)^n(2l+k+1).$$

This gives a proper form for the coefficients of $p_n(z)$ in terms of $w_m(z)$. It remains to be shown that the coefficient of $w_0(z)$ vanishes, or $\beta_{n,0}=0$ for all n, where

$$\beta_{n,0}=\sum_{j,l}(-1)^{l+1}\binom{j}{l}2^{-j-1}l^n(l+1)^n(2l+1).$$

Consider

$$t_n=\sum_{k=0}^{n}\binom{n}{k}4^{n-k}\beta_{n-k,0};$$

since this is a triangular system of the $\beta_{n-k,0}$ in terms of the t_n, all $\beta_{j,0}$ are zero if we prove that all t_n are zero for $n=0,1,2,\ldots$. For t_n, there comes the expression

$$t_n=\sum_{k,j,l}\binom{n}{k}4^{n-k}(-1)^{l+1}\binom{j}{l}2^{-j-1}(l^2+l)^{n-k}(2l+1)=\sum_{j,l}(-1)^{l+1}\binom{j}{l}2^{-j-1}(2l+1)^{2n+1}.$$

Consider

$$T_n(z)=\sum_j 2^{-j-1}\sum_l(-1)^{l+1}\binom{j}{l}(2z+2l+1)^{2n+1};$$

then $t_n=T_n(0)$, and with $f(z)=(2z+1)^{2n+1}$ we have (using the notation of Lemma 2)

$$T_n(z)=\sum_j 2^{-j-1}\sum_l(-1)^{l+1}\binom{j}{l}f(z+l)$$

$$=-\sum_j 2^{-j-1}(-1)^j\Delta^j f(z)$$

$$=-\frac{1}{2}\sum_j\left(-\frac{\Delta}{2}\right)^j f(z)$$

$$=-\frac{1}{2}\frac{1}{1+\Delta/2}f(z)$$

$$=\frac{-1}{1+E}f(z).$$

Hence $T_n(z)$ is the polynomial solution of $T_n(z+1)+T_n(z)=-(2z+1)^{2n+1}$. Replacing herein z by $z-1/2$ leads to $T_n(z+1/2)+T_n(z-1/2)=-(2z)^{2n+1}$; using Lemma 1 implies that $T_n(z)$ is an odd function of z, thus $t_n=T_n(0)=0$. Combining all results now leads to (34) and (35).

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SU3 isoscalar factors

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A summary of the properties of the Wigner–Clebsch–Gordan coefficients and isoscalar factors for the group SU3 in the SU2⊗U1 decomposition is presented. The outer degeneracy problem is discussed in detail with a proof of a conjecture (Braunschweig's) which has been the basis of previous work on the SU3 coupling coefficients. Recursion relations obeyed by the SU3 isoscalar factors are produced, along with an algorithm which allows numerical determination of the factors from the recursion relations. The algorithm produces isoscalar factors which share all the symmetry properties under permutation of states and conjugation which are familiar from the SU2 case. The full set of symmetry properties for the SU3 Wigner–Clebsch–Gordan coefficients and isoscalar factors are displayed. © *1996 American Institute of Physics.* [S0022-2488(96)01208-X]

I. INTRODUCTION

The group SU3 continues to be useful in modeling symmetries observed in particle and nuclear physics. In the late 1950s application was found in classification of "elementary" hadrons, and in the description of rotational states of nonspherical nuclei. Its utility persists as the color symmetry of quantum chromodynamics, various models for collective nuclear motion, and elsewhere.

The Wigner–Clebsch–Gordan coefficients (WCG) are of particular interest. These can be defined as the expansion coefficients of a composite state of good SU3 quantum numbers in terms of direct products of two individual SU3 classified states, paralleling Wigner's original use of SU2 in the treatment of quantum angular momentum. The WCG can also be developed as the matrix elements of a set of tensor operators which have distinctive properties under the transformations of SU3. These two viewpoints on the WCG are formally identical, and their algebraic connection is expressed by the Wigner–Eckart Theorem. The SU3 case presents a complication that is absent in the SU2 recoupling problem—that of the *outer degeneracy*. The complete determination of WCGs in SU3 requires a criterion outside the SU3 group to completely classify composite states, and thus to fully define numerical values for the WCG. In *this* process, the two perspectives on the WCG mentioned above suggest quite different mechanisms.

Biedenharn and co-workers,[1–3] adopting the operator point of view, have developed a set of canonical SU3-labeled unit tensor operators, whose matrix elements become the "canonical WCGs." The canonical operators acquire SU3 labels by virtue of their behavior under the transformations of the group. As well, each produces a unique set of shifts, i.e., its action when operating on a state from a particular irreducible representations (irrep) produces states from a unique second irrep; and in cases of nontrivial outer degeneracy there is a distinct operator for each degeneracy index. The uniqueness of the operators, and thus their designation as canonical, comes from their null space properties. The *characteristic null space* of an operator is the union of all irreps which identically yield zero under the action of the operator. In the case of a tensor operator of degeneracy one, the null space is uniquely determined by the group properties of the operator and the state operated upon: for higher degeneracy the operators for distinct degeneracy labels are chosen to have a null space each larger than the previous and completely containing it.

Adopting the alternative viewpoint—the WCGs as coupling coefficients which give the amplitude for the joining of two SU3 states to a composite state of good SU3 quantum numbers—coefficients which exhibit symmetry under interchange of the two states being coupled are sug-

gested (a symmetry missing from the canonical coefficients).[4] The WCGs for those couplings which have degeneracy 1 possess this symmetry, and indeed all the symmetries under permutation of irreps of the familiar SU2 Clebsch–Gordan coefficients. It has been proven that such permutation symmetric WCGs for the SU3 case with degeneracy >1 exist[5–7] and examples of such SU3 WCGs have been developed.[8,9]

In the sections which follow, new results pertaining to the SU3 WCGs are presented which simplify evaluation of the WCGs, and which are independent of the particular scheme adopted for outer degeneracy resolution. In particular, a collection of recursion relations are defined for the isoscalar factors. An algorithm is presented which utilizes these recursion relations to generate a set of WCGs demonstrating all the Racah symmetries familiar from SU2. This algorithm has been used in a successful C language implementation.

II. DEFINITIONS AND NOTATION

A linear vector space which carries an irrep of SU3 is fully specified by two integers (p,q), henceforth referred to as the *irrep labels*. The dimension of the space is

$$d=(p+1)(q+1)(p+q+2)/2. \tag{1}$$

A complete set of d orthogonal vectors within the irrep can be labeled by three further integers (k,l,m), the *subspace labels*, which satisfy the *betweenness conditions*

$$p+q\geqslant k\geqslant q\geqslant l\geqslant 0; \quad k\geqslant m\geqslant l. \tag{2}$$

A fully specified member of the orthonormal spanning set for the irrep is denoted by the ket

$$|p,q;k,l,m\rangle.$$

The WCGs are the coefficients (C) of the expansion of a composite SU3 state ket in terms of products of SU3 kets,

$$|\mathscr{P};\kappa\rangle=\sum C^{[\mathscr{P}_1]\ \ [\mathscr{P}_2]\ \ [\mathscr{P}]}_{[\kappa_1]\ \ [\kappa_2]\ \ [\kappa]}\ |\mathscr{P}_1;\kappa_1\rangle|\mathscr{P}_2;\kappa_2\rangle, \tag{3}$$

where $\mathscr{P}$ is shorthand for the pair (p,q) and κ for the set (k,l,m); the sum extends over subspace labels of κ_1 and κ_2, and $n=0,1,...$ labels the outer degeneracy. The Wigner–Eckart Theorem relates the WCGs to matrix elements of operators $T^n_{p,q;k,l,m}$, which transform like tensors under the operations of SU3:

$$\langle p,q;k,l,m|T^n_{p_1,q_1;k_1,l_1,m_1}|p_2,q_2;k_2,l_2,m_2\rangle=C^{[\mathscr{P}_1]\ \ [\mathscr{P}_2]\ \ [\mathscr{P}]}_{[\kappa_1]\ \ [\kappa_2]\ \ [\kappa]}\langle p,q\|T^n_{p_1,q_1}\|p_2,q_2\rangle, \tag{4}$$

where

$$\langle p,q\|T^n_{p_1,q_1}\|p_2,q_2\rangle,$$

the *reduced matrix element*, is a complex number which depends only upon the three sets of irrep labels. (The unit tensor operators of the Biedenharn scheme are so named since each has a reduced matrix element of one.)

The ket labeling scheme described above represents the decomposition SU3⊃SU2⊗U1. The labels (k,l,m) are the quantum numbers of the SU2 subgroup, and are related to the isospin (I) and its z component (I_z) by

$$I=\frac{k-l}{2}, \tag{5}$$

$$I_z=m-\frac{k+l}{2}, \tag{6}$$

and the U1 subgroup with the hypercharge (Y) given by

$$Y=k+l-\tfrac{2}{3}(p+2q). \tag{7}$$

The WCG of Eq. (3) will vanish unless the subspace labels obey the relations

$$I_1+I_2\geqslant I,$$
$$|I_1-I_2|\leqslant I, \tag{8}$$

$$I_{1_z}+I_{2_z}=I_z, \tag{9}$$

$$Y_1+Y_2=Y. \tag{10}$$

This decomposition allows factoring of an SU2 Clebsch–Gordan coefficient from the SU3 WCG as follows:

$$C\begin{matrix}[\mathscr{P}_1] & \overset{n}{[\mathscr{P}_2]} & [\mathscr{P}] \\ [\kappa_1] & [\kappa_2] & [\kappa]\end{matrix}=C\begin{matrix}I_1 & I_2 & I \\ I_{1_z} & I_{2_z} & I_z\end{matrix}F^n(p,q,k,l;p_1,q_1,k_1,l_1;p_2,q_2,k_2,l_2), \tag{11}$$

where the factor F, which is independent of the m subspace labels, is called the *isoscalar factor* (ISF). In subsequent usage, when their values are obvious from the context, the p and q values will be suppressed in the notation for the ISF.

A particular set of subspace labels, $k=m=p+q$, $l=0$, will play an important role in the present consideration. This set, referred to as the *state of highest weight* (SHW) for a particular irrep, will be referred to by the replacement $(k=p+q,\ l=0,\ m=p+q)\rightarrow$SHW and likewise in the isoscalar factor by $(p,q,k=p+q,\ l=0)\rightarrow(p,q,\text{SHW})$.

III. OUTER DEGENERACY

The Clebsch–Gordan series for SU3,

$$(p_1,q_1)\otimes(p_2,q_2)=\sum_i \eta_i(p_i',q_i'), \tag{12}$$

indicates the number of distinct times (η_i) the irrep (p_i',q_i') appears in the outer product of irreps (p_1,q_1) and (p_2,q_2). The circumstance of $\eta_i>1$ is a feature of SU3 referred to as *outer degeneracy*, and the coefficients η_i will be referred to herein as the *degeneracy* of the coupling $(p_1,q_1)\otimes(p_2,q_2)\rightarrow(p_i',q_i')$.

The value of the degeneracy is a function of the six irrep labels and can be deduced from the betweenness conditions of Eq. (2) for each irrep, and the requirements of the SU2 and U1 subgroups, given in Eqs. (8)–(10). These latter requirements follow from the corresponding Clebsch–

Gordan series for SU2 (triangularity of three Euclidian vectors in two dimensions) and for U1 (scalar addition). Various ways of evaluating the degeneracy appear in the literature.[10,11] An equivalent expression for the degeneracy consistent with present notation is

$$\eta=\max(\eta'+1-\max(\gamma,\sigma),0),$$
$$\eta'=\min(p_1+\sigma,p_2+\sigma,q+\sigma,q_1+\gamma,q_2+\gamma,p+\gamma,2(\sigma+\gamma),p_1+q_1-\gamma-\sigma,p_2+q_2-\gamma-\sigma) \tag{13}$$

where $\gamma\equiv(p_1+p_2-p)/3$, and $\sigma\equiv(q_1+q_2-q)/3$.

This expression can be used to prove Braunschweig's conjecture which has been used by several authors[12–14] in work related to determination of WCGs for SU3. The conjecture suggests that the number of nonvanishing values of the WCG,

$$C^{\overset{n}{[\mathscr{P}_1]\quad[\mathscr{P}_2]\quad[\mathscr{P}]}}_{[\mathrm{SHW}]\quad[\kappa_2]\quad[\mathrm{SHW}]'} \tag{14}$$

is no less than the degeneracy of the irrep coupling. The value for the subspace label m_2 is fixed by Eq. (9) and l_2 is dependent upon k_2 through Eq. (10)

$$k_2+l_2=p_2+q_2-\gamma+\sigma, \tag{15}$$

so counting the number of nonvanishing WCGs of this type can be accomplished by determining the range of k_2 values. Upper and lower limits on k_2 come from the triangularity expressions of Eq. (8) combined with Eq. (15), producing

$$k_2\geq p_2+q_2-2\gamma-\sigma, \quad k_2\geq\gamma+2\sigma, \tag{16}$$
$$k_2\leq p+q+\gamma+2\sigma.$$

The betweenness relations for state 2 give further limits on $k_2(p_2+q_2\geq k_2\geq q_2)$ and on $l_2(q_2\geq l_2\geq 0)$, which when combined with Eq. (15) produce

$$k_2\geq\sigma-\gamma+p_2, \quad k_2\leq\sigma-\gamma+p_2+q_2. \tag{17}$$

The limits on k_2 are thus

$$\max(p_2+q_2-2\gamma-\sigma,\gamma+2\sigma,q_2,p_2+\sigma-\gamma)\leq k_2\leq\min(p_2+q_2+\sigma-\gamma,p_2+q_2,p+q+\gamma+2\sigma), \tag{18}$$

which implies that the total number of k_2 values producing nonvanishing WCGs in this case is given by

$$1+\min(\gamma+2\sigma,\sigma+2\gamma,p_2+q_2-\sigma-2\gamma,p_2+q_2-\gamma-2\sigma,q_2,q_2$$
$$+\gamma-\sigma,p_1+q_1,p+q,p+q-q_2+\gamma+2\sigma,p+q-p_2+2\gamma+\sigma). \tag{19}$$

A term-by-term comparison of this expression with that for the degeneracy [Eq. (13)] reveals that the number of k_2 values producing nonvanishing WCGs of the form of Eq. (14) is greater than or equal to the degeneracy. This inequality is sufficient for the uses of the previously cited references, and has been important in the development of the algorithm presented later in this paper.

IV. RECURSION RELATIONS

An efficient scheme for evaluation of the SU3 ISF *independent of the method chosen for resolution of outer degeneracy* involves use of recursion relations for these quantities, which can be derived using the group generators.[15] Explicit expressions for the generators depend upon a choice of signs of the matrix elements of the generators between elements of the fundamental three-dimensional representation: those given below follow the phase convention of de Swart.[16] The actions of these generators on the orthonormal kets previously defined are

$$\hat{T}_+|p,q;k,l,m\rangle=\sqrt{(k-m)(m-l+1)}|p,q;k,l,m+1\rangle, \tag{20}$$

$$\hat{T}_-|p,q;k,l,m\rangle=\sqrt{(k-m+1)(m-l)}|p,q;k,l,m-1\rangle, \tag{21}$$

$$\hat{V}_+|p,q;k,l,m\rangle=\sqrt{\frac{(k+2)(m-l+1)(k-q+1)(p+q-k)}{(k-l+1)(k-l+2)}}|p,q;k+1,l,m+1\rangle + \sqrt{\frac{(l+1)(k-m)(q-l)(p+q-l+1)}{(k-l)(k-l+1)}}|p,q;k,l+1,m+1\rangle, \tag{22}$$

$$\hat{V}_-|p,q;k,l,m\rangle=\sqrt{\frac{(k+1)(m-l)(k-q)(p+q-k+1)}{(k-l)(k-l+1)}}|p,q;k-1,l,m-1\rangle + \sqrt{\frac{l(k-m+1)(q-l+1)(p+q-l+2)}{(k-l+1)(k-l+2)}}|p,q;k,l-1,m-1\rangle, \tag{23}$$

$$\hat{U}_+|p,q;k,l,m\rangle=\sqrt{\frac{(k+2)(k-m+1)(k-q+1)(p+q-k)}{(k-l+1)(k-l+2)}}|p,q;k+1,l,m\rangle - \sqrt{\frac{(m-l)(l+1)(q-l)(p+q-l+1)}{(k-l)(k-l+1)}}|p,q;k,l+1,m\rangle, \tag{24}$$

$$\hat{U}_-|p,q;k,l,m\rangle=\sqrt{\frac{(k+1)(k-m)(k-q)(p+q-k+1)}{(k-l)(k-l+1)}}|p,q;k-1,l,m\rangle - \sqrt{\frac{l(m-l+1)(q-l+1)(p+q-l+2)}{(k-l+1)(k-l+2)}}|p,q;k,l-1,m\rangle. \tag{25}$$

Three diagonal operators indicate the values of the subspace labels for a ket:

$$\hat{T}_3|p,q;k,l,m\rangle=I_z|p,q;k,l,m\rangle, \tag{26}$$

$$\hat{Y}|p,q;k,l,m\rangle=Y|p,q;k,l,m\rangle, \tag{27}$$

$$\hat{T}^2|p,q;k,l,m\rangle=\tfrac{1}{2}(\hat{T}_+\hat{T}_-+\hat{T}_-\hat{T}_++2(\hat{T}_3)^2)|p,q;k,l,m\rangle=I(I+1)|p,q;k,l,m\rangle, \tag{28}$$

making use of the definitions of Eqs. (6) and (7). The operators $\hat{T}_+$ and $\hat{T}_-$ move up and down in the variable I_z, and thus have no effect on the ISF. The remaining four nondiagonal (ladder) operators form the basis of the derivation of the recursion relations.

Consider a composite state of highest weight:

$$|\mathscr{P};\mathrm{SHW}\rangle=\sum C^{[\mathscr{P}_1]\quad [\mathscr{P}_2]\quad [\mathscr{P}]}_{[\kappa_1]\quad [\kappa_2]\quad [\mathrm{SHW}]}\ |\mathscr{P}_1;\kappa_1\rangle|\mathscr{P}_2;\kappa_2\rangle. \tag{29}$$

The action of $\hat{V}_+$ on this ket must vanish since each of the two states it produces have $m=p+q+1$, which violates betweenness. Linearity of the generators (e.g., $\hat{V}_+=\hat{V}_{1+}+\hat{V}_{2+}$) implies from Eq. (29) that

$$\hat{V}_+|\mathscr{P};\mathrm{SHW}\rangle=0=\sum C^{[\mathscr{P}_1]\quad [\mathscr{P}_2]\quad [\mathscr{P}]}_{[\kappa_1]\quad [\kappa_2]\quad [\mathrm{SHW}]}\ (|\mathscr{P}_2;\kappa_2\rangle\hat{V}_{1+}|\mathscr{P}_1;\kappa_1\rangle + |\mathscr{P}_1;\kappa_1\rangle\hat{V}_{2+}|\mathscr{P}_2;\kappa_2\rangle). \tag{30}$$

Use of the defining equation for $\hat{V}_+$ [Eq. (22)] changes this expression into a summed four-term expression which must vanish. The orthogonality of any two SU3 kets with different subspace labels allows this sum to be transformed into a four-term recursion relation for the WCG:

$$\begin{aligned}
0=&\sqrt{\frac{(k_1+1)(m_1-l_1)(k_1-q_1)(p_1+q_1-k_1+1)}{(k_1-l_1)(k_1-l_1+1)}}\\
&\times C^{[\mathscr{P}_1]\quad [\mathscr{P}_2]\quad [\mathscr{P}]}_{[k_1-1,l_1,m_1-1]\quad [k_2,l_2,m_2]\quad [\mathrm{SHW}]}\\
&+\sqrt{\frac{(k_2+1)(k_2-q_2)(p_2+q_2-k_2+1)(m_2-l_2+1)}{(k_2-l_2)(k_2-l_2+1)}}\\
&\times C^{[\mathscr{P}_1]\quad [\mathscr{P}_2]\quad [\mathscr{P}]}_{[k_1,l_1,m_1]\quad [k_2-1,l_2,m_2-1]\quad [\mathrm{SHW}]}\\
&+\sqrt{\frac{l_1(q_1-l_1+1)(k_1-m_1+1)(p_1+q_1-l_1+2)}{(k_1-l_1+1)(k_1-l_1+2)}}\\
&\times C^{[\mathscr{P}_1]\quad [\mathscr{P}_2]\quad [\mathscr{P}]}_{[k_1,l_1-1,m_1-1]\quad [k_2,l_2,m_2]\quad [\mathrm{SHW}]}\\
&+\sqrt{\frac{l_2(k_2-m_2+1)(q_2-l_2+1)(p_2+q_2-l_2+2)}{(k_2-l_2+1)(k_2-l_2+2)}}\\
&\times C^{[\mathscr{P}_1]\quad [\mathscr{P}_2]\quad [\mathscr{P}]}_{[k_1,l_1,m_1]\quad [k_2,l_2-1,m_2-1]\quad [\mathrm{SHW}]}.
\end{aligned} \tag{31}$$

This should be valid for any set of projection quantum numbers, thus for $k_1=m_1$ which allows the replacement of the WCG in this expression by products of ISF and simple SU2 Clebsch–Gordan coefficients whose values can be expressed analytically.[17] The result of this replacement is a four-term recursion relation among the ISFs for coupling to a state of highest weight:

$$\begin{aligned}
0=&a_1F^n(\mathrm{SHW}:k_1-1,l_1;k_2,l_2)+a_2F^n(\mathrm{SHW}:k_1,l_1;k_2-1,l_2)-a_3F^n(\mathrm{SHW}:k_1,l_1-1;k_2,l_2)\\
&+a_4F^n(\mathrm{SHW}:k_1,l_1;k_2,l_2-1),
\end{aligned}$$

where

$$a_1=\sqrt{\frac{(k_1+1)(k_1-q_1)(p_1+q_1-k_1+1)(p+q+2I_1+2I_2+3)(p+q+2I_1-2I_2+1)}{I_1(2I_1+1)}},$$

$$a_2=\sqrt{\frac{(k_2+1)(k_2-q_2)(p_2+q_2-k_2+1)(p+q+2I_1+2I_2+3)(p+q-2I_1+2I_2+1)}{I_2(2I_2+1)}},$$

$$a_3=\sqrt{\frac{l_1(q_1-l_1+1)(p_1+q_1-l_1+2)(-p-q+2I_1+2I_2+1)(p+q-2I_1+2I_2+1)}{(2I_1+1)(I_1+1)}}, \tag{32}$$

$$a_4=\sqrt{\frac{l_2(q_2-l_2+1)(p_2+q_2-l_2+2)(-p-q+2I_1+2I_2+1)(p+q+2I_1-2I_2+1)}{(2I_2+1)(I_2+1)}}.$$

Similarly,

$$\hat{U}_{-1}|\mathscr{F};\mathrm{SHW}\rangle=0 \tag{33}$$

since the two kets produced by this operation both violate betweenness. By an analogous set of steps one derives a second, distinct recursion relation:

$$0=b_1F^n(\mathrm{SHW}:k_1+1,l_1;k_2,l_2)-b_2F^n(\mathrm{SHW}:k_1,l_1;k_2+1,l_2)+b_3F^n(\mathrm{SHW}:k_1,l_1+1;k_2,l_2)$$
$$+b_4F^n(\mathrm{SHW}:k_1,l_1;k_2,l_2+1),$$

where

$$b_1=\sqrt{\frac{(k_1+2)(k_1-q_1+1)(p_1+q_1-k_1)(-p-q+2I_1+2I_2+1)(p+q-2I_1+2I_2+1)}{(2I_1+1)(I_1+1)}},$$

$$b_2=\sqrt{\frac{(k_2+2)(k_2-q_2+1)(p_2+q_2-k_2)(-p-q+2I_1+2I_2+1)(p+q+2I_1-2I_2+1)}{(2I_2+1)(I_2+1)}},$$

$$b_3=\sqrt{\frac{(l_1+1)(q_1-l_1)(p_1+q_1-l_1+1)(p+q+2I_1+2I_2+3)(p+q+2I_1-2I_2+1)}{I_1(2I_1+1)}}, \tag{34}$$

$$b_4=\sqrt{\frac{(l_2+1)(q_2-l_2)(p_2+q_2-l_2+1)(p+q+2I_1+2I_2+3)(p+q-2I_1+2I_2+1)}{I_2(2I_2+1)}}.$$

One can "step down" from the ISFs for the coupled state of highest weight to ISFs for any other k,l values by use of two relations derived in an analogous fashion from the actions of the operators $\hat{V}_-$ and $\hat{U}_+$, respectively:

$$F^n(k,l:k_1,l_1;k_2,l_2)=\alpha(c_1F^n(k+1,l-1:k_1,l_1;k_2,l_2)+c_2F^n(k,l-1:k_1,l_1-1;k_2,l_2)$$
$$-c_3F^n(k,l-1:k_1,l_1;k_2-1,l_2)+c_4F^n(k,l-1:k_1,l_1;k_2,l_2-1), \tag{35}$$

where

$$\alpha=\frac{k-l+2}{\sqrt{2l(q-l+1)(p+q-l+2)}},$$

$$c_1=\sqrt{\frac{(k+2)(k-q+1)(p+q-k)(I_1+I_2-I)(-I_1+I_2+I+1)}{(I+1)^2(I_1+I_2+I+2)(I_1-I_2+I+1)}},$$

$$c_2=\sqrt{\frac{4I_1(q_1-l_1+1)(p_1+q_1-l_1+2)(2I_1+1)}{(2I_1+2)(2I_1+2I_2+2I+4)(2I_1-2I_2+2I+2)}},$$

$$c_3=\sqrt{\frac{(k_2+1)(k_2-q_2)(p_2+q_2-k_2+1)(I_1+I_2-I)}{I_2(2I_2+1)(I_1-I_2+I+1)}},$$

$$c_4=\sqrt{\frac{l_2(q_2-l_2+1)(p_2+q_2-l_2+2)(-I_1+I_2+I+1)}{(2I_2+1)(I_2+1)(I_1+I_2+I+2)}};$$

and

$$F^n(k,0:k_1,l_1;k_2,l_2)=\beta(d_1F^n(k+1,0:k_1+1,l_1;k_2,l_2)+d_2F^n(k+1,0:k_1,l_1;k_2+1,l_2)$$
$$+d_3F^n(k+1,0:k_1,l_1;k_2,l_2+1)), \tag{36}$$

where

$$\beta=\sqrt{\frac{(k+2)}{2(k-q+1)(p+q-k)}},$$

$$d_1=\sqrt{\frac{(k_1+2)(k_1-q_1+1)(p_1+q_1-k_1)(2I_1+1)}{(I_1+1)(I_1+I_2+I+2)(I_1-I_2+I+1)}},$$

$$d_2=\sqrt{\frac{(k_2+2)(k_2-q_2+1)(p_2+q_2-k_2)(-I_1+I_2+I+1)}{(2I_2+1)(I_2+1)(I_1+I_2+I+2)}},$$

$$d_3=\sqrt{\frac{(l_2+1)(q_2-l_2)(p_2+q_2-l_2+1)(I_1+I_2-I)}{I_2(2I_2+1)(I_1-I_2+I+1)}}.$$

The second of these two expressions is not the most such general relation which can be derived, but when used in combination with the first, it is sufficient to determine the value of any ISF for the given irrep coupling, once the values of the ISFs for k,l=SHW are known.

V. DETERMINING THE ISOSCALAR FACTORS

To move from the recursion relations to determination of the ISF, a sign convention and a resolution scheme for outer degeneracy must be chosen. For a given coupling,

$$(p_1,q_1)\otimes(p_2,q_2)\rightarrow(p,q),$$

the degeneracy is determined by Eq. (13). For cases of degeneracy $\eta=1$, the choice of sign of one of the nonvanishing ISFs for (k,l)=SHW is sufficient to determine all the others. In practice, one such ISF is set equal to 1; Eqs. (32) and (34) are used to generate all others from this one; and all are multiplied by a common factor to enforce the normalization condition

$$\sum_{k_1,l_1,k_2,l_2}(F(\mathrm{SHW}:k_1,l_1;k_2,l_2))^2=1. \tag{37}$$

Even in such simple cases, the particular ISF to initialize must be chosen as one which allows use of the recursion relations (32) and (34) to determine neighboring values, and a recursive path from the starting point to arbitrary ISFs must be deduced.

When the (k,l)=SHW ISFs are all known, Eq. (36) can be used to deduce all $k<p+q$, $l=0$ ISFs, and from them Eq. (35) implies all $l>0$ cases.

The most delicate problem is the determination of an algorithm which uniquely determines all ISFs in cases of outer degeneracy two or higher. Such an algorithm has been developed and implemented in C language codes for evaluation of arbitrary ISFs as floating point values, and as exact precision square roots of a ratio of integers.[18] The ISFs produced by this algorithm share all the symmetries under irrep exchange and conjugation with the familiar SU2 Clebsch–Gordan coefficients.

The logic of the algorithm can be made clearer through a change of variables. Of the four integers, k_1,l_1,k_2,l_2, used heretofore as parameters of the isoscalar factor for a coupling to a state of highest weight, only three are independent. The hypercharge conservation relation (10) implies

$$k_1+l_1+k_2+l_2=\tfrac{1}{3}(2(p_1+p_2)+4(q_1+q_2)+p-q).$$

Use of the definition

$$s\equiv k_1-l_1+k_2-l_2$$

allows the ISFs to be expressed as $F^n(\mathrm{SHW}{:}s,k_1,l_1)$. The degeneracy index $n=0,1,\ldots,\eta-1$ is necessary for couplings with degeneracy $\eta>1$. The algorithm works as follows:

(i) Make the following assignments for $0\leqslant n<\eta$, $0\leqslant n'<\eta$; $F^n(\mathrm{SHW}{:}s_{\max}-2n',k_{1\,\min},l_{1\,\min})=\delta_{n,n'}$, where δ is the Kroneker delta.

(ii) Using these assignments, the recursion relations (32) and (34) are adequate to determine all ISFs (with k,l=SHW) for $s_{\max}\geqslant s\geqslant s_{\max}-2(\eta-1)$.

(iii) The ISFs (with k,l=SHW) for remaining values of s can be determined without further assignments, evaluating each set of values for fixed s before moving to lower s. To move to a lower s value, the recursion relation reduces to only three terms either at $k_1=k_{1\,\max}$, $l_1=l_{1\,\min}$; or at $k_1=k_{1\,\min}$, $l_1=l_{1\,\max}$. This allows determination of one ISF for the new s value, which then allows the evaluation of all others at this s value using the full four-term recursion relation. This stepdown procedure fails in a small subset of cases, whereupon one must take advantage of permutation symmetry (discussed below) to move to the lower value of s.

(iv) The $F^0(\mathrm{SHW}{:}s,k_1,k_2)$ values, once normalized, are proper isoscalar factors. A linear combination of the F^0s and the F^1s, made orthogonal to F^0 and normalized, become proper $F^1(\mathrm{SHW}{:}s,k_1,k_2)$ values. Likewise, using the Gram–Schmidt orthogonalization procedure, each set of F^n with higher n is constructed from those with lower ns.

(v) Remaining ISFs for values of $k,l\neq$SHW can be determined in a straightforward way using the remaining recursion relations, (35) and (36).

In this description, $s_{\max}$ is the maximum value of s for which a nonvanishing ISF occurs for a coupling of fixed p, q, p_1, q_1, p_2, q_2 values: $k_{1\,\min}$, $l_{1\,\min}$, $k_{1\,\max}$, $l_{1\,\max}$ are the minimum and maximum values of the k_1 and l_1 variables for a particular value of s.

VI. SYMMETRIES OF THE ISOSCALAR FACTOR

The symmetries of the SU2 Clebsch–Gordan coefficient under permutation of irreps (j_i,m_i) and under conjugation $(j,m\rightarrow j,-m)$, known as the Racah symmetries, are well known and frequently utilized to simplify tabulations of coefficients and recoupling calculations. For SU3 couplings of degeneracy one, a complete set of Racah symmetries can be demonstrated. The

algorithm described in Sec. V extends these symmetries to couplings of arbitrary degeneracy, in contrast to some other degeneracy resolution schemes. Once the symmetries of the SU3 WCG are known, one can use the symmetry relations for the SU2 Clebsch–Gordan coefficients to deduce symmetry properties of the SU3 isoscalar factors.

Derivation of the symmetry relations for the SU3 WCG is straightforward, albeit tedious. If one applies the V_+ operator [Eq. (22)] to both sides of the defining expression for the WCG [Eq. (3)], the result is a linear expression involving six WCGs of various indices and corresponding coefficients which sum to zero. Under each of the transformations

(1) $(p_1,q_1;k_1,l_1,m_1)\leftrightarrow(p_2,q_2;k_2,l_2,m_2)$, referred to as $(1\leftrightarrow 2)$;
(2) $(p_1,q_1;k_1,l_1,m_1)\rightarrow(q,p;p+q-l,p+q-k,p+q-m)$ and $(p,q;k,l,m)\rightarrow(q1,p1;p1+q1-l1,p1+q1-k1,p1+q1-m1)$, referred to as $(1\leftrightarrow\bar{3})$; and
(3) $(p,q;k,l,m)\rightarrow(q,p;p+q-l,p+q-k,p+q-m)$ and similarly for the states p_1,q_1 and p_2,q_2, referred to as *conjugation*,

the coefficients in the six term expression of WCGs transform among one another in pairs, easily exhibiting the fact that the transformed WCGs (within a sign which depends on the k,l,m indices) obey the same six term recursion relations as the original WCGs.

The symmetry transformations can also involve a sign change which depends upon the p and q variables. This is fully dependent upon another sign convention which must be chosen in order to fully specify the WCGs and ISFs. Convenient choices are

$$C^{\,j_1\quad j_2\quad j}_{m_1=j_1\quad m_2=-j_2\quad >0},$$

the familiar Condon and Shortley phase convention,[19] and

$$F^n(\mathrm{SHW{:}SHW}_1;k_{2\,\max},l_{2\,\min})>0,$$

with the s value of the F chosen to be positive given as $s_{\max}-n$. To derive the p,q dependence of the phase under one of the symmetry transformations, begin with a SU3 WCG which is positive under this convention; apply the transformation; and determine the sign of the transformed WCG relative to that which is positive by convention among the transformed coefficients, using the recursion relations derived earlier. This sign, which will depend upon the six p,q values only, becomes part of the symmetry relation.

The absolute magnitude of the ratio of a WCG to its permuted version results from the normalization condition

$$\sum_{\kappa_1,\kappa_2}\left(C^{[\mathscr{P}_1]\quad [\mathscr{P}_2]\quad [\mathscr{P}]}_{[\kappa_1]\quad [\kappa_2]\quad [\kappa]}\right)^2=1. \tag{38}$$

It is straightforward to show that two of the transformations—$(1\leftrightarrow 2)$ and conjugation—produce no change in normalization and thus require no constant term; and the third—$(1\leftrightarrow\bar{3})$—requires a constant equal to the square root of the ratio of the dimension of the irreps $\mathscr{P}_1$ and $\mathscr{P}$.

When one considers couplings which have degeneracy greater than one, each set of distinct WCG's (labeled by the index n) has a unique element chosen as positive by convention. As a result, there is an additional phase contribution of $(-1)^n$ in each of the transformations considered here.

The resulting symmetry relations are as follows:

$$C\begin{matrix}[\mathscr{P}_1] & \overset{n}{[\mathscr{P}_2]} & [\mathscr{P}] \\ [\kappa_1] & [\kappa_2] & [\kappa]\end{matrix}=(-1)^{\gamma+\sigma+\max(\gamma,\sigma)+n}C\begin{matrix}[\mathscr{P}_2] & \overset{n}{[\mathscr{P}_1]} & [\mathscr{P}] \\ [\kappa_2] & [\kappa_1] & [\kappa]\end{matrix} \tag{39}$$

for the $(1\leftrightarrow 2)$ transformation;

$$C\begin{matrix}[\mathscr{P}_1] & \overset{n}{[\mathscr{P}_2]} & [\mathscr{P}] \\ [\kappa_1] & [\kappa_2] & [\kappa]\end{matrix}=(-1)^{m_2+n}\sqrt{\frac{(p+1)(q+1)(p+q+2)}{(p_1+1)(q_1+1)(p_1+q_1+2)}}C\begin{matrix}[\tilde{\mathscr{P}}] & \overset{n}{[\mathscr{P}_2]} & [\tilde{\mathscr{P}}_1] \\ [\tilde{\kappa}] & [\kappa_2] & [\tilde{\kappa}_1]\end{matrix} \tag{40}$$

for the $(1\leftrightarrow\bar{3})$ transformation (where $\tilde{\mathscr{P}}$ represents the ordered pair q,p and $\tilde{\kappa}$ represents $p+q-l$, $p+q-k$, $p+q-m$); and

$$C\begin{matrix}[\mathscr{P}_1] & \overset{n}{[\mathscr{P}_2]} & [\mathscr{P}] \\ [\kappa_1] & [\kappa_2] & [\kappa]\end{matrix}=(-1)^{\gamma+\sigma+\min(\gamma,\sigma)+n}C\begin{matrix}[\tilde{\mathscr{P}}_1] & \overset{n}{[\tilde{\mathscr{P}}_2]} & [\tilde{\mathscr{P}}] \\ [\tilde{\kappa}_1] & [\tilde{\kappa}_2] & [\tilde{\kappa}]\end{matrix} \tag{41}$$

for the conjugation transformation.

No additional information is given by repeating this procedure with the ladder operators $\hat{V}_-$ and $\hat{U}_+$ since they are related to the two operators already considered by Hermitian conjunction: similar treatment using $\hat{T}_+$ and $\hat{T}_-$ generate the symmetry relations for the SU2 Clebsch–Gordan coefficients.

Corresponding symmetry relations for the isoscalar factors follow from the above combined with the symmetry relations for the SU2 Clebsch–Gordan coefficients in the Condon and Shortley phase conventions. They are

$$F^n(\mathscr{P},\kappa:\mathscr{P}_1,\kappa_1;\mathscr{P}_2,\kappa_2)=(-1)^{\gamma+\sigma+\max(\gamma,\sigma)+n+l_1+l_2-l}F^n(\mathscr{P},\kappa:\mathscr{P}_2,\kappa_2;\mathscr{P}_1,\kappa_1) \tag{42}$$

for the $(1\leftrightarrow 2)$ transformation [here κ represents the pair (k,l)];

$$F^n(\mathscr{P},\kappa:\mathscr{P}_1,\kappa_1;\mathscr{P}_2,\kappa_2)=(-1)^{l_2+n}\sqrt{\frac{(p+1)(q+1)(p+q+2)(k_1-l_1+1)}{(p_1+1)(q_1+1)(p_1+q_1+2)(k-l+1)}}\times F^n(\tilde{\mathscr{P}}_1,\tilde{\kappa}_1:\tilde{\mathscr{P}},\tilde{\kappa};\mathscr{P}_2,\kappa_2) \tag{43}$$

for the $(1\leftrightarrow\bar{3})$ transformation; and

$$F^n(\mathscr{P},\kappa:\mathscr{P}_1,\kappa_1;\mathscr{P}_2,\kappa_2)=(-1)^{\gamma+\sigma+\min(\gamma,\sigma)+n+l_2+l_2-l}F^n(\tilde{\mathscr{P}},\tilde{\kappa}:\tilde{\mathscr{P}}_1,\tilde{\kappa}_1;\tilde{\mathscr{P}}_2,\tilde{\kappa}_2) \tag{44}$$

for the conjunction transformation.

The choice of a resolution procedure which yields symmetries such as these produces considerable simplifications in calculations of physical states, reduces the complexity of definitions of $6-j$ and $9-j$ type recoupling coefficients, and significantly shortens databases and printed tables of WCGs and ISFs.

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Errata: Fluctuations of a spherical gravitational impulsive wave [J. Math. Phys. 34, 690–699 (1993)] and Fluctuations of a rotating impulsive wave [J. Math. Phys. 35, 3043–3050 (1994)]

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There are two main common errors in these papers.

1. The Greens function, used in Eq. (25) of the paper published in J. Math. Phys. **34**, 690–699 (1993) has to be multiplied by u/u' when applied to the inhomogenous term. The same expression is also used in the article, J. Math. Phys. **35**, 3043–3050 (1994). This modifies Eq. (28) of the first article as

$$g_1=\frac{1}{iu}\left(\frac{k_1x+k_2y}{x^2+y^2}+\frac{iR}{2}\log(x^2+y^2)\right)$$

and Eq. (26) of the second article as

$$f_1=\frac{2}{iu}\frac{k_y-k_2x}{x^2+y^2}+iR\tan^{-1}\frac{y}{x}.$$

The following expressions change accordingly.

The final expression which does not appear explicitly in these references reads

$$G_F^{(1)}=\frac{1}{32\pi}\frac{1}{(u-u')(v-v')}\left[\frac{\Theta(v)v-\Theta(v')v'}{(v-v')}\right]\left[\frac{\delta}{2}\log(x^2+y^2)-2\epsilon\tan^{-1}y/x\right]$$
$$+\left(\frac{\Theta(v)u'-\Theta(v')u}{(u-u')}\right)[\delta\log(x^2+y^2)-4\epsilon\tan^{-1}y/x]$$
$$+(\Theta(v)+\Theta(v'))\left[\frac{\delta}{4}\log(x^2+y^2)-2\epsilon\tan^{-1}y/x\right].$$

Here the terms proportional to δ give the result in the first paper and those proportional to ϵ give the result in the second paper. We could not find the finite part of these expressions as u goes to u' and v goes to v'.

2. The symmetrization of the final expression in the above mentioned articles is not correct. As seen in this expression upon proper symmetrization the Hadamard form for the Greens function is obtained, contrary to the claims made in these two articles.

Canonical commutation relations, the Weierstrass Zeta function, and infinite dimensional Hilbert space representations of the quantum group $U_q(\mathfrak{sl}_2)$

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A two-dimensional quantum system of a charged particle interacting with a vector potential determined by the Weierstrass Zeta function is considered. The position and the physical momentum operators give a representation of the canonical commutation relations with two degrees of freedom. If the charge of the particle is not an integer (the case corresponding to the *Aharonov–Bohm effect*), then the representation is inequivalent to the Schrödinger representation. It is shown that the inequivalent representation induces infinite-dimensional Hilbert space representations of the quantum group $U_q(\mathfrak{sl}_2)$. Some properties of these representations of $U_q(\mathfrak{sl}_2)$ are investigated. © *1996 American Institute of Physics.*
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I. INTRODUCTION

In a previous paper,[1] we considered a quantum system of a charged particle moving in the Euclidean plane $\mathbf{R}^2$ under the influence of a perpendicular magnetic field, which may be strongly singular at some fixed points $\mathbf{a}_1,...,\mathbf{a}_N$ in $\mathbf{R}^2$. If the magnetic field is concentrated on the discrete set $\{\mathbf{a}_n\}_{n=1}^N$ in the sense of distribution, then the position and the physical momentum operators give a representation of the canonical commutation relations (CCRs) (Heisenberg relations) with two degrees of freedom.

Here we recall some technical terms in the representation theory of CCR. A set $\{\mathscr{H},\mathscr{D},\{Q_j,P_j\}_{j=1}^d\}$ consisting of a Hilbert space $\mathscr{H}$, a dense subspace $\mathscr{D}$ of $\mathscr{H}$, and self-adjoint operators Q_j, P_j, $(j=1,\ldots,d)$ is called a representation of the CCR with d degrees of freedom if $\mathscr{D}\subset\cap_{j,k=1}^d[D(Q_jQ_k)\cap D(Q_jP_k)\cap D(P_kQ_j)\cap D(P_jP_k)]$ [$D(T)$ denotes the domain of operator T] and the CCR,

$$[Q_j,Q_k]=0,\quad [P_j,P_k]=0,\quad [Q_j,P_k]=i\delta_{jk},\quad j,k=1,\ldots,d,$$

hold on $\mathscr{D}$, where $[S,T]:=ST-TS$. Following Putnam,[2] we say that a set $\{Q_j,P_j\}_{j=1}^d$ of self-adjoint operators on a Hilbert space is a *Schrödinger d system* if it is unitarily equivalent to a direct sum of the Schrödinger representation of the CCR with d degrees of freedom. A representation $\{\mathscr{H},\mathscr{D},\{Q_j,P_j\}_{j=1}^d\}$ of CCR is called *equivalent* (resp., *inequivalent*) if $\{Q_j,P_j\}_{j=1}^d$ is (resp., not) a Schrödinger d system.

In Ref. 1 the following facts were shown: (i) the representation of CCR mentioned above is equivalent if and only if the magnetic flux is locally quantized (i.e., the magnetic flux at each point $\mathbf{a}_n$ $(n=1,\ldots,N)$ is an integer multiple of $2\pi/\alpha$, where α is the charge of the particle); (ii) the inequivalent representation appearing in the case where the magnetic flux is not locally quantized may be regarded as a mathematical form of the *Aharonov–Bohm effect*.[3] A geometric construction of a representation of CCR that is unitarily equivalent to the one given in Ref. 1 was considered by Kurose and Nakazato,[4] and more detailed properties of the representation were discussed.

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To investigate differences between the equivalent and the inequivalent representations of CCR in Ref. 1, an analysis has been made on Dirac–Weyl operators defined in terms of the physical momentum operator.[5] Moreover, the framework and results in Ref. 1 were extended to the case of a non-Abelian gauge theory.[6,7]

Recently Wiegmann and Zabrodin[8] considered a quantum system of a particle on a two-dimensional square lattice in a magnetic field and showed that magnetic translations on the lattice are related to finite-dimensional representations of the quantum group $U_q(\mathfrak{sl}_2)$. Inspired by their work, we investigate in this paper if there is any connection between the quantum system considered in Ref. 1 and representations of $U_q(\mathfrak{sl}_2)$. We shall show that, for a vector potential determined by the Weierstrass Zeta function, special elements of the unitary groups generated by the components of the physical momentum operator induce representations of $U_q(\mathfrak{sl}_2)$ on the Hilbert space $L^2(\mathbf{R}^2)$. This establishes a connection of a classical special function to $U_q(\mathfrak{sl}_2)$. A particular feature of the representations of $U_q(\mathfrak{sl}_2)$ given in this paper is that they have no finite-dimensional irreducible components.

The present paper is organized as follows. In Sec. II we consider a quantum system of a charged particle in $\mathbf{R}^2$ under the influence of a perpendicular magnetic field that may be singular at points in an *infinite lattice* [see (2.1)]. This is an extension of the framework of Ref. 1 to the case where the number of possible singular points of the magnetic field is infinite. Fundamental results in Ref. 1 continue to hold in the present case too with no significant modifications. As in the case of Ref. 1, the position operator and the physical momentum operator $\mathbf{P}=(P_1,P_2)$ of the particle give a representation of the CCR with two degrees of freedom if the magnetic field is concentrated on the infinite lattice. Spectral properties of the unitary operators generated by P_1 and P_2 are analyzed. Also, we show that, under some conditions for the vector potential of the magnetic field, P_1 and P_2 have permutation-reflection symmetries.

In Secs. III–V, we consider the special case where the vector potential $A=A_1\,dx+A_2\,dy$ (a 1-form) of the magnetic field is given by the Weierstrass Zeta function ζ in such a way that $\zeta=A_2+iA_1$ [see (3.2)–(3.4)]. We first show in Sec. III that, if the charge of the particle is not an integer, then special elements of the unitary groups generated by P_1 and P_2 give representations of the quantum plane. Unitary equivalences of these representations are discussed. As is shown in Ref. 8, a representation of the quantum plane with some additional properties induces representations of $U_q(\mathfrak{sl}_2)$. Applying this idea, we construct in Secs. IV and V representations of $U_q(\mathfrak{sl}_2)$ on $L^2(\mathbf{R}^2)$ and investigate some properties of them.

II. A CHARGED PARTICLE IN A MAGNETIC FIELD WITH POSSIBLE SINGULARITIES ON AN INFINITE LATTICE

A. Representation of CCR

We consider a quantum system of a charged particle with charge $\alpha\in\mathbf{R}\backslash\{0\}$ moving in the plane $\mathbf{R}^2=\{\mathbf{r}=(x,y)|x,y\in\mathbf{R}\}$ under the influence of a perpendicular magnetic field B that may be singular at points in the infinite lattice,

$$\mathbf{Z}^2_{\omega_1,\omega_2}:=\{\mathbf{\Omega}_{m,n}=(\omega_1 m,\omega_2 n)|m,n\in\mathbf{Z}\},\tag{2.1}$$

where ω_j, $j=1,2$, are positive constants and $\mathbf{Z}$ is the set of integers. A vector potential of the magnetic field B is given by a *continuously differentiable* real 1-form $A=A_1\,dx+A_2\,dy$ on the nonsimply connected domain

$$\mathbf{M}=\mathbf{R}^2\backslash\mathbf{Z}^2_{\omega_1,\omega_2},\tag{2.2}$$

such that

$$B=D_xA_2-D_yA_1,\tag{2.3}$$

in the distribution sense, where D_x and D_y are the generalized partial differential operators in the variables x and y, respectively. We say that A is *flat on* $\mathbf{M}$ if $B=0$ on $\mathbf{M}$, i.e., B is concentrated on $\mathbf{Z}^2_{\omega_1,\omega_2}$ (in the sense of distribution).

Throughout this paper we use a physical unit system such that $\hbar$ (the Planck constant divided by 2π)$=c$ (the light velocity)$=1$. Let (Q_1,Q_2) be the position operator of the particle, i.e., Q_1 and Q_2 are the maximal multiplication operators by x and y acting in the Hilbert space $L^2(\mathbf{M})\cong L^2(\mathbf{R}^2)$, respectively. The physical (kinetic) momentum operator $\mathbf{P}=(P_1,P_2)$ of the particle is defined by the operators

$$P_j=p_j-\alpha A_j, \quad j=1,2, \tag{2.4}$$

acting in $L^2(\mathbf{R}^2)$, where (p_1,p_2) is the momentum operator of the free particle:

$$p_1=-iD_x, \quad p_2=-iD_y. \tag{2.5}$$

We denote by $C_0^m(\mathbf{M})$ $(m=0,1,2,\ldots)$ the space of m times continuously differentiable functions on $\mathbf{M}$ with bounded support in $\mathbf{M}$. In the same way as in Ref. 1, we can prove the following fact.

Lemma 2.1:

(i) *Each P_j is essentially self-adjoint on $C_0^1(\mathbf{M})$. (We denote the closure of P_j by the same symbol.)*

(ii) *Suppose that A is flat on $\mathbf{M}$. Then $\{L^2(\mathbf{R}^2), C_0^2(\mathbf{M}), \{Q_j,P_j\}_{j=1}^2\}$ is a representation of the CCR with two degrees of freedom.*

The analysis of the representation $\{L^2(\mathbf{R}^2), C_0^2(\mathbf{M}), \{Q_j,P_j\}_{j=1}^2\}$ in Lemma 2.1 can be done in quite the same way as in the case where $\mathbf{Z}^2_{\omega_1,\omega_2}$ is replaced by a finite discrete set in $\mathbf{R}^2$ (see Refs. 1, 4, and 6). Hence, as for that, we describe only results needed later. Let

$$\mathbf{S}_1=\mathbf{R}\backslash\{m\omega_1\}_{m\in\mathbf{Z}}, \quad \mathbf{S}_2=\mathbf{R}\backslash\{n\omega_2\}_{n\in\mathbf{Z}}.$$

For $(x,y)\in\mathbf{R}\times\mathbf{S}_2$, we can define

$$U_1(x,y)=\exp\left(-i\alpha\int_0^x A_1(x',y)dx'\right). \tag{2.6}$$

Then U_1 defines a unique unitary operator as a multiplication operator on $L^2(\mathbf{R}^2)$. Similarly, the function

$$U_2(x,y)=\exp\left(-i\alpha\int_0^y A_2(x,y')dy'\right), \quad (x,y)\in\mathbf{S}_1\times\mathbf{R}, \tag{2.7}$$

defines a unique unitary operator as a multiplication operator on $L^2(\mathbf{R}^2)$. We then have *operator equalities*,

$$P_j=U_j^{-1}p_jU_j, \quad j=1,2. \tag{2.8}$$

It follows from these relations that, for all $t\in\mathbf{R}$, $\psi\in L^2(\mathbf{R})$, and for almost everywhere (a.e.) (x,y),

$$(e^{itP_1}\psi)(x,y)=\exp\left(-i\alpha\int_x^{x+t} A_1(x',y)dx'\right)\psi(x+t,y), \tag{2.9}$$

$$(e^{itP_2}\psi)(x,y)=\exp\left(-i\alpha\int_y^{y+t}A_2(x,y')dy'\right)\psi(x,y+t). \tag{2.10}$$

Let $C_\pm(x,y;s,t)$ $(x,y,s,t\in\mathbf{R})$ be hook-shaped paths from (x,y) to $(x+s,y+t)$ given by

$$C_-(x,y;s,t)=\{(x+\theta s,y)|0\leqslant\theta\leqslant 1\}\cup\{(x+s,y+\theta t)|0\leqslant\theta\leqslant 1\},$$

$$C_+(x,y;s,t)=\{(x,y+\theta t)|0\leqslant\theta\leqslant 1\}\cup\{(x+\theta s,y+t)|0\leqslant\theta\leqslant 1\},$$

and set

$$C(x,y;s,t)=C_+(x,y;s,t)^{-1}\circ C_-(x,y;s,t), \tag{2.11}$$

the rectangular path: $(x,y)\to(x+s,y)\to(x+s,y+t)\to(x,y+t)\to(x,y)$. For $s,t\in\mathbf{R}$, we set

$$\mathbf{S}_1^{(s)}=\mathbf{R}\backslash\{\omega_1 m,\omega_1 m-s|m\in\mathbf{Z}\},\quad \mathbf{S}_2^{(t)}=\mathbf{R}\backslash\{\omega_2 n,\omega_2 n-t|n\in\mathbf{Z}\}, \tag{2.12}$$

and define

$$\mathbf{M}_{s,t}=\mathbf{S}_1^{(s)}\times\mathbf{S}_2^{(t)},\quad s,t\in\mathbf{R}. \tag{2.13}$$

For each $s,t\in\mathbf{R}$, we can define a function $\Phi_{s,t}^A$ on $\mathbf{M}_{s,t}$ by

$$\Phi_{s,t}^A(x,y)=\int_{C(x,y;s,t)}A,\quad (x,y)\in\mathbf{M}_{s,t}, \tag{2.14}$$

which physically means the magnetic flux passing through the interior domain of the closed curve $C(x,y;s,t)$. Since $\mathbf{R}^2\backslash\mathbf{M}_{s,t}$ is a null set with respect to the two-dimensional Lebesgue measure, one can regard $\Phi_{s,t}^A$ as a real-valued function on $\mathbf{R}^2$, which is a.e. finite. Hence $\Phi_{s,t}^A$ defines a unique self-adjoint multiplication operator on $L^2(\mathbf{R}^2)$. We denote this operator by the same symbol. The following theorem gives commutation relations for the one parameter unitary groups generated by Q_j and P_j, $j=1,2$.

Theorem 2.2. (cf. Theorem 2.1 in Ref. 1): *For all* $s,t\in\mathbf{R}$,

$$e^{isQ_j}e^{itP_k}=e^{-ist\delta_{jk}}e^{itP_k}e^{isQ_j}, \tag{2.15}$$

$$e^{isP_1}e^{itP_2}=e^{-i\alpha\Phi_{s,t}^A}e^{itP_2}e^{isP_1}. \tag{2.16}$$

Following Ref. 1, we say that *the magnetic flux is locally quantized if, for all* $s,t\in\mathbf{R}$, $\Phi_{s,t}^A$ *is a* $2\pi\mathbf{Z}/\alpha$*-valued function on* $\mathbf{M}_{s,t}$.

Theorem 2.2 implies the following characterization of the representation $\{Q_j,P_j\}_{j=1}^2$ of CCR in the case where A is flat [Lemma 2.1(ii)].

Theorem 2.3: *Suppose that* A *is flat on* $\mathbf{M}$. *Then the representation* $\{Q_j,P_j\}_{j=1}^2$ *of CCR is equivalent if and only if the magnetic flux is locally quantized*.

Remark: (i) In the case where the magnetic flux is not locally quantized, formula (2.16) may be regarded as a mathematical form of the *Aharonov–Bohm effect*.[9] Thus the inequivalent representation of $\{Q_j,P_j\}_{j=1}^2$ corresponds to the Aharonov–Bohm effect.

(ii) In operator theory, two self-adjoint operators, S and T, on a Hilbert space are said to be *strongly commuting* if their spectral measures commute. It is well known that S and T are strongly commuting if and only if $e^{iaS}e^{ibT}=e^{ibT}e^{iaS}$ for all $a,b\in\mathbf{R}$ (Theorem VIII.13 in Ref. 10). It follows from this fact and (2.16) that P_1 and P_2 *are strongly commuting if and only if the magnetic flux is locally quantized*.

Let $\omega_0>0$ be a number such that, for all $(m,n),(m',n')\in\mathbf{Z}^2$ with $(m,n)\neq(m',n')$, $\{\mathbf{r}||\mathbf{r}-\mathbf{\Omega}_{m,n}|<\omega_0\}\cap\{\mathbf{r}||\mathbf{r}-\mathbf{\Omega}_{m',n'}|<\omega_0\}=\emptyset$. The following fact is easily proven.

Lemma 2.4: Suppose that A is flat. Let $0<\delta<\omega_0$. Then

$$\gamma_{m,n}(A):=\int_{|\mathbf{r}-\mathbf{\Omega}_{m,n}|=\delta}A \tag{2.17}$$

is independent of δ, where the orientation of the integral on the right-hand side (rhs) is taken to be anticlockwise. Moreover, for all $s,t\in\mathbf{R}$,

$$\Phi^A_{s,t}(x,y)=\epsilon(s)\epsilon(t)\sum_{\mathbf{\Omega}_{m,n}\in D(x,y;s,t)}\gamma_{m,n}(A),\quad (x,y)\in\mathbf{M}_{s,t},$$

where $D(x,y;s,t)$ is the interior domain of $C(x,y;s,t)$ and $\epsilon(t)$ is the sign function: $\epsilon(t)=1$ for $t\geqslant 0$; $\epsilon(t)=-1$ for $t<0$.

Theorem 2.3 and Lemma 2.4 imply the following fact.

Theorem 2.5: *Suppose that A is flat. Then the representation $\{Q_j,P_j\}_{j=1}^2$ of CCR is equivalent if and only if $\gamma_{m,n}(A)\in 2\pi\mathbf{Z}/\alpha$ for all $m,n\in\mathbf{Z}$.*

B. Spectral properties

For later use, we investigate spectral properties of some unitary operators. For a densely defined closed linear operator T on a Hilbert space, we denote by $\sigma(T)$ [resp., $\sigma_p(T)$] the spectrum (resp., point spectrum) of T. We set

$$\mathbb{T}=\{z\in\mathbf{C}||z|=1\}. \tag{2.18}$$

Lemma 2.6:

(i) *$\sigma(P_j)=\mathbf{R}$, $\sigma_p(P_j)=\emptyset$, $j=1,2$.*

(ii) *For all $t\in\mathbf{R}\backslash\{0\}$ and $j=1,2$, $\sigma(e^{itP_j})=\mathbb{T}$, $\sigma_p(e^{itP_j})=\emptyset$.*

Proof: (i) By (2.8), we have $\sigma(P_j)=\sigma(p_j)=\mathbf{R}$, $\sigma_p(P_j)=\sigma_p(p_j)=\emptyset$. (ii) This follows from part (i) and the spectral mapping theorem. ■

Lemma 2.7: For all $s,t\in\mathbf{R}\backslash\{0\}$,

$$\sigma_p(e^{isP_1}e^{itP_2})=\emptyset,\quad \sigma_p(e^{itP_2}e^{isP_1})=\emptyset. \tag{2.19}$$

Proof: It follows from (2.9) and (2.10) that, for all $s,t\in\mathbf{R}$,

$$e^{isP_1}e^{itP_2}=\exp\left(-i\alpha\int_{C_-(x,y;s,t)}A\right)e^{isp_1}e^{itp_2}, \tag{2.20}$$

$$e^{itP_2}e^{isP_1}=\exp\left(-i\alpha\int_{C_+(x,y;s,t)}A\right)e^{itp_2}e^{isp_1}. \tag{2.21}$$

Since $e^{isP_1}e^{itP_2}$ is unitary, we have $\sigma_p(e^{isP_1}e^{itP_2})\subset\mathbb{T}$. Suppose that there exists a vector $\psi\in L^2(\mathbf{R}^2)$ and a constant $\lambda\in\mathbb{T}$ such that $e^{isP_1}e^{itP_2}\psi=\lambda\psi$. Then, by (2.20), we have $\exp(e^{-i\alpha}\int_{C_-(x,y;s,t)}A)\psi(x+s,y+t)=\lambda\psi(x,y)$ a.e. (x,y). Hence $|\psi(x,y)|=|\psi(x+s,y+t)|$ a.e. (x,y), which, together with the fact $\psi\in L^2(\mathbf{R}^2)$, implies $\psi=0$. Thus the first formula of (2.19) follows. Similarly, using (2.21), we can prove the second one of (2.19). ■

Proposition 2.8: Consider the case where the magnetic flux is locally quantized. Then, for all $t,s\in\mathbf{R}\backslash\{0\}$,

$$\sigma(e^{isP_1}e^{itP_2})=\sigma(e^{itP_1}e^{isP_2})=\mathbb{T}.$$

Proof: Under the present assumption, P_1 and P_2 strongly commute [see Remark (ii) after Theorem 2.3]. Hence, by the two variable functional calculus, we see that sP_1+tP_2 is essentially self-adjoint and $e^{isP_1}e^{itP_2} = e^{itP_2}e^{isP_1} = e^{i(\overline{sP_1+tP_2})}$, where $\overline{sP_1+tP_2}$ is the closure of sP_1+tP_2. By the two variable functional calculus and Lemma 2.6(i), we have $\sigma(\overline{sP_1+tP_2}) = \mathbf{R}$. Thus, by the spectral mapping theorem, we obtain the desired result. ■

Remark: We have been unable to identify $\sigma(e^{isP_1}e^{itP_2})$ and $\sigma(e^{itP_2}e^{isP_1})$ in the case where the magnetic field is not locally quantized. It would be interesting to see if there appears any difference from the case where the magnetic field is locally quantized. In the case of Dirac–Weyl operators defined in terms of P_1 and P_2, such differences exist; see Ref. 5. We leave this problem as an open problem.

C. Permutation-reflection symmetry of the physical momentum operator

Let $R_j : L^2(\mathbf{R}^2) \to L^2(\mathbf{R}^2)$, $j=1,2$, be the unitary operators defined by

$$(R_1\psi)(x,y) = \psi(-y,x), \quad (R_2\psi)(x,y) = \psi(y,-x), \quad \psi \in L^2(\mathbf{R}^2). \tag{2.22}$$

Then it is easy to see that

$$R_1R_2 = R_2R_1 = I, \tag{2.23}$$

$$R_1p_1R_1^{-1} = -p_2, \quad R_1p_2R_1^{-1} = p_1, \tag{2.24}$$

$$R_2p_1R_2^{-1} = p_2, \quad R_2p_2R_2^{-1} = -p_1. \tag{2.25}$$

As usual, we denote by $z=x+iy$ the point in the complex plane $\mathbf{C}$ corresponding to $\mathbf{r}=(x,y)\in\mathbf{R}^2$. We set

$$\widetilde{A}(z) = A_2(x,y) + iA_1(x,y). \tag{2.26}$$

Proposition 2.9:
(i) *Suppose that*

$$\widetilde{A}(iz) = -i\widetilde{A}(z). \tag{2.27}$$

Then

$$R_1P_1R_1^{-1} = -P_2, \quad R_1P_2R_1^{-1} = P_1. \tag{2.28}$$

(ii) *Suppose that*

$$\widetilde{A}(iz) = i\widetilde{A}(-z). \tag{2.29}$$

Then

$$R_2P_1R_2^{-1} = P_2, \quad R_2P_2R_2^{-1} = -P_1. \tag{2.30}$$

Proof: (i) Condition (2.27) is equivalent to that

$$A_2(-y,x) = A_1(x,y), \quad A_1(-y,x) = -A_2(x,y).$$

Hence, for all $\psi \in C_0^1(\mathbf{M})$,

$$R_1P_1R_1^{-1}\psi = -P_2\psi, \quad R_1P_2R_1^{-1}\psi = P_1\psi. \tag{2.31}$$

Since R_1 leaves $C_0^1(\mathbf{M})$ invariant bijectively and P_j, $j=1,2$, are essentially self-adjoint on $C_0^1(\mathbf{M})$ [Lemma 2.1(i)], the vector equations in (2.31) extend to operator equalities (2.28).

(ii) Similar to part (i). ■

In Sec. III, we shall consider the case of a vector potential satisfying (2.27) and (2.29).

D. Small coupling limit

Finally we consider the small coupling limit $\alpha\to 0$ of P_j.

Lemma 2.10: For all $t\in\mathbf{R}$ and $j=1,2$,

$$\text{s-lim}_{\alpha\to 0}\ e^{itP_j}=e^{itp_j}, \tag{2.32}$$

where s-lim *denotes strong limit.*

Proof: For all $\psi\in C_0^1(\mathbf{M})$, we have $P_j\psi\to p_j\psi$ ($\alpha\to 0$). Note that $C_0^1(\mathbf{M})$ is a common core of P_j and p_j. Hence, by general convergence theorems [Theorem VIII.25 (a) and Theorem VIII.21 in Ref. 10], we obtain (2.32). ■

III. A VECTOR POTENTIAL GIVEN BY THE WEIERSTRASS ZETA FUNCTION AND REPRESENTATIONS OF THE QUANTUM PLANE

We now specialize the vector potential A. We set

$$\Omega_{m,n}=m\omega_1+in\omega_2,\quad m,n\in\mathbf{Z}. \tag{3.1}$$

Let $\zeta(z)$ ($z\in\mathbf{C}$) be the Weierstrass Zeta function with poles at $z=\Omega_{m,n}, m,n\in\mathbf{Z}$:

$$\zeta(z)=\frac{1}{z}+\sum_{(m,n)\in\mathbf{Z}^2\setminus\{(0,0)\}}\left(\frac{1}{z-\Omega_{m,n}}+\frac{1}{\Omega_{m,n}}+\frac{z}{\Omega_{m,n}^2}\right). \tag{3.2}$$

In what follows, we assume that the vector potential A is given by $A=A_1\,dx+A_2\,dy$ with

$$A_1(\mathbf{r})=\text{Im}\ \zeta(z),\quad A_2(\mathbf{r})=\text{Re}\ \zeta(z), \tag{3.3}$$

so that

$$\zeta(z)=A_2(\mathbf{r})+iA_1(\mathbf{r}). \tag{3.4}$$

Then, by the Cauchy–Riemann equation, A is flat on $\mathbf{M}$.

In the present case, the constant $\gamma_{m,n}(A)$ defined by (2.17) is computed as

$$\gamma_{m,n}(A)=2\pi, \tag{3.5}$$

independently of $(m,n)\in\mathbf{Z}^2$. Hence *the magnetic flux is locally quantized if and only if α is an integer*. Thus the local quantization of the magnetic flux is equivalent to the ''charge quantization.'' *The representation $\{Q_j,P_j\}_{j=1}^2$ of CCR in the present case is an inequivalent representation if and only if α is not an integer*.

Let

$$q_\alpha=e^{2\pi i\alpha}. \tag{3.6}$$

Lemma 3.1: For all $m,n\in\mathbf{Z}$,

$$e^{in\omega_2P_2}e^{im\omega_1P_1}=q_\alpha^{nm}e^{im\omega_1P_1}e^{in\omega_2P_2}. \tag{3.7}$$

Proof: For all $(x,y) \in \mathbf{M}_{\omega_1,\omega_2}$, $D(x,y;\omega_1,\omega_2)$ contains only one point in the lattice $\mathbf{Z}^2_{\omega_1,\omega_2}$. Hence, by Lemma 2.4 and (3.5), $\Phi^A_{\omega_1,\omega_2} = 2\pi$, a.e., which, together with (2.16), implies (3.7) with $m=n=1$. Using this relation repeatedly, we obtain (3.7) with $m,n \in \mathbf{N}\cup\{0\}$, whose adjoint gives (3.7) with $m,n<0$. Noting that e^{itP_j} $(t\in\mathbf{R})$ is invertible with $(e^{itP_j})^{-1} = e^{-itP_j}$, we obtain (3.7) with $m\geqslant 0, n<0$ or $m\leqslant 0, n>0$. ∎

Relation (3.7) naturally leads us to the *quantum plane*,[11] which is defined to be the algebra generated by two elements X,Y subject to the relation

$$qXY = YX,$$

with q a parameter.[12] We denote the quantum plane by $\mathbf{C}^2_q$.

For an algebra $\mathfrak{U}$, a set (π,V) of a complex vector space V and an algebraic homomorphism $\pi:\mathfrak{u}\to\mathrm{End}(V)$ is called a representation of $\mathfrak{U}$.

We denote by $\mathfrak{B}(L^2(\mathbf{R}^2))$ the $*$ algebra of bounded linear operators on $L^2(\mathbf{R}^2)$. The following theorem immediately follows from Lemma 3.1.

Theorem 3.2: *The following correspondence* $\pi_\alpha:\{X,Y\}\to\mathfrak{B}(L^2(\mathbf{R}^2))$ *defines a representation of* $\mathbf{C}^2_{q_\alpha}$ *on* $L^2(\mathbf{R}^2)$*:*

$$\pi_\alpha(X) = e^{i\omega_1 P_1}, \quad \pi_\alpha(Y) = e^{i\omega_2 P_2}. \tag{3.8}$$

It should be noted that, in the representation $(\pi_\alpha, L^2(\mathbf{R}^2))$, $\pi_\alpha(X)$ and $\pi_\alpha(Y)$ are unitary operators. Also, $q_\alpha \neq 1$ if and only if $\alpha \notin \mathbf{Z}$.

We have

$$\lim_{\alpha\to 0} q_\alpha = 1, \tag{3.9}$$

which means that the small coupling limit $\alpha\to 0$ corresponds to the ''classical limit'' of deformation by the parameter q_α.

The representation $(\pi_\alpha, L^2(\mathbf{R}^2))$ has a nontrivial classical limit.

Proposition 3.3:

$$\text{s-}\lim_{\alpha\to 0} \pi_\alpha(X) = e^{i\omega_1 p_1} \neq I, \quad \text{s-}\lim_{\alpha\to 0} \pi_\alpha(Y) = e^{i\omega_2 p_2} \neq I,$$

where I denotes the identity operator on $L^2(\mathbf{R}^2)$*.*

Proof: This follows from Lemma 2.10. ∎

For a subalgebra $\mathfrak{M}$ of $\mathfrak{B}(L^2(\mathbf{R}^2))$, we denote by $\mathfrak{M}'$ the commutant of $\mathfrak{M}$:

$$\mathfrak{M}' = \{T \in \mathfrak{B}(L^2(\mathbf{R}^2)) \mid TS = ST, S \in \mathfrak{M}\}. \tag{3.10}$$

Let $\mathfrak{E}_\alpha$ be the algebra generated by $\{e^{i\omega_1 P_1}, e^{i\omega_2 P_2}\}$:

$$\mathfrak{E}_\alpha = \pi_\alpha(\mathbf{C}^2_q\alpha).$$

Lemma 3.4: $e^{\pm 2\pi i Q_1/\omega_1}$, $e^{\pm 2\pi i Q_2/\omega_2} \in \mathfrak{E}'_\alpha$.

Proof: This follows from (2.15). ∎

By Lemma 3.1, we have

$$q_\alpha e^{-i\omega_2 P_2} e^{i\omega_1 P_1} = e^{i\omega_1 P_1} e^{-i\omega_2 P_2}, \quad q_\alpha e^{i\omega_2 P_2} e^{-i\omega_1 P_1} = e^{-i\omega_1 P_1} e^{i\omega_2 P_2}, \tag{3.11}$$

$$q_\alpha e^{-i\omega_1 P_1} e^{-i\omega_2 P_2} = e^{-i\omega_2 P_2} e^{-i\omega_1 P_1}. \tag{3.12}$$

Hence, each of $\{e^{-i\omega_2 P_2}, e^{i\omega_1 P_1}\}$, $\{e^{i\omega_2 P_2}, e^{-i\omega_1 P_1}\}$, and $\{e^{-\omega_1 P_1}, e^{-i\omega_2 P_2}\}$ gives a representation of $\mathbf{C}^2_{q_\alpha}$. We denote these representations by $(\pi_\alpha^{(j)}, L^2(\mathbf{R}^2))$, $j=1,2,3$, respectively.

Proposition 3.5: Suppose that

$$\omega_1 = \omega_2 . \tag{3.13}$$

Then, each representation $(\pi_\alpha^{(j)}, L^2(\mathbf{R}^2))$ *is unitarily equivalent to* $(\pi_\alpha, L^2(\mathbf{R}^2))$.

Proof: It is easy to check that, if (3.13) is satisfied, then (2.27) and (2.29) hold with $\widetilde{A}(z)$ replaced by $\zeta(z)$. Hence we have (2.28) and (2.30), which imply that, for all $t \in \mathbf{R}$,

$$R_1 e^{itP_1} R_1^{-1} = e^{-itP_2}, \quad R_1 e^{itP_2} R_1^{-1} = e^{itP_1}, \quad R_2 e^{itP_1} R_2^{-1} = e^{itP_2}, \quad R_2 e^{itP_2} R_2^{-1} = e^{itP_1}. \tag{3.14}$$

These relations give a unitary equivalence between $(\pi_\alpha, L^2(\mathbf{R}^2))$ and $(\pi_\alpha^{(j)}, L^2(\mathbf{R}^2))$ $(j=1,2)$. Moreover, (3.14) implies that

$$R_1^2 e^{itP_1} R_1^{-2} = e^{-itP_1}, \quad R_2^2 e^{itP_2} R_2^{-2} = e^{-itP_2}.$$

It is easy to see that $R_1^2 = R_2^2$. Thus, the unitary equivalence between $(\pi_\alpha, L^2(\mathbf{R}^2))$ and $(\pi_\alpha^{(3)}, L^2(\mathbf{R}^2))$ follows. ■

Remark: (i) In the case $\omega_1 \neq \omega_2$, we have been unable to clarify whether $(\pi_\alpha, L^2(\mathbf{R}^2))$, $(\pi_\alpha^{(j)}, L^2(\mathbf{R}^2))$, $j=1,2,3$, are unitarily equivalent to each other or not.

(ii) Relation (2.15) implies that

$$q_\alpha e^{2\pi i \alpha Q_j/\omega_j} e^{i\omega_j P_j} = e^{i\omega_j P_j} e^{2\pi i \alpha Q_j/\omega_j}, \quad j=1,2.$$

Hence, for each $j=1,2$ $\{e^{2\pi i \alpha Q_j/\omega_j}, e^{i\omega_j P_j}\}$ gives a representation of $\mathbf{C}^2_{q_\alpha}$. It is a problem to clarify whether these representations and the representations $(\pi_\alpha, L^2(\mathbf{R}^2))$, $(\pi_\alpha^{(j)}, L^2(\mathbf{R}^2))$, $j=1,2,3$, are unitarily equivalent to each other or not.

In this paper we concentrate our attention on the representation $(\pi_\alpha, L^2(\mathbf{R}^2))$. The methods developed in what follows apply also to the other representations of the quantum plane.

(iii) Consider the case where α is a rational number: $\alpha = p/r$ with $p \in \mathbf{Z}$ and $r \in \mathbf{Z}\backslash\{0\}$. Then $q_\alpha^r = 1$. It follows from (3.7) that, for all m, $n \in \mathbf{Z}$ with $mn = r$, $e^{im\omega_1 P_1}$ and $e^{in\omega_2 P_2}$ commute. But, if α is irrational, then $e^{im\omega_1 P_1}$ and $e^{in\omega_2 P_2}$ do not commute for all m, $n \in \mathbf{Z}\backslash\{0\}$.

IV. REPRESENTATION OF $U_q(\mathfrak{sl}_2)$ (I)

For a complex number $q \in \mathbf{C}\backslash\{0,1,-1\}$, the quantum group $U_q(\mathfrak{sl}_2)$ is defined to be the algebra generated by four elements E, F, K, K^{-1} subject to the following relations:[13]

$$KK^{-1} = K^{-1}K = 1,$$

$$KEK^{-1} = q^2 E, \quad KFK^{-1} = q^{-2} F,$$

$$[E,F] = \frac{K - K^{-1}}{q - q^{-1}}.$$

The Casimir element C of $U_q(\mathfrak{sl}_2)$ is defined by

$$C = \frac{qK - 2 + q^{-1}K^{-1}}{(q - q^{-1})^2} + FE. \tag{4.1}$$

Given a representation (π, V) of the quantum plane $\mathbf{C}^2_q$ such that $\pi(X)$ and $\pi(Y)$ are bijective, we can construct a representation of $U_q(\mathfrak{sl}_2)$.

Lemma 4.1 (cf. Ref. 8): *Let (π,V) be as above and $a,b,a',b' \in \mathbf{C}$ be constants satisfying*

$$abq = a'b'q^{-1} = -\frac{1}{(q-q^{-1})^2}. \tag{4.2}$$

Then the following correspondence Π:$\{E,F,K,K^{-1}\} \to \mathrm{End}(V)$ defines a representation of $U_q(\mathfrak{sl}_2)$:

$$\Pi(E) = \pi(X)(a\pi(X) + a'\pi(X)^{-1})\pi(Y)^{-1},$$

$$\Pi(F) = \pi(Y)(b\pi(X) + b'\pi(X)^{-1})\pi(X)^{-1},$$

$$\Pi(K) = \pi(X)^2, \quad \Pi(K^{-1}) = \pi(X)^{-2}.$$

In this representation, we have

$$\Pi(C) = a'b + ab' - \frac{2}{(q-q^{-1})^2}. \tag{4.3}$$

Proof: Direct computations. ∎

Remark: By (4.2), we can write $\Pi(C)$ as

$$\Pi(C) = (a' + aq)(b + b'q^{-1}).$$

In the rest of the paper, we assume that A_j, $j=1,2$, are given by (3.3) and

$$\alpha \notin \frac{\mathbf{Z}}{2}. \tag{4.4}$$

Hence $q_\alpha^2 \neq 1$.

Let a_α, a'_α, b_α, b'_α be constants satisfying

$$a_\alpha b_\alpha q_\alpha = a'_\alpha b'_\alpha q_\alpha^{-1} = -\frac{1}{(q_\alpha - q_\alpha^{-1})^2} = \frac{1}{4\sin^2 2\pi\alpha}. \tag{4.5}$$

By Lemma 4.1 and Theorem 3.2, we have the following theorem.

Theorem 4.2: *The following correspondence Π_α:$\{E,F,K,K^{-1}\} \to \mathfrak{B}(L^2(\mathbf{R}^2))$ defines a representation of $U_{q_\alpha}(\mathfrak{sl}_2)$ on $L^2(\mathbf{R}^2)$:*

$$\Pi_\alpha(E) = e^{i\omega_1 P_1}(a_\alpha e^{i\omega_1 P_1} + a'_\alpha e^{-i\omega_1 P_1})e^{-i\omega_2 P_2},$$

$$\Pi_\alpha(F) = e^{i\omega_2 P_2}(b_\alpha e^{i\omega_1 P_1} + b'_\alpha e^{-i\omega_1 P_1})e^{-i\omega_1 P_1},$$

$$\Pi_\alpha(K) = e^{2i\omega_1 P_1}, \quad \Pi_\alpha(K^{-1}) = e^{-2i\omega_1 P_1}.$$

We investigate basic properties of the representation $(\Pi_\alpha, L^2(\mathbf{R}^2))$.

Theorem 4.3: *The representation $(\Pi_\alpha, L^2(\mathbf{R}^2))$ has no weight vectors. In particular, there exists no nonzero finite-dimensional subspace W such that (Π_α, W) gives a representation of $U_{q_\alpha}(\mathfrak{sl}_2)$.*

Proof: A weight vector of weight $\lambda \in \mathbf{C}$ in the representation $(\Pi_\alpha, L^2(\mathbf{R}^2))$ is a nonzero vector ψ satisfying $\Pi_\alpha(K)\psi = q_\alpha^\lambda \psi$. Hence ψ is an eigenvector of $e^{2i\omega_1 P_1}$. But, by Lemma 2.6(ii), $e^{2i\omega_1 P_1}$ has no eigenvectors. The last assertion in Theorem 4.3 follows from the well-known fact that any nonzero finite-dimensional $U_q(\mathfrak{sl}_2)$-module contains a highest weight vector (Proposition VI.3.3 in Ref. 11). ∎

Let

$$\mathfrak{U}_\alpha = \Pi_\alpha(U_{q_\alpha}(\mathfrak{sl}_2)). \tag{4.6}$$

Theorem 4.4: *Suppose that* $a'_\alpha = \overline{b_\alpha}$, $b'_\alpha = \overline{a_\alpha}$ ($\overline{z}$ *denotes the complex conjugate of the complex number* z). *Then*

(i) $\mathfrak{U}_\alpha$ *is a* $*$ *subalgebra of* $\mathfrak{B}(L^2(\mathbf{R}^2))$.

(ii) *The representation* $(\Pi_\alpha, L^2(\mathbf{R}^2))$ *is completely reducible.*

Proof: (i) In the present assumption, we have

$$\Pi_\alpha(E)^* = \Pi_\alpha(F),$$

where T^* denotes the adjoint of operator T. It is obvious that $\Pi_\alpha(K)^* = \Pi_\alpha(K^{-1})$. Hence it follows that $\mathfrak{U}_\alpha$ is self-adjoint (i.e., $T \in \mathfrak{U}_\alpha \Rightarrow T^* \in \mathfrak{U}_\alpha$). Thus part (i) follows.

(ii) As in Lemma 3.4, we have

$$\{e^{\pm 2\pi i Q_j/\omega_j}\}_{j=1}^2 \subset \mathfrak{U}'_\alpha, \tag{4.7}$$

which implies that $\mathfrak{U}'_\alpha \neq \mathbf{C}I$. As proven in part (i), $\mathfrak{U}_\alpha$ is self-adjoint. Hence $\mathfrak{U}_\alpha$ is not irreducible (Proposition 2.3.8 in Ref. 14). Let W be any closed subspace of $L^2(\mathbf{R}^2)$, which is invariant under the action of $\mathfrak{U}_\alpha$. Since $\mathfrak{U}_\alpha$ is self-adjoint, it follows that $W^\perp$ [the orthogonal complement of W in $L^2(\mathbf{R}^2)$] is also invariant under the action of $\mathfrak{U}_\alpha$. Thus $(\Pi_\alpha, L^2(\mathbf{R}^2))$ is completely reducible. ■

For a subset $\mathfrak{M}$ of $\mathfrak{B}(L^2(\mathbf{R}^2))$, we denote by $\overline{\mathfrak{M}}$ the closure of $\mathfrak{M}$ with respect to the operator norm.

We denote by $\mathfrak{F}_\alpha$ the algebra generated by $e^{\pm 2i\omega_1 P_1}$, $e^{\pm i\omega_2 P_2}$, which is a $*$ subalgebra of $\mathfrak{B}(L^2(\mathbf{R}^2))$, so that $\overline{\mathfrak{F}_\alpha}$ is a C^* subalgebra.

Theorem 4.5: *Suppose that* $|a_\alpha| \neq |a'_\alpha|$, $|b_\alpha| \neq |b'_\alpha|$. *Then*

(i)

$$\overline{\mathfrak{F}_\alpha} = \overline{\mathfrak{U}_\alpha}. \tag{4.8}$$

(ii) $\overline{\mathfrak{U}_\alpha}$ *is completely reducible.*

Proof: (i) For simplicity, we set $a = a_\alpha$, $a' = a'_\alpha$, $b = b_\alpha$, $b' = b'_\alpha$. We have

$$\Pi_\alpha(E) = Se^{-i\omega_2 P_2}, \quad \Pi_\alpha(F) = e^{i\omega_2 P_2}T, \tag{4.9}$$

with

$$S = ae^{2i\omega_1 P_1} + a', \quad T = b + b'e^{-2i\omega_1 P_1}.$$

Hence it follows that $\mathfrak{U}_\alpha \subset \mathfrak{F}_\alpha$, implying

$$\overline{\mathfrak{U}_\alpha} \subset \overline{\mathfrak{F}_\alpha}. \tag{4.10}$$

To prove the converse inclusion relation, we express $e^{\pm i\omega_2 P_2}$ in terms of $\Pi_\alpha(E)$, $\Pi_\alpha(F)$, $\Pi_\alpha(K)$, and $\Pi_\alpha(K^{-1})$. We first consider the case $|a|/|a'| < 1$. We can write

$$S = a\Pi_\alpha(K) + a' = a'\left(1 + \frac{a}{a'}\,\Pi_\alpha(K)\right).$$

We have $\|a\Pi_\alpha(K)/a'\| = |a|/|a'| < 1$, where $\|L\|$ with operator $L \in \mathfrak{B}(L^2(\mathbf{R}^2))$ denotes the operator norm of L. Hence, S is bijective with

$$S^{-1}=\frac{1}{a'}\sum_{n=0}^{\infty}(-1)^n\left(\frac{a}{a'}\right)^n\Pi_\alpha(K)^n$$

in the operator norm topology. Therefore we obtain

$$e^{-i\omega_2 P_2}=S^{-1}\Pi_\alpha(E)\in\overline{\mathfrak{U}_\alpha}.$$

In the case $|a|/|a'|>1$, we write

$$S=a\Pi_\alpha(K)\left(1+\frac{a'}{a}\,\Pi_\alpha(K^{-1})\right).$$

Then, in the same way as in the preceding case, we can show that S is bijective with

$$S^{-1}=a^{-1}\sum_{n=0}^{\infty}(-1)^n\left(\frac{a'}{a}\right)^n\Pi_\alpha(K^{-1})^{n+1},$$

in the operator norm topology. Hence $e^{-i\omega_2 P_2}\in\overline{\mathfrak{U}_\alpha}$. Similarly, the second relation in (4.9) implies that $e^{i\omega_2 P_2}\in\overline{\mathfrak{U}_\alpha}$. Thus, $\overline{\mathfrak{F}_\alpha}\subset\overline{\mathfrak{U}_\alpha}$, which, together with (4.10), gives (4.8).

(ii) Relation (4.7) implies that

$$\{e^{\pm 2\pi i Q_j/\omega_j}\}_{j=1}^2\subset\overline{\mathfrak{U}'_\alpha}.$$

By the preceding result, $\overline{\mathfrak{U}_\alpha}$ is self-adjoint (in fact, a C^* subalgebra). Thus, by the same reasoning as in the proof of Theorem 4.4(ii), we obtain the desired result. ■

Remark: In the case $a_\alpha=\pm a'_\alpha$, S is injective, but not surjective [Lemma 2.6(ii)]. Hence S^{-1} is unbounded. The same applies to T in the case $b_\alpha=\pm b'_\alpha$.

For $(m,n)\in\mathbf{Z}^2$, we define a function $F_{m,n}(x,y)$ by

$$F_{m,n}(x,y)=\begin{cases}\exp\left(-i\alpha\displaystyle\int_{C_-(x,y;2m\omega_1,n\omega_2)}A\right); & (x,y)\in\mathbf{M}_{\omega_1,\omega_2},\\ 0; & (x,y)\notin\mathbf{M}_{\omega_1,\omega_2}.\end{cases}\tag{4.11}$$

For $\psi\in L^2(\mathbf{R}^2)$, we set

$$\psi_{m,n}(x,y)=\psi(x+2m\omega_1,y+n\omega_2),\quad (m,n)\in\mathbf{Z}^2.\tag{4.12}$$

Corollary 4.6: Suppose that $|a_\alpha|\neq|a'_\alpha|$, $|b_\alpha|\neq|b'_\alpha|$. Let W be any irreducible closed subspace of the representation $(\Pi_\alpha,L^2(\mathbf{R}^2))$. Then each nonzero vector $\psi\in W$ is cyclic and W is generated by vectors of the form $F_{m,n}\psi_{m,n}$, $(m,n)\in\mathbf{Z}^2$.

Proof: The first half is due to a general fact (Proposition 2.3.8 in Ref. 14). By Theorem 4.5(i), W is generated by vectors of the form

$$\phi_{m,n}=e^{2im\omega_1 P_1}e^{in\omega_2 P_2}\psi,\quad (m,n)\in\mathbf{Z}^2.$$

Using (2.20), we see that $\phi_{m,n}=F_{m,n}\psi_{m,n}$. ■

Corollary 4.6 clarifies the structure of any irreducible closed subspace W of the representation $(\Pi_\alpha,L^2(\mathbf{R}^2))$ in the case $|a_\alpha|\neq|a'_\alpha|$, $|b_\alpha|\neq|b'_\alpha|$. By Theorem 4.3, $\dim W=\infty$.

V. REPRESENTATION OF $U_q(\mathfrak{sl}_2)$ (II)

In this section, we construct representations of $U_q(\mathfrak{sl}_2)$ that are different from the one given in Sec. IV.

Lemma 5.1 (cf. Ref. 8): *Suppose that* $q \in \mathbf{C}\backslash\{0,1,-1\}$. *Let* (π,V) *be a representation of* $\mathbf{C}^2_{q^2}$ *[i.e.,* $q^2\pi(X)\pi(Y)=\pi(Y)\pi(X)$*] with the following properties.*

(i) $\pi(X)$ *and* $\pi(Y)$ *are bijective on* V.

(ii) *There exists a bijection* $Z \in \mathrm{End}(V)$ *such that* $Z^2=\pi(Y)^{-1}\pi(X)$.

Let $c_\pm$ and $d_\pm$ be constants satisfying

$$c_\pm d_\pm = \pm\frac{1}{(q-q^{-1})^2}. \tag{5.1}$$

Then the following correspondences $\Pi_\pm:\{E,F,K,K^{-1}\}\to\mathrm{End}\,(V)$ *define representations of* $U_q(\mathfrak{sl}_2)$*:*

$$\Pi_\pm(E)=c_\pm Z(\pi(X)^{-1}+\pi(Y)^{-1}),$$

$$\Pi_\pm(F)=d_\pm(\pi(X)+\pi(Y))Z^{-1},$$

$$\Pi_\pm(K)=\pm q^{-1}\pi(Y)^{-1}\pi(X),$$

$$\Pi_\pm(K^{-1})=\pm q\,\pi(X)^{-1}\pi(Y).$$

In these representations, we have

$$\Pi_\pm(C)=\pm\frac{(1+q^2)\pi(Y)^{-1}\pi(X)+(1+q^{-2})\pi(X)^{-1}\pi(Y)}{(q-q^{-1})^2}. \tag{5.2}$$

Proof: Direct computations. ■

To apply Lemma 5.1 with the representation $(\pi_\alpha, L^2(\mathbf{R}^2))$ of $\mathbf{C}^2_{q_\alpha}$ given in Theorem 3.2, we need the following lemma.

Lemma 5.2: Let U *be a unitary operator on a Hilbert space* $\mathscr{H}$. *Then there exists a unitary operator* T *on* $\mathscr{H}$ *such that*

$$T^2=U. \tag{5.3}$$

Proof: By the spectral theorem for unitary operators, there exists a unique resolution of identity $F(\theta)$ such that $F(0)=0$, $F(2\pi)=I$, and $U=\int_0^{2\pi}e^{i\theta}\,dF(\theta)$. Let $T=\int_0^{2\pi}e^{i\theta/2}\,dF(\theta)$. Then, by the functional calculus, T is unitary and (5.3) holds. ■

The operator $e^{-i\omega_2 P_2}e^{i\omega_1 P_1}$ is unitary on $L^2(\mathbf{R}^2)$. Hence, by Lemma 5.2, there exists a unitary operator Z_α on $L^2(\mathbf{R}^2)$ satisfying

$$Z_\alpha^2=e^{-i\omega_2 P_2}e^{i\omega_1 P_1}. \tag{5.4}$$

Let

$$q_\alpha^{1/2}:=e^{i\pi\alpha}. \tag{5.5}$$

Applying Lemma 5.1 with $\pi(X)=e^{i\omega_1 P_1}$, $\pi(Y)=e^{i\omega_2 P_2}$, we obtain the following theorem.

Theorem 5.3: *Let* $c_\pm(\alpha)$ *and* $d_\pm(\alpha)$ *be constants satisfying*

$$c_\pm(\alpha)d_\pm(\alpha)=\pm\frac{1}{(q_\alpha^{1/2}-q_\alpha^{-1/2})^2}=\mp\frac{1}{4\sin^2\pi\alpha}. \tag{5.6}$$

Then the following correspondences $\Pi_\alpha^\pm : \{E,F,K,K^{-1}\} \to \mathfrak{B}(L^2(\mathbf{R}^2))$ *define representations of* $U_q(\mathfrak{sl}_2)$ *with* $q = q_\alpha^{1/2}$:

$$\Pi_\alpha^\pm(E) = c_\pm(\alpha) Z_\alpha (e^{-i\omega_1 P_1} + e^{-i\omega_2 P_2}),$$

$$\Pi_\alpha^\pm(F) = d_\pm(\alpha)(e^{i\omega_1 P_1} + e^{i\omega_2 P_2}) Z_\alpha^{-1},$$

$$\Pi_\alpha^\pm(K) = \pm q_\alpha^{-1/2} e^{-i\omega_2 P_2} e^{i\omega_1 P_1},$$

$$\Pi_\alpha^\pm(K^{-1}) = \pm q_\alpha^{1/2} e^{-i\omega_1 P_1} e^{i\omega_2 P_2}.$$

In these representations, we have

$$\Pi_\alpha^\pm(C) = \pm \frac{(1+q_\alpha) e^{-i\omega_2 P_2} e^{i\omega_1 P_1} + (1+q_\alpha^{-1}) e^{-i\omega_1 P_1} e^{i\omega_2 P_2}}{(q_\alpha^{1/2} - q_\alpha^{-1/2})^2}. \tag{5.7}$$

By Lemma 2.7, we obtain the following theorem.

Theorem 5.4: *The representations* $(\Pi_\alpha^\pm, L^2(\mathbf{R}^2))$ *have no weight vectors. In particular, there exist no nonzero finite-dimensional subspaces* $W_\pm$, *such that* $(\Pi_\alpha^\pm, W_\pm)$ *give representations of* $U_{q_\alpha^{1/2}}(\mathfrak{sl}_2)$.

Let

$$\mathfrak{U}_\alpha^\pm = \Pi_\alpha^\pm(U_{q_\alpha^{1/2}}(\mathfrak{sl}_2)). \tag{5.8}$$

Theorem 5.5: *Let* $\overline{c_\pm(\alpha)} = d_\pm(\alpha)$. *Then*

(i) $\mathfrak{U}_\alpha^\pm$ *are* $*$ *subalgebras of* $\mathfrak{B}(L^2(\mathbf{R}^2))$.

(ii) $(\Pi_\alpha^\pm, L^2(\mathbf{R}^2))$ *are completely reducible.*

Proof: Under the assumption, $\mathfrak{U}_\alpha^\pm$ are self-adjoint, since we have

$$\Pi_\alpha^\pm(E)^* = \Pi_\alpha^\pm(F), \quad \Pi_\alpha^\pm(K)^* = \Pi_\alpha^\pm(K^{-1}).$$

Note that, if $T \in \mathfrak{B}(L^2(\mathbf{R}^2))$ commutes with $e^{-i\omega_2 P_2} e^{i\omega_1 P_1}$, then T commutes with Z_α. In particular, Z_α commutes with $e^{2\pi i Q_j/\omega_j}$, $j=1,2$. Hence $\{e^{2\pi i Q_j/\omega_j}\}_{j=1}^2 \subset \mathfrak{U}_\alpha^{\pm\prime}$. Thus, by the same reasoning as in the proof of Theorem 4.4, we obtain the desired result. ■

Note that $q_{2\alpha}^{1/2} = q_\alpha$. Hence $(\Pi_{2\alpha}^\pm, L^2(\mathbf{R}^2))$ are representations of $U_q(\mathfrak{sl}_2)$ with $q = q_\alpha$. It is natural to ask if these representations are equivalent to the representation $(\Pi_\alpha, L^2(\mathbf{R}^2))$ constructed in the preceding section.

Theorem 5.6: *The representations* $(\Pi_{2\alpha}^\pm, L^2(\mathbf{R}^2))$ *are not equivalent to* $(\Pi_\alpha, L^2(\mathbf{R}^2))$.

Proof: By (5.7), (2.20), and (2.21), we have, for all $\psi \in L^2(\mathbf{R}^2)$,

$$(\Pi_{2\alpha}^\pm(C)\psi)(x,y) = \pm \frac{1+q_\alpha^2}{(q_\alpha - q_\alpha^{-1})^2} \exp\left(-2i\alpha \int_{C_+(x,y;\omega_1,-\omega_2)} A \right) \psi(x+\omega_1, y-\omega_2)$$
$$\pm \frac{1+q_\alpha^{-2}}{(q_\alpha - q_\alpha^{-1})^2} \exp\left(-2i\alpha \int_{C_-(x,y;-\omega_1,\omega_2)} A \right) \psi(x-\omega_1, y+\omega_2), \quad \text{a.e.}$$

From this expression, it is seen that $\Pi_{2\alpha}^\pm(C)$ are not scalar multiples of the identity. [For example, consider a function $\psi \in L^2(\mathbf{R}^2)$, $\psi \neq 0$, with support in $S = (0,\omega_1) \times (0,\omega_2)$. Then the support of $\Pi_{2\alpha}^\pm(C)\psi$ is outside of S.] On the other hand, by (4.3), $\Pi_\alpha(C)$ is a scalar multiple of the identity. Thus, the desired result follows. ■

We can prove a more detailed fact on the inequivalence between $(\Pi^{\pm}_{2\alpha}, L^2(\mathbf{R}^2))$ and $(\Pi_\alpha, L^2(\mathbf{R}^2))$. For this purpose, we prepare a lemma. Let

$$h^{\pm}_\alpha(\lambda) = \pm \frac{(1+q_\alpha)\lambda + (1+q_\alpha^{-1})\overline{\lambda}}{(q_\alpha^{1/2} - q_\alpha^{-1/2})^2}, \quad \lambda \in \mathbf{C}. \tag{5.9}$$

Note that $h^{\pm}_\alpha$ are real valued.

Lemma 5.7:

(i)

$$\sigma(\Pi^{\pm}_\alpha(C)) = \{h^{\pm}_\alpha(\lambda) | \lambda \in \sigma(e^{-i\omega_2 P_2} e^{i\omega_1 P_1})\}. \tag{5.10}$$

In particular,

$$\sigma(\Pi^{\pm}_\alpha(C)) \subset [-R_\alpha, R_\alpha], \tag{5.11}$$

where

$$R_\alpha = \frac{2|1+q_\alpha|}{|q_\alpha^{1/2} - q_\alpha^{-1/2}|^2} = \frac{|\cos \pi\alpha|}{\sin^2 \pi\alpha}. \tag{5.12}$$

(ii)

$$\sigma_p(\Pi^{\pm}_\alpha(C)) = \emptyset. \tag{5.13}$$

Proof: (i) We first note that

$$U_\alpha := e^{-i\omega_2 P_2} e^{i\omega_1 P_1}$$

is unitary and $U_\alpha^{-1} = e^{-i\omega_1 P_1} e^{i\omega_2 P_2}$. We have

$$\Pi^{\pm}_\alpha(C) = \pm \frac{(1+q_\alpha)U_\alpha + (1+q_\alpha^{-1})U_\alpha^{-1}}{(q_\alpha^{1/2} - q_\alpha^{-1/2})^2}.$$

Relation (5.10) follows from this expression and the spectral mapping theorem for unitary operators. It is easy to see that there exists a constant $\delta_\alpha \in [0, 2\pi)$ such that

$$h^{\pm}_\alpha(e^{i\theta}) = \pm R_\alpha \cos(\theta + \delta_\alpha), \quad \theta \in \mathbf{R}. \tag{5.14}$$

Hence (5.11) follows.

(ii) Suppose that $\sigma_p(\Pi^{+}_\alpha(C)) \neq$ and $\lambda \in \sigma_p(\Pi^{+}_\alpha(C))$. Then, by (5.11), $-R_\alpha \leqslant \lambda \leqslant R_\alpha$ and there exists a nonzero vector $\psi \in L^2(\mathbf{R}^2)$ such that $\Pi^{+}_\alpha(C)\psi = \lambda\psi$. Let E be the spectral measure of U_α:

$$U_\alpha = \int_0^{2\pi} e^{i\theta}\, dE(\theta).$$

Then we have

$$0 = \|\Pi^{+}_\alpha(C)\psi - \lambda\psi\|^2 = \int_0^{2\pi} |h^{+}_\alpha(e^{i\theta}) - \lambda|^2 d\|E(\theta)\psi\|^2,$$

which implies that the support of the measure $\|E(\cdot)\psi\|^2$ is included in the set $\{\theta\in[0,2\pi]|h_\alpha^+(e^{i\theta})=\lambda\}$. By (5.14), the equation $h_\alpha^+(e^{i\theta})=\lambda$ has at most two solutions: $\theta_j\in[0,2\pi)$, $j=1,2$. This implies that one of $E(\{\theta_j\})\psi$ $(j=1,2)$ is not zero and an eigenvector of U_α with eigenvalue $e^{i\theta_j}$. But this contradicts Lemma 2.7. Thus $\sigma_p(\Pi_\alpha^+(C))$ must be empty. Similarly, we can prove $\sigma_p(\Pi_\alpha^-(C))=\emptyset$. ■

Theorem 5.8: *Let* (Π_α,W) *be any irreducible component of* $(\Pi_\alpha,L^2(\mathbf{R}^2))$ $(W\subset L^2(\mathbf{R}^2))$. *Then* (Π_α,W) *is not equivalent to any irreducible component of* $(\Pi_{2\alpha}^{\pm},L^2(\mathbf{R}^2))$.

Proof: By Lemma 5.7(ii), $\Pi_{2\alpha}^{\pm}(C)$ are not scalar multiples of the identity in any irreducible components of $(\Pi_{2\alpha}^+,L^2(\mathbf{R}^2))$. Thus, the desired result follows. ■

Remark: It is an open problem to clarify whether $(\Pi_\alpha^+,L^2(\mathbf{R}^2))$ is equivalent to $(\Pi_\alpha^-,L^2(\mathbf{R}^2))$ or not.

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The Heisenberg dynamics of spin systems: A quasi*-algebras approach

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The problem of the existence of the thermodynamical limit of the algebraic dynamics for a class of spin systems is considered in the framework of a generalized algebraic approach in terms of a special class of quasi*-algebras, called CQ^*-algebras. Physical applications to (almost) mean-field models and to bubble models are discussed. © *1996 American Institute of Physics.*
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I. INTRODUCTION

When working with spin systems it is not difficult to build up simple models for which the algebraic approach developed by Haag and Kastler[1] fails. In this approach, the observable algebra $\mathfrak{U}$ of the system is taken to be a quasilocal C^*-algebra. But already for reasonably simple interactions, e.g., for mean-field models, the thermodynamical limit of the local Heisenberg dynamics does not converge in the usual spin C^*-algebra $\mathfrak{U}_S$. One possible way to overcome this difficulty consists in weakening the Haag–Kastler axioms by assuming that the observable algebra of the system is a more general structure than a C^*-algebra. In Refs. 2, and 3, Lassner proposed to define on the algebra $\mathfrak{U}_0$ generated by all the local algebras $\mathfrak{U}_V$ a different topology (that he called *physical*), constructed *ad hoc* to allow the thermodynamical limit of the local Heisenberg dynamics to live in the completion of $\mathfrak{U}_0$ with respect to this topology.

In Ref. 4 we introduced a particular class of quasi*-algebras, called CQ^*-algebras, with the scope of providing an intermediate structure between a general quasi*-algebra and a C^*-algebra, which still allows a solution of the problems mentioned above. A CQ^*-algebra can be thought, roughly speaking, as the completion of a C^*-algebra with respect to a certain weaker norm.

In Ref. 4 we proved that, at least for certain representations of $\mathfrak{U}_0$, the thermodynamical limit can be found for the so-called *almost* mean-field models[5,6] in the CQ^*-algebra of operators, where the representations take their values.

In this paper we consider the same problem from a more general point of view (i.e., without specifying, as far as it is possible, the local Hamiltonian), and we investigate on the properties that a spin model should satisfy in order that the existence of the thermodynamical limit of the local dynamics can be obtained in the CQ^*-algebras framework (or at least in a quasi*-algebra, which is obtained as the projective limit of CQ^*-algebras).

In Sec. II we construct the spin CQ^*-algebra and study the derivation δ arising as the limit of the local derivations δ_V, for finite V, where $\delta_V(A)=[H_V,A]$, $A\in\mathfrak{U}$. The integration of the derivation δ is then discussed both in the purely algebraic setup and, under representations, making use of the so-called *effective Hamiltonians*.

In Sec. III, we exhibit examples of spin models satisfying the assumptions of Sec. II. In particular, we rediscuss in this different framework the almost mean-field models studied in Refs.

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5 and 6 and some other models (bubble models) that are obtained by unitary transformations of the previous ones and have nevertheless a physical meaning on their own.

The basic definitions and properties of quasi*-algebras and of CQ^*-algebras are collected in the Appendix.

II. SPIN LATTICE SYSTEMS

Let V be a finite region of a d-dimensional lattice and $|V|$ the number of points in V. The local C^*-algebra $\mathfrak{U}_V$ is generated by the Pauli operators, $\sigma_p=(\sigma_p^1,\sigma_p^2,\sigma_p^3)$ and by the unit 2×2 matrix I_p at every point $p\in V$. The σ_p's are copies of the Pauli matrices,

$$\sigma^1=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},\quad \sigma^2=\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix},\quad \sigma^3=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}.$$

$\mathfrak{U}_V$ is isomorphic to the C^*-algebra of all $2^{|V|}\times 2^{|V|}$ matrices on the $2^{|V|}$-dimensional complex Hilbert space $\mathscr{H}_V=\otimes_{p\in V}C_p^2$, where C_p^2 is the two-dimensional complex Hilbert space at p. If $V\subset V'$ and $A_V\in\mathfrak{U}_V$, then $A_V\to A_{V'}=A_V\otimes(\otimes_{p\in V'\setminus V}I_p)$ defines the natural imbedding of $\mathfrak{U}_V$ into $\mathfrak{U}_{V'}$.

Let $n=(n^1,n^2,n^3)$ be a unit vector in $\mathbb{R}^3$, and put

$$(\sigma\cdot n)=n^1\sigma^1+n^2\sigma^2+n^3\sigma^3.$$

Then, denoting as $Sp(\sigma\cdot n)$ the spectrum of $\sigma\cdot n$, we have

$$Sp(\sigma\cdot n)=\{1,-1\}.$$

Let $|n\rangle$ be a unit eigenvector associated with 1. Let $\{n\}=\{n_1,n_2,\ldots\}$ be an infinite sequence of unit vectors in $\mathbb{R}^3$ and $|\{n\}\rangle=\otimes_p|n_p\rangle$ the corresponding unit vector in the infinite tensor product, $\mathscr{H}_\infty=\otimes_p C_p^2$. We put

$$\mathfrak{U}_0=\bigcup_V \mathfrak{U}_V$$

and

$$\mathscr{D}_{\{n\}}^0=\mathfrak{U}_0|\{n\}\rangle,$$

and we denote the closure of $\mathscr{D}_{\{n\}}^0$ in $\mathscr{H}_\infty$ by $\mathscr{H}_{\{n\}}$. As we saw above, to any sequence $\{n\}$ of three-vectors it corresponds a state $|\{n\}\rangle$ of the system. Such a state defines a realization $\pi_{\{n\}}(\mathfrak{U}_0)$ in the Hilbert space $\mathscr{H}_{\{n\}}$. This representation is faithful, since the norm completion $\mathfrak{U}_S$ of $\mathfrak{U}_0$ is a simple C^*-algebra. To define it one starts with constructing a special basis for $\mathscr{H}_{\{n\}}$. This is obtained from the *ground* state $|\{n\}\rangle$ by *flipping* a finite number of spins.

Let $(n,n^{(1)},n^{(2)})$ be an orthonormal basis of $\mathbb{R}^3$. We put

$$n^{\pm}=\tfrac{1}{2}(n^{(1)}\pm in^{(2)})$$

and

$$|m,n\rangle=(\sigma\cdot n^-)^m|n\rangle\quad (m=0,1).$$

Then we have

$$(\sigma\cdot n)|m,n\rangle=(-1)^m|m,n\rangle\quad (m=0,1).$$

Thus the set $\{|\{m\},\{n\}\rangle = \otimes_p |m_p, n_p\rangle;\ m_p = 0,1,\ \Sigma_p m_p < \infty\}$ forms an orthonormal basis in $\mathscr{H}_{\{n\}}$.[7] In this space we define the unbounded self-adjoint operator M by

$$M|\{m\},\{n\}\rangle = \left(\sum_p m_p\right)|\{m\},\{n\}\rangle.$$

M counts the number of the flipped spins in $|\{m\},\{n\}\rangle$ with respect to the ground state $|\{n\}\rangle$. Of course M depends on $\{n\}$, but we will not explicitly indicate this fact whenever no confusion arises.

Next we consider the natural representation $\pi_{\{n\}}$ of $\mathfrak{U}_0$ into some class of operators in the Hilbert space $\mathscr{H}_{\{n\}}$. The representation $\pi_{\{n\}}$ is defined on the basis vectors $\{|\{m\},\{n\}\rangle\}$ by

$$\pi_{\{n\}}(\sigma_p^i)|\{m\},\{n\}\rangle = \sigma_p^i |m_p, n_p\rangle \otimes \left(\prod_{p' \neq p} \otimes |m_{p'}, n_{p'}\rangle\right) \quad (i = 1,2,3).$$

This definition is then extended in an obvious way to the whole space $\mathscr{H}_{\{n\}}$. It turns out that $\pi_{\{n\}}$ is a *bounded* representation of $\mathfrak{U}_0$ into $\mathscr{H}_{\{n\}}$.

But in view of the definition of a new topology on $\mathfrak{U}_0$, different from that induced by its C^*-norm, it is quite unconvenient to consider $\pi_{\{n\}}$ as a bounded representation of $\mathfrak{U}_0$ into $\mathscr{H}_{\{n\}}$. For this reason, we will consider more appropriate domains where the representation $\pi_{\{n\}}$ lives.

First we can put

$$\mathscr{D}_{\{n\}} = \bigcap_k \mathscr{D}(M^k).$$

Then very simple estimates show that $\pi_{\{n\}}(A)$ leaves $\mathscr{D}_{\{n\}}$ invariant, for any $A \in \mathfrak{U}_0$.[2] It turns out that $\pi_{\{n\}} : \mathfrak{U}_0 \to \mathscr{L}^\dagger(\mathscr{D}_{\{n\}})$.

With this choice one can follow the approach developed in Refs. 2, 5, and 6 and define a *physical topology* on $\mathfrak{U}_0$ as the weakest locally convex topology, such that each $\pi_{\{n\}}$ is continuous from $\mathfrak{U}_0$ into $\mathscr{L}^\dagger(\mathscr{D}_{\{n\}})$, this latter endowed with the so-called quasiuniform topology $\tau_{\{n\}}$.[2]

There is, however, a different and, in our opinion, simpler possible choice.

As seen above, the operator M is a number operator. Therefore, the operator e^M is a densely defined self-adjoint operator. Let $\mathscr{D}$ denote its domain. Then $\mathscr{D}$ can be made into a Hilbert space, denoted as $\mathscr{H}_M$, in a canonical way. The norm in $\mathscr{H}_M$ is given by

$$\|f\|_M = \|e^M f\|, \quad f \in \mathscr{H}_M.$$

Taking the conjugate dual $\mathscr{H}_{\overline{M}}$ of $\mathscr{H}_M$, with respect to the scalar product of $\mathscr{H}_{\{n\}}$, we get the triplet of Hilbert spaces,

$$\mathscr{H}_M \subset \mathscr{H}_{\{n\}} \subset \mathscr{H}_{\overline{M}}.$$

Now we can consider the CQ^*-algebra $(\mathscr{B}(\mathscr{H}_M, \mathscr{H}_{\overline{M}}), *, \mathscr{B}(\mathscr{H}_M), \flat)$ of bounded operators acting in the triplet (see the Appendix).

The norm of $\mathscr{B}(\mathscr{H}_M, \mathscr{H}_{\overline{M}})$ can be written in terms of the norm in $\mathscr{B}(\mathscr{H}_{\{n\}})$ by

$$\|X\|_{M,\overline{M}} = \|e^{-M} X e^{-M}\|, \quad X \in \mathscr{B}(\mathscr{H}_M, \mathscr{H}_{\overline{M}}).$$

Similarly, the norm in $\mathscr{B}(\mathscr{H}_M)$ becomes

$$\|X\|_M = \|e^M X e^{-M}\|, \quad X \in \mathscr{B}(\mathscr{H}_M).$$

Also in this case it is not difficult to prove that $\pi_{\{n\}}(A)$ maps $\mathscr{H}_M$ into itself, for each $A \in \mathfrak{U}_0$. Then if we look at $\pi_{\{n\}}(A)$ as a bounded operator in $\mathscr{H}_M$, we get, taking into account the fact that $\pi_{\{n\}}$ can be viewed as the restriction to $\mathfrak{U}_0$ of a *-representation of the simple C^*-algebra $\mathfrak{U}_S$,

$$\|\pi_{\{n\}}(A)\|_M = \|A\|, \quad \forall A \in \mathfrak{U}_0,$$

where the norm on the right-hand side is the C^*-norm of $\mathfrak{U}_0$.

On the other hand, the CQ^*-norm,

$$\|\pi_{\{n\}}(A)\|_{M,\overline{M}} = \|e^{-M}\pi_{\{n\}}(A)e^{-M}\|,$$

is, in general, different from $\|A\|$.

Of course, to each $\{n\}$ it corresponds a CQ^*-algebra of the kind discussed above. This algebraic setup could also be taken as a reasonable framework, where discussing problems like the existence of the thermodynamical limit of the local Heisenberg dynamics. The results would, however, depend on $\{n\}$ and hence on the representation $\pi_{\{n\}}$. This has been done, for instance, in Ref. 5, for the so-called *almost-mean-field* models. Nevertheless, in that case the dependence on the representation is not crucial at all, provided that the states $\{n\}$ are chosen in a suitable family of *relevant* states. We will come back to this point in the next section.

For general models, however, this dependence on the representation cannot be easily eliminated. For this reason it might be convenient to define a topology that takes into account the whole class $\mathscr{F}$ of states under consideration. This topology, which we call *weak physical topology* and denote by $\tau_{\mathscr{F}}$ is defined by the family of seminorms (we will explicitly write the dependence of M on $\{n\}$):

$$A \in \mathfrak{U}_0 \to \|e^{-M_{\{n\}}}\pi_{\{n\}}(A)e^{-M_{\{n\}}}\|, \quad \{n\} \in \mathscr{F}.$$

Of course, $\tau_{\mathscr{F}}$ is the weakest locally convex topology, such that each $\pi_{\{n\}}$ is continuous from $\mathfrak{U}_0$ into $(\mathscr{B}(\mathscr{H}_M,\mathscr{H}_{\overline{M}}),*,\mathscr{B}(\mathscr{H}_M),\flat)$. The completion of $\mathfrak{U}_0[\tau_{\mathscr{F}}]$ will be denoted with $\mathfrak{U}$. The new seminorms above will take the place of the seminorms $\|A\|^{f,k} = \max\{\|M^k A f(M)\|, \|f(M)AM^k\|\}$ introduced in Refs. 5 and 6 to deal with the thermodynamical limit, where f runs in a suitable set of functions. We prefer to use the topology $\tau_{\mathscr{F}}$ because it is directly linked to the family of CQ^*-algebras shown above (it is indeed the projective limit of the norms of that family), and it still allows a complete discussion of the questions arose. The following proposition is now obvious.

Lemma II.1: Let $\mathfrak{U}$ *denote the completion of* $\mathfrak{U}_0[\tau_{\mathscr{F}}]$. *Then* $(\mathfrak{U}[\tau_{\mathscr{F}}],\mathfrak{U}_0)$ *is a topological quasi* *-*algebra*.

A. The thermodynamical limit

The possibility of defining a topology $\tau_{\mathscr{F}}$ for a specific model relies on the particular form of the Hamiltonian and, of course, on the possibility of choosing a family $\mathscr{F}$ of *relevant* states.

To begin with, let H_V be the finite volume Hamiltonian of the system and put

$$\delta_V(A) = i[H_V, A], \quad A \in \mathfrak{U}_0$$

and

$$\delta_V^k(A) = i[H_V, A]_k, \quad A \in \mathfrak{U}_0,$$

where $[H_V, A]_1 = [H_V, A]$ and $[H_V, A]_k = [H_V, [H_V, A]_{k-1}]$.

Proposition II.2: Let the finite volume Hamiltonian H_V *of the system be a polynomial* $p_V(S_V^i, \sigma_k^j)$ *in the variables* S_V^i *with* $S_V^i \in \mathfrak{U}_0$, $i = 1,2,\ldots,N$ *and a continuous function of the* σ_k^j*'s.*

Assume that (i) $\forall A \in \mathfrak{U}_0$, $[H_V, A]$ *depends on V only through the* S_V^i*'s*; (ii) $\lim_{|V|\to\infty}(S_V^i)^n$ *exists in* $\mathfrak{U}[\tau_{\mathscr{T}}]$, $\forall n \in \mathbb{N}$, $i=1,2,\ldots,N$.
Then, for each $A \in \mathfrak{U}_0$ *and for any* $k \in \mathbb{N}$ *the limits*

$$\lim_{|V|\to\infty} \delta_V^k(A)$$

exist in $\mathfrak{U}[\tau_{\mathscr{T}}]$. *Setting* $\delta(A) = \tau_{\mathscr{T}} - \lim_{|V|\to\infty} \delta_V(A)$, $A \in \mathfrak{U}_0$, *then* δ *has the properties* (a) $\delta(A)^* = \delta(A)^*$, $\forall A \in \mathfrak{U}_0$; (b) $\delta(AB) = \delta(A)B + A\delta(B)$, $\forall A, B \in \mathfrak{U}_0$.

Proof: By induction on k, one can show that, as well as for $k=1$, $\delta_V^k(A)$ is a polynomial in $\vec{S}_V$ and does not depend explicitly on V. Therefore, by (ii)

$$\tau_{\mathscr{T}} - \lim_{|V|\to\infty} \delta_V^k(A) \equiv \delta^{(k)}(A)$$

exist in $\mathfrak{U}$, for each $A \in \mathfrak{U}_0$ and for any $k \in \mathbb{N}$. (The notation $\delta^{(k)}$ is used to stress the fact that the powers of δ are not well defined, in general.)

Of course, by the $\tau_{\mathscr{T}}$ continuity of the involution and by the separate continuity of the multiplication one has, for any $A, B \in \mathfrak{U}_0$,

$$\delta(A^*) = \tau_{\mathscr{T}} - \lim_{|V|\to\infty} \delta_V(A^*) = \tau_{\mathscr{T}} - \lim_{|V|\to\infty} \sigma_V(A)^* = \delta(A)^*$$

and

$$\delta(AB) = \tau_{\mathscr{T}} - \lim_{|V|\to\infty} \delta_V(AB) = \tau_{\mathscr{T}} - \lim_{|V|\to\infty} (\delta_V(A)B + A\delta_V(B)) = \delta(A)B + A\delta(B).$$

□

Example II.3: The assumption (i) of the above proposition seems to be very strong. In spite of this appearance, it is fulfilled by several interesting models such as the (almost) mean-field spin models considered Refs. 5 and 6. For the Heisenberg model, for instance, the local Hamiltonian has the form

$$H_V = \frac{J}{|V|^\gamma} \sum_{p,q \in V} \sum_{i=1}^{3} \sigma_p^i \sigma_q^i, \tag{2.1}$$

with $\frac{1}{2} < \gamma \leqslant 1$, and the operators S_V^i are defined as

$$S_V^i = \frac{1}{|V|^\gamma} \sum_{p \in V} \sigma_p^i, \quad i = 1,2,3.$$

In this case one can show that, if $A \in \mathfrak{U}_{V'}$, then all the repeated commutators $[H_V, A]_k$ depend on the means S_V^i and on operators belonging to $\mathfrak{U}_{V'}$.

Analogous conclusions are obtained even for non-mean-field models like, for instance, the one defined by the following Hamiltonian:

$$H_V = \sum_{p,q \in V} \sum_{i=1}^{3} J_{p,q} (\sigma_p^i - \overline{\sigma^i})(\sigma_q^i - \overline{\sigma^i}), \tag{2.2}$$

where $\overline{\sigma^i}$ is the ith component of a fixed three vector (times the unit matrix).[8] Here the relevant V-dependent variables are

$$S_V^i(q)=\sum_{p\in V} J_{p,q}(\sigma_p^i-\overline{\sigma^i}),\quad i=1,2,3;\quad p=1,2,\ldots,|V|.$$

Remark II.4: The linear map δ defined in Proposition II.2 may be regarded as a *-derivation of $\mathfrak{U}_0$ defined on the domain

$$D(\delta)=\{A\in\mathfrak{U}_0:\delta(A)\in\mathfrak{U}_0\},\tag{2.3}$$

which is, as is readily checked, a *-subalgebra of $\mathfrak{U}_0$. This is, however, an unnecessary limitation. As we have seen in Proposition II.2, δ is, indeed, everywhere defined in $\mathfrak{U}_0$ [and of course the products in (b) make sense in the quasi *-algebra $\mathfrak{U}$). So, it would be natural to consider it as a *-derivation of the quasi*-algebra $(\mathfrak{U},\mathfrak{U}_0)$ in the sense of Ref. 9. This is, however, not always possible since, in general, δ is not continuous from $\mathfrak{U}_0[\tau_{\mathscr{F}}]$ into $\mathfrak{U}[\tau_{\mathscr{F}}]$.

The derivations δ_V and δ describe, at an infinitesimal level, respectively, the finite and the infinite volume dynamics of the system. What is, in general, expected is that they are generators of one-parameter groups of automorphisms of the completion of $\mathfrak{U}_0$ in a suitably chosen topology. This is certainly true for δ_V, $|V|<\infty$, since

$$\alpha_V^t(A)=e^{iH_Vt}Ae^{-iH_Vt},\quad A\in\mathfrak{U}_0,$$

is well defined, because $H_V\in\mathfrak{U}_V$ (and so does e^{iH_Vt}). The local dynamics α_V^t can be extended to the whole spin C^*-algebra $\mathfrak{U}_S$ and, as a function of t, is a one-parameter group of *-automorphisms of $\mathfrak{U}_S$. Since δ_V is bounded in $\mathfrak{U}_0$, we also get

$$\alpha_V^t(A)=\sum_{k=0}^{\infty}\frac{(it)^k}{k!}\delta_V^k(A),\quad A\in\mathfrak{U}_0,$$

and we know that $\delta_V^k(A)$ is $\tau_{\mathscr{F}}$ convergent to what we called $\delta^{(k)}(A)$. The problem of finding the limit for $|V|\to\infty$ of $\alpha_V^t(A)$ is then solved if we can control in a reasonable way the behavior of $\|\pi_{\{n\}}(\delta_V^k(A))\|_{M,\overline{M}}$ when $|V|$ grows to infinity.

Many models allow, indeed, some useful estimate of the norm of $\delta_V^k(A)$. This is true, for instance, for all mean-field models whose Hamiltonian is a polynomial of the three components of the mean spin.[10]

Lemma II.5: Assume that the local Hamiltonian H_V of a spin model can be written in the form

$$H_V=|V|p(S_V^1,S_V^2,S_V^3),$$

where p is a polynomial and

$$S_V^i=\frac{1}{|V|}\sum_{p\in V}\sigma_p^i,\quad i=1,2,3.$$

Then there exist two constants C_1, $C_2>0$ such that

$$\|\pi_{\{n\}}(\delta_V^k(A))\|_{M,\overline{M}}\leqslant\frac{C_1}{q}\max(2,\|A\|)C_2^k|V'|^k(k-1)!,\quad \forall A\in\mathfrak{U}_{V'}.$$

The constant C_1 depends only on $\{n\}$, C_2 depends only on the degree and on the form of the polynomial p, and $q\geqslant 1$ is the degree of the polynomial p.

Proof: In Ref. 10 it has been proved that, under the same assumptions, there exists $C_2>0$ such that

$$\|\delta_V^k(A)\| \leqslant \frac{1}{q}\max(2,\|A\|)C_2^k|V'|^k(k-1)!, \quad \forall A \in \mathfrak{U}_{V'}.$$

The statement then follows from the fact that $\|\pi_{\{n\}}(X)\|_{M,\overline{M}} \leqslant \|\pi_{\{n\}}(I)\|_{M,\overline{M}}\|X\|$, for each $X \in \mathfrak{U}_0$ and choosing $C_1 = \|\pi_{\{n\}}(I)\|_{M,\overline{M}}$. □

Proposition II.6: In the hypotheses of Lemma II.5, for each $A \in \mathfrak{U}_0$ there exists a positive number r_A such that the local dynamics

$$\alpha_V^t(A) = e^{iH_V t}Ae^{-iH_V t}$$

converges in the topology $\tau_{\mathscr{T}}$, when $|V| \to \infty$, to a limit that we denote by $\alpha^t(A)$, for any t with $|t| < r_A$.

Proof: If $A \in \mathfrak{U}_0$, then $A \in \mathfrak{U}_{V'}$ for some V'. Making use of Lemma II.5 we get

$$\left\| \sum_{k=0}^{\infty} \frac{(it)^k}{k!}\pi_{\{n\}}(\delta_V^k(A)) \right\|_{M,\overline{M}} \leqslant \sum_{k=0}^{\infty} \frac{|t|^k}{k}\frac{C_1}{q}\max(2,\|A\|)C_2^k|V'|^k.$$

The series on the right-hand side has a radius of convergence $r_A = 1/C_2|V'|$. □

It is worth noticing that the path followed in Ref. 5 depends strictly on the form of H_V since those results were mostly obtained by direct estimates. In the perspective we are following now, i.e., trying to obtain results for certain classes of interactions rather than for a specific one, it is not useful therefore to follow that approach. A more general strategy, for mean spin models, based on abstract results on differential equations can be found in Ref. 11.

Another possible approach to the problem of the existence of the thermodynamical limit makes use of the possibility of defining an *effective Hamiltonian.*

We will indicate with the same symbol the representation $\pi_{\{n\}}$ and its continuous extension to $\mathfrak{U}$ (this extension exists by the definition itself of the topology).

Definition II.7: We say that the model admits an effective Hamiltonian if for each $\{n\} \in \mathscr{T}$ there exists a self-adjoint operator $H_{\text{eff}}^{\{n\}}$ in $\mathscr{H}_{\{n\}}$ with the property

$$\pi_{\{n\}}(\delta(A)) = i[H_{\text{eff}}^{\{n\}}, \pi_{\{n\}}(A)], \quad \forall A \in \mathfrak{U}_0.$$

This equation is understood in the following weak sense:

$$\langle \pi_{\{n\}}(\delta(A))\phi, \psi\rangle = i\{\langle \pi_{\{n\}}(A)\phi, H_{\text{eff}}^{\{n\}}\psi\rangle - \langle H_{\text{eff}}^{\{n\}}\phi, \pi_{\{n\}}(A^*)\psi\rangle\},$$

$$\forall \phi, \psi \in D(H_{\text{eff}}^{\{n\}}), \quad \forall A \in \mathfrak{U}_0.$$

Remark II.8: This definition says, in practice, that the derivation on $\pi_{\{n\}}(\mathfrak{U}_0)$,

$$\delta_{\{n\}}(\pi_{\{n\}}(A)) = \pi_{\{n\}}(\delta(A))$$

is spatial and the implementing operator is self-adjoint. As is known, both these conditions require quite strong assumptions to be fulfilled.

For instance, if the states $|\{n\}\rangle$ with $\{n\} \in \mathscr{T}$ satisfy the condition

$$\langle\{n\}|\pi_{\{n\}}(\delta(A))|\{n\}\rangle = 0, \quad \forall A \in \mathfrak{U}_0, \tag{2.4}$$

then, as is known (Ref. 12, Sec. 3.2.2), the effective Hamiltonians $H_{\text{eff}}^{\{n\}}$ exist as self-adjoint operators in $\mathscr{H}_{\{n\}}$.

Equation (2.4) is fulfilled, for instance, by the almost mean-field Ising model,[5] for a suitable choice of the family $\mathscr{T}$ of states. This will be discussed in the next section.

If the model admits an effective Hamiltonian, then one can consider the subset $\mathscr{D}$ of $D(\delta)$ consisting of all the *generalized analytic elements* of δ, i.e., $A\in\mathscr{D}$ iff

$$e^{iH_{\rm eff}^{\{n\}}t}\pi_{\{n\}}(A)e^{-iH_{\rm eff}^{\{n\}}t}=\sum_{k=0}^{\infty}\frac{(it)^k}{k!}\,\pi_{\{n\}}(\delta^{(k)}(A)),$$

where the series on the right-hand side is understood to converge with respect to $\|\ \|_{M_{\{n\}},\overline{M}_{\{n\}}}$.

Proposition II.9: Let $\mathscr{F}_0\subset\mathscr{F}$ be a set of states such that for each $\{n\}\in\mathscr{F}_0$, $M_{\{n\}}$ and $H_{\rm eff}^{\{n\}}$ commute strongly (i.e., their spectral families commute). Then, for each $A\in\mathscr{D}$, the series $\Sigma_{k=0}^{\infty}[(it)^k/k!](\delta^{(k)}(A))$ converges, with respect to the topology $\tau_{\mathscr{F}_0}$, to an element of $\mathfrak{U}$ that we call $\alpha_t(A)$. Moreover, α_t can be extended to the closure $\overline{\mathscr{D}}$ of $\mathscr{D}$ in $\mathfrak{U}[\tau_{\mathscr{F}_0}]$.
If $\overline{\mathscr{D}}=\mathfrak{U}$, then α_t is a one-parameter group of automorphisms of $\mathfrak{U}$.

Proof: For $A\in\mathscr{D}$, we get

$$\left\|\sum_{k=0}^{\infty}\frac{t^k}{k!}\,(\delta^{(k)}(\pi_{\{n\}}(A)))\right\|_{M_{\{n\}},\overline{M}_{\{n\}}}=\left\|e^{-M_{\{n\}}}\left(\sum_{k=0}^{\infty}\frac{t^k}{k!}\,\pi_{\{n\}}(\delta^{(k)}(A))\right)e^{-M_{\{n\}}}\right\|$$
$$=\|e^{-M_{\{n\}}}e^{iH_{\rm eff}^{\{n\}}t}\pi_{\{n\}}(A)e^{-iH_{\rm eff}^{\{n\}}t}e^{-M_{\{n\}}}\|=\|\pi_{\{n\}}(A)\|_{M_{\{n\}},\overline{M}_{\{n\}}}. \tag{2.5}$$

Thus, the series

$$\sum_{k=0}^{\infty}\frac{(it)^k}{k!}\,(\delta^{(k)}(A))$$

is $\tau_{\mathscr{F}_0}$ convergent and we define $\alpha_t(A)$ as its limit. Equation (2.5) also implies the continuity of α_t. Then α_t can be extended to $\overline{\mathscr{D}}$. If $\overline{\mathscr{D}}=\mathfrak{U}$, the group property can be easily derived, under representation, for $A\in\mathfrak{U}_0$, making use of the effective Hamiltonian and then by pullback of the faithful representation $\pi_{\{n\}}$. For an arbitrary element of $\mathscr{D}$, the statement follows by continuous extension. □

Remark II.10: As noticed above, there could be some difference between $\delta^{(k)}(A)=\tau_{\mathscr{F}}-\lim_{V\to\infty}\delta_V^k(A)$ and $\delta^k(A)$, since the latter might not be well defined for an arbitrary $A\in\mathfrak{U}_0$. However, even when $\delta^k(A)$ is well defined, for any k (think of the case of an everywhere defined δ), there is no reason for $\delta^{(k)}(A)$ and $\delta^k(A)$ to coincide, since, in general, the convergence of $\delta_V^k(A)$ is not uniform in V.

Even the algebraic dynamics α_t is not, in general, the $\tau_{\mathscr{F}}$ limit of α_V^t in spite of the fact that $\delta(A)=\tau_{\mathscr{F}}-\lim_{V\to\infty}\delta_V(A)$.

If the derivation $\delta_{\{n\}}$ is continuous, some information can be obtained without making reference to the effective Hamiltonians.

Proposition II.11: Assume that for each $\{n\}\in\mathscr{F}$ there exists $C_{\{n\}}>0$, such that

$$\|\pi_{\{n\}}(\delta(A))\|_{M,\overline{M}}\leqslant C_{\{n\}}\|\pi_{\{n\}}(A)\|_{M,\overline{M}},\quad\forall A\in\mathscr{D}, \tag{2.6}$$

where $\mathscr{D}$ is a dense-subalgebra of $\mathfrak{U}$. Then* (i) *δ has a unique extension to $\mathfrak{U}$*; (ii) *for each $A\in\mathscr{D}$, the series $\Sigma_{k=0}^{\infty}[(it)^k/k!](\delta^{(k)}(A))$ converges, with respect to the topology $\tau_{\mathscr{F}}$, to an element of $\mathfrak{U}$ that we call $\alpha_t(A)$*; (iii) *$\{\alpha_t\}_{t\in\mathbb{R}}$ is a one-parameter group of automorphisms of $\mathfrak{U}$.*

Proof: (i) The inequality (2.6) implies the $\tau_{\mathscr{F}}$ continuity of δ on $\mathscr{D}$. So there exists a unique continuous extension (which we denote with the same symbol) of δ to $\mathfrak{U}$ for which (2.6) still holds.

(ii) From (2.6) it follows also, by an induction argument, that

$$\|\pi_{\{n\}}(\delta^{(k)}(A))\|_{M,\overline{M}} \leqslant C_{\{n\}}^k \|\pi_{\{n\}}(A)\|_{M,\overline{M}}, \quad \forall A \in \mathfrak{U},$$

and so

$$\left\| \sum_{k=0}^{\infty} \frac{(it)^k}{k!} \pi_{\{n\}}(\delta^k(A)) \right\|_{M,\overline{M}} \leqslant \sum_{k=0}^{\infty} \frac{|t|^k}{k!} C_{\{n\}}^k \|\pi_{\{n\}}(A)\|_{M,\overline{M}} \quad , \forall A \in \mathfrak{U}.$$

The series on the left-hand side converges therefore in $\mathfrak{U}$ to an element that we call $\alpha_t(A)$.

(iii) follows from a simple standard calculation. □

We will now give another existence theorem for the dynamics in representation whose assumptions, indeed very strong, are satisfied by many models.

Proposition II.12: Let H_{eff} be such that for all $X \in \mathfrak{U}_0$ there exist two positive constants, $L_{X,\{n\}}$, M_X such that

$$\|[H_{\text{eff}}, \pi_{\{n\}}(X)]_k\|_{M_{\{n\}},\overline{M}_{\{n\}}} \leqslant M_X^k L_{X,\{n\}},$$

for all $k \in N$. Therefore the series $\Sigma_{k=0}^{\infty}[(it)^k/k!]\pi_{\{n\}}((\delta^{(k)}(X)))$ converges, with respect to the norm $\|\ \|_{M_{\{n\}},\overline{M}_{\{n\}}}$, to $e^{iH_{\text{eff}}t}\pi_{\{n\}}(X)e^{-iH_{\text{eff}}t}$, for each $\{n\} \in \mathscr{F}$. Therefore the series $\Sigma_{k=0}^{\infty}[(it)^k/k!](\delta^{(k)}(X))$ converges in $\mathfrak{U}[\tau_{\mathscr{F}}]$ to an element that we call $\alpha_t(X)$.

The proof is straightforward so that we will omit it. It is more interesting here to provide some examples satisfying the above hypotheses.

We consider first the almost mean-field Ising model. The effective Hamiltonian is given by $H_{\text{eff}}^{\mathscr{J}} = 2J\eta n_3 \Sigma_p[\pi_{\{n\}}(\sigma_p^3) - n_p^3]$. Let $A_k \equiv \sigma_{p_1}^{i_1} \cdots \sigma_{p_k}^{i_k}$ be an element of the basis of $\mathfrak{U}_0$. By a direct estimate we deduce that

$$\|[H_{\text{eff}}, \pi_{\{n\}}(A_k)]_l\|_{M_{\{n\}},\overline{M}_{\{n\}}} \leqslant C_{\{n\}}(4Jk)^l.$$

This inequality can be extended to a general element of $\mathfrak{U}_0$ simply using the linearity. Analogous estimates also hold for the almost mean-field Heisenberg model, for the van der Waals spin model,[13] and also for the (long-range) Ising model described by (2.2).

III. PHYSICAL APPLICATIONS

This section is devoted to discussing some explicit physical spin models that fit well in the framework discussed above. In particular, we will consider once more the almost mean-field spin models discussed in Refs. 5 and 6. After that we will also introduce more spin models, unitarily equivalent to these ones, which describes different physical situations.

A. (Almost) mean-field spin models

As before, the basic mathematical ingredient for the study of this model is the spin *-algebra $\mathfrak{U}_0$. Its norm completion, $\mathfrak{U}_S$, is not, as is known, rich enough for a comprehensive discussion of the thermodynamical limit of the algebraic dynamics.

The finite volume Hamiltonian that describes the Ising model is

$$H_V^{\mathscr{J}} = \frac{1}{|V|^{\gamma}} \sum_{i,j \in V} \sigma_i^3 \sigma_j^3, \tag{3.1}$$

while for the Heisenberg model

$$H_V^{\mathscr{H}} = \frac{1}{|V|^{\gamma}} \sum_{i,j \in V} \sum_{\alpha=1}^{3} \sigma_i^{\alpha} \sigma_j^{\alpha}. \tag{3.2}$$

For $\gamma=1$ these are typical mean-field models, extensively discussed in the literature.[7,2,11] The case $\gamma<1$ has been considered in Refs. 5 and 6.

The local Heisenberg equations of motion for both models are given by

$$\frac{d}{dt}\,\alpha_V^t(\sigma_p^i)=i[H_V,\alpha_V^t(\sigma_p^i)],\quad i=1,2,3, \tag{3.3}$$

whose solution can be easily computed as in Refs. 5 and 6.

As is known, the thermodynamical limit of $\alpha_V^t(A)$, $A\in\mathfrak{U}_0$ does not belong to $\mathfrak{U}_S$.

All the approaches suggested in the previous section, make reference to a family $\mathscr{F}$ of relevant states. For these models we choose

$$\mathscr{F}=\left\{\{n\}=\{n_1,n_2,n_3,\ldots\}:\lim_{|V|,\infty}\frac{1}{|V|^\gamma}\sum_{p\in V}n_p=\eta n,\quad |\eta|\leqslant 1\right\},$$

where n is a fixed unit vector in $\mathbb{R}^3$, which, for Ising models, has to be chosen, as well as the n_p's for large p, of the form $(0,0\pm 1)$. In the first approach, which is closer to that developed in Refs. 5 and 6, we will make use of the *weak physical topology* $\tau_{\mathscr{F}}$ defined in the previous section.

Of course, our aim is to make use of Proposition II.2. For this reason we need to find local observables S_V^i fulfilling the conditions given there. This role will be played by the ''almost'' mean spin operators. They do indeed converge, together with their powers, in the weak physical topology. This can be easily shown with analogous techniques as the ones used in Refs. 5 and 6. We prove in detail the convergence of

$$S_V^3\equiv\frac{1}{|V|^\gamma}\sum_{p\in V}\sigma_p^3, \tag{3.4}$$

for the ''almost'' Ising model in the $\tau_{\mathscr{F}}$ topology. Using the same notations as in the cited papers, and in particular by means of the spectral decomposition $M=\Sigma_{n=0}^{\infty}mP_m$, neglecting the n dependence in this formula, we have

$$\|\pi_{\{n\}}(S_V^3)-\eta n_3\|_{M_{\{n\}},\overline{M}_{\{n\}}}=\sum_{l,k=0}^{\infty}e^{-l}e^{-k}\|P_l(\pi_{\{n\}}(S_V^3)-\eta n_3)P_k\|,$$

and this last contribution can be estimated as in Ref. 5. We get, indeed,

$$\|\pi_{\{n\}}(S_V^3)-\eta n_3\|_{M_{\{n\}},\overline{M}_{\{n\}}}\leqslant\left|\frac{1}{|V|^\gamma}\sum_{p\in V}n_p^3-\eta n_3\right|\sum_l e^{-2l}+\frac{2}{|V|^\gamma}\sum_l e^{-2l+1}\to 0.$$

Moreover, even the powers converge in this topology, as is easily seen.

As far as the convergence of the algebraic dynamics α_V^t is concerned, it is also possible, and perhaps more convenient, to make use of the effective Hamiltonian H_{eff}. Both for the Ising and the Heisenberg models these effective Hamiltonian do really exist and allow us to treat both models in the same way. Indeed, at least for the Ising model, each state in the family $\mathscr{F}$ satisfies Eq. (2.4). For instance, if $A=\sigma_p^i$ then $\delta_V(A)=S_V^3(c_1\sigma_p^1+c_2\sigma_p^2)$ plus terms going to zero when $|V|\to\infty$, where c_1 and c_2 are complex numbers. If now $\{n\}\in\mathscr{F}$ it follows that for large p $\lim_{V\to\infty}\langle\{n\}|S_V^3(c_1\sigma_p^1+c_2\sigma_p^2)|\{n\}\rangle=0$. These effective Hamiltonians are given, for Ising and the Heisenberg models, respectively, by the two self-adjoint operators in $\mathscr{H}_{\{n\}}$:

$$H_{\text{eff}}^{\mathscr{I}}=2J\eta n_3\sum_p\left[\pi_{\{n\}}(\sigma_p^3)-n_p^3\right]$$

and

$$H_{\text{eff}}^{\mathscr{H}}=2J\eta\sum_p\ [\pi_{\{n\}}(\sigma_p)\cdot n-\epsilon_p].$$

Here n, n_p, and η are the quantities entering in the definition of the family $\mathscr{F}$, while ϵ_p is a sequence consisting of elements equal either to 1 or to -1, such that

$$\lim_{|V|\to\infty}\frac{1}{|V|^\gamma}\sum_{p\in V}\epsilon_p=\eta.$$

These sequences can be used to define a subset $\mathscr{F}_0$ of $\mathscr{F}$ just by considering, for a fixed three-vector n, the sequence $\{n_p\}$ where $n_p=\epsilon_p n$. The states in $\mathscr{F}_0$ are such that $H_{\text{eff}}^{\mathscr{H}}$ commutes with $M_{\{n\}}$; see Ref. 6. These effective Hamiltonians both satisfy the following condition:

$$[H_{\text{eff}},\pi_{\{n\}}(A)]=\pi_{\{n\}}(\lim_{|V|\to\infty}[H_V,A]),$$

for all $A\in\mathfrak{U}_0$. As in Ref. 6 we can therefore prove that the following equality holds true:

$$e^{iH_{\text{eff}}t}\pi_{\{n\}}(A)e^{-iH_{\text{eff}}t}=\sum_{k=0}^{\infty}\frac{(it)^k}{k!}\,\pi_{\{n\}}(\delta^{(k)}(A)),$$

where the convergence of the series is intended in the usual matrix norm, which also implies convergence in the $\tau_{\mathscr{F}}$ topology. Furthermore, in the Ising model and in the Heisenberg model, if we restrict to $\mathscr{F}_0$, it is certainly possible to define the algebraic dynamics as the following infinite sum:

$$\alpha_t(A)=\sum_{k=0}^{\infty}\frac{t^k}{k!}\,(\delta^{(k)}(A)),$$

since one can prove that the series again converges with respect to the $\tau_{\mathscr{F}}$ or $\tau_{\mathscr{F}_0}$ topology, respectively. Obviously we have $\alpha_t(A)\in\mathfrak{U}$ for all $A\in\mathfrak{U}_0$.

As mentioned in Sec. II, for each $\{n\}\in\mathscr{F}$ the problem of the existence of the thermodynamical limit of α_V^t can be considered in each CQ^*-algebra $(\mathscr{B}(\mathscr{H}_M,\mathscr{H}_{\overline{M}}),*,\mathscr{B}(\mathscr{H}_M),\flat)$. This can be useful when the family $\mathscr{F}$ of states is so poor as to consist of only one state.

This is not the case of the (almost) mean-field models, since for them the family $\mathscr{F}$ is quite rich. Nevertheless, it still makes sense to consider for these models this CQ^*-algebraic approach.

From the first part of this section we know, in fact, that the almost ergodic means S_V^i converge in the topology $\tau_{\mathscr{F}}$, so that they converge with respect to each norm $\|\cdots\|_{M_{\{n\}},\overline{M}_{\{n\}}}=\|\,e^{-M_{\{n\}}}\cdots e^{-M_{\{n\}}}\|$ for any choice of the sequence $\{n\}$ in the set $\mathscr{F}$, and the same obviously holds true, even for the finite volume dynamics α_V^t. Therefore, in each of these CQ^*-algebras the thermodynamical limit of α_V^t is well defined, even if it is necessarily representation dependent. This is not a major problem in the models we are considering since something nice happens here: as far as the sequence $\{n\}$ is chosen in $\mathscr{F}$, or in $\mathscr{F}_0$ for the Heisenberg model, $\alpha_V^t(A)$ converges always to the same element, modulo $\pi_{\{n\}}(I)$. For instance, in the Ising model, $\pi_{\{n\}}(S_V^3)$ converges to $2Jt\eta n_3\pi_{\{n\}}(I)$ in any norm $\|\ \|_{M_{\{n\}},\overline{M}_{\{n\}}}$, where η and n_3 are fixed by the definition of $\mathscr{F}$. A consequence of this fact is the convergence of $\pi_{\{n\}}(\alpha_V^t(A))$ for each $A\in\mathfrak{U}_0$.

Of course, this procedure strongly relies on the specific models we are considering, since there is no reason *a priori* to be sure that the limit of a certain α_V^t does not depend on the way in which this limit is performed!

B. Spin models with bubbles

In this section we discuss some more models with a direct physical meaning that are unitarily equivalent to those discussed above and whose thermodynamical behavior can easily be determined. We will see that the models below still give rise to finite volume algebraic dynamics converging when $|V|\to\infty$.

We start with proving a first *equivalence* result, which relates different Hamiltonians. Let us consider a certain finite lattice region Ω, which we may suppose to be contained in any volume V for $|V|>|\Omega|$.

Let us now define the finite volume Hamiltonian,

$$H_V^{\rm tr}=\frac{1}{|V|^{\gamma}}\sum_{p,q\in V} T_pT_q\,, \tag{3.5}$$

where $T_p=(\gamma\cdot\sigma)_p$

We have the following.

Proposition III.1: Let H_V^{tr} be as in (3.5) and suppose that, $\forall p\notin\Omega, T_p=\sigma_p^3$. A unitary operator U of the form

$$U=\exp\left\{i\sum_p m_p\cdot\sigma_p\right\},$$

such that $H_V^{tr}=UH_V^{\mathcal{T}}U^*$ exists if and only if each vector γ_p has a norm equal to unity. In this case one finds explicitly

$$m_p=\begin{cases}\left(\dfrac{\pi\sqrt{2}\,\gamma_p^1}{4\sqrt{1+\gamma_p^3}},\dfrac{\pi\sqrt{2}\,\gamma_p^2}{4\sqrt{1+\gamma_p^3}},\dfrac{\pi\sqrt{2}\,\gamma_p^3}{4\sqrt{1+\gamma_p^3}}\right), & \forall p\in\Omega,\\ 0, \quad otherwise.\end{cases} \tag{3.6}$$

Proof: We prove first the necessity. If such a U exists it must necessarily transform σ_p^3 into T_p, so that $T_p=U\sigma_p^3U^*$, $\forall p\in V$. Indicating with $\|\ \|_V$ the vector norm and with $\|\ \|$ the C^* norm, and using some easy properties of the σ matrices, we must have simultaneously $\|T_p\|=\|(\gamma\cdot\sigma)_p\,,\|=\|\gamma_p\|_V$ and $\|T_p\|=\|U\sigma_p^3U^*\|=\|\sigma_p^3\|=1$.

Vice versa, let us suppose that $\|\gamma_p\|=1$. We want to show that it is possible to choose an operator U as above that maps one Hamiltonian into the other. The proof is straightforward. We have to solve the following system (in which we have omitted the lattice site index):

$$\begin{cases}-\dfrac{\sin(2m)}{m}\,m_2+2m_3m_1\left(\dfrac{\sin(m)}{m}\right)^2=\gamma_1,\\ \dfrac{\sin(2m)}{m}\,m_1+2m_3m_2\left(\dfrac{\sin(m)}{(m)}\right)^2=\gamma_2,\\ \cos(2m)+2m_3^2\left(\dfrac{\sin(m)}{m}\right)^2=\gamma_3.\end{cases} \tag{3.7}$$

where $m^2=m_1^2+m_2^2+m_3^2$. It is now very easy to verify that the solution (3.6) satisfies, in the hypothesis $\|\gamma_p\|_V=1$, the above system and corresponds to $m=\pi/2$. □

The models described by $H_V^{\rm tr}$ can all be thought of as *bubble* models. They describe, in fact, a situation in which inside a certain bubble of finite size, Ω, the spin variables are not necessarily in the z direction, while outside this region all the spins are polarized along z. From the

literature,[11,5,6] it is reasonable to expect that the algebraic dynamics of this bubble model still converges. This should essentially follow from the fact that the family $\mathscr{F}$ is closed under local transformations.

Here we will adopt a different approach, which allows us to conclude directly that the thermodynamical limit exists. Let us define

$$\widetilde{\alpha}^t_V(A) \equiv e^{iH^{\mathrm{tr}}_V t} A e^{-iH^{\mathrm{tr}}_V t},$$

where $A \in \mathfrak{U}_0$. We now verify that, for each $A \in \mathfrak{U}_0$, $\widetilde{\alpha}'_V(A)$ is a Cauchy net in the topology $\tau_{\mathscr{F}}$. This depends on the fact that $\alpha'_V(A)$ is, in turn, a $\tau_{\mathscr{F}}$-Cauchy net. We have, indeed,

$$\begin{aligned}\|\pi_{\{n\}}(\widetilde{\alpha}^t_V(A) - \widetilde{\alpha}^t_{V'}(A))\|_{M_{\{n\}},\overline{M_{\{n\}}}} &= \|\pi_{\{n\}}(U(\alpha^t_V(\widetilde{A}) - \alpha^t_{V'}(\widetilde{A}))U^*)\|_{M_{\{n\}},\overline{M_{\{n\}}}} \\ &\leqslant \|\pi_{\{n\}}(\alpha^t_V(\widetilde{A}) - \alpha^t_{V'}(\widetilde{A}))\|_{M_{\{n\}},\overline{M_{\{n\}}}} \to 0,\end{aligned}$$

where $\widetilde{A} \equiv U^* A U$. Here we took into account the inequality

$$\|\pi_{\{n\}}(XY)\|_{M_{\{n\}},\overline{M_{\{n\}}}} \leqslant \|\pi_{\{n\}}(X)\|_{M_{\{n\}},\overline{M_{\{n\}}}} \|Y\|, \quad \forall X, Y \in \mathfrak{U}_0,$$

and we made use of the fact that $e^{iH^{\mathrm{tr}}_V t} A e^{-iH^{\mathrm{tr}}_V t} = U e^{iH_V t} \widetilde{A} e^{-iH_V t} U^*$. Convergence to zero of the above limit when both V and V' diverge is ensured by the existence of the dynamics α_t on the whole $\mathfrak{U}_0$.

Of course, the group property of α_t is also shared by $\widetilde{\alpha}_t$, like the other properties discussed for the original model.

A similar conclusion can also be stated for the Heisenberg model. Even in this case it is possible to consider bubble models related to this and to study the thermodynamical limit of the algebraic dynamics.

Proposition III.2: Let H^{tr}_V be

$$H^{\mathrm{tr}}_V = \frac{1}{|V|^\gamma} \sum_{p,q \in V} \sum_{i=1}^{3} T^i_p T^i_q,$$

and suppose that $\forall p \notin \Omega, T^i_p = \sigma^i_p$. *A unitary operator* U *of the form*

$$U = \exp\left\{ i \sum_p m_p \cdot \sigma_p \right\},$$

such that $H^{\mathrm{tr}}_V = U H^{\mathscr{H}}_V U^*$ *exists only if the vectors* γ^i_p *form, for any* $p \in V$, *a set of right-handed versors*.

The proof is very simple and will be omitted here. It is more useful to notice that we can only prove a necessary condition for the transformation between the two Hamiltonians to be possible. Nevertheless, it is reasonable to expect that the above condition is also sufficient for the existence of the operator U. Its geometrical interpretation is clear: we start with an orthonormal system of normalized vectors and we obtain another analogous system of vectors. *Vice versa*, to get an orthonormal system of normalized vectors we expect that the starting point should be a triplet of similar versors.

Then, in conclusion, also these bubble models, as well as any other unitarily equivalent model, can be setted in the framework discussed in Sec. II.

APPENDIX A: AN OVERVIEW OF MATHEMATICAL DEFINITIONS

In this appendix we collect some basic facts on partial *-algebras, quasi *-algebras, and CQ^*-algebras, which are needed for a better understanding of the paper. For more details we refer to Refs. 14, 15, 16, 2, 3, and 4 and to Refs. 17 and 18 for reviews.

A partial *-algebra is a vector space $\mathfrak{A}$ with involution $A\to A^*$ [i.e., $(A+\lambda B)^*=A^*+\overline{\lambda}B^*$; $A=A^{**}$] and a subset $\Gamma\subset\mathfrak{A}\times\mathfrak{A}$, such that (i) $(A,B)\in\Gamma$ implies $(B^*,A^*)\in\Gamma$; (ii) (A,B) and $(A,C)\in\Gamma$ imply $(A,B+\lambda C)\in\Gamma$; and (iii) if $(A,B)\in\Gamma$, then there exists an element $AB\in\mathfrak{A}$, and for this multiplication the distributive property holds in the following sense: if $(A,B)\in\Gamma$ and $(A,C)\in\Gamma$ then

$$AB+AC=A(B+C).$$

Furthermore $(AB)^*=B^*A^*$.

The product is not required to be associative.

The partial *-algebra $\mathfrak{A}$ is said to have a unit if there exists an element I (necessarily unique) such that $I^*=I$, $(I,A)\in\Gamma$, $IA=AI=A$, $\forall A\in\mathfrak{A}$.

If $(A,B)\in\Gamma$ then we say that A is a left multiplier of B [and write $A\in L(B)$] or B is a right multiplier of A [$B\in R(A)$]. For $\mathscr{S}\subset\mathfrak{A}$ we put $L.\mathscr{S}=\cap_{A\in\mathscr{S}}L(A)$; the set $R.\mathscr{S}$ is defined in an analogous way. The set $M.\mathscr{S}=L.\mathscr{S}\cap R.\mathscr{S}$ is called the set of universal multipliers of $\mathscr{S}$.

Following Lassner,[2,3] we call quasi *-algebras a special family of partial *-algebras: namely, those for which the set $M\mathfrak{A}$ of universal multipliers is a *-algebra.

Let $\mathfrak{A}$ be a linear space and $\mathfrak{A}_0$ a *-algebra contained in $\mathfrak{A}$. We say that $\mathfrak{A}$ is a quasi *-algebra with distinguished *-algebra $\mathfrak{A}_0$ (or, simply, over $\mathfrak{A}_0$) if (i) the right and left multiplications of an element of $\mathfrak{A}$ and an element of $\mathfrak{A}_0$ are always defined and linear; and (ii) an involution * (which extends the involution of $\mathfrak{A}_0$) is defined in $\mathfrak{A}$ with the property $(AB)^*=B^*A^*$ whenever the multiplication is defined.

A quasi *-algebra $(\mathfrak{A},\mathfrak{A}_0)$ is said to have a unit I if there exists an element $I\in\mathfrak{A}_0$ such that $AI=IA=A$, $\forall A\in\mathfrak{A}$.

A quasi *-algebra $(\mathfrak{A},\mathfrak{A}_0)$ is said to be a topological quasi *-algebra if in $\mathfrak{A}$ is defined a locally convex topology ξ such that (a) the involution is continuous and the multiplications are separately continuous; and (b) $\mathfrak{A}_0$ is dense in $\mathfrak{A}[\xi]$.

In Ref. 4 we considered a special class of quasi *-algebras, called CQ^*-algebras, which arise as completions of C^*-algebras.

*Definition 1: A rigged quasi *-algebra $\mathfrak{A}$ is a partial *-algebra for which there exist two vector subspaces $\mathfrak{A}_\flat$ and $\mathfrak{A}_\sharp$, such that* (i) $(\mathfrak{A}_\flat)^*=\mathfrak{A}_\sharp$; (ii)

$$\Gamma\{(A,B)\in\mathfrak{A}\times\mathfrak{A}:A\in\mathfrak{A}_\sharp \quad or \quad B\in\mathfrak{A}_\flat\};$$

and (iii) *both $\mathfrak{A}_\flat$ and $\mathfrak{A}_\sharp$ are algebras with respect to the partial multiplication $(A,B)\in\Gamma\to AB\in\mathfrak{A}$ defined in $\mathfrak{A}$.*

The multiplication $(A,B)\in\Gamma\to AB\in\mathfrak{A}$ is supposed to be (weakly) semiassociative; *i.e.* $(AB)C=A(BC)\forall A\in\mathfrak{A}$ *and* $\forall B,C\in\mathfrak{A}_\flat$.

*Definition 2: A rigged quasi *-algebra $\{\mathfrak{A},*,\mathfrak{A}_\flat,\flat\}$ is called a CQ^*-algebra if (i) $\mathfrak{A}$ is a Banach space under the norm and $\|A^*\|=\|A\|$, $\forall A\in\mathfrak{A}$; (ii) $\mathfrak{A}_\flat$ is a C^*-algebra with respect to the norm $\|\ \|_\flat$ and to the involution $\flat$; (iii) $\mathfrak{A}_\sharp$ carries the norm $\|\ \|_\sharp$, defined by $\|A\|_\sharp\equiv\|A^*\|_\flat$ (thus the involution * is an isometric anti-isomorphism of $\mathfrak{A}_\flat$ onto $\mathfrak{A}_\sharp$) and $A^{\sharp *}=A^{*\flat}$, $\forall A\in\mathfrak{A}_\sharp$; (iv) $\|B\|_\flat=\sup_{\|A\|\le 1}\|AB\|$; and (v) $\mathfrak{A}_0=\mathfrak{A}_\flat\cap\mathfrak{A}_\sharp$ is $\|\ \|_\flat$ dense in $\mathfrak{A}_\flat$ and $\mathfrak{A}_\flat$ is $\|\ \|$ dense in $\mathfrak{A}$.*

A very interesting example of CQ^*-algebras is provided by the families of bounded operators acting in a triplet of Hilbert spaces.

Let $\mathscr{H}$ be a Hilbert space with scalar product $\langle\cdot,\cdot\rangle$ and $\lambda(\cdot,\cdot)$ a positive sesquilinear closed form defined on a dense domain $\mathscr{D}_\lambda\subset\mathscr{H}$. Then $\mathscr{D}_\lambda$ becomes a Hilbert space, that we denote by $\mathscr{H}_\lambda$, with respect to the scalar product

$$\langle f,g\rangle_\lambda = \langle f,g\rangle + \lambda(f,g).$$

Let $\mathscr{H}_\lambda^-$ be the Hilbert space of conjugate linear forms on $\mathscr{H}_\lambda$.

In this way one gets the triplet of Hilbert spaces,

$$\mathscr{H}_\lambda \subset \mathscr{H} \subset \mathscr{H}_\lambda^-.$$

Let $\mathscr{B}(\mathscr{H}_\lambda, \mathscr{H}_\lambda^-)$ be the Banach space of bounded operators from $\mathscr{H}_\lambda$ into $\mathscr{H}_\lambda^-$ and let us denote with $\|A\|_{\lambda\lambda}^-$ the natural norm of $A \in \mathscr{B}(\mathscr{H}_\lambda, \mathscr{H}_\lambda^-)$.

The involution in $\mathscr{B}(\mathscr{H}_\lambda, \mathscr{H}_\lambda^-)$, is defined in the following way: to each element $A \in \mathscr{B}(\mathscr{H}_\lambda, \mathscr{H}_\lambda^-)$, we associate the linear map A^* from $\mathscr{H}_\lambda$ into $\mathscr{H}_\lambda^-$, defined by the equation

$$\langle A^* f,g\rangle = \overline{\langle Ag,f\rangle}, \quad \forall f,g \in \mathscr{H}_\lambda.$$

Then one has $A^* \in \mathscr{B}(\mathscr{H}_\lambda, \mathscr{H}_\lambda^-)$ and $\|A^*\|_{\lambda\lambda}^- = \|A\|_{\lambda\lambda}^-, \forall A \in \mathscr{B}(\mathscr{H}_\lambda, \mathscr{H}_\lambda^-)$.

Let $\mathscr{B}(\mathscr{H}_\lambda)$ denotes the C^*-algebra of bounded operators on $\mathscr{H}_\lambda$ [the usual involution of $\mathscr{B}(\mathscr{H}_\lambda)$ will be denoted here as $\flat$] and $\mathscr{B}(\mathscr{H}_\lambda^-)$ the C^*-algebra of bounded operators on $\mathscr{H}_\lambda^-$ [the natural involution of $\mathscr{B}(\mathscr{H}_\lambda^-)$ is denoted as $\sharp$]. Then, both $\mathscr{B}(\mathscr{H}_\lambda)$ and $\mathscr{B}(\mathscr{H}_\lambda^-)$ are contained in $\mathscr{B}(\mathscr{H}_\lambda, \mathscr{H}_\lambda^-)$ and $A \in \mathscr{B}(\mathscr{H}_\lambda)$ if, and only if, $A^* \in \mathscr{B}(\mathscr{H}_\lambda^-)$. Moreover, $B^\flat{}^* = B^{*\sharp}, \forall B \in \mathscr{B}(\mathscr{H}_\lambda)$.

With the algebraic operations defined in the natural way $(\mathscr{B}(\mathscr{H}_\lambda, \mathscr{H}_\lambda^-), *, \mathscr{B}(\mathscr{H}_\lambda), \flat)$ is a rigged quasi *-algebra. The distinguished *-algebra of $\mathscr{B}(\mathscr{H}_\lambda, \mathscr{H}_\lambda^-)$ is

$$\mathscr{B}^+(\mathscr{H}_\lambda) = \{A \in \mathscr{B}(\mathscr{H}_\lambda, \mathscr{H}_\lambda^-) : A, A^* \in \mathscr{B}(\mathscr{H}_\lambda)\}.$$

Moreover, $(\mathscr{B}(\mathscr{H}_\lambda, \mathscr{H}_\lambda^-), *, \mathscr{B}(\mathscr{H}_\lambda), \flat)$ is a CQ^*-algebra if $\mathscr{B}(\mathscr{H}_\lambda, \mathscr{H}_\lambda^-)$ and $\mathscr{B}(\mathscr{H}_\lambda)$ carry their natural norms. In fact, $\mathscr{B}^+(\mathscr{H}_\lambda)$ is dense in $\mathscr{B}(\mathscr{H}_\lambda, \mathscr{H}_\lambda^-)$, and the other requirements of the definition of CQ^*-algebra are also fulfilled. For the details see Ref. 4, Example 3.3.

The CQ^*-algebras considered in Secs. I and II of this paper are all of this kind. They are obtained when the form λ is taken as the form associated to the closed operator e^M.

The general structure of CQ^*-algebras simplifies for the so-called proper CQ^*-algebras.

Definition 3: A CQ^*-algebra $\{\mathfrak{U}, *, R\mathfrak{U}, \flat\}$ is called proper if $R\mathfrak{U} = L\mathfrak{U}$ and if $A^\flat = A^\sharp, \forall A \in R\mathfrak{U}$.

In Ref. 4 it is proved that from the above definition it follows that (i) $\|A\|_\sharp = \|A\|_\flat, \forall A \in R\mathfrak{U}$; (ii) all the Abelian CQ^*-algebras (i.e., $R\mathfrak{U} = L\mathfrak{U}$ and $AB = BA, \forall A \in \mathfrak{U}, B \in R\mathfrak{U}$) are proper.

As said before, CQ^*-algebras arise naturally as completions of C^*-algebras with respect to a weaker norm. Indeed the following is true.

Proposition 4: Let $\mathscr{C}$ be a C^*-algebra with norm $\|\ \|_1$ and involution $*$. Let $\|\ \|$ be another norm on $\mathscr{C}$, weaker than $\|\ \|_1$ and such that (i) $\|A\| = \|A^*\|, \forall A \in \mathscr{C}$; (ii) $\|AB\| \leq \|A\| \|B\|_1, \forall A, B \in \mathscr{C}$. *Then the completion $\hat{\mathscr{C}}$ of $\mathscr{C}$, with its natural norm, is a proper CQ^*-algebra over $\mathscr{C}$, with $* = \flat$.*

A more detailed study of CQ^*-algebras has been undertaken in Ref. 19.

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Gamow states as continuous linear functionals over analytical test functions

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The space of analytical test functions ξ, rapidly decreasing on the real axis (i.e., Schwartz test functions of the type $\mathscr{S}$ on the real axis), is used to construct the rigged Hilbert space (RHS) $(\xi,\mathscr{H},\xi')$. Gamow states (GS) can be defined in RHS starting from Dirac's formula. It is shown that the expectation value of a self-adjoint operator acting on a GS is real. We have computed exactly the probability of finding a system in a GS and found that it is finite. The validity of recently proposed approximations to calculate the expectation value of self-adjoint operators in a GS is discussed. © *1996 American Institute of Physics.* [S0022-2488(96)00209-5]

I. INTRODUCTION

The proper treatment of the continuum and the inclusion of decaying states belonging to it in the definition of Green's functions of physical interest is a long-standing problem in various fields of physics. The mathematical consequences of the inclusion of the continuum in the scattering of particles by a central potential have been explored by Gamow long ago.[1] A modern review of the scattering theory can be found in Ref. 2 where the basic elements of the involved radial differential equations are presented in great detail. The use of these states, as it has been shown by Gamow,[1] is of central importance in building the physical interpretation of the α-decay mode of heavy atomic nuclei.[3] The so-called Gamow resonant states [for simplicity Gamow states (GS)] fulfill purely outgoing boundary conditions with an exponential behavior at infinity.[2] Several methods have been proposed since the publication of Gamow's work,[4] particularly in connection with the normalizability of Green's functions in the presence of GS and in the treatment of completeness relations.[5] The mathematical equivalence between some of these methods has been discussed recently and the correspondence between Bergreen's and Mittag-Lefler's representations has been explored at length.[6] Presently a rich literature is available regarding the application of these concepts to nuclear reactions and to nuclear structure problems.[7]

The amount of information about mathematical properties of representations which include GS is also very rich. The use of decaying states of complex energy in the framework of the Hamiltonian formalism, and the use of deformed contours to compute survival amplitudes, has been reported in Ref. 8 by Sudarshan and co-workers. The formulation of quantum mechanics in the rigged Hilbert space (RHS) has been also studied by Bohm.[9] In Ref. 10 it is shown that idealized resonances are described, within the RHS, by generalized eigenvectors of a self-adjoint Hamiltonian with complex eigenvalues and a Breit–Wigner energy distribution. Similar arguments have been advanced by Gadella.[11,12,13] Among the difficulties posed by the use of GS one can mention the appearance of the exponential catastrophe and the need to include nonphysical

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states of negative energy in the definition of GS by an integral on the real axis.[14] A nonrigorous cure for the exponential catastrophe would be the use of some regularization techniques, such as the one proposed by Zel'dovich.[15] However, and with reference to explicit numerical applications, the use of these techniques does not guarantee the stability of the results since the onset of the exponential dominance of the GS can manifest itself at physical scales.[5] Among the recent references on GS we shall mention the work of T. Berggren,[16] where the possibility of defining expectation values of operators in a resonant state is considered. In the present work we shall focus our attention on the mathematical aspects of representations which include Gamow states. At variance with the usually adopted approach, i.e., by using the class of functions known as Hardy class functions,[11–13] we shall use tempered ultradistributions.[17,–20] The space of analytical functionals ξ' (tempered ultradistributions) is the minimal space whose Fourier antitransform accomodates real exponential functions as distributions. In the first part of this work the definition of the space of analytical test functions ξ is given and the corresponding RHS is constructed. Then Dirac's formulation of quantum mechanics in RHS is shown, the structure of GS is given explicitly, and the norm of GS in RHS is calculated. The contribution of GS to $P(E)$, the probability distribution of a system at energy E, is obtained and the relation with the Breit–Wigner weighted energy distribution is studied. Next, some examples of GS as analytical functionals are given. Finally, a comparison with Berggren's results on expectation values with resonant states is presented.

II. THE RIGGED HILBERT SPACE ($\xi,\mathscr{H},\xi'$)

Let us consider the space ξ of entire analytical test functions $\hat{\phi}(z)$ rapidly decreasing on the real axis, i.e., $\hat{\phi}(z)|_{y=0}=\phi(x)$ is a test function of the Schwartz space $\mathscr{S}$ (see Refs. 17–21).

The structure of a countable normed space of ξ is given by the family of norms

$$\|\hat{\phi}\|_n=\sup_{|z|=n}|\hat{\phi}(z)|, \quad n\in\mathscr{N}. \tag{1}$$

These norms are compatible since

$$\|\hat{\phi}\|_n<\|\hat{\phi}\|_{n+1}. \tag{2}$$

In ξ we define the scalar product

$$\langle\hat{\psi},\hat{\phi}\rangle=\int_{-\infty}^{+\infty}dE\ \overline{\hat{\psi}}(E)\hat{\phi}(E) \tag{3}$$

and the norm

$$\|\hat{\phi}\|^2=\langle\hat{\phi},\hat{\phi}\rangle. \tag{4}$$

The space ξ is completed by using the norm of Eq. (4); the resulting space is the Hilbert space $\mathscr{H}$ of square-integrable functions ($\xi\subset\mathscr{H}$).

If ξ' are linear continuous functionals (distributions) over ξ, we have (Refs. 17–21)

$$\xi\subset\mathscr{H}\subset\xi'. \tag{5}$$

Here ξ is a nuclear space (see Ref. 22) and $(\xi,\mathscr{H},\xi')$ is a RHS or a Guelfand's triplet (GT). In this RHS a linear and symmetric operator A acting on ξ, which admits a self-adjoint prolongation $\overline{A}$ acting on $\mathscr{H}$, has a complete set of eigen-functionals on ξ' with real generalized eigenvalues.[23,24] Let us introduce the GT $(\tilde{\xi},\mathscr{H},\tilde{\xi}')$ which is related to the GT given in Eq. (5) by the Fourier transform

$$\phi(t)=\mathscr{F}^{-1}\{\hat{\phi}(E)\}=\frac{1}{2\pi}\int_{-\infty}^{+\infty}e^{iEt}\hat{\phi}(E)dE. \tag{6}$$

If $\hat{\psi}(E)\in\xi'$, we define $\psi(t)$ by

$$\langle\psi(t),\phi(t)\rangle=\frac{1}{2\pi}\langle\hat{\psi}(E),\hat{\phi}(E)\rangle. \tag{7}$$

Consequently, one has

$$\psi(t)=\mathscr{F}^{-1}\{\hat{\psi}(E)\} \tag{8}$$

with

$$\phi(t)\in\widetilde{\xi},\quad \psi(t)\in\widetilde{\xi}'. \tag{9}$$

The Schwartz space $\mathscr{S}'$ (of tempered distributions) is included in ξ' and in $\widetilde{\xi}'$ ($\mathscr{S}'\subset\xi'$). The distributions of $\mathscr{S}'$ fulfill Dirac's formula[17]

$$S(x)=\int_{-\infty}^{+\infty}\delta(x-y)S(y)dy. \tag{10}$$

The extension to ξ' of Dirac's formula is given by[17]

$$\hat{\psi}_c(z)=\frac{1}{2\pi i}\int_{-\infty}^{+\infty}\frac{1}{E-z}\,\hat{\psi}(E)dE, \tag{11}$$

where

$$\hat{\psi}(E)=\hat{\psi}_c(E+i0)-\hat{\psi}_c(E-i0). \tag{12}$$

Related to the RHS $(\widetilde{\xi},\mathscr{H},\widetilde{\xi}')$ [and $(\xi,\mathscr{H},\xi')$], it exists the abstract GT $(\xi_a,\mathscr{H}_a,\xi_a')$. This relation is established with the help of the operator $\hat{x}$, representing in $\mathscr{H}_a$ the position operator x of $\mathscr{H}$. The operator $\hat{x}$ has a complete set of eigenfunctions in ξ_a'. We use for them Dirac's notation $|x\rangle$. To each abstract ket $|\phi\rangle\in\xi_a$ it corresponds a function $\langle x|\phi\rangle=\phi(x)\in\widetilde{\xi}$. In other words, to each function $\phi(x)\in\widetilde{\xi}$, it corresponds an abstract ket $|\phi\rangle\in\xi_a$, such that $\langle x|\phi\rangle=\phi(x)$. This procedure establishes the above-mentioned relation between $\widetilde{\xi}$ and ξ_a. When the space ξ is completed we obtain the Hilbert space $\mathscr{H}$, while the correspondence just established leads to the complete abstract space $\mathscr{H}_a(\supset\xi_a)$. Finally, any linear continuous functional ψ in $\widetilde{\xi}'$ is made to correspond to that abstract ket, $|\psi\rangle\in\xi_a'$, such that

$$\psi(\phi)=\langle\psi|\phi\rangle \tag{13}$$

for all $\phi\in\widetilde{\xi}$.

These relations represent Dirac's formalism of quantum mechanics in a RHS. For more details see the works cited in Ref. 25.

The principal difference between the triplets defined above and those considered in Ref. 11 are due to the fact that our space ξ is formed by ''ultra analytic'' test functions; i.e., any $\phi\in\xi$ is entire-analytic and rapidly decreasing on the real axis. The dual space ξ' is formed by ''ultradistributions'' (see Refs. 17–20). The space $\widetilde{\xi}'$ is the minimal space that contains real exponentials. It also allows the representation of any ultradistribution by a pair of analytic functions that can be determined by Eqs. (11) and (12).

Let us now introduce a self-adjoint operator $H \in \mathscr{H}$, such that

$$H|E\rangle = E|E\rangle, \quad E_0 < E < E_1. \tag{14}$$

We shall consider all the $\hat{\psi} \in \xi'$ with support (in the sense of Ref. 17) in the interval (E_0, E_1). This means that $\hat{\psi}$ can be determined from the discontinuity $\psi(E)$ of the pair of analytic functions on the real axis. Furthermore, $\psi(E) = 0$ if $E \notin (E_0, E_1)$.

Following Eq. (11) one can write

$$\hat{\psi}(E_G) = \frac{1}{2\pi i} \int_{E_0}^{E_1} \frac{1}{E - E_G} \hat{\psi}(E) dE \tag{15}$$

and

$$(\hat{\psi}(E_G))^* = \frac{1}{2\pi i} \int_{E_0}^{E_1} \frac{1}{E_G^* - E} (\hat{\psi}(E))^* \, dE \tag{16}$$

with

$$E_G = E_D + i\Gamma, \quad \Gamma > 0.$$

In Dirac's notation, $\hat{\psi}(E) = \langle E|\psi\rangle$. Thus

$$\hat{\psi}(E_G) = \frac{1}{2\pi i} \int_{E_0}^{E_1} \frac{1}{E - E_G} \langle E|\psi\rangle dE, \tag{17}$$

$$(\hat{\psi}(E_G))^* = \frac{1}{2\pi i} \int_{E_0}^{E_1} \frac{1}{E_G^* - E} \langle \psi|E\rangle dE. \tag{18}$$

We can also write Eq. (17) as

$$\hat{\psi}(E_G) = \frac{1}{2\pi i} \int_{E_0}^{E_1} \frac{1}{E - E_G} \langle E|dE|\psi\rangle.$$

We now define

$$\langle E_G| = \frac{1}{2\pi i} \int_{E_0}^{E_1} \frac{1}{E - E_G} \langle E|dE \tag{19}$$

and

$$|E_G^*\rangle = \frac{1}{2\pi i} \int_{E_0}^{E_1} \frac{1}{E_G^* - E} |E\rangle dE. \tag{20}$$

In consequence,

$$\hat{\psi}(E_G) = \langle E_G|\psi\rangle, \tag{21}$$

$$(\hat{\psi}(E_G))^* = \langle \psi|E_G^*\rangle. \tag{22}$$

The state $|E_G^*\rangle$ is by definition a Gamow state. Note that if $\hat{\psi}(E)$ is the discontinuity of $\hat{\psi}_c(z)$ on the real axis, then $E^n \hat{\psi}(E)$ is the discontinuity of $z^n \hat{\psi}(z)$ also on the real axis.

Then we have [cf. Eq. (20)]

$$E_G{}^{*n}|E_G{}^*\rangle = \frac{1}{2\pi i}\int_{E_0}^{E_1}\frac{1}{E_G{}^*-E}\,E^n|E\rangle dE,$$

i.e.,

$$H^n|E_G{}^*\rangle = \frac{1}{2\pi i}\int_{E_0}^{E_1}\frac{1}{E_G{}^*-E}\,H^n|E\rangle dE \tag{23}$$

$$= E_G{}^{*n}|E_G{}^*\rangle, \tag{24}$$

and $|E_G{}^*\rangle$ is an eigenstate of H.

The states $|E_G{}^*\rangle$ are normalizable and the norm is given by

$$\langle E_G|E_G^*\rangle = \frac{1}{4\pi^2\Gamma}\left[\arctan\left(\frac{E_1-E_D}{\Gamma}\right)-\arctan\left(\frac{E_0-E_D}{\Gamma}\right)\right]. \tag{25}$$

With this normalization, and for the $E_1\to\infty$ and $E_0\to-\infty$, the normalized GS can be cast in the more familiar form of Ref. 14.

In consequence, the diagonal matrix element of H between GS is given by the expression

$$\langle E_G|H|E_G^*\rangle = E_D+\frac{\Gamma}{2}\,\frac{\ln\left[\dfrac{(E_1-E_D)^2+\Gamma^2}{(E_0-E_D)^2+\Gamma^2}\right]}{\left[\arctan\left(\dfrac{E_1-E_D}{\Gamma}\right)-\arctan\left(\dfrac{E_0-E_D}{\Gamma}\right)\right]}. \tag{26}$$

With this result it is readily seen that the imaginary part of the diagonal matrix element satisfies

$$\mathrm{Im}\langle E_G|H|E_G^*\rangle = 0, \tag{27}$$

and that for the limits $E_0\to-\infty$ and $E_1\to+\infty$ one has

$$\langle E_G|H|E_G^*\rangle = E_D\,. \tag{28}$$

The time evolution of a GS is given by

$$\langle\psi|e^{-iHt}|E_G{}^*\rangle = e^{-iE_G{}^*t}(\hat{\psi}(E_G))^* \tag{29}$$

as a consequence of Eqs. (11) and (23).

The probability distribution associated to a GS is given by

$$P(E)=|\langle E|E_G^*\rangle|^2=\frac{\Gamma}{(E-E_D)^2+\Gamma^2}\cdot\frac{1}{\left[\arctan\left(\dfrac{E_1-E_D}{\Gamma}\right)-\arctan\left(\dfrac{E_0-E_D}{\Gamma}\right)\right]}. \tag{30}$$

In the limit $E_1\to+\infty$, $E_0\to-\infty$, the above equation yields

$$P(E)=\frac{\Gamma/\pi}{(E-E_D)^2+\Gamma^2}, \tag{31}$$

which is the Breit–Wigner form proposed by Ref. 16.

Let us introduce the self-adjoint operator A, which is acting on $\mathscr{H}_a$,

$$A=\int_{-\infty}^{+\infty}|\lambda\rangle\lambda\, d\sigma_a(\lambda)\langle\lambda|, \tag{32}$$

where $\sigma_a(\lambda)$ is given by

$$\sigma_a(\lambda)=\begin{cases}\displaystyle\sum_{n=-\infty}^{+\infty}\Theta(\lambda-\lambda_n), & \lambda<\lambda_0\\ \lambda, & \lambda_0<\lambda<\lambda_1,\end{cases} \tag{33}$$

and where Θ is a Heaviside step function. The expectation value of A between GS

$$\langle E_G|A|E_G{}^*\rangle=\int_{-\infty}^{+\infty}\langle E_G|\lambda\rangle\lambda\, d\sigma_a(\lambda)\langle\lambda|E_G{}^*\rangle \tag{34}$$

is real since $\langle E_G|\lambda\rangle=(\langle\lambda|E_G^*\rangle)^*$. So far, the results which we have presented are based on the use of the theory of tempered ultradistributions. In order to illustrate them we shall discuss some simple examples.

For the first case we have adopted the plane waves

$$\langle E|x\rangle=\frac{e^{-iEx}}{\sqrt{2\pi}}.$$

From Eq. (11) one obtains

$$\langle E_G|x\rangle=\sqrt{2\Gamma}\ \mathrm{sgn}[\mathrm{Im}(E_G)]e^{-iE_Gx} \tag{35}$$

for the wavefunction of a GS.[26]

The second example is given by the function

$$\langle E|x\rangle=[\Theta(E-E_0)-\Theta(E-E_1)]\frac{e^{-iEx}}{\sqrt{2\pi}},$$

and for this case Eq. (11) yields

$$\langle E_G|x\rangle=\frac{C}{2\pi i}\,[\ln(E_G-E_1)-\ln(E_G-E_0)]e^{-iE_Gx}, \tag{36}$$

where C is a constant.[26]

As it can be seen from these examples, the GS can be obtained as tempered ultradistributions.

III. BERGGREN APPROXIMATION

In the following we shall discuss the validity of the approximation proposed by Berggren[16] to calculate the expectation value of an operator in a resonant state. Following Berggren's notation, let us introduce the state $|k,\hat{k},l\rangle$ and the continuum wavefunction $\langle\mathbf{x}|k,\hat{k},l\rangle=\phi_k^{(+)}(\mathbf{r})$.

Then, since the energy E is given by

$$E(\mathbf{k})=\frac{k^2}{2m}, \tag{37}$$

the GS can be defined by

$$|E_G{}^*\rangle = \frac{\sqrt{\Gamma}}{i\sqrt{\pi/2}} \int_0^{+\infty} \frac{|E(\mathbf{k}),\hat{k},l\rangle}{E_G{}^* - E}\, dE. \tag{38}$$

One can write

$$|k,\hat{k},l\rangle = \sqrt{\frac{k}{m}}\, |E(\mathbf{k}),\hat{k},l\rangle \tag{39}$$

and, consequently,

$$|E_G{}^*\rangle = \frac{\sqrt{\Gamma}}{i\sqrt{\pi/2}} \int_0^{+\infty} \sqrt{\frac{k}{m}}\, \frac{|k,\hat{k},l\rangle}{E_G{}^* - E(\mathbf{k})}\, dk, \tag{40}$$

$$\langle E_G|A|E_G{}^*\rangle = \frac{2\Gamma}{\pi} \sum_{l,l'} \int_0^{+\infty} dk \int_0^{+\infty} dk'\, \frac{\sqrt{kk'}}{m}\, \frac{\langle k',\hat{k}',l'|A|k,\hat{k},l\rangle}{(E(\mathbf{k}') - E_G)(E(\mathbf{k}) - E_G{}^*)} \tag{41}$$

[see Eq. (2) of Ref. 16]. We are now in a position to compare the result provided by the present method, about the expectation value of an operator in a resonant GS, and Berggren's conjecture, namely,

$$\langle A\rangle = \mathrm{Re}\langle E_G{}^*|A|E_G{}^*\rangle, \tag{42}$$

where

$$\langle E_G{}^*|A|E_G{}^*\rangle = \frac{2\Gamma}{\pi} \sum_{l,l'} \int_0^{+\infty} dk \int_0^{+\infty} dk'\, \frac{\sqrt{kk'}}{m}\, \frac{\langle k',\hat{k}',l'|A|k,\hat{k},l\rangle}{(E(\mathbf{k}') - E_G{}^*)(E(\mathbf{k}) - E_G{}^*)}. \tag{43}$$

The relation between Eqs. (40) and (42) can be expressed as

$$\begin{aligned}\langle A\rangle = \langle E_G|A|E_G{}^*\rangle = \mathrm{Re}\langle E_G{}^*|A|E_G{}^*\rangle &- \frac{2i\Gamma^2}{\pi} \sum_{l,l'} \int_0^{+\infty} dk \int_0^{+\infty} dk'\, \frac{\sqrt{kk'}}{m}\, [E(\mathbf{k}) - E(\mathbf{k}')] \\ &\times \frac{\langle k',\hat{k}',l'|A|k,\hat{k},l\rangle}{|E(\mathbf{k}') - E_G|^2 |E(\mathbf{k}) - E_G|^2} \\ &+ \frac{4\Gamma^3}{\pi} \sum_{l,l'} \int_0^{+\infty} dk \int_0^{+\infty} dk'\, \frac{\sqrt{kk'}}{m}\, \frac{\langle k',\hat{k}',l'|A|k,\hat{k},l\rangle}{|E(\mathbf{k}') - E_G|^2 |E(\mathbf{k}) - E_G|^2}.\end{aligned} \tag{44}$$

It means that the result obtained by Berggren[16] is valid at leading order in Γ. At this order one obtains, from the above equation,

$$\langle A\rangle = \langle E_G|A|E_G{}^*\rangle = \mathrm{Re}\langle E_G{}^*|A|E_G{}^*\rangle. \tag{45}$$

The contributions of higher-order terms, for any value of Γ, is given by Eq. (43). From this equation it is seen that the expectation value of the operator A in a GS differs from the estimate $\mathrm{Re}\langle E_G{}^*|A|E_G{}^*\rangle$ and that it shows a power-law dependence upon Γ.

IV. CONCLUSIONS

In this work we have presented a mathematical representation of GS based on the theory of tempered ultradistributions. The use of them has been shown to be useful, particularly in discussing the normalization of GS. The connection with Berggren's approximation, concerning the expectation value of an operator on a resonant state, has been established. We have shown that Berggren's expansion is valid at leading order in the imaginary part of the energy E_G. A general expression for this expectation value has been introduced which is not restricted by any prior assumption about the order of magnitude of the imaginary part of E_G as compared with the value of the real part of it. These results show that the space of ultradistributions together with the RHS discussed seems to be an appropriate framework for the description of GS and its main properties.

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Solvable quantum version of an integrable Hamiltonian system

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Solvable quantum versions of the classical dynamical system characterized by the Hamiltonian $H=\Sigma_{j,k=1}^{n}\ p_j p_k[\lambda+\mu\cos(q_j-q_k)]$ are presented. The eigenvalues of the quantum Hamiltonians are exhibited, as well as the corresponding eigenfunctions. © *1996 American Institute of Physics.* [S0022-2488(96)04009-1]

I. INTRODUCTION

It has been recently pointed out that the dynamical system characterized by the Hamiltonian

$$H=\sum_{j,k=1}^{n}\ p_j p_k\ \exp(-|q_j-q_k|) \tag{1.1}$$

is completely integrable.[1,2] Motivated by this remarkable discovery, one of us investigated the integrability of analogous systems and found that the Hamiltonian

$$H=\sum_{j,k=1}^{n}\ p_j p_k[\lambda+\mu\ \cos(q_j-q_k)] \tag{1.2}$$

is integrable.[3] Subsequently, it was shown that the more general Hamiltonian

$$H=\sum_{j,k=1}^{n}\ p_j p_k[\lambda+\mu\ \cos(q_j-q_k)+\mu'\ \sin|q_j-q_k|] \tag{1.3}$$

of which H (1.1) and H (1.2) are special cases, is also integrable.[4]

Not only is the system characterized by the Hamiltonian (1.2) completely integrable, it also turns out that the corresponding equations of motion *can be solved explicitly in terms of elementary functions*. This result led to the suggestion that there might exist *solvable quantum versions* of this model.[3] In the present paper this conjecture is validated.

Below, in Sec. II, three quantum versions of H (1.2) are introduced. For the special case $n=2$, the eigenvalues and eigenfunctions of these three quantum Hamiltonians are displayed in Sec. III. For the third of these quantum versions, the solution to the eigenvalue problem is exhibited for arbitrary n in Sec. IV; for the second, in Sec. V. In both these cases, the solutions live in the Hilbert space characterized by periodic boundary conditions (of period 2π), with the additional restriction that *all momenta be non-negative*; as explained below, this latter restriction is a rather natural requirement in the former case (third model), less so in the latter (second model). The proofs of these results are given in Sec. VI. In Sec. VII we conclude the paper by briefly listing some open problems.

Let us end this introduction by mentioning that the analogous classical dynamical system characterized by the Hamiltonian

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$$H=\lambda n\sum_{j=1}^{n} p_j+\mu\sum_{j,k=1}^{n}(p_jp_k)^{1/2}\cos(q_j-q_k) \tag{1.4}$$

is also explicitly solvable in terms of elementary functions,[5] and that also for this system there exists a solvable quantum version.[6]

II. QUANTUM HAMILTONIANS

The quantization is generally achieved via the standard representation

$$p_j=\frac{\hbar}{i}\frac{\partial}{\partial q_j}, \tag{2.1}$$

which entails the commutation rule

$$[q_j,p_k]=i\hbar\,\delta_{jk}. \tag{2.2}$$

Hereafter we generally set $\hbar=1$, except when we deem appropriate to display explicitly the dependence on $\hbar$.

A natural quantum version of the Hamiltonian (1.2) is given by

$$H^{(1)}=\lambda P^2+\mu\sum_{j,k=1}[\alpha\cos(q_j-q_k)\,p_jp_k+\beta\,p_jp_k\cos(q_j-q_k)+(1-\alpha-\beta)\,p_j\cos(q_j-q_k)\,p_k], \tag{2.3}$$

where α and β denote two arbitrary constants. Here, and always below

$$P=\sum_{j=1}^{n} p_j. \tag{2.4}$$

It is clear that the quantum Hamiltonian $H^{(1)}$, see Eq. (2.3), is Hermitian if λ,μ,α,β are real and $\alpha=\beta$.

Two other quantizations of the classical Hamiltonian H (1.2) read as follows:

$$H^{(2)}=\lambda P^2+\mu A^+A \tag{2.5a}$$

with

$$A=\sum_{j=1}^{n} a_j,\quad A^+=\sum_{j=1}^{n} a_j^+, \tag{2.6a}$$

$$a_j=\exp(-iq_j)p_j,\quad a_j^+=p_j\exp(iq_j), \tag{2.6b}$$

and

$$H^{(3)}=\lambda P^2+\tfrac{1}{4}\mu B^+B \tag{2.7a}$$

with

$$B=\sum_{j=1}^{n} b_j^2,\quad B^+=\sum_{j=1}^{n}(b_j^+)^2, \tag{2.8a}$$

$$b_j = \exp(-iq_j/2)(2p_j)^{1/2}, \quad b_j^+ = (2p_j)^{1/2}\exp(iq_j/2). \tag{2.8b}$$

Clearly, both $H^{(2)}$ and $H^{(3)}$ are Hermitian (provided λ and μ are real), because A^+ is the Hermitian conjugate of A and B^+ is the Hermitian conjugate of B. In terms of the original operators q_j, p_j the latter two Hamiltonians read as follows:

$$H^{(2)} = \lambda P^2 + \mu \sum_{j,k=1}^{n} p_j \exp[i(q_j - q_k)]p_k \tag{2.5b}$$

$$= \lambda P^2 + \mu \sum_{j,k=1}^{n} p_j \cos(q_j - q_k)p_k + \mu \frac{\hbar}{2} \sum_{j,k=1, j\neq k}^{n} \cos(q_j - q_k)(p_j + p_k), \tag{2.5c}$$

and

$$H^{(3)} = \lambda P^2 + \mu \sum_{j=1}^{n} p_j(p_j - \hbar/2) + \mu \sum_{j,k=1, j\neq k}^{n} \exp[i(q_j - q_k)][(p_j + \hbar)(p_j + \hbar/2)p_k(p_k - \hbar/2)]^{1/2}. \tag{2.7b}$$

To obtain the formula for $H^{(3)}$ we used the formal operator identity

$$(p_j + a)^{1/2}\exp(ibq_k) = \exp(ibq_k)(p_j + a + b\hbar\delta_{jk})^{1/2}. \tag{2.9}$$

It is obvious from the above expressions that the Hamiltonians $H^{(r)}$, $r = 1,2,3$, reduce to the classical Hamiltonian (1.2) when $\hbar = 0$ and q_j, p_j are treated as ordinary variables instead of (noncommuting) operators.

The rest of this paper is devoted to the investigation of the eigenvalue (or Schrödinger) equations,

$$H^{(r)}\Psi^{(r)}(\mathbf{q}) = E^{(r)}\Psi^{(r)}(\mathbf{q}), \quad r = 1,2,3, \tag{2.10}$$

for these 3 quantum Hamiltonians.

III. SOLUTIONS IN THE TWO-BODY CASE ($n=2$)

In this section we exhibit the eigenvalues $E^{(r)}$ and the eigenfunctions $\Psi^{(r)}(\mathbf{q})$ of the quantum Hamiltonians of the preceding Section, see Eq. (2.10), in the special case of two particles ($n=2$). The verification of these results is left as an exercise for the diligent reader (in the cases of $H^{(3)}$ and $H^{(2)}$ see also below)

$$E^{(1)} = \lambda k^2 + \mu[k^2 + 2\alpha m - 2\beta(m+1) - m(m+1)] \tag{3.1a}$$

$$\Psi^{(1)} = \exp[ik(q_1 + q_2)/2]\ \sin^m[(q_1 - q_2)/2]\ F(a_+, a_-, c; \sin^2[(q_1 - q_2)/2]), \tag{3.1b}$$

$$a_\pm = (1 + m - \alpha + \beta \pm [k^2 - 4\beta + (1 - \alpha + \beta)^2]^{1/2})/2, \tag{3.1c}$$

$$c = a_+ + a_- + 1/2 = m - \alpha + \beta + 3/2. \tag{3.1d}$$

$$E^{(2)} = \lambda k^2 + \mu[k^2 + k - m(m+1)], \tag{3.2a}$$

$$\Psi^{(2)} = \exp[ik(q_1 + q_2)/2]\ \sin^m[(q_1 - q_2)/2]\ F(a, b, c; \sin^2[(q_1 - q_2)/2]), \tag{3.2b}$$

$$a=1+(m+k)/2, \quad b=(m-k)/2, \quad c=a+b+1/2=m+3/2. \tag{3.2c}$$

$$E^{(3)}=\lambda k^2+\mu(k^2-m^2), \tag{3.3a}$$

$$\Psi^{(3)}=\exp(ikq_2)\, f(q_1-q_2), \tag{3.3b}$$

$$f(q)=\sum_{l=0}^{k} c_l \exp(ilq), \tag{3.3c}$$

$$c_l=\{(2l)![2(k-l)]!\}^{1/2} \sum_{l'=0}^{\min(k-m,l)} (-1)^{l-l'} \binom{k-m}{l'} \binom{2m}{2(l-l')}. \tag{3.3d}$$

In the above formulas m and k are the two quantum numbers that identify the eigenvalues and the eigenfunctions. The significance of k is revealed by the formula [see Eq. (2.4)]

$$P\Psi^{(r)}(\mathbf{q})=k\Psi^{(r)}(\mathbf{q}), \quad r=1,2,3. \tag{3.5}$$

In Eqs. (3.1b) and (32.b), $F(-,-,-;-)$ denotes the Gauss hypergeometric function;[7] note that in both cases the hypergeometric function belongs to the special class for which there holds a quadratic transformation [see Eq. (2.11.2) of Ref. 7]. The functions $\Psi^{(1)}(\mathbf{q})$ and $\Psi^{(2)}(\mathbf{q})$ satisfy the eigenvalue equation (2.10) for *any* value of m and k. However, the restriction that (the real part of) m be *non-negative* is required to avoid that these wave functions diverge at $q_1=q_2$, and the requirement that m and k be *integers* with $m+k$ *even* is necessary and sufficient to guarantee that these wave functions are periodic in q_1 and q_2 with period 2π. Under these conditions the quantities a,b in (3.2c) are also *integers*; if either of them in *not positive* then the hypergeometric function in the r.h.s. of Eq. (3.2b) becomes a *polynomial*. Likewise, the constants $a_{\pm}$, see Eq. (3.1c), become *integers* if $\alpha=(s-1)^2$ and $\beta=s^2$ with s integer; then $a_{\pm}=s+(m\pm k)/2$.

For the eigenvalue problem (2.10) with $r=3$, see Eq. (3.3), we have assumed that the quantum numbers k and m are *non-negative integers* with $m\leqslant k$. As a consequence, the eigenfunction $\Psi^{(3)}(\mathbf{q})$, see Eqs. (3.3b)–(3.3d) is periodic with period 2π in q_1,q_2, and it moreover contains *only non-negative powers* of $\exp(iq_1)$ and $\exp(iq_2)$. The significance of this restriction is discussed in the next section.

IV. EIGENVALUES AND EIGENFUNCTIONS OF $H^{(3)}$

When investigating the eigenvalues and eigenfunctions of the quantum Hamiltonian $H^{(3)}$, see Eq. (2.7), we restrict consideration to the Hilbert space spanned by the basis

$$\exp(i\mathbf{m}\cdot\mathbf{q})\equiv\exp\left(i\sum_{j=1}^{n} m_j q_j\right), \quad \mathbf{m}\equiv(m_1,\ldots,m_n)\in\mathbf{N}^n \tag{4.1}$$

(i.e., with $m_1,\ldots,m_n$ being *non-negative integers*), endowed with the standard inner product for square integrable functions with period 2π ($\langle f,g\rangle=\int_0^{2\pi}\cdots\int_0^{2\pi} f^*(\mathbf{q})g(\mathbf{q})dq_1\cdots dq_n$). Requiring that all components m_j of $\mathbf{m}$ be *integers* corresponds to imposing *periodic* boundary conditions (with period 2π, for all the variables q_j); the restriction that they be *non-negative* is to avoid any difficulty with the definition of the pseudo-differential operators $p_j^{1/2}$ [see Eq. (2.8b)], whose action on the basis (4.1) is specified by the formula [see Eq. (2.1)]

$$p_j^{1/2}\exp(i\mathbf{m}\cdot\mathbf{q})=m_j^{1/2}\exp(i\mathbf{m}\cdot\mathbf{q}). \tag{4.2}$$

The restriction to this ''non-negative momenta'' subspace is *self-consistent*, because acting with $H^{(3)}$, see Eq. (2.7), on any function that is representable as a superposition of these basis elements

yields a function that is again representable as a superposition of these basis elements; indeed, this is clearly a property inherited from the operators b_j, b_j^+ [see Eqs. (2.8) and (4.2)].

Let us now turn to a description of the eigenvalues and eigenfunctions of $H^{(3)}$ in the above mentioned Hilbert space. The proofs of the following results are given in Sec. VI.

The solution of the eigenvalue equation (2.10) for $r=3$ and *arbitrary* particle number $n \geqslant 2$ is given by the eigenvalues

$$E^{(3)} = \lambda k^2 + \mu[k^2 + (\tfrac{n}{2} - 1)k - m(m + \tfrac{n}{2} - 1)], \tag{4.3}$$

and by the eigenfunctions

$$\Psi^{(3)}(\mathbf{q}) = \sum_{l_1,\ldots,l_n=0, l_1+\ldots+l_m=k}^{n} c(\mathbf{m},\mathbf{l}) \left(\prod_{j=1}^{n} (2l_j)! \right)^{1/2} \exp\left(i \sum_{j=1}^{n} l_j q_j \right), \tag{4.4a}$$

where the coefficients $c(\mathbf{m},\mathbf{l})$ are defined by the expansion formula

$$\left(\sum_{j=1}^{n} x_j^2 \right)^{k-m} H_{2m}(\mathbf{x}) = \sum_{l_1,\ldots,l_n=0, l_1+\ldots+l_n=k}^{k} c(\mathbf{m},\mathbf{l}) \prod_{j=1}^{n} x_j^{2l_j}. \tag{4.4b}$$

Just as in the treatment of $H^{(3)}$ given in Sec. III (for $n=2$), the numbers k and m are *non-negative integers* with $m \leqslant k$; they are the quantum numbers labeling the eigenvalues $E^{(3)}$, see Eq. (4.3). One again has [see Eq. (3.5)]

$$P\Psi^{(3)}(\mathbf{q}) = k\Psi^{(3)}(\mathbf{q}). \tag{4.5}$$

The function $H_{2m}(\mathbf{x})$ in the defining relation (4.4b) for the coefficients $c(\mathbf{m},\mathbf{l})$ denotes a *harmonic* polynomial of degree $2m$, i.e., an even homogeneous polynomial of degree $2m$ in the variables $x_1,\ldots,x_n$ satisfying the (n-dimensional) Laplace equation

$$\Delta H_{2m}(\mathbf{x}) = 0. \tag{4.6}$$

For a given m (and $n \geqslant 3$) there exist $(4m+n-2)!(2m+n-3)!/[(n-2)!(2m)!]$ such *independent* harmonic polynomials [see Eq. (11.2.2) of Ref. 7]; this is, therefore, also the multiplicity of the eigenvalue $E^{(3)}$, see Eq. (4.3), in the generic case (λ and μ incommensurate); note that the multiplicity does not depend on k. Rather explicit formulas for these polynomials (in terms of Gegenbauer polynomials) can be found in Eq. (11.2.21) of Ref. 7.

V. EIGENVALUES AND EIGENFUNCTIONS OF $H^{(2)}$

In this section we exhibit the eigenvalues and eigenfunctions of the Hamiltonian $H^{(2)}$, see Eq. (2.5), again in the Hilbert space spanned by the basis (4.1). The restriction to *integer* values of the quantum numbers m_j corresponds again to the imposition of *periodic* boundary conditions (of period 2π, for all the variables q_j); the additional restriction that they all be *non-negative* (namely, the restriction to work in the space with only *non-negative momenta*), although *self-consistent* (as in the previous case), has no cogent justification (contrary to the previous case).

The proofs of the following results are given in Sec. VI.

The eigenvalues $E^{(2)}$ of $H^{(2)}$, see Eq. (2.10), are given by the formula

$$E^{(2)} = \lambda k^2 + \mu[k^2 + (n-1)k - m(m+n-1)], \tag{5.1}$$

with k and m *non-negative integers* and $m \leqslant k$; note the analogy, and yet the difference, of $E^{(2)}$, see Eq. (5.1), with $E^{(3)}$, see Eq. (4.3).

The corresponding eigenfunctions of $\Psi^{(2)}$, see Eq. (2.10), are again also eigenfunctions of P,

$$P\Psi^{(2)}=k\Psi^{(2)}, \tag{5.2}$$

so that the quantum number k has the same significance as in the preceeding sections [see Eqs. (3.5) and (4.5)]; and they are given by the explicit formulas

$$\Psi^{(2)}(\mathbf{q})=(A^{+})^{k-m}\Phi(\mathbf{q}), \tag{5.3}$$

$$\Phi(\mathbf{q})=\left[\sum_{j=1}^{n}\gamma_j\exp(iq_j)\right]^m, \tag{5.4a}$$

with A^{+} defined by Eqs. (2.6) and (2.1), and where the n constants γ_j are arbitrary except for the single restriction

$$\sum_{j=1}^{n}\gamma_j=0. \tag{5.4b}$$

For $n=2$ the simultaneous validity of Eq. (3.2b), and of Eq. (5.3) with Eq. (5.4), entails the following intriguing (possibly new!?) representation of (even) Gegenbauer polynomials:[8]

$$C_{2p}^{m+1}(\cos x)=(-)^p 2^{-2p}[(2p)!]^{-1}(\sin x)^{-m}\exp[-i(m+2p)y]\cdot\left\{\left(\frac{\partial}{\partial y}+\frac{\partial}{\partial x}\right)\exp[i(x+y)]+\left(\frac{\partial}{\partial y}-\frac{\partial}{\partial x}\right)\exp[i(y-x)]\right\}^{2p}\cdot\exp(imy)(\sin x)^m, \tag{5.5a}$$

$$C_{2p}^{m+1}(\cos x)=[(2p)!]^{-1}(\sin x)^{-m}\cdot\left\{\left[(m+2p+1)\cos x+(\sin x)\frac{\partial}{\partial x}\right]\times\left[(m+2p)\cos x+(\sin x)\frac{\partial}{\partial x}\right]\cdot\left[(m+2p-1)\cos x+(\sin x)\frac{\partial}{\partial x}\right]\cdots\left[(m+3)\cos x+(\sin x)\frac{\partial}{\partial x}\right]\cdot\left[(m+2)\cos x+(\sin x)\frac{\partial}{\partial x}\right]\right\}(\sin x)^m, \tag{5.5b}$$

with m and p *non-negative integers*. The formula (5.5a) has been obtained by setting $k-m=2p$, $q_1=y+x$, $q_2=y-x$, and using the second of Eqs. (10.9.21) of Ref. 8. The formula (5.5b) is easily obtained from (5.5a) using the (operator) identity

$$\left(\frac{\partial}{\partial y}+\frac{\partial}{\partial x}\right)\exp[i(x+y)]+\left(\frac{\partial}{\partial y}-\frac{\partial}{\partial x}\right)\exp[i(y-x)]=2\left[\frac{\partial}{\partial y}\cos x+i\frac{\partial}{\partial x}\sin x\right]\exp(iy). \tag{5.6}$$

The normalization constant for these equations has been determined by setting $\cos x=z$ in Eq. (5.5b) and then evaluating the dominant term (as z diverges).

Of course an equivalent representation to Eqs. (5.4) reads

$$\Phi(\mathbf{q})=\left\{\sum_{j=1,j\neq k}^{n}\gamma_j[\exp(iq_j)-\exp(iq_k)]\right\}^m, \tag{5.7}$$

with k arbitrary, $1 \leqslant k \leqslant n$, and now with the $n-1$ arbitrary constants γ_j, $j=1,\ldots,n$, $j \neq k$, unrestricted. By expanding the right-hand-side in powers of the constants γ_j, one obtains $N(n,m)=\binom{n+m-2}{m} \equiv (n+m-2)!/[(n-2)!m!]$ different functions, as coefficients of different powers of the $n-1$ constants γ_j; all these functions yield, via Eq. (5.3), different eigenfunctions, all of which satisfy both eigenvalue equations, (5.2), and (2.10) with $r=2$ and with Eq. (5.1). Hence $N(n,m)$ gives the multiplicity (or at least, a lower bound to the multiplicity) of the eigenvalue (5.1) (in the generic case with λ and μ incommensurate).

VI. PROOFS

To derive the results of Sec. IV one first observes that the operators b_j^+ and b_j, see Eq. (2.8b), satisfy the commutation rules

$$[b_j,\ b_j^+]=\delta_{jk}. \tag{6.1}$$

Hence another representation for these operators, also consistent with these commutation relations, is given by

$$b_j^+ = x_j, \quad b_j = \frac{\partial}{\partial x_j}. \tag{6.2}$$

In the latter representation the Hamiltonian (2.7a) reads

$$H^{(3)} = \tfrac{1}{4}(\lambda N + \mu r^2 \Delta), \tag{6.3a}$$

with

$$N = \sum_{j=1}^{n} x_j \frac{\partial}{\partial x_j}, \quad r^2 = \sum_{j=1}^{n} x_j^2, \quad \Delta = \sum_{j=1}^{n} \frac{\partial^2}{\partial x_j^2}. \tag{6.3b}$$

Now let $H_{2m}(\mathbf{x})$ be a *harmonic* polynomial of degree $2m$ and define

$$\phi(\mathbf{x}) = r^{2(k-m)} H_{2m}(\mathbf{x}), \tag{6.4}$$

so that $\phi(\mathbf{x})$ is a homogeneous *polynomial* in the x_j's of degree $2k$ (here the assumption $k-m \geqslant 0$ plays an essential role). Then it is clear from the representation (6.3a) that

$$H^{(3)}\phi(\mathbf{x}) = E^{(3)}\phi(\mathbf{x}), \tag{6.5}$$

with $E^{(3)}$ given by Eq. (4.3).

It remains to transform back to the variables q_j, $j=1,\ldots,n$. To this end one observes that in both representations the ground state wave function is a constant [constant functions are annihilated by both representations of b_j, see Eqs. (2.8b) and (6.2)]. By comparing the action of the creation operators b_j^+ on the ground state in both representations one arrives at the transformation rule

$$x_j^{2l} \to [(2l)!]^{1/2} \exp(ilq_j). \tag{6.6}$$

Hence, to obtain the eigenfunction $\Psi^{(3)}(\mathbf{q})$ one must first expand $\phi(\mathbf{x})$, see Eq. (6.4), in powers of the variables x_j, and then perform the substitution (6.6). This yields Eq. (4.4).

Let us now proceed to prove the results of Sec. V.

It is easily seen that the following formulas are implied by the definitions (2.6) with Eqs. (2.1), (2.2), (2.4):

$$[a_j, a_k^+] = \delta_{jk}(1+2p_j), \tag{6.7}$$

$$[P, A^m] = -mA^m, \quad m = 0,1,2,\ldots, \tag{6.8a}$$

$$[P, (A^+)^m] = m(A^+)^m, \quad m = 0,1,2,.., \tag{6.8b}$$

$$[A, (A^+)^m] = (A^+)^{m-1} m(m+n-1+2P), \quad m = 0,1,2,.., \tag{6.9a}$$

$$[A^+A, (A^+)^m] = (A^+)^m m(m+n-1+2P), \quad m = 0,1,2,\ldots, \tag{6.9b}$$

$$[P, A^+A] = 0. \tag{6.10}$$

Using the explicit definition (5.4) of $\Phi(\mathbf{q})$ it is easy to show that this function satisfies the two equations

$$P\Phi(\mathbf{q}) = m\Phi(\mathbf{q}), \tag{6.11}$$

$$A\Phi(\mathbf{q}) = 0. \tag{6.12}$$

Hence, using Eqs. (6.8b) and (6.9b), it is easy to show that $\Psi^{(2)}$, see Eq. (5.3), satisfies Eq. (5.2) as well as Eq. (2.10) with Eq. (5.1).

VII. OUTLOOK

We conclude by briefly mentioning some open problems associated with these quantum versions of the Hamiltonian (1.2) (for a list of open problems extant in the classical context see Ref. 4).

For the two-body case ($n=2$), the results of Sec. III provide the complete solution of the quantum problem for the 3 Hamiltonians $H^{(r)}$, $r=1,2,3$, introduced in Sec. II, in the guise of rather explicit solutions of the relevant Schrödinger equations. This opens the possibility to investigate other prescriptions for quantization (for instance, different boundary conditions) than those detailed above; a task that we consider sufficiently easy, for $n=2$, not to warrant any additional elaboration here. The question of exploring more fully other quantizations in the many-body case ($n>2$) is on the other hand an interesting open problem; and also open and interesting is the problem to solve, in some appropriate Hilbert space, the eigenvalue equation (2.10) with $r=1$ (for $n>2$), as well as the problem to solve Eq. (2.10) with $r=2$ (for $n>2$) in the larger Hilbert space characterized by the basis (4.1) *without* the restriction that the integers m_j be *non-negative* (note that, in the $n=2$ case, the eigenfunctions are then given by Eq. (3.2b) with a *nonpolynomial* hypergeometric function).

Let us end by mentioning that the question of the existence of a *solvable* quantum version of the more general Hamiltonian (1.3) constitutes an interesting, and probably difficult, open problem.

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Coherent state path-integral representation of supersymmetric lattice models

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A kind of high-temperature superconductivity related lattice model is investigated within the framework of supergroup coherent state path-integral representation. Symmetry properties are analyzed and the Hamiltonians are written in the symmetric form explicitly in terms of generators of the supergroup $U(N/M)$. By a standard approach, general supergroup coherent states are constructed. Holstein–Primakoff realizations of the supergroup $U(N/M)$ on the coset space $U(N/M)/[U(1)\otimes U(N-1/M)]$ are obtained. Vacuum persistence amplitudes are expressed in terms of parameters on the coset space $U(2/M)/[U(1)\otimes U(1/M)]$. Symmetry-breaking terms in the Hamiltonian are taken into account separately. The Lagrangians of these models are quadratic in Grassmann variables. Thus fermionic fields can be integrated out. The nonlinear σ model is arrived at as effective continuum field theory describing the low-energy excitations of the supersymmetric lattice models.
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I. INTRODUCTION

It is well known that the Bardeen, Cooper, and Schrieffer (BCS) theory[1] gives viable mechanisms for superconductivity in metals and superfluidity of liquid He_3. This theory has also successfully explained a variety of related phenomena in diverse areas of physics. However, the discovery of copper-oxide superconductivity[2,3] with critical temperature as high as 120 K raised doubts about it. Due to the nature of the phonon-mediated electron–electron interaction in BCS theory, there are upper bounds on the critical temperatures much lower than those achieved with the copper oxides. The lack of a significant isotope effect with substitution of the oxygen sites seems to rule out the possibility that the phonon Debye frequency is the characteristic energy scale entering in the fundamental equations of the high-temperature superconductivity. Because the superconductiviting phase occurs near a metal-insulator transition, an antiferromagnetic as well as a structural instability, the phase diagram of high T_c superconductivity materials is rich. There is a growing suspicion that a different mechanism may be responsible for the high T_c superconductivity. Anderson[4,5] suggested that the novel quantum spin fluctuations in the CuO_2 planes may be responsible for the superconductivity. Interesting magnetic properties revealed by neutron-scattering experiments provide further support for this idea. It was conjectured that such fluctuations might destroy the antiferromagnetic long-range order in the ground state, giving rise to a new state of the spin system, a quantum spin-liquid state. The superconductivity in these materials was then conjectured to arise from the behavior of a novel quantum fluid created out of a highly correlated set of electronic degrees of freedom.

Anderson argued that the appropriate model for the high T_c superconductivity is the two-dimensional single-band Hubbard model[6] in the strong on-site Coulomb repulsion limit,

$$H_{\text{Hubb.}}=-t\sum_{\langle jk\rangle}\sum_{\sigma=\pm 1}(c_{j\sigma}^{\dagger}c_{k\sigma}+c_{k\sigma}^{\dagger}c_{j\sigma})+U\sum_{j}\ c_{j1}^{\dagger}c_{j1}c_{j,-1}^{\dagger}c_{j,-1}, \tag{1}$$

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where t is the hopping matrix elements and U is the on-site Coulomb interaction. In this model the fermion creation operators create electrons at the outer $d_{x^2-y^2}$ orbital of the Cu atoms, which is hybridized in an antibonding symmetry with the P_x and P_y orbitals of the two oxygen atoms in the CuO_2 cell.

Standard strong-coupling perturbation treatment of the single-band Hubbard Hamiltonian produces the effective $t-J$ model[7,8] with the superexchange coupling $J=4t^2/U$,

$$H_{t-J}=-t\sum_{\langle jk\rangle}\sum_{\sigma=\pm 1}(c_{j\sigma}^{\dagger}c_{k\sigma}+c_{k\sigma}^{\dagger}c_{j\sigma})+J\sum_{\langle jk\rangle}(S_j^{\dagger}S_k+S_k^{\dagger}S_j+2S_j^3S_k^3). \tag{2}$$

The $t-J$ Hamiltonian is an interesting model on its own. This model can be obtained in the strong-coupling limit from a more realistic model that takes into account the more detailed orbital structure of the CuO_2 cell, even when the holes created by doping sit primarily on the oxygen sites.[9]

At half-filling, apart from a constant, the $t-J$ Hamiltonian is equivalent to the spin-$\frac{1}{2}$ antiferromagnetic Heisenberg model on a square lattice,

$$H_{\text{Heisen.}}=J\sum_{\langle jk\rangle}(S_j^{\dagger}S_k+S_k^{\dagger}S_j+2S_j^3S_k^3). \tag{3}$$

The spin model has been studied for many years.[10,11] Since the 1950s, the importance of field theory to condensed matter physics, and vice versa, has been recognized based on the pioneer works of Landau and Feynman. Conformal field theory describes effectively critical phenomena. The renormalization group, which is developed initially by field theorists, has become the main tool for the interpretations of experimental data, the conceptual framework, and the computational algorithm in condensed matter physics. Haldane first used the $SU(2)$ group coherent state path-integral representation[12] to map the spin operators to unit 3-vectors on the large spin limit,

$$\mathbf{S}_j\rightarrow s\boldsymbol{\varphi}_j,\quad \boldsymbol{\varphi}_j\cdot\boldsymbol{\varphi}_j=1, \tag{4}$$

and the system becomes classical. On the other hand, in the long-wavelength limit the system approaches a continuum field theory appropriate for the study of low-energy excitations. When both approximations are used in conjunction the system is described by a nonlinear σ model,

$$L=\frac{1}{2g}\,\partial_\mu\boldsymbol{\varphi}\cdot\partial^\mu\boldsymbol{\varphi}, \tag{5}$$

with the constraint $\boldsymbol{\varphi}\cdot\boldsymbol{\varphi}=1$.

Semiclassically we assume spontaneous symmetry breaking[13] and write

$$\boldsymbol{\varphi}=\left(\varphi_1,\varphi_2,\sqrt{1-\sum_{i=1}^{2}\varphi_i\varphi_i}\right)\doteq(\varphi_1,\varphi_2,1). \tag{6}$$

Then we have

$$L=\frac{1}{2g}\sum_{i=1}^{2}2\,\partial_\mu\varphi_i\,\partial^\mu\varphi_i=\frac{1}{2g}\,\partial_\mu\phi\,\partial^\mu\phi^{\dagger}, \tag{7}$$

where we have used the notations $\phi=\varphi_1+i\varphi_2$, $\phi^{\dagger}=\varphi_1-i\varphi_2$.

It is widely believed that the quantum nonlinear σ model provides an accurate description of the long-wavelength, low-energy properties of the spin system, even in the small spin regime. Affleck and Randjbar-Daemi, Salam, and Strathdee (RSS) have generalized the approach to $SU(N)$ and general Lie group cases.[14,15]

By defining the so-called spin-hole coherent states,

$$|\Omega,\xi\rangle_s=|\Omega\rangle_s|0\rangle+|\Omega\rangle_{s-1/2}\xi f^\dagger|0\rangle, \tag{8}$$

Auerbach and Larson[16] used the coherent state representation to deal with the $t-J$ model. By a Hartree–Fock approximation, a model that is quadratic in the Grassmann variables is arrived. The effective Lagrangian of the $t-J$ model is of the form

$$L^{\rm eff}_{t-J}=\sum_j\ (2s-\rho_j)\mathbf{A}(\Omega_j)\cdot\dot{\Omega}_j-H^J(\Omega)-\beta^{-1}T\ \log\left[1+T_\tau\ \exp\left(-\int_0^\beta d\tau(H^f(\Omega_j)-\mu)\right)\right]. \tag{9}$$

However, no σ-type field theory was obtained explicitly. They argued that although the expansion around the Néel state is formally controlled by the large spin size s, at low doping the success of this approximation for the $s=\frac{1}{2}$ antiferromagnetism can be relied on.

The spin–spin interactions are essential to the high T_c superconductivity related lattice models. As Haldane has shown in the absence of doping the spin–spin interactions can be presented by the $2+1$-dimensional nonlinear σ model. It is natural to hope that, at least in the low doping case, the spin–spin interactions, in general, should be described by a σ-type field theory.

It is well known that the novel feature of supersymmetry is that it operates between bosons and fermions, the odd generators of the supergroup corresponding to transformations between bosons and fermions. Thus supersymmetry provides a unified description of mixed systems of bosons and fermions. Supersymmetry is introduced originally for applications in high-energy physics and becomes more and more popular in other fields of physics.

In this paper, we begin with discussing the symmetry properties of these models and rewrite the Hamiltonians in a supersymmetric form. Here the supergroup $U(N/M)$[17–19] plays a fundamental role. The Hamiltonians are written in terms of the generators of $U(N/M)$. For convenience, we introduce the Schwinger boson (slave fermion) representation.[20,21] This representation is widely used by condensed matter physicists in dealing with doping problems of high T_c superconductivity. The total particle number of bosons and fermions is used to label representations of $U(N/M)$. The elements of $U(N/M)$ are identified as transformations among states that have the same total particle number. To arrive at a path-integral representation of the supersymmetric models, we construct supergroup coherent states[18,22] from unitary irreducible representations of the supergroup. The supergroup coherent states have a natural topological coset space structure $U(N/M)/[U(1)\otimes U(N-1/M)]$. Parametrization of the coset space is presented explicitly. A complex projective representation of $U(N/M)/[U(1)\otimes U(N-1/M)]$ is introduced. We show that two important properties of ordinary group coherent states are maintained by the supergroup coherent states, i.e., they are, in general, nonorthogonal but are normalized to unity. According to Schurr's lemma, we also give the resolution of identity of the supergroup coherent states. This is crucial for obtaining a path-integral representation. Following the method of RSS,[15] we express the vacuum persistence amplitudes of the supersymmetric systems in terms of parameters on the coset space $U(2/M)/[U(1)\otimes U(1/M)]$ through the Holstein–Primakoff realizations.[23] To agree with the Néel character (at least short range) of the high T_c superconductivity materials, we give two kinds of parametrizations of the coset space on bipartite lattices. After taking account of the symmetry-breaking terms of the Hamiltonians, we get a Lagrangian that describes sensibly the spin fluctuations of the high T_c superconductivity materials. It should be noticed that the Lagrangian is quadratic in Grassmann variables. Thus we can integrate out the fermionic fields and get an

effective Lagrangian that only involves bosonic fields. This is just the familiar nonlinear σ model. This result proves the predictions of the weak-coupling mean-field theory in the Fermion coherent state path-integral representation.

This paper is organized as follows. In Sec. II, we show symmetry properties of the high T_c superconductivity related lattice models. Section III is devoted to discussing the Schwinger boson representations of the supergroup. Supergroup coherent states are constructed in Sec. IV. We give the supergroup coherent state path-integral representations of these models in Sec. V. Concluding remarks are given in Sec. VI.

II. HIGH T_c SUPERCONDUCTIVITY RELATED SUPERSYMMETRIC LATTICE MODELS

The existence of antiferromagnetism in the absence of doping is an evidence for strong electron correlations for the high T_c materials. The extended Hubbard model[24–26] is one of the simplest models for describing the electron correlations on a two-dimensional lattice, which includes nearest-neighbor interactions such as density–density and spin–spin coupling and additional interactions such as a bond charge term and a pair hopping term. The Hamiltonian of the model is given by

$$\begin{aligned} H_{\text{Hubb.}} = & -t\sum_{\langle jk\rangle}\sum_{\sigma=\pm 1}(c_{j\sigma}^{\dagger}c_{k\sigma}+c_{k\sigma}^{\dagger}c_{j\sigma})-\frac{t}{2}\sum_{\langle jk\rangle}(n_j-1)(n_k-1)+t\sum_{\langle jk\rangle}(c_{j1}^{\dagger}c_{j,-1}c_{k,-1}^{\dagger}c_{k1} \\ & +c_{j,-1}^{\dagger}c_{j1}c_{k1}^{\dagger}c_{k,-1})+t\sum_{\langle jk\rangle}\sum_{\sigma=\pm 1}(c_{j\sigma}^{\dagger}c_{k\sigma}+c_{k\sigma}^{\dagger}c_{j\sigma})(n_{j,-\sigma}+n_{k,-\sigma}) \\ & -t\sum_{\langle jk\rangle}(c_{j1}^{\dagger}c_{j,-1}^{\dagger}c_{k,-1}c_{k1}+c_{k1}^{\dagger}c_{k,-1}^{\dagger}c_{j-1}c_{j1})-4t\sum_{j}\left(n_{j1}-\frac{1}{2}\right)\left(n_{j,-1}-\frac{1}{2}\right) \\ & +U\sum_{j}c_{j1}^{\dagger}c_{j1}c_{j,-1}^{\dagger}c_{j,-1}, \end{aligned} \tag{10}$$

where the operator $c_{j\sigma}$ ($c_{j\sigma}^{\dagger}$) [$j=1,2,\ldots,L$ (total number of lattice sites)] describe electrons on the lattice and satisfy the anticommutation relation,

$$\{c_{j\sigma},c_{k\sigma'}\}=0,\quad \{c_{j\sigma},c_{k\sigma'}^{\dagger}\}=\delta_{jk}\delta_{\sigma\sigma'},\quad \{c_{j\sigma}^{\dagger},c_{k\sigma'}^{\dagger}\}=0. \tag{11}$$

Here we have used the notations $n_{j\sigma}=c_{j\sigma}^{\dagger}c_{j\sigma}$ and $n_j=\Sigma_{\sigma=\pm 1}n_{j\sigma}$, $\Sigma_{\langle jk\rangle}$ implies the sum over the nearest neighbors, in which the pairs (j,k) and (k,j) have to be counted once each so that the sum can be always considered as symmetric under interchanging $j\leftrightarrow k$.

The Hilbert space of the extended Hubbard model is spanned by the states of the form

$$|a_1\rangle\otimes|a_2\rangle\otimes\cdots\otimes|a_j\rangle\otimes\cdots\otimes|a_L\rangle, \tag{12}$$

where $|a_j\rangle\in\{|1_j\rangle=c_{j1}^{\dagger}|0\rangle_j,|2_j\rangle=c_{j,-1}^{\dagger}|0\rangle_j,|3_j\rangle=|0\rangle_j,|4_j\rangle=c_{j1}^{\dagger}c_{j,-1}^{\dagger}|0\rangle_j\}$. Here $|0\rangle_j$ is defined as $c_{j\sigma}|0\rangle_j=0$ and the vacuum $|0\rangle=\otimes|0\rangle_j$ satisfies $c_{j\sigma}|0\rangle=0$.

The system has $SU(2)$ spin symmetry. The spin operator $\mathbf{S}_j$ is defined by

$$\mathbf{S}_j=\frac{1}{2}\sum_{\sigma,\sigma'=\pm 1}c_{j\sigma}^{\dagger}\boldsymbol{\tau}_{\sigma\sigma'}c_{j\sigma'}, \tag{13}$$

where $\boldsymbol{\tau}$ are the three Pauli matrices,

$$\tau_1=\begin{pmatrix}0&1\\1&0\end{pmatrix},\quad \tau_2=\begin{pmatrix}0&-i\\i&0\end{pmatrix},\quad \tau_3=\begin{pmatrix}1&0\\0&-1\end{pmatrix}. \tag{14}$$

Another symmetry of the system is the so-called η pairing[27,28] generated by

$$\eta_j = c_{j1}c_{j,-1}, \quad \eta_j^\dagger = c_{j,-1}^\dagger c_{j1}^\dagger, \quad \eta_j^3 = -\tfrac{1}{2}(n_j - 1). \tag{15}$$

Together with the spin $SU(2)$ symmetry, this gives an $SO(4)$ symmetry.

In terms of the operators of spin and η spin, the extended Hubbard Hamiltonian is of the form

$$\begin{aligned} H_{\text{Hub.}} = & -t\sum_{\langle jk\rangle}\sum_{\sigma=\pm 1}(c_{j\sigma}^\dagger c_{k\sigma} + c_{k\sigma}^\dagger c_{j\sigma}) - \frac{t}{2}\sum_{\langle jk\rangle}(n_j - 1)(n_k - 1) + t\sum_{\langle jk\rangle}(S_j^\dagger S_k + S_k^\dagger S_j + 2S_j^3 S_k^3) \\ & + t\sum_{\langle jk\rangle}\sum_{\sigma=\pm 1}(c_{j\sigma}^\dagger c_{k\sigma} + c_{k\sigma}^\dagger c_{j\sigma})(n_{j,-\sigma} + n_{k,-\sigma}) - t\sum_{\langle jk\rangle}(\eta_j^\dagger \eta_k + \eta_k^\dagger \eta_j + 2\eta_j^3 \eta_k^3) \\ & - 4t\sum_j \left(n_{j1} - \frac{1}{2}\right)\left(n_{j,-1} - \frac{1}{2}\right) + U\sum_j c_{j1}^\dagger c_{j1} c_{j,-1}^\dagger c_{j,-1}. \end{aligned} \tag{16}$$

The above Hamiltonian can be divided formally into two parts, the supersymmetric part $H_{\text{Hub.}}^0$ and the symmetry-breaking part $H_{\text{Hub.}}^{\text{int}}$,

$$\begin{aligned} H_{\text{Hub.}}^0 = & -t\sum_{\langle jk\rangle}\sum_{\sigma=\pm 1}(c_{j\sigma}^\dagger c_{k\sigma} + c_{k\sigma}^\dagger c_{j\sigma}) - \frac{t}{2}\sum_{\langle jk\rangle}(n_j - 1)(n_k - 1) + t\sum_{\langle jk\rangle}(S_j^\dagger S_k + S_k^\dagger S_j + 2S_j^3 S_k^3) \\ & + t\sum_{\langle jk\rangle}\sum_{\sigma=\pm 1}(c_{j\sigma}^\dagger c_{k\sigma} + c_{k\sigma}^\dagger c_{j\sigma})(n_{j,-\sigma} + n_{k,-\sigma}) - t\sum_{\langle jk\rangle}(\eta_j^\dagger \eta_k + \eta_k^\dagger \eta_j + 2\eta_j^3 \eta_k^3) \\ & - 4t\sum_j \left(n_{j1} - \frac{1}{2}\right)\left(n_{j,-1} - \frac{1}{2}\right), \\ H_{\text{Hub.}}^{\text{int}} = & U\sum_j c_{j1}^\dagger c_{j1} c_{j,-1}^\dagger c_{j,-1}. \end{aligned} \tag{17}$$

As we know there are four states at each lattice site, two of them are fermionic and the others are bosonic. The terms H_{jk}^0 $(t=1)$ act as a minus graded permutation[29] of the electron states at sides j and k. By ''graded'' we mean that there is an extra minus sign if the two states that are permuted are both single electron states. For example,

$$\begin{aligned} H_{jk}^0 c_{j1}^\dagger |0\rangle &= -c_{k1}^\dagger |0\rangle, \\ H_{jk}^0 c_{j1}^\dagger c_{k,-1}^\dagger |0\rangle &= c_{j,-1}^\dagger c_{k1}^\dagger |0\rangle. \end{aligned} \tag{18}$$

Thus the symmetric part $H_{\text{Hub.}}^0$ can be written as an invariant form in terms of generators of the supergroup $U(2/2)$,

$$H_{\text{Hub.}}^0 = -t\sum_{\langle jk\rangle}\sum_{\alpha,\beta=1}^{16} \text{Str}(X^\alpha X^\beta) X^\alpha X^\beta. \tag{19}$$

The supergroup $U(2/2)$ here is the group of the unitary rotations of the four allowed states, $|a_j\rangle$ $(a=1,\ldots,4)$, into one another.

It is easy to show that the off-diagonal matrix element $(j \neq k)$ $\langle \Phi_m | c_{j,-1}^\dagger c_{j1}^\dagger c_{k1} c_{k,-1} | \Phi_m \rangle / \langle \Phi_m | \Phi_m \rangle$ is constant for long distances $|j-k|$. Here $|\Phi_m\rangle = (\eta^\dagger)^m |0\rangle$. Indeed we have

$$\frac{\langle\Phi_m|c^\dagger_{j,-1}c^\dagger_{j1}c_{k1}c_{k,-1}|\Phi_m\rangle}{\langle\Phi_m|\Phi_m\rangle}=\frac{m(L-m)}{L(L-1)}. \tag{20}$$

This fact established the properties of off-diagonal-long-range-order (ODLRO) for the state $|\Phi_m\rangle$. In the thermodynamic limit we have ODLRO as soon as $m/L\to D$ becomes finite. The ODLRO is characteristic for superconductivity.[30]

If the double occupied sites are kinetically forbidden, the restricted Hilbert space of the system now consists of configurations made of empty sites (holes) and up and down spins ($|a_j\rangle$, $a=1,2,3$). The kinetic term will allow for charge motion since empty sites will be able to move. These holes carry electric charge but they have no spin. The effective Hamiltonian now has the form of the t-J model,

$$H_{t-J}=-t\sum_{\langle jk\rangle}\sum_{\sigma=\pm1}(c^\dagger_{j\sigma}c_{k\sigma}+c^\dagger_{k\sigma}c_{j\sigma})+J\sum_{\langle jk\rangle}\left(S^\dagger_jS_k+S^\dagger_kS_j+2S^3_jS^3_k-\frac{n_jn_k}{4}\right). \tag{21}$$

Notice that H_{t-J} acts on the Hilbert space, where no double occupancy of sites are allowed.

Also, the $t-J$ Hamiltonian can be divided into a symmetric part H^0_{t-J} and a symmetry-breaking part $H^{\rm int}_{t-J}$,[31–33]

$$\begin{aligned}H^0_{t-J}&=-t\sum_{\langle jk\rangle}\sum_{\sigma=\pm1}(c^\dagger_{j\sigma}c_{k\sigma}+c^\dagger_{k\sigma}c_{j\sigma})+2t\sum_{\langle jk\rangle}\left(S^\dagger_jS_k+S^\dagger_kS_j+2S^3_jS^3_k-\frac{n_jn_k}{4}\right),\\ H^{\rm int}_{t-J}&=(J-2t)\sum_{\langle jk\rangle}\left(S^\dagger_jS_k+S^\dagger_kS_j+2S^3_jS^3_k-\frac{n_jn_k}{4}\right).\end{aligned} \tag{22}$$

H^0_{t-J} is of $U(2/1)$ supersymmetric invariance. It generates the unitary rotations among the allowed states of the $t-J$ model, $|a_j\rangle$ ($a=1,2,3$). And the terms H^0_{jk} act as a minus graded permutations of these states.

At the half-filled case of the extended Hubbard model, only the spin up and down states $|a_j\rangle$ ($a=1,2$) are allowed and no fermionic states are left. The permutation group in this case becomes as the Lie group $U(2)$. And the symmetric Hamiltonian reduces to the usual spin-$\frac{1}{2}$ quantum Heisenberg Hamiltonian,

$$H_{\rm Heisen.}=J\sum_{\langle jk\rangle}(S^\dagger_jS_k+S^\dagger_kS_j+2S^3_jS^3_k). \tag{23}$$

Generally speaking, from n states $|a\rangle$ ($a=1,2,\ldots,n$), which satisfy

$$\langle a|b\rangle=\delta^{ab}, \tag{24}$$

one can construct $n\times n$ independent real operators X^{ab},

$$X^{ab}=|a\rangle\langle b|,\quad a,b=1,2,\ldots,n. \tag{25}$$

With the local states $|a_j\rangle$ that satisfy the relation

$$\langle a_j|b_k\rangle=\delta_{jk}\delta^{ab}, \tag{26}$$

we can define the local operators $X^{ab}_j=|a_j\rangle\langle b_j|$.

With the local Hubbard operators X^{ab}_j the extended Hubbard Hamiltonian can be cast into the following form:

$$H_{\text{Hub.}}=-t\sum_{\langle jk\rangle}\sum_{a,c=1}^{4}X_j^{ac}X_k^{ca}(-1)^{F(a)\cdot F(c)}+U\sum_j X_j^{44}, \tag{27}$$

where F is the graded number,

$$F(x)=\begin{cases}1, & \text{for } x=1,2,\\ 0, & \text{for } x=3,4.\end{cases}$$

The $t-J$ and Heisenberg Hamiltonians in terms of the local Hubbard operators are

$$H_{t-J}=-t\sum_{\langle jk\rangle}\sum_{a,c=1}^{3}X_j^{ac}X_k^{ca}(-1)^{F(a)\cdot F(c)}+(J-2t)\sum_{\langle jk\rangle}\sum_{a,c=1}^{2}X_j^{ac}X_k^{ca}; \tag{28}$$

$$H_{\text{Heisen.}}=J\sum_{\langle jk\rangle}\sum_{a,c=1}^{2}X_j^{ac}X_k^{ca}. \tag{29}$$

We clearly see that the extended Hubbard model, the t-J model, and Heisenberg model can be described in a unified manner. The Hamiltonians of these models can be written into a supersymmetric form explicitly in terms of the generators of the supergroup $U(2/M)$. In the following, we investigate the supergroup coherent state path-integral presentations of the $U(2/M)$ models.

It should be noticed that, so far, the discussion has been entirely about the $s=\frac{1}{2}$ case. Before going ahead further, we would like to generalize to high s. Let us imagine that the band electrons have an orbital degeneracy labeled by an index $a=1,2,\ldots,\mathcal{N}$, where $\mathcal{N}$ is the number of degenerate bands. The total band spin at a given site j is now given by $\mathbf{S}_j=\frac{1}{2}\Sigma_{\sigma,\sigma'=\pm1}\Sigma_{a=1}^{\mathcal{N}}c_{j\sigma,a}^{\dagger}\boldsymbol{\tau}_{\sigma\sigma'}c_{j\sigma',a}$. This system still has the global $SU(2)$ invariant of spin rotations. At the half-filling case, the local spin gets to be as large as possible. The equivalent Heisenberg model has a total spin quantum number s at each site equal to $s=\mathcal{N}/2$. The limit $\mathcal{N}\to\infty$ is the same as the semiclassical limit $s\to\infty$.[34]

III. SCHWINGER BOSONS (SLAVE FERMIONS) REPRESENTATIONS

Arovas and Auerbach[21] introduced two commuting Schwinger bosons b^i ($b^{i\dagger}$) ($i=1,2$) to describe states of spin. The operator b^i ($b^{i\dagger}$) obeys the commutation relation

$$[b^i,b^{j\dagger}]=\delta^{ij}, \tag{30}$$

and satisfies the constraint

$$\sum_{i=1}^{2}b^{i\dagger}b^i=1. \tag{31}$$

The bilinear forms of the Schwinger bosons yield the spin operators

$$\mathbf{S}=\frac{1}{2}(b^{1\dagger},b^{2\dagger})\boldsymbol{\tau}\begin{pmatrix}b^1\\ b^2\end{pmatrix}. \tag{32}$$

Furthermore, a slave fermion f ($f^{\dagger}$)[16] and the two Schwinger bosons can be used to represent the allowed states of the projected Hilbert space of the $t-J$ model. The slave fermion obeys the anticommutation relation

$$\{f^{\dagger},f\}=1, \tag{33}$$

and satisfies the constraints

$$\sum_{i=1}^{2} b^{i\dagger}b^{i}+f^{\dagger}f=1. \tag{34}$$

The $t-J$ model is faithfully represented by

$$H^{t-J}=t\sum_{\langle jk\rangle} f_j^{\dagger}f_k\mathscr{T}_{jk}-J\sum_{\langle jkl\rangle}(\delta_{jl}-f_l^{\dagger}f_j)\mathscr{A}_{lk}^{\dagger}\mathscr{A}_{lk}(1-f_k^{\dagger}f_k), \tag{35}$$

where

$$\mathscr{A}_{jk}=b_j^{1\dagger}b_k^{2\dagger}-b_j^{2\dagger}b_k^{1\dagger},\quad \mathscr{T}_{jk}=b_k^{1\dagger}b_j^{1\dagger}-b_k^{2\dagger}b_j^{2\dagger}.$$

Here $\langle jkl\rangle$ are triads of nearest neighbors.

In the general case, to denote the allowed states of the high-temperature superconductivity related lattice models, one can introduce a set of Schwinger bosons and slave fermions at each site, b^i $(b^{i\dagger})$ $(i=1,2,\ldots,N)$ and f^{α} $(f^{\alpha\dagger})$ $(\alpha=1,2,\ldots,M)$, which satisfy the following commutation (anticommutation) relations:

$$\begin{gathered}[b^i,b^{j\dagger}]=\delta^{ij},\quad i,j=1,2,\ldots,N,\\ \{f^{\alpha},f^{\beta\dagger}\}=\delta^{\alpha\beta},\quad \alpha,\beta=1,2,\ldots,M,\\ [b^i,f^{\alpha}]=0=[b^i,f^{\dagger\alpha}],\quad \{f^{\alpha},f^{\beta}\}=0=[b^i,b^j].\end{gathered} \tag{36}$$

For the sake of compactness, we denote the boson and fermion operators generically as ξ^A $(\xi^{\dagger A})$,

$$\begin{gathered}\xi^A(\xi^{A\dagger}),\quad A=1,2,\ldots,N+M,\\ \xi^i\equiv b^i,\quad i=1,2,\ldots,N,\\ \xi^{N+\alpha}\equiv f^{\alpha},\quad \alpha=1,2,\ldots,M,\end{gathered} \tag{37}$$

and write symbolically

$$[\xi^A,\xi^{B\dagger}\}=\delta^{AB}, \tag{38}$$

where the product [,} is to be understood as an anticommutator between any two fermionic components and as a commutator otherwise.

It is well known that the bosonic bilinears $b^ib^{j\dagger}$ and the fermionic bilinears $f^{\alpha}f^{\beta\dagger}$ generate the Lie algebras $u(N)$ and $u(M)$ under commutation, respectively. The Bose–Fermi bilinears $b^if^{\alpha\dagger}$ and $f^{\alpha}b^{i\dagger}$ close into the set $b^ib^{j\dagger}$ and $f^{\alpha}f^{\beta\dagger}$ under anticommutation,

$$\begin{gathered}\{f^{\alpha\dagger}b^i,b^{j\dagger}f^{\beta}\}=f^{\alpha\dagger}f^{\beta}\delta^{ij}+b^{j\dagger}b^i\delta^{\alpha\beta},\\ \{f^{\alpha\dagger}b^i,f^{\beta\dagger}b^j\}=0=\{b^{i\dagger}f^{\alpha},b^{j\dagger}f^{\alpha}\}.\end{gathered} \tag{39}$$

Thus, considering the boson-fermion bilinears as the odd generators and bosonic bilinears and fermionic bilinears as the even generators, one finds that the operators $\xi^{A\dagger}\xi^B$ form the superalgebra $u(N/M)$.[17,18]

Indeed, we have

$$\begin{gathered}X^{AB}=\xi^{A\dagger}\xi^B,\\ [X^{AC},X^{BD}\}=X^{AD}\delta^{BC}\pm X^{BC}\delta^{AD}.\end{gathered} \tag{40}$$

Thus X^{AB} generates the supergroup $U(N/M)$.

The Fock space of the system is of the form

$$
\begin{gathered}
|0\rangle = \text{vacuum}, \\
b^{i\dagger}|0\rangle, \quad f^{\alpha\dagger}|0\rangle = 1-\text{particle states}, \\
b^{i_1\dagger}b^{i_2\dagger}|0\rangle, \quad b^{i\dagger}f^{\alpha\dagger}|0\rangle, \quad f^{\alpha_1\dagger}f^{\alpha_2\dagger}|0\rangle = 2-\text{particle states}, \\
\vdots \\
b^{i_1\dagger}b^{i_2\dagger}\cdots b^{i_k\dagger}f^{\alpha_1\dagger}f^{\alpha_2\dagger}\cdots f^{\alpha_{\mathscr{L}-k}\dagger}|0\rangle = \mathscr{L}-\text{particle states}.
\end{gathered}
\tag{41}
$$

Generally, the $\mathscr{L}$-particle states may contain k bosons and $\mathscr{L}-k$ fermions, where $1\leqslant k\leqslant\mathscr{L}$.

It is easy to see that the total particle number operator,

$$
N_{bf} = \sum_i b^{i\dagger}b^i + \sum_\alpha f^{\alpha\dagger}f^\alpha = \sum_A \xi^{A\dagger}\xi^A, \tag{42}
$$

has the fixed eigenvalue $\mathscr{L}$ for the $\mathscr{L}$-particle states of any value of k, $1\leqslant k\leqslant\mathscr{L}$. It should be used to label the Fock space of the supersymmetric systems.

Supposing that the systems we are interested in are of $\mathscr{N}$-fold orbital degeneracy, we would focus on the $\mathscr{N}$-particle states of the Fock space. The $\mathscr{N}$-particle states may be written in terms of the operator $\xi^{A\dagger}$,

$$
\xi^{A_1\dagger}\xi^{A_2\dagger}\cdots\xi^{A_{\mathscr{N}}\dagger}|0\rangle. \tag{43}
$$

If we analyze the $\mathscr{N}$-particle state as a tensor in the boson and fermion indices, we find it is symmetric in bosonic indices $(i_1, i_2, \ldots, i_k)$ and antisymmetric in the fermionic indices $(\alpha_1, \alpha_2, \ldots, \alpha_{\mathscr{N}-k})$. Thus, in terms of Young tableau, we may represent it as

$$
\left(\begin{array}{ll} \underbrace{\heartsuit\,\heartsuit\cdots\heartsuit\,\heartsuit}_{k}, & \left.\begin{array}{l}\heartsuit\\ \heartsuit\\ \vdots\\ \heartsuit\\ \vdots\\ \heartsuit\\ \heartsuit\end{array}\right\}\mathscr{N}-k \end{array}\right). \tag{44}
$$

It indicates a direct product of a symmetric representation of $U(N)$ and an antisymmetric representation of $U(M)$. Thus, in terms of $U(N)\otimes U(M)$ representations, the $\mathscr{N}$-particle state are the direct sum,

$$
\left(\underbrace{\heartsuit\,\heartsuit\cdots\heartsuit\,\heartsuit}_{\mathscr{N}},0\right)\otimes\left(\underbrace{\heartsuit\,\heartsuit\cdots\heartsuit\,\heartsuit}_{\mathscr{N}\text{-}1},\heartsuit\right)\otimes\left(\underbrace{\heartsuit\,\heartsuit\cdots\heartsuit\,\heartsuit}_{\mathscr{N}\text{-}2},\begin{array}{l}\heartsuit\\ \heartsuit\end{array}\right)\otimes\cdots\otimes\left(0,\left.\begin{array}{l}\heartsuit\\ \heartsuit\\ \vdots\\ \heartsuit\\ \heartsuit\end{array}\right\}\mathscr{N}\right). \tag{45}
$$

We will indicate the supertensor by a super Young tableau,

$$\left(\underbrace{\spadesuit\spadesuit\cdots\spadesuit\spadesuit}_{\mathcal{N}} \right). \tag{46}$$

Thus, the $U(N/M)$ supertableau, if decomposed into its $U(N)\otimes U(M)$ parts, is seen to be Eq. (45).

Therefore, the $\mathcal{N}$-particle state may be understood as a collection of irreducible representations of the $U(N)\otimes U(M)$ subgroup. X^{ij} ($X^{\alpha\beta}$) kills a boson (fermion) and creates another boson (fermion) and $X^{\alpha i}$ ($X^{i\alpha}$) kills a boson (fermion) and creates a fermion (boson). Thus,

$$X^{ij}\left|\left(\begin{array}{c}\overbrace{\heartsuit\cdots\heartsuit *\cdots\heartsuit\heartsuit}^{j}\\ \underbrace{\qquad\qquad\qquad}_{k}\end{array},\ \left.\begin{array}{c}\heartsuit\\ \heartsuit\\ \vdots\\ \heartsuit\\ \heartsuit\end{array}\right\}\mathcal{N}-k\right)\right\rangle\rangle=\left|\left(\begin{array}{c}\overbrace{\heartsuit\cdots\heartsuit *\cdots\heartsuit\heartsuit}^{i}\\ \underbrace{\qquad\qquad\qquad}_{k}\end{array},\ \left.\begin{array}{c}\heartsuit\\ \heartsuit\\ \vdots\\ \heartsuit\\ \heartsuit\end{array}\right\}\mathcal{N}-k\right)\right\rangle\rangle,$$

$$X^{\alpha\beta}\left|\left(\underbrace{\heartsuit\heartsuit\cdots\heartsuit\heartsuit}_{k},\ \beta\left\{\begin{array}{c}\heartsuit\\ \vdots\\ \heartsuit *\\ \vdots\\ \heartsuit\\ \heartsuit\end{array}\right\}\mathcal{N}-k\right)\right\rangle\rangle=\left|\left(\underbrace{\heartsuit\heartsuit\cdots\heartsuit\heartsuit}_{k},\ \alpha\left\{\begin{array}{c}\heartsuit\\ \vdots\\ \heartsuit *\\ \vdots\\ \heartsuit\\ \heartsuit\end{array}\right\}\mathcal{N}-k\right)\right\rangle\rangle, \tag{47}$$

$$X^{\alpha i}\left|\left(\underbrace{\heartsuit\heartsuit\cdots\heartsuit\heartsuit}_{k},\ \left.\begin{array}{c}\heartsuit\\ \heartsuit\\ \vdots\\ \heartsuit\\ \heartsuit\end{array}\right\}\mathcal{N}-k\right)\right\rangle\rangle=\left|\left(\underbrace{\heartsuit\heartsuit\cdots\heartsuit\heartsuit}_{k-1},\ \left.\begin{array}{c}\heartsuit\\ \heartsuit\\ \vdots\\ \heartsuit\\ \heartsuit\end{array}\right\}\mathcal{N}-k+1\right)\right\rangle\rangle,$$

$$X^{i\alpha}\left|\left(\underbrace{\heartsuit\heartsuit\cdots\heartsuit\heartsuit}_{k},\ \left.\begin{array}{c}\heartsuit\\ \heartsuit\\ \vdots\\ \heartsuit\\ \heartsuit\end{array}\right\}\mathcal{N}-k\right)\right\rangle\rangle=\left|\left(\underbrace{\heartsuit\heartsuit\cdots\heartsuit\heartsuit}_{k+1},\ \left.\begin{array}{c}\heartsuit\\ \heartsuit\\ \vdots\\ \heartsuit\\ \heartsuit\end{array}\right\}\mathcal{N}-k-1\right)\right\rangle\rangle,$$

so that the $X^{\alpha i}$ ($X^{i\alpha}$) acts as a ladder operator hopping to the right (left) in Eq. (45). If we apply all the operators X^{AB} taken to any power on the $\mathcal{N}$-particle state, we remain within the set of $\mathcal{N}$-particle states. This shows that the super-tableau (46) represents an irreducible set of states under all transformations of supergroup $U(N/M)$.

IV. SUPERGROUP COHERENT STATES

Consider an arbitrary quantum mechanical lattice model, whose Hamiltonian is expressed in terms of generators of a supergroup G, $X_j^l \in g$,

$$H = H(X_j^l). \tag{48}$$

We are now interested only in the case of the Hamiltonian involving linear and quadratic terms of X_j^l,

$$H = \sum_{j,k} \sum_{l,m} c_{lm}^{jk} X_j^l X_k^m + \sum_j \sum_l c_j^l X_j^l. \tag{49}$$

The superalgebra g spanned by the operators X_j^l is closed under commutation (anticommutation),

$$[X_j^k, X_j^l\} = \sum_k c_m^{kl} X_j^m, \tag{50}$$

where c_m^{kl} are the structure constants of g.

The group-theoretic approach to coherent states involves the use of unitary group representations.[35–37] We know that the standard supergroup elements connected to the identity are obtained by exponentiating superalgebra elements. There is thus one-to-one correspondence between such elements of the supergroup and points in the flat superspace $RM_L^{m,n}$,[38–40] which is the Cartesian product of m copies of RB_{L0} with n copies of RB_{L1}. A Grassmann algebra RB_L is an associative algebra generated by identity 1 and by L elements β_a ($a=1,2,\ldots,L$) obeying the anticommutation relations $\{\beta_a, \beta_b\} = 0$. The algebra is spanned by the identity and all independent nonvanishing products of β_a. There are 2^L linear independent basis elements. The subset of basis elements consisting of identity and all even products of the generators spans the even part RB_{L0} of RB_L; the remaining basis elements span the odd part RB_{L1}.

The set of left translations on a supergroup forms a supermodule W. This is the direct product of RB_L with a superalgebra. We denote the superalgebra generators[41] by X^1, $X^2,\ldots,X^m$; X^{m+1}, $X^{m+2},\ldots,X^{m+n}$. To obtain a unitary representation $T(g)$, we must work with the super-Hermitian basis of the superalgebra by choosing the generators so that $X^{j\dagger} = X^j$ for $j=1,2,\ldots,m$ and $X^{j\dagger} = -X^j$ otherwise. Thus, the operator

$$\begin{gathered} T(g) = \exp\left(\sum_{j=1}^{N^2+M^2} iA^j X^j + \sum_{j=1}^{2NM} i\theta^j X^{m+j} \right), \\ X^{j\dagger} = X^j, \quad \text{for } j = 1,2,\ldots,N^2+M^2, \\ X^{j\dagger} = -X^j, \quad \text{for } j = N^2+M^2+1,\ N^2+M^2+2,\ldots,(N+M)^2, \\ A^j \in RB_{L0}, \quad \theta^j \in RB_{L1}, \end{gathered} \tag{51}$$

defines an unitary representation of the supergroup $U(N/M)$.

To go to the super-Hermitian basis we must choose Hermitian combinations of the even generators and anti-Hermitian combinations of the odd ones. For the even generators we thus choose

$$X^k=\begin{cases} X^{ij}+X^{ji}, \\ i(X^{ij}-X^{ji}), \\ X^{\alpha\beta}+X^{\beta\alpha}, \\ i(X^{\alpha\beta}-X^{\beta\alpha}), \end{cases} \qquad k=1,2,\ldots,N^2+M^2. \tag{52}$$

And for the odd generators we choose the following anti-Hermitian operators:

$$X^k=\begin{cases} X^{\alpha i}-X^{i\alpha}, \\ i(X^{\alpha i}+X^{i\alpha}), \end{cases} \qquad k=N^2+M^2+1,\ldots,(N^2+M^2). \tag{53}$$

For the Hamiltonian (49), the Hilbert space V^Λ is a direct sum of unitary irreducible representations Γ_j of the supergroup G at each site of the lattice. In principle, we can choose an arbitrary state $|\Phi_0\rangle=|\Lambda\rangle$ within each unitary irreducible representation Γ_j^Λ, which can be normalized to unity $\langle\Phi_0|\Phi_0\rangle=1$. Acting by unitary representation Γ_j^Λ on the reference state Λ, we get the supergroup coherent states.

It should be noticed that there is a subgroup of $U(N/M)$ that consists of all the group elements h that leaves the reference state invariant up to a phase factor, called the maximum-stability subgroup H, i.e.,

$$h|\Lambda\rangle=|\Lambda\rangle e^{i\psi(h)}, \quad h\in H. \tag{54}$$

Every element g of the supergroup $U(N/M)$ can be uniquely decomposed into a product of two elements, one in H and the other in the quotient $U(N/M)/H$,

$$g=\Omega h, \quad g\in U(N/M), \quad h\in H, \quad \Omega\in U(N/M)/H, \tag{55}$$

so that we have

$$g|\Lambda\rangle=\Omega h|\Lambda\rangle=\Omega|\Lambda\rangle e^{i\psi(h)}. \tag{56}$$

$|SC\rangle\equiv\Omega|\Lambda\rangle$ is the supergroup coherent states. This definition of supergroup coherent states guarantees that there is a one-to-one correspondence with the coset space $U(N/M)/H$, so that the coordinates of the supergroup coherent states, $z^i\in RB_{L0}(\mu=1,2,\ldots,p)$, $z^\alpha\in RB_{L1}$ $[\alpha=1,2,\ldots,q$; and $p+q=\dim U(N/M)/H]$, may be chosen in any convenient parametrize representatives, $T(\Omega)$, from the cosets $U(N/M)/H$.

It is easy to see that

$$\begin{gathered} X^{\alpha\beta}\frac{1}{\sqrt{\mathcal{N}!}}(b^{1\dagger})^{\mathcal{N}}|0\rangle=0, \\ X^{ij}\frac{1}{\sqrt{\mathcal{N}!}}(b^{1\dagger})^{\mathcal{N}}|0\rangle=0, \quad \text{for } j\neq 1, \\ X^{i\alpha}\frac{1}{\sqrt{\mathcal{N}!}}(b^{1\dagger})^{\mathcal{N}}|0\rangle=0, \\ X^{\alpha i}\frac{1}{\sqrt{\mathcal{N}!}}(b^{1\dagger})^{\mathcal{N}}|0\rangle=0, \quad \text{for } i\neq 1. \end{gathered} \tag{57}$$

These operators span a subalgebra $u(1)\otimes u(N-1/M)$ of $u(N/M)$. The corresponding supergroup $U(1)\otimes U(N-1/M)$ is just the stability subgroup of $U(N/M)$, which leaves the state $(1/\sqrt{\mathcal{N}!})\times(b^{1\dagger})^{\mathcal{N}}|0\rangle$ invariant.

Choosing $(1/\sqrt{\mathcal{N}!})(b^{1\dagger})^{\mathcal{N}}|0\rangle$ as the reference state $|\Lambda\rangle$ in the representation denoted by the super Young tableau (46), we obtain the supergroup coherent states by acting

$$\Omega=\exp\left(\sum_{j=1}^{N}\eta^{j}X^{1j}+\sum_{\alpha=1}^{M}\eta^{\alpha}X^{1\alpha}-\sum_{j=1}^{N}\eta^{j\dagger}X^{j1}-\sum_{\alpha=1}^{M}\eta^{\alpha\dagger}X^{1\alpha}\right), \tag{58}$$

on the chosen reference state $(1/\sqrt{\mathcal{N}!})(b^{1\dagger})^{\mathcal{N}}|0\rangle$,

$$|SC\rangle=\Omega|\Lambda\rangle=\exp\left(\sum_{j=1}^{N}\eta^{j}X^{1j}+\sum_{\alpha=1}^{M}\eta^{\alpha}X^{1\alpha}-\sum_{j=1}^{N}\eta^{j\dagger}X^{j1}-\sum_{\alpha=1}^{M}\eta^{\alpha\dagger}X^{1\alpha}\right)\frac{1}{\sqrt{\mathcal{N}!}}(b^{1\dagger})^{\mathcal{N}}|0\rangle, \tag{59}$$

where $\eta^{j}\in CB_{L0}$, $\eta^{\alpha}\in CB_{L1}$, and CB_{L0}, CB_{L1} denotes the even and odd part of a complex Grassmann algebra with L elements, respectively.

These supergroup coherent states have a natural topological coset space $U(N/M)/[U(1)\otimes U(N-1/M)]$.

The fundamental representation of the superalgebra $u(N/M)$ is generated by the $(N+M)$-dimensional matrices,

$$(X^{AB})_{mn}=\delta^{A}_{m}\delta^{B}_{n}. \tag{60}$$

Thus, we have

$$\Omega=\exp\left(\sum_{j=1}^{N}\eta^{j}X^{1j}+\sum_{\alpha=1}^{M}\eta^{\alpha}X^{1\alpha}-\sum_{j=1}^{N}\eta^{j\dagger}X^{j1}-\sum_{\alpha=1}^{M}\eta^{\alpha\dagger}X^{1\alpha}\right)=\exp\begin{pmatrix}\bigcirc & \eta\\ -\eta^{\dagger} & \bigcirc\end{pmatrix}, \tag{61}$$

where η is an $(N+M-1)$-component rank vector with the first $(N-1)$ elements ordinary complex numbers while the last M elements complex Grassmann numbers. Therefore, in the fundamental representation, the finite transformation Ω is of the form

$$(\Omega)^{D}_{C}(z)=\begin{pmatrix}\sqrt{1-zz^{\dagger}} & z\\ -z^{\dagger} & \sqrt{1-z^{\dagger}z}\end{pmatrix}, \tag{62}$$

where $z=\eta(\sin\sqrt{\eta^{\dagger}\eta}/\sqrt{\eta^{\dagger}\eta})$, is also an $(N+M-1)$-component rank vector with the same grad with η. This is a supersymmetric generalization of the bosonic case discussed in Ref. 15.

If we explicitly introduce a complex projective representation τ of $U(N/M)/[U(1)\otimes U(N-1/M)]$,

$$\tau=\frac{z}{\sqrt{1-z^{\dagger}z}}, \tag{63}$$

any group transformation g acting on the coset space $U(N/M)/[U(1)\otimes U(N-1/M)]$ must be a holomorphic transformation,

$$\tau'=g\tau=\frac{A\tau+B}{C\tau+D}, \tag{64}$$

where

$$g=\begin{pmatrix} A & B \\ C & D \end{pmatrix} \in U(N+M),$$

$A(D)$ is a 1×1 $((N+M-1)\times(N+M-1))$ complex matrix, $B(C)$ is a $1\times(N+M-1)$ $((N+M-1)\times 1)$ matrix.

Just as the ordinary group coherent states, two important algebraic properties are maintained by the supergroup coherent states. From the definition of the supergroup coherent states, we have

$$\langle SC(z)|SC(z')\rangle=\langle\Lambda|\Omega^{-1}(z)\Omega(z')|\Lambda\rangle=\langle\Lambda|\Omega(z'')|\Lambda\rangle e^{i\psi}\neq 0, \tag{65}$$

and

$$\langle SC(z)|SC(z)\rangle=\langle\Lambda|\Omega^{-1}(z)\Omega(z)|\Lambda\rangle=\langle\Lambda|\Lambda\rangle=1. \tag{66}$$

Thus the supergroup coherent states are generally nonorthogonal but normalized to unity.

Define the operator O as

$$O=\int |SC(z)\rangle d\mu(\Omega(z))\langle SC(z)|, \tag{67}$$

we obtain that

$$gO=\int g|SC(z)\rangle d\mu(\Omega(z))\langle SC(z)|g^{-1}g=\int |SC(z')\rangle e^{i\phi'(h)}d\mu(\Omega(z'))e^{-i\phi'(h)}\langle SC(z')|g$$

$$=Og, \quad g\in U(N/M), \tag{68}$$

where $d\mu(\Omega)$ is the supergroup-invariant measure of $U(N/M)$ possessing the property $d\mu(\Omega(z))=d\mu(\Omega(z'))$.

Therefore, according to Schurr's lemma, the operator O must be proportional to the identity operator. Hence, with an appropriately normalized measure $d\mu$, we can get

$$\int |SC(z)\rangle d\mu(\Omega(z))\langle SC(z)|=1. \tag{69}$$

The supergroup coherent states can be expanded in a complete orthonormal basis $|\lambda\rangle$,

$$|SC(z)\rangle=\sum_{\lambda} |\lambda\rangle\langle\lambda|SC(z)\rangle, \tag{70}$$

and it is possible to project the orthonormal basis vectors from the supergroup coherent states by making use of Eq. (69),

$$|\lambda\rangle=\int d\mu(\Omega(z))|SC(z)\rangle\langle SC(z)|\lambda\rangle. \tag{71}$$

The supergroup coherent states therefore constitute an overcomplete basis.

V. PATH-INTEGRAL REPRESENTATIONS

Typically we are interested in studying both zero-temperature and finite-temperature properties of a system. At finite temperature, the equilibrium properties are determined by the partition function

$$Z=\mathrm{Tr}\ e^{-H/k_BT}. \tag{72}$$

At zero temperature we are interested in the vacuum persistence amplitudes,

$$Z=\mathrm{Tr}\ \hat{T}\ \exp\left(-\frac{i}{\hbar}\int_{-\infty}^{\infty}H\ d\tau\right), \tag{73}$$

where $\hat{T}$ is the time order operator.

In this section, we generalize the method of RSS[15] to supersymmetric systems and give the supergroup coherent state path-integral representation of the high T_c superconductivity related lattice models. For a supersymmetric system with the supergroup theoretic Hamiltonian H, the standard path integral is derived as follows. We first split up the time interval τ into N_τ segments of infinitesimal length $\Delta\tau$ such that $N_\tau\cdot\Delta\tau=\tau$. For infinitesimal intervals $\Delta\tau\to 0$, we can write

$$Z=\mathrm{Tr}\ \hat{T}\ \exp\left(-\frac{i}{\hbar}\sum_{j=1}^{N_\tau}H(\tau_j)\Delta\tau\right)=\mathrm{Tr}\ \hat{T}\prod_{j=1}^{N_\tau}\exp\left(-\frac{i}{\hbar}H(\tau_j)\Delta\tau\right). \tag{74}$$

Then we insert the resolution of identity (69) at each intermediate time τ_j. We get

$$\begin{aligned}
Z=&\lim_{\Delta\tau\to 0}\int\left\langle SC(z_f)\left|e^{-iH\,\Delta\tau/\hbar}\right|SC\left(z_f-\frac{dz}{d\tau}\Delta\tau\right)\right\rangle d\mu\left(\Omega\left(z_f-\frac{dz}{d\tau}\Delta\tau\right)\right)\\
&\times\left\langle SC\left(z_f-\frac{dz}{d\tau}\Delta\tau\right)\left|e^{-iH\,\Delta\tau/\hbar}\right|SC\left(z_f-\frac{dz}{d\tau}2\,\Delta\tau\right)\right\rangle d\mu\left(\Omega\left(z_f-\frac{dz}{d\tau}2\,\Delta\tau\right)\right)\\
&\times\left\langle SC\left(z_f-\frac{dz}{d\tau}2\,\Delta\tau\right)\right|\cdots\left|SC\left(z_i+\frac{dz}{d\tau}\Delta\tau\right)\right\rangle d\mu\left(\Omega\left(z_i+\frac{dz}{d\tau}\Delta\tau\right)\right)\\
&\times\left\langle SC\left(z_i+\frac{dz}{d\tau}\Delta\tau\right)\left|e^{-iH\,\Delta\tau/\hbar}\right|SC(z_i)\right\rangle\\
=&\int\mathscr{D}[d\mu(\Omega(\tau))]\exp\left(\frac{i}{\hbar}\int_{-\infty}^{\infty}L\ d\tau\right),
\end{aligned} \tag{75}$$

where $\mathscr{D}[d\mu(\Omega(\tau))]$ is the functional measure of the path integral and L is the Lagrangian of the system.

The overlap between neighboring coherent states is

$$\langle SC(z+dz)|SC(z)\rangle=\langle\Lambda|\Omega^{-1}(z+dz)\Omega(z)|\Lambda\rangle=1-\tfrac{1}{2}\mathscr{N}(z\ dz^\dagger-dz\ z^\dagger). \tag{76}$$

Hence, the Lagrangian of the system takes the form

$$L=-\frac{\hbar}{2i}\mathscr{N}(z\ \partial_\tau z^\dagger-\partial_\tau z\ z^\dagger)-H(z,z^\dagger). \tag{77}$$

The canonical momenta of the system are

$$\pi_i=\frac{\partial L}{\partial\dot{z}^i}=\frac{\hbar}{i}\mathscr{N}z^{i\dagger}. \tag{78}$$

Canonical quantization gives the commutation rules,

$$[z^i,z^j\}=0,\quad [z^i,z^{j\dagger}\}=\frac{1}{\mathcal{N}}\delta_{ij},\quad [z^{i\dagger},z^{j\dagger}\}=0. \tag{79}$$

To construct the generators out of these operators it is helpful to consider first their coherent state expectation values,

$$\begin{aligned}\langle SC(z)|X^{AB}|SC(z)\rangle&=\langle\Lambda|\Omega^{-1}(z)X^{AB}\Omega(z)|\Lambda\rangle=(\Omega^{-1}(z))^{AC}\langle\Lambda|X^{CD}|\Lambda\rangle(\Omega(z))^{DB}\\&=\mathcal{N}(\Omega^{-1}(z)Y\Omega(z))^{AB},\end{aligned} \tag{80}$$

where

$$Y=\begin{pmatrix}\mathcal{N} & 0\\ 0 & 0\end{pmatrix}.$$

With the matrices $\Omega(z)$ given by Eq. (62) one obtains

$$\langle SC(z)|X^{AB}|SC(z)\rangle=\begin{pmatrix}\mathcal{N}(1-zz^\dagger) & \mathcal{N}\sqrt{1-zz^\dagger}z\\ \mathcal{N}z^\dagger\sqrt{1-zz^\dagger} & \mathcal{N}z^\dagger z\end{pmatrix}. \tag{81}$$

The classical expressions on the rhs of the above equation suggest the following operator realization:

$$\begin{aligned}X^{11}(z)&=\mathcal{N}\left(1-\sum_{k=1}^{N+M-1}z^{k\dagger}z^k\right),\\ X^{1(j+1)}(z)&=\mathcal{N}\sqrt{1-\sum_{k=1}^{N+M-1}z^{k\dagger}z^k}z^j,\quad j=1,2,\ldots,N+M-1,\\ X^{(i+1)1}(z)&=\mathcal{N}z^{i\dagger}\sqrt{1-\sum_{k=1}^{N+M-1}z^{k\dagger}z^k},\quad i=1,2,\ldots,N+M-1,\\ X^{(i+1)(j+1)}(z)&=\mathcal{N}z^{i\dagger}z^j.\end{aligned} \tag{82}$$

It is easy to verify, using the commutation rules (79), that these operators satisfy the superalgebra $u(N/M)$.

From now on we discuss the high-temperature superconductivity related lattice models and so that we restrict ourselves at the case of $N=2$. We expect that the high-temperature superconductivity materials, at least the short-range order, should have Néel character, it is natural to consider the staggered and uniform components of the z field, i.e., on sublattice A we use the above z parametrization and on sublattice B we use another set of parametrization. Making use of a parameter transformation of the supergroup coherent states.

$$\begin{aligned}z^1&\to -z^1\sqrt{1-\sum_{i=1}^{1+M}z^{i\dagger}z^i},\quad z^{1\dagger}\to -\sqrt{1-\sum_{i=1}^{1+M}z^{i\dagger}z^i}z^{1\dagger},\\ z^i&\to\frac{z^{1\dagger}}{\sqrt{z^{1\dagger}z^1}}z^i,\quad i=2,3,\ldots,1+M,\\ z^{i\dagger}&\to z^{i\dagger}\frac{z^{1\dagger}}{\sqrt{z^{1\dagger}z^1}},\quad i=2,3,\ldots,1+M,\end{aligned} \tag{83}$$

we get the other set of expectations of X_j^{ac},

$$\langle SC(z')|X^{ac}|SC(z')\rangle$$

$$=\begin{pmatrix} \mathcal{N}z^{1\dagger}z^1 & -\mathcal{N}\sqrt{1-\sum_{i=1}^{1+M} z^{i\dagger}z^i}\,z^1 & \mathcal{N}z^{1\dagger}z' \\ -\mathcal{N}z^{1\dagger}\sqrt{1-\sum_{i=1}^{1+M} z^{i\dagger}z^i} & \mathcal{N}\left(1-\sum_{i=1}^{1+M} z^{i\dagger}z^i\right) & -\mathcal{N}\sqrt{1-\sum_{i=1}^{1+M} z^{i\dagger}z^i}\,z' \\ \mathcal{N}z'^{\dagger}z^1 & -\mathcal{N}z'^{\dagger}\sqrt{1-\sum_{i=1}^{1+M} z^{i\dagger}z^i} & \mathcal{N}z'^{\dagger}z' \end{pmatrix}, \tag{84}$$

where we have used the notation $z'=(z^2,z^3,\ldots,z^{1+M})$.

This set of expectations arise another Holstein–Primakoff realization of the superalgebra $u(2/M)$,

$$X^{11}(z)=\mathcal{N}z^{1\dagger}z^1,\quad X^{12}(z)=-\mathcal{N}\sqrt{1-\sum_{k=1}^{1+M} z^{k\dagger}z^k}\,z^1,$$

$$X^{1(j+1)}=\mathcal{N}z^{1\dagger}z^j,\quad j=2,3,\ldots,1+M,$$

$$X^{21}(z)=-\mathcal{N}z^{1\dagger}\sqrt{1-\sum_{k=1}^{1+M} z^{k\dagger}z^k},$$

$$X^{22}=\mathcal{N}\left(1-\sum_{k=1}^{1+M} z^{k\dagger}z^k\right),\quad X^{2(j+1)}=-\mathcal{N}\sqrt{1-\sum_{k=1}^{1+M} z^{k\dagger}z^k}\,z^j, \tag{85}$$

$$X^{(i+1)1}=\mathcal{N}z^{i\dagger}z^1,\quad i=2,3,\ldots,1+M,$$

$$X^{(i+1)2}=-\mathcal{N}z^{i\dagger}\sqrt{1-\sum_{k=1}^{1+M} z^{k\dagger}z^k},$$

$$X^{(i+1)(j+1)}(z)=\mathcal{N}z^{i\dagger}z^j.$$

Let H^0 be the Hamiltonian for the system with $U(2/M)$ symmetry on a two-dimensional lattice,

$$H^0=-t\sum_{\langle jk\rangle}\sum_{a,c=1}^{2+M} X_j^{ac}X_k^{ca}(-1)^{F(a)\cdot F(c)}, \tag{86}$$

where

$$F(x)=\begin{cases}1, & x=1,2,\\ 0, & x=3,4,\ldots,2+M.\end{cases}$$

Then we have

$$
\begin{aligned}
H^0(z)&=\langle SC(z)|H|SC(z)\rangle\\
&=-t\sum_{\langle jk\rangle}\sum_{a,c=1}^{2+M}\langle X_j^{ac}\rangle\langle X_k^{ca}\rangle(-1)^{F(a)\cdot F(c)}\\
&=\frac{t}{2}\sum_{\langle jk\rangle}\sum_{a,c=1}^{2}(\langle X_j^{ac}\rangle+\langle X_k^{ac}\rangle)(\langle X_j^{ca}\rangle+\langle X_k^{ca}\rangle)-t\sum_j\sum_{a,c=1}^{2}\langle X_j^{ac}\rangle\langle X_j^{ca}\rangle\\
&\quad+\frac{t}{2}\sum_{\langle jk\rangle}\sum_{a=1}^{2}\sum_{c=3}^{2+M}(\langle X_j^{ac}\rangle+\langle X_k^{ac}\rangle)(\langle X_j^{ca}\rangle-\langle X_k^{ca}\rangle)\\
&\quad+\frac{t}{2}\sum_{\langle jk\rangle}\sum_{a=3}^{2+M}\sum_{c=1}^{2}(\langle X_j^{ac}\rangle+\langle X_k^{ac}\rangle)(\langle X_j^{ca}\rangle-\langle X_k^{ca}\rangle)\\
&\quad+\frac{t}{2}\sum_{\langle jk\rangle}\sum_{a,c=3}^{2+M}(\langle X_j^{ac}\rangle-\langle X_k^{ac}\rangle)(\langle X_j^{ca}\rangle-\langle X_k^{ca}\rangle)-t\sum_j\sum_{a,c=3}^{2+M}\langle X_j^{ac}\rangle\langle X_j^{ca}\rangle. \qquad (87)
\end{aligned}
$$

We will not consider here frustrated systems. Thus, and for the sake of simplicity, we will consider the case of $U(2/M)$ models on bipartite lattices. We split the staggered z_j^1 field into a slowly very piece $\phi(j)$, the order parameter field, and a small rapidly varying part, $\xi(j)$,

$$
\begin{aligned}
z_j^1&=\phi(j)+a_0\xi(j), \quad \text{for sublattice } A,\\
z_j^1&=\phi(j)-a_0\xi(j), \quad \text{for sublattice } B,
\end{aligned} \qquad (88)
$$

where a_0 denotes the lattice spacing.

We work with the constraint that requires that

$$
\sum_{a,c=1}^{2+M}\langle X^{ac}(z)\rangle\langle X^{ca}(z)\rangle(-1)^{F(a)\cdot F(c)}=\sum_{a,c=1}^{2+M}\langle X^{ac}(\phi)\rangle\langle X^{ca}(\phi)\rangle(-1)^{F(a)\cdot F(c)}. \qquad (89)
$$

By making use of the large $\mathcal{N}$ approximation, we obtain

$$
H^0(\phi,\xi;z')=\frac{t\mathcal{N}^2}{2}\int dx\,dy\left(\partial_\mu\phi\;\partial^\mu\phi^\dagger+4\xi\xi^\dagger+4\sum_{k=2}^{1+M}z^{k\dagger}z^k\right), \qquad (90)
$$

where $\partial_\mu\phi\;\partial^\mu\phi^\dagger\equiv\partial_x\phi\;\partial_x\phi^\dagger+\partial_y\phi\;\partial_y\phi^\dagger$.

We know that the Lagrangian of the $U(2/M)$ model is

$$
L^0(z)=-\frac{i\hbar}{2}\mathcal{N}\sum_j\left\{(-1)^{S(j)}(z_j^1\;\partial_\tau z_j^{1\dagger}-\partial_\tau z_j^1\;z_j^{1\dagger})+\sum_{i=2}^{1+M}(z_j^i\;\partial_\tau z_j^{i\dagger}-\partial_\tau z_j^i\;z_j^{i\dagger})\right\}-H^0(z), \qquad (91)
$$

where

$$
S(j)=\begin{cases}0, & \text{for sublattice } A,\\ 1, & \text{for sublattice } B.\end{cases}
$$

To complete the discussion of the continuum limit, it is necessary to consider the kinetic term,

$$-\frac{i\hbar}{2}\mathcal{N}\sum_j\left\{(-1)^{S(j)}(z_j^1\ \partial_\tau z_j^{1\dagger}-\partial_\tau z_j^1\ z_j^{1\dagger})+\sum_{i=2}^{1+M}(z_j^i\ \partial_\tau z_j^{i\dagger}-\partial_\tau z_j^i\ z_j^{i\dagger})\right\}.$$

Substituting Eq. (88), we obtain, after discarding a total derivative,

$$-\frac{i\hbar}{2}\mathcal{N}\sum_j(-1)^{S(j)}(z_j^1\ \partial_\tau z_j^{1\dagger}-\partial_\tau z_j^1\ z_j^{1\dagger})\doteq\frac{-i\hbar\mathcal{N}}{a_0}\int dx\ dy(\xi\ \partial_\tau\phi^\dagger-\partial_\tau\phi\ \xi^\dagger).\tag{92}$$

Thus, the Lagrangian becomes as

$$L^0(\phi,\xi;z_i)=-\frac{i\hbar\mathcal{N}}{a_0}\int dx\ dy(\xi\ \partial_\tau\phi^\dagger-\partial_\tau\phi\ \xi^\dagger)-\frac{i\hbar\mathcal{N}}{2a_0^2}\int dx\ dy\sum_{i=2}^{1+M}(\partial_\tau z^i\ z^{i\dagger}+\partial_\tau z^{i\dagger}\ z^i)$$
$$-\frac{t\mathcal{N}^2}{2}\int dx\ dy\left(\partial_\mu\phi\ \partial^\mu\phi^\dagger+4\xi\xi^\dagger+4\sum_{i=2}^{1+M}z^{i\dagger}z^i\right).\tag{93}$$

The auxiliary fields ξ can be eliminated by solving the Euler–Lagrange equation $\delta L/\delta\xi=0$,

$$2t\mathcal{N}^2\xi^\dagger=-\frac{i\hbar\mathcal{N}}{a_0}\partial_\tau\phi^\dagger,\quad 2t\mathcal{N}^2\xi=\frac{i\hbar\mathcal{N}}{a_0}\partial_\tau\phi.\tag{94}$$

Therefore, we obtain

$$L^0(\phi,z_i)\doteq\int dx\ dy\left(\frac{\hbar^2}{2ta_0^2}\partial_\tau\phi\ \partial_\tau\phi^\dagger-\frac{t\mathcal{N}^2}{2}\partial_\mu\phi\ \partial^\mu\phi^\dagger\right)$$
$$-\int dx\ dy\sum_{i=2}^{1+M}\left(\frac{i\hbar\mathcal{N}}{2a_0^2}(\partial_\tau z^i\ z^{i\dagger}+\partial_\tau z^{i\dagger}\ z^i)+2t\mathcal{N}^2z^{i\dagger}z^i\right).\tag{95}$$

To deal with the realistic models related to high-temperature superconductivity, we must consider the interactive Hamiltonian. The whole Lagrangian of the two-dimensional (2-D) extended Hubbard model is

$$L_{\text{Hub.}}(\phi,z_i)\doteq\int dx\ dy\left(\frac{\hbar^2}{2ta_0^2}\partial_\tau\phi\ \partial_\tau\phi^\dagger-\frac{t\mathcal{N}^2}{2}\partial_\mu\phi\ \partial^\mu\phi^\dagger\right)$$
$$-\int dx\ dy\sum_{i=2}^{3}\left(\frac{i\hbar\mathcal{N}}{2a_0^2}(\partial_\tau z^i\ z^{i\dagger}+\partial_\tau z^{i\dagger}\ z^i)+2t\mathcal{N}^2z^{i\dagger}z^i\right)-\frac{U}{a_0^2}\int dx\ dy\ z^{3\dagger}z^3.\tag{96}$$

The Lagrangian of the $t-J$ model on the two-dimensional lattice is

$$L_{t-J}(\phi,z_i)\doteq\int dx\ dy\left(\frac{\hbar^2}{2Ja_0^2}\partial_\tau\phi\ \partial_\tau\phi^\dagger-\frac{J\mathcal{N}^2}{2}\partial_\mu\phi\ \partial^\mu\phi^\dagger\right)$$
$$-\int dx\ dy\left(\frac{i\hbar\mathcal{N}}{2a_0^2}(\partial_\tau z^2\ z^{2\dagger}+\partial_\tau z^{2\dagger}\ z^2)+2t\mathcal{N}^2z^{2\dagger}z^2\right).\tag{97}$$

And the Lagrangian of the 2-D Heisenberg model is simply

$$L_{\text{Heisen.}}(\phi,z_i)\doteq\int dx\ dy\left(\frac{\hbar^2}{2Ja_0^2}\partial_\tau\phi\ \partial_\tau\phi^\dagger-\frac{J\mathcal{N}^2}{2}\partial_\mu\phi\ \partial^\mu\phi^\dagger\right).\tag{98}$$

Making use of the property of Grassmann integrals,

$$\int \mathscr{D}z^{i\dagger}\,\mathscr{D}z^{i}\,\exp\left(-\int z^{i\dagger}Mz^{i}\right)=\mathrm{Det}\;M,\quad z^{i},z^{i\dagger}\in CB_{L1}, \tag{99}$$

we can integrate out the fermionic fields and obtain an effective Lagrangian that involves only a bosonic part,

$$L^{\mathrm{eff}}_{\mathrm{Hub.}}(\phi)=\int dx\;dy\left(\frac{\hbar^{2}}{2ta_{0}^{2}}\,\partial_{\tau}\phi\;\partial_{\tau}\phi^{\dagger}-\frac{t\mathscr{N}^{2}}{2}\,\partial_{\mu}\phi\;\partial^{\mu}\phi^{\dagger}\right)$$
$$-i\;\ln\left(\mathrm{Det}\left(\frac{i\hbar\mathscr{N}}{a_{0}^{2}}\,\partial_{\tau}+2t\mathscr{N}^{2}\right)\mathrm{Det}\left(\frac{i\hbar\mathscr{N}}{a_{0}^{2}}\,\partial_{\tau}+2t\mathscr{N}^{2}+\frac{U}{a_{0}^{2}}\right)\right); \tag{100}$$

$$L^{\mathrm{eff}}_{t-J}(\phi)=\int dx\;dy\left(\frac{\hbar^{2}}{2Ja_{0}}\,\partial_{\tau}\phi\;\partial_{\tau}\phi^{\dagger}-\frac{J\mathscr{N}^{2}}{2}\,\partial_{\mu}\phi\;\partial^{\mu}\phi^{\dagger}\right)-i\;\ln\,\mathrm{Det}\left(\frac{i\hbar\mathscr{N}}{a_{0}^{2}}\,\partial_{\tau}+2t\mathscr{N}^{2}\right). \tag{101}$$

Therefore, up to a constant, the low-energy excitations of the extended Hubbard model, $t-J$ model and Heisenberg model is described, in a unified manner, by the nonlinear σ model. In other words, the nonlinear σ model gives a sensible description of the spin fluctuations of the high T_c superconductivity materials. This agrees with the predictions of the weak-coupling mean-field theory.

VI. CONCLUDING REMARKS

In this paper, we have shown that the supergroup $U(N/M)$ plays an important role in a kind of high-temperature superconductivity related lattice model. To arrive at a continuum field theory description of these models, we constructed supergroup coherent states by a standard approach. A nonlinear σ model was obtained as an effective field theory of low-energy excitations of spin–spin interactions of high T_c superconductivity materials in the supergroup coherent state path-integral representation. This result is within our expectations, the spin–spin interactions can be described by the nonlinear σ model in the absence of doping and doping do not violate the Néel ground state, at least in the low doping case. This also proves the prediction of weak-coupling mean-field theory in fermion coherent state path-integral representation. In the fermion coherent state path-integral representation,[34,42,43] the Lagrangian of the Hubbard model is of the form

$$L=\frac{i}{\hbar}\sum_{\langle jk\rangle}\sum_{\sigma=\pm1}\Phi^{\dagger}_{j\sigma}\;\partial_{\tau}\Phi_{k\sigma}+2t\sum_{\langle jk\rangle}\sum_{\sigma=\pm1}\Phi^{\dagger}_{j\sigma}\Phi_{k\sigma}+\frac{U}{6}\sum_{j}\;(\Phi^{\dagger}_{j\sigma}\boldsymbol{\tau}_{\sigma\sigma'}\Phi_{j\sigma'})^{2}. \tag{102}$$

The associated path-integral contains quartic terms, the interaction, and hence we do not know how to complete the partition function. Introducing a vector real boson field $\boldsymbol{\phi}$ and using the Hubbard–Stratonovich transformation,[44,45]

$$\int d\boldsymbol{\phi}\,\exp\left(-\frac{i}{\hbar}\left(\frac{1}{2}\,\boldsymbol{\phi}^{2}+\lambda\,\boldsymbol{\phi}\Phi^{\dagger}\boldsymbol{\tau}\Phi\right)\right)=\mathrm{const}\times\exp\left(\frac{i}{2\hbar}\,\lambda^{2}(\Phi^{\dagger}\boldsymbol{\tau}\Phi)^{2}\right), \tag{103}$$

one can get an equivalent Lagrangian of the Hubbard model,

$$L'=\frac{i}{\hbar}\sum_{\langle jk\rangle}\sum_{\sigma=\pm1}\Phi^{\dagger}_{j\sigma}\;\partial_{\tau}\Phi_{k\sigma}+2t\sum_{\langle jk\rangle}\sum_{\sigma=\pm1}\Phi^{\dagger}_{j\sigma}\Phi_{k\sigma}-\sqrt{\frac{U}{3}}\sum_{j}\;\boldsymbol{\phi}_{j}\Phi^{\dagger}_{j\sigma}\boldsymbol{\tau}_{\sigma\sigma'}\Phi_{j\sigma'}-\frac{1}{2}\sum_{j}\;\boldsymbol{\phi}^{2}_{j}. \tag{104}$$

The $\boldsymbol{\phi}$ fields represent the collective modes associated with spin fluctuations. The effective Lagrangian is given by

$$L^{\text{eff}}(\boldsymbol{\phi}) = -\frac{1}{2}\sum_j \boldsymbol{\phi}^2 - i \ln \text{Det}\left(\frac{i}{\hbar}\partial_\tau - M(\boldsymbol{\phi})\right), \tag{105}$$

where $M(\boldsymbol{\phi})$ is a functional matrix of the $\boldsymbol{\phi}$ fields. On the mean-field-theory approximation, the effective Lagrangian shows the relevant nonlinear effects. The properties of the effective Lagrangian suggests that the nonlinear σ model,

$$L^{\text{eff}} = \frac{\rho}{2}\left(\partial_\tau \boldsymbol{\phi}\cdot\partial_\tau \boldsymbol{\phi} - v_s^2\ \partial_\mu \boldsymbol{\phi}\cdot\partial^\mu \boldsymbol{\phi}\right) + \cdots\ , \tag{106}$$

describes the slow spin fluctuations. In this paper we have proved the assumption but not used any approximation, except large spin and long wavelength.

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Two-body wave equations in curved space–time

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Two scalar particles undergoing mutual interaction are considered in a prescribed curved space–time. Both masses are finite (recoil is not neglected). For a description of this system we propose a pair of coupled Klein–Gordon equations; they involve two-body-sector extensions of the Laplace–Beltrami operator, plus a term that takes mutual interaction into account. Besides the problem of compatibility, we discuss several requirements that seem more or less necessary from a physical point of view. Particular attention is devoted to the preservation of space–time symmetries (isometric invariance). Composition of curvature with mutual interaction is a nonlinear problem, but it can be explicitly solved in a toy model of static orthogonal space–time. Moreover, we check that isometric invariance and other physical requirements are satisfied in this example. © *1996 American Institute of Physics.* [S0022-2488(96)02708-9]

I. INTRODUCTION

The perturbation of energy levels of an atom in curved space–time is of considerable theoretical interest. Several years ago, Parker pointed out the possibility to consider a hydrogen atom as a probe of space–time curvature.[1] We would like to add that, *in principle*, also the elementary quark model of composite hadrons should be somehow affected by the presence of an extremely strong gravitational field.

Of course, curvature effects on the *internal* structure of composite systems are of very small magnitude and cannot be directly observed in accessible regions of space–time. For an atomic system, a significant effect would require a radius of curvature of the order of 10^{-3} cm (a molecule should be more sensitive).

Nevertheless, regions of such large curvature might exist in the neighborhood of small black holes left over from the early stage of the universe. And one must bear in mind that observations of more and more remote regions of space provides us with information about the early universe, a laboratory of large curvature.

All these reasons have motivated an abundant flow of papers about quantum mechanics of atoms in curved space–time.[1–3] Most authors have systematically neglected the recoil of the nucleus. It was the merit of Fischbach, Freeman, and Cheng[3] to point out that taking recoil into account may, in weak gravitational fields, introduce a correction of the same magnitude as the gravitational perturbations (and this remark is more drastically relevant for positronium). They realized that a fully relativistic treatment of two-body dynamics in the presence of gravity is a difficult problem, and they undertook to solve it along the lines of the Bakamjian–Thomas formalism.[4] In this context they devoted special attention to the problem of separating relative variables from the center-of-mass coordinates, a delicate question previously considered by Krajcik and Foldy.[5]

However, the modern developments of relativistic particle dynamics[6–9] allow for a more sophisticated and more efficient framework. In our opinion it has now become natural and reasonable to look after a *manifestly covariant* description of mutually interacting particles moving in a prescribed Riemannian space–time.

Insofar as pair creation can be neglected (and taking recoil into account does not change the conditions under which this approximation is valid, so one is referred to the literature quoted

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above in order to discuss this point) any arbitrary, but fixed, number of particles could be, in principle, considered. But in practice, we are in a position to undertake the study of *two-body* quantum mechanics because the progresses obtained up to now in flat space–time have essentially concerned the two-body sector.

Our approach to the quantum mechanics of composite systems was obtained by quantizing ''predictive relativistic mechanics.''[6] It agrees with the possibility of considering relativistic particle dynamics as a constraint theory[7] (papers in this field are currently referred to in the literature as constraint relativistic mechanics). This standpoint implies eliminating the field that underlies the mutual interaction, thus *only the particle degrees of freedom* are explicitly considered, and eventually coupled to gravity.

The basic equations for two interacting scalar particles are a pair of Klein–Gordon equations coupled by appropriate terms that carry the mutual interaction and must ensure compatibility.[6] This term can be either phenomenological or motivated by consideration of quantum field theory. In this latter case, the contact between coupled Klein–Gordon equations and the standard methods of quantum electrodynamics in the two-body sector has been firmly established, see Todorov for the quasipotential approach[9] and Sazdjian[10] for the relationship to Bethe–Salpeter equation (BS equation). In fact, the coupled equations of relativistic quantum mechanics present several advantages over the BS equation.

Turning now to the situation where gravity is present as an external field, we observe that, in spite of promising advances, quantum theory is not yet developed in curved space–time as far as to produce a tractable version of the BS equation, taking curvature effects into account. Thus, a formulation of two-body dynamics in curved space–time using a pair of wave equations would be very convenient.

In principle, generalizing quantum mechanics to a Lorentzian manifold M_4 is straightforward if the d'Alembert symbol is replaced by the Laplace Beltrami operator (for simplicity we consider minimal coupling). So let us write

$$2H_a\Psi = m_a^2\Psi, \quad a=1,2, \tag{1.1}$$

where the particle masses are m_1, m_2. The wave function Ψ depends on eight arguments, namely the coordinates of a couple q_1, q_2 taken in $M_4 \times M_4$. It is always possible to write $H_a = K_a + V_a$, where K_1, K_2, respectively, refer to particles 1 and 2, namely

$$K_a = -\tfrac{1}{2}\, g(a)^{\alpha\beta}\boldsymbol{\nabla}_{a\alpha}\boldsymbol{\nabla}_{a\beta}, \tag{1.2}$$

whereas V_1, V_2 are considered as describing the mutual interaction. In view of our knowledge of the flat-space–time theory,[6] we expect to have in most cases of interest the unipotential simplification $V_1 = V_2 = V$.

To avoid unnecessary complications we assume that space–time M_4 has the trivial topology. It is clear that Eqs. (1.1) must be mutually compatible. By natural generalization of the flat-space–time theory, we require a strong *compatibility condition*, namely

$$[H_1, H_2] = 0. \tag{1.3}$$

At this stage it is already a practical problem to determine in closed form which interaction term can be added to the Laplace–Beltrami operators without violating condition (1.3). This problem was solved years ago[6] for an isolated system in Minkowski space (the word isolated refers to the absence of an external field). Even if one remains in flat space–time, the presence of external fields is a difficulty, because *relativistic interactions cannot be linearly composed*. In the flat case however, some results have been obtained, for external potentials with special symmetries.[11–14]

In the present case we consider a system that is submitted to no external force but gravity. Physically, this situation is analogous to the flat case in the presence of an external potential. But we have a lot of extra complications due to the geometric nature of General Relativity.

Our main goal is to construct closed-form examples of a pair of wave equations, mutually consistent in the presence of a curvature field. But we shall also discuss the general features of such equations, with special care for a set of reasonable requirements one should impose to them. Among these conditions isometric invariance plays the role of a generalization of the Poincaré invariance usually required in the flat case.

We first recollect, in Sec. II, several well-known results about the manifestly covariant formulation of two-body dynamics in flat space–time. In this framework, and in order to make possible a contact with the work of Fishbach *et al.*, we propose a relativistic covariant version of the concept of center of mass, and we outline its connection with the separation of canonical variables we are currently using.

In Sec. III we address the general problem of two mutually interacting particles imbedded in a curved space–time. An axiomatic discussion (focusing on invariance properties) provides a set of necessary conditions restricting the possible choice of H_1 and H_2. Then it will be interesting to exhibit an example satisfying all (or part of) these minimal requirements. Keeping this goal in mind, a preliminary work is in order. That is why in Sec. IV we recall some standard facts about the motion of a test particle *alone* in a curved space–time with possible isometries. In addition, we systematically introduce a flat background metric and put special emphasis on the role of isometries.

We return to the two-body case in Sec. V. Finally, a specific form of the metric tensor will be assumed. The particular symmetry enjoyed by this metric singles out a natural flat background where standard methods of *special relativistic quantum mechanics in external fields* can be finally applied. Moreover, this metric is invariant under time translation in a strong sense, which allows for solving (in closed form) the compatibility problem. We ultimately discuss whether the outcome of this procedure satisfies the conditions we have previously demanded. Section VI will be devoted to concluding remarks.

Notation: Particle labels $a,b=1,2$. Space–time manifold M_4. Partial differentiation with respect to coordinates are noted as $\partial_\mu=\partial/\partial q^\mu$, $\partial_{a\mu}=\partial/\partial q_a^\mu$. The use of q_1,q_2 is not a typographic fancy; we mean to recall that in the classical limit ($\hbar\to 0$) the arguments of the wave function should, in principle, reduce to the canonical coordinates of a covariant Hamiltonian formulation and cannot coincide with the physical coordinates (say x_1,x_2) in the *large* (that is unconstrained) *phase space*, where the standard Poisson brackets are implemented.[6]

Greek labels are omitted whenever no confusion is possible. When we consider a flat background metric $\underline{g}_{\mu\nu}$, its reciprocal tensor is $\underline{g}^{\alpha\beta}$. The determinants are g and $\underline{g}$, respectively. Of course, Cartesian coordinates refer to $\underline{g}_{\mu\nu}$.

Scalar products indicated by a dot always refer to the flat metric. For instance $p^2=p\cdot p$ stands for $\underline{g}^{\mu\nu}p_\mu p_\nu$. Indices will be rised (lowered) with help of the flat metric only. $p_{a\alpha}$ is the operator with components $-i\partial/\partial q_a^\alpha$ in the Cartesian coordinates.

Angular momentum in flat space–time is $m^{\alpha\beta}=q^\alpha p^\beta-q^\beta p^\alpha$.

Dependence on the coordinates and/or momenta of particle a is indicated as in $g(a)=g(q_a)$, etc.

In Cartesian coordinates, we separate canonical variables in two groups as follows:

$$z^\alpha=q_1^\alpha-q_2^\alpha,\quad y=\tfrac{1}{2}(p_1-p_2), \tag{1.4}$$

$$P=p_1+p_2,\quad Q=\tfrac{1}{2}(q_1^\alpha+q_2^\alpha), \tag{1.5}$$

hence the commutators

$$[z^\alpha, y_\beta] = [Q^\alpha, P_\beta] = i\,\delta^\alpha_\beta. \tag{1.6}$$

The total angular momentum is defined as

$$M = q_1 \wedge p_1 + q_2 \wedge p_2 = Q \wedge P + z \wedge y,$$

which allows for checking that P and M actually generate the Lie algebra of the Poincaré group.

Projection orthogonal to P is performed with help of the tensor $\Pi^\mu_\nu = \delta^\mu_\nu - P^\mu P_\nu / P^2$. As in Ref. 12, we define

$$Z = z^2 P^2 - (z \cdot P)^2. \tag{1.7}$$

The superscript (0), like for instance in $V^{(0)}$, refers to the isolated system (no curvature involved).

Throughout this paper, *symmetric operators will be referred to as Hermitian*. Isometry always refers to the Riemannian metric, never to the metric of Hilbert space.

Definition: A flat metric $\overline{g}$ is said to be *isometrically admissible* with respect to g if any isometry of g is an isometry of $\overline{g}$.

II. TWO-BODY DYNAMICS IN FLAT SPACE–TIME

In order to avoid misunderstandings, the reader who is not familiar with constraint relativistic mechanics is cautioned that the field that carries mutual interaction does not explicitly appear in the system of coupled equations (1.1).

For the moment, let us postpone the question of coupling this picture to the curvature field, and consider the dynamics of an isolated two-body system in flat space–time.

One may think of two scalar particles of the same nature (like, e.g., pions undergoing electromagnetic interactions). Both constituent particles correspond to the same matter field. This field is considered in the two-body sector and interacts with some mediating field (like photon, gluon, etc.), which carries mutual interaction between the particles. Standard methods of quantum field theory allow for elimination of the mediating field. For instance, the quasipotential approach gives rise to a differential equation complemented with an extra equation, which handles the problem of relative time. Alternatively, one may use the integrodifferential Bethe–Salpeter equation (BS), which is characterized by its kernel. Of course, any term in the Lagrangian that couples the matter field with the mediating field will result in a contribution to the quasipotential equation, or equivalently a contribution to the BS kernel. So the analytic form of this kernel reflects the interaction between the matter field and the mediating field. Under reasonably general assumptions, it has been proved that the BS equation can be transformed into a pair of coupled *differential* equations of the form (1.1) (naturally approximations may be made, some diagrams may be considered as dominant, etc.; the reader is referred to Sazdjian[11] for details). In practice, any potential of the form $V^{(0)} = f(Z, P^2, y \cdot P)$ or simply $f(Z, P^2)$ is general enough to accommodate most relevant examples of interaction between scalar constituents.

We insist that our approach is self-contained within the two-body sector. Like in the BS equation, our wave function is a (c-number) scalar depending on two points of space–time. But in the absence of a mediating field, it would reduce to a superposition of products of (classical, complex) Klein–Gordon fields.

Wave equations are of the form (1.1). The couple q_1, q_2 has Cartesian coordinates q_1^α, q_2^β in $M_4 \times M_4$.

The multiplicative operators q_1, q_2 are canonically conjugate to the operators $p_1 = -i\partial/\partial q_1$, $p_2 = -i\partial/\partial q_2$. The Lie algebra of the Poincaré group has the generators $P = p_1 + p_2$, $M = q_1 \wedge p_1 + q_2 \wedge p_2$. Notice that these formulas are valid, irrespective of the mutual interaction exerted between the particles. P^α is interpreted as total momentum, since its components generate space–time translations. It is remarkable that if we define $z^\alpha = q_1^\alpha - q_2^\alpha$, this operator is invariant under translation. It is therefore natural to regard z as a relative quantity and to complete the

commuting set P^α, z^β by eight more variables in order to obtain a new set of 16 canonical variables. After this, we end up with two separate kinds of variables. In fact, the interpretation of z can be justified by a precise analysis in terms of the *physical* coordinates of the particles, provided one gets back to the level of *classical* (relativistic) mechanics, where the concept of world line still makes sense. For this purpose let us sketch the classical Hamiltonian formulation underlaying our description of two-particle systems by coupled wave equations. We follow the line of a two-time formalism, which considers the proper times as independent parameters. Phase space is a 16-dimensional symplectic space with *canonical* coordinates satisfying the standard Poisson bracket relations $\{q_a^\alpha, p_{b\beta}\} = \delta_{ab}\delta_\beta^\alpha$, etc. In terms of these canonical coordinates, the motion is governed by Hamiltonian equations of the form.

$$\frac{\partial A}{\partial \tau_a} = \{A, H_a\}, \tag{2.1}$$

where H_1, H_2 are the Hamiltonian generators and τ_1, τ_2 are proportional to the proper times (these Hamiltonians, identified as half-squared masses, should not be confused with the Dirac Hamiltonian H_{D}, which arises in the constraints approach and is numerically zero). They are mutually in involution, which ensures that equations of the form (2.1) are consistent. In fact, H_1, H_2 generate a two-parameter Abelian group. The orbits of this group are eventually identified as the Cartesian products $\Gamma_1 \times \Gamma_2$, where Γ_1 (resp., Γ_2) is the lift in phase space of the world line of particle 1 (resp., particle 2). A complication associated with the famous No-Interaction Theorem[15] is that, in general, Poincaré invariance implies that the physical positions x_1^α, x_2^β cannot be canonical. They coincide with the canonical coordinates *only* on a certain submanifold (Σ). [This point is sometimes hidden in the constraints formulation, because this alternative approach deals with a submanifold of (Σ).] The Poisson bracket $\{x_1^\alpha, x_2^\beta\}$ differs from the metric tensor $\eta^{\alpha\beta}$ (its precise value is model dependent). Throughout the whole phase space, x_1, x_2 may be complicated functions of the canonical variables. Specifying the manifold (Σ) is actually a boundary condition that achieves the definition of the system we consider. In a large class of models one assumes that the equation of (Σ) is simply $P \cdot z = 0$. It is clear that every point of (Σ) also satisfies

$$P \cdot (x_1 - x_2) = 0. \tag{2.2}$$

Provided P is time-like, this equation expresses that in the frame where $\mathbf{P}=0$ (rest frame of the system) one has $x_1^0 = x_2^0$. Therefore (Σ) is called the equal-time surface; the points located on it have equal-time coordinates in the system rest frame. Finally, the connection between z and the physical relative coordinates is as follows: *In restriction to* (Σ) *and in the rest frame*, $z^0 = 0$ and $\mathbf{z} = \mathbf{q}_1 - \mathbf{q}_2 = \mathbf{x}_1 - \mathbf{x}_2$.

We pursue the task of forming a new set of canonical coordinates by completion of P, z with conjugate quantities. Limiting ourselves to a linear transformation (from individual coordinates to the new set) we can define

$$Q = \lambda q_1 + (1-\lambda) q_2, \quad y = (1-\lambda) p_1 - \lambda p_2, \tag{2.3}$$

and we can check $\{Q^\alpha, P_\beta\} = \{z^\alpha, y_\beta\} = \delta_\beta^\alpha$, $\{Q^\alpha, Q^\beta\} = \{y^\alpha, y^\beta\} = 0$. For any choice of the positive constant $\lambda < 1$, we obtain two separate sets of canonical variables. With an obvious abuse of language, a popular terminology refers to Q, P and z, y, respectively, as center-of-mass variables and relative variables. For computational simplicity we take $\lambda = \frac{1}{2}$. Still, some explanation is necessary in order to somehow relate Q with the physical center of mass. Here we hit the delicate question of defining this concept in a covariant framework,[5,16,17] but we shall not discuss here the various definitions of relativistic center of mass. We simply propose to consider the quantities

$$\Xi = \frac{M\cdot P}{P^2} + \frac{P\cdot Q}{P^2}\,P, \tag{2.4}$$

as the space–time coordinates of the center of mass. This definition may be justified as follows:

(i) It is manifestly covariant.

(ii) Owing to the constancy of M and P, the quantities Ξ^α are the coordinates of a point that moves on a straight line when τ_1,τ_2 run from $-\infty$ to $+\infty$, and this line is parallel to P.

(iii) For the configurations taken on the equal-time surface, Ξ reduces to

$$\Xi^\alpha_\Sigma = \frac{P\cdot p_1}{P^2}\,x_1^\alpha + \frac{P\cdot p_2}{P^2}\,x_2^\alpha \tag{2.5}$$

[hint $P^2/2 \pm y\cdot P = P\cdot p_1$ (resp. $P\cdot p_2$)]. Therefore, in the rest frame (defined by P^α) the spatial component of Ξ_Σ coincides with definition (c) of Pryce[16] (average of the coordinates weighted by the energies).

(iv) One easily computes $\{(M\cdot P/P^2)^\alpha, P^\beta\} = \Pi^{\alpha\beta}$ and $\{T, P^\beta\} = P^\beta/P^2$, whence we derive equations of motion in single-particle form,

$$\{\Xi^\alpha, P^\beta\} = \eta^{\alpha\beta}, \quad \left\{\Xi^\alpha, \frac{P^2}{2}\right\} = P^\alpha, \quad P^\alpha = \text{const.} \tag{2.6}$$

However, the components of Ξ have nonvanishing Poisson brackets among themselves and cannot be taken as canonical coordinates. This is reminiscent of definition (c) in Pryce,[16] and agrees with a remark made by Llosa.[17]

In the rest frame and at equal times, the spatial piece of Ξ finally reduces to the object that is called ''center of energy'' by Feshman *et al.*,[3] and agrees with the definition of Lightman and Lee,[18] in the classical limit. Finally, it is easy to see how Ξ differs from Q, if we notice that Ξ can be equivalently written as

$$\Xi = Q + \left(\frac{y\cdot P}{P^2}\right) z + \left(\frac{z\cdot P}{P^2}\right) y. \tag{2.7}$$

The second term on the right-hand side expresses that Ξ involves a weighted average: this term vanishes in the case of equal masses (then $P\cdot p_1 = P\cdot p_2$). The last term on the right-hand side vanishes at equal times.

Ξ^α has four components, but the contraction $\Xi\cdot P$ is identical with $Q\cdot P$ and is trivially related to the proper time of the center of mass.

Still, we must remember that this picture is limited to isolated systems. In the presence of external fields, we naturally retain the interpretation that P is the total momentum, but it is not constant anymore. Moreover, the use of the surface $P\cdot z = 0$ for a boundary condition in this case is probably questionable, and no reasonable modification of it, adapted to the external field, is known for the moment. As a result, the relationship between z^α and $x_1^\alpha - x_2^\alpha$ is not anymore well defined when external coupling is turned on.

Also, it remains an open problem as to know how Eq. (2.6) are modified and whether they keep a single-particle form, in the presence of curvature. A similar question was earlier discussed in Refs. 3 and 18, but substantial differences existing between their formulation and ours make it difficult to transpose their conclusions.

Nevertheless, the variables Q, P, z, y introduced by (1.4), (1.5) remain canonical whatsoever and they split anyway into two separate groups. In the presence of an external field, like, for instance, gravity, their labeling as ''center-of-mass variables'' and ''relative variables'' is a manifest abuse of language, and should be avoided in a rigorous terminology.

Still, they provide a powerful tool in order to organize tractable calculations (see Ref. 12).

III. GENERAL FRAMEWORK

We now turn to the case where curvature is present (no other external force is being considered).

A. Compatibility

The wave equations have the form (1.1). We naturally require the strong condition (1.3), which ensures compatibility. Assuming that $V_1=V_2=V$, condition (1.3) reduces to

$$[K_1-K_2,V]=0. \tag{3.1}$$

B. Hermiticity

In order to have a consistent mathematical setting, the squared-mass operators on the left-hand side of (1.1) (and eventually the generators of transformations induced by space–time symmetries, if any) must be considered as acting in some well-defined Hilbert space; this remains true even if the wave function cannot actually belong to this Hilbert space.

Therefore we shall naturally assume that H_1,H_2 are operators in

$$L^2(\mathbf{R}^8)=L^2(\mathbf{R}^8,\sqrt{|g(1)|}\sqrt{|g(2)|}d^4q_1\ d^4q_2).$$

Here the following observation is in order. In the absence of mutual interaction we can write (1.1) in the form of independent Klein–Gordon equations,

$$2K_a\Psi=m_a^2\Psi, \tag{3.2}$$

where $2K_a$ is the Laplace Beltrami operator in terms of the coordinates of particle a. It is well known[19] that this operator is Hermitian when considered as acting in $L_a^2=L^2(\mathbf{R}^4,\sqrt{|g(a)|}d^4q_a)$, thus K_1 and K_2, extended as operators acting in $L^2(\mathbf{R}^8)=L_1^2\otimes L_2^2$ are both Hermitian. Despite the fact that the four-fold integrals defining L_1^2 and L_2^2 have no direct physical interpretation, this property of hermiticity is very fortunate from a formal point of view. Already in special relativity, it has been demonstrated that off-shell Hilbert spaces of the form $L^2(\mathbf{R}^4)$ or $L^2(\mathbf{R}^8)$ provide the most convenient framework for handling Feynmann's propagators in a manifestly covariant way [for instance, $1/(p^2+U-m^2\pm i\epsilon)$, where U is an external potential, naturally makes sense as the resolvent of an operator in $L^2(\mathbf{R}^4,d^4q)$, and similar observations can be made when interparticle interaction is considered[20]]. We extend this philosophy to curved space–time and require hermiticity as well in the presence of mutual interactions.

In other words, we demand that H_1,H_2 are Hermitian operators in the Hilbert space $L^2(\mathbf{R}^8)$.

At a deeper level of accuracy one would raise the question of self-adjointness, in connection with the possibility of developing a manifestly covariant scattering theory in terms of scalar evolution parameters. Indeed, there are two possibilities in relativistic dynamics.

(For simplicity of the present argument, let us provisionally consider the case of a single particle.) The most popular point of view consists in using the time coordinate as an indicator of evolution (say q^0 in some coordinate system); then the Klein–Gordon equation is interpreted as the relativistic generalization of the time-depending Schrödinger equation.

Another approach, in the spirit of Schwinger's ''proper time method''[21] assigns this role to a scalar parameter, which coincides with proper time (or a suitable generalization of it) in the classical limit $\hbar\to 0$; now the Klein–Gordon equation is a mass-shell reduction of the Stückelberg equation,[22] and the D'Alembert operator is trivially proportional to the generator of the motion. In this case, self-adjointness of the D'Alembert operator with respect to the *four-space* scalar product (involving integration over d^4q) would be a precious information in order to set up a complete quantum theory.

Although we have a preference for the latter point of view (which has been extended to many-body systems[20,23]), we shall not discuss further the evolutive aspects of the wave equations.

Returning to the problem of two-body quantum mechanics in curved space–time, we shall be contented, in this first attempt, with the property of hermiticity (symmetry) and leave the question of self-adjointness for future investigations (notice that even in the one-body case, self-adjointness in the four-space scalar product has received so far very little attention, if any).

C. Coupling separability

The above conditions are not yet sufficient from a physical point of view. Indeed, one expects to find the *correct limits when either the curvature or the mutual interaction is absent*.

When the curvature identically vanishes, one should recover an isolated system of particles interacting in Minkowski space–time.

When the mutual interaction is zero, the wave equations should describe independent particles, each one being free in curved space–time (in other words, submitted only to the curvature field associated with the metric).

These situations will be referred to as the *no-field limit* and the *independent-particles limit*, respectively.

As simple as it might seem, the formulation of correct limits is problematic in curved space–time. First of all, *the notion of an isolated system is generally ambiguous*. Strictly speaking, the absence of curvature does not correspond to a well-specified Minkowski space.

But, in practice, there are cases where this difficulty can be bypassed.

(i) One may consider a particular solution of the Einstein equations. This solution necessarily depends on the Newton constant, and we obtain a flat metric if we replace this constant by zero.

(ii) Particular symmetries may select a flat metric in a natural way (asymptotically flat space–times, plane waves, etc.). Another example: $ds^2=dt^2-d\sigma^2$, where $d\sigma^2$ enjoys spherical symmetry (but not more).

Besides this problem about the unicity of a flat background, additional care is needed because the most natural flat background and the Riemannian metric do not define the same Hilbert space. Indeed, the quotient $\overline{g/g}$ of scalar densities is a scalar, and, in general, it is not a constant (the case of a plane wave, in the weak field approximation and TT gauge, is an exception). One might be tempted to consider only flat metrics satisfying $\overline{g/g}=$const. as eligible for a flat background. But generally, this procedure does not respect the symmetries of the pseudo-Riemannian metric $g_{\mu\nu}$. Indeed, it may happen that none of the background metrics selected in this manner is isometrically admissible.

Fortunately, the technical complication of having distinct Hilbert spaces will be easily handled by a change of wave function that amounts to reformulating the wave equations in terms of a new wave function $\tilde{\Psi}$, an (improper) element of

$$\overline{L^2}(\mathbf{R}^8)=L^2(\mathbf{R}^8,\sqrt{\overline{g(1)}\,\overline{g(2)}}d^4q_1\,d^4q_2),$$

and in terms of modified operators that are Hermitian (symmetric) in this new Hilbert space. This approach can be considered as a change of representation, performed with the help of a unitary transformation from L^2 to $\overline{L^2}$. This method allows for application of flat-space techniques: Cartesian coordinates, etc.

D. Isometric invariance

It may happen that space–time admits some isometries. If we first consider the motion of a single test particle, each isometry of space–time is associated with a conserved quantity: its generator.

A natural generalization of flat-space theory consists in requiring that the generators of these isometries must be constants of the two-body motion, even in the presence of a mutual interaction.

Whereas an *isolated system* in Minkowski space is characterized by Poincaré symmetry (Poincaré invariance from the active point of view), *it is natural to require that an isolated system in curved space–time be at least invariant under the infinitesimal unitary transformations associated with space–time isometries*. This should hold true as well for two-body as for one-body systems, and also when the constituent particles undergo mutual interaction. For this aim it is not sufficient that the interaction term be Poincaré invariant in its no-field limit, say $V^{(0)}$. Indeed, this term is modified by the presence of curvature (namely $V \neq V^{(0)}$) in order to keep compatibility satisfied.

The question of whether this condition is sufficient goes beyond the scope of this paper (when space–time has no isometry at all, this condition becomes empty; is it still possible to define isolated systems?).

Remark: When we perform a change of wave function, some unitary transformation of the whole picture is necessary. This transformation maps $L^2(\mathbf{R}^8)$ either onto itself or onto a different Hilbert space, and obviously keeps the compatibility conditions satisfied. When identifying the no-field and independent-particle limits, one must take this change of representation into account. For instance, after transformation (4.5) below, the independent-particle limit is characterized by the half-squared-mass operators $\tilde{K}_1, \tilde{K}_2$, which are Hermitian in $L^2(\mathbf{R}^8)$. We first recall a few results of Riemannian geometry (see the Appendix).

If ξ generates infinitesimal isometries of g, then, in the standard notation of differential geometry the Lie derivative operator satisfies $\mathscr{L}_\xi \Delta = \Delta \mathscr{L}_\xi$. When f is a 0-form, that is a scalar function, we simply have $\mathscr{L}_\xi f = \xi^\alpha \partial_\alpha f$. Moreover, $\xi^\alpha \partial_\alpha$ is skew symmetric with respect to the scalar product that defines $L^2(\mathbf{R}^4)$.

Isometries are implemented as quantum operators in the following way. With any vector field ξ^α leaving $g_{\mu\nu}$ invariant, we associate the operator $X = -i\xi^\mu \partial_\mu$ acting in $L^2(\mathbf{R}^4, d^4q)$. It is clear that X is Hermitian.

In the two-body sector ones deal with $L^2(\mathbf{R}^8) = L_1 \otimes L_2$. The isometric vector ξ^α induces the operators

$$J_1 = -i\xi^\alpha(1)\partial_{1\alpha}, \quad J_2 = -i\xi^\alpha(2)\partial_{2\alpha}, \tag{3.3}$$

respectively acting in L_1, L_2. Then J_1, J_2 are extended to $L^2(\mathbf{R}^8)$ as $J_1 \otimes 1$ and $1 \otimes J_2$, respectively. Considered as operators in $L^2(\mathbf{R}^8)$, they are the *individual isometries* (for instance, in the limit of free motion in flat space–time, linear and angular momenta of each particle are trivial examples of individual isometries). Finally, the *total isometry* induced by ξ^μ is $J = J_1 + J_2$.

IV. THE ONE-BODY PROBLEM

In the Klein–Gordon equation $2K\psi = m^2\psi$, the D'Alembert symbol is replaced by the Laplace–Beltrami operator. In other words,

$$-2K\psi = \frac{1}{\sqrt{|g|}} \partial_\mu (\sqrt{|g|} g^{\mu\nu} \partial_\nu \psi).$$

K transforms as a scalar and is Hermitian[19] in the space $L^2(\mathbf{R}^4, \sqrt{|g|} d^4q)$. Moreover, if the contravariant vector field $\xi^\mu(q)$ is the infinitesimal generator of a one-parameter group of transformations leaving g invariant, then a *classical* constant of geodesic motion is the function $\xi^\mu \pi_\mu$, a scalar on the cotangent bundle $T^*(M_4)$ endowed with coordinates q^α, π_β and with the standard Poisson brackets.

Its quantum counterpart is the differential operator $X = -i\xi^\mu \partial_\mu$.

But the partial differentiation operator ∂_μ present in the above expression of $K\psi$ is neither a vector nor Hermitian in the sense of Hilbert space L^2.

Nevertheless, if we now introduce any flat metric $\overline{g_{\mu\nu}}$, then the operator defined as $p_\mu = -i\partial_\mu$ in the Cartesian coordinates associated with $\overline{g}$ does transform as a vector and is Hermitian in the space $\overline{L^2}(\mathbf{R}^4) = L^2(\mathbf{R}^4, \sqrt{|\overline{g}|}d^4q)$ endowed with the scalar product

$$\langle \chi, \omega \rangle = \int \chi^* \omega \sqrt{|\overline{g}|} d^4q. \tag{4.1}$$

Moreover, we have $X = \xi \cdot p$.

Using Cartesian coordinates makes it trivial to check that we can write

$$2K = \frac{1}{\sqrt{|g|}} p_\mu \sqrt{|g|} g^{\mu\nu} p_\nu. \tag{4.2}$$

This situation suggests a change of wave function, say

$$\widetilde{\psi} = \Gamma \psi,$$

where the ''bimetric'' scalar Γ is

$$\Gamma = |g/\overline{g}|^{1/4}, \tag{4.3}$$

that is to say, $\sqrt{|g|} = \Gamma^2 \sqrt{|\overline{g}|}$. The Klein–Gordon equation can now be written as

$$2\widetilde{K}\widetilde{\psi} = m^2 \widetilde{\psi}, \tag{4.4}$$

where, for all operator A,

$$\widetilde{A} = \Gamma A \Gamma^{-1}. \tag{4.5}$$

In this formula Γ is understood as a multiplicative operator acting on functions $f(q)$. Notice that $\widetilde{K}$ is Hermitian in $\underline{L^2}$, we say flat Hermitian. Equation (4.3) is a unitary transformation from $L^2(\mathbf{R}^4, \sqrt{|g|}d^4q)$ to $\underline{L^2}(\mathbf{R}^4)$. The multiplicative operator Γ (and, more generally, any function of q) is Hermitian in both $L^2(\mathbf{R}^4)$ and $L^2(\mathbf{R}^4)$.

Applying rule (4.5) to Eq. (4.1), we immediately find

$$2\widetilde{K} = \Gamma^{-1} p_\mu \Gamma g^{\mu\nu} \Gamma p_\nu \Gamma^{-1}, \tag{4.6}$$

which is manifestly flat Hermitian. We define an *effective* external potential F by setting

$$\widetilde{K} = \tfrac{1}{2}p^2 + F. \tag{4.7}$$

From its very definition, F is flat Hermitian. So finally, both $\widetilde{K}$ and F are Hermitian in $\overline{L^2}$.

Notice that we could write F down in closed form, by elementary commutator algebra, starting from (4.6) and splitting the contravariant metric tensor as $g^{\mu\nu} = \overline{g^{\mu\nu}} + h^{\mu\nu}$. Of course, the contravariant components of $\overline{g}$ reduce to $\eta^{\mu\nu} = \mathrm{diag}(1,-1,-1,-1)$ in Cartesian coordinates.

Let us now consider the behavior of infinitesimal isometries.

If ξ generates infinitesimal isometries of $g_{\mu\nu}$, it follows that $\xi^\alpha \partial_\alpha$ commutes with K [both being considered as operators in $L^2(\mathbf{R}^4)$]. After introduction of an auxiliary flat metric $\overline{g}$, we can write $X = -i\xi^\alpha \partial_\alpha = \xi \cdot p$ and $[\xi \cdot p, K] = 0$, where $\xi \cdot p$ and K are Hermitian in $L^2(\mathbf{R}^4)$.
Henceforth we assume that $\overline{g}$ is isometrically admissible.

Proposition 1: Assume that ξ is an isometry of both g and $\overline{g}$. Then transformation (4.5) leaves $X = \xi \cdot p$ unchanged, so $\widetilde{X} = X$. In other words, in the Poincaré Lie algebra associated with the flat

metric, any element that leaves also g invariant is unchanged by transformation (4.5). *Moreover,* $\tilde{K}$ *as well as* K *commutes with* X*, and* X *is Hermitian in both* L^2 *and* $\overline{L^2}$.

Proof: ξ being isometry of g and $\overline{g}$ implies that the Lie derivative of the bimetric scalar vanishes, say $\xi^\alpha \partial_\alpha \Gamma = 0$, thus the multiplicative operator Γ satisfies $[\xi\cdot p, \Gamma] = 0$. We have seen that $\xi^\alpha \partial_\alpha$ commutes with the Laplace Beltrami operator Δ. After transformation (4.5) we get $[\tilde{K}, \xi\cdot p] = 0$. We have already proved that $\xi\cdot p$ is Hermitian in L^2. But according to our assumption, there exist, *in Cartesian coordinates*, a constant vector C^α and a skew-symmetric tensor $C^{\alpha\beta}$, such that

$$X = \xi^\alpha p_\alpha = C^\alpha p_\alpha + C^{\alpha\beta} m_{\alpha\beta}. \tag{4.8}$$

In this form, it is manifest that $\xi\cdot p$ is Hermitian also in the sense of $\overline{L^2}$.

Corollary 2: If $\mathscr{L}_\xi g = \mathscr{L}_\xi \overline{g}$ *then* $[\xi\cdot p, F] = 0$. This is now obvious from Eq. (4.7) and shows the importance of having $\overline{g}$ isometrically admissible.

Example: We now consider a line element of the simple form,

$$ds^2 = d(q^0)^2 - R^2(r)\, d\mathbf{q}^2, \tag{4.9}$$

where $d\mathbf{q}^2$ is a shorthand notation for $\delta_{ij}\, dq^i\, dq^j$ and r is $\sqrt{\mathbf{q}^2}$. This metric defines a particular case of static orthogonal space–time. We assume that R is everywhere finite and differentiable as many times as necessary. Space sections are supposed to be isotropic but *not* homogeneous. They have a unique center of spherical symmetry; thus the form (4.9) of the metric is unique up to a change,

$$q'^k = \Lambda q^k, \quad R' = \Lambda^{-1} R,$$

but we fix the space coordinates by requiring that $R(\mathbf{q}=0) = 1$.

Our assumptions imply that

$$R^2 \neq \frac{\text{const}}{(1 + \frac{1}{4} k r^2)^2}.$$

This restriction excludes the particular case of an Einstein static space–time.

A preferred background metric is, of course, $d\overline{s^2} = d(q^0)^2 - d\mathbf{q}^2$.

Notice that the metrics $g_{\mu\nu}$ and $\overline{g_{\mu\nu}}$ coincide on the line $q^k = 0$, world line of the center of spherical symmetry.

Both metrics are invariant under time translation and space rotations, and $g_{\mu\nu}$ has no further symmetry. Each generator of these isometries (considered as a Hermitian operator in L^2) commutes with K.

Alternatively, when the state of the particle is represented by $\tilde{\psi}$ and its motion described by Eq. (4.4), the infinitesimal rotations and the time translation keep being represented by the same operators m_{ij}, p_0. Because Γ in (4.5) is rotational invariant, and does not depend on time, these operators are not affected by (4.5) and are Hermitian in both Hilbert spaces $L^2(\mathbf{R}^4)$ and $\overline{L^2}(\mathbf{R}^4)$.

According to this particular form of g and $\overline{g}$, p_0 and m_{ij} are unchanged by (4.5). In other words, $\tilde{p}_0 = p_0$ and $\tilde{m}_{ij} = m_{ij}$.

It is clear that $d\overline{s^2}$ defines $\overline{g_{\mu\nu}}$ as an isometrically admissible background metric. In the present example, Eq. (4.8) is satisfied with $C^\alpha = (1,0,0,0)$ and $C^{\alpha\beta}$ reduces to C^{jk}.

Now our claim is that, owing to the assumptions made on the line element (4.9), both $[F, p_0]$ and $[F, q^0]$ vanish. According to the terminology introduced in a previous work,[12] we formulate this statement as follows.

Proposition 3: Owing to the form (4.9) of the metric $g_{\mu\nu}$*, the effective potential* F *defined by (4.7) is strongly invariant by time translation.*

Proof: Commutation with p_0 is straightforward. Indeed Γ only depends on **q**, thus $[\Gamma,p_0]=0$; for a similar reason $[g^{\mu\nu},p_0]=0$, and obviously p_μ commutes with p_0.

According to (4.7), in order to prove that also $[F,q^0]$ vanishes it will be sufficient to prove that $[2\widetilde{K},q^0]$ coincides with $[p^2,q^0]$.

We observe that

$$[p^2,q^0]=-2ip_0.$$

Using (4.6) we easily compute

$$[2\widetilde{K},q^0]=-ig^{0\nu}\Gamma p_\nu\Gamma^{-1}-i\Gamma^{-1}p_\mu\Gamma g^{\mu 0}.$$

But g^{0j} is zero, thus only g^{00} survives. We are left with

$$2[\widetilde{K},q^0]=-i\Gamma p_0\Gamma^{-1}-i\Gamma^{-1}p_0\Gamma,$$

where $[\Gamma,p_0]$ vanishes, thus finally $2[\widetilde{K},p_0]=-2ip_0$, which completes the proof of our statement.

Loosely speaking, F depends only on **q** and **p**; we say that it is purely transverse.

Proposition 4: Owing to the form (4.9) of the metric, the effective potential F is (simply) invariant by space rotations.

Proof: From Proposition 1 we know that K and $\widetilde{K}$ commute with X, in particular, when $X=C^{ij}m_{ij}$. Obviously, p^2 is invariant under space rotations. Finally, a glance at (4.7) ensures rotation invariance of F.

V. THE TWO-BODY PROBLEM

Assuming the unipotential simplification, we write

$$H_a=K_a+V. \tag{5.1}$$

Our problem reduces to the determination of V by solving (3.1). Insofar as we consider gravity as an external field applied to the system, a natural approach consists in determining V by its no-field limit, say $V^{(0)}$. Indeed, in the absence of gravity, the most general form of $V^{(0)}$ allowing for compatibility and Poincaré invariance is well known.[6] As mentioned in Sec. II, a potential of the form $V^{(0)}=f(Z,P^2,y\cdot P)$ is general enough for our purpose.

Some care is needed, however, because, in general, for an arbitrarily specified metric $g_{\mu\nu}$, the no-field limit has no intrinsic meaning.

Anyway, this point of view requires introduction of an auxiliary flat metric $\overline{g_{\mu\nu}}$, and leads to the following developments.

Define $\Gamma_a=|g(a)/\overline{g(a)}|^{1/4}$ and $\Gamma_1\Gamma_2=\Gamma_{12}$.

Since $L^2(\mathbf{R}^8,\sqrt{g_1g_2}d^4q_1,d^4q_2)=L^2(\mathbf{R}^4,\sqrt{|g(1)|}d^4q_1)\otimes L^2(\mathbf{R}^4,\sqrt{|g(2)|}d^4q_2)$, there is no confusion if now $\widetilde{A}$ denotes the product $\Gamma_{12}A\Gamma_{12}^{-1}$ for all A acting in $L^2(\mathbf{R}^8)$. Indeed, when A is a product A_1A_2 of operators acting in $L^2(1)$ and $L^2(2)$, respectively, we can check that $\widetilde{A}=\widetilde{A}_1\widetilde{A}_2$.

The lack of Poincaré symmetry is partially redeemed by considering the operators induced in $\overline{L^2}(\mathbf{R}^8)$ by the isometries of g. Let the contravariant vector field ξ generate a one-parameter group of isometries of space–time. In Sec. III D we have introduced the operators J_1,J_2, respectively, acting in $L^2(\mathbf{R}^4\sqrt{|g(1)|},d^4q_1)$ and in $L^2(\mathbf{R}^4\sqrt{|g(2)|},d^4q_2)$. Their extension to $L^2(\mathbf{R}^8)$ is straightforward.

In the presence of an auxiliary flat metric we can write $J_1=\xi(1)\cdot p_1$, $J_2=\xi(2)\cdot p_2$. Provided the auxiliary metric $\overline{g}$ is isometrically admissible, we apply Proposition 1 and obtain

$$J_1=C\cdot p_1+C^{\mu\nu}m_{1\mu\nu}, \tag{5.2}$$

$$J_2 = C \cdot p_2 + C^{\mu\nu} m_{2\mu\nu}, \tag{5.3}$$

for some constant vector C^α and tensor $C^{\mu\nu}$.

Now consider the *total isometry* induced by ξ, say $J = J_1 + J_2$. Proposition 1 implies that $\tilde{J}_a = J_a$, hence $\tilde{J} = J$.

From the properties of the motion in the absence of mutual interaction, or equivalently from Proposition 1 extended by the tensor product, we obtain

$$[K_a, J_b] = [\tilde{K}_a, J_b] = 0, \quad a,b = 1,2. \tag{5.4}$$

It is clear that

$$J = C \cdot P + C^{\alpha\beta} M_{\alpha\beta}. \tag{5.5}$$

Existence of nonvanishing coefficients $C^\alpha, C^{\mu\nu}$ ensures that some elements of the Poincaré algebra survive as symmetries of the motion in the presence of curvature.

Axiom (D) of Sec. III (isometric invariance) can be precisely understood as follows: For all isometry-generating vector field ξ, the corresponding operator of total isometry J must be a constant of the two-body motion.

Later on, we shall apply the above formula in order to check that this condition is actually satisfied by two-body motion in the particular space–time (4.9).

Let us now turn to the problem of compatibility. Condition (3.1) is transformed into

$$[\tilde{K}_1 - \tilde{K}_2, \tilde{V}] = 0. \tag{5.6}$$

In view of (4.7) we define effective external potentials $F_a = F(q_a, p_a)$ by the formulas

$$\tilde{K}_a = \tfrac{1}{2} p_a^2 + F_a. \tag{5.7}$$

It is clear that $\tilde{K}_a$ and F_b are Hermitian in $\overline{L^2}(\mathbf{R}^8)$.

Example: In general, the decomposition (5.7) would have no intrinsic significance (assuming that we rely on General Relativity as the true theory of gravity). But we shall now specialize to the particular case of the line element (4.9). The assumptions made about the function $R^2(r)$ ensure without ambiguity a preferred flat background.

For the metric (4.9) we have seen that C has components (1,0,0,0) and C reduces to its space-by-space components. Any isometry of $g_{\mu\nu}$ satisfies

$$J = C^0 P_0 + C^{ij} M_{ij}. \tag{5.8}$$

Extension of Propositions 3 and 4 to the two-body sector is straightforward and implies that the effective potentials F_1, F_2 are strongly invariant under time translations, and simply invariant by space rotations.

As a result, compatibility can now be solved by a flat-space technique, using the Bijtebier ansatz.[11] Closed form expressions will be written at the price of a change of representation. The *external-field representation* is formally given by

$$A' = e^{iB} A e^{-iB}, \quad \forall A, \tag{5.9}$$

where $B = TL$ and

$$T = y_T \cdot P_T + F_1 - F_2, \tag{5.10}$$

$$L = L_\alpha z^\alpha, \quad L_\alpha = \frac{P_L^\alpha}{P_L^2}. \tag{5.11}$$

In order to keep contact with a generalized formulation of this method we use our notation of Ref. 12. The space of four-vectors is decomposed along longitudinal and transverse directions. Each four-vector has a unique transverse (resp., longitudinal) part. Subscripts T and L refer to this splitting.

But here, like in Ref. 11, the longitudinal part has only the time component. Longitudinal canonical variables commute with the transverse ones, F_1, F_2 depend only on transverse variables and $[T,L]=0$.

The wave equations will be now written as

$$2\widetilde{H}'_a\widetilde{\Psi}' = m_a^2\widetilde{\Psi}', \tag{5.12}$$

where $\widetilde{H}'_a = \widetilde{K}'_a + \widetilde{V}'$. In order to avoid cumbersome notation we systematically write $\widetilde{K}'$ for $(\widetilde{K})'$, etc. One must keep in mind that

$$\widetilde{\Psi}' = e^{iB}\Gamma\Psi, \quad \widetilde{H}'_a = e^{iB}\Gamma H_a \Gamma^{-1} e^{-iB}, \tag{5.13}$$

and so on.

In the present notation, (5.7) can be identified as (2.7) of Ref. 12, where K_a and G_a have been replaced by $\widetilde{K}_a$ and F_a, respectively. Along this line $\widetilde{K}'_a$ can be explicitly computed; see Eqs. (3.36) of Ref. 12, or Eqs. (2.24) and (2.25) of Ref. 14. One finds

$$\widetilde{K}'_a = \widetilde{K}_a - T(L\cdot y \pm \tfrac{1}{2}) + \tfrac{1}{2}T^2 L\cdot L, \tag{5.14}$$

with $+1$ (resp., -1) for $a=1$ (resp., $a=2$). Hence, using the identity $p_1^2+p_2^2 = \frac{1}{2}P^2 + 2y^2$, we get

$$\widetilde{K}'_1 + \widetilde{K}'_2 = \frac{P^2}{4} + y^2 + F_1 + F_2 - 2T(L\cdot y) + T^2 L\cdot L, \tag{5.15}$$

$$\widetilde{K}'_1 - \widetilde{K}'_2 = y_L \cdot P_L. \tag{5.16}$$

In fact, B was tailored in order to obtain (5.16). Now define

$$\mu = \tfrac{1}{2}(m_1^2 + m_2^2), \quad \nu = \tfrac{1}{2}(m_1^2 - m_2^2),$$

and replace the wave equations by their sum and difference. We get

$$(\widetilde{H}'_1 + \widetilde{H}'_2)\widetilde{\Psi}' = \mu\widetilde{\Psi}', \tag{5.17}$$

$$(\widetilde{H}'_1 - \widetilde{H}'_2)\widetilde{\Psi}' = \nu\widetilde{\Psi}'. \tag{5.18}$$

According to the assumptions made about the metric, there is a unique ''laboratory frame.'' Transverse and longitudinal decomposition simply refers to space and time splitting, thus B takes on the form given by Bijtebier in Ref. 11. In other words,

$$L\cdot L = \frac{1}{P_0^2}, \quad L\cdot y = \frac{y_0}{P_0}, \quad y_L\cdot P_L = y^0\cdot P^0, \tag{5.19}$$

$$T = -\mathbf{y}\cdot\mathbf{P} + F_1 - F_2, \quad L = \frac{z^0}{P^0}. \tag{5.20}$$

These expressions are inserted into (5.15) and (5.16), and one makes the ansatz

$$\widetilde{V}' = f(\hat{Z}, P^2, y^0 P^0), \tag{5.21}$$

$$\hat{Z} = -\mathbf{z}^2 P^2 - (\mathbf{z}\cdot\mathbf{P})^2. \tag{5.22}$$

We finally obtain

$$\widetilde{H}_1' + \widetilde{H}_2' = \frac{P^2}{4} + y^2 + F_1 + F_2 - 2T\,\frac{y_0}{P_0} + \frac{T^2}{P_0^2} + f(\hat{Z}, P^2, y^0 P^0), \tag{5.23}$$

whereas the difference of squared mass operators is simply

$$\widetilde{H}_1' - \widetilde{H}_2' = y_0 P_0 . \tag{5.24}$$

In these formulas T is simply $F_1 - F_2 - \mathbf{y}\cdot\mathbf{P}$ and F_1, F_2 are given by (5.7).

At this stage, *invariance under time translation and space rotations is manifest, which demonstrates, according to (5.8), that axiom D of Sec. III is actually satisfied*.

Since P_0 and $y_0 P_0$ are constants of the motion, the wave equations (5.17) and (5.18) undergo a reduction. The dependence on the ''relative time'' is factorized out by diagonalization of these quantities. If E is eigenvalue of P^0, we write

$$\widetilde{\Psi}'(z, Q) = \exp\, i\left(EQ^0 + \frac{\nu}{E}\, z^0 \right) \Phi(\mathbf{z}, \mathbf{Q}). \tag{5.25}$$

We are left with six degrees of freedom.

Remark: The line followed from Eq. (5.10) to Eqs. (5.15) and (5.24) was the most natural from a heuristic or pedagogic point of view. Let us, however, stress that the possibility of explicitly computing operators of the form $e^{iB} A e^{-B}$ without question about the self-adjointness of B is essentially founded on the fact that a multiple commutator,

$$[B^{[n]}, A] = [B[B \cdots [B, A] \cdots]],$$

vanishes for some finite integer n. Beside the case of squared-mass operators, a trivial example is given by P_0 and M_{ij}. Obviously, P_0' and M_{ij}' exist and simply $P_0' = P_0$, $M_{ij}' = M_{ij}$. It stems from (5.8) that J' exists and $J' = J$. But we have previously seen that $\widetilde{J} = J$, thus finally $\widetilde{J}' = J$. So the Lie algebra generated by the isometries of $g_{\mu\nu}$ is kept unchanged under transformations $A \to \widetilde{A} \to \widetilde{A}'$.

In our present knowledge, there is no evidence that B is essentially self-adjoint on some dense domain in $L^2(\mathbf{R}^8)$. This difficulty is not specific of a curvature field. We have already pointed it out, in the case where the external field is electromagnetic. In the present state of the art, we cannot discard the possibility that A' may not exist or may be ambiguously defined, *when A is an operator other than those we explicitly consider here*.

For instance, can we actually transform the generator of a Lorentz rotation mixing space and time? Fortunately we are not concerned with such an operator because it does not leave the metric (4.9) invariant and therefore is not a symmetry of our system.

All we need is to represent the pieces of Poincaré algebra that survive the application of a curvature field. And, in fact, the Lie algebra generated by H_1, H_2 and the total isometries of $g_{\mu\nu}$ is respected by the transformation (5.9).

Notice that $\widetilde{P}_0 = P_0$ and if $M = (q \wedge p)_1 + (q \wedge p)_2$ then $\widetilde{M}_{ij} = M_{ij}$.

In view of these considerations, a rigorous exposition should start with (5.17) and (5.18) from the outset, $\widetilde{H}_1'$ and $\widetilde{H}_2'$ being given by (5.23) and (5.24). Then checking that $\widetilde{H}_1'$ and $\widetilde{H}_2'$ commute

to each other is a mere exercise. In this approach we postulate the wave equation in the form (5.12). The squared mass operators are explicitly given by application of (5.23) and (5.24).

For the sake of the principles formulated in Sec. III, we may observe that it is always possible to construct a representation in terms of operators acting in L^2, making the change of wave function $\hat{\Psi}=\Gamma^{-1}\widetilde{\Psi}'$ and the operator transformation $\hat{H}_a = \Gamma^{-1}\widetilde{H}'_a\Gamma$, which maps $\overline{L^2}$ back onto L^2. (Beware that $[\Gamma, B]$ does not vanish. H does not coincide with $\hat{H}$.) But only the external-field representation is tractable.

A. No-field limit

In the absence of curvature, B does not vanish, but it reduces to

$$b=(y_T\cdot P_T)L=-\mathbf{y}\cdot\mathbf{P}\,\frac{z^0}{P^0},$$

which has been proved to be essentially self-adjoint in some dense domain of $\overline{L^2}$.[14] Thus, all operators of the form $e^{ib}Ae^{-ib}$ are well defined and the no-field limit of the external-field representation is unitarily equivalent to the customary representation describing two interacting particles in flat space–time.

However, the no-field limits of $\widetilde{H}'_1,\widetilde{H}'_2$, say $\widetilde{H}'^{(0)}_1,\widetilde{H}'^{(0)}_2$ do not show up the familiar form one usually encounters for a two-body system isolated in Minkowski space. In particular, their Poincaré invariance arises ''in disguise,'' owing to the fact that the generators of (flat) space–time displacements are not represented in the conventional fashion.

But one may easily revert to the primitive representation by the transformation

$$H^{(0)}_a=\Gamma^{-1}e^{-ib}\widetilde{H}'^{(0)}_a e^{ib}\Gamma.$$

This peculiarity is not characteristic of gravity. It already occurs when one turns off an external field in special relativity.[11,14]

B. Independent-particle limit

The case of two independent particles moving in curved space–time without mutual interaction is more tricky.

The wave equations of the external-field representation are given in terms of $\widetilde{K}'_1,\widetilde{K}'_2$.

But there is no rigorous evidence that these operators be unitarily equivalent to $\widetilde{K}_1,\widetilde{K}_2$. However, the important structure here is the Lie algebra generated by K_1,K_2 and the *individual isometries* of the form $J_1=-i\xi^\alpha\partial_{1\alpha}$, $J_2=-i\xi^\alpha\partial_{2\alpha}$. We wish to stress that in (5.9) the transformed version of all the individual isometries is well-defined. In fact, J_1,J_2 commute with Γ_{12} and with B, thus they keep their form unchanged under the transformations generated by these operators.

Finally, the commutation relations among $\widetilde{K}_1$, $\widetilde{K}_2$, P^0, M_{ij} are not altered when going over to $\widetilde{K}'_1$, $\widetilde{K}'_2$, P^0, M_{ij}.

VI. CONCLUSION

The equations of motion proposed here fully take into account the two-body structure of the system. Hence, some questions raised by Fishbach *et al.* are answered. The way we separate canonical variables in two sets was mainly motivated by computational simplicity. Insofar as the contact with noncovariant theories can be made explicit, our choice turns out to be more in the spirit of a ''center of energy'' according to Ref. 3 rather than of a center of mass in the sense of Krajcik and Foldy. More precisely, our canonical variable Q is simply related with Ξ through Eq.

(2.7). Then the spatial part of Ξ can be identified with the ''center of energy'' evoked by Fischer *et al.*,[3] following Ref. 18. After this reduction is made, the contact with the definition of Ref. 5 can be obtained like in Ref. 3.

In principle, our equations of motion could permit us to formulate as well the scattering of a bound state *by* the gravitational field (with some reservations about the intrinsic meaning of this concept, we may return to this question in future work) as the $1+1$ scattering of two particles *in the presence of* curvature. They also should allow for investigating changes in the spectrum of bound states.

Unfortunately it is generally not possible to write these equations in closed form; exact solutions of the compatibility condition are exceptional, they require a special symmetry of the metric tensor. But this complication is by no means a characteristic peculiarity of the gravitational field; it arises as well in special relativity when we consider two bodies interacting in an external field, as soon as recoil effects are taken into account. When the metric has the suitable symmetry, formulas (5.23) and (5.24) permit writing Eqs. (5.17) and (5.18) explicitly by a method that is, to a large extent, independent of the form of the mutual interaction.

In the absence of curvature, an essential structure was the Lie algebra spanned by the squared-mass operators and the generators of the Poincaré group. Here analogously, the algebra spanned by H_1, H_2 and the total isometries (if any) play a similar role.

In addition to compatibility, a list of physically reasonable conditions has been discussed. In order to implement these requirements in a tractable model, we have considered a special case of static orthogonal space–time. In this example, the existence of a preferred flat background allows for regarding the curvature field as an external field in Minkowski space–time. In a representation using Hilbert space L^2, we have applied standard methods of relativistic quantum mechanics of particles, and explicitly solved the compatibility problem in a way that respects the symmetries of the Riemannian metric. Relative time was finally eliminated.

In this model, Axioms A, B, and D are strictly satisfied. Axiom C is rigorously satisfied insofar as the no-field limit is concerned, and (at least) formally satisfied in the case of the independent-particle limit.

Of course, the example given in Sec. V is not very useful for practical applications because no reasonable stress-energy tensor is expected to support a line element of the form (4.9) through Einstein equations. For this reason we prefer to speak of a *curvature field* rather than of a gravitational field.

Nevertheless, one must realize that no other solution of the compatibility condition (1.3) is available in closed form at the present time, except in the trivial case of Minkowski space. The present example is at least nontrivial, as it has a nonzero curvature. Our model, being defined in closed form, ensures that the general framework developed in Sec. III is not empty. Moreover it is an illustration of the role of isometries.

If one wishes to consider realistic space–times, it is possible to seek for solutions in the form of series expansions.

In this paper, for simplicity, we have considered scalar particles only. The general framework can be set forth also for fermions, provided K_1, K_2 are replaced by Dirac operators and the right-hand side of (1.1) become linear in the masses. But adapting to fermions the method displayed in Sec. V requires further work.

APPENDIX: PROPERTIES OF ISOMETRIES

In standard notations of differential geometry, the four-dimensional Laplace–Beltrami operator is

$$\Delta = \delta d + d\delta.$$

Claim: If ξ is an isometry and f a differential form, then $\mathscr{L}_\xi \Delta f = \Delta \mathscr{L}_\xi f$.

For a p form, the general proof rests on the identities $\delta = *^{-1} d *$ and $* \mathscr{L} = (-1)^p \mathscr{L} *$. When f is a function, that is a 0 form, we simply have

$$2Kf = \Delta f = \delta\, df.$$

Claim: If ξ is an isometry, then $\xi^\alpha \partial_\alpha$ is skew Hermitian in $L^2(\mathbf{R}^4)$.
Proof:

$$\int_\Omega (\xi^\alpha\ \partial_\alpha \phi^*)\psi \sqrt{|g|}\, d^4q = \int_\Omega \nabla_\alpha \partial_\alpha (\xi^\alpha \phi^* \psi)\sqrt{|g|}\, d^4q - \int_\Omega (\xi^\alpha\ \partial_\alpha \psi)\phi^* \sqrt{|g|}\, d^4q$$

$$- \int_\Omega (\nabla_\alpha \xi^\alpha)\phi^* \psi \sqrt{|g|}\, d^4q.$$

The first term gets transformed into the flux of $\xi^\alpha \phi^* \psi$ across the three-dimensional surface $\partial\Omega$. In the limit where Ω extends to infinity *in all space–time directions*, then ϕ and ψ vanish on $\partial\Omega$ (they are supposed to be squared integrable), therefore this first term yields no contribution. The last term also vanishes since $\nabla \cdot \xi$ is obviously zero. We are left with

$$\int\ (\xi \cdot \partial \phi^*)\psi \sqrt{|g|}\, d^4q = -\int\ \phi^* (\xi \cdot \partial \psi)\sqrt{|g|}\, d^4q;$$

in other words, $\xi^\alpha \partial_\alpha$ is skew symmetric in L^2.

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Squeezing Bogoliubov transformations on the infinite mode CCR-algebra

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A detailed analysis of and a general decomposition theorem for in general unbounded symplectic transformations on an arbitrary complex pre-Hilbert space (one–boson test function space) are given. The structure of strongly continuous symplectic groups on such spaces is determined. The connection between quadratic Hamiltonians, Bogoliubov transformations, and symplectic transformations is discussed in the Fock representation, and their relevance for squeezing operations in quantum optics is pointed out. The results for this rather general class of transformations are proved in a self-contained fashion. © *1996 American Institute of Physics.* [S0022-2488(96)01308-4]

I. INTRODUCTION

In recent developments in quantum optics the squeezed states of light have acquired a broad interest since by noise reduction they promise to increase the accuracy of certain measurement devices and to improve the transmission rate in optical communication techniques.

In the theoretical descriptions of squeezing processes the Hamiltonians most frequently are approximated by quadratic expressions

$$H_q=\frac{1}{2}\sum_{n=1}^{N}\left(\zeta_n a_n^* a_n^* + \overline{\zeta_n} a_n a_n\right) \tag{1.1}$$

of the light field (interaction picture), where the $\zeta_n \in \mathbb{C}$ arise from a classical (macroscopic) pumping field, and the $a_n^* \equiv a^*(e_n)$ are the creation [resp. the $a_n \equiv a(e_n)$ the annihilation] operators of the orthonormalized modes $\{e_1,\ldots,e_N\}$. Here N commonly is assumed to be finite.[1] In the literature the Hamiltonian (1.1) usually is referred to as the degenerate case of squeezing. However, in the smeared field formalism[2] the nondegenerate squeezing Hamiltonians may be transformed into the form (1.1) by superposing the idler and the signal modes.[3,4] There are also some investigations on infinite (resp. continuous) mode squeezing.[5] Calculating the time evolution associated with (1.1) leads to a one-parameter group of Bogoliubov transformations on the algebra of observables.

A rigorous smeared boson field theory is based on an arbitrary one-boson testfunction space E, which is a complex pre-Hilbert space with norm completion $\mathscr{H}$. The choice of E determines the specific boson system and the modes taken into account. For bosons with the spin s, E is a subspace of $\mathsf{L}^2(\Lambda)\otimes\mathbb{C}^{2s+1}$. For photons the quantization procedure in the Coulomb gauge leads to a test function space E consisting of divergence-free (i.e., $\boldsymbol{\nabla}\cdot f=0$), square-integrable functions f: $\Lambda\to\mathbb{C}^3$ on the quantization volume $\Lambda\subseteq\mathbb{R}^3$ in position space. The algebra of observables is the C^*-Weyl algebra $\mathscr{W}(E)$ over E generated by the unitary Weyl operators $W(f),f\in E$ (sometimes called displacement operators), which in regular representations are given in terms of the smeared creation and annihilation operators, $W(f)=\exp\{i2^{-1/2}(a^*(f)+a(f))\}$, and which satisfy the Weyl form of the canonical commutation relations (CCR), cf. the beginning of Sec. III.

The Bogoliubov transformations α on $\mathscr{W}(E)$ (as, e.g., those generated by the quadratic Hamiltonians from above) are in one-to-one correspondence with the symplectic transformations T on E (i.e., T acts real-linearly and bijectively on E and leaves the imaginary part of the scalar product $\langle .|. \rangle$ invariant), such that $\alpha(W(f))=W(Tf)\ \forall f\in E$, in which case we write $\alpha=\alpha_T$.

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Symplectic and Bogoliubov transformations belong to the basic structure of a boson quantum field theory. From the beginning of the operator-algebraic Weyl theory they have been studied with respect to different points of view. In the theoretical developments of squeezing for modern measurement and communication devices they are of a special importance (see above). Both for the structural investigations and for practical applications the use of unbounded symplectic transformations on an incomplete pre-Hilbert space E is unavoidable (as will be substantiated by future work).

Here, we present a new approach using the (unique) decompositions of real-linear operators into their complex-linear and complex-antilinear parts. The fixed complex structure inherent in the complex-linearity of the test function space E allows a systematic study of the general structure of symplectic transformations, especially of symplectic one-parameter groups with their generators and unitary implementations (here in Fock space). Beside new results we also collect and generalize some older ones, which are scattered in an incoherent fashion over a series of articles. Here we present a self-contained exposition, where all statements are proved by means of a direct and complete argumentation and are illustrated by several examples.

In Sec. II we first give a detailed analysis of the algebraic relations for the (complex) linear part and the antilinear (conjugate linear) part of a symplectic T. Then we verify that every symplectic T on E uniquely is decomposable into a unitary U, a self-adjoint positive S, and an antilinear involution J (as operators on $\mathscr{H}$), so that

$$T = U\,\cosh(S) + UJ\,\sinh(S). \tag{1.2}$$

This formula may be considered as the polar decomposition of the real-linear, symplectic T. It generalizes the special finite-dimensional examples, which gave rise to the developments of the squeezing theory.[1] If E is a proper dense subspace of $\mathscr{H}$, then T (or equivalently S) may be unbounded. For $E=\mathscr{H}$, however, T always has to be bounded (cf. Lemma 2.9). In Sec. II B we completely characterize strongly continuous symplectic one-parameter groups $\{T_t | t\in\mathbb{R}\}$ on $\mathscr{H}$ with the growth property $||T_t|| \leqslant \exp\{\beta|t|\} \forall t\in\mathbb{R}$ for some $\beta\geqslant 0$, as those which have a generator with bounded antilinear part.

The decomposition formula (1.2) is a useful tool for calculating squeezing properties (e.g., the variances) of Bogoliubov transformed (i.e., squeezed) states. This application is deferred to papers to follow.[6]

Section III is devoted to unitary implementations of the Bogoliubov transformations α_T with respect to the Fock representation of $\mathscr{W}(E)$. This investigation is inspired by Ref. 7 where, however, functional techniques are used exclusively. In Sec. III A we first give a slight generalization of Shale's result:[8] α_T is unitarily implementable in Fock space, if and only if the antilinear part of T is of Hilbert–Schmidt class, which especially yields T to be bounded. Then we calculate the transition probability of Glauber vectors with squeezed Glauber vectors [Lemma 3.4 and Eq. (A1)], a result which resembles a functional formula in Ref. 7. It is found for the one mode case also in some quantum optical articles.[1] Section III B deals with the connection between general quadratic Hamiltonians in Fock space and one-parameter groups of symplectic transformations on $\mathscr{H}$. Let $H := H_q + H_C$, where H_q is from (1.1) with $N=\infty$, and H_C denotes the free evolution Hamiltonian on Fock space uniquely associated with the self-adjoint linear one-boson Hamiltonian C on the complex one-boson Hilbert space $\mathscr{H}$. Then with the self-adjoint antilinear $D=\Sigma_{n=1}^{\infty}\zeta_n\langle .|e_n\rangle e_n$ on $\mathscr{H}$, we show the group $T_t := \exp\{ti(C-D)\}$, $t\in\mathbb{R}$, to consist of bounded symplectic transformations T_t on $\mathscr{H}$, which on the second quantized level are implemented by $\exp\{itH\}$, i.e.,

$$\exp\{itH\}W(f)\exp\{-itH\} = \alpha_{T_t}(W(f)) = W(T_t f) \quad \forall f\in\mathscr{H} \quad \forall t\in\mathbb{R}. \tag{1.3}$$

Here C may be unbounded. However, the condition that the Fock vacuum vector is contained in the domain of definition of the self-adjoint H on Fock space is equivalent to D being an antilinear Hilbert–Schmidt operator on $\mathscr{H}$, i.e., $\Sigma_{n=1}^{\infty}|\zeta_n|^2<\infty$, which also yields the Hilbert–Schmidt property of the antilinear parts of the symplectic transformations T_t.

Especially for $C=0$, and hence $H_C=0$, one obtains the formula (cf. Corollary 3.10)

$$T_t=\exp\{-itD\}=\cosh(tS)+J\,\sinh(tS)=\sum_{n=1}^{\infty}\left[\cosh(t|\zeta_n|)\langle e_n|.\rangle e_n-i\,\frac{\zeta_n}{|\zeta_n|}\,\sinh(t|\zeta_n|)\langle .|e_n\rangle e_n\right]$$

with $S=\Sigma_{n=1}^{\infty}|\zeta_n|\langle e_n|.\rangle e_n$ and $Je_n=-i(\zeta_n/|\zeta_n|)e_n\forall n\in\mathbb{N}$. Then Eq. (1.3) expressed in terms of annihilation and creation operators in Fock space gives for every $n\in\mathbb{N}$ and $t\in\mathbb{R}$

$$\exp\{itH_q\}a(e_n)\exp\{-itH_q\}=\cosh(t|\zeta_n|)a(e_n)-i\,\frac{\zeta_n}{|\zeta_n|}\,\sinh(t|\zeta_n|)a^*(e_n).$$

If $\Sigma_{n=1}^{\infty}|\zeta_n|^2=\infty$, then H_q has no meaning as an operator on Fock space.[4]

As indicated above, there occur on the one-particle level complex-linear, complex-antilinear, and real-linear operators. If not stated otherwise, we always mean with the expressions ''operator'' and ''linear operator'' complex-linear mappings. On the level of the second quantization (C^*-algebraic level, and operators on Fock space), however, we are concerned with complex-linear operators, only.

II. SYMPLECTIC TRANSFORMATIONS

Let E be an arbitrary complex pre-Hilbert space with (right-linear) scalar product $\langle .|.\rangle$ and norm-completion $\mathscr{H}$. The imaginary part of the scalar product is a nondegenerate symplectic form on E.

Definition 2.1 (Symplectic Transformation): A mapping $T: E\to E$ is called a symplectic transformation on E, if it is real-linear, surjective [that is, $T(E)=E$] and fulfills

$$\mathrm{Im}\langle Tf|Tg\rangle=\mathrm{Im}\langle f|g\rangle\quad\forall f,g\in E. \tag{2.1}$$

The set of all symplectic transformation on E we denote by $\mathscr{T}(E)$.

Relation (2.1) implies the injectivity of T, and thus each symplectic transformation T acts bijective on E. The inverse mapping $T^{-1}: E\to E$ is a symplectic transformation on E, too. Hence $\mathscr{T}(E)$ forms a group. We have, e.g., $U\in\mathscr{T}(E)$ for each unitary U on $\mathscr{H}$ with $U(E)=E$, which gives a subgroup of $\mathscr{T}(E)$.

A. The general form of a symplectic transformation

Since E and $\mathscr{H}$ are complex-linear vector spaces each real-linear operator $T: E\to\mathscr{H}$ decomposes uniquely into its (complex-) linear part T_l and its (complex-) antilinear part T_a, that is, $T=T_l+T_a$ with

$$T_l:=\tfrac{1}{2}(T-iTi)\quad\text{and}\quad T_a:=\tfrac{1}{2}(T+iTi). \tag{2.2}$$

In the following we consider T_l and T_a for a symplectic $T\in\mathscr{T}(E)$ as (not necessarily bounded) operators on the Hilbert space $\mathscr{H}$ with the dense domain of definition E and range contained in E.

Let us refer some common notations (cf. Ref. 9, Section VIII.1), which are used throughout the paper. The orthogonal complement of a subset $K\subseteq\mathscr{H}$ is denoted by $K^{\perp}$, its closure by $\bar{K}$. The (complex-) linear hull $\mathsf{LH}(K)$ of $K\subset\mathscr{H}$ consists of all finite linear combinations of elements of K. A linear (resp. antilinear) operator B on $\mathscr{H}$ is a linear (resp. antilinear) mapping from its domain $\mathscr{D}(B)$, a complex-linear subspace of $\mathscr{H}$, into $\mathscr{H}$. B is called densely defined, if $\mathscr{D}(B)$ is dense in $\mathscr{H}$. The adjoint B^* of a densely defined linear (resp. antilinear) operator B on $\mathscr{H}$ is given by

$$\mathscr{D}(B^*) := \{g \in \mathscr{H} | f \in \mathscr{D}(B) \mapsto \langle g|Bf\rangle \text{ is } \|.\|\text{-continuous}\}$$

and by setting $\langle B^*g|f\rangle := \langle g|Bf\rangle$ for linear B, and $\langle f|B^*g\rangle := \langle g|Bf\rangle$ for antilinear B, respectively. In general B^* is a closed linear (resp. antilinear) operator on $\mathscr{H}$, but not necessarily densely defined. $\ker(B)$ is the kernel and $\mathrm{ran}(B)$ the range of B. For closable B we write B for its closure. $B|_K$ denotes the restriction of B to the subspace $K \subseteq \mathscr{D}(B)$. K is a core for the closed B, if $\overline{B|_K} = B$. B leaves K invariant, if $K \subseteq \mathscr{D}(B)$ and $B(K) \subseteq K$. B is called positive, $B \geqslant 0$, if $\langle f|Bf\rangle \geqslant 0 \forall f \in \mathscr{D}(B)$. We write $A \subseteq B$, if $\mathscr{D}(A) \subseteq \mathscr{D}(B)$ and $A = B|_{\mathscr{D}(A)}$. A densely defined B is called symmetric if $B \subseteq B^*$, essentially self-adjoint if $B = B^*$, and self-adjoint if $B = B^*$. For closed densely defined B one has that $0 \leqslant B^*B$ is self-adjoint and linear, and one puts $|B| := \sqrt{B^*B}$. For the closed linear (resp. antilinear) B one has the (unique) polar decomposition $B = V|B|$ where V is the unique linear (resp. antilinear) partial isometry with initial space $(\ker(B))^\perp = \overline{\mathrm{ran}(|B|)}$ and final space $\overline{\mathrm{ran}(B)}$. For bounded linear (resp. antilinear) operators A on $\mathscr{H}$ we always assume $\mathscr{D}(A) = \mathscr{H}$, which gives $\mathscr{D}(A^*) = \mathscr{H}$ and $\|A\| = \|A^*\|$.

Theorem 2.2: *Let $T: E \to \mathscr{H}$ be a real-linear operator. We have the following equivalences:*

(*i*) $T \in \mathscr{T}(E)$ (*especially,* $T(E) = E$).

(*ii*) *T, T_l, and T_a fulfill the following relations:*

(*a*) $T(E) = E$ [*implying* $T_l(E) \subseteq E$, and $T_a(E) \subseteq E$], $E \subseteq \mathscr{D}(T_l^*)$, $E \subseteq \mathscr{D}(T_a^*)$ (*implying the closability of T_l and T_a*),

(b) $T_l^* T_a = T_a^* T_l$ and $T_l^* T_l - T_a^* T_a = \mathbb{1}_E$.

(*iii*) *T, T_l, and T_a fulfill the following relations:*

(a) $T(E) = E$,

(b) $\langle T_l f|T_a g\rangle = \langle T_l g|T_a f\rangle$ *and* $\langle T_l f|T_l g\rangle - \langle T_a g|T_a f\rangle = \langle f|g\rangle \forall f, g \in E$.

(iv) *T_l and T_a fulfill the following relations:*

(a) $E \subseteq \mathscr{D}(T_l^*)$, $E \subseteq \mathscr{D}(T_a^*)$, and, *$T_l, T_a, T_l^*, T_a^*$ leave E invariant,*

(b) $T_l^* T_a = T_a^* T_l$, $T_l^* T_l - T_a^* T_a = \mathbb{1}_E$,

(c) $T_l T_a^*|_E = T_a T_l^*|_E$ *and* $T_l T_l^*|_E - T_a T_a^*|_E = \mathbb{1}_E$.

Moreover, if T is a symplectic transformation on E, then

$$T_l^* \supseteq \tfrac{1}{2}(T^{-1} - iT^{-1}i), \quad T_a^* \supseteq -\tfrac{1}{2}(T^{-1} + iT^{-1}i), \tag{2.3}$$

and, for the symplectic transformation $T^{-1}: E \to E$, it holds

$$T^{-1} = T_l^*|_E - T_a^*|_E, \quad (T^{-1})_l = T_l^*|_E, \quad (T^{-1})_a = -T_a^*|_E. \tag{2.4}$$

Proof: (i)$\Rightarrow$(ii): Observing $\langle f|Tg\rangle = \mathrm{Im}(i\langle f|Tg\rangle) + i\,\mathrm{Im}\langle f|Tg\rangle$ one uses (2.1) to calculate

$$\langle f|(T - iTi)g\rangle = \langle (T^{-1} - iT^{-1}i)f|g\rangle, \quad \langle f|(T + iTi)g\rangle = -\langle g|(T^{-1} + iT^{-1}i)f\rangle,$$

which leads to (2.3) and (2.4), and also shows (ii)(a). Now (2.1) implies

$$\underbrace{(T_l^* T_l - T_a^* T_a - \mathbb{1}_E)}_{\text{linear}} f + \underbrace{(T_l^* T_a - T_a^* T_l)}_{\text{antilinear}} f = 0 \quad \forall f \in E.$$

Now observe that E is a complex-linear vector space, and we may replace f by if. (ii)$\Rightarrow$(iii): (iii)(b) is another formulation of (ii)(b). (iii)$\Rightarrow$(i): (iii)(b) yields (2.1). (i)$\Rightarrow$(iv) is obtained by applying (i)$\Leftrightarrow$(ii) to T and T^{-1} from (2.4). (iv)$\Rightarrow$(ii): Let $\widetilde{T} := T_l^*|_E - T_a^*|_E$. With (iv)(c) one easily checks $T\widetilde{T} = \mathbb{1}_E$, which proves (ii)(a). ∎

Corollary 2.3: Let $T \in \mathscr{T}(E)$. It holds $\||\overline{T_l}|f\| = \|\overline{T_l} f\| \geqslant \|f\| \forall f \in \mathscr{D}(|\overline{T_l}|) = \mathscr{D}(\overline{T_l})$, and $\overline{\mathrm{ran}(|\overline{T_l}|)} = \mathscr{H}$. If $\mathscr{H}$ is separable, or, if T_l is bounded, then $\mathrm{ran}(T_l) = \overline{\mathrm{ran}(T_l)} = \mathscr{H}$, i.e., *$|\overline{T_l}|^{-1}$ and $(T_l)^{-1}$ are bounded with domain $\mathscr{H}$.*

Proof: From Theorem 2.2(iv) follows $\||\overline{T_l}|f\| = \|\overline{T_l}f\| \geqslant \|f\| \forall f \in \mathscr{D}(|\overline{T_l}|) = \mathscr{D}(\overline{T_l})$ and $\|T_l^* f\| \geqslant \|f\| \forall f \in E$. Since $|\overline{T_l}|$ is self-adjoint we have $\mathscr{H} = \ker(|\overline{T_l}|)^\perp = \overline{\mathrm{ran}(|\overline{T_l}|)}$ (e.g., Ref. 10, Proposition X.1.13). Since also $|\overline{T_l}|^{-1}$ is closed and $\||\overline{T_l}|^{-1} g\| \leqslant \|g\|$, we actually have $\mathrm{ran}(|\overline{T_l}|) = \mathscr{H}$. The same argument for $\overline{T_l}$ yields $\mathrm{ran}(\overline{T_l}) = \mathrm{ran}(T_l) =: \mathscr{K}$ to be closed. Assume $\mathscr{K}$ to be a proper subspace of $\mathscr{H}$. Then there is an $f \in E$ with $f \notin \mathscr{K}$. Choose an ONB (orthonormal base) $\mathscr{O}$ of the linear hull $\mathsf{LH}\{\mathrm{ran}(T_l), f\} \subseteq E$, the existence of which is ensured by the separability of $\mathscr{H}$ (e.g., Ref. 11, Section 3.3). Then there exists an $e \in \mathscr{O}$ with $e \in E \cap \mathscr{K}^\perp$. But $\mathscr{K}^\perp = \ker(T_l^*)$, and thus $1 = \|e\| \leqslant \|T_l^* e\| = 0$, a contradiction. The proof for bounded T_l is obvious. ■

Corollary 2.4: Suppose $\mathscr{H}$ separable, and let $T \in \mathscr{T}(E)$. Then E is a core for T_l^*, T_a^*, $T_l^* \overline{T_l}$, $T_a^* \overline{T_a}$, $\overline{T_l} T_l^*$, and $\overline{T_a} T_a^*$.

Proof: Replacing T_a by $-T_a$ from Theorem 2.2(iv) follows that $\hat{T} := T_l - T_a \in \mathscr{T}(E)$ with $\hat{T}^{-1} = T_l^*|_E + T_a^*|_E \in \mathscr{T}(E)$. Hence $S := \hat{T}^{-1} T \in \mathscr{T}(E)$. But $S_l = T_l^* T_l + T_a^* T_a = 2 T_l^* T_l - \mathbb{1}_E$ is symmetric with $\mathrm{ran}(S_l) = \mathscr{H}$ by Corollary 2.3. Hence $\overline{S_l}$ is self-adjoint by Ref. 11, Theorem 5.19, and so is $\overline{T_l^* T_{le}} = \frac{1}{2}(\overline{S_l} + \mathbb{1})$. But $\overline{T_l^* T_l} \subseteq \overline{T_l^*}\,\overline{T_l}$, and thus $\overline{T_l^* T_l} = \overline{T_l^*}\,\overline{T_l}$ (e.g., Ref. 11, Theorem 5.31), which proves E to be a core for $\overline{T_l^* T_l}$. Because of $\mathrm{ran}(T_l) \subseteq E$ and $\mathscr{D}(T_l^*) \supseteq E$ this yields $T_l^* \overline{T_l} = \overline{T_l^*|_E}\,\overline{T_l}$. But $\overline{T_l^*|_E} \subseteq T_l^*$ gives $\overline{T_l} = \overline{T_l^{**}} \subseteq \overline{T_l^*|_E}^*$, and hence $T_l^* \overline{T_l} = \overline{T_l^*|_E}\,\overline{T_l^*|_E}^*$, which with Ref. 11, Theorem 5.40, leads to $\overline{T_l} = \overline{T_l^*|_E}^*$, respectively $T_l^* = \overline{T_l^*|_E}$. Now use $T_l^* T_l = T_a^* T_a + \mathbb{1}_E$, and the same argumentation for $T^{-1} \in \mathscr{T}(E)$. ■

Theorem 2.5 (Decomposition): *Let $T \in \mathscr{T}(E)$. Suppose $\mathscr{H}$ separable or T_l (or equivalently T_a) bounded. Then on $\mathscr{H}$ there exist a positive self-adjoint operator S, a unitary U, and an antilinear involution J (that is, $J = J^* = J^{-1}$), so that*

(a) *E is a subspace of the domains of $U \cosh(S)$, $UJ \sinh(S)$, $\cosh(S) U^*$, $J \sinh(S) U^*$, and these operators leave E invariant.*

(b) *J commutes with S in the sense of $J\phi(S) = \overline{\phi(S)} J$ for every Borel measurable function $\phi: [0,\infty[\to \mathbb{C}$ (here ϕ is the complex-conjugate function). Especially, $J(\ker(S)) = \ker(S)$ and $J(\ker(S)^\perp) = \ker(S)^\perp$.*

(c) *$T_l = U \cosh(S)|_E$ and $T_a = UJ \sinh(S)|_E$.*

(d) *E is a core for $\cosh(S)$, $\sinh(S)$, $\cosh(S)^2$, and $\sinh(S)^2$.*

(e) *Let $\widetilde{U}$ be a unitary, $\widetilde{S}$ a self-adjoint operator with $\mathscr{D}(\exp\{\pm\widetilde{S}\}) \supseteq E$, and $\widetilde{J}$ an antilinear involution on $\mathscr{H}$, such that $T = \widetilde{U} \cosh(\widetilde{S})|_E + \widetilde{U}\widetilde{J} \sinh(\widetilde{S})|_E$. We have $\widetilde{U} = U$, $|\widetilde{S}| = S$, $\widetilde{J}$ commutes with $\widetilde{S}$, $\widetilde{J} f = -Jf$ for $f \in \widetilde{P}(]-\infty, 0[)\mathscr{H}$, and $\widetilde{J} g = Jg$ for $g \in \widetilde{P}([0,\infty[)\mathscr{H}$, where $\widetilde{P}$ is the projection-valued measure associated with $\widetilde{S}$. Especially, if $\widetilde{S} \geqslant 0$, then $\widetilde{S} = S$ and $\widetilde{J} g = Jg \forall g \in \ker(S)^\perp$.*

Proof: $T_l^* T_l - T_a^* T_a = \mathbb{1}_E$ implies $\|\overline{T_l} f\|^2 = \|\overline{T_a} f\|^2 + \|f\|^2 \forall f \in D_1 := \mathscr{D}(\overline{T_l}) = \mathscr{D}(\overline{T_a})$. For the proof we drop the bar for the closures. We get $\mathscr{D}(|T_l|^2) = \mathscr{D}(|T_a|^2)$ and $|T_l|^2 = |T_a|^2 + \mathbb{1}$, which gives

$$\exp\{it|T_l|^2\} = \exp\{it\} \exp\{it|T_a|^2\} \quad \forall t \in \mathbb{R}, \tag{2.5}$$

and the closed subspace $\mathscr{K} := \ker(|T_a|) = \{f \in D_1 \,||T_l| f = f\}$. Thus, $\exp\{it|T_l|^2\}(\mathscr{K}) = \mathscr{K} \forall t \in \mathbb{R}$, and $\mathscr{K}$ is a reducing subspace for $|T_l|^2$ and for $|T_l|$ (cf. Ref. 11, Theorem 7.39). Since E is a core for T_l^* and T_a^* (Corollary 2.4), the same argumentation holds for $T^{-1} = T_l^*|_E - T_a^*|_E$ with $D_1^* := \mathscr{D}(T_l^*) = \mathscr{D}(T_a^*)$ and $\mathscr{K}^* := \ker(|T_a^*|)$.

Since cosh is bijective from $[0,\infty[$ onto $[1,\infty[$ we may define $S \geqslant 0$ by $|T_l| =: \cosh(S)$, and thus $|T_a| = \sinh(S)$. Obviously, $\mathscr{K} = \ker(S)$.

Let $T_l = U|T_l|$ be the polar decomposition, for which U is a unitary because of Corollary 2.3. From $T_l^* = |T_l| U^*$ it follows $U^*(D_1^*) = D_1$. From $|T_l^*| U = U|T_l|$ we obtain $|T_l^*| Uf = U|T_l| f = Uf \forall f \in \mathscr{K}$, and hence $U(\mathscr{K}) = \mathscr{K}^*$.

Let $T_a = V|T_a|$ be the polar decomposition with the antilinear partial isometry V from $\overline{\mathrm{ran}(|T_a|)} = \mathscr{K}^{\perp}$ onto $\overline{\mathrm{ran}(T_a)} = \mathscr{K}^{*\perp}$. We continue V to an antiunitary on $\mathscr{H}$: let I be an arbitrary antilinear involution on $\mathscr{K}$ and define $Vf := UIf$ for $f \in \mathscr{K}$.

With $|T_l^*|^2 = U|T_l|^2U^*$ and $|T_a^*|^2 = V|T_a|^2V^*$ and (2.5) we calculate

$$U\exp\{it|T_l|^2\}U^* = \exp\{it|T_l^*|^2\} = \exp\{it\}\exp\{it|T_a^*|^2\} = \exp\{it\}V\exp\{-it|T_a|^2\}V^*$$
$$= V\exp\{-it\}\exp\{-it|T_a|^2\}V^* = V\exp\{-it|T_l|^2\}V^* \quad \forall t \in \mathbb{R},$$

implying $V^*U\exp\{it|T_l|^2\} = \exp\{-it|T_l|^2\}V^*U$. With Fourier transformation and standard arguments one now easily checks (b) for $J := V^*U$.

Here $\mathscr{K}^{\perp}$ is a reducing subspace for $|T_l|$, hence $|T_a||T_l|\exp\{-2\tau|T_l|\}|_{\mathscr{K}^{\perp}}$ for $\tau > 0$ is a bounded, injective, self-adjoint operator on $\mathscr{K}^{\perp}$ with range dense in $\mathscr{K}^{\perp}$. Because J commutes with $|T_l|$, for all $f, g \in \mathscr{K}^{\perp}$ one easily calculates with Theorem 2.2(iii)

$$\langle f|J^*|T_a||T_l|\exp\{-2\tau|T_l|\}g\rangle$$
$$= \langle T_l\exp\{-\tau|T_l|\}f|T_a\exp\{-\tau|T_l|\}g\rangle$$
$$= \langle T_l\exp\{-\tau|T_l|\}g|T_a\exp\{-\tau|T_l|\}f\rangle$$
$$= \langle f|J|T_a||T_l|\exp\{-2\tau|T_l|\}g\rangle,$$

which yields $J = J^*$ on $\mathscr{K}^{\perp}$. $J = I$ on $\mathscr{K}$ is obvious, and thus $J = J^*$ on the whole of $\mathscr{H}$.

We prove (e): From the uniqueness of the decomposition (2.2) it follows $T_l|_E = \widetilde{U}\cosh(\widetilde{S})|_E = U\cosh(S)|_E$, which implies $\mathscr{D}(\overline{\cosh(\widetilde{S})|_E}) = D_1 = \mathscr{D}(\cosh(S))$. Since $\widetilde{U}$ is unitary and $\mathrm{ran}(T_l) = \mathscr{H}$, we have $\mathrm{ran}(\overline{\cosh(\widetilde{S})|_E}) = \mathscr{H}$, which by Ref. 11, Theorem 5.19 implies the self-adjointness of $\overline{\cosh(\widetilde{S})|_E}$ and finally $\overline{\cosh(\widetilde{S})|_E} = \cosh(\widetilde{S})$. The uniqueness of the polar decomposition now yields $U = U$ and $\cosh(\widetilde{S}) = \cosh(S)$, which gives $|\widetilde{S}| = S$ [since $\cosh(x) = \cosh(|x|)\forall x \in \mathbb{R}$]. The spectral calculus and $U^*T_a = J\sinh(\widetilde{S}) = J\sinh(S)$ proves the rest.

(a) is a consequence of Theorem 2.2(iv). (d) follows from Corollary 2.4. ■

For $T \in \mathscr{T}(E)$ part (e) of the above theorem gives the uniqueness of the decomposition $T = U\cosh(S)|_E + UJ\sinh(S)|_E$ with positive self-adjoint $S \geqslant 0$. Since J commutes with S, only its action on $\ker(S)^{\perp}$ is of interest, i.e., J is arbitrarily changeable on $\ker(S)$. We also give the converse statement, which is very helpful for explicit constructions of symplectic transformations T, which may be performed as in Example 2.7 below.

Corollary 2.6: Let be U a unitary, S a self-adjoint operator (not necessarily positive), and J an antilinear involution on $\mathscr{H}$*, so that* (a) *and* (b) *of Theorem 2.5 are fulfilled. Then* $U\cosh(S)|_E + UJ\sinh(S)|_E$ *is an element of* $\mathscr{T}(E)$.

Proof: T so defined being symplectic on E is a consequence of Theorem 2.2(iv). ■

Example 2.7: Let $m \in \mathbb{N}$ and $n \in \mathbb{N} \cup \{0, \infty\}$. *Assume* $E := \mathscr{C}_c^n(\mathbb{R}^m)$, *the complex-valued, n-times continuously differentiable functions on* $\mathbb{R}^m$ *with compact support. We choose* $\mathscr{H} = \mathsf{L}^2(\mathbb{R}^m)$ *with respect to the Lebesgue measure* $\mathrm{d}^m x$ *as the completion of E. Define S to be the operator of multiplication with the arbitrary but n-times continuously differentiable function* $s: \mathbb{R}^m \to \mathbb{R}$, *and J to be the complex conjugation,* $Jf = \bar{f}$, $f \in \mathscr{H}$. *The unitary U on* $\mathscr{H}$ *we construct by* $(Uf)(x) := \exp\{i\theta(x)\}f(Rx - a)$, $x \in \mathbb{R}^m$, $f \in \mathscr{H}$, *with some real-valued, n-times continuously differentiable function* θ, *the rotation* $R \in \mathsf{SO}(m)$, *and* $a \in \mathbb{R}^m$.

The operators U, J, $\cosh(S)$, *and* $\sinh(S)$ *leave E invariant, and consequently by the above corollary* $U\cosh(S)|_E + UJ\sinh(S)|_E =: T \in \mathscr{T}(E)$. *Moreover,* $\ker(S) = \mathsf{L}^2(N(S))$ *where* $N(S) := \{x \in \mathbb{R}^m | s(x) = 0\}$.

Sometimes we consider $\mathscr{H}$ as a real Hilbert space with scalar product $(.|.) := \mathrm{Re}\langle .|. \rangle$, which we denote by $\mathscr{H}_r$. The adjoint of the real-linear operator A on $\mathscr{H}_r$ is denoted by A^+, $(f|Ag) = (A^+f|g)$ for all $f \in \mathscr{D}(A)$ and $g \in \mathscr{D}(A^+)$. The absolute value of the closed real-linear A

on $\mathscr{H}_r$ is denoted by $|A|_r := \sqrt{A^+A}$. Similarly to the complex case, for a closed real-linear operator A on a real Hilbert space one has the (unique) polar decomposition $A = V|A|_r$, where the (unique) partial isometry is real-linear with initial space $\overline{\mathrm{ran}(|A|_r)}$ and final space $\overline{\mathrm{ran}(A)}$ (cf., e.g., Ref. 11).

Corollary 2.8: Let $T \in \mathscr{T}(E)$. Then T is a closable real-linear operator on the real Hilbert space $\mathscr{H}_r$. And the decomposition $T = U(\cosh(S)|_E + J \sinh(S)|_E)$ according Theorem 2.5 with the unitary U, the positive $S = S^*$, and the antilinear involution J on $\mathscr{H}$ gives the polar decomposition of the closure $T = U|T|_r$, $|T|_r = \cosh(S) + J \sinh(S)$.

Proof: Obviously, $T^+ \supseteq T_l^* + T_a^*$ is densely defined and hence T is closable. Now observe that $\cosh(S) + J \sinh(S)$ is a positive real-linear operator on $\mathscr{H}_r$. ■

B. Strongly continuous symplectic groups

We give here the case of bounded $T \in \mathscr{T}(E)$ a special treatment. If $\|Tf\| \leqslant c\|f\| \forall f \in E$ for some $c > 0$, then $\|\pm iTif\| \leqslant c\|f\|$, thus T_l and T_a are bounded. Conversely, T_l to be bounded is equivalent for T_a to be bounded, which implies T to be bounded. In this case T is continuously extendable to an element of $\mathscr{T}(\mathscr{H})$.

Lemma 2.9: Let $T \in \mathscr{T}(\mathscr{H})$. Then T, T_l and T_a are bounded.

Proof: Theorem 2.2 gives $\mathscr{D}(T_l) = \mathscr{D}(T_a) = \mathscr{D}(T_l^*) = \mathscr{D}(T_a^*) = \mathscr{H}$. The boundedness now follows from the closed graph theorem (e.g., Ref. 11, Theorem 5.7). ■

Let $C = C^*$ be a self-adjoint linear (possibly unbounded) operator on $\mathscr{H}$. Then $u_t := \exp\{itC\}$, $t \in \mathbb{R}$, defines a strongly continuous one-parameter group u of isometries on the real Hilbert space $\mathscr{H}_r$. We perturb u with the antilinear self-adjoint bounded $D = D^*$ on $\mathscr{H}$. The perturbed (strongly continuous) group on $\mathscr{H}_r$ is denoted by $\exp\{t(iC + D)\}$ with generator $iC + D$ and may be calculated by a perturbation expansion (cf. Ref. 12, Section 3.1). The linear part of $\exp\{t(iC + D)\}$ is given by summing over the even powers in the expansion series, and the antilinear part by summing over the odd ones.

Theorem 2.10: *The following statements are valid:*

(a) *Let $C = C^*$ be a linear operator on $\mathscr{H}$, and let $D = D^*$ be an antilinear bounded operator on $\mathscr{H}$. Then $T_t := \exp\{t(iC + D)\} \in \mathscr{T}(\mathscr{H})$ with $\|T_t\| \leqslant \exp\{\|D\||t|\}$ for all $t \in \mathbb{R}$.*

(b) *Let $\{T_t | t \in \mathbb{R}\} \subset \mathscr{T}(\mathscr{H})$ be a strongly continuous group with growth $\|T_t\| \leqslant \exp\{\beta|t|\} \forall t \in \mathbb{R}$ for some $\beta \geqslant 0$. Then there exists a unique linear $C = C^*$ and a unique antilinear bounded $D = D^*$ on $\mathscr{H}$ with $T_t = \exp\{t(iC + D)\} \forall t \in \mathbb{R}$.*

Proof: (a): $D = D^*$ implies $\mathrm{Im}\langle f | Dg\rangle = \mathrm{Im}\langle -Df | g\rangle \forall f, g \in \mathscr{H}$. Calculating with the perturbation series (e.g., Ref. 12, Theorem 3.1.33) gives $\mathrm{Im}\langle T_{-t} f | g\rangle = \mathrm{Im}\langle f | T_t g\rangle \forall f, g \in \mathscr{H}$. But $T_{-t} = T_t^{-1}$, thus $T_t \in \mathscr{T}(\mathscr{H})$. (b): From (2.4) follows $(T_{-t})_l + (T_{-t})_a = T_{-t} = T_t^{-1} = (T_t)_l^* - (T_t)_a^*$, which gives $(T_{-t})_l = (T_t)_l^*$ and $(T_{-t})_a = -(T_t)_a^*$. Let now all be as in Lemma A1 for our group T_t on the real Hilbert space $\mathscr{H}_r$. For the adjoint group T_t^+ we have $T_t^+ = (T_t)_l^* + (T_t)_a^* = (T_{-t})_l - (T_{-t})_a = -iT_{-t}i$, that is, $\exp\{tG^+\} = -i \exp\{-tG\}i \forall t \in \mathbb{R}$, which gives $f \in \mathscr{D}(G^+)$, if and only if $if \in \mathscr{D}(G)$. Hence, $\mathscr{D}(G) = \mathscr{D}(G^+)$ implies $\mathscr{D}(G)$ to be a complex dense subspace of $\mathscr{H}$, and, consequently, $G^+ = iGi$. Comparing with (2.2) gives $\Lambda = G_l$ to be (complex) linear and $D \supseteq G_a$ to be antilinear. Put $C := -i\Lambda$. From $\Lambda = -\Lambda^+$ and $D = D^+$ now follows $C = C^*$, and $D = D^*$, the adjoints with respect to the complex scalar product $\langle .|. \rangle$. ■

Theorem 2.10 completely characterizes the strongly continuous symplectic goups $\{T_t | t \in \mathbb{R}\} \subset \mathscr{T}(\mathscr{H})$ with growth $\|T_t\| \leqslant \exp\{\beta|t|\} \forall t \in \mathbb{R}$ for some $\beta \geqslant 0$. In general, a strongly continuous symplectic goup $\{V_t | t \in \mathbb{R}\} \subset \mathscr{T}(\mathscr{H})$ has the growth property $\|V_t\| \leqslant c \exp\{\beta|t|\} \forall t \in \mathbb{R}$ for some $\beta \geqslant 0$ and $c \geqslant 1$ (Ref. 12, Proposition 3.1.3). If there does not exist a $\beta \geqslant 0$ so that c may be chosen as $c = 1$, then by Theorem 2.10 the antilinear part, if it exists as a densely defined (closed) operator, of the generator of the group $\{V_t | t \in \mathbb{R}\}$ cannot be bounded.

Example 2.11. Let $\mathscr{H}$ be a separable complex Hilbert space with fixed ONB $\{e_k | k \in \mathbb{N}\}$, *and*

C,S,R positive, self-adjoint linear operators on $\mathscr{H}$ with $Ce_k=c_ke_k$, $Se_k=s_ke_k$, $Re_k=r_ke_k$ where $c_k>0$, $s_k\geqslant 0$, and $r_k>0\,\forall k\in\mathbb{N}$. S and R are supposed to be bounded. Finally let J be the antilinear involution on $\mathscr{H}$ satisfying $Je_k=e_k\,\forall k\in\mathbb{N}$. Obviously, C, S, R, and J mutually commute.

By Theorem 2.10 the exponentials $T_t:=\exp\{it(C-JS)\}$, $t\in\mathbb{R}$, define a strongly continuous one-parameter group of symplectic transformations $T_t\in\mathscr{T}(\mathscr{H})$. Another symplectic group of this kind is introduced by $\hat{T}_t:=TT_tT^{-1}$, where $T:=\exp\{JR\}=\cosh(R)+J\sinh(R)\in\mathscr{T}(\mathscr{H})$.

It holds $\hat{T}_t=\exp\{it(\hat{C}-J\hat{S})\}\,\forall t\in\mathbb{R}$ with the self-adjoint linear operators on $\mathscr{H}$

$$\begin{aligned}\hat{C}&:=2(\sinh(R)^2C+\cosh(R)\sinh(R)S)+C,\\ \hat{S}&:=2(\sinh(R)^2S+\cosh(R)\sinh(R)C)+S,\end{aligned}\tag{2.6}$$

which also have the e_k, $k\in\mathbb{N}$, as eigenvectors.

From (2.6) *it is seen that, for unbounded C, it may happen that $\hat{S}$ is unbounded, too. Hence the antilinear part $-iJ\hat{S}$ of the generator is unbounded* (e.g., *if $R\geqslant\mathbb{1}$, then $\hat{S}\geqslant C$*), *which by Theorem 2.10 implies the growth estimate $\|\hat{T}_t\|\leqslant c\exp\{\beta|t|\}\,\forall t\in\mathbb{R}$ with some $c>1$ and $\beta\geqslant 0$. Also, it is not possible to find a $\beta>0$ such that c may be chosen as $c=1$. Especially, because of $\|T\|=\|T^{-1}\|=\exp\{\|R\|\}$ and Theorem 2.10*(a), *we find the growth property $\|\hat{T}_t\|\leqslant\exp\{2\|R\|\}\exp\{\|S\||t|\}\,\forall t\in\mathbb{R}$.*

A continuation of this example is found at the end of Sec. III. The following lemma is used in the sequel.

Lemma 2.12: Let $D=D^*$ be an antilinear bounded operator on $\mathscr{H}$. Then there exists an antilinear involution J on $\mathscr{H}$ so that $D=J|D|$ and J commutes with D and $|D|$. Moreover, J is uniquely determined on $\ker(D)^\perp$.

Proof: The self-adjointness of D yields $\ker(|D|)=\ker(D)=\ker(D^*)$. Hence the initial space and final space is $\ker(D)^\perp$ for the antilinear partial isometry V occuring in the polar decomposition $D=V|D|$. The self-adjointness of D also yields V to commute with $|D|$ and D, and $V=V^*$. Hence V is an antilinear involution on $\ker(D)^\perp$, which we extend to an antilinear involution J on $\mathscr{H}$.

Example 2.13: Let D and J be as in Lemma 2.12. Then $T_t=\exp\{tD\}\in\mathscr{T}(\mathscr{H})$ with $(T_t)_l=\cosh(t|D|)$ and $(T_t)_a=J\sinh(t|D|)\,\forall t\in\mathbb{R}$.

III. UNITARY IMPLEMENTATIONS ON FOCK SPACE

The one-boson test function space E is a complex pre-Hilbert space with norm-completion $\mathscr{H}$. The C^*-algebra of the boson system is the Weyl algebra $\mathscr{W}(E)$ over E. $\mathscr{W}(E)$ is generated by the unitary Weyl operators $W(f)$, $f\in E$, satisfying (Ref. 12, Theorem 5.2.8)

$$W(f)W(g)=\exp\left\{-\frac{i}{2}\,\mathrm{Im}\langle f|g\rangle\right\}W(f+g),\quad W(f)^*=W(-f)\,\forall f,g\in E.\tag{3.1}$$

$\mathscr{S}\equiv\mathscr{S}(\mathscr{W}(E))$ denotes the state space of $\mathscr{W}(E)$. A state $\omega\in\mathscr{S}$ is called *regular*, if for each $f\in E$ the map $t\in\mathbb{R}\mapsto\langle\omega;W(tf)\rangle$ is continuous [$\langle\omega;M\rangle$ denotes the expectation value of ω with $M\in\mathscr{W}(E)$]. In the GNS representation $(\Pi_\omega,\mathscr{H}_\omega,\Omega_\omega)$ (e.g., Ref. 12, Subsection 2.3.3) of the regular $\omega\in\mathscr{S}$ the self-adjoint field operators are given by $\Phi_\omega(f):=-i(\mathrm{d}/\mathrm{d}t)\Pi_\omega(W(tf))|_{t=0}$, $f\in E$. The functional $f\in E\mapsto\Phi_\omega(f)$ is real-linear and the field operators satisfy the CCR on suitable dense domains, $[\Phi_\omega(f),\Phi_\omega(g)]\subseteq i\,\mathrm{Im}\langle f|g\rangle\mathbb{1}$, $\forall f,g\in E$. The CCR for the smeared annihilation and creation operators, $a_\omega(f):=2^{-1/2}(\Phi_\omega(f)+i\Phi_\omega(if))$ and $a_\omega^*(f):=2^{-1/2}(\Phi_\omega(f)-i\Phi_\omega(if))$, respectively, write as $[a_\omega(f),a_\omega(g)]=[a_\omega^*(f),a_\omega^*(g)]=0$, and $[a_\omega(f),a_\omega^*(g)]\subseteq\langle f|g\rangle\mathbb{1}$, where the $a_\omega^*(f)$ and $a_\omega(f)$, $f\in E$, are densely defined and closed. Furthermore, $a_\omega(f)^*=a_\omega^*(f)$, the map $f\in E\mapsto a_\omega(f)$ is antilinear, and $f\in E\mapsto a_\omega^*(f)$ is linear (e.g., Ref. 12, Lemma 5.2.12).

The Fock vacuum state $\omega_{\mathrm{F}}\in\mathscr{S}$ is given by its characteristic function

$$\langle \omega_F; W(f)\rangle = \exp\{-\tfrac{1}{4}\|f\|^2\} \quad \forall f \in E. \tag{3.2}$$

Its GNS representation $(\Pi_F, F_+(\mathscr{H}), \Omega_F)$ is identical to the usual Fock representation Π_F on the symmetric Fock space $F_+(\mathscr{H}) = \oplus_{n=0}^{\infty} \mathbb{P}_+(\otimes_n \mathscr{H})$, where $\mathbb{P}_+$ is the symmetrization operator and $\otimes_n \mathscr{H}$ the n-fold tensor product of $\mathscr{H}$ with itself, and with the vacuum vector $\Omega_F = (1,0,0,\ldots) \in F_+(\mathscr{H})$ as cyclic vector. $\mathbb{P}_+(\otimes_n \mathscr{H})$ is called the n-particle subspace of $F_+(\mathscr{H})$. The Fock field, creation, annihilation, and Weyl operators are denoted by $\Phi_F(f)$, $a_F^*(f)$, $a_F(f)$, and $W_F(f)$, $f \in \mathscr{H}$ [$\Pi_F(W(f)) = W_F(f)$ for $f \in E$], respectively. We remark that $a_F(g)\Omega_F = 0$ $\forall g \in \mathscr{H}$, and $a_F^*(g)\mathbb{P}_+(f_1 \otimes \cdots \otimes f_n) = \sqrt{n+1}\,\mathbb{P}_+(g \otimes f_1 \otimes \cdots \otimes f_n) \forall g, f_j \in \mathscr{H}, \forall n \in \mathbb{N} \cup \{0\}$ (e.g., Ref. 12, Subsection 5.2.1; Ref. 9, Section X.7).

For each $T \in \mathscr{T}(E)$ there is a (unique)*-automorphism α_T on the Weyl algebra $\mathscr{W}(E)$ with $\alpha_T(W(f)) = W(Tf) \forall f \in E$, the *Bogoliubov transformation* associated with T. The dual transformation ν_T, $\langle \nu_T(\omega); M\rangle = \langle \omega; \alpha_T(M)\rangle$, $\omega \in \mathscr{S}$, $M \in \mathscr{W}(E)$, is an affine bijection on $\mathscr{S}$. Obviously, $(\nu_T)^{-1} = \nu_{T^{-1}}$, and, the state $\omega \in \mathscr{S}$ is regular, if and only if $\nu_T(\omega)$ is so. Especially, $\nu_T(\omega_F)$ is regular.

A. Bogoliubov transformations in the Fock representation

Here we turn our interest to those cases for which the Bogoliubov transformation α_T is unitarily implementable in Fock space. For finite-dimensional $E = \mathscr{H}$ [for each $T \in \mathscr{T}(E)$] this is a consequence of the Stone–von Neumann uniqueness theorem (e.g., Ref. 12, Corollary 5.2.15), which implies the irreducible GNS representation $[\Pi_F \circ \alpha_T, F_+(\mathscr{H}), \Omega_F]$ of the pure state $\nu_T(\omega_F)$ to be unitarily equivalent to the Fock representation $(\Pi_F, F_+(\mathscr{H}))$. For separable $E = \mathscr{H}$ the problem is solved in Ref. 8 (cf. also Refs. 7 and 13, Section 9), which is equivalent to the result of Ref. 14. The formulation of Shale's theorem presented here makes no use of the separability of $\mathscr{H}$ and allows also E to be a proper, dense, complex subspace of $\mathscr{H}$ (cf. Lemma 2.9). It is derived in a way different from Refs. 8 and 14. We refer some common notions (e.g., Ref. 9, Section VI.6): A bounded linear (resp. antilinear) operator D on $\mathscr{H}$ is called Hilbert–Schmidt, if its Hilbert–Schmidt norm $\|D\|_{HS} := (\Sigma_{e \in \mathscr{O}} \|De\|^2)^{1/2}$ is finite, here $\|.\|_{HS}$ does not depend on the specific ONB $\mathscr{O}$ chosen for $\mathscr{H}$; D is called to be of trace class, if $\mathrm{tr}[|D|] < \infty$, where $\mathrm{tr}[.]$ denotes the usual trace on $\mathscr{H}$.

Theorem 3.1: *Let $T \in \mathscr{T}(E)$. We have the following equivalences:*

(i) *$\nu_T(\omega_F)$ is normal with respect to the Fock representation $(\Pi_F, F_+(\mathscr{H}))$;*

(ii) *α_T is unitarily implementable with respect to the Fock representation $(\Pi_F, F_+(\mathscr{H}))$, that is, there exists a unitary U_T on $F_+(\mathscr{H})$ with $\Pi_F(\alpha_T(M)) = U_T \Pi_F(M) U_T^* \forall M \in \mathscr{W}(E)$;*

(iii) *$|\overline{T_a}|$ is Hilbert–Schmidt on $\mathscr{H}$, which is equivalent for $|T_l| - \mathbb{1}$ to be of trace class;*

(iv) *$|T|_r - \mathbb{1}$ is a real-linear Hilbert–Schmidt operator on the real Hilbert space $\mathscr{H}_r$ (see Corollary 2.8), which is equivalent for $T^+T - \mathbb{1}$ to be Hilbert–Schmidt (cf. Refs. 8 and 13).*

If some of these assertions (and hence all) are valid, then U_T of (ii) is unique up to a phase. Moreover, $U_T\Omega_F = e^{i\vartheta}\Omega_F$ for some $\vartheta \in [0, 2\pi[$, if and only if $T_a = 0$.

Proof: (i)⇒(ii): $\nu_T(\omega_F)$ is pure. Hence, since $\nu_T(\omega_F)$ is Π_F-normal and by the irreducibility of Π_F (Ref. 12, Proposition 5.2.4), there exists a normalized $\eta_T \in F_+(\mathscr{H})$ so that $(\Pi_F, F_+(\mathscr{H}), \eta_T)$ is a GNS representation of $\nu_T(\omega_F)$. On the other side, $(\Pi_F \circ \alpha_T, F_+(\mathscr{H}), \Omega_F)$ is a GNS representation of $\nu_T(\omega_F)$, too, which has to be unitarily equivalent to $(\Pi_F, F_+(\mathscr{H}), \eta_T)$.

(ii)⇒(iii): First, $f \in E \mapsto \langle U_T^* \Omega_F | W_F(f) U_T^* \Omega_F\rangle = \exp\{-\tfrac{1}{4}\|Tf\|^2\}$ is continuous [e.g., Ref. 12, Proposition 5.2.4(4)], from which it follows that T is bounded. We extend the bounded T_l and T_a to all of $\mathscr{H}$ without changing the notation. From $\Phi_F(Tf) = U_T \Phi_F(f) U_T^*$ follows $U_T a_F(f) U_T^* = a_F(T_l f) + a_F^*(T_a f)$. Let $U_T\Omega_F = \oplus_{n=0}^{\infty} \xi_n$ with $\xi_n \in \mathbb{P}_+(\otimes_n \mathscr{H})$, especially, $\xi_0 = \alpha_0 \Omega_F$, i.e., $\alpha_0 = \langle \Omega_F | U_T \Omega_F\rangle$. Then $(a_F(T_l f) + a_F^*(T_a f)) U_T \Omega_F = U_T a_F(f) \Omega_F = 0 \; \forall f \in E$. With Corollary 2.3 we obtain the recursive system of equations: $a_F(g)\xi_{n+1} = -a_F^*(T_a (T_l)^{-1} g)\xi_{n-1}$ for all $g \in \mathscr{H}$

and each $n \geqslant 0$. Especially for $n=0$ it follows $\xi_1=0$, and thus, $\xi_{2k+1}=0\ \forall k \in \mathbb{N}$. $U_T\Omega_F \neq 0$ implies $\alpha_0 \neq 0$. For $n=1$ we have $a_F(g)\xi_2 = -\alpha_0 T_a (T_l)^{-1} g$, which with $\xi_2 = \mathbb{P}_+ \xi_2$ yields

$$\sqrt{2}\langle g \otimes h | \xi_2 \rangle = \langle a_F^*(g) h | \xi_2 \rangle = \langle h | a_F(g) \xi_2 \rangle = -\alpha_0 \langle h | T_a (T_l)^{-1} g \rangle. \tag{3.3}$$

With an ONB $\{e_j | j \in I\}$ of $\mathscr{H}$ we finally obtain

$$\infty > \frac{\|\xi_2\|^2}{|\alpha_0|^2} = \sum_{i,j \in I} |\langle e_i \otimes e_j | \alpha_0^{-1} \xi_2 \rangle|^2 = \frac{1}{2} \sum_{i,j \in I} |\langle e_j | T_a (T_l)^{-1} e_i \rangle|^2 = \frac{1}{2} \| |T_a| |T_l|^{-1} \|_{\mathrm{HS}}^2,$$

where we used the decomposition $T_l = U|T_l|$ and $T_a = UJ|T_a|$ with $|T_l| = \cosh(S)$ and $|T_a| = \sinh(S)$ from Theorem 2.5. Since $|T_l|$ is bounded, the assertion follows from the fact that the Hilbert–Schmidt class is a two-sided *-ideal in the bounded operators on $\mathscr{H}$.

$|T_l| \geqslant \mathbb{1}$ and $(|T_l|-\mathbb{1})(|T_l|+\mathbb{1}) = |T_l|^2 - \mathbb{1} = |T_a|^2$ imply $0 \leqslant |T_l| - \mathbb{1} \leqslant |T_a|^2$. Hence $|T_l| - \mathbb{1}$ is of trace class, if and only if $|T_a|^2$ is so (the trace class is a two-sided *-ideal in the bounded operators on $\mathscr{H}$).

(iii)$\Rightarrow$(i): The field, creation, and annihilation operators associated with the GNS representation $(\Pi_F \circ \alpha_T,\ F_+(\mathscr{H}),\ \Omega_F)$ of $\nu_T(\omega_F)$ we denote by $\Phi_T(f)$, $a_T^*(f)$, and $a_T(f)$, respectively. Obviously, $\Phi_T(f) = \Phi_F(Tf)$ and $a_T(f) = a_F(T_l f) + a_F^*(T_a f)\ \forall f \in E$. Since $|T_a|$ is Hilbert–Schmidt and commutes with J (Theorem 2.5) there exists an ONB $\mathscr{O}$ for $\mathscr{H}$ consisting of eigenvectors for $|T_a|$ with $Je = e\ \forall e \in \mathscr{O}$. Let $\mathscr{T}$ be a finite subset of $\mathscr{O}$, $P_{\mathscr{T}}$ the orthogonal projection onto $\mathsf{LH}\{\mathscr{T}\}$, and $h \in \mathsf{LH}\{\mathscr{T}\}$. Using the commutation relations

$$a_F(g) W_F(h) = W_F(h) \left(a_F(g) + \frac{i}{\sqrt{2}} \langle g | h \rangle \right), \quad a_F^*(g) W_F(h) = W_F(h) \left(a_F^*(g) - \frac{i}{\sqrt{2}} \langle h | g \rangle \right), \tag{3.4}$$

$|T_l|^2 = |T_a|^2 + \mathbb{1}$, and the Cauchy–Schwarz inequality, we obtain for each $g \in \mathscr{H}$

$$\|a_T(g) W_F(Uh) \Omega_F\|^2 = \tfrac{1}{2} |\langle g | (|T_l| - J|T_a|) h \rangle|^2 + \| |T_a| g \|^2 \leqslant \mathrm{tr}[|g\rangle\langle g| (c(h) P_{\mathscr{T}} + T_a^* T_a)]$$

with $c(h) \geqslant 0$ only depending on h. Let $\mathscr{F}$ be an ONB of the arbitrary finite-dimensional complex subspace $F \subseteq E$ with associated orthogonal projection P_F. Then

$$\sum_{e \in \mathscr{T}} \|a_T(e) W_F(Uh) \Omega_F\|^2 \leqslant \mathrm{tr}[P_F (c(h) P_{\mathscr{T}} + T_a^* T_a)] \leqslant \mathrm{tr}[c(h) P_{\mathscr{T}} + T_a^* T_a] < \infty.$$

But the set of vectors $W_F(Uh)\Omega_F$ with $h \in \mathsf{LH}(\mathscr{O})$ is total in $\mathscr{H}$. Hence a Fock-number operator for $\nu_T(\omega_F)$ exists and Ref. 12. Theorem 5.2.14 yields (i).

The equivalence (iii)$\Leftrightarrow$(iv) is easily checked with the decomposition of Theorem 2.5 and Corollary 2.8. Furthermore, the relations $|T|_r + \mathbb{1} \geqslant \mathbb{1}$ and $(|T|_r - \mathbb{1})(|T|_r + \mathbb{1}) = |T|_r^2 - \mathbb{1}$ imply $0 \leqslant |T|_r - \mathbb{1} \leqslant T^+ T - \mathbb{1}$. Hence $|T|_r - \mathbb{1}$ is Hilbert–Schmidt, if and only if $T^+ T - \mathbb{1}$ is so.

Let us prove the uniqueness of U_T: Assume U_T and $\widetilde{U}_T$ to implement α_T. Then $\widetilde{U}_T^* U_T$ is a unitary element of the commutant $\Pi_F(\mathscr{W}(E))'$. But Π_F is irreducible. Now, $T_a = 0$, if and only if T is unitary ($S=0$ in Theorem 2.5). This holds, if and only if $\nu_T(\omega_F) = \omega_F$, which is equivalent to $\eta_T = e^{i\vartheta} \Omega_F$ for some $\vartheta \in [0, 2\pi[$, where η_T is the cyclic vector from above. ■

Let us remark, that, e.g., Example 2.7 does not fulfill the requirements of Theorem 3.1.

Corollary 3.2: Let $T \in \mathscr{T}(E)$. Then the GNS representation of the pure state $\nu_T(\omega_F)$ is $(\Pi_F \circ \alpha_T, F_+(\mathscr{H}), \Omega_F)$, and the associated field and annihilation operators, $\Phi_T(f)$ resp. $a_T(f)$, are given as

$$\Phi_T(f) = \Phi_F(Tf), \quad a_T(f) = a_F(T_l f) + a_F^*(T_a f), \quad f \in E.$$

There exists a normalized vector $\xi_T \in F_+(\mathscr{H})$ with $a_T(f)\xi_T = 0 \forall f \in E$, *if and only if the equivalent assertions (i)–(iv) of Theorem 3.1 are valid, in which case* ξ_T *uniquely (up to a phase) is given by* $\xi_T = U_T\Omega_F$.

Definition 3.3: Let $\mathscr{T}_F(E)$ *be the subgroup of those symplectic transformations* $T \in \mathscr{T}(E)$ *for which* $|\overline{T_a}|$ *is a Hilbert–Schmidt operator on* $\mathscr{H}$.

Each $T \in \mathscr{T}_F(E)$ extends continuously to an element of $\mathscr{T}_F(\mathscr{H})$, in which sense $\mathscr{T}_F(E)$ is a subgroup of $\mathscr{T}_F(\mathscr{H})$. Because the unitaries U_T, $T \in \mathscr{T}_F(\mathscr{H})$, are unique up to a phase, $T \mapsto U_T$ is a projective representation of $\mathscr{T}_F(\mathscr{H})$; some properties of this are discussed in Ref. 8.

In the following we use the determinant $\det(R)$ of a bounded (linear) operator R on $\mathscr{H}$. $\det(R)$ exists if $R - \mathbb{1}$ is of trace class, and it is approximable from finite dimensions with the usual determinant. $\det(R) = 0$, if $0 \in \sigma(R)$, with $\sigma(R)$ the spectrum of R. If $0 \notin \sigma(R)$, we have the formula $\det(R) = \exp\{\mathrm{tr}[\ln(R)]\}$, where $\ln(R)$ is well defined (cf. Ref. 8 Lemma 2.1; Ref. 15, Sections VII.3 and XI.6; Ref. 7, p. 8; and Ref. 16, Subsection X.I.4).

Lemma 3.4: Let $T \in \mathscr{T}_F(\mathscr{H})$. *Then the unitary* U_T *implementing* α_T *in the Fock representation* $(\Pi_F, F_+(\mathscr{H}))$ *is characterized uniquely by the following transition amplitude, which holds for all* $g, h \in \mathscr{H}$:

$$\langle W_F(g)\Omega_F | U_T W_F(h)\Omega_F\rangle = \langle \Omega_F | U_T\Omega_F\rangle \exp\{\tfrac{1}{2}\langle (T_l)^{-1}g | h\rangle + \tfrac{1}{4}(\langle g | T_a (T_l)^{-1} g\rangle - \langle (T_l)^{-1} T_a h | h\rangle - \|g\|^2 - \|h\|^2)\} \tag{3.5}$$

with $|\langle \Omega_F | U_T\Omega_F\rangle| = (\det(|T_l|))^{-1/2}$. *One has* $\det(|T_l|) \neq 0$, *since* $0 \notin \sigma(T_l)$ *by Corollary 2.3.*

Proof: $U_T a_F(g) U_T^* = a_F(T_l g) + a_F^*(T_a g)$, and $-i\sqrt{2}(\mathrm{d}/\mathrm{d}t) W_F(tf)\Omega_F = W_F(tf) a_F^*(f)\Omega_F$, and (3.4) lead to the following differential equations (for each $f \in \mathscr{H}$ in dependence of the parameter $t \in \mathbb{R}$):

$$\begin{aligned} 0 &= \langle W_F(tf)\Omega_F | U_T a_F((T_l)^{-1} f)\Omega_F\rangle \\ &= \langle a_F^*(f) W_F(tf)\Omega_F | U_T\Omega_F\rangle + \langle a_F(T_a (T_l)^{-1} f) W_F(tf)\Omega_F | U_T\Omega_F\rangle \\ &= i\sqrt{2}\,\frac{\mathrm{d}}{\mathrm{d}t}\langle W_F(tf)\Omega_F | U_T\Omega_F\rangle + \frac{i}{\sqrt{2}}\, t(\|f\|^2 - \langle f | T_a (T_l)^{-1} f\rangle)\langle W_F(tf)\Omega_F | U_T\Omega_F\rangle, \end{aligned}$$

the solutions of which give (3.5) for $h = 0$. $U_T W_F(h)\Omega_F = W_F(Th) U_T\Omega_F$, the Weyl relations and the decomposition of Theorem 2.5, $T_l = U|T_l|$ and $T_a = UJ|T_a|$ with $|T_l|^2 = |T_a|^2 + \mathbb{1}$, and $[|T_l|, J] = 0$ imply (3.5) for every $g, h \in \mathscr{H}$. For determining $|\langle \Omega_F | U_T\Omega_F\rangle|$ we use Subsection B of the Appendix. Choose an ONB $\mathscr{O}$ for $\mathscr{H}$ consisting of eigenvectors of $|T_a|$ with $Je = e \forall e \in \mathscr{O}$. Let $\mathscr{L}$ be the set of all finite-dimensional complex subspaces $\mathscr{V} \subseteq \mathsf{LH}(U\mathscr{O})$. Then $1 = \| U_T\Omega_F\|^2 = \sup_{\mathscr{V} \in \mathscr{L}} \|\Gamma(P_{\mathscr{V}}) U_T\Omega_F\|^2$ ($\Gamma(P_{\mathscr{V}})$ is defined in Subsection B of the Appendix). For each $\mathscr{V} \in \mathscr{L}$ choose the ONB as a subset of $U\mathscr{O}$. Then with (3.5) by direct calculation of the integrals (A2) one obtains the result. ∎

B. Hamiltonians for symplectic one-parameter groups

Assume $\{T_t | t \in \mathbb{R}\}$ to be a strongly continuous one-parameter group of symplectic transformations $T_t \in \mathscr{T}_F(\mathscr{H})$ with associated Bogoliubov transformations α_{T_t} on the Weyl algebra $\mathscr{W}(\mathscr{H})$. Whenever the group $\{T_t | t \in \mathbb{R}\}$ is nontrivial, then the associated group $\{\alpha_{T_t} | t \in \mathbb{R}\}$ on $\mathscr{W}(\mathscr{H})$ is not strongly continuous, because of $\|W(f) - W(g)\| = 2$ for $f \neq g$ (e.g., Ref. 12, Theorem 5.2.8). Nevertheless it may be possible to implement this group of Bogoliubov transformations by a strongly continuous unitary group in some representations of $\mathscr{W}(\mathscr{H})$. In the present subsection we are asking for self-adjoint operators H on $F_+(\mathscr{H})$ such that $\exp\{itH\}$ unitarily implements α_{T_t} with respect to the Fock representation $(\Pi_F, F_+(\mathscr{H}))$ for every $t \in \mathbb{R}$, that is,

$$\exp\{itH\}W_{\mathrm{F}}(f)\exp\{-itH\}=W_{\mathrm{F}}(T_t f)=(\Pi_{\mathrm{F}}\circ\alpha_{T_t})(W(f)) \quad \forall f\in\mathscr{H}. \tag{3.6}$$

The next two theorems completely solve this problem for H satisfying the additional property $\Omega_{\mathrm{F}}\in\mathscr{D}(H)$. We need some preparatory considerations.

For the self-adjoint linear C on $\mathscr{H}$ the self-adjoint operator $a_{\mathrm{F}}^*Ca_{\mathrm{F}}$ on $F_+(\mathscr{H})$ is the second quantization of C, often also denoted by $\mathrm{d}\Gamma(C)$; especially $a_{\mathrm{F}}^*\mathbb{1}a_{\mathrm{F}}=:N$ is the number operator on the Fock space $F_+(\mathscr{H})$ (cf., e.g., Ref. 12, Subsection 5.2.1, or Ref. 9, Section X.7), whose eigenspace with eigenvalue $n\in\mathbb{N}$ consists just of the n-particle subspace $\mathbb{P}_+(\otimes_n\mathscr{H})$ of $F_+(\mathscr{H})$. We want to define the quadratic operators $a_{\mathrm{F}}^*Da_{\mathrm{F}}^*$ and $a_{\mathrm{F}}Da_{\mathrm{F}}$.

Definition 3.5: For each antilinear finite rank operator D on $\mathscr{H}$ [i.e., ran(D) *is of finite dimension; e.g., Ref. 11, Theorem 6.1] with (nonunique) decomposition* $D=\Sigma_{j=1}^p\langle\cdot|f_j\rangle g_j$ *(where* $p\in\mathbb{N}$, *and* $f_j,g_j\in\mathscr{H}$ for $j\in\{1,\ldots,p\}$) *we define*

$$a_{\mathrm{F}}^*Da_{\mathrm{F}}^*:=\sum_{j=1}^p a_{\mathrm{F}}^*(f_j)a_{\mathrm{F}}^*(g_j), \quad a_{\mathrm{F}}Da_{\mathrm{F}}:=\sum_{j=1}^p a_{\mathrm{F}}(f_j)a_{\mathrm{F}}(g_j).$$

We mention that this definition is independent from the specific decomposition of D, *and* that $\mathscr{D}(N)\subseteq\mathscr{D}(a_{\mathrm{F}}^*Da_{\mathrm{F}}^*)$ *and* $\mathscr{D}(N)\subseteq\mathscr{D}(a_{\mathrm{F}}Da_{\mathrm{F}})$.

Obviously, $(a_{\mathrm{F}}^*Da_{\mathrm{F}}^*)^*\supseteq a_{\mathrm{F}}Da_{\mathrm{F}}$ and $(a_{\mathrm{F}}Da_{\mathrm{F}})^*\supseteq a_{\mathrm{F}}^*Da_{\mathrm{F}}^*$. Because creation operators commute with each other, we have $a_{\mathrm{F}}^*Da_{\mathrm{F}}^*=a_{\mathrm{F}}^*D^*a_{\mathrm{F}}^*$, resp. $a_{\mathrm{F}}Da_{\mathrm{F}}=a_{\mathrm{F}}D^*a_{\mathrm{F}}$. Hence we may restrict ourselves to self-adjoint antilinear finite rank operators D. $\mathsf{HS}_a^{sa}(\mathscr{H})$ denotes the complex-linear vector space of self-adjoint antilinear Hilbert–Schmidt operators on $\mathscr{H}$. It is well known that the self-adjoint antilinear finite rank operators on $\mathscr{H}$ are $\|.\|_{\mathsf{HS}}$-dense in $\mathsf{HS}_a^{sa}(\mathscr{H})$.

Lemma 3.6: It holds:

(a) *Let D be an antilinear finite rank operator on $\mathscr{H}$. Then*

$$\|a_{\mathrm{F}}^*Da_{\mathrm{F}}^*\psi\|\leqslant\|D\|_{\mathsf{HS}}\|((N+1)(N+2))^{1/2}\psi\| \quad \forall\psi\in\mathscr{D}(N),$$

and the same inequality holds for $a_{\mathrm{F}}Da_{\mathrm{F}}$. Hence $a_{\mathrm{F}}^*Da_{\mathrm{F}}^*$ and $a_{\mathrm{F}}Da_{\mathrm{F}}$ can be defined for arbitrary $D\in\mathsf{HS}_a^{sa}(\mathscr{H})$ by continuous approximation of D by finite rank operators, with the domain $\mathscr{D}(a_{\mathrm{F}}^*Da_{\mathrm{F}}^*):=\mathscr{D}(N)=:\mathscr{D}(a_{\mathrm{F}}Da_{\mathrm{F}})$. The mapping $D\in\mathsf{HS}_a^{sa}(\mathscr{H})\mapsto a_{\mathrm{F}}^*Da_{\mathrm{F}}^*$ is (complex-) linear, and $D\in\mathsf{HS}_a^{sa}(\mathscr{H})\mapsto a_{\mathrm{F}}Da_{\mathrm{F}}$ is antilinear.

(b) *Let be $C=C^*$ linear with core $\mathscr{D}_C\subseteq\mathscr{H}$,* and $D=D^*\in\mathsf{HS}_a^{sa}(\mathscr{H})$. *Then*

$$H:=\tfrac{1}{2}(a_{\mathrm{F}}^*Da_{\mathrm{F}}^*+a_{\mathrm{F}}Da_{\mathrm{F}})+a_{\mathrm{F}}^*Ca_{\mathrm{F}}$$

is essentially self-adjoint on the linear hull L of vectors $\mathbb{P}_+(f_1\otimes\cdots\otimes f_n)$ with $f_1,\ldots,f_n\in\mathscr{D}_C$ and $n\in\mathbb{N}\cup\{0\}$. Especially, $\|H\Omega_{\mathrm{F}}\|=(1/\sqrt{2})\|D\|_{\mathsf{HS}}$.

Proof: We omit the index F standing for Fock. (a): We decompose $D=\Sigma_{j=1}^p\alpha_j\langle\cdot|f_j\rangle g_j$ with $\alpha_j\in\mathbb{C}$ and $f_j,g_j\in\mathscr{H}$ such that $\{f_1,\ldots,f_p\}$ is an orthonormal system of $\mathscr{H}$ and $\{g_1,\ldots,g_p\}$, too. Define the linear operator $X_n:\otimes_n\mathscr{H}\to\otimes_{n+2}\mathscr{H}$, $\xi\mapsto\sqrt{(n+1)(n+2)}\Sigma_{j=1}^p\alpha_j f_j\otimes g_j\otimes\xi$. Then $\|X_n\|=\sqrt{(n+1)(n+2)}\|D\|_{\mathsf{HS}}$. Now observe that $a^*Da^*=\oplus_n\mathbb{P}_+X_n\mathbb{P}_+$.

(b): We show that $\mathrm{ran}(H|_L-z)$ is dense in $F_+(\mathscr{H})$ for each $z\in\mathbb{C}$ with $\mathrm{Im}(z)\neq0$, which gives the essential self-adjointness of $H|_L$ (e.g., Ref. 11, Theorem 5.21). Let $\eta=\oplus_k\eta_k\in F_+(\mathscr{H})$, $\eta_k\in\mathbb{P}_+(\otimes_k\mathscr{H})$, with $\eta\perp\mathrm{ran}(H|_L-z)$. Because of (a) especially for vectors $\xi\in L\cap\mathbb{P}_+(\otimes_k\mathscr{H})$ we obtain $2\langle(a^*Ca-z)\xi|\eta_k\rangle+\langle\xi|aDa\,\eta_{k+2}\rangle+\langle\xi|a^*Da^*\eta_{k-2}\rangle=0$. But a^*Ca is essentially selfadjoint on $L\cap\mathbb{P}_+(\otimes_k\mathscr{H})$ as an operator on $\mathbb{P}_+(\otimes_k\mathscr{H})$, which implies $\eta_k\in\mathscr{D}(a^*Ca)$ and $2a^*Ca\,\eta_k+aDa\,\eta_{k+2}+a^*Da^*\eta_{k-2}=\overline{z}\,\eta_k\,\forall k\in\mathbb{N}$. Taking the imaginary part of the inner product with η_k, one obtains

$$\mathrm{Im}(z)\|\eta_k\|^2=\mathrm{Im}\langle\eta_{k+2}|a^*Da^*\eta_k\rangle-\mathrm{Im}\langle\eta_k|a^*Da^*\eta_{k-2}\rangle.$$

Consequently, $\mathrm{Im}(z)\Sigma_{k=0}^{n}\|\eta_k\|^2=\mathrm{Im}\langle\eta_{n+2}|a^*Da^*\eta_n\rangle+\mathrm{Im}\langle\eta_{n+1}|a^*Da^*\eta_{n-1}\rangle$. Hence with the estimations of (a) we get for each $n\in\mathbb{N}$

$$|\mathrm{Im}(z)|\sum_{k=0}^{n}\|\eta_k\|^2\leqslant\sqrt{(n+1)(n+2)}\||D|\|_{\mathsf{HS}}(\|\eta_{n+2}\|+\|\eta_{n+1}\|+\|\eta_n\|+\|\eta_{n-1}\|). \tag{3.7}$$

Assume $\eta\neq0$. Then there is an $n_0\in\mathbb{N}$ with $\Sigma_{k=0}^{n_0}\|\eta_k\|^2=:c>0$. Equation (3.7) now gives

$$4\sum_{n=n_0-1}^{\infty}\|\eta_n\|^2\geqslant\frac{|\mathrm{Im}(z)|c}{\||D|\|_{\mathsf{HS}}}\sum_{n=n_0}^{\infty}((n+1)(n+2))^{-1/2}=\infty,$$

which is a contradiction to $\|\eta\|^2=\Sigma_k\|\eta_k\|^2<\infty$. Thus $\eta=0$ and $\mathrm{ran}(H|_L-z)$ is dense.

Now use the decomposition (3.8) from below. Then $H\Omega_{\mathrm{F}}=\frac{1}{2}a^*Da^*\Omega_{\mathrm{F}}=2^{-1/2}\Sigma_k d_k e_k\otimes e_k$, which gives $\|H\Omega_{\mathrm{F}}\|^2=\frac{1}{2}\|D\|_{\mathsf{HS}}^2$. ∎

Let be $D=D^*\in\mathsf{HS}_a^{sa}(\mathscr{H})$ and J an antilinear involution on $\mathscr{H}$ from Lemma 2.12, i.e., $D=J|D|$ and J commutes with D and $|D|$. We select an ONB $\{e_k|k\in I\}$ of $\mathscr{H}$ consisting of eigenvectors for $|D|$ so that $Je_k=e_k\forall k\in I$, i.e., $|D|e_k=d_ke_k$ with $d_k\geqslant0\forall k\in I$ and $\Sigma_{k\in I}d_k^2<\infty$. Hence the antilinear $D\in\mathsf{HS}_a^{sa}(\mathscr{H})$ may be represented as $D=\Sigma_{k\in I}d_k\langle.|e_k\rangle e_k$, and by Lemma 3.6(a) we have

$$a_{\mathrm{F}}^*Da_{\mathrm{F}}^*\psi=\sum_{k\in I}d_ka_{\mathrm{F}}^*(e_k)a_{\mathrm{F}}^*(e_k)\psi\quad\forall\psi\in\mathscr{D}(N), \tag{3.8}$$

where the series converge with respect to the norm on $F_+(\mathscr{H})$ (the analogous equation is valid for $a_{\mathrm{F}}Da_{\mathrm{F}}$). This implies that, for $N=\infty$ in the case $\Sigma_{n=1}^{\infty}|\zeta_n|^2<\infty$, the Hamiltonian H_q from the introduction is a well-defined self-adjoint operator in the Fock representation (observe that, for each $n\in\mathbb{N}$, we have $\zeta_n\langle.|e_n\rangle e_n=|\zeta_n|\langle.|z_ne_n\rangle(z_ne_n)$ and $\zeta_na_n^*a_n^*\equiv\zeta_na_{\mathrm{F}}^*(e_n)^2=|\zeta_n|a_{\mathrm{F}}^*(z_ne_n)^2$, where $z_n:=\exp\{(i/2)\arg(\zeta_n)\}$), and the power series in (1.1) converges in the strong resolvent sense by Ref. 11, Theorem 9.16.

Theorem 3.7: *Let $C=C^*$ be a linear operator on $\mathscr{H}$ and $D=D^*$ an antilinear Hilbert–Schmidt operator on $\mathscr{H}$, and let $H=\frac{1}{2}(a_{\mathrm{F}}^*Da_{\mathrm{F}}^*+a_{\mathrm{F}}Da_{\mathrm{F}})+a_{\mathrm{F}}^*Ca_{\mathrm{F}}$ be the self-adjoint operator on $F_+(\mathscr{H})$ from Lemma 3.6. Then, for each $t\in\mathbb{R}$ it holds $T_t:=\exp\{it(C-D)\}\in\mathscr{T}_{\mathrm{F}}(\mathscr{H})$ (cf. Theorem 2.10), and $\exp\{itH\}$ unitarily implements α_{T_t} with respect to the Fock representation $(\Pi_{\mathrm{F}},F_+(\mathscr{H}))$ [see Eq. (3.6)].*

Moreover, $\langle\Omega_{\mathrm{F}}|\exp\{itH\}\Omega_{\mathrm{F}}\rangle=(\det((T_{-t})_l\exp\{itC\}))^{-1/2}$, where $(T_{-t})_l\exp\{itC\}-\mathbb{1}$ is of trace class, and $\langle W_{\mathrm{F}}(g)\Omega_{\mathrm{F}}|\exp\{itH\}W_{\mathrm{F}}(h)\Omega_{\mathrm{F}}\rangle$ is given by Eq. (3.5) with $U_{T_t}\equiv\exp\{itH\}$ for every $f,g\in\mathscr{H}$ and all $t\in\mathbb{R}$.

Proof: We omit the index F. That $T_t\in\mathscr{T}_{\mathrm{F}}(\mathscr{H})$ immediately follows from the Theorems 2.10 and 3.1 with the perturbation expansion. For antilinear $X=X^*$ of Hilbert–Schmidt class we put $H(X):=\frac{1}{2}(a^*Xa^*+aXa)$. Let $U_t:=\exp\{ita^*Ca\}$ and $u_t:=\exp\{itC\}$. We use $U_t\Phi(h)U_{-t}=\Phi(u_th)$ and (3.8) applied to X for deriving $U_tH(X)U_{-t}=H(u_tXu_{-t})$, and the CCR for checking $i[H(X),\Phi(h)]=\Phi(-iXh)$ for each $h\in\mathscr{H}$. With the Dyson expansion for the perturbation $H(D)$ (e.g., Ref. 12, Proposition 5.4.1) we obtain

$$\begin{aligned}&\exp\{itH\}\Phi(f\,)\exp\{-itH\}\\&\quad=\sum_{n=0}^{\infty}\int_0^t\mathrm{d}t_1\int_0^{t_1}\mathrm{d}t_2\cdots\\&\quad\times\int_0^{t_{n-1}}\mathrm{d}t_n i^n[U_{t_n}H(D)U_{-t_n},[\ldots[U_{t_n}H(D)U_{-t_n},U_t\Phi(f\,)U_{-t}]\ldots]]\end{aligned}$$

$$
\begin{aligned}
&= \sum_{n=0}^{\infty} \int_0^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 \cdots \int_0^{t_{n-1}} \mathrm{d}t_n i^n [H(u_{t_n} D u_{-t_n}), [\ldots [H(u_{t_1} D u_{-t_1}), \Phi(u_t f)]\ldots]] \\
&= \sum_{n=0}^{\infty} \int_0^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 \cdots \int_0^{t_{n-1}} \mathrm{d}t_n \Phi(u_{t_n}(-iD) u_{-t_n} \cdots u_{t_1}(-iD) u_{-t_1} u_t f) \\
&= \Phi(T_t f),
\end{aligned}
$$

which converges for small t on finite particle vectors because of the estimations of Lemma 3.6 (detailed estimations of the perturbation terms may be done analoguously to Ref. 17).

We calculate $\langle \Omega_{\mathrm{F}} | \exp\{itH\} \Omega_{\mathrm{F}} \rangle$. Equation (3.8) yields $H\Omega_{\mathrm{F}} = \frac{1}{2} a^* D a^* \Omega_{\mathrm{F}} = 2^{-1/2} \Sigma_k d_k e_k \otimes e_k$, from which with Eq. (3.3) we obtain the differential equation

$$
\begin{aligned}
\frac{1}{i} \frac{\mathrm{d}}{\mathrm{d}t} \langle \Omega_{\mathrm{F}} | \exp\{itH\} \Omega_{\mathrm{F}} \rangle &= \langle H\Omega_{\mathrm{F}} | \exp\{itH\} \Omega_{\mathrm{F}} \rangle \\
&= \sum_k \frac{d_k}{\sqrt{2}} \langle e_k \otimes e_k | \exp\{itH\} \Omega_{\mathrm{F}} \rangle \\
&\overset{(3.3)}{=} -\sum_k \frac{d_k}{2} \langle e_k | (T_t)_a ((T_t)_l)^{-1} e_k \rangle \langle \Omega_{\mathrm{F}} | \exp\{itH\} \Omega_{\mathrm{F}} \rangle \\
&= -\tfrac{1}{2} \overline{\mathrm{tr}[D(T_t)_a ((T_t)_l)^{-1}]} \langle \Omega_{\mathrm{F}} | \exp\{itH\} \Omega_{\mathrm{F}} \rangle. \qquad (3.9)
\end{aligned}
$$

Obviously, $\mathrm{d}(T_t)_l/\mathrm{d}t = (\mathrm{d}T_t/\mathrm{d}t)_l = i(C(T_t)_l - D(T_t)_a)$. Hence, putting $M_t := u_{-t}(T_t)_l$ we obtain $iM_t^{-1} \mathrm{d}M_t/\mathrm{d}t = ((T_t)_l)^{-1} D(T_t)_a$ to be of trace class, which with the formula $\det(M_t) = \exp\{\mathrm{tr}[\ln(M_t)]\}$ implies

$$
-2i\sqrt{\det(M_t)} \, \frac{\mathrm{d}(\det(M_t))^{-1/2}}{\mathrm{d}t} = \mathrm{tr}[((T_t)_l)^{-1} D(T_t)_a] = \mathrm{tr}[D(T_t)_a ((T_t)_l)^{-1}].
$$

Comparing with (3.9) yields $\langle \Omega_{\mathrm{F}} | \exp\{itH\} \Omega_{\mathrm{F}} \rangle = \overline{(\det(M_t))^{-1/2}} = (\det((T_t)_l^* u_t))^{-1/2}$. Now observe $T_{-t} = T_t^{-1}$, and hence $(T_t)_l^* = (T_{-t})_l$ by Eq. (2.4). That $(T_{-t})_l u_t - \mathbb{1}$ (resp. $M_t - \mathbb{1}$) are of trace class follows immediately from the perturbation expansion. ■

Theorem 3.8: *For each $t \in \mathbb{R}$ let $T_t \in \mathscr{T}_{\mathrm{F}}(\mathscr{H})$, and let H be a self-adjoint operator on $F_+(\mathscr{H})$ such that* $\exp\{itH\}$ *unitarily implements α_{T_t} with respect to $(\Pi_{\mathrm{F}}, F_+(\mathscr{H}))$ for every $t \in \mathbb{R}$* [cf. *Eq. (3.6)*]. *Then $\{T_t | t \in \mathbb{R}\}$ is a strongly continuous group, and we have the following equivalences*

(i) $\Omega_{\mathrm{F}} \in \mathscr{D}(H)$,

(ii) *there exists a linear operator $C = C^*$ on $\mathscr{H}$ and an antilinear Hilbert–Schmidt operator $D = D^*$ on $\mathscr{H}$ with $T_t = \exp\{it(C-D)\} \forall t \in \mathbb{R}$* (cf. *Theorem 2.10*).

If (i) and (ii) are fulfilled, then the (linear, resp. *antilinear) self-adjoint operators C and D are uniquely given, and it is $H = \frac{1}{2}(a_{\mathrm{F}}^* D a_{\mathrm{F}}^* + a_{\mathrm{F}} D a_{\mathrm{F}}) + a_{\mathrm{F}}^* C a_{\mathrm{F}} + \kappa \mathbb{1}$ for $a \kappa \in \mathbb{R}$.*

Proof: That $\{T_t | t \in \mathbb{R}\}$ forms a group is immediate. Let us check its strong continuity: With the Weyl relations (3.1) and (3.2) we obtain for each $f \in \mathscr{H}$

$$1=\lim_{t\to 0}|\langle W_{\mathrm{F}}(f\,)\Omega_{\mathrm{F}}|\exp\{itH\}W_{\mathrm{F}}(f\,)\exp\{-itH\}\Omega_{\mathrm{F}}\rangle|\overset{(3.6)}{=}\lim_{t\to 0}|\langle W_{\mathrm{F}}(f\,)\Omega_{\mathrm{F}}|W_{\mathrm{F}}(T_t f\,)\Omega_{\mathrm{F}}\rangle|$$

$$\overset{(3.1)}{=}\lim_{t\to 0}|\langle\Omega_{\mathrm{F}}|W_{\mathrm{F}}(T_t f-f\,)\Omega_{\mathrm{F}}\rangle|\overset{(3.2)}{=}\lim_{t\to 0}\exp\{-\tfrac{1}{4}\|T_t f-f\|^2\}.$$

Hence there exists the generator $G, T_t=\exp\{tG\}$, a closed real-linear operator on $\mathscr{H}$ with dense real-linear domain $\mathscr{D}(G)$.

Because of Theorem 3.7 and since the U_{T_t} are unique up to a phase by Theorem 3.1, it suffices to prove (i)⇒(ii). Let $H':=H-\langle\Omega_{\mathrm{F}}|H\Omega_{\mathrm{F}}\rangle\mathbb{1}$. Then Eq. (3.5) gives for each $g\in\mathscr{H}$ and all $t\in\mathbb{R}$

$$\langle W_{\mathrm{F}}(g)\Omega_{\mathrm{F}}|\exp\{itH'\}\Omega_{\mathrm{F}}\rangle=\langle\Omega_{\mathrm{F}}|\exp\{itH'\}\Omega_{\mathrm{F}}\rangle\exp\{\tfrac{1}{4}(\langle g|(T_t)_a((T_t)_l)^{-1}g\rangle-\|g\|^2)\}. \tag{3.10}$$

Since $\Omega_{\mathrm{F}}\in\mathscr{D}(H')$ we may differentiate $d/dt\cdots|_{t=0}$, and it follows that

$$\frac{d}{dt}\langle g|(T_t)_a((T_t)_l)^{-1}g\rangle\bigg|_{t=0}=\frac{d}{dt}\langle g|T_t((T_t)_l)^{-1}g\rangle\bigg|_{t=0}=:q(g)$$

exists for all $g\in\mathscr{H}$. But $q(g)=\langle g|Gg\rangle\forall g\in\mathscr{D}(G)$. We define the (complex-) bi-antilinear form $d(f,g):=\frac{1}{4}(q(f+g)-q(f-g))$ with $\mathscr{D}(d)=\mathscr{H}$, which satisfies $d(f,g)=d(g,f\,)\forall f,\ g\in\mathscr{H}$. Hence (3.10) implies $\langle W_{\mathrm{F}}(g)\Omega_{\mathrm{F}}|H'\Omega_{\mathrm{F}}\rangle=\frac{1}{4}d(g,g)\exp\{-\frac{1}{4}\|g\|^2\}\forall g\in\mathscr{H}$. Now let $\mathscr{V}$ be an arbitrary finite-dimensional complex subspace $\mathscr{V}\subseteq\mathscr{H}$ with ONB $\{e_1,\ldots,e_m\}$, where $m:=\dim_{\mathbb{C}}\mathscr{V}$. Then Proposition A3 and Lemma A2 from the Appendix yield

$$\|\Gamma(P_{\mathscr{V}})H'\Omega_{\mathrm{F}}\|^2=\frac{1}{2}\sum_{k,l=1}^{m}|d(e_k,e_l)|^2=\frac{1}{2}\|D_{\mathscr{V}}\|_{\mathsf{HS}}^2\geqslant\frac{1}{2}\|D_{\mathscr{V}}\|^2, \tag{3.11}$$

where $D_{\mathscr{V}}=D_{\mathscr{V}}^*$ is the antilinear operator on $\mathscr{V}$ with $d(f,g)=\langle f|D_{\mathscr{V}}g\rangle\forall f,\ g\in\mathscr{V}$. Consequently $|d(f,g)|\leqslant\sqrt{2}\|H'\Omega_{\mathrm{F}}\|\,\|f\|\,\|g\|\forall f,\ g\in\mathscr{H}$, and the form d is bounded, which implies the existence of an antilinear bounded $D=D^*$ on $\mathscr{H}$ with $d(f,g)=\langle f|-iDg\rangle\forall f,\ g\in\mathscr{H}$. Equation (3.11) finally gives $\||D|\|_{\mathsf{HS}}=\sqrt{2}\|H'\Omega_{\mathrm{F}}\|$, i.e., $|D|$ is Hilbert–Schmidt.

Now consider $\mathscr{H}$ as a real Hilbert space with scalar product $(.|.):=\mathrm{Re}\langle.|.\rangle$. Since $d(g,g)=q(g)=\langle g|Gg\rangle\forall g\in\mathscr{D}(G)$, we have that $\mathrm{Re}(d(f,g))$ is a real-bilinear form on $\mathscr{H}$ with

$$(f|-iDg)=(-iDf|g)=\mathrm{Re}(d(f,g))=\tfrac{1}{2}((f|Gg)+(Gf|g))\quad\forall f,g\in\mathscr{D}(G),$$

which for $\Lambda:=G+iD$ implies $0=(f|\Lambda g)+(\Lambda f|g)$. Hence $\Lambda=-\Lambda^+$ by Lemma A1, where Λ^+ is the adjoint of Λ with respect to the real scalar product $(.|.)$. Then, as in the proof of Theorem 2.10, it follows: $C:=-i\Lambda$ is complex-linear and self-adjoint with respect to the complex scalar product $\langle.|.\rangle$, i.e., $C=C^*$. ■

Corollary 3.9: Let $\{T_t|t\in\mathbb{R}\}\subset\mathscr{T}_{\mathrm{F}}(\mathscr{H})$ *be a strongly continuous group. Assume the existence of a* $T\in\mathscr{T}_{\mathrm{F}}(\mathscr{H})$ *such that* $T^{-1}T_tT=\exp\{it(C-D)\}\ \forall t\in\mathbb{R}$ *for some linear* $C=C^*$ *and* $D\in\mathsf{HS}_a^{sa}(\mathscr{H})$ (*or, equivalently* $T^{-1}GT=i(C-D)$ *for the generator* G *of* $T_t=\exp\{tG\}$). *Then* $\exp\{itH\}$ *unitarily implements* α_{T_t} *with respect to* Π_{F} *for every* $t\in\mathbb{R}$ [*cf. Eq. (3.6)*], *where* $H=U_T[\frac{1}{2}(a_{\mathrm{F}}^*Da_{\mathrm{F}}^*+a_{\mathrm{F}}Da_{\mathrm{F}})+a_{\mathrm{F}}^*Ca_{\mathrm{F}}]U_T^*$.

For $C=0$ the situation is somewhat simpler, which is shown by the following

Corollary 3.10: Let $D=D^*$ *be antilinear and bounded on* $\mathscr{H}$, *and* J *the antilinear involution from Lemma 2.12. Then*

$$T_t:=\exp\{-itD\}=\cosh(t|D|)-iJ\,\sinh(t|D|)\in\mathscr{T}(\mathscr{H})$$

for all $t\in\mathbb{R}$ (cf. *Example 2.13). Moreover, we have the following equivalences:*

(i) $|D|$ *is a Hilbert–Schmidt operator on* $\mathscr{H}$,

(ii) $T_t \in \mathscr{T}_{\mathrm{F}}(\mathscr{H})$ *for some real* $t \neq 0$,
(iii) $T_t \in \mathscr{T}_{\mathrm{F}}(\mathscr{H})$ *for all* $t \in \mathbb{R}$,
(iv) *there exists a unitary* U_{T_t} on $F_+(\mathscr{H})$, *which unitarily implements* α_{T_t} *with respect to* Π_{F} *for some real* $t \neq 0$.

If these conditions are valid, then U_{T_t} *from (iv) is uniquely (up to a phase) given by* $U_{T_t} = \exp\{itH\}$ with $H = \frac{1}{2}(a_{\mathrm{F}}^* D a_{\mathrm{F}}^* + a_{\mathrm{F}} D a_{\mathrm{F}})$.

Proof: The decomposition of T_t follows from the exponential series. Because of Theorems 3.7 and 3.8 it remains to prove and (iv)⇒(ii)⇒(i). However, V_t implementing α_{T_t} with respect to Π_{F} implies $T_t \in \mathscr{T}_{\mathrm{F}}(\mathscr{H})$ by definition. Theorem 3.1 yields $\sinh(t|D|)$ to be Hilbert–Schmidt for a $t \neq 0$. Thus there exists an ONB $\{e_k | k \in I\}$ for $\mathscr{H}$ consisting of eigenvectors for $|D|$, $|D| e_k = d_k e_k, d_k \geqslant 0$, satisfying

$$\infty > \sum_{n=1}^{\infty} \sinh(t d_k)^2 = \frac{1}{2} \sum_{n=1}^{\infty} (\cosh(2t d_k) - 1) \geqslant t^2 \sum_{n=1}^{\infty} d_k^2,$$

which gives (i). The rest follows from Theorems 3.1 and 3.7. ■

Let us continue Example 2.11.

Example 3.11: Let all be as in Example 2.11. In addition assume R to be Hilbert–Schmidt and $T \in \mathscr{T}_{\mathrm{F}}(\mathscr{H})$. *Then, by Theorem 3.1 the latter is equivalent with* $\sinh(R)$ *being Hilbert–Schmidt on* $\mathscr{H}$, *and Theorem 3.7 implies* $T_t \in \mathscr{T}_{\mathrm{F}}(\mathscr{H}) \forall t \in \mathbb{R}$. *Since* $\mathscr{T}_{\mathrm{F}}(\mathscr{H})$ *is a group, we have* $T_t \in \mathscr{T}_{\mathrm{F}}(\mathscr{H}) \forall t \in \mathbb{R}$.

Even in this case C may be chosen such that $\hat{S}$ *is unbounded. For example, define C by* $c_k := k/\sinh(r_k) \forall k \in \mathbb{R}$. *Then (2.6) yields* $\hat{S}$ *to be unbounded.*

APPENDIX

1. On generators of groups on real Hilbert spaces

For the proof of Theorem 2.10 we need some group theoretical results on real Hilbert spaces. Here in the first part of the Appendix we exclusively are concerned with a real Hilbert space $\mathscr{H}_r$ with scalar product $(.|.)$, and with real-linear operators having real-linear domains. The adjoint of the (real-linear) operator A on $\mathscr{H}_r$ is denoted by A^+. Let us mention that each weakly continuous (semi-) group on $\mathscr{H}_r$ is strongly continuous and its weak and strong generators coincide (Ref. 12, Corollary 3.1.8).

Lemma A1: Let $\{T_t | t \in \mathbb{R}\}$ *be a strongly continuous group on* $\mathscr{H}_r$ *with generator G*, i.e., $T_t = \exp\{tG\}$, $t \in \mathbb{R}$, *and growth* $\|T_t\| \leqslant \exp\{\beta|t|\} \forall t \in \mathbb{R}$ for some $\beta \geqslant 0$. *It follows* $\mathscr{D}(G) = \mathscr{D}(G^+)$, G^+ *is the generator of the adjoint group* $\{T_t^+ | t \in \mathbb{R}\}$, and G *decomposes uniquely as* $G = \Lambda + D$ *with the closed operator* $\Lambda = -\Lambda^+$ *and the bounded operator* $D = D^+$. *Especially,* $D \supseteq \frac{1}{2}(G + G^+)$ *and* $\Lambda = \frac{1}{2}(G - G^+)$.

Proof: G is closed with dense domain $\mathscr{D}(G)$ (Ref. 12, Theorem 3.1.22). Hence $\{T_{\pm t} \exp\{-\beta t\} | t \geqslant 0\}$ defines two semigroups of contractions. Differentiating $\|T_{\pm t} \exp\{-\beta t\} f\|^2 \leqslant \|f\|^2$ for $t \geqslant 0$ yields

$$0 \geqslant \frac{\mathrm{d}}{\mathrm{d}t} \| T_{\pm t} \exp\{-\beta t\} f \|^2 \Big|_{t=0} = 2(f | (\pm G - \beta) f) \quad \forall f \in \mathscr{D}(G),$$

which gives $-\beta \|f\|^2 \leqslant (f|Gf) \leqslant \beta \|f\|^2 \forall f \in \mathscr{D}(G)$. Let us define on $\mathscr{D}(G)$ the symmetric (real)-bilinear form $s(f,g) = \frac{1}{2}((f|Gg) + (Gf|g))$. Then $-\beta \|f\|^2 \leqslant s(f,f) \leqslant \beta \|f\|^2 \forall f \in \mathscr{D}(G)$ implies the boundedness of s (which we extend to all of $\mathscr{H}_r$) and the existence of a bounded operator $D = D^+$ on $\mathscr{H}_r$ with $s(f,g) = (f|Dg) \forall f,g \in \mathscr{H}_r$ (Ref. 9, Theorem VIII.15). Let $\Lambda := G - D$. Then

$$0 = \tfrac{1}{2}((f|Gg) + (Gf|g)) - (f|Dg) = \tfrac{1}{2}((f|\Lambda g) + (\Lambda f|g))$$

from which follows $\Lambda \subseteq -\Lambda^+$.

On the other side the adjoint group is weakly (and hence strongly) continuous with generator G^+. Now $G^+=\Lambda^+ + D$ and the same procedure as above yield $\Lambda^+ \subseteq -\Lambda^{++}$. But G is closed, and thus Λ is so, which gives $\Lambda^{++}=\Lambda$ (Ref. 11, Theorem 5.3). Uniqueness follows from $D \supseteq \frac{1}{2}(G+G^+)$ and $\Lambda=\frac{1}{2}(G-G^+)$. ■

2. Second quantized projections

Here we prove some results, which we need for Lemma 3.4 and Theorem 3.7. On $\mathbb{C}^m \cong \mathbb{R}^{2m}$ we denote by $d^{2m}\alpha$ the Lebesgue measure $\mathrm{dRe}(\alpha_1)\,\mathrm{dIm}(\alpha_1)\cdots\mathrm{dRe}(\alpha_m)\,\mathrm{dIm}(\alpha_m)$ for $\alpha=(\alpha_1,...,\alpha_m)\in\mathbb{C}^m$.

Lemma A2: For $m\in\mathbb{N}$ let $E:\mathbb{C}^m\to\mathbb{C}$, $\alpha\mapsto\exp\{-\frac{1}{2}\Sigma_{k=1}^m|\alpha_k|^2\}$. Then for every $p_k, q_k \in \mathbb{N}\cup\{0\}$ we have

$$\int_{\mathbb{R}^{2m}} E(\alpha)\overline{\alpha_1}^{p_1}\cdots\overline{\alpha_m}^{p_m}\alpha_1^{q_1}\cdots\alpha_m^{q_m}\,\mathrm{d}^{2m}\alpha=(\delta_{p_1,q_1}\cdots\delta_{p_m,q_m})(2\pi)^m(2^{p_1}(p_1!)\cdots 2^{p_m}(p_m!))$$

where $\delta_{k,l}=0$ for $k\neq l$ and $\delta_{k,l}=1$ for $k=1$.

Proof: We have $\overline{\alpha_k}E(\alpha) = -2(\partial E/\partial\alpha_k)(\alpha)$ and $\alpha_k E(\alpha) = -2(\partial E/\partial\overline{\alpha_k})(\alpha)$. Now use integration by parts, $\int(\partial E/\partial\alpha_k)F\,\mathrm{d}^{2m}\alpha=-\int E(\partial F/\partial\alpha_k)\mathrm{d}^{2m}\alpha$ and $\int(\partial E/\partial\overline{\alpha_k})F\,\mathrm{d}^{2m}\alpha = -\int E(\partial F/\partial\alpha_k)\mathrm{d}^{2m}\alpha$. ■

From now on we are exclusively concerned with complex-linear spaces and operators. Let $\mathscr{H}$ be a Hilbert space. On the Fock space $F_+(\mathscr{H})=\oplus_{n=0}^\infty \mathbb{P}_+(\otimes_n\mathscr{H})$ the Glauber vectors are given as $\mathscr{G}(h)=W_F(-i\sqrt{2}h)\Omega_\mathrm{F}$, $h\in\mathscr{H}$ (cf., e.g., Ref. 18, Section 8.1), where

$$W_\mathrm{F}(g)\Omega_\mathrm{F}=\exp\{-\tfrac{1}{4}\|g\|^2\}\left[\bigoplus_{n=0}^{\infty}\left(\frac{i}{\sqrt{2}}\right)^n\frac{1}{\sqrt{n!}}(\otimes_n g)\right],\quad g\in\mathscr{H}. \tag{A1}$$

For a subspace $\mathscr{V}$ of $\mathscr{H}$ with associated orthogonal projection $P_\mathscr{V}$ from $\mathscr{H}$ onto $\mathscr{V}$ let $\Gamma(P_\mathscr{V}):=\oplus_{n=0}^\infty(\otimes_n P_\mathscr{V})$ (second quantization, cf. Ref. 12, Subsection 5.2.1, or Ref. 9, Section X.7), which is an orthogonal projection in $F_+(\mathscr{H})$. As a consequence of Lemma A2 we obtain:

Proposition A3: Let $\mathscr{V}$ be an m-dimensional subspace of $\mathscr{H}$ with arbitrary ONB *$\{e_k|k=1,\ldots,m\}$, $m\in\mathbb{N}$. Then for each $\psi\in F_+(\mathscr{H})$ we have*

$$\|\Gamma(P_\mathscr{V})\psi\|^2=\frac{1}{(2\pi)^m}\int_{\mathbb{R}^{2m}}|\langle W_\mathrm{F}\left(\sum_{k=1}^m\alpha_k e_k\right)\Omega_\mathrm{F}|\psi\rangle|^2\,\mathrm{d}^{2m}\alpha. \tag{A2}$$

Proof: Let $\psi=\oplus_{n=0}^\infty\psi_n$ with $\psi_n\in\mathbb{P}_+(\oplus_n\mathscr{H})$. Then

$$\left\langle\otimes_n\left(\sum_{k=1}^m\alpha_k e_k\right)\middle|\psi_n\right\rangle=\sum_{\text{a.p.:}n_1,\ldots,n_m}\frac{n!}{n_1!\cdots n_m!}\,\alpha_1^{n_1}\cdots\alpha_m^{n_m}\langle\mathbb{P}_+(e_1\otimes\cdots e_m)|\psi_n\rangle,$$

where $\Sigma_{\text{a.p.:}n_1,\ldots,n_m}$ runs over all possibilities for $n_k\in\{0,\ldots,n\}$ with $\Sigma_{k=1}^m n_k=n$ and e_k appears n_k times in $\langle\mathbb{P}_+(e_1\otimes\cdots e_m)|\psi_n\rangle\equiv\langle n_1,\ldots,n_m|\psi_n\rangle$. Now for $M\in\mathbb{N}$ let

$$G_M(\alpha):=\sqrt{E(\alpha)}\sum_{n=0}^M\left(\frac{-i}{\sqrt{2}}\right)^n\frac{1}{\sqrt{n!}}\sum_{\text{a.p.:}n_1,\ldots,n_m}\frac{n!}{n_1!\cdots n_m!}\,\alpha_1^{n_1}\cdots\alpha_m^{n_m}\langle n_1,\ldots,n_m|\psi_n\rangle,$$

for which $\lim_{M\to\infty}G_M(\alpha)=\langle W_F(\Sigma_{k=1}^m\alpha_k e_k)\Omega_\mathrm{F}|\psi\rangle\forall\alpha\in\mathbb{C}^m$ by Eq. (A1). Now remember that $\{\sqrt{n!/n_1!\ldots n_m!}|n_1,\ldots,n_m\rangle|\Sigma_{k=1}^m n_k=n\}$ forms an ONB for $\mathbb{P}_+(\otimes_n\mathscr{H})$, and use Lemma A2 to deduce

$$\int_{\mathbb{R}^{2m}}|G_M(\alpha)|^2\,\mathrm{d}^{2m}\alpha=(2\pi)^m\sum_{n=0}^M\|\Gamma(P_\mathscr{V})\psi_n\|^2,$$

which implies that $\lim_M\int\cdots=\int\lim_M\cdots$. ■

Consider the linear space $\mathscr{M}$ of mappings $\Theta:\mathscr{H}\to\mathbb{C}$, $f\mapsto\Theta(f)$, for which for each finite-dimensional subspace $\mathscr{V}\subseteq\mathscr{H}$ the functions $\alpha\in\mathbb{C}^m\cong\mathbb{R}^{2m}\mapsto\Theta(\Sigma_{k=1}^m\alpha_k e_k)$ are measurable, where $\{e_k|k=1,\ldots,m\}$ is an ONB of $\mathscr{V}$. Obviously, $\int_{\mathbb{R}^{2m}}\Theta(\Sigma_{k=1}^m\alpha_k e_k)\mathrm{d}^{2m}\alpha$ does not depend on the ONB of $\mathscr{V}$, and thus one puts $[1/(2\pi)^m]\mathrm{d}^{2m}\alpha\equiv\mathrm{d}\mu_{\mathscr{V}}(f)$. If $\mathscr{S}$ is the collections of all finite-dimensional subspaces of $\mathscr{H}$ ordered by inclusion, one constructs the *continual integral* Hilbert space $\mathscr{K}_c(\mathscr{H})$ to consist of those $\Theta\in\mathscr{M}$ for which $\lim_{\mathscr{V}\in\mathscr{S}}\int_{\mathscr{V}}|\Theta(f)|^2\,d\mu_{\mathscr{V}}(f)<\infty$. Since $\lim_{\mathscr{V}\in\mathscr{S}}\|\Gamma(P_{\mathscr{V}})\psi\|=\|\psi\|\forall\psi\in F_+(\mathscr{H})$, from Eq. (A2) follows that $F_+(\mathscr{H})$ and $\mathscr{K}_c(\mathscr{H})$ are unitarily equivalent in the sense that $\psi\in F_+(\mathscr{H})$ corresponds to the functional $f\in\mathscr{H}\mapsto\langle W_{\mathrm{F}}(f)\Omega_{\mathrm{F}}|\psi\rangle$ in $\mathscr{K}_c(\mathscr{H})$ (cf., e.g., Ref. 7).

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[2] In the smeared field formalism the creation and annihilation operators ''smeared'' by the ''test function'' $f\in\mathscr{H}$ are given as $a^*(f)=\Sigma_{n=1}^N\langle e_n|f\rangle a^*(e_n)$ resp. $a(f)=\Sigma_{n=1}^N\overline{\langle e_n|f\rangle}a(e_n)$, where $f=\Sigma_{n=1}^N\langle e_n|f\rangle e_n$ decomposes according to the orthonormal base $\{e_1,\ldots,e_N\}$ of the complex one-particle (test function) Hilbert space $\mathscr{H}$ with right-linear scalar product $\langle.|.\rangle$. Here $a(f)$ and $a^*(f)$ are adjoint to each other. The mapping $f\in\mathscr{H}\mapsto a^*(f)$ is complex-linear, $f\in\mathscr{H}\mapsto a(f)$ is complex-antilinear, and the canonical commutation relations (CCR) with the commutator $[A,B]=AB-BA$ written as

$$[a(f),a(g)]=[a^*(f),a^*(g)]=0,\quad [a(f),a^*(g)]=\langle f|g\rangle\mathbb{1},\quad \forall f,g\in\mathscr{H}.$$

[3] One has $\Sigma_k(\eta_k a^*(e_{s,k})a^*(e_{i,k})+\overline{\eta_k}a(e_{s,k})a(e_{i,k}))$ for the quadratic Hamiltonians associated with nondegenerate squeezing, where the index s stands for the signal modes $e_{s,k}$ and i for the idler modes $e_{i,k}$ (which all are supposed to be mutually orthogonal and normalized, and which generate the one-photon test function Hilbert space $\mathscr{H}$) and $\eta_k\in\mathbb{C}$. The combined orthonormalized modes e_n are chosen as $2^{-1/2}(e_{s,k}\pm e_{i,k})$, and the form (1.1) is obtained from the simple transformations $a^{\#}(f)a^{\#}(g)=4^{-1}(a^{\#}(f+g)^2-a^{\#}(f-g)^2)$ for arbitrary one-photon testfunctions $f,g\in\mathscr{H}$, which is valid for both the smeared creation [i.e., $a^{\#}(h)\equiv a^*(h)$] and annihilation operators [i.e., $a^{\#}(h)\equiv a(h)$ (Ref. 4)].

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Path integral solution of the Schrödinger equation in curvilinear coordinates: A straightforward procedure

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A new axiomatic formulation of path integrals is used to construct a path integral solution of the Schrödinger equation in curvilinear coordinates. An important feature of the formalism is that a coordinate transformation in the variables of the wavefunction does not imply a change of variable of integration in the path integral. Consequently, a transformation from Euclidean to curvilinear coordinates is simple to handle; there is no need to introduce ''quantum corrections'' into the action functional. Furthermore, the paths are differentiable: hence, issues related to stochastic paths do not arise. The procedure for constructing the path integral solution of the Schrödinger equation is straightforward. The case of the Schrödinger equation in spherical coordinates for a free particle is presented in detail. © *1996 American Institute of Physics.* [S0022-2488(96)02809-5]

I. INTRODUCTION

The generalization of the Feynman path integral to non-Euclidean coordinates has been a long and sometimes confusing process. Already in 1948, Feynman[1] realized that a naive change of variables in the path integral would not yield the required result. Later, Edwards and Gulyaev,[2] working in configuration space, considered a free particle in polar coordinates and found that the correct Green's function for the associated Schrödinger equation could only be obtained if they kept terms of higher order in the expansion parameter than one would expect. On the other hand, Arthurs,[3] working on phase space, found that higher-order terms were not required as long as a suitable Hamiltonian was used. Peak and Inomata[4] also considered the path integral in polar coordinates (see also Ref. 5). *All of these studies found that extra terms were needed in the action functional to account for the change from Euclidean to polar coordinates.* The extra terms were later interpreted as a consequence of the stochastic nature of the paths used in the integration.

An added source of confusion was the ambiguity in the definition of the time-sliced path integral. The definition does not specify at which point of the time interval one is to evaluate the short-time propagator. Each choice leads to a different result. Eventually, it was realized that this ambiguity was directly related to the operator ordering ambiguity.[6–13]

Despite improved understanding, expressing the solution of a given Schrödinger equation in terms of the conventional definition of a path integral remains a difficult task in general.

An axiomatic formulation of path integrals currently being developed by Cartier and DeWitt-Morette[14] remedies this situation. (Alternative mathematical approaches to formulating the Feynman path integral can be found in the literature.[15–18]) The key to the formulation's *utility* is that it emphasizes the infinite-dimensional space of paths rather than the finite-dimensional manifold where the paths take their values. Moreover, in order that actions be finite, the paths are differentiable—unlike the continuous paths in conventional path integrals. A change of coordinates (on the manifold where the paths take their values) is easy to handle, and a key theorem allows for the construction of a path integral solution for the Schrödinger equation in curvilinear coordinates.

We will show that the construction requires only the transformation from Euclidean to curvilinear coordinates and knowledge of the free part of the action functional. Notably, no ''extra terms'' are needed in the action functional. The procedure is general and simple to use. Of course,

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the resulting path integral may not always be easy to evaluate. It can be solved exactly for a free particle in d-dimensions, and the three-dimensional spherical coordinate case is worked out in detail. The scope of this paper is confined to curvilinear coordinate systems so only *flat* configuration space will be considered.

II. TWO APPROACHES TO PATH INTEGRALS

In this section we present both the usual derivation of the path integral as a solution of the Schrödinger equation and the new axiomatic formulation of Cartier/DeWitt-Morette. Although the first derivation is thoroughly familiar to most physicists, we present a brief review: it is important to have the salient features in mind in order to better appreciate how the Cartier/DeWitt-Morette formalism handles the Schrödinger equation in curvilinear coordinates. The purpose of this section is not to give a thorough comparison between the formalisms but to point out two particularly relevant issues related to a change of coordinates on a flat configuration space.

A. The ''time-slicing'' method

The conventional definition of a path integral as the matrix elements of the evolution operator in quantum mechanics employs two principal ideas. First, the Trotter–Kato–Nelson product formula is used to represent the evolution operator, $\hat{U}(t_f,t_i):=\exp[-i(t_f-t_i)\hat{H}(q,p)]$ $=\exp[-i(t_f-t_i)\{\hat{T}(p)+\hat{V}(q)\}]$, in the form

$$\begin{aligned}\exp[-i(t_f-t_i)\hat{H}(q,p)/\hbar]&=(\exp[-i(t_f-t_i)\hat{H}(q,p)/N\hbar])^N\\&=\lim_{N\to\infty}(\exp[-i(t_f-t_i)\hat{T}(p)/N\hbar]\\&\quad\times\exp[-i(t_f-t_i)\hat{V}(q)/N\hbar])^N.\end{aligned}\tag{1}$$

Here (q,p) is a point in the phase space of the associated classical system, which we take to be the cotangent bundle T^*M of the d-dimensional configuration space M. We assume M is equipped with a metric g. More general Hamiltonians can be considered which will raise the issue of operator ordering.

Essentially, this is a time-slicing technique. That is, the time interval $[t_i,\ t_f]$ is divided into N small pieces $[t_i,\ t_1]\cup\cdots\cup[t_{N-1},\ t_f]$, and the effect of the evolution operator for the full time interval is replaced by the short-time evolution operators over each piece of the divided time interval. In the limit as the number of small intervals goes to infinity and their length goes to zero, the last line of Eq. (1) becomes exact.

The second step is to insert the mixed representation identity operator

$$\mathbf{1}=\int_{T^*M}\frac{dqdp}{2\pi\hbar}\,|q\rangle\langle q\|p\rangle\langle p|\tag{2}$$

a total of N times between each term in the product in the last line of Eq. (1). We remark that $dqd\tilde{p}:=dqdp/2\pi\hbar$ is the Liouville measure in the associated phase space.

In the coordinate basis, the final state $|q_f\rangle:=\hat{U}(t_f,t_i)|q_i\rangle$ can thus be represented as

$$\begin{aligned}|q_f\rangle=e^{[-i(t_f-t_i)\hat{H}(q,p)/\hbar]}|q_i\rangle&=\lim_{N\to\infty}(e^{[-i(t_f-t_i)\hat{T}(p)/N\hbar]}e^{[-i(t_f-t_i)\hat{V}(q)/N\hbar]})^N|q_i\rangle\\&=\lim_{N\to\infty}\prod_{n=1}^{N}\int_{T^*M}dq_nd\tilde{p}_n\,e^{[ip_n(q_n-q_{n-1})/\hbar]}\\&\quad\times e^{[-i(t_f-t_i)\{T(p_n)+V(q_{n-1})\}/N\hbar]}|q_N\rangle,\end{aligned}\tag{3}$$

where $q_n := q(\overline{t_n})$ and $p_n := p(\overline{t_n})$ for some $\overline{t_n} \in [t_n, t_{n+1}]$. If the q_n and p_n are interpreted as particular values of position and momentum along some trajectory in phase space, then Eq. (3) can be interpreted as an integral over all paths in phase space such that $q_0 = q_i$. Notice that we must integrate over all values of q_N so that Eq. (3) is an integration over paths with only one endpoint fixed.

From Eq. (3), the matrix elements of the evolution operator, $\langle q_f|\hat{U}(t_f,t_i)|q_i\rangle$, are given by

$$\langle q(t_f)|q(t_i)\rangle := \langle q_f|\hat{U}(t_f,t_i)|q_i\rangle = \langle q_f|e^{[-i(t_f-t_i)\hat{H}(q,p)/\hbar]}|q_i\rangle$$

$$= \lim_{N\to\infty} \prod_{n=1}^{N} \int_{T^*M} dq_n d\tilde{p}_n \delta(q_f - q_N)$$

$$\times e^{[ip_n(q_n-q_{n-1})/\hbar]} e^{[i(t_f-t_i)\{T(p_n)+V(q_{n-1})\}/N\hbar]}, \tag{4}$$

where we have used $\langle q_f|q_N\rangle = \delta(q_f - q_N)$. We emphasize that the integration is over paths with only one fixed endpoint—the other endpoint being fixed by the delta function.

For the special case of a flat configuration space, Eq. (4) is often written schematically as

$$\langle q(t_f)|q(t_i)\rangle = \int \mathscr{D}q\mathscr{D}p\, \delta(q_f - q_N) \exp\left(\frac{i}{\hbar}\int_{t_i}^{t_f} \{\mathbf{p}\cdot\dot{\mathbf{q}} - H(q,p)\}dt\right), \tag{5}$$

where the domain of integration is understood to be the space of paths which take their values in phase space and which have one fixed endpoint, i.e., $q_0 = q_i$. [It should be kept in mind that Eq. (5) is only a shorthand notation for Eq. (4).[19]]

Finally, if the Hamiltonian is quadratic in the momentum, the integration over momentum variables in Eq. (4) can be done explicitly, resulting in the usual configuration space path integral.

There are two important points to be made concerning this construction of the path integral. Both points are direct consequences of the use of the Trotter–Kato–Nelson product formula and the resolution of the identity operator.

The first point is that time-slicing introduces an ambiguity associated with the choice of $\overline{t_n}$. Should $\overline{t_n}$ be taken to be the beginning of the time interval, somewhere between, the end, or a combination of points? In fact, the ambiguity in the choice of $\overline{t_n}$ is related to the operator ordering problem; each choice of $\overline{t_n}$ corresponds to a different Hamiltonian operator (see, for example, Refs. 6–13).[20–22]

The second point is that the use of the resolution of the identity operator introduces an explicit choice of representation and, hence, an explicit choice of coordinates on phase space. Indeed, the whole time-sliced path integral game is played with particular values of paths *in phase space*. Changing coordinates on the phase space manifold changes the expression in Eq. (3). Exactly how to change the expression under a change of coordinates is not as straightforward as one might expect. In general, an extra ''quantum potential'' term must be added to the action functional to obtain the correct result. The extra term can be attributed to the stochastic nature of the time-sliced paths.

B. The new formalism

We will now contrast the time-slicing method with the Cartier/DeWitt-Morette formalism. In particular, we will see how the two points above do not become an issue. Only a general sketch of the relevant ideas is presented, and we will confine ourselves to paths which take their values in configuration space. More complete details can be found elsewhere.[14,23]

The new method is fundamentally different from the time-slicing technique. The underlying theme is an *emphasis on an infinite-dimensional space* of paths and a *shift away from the finite-*

dimensional manifold where the paths take their values. This allows for a solid mathematical formalism which, we believe, is advantageous despite the inherent complexity of working with the infinite-dimensional function (path) space.

1. Definition of the path integral

The generic path integral requires three well-defined components for its construction: (1) a domain of integration which is an infinite-dimensional function space, (2) an integrator defined on the domain of integration, and (3) an integrand or integrable functional. Given these three ingredients, a value can be assigned to the path integral.

The **domain of integration** $\boldsymbol{X}$ is a real, separable Banach space and $x \in \boldsymbol{X}$ are taken to be $L^{2,1}$ functions.[24] We denote the dual space of $\boldsymbol{X}$ by $\boldsymbol{X}'$ and the duality by $\langle x', x\rangle_{\boldsymbol{X}}$ where $x' \in \boldsymbol{X}'$.

Assume there exists a continuous, symmetric, nondegenerate linear map $D:\boldsymbol{X}\to\boldsymbol{X}'$ and denote its inverse by the map $G:\boldsymbol{X}'\to\boldsymbol{X}$. Then a quadratic form on $\boldsymbol{X}$ is defined by $Q(x)=\langle Dx, x\rangle_{\boldsymbol{X}}$, and a quadratic form on $\boldsymbol{X}'$ is defined by $W(x')=\langle x', Gx'\rangle_{\boldsymbol{X}}$. An **integrator** $\mathscr{D}_{Q,W}x$ for a path integral can be defined by the relation

$$\int_{\boldsymbol{X}} e^{\{\pi i Q(x) - 2\pi i \langle x', x\rangle_{\boldsymbol{X}}\}} \mathscr{D}_{Q,W}x = e^{\{-\pi i W(x')\}}. \tag{6}$$

We emphasize that the integrator is defined *implicitly* in terms of Q and W by Eq. (6). (More exotic integrators can be defined, but we choose the familiar example of a Gaussian integrator for illustration purposes.)

Now, since $\boldsymbol{X}'$ is separable and complete, it is possible to define complex Borel measures μ on $\boldsymbol{X}'$. This allows one to relate a class of **integrable functionals** Φ_Q to the fiducial integrand $\exp\{\pi i Q(x)\}$ by the relation

$$F_\mu(x) = \int_{\boldsymbol{X}'} e^{\{\pi i Q(x) - 2\pi i \langle x', x\rangle_{\boldsymbol{X}}\}} d\mu(x'), \tag{7}$$

where $F_\mu \in \Phi_Q$.

This construction implies the functional integral satisfies

$$\int_X F_\mu(x) \mathscr{D}_{Q,W}x = \int_{\boldsymbol{X}'} e^{\{-\pi i W(x')\}} d\mu(x'). \tag{8}$$

The right-hand side of Eq. (8) should not be construed as a means to evaluate the left-hand side. Indeed, the measure μ associated with a given $F_\mu \in \Phi_Q$ is not usually known. Equation (8) is a consequence of relations (6) and (7) and is useful for determining when the integral exists or for proving general theorems—neither of which requires the specific form of μ.

2. Parametrizing the space of paths

We need to say a few things about the domain of integration. For quantum mechanical applications, one is usually interested in a path integral over all paths $x:\mathrm{T}\to N$ where $\mathrm{T}=[t_i, t_f]\subset\mathbb{R}$ and N is an n-dimensional manifold. However, in general, the space of paths which take their values in a manifold N will not be a Banach space $\boldsymbol{X}$. For suppose that we are interested in all paths which have the same fixed endpoints at $t=t_i$. Then $x_1+x_2\in\boldsymbol{X}$ if and only if $x(t_i)=0 \forall x\in\boldsymbol{X}$. This follows because $(x_1+x_2)(t_i)=x_1(t_i)+x_2(t_i)$ for vanishing endpoints only. So the space of paths with nonvanishing fixed endpoints is not a vector space and, therefore, is not a Banach space.

However, if we restrict attention to the space of paths which have only one endpoint fixed in N (that is, a space of pointed paths), then the space of such paths is contractible. Consequently, it

can be parametrized by a space of pointed paths which take their values in a flat manifold $\mathbb{R}^n$ and have their fixed endpoint at the origin of $\mathbb{R}^n$. But, this parameter space of paths *is* a Banach space. Hence, *integration on a space of pointed paths can be defined in terms of integration on the parameter space*.[14]

The situation is analogous to integration on finite-dimensional manifolds. There one does not know how to integrate on a general manifold. Instead, one defines the integral by parametrizing points in the general manifold by points in flat manifolds where one knows how to integrate. For functional integrals, we do not know how to integrate over a general function space so we parametrize it with a Banach space where the rules of functional integration are established.

The details of the parametrization for our particular case follow. Let there be r linearly independent vector fields which generate a vector subspace $R_m \subseteq T_m M$ at each $m \in M$, and denote them by $\boldsymbol{X}_{(\alpha)}$ where $\alpha \in \{1,...,r\}$. Let $\mathscr{P}_f^R M$ denote the space of pointed $L^{2,1}$ paths with fixed *final* point $x(t_f) = m_f \in M \forall x \in \mathscr{P}_f^R M$ and such that $\dot{\mathbf{x}}(t) \in R_{x(t)}$. Denote by $\mathscr{P}_0 \mathbb{R}^d =: \boldsymbol{Z}_i$ the space of $L^{2,1}$ paths with fixed *initial* point $z(t_i) = 0 \in \mathbb{R}^d \ \forall z \in \boldsymbol{Z}_i$.[25]

Since the paths in $\mathscr{P}_f^R M$ are $L^{2,1}$ and since the set $\{\boldsymbol{X}_{(\alpha)}(x(t))\}$ spans $R_{x(t)}$, it follows that there exist functions $\dot{z}^\alpha(t)$ such that

$$\dot{\mathbf{x}}(t) = \boldsymbol{X}_{(\alpha)}(x(t))\dot{z}^\alpha(t), \quad x(t_f) = m_f. \tag{9}$$

This differential equation associates a path $z \in \boldsymbol{Z}_i$ with each path $x \in \mathscr{P}_f^R M$. If the map $x \mapsto z$ can be inverted, then, given some $z \in \boldsymbol{Z}_i$, Eq. (9) has a unique solution $x \in \mathscr{P}_f^R M$. Denote this solution by $x(t,z) = m_f \cdot \boldsymbol{\Sigma}(t,z)$ where $\Sigma(t,z): M \to M$ is a global transformation on M such that $x(t_i,z) = m_f \cdot \boldsymbol{\Sigma}(t_i,z) = m_f$.

We now have a parametrization $P: \boldsymbol{Z}_i \to \mathscr{P}_f^R M$ by the solution of Eq. (9). That is, we have parametrized the space of pointed paths $\mathscr{P}_f^R M$ by the space of paths $\boldsymbol{Z}_i$. Since we know how to do a functional integral on $\boldsymbol{Z}_i$, we simply define

$$\int_{\mathscr{P}_f^R M} F(x) \mathscr{D}x := \int_{\boldsymbol{Z}_i} F(x(z)) \mathscr{D}_{Q,W} z, \tag{10}$$

where $\mathscr{D}_{Q,W} z$ is characterized by Eq. (6) with $\boldsymbol{X} = \boldsymbol{Z}_i$. Of course, for this definition to be useful, the right-hand side must be independent of the parametrization used. That is, we must get the same answer if we use the parametrization $\widetilde{P}: \widetilde{\boldsymbol{Z}}_i \to \mathscr{P}_f^R M$ by $\widetilde{z} \mapsto x$. But, this just means that the functional integral must be invariant under a change of variable of integration.

Inspection of Eq. (9) shows that a change of variable of integration is not directly associated with a change of coordinates on the manifold M. A change of coordinates on M implies a change in the components of the vector fields $\dot{\mathbf{x}}$ and $\boldsymbol{X}_{(\alpha)}$ but there is no change in the coordinates of z: the parametrization changes, but the integration variables do not. The point is that, in contrast to the time-slicing method, a change of coordinates on the manifold M is *not* associated with a change of variable of integration.

3. Key theorem

A key result of Cartier/DeWitt-Morette is that the path integral which has been defined above is the solution of a Schrödinger-type partial differential equation:

Theorem[14]: Let $\mathscr{P}_f^R M$ be the space of $L^{2,1}$ paths with fixed endpoints $x(t_f) = m_f \in M$ whose velocity vectors are elements of $R \subseteq TM$. Parametrize $\mathscr{P}_f^R M$ by $\boldsymbol{Z}_i$. Let $S_0(x)$ be the free action of a particle given by $S_0(x) = \int_T g_{x(t)}(\dot{\mathbf{x}}(t), \dot{\mathbf{x}}(t)) dt$, and let $V: M \to \mathbb{R}$ be a well-behaved scalar potential. Let $\psi: M \to \mathbb{C}^n$ be any integrable $C^\infty(M)$ function with compact support. Then the path integral

$$\Psi(t_f,m_f):=(U_{t_f}\psi)(m_f):=\int_{\mathscr{P}_f^D M}\psi(x)e^{[\pi i S_0(x)+\int_T V(x)dt]}\mathscr{D}x$$

$$=\int_{\mathbf{Z}_i}\psi(x(t_f,z))e^{[\pi i S_0(x(z))+\int_T V(x(t,z))dt]}\mathscr{D}_{Q,W}z$$

$$=\int_{\mathbf{Z}_i}\psi(m_f\cdot\Sigma(t_f,z))e^{[\int_T V(m_f\cdot\Sigma(t,z))dt]}e^{[\pi i Q(z)]}\mathscr{D}_{Q,W}z \tag{11}$$

is a solution of the partial differential equation

$$\frac{\partial\Psi(t_f,m_f)}{\partial t_f}=\left[\frac{i}{4\pi}\,g^{\alpha\beta}\mathscr{L}_{\mathbf{X}_{(\alpha)}}\mathscr{L}_{\mathbf{X}_{(\beta)}}+V\right]\Bigg|_{m_f}\Psi(t_f,m_f),$$

$$\Psi(t_i,m_f)=\psi(m_f). \tag{12}$$

Moreover, the functional operator U_{t_f}, which evolves the function ψ from t_i to t_f, satisfies the group property $U_{t_2}\circ U_{t_1}=U_{t_2+t_1}$.

Here $g^{\alpha\beta}g_{\beta\gamma}=\delta^{\alpha}_{\gamma}$, $\mathscr{L}_{\mathbf{X}_{(\alpha)}}$ is the Lie derivative in the direction $\boldsymbol{X}_{(\alpha)}$, and $g_{\alpha\beta}$ is a symmetric nondegenerate matrix on $\boldsymbol{Z}_i$ defined by

$$S_0(x(z))=\int_T g_{x(t)}(\dot{\mathbf{x}}(t,z),\dot{\mathbf{x}}(t,z))dt=\int_T g_{x(t)}(\mathbf{X}_{(\alpha)}(x(t)),\boldsymbol{X}_{(\beta)}(x(t)))\dot{z}^{\alpha}(t)\dot{z}^{\beta}(t)dt$$

$$=:\int_T g_{\alpha\beta}\dot{z}^{\alpha}(t)\dot{z}^{\beta}(t)dt$$

$$=:Q(z). \tag{13}$$

Equation (11) is the Cartier/DeWitt-Morette analog of the time-sliced configuration space path integral. This theorem allows one to associate a *unique* action functional[25] with a Hamiltonian operator associated with a given Schrödinger equation. Again, this should be contrasted with the discussion above concerning the analogous situation for conventional path integrals.

III. CURVILINEAR COORDINATES

In this section we will first give a simple example—the Schrödinger equation for a free particle in spherical coordinates—to see how a change of coordinates is handled in the new formalism. Then we will present the recipe for the general case. Throughout this section we consider only flat configuration space path integrals. When configuration space is a nontrivial (pseudo)Riemannian manifold, one can use the Cartan development to parametrize the space of pointed paths on the manifold by the space of pointed paths on the tangent space at a point of the manifold.[14] This procedure does not alter the methods or results of this or the next section.

A. Spherical coordinates

Consider a free particle on $\mathbb{R}^3$. We want to calculate the Green's function of the Schrödinger equation in spherical coordinates $(r,\theta,\phi)=:\mathbf{r}$ on $\mathbb{R}^3$. This is equivalent to finding the point-to-point transition amplitude $\langle\mathbf{r}(t_f)|\mathbf{r}(t_i)\rangle=:\mathscr{K}(t_f,\mathbf{r}_f;t_i,\mathbf{r}_i)$. The point-to-point transition amplitude can be obtained from the path integral in Eq. (11) by taking the initial functional ψ to be a delta functional. This choice ''ties down'' the other ends of the paths (recall that we deal with pointed paths).

Cover $\mathbb{R}^3$ with an atlas of spherical coordinates such that $\mathbf{r}_f$ and $\mathbf{r}_i$ lie in the same patch. Note that the space of paths $\mathscr{P}_f^R\mathbb{R}^3$ is not a Banach space so we parametrize by the space of paths $\mathbf{Z}_i=\mathscr{P}_0\mathbb{R}^3$. According to Eq. (11), we have to solve the following functional integral:

$$\mathscr{K}(t_f,\mathbf{r}_f;t_i,\mathbf{r}_i)=\int_{\mathbf{Z}_i}\delta(\mathbf{r}_f\cdot\Sigma(t_f,z)-\mathbf{r}_i)e^{[\pi iS_0(\mathbf{r}(z))]}\mathscr{D}_{Q,W}z \tag{14}$$

where

$$S_0(\mathbf{r})=\frac{1}{2\pi\hbar}\int_{\mathrm{T}}(\dot{r}^2+r^2\dot{\theta}^2+r^2\sin^2\theta\dot{\phi}^2)dt.$$

The first step in solving Eq. (14) is to find a simplifying parametrization. From the form of the action functional, the indicated parametrization is fairly obvious. Take Euclidean coordinates for $z(t)\in\mathbb{R}^3$ [then Eq. (14) will be easy to solve] and consider the transformation between spherical and Euclidean coordinates:

$$\begin{aligned}
r&=\sqrt{(z^1)^2+(z^2)^2+(z^3)^2},\\
\theta&=\cos^{-1}\left(\frac{z^3}{\sqrt{(z^1)^2+(z^2)^2+(z^3)^2}}\right),\\
\phi&=\tan^{-1}\left(\frac{z^2}{z^1}\right).
\end{aligned} \tag{15}$$

Then the parametrization corresponding to Eq. (9) which transforms spherical coordinates to Euclidean coordinates is

$$\begin{aligned}
dr(t)&=\sin\theta(t)\cos\phi(t)dz^1(t)+\sin\theta(t)\sin\phi(t)dz^2(t)+\cos\theta(t)dz^3(t),\\
d\theta(t)&=\frac{\cos\theta(t)\cos\phi(t)}{r(t)}dz^1(t)+\frac{\cos\theta(t)\sin\phi(t)}{r(t)}dz^2(t)-\frac{\sin\theta(t)}{r(t)}dz^3(t),\\
d\phi(t)&=\frac{-\sin\phi(t)}{r(t)\sin\theta(t)}dz^1(t)+\frac{\cos\phi(t)}{r(t)\sin\theta(t)}dz^2(t),\\
r(t_f)&=r_f,\quad \theta(t_f)=\theta_f,\quad \phi(t_f)=\phi_f,
\end{aligned} \tag{16}$$

and the solution is

$$\begin{aligned}
r(t,z)&=\{(r_f\sin\theta_f\cos\phi_f+z^1(t))^2+(r_f\sin\theta_f\sin\phi_f+z^2(t))^2\\
&\quad+(r_f\cos\theta_f+z^3(t))^2\}^{1/2},\quad 0<r<\infty\\
\cos\theta(t,z)&=\left(\frac{r_f\cos\theta_f+z^3(t)}{r(t)}\right),\quad 0\leqslant\theta<\pi,\\
\tan\phi(t,z)&=\left(\frac{r_f\sin\theta_f\sin\phi_f+z^2(t)}{r_f\sin\theta_f\cos\phi_f+z^1(t)}\right),\quad 0\leqslant\phi<2\pi.
\end{aligned} \tag{17}$$

Hence, the parametrized action functional is given by

$$S_0(\mathbf{r}(z))=Q(z)=\frac{1}{2\pi\hbar}\int_{\mathrm{T}}\{(\dot{z}^1)^2+(\dot{z}^2)^2+(\dot{z}^3)^2\}dt \tag{18}$$

so that $g^{\alpha\beta}=(2\pi\hbar)\delta^{\alpha\beta}$.

The delta functional becomes

$$\begin{aligned}&\delta^3\{r(t_f,z)-r_i,\theta(t_f,z)-\theta_i,\phi(t_f,z)-\phi_i\}\\&\quad=r_i^2\sin\theta_i\delta^3\begin{pmatrix}r_f\sin\theta_f\cos\phi_f-r_i\sin\theta_i\cos\phi_i+z^1(t_f),\\ r_f\sin\theta_f\sin\phi_f-r_i\sin\theta_i\sin\phi_i+z^2(t_f),\\ r_f\cos\theta_f-r_i\cos\theta_i+z^3(t_f)\end{pmatrix},\end{aligned} \tag{19}$$

where the right-hand side follows from Eq. (17) and the well-known identity $\delta^3(f(x))=\Sigma_{x_0}\delta^3(x-x_0)/|\det f'(x_0)|$ with $f(x_0)=0$. Note that the delta functional depends only on a single value of the paths, i.e., $z(t_f)$. Thus it is actually just a delta *function*.

Substitute Eqs. (18) and (19) into Eq. (14). The integral can be simplified by making use of the linear map $L:\mathbf{Z}_i\to\mathbb{R}^3$ by $z^\alpha\mapsto u^\alpha=z^\alpha(t_f)$. The integral reduces to a finite integral (see, for example, Ref. 14)

$$\int_{\mathbb{R}^3}e^{[\pi iQ(u)]}r_i^2\sin\theta_i\delta^3\begin{pmatrix}r_f\sin\theta_f\cos\phi_f-r_i\sin\theta_i\cos\phi_i+u^1,\\ r_f\sin\theta_f\sin\phi_f-r_i\sin\theta_i\sin\phi_i+u^2,\\ r_f\cos\theta_f-r_i\cos\theta_i+u^3,\end{pmatrix}|\det 2\pi i\hbar G(t_f,t_f)|^{1/2}d^3u, \tag{20}$$

where $Q(\mathbf{u})=\mathbf{u}^2/2G(t_f,t_f)$. Here $G(t,s)$ is the Green's function for $Q(z)$ for $z\in\mathbf{Z}_i$. It is easy to check that $G(t,s)=\theta(t-s)(t-t_i)+\theta(s-t)(s-t_i)$ so that $G(t_f,t_f)=(t_f-t_i)$.

Therefore, the final expression for the transition amplitude is

$$\mathscr{K}(t_f,\mathbf{r}_f;t_i,\mathbf{r}_i)=r_i^2\sin\theta_i[2\pi i\hbar(t_f-t_i)]^{-3/2}\exp\left\{\frac{i}{\hbar}\frac{|\mathbf{r}_f-\mathbf{r}_i|^2}{2(t_f-t_i)}\right\}. \tag{21}$$

This is the propagator for a free particle in $\mathbb{R}^3$ expressed in spherical coordinates.

According to the key theorem, the transition amplitude (21) is the solution of a partial differential equation. By inspecting Eq. (16), we identify

$$\begin{aligned}\boldsymbol{X}_{(1)}&=\left(\sin\theta\cos\phi,\frac{\cos\theta\cos\phi}{r},\frac{-\sin\phi}{r\sin\phi}\right),\\ \boldsymbol{X}_{(2)}&=\left(\sin\theta\sin\phi,\frac{\cos\theta\sin\phi}{r},\frac{\cos\phi}{r\sin\theta}\right),\\ \boldsymbol{X}_{(3)}&=\left(\cos\theta,\frac{-\sin\theta}{r},0\right).\end{aligned} \tag{22}$$

The corresponding Lie derivatives are

$$\begin{aligned}\mathscr{L}_{\boldsymbol{X}_{(1)}}&=\sin\theta\cos\phi\frac{\partial}{\partial r}+\frac{\cos\phi}{r}\frac{\partial}{\partial\theta}-\frac{\sin\phi}{r\sin\theta}\frac{\partial}{\partial\phi},\\ \mathscr{L}_{\boldsymbol{X}_{(2)}}&=\sin\theta\sin\phi\frac{\partial}{\partial r}+\frac{\sin\phi}{r}\frac{\partial}{\partial\theta}+\frac{\cos\phi}{r\sin\theta}\frac{\partial}{\partial\phi},\\ \mathscr{L}_{\boldsymbol{X}_{(3)}}&=\cos\theta\frac{\partial}{\partial r}-\frac{\sin\theta}{r}\frac{\partial}{\partial\theta}.\end{aligned} \tag{23}$$

Substituting these Lie derivatives and the transition amplitude into Eq. (12) verifies the partial differential equation

$$\frac{\partial \mathscr{K}}{\partial t_f} = \frac{i\hbar}{2}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)\Bigg|_{\mathbf{r}_f}\mathscr{K},$$
$$\lim_{t_f\to t_i}\mathscr{K}(t_f,\mathbf{r}_f;t_i,\mathbf{r}_i) = \delta(r_f-r_i)\,\delta(\theta_f-\theta_i)\,\delta(\phi_f-\phi_i), \tag{24}$$

and we have succeeded in solving the Schrödinger equation in spherical coordinates. Note that the constant $r_i^2\sin\theta_i$ in Eq. (21) is consistent with Eq. (24) since

$$\begin{aligned}(r_i^2\sin\theta_i)^{-1}\lim_{t_f\to t_i}\mathscr{K}(t_f,\mathbf{r}_f;t_i,\mathbf{r}_i) &= (r_i^2\sin\theta_i)^{-1}\delta(r_f-r_i)\,\delta(\theta_f-\theta_i)\,\delta(\phi_f-\phi_i)\\ &= \delta(x_f-x_i)\,\delta(y_f-y_i)\,\delta(z_f-z_i)\\ &= \lim_{t_f\to t_i}\mathscr{K}(t_f,\mathbf{x}_f;t_i,\mathbf{x}_i).\end{aligned} \tag{25}$$

B. The general case

To obtain the path integral solution of the Schrödinger equation in *general* curvilinear coordinates for an interacting particle in Euclidean space, we just outline the necessary steps. The calculations follow the example in the previous section. Of course for generic interactions the path integral cannot be solved exactly.

(1) Write the equations for the transformation $x=f(z)$ from Euclidean to curvilinear coordinates.
(2) Use the derivatives $\mathbf{dx}=f'\mathbf{dz}$ to define the parametrization and to identify the vector fields $X_{(\alpha)}$, which will be the columns of f'.
(3) Use the free part of the action functional to define the quadratic form Q. Hence, determine $g_{\alpha\beta}$.
(4) Use Eq. (11) to solve the Schrödinger equation given by Eq. (12).
(5) If a point-to-point transition is desired, take the initial functional in the path integral to be a delta functional.

IV. CONCLUSIONS

A new formulation of path integrals has been used to study the relationship between coordinate transformations on a flat configuration space and the path integral solution of the transformed Schrödinger equation. The variables of the path integral are $L^{2,1}$ functions which do not share the stochastic properties of paths in the conventional path integral. In particular, no ''quantum potential'' corrections to the action functional are required under a change from Euclidean to curvilinear coordinates. Moreover, a unique integrator is associated with the Hamiltonian operator encoded in the Schrödinger equation. Given a coordinate transformation, it is straightforward to write down the path integral solution of the transformed Schrödinger equation.

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[20] Closely related to the t_n ambiguity and operator ordering is the fact that the ''paths'' in Eq. (3) behave like Brownian paths in the sense that $(dx)^2 \sim dt$. This leads to an often fruitful analogy with stochastic calculus and Wiener integrals. However, analytically continuing Wiener integrals to include the case of quantum mechanics is not possible in general (see, for example, Refs. 21 and 22), and the correspondence between path integrals and Wiener integrals is strictly formal.
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[24] A function is $L^{2,1}$ if $\int_T |dx/dt|^2 \, dt < \infty$. We choose $L^{2,1}$ functions because of their relevance to physics. Specifically, the Lagrangian density requires derivatives, and the kinetic energy must be finite.
[25] For our purpose, it is convenient but not necessary to fix the *final* endpoints for the paths $x \in \mathscr{P}_f^R M$ and the *initial* endpoints for the paths $z \in \boldsymbol{Z}_i$: fixing any combination of initial and/or final points is allowed.
[26] Strictly speaking, the action functional is only unique up to definition (13) which relates the free-particle action to the quadratic form that characterizes the integrator.

A symmetry of massless fields

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It is proved that there exists an additional intrinsic symmetry in the left-handed and right-handed fermions (and other fields). The corresponding group of transformations is induced by the Poincaré translations in the space–time manifold. This symmetry predicts an additional intrinsic energy-momentum for fermions. Considering this symmetry as local leads to introduction of a gauge field and of a nonintegrable phase angle, the corresponding Berry-type phase depends on the topology of the Riemannian space–time manifold as determined by the vierbein. This additional symmetry provides us with the possibility of considering the fermions as gauge fields on the nonvector bundle. © *1996 American Institute of Physics.* [S0022-2488(96)02109-3]

I. INTRODUCTION

In the theory of elementary particles we customarily invoke the principles of symmetry. The discovery of symmetries has brought order into the complexity of data and phenomena; it has made possible several developments of science. ''Symmetry is one idea by which man through the ages has tried to comprehend and create order, beauty, and perfection'' as H. Weyl has expressed it so concisely.

In elementary particle physics the inherent symmetries of the fields considered have allowed us either to derive or to incorporate many important properties of the particles, mainly through the conservation rules (the conserved quantities as invariants of the symmetry groups considered) and the associated selection rules for possible interactions.

In this paper we will analyze an additional intrinsic symmetry in the left-handed and right-handed fermion fields. The corresponding group transformation on the null twistor space can be induced by the Poincaré translation in the space–time manifold. This symmetry predicts an additional intrinsic energy-momentum for the fermion. By extension this could be applied to other massless fields.

It is known that gauge fields in physics are established as connections on a vector bundle. The theory of a gauge field on a nonvector bundle should deserve more attention.[1] We show that an additional symmetry provides us with the possibility to construct the theory where the fermionic fields, commonly regarded as matter fields, become the gauge fields on the nonvector bundle. This opens a new approach in the pursuit of great unification of physical fields.

First we show that the Poincaré group can be considered as a chiral group. The complexification of $R_{1,3}$, the Clifford algebra of space–time $R^{1,3}$, will be used for this purpose ($R_{1,3}$ is called space–time real geometrical algebra). This is the algebra generated by representing a space–time vector tetrad by γ_μ, $\mu=0,1,2,3$, and the definitions of the multiple index quantities and of geometric multiplication:

$$\gamma_\mu\gamma_\nu=g_{\mu\nu}\mathbf{1}+\gamma_{\mu\nu}, \quad \gamma_{\mu\nu}=-\gamma_{\nu\mu},$$

where $g_{\mu\nu}$ is the scalar metric, $\mathbf{1}$ is the unit of the algebra, the $\gamma_{\mu\nu}$ are bivectors;

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$$\gamma_{\mu\nu}\gamma_\lambda=\gamma_\mu g_{\nu\lambda}-g_{\mu\lambda}\gamma_\nu+\gamma_{\mu\nu\lambda},$$

defining the trivectors, totally antisymmetric in all three indexes,

$$\gamma_{\mu\nu\lambda}=-\gamma_{\mu\lambda\nu}=-\gamma_{\nu\mu\lambda}=\gamma_{\lambda\mu\nu};$$

and the pseudoscalar γ_5 or space–time volume tetravector

$$\gamma_{\mu\nu\lambda}\gamma_\rho=\gamma_{\mu\nu}g_{\lambda\rho}-\gamma_{\mu\lambda}g_{\nu\rho}+\gamma_{\nu\lambda}g_{\mu\rho}+\gamma_5.$$

The indexes are given a definite order and the definitions are consistent with the change of sign with the exchange of two adjacent indexes.

The reversion of all indexes is denoted by a tilde over a multivector $\tilde{\gamma}_{\mu\nu}=\gamma_{\nu\mu}$, $\tilde{\gamma}_{\mu\nu\lambda}=\gamma_{\lambda\nu\mu}$, etc.

Second we consider the symmetry generated by these quantities when combined in a form suitable to have a representation of the Poincaré group. This is then used to study fermion fields.

This brings the necessity of studying the gauge theory of the translation group as an extension of the simplest gauge groups for fermions.

We end with some final consideration about the significance of this analysis.

II. THE POINCARÉ GROUP REPRESENTATION AS A CHIRAL GROUP IN SPACE–TIME ALGEBRA

The equations describing physical relations in space–time (or in ordinary three-dimensional space) should be covariant under both Lorentz transformations $\mathbb{L}$ and changes of origin d of the coordinate system. This set of operations, called the Poincaré group, of which rotations and changes of origin in ordinary three-dimensional space are subgroups, is characterized by the pair $\{\mathbb{L},d\}$.

The group transformation is $\{\mathbb{L}_2,d_2\}\{\mathbb{L}_1,d_1\}=\{\mathbb{L}_3,d_3\}$. In the geometric algebra of space–time $R^{1,3}$ (the Clifford algebra $R_{1,3}$) a position vector $\chi_0=\chi^\mu\gamma_\mu$ is transformed. With the use of the boosters and rotors $\mathbb{L}$,

$$\chi_0\rightarrow\chi_1=\mathbb{L}_1\chi_0\tilde{\mathbb{L}}_1+d_1\rightarrow\chi_2=\mathbb{L}_2\chi_1\tilde{\mathbb{L}}_2+d_2, \tag{1}$$

or

$$\chi_2=\mathbb{L}_2\mathbb{L}_1\chi_0\tilde{\mathbb{L}}_1\tilde{\mathbb{L}}_2+\mathbb{L}_2d_1\tilde{\mathbb{L}}_2+d_2, \tag{2}$$

$$\chi_2=\mathbb{L}_3\chi_0\tilde{\mathbb{L}}_3+d_3, \tag{3}$$

defining (the tilde operation reverses the product of two multivectors)

$$\mathbb{L}_3=\mathbb{L}_2\mathbb{L}_1 \quad \text{and} \quad d_3=\mathbb{L}_2d_1\tilde{\mathbb{L}}_2+d_2. \tag{4}$$

The ''multiplication'' of the Poincaré group is well defined but cumbersome. There are several representations, some of which are reasonable to handle. For example, the use of the matrix form (here the $\mathbb{L}_i$ are square matrices and the χ_i and d_i column matrices, the 0^l are row matrices)

$$\begin{pmatrix}\mathbb{L}_1 & d_1\\ 0^l & \mathbf{1}\end{pmatrix}\begin{pmatrix}\chi_0\\ 1\end{pmatrix}=\begin{pmatrix}\mathbb{L}_1\chi_0+d_1\\ 1\end{pmatrix} \tag{5}$$

and

$$\begin{pmatrix} \mathbb{L}_2 & d_2 \\ 0^l & \mathbf{1} \end{pmatrix}\begin{pmatrix} \chi_1 \\ 1 \end{pmatrix}=\begin{pmatrix} \mathbb{L}_2\chi_1+d_2 \\ 1 \end{pmatrix} \tag{6}$$

or

$$\begin{pmatrix} \mathbb{L}_3 & d_3 \\ 0^l & \mathbf{1} \end{pmatrix}\begin{pmatrix} \chi_0 \\ 1 \end{pmatrix}=\begin{pmatrix} \mathbb{L}_2 & d_2 \\ 0^l & \mathbf{1} \end{pmatrix}\begin{pmatrix} \mathbb{L}_1 & d_1 \\ 0^l & \mathbf{1} \end{pmatrix}\begin{pmatrix} \chi_0 \\ 1 \end{pmatrix}. \tag{7}$$

Then

$$\begin{pmatrix} \mathbb{L}_3 & d_3 \\ 0^l & \mathbf{1} \end{pmatrix}=\begin{pmatrix} \mathbb{L}_2\mathbb{L}_1 & \mathbb{L}_2 d_1+d_2 \\ 0^l & \mathbf{1} \end{pmatrix} \tag{8}$$

clearly shows that the ''product'' of group elements are elements of the group. Group multiplication is matrix multiplication here.

In geometric algebra there is a representation of the elements of the group which allows *geometric multiplication* as the group (non-Abelian) multiplication:

$$\{\mathbb{L}_2,d_2\}\{\mathbb{L}_1,d_1\}=\{\mathbb{L}_3,d_3\}.$$

For this geometric algebra representation we use the product of the elements $(1+\varepsilon d)$ and $\mathbb{L}$, which separately have as group multiplication the geometric product

$$\mathbb{L}_3=\mathbb{L}_2\mathbb{L}_1 \quad \text{and} \quad (1+\varepsilon d_3)=(1+\varepsilon d_2)(1+\varepsilon d_1), \tag{9}$$

where $d_3=d_2+d_1$ and $\varepsilon d_2\varepsilon d_1=0$, requiring that either $\{\varepsilon^2=0,\ \varepsilon d=d\varepsilon\}$ or $\{\varepsilon_+\varepsilon_-=0,\ \varepsilon_+ d=d\varepsilon_-\}$. In the first case $\varepsilon^2=0$ is a nilpotent operation commuting with the vectors d. In the second case $\varepsilon_+(\varepsilon_-)$ is a projector operator

$$\varepsilon_+\varepsilon_-=\varepsilon_-\varepsilon_+=0, \quad \varepsilon_++\varepsilon_-=1, \tag{10}$$

which can be written in terms of a unit multivector e, $e^2=\mathbf{1}$ which, $ed=-de$, anticommutes with the vectors d. The $\varepsilon_+=\frac{1}{2}(1+e)$ and $\varepsilon_-=\frac{1}{2}(1-e)$. In general a suitable $\{\varepsilon;\varepsilon^2=0,\ \varepsilon d=d\varepsilon\}$ or $\{e;e^2=1,\ ed=-de\}$ can only be found in an algebra of a dimension higher than the Clifford algebra $R_{p,q}$ corresponding to the space $R^{p,q}$. The formal definition of ε or e is enough for the purpose of studying the Poincaré group but the possibility of physical usefulness or insight would be lost.

In the Dirac algebra $\mathscr{D}$ corresponding to $R_{1,3}$ one usually admits its complexification, corresponding to the use of $R_{0,5}\simeq R_{2,3}\simeq R_{4,1}$, that is $\mathscr{D}=\{R_{1,3}\oplus iR_{1,3}\simeq R_{0,5}\}$. The commonly used operators $i\gamma_5=i\gamma_0\gamma_1\gamma_2\gamma_3$ and $i\gamma_{12}=i\gamma_1\gamma_2$ are good examples of this complexification of the algebra. It is $i\gamma_5$ which has the property $i\gamma_5\gamma_\mu=-\gamma_\mu i\gamma_5$, and $(i\gamma_5)^2=1$ required for the use in (9) and (10). Then the group of translations Γ has two isomorphic representations $\Gamma:d\to d'$, which are $(1+\mathbb{P}_R d)$ and $(1+\mathbb{P}_L d)$ where

$$\begin{gathered} \mathbb{P}_R=\tfrac{1}{2}(1+i\gamma_5) \ \text{ and } \ \mathbb{P}_L=\tfrac{1}{2}(1-i\gamma_5), \\ \mathbb{P}_R+\mathbb{P}_L=1, \quad \mathbb{P}_R\mathbb{P}_L=\mathbb{P}_L\mathbb{P}_R=0 \quad \text{and} \quad \mathbb{P}_R\mathbb{P}_R=\mathbb{P}_R, \quad \mathbb{P}_L\mathbb{P}_L=\mathbb{P}_L, \quad \mathbb{P}_R d=d\mathbb{P}_L. \end{gathered} \tag{11}$$

Here the $\mathbb{P}_R$ and $\mathbb{P}_L$ are the operators for right-handed and left-handed projection, respectively: $\psi=\mathbb{P}_R\psi+\mathbb{P}_L\psi=R_0+L_0$.

The Lorentz transformations $\mathbb{L}$,

$$\mathbb{L}:\chi\to\chi'=\mathbb{L}\chi\tilde{\mathbb{L}}, \quad \mathbb{L}\tilde{\mathbb{L}}=\tilde{\mathbb{L}}\mathbb{L}=1, \tag{12}$$

do form a multiplication group

$$\mathbb{L}_3=\mathbb{L}_2\mathbb{L}_1, \quad \tilde{\mathbb{L}}_3=\tilde{\mathbb{L}}_1\tilde{\mathbb{L}}_2, \tag{13}$$

which can be used to construct, together with the $(1+\varepsilon d)$, a set of two *representations* of the Poincaré group.

The representations of the Poincaré group are

$$\mathbb{P}_i^{(L)}=(1+\mathbb{P}_L d_i)\mathbb{L}_i; \quad \mathbb{P}_i^{(R)}=(1+\mathbb{P}_R d_i)\mathbb{L}_i, \tag{14}$$

and ($A=L,R$ and, as a reminder, $\mathbb{L}_j\mathbb{P}_L=\mathbb{P}_L\mathbb{L}_j$)

$$\begin{aligned}\mathbb{P}_k^{(A)}&=\mathbb{P}_j^{(A)}\mathbb{P}_i^{(A)}=(1+\mathbb{P}_L d_j)\mathbb{L}_j(1+\mathbb{P}_L d_i)\mathbb{L}_i,\\ \mathbb{P}_k^{(A)}&=(1+\mathbb{P}_L(d_j+\mathbb{L}_j d_i\mathbb{L}_j))\mathbb{L}_j\mathbb{L}_i,\\ \mathbb{P}_k^{(A)}&=(1+\mathbb{P}_L d_k)\mathbb{L}_k.\end{aligned} \tag{15}$$

The operators $(1+\mathbb{P}_A d)$ then become an important part of the study of the invariances and the symmetries related to relativistic quantum theory of particle and interaction fields. Their use in constructing a new representation of the Poincaré Lie algebra (see below) is thus both straightforward and clarifies the reason for some features of the theory of elementary particles.

III. INTRINSIC SYMMETRY OF FERMION

In this section we will show now that there exists a new intrinsic symmetry for the left-handed and right-handed fermions, which corresponds to a special Poincaré translation in the phase space of the spinor space.

One knows that any fermion field can be written as a superposition of handness states:

$$\Psi=(\mathbb{P}_L+\mathbb{P}_R)\Psi=\left(\frac{1-i\gamma_5}{2}\right)\Psi+\left(\frac{1+i\gamma_5}{2}\right)\Psi=L_0+R_0. \tag{16}$$

In the standard Weinberg–Salam model,[2] the left-handed fermion L_0 and right-handed fermion R_0 are treated on different levels. All left-handed components L_0 are supposed to form SU(2) doublets while the right-handed components R_0 are SU(2) singlets. From the mathematical point of view they are mathematically independent quantities.

The Lagrangian in the standard model for a fermion field with electroweak interactions and a symmetry breaking mass term is

$$\begin{aligned}\mathbf{L}=&+\frac{1}{2}\overline{L_0}i\gamma^\mu\left(\frac{1-i\gamma_5}{2}\right)\left(\partial_\mu L_0+\frac{ig'}{2}B_\mu L_0-\frac{ig}{2}A_\mu^i\tau_i L_0\right)-\frac{1}{2}\left(\partial_\mu\overline{L_0}-\frac{ig'}{2}B_\mu\overline{L_0}\right.\\ &\left.+\frac{ig}{2}\overline{L_0}\tau_i A_\mu^i\right)i\gamma^\mu\left(\frac{1-i\gamma_5}{2}\right)L_0+\frac{1}{2}\overline{R_0}i\gamma^\mu\left(\frac{1+i\gamma_5}{2}\right)(\partial_\mu R_0+ig'B_\mu R_0)-\frac{1}{2}(\partial_\mu\overline{R_0}\\ &-ig'B_\mu\overline{R_0})i\gamma^\mu\left(\frac{1+i\gamma_5}{2}\right)R_0-g_e\left[\overline{R_0}\Phi^\dagger\left(\frac{1-i\gamma_5}{2}\right)L_0+\overline{L_0}\left(\frac{1+i\gamma_5}{2}\right)\Phi R_0\right],\end{aligned} \tag{17}$$

where the τ_i ($i=1,2,3$) are Pauli matrices, Φ is a Higgs–Goldstone field, and B_μ and A_μ^i are U(1) and SU(2) gauge fields, respectively.

By introducing new special arbitrary phase-angles (which do not change the Lagrangian), we can generalize the left-handed and right-handed spinors through a Clifford algebra valued phase factor in the following form:[3]

$$L_0 \to L \equiv \exp\left[b^a i\gamma_a \left(\frac{1-i\gamma_5}{2} \right) \right] L_0 = \left[1 + b^a i\gamma_a \left(\frac{1-i\gamma_5}{2} \right) \right] L_0 ,$$
$$R_0 \to R \equiv \exp\left[b^a i\gamma_a \left(\frac{1+i\gamma_5}{2} \right) \right] R_0 = \left[1 + b^a i\gamma_a \left(\frac{1+i\gamma_5}{2} \right) \right] R_0 . \tag{18}$$

The last equalities arise because the exponential has a truncated expansion from $\gamma_\alpha \mathbb{P}_L = \mathbb{P}_R \gamma_\alpha$ and $\mathbb{P}_L \mathbb{P}_R = \mathbb{P}_R \mathbb{P}_L = 0$. The corresponding Dirac conjugate spinors are

$$\overline{L} = \overline{L_0} \left[1 - b^a i\gamma_a \left(\frac{1-i\gamma_5}{2} \right) \right],$$
$$\overline{R} = \overline{R_0} \left[1 - b^a i\gamma_a \left(\frac{1+i\gamma_5}{2} \right) \right], \tag{19}$$

with $\overline{L}L = \overline{L_0} L_0$ and $\overline{R}R = \overline{R_0} R_0$.

In principle, L (resp. R) is not just a conventional left (resp. right)-handed spinor, as far as it includes left (resp. right)-handed ''phase angles b^a''. We choose to call L (resp. R) as ''generalized left (resp. right)-handed spinor''. In fact L (or R) are closely related to the ''null twistors'' which were studied early by Penrose.[4] (See Ref. 5 for the geometric algebra formulation of twistors.) The objects (18) and (19) are faithful representations of the full Poincaré group and not only, as spinors are, of the Lorentz group. The geometry of these spinors is clearest in the terms of projective twistor space. Considering L to be fixed and solving for real solutions $b^a \in M$ of Eq. (18), it turns out that a solution exists only if $LL = 0$. These solutions for b^a in real Minkowski space M constitute a null straight line (null geodesics), and every null straight line in Minkowski space M arises in this way. So a point in Minkowski space is said to be ''incident'' with the null twistor. This is the so-called standard flat-space twistor correspondence.

The generalized left (or right)-handed spinor (null twistor) can be defined by using (the idempotent) projector operator $P_L = [1 + b^\mu i\gamma_\mu((1-i\gamma_5)/2)]((1-i\gamma_5)/2)$, which satisfies $P_L P_L = P_L$. It can be considered as generalization of $(P_L)_0 = ((1-i\gamma_5)/2)$. We define its complement V by $P_L + V = 1$; it also satisfies $VV = V$. Any spinor can then be decomposed in two parts:

$$\psi = P_L(\psi) + V(\psi) = L + V(\psi). \tag{20}$$

It is important to notice that under a new $S^\alpha_{-\beta} \in G_T$ transformation of a chiral group G_T [see the definition of $S^\alpha_{-\beta}$ in Eq. (22)], the spinor ψ transforms as

$$\widetilde{\psi} = S_- \psi = S_-(L + V(\psi)) = S_- L + V(\psi). \tag{21}$$

This means that in the spinor space $S^\alpha_{-\beta} \in G_T$ acts only on its projective subspace (projective null twistor space), which can be considered as representation space of this group G_T.

Notice also that although we bear firmly in mind that L and R include arbitrary ''phase angles b^a'', these parameters will disappear from the Lagrangian (17) when we replace L_0 and R_0 by L and R. This means that the standard model is invariant under the following transformation[3]

$$\widehat{R^\alpha} = S^\alpha_{+\beta} R^\beta = \left[1 - k\sigma^\mu i\gamma_\mu \left(\frac{1+i\gamma_5}{2} \right) \right]^\alpha_\beta R^\beta ,$$
$$\widehat{L^\alpha} = S^\alpha_{-\beta} L^\beta = \left[1 - k\sigma^\mu i\gamma_\mu \left(\frac{1-i\gamma_5}{2} \right) \right]^\alpha_\beta L^\beta , \tag{22}$$

$$S_+\left[\gamma_\mu\left(\frac{1+i\gamma_5}{2}\right)\right](S_+)^{-1}=\gamma_\mu\left(\frac{1+i\gamma_5}{2}\right),$$

$$S_-\left[\gamma_\mu\left(\frac{1-i\gamma_5}{2}\right)\right](S_-)^{-1}=\gamma_\mu\left(\frac{1-i\gamma_5}{2}\right).$$

The matrices $S^{\alpha}_{\pm\beta}$ with parameters σ^μ constitute a four-dimensional Abelian subgroup of SU(2,2). For some physical considerations we can consider σ^μ as parameters of Poincaré translation in the phase space of the spinor space induced by translation $\widehat{x^\mu} = x^\mu + \sigma^\mu$ in the space–time manifold. The generators of Poincaré group can be taken[6,7] therefore as elements of the multivector Clifford algebra of the complex space–time geometric algebra $M=s+v+b+t+p$, where s denotes scalar, v denotes vector, b denotes bivector, t denotes trivector, and p denotes pseudoscalar part, as

$$P^{\pm}_{\mu}=i\partial_\mu-k\gamma_\mu\left(\frac{1\pm i\gamma_5}{2}\right),$$

$$L_{\mu\nu}=ix_\nu\partial_\mu-ix_\mu\partial_\nu+\frac{i}{4}(\gamma_\mu\gamma_\nu-\gamma_\nu\gamma_\mu). \tag{23}$$

We can verify that these sets of generators satisfy the usual commutation relations of the Poincaré Lie algebra (''Poisson brackets'' relations)

$$[P^{\pm}_{\mu},P^{\pm}_{\nu}]=0,$$

$$[L_{\mu\nu},L_{\lambda\rho}]=ig_{\mu\lambda}L_{\mu\rho}-ig_{\mu\lambda}L_{\nu\rho}+ig_{\nu\rho}L_{\lambda\mu}-ig_{\mu\rho}L_{\lambda\nu}, \tag{24}$$

$$[P^{\pm}_{\mu},L_{\nu\lambda}]=ig_{\mu\nu}P^{\pm}_{\lambda}-ig_{\mu\lambda}P^{\pm}_{\nu}.$$

These generators have been studied as generators of a subgroup of the conformal group by Barut and Raczka.[8] Some interesting results in this direction have previously been obtained by Dirac[9] and Hepner.[10] We remind the reader that a choice like (23) is in itself a dynamical model. Also, there exist representations of M suitable for any spin and not only for spin $\frac{1}{2}$ fermions.[5,7]

Returning to the consideration of the standard model, we know that, under the gauge group SU(2) transformations, L and R transform in completely different ways, and now we see that under the Poincaré translation they also transform in different ways. We can easily visualize this situation by the example of two different kinds of screws. When we screw both, the clockwise and the counterclockwise screws with the same rotation direction, we can observe that if the former is screwed (translated) in, the latter is screwed (translated) out. The phase angles involved by (22) correspond to a so-called complex duality rotation $v\rightarrow it$, $t'=i\gamma_5 v'$, where vectors and trivectors are mapped in the $v-t$ plane.

According to Dirac,[11] the task of constructing a relativistic dynamics is equivalent to constructing a representation of the inhomogeneous Lorentz group. In other words, ''to construct the theory of a dynamical system, one must obtain expressions for ten fundamental quantities that satisfy the 'Poisson brackets' relations [i.e., Eq. (24)]. The problem of finding a new dynamical system reduces to the problem of finding a new solution of these equations.''

The existence of an additional intrinsic symmetry introduced by enlarging the representation of P_μ predicts an additional intrinsic energy-momentum term for fermions, which is generated, as discussed below, by the additional second term $i\gamma_\mu((1\pm i\gamma_5)/2)$ in the $P^{\pm}_{\mu}$. However, since the additional term $i\gamma_\mu((1\pm i\gamma_5)/2)$ is nilpotent, it turns out that the rest mass corresponding to the additional intrinsic energy-momentum of a given handness fermion is zero.

Let

$$W_{\mu}^{\pm}=-\tfrac{1}{2}\epsilon_{\mu\nu\lambda\rho}L^{\nu\lambda}P^{\pm\rho} \tag{25}$$

be the new Pauli–Lubanski vector. Consider now the following linear combinations of $(P^{\pm})^2$ and $(W^{\pm})^2$,

$$\begin{aligned} C_1&=\tfrac{3}{2}(P_{\mu}^{\pm}+\tfrac{2}{3}W_{\mu}^{\pm})(P^{\pm\mu}+\tfrac{2}{3}W^{\pm\mu})=\tfrac{3}{2}(P^{\pm})^2+\tfrac{2}{3}(W^{\pm})^2=-\partial_{\mu}\partial^{\mu},\\ C_2^{\pm}&=\left(P_{\mu}^{\pm}+\frac{2}{\sqrt{3}}\,W_{\mu}^{\pm}\right)\left(P^{\pm\mu}+\frac{2}{\sqrt{3}}\,W^{\pm\mu}\right)=(P^{\pm})^2+\frac{4}{3}\,(W^{\pm})^2=4ki\,\gamma_{\mu}\left(\frac{1\pm i\gamma_5}{2}\right)\partial_{\mu}, \end{aligned} \tag{26}$$

which commute with all the ten generators of the Poincaré group. The first of these Casimir operators, which corresponds to the orbital energy-momentum, is associated with the rest mass m^2. The second is associated with an internal-orbital interaction. [The invariance of the $C_2^{\pm}$ depends on the invariance of the $\mathbb{P}_L$ and $\mathbb{P}_R$ (see Ref. 7).]

We can also approach these issues from an equivalent but different perspective. Since the Lagrangian (39) is invariant under the translational transformation (23), the Noether conserved quantity for the left-handed fermion is the energy-momentum tensor density

$$T_{\nu}^{-\mu}=\frac{i}{2}\,[(\overline{L_0}\gamma^{\mu}(\partial_{\nu}L_0)-(\partial_{\nu}\overline{L_0})\,\gamma^{\mu}L_0)]+\frac{ik_2}{2}\,[(\overline{L_0}\gamma_{\nu}(\partial^{\mu}L_0)-(\partial^{\mu}\overline{L_0})\,\gamma_{\nu}L_0))] \tag{27}$$

here k_2 depends on k_1 and k. The energy-momentum vector is

$$\begin{aligned} P_{\mu}^{-}&=\int d^3x T_{\mu}^{-0},\\ P_{\mu}^{-}&=\int d^3x\,\frac{i}{2}\,[\overline{L_0}\gamma^0(\partial_{\mu}L_0)-(\partial_{\mu}\overline{L_0})\,\gamma^0L_0+k_2(\overline{L_0}\gamma_{\mu}(\partial_0L_0)-(\partial_0\overline{L_0})\,\gamma_{\mu}L_0)]. \end{aligned} \tag{28}$$

The additional second part corresponds to the intrinsic energy momentum for the left-handed fermion. Its form is similar to the U(1) charged current. This opens the possibility that a chiral field behaves as a field with an intrinsic energy momentum current, and intrinsic charged current.

IV. GAUGE THEORY OF THE TRANSLATION GROUP

The gauge theory of the Poincaré group was brought into consideration by Kibble, Frolov and Sciama at the beginning of 1960s. Their work generalizes Utiyama's gauge version of gravity which left open the question on the gauge status of the tetrad gravitational fields.[12] In the same period of time, the gauge potentials of spatial translations were considered in the gauge theory of dislocations in continuous media.[13]

The Poincaré group combines the group of Lorentz rotations L_b^a and the group of translations σ^a in the four-dimensional Minkowski space–time in the form

$$\widehat{y^a}=L_b^a y^b+\sigma^a. \tag{29}$$

Localization, that is making this L_b^a and σ^a position-dependent $L_b^a(x)$ and $\sigma^a(x)$, of these transformations leads in the usual analysis to the introduction of gauge fields (notice that, different from the coordinate frame vectors x^{μ}, the free y^b are components of the nonvector bundle). The covariant derivative ∇_{μ} of the section $y^a(x)$ can be defined as the sum

$$\nabla_{\mu}(y^a)=\partial_{\mu}y^a-\Gamma_{\mu b}^a y^b-N_{\mu}^a. \tag{30}$$

The transformation properties of the above connections in relation to (29) are

$$\widehat{\nabla}_\mu(\widehat{y^a}) \equiv \left(\frac{\partial \widehat{y^a}}{\partial y^b}\right) \nabla_\mu y^b = L^a_b(\nabla_\mu y^b) \tag{31}$$

and (notice that the following are, in fact, definitions of Γ and N)

$$\widehat{\Gamma^a_{\mu b}} = L^a_d \Gamma^d_{\mu c}(L^{-1})^c_b + L^a_{d,\mu}(L^{-1})^d_b, \tag{32}$$

$$\widehat{N^a_\mu} = L^a_b N^b_\mu + \partial_\mu \sigma^a - [L^a_d \Gamma^d_{\mu c}(L^{-1})^c_b + L^a_{d,\mu}(L^{-1})^d_b]\sigma^b. \tag{33}$$

As it can be shown that the gauge fields $\Gamma^a_{\mu b}$ are related and can be expressed in terms of the Christoffel symbols and tetrads, it can be shown therefore that they correspond to the gravitational field. Also, and in the same way, from physical considerations it is possible to select a special, metric-compatible, gauge potential of the localized Poincaré translation such that

$$\nabla_\mu(y^a) = \partial_\mu y^a - \Gamma^a_{\mu b} y^b - N^a_\mu = e^a_\mu, \tag{34}$$

where e^a_μ is the vierbein field. This invariant condition implies that there is always a certain translation gauge where N^a_μ coincides with e^a_μ. In this case the curvature tensor corresponding to the translational connection

$$F^a_{\mu\nu} = N^a_{\nu,\mu} - N^a_{\mu,\nu} + \Gamma^a_{\nu b} N^b_\mu - \Gamma^a_{\mu b} N^b_\nu = e^a_{\nu,\mu} - e^a_{\mu,\nu} + \Gamma^a_{\nu b} e^b_\mu - \Gamma^a_{\mu b} e^b_\nu. \tag{35}$$

plays the role of the Cartan torsion.

Now we have stated the necessary definitions and we proceed to analyze the gauge theory of the Poincaré translation (23) in the phase space of the (chiral projected) spinor space which (as we mentioned in the previous section) is induced by translations in the tangent bundle of the space–time manifold. The covariant derivatives of generalized left-handed spinor are defined as

$$\nabla_\mu(L^\beta) \equiv \partial_\mu L^\beta - N^a_\mu i \left[\gamma_a\left(\frac{1-i\gamma_5}{2}\right)\right]^\beta_\gamma L^\gamma - \frac{1}{4}\Gamma^a_{\mu b}(\gamma_a\gamma^b - \gamma^b\gamma_a)^\beta_\gamma L^\gamma. \tag{36}$$

In analogy to (34), without losing the invariant property of the theory, we can consider only the metric compatible translation connection N^a_μ, i.e., assume that

$$\nabla_\mu(b^a) = \partial_\mu b^a - \Gamma^a_{\mu d} b^d - N^a_\mu = k_1 e^a_\mu, \tag{37}$$

where $b^a(x)$ are phase angles of generalized left-handed spinor

$$L = \exp\left[b^a i\gamma_a\left(\frac{1-i\gamma_5}{2}\right)\right] L_0 = \left[1 + b^a i\gamma_a\left(\frac{1-i\gamma_5}{2}\right)\right] L_0 \tag{38}$$

(see Ref. 14 for further discussions of this point and of the importance of twistor-spin $\frac{1}{2}$-fields). We now restrict ourselves to emphasize the new translational symmetry of the spinors to the case where the gravitational field and the torsion are zero (i.e., $\Gamma^a_{\mu d} = T^a_{\mu d} = 0$). We can rewrite the Lagrangian $\mathbf{L}$ of the Dirac field in the same form as that for bosons:

$$\mathbf{L} = \frac{-1}{k_1}(\overline{\nabla_\mu L})(\nabla_\mu L) + \frac{-1}{k_1}(\overline{\nabla_\mu R})(\nabla_\mu R) - m\left[\overline{L}\left(\frac{1+i\gamma_5}{2}\right)R + \overline{R}\left(\frac{1-i\gamma_5}{2}\right)L\right]. \tag{39}$$

In the torsion-free case, the curvature tensor corresponding to the above connection,

$$F^{\alpha}_{\beta\mu\nu}=F^{d}_{\mu\nu}i\left[\gamma_d\left(\frac{1\mp i\gamma_5}{2}\right)\right]^{\alpha}_{\beta}=0 \tag{40}$$

[here $F^{a}_{\mu\nu}$ is defined as (35)]. So we could naively state that the fermions have nowhere experienced any ''force.'' However, as the Aharonov–Bohm experiment shows, in quantum mechanics the actual value of the potential plays a role (i.e., in determining some observable effect such as interference) not expected on classical theories. As stressed by C. N. Yang, the knowledge on the field strengths $F_{\mu\nu}$ under-describes electromagnetism while the knowledge on the potential over-describes the physical situation, leading to the attempt of using the nonintegrable phases to characterize a gauge theory. The existence of Berry phases within the well-known framework of the adiabatic approximation requires the study of the question of phases and angles in quantum mechanics. The nonintegrable phases for left-handed fermion are defined as

$$L'=\exp\left\{\beta^a i\gamma_a\left(\frac{1-i\gamma_5}{2}\right)\right\}\cdot L_0=\exp\left\{\left(b^a+\int N^a_\mu dx^\mu\right)i\gamma_a\left(\frac{1-i\gamma_5}{2}\right)\right\}\cdot L_0, \tag{41}$$

where the N^a_μ are metric compatible and satisfy

$$\nabla_\mu(b^a)=\partial_\mu b^a-\Gamma^a_{\mu d}b^d-N^a_\mu=k_1 e^a_\mu. \tag{42}$$

We see then that the Berry-type phases in the fermion fields depend on the topology of the space–time manifold which is determined by the vierbein e^a_μ. Moreover the U(1) phase in $\exp(i\alpha)$ is determined only up to a term $\exp(i2n\pi)$ where n is *integer*. In contrast with the U(1) case, the 'phases β^a' in (41) are only determined to a *null straight line* in the Minkowski space–time.

It is interesting to notice that in the theory of continuous media,[13] $\Gamma^a_{\mu d}$ corresponds to the disclination and N^a_μ corresponds to the dislocation fields, both of which have their origin from line defects.

V. GAUGE FIELD THEORY FOR FERMION FIELDS

To study, under the previous point of view, the Lagrangian of chiral fermion fields, let us begin with the definition of the extended Poincaré group (we remind that this extension is different from the group used in supersymmetry theory) considering also the standard U(1)×SU(2) gauge groups in the spinor space:

$$\begin{aligned}
\widehat{y^d}&=y^d+h^d,\\
\widehat{y^A}&=\exp(ig_1h^5)S^A_B(\sigma^i)y^B,\\
\widehat{\theta^\beta}&=\exp(ig_2h^5)\left[1+h^d i\gamma_d\left(\frac{1-i\gamma_5}{2}\right)\right]^{\beta}_{\alpha}\theta^\alpha+\xi^\beta,\\
\widehat{\overline{\theta_\beta}}&=\exp(-ig_2h^5)\overline{\theta_\alpha}\left[1-h^d i\gamma_d\left(\frac{1-i\gamma_5}{2}\right)\right]^{\alpha}_{\beta}+\overline{\xi_\beta}.
\end{aligned} \tag{43}$$

Here h^d, h^5, σ^i, ξ^β, and $\overline{\xi_\beta}$ (for simplicity denoted sometimes as ξ and $\overline{\xi}$) are group parameters of the Poincaré translation, the U(1), the SU(2), and the spinor translation groups, respectively. Experimentalists assert that they have not observed fermions with $V+A$ weak interactions. So, for a reason that will be clear shortly, we will work here with left-Poincaré-translation only. The generators of the corresponding Lie algebra are

$$T_d=\partial_d+i\left[\gamma_d\left(\frac{1-i\gamma_5}{2}\right)\right]^{\beta}_{\alpha}\theta^{\alpha}\frac{\partial}{\partial\theta^{\beta}}-i\overline{\theta}\left[\gamma_a\left(\frac{1-i\gamma_5}{2}\right)\right]\frac{\partial}{\partial\overline{\theta}},$$

$$T_5=ig_1y^A\frac{\partial}{\partial y^A}+ig_2\theta^{\beta}\frac{\partial}{\partial\theta^{\beta}}-ig_2\overline{\theta}\frac{\partial}{\partial\overline{\theta}},$$

$$T_i=\tau^A_{iB}y^B\frac{\partial}{\partial y^A},\quad T_{\beta}=\frac{\partial}{\partial\theta^{\beta}},\quad \overline{T^{\beta}}=\frac{\partial}{\partial\overline{\theta}_{\beta}}. \tag{44}$$

The nonzero commutation relations among these generators are

$$\begin{aligned}
&[T_i,T_j]=c^k_{ij}T_k,\\
&[T_d,T_{\beta}]=-T_{\gamma}\left[i\gamma_d\left(\frac{1-i\gamma_5}{2}\right)\right]^{\gamma}_{\beta},\\
&[T_d,\overline{T^{\beta}}]=\left[i\gamma_d\left(\frac{1-i\gamma_5}{2}\right)\right]^{\beta}_{\gamma}\overline{T^{\gamma}},\\
&[T_5,T_{\beta}]=-ig_2T_{\beta},\quad [T_5,\overline{T^{\beta}}]=ig_2\overline{T^{\beta}}.
\end{aligned} \tag{45}$$

In the local coordinate neighborhood $E_u(x,y)$, where $y=(y^d,y^A,\theta^{\alpha},\overline{\theta_{\beta}})$ and $x=\{x^{\mu}\}$ are coordinates in the base space (Minkowski space–time), let

$$Z_{\mu}=\partial_{\mu}+N^d_{\mu}T_d+B^5_{\mu}T_5+A^i_{\mu}T_i+W^{\beta}_{\mu}T_{\beta}+\overline{W}_{\beta\mu}\overline{T^{\beta}} \tag{46}$$

be the horizontal vector. Then the functions $N^d_{\mu}(x)$, $B^5_{\mu}(x)$, $A^i_{\mu}(x)$, $W^{\beta}_{\mu}(x)$, and $\overline{W}_{\beta\mu}(x)$ define connections in a wider sense (gauge fields on nonvector bundle). The covariant derivatives of a section $y(x)=[y^d(x^{\mu}),y^A(x^{\mu}),\theta^{\beta}(x^{\mu}),\theta_{\beta}(x^{\mu})]$ can be defined as

$$\begin{aligned}
&\nabla_{\mu}(y^a)\equiv\partial_{\mu}y^a-N^a_{\mu},\\
&\nabla_{\mu}(y^A)\equiv\partial_{\mu}y^A-ig_1B^5_{\mu}y^A-A^i_{\mu}\tau^A_{iB}y^B,\\
&\nabla_{\mu}(\theta^{\beta})\equiv\partial_{\mu}\theta^{\beta}-ig_2B^5_{\mu}\theta^{\beta}-N^d_{\mu}\left[i\gamma_d\left(\frac{1-i\gamma_5}{2}\right)\right]^{\beta}_{\alpha}\theta^{\alpha}-W^{\beta}_{\mu},\\
&\nabla_{\mu}(\overline{\theta_{\beta}})\equiv\partial_{\mu}\overline{\theta_{\beta}}+ig_2B^5_{\mu}\overline{\theta_{\beta}}+N^d_{\mu}\overline{\theta_{\alpha}}\left[i\gamma_d\left(\frac{1-i\gamma_5}{2}\right)\right]^{\alpha}_{\beta}-\overline{W}_{\beta\mu}.
\end{aligned} \tag{47}$$

The corresponding curvature tensor is defined by

$$\begin{aligned}
[Z_{\mu},Z_{\nu}]&\equiv F^d_{\mu\nu}T_d+F^5_{\mu\nu}T_5+F^i_{\mu\nu}T_i+F^{\beta}_{\mu\nu}T_{\beta}+\overline{F}_{\beta\mu\nu}\overline{T^{\beta}}\\
&=(\partial_{\mu}N^d_{\nu}-\partial_{\nu}N^d_{\mu})T_d+(\partial_{\mu}B^5_{\nu}-\partial_{\nu}B^5_{\mu})T_5+(\partial_{\mu}A^i_{\nu}-\partial_{\nu}A^i_{\mu}+c^i_{jk}A^j_{\mu}A^k_{\nu})T_i\\
&\quad+\left\{\partial_{\mu}W^{\beta}_{\nu}-\partial_{\nu}W^{\beta}_{\mu}-ig_2B^5_{\mu}W^{\beta}_{\nu}+ig_2B^5_{\nu}W^{\beta}_{\mu}+N^d_{\nu}\left[i\gamma_d\left(\frac{1-i\gamma_5}{2}\right)\right]^{\beta}_{\alpha}W^{\alpha}_{\mu}\right.
\end{aligned}$$

$$-N_\mu^d\left[i\gamma_d\left(\frac{1-i\gamma_5}{2}\right)\right]_\alpha^\beta W_\nu^\alpha\Big\}T_\beta+\Big\{\partial_\mu\overline{W_{\beta\nu}}-\partial_\nu\overline{W_{\beta\mu}}+ig_2B_\mu^5\overline{W_{\beta\nu}}-ig_2B_\nu^5\overline{W_{\beta\mu}}$$

$$-N_\nu^d\overline{W_{\alpha\mu}}\left[i\gamma_d\left(\frac{1-i\gamma_5}{2}\right)\right]_\beta^\alpha+N_\mu^d\overline{W_{\alpha\nu}}\left[i\gamma_d\left(\frac{1-i\gamma_5}{2}\right)\right]_\beta^\alpha\Big\}\overline{T^\beta}. \tag{48}$$

Here $F_{\mu\nu}^5$ and $F_{\mu\nu}^i$ are the electromagnetic field and the Yang–Mills fields, respectively. As we noted before, it is possible to choose a special metric-compatible gauge potential N_μ^d such that

$$\nabla_\mu(y^a)=\partial_\mu y^a-N_\mu^a=e_\mu^a. \tag{49}$$

The torsion-free case corresponds to $F_{\mu\nu}^d=0$. In the same way we can introduce a covariant condition for $\nabla_\mu(\theta^\alpha)$ (i.e., a restriction for the gauge field W_μ^β). According to Eq. (20), by using the projector operators $P_L=[1+y^a i\gamma_\mu((1-i\gamma_5)/2)]((1-i\gamma_5)/2)$ and V, it can be decomposed in to two parts $\nabla_\mu\theta^\alpha=P_L(\nabla_\mu\theta^\alpha)+V(\nabla_\mu\theta^\alpha)$. Under a $S_{-\beta}^\alpha\in G_T$ transformation

$$\widehat{\nabla_\mu\theta^\beta}=S_{-\alpha}^\beta[\nabla_\mu\theta^\alpha]=S_{-\alpha}^\beta[P_L(\nabla_\mu\theta^a)]+V(\nabla_\mu\theta^\beta), \tag{50}$$

which means that only the components $P_L(\nabla_\mu\theta^\alpha)$ are affected by the transformation $S_{-\beta}^\alpha\in G_T$. So, without losing the invariant properties of the theory, we can assume that $V(\nabla_\mu\theta^\alpha)=0$. In other words, the $\nabla_\mu\theta^\alpha$ can be assumed to have the following form:

$$\begin{aligned}\nabla_\mu\theta=L_\mu&=\left[1+y^d i\gamma_d\left(\frac{1-i\gamma_5}{2}\right)\right]L_{0\mu},\\ \nabla_\mu\overline{\theta}=\overline{L}_\mu&=\overline{L_{0\mu}}\left[1-y^d i\gamma_d\left(\frac{1-i\gamma_5}{2}\right)\right].\end{aligned} \tag{51}$$

In this case, instead of W_μ^β and $\overline{W_{\beta\mu}}$, we can use $L_{0\mu}^\beta$ and $\overline{L_{0\mu\beta}}$ in $F_{\mu\nu}^\beta$ and $\overline{F_{\beta\mu\nu}}$. So the Yang–Mills-type Lagrangian is

$$\begin{aligned}\mathbf{L}&=-\tfrac{1}{4}F_{\mu\nu}^5F_{\mu\nu}^5-\tfrac{1}{4}F_{\mu\nu}^iF_{\mu\nu}^i-\tfrac{1}{2}\overline{F_{\beta\mu\nu}}F_{\mu\nu}^\beta\\ &=-\tfrac{1}{4}F_{\mu\nu}^5F_{\mu\nu}^5-\tfrac{1}{4}F_{\mu\nu}^iF_{\mu\nu}^i+6\overline{R_0}i\gamma_\mu(\partial_\mu R_0+ig_2B_\mu^5R_0)-6(\partial_\mu\overline{R_0}-ig_2B_\mu^5\overline{R_0})i\gamma_\mu R_0\\ &\quad-\overline{L_{0\nu}^T}i\gamma_\mu(\partial_\mu L_{0\nu}^T+ig_2B_\mu^5L_{0\nu}^T)+(\partial_\mu\overline{L_{0\nu}^T}-ig_2B_\mu^5\overline{L_{0\nu}^T})i\gamma_\mu L_{0\nu}^T-2[\overline{L_{0\mu}^T}R_0+\overline{R_0}L_{0\mu}^T]_{,\mu},\end{aligned} \tag{52}$$

where the vector-spinor $L_{0\mu}^\beta$ has been decomposed into two parts:

$$L_{0\mu}=L_{0\mu}^T+i\gamma_\mu\left(\frac{-i}{4}\gamma_\mu L_{0\mu}\right)=L_{0\mu}^T+i\gamma_\mu R_0. \tag{53}$$

We can verify that the above Lagrangian includes the Dirac Lagrangian of the charged right-handed fermion R_0. One can ignore the last divergence term, as this term may be integrated up to the topological quantum number. Performing the variation of this Lagrangian with respect to $L_{0\mu}^T$, and using the method of Lagrange multipliers, we can prove that $L_{0\mu}^T=L_{02\mu}^T+D_\mu L_{01}$ (here $D_\mu=\partial_\mu-ig_2B_\mu^5$) includes a spin $\frac{1}{2}$ charged left-handed spinor singlet $L_{01}\equiv\frac{1}{2}D_\nu L_{0\nu}^T$ which satisfies the massless Dirac equation and the spin $\frac{3}{2}$ charged left-handed vector-spinor field $L_{02\mu}^T$ (with the condition for Rarita–Schwinger fields $\gamma_\mu L_{02\mu}^T=0$) which satisfies $\gamma_\mu D_\mu L_{02\nu}^T=(\gamma_\nu+F_{\nu\mu}^5\gamma_\mu)L_{01}$.

If W_μ^β [in addition to Eq. (51)] satisfies following invariant condition (twistor equation),

$$\gamma_\nu\left(\frac{1-i\gamma_5}{2}\right)\nabla_\mu\theta+\gamma_\mu\left(\frac{1-i\gamma_5}{2}\right)\nabla_\nu\theta=\frac{1}{2}\,g_{\mu\nu}\gamma_\lambda\left(\frac{1-i\gamma_5}{2}\right)\nabla_\lambda\theta, \tag{54}$$

then we can prove that the above Lagrangian includes only a right-handed spinor singlet $R_0=(-i/4)\,\gamma_\mu L_{0\mu}$ (i.e., $L_{0\mu}=i\gamma_\mu R_0$).

VI. SOME FINAL CONSIDERATIONS

It is important to notice that if the base space is a Riemannian space with Christoffel connections $\{^{\nu}_{\mu}\}$, then the derivative of any space–time vector $\partial_\mu B_\nu$ must be replaced by the covariant derivative $D_\mu(B_\nu)\equiv\partial_\mu B_\nu+B_\lambda\{^{\lambda}_{\mu\nu}\}$.

Moreover, in analogy to the Kaluza–Klein[15] theory, the base space can be enlarged, and then more gauge components must be introduced.[16] Let us consider for example the case with five-dimensional base space. We know that the physical charged field has an arbitrary phase angle, denoted here by x^5, and subjected to the condition of cyclicity, i.e., $\Psi(x^\mu,x^5)=\Psi(x^\mu)\exp(-ig_1x^5)$. The Lagrangian does not depend on this phase angle. This condition reflects the independence of observed physical phenomena on the fifth coordinate of the base space and is called the condition of cylindricity. It implies the orthogonality of space–time manifold with the phase manifold. If we admit that in Eq. (43) the parameters of the (local) gauge group $\xi^\beta(x^\mu,x^5)$ are not only functions of the space–time coordinate x^μ but also functions of the phase angle x^5, that leads to the introduction of the additional gauge fields L_5^β and $L_{\beta5}$ such that

$$\begin{aligned} Z_\mu&=\partial_\mu+N_\mu^d T_d+B_\mu^5 T_5+A_\mu^i T_i+W_\mu^\beta T_\beta+\overline{W}_{\beta\mu}\overline{T^\beta},\\ Z_5&=\partial_5+a_1L_5^\beta T_\beta+a_2\overline{L}_{\beta5}\overline{T^\beta}. \end{aligned} \tag{55}$$

For simplicity let us consider only the case with $W_{0\mu}=i\gamma_\mu R_0$. As mentioned above, in analogy to the Kaluza–Klein theory, we can introduce the ansatz of ''dimensional reduction,'' i.e., taking the fields N_μ^d, B_μ, and A_μ^i to be independent of the extra coordinate x^5, and the fermion fields R_0 and L_5^β subjected to the condition of cyclicity. We get then additional components of the curvature tensor

$$[Z_\mu,\,Z_5]=F_{\mu5}^\beta T_\beta+\overline{F}_{\beta\mu5}\overline{T^\beta} \tag{56}$$

and additional Lagrangian terms $(\overline{F}_{\beta\mu5}F_{\mu5}^\beta)$ which include the Dirac Lagrangian of the left-handed fermion and the fermionic mass term.

In a similar form, we can enlarge the base space M to include the representation space of the SU(2) group, i.e., $\mathbf{x}=(x^\mu,x^5,x^A)$. And then, the total Lagrangian will include a left-handed SU(2) spinor-doublet and a doublet of a Higgs–Goldstone complex scalar field.

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Quantum Boltzmann equation for photons

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The quantum Boltzmann equation is derived for photons. The form of the scattering and absorption terms for the case of photon diffusion is discussed in detail. We show how the structure factor of the scattering centers enters into the scattering rate of the photons. © *1996 American Institute of Physics.*
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I. INTRODUCTION

The quantum Boltzmann equation (QBE) is derived for photons. As far as we know, this is the first derivation of this fundamental equation. We expect the main application of this result is to photon diffusion in matter. We distinguish the QBE from the usual Boltzmann equation. The latter has been studied widely. We explain below the differences between these two equations. We also show how the usual Boltzmann equation is derived from the QBE.

Photons diffuse through many different kinds of materials, such as clouds, stellar atmospheres, cermats, and human tissue.[1–7] The Boltzmann equation for photons is routinely used to describe the diffusion of light in these materials.

In the Boltzmann equation for photons, the usual practice is to have a differential equation for the number density of photons $f(\hat{q},\mathbf{r},t)$ of frequency ω, which depends upon the direction of the photons $\hat{q}$, the position in the medium $\mathbf{r}$ and the time t. The usual equation is

$$\left[\frac{\partial}{\partial t}+c\hat{q}\cdot\boldsymbol{\nabla}_r+\left(\frac{1}{\tau_a}+\frac{1}{\tau_s}\right)\right]f(\hat{q},\mathbf{r},t)=\frac{1}{\tau_s}\int\frac{d\Omega'}{4\pi}P(\hat{q},\hat{q}')f(\hat{q}',\mathbf{r},t), \tag{1}$$

where the lifetimes are for absorption τ_a and scattering τ_s. The scattering term on the right contains the information $P(\hat{q},\hat{q}')$ for scattering between $\mathbf{q}$ and $\mathbf{q}'$. The scattering integral is over all of the 4π solid angle of the $\hat{q}'$ variable. This equation is well-known and well studied.[1–7]

The quantum Boltzmann equation (QBE) is an equation of motion for the photon Green's function when the system is not in equilibrium. There are several types of correlation function, such as retarded, advanced, etc.[8] An important one is

$$\mathscr{D}^{<}_{\mu\nu}(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2)=-i\langle A_\nu(\mathbf{r}_2,t_2)A_\mu(\mathbf{r}_1,t_1)\rangle, \tag{2}$$

where the vector potential is $A_\mu(\mathbf{r},t)$. From this definition one derives an equation of motion for the Wigner distribution function (WDF) $\mathscr{D}_{\mu\nu}(\mathbf{q},\omega;\mathbf{r},t)$. This equation is the QBE. It is different than the usual Boltzmann equation described in the previous paragraph. It is a tensor quantity, rather than a scalar. Also, it has more variables in its arguments, since $\mathbf{q}$ and ω are assumed to be independent variables. The QBE is the more fundamental equation. From it we derive the Boltzmann equation (1). This derivation gives us definitions of quantities such as the life times for absorption τ_a and scattering τ_s.

There has been prior work on the closely related problem of evaluating the correlation of the electric field with itself at two different points in space and time $\langle E^*(\mathbf{r}_1,t_1)E(\mathbf{r}_2,t_2)\rangle$. Zubairy and Wolf[9] derived an equation for the correlation function of free fields. Their result is very different than ours since they are not using Wigner distribution functions. Later work has discussed free

field propagation from partially coherent sources.[10] An important line of work was the development of theories on weak localization and coherent backscattering of photons.[11–13] There they evaluated the average electric field in the coherent potential approximation, and then used perturbation theory to get the correlation functions of the field with itself. We discuss these results further in the final section of this paper.

The general procedure is similar to that for phonons, since both particles are boson fields. There have been numerous derivations of the QBE for phonons.[14–21] However, the interaction between photons and matter is strong, so that several scattering terms must be retained in the interaction. The same terms are not kept in the QBE for phonons since the interaction there is weaker. Also, phonon scattering is dominated by anharmonic effects, and these processes are unimportant for photon diffusion. So the QBE for the two systems are different in detail.

The derivation proceeds in three stages. The next is to derive the QBE for noninteracting photons. This allows us to introduce the notation and to set up the general formalism. Sections III and IV discuss the interactions between the photon and the media. We derive the photon Green's function for systems in equilibrium. Here, we derive the important self-energy terms which also contribute to the nonequilibrium case. Section V has the case where photons diffuse through matter. Here, we assume the scattering centers are fixed. We identify the limits of coherent and incoherent scattering. The last section contains a brief discussion and summary of the results.

II. NONINTERACTING PHOTONS

The Green's function for photons is the correlation function of the vector potential $A_\mu(\mathbf{r},t)$ at two different points in space and time

$$\mathscr{D}^{<}_{\mu\nu}(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2) = -i\langle A_\nu(\mathbf{r}_2,t_2)A_\mu(\mathbf{r}_1,t_1)\rangle. \tag{3}$$

The QBE for photons is the equation of motion for this correlation function. The derivation requires other correlation functions, which are defined as[8]

$$\mathscr{D}^{>}_{\mu\nu}(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2) = -i\langle A_\mu(\mathbf{r}_1,t_1)A_\nu(\mathbf{r}_2,t_2)\rangle, \tag{4}$$

$$\mathscr{D}^{t}_{\mu\nu} = \theta(t_1-t_2)\mathscr{D}^{>}_{\mu\nu} + \theta(t_2-t_1)\mathscr{D}^{<}_{\mu\nu}, \tag{5}$$

$$\mathscr{D}^{\overline{t}}_{\mu\nu} = \theta(t_1-t_2)\mathscr{D}^{<}_{\mu\nu} + \theta(t_2-t_1)\mathscr{D}^{>}_{\mu\nu}, \tag{6}$$

$$\mathscr{D}^{r}_{\mu\nu} = \theta(t_1-t_2)[\mathscr{D}^{>}_{\mu\nu} - \mathscr{D}^{<}_{\mu\nu}]. \tag{7}$$

The superscripts $t,\overline{t},r$ denote the time-ordered, anti-time-ordered, and retarded Green's functions.

The Hamiltonian for photons depends upon the gauge. Here we use the gauge $\nabla\cdot\mathbf{A}=0$ which makes the scalar potential instantaneous. Then the noninteracting Hamiltonian for photons is given in terms of the electric and magnetic fields

$$H_0 = \int \frac{d^3r}{8\pi}\,[E^2+B^2], \tag{8}$$

$$\mathbf{E} = -\frac{1}{c}\frac{\partial \mathbf{A}}{\partial t}, \tag{9}$$

$$\mathbf{B} = \nabla\times\mathbf{A}. \tag{10}$$

The fields are quantized. The electric field is the conjugate momentum to the vector potential, so that the basic commutation relation is

$$[E_\mu(\mathbf{r}_1,t),A_\nu(\mathbf{r}_2,t)]=4\pi i\hbar c\,\delta_{\mu\nu}\delta^3(\mathbf{r}_1-\mathbf{r}_2). \tag{11}$$

The commutator is defined at equal times. The first equation of motion

$$\frac{\partial}{\partial t}A_\mu=i[H_0,A_\mu]=-cE_\mu \tag{12}$$

which reproduces Eq. (9). The second equation of motion is

$$\frac{\partial^2}{\partial t^2}\mathbf{A}=-ic[H_0,\mathbf{E}] \tag{13}$$

$$=c^2\boldsymbol{\nabla}\times(\boldsymbol{\nabla}\times\mathbf{A}). \tag{14}$$

The term on the right comes from the commutator of the electric and magnetic fields. We use the fact that $\boldsymbol{\nabla}\times(\boldsymbol{\nabla}\times\mathbf{A})=\nabla^2\mathbf{A}-\boldsymbol{\nabla}\boldsymbol{\nabla}\cdot\mathbf{A}$ and the second term is zero by our gauge condition. This expression is the standard equation of motion for the vector potential. For noninteracting photons, the equation of motion for the Green's functions are either of the two expressions

$$\left[\frac{\partial^2}{\partial t_1^2}-c^2\nabla_1^2\right]D^<_{\mu\nu}(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2)=0, \tag{15}$$

$$\left[\frac{\partial^2}{\partial t_2^2}-c^2\nabla_2^2\right]D^<_{\mu\nu}(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2)=0. \tag{16}$$

The above two expressions are equations of motion for the Green's function.

The equation we want is obtain by subtracting them. First we must go to a center-of-mass coordinate system.

$$\mathbf{r}=\mathbf{r}_1-\mathbf{r}_2, \tag{17}$$

$$\mathbf{R}=\frac{\mathbf{r}_1+\mathbf{r}_2}{2}, \tag{18}$$

$$t=t_1-t_2, \tag{19}$$

$$T=\frac{t_1+t_2}{2}, \tag{20}$$

$$\mathscr{D}(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2)\rightarrow\mathscr{D}(\mathbf{r},t;\mathbf{R},T). \tag{21}$$

Here, the symbol T denotes center-of-mass time, and not temperature or time ordering. If we subtract our two equations (15) and (16), and convert to c.m. coordinates, then we find

$$2\left[\frac{\partial^2}{\partial t\partial T}-c^2\boldsymbol{\nabla}r\cdot\boldsymbol{\nabla}R\right]\mathscr{D}^<_{\mu\nu}(\mathbf{r},t;\mathbf{R},T)=0. \tag{22}$$

The next step is to Fourier transform the relative variables to $(\mathbf{q},\omega)$

$$\mathscr{D}^<(\mathbf{q},\omega;\mathbf{R},T)=\int d^3r\; e^{-i\mathbf{q}\cdot\mathbf{r}}\int dt\; e^{i\omega t}\mathscr{D}^<_{\mu\nu}(\mathbf{r},t;\mathbf{R},T) \tag{23}$$

$$\left[\omega\,\frac{\partial}{\partial T}+c^2\mathbf{q}\cdot\boldsymbol{\nabla}_R\right]\mathscr{D}^{<}_{\mu\nu}(\mathbf{q},\omega;\mathbf{R},T)=0. \tag{24}$$

Notice that the last equation is similar to a Boltzmann equation, in that there is a term with a derivative with respect to time (T) and another term with a derivative with respect to position ($\boldsymbol{\nabla}_R$). It is solved by any function of the form $f(\omega\mathbf{q}\cdot\mathbf{R}-c^2q^2T)$. Further terms are provided by the interactions.

In discussing the interactions it is useful to introduce a matrix formalism for the various Green's functions[8]

$$\widetilde{\mathscr{D}}=\begin{pmatrix}\mathscr{D}^{t} & -\mathscr{D}^{<}\\ \mathscr{D}^{>} & -\mathscr{D}^{\overline{t}}\end{pmatrix}, \tag{25}$$

$$\left(\omega\,\frac{\partial}{\partial T}+c^2\mathbf{q}\cdot\boldsymbol{\nabla}_R\right)\widetilde{\mathscr{D}}(\mathbf{q},\omega;\mathbf{R},T)=0. \tag{26}$$

Each Green's function obeys the homogeneous Boltzmann equation for noninteracting particles. Another equation we shall need is

$$\left(\frac{\partial^2}{\partial t_1^2}-c^2\nabla_1^2\right)\widetilde{\mathscr{D}}(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2)=4\pi c^2\delta_{\mu\nu}\delta(t_1-t_2)\,\delta(\mathbf{r}_1-\mathbf{r}_2)\widetilde{I}, \tag{27}$$

where $\widetilde{I}$ is the unit matrix. We also give the noninteracting Green's functions, where η is infinitesimal

$$\mathscr{D}^{r}_{\mu\nu}(\mathbf{k},\omega)=\frac{4\pi c^2\hbar(\delta_{\mu\nu}-\hat{k}_\mu\hat{k}_\nu)}{\omega^2-c^2k^2+i\eta}, \tag{28}$$

$$\mathscr{D}^{<}_{\mu\nu}(\mathbf{k},\omega)=-iB(\mathbf{k},\omega)n(\omega), \tag{29}$$

$$\mathscr{D}^{>}_{\mu\nu}(\mathbf{k},\omega)=-iB(\mathbf{k},\omega)[n(\omega)+1], \tag{30}$$

$$B(\mathbf{k},\omega)=\frac{(2\pi c)^2\hbar}{ck}\,(\delta_{\mu\nu}-\hat{k}_\mu\hat{k}_\nu)[\delta(\omega-ck)-\delta(\omega+ck)], \tag{31}$$

$$n(\omega)=\frac{1}{e^{\beta\omega}-1}, \tag{32}$$

$$\mathscr{D}^{t}=\mathscr{D}^{r}+\mathscr{D}^{<}=\mathscr{D}^{>}+\mathscr{D}^{a}, \tag{33}$$

$$\mathscr{D}^{\overline{t}}=\mathscr{D}^{>}-\mathscr{D}^{r}=\mathscr{D}^{<}-\mathscr{D}^{a}. \tag{34}$$

III. PHOTONS INTERACTIONS WITH CELLS

We assume the scattering is done by particles located at points $\mathbf{R}_j$ which are fixed in position. Each scatterer is an object such as a droplet or cell which can absorb and scatter radiation. Let $\hbar\omega_l$ denote the energy of an optical transition which has a matric element $r_{l\mu}=\langle f|r_\mu|i\rangle$ between the initial and final state of that transition. The position and momentum operators for these optical transitions are[22]

$$X_\mu = \sum_l r_{l\mu}(b_l + b_l^\dagger), \tag{35}$$

$$P_\nu = -im\sum_l r_{l\nu}\omega_l(b_l - b_l^\dagger), \tag{36}$$

where b_l and $b_l^\dagger$ are the boson quantum operators of the Frenkel exciton. These position and momentum operators obey the usual commutation relation,

$$[X_\mu, P_\nu] = 2im\sum_l r_{l\mu}r_{l\nu}\omega_l = iN_c\hbar\delta_{\mu\nu}, \tag{37}$$

$$2m\sum_l r_{l\mu}r_{l\nu}\omega_l = \hbar N_c\delta_{\mu\nu}. \tag{38}$$

The last identity is the f-sum rule, where N_c is the number of electrons in the cell.

The dynamic dipole moment of the cell is eX_μ. The polarizability is the correlation of the dynamic moment with itself[22]

$$\alpha_{\mu\nu}(i\omega_n) = -\frac{e^2}{\hbar}\int_0^\beta d\tau\, e^{i\omega_n\tau}\langle T_\tau X_\mu(\tau)X_\nu(0)\rangle \tag{39}$$

$$= \frac{2e^2}{\hbar}\sum_l \frac{r_{l\mu}r_{l\nu}\omega_l}{(i\omega_n)^2 - \omega_l^2} \tag{40}$$

which has the units of volume. Here, we are using the formalism[23] at nonzero temperature, where the frequencies are imaginary $i\omega_n = 2\pi i k_B T n/\hbar$. The symbol T_τ denotes the τ-ordering operator. Our analysis will also require that we evaluate the correlation function of the momentum with itself. A short calculation gives

$$\mathscr{P}_{\mu\nu}(i\omega_n) = -\frac{e^2}{\hbar m^2}\int_0^\beta d\tau\, e^{i\omega_n\tau}\langle P(\tau)P(0)\rangle \tag{41}$$

$$= (i\omega_n)^2\alpha_{\mu\nu}(\omega_n) - \frac{e^2N_c}{m}\delta_{\mu\nu}, \tag{42}$$

where we have used the f-sum rule to derive the last expression.

The interaction between the photons and the electrons in the cell is written as

$$V = -\frac{e}{mc}\sum_j \mathbf{P}_j\cdot\mathbf{A}(\mathbf{R}_j, t) + \frac{e^2}{2mc^2}\sum_j A^2(\mathbf{R}_j, t). \tag{43}$$

The symbol $\mathbf{P}_j$ denotes the momentum operator (36) for the cell j at position $\mathbf{R}_j$. This momentum operator denotes the motion of the electrons within the cell or droplet. Another term, which we do not write, is contributed by the center-of-mass motion of the cell or droplet.

IV. HOMOGENEOUS SYSTEMS IN EQUILIBRIUM

A. Dyson's equation

First we discuss the result for homogeneous systems in equilibrium. Here, the only Green's function we need is found at complex frequencies $i\omega_n$.[8] There is no dependence upon the variables $(\mathbf{R},T)$. Dyson's equation in the Matsubara notation is

$$\mathscr{D}_{\mu\nu}(\mathbf{k},i\omega_n)=\mathscr{D}^{(0)}_{\mu\nu}(\mathbf{k},i\omega_n)+\mathscr{D}^{(0)}_{\mu\phi}(\mathbf{k},i\omega_n)M_{\phi\lambda}(\mathbf{k},i\omega_n)\mathscr{D}_{\lambda\nu}(\mathbf{k},i\omega_n), \tag{44}$$

$$\mathscr{D}^{(0)}_{\mu\nu}(\mathbf{k},i\omega_n)=\frac{4\pi c^2(\delta_{\mu\nu}-\hat{k}_\mu\hat{k}_\nu)}{(i\omega_n)^2-c^2k^2}. \tag{45}$$

The self-energy function of the photon is[22] $M_{\mu\nu}$. It is a matrix because the Green's function is also a matrix. Repeated indices imply summation.

The interaction in Eq. (43) has two types of self-energy terms. The first contains two factors of the $\mathbf{P}\cdot\mathbf{A}$ interaction, and contains the correlation function evaluated in Eq. (42). The second self-energy comes from the A^2 term in the interaction. It produces a term which is equal, and opposite in sign, to the second term in Eq. (42). The sum of the two self-energy terms is just the first term in Eq. (42) divided by c^2. When we solve Dyson's equation for homogeneous systems in equilibrium, we find the Green's function for photons of

$$\mathscr{D}_{\mu\nu}(\mathbf{k},i\omega_n)=\frac{4\pi c^2(\delta_{\mu\nu}-\hat{k}_\mu\hat{k}_\nu)}{(i\omega_n)^2\epsilon(\mathbf{k},i\omega_n)-c^2k^2}, \tag{46}$$

$$\epsilon(\mathbf{k},i\omega_n)=1+4\pi n_s\alpha(\mathbf{k},i\omega_n), \tag{47}$$

where n_s is the density of scattering centers. Here, we have derived the well-known result that the interactions produce a dielectric function $\epsilon(\mathbf{k},i\omega_n)$ which then modifies the dispersion of the photons.

B. Local field corrections

The above derivation does not include the Lorenz–Lorentz local field corrections to the dielectric function. This contribution can be included by a more careful derivation, as done in Ref. 22. One must add another interaction term which includes the dipole–dipole interaction between the fluctuations eX_j at different sites

$$V_d=e^2\sum_{ij}X_{i\mu}\phi_{\mu\nu}(\mathbf{R}_{ij})X_{j\nu}, \tag{48}$$

$$\phi_{\mu\nu}(\mathbf{R})=\frac{\delta_{\mu\nu}}{R^3}-\frac{3R_\mu R_\nu}{R^5}. \tag{49}$$

A wave vector dependent polarizability for the scattering media can be defined as

$$\alpha_{\mu\nu}(\mathbf{k},i\omega_n)=-e^2\sum_{j\neq i}e^{i\mathbf{k}\cdot\mathbf{R}_{ji}}\int_0^\beta d\tau\, e^{i\omega_n\tau}\langle T_\tau X_j(\tau)X(\tau)\rangle. \tag{50}$$

Here, one starts at one scattering site i and sums over all other scattering sites $j\neq i$. The technique for evaluating this sum, with random scattering centers, is explained in the next section. Now we show that one can derive a Dyson's equation for the polarizability using the dipole–dipole interaction plus the $p\cdot A$ interaction

$$\alpha_{\mu\nu}(\mathbf{k},i\omega_n)=\alpha_{\mu\nu}(i\omega_n)+\alpha_{\mu\phi}(i\omega_n)[t_{\phi\lambda}(\mathbf{k})+d_{\phi\lambda}(\mathbf{k},i\omega_n)]\alpha_{\lambda\nu}(\mathbf{k},i\omega_n), \tag{51}$$

$$t_{\mu\nu}(\mathbf{k})=\sum_{j\neq i} e^{i\mathbf{k}\cdot\mathbf{R}_{ji}}\phi_{\mu\nu}(\mathbf{R}_{ji}), \tag{52}$$

$$d_{\mu\nu}(\mathbf{k},i\omega_n)=\frac{\omega_n^2}{c^2}\sum_{j\neq i} e^{i\mathbf{k}\cdot\mathbf{R}_{ji}}\mathscr{D}_{\mu\nu}(\mathbf{R}_{ji},i\omega_n). \tag{53}$$

The symbol $\alpha_{\mu\nu}(i\omega_n)$ denotes the polarizability of a single scattering center, while $\alpha_{\mu\nu}(\mathbf{k},i\psi_n)$ denotes the polarizability in the actual media, including local field corrections. The Lorentz–Lorenz form of the dielectric function is obtained using the expressions

$$t_{\mu\nu}(\mathbf{k})=4\pi n_s[\hat{k}_\mu\hat{k}_\nu-\tfrac{1}{3}\delta_{\mu\nu}], \tag{54}$$

$$d_{\mu\nu}(\mathbf{k},i\omega_n)\ll 1. \tag{55}$$

Here, n_s is the density of scattering sites. This result is derived in the next section.

The photon polarization is perpendicular to the photon wave vector $\mathbf{k}$. This is ensured by the factor $(\delta_{\mu\nu}-\hat{k}_\mu\hat{k}_\nu)$. From now on we assume that all Green's functions have this factor and write

$$\mathscr{D}_{\mu\nu}(\mathbf{k},i\omega_n)=(\delta_{\mu\nu}-\hat{k}_\mu\hat{k}_\nu)\mathscr{D}(\mathbf{k},i\omega_n). \tag{56}$$

All Green's functions have a scalar factor $\mathscr{D}$ times this polarization factor. We also do this with our nonequilibrium Green's functions. Similarly, in Dyson's equation, the self-energy $M_{\mu\nu}$ becomes a scalar since its tensor components are averaged over the photon polarization. We also assume that the polarizability $\alpha_{\mu\nu}=\delta_{\mu\nu}\alpha$ is isotropic.

C. Averaging over scattering centers

Here, we wish to reexamine the above self-energy terms, and to consider carefully the method of averaging over the positions of the scattering sites $\mathbf{R}_j$. We discuss the averaging for the A^2 term in the interaction, since this self-energy is easier. However, exactly the same analysis applies to the $p\cdot A$ term. In evaluating the perturbation expansion for the S matrix, the first term which gives a self-energy has the factor

$$\frac{e^2N_c}{2mc^2}\sum_j\int d^3r_1\, e^{-i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}_2)}\int_0^\beta d\tau_1\int_0^\beta d\tau\, e^{i\omega_n\tau}\langle T_\tau A_\mu(\mathbf{r}_1,\tau)A^2(\mathbf{R}_j,\tau_1)A_\nu(\mathbf{r}_2,0)\rangle$$

$$=\frac{e^2N_c}{mc^2}\sum_j\int d^3r_1\, e^{-i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}_2)}\int_0^\beta d\tau_1\int_0^\beta d\tau\, e^{i\omega_n\tau}\mathscr{D}_{\mu\phi}(\mathbf{r}_1-\mathbf{R}_j,\tau-\tau_1)\mathscr{D}_{\phi,\nu}(\mathbf{R}_j-\mathbf{r}_2,\tau_1)$$

$$=\frac{e^2N_c}{mc^2}\mathscr{D}_{\mu\phi}(\mathbf{k},i\omega_n)\,\frac{1}{\Omega}\sum_{j\mathbf{q}} D_{\phi\nu}(\mathbf{q},i\omega_n)e^{i(\mathbf{k}-\mathbf{q})\cdot(\mathbf{R}_j-\mathbf{r}_2)},$$

where Ω is the volume. In the double sum over $(j,\mathbf{q})$, the nonzero term is where $\mathbf{q}=\mathbf{k}$ and then the sum over j gives N_s $(n_s=N_s/\Omega)$. Thus this term is

$$\frac{e^2N_cn_s}{mc^2}\mathscr{D}_{\mu\phi}(\mathbf{k},i\omega_n)\mathscr{D}_{\phi\nu}(\mathbf{k},i\omega_n). \tag{57}$$

This term leads to a self-energy of

$$\frac{e^2 N_c n_s}{m}\,\delta_{\mu\nu}. \tag{58}$$

This is the term in the first order of perturbation theory. It cancels the second term in Eq. (42).

Let us now examine the same interaction in the second order of perturbation theory. The correlation function is

$$\langle T_\tau A_\mu(\mathbf{r}_1,\tau)A^2(\mathbf{R}_i,\tau_1)A^2(\mathbf{R}_j,\tau_2)A_\nu(\mathbf{r}_2,0)\rangle \tag{59}$$

$$=4\mathscr{D}_{\mu\phi}(\mathbf{r}_1-\mathbf{R}_i,\tau-\tau_1)\mathscr{D}_{\phi\lambda}(\mathbf{R}_i-\mathbf{R}_j,\tau_1-\tau_2)\mathscr{D}_{\lambda\nu}(\mathbf{R}_j-\mathbf{r}_2,\tau_2). \tag{60}$$

There is now a double sum over the positions (i,j) of the scattering centers. We chose to omit the term where the photons successively interact with the same scattering center. This term does not contribute to scattering, and merely renormalizes the charge on the electron. So in the above expression we specify that $i\neq j$.

When we express the photon Green's functions of position as functions of wave vector, we find the factor

$$\sum_{i\neq j} e^{i(\mathbf{q}-\mathbf{k})\cdot(\mathbf{R}_i-\mathbf{R}_j)}=N_s^2\delta_{\mathbf{q}=\mathbf{k}}+N_s[S(\mathbf{q}-\mathbf{k})-1]. \tag{61}$$

The first term on the right $N_s^2\delta_{\mathbf{q}=\mathbf{k}}$ gives the square of the self-energy found in first-order. The second term gives a new contribution to the self-energy. The factor of $S(\mathbf{q}-\mathbf{k})$ is the *static structure factor*.[24] It is the term which depends on the arrangement and density of the scattering centers. The $p\cdot A$ term has a similar expression, and the again there is cancellation.

We must now determine the form for $S(q)$. There are three constraints:

(1) It vanishes at $q\to 0$.
(2) It goes to one at $qa\gg 1$ where a is a length typical of the separation between scattering centers.
(3) It obeys an important sum rule

$$\int \frac{d^3q}{(2\pi)^3}[1-S(q)]=n_s, \tag{62}$$

where n_s is the density of scattering centers.

A formula which obeys the second and third constraints is

$$1-S(q)=\frac{8\pi a^3 n_s}{[1+(qa)^2]^2}. \tag{63}$$

One can make it obey the first constraint by choosing $8\pi n_s a^3=1$ which serves to define a precisely. We do not assert that the random distribution of scattering centers always has this form for $S(q)$. Instead, we note that this choice is the simplest one which obeys all of the constraints. We shall use it in the evaluation of integrals. If the wave vector of light is k, our results for $(ka)\gg 1$ and also $(ka)\ll 1$ are independent of the choice of $S(q)$. However, having a specific form for $S(q)$ allows a reasonable interpolation between these limits.

We now can evaluate the sums over the scattering centers in Eqs. (52) and (53). First evaluate Eq. (52) which can be written

$$t_{\mu\nu}(\mathbf{k})=n_s\int d^3r\; g(\mathbf{r})\,\phi_{\mu\nu}(\mathbf{r}), \tag{64}$$

where $g(\mathbf{r})$ is the pair distribution function. We rewrite $g=(g-1)+1$. The ''1'' term is just the Fourier transform of $\phi_{\mu\nu}$ which is called $T_{\mu\nu}(\mathbf{k})$. The fourier transform of $n_s(g-1)$ is $(S-1)$ so that we derive the expression

$$T_{\mu\nu}(\mathbf{k})=4\pi\hat{k}_\mu\hat{k}_\nu, \tag{65}$$

$$t_{\mu\nu}(\mathbf{k})=n_sT_{\mu\nu}(\mathbf{k})-\int\frac{d^3q}{(2\pi)^3}[1-S(\mathbf{k}-\mathbf{q})]T_{\mu\nu}(\mathbf{q}) \tag{66}$$

$$=4\pi n_s\{\hat{k}_\mu\hat{k}_\nu-\tfrac{1}{2}[(1-\xi)\delta_{\mu\nu}-(1-3\xi)\hat{k}_\mu\hat{k}_\nu]\}, \tag{67}$$

$$\xi=\left[1+\frac{1}{\lambda^2}\right]\left[1-\frac{1}{\lambda}\tan^{-1}(\lambda)\right], \tag{68}$$

$$\lambda=ka. \tag{69}$$

A similar analysis for the summation over the photon Green's functions yields the expression

$$d_{\mu\nu}=q_n^2\left\{n_s\mathscr{D}_{\mu\nu}(\mathbf{k},i\omega_n)-\int\frac{d^3q}{(2\pi)^3}[1-S(\mathbf{q}-\mathbf{k})]\mathscr{D}_{\mu\nu}(\mathbf{q},i\omega_n)\right\}. \tag{70}$$

However, we drop the first term. We have already counted it in the self-energy of the photon, and including it here is double counting. The second term is new, and is the contribution we want

$$d_{\mu\nu}=-q_n^2\int\frac{d^3q}{(2\pi)^3}[1-S(\mathbf{q}-\mathbf{k})]\mathscr{D}_{\mu\nu}(\mathbf{q},i\omega_n) \tag{71}$$

$$=4\pi n_sz^2\left\{\frac{(\delta_{\mu\nu}-\hat{k}_\mu\hat{k}_\nu)}{\lambda^2+(1+z)^2}+\frac{\zeta}{2}(\delta_{\mu\nu}-3\hat{k}_\mu\hat{k}_\nu)\right\}, \tag{72}$$

$$\zeta=\frac{1}{\lambda^2z}-\frac{1}{\lambda^3z^2}\left[(1+\lambda^2)\tan^{-1}(\lambda)-(1+\lambda^2-z^2)\tan^{-1}\left(\frac{\lambda}{1+z}\right)\right], \tag{73}$$

$$z=aq_n=\frac{\omega_na}{c}. \tag{74}$$

These complicated expressions become simple in the two important limits.

1. $(ka)^2\ll 1$

Here, the scattering centers are close together on the scale of the wave length of light. Then one finds that $\xi=1/3+O(\lambda^2)$ and $\zeta=-2/[3(1+z)^2]$ which gives

$$t_{\mu\nu}(\mathbf{k})=-\frac{4\pi n_s}{3}[\delta_{\mu\nu}-3\hat{k}_\mu\hat{k}_\nu], \tag{75}$$

$$d_{\mu\nu}(\mathbf{k},i\omega_n)=\frac{8\pi n_s}{3}\delta_{\mu\nu}\frac{z^2}{(1+z)^2}. \tag{76}$$

Eventually we will analytically extend the imaginary frequency to the complex space $i\omega_n\to\omega$ and then $z^2\to-\lambda^2$. In this limit the term $d_{\mu\nu}$ is negligible while the term $t_{\mu\nu}$ gives a dielectric function

of the Lorentz–Lorenz form, with the local field correction. It is suitable for light propagating through fluids such as water, where the scattering centers are close together. The wavelets from the scattering add together to form a new wave, in agreement with Huygens principle.

2. $(ka)^2 \gg 1$

Here, the scattering centers are far apart on the scale of the wave length of light. In this limit we find that $\zeta \to O(1/\lambda^2 z)$ and

$$\xi \to 1 - \frac{\pi}{2\lambda} + O(1/\lambda^2), \tag{77}$$

$$t_{\mu\nu}(\mathbf{k}) = -\frac{\pi^2 n_s}{\lambda}[\delta_{\mu\nu} - 3\hat{k}_\mu \hat{k}_\nu]. \tag{78}$$

The factor $t_{\mu\nu}$ is now of order $O(1/\lambda)$ so the local field correction is small. There are not enough scattering centers, in the vicinity of each other, to provide such a correction. Similarly, the factor of $d_{\mu\nu}$ is also of $O(n_s/\lambda)$ or else $O(n_s/z)$ and is also negligible.

The case of photon diffusion has $\lambda, z \gg 1$. Here, there is no local field correction. So we generally neglect this contribution to the polarizability.

We end this section by giving the final expression for the dielectric function of the media in equilibrium

$$\epsilon(\mathbf{k}, i\omega_n) = 1 + 4\pi n_s \alpha_L(\mathbf{k}, i\omega_n)\left\{1 + 4\pi (i\omega_n)^2 \alpha_L(\mathbf{k}, i\omega_n) \int \frac{d^3q}{(2\pi)^3} \frac{\zeta(\hat{q}\cdot\hat{k})}{\omega_n^2 + c^2 q^2}[1 - S(\mathbf{q}-\mathbf{k})]\right\}, \tag{79}$$

$$\alpha_L(\mathbf{k}, i\omega_n) = \frac{\alpha(i\omega_n)}{1 + 4\pi n_s \alpha(i\omega_n) t_{\mu\mu}(\mathbf{k})}, \tag{80}$$

$$\zeta(\hat{q}\cdot\hat{k}) = \tfrac{1}{2}[1 + (\hat{q}\cdot\hat{k})^2]. \tag{81}$$

The polarization factor $\zeta(\hat{q}\cdot\hat{k})$ needs to be explained. We assume that the polarizabilities $\alpha_{\mu\nu}$ are isotropic. Then in Dyson's equation we have the combination of polarization factors

$$\rho_{\mu\nu} = (\delta_{\mu\phi} - \hat{k}_\mu \hat{k}_\phi)(\delta_{\phi\lambda} - \hat{q}_\phi \hat{q}_\lambda)(\delta_{\lambda\nu} - \hat{k}_\lambda \hat{k}_\nu) \tag{82}$$

$$= \delta_{\mu\nu} - \hat{k}_\mu \hat{k}_\nu - \hat{q}_\mu \hat{q}_\nu + (\hat{q}_\mu \hat{k}_\nu + \hat{k}_\mu \hat{q}_\nu)(\hat{q}\cdot\hat{k}) - \hat{k}_\mu \hat{k}_\nu (\hat{q}\cdot\hat{k})^2. \tag{83}$$

After doing the integrals over the variable d^3q we are left with a contribution to the Green's function which must have a net dependence of $(\delta_{\mu\nu} - \hat{k}_\mu \hat{k}_\nu)$. This latter expression can be averaged by taking the sum with $\mu = \nu$ which is two. Applying the same sum to $\rho_{\mu\nu}$ gives $1 + (\hat{q}\cdot\hat{k})^2$ and dividing by two gives ζ.

In the expression for the dielectric function, we treat differently the two factors of $t_{\mu\nu}$ and $d_{\mu\nu}$. The former contributes to the local field correction for the polarizability. The latter does not. Instead, it is just a correction to the dielectric constant. This difference occurs because $d_{\mu\nu}$ is a self-energy correction to the photon Green's function. Higher-order terms in the perturbation series are examined in Ref. 25.

V. NONEQUILIBRIUM

A. QBE

Now we consider how these interactions contribute to the QBE for photons. We assume here that the scattering centers are fixed in space.

We begin by writing Dyson's equation in real space, and introduce a four vector notation $x=(\mathbf{r},t)$. Then operating upon this equation with the left-hand side of Eq. (27)

$$\begin{aligned}\widetilde{\mathscr{D}}_{\mu\nu}(x_1;x_2)&=\widetilde{\mathscr{D}}^{(0)}_{\mu\nu}(x_1;x_2)+\int dx_3\ dx_4\ \widetilde{\mathscr{D}}^{(0)}_{\mu\phi}(x_1;x_3)\widetilde{M}_{\phi\lambda}(x_3;x_4)\widetilde{\mathscr{D}}_{\lambda\nu}(x_4;x_2)\\&\quad\times\left[\frac{\partial^2}{\partial t_1^2}-c^2\nabla_1^2\right]\widetilde{\mathscr{D}}_{\mu\nu}(x_1;x_2)\\&=4\pi c^2\delta_{\mu\nu}\delta(x_1-x_2)\widetilde{I}+4\pi c^2\\&\quad\times\int dx_3\ \widetilde{M}_{\mu\lambda}(x_1;x_3)\widetilde{\mathscr{D}}_{\lambda\nu}(x_3;x_2)\left[\frac{\partial^2}{\partial t_2^2}-c^2\nabla_2^2\right]\widetilde{\mathscr{D}}_{\mu\nu}(x_1;x_2)\\&=4\pi c^2\delta_{\mu\nu}\delta(x_1-x_2)\widetilde{I}+4\pi c^2\int dx_3\ \widetilde{\mathscr{D}}_{\mu\phi}(x_1;x_3)\widetilde{M}_{\phi\nu}(x_3;x_2).\end{aligned}$$

We have given the equations obtained when one takes derivatives either with respect to the x_1 or to the x_2 variable. The QBE is obtained by subtracting these last two equations, and then changing to center-of-mass variables

$$\begin{aligned}2i\left(\omega\frac{\partial}{\partial T}+c^2\mathbf{q}\cdot\boldsymbol{\nabla}\right)\widetilde{\mathscr{D}}(\mathbf{q},\omega;\mathbf{R},T)&=4\pi c^2[\widetilde{M}(\mathbf{q},\omega;\mathbf{R},T)\widetilde{\mathscr{D}}(\mathbf{q},\omega;\mathbf{R},T)\\&\quad-\widetilde{\mathscr{D}}(\mathbf{q},\omega;\mathbf{R},T)\widetilde{M}(\mathbf{q},\omega;\mathbf{R},T)].\end{aligned}\tag{84}$$

The matrix $\widetilde{M}$ has the same arrangement of elements as Eq. (25). We have neglected terms which contain derivatives with respect to the variables $\mathbf{R}$ and T. The left-hand side of this equation has the same terms we have for the noninteracting QBE. The terms on the right involving the self-energy operator $\widetilde{M}$ are the contributions of the interactions. This factor is nonzero since the two matrices do not commute. The various terms which contribute to the self-energy in equilibrium also contribute to the scattering and interactions in nonequilibrium. We now examine these various terms to see how they enter into the QBE for photons.

An important question is whether the scattering center remains in thermal equilibrium. When the photons diffuse they are not in thermal equilibrium. Whether the scattering centers remain in equilibrium depends upon their connection to the heat bath. If the scattering centers are the cells of the body, they are probably well connected to a heat bath. We will assume this to be the case. The cells absorb radiation, and convert it to heat. A counter example is when the scattering is done by individual atoms in a gas. The atoms have no place to dissipate their energy except by reradiating the absorbed photons. Then the atoms are out of equilibrium along with the photons.

B. First-order scattering

There are two scattering terms. As for the case of equilibrium, the lowest order term is from $\mathscr{P}(\omega)$ which gives $\widetilde{M}=n_s(\omega/c)^2\widetilde{\alpha}(\omega)$. The commutator of the two matrices is

$$\widetilde{\alpha}\widetilde{\mathscr{D}}-\widetilde{\mathscr{D}}\widetilde{\alpha}=[\alpha^{>}\mathscr{D}^{<}-\alpha^{<}\mathscr{D}^{>}]\begin{pmatrix}1&-1\\1&-1\end{pmatrix}.\tag{85}$$

In equilibrium we have that

$$\alpha^{<} = -in(\omega)A(\omega), \tag{86}$$

$$\alpha^{>} = -i[n(\omega)+1]A(\omega), \tag{87}$$

$$A(\omega) = 2\pi \frac{e^2}{\hbar} \sum_l r_{l\mu}^2 [\delta(\omega-\omega_l) - \delta(\omega+\omega_l)]. \tag{88}$$

We assume that the photons are only slightly out of equilibrium. The photon Green's functions $\mathscr{D}^{<}$ and $\mathscr{D}^{>}$ both equal their equilibrium part plus a nonequilibrium term $\delta\mathscr{D}$. The QBE for the nonequilibrium part is, including only the absorption term in the scattering part,

$$\left[\omega \frac{\partial}{\partial T} + c^2 \mathbf{q}\cdot\boldsymbol{\nabla}_R + 2\pi n_s \omega^2 A(\omega)\right]\delta\mathscr{D} = 0. \tag{89}$$

The last term in brackets is due to photon absorption at the cells, where n_s is the volume density of such scatterers, and $A(\omega)$ is the spectral function of the polarizability.

C. Second-order scattering

There is a self-energy term in the equilibrium case (60) which is due to a double scattering event. Here, we consider how the same term enters into the scattering term for the QBE. For this case we can write the matrix $\widetilde{M}$ as

$$\widetilde{M} = n_s \left(\frac{\omega}{c}\right)^4 \widetilde{\alpha}\widetilde{D}'\widetilde{\alpha}, \tag{90}$$

$$\widetilde{D}' = \frac{1}{2\Omega} \sum_{\mathbf{q}'} [1+(\hat{q}\cdot\hat{q}')^2][S(\mathbf{q}-\mathbf{q}')-1]\widetilde{\mathscr{D}}(\mathbf{q}',\omega;\mathbf{R},T). \tag{91}$$

In order to evaluate the scattering term we need the combination of matrix multiplications

$$\widetilde{N} = \widetilde{\alpha}\widetilde{D}'\widetilde{\alpha}\widetilde{\mathscr{D}} - \widetilde{\mathscr{D}}\widetilde{\alpha}\widetilde{D}'\widetilde{\alpha}. \tag{92}$$

This expression is complicated. For the QBE we only need the component N_{12} of the 2×2 matrix which gives the contribution to $\mathscr{D}^{<}$. After much algebra we find

$$N_{12} = -D^{<}[D_r'\alpha_r^2 - D_a'\alpha_a^2] + (D^{>}-D^{<})[\alpha^{<}(\alpha_r D_r' + \alpha_a D_a') + \alpha_r\alpha_a D^{<\prime}]. \tag{93}$$

Usually we assume that the system is only slightly out of equilibrium. Then we set the photon Green's functions to an equilibrium part plus a nonequilibrium part $D \to D + \delta D$, etc. The term containing only equilibrium factors vanishes. We linearize the equations and retain only the terms proportional to one power of the nonlinear component.

$$\delta N_{12} = \delta D'\alpha_r\alpha_a[D^{>}-D^{<}] - \delta\mathscr{D}[D_r'\alpha_r^2 - D_a'\alpha_a^2]. \tag{94}$$

Factors such as $D^{>}, D^{<}, D_r', D_a'$ are evaluated using their equilibrium values. The first term on the right is due to the nonequilibrium $\delta D'$. It is due to the photons scattering back into the distribution. The term proportional to $\delta\mathscr{D}$ is scattering out of the distribution of photons. The rates of these two process are not equal. However, we can rearrange this expression to give

$$\delta N_{12} = i\alpha_r\alpha_a[B\,\delta D' - B'\,\delta\mathscr{D}] + 2iA\,\delta\mathscr{D}\Re\{\alpha_r\mathscr{D}_r\}. \tag{95}$$

The last term on the right is a contribution to the absorption coefficient. The first two terms give the scattering in and out of the photons from the distribution. These terms are now symmetrical.

When photons diffuse they scatter without changing frequencies. In the expression for $[1-S(\mathbf{q}-\mathbf{k})]$ the two wave vectors will have the same magnitude: $|\mathbf{q}|=|\mathbf{k}|$. This factor depends mainly on the scattering angle θ between these two vectors. Define $\mu=\cos(\theta)$ so that $\mathbf{q}\cdot\mathbf{k}=k^2\mu$ then our expression for the structure factor becomes

$$[1-S(\mathbf{q}-\mathbf{k})]=\frac{1}{[1+2(ka)^2(1-\mu)]^2}. \tag{96}$$

In the diffusion regime, where $ka\gg 1$, then this function is highly peaked for forward scattering ($\mu\sim 1$). Thus we have shown that photon scattering is peaked in the forward direction. This is well known to workers in the field. However, they have attributed the forward scattering to the properties of a single cell, which is approximated as a water droplet. Here, we note that another contribution to the forward scattering is the distribution of cells.

D. *J* algebra

So far we have treated the self-energies in the first two orders of perturbation. We wish to sum subsets of diagrams to all orders of perturbation. We have found a simple method of doing this using an algebra based on a matrix we call $\tilde{J}$

$$\tilde{J}=\begin{pmatrix}1 & -1\\ 1 & -1\end{pmatrix}. \tag{97}$$

Now it is possible to prove some theorems

$$(1)\,\tilde{J}\tilde{J}=0, \tag{98}$$

$$(2)\,\tilde{\alpha}\tilde{J}=\alpha_r\tilde{J}, \tag{99}$$

$$(3)\,\tilde{J}\tilde{\alpha}=\alpha_a\tilde{J}, \tag{100}$$

where products of matrices imply matrix multiplication.

The first theorem is obvious by inspection. The second and third are proved similarly, and it is sufficient to prove one, say the second. From the definition of the matrices we get

$$\tilde{\alpha}\tilde{J}=\begin{pmatrix}\alpha^t & -\alpha^<\\ \alpha^> & -\overline{\alpha^t}\end{pmatrix}\begin{pmatrix}1 & -1\\ 1 & -1\end{pmatrix} \tag{101}$$

$$=\begin{pmatrix}\alpha^t-\alpha^< & -\alpha^t+\alpha^<\\ \alpha^>-\overline{\alpha^t} & -\alpha^>+\overline{\alpha^t}\end{pmatrix} \tag{102}$$

$$=\alpha^r\begin{pmatrix}1 & -1\\ 1 & -1\end{pmatrix}, \tag{103}$$

where we have used the identities that $\alpha^r=\alpha^t-\alpha^<=\alpha^>-\overline{\alpha^t}$.

These results allow us to evaluate in a simple way any product of matrices containing one $\tilde{J}$ matrix. An example is

$$\tilde{\alpha}\tilde{D}\tilde{J}\tilde{\alpha}=\alpha_r\alpha_a D_r\tilde{J}. \tag{104}$$

Any matrix to the left of $\tilde{J}$ gets replaced by its retarded function, and any matrix to the right of $\tilde{J}$ gets replaced by its advanced function. Any string with two of them is zero.

This simple algebra allows us to evaluate in a simple way the perturbation series for the photon self-energies. The photon Green's function matrix is evaluated as an equilibrium term plus a nonequilibrium term δD which is the same for every element of the matrix

$$\mathscr{D} \to \mathscr{D} + \delta D \tilde{J}. \tag{105}$$

The nonequilibrium term is proportional to the $\tilde{J}$ matrix. As an example, consider the second-order self-energy evaluated in the prior section

$$\tilde{N} = \tilde{\alpha}\tilde{D}'\tilde{\alpha}\tilde{D} - \tilde{D}\tilde{\alpha}\tilde{D}'\tilde{\alpha}. \tag{106}$$

We find the term proportional to one power of the nonequilibrium part

$$\delta\tilde{N} = \delta D[\tilde{\alpha}\tilde{D}'\tilde{\alpha}\tilde{J} - \tilde{J}\tilde{\alpha}\tilde{D}'\tilde{\alpha}] + \delta D'[\tilde{\alpha}\tilde{J}\tilde{\alpha}\tilde{D} - \tilde{D}\tilde{\alpha}\tilde{J}\tilde{\alpha}] \tag{107}$$

$$= \delta D[\alpha_r^2 D_r' - \alpha_a^2 D_a'] + \alpha_r \alpha_a \delta D'[D_a - D_r]. \tag{108}$$

This gives the prior result, and by a derivation which takes only a few lines. Similarly, in the next higher order of perturbation theory we find

$$\tilde{N} = \tilde{\alpha}\tilde{D}'\tilde{\alpha}\tilde{D}'\tilde{\alpha}\tilde{D} - \tilde{D}\tilde{\alpha}\tilde{D}'\tilde{\alpha}\tilde{D}'\tilde{\alpha}, \tag{109}$$

$$\delta\tilde{N} = \delta D\tilde{J}[\alpha_r^3 D_r'^2 - \alpha_a^3 D_a'^2] + \delta D'\tilde{J}\alpha_r\alpha_a[\alpha_r D_r' + \alpha_a D_a'][D_a - D_r]. \tag{110}$$

Continuing in his way we can easily derive the expressions for terms in the higher order of perturbation theory. Then it is possible to sum the series and we finally obtain the total result

$$\begin{aligned}
\delta\tilde{N} &= \delta D\tilde{J}\left[\frac{\alpha_r}{1-\alpha_r D_r'} - \frac{\alpha_a}{1-\alpha_a D_a'}\right] \\
&= \frac{\alpha_r\alpha_a\delta D'}{(1-\alpha_r D_r')(1-\alpha_a D_a')}\,\tilde{J}[D_r - D_a] \\
&= \frac{\alpha_r\alpha_a}{(1-\alpha_r D_r')(1-\alpha_a D_a')}\,\tilde{J}[\delta D(D_r' - D_a') - \delta D'(D_r - D_a)] + \frac{(\alpha_r - \alpha_a)\delta D}{(1-\alpha_r D_r')(1-\alpha_a D_a')}\,\tilde{J}.
\end{aligned} \tag{111}$$

We have presented two equivalent expressions. In the second expression, we have grouped them such that the first two terms describe scattering, while the last term describes absorption.

The effect of the higher-order terms is to provide terms in the denominator such as $(1 - \alpha_r D_r')$ and $(1 - \alpha_a D_a')$. These provide local field corrections to the polarizabilities of the scattering centers. As remarked earlier, for the case of photon diffusion these terms are negligible. We omit them since we are primarily interested in this case. Then the absorption term is given by the expression derived from the first-order scattering. The QBE we have derived so far, including second order terms, is

$$\begin{aligned}
&\left[\omega\,\frac{\partial}{\partial T} + c^2\mathbf{q}\cdot\boldsymbol{\nabla} + 2\pi c^2(\Gamma_a(\omega) + \Gamma_s(\mathbf{q},\omega)]\,\delta D(\mathbf{q},\omega;\mathbf{R},T)\right. \\
&\quad = 2\pi c^2 n_s B(\mathbf{q},\omega;\mathbf{R},T)\int \frac{d^3k}{(2\pi)^3}\,\delta D(\mathbf{k},\omega;\mathbf{R},T)\,\frac{d\sigma(\hat{q}\cdot\hat{k})}{d\Omega}\,[1 - S(\mathbf{q}-\mathbf{k})],
\end{aligned} \tag{112}$$

$$\Gamma_a(\omega) = n_s \left(\frac{\omega}{c}\right)^2 A(\omega), \tag{113}$$

$$\Gamma_s(\mathbf{q},\omega;\mathbf{R},T) = n_s \int \frac{d^3k}{(2\pi)^3} B(\mathbf{k},\omega;\mathbf{R},T) \frac{d\sigma(\hat{q}\cdot\hat{k})}{d\Omega} [1 - S(\mathbf{q}-\mathbf{k})], \tag{114}$$

$$\frac{d\sigma(\hat{q}\cdot\hat{k})}{d\Omega} = \left(\frac{\omega}{c}\right)^4 \alpha(\omega)^2 \frac{1}{2}[1 + (\hat{q}\cdot\hat{k})^2]. \tag{115}$$

This QBE is the main result of this calculation. In the next section we discuss various moments of this equation.

We have written the scattering in terms of the differential cross section for the photon scattering. We also give the cross section for Rayleigh scattering. Another important scattering source is Mie scattering from a dielectric sphere. Mie scattering is the correct theory if the scattering centers are spheres. Examples are water droplets in clouds or else latex balls suspended in water. The theory of Mie scattering is given in standard textbooks.[26] A very interesting test of the theory is given by Zaccanti and Bruscaglioni.[27] They show that the Mie scattering is highly peaked in the forward direction when $a \gg \lambda$, where a is the radius of the spheres.

VI. MOMENTS

One of our goals is to derive Eq. (1). Since it does not depend upon the frequency variable ω then this equation is obtained from our QBE by an integration over frequency.

''Moment equations'' are the name applied to macroscopic equations obtained by integrating the QBE over frequency, over wave vector, or both. Functions of frequency and wave vector are inserted into these integrals to give various macroscopic equations. We know in advance that we should obtain equations which depend upon macroscopic quantities such as

(1) The number density of photons $f(\mathbf{q},\mathbf{r},t)$.

(2) The photon energy density which depends upon electric **E** and magnetic **B** fields

$$\mathscr{E}(\mathbf{R},T) = \frac{1}{8\pi}[E^2(\mathbf{R},T) + B^2(\mathbf{R},T)]. \tag{116}$$

(3) The Poynting vector for energy flux

$$\mathbf{S}(\mathbf{R},T) = \frac{c}{4\pi} \mathbf{E}\times\mathbf{B}. \tag{117}$$

Since the last two quantities do not depend upon **q** or ω they are moments obtained by integrating over both $d\omega$ and d^3q.

A. Equilibrium moments

A useful introduction to this topic is obtained by taking moments of the equilibrium functions. They provide a guide to possible macroscopic variables. The basic definitions are in Eqs. (29) and (31). The polarization tensor $(\delta_{\mu\nu} - \hat{q}_\mu \hat{q}_\nu)$ is evaluated by taking its trace which is 2

$$i\sum_\mu \mathscr{D}^<_{\mu\nu}(\mathbf{q},\omega) = 2B(q,\omega)n(\omega), \tag{118}$$

$$B(q,\omega) = \frac{(2\pi c)^2\hbar}{\omega_q}[\delta(\omega-\omega_q) - \delta(\omega+\omega_q)], \tag{119}$$

$$\Lambda_n(q)=\int \frac{d\omega}{2\pi}\,\omega^n B(q,\omega)n(\omega), \tag{120}$$

$$\Lambda_0=\frac{(2\pi c)^2\hbar}{\omega_q}\,[2n(\omega_q)+1], \tag{121}$$

$$\Lambda_1=-(2\pi c)^2\hbar, \tag{122}$$

$$\Lambda_2=(2\pi c)^2\hbar\,\omega_q[2n(\omega_q)+1]. \tag{123}$$

The moment Λ_0 appears to be the particle density, while Λ_2 is the energy density. The moment Λ_1 is just a constant. The even moments are proportional to the photon occupation number $n(\omega_q)$. They are candidates for being a distribution function. The odd moments are not proportional to the photon density.

B. Nonequilibrium moments

Here, we evaluate the same moments using the nonequilibrium distributions. We define them as

$$\Xi_n(\mathbf{q},\mathbf{R},T)=i\int \frac{d\omega}{2\pi}\,\omega^n\sum_\mu \mathscr{D}^<_{\mu\mu}(\mathbf{q},\omega;\mathbf{R},T)$$
$$=i^n\int dt\,\delta(t)\int d^3r\; e^{-i\mathbf{q}\cdot\mathbf{r}}\frac{\partial^n}{\partial t^n}\sum_\mu\left\langle A_\mu\left(\mathbf{R}+\frac{\mathbf{r}}{2};T+\frac{t}{2}\right)A_\mu\left(\mathbf{R}-\frac{\mathbf{r}}{2};T-\frac{t}{2}\right)\right\rangle. \tag{124}$$

We have used the definition of the correlation functions as a Wigner distribution function. From now on, in this section, the summation over μ is intended, but is not written explicitly. The first moments are as follows.

1. $n=0$. Here, there are no time derivatives. This suggests the following definition for the photon density:

$$f(\mathbf{q},\mathbf{R},T)=\frac{\omega_q}{(2\pi c)^2\hbar}\int d^3r\; e^{-i\mathbf{q}\cdot\mathbf{r}}\left\langle A_\mu\left(\mathbf{R}+\frac{\mathbf{r}}{2};T\right)A_\mu\left(\mathbf{R}-\frac{\mathbf{r}}{2};T\right)\right\rangle. \tag{125}$$

2. $n=1$. Here, there is a single time derivative. We use the notation $A(\pm)$ to denote $A_\mu(\mathbf{R}\pm\frac{\mathbf{r}}{2},T)$. In the following equations, we use the fact that the time derivative of the vector potential is proportional to the electric field

$$\Xi_1=\frac{i}{2}\int d^3r\; e^{-i\mathbf{q}\cdot\mathbf{r}}\langle\dot{A}(+)A(-)-A(+)\dot{A}(-)\rangle \tag{126}$$

$$=-\frac{ic}{2}\int d^3r\; e^{-i\mathbf{q}\cdot\mathbf{r}}\langle E(+)A(-)-A(+)E(-)\rangle. \tag{127}$$

The quantity in brackets would be the commutator of the electric field with the vector potential, except that the space arguments in the last term are interchanged. So this moment has a complex behavior. It is not a simple constant, as it was for the equilibrium case.

3. $n=2$. There are two time derivatives which can be expressed as

$$\Xi_2=-\frac{1}{4}\int d^3r\; e^{-i\mathbf{q}\cdot\mathbf{r}}\langle\ddot{A}(+)A(-)+A(+)\ddot{A}(-)-2\dot{A}(+)\dot{A}(-)\rangle \tag{128}$$

$$= -\int d^3r\ e^{-i\mathbf{q}\cdot\mathbf{r}}\left[\frac{\partial^2}{4\partial T^2}\langle A(+)A(-)\rangle - \langle \dot{A}(+)\dot{A}(-)\rangle\right]. \tag{129}$$

The first term in brackets is the second time (i.e., T) derivative of $f(\mathbf{q},\mathbf{R},T)$. The last term in the bracket is just the correlation function of the electric field with itself $c^2\langle E(+)E(-)\rangle$ and is related to the energy density. For equilibrium moments the second moment was proportional to the density of photons

$$(2\pi)^2\hbar W(\mathbf{q},\mathbf{R},T) = \int d^3r\ e^{-i\mathbf{q}\cdot\mathbf{r}}\langle E_\mu(\mathbf{R}+\tfrac{1}{2}\mathbf{r},T)E_\mu(\mathbf{R}-\tfrac{1}{2}\mathbf{r},T)\rangle. \tag{130}$$

It is reasonable to suggest that the distribution W, from the energy density, is proportional to $f(\mathbf{q},\mathbf{R},T)$. We can express even moments in terms of this distribution function. However, the odd moments must be another function.

C. Boltzmann equation

Now we turn to the derivation of Eq. (1). The obvious way to obtain this equation is to integrate the QBE over all frequency: to take its zeroth moment. For this discussion, we focus initially on the first two terms in the QBE which are

$$\left[\omega\frac{\partial}{\partial T} + c^2\mathbf{q}\cdot\boldsymbol{\nabla}\right]\mathscr{D} = . \tag{131}$$

If we integrate this equation over all frequency, then there is a problem. The first term has the first moment while the second term has a zeroth moment. These two moments are fundamentally different, since one is proportional to the density of photons while the odd moment is something else. This problem is not corrected by multiplying the equation by any power of ω, since one term will be an even moment and the other will be an odd moment.

We examined the references on the QBE for phonons, to see how previous authors solved the problem there. They obtained a BE by a procedure which we regard as incorrect. They *assumed* that[9–16]

$$\mathscr{D}^< = C(q)\,\delta(\omega-\omega_q)f(\mathbf{q},\mathbf{R},T), \tag{132}$$

where $C(q)$ is a function of q. With this assumption, the zeroth moment of frequency gives an equation similar to Eq. (1). However, our moment analysis has shown this assumption is incorrect. There is no reason to omit the contribution from negative frequencies.

We decided to proceed by deriving two distribution functions. The first is $f(\mathbf{q},\mathbf{R},T)$ which is defined in Eq. (125), and which is related to the density of photons. The second we define as $g(\mathbf{q},\mathbf{R},T)$ is related to the odd moments of the distribution function

$$(2\pi c)^2\hbar g(\mathbf{k},\mathbf{R},T) = \int \frac{d\omega}{2\pi}\,\omega\mathscr{D}(\mathbf{k},\omega,\mathbf{R},T). \tag{133}$$

This correlation is proportional to the bracket in Eq. (127). Using this definition, we can now take moments of the Boltzmann equation. In doing the frequency integral, we examine the parity of the terms multiplying $\mathscr{D}$ in the frequency integrand. If these terms are even in frequency, such as ω^{2n} or else $\omega A(\omega)$, then this integral is proportional to $f(\mathbf{q},\mathbf{R},T)$. However, if these factors are odd functions of frequency, then we suppose the integral is proportional to $g(\mathbf{q},\mathbf{R},T)$. The division of terms into odd and even functions of frequency allows us to define the absorption and scattering terms.

1. n=0

We take the frequency integral of the QBE in Eq. (112) and derive

$$\frac{\partial}{\partial T}\, g + c\hat{q}\cdot\nabla f + \left(\frac{1}{\tau_a}+\frac{1}{\tau_s}\right) g = \frac{1}{\tau_s}\int \frac{d\Omega'}{4\pi}\, P(\hat{q}\cdot\hat{k}) g(\mathbf{k},\mathbf{R},T), \tag{134}$$

$$\frac{1}{\tau_a} = 2\pi n_s \omega_q A(\omega_q), \tag{135}$$

$$\frac{1}{\tau_s} = \frac{(2\pi)^3 c^4}{\omega_q^2}\, n_s \int \frac{d^3k}{(2\pi)^3}\, \delta(\omega_k-\omega_q)\, \frac{d\sigma(\hat{q}\cdot\hat{k})}{d\Omega}\, [1-S(\mathbf{q}-\mathbf{k})]$$

$$= c n_s \int d\Omega'\, \frac{d\sigma(\cos(\theta))}{d\Omega'}\, [1-S(2q\ \sin(\theta/2))], \tag{136}$$

$$P(\hat{q}\cdot\hat{k}) = c\tau_s n_s\, \frac{d\omega(\cos(\theta))}{d\Omega'}\, [1-S(2q\ \sin(\theta/2))]. \tag{137}$$

Note that the structure factor $1-S$ enters into the definition of the scattering function $P(\hat{q}\cdot\hat{k})$. Previous workers only included the scattering cross section in this function.

2. n=1

Here, we multiply the QBE by ω and integrate over all frequencies. Sorting integrands according to whether they are even or odd functions of frequency produces the following equation:

$$\frac{\partial}{\partial T}\left[W - \frac{1}{4\omega_q^2}\frac{\partial^2}{\partial T^2}\, f\right] + c\hat{q}\cdot\nabla g + \left(\frac{1}{\tau_a}+\frac{1}{\tau_s}\right) f = \frac{1}{\tau_s}\int \frac{d\Omega'}{4\pi}\, P(\hat{q}\cdot\hat{k}) f(\mathbf{k},\mathbf{R},T). \tag{138}$$

The terms for absorption and scattering are the same ones in Eq. (134). We make two approximations on this expression. First, we neglect the triple time derivative of f. Since we are interested in diffusion, then they should give a very small contribution. Second, we assume the energy density is just the phonon frequency multiplied by f. If this is true, then $W=f$. With these two assumptions, Eq. (138) becomes

$$\frac{\partial}{\partial T}\, f + c\hat{q}\cdot\nabla g + \left(\frac{1}{\tau_a}+\frac{1}{\tau_s}\right) f = \frac{1}{\tau_s}\int \frac{d\Omega'}{4\pi}\, P(\hat{q}\cdot\hat{k}) f(\mathbf{k},\mathbf{R},T). \tag{139}$$

When we compare Eqs. (134) and (139) we see they are similar. One is found from the other by exchanging f and g. It makes sense to alternately add these two equations, or subtract them

$$f^{(\pm)} = f \pm g,$$

$$\left[\frac{\partial}{\partial T} + c\hat{q}\cdot\nabla + \left(\frac{1}{\tau_a}+\frac{1}{\tau_s}\right)\right] f^{(+)} = \frac{1}{\tau_s}\int \frac{d\Omega'}{4\pi}\, P(\hat{q}\cdot\hat{k}) f^{(+)}(\mathbf{k},\mathbf{R},T),$$

$$\left[\frac{\partial}{\partial T} - c\hat{q}\cdot\nabla + \left(\frac{1}{\tau_a}+\frac{1}{\tau_s}\right)\right] f^{(-)} = \frac{1}{\tau_s}\int \frac{d\Omega'}{4\pi}\, P(\hat{q}\cdot\hat{k}) f^{(-)}(\mathbf{k},\mathbf{R},T). \tag{40}$$

The first of these two equations is the same as Eq. (1). Thus we have derived this equation, which was one of the goals of this paper. We now see that it is the Boltzmann equation for the combination $f^{(+)}=f+g$. We associate this function with photons of positive frequency. We have also derived a second equation for $f^{(-)}=f-g$. We associate this function with photons of negative

frequency. Without any interactions, then $f^{(+)}=F(\mathbf{q}\cdot\mathbf{R}-\omega T)$ while $f^{(-)}=F(\mathbf{q}\cdot\mathbf{R}+\omega T)$. Obviously $f^{(+)}$ corresponds to the physics convention that a wave of positive $\mathbf{q}$ and positive frequency moves in the direction $\mathbf{R}$ with increasing time.

VII. DISCUSSIONS

We have provided the first derivation of the quantum Boltzmann equation for photons. We have showed how the usual Boltzmann equation for the photon density can be derived from this QBE by taking moments. One result of this derivation is an explicit expression for the scattering term in the Boltzmann equation. This function contains a factor which relates to the distribution of scattering centers. We also showed that there are negligible local field corrections for the case of photon diffusion, which is the primary application of the QBE. Finally, we introduced a matrix $\tilde{J}$ which makes the discussion of perturbation expansions very easy.

Stephen[12] has discussed the phenomena of photon diffusion and coherent backscattering. His analysis is derived from the correlation function of the electric field with itself. His analysis starts from a different point, the electric field in the coherent potential approximation. We tried and failed to derive coherent backscattering using our formalism. We summed several sets of diagrams, besides those reported here. We summed every set we could imagine. But none gave coherent backscattering. We are still working on this problem.

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On the vacuum stability in the Efimov–Fradkin model at finite temperature

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The behavior of the nontruncated and truncated Efimov–Fradkin models ($\mathscr{L}_{\rm int}=-\Sigma_{n=3}^{N}\lambda_n\varphi^n$) at finite temperature in a generic D-dimensional flat space–time was investigated. The thermal contribution to the renormalized mass and coupling constants are obtained in the one-loop approximation by the use of a mix between dimensional and the Epstein zeta function analytic regularization and a modified minimal subtraction procedure. We proved that for $D_c(N-1)\leqslant D$ there is not a temperature for which at least one of the renormalized coupling constants becomes zero, where $D_c(N-1)$ is the critical spacetime dimension for the renormalized coupling constant λ_{N-1}. For $D_c(N)\leqslant D<D_c(N-1)$ only the renormalized coupling constant λ_{N-1} becomes zero at some temperature β_{N-1}^{-1}. For $D<D_c(N)$ the renormalized coupling constants $\lambda_{N-1}(\beta)$ and $\lambda_N(\beta)$ become zero at temperatures β_{N-1}^{-1} and β_N^{-1}, respectively. In the latter situation, for temperatures $\beta_{N-1}^{-1}<\beta^{-1}<\beta_N^{-1}$ the effective potential has a global minimum. For temperatures above β_N^{-1}, the system can develop a first order phase transition, where the origin corresponds to a metastable vacuum. In the nontruncated model, corresponding to a nonpolynomial Lagrange density, for $D\geqslant 2$ all the coupling constants remain positive for any temperature. © *1996 American Institute of Physics.*
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I. INTRODUCTION

In this paper an attempt is made to understand the vacuum stability mechanism in scalar models at finite temperature assuming polynomial and nonpolynomial Lagrange densities. It is of common knowledge that the ultraviolet divergences that arise in models with nonpolynomial Lagrange densities are not worse graph by graph than those encountered in polynomial renormalizable models.[1] This result was obtained using a summation method introduced by Efimov and Fradkin.[2,3] The idea of the method is to investigate the Borel summability of the divergent perturbative series.[4] The interaction Lagrange density of these models may be expanded in a power series of the type,

$$\mathscr{L}_{\rm int}=-\lim_{N\to\infty}\sum_{n=3}^{N}\lambda_n\varphi^n(x), \tag{1}$$

where $\varphi(x)$ is a Hermitian scalar field and λ_n are the coupling constants of the model.

Instead of regularizing the model using a ultraviolet cutoff Λ in the Euclidean momenta, or assuming the existence of a spacetime microscopic structure, characterized by a lattice spacing a, we preferred to regularize it by using a combination of two different methods: the dimensional[5] and analytic regularization methods.[6] The advantage of this technique lies in the fact that the dependence of mass and coupling constant with the temperature appear in a very straightforward

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way. A recent discussion on the relation between the cutoff method and analytical regularization procedures to obtain the Casimir energy in an arbitrary ultrastatic spacetime with or without boundaries, may be found in Svaiter and Svaiter.[7] Upon the application of the analytic regularization method, a mass parameter μ is introduced, in order to deal with dimensionless quantities in the analytic extensions. It is not difficult to show that the canonical dimension of the coupling constants of the model are given by

$$\lambda_n = \mu^{D-(n/2)(D-2)}, \tag{2}$$

where D is the space–time dimension. Each coupling constant in the expansion given by Eq. (1) has a critical dimension $D_c(n)$. By critical dimension of each coupling constant we mean a space–time dimension such that below it the coupling constant may be a large quantity due to its positive dimension $D-(n/2)(D-2)$ in terms of μ (or using the critical phenomena language, in terms of the original scale $1/a$, where a is the lattice spacing). We define the critical space–time dimension $D_c(n)=2n/(n-2)$, as the space–time dimension where the renormalized coupling constant λ_n is dimensionless. Below $D_c(n)$, the model is superrenormalizable. We demonstrate that in the superrenormalizable case above some temperature the system may suffer a first order phase transition.

In two recent papers studying the $\lambda\varphi^4$ model, the possibility of changing the sign of the renormalized coupling constant was raised.[8,9] In the first one, the thermal and topological contributions to the renormalized mass and renormalized coupling constant in the one-loop approximation were obtained.[8] In the second one we extended the study of the $\lambda\varphi^4$ model at finite temperature to a generic D-dimensional space–time with trivial topology of the spacelike section and we also discussed the behavior with the temperature of the Gross–Neveu model, which is an ultraviolet asymptotically free model. In the Gross–Neveu model, we proved that for $D=3$ the thermal contribution to the renormalized coupling constant is zero. On the other hand, for $D\neq 3$ our results are inconclusive.[9] Studying the $\lambda\varphi^4$, model we obtained more concrete results. Still using the effective potential and the one-loop approximation, we presented the thermal contribution to the renormalized mass and coupling constant. The thermal renormalized coupling constant is given by

$$\lambda(\beta)=\lambda(\infty)+\Delta\lambda(\beta), \tag{3}$$

where $\lambda(\infty)$ is the temperature independent renormalized coupling constant and $\Delta\lambda(\beta)$ is its thermal correction. Using the fact that $\Delta\lambda(\beta)$ is negative, we proved that for $D<4$, at sufficiently high temperatures, the system may suffer a first order phase transition with a metastable vacuum at the origin.

In the majority of the papers in the literature the temperature dependence of the renormalized coupling constant is neglected. This approach is reasonable if we are interested in studying a second order phase transition. In this case, the variation of the squared mass with the temperature is the most important fact. Therefore, it is sufficient to consider the renormalized coupling constant as independent of the temperature, and the sign of the squared mass drives the second order phase transition. The situation that we are interested in discussing here is quite different, since the goal of our investigation is not the behavior of the system in the neighborhood of a second order phase transition. Our intention is to study the model in the high temperature regime (far from a critical temperature), where the possibility of vanishing some renormalized coupling constant with a first order phase transition at some temperature arises.

We would like to emphasize that the study of the dependence of the coupling constant with the temperature is not new in the literature. Many authors have studied such dependence in scalar models[10] and also in non-Abelian gauge theories.[11] In the former case, since QCD is an asymptotically free theory, it can be shown that as the temperature increases, the temperature dependent renormalized coupling constant goes to zero. As we discussed, in the $\lambda\varphi^4$ model if $D<4$, for temperatures β^{-1} above the temperature β_T^{-1} the renormalized coupling constant $\lambda(\beta)$ becomes

negative and the origin is a metastable vacuum. This kind of problem occurs with nonasymptotical models. The growth of the coupling constant at large momenta corresponds to the temperature growth (in modulus) of the renormalized coupling constant.

Even in the absence of temperature, the instability of the vacuum of models using scalar fields has been discussed in the literature. An enlightening discussion has been done by Linde.[12] Studying the $O(N)$ model and performing an $1/N$ expansion of the effective potential, this author showed that the effective potential is a double-valued function of the field φ [where the field $\Phi=(\varphi_1,...,\varphi_N)$ has a classical part $\Phi=\sqrt{N}(\varphi,0,...,0)$]. In the upper branch appears a tachyonic pole that leads us to disregard it as a nonphysical one, remaining the effective potential described by a unique curve that for large values of the classical field is not bounded from below.

We would like to stress that the situation treated in this paper is very similar to the examples where renormalized quantities depend on the geometric parameters of the spacelike section. The simplest example is the renormalized vacuum energy of scalar fields confined in a parallelepipedal box, where the sign of the energy may depend on the relative lengths of the cavity. Indeed the sign of the Casimir energy may depend on the spacetime dimension, the type of boundary conditions, etc.,[13] but we would like to emphasize only the dependence of the Casimir energy on the ratio of the sizes of the box [imposing a Dirichlet boundary condition] to give a rough idea of what kind of behavior we expect in situations where regularization and renormalization procedures are obligatory. Note that the possibility of obtaining a negative renormalized coupling constant in the $\lambda\varphi^4$ model was conjectured by Nash a long time ago.[14]

In this paper, we will investigate the one-loop renormalization of the truncated and nontruncated Efimov–Fradkin model assuming thermal equilibrium with a reservoir at temperature β^{-1}. Using the one-loop effective potential discussed briefly in Refs. 8 and 9, we will show that if $D\geqslant D_c(N-1)$, all the renormalized coupling constants of the truncated model are positive for any temperature (note that for reasons of stability in the tree level N must be even). For $D_c(N-1)>D\geqslant D_c(N)$ only the renormalized coupling constant $\lambda_{N-1}(\beta)$ becomes zero at some temperature β_{N-1}^{-1}. For $D_c(N)>D$, the renormalized coupling constants $\lambda_{N-1}(\beta)$ and $\lambda_N(\beta)$ become zero at the temperatures β_{N-1}^{-1} and β_N^{-1}, respectively.

The outline of the paper is the following: in Sec. II the effective potential is presented. In Sec. III the thermal contribution to the renormalized mass and coupling constant are presented in the truncated model ($N=4$). In Sec. IV we repeat the calculations of the truncated model for $N>4$ and in the nontruncated model. Finally, we discuss some applications of our results in curved spacetime and high order behavior of perturbation theory. Conclusions are given in Sec. V. In this paper we use $\hbar=c=1$.

II. THE ONE-LOOP EFFECTIVE POTENTIAL OF THE EFIMOV–FRADKIN MODEL AT ZERO AND FINITE TEMPERATURE

In this section we will generalize some results obtained in Refs. 8 and 9. Suppose we have a D-dimensional flat space–time with trivial topology of the spacelike section and Bose fields in thermal equilibrium with a reservoir at temperature β^{-1}. Let us assume the following Lagrange density associated with a massive neutral scalar field,

$$\mathscr{L}=\frac{1}{2}(\partial_\mu\varphi)^2-\frac{1}{2}m^2\varphi^2-\sum_{n!}^{\infty}\frac{\lambda_n}{n!}\varphi^n+\text{counterterms}. \tag{4}$$

Since the model is nonrenormalizable, the counterterms have meaning only in the context of a finite number of loops. Note that we are not assuming inversion symmetry in the model, i.e., $V(\varphi_0)=V(-\varphi_0)$. If we assume it, the only surviving terms will be the even powers of the field. The time ordered products of the fields can be continued analytically to imaginary times, and we define a Euclidean action integrating the analytic continuation to imaginary times in the Lagrange

density. After a Wick rotation, defining the normalized expectation value of the field by $\varphi_0=\langle 0|\varphi|0\rangle/\langle 0|0\rangle$, the zero temperature effective potential is given in the one-loop approximation by

$$V(\varphi_0)=V_{\mathrm{I}}(\varphi_0)+V_{\mathrm{II}}(\varphi_0), \tag{5}$$

where

$$V_{\mathrm{I}}(\varphi_0)=\frac{1}{2}\,m^2\varphi_0^2+\sum_{n=3}^{\infty}\frac{\lambda_n}{n!}\,\varphi_0^n+\text{counterterms}, \tag{6}$$

and

$$V_{\mathrm{II}}(\varphi_0)=\sum_{s=1}^{\infty}\frac{(-1)^{s+1}}{2s}\left(\sum_{n=3}^{\infty}\frac{1}{(n-2)!}\,\lambda_n\varphi_0^{n-2}\right)^s\int\frac{d^Dq}{(2\pi)^D}\,\frac{1}{(\omega^2+\mathbf{q}^2+m^2)^s}. \tag{7}$$

There is no difficulty in extending the above results, assuming that the system is in thermal equilibrium with a reservoir at temperature β^{-1}. In the study of quantum fields at finite temperature two different approaches are currently used. The first one is the real time formalism in the canonical[15] or path integral approach.[16] The second one, is the Euclidian time formalism and will be used from now on in this paper. After a Wick rotation, the functional integral runs over the fields that satisfy periodic boundary conditions in Euclidian time. The effective action may be defined, as in the zero temperature case, by a functional Legendre transformation. Regularization and renormalization procedures follow the same steps taken in the zero temperature case, since temperature effects do not change the ultraviolet behavior of the model. Summing up, to study temperature effects in Bose fields we must perform the following replacements in the Euclidian region:

$$\int\frac{d\omega}{2\pi}\rightarrow\frac{1}{\beta}\sum_{n'}\,, \tag{8}$$

and

$$\omega\rightarrow\omega_{n'}=\frac{2\pi n'}{\beta}, \tag{9}$$

where $\omega_{n'}=2\pi n'/\beta$ are the Matsubara frequencies. Introducing a mass parameter μ and defining the dimensionless quantities,

$$c^2=\frac{m^2}{4\pi^2\mu^2}, \tag{10}$$

$$(\beta\mu)^2=a^{-1}, \tag{11}$$

and

$$k^i=\frac{q^i}{2\pi\mu}, \tag{12}$$

the Born terms plus the one-loop contributions to the effective potential are given by

$$V(\beta,\varphi_0)=V_{\mathrm{I}}(\varphi_0)+V_{\mathrm{II}}(\beta,\varphi_0),$$

where

$$V_{\mathrm{I}}(\beta,\varphi_0)=\frac{1}{2}\,m^2\varphi_0^2+\sum_{n=3}^{\infty}\,\frac{\lambda_n}{n!}\,\varphi_0^n+\text{counterterms},\tag{13}$$

and

$$V_{\mathrm{II}}(\beta,\varphi_0)=\sqrt{a}\mu^D\sum_{s=1}^{\infty}\,\frac{(-1)^{s+1}}{2s}\left(\sum_{n=3}^{\infty}\,\frac{\lambda_n\varphi_0^{n-2}}{4\pi^2\mu^2(n-2)!}\right)^s\sum_{n'=-\infty}^{\infty}\int d^dk\,\frac{1}{(an'^2+\mathbf{k}^2+c^2)^s}.\tag{14}$$

Owing to the discreteness of the Matsubara frequencies, an analytic regularization procedure will be used. Defining the inhomogeneous Epstein zeta function as

$$A_N^{c^2}(s,a_1,a_2,\ldots,a_N)=\sum_{n_1,n_2,\ldots,n_N=-\infty}^{\infty}(a_1n_1^2+a_2n_2^2+\cdots+a_Nn_N^2+c^2)^{-s},\tag{15}$$

we will see that its analytic continuation will be used to regularize the model. Before showing how this analytic continuation works, and in order to simplify Eq. (14), it is convenient to define g_n and ϕ as the new coupling constants and an adimensional (for $D=4$) vacuum expectation value of the field

$$g_n=\frac{\lambda_n}{4\pi^2\mu^{4-n}(n-2)!},\tag{16}$$

and

$$\frac{\varphi_0}{\mu}=\phi.\tag{17}$$

Substituting Eq. (16) and Eq. (17) in Eq. (14) we obtain

$$V_{\mathrm{II}}(\beta,\phi)=\mu^D\sqrt{a}\sum_{s=1}^{\infty}\,\frac{(-1)^{s+1}}{2s}\left(\sum_{n=3}^{\infty}\,g_n\phi^{n-2}\right)^s\sum_{n'=-\infty}^{\infty}\int d^dk\,\frac{1}{(an'^2+c^2+\mathbf{k}^2)^s}.\tag{18}$$

Since the spatial section of the space–time is noncompact, in order to deal with the divergences in the integral of Eq. (18), we will first use dimensional regularization. From the well-known formula,

$$\int\,\frac{d^dk}{(k^2+b^2)^s}=\frac{\pi^{d/2}}{\Gamma(s)}\,\Gamma\left(s-\frac{d}{2}\right)\,\frac{1}{b^{2s-d}},\tag{19}$$

and defining $f(D,s)$ as

$$f(D,s)=f(d+1,s)=\frac{(-1)^{s+1}}{2s}\,\pi^{d/2}\Gamma\left(s-\frac{d}{2}\right)\,\frac{1}{\Gamma(s)},\tag{20}$$

it is possible to write $V_{\mathrm{II}}(\beta,\phi)$ in terms of the inhomogeneous Epstein zeta function given by Eq. (15) as

$$V_{\mathrm{II}}(\beta,\phi)=\mu^{D}\sqrt{a}\sum_{s=1}^{\infty} f(D,s)\left(\sum_{n=3}^{\infty} g_n\phi^{n-2}\right)^{s} A_1^{c^2}\left(s-\frac{d}{2},a\right). \tag{21}$$

The terms $s\leqslant D/2$ are divergent, which implies that the effective potential is not yet regularized. To complete the regularization, let us assume that each term in the series of the one-loop effective potential $V(\beta,\phi)$ is replaced by its analytic extension, defined at the beginning in a open connected set of points of the complex plane s. Since we discussed carefully the process of the analytic continuation in the previous works, here we will only sketch this derivation. First, it is necessary to write Eq. (21) in terms of the modified inhomogeneous Epstein zeta function as we did in the above quoted works. For $\mathrm{Re}(s)>N/2$, the modified inhomogeneous Epstein zeta function, $E_N^{c^2}(s,a_1,a_2,\ldots,a_N)$ converges and represents an analytic function of s, so $\mathrm{Re}(s)>N/2$ is the largest possible convergence domain of the series. The next step is to establish a connection between the terms of the series defining the inhomogeneous Epstein zeta function and the Euler integral representation of the gamma function. For instance, in the case of only one sum this connection is of the type

$$\frac{1}{(n+a)^s}=\frac{1}{\Gamma(s)}\int_0^{\infty} t^{s-1}e^{-t(n+a)}dt.$$

Summing over n in both sides, we obtain in the left-hand side the inhomogeneous Riemann zeta function and in the right-hand side a still divergent integral. We split the integral into two parts, the first one defines an entire function $Q(s)$ and the second one $P(s)$ contains the divergences. Then we use a Bernoulli representation for the integrand of $P(s)$ and the Weierstrass theorem to exchange the sum and integral operations. This allows us to show that $P(s)$ extends to a meromorphic function of s having simple poles. The generalization the case of a multiple sum goes along the same lines.

Therefore, using the results of Ref. 17 we rewrite Eq. (21) as

$$V_{\mathrm{II}}(\beta,\phi)=\mu^{D}\sum_{s=1}^{\infty}\left(\sum_{n=3}^{\infty} g_n\phi^{n-2}\right)^{s} h(D,s)\left[\frac{1}{2^{D/2-s+2}}\,\Gamma\left(s-\frac{D}{2}\right)\left(\frac{m}{\mu}\right)^{D-2s}+\sum_{n'=1}^{\infty}\left(\frac{m}{\mu^2\beta n'}\right)^{D/2-s} K_{D/2-s}(mn'\beta)\right], \tag{22}$$

where

$$h(D,s)=\frac{1}{2^{D/2-s-1}}\,\frac{1}{\pi^{D/2-2s}}\,\frac{(-1)^{s+1}}{s}\,\frac{1}{\Gamma(s)}. \tag{23}$$

Although Eq. (22) is ill defined, in the one-loop approximation it is possible to find the exact form of the counterterms in such a way that, mass and coupling constants (and consequently) the effective potential are finite quantities. To extract the singularities from the analytic extensions, let us define the mass squared as the value of the inverse propagator at zero momentum and the coupling constant λ_n as the proper n-point function at zero external momentum. In fact, the true physical mass is defined as the value of p^2 at which the inverse propagator vanishes. However, the two values are related by a finite renormalization. In the next section, we will develop such an idea in a very simple case: the truncated ($N=4$) Efimov–Fradkin model and, subsequently, present the temperature dependent renormalized squared mass and coupling constants of the model.

III. THE RENORMALIZED MASS AND COUPLING CONSTANTS IN THE TRUNCATED ($N=4$) EFIMOV–FRADKIN MODEL

The goal of this section is to study how temperature effects lead to instabilities in scalar massive models. For the sake of simplicity and in order to obtain some insight about the thermal contribution to the renormalized mass and coupling constants in the nontruncated Efimov–Fradkin model, let us suppose the truncated model, i.e., $\lambda_n=0$ for $n>4$. We remark that the theory defined only with the term λ_3 is not consistent in any spacetime dimension since the energy is not bounded below, and so no ground state can exist in the interacting theory. The inclusion of λ_4 introduces a global minimum in the model. Defining

$$f(D,s)=\frac{1}{2^{D/2-s+2}}\,\Gamma\left(s-\frac{D}{2}\right),$$

it is possible to write $V_{\mathrm{II}}(\beta,\phi)$ as

$$V_{\mathrm{II}}(\beta,\phi)=\mu^D\sum_{s=1}^{\infty}\sum_{k=0}^{s}h(D,s)C_s^k g_3^{s-k}g_4^k\phi^{s+k}\left[f(D,s)\left(\frac{m}{\mu}\right)^{D-2s}+\sum_{n=1}^{\infty}\left(\frac{m}{\mu^2\beta n}\right)^{D/2-s}K_{D/2-s}(mn\beta)\right]. \tag{24}$$

In order to find the exact form of the counterterms that will render the model finite, let us consider the renormalization conditions for the nontruncated model

$$\frac{\partial^2}{\partial\phi^2}\,V(\beta,\phi)\big|_{\phi=0}=\mu^2m^2, \tag{25}$$

and

$$\frac{\partial^n}{\partial\phi^n}\,V(\beta,\phi)\big|_{\phi=0}=\mu^n\lambda_n,\quad n=3,4,\ldots\ . \tag{26}$$

We should point out that, strictly speaking, there is no need for wave function renormalization because the vacuum expectation value of the field has been chosen to be a constant. Using Eqs. (6), (24), (25), and (26), it is possible to find the exact form of the counterterms in such a way that they cancel the pole contribution of the analytic extensions. In the neighborhood of the poles, the regular part of the analytic extension of the inhomogeneous Epstein zeta function has two contributions: one which is independent of the temperature (this contribution can be absorbed in the counterterms), and another that depends on it. The thermal contribution to the renormalized coupling constant is proportional to the regular part of the analytic extension of the inhomogeneous Epstein zeta function in the neighborhood of some poles for the ultraviolet divergent graphs. Of course, nonultraviolet divergent graphs do not need to be regularized giving a finite thermal contribution to the renormalized quantities.

Note that we are choosing the renormalization conditions at $\varphi_0=0$. This may be done in the truncated model even if the minimum of the effective potential is not at $\varphi_0=0$, since the renormalization point is totally arbitrary. The values of the renormalized quantities obtained using $\varphi_0=0$ as the renormalization point are related to the corresponding quantities obtained in the true vacuum $\varphi_0\neq0$ by the equations,

$$m^2\big|_{\varphi_0}=\tfrac{1}{2}\,m^2+\tfrac{1}{2}\,\lambda_3\varphi_0+\tfrac{1}{4}\,\lambda_4\varphi_0^2, \tag{27}$$

FIG. 1. The two graphs that contribute to the temperature dependent renormalized mass m^2. Note that they are ultraviolet divergent for $D=4$.

$$\lambda_3|_{\varphi_0}=\frac{1}{3!}\,(\lambda_3+\lambda_4\varphi_0), \tag{28}$$

and finally

$$\lambda_4|_{\varphi_0}=\lambda_4. \tag{29}$$

Analyzing the sign of the thermal corrections to the renormalized physical parameters evaluated at $\phi=0$, the sign of Eqs. (27) and (29) does not change. This is expected since the metastable behavior and the existence of a global minimum cannot depend upon the choice of the renormalization point. For the case of the coupling constant $\lambda_3(\beta)$ with the restrictive condition $|\varphi_0\lambda_4|<|\lambda_3|$, all the forthcoming conclusions also apply.

Let us call $\Delta m^2(D,\beta,m,\lambda_3,\lambda_4,\mu)$ and $\Delta\lambda_n(D,\beta,m,\lambda_3,\lambda_4,\mu)$, $n=3,4$ the thermal squared mass and thermal coupling constants, respectively. In the following, in order to simplify the notation we keep explicitly only the β dependence of the renormalized quantities. Thus,

$$m^2(\beta)=m^2+\Delta m^2(\beta), \tag{30}$$

$$\lambda_n(\beta)=\lambda_n+\Delta\lambda_n(\beta), \quad n=3,4, \tag{31}$$

and for the sake of simplicity in the notation in the rest of this section, we call $\lambda_3(\beta)=\sigma(\beta)$ and $\lambda_4(\beta)=\lambda(\beta)$. From now on we will disregard the combinatorics factors in front of Feynman diagrams, since they are always real positive numbers, and cannot change qualitatively the forthcoming results concerning the sign of the renormalized physical parameters. We are interested only in the connected one particle irreducible diagrams (1PI) which means that in the approximation we are making here, we have two graphs that contribute to the temperature dependent renormalized squared mass (see Fig. 1), the terms $s=1$, $k=1$ (of order λ) and $s=2$, $k=0$ (of order σ^2). It is not difficult to show that the case $s=1$, $k=1$ gives a positive contribution,

$$\Delta m^2_{g_4}(\beta)-\Delta m^2_{g_4}(\infty)=\mu^{D-2}h(D,1)g_4\sum_{n=1}^{\infty}\left(\frac{m}{\mu^2\beta n}\right)^{D/2-1}K_{D/2-1}(mn\beta). \tag{32}$$

In the same way, the contribution from the term $s=2$, $k=0$ is negative and it is given by

$$\Delta m^2_{g_3}(\beta)-\Delta m^2_{g_3}(\infty)=\mu^{D-2}h(D,2)g_3^2\sum_{n=1}^{\infty}\left(\frac{m}{\mu^2\beta n}\right)^{D/2-2}K_{D/2-2}(mn\beta). \tag{33}$$

Using general properties of the Bessel function $K_n(z)$, we obtain that the leading contribution comes from the graph given by Fig. 1(a), i.e., $\Delta m^2_{g_4}(\beta)-\Delta m^2_{g_4}(\infty)+\Delta m^2_{g_3}(\beta)-\Delta m^2_{g_3}(\infty)>0$, and the thermal correction to the renormalized squared mass is always positive. Using the proper time method, Braden obtained the same expression for the thermal mass in the $\lambda\varphi^4$ model [see Eq. (32)]. This author also discussed the two-loop correction to the mass and proved that the coun-

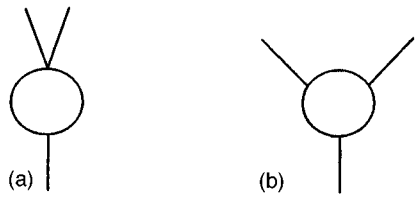

FIG. 2. The two graphs that contribute to the renormalized coupling constant $\sigma(\beta)$. Note that only the first one is ultraviolet divergent for $D=4$.

terterms are temperature independent.[18] Note that the nonleading contribution coming from the graph of Fig. 1(b) is negative, going in the direction of the vanishing of the mass. In other words, in the truncated model with only nonzero λ_3 coupling constant (disregarding the problem of the unboundedness of the effective potential even in the tree level approximation), the thermal squared mass will become zero and negative at high temperatures. Various investigations have been made in theories with cubic coupling. Gross, Perry, and Yaffe[19] calculated the thermal mass of a graviton coupled with massless fermions in the one-loop approximation. These authors found that the thermal mass squared was negative and the graviton developed an imaginary mass at some temperature. This lead the authors to conclude that the hot flat space–time is unstable. The thermal graviton one-loop correction was also analyzed by Kikuchi, Moriya, and Tsukahara and Holstein.[20] It was also shown that the thermal effects destabilize the hot curved space–time.

The situations that we are interested in discussing are the ones in which some renormalized coupling constant $\lambda_n(\beta)$ vanishes by temperature effects. As we discussed above, if $D<D_c(n)$ this situation can be realized. It is important to note that in this region the model is superrenormalizable, and when the fields are massless, perturbative expansion suffers from severe infrared divergences. Since the thermal squared mass is always positive and we are interested in the high temperature regime, this problem does not afflict us, i.e., infrared divergences never appear in our calculations at least in the one-loop aproximation. It should be noted that this fact does not occur in higher order-loop calculations. If we consider N self-energy insertions of $O(\lambda)$ (a ring correction) into a single loop, its contribution is infrared divergent in the case of the zero mass of the field. In other words, on the perturbative level the thermal mass generation does not prevent the appearance of infrared divergences in higher order loop diagrams.

Let us now study the thermal contribution to the renormalized coupling constants. Initially, for the thermal renormalized coupling constant $\sigma(\beta)$ we obtain,

$$\sigma(\beta)=\sigma(\infty)+\Delta\sigma_{g_3}(\beta)+\Delta\sigma_{g_3g_4}(\beta). \tag{34}$$

As in the previous case, it is necessary to study the cases $s=2$, $k=1$ and $s=3$, and $k=0$ (see Fig. 2). In the case of $s=2$, $k=1$ [of order $\sigma\lambda$, see Fig. 2(a)], it is not difficult to show that it gives a negative contribution,

$$\Delta\sigma_{g_3g_4}(\beta)-\Delta\sigma_{g_3g_4}(\infty)=2\mu^{D-3}h(D,2)g_3g_4\sum_{n=1}^{\infty}\left(\frac{m}{\mu^2\beta n}\right)^{D/2-2}K_{D/2-2}(mn\beta). \tag{35}$$

For the second case, $s=3$, $k=0$ [of the order σ^3, see Fig. 2(b)] the contribution is positive,

$$\Delta\sigma_{g_3}(\beta)-\Delta\sigma_{g_3}(\infty)=\mu^{D-3}h(D,3)g_3^3\sum_{n=1}^{\infty}\left(\frac{m}{\mu^2\beta n}\right)^{D/2-3}K_{D/2-3}(mn\beta). \tag{36}$$

The thermal correction to the renormalized coupling constant $\sigma(\beta)$ is given by

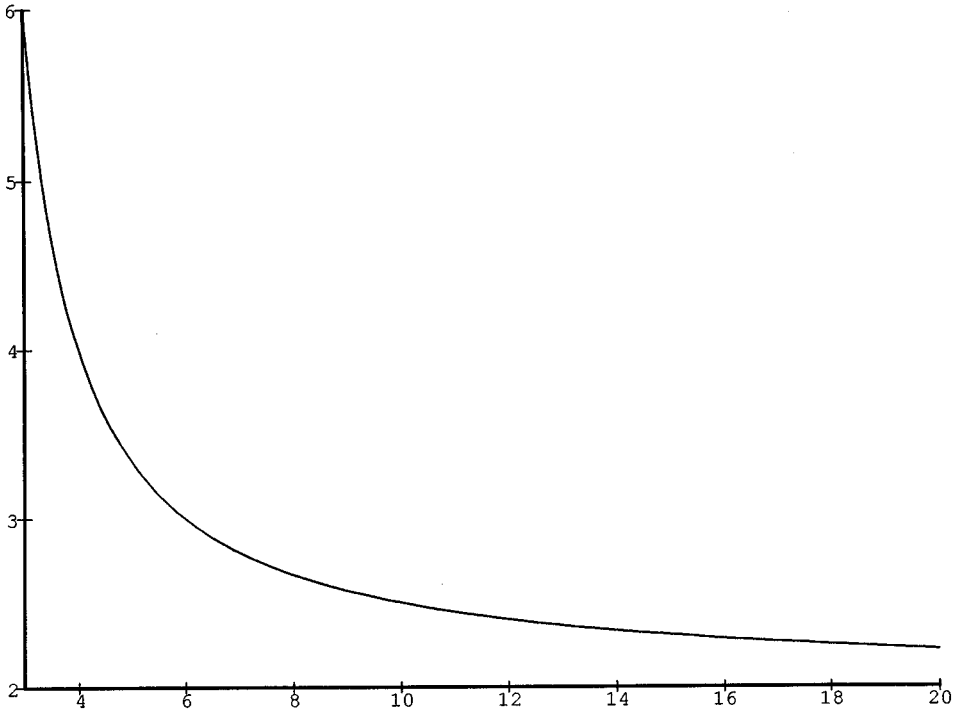

FIG. 3. The critical dimension as a function of n for each coupling constant λ_n.

$$[\Delta\sigma_{g_3g_4}(\beta)-\Delta\sigma_{g_3g_4}(\infty)]+[\Delta\sigma_{g_3}(\beta)-\Delta\sigma_{g_3}(\infty)]. \tag{37}$$

The term between the first brackets of Eq. (37) dominates over the second one, and the thermal correction to the renormalized coupling constant $\sigma(\beta)$ is negative. We have the interesting situation where the renormalized coupling constant $\sigma(\beta)$ attains its maximum at zero temperature ($\beta^{-1}=\infty$), and decreases monotonically as the temperature increases. In other words, the thermal contribution to the renormalized coupling constant $\Delta\sigma(\beta)$ is negative, and increases in modulus with the temperature. As we discussed in the previous sections, for $D<D_c(n)$ the coupling constant may be a large quantity. From Eq. (2), it is not difficult to show that $D_c(n)=2n/(n-2)$ (see Fig. 3). Since the thermal contribution to the renormalized coupling constant is negative, there is a temperature β_3^{-1} where $\sigma(\beta)$ vanishes if $D<6$. Above this temperature $\sigma(\beta)$ becomes negative. As we will see, even if $D<4$, there is a finite range of temperatures where $\lambda(\beta)$ is still positive. The thermal contribution to the renormalized coupling constant $\lambda(\beta)$ also can be calculated. The complete expression for $\lambda(\beta)$ is

$$\lambda(\beta)=\lambda(\infty)+\Delta\lambda_{g_3}(\beta)+\Delta\lambda_{g_3g_4}(\beta)+\Delta\lambda_{g_4}(\beta). \tag{38}$$

As in the previous case we need to study the graphs $s=2$, $k=2$, $s=3$, $k=1$, and $s=4$, $k=0$ (see Fig. 4). For the first case $s=2$, $k=2$ (of order λ^2), we get a negative contribution [see Fig. 4(a)],

$$\Delta\lambda_{g_4}(\beta)-\Delta\lambda_{g_4}(\infty)=\mu^{D-4}h(D,2)g_4^2\sum_{n=1}^{\infty}\left(\frac{m}{\mu^2\beta n}\right)^{D/2-2}K_{D/2-2}(mn\beta). \tag{39}$$

For the case $s=3$, $k=1$ [of the order $\sigma^2\lambda$, Fig. 4(b)] we obtain a positive contribution

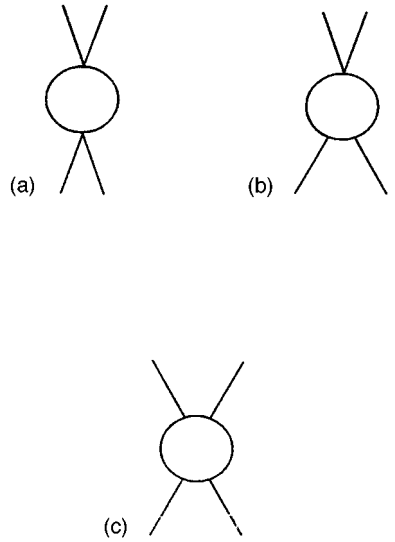

FIG. 4. The three graphs that contribute to the renormalized coupling constant $\lambda(\beta)$. Again, only the first is ultraviolet divergent in $D=4$.

$$\Delta\lambda_{g_3g_4}(\beta)-\Delta\lambda_{g_3g_4}(\infty)=3\mu^{D-4}h(D,3)g_3^2g_4\sum_{n=1}^{\infty}\left(\frac{m}{\mu^2\beta n}\right)^{D/2-3}K_{D/2-3}(mn\beta). \tag{40}$$

Finally, in the last case, $s=4$, $k=0$ [of the order σ^4, Fig. 4(c)] we obtain a negative contribution given by

$$\Delta\lambda_{g_3}(\beta)-\Delta\lambda_{g_3}(\infty)=\mu^{D-4}h(D,4)g_3^4\sum_{n=1}^{\infty}\left(\frac{m}{\mu^2\beta}\right)^{D/2-4}K_{D/2-4}(mn\beta). \tag{41}$$

The thermal correction to the renormalized coupling constant $\lambda(\beta)$ is the sum of the contributions from the three graphs of Fig. 4, which gives

$$[\Delta\lambda_{g_3}(\beta)-\Delta\lambda_{g_3}(\infty)]+[\overline{\Delta\lambda}_{g_3g_4}(\beta)-\Delta\lambda_{g_3g_4}(\infty)]+[\Delta\lambda_{g_4}(\beta)-\Delta\lambda_{g_4}(\infty)]. \tag{42}$$

The term between the last brackets in Eq. (42) dominates over the others and, since its contribution is negative, the thermal correction to the renormalized coupling constant $\lambda(\beta)$ is negative. The important conclusion from the above discussion is the following: the critical dimension for λ is $D=4$, which implies that if we take $D<4$ there is a temperature such that $\lambda(\beta)$ becomes zero. Let us call β_4^{-1} this temperature. If the system is heated above this temperature β_4^{-1}, the renormalized coupling constant $\lambda(\beta)$ becomes negative. Note that we have two different temperatures (for $D<4$) where $\sigma(\beta)$ and $\lambda(\beta)$ vanish. First $\sigma(\beta)$ becomes zero at β_3^{-1} [where $\lambda(\beta)$ is still positive] and after at β_4^{-1} the renormalized coupling constant $\lambda(\beta)$ becomes zero [where $\sigma(\beta)$ is negative]. For temperatures $\beta^{-1}>\beta_4^{-1}$ the system can develop a first order phase transition with the decay of a false vacuum.[21]

Finally, the effective potential as a function of the temperature and the vacuum expectation value of the field for $D<4$, $m^2=\mu=\lambda=1$ may be plotted in a ''toy'' model. The temperature is the parameter that allows us to interpolate between the two configurations: a stable vacuum at low temperatures and a metastable state at temperatures $\beta^{-1}>\beta_4^{-1}$ (see Fig. 5). In the next section we

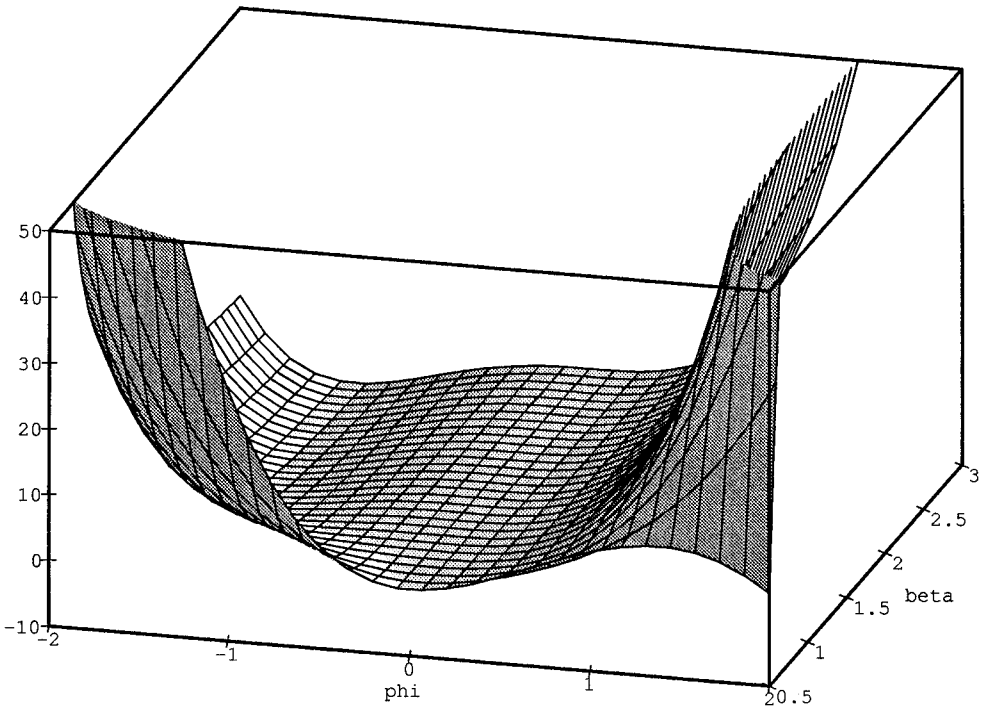

FIG. 5. The effective potential as a function of the vacuum expectation value of the field and the inverse of the temperature. For low temperatures, it has a global minimum and for temperature $\beta^{-1}>\beta_{g4}^{-1}$, the potential has a metastable vacuum.

will repeat the calculations that we have done in this section to the truncated ($N>4$) and also in the nontruncated modes.

IV. THE RENORMALIZED MASS AND COUPLING CONSTANTS IN THE TRUNCATED ($N>4$) AND THE NONTRUNCATED MODELS

In this section we will suppose a general truncated model, i.e., $\lambda_n=0$ for $n>N>4$. Since we intend to disregard at the tree level the problem of the unboundedness of the energy density, we assume that N is an even integer. The calculations are now formally identical to the previous ones. The only difference is the richness coming from the distinct graphs contributing to the thermal renormalized coupling constants. For reasons that will become clear later we will study two different situations,

$$\text{(i)}\quad D<D_c(N-1),$$

$$\text{(ii)}\quad D\geqslant D_c(N-1).$$

For $D<D_c(N-1)$, let us investigate the thermal renormalized coupling constants $\lambda_{N-2}(\beta)$, $\lambda_{N-1}(\beta)$ and $\lambda_N(\beta)$, separately. We must analyze the leading diagrams giving contributions to the renormalized coupling constants $\lambda_{N-2}(\beta)$, $\lambda_{N-1}(\beta)$, and $\lambda_N(\beta)$. In this case, it is not difficult to show that there is a positive contribution to the renormalized coupling constant $\lambda_{N-2}(\beta)$ given by the graph $s=1$ in Fig. 6. This is because the leading contribution comes from the graph with the smaller value of s. An example of nonleading contributions are those given by the graphs in Fig. 7. The leading thermal contribution gives

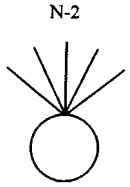

FIG. 6. The graph that gives the leading contribution to the renormalized coupling constant $\lambda_{N-2}(\beta)$.

$$\lambda_{N-2}(g_N,\beta)-\lambda_{N-2}(g_N,\infty)\cong\mu^{D-N+2}h(D,1)g_N\sum_{n=1}^{\infty}\left(\frac{m}{\mu^2\beta n}\right)^{D/2-1}K_{D/2-1}(mn\beta). \quad (43)$$

The result above can be generalized to the other coupling constants $\lambda_3,...,\lambda_{N-3}$. Thus, the renormalized coupling constants $\lambda_3,...,\lambda_{N-2}$ are always positive, for any D space–time dimension. The situation changes in the case of the coupling constant $\lambda_{N-1}(\beta)$. In this case the leading graphs are given in Fig. 8. The thermal contribution from these graphs to the renormalized coupling constant λ_{N-1} is given by

$$\lambda_{N-1}(g_N,g_{N-1},\ldots,g_3,\beta)-\lambda_{N-1}(g_N,g_{N-1},\ldots,g_3,\infty)$$

$$\cong\mu^{D-N+1}h(D,2)(g_Ng_3+g_{N-1}g_4+\cdots)\sum_{n=1}^{\infty}\left(\frac{m}{\mu^2\beta n}\right)^{D/2-2}K_{D/2-2}(mn\beta), \quad (44)$$

which is a negative expression, implying that for $D<D_c(N-1)$ it must have a temperature where $\lambda_{N-1}(\beta)$ vanishes. Finally, for the coupling constant $\lambda_N(\beta)$, the leading graphs are given by Fig. 9. A straightforward calculation gives for the thermal contribution to the renormalized coupling constant λ_N the value

$$\lambda_N(g_N,g_{N-1},\ldots,g_3,\beta)-\lambda_N(g_N,g_{N-1},\ldots,g_3,\infty)$$

$$=\mu^{D-N}h(D,2)(g_Ng_4+g_{N-1}g_5+\cdots)\sum_{n=1}^{\infty}\left(\frac{m}{\mu^2\beta n}\right)^{D/2-2}K_{D/2-2}(mn\beta). \quad (45)$$

As in the previous case, the coupling constant λ_N also becomes zero at the temperature β_N^{-1} if $D<D_c(N)$. From the same arguments related to the critical dimension of each coupling constant, for $D\geqslant D_c(N-1)$ all the renormalized coupling constants are positive for any temperature. A very interesting situation is the case where $D_c(N)\leqslant D<D_c(N-1)$. Although the coupling constant λ_{N-1} becomes negative above the temperature β_{N-1}^{-1}, the effective potential has a global

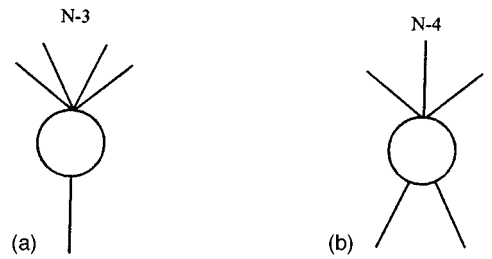

FIG. 7. The graphs that give nonleading contributions to the renormalized coupling constant $\lambda_{N-2}(\beta)$.

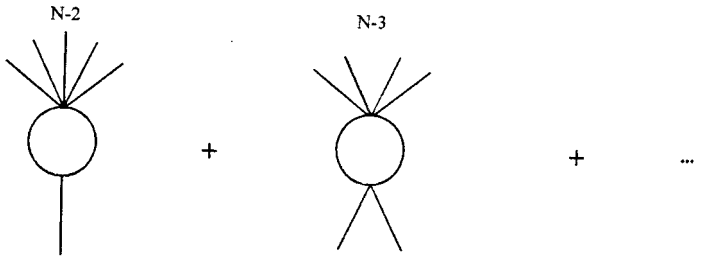

FIG. 8. The graphs that give the leading contribution to the renormalized coupling constant $\lambda_{N-1}(\beta)$.

minimum, since the renormalized coupling constant $\lambda_N(\beta)$ is positive for any temperature. In this case, the ground state of the model is stable. Note that we are using the renormalization conditions at $\phi=0$. Imposing only even powers of the field in Eq. (1), all the above conclusions apply. Including odd powers of the field, the global minimum of the effective potential is not at $\phi=0$. Let us suppose that the minimum occurs at some value $\phi\neq 0$. It is possible to show that the results concerning the sign of the renormalized coupling constant $\lambda_N(\beta)$ and squared mass do not change. From a physical point of view this could not be otherwise, since the critical behavior of the system and the existence or not of vacuum decay should not be affected by a change of the renormalization point. Summing up, in the truncated model we have tunneling between different vacua if $D<D_c(N)$, where $D_c(N)$ is the critical dimension of λ_N.

The above discussions can be summarized as follows. In a massive scalar superrenormalizable model at finite temperature, there is a temperature β_N^{-1} such that the renormalizable coupling constant $\lambda_N(\beta)$ becomes zero. Above such temperature there is tunneling between different vacua.

Particularly important is the connection between our investigations and instanton solutions in scalar models. It is well known that in $D=4$ the massive $\lambda\varphi^4$ model does not admit real instanton solutions. In the massless case, also, there are no real instanton solutions (with positive action), nevertheless, a complex instanton solution (with negative action) is known.[22] The instanton solution is related to the fact that the renormalized coupling constant λ is negative. It is not difficult to see the connection between the mechanism studied by us and the possible existence of instantons, since in our case the renormalized coupling constant may become negative as the temperature changes. In the simplest case of massive $\lambda\varphi^4$ and $D<4$, instantons could exist in the model for $\beta^{-1}>\beta_4^{-1}$.

As noted a long time ago by Dyson, in QED, for negative coupling constant e^2, the Hamiltonian is unbounded below and the vacuum is a metastable state.[23] In this situation, particles and antiparticles would repel each other, increasing the distance between them and pairs of particle, and antiparticles would be continually created. In the vacuum energy (the sum of all connected diagrams having n vertices and no external legs) appears an imaginary part. As it was noted originally by Bender and Wu studying the quantum anharmonic oscillator, there is a relation between the nth Rayleigh–Schrodinger coefficient and the lifetime of the unstable states of a negatively coupled anharmonic oscillator.[24] The idea was used also in field theory by Parisi and others.[25–27] Asymptotic estimates in perturbation theory can be obtained by computing the imaginary part of the Green's functions for small negative coupling constant. More recently, Fainberg and Yofa also calculated the high order corrections to the instantons contribution to the Green's functions in the regime $\lambda<0$.[28]

The effects we have described in this paper may also be applied to cosmological phase transition problems. The study of phase transition in cosmological models has been widely discussed in the literature. For a complete review see Ref. 29 and other references, therein. It is shown that in the evolution of the universe, metastable vacuum states may appear. The decay of such metastable states is materialized in the Lorentzian space–time as nucleation of a bubble of

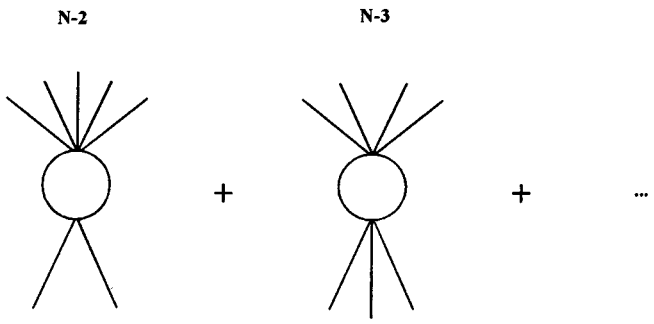

FIG. 9. The graphs that give leading contributions to the renormalized coupling constant $\lambda_N(\beta)$.

true vacuum in the false vacuum phase. Frequently, in the study of the false vacuum decay, it is assumed that the system is ''prepared'' in a metastable state. Such metastable states appear naturally in our formalism by temperature effects that change the sign of renormalized coupling constants. For instance, as we have seen before, in the truncated model ($N=4$) for $4\leqslant D<6$, the coefficient of the φ^3 term becomes negative above the temperature β_3^{-1}. This is a natural realization of the potential studied by Gleiser *et al.*[30] and Vilenkin and Ford.[31] If we assume that the universe expands and supercools, the possibility of the creation of bubbles of true vacuum arises, nevertheless, there are subtleties in this process. Back to Lorentzian time, let us define $\Delta\tau$ as the time necessary to the temperature of the environment to drop down to β_4^{-1}, where the vacuum state becomes stable. On the other hand, if the mean life of the metastable state Δt is larger than $\Delta\tau$ there is no nucleation of the bubbles at all. Only if $\Delta t<\Delta\tau$, there would be a finite probability of nucleation of bubbles.

In the case of ''real'' cosmological evolution, it is necessary to include gravity; nontrivial problems may appear, as for example the possibility of the presence of horizon. For a careful analysis of these situations, see Ref. 32. We cannot disregard the possibility that particle creation associated with the tunneling process will destroy the above scenario. Particle creation that occurs in the process of nucleation of bubbles was analyzed by Rubakov.[33] We still do not know how to introduce these effects in our model. The discussion of tunneling effects, instantons, and how they contribute to high order estimates in perturbation theory will be presented in a forthcoming paper.[34]

V. CONCLUSION

The purpose of this paper has been to discuss the effect of keeping local terms with higher powers of the field in the Lagrange density of a neutral scalar field. We also assume that the system is in thermal equilibrium with a reservoir at temperature β^{-1}. We proved that in the truncated Efimov–Fradkin model, (i) for $D\geqslant D_c(N-1)$ there is no a temperature where at least one of the coupling constants becomes zero; (ii) for $D_c(N-1)>D\geqslant D_c(N)$, there exists a temperature β_{N-1}^{-1}, where only the renormalized coupling constant $\lambda_{N-1}(\beta)$ becomes zero and all the other renormalized coupling constants remain positive; and (iii) for $D<D_c(N)$, the coupling constants $\lambda_{N-1}(\beta)$ and $\lambda_N(\beta)$ become zero at some temperatures β_{N-1}^{-1} and β_N^{-1}, respectively.

It is clear that in the nontruncated case, all the renormalized coupling constants remain positive for $D\geqslant 2$. We would like to point out that some care must be taken in order not to extrapolate the results of this paper to regions outside the domain of validity of the approximation we have done, i.e., beyond the one-loop level. As we discussed in the previous section, a natural extension of the ideas of the paper is to include gravitation, although there is some subtleness related to this approach. The techniques of the paper with the Euclidian path approach can only be implemented

in some special cases (for example, Schwarzschild or de Sitter spacetime), i.e., to continue analytically to Euclidian space the metric must have a section in the complexified spacetime on which the metric is real and positive-definite. In spacetime metrics where this property works, all the calculations can be repeated, of course, with the subtleness of the curved metric.

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The Lax pair by dimensional reduction of Chern–Simons gauge theory

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We show that the Nonlinear Schrödinger Equation and the related Lax pair in $1+1$ dimensions can be derived from $2+1$-dimensional Chern–Simons Topological Gauge Theory. The spectral parameter, a main object for the Loop algebra structure and the Inverse Spectral Transform, has to appear as a homogeneous part (condensate) of the statistical gauge field, connected with the compactified extra space coordinate. In terms of solitons, a natural interpretation for the one-dimensional analog of Chern–Simons Gauss law is given. © *1996 American Institute of Physics.* [S0022-2488(96)02308-0]

I. INTRODUCTION

It has been known for many years that intimate relations between the dimensional reduction procedure and nonlinear models exist. A first example of such relations was suggested by Kaluza and Klein[1] for unification of gravitation and electromagnetism in a five-dimensional theory of gravity. Then, the idea was remarkably developed in the context of dual models and the string theory.[2] It turns out that the Yang–Mills theory in $4+N$ dimensions leads, via dimensional reduction, to a Yang–Mills+Higgs scalars coupled theory with specific couplings.[3] In this context we can suppose that the integrability of some nonlinear models can be related to the dimensional reduction procedure. This guess is indicated by a ''folk theorem'' that dimensional reduction from higher dimensions enlarges the symmetry G to its affine extension.[4,5] Then, some infinite-dimensional symmetries, appearing as the hidden symmetries of integrable models, shall have a geometrical meaning. Thus, by dimensional reduction, many $0+1$- and $1+1$-dimensional integrable models were embedded to the self-dual Yang–Mills (SDYM) equations.[6] By suitable reduction, the Lax pair associated with the corresponding low-dimensional model has appeared from the Lax pair for SDYM.[7] Moreover, one believes even that the self-dual Yang–Mills equations are a universal integrable system from which all the others could be obtained by proper reductions.[6] This program, still being intensively studied, requires that there should be a linear system for equations of the zero-curvature type (the Lax pair). However, the origin of the linear system remains a *terra incognita*. As well as the most mysterious part of the linear problem—the spectral parameter. From the algebraic point of view, the presence of a spectral parameter in the linear problem with Lie algebra $\mathcal{G}$ announces the appearance of an enlarged, loop algebra structure $\mathcal{G}\times C[\lambda,\lambda^{-1}]$, associated with the hidden non-Abelian symmetry of the model. An important point is that the spectral parameter is present in the linear problem and absent in the related evolution equation. Since the last one arises from the zero-curvature condition (ZCC) for the associated flat connections, it suggests a gauge-theoretical formulation of this phenomena. According to this observation we expect the existence of non-Abelian gauge theory, which includes the spectral parameter as a gauge degree of freedom. Hence, the isospectral deformation defined by the nonlinear evolution equation should appear as a gauge invariant condition.

Thus, we search for non-Abelian gauge theory with symmetries not less than the integrable one. Usually, in high-energy physics, the unification procedure means an embedding to a larger

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symmetry group. Apparently most drastic possibilities for unification provide the Topological Field Theory (TFT).[8] As is well known,[9] TFT admits a huge diffeomorphism symmetry, which is realized by gauge transformations. Resulting reparametrization invariance of the model leads to the trivial dynamics, frozen in the reparametrization of gauge (unphysical) parameters. The dimensional reduction idea is very useful in the TFT.[10] Thus, three-dimensional Chern–Simons gauge field theory[11] can be reduced from four-dimensional TFT. By a subsequent reduction to two dimensions the conformal field theory was obtained.[12] A general reduction of CS theory leads to two-dimensional TFT, known as the BF theory.[13,14] Furthermore, two linear gravities—based on the de Sitter group or a central extension of the Poincaré group—were derived from three-dimensional TFT.[15] These results suggest that TFT could be a good candidate for the universal model, properly reducing which conformal invariant and integrable systems can be obtained. The question is how to constrain the model to have an integrable two-dimensional system.

Earlier we showed that for nonlinear σ models some constraint equations naturally arise. The idea, inspired by the gauge relation between one-dimensional integrable models, is to use variables from the tangent space to the nonlinear manifold.[16] By this approach, some evolution σ models like the Heisenberg Model (HM) and the Topological Magnet[17] are reformulated as the $U(1)$ gauge invariant field theory.[18–20] A mapping of the model to the three-dimensional zero-curvature condition (or to the CS theory) implies that the field connection should satisfy the proper constraint. In contrast with time reparametrization invariance of CS theory, the reduced system evolves according to the related σ model. For the integrable evolution,[19] it means a breaking of continual TFT symmetry up to a discrete time hierarchy of integrable models.

In the present paper we show that $2+1$-dimensional HM, considered as a constraint for CS theory, by dimensional reduction provides not only the integrable model, the Nonlinear Schrödinger Equation (NLSE), but also the corresponding Lax pair. The spectral parameter appears automatically in a correct way and has the meaning of the homogeneous (condensate) part for the statistical gauge field, related with the extra space dimension. Moreover, the nonhomogeneous structure of the field is related to the Bäcklund transformations for NLSE. In Sec. II, we present the general formalism of constructing the gauge invariant field theory, associated with the nonlinear σ model. Section III describes the related formulation of the non-Abelian CS theory. In Sec. IV, we illustrate the general approach with two important examples. Dimensional reduction for $2+1$ HM will be considered in Sec. V. In the conclusion we discuss some physical ideas to explain our results. We interpret the one-dimensional analog of CS Gauss law in terms of solitons for integrable models.

II. MOVING FRAME AND ADJOINT REPRESENTATION OF ZCC

In this section we present a general formalism connecting a zero curvature equations on A_1 algebra [$SU(2)$ or any noncompact version of it] in the adjoint representation with the moving trihedral.[21,22] This formalism allows us to formulate a nonlinear σ model as the Abelian gauge field theory.

Let us consider the group A_1 with element g, generated by τ_i $(i=1,2,3)$, satisfying

$$\tau_i \tau_j = h_{ij} + i c_{ijk} \tau_k , \tag{2.1}$$

where h_{ij} and c_{ijk} are the Killing metric and structure constants of A_1. We define an orthonormal trihedral set of unit vectors $\mathbf{n}_i$ and $\mathbf{e}_i$, and matrices N_i and E_i correspondingly, in the adjoint representation,

$$N_i = (\mathbf{n}_i, \tau) = \mathbf{n}_i^k \tau_k = h_{kl} \mathbf{n}_i^k \tau^l = g \tau_i g^{-1}, \tag{2.2a}$$

$$E_i = (\mathbf{e}_i, \tau) = \mathbf{e}_i^k \tau_k = h_{kl} \mathbf{e}^k \tau^l = g^{-1} \tau_i g. \tag{2.2b}$$

Using (2.1), the orthonormality of the trihedral are expressed by the relations

$$N_i N_j = h_{ij} + i c_{ijk} N_k , \tag{2.3a}$$

$$E_i E_j = h_{ij} + i c_{ijk} E_k . \tag{2.3b}$$

The Killing metric h_{ij} and structure constants $c_{ijk} = -c_{jik}$ defines the inner and cross products between three-vectors, transforming in the adjoint representation of A_1:

$$(\mathbf{n}_i \mathbf{n}_j) = h_{ij} , \tag{2.4a}$$

$$\mathbf{n}_i \wedge \mathbf{n}_j = c_{ijk} \mathbf{n}_k \tag{2.4b}$$

(and the similar equations for $\mathbf{e}_i$ vectors). Matrices N_i and E_i are connected by the similarity transformation,

$$N_i = g^2 E_i g^{-2}, \tag{2.5}$$

while related $\mathbf{n}_i$ and $\mathbf{e}_i$ vectors satisfy

$$(\mathbf{n}_i)^j h_{jj} = (\mathbf{e}_j)^i h_{ii} \tag{2.6}$$

(no summation). Due to this relation, in the present paper we restrict ourselves only with $\mathbf{n}_i$ vectors.

Let $\mathbf{n}_i = \mathbf{n}_i(x)$ are smooth vector fields that define at each space coordinate $\mathbf{x} = (x^1, x^2, x^3)$ of M the three vectors $(\mathbf{n}_1(x), \mathbf{n}_2(x), \mathbf{n}_3(x))$, forming an orthonormal basis called the moving frame.

We can introduce the left- and right-invariant chiral currents,

$$J^R_\mu = g^{-1} \partial_\mu g, \tag{2.7a}$$

$$J^L_\mu = \partial_\mu g \; g^{-1} \tag{2.7b}$$

($\mu = 1,2,3$). They are connected by simple transformation,

$$J^R_\mu = g^{-1} J^L_\mu g. \tag{2.8}$$

The trihedral moves according to the equations,

$$\partial_\mu N_i = [J^L_\mu, N_i] = g[J^R_\mu, \tau_i] g^{-1}, \tag{2.9a}$$

$$\partial_\mu E_i = g^{-1}[\tau_i, J^L_\mu] g = [E_i, J^R_\mu], \tag{2.9b}$$

or in the three-dimensional representation,

$$\partial_\mu N_i = (J^R_\mu)^{(ad)}_{ik} N_k , \tag{2.10a}$$

$$\partial_\mu E_i = -(J^L_\mu)^{(ad)}_{ik} E_k , \tag{2.10b}$$

where $(J^R_\mu)_{ik}$ and $(J^L_\mu)_{ik}$ are matrices in the adjoint representation,

$$(J^{R,L}_\mu)^{(ad)}_{ik} = -i c_{ijk} (J^{R,L}_\mu)_j = i (J^{R,L}_\mu)_j c_{jik} , \tag{2.11}$$

and $J^{R,L}_\mu = \Sigma (J^{R,L}_\mu)_j \frac{1}{2} \tau_j$. Related rotation of the moving frame is given by the equations

$$\partial_\mu \mathbf{n}_i = (J^R_\mu)^{(ad)}_{ik}\mathbf{n}_k, \quad \partial_\mu \mathbf{e}_i = -(J^L_\mu)^{(ad)}_{ik}\mathbf{e}_k.$$

Matrices $J^{R,L}_\mu$ have the symmetry property

$$(J^{R,L}_\mu)^{(ad)}_{ij} h_{jj} = -(J^{R,L}_\mu)^{(ad)}_{ji} h_{ii}.$$

For $SU(2)$ case $h_{ij}=\delta_{ij}$, $c_{ijk}=\epsilon_{ijk}$ and the matrices (2.11) are antisymmetric.

The zero-curvature conditions for chiral currents (2.7) have the form

$$\partial_\mu J^R_\nu - \partial_\nu J^R_\mu + [J^R_\mu, J^R_\nu] = 0, \tag{2.12a}$$

$$\partial_\mu J^L_\nu - \partial_\nu J^L_\mu - [J^L_\mu, J^L_\nu] = 0. \tag{2.12b}$$

In the following discussion we are concerned mainly on the J^R_μ matrix and skip the R index.

Let us decompose the matrix J_μ to the diagonal and off-diagonal parts,

$$J_\mu = J^{(0)}_\mu + J^{(1)}_\mu,$$

parametrized in the form

$$J^{(0)}_\mu = \frac{i}{4}\sigma_3 V_\mu, \tag{2.13a}$$

$$J^{(1)}_\mu = \begin{pmatrix} 0 & -\kappa^2\overline{q_\mu} \\ q_\mu & 0 \end{pmatrix}, \tag{2.13b}$$

where $\kappa^2=+1$ for $SU(2)$ and $\kappa^2=-1$ for $SU(1,1)$ case. Then,

$$c_{ijk} = \kappa^2 \epsilon_{ijk} h_{kk},$$

and in the adjoint representation we have

$$(J_\mu)^{(ad)} = \frac{1}{2}\begin{pmatrix} 0 & V_\mu & 4\kappa^2\,\mathrm{Re}(q_\mu) \\ -V_\mu & 0 & 4\kappa^2\,\mathrm{Im}(q_\mu) \\ -4\,\mathrm{Re}(q_\mu) & -4\,\mathrm{Im}(q_\mu) & 0 \end{pmatrix}. \tag{2.14}$$

The moving frame rotates with x variation according to equations

$$\partial_\mu \mathbf{n}_1 = -\tfrac{1}{2}V_\mu \mathbf{n}_2 - 2\kappa^2(\mathrm{Re}\ q_\mu)\mathbf{n}_3, \tag{2.15a}$$

$$\partial_\mu \mathbf{n}_2 = \tfrac{1}{2}V_\mu \mathbf{n}_1 - 2\kappa^2(\mathrm{Im}\ q_\mu)\mathbf{n}_3, \tag{2.15b}$$

$$\partial_\mu \mathbf{n}_3 = 2(\mathrm{Re}\ q_\mu)\mathbf{n}_1 + 2(\mathrm{Im}\ q_\mu)\mathbf{n}_2. \tag{2.15c}$$

If we denote $U_\mu \equiv (\mathrm{Re}(q_\mu), \mathrm{Im}(q_\mu))$, the system can be written in a more compact form,

$$\partial_\mu \mathbf{n}_i = -\tfrac{1}{2}V_\mu \epsilon_{ij}\mathbf{n}_j - 2\kappa^2 U_{i\mu}\mathbf{s}, \tag{2.16a}$$

$$\partial_\mu \mathbf{s} = 2U_{i\mu}\mathbf{n}_i. \tag{2.16b}$$

The vector $\mathbf{s}\equiv\mathbf{n}_3$ satisfies the constraint

$$(\mathbf{s}(x), \mathbf{s}(x)) = h_{33}, \tag{2.17}$$

where $h_{33}=1$ for $SU(2)$ and $SU(1,1)$ [and $h_{33}=-1$ for $SL(2,R)$]. It belongs to the two-dimensional sphere S^2 or pseudosphere $S^{1,1}$ correspondingly.

Fields V_μ and q_μ are given by projections,

$$V_\mu=-2\kappa^2(\mathbf{n}_2,\partial_\mu\mathbf{n}_1),\quad \mathrm{Re}(q_\mu)=-\frac{\kappa^2}{2}(\mathbf{s},\partial_\mu\mathbf{n}_1),\quad \mathrm{Im}(q_\mu)=-\frac{\kappa^2}{2}(\mathbf{s},\partial_\mu\mathbf{n}_2). \tag{2.18}$$

Two vector fields $(\mathbf{n}_1(x),\mathbf{n}_2(x))$ at each $\mathbf{x}$ form a basis in the tangent space to the corresponding manifold for $\mathbf{s}(x)$. But vectors $\mathbf{n}_1$ and $\mathbf{n}_2$ are not uniquely determined by Eq. (2.4).[16]

If we choose other $\mathbf{n}_1',\mathbf{n}_2'$ as a rotated basis,

$$\mathbf{n}_1'=\cos\alpha\mathbf{n}_1-\sin\alpha\mathbf{n}_2,\quad \mathbf{n}_2'=\cos\alpha\mathbf{n}_2+\sin\alpha\mathbf{n}_1, \tag{2.18}$$

related V_μ' and q_μ' defined by (2.18) are the $U(1)$ gauge transformed fields,

$$V_\mu'=V_\mu+2\partial_\mu\alpha,\quad q_\mu'=e^{i\alpha}q_\mu. \tag{2.19}$$

The expression for the q_μ field is simplified if we introduce a complex basis,

$$\mathbf{n}_+=\mathbf{n}_1+i\mathbf{n}_2,\quad \mathbf{n}_-=\mathbf{n}_1-i\mathbf{n}_2, \tag{2.20}$$

satisfying the following relations:

$$(\mathbf{n}_+,\mathbf{n}_+)=0=(\mathbf{n}_-,\mathbf{n}_-), \tag{2.20a}$$

$$(\mathbf{n}_+,\mathbf{n}_-)=2\kappa^2, \tag{2.20b}$$

$$\mathbf{n}_+\times\mathbf{s}=i\mathbf{n}_+,\quad \mathbf{n}_-\times\mathbf{s}=-i\mathbf{n}_-,\quad \mathbf{n}_-\times\mathbf{n}_+=2i\kappa^2\mathbf{s}. \tag{2.20c}$$

Then

$$q_\mu=\frac{\kappa^2}{2}(\partial_\mu\mathbf{s},\mathbf{n}_+),\quad \overline{q_\mu}=\frac{\kappa^2}{2}(\partial_\mu\mathbf{s},\mathbf{n}_-). \tag{2.21}$$

In terms of (2.20), the moving frame equations (2.16) become

$$D_\mu\mathbf{n}_+=-2\kappa^2q_\mu\mathbf{s}, \tag{2.22a}$$

$$\partial_\mu\mathbf{s}=q_\mu\mathbf{n}_-+\overline{q_\mu}\mathbf{n}_+, \tag{2.22b}$$

where $D_\mu\equiv\partial_\mu-i/2V_\mu$ is the covariant derivative.

This form is explicitly invariant under the local $U(1)$ gauge transformations,

$$\mathbf{s}\to\mathbf{s},\quad \mathbf{n}_+\to e^{i\alpha}\mathbf{n}_+,\quad \mathbf{n}_-\to e^{-i\alpha}\mathbf{n}_-, \tag{2.23}$$

which are just the local rotations in the tangent to the vector $\mathbf{s}$ plane.

As follows from Eqs. (2.22), fields V_μ and q_μ are subject to the system

$$D_\mu q_\nu=D_\mu q_\mu, \tag{2.24a}$$

$$[D_\mu,D_\nu]=-2\kappa^2(\overline{q_\mu}q_\nu-\overline{q_\nu}q_\mu). \tag{2.24b}$$

To describe a time evolution of the three-dimensional physical system, we need to introduce the space-time $M_3=T\times M_2$ decomposition, where T is associated with the time variable $x_3=t$ and M_2 is a two-dimensional space manifold. In this case a time evolution of the moving frame,

$$D_0\mathbf{n}_+ = -2\kappa^2 q_0 \mathbf{s}, \tag{2.25a}$$

$$\partial_0 \mathbf{s} = q_0 \mathbf{n}_- + \overline{q_0}\mathbf{n}_+ , \tag{2.25b}$$

is completely arbitrary due to the arbitrariness of q_0. We recall that q_0 as well as V_0 are Lagrange multipliers of the CS TFT appearing in front of the CS Gauss law of the theory [see Eq. (3.12)]. Moreover, Eq. (2.25b) shows that evolution of the spin vector $\mathbf{s}$ associated with CS TFT, $U(1)$ being gauge invariant, remains completely arbitrary. In this sense the TFT are related to the nonlinear σ model with an arbitrary evolution (reparametrization invariance) or, what is the same, without any evolution, modulo $U(1)$ gauge transformations.

Formally, we can represent Eq. (2.25b) as the spin precession equation,

$$\partial_0 \mathbf{s} = \mathbf{s} \times \mathbf{H}, \tag{2.26}$$

in an arbitrary $U(1)$ gauge invariant magnetic field,

$$\mathbf{H} = i(\overline{q_0}\mathbf{n}_+ - q_0 \mathbf{n}_-). \tag{2.27}$$

Nevertheless, to the above results a topological restriction on the possible spin configurations exists. Indeed, we can imagine that the space M_2 is compact. For example, if we suppose that the value of the spin vector $\mathbf{s} \in S^2$ [$SU(2)$ case] at infinity is fixed $\mathbf{s} \to (0,0,1)$. Then, all smooth configurations describing the mapping of (x_1, x_2) into $\mathbf{s}(x)$, independently of the evolution, are classified by the integer-valued degree of mapping of $S^2 \to S^2$, or the topological charge:

$$Q = \frac{1}{8\pi} \int \epsilon_{ij} \mathbf{s}(\partial_i \mathbf{s} \times \partial_j \mathbf{s}) d^2x = \frac{1}{8\pi} \int \epsilon_{ij}\, \partial_i V_j\, d^2x. \tag{2.28}$$

In terms of our gauge fields, the topological charge density has the form

$$\epsilon_{ij} \mathbf{s}(\partial_i \mathbf{s} \times \partial_j \mathbf{s}) = \epsilon_{ij} \partial_i V_j = B, \tag{2.29}$$

of the radial (along the $\mathbf{s}$) oriented magnetic field $\mathbf{B}$ associated with the vector potential V_j. As well known, Eq. (2.28) states that the winding number of mapping $S^2 \to S^2$ coincides with the winding number of the mapping of the circle S^1 at $x_1^2 + x_2^2 \to \infty$ into the Abelian gauge group manifold. It means that all $U(1)$ gauge transformations (2.19) also fall into topologicoal classes characterized by winding number (2.28). Just substituting (2.19) in to (2.28) we find that under Abelian gauge transformations

$$V_j \to V_j + 2\partial_j \alpha, \tag{2.30}$$

Q transforms as

$$Q \to Q + \frac{1}{4\pi} \int \epsilon_{ij} \partial_i \partial_j \alpha d^2x. \tag{2.31}$$

For a smooth gauge transformation the second term vanishes and Q is invariant.

More generally, if M_2 is a compact Riemann surface of genus g, $M_2 = \Sigma_g$, the charge Q in (2.28) is the first Chern class c_1, which is an integer.[23]

However, if M_2 admits some singular points, Q could be an arbitrary number. Let us consider a potential V_j with charge Q. We perform a singlar at $\mathbf{x}=0$ rotation (2.31) of $(\mathbf{n}_1, \mathbf{n}_2)$ with angle

$$\alpha(\mathbf{x}) = N\theta(\mathbf{x}), \tag{2.32}$$

where $\theta(\mathbf{x}) = \arctan(x_2/x_1)$. Then, using unconventional representation for the planar δ-function[24]

$$\epsilon_{ij}\partial_i\partial_j\theta=(\partial_1\partial_2-\partial_2\partial_1)\theta=2\pi\delta^2(x), \tag{2.33}$$

we find that $\Delta Q = N/2$.

As evident, instead of integer N we can use an arbitrary real number which gives us arbitrary Q. This singular gauge transformation is related with a point vortex creation at $\mathbf{x}=0$ and is described by the anyon potential

$$V_i^A=2\frac{\partial}{\partial x_i}\alpha(\mathbf{x})=2N\frac{\partial}{\partial x_i}\theta(\mathbf{x})=-2N\epsilon_{ij}\partial_j\ \ln|\mathbf{x}|=-2N\epsilon_{ij}\frac{x_j}{|\mathbf{x}|}. \tag{2.34}$$

In a more general situation, for n point vortices located at $\mathbf{x}_1, \ldots, \mathbf{x}_n$, with related strength $N_p(p = 1, \ldots, n)$, the vector potential

$$V_i^A(\mathbf{x};\mathbf{x}_1, \ldots, \mathbf{x}_n)=-2\epsilon_{ij}\sum_{p=1}^{n} N_p\frac{(x^j-x_p^j)}{|\mathbf{x}-\mathbf{x}_p|^2}=-2\epsilon_{ij}\partial_j\sum_{p=1}^{n} N_p\ \ln|\mathbf{x}-\mathbf{x}_p|, \tag{2.35}$$

produces the magnetic field vanishing almost everywhere,

$$B(\mathbf{x})=\epsilon_{ij}\ \partial_i V_j=4\pi\sum_{p=1}^{n} N_p\delta^2(x-x_p). \tag{2.36}$$

The corresponding charge changes as

$$\Delta Q=\frac{1}{2}\sum_{p=1}^{n} N_p. \tag{2.37}$$

III. CHERN–SIMONS GAUGE THEORY REDUCTION

In the previous section we introduced the chiral fields J_μ (2.7) satisfying the zero curvature condition (2.12). The last one, in term of components (2.13), is described by the system (2.24). For fields V_μ and q_μ, subject to (2.24), the moving frame can be reconstructed from Eq. (2.16). Moreover, the current J_μ can be considered as a non-Abelian pure gauge potential. Then, the zero-curvature equations (2.12) are of the Lagrangian form for the pure non-Abelian Chern–Simons functional.

The Chern–Simons action is defined as follows:

$$S[J]=\frac{k}{4\pi}\int_M \mathrm{Tr}\left(J\wedge dJ+\frac{2}{3}J\wedge J\wedge J\right), \tag{3.1}$$

where M is an oriented three-dimensional manifold, J is a gauge connection with values in the Lie algebra $\mathcal{G}$. Action (3.1) is manifestly independent from the space metric, so it was interpreted by Witten as a general covariant theory or topological field theory.[8]

The classical equations of motion following from action (3.1) have the form

$$F=dJ+J\wedge J=0, \tag{3.2}$$

of the zero-curvature condition.

To adopt the canonical approach to the problem, one considers a region of the three-manifold to be isomorphic to $M_3=T\times M_2$, where we interpret T as the time. Then, for the gauge field we have $J_\mu=(J_0,J_j)$, where J_0 is the time component and the action (3.1) takes the form

$$S(J)=-\frac{k}{4\pi}\int_{\Sigma}\int dt\ \epsilon^{ij}\ \mathrm{Tr}\left(J_i\frac{\partial}{\partial t}J_j-J_0F_{ij}\right), \tag{3.3a}$$

where

$$F_{ij}=\partial_iJ_j-\partial_jJ_i+[J_i,J_j]. \tag{3.3b}$$

In the basis

$$T_a=\tfrac{1}{2}\tau_a \quad (a=1,2,3), \tag{3.4a}$$

$$[T_a,T_b]=ic_{abc}T_c, \tag{3.4b}$$

with

$$\mathrm{Tr}(T_aT_b)=\tfrac{1}{2}h_{ab} \tag{3.4c}$$

[see Eq. (2.1)], we have the Poisson brackets for components $J_\mu=\Sigma_{a=1}^{3}(J_\mu)_aT_a$:

$$\{J_i^a(x),J_j^b(y)\}=\frac{4\pi}{k}\epsilon_{ij}h^{ab}\delta^2(x-y). \tag{3.5}$$

Then, in terms of V_μ and q_μ fields,

$$\{V_i(x),V_j(y)\}=-\frac{16\pi}{k}\epsilon_{ij}h_{33}\delta^2(x-y), \tag{3.6}$$

$$\{\mathrm{Re}(q_i(x)),\mathrm{Re}(q_j(y))\}=-\frac{\pi}{k}\epsilon_{ij}h_{11}\delta^2(x-y), \tag{3.7a}$$

$$\{\mathrm{Im}(q_i(x)),\mathrm{Im}(q_j(y))\}=-\frac{\pi}{k}\epsilon_{ij}h_{22}\delta^2(x-y). \tag{3.7b}$$

The last two relations have a more appropriate form if we introduce new fields (this idea was inspired by the gauge relation between 1+1-dimensional NLSE and HM),

$$\psi_\pm=\frac{1}{2\sqrt{\pi}}(q_1\pm iq_2). \tag{3.8}$$

They are directly related with the complex structure on the manifold M_2 in terms of

$$z=x_1+ix_2, \quad \overline{z}=x_1-ix_2. \tag{3.9}$$

The Poisson brackets for the $\psi_\pm$ fields are

$$\{\psi_+(x),\overline{\psi_+}(y)\}=\frac{i}{2k}(h_{11}+h_{22})\delta^2(x-y), \tag{3.10a}$$

$$\{\psi_-(x),\overline{\psi_-}(y)\}=-\frac{i}{2k}(h_{11}+h_{22})\delta^2(x-y). \tag{3.10b}$$

As evident, new fields defined by (3.8) are convenient only for $SU(2)$ and $SU(1,1)$ cases. For $SL(2,R)$ case brackets (3.10) are vanishing and more convenient to use other variables. We can rewrite the brackets in a compact form,

$$\{V_i(x),V_j(y)\}=-\frac{16\pi}{k}\,\epsilon_{ij}\delta^2(x-y), \tag{3.11a}$$

$$\{\psi_+(x),\overline{\psi_+}(y)\}=\frac{i}{k}\,\kappa^2\delta^2(x-y), \tag{3.11b}$$

$$\{\psi_-(x),\overline{\psi_-}(y)\}=-\frac{i}{k}\,\kappa^2\delta^2(x-y), \tag{3.11c}$$

where $\kappa^2=+1$ for $SU(2)$ and $\kappa^2=-1$ for $SU(1,1)$.

The brackets (3.11) allow us to interpret V_μ as an Abelian CS field (the statistical field) and ψ_+,ψ_- as charged matter fields.[18–20]

The action in terms of these fields on the plane has the form

$$\begin{aligned}S=\int dt\int d^2x\Big\{&-\frac{k}{32\pi}\,\epsilon^{\mu\nu\lambda}V_\mu\,\partial_\nu V_\lambda\\&+\frac{ik}{2}\,[(\psi_+\,\overline{D_0\psi_+}-\overline{\psi_+}\,D_0\psi_+)-(\psi_-\,\overline{D_0\psi_-}-\overline{\psi_-}\,D_0\psi_-)]\\&-\frac{k}{2\pi}\,iq_0(\overline{D_-}\,\overline{\psi_+}-\overline{D_+}\,\overline{\psi_-})+\frac{k}{2\pi}\,i\overline{q_0}(D_-\psi_+-D_+\psi_-)\Big\},\end{aligned} \tag{3.12}$$

where $D_\pm=D_1\pm iD_2=\partial_\pm-i/2V_\pm$, $V_\pm=V_1\pm iV_2$. From (3.3) we recognize that the time components V_0 and q_0 of the gauge potential J_0 are the Lagrange multipliers, arbitrariness of which guarantees the gauge invariance (covariance) of the topological action.

Related constraints (3.3a) in components $F=\Sigma_{a=1}^3F_aT_a$ generate $su(2)$ or $su(1,1)$ algebra,

$$\{G_a(\mathbf{x}),G_b(\mathbf{y})\}=c_{abc}G_c(\mathbf{x})\,\delta^2(x-y), \tag{3.13}$$

where rescaled constraints $G^a=-(ik/8\pi)F^a$ have the form

$$G_+=G_1+iG_2=-\frac{k}{2\pi}\,(D_-\psi_+-D_+\psi_-), \tag{3.14a}$$

$$G_-=G_1-iG_2=-\frac{k}{2\pi}\,(\overline{D_-}\,\overline{\psi_+}-\overline{D_+}\,\overline{\psi_-}), \tag{3.14b}$$

$$G_3=\frac{k}{8\pi}\,[(\partial_1V_2-\partial_2V_1)+8\pi(|\psi_+|^2-|\psi_-|^2)]. \tag{3.14c}$$

The physical subspace of the TFT is defined by the constraint surface

$$G_\pm=0,\quad G_0=0,$$

and any breaking of the topological symmetry relates with a deviation from this surface. Constraints (3.14) form a part of the Euler–Lagrange equations for the action (3.12):

$$D_0\psi_\pm=\frac{1}{2\sqrt{\pi}}D_\pm q_0, \tag{3.15a}$$

$$[D_+,D_-]=8\pi\kappa^2(|\psi_+|^2-|\psi_-|^2), \tag{3.15b}$$

$$[D_0,D_\pm]=-4\sqrt{\pi}\kappa^2(\overline{q_0}\psi_\pm-\overline{\psi_\pm}q_0), \tag{3.15c}$$

$$D_+\psi_-=D_-\psi_+. \tag{3.15d}$$

A solution of these equations defines the moving frame according to

$$D_0\mathbf{n}_+=-2q_0\mathbf{s}, \tag{3.16a}$$

$$\partial_0\mathbf{s}=q_0\mathbf{n}_-+\overline{q_0}\mathbf{n}_+, \tag{3.16b}$$

$$D_\pm\mathbf{n}_+=-4\sqrt{\pi}\psi_\pm\mathbf{s}, \tag{3.16c}$$

$$\partial_\pm\mathbf{s}=2\sqrt{\pi}(\psi_\pm\mathbf{n}_-+\overline{\psi_\mp}\mathbf{n}_+), \tag{3.16d}$$

where fields $V_0,V_\pm$, and $q_0,\psi_\pm$ are given by relations

$$V_0=-i(\partial_0\mathbf{n}_+,\mathbf{n}_-),\quad V_\pm=-i(\partial_\pm\mathbf{n}_+,\mathbf{n}_-), \tag{3.17a}$$

$$q_0=\frac{1}{2}(\partial_0\mathbf{s},\mathbf{n}_+),\quad \psi_\pm=\frac{1}{4\sqrt{\pi}}(\partial_\pm\mathbf{s},\mathbf{n}_+). \tag{3.17b}$$

We note that the system (3.15), as well as (3.16), is invariant under conformal transformations,

$$z'=f(z),\quad \overline{z'}=\overline{f(z)},\quad V_-=f'V'_-,\quad V_+=\overline{f'}V'_+,\quad \psi_-=f'\psi'_-,\quad \psi_+=\overline{f'}\psi'_+.$$

At the end of this section we reproduce some useful formulas,

$$(\partial_\pm\mathbf{s},\partial_\pm\mathbf{s})=16\pi\psi_\pm\overline{\psi_\mp}, \tag{3.18}$$

$$(\partial_+\mathbf{s},\partial_-\mathbf{s})=8\pi(|\psi_+|^2+|\psi_-|^2), \tag{3.19}$$

$$\partial_+\mathbf{s}\times\partial_-\mathbf{s}=8i\pi(|\psi_+|^2-|\psi_-|^2). \tag{3.20}$$

IV. NONLINEAR σ-MODEL EXAMPLES

In this section we describe some simple two-dimensional models in the formalism of Sec. II. The first model is conformal invariant, while the second one is just integrable. In both cases time evolution is defined by the Lagrange multipliers q_0,V_0 and has an arbitrary character. Imposing equations of motion for the model as constraints on the field variables, we restrict the phase space of CS TFT.

A. 2+0-dimensional σ model

As a first simple example we consider the Euclidean nonlinear σ model for the classical spin vector $\mathbf{s}$,

$$\partial_+\,\partial_-\mathbf{s}+(\partial_+\mathbf{s},\partial_-\mathbf{s})\mathbf{s}=0. \tag{4.1}$$

The model is conformal invariant. This fact guarantees that the conformal invariance of the CS TFT (3.12), supplied with Eq. (4.1), will be preserved.

Due to Eqs. (3.16c), (3.16d), (3.19), and the relation

$$\partial_+ \partial_- \mathbf{s} = 2\sqrt{\pi}[(D_-\psi_+)\mathbf{n}_- + (\overline{D_-}\,\overline{\psi_+})\mathbf{n}_+) - 8\pi(|\psi_+|^2 + |\psi_-|^2)\mathbf{s}, \tag{4.2}$$

the moving frame (3.16) and the field equations (3.15), consistent with Eq. (4.1), should be supplied with additional constraints

$$D_-\psi_+ = D_+\psi_- = 0. \tag{4.3}$$

The resulting system (3.15) decouples on the evolutionary part,

$$D_0\psi_\pm = \frac{1}{2\sqrt{\pi}} D_\pm q_0, \tag{4.4a}$$

$$[D_0, D_\pm] = -4\sqrt{\pi}\kappa^2(\overline{q_0}\psi_\pm - \overline{\psi_\pm} q_0), \tag{4.4b}$$

which contains arbitrary Lagrange multipliers q_0, V_0 and the spatial part

$$D_-\psi_+ = D_+\psi_- = 0, \tag{4.5a}$$

$$[D_+, D_-] = 8\pi\kappa^2(|\psi_+|^2 - |\psi_-|^2). \tag{4.5b}$$

The last system (4.5) is completely equivalent to the σ model (4.1) and has remarkable properties.[18] Most interesting for TFT may be that Eqs. (4.5), known as the Hitchin equations, can be formulated on an arbitrary Riemann surface.

The system (4.5) [in contrast to Eqs. (4.4)] is also invariant under simple transformation,

$$\psi_+ \to e^{i\gamma}\psi_+, \quad \psi_- \to e^{-i\gamma}\psi_-, \quad V_\pm \to V_\pm, \tag{4.6}$$

where γ=const. This transformation for the σ model is known as the Pohlmeyer's $R^{(\gamma)}$ transformation.[25] It relates to a ''hidden'' symmetry of the model and generates an infinite set of nonlocal conservation laws.[16] It seems not obvious as this symmetry acts in the CS TFT (3.12).

If we attempt to describe the symmetry transformation (4.6) as the global $U(1)$ gauge transformation (2.19), (2.23), we immediately obtain that one of the fields ψ_+, ψ_- should vanish. As a result, the system (4.5) reduces to the self-(anti-)dual Chern–Simons equations:[24]

$$D_\pm\psi_\mp = 0, \tag{4.7a}$$

$$[D_+, D_-] = \pm 8\pi\kappa^2|\psi_\mp|^2, \tag{4.7b}$$

related with the Liouville equation. The instantons (topological solitons) of the model (4.1) correspond to the Chern–Simons solitons of the model (4.7),[18] while the topological charge (2.28) becomes of the electric charge form

$$Q_\pm = \pm\int |\psi_\pm|^2 \, d^2x.$$

Solutions other than solitons, when both ψ_+ and $\psi_- \neq 0$, are described by the conformal Sinh-Gordon equation[26] (Toda hierarchy) reduced from (4.5).[18] It is worth noting that both of the systems (4.5) and (4.7) is conformal and R invariant. However, only the self-dual system (4.7)

admits the Pohlmeyer's symmetry (4.6), as a gauge symmetry. This fact intimately relates with the Darboux and C integrability of the Liouville equation[27,28] and with special properties of the CS action, admitting diffeomorphism invariance as the gauge invariance.

B. (1+1)-Heisenberg model

If in the previous case we considered the conformal invariant integrable model, now we like to break the conformal invariance, but preserve integrability. This is the well-known classical continuous isotropic Heisenberg model, describing precession of the spin **s** according to the Landau–Lifshitz equation,

$$\partial_0 \mathbf{s} = \mathbf{s} \times \partial_j \, \partial^j \mathbf{s}, \tag{4.8}$$

where **s** belongs to the two-dimensional sphere S^2 (or pseudosphere $S^{1,1}$).[31]

In this section we examine only the 1+1-dimensional case (the 2+1 -dimensional model is considered in Sec. V). We will treat here both coordinates as the space coordinates. Then the model

$$\partial_1 \mathbf{s} = \mathbf{s} \times \partial_2^2 \mathbf{s}, \tag{4.9}$$

is some kind of two-dimensional σ model.

Substituting

$$\partial_1 \mathbf{s} = q_1 \mathbf{n}_- + \overline{q_1} \mathbf{n}_+ , \tag{4.10a}$$

$$\partial_2^2 \mathbf{s} = D_2 \mathbf{n}_- + \overline{D_2} \mathbf{n}_+ - 4|q_2|^2 \mathbf{s}, \tag{4.10b}$$

to Eq. (4.9), we find the constraint between components,

$$q_1 = i \, D_2 q_2 , \tag{4.11}$$

where the covariant derivative $D_2 = \partial_2 - (i/2)V_2$. Equation (4.11) allows us to exclude the q_1 field from equations.

The moving frame equations (2.22) now read as

$$D_1 \mathbf{n}_+ = -2i\kappa^2 \, D_2 q_2 \, \mathbf{s}, \tag{4.12a}$$

$$D_2 \mathbf{n}_+ = -2\kappa^2 q_2 \mathbf{s}, \tag{4.12b}$$

$$\partial_1 \mathbf{s} = i \, D_2 q_2 \mathbf{n}_- - i \, \overline{D_2} \overline{q_2} \mathbf{n}_+ , \tag{4.12c}$$

$$\partial_2 \mathbf{s} = q_2 \mathbf{n}_- + \overline{q_2} \mathbf{n}_+ , \tag{4.12d}$$

while the field equations are

$$i \, D_1 q_2 + D_2^2 q_2 = 0, \tag{4.13a}$$

$$\partial_1 V_2 - \partial_2 V_1 = -4\kappa^2 \partial_2 |q_2|^2 . \tag{4.13b}$$

In terms of redefined fields,

$$A_1 = V_1 + 4\kappa^2 |q_2|^2, \quad A_2 = V_2 , \tag{4.14}$$

(4.13) becomes the $U(1)$ gauged Nonlinear Schrödinger Equation,

$$i\left(\partial_1-\frac{i}{2}A_1\right)q_2+\left(\partial_2-\frac{i}{2}A_2\right)^2 q_2-2\kappa^2|q_2|^2q_2=0, \tag{4.15a}$$

$$\partial_1 A_2-\partial_2 A_1=0. \tag{4.15b}$$

The second equation allows one to exclude the potentials A_1 and A_2 by the $U(1)$ gauge transformation. If $A_j=2\partial_j\lambda$, we define a new, gauge invariant $\Phi=qe^{i\lambda}$ subject to the Nonlinear Schrödinger equation,

$$i\ \partial_1\Phi+\partial_2^2\Phi-2\kappa^2|\Phi|^2\Phi=0. \tag{4.16}$$

As is well known, this equation is integrable and admits an infinite number of conservation laws, interpreted as continuity equations in our case.

The topological charge (2.28) appears now as

$$Q=-\kappa^2\frac{2}{\pi}\int d^2x\ \partial_2|\Phi|^2=-\kappa^2\frac{2}{\pi}\int dx_1(|\Phi(x_1,x_2=L_+)|^2-|\Phi(x_1,x_2=L_-)|^2),$$

where $L_\pm$ are the boundary values in the second space direction. The usual evolution form for NLSE, when $x_1=t$, $x_2=x$, gives the meaning of

$$Q=\frac{1}{4\pi}\int \mathbf{s}\ \partial_t\mathbf{s}\times\partial_x\mathbf{s}\ dt\ dx=-\kappa^2\frac{2}{\pi}\int_{x=C}dt|\Phi(x,t)|^2,$$

as a one dimensional Wess–Zumino term. It turns out that well-known soliton solutions on an infinite space line (the plane for M_2) and periodic solutions on the finite interval (the cylinder for M_2) always have vanishing Q. A nonvanishing contribution should appear for the compact on (x,t) boundary conditions (the Riemann surface for M_2).

It is worth noting that integrability of models (4.9) and (4.16) is connected with the Lax pair representation or ZCC with an arbitrary spectral parameter. The loop algebra structure provides nonlocal conserved quantities, generating non-Abelian algebra for the NLSE.[29] They arise as a hidden non-Abelian structure of the model (4.16). We understand now the geometrical meaning of this structure, since the model phase space can be considered as the tangent plane to the two-dimensional manifold, being a sphere for $\kappa^2=1$ and a pseudosphere for $\kappa^2=-1$.[31] Moreover, in the next section we show that the spectral parameter has an origin from the extra space direction.

V. DIMENSIONAL REDUCTION OF 2+1 HM

From the action (3.3) or (3.12) we conclude that evolution of the model is completely defined by Lagrange multipliers. Usually to fix gauge freedom one uses the Hamiltonian gauge, when

$$q_0=0,\quad V_0=0.$$

Thus, all considered field configurations are static. In this case reparametrization invariance of the theory corresponds to an arbitrary time dependence for parameters of the moduli space. But if we like to study an integrable deformation of the topological symmetry we need to consider less restricted gauge conditions, providing integrable dynamics.

In the present section we choose a different gauge condition. Since evolution equation for σ models in tangent space reduces to constraints on the phase space variables, we can choose this constraint as a new gauge condition. Then, in this gauge the resulting CS theory should have the corresponding time evolution.[18–20]

We consider the HM (4.8) in 2+1 dimensions,

$$\partial_0 \mathbf{s} = \mathbf{s} \times (\partial_1^2 + \partial_2^2)\mathbf{s}, \tag{5.1}$$

with $(\mathbf{s}, \mathbf{s}) = 1$.

From the moving frame equations (2.22), we conclude that Eq. (5.1) leads to the constraint on q_0:

$$q_0 = i\, D_1 q_1 + i\, D_2 q_2 . \tag{5.2}$$

This relation allows one to exclude q_0 from the system (2.22), and we have

$$D_0 \mathbf{n}_+ = -2i\kappa^2 (D_k q_k)\mathbf{s}, \tag{5.3a}$$

$$D_k \mathbf{n}_+ = -2\kappa^2 q_k \mathbf{s}, \tag{5.3b}$$

$$\partial_0 \mathbf{s} = i(D_k q_k)\mathbf{n}_- - i(\overline{D_k q_k})\mathbf{n}_+ , \tag{5.3c}$$

$$\partial_k \mathbf{s} = q_k \mathbf{n}_- + \overline{q_k}\mathbf{n}_+ \quad (k = 1,2). \tag{5.3d}$$

Remaining field variables should satisfy the system

$$iD_0 q_k + D_k D_l q_l = 0, \tag{5.4a}$$

$$D_k q_l = D_l q_k \quad (k,l = 1,2), \tag{5.4b}$$

$$[D_k, D_l] = -2\kappa^2 (\overline{q_k} q_l - q_k \overline{q_l}), \tag{5.4c}$$

$$[D_0, D_k] = 2i\kappa^2 (q_k\, \overline{D_l q_l} + \overline{q_k}\, D_l q_l). \tag{5.4d}$$

In terms of complex fields (3.8),

$$\psi_\pm = \frac{1}{2\sqrt{\pi}} (q_1 \pm i q_2), \tag{5.5}$$

we have for the moving frame

$$D_0 \mathbf{n}_+ = -4i\sqrt{\pi}(D_- \psi_+)\mathbf{s} + 4i\pi\kappa^2 (|\psi_+|^2 + |\psi_-|^2)\mathbf{n}_+ , \tag{5.6a}$$

$$D_\pm \mathbf{n}_+ = -4\sqrt{\pi}\psi_\pm \mathbf{s}, \tag{5.6b}$$

$$\partial_0 \mathbf{s} = 2i\sqrt{\pi}((D_- \psi_+)\mathbf{n}_- - (\overline{D_-}\,\overline{\psi_+})\mathbf{n}_+), \tag{5.6c}$$

$$\partial_\pm \mathbf{s} = 2\sqrt{\pi}(\psi_\pm \mathbf{n}_- + \overline{\psi_\mp}\mathbf{n}_+), \tag{5.6d}$$

and for the field equations,

$$i\, D_0 \psi_\pm + (D_1^2 + D_2^2)\psi_\pm + 8\pi\kappa^2 |\psi_\pm|^2 \psi_\pm = 0, \tag{5.7a}$$

$$D_- \psi_+ = D_+ \psi_- , \tag{5.7b}$$

$$[D_+, D_-] = 8\pi\kappa^2 (|\psi_+|^2 - |\psi_-|^2), \tag{5.7c}$$

$$[D_0, D_\pm] = 8i\pi\kappa^2 (\overline{\psi_\mp}\, D_\pm \psi_\mp + \psi_\pm\, \overline{D_\mp}\,\overline{\psi_\pm}) - 4i\pi\kappa^2 \partial_\pm (|\psi_+|^2 + |\psi_-|^2). \tag{5.7d}$$

The covariant derivatives in the system (5.6) and (5.7) are defined as before [see Eq. (3.12)]:

$$D_{\pm}=\partial_{\pm}-\frac{i}{2}A_{\pm},\quad D_0=\partial_0-\frac{i}{2}A_0, \tag{5.8}$$

with $A_{\pm}=V_{\pm}$, but redefined as

$$A_0=V_0-8\pi\kappa^2(|\psi_+|^2+|\psi_-|^2). \tag{5.9}$$

For the static field configurations, Eq. (5.1) reduces to the σ model (4.1), considered before. Now we are going to perform a dimensional reduction of the model to have an integrable evolution system. Let $M=T\times R\times S$, where R is the real line associated with the x_1 space coordinate and S is compactified on the circle second space coordinate x_2. As usual, for zero modes we are looking for equations independent of x_2,

$$i\ D_0\psi_{\pm}+\left[D_1^2+\left(\frac{i}{2}A_2\right)^2\right]\psi_{\pm}+8\pi\kappa^2|\psi_{\pm}|^2\psi_{\pm}=0, \tag{5.10a}$$

$$\left(\partial_1-\frac{i}{2}A_-\right)\psi_+=\left(\partial_1-\frac{i}{2}A_+\right)\psi_-, \tag{5.10b}$$

$$\partial_1 A_2=-8\pi\kappa^2(|\psi_+|^2-|\psi_-|^2), \tag{5.10c}$$

$$\partial_0 A_1-\partial_1 A_0=8\pi\kappa^2 A_2(|\psi_+|^2-|\psi_-|^2), \tag{5.10d}$$

$$\partial_0 A_2=-8i\pi\kappa^2[(\overline{\psi_+}\ \partial_1\psi_+-\psi_+\ \partial_1\overline{\psi_+})-(\overline{\psi_-}\ \partial_1\psi_--\psi_-\ \partial_1\overline{\psi_-})-iA_1(|\psi_+|^2-|\psi_-|^2)]. \tag{5.10e}$$

If instead of the potential A_0 we introduce

$$\mathscr{A}_0=A_0-\tfrac{1}{2}A_2^2,\quad \mathscr{A}_1=A_1,\quad \mathscr{A}_2=A_2, \tag{5.11}$$

Eq. (5.10d) becomes of the vanishing field strength form

$$\partial_0\mathscr{A}_1-\partial_1\mathscr{A}_0=0, \tag{5.12d}$$

and for the remain equations we have

$$i\ \mathscr{D}_0\psi_{\pm}+\mathscr{D}_1^2\psi_{\pm}+8\pi\kappa^2|\psi_{\pm}|^2\psi_{\pm}=0, \tag{5.12a}$$

$$\left(\partial_1-\frac{i}{2}\mathscr{A}_-\right)\psi_+=\left(\partial_1-\frac{i}{2}\mathscr{A}_+\right)\psi_-, \tag{5.12b}$$

$$\partial_1\mathscr{A}_2=-8\pi\kappa^2(|\psi_+|^2-|\psi_-|^2), \tag{5.12c}$$

$$\partial_0\mathscr{A}_2=-8i\pi\kappa^2[(\overline{\psi_+}\ \mathscr{D}_1\psi_+-\psi_+\ \overline{\mathscr{D}_1}\,\overline{\psi_+})-(\overline{\psi_-}\ \mathscr{D}_1\psi_--\psi_-\ \overline{\mathscr{D}_1}\,\overline{\psi_-}), \tag{5.12e}$$

where $\mathscr{D}_0=\partial_0-(i/2)\mathscr{A}_0$, $\mathscr{D}_1=\partial_1-(i/2)\mathscr{A}_1$. Comparing Eqs. (5.12a) and (5.12d) with gauged NLSE (4.15a)–(4.15b), we recognize complete equivalence. Using the same as before procedure, we can compensate the gauge potentials via $U(1)$ rotation,

$$\mathscr{A}_0=2\ \partial_0\lambda,\quad \mathscr{A}_1=2\ \partial_1\lambda,\quad \Phi_{\pm}=\psi_{\pm}e^{i\lambda}. \tag{5.13}$$

Thus, we find that both of the Φ_+, Φ_- fields satisfy the NLSE,

$$i\ \partial_0\Phi_\pm+\partial_1^2\Phi_\pm+8\pi\kappa^2|\Phi_\pm|^2\Phi_\pm=0, \tag{5.14}$$

and the set of relations connecting $\mathscr{A}_2$ with Φ_+, Φ_- fields,

$$\partial_1\Phi_+-\partial_1\Phi_-=1/2.\mathscr{A}_2(\Phi_++\Phi_-), \tag{5.15a}$$

$$\partial_1.\mathscr{A}_2=-8\pi\kappa^2(|\Phi_+|^2-|\Phi_-|^2), \tag{5.15b}$$

$$\partial_0.\mathscr{A}_2=-8i\pi\kappa^2[(\overline{\Phi}_+\ \partial_1\Phi_+-\Phi_+\ \partial_1\overline{\Phi}_+)-(\overline{\Phi}_-\ \partial_1\Phi_--\Phi_-\ \partial_1\overline{\Phi}_-)]. \tag{5.15c}$$

The system (5.15) allows one to define the $\mathscr{A}_2$ field in explicit form,

$$\mathscr{A}_2=\epsilon_\pm\sqrt{\alpha_0^2-16\pi\kappa^2|\Phi_+-\Phi_-|^2}, \tag{5.16}$$

where α_0 is an integration constant, $\epsilon_\pm=\pm1$. I can easily show that if both Φ_+ and Φ_- are solutions of the NLSE (5.14), then the evolution for $\mathscr{A}_2$ (5.16) is satisfied to Eq. (5.15c).

But Eq. (5.15a) with condition (5.16) is just the space part of the Bäcklund transformations for NLSE (5.14). The related time part can be easily reconstructed from the system (5.15). Thus, a surprising moment arising from the (2+1)-dimensional reduction is an interpretation of the Bäcklund transformation for NLSE in terms of the Abelian Chern–Simons gauge field, associated with the extra space coordinate x_2.

When $\Phi_+=\Phi_-$ the $\mathscr{A}_2=\epsilon_\pm\alpha_0=$const. As we show immediately, this constant has the meaning of the spectral parameter. When $\Phi_+\neq\Phi_-$, that means a soliton creation $\mathscr{A}_2$ is an inhomogeneous function measuring the departure of Φ_+ from Φ_-.

To clarify the meaning of the homogeneous part α_0, we turn now to the chiral current (2.7a),

$$J_\mu=g^{-1}\ \partial_\mu g=\frac{i}{4}\ \sigma_3V_\mu+\begin{pmatrix}0 & -\kappa^2\overline{q_\mu}\\ q_\mu & 0\end{pmatrix}. \tag{5.17}$$

We can carry out the $U(1)$ gauge transformation (5.13),

$$g\to ge^{(i/4)\lambda\sigma_3}. \tag{5.18}$$

As a result we have

$$J_1=\sqrt{\pi}\begin{pmatrix}0 & -\kappa^2(\overline{\Phi}_++\overline{\Phi}_-)\\ \Phi_++\Phi_- & 0\end{pmatrix},$$

$$J_2=\frac{i}{4}\ \sigma_3.\mathscr{A}_2-i\sqrt{\pi}\begin{pmatrix}0 & \kappa^2(\overline{\Phi}_+-\overline{\Phi}_-)\\ \Phi_+-\Phi_- & 0\end{pmatrix},$$

$$J_0=\frac{i}{8}\ \sigma_3[\mathscr{A}_2^2+16\pi\kappa^2(|\Phi_+|^2+|\Phi_-|^2)]+i\sqrt{\pi}\begin{pmatrix}0 & \kappa^2(\overline{\mathscr{D}}_-\overline{\Phi}_++\overline{\mathscr{D}}_+\overline{\Phi}_-)\\ \mathscr{D}_-\Phi_++\mathscr{D}_+\Phi_- & 0\end{pmatrix}.$$

Using (5.7b),

$$\mathscr{D}_-\Phi_+=\mathscr{D}_+\Phi_-,$$

we can rewrite it as

$$J_+=-\frac{1}{4}\ \sigma_3.\mathscr{A}_2+2\sqrt{\pi}\begin{pmatrix}0 & -\kappa^2\overline{\Phi}_-\\ \Phi_+ & 0\end{pmatrix}, \tag{5.19a}$$

$$J_0=\frac{i}{8}\,\sigma_3[\mathscr{A}_2^2+16\pi\kappa^2(|\Phi_+|^2+|\Phi_-|^2)]+2i\sqrt{\pi}\begin{pmatrix}0 & \kappa^2\,\overline{\mathscr{D}}_+\overline{\Phi}_-\\ \mathscr{D}_-\Phi_+ & 0\end{pmatrix}. \tag{5.19b}$$

Now, let

$$\Phi_+=\Phi_-\equiv\frac{1}{2\sqrt{\pi}}\,\Phi, \tag{5.20}$$

then, from (5.16),

$$\mathscr{A}_2=\epsilon_\pm\alpha_0\equiv 4\lambda_0. \tag{5.21}$$

As a result we have the well-known Lax pair for NLSE,

$$J_+=-\lambda_0\sigma_3+\begin{pmatrix}0 & -\kappa^2\overline{\Phi}\\ \Phi & 0\end{pmatrix}, \tag{5.22a}$$

$$J_0=i\sigma_3[2\lambda_0^2+\kappa^2|\Phi|^2]+i\begin{pmatrix}0 & \kappa^2(\partial_1+2\lambda_0)\overline{\Phi}\\ (\partial_1-2\lambda_0)\Phi & 0\end{pmatrix}. \tag{5.22b}$$

The Lax pair for the 1+1 HM model (4.9) can be constructed from (5.22) by the usual procedure of the gauge transformation, in terms of (2.2) trihedral N_3.[30,31]

It is clear now that constant λ_0 has a meaning of the spectral parameter. The remarkable fact is that J_+ consists of two parts: J_1 part is independent of the spectral parameter and J_2 is completely defined in terms of it.

As known, in order to investigate the infrared properties of the theory, we can expand the gauge field $\mathscr{A}_2$ in a Fourier series and separate out the part that plays the main role at long distances. This is the constant in space (x_1) term,

$$\mathscr{A}_2\cong 4\lambda_0\left(1+\frac{\pi\kappa^2}{2\lambda_0^2}\,|\Phi_+-\Phi_-|^2+\cdots\right). \tag{5.23}$$

Thus, we can interpret the spectral parameter as a condensate value for the Chern–Simons gauge field $\mathscr{A}_2$ associated with the extra dimension.

As we see, the Lax pair with the spectral parameter flow, defining all the miracles of soliton mathematics, has a simple interpretation in terms of an extra space direction and CS TFT.

VI. CONCLUSION

In conclusion I would like to emphasize some points. First, as shown above, the non-Abelian TFT (3.1) represented in the form (3.12) could be interpreted as the Abelian Chern–Simons gauge theory interacting with a doublet of matter fields.[20] Usually, the Abelian gauge field is called the ''statistical field'' since it defines the anyonic statistics for matter fields. For a more direct relation we need to rescale the ''matter'' fields,

$$\psi_\pm=\frac{1}{\sqrt{k}}\,\Psi_\pm,$$

to have normal canonical brackets (3.11). Then, the Chern–Simons Gauss law (3.15b) becomes

$$\partial_1 V_2 - \partial_2 V_1 = -\frac{8\pi\kappa^2}{k}\,(|\Psi_+|^2 - |\Psi_-|^2).$$

From this form we recognize that the coupling constant k for the non-Abelian theory (3.1) coincides with the statistical parameter for fractional statistics. It means that in quantized (3.1) theory the matter fields could appear (after singular gauge transformation) as anyons.[20]

The 1+1-dimensional reduction of the model (5.7) shows that two components $\mathscr{A}_0$, $\mathscr{A}_1$ of the statistical gauge field can be removed by gauge transformation. But component $\mathscr{A}_2$ (5.16) related to the extra space coordinate has a deep physical meaning. Thus, for infrared properties of the Chern–Simons theory (3.12), the constant in space vector potential,

$$A_i(x) = X_i(t) + \cdots,$$

depending only of time, is relevant. The corresponding Chern–Simons term in (3.12),

$$\frac{k}{16\pi}\,\dot{\mathbf{X}}\times\mathbf{X},$$

has a simple physical interpretation. If we consider (X_1, X_2) as coordinates of the charged particle in the plane, and switch on the magnetic field orthogonal to the plane, the Lorentz force will arise. It connects two directions X_1, X_2 in such a way that energy from the first direction will flow to the second one. In our case it means that due to the Chern–Simons structure in the topological action (3.12), our 1+1-dimensional gauge theory (5.14), (5.15) continue to feel an extra space coordinate. But all dependence of the extra space coordinate is hidden in the spectral parameter (5.21). Of course, the gauge invariant nonlinear equations (5.14) are independent of x_2 and λ_0.

Thus, the potential (5.16) generally includes two parts. A part with the spectral parameter only is a constant, and has meaning of the ''condensate'' for the statistical gauge field, while the nonhomogeneous part of $\mathscr{A}_2$ comes from the deviation between two solutions of the NLSE (5.14). We know that (5.15)–(5.16) is an elementary Bäcklund transformation for NLSE. If one of the fields is vanishing, it provides the one-soliton solution for the second one. Corresponding value of $\mathscr{A}_2$ we call the one-soliton gauge potential. This allows us to formulate a gauge invariance principle. The statistical gauge field is a homogeneous, globally defined field in the case (5.20). When condition (5.20) is broken, that means a soliton is created, the gauge field $\mathscr{A}_2$ becomes a local function of coordinate x_1. Hence, we observe that the statistical gauge field is an inseparable phenomena accompanying the soliton creation. It is a relic of the Chern–Simons Gauss law, which states the creation of magnetic flux by a particle creation. According to this, in anyon physics, we interpret the physical excitations as particles with an attached magnetic flux. Consequently, even the one-dimensional solitons are excitations attached with a statistical magnetic field. Indeed, if we put one of the fields, say $\Phi_- = 0$, from Eq. (5.15b) follows the one-dimensional (!) CS Gauss law,

$$B(x) = \frac{8\pi\kappa^2}{k}\,|\Psi_+|^2.$$

For a soliton with large amplitude $\eta = \mathrm{Im}\,\lambda_0$, we can write approximately

$$B(x) \approx \frac{16\pi\kappa^2}{k}\,\eta\,\delta(x).$$

This relation should be compared with a two-dimensional ''prototype'' (2.36). It shows explicitly that one soliton is always attached to the ''magnetic'' field. The line integral (''one-dimensional flux''),

$$\int B\, dx = \frac{8\pi\kappa^2}{k} \int |\Psi_+|^2\, dx = \frac{16\pi\kappa^2}{k}\, \eta,$$

is time independent and the well-known first integral of NLSE. It has a simple interpretation of the rescaled soliton amplitude Im λ_0 and really is inseparable from the soliton in any collisions.

The above discussion, appearing exactly 120 yr after Bäcklund's first paper on his transformation theory,[32] implies a new, physical interpretation of the Bäcklund transformation. It gives BT explicitly in terms of an inhomogeneous Abelian CS gauge field and indicates the deep relation between CS TFT and BT. We conjecture that results have the general meaning and are applicable to other integrable models. In fact, all that we need are constraints for CS theory, arising from the nonlinear σ model. Thus, earlier we showed[19] that the classical spin model in planar condensed media, the so-called Topological Magnet,[17] provides for gauge invariant fields the Davey–Stewartson equations. Dimensional reduction in this case also leads to the NLSE and related BT. Our result suggests that while the Lax pair depends on an additional spectral parameter, which is remnant of the three-dimensional theory, the reduced Nonlinear Evolution Equation is gauge invariant and independent of that parameter. It would be interesting to obtain in this way the Lax pair for the SDYM from proper TFT in higher then four dimensions.

Finally, we remark on the possibility of tracking the connection between quantum exactly soluble TFT and integrable models in the spirit of Ref. 33. In this case, ideas of dissipative dynamics associated with CS theory[34] could be relevant to treat the indefinite metric structure of TFT.

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Anomalous thresholds and edge singularities in electrical impedance tomography

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Studies of models of current flow behaviour in electrical impedance tomography (EIT) have shown that the current density distribution varies extremely rapidly near the edge of the electrodes used in the technique. This behaviour imposes severe restrictions on the numerical techniques used in image reconstruction algorithms. In this paper we have considered a simple two dimensional case and we have shown how the theory of end point/pinch singularities which was developed for studying the anomalous thresholds encountered in elementary particle physics can be used to give a complete description of the analytic structure of the current density near to the edge of the electrodes. As a byproduct of this study it was possible to give a complete description of the Riemann sheet manifold of the eigenfunctions of the logarithmic kernel. These methods can be readily extended to other weakly singular kernels. © *1996 American Institute of Physics.* [S0022-2488(96)02307-9]

I. INTRODUCTION

There are numerous examples of practical situations where electric current is used to probe the interior of some object of interest. One emerging technology which specifically uses this approach has become known as electrical impedance tomography (EIT). This is a method of medical and industrial imaging in which electrical currents are applied to the surface of an object and the induced surface voltage is measured. These data are then used to produce an image of the conductivity distribution in the interior of the object. An extensive literature exists on EIT.[1]

The particular feature of EIT which is of interest to us here is related to the observation that in practice the electric current can be applied only through a finite number of electrodes—currently in the range 16–64 for two dimensional applications. The consequences of this fact and the appropriate mathematical modelling of the electrodes have been discussed in a number of papers.[2–4]

In medical applications one of the significant problems for EIT is the existence of a thin layer of material of high, but unknown, contact impedance lying between the current drive electrodes and the body. Various models have been proposed to describe this phenomenon but one which has strong experimental support[5] is to suppose that on the (finite size) electrodes the electric potential, Φ, is related to the electric current $\sigma(\partial\Phi/\partial n)$ by

$$\Phi + \mathcal{Z}\sigma \frac{\partial \Phi}{\partial n} = V$$

where σ is the conductivity just below the electrode, $\mathcal{Z}$ is the contact impedance and V is the potential of the electrode (a constant). The induced voltage, Φ, is found by making measurements on high impedance electrodes, also attached to the surface.

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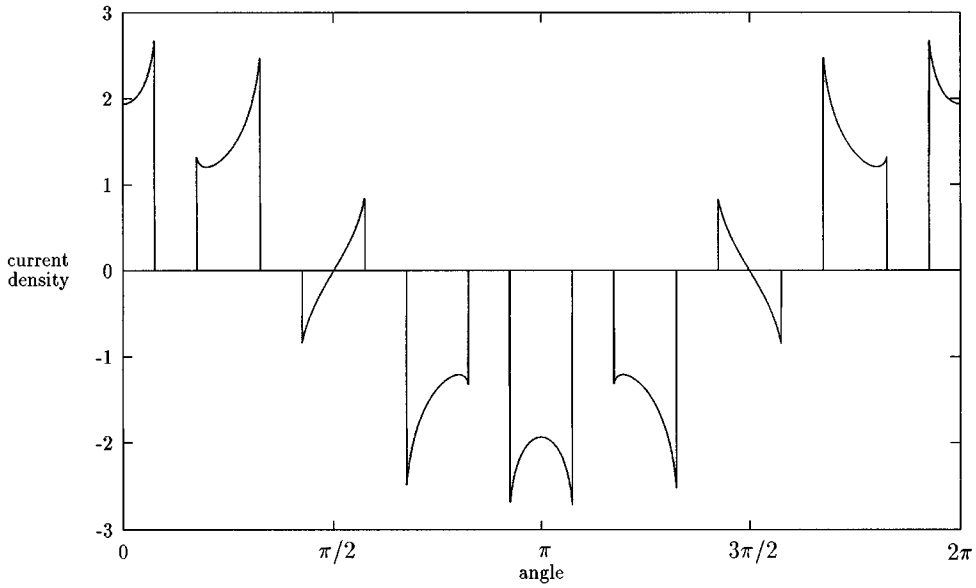

FIG. 1. The current density distribution obtained solving Eq. (6) numerically for the case of 8 electrodes, each having a contact impedance equal to 0.22.

This model has been studied numerically using a boundary Fourier technique[2] for the case of constant $\mathscr{Z}$ and an interesting phenomenon which was observed was the appearance of very sharp peaks in the current density distribution at the edge of the electrodes. More recently the model has been studied numerically for non-constant $\mathscr{Z}$ using the weakly singular integral equation described in Eq. (6) below. Although the singularity is weak, its existence has important consequences for the numerical treatment of this equation. Details of this work will be given elsewhere[6] but the point which we wish to emphasize here is that the distinctive sharp peak behaviour occurs for a wide range of conductivity distributions and contact impedance forms. In Fig. 1 we show typical results for the current density distribution in the case of eight electrodes with an input current on the lth electrode of $\cos\theta_l$.

An unwelcome consequence of the sharpness of these peaks is that the direct numerical modelling of the potential with the finite element method has become an excessively substantial task due to the high number of mesh points needed near to the edge of the electrodes in order to accommodate the rapid variation of the normal derivative of the potential. The aim of this article is to give an explicit analytic description of these singularities in a form which should substantially improve the speed of the numerical computation.

Since the appearance of the peaks is a boundary phenomenon which is very little influenced by the actual values of the conductivity σ inside the disk—see the discussion in Section III about the *dominant singular integral equation*—we shall focus our attention on the constant σ case. In this case the governing partial differential equation is Laplace's equation and our problem becomes one in potential theory. Consequently, we shall study the electrode model defined above for the standard domain of the unit disk. The importance of the unit disk stems from the fact that the potential problem for any simply connected two dimensional domain can be reduced to the unit disk by an appropriate conformal mapping.

In earlier investigations of these peaks it had been shown[4] that this problem can be solved explicitly in the *zero* contact impedance case ($\mathscr{Z}\equiv 0$), for the case of two electrodes. In this specific case one finds that near the edge of the electrodes

$$\frac{\partial \Phi}{\partial n} \sim \frac{1}{\sqrt{x}}$$

where x is the distance, along the boundary, from the edge of the electrode. Thus the normal derivative of Φ becomes infinite at the edge of the electrodes. However if the contact impedance $\mathcal{Z}$ is not zero, although $\partial\Phi/\partial n$ still has sharp peaks at the edge of the electrodes (see Fig. 1), it remains finite since both Φ and V are finite and since $\partial\Phi/\partial n \equiv (V-\Phi)/(\mathcal{Z}\sigma)$. This shows that the nature of the singularities in the $\mathcal{Z}\neq 0$ case *cannot* be obtained from that encountered in the soluble $\mathcal{Z}\equiv 0$ model. Thus, in order to have a correct understanding of these singularities some deeper investigations are necessary and this represents the main goal of the present paper.

Overview of the paper

After a short description of the mathematical model in Section II, in Section III we formulate the boundary problem as an integral equation. As shown there the kernel of this integral equation has a weak (logarithmic) singularity, and this has direct consequences for the singularities of the solution near the electrodes edges. We will describe these singularities in terms of an asymptotic series for the potential.

In pursuing this program we shall have to step off the real axis into the neighbouring complex plane. This will be necessary since we will write the solution of the integral equation as an infinite sum of the free term and the eigenfunctions of the weakly singular kernel. As one knows, there are many examples of series uniformly and absolutely convergent on the real axis which cannot be differentiated term by term [for example $\Sigma_{n=1}\cos(nx)/n^2$ converges uniformly, while the kth derivatives of its terms contain factors of the form n^{k-2} which spoil any convergence], but in deriving asymptotic expressions we will often have to perform this kind of operation. However, in contrast to what happens on a real interval, in the complex plane there exists a marvelous theorem which states that given a sequence $\{f_i\}$ of functions holomorphic in some domain Ω which converge uniformly, $f_i \to f$, on all compact subsets of Ω, then (a) f is a holomorphic function in Ω and (b) f_i' as well as the higher derivatives $f_i^{(n)}$ tend uniformly towards f' and $f^{(n)}$ on any compact subset of Ω. In some way by walking in the complex plane around the singularity one has a better view of what really happens there.

In studying the analytic properties of the free term (Section IV) and of the eigenfunctions (Section V), we shall use techniques similar to those from the ''pinch and end point singularities theory'' which was developed some time ago by Eden, Landshoff, Olive and Polkinghorne[7] in elementary particle physics. However our problem is more complex than that related to the Feynman graphs in two respects. First we will have to consider moving cuts rather than moving poles, and second we will no longer have integrals over some explicitly given functions, but integrals over the *a priori* unknown eigenfunctions whose singularities we are trying to find.

Handling infinite series can also be dangerous because spurious singularities may creep in as happens, for example, with the common geometric series. The proof that this does not happen in the neighbourhood of the singular point is given in the first subsection of the Section V. The analytic properties of the eigenfunctions and the recursive procedure to compute the coefficients in the asymptotic expansions are given in Section V B [see Eq. (67)]. From this expansion it follows that the spikes of the current density near the edge of the electrodes are of the form

$$\frac{\partial \Phi}{\partial n} \sim \sum_{m=1}^{r} \sum_{k=1}^{m} c_{mk} x^m \cdot \log^k(x) + \mathcal{O}(x^{r+1-\varepsilon}) + \text{regular part},$$

where x is the distance along the boundary from the edge of the electrode and c_{mk} some real coefficients. Since the derivative of $x\log(x)$ is $1+\log(x)$, this means that although these spikes are *finite* they have *infinite derivatives*.

II. THE MATHEMATICAL MODEL FOR EIT

The usual model used to describe the forward problem in EIT is obtained by considering the object as consisting of isotropic material with conductivity distribution σ contained in an open, simply connected region Ω surrounded by a reasonably smooth boundary $\partial\Omega$. On the surface, $\partial\Omega$, a number, L, of electrodes are attached and electrical current is applied.

In this case Maxwell's equations give:

$$\nabla\cdot(\sigma\nabla\Phi)=0 \quad \text{in} \quad \Omega. \tag{1}$$

Further, the total current driven on the lth electrode $I_l = \int_{\Gamma_l}\sigma(\partial\Phi/\partial n)$ is a known quantity and there is no current outflow outside the region covered by the electrodes, $\Gamma=\Gamma_1\cup\Gamma_2\cup\cdots\cup\Gamma_L$. If we now introduce our electrode model mentioned earlier to the case when σ is constant and Ω is the unit disk, the physical problem is equivalent to the mathematical problem of solving the following boundary value problem:

$$\nabla^2\Phi(z)=0 \quad \text{in} \quad \Omega, \tag{2}$$

$$\frac{\partial\Phi}{\partial n}=0 \quad \text{on} \quad \partial\Omega\backslash\Gamma,$$

$$\frac{\partial\Phi}{\partial n}=\frac{1}{\mathscr{Z}_l(z)}\,[V_l-\Phi(z)] \quad \text{on the electrode} \quad \Gamma_l\subset\partial\Omega, \tag{3}$$

$$\int_{\Gamma_l}\frac{\partial\Phi}{\partial n}\,d\theta=I_l, \quad l=1,\ldots,L,$$

for constant induced voltage, V_l, and total current driven, I_l, on each electrode. Here $\mathscr{Z}_l$ represents the contact (the ''skin'') impedance and $\Phi(z=e^{i\theta}\in\Gamma_l)$ is the potential just underneath ''the skin''.

III. THE INTEGRAL EQUATION

If the values of the normal derivative

$$\left.\frac{\partial\Phi}{\partial n}\right|_{z=e^{i\theta}}$$

were known everywhere on the boundary $\partial\Omega$ of the unit disk, we would be considering a classical Neumann problem, which is readily solved by means of the formula

$$\Phi(z)=\int_0^{2\pi}\mathscr{N}(z,e^{i\theta'};0)\left.\frac{\partial\Phi}{\partial n}\right|_{z'=e^{i\theta'}}d\theta'+\text{const.}, \tag{4}$$

where the Neumann kernel $\mathscr{N}(z,z';0)$ is

$$\mathscr{N}(z,z';0)=-\frac{1}{\pi}\log|z-z'|,$$

with $z'=e^{i\theta'}$ on the unit circle.

If we integrate the kernel with the values of the normal derivative $\partial\Phi/\partial n$ on the unit circle, we obtain a function Φ which is harmonic throughout the unit disk, which vanishes at $z=0$ and which

has the prescribed normal derivative values on the boundary. Similar kernels $\mathcal{N}(z,z';z_0)$ producing functions vanishing at $z=z_0$ rather that at $z=0$ can be written easily,[8] but the knowledge of the normal derivative determines Φ only up to a constant.

For what follows it is interesting to continue the Neumann integral (4) up to the boundary. Since

$$|e^{i\theta}-e^{i\theta'}|^2 \equiv 2[1-\cos(\theta'-\theta)],$$

if z and z' are of the form $z=e^{i\theta}$ and $z'=e^{i\theta'}$ the Neumann kernel on the unit circle reads:

$$\mathcal{N}(e^{i\theta},e^{i\theta'};0) = -\frac{1}{2\pi}\log\{2[1-\cos(\theta'-\theta)]\},$$

$$= -\frac{1}{\pi}\log\left|2\sin\left(\frac{\theta'-\theta}{2}\right)\right|. \tag{5}$$

In our case the normal derivative is known explicitly only on that part of the boundary which lies between the electrodes (i.e., on $\partial\Omega\backslash\Gamma$) where $\partial\Phi/\partial n$ is identical to zero. However, since the integral representation (4) can be continued up to the boundary, conditions (3) yield a linear integral equation for the boundary values $\rho(\theta)\equiv\Phi(e^{i\theta})$ of the potential:

$$\rho(\theta) = -\frac{1}{\pi}\sum_{l=1}^{L} V_l \int_{\Gamma_l}\frac{d\theta'}{\mathcal{Z}_l(\theta')}\log\left|2\sin\left(\frac{\theta'-\theta}{2}\right)\right| + \frac{1}{\pi}\sum_{l=1}^{L}\int_{\Gamma_l}\frac{d\theta'}{\mathcal{Z}_l(\theta')}\log\left|2\sin\left(\frac{\theta'-\theta}{2}\right)\right|\rho(\theta'). \tag{6}$$

Although the kernel

$$-\frac{1}{\pi}\log\left|2\sin\left(\frac{\theta'-\theta}{2}\right)\right|$$

becomes infinite each time θ' equals θ, this logarithmic singularity is weak enough to be L^2 integrable. The kernel is therefore of Hilbert–Schmidt type and so one can benefit from all the advantages of Fredholm integral equations of the second kind, namely the existence and uniqueness of an L^2 solution $\rho(\theta)$.

Equation (6) may be rewritten in a form which exhibits the logarithmic singularities of the kernel. Taking $e^{i\theta}\in\Gamma_{l_0}$ we may write

$$\begin{aligned}\rho(\theta) = &-\frac{1}{\pi}\sum_{l\neq l_0}\int_{\Gamma_l}\log\left|2\sin\left(\frac{\theta'-\theta}{2}\right)\right|\frac{[V_l-\rho(\theta')]}{\mathcal{Z}_l(\theta')}\,d\theta' \\ &-\frac{1}{\pi}\int_{\Gamma_{l_0}}\log\left|\frac{\sin\left(\frac{\theta'-\theta}{2}\right)}{\left(\frac{\theta'-\theta}{2}\right)}\right|\frac{[V_{l_0}-\rho(\theta')]}{\mathcal{Z}_{l_0}(\theta')}\,d\theta' - \frac{1}{\pi}V_{l_0}\int_{\Gamma_{l_0}}\frac{d\theta'}{\mathcal{Z}_{l_0}(\theta')}\log|\theta'-\theta| \\ &+\frac{1}{\pi}\int_{\Gamma_{l_0}}\frac{d\theta'}{\mathcal{Z}_{l_0}(\theta')}\log|\theta'-\theta|\rho(\theta').\end{aligned} \tag{7}$$

In order to study the local behaviour of the solution $\rho(\theta)$ near the edges of the l_0th electrode, we absorb the first two terms which are continuous into the ''free term'' of the so called *dominant singular integral equation*,[9] which is of the form:

$$f(x)=g(x)+\lambda\int_0^1 K(x,t)f(t)dt, \quad 0\leqslant x\leqslant 1, \tag{8}$$

$$K(x,t)\equiv\log|t-x|. \tag{9}$$

Here the points $x=0$ and $x=1$ correspond to the edges of the electrode under consideration. Equation (8) can be readily deduced from (7) by a suitable change of variables and functions in the $\mathscr{Z}_l(\theta)$ constant case, but as we shall show elsewhere[10] the discussion for the general case (non-constant $\mathscr{Z}_l$, non-constant σ) is fairly similar. When we follow this procedure we find that, as well as the first two terms from Eq. (7) which are regular, the function $g(x)$ contains the term

$$-V_{l_0}\Big/\pi\int_{\Gamma_{l_0}} d\theta'\log|\theta'-\theta|/\mathscr{Z}_{l_0}(\theta'),$$

so that after the changes of variables $g(x)$ has the form

$$g(x)=\int_0^1 \log|t-x|w(t)dt+\text{regular part}.$$

For the convenience of some subsequent proofs we shall also be interested in the iterated equations obtained by replacing $f(t)$ under the integral by the right hand side of the integral equation (8):

$$\begin{aligned} f(x)&=g_2(x)+\lambda^2\int_0^1 K_2(x,t)f(t)dt,\\ f(x)&=g_3(x)+\lambda^3\int_0^1 K_3(x,t)f(t)dt,\ldots \end{aligned} \tag{10}$$

and so on, where

$$\begin{aligned} g_2(x)&=g(x)+\lambda\int_0^1 K(x,t)g(t)dt,\\ g_3(x)&=g_2(x)+\lambda^2\int_0^1 K_2(x,t)g(t)dt,\ldots \end{aligned} \tag{11}$$

and

$$\begin{aligned} K_2(x,t)&=\int_0^1 K(x,\tau)K(\tau,t)d\tau,\\ K_3(x,t)&=\int_0^1 K_2(x,\tau)K(\tau,t)d\tau,\ldots\ . \end{aligned} \tag{12}$$

If this iteration had been continued indefinitely we would have found the Neumann series for f. Since these series usually converge only for very small values of λ, we shall not use them but stop after a finite number of terms and take advantage of the fact that the eigenvalues of $K_j(x,t)$ are the powers $\{\lambda_n^j\}$ of the eigenvalues $\{\lambda_n\}$ of $K(x,t)$. Indeed this will be quite helpful in some subsequent convergence proofs.

IV. SINGULARITY OF THE FREE TERM

In this and in the next section we shall try to find the analytic structure of the edge singularities of the solution without solving the integral equation, the latter being possible only numerically

or in some very special cases.[4] To this aim we shall use methods similar to those from the theory of the pinch or of the end point singularities,[7] well known to particle physicists working in analytic S-matrix theory. As a preparation to what follows it is probably helpful to look to the corresponding chapters from the classical book of Eden, Landshoff, Olive and Polkinghorne.[7]

In this section we shall deal with the free term $g(x)$ of Eq. (8). As mentioned in the Introduction, in order to find the analytic structure of the singularities we have to step into the neighbouring complex plane. We shall start our investigations with some negative values z_0 of z for which $\log|t-z|=\log(t-z)$ since the integration variable t is between 0 and 1. Having to perform analytic continuations we prefer to handle holomorphic expressions ($\log|t-z|$ *is not* a holomorphic function of z) and so, instead working with $g(x)$ we shall focus our attention on functions of the kind

$$F(z)=\int_0^1 \log(t-z)w(t)dt \tag{13}$$

where the weight $w(t)$ is a function of t, which is holomorphic (no cuts or other singularities) in neighbourhoods of $t=0$ and $t=1$. Although the holomorphic extension $F(z)$ is different from $g(x)$, it is closely related to it since, up to regular terms $\mathrm{Re}\,F(x\pm i\epsilon)=g(x)$ for $x\in[0,1]$ and $\epsilon\searrow 0$. Since the weight $w(t)$ may differ very much from one case to another, integral (13) cannot be performed explicitly. Therefore it will be interesting to have a mathematical procedure which should be able to predict the form of the singularity *without* actually performing the integrals. However, in order to have a partial check of the results which will be obtained below, we note that in the simplest case $w\equiv 1$ we obtain $F_{w\equiv 1}(z)=z\log(-z)+(1-z)\log(1-z)-1$.

As mentioned at the end of the last section, if λ is small enough the Neumann series converge and so the solution can be written in terms of the free terms g_j of the iterated equations. Therefore at the end of this section we shall discuss briefly the singularity of the iterated functions $g_j(x)$ since they provide a check of the results obtained in Section V in the general case.

A. Different ways of defining a cut

We recall that the features which are important when considering the cut structure of complex functions are the locations of the branch points and not the way in which the cut is taken. Indeed, the cut can be deformed or trailed as will become apparent below, in Figs. 3 to 5. As a first example, consider the function $F_{w\equiv 1}(z)$ given above. To define the cut of the first term $z\log(-z)$, we first introduce the function $Z(z)=-z$ and ask then that the cut of $\log Z(z)$ should run along the positive Z real axis. One achieves this by writing $Z=|Z|\exp(i\phi)$ and requiring ϕ to be in the range $[0,2\pi)$. With these conditions the cut of the first term, $z\log(-z)$, of $F_{w\equiv 1}(z)$ runs along the negative z real axis. The function $z\log(-z)$ is real and equal to $z\log|-z|\equiv-|z|\log|z|$ below the cut. Above the cut it will contain an additional imaginary part equal to $2i\pi z$. There will be no cut along the positive z real axis; here the value of $z\log(-z)$ is equal to $z\log|z|+i\pi z$ both above and below the real axis.

It is not compulsory to take the cut of the second term of $F_{w\equiv 1}(z)$ to the left. Indeed, if we define a new variable $Z(z)=1-z$, we can redefine the ''fundamental Riemann sheet'' of $\log Z$ by requiring that the argument ϕ of Z to be between $-\pi$ and π rather than between 0 and 2π, so that the cut of $\log Z=\log(1-z)$ will run along the negative real Z axis. Summarising $F_{w\equiv 1}(z)$ has no cut on the interval $[0,1]$ but two cuts running from $-\infty$ to 0 and from 1 to ∞.

The possible patterns for the cut of the logarithm are not exhausted by the cases discussed above. To have a further example let us consider for instance the function $Z(z)\equiv 1+z$ and begin with a cut of $\log Z$ running along the negative Z real axis. In this case the cut of $\log(z+1)$ looks as in Fig. 2a where the $\pm i\pi$ *zones* mean that the values just above or beneath the cut differ by $\pm i\pi$ from the mean value across the cut. (For illustration purposes we have slightly deplaced the cut: as it stands it corresponds to the function $\log[z-(-1-i\epsilon)]$, $\epsilon>0$.)

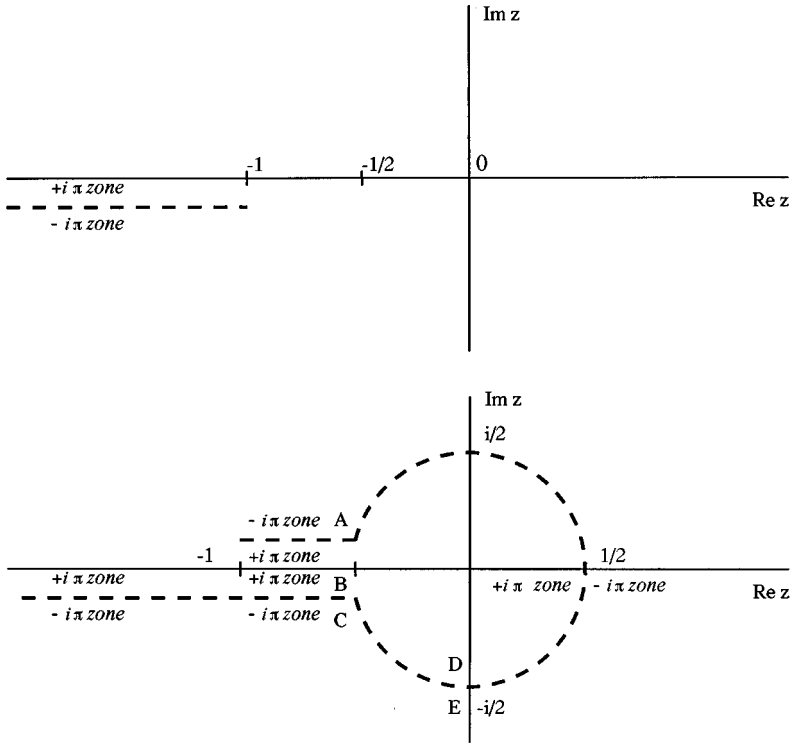

FIG. 2. (a) and (b) Example of two different definitions of the cut of $\log(z+1)$.

However we could alternatively define the cuts to run as in Fig. 2b where again the $\pm i\pi$ *zones* mean that the values of the logarithm differ by $\pm i\pi$ from the mean value across the cut (which is not necessarily real). With these specifications one finds immediately that the value of $\log(z+1)$ at the points A, B and C are, up to epsilons, equal respectively to $\log|z_A+1|$, to $\log|z_A+1|+2i\pi$ and again to $\log|z_A+1|$. As a further example, the values of $\log(z+1)$ at the points $D(z=-i/2+i\epsilon)$ and $E(z=-i/2-i\epsilon)$ are respectively $\log\sqrt{5/4} - (26.5/180)i\pi + 2i\pi$ and $\log\sqrt{5/4} - (26.5/180)i\pi$, while the mean value across the cut is there equal to $\log\sqrt{5/4} - (26.5/180)i\pi + i\pi$.

B. "Hooking" the integration contour

Let us come back to the function $F(z)$. In what follows it is important to consider separately the parameter (the "control") z-plane, and the complex t-plane where the integration is performed. As stated above, our aim is to find the singularities of $F(z)$, in the "control" z-plane, without performing the integration explicitly. Since our final goal is the description of the singularity of $F(z)$ at $z=0$, in this section we shall consider only analytic continuations performed in some neighborhood of the origin. A similar discussion can be made for the other end point $z=1$.

Suppose that initially z lies somewhere immediately below the negative real axis in the complex z-plane: $z=z_0\equiv x_0-i\epsilon$, where $x_0<0$ and $\epsilon>0$. The function $\log(t-z)$ from the integral of Eq. (13) has, *as a function of* t (i.e. in the complex t-plane where the integration is performed), a cut running parallel to the real t-axis from $t=-\infty$ to $t=z$ (see the dashed line in Fig. 3). From the point of view of the integration t-space, z is a parameter. Suppose now that z moves towards a point $z_a=x_a-i\epsilon$ ($x_a>0$) and then returns to z_0 ($x_0<0$) without crossing the integration contour.

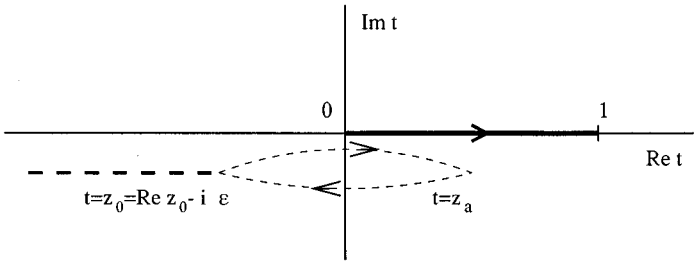

FIG. 3. Integration path (full line) and cut of the logarithm (dashed).

Correspondingly, the head of the cut of the logarithm (as a function of t) will move in the t-plane as shown in Fig. 3, but, since it will never cross the integration contour, the value of $F(z_0)$ will be identical with the value that the function $F(z)$ had before the point z began to move from z_0.

The situation is however different if the path followed by the point z in the control complex z-plane crosses the segment $[0,1]$ before returning to the initial position $z=z_0$. Here again the path followed by the ''head'' of the cut begins at z_0 and ends at the same point, but this time it winds around the integration end point $t=0$, crossing the real axis at $t=z_b$ as shown in Figs. 4 and 5.

A genuine analytic continuation of the function $F(z)$ should, of course, be at least continuous, i.e. have no jumps or other discontinuities. Therefore, even before the end point $t=z$ of the singularity of the logarithm reaches the point $t=z_b$ which lies on the real axis between 0 and 1 (see Fig. 4), we shall use the freedom we have to deform the integration contours inside the analyticity domain of the integrand without altering in any way the value of the integral $F(z)$.

Since the branch point $t=z$ ''trails'' behind it the cut of the logarithm when z moves further through points z_c in the upper half z-plane (Fig. 4) towards z_0, the value we obtain for the analytic continuation $F^{(1)}(z_0)$ of the initial integral will be given by the integral along the path C in Fig. 5 (the dashed line in Fig. 5 represents the cut of the logarithm; as it stands, the cut ends at the conjugate point $\overline{z_0}=x_0+i\epsilon$ rather than at z_0). Since the value of the logarithm on the lower lip of the emerging part of the cut contains an additional $2\pi i$ with respect to that on the upper lip (recall the discussions about the points A and B from Fig. 2b), the integral on the part of the contour around the cut (see Fig. 5) is

$$\int_0^{z_0}(\log|t-z_0|+i\pi)w(t)dt+\int_{z_0}^{0}(\log|t-z_0|-i\pi)w(t)dt=-2i\pi\int_{z_0}^{0}w(t)dt.$$

Here we have supposed that the weight $w(t)$ has no singularities at $z=0$. Such a point z_0 where the integration starts and which is below the initial integration threshold is called an ''anomalous threshold'' in elementary particle physics.

The new value $F^{(1)}(z_0)$ of $F(z)$ obtained by means of this analytic continuation process is hence

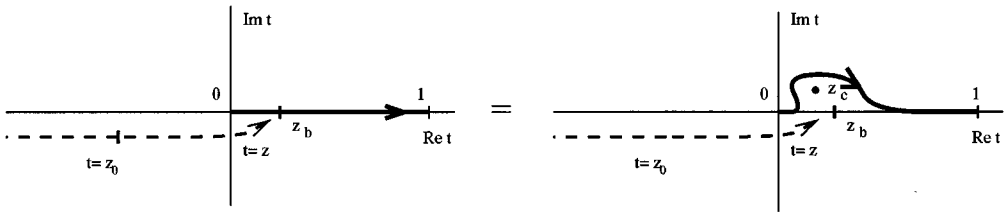

FIG. 4. The integrals over $[0,1]$ and over the deformed path are identical if $w(t)$ is holomorphic.

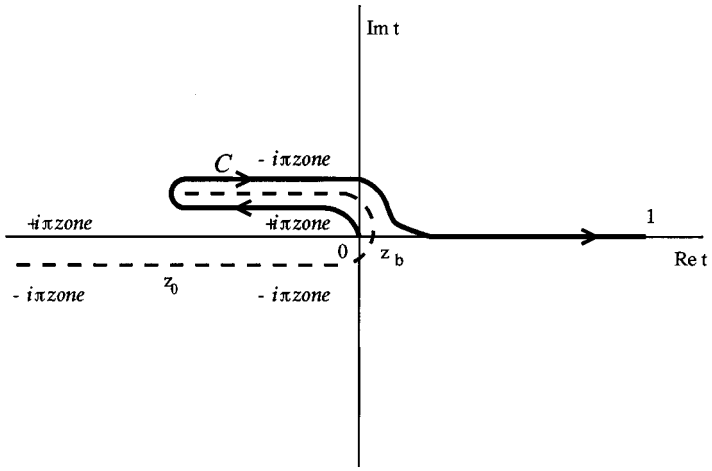

FIG. 5. The moving cut deforms the integration contour and produces an anomalous threshold.

$$F^{(1)}(z_0)=2i\pi\int_0^{z_0} w(t)dt+\int_0^1 \log(t-z_0)w(t)dt, \tag{14}$$

where the logarithm has the same determination as in Eq. (13) (i.e., a cut like in Fig. 3). There are many ways of defining the Riemann sheets of $F(z)$ but here we describe only two of them:

(i) If we define $F(x+iy)$ for any point in the upper half z-complex plane to coincide with the function $F^{(1)}(x+iy)$ defined above, i.e. $F(x+iy)\equiv F^{(1)}(x+iy)$ $(y>0)$, we have implicitly required that the function $F(z)$ should have no cuts on the segment [0,1] but only on other parts of the real axis. For instance, from the above discussion it follows that along the negative real axis $F(z)$ will have a discontinuity

$$\begin{aligned}\Delta F(x)&=F(x+i\epsilon)-F(x-i\epsilon)\equiv F^{(1)}(x+i\epsilon)-F(x-i\epsilon)\\&=2i\pi\int_0^x w(t)dt, \quad x\in\text{negative real axis},\end{aligned} \tag{15}$$

which means that $F(z)$ has indeed a cut along the negative real axis. This definition of the ''fundamental'' Riemann sheet of $F(z)$ coincides with that for the simple example of $F_{w\equiv 1}(z)$ discussed in the previous subsection.

(ii) Alternatively we could have required that the function $F(z)$ should have no cuts along the negative real axis. This amounts to redefining its ''fundamental'' Riemann sheet: we start again from our $z_0\equiv x_0-i\epsilon$ with $x_0<0$, ask that $F^{(0)}(z_0)\equiv F(z_0)$ but then require that the values of $F^{(0)}(z)$ above the real axis should merge, for $\mathrm{Re}\, z<0$, with those below the axis. We, therefore, *define* $F^{(0)}(z)$ for $\mathrm{Re}\, z<0$ as

$$F^{(0)}(z)=\int_0^1 \log(t-z)w(t)dt. \tag{16}$$

This definition which initially has been given only for $\mathrm{Re}\, z<0$ may then be extended to the whole complex plane cut along the real segment [0,1] (and further, along the positive real axis up to infinity; but, as mentioned at the beginning of this subsection, in order to keep the discussion simple we shall not consider what happens beyond the end point $z=1$). According to the definition (ii), the function $F^{(0)}(z)$ will have no cuts along the real negative axis, but in return, will have

different values along the upper and the lower lip of the real segment [0,1]. In the lower half plane $F^{(0)}(z)$ coincides with the function $F(z)$ corresponding to the previous definition (i) of the fundamental Riemann sheet, but not any longer for $\mathrm{Im}\, z>0$ where $F(z)$ was identical to $F^{(1)}(z)$. However, since by the construction of the function $F^{(1)}(z)$ [see the discussion preceding Eq. (14)] we had

$$F^{(0)}(x-i\epsilon)=F^{(1)}(x+i\epsilon)+\mathcal{O}(\epsilon), \quad \text{for } \epsilon>0 \quad \text{and } 0<x<1, \tag{17}$$

it follows that $F^{(1)}(z)$ represents now the analytic continuation of $F^{(0)}(z)$ on the next Riemann sheet—call it sheet (1)—when one crosses the segment [0,1] in the *upward* direction.

On the other hand, starting from the values $F^{(0)}(x+i\epsilon)$ from the upper lip of the segment [0,1] and continuing them *downwards*, one gets the function $F^{(-1)}(z)$:

$$F^{(-1)}(x-i\epsilon)=F^{(0)}(x+i\epsilon)+\mathcal{O}(\epsilon), \quad \text{for } \epsilon>0 \quad \text{and } 0<x<1, \tag{18}$$

which is obtained by deforming the integration contour in the lower half plane. Hence, $F^{(-1)}(z)$ will have the form

$$F^{(-1)}(z_0)=-2i\pi\int_0^{z_0} w(t)dt+\int_0^1 \log(t-z_0)w(t)dt, \tag{19}$$

where, again, the logarithm has the same determination as in Eqs. (13) and (16). Further, we see that the jump of $F^{(0)}$ across the cut [0,1] is

$$\Delta F^{(0)}(x)=-2i\pi\int_0^z w(t)dt, \quad \text{for } 0<x<1.$$

The functions $F^{(-1)}$, $F^{(0)}$, $F^{(1)}$ living on the Riemann sheets (-1), (0), (1) represent in fact a unique analytic function $F(z)$, the various branches $F^{(-1)}(z)$, $F^{(0)}(z)$, $F^{(1)}(z)$ being nothing but its values on a cutting up of the initial Riemann manifold along some arbitrarily given cuts.

If the function w is holomorphic in some neighbourhood of the origin it admits there an expansion of the form

$$w(t)=a_0+a_1t+a_2t^2+\cdots, \tag{20}$$

and so, from Eq. (15) we find

$$\Delta F(x)=2i\pi\left[a_0x+\frac{a_1}{2}x^2+\frac{a_2}{3}x^3+\cdots\right]. \tag{21}$$

A function which has precisely the same jump along the negative axis is given by

$$\left[a_0+\frac{a_1}{2}z+\frac{a_2}{3}z^2+\cdots\right]z\log z \tag{22}$$

which provides a mathematically correct and at the same time extremely simple description of the singularity of $F(z)$ near the point $z=0$.

Before closing this section we shall discuss briefly the structure of the singularities at the origin of the free terms $g_2(z)$, $g_3(z),\ldots,$ $g_j(z)$ of the iterated equations (10). In contrast to $g(z)$, these functions are written as integrals of the form (13) over weights $w(t)$ which are no longer holomorphic but contain the singularities of $g(z)$, $g_2(z),\ldots,$ $g_{j-1}(z)$ respectively. By straightforward integration we find that the general term of the iterated function $g_j(z)$ is

$$z^m \log^k(z), \quad \text{with } k=0,1,\ldots,j \text{ and } m\geqslant k. \tag{23}$$

At this stage we may wonder whether the left hand cuts of the powers of $\log(t)$ appearing under the integrals will not interfere with the above analytic continuation process. This does not occur since the real part of t becomes negative only along the loop in Fig. 5 around the emerging part of the cut of $\log(t-z)$ which is always at the same side of the negative real axis, i.e. always in the same ''$+i\pi$ *zone*'' of the function $\log(t)$. This means that

$$\Delta\left[\int_0^1 \log(t-z)t^m \log^k(t)dt\right]=2i\pi\int_0^z t^m(\log|t|+i\pi)^k dt, \quad z\in\text{negative real axis}. \tag{24}$$

V. SINGULARITIES OF THE SOLUTION OF THE FULL EQUATION

As mentioned in the Introduction, the specific difficulties of our problem are twofold. We have first to handle moving cuts; this question has been largely discussed in the previous section devoted to the free term. Second—and this is probably the main difference with respect to the classical papers on pinch and end point singularities—we will have to cope with the fact that the singularities of the function under the integral are *a priori* unknown, this function being the solution of the integral equation whose analytic properties we are trying to establish. In this section we shall address this second problem by solving it first for the eigenfunctions which are the natural building blocks of the solution, with the hope that their analytic properties (together with those of the free term) will be transmitted to the solution itself. Of course, this is not at all obvious since we will deal with infinite series and so new singularities may creep in. Therefore before we embark in Section V B on the study of the Riemann sheet structure and the asymptotic expansion of the eigenfunctions, we will first make sure in Section V A that the analytic properties of the eigenfunctions do exhaust the holomorphic characteristics of the solution. This is probably not entirely pedagogical, but reflects fairly well the way in which our work progressed. We shall have often to refer in Section V A to various analytic properties of the eigenfunctions which will be proved only later in Section V B.

This type of analysis presented here is not restricted to this particular integral equation, but we hope that it provides a working example of how one could proceed in problems involving other kinds of weakly singular kernels. To this end we tried to avoid as much as possible any special properties of the logarithmic kernel—for instance the fact that its null-space ker **K** is empty—and show how we can proceed in the general case. At a first reading or if not particularly interested in these mathematical proofs but only in the practical aspects of the asymptotic expansion, the reader may read only Section V A 1, skip the remainder of the Section V A and pass directly to Section V B.

A. The absence of summation singularities

We shall proceed in a number of stages:

In Section *V A 1* we discuss the role of eigenfunction expansions in describing the generic singularities of the solution. In both Sections *V A 1* and *V A 2* we recall some facts from the theory of integral equations and we identify a class of functions $\{\psi\}$ which can be expanded in terms of the eigenfunctions. We discuss also the possible appearance of additional singularities due to problems of convergence of infinite sums of functions.

The convergence proofs are provided in two separate subsections. In Section *V A 3* we discuss the continuity of these ψ-functions on the real segment $[0,1]$ and we show that their eigenfunction expansions converge uniformly there. However, in order to be able to consider the holomorphic properties of the solution $f(z)$ we need a number of results in the complex z-plane. These are derived in Section *V A 4* where, in particular, we prove that no additional singularities appear as a result of the summation of the series. The convergence of the asymptotic parts of the eigenfunctions is discussed in Section *V A 5*.

1. Generic singularities and eigenfunction expansions

When discussing the possible singularities of the solution of an integral equation we are faced with an apparent paradox. Independently of the specific form of the integral kernel, we may always proceed as a numerical analyst usually does when checking the correctness of computer code: start in the right hand side of Eq. (8) with some ''nice'' function $f(t)$ which has no singularities, integrate it with the kernel and then choose the free term $g(x)$ to recover the initial function $f(x)$. So, irrespective of the (integrable) singularities of the kernel, the solution $f(x)$ might be a polynomial, a simple trigonometric function or anything else. One may feel that this type of solution is quite exceptional but this example is enough to show that one *cannot* speak about ''the general singularity'' of the solution of an integral equation with a given singular kernel. However one is fully entitled to ask oneself what may happen in the non-exceptional situations, i.e. in the *generic* case.

To this end it is enlightening to express the solution of the integral equation (8) for our logarithmic kernel in terms of the eigenfunctions $u_n(x)$ of $K(x,t)$, defined by

$$u_n(x)=\lambda_n\int_0^1 K(x,t)u_n(t)dt, \quad \text{with } K(x,t)\equiv\log|t-x|, \tag{25}$$

as the series

$$f(x)=g(x)+\sum_{n=0}^{\infty}\frac{\lambda}{\lambda_n-\lambda}\,g_n u_n(x), \tag{26}$$

derived below in Section *V A 2*, where

$$g_n\overset{\text{def}}{=}\int_0^1 g(x)u_n(x)dx. \tag{27}$$

From expansion (26) it is obvious that in the generic case when small changes in the form of the function $g(x)$ and hence in $\{g_n\}$ are allowed, both the singularities of the free term $g(x)$ and of the eigenfunctions $u_n(x)$ will appear in the solution $f(x)$ since they will no longer cancel identically.

2. The functions $\psi(x)$

In what follows we shall use systematically the notation $\psi(x)$ for the functions from the range Ran **K** of the integral operator. The properties of these functions are used in the derivation of expansion (26) which plays a central role for the analytic properties of f as a superposition of those of g and of the u_n. However we should exercise great care at this point since additional singularities may creep in. We should have in mind the case of the sequence of functions $1,1+z,1+z+z^2,\ldots$. In the open unit disk this sequence tends to the function $1/(1-z)$ which has a pole at $z=1$, whereas all the functions in the sequence are holomorphic in an arbitrary large disk. Later in Section *V A 4* we will use a theorem of Vitali and/or of Morera to prove that no additional singularities appear in a neighbourhood of the origin. The theorem of Vitali, for instance, is partially based on the requirement that the elements of the sequence of partial sums should be uniformly bounded, which is clearly not valid in the counter-example with the geometric series if $|z|\geqslant 1$. Hence we have to make sure that in our case all the requirements of these theorems are fulfilled.

In order to obtain Eq. (26) we first multiply the integral equation (8) by an eigenfunction $u_n(x)$, integrate over the variable x and use the symmetry of the kernel to get

$$f_n=g_n+\frac{\lambda}{\lambda_n}f_n, \tag{28}$$

where the coefficients f_n are defined from $f(x)$ by integrals similar to those in Eq. (27).

From Eq. (28) we find $f_n=\lambda_n g_n/(\lambda_n-\lambda)$, but we should avoid expressing the solution $f(x)$ as a sum $\Sigma f_n u_n(x)$ since the latter might not converge pointwise and/or the eigenfunctions $\{u_n\}$ might not represent a complete system of orthonormal functions. In the special case of the logarithmic kernel (25) it happens (see Appendix) that the $\{u_n\}$ do represent such a complete orthonormal system, but for an arbitrary kernel K, $\ker \mathbf{K}$ is not empty and so they do not.

Many of the textbook theorems concerning expansions of the type (26) rely on the continuity of the kernel in the square $[0,1]\times[0,1]$. Since this is certainly not the case for our logarithmic kernel, some supplementary work is necessary to adapt the proofs to our specific conditions. In the simple cases where the kernel is continuous one usually takes advantage of this fact to prove that for any square integrable—even singular—function $\varphi(t)$, the function

$$\psi(x)\overset{\text{def}}{=}\int_0^1 K(x,t)\varphi(t)dt \tag{29}$$

from $\mathrm{Ran}\,\mathbf{K}$ is (a) continuous for $x\in[0,1]$, and (b) expressible in the form of an uniformly convergent expansion

$$\begin{aligned}\psi(x)&=\sum_{n=0}^{\infty}\psi_n u_n(x),\\ &\equiv\sum_{n=0}^{\infty}\varphi_n/\lambda_n u_n(x)\end{aligned} \tag{30}$$

where ψ_n and φ_n are defined by

$$\psi_n=\int_0^1\psi(t)u_n(t)dt,\quad \varphi_n=\int_0^1\varphi(t)u_n(t)dt.$$

Here the relation which connects the coefficients ψ_n and φ_n can be obtained by multiplying Eq. (29) by $u_n(x)$, integrating and using the symmetry of the kernel

$$\psi_n=\varphi_n/\lambda_n\,. \tag{31}$$

The solution $f(x)$ itself does not in general have a representation of the ψ-kind (29), but it is clear from the integral equation (8) that the difference $f(x)-g(x)$ is a true ψ-kind function. Hence it can be expanded as the sum $\Sigma(f_n-g_n)u_n(x)$, which in turn, using the relation (28) between f_n and g_n, yields the representation (26) for the solution of the integral equation in terms of the free term $g(x)$ and of the eigenfunctions $u_n(x)$.

In Section *V A 3* we shall prove that the properties (a) and (b) and hence the expandibility of $f(x)-g(x)$ are also valid in the case of the logarithmic kernel. Before showing that let us notice that if $\ker\mathbf{K}$ is empty as is the case—see the Appendix—with the logarithmic kernel, or if φ is chosen from the orthogonal complement $\ker^{\perp}\mathbf{K}$ of $\ker\mathbf{K}$, we also have

$$\left\|\varphi(x)-\sum_{n=0}^{\infty}\varphi_n u_n(x)\right\|_{L^2}=0. \tag{32}$$

However, in contrast with what happens with the ψ-kind functions, Eq. (32) represents only a convergence in the mean, i.e. $\varphi(x)$ does not have, in general, an expansion of the form (30) which converges uniformly. For the study of the analytic properties of the solution we shall need finer properties than those offered by L^2-space arguments, since, for instance, holomorphy and uniform convergence of the partial sums are essential for the Morera theorem to be used in Section *V A 4*.

3. Continuity of $\psi(x)$ in the logarithmic case and the uniform convergence of the $\psi^{(j)}(x)$ on the segment [0,1]

This section deals with the properties of the ψ-kind functions (29) on the segment $[0,1]$ for the logarithmic kernel (9). The arguments are quite similar to those which are used in the case of the continuous kernels, but we shall discuss them briefly here as a preparation for the next section and as well as to make this paper self-contained.

Our logarithmic kernel becomes infinite each time the integration variable t equals x. However, the continuity (a) of $\psi(x)$ on the interval $[0,1]$ (including at its end points) can be proved in a straightforward manner using the Schwarz inequality. Indeed, for any L^2 function $\|\varphi\|_{L^2} \leqslant M$ and for any points x and $x+\delta$ belonging to the (closed) segment $[0,1]$, we have

$$|\psi(x+\delta)-\psi(x)|^2 \leqslant \int_0^1 [\log|t-(x+\delta)|-\log|t-x|]^2 dt \times M^2, \tag{33}$$

where the integral $\int_0^1 |\varphi(t)|^2 dt$ has been replaced by the bound on the L^2-norm. If δ is small enough, it can be shown that the integral on the right hand side of (33) can be made smaller than any given nonzero ϵ^2/M^2, which proves the continuity of all the ψ-kind functions of the form (29). Since the eigenfunctions $u_n(x)$ by their very definition (25) are also functions of the ψ-kind, we have hence implicitly proved their continuity on the segment $[0,1]$, including at the end points $x=0$ and $x=1$.

We shall now show, (b), that for $x \in [0,1]$ the finite sums

$$\psi^{(j)}(x) = \sum_{n=0}^{j} \psi_n u_n(x) \tag{34}$$

converge uniformly to the function $\psi(x)$ defined in Eq. (29).

To this end we shall show first that the functions $\psi^{(j)}(x)$ converge uniformly to some (continuous) function $\psi^{(\infty)}(x)$: a similar proof may be used then for the uniform convergence of the analytic extensions $\Psi^{(j)}(z)$ which will be introduced in the next section. From Eq. (31) and from the definition (25) of the eigenfunctions $\{u_n(x)\}$ we have

$$\left|\sum_{j+1}^{j+k} \psi_n u_n(x)\right|^2 \equiv \left|\sum_{j+1}^{j+k} \frac{\varphi_n}{\lambda_n} \cdot \lambda_n \int_0^1 K(x,t) u_n(t) dt\right|^2 = \left|\int_0^1 K(x,t) \sum_{j+1}^{j+k} \varphi_n u_n(t) dt\right|^2,$$

which, using the Schwarz inequality and the fact that the basis $\{u_n(t)\}$ is orthonormal, yields

$$\left|\sum_{j+1}^{j+k} \psi_n u_n(x)\right|^2 \leqslant \int_0^1 \left|K(x,t)\right|^2 dt \cdot \int_0^1 \left|\sum_{j+1}^{j+k} \varphi_n u_n(t)\right|^2 dt = \int_0^1 |K(x,t)|^2 dt \cdot \sum_{j+1}^{j+k} \varphi_n^2. \tag{35}$$

For each fixed value of x, $0 \leqslant x \leqslant 1$, the kernel $K(x,t) \equiv \log|t-x|$ regarded as a function of t is in $L^2[0,1]$, and so,

$$\int_0^1 K^2(x,t) dt < M^2 < \infty.$$

Since the function φ is also in L^2, $\Sigma_{j+1}^{j+k} \varphi_n^2$ tends to zero for $\forall k$ as j increases. Hence the right hand side of (35) can be made arbitrarily small irrespective of the value of x. This means that the sequence $\psi^{(j)}(x)$ converges *uniformly* to some limit $\psi^{(\infty)}(x)$. Now from the continuity of the eigenfunctions $\{u_n(x)\}$ which we have proved above, it follows that the finite combinations $\{\psi^{(j)}(x)\}$ are continuous. Since the $\{\psi^{(j)}(x)\}$ converge *uniformly*, the limit $\psi^{(\infty)}(x)$ is also continuous.

On the other hand, by projecting the kernel onto the basis $\{u_n\}$ we obtain ''the coefficients'' $u_n(x)/\lambda_n$. Bessel's inequality then ensures that any sum over the $u_n^2(x)/\lambda_n^2$ is bounded:

$$\sum_{n=0}^{\infty} \frac{u_n^2(x)}{\lambda_n^2} \leqslant \int_0^1 K^2(x,t)dt (<\infty). \tag{36}$$

Integrating with respect to x we see that $\Sigma 1/\lambda_n^2$ must also converge and hence the $|\lambda_n|$ must tend to infinity with n. This fact will help us to prove that $\psi^{(\infty)}(x)$ is in fact identical to the function $\psi(x)$ defined in Eq. (29).

Indeed, since both functions $\psi(x)$ and $\psi^{(\infty)}(x)$ are continuous, it is enough to show that the L^2-norm of their difference is zero. To this end we notice that the difference between $\psi(x)$ and the functions $\psi^{(j)}(x)$ can be written as

$$\psi(x) - \psi^{(j)}(x) = \int_0^1 K^{(j+1)}(x,t)\varphi(t)dt \tag{37}$$

where $K^{(j+1)}(x,t)$ is the truncated kernel

$$K^{(j+1)}(x,t) = K(x,t) - \sum_{n=0}^{j} \frac{u_n(x)u_n(t)}{\lambda_n}, \tag{38}$$

where we have supposed that the eigenvalues have been labelled according their increasing moduli: $|\lambda_0| \leqslant |\lambda_1| \leqslant \cdots$. Unlike the procedure followed before, we shall not try to use the Schwarz inequality to prove directly the pointwise convergence of the $\psi^{(j)}(x)$, but we shall go instead through L^2-space arguments. Since the first $j+1$ eigenfunctions $u_0(x),\ u_1(x),\ldots,u_j(x)$ are all in the null space ker $\mathbf{K}^{(j+1)}$ of the truncated kernel (38), it follows that its eigenvalue with smallest absolute value is λ_{j+1}. If we denote by $K_2^{(j+1)}(x,y)$ the iterated truncated kernel

$$K_2^{(j+1)}(x,y) = \int K^{(j+1)}(x,t)K^{(j+1)}(t,y)dt, \tag{39}$$

its smallest eigenvalue μ will be λ_{j+1}^2. However for any symmetric Hilbert-Schmidt kernel $\mathscr{K}(x,y)$ we have

$$\sup_{\|\varphi\|=M} \left| \int \int \mathscr{K}(x,y)\varphi(x)\varphi(y)dxdy \right| = \frac{M^2}{|\mu|}$$

where μ is the smallest eigenvalue of $\mathscr{K}$. Hence, taking the integral over the square of the modulus of the left hand side of Eq. (37) we obtain

$$\|\psi - \psi^{(j)}\|_{L^2}^2 = \left| \int \int K_2^{(j+1)}(x,y)\varphi(x)\varphi(y)dxdy \right| \leqslant \frac{M^2}{\lambda_{j+1}^2} \tag{40}$$

which means that $\|\psi - \psi^{(j)}\|_{L^2} \leqslant M/|\lambda_{j+1}|$. Since $1/|\lambda_{j+1}|$ tends to zero as j increases, so does $\|\psi - \psi^{(j)}\|_{L^2}$. Now, from the uniform convergence $\|\psi^{(j)} - \psi^{(\infty)}\|_{L^{(\infty)}} \to 0$ which has proved above [see Eq. (35)], we have immediately also the L^2 convergence

$$\|\psi^{(j)} - \psi^{(\infty)}\|_{L^2} \to 0. \tag{41}$$

From the triangle inequality we have

$$\|\psi - \psi^{(\infty)}\|_{L^2} \leqslant \|\psi - \psi^{(j)}\|_{L^2} + \|\psi^{(j)} - \psi^{(\infty)}\|_{L^2}, \tag{42}$$

where from Eqs. (40) and (41) we see that the left hand side, which is independent of j, can be made arbitrarily small by a suitable choice of j in the right hand side. This means that $\|\psi - \psi^{(\infty)}\|_{L^2} \equiv 0$ which, since both $\psi(x)$ and $\psi^{(\infty)}(x)$ are continuous, proves that the two functions are identical.

4. The functions $\Psi^{(j)}(z)$ and the theorems of Morera and Vitali

In order to be able to study the nature of the singularities of the functions of ψ-kind, we will have to step off the real axis into the complex z-plane. We shall be particularly interested in the complex plane singularities and the asymptotic expansions near $z=0$ of eigenfunction expansions of the form (26), related to the solution $f(x)$ of the integral equation. To this end we shall need to know some analytic properties of the eigenfunctions $\{u_n\}$. These will be derived in section V B where, similarly to the function $F^{(0)}(z)$ [see Eq. (16) from Section IV], we shall define the analytic functions

$$U_n^{(0)}(z) \overset{\text{def}}{=} \lambda_n \int_0^1 \log(t-z) u_n(t)\, dt, \quad n=1,2,3,\ldots . \tag{43}$$

Although these functions do not yet represent the analytic continuation of the eigenfunctions $u_n(x)$ which are defined on the real segment $[0,1]$, they are closely related to them. This specific choice is based, as for $F^{(0)}(z)$, on the fact that for real negative z we have $\log(t-z) \equiv \log|t-z|$, since the integration variable t on the right hand side of Eq. (43) is always between 0 and 1. In contrast to the function $\log|t-z|$ (which is *not* holomorphic because of the modulus), the function $\log(t-z)$ can be extended analytically in the whole (cut) complex z-plane.

As will become apparent in Section V B, the analytic functions $U_n^{(0)}(z), U_n^{(1)}(z), U_n^{(-1)}(z),...$ which are the analogues of the functions $F^{(0)}(z), F^{(1)}(z), F^{(-1)}(z),...$, defined in Eqs. (16), (14) and (19), have an infinite Riemann sheet structure; the superscript in parentheses indicates the Riemann sheet under consideration. From the definition of the Riemann sheets and the continuity properties across the cut, we have, similar to Eqs. (17)–(18), for any real x between 0 and 1:

$$U_n^{(k)}(x+i\epsilon) = U_n^{(k-1)}(x-i\epsilon) + \mathcal{O}(\epsilon), \quad \epsilon > 0, \quad x \in [0,1]. \tag{44}$$

As will be shown in Section *V B 3*, the eigenfunctions $u_n(x)$ defined on the interval $[0,1]$ can be written as simple combinations of the boundary values of $U_n^{(0)}(z)$, $U_n^{(1)}(z)$ and $U_n^{(-1)}(z)$ on the upper and lower lips of the cut:

$$\begin{aligned} u_n(x) &= \frac{1}{2}\left[U_n^{(0)}(x+i\epsilon) + U_n^{(1)}(x+i\epsilon)\right], \quad \epsilon \searrow 0, \quad 0<x<1, \\ u_n(x) &= \frac{1}{2}\left[U_n^{(0)}(x-i\epsilon) + U_n^{(-1)}(x-i\epsilon)\right], \quad \epsilon \searrow 0, \quad 0<x<1. \end{aligned} \tag{45}$$

Hence, in analogy with the function $\psi(x)$ and the finite sums $\psi^{(j)}(x)$ defined in the previous subsection for $x \in [0,1]$, we shall define now for z in some given region Ω of the complex plane, the holomorphic functions

$$\Psi(z) \overset{\text{def}}{=} \int_0^1 \log(t-z)\varphi(t)\, dt, \quad \varphi \in L^2[0,1], \tag{46}$$

$$\Psi^{(j)}(z) \overset{\text{def}}{=} \sum_{n=0}^{j} \psi_n U_n^{(0)}(z) \equiv \sum_{n=0}^{j} \frac{\varphi_n}{\lambda_n} U_n^{(0)}(z). \tag{47}$$

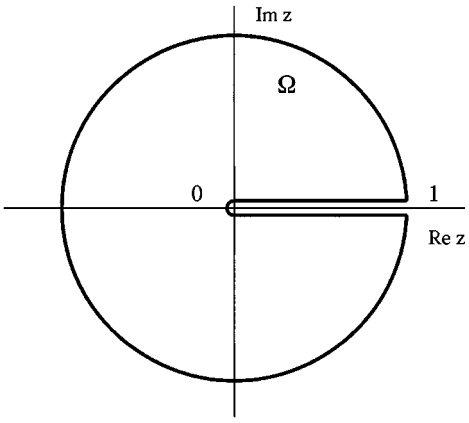

FIG. 6. The open set Ω.

Since we are mainly interested in the behavior of the solution near the origin, it is sufficient to take the region Ω to be the (open) unit disk cut along the real segment [0,1] (see Fig. 6), but any other (cut) disk of radius R is also acceptable. The holomorphy of $\Psi(z)$ in Ω follows from the theorem of Morera which states that iff[11,12] the function $\Psi(z)$ *is continuous* in the open set Ω and iff

$$\int_{\partial\Delta} \Psi(z)dz = 0 \tag{48}$$

along the border of *every* closed triangle $\Delta \subset \Omega$ (i.e. along any reasonable regular closed contour), then the function $\Psi(z)$ *is holomorphic* in Ω. It is clear that these two conditions are met by any function having the representation (46) for $z \in \Omega$. The continuity of $\Psi(z)$ can be established in a similar way to that of the functions $\psi(x)$ [see Eq. (33)], while the vanishing of the integrals (48) follows—after the interchange of the integral over $t \in [0,1]$ and integrals in the z complex plane—from the holomorphy of $\log(t-z)$ as a function of $z \in \Omega$. The theorem of Fubini[11] permits this interchange of the integration order since the function $F(z,t) \equiv \log(t-z)\varphi(t)$ is in $L^1[\partial\Delta \times [0,1]]$ we are interested in. The holomorphy of the functions $\Psi^{(j)}(z)$ is an immediate consequence of the fact that they are finite sums of holomorphic functions.

We denote by $\Psi^{\infty}(z)$ the limit of the sequence $\{\Psi^{(j)}(z)\}$ wherever this limit exists. We will show that *there are no new singularities* which enter the region Ω as a result of the summation process, i.e., that the limit $\Psi^{\infty}(z)$ is holomorphic in Ω. This is an important point: remember the counterexample with the geometric series from the beginning of Section *V A 2*.

In studying the analytic properties of the function $\Psi^{\infty}(z)$, the crucial property is again the uniform convergence—to be proved below—of the sequence $\{\Psi^{(j)}(z)\}$. This might seem surprising since on the real line there exist examples of sequences of infinitely differentiable functions which converge uniformly to functions which are nowhere differentiable. However, in the complex plane the uniform convergence of the sequences can be used in conjunction with the theorem of Morera to prove the holomorphy of their limits. Indeed, as a first consequence of the uniform convergence of the sequence $\{\Psi^{(j)}(z)\}$ one obtains the continuity of its limit $\Psi^{\infty}(z)$. Secondly, the identities

$$\int_{\partial\Delta} \Psi^{\infty}(z)dz = 0 \tag{49}$$

follow from the vanishing of the corresponding integrals over the holomorpic functions $\Psi^{(j)}(z)$ and from the fact that, because of uniform convergence, the integration and the limiting processes can be interchanged.

To prove the uniform convergence of $\{\Psi^{(j)}(z)\}$ for $z \in \Omega$ we shall proceed similarly to the method used on the interval [0,1]. Since the sums (47) are finite, they commute with the integral (43) from the definition of $U_n^{(0)}(z)$ and so

$$\Psi^{(j)}(z) \equiv \sum_{n=0}^{j} \frac{\varphi_n}{\lambda_n} U_n^{(0)}(z) = \int_0^1 \log(t-z) \sum_{n=0}^{j} \varphi_n u_n(t) dt. \tag{50}$$

Using arguments similar to those which led to Eq. (35), we find

$$\left| \sum_{j+1}^{j+k} \psi_n U_n^{(0)}(z) \right|^2 \leqslant \int_0^1 |\log(t-z)|^2 dt \cdot \sum_{j+1}^{j+k} \varphi_n^2 \tag{51}$$

where, for all $z \in \Omega$, the integral over the logarithm is bounded while the sum over the coefficients φ_n^2 tends to zero as j becomes large. This proves the uniform convergence of the sequence $\{\Psi^{(j)}(z)\}$ in Ω and hence, by the theorem of Morera, that the function $\Psi^{\infty}(z)$ has no singularities in the region Ω.

These results can also be proved using a theorem of Vitali[13] which states that if (a) the functions $\Psi^{(j)}(z)$ are holomorphic for $z \in \Omega$, (b) the sequence converges uniformly on some subset Σ of Ω which has an accumulation point inside Ω and (c) the functions $\Psi^{(j)}(z)$ are *uniformly bounded* in Ω, then the functions $\Psi^{(j)}(z)$ tend uniformly towards a function $\Psi^{\infty}(z)$ which is holomorphic in Ω. Note that the subset Σ may be the segment just above the real interval [0,1] where the uniform convergence has been proved in Section *V A 3*.

Using Vitali's theorem we can easily find the regions where $\Psi^{\infty}(z)$ is holomorphic, by looking at the sets where the $\Psi^{(j)}(z)$ are bounded. In this way we can verify that unlike the functions $U_n^{(0)}(z)$ which can be continued on higher Riemann sheets, the limit $\Psi^{\infty}(z)$ generally *does not exist* there. This is so because the uniform boundness condition (c) is no longer fulfilled outside the first Riemann sheet (unless the coefficients ψ_n decrease exponentially quickly). The reason is the existence of the factor $\exp[i\lambda_n(z-t)]$ in the higher Riemann sheet continuations $U_n^{(k)}(z)$ of the functions $U_n^{(0)}(z)$—see Eq. (65) from Section *V B 4*—which grows exponentially with λ_n if $(z-t)$ is complex.

Finally we shall show that, similar to $\psi^{(\infty)}$ on the real segment, the limit $\Psi^{\infty}(z)$ coincides inside Ω with the function $\Psi(z)$ defined in Eq. (46). This is a direct consequence of the fact that the set $\ker \mathbf{K}$ is empty in the case of the logarithmic kernel. Indeed, replacing $U_n^{(0)}(z)$ in Eq. (47) by its definition (43), Eq. (46) and the Schwarz inequality give

$$|\Psi(z) - \Psi^{(j)}(z)|^2 \leqslant \left\| \varphi(x) - \sum_{0}^{j} \varphi_n u_n(x) \right\|_{L^2}^2 \int_0^1 |\log(t-z)|^2 dt \tag{52}$$

where the right hand side tends to zero when j grows. [For kernels other than the logarithmic one with non empty null space, we can define appropriate Ψ-functions so that the corresponding φ-functions are contained in $\ker^{\perp}\mathbf{K}$. The simplest way to do this is to begin with a Neumann series but stop after few iterations so that the new $\varphi(x)$ should belong itself to Ran $\mathbf{K}$.]

5. Sums of asymptotic expressions

One of the goals of Section V B is to derive asymptotic expressions valid for $z \to 0$ for the analytic extensions $U_n^{(0)}(z)$ of the eigenfunctions:

$$U_n^{(0)}(z) = U_{n,\mathrm{asy}}^{(0)}(z) + U_{n,\mathrm{rem}}^{(0)}(z). \tag{53}$$

The remainder $U^{(0)}_{n,\mathrm{rem}}(z)$ behaves like $\mathcal{O}(|z|^{k-\eta})$ where k is some given positive integer and $\eta>0$ but otherwise arbitrary small. However, the coefficients of the asymptotic terms $U^{(0)}_{n,\mathrm{asy}}(z)$ contain some (fixed) positive power of the eigenvalue λ_n, depending on the value of the exponent k. Since the $\{\lambda_n\}$ tend to infinity with n, we should choose carefully an appropriate definition for the $\{\Psi^{(j)}_{\mathrm{asy}}\}$ in order to secure their convergence.

The simplest way to solve this problem is to use the iterated integral equations (10) discussed in Section III. The eigenfunctions of the iterated kernels $K_r(x,t)$ (12) are identical with those of the initial one, the only change being that the eigenvalues are now $(\lambda_n)^r$. This introduces a beneficial factor $1/\lambda_n^r$ in the coefficients $\psi_{r,n}$ of the new functions

$$\psi_r(x)=\int_0^1 K_r(x,t)\varphi(t)dt, \tag{54}$$

which are now

$$\psi_{r,n}=\frac{\varphi_n}{\lambda_n^r}. \tag{55}$$

This ensures the separate convergence of the series

$$\Psi^{(j)}_{\mathrm{asy}}(z)=\sum_{n=0}^{j}\psi_{r,n}U^{(0)}_{n,\mathrm{asy}}(z)=\sum_{n=0}^{j}\frac{\varphi_n}{\lambda_n^r}U^{(0)}_{n,\mathrm{asy}}(z) \tag{56}$$

and

$$\Psi^{(j)}_{\mathrm{rem}}(z)=\sum_{n=0}^{j}\psi_{r,n}U^{(0)}_{n,\mathrm{rem}}(z)=\sum_{n=0}^{j}\frac{\varphi_n}{\lambda_n^r}U^{(0)}_{n,\mathrm{rem}}(z).$$

As a result the asymptotic expansion of the solution of the integral equation will contain terms of the form $z^m\log^k(z)$, $k\leqslant r$, $m\geqslant k$, as do the iterated free term [see Eq. (23)] and the asymptotic terms $U^{(0)}_{n,\mathrm{asy}}(z)$.

The initial range of validity of the asymptotic expressions derived above is the cut open disk Ω and so does not yet extend on the real segment $[0,1]$. We are of course interested to show the correctness of these asymptotic series also on some small real interval $0\leqslant x\leqslant x_0$. As has been shown above, the theorem of Vitali fails to work on higher Riemann sheets since the functions $U^{(1)}_n(z)$ and $U^{(-1)}_n(z)$ are no longer uniformly bounded and so the sequence $\{\Psi^{(j)}(z)\}$ does not converge any more there. However it is interesting and important for what follows to note that the sequence $\{\Psi^{(j)}(z)\}$ related to our integral equation with logarithmic kernel converges uniformly also on the closure $\overline{\overline{\Omega}}$ of Ω, i.e. the function $\Psi^{\infty}(z)$ is well defined and continuous (because of the uniform convergence) on the real interval $[0,1]$, both when approached from above and below. We have used the symbol $\overline{\overline{\Omega}}$ to emphasize the fact that in all this discussion the open set Ω has to be considered as an open subset of the whole Riemann manifold of the solution of the integral equation rather than of the z complex plane (whereas normally the closure $\overline{\Omega}$ coincides with the unit disk $|z|\leqslant 1$). The set $\overline{\overline{\Omega}}$ contains the interval $[0,1]$ twice (see Fig. 7) corresponding to the fact that the function $\Psi(z)$ has different limits when z approaches the interval $[0,1]$ from above or below.

To prove that the sequence $\{\Psi^{(j)}(z)\}$ converges uniformly also on the interval $[0,1]$ it is sufficient to note that when $z\in[0,1]$, $|\log(t-z)|$ is equal to $|\log|t-z||$ if $t>z$, or to $|\log|t-z|\pm i\pi|$ if $t<z$. Here the sign of $i\pi$ depends on whether z approaches the real axis from above or from below. However in both cases the integral from Eq. (52) is bounded and hence, the right hand side of (52) can be made as small as one wishes by taking j to be sufficiently large.

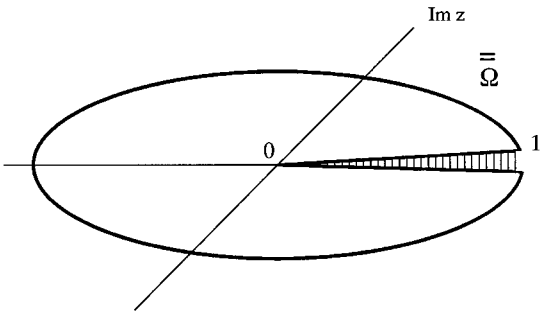

FIG. 7. The closure $\bar{\bar{\Omega}}$ of Ω drawn as a three dimensional picture in order to emphasize that the interval [0,1] is included twice.

It has been already shown in the previous subsection that limit $\Psi^{\infty}(z)$ coincides with the holomorphic function $\Psi(z)$ throughout the open set Ω. The limit $\Psi^{\infty}(z)$ does not exist beyond the two real segments [0,1] from the border of $\bar{\bar{\Omega}}$ but is continuous up to and on them, because of the uniform convergence of the sequence $\{\Psi^{(j)}(z)\}$. The function $\Psi^{\infty}(z)$ is hence defined, by continuity, in an unambiguous way on the two real intervals on the boundary of $\bar{\bar{\Omega}}$. It coincides there with $\Psi(z)$, as everywhere else in the closed set $\bar{\bar{\Omega}}$.

In this way we have shown that the asymptotic series $\Psi^{\infty}_{\text{asy}}(z)$ obtained using the asymptotic expansions of $U_n^{(0)}(z)$ are valid in a neighbourhood of the origin in $\bar{\bar{\Omega}}$, and therefore on the (two) real intervals $[0,x_0]$. This means that the remainder $\Psi^{\infty}_{\text{rem}}(z)$ of the asymptotic series is bounded by $\mathcal{O}(|z|^{k-\eta})$ on the real interval $[0,x_0]$ as well as in the open set Ω.

B. Continuation of the eigenfunctions to the complex plane

In this subsection we shall study the singularities of the eigenfunctions. To this end, similar to the analytic extension $F^{(0)}$ of the free term from Section IV we shall introduce in Section *V B 2* the analytic extensions $U_n^{(0)}$ of the eigenfunctions $u_n(x)$.

In trying to continue $U_n^{(0)}$ analytically on higher Riemann sheets, i.e. in trying to construct the function $U_n^{(1)}$ as we did with the free term in Section IV, we face a specific difficulty related to the fact that the eigenfunctions $u_n(x)$ as they stand are defined only on the segment [0,1]. This means that we could no longer ''hook'' the integration contour, as we did in Section IV where the weight $w(t)$, being analytic, was well defined not only on the real segment but also on the various complex plane deformations of the initial integration path.

This point will be solved in Section V B 3 where the eigenfunctions $u_n(x)$ will be expressed as linear combinations of $U_n^{(0)}$ and its Riemann sheet continuations. Another consequence of this fact will be the Volterra integral equation which relates $U_n^{(1)}$ to $U_n^{(0)}$ or vice versa (Section *V B 4*). This Volterra integral equation can be solved effectively, providing explicit expressions for $U_n^{(1)}$ or $U_n^{(-1)}$ in terms of $U_n^{(0)}$. Finally, in Section *V B 5* this integral equation is used in order to derive the asymptotic series which describe the singularities of the eigenfunctions around the origin.

1. Eigenfunctions of the logarithmic kernel

It has been proved in the Section *V A 3* that, in spite of the logarithmic singularity in the integrand, the eigenfunctions $\{u_n\}$ defined by

$$u_n(x)=\lambda_n\int_0^1 \log|t-x|u_n(t)dt \tag{57}$$

are continuous functions. The graphs of some of these eigenfunctions are depicted in Fig. 8 and

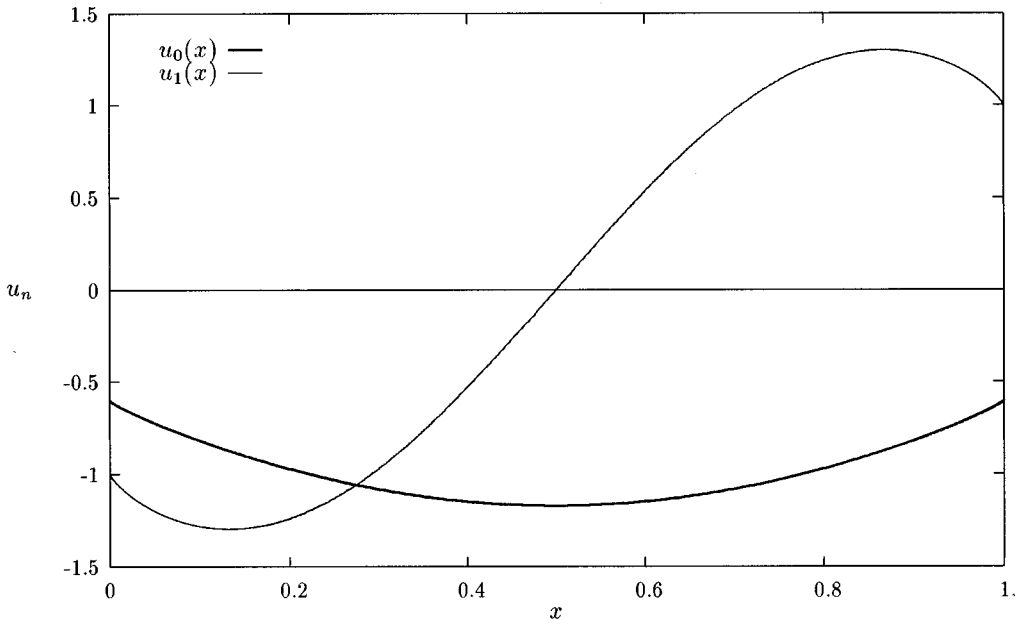

FIG. 8. The eigenfunctions $u_0(x)$ and $u_1(x)$.

Fig. 9. Although these eigenfunctions are finite and look well behaved at the end points 0 and 1 of the fundamental domain (they are there continuous), their derivatives are there infinite. It is the aim of the following subsections to give a full analytic description of the singularities of $u_n(x)$ at these end points.

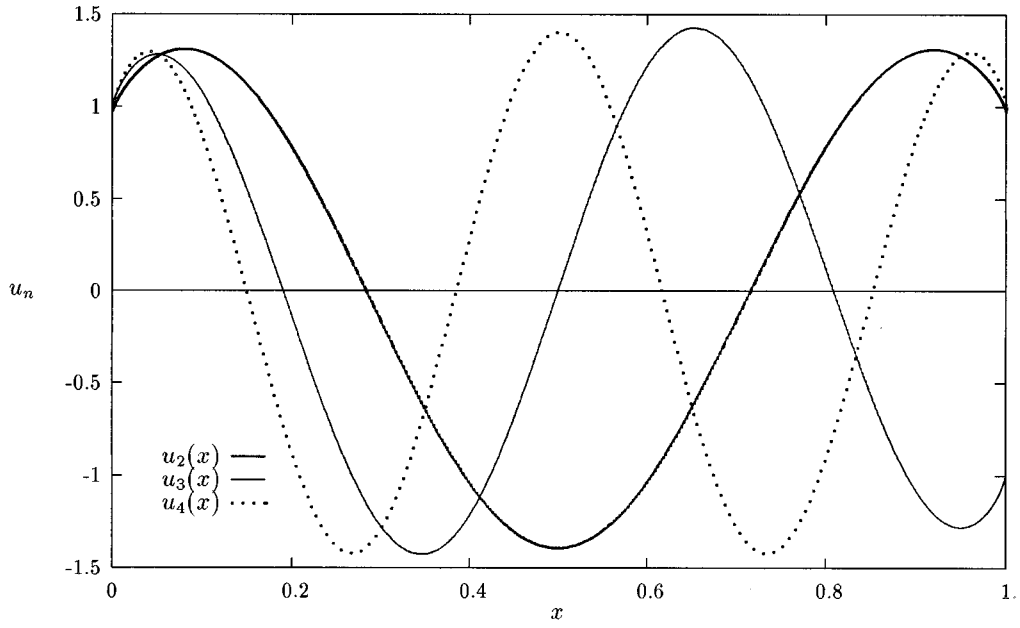

FIG. 9. The eigenfunctions $u_2(x)$, $u_3(x)$ and $u_4(x)$.

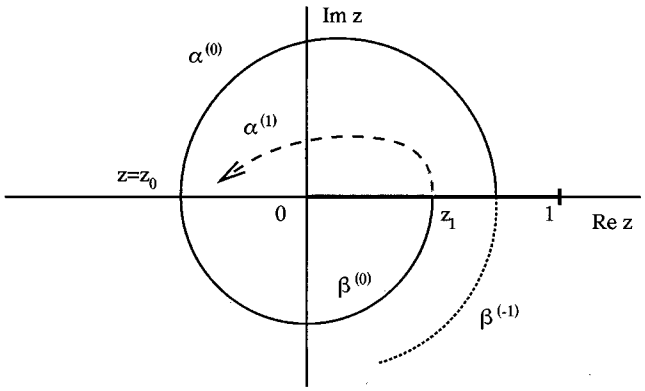

FIG. 10. Higher Riemann sheet continuations paths of $U_n^{(0)}$.

Notice that initially, in order to compute the eigenfunctions $u_n(x)$ it has been sufficient to take the range of the variable x to be the same as that of the integration variable t. Usually to compute the function from the left hand side of an integral equation for values of the variable x outside this initial range, we take the so-called Nystrøm continuation, which consists simply of substituting the new values of x in the right hand side of the equation. However this is possible *only* if the kernel is holomorphic in some given region and so this method is not applicable in our case because of the modulus function inside the logarithm which spoils holomorphy. Thus if in Eq. (57) we take x to be negative, the left hand side ''$u_n(x)$'' *is not* the analytic continuation of the function $u_n(t)$ which appears on the right hand side.

2. The functions $U_n^{(0)}(z)$ and their analytic continuations $U_n^{(\pm k)}(z)$

The function $u_n(x)$, which was defined in this naive way for negative values of x, may be used to introduce a new function $U_n^{(0)}(z)$ which is analytic and, although different from $u_n(x)$ when $x \in [0,1]$, is intimately related to it. Noticing that for $x<0$ *and* $\forall t \in [0,1]$ we have $\log|t-x| = \log(t-x)$, we shall define $U_n^{(0)}(z)$ by

$$U_n^{(0)}(z) \overset{\text{def}}{=} \lambda_n \int_0^1 \log(t-z) u_n(t)\, dt, \quad n=1,2,3,\ldots . \tag{58}$$

Taking the cut of $\log(Z) \equiv \log(t-z)$ along the real negative axis of the complex $Z \equiv t-z$ plane, $U_n^{(0)}(z)$ is a complex function of real type, $U_n^{(0)}(z) = \overline{U_n^{(0)}(\overline{z})}$, having, as we shall show later, a branch point at the origin and a cut lying on the positive real axis. Since we are interested in the singularity of the function near the origin we shall consider the detailed behaviour of $U_n^{(0)}(z)$ only in the neighbourhood of $z=0$. A similar analysis can be performed at the point $z=1$.

The superscript ($^{(0)}$ in the present case) of $U_n^{(k)}(z)$ denotes the Riemann sheet under consideration. Our notation will be such that, by crossing the cut of $U_n^{(k)}$ between $z=0$ and $z=1$ in *an anti-clockwise* way, the value of the superscript increases by 1: see, in Fig. 10, the full line $\alpha^{(0)}-\beta^{(0)}$ from the sheet (0), which is continued by the dashed line $\alpha^{(1)}$ lying on sheet (1). Conversely, crossing the cut between 0 and 1 in the *clockwise* direction, we pass from the full line $\alpha^{(0)}$ from the sheet (0) to the dotted line $\beta^{(-1)}$ from the sheet (-1).

We will want to continue the function $U_n^{(0)}(z)$ defined by the right hand side integral from Eq. (58), starting from some point $z=z_0$ ($z_0<0$), along the full line path $\beta^{(0)}$ and the dashed line $\alpha^{(1)}$, back to z_0, obtaining in this way the value $U_n^{(1)}(z_0)$ of $U_n(z)$ on the next Riemann sheet. But in so doing we will need to deform the integration contour on the right hand side of Eq. (58) into the upper half complex t-plane as we did in the case of the free term in Section IV. We are faced,

however, with the difficulty that $u_n(t)$, as it stands, is defined only on the real segment $0 \leqslant t \leqslant 1$. We therefore need to express $u_n(t)$ as the value of some analytic function on the upper edge of the cut. Here we will be interested only in the *upper lip* of the cut, since moving in an anti-clockwise direction, the analytic continuation path will hook and deform the integration contour into the *upper half* of the complex t-plane (see the curve C from Fig. 5).

3. Expressing $u_n(t)$, $0<t<1$, in terms of $U_n^{(0)}(t+i\epsilon)$ and $U_n^{(1)}(t+i\epsilon)$

Our first concern will be to rewrite the functions appearing under the integral sign of Eq. (58) as combinations of analytic functions. To this end we again use the definition (58) and start from some point $z=z_0$, $z_0<0$. We first continue $U_n^{(0)}(z)$ along a path lying in the lower half z-plane to a point $z_-=z_1-i\epsilon$, $0<z_1<1$, $\epsilon>0$, below the segment $[0,1]$ (along the path $\beta^{(0)}$ from Fig. 10). If the cut of $\log(Z)\equiv\log(t-z)$ is taken to run along the negative real Z-axis, we have

$$\lim_{\epsilon \searrow 0} \log[t-(z_1-i\epsilon)] = \begin{cases} \log|t-z_1|+i\pi & \text{if } t<z_1, \\ \log|t-z_1| & \text{if } t>z_1. \end{cases}$$

We now split the integral along the segment $[0,1]$ into one between 0 and z_1 (where, of course, $t<z_1$ and so the integral runs along the upper lip of the cut of the logarithm), and a second one, between z_1 and 1, where the integration points stay apart from the cut of the logarithm. In this way we get

$$\begin{aligned} U_n^{(0)}(z_1-i\epsilon) &= \lambda_n \int_0^{z_1} \log|t-z_1| u_n(t)dt + \pi i \lambda_n \int_0^{z_1} u_n(t)dt + \lambda_n \int_{z_1}^{1} \log|t-z_1| u_n(t)dt \\ &= u_n(z_1) + \pi i \lambda_n \int_0^{z_1} u_n(t)dt, \end{aligned} \tag{59}$$

where the last equality follows simply from the fact that the first and the third terms combine to give exactly the right hand side of Eq. (57).

Similarly we can make an analytic continuation from $z=z_0<0$ (along the path $\alpha^{(0)}$ from Fig. 10) to the point $z_+=z_1+i\epsilon$ above the cut, to obtain

$$\begin{aligned} U_n^{(0)}(z_1+i\epsilon) &= \lambda_n \int_0^{z_1} \log|t-z_1| u_n(t)dt - \pi i \lambda_n \int_0^{z_1} u_n(t)dt + \lambda_n \int_{z_1}^{1} \log|t-z_1| u_n(t)dt \\ &= u_n(z_1) - \pi i \lambda_n \int_0^{z_1} u_n(t)dt. \end{aligned} \tag{60}$$

The integral over $u_n(t)$ can be eliminated between Eqs. (59) and (60) by taking the sum of the right hand sides, so that

$$\begin{aligned} u_n(z_1) &= \frac{1}{2}\,[U_n^{(0)}(z_1+i\epsilon)+U_n^{(0)}(z_1-i\epsilon)] + \mathcal{O}(\epsilon) \\ &= \frac{1}{2}\,[U_n^{(0)}(z_1+i\epsilon)+U_n^{(1)}(z_1+i\epsilon)] + \mathcal{O}(\epsilon). \end{aligned} \tag{61}$$

Here the last line of Eq. (61) follows from the fact that the values of $U_n^{(1)}$ of the function U_n on the next Riemann sheet on the *upper lip* of the cut, merge, by definition [see also Eq. (17)], with those of $U_n^{(0)}$ *below* the cut:

$$U_n^{(0)}(z_1-i\epsilon) = U_n^{(1)}(z_1+i\epsilon) + \mathcal{O}(\epsilon), \quad 0<z_1<1.$$

4. A Volterra equation for $U_n^{(1)}(z)$

We shall now be able to deform the integration contour in the complex t-plane in the same way as we did in Section IV. Recalling that by the analytic continuation of $U_n^{(0)}(z)$ along the path $\beta^{(0)}-\alpha^{(1)}$ from Fig. 10 one obtains the function $U_n^{(1)}(z)$, we find

$$U_n^{(1)}(z_0)=\lambda_n\int_C \log(t-z_0)\,\frac{U_n^{(0)}(t)+U_n^{(1)}(t)}{2}\,dt, \tag{62}$$

where the integration contour C is shown in Fig. 5 and where we have replaced $u_n(t)$ under the integrand by its holomorphic expression (61). The dashed line represents the cut of $\log(t-z_0)$ in the complex t-plane, where, again, the $+i\pi$-*zone* and $-i\pi$-*zone* mean that the logarithm differs there by $+i\pi$ and $-i\pi$ with respect to its mean value across the cut. In the region $\mathrm{Re}\,t<0$, both $U_n^{(0)}$ and $U_n^{(1)}$ are holomorphic. So—recollect the discussion from Section IV which led to Eq. (14)—the integral over the $\mathrm{Re}\,t<0$ half-plane part of the contour C yields

$$-i\pi\lambda_n\int_{z_0}^{0}[U_n^{(0)}(t)+U_n^{(1)}(t)]dt,$$

while the rest of the integral, between $t=0$ and $t=1$, is identical with that from definition (58) of the function $U_n^{(0)}(z_0)$. So, Eq. (62) can be rewritten in the form

$$U_n^{(1)}(z)=U_n^{(0)}(z)+i\pi\lambda_n\int_0^z[U_n^{(0)}(t)+U_n^{(1)}(t)]dt, \tag{63}$$

which is valid for any z in the cut complex plane since it involves only analytic expressions. Equation (63) can be regarded as a Volterra integral equation for $U_n^{(1)}(z)$ if the function $U_n^{(0)}(z)$ is known, or equally, as a Volterra integral equation for $U_n^{(0)}(z)$ if $U_n^{(1)}(z)$ were known.

This equation can be solved by differentiation. We find immediately

$$\frac{dU_n^{(1)}(z)}{dz}-\frac{dU_n^{(0)}(z)}{dz}=+i\pi\lambda_n[U_n^{(0)}(z)+U_n^{(1)}(z)], \tag{64}$$

or, rearranging the terms,

$$\frac{dU_n^{(1)}(z)}{dz}-i\pi\lambda_nU_n^{(1)}(z)=\frac{dU_n^{(0)}(z)}{dz}+i\pi\lambda_nU_n^{(0)}(z).$$

This can be rewritten in the form

$$\exp(+i\pi\lambda_nz)\,\frac{d}{dz}\,[\exp(-i\pi\lambda_nz)U_n^{(1)}(z)]=\exp(-i\pi\lambda_nz)\,\frac{d}{dz}\,[\exp(+i\pi\lambda_nz)U_n^{(0)}(z)].$$

Now, from Eq. (63) it is obvious that $U_n^{(1)}(0)=U_n^{(0)}(0)$. This is an initial condition which permits us to write the solution of the Volterra equation as

$$U_n^{(1)}(z)=U_n^{(0)}(z)+2i\pi\lambda_n\int_0^z\exp[i\pi\lambda_n(z-t)]U_n^{(0)}(t)dt. \tag{65}$$

Similarly we can step backwards and express $U_n^{(0)}$ with respect to $U_n^{(1)}$, or $U_n^{(-1)}$ with respect to $U_n^{(0)}$:

$$U_n^{(-1)}(z)=U_n^{(0)}(z)-2i\pi\lambda_n\int_0^z \exp[-i\pi\lambda_n(z-t)]U_n^{(0)}(t)dt. \tag{66}$$

5. Asymptotic expansion

To begin with, we shall suppose that each of the functions $U_n^{(0)}(z)$ admits an expansion around the origin of the form

$$U_n^{(0)}(z)=U_{n,\mathrm{asy}}^{(0)}(z)+U_{n,\mathrm{rem}}^{(0)}(z)\equiv\sum_{k=0}^{r} a_k z^k+\sum_{m=1}^{r}\sum_{k=1}^{r} b_{mk}z^m\cdot\log^k(-z)+U_{n,\mathrm{rem}}^{(0)}(z), \tag{67}$$

where $U_{n,\mathrm{rem}}^{(0)}$ is $\mathcal{O}(|z|^{r+1-\eta})$. The choice of these series may look very restrictive, but once we have shown their consistency, their uniqueness follows from the uniqueness of the solution of a linear integral equation with a Hilbert-Schmidt kernel. In Eq. (67) the sum $\Sigma_{k=0}^{r}a_k z^k$ comes from the holomorphic part of $U_n^{(0)}$ around $z=0$. Taking as before the cut of $\log(Z)\equiv\log(-z)$ along the negative real Z-axis, the right hand side of Eq. (67) will be holomorphic throughout the domain Ω which has a cut running along the positive real axis (see Fig. 6). From the definition (58) we see that $U_n^{(0)}(z)$ is a real-analytic function [i.e. $U_n^{(0)}(z)=\overline{U_n^{(0)}(\overline{z})}$] and so the coefficients a_k ($k=0,1,2...$) and b_{mk} ($m,k=1,2,...$) have to be real. The coefficients b_{mk} are then determined in a recursive manner from the coefficients a_k of the regular part.

In order to find the coefficients b_{mk} we first notice that the analytic continuation of $U_{n,\mathrm{asy}}^{(0)}$ across the cut yields

$$U_{n,\mathrm{asy}}^{(1)}(z)=\sum_{k=0}^{r} a_k z^k+\sum_{m=1}^{r}\sum_{k=1}^{r} b_{mk}z^m\cdot[\log(-z)+2i\pi]^k. \tag{68}$$

Inserting the expressions (67) and (68) in Eq. (64) we may then compare the various terms appearing in the left and right hand sides. This comparison can be done for any z in the open set Ω, for instance for negative real z, in order to be away from the cut of $\log(-z)$. Taking the limit $z\to 0$ in both sides we remark that

$$b_{1k}=0,\quad k=2,3,\ldots, \tag{69}$$

as a consequence of the fact that the differences of terms of the type $z[\log(-z)+2i\pi]^k$ and $z\log^k(-z)$ from the left hand side of Eq. (64) yield, by differentiation, terms which tend to infinity and which are not compensated by similar terms from the right hand side. Looking at the constant terms we get

$$b_{11}=\lambda_n a_0. \tag{70}$$

Similarly, by differentiating with respect to z both sides of Eq. (64) we obtain

$$b_{mk}=0\quad \text{if } k\geqslant m+1, \tag{71}$$

while the coefficients b_{mk} with $k\leqslant m$ can be expressed iteratively by means of the coefficients a_k. So, for instance, we find

$$b_{21}=\frac{2a_1\lambda_n-a_0\lambda_n^2}{4},\quad b_{22}=\frac{a_0\lambda_n^2}{4}. \tag{72}$$

We tried to check numerically the accuracy of this asymptotic expansion in regions close to the singularity. To this end we took two terms from the holomorphic part of $U_{n,\mathrm{asy}}^{(0)}(z)$, and expressed

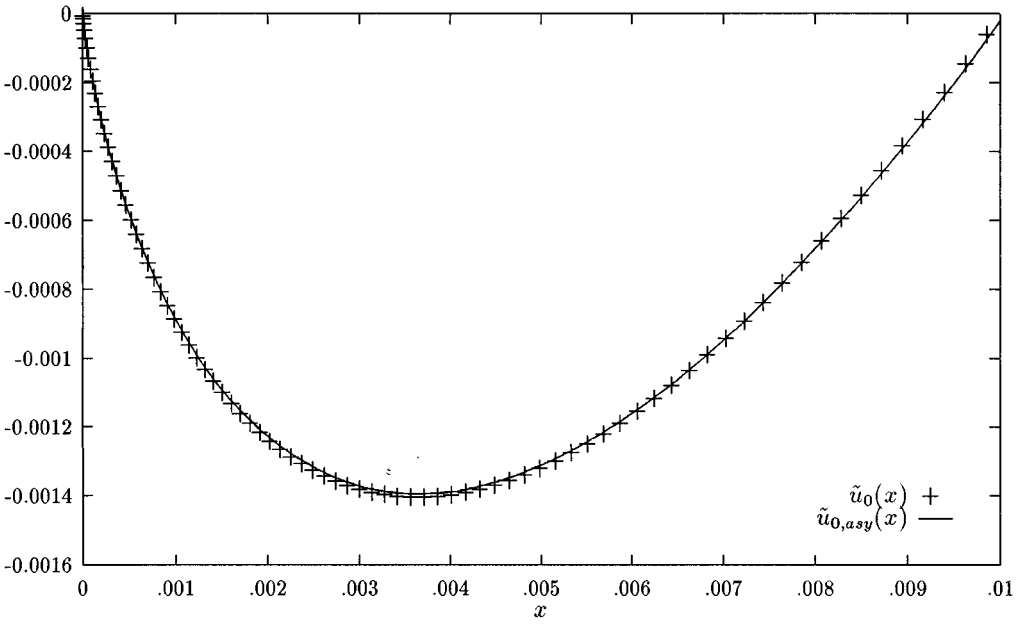

FIG. 11. One parameter asymptotic fit of $\tilde{u}_0(x)$.

the corresponding b_{mk} coefficients in terms of the first two coefficients a_0 and a_1. Since a_0 is determined by the value at $x=0$ of the eigenfunctions which, in turn, is determined by the normalization condition, we have in fact *only one free parameter*, the coefficient a_1. Using the above expressions for b_{11}, b_{21} and b_{22} in terms of a_0 (given) and a_1 (free), we have chosen a_1 to obtain the best fit to the first few eigenfunctions, in the region [0,0.01] near the origin where we expected the asymptotic expansion to hold. When we plot the function $u_n(x)$ together with our asymptotic expansion the two curves appear identical on the interval [0,0.01]. In order to show the slight difference in these functions we have defined a new function $\tilde{u}_n(x)=u_n(x)-u_n(0)-[u_n(x_1)-u_n(0)]x/x_1$ which has its end points $\tilde{u}_n(0)$ and $\tilde{u}_n(0.01)$ at the same height and so permits the use of a much enlarged y-axis scale. The corresponding plots for the two first eigenfunctions are presented in Figs. 11 and 12. Although as it has been already stressed, these curves are just one parameter fits and that moreover we have restricted ourselves only to the first terms in the asymptotic expression, the agreement between these asymptotic expressions (the full lines) with the computer calculated points of the eigenfunctions (the crosses) is really excellent.

VI. RESUME AND CONCLUSIONS

As indicated in the Introduction, the numerical calculations related to the solution of the inverse problem for EIT are seriously hampered by the high number of mesh points necessary to take into account the sharp peaks of the current density near the edge of the electrodes. Since these peaks seemed to be intrinsic objects describable by only a small numbers of parameters we have investigated the details of their analytic structure. To this end we have studied the Riemann sheet structure of the eigenfunctions of the dominant singular integral equation relating to the solution of the mixed boundary problem for the potential, and derived asymptotic expressions both for the eigenfunctions and for the solution of the integral equation. These asymptotic expressions provide very simple parametrisations for the anomalous thresholds, whose effectiveness can be judged from the Figs. 11 and 12.

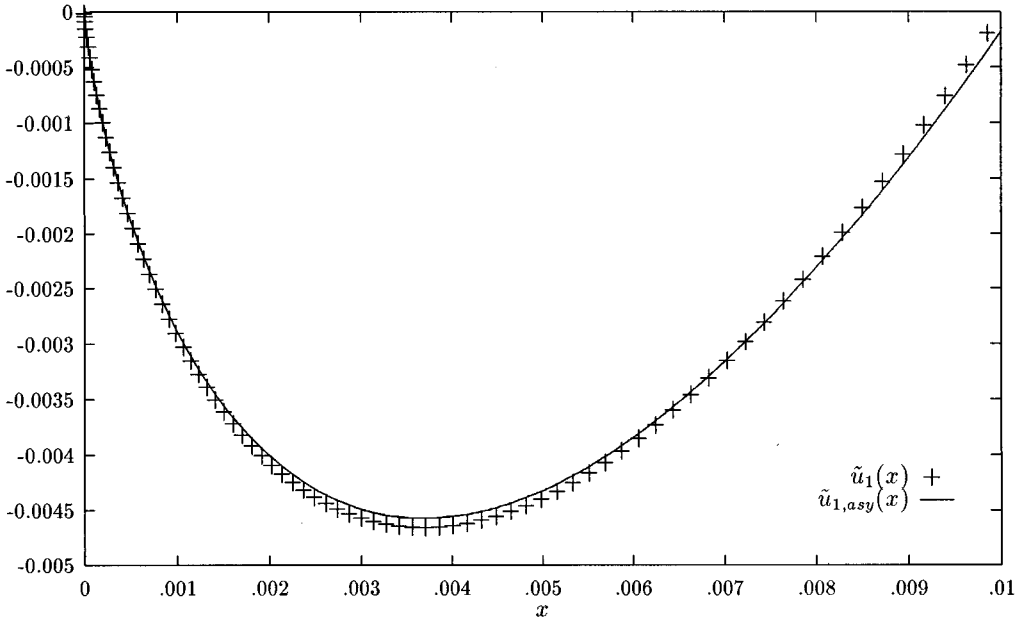

FIG. 12. One parameter asymptotic fit of $\tilde{u}_1(x)$.

The paper is constructed as follows: In the Introduction and in Section II the mathematics of the EIT modelling is discussed while the corresponding weakly singular integral equation is given in Section III. In Section IV we have discussed the effect on the singularities of the free term of the moving cut of the logarithm which ''hooks'' the integration contour. The *generic singularities* of the solution of the integral equation are then described as a superposition of those of the free term and of the eigenfunctions which were derived in Section V B. Section V A contains the proof that although we deal with infinite series, no new singularities appear in the neighbourhood of the origin, i.e. the singularities of the solution are really those of the eigenfunctions and of the free term. We also determine the limits of the domain where the eigenfunction sum converges unconditionally and show how one can extend the validity of the asymptotic series also on the real segment [0,1].

We hope that the discussion of the analytic properties of the eigenfunctions and solution of this quite special, logarithmic singular equation, will provide a working example which might be useful also for the study of the singularities of the solution of other weakly singular integral equations. The discontinuities across the cuts will certainly be different, but the general discussion will probably be fairly similar.

ACKNOWLEDGMENTS

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APPENDIX: COMPLETENESS OF THE BASIS $\{u_n\}$

Following a proof given by Auberson,[14] we shall show in what follows that ker **K**, the null space of the logarithmic kernel, is empty and so the eigenfunctions $\{u_n\}_{n=0,1,2\ldots}$ do span the whole Hilbert space of the L^2 functions on [0,1].

Suppose that ker $\mathbf{K}\neq\{0\}$, i.e. that there exists at least one non zero L^2-function ϕ such that

$$\int_0^1 \log|x-y|\,\phi(y)\,dy=0. \tag{A1}$$

Defining the function

$$v(x)\overset{\text{def}}{=}\int_0^x \phi(y)\,dy, \tag{A2}$$

we have

$$\text{(a)}\quad \frac{dv(x)}{dx}=\phi(x)\ \text{ almost everywhere,}$$

$$\text{(b)}\quad v(0)=0.$$

We can easily prove that the function $v(x)$ satisfies a Hölder condition of index 1/2

$$|v(x_1)-v(x_2)|\leqslant A|x_1-x_2|^{1/2},\quad \text{for } \forall x_1,x_2\in(0,1),$$

where A is a positive constant.

By integrating the left hand side of Eq. (A1) by parts we find

$$\int_0^1 \log|x-y|\,\phi(y)\,dy=v(1)\log(1-x)-\mathscr{P}\int_0^1 \frac{v(y)}{y-x}\,dy$$

so that from Eq. (A1) we obtain

$$\mathscr{P}\int_0^1 \frac{v(y)}{y-x}\,dy=v(1)\log(1-x), \tag{A3}$$

If we now consider the following function

$$F(z)\overset{\text{def}}{=}\sqrt{z(z-1)}\int_0^1 \frac{v(y)}{y-z}\,dy\quad \text{for } z\in D \tag{A4}$$

where D is the complex z-plane cut along the segment [0,1], we can show that

(i) F is a holomorphic function in D;
(ii) $\lim_{z\to\infty}F(z)=-\int_0^1 v(y)\,dy$;
(iii) $\operatorname{Im} F(x+i\epsilon)=\sqrt{x(1-x)}\,\mathscr{P}\int_0^1[v(y)/(y-x)]\,dy=\sqrt{x(1-x)}\,v(1)\log(1-x)$, for $x\in(0,1)$;
(iv) $\operatorname{Re} F(x+i\epsilon)=-\pi\sqrt{x(1-x)}\,v(x)$, for $x\in(0,1)$.

The properties (i)–(iii) imply that

$$F(z)=\frac{v(1)}{\pi}\int_0^1 \frac{\sqrt{y(1-y)}\log(1-y)}{y-z}\,dy-\int_0^1 v(y)\,dy,\quad z\in D, \tag{A5}$$

while from (iv) it follows that for $x \in (0,1)$ we have

$$-\pi\sqrt{x(1-x)}v(x)=\frac{v(1)}{\pi}\mathscr{P}\int_0^1 \frac{\sqrt{y(1-y)}\log(1-y)}{y-x}\,dy-\int_0^1 v(y)dy. \tag{A6}$$

Taking now the limits $x\searrow 0$ and $x\nearrow 1$ we find

$$\frac{v(1)}{\pi}\int_0^1 \sqrt{\frac{1-y}{y}}\log(1-y)dy-\int_0^1 v(y)dy=0, \tag{A7}$$

$$-\frac{v(1)}{\pi}\int_0^1 \sqrt{\frac{y}{1-y}}\log(1-y)dy-\int_0^1 v(y)dy=0. \tag{A8}$$

Subtracting (A8) from (A7) we see that $v(1)=0$ and hence, from Eq. (A6),

$$v(x)=\frac{1}{\pi\sqrt{x(1-x)}}\int_0^1 v(y)dy\equiv\frac{C}{\pi\sqrt{x(1-x)}}. \tag{A9}$$

Now, since $v(1)$ is zero, the constant C also has to be zero and so $v(x)$ has to vanish identically [it had to be so since neither the right hand side of Eq. (A9) and even less its derivative are L^2]. This implies that ker**K** is an empty set and so the eigenfunctions $\{u_n\}$ of the logarithmic kernel form a complete L^2 basis on the segment [0,1].

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Localized solutions of the Dirac–Maxwell equations

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The full classical Dirac–Maxwell equations are considered in a somewhat novel form and under various simplifying assumptions. A reduction of the equations is performed in the case when the Dirac field is static. A further reduction of the equations is made under the assumption of spherical symmetry. These static spherically symmetric equations are examined in some detail and a numerical solution presented. Some surprising results emerge from this investigation: (i) Spherical symmetry necessitates the existence of a magnetic monopole. (ii) There exists a uniquely defined solution, determined only by the demand that the solution be analytic at infinity. (iii) The equations describe highly compact objects with an inner onion like shell structure. © *1996 American Institute of Physics.*
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I. INTRODUCTION

It is an interesting exercise to compare the current development of a quantum theory of gravitation, from the fully non-linear Einstein theory, to the development of QED from the linearized Dirac–Maxwell theory. The most startling difference is the large body of work on the classical, non-linear, theory of gravitation (general relativity)—a theory which includes, in a self consistent manner, the interactions of the gravitational field itself. There is no comparable body of work on the full Dirac–Maxwell theory (Dirac equations with electromagnetic interaction, Maxwell equations with Dirac field source—the so-called ''self interaction''). Of course this situation arose, historically, because of the rapid development and stunning success of QED.

Einstein's equations provide a much better description of gravity than do the linear spin-2 equations. Indeed, one can ''derive'' classical general relativity from the linear, massless spin-2 theory by summing all the Feynman diagrams to tree level—see Refs. 1 and 2. The full Dirac–Maxwell equations should provide a much better description of electronic matter than their linearized counterparts (in which self terms are ignored).

Explicit solutions to the Dirac–Maxwell equations are rare, see Ref. 3. Uniqueness and existence results for this system have been known for some time, see Ref. 4 and references therein. More recently, existence results have been obtained for ''soliton like'' solutions.[5,6] Theorem 1 of Ref. 5 proves the existence of solutions to the Dirac–Maxwell equations as a critical point of the Dirac–Maxwell action functional in the Sobelev space $H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$; with the Dirac spinor being a smooth function exponentially decreasing at infinity, together with all its derivatives. The solutions presented here are quite different, they are singular at the origin and behave like $1/r^4$ near infinity.

There exist a number of solutions to the Yang–Mills–Dirac and Yang–Mills–Dirac–Higgs equations, see Ref. 7 and the comprehensive list of references contained therein.

The paper is organized as follows: in Sec. II we write the equations in 2-spinor form, this description then allows us to (covariantly) solve the Dirac equations for the electromagnetic potential and so write down a complete set of equations in terms of the Dirac field. In Sec. III we examine the static and spherically symmetric reductions of the equations. In Sec. IV we deal with

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some general properties of the static spherically symmetric system and in Sec. V present a numerical solution to this system.

II. The Dirac–Maxwell Equations

In standard notation the Dirac-Maxwell equations are

$$\gamma^{\alpha}(\partial_{\alpha}-ieA_{\alpha})\psi+im\psi=0, \quad F_{\alpha\beta}=A_{\beta,\alpha}-A_{\alpha,\beta},$$
$$\partial^{\alpha}F_{\alpha\beta}=-4\pi ej_{\beta}=-4\pi e\overline{\psi}\gamma_{\beta}\psi. \tag{1}$$

Employing the γ_5-diagonal or van der Waerden description, see for example Ref. 8, we have

$$\gamma^{\alpha}=\sqrt{2}\begin{pmatrix} 0 & \sigma^{\alpha}_{B\dot{B}} \\ \sigma^{\alpha A\dot{A}} & 0 \end{pmatrix},$$

with $\sigma^{\alpha}_{A\dot{A}}$ the van der Waerden symbols, i.e.

$$(\sigma^{0}_{A\dot{A}})=\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{and} \quad (\sigma^{j}_{A\dot{A}})=\frac{1}{\sqrt{2}}\times \text{Pauli Matrix}, \quad j=1,2,3.$$

Where $A,B=0,1$ and $\dot{A},\dot{B}=\dot{0},\dot{1}$ are two-spinor indices (see Ref. 8). The Dirac bispinor, ψ is

$$\psi=\begin{pmatrix} u_A \\ \overline{v^{\dot{B}}} \end{pmatrix} \quad \text{and} \quad \overline{\psi}=(v^{B},\overline{u_{\dot{A}}}).$$

So that the Dirac equations become

$$(\partial^{A\dot{A}}-ieA^{A\dot{A}})u_A+\frac{im}{\sqrt{2}}\,\overline{v^{\dot{A}}}=0, \quad (\partial^{A\dot{A}}+ieA^{A\dot{A}})v_A+\frac{im}{\sqrt{2}}\,\overline{u^{\dot{A}}}=0, \tag{2}$$

where $\partial^{A\dot{A}}\equiv\sigma^{\alpha A\dot{A}}\partial_{\alpha}$, $A^{A\dot{A}}=\sigma^{\alpha A\dot{A}}A_{\alpha}$.

The Maxwell equations are

$$\partial^{\alpha}F_{\alpha\beta}=-4\pi ej_{\beta}=-4\pi e\sigma^{A\dot{A}}_{\beta}(u_A\overline{u_{\dot{A}}}+v_A\overline{v_{\dot{A}}}). \tag{3}$$

In the linearized theory the ''self current'' j_{β} is ignored. We now eliminate the potential $A^{A\dot{A}}$ using (2)-another approach is to eliminate ''A^{self}_{α}'' using the formal Green's function[3,9]—we will use purely algebraic methods. From Eqs. (2) we have

$$v^{A}\partial^{B\dot{A}}u_B+u^{A}\partial^{B\dot{A}}v_B+\frac{im}{\sqrt{2}}\,(v^{A}\overline{v^{\dot{A}}}+u^{A}\overline{u^{\dot{A}}})=ie[A^{B\dot{A}}(v^{A}u_B-u^{A}v_B)]. \tag{4}$$

However, because of the two-dimensionality of the 2-spinor space we have

$$v_Au_B-u_Av_B=\epsilon_{AB}(u^{C}v_C).$$

Here, $\epsilon_{01}=\epsilon^{01}=1$, $\epsilon_{10}=\epsilon^{10}=-1$, $\epsilon^{00}=\epsilon_{00}=\epsilon^{11}=\epsilon_{11}=0$; we define $\xi^{A}=\epsilon^{AB}\xi_B$ and $\xi_A=\epsilon_{BA}\xi^{B}$.

We assume that $u^{C}v_C\neq0$ almost everywhere. Now, $j^{\alpha}j_{\alpha}=|u^{A}v_A|^2$, so $u^{C}v_C\equiv0$ implies that the current vector, j, is null—a massive neutrino field.

We can now solve (4) for the electromagnetic potential A,

$$A^{A\dot{A}}=\frac{i}{e(u^c v_c)}\left\{v^A\partial^{B\dot{A}}u_B+u^A\partial^{B\dot{A}}v_B+\frac{im}{\sqrt{2}}\,(u^A\overline{u^{\dot{A}}}+v^A\overline{v^{\dot{A}}})\right\}. \tag{5}$$

Notice that, from (5), under the gauge transformation

$$\begin{pmatrix} u_A \\ \overline{v^{\dot{B}}}\end{pmatrix}\to e^{i\chi}\begin{pmatrix} u_A \\ \overline{v^{\dot{B}}}\end{pmatrix}\quad\text{we have}\quad A_\alpha\to A_\alpha+\frac{1}{e}\,\partial_\alpha\chi$$

as we should expect!

The four complex equations (2) actually over determine the four *real* quantities A_α. We must impose on (5) the condition that A_α is real. These reality conditions can be written as

$$\overline{(A^{A\dot{A}}u_A\overline{u_{\dot{A}}})}=A^{A\dot{A}}u_A\overline{u_{\dot{A}}},\quad \overline{(A^{A\dot{A}}v_A\overline{v_{\dot{A}}})}=A^{A\dot{A}}v_A\overline{v_{\dot{A}}},\quad \overline{(A^{A\dot{A}}u_A\overline{v_{\dot{A}}})}=A^{A\dot{A}}v_A\overline{u_{\dot{A}}}.$$

With the use of (5) these reality conditions become

$$\begin{aligned}\partial^{A\dot{A}}(u_A\overline{u_{\dot{A}}})&=-\frac{im}{\sqrt{2}}\,(u^C v_C-\overline{u^{\dot{C}}}\,\overline{v_{\dot{C}}}),\\ \partial^{A\dot{A}}(v_A\overline{v_A})&=\frac{im}{\sqrt{2}}\,(u^C v_C-\overline{u^{\dot{C}}}\,\overline{v_{\dot{C}}}),\\ u_A\partial^{A\dot{A}}\overline{v_{\dot{A}}}-\overline{v_{\dot{A}}}\partial^{A\dot{A}}u_A&=0.\end{aligned} \tag{6}$$

These equations constitute four real first order equations for the four complex quantities u^A and v^A. A further four real third order equations for these quantities is obtained upon substitution of (5) into the Maxwell equations (3). Note that adding the first two equations of (6) leads to the equation of conservation for j^α.

III. REDUCTION OF THE SYSTEM

A. The static equations

Firstly, we impose the condition that the field is static. We assume that there exists a Cartesian Lorentz frame in which $j^\alpha=\delta_0^\alpha j^0$. Imposing this condition one quickly finds that

$$v^A=e^{i\chi}\sqrt{2}\sigma^{0A\dot{A}}\overline{u_{\dot{A}}},\ \text{with}\ \chi\ \text{a real function.}$$

The current vector is now

$$j^\alpha=\sqrt{2}(u^0\overline{u^0}+u^1\overline{u^1})\,\delta_0^\alpha.$$

The reality conditions are

$$\begin{aligned}\partial_{A\dot{A}}(u^A\overline{u^A})&=\frac{-2m}{\sqrt{2}}\,(|u^0|^2+|u^1|^2)\sin\chi,\\ (\partial_{0\dot{0}}+\partial_{1\dot{1}})(|u^0|^2+|u^1|^2)&=0,\\ u^0(\partial_{0\dot{0}}+\partial_{1\dot{1}})u^1-u^1(\partial_{0\dot{0}}+\partial_{1\dot{1}})u^0&=i[u^0u^1(\partial_{0\dot{0}}-\partial_{1\dot{1}})+(u^1)^2\partial_{1\dot{0}}-(u^0)^2\partial_{1\dot{1}}]\chi,\end{aligned}$$

the expressions for the potential $A^{A\dot{A}}$ can now be written down, although we will not do this at this stage.

Now under a gauge transformation we have

$$u^A \to e^{i\mu} u^A \quad \text{and} \quad A_\alpha \to A_\alpha + \frac{1}{e}\,\partial_\alpha \mu.$$

We fix the gauge by defining real functions X, Y and η as follows:

$$u^0 = X e^{i/2(\chi+\eta)}, \quad u^1 = Y e^{i/2(\chi-\eta)}.$$

Our equations can be given in a particularly suggestive three vector form by writing (in our Cartesian coordinates)

$$l = (\sigma^{\alpha}_{A\dot{A}} u^A \overline{u^A}) = \left(l^0, \frac{1}{\sqrt{2}}\,\mathbf{V} \right)$$

with

$$l^0 = \frac{1}{\sqrt{2}}\,(X^2 + Y^2)$$

and

$$\mathbf{V} = (2XY\,\cos\,\eta, 2XY\,\sin\,\eta, X^2 - Y^2).$$

The reality conditions become

$$\frac{\partial}{\partial t}\,(X^2+Y^2) = 0, \quad \boldsymbol{\nabla}\cdot\mathbf{V} = -2m(X^2+Y^2)\sin\,\chi, \quad \frac{\partial \mathbf{V}}{\partial t} + (\boldsymbol{\nabla}\chi)\times\mathbf{V} = \mathbf{0}.$$

With electromagnetic potential

$$A^0 = \frac{m}{e}\,\cos\,\chi + \frac{(X^2-Y^2)}{2e(X^2+Y^2)}\,\frac{\partial \eta}{\partial t} + \frac{(\boldsymbol{\nabla}\chi)\cdot\mathbf{V}}{2e(X^2+Y^2)},$$

$$\mathbf{A} = \frac{1}{2e(X^2+Y^2)}\left[\frac{\partial \chi}{\partial t}\,\mathbf{V} + (X^2-Y^2)\boldsymbol{\nabla}\eta - \boldsymbol{\nabla}\times\mathbf{V} \right], \quad \text{where } \mathbf{A} = (A^1, A^2, A^3).$$

The full system is given by the above two sets of equations and the Maxwell equations.

B. Spherical symmetry

We now impose spherical symmetry upon our static system. A minimal requirement that the Dirac field be static and spherically symmetric (in any gauge) is that the vector l, above, is spherically symmetric. We require

$$[X_i, l] = 0,$$

where the X_i, $i=1,2,3$, are the three (vector) generators of rotations.

These conditions imply that l has time and radial components only and that these components are functions of (t,r) only, $r = \sqrt{(x^1)^2+(x^2)^2+(x^3)^2}$.

Using the notation above we have

$$X^2+Y^2=R=R(r), \quad \text{only} \quad \mathbf{V}=|\mathbf{V}|\hat{\mathbf{r}}=R\hat{\mathbf{r}},$$

where $\hat{\mathbf{r}}=(\sin\theta\cos\phi,\sin\theta\sin\phi,\cos\theta)$ in terms of the polar coordinates r, θ, ϕ. We have

$$X=\sqrt{R}\,\cos(\theta/2), \quad Y=\sqrt{R}\,\sin(\theta/2), \quad \eta=\phi.$$

The Dirac bispinor is now

$$\psi=\sqrt{R}\begin{pmatrix} -e^{(i/2)(\chi-\phi)}\sin(\theta/2) \\ e^{(i/2)(\chi+\phi)}\cos(\theta/2) \\ -e^{-(i/2)(\chi+\phi)}\sin(\theta/2) \\ e^{-(i/2)(\chi-\phi)}\cos(\theta/2) \end{pmatrix}.$$

The equations are now as follows

$$\chi=\chi(r), \quad R=R(r), \quad \mathbf{A}=\frac{1}{2e}\frac{\cot\theta}{r}\hat{\phi},$$

$$A^0=\frac{m}{e}\cos\chi+\frac{1}{2e}\frac{d\chi}{dr},$$

$$\frac{d}{dr}(r^2R)=-2mr^2R\sin\chi, \quad \frac{d}{dr}\left(r^2\frac{dA_0}{dr}\right)=4\sqrt{2}\pi e r^2R. \tag{7}$$

The really surprising result here is the unavoidable appearance of the magnetic monopole term

$$\mathbf{A}=\frac{1}{2e}\frac{\cot\theta}{r}\hat{\phi}.$$

Here $\hat{\phi}$ is the usual azimuthal unit vector, in terms of a coordinate basis $A=-(1/2e)\cos\theta d\phi$.

We should also impose a normalization condition (or finite total charge condition) on any solution

$$\int j^\alpha dS_\alpha<\infty$$

on any space like hypersurface. This leads to the condition

$$\int_{r=0}^{\infty} r^2Rdr<\infty.$$

To end this section we rewrite the determining radial equations in a more transparent form by introducing the following new (dimensionless) variables

$$\rho=2mr, \quad a=\frac{e}{m}A^0, \quad q=4\pi\sqrt{2}\,\frac{e^2}{m}\,r^2R.$$

$$\frac{d\chi}{d\rho}=a-\cos\chi, \quad \frac{d}{d\rho}\left(\rho^2\frac{da}{d\rho}\right)=q, \quad \frac{dq}{d\rho}=-q\sin\chi. \tag{8}$$

IV. STATIC SPHERICAL SYMMETRY: GENERAL PROPERTIES

The system of equations (8) possesses the discrete symmetry

$$\chi \to \pi - \chi, \quad a \to -a, \quad q \to -q. \tag{9}$$

This is just the operation of charge conjugation; q needs to be reinterpreted (it was originally defined as non-negative) to account for the change in sign of the charge which manifests itself on the right hand side of the second equation of (8). We write $q=\epsilon Q$, with $\epsilon^2=1$ and $Q \geqslant 0$, so $Q=\sqrt{2}(e^2/m)r^2R$; then, under (9), we have $\epsilon \to -\epsilon$ and $Q \to Q$.

Our equations read,

$$\frac{d\chi}{d\rho}=a-\cos\,\chi, \quad \frac{da}{d\rho}=\frac{\epsilon f}{\rho^2}, \quad \frac{df}{d\rho}=Q, \quad \frac{dQ}{d\rho}=-Q\,\sin\,\chi, \tag{10}$$

where we have introduced the new variable f to give a set of four first order, ordinary differential equations. This new variable is directly related to the magnitude total (Dirac field) charge contained in a ball of radius r, $B(r)$,

$$e\int_{B(r)} j^{\alpha}dS_{\alpha}=e\int_{B(r)} j^0 d^3x=4\pi e\sqrt{2}\int_{s=0}^{r} s^2R(s)ds=\frac{2\pi}{e}\int_{\sigma=0}^{\rho} Q d\sigma=\frac{1}{2e}\,(f(\rho)-f(0)).$$

In view of this—and the fact that $df/dp=Q=\epsilon q$ is proportional to the charge density on a shell of radius r—we will use the following condition on our system (10):

$$\left[\begin{array}{l}\text{On } \rho>0,\ f \text{ is a bounded } C^1 \text{ function, with bounded first derivative.}\\ \text{Both } f \text{ and } \dfrac{df}{d\rho} \text{ have well defined limits as } \rho\to\infty.\end{array}\right. \tag{C1}$$

We will now develop some qualitative results which indicate the types of solution which can exist under rather general (and physically reasonable) conditions.

Lemma 1: Suppose (χ,a,f,Q) is a solution of (10) on $\rho>0$, then under C1 the function a is C^2 on $\rho>0$ with a and $da/d\rho$ bounded on intervals $\rho\geqslant\rho_1>0$ and ρa bounded on $0\leqslant\rho\leqslant\rho_1<\infty$. If $f(0)\neq 0$ or $df/d\rho(0)=Q(0)>0$ then a is unbounded as $\rho\to 0$.

Proof: We first establish that Q and f have well defined limits as ρ approaches 0. We are assuming that the solution (χ,a,f,Q) exists on $\rho>0$, so for $\rho_2>\rho_1>0$ and using Eq. (10), we have

$$|Q(\rho_2)-Q(\rho_1)|=\left|\int_{\rho_1}^{\rho_2} Q(\sigma)\sin\,\chi(\sigma)d\sigma\right|$$

$$\leqslant\int_{\rho_1}^{\rho_2}|Q\,\sin\,\chi|d\sigma<M_1(\rho_2-\rho_1), \text{ here } M_1=\sup_{\mathbf{R}^+}Q<\infty.$$

Letting ρ_1 and ρ_2 approach zero, we have $|Q(\rho_2)-Q(\rho_1)|\to 0$. Using Cauchy's criterion we conclude that $Q(0^+)$ exists. A similar argument can be given to demonstrate the existence of $f(0^+)$.

The boundedness of $da/d\rho$, on $\rho\geqslant\rho_1$ follows from

$$\epsilon\frac{da}{d\rho}=f/\rho^2$$

Integrate this expression to bound a on $\rho\geqslant\rho_1>0$.

Write $\Omega=\epsilon\rho a$, then

$$\rho\,\frac{d\Omega}{d\rho}-\Omega=f,\ \text{ and }\quad \rho\,\frac{d^2\Omega}{d\rho^2}=Q.$$

From the second of these equations we have, on $(0,\rho_1]$,

$$-M_1\,\ln\!\left(\frac{\rho_1}{\rho}\right)+\frac{d\Omega}{d\rho}\,(\rho_1)\leqslant\frac{d\Omega}{d\rho}\,(\rho)\leqslant\frac{d\Omega}{d\rho}\,(\rho_1).$$

So we have (note as a is C^2 away from $\rho=0$ so is Ω)

$$\rho\,\frac{d\Omega}{d\rho}\to 0,\ \text{ as }\ \rho\to 0.$$

Hence from the first of the Ω equations we see that Ω has a well defined limit as $\rho\to 0$, in fact

$$\lim_{\rho\to 0}\,\Omega(\rho)=-f(0).$$

An immediate consequence is that if $f(0)\neq 0$ then a is unbounded as $\rho\to 0$.

Now from (10) we have $Q\geqslant Q(0)e^{-\rho}$, so that $f(\rho)-f(0)\geqslant(df/d\rho)(0)(1-e^{-\rho})$—recall $df/d\rho=\epsilon q=Q$. Given the earlier result we may $f(0)=0$ otherwise a is unbounded. We can now integrate our $da/d\rho$ equation with this bound for f,

$$\epsilon(a(\rho)-a(\rho_1))\leqslant-\frac{df}{d\rho}\,(0)\left[\frac{(1-e^{-\rho})}{\rho}-\frac{(1-e^{-\rho_1})}{\rho_1}\right]-\frac{df}{d\rho}\,(0)\int_{\sigma=\rho}^{\rho_1}\frac{e^{-\sigma}}{\sigma}\,d\sigma.$$

As $\rho\to 0$ the integral on the right side of the inequality diverges to $+\infty$.

Lemma 2: Suppose (χ,a,f,Q) is a solution of (10) on $\infty>\rho>0$, then under C1 the function χ is C^1 with $d\chi/d\rho$ bounded on intervals $\rho\geqslant\rho_1>0$. If $f(0)\neq 0$ then χ is unbounded as $\rho\to 0$.

Proof: The regularity of χ—on its presumed interval of existence—is established using standard theory (see, for example, Ref. 10 or 11) after first noting that the right side of

$$\frac{d\chi}{d\rho}=a-\cos\,\chi$$

is C^2 in ρ (treating a as a known function and using lemma 1) and C^∞ in χ.

From the above equation we also have

$$\epsilon a-1\leqslant\epsilon\,\frac{d\chi}{d\rho}\leqslant\epsilon a+1,$$

which gives the required bounds (using lemma 1). Working on $(0,\rho_1)$ we have (as in the proof of lemma 1)

$$C_0+\frac{f(0)}{\rho}\leqslant\epsilon\,\frac{d\chi}{d\rho}\leqslant C_1+\frac{f(\rho_1)}{\rho},$$

where $C_0=\epsilon a(\rho_1)-1-f(0)/\rho_1$ and $C_1=\epsilon a(\rho_1)+1-f(\rho_1)/\rho_1$.

Integrating,

$$C_2-C_1(\rho_1-\rho)+f(\rho_1)\ln(\rho)\leqslant\epsilon\chi\leqslant C_3-C_0(\rho_1-\rho)+f(0)\ln(\rho),$$

with $C_2=\epsilon\chi(\rho_1)-f(\rho_1)\ln(\rho_1)$ and $C_3=\epsilon\chi(\rho_1)-f(0)\ln(\rho_1)$. If $f(0)<0$ choose ρ_1 near 0 so that $f(\rho_1)<0$ and we have from our last inequality that $\epsilon\chi\to\infty$ as $\rho\to 0$. If $f(0)>0$ our inequality yields $\epsilon\chi\to-\infty$ as $\rho\to 0$.

There is one other condition which makes sense ''physically'': if we have an isolated system we expect the charge density should go to zero at infinity.

$$\left[\frac{df}{d\rho}=Q\to 0, \text{ as } \rho\to\infty. \tag{C2}\right.$$

Lemma 3: Suppose (χ,a,f,Q) is a solution of (10) on $\rho>0$ under conditions C1 and C2. Then $-1\leqslant a_\infty\leqslant 1$ where $a\to a_\infty$ as $\rho\to\infty$.

Proof: We first establish that a has a well defined limit, written as a_∞, as $\rho\to\infty$; for $\rho_2>\rho_1>0$, we have

$$|a(\rho_2)-a(\rho_1)|=\left|\int_{\rho_1}^{\rho_2}\frac{f(\sigma)d\sigma}{\sigma^2}\right|<M_2\left(\frac{1}{\rho_1}-\frac{1}{\rho_2}\right), \text{ where } M_2=\sup_{\mathbb{R}^+}|f|.$$

Letting ρ_1 and ρ_2 approach ∞, we conclude that the limit $a\to a_\infty$ exists.

From the first and second equations of (10) we have

$$\frac{d}{d\rho}\ln|a-\cos\chi|=\left(\frac{da}{d\rho}+\sin\chi\,\frac{d\chi}{d\rho}\right)\Big/(a-\cos\chi)=\sin\chi-\frac{f}{\rho^2(a-\cos\chi)}.$$

Consequently, on $\rho\geqslant\rho_1>0$, integrating the last equation of (10) we have

$$-\ln[Q/Q(\rho_1)]=\int_{\rho_1}^{\rho}\sin\chi(\sigma)d\sigma=\ln\left|\frac{a-\cos\chi}{a(\rho_1)-\cos\chi(\rho_1)}\right|+\int_{\rho_1}^{\rho}\frac{f(\sigma)d\sigma}{[\sigma^2(a(\sigma)-\cos\chi(\sigma))]}.$$

Now assume $a_\infty>1$. In fact, this also takes care of the case $a_\infty<-1$, since under the discrete conjugation symmetry, (9), $a\to -a$ and in particular $a_\infty\to -a_\infty$. Working on $\rho\geqslant\rho_1>0$ we have, for ρ_1 large enough,

$$a(\rho)>1+\alpha_0>0, \text{ for } \rho\geqslant\rho_1 \text{ and some constant } \alpha_0.$$

Then, as $a-1\leqslant(d\chi/d\rho)\leqslant a+1$, so

$$0<\alpha_0<\frac{d\chi}{d\rho}<M, \text{ where } M \text{ is a finite constant—see lemma 1,}$$

$$\text{i.e., } \quad \alpha_0<a-\cos\chi<M.$$

Clearly both terms on the right side of our equation for $-\ln[Q/Q(\rho_1)]$ are bounded. This contradicts our assumption C2 that $Q\to 0$ as $\rho\to\infty$.

The constant a_∞ can be removed from the potential via a gauge transformation. Under $\psi\to e^{-ima_\infty t}\psi$, we have $a\to a-a_\infty$. After this transformation the Dirac field ψ has time dependence e^{-iEt}, where $-m\leqslant E=\alpha_\infty m\leqslant m$.

The three lemmas give a basic characterization of the solutions obeying C1 and C2. If $f(0)\neq 0$ or $Q(0)>0$ then a diverges at the origin, these are solutions which can be pictured as a Dirac field surrounding a central charged monopole—the numerical solution of Sec. 4 is of this type. There is also the possibility of solutions with a and R (recall: $Q=\sqrt{2}(e^2/m)r^2R$) everywhere bounded, such solutions were suggested by the work of Wakano,[12] who examined numerical solutions for what could be called ''half linearized'' Dirac Maxwell equations—''half linearized'': if the elec-

trostatic potential is ''dominant'' ignore the Maxwell equation involving the electromagnetic vector potential and vice versa. In fact, as the following theorem demonstrates, no such solutions exist.

Theorem: *There does not exist a non-trivial solution of (10) on $\rho\geqslant 0$ under conditions C1 and C2 with a and $P=Q/\rho^2$ bounded on $\rho\geqslant 0$.*

Proof: From lemma 1 we have, $f(0)=Q(0)=0$. Next we establish that both χ and a have well defined limits as $\rho\to 0$. Note that $d\chi/d\rho=a+1-\cos\chi$ is bounded, under the hypothesis of the theorem, as $\rho\to 0$; hence, by an argument of the sort used previously, $\chi\to\chi(0)=\chi_0$, say, as $\rho\to 0$. We also have

$$f=\int_{\sigma=0}^{\rho} Q(\sigma)d\sigma=\int_{\sigma=0}^{\rho}\sigma^2 P(\sigma)d\sigma\geqslant 0.$$

Using the mean value theorem we have, for some $\rho_1,\rho>\rho_1>0$

$$f(\rho)=\rho\rho_1^2 P(\rho_1)<\rho^3 M_3,\quad \text{where}\quad M_3=\sup_{\mathbb{R}^+} P<\infty.$$

Thus

$$|a(\rho_2)-a(\rho_1)|=\left|\int_{\rho_1}^{\rho_2}\frac{f(\rho)d\rho}{\rho^2}\right|<\int_{\rho_1}^{\rho_2}\rho M_3 d\rho=\frac{1}{2}M_3(\rho_2^2-\rho_1^2).$$

Letting $\rho_1,\rho_2\to 0$ establishes the existence of the limit for a, we write

$$\lim_{\rho\to 0} a=a_0.$$

Now we use an argument similar to that used in the proof of lemma 3 to show that $d\chi/d\rho=a-\cos\chi\to 0$, as $\rho\to 0$. On $(0,\rho_1)$ we have

$$(*)-\ln[Q(\rho_1)/Q(\rho)]=\ln\left|\frac{a(\rho_1)-\cos\chi(\rho_1)}{a-\cos\chi}\right|+\int_{\sigma=\rho}^{\rho_1}\frac{f(\sigma)d\sigma}{\sigma^2[a(\sigma)-\cos\chi(\sigma)]}.$$

Assume, $(d\chi/d\rho)(0)=a_0-\cos\chi_0\neq 0$. Then, choosing ρ_1 near 0 so that $(d\chi/d\rho)(\rho)(d\chi/d\rho)(0)>0$, for $\rho_1>\rho>0$, we have

$$\left|\int_{\rho}^{\rho_1}\frac{f(\sigma)d\sigma}{\sigma^2[a(\sigma)-\cos\chi(\sigma)]}\right|<M_3\int_{\rho}^{\rho_1}\frac{\sigma d\sigma}{\left|\frac{d\chi}{d\rho}(\sigma)\right|}.$$

The right side of this inequality is bounded as $\rho\to 0$. Consequently, the right side of $(*)$ is bounded as $\rho\to 0$. But this contradicts the assumption of the theorem that $Q=\rho^2 P\to 0$ as $\rho\to 0$. Thus

$$\frac{d\chi}{d\rho}(0)=a_0-\cos\chi_0=0,\quad\text{or}\quad a_0=\cos\chi_0.$$

We now assume $\epsilon=+1$, the case $\epsilon=-1$ can (of course!) be obtained by conjugation. As $da/d\rho=f/\rho^2<0$ on $\rho>0$, so

$$a_0=\cos\chi_0<a<a_\infty\leqslant 1$$

on $\rho>0$.

Define new variables

$$U=\sqrt{Q}\,\cos(\chi/2),\quad\text{and}\quad V=\sqrt{Q}\,\sin(\chi/2).$$

We have

$$\frac{dU}{d\rho}=-\frac{1}{2}(a+1)V,\quad\text{and}\quad\frac{dV}{d\rho}=\frac{1}{2}(a-1)U.$$

The pair U and V also satisfy the following linear, second order equations

$$\frac{d^2U}{d\rho^2}-\frac{f}{\rho^2(a+1)}\frac{dU}{d\rho}+\frac{1}{4}(a^2-1)U=0,$$

and (11)

$$\frac{d^2V}{d\rho^2}-\frac{f}{\rho^2(a-1)}\frac{dV}{d\rho}+\frac{1}{4}(a^2-1)V=0.$$

We note that $f/\rho^2(a+1)$ is bounded on intervals $[0,\rho_2]$, with $0\leqslant\rho_2<\infty$ and that $f/\rho^2(a-1)$ is bounded on $(0,\infty]$—in the first case we may have $a_\infty=-2$, whereas we may have $a_0=0$ in the second; we also have

$$\tfrac{1}{4}(a^2-1)\leqslant 0,\quad\text{on}\quad\rho\geqslant 0.$$

From the definitions of U and V we have $U,V\to 0$ as $\rho\to 0$ or ∞. Thus, by the maximum principle for odes (see Ref. 13), we conclude $U\equiv V\equiv 0$, so $Q\equiv 0$. There do not exist non-trivial solutions.

V. NUMERICAL SOLUTIONS

Numerical solutions to the system (10), with $\epsilon=1$, were sought by first expanding in a power series from either $s=0$ ($\rho=\infty$, with $s=1/\rho$) or $\rho=0$ and then evolving the system in s or ρ, respectively, using a MATLAB interface to the NAG library.[14]

A. Solutions near $\rho=0$

In lemma 1 we found that $\Omega=\rho a$ was bounded, near $\rho=0$, with

$$\lim_{\rho\to 0}\Omega(\rho)=f(0)$$

It is natural then to seek solutions of the form $a=\Omega(\rho)/\rho$, near $\rho=0$, with Ω analytic in ρ. From (10) it can be seen that both f and Q must be analytic, with $Q(0)=0$.

However, with Q analytic and $Q(0)=0$, the last equation of (10) can only be satisfied with $Q\equiv 0$–which implies $a=c_0+c_1/\rho$, we will refer to such solutions as trivial. The behavior of the system near $\rho=0$ may be quite complex; from the proof of the theorem (see Eqs. (11)), with $a=\Omega/\rho$, we see that near $\rho=0$ the second order equations for U and V have indicial equation (see Ref. 15)

$$\lambda^2+\tfrac{1}{4}\Omega(0)^2=0.$$

This implies that U and V have behavior

$$U\ \text{ or }\ V\sim\omega_1(\rho)\cos\left(\frac{\Omega(0)}{2}\ln\rho\right)+\omega_2(\rho)\sin\left(\frac{\Omega(0)}{2}\ln\rho\right),\ \text{ near }\ \rho=0.$$

B. Solutions near $\rho=\infty$

Near $\rho=\infty$ we expect $a\sim a_\infty+c_1/\rho+c_2/\rho^2+\cdots$. Assuming a is analytic in $s=1/\rho$, near $s=0$, then implies that f, Q and $\sin\chi$ are also analytic in s, in fact

$$f=\frac{da}{ds},\quad Q=s^2\frac{d^2a}{ds^2},\quad \text{and}\quad \sin\chi=2s+s^2\left(\frac{d^3a/ds^3}{d^2a/ds^2}\right).$$

With the assumption that χ is analytic near $s=0$ a uniquely defined (up to conjugacy) power series results if we demand that the solution be non-trivial (χ does have the freedom to add integer multiples of 2π).

The resulting power series has no free parameters, it is uniquely determined. The lower order portion of the power series solution is as follows

$$\chi=\pi-2s-\frac{1}{21}s^3-\frac{3}{520}s^5+O(s^7),$$

$$a=-1+4s^2-\frac{3}{7}s^4+\frac{341}{5096}s^6+O(s^7),$$

$$f=-8s+\frac{12}{7}s^3-\frac{1023}{2548}s^5+O(s^7),$$

$$Q=8s^2-\frac{36}{7}s^4+\frac{5115}{2548}s^6+O(s^7).$$

Using the power series to determine initial conditions it was found that the numerical results were very stable for a good range of initial values for s ($s_0=0.000001$ to $s_0=0.01$), the results were somewhat unstable for $s_0<0.0000001$. The results presented in figures 1 to 4 were obtained by first shooting from near $s=0$ towards $\rho=0$ and then using the final values of this run as initial conditions to shoot from near $\rho=0$ towards $s=0$, to verify the solution. We also note, from the above power series, that $a_\infty=-1$. So in the gauge for which $a\to 0$ as $\rho\to\infty$ the Dirac field has time dependence e^{imt}.

In Figs. 1–4 χ, $a-a_\infty=a+1$, $f(r)-f(0)$ (proportional to the ''electron'' charge interior to a ball radius r) and Q are plotted against the radial distance measured in units of the Compton wavelength (i.e. against $\frac{1}{2}\rho=mr$).

Interpretation: The solution represented in Figs. 1–4 can be thought of as a central, charged monopole (point source), surrounded by an oppositely charged Dirac field-near ∞ the electrostatic potential behaves as $A^0=(m/e)a\sim -m/e+[1/(me)/r^2]$ and near $r=0$ the potential behaves as $A^0\sim -m/e+[(\gamma/e)r]$ (where $\gamma\approx 5.7037$ is the magnitude of the slope of the line in Fig. 5, where $a+1$ is plotted against $1/(mr)$).

At about one half the Compton wavelength from the center there is a shielding effect and the Coulomb nature of the central charge becomes apparent. [We assume that the constants appearing in the Dirac equation, i.e., e and m have there usual meaning—e the square root of the fine structure constant and m the inverse of the (reduced) Compton wavelength.]At large distances from the center the electrostatic charges ''cancel'' each other. We can calculate the magnitude of the total charge due to the Dirac field (see Sec. III A 3.1), with $f(0)$ calculated numerically ($f(\infty)=0$, in this case),

$$e\int_{\mathbb{R}^3}j^\alpha dS_\alpha=\frac{1}{2e}\,(f(\infty)-f(0))\approx\frac{1}{2e}\,11.407391.$$

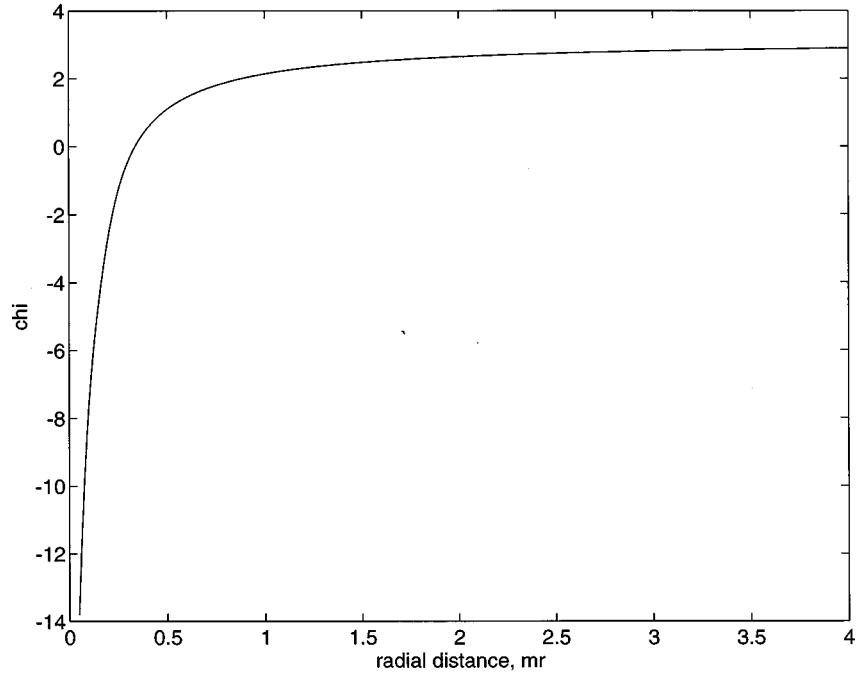

FIG. 1. The angular variable, χ.

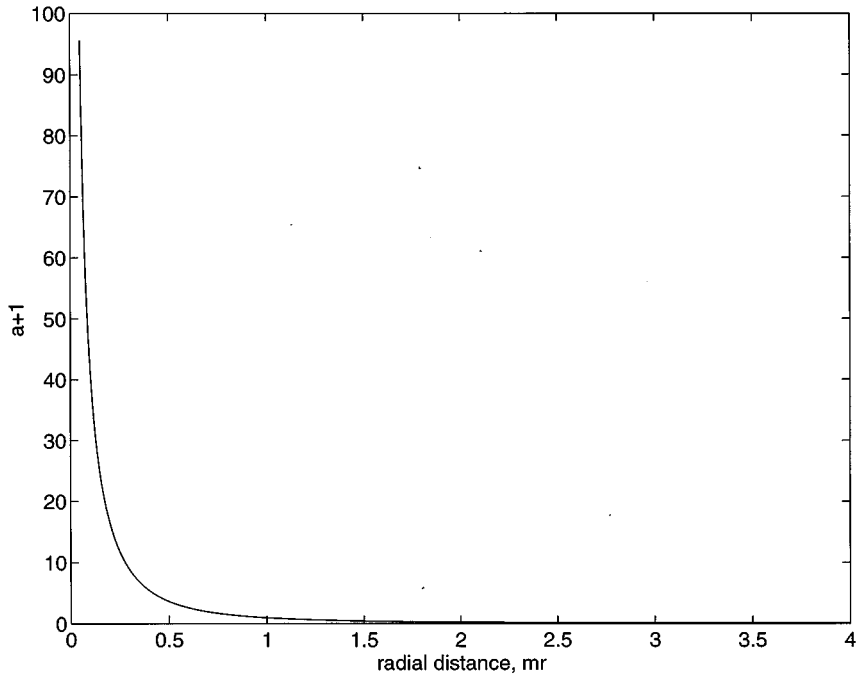

FIG. 2. The potential, $a+1$.

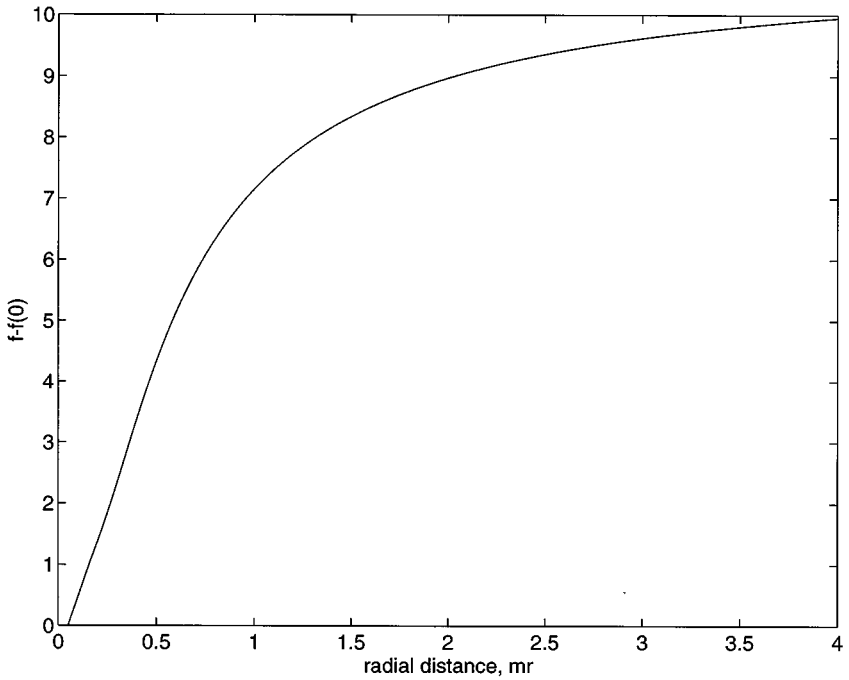

FIG. 3. The ''charge'' interior to $B(r)$, $f-f(0)$.

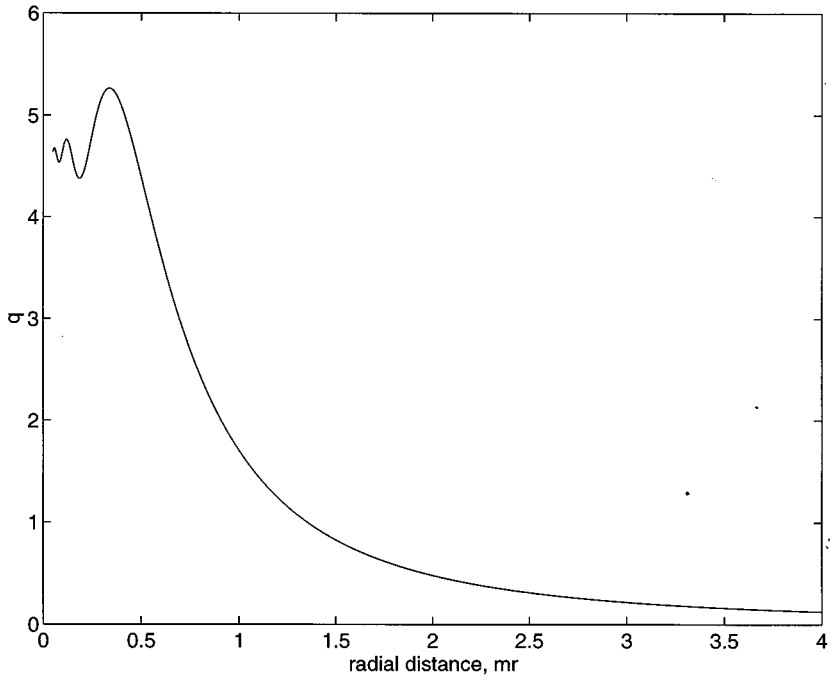

FIG. 4. The ''charge'' on a shell, radius mr, q.

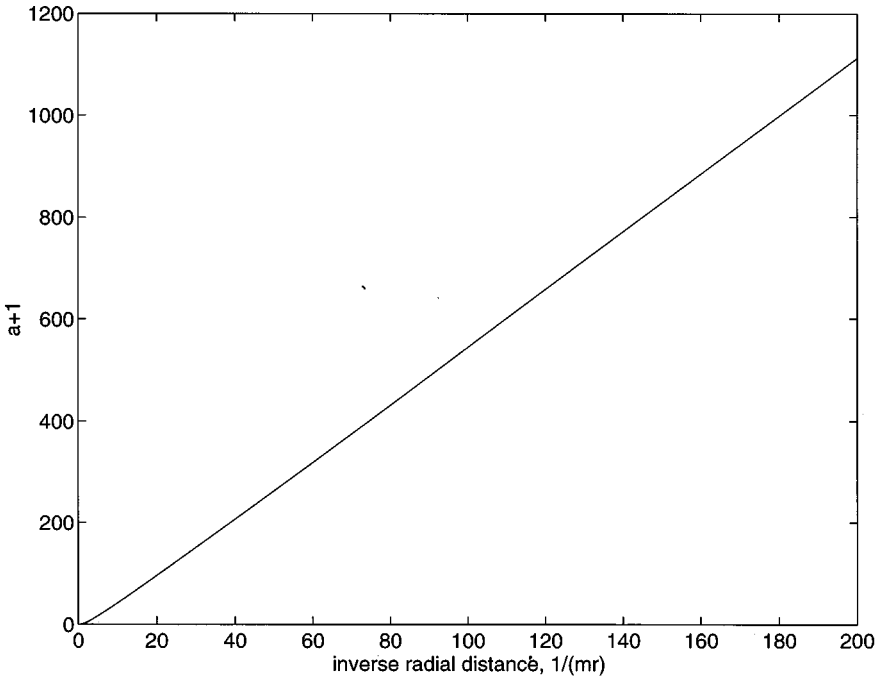

FIG. 5. The potential, a, from infinity.

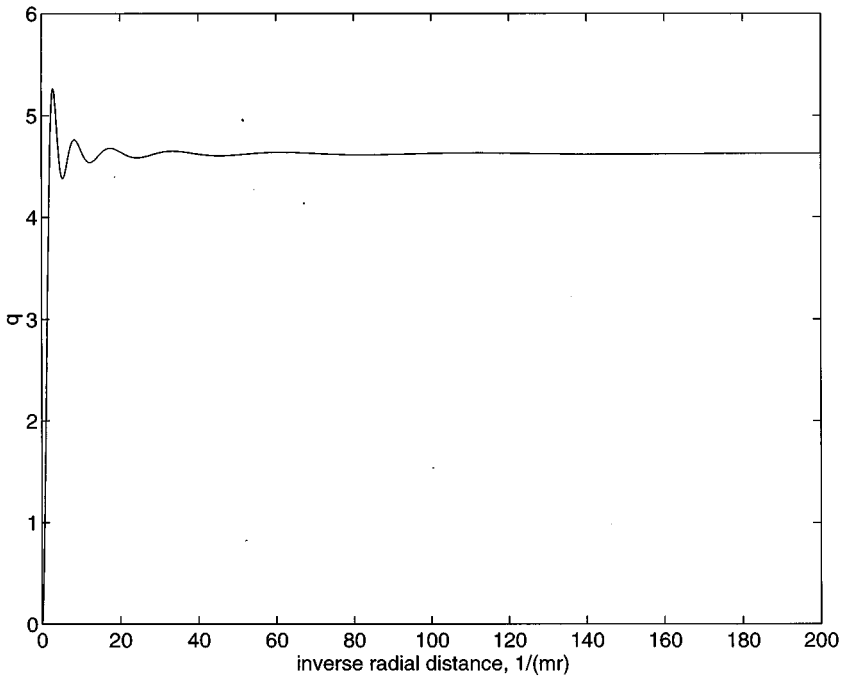

FIG. 6. The shell ''charge,'' q, from infinity.

This calculation results in a charge of the same magnitude as the central charge.

The object is highly compact, with a radius of about a (reduced) Compton wavelength—see Figs. 4 and 6. It has an onion like structure consisting of an infinite series of spherical shells—the local maxima of Q occur at points, $\rho=\rho_m$, where $\sin(\chi(\rho_m))=0$, however from lemma 2 we see that χ must diverge as $\rho\to 0$ (in the present case) so there will be an infinite number of shells.

The ''mass'' of the Dirac field may be defined as

$$m\int_{\mathbb{R}^3} j^\alpha dS_\alpha=\frac{m}{2e^2}\,(f(\infty)-f(0))\approx 11.407391\,\frac{m}{2e^2}.$$

To finish we calculate the energy-momentum of the system. The symmetric energy-momentum tensor is

$$T_{\alpha\beta}=T^D_{\alpha\beta}+T^{em}_{\alpha\beta},\quad \text{with}$$

$$T^D_{\alpha\beta}=\frac{i}{4}\,[\sigma_\alpha^{A\dot A}(\overline{u_{\dot A}}u_{A,\beta}+v_A\overline{v_{\dot A,\beta}})+\sigma_\beta^{A\dot A}(\overline{u_{\dot A}}u_{A,\alpha}+v_A\overline{v_{\dot A,\alpha}})$$

$$-\sigma_\alpha^{A\dot A}(u_A\overline{u_{\dot A,\beta}}+\overline{v_{\dot A}}v_{A,\beta})-\sigma_\beta^{A\dot A}(u_A\overline{u_{\dot A,\alpha}}+\overline{v_{\dot A}}v_{A,\alpha})]+eA_{(\alpha j\beta)},$$

$$T^{em}_{\alpha\beta}=-\frac{1}{4\pi}\left(F_{\alpha\gamma}F^\gamma_\beta-\frac{1}{4}\,\eta_{\alpha\beta}F_{\mu\nu}F^{\mu\nu}\right).$$

These expressions are derived from the Lagrangian

$$L=\frac{i}{2}\,(\overline{u_{\dot A}}\partial^{A\dot A}u_A-u_A\partial^{A\dot A}\overline{u_{\dot A}}-\overline{v_{\dot A}}\partial^{A\dot A}v_A+v_A\partial^{A\dot A}\overline{v_{\dot A}})-\frac{m}{\sqrt{2}}\,(u_Av^A+\overline{u_{\dot A}}\dot{\bar v}^{\dot A})+ej_\alpha A^\alpha-\frac{1}{16\pi}\,F_{\alpha\beta}F^{\alpha\beta}.$$

Notice that in the absence of the electromagnetic field, for a Dirac field with time dependence e^{-iEt}, the energy density T^D_{00} is

$$T^D_{00}=Ej_0.$$

In the present case we have

$$T^D_{00}=j_0eA_0=\frac{m^2}{e^2}\,\frac{Qa}{4\pi r^2},\qquad T^{em}_{00}=\frac{m^2}{2e^2}\left[\rho^2\left(\frac{da}{d\rho}\right)^2+\frac{1}{\rho^2}\right]\left(\frac{1}{4\pi r^2}\right).$$

These expressions include terms due to the central Coloumb and magnetic monopole fields, they lead to an infinite total energy when integrated over $\mathbb{R}^3$. Formally then, the total energy is

$$E=\frac{m}{4e^2}\int_0^\infty\left[\frac{f^2}{\rho^2}+\frac{1}{\rho^2}+2Qa\right]d\rho.$$

Finally, it is perhaps worth mentioning that the highly localized ''multi-electron fields'' described here may in fact have applications to objects described in recent experimental work[16]-''geonium'' or ''kilo-e'' objects-consisting of highly localized (point like, from the experimental viewpoint) collections of electrons in atomic traps.

ACKNOWLEDGMENTS

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A manifestly reciprocal theory of scattering in the presence of elastic media

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The role of elastic waves in the scattering problem is examined in the context of modern field theory. This effort builds upon a previously published, and since successfully applied formalism for solving the acoustic and electromagnetic scattering problems. It specifically addresses the scattering of acoustic waves from a fluid-solid interface, as well as the scattering of elastodynamic waves from surfaces satisfying the zero-displacement, stress-free, and solid–solid boundary conditions. Expressions for the change in the scattering amplitude due to a perturbation in the scattering surface are derived directly from the requirement of time reversal symmetry (also known as reciprocity). These results constitute formal statements of the composite (or two-scale) model. In a typical application, the perturbation usually corresponds to Bragg scattering and is treated statistically, while the reference surface provides tilt, shadowing, and multiple scattering, and is usually treated deterministically. Used in this way, the new formalism effectively allows existing numerical and operator expansion methods to be used to calculate the scattering from rougher and/or higher dimensional surfaces than would otherwise be possible. An alternate application of the formalism is illustrated using the fluid-solid boundary as an example. A new manifestly reciprocal expression for the scattering amplitude is presented, as are the small slope and ''local'' two-scale approximations for this problem. (By local, it is meant that only local phenomena such as the tilt of the reference surface are automatically included. However, since the result is manifestly reciprocal, it is fairly straightforward to incorporate a non-local effect such as shadowing.) During the course of the discussion, the classical scattering problem is reexamined from an entirely new perspective. [S0022-2488(96)02009-9]

I. INTRODUCTION

A new approach for calculating the far-field scattering of acoustic and electromagnetic waves from rough surfaces has recently been developed[1–5]. The formalism is constructed around the property of time-reversal symmetry (also known as reciprocity). Well-known proofs for the reciprocity of acoustic and electromagnetic scattering in a time-independent environment were modified to produce formal statements of the composite-roughness (i.e., two-scale) model. These consist of approximate expressions for the change in the scattering amplitude corresponding to a small perturbation of a reference surface. The expressions are good to first order in the perturbation, but exact with respect to the reference surface. By construction, they manifestly exhibit reciprocity. Two basic strategies have been used to develop practically useful applications of this fundamental formal result.

On the one hand, the formal statement of the composite-roughness model can be used directly to generate an entirely new approach for calculating the field scattered from a rough surface. Let the unperturbed reference surface include those features of the scattering surface which are large compared to the wavelength of the field, and let the perturbation contain all the smaller features. Since the result is *exact* with respect to the large features, non-local effects such as shadowing, multiple scattering, and diffraction can be calculated using high-order perturbation theory,[1] or

non-perturbative numerical or analytic techniques.[6] Bragg scattering is associated with the small surface features, and it is calculated using perturbation theory, and typically treated stochastically. Note that non-perturbative techniques are usually considered to be inappropriate for use with very rough scattering surfaces, but in the two-scale context provided by the new formalism, these restrictions are effectively circumvented. Direct application of the new composite model also leads to another related line of development. If only local effects are of interest, the formal statements of the composite model can be used to generate entirely new expansions of the scattering amplitude good to second order in the ratio of the acoustic wavelength to the radius of curvature of the scattering surface, and, most significantly, also good to much higher orders in the slope.[3] (The distinctive feature of these results is the presence of an arctangent in the integrand.)

Following the alternate basic strategy, the formal statement of the composite model is used to generate a second fundamental result. The expressions for the *change* in the scattering amplitude, when applied to an infinitesimal translation, become generating functions for new representations of the scattering amplitude *itself*. Unlike the traditional representations of the scattering amplitude, these manifestly exhibit reciprocity. In the investigation of acoustic and electromagnetic scattering, approximation schemes such as perturbation theory, the small slope approximation, and the composite model were easily derived for a number of boundary conditions.[3] In some cases, this was the first time the results had been derived anywhere.

The utility of the manifestly reciprocal representations of the scattering amplitude is not restricted to the problem of scattering from rough surfaces alone. The formalism has also led to breakthroughs in the study of scattering from finite objects. When applied to planar objects, it provides an exact formula for the scattering amplitude in terms of a line integral around the edge of the scatterer. Useful approximations can be obtained by approximating the integrand with solutions to the local half-plane problem. These insights have recently been used by Dashen, Abawi, and Wandzura[7,8] to examine the scattering from planar objects, edges, and corners.

In this paper the formalism will be extended to include elastic solids. The formal statement of the composite model and the manifestly reciprocal representation of the scattering amplitude will be derived for scattering from a fluid–solid interface as well as for the interface between two elastic solids. In addition, the manifestly reciprocal expression for the scattering amplitude will be used to generate new composite model and small slope approximations for the case of the fluid–solid interface.

The limiting properties of these results will be considered. It will be shown that, in the limit as the shear waves disappear (i.e., as the shear velocity approaches zero), the results for scattering from a fluid–solid interface approach previously derived results for the fluid–fluid interface (see Ref. 3).

The formal mathematical results to be presented in this paper are applicable to several physical problems. A typical application of the results for scattering from a fluid–solid interface would be acoustic scattering from some parts of the ocean bottom. This would include areas where there is a solid rock layer either directly underwater, or submerged beneath a muddy bottom that acoustically behaves like a liquid. The solid–solid results may find application in the study of seismic waves, specifically where the scattering between layers of the Earth's crust is involved. These results may also find application in the field of non-destructive testing, where scattering from the interface between different materials would be described by the solid–solid scattering formalism.

II. A FORMAL STATEMENT OF THE COMPOSITE ROUGHNESS MODEL

A. The general procedure

The derivations in this paper parallel the procedure developed in Refs. 2 and 3. For additional insight into the notation, the strategy employed, and the underlying physical assumptions, the reader is referred to those references. Elements of the notation for elastodynamic wave scattering developed in Ref. 9 (pp. 46–50) and Refs. 10–12 will also be used below.

A small displacement of the material in an elastic solid is given by the vector $\vec{u}$ while the components of the stress tensor are defined to be

$$\tau_{ij} \equiv \lambda(\vec{\nabla}\cdot\vec{u})\,\delta_{ij} + \mu(\nabla_i u_j + \nabla_j u_i), \tag{2.1}$$

where λ and μ are the Lamé constants, physical parameters characteristic of the solid. In dyadic notation, this is written as

$$\overleftrightarrow{\tau} \equiv \lambda \overleftrightarrow{\mathbf{1}}(\vec{\nabla}\cdot\vec{u}) + \mu(\vec{\nabla}\vec{u} + \vec{u}\vec{\nabla}_{\hookleftarrow}), \tag{2.2}$$

(where the subscript ''$\hookleftarrow$'' indicates that the differential operator operates to the left). The environment is assumed to be time-independent. Then, considering each frequency ω independently, wave propagation is given by the equation

$$\vec{\nabla}\cdot\overleftrightarrow{\tau} = -\rho\omega^2\vec{u}, \tag{2.3}$$

where ρ is the density of the solid.

Reciprocity is proven using the elastodynamic equivalent of what is called Lorentz's Lemma in electromagnetic theory. This procedure is outlined in Ref. 12 (pp. 155–156). Recall that Lorentz's Lemma states that, for any two independent fields labeled 1 and 2 which satisfy the time-independent problem at a given fixed frequency ω, the vector

$$\vec{E}_1 \times \vec{H}_2 - \vec{E}_2 \times \vec{H}_1$$

must be a divergence-free vector. This follows from Maxwell's equations in the absence of free charges. The analogous divergence-free vector for elastodynamic waves is

$$\overleftrightarrow{\tau}_1\cdot\vec{u}_2 - \overleftrightarrow{\tau}_2\cdot\vec{u}_1.$$

This follows immediately from the equation of motion (2.3) and the equality

$$\overleftrightarrow{\tau}_1 : \vec{\nabla}\vec{u}_2 = \overleftrightarrow{\tau}_2 : \vec{\nabla}\vec{u}_1,$$

which in turn follows directly from the definition of the stress tensor (2.1). (Note that '':'' is the double dot product defined by $A:B \equiv A_{ij}B_{ji}$, where repeated indices are summed.) It follows that for any closed surface with normal $\hat{n}$ (we follow the convention that $\hat{n}$ points into the region bounded by S),

$$\int_S dS\hat{n}\cdot[\overleftrightarrow{\tau}_1\cdot\vec{u}_2 - \overleftrightarrow{\tau}_2\cdot\vec{u}_1] = 0. \tag{2.4}$$

Reciprocity follows from this equality as follows.

- S is chosen to be the sum of the scattering surface S_0 and the sphere at infinity S_∞ (or the hemisphere at infinity for a plane scatterer).
- The two solutions correspond to incoming plane waves labeled by the directions $\hat{k}_1$ and $\hat{k}_2$, respectively.
- $\hat{k}_2$ is identified with the negative of the normalized position vector of the observer (i.e., $\hat{k}_2 = -\hat{r}$). The solution labeled by ''2'' is then called the reciprocal solution. $\hat{r}$ is sometimes referred to below as the outgoing direction.

Evaluation of equation (2.4) shows that the scattering amplitude remains unchanged under the exchange $\hat{k}_1 \to \hat{k}_2$; $\hat{k}_2 \to \hat{k}_1$ (this step takes some effort; see Ref. 12). To put it another way, in the asymptotic limit, the magnitude and phase of the scattered wave are unchanged by reversing the

incoming and outgoing directions, and exchanging their roles. This is the reciprocity theorem. There are some minor complications related to the tensor nature of elastodynamic waves, but these will be addressed below as they become directly relevant to the discussion.

Following the technique outlined in Ref. 2, the new formalism emerges when the two solutions are chosen so that they correspond to not only to different incoming directions, *but also to scattering from different scattering surfaces*—the solution labeled by ''2'' scatters from a reference surface S_2 and the solution labeled by ''1'' scatters from a perturbed surface S_1. In equation (2.4), choose S to be S_2+S_∞ and define R_∞ to be the negative of the contribution from S_∞, the sphere (or hemisphere) at infinity (unless S_2 is a closed surface and the integrand is evaluated using the field *inside* S_2; then $S=S_2$, and just set $R_\infty=0$). We have

$$R_\infty=\int_{S_2} dS_2[\hat{n}_2\cdot\vec{\tau}_1(\vec{x_2})\cdot\vec{u}_2(\vec{x_2})-\hat{n}_2\cdot\vec{\tau}_2(\vec{x_2})\cdot\vec{u}_1(\vec{x_2})]. \tag{2.5}$$

Consider the following mapping from S_2 to S_1. At the point $\vec{x_2}$ draw a normal to S_2 and follow it until intersects S_1 at point $\vec{x_1}$. The normal distance ξ from $\vec{x_1}$ to $\vec{x_2}$ is positive if $\vec{x_1}$ lies within the scattering region for S_2 and negative if the opposite is true. (This geometry is sketched in Figure 1 of Ref. 2.) It is implicitly assumed that the perturbation is small enough with respect to the radius of curvature of the reference surface (i.e., the reference surface is smooth) that the transformation is single-valued, and that the solution can be analytically continued beyond the scattering surface (see Refs. 2 and 13 for a further discussion of this topic). We now calculate (2.5) to first order. The details are given in Appendix A.

Here

$$\begin{aligned}
R_\infty=&\int_{S_2} dS_2[\hat{n}_1\cdot\vec{\tau}_1(\vec{x_1})\cdot\vec{u}_2(\vec{x_2})-\hat{n}_2\cdot\vec{\tau}_2(\vec{x_2})\cdot\vec{u}_1(\vec{x_1})]-\int dS\xi\,\mathrm{Tr}(\vec{\varrho})\hat{n}\cdot\vec{\tau}_1\cdot\vec{u}_2\\
&+\int dS\xi[\hat{n}\cdot\vec{\tau}_2\cdot\vec{\varrho}\cdot\vec{u}_1+\hat{n}\cdot\vec{\tau}_1\cdot\vec{\varrho}\cdot\vec{u}_2]\\
&-\int dS\xi[\hat{n}\cdot\vec{\tau}_2\cdot(\vec{\mathbf{1}}-\hat{n}\hat{n})\cdot\vec{\nabla}(\vec{u}_1\cdot\hat{n})+\hat{n}\cdot\vec{\tau}_1\cdot(\vec{\mathbf{1}}-\hat{n}\hat{n})\cdot\vec{\nabla}(\vec{u}_2\cdot\hat{n})]-\int dS\xi[\vec{\nabla}\cdot(\vec{\tau}_1\cdot\vec{u}_2)]\\
&+\int dS\xi[\hat{n}\cdot\vec{\tau}_2\cdot\hat{n}[\hat{n}\hat{n}:\vec{\nabla}\vec{u}_1]+\hat{n}\cdot\vec{\tau}_1\cdot\hat{n}[\hat{n}\hat{n}:\vec{\nabla}\vec{u}_2]]\\
&+2\int dS\xi\left[\frac{\hat{n}\cdot\vec{\tau}_2\cdot(\vec{\mathbf{1}}-\hat{n}\hat{n})\cdot\vec{\tau}_1\cdot\hat{n}}{\mu}\right]+O(\xi^2).
\end{aligned} \tag{2.6}$$

The dyadic $\vec{\varrho}$ is the curvature tensor, and it is a geometrical characteristic of the scattering surface defined by equation (A9). (It should not be confused with the scalar ρ, which is the density of the material.) Equation (2.6) is an intermediate result. It is best thought of as a mathematical identity, presented here as a lemma, which underlies the results that will be presented later in this paper. Subsequent to equation (2.6), the calculations for scattering from a fluid–solid interface and a solid–solid interface part ways.

In what follows, $\vec{\nabla}\cdot(\vec{\tau}_1\cdot\vec{u}_2)$ will generally be rewritten as

$$\vec{\nabla}\cdot(\vec{\tau}_1\cdot\vec{u}_2)=(\vec{\nabla}\cdot\vec{\tau}_1)\cdot\vec{u}_2+\vec{\tau}_1:\vec{\nabla}\vec{u}_2=-\rho\omega^2\vec{u}_1\cdot\vec{u}_2+\vec{\tau}_1:\vec{\nabla}\vec{u}_2.$$

On terms which are manifestly $O(\xi)$ there is no need to specify whether the field is evaluated at $\vec{x_1}$ or at $\vec{x_2}$, because the resulting effect on R_∞ is of $O(\xi^2)$. It also does not matter whether the solutions correspond to scattering from the reference surface or from the perturbed surface, since

here too the difference contributes at $O(\xi^2)$. The labels ''1'' and ''2'' in this case only refer to properties of the incident fields such as the direction of the wavevector and sometimes, as we will see below, whether the incoming wave is longitudinal or transverse and specifying the incoming polarization for the latter case.

Because of its general nature, equation (2.6) and its components do not easily lend themselves to straightforward physical interpretation. However, there are some things we can say, even at this early stage of the calculation. In what follows, as was done in the reciprocity proof outlined earlier, the direction of the incident wavevector labeled by ''2'' will always be interpreted as being the negative of the direction of the observer in the original problem; thus, the solution labeled ''2'' almost corresponds to the reciprocal problem (''almost'' because it scatters from the reference surface, but we are just a step or two away from eliminating the only terms where the distinction still matters). Then, using very general arguments, it is shown in Appendix B that R_∞ is (more or less) proportional to δT, the difference between the scattering amplitude for the perturbed surface T and that for the reference surface T_0; i.e., symbolically,

$$R_\infty \propto \delta T \equiv T - T_0 .$$

(Recall that ''$\equiv$'' implies a definition.) Note that this implies that R_∞ must be at least first order in ξ, and that the first term on the right-hand side of equation (2.6), although it does not explicitly *appear* to be at least of $O(\xi)$, must reduce to an expression which is. It is also shown in Appendix B that if neither field ''1'' nor field ''2'' is incoming from a half-space, then the contribution from the hemisphere at ∞ bounding that half-space is zero (i.e., $R_\infty = 0$), even if there are transmitted waves in the half-space.

We are now in a position to recognize the power of this approach. Once the expression has been recast so that only terms manifestly proportional to ξ remain, then we have an expression for scattering from the perturbed surface, which can be evaluated using only solutions for scattering from the *un*perturbed surface. The proviso that only terms manifestly proportional to ξ remain is satisfied by invoking specific boundary conditions to evaluate the offending terms [i.e., the first line on the right hand side of (2.6)]. Four boundary conditions are of interest here (see e.g., Ref. 10, pp. 27–29):

- fixed rigid boundary: $\vec{u} = 0$ on the interface;
- free boundary: $\hat{n} \cdot \vec{\tau} = 0$ on the interface;
- boundary between two elastic solids (i.e., the solid–solid interface): $\vec{u}$ and $\hat{n} \cdot \vec{\tau}$ continuous on the interface;
- slip boundary condition (the fluid–solid interface is a special case of this condition): $\hat{n} \cdot \vec{u}$ and $\hat{n} \cdot \vec{\tau} \cdot \hat{n}$ are continuous and $\hat{n} \cdot \vec{\tau} \cdot (\vec{\mathbf{1}} - \hat{n}\hat{n}) = 0$ on the interface.

Note that the terms in equation (2.6) which are not manifestly proportional to ξ vanish automatically in the first two cases. For the solid–solid interface, subtract equation (2.6) for the region below the interface (i.e., corresponding to the half-space without an incoming plane wave, or the interior region for a finite scatterer) from the same equation evaluated for the solution above the interface (recalling that $R_\infty = 0$ in the former case, $R_\infty \propto \delta T$ in the latter case). The continuity conditions ensure that the first line on the right hand side of (2.6) cancels, and the result is an equation for δT with an integrand manifestly proportional to ξ. (Recall that δT was defined just above as the change in the scattering amplitude due to the perturbation of the surface.)

Thus, we have outlined how the first three boundary conditions may be used to eliminate the $O(\xi^{\,0})$ terms in equation (2.6). However, for the slip boundary condition, more work is needed. This will be considered in the next section, where the problem of scattering from a fluid–solid interface is considered.

B. The fluid–solid interface

The fluid–solid interface is subject to the fourth set of boundary conditions listed in the previous section, the slip boundary conditions. According to these conditions, $\hat{n}\cdot\vec{\vec{\tau}}$ and $\vec{u}$ are no longer required to be continuous along the interface. However, $\hat{n}\cdot\vec{\vec{\tau}}\cdot\hat{n}$ and $\hat{n}\cdot\vec{u}$ are continuous, and furthermore, we have $\hat{n}\cdot\vec{\vec{\tau}}=\hat{n}\cdot\vec{\vec{\tau}}\cdot\hat{n}\hat{n}$ on the surface, so that

$$R_\infty=\int_{S_2} dS_2[\hat{n}_1\cdot\vec{\vec{\tau}}_1(\vec{x_1})\cdot\hat{n}_1\hat{n}_1\cdot\vec{u}_2(\vec{x_2})-\hat{n}_2\cdot\vec{\vec{\tau}}_2(\vec{x_2})\cdot\hat{n}_2\hat{n}_2\cdot\vec{u}_1(\vec{x_1})]+O(\xi). \tag{2.7}$$

Next, use equation (A1) to match up $\vec{u}_2(\vec{x_2})$ with $\hat{n}_2$ and $\vec{u}_1(\vec{x_1})$ with $\hat{n}_1$, and then integrate by parts. The details are given in Appendix C, leading to the result

$$\begin{aligned}R_\infty=&\int_{S_2} dS_2[\hat{n}_1\cdot\vec{\vec{\tau}}_1(\vec{x_1})\cdot\hat{n}_1\hat{n}_2\cdot\vec{u}_2(\vec{x_2})-\hat{n}_2\cdot\vec{\vec{\tau}}_2(\vec{x_2})\cdot\hat{n}_2\hat{n}_1\cdot\vec{u}_1(\vec{x_1})]+\int dS\xi\,\mathrm{Tr}(\vec{\vec{\varrho}})\hat{n}\cdot\vec{u}_1\tau^2_{nn}\\&+\int dS\xi\rho\omega^2\vec{u}_1\cdot\vec{u}_2+\int dS\xi[\vec{u}_2\cdot(\vec{\vec{1}}-\hat{n}\hat{n})\cdot\vec{\nabla}(\tau^1_{nn})+\vec{u}_1\cdot(\vec{\vec{1}}-\hat{n}\hat{n})\cdot\vec{\nabla}(\tau^2_{nn})]\\&-\int dS\xi\frac{\vec{\vec{\tau}}_1:\vec{\vec{\tau}}_2}{2\mu}+\int dS\xi\frac{\lambda}{2\mu}\frac{\mathrm{Tr}(\vec{\vec{\tau}}_1)\,\mathrm{Tr}(\vec{\vec{\tau}}_2)}{3\lambda+2\mu}+\int dS\xi\left[\frac{\mathrm{Tr}(\vec{\vec{\tau}}_1)}{3\lambda+2\mu}\tau^2_{nn}+\frac{\mathrm{Tr}(\vec{\vec{\tau}}_2)}{3\lambda+2\mu}\tau^1_{nn}\right],\end{aligned} \tag{2.8}$$

where $\tau_{nn}\equiv\hat{n}\cdot\vec{\vec{\tau}}\cdot\hat{n}$. Note that the $O(\xi^0)$ terms are now continuous across the interface and may be canceled by subtraction of the equivalent equation below the surface.

Now, take the limit as the solid becomes a fluid (i.e., let $\mu\to 0$). It is shown in Appendix D that in this limit (2.8) reduces to

$$\begin{aligned}R_\infty=&\int_{S_2} dS_2[\hat{n}_1\cdot\vec{\vec{\tau}}_1(\vec{x_1})\cdot\hat{n}_1\hat{n}_2\cdot\vec{u}_2(\vec{x_2})-\hat{n}_2\cdot\vec{\vec{\tau}}_2(\vec{x_2})\cdot\hat{n}_2\hat{n}_1\cdot\vec{u}_1(\vec{x_1})]\\&+\int dS\xi\,\mathrm{Tr}(\vec{\vec{\varrho}})\hat{n}\cdot\vec{u}_1\tau^2_{nn}+\int dS\xi\rho\omega^2\hat{n}\cdot\vec{u}_1\hat{n}\cdot\vec{u}_2\\&-\int dS\xi\rho\omega^2\vec{u}_1\cdot(\vec{\vec{1}}-\hat{n}\hat{n})\cdot\vec{u}_2+\int dS\xi\frac{k^2}{\rho\omega^2}\tau^1_{nn}\tau^2_{nn}.\end{aligned} \tag{2.9}$$

Equations (2.8) and (2.9) will shortly be subtracted from one another to produce an expression for the change in the scattering amplitude δT corresponding to the perturbation of a fluid–solid interface. However, we first briefly digress to more closely examine equation (2.9). This is done in order to develop a better physical understanding of this equation, and to determine the precise relationship between R_∞ and δT, when the latter is defined in terms of the conventions used in reference 2 (which in turn are conventions commonly used in acoustics).

Thus, note that for an acoustic field in a fluid:

$$\vec{u}\to\frac{\vec{\nabla}P}{\rho\omega^2};\quad \vec{\vec{\tau}}\to -P\vec{\vec{1}},$$

where P is the pressure wave. Making these substitutions, we find

$$R_\infty = -\frac{1}{\rho\omega^2}\left\{ \int_{S_2} dS_2[P_1(\vec{x}_1)\hat{n}_2\cdot\vec{\nabla}P_2(\vec{x}_2) - P_2(\vec{x}_2)\hat{n}_1\cdot\vec{\nabla}P_1(\vec{x}_1)] + \int dS\xi\ \mathrm{Tr}(\overleftrightarrow{\mathcal{G}})(\hat{n}\cdot\vec{\nabla}P_1)P_2 \right.$$
$$\left. - \int dS\xi\hat{n}\cdot\vec{\nabla}P_1\hat{n}\cdot\vec{\nabla}P_2 + \int dS\xi[\vec{\nabla}P_1\cdot(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})\cdot\vec{\nabla}P_2 - k^2P_1P_2] \right\}$$
$$= -\frac{1}{\rho\omega^2}R_\infty^{fluid} = -\frac{1}{\rho\omega^2}\delta T^{fluid}, \tag{2.10}$$

where R_∞^{fluid} and δT^{fluid} are analogous quantities for the problem of acoustic propagation through a fluid as discussed in reference 2. (Recall that δT represents the correction to the scattering amplitude for the perturbed surface; i.e., $T = T_0 + \delta T$ where T_0 is for scattering from the reference surface.) The identification of R_∞^{fluid} with δT^{fluid} implies that both the incoming and outgoing directions lie in the region bounded by S_2 and the sphere at infinity (i.e., we are looking at reflection back into the same medium, not transmission into the medium on the other side of the interface). We will implicitly continue to make this assumption in what follows.

Note that in Appendix B, we have the result

$$R_\infty = \frac{\rho\omega^2}{k_p^2}\delta T^{pp}, \tag{2.11}$$

where pp stands for ''scattering between scalar components of an elastodynamic wave.'' This gives the apparent result

$$\delta T^{pp} \overset{?}{=} -\frac{k_p^2}{(\rho\omega^2)^2}\delta T^{fluid}.$$

It is very important to note that this would be an erroneous conclusion! Equality (2.11) assumes that the incoming displacement wave has an amplitude of 1, whereas (2.10) assumes that the incoming pressure wave is normalized to unity. Once the different assumptions are accounted for, we indeed find

$$\delta T^{pp} = \delta T^{fluid}.$$

In our study of the fluid–solid interface, we will assume that there is a *normalized incoming pressure* wave in the fluid.

We now follow the strategy which was used in reference 2 to calculate the scattering from a two-fluid or a two-dielectric interface. Equation (2.8) is evaluated in the solid. Since it is assumed here that there is no incoming wave in the solid, and that the outgoing direction points somewhere into the fluid, it follows that $R_\infty^{solid} = 0$. Equation (2.9) is evaluated in the fluid, where $R_\infty = -\delta T/\rho_I\omega^2$ with ρ_I the density of the fluid. Henceforth, the superscript ''I'' refers to quantities evaluated on the fluid side, while the superscript ''II'' refers to those quantities evaluated on the solid side. (Later, when we consider the interface between two solids, this will, of course, be generalized, where I will refer to the side with an incoming wave.) Now, subtract the equations and use the boundary conditions (continuity of $\hat{n}\cdot\vec{u}, \tau_{nn}$) to simplify the result. Note that the continuity of τ_{nn} implies that the transverse derivative $(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})\cdot(\vec{\nabla}\tau_{nn})$ must be continuous as well, so that

$$(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})\cdot(\vec{\nabla}\tau_{nn}^{II}) = (\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})\cdot(\vec{\nabla}\tau_{nn}^{I}) = -\rho_I\omega^2(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})\cdot\vec{u}^I.$$

(There is a minor point that may cause some confusion here. In the above derivations, it was always assumed that the normal points into the volume enclosed by S. Thus, strictly speaking, below the interface, $\hat{n}$ should be replaced by its negative. However, $\hat{n}\rightarrow-\hat{n}$ also implies that $\vec{\varrho}\rightarrow-\vec{\varrho}$ and $\xi\rightarrow-\xi$ and it turns out that all terms in these equations have the same parity! This makes comparison and subtraction of the two equations completely straightforward.)

Combining these results, we have the following equation applicable to the case when an acoustic wave is incident from the fluid side of a fluid–solid interface and scatters back into the fluid,

$$-\frac{\delta T}{\rho_I\omega^2}=\int dS\xi\omega^2(\rho_I-\rho_{II})\hat{n}\cdot\vec{u}_1\hat{n}\cdot\vec{u}_2+\int dS\xi\omega^2(\rho_I-\rho_{II})\vec{u}_1^{II}\cdot(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})\cdot\vec{u}_2^{II}-\int dS\xi\rho_I\omega^2(\vec{u}_1^{I}-\vec{u}_1^{II})\cdot(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})\cdot(\vec{u}_2^{I}-\vec{u}_2^{II})+\int dS\xi\left(\frac{k_I^2}{\rho_I\omega^2}+\frac{1}{2\mu_{II}}\right)\tau_{nn}^1\tau_{nn}^2+\int dS\xi\frac{\overleftrightarrow{\tau}_1^{TII}:\overleftrightarrow{\tau}_2^{TII}}{2\mu_{II}}-\int dS\xi\left(\frac{\lambda_{II}}{2\mu_{II}}\right)\frac{\mathrm{Tr}(\overleftrightarrow{\tau}_1^{II})\,\mathrm{Tr}(\overleftrightarrow{\tau}_2^{II})}{3\lambda_{II}+2\mu_{II}}-\int dS\xi\left[\frac{\mathrm{Tr}(\overleftrightarrow{\tau}_1^{II})}{3\lambda_{II}+2\mu_{II}}\tau_{nn}+\frac{\mathrm{Tr}(\overleftrightarrow{\tau}_2^{II})}{3\lambda_{II}+2\mu_{II}}\tau_{nn}\right]. \tag{2.12}$$

The superscript ''T'' denotes the transverse components of τ defined by

$$\overleftrightarrow{\tau}^{T}\equiv(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})\cdot\overleftrightarrow{\tau}\cdot(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})=\begin{pmatrix}\tau_{t_1t_1}\tau_{t_1t_2}\\ \tau_{t_2t_1}\tau_{t_2t_2}\end{pmatrix}. \tag{2.13}$$

Implicit in the last equality is the choice of a *local* coordinate system such that

$$\hat{n}\perp\hat{t}_1\perp\hat{t}_2.$$

Often, $\hat{t}_1$ is chosen to be in the plane of incidence.

In (2.12), note that there are no I/II labels on $\hat{n}\cdot\vec{u}$ and τ_{nn}, since these quantities are the same on both sides. In interpreting this equation, it is also worthwhile to note that the labels 1 and 2 at this point refer to the fact that the quantities in question are, in the former case, solutions to the problem of scattering for an incoming plane wave with wave-vector $\vec{k}$, and in the latter case to the reciprocal problem with incoming wave-vector $-\vec{q}$. Also note that

$$\tau_{nn}=\frac{\mathrm{Tr}(\overleftrightarrow{\tau}^{I})}{3}.$$

The trace of the stress tensor is a physically significant quantity. Note that

$$\frac{\mathrm{Tr}(\overleftrightarrow{\tau})}{3\lambda+2\mu}=\vec{\nabla}\cdot\vec{u}=\Delta,$$

where Δ is the ''dilatation'' (i.e., the increase in volume per unit volume). Δ basically propagates with the longitudinal (i.e., p-, primary, or pressure) wave. Beyond this observation, the physical interpretation of the terms in equation (2.12) generally will become clear only gradually. Particularly helpful in this regard will be section III D, where certain limits are taken as the solid in region II becomes a liquid.

Result (2.12) is, in fact, more general than implied here. In deriving this equation, it was implicitly assumed that ρ_I is constant on the sphere at ∞, but nowhere was it assumed that ρ,

λ, or μ are constant in the vicinity of the scattering surface. The same applies for the results to follow in this section as well as those derived in section II C to follow. For a further discussion of this issue, see Ref. 2.

Following Ref. 2, let $\vec{d}$ be an infinitesimal constant translation so that consequently $\delta T = -i\vec{Q}\cdot\vec{d}\,T(\vec{q},\vec{k})$ and $\xi = -\hat{n}\cdot\vec{d}$ [where $T(\vec{q},\vec{k})$ is the scattering amplitude from the surface before it is translated and $\vec{Q}\equiv\vec{k}-\vec{q}$]. Parameterize the surface S using the 2-dimensional vector **x**, the projection of the coordinates of points on S onto a plane. Since $\vec{d}$ is arbitrary, we have

$$
\begin{aligned}
-\frac{iQ_z T(\vec{q},\vec{k})}{\rho_I\omega^2} &= \int d^2x(\rho_I-\rho_{II})\omega^2\hat{n}\cdot\vec{u}_1\hat{n}\cdot\vec{u}_2 + \int d^2x(\rho_I-\rho_{II})\omega^2\vec{u}_1^{II}\cdot(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})\cdot\vec{u}_2^{II} \\
&\quad - \int d^2x\rho_I\omega^2(\vec{u}_1^{I}-\vec{u}_1^{II})\cdot(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})\cdot(\vec{u}_2^{I}-\vec{u}_2^{II}) + \int d^2x\left(\frac{k_I^2}{\rho_I\omega^2}+\frac{1}{2\mu_{II}}\right)\tau_{nn}^1\tau_{nn}^2 \\
&\quad + \int d^2x\frac{\overleftrightarrow{\tau}_1^{TII}:\overleftrightarrow{\tau}_2^{TII}}{2\mu_{II}} - \int d^2x\left(\frac{\lambda_{II}}{2\mu_{II}}\right)\frac{\mathrm{Tr}(\overleftrightarrow{\tau}_1^{II})\,\mathrm{Tr}(\overleftrightarrow{\tau}_2^{II})}{3\lambda_{II}+2\mu_{II}} \\
&\quad - \int d^2x\left[\frac{\mathrm{Tr}(\overleftrightarrow{\tau}_1^{II})}{3\lambda_{II}+2\mu_{II}}\frac{\mathrm{Tr}(\overleftrightarrow{\tau}_2^{I})}{3} + \frac{\mathrm{Tr}(\overleftrightarrow{\tau}_2^{II})}{3\lambda_{II}+2\mu_{II}}\frac{\mathrm{Tr}(\overleftrightarrow{\tau}_1^{I})}{3}\right],
\end{aligned}
\tag{2.14}
$$

where Q_z is the component of $\vec{Q}$ in the direction normal to the reference plane (with positive direction pointing into the fluid). Note that line 5 of equation (2.14) can be combined with the second term of line 4 using the following equality:

$$
\tau_{nn}^1\tau_{nn}^2 + \overleftrightarrow{\tau}_1^{TII}:\overleftrightarrow{\tau}_2^{TII} = \overleftrightarrow{\tau}_1^{II}:\overleftrightarrow{\tau}_2^{II}. \tag{2.15}
$$

This equality follows from equation (E2) and the boundary condition $\hat{n}\cdot\overleftrightarrow{\tau}\cdot(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n}) = 0$.

Equation (2.14) is somewhat related to an important previous result obtained by Berman and Dacol and given by Ref. 5, equation (2). The latter is valid in general for the scattering of an acoustic wave, where both the incident wave and the observer are in the fluid (i.e., $-\vec{k}$ and $\vec{q}$ both point into the fluid, and the scattering is from an interface obeying either the Dirichlet, Neumann, impedance, fluid–fluid, or fluid–solid boundary conditions). The work outlined in Ref. 5 is also based on the technique proposed by Dashen and outlined in Refs. 1, 2, and consequently the resultant expression for the scattering amplitude manifestly exhibits reciprocity. Equation (2.14) and Ref. 5 [equation (2)] are both exact, and must ultimately be equivalent, but there are significant differences in their practical implementation. For example, the latter depends only on the field evaluated on the fluid (i.e., incoming) side, and this arguably leads to a (formal) simplification of the problem. On the other hand, the integrand of (2.14) depends on the displacement vector $\vec{u}$ and the stress tensor $\overleftrightarrow{\tau}$ only, both of which have a straightforward physical interpretation, while equation (2) of Ref. 5 explicitly depends on quantities such as $\vec{\nabla}\vec{u}$ which can be simplified further (see, for example, the last few lines of Appendix I). There is a great deal of physical information ''hiding'' in these terms. We will see in section III D that the comparative physical transparency of equation (2.14) leads, for example, to a straightforward examination of the difference between the Dirichlet, Neumann, fluid–fluid, and fluid–solid boundary value problems. Such an increase in physical transparency can also be a significant asset in simplifying the results. The scattering problem is potentially very complex, and the extensive use of physical intuition can be crucial in making the problem tractable (see once again, for example, section III below).

C. Full elastodynamic scattering

When the scattered wave is a full elastodynamic wave, then the problem involves a complication that does not seem at first glance to be present when the scattered wave is a (scalar) acoustic wave, namely that the scattering amplitude behaves as a tensor quantity. However, this property can be viewed as a straightforward generalization of concepts familiar from the scalar problem. For the acoustic problem, the scattering amplitude can be interpreted as a tensor, with the indices being the (continuous) variables specifying the direction of the incoming wave and the angular coordinates of the observer (i.e., the vectors $\vec{k}$ and $\vec{q}$, respectively). For the electromagnetic problem, the scattering amplitude is additionally labeled by the polarization of the incoming wave (having implicitly decomposed the incident wave into components of this form) and the polarization components of the outgoing wave being sampled by the observer (again assuming such a decomposition). Thus two more continuous tensor indices are added to the scattering amplitude. Finally, for elastodynamic waves, it is also necessary to decompose the incident field into scalar or vector components of the field and to similarly specify whether the observer is sampling the scalar or vector components of the outgoing waves. Now the new relevant tensor indices take on one of two discrete possible values (corresponding to ''scalar or vector'').

The decomposition of the field (in terms of plane waves, polarizations, etc.), which is necessary for defining the scattering amplitude as a tensor, is also intimately connected with the concept of reciprocity. In particular, it is the ''spectral'' components of the wave after it has been decomposed in this way, which are reciprocal. Conversely, a theory constructed from the reciprocity principle very naturally leads to the scattering amplitude tensor. As demonstrated below, the scattering amplitude can be written in terms of products of the solution to the problem at hand, and the solution of the reciprocal problem. The reciprocal problem is defined such that the incoming wave is characterized by the tensor quantities corresponding to those ''components'' of the outgoing solution of the original problem which are being sampled by the observer. The key insight which allows the formalism previously developed for the electromagnetic and acoustic problems (and in section II B above for the problem of scattering from the fluid–solid interface) to be extended to elastodynamic waves is the recognition that decomposing an elastodynamic wave into scalar and vector components is entirely analogous to specifying the polarization or the direction of propagation of the wave. (This insight is implicitly used, for example, in the reciprocity proof given on pp. 155–154 of Ref. 12.)

Armed with this insight, it is once again possible to derive a formal two-scale expression for the scattering amplitude of elastodynamic waves which is exact with respect to a reference surface, and good to first order in a perturbation. This is evaluated explicitly for the zero displacement boundary condition, the free boundary condition, and the continuity boundary condition found at the interface between two elastic solids. (The latter may be applicable to the study of scattering from sub-bottom layers. The two former are expected to apply to certain seismic problems.) These results are analogous to those obtained for scattering from the fluid–solid interface as well as for the electromagnetic and acoustic problems.

We are now ready to examine the details. It is shown in Appendix E that equation (2.6) reduces to

$$
\begin{aligned}
R_\infty = & \int_{S_2} dS_2[\hat{n}_1 \cdot \vec{\vec{\tau}}_1(\vec{x_1}) \cdot \vec{u}_2(\vec{x_2}) - \hat{n}_2 \cdot \vec{\vec{\tau}}_2(\vec{x_2}) \cdot \vec{u}_1(\vec{x_1})] - \int dS \xi \, \mathrm{Tr}(\vec{\vec{\varrho}}) \hat{n} \cdot \vec{\vec{\tau}}_1 \cdot \vec{u}_2 \\
& + \int dS \xi [\hat{n} \cdot \vec{\vec{\tau}}_2 \cdot \vec{\vec{\varrho}} \cdot \vec{u}_1 + \hat{n} \cdot \vec{\vec{\tau}}_1 \cdot \vec{\vec{\varrho}} \cdot \vec{u}_2] \\
& - \int dS \xi [\hat{n} \cdot \vec{\vec{\tau}}_2 \cdot (\vec{\vec{1}} - \hat{n}\hat{n}) \cdot \vec{\nabla}(\vec{u}_1 \cdot \hat{n}) + \hat{n} \cdot \vec{\vec{\tau}}_1 \cdot (\vec{\vec{1}} - \hat{n}\hat{n}) \cdot \vec{\nabla}(\vec{u}_2 \cdot \hat{n})]
\end{aligned}
$$

$$+\int dS\xi\rho\omega^2\vec{u}_1\cdot\vec{u}_1+\int dS\xi\frac{\tau^1_{nn}\tau^2_{nn}+2\hat{n}\cdot\vec{\tau}_1\cdot(\vec{\mathbf{1}}-\hat{n}\hat{n})\cdot\vec{\tau}_2\cdot\hat{n}}{2\mu}$$

$$-\int dS\xi\frac{\vec{\tau}^T_1:\vec{\tau}^T_2}{2\mu}+\int dS\xi\frac{\lambda}{2\mu}\frac{\mathrm{Tr}(\vec{\tau}^T_1)\ \mathrm{Tr}(\vec{\tau}^T_2)}{3\lambda+2\mu}-\int dS\xi\frac{\lambda}{2\mu}\frac{\tau^1_{nn}\tau^2_{nn}}{3\lambda+2\mu}. \tag{2.16}$$

Note that for the three elastodynamic boundary conditions being considered here (i.e., $\vec{u}=0$; $\hat{n}\cdot\vec{\tau}=0$; continuity of $\vec{u}$, $\hat{n}\cdot\vec{\tau}$) the first four lines of equation (2.16) are either zero, or cancel at the interface. [In particular, consider the 4th line of equation (2.16). For the zero-displacement boundary condition ($\vec{u}=0$), $\vec{u}\cdot\hat{n}=0$ on S implies that $\vec{\nabla}(\vec{u}\cdot\hat{n})\|\hat{n}$ and thus $(\vec{\mathbf{1}}-\hat{n}\hat{n})\cdot\vec{\nabla}(\vec{u}\cdot\hat{n})=0$. For the stress-free boundary condition ($\hat{n}\cdot\vec{\tau}=0$) the term is trivially zero. For the solid–solid boundary condition, we have $\vec{u}$ continuous on S, which implies that $\hat{n}\cdot(\vec{u}^I-\vec{u}^{II})=0$ everywhere on S. Thus $\vec{\nabla}(\hat{n}\cdot(\vec{u}^I-\vec{u}^{II}))$ is proportional to $\hat{n}$, and

$$(\vec{\mathbf{1}}-\hat{n}\hat{n})\cdot\vec{\nabla}(\hat{n}\cdot(\vec{u}^I-\vec{u}^{II}))=0,$$

establishing that $(\vec{\mathbf{1}}-\hat{n}\hat{n})\cdot\vec{\nabla}(\hat{n}\cdot\vec{u})$ is continuous across the interface and the term in question cancels when contributions from the two sides are subtracted.]

Also note that from Appendix B we have $R_\infty=a^{ch}\delta T^{ch}$ where the superscript ch stands for the four possible channels pp, sp, ps, and ss; and a^{ch} is given by

$$a^{pp}=\rho\omega^2/k_p^2,\quad a^{sp}=\rho\omega^2/k_s^{1/2}k_p^{3/2},$$
$$a^{ps}=\rho\omega^2/k_s^{3/2}k_p^{1/2},\quad a^{ss}=\rho\omega^2/k_s^2, \tag{2.17}$$

where we are implicitly assuming that the *incoming* wave corresponding to the solution labeled by 1 contains only the type of wave (s or p) given by the 2nd label in ch, is normalized to unity, and approaches from a direction given by $\hat{k}$, while the *incoming* wave corresponding to the solution labeled by 2 contains only the type of wave given by the 1st label in ch, is also normalized to unity, and approaches from a direction given by $-\hat{q}=-\hat{r}$ (where $\hat{r}$ specifies the angular coordinates of the observer).

We are now ready to consider specific cases. Along with equation (2.12), they are the *fundamental results* of this paper.

1. The zero-displacement boundary condition

For the zero-displacement boundary condition, $\vec{u}=0$. This corresponds to scattering from an infinitely rigid wall. It is shown in Appendix F that in this case, equation (2.16) reduces to

$$a^{ch}\delta T^{ch}=\int dS\xi\left[\frac{\tau^1_{nn}\tau^2_{nn}}{\lambda+2\mu}+\frac{\hat{n}\cdot\vec{\tau}_1\cdot(\vec{\mathbf{1}}-\hat{n}\hat{n})\cdot\vec{\tau}_2\cdot\hat{n}}{\mu}\right]. \tag{2.18}$$

2. The stress-free boundary condition

The stress-free boundary condition ($\hat{n}\cdot\vec{\tau}=0$) is relevant to the problem of scattering from a free surface (i.e., the boundary between a solid and a vacuum such as, for example, an air–rock interface). When this condition applies, equation (2.16) immediately reduces to

$$a^{ch}\delta T^{ch}=\int dS\xi\left[\rho\omega^2\vec{u}_1\cdot\vec{u}_2-\frac{\vec{\tau}^T_1:\vec{\tau}^T_2}{2\mu}+\frac{\lambda}{2\mu}\frac{\mathrm{Tr}(\vec{\tau}^T_1)\ \mathrm{Tr}(\vec{\tau}^T_2)}{3\lambda+2\mu}\right]. \tag{2.19}$$

The reader should be aware of the availability of an additional technique for solving this type of boundary value problem. De Santo[14] has developed a diagrammatic approach for modeling the scattering of elastodynamic waves from surfaces obeying stress-free boundary conditions. Of particular relevance to the discussion here, it should be noted that this method may find use in solving for $\vec{u}$ and $\vec{\vec{\tau}}$ of the reference problem.

3. The solid–solid boundary condition

For the solid–solid boundary condition ($\vec{u}$, $\hat{n}\cdot\vec{\vec{\tau}}$ continuous) we subtract equation (2.16) on the two sides of the interface and use the continuity conditions to obtain

$$a^{ch}\delta T^{ch}=\int dS\xi(\rho_I-\rho_{II})\omega^2\vec{u}_1\cdot\vec{u}_2+\int dS\xi\left(\frac{1}{\mu_I}\frac{\lambda_I+\mu_I}{3\lambda_I+2\mu_I}-\frac{1}{\mu_{II}}\frac{\lambda_{II}+\mu_{II}}{3\lambda_{II}+2\mu_{II}}\right)\tau^1_{nn}\tau^2_{nn}$$
$$+\int dS\xi\left(\frac{1}{\mu_I}-\frac{1}{\mu_{II}}\right)\hat{n}\cdot\vec{\vec{\tau}}_1\cdot(\vec{\vec{1}}-\hat{n}\hat{n})\cdot\vec{\vec{\tau}}_2\cdot\hat{n}-\int dS\xi\left[\frac{\vec{\vec{\tau}}_1^{TI}:\vec{\vec{\tau}}_2^{TI}}{2\mu_I}-\frac{\vec{\vec{\tau}}_1^{TII}:\vec{\vec{\tau}}_2^{TII}}{2\mu_{II}}\right]$$
$$+\int dS\xi\left[\frac{\lambda_I}{2\mu_I}\frac{\mathrm{Tr}(\vec{\vec{\tau}}_1^{TI})\,\mathrm{Tr}(\vec{\vec{\tau}}_2^{TI})}{3\lambda_I+2\mu_I}-\frac{\lambda_{II}}{2\mu_{II}}\frac{\mathrm{Tr}(\vec{\vec{\tau}}_1^{TII})\,\mathrm{Tr}(\vec{\vec{\tau}}_2^{TII})}{3\lambda_{II}+2\mu_{II}}\right]. \tag{2.20}$$

The off-diagonal element of $\vec{\vec{\tau}}^T$, $\tau_{t_1t_2}$ obeys the simple boundary condition given in Appendix G, but this does not lead to an apparent simplification of the formal result equation (2.20). Once again, note that De Santo[15] has developed a boundary integral equation approach, which facilitates numerical calculations modeling the scattering of elastodynamic waves from solid–solid interfaces. This method could be useful in solving the reference problem.

III. EXAMPLE: THE ''SMALL SLOPE'' AND '' 'LOCAL' TWO-SCALE'' APPROXIMATIONS FOR THE FLUID-SOLID INTERFACE

To illustrate the results obtained in section II, we now use the formalism for the fluid–solid boundary [specifically, equation (2.14)] to derive both the small slope and the ''local'' two-scale (i.e., composite model) approximations. The approach follows that pursued for the acoustic and electromagnetic problems as outlined in references 1, 3. For a more complete discussion concerning the origin of this type of approximation, see references 16–22.

The approximations considered here are used to model scattering from a fluid-elastic interface S which can naturally be parameterized by the coordinates $\vec{x}=(\mathbf{x},h(\mathbf{x}))$ where $\mathbf{x}$ is a 2-dimensional vector specifying coordinates in a plane, and $h(\mathbf{x})$ is a single-valued function which averages to zero when $\mathbf{x}$ is allowed to vary over the entire plane.

Note that in this paper, as in references 2–4, a bold-faced variable indicates a 2-dimensional vector, while a variable with an arrow on top represents a 3-dimensional vector. We are implicitly employing a Cartesian coordinate system oriented such that the direction of the positive z-axis (given by the unit vector $\hat{z}$) is given by $\hat{z}=\hat{n}$, where $\hat{n}$ is the unit vector normal to the plane pointing *into* the fluid. (Keep in mind that the wave is assumed to be incident from the fluid side.) Concerning an additional point of notation, the vector $\vec{r}$ will be used to denote an arbitrary point in space, while $\vec{x}$ (or $\vec{x}_0$) denotes the (3-dimensional) coordinates of a point on a scattering (or reference) surface.

Typically, $h(\mathbf{x})$ is a statistical quantity, often, but not necessarily always, characterized by Gaussian statistics (e.g., see reference 1). The formalism described in this section may, for example, be applicable to modeling acoustic scattering from the sea floor in certain regions of the world's oceans.

The small slope approximation is good to 2nd order in both the slope and the radius of curvature of the scattering surface [i.e., Error $= O(\nabla h, \nabla\nabla h/\kappa)$ where κ is the smallest of the various wavenumbers characterizing the field]. This approximation differs from 1st order perturbation theory primarily because it is good to all orders in $Q_z h$.

The ''local'' two-scale approximation assumes, in addition, the existence of a reference surface S_0 given by $\vec{x}_0=(\mathbf{x},h_0(\mathbf{x}))$. This approximation is here called ''local'' because the particular two-scale model being developed in this section measures the tilt of the reference surface, but does not include non-local effects such as shadowing and multiple scattering. It is formally accurate to 1st order in the radius of curvature of the *reference* surface S_0, but it retains accuracy to much higher orders with respect to the slope of S_0. Thus, the ''local'' two-scale approximation is typically appropriate for use when a reference surface is available so that most of the slope of S is due to the ''tilt'' of the reference surface [i.e., for $\delta h \equiv h(\mathbf{x})-h_0(\mathbf{x})$, we have $\nabla(\delta h)\ll\nabla h_0$], while the radius of the curvature of the reference surface S_0 remains small relative to all of the wavelengths associated with the field (see discussion in section II of Ref. 1). The ''local'' two-scale approximation is also well suited to instances when there are large scale features present which are best described deterministically, while superimposed on these one finds small scale surface features which can only be conveniently characterized statistically. Such a scenario may apply to some of the ocean bottom scattering problems referred to just above. In such cases, a non-local effect like shadowing, if important, must be inserted by hand. Since the formalism is manifestly reciprocal, this is not too difficult (see comments towards the end of section IV in reference 2). As will be shown below, following our approach, the ''local'' two-scale approximation turns out to be closely related to the small slope approximation.

A. The general procedure

We begin by deriving the small slope approximation, and then generalizing the result to the ''local'' two-scale approximation. In so doing, we follow a very general procedure developed in section II of reference 3. The starting point for this approach is the general form for the scattering amplitude given by equation (2.2) of reference 3:

$$T_0(\vec{q},\vec{k})=\frac{i}{Q_z}\int d^2x A_0(\vec{q},\vec{k}) \tag{3.1}$$

(recalling that $\vec{Q}\equiv\vec{k}-\vec{q}$). Note that the equation for a fluid–solid interface, equation (2.14), has this form, allowing A_0 to be expressed in terms of the displacement vector $\vec{u}$ and the stress tensor $\overleftrightarrow{\tau}$ evaluated on the two sides of the interface. T_0 and A_0 are taken to refer to the problem of scattering from a reference surface S_0. The scattering amplitude T corresponding to the surface $S=(\mathbf{x},h_0(\mathbf{x})+\delta h(\mathbf{x}))$ is given by equation (2.6) in reference 3:

$$T(\vec{q},\vec{k})=\frac{i}{Q_z}\int d^2x e^{iQ_z\delta h}A_0(\vec{q},\vec{k})+O\left((\nabla\delta h)^2,\left(\frac{\nabla\nabla\delta h}{\kappa}\right)^2\right) \tag{3.2}$$

[through $O(\delta h)$, this result follows directly from (2.12); higher orders in $Q_z\delta h$ essentially come by considering the phase shift associated with a constant translation, but some effort is needed to rigorously eliminate the possibility of cross-terms between higher orders of $Q_z\delta h$ and 1st order in derivatives of δh; see appendix A of Ref. 3]. The small slope follows when the reference surface is chosen to be the plane $h_0=0$. [This case is a little unusual since (3.1) will give δ-functions corresponding to specular scattering directions, but this does not invalidate the method.]

Thus, the small slope approximation can be obtained as follows. Set $A_0(\vec{q},\vec{k})$ equal to $\rho_I\omega^2$ times the integrand of equation (2.14), and evaluate it with $\vec{u}^I$, $\overleftrightarrow{\tau}^I$, $\vec{u}^{II}$, and $\overleftrightarrow{\tau}^{II}$ chosen to be the

solutions to the flat plane problem. Then insert the resulting expression for $A_0(\vec{q},\vec{k})$ into equation (3.2). Note that the effect of the phase factor $\exp(iQ_z\delta h)$ in equation (3.2) is simply to shift the phase to that of the incoming wave at the interface.

The ''local'' two-scale approximation is obtained from the small slope result when the normal to the plane $\hat{z}$ is replaced by $\hat{n}_0$, the normal to some reference surface S_0. Furthermore, the phase of all the components of the solution must now be set equal to the phase of the incoming wave evaluated on the reference surface S_0. In other words, define

$$\mathbf{k}\equiv(\vec{\mathbf{1}}-\hat{z}\hat{z})\cdot\vec{k}= \text{ horizontal component of } \vec{k}$$

and consider the solution to the flat plane problem. On the interface (i.e., the $z=0$ plane) the incident, reflected, and both the transmitted waves have the same phase given by $\exp(i\mathbf{k}\cdot\mathbf{x})$ (a more detailed discussion will be presented when the problem is solved below). In going from the small slope to the two-scale approximation, this gets replaced according to the prescription

$$e^{i\mathbf{k}\cdot\mathbf{x}}\rightarrow e^{i\mathbf{k}\cdot\mathbf{x}}e^{ik_zh_0}=e^{i\vec{k}\cdot\vec{x}_0}.$$

What has effectively been done here is to treat the reference surface as being locally flat, with an additional phase shift accounting for the fact that the origin is no longer on the plane. If there were no curvature to the surface, the result would be exact. (If this all seems unclear, see reference 3, section II for further discussion concerning this procedure.) Finally, note that once again, the phase factor $\exp(iQ_z\delta h)$ in equation (3.2) will effectively bring the phase up to $\exp(i\vec{k}\cdot\vec{x})$, where $\vec{x}$ is on the actual scattering surface.

Henceforth, we will conduct our calculation in a general notation which will apply to both the small slope and the two-scale approximation. This is possible essentially because the small slope is, formally speaking, a special case of the local two-scale approximation, although a close inspection of the procedure described in the preceding paragraph, as well as a comparison of the error terms, will indicate that some caution must be exercised before taking this connection too literally.

From now on, we will therefore use $\hat{n}$ to stand for either $\hat{z}$ (small slope) or $\hat{n}_0$ (''local'' two-scale). The phase on the reference interface is given by $\exp(i\vec{k}\cdot\vec{x}_0)$ where $\vec{x}=(\mathbf{x},0)$ for the small slope calculation, and $\vec{x}=(\mathbf{x},h_0)$ for the small slope calculation. It will also be useful to define the quantity

$$\mathbf{k}_\perp\equiv(\vec{\mathbf{1}}-\hat{n}\hat{n})\cdot\vec{k}.$$

This is the component of the vector in the tangent plane of the reference surface for the ''local'' two-scale approximation, and the horizontal component $\mathbf{k}$ (i.e., in the x-y plane) of the wave vector in the small slope approximation.

B. Solution for the flat plane problem

Keeping in mind that in the flat plane problem, the unit vector $\hat{n}$ is the constant vector $\hat{z}$, the general form of the pressure field resulting when a normalized incoming plane wave scatters from a flat interface is

$$P=e^{i\vec{k}_i\cdot\vec{r}}+Be^{i\vec{k}_R\cdot\vec{r}},$$
$$\vec{k}_i=(\mathbf{k}_\perp,k_{in});\quad \vec{k}_R\equiv(1-2\hat{n}\hat{n})\cdot\vec{k}_i=(\mathbf{k}_\perp,-k_{in}). \tag{3.3}$$

In presenting solutions to the flat plane problem, we will henceforth append the subscript i to the incoming wavevector (i.e., $\vec{k}\rightarrow\vec{k}_i$). As always, the time dependence $\exp(-i\omega t)$ has been dropped.

(Note that throughout this paper, we have implicitly decomposed the scattering problem for an arbitrary incoming field into the problem of scattering each individual plane wave component of the incoming field. This is a standard procedure for problems where the medium does not vary as a function of the time. See reference 1, section II for more details.)

B will be derived from the boundary conditions below. The general form of the solution and the definition of $\vec{k}_R$ follow from the requirement that the horizontal component of the wavenumber must be conserved at a flat interface. This is a well known result and can be deduced from very general arguments [see, for example, reference 23, equation (7.34)]. Note that $k_i=|\vec{k}_i|=|\vec{k}_R|=\omega/c_I$ where c_I is the speed of sound in the fluid.

Now, use

$$\vec{u}^I=\frac{\vec{\nabla}P}{\rho_I\omega^2}, \tag{3.4}$$

the definition of $\vec{\vec{\tau}}$ [equation (2.1)], and the Helmholtz equation for P to show

$$\vec{\vec{\tau}}^I=\lambda_I\vec{\nabla}\cdot\vec{u}^I=-P\vec{\vec{1}}, \tag{3.5}$$

and consequently

$$\vec{u}^I=\frac{i}{\rho_I\omega^2}(\vec{k}_i e^{i\vec{k}_i\cdot\vec{r}}+B\vec{k}_R e^{i\vec{k}_R\cdot\vec{r}}), \tag{3.6}$$

$$\vec{\vec{\tau}}^I=-(e^{i\vec{k}_i\cdot\vec{r}}+Be^{i\vec{k}_R\cdot\vec{r}})\vec{\vec{1}}. \tag{3.7}$$

Also in the solid, we have in general both outgoing primary (p) and secondary (s) waves:

$$\vec{u}^{II}=C[\hat{k}_p e^{i\vec{k}_p\cdot\vec{r}}-A_S\hat{t}e^{i\vec{k}_s\cdot\vec{r}}], \tag{3.8}$$

where C, A_S, and $\hat{t}$ will be determined below. Once again using the definition of $\vec{\vec{\tau}}$ equation (2.1) we have

$$\vec{\vec{\tau}}^{II}=iC[k_p(\lambda_{II}\vec{\vec{1}}+2\mu_{II}\hat{k}_p\hat{k}_p)e^{i\vec{k}_p\cdot\vec{r}}-\mu_{II}k_sA_S(\hat{k}_s\hat{t}+\hat{t}\hat{k}_s)e^{i\vec{k}_s\cdot\vec{r}}]. \tag{3.9}$$

Note that $k_p=|\vec{k}_p|=\omega/c_p$, $k_s=|\vec{k}_s|=\omega/c_s$, where

$$c_p=\sqrt{\frac{\lambda_{II}+2\mu_{II}}{\rho_{II}}},\quad c_s=\sqrt{\frac{\mu_{II}}{\rho_{II}}} \tag{3.10}$$

are the propagation speeds for the primary and secondary waves, respectively. We also have

$$\begin{aligned}\vec{k}_p&=(\mathbf{k}_\perp,k_{pn})\ \text{ with }\ k_{pn}=\operatorname{sgn}(k_{in})\sqrt{k_p^2-\mathbf{k}_\perp\cdot\mathbf{k}_\perp},\\ \vec{k}_s&=(\mathbf{k}_\perp,k_{sn})\ \text{ with }\ k_{sn}=\operatorname{sgn}(k_{in})\sqrt{k_s^2-\mathbf{k}_\perp\cdot\mathbf{k}_\perp},\end{aligned} \tag{3.11}$$

where the principal values of the square roots must be taken (i.e., positive if the argument of the square root is positive, a positive number times i if it is negative). Note that if the positive z-axis points *into* the fluid and therefore in the direction of the normal $\hat{n}$ (all this is generally assumed in this paper), then $\operatorname{sgn}(k_{in})$ corresponds to a ''$-$'' sign.

It is easily verified that the boundary condition $\hat{n}\cdot\vec{\vec{\tau}}^{\,II}\cdot(1-\hat{n}\hat{n})=0$ implies that $(1-\hat{n}\hat{n})\cdot\hat{t}\propto\mathbf{k}_\perp$ (independent of C or A_S). Note that this constrains $\hat{t}$ to the plane of incidence and therefore implies that the shear wave is linearly polarized for this (the flat plane) problem.

By additionally recognizing that $\hat{t}\perp\vec{k}_s$, and recalling that $\hat{t}$ is normalized to unity, we can conclude that $\hat{t}$ must (aside from an overall phase which can be absorbed in A_S) be given by

$$\hat{t}=\hat{k}_s\times\frac{\hat{n}\times\mathbf{k}_\perp}{|\mathbf{k}_\perp|}=\frac{\hat{n}|\mathbf{k}_\perp|^2-\mathbf{k}_\perp k_{sn}}{|\mathbf{k}_\perp|k_s}. \tag{3.12}$$

Substituting this result back into the equation $\hat{n}\cdot\vec{\tau}^{\,II}\cdot(1-\hat{n}\hat{n})=0$, applying some straightforward algebra, including the result

$$1-\frac{k_{sn}^2}{|\mathbf{k}_\perp|^2}=2\left(1-\frac{k_s^2}{2|\mathbf{k}_\perp|^2}\right),$$

we find

$$A_S=\frac{k_s k_{pn}}{|\mathbf{k}_\perp|k_p(1-k_s^2/2|\mathbf{k}_\perp|^2)}. \tag{3.13}$$

The continuity conditions on $\hat{n}\cdot\vec{u}$ and τ_{nn} provide two equations for the two remaining unknowns B and C. After some (mostly) straightforward algebra, we find

$$B=\frac{\alpha+\beta-\delta}{\alpha+\beta+\delta},\quad C=\frac{-2i}{\alpha+\beta+\delta},$$

where

$$\alpha=-k_p\left(\lambda_{II}+2\mu_{II}\frac{k_{pn}^2}{k_p^2}\right)=\frac{k_s}{k_p}\frac{2\mu_{II}}{A_S}\frac{k_{pn}}{k_p}|\mathbf{k}_\perp,$$

$$\beta=2\mu_{II}\left(\frac{k_{sn}}{k_s}\right)|\mathbf{k}_\perp|A_S,\quad \delta=\frac{\rho_I\omega^2}{k_{in}}\left(\frac{k_s}{2|\mathbf{k}_\perp|}\right)A_S, \tag{3.14}$$

where the expression for α in terms of A_S makes use of a lemma derived in Appendix H. This is the only tricky part related to the derivation of equation (3.14). The form of the solution given by this equation follows directly from the boundary conditions. It is also well suited for verification of energy conservation (i.e., $|B|^2\leqslant 1$) even when the transmitted waves become evanescent (i.e., k_{pn} imaginary, or k_{pn} and k_{sn} both imaginary; k_{sn} only imaginary is impossible).

For practical applications to be discussed below, it will also be useful to have the following alternate form of the solution available:

$$B=\frac{a-1}{a+1},\quad C=\frac{-b}{ik_p\mu_{II}(\lambda_{II}/2\mu_{II}+1)}\frac{1}{a+1},$$

where

$$a=\frac{\alpha+\beta}{\delta}=\frac{\rho_{II}}{\rho_I}\frac{k_{in}}{k_{pn}}\left[1-\frac{4|\mathbf{k}_\perp|^2k_{sn}(k_{sn}-k_{pn})}{k_s^4}\right],$$

$$b=\frac{\rho_{II}}{\rho_I}\frac{k_{in}}{k_{pn}}\left(1-\frac{2|\mathbf{k}_\perp|^2}{k_s^2}\right). \tag{3.15}$$

Generally straightforward algebra is needed to obtain result (3.15). The only ''tricky'' step comes in eliminating the explicit ω^2 from C by making the substitution

$$k_p^2=\frac{\rho_{II}\omega^2}{2\mu_{II}(1+\lambda_{II}/2\mu_{II})}. \tag{3.16}$$

C. Approximate representations of the scattering amplitude

1. Derivation

To evaluate the integrand A_0 in equation (3.2), it is necessary to evaluate the displacement vector and stress tensor on the reference surface. As stated above, for the small slope approximation, this means taking the flat plane solution [as given by equations (3.6)–(3.9], and evaluating it on the interface, which is called S_0 [recall, this is the plane $(\mathbf{x},0)$ for the small slope approximation]. Thus, we have

$$e^{i\vec{k}_i\cdot\vec{x}}|_{S_0}=e^{i\vec{k}_R\cdot\vec{x}}|_{S_0}=e^{i\vec{k}_p\cdot\vec{x}}|_{S_0}=e^{i\vec{k}_s\cdot\vec{x}}|_{S_0}=e^{i\mathbf{k}_\perp\cdot\vec{x}}. \tag{3.17}$$

For the ''local'' two-scale approximation, let $\hat{n}\rightarrow\hat{n}_0$ and make the following replacement (as discussed above):

$$\left.\begin{matrix} e^{i\vec{k}_R\cdot\vec{x}}|_{S_0} \\ e^{i\vec{k}_p\cdot\vec{x}}|_{S_0} \\ e^{i\vec{k}_s\cdot\vec{x}}|_{S_0} \end{matrix}\right\} \rightarrow e^{i\vec{k}_i\cdot\vec{x}}|_{S_0}+O\left(\frac{1}{R_c}\right), \tag{3.18}$$

where $1/R_c\propto\nabla\nabla h_0$ is the reciprocal of the radius of curvature of the reference surface S_0 given by $(\mathbf{x},h_0)$ (i.e., at each point, assume that the reference surface is locally flat). (For more information concerning the relationship of $\nabla\nabla h_0$ to the geometric quantity R_c, see reference 2, Appendix B.) Once again note that the extra phase in equation (3.2) formally implies that the phase is evaluated on the ''true'' scattering surface S rather than on the reference surface S_0, but the normal vector $\hat{n}$ is evaluated on the reference surface (i.e., $\hat{n}=\hat{z}$ for the small slope, $\hat{n}=\hat{n}_0$ for the ''local'' two-scale).

Thus effectively, for the small slope and two-scale approximations, we can now substitute the following quantities directly into equation (2.14):

$$\vec{u}_1^I=\frac{i}{\rho_I\omega^2}(\vec{k}_i+B\vec{k}_R)e^{i\vec{k}_i\cdot\vec{x}},\quad \vec{\vec{\tau}}_1^I=-(1+B)\vec{\vec{1}}e^{i\vec{k}_i\cdot\vec{x}},$$

$$\vec{u}_1^{II}=C[\hat{k}_p-A_S\hat{t}]e^{i\vec{k}_i\cdot\vec{x}}, \tag{3.19}$$

$$\vec{\vec{\tau}}_1^{II}=iC[k_p(\lambda_{II}\vec{\vec{1}}+2\mu_{II}\hat{k}_p\hat{k}_p)-\mu_{II}k_sA_S(\hat{k}_s\hat{t}+\hat{t}\hat{k}_s)]e^{i\vec{k}_i\cdot\vec{x}},$$

where the quantities $\hat{k}_R$, $\hat{k}_p$, $\hat{k}_s$, $\hat{t}$, B, C, and A_S are all evaluated using $\hat{n}$ of the reference surface ($\hat{z}$ or $\hat{n}_0$) and the position vector $\vec{x}$ in the phase lies on the scattering surface S. For the same quantities labeled by the subscript ''2,'' just replace $\vec{k}$ with $-\vec{q}$.

Recall that the error introduced when substitutions (3.19) are made into (2.14) is $O((\nabla h)^2, (\nabla\nabla h)^2)$ for the small slope approximation and $O(\nabla\nabla h_0)$ for the ''local'' two-scale approximation. *For these two approximations*, we can further simplify the expression for the scattering amplitude T, equation (2.14), as follows:

$$\frac{-iQ_zT}{\rho_1\omega^2}=\int d^2x[\text{ Integrand}]$$

$$\begin{aligned}\text{Integrand}=&(\rho_I-\rho_{II})\omega^2\hat{n}\cdot\hat{u}_1\hat{n}\cdot\hat{u}_2+[(\rho_I-\rho_{II})\omega^2+2\mu_{II}\vec{k}_i\cdot(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})\cdot\vec{q}_i]\vec{u}_1^{II}\cdot(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})\cdot\vec{u}_2^{II}\\&-\rho_I\omega^2(\vec{u}_1^I-\vec{u}_1^{II})\cdot(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})\cdot(\vec{u}_2^I-\vec{u}_2^{II})+\left(\frac{k_i^2}{\rho_I\omega^2}+\frac{1}{2\mu_{II}}\right)\tau_{nn}^1\tau_{nn}^2\\&+\frac{\lambda_{II}}{(3\lambda_{II}+2\mu_{II})^2}\left(1+\frac{\lambda_{II}}{2\mu_{II}}\right)[\text{ Tr}(\overleftrightarrow{\tau}_1^{II})\text{ Tr}(\overleftrightarrow{\tau}_2^{II})]\\&-\frac{1}{(3\lambda_{II}+2\mu_{II})}\left(1+\frac{\lambda_{II}}{2\mu_{II}}\right)[\text{ Tr}(\overleftrightarrow{\tau}_1^{II})\tau_{nn}^2+\text{ Tr}(\overleftrightarrow{\tau}_2^{II})\tau_{nn}^1].\end{aligned}\tag{3.20}$$

The derivation is given in Appendix I. We will see below that the three terms manifestly of order $1/\mu$ cancel in the limit as $\mu\to 0$ (i.e., they are associated with the elastic solid only and disappear in the limit as the solid becomes a fluid).

Note that the only quantities needed are $\vec{u}^I$, $\vec{u}^{II}$, τ_{nn}, and $\text{Tr}(\overleftrightarrow{\tau}^{II})$. *Suppressing the phase factor* $\exp(i\vec{k}_i\cdot\vec{x})$ [or $\exp(-i\vec{q}_i\cdot\vec{x})$], we have, using equations (3.15) and (3.19):

$$\text{Tr}(\overleftrightarrow{\tau}^{II})=iCk_p(3\lambda_{II}+2\mu_{II})=\frac{-b(3\lambda_{II}+2\mu_{II})}{\mu_{II}\left(1+\dfrac{\lambda_{II}}{2\mu_{II}}\right)}\frac{1}{a+1},$$

$$\tau_{nn}=-(1+B)=\frac{-2a}{a+1},\tag{3.21}$$

$$\vec{u}^I=\frac{i}{\rho_I\omega^2}[k_{in}(1-B)\hat{n}+(1+B)\mathbf{k}_\perp]=\frac{2i}{\rho_I\omega^2}\frac{1}{a+1}[k_{in}\hat{n}+a\mathbf{k}_\perp].$$

Recasting $\vec{u}^{II}$ is trickier. The result is

$$\begin{aligned}\vec{u}^{II}&=\frac{2i}{\rho_I\omega^2}\frac{1}{a+1}[k_{in}\hat{n}+\xi\mathbf{k}_\perp],\\\xi&=\frac{k_{in}}{k_{pn}k_s^2}[(k_{sn}-k_{pn})^2-k_p^2]=\frac{k_{in}}{k_{pn}}\left(1-2\frac{\vec{k}_s\cdot\vec{k}_p}{k_s^2}\right).\end{aligned}\tag{3.22}$$

The details of the derivation are given in Appendix J.

2. Key result

In Appendix K, it is shown that substituting the results (3.21) and (3.22) into equation (3.20) leads to the result

$$\begin{aligned}T(\vec{q}_i,\vec{k}_i)=\frac{i}{Q_{iz}}\int d^2x e^{i\vec{Q}_i\cdot\vec{x}}\Bigg[&\left(1-\frac{\rho_{II}}{\rho_I}\right)\frac{4k_{in}q_{in}}{(a_1+1)(a_2+1)}\\&+4\left(1-\frac{\rho_{II}}{\rho_I}\right)\vec{k}_i\cdot(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})\cdot\vec{q}_i\frac{\xi_1\xi_2}{(a_1+1)(a_2+1)}\end{aligned}$$

$$+\frac{8\rho_{II}}{\rho_I k_s^2}[\vec{k}_i\cdot(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})\cdot\vec{q}_i]^2\frac{\xi_1\xi_2}{(a_1+1)(a_2+1)}-4\vec{k}_i\cdot(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})\cdot\vec{q}_i\frac{(a_1-\xi_1)(a_2-\xi_2)}{(a_1+1)(a_2+1)}$$

$$+4k_i^2\frac{a_1a_2}{(a_1+1)(a_2+1)}+2k_s^2\frac{\rho_I}{\rho_{II}}\frac{(a_1-b_1)(a_2-b_2)}{(a_1+1)(a_2+1)}-4k_p^2\frac{\rho_I}{\rho_{II}}\frac{b_1b_2}{(a_1+1)(a_2+1)}\Bigg], \tag{3.23}$$

where a_1 and b_1 are simply a and b given in equation (3.15), and ξ_1 is similarly given by equation (3.22). For the quantities labeled by the subscript ''2'' just substitute $-\vec{q}_i$ for $\vec{k}_i$ everywhere. Recall that $\vec{k}_p$, $\vec{k}_s$, and $\mathbf{k}_\perp$ are all derived from $\vec{k}_i$ using equations (3.11), and that $-\vec{q}_p$, $-\vec{q}_s$, and $-\mathbf{q}_\perp$ are similarly defined. Since equation (3.23) directly provides the small slope ($\hat{n}=\hat{z}$) and ''local'' two-scale ($\hat{n}=\hat{n}_0$) approximations for the scattering amplitude corresponding to a fluid–solid interface, it is one of the major results of this paper.

3. Discussion

Note the following change in notation as compared with previous equations involving the scattering amplitude [such as (3.1), (3.2), and (3.20)]. We are now appending the subscript i onto the vectors $\vec{k}$, $\vec{q}$, and $\vec{Q}$ in order to bring our notation in line with that used to discuss the flat plane problem. Recall that this change was made in order to clearly distinguish these wavevectors from those related to the p- and s-waves in the solid (i.e., medium II).

Note that it is possible to make the substitution $\rho_{II}/k_s^2=\mu_{II}/\omega^2$ in the third line of equation (3.23). We will see below that the 3rd and 6th lines disappear in the limit as the solid becomes a fluid (i.e., $\mu_{II}\to 0$).

In examining (3.23), also keep in mind that $\hat{n}=\hat{z}$ for the small slope approximation and that $\hat{n}=\hat{n}_0$ for the ''local'' two-scale approximation. Recall that the error for the small slope version of the result is of order $O((\nabla h)^2,([\nabla\nabla h]/k_i)^2)$ (where $\nabla\nabla h=1/R_c$, R_c is the local radius of curvature of the interface). The error for the ''local'' two-scale version ($\hat{n}=\hat{n}_0$) of the result is $O([\nabla\nabla h_0]/k_i)$ (where $\nabla\nabla h_0=1/R_{0c}$, R_{0c} is the local radius of curvature of the reference surface).

The small slope version of result (3.23) must be equivalent to the expression for the small slope scattering amplitude (also for scattering from a fluid–solid interface) given in references 24 and 25. (To be specific, in reference 24, evaluate equation ((23) with ϕ given by equations (25) (use 1st order only) and (31); in reference 25, evaluate equation (2) with ϕ_0 given by equation (6) and ϕ_1 given by equation (7).] Note that, as remarked in reference 24, it is difficult to see reciprocity in the previously published version of this result, but reciprocity is easy to see in equation (3.23).

D. Limiting cases

Consider the limit as the 2nd Lamé constant $\mu_{II}\to 0$, while the density in the solid ρ_{II} remains non-zero. As is demonstrated in Appendix L, this leads to

$$T(\vec{q}_i,\vec{k}_i)=\frac{i}{Q_{iz}}\int d^2x e^{i\vec{Q}_i\cdot\vec{x}}\Bigg[\left(1-\frac{\rho_{II}}{\rho_I}\right)k_{in}q_{in}(2-A_{\vec{k}_i})(2-A_{-\vec{q}_i})$$

$$+\left(\frac{\rho_I}{\rho_{II}}-1\right)\vec{k}_i\cdot(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})\cdot\vec{q}_iA_{\vec{k}_i}A_{-\vec{q}_i}+\left(k_i^2-\frac{\rho_I}{\rho_{II}}k_p^2\right)A_{\vec{k}_i}A_{-\vec{q}_i}\Bigg]+O(\mu_{II}^{1/2}), \tag{3.24}$$

where

$$A_{\vec{k}_i} \equiv \frac{2a_1}{a_1+1}; \quad A_{-\vec{q}_i} \equiv \frac{2a_2}{a_2+1}.$$

[Recall that a_1 (and analogously a_2) are given by equation (3.15).] As would be expected, this is the 2-fluid result given in equation (C12) of Appendix C in reference 3 (with the identification $k_p = k_{II}$, $k_i = k_I$, $\vec{k}_i = \vec{k}$, $\vec{q}_i = \vec{q}$, and $\vec{Q}_i = \vec{Q}$).

On the other hand, taking the limit $\mu_{II} \to \infty$, we recover

$$T(\vec{q}_i, \vec{k}_i) = \frac{i}{Q_{iz}} \int d^2x \; e^{i\vec{Q}_i \cdot \vec{x}} [-4\vec{k}_i \cdot (\vec{\mathbf{1}} - \hat{n}\hat{n}) \cdot \vec{q}_i + 4k_i^2] + O\left(\frac{1}{\mu_{II}}\right). \tag{3.25}$$

The derivation is given in Appendix M. Note that the object in parentheses can be rewritten as

$$4[k_{in} q_{in} - \vec{k}_i \cdot \vec{q}_i + k_i^2],$$

and we recover the result for Neumann boundary conditions at the interface given by equation (C11) in reference 3.

Finally, if we let $\mu_{II} \to 0$, $\rho_{II} \to 0$ simultaneously, we obtain

$$T(\vec{q}_i, \vec{k}_i) = \frac{i}{Q_{iz}} \int d^2x \; e^{i\vec{Q}_i \cdot \vec{x}} 4k_{in} q_{in} + O(\mu_{II}, \rho_{II}). \tag{3.26}$$

The derivation is sketched in Appendix N. This is the result for scattering from Dirichlet boundary conditions, equation (C10) in Ref. 3.

IV. AN IMPORTANT CAVEAT CONCERNING PERTURBATIVE SCATTERING THEORY

As several researchers have noted (see reference 9 (pp. 41,100), and reference [26]–28), perturbative approaches for calculating the scattering amplitude do not, in general, conserve energy. This phenomenon is most easily seen at very shallow grazing angles. Specifically, for the Neumann boundary conditions, the cross-section remains non-zero as the grazing angle approaches zero. For example, consider the small slope ($\hat{n} = \hat{z}$) versions of equations (3.24), (3.25), and (3.26). In equations (3.24) and (3.26), the scattering amplitude goes to zero as the angle of incidence becomes very shallow, but for equation (3.25), it does not! On the other hand, the scattered energy *must always* go to zero, because energy conservation requires that the scattered wave disappear as the grazing angle becomes very small, since all the flux associated with the incoming wave is traveling horizontally, and is thus unavailable for diffuse scattering (i.e., the energy actually incident on a patch of surface goes to zero). It is important to keep in mind that this is a particularly blatant example of what is in fact a more general problem: *that perturbative scattering theory does not conserve energy*.

This violation of energy conservation, of course, casts doubt on the validity of the perturbative approach to surface scattering. However, there are physical and mathematical grounds for concluding that this phenomenon is only important at very shallow grazing angles ($1° - 2°$).[26,28] Physically, the problem is the result of an interaction between the interface wave and the scattering process [reference 9, (p. 100) and reference 28] (i.e., the surface effectively comes out and ''grabs'' the incoming wave). A significant interaction between scattering and an interface wave would reasonably be expected to occur at very shallow grazing angles where the incoming wave can be thought of as spending a great deal of time close to the interface (without actually touching it). More specifically, use an intuitive picture taken from ray theory, and think of a given ray at shallow grazing angle as spending more time in a thin band near the surface, where it is able to interact with the interface wave. In addition, note that the purely formal mathematical argument

presented in the previous paragraph also points to the fact that the breakdown of unitarity (i.e., energy conservation) becomes most apparent as the grazing angle becomes very shallow.

In light of these insights, there is reason to believe that use of an approach based on formulas (2.12), (2.18), (2.19), and (2.20) may mitigate these problems. Note that our formulas are formally *exact* with respect to the reference solution. Therefore, provided one chooses a reference surface so that the corresponding solution includes interaction between the interface wave and the scattering, it may be possible to circumvent this problem within the context of perturbation theory. There are some tricky issues being raised here, and pursuit of such a project requires original and possibly subtle uses of the formalism. For example, note that the reference surface is typically chosen so that the perturbation δh corresponds to components of the surface wavenumber spectrum on the order of the Bragg wavenumber and larger. (See, e.g., Ref. 1 (section I) for a discussion of Bragg scattering and Bragg waves.) Such a choice for δh would not mitigate the unitarity problem, which already shows up for Bragg scattering. (To be specific, note that Bragg scattering can be extracted directly from the small slope approximation by expanding in $Q_z h$, and dropping the specular component. At lowest order, we are left with a quantity proportional to the spectral component of the surface roughness parameter evaluated at the Bragg wavevector $\widetilde{\delta h}(\mathbf{Q})$ (recalling that $\mathbf{Q}$ is the projection onto the x-y plane of $\vec{Q} \equiv \vec{k} - \vec{q}$). Consequently the average cross-section is proportional to the surface roughness spectrum $S(\mathbf{Q})$; e.g., see Ref. 1 [equation (61)] and Ref. 4 (equation (4.6)]. This approximation corresponds to the specific physical effect known as Bragg scattering (i.e., the surface scatters like a diffraction grating). The isolation of this physical effect from other physical phenomena, such as interface waves, results directly from treating the surface roughness on the order of the Bragg scale using perturbation theory. As suggested above, this decoupling is believed to be the physical reason behind the breakdown of unitarity. (Note that such decoupling is also inherent in the formal statement of the composite model when δh is chosen on the order of the Bragg scale.)

However, it *would* be legitimate to choose δh corresponding to surface spectral components having wavenumbers larger than the Bragg value (i.e., smaller scale phenomena). Essentially this strategy was successfully employed by Orris and Dashen in Ref. 29. That study examined acoustic scattering from the Dirichlet and Neumann boundary conditions. We will leave the application to scattering involving elastic solids as a possible future research direction.

For the time being, users of perturbative scattering theory in general, and results (2.12), (2.18), (2.19), and (2.20) in particular, need to be aware of this issue, and remain on the lookout for future developments.

V. CONCLUSION

A. Summary of the basic approach

The technique of constructing a physical theory from a symmetry principle has been a hallmark of modern physics. The concept was foreshadowed by the work of Fermat and Hamilton in which geometrical optics and classical mechanics, respectively, were deduced from a variational principle. More recently, the connection between symmetry principles, conservation laws, and the field equations was firmly established by Noether's theorem (see Ref. 30 for a review of this topic). The concept reached its full fruition with the subsequent development of gauge theories, which form the basis of elementary particle physics, and therefore of modern cosmology (see, e.g., Ref. 31 for an overview).

Recently a similar approach has been applied to a reexamination of a more mundane physical problem, the scattering of acoustic and electromagnetic waves from interfaces. In Refs. 1–4, a new formal approach for describing such scattering was bootstrapped from the principle of time-reversal symmetry (also called reciprocity). In this paper, the new approach has been extended to scattering problems where elastodynamic waves are involved as well.

The overall strategy employed builds upon the previously known proof for the reciprocity theorem (see, e.g., Ref. 12). The basic ingredients of this proof are the two quantities known to be associated with the energy propagation vector. In acoustics, the two field quantities involved in energy propagation are the pressure p and the displacement $\vec{u}$, for the electromagnetic field it is the electric field $\vec{E}$ and the magnetic field $\vec{H}$, and for elastodynamic waves the relevant quantities are the displacement $\vec{u}$ and the stress tensor $\vec{\tau}$. Furthermore, two independent sets of solutions to the field equations are considered (labeled here by the subscripts ''1'' and ''2''). These ingredients are combined to form a divergence-free vector. For the electromagnetic field, this result has a name, ''Lorentz's Lemma,'' but the concept also applies to acoustic and elastodynamic fields. The elastodynamic equivalent of Lorentz's Lemma is

$$\vec{\nabla}\cdot(\vec{\tau}_1\cdot\vec{u}_2-\vec{\tau}_2\cdot\vec{u}_1)=0.$$

Remarkably, this and all versions of Lorentz's Lemma involve two completely independent solutions to the field equations *in any region where both solutions are valid*. In order to prove reciprocity, the solutions are chosen to correspond to scattering from the same surface, differing only in the incoming and outgoing geometries.

Specifically, it is assumed that the problem has been decomposed so that the incoming wave is a plane wave with wavevector $\vec{k}$. The reciprocal problem concerns a plane wave incoming from the angular coordinates of the observer (i.e., with wavevector $-\vec{q}$). Reciprocity implies that the scattering amplitude is invariant under the exchange $\vec{q}\rightarrow-\vec{k}$, $\vec{k}\rightarrow-\vec{q}$. This result emerges when Lorentz's Lemma is integrated over the scattering volume, and Gauss' Law is used to convert the volume integral to a surface integral over the boundaries of the scattering region. The change in the scattering amplitude under the reciprocity exchange [i.e., $\delta T\equiv T(\vec{q},\vec{k})-T(-\vec{k},-\vec{q})$] is proportional to the contribution from the sphere at infinity, while the boundary conditions ensure that the scattering surface does not contribute to the surface integral. Thus, $\delta T=0$, so that the scattering amplitude remains unaffected by the exchange, and reciprocity is established.

In fact, this simple picture only applies to the acoustic case. The electrodynamic and elastodynamic problems are a little more complicated. For the electromagnetic field, it is additionally necessary to include the polarization of the incoming wave, and to specify the polarization to be observed. In the elastodynamic case, it is also necessary to further decompose the incoming wave into primary (p-wave) and secondary (s-wave) components, and consider the scattering of each separately (the problems legitimately separate, no information is lost). Similarly, it is necessary to specify whether the observer is viewing the p- or s-components of the scattered wave. Reciprocity is only preserved once the problem has been decomposed in this way. The key insight is the realization that the extra decompositions outlined in this paragraph are not fundamentally different from the specification of $\vec{k}$ and $\vec{q}$.

In this paper and its predecessors,[1–4] the same procedure is followed, but with a crucially important innovation. The two solutions are now chosen not only to correspond to reciprocal geometries, but to scattering from different surfaces as well (with one ultimately serving as a reference surface). The reciprocity theorem and boundary conditions are then used to obtain expressions for the change in the scattering amplitude associated with the difference between the two scattering surfaces. The results are given by equation (2.12) for the scattering of an acoustic wave from a fluid–solid interface, and by equations (2.18), (2.19), and (2.20) for the scattering of elastodynamic waves from boundaries obeying the zero-displacement, stress-free, and solid–solid boundary conditions, respectively.

In this paper, the observer and the incoming waves are always chosen to be on the same side of the scattering surface. The generalization is very straightforward, as can be seen in analogous work in Ref. 3. It will be considered in future research as it is needed for specific applications.

B. Overview of the results

Formulas (2.12), (2.18), (2.19), and (2.20) are the fundamental results of this paper. All subsequent results follow from these equations. As stated just above, the four formulas correspond to the four types of scattering problem usually cited in connection with elastodynamic fields. They each constitute a formal statement of the two-scale (i.e., composite-roughness) model, being exact with respect to the reference surface and 1st order with respect to the perturbation (i.e., the normal distance between the surfaces). Typically, since *the reference surface is usually smoother* than the true scattering surface, the solution to reference problem can be found using more conventional techniques [such as numerical techniques; e.g., see Ref. 6; Milder's operator expansion method (see, e.g., Refs. 32, 33) also turns out to be very useful]. When the new scattering formalism is used in this way, it is effectively extending the range of utility of these techniques, making them apply to rougher surfaces than would otherwise be possible. Such applications of the formalism derived above will be a topic of upcoming research.

To provide a comparatively modest illustration of the utility of these results, the formalism was first used to derive a new manifestly reciprocal expression for the scattering amplitude corresponding to scattering from a fluid–solid interface. This is given in equation (2.14). The expression is derived from the 1st order perturbative equation (2.12) by considering an *infinitesimal* translation, and it is therefore exact.

Equations (2.12) and (2.14) are then used to obtain the small slope and ''local'' two-scale approximations for the problem of scattering from a rough, but approximately planar fluid–solid interface (i.e., assume that the interface is a surface which can be parameterized as a single valued function of coordinates on a plane). The result for both approximations is given by equation (3.23), with the small slope approximation emerging when the reference surface is chosen to be a plane, while for the two-scale result, the reference surface is formally arbitrary, but its curvature must be small relative to the wavelength of the field. An examination of equation (3.23) reveals that formally, this simply implies that the normal $\hat{n}$ is taken to be a constant unit vector $\hat{z}$ for the small slope approximation, and $\hat{n}_0$, the normal to the reference surface, for the ''local'' two-scale approximation. The approximation is called ''local'' because it is of lowest order, and therefore does not include non-local effects such as shadowing or multiple scattering. From equations (3.24), (3.25), and (3.26), it is clear that in the proper limits, equation (3.23) reduces to the corresponding previously known acoustic results.

Finally, in section IV, there was a brief discussion of the issue of energy non-conservation in perturbative scattering theory and its relevance to the results presented above. The reader is reminded that all perturbative scattering results, including those in this paper, can occasionally be affected by this issue, particularly at very shallow grazing angles. On the other hand, it was also pointed out that the formalism presented here can, for some purposes, be used to circumvent this problem.

C. Significance of the results

The work presented in this paper will form the basis for a number of future research projects. The most immediate application will be a study of acoustic scattering from the ocean bottom. There is reason to believe that there are regions of the world's oceans where the sea floor can be modeled as an elastic solid. Furthermore, it is also observed that at shallow grazing angles, or moderately high frequencies (>5 kHz), scattering from the interface between the ocean and the bottom dominate the near-bottom scattering results (as opposed to, say, volume scattering in the sub-bottom). The goal of theoretical research in this area would be to provide an expression for the scattering strength in terms of the roughness spectrum for the fine structure of the bottom (i.e., features on the order of a wavelength, typically: boulders, small dunes, etc.), its material parameters (e.g., density, the Lamé constants), and large-scale location-specific features of the bathymetry (e.g., underwater mountains, ridges, etc.). Equation (2.12) would form the basis of such a

study. The fine structure would be treated as a perturbation and considered statistically. The problem of scattering from the large scale structure would be treated as a deterministic problem to be solved numerically.

It is important to understand the way in which a formula such as (2.12) becomes useful for describing scattering from a rough surface such as the sea floor. The complicated multi-scale topography of such a surface makes scattering calculations very difficult, because there is no single method suitable for calculating the scattering from both large and small scale surface features. Large scale features (i.e., those characterized by scales significantly greater than the wavelength of the field) are associated with non-local scattering effects such as diffraction, shadowing, and multiple scattering, while small scales (on the order of a wavelength) are responsible for Bragg scattering (i.e., the surface acts like a diffraction grating). The former type of effect lends itself to numerical calculation (or to an exact solution in a handful of cases). On the other hand, use of perturbation theory is greatly complicated by the fact that non-local effects are associated with higher orders, which are in general very difficult to calculate. Bragg scattering, however, already emerges from lowest order perturbation theory, which is therefore the method of choice for calculating this phenomenon. Numerical calculations of Bragg scattering would on the other hand require such fine grids that a rigorous application of this technique would be prohibitively expensive in terms of time and computing resources. This problem becomes particularly acute when the full 3-dimensional scattering problem is considered.

Equations such as (2.12) [and similarly (2.18), (2.19), and (2.20)] solve this quandary provided that the perturbation δh is chosen judiciously. Used in this context, δh should correspond to surface features on the order of the Bragg wavelength and smaller. Thus, non-local events can be calculated numerically, and Bragg scattering can be handled perturbatively. Alternately, consider equations (2.14) and especially (3.23). Since these equations are manifestly reciprocal, the most important non-local effect, shadowing, can be inserted by hand [by using ray tracing to see which points on the surface are shielded from either the source or the observer, and setting the contribution to the surface integral to zero at those points. Note that for traditional, non-reciprocal expressions for the scattering amplitude, this is only really possible for a monostatic (i.e., backscattering) geometry, while with the new formalism, this can be done for the full bistatic problem. See Ref. 2 for further discussion of this issue].

Thus, it is fair to conclude that the study of non-local effects in rough surface scattering constitutes an important application of the formalism developed here. Note that such effects are particularly important at shallow grazing angles, which is precisely where surface scattering becomes most important relative to other (e.g., volume scattering) effects. In particular, note that this observation holds for the problem of scattering from the ocean bottom, or from layers in the sub-bottom.

The issue of rough surface scattering is only one of many possible applications of the results in this paper. As mentioned in the Introduction, Dashen, Abawi, and Wandzura[7,8] have used the acoustic version of this formalism to examine the scattering from planar objects bounded by edges and corners. The scattering from such objects is usually expressed as an integral over a two-dimensional surface, but in Refs. 7, 8, it is shown that such expressions reduce to (one-dimensional) line integrals, which are naturally much easier to evaluate. Because of shadowing, the illuminated area of a finite three-dimensional scatterer consists of such planar areas bounded by edges and corners, and therefore, the results obtained for the scattering from bounded two-dimensional surfaces (embedded in three-dimensional space) can be used to develop an entirely new approach to modeling scattering from typical three-dimensional scatterers (i.e., those bounded by a *closed* two-dimensional surface).

Thus, this paper adds another building block to the structure of a new theory for the scattering of classical fields. This new approach fully incorporates the insights gained from modern field theory.

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APPENDIX A: DERIVATION OF EQUATION (2.6)

In this appendix, the details of the calculation leading from equation (2.5) to equation (2.6) are provided. In Figure 2 of Ref. 2, a coordinate system locally tangent to the surface S_2 is used to show that

$$\hat{n}_1 = \hat{n}_2 - (1 - \hat{n}\hat{n}) \cdot \vec{\nabla} \xi, \tag{A1}$$

where the labels ''1'' and ''2'' are dropped if the result is the same to first order in ξ. We also have

$$\vec{\tau}_1(\vec{x_2}) = \vec{\tau}_1(\vec{x_1}) - \xi(\hat{n} \cdot \vec{\nabla}) \vec{\tau}_1, \quad \vec{u}_1(\vec{x}_2) = \vec{u}_1(\vec{x}_1) - \xi(\hat{n} \cdot \vec{\nabla}) \vec{u}_1,$$

so that

$$R_\infty = \int_{S_2} dS_2 [\hat{n}_1 \cdot \vec{\tau}_1(\vec{x_1}) \cdot \vec{u}_2(\vec{x_2}) - \hat{n}_2 \cdot \vec{\tau}_2(\vec{x_2}) \cdot \vec{u}_1(\vec{x_1})] + \int dS [\vec{\nabla} \xi \cdot (1 - \hat{n}\hat{n}) \cdot \vec{\tau}_1 \cdot \vec{u}_2$$
$$- \xi \hat{n} [(\hat{n} \cdot \vec{\nabla}) \vec{\tau}_1] \cdot \vec{u}_2 + \xi \hat{n} \cdot \vec{\tau}_2 \cdot [(\hat{n} \cdot \vec{\nabla}) \vec{u}_1]]. \tag{A2}$$

Note that, on terms of $O(\xi)$, there is no need to specify whether the field is evaluated at $\vec{x}_1$ or $\vec{x}_2$. Also note that on such terms, the subscripts have been dropped from dS since to this order, dS_1, dS_2, or the area element on any intermediate surface are all the same. Therefore, when considering terms of $O(\xi)$, the surfaces are equivalent, and the label S will henceforth stand for S_1, S_2, or any surface in between. A corresponding coordinate on one of these surfaces will simply be given by $\vec{x}$; no subscript is necessary.

The term in (A2) involving $\vec{\nabla} \xi$ will now be integrated by parts. For this step, the surface S is parameterized so that $\vec{x}$ is given by the Cartesian coordinates $(\mathbf{x}, h(\mathbf{x}))$ where $\mathbf{x}$ is a two-dimensional vector. Let ∇ be the associated two-dimensional gradient vector. Then, as in Appendix B of Ref. 2, it follows that

$$\hat{n} = n_z(-\nabla h, 1), \tag{A3}$$

$$n_z \equiv \frac{1}{\sqrt{1 + (\nabla h)^2}}, \tag{A4}$$

$$dS = d^2\mathbf{x}/n_z. \tag{A5}$$

Also note that

$$(1 - \hat{n}\hat{n}) \cdot \vec{\nabla} \xi = (1 - \hat{n}\hat{n}) \cdot \nabla \xi,$$

or more generally,

$$(1-\hat{n}\hat{n})\cdot\vec{\nabla}f(\mathbf{x},y)=(1-\hat{n}\hat{n})\cdot\nabla f(\mathbf{x},h(\mathbf{x})), \tag{A6}$$

for any function f of the coordinates evaluated on the surface S [see Ref. 2, equation (B16)].

These results are substituted into the second term of equation (A2), and an integration by parts is performed. The contribution from the edge of S is zero: for a closed surface where the parameterization is broken into pieces, the edge contribution from adjacent pieces cancels, and there is no overall edge; similarly for an infinite surface, the edge is out at infinity and therefore does not contribute to the scattering amplitude. The result is

$$\int \frac{d^2\mathbf{x}}{n_z}\nabla\xi\cdot(1-\hat{n}\hat{n})\cdot\vec{\tau}_1\cdot\vec{u}_2=-\int d^2\mathbf{x}\xi\nabla\cdot\left(\frac{1-\hat{n}\hat{n}}{n_z}\right)\cdot\vec{\tau}_1\cdot\vec{u}_2 - \int d^2\mathbf{x}\xi\left(\frac{\delta^{ij}-n^in^j}{n_z}\right):\vec{\nabla}^i(\vec{\tau}_1\cdot\vec{u}_2)^j. \tag{A7}$$

Use equation (B21) in Ref. 2 to show

$$\nabla\cdot\left(\frac{1-\hat{n}\hat{n}}{n_z}\right)=\frac{\mathrm{Tr}(\vec{\varrho})}{n_z}\hat{n}, \tag{A8}$$

where

$$\vec{\varrho}\equiv-(\vec{\mathbf{1}}-\hat{n}\hat{n})\cdot\vec{\nabla}\hat{n} \tag{A9}$$

is the curvature tensor, and ''Tr'' is the trace. Use this result, along with straightforward simplifications and cancellations to obtain

$$R_\infty=\int_{S_2}dS_2[\hat{n}_1\cdot\vec{\tau}_1(\vec{x_1})\cdot\vec{u}_2(\vec{x_2})-\hat{n}_2\cdot\vec{\tau}_2(\vec{x_2})\cdot\vec{u}_1(\vec{x_1})]-\int dS\xi\vec{\nabla}\cdot(\vec{\tau}_1\cdot\vec{u}_2) - \int dS\xi\,\mathrm{Tr}(\vec{\varrho})\hat{n}\cdot\vec{\tau}_1\cdot\vec{u}_2+\int dS\xi[(\hat{n}\cdot\vec{\tau}_1)\cdot[(\hat{n}\cdot\vec{\nabla})\vec{u}_2]+(\hat{n}\cdot\vec{\tau}_2)\cdot[(\hat{n}\cdot\vec{\nabla})\vec{u}_1]]. \tag{A10}$$

Note that the result is independent of the parameterization. The parameterization was only used to perform the integration by parts and it will not be used again in the derivation. As shown in Ref. 6, it is possible to perform this type of integration by parts using techniques from analytic geometry, without recourse to such a parameterization at all. Also note that on terms of $O(\xi)$ the subscripts have been dropped from S. To the order considered here, S_1, S_2 or any intermediate surface are all equivalent.

Decompose the term

$$\int dS\xi(\hat{n}\cdot\vec{\tau}_2)\cdot[(\hat{n}\cdot\vec{\nabla})\vec{u}_1] \tag{A11}$$

as follows:

$$\int dS\xi(\hat{n}\cdot\vec{\tau}_2\cdot\hat{n})(\hat{n}\hat{n}:\vec{\nabla}\vec{u}_1)+\int dS\xi(\hat{n}\cdot\vec{\tau}_2)\cdot(\vec{\mathbf{1}}-\hat{n}\hat{n})\cdot[(\hat{n}\cdot\vec{\nabla})\vec{u}_1]. \tag{A12}$$

Use the definition of $\vec{\tau}$, equation (2.1), to obtain the expressions

$$\hat{n}\hat{n}:\vec{\nabla}\vec{u}_1=\frac{\hat{n}\cdot\vec{\vec{\tau}}_1\cdot\hat{n}}{2\mu}-\frac{\lambda}{2\mu}\vec{\nabla}\cdot\vec{u}_1,$$

$$(\vec{\vec{1}}-\hat{n}\hat{n})\cdot[(\hat{n}\cdot\vec{\nabla})\vec{u}_1]=\frac{(\vec{\vec{1}}-\hat{n}\hat{n})\cdot\vec{\vec{\tau}}_1\cdot\hat{n}}{\mu}-n^i(\vec{\vec{1}}-\hat{n}\hat{n})\vec{\nabla}u_1^i.$$

These are substituted into (A12) above. After a little bit of algebra, and once again using the definition of $\vec{\vec{\tau}}$ [equation (2.1)], we are left with

$$\int dS\xi(\hat{n}\cdot\vec{\vec{\tau}}_2)\cdot[(\hat{n}\cdot\vec{\nabla})\vec{u}_1]=\int dS\xi\left[\frac{\hat{n}\cdot\vec{\vec{\tau}}_2\cdot(\vec{\vec{1}}-\hat{n}\hat{n})\cdot\vec{\vec{\tau}}_1\cdot\hat{n}}{\mu}-\hat{n}\cdot\vec{\vec{\tau}}_2\cdot(1-2\hat{n}\hat{n})\cdot(\vec{\nabla}u_1^i)n^i\right]. \tag{A13}$$

Now, consider the second term on the right side of (A13) above. Use $(\vec{\nabla}u^i)n^i=\vec{\nabla}(\vec{u}\cdot\hat{n})-u^i\vec{\nabla}n^i$ and the definition of the curvature tensor $\vec{\vec{\mathcal{Q}}}$ given above to obtain

$$\begin{aligned}-\int dS\xi\hat{n}\cdot\vec{\vec{\tau}}_2\cdot(1-2\hat{n}\hat{n})\cdot(\vec{\nabla}u_1^i)n^i&\\ =\int dS\xi[-\hat{n}\cdot\vec{\vec{\tau}}_2\cdot(\vec{\vec{1}}-\hat{n}\hat{n})\cdot\vec{\nabla}(\vec{u}_1\cdot\hat{n})+\hat{n}\cdot\vec{\vec{\tau}}_2\cdot\vec{\vec{\mathcal{Q}}}\cdot\vec{u}_1+\hat{n}\cdot\vec{\vec{\tau}}_2\cdot\hat{n}[\hat{n}\hat{n}:\vec{\nabla}\vec{u}_1]],&\end{aligned} \tag{A14}$$

and we obtain the useful result

$$\begin{aligned}\int dS\xi\hat{n}\cdot\vec{\vec{\tau}}_2\cdot(\hat{n}\cdot\vec{\nabla})\vec{u}_1=\int dS\xi\frac{\hat{n}\cdot\vec{\vec{\tau}}_2\cdot(\vec{\vec{1}}-\hat{n}\hat{n})\cdot\vec{\vec{\tau}}_1\cdot\hat{n}}{\mu}-\int dS\xi\hat{n}\cdot\vec{\vec{\tau}}_2\cdot(\vec{\vec{1}}-\hat{n}\hat{n})\cdot\vec{\nabla}(\vec{u}_1\cdot\hat{n})&\\ +\int dS\xi\hat{n}\cdot\vec{\vec{\tau}}_2\cdot\vec{\vec{\mathcal{Q}}}\cdot\vec{u}_1+\int dS\xi\hat{n}\cdot\vec{\vec{\tau}}_2\cdot\hat{n}[\hat{n}\hat{n}:\vec{\nabla}\vec{u}_1].&\end{aligned} \tag{A15}$$

Finally, take this result and the same with the labels ''1'' and ''2'' exchanged, and substitute into (A10) to obtain equation (2.6).

APPENDIX B: THE CONTRIBUTION FROM THE SPHERE AT INFINITY FOR AN INFINITE ELASTIC MEDIUM

This is a generalization of the calculation presented in Appendix A of Ref. 2. The formal conventions presented in Ref. 12 (pp. 153–154) are used. As indicated in the reference, just as the acoustic and electromagnetic scattering problems can be decomposed so that scattering by each plane wave component of the incoming signal may be considered separately, so too can the elastodynamic scattering problem be decomposed, with the additional property that scattering by the incoming *p*-wave components and by the incoming *s*-wave components are decoupled as well. However, since incoming *p*-waves or *s*-waves scatter *into* waves of both types, when constructing a reciprocal theory, it will be convenient to consider incoming waves which consist of both *p*-waves and *s*-waves. However, it is sufficient to combine only plane waves incoming from a common direction $\hat{k}^{in}$.

Thus, an incoming plane wave is given by

$$\vec{u}^i=(k_pk_s^{-1})^{3/2}u^{ip}e^{ik_p\hat{k}^{in}\cdot\vec{r}}\hat{k}^{in}+u^{is}e^{ik_s\hat{k}^{in}\cdot\vec{r}}\hat{t}^{in}, \tag{B1}$$

$$\vec{\vec{\tau}}^i=ik_p(k_pk_s^{-1})^{3/2}[\lambda\vec{\vec{1}}+2\mu\hat{k}^{in}\hat{k}^{in}]u^{ip}e^{ik_p\hat{k}^{in}\cdot\vec{r}}+ik_s\mu[\hat{k}^{in}\hat{t}^{in}+\hat{t}^{in}\hat{k}^{in}]u^{is}e^{ik_s\hat{k}^{in}\cdot\vec{r}}, \tag{B2}$$

and the scattered wave has the form

$$\vec{u}^{sc}=(k_p k_s^{-1})^{3/2}\frac{A^p}{k_p}\frac{e^{ik_p r}}{r}\hat{r}+\frac{A^s}{k_s}\frac{e^{ik_s r}}{r}\hat{t}^{sc}, \tag{B3}$$

$$\vec{\vec{\tau}}^{sc}=i(k_p k_s^{-1})^{3/2}[\lambda\vec{\vec{1}}+2\mu\hat{r}\hat{r}]A^p\frac{e^{ik_p r}}{r}+i\mu[\hat{r}\hat{t}^{sc}+\hat{t}^{sc}\hat{r}]A^s\frac{e^{ik_s r}}{r}. \tag{B4}$$

The precise value of the unit vector $\hat{t}^{sc}$ depends on the details of the scattering process, and varies with $\hat{r}$, but it does not need to be specified for the present purposes. However, it is important to note that $\hat{k}^{in}\perp\hat{t}^{in}$ and $\hat{r}\perp\hat{t}^{sc}$. Furthermore,

- p denotes the primary wave (also known as pressure; or compressional; or longitudinal wave);
- s denotes the secondary wave (also known as shear; or equivolume wave);
- in denotes the incoming wave (in this appendix only; elsewhere in is used to denote the normal component of a vector labeled by i);
- sc denotes the scattered wave.

The wavenumbers are given by $k_p=\omega/c_p$, $k_s=\omega/c_s$, where

$$c_p=\sqrt{\frac{\lambda+2\mu}{\rho}},\quad c_s=\sqrt{\frac{\mu}{\rho}}$$

are the velocities of the two waves. Note that u^{ip} and u^{is} are completely independent.

Recall that we are calculating R_∞, the negative of the contribution from the sphere at infinity,

$$R_\infty=-\int_{S_\infty}dS(-\hat{r})\cdot[\vec{\vec{\tau}}_1\cdot\vec{u}_2-\vec{\vec{\tau}}_2\cdot\vec{u}_1], \tag{B5}$$

where

$$\int_{S_\infty}dS\Leftrightarrow\lim_{r\to\infty}r^2\int_0^{2\pi}d\phi\int_0^{\pi}\sin(\theta)d\theta\Leftrightarrow\lim_{r\to\infty}r^2\int d\Omega, \tag{B6}$$

with ϕ and θ polar angles and Ω a unit of solid angle. Use $\vec{u}=\vec{u}^{in}+\vec{u}^{sc}$ and $\vec{\vec{\tau}}=\vec{\vec{\tau}}^{in}+\vec{\vec{\tau}}^{sc}$ to obtain

$$R_\infty=\int_{S_\infty}dS[[\hat{r}\cdot(\vec{\vec{\tau}}_1^{in}\cdot\vec{u}_2^{in})+\hat{r}\cdot(\vec{\vec{\tau}}_1^{sc}\cdot\vec{u}_2^{sc})+\hat{r}\cdot(\vec{\vec{\tau}}_1^{in}\cdot\vec{u}_2^{sc})+\hat{r}\cdot(\vec{\vec{\tau}}_1^{sc}\cdot\vec{u}_2^{in})]-(1\leftrightarrow2)], \tag{B7}$$

where $(1\leftrightarrow2)$ stands for ''same as the preceding term with labels 1 and 2 exchanged.''

1. Consider $B_1=\int_{S_\infty}dS[\hat{r}\cdot(\vec{\vec{\tau}}_1^{in}\cdot\vec{u}_2^{in})-(1\leftrightarrow2)]$

The incoming plane waves are solutions to the elastodynamic equation of motion in absence of a scattering surface S_2, and, following the discussion above equation (2.4), the integrand is therefore divergence-free over all space (or the half-space as the case may be). Once again, application of Gauss's law leads us to conclude that $B_1=0$. [Another way of saying this: there is no scattering surface S_0, and equation (2.4) with S_0 being the null set remains valid with S set equal to S_∞.]

2. Consider $B_2=\int_{S_\infty} dS[\hat{r}\cdot(\vec{\vec{\tau}}_1^{sc}\cdot\vec{u}_2^{sc})-(1\leftrightarrow 2)]$

From (B3) and (B4), it follows that

$$\hat{r}\cdot(\vec{\vec{\tau}}_1^{sc}\cdot\vec{u}_2^{sc})=i\frac{(k_pk_s^{-1})^3}{k_p}(\lambda+2\mu)\frac{e^{2ik_pr}}{r^2}A_1^pA_2^p+i\mu\frac{e^{2ik_pr}}{r^2}A_1^sA_2^s(\hat{t}_1^{sc}\cdot\hat{t}_2^{sc}), \tag{B8}$$

which is completely symmetric under the exchange $(1\leftrightarrow 2)$, so that $B_2=0$.

It has thus been established that for elastodynamic waves, as for scalar and electrodynamic waves, only cross terms between incoming planar and scattered spherical waves contribute to the surface integral evaluated on the sphere at infinity.

3. Consider $B_3=\int_{S_\infty} dS[\hat{r}\cdot(\vec{\vec{\tau}}_1^{in}\cdot\vec{u}_2^{sc})-(1\leftrightarrow 2)]$

Use (B3), (B2), (B6), and the orthogonality relation $\hat{r}\perp\hat{t}^{sc}$ to obtain

$$\begin{aligned}B_3=\lim_{r\to\infty}\int d\Omega r^2\Bigg(\Bigg[&i\frac{k_p^3}{k_s^3}A_2^pu_1^{ip}(\lambda+2\mu(\hat{k}^{in}\cdot\hat{r})^2)\frac{e^{ik_pr}}{r}e^{ik_p\hat{k}^{in}\cdot\vec{r}}\\&+i\mu A_2^su_1^{is}(\hat{r}\cdot\hat{k}_1^{in}\hat{t}_1^{in}\cdot\hat{t}_2^{sc}+\hat{r}\cdot\hat{t}_1^{in}\hat{k}_1^{in}\cdot\hat{t}_2^{sc})\frac{e^{ik_sr}}{r}e^{ik_s\hat{k}^{in}\cdot\vec{r}}\\&+(\text{ a term proportional to }\hat{r}\cdot\hat{t}_1^{in})+(\text{ a term proportional to }\hat{k}_1^{in}\cdot\hat{t}_1^{sc})\Bigg]-(1\leftrightarrow 2)\Bigg).\end{aligned} \tag{B9}$$

It will shortly be shown that the terms proportional to $\hat{r}\cdot\hat{t}_1^{in}$ and $\hat{k}_1^{in}\cdot\hat{t}_1^{sc}$ do not contribute to the integral.

As in Appendix A of Ref. 2 use the stationary phase to evaluate the integral. This turns out to be exact in the limit $r\to\infty$. We use the following polar coordinates to evaluate the integral over the solid angle:

$$\hat{r}=\cos\,\phi\,\sin\,\theta\hat{x}+\sin\,\phi\,\sin\,\theta\hat{y}+\cos\,\theta\hat{z}\ .$$

Perform a change variables using $\eta\equiv\cos\,\theta$ and pick $\hat{x}=\hat{k}_a^{in}$ (where subscript a stands for 1 or 2 as needed). The axes are oriented so that $\hat{k}_a^{in}$ points in the direction of the x-axis rather than the more common choice of the z-axis so that the stationary phase points do not occur at the endpoints of an integration. Similarly, let ϕ go from $-\pi/2$ to $3\pi/2$ rather than 0 to 2π.

The result is a sum of integrals all with the basic form

$$\lim_{r\to\infty}\int_{-1}^{1}d\eta\int_{-\pi/2}^{3\pi/2}d\phi F(\hat{r})e^{ikr\sqrt{1-\eta^2}\,\cos\,\phi},$$

where $F(\hat{r})$ is slowly varying near the stationary phase points $\hat{r}=\pm\hat{k}_a^{in}$ Note that this equality combined with the orthogonality relations given above ($\hat{k}^{in}\perp\hat{t}^{in}$ and $\hat{r}\perp\hat{t}^{sc}$) implies that the terms proportional to $\hat{r}\cdot\hat{t}_1^{in}$ and $\hat{k}_1^{in}\cdot\hat{t}_1^{sc}$ do not contribute to integral (B9).

In the limit $r\to\infty$, the integrand is non-zero only within an arbitrarily small range about the stationary phase points, so we can extend the η- and ϕ-integrations to $\pm\infty$. To properly evaluate the limit, it is necessary to expand the argument of the exponential $ikr\sqrt{1-\eta^2}\,\cos\,\phi$ about the stationary phase variables. Also shift integration variables so that $\phi-\pi$ goes to ϕ where the expansion was about the point $\phi=\pi$. Now, we have

$$\lim_{r\to\infty}\int_{-1}^{1} d\eta \int_{-\pi/2}^{3\pi/2} d\phi\, rF(\hat{r})e^{ik\hat{k}_a\cdot\vec{r}}$$

$$= \lim_{r\to\infty}\sum_{+/-} e^{\pm ikr} rF(\pm\hat{k}_a)\int_{\infty}^{-\infty}\int_{\infty}^{-\infty} d\eta\, d\phi\, \exp\left[\frac{ikr}{2}(\eta \quad \phi)\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}\begin{pmatrix}\eta\\ \phi\end{pmatrix}\right]$$

$$= -2\pi i \lim_{r\to\infty}\left[\left(\sum_{+/-} e^{\pm ikr}F(\pm\hat{k}_a)\right)\right]. \tag{B10}$$

Finally, using $\lambda+2\mu=\omega^2\rho/k_p^2$ and $\mu=\omega^2\rho/k_s$ we have

$$B_3=\left[\begin{matrix}+\\+\end{matrix}\frac{2\pi\rho\omega^2}{k_s^3}A_2^p(\pm\hat{k}_1^{in})u_1^{ip}e^{i(1\pm1)k_pr}\begin{matrix}+\\-\end{matrix}\frac{2\pi\rho\omega^2}{k_s^3}A_2^s(\pm\hat{k}_1^{in})u_1^{is}(\hat{t}_1^{in}\cdot\hat{t}_2^{sc})e^{i(1\pm1)k_sr}\right]-(1\leftrightarrow2). \tag{B11}$$

4. Consider $B_4=\int_{S_\infty} dS[\hat{r}\cdot(\overleftrightarrow{\tau}_1^{sc}\cdot\vec{u}_2^{in})-(1\leftrightarrow2)]$

Perform exactly the same procedure as that used in the previous section to obtain

$$B_4=\left[\begin{matrix}+\\-\end{matrix}\frac{2\pi\rho\omega^2}{k_s^3}A_1^p(\pm\hat{k}_2^{in})u_2^{ip}e^{i(1\pm1)k_pr}\begin{matrix}+\\+\end{matrix}\frac{2\pi\rho\omega^2}{k_s^3}A_1^s(\pm\hat{k}_2^{in})u_2^{is}(\hat{t}_1^{sc}\cdot\hat{t}_2^{in})e^{i(1\pm1)k_sr}\right]-(1\leftrightarrow2). \tag{B12}$$

5. Combine results

Combining $R_\infty=B_1+B_2+B_3+B_4$, we have

$$\begin{aligned}R_\infty=\Bigg[&\begin{matrix}+\\+\end{matrix}\frac{2\pi\rho\omega^2}{k_s^3}A_2^p(\pm\hat{k}_1^{in})u_1^{ip}e^{i(1\pm1)k_pr}\begin{matrix}+\\-\end{matrix}\frac{2\pi\rho\omega^2}{k_s^3}A_2^s(\pm\hat{k}_1^{in})u_1^{is}(\hat{t}_1^{in}\cdot\hat{t}_2^{sc})e^{i(1\pm1)k_sr}\\
&\begin{matrix}-\\-\end{matrix}\frac{2\pi\rho\omega^2}{k_s^3}A_1^p(\pm\hat{k}_2^{in})u_2^{ip}e^{i(1\pm1)k_pr}\begin{matrix}-\\+\end{matrix}\frac{2\pi\rho\omega^2}{k_s^3}A_1^s(\pm\hat{k}_2^{in})u_2^{is}(\hat{t}_2^{in}\cdot\hat{t}_1^{sc})e^{i(1\pm1)k_sr}\\
&\begin{matrix}+\\-\end{matrix}\frac{2\pi\rho\omega^2}{k_s^3}A_1^p(\pm\hat{k}_2^{in})u_2^{ip}e^{i(1\pm1)k_pr}\begin{matrix}+\\+\end{matrix}\frac{2\pi\rho\omega^2}{k_s^3}A_1^s(\pm\hat{k}_2^{in})u_2^{is}(\hat{t}_1^{sc}\cdot\hat{t}_2^{in})e^{i(1\pm1)k_sr}\\
&\begin{matrix}-\\+\end{matrix}\frac{2\pi\rho\omega^2}{k_s^3}A_2^p(\pm\hat{k}_1^{in})u_1^{ip}e^{i(1\pm1)k_pr}\begin{matrix}-\\-\end{matrix}\frac{2\pi\rho\omega^2}{k_s^3}A_2^s(\pm\hat{k}_1^{in})u_1^{is}(\hat{t}_2^{sc}\cdot\hat{t}_1^{in})e^{i(1\pm1)k_sr}\Bigg],\end{aligned} \tag{B13}$$

where there is an implicit $r\to\infty$ in this equation. When similar terms are summed together, they combine to give the equation

$$R_\infty=\frac{4\pi\rho\omega^2}{k_s^3}[A_2^p(-\hat{k}_1^{in})u_1^{ip}-A_2^s(-\hat{k}_1^{in})u_1^{is}(\hat{t}_1^{in}\cdot\hat{t}_2^{sc})-A_1^p(-\hat{k}_2^{in})u_2^{ip}+A_1^s(-\hat{k}_2^{in})u_2^{is}(\hat{t}_2^{in}\cdot\hat{t}_1^{sc})]. \tag{B14}$$

Note that terms proportional to $\exp(i2k_pr)$ have canceled. Now, define

$$\vec{u}_a^{ip}\equiv u^{ip}\hat{k}_a^{in};\quad \vec{u}_a^{is}\equiv u^{is}\hat{t}_a^{in},$$

$$\vec{A}_a^p(\hat{r})\equiv A_a^p(\hat{r})\hat{r};\quad \vec{A}_a^s(\hat{r})\equiv A_a^s(\hat{r})\hat{t}_a^{sc}, \tag{B15}$$

and so

$$R_\infty=\frac{4\pi\rho\omega^2}{k_s^3}[-\vec{u}_1^{ip}\cdot\vec{A}_2^p(-\hat{k}_1^{in})-\vec{u}_1^{is}\cdot\vec{A}_2^s(-\hat{k}_1^{in})+\vec{u}_2^{ip}\cdot\vec{A}_1^p(-\hat{k}_2^{in})+\vec{u}_2^{is}\cdot\vec{A}_1^s(-\hat{k}_2^{in})]. \quad \text{(B16)}$$

Now, following equations (2.63)–(2.64) in Ref. 12, assume that $\vec{A}^p$ and $\vec{A}^s$ depend linearly on $\vec{u}^{ip}$ and $\vec{u}^{is}$:

$$\begin{aligned}\vec{A}_a^p(-\hat{k}_b^{in})&=\vec{\vec{A}}_a^{pp}(-\hat{k}_b^{in},\hat{k}_a^{in})\cdot\vec{u}_a^{ip}+\vec{\vec{A}}_a^{ps}(-\hat{k}_b^{in},\hat{k}_a^{in})\cdot\vec{u}_a^{is},\\ \vec{A}_a^s(-\hat{k}_b^{in})&=\vec{\vec{A}}_a^{sp}(-\hat{k}_b^{in},\hat{k}_a^{in})\cdot\vec{u}_a^{ip}+\vec{\vec{A}}_a^{ss}(-\hat{k}_b^{in},\hat{k}_a^{in})\cdot\vec{u}_a^{is},\end{aligned} \quad \text{(B17)}$$

where, for now, the dependence on $\hat{t}_a$ and $\hat{t}_b$ has been suppressed. Note the dyad $\vec{\vec{A}}$ does *not* depend on the magnitudes u_a^{ip} and u_a^{is}. Now,

$$\begin{aligned}R_\infty=\frac{4\pi\rho\omega^2}{k_s^3}\{&\vec{u}_2^{ip}\cdot[-[\vec{\vec{A}}_2^{pp}(-\hat{k}_1^{in},\hat{k}_2^{in})]^t+\vec{\vec{A}}_1^{pp}(-\hat{k}_2^{in},\hat{k}_1^{in})]\cdot\vec{u}_1^{ip}\\ &+\vec{u}_2^{ip}\cdot[-[\vec{\vec{A}}_2^{ps}(-\hat{k}_1^{in},\hat{k}_2^{in})]^t+\vec{\vec{A}}_1^{sp}(-\hat{k}_2^{in},\hat{k}_1^{in})]\cdot\vec{u}_1^{ip}\\ &+\vec{u}_2^{ip}\cdot[-[\vec{\vec{A}}_2^{sp}(-\hat{k}_1^{in},\hat{k}_2^{in})]^t+\vec{\vec{A}}_1^{ps}(-\hat{k}_2^{in},\hat{k}_1^{in})]\cdot\vec{u}_1^{ip}\\ &+\vec{u}_2^{ip}\cdot[-[\vec{\vec{A}}_2^{ss}(-\hat{k}_1^{in},\hat{k}_2^{in})]^t+\vec{\vec{A}}_1^{ss}(-\hat{k}_2^{in},\hat{k}_1^{in})]\cdot\vec{u}_1^{ip}\},\end{aligned} \quad \text{(B18)}$$

where superscript t stands for ''transpose the matrix.'' Setting $S_1=S_2$, it follows that $R_\infty=0$. With u_1, u_2 properly set to 0 or 1, we recover reciprocity relations (2.66)–(2.69) or Ref. 12:

$$\begin{aligned}[\vec{\vec{A}}_2^{pp}(-\hat{k}_1^{in},\hat{k}_2^{in})]^t&=\vec{\vec{A}}_2^{pp}(-\hat{k}_2^{in},\hat{k}_1^{in}),\\ [\vec{\vec{A}}_2^{ps}(-\hat{k}_1^{in},\hat{k}_2^{in})]^t&=\vec{\vec{A}}_2^{sp}(-\hat{k}_2^{in},\hat{k}_1^{in}),\\ [\vec{\vec{A}}_2^{sp}(-\hat{k}_1^{in},\hat{k}_2^{in})]^t&=\vec{\vec{A}}_2^{ps}(-\hat{k}_2^{in},\hat{k}_1^{in}),\\ [\vec{\vec{A}}_2^{ss}(-\hat{k}_1^{in},\hat{k}_2^{in})]^t&=\vec{\vec{A}}_2^{ss}(-\hat{k}_2^{in},\hat{k}_1^{in}),\end{aligned} \quad \text{(B19)}$$

where note that the subscript 2 on $\vec{\vec{A}}$ reminds us that the scattering surface is S_2.

Return to the problem $S_1 \neq S_2$. Define

$$\delta\vec{\vec{A}}\equiv\vec{\vec{A}}_1-\vec{\vec{A}}_2,$$

and let

$$\begin{aligned}-\hat{k}_2^{in}&\equiv\vec{q},\\ \hat{k}_1^{in}&\equiv\vec{k}.\end{aligned} \quad \text{(B20)}$$

This gives us the important result

$$R_\infty=\frac{4\pi\rho\omega^2}{k_s^3}[\vec{u}_2^{ip}\cdot\delta\vec{\vec{A}}^{pp}\cdot\vec{u}_1^{ip}+\vec{u}_2^{is}\cdot\delta\vec{\vec{A}}^{sp}\cdot\vec{u}_1^{ip}+\vec{u}_2^{ip}\cdot\delta\vec{\vec{A}}^{ps}\cdot\vec{u}_1^{is}+\vec{u}_2^{is}\cdot\delta\vec{\vec{A}}^{ss}\cdot\vec{u}_1^{is}]. \quad \text{(B21)}$$

Alternately, use

$$\vec{u}_2^{ip} = -u_2^{ip}\hat{q}; \quad \vec{u}_1^{ip} = u_1^{ip}\hat{k},$$

$$\vec{u}_2^{is} = u^{is}\hat{t}_{-\hat{q}} = u_2^{is}\hat{t}_{\hat{q}}^{*}; \quad \vec{u}_1^{is} = u_1^{is}\hat{t}_{\hat{k}},$$

and define

$$\begin{aligned}
T^{pp}(\hat{q};\hat{k}) &\equiv \frac{4\pi}{k_p}(-\hat{q})\cdot\vec{\vec{A}}^{pp}(\hat{q},\hat{k})\cdot\hat{k},\\
T^{sp}(\hat{q},\hat{t}_{\hat{q}};\hat{k}) &\equiv \frac{4\pi}{k_s}\hat{t}_{\hat{q}}^{*}\cdot\vec{\vec{A}}^{sp}(\hat{q},\hat{k})\cdot\hat{k},\\
T^{ps}(\hat{q};\hat{k},\hat{t}_{\hat{k}}) &\equiv \frac{4\pi}{k_p}(-\hat{q})\cdot\vec{\vec{A}}^{ps}(\hat{q},\hat{k})\cdot\hat{t}_{\hat{k}},\\
T^{ss}(\hat{q},\hat{t}_{\hat{q}};\hat{k},\hat{t}_{\hat{k}}) &\equiv \frac{4\pi}{k_s}\hat{t}_{\hat{q}}^{*}\cdot\vec{\vec{A}}^{ss}(\hat{q},\hat{k})\cdot\hat{t}_{\hat{k}}.
\end{aligned} \tag{B22}$$

Note that we have absorbed the factor 1/ outgoing wavenumber [see equation (B3)] into the definition of the scattering amplitude T, bringing it in line with the convention pursued in Ref. 2–4. Also note that the $\hat{t}$ dependence has now been inserted explicitly. It is left out in some instances since a p-wave has no polarization, and it will be shown below that (as with the reciprocity calculation outlined above and in Ref. 12) a judicious choice of u_a^{ip} and u_a^{is} completely decouples the different channels pp, ps, sp, and ss. Also note that reversing the direction of the wavevector is the same as changing the sign of the phase of the plane wave which implies taking the complex conjugate of the amplitude. We follow the convention that the phase shift of the s-wave relative to the p-wave is in the unit polarization vector $\hat{t}$, and thus $\hat{t}_{-\hat{q}} = \hat{t}_{\hat{q}}^{*}$. We now have the very important result

$$\begin{aligned}
R_\infty = \frac{\rho\omega^2}{k_s^3}[&k_p u_2^{ip}\,\delta T^{pp}(\hat{q};\hat{k})u_1^{ip} + k_s u_2^{is}\,\delta T^{sp}(\hat{q},\hat{t}_{\hat{q}};\hat{k})u_1^{ip} + k_p u_2^{ip}\,\delta T^{ps}(\hat{q};\hat{k},\hat{t}_{\hat{k}})u_1^{is}\\
&+ k_s u_2^{is}\,\delta T^{ss}(\hat{q},\hat{t}_{\hat{q}};\hat{k},\hat{t}_{\hat{k}})u_1^{is}].
\end{aligned} \tag{B23}$$

Finally, to find the four δT's, let

$$\begin{matrix}(k_p k_s^{-1})^{3/2}u_1^{ip} \\ u_1^{is}\end{matrix}\;;\;\begin{matrix}(k_p k_s^{-1})^{3/2}u_2^{ip} \\ u_2^{is}\end{matrix} = \begin{cases}1,\\ 0,\end{cases}$$

in 1,2 pairs, and solve the resulting four independent problems separately. Specifically, recall that R_∞ is an integral over the scattering surface of the solutions, *given* certain specified plane waves. Thus writing R_∞ as a function of the u^i's:

$$R_\infty = R_\infty([(k_p k_s^{-1})^{3/2}u_2^{ip}], u_2^{is}; [(k_p k_s^{-1})^{3/2}u_1^{ip}], u_1^{is}),$$

we have

$$\delta T^{pp}(\hat{q};\hat{k}) = R_\infty(1,0;1,0)\left[\frac{k_p^2}{\rho\omega^2}\right],$$

$$\delta T^{sp}(\hat{q},\hat{t}_{\hat{q}};\hat{k}) = R_\infty(0,1;1,0)\left[\frac{k_s^{1/2}k_p^{3/2}}{\rho\omega^2}\right],$$

$$\delta T^{ps}(\hat{q};\hat{k},\hat{t}_{\hat{k}}) = R_\infty(1,0;0,1)\left[\frac{k_s^{3/2}k_p^{1/2}}{\rho\omega^2}\right], \tag{B24}$$

$$\delta T^{ss}(\hat{q},\hat{t}_{\hat{q}};\hat{k},\hat{t}_{\hat{k}}) = R_\infty(0,1;0,1)\left[\frac{k_s^2}{\rho\omega^2}\right].$$

Since the right hand side cannot depend on $\hat{t}_a$ if $u_a^{is}=0$, we now see why some $\hat{t}_a$'s were left out beginning with equation (B22).

As in Ref. 2, by choosing $\xi=\hat{n}$, we obtain new manifestly reciprocal expressions for $\vec{Q}^{pp}T^{pp}$,$\vec{Q}^{sp}T^{sp}$,$\vec{Q}^{ps}T^{ps}$, and $\vec{Q}^{ss}T^{ss}$ where $\vec{Q}^{pp}\equiv k_p\hat{k}-k_p\hat{q}$, $\vec{Q}^{ps}\equiv k_s\hat{k}-k_p\hat{q}$, etc . The bottom line is that in this formulation, the different channels pp, sp, ps, and ss are treated separately. The result is a scattering matrix which solves the general problem.

Note that acoustics essentially involves finding T^{pp} (scattering from scalar wave to scalar wave) whereas the electromagnetic problem (described in Ref. 2) more or less amounts to finding T^{ss} (scattering from transverse vector wave to transverse vector wave). The elastodynamic problem differs in that it involves more than one such channel.

APPENDIX C: DETAILS IN DERIVATION OF EQUATION (2.8)

Begin with equation (2.6) with the $O(\xi^0)$ term given by (2.7). Use the boundary condition $\hat{n}\cdot\vec{\tau}\cdot(1-\hat{n}\hat{n})=0$ to drop the 3rd, 4th, and 7th rows of (2.6). It is also necessary to recall the definition of the curvature tensor (A9), and to insert $\hat{n}\hat{n}$ between $\vec{\tau}_1$ and $\vec{u}_2$ in the 2nd row of (2.6). Next, use equation (A1) to replace $\hat{n}_1$ in $\hat{n}_1\cdot\vec{u}_2(\vec{x}_2)$ and $\hat{n}_2$ in $\hat{n}_2\cdot\vec{u}_1(\vec{x}_1)$. The result is

$$R_\infty = \text{O}(\xi^0)\text{ terms which cancel at the interface } -\int dS\hat{n}\cdot\vec{\tau}_1\nabla\xi\cdot(1-\hat{n}\hat{n})\cdot\vec{u}_2$$
$$-\int dS\hat{n}\cdot\vec{\tau}_2\nabla\xi\cdot(1-\hat{n}\hat{n})\cdot\vec{u}_1 + O(\xi)\text{ terms included previously in equation (2.6).} \tag{C1}$$

Note that $I=-\int dS\hat{n}\cdot\vec{\tau}_1\cdot\nabla\xi\cdot(1-\hat{n}\hat{n})\cdot\vec{u}_2$ and the next term with labels 1 and 2 exchanged have the same sign (generally such pairs have come with opposite signs). This is no misprint; it follows from the fact that equation (A1) is not symmetric under the exchange $(1\leftrightarrow 2)$.

Consider

$$I=-\int dS\hat{n}\cdot\vec{\tau}_1\cdot\nabla\xi\cdot(1-\hat{n}\hat{n})\cdot\vec{u}_2.$$

We follow the technique outlined in Appendices B and C in Ref. 2. To integrate this result by parts, write dS as d^2x/n_z where n_z is the z-component of $\hat{n}$ for some coordinate system and d^2x is $dx\,dy$ for the same coordinate system. Perform the integration by parts. Use from Ref. 2

$$\nabla\cdot\left(\frac{\vec{\mathbf{1}}-\hat{n}\hat{n}}{n_z}\right)=\frac{\hat{n}}{n_z}\,\text{Tr}(\vec{\varrho}) \tag{C2}$$

[see the comments below equation (C11), or equation (B21) and the comment above (B23); all in Ref. 2), and also recall equation (A6). Putting these results together, we have

$$I=\int dS\xi\ \mathrm{Tr}(\vec{\vec{g}})\hat{n}\cdot\vec{u}_2\tau^1_{nn}+\int dS\xi(\vec{\vec{1}}-\hat{n}\hat{n}):\vec{\nabla}\vec{u}_2\tau^1_{nn}+\int dS\xi\vec{u}_2\cdot(\vec{\vec{1}}-\hat{n}\hat{n})\cdot\vec{\nabla}\tau^1_{nn}\ . \tag{C3}$$

Get the same result with labels 1 and 2 exchanged. Note that the terms involving $\hat{n}\hat{n}:\vec{\nabla}\vec{u}$ will cancel the 6th row of equation (2.6). To recapitulate, we have succeeded in eliminating the 3rd, 4th, 6th, and 7th rows of equation (2.6). Substitute into equation (2.6) the remaining results obtained so far in this appendix to obtain

$$\begin{aligned}R_\infty=&\int_{S_2}dS_2[\hat{n}_1\cdot\vec{\vec{\tau}}_1(\vec{x_1})\cdot\hat{n}_1\hat{n}_2\cdot\vec{u}_2(\vec{x_2})-\hat{n}_2\cdot\vec{\vec{\tau}}_2(\vec{x_2})\cdot\hat{n}_2\hat{n}_1\cdot\vec{u}_1(\vec{x_1})]+\int dS\xi\ \mathrm{Tr}(\vec{\vec{g}})\hat{n}\cdot\vec{u}_1\hat{n}\cdot\vec{\vec{\tau}}_2\cdot\hat{n}\\&+\int dS\xi\rho\omega^2\vec{u}_1\cdot\vec{u}_2-\int dS\xi\vec{\vec{\tau}}_1:\vec{\nabla}\vec{u}_2+\int dS\xi[(\vec{\nabla}\cdot\vec{u}_2)\tau^1_{nn}+(\vec{\nabla}\cdot\vec{u}_1)\tau^2_{nn}]\\&+\int dS\xi[\vec{u}_2\cdot(\vec{\vec{1}}-\hat{n}\hat{n})\cdot\vec{\nabla}(\tau^1_{nn})+\vec{u}_1\cdot(\vec{\vec{1}}-\hat{n}\hat{n})\cdot\vec{\nabla}(\tau^2_{nn})].\end{aligned} \tag{C4}$$

Since $\vec{\vec{\tau}}$ is symmetric, we have (summing repeated indices i,j; covariance/contravariance notation is *NOT* being used here in this paper)

$$\begin{aligned}\vec{\vec{\tau}}_1:\vec{\nabla}\vec{u}_2=\frac{1}{2}\tau_1^{ij}(\nabla^i u_2^j+\nabla^j u_2^i)&=\frac{1}{2}\tau_1^{ij}\frac{\tau_2^{ij}-\lambda\vec{\nabla}\cdot\vec{u}_2\delta^{ij}}{\mu}\\&=\frac{\vec{\vec{\tau}}_1:\vec{\vec{\tau}}_2}{2\mu}-\frac{\lambda}{2\mu}\mathrm{Tr}(\vec{\vec{\tau}}_1)\vec{\nabla}\cdot\vec{u}_2\\&=\frac{\vec{\vec{\tau}}_1:\vec{\vec{\tau}}_2}{2\mu}-\frac{\lambda}{2\mu}\frac{\mathrm{Tr}(\vec{\vec{\tau}}_1)\ \mathrm{Tr}(\vec{\vec{\tau}}_2)}{3\lambda+2\mu},\end{aligned} \tag{C5}$$

and equation (2.8) follows immediately.

APPENDIX D: DETAILS IN THE DERIVATION OF EQUATION (2.9)

Note the fact that for a standard acoustic field in a fluid,

$$\tau_{nn}=-P\Rightarrow\vec{\nabla}(\tau_{nn})=-\vec{\nabla}P=-\rho\omega^2\vec{u}.$$

Also note the following three lemmas *valid for an acoustic field in a fluid.*

Lemma 1:

$$\frac{\vec{\vec{\tau}}_1:\vec{\vec{\tau}}_2}{2\mu}=\frac{3\lambda^2}{2\mu}\vec{\nabla}\cdot\vec{u}_1\vec{\nabla}\cdot\vec{u}_2+\frac{2k^2}{\rho\omega^2}\tau^1_{nn}\tau^2_{nn}+O(\mu). \tag{D1}$$

Lemma 2:

$$\frac{\lambda}{2\mu}\frac{\mathrm{Tr}(\vec{\vec{\tau}}_1)\ \mathrm{Tr}(\vec{\vec{\tau}}_2)}{3\lambda+2\mu}=\frac{3\lambda^2}{2\mu}\vec{\nabla}\cdot\vec{u}_1\vec{\nabla}\cdot\vec{u}_2+\frac{k^2}{\rho\omega^2}\tau^1_{nn}\tau^2_{nn}+O(\mu). \tag{D2}$$

Lemma 3:

$$\frac{\mathrm{Tr}(\overleftrightarrow{\tau}_1)}{3\lambda+2\mu}\tau^2_{nn}+\frac{\mathrm{Tr}(\overleftrightarrow{\tau}_2)}{3\lambda+2\mu}\tau^1_{nn}=\frac{2k^2}{\rho\omega^2}\tau^1_{nn}\tau^2_{nn}+O(\mu). \tag{D3}$$

Given these results, (2.9) follows immediately from (2.8).

Proof of Lemma 1: Begin with

$$\overleftrightarrow{\tau}_1:\overleftrightarrow{\tau}_2=\tau^1_{nn}\tau^2_{nn}+2\hat{n}\cdot\overleftrightarrow{\tau}_1\cdot(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})\cdot\overleftrightarrow{\tau}_2\cdot\hat{n}+\overleftrightarrow{\tau}^T_1:\overleftrightarrow{\tau}^T_2,$$

where the superscript T denotes components perpendicular to the normal $\hat{n}$ [see also equation (2.13)].

The ''cross term'' $2\hat{n}\cdot\overleftrightarrow{\tau}_1\cdot(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})\cdot\overleftrightarrow{\tau}_2\cdot\hat{n}$ is zero on S by the slip boundary condition $\hat{n}\cdot\tau_1\cdot(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})=0$. It is also worth noting that, even away from the surface, any off-diagonal component of $\overleftrightarrow{\tau}$ is automatically $O(\mu)$ so a product of such terms must be $O(\mu^2)$.

From the definition of $\overleftrightarrow{\tau}$, equation (2.1), we have

$$\tau_{nn}=\lambda\vec{\nabla}\cdot\vec{u}+2\mu\hat{n}\hat{n}:\vec{\nabla}\vec{u}.$$

From $\vec{u}=\vec{\nabla}P/\rho\omega^2$ and the Helmholtz equation for P, we have

$$\lambda\vec{\nabla}\cdot\vec{u}=-P+O(\mu)(=\tau_{nn}+O(\mu)), \tag{D4}$$

and thus

$$\tau^1_{nn}\tau^2_{nn}=\lambda^2\vec{\nabla}\cdot\vec{u}_1\vec{\nabla}\cdot\vec{u}_2-\frac{2\mu}{\rho\omega^2}(\hat{n}\hat{n}:\vec{\nabla}\vec{\nabla}P_2)P_1-\frac{2\mu}{\rho\omega^2}(\hat{n}\hat{n}:\vec{\nabla}\vec{\nabla}P_1)P_2+O(\mu^2). \tag{D5}$$

Now, consider

$$\overleftrightarrow{\tau}^T_1:\overleftrightarrow{\tau}^T_2=\tau^1_{t_1t_1}\tau^2_{t_1t_1}+\tau^1_{t_2t_2}\tau^2_{t_2t_2}+2\tau^1_{t_1t_2}\tau^2_{t_2t_1},$$

where the indices t_1 and t_2 label components in the ''T'' direction (i.e., $\perp\hat{n}$). Note once again that the cross term is $O(\mu^2)$. From equation (2.1), we have

$$\tau_{t_it_i}=\lambda\vec{\nabla}\cdot\vec{u}+\frac{2\mu}{\rho\omega^2}\hat{t}_i\hat{t}_i:\vec{\nabla}\vec{\nabla}P+O(\mu^2).$$

Consequently, also recalling equation (D4), we have

$$\tau^1_{t_it_i}\tau^2_{t_it_i}=\lambda^2\vec{\nabla}\cdot\vec{u}_1\vec{\nabla}\cdot\vec{u}_2-\frac{2\mu}{\rho\omega^2}(\hat{t}_i\hat{t}_i:\vec{\nabla}\vec{\nabla}P_2)P_1-\frac{2\mu}{\rho\omega^2}(\hat{t}_i\hat{t}_i:\vec{\nabla}\vec{\nabla}P_1)P_2+O(\mu^2). \tag{D6}$$

Summing our results, and using

$$\hat{t}_1\hat{t}_1+\hat{t}_2\hat{t}_2+\hat{n}\hat{n}=1, \tag{D7}$$

as well as

$$1:\vec{\nabla}\vec{\nabla}P=\nabla^2P=-k^2P=k^2\tau_{nn},$$

to simplify the result, we have equation (D1).

Proof of Lemma 2: Note that

$$\mathrm{Tr}(\overleftrightarrow{\tau}) = (3\lambda + 2\mu)\vec{\nabla}\cdot\vec{u},$$

to obtain

$$\frac{\lambda}{2\mu}\frac{\mathrm{Tr}(\overleftrightarrow{\tau}_1)\,\mathrm{Tr}(\overleftrightarrow{\tau}_2)}{3\lambda+2\mu} = \frac{\lambda}{2\mu}(3\lambda+2\mu)\vec{\nabla}\cdot\vec{u}_1\vec{\nabla}\cdot\vec{u}_2 = \frac{3\lambda^2}{2\mu}\vec{\nabla}\cdot\vec{u}_1\vec{\nabla}\cdot\vec{u}_2 + \lambda\vec{\nabla}\cdot\vec{u}_1\vec{\nabla}\cdot\vec{u}_2. \quad \text{(D8)}$$

Simplify using (D4) and $1/\lambda = k^2/\rho\omega^2$ to obtain equation (D2).

Proof of Lemma 3: We have

$$\frac{\mathrm{Tr}(\overleftrightarrow{\tau}_1)}{3\lambda+2\mu}\tau^2_{nn} + \frac{\mathrm{Tr}(\overleftrightarrow{\tau}_2)}{3\lambda+2\mu}\tau^1_{nn} = 2\lambda\vec{\nabla}\cdot\vec{u}_1\vec{\nabla}\cdot\vec{u}_2 = \frac{2}{\lambda}P_1P_2 + O(\mu) = \frac{2k^2}{\rho\omega^2}\tau^1_{nn}\tau^2_{nn} + O(\mu). \quad \text{(D9)}$$

APPENDIX E: DETAILS IN THE DERIVATION OF EQUATION (2.16)

Once again, begin with equation (2.6), and simplify using equation (C5) as well as the equation

$$\frac{\tau_{nn}}{2\mu} - \frac{\lambda}{2\mu}\frac{\mathrm{Tr}(\overleftrightarrow{\tau})}{3\lambda+2\mu} = \hat{n}\hat{n}:\vec{\nabla}\vec{u},$$

obtained directly from the definition of the stress tensor, equation (2.1). Thus we have

$$\begin{aligned} R_\infty = {} & \text{terms which are zero or cancel at the boundary} + \int dS\,\xi\rho\omega^2\vec{u}_1\cdot\vec{u}_1 \\ & + \int dS\,\xi\left[-\frac{\overleftrightarrow{\tau}_1:\overleftrightarrow{\tau}_2}{2\mu} + \frac{\lambda}{2\mu}\frac{\mathrm{Tr}(\overleftrightarrow{\tau}_1)\,\mathrm{Tr}(\overleftrightarrow{\tau}_2)}{3\lambda+2\mu}\right] + \int dS\,\xi\left[\frac{\tau^1_{nn}\tau^2_{nn}}{\mu} + \frac{2}{\mu}\overleftrightarrow{\tau}_1\cdot(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})\cdot\overleftrightarrow{\tau}_2\cdot\hat{n}\right] \\ & - \int dS\,\xi\left[\frac{\lambda}{2\mu}\frac{\tau^2_{nn}\,\mathrm{Tr}(\overleftrightarrow{\tau}_1)}{3\lambda+2\mu} + \frac{\lambda}{2\mu}\frac{\tau^1_{nn}\,\mathrm{Tr}(\overleftrightarrow{\tau}_2)}{3\lambda+2\mu}\right]. \end{aligned} \quad \text{(E1)}$$

Note that

$$\overleftrightarrow{\tau}_1:\overleftrightarrow{\tau}_2 = \overleftrightarrow{\tau}^T_1:\overleftrightarrow{\tau}^T_2 + \tau^1_{nn}\tau^2_{nn} + 2\tau^1_{nt_1}\tau^2_{t_1n} + 2\tau^1_{nt_2}\tau^2_{t_2n} = \overleftrightarrow{\tau}^T_1:\overleftrightarrow{\tau}^T_2 + \tau^1_{nn}\tau^2_{nn} + 2\hat{n}\cdot\overleftrightarrow{\tau}_2\cdot(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})\cdot\overleftrightarrow{\tau}_1\cdot\hat{n}. \quad \text{(E2)}$$

This equality will combine the 1st term in the 3rd line with the 4th line of equation (E1). Also to combine the second term in the 3rd line with the last line of (E1), let $a=\tau_{nn}$, $b=\tau_{t_1t_1}$, $c=\tau_{t_2t_2}$, to obtain

$$\begin{aligned} & \mathrm{Tr}(\overleftrightarrow{\tau}_1)\,\mathrm{Tr}(\overleftrightarrow{\tau}_2) - \tau^1_{nn}\,\mathrm{Tr}(\overleftrightarrow{\tau}_2) - \tau^2_{nn}\,\mathrm{Tr}(\overleftrightarrow{\tau}_1) \\ & \quad = (a_1+b_1+c_1)(a_2+b_2+c_2) - a_1(a_2+b_2+c_2) - a_2(a_1+b_1+c_1) \\ & \quad = (b_1+c_1)(b_2+c_2) - a_1a_2 = \mathrm{Tr}(\overleftrightarrow{\tau}^T_1)\,\mathrm{Tr}(\overleftrightarrow{\tau}^T_2) - \tau^1_{nn}\tau^2_{nn}. \end{aligned} \quad \text{(E3)}$$

Combining these results, we are left with equation (2.16).

APPENDIX F: DETAILS OF DERIVATION OF (2.18)

Setting $\vec{u}=0$ in (2.16), we are left with the last four lines only. To evaluate these, we need to obtain two intermediate results.

1. Evaluate $\overleftrightarrow{\tau}_1^T : \overleftrightarrow{\tau}_2^T$ when $\vec{u}=0$

Expanding this quantity, we have

$$\overleftrightarrow{\tau}_1^T : \overleftrightarrow{\tau}_2^T = \tau^1_{t_1t_1}\tau^2_{t_1t_1} + \tau^1_{t_2t_2}\tau^2_{t_2t_2} + 2\tau^1_{t_2t_1}\tau^2_{t_2t_1}. \tag{F1}$$

Consider $\tau_{t_2t_1} = \mu \hat{t}_1 \hat{t}_2 : (\vec{\nabla}\vec{u} + \vec{u}\vec{\nabla}_{\hookleftarrow})$. Recall $\vec{u}=0$ implies that $\vec{\nabla}u^i \| \hat{n} \perp \hat{t}$ so that $\hat{t}\cdot\vec{\nabla}\vec{u}=0$ and $\tau_{t_2t_1}=0$.

Next, consider $\tau_{t_1t_1} = \tau_{t_2t_2} = \lambda\vec{\nabla}\cdot\vec{u}$, where again we have used $\vec{\nabla}u^i \perp \hat{t}$. Since $\vec{\nabla}u^i \| \hat{n}$ we have $(\overleftrightarrow{\mathbf{1}} - \hat{n}\hat{n}) : \vec{\nabla}\vec{u} = 0$, or $\vec{\nabla}\cdot\vec{u} = \hat{n}\hat{n} : \vec{\nabla}\vec{u}$ (note, this result is only valid for the special case $\vec{u}=0$ on S). Thus $\tau_{nn} = (\lambda + 2\mu)\vec{\nabla}\cdot\vec{u}$, and

$$\tau_{t_1t_1} = \tau_{t_2t_2} = \lambda\vec{\nabla}\cdot\vec{u} = \frac{\lambda\tau_{nn}}{\lambda+2\mu}. \tag{F2}$$

Substituting into equation (F1), it follows that

$$\overleftrightarrow{\tau}_1^T : \overleftrightarrow{\tau}_2^T = \frac{2\lambda^2}{(\lambda+2\mu)^2}\tau^1_{nn}\tau^2_{nn}. \tag{F3}$$

2. Evaluate Tr($\overleftrightarrow{\tau}^T$)

From equation (F2), it follows immediately that

$$\mathrm{Tr}(\overleftrightarrow{\tau}^T) = \frac{2\lambda}{\lambda+2\mu}\tau_{nn}.$$

3. Combine results

Substituting these results into (2.16) we find

$$R_\infty = \int dS\xi \left[\frac{\hat{n}\cdot\overleftrightarrow{\tau}_1\cdot(\overleftrightarrow{\mathbf{1}} - \hat{n}\hat{n})\cdot\overleftrightarrow{\tau}_2\cdot\hat{n}}{\mu} + \frac{\tau^1_{nn}\tau^2_{nn}}{2\mu}\left(1 - \frac{2\lambda^2}{(\lambda+2\mu)^2} + \frac{4\lambda^3}{3\lambda+2\mu}\frac{1}{(\lambda+2\mu)^2} - \frac{\lambda}{3\lambda+2\mu}\right)\right]. \tag{F4}$$

The object in parentheses on the second line of equation (F4) simplifies to $2\mu/(\lambda+2\mu)$, and equation (2.18) follows immediately. Note that this result is valid for the zero displacement ($\vec{u}=0$) boundary condition only.

APPENDIX G: THE SOLID-SOLID BOUNDARY CONDITION FOR THE OFF-DIAGONAL ELEMENT OF $\overleftrightarrow{\tau}^T$

On the interface between two elastic solids labeled I and II, the off-diagonal element of $\overleftrightarrow{\tau}^T$, $\tau_{t_1t_2}$, obeys a simple boundary condition:

$$\frac{\tau^I_{t_1t_2}}{\mu_I} - \frac{\tau^{II}_{t_1t_2}}{\mu_{II}} = 0. \tag{G1}$$

The proof is fairly simple. Note that

$$\tau_{t_1t_2}=\mu\hat{t}_1\cdot(\vec{\nabla}\vec{u})\cdot\hat{t}_2+\mu\hat{t}_2\cdot(\vec{\nabla}\vec{u})\cdot\hat{t}_1,$$

so that

$$\frac{\tau^I_{t_1t_2}}{\mu_I}-\frac{\tau^{II}_{t_1t_2}}{\mu_{II}}=\hat{t}_1\cdot[\vec{\nabla}(\vec{u}^I-\vec{u}^{II})]\cdot\hat{t}_2+(1\leftrightarrow 2)=0,$$

since $\vec{u}^I-\vec{u}^{II}=0$ on S, and therefore $\vec{\nabla}(\vec{u}^I-\vec{u}^{II})^i\|\hat{n}\perp\hat{t}$. Q.E.D.

APPENDIX H: LEMMA USEFUL FOR EXPRESSING α IN TERMS OF A_S

Note that

$$k_s^2=\frac{c_p^2}{c_s^2}k_p^2=\frac{\lambda_{II}+2\mu_{II}}{\mu_{II}},$$

so that

$$\frac{1}{1-k_s^2/2|\mathbf{k}_\perp|^2}=\frac{1}{1-(1+\lambda_{II}/2\mu_{II})(k_p^2/|\mathbf{k}_\perp|^2)}=\frac{|\mathbf{k}_\perp|^2}{-k_{pn}^2-(\lambda_{II}/2\mu_{II})k_p^2}$$
$$=\frac{|\mathbf{k}_\perp|^2 2\mu_{II}}{-k_p^2(\lambda_{II}+2\mu_{II}(k_{pn}^2/k_p^2))}=\frac{|\mathbf{k}_\perp|^2 2\mu_{II}}{k_p\alpha}. \tag{H1}$$

It follows immediately that

$$\alpha=\frac{k_s}{k_p}\frac{2\mu_{II}}{A_S}\frac{k_{pn}}{k_p}|\mathbf{k}_\perp|. \tag{H2}$$

APPENDIX I: SIMPLE FORM OF THE SCATTERING AMPLITUDE FOR SMALL SLOPE AND "LOCAL" TWO-SCALE APPROXIMATIONS

In this appendix, equation (3.20) will be derived from equation (2.14) by making the approximation that the surface is locally flat. In order to do so, it is necessary to simplify the term involving $\overleftrightarrow{\tau}_1^{II}:\overleftrightarrow{\tau}_2^{II}$. *Suppressing the label II* (i.e., inside the solid) for now, and summing repeated indices j and k, we have $\overleftrightarrow{\tau}_1^{II}:\overleftrightarrow{\tau}_2^{II}=\tau_1^{jk}\tau_2^{jk}$. Recall that $\tau^{jk}=\lambda\vec{\nabla}\cdot\vec{u}\,\delta^{jk}+\mu(\nabla^j u^k+\nabla^k u^j)$ and define $\sigma^{jk}\equiv\nabla^j u^k+\nabla^k u^j$. It follows that

$$\tau_1^{jk}\tau_2^{jk}=(3\lambda^2+4\mu\lambda)(\vec{\nabla}\cdot\vec{u}_1)(\vec{\nabla}\cdot\vec{u}_2)+\sigma_1^{jk}\sigma_2^{jk}, \tag{I1}$$

where use was made of $\delta^{jk}\delta^{jk}=3$ and $\sigma^{jk}\delta^{jk}=2\mu\vec{\nabla}\cdot\vec{u}$. Next, we consider $\overleftrightarrow{\sigma}_1:\overleftrightarrow{\sigma}_2=\sigma_1^{jk}\sigma_2^{jk}$. We can decompose $\overleftrightarrow{\sigma}$ using

$$\overleftrightarrow{\sigma}=(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})\cdot\overleftrightarrow{\sigma}\cdot(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})+\hat{n}\hat{n}\cdot\overleftrightarrow{\sigma}\cdot(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})+(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})\cdot\overleftrightarrow{\sigma}\cdot\hat{n}\hat{n}+\sigma_{nn}\hat{n}\hat{n}.$$

Recall the boundary condition

$$0=\hat{n}\hat{n}\cdot\overleftrightarrow{\tau}\cdot(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})=\hat{n}\hat{n}\cdot\overleftrightarrow{\sigma}\cdot(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})$$

and define

$$\overleftrightarrow{\sigma}^T\equiv(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})\cdot\overleftrightarrow{\sigma}\cdot(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})$$

to obtain

$$\vec{\vec{\sigma}} \equiv \vec{\vec{\sigma}}^T + \sigma_{nn}\hat{n}\hat{n}$$

and thus

$$\vec{\vec{\sigma}}^1 : \vec{\vec{\sigma}}^2 = \vec{\vec{\sigma}}^{1T} : \vec{\vec{\sigma}}^{2T} + \sigma^1_{nn}\sigma^2_{nn}. \tag{I2}$$

Now we need σ^T_{jk} evaluated for the ''locally flat'' scattering surface approximation. Using the equation for $\vec{u}^{II}$ (3.8), and recalling

$$(\vec{\vec{1}} - \hat{n}\hat{n}) \cdot \vec{k}_p = (\vec{\vec{1}} - \hat{n}\hat{n}) \cdot \vec{k}_s = (\vec{\vec{1}} - \hat{n}\hat{n}) \cdot \vec{k}_i = \mathbf{k}_\perp ,$$

we have

$$(\vec{\vec{1}} - \hat{n}\hat{n}) \cdot \vec{\nabla} \equiv \nabla_\perp \propto \mathbf{k}_\perp$$

(to be precise, the transverse component of the gradient brings down $i\mathbf{k}_\perp$). From equation (3.22), we also have (on the boundary)

$$\vec{u}^{II}_T \propto \mathbf{k}_\perp ,$$

so that (still suppressing the label ''*II*'')

$$\nabla^j_\perp u^k_\perp + \nabla^k_\perp u^j_T = 2\nabla^j_\perp u^k_T .$$

Thus, since $\nabla_\perp$ brings down an $i\mathbf{k}_\perp$ (or a $-i\mathbf{q}_\perp$), we have

$$\begin{aligned} \vec{\vec{\sigma}}^{1T} : \vec{\vec{\sigma}}^{2T} &= i\mathbf{k}^j_\perp u^k_{1T}(-i\mathbf{q}^j_\perp) u^k_{2T} 4\mu^2 = \mathbf{k}_\perp \cdot \mathbf{q}_\perp \vec{u}_1 \cdot (\vec{\vec{1}} - \hat{n}\hat{n}) \cdot \vec{u}_2 4\mu^2 \\ &= 4\mu^2 \vec{k}_i \cdot (\vec{\vec{1}} - \hat{n}\hat{n}) \cdot \vec{q}_i \vec{u}_1 \cdot (\vec{\vec{1}} - \hat{n}\hat{n}) \cdot \vec{u}_2 . \end{aligned} \tag{I3}$$

To complete our evaluation of equation (I2), we also have the result

$$\sigma^1_{nn}\sigma^2_{nn} = 4\mu^2 (\hat{n}\hat{n} : \vec{\nabla}\vec{u}_1)(\hat{n}\hat{n} : \vec{\nabla}\vec{u}_2). \tag{I4}$$

Use (I3) and (I4) to evaluate (I2), then substitute that result into (I1), and also make the substitution

$$\vec{\nabla} \cdot \vec{u} = \frac{\vec{\vec{\tau}}}{3\lambda + 2\mu}.$$

Thus, we obtain

$$\begin{aligned} \vec{\vec{\tau}}_1 : \vec{\vec{\tau}}_2 = {} & \frac{3\lambda^2 + 4\mu\lambda}{(3\lambda + 2\mu)^2} \operatorname{Tr}(\vec{\vec{\tau}}_1) \operatorname{Tr}(\vec{\vec{\tau}}_2) + 4\mu^2 (\hat{n}\hat{n} : \vec{\nabla}\vec{u}_1)(\hat{n}\hat{n} : \vec{\nabla}\vec{u}_2) \\ & + 4\mu^2 \vec{k}_i \cdot (\vec{\vec{1}} - \hat{n}\hat{n}) \cdot \vec{q}_i \vec{u}_1 \cdot (\vec{\vec{1}} - \hat{n}\hat{n}) \cdot \vec{u}_2 , \end{aligned} \tag{I5}$$

where the 1st and 2nd lines are universally valid, but the 3rd line ignores the curvature of the scattering surface. Now, split the 1st term using

$$\frac{3\lambda^2 + 4\mu\lambda}{(3\lambda + 2\mu)^2} = \frac{3\lambda^2 + 2\mu\lambda}{(3\lambda + 2\mu)^2} + \frac{2\mu\lambda}{(3\lambda + 2\mu)^2},$$

and also restore the label II to obtain

$$\vec{\tau}_1^{II}:\vec{\tau}_2^{II}=\frac{1}{2\mu_{II}}\frac{\lambda_{II}}{3\lambda_{II}+2\mu_{II}}\,\mathrm{Tr}(\vec{\tau}_1^{II})\,\mathrm{Tr}(\vec{\tau}_2^{II})+\frac{\lambda_{II}}{(3\lambda_{II}+2\mu_{II})^2}\,\mathrm{Tr}(\vec{\tau}_1^{II})\,\mathrm{Tr}(\vec{\tau}_2^{II})$$
$$+2\mu_{II}(\hat{n}\hat{n}:\vec{\nabla}\vec{u}_1^{II})(\hat{n}\hat{n}:\vec{\nabla}\vec{u}_2^{II})+2\mu_{II}\vec{k}_i\cdot(\vec{\mathbf{1}}-\hat{n}\hat{n})\cdot\vec{q}_i\vec{u}_1^{II}\cdot(\vec{\mathbf{1}}-\hat{n}\hat{n})\cdot\vec{u}_2^{II}. \tag{I6}$$

Note that the 1st term on the right hand side of this equation will cancel line 6 of equation (2.14). Thus, substituting the result (I6) into equation (2.14) gives

$$\frac{-iQ_zT}{\rho_1\omega^2}=\int d^2x[\ \text{Integrand}]$$

$$\text{Integrand}=(\rho_I-\rho_{II})\omega^2\hat{n}\cdot\hat{u}_1\hat{n}\cdot\hat{u}_2+[(\rho_I-\rho_{II})\omega^2+2\mu_{II}\vec{k}_i\cdot(1-\hat{n}\hat{n})\cdot\vec{q}_i]\vec{u}_1^{II}\cdot(1-\hat{n}\hat{n})\cdot\vec{u}_2^{II}$$
$$-\rho_I\omega^2(\vec{u}_1^{I}-\vec{u}_1^{II})\cdot(\vec{\mathbf{1}}-\hat{n}\hat{n})\cdot(\vec{u}_2^{I}-\vec{u}_2^{II})+\frac{k_i^2}{\rho_I\omega^2}\tau_{nn}^1\tau_{nn}^2$$
$$+\frac{\lambda_{II}}{(3\lambda_{II}+2\mu_{II})^2}[\ \mathrm{Tr}(\vec{\tau}_1^{II})\,\mathrm{Tr}(\vec{\tau}_2^{II})]-\frac{1}{3\lambda_{II}+2\mu_{II}}[\ \mathrm{Tr}(\vec{\tau}_1^{II})\tau_{nn}^2+\ \mathrm{Tr}(\vec{\tau}_2^{II})\tau_{nn}^1]$$
$$+2\mu_{II}(\hat{n}\hat{n}:\vec{\nabla}\vec{u}_1^{II})(\hat{n}\hat{n}:\vec{\nabla}\vec{u}_2^{II}). \tag{I7}$$

Note that the 2nd part of line 2 (involving $\vec{k}_i$ and $\vec{q}_i$) is the only instance where the ''flat scattering surface'' approximation comes in. The remainder of the equation is exact.

Finally, simplify the term involving $\hat{n}\hat{n}:\vec{\nabla}\vec{u}$. The equation,

$$\tau_{nn}=\lambda\vec{\nabla}\cdot\vec{u}+2\mu\hat{n}\hat{n}:\vec{\nabla}\vec{u},$$

can be inverted to solve for $\hat{n}\hat{n}:\vec{\nabla}\vec{u}$. This leads to

$$2\mu_{II}(\hat{n}\hat{n}:\vec{\nabla}\vec{u}_1^{II})(\hat{n}\hat{n}:\vec{\nabla}\vec{u}_2^{II})=\frac{1}{2\mu_{II}}\tau_{nn}^1\tau_{nn}^2+\frac{1}{2\mu_{II}}\frac{\lambda_{II}^2}{(3\lambda_{II}+2\mu_{II})^2}\,\mathrm{Tr}(\vec{\tau}_1^{II})\,\mathrm{Tr}(\vec{\tau}_2^{II})$$
$$-\frac{1}{2\mu_{II}}\frac{\lambda_{II}}{3\lambda_{II}+2\mu_{II}}[\ \mathrm{Tr}(\vec{\tau}_1^{II})\tau_{nn}^2+\ \mathrm{Tr}(\vec{\tau}_2^{II})\tau_{nn}^1].$$

Substituting this result into equation (I7), we finally obtain equation (3.20).

APPENDIX J: DETAILS OF THE DERIVATION OF EQUATION (3.22)

In this appendix, equation (3.22) is derived beginning with the 3rd part of equation (3.19):

$$\vec{u}_1^{II}=C[\hat{k}_p-A_S\hat{t}]e^{i\vec{k}_i\cdot\vec{x}}.$$

The phase factor $e^{i\vec{k}_i\cdot\vec{x}}$ will be suppressed for the rest of the discussion in this appendix.

Decompose $\vec{u}^{II}$ according to

$$\vec{u}^{II}=(\vec{u}^{II}\cdot\hat{n})\hat{n}+\vec{u}^{II}\cdot(\vec{\mathbf{1}}-\hat{n}\hat{n}), \tag{J1}$$

and note that $\vec{u}^{II}\cdot\hat{n}=\vec{u}^{I}\cdot\hat{n}$ and that $\vec{u}^{I}$ can be evaluated using equation (3.21) to give

$$\vec{u}^{II}\cdot\hat{n}=\frac{i}{\rho_I\omega^2}(1-B)k_{in}=\frac{i}{\rho_I\omega^2}\,\frac{2}{a+1}k_{in}\,. \tag{J2}$$

Using equation (3.12), it is easy to show that

$$\vec{u}^{II}\cdot(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})=\frac{C\mathbf{k}_\perp}{k_p}\left[1+\frac{A_S k_p k_{sn}}{|\mathbf{k}_\perp|}k_s\right]. \tag{J3}$$

When A_S is further evaluated using equation (3.13), it follows that

$$\vec{u}_{II}\cdot(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})=\frac{C\mathbf{k}_\perp}{k_p}\left[\frac{|\mathbf{k}_\perp|^2-k_s^2/2+k_{pn}k_{sn}}{|\mathbf{k}_\perp|^2-k_s^2/2}\right]. \tag{J4}$$

From equation (3.15), we have

$$C=\frac{-2b}{ik_p(\lambda_{II}+2\mu_{II})}\,\frac{1}{a+1},$$

where a and b are also given in (3.15). Substitute

$$b=\frac{\rho_{II}}{\rho_I}\,\frac{k_{in}}{k_{pn}}\left(1-\frac{2|\mathbf{k}_\perp|^2}{k_s^2}\right)$$

into C, and use equation (3.16) to make the substitution

$$\lambda_{II}+2\mu_{II}=\frac{\rho_{II}\omega^2}{k_p^2}.$$

After just a little algebra, we have

$$C=\frac{2ik_p}{\rho_I\omega^2}\,\frac{k_{in}}{k_{pn}}\,\frac{-2}{k_s^2}\left[|\mathbf{k}_\perp|^2-\frac{k_s^2}{2}\right]\frac{1}{a+1}.$$

Also, use

$$|\mathbf{k}_\perp|^2+k_{sn}^2=k_s^2\quad\text{and}\quad-|\mathbf{k}_\perp|^2=k_{pn}^2-k_p^2$$

to show that

$$|\mathbf{k}_\perp|^2-\frac{k_s^2}{2}+k_{pn}k_{sn}=-\frac{1}{2}((k_{sn}-k_{pn})^2-k_p^2).$$

Combining these results, we obtain

$$\vec{u}_{II}\cdot(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})=\mathbf{k}_\perp\,\frac{2i}{\rho_I\omega^2}\,\frac{\xi}{a+1}, \tag{J5}$$

with ξ as defined in equation (3.22). Substituting equations (J2) and (J5) back into equation (J1), we finally obtain equation (3.22).

To obtain the alternate form for ξ, note that

$$\frac{(k_{sn}-k_{pn})^2-k_p^2}{k_s^2}=\frac{k_{sn}^2+k_{pn}^2-2k_{sn}k_{pn}-k_p^2}{k_s^2}=\frac{k_s^2-|\mathbf{k}_\perp|^2+k_p^2-|\mathbf{k}_\perp|^2-2k_{sn}k_{pn}-k_p^2}{k_s^2}$$

$$=1-2\frac{|\mathbf{k}_\perp|^2+k_{sn}k_{pn}}{k_s^2}=1-2\frac{\vec{k}_s\cdot\vec{k}_p}{k_s^2}. \tag{J6}$$

APPENDIX K: DETAILS OF THE DERIVATION OF EQUATION (3.23)

We need to use the results (3.21) and (3.22) to evaluate the quantities in equation (3.20). This is absolutely straightforward, and the result is

$$\begin{aligned}
&e^{i\vec{Q}_i\cdot\vec{x}}(a_1+1)(a_2+1)[\text{ Integrand}]\\
&=\frac{(\rho_I-\rho_{II})}{\rho_I^2\omega^2}4k_{in}q_{in}+\frac{(\rho_I-\rho_{II})}{\rho_I^2\omega^2}\vec{k}_i\cdot(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})\cdot\vec{q}_i 4\xi_1\xi_2+\frac{8\mu_{II}[\vec{k}_i\cdot(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})\cdot\vec{q}_i]^2}{\rho_I^2\omega^4}\xi_1\xi_2\\
&-\frac{1}{\rho_I\omega^2}\vec{k}_i\cdot(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})\cdot\vec{q}_i 4(a_1-\xi_1)(a_2-\xi_2)+\frac{k_i^2}{\rho_I\omega^2}4a_1a_2+\frac{1}{2\mu_{II}}4a_1a_2\\
&+\frac{\lambda_{II}}{(3\lambda_{II}+2\mu_{II})^2}\left(1+\frac{\lambda_{II}}{2\mu_{II}}\right)\frac{b_1b_2(3\lambda_{II}+2\mu_{II})^2}{\mu_{II}^2(1+\lambda_{II}/(2\mu_{II}))^2}\\
&-\frac{1}{(3\lambda_{II}+2\mu_{II})}\left(1+\frac{\lambda_{II}}{2\mu_{II}}\right)\frac{2(b_1a_2+b_2a_1)(3\lambda_{II}+2\mu_{II})}{\mu_{II}(1+\lambda_{II}/(2\mu_{II}))}.
\end{aligned}\tag{K1}$$

Note the immediate cancellation of $3\lambda_{II}+2\mu_{II}$ and $1+\lambda_{II}/(2\mu_{II})$ in the last two lines of equation (K1) above. Furthermore, to evaluate the last 3 terms, note that

$$\frac{1}{\mu_{II}}=\frac{1}{\rho_{II}\omega^2}\frac{\rho_{II}\omega^2}{\mu_{II}}=\frac{k_s^2}{\rho_{II}\omega^2}=\frac{k_s^2}{\rho_I\omega^2}\frac{\rho_I}{\rho_{II}},$$

so that these 3 terms become

$$\begin{aligned}
&\frac{2k_s^2}{\rho_I\omega^2}\frac{\rho_I}{\rho_{II}}a_1a_2+\frac{2\lambda_{II}}{\lambda_{II}+2\mu_{II}}\frac{k_s^2}{\rho_I\omega^2}\frac{\rho_I}{\rho_{II}}b_1b_2-\frac{2k_s^2}{\rho_I\omega^2}\frac{\rho_I}{\rho_{II}}(b_1a_2+b_2a_1)\\
&\quad=\frac{2(\lambda_{II}+2\mu_{II})}{\lambda_{II}+2\mu_{II}}\frac{k_s^2}{\rho_I\omega^2}\frac{\rho_I}{\rho_{II}}b_1b_2+\frac{2k_s^2}{\rho_I\omega^2}\frac{\rho_I}{\rho_{II}}a_1a_2\\
&\qquad-\frac{2(2\mu_{II})}{\lambda_{II}+2\mu_{II}}\frac{k_s^2}{\rho_I\omega^2}\frac{\rho_I}{\rho_{II}}b_1b_2-\frac{2k_s^2}{\rho_I\omega^2}\frac{\rho_I}{\rho_{II}}(b_1a_2+b_2a_1)\\
&\quad=\frac{2k_s^2}{\rho_I\omega^2}\frac{\rho_I}{\rho_{II}}(a_1a_2+b_1b_2-b_1a_2-b_2a_1)-\frac{4\mu_{II}}{\lambda_{II}+2\mu_{II}}\frac{k_s^2}{\rho_I\omega^2}\frac{\rho_I}{\rho_{II}}b_1b_2.
\end{aligned}$$

Simplify using

$$\frac{\mu_{II}}{\lambda_{II}+2\mu_{II}}=\frac{k_p^2}{k_s^2}\quad\text{and}\quad(a_1-b_1)(a_2-b_2)=a_1a_2+b_1b_2-b_1a_2-b_2a_1.$$

Now substitute all this into equation (K1) to obtain

$$e^{i\vec{Q}_i\cdot\vec{x}}\rho_I\omega^2(a_1+1)(a_2+1)[\text{ Integrand}]$$
$$=\left(1-\frac{\rho_I}{\rho_{II}}\right)4k_{in}q_{in}+4\left(1-\frac{\rho_I}{\rho_{II}}\right)\vec{k}_i\cdot(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})\cdot\vec{q}_i\xi_1\xi_2+\frac{8\mu_{II}}{\rho_I\omega^2}[\vec{k}_i\cdot(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})\cdot\vec{q}_i]^2\xi_1\xi_2$$
$$-4\vec{k}_i\cdot(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})\cdot\vec{q}_i(a_1-\xi_1)(a_2-\xi_2)+4k_i^2a_1a_2+2k_s^2\frac{\rho_I}{\rho_{II}}(a_1-b_1)(a_2-b_2)-4k_p^2\frac{\rho_I}{\rho_{II}}b_1b_2. \tag{K2}$$

Optionally, use $\mu_{II}/(\rho_I\omega^2)=(1/k_s^2)(\rho_{II}/\rho_I)$ in line 3. Having now evaluated the integrand in equation (3.20), equation (3.23) follows immediately.

APPENDIX L: THE LIMIT AS THE SOLID IN REGION *II* BECOMES A FLUID

In this appendix, we examine the two *(locally) flat reference surface approximations* in the limit as $\mu_{II}\to 0$. (i.e., as the solid in region *II* becomes a fluid). The result is equation (3.24).

In this limit, we have from equations (3.10) and (3.11) that

$$1/k_s^2=O(\mu_{II}),\quad k_{sn}=O(\mu_{II}^{-1/2}),$$

and further, substituting into equations (3.15) and (3.22), we find

$$a=\frac{\rho_{II}}{\rho_I}\frac{k_{in}}{k_{pn}}+O(\mu_{II}),\quad b=a+O(\mu_{II}),$$

$$\xi=\frac{k_{in}}{k_{pn}}+O(\mu_{II}^{1/2})=\frac{\rho_I}{\rho_{II}}a+O(\mu_{II}^{1/2}).$$

Note that $a-b=O(\mu_{II})$, so that

$$(a_1-b_1)(a_2-b_2)=O(\mu_{II}^2),$$

and we have

$$T(\vec{q}_i,\vec{k}_i)=\frac{i}{Q_{iz}}\int d^2x e^{i\vec{Q}_i\cdot\vec{x}}\left[\left(1-\frac{\rho_{II}}{\rho_I}\right)\frac{4k_{in}q_{in}}{(a_1+1)(a_2+1)}\right.$$
$$+4\left(\frac{\rho_I^2}{\rho_{II}^2}-\frac{\rho_I}{\rho_{II}}\right)\vec{k}_i\cdot(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})\cdot\vec{q}_i\frac{a_1a_2}{(a_1+1)(a_2+1)}$$
$$-4\vec{k}_i\cdot(\overleftrightarrow{\mathbf{1}}-\hat{n}\hat{n})\cdot\vec{q}_i\left(1-\frac{\rho_I}{\rho_{II}}\right)^2\frac{a_1a_2}{(a_1+1)(a_2+1)}$$
$$\left.+4k_i^2\frac{a_1a_2}{(a_1+1)(a_2+1)}-4k_p^2\frac{\rho_I}{\rho_{II}}\frac{a_1a_2}{(a_1+1)(a_2+1)}\right]+O(\mu_{II}^{1/2}). \tag{L1}$$

Define

$$\frac{2a}{a+1}\equiv A,$$

with the identification of the subscripts $1\leftrightarrow\vec{k}_i$, $2\leftrightarrow-\vec{q}_i$ and note that

$$\frac{\rho_I^2}{\rho_{II}^2}-\frac{\rho_I}{\rho_{II}}-\left(1-\frac{\rho_I}{\rho_{II}}\right)^2=\frac{\rho_I}{\rho_{II}}-1$$

to obtain equation (3.24).

APPENDIX M: THE LIMIT AS THE SOLID IN REGION *II* BECOMES INFINITELY STIFF

In this appendix, we examine the two *(locally) flat reference surface approximations* in the limit as $\mu_{II}\to\infty$. The result is equation (3.25)

We have

$$\begin{aligned} k_{sn}&=-\sqrt{k_s^2-|\mathbf{k}_\perp|^2}=-i|\mathbf{k}_\perp|\left(1-\frac{\rho_{II}\omega^2}{2\mu_{II}|\mathbf{k}_\perp|^2}\right)+O\left(\frac{1}{\mu_{II}^2}\right),\\ k_{pn}&=-\sqrt{k_p^2-|\mathbf{k}_\perp|^2}=-i|\mathbf{k}_\perp|\left(1-\frac{\rho_{II}\omega^2}{4\mu_{II}|\mathbf{k}_\perp|^2}\right)+O\left(\frac{1}{\mu_{II}^2}\right), \end{aligned} \tag{M1}$$

so that

$$k_{sn}-k_{pn}=\frac{ik_s^2}{4|\mathbf{k}_\perp|}. \tag{M2}$$

Thus, substituting into equation (3.15), we find

$$a_1=i|\mathbf{k}_\perp|\frac{\rho_{II}}{\rho_I}\frac{(-k_{in})}{k_s^2}+O(\mu_{II}^0)\to\infty.$$

Since $1/k_s^2\propto\mu_{II}$, we have $a_1\to\infty$ and

$$\frac{1}{a_1+1}=O\left(\frac{1}{\mu_{II}}\right)\quad\text{and}\quad\frac{a_1}{a_1+1}\to 1.$$

By also substituting the results (M1) in the equation for b in equation (3.15), we obtain

$$b_1=2a_1+O(\mu_{II}^0),$$

so that $(a_1-b_1)/(a_1+1)$ and $b_1/(a_1+1)$ are both $O(\mu_{II}^0)$ (i.e., just finite numbers).

We also have

$$k_p^2=\frac{k_s^2}{2}+O\left(\frac{1}{\mu_{II}^2}\right),$$

so that, using equations (3.22) and (M2),

$$\xi_1=-\frac{k_{in}}{i|\mathbf{k}_\perp|}\left[\frac{1}{k_s^2}\left(\frac{ik_s^2}{4|\mathbf{k}_\perp|}\right)^2-\frac{k_p^2}{k_s^2}\right]=-\frac{(-k_{in})}{2i|\mathbf{k}_\perp|}+O\left(\frac{1}{\mu_{II}}\right),$$

and consequently that

$$\frac{\xi_1}{a_1+1}=O\left(\frac{1}{\mu_{II}}\right).$$

Note that k_p^2 and k_s^2 are both $O(1/\mu_{II})$. Substituting these results, and the analogous ones with the subscript ''2'' into equation (3.23), equation (3.25) follows immediately.

APPENDIX N: THE LIMIT AS THE SOLID IN REGION *II* BECOMES A GAS

Once again, consider equation (3.23), and this time let the solid in medium II become gas-like (i.e., let both μ_{II} and ρ_{II} go to 0). In Appendix L above, it was shown that taking $\mu_{II}\to 0$ first, we recover the two-fluid result. It is well-known, and easy to verify that for a two-fluid interface, as the density of medium II approaches zero, Dirichlet boundary conditions are satisfied at the interface. Therefore, we will not reproduce a proof for that case here. Instead, let us take $\rho_{II}\to 0$ first, and only then let $\mu_{II}\to 0$ (i.e., assume the density ρ_{II} goes to zero more rapidly than the second Lamé constant μ_{II}).

If $\rho_{II}\to 0$, with μ_{II} not yet 0, we have [cf. equations (M1) and (M2)]

$$\begin{aligned} k_p^2=\frac{\rho_{II}\omega^2}{\lambda_{II}+2\mu_{II}}\Rightarrow k_{pn}=-i|\mathbf{k}_\perp|\left(1-\frac{\rho_{II}\omega^2}{2(\lambda_{II}+2\mu_{II})|\mathbf{k}_\perp|^2}\right)+O(\rho_{II}^2),\\ k_s^2=\frac{\rho_{II}\omega^2}{\mu_{II}}\Rightarrow k_{sn}=-i|\mathbf{k}_\perp|\left(1-\frac{\rho_{II}\omega^2}{2\mu_{II}|\mathbf{k}_\perp|^2}\right)+O(\rho_{II}^2), \end{aligned} \tag{N1}$$

and thus

$$k_{sn}-k_{pn}=-\frac{i\rho_{II}\omega^2}{2|\mathbf{k}_\perp|}\left(\frac{1}{\lambda_{II}+2\mu_{II}}-\frac{1}{\mu_{II}}\right)+O(\rho_{II}^2). \tag{N2}$$

Therefore, we have from equation (3.15),

$$\begin{aligned} a_1=-\frac{2ik_{in}\mu_{II}|\mathbf{k}_\perp|}{\rho_I\omega^2}\left(1-\frac{\mu_{II}}{\lambda_{II}+2\mu_{II}}\right)+O(\rho_{II}),\\ b_1=-\frac{2ik_{in}\mu_{II}|\mathbf{k}_\perp|}{\rho_I\omega^2}+O(\rho_{II}). \end{aligned} \tag{N3}$$

Furthermore, substituting results (N1) and (N2) into equation (3.22), we have

$$\xi_1=-\frac{ik_{in}}{|\mathbf{k}_\perp|}\frac{\mu_{II}}{\lambda_{II}+2\mu_{II}}+O(\rho_{II}). \tag{N4}$$

Once again, the results with the subscript ''2'' are virtually identical. Finally, letting $\mu_{II}\to 0$, we have $a,b,\xi=O(\mu_{II})\to 0$, and equation (3.24) follows immediately as these results are substituted into equation (3.23).

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Invariant of dynamical systems: A generalized entropy

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In this work the concept of entropy of a dynamical system, as given by Kolmogorov, is generalized in the sense of Tsallis. It is shown that this entropy is an isomorphism invariant, being complete for Bernoulli schemes. © *1996 American Institute of Physics.* [S0022-2488(96)03309-9]

I. INTRODUCTION

Ergodic theory not only is an important chapter of Statistical Physics but also it constitutes by itself an entire branch of Mathematics.

A basic result of ergodic theory is the isomorphism theorem for Bernoulli schemes, initially proved by Ornstein.[1] This theorem involves the concept of entropy.

Entropy was introduced by Shannon, in his mathematical theory of communications, as a measure of the amount of information[2] and generalized in the context of dynamical systems by Kolmogorov.[3] Subsequently, Sinai[4] proved Kolmogorov's entropy to be an isomorphism invariant, Meshalkin[5] demonstrated that some special Bernoulli schemes are always isomorphic whereas Ornstein's isomorphism theorem showed the isomorphism to be complete. A nice proof of this last result, which enables us to construct finitary isomorphisms, was later given by Keane and Smorodinsky based on coding-theoretical arguments.[6]

Generalizations of Shannon's entropy have been introduced by Rényi[7] and, more recently, on a multifractal basis, by Tsallis.[8] These generalized entropies have found a wide field of applications in the last few years. In particular, they enable us to explain a variety of physical phenomena such as the behavior of self-gravitating systems, the anomalous diffusion, Euler turbulence, and so on.[9–15]

In this work we generalize the concept of Tsallis entropy to abstract dynamical systems in the same spirit as Kolmogorov did for Shannon entropy and study its invariance under isomorphisms. Our main result is that the new generalized entropy we consider is also an isomorphism invariant of dynamical systems. Moreover, it is a complete invariant for Bernoulli schemes. It should be noted that very recently Zanette has studied the dynamics of multifractal generation using a generalization of the Kolmogorov entropy.[16] Zanette's generalization, however, is a particular case of the more general definition that we consider in this paper.

In the next section we give a brief review of the main concepts concerning dynamical systems, Bernoulli schemes, and isomorphisms. Section III will be devoted to introducing the new generalized entropy, whereas in Sec. IV we prove its properties we are interested in here, namely, the isomorphism invariance and the complete invariance for Bernoulli schemes.

II. DYNAMICAL SYSTEMS AND BERNOULLI SCHEMES

The idea of measure-preserving transformation,[17] mathematically generalizes the physical concept of a dynamical system. Here we understand by a physical dynamical system a collection of particles or states, the temporal evolution of which is determined by some physical law in such a way that Liouville's theorem is verified.

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From a mathematical point of view a dynamical system or, more precisely, a measure-preserving dynamical system, also simply called a measure-preserving transformation, is a quadruple $(X,\mathscr{A},\mu,T)$ where X is a set, $\mathscr{A}$ a σ-algebra, μ a measure on $\mathscr{A}$, and T is a mapping of the underlying set X to itself that is measurable and preserves the measure μ, i.e. *for any* $A\in\mathscr{A}$, $T^{-1}A\in\mathscr{A}$ *and* $\mu(T^{-1}A)=\mu(A)$ [$\mu(\cdot)$ denotes the measure of an element $\cdot$ of $\mathscr{A}$].

Bernoulli schemes are particular cases of measure-preserving dynamical systems of great importance in ergodic theory. Thus, a Bernoulli scheme is also a quadruple $(X,\mathscr{A},\mu,T,)$, where X is now a *sample space* associated with the possible results arising in a probabilistic experiment, say 1,2,...,n, having respective probabilities $p_1,p_2,\ldots,p_n$ (we use the notation of Ref. 17):

$$X=\{1,2,\ldots,n\}^Z=\{x=(\cdots x_{-1},x_0,x_1,\ldots):x_i\in\{1,2,\ldots,n\},\quad \text{for all } i\in Z\}. \tag{1}$$

The σ-algebra $\mathscr{A}$ on X and the measure μ are the standard ones for this kind of probabilistic experiment. Thus, $\mu=(p_1,p_2,\ldots,p_n)^Z$, assuming that the individual experiments are independent. Finally, the measure-preserving transformation T is the *shift* on X defined $Tx=x'$, where $x_i'=x_{i+1}$. As usual we denote the above Bernoulli scheme by $BS(p)$.

To finish with this brief review let us recall the concept of isomorphism between two dynamical system $S=(X,\mathscr{A},\mu,T)$ and $S'=(X',\mathscr{A}',\mu',T')$. S and S' are isomorphic if there exists a measurable mapping $f:X\to X'$, which is a bijection such that *(i) for any* $A'\in\mathscr{A}'$, $\mu(f^{-1}A')=\mu'(A')$ and *(ii) for all* x, $f(Tx)=T'(fx)$.

III. GENERALIZED ENTROPY

The Kolmogorov–Shannon entropy is constructed considering that, within Shannon's information theory, the amount of information we have if we know that a point $x\in X$ belongs to some fixed set of a partition $C=\{C_1,C_2,\ldots,C_m\}$ of X is

$$H_1(C)=-\sum_{i=1}^{m}\mu(C_i)\log\,\mu(C_i). \tag{2}$$

A generalization of this magnitude has been given, among others, by Tsallis.[8] In our context it reads as

$$H_q(C)=(q-1)^{-1}\left(1-\sum_{i=1}^{m}[\mu(C_i)]^q\right), \tag{3}$$

where q is any real number. We observe that for $q\to 1$, Shannon's expression (2) is recovered. Equation (3) enables us to give a generalized formulation of information theory in such a way that the relevant relationships of Shannon's information theory are preserved.[18]

To define our generalized entropy we follow Ref. 17. We firstly consider a finite partition $B=\{B_1,B_2,\ldots,B_k\}$ of the sample space, i.e., $\cup_{i=1}^{k}B_i=X$; $B_i\cap B_j=\phi\,\forall\, i\neq j$. Then we take n points on the orbit of X: $x,Tx,T^2x,\ldots,T^{n-1}x$. B being a partition, for each of these points there exists only one set B_i to which it belongs. We associate to each x a string $l=(l_0,l_1,\ldots,l_{n-1})$, called the name of x, where $T^ix\in B_{l_i}$. From B we construct a new partition $B^n=\{B^n(l)\colon l$ is any name of length $n\}$, where $B^n(l)$ is the set of x with name l.

Thus, we define a generalized mean entropy (Kolmogorov–Tsallis entropy) of the measure-preserving transformation T by

$$h_q(T)=(q-1)^{-1}[1-\exp(\tilde{h}_q(T))], \tag{4}$$

where

$$\widetilde{h}_q(T)=\sup_B \widetilde{h}_q(B,T) \tag{5}$$

and

$$\widetilde{h}_q(B,T)=\overline{\lim_{n\to\infty}}\frac{1}{n}\{\log[1+(1-q)H_q(B^n)]\}. \tag{6}$$

In particular, for a Bernoulli scheme $BS(p)$, we have $\mu(B^n(l)) = p_{l_0}p_{l_1}\cdots p_{l_{n-1}}$ for each name l of length n. Therefore, using for the partition B^n the generator $B_i = \{x: x_0=i\}$, $1\leqslant i\leqslant k$ we obtain

$$[\widetilde{h}_q(T)]_{BS(p)}=\log\sum_{i=1}^{n} p_i^q, \tag{7}$$

which yields Tsallis' entropy for arbitrary q,

$$[h_q(T)]_{BS(p)}=(q-1)^{-1}\left[1-\sum_{i=1}^{n} p_i^q\right], \tag{8}$$

and Shannon's expression,

$$[h_1(T)]_{BS(p)}=-\sum_{i=1}^{n} p_i\log(p_i), \tag{9}$$

for $q\to 1$.

IV. ISOMORPHISM THEOREMS FOR THE GENERALIZED ENTROPY

Let us consider two isomorphic measure-preserving dynamical systems $S=(X,\mathscr{A},\mu,T)$, $S'=(X',\mathscr{A}',\mu',T')$ [with $0<\mu,\ \mu'\leqslant 1$ and $\mu(X)=\mu'(X')=1$] and an arbitrary partition of X of size n, say $B=\{B_1,B_2,\ldots,B_n\}$. Then, if f is a bijection between X and X', the set $C=\{C_1,C_2,\ldots,C_n\}$, where $C_i=f(B_i)$ for each $i=1,2,\ldots,n$, is a partition of X' also. Let $l=(l_0,l_1,\ldots,l_{n-1})$ and $l'=(l'_0,l'_1,\ldots,l'_{n-1})$ be the names of a given point $x\in X$ with relation to B and of $y=f(x)$ with relation to C, respectively.

Since S and S' are assumed to be isomorphic, thus $T^ix\in B_{l_i}\to fT^ix=(T')^ifx\in C_{l'_i}$. On the other hand, we also know that $fT^ix\in f(B_{l_i})=C_{l_i}$ because of the form in which the partition was constructed. Therefore $l'_i=l_i$ for all $i=0,1,\ldots,n-1$ and both names l and l' are the same one. Consequently, the quantities $H_q(B^n)=(q-1)^{-1}(1-\sum_l[\mu(B^n(l))]^q)$ and $H'_q(C^n)=(q-1)^{-1}(1-\sum_l[\mu'(C^n(l))]^q)$, and hence also $\widetilde{h}_q(B,T)$ and $\widetilde{h}'_q(C,T)$, are equal because, S and S' being isomorphic, we have $\mu'(C^n(l_i))=\mu'(fB^n(l_i))=\mu(f^{-1}fB^n(l_i))=\mu(B^n(l_i))$. Then, from Eq. (5), we get $\widetilde{h}_q(T)\geqslant\widetilde{h}_q(B,T)=\widetilde{h}'_q(C,T')$ and $\widetilde{h}'_q(T')\geqslant\widetilde{h}'_q(C,T)=\widetilde{h}_q(B,T)$, which implies $\widetilde{h}_q(T)\leqslant\widetilde{h}'_q(T')$ and $\widetilde{h}'_q(T')\leqslant\widetilde{h}_q(T)$ or $\widetilde{h}_q(T)=\widetilde{h}'_q(T')$. Consequently, $h_q(T)=\widetilde{h}'_q(T')$. In this way, we have demonstrated the following theorem.

Theorem 1: *If two measure-preserving dynamical systems are isomorphic then the associated generalized (Kolmogorov–Tsallis) entropies as defined by Eqs. (4)–(6) are equal.*

The complete isomorphism is proved just for Bernoulli schemes and reads as the following.

Theorem 2: *Two Bernoulli schemes with the same generalized (Kolmogorov–Tsallis) entropies as given by Eq. (8) are finitarily isomorphic.*

Remark: we recall that an isomorphism f between two Bernoulli schemes is *finitary* if, given an element x of the sample space X [see Eq. (1)], there exist two integers $n_1\leqslant n_2$ such that for any

other $x' \in X$ that verifies $x'[n_1,n_2]=x[n_1,n_2]$, the zero coordinates $[f(x)]_0,[f(x')]_0$ and $[f^{-1}(x)]_0,[f^{-1}(x')]_0$ are, respectively, equal. Here we denote with $x[n_1,n_2]$ the word $x_{n_1}x_{n_a+1}\cdots x_{n_{2-1}}x_{n_2}$.

Proof: The demonstration is based on the following lemma, which was proved by Keane and Smorodinsky[6] in the case $q\to 1$.

Lemma: given two Bernoulli schemes $BS(p)$ and $BS(p')$, where $p=(p_0,p_1\cdots p_{a-1})$ and $p' = (p'_0,p'_1\cdots p'_{b-1})$ (with $a\geqslant 3$; $b\geqslant 3$) for which $[h_q(T)]_{BS(p)}=[h_q(T)]_{BS(p')}$, we can find a third probability vector $r=(r_0,r_1,\ldots,r_{c-1})$ with the same entropy and $r_0=p_i$ and $r_1 = p'_j$ for some i,j.

To prove it we take into account that, without loss of generality, we can assume that the vectors are ordered $p_0\geqslant p_{1\geqslant}\cdots\geqslant p_{a-1}$ and $p'_0\geqslant p'_{1\geqslant}\cdots\geqslant p'_{b-1}$ with $p_{a-1}\geqslant p'_{b-1}$. Let us consider an auxiliary triple $r' = (p_0,p'_{b-1},1-(p_0+p'_{b-1}))$ whose generalized entropy is $[h_q(T)]_{BS(r')}$. It can be shown that Tsallis entropy, Eq. (8) is a strictly decreasing function of q and that $[h_q(T)]_{BS(r')}\leqslant[h_q(T)]_{BS(p)}=[h_q(T)]_{BS(p')}$ for any q. So we can increase the entropy until we reach the entropy $[h_q(T)]_{BS(r)}=[h_q(T)]_{BS(p)}$ by successively splitting the auxiliary vector: $r'\to r''=(p_0,p'_{b-1},r_3,1-(p_0+p'_{b-1}+r_3))\to\cdots\to r$.

Remark: For $a=2$ (or $b=2$) it is still possible[6] to prove the lemma by a convenient election of the components of the vector r.

The previous lemma put us in the conditions for constructing a finitary isomorphism between the two Bernoulli schemes following the coding technic of Keane and Smorodinsky.[6] This observation proves Theorem 2.

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R-matrix theory, formal Casimirs and the periodic Toda lattice

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The nonunitary r-matrix theory and the associated bi- and triHamiltonian schemes are considered. The language of Poisson pencils and of their formal Casimirs is applied in this framework to characterize the biHamiltonian chains of integrals of motion, pointing out the role of the Schur polynomials in these constructions. This formalism is subsequently applied to the periodic Toda lattice. Some different algebraic settings and Lax formulations proposed in the literature for this system are analyzed in detail, and their full equivalence is exploited. In particular, the equivalence between the loop algebra approach and the method of differential-difference operators is illustrated; moreover, two alternative Lax formulations are considered, and appropriate reduction algorithms are found in both cases, allowing us to derive the multiHamiltonian formalism from r-matrix theory. The systems of integrals for the periodic Toda lattice known after Flaschka and Hénon, and their functional relations, are recovered through systematic application of the previously outlined schemes.
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I. INTRODUCTION

The multiHamiltonian formalism is a known geometrical tool in the theory of the integrable Hamiltonian systems; this scheme can be formulated in an elegant way using the theory of the so-called pencils of Poisson structures and of their formal Casimirs.[1] A celebrated scheme to generate a biHamiltonian structure on (the dual of) an associative algebra is provided by r-matrix theory.[2–4] Recently, the theory was extended, independently, by Oevel and Ragnisco[5] and Li and Parmentier[6] to the so-called nonunitary case, in which the r-matrix is not skew-symmetric. In the best known applications, the r-matrix is induced by a splitting of the algebra into the direct sum of two Lie subalgebras; in this case, the construction of the first Poisson structure is closely related to the earlier Adler–Kostant–Symes (AKS) scheme.[7–9]

A typical application of the nonunitary r-matrix scheme is the finite Toda lattice with fixed ends. This system is discussed in both Refs. 5 and 6; for a recent review of the fixed ends Toda-type lattices, see Ref. 10. The infinite Toda chain (and some generalizations of it) was also treated within the nonunitary scheme, see Ref. 11. Less material seems to be available on the multiHamiltonian formalism for the periodic case.

The aim of this article is to discuss some topics in the above mentioned areas, deserving in our opinion a further analysis or illustration. We are interested in the following items:

(i) to get a deeper insight into the functional relations between the Casimirs of a Poisson pencil (i.e., between the chains of integrals in involution) at three different levels: the general

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biHamiltonian framework, the *r*-matrix scheme and the specific case of the periodic Toda lattice;

(ii) to point out the connections between the different algebraic environments proposed in the literature for the periodic Toda lattice; we refer to the loop algebra setting of Adler–van Moerbeke[12] and the differential-difference calculus of Kupershmidt;[13]

(iii) to compare two different Lax formulations proposed for the periodic lattice;

(iv) to discuss the multiHamiltonian structure as a reduction of the *r*-matrix scheme, for both the Lax formulations in item (iii).

Concerning item (i), we will point out that, for any Poisson pencil, the functional relations between different Casimirs are strictly related to the theory of Schur polynomials, or some natural generalization of it.[14] In the application we will propose to the *r*-matrix framework, the representation of the Casimirs as formal power series is particularly elegant; we think that the formal traces and the formal determinants introduced for this purpose deserve some interest by themselves.

In order to introduce items (ii) and (iii), we start from the evolution equations of the periodic Toda lattice. Using the Flaschka variables, we can describe the phase space of the lattice with n particles as a set of pairs $x=(a,b)$, where $a=(a_\alpha)$ and $b=(b_\alpha)$ are real periodic sequences of period n; the equations of motion are

$$\dot{a}=2ab-2ab_{[1]}, \quad \dot{b}=4a_{[-1]}^2-4a^2, \tag{1.1}$$

where $a_{[-1]}$ denotes the sequence $(a_{\alpha-1})$, and $b_{[1]}$ the sequence $(b_{\alpha+1})$.

To set up the Lax formulation, one must first of all choose the algebra in which the Lax operator lives. The framework of loop algebras was strongly supported by Adler and van Moerbeke;[12] these authors employ for Eq. (1.1) the Lax pair $dL/dt=[L,B_1]$, based on the $n\times n$ matrices

$$L(x):=\begin{pmatrix} b_1 & a_1 & 0 & .. & .. & 0 & \lambda^{-1}a_n \\ a_1 & b_2 & a_2 & 0 & .. & .. & 0 \\ 0 & a_2 & b_3 & a_3 & .. & .. & .. \\ .. & .. & .. & .. & .. & .. & .. \\ .. & .. & .. & .. & .. & a_{n-2} & 0 \\ 0 & .. & .. & 0 & a_{n-2} & b_{n-1} & a_{n-1} \\ \lambda a_n & 0 & .. & .. & 0 & a_{n-1} & b_n \end{pmatrix},$$

$$B_1(x):=2\begin{pmatrix} 0 & a_1 & 0 & .. & .. & .. & -\lambda^{-1}a_n \\ -a_1 & 0 & a_2 & 0 & .. & .. & 0 \\ 0 & -a_2 & 0 & .. & .. & .. & .. \\ .. & 0 & .. & .. & .. & 0 & .. \\ .. & .. & .. & .. & 0 & a_{n-2} & 0 \\ 0 & .. & .. & 0 & -a_{n-2} & 0 & a_{n-1} \\ \lambda a_n & .. & .. & .. & 0 & -a_{n-1} & 0 \end{pmatrix}. \tag{1.2}$$

Here, λ is a free parameter, and the Lax equation for the matrices in Eq. (1.2) is satisfied identically in λ. Both $L(x)$ and $B_1(x)$ are regarded in Ref. 12 as elements of the loop algebra $gl(n)(\lambda,\lambda^{-1}]$, made of formal Laurent series in λ and λ^{-1} with coefficients in the algebra $gl(n,\mathbb{R})$ of real $n\times n$ matrices.

Using the loop algebra, one can produce other Lax representations for the periodic Toda lattice, which are alternative to the scheme (1.2). In order to illustrate one of them, we remark that the evolution equations (1.1) are equivalent (up to rescaling by a common factor $\frac{1}{2}$) to

$$\dot{c}=2cb-2cb_{[1]}, \quad \dot{b}=2c_{[-1]}-2c, \tag{1.3}$$

if one stipulates that $c=a^2$. Equation (1.3) admits the Lax formulation $dV/dt=[V,C_1]$, where, at each point $y=(c,b)$,

$$V(y):=\begin{pmatrix} b_1 & 1 & 0 & .. & .. & 0 & \lambda^{-1}c_n \\ c_1 & b_2 & 1 & 0 & .. & .. & 0 \\ 0 & c_2 & b_3 & 1 & .. & .. & .. \\ .. & .. & .. & .. & .. & .. & .. \\ .. & .. & .. & .. & .. & 1 & 0 \\ 0 & .. & .. & 0 & c_{n-2} & b_{n-1} & 1 \\ \lambda & 0 & .. & .. & 0 & c_{n-1} & b_n \end{pmatrix},$$

$$C_1(y):=2\begin{pmatrix} b_1 & 1 & 0 & .. & .. & .. & 0 \\ 0 & b_2 & 1 & 0 & .. & .. & .. \\ 0 & 0 & b_3 & 1 & .. & .. & .. \\ .. & .. & .. & .. & .. & .. & .. \\ .. & .. & .. & .. & b_{n-2} & 1 & 0 \\ 0 & .. & .. & 0 & 0 & b_{n-1} & 1 \\ \lambda & .. & .. & .. & 0 & 0 & b_n \end{pmatrix}. \tag{1.4}$$

This generalizes to the periodic case a Lax scheme well known for the fixed ends lattice.[10,15]

The formulations (1.2) and (1.4) have counterparts in the environment of differential-difference calculus of Kupershmidt.[13] In the quoted reference, Kupershmidt defines a discrete analogue of the algebra of formal pseudo-differential operators, where the derivation ∂ is replaced by a shift operator Δ; the formalism can be applied, in particular, to the periodic lattices. Here, we will employ the term Kupershmidt algebra and the symbol $\mathbb{R}_n(\Delta,\Delta^{-1}]$ to denote a suitably defined algebra of (formal) differential-shift operators, obtained essentially by realizing the abstract scheme of Ref. 13 in the periodic case; we will make clear that $\mathbb{R}_n(\Delta,\Delta^{-1}]$ is algebraically isomorphic to the loop algebra $gl(n)(\lambda,\lambda^{-1}]$ of Ref. 12. Using this isomorphism, one easily constructs the equivalent of the Lax scheme (1.2); the matrices appearing in these equations correspond to the operators

$$L(x):=a\Delta+b+a_{[-1]}\Delta^{-1}, \quad B_1(x):=2a\Delta-2a_{[-1]}\Delta^{-1}. \tag{1.5}$$

More generally, one can write the Lax pairs $dL/dt_k=[L,B_k]$ ($k=1,2,3,...$) for the full hyerarchy of commuting Toda flows, recovering Eq. (1.1) for $k=1$; the operators $B_k(x)$ are constructed by translating to $\mathbb{R}_n(\Delta,\Delta^{-1}]$ the homologous prescriptions of Ref. 12 for the loop algebra setting.

The differential-difference equivalent of the Lax scheme (1.4) rests on the operators

$$V(y):=\Delta+b+c_{[-1]}\Delta^{-1}, \quad C_1(y):=2(\Delta+b), \tag{1.6}$$

which are just the Lax pair of Ref. 13 for the Toda lattice. More generally, a full hierarchy of commuting vector fields is generated in this reference prescribing the Lax equations $dV/dt_k=[V,C_k]$ ($k=1,2,3,...$), with a suitable rule to define the companion operators $C_k(y)$; the flow (1.3) is recovered for $k=1$.

Let us come to item (iv), i.e., to the triHamiltonian formulation of the periodic Toda system. As a matter of fact, the Poisson tensors of the fixed end case can be adjusted a posteriori so as to

fit the periodicity condition;[16] however, the interest in the periodic problem is not just in the final expression for the Poisson structures, but in their systematic derivation by means of appropriate reduction methods.

A construction of the first Poisson structure, based on the AKS scheme, can be found in Ref. 12. A derivation of the second Poisson tensor in the framework of loop algebras has been recently proposed in Ref. 17, but the Lax matrices employed therein are different from both $L(x)$ in Eq. (1.2) and $V(y)$ in Eq. (1.4), and require a generalization of the standard r-matrix scheme of Refs. 5 and 6. On the contrary, we show in this article that the first, the second and even the third Poisson tensors of the periodic Toda lattice can be constructed, for both the Lax schemes (1.5) and (1.6), inside the standard r-matrix theory, using appropriate splittings.

From a technical viewpoint, in our analysis we draw some advantage using the formal differential-difference calculus of Ref. 13. However, the splitting we employ for the Lax scheme (1.5) is just the correspondent in $\mathbb{R}_n(\Delta,\Delta^{-1}]$ of the one proposed in Ref. 12 in connection with the AKS scheme. The alternative splitting required for the Lax scheme (1.6) is suggested by the prescription of Ref. 13 for the companion operators $C_k(y)$ associated to the full hierarchy. This splitting is the correspondent of the one employed in Ref. 11 for the infinite Toda chain; in the periodic case, the reduction of the r-matrix structures requires some supplementary caution, yielding to replace the usual restriction schemes with a slightly more involved restriction/projection algorithm. This refinement is necessary, in particular, for the third Poisson structure.

The article is organized as follows. Section II is devoted to bi- and triHamiltonian structures and their reduction techniques, to formal Casimirs and Schur polynomials. The nonunitary r-matrix theory is reviewed in Sec. III. The isomorphism between the loop algebra $gl(n)(\lambda,\lambda^{-1}]$ and the Kupershmidt algebra $\mathbb{R}_n(\Delta,\Delta^{-1}]$ is exploited in Sec. IV. The r-matrix triHamiltonian structure in $\mathbb{R}_n(\Delta,\Delta^{-1}]$ and its restriction for the Lax scheme (1.5) are presented in Sec. V. In Sec. VI, the Flaschka and Hénon integrals of the Toda lattice are interpreted in terms of the biHamiltonian recursion and the Schur polynomials. In Sec. VII we deal with the Lax scheme (1.6) and the associated r-matrix; the reduction of the triHamiltonian structure is performed, and the relations with the Lax scheme (1.5) are illustrated in terms of gauge equivalence (as in Ref. 15 for the nonperiodic case).

II. MULTIHAMILTONIAN STRUCTURES AND RECURSION SCHEMES

A. Hamiltonian and multiHamiltonian manifolds

A wide literature is available on this topic (see, for example, Refs. 18–26 and quotations therein). If $\mathscr{V}$ is a manifold and $v\in\mathscr{V}$, we denote by $T_v\mathscr{V}$ the tangent space and by $T_v^*\mathscr{V}$ the cotangent space at v; the latter generally means a vector space in separating duality with $T_v\mathscr{V}$ through some bilinear pairing (which is a standard procedure in this framework; see, e.g., Refs. 8 and 12). Tangent vectors and covectors will often be indicated, respectively, by $\dot{v}$ and δv, and the pairing by $\langle \delta v,\dot{v}\rangle$.

A (2,0) tensor on the manifold $\mathscr{V}$ is a map $v\mapsto Q_v$ where, for each $v\in\mathscr{V}$, Q_v is a linear operator from $T_v^*\mathscr{V}$ to $T_v\mathscr{V}$. A Poisson tensor means a skew-symmetric (2,0) tensor Q such that the bracket $\{f,l\}_Q:=\langle df,Qdl\rangle$ (f,l real functions on $\mathscr{V}$) satisfies the Jacobi identity. If Q is a Poisson tensor, for each function $h:\mathscr{V}\to\mathbb{R}$, the vector field $X:=Qdh$ is called the Hamiltonian vector field corresponding to h (and it is also said that h is a Hamiltonian function for X w.r.t. Q). A function h is said to be a Casimir of Q if $Qdh=0$. The manifold $\mathscr{V}$, equipped with a Poisson tensor Q, is called a Poisson, or Hamiltonian manifold.

Two Poisson tensors Q,P are said to be compatible in the sense of Magri[21] if, for each $\xi\in\mathbb{R}$, the linear combination $Q+\xi P$ is again a Poisson tensor; similarly, three Poisson tensors Q,P,S are compatible if $Q+\xi P+\eta S$ is Poisson for each $\xi,\eta\in\mathbb{R}$. The manifold $\mathscr{V}$, equipped with a pair (resp. a triple) of compatible Poisson tensors is said to be biHamiltonian (resp. triHamiltonian).

If h_k ($k=1,2,3,\ldots$) is a sequence of real functions on the biHamiltonian manifold $\mathscr{V}$, we say that the h_k's satisfy a biHamiltonian recursion scheme if

$$Pdh_k = Qdh_{k+1} \quad (k=1,2,3,\ldots); \tag{2.1}$$

if $\mathscr{V}$ carries a third compatible Poisson tensor, and it is also

$$Sdh_{k-1} = Pdh_k \quad (k=2,3,\ldots), \tag{2.2}$$

we say that there is a triHamiltonian recursion scheme. These relations imply that the functions h_k are mutually in involution w.r.t. the Poisson brackets corresponding to both Q and P (or Q, P, S). The Hamiltonian functions h_k and the vector fields X_k are said to form a biHamiltonian (or triHamiltonian) hierarchy.

B. BiHamiltonian recursion, formal power series and Schur polynomials

Let $\mathscr{U}$ be an arbitrary real associative algebra with unit. We consider the space $\mathscr{U}[z]$ of the formal power series $U=\Sigma_{k=0}^{\infty} U_k z^k$ in one indeterminate z with coefficients $U_k \in \mathscr{U}$ (when it is convenient, we also write $U(z)$ instead of U). $\mathscr{U}[z]$ is an associative algebra with the usual Cauchy product of series.

Let $\mathscr{U}_0[z]$ be the subalgebra of $\mathscr{U}[z]$ formed by the series U without zero order term: $U_0=0$. If $\mathbb{R}[w]$ is the commutative algebra of formal series $E(w)=\Sigma_{k=0}^{\infty} e_k w^k$, with real coefficients e_k, we can define a composition law $\mathbb{R}[w]\times\mathscr{U}_0[z]\to\mathscr{U}[z]$, $(E,U)\mapsto E(U)$, where

$$E(U) := \sum_{k=0}^{\infty} e_k U^k = e_0 + e_1(U_1 z + U_2 z^2 + \ldots) + e_2(U_1 z + U_2 z^2 + \ldots)^2 + \ldots . \tag{2.3}$$

Now, let $\mathscr{V}$ be a biHamiltonian manifold with the Poisson tensors Q, P; we apply the above notions to the commutative algebra $\mathscr{U}$ of the smooth real functions on $\mathscr{V}$. Assume we are given a sequence of functions h_k on $\mathscr{V}$, and define a formal power series $h := \Sigma_{k=1}^{\infty} h_k z^k$ in the indeterminate z. Consider the condition

$$(Q - zP)dh = 0; \tag{2.4}$$

this equation is satisfied (identically in z) iff the functions h_k obey to the recursion scheme (2.1) and h_1 is a Casimir of Q, i.e., $Qdh_1=0$. The condition (2.4) can be interpreted saying that h is a (formal) Casimir for the Poisson pencil $Q-zP$; so, the biHamiltonian hierarchies starting from a Casimir of Q correspond bijectively to the Casimirs of the Poisson pencil $Q-zP$.[1]

Proposition 2.1: Let h_k ($k=1,2,3,...$) be a biHamiltonian hierarchy starting from a Casimir of Q, so that $h := \Sigma_{k=1}^{\infty} h_k z^k$ is a Casimir of the Poisson pencil $Q-zP$. Consider a formal series $E(w)=\Sigma_{k=1}^{\infty} e_k w^k$ with real coefficients e_k, and put $f := E(h) = e_1(h_1 z + h_2 z^2 + \ldots) + e_2(h_1 z + h_2 z^2 + \ldots)^2 + \ldots$. Then f is also a Casimir of $Q-zP$; so, if we write $f=\Sigma_{k=1}^{\infty} f_k z^k$, the functions f_k form a biHamiltonian hierarchy starting from a Casimir f_1 of Q.

Proof: From the definition of f it follows that $df = E'(h)dh$, where $E'(w) := e_1 + 2e_2 w + \ldots$ is the term by term derivative of E. From here and Eq. (2.4) we immediately infer $(Q-zP)df=0$. ◇

It is interesting to give explicit formulas for the functions f_k of the above Proposition in terms of the h_k's and the coefficients e_k. For each real formal series $E(w) := \Sigma_{k=1}^{\infty} e_k w^k$, define a family of polynomials $S_k(t_1,t_2,t_3,\ldots)$ in infinitely many variables t_j ($j=1,2,3,...$) stipulating that

$$E\left(\sum_{k=1}^{\infty} t_k z^k\right) = \sum_{k=1}^{\infty} S_k(t_1,t_2,t_3,\ldots) z^k. \tag{2.5}$$

Using some standard combinatorics, it can be shown that, for each k,

$$S_k(t_1,t_2,t_3,\ldots)=\sum_{k_1+2k_2+3k_3+\ldots=k} e_{k_1+k_2+k_3+\ldots}\,\frac{(k_1+k_2+k_3+\ldots)!}{k_1!k_2!k_3!\ldots}\,t_1^{k_1}t_2^{k_2}t_3^{k_3}\ldots\,. \tag{2.6}$$

In the above sum $k_1,k_2,k_3,\ldots$ are positive integers; note that S_k depends only on the first k variables $t_1,\ldots,t_k$. We will say that the S_k's are the generalized Schur polynomials generated by the formal series E.

The functions in Prop. 2.1 are related by $f_k=S_k(h_1,h_2,h_3,\ldots)$. The fact that the f_k's are functions of the Hamiltonians $h_{k'}$ implies that they are in involution (and also commute with all the $h_{k'}$) w.r.t. any Poisson bracket in which the $h_{k'}$ are themselves in involution.

The relation between the functions f_k and $h_{k'}$ can be inverted if the first coefficient e_1 in the series E is nonzero. In this case, there is a unique formal series $E^{-1}(u)=\Sigma_{k=1}^{+\infty}\tilde{e}_k u^k$ such that $E^{-1}(E(w))=w$, and we can write $h=E^{-1}(f)$; this implies $h_k=S_k(f_1,f_2,f_3,\ldots)$, where the S_k are the generalized Schur polynomials generated by E^{-1}. In Sec. III and VI, we will be interested in particular in the choice $E(w)=1-e^{-w}$, giving $e_k=(-1)^{k+1}/k!$ and

$$S_k(t_1,t_2,t_3,\ldots)=\sum_{k_1+2k_2+3k_3+\ldots.=k} \frac{(-1)^{1+k_1+k_2+k_3+\ldots.}}{k_1!k_2!k_3!\ldots}\,t_1^{k_1}t_2^{k_2}t_3^{k_3}\ldots\,. \tag{2.7}$$

Up to trivial sign changes, the S_k are the ordinary Schur polynomials.[27] The inverse of E is the formal series $E^{-1}(u)=-\ln(1-u)$, with coefficients $\tilde{e}_k=1/k$, which generates the polynomials

$$\tilde{S}_k(t_1,t_2,t_3,\ldots)=\sum_{k_1+2k_2+3k_3+\ldots=k} \frac{(k_1+k_2+k_3+\ldots-1)!}{k_1!k_2!k_3!\ldots}\,t_1^{k_1}t_2^{k_2}t_3^{k_3}\ldots\,. \tag{2.8}$$

With this choice of E, the first functions in the biHamiltonian chains of Prop. 2.1 are related by

$$\begin{gathered} f_1=h_1,\quad f_2=-\tfrac{1}{2}h_1^2+h_2,\quad f_3=\tfrac{1}{6}h_1^3-h_1h_2+h_3,\\ f_4=-\tfrac{1}{24}h_1^4-\tfrac{1}{2}h_2^2+\tfrac{1}{2}h_2h_1^2-h_1h_3+h_4,\ldots\,. \end{gathered} \tag{2.9}$$

C. Reduction schemes for Poisson structures

The schemes presented in Ref. 23 are sufficient for our purposes; for a more general formulation, see Ref. 24. Let $(\mathscr{V},Q)$ be a Poisson manifold, and $j:\mathscr{M}\to\mathscr{V}$ an embedding of another manifold $\mathscr{M}$ into $\mathscr{V}$ (i.e., a map such that $j(\mathscr{M})$ is a submanifold of $\mathscr{V}$ and j is a diffeomorphism between $\mathscr{M}$ and its image); in practical applications, $\mathscr{M}$ plays the role of a ''coordinate space'' for the submanifold $j(\mathscr{M})$. For $m\in\mathscr{M}$ and $v=j(m)$, we denote by $T_mj:T_m\mathscr{M}\to T_v\mathscr{V}$ the tangent map; its image $\mathrm{Im}T_mj\subset T_v\mathscr{V}$ is the tangent space at v of the submanifold $j(\mathscr{M})$.

Proposition 2.2: Assume that, for each $m\in\mathscr{M}$ and $v=j(m)$, it is $\mathrm{Im}Q_v\subset\mathrm{Im}T_mj$. Let $\delta v\in T_v^*\mathscr{V}$ be any covector extending a given covector $\delta m\in T_m^*\mathscr{M}$, i.e., such that

$$\langle\delta v,(T_mj)\dot{m}\rangle=\langle\delta m,\dot{m}\rangle \tag{2.10}$$

for each $\dot{m}\in T_m\mathscr{M}$; then the tangent vector $Q_v\delta v\in\mathrm{Im}T_mj$ is fully determined by δm and does not depend on the chosen extension δv. The (2,0) tensor on $\mathscr{M}$, denoted again by Q and defined by

$$Q_m\delta m:=(T_mj)^{-1}Q_v\delta v, \tag{2.11}$$

is a Poisson tensor. ◇

Another restriction scheme can be obtained by weakening the assumptions of Prop. 2.2, as explained hereafter.

Proposition 2.3: Assume that, for each $m \in \mathscr{M}$ and $\delta m \in T^*_m \mathscr{M}$, the following conditions are satisfied at the point $v = j(m)$:

(a) there is at least one covector $\delta v \in T^*_v \mathscr{V}$ extending δm in the sense of Eq. (2.10), and such that $Q_v \delta v \in \mathrm{Im} T_m j$;

(b) for δv as in (a), $Q_v \delta v$ is fully determined by δm (i.e., we have $Q_v \delta v' = Q_v \delta v$ for any other covector $\delta v'$ as in (a)).

Then a Poisson tensor is induced on $\mathscr{M}$. This tensor, denoted again by Q, is defined as in Eq. (2.11), with δv as in item (a). ◇

Definition 2.4: If the conditions of Prop. 2.2 are satisfied, we say that Q can be properly restricted from $\mathscr{V}$ to $\mathscr{M}$ along j. Under the conditions of Prop. 2.3, we say that it can be *Dirac restricted* along j. In both cases, the Poisson tensor induced on $\mathscr{M}$ is called the restriction of Q. ◇

In the case of bi- or triHamiltonian manifolds, the compatibility of the Poisson structures is preserved by both types of restriction. The restriction operation can also be applied to Hamiltonian functions and vector fields [a vector field X on $\mathscr{V}$ is restrictable to $\mathscr{M}$ along j if it is tangent to the submanifold $j(\mathscr{M})$].

We now discuss the projection of the Poisson structures.

Let $(\mathscr{V}, Q)$ be a Poisson manifold, and $\pi: \mathscr{V} \to \mathscr{W}$ a projection of the manifold $\mathscr{V}$ onto another manifold $\mathscr{W}$. For $v \in \mathscr{V}$ and $w = \pi(v)$, we consider the tangent map $T_v \pi: T_v \mathscr{V} \to T_w \mathscr{W}$ and its adjoint $T^*_v \pi: T^*_w \mathscr{W} \to T^*_v \mathscr{V}$.

Proposition 2.5: For each $w \in \mathscr{W}$ and $v \in \mathscr{V}$ such that $\pi(v) = w$, let us consider the map $T_v \pi \circ Q_v \circ T^*_v \pi: T^*_w \mathscr{W} \to T_w \mathscr{W}$. Assume that this map be completely determined by w, i.e., that it does not change if v is replaced by another point $v' \in \pi^{-1}(w)$. Then the (2,0) tensor on $\mathscr{W}$, denoted with $\tilde{Q}$ and defined by

$$\tilde{Q}_w \delta w := (T_v \pi \circ Q_v \circ T^*_v \pi)(\delta w), \tag{2.12}$$

is a Poisson tensor. ◇

Definition 2.6: We say that the Poisson tensor $\tilde{Q}$ is the projection of Q and $\mathscr{V}$ onto $\mathscr{W}$ along π. ◇

The projection operation preserves the compatibility of Poisson tensors. A function $h: \mathscr{V} \to \mathbb{R}$ is said to be projectable onto W if $h(v) = h(v')$ for each pair v, v' such that $\pi(v) = \pi(v')$; in this case, h induces in an obvious way a real function $\tilde{h}$ on $\mathscr{W}$, called the projection of h. A vector field X on $\mathscr{V}$ is said to be projectable if, for w in $\mathscr{W}$ and $v \in \pi^{-1}(w)$, the vector $(T_v \pi) X(v) \in T_w \mathscr{W}$ depends only on w; in this case, the vector field $\tilde{X}$ induced in the obvious way on $\mathscr{W}$ is called the projection of X.

III. *R*-MATRIX THEORY: A REVIEW

A. The nonunitary case (Refs. 5,6)

Let $\mathfrak{g}$ be a real associative algebra with unit 1 and typical elements $V, W, Z, \ldots$; then $\mathfrak{g}$ is a Lie algebra w.r.t. the commutator $[V, W] := VW - WV$.

Definition 3.1: An r-matrix on $\mathfrak{g}$ is a linear operator $R: \mathfrak{g} \to \mathfrak{g}$ satisfying the modified Yang-Baxter equation

$$[RV, RW] - R[V, RW] - R[RV, W] + [V, W] = 0. \tag{3.1}$$

◇

Here and in the sequel, we assume that $\mathfrak{g}$ carries a traceform, i.e., a linear functional $\mathrm{Tr}: \mathfrak{g} \to \mathbb{R}$ such that the bilinear form $\langle , \rangle: \mathfrak{g} \times \mathfrak{g} \to \mathbb{R}$, $\langle V, W \rangle := \mathrm{Tr}(VW)$ is symmetric and nondegenerate; the pairing $\langle , \rangle$ will be employed to identify $\mathfrak{g}$ with its dual space $\mathfrak{g}^*$ (in the infinite-dimensional case, the

statement $\mathfrak{g}\approx\mathfrak{g}^*$ can be viewed as the definition of $\mathfrak{g}^*$, see Ref. 2). From a geometrical viewpoint, we can regard $\mathfrak{g}$ as a manifold, with $T_V\mathfrak{g}\approx\mathfrak{g}$ and $T_V^*\mathfrak{g}\approx\mathfrak{g}$ at each point V (so, a typical element of $\mathfrak{g}$ is written as δV when it is viewed as a covector).

Let $R:\mathfrak{g}\to\mathfrak{g}$ be a linear operator with adjoint $R^*:\mathfrak{g}\to\mathfrak{g}$ (satisfying the condition $\langle R^*V,W\rangle=\langle V,RW\rangle$).

Definition 3.2: Q, P and S denote, respectively, the (2,0) tensors on the manifold $\mathfrak{g}$ defined at each point V setting Q_V, P_V, $S_V:T_V^*\mathfrak{g}\approx\mathfrak{g}\to T_V\mathfrak{g}\approx\mathfrak{g}$,

$$Q_V\delta V:=[V,R\delta V]+R^*[V,\delta V], \tag{3.2}$$

$$P_V\delta V:=[V,R(V.\delta V)]+V.R^*[V,\delta V], \tag{3.3}$$

$$S_V\delta V:=\tfrac{1}{2}[V,R(V\delta VV)]+\tfrac{1}{2}V(R^*[V,\delta V])V. \tag{3.4}$$

In Eq. (3.3), . denotes the symmetrized product, so $V.\delta V=1/2(V\delta V+\delta VV)$.

We will say that Q, P and S are, respectively, the linear, quadratic and cubic tensor induced by R (this is motivated by their dependence on the footpoint V). ◇

Proposition 3.3:[5,6] If R and its skew-symmetric part $1/2(R-R^*)$ are r-matrices, Q, P and S are compatible Poisson tensors. The functions $h_k:\mathfrak{g}\to\mathbb{R}$, $h_k(V):=1/k\mathrm{Tr}V^k$ ($k=1,2,3,....$) satisfy the triHamiltonian recursion schemes (2.1)–(2.2); the vector fields $X_k:=Pdh_k$ are given explicitly by $X_k(V)=[V,R(V^k)]$. Finally, the function h_1 is a Casimir of Q if $[V,R(1)]=0$ for each $V\in\mathfrak{g}$. ◇

B. The split case of *r*-matrix theory

Given an associative algebra $\mathfrak{g}$ with unit, assume that there is a vector space decomposition $\mathfrak{g}=\mathfrak{g}_+\oplus\mathfrak{g}_-$. If $\mathfrak{g}$ is equipped with a traceform, we can define the annihilators

$$\mathfrak{g}^\pm:=(\mathfrak{g}_\pm)^\perp=\{W\in\mathfrak{g}\,|\,\langle W,V\rangle=0\quad\text{for each}\quad V\in\mathfrak{g}_\pm\}. \tag{3.5}$$

Due to the symmetry and nondegeneracy of $\langle,\rangle$ one easily infers that $\mathfrak{g}=\mathfrak{g}^+\oplus\mathfrak{g}^-$, and that the dual of $\mathfrak{g}^\mp$ can be identified with $\mathfrak{g}_\pm:(\mathfrak{g}^\mp)^*\approx\mathfrak{g}_\pm$. For each $V\in\mathfrak{g}$, we denote with $V_\pm$ and $V^\pm$ its components according to the previous direct sum decompositions of $\mathfrak{g}$. Let $\Pi_\pm,\Pi^\mp:\mathfrak{g}\to\mathfrak{g}$ be the projections corresponding to these decompositions. Then $\Pi^\mp$ is the adjoint of $\Pi_\pm$, and $R:=\Pi_+-\Pi_-$ has adjoint $R^*=\Pi^--\Pi^+$.

It is known that, if $\mathfrak{g}_\pm$ are Lie subalgebras of $\mathfrak{g}$, R is an r-matrix. Assume that $1/2(R-R^*)$ is also an r-matrix and consider the triHamiltonian structure of Def. 3.2. Explicitating R and R^* in Eqs. (3.2)–(3.4) one finds[5] that each of the tensors Q, P and S can be written as follows, in two equivalent ways:

$$Q_V\delta V=2[V,(\delta V)_+]-2[V,\delta V]^+=-2[V,(\delta V)_-]+2[V,\delta V]^-, \tag{3.6}$$

$$P_V\delta V=2[V,(V.\delta V)_+]-2V.[V,\delta V]^+=-2[V,(V.\delta V)_-]+2V.[V,\delta V]^-, \tag{3.7}$$

$$S_V\delta V=[V,(V\delta VV)_+]-V[V,\delta V]^+V=-[V,(V\delta VV)_-]+V[V,\delta V]^-V. \tag{3.8}$$

The vector fields $X_k:=Pdh_k$ of Prop. 3.3 are given in this case by

$$X_k=2[V,(V^k)_+]=-2[V,(V^k)_-]. \tag{3.9}$$

In many applications, but not in the one considered in this article, the splitting is such that $\mathfrak{g}^\pm=\mathfrak{g}_\pm$, implying $R^*=-R$: this is the so-called unitary case.

C. Split case: The reduction to $\mathfrak{g}^+$

Let the assumptions of Prop. 3.3 be satisfied, and consider the triHamiltonian structure (3.6) –(3.8) on $\mathfrak{g}$. Let us regard $\mathfrak{g}^+$ as a manifold: at each point $L \in \mathfrak{g}^+$, $T_L\mathfrak{g}^+ \approx \mathfrak{g}^+$ and $T_L^*\mathfrak{g}^+ \approx \mathfrak{g}_-$. We consider the embedding $j: \mathfrak{g}^+ \to \mathfrak{g}$ given by the identity map, and apply Prop. 2.2.

Proposition 3.4 (Ref. 5): The Poisson tensor Q of Eq. (3.6) can be (properly) restricted to $\mathfrak{g}^+$; at any point $L \in \mathfrak{g}^+$ the restricted tensor, denoted again with Q, is given by

$$Q_L \delta L = -2[L, \delta L]^+ \tag{3.10}$$

for each $\delta L \in \mathfrak{g}_-$. The tensor P of Eq. (3.7) can be (properly) restricted to $\mathfrak{g}^+$ if this subspace is closed in the symmetrized product, i.e., $L.L' \in \mathfrak{g}^+$ for each $L, L' \in \mathfrak{g}^+$; the restricted Poisson tensor is given by

$$P_L \delta L = 2[L, (L.\delta L)_+] - 2L.[L, \delta L]^+. \tag{3.11}$$

Finally, the tensor S of Eq. (3.8) can be (properly) restricted to $\mathfrak{g}^+$ if $LL'L \in \mathfrak{g}^+$ for each, $L, L' \in \mathfrak{g}^+$, and the restricted Poisson tensor is given by

$$S_L \delta L = [L, (L\,\delta L L)_+] - L[L, \delta L]^+ L. \tag{3.12}$$

Each of the two summands in Eq. (3.11), as well as in Eq. (3.12), belongs to $\mathfrak{g}^+$. ◇

Under the assumptions of the previous Proposition, the recursion scheme (2.1),(2.2) is again satisfied on $\mathfrak{g}^+$ by the restrictions of the functions h_k; the vector fields X_k in Eq. (3.9) are tangent to this submanifold.

D. Formal Casimirs and other biHamiltonian hierarchies

Let $\mathfrak{g}$ be an algebra equipped with an abstract r-matrix, as in Sec. III A. We consider the associative algebra $\mathfrak{g}[z]$ of formal series $W = \Sigma_{k=0}^{\infty} W_k z^k$, with coefficients $W_k \in \mathfrak{g}$; let $\mathfrak{g}_0[z]$ consist of the series with $W_0 = 0$. Using the real formal series $\ln(1+w) := \Sigma_{k=1}^{\infty} (-1)^{k+1} (1/k) w^k \in \mathbb{R}[w]$, for each $W \in \mathfrak{g}_0[z]$ we define the element

$$\ln(1+W) := \sum_{k=1}^{\infty} (-1)^{k+1} \frac{1}{k} (W_1 z + W_2 z^2 + \ldots)^k \in \mathfrak{g}_0[z]. \tag{3.13}$$

Equivalently, we can consider the series $U = 1 + W$ and define $\ln U$ for each $U = \Sigma_{k=0}^{\infty} U_k z^k \in \mathfrak{g}[z]$ $U_0 = 1$.

If $W = \Sigma_{k=1}^{\infty} W_k z^k$, the exponential $e^W := 1 + \Sigma_{k=1}^{\infty} (1/k!) W^k$ is also well defined, and we have $\ln(e^W) = W$ in the sense of formal series composition. Similarly, for $U = 1 + \Sigma_{k=1}^{\infty} (1/k!) U^k z^k$ we have $e^{\ln U} = U$.

We observe that the traceform $\mathrm{Tr}: \mathfrak{g} \to \mathbb{R}$ induces a linear function $\mathrm{Tr}: \mathfrak{g}[z] \to \mathbb{R}[z]$, $\mathrm{Tr}W := \Sigma_{k=0}^{\infty} (\mathrm{Tr} W_k) z^k$. Also, if $U \in \mathfrak{g}[z]$ and $U_0 = 1$, we put $\mathrm{Det}\, U := e^{\mathrm{Trln} U}$ (here, we have a composition of the real formal series $\mathrm{Trln}\, U$ and $e^w := \Sigma_{k=0}^{\infty} (1/k!) w^k$). It is not difficult to check that $\mathrm{Trln} U = \ln \mathrm{Det}\, U$.

We now refer to the r-matrix Poisson tensors Q, P of $\mathfrak{g}$ and consider the hierarchy of Hamiltonian functions $h_k: \mathfrak{g} \to \mathbb{R}$, $h_k(V) = 1/k \mathrm{Tr} V^k$ $(k = 1,2,3,\ldots)$. We recall that h_1 is a Casimir of Q if $R(1)$ is in the center of $\mathfrak{g}$; we will assume this condition to be satisfied. On the grounds of Sec. II B, the formal series $h := \Sigma_{k=1}^{\infty} h_k z^k$ is a Casimir of the Poisson pencil $Q - zP$. From here one can generate by composition other Casimirs; in particular, composing with the series $1 - e^{-w}$ one gets the formal Casimir

$$f := 1 - e^{-h} = \sum_{k=1}^{\infty} f_k z^k. \tag{3.14}$$

The functions f_k, which can be expressed as Schur polynomials in the h_k's (see Sec. II B.), also satisfy a biHamiltonian recursion scheme w.r.t. Q and P. It is straightforward to check the following.

Proposition 3.5: At each point $V \in \mathfrak{g}$, we have

$$h(V) = -\operatorname{Tr} \ln(1 - zV) = -\ln \operatorname{Det}(1 - zV), \quad f(V) = 1 - \operatorname{Det}(1 - zV). \tag{3.15}$$

◇

Using the Hamiltonians f_k ($k = 1,2,3,...$), we can define a sequence of commuting vector fields $Y_k := P df_k = Q df_{k+1}$. Since $f_1 = h_1$, we infer that $Y_1 = X_1$ is as in Prop. 3.3. The Hamiltonians f_k and $h_{k'}$ are in mutual involution w.r.t. the Q, P (and S) Poisson brackets for each k and k'.

Definition 3.6: The formal Casimirs h and f are called, respectively, the Flaschka Casimir and the Hénon Casimir; similarly, the functions h_k and f_k are referred to as the Flaschka and Hénon integrals. ◇

We use the above names for a historical reason; the integrals of motion of the periodic Toda lattice first constructed by these authors in Refs. 28 and 29 arise by simply specializing the above formalism to a particular algebra $\mathfrak{g}$, that will be described in the next section.

IV. THE ALGEBRAIC FRAMEWORK FOR THE PERIODIC TODA LATTICE

A. The Kupershmidt algebra $\mathbb{R}_n(\Delta,\Delta^{-1}]$

Throughout the rest of the article, n is a fixed positive integer.

Definition 4.1: Let $v = (v_\alpha)_{\alpha \in \mathbb{Z}}$ be a real sequence. For each $\nu \in \mathbb{Z}$, the ν-shift of v is the sequence $v_{[\nu]} := (v_{\alpha+\nu})_{\alpha \in \mathbb{Z}}$. It is said that v is n-periodic if $v_{[n]} = v$; $\mathbb{R}_n$ denotes the (n-dimensional) vector space of these sequences. For each $v \in \mathbb{R}_n$, we put $\Sigma_0 v := \Sigma_{j=1}^n v_j$, $\langle v \rangle := 1/n \Sigma_0 v$. ◇

Definition 4.2: The Kupershmidt algebra $\mathbb{R}_n(\Delta,\Delta^{-1}]$ consists of the formal Laurent series

$$V = \sum_{\sigma \in \mathbb{Z}} v_\sigma \Delta^\sigma, \tag{4.1}$$

where Δ is an indeterminate; each v_σ is an n-periodic sequence (of elements $v_{\sigma|\alpha}$); $v_\sigma = 0$ for $\sigma \gg 0$.[30] The product of V as above with $V' = \Sigma_{\sigma \in \mathbb{Z}} v'_\sigma \Delta^\sigma$ is

$$VV' := \sum_{\sigma \in \mathbb{Z}} \left(\sum_{\mu \in \mathbb{Z}} v_\mu v'_{\sigma - \mu[\mu]} \right) \Delta^\sigma. \tag{4.2}$$

The elements of $\mathbb{R}_n(\Delta,\Delta^{-1}]$ will be called (formal) differential-shift operators. ◇

This definition is modelled on Ref. 13; note that the sum over μ on the r.h.s. of Eq. (4.2) involves only a finite number of nonzero summands, due to the assumptions $v_\mu = 0$ and $v'_\mu = 0$ for $\mu \gg 0$.

It is easily checked that the product (4.2) is associative. This product can be characterized through the multiplication rules for the elements Δ^μ ($\mu \in \mathbb{Z}$) and $v\Delta^0 := v$ (where v is an arbitrary n-periodic sequence). It is $\Delta^\mu \Delta^\nu = \Delta^{\mu+\nu}$ and $\Delta^\mu v = v_{[\mu]} \Delta^\mu$; for each pair of sequences $v, v' \in \mathbb{R}_n$, the product vv' in $\mathbb{R}_n(\Delta,\Delta^{-1}]$ is just the ordinary pointwise product. The sequence with all elements equal to 1 is the unit element of this algebra.

The composition law (4.2) and the denomination of differential-shift operators can be understood in terms of a representation of the algebra $\mathbb{R}_n(\Delta,\Delta^{-1}]$ on an appropriate space $\mathbb{R}(\infty]$ of real infinite sequences; in this representation, Δ^μ acts as the shift operator by μ, and each sequence v acts as a pointwise multiplication operator. One easily proves the following

Proposition 4.3: Let $\mathbb{R}(\infty]$ denote the vector space of sequences $\psi = (\psi_\alpha)_{\alpha\in\mathbb{Z}}$ such that $\psi_\alpha=0$ for $\alpha\ll 0$; consider the algebra $\mathscr{G}in(\mathbb{R}(\infty])$ of the linear operators on $\mathbb{R}(\infty]$. Then the map π: $\mathbb{R}_n(\Delta,\Delta^{-1}]\to\mathscr{G}in(\mathbb{R}(\infty])$ defined by

$$(\pi(V)\psi)_\alpha := \sum_{\sigma\in\mathbb{Z}} v_{\sigma|\alpha}\psi_{\alpha+\sigma} \tag{4.3}$$

is a faithful representation of the algebra $\mathbb{R}_n(\Delta,\Delta^{-1}]$. In particular, for each integer μ and each $v\in\mathbb{R}_n$, it is

$$(\pi(\Delta^\mu)\psi)_\alpha=\psi_{\alpha+\mu}, \quad (\pi(v)\psi)_\alpha=v_\alpha\psi_\alpha. \tag{4.4}$$

◇

The algebra $\mathbb{R}_n(\Delta,\Delta^{-1}]$ also carries a trace, given by

$$\mathrm{Tr}V := \sum_0 v_0 = \sum_{i=1}^n v_{0|i} \tag{4.5}$$

for V as in Eq. (4.1). The bilinear form $\langle,\rangle$: $\mathbb{R}_n(\Delta,\Delta^{-1}]\times\mathbb{R}_n(\Delta,\Delta^{-1}]\to\mathbb{R}$, $\langle V,V'\rangle := \mathrm{Tr}(VV')$ is symmetric and nondegenerate.

B. Other realizations of the Kupershmidt algebra

The algebraic setting for the periodic Toda lattice proposed by Adler and van Moerbeke is based on the loop algebra $gl(n)(\lambda,\lambda^{-1}]$ of formal Laurent series in a parameter λ, where the coefficients are $n\times n$ real matrices. In this subsection, we show that $gl(n)(\lambda,\lambda^{-1}]$ is isomorphic to $\mathbb{R}_n(\Delta,\Delta^{-1}]$; the link between the two is a third algebra $gl_n[\infty)$, consisting of infinite n-periodic matrices, already considered in Ref. 12. These facts will be illustrated using the natural linear representations possessed by the three algebras, and finally summarized through the commutative diagram (4.14).

Definition 4.4: Throughout this article, an infinite matrix means a family $M = (M_{\alpha\beta})_{\alpha,\beta\in\mathbb{Z}}$ with $M_{\alpha\beta}\in\mathbb{R}$ for each α,β and with the additional property $M_{\alpha\beta}=0$ for $\beta-\alpha\gg 0$. An infinite matrix M is said to be n-periodic if $M_{\alpha+n,\beta+n}=M_{\alpha\beta}$ for each $\alpha,\beta\in\mathbb{Z}$; $gl_n[\infty)$ denotes the set of such matrices. ◇

We observe that, for each integer σ, the matrix elements $M_{\alpha\beta}$ with $\beta-\alpha=\sigma$ form the σ-th diagonal of M. So, a matrix in $gl_n[\infty)$ has zero entries above the κ-th diagonal for some integer κ, and the elements of each one of its diagonals form an n-periodic sequence. $gl_n[\infty)$ is an associative algebra with the usual matrix product. It carries a trace, given by $\mathrm{Tr}M := \Sigma_{j=1}^n M_{jj}$.

Definition 4.5: Let $\mathbb{R}(\infty]$ be the vector space of sequences appearing in Prop. 4.3. The tautological representation of $gl_n[\infty)$ on $\mathbb{R}(\infty]$ is the map π': $gl_n[\infty)\to\mathscr{G}in(\mathbb{R}(\infty])$ given by

$$(\pi'(M)\psi)_\alpha := \sum_{\beta\in\mathbb{Z}} M_{\alpha\beta}\psi_\beta. \tag{4.6}$$

◇

Proposition 4.6: Let π be the representation of $\mathbb{R}_n(\Delta,\Delta^{-1}]$ on $\mathbb{R}(\infty]$ considered in Prop. 4.3. There is a unique algebraic isomorphism Ψ: $\mathbb{R}_n(\Delta,\Delta^{-1}]\to gl_n[\infty)$ such that $\pi(V)=\pi'(\Psi(V))$ for each $V\in\mathbb{R}_n(\Delta,\Delta^{-1}]$. The expressions in components of the relations $M=\Psi(V)$ and $V=\Psi^{-1}(M)$ are

$$M_{\alpha\beta}=v_{\beta-\alpha|\alpha}, \quad v_{\sigma|\alpha}=M_{\alpha,\alpha+\sigma}, \tag{4.7}$$

for V as in Eq. (4.1) and α,β,σ arbitrary integers. Furthermore, Ψ is trace preserving.

Proof: It amounts to simple manipulations on indices. Note that, according to Eq. (4.7), the σ-th diagonal of the matrix M is fully determined by the sequence v_σ. ◇

We finally come to the loop algebra $gl(n)(\lambda,\lambda^{-1}]$.

Definition 4.7: $gl(n)(\lambda,\lambda^{-1}]$ is the set of formal Laurent series

$$A=\sum_{\rho\in Z} A_\rho\lambda^\rho \tag{4.8}$$

in an indeterminate λ, where, for each ρ, $A_\rho=(A_{\rho|jl})_{j,l=1,\ldots,n}$ is an $n\times n$ real matrix and $A_\rho=0$ for $\rho\gg 0$. ◇

$gl(n)(\lambda,\lambda^{-1}]$ is an associative algebra w.r.t. the usual Cauchy product of series. For each $A=\Sigma_\rho A_\rho\lambda^\rho$ we put $\mathrm{Tr}\,A:=\mathrm{tr}\,A_0$, where tr is the usual trace for $n\times n$ matrices (i.e., $\mathrm{tr}A_0=\Sigma_{j=1}^n A_{0|jj}$). The bilinear form $\langle,\rangle$: $gl(n)(\lambda,\lambda^{-1}]\times gl(n)(\lambda,\lambda^{-1}]\to\mathbb{R}$, $\langle A,A'\rangle:=\mathrm{Tr}(AA')$ is symmetric and nondegenerate.

Definition 4.8: Let $\mathbb{R}^n(\lambda,\lambda^{-1}]$ be the space of formal series $x=\Sigma_{\rho\in\mathbb{Z}}x_\rho\lambda^\rho$, where, for each ρ, $x_\rho=(x_{\rho|i})_{i=1,\ldots,n}$ is in $\mathbb{R}^n$ and $x_\rho=0$ for $\rho\gg 0$. The tautological representation of $gl(n)(\lambda,\lambda^{-1}]$ on this vector space is the map $\pi'':gl(n)(\lambda,\lambda^{-1}]\to\mathcal{S}in(\mathbb{R}^n[\lambda,\lambda^{-1}))$ given by

$$\pi''(A)x:=\sum_{\rho\in\mathbb{Z}}\left(\sum_{\mu\in\mathbb{Z}}A_\mu x_{\rho-\mu}\right)\lambda^\rho. \tag{4.9}$$

◇

Now, we introduce a linear isomorphism between the vector spaces of the representations π',π''; this isomorphism is the map $\mathcal{I}:\mathbb{R}(\infty]\to\mathbb{R}^n(\lambda,\lambda^{-1}]$, $\psi\mapsto\mathcal{I}\psi=\Sigma_{\rho\in\mathbb{Z}}x_\rho\lambda^\rho$, where

$$x_{\rho|i}:=\psi_{i-n\rho}. \tag{4.10}$$

By composition with $\mathcal{I}$ and $\mathcal{I}^{-1}$, the linear operators on $\mathbb{R}(\infty]$ are applied bijectively into the linear operators on $\mathbb{R}^n(\lambda,\lambda^{-1}]$.

Proposition 4.9: There is a unique algebraic isomorphism $\Phi:gl_n[\infty)\to gl(n)(\lambda,\lambda^{-1}]$ such that

$$\pi''(\Phi(M))=\mathcal{I}\pi'(M)\mathcal{I}^{-1} \tag{4.11}$$

for each $M\in gl_n[\infty)$. For $M=(M_{\alpha\beta})$ and $A=\Sigma_\rho A_\rho\lambda^\rho\in gl(n)(\lambda,\lambda^{-1}]$, the expressions in components of the equations $A=\Phi(M)$ and $M=\Phi^{-1}(A)$ are

$$A_{\rho|jl}=M_{j,l+n\rho}, \quad M_{j+n\nu,l+n\mu}=A_{\mu-\nu|jl} \tag{4.12}$$

for each $\rho,\mu,\nu,\in\mathbb{Z}$ and $j,l=1,\ldots,n$. Finally, Φ is trace preserving.

Proof: The uniqueness of the isomorphism Φ satisfying Eq. (4.11) follows from the fact that π' and π'' are faithful. To show the existence, we define Φ to be the map that associates to each $M \in gl_n[\infty)$ the element $A \in gl(n)(\lambda,\lambda^{-1}]$ as in the first Eq. (4.12); it can be checked by direct computation that Φ is one-to-one, with inverse as in the second Eq. (4.12), and that Eq. (4.11) holds.

We note that we can write $\Phi = (\pi'')^{-1} \circ Ad_{\mathcal{J}} \circ \pi'$ where $Ad_{\mathcal{J}}: \mathcal{S}in(\mathbb{R}^n(\lambda,\lambda^{-1}]) \to \mathcal{S}in(\mathbb{R}(\infty])$ is the map given by $Ad_{\mathcal{J}}(L) := \mathcal{J} L \mathcal{J}^{-1}$. So, Φ is a composition of algebraic isomorphisms, and therefore it is itself an isomorphism. The preservation of the trace under Φ follows immediately from Eq. (4.12). ◇

The isomorphism Φ appearing in the previous Proposition was introduced in Ref. 12; here, the infinite periodic matrix $M = \Phi^{-1}(A)$ corresponding to an element $A \in gl(n)(\lambda,\lambda^{-1}]$ is described by glueing together infinitely many $n \times n$ blocks:

$$M = \begin{pmatrix} \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & A_0 & A_1 & A_2 & A_3 & \cdots \\ \cdots & A_{-1} & A_0 & A_1 & A_2 & \cdots \\ \cdots & A_{-2} & A_{-1} & A_0 & A_1 & \cdots \\ \cdots & A_{-3} & A_{-2} & A_{-1} & A_0 & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix} \tag{4.13}$$

(with a fixed basepoint). So, M is organized in block diagonals, and the ρ-th block diagonal contains infinitely many copies of A_ρ for each $\rho \in \mathbb{Z}$.

Of course, Propositions 4.6 and 4.9 imply the following.

Corollary 4.10: The map $\Phi \circ \Psi: \mathbb{R}_n(\Delta,\Delta^{-1}] \to gl(n)(\lambda,\lambda^{-1}]$ is a trace preserving, algebraic isomorphism. ◇

We can summarize the above results in the following commutative diagram:

$$\begin{array}{ccccc} & & \mathcal{S}in(\mathbb{R}(\infty]) & \xrightarrow[Ad_{\mathcal{J}}]{} & \mathcal{S}in(\mathbb{R}^n(\lambda,\lambda^{-1}]) \\ & \overset{\pi}{\nearrow} & \uparrow \pi' & & \uparrow \pi'' \\ \mathbb{R}_n(\Delta,\Delta^{-1}] & \xrightarrow[\Psi]{} & gl_n[\infty) & \xrightarrow[\Phi]{} & gl(n)(\lambda,\lambda^{-1}] \end{array} \tag{4.14}$$

(with $Ad_{\mathcal{J}}$ as in the proof of Prop. 4.9).

C. Finite order elements of $\mathbb{R}_n(\Delta,\Delta^{-1}]$: Adjunction and projection on $gl(n,\mathbb{C})$

A generic element V of the Kupershmidt algebra is a formal Laurent series as in Eq. (4.1). We now consider the elements which are finite sums: $v_\sigma \neq 0$ for finitely many values of σ; these form a subalgebra of $\mathbb{R}_n(\Delta,\Delta^{-1}]$. The counterparts of this subalgebra in $gl_n[\infty)$ and $gl(n)(\lambda,\lambda^{-1}]$ are formed, respectively, by the n-periodic matrices with finitely many nonzero diagonals and by the elements A as in Eq. (4.8), with $A_\rho \neq 0$ for finitely many values of ρ.

Definition 4.11: $\mathbb{R}_n(\Delta,\Delta^{-1})$ is the subalgebra of $\mathbb{R}_n(\Delta,\Delta^{-1}]$ formed by the elements V as in Eq. (4.1) such that $v_\sigma = 0$ for $|\sigma| \gg 0$.

$gl_n(\infty)$ is the subalgebra of $gl_n[\infty)$ formed by n-periodic matrices M such that $M_{\alpha\beta} = 0$ for $|\beta - \alpha| \gg 0$.

$gl(n)(\lambda,\lambda^{-1})$ is the subalgebra of $gl(n)(\lambda,\lambda^{-1}]$ formed by the elements A as in Eq. (4.8) such that $A_\rho = 0$ for $|\rho| \gg 0$. ◇

It is easily checked that these three algebras are mapped into each other by the isomorphisms Φ and Ψ in the diagram (4.14). In each of them, we can introduce an adjunction operation, which

is preserved by the transformations Φ and Ψ; so, we have three involutive algebras, which are mutually isomorphic. Also, these adjunctions are trace invariant: each element and its adjoint have equal traces. All these statements are easily checked, on the grounds of the following.

Definition 4.12: The adjoints of the elements $V \in \mathbb{R}_n(\Delta,\Delta^{-1})$, $M \in gl_n(\infty)$ and $A \in gl(n)(\lambda,\lambda^{-1})$, denoted with the suffix *, are defined by

$$V^*:=\sum_\sigma v_{-\sigma[\sigma]}\Delta^\sigma, \quad (M^*)_{\alpha\beta}:=M_{\beta\alpha}, \quad A^*:=\sum_\rho A^*_{-\rho}\lambda^\rho. \tag{4.15}$$

In the third equation, $A^*_{-\rho}$ is the usual transpose of the $n\times n$ matrix $A_{-\rho}$. ◇

The above adjunction in $\mathbb{R}_n(\Delta,\Delta^{-1}]$ can be characterized as the only involution such that $v^*=v$ for each sequence $v \in \mathbb{R}_n$ and $\Delta^*=\Delta^{-1}$. The involution in $gl(n)(\lambda,\lambda^{-1})$ is uniquely fixed stipulating that $\lambda^*=1/\lambda$ and that * coincides with the usual transposition on the $n\times n$ real matrices.[12]

The three algebras of Def. 4.11 can be projected homomorphically onto the algebra $gl(n,\mathbb{C})$ of the complex $n\times n$ matrices; there are infinitely many projections, one for each $\xi \in \mathbb{C}$. In the case of $gl(n)(\lambda,\lambda^{-1})$, the projections are the evaluation maps

$$Ev_\xi : gl(n)(\lambda,\lambda^{-1}) \to gl(n,\mathbb{C}), \quad A=\sum_\rho A_\rho\lambda^\rho \mapsto A(\xi):=\sum_\rho A_\rho\xi^\rho. \tag{4.16}$$

For each fixed ξ, Ev_ξ is an algebraic morphism (moreover, if $\xi=\pm i$, Ev_ξ maps the adjoint A^* into the Hermitian conjugate of the matrix $A(\xi)$). The diagram

$$\mathbb{R}_n(\Delta,\Delta^{-1}) \underset{\Psi}{\to} gl_n(\infty) \underset{\Phi}{\to} gl(n)(\lambda,\lambda^{-1}) \underset{Ev_\xi}{\to} gl(n,\mathbb{C}) \tag{4.17}$$

indicates how to obtain, by composition with Φ and Ψ, the homomorphic projections of $gl_n(\infty)$ and $\mathbb{R}_n(\Delta,\Delta^{-1})$ onto $gl(n,\mathbb{C})$. In view of the application to be discussed in Sec. VI, it is interesting to observe that Ev_ξ is not trace preserving: for each $A \in gl_n(\infty)$ and $\xi \in \mathbb{C}$, it is $\mathrm{tr}A(\xi) = \mathrm{Tr}A + \Sigma_{\rho\in\mathbb{Z}\setminus\{0\}}\mathrm{tr}(A_\rho)\xi^\rho$.
On the other hand, if A is the image under $\Phi\circ\Psi$ of an operator $V \in \mathbb{R}_n(\Delta,\Delta^{-1})$, it is $\mathrm{Tr}A=\mathrm{Tr}V$ and the diagonal elements of the matrices A_ρ are $A_{\rho|jj}=v_{n\rho|j}$. So,

$$\mathrm{tr}A(\xi)=\mathrm{Tr}V+\sum_{\rho\in\mathbb{Z}\setminus\{0\}}\left(\sum_{j=1}^n v_{n\rho/j}\right)\xi^\rho=\mathrm{Tr}V+\sum_{\rho\in\mathbb{Z}\setminus\{0\}}\mathrm{Tr}(V\Delta^{-n\rho})\xi^\rho. \tag{4.18}$$

In the application to the periodic Toda lattice, this equation will be basic in proving a number of statements on the Flaschka and Hénon integrals.

V. THE TRIHAMILTONIAN STRUCTURE OF THE PERIODIC TODA LATTICE: DERIVATION FROM THE ADLER–VAN MOERBEKE SPLITTING

In this section, we apply the theoretical schemes of Secs. II and III to construct the triHamiltonian structure of the periodic Toda lattice. Here the abstract algebra $\mathfrak{g}$ of Sec. III is taken to be the Kupershmidt algebra $\mathbb{R}_n(\Delta,\Delta^{-1}]$; the traceform Tr is as in Eq. (4.5). The splitting we introduce in $\mathfrak{g}=\mathbb{R}_n(\Delta,\Delta^{-1}]$ can be as well described in terms of the other two realizations of the Kupershmidt algebra given in Sec. IV. The description in terms of the loop algebra $gl(n)(\lambda,\lambda^{-1}]$ corresponds to the original treatment of the Toda lattice given in Ref. 12, where, in place of *r*-matrix theory, the earlier AKS scheme was employed, and only the first Poisson structure was considered. The realization in terms of infinite *n*-periodic matrices strongly emphasizes the analogy with the setting proposed by Refs. 5 and 6 for the finite nonperiodic Toda lattice. In any case, working with $\mathbb{R}_n(\Delta,\Delta^{-1}]$ seems more convenient from the computational viewpoint.

A. The splitting and the *r*-matrix

We start with the following.

Definition 5.1: Let $V=\Sigma_{\sigma\in\mathbb{Z}}v_\sigma\Delta^\sigma$ be in $\mathbb{R}_n(\Delta,\Delta^{-1}]$. We say that V is
symmetric if $V\in\mathbb{R}_n(\Delta,\Delta^{-1})$ and $V^*=V$;
skew-symmetric if $V\in\mathbb{R}_n(\Delta,\Delta^{-1})$ and $V^*=-V$;
of positive (resp. negative) type if $v_\sigma=0$ for $\sigma\leqslant 0$ (resp. $\sigma\geqslant 0$);
of nonnegative (resp. nonpositive) type if $v_\sigma=0$ for $\sigma<0$ (resp. $\sigma>0$). ◇

Definition 5.2: $\mathfrak{g}_\pm$ and $\mathfrak{g}^\pm$ are the linear subspaces of $\mathfrak{g}=\mathbb{R}_n(\Delta,\Delta^{-1}]$ defined by

$$\mathfrak{g}_+ :=\{B\in\mathfrak{g}\,|\,B \text{ is skew-symmetric}\}, \tag{5.1}$$

$$\mathfrak{g}_- :=\{T\in\mathfrak{g}\,|\,T \text{ is of nonpositive type}\}, \tag{5.2}$$

$$\mathfrak{g}^+ :=\{L\in\mathfrak{g}\,|\,L \text{ is symmetric}\}, \tag{5.3}$$

$$\mathfrak{g}^- :=\{N\in\mathfrak{g}\,|\,N \text{ is of negative type}\}. \tag{5.4}$$

◇

The following statements are easily checked:

Proposition 5.3: The subspaces $\mathfrak{g}_\pm$ are Lie subalgebras of $\mathfrak{g}$, and $\mathfrak{g}=\mathfrak{g}_+\oplus\mathfrak{g}_-$ (vector space direct sum); $\mathfrak{g}^\pm$ is the orthogonal of $\mathfrak{g}_\pm$ in the pairing $\langle,\rangle$. Finally, for each $L,L'\in\mathfrak{g}^+$ one has $L\cdot L'$ and $LL'L\in\mathfrak{g}^+$. ◇

For each $V=\Sigma_{\sigma\in\mathbb{Z}}v_\sigma\Delta^\sigma$, we put $V_{>0}:=\Sigma_{\sigma>0}v_\sigma\Delta^\sigma$, $V_{\geqslant 0}:=\Sigma_{\sigma\geqslant 0}v_\sigma\Delta^\sigma$ and define $V_{<0}$, $V_{\leqslant 0}$ in a similar way. Then

$$V_+=V_{>0}-(V_{>0})^*,\quad V_-=V_{\leqslant 0}+(V_{>0})^*, \tag{5.5}$$

$$V^+=V_{\geqslant 0}+(V_{>0})^*,\quad V^-=V_{<0}-(V_{>0})^*. \tag{5.6}$$

The expressions for V_+ and V^+ can be written equivalently in terms of the symmetrizations and skew-symmetrizations $V^{\mathrm{sym}}:=1/2(V+V^*)$, $V^{\mathrm{skew}}:=1/2(V-V^*)$. For each $V=\Sigma_\sigma v_\sigma\Delta^\sigma$, it is $V_+=2(V_{>0})^{\mathrm{skew}}$, $V^+=v_0+2(V_{>0})^{\mathrm{sym}}$. From the projections corresponding to the above splitting of $\mathfrak{g}$, we construct the operator $R:=\Pi_+-\Pi_-$, whose adjoint is $R^*=\Pi^--\Pi^+$. We note that $\frac{1}{2}(R-R^*)V=V_{>0}-V_{<0}$; it can be checked by direct computation that this operator satisfies the modified Yang–Baxter equation (3.1). From here, from Prop. 5.3 and from the general *r*-matrix theory reviewed in Sec. III, we draw the following conclusions:

Proposition 5.4: R and $\frac{1}{2}(R-R^*)$ are *r*-matrices on $\mathfrak{g}$; $\mathfrak{g}$ is a triHamiltonian manifold with the Poisson tensors (3.6)–(3.8). Furthermore, each of these Poisson tensors can be (properly) restricted to the subspace $\mathfrak{g}^+$, the restrictions being as in Eqs. (3.10)–(3.12). ◇

B. Restriction to the Flaschka submanifold

Let us consider the manifold $\mathbb{R}_n\times\mathbb{R}_n$; a typical point will be written as $x=(a,b)$. Both the tangent and cotangent space at x are obviously identified with $\mathbb{R}_n\times\mathbb{R}_n$; tangent vectors and covectors will be represented as pairs $\dot{x}=(\dot{a},\dot{b})$ and $\delta x=(\delta a,\delta b)$, with the pairing $\langle\delta x,\dot{x}\rangle:=\Sigma_\circ(\delta a\dot{a}+\delta b\dot{b})$.

Definition 5.5: For each $x=(a,b)$, let us put

$$L(x):=a\Delta+b+\Delta^{-1}a=b+2(a\Delta)^{\mathrm{sym}} \tag{5.7}$$

(in agreement with Eq. (1.5)). The embedding $\mathbb{R}_n\times\mathbb{R}_n\to\mathfrak{g}^+$, $x\mapsto L(x)$ will also be denoted by j. Its image $\mathscr{F}$, i.e., the set of all the operators (5.7), will be called the Flaschka submanifold. ◇

At any point x, the tangent map $T_xj\colon \mathbb{R}_n\times\mathbb{R}_n\to\mathfrak{g}^+$ sends $\dot{x}=(\dot{a},\dot{b})$ into

$$\dot{L}=\dot{a}\Delta+\dot{b}+\Delta^{-1}\dot{a}=\dot{b}+2(\dot{a}\Delta)^{\mathrm{sym}}; \tag{5.8}$$

the set of these operators is the tangent space of the Flaschka submanifold $\mathscr{F}$. Recalling Eq. (4.13) and the diagram (4.14), the following can be checked.

Proposition 5.6: For each $x\in\mathbb{R}_n\times\mathbb{R}_n$, $L(x)$ is the image under $\Psi^{-1}.\Phi^{-1}$ of the Lax matrix in Eq. (1.2). ◇

Proposition 5.7: The linear, quadratic and cubic Poisson tensors (3.10)–(3.12) can be properly restricted from $\mathfrak{g}^+$ to $\mathbb{R}_n\times\mathbb{R}_n$ along j. The restricted Poisson tensors, denoted again with Q, P and S, have the following expressions:

$$Q_x dx=\dot{x},\quad \begin{cases}\dot{a}:=2a\,\delta b-2a\,\delta b_{[1]},\\ \dot{b}:=2a_{[-1]}\delta a_{[-1]}-2a\,\delta a\end{cases} \tag{5.9}$$

$$P_x\delta x=\dot{x},\quad \begin{cases}\dot{a}:=aa_{[-1]}\delta a_{[-1]}-aa_{[1]}\delta a_{[1]}+2ab\,\delta b-2ab_{[1]}\delta b_{[1]},\\ \dot{b}:=2a_{[-1]}b\,\delta a_{[-1]}-2ab\,\delta a+4a_{[-1]}^2\delta b_{[-1]}-4a^2\,\delta b_{[1]}\end{cases} \tag{5.10}$$

$$S_x\delta x=\dot{x},\quad \begin{cases}\dot{a}:=a_{[-1]}ab\,\delta a_{[-1]}-aa_{[1]}b_{[1]}\delta a_{[1]}+a_{[-1]}^2a\,\delta b_{[-1]}-aa_{[1]}^2\delta b_{[2]}\\ \qquad +a(a^2+b^2)\,\delta b-a(a^2+b_{[1]}^2)\,\delta b_{[1]},\\ \dot{b}:=a_{[-2]}a_{[-1]}^2\delta a_{[-2]}-a^2a_{[1]}\delta a_{[1]}+a_{[-1]}(a_{[-1]}^2+b^2)\,\delta a_{[-1]}\\ \qquad -a(a^2+b^2)\,\delta a+2a_{[-1]}^2(b_{[-1]}+b)\,\delta b_{[-1]}-2a^2(b+b_{[1]})\,\delta b_{[1]}.\end{cases} \tag{5.11}$$

Proof: We refer to Prop. 2.2 for the notion of proper restriction. Let us consider a point $x=(a,b)\in\mathbb{R}_n\times\mathbb{R}_n$ and its image $L=L(x)$ in the Flaschka submanifold $\mathscr{F}$. Our procedure is divided in the following steps:

(i)–(iii) to show that $Q_L\delta L, P_L\delta L, S_L\delta L$ are tangent to $\mathscr{F}$, for each covector $\delta L\in T_L^*\mathfrak{g}^+\approx\mathfrak{g}_-$;

(iv) to characterize the covectors δL extending a given covector $\delta x=(\delta a,\delta b)$ at x, in the sense of Eq. (2.10).

Each of the four items is treated in the sequel. If κ is an integer, we write $\mathscr{O}(\Delta^\kappa)$ to denote any element of $\mathfrak{g}$ containing only the powers of Δ of exponent $\leqslant\kappa$, i.e., of the form $\Sigma_{\sigma\leqslant\kappa}v_\sigma\Delta^\sigma$.

(i) Let us show that $Q_L\delta L=-2[L,\delta L]^+$ is tangent to the Flaschka submanifold for each $\delta L\in\mathfrak{g}_-$. An element of $\mathfrak{g}_-$ can be written as

$$\delta L=p+\Delta^{-1}q+\mathscr{O}(\Delta^{-2}), \tag{5.12}$$

where $p,q\in\mathbb{R}_n$ are arbitrary. This implies

$$[L,\delta L]=(ap_{[1]}-ap)\Delta+(aq-a_{[-1]}q_{[-1]})+\mathscr{O}(\Delta^{-1}); \tag{5.13}$$

$$[L,\delta L]^+=(aq-a_{[-1]}q_{[-1]})+2\{(ap_{[1]}-ap)\Delta\}^{sym}. \tag{5.14}$$

So, $Q_L\delta L$ has the form (5.8) (and is henceforth tangent to the Flaschka submanifold) with coefficients

$$\dot{a}=2ap-2ap_{[1]},\quad \dot{b}=2a_{[-1]}q_{[-1]}-2aq. \tag{5.15}$$

(ii) Similar computations are required to prove that $P_L\delta L$ is tangent to $\mathscr{F}$ for each $\delta L \in \mathfrak{g}_-$. We use again Eq. (5.12) and evaluate separately the two terms $2[\mathrm{L},(L.\delta L)_+]$ and $2L.[L,\delta L]^+$ giving $P_L\delta L$ according to Eq. (3.11). The results are

$$2[L,(L.\delta L)_+]=2(a_{[-1]}^2-a^2)p+2a_{[-1]}^2p_{[-1]}-2a^2p_{[1]} \\ +2\{a(bp-b_{[1]}p_{[1]}+bp_{[1]}-b_{[1]}p)\Delta+aa_{[1]}(p_{[2]}-p)\Delta^2\}^{sym}, \quad (5.16)$$

$$2L.[L,\delta L]^+=2(a_{[-1]}^2-a^2)p-2a_{[-1]}^2p_{[-1]}+2a^2p_{[1]}+2b(aq-a_{[-1]}q_{[-1]})+2\{a(a_{[1]}q_{[1]} \\ -q_{[-1]}q_{[-1]}-bp+b_{[1]}p_{[1]}+bp_{[1]}-b_{[1]}p)\Delta+aa_{[1]}(p_{[2]}-p)\Delta^2\}^{sym}. \quad (5.17)$$

Subtracting Eq. (5.17) from (5.16), we obtain that $P_L\delta L$ is tangent to the Flaschka submanifold and of the form (5.8), with coefficients

$$\dot a=aa_{[-1]}q_{[-1]}-aa_{[1]}q_{[1]}+2abp-2ab_{[1]}p_{[1]}, \\ \dot b=2a_{[-1]}bq_{[-1]}-2abq+4a_{[-1]}^2p_{[-1]}-4a^2p_{[1]}. \quad (5.18)$$

(iii) The computation of $S_L\delta L$ according to Eq. (3.12) requires the separate evaluation of the terms $[L,(L\,\delta L L)_+]$ and $L[L,\delta L]^+L$. We have

$$[L,(L\,\delta L L)_+]=k+2\{m\Delta+r\Delta^2+s\Delta^3\}^{sym}, \quad (5.19)$$

$$L[L,\delta L]^+L=u+2\{w\Delta+r\Delta^2+s\Delta^3\}^{sym}, \quad (5.20)$$

where $k,m,\ldots,w$ are given by

$$k:=2a_{[-1]}^2bp-2a^2bp+2a_{[-1]}^2b_{[-1]}p_{[-1]}-2a^2b_{[1]}p_{[1]}+2a_{[-1]}^3q_{[-1]}-2a^3q,$$

$$m:=aa_{[-1]}^2p-aa_{[1]}^2p_{[1]}+ab^2p-ab_{[1]}^2p_{[1]}+abb_{[1]}p_{[1]}-abb_{[1]}p+a^2bq-a^2b_{[1]}q,$$

$$r:=aa_{[1]}bp_{[1]}-aa_{[1]}bp+aa_{[1]}b_{[2]}p_{[2]}-aa_{[1]}b_{[2]}p_{[1]}+aa_{[1]}^2q_{[1]}-a^2a_{[1]}q,$$

$$s:=aa_{[1]}a_{[2]}p_{[2]}-aa_{[1]}a_{[2]}p_{[1]}, \quad (5.21)$$

$$u:=2a_{[-1]}^2bp-2a^2bp+2a^2bp_{[1]}-2a_{[-1]}^2bp_{[-1]}+a_{[-1]}^3q_{[-1]}-a^3q+ab^2q \\ -a_{[-1]}b^2q_{[-1]}+a^2a_{[1]}q_{[1]}-a_{[-2]}a_{[-1]}^2q_{[-2]},$$

$$w:=aa_{[-1]}^2p-aa_{[-1]}^2p_{[-1]}+a^3p_{[1]}-a^3p+abb_{[1]}p_{[1]}-abb_{[1]}p+aa_{[1]}^2p_{[2]} \\ -aa_{[1]}^2p_{[1]}+aa_{[1]}b_{[1]}q_{[1]}-aa_{[-1]}bq_{[-1]}+a^2bq-a^2b_{[1]}q.$$

Subtracting Eq. (5.20) from Eq. (5.19), we obtain that $S_L\delta L$ is as in Eq. (5.8) (and henceforth tangent to the Flaschka submanifold) with coefficients

$$\dot a=a_{[-1]}abq_{[-1]}-aa_{[1]}b_{[1]}q_{[1]}+a_{[-1]}^2ap_{[-1]}-aa_{[1]}^2p_{[2]}+a(a^2+b^2)p-a(a^2+b_{[1]}^2)p_{[1]}, \\ \dot b=a_{[-2]}a_{[-1]}^2q_{[-2]}-a^2a_{[1]}q_{[1]}+a_{[-1]}(a_{[-1]}^2+b^2)q_{[-1]}-a(a^2+b^2)q \\ +2a_{[-1]}^2(b_{[-1]}+b)p_{[-1]}-2a^2(b+b_{[1]})p_{[1]}. \quad (5.22)$$

(iv) On the grounds of the results in items (i)–(iii), the Poisson tensors Q, P and S can be properly restricted to $\mathbb{R}_n\times\mathbb{R}_n$ along j. Now, consider (at a point $L=L(x)$) a covector $\delta L\in\mathfrak{g}_-$, written as in Eq. (5.12); for each $\dot{L}$ as in (5.8), we have

$$\mathrm{Tr}(\delta L\dot{L})=\mathrm{Tr}(p\dot{a}\Delta+q_{[-1]}\dot{a}_{[-1]}+p\dot{b}+l(\Delta^{-1}))=\sum_0(q\dot{a}+p\dot{b}). \tag{5.23}$$

By definition, δL extends a covector $\delta x=(\delta a,\delta b)\in\mathbb{R}_n\times\mathbb{R}_n$ if $\langle\delta L,\dot{L}\rangle=\langle\delta x,\dot{x}\rangle=\Sigma_0(\delta a\dot{a}+\delta b\dot{b})$ for each $\dot{x}=(\dot{a},\dot{b})\in\mathbb{R}_n\times\mathbb{R}_n$. From Eq. (5.23), it is seen that this happens if $q=\delta a$, $p=\delta b$. Inserting this result in Eqs. (5.15), (5.18), and (5.22), we conclude that the restricted Poisson tensors Q, P and S are as in Eqs. (5.9)–(5.11). ◇

VI. RECURSION SCHEMES ON THE FLASCHKA SUBMANIFOLD

Throughout this section, the restrictions of Q,P,S,h_k,X_k ($k=1,2,3...$) from $\mathfrak{g}^+$ to $\mathbb{R}_n\times\mathbb{R}_n$ along j are denoted with the same symbols. At each point $x=(a,b)$, the Hamiltonians are

$$h_1(x)=\mathrm{Tr}L(x)=\sum_0 b,\quad h_2(x)=\frac{1}{2}\,\mathrm{Tr}\,L^2(x)=\sum_0\left(\frac{1}{2}\,b^2+a^2\right),$$
$$h_3(x)=\frac{1}{3}\,\mathrm{Tr}\,L^3(x)=\sum_0\left(\frac{1}{3}\,b^3+a^2b+a^2b_{[1]}\right), \tag{6.1}$$

and so on. We have $Q_xd_xh_1=0$, and

$$X_k(x)=P_xd_xh_k=Q_xd_xh_{k+1}=S_xd_xd_{k-1}. \tag{6.2}$$

$X_1(x)$ has components $\dot{a}$ and $\dot{b}$ as in Eq. (1.1). The Lax formulation (1.5) for this vector field follows from Eq. (3.9); the companion $B_1(x)$ in Eq. (1.5) is just $2(L(x))_+$, and, more generally, each vector field X_k on $\mathbb{R}_n\times\mathbb{R}_n$ admits a Lax formulation $dL/dt_k=[L,B_k]$, with $B_k(x)=2(L^k(x))_+$.

Let us choose one of the three Poisson structures, say Q. By construction, all vector fields X_k belong to $\mathrm{Im}\,Q$, so they are tangent to the symplectic leaves of the Poisson tensor;[31] on each symplectic leaf, one can discuss the Arnold–Liouville integrability of the Toda hierarchy. It is known from the literature[12] that only $n-1$ vector fields in the sequence X_k ($k=1,2,3,...$) are linearly independent at a generic point x of $\mathbb{R}_n\times\mathbb{R}_n$; the property of being generically independent is satisfied for instance by the first $n-1$ fields. On the other hand, $n-1$ is just half the dimension of a generic symplectic leaf of Q, so the complete integrability of the system is ensured. Let us consider on $\mathbb{R}_n\times\mathbb{R}_n$ the Hamiltonians h_k for the first $n+1$ values of k. To compute them, it is not even necessary to employ the operator $L(x)$; in fact, it suffices to consider a finite matrix $\Lambda(x)$ and the ordinary traces of its powers.

Proposition 6.1: At each point $x=(a,b)$, consider the $n\times n$ matrix

$$\Lambda(x):=\begin{pmatrix} b_1 & a_1 & 0 & .. & .. & 0 & -ia_n\\ a_1 & b_2 & a_2 & 0 & .. & .. & 0\\ 0 & a_2 & b_3 & a_3 & .. & .. & ..\\ .. & .. & .. & .. & .. & .. & ..\\ .. & .. & .. & .. & .. & a_{n-2} & 0\\ 0 & .. & .. & 0 & a_{n-2} & b_{n-1} & a_{n-1}\\ ia_n & 0 & .. & .. & 0 & a_{n-1} & b_n \end{pmatrix} \tag{6.3}$$

(obtained setting $\lambda = i$ in Eq. (1.2), where i is the imaginary unit). Then $h_k(x) = (1/k)\mathrm{tr}\,\Lambda^k(x)$ for $k = 1,2,\ldots,n+1$.

Proof: With the notations of Sec. IV, the matrix (6.3) is related to the operator $L(x) = a\Delta + b + a_{[-1]}\Delta^{-1}$ by the equation $\Lambda(x) = Ev_i(\Psi \circ \Phi(L(x)))$, and a similar relation holds for the powers of $\Lambda(x)$ and $L(x)$. The thesis is proved if we show that $\mathrm{tr}\,\Lambda^k(x) = \mathrm{Tr}\,L^k(x)$ for $k = 1,2,\ldots,n+1$. On the grounds of Eq. (4.18), for each positive integer k we have

$$\mathrm{tr}\,\Lambda^k(x) - \mathrm{Tr}\,L^k(x) = \sum_{\rho \in \mathbb{Z}\setminus\{0\}} i^\rho \mathrm{Tr}(L^k(x)\Delta^{-n\rho}); \tag{6.4}$$

from the explicit expression of the operator $L(x)$, one infers that the r.h.s. of this equation is zero for $k \leqslant n+1$. ◇

Remark 6.2: The finite matrix $\Lambda(x)$ is also a Lax operator for the periodic Toda lattice. Due to this fact, one might conjecture that the whole theory of the periodic Toda lattice can be developed using the finite-dimensional algebra $\mathfrak{g} = gl(n,\mathbb{C})$ of $n \times n$ complex matrices instead of the infinite-dimensional algebra $\mathfrak{g} = \mathbb{R}_n(\Delta,\Delta^{-1}]$ employed in this article. Unfortunately, it is not known how to construct an r-matrix in $gl(n,\mathbb{C})$, so as to induce the Toda multiHamiltonian structure on the submanifold described by Eq. (6.3). Working with the finite $n \times n$ matrices one introduces some ''boundary effects'' related to the presence of the element a_n in the corners of the matrix $\Lambda(x)$; the price for the elimination of such effects is the infinite dimensionality of $\mathfrak{g} = \mathbb{R}_n(\Delta,\Delta^{-1}]$.

We now recall that in Sec. III D we have considered on $\mathfrak{g}$ or $\mathfrak{g}^+$ an alternative sequence of Hamiltonian functions f_k ($k = 1,2,3,...$), in such a way that, at each point L, $\mathrm{Det}(1 - zL) = 1 - \Sigma_{k=1}^{\infty} f_k(L) z^k$. This chain also satisfies a biHamiltonian recursion scheme w.r.t. Q and P; the f_k's can be expressed as Schur polynomials in the h_k's via Eq. (2.5).

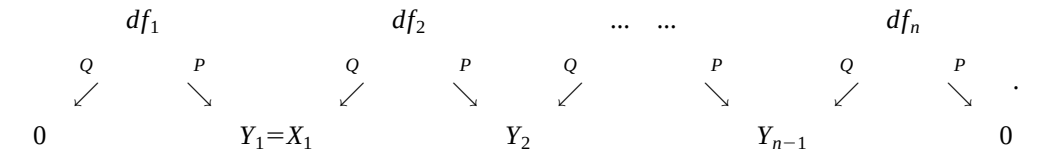
Proposition 6.3: $f_1(x),\ldots,f_n(x)$ are the coefficients of the characteristic polynomial of $\Lambda(x)$, i.e., $\det(\Lambda(x) - \zeta) = (-1)^n(\zeta^n - f_1(x)\zeta^{n-1} - f_2(x)\zeta^{n-2} - \ldots - f_n(x))$. Furthermore, it is $f_{n+1}(x) = 0$.

Proof: Let us recall that, for each k, we have $f_k(x) = S_k(h_1(x),h_2(x),h_3(x),\ldots)$, where S_k is the Schur polynomial defined as in Eq.(2.6); in particular, $f_1(x),\ldots,f_{n+1}(x)$ depend only on $h_1(x),\ldots,h_{n+1}(x)$, which can be computed from the traces of the finite matrix $\Lambda(x)$ and its powers (Prop. 6.1). The thesis follows from this and from elementary matrix theory:[32,33] in fact, if we consider any $n \times n$ matrix Λ and set $t_j := (1/j)\mathrm{tr}\Lambda^j$, then the Schur polynomials $S_k(t_1,t_2,t_3,\ldots)$ for $k \leqslant n$ are known to give the coefficients of $\det(\Lambda - \zeta)$ (this fact is related to the so-called Leverrier method for computing the characteristic polynomial[33,34]). Also, it is known that $S_k(t_1,t_2,t_3,\ldots) = 0$ for $k \geqslant n+1$, which means that the characteristic polynomial has degree n. From here we infer the thesis.[35] ◇

In Sec. III D we proposed the denomination of Flaschka and Hénon integrals for the functions h_k and f_k on an arbitrary r-matrix algebra $\mathfrak{g}$ (not necessarily the one considered here). In the present case, considering the functions h_k and f_k on the ''space of coordinates'' $\mathbb{R}_n \times \mathbb{R}_n$ of the Flaschka submanifold, we recover for $k = 1,\ldots,n$ the systems of integrals first constructed in Refs. 28 and 29 for the Toda lattice. The expression of the f_k's as polynomials in the h_k's for the first values of k was found by Hénon; our formulas (2.7)–(2.8) provide a general rule, based on the theory of the Schur polynomials.

Our framework also allows us to derive a property of the Hénon integrals, which has some interest from the biHamiltonian viewpoint. In general, for a finite dimensional system the biHamiltonian approach acquires a more elegant form if one is able to exhibit a finite hierarchy where both the initial and the final Hamiltonian are Casimirs. The chain $f_1,\ldots,f_n$ possesses this property:

Proposition 6.4: The Hénon integrals $f_1,\ldots,f_n$ and the vector fields $Y_1 = Pdf_1,\ldots,Y_{n-1} = Pdf_{n-1}$ on $\mathbb{R}_n \times \mathbb{R}_n$ form a finite biHamiltonian hierarchy, starting from a Casimir of Q and ending with a Casimir of P:



(6.5)

Proof: The recurrence relations and the property $Qdf_1=0$ hold in general on $\mathfrak{g}$ or $\mathfrak{g}^+$, so they are also satisfied by the restrictions to $\mathbb{R}_n\times\mathbb{R}_n$ along j. The statement that $Pdf_n=0$ on $\mathbb{R}_n\times\mathbb{R}_n$ follows from $Pdf_n=Qdf_{n+1}$ and the fact that $f_{n+1}=0$. ◇

Let us present explicitly the finite biHamiltonian chain for $n=3$. We have

$$f_1(x)=h_1(x)=b_1+b_2+b_3,\quad f_2(x)=a_1^2+a_2^2+a_3^2-b_1b_2-b_2b_3-b_3b_1,$$
$$f_3(x)=b_1b_2b_3-a_1^2b_3-a_2^2b_1-a_3^2b_2. \tag{6.6}$$

The vector field $Y_1=X_1$ is as in Eq. (1.1) and $Y_2(x)=(\dot{a},\dot{b})$, where

$$\dot{a}=2a(a_{[-1]}^2-a_{[1]}^2)+2ab_{[-1]}(b_{[1]}-b),$$
$$\dot{b}=4a^2b_{[-1]}-4a_{[-1]}^2b_{[1]}. \tag{6.7}$$

It turns out that Y_1 and Y_2 are independent on a generic subset of $\mathbb{R}_3\times\mathbb{R}_3$; so they can be employed to prove Liouville integrability of the system on the symplectic leaves of Q (or P), which are four-dimensional in the present case. For $n=4$, we have a chain of Hamiltonians $f_1,\ldots,f_4$ with three generically independent vector fields Y_1,Y_2,Y_3, and so on.

VII. THE TODA TRIHAMILTONIAN STRUCTURE: DERIVATION FROM THE KUPERSHMIDT LAX OPERATOR

In this section, we consider the alternative formulation of the periodic Toda lattice in which the evolution equations of the system have the form (1.3), and the associated Lax pair is given in terms of the operators (1.6); this is the setting adopted in Ref. 13. The algebra $\mathfrak{g}$ supporting this formulation is again $\mathbb{R}_n(\Delta,\Delta^{-1}]$.

A. Another splitting of $\mathbb{R}_n(\Delta,\Delta^{-1}]$

The alternative choice is suggested by the prescription of Ref. 13 for the Lax pairs $dV/dt_k=[V,C_k]$ of the Toda hierarchy, which is $C_k(y)=2(V^k(y))_{\geqslant 0}$. The same splitting was employed in Ref. 11 for the infinite Toda chain and some generalizations of it (in that paper, the reduction was performed for the first two associated Poisson structures, and not for the third one). In the sequel, the symbols $_{\geqslant 0,>0}$, etc., are intended as in Sec. V.

Definition 7.1: $\mathfrak{g}_\pm$ and $\mathfrak{g}^\pm$ are the linear subspaces of $\mathfrak{g}=\mathbb{R}_n(\Delta,\Delta^{-1}]$ defined by

$$\mathfrak{g}_+:=\{C\in\mathfrak{g}\,|\,C \text{ is of nonnegative type}\}, \tag{7.1}$$

$$\mathfrak{g}_-:=\{N\in\mathfrak{g}\,|\,N \text{ is of negative type}\}, \tag{7.2}$$

$$\mathfrak{g}^+:=\{D\in\mathfrak{g}\,|\,D \text{ is of positive type}\}, \tag{7.3}$$

$$\mathfrak{g}^-:=\{Z\in\mathfrak{g}\,|\,Z \text{ is of nonpositive type}\}. \tag{7.4}$$

◇

Proposition 7.2: The subspaces $\mathfrak{g}_{\pm}$ are Lie subalgebras of $\mathfrak{g}$, and $\mathfrak{g}=\mathfrak{g}_{+}\oplus\mathfrak{g}_{-}$ (vector space direct sum); $\mathfrak{g}^{\pm}$ is the orthogonal of $\mathfrak{g}_{\pm}$ in the pairing $\langle,\rangle$. ◇

For each $V\in\mathfrak{g}$, the components according to the splitting of Def. 7.1 are $V_{+}=V_{\geqslant 0}$, $V_{-}=V_{<0}$, $V^{+}=V_{>0}$, $V^{-}=V_{\leqslant 0}$. Of course, the operator $\mathscr{R}$ on $\mathfrak{g}$ and its adjoint $\mathscr{R}^{*}$ given by $\mathscr{R}(V):=V_{+}-V_{-}$, $\mathscr{R}^{*}(V)=V^{-}-V^{+}$ are now different from the operators R and R^{*} considered in Sec. V, but, incidentally, the skew-symmetrization $\frac{1}{2}(\mathscr{R}-\mathscr{R}^{*})$ is again as in Eq.(5.8). We have the following.

Proposition 7.3: $\mathscr{R}$ and $\frac{1}{2}(\mathscr{R}-\mathscr{R}^{*})$ are r-matrices on $\mathfrak{g}$; $\mathfrak{g}$ is a triHamiltonian manifold with the Poisson tensors (3.6)–(3.8). ◇

We will employ script letters to denote these Poisson tensors, which have the form

$$\mathscr{Q}_{v}\delta V=2[V,(\delta V)_{\geqslant 0}]-2[V,\delta V]_{>0}=-2[V,(\delta V)_{<0}]+2[V,\delta V]_{\leqslant 0}, \tag{7.5}$$

$$\mathscr{P}_{v}\delta V=2[V,(V.\delta V)_{\geqslant 0}]-2V.[V,\delta V]_{>0}=-2[V,(V.\delta V)_{<0}]+2V.[V,\delta V]_{\leqslant 0}, \tag{7.6}$$

$$\mathscr{S}_{v}\delta V=[V,(V\delta VV)_{\geqslant 0}]-V[V,\delta V]_{>0}V=-[V,(V\delta VV)_{<0}]+V[V,\delta V]_{\leqslant 0}V. \tag{7.7}$$

The functions $h_{k}(V)=(1/k)\mathrm{Tr}V^{k}$ satisfy the triHamiltonian recursion relations (2.1) and (2.2) w.r.t. $\mathscr{Q}$, $\mathscr{P}$ and $\mathscr{S}$; also, the functions f_{k} forming the Hénon Casimir give rise to a biHamiltonian recursion with $\mathscr{Q}$ and $\mathscr{P}$. Using these Hamiltonian functions, we can define infinitely many commuting vector fields $\mathscr{X}_{k}:=\mathscr{P}dh_{k}$ and $\mathscr{Y}_{k}:=\mathscr{P}df_{k}$; we have

$$\mathscr{X}_{k}(V)=2[V,(V^{k})_{\geqslant 0}]. \tag{7.8}$$

B. Restriction of the triHamiltonian structure

Let us consider the manifold $\mathbb{R}_{*}\times\mathbb{R}_{n}\times\mathbb{R}_{n}$, where $\mathbb{R}_{*}:=\mathbb{R}\backslash\{0\}$. A typical point is written as $z=(K,d,b)$; here, K is a nonzero real number, while d and b are n-periodic sequences. Both the tangent and cotangent space at z are identified with $\mathbb{R}\times\mathbb{R}_{n}\times\mathbb{R}_{n}$; tangent vectors and covectors are represented as triples $\dot{z}=(\dot{K},\dot{d},\dot{b})$ and $\delta z=(\delta K,\delta d,\delta b)$, with the pairing $\langle\delta z,\dot{z}\rangle:=\delta K\dot{K}+\Sigma_{0}(\delta d\dot{d}+\delta b\dot{b})$.

Definition 7.4: For each $z=(K,d,b)$ we put

$$V(z):=K\Delta+b+\Delta^{-1}d. \tag{7.9}$$

The embedding $\mathbb{R}_{*}\times\mathbb{R}_{n}\times\mathbb{R}_{n}\to\mathfrak{g}$, $z\mapsto V(z)$ will also be denoted by J. Its image $\mathscr{H}$, i.e., the set of all the operators (7.9), will be called the *extended Kupershmidt submanifold.* ◇

We note that, for $K=1$ and $d=c$, the operator (7.9) becomes the Kupershmidt Lax operator in Eq. (1.6).

At any point z, the tangent map $T_{z}J:\mathbb{R}\times\mathbb{R}_{n}\times\mathbb{R}_{n}\to\mathfrak{g}$ sends $\dot{z}=(\dot{K},\dot{d},\dot{b})$ into

$$\dot{V}=\dot{K}\Delta+\dot{b}+\Delta^{-1}\dot{d}; \tag{7.10}$$

the set of these operators is the tangent space of the submanifold $\mathscr{H}$ at $V(z)$.

Our aim is to restrict the r-matrix triHamiltonian structure (7.5)–(7.7) to $\mathbb{R}_{*}\times\mathbb{R}_{n}\times\mathbb{R}_{n}$ along J. As we shall see, the linear Poisson tensor fits the proper restriction scheme. This technique is not appropriate for the quadratic and the cubic ones, and the more subtle machinery of the Dirac reduction must be invoked; in a sense, this is a price one has to pay for having chosen an apparently simpler splitting than in Sec. V.

Proposition 7.5: The three Poisson tensors (7.6)–(7.8) can be restricted from $\mathfrak{g}$ to $\mathbb{R}_{*}\times\mathbb{R}_{n}\times\mathbb{R}_{n}$ along J (the first one in the proper sense, the other two in the Dirac sense). The restrictions have the following expressions:

$$\mathscr{Q}_z\delta z=\dot z,\begin{cases}\dot K:=0,\\ \dot d:=2d\,\delta b-2d\,\delta b_{[1]},\\ \dot b:=2d_{[-1]}\delta d_{[-1]}-2d\,\delta d,\end{cases}\tag{7.11}$$

$$\mathscr{P}_z\delta z=\dot z,\begin{cases}\dot K:=0,\\ \dot d:=2d(d_{[-1]}\delta d_{[-1]}-d_{[1]}\delta d_{[1]}+b\,\delta b-b_{[1]}\delta b_{[1]}),\\ \dot b:=2b(d_{[-1]}\delta d_{[-1]}-d\,\delta d)+2K(d_{[-1]}\delta b_{[-1]}-d\,\delta b_{[1]}),\end{cases}\tag{7.12}$$

$$\mathscr{S}_z\delta z=\dot z,\begin{cases}\dot K:=-K\langle(b-b_{[1]})d\,\delta d\rangle+K^2\langle d(\delta b-\delta b_{[1]})\rangle,\\ \dot d=2d(bd_{[-1]}\delta d_{[-1]}-b_{[1]}d_{[1]}\delta d_{[1]})+Kd(d_{[-1]}\delta b_{[-1]}-d_{[1]}\delta b_{[2]})\\ \quad+d(Kd+b^2)\delta b-d(Kd+b_{[1]}^2)\delta b_{[1]}+d(b_{[1]}-b)\langle d\,\delta d\rangle\\ \quad+d\langle(b-b_{[1]})d\,\delta d\rangle-Kd\langle d(\delta b-\delta b_{[1]})\rangle+1/n\;Kd(b-b_1)\delta K,\\ \dot b=K(d_{[-2]}d_{[-1]}\delta d_{[-2]}-dd_{[1]}\delta d_{[1]})+d_{[-1]}(Kd_{[-1]}+b^2)\delta d_{[-1]}\\ \quad-d(Kd+b^2)\delta d+Kd_{[-1]}(b_{[-1]}+b)\delta b_{[-1]}-Kd(b+b_{[1]})\delta b_{[1]}\\ \quad+K(d-d_{[-1]})\langle d\,\delta d\rangle-1/n\;K^2(d-d_{[-1]})\delta K.\end{cases}\tag{7.13}$$

(Recall that, for each sequence $v\in\mathbb{R}_n$, $\langle v\rangle$ denotes the average of v over a period, see Def. 4.1).

Proof: Let us consider any point $z=(K,d,b)$ and its image $V=V(z)$ in the submanifold $\mathscr{H}$. Our procedure is divided in the following steps:
(i) to compute $\mathscr{Q}_v\delta V$, $\mathscr{P}_v\delta V$ and $\mathscr{S}_v\delta V$ for an arbitrary $\delta V\in T_v^*\mathfrak{g}\approx\mathfrak{g}$;
(ii) to find the most general covector $\delta V\in\mathfrak{g}$ extending a given $\delta z=(\delta K,\delta d,\delta b)$ in the sense of Eq. (2.10);
(iii)–(v) to check restrictability, and make explicit the restrictions of $\mathscr{Q}$, $\mathscr{P}$ and $\mathscr{S}$.

In the sequel, if κ is an integer, we write $u(\Delta^\kappa)$ to denote any element of $\mathfrak{g}$ in which the powers of Δ occur with exponents $\geqslant\kappa$. We also employ the notation $\ell(\Delta^k)$ as in Sec. V, to denote the operators in which the powers of Δ have exponents $\leqslant k$.

(i) We must compute $\mathscr{Q}_v\delta V$ for an arbitrary $\delta V\in\mathfrak{g}$. Let us start from the particular case $\delta V=u(\Delta^2)$. Then $[V,\delta V]_{\leqslant 0}=0$, and from the second representation in Eq. (7.5) we infer $\mathscr{Q}_v\delta V=0$. Similarly, from the first representation in Eq. (7.5) we infer that $\mathscr{Q}_v\delta V=0$ for $\delta V=\ell(\Delta^{-1})$. A general covector in $\mathfrak{g}$ can be written as

$$\delta V=u(\Delta^2)+q\Delta+p+\ell(\Delta^{-1}),\tag{7.14}$$

with arbitrary coefficients $q,p\in\mathbb{R}_n$. Only the middle term $q\Delta+p$ gives a nonzero result on application of $\mathscr{Q}$; from the second Eq. (7.5), we conclude that

$$\mathscr{Q}_v\delta V=2[K\Delta+b+\Delta^{-1}d,q\Delta+p]_{\leqslant 0}=2(d_{[-1]}q_{[-1]}-dq)+2\Delta^{-1}(dp-dp_{[1]}).\tag{7.15}$$

This means that the vector $\mathscr{Q}_v\delta V$ is of the form (7.10), and henceforth tangent to $\mathscr{H}$, with coefficients

$$\dot K=0,\quad \dot d=2dp-2dp_{[1]},\quad \dot b=2d_{[-1]}q_{[-1]}-2dq.\tag{7.16}$$

We now compute $\mathscr{P}_v\delta V$ for an arbitrary $\delta V\in\mathfrak{g}$; the second and the first representations in Eq. (7.6) can be used to prove that $\mathscr{P}_v\delta V=0$ both for $\delta V=u(\Delta^2)$ and for $\delta V=\ell(\Delta^{-2})$. We write a general $\delta V\in\mathfrak{g}$ as

$$\delta V=u(\Delta^2)+q\Delta+p+r\Delta^{-1}+\ell(\Delta^{-2});\tag{7.17}$$

then only the middle terms in q,p,r contribute under application of $\mathscr{P}$, and the result is

$$\mathscr{P}_v \delta V = k\Delta + l + \Delta^{-1} m, \tag{7.18}$$

$$k := K(d_{[-1]}q_{[-1]} - d_{[1]}q_{[1]}) + K^2(r_{[2]} - r),$$

$$l := 2d_{[-1]}bq_{[-1]} - 2bdq + 2K(d_{[-1]}p_{[-1]} - dp_{[1]}),$$

$$m := d_{[-1]}dq_{[-1]} - dd_{[1]}q_{[1]} + 2bdp - 2b_{[1]}dp_{[1]} - Kd(r_{[2]} - r).$$

Note that this vector is not generally tangent to $\mathscr{H}$, because the coefficient k of Δ is not constant.

We finally compute $\mathscr{S}_v \delta V$. An arbitrary covector in $\mathfrak{g}$ can be written as

$$\delta V = u(\Delta^2) + q\Delta + p + r\Delta^{-1} + s\Delta^{-2} + \mathscr{O}(\Delta^{-3}); \tag{7.19}$$

only the middle terms in p,q,r,s give a nonzero result on application of $\mathscr{S}$, and it is found that

$$\mathscr{S}_v \delta V = g\Delta^2 + k\Delta + l + \Delta^{-1} m, \begin{cases} g := K^2(dq - d_{[1]}q_{[1]}) + K^3(r_{[2]} - r_{[1]}), \\ k := Kd(b_{[1]} - b)q + K(bd_{[-1]}q_{[-1]} - b_{[1]}d_{[1]}q_{[1]}) \\ \quad + K^2 d(p - p_{[1]}) + K^2(b_{[1]}r_{[2]} - br) + K^3(s_{[2]} - s_{[1]}), \\ l := K(d_{[-2]}d_{[-1]}q_{[-2]} - dd_{[1]}q_{[1]}) + d_{[-1]}b^2 q_{[-1]} \\ \quad - db^2 q + Kd_{[-1]}(b_{[-1]} + b)p_{[-1]} - Kd(b + b_{[1]})p_{[1]} \\ \quad + K^2(d_{[-1]}r - dr_{[1]}), \\ m := bdd_{[-1]}q_{[-1]} - b_{[1]}dd_{[1]}q_{[1]} + Kdd_{[-1]}p_{[-1]} \\ \quad - Kdd_{[1]}p_{[2]} + b^2 dp - b_{[1]}^2 dp_{[1]} + Kbd(r + r_{[1]}) \\ \quad - Kb_{[1]}d(r_{[1]} + r_{[2]}) - K^2 d(s_{[2]} - s_{[1]}). \end{cases} \tag{7.20}$$

The vector (7.20) is not generally tangent to $\mathscr{H}$, due to the term in Δ^2 and the fact that the coefficient k of Δ is not constant.

(ii) Let us consider (at the point $V = V(z)$) a covector $\delta V \in \mathfrak{g}$, written as in Eq. (7.14); for each $\dot{V}$ as in (7.10), we have

$$\langle \dot{V}, \delta V \rangle = \sum_0 (\dot{K}r + \dot{d}q + \dot{b}p) = \dot{K}\sum_0 r + \sum_0 (\dot{d}q + \dot{b}p). \tag{7.21}$$

By definition, δV extends a covector $\delta z = (\delta K, \delta d, \delta b) \in \mathbb{R}\times\mathbb{R}_n\times\mathbb{R}_n$ if $\langle \delta V, \dot{V}\rangle = \langle \delta z, \dot{z}\rangle = \delta K\dot{K} + \Sigma_0(\delta d\dot{d} + \delta b\dot{b})$ for each $\dot{z} = (\dot{K}, \dot{d}, \dot{b}) \in \mathbb{R}\times\mathbb{R}_n\times\mathbb{R}_n$. From Eq. (7.21), it is seen that this happens iff

$$q = \delta d, \quad p = \delta b, \quad \sum_0 r = \delta K, \tag{7.22}$$

i.e., $\langle r\rangle = (1/n)\delta K$. So, q,p and the average of r are uniquely fixed, while the remaining parts $u(\Delta^2), l(\Delta^{-2})$ of δV are arbitrary.

(iii) We have seen that $\mathscr{Q}_v \delta V$ is automatically tangent to $\mathscr{H}$, so we have a proper restriction of $\mathscr{Q}$ to $\mathbb{R}_*\times\mathbb{R}_n\times\mathbb{R}_n$ along J. Equations (7.16) and (7.22) yield the expression (7.11) for the reduced tensor.

(iv) Let us consider any extension δV of a given covector δz. The expression of $\mathscr{P}_v \delta V$ is as in Eq. (7.18), with q, p and r as in Eq. (7.22). The vector $\mathscr{P}_v \delta V$ is tangent to $\mathscr{H}$ iff the coefficient k is a constant $\dot{K}$. So, we are led to the equation

$$\dot{K} = K(d_{[-1]}\delta d_{[-1]} - d_{[1]}\delta d_{[1]}) + K^2(r_{[2]} - r). \tag{7.23}$$

The r.h.s. of this equation has zero average, so the constant $\dot{K}$ must be zero. From here, it follows $r_{[2]}-r=1/K(d_{[1]}\delta d_{[1]}-d_{[-1]}\delta d_{[-1]})$, which implies

$$r=\frac{1}{K}\,d_{[-1]}\delta d_{[-1]}+w, \tag{7.24}$$

where w is an element of $\mathbb{R}_n$ such that $w_{[2]}-w=0$. Also, w must be such that the condition $\langle r\rangle=(1/n)\,\delta\dot{K}$ be satisfied.[36] Inserting these results into Eq. (7.18), we obtain $P_v\delta V=\dot{b}+\Delta^{-1}\dot{d}$, with d and $\dot{b}$ as in Eq. (7.12). This means that P is Dirac restrictable to $\mathbb{R}_*\times\mathbb{R}_n\times\mathbb{R}_n$ along J, yielding the reduced tensor (7.12).

(v) To restrict the third Poisson tensor $\mathscr{S}$, we reconsider the most general δV extending a given covector δz. Then $\mathscr{S}_v\delta V$ is as in Eq. (7.20), with $q=\delta d$, $p=\delta b$, and we must also take into account that $\langle r\rangle=(1/n)\,\delta K$.

$\mathscr{S}_v\delta V$ is tangent to $\mathscr{H}$ iff $g=0$ and k is a constant $\dot{K}$. We regard these two constraints as equations for r and s; the equation $g=0$ and the condition on the average of r imply

$$r=\frac{1}{K}\,d_{[-1]}\delta d_{[-1]}-\frac{1}{K}\,\langle d\,\delta d\rangle+\frac{1}{n}\,\delta K. \tag{7.25}$$

Due to this outcome, the equation $k=\text{const.}=\dot{K}$ becomes

$$\dot{K}=Kd(b_{[1]}-b)\,\delta d+K^2d(\,\delta b-\delta b_{[1]})-K(b_{[1]}-b)\langle d\,\delta d\rangle+\frac{1}{n}\,K^2(b_{[1]}-b)\,\delta K+K^3(s_{[2]}-s_{[1]}). \tag{7.26}$$

Taking the average of both sides in this equation, we obtain

$$\dot{K}=K\langle d(b_{[1]}-b)\,\delta d\rangle+K^2\langle d(\,\delta b-\delta b_{[1]})\rangle; \tag{7.27}$$

Eq. (7.26) also determines the difference $s_{[2]}-s_{[1]}$. With these tangency prescriptions, $S_v\delta V$ is fully determined. These results mean that the third tensor $\mathscr{S}$ is Dirac restrictable; the explicit expression of the restriction is immediately found to be as in Eq. (7.13), and this concludes the proof. ◇

From the proper reducibility of $\mathscr{Q}$ and from the representations $\mathscr{X}_k=\mathscr{Q}dh_{k+1}$, $\mathscr{Y}_k=\mathscr{Q}df_{k+1}$, it follows that the vector fields $\mathscr{X}_k$ and $\mathscr{Y}_k$ are also restrictable from $\mathfrak{g}$ to $\mathbb{R}_*\times\mathbb{R}_n\times\mathbb{R}_n$ along J. The symbols $\mathscr{X}_k$, h_k, etc. will be maintained to denote the restrictions of the vector fields and the Hamiltonians, which satisfy the usual recursion schemes w.r.t. the restricted Poisson tensors $\mathscr{Q}$, $\mathscr{P}$ and $\mathscr{S}$. For $z=(K,d,b)$, we find

$$h_1(z)=\sum_0 b,\quad h_2(z)=\sum_0\left(\frac{1}{2}\,b^2+Kd\right),\quad h_3(z)=\sum_0\left(\frac{1}{3}\,b^3+Kdb+Kdb_{[1]}\right), \tag{7.28}$$

and so on; the components of the vector field $\mathscr{X}_1$ at z are

$$\dot{K}=0,\quad \dot{d}=2d(b-b_{[1]}),\quad \dot{b}=2K(d_{[-1]}-d). \tag{7.29}$$

C. A projection of the triHamiltonian scheme

Let us consider the product $\mathbb{R}_n\times\mathbb{R}_n$, and denote with $y=(c,b)$ a typical point. Tangent vectors and covectors at y are represented as pairs $\dot{y}=(\dot{c},\dot{b})$ and $\delta y=(\delta c,\delta b)$, respectively, with the duality $\langle\delta y,\dot{y}\rangle=\Sigma_0(\delta c\dot{c}+\delta b\dot{b})$.

Definition 7.6: π:$\mathbb{R}_*\times\mathbb{R}_n\times\mathbb{R}_n\to\mathbb{R}_n\times\mathbb{R}_n$ is the projection given by

$$\pi(K,d,b):=(Kd,b). \tag{7.30}$$

◇

For $z=(K,d,b)$ and $y=\pi(z)$, the tangent map $T_z\pi:\mathbb{R}\times\mathbb{R}_n\times\mathbb{R}_n\to\mathbb{R}_n\times\mathbb{R}_n$ sends a vector $\dot z=(\dot K,\dot d,\dot b)$ into the vector $\dot y=(\dot c,\dot b)$, with $\dot c=\dot K d+K\dot d$. The cotangent map $T_z^*\pi:\mathbb{R}_n\times\mathbb{R}_n\to\mathbb{R}\times\mathbb{R}_n\times\mathbb{R}_n$ is defined by the condition $\langle (T_z^*\pi)\,\delta y,\dot z\rangle=\langle \delta y,(T_z\pi)\dot z\rangle$ for each δy and $\dot z$; $T_z^*\pi$ sends $\delta y=(\delta c,\delta b)$ into $\delta z=(\delta K,\delta d,\delta b)$, with $\delta K=\Sigma_0(d\,\delta c),\delta d=K\,\delta c$.

Our aim in this subsection is to project along π the triHamiltonian structure of Prop. 7.5. Before passing to this operation, we suggest a geometrical interpretation for the map (7.30), recalling that its domain $\mathbb{R}_*\times\mathbb{R}_n\times\mathbb{R}_n$ is the ''coordinate space'' of the extended Kupershmidt submanifold $\mathscr{H}$. According to this interpretation, the codomain $\mathbb{R}_n\times\mathbb{R}_n$ of π is the coordinate space for a quotient $\mathscr{H}/\!\sim$, where $\sim$ is an appropriately defined equivalence relation, and π corresponds to the quotient map. The relation $\sim$ arises from the remark that an arbitrary element $V=V(K,d,b)$ of $\mathscr{H}$ can be written as

$$V=\widetilde\Delta+b+\widetilde\Delta^{-1}c,\quad c:=Kd,\quad \widetilde\Delta:=K\Delta. \tag{7.31}$$

Some interesting conclusions can be drawn from this representation; for example, we will show that the traces $\mathrm{Tr}\,V^k(K,d,b)$ depend only on b and the product $Kd=c$.

Definition 7.7: Given the operators $V=V(K,d,b)$ and $V'=V(K',d',b')$ in $\mathscr{H}$, we write $V\sim V'$ if $b=b'$ and $Kd=K'd'$. ◇

This is clearly an equivalence relation. There is a natural diffeomorphism $I:(\mathscr{H}/\!\sim)\to\mathbb{R}_n\times\mathbb{R}_n$, which associates to any point $V(K,d,b)\,\mathrm{mod}\,\sim$ in the quotient space the pair $(c,b):=(Kd,b)$. Employing I and the diffeomorphism $J^{-1}:\mathscr{H}\to\mathbb{R}_*\times\mathbb{R}_n\times\mathbb{R}_n$, we conclude that the quotient map $\mathscr{H}\to\mathscr{H}/\!\sim$ is just the composition $I^{-1}\circ\pi\circ J^{-1}$, with π as in Eq. (7.30). By elementary computations, one can prove the following.

Proposition 7.8: The Poisson tensors (7.11)–(7.13) carried by $\mathbb{R}_*\times\mathbb{R}_n\times\mathbb{R}_n$ can be projected onto $\mathbb{R}_n\times\mathbb{R}_n$ along π, in the sense of Prop. 2.5. The projected tensors, denoted with the same letters plus a superscript $\sim$, have the following expressions:

$$\widetilde{\mathscr{Q}}_y\,\delta y=\dot y,\quad \begin{cases}\dot c:=2c\,\delta b-2c\,\delta b_{[1]},\\ \dot b:=2c_{[-1]}\delta c_{[-1]}-2c\,\delta,\end{cases} \tag{7.32}$$

$$\widetilde{\mathscr{P}}_y\,\delta y=\dot y,\quad \begin{cases}\dot c:=2c(c_{[-1]}\delta c_{[-1]}-c_{[1]}\delta c_{[1]}+b\,\delta b-b_{[1]}\delta b_{[1]}),\\ \dot b:=2b(c_{[-1]}\delta c_{[-1]}-c\,\delta c)+2(c_{[-1]}\delta b_{[-1]}-c\,\delta b_{[1]}),\end{cases} \tag{7.33}$$

$$\widetilde{\mathscr{S}}_y\,\delta y=\dot y,\quad \begin{cases}\dot c=2c(bc_{[-1]}\delta c_{[-1]}-b_{[1]}c_{[1]}\delta c_{[1]})+c(c_{[-1]}\delta b_{[-1]}-c_{[1]}\delta b_{[2]})\\ \quad +c(c+b^2)\,\delta b-c(c+b_{[1]}^2)\,\delta b_{[1]},\\ \dot b=c_{[-2]}c_{[-1]}\delta c_{[-2]}-cc_{[1]}\delta c_{[1]}+c_{[-1]}(c_{[-1]}+b^2)\,\delta c_{[-1]}\\ \quad -c(c+b^2)\,\delta c+c_{[-1]}(b_{[-1]}+b)\,\delta b_{[-1]}-c(b+b_{[1]})\,\delta b_{[1]}.\end{cases} \tag{7.34}$$

◇

Proposition 7.9: The Hamiltonian functions h_k,f_k and the vector fields $\mathscr{X}_k,\mathscr{Y}_k$ on $\mathbb{R}_*\times\mathbb{R}_n\times\mathbb{R}_n$ are projectable onto $\mathbb{R}_n\times\mathbb{R}_n$ along π.

Proof: The projectability of the vector fields follows from the previous Prop. 7.8, if one shows that the Hamiltonians can be projected. The f_k's are functions of the h_k's, so it suffices to show the projectability of each function $h_k(K,d,b)=1/k\ \mathrm{Tr}\,V^k(K,d,b)$. To this purpose, we recall that each

operator $V=V(K,d,b)\in\mathscr{H}$ can be written as in Eq. (7.31), using the rescaled shift operator $\tilde{\Delta}=K\Delta$. From Eq. (7.31), it follows that we can write $V=\Sigma_{\sigma=-1,0,1}v_\sigma\tilde{\Delta}^\sigma$, with $v_{-1}:=c_{[-1]}$, $v_0:=b$, $v_1:=1$. For each positive integer k, it is

$$V^k(K,d,b)=\sum_{\sigma=-k}^{k}v_{k,\sigma}(c,b)\tilde{\Delta}^\sigma=\sum_{\sigma=-k}^{k}K^\sigma v_{k,\sigma}(c,b)\Delta^\sigma, \tag{7.35}$$

where the coefficients $v_{k,\sigma}(c,b)\in\mathbb{R}_n$ are suitable functions of c and b. By taking the traces, we obtain $h_k(K,d,b)=(1/k)\Sigma_0 v_{k,0}(c,b)$; so, each h_k depends only on c,b and the projectability is proved. ◇.

Definition 7.10: The projections along π of the Hamiltonians and vector fields will be indicated with the same letters plus a superscript $\sim$: $\tilde{h}_k,\tilde{f}_k,\tilde{\mathscr{X}}_k,\tilde{\mathscr{Y}}_k$. ◇

At each point $y=(c,b)$, we have

$$\tilde{h}_1(y)=\sum_0 b,\quad \tilde{h}_2(y)=\sum_0\left(\frac{1}{2}b^2+c\right),\quad \tilde{h}_3(y)=\sum_0\left(\frac{1}{3}b^3+cb+cb_{[1]}\right), \tag{7.36}$$

and so on; the first vector field $\tilde{\mathscr{X}}_1$ has components $\dot{c},\dot{b}$ as in Eq. (1.3); here, it was already observed that the flow of $\tilde{\mathscr{X}}_1$ gives the time evolution of the Toda lattice, the connection with the Flaschka variables being the transformation $c=a^2$.

D. The Kupershmidt submanifold and the Lax formalism for the vector fields $\tilde{\mathscr{X}}_k$

The Lax formalism for the Toda lattice set up in Ref. 13 does not envolve directly the manifold $\mathscr{H}$ of Def. 7.4, but rather the subset of operators obtained setting $K=1$ in Eq. (7.9).

Definition 7.11: For each $y=(c,b)\in\mathbb{R}_n\times\mathbb{R}_n$, we put

$$V(y):=\Delta+b+\Delta^{-1}c. \tag{7.37}$$

The embedding $\mathbb{R}_n\times\mathbb{R}_n\to\mathfrak{g}$, $y\mapsto V(y)$ will be be denoted by Σ. Its image $\mathscr{K}\subset\mathscr{H}$ will be called the Kupershmidt submanifold. ◇

Recalling the diagram (4.14) and Eq. (4.13), one can check that, for each $y=(c,b)$, $V(y)$ is the image under the map $\Psi_\circ^{-1}\Phi^{-1}$ of the homologous element of the loop algebra $gl(n)(\lambda,\lambda^{-1}]$ in Eq. (1.4). If we think geometrically in terms of the equivalence relation $\sim$ on $\mathscr{H}$ and employ the diffeomorphism $I:(\mathscr{H}/\sim)\to\mathbb{R}_n\times\mathbb{R}_n$ (see the previous subsection), we can describe $\Sigma\circ I$ as a section of the quotient bundle $\mathscr{H}\to\mathscr{H}/\sim$.

It is straightforward to check that the Poisson tensors $\mathscr{Q},\mathscr{P}$ (Eqs. (7.6)–(7.7)) can be restricted directly from $\mathfrak{g}$ to $\mathbb{R}_n\times\mathbb{R}_n$ along Σ (the first one properly, the second in the Dirac sense). Performing the necessary computations, one finds that the restrictions coincide exactly with the tensors $\tilde{\mathscr{Q}}$ and $\tilde{\mathscr{P}}$ of Eqs. (7.32-33), previously obtained by the restriction/projection algorithm of Secs. VII B and C. Also, the vector fields $\mathscr{X}_k$ on $\mathfrak{g}$ are restrictable via Σ; the restrictions coincide with the vector fields $\tilde{\mathscr{X}}_k$, constructed previously with the restriction/projection method. The Lax formulation for these fields follows immediately from Eq. (7.8), with the Lax operator (7.37); this final result agrees with the Lax scheme of Ref. 13.

On the contrary, the third r-matrix Poisson tensor carried by $\mathfrak{g}$ (Eq. (7.7)) cannot be restricted: the tangency constraints for $\mathscr{S}_v\delta V$ appearing if one tries a Dirac reduction have no periodic solution in general.

E. A comparison with the framework of Sec. V

Let $\mathbb{R}_n^+$ denote the open subset of $\mathbb{R}_n$ formed by the periodic sequences $v=(v_\alpha)_{\alpha\in\mathbb{Z}}$ with $v_\alpha>0$ for each α.

Definition 7.12: $F:\mathbb{R}_n^+\times\mathbb{R}_n\to\mathbb{R}_n^+\times\mathbb{R}_n$ is the diffeomorphism given by

$$F(a,b):=(a^2,b). \tag{7.38}$$

◇

A point to which F is applied will be typically denoted with x or (a,b) as above; its image under F will be generally written as $y=(c,b)$. The inverse map is obviously given by $F^{-1}(c,b)=(\sqrt{c},b)$.

Proposition 7.13: Consider on $\mathbb{R}_n^+\times\mathbb{R}_n$ the Poisson structures Q, P and S given by Eqs. (5.9)–(5.11), and $\tilde{Q}$, $\tilde{P}$ and $\tilde{S}$ as in Eqs. (7.32)–(7.34). Denoting by F_* the push-forward along F, we have $F_*Q=2\tilde{Q}$, $F_*P=2\tilde{P}$, $F_*S=2\tilde{S}$.

Proof: Let us consider, for example, the tensor Q; at any point $y=(c,b)$, it is

$$(F_*Q)_y:=(T_xF\circ Q_x\circ T_x^*F)|_{x=F^{-1}(y)}, \tag{7.39}$$

where T_xF and T_x^*F denote, respectively, the tangent map of F at x and its adjoint, given by $(T_xF)(\dot{a},\dot{b})=(2a\dot{a},\dot{b})$, $(T_x^*F)(\delta c,\delta b)=(2a\delta c,\delta b)$. A straightforward computation gives $F_*Q=2\tilde{Q}$; the analogous relations for $\tilde{P}$ and $\tilde{S}$ are proved similarly. ◇

To complete the comparison with Sec. V, we point out a relevant connection between the operators $V(K,d,b)$, given by Eq. (7.9), and $L(a,b)$ in Eq. (5.7), existing if $Kd=a^2$. This relation can be illustrated in terms of the following.

Definition 7.14: Two operators $L,V\in\mathfrak{g}$ are said to be gauge equivalent if there exists an n-periodic sequence $s=(s_\alpha)_{\alpha\in\mathbb{Z}}$ such that $s_\alpha\neq 0$ for each α, and

$$sL\,\frac{1}{s}=V, \tag{7.40}$$

intending the l.h.s. of the above equation as the product in $\mathfrak{g}$ among L, the sequence s and its reciprocal $(1/s):=(1/s_\alpha)$. ◇

Proposition 7.15: For each $(a,b)\in\mathbb{R}_n^+\times\mathbb{R}_n$, there exist $K>0$, $d\in\mathbb{R}_n^+$ and a never zero sequence $s\in\mathbb{R}_n$ such that $Kd=a^2$ and

$$sL(a,b)\,\frac{1}{s}=V(K,b,d). \tag{7.41}$$

Proof: For each sequence $v\in\mathbb{R}_n$, we put $\Pi_0 v:=\Pi_{\alpha=1}^n v_\alpha$. Equation (7.41) is satisfied setting $K:=(\Pi_0 a)^{1/n}$, $d:=a^2/K$ and taking for s a periodic solution[37] of the equation $s_{[1]}=(a/K)s$. ◇

The previous result can be used to prove that the diffeomorphism F transforms the Hamiltonians $h_k(a,b)$ of Sec. V into the Hamiltonians $\tilde{h}_k(c,b)$ of Sec. VII C.

Proposition 7.16: For $(a,b)\in\mathbb{R}_n^+\times\mathbb{R}_n$ and $(c,b)=F(a,b)$, it is $\tilde{h}_k(c,b)=h_k(a,b)$.

Proof: By definition, $\tilde{h}_k(c,b):=(1/k)\mathrm{Tr}\,V^k(K,d,b)$, where $V(K,d,b)$ is any operator with $Kd=c$; also, we know that $h_k(a,b)=(1/k)\mathrm{Tr}\,L^k(a,b)$. We can choose K and d as in the previous Proposition, so as to set up a gauge equivalence; then

$$\mathrm{Tr}\,V^k(K,d,b)=\mathrm{Tr}\left(sL^k(a,b)\,\frac{1}{s}\right)=\mathrm{Tr}\left(\frac{1}{s}\,sL^k(a,b)\right)=\mathrm{Tr}\,L^k(a,b). \tag{7.42}$$

◇

Corollary 7.17: Consider on $\mathbb{R}_n^+\times\mathbb{R}_n$ the vector fields $X_k=P\,dh_k$ of Secs. V and VI and $\tilde{\mathscr{X}}_k=\tilde{\mathscr{P}}d\tilde{h}_k$ of Sec. VII C. For each k, it is $F_*X_k=2\tilde{\mathscr{X}}_k$ $(k=1,2,3,\ldots)$. ◇

Here, $F_* X_k$ stands for the push-forward, i.e., the vector field $y \mapsto (T_x F) X_k(x)|_{x=F^{-1}(y)}$; the thesis follows from Props. 7.13 and 7.16. Of course, two statements similar to Prop. 7.16 and Corollary 7.17 hold for the Hamiltonians $f_k, \tilde{f}_k$ and the associated vector fields $Y_k, \tilde{Y}_k$.

VIII. COMMENTS

This article is devoted to the periodic Toda lattice, but the r-matrix methods can be as well applied to other lattices. The system in $2N$ field variables $b, c_1, \ldots, c_{2N-1}$, described by the ''Kupershmidt-like'' Lax operator

$$V = \Delta + b + \sum_{k=1}^{2N-1} \Delta^{-k} c_k, \tag{8.1}$$

was treated in Ref. 11 in the infinite nonperiodic case; its periodic counterpart can be discussed assuming $b, c_1, \ldots, c_{2N-1}$ to be n-periodic sequences. For $N=1$, one reobtains the Toda theory in the field variables b and $c_1 := c$ [see Eq. (7.37)].

As a generalization, it is possible to analyze the theory in infinitely many field variables $b, c_k \in \mathbb{R}_n(\Delta, \Delta^{-1}]$, described by the Lax operator

$$V = \Delta + b + \sum_{k=1}^{+\infty} \Delta^{-k} c_k, \tag{8.2}$$

which can be regarded as a periodic analogue of the so-called ''full Kostant Toda lattice,'' or a discrete version of the KP theory (for the multi-Hamiltonian structure of this system, independently of r-matrix theory, see Ref. 13).

Finally, the treatment of Sec. V could be extended to the system in $2N$ field variables $b, a_1, \ldots, a_{2N-1} \in \mathbb{R}_n(\Delta, \Delta^{-1}]$, described by the symmetric Lax operator

$$L = \sum_{k=1}^{2N-1} a_k \Delta^k + b + \sum_{k=1}^{2N-1} \Delta^{-k} a_k. \tag{8.3}$$

It should be noticed that, with the exception of the Toda case $N=1$, the systems in Eqs. (8.1) and (8.3) are essentially different: in fact, their Lax operators are not gauge equivalent.

Also, it would be of interest to analyze the continuous limits of the above lattices; for example, these could be treated with the methods proposed in Ref. 38; work on this point is in progress, and it turns out that the limiting systems can be classified in terms of the Drinfeld–Sokolov scheme for KdV-type hierarchies.[39]

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[36] If n is odd, any sequence $w \in \mathbb{R}_n$ such that $w_{[2]}-w=0$ is constant: $w_\alpha = H$ for each $\alpha \in \mathbb{Z}$; the supplementary requirement on the average of r uniquely fixes H. If n is even, it is $w_{[2]}-w=0$ if there are two constants H and H' such that $w_\alpha = H$ for α even and $w_\alpha = H'$ for α odd. The condition on the average of r fixes the sum $H+H'$.
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Symplectic completion of symplectic jets

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In this paper, we outline a method for symplectic integration of three degree-of-freedom Hamiltonian systems. We start by representing the Hamiltonian system as a symplectic map. This map (in general) has an infinite Taylor series. In practice, we can compute only a finite number of terms in this series. This gives rise to a truncated map approximation of the original map. This truncated map is however not symplectic and can lead to wrong stability results when iterated. In this paper, following a generalization of the approach pioneered by Irwin (SSC Report No. 228, 1989), we factorize the map as a product of special maps called ''jolt maps'' in such a manner that symplecticity is maintained. © *1996 American Institute of Physics.* [S0022-2488(96)03509-8]

I. INTRODUCTION

Consider a complicated periodic Hamiltonian system that is non-integrable. Suppose we are interested in the long-term stability of particles being transported through this system. Since the system is assumed to be nonintegrable, it is very difficult to give stability criteria in an analytic form. A possible solution is to numerically follow the trajectories of particles through the system for a large number of periods (a process that goes by the name of tracking). One could then attempt to infer the stability of motion in the system by analyzing these tracking results.

The most straightforward method that can be used to perform this long term tracking is numerical integration. However, this method is too slow for analyzing the stability of very complicated systems. Therefore, we need a method that is both fast and accurate.

Several symplectic integration methods have been discussed in the literature. Ruth,[1] Feng,[2] Channel and Scovel,[3] Yoshida,[4] Berg *et al.*[5] and others have derived symplectic integrators using generating functions. These are typically implicit methods and using these methods requires one to use Newton's method with its attendent questions of convergence, etc. Another approach is through solvable maps.[6,7] But this method has not been explored in great detail. In this paper, following Irwin,[8] we explore a more direct method of symplectic integration.

The method that we will use is the iteration of symplectic maps[9] representing the Hamiltonian system. We start by defining certain mathematical objects. Let us denote the collection of six phase space variables q_i, p_i $(i=1,2,3)$ by the symbol z:

$$z=(q_1,p_1,q_2,p_2,q_3,p_3). \tag{1.1}$$

The Lie operator corresponding to a phase space function $f(z)$ is denoted by $:f(z):$. It is defined by its action on a phase-space function $g(z)$ as shown below

$$:f(z):g(z)=[f(z),g(z)]. \tag{1.2}$$

Here $[f(z),g(z)]$ denotes the usual Poisson bracket of the functions $f(z)$ and $g(z)$. Next, we define the exponential of a Lie operator. It is called a Lie transformation and is given as follows:

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$$e^{:f(z):}=\sum_{n=0}^{\infty}\frac{:f(z):^n}{n!}. \tag{1.3}$$

Powers of $:f(z):$ that appear in the above equation are defined recursively by the relation

$$:f(z):^n g(z)=:f(z):^{n-1}[f(z),g(z)], \tag{1.4}$$

with

$$:f(z):^0 g(z)=g(z). \tag{1.5}$$

For further details regarding Lie operators and Lie transformations, see Ref. 9.

The time evolution of the Hamiltonian system over one period can be represented by a symplectic map $\mathscr{M}$.[9] Symplectic maps are maps whose Jacobian matrices $M(z)$ satisfy the following symplectic condition:

$$\widetilde{M(z)}JM(z)=J, \tag{1.6}$$

where $\widetilde{M}$ is the transpose of M and J is an antisymmetric matrix defined as follows:

$$J=\begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 \end{pmatrix}. \tag{1.7}$$

Matrices M satisfying Eq. (1.6) are called symplectic matrices and the corresponding maps $\mathscr{M}$ symplectic maps. It can be shown[9] that the set of all $\mathscr{M}$'s forms an infinite dimensional Lie group of symplectic maps. On the other hand, the set of all real 6×6 symplectic matrices forms the finite dimensional real symplectic group Sp(6,R).

Using the Dragt–Finn factorization theorem,[9,10] the symplectic map $\mathscr{M}$ can be factorized as shown below:

$$\mathscr{M}=\hat{M}e^{:f_3:}e^{:f_4:}\ldots e^{:f_n:}\ldots \ . \tag{1.8}$$

Here $\hat{M}$ gives the linear part of the map and hence has an equivalent representation in terms of the Jacobian matrix $M(0)$ of the map $\mathscr{M}$ at the origin:[9]

$$\hat{M}z_i=M_{ij}z_j=(Mz)_i. \tag{1.9}$$

Thus, $\hat{M}$ is said to be the Lie transformation corresponding to the 6×6 matrix M belonging to Sp(6,R). The infinite product of Lie transformations $\exp(:f_n:)$ $(n=3,4,\ldots)$ in Eq. (1.8) represents the nonlinear part of $\mathscr{M}$. Here $f_n(z)$ denotes a homogeneous polynomial (in z) of degree n uniquely determined by the factorization theorem.

The above map $\mathscr{M}$ is called the one-period map for the system. It gives the final state $z^{(1)}$ of a particle after one period as a function of its initial state $z^{(0)}$:

$$z^{(1)}=\mathscr{M}z^{(0)}. \tag{1.10}$$

To obtain the state of a particle after N periods, one has to merely iterate the above mapping N times, i.e.,

$$z^{(N)}=\mathcal{M}^N z^{(0)}. \tag{1.11}$$

It is obvious that one cannot use $\mathcal{M}$ in the form given in Eq. (1.8) for any practical computations. It involves an infinite number of Lie transformations. Therefore, we have to truncate $\mathcal{M}$ by stopping after a finite number of Lie transformations:

$$\mathcal{M}\approx\hat{M}e^{:f_3:}e^{:f_4:}\cdots e^{:f_P:}. \tag{1.12}$$

However, we are still not out of the woods. Each exponential $e^{:f_n:}$ in $\mathcal{M}$ contains an infinite number of terms in its Taylor series expansion. One possible solution is to truncate the Taylor series generated by the Lie transformations to order P. We denote this truncated map by $\mathcal{M}_P$. As a power series in the six phase space variables, it is given as follows:

$$\mathcal{M}_P z=M(1+:f_3:+\cdots)(1+:f_4:+\cdots)$$

$$\cdots(1+:f_p:+\cdots)z, \tag{1.13}$$

where we have to truncate the power series in such a way that the highest order term generated is z^{P-1}. If we did not impose this restriction, we would generate terms of order z^P and higher. Then, to be consistent, we would be forced to include in our map, $:f_n:$'s for n greater than P (since these also generate terms of order z^P and higher).

Equation (1.13) can be rewritten as follows:

$$\mathcal{M}_P z=h_1(z)+h_2(z)+\cdots+h_{P-1}(z), \tag{1.14}$$

where $h_n(z)$ denotes a polynomial of degree n in z. Since we have decided to consistently drop terms of order z^P and higher, we can define the following equivalence relation between maps of order P:

$$\mathcal{M}_P\sim\mathcal{M}'_P \quad \text{if } \mathcal{M}_P z-\mathcal{M}'_P z=h_P(z)+\text{higher order terms}. \tag{1.15}$$

This can be rephrased in terms of partial derivatives as follows. Maps $\mathcal{M}_P$ and $\mathcal{M}'_P$ are equivalent if all the partial derivatives of $\mathcal{M}_P z$ and $\mathcal{M}'_P z$ up to order $P-1$ are equal. An equivalence class with respect to this equivalence relation is called a jet of order P. Since the map $\mathcal{M}_P$ is obtained from a symplectic map $\mathcal{M}$, we call $\mathcal{M}_P$ (or more accurately, the equivalence class to which it belongs) a symplectic jet of order P. We stress that, despite its name, $\mathcal{M}_P$ is not symplectic.

We note that symplectic jets of order P have the following properties. A symplectic jet maps $\mathbb{R}^6$ into $\mathbb{R}^6$. It maps the origin of $\mathbb{R}^6$ into itself. It is invertible. And the composition of two symplectic jets $\mathcal{M}_P$ and $\mathcal{M}'_P$ is defined as follows:

$$\mathcal{M}_P\cdot\mathcal{M}'_P=(\mathcal{M}\cdot\mathcal{M}')_P. \tag{1.16}$$

This is again a symplectic jet of order P. And finally, there exists an identity given by the following equivalence class:

$$\mathcal{M}^0_P z=z+h_P(z)+\text{higher order terms}. \tag{1.17}$$

Therefore, the set of all symplectic jets of order P forms a group. It can be shown that it is actually a Lie group. This Lie group formed by the set of all symplectic jets of order P is called the symplectic jet group Spj(6;P).

However, the above solution of truncating the Taylor series has a severe shortcoming. As mentioned above, the mapping $\mathcal{M}_P$ generated by the truncated Taylor series is no longer symplectic. Therefore, repeated iterations of this mapping can lead to spurious growth (or damping) in

the amplitude of motion of the particle being tracked. Obviously, this can lead to wrong conclusions regarding the stability of the system. Therefore it is important to preserve the symplectic nature of $\mathscr{M}_P$ when using it for long term tracking. For this purpose, we need to ensure that each factor in $\mathscr{M}_P$ takes the form $e^{:g:}$. On the other hand, for the numerical tracking scheme to be practical, we need to ensure that we evaluate only a finite number of terms. In this paper, we discuss how to reconcile these two apparently contradictory objectives.

The basic goal of this paper is to refactorize $\mathscr{M}_P$ [cf. Eq. (1.13)] as a product of symplectic maps that can be evaluated exactly. Since we do not truncate the Taylor series, we preserve the symplectic nature of the map even when we evaluate it. Another attractive feature of these special maps is that their inverses can also be evaluated exactly. The process of refactorizing a map into a product of symplectic maps characterized by these nice features is called ''symplectic completion''. Since the map that is being refactorized is $\mathscr{M}_P$, a symplectic jet, this refactorization procedure is called ''symplectic completion of symplectic jets''. And this will be the subject of this paper.

We start by defining jolt maps in Section II. In Section III, we formulate the problem of symplectic completion of $\mathscr{M}_P$ in terms of these jolt maps. Here, we follow the procedure first outlined by Irwin.[8] To get a better understanding of the problem, we first solve a model problem in Section IV. In Section V, we formulate a solution to the problem of symplectic completion of symplectic jets. In Section VI, we optimize the number of jolt maps required so that an efficient numerical algorithm is obtained.

II. JOLT MAPS

Consider the symplectic map given by $e^{:g(z):}$ where $g(z)$ is a function of the phase space variables z. It is called a jolt map if $:g(z):$ is a nilpotent operator of rank 2, i.e., if the following condition is satisfied:

$$:g(z):^2 z = 0. \tag{2.1}$$

The function $g(z)$ is then called a jolt function. We note that jolt maps have only two nonzero terms in their Taylor series expansions [cf. Eq. (1.3)]. The term jolt map was first introduced in Ref. 11.

Examples of jolt maps are given by the following theorem.

Theorem 1: *The following maps are jolt maps*

$$\text{(i)}\quad \hat{R} e^{:q_1^n:} \hat{R}^{-1} = e^{:\hat{R} q_1^n:}, \tag{2.2}$$

$$\text{(ii)}\quad \hat{R} e^{:f(q_1,q_2,q_3):} \hat{R}^{-1} = e^{:\hat{R} f(q_1,q_2,q_3):}. \tag{2.3}$$

Here $f(q_1,q_2,q_3)$ is an nth degree polynomial in variables q_1, q_2, and q_3. Finally, $\hat{R}$ is the Lie transformation corresponding to a 6×6 *matrix R belonging to any subgroup of* Sp(6,R) *[including* Sp(6,R) *itself]. It is given by the following relation [cf. Eq. (1.9)]:*

$$\hat{R} z_i = R_{ij} z_j = (Rz)_i. \tag{2.4}$$

See Appendix A for a proof of this theorem. In this theorem, note that the second statement contains the first statement as a special case. However, a separate (and simpler) proof is given even for the first statement since we will be using this later in the paper.

III. FORMULATION OF THE PROBLEM OF JOLT FACTORIZATION

Our goal is to refactorize $\mathscr{M}_P$ [cf. Eq. (1.13)] in terms of a finite number of jolt maps. The first step towards achieving this goal is to formulate the problem in an appropriate form. The best way to mathematically formulate the problem appears to be as follows[8]:

Problem 1: *Given the map $\mathscr{M}_P$, find another map $\mathscr{J}$ specified by the following product of K jolt maps*:

$$\mathscr{J}=\hat{M}e^{:g_3^{(1)}+g_4^{(1)}+\cdots+g_P^{(1)}:}e^{:g_3^{(2)}+g_4^{(2)}+\cdots+g_P^{(2)}:}\cdots e^{:g_3^{(K)}+g_4^{(K)}+\cdots+g_P^{(K)}:} \tag{3.1}$$

such that this map agrees with $\mathscr{M}_P$ to order P, i.e.,

$$\mathscr{J}\cong\mathscr{M}_P \quad \text{to order } P. \tag{3.2}$$

Here $g_n^{(i)}$'s are (homogeneous) jolt polynomials of degree n given by the following relation:

$$g_n^{(i)}=\beta_n^{(i)}\hat{R}_i q_1^n, \quad i=1,2,\ldots,K, \tag{3.3}$$

where $\beta_n^{(i)}$ is a real coefficient. The matrices R_i belong to a subgroup of Sp(6,R) *[including* Sp(6,R) *itself] and $\hat{R}_i$ denotes the Lie transformation corresponding to these matrices [cf. Eq. (2.4)]*.

Before proceeding further, we note that Eq. (3.1) can be rewritten in the following form:

$$\mathscr{J}=\hat{M}e^{:g^{(1)}:}e^{:g^{(2)}:}\cdots e^{:g^{(K)}:}, \tag{3.4}$$

where

$$g^{(i)}=g_3^{(i)}+g_4^{(i)}+\cdots g_P^{(i)} \quad i=1,2,\ldots,K. \tag{3.5}$$

From Eq. (3.3) and Theorem 1 [cf. Eq. (2.2)] it is seen that $g^{(i)}$'s are jolt polynomials (a sum of jolt polynomials is easily shown to be another jolt polynomial). Consequently, $\exp(:g^{(i)}:)$'s are jolt maps.

In order to solve the above problem, we need to determine the various unknown quantities appearing in the above equations—the number of jolt maps K, the matrices R_i, and the coefficients $\beta_n^{(i)}$. It turns out that K and R_i can be determined independent of the details of the map $\mathscr{M}_P$. They depend only on the order P of the map. This will be explicitly demonstrated shortly. For the moment, we will assume that K and R_i have already been fixed. This reduces our task to merely finding the coefficients $\beta_n^{(i)}$'s such that Eq. (3.2) is satisfied. We now proceed to solve for these coefficients order by order.

Since the linear part of a symplectic map can be evaluated exactly, there is no need to refactorize it in terms of jolt maps. Hence, we have already chosen the linear parts of the maps $\mathscr{M}_P$ and $\mathscr{J}$ to be the same. Therefore, we need to refactorize only the nonlinear part of $\mathscr{M}_P$. We start by comparing terms of order 3 in $\mathscr{M}_P$ and $\mathscr{J}$ respectively. The third-order term in $\mathscr{M}_P$ is given by f_3. To obtain the third-order term in $\mathscr{J}$, we need to cast it in the standard Dragt–Finn form. This is accomplished by using the Baker–Campbell–Hausdorff (BCH) formula[10] given below:

$$\exp(t:f:)\exp(s:g:)=\exp(t:f:+s:g:+ts:[f,g]:/2+\cdots). \tag{3.6}$$

We get the following result to third order:

$$\mathscr{J}\cong\hat{M}e^{:h_3:}, \tag{3.7}$$

where

$$h_3=\sum_{i=1}^{K} g_3^{(i)}. \tag{3.8}$$

Therefore, $\mathscr{J}$ and $\mathscr{M}_P$ will be equal to order 3 if the following equality is satisfied [cf. Eq. (3.3)]:

$$\sum_{i=1}^{K} \beta_3^{(i)} \hat{R}_i q_1^3 = f_3. \tag{3.9}$$

In other words, we have to determine $\beta_3^{(i)}$'s such that the above equation is satisfied.

Next, we compare terms of order 4 in $\mathscr{M}_P$ and $\mathscr{J}$. The fourth-order term in $\mathscr{M}_P$ is given by f_4. Using the BCH formula, the Dragt–Finn factorization of $\mathscr{J}$ correct to fourth order is given by the following result:

$$\mathscr{J} \cong \hat{M} e^{:h_3:} e^{:h_4:}, \tag{3.10}$$

where

$$h_4=\sum_{i=1}^{K} g_4^{(i)} + \frac{1}{2} \sum_{j<k} [g_3^{(j)}, g_3^{(k)}]. \tag{3.11}$$

The second term on the right hand side of the above equation is a fourth-order term produced by the concatenation of third-order terms in Eq. (3.1). Equating the fourth-order terms of $\mathscr{M}_P$ and $\mathscr{J}$ we get the relation [cf. Eq. (3.3)]

$$\sum_{i=1}^{K} \beta_4^{(i)} \hat{R}_i q_1^4 = f_4 - \frac{1}{2} \sum_{j<k} \beta_3^{(j)} \beta_3^{(k)} [\hat{R}_j q_1^3, \hat{R}_k q_1^3] \equiv f_4'. \tag{3.12}$$

Here f_4' includes the fourth-order terms produced by concatenation of lower order terms. By choosing $\beta_4^{(i)}$'s such that the above equation is satisfied, we ensure that $\mathscr{J}$ and $\mathscr{M}_P$ agree to fourth order.

This process can be continued in a similar fashion to deal with the higher order terms. At the nth order, we have to choose $\beta_n^{(i)}$'s such that the following equality is satisfied:

$$\sum_{i=1}^{K} \beta_n^{(i)} \hat{R}_i q_1^n = f_n'. \tag{3.13}$$

Here f_n' includes the unwanted nth-order terms produced by $g_l^{(i)}$ $(l<n)$.

We are now in a position to determine the number of jolt maps K and the matrices R_i. We will show that they are independent of the map $\mathscr{M}_P$. We note that f_n' involves $N(n)$ independent coefficients where $N(n)$ is given by the relation[8]

$$N(n)=\binom{n+5}{n}. \tag{3.14}$$

Thus, we need at least $N(n)$ $\beta_n^{(i)}$'s to solve the above equation. Since $N(n)$ is a monotonically increasing function of n, the maximum number of $\beta_n^{(i)}$'s are required when n is equal to P (the maximum order). Thus we need $N(P)$ $\beta_n^{(i)}$'s to solve Eq. (3.13) for all n. This fixes K to be equal to $N(P)$. Moreover, $\hat{R}_i q_1^n$ $(i=1,\ldots,K)$ should be linearly independent quantities. This imposes restrictions on the matrices R_i that we can choose. Both these conditions are independent of f_n', i.e., they are independent of the map $\mathscr{M}_P$. They depend only on the maximum order P. Therefore both K and R_i's can be fixed in advance independent of the map to be represented.

Once K and the R_i's are fixed, we start by first solving Eq. (3.9) for $\beta_3^{(i)}$'s. We then proceed order by order until we reach the Pth-order equation. At the nth order, we have to solve Eq. (3.13). The right hand side involves $N(n)$ independent coefficients. Since $N(n)$ is less than K $(=N(P))$ for n less than P, we have more $\beta_n^{(i)}$'s than necessary to solve this equation, i.e., the $\beta_n^{(i)}$'s are underdetermined. The naive solution would be to set these extra $\beta_n^{(i)}$'s to zero

$$\beta_n^{(i)}=0 \quad \text{for } i>N(n). \tag{3.15}$$

But there is a better solution. We fix these extra $\beta_n^{(i)}$'s by requiring that $\Sigma_{i=1}^{K}(\beta_n^{(i)})^2$ be a minimum. The reason for this is simple. We have seen that the nth-order jolt polynomials produce higher order terms [for example, see Eq. (3.11)] upon concatenation. These higher order terms depend on the coefficients $\beta_n^{(i)}$ [for example, see Eq. (3.12)]. Therefore, by minimizing the sum of the squares of these coefficients, we reduce the magnitude of the unwanted higher order terms produced by concatenation of lower order terms.

Putting everything together, the problem of obtaining a jolt map factorization can be reduced to the following general problem:

Problem 2: *Given a nth degree homogeneous polynomial f_n and K matrices R_i, find the coefficients $\beta_n^{(i)}$'s such that the following conditions are satisfied:*

$$\text{(i)} \quad \sum_{i=1}^{K} \beta_n^{(i)} \hat{R}_i q_1^n = f_n \tag{3.16}$$

and

$$\text{(ii)} \quad \sum_{i=1}^{K} [\beta_n^{(i)}]^2 \text{ is a minimum.} \tag{3.17}$$

IV. A MODEL PROBLEM AND ITS SOLUTION

Before attempting to solve the general problem outlined above, we will first solve a model problem in this section. This model problem is deliberately designed to be quite similar to the problem of jolt factorization [cf. Eqs. (3.16) and (3.17)]. Therefore, solving this problem will enable us to get a feel for the issues involved in the solution of the jolt factorization problem.

Consider an arbitrary vector v in the two dimensional $x-y$ plane. It can be expressed as follows:

$$v=v_x e_x+v_y e_y, \tag{4.1}$$

where e_x and e_y are the usual unit vectors along the x and y axes, respectively, and v_x and v_y are the corresponding vector components. Next, we construct a new set of N basis vectors e_i (where N is an integer greater than 2) in the $x-y$ plane using the following procedure:

$$e_i=R(\theta_i)e_x, \quad i=1,2,\ldots,N, \tag{4.2}$$

where

$$R(\theta_i)e_x=\cos(\theta_i)e_x+\sin(\theta_i)e_y \tag{4.3}$$

and

$$\theta_i=(k-1)\,\frac{2\pi}{N}. \tag{4.4}$$

We are now in a position to state the problem—express v in the new basis given by the N e_i's. Of course, only two basis vectors are actually needed to express the vector v. Since we have extra basis vectors, we need to impose a constraint. Taking this into account, the problem can be formulated as follows.

Problem 3: *Given the vector v [cf. Eq. (4.1)], find coefficients* β_i *such that the following conditions are satisfied*:

$$\text{(i)} \quad v=\sum_{i=1}^{N} \beta_i e_i=\sum_{i=1}^{N} \beta_i R(\theta_i)e_x \tag{4.5}$$

and

$$\text{(ii)} \quad \sum_{i=1}^{N} \beta_i^2 \text{ is a minimum.} \tag{4.6}$$

The reader will immediately notice the striking similarity between this problem and the problem of jolt factorization [cf. Eqs. (3.16) and (3.17)].

Instead of solving this particular problem, we will solve the more general problem obtained by going to the continuum limit. Its solution will then contain the solution to the original (discrete) problem as a special case. The generalized problem is given as follows.

Generalized Problem 1: *Given the vector v [cf. Eq. (4.1)], find the function* $g(\theta)$ *such that the following conditions are satisfied:*

$$\text{(i)} \quad v=\frac{1}{2\pi}\int_0^{2\pi} d\theta\, g(\theta)R(\theta)e_x \tag{4.7}$$

and

$$\text{(ii)} \quad \frac{1}{2\pi}\int_0^{2\pi} d\theta\, g^2(\theta) \text{ is a minimum,} \tag{4.8}$$

where

$$R(\theta)e_x=\cos(\theta)e_x+\sin(\theta)e_y\,. \tag{4.9}$$

We solve this generalized problem as follows. We first find functions $g_x(\theta)$ and $g_y(\theta)$ satisfying the following relations:

$$\frac{1}{2\pi}\int_0^{2\pi} d\theta\, g_x(\theta)R(\theta)e_x=e_x\,, \tag{4.10}$$

$$\frac{1}{2\pi}\int_0^{2\pi} d\theta\, g_y(\theta)R(\theta)e_x=e_y\,. \tag{4.11}$$

In other words, the functions $g_x(\theta)$ and $g_y(\theta)$ project out the unit vectors e_x and e_y, respectively. Substituting Eq. (4.9) in the above expressions, we obtain the relations

$$\frac{1}{2\pi}\int_0^{2\pi} d\theta\, g_x(\theta)[\cos(\theta)e_x+\sin(\theta)e_y]=e_x\,, \tag{4.12}$$

$$\frac{1}{2\pi}\int_0^{2\pi} d\theta\, g_y(\theta)[\cos(\theta)e_x+\sin(\theta)e_y]=e_y. \tag{4.13}$$

The cosine and sine functions satisfy the following orthonormality conditions:

$$\frac{1}{2\pi}\int_0^{2\pi} d\theta\, \cos(m\theta)\cos(m'\theta)=\frac{1}{2}\,\delta_{mm'}+\frac{1}{2}\,\delta_{m0}\delta_{m'0}, \tag{4.14}$$

$$\frac{1}{2\pi}\int_0^{2\pi} d\theta\, \sin(m\theta)\sin(m'\theta)=\frac{1}{2}\,\delta_{mm'}-\frac{1}{2}\,\delta_{m0}\delta_{m'0}, \tag{4.15}$$

$$\frac{1}{2\pi}\int_0^{2\pi} d\theta\, \cos(m\theta)\sin(m'\theta)=0, \tag{4.16}$$

where m and m' are arbitrary integers. Using these orthonormality relations, we get the following solution for $g_x(\theta)$ and $g_y(\theta)$:

$$g_x(\theta)=2\cos(\theta);\quad g_y(\theta)=2\sin(\theta). \tag{4.17}$$

Consider the following function

$$g(\theta)=v_x g_x(\theta)+v_y g_y(\theta). \tag{4.18}$$

Substituting this function into the right hand side of Eq. (4.7), we get the following result:

$$\frac{1}{2\pi}\int_0^{2\pi} d\theta[v_x g_x(\theta)+v_y g_y(\theta)]R(\theta)e_x. \tag{4.19}$$

Using Eqs. (4.10) and (4.11), we obtain the relation [cf. Eq. (4.1)]

$$\frac{1}{2\pi}\int_0^{2\pi} d\theta\, g(\theta)R(\theta)e_x=v_x e_x+v_y e_y=v. \tag{4.20}$$

This proves that the function $g(\theta)$ given in Eq. (4.18) is a solution satisfying Eq. (4.7).

Next, we have to show that it also satisfies Eq. (4.8). Using the standard Fourier series expansion, the most general function satisfying Eq. (4.7) is found to be

$$g(\theta)=2v_x\cos(\theta)+2v_y\sin(\theta)+b_0+\sum_{n=2}^{\infty} b_n\cos(n\theta)+\sum_{n=2}^{\infty} a_n\sin(n\theta). \tag{4.21}$$

Using the orthonormality relations [cf. Eqs. (4.14), (4.15), and (4.16)], it is easily verified that this is indeed a solution to Eq. (4.7). Substituting this result into Eq. (4.8), we get the relation

$$\frac{1}{2\pi}\int_0^{2\pi} d\theta\, g^2(\theta)=2(v_x^2+v_y^2)+b_0^2+\sum_{n=2}^{\infty}(a_n^2+b_n^2)/2. \tag{4.22}$$

This is a minimum only if the following condition is satisfied:

$$b_0=0;\quad a_n=b_n=0\quad n>1. \tag{4.23}$$

Imposing these conditions on the general solution [cf. Eq. (4.21)], we get back the particular solution given in Eq. (4.18). Thus, the function $g(\theta)$ displayed below is indeed the solution to the generalized problem stated in Eqs. (4.7) and (4.8):

$$g(\theta)=2v_x\cos(\theta)+2v_y\sin(\theta). \tag{4.24}$$

This solution satisfies the following relation [cf. Eqs. (4.22) and (4.23)]

$$\frac{1}{2\pi}\int_0^{2\pi} d\theta\, g^2(\theta)=2(v_x^2+v_y^2). \tag{4.25}$$

The discrete version of the generalized problem is given as follows: Given the vector v [cf. Eq. (4.1)], find values $g(\theta_i)$ $(i=1,2,\ldots,N)$ such that the following conditions are satisfied:

$$\text{(i)}\quad v=\frac{1}{N}\sum_{i=1}^{N} g(\theta_i)R(\theta_i)e_x \tag{4.26}$$

and

$$\text{(ii)}\quad \frac{1}{N}\sum_{i=1}^{N}[g(\theta_i)]^2 \text{ is a minimum.} \tag{4.27}$$

Comparing this with our original problem [cf. Eqs. (4.5) and (4.6)], we make the following identification:

$$\beta_i=g(\theta_i)/N. \tag{4.28}$$

If we choose the angles θ_i to be equally spaced over the interval $[0,2\pi]$ [as we did in the original problem, cf. Eq. (4.4)], $\cos(\theta_i)$ and $\sin(\theta_i)$ still form an othogonal set. Therefore, the solution $g(\theta)$ [cf. Eq. (4.24)] to the continuum problem is the solution even for the discrete version. The only difference is that $g(\theta)$ is now evaluated only at the discrete set of angles θ_i. Therefore, the coefficients β_i satisfying Eqs. (4.5) and (4.6) are given as follows [cf. Eqs. (4.24) and (4.28)]:

$$\beta_i=[2v_x\cos(\theta_i)+2v_y\sin(\theta_i)]/N. \tag{4.29}$$

The discrete version of Eq. (4.25) is found to be

$$\frac{1}{N}\sum_{i=1}^{N}[g(\theta_i)]^2=2(v_x^2+v_y^2). \tag{4.30}$$

Substituting Eq. (4.28) into this expression, we get the relation

$$\sum_{i=1}^{N}\beta_i^2=\frac{2}{N}(v_x^2+v_y^2). \tag{4.31}$$

We notice that the sum of the squares of the coefficients decreases as the number N of basis vectors increases. We also note that the basis vectors e_i [cf. Eq. (4.2)] form a discrete subgroup of the rotation group if the angles θ_i are equally spaced over the interval $[0,2\pi]$.

V. SOLUTION TO THE PROBLEM OF JOLT FACTORIZATION

In this section, we return to the problem of jolt factorization [cf. Eqs. (3.16) and (3.17)]. In Section II, we had concluded that the problem of obtaining a jolt factorization is equivalent to the

determination of the coefficients $\beta_n^{(i)}$ subject to the conditions given in Eqs. (3.16) and (3.17). Hence, we will achieve our goal if we determine these $\beta_n^{(i)}$'s. However, in the previous section, we had discovered that the solution to such problems is facilitated by going over to the continuum limit. Therefore, we do the same for the problem of jolt factorization and obtain the following generalized problem.

Generalized Problem 2: *Given an nth degree homogeneous polynomial f_n and a subgroup G of* Sp(6,R) *on which invariant integration is well defined, find the function $g(u)$ such that the following conditions are satisfied:*

$$\text{(i)} \quad f_n = \int_G du\ g(u)\hat{R}(u)q_1^n \tag{5.1}$$

and

$$\text{(ii)} \quad \int_G du\ g^2(u) \quad \text{is a minimum.} \tag{5.2}$$

Here u denotes a general element of the group G and $\hat{R}(u)$ denotes the Lie transformation corresponding to u. All integrations are invariant integrations performed over the group G.

First we need to choose the group G. We cannot take G to be Sp(6,R) since Sp(6,R) is a noncompact group and therefore its invariant integrals cannot be normalized. We therefore integrate over a compact subgroup of Sp(6,R). The largest compact subgroup of Sp(6,R) is the unitary group U(3). However, we prefer to use SU(3) since it is more convenient for our purposes. If needed, it is possible to generalize the invariant integrals over SU(3) to those over U(3).

Having chosen G to be SU(3), we are now in a position to solve the problem. First, we notice the strong similarity between the present problem and the model problem that was solved in the previous section. Therefore, we will closely follow the procedure used to solve the model problem.

We need to determine the function $g(u)$. For this, we expand all quantities in terms of certain basis vectors. Since we are working with SU(3), it is natural that we use SU(3) basis vectors. Appendix B defines these basis vectors in terms of phase space variables (see Ref. 7 for additional details). Further, one can show[7] that any homogeneous polynomial f_n in the phase space variables can be decomposed in terms of these vectors.

We will denote by $|j;m\rangle$ the basis vectors uniquely labeled according to their transformation properties under SU(3). Here, j denotes the collection of indices j_1 and j_2 labeling the representation and m denotes the collection of indices I, I_3, and Y labeling vectors within the representation. (These basis vectors are analogous to the basis vectors e_x and e_y of the model problem.)

We expand the given homogeneous polynomial f_n in this basis as follows

$$f_n = \sum_{j,m} \phi_m^j |j;m\rangle \quad j \leqslant n. \tag{5.3}$$

A word on the notation used here. Since j stands for a collection of indices j_1 and j_2, $j \leqslant n$ actually means that $j_1 + j_2 \leqslant n$. Here, the ϕ_m^j's are coefficients multiplying the basis vectors. [This expansion is analogous to the one given in Eq. (4.1) for v in the model problem.] Thus, the left hand side of Eq. (5.1) has been expanded in terms of $|j;m\rangle$. However the right hand side is in terms of an integral over SU(3). Therefore, we will rewrite $|j;m\rangle$ in terms of an integral over SU(3) such that a direct comparison of the two sides is possible.

We proceed as follows. Suppose we can find a function $g_m^j(u)$ satisfying the following relation:

$$\int_{\mathrm{SU}(3)} du\ g_m^j(u)\hat{R}(u)q_1^n=|j;m\rangle,\quad j\leqslant n. \tag{5.4}$$

In other words, the function $g_m^j(u)$ projects out the basis vector $|j;m\rangle$. (This function is analogous to the functions g_x and g_y in the model problem.) Substituting this equation and Eq. (5.3) in Eq. (5.1) we get

$$\sum_{j,m}\ \phi_m^j\int_{\mathrm{SU}(3)} du\ g_m^j(u)\hat{R}(u)q_1^n=\int_{\mathrm{SU}(3)} du\ g(u)\hat{R}(u)q_1^n,\quad j\leqslant n. \tag{5.5}$$

Comparing both sides, we see that

$$g(u)=\sum_{j,m}\ \phi_m^j g_m^j(u),\quad j\leqslant n. \tag{5.6}$$

All that remains to be done is to determine $g_m^j(u)$ satisfying Eq. (5.4). To do this, we rewrite $\hat{R}(u)q_1^n$ in terms of SU(3) basis vectors. As a first step, we expand q_1^n in this basis (see Appendix B for a proof of this result):

$$q_1^n=\sum_{j\leqslant n}\ \xi^j|j;m_j\rangle. \tag{5.7}$$

We note two important features of this expansion (see Appendix B for a proof). First, the coefficients ξ^j are all nonzero:

$$\xi^j\neq 0,\quad j\leqslant n. \tag{5.8}$$

Second, each representation occurs *only* once. This is indicated by the fact that there is no summation over the indices m that label vectors within a representation. In summary, each representation (labeled by $j\leqslant n$) occurs once and only once in the expansion of q_1^n. This result will play a crucial role in the discussion that follows.

To get $\hat{R}(u)q_1^n$ we act on both sides of Eq. (5.7) with $\hat{R}(u)$, obtaining the following result:

$$\hat{R}(u)q_1^n=\sum_{j\leqslant n}\ \xi^j\hat{R}(u)|j;m_j\rangle. \tag{5.9}$$

Since the basis vectors $|j;m\rangle$ form a complete set for each j, they satisfy the relation

$$\sum_m\ |j;m\rangle\langle j;m|=1\quad\forall j. \tag{5.10}$$

Inserting this result into the right hand side of Eq. (5.9), we get the following relation:

$$\hat{R}(u)q_1^n=\sum_{j,m}\ \xi^j|j;m\rangle\langle j;m|\hat{R}(u)|j;m_j\rangle,\quad j\leqslant n. \tag{5.11}$$

However, we have the following standard result from representation theory of SU(3):

$$\langle j,m|\hat{R}(u)|j;m_j\rangle=\mathscr{D}^{\,j}{}_{mm_j}(u). \tag{5.12}$$

Substituting this into Eq. (5.11), we obtain the result

$$\hat{R}(u)q_1^n=\sum_{j,m}\xi^j\mathscr{D}^j_{mm_j}(u)|j;m\rangle,\quad j\leqslant n. \tag{5.13}$$

Inserting Eq. (5.13) into Eq. (5.4), we get the result

$$\int_{\mathrm{SU}(3)}du\ g^j_m(u)\sum_{j',m'}\xi^{j'}\mathscr{D}^{j'}_{m'm_{j'}}(u)|j',m'\rangle=|j;m\rangle,\quad j\leqslant n. \tag{5.14}$$

The functions $\mathscr{D}^j(u)$ satisfy the following orthogonality relations

$$\int_{\mathrm{SU}(3)}du\overline{\mathscr{D}}^j_{ab}(u)\mathscr{D}^{j'}_{a'b'}(u)=\frac{1}{d}\ \delta_{jj'}\delta_{aa'}\delta_{bb'}. \tag{5.15}$$

Here $\overline{\mathscr{D}}^j$ is the complex conjugate of the representation $\mathscr{D}^j$ and $d=(j_1+1)(j_2+1)\times((j_1+j_2)/2+1)$ is the dimension of the SU(3) representation labeled by j. Using these orthogonality relations, it is easily verified that the expression given below for $g^j_m(u)$ satisfies Eq. (5.14)

$$g^j_m(u)=\frac{d}{\xi^j}\overline{\mathscr{D}}^j_{mm_j}(u),\quad j\leqslant n. \tag{5.16}$$

We note that this expression is well defined since ξ^j is nonzero for $j\leqslant n$ [cf. Eq. (5.8)].

Having determined $g^j_m(u)$, we immediately obtain the required solution $g(u)$ [cf. Eq. (5.6)]:

$$g(u)=\sum_{j,m}\ \frac{d\phi^j_m}{\xi^j}\overline{\mathscr{D}}^j_{mm_j}(u),\quad j\leqslant n. \tag{5.17}$$

This is a solution satisfying Eq. (5.1). We need to verify that it also satisfies Eq. (5.2).

Again, we proceed as we did in the model problem. The most general solution $g(u)$ satisfying Eq. (5.1) is of the following form:

$$g(u)=\sum_{j,m}\ \frac{d\phi^j_m}{\xi^j}\overline{\mathscr{D}}^j_{mm_j}(u)+\sum_{j',a,b}c^{j'}_{ab}\overline{\mathscr{D}}^{j'}_{ab}(u). \tag{5.18}$$

Here the indices j', a, and b are required to satisfy the condition

$$\int_{\mathrm{SU}(3)}du\overline{\mathscr{D}}^{j'}_{ab}(u)\hat{R}(u)q_1^n=0. \tag{5.19}$$

This condition ensures that the extra terms added to obtain the general solution do not contribute to the integral in Eq. (5.1). However, these extra terms do contribute to the integral in Eq. (5.2). This is easily seen by substituting the general solution given in Eq. (5.18) into Eq. (5.2). We obtain the relation

$$\int_{\mathrm{SU}(3)}du\ g^2(u)=\sum_{j,m}\ d\left|\frac{\phi^j_m}{\xi^j}\right|^2+\sum_{j',a,b}|c^{j'}_{ab}|^2. \tag{5.20}$$

The above expression is minimized only if the following conditions are satisfied:

$$c^{j'}_{ab}=0\quad\forall j',a,b. \tag{5.21}$$

Imposing these conditions on the general solution [cf. Eq. (5.18)], we get back the particular solution given in Eq. (5.17). In summary, the function $g(u)$ given in Eq. (5.17) is the solution satisfying both Eqs. (5.1) and (5.2).

Having solved the problem in the continuum limit, we now return to the discrete version. Following the analogy with the model problem, we replace the integral over SU(3) by a sum over a discrete subgroup Γ of SU(3).[7] Since the elements of the discrete subgroups satisfy the same group properties as elements of the original group, the solution for the continuum problem would still be a solution to the discrete problem. There are several discrete subgroups of SU(3) that could be used. They are listed in detail in Appendix C. One should choose a subgroup of SU(3) whose order is greater than or equal to K. The above procedure leads us to the following result:

$$f_n=\frac{1}{K}\sum_{i=1}^{K} g(u_i)\hat{R}(u_i)q_1^n, \quad u_i\in\Gamma, \tag{5.22}$$

where $g(u)$ is given by Eq. (5.17). Comparing this with Eq. (3.16), we get the following solution for the coefficients $\beta_n^{(i)}$:

$$\beta_n^{(i)}=g(u_i)/K. \tag{5.23}$$

VI. OPTIMIZATION OF THE NUMBER OF JOLT MAPS

We achieved our primary goal of finding a jolt factorization of the map $\mathscr{M}_P$ in the previous section. We now seek to optimize this solution. More specifically, we attempt to reduce the number of jolt maps to a minimum.

We start with the following result from the previous section:

$$f_n=\int_{\mathrm{SU(3)}} du\; g(u)\hat{R}(u)q_1^n, \tag{6.1}$$

where $g(u)$ is given by Eq. (5.17). Here, we take a single jolt monomial q_1^n and act on it with the group SU(3). An alternative procedure is considered below. We will show that it reduces the number of jolt maps required by a substantial amount.

First, we factor SU(3) into the orthogonal group SO(3) and SU(3)/SO(3). The group SO(3) is taken to be the rotation group in the q_1, q_2, q_3 space. We will provide the reason for employing this factorization later. For the sake of notational convenience, let us denote SU(3)/SO(3) by G'. To proceed further, we write u [belonging to the group SU(3)] as the following product of elements belonging to G' and SO(3):

$$u=c\cdot r, \quad u\in\mathrm{SU(3)}, \quad c\in G', \quad r\in\mathrm{SO(3)}. \tag{6.2}$$

Then, it can be shown[12] that the following relation holds between the measure du for SU(3) and the measures dc and dr for G' and SO(3), respectively:

$$du=dc\cdot dr. \tag{6.3}$$

Substituting these results into the expression for f_n [cf. Eq. (6.1)], we obtain the relation

$$f_n=\int_{G'} dc\int_{\mathrm{SO(3)}} dr\;\; g(c\cdot r)\hat{R}(c\cdot r)q_1^n. \tag{6.4}$$

Letting the SO(3) part of $\hat{R}(c\cdot r)$ act first on q_1^n, we get the following result:

$$\hat{R}(c\cdot r)q_1^n=\hat{R}(c)\sum_{k=1}^{N'(n)} d_k(r)P_k^{(n)}(q_1,q_2,q_3). \tag{6.5}$$

Here we have used the following relation:

$$\hat{R}(r)q_1^n=\sum_{k=1}^{N'(n)} d_k(r)P_k^{(n)}(q_1,q_2,q_3), \quad r\in \mathrm{SO}(3), \tag{6.6}$$

where $P_k^{(n)}(q_1,q_2,q_3)$ denotes a nth degree basis monomial in variables q_1, q_2, and q_3:

$$P_k^{(n)}(q_1,q_2,q_3)=q_1^{n_1}q_2^{n_2}q_3^{n_3}, \quad n_1\geqslant n_2\geqslant n_3, \ \ n_1+n_2+n_3=n. \tag{6.7}$$

The number $N'(n)$ of nth degree basis monomial in three variables is given by the following relation:[7]

$$N'(n)=\binom{n+2}{n}. \tag{6.8}$$

Substituting Eq. (6.5) into Eq. (6.4), we get the relation

$$f_n=\int_{G'} dc\hat{R}(c)\int_{\mathrm{SO}(3)} dr\ g(c\cdot r)\sum_{k=1}^{N'(n)} d_k(r)P_k^{(n)}(q_1,q_2,q_3). \tag{6.9}$$

Next, we define a function $h_k(c)$ by the following relation:

$$h_k(c)\equiv\int_{\mathrm{SO}(3)} dr\ g(c\cdot r)\sum_{k=1}^{N'(n)} d_k(r). \tag{6.10}$$

We have already calculated $g(c\cdot r)$. It is nothing but the function $g(u)$ given in Eq. (5.17). Thus, $h_k(c)$ is well defined and can be calculated. Inserting Eq. (6.10) into Eq. (6.9), we obtain the following result:

$$f_n=\int_{G'} dc\hat{R}(c)\sum_{k=1}^{N'(n)} h_k(c)P_k^{(n)}(q_1,q_2,q_3). \tag{6.11}$$

Next, we need to obtain the discrete version of the above equation. This is again done by going over to a discrete sum over SU(3)/SO(3). Starting from a discrete subgroup of SU(3), one can go over to SU(3)/SO(3) following the procedure outlined in Appendix C. We obtain the following solution:

$$f_n=\int_{G'} dc\hat{R}(c)\sum_{k=1}^{N'(n)} h_k(c)P_k^{(n)}(q_1,q_2,q_3)=\frac{1}{K(G')}\sum_{l=1}^{K(G')}\hat{R}(c_l)\sum_{k=1}^{N'(n)} h_k(c_l)P_k^{(n)}(q_1,q_2,q_3). \tag{6.12}$$

Here, $K(G')$ gives the number of jolt maps required.

We now turn to the task of determining the number of jolt maps $K(G')$. It depends on G' as indicated. We have already seen in Section V that K is determined by looking at the equation for n equal to P (the maximum order). Setting n equal to P in the above expression, we obtain the following result:

$$f_P=\frac{1}{K(G')}\sum_{l=1}^{K(G')}\hat{R}(c_l)\sum_{k=1}^{N'(P)}h_k(c_l)P_k^{(P)}(q_1,q_2,q_3). \tag{6.13}$$

Since the Pth degree homogeneous polynomial f_P on the left hand side has $N(P)$ independent coefficients [cf. Eq. (3.14)], we need $N(P)$ linearly independent vectors on the right hand side. Only then, we can express any f_P in terms of these vectors.

We are now in a position to justify our decision to factor SU(3) into SO(3) and SU(3)/SO(3). Suppose we had not factorized SU(3) as above. Then the analogue of the above equation would be

$$f_P=\frac{1}{K'}\sum_{k=1}^{K'}g(u_i)\hat{R}(u_i)q_1^P, \tag{6.14}$$

where u_i belongs to a discrete subgroup of SU(3). Since we need $N(P)$ independent coefficients to describe f_P, K' has to equal $N(P)$. On the other hand, with factorization we need only $N''(P)$ jolts in Eq. (6.13) where

$$N''(P)=N(P)/N'(P). \tag{6.15}$$

This can be seen as follows. Equation (6.13) can be rewritten to give

$$f_P=\frac{1}{K(G')}\sum_{l=1}^{K(G')}\hat{R}(c_l)H_l(q_1,q_2,q_3), \tag{6.16}$$

where

$$H_l(q_1,q_2,q_3)=\sum_{k=1}^{N'(P)}h_k(c_l)P_k^{(P)}(q_1,q_2,q_3). \tag{6.17}$$

Now, the linear combination of $N'(P)$ jolt polynomials given by $H_l(q_1,q_2,q_3)$ is again a jolt polynomial. Since the jolt polynomial $H_l(q_1,q_2,q_3)$ itself has $N'(P)$ independent coefficients, $K(G')$ needs to be equal only to $N''(P)$ [cf. Eq. (6.15)] in order to give a total of $N(P)$ independent coefficients. On the other hand, in Eq. (6.14), we only have a single jolt monomial q_1^P and hence a single coefficient. Therefore, K' has to equal $N(P)$ in this case.

The above discussion demonstrates that a fewer number of jolts are required when SU(3) is factored into G' and SO(3). We now argue that factorizing SU(3) into a different set of factors does not give an even better result. First, we note that q_1, q_2, q_3 space (or equivalently, p_1, p_2, p_3 space) gives the maximal subspace of commuting jolt polynomials. We cannot choose any group larger than SO(3) since it is shown in Appendix D that SO(3) is the largest subgroup of Sp(6,R) that leaves the q_1, q_2, q_3 space invariant. If we choose a group smaller than SO(3), we will not get all the $N'(P)$ jolt monomials. Then $K(G')$ might have to be larger to get $N(P)$ independent coefficients. Therefore, factoring SU(3) into G' and SO(3) does appear to be the best compromise.

For P equal to 6, $N''(P)$ is equal to 17 from the above procedure [cf. Eqs. (6.15), (3.14) and (6.8)]. From Appendix C, we find that starting from (a similarity transformation of) a discrete subgroup of order 108 of SU(3), one can go over to a set of 18 elements belonging to SU(3)/SO(3). Thus, the number of jolt maps $K(G')$ required for $P=6$ is 18. For this case, we have verified that we do get the required number of linearly independent vectors on the right hand side of Eq. (6.13). Irwin[8] factorizes G as U(1)×U(1)×U(1). Using this factorization, for $P=6$, one

needs 27 jolt maps. Thus, we find that the number of jolt maps required in our case is less. When using our factorization for long-term stability analysis of Hamiltonian systems, this can lead to substantial savings in computer time.

VII. SUMMARY

When a nonlinear symplectic map is used in numerical calculations, one is forced to truncate the map at a given order in phase space variables. This truncated map (also known as a symplectic jet) violates the symplectic condition and typically exhibits spurious damping or growth when used to analyze long-term behavior of particle trajectories. We therefore approximated the map by a finite product of symplectic jolt maps which constitutes a symplectic completion of the jet. The action of jolt maps on phase space functions can be evaluated exactly and this should lead to better predictions of long-term stability in complicated Hamiltonian systems. Further, our jolt factorization was optimized so that the number of jolt maps required was significantly reduced. This can result in substantial savings in computer time when used for long-term stability studies. Finally, for $P=6$, we explicitly demonstrated that a fewer number of jolt maps were required as compared to Irwin's procedure.[8] We believe this will be true even for a general P since we are using a bigger group.

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APPENDIX A: EXAMPLES OF JOLT MAPS

Proof of Theorem 1: (i) The equality in Eq. (2.2) follows from Eq. (2.4) and properties of Lie transformations.[9] To show that $e^{:\hat{R}q_1^n:}$ is a jolt map, we start by making the following identification:

$$\exp(:\hat{R}q_1^n:)=\exp(:(\hat{R}q_1)^n:), \tag{A1}$$

where [cf. Eq. (2.4)]

$$\hat{R}q_1=R_{11}q_1+R_{12}p_1+\cdots+R_{16}p_3. \tag{A2}$$

The action of the Lie operator $:(\hat{R}q_1)^n:$ on the phase space variables is given by the relations

$$\begin{aligned} :(\hat{R}q_1)^n:z_i&=-n(\hat{R}q_1)^{n-1}R_{1i+1}, \quad i=1,3,5,\\ :(\hat{R}q_1)^n:z_i&=n(\hat{R}q_1)^{n-1}R_{1i-1}, \quad i=2,4,6. \end{aligned} \tag{A3}$$

Now, consider the action of $:(\hat{R}q_1)^n:^2$ on the phase space variables. Using Eq. (A3) we obtain the following result:

$$\begin{aligned} :(\hat{R}q_1)^n:^2z_i&=-nR_{1i+1}[(\hat{R}q_1)^n,(\hat{R}q_1)^{n-1}], \quad i=1,3,5,\\ :(\hat{R}q_1)^n:^2z_i&=nR_{1i-1}[(\hat{R}q_1)^n,(\hat{R}q_1)^{n-1}], \quad i=2,4,6. \end{aligned} \tag{A4}$$

But[9]

$$[(\hat{R}q_1)^n,(\hat{R}q_1)^{n-1}]=\hat{R}[q_1^n,q_1^{n-1}]=0. \tag{A5}$$

This proves that $e^{:\hat{R}q_1^n:}$ is a jolt map.

(ii) We note that the equality in Eq. (2.3) follows from Eq. (2.4) and properties of Lie transformations.[9] We also note that the following equality is satisfied:[9]

$$\hat{R}f(q_1,q_2,q_3)=f(\hat{R}q_1,\hat{R}q_2,\hat{R}q_3). \tag{A6}$$

Consider

$$:\hat{R}f(q_1,q_2,q_3):z_i=[f(\hat{R}q_1,\hat{R}q_2,\hat{R}q_3),z_i]. \tag{A7}$$

Since $\hat{R}q_i$ is linear in the phase space variables, the right hand side can be a function only of $\hat{R}q_i$'s. Denote this function by h. Thus

$$:\hat{R}f(q_1,q_2,q_3):z_i=h(\hat{R}q_1,\hat{R}q_2,\hat{R}q_3)=\hat{R}h(q_1,q_2,q_3), \tag{A8}$$

where the last equality follows from standard properties of Lie transformations.[9]

Next, consider the action of $:\hat{R}f:^2$ on the phase space variables. Using Eq. (A8) we get

$$:\hat{R}f(q_1,q_2,q_3):^2z_i=[\hat{R}f(q_1,q_2,q_3),\hat{R}h(q_1,q_2,q_3)]. \tag{A9}$$

Again using properties of Lie transformations,[9] we obtain

$$:\hat{R}f(q_1,q_2,q_3):^2z_i=\hat{R}[f(q_1,q_2,q_3),h(q_1,q_2,q_3)]. \tag{A10}$$

Since q_i's commute with one another, the Poisson bracket on the right hand side is identically zero. Therefore, $e^{:\hat{R}f(q_1,q_2,q_3):}$ is indeed a jolt map. This completes the proof of the theorem.

APPENDIX B: REPRESENTATIONS OF SU(3) CARRIED BY $q_1^{(n)}$

In this appendix, we prove a theorem regarding the representations of SU(3) carried by the monomial q_1^n. The proof will be a constructive one. Therefore, as a by-product, we obtain the explicit decomposition of q_1^n in terms of the SU(3) basis vectors. We end this appendix with an example. Using the formulas derived during the course of proving the theorem, we decompose q_1^4 in terms of the SU(3) basis vectors.

Let us denote the SU(3) basis vectors by $|j_1,j_2;I,I_3,Y\rangle$. Here j_1 and j_2 label the irreducible representations of SU(3) and I, I_3 and Y label weight vectors within the irreducible representation. It can be shown[13–15] that these basis vectors are associated with harmonic functions on the 5-sphere S^5. The 5-sphere is defined by the relation

$$Z_1^*Z_1+Z_2^*Z_2+Z_3^*Z_3=r^2=1, \tag{B1}$$

where

$$Z_j\equiv\frac{1}{\sqrt{2}}(q_j+ip_j), \tag{B2}$$

$$Z_j^*\equiv\frac{1}{\sqrt{2}}(q_j-ip_j). \tag{B3}$$

Since we are interested in functions defined on the 5-space S^5, it is convenient to parametrize S^5 in terms of polar coordinates ϕ_1, ϕ_2, ϕ_3, θ and ξ. These coordinates are related to the complex phase space variables by the following relations:

$$Z_1 = re^{i\phi_1} \cos\,\theta, \tag{B4}$$

$$Z_2 = re^{i\phi_2} \sin\,\theta \cos\,\xi, \tag{B5}$$

$$Z_3 = re^{i\phi_3} \sin\,\theta \sin\,\xi, \tag{B6}$$

where

$$0 \leqslant \phi_1, \phi_2, \phi_3 \leqslant 2\pi; \quad 0 \leqslant \theta, \xi \leqslant \pi/2. \tag{B7}$$

It can be shown[15] that states within the irreducible representation (j_1, j_2) can be associated with harmonic functions defined on S^5 as shown below:

$$|j_1, j_2; I, I_3, Y\rangle = \frac{1}{\sin\,\theta}\, d^{(1/2)(j_1+j_2+1)}_{(1/6)(j_1-j_2-3Y+6I+3),(1/6)(j_1-j_2-3Y-6I-3)}(2\theta) d^{(I)}_{(1/3)(j_1-j_2)+1/2Y, I_3} \times (2\xi) e^{(1/3)i(j_1-j_2)(\phi_1+\phi_2+\phi_3)} e^{iI_3(\phi_2-\phi_3)} e^{(1/2)iY(-2\phi_1+\phi_2+\phi_3)}. \tag{B8}$$

Here $d^{(j)}_{m',m}(\beta)$ are the usual d-functions that characterize the irreducible representation (j) of SU(2). The sign convention for the d-function is taken to be that given in Edmonds,[16] i.e.,

$$d^{(j)}_{m',m}(\beta) = \langle jm' | \exp(+i\beta J_y/h) | jm \rangle. \tag{B9}$$

where $|jm\rangle$ denotes states within the representation (j) of SU(2).

The d-functions can be computed using the following formula:[17]

$$d^{(j)}_{m',m}(\beta) = [(j+m')!(j-m')!(j+m)!(j-m)!]^{1/2} \times \sum_s \frac{(-1)^s \left(\cos\frac{\beta}{2}\right)^{2j+m-m'-2s} \left(\sin\frac{\beta}{2}\right)^{m'-m+2s}}{(j+m-s)!\,s!\,(m'-m+s)!\,(j-m'-s)!}, \tag{B10}$$

where the summation index s ranges over all integral values such that the factorials in the denominator are non-negative. The d-functions can also be computed using the following recursion relation:[17]

$$d^{(j)}_{m',m}(\beta) = \left(\frac{j-m'}{j-m}\right)^{1/2} d^{(j-1/2)}_{m'+1/2,m+1/2}(\beta) \cos\frac{\beta}{2} + \left(\frac{j+m'}{j-m}\right)^{1/2} d^{(j-1/2)}_{m'-1/2,m+1/2}(\beta) \sin\frac{\beta}{2}, \quad \text{if } j \neq m. \tag{B11}$$

If j is equal to m, the following relation can be used:

$$d^{(j)}_{m',j}(\beta) = (-1)^{j-m'} \left[\frac{(2j)!}{(j+m')!(j-m')!}\right]^{1/2} \left(\cos\frac{\beta}{2}\right)^{j+m'} \left(\sin\frac{\beta}{2}\right)^{j-m'}. \tag{B12}$$

Two additional formulas which facilitate computation of the d-functions are given below

$$d^{(j)}_{m',m}(\beta) = (-1)^{m'-m} d^{(j)}_{m,m'}(\beta), \tag{B13}$$

$$d^{(j)}_{m',m}(\beta) = (-1)^{m'-m} d^{(j)}_{-m',-m}(\beta), \tag{B14}$$

We are now in a position to state and prove the theorem on the SU(3) content of q_1^n.

Theorem 2: *The monomial q_1^n contains only those representations (j_1,j_2) of* SU(3) *for which j_1+j_2 is less than or equal to n. Moreover, each such representation occurs once and only once in q_1^n.*

Proof: From Eq. (B4), we obtain the following expression for q_1^n in terms of the coordinates that parametrize the 5-sphere:

$$q_1^n=2^{n/2}(\text{Re } Z_1)^n=2^{n/2}r^n \cos^n \phi_1 \cos^n \theta. \tag{B15}$$

However, $\cos^n \phi_1$ satisfies the relation[18]

$$\cos^n \phi_1=\sum_{\substack{j_1+j_2=n \\ j_1\geqslant j_2}} a_{j_1j_2} \cos[(j_1-j_2)\phi_1], \tag{B16}$$

where

$$a_{j_1j_2}=\frac{1}{2^{n-1}}\binom{n}{j_2}, \quad j_1+j_2=n, \ j_1>j_2, \tag{B17}$$

$$a_{j_1j_2}=\frac{1}{2^n}\binom{n}{j_2}, \quad j_1+j_2=n, \ j_1=j_2. \tag{B18}$$

Notice that we have denoted the summation indices by j_1 and j_2 in anticipation of results to come. Substituting Eq. (B16) into Eq. (B15), we obtain the result

$$q_1^n=2^{n/2}r^n \sum_{\substack{j_1+j_2=n \\ j_1\geqslant j_2}} a_{j_1j_2} \cos[(j_1-j_2)\phi_1]\cos^{j_1+j_2} \theta. \tag{B19}$$

The above result has to be expressed in terms of the SU(3) state vectors given by $|j_1,j_2;I,I_3,Y\rangle$ [cf. Eq. (B8)]. However, q_1^n does not depend on the coordinates ϕ_2, ϕ_3, and ξ. Therefore, only those SU(3) state vectors that satisfy the following conditions can occur in the expansion of q_1^n:

$$I=I_3=0, \quad Y=-2(j_1-j_2)/3. \tag{B20}$$

Imposing these conditions on a general $|j_1,j_2;I,I_3,Y\rangle$ [cf. Eq. (B8)], we obtain the relation

$$|j_1,j_2;0,0,-2(j_1-j_2)/3\rangle=\frac{1}{\sin \theta} d^{(1/2)(j_1+j_2+1)}_{(1/2)(j_1-j_2+1),(1/2)(j_1-j_2-1)}(2\theta)e^{i(j_1-j_2)\phi_1}. \tag{B21}$$

As expected, these vectors do not depend on the coordinates ϕ_2, ϕ_3, and ξ. The d-function appearing in the above expression satisfies the following property [cf. Eqs. (B13) and (B14)]:

$$d^{(1/2)(j_1+j_2+1)}_{(1/2)(j_1-j_2+1),(1/2)(j_1-j_2-1)}(2\theta)=d^{(1/2)(j_2+j_1+1)}_{(1/2)(j_2-j_1+1),(1/2)(j_2-j_1-1)}(2\theta). \tag{B22}$$

That is, this function is invariant under the exchange of the indices j_1 and j_2. Using this property and Eq. (B21), we obtain the following result:

$$\begin{aligned}&\tfrac{1}{2}\left[|j_1,j_2;0,0,-2(j_1-j_2)/3\rangle+|j_2,j_1;0,0,-2(j_2-j_1)/3\rangle\right] \\ &\quad=\cos[(j_1-j_2)\phi_1]\frac{1}{\sin \theta} d^{(1/2)(j_1+j_2+1)}_{(1/2)(j_1-j_2+1),(1/2)(j_1-j_2-1)}(2\theta), \quad j_1\geqslant j_2.\end{aligned} \tag{B23}$$

Here we have also used the standard relation

$$\tfrac{1}{2}\,[e^{i(j_1-j_2)\phi_1}+e^{-i(j_1-j_2)\phi_1}]=\cos[(j_1-j_2)\phi_1]. \tag{B24}$$

Comparing Eq. (B23) with the summand on the right hand side of Eq. (B19), we note that we somehow have to generate the function $\cos^{j_1+j_2}\theta$ out of the d-functions by taking appropriate linear combinations. In order to accomplish this, we first need explicit expressions for the d-functions. From Eq. (B10), we get the following result:

$$\frac{1}{\sin\,\theta}\,d^{(1/2)(j_1+j_2+1)}_{(1/2)(j_1-j_2+1),(1/2)(j_1-j_2-1)}(2\theta)$$
$$=[j_1!(j_1+1)!j_2!(j_2+1)!]^{1/2}\sum_{s=0}^{j_2}\frac{(-1)^s(\cos\,\theta)^{j_1+j_2-2s}(\sin\,\theta)^{2s}}{s!(s+1)!(j_1-s)!(j_2-s)!},\quad j_1\geqslant j_2. \tag{B25}$$

Using the standard binomial theorem, we obtain the relation

$$(\sin\,\theta)^{2s}=(1-\cos^2\,\theta)^s=\sum_{k=0}^{s}\binom{s}{k}(-1)^{s-k}(\cos^2\,\theta)^{s-k}. \tag{B26}$$

Substituting this relation into Eq. (B25), we get

$$\frac{1}{\sin\,\theta}\,d^{(1/2)(j_1+j_2+1)}_{(1/2)(j_1-j_2+1),(1/2)(j_1-j_2-1)}(2\theta)$$
$$=[j_1!(j_1+1)!j_2!(j_2+1)!]^{1/2}\sum_{s=0}^{j_2}\frac{1}{s!(s+1)!(j_1-s)!(j_2-s)!}$$
$$\times\sum_{k=0}^{s}\binom{s}{k}(-1)^k(\cos\,\theta)^{j_1+j_2-2k},\quad j_1\geqslant j_2. \tag{B27}$$

We had noticed earlier [cf. Eq. (B23)] that the sum of the state vectors $|j_1,j_2;0,0,-2(j_1-j_2)/3\rangle$ and $|j_2,j_1;0,0,-2(j_2-j_1)/3\rangle$ is proportional to $\cos[(j_1-j_2)\phi_1]$ [cf. Eq. (B23)]. This remains true even if we make the following substitution:

$$j_1\to j_1-i,\quad j_2\to j_2-i, \tag{B28}$$

where i is some integer. More specifically, we have the following relation:

$$\tfrac{1}{2}\,[|j_1-i,j_2-i;0,0,-2(j_1-j_2)/3\rangle+|j_2-i,j_1-i;0,0,-2(j_2-j_1)/3\rangle]$$
$$=\frac{1}{\sin\,\theta}\,d^{(1/2)(j_1+j_2+1-2i)}_{(1/2)(j_1-j_2+1),(1/2)(j_1-j_2-1)}(2\theta)\cos[(j_1-j_2)\phi_1],\quad j_1\geqslant j_2,\ \ i\leqslant j_2, \tag{B29}$$

where

$$\frac{1}{\sin\theta}\, d^{(1/2)(j_1+j_2+1-2i)}_{(1/2)(j_1-j_2+1),(1/2)(j_1-j_2-1)}(2\theta)$$
$$=[(j_1-i)!(j_1+1-i)!(j_2-i)!(j_2+1-i)!]^{1/2}$$
$$\times\sum_{s=0}^{j_2-i}\frac{1}{s!(s+1)!(j_1-s-i)!(j_2-s-i)!}\sum_{k=0}^{s}\binom{s}{k}$$
$$\times(-1)^k(\cos\theta)^{j_1+j_2-2k-2i},\quad j_1\geqslant j_2. \tag{B30}$$

Therefore, the most general combination of vectors that still gives a quantity proportional to $\cos[(j_1-j_2)\phi_1]$ is as follows:

$$2^{n/2}r^n\sum_{i=0}^{j_2}\frac{A_i^{(j_1,j_2)}}{2}\left[|j_1-i,j_2-i;0,0,-2(j_1-j_2)/3\rangle+|j_2-i,j_1-i;0,0,-2(j_2-j_1)/3\rangle\right]$$
$$=2^{n/2}r^n\cos[(j_1-j_2)\phi_1]\sum_{i=0}^{j_2}A_i^{(j_1,j_2)}\frac{1}{\sin\theta}\, d^{(1/2)(j_1+j_2+1-2i)}_{(1/2)(j_1-j_2+1),(1/2)(j_1-j_2-1)}(2\theta),\quad j_1\geqslant j_2. \tag{B31}$$

Comparing the right hand side of the above equation with the summand in the expression for q_1^n [cf. Eq. (B19)], we obtain the condition

$$\sum_{i=0}^{j_2}A_i^{(j_1,j_2)}\frac{1}{\sin\theta}\, d^{(1/2)(j_1+j_2+1-2i)}_{(1/2)(j_1-j_2+1),(1/2)(j_1-j_2-1)}(2\theta)=\cos^{j_1+j_2}\theta. \tag{B32}$$

In other words, we need to find coefficients $A_i^{(j_1,j_2)}$ such that the above condition is satisfied. Then, we would have succeeded in decomposing q_1^n in terms of the SU(3) state vectors. We proceed as follows. First, we interchange the summations over indices s and k in Eq. (B30) to obtain the relation

$$\frac{1}{\sin\theta}\, d^{(1/2)(j_1+j_2+1-2i)}_{(1/2)(j_1-j_2+1),(1/2)(j_1-j_2-1)}(2\theta)$$
$$=B_i^{(j_1,j_2)}\sum_{k=0}^{j_2-i}(-1)^k(\cos\theta)^{j_1+j_2-2k-2i}$$
$$\times\sum_{s=k}^{j_2-i}\frac{1}{s!(s+1)!(j_1-s-i)!(j_2-s-i)!}\binom{s}{k},\quad j_1\geqslant j_2,\ \ i\leqslant j_2, \tag{B33}$$

where

$$B_i^{(j_1,j_2)}=[(j_1-i)!(j_1+1-i)!(j_2-i)!(j_2+1-i)!]^{1/2}. \tag{B34}$$

Inserting Eq. (B33) into Eq. (B32), we get the condition

$$\sum_{i=0}^{j_2}A_i^{(j_1,j_2)}B_i^{(j_1,j_2)}\sum_{k=0}^{j_2-i}(-1)^k(\cos\theta)^{j_1+j_2-2k-2i}$$
$$\times\sum_{s=k}^{j_2-i}\frac{1}{s!(s+1)!(j_1-s-i)!(j_2-s-i)!}\binom{s}{k}=\cos^{j_1+j_2}\theta,\quad j_1\geqslant j_2. \tag{B35}$$

The coefficient $C_l^{(j_1,j_2)}$ of $\cos^{j_1+j_2-2l}\theta$ on the left hand side of the above equation is given by the expression (where $l=i+k$)

$$C_l^{(j_1,j_2)}=\sum_{k=0}^{l}(-1)^k A_{l-k}^{(j_1,j_2)}B_{l-k}^{(j_1,j_2)} \times\sum_{s=k}^{j_2-l+k}\frac{1}{s!(s+1)!(j_1-s-l+k)!(j_2-s-l+k)!}\binom{s}{k},\quad j_1\geqslant j_2. \tag{B36}$$

The above expression can be simplified by using the following substitution

$$s'=s-k. \tag{B37}$$

Making this substitution in Eq. (B36), we get the relation

$$C_l^{(j_1,j_2)}=\sum_{k=0}^{l}\frac{(-1)^k}{k!}A_{l-k}^{(j_1,j_2)}B_{l-k}^{(j_1,j_2)}\sum_{s'=0}^{j_2-l}\frac{1}{s'!(s'+k+1)!(j_1-s'-l)!(j_2-s'-l)!},\quad j_1\geqslant j_2. \tag{B38}$$

In order to satisfy Eq. (B35), we need to impose the following conditions

$$C_0^{(j_1,j_2)}=1, \tag{B39}$$

$$C_l^{(j_1,j_2)}=0,\quad l=1,2,\ldots,j_2. \tag{B40}$$

Inserting the expression for $C_l^{(j_1,j_2)}$ into the above equations, we obtain the following results:

$$A_0^{(j_1,j_2)}=\frac{1}{B_0^{(j_1,j_2)}S_{00}^{(j_1,j_2)}},$$

$$A_l^{(j_1,j_2)}=\frac{1}{B_l^{(j_1,j_2)}S_{l0}^{(j_1,j_2)}}\sum_{k=1}^{l}\frac{(-1)^{k+1}}{k!}A_{l-k}^{(j_1,j_2)}B_{l-k}^{(j_1,j_2)}S_{lk}^{(j_1,j_2)},\quad 1\leqslant l\leqslant j_2, \tag{B41}$$

where

$$S_{lk}^{(j_1,j_2)}=\sum_{s'=0}^{j_2-l}\frac{1}{s'!(s'+k+1)!(j_1-s'-l)!(j_2-s'-l)!}. \tag{B42}$$

From Eqs. (B19), (B31), and (B32), we finally get the following decomposition for q_1^n:

$$q_1^n=2^{n/2}r^n\sum_{\substack{j_1+j_2=n\\ j_1\geqslant j_2}}\frac{a_{j_1j_2}}{2} \times\sum_{i=0}^{j_2}A_i^{(j_1,j_2)}[|j_1-i,j_2-i;0,0,-2(j_1-j_2)/3\rangle+|j_2-i,j_1-i;0,0,-2(j_2-j_1)/3\rangle]. \tag{B43}$$

We note that all representations (j_1,j_2) (with j_1+j_2 less than or equal to n) appear in the decomposition (since the coefficients $A_i^{(j_1,j_2)}a_{j_1j_2}$ are seen to be nonzero for all valid j_1, j_2, and i). Furthermore, from each representation (j_1,j_2), only one vector $|j_1,j_2;0,0,-2(j_1-j_2)/3\rangle$ appears in the decomposition. This proves the theorem.

As an example, we obtain the decomposition of q_1^4. Using the above formulas we get the following results:

$$a_{40}=1/8, \quad a_{31}=1/2, \quad a_{22}=3/8; \tag{B44}$$

$$A_0^{(4,0)}=1/\sqrt{5}, \quad A_0^{(3,1)}=1/5\sqrt{2}, \quad A_1^{(3,1)}=\sqrt{3}/5; \tag{B45}$$

$$A_0^{(2,2)}=1/10, \quad A_1^{(2,2)}=4/15, \quad A_2^{(2,2)}=1/6. \tag{B46}$$

Substituting these results into Eq. (B43), we obtain the following decomposition

$$\begin{aligned} q_1^4=&\frac{r^4}{4\sqrt{5}}[|4,0;0,0,-8/3\rangle+|0,4;0,0,8/3\rangle]+\frac{r^4}{5\sqrt{2}}[|3,1;0,0,-4/3\rangle+|1,3;0,0,4/3\rangle] \\ &+\frac{\sqrt{3}r^4}{5}[|2,0;0,0,-4/3\rangle+|0,2;0,0,4/3\rangle]+\frac{3}{20}r^4|2,2;0,0,0\rangle+\frac{2}{5}r^4|1,1;0,0,0\rangle \\ &+\frac{1}{4}r^4|0,0;0,0,0\rangle. \end{aligned} \tag{B47}$$

APPENDIX C: DISCRETE SUBGROUPS OF SU(3)

In this appendix, we study the discrete subgroups of SU(3) which are required in Sections V and VI. We start by defining the following matrices:

$$A(\alpha,\beta)=\begin{pmatrix} e^{i\alpha} & 0 & 0 \\ 0 & e^{i\beta} & 0 \\ 0 & 0 & e^{-i(\alpha+\beta)} \end{pmatrix}, \tag{C1}$$

$$B(\alpha,\beta)=\begin{pmatrix} e^{i\alpha} & 0 & 0 \\ 0 & 0 & e^{i\beta} \\ 0 & e^{i(\pi-\alpha-\beta)} & 0 \end{pmatrix}, \tag{C2}$$

$$E(\alpha,\beta)=\begin{pmatrix} 0 & e^{i\alpha} & 0 \\ 0 & 0 & e^{i\beta} \\ e^{-i(\alpha+\beta)} & 0 & 0 \end{pmatrix}, \tag{C3}$$

$$V=\frac{1}{\sqrt{3}i}\begin{pmatrix} 1 & 1 & 1 \\ 1 & \omega & \omega^2 \\ 1 & \omega^2 & \omega \end{pmatrix}, \tag{C4}$$

$$V'=\frac{1}{\sqrt{3}i}\begin{pmatrix} 1 & 1 & \omega^2 \\ 1 & \omega & \omega \\ \omega & 1 & \omega \end{pmatrix}, \tag{C5}$$

$$W=\frac{1}{2}\begin{pmatrix} -1 & \mu_2 & \mu_1 \\ \mu_2 & \mu_1 & -1 \\ \mu_1 & -1 & \mu_2 \end{pmatrix}, \tag{C6}$$

$$Z=\frac{-1}{\sqrt{7}i}\begin{pmatrix} a & b & c \\ b & c & a \\ c & a & b \end{pmatrix}, \tag{C7}$$

where

$$\omega=e^{i2\pi/3}, \tag{C8}$$

$$\mu_1=\tfrac{1}{2}(-1+\sqrt{5}), \quad \mu_2=\tfrac{1}{2}(-1-\sqrt{5}), \tag{C9}$$

$$a=\xi^4-\xi^3, \quad b=\xi^2-\xi^5, \tag{C10}$$

$$c=\xi-\xi^6, \quad \xi^7=1. \tag{C11}$$

The discrete subgroups of SU(3) are listed below along with their generators.[19,20] First, we list the crystal-like subgroups. They are denoted by $\Gamma(n)$ where n denotes the order of the group:

(1) $\Gamma(60)$:$A(0,\pi)$, $E(0,0)$, and W;
(2) $\Gamma(108)$:$A(0,2\pi/3)$, $E(0,0)$, and V;
(3) $\Gamma(168)$:$A(2\pi/7,4\pi/7)$, $E(0,0)$, and Z;
(4) $\Gamma(216)$:$A(0,2\pi/3)$, $E(0,0)$, V, and V';
(5) $\Gamma(648)$:$A(0,2\pi/3)$, $E(0,0)$, V, and $A(4\pi/9,4\pi/9)$;
(6) $\Gamma(1080)$:$A(0,\pi)$, $E(0,0)$, W, and $B(\pi,5\pi/3)$.

Next, we list the dihedral-like groups and the disconnected groups. They are denoted by $\Delta(n)$ where n denotes the order of the group:

(1) $\Delta(3m^2)$:$A(j2\pi/m,k2\pi/m)$ and $E(0,0)$ where j and k are integers;
(2) $\Delta(6m^2)$:$A(j2\pi/m,k2\pi/m)$, $E(0,0)$, and $B(j2\pi/m,k2\pi/m)$ where j and k are integers;
(3) $\Delta(3\infty^2)$:$A(\alpha,\beta)$ and $E(0,0)$;
(4) $\Delta(6\infty^2)$:$A(\alpha,\beta)$, $E(0,0)$, and $B(\alpha,\beta)$.

In Section VI, we will also be interested in discrete elements of SU(3)/SO(3). We obtain discrete elements of SU(3)/SO(3) by the following procedure. We start with a discrete subgroup $\Gamma(n)$ of SU(3). Next, we identify the subgroup $\Gamma'(n')$ of $\Gamma(n)$ that belongs to SO(3) [where n' is the order of $\Gamma'(n')$]. This is easily accomplished once it is realized that an element $\Gamma_i \in \Gamma(n)$ belongs to SO(3) if and only if all its matrix elements are real. For example, it is seen that all of $\Gamma(60)$ also belongs to SO(3) since each of its elements is real. Next, we construct the $\Gamma(n)/\Gamma'(n')$ as follows. For every element Γ_i belonging to $\Gamma(n)$, we form the right coset $\Gamma'(n')\Gamma_i$. There will be n/n' distinct right cosets. From each distinct coset, we select one element to be the coset representative. These n/n' coset representatives belong to $\Gamma(n)/\Gamma'(n')$. Thus we get a collection of n/n' discrete elements of SU(3)/SO(3). Values for n' and n/n' for the various crystal groups are given below:

(1) $\Gamma(60)$:$n'=60$, $n/n'=1$;
(2) $\Gamma(108)$:$n'=6$, $n/n'=18$;
(3) $\Gamma(168)$:$n'=6$, $n/n'=28$;
(4) $\Gamma(216)$:$n'=6$, $n/n'=36$;

(5) $\Gamma(648): n' = 6,\ n/n' = 108;$
(6) $\Gamma(1080): n' = 60,\ n/n' = 18.$

Finally, we should mention that we rarely make direct use of the complex 3×3 matrices Γ_i belonging to $\Gamma(n)$. We need objects that act on the six dimensional phase space. Therefore, we first embed these complex 3×3 matrices into the compact part of Sp(6,R) following the procedure outlined in Appendix D. The real 6×6 matrices that are obtained as a result of this embedding (and the Lie transformations corresponding to these matrices) can act on phase space variables. It is these real 6×6 matrices that are used in Sections V and VI.

APPENDIX D: LARGEST SUBGROUP OF SU(3) THAT LEAVES COORDINATE SPACE INVARIANT

In this appendix, we prove a theorem satisfied by the special orthogonal group SO(3). The result of this theorem will be used in Section VI. Throughout this appendix, we will work in the rearranged basis of phase space variables given by $z=(q_1,q_2,q_3,p_1,p_2,p_3)$ for convenience. Symplectic matrices in the rearranged basis are related to those in the original basis by a simple similarity transformation.

Theorem 3: *Let $V^{(m)}$ be the vector space formed by homogeneous polynomials of degree m in variables q_1, q_2, and q_3. Then,* SO(3) *is the largest subgroup of* SU(3) *that leaves $V^{(m)}$ invariant.*

Proof: We first prove the following lemma.

Lemma 1: SO(3) *is the largest subgroup of* SU(3) *that leaves $V^{(1)}$ invariant.*

Proof: Consider a complex 3×3 matrix R belonging to SU(3). It satisfies the following conditions:

$$R^{\dagger}=R^{-1};\quad \det R=1. \tag{D1}$$

It can be decomposed into its real and imaginary parts as follows

$$R=-D+iC, \tag{D2}$$

where C and D are real 3×3 matrices.

Since the matrix R has to act on functions of phase space variables, we first need to embed it in the compact part of Sp(6,R). Following the procedure outlined in Ref. 7, the real 6×6 symplectic matrix U^s (in the rearranged basis) corresponding to the unitary matrix R is given by the relation

$$U^s=V^s\begin{pmatrix} R & 0 \\ 0 & R^* \end{pmatrix}(V^s)^{-1}, \tag{D3}$$

where V^s is given by[9]

$$V^s=\frac{1}{\sqrt{2}}\begin{pmatrix} I & iI \\ iI & I \end{pmatrix}. \tag{D4}$$

Here I is a 3×3 identity matrix. Upon evaluating this equation, we obtain the following result:

$$U^s=\begin{pmatrix} -D & C \\ -C & -D \end{pmatrix}. \tag{D5}$$

Next, consider a general 6-vector v^s belonging to $V^{(1)}$. It is given by the relation

$$v^s=(v_3^s,0_3) \tag{D6}$$

where v_3^s and 0_3 are 3-vectors defined as follows:

$$v_3^s=(a,b,c), \quad a,b,c\in\mathscr{R} \tag{D7}$$

$$0_3=(0,0,0). \tag{D8}$$

The action of U^s on v^s is given by the following relation:

$$U^s v^s=\begin{pmatrix} -Dv_3^s \\ -Cv_3^s \end{pmatrix}. \tag{D9}$$

Therefore, $U^s v^s$ belongs to $V^{(1)}$ if and only if the following condition is satisfied [cf. Eq. (D6)]

$$Cv_3^s=0. \tag{D10}$$

Since v_3^s is an arbitrary 3-vector, this implies that C is a zero matrix:

$$C=0. \tag{D11}$$

Substituting Eq. (D11) into Eq. (D5), the most general element belonging to the compact part of Sp(6,R) that leaves $V^{(1)}$ invariant is found to have the following form:

$$U_*^s=\begin{pmatrix} -D & 0 \\ 0 & -D \end{pmatrix}. \tag{D12}$$

We convert this into an element of SU(3) using the following procedure.[8] Given a 6×6 matrix U^s belonging to the compact part of Sp(6,R), one can extract the complex 3×3 matrix R belonging to SU(3) from it through the following relation:

$$(V^s)^{-1}U^sV^s=\begin{pmatrix} R & 0 \\ 0 & R^* \end{pmatrix}. \tag{D13}$$

From the above equation, we obtain the SU(3) element R_* corresponding to U_*^s as

$$R_*=-D. \tag{D14}$$

However, since this is supposed to be an element of SU(3), it has to satisfy the conditions given in Eq. (D1). Imposing these conditions on R_* and noting that R_* is real, we obtain the following restrictions on R_*:

$$\widetilde{R}_*=R_*^{-1}; \quad \det R_*=1, \tag{D15}$$

where $\widetilde{R}_*$ is the transpose of R_*. But these are precisely the conditions satisfied by an element of SO(3). This proves the lemma.

We now return to the proof of the theorem. Consider an element $P_k^{(m)}$ belonging to $V^{(m)}$:

$$P_k^{(m)}=a_1q_1^m+a_2q_1^{m-1}q_2+\cdots+a_Nq_3^m, \tag{D16}$$

where [cf. Eq. (6.8)]

$$N=\begin{pmatrix} m+2 \\ m \end{pmatrix}. \tag{D17}$$

The action of $\hat{U}^s$ (the Lie transformation corresponding to the matrix U^s) on $P_k^{(m)}$ is given as follows:

$$\hat{U}^s P_k^{(m)} = a_1(\hat{U}^s q_1)^m + a_2(\hat{U}^s q_1)^{m-1}(\hat{U}^s q_2) + \cdots + a_N(\hat{U}^s q_3)^m. \tag{D18}$$

Therefore, the condition that ''U^s leaves $V^{(1)}$ invariant'' is sufficient to ensure that $\hat{U}^s$ leaves $V^{(m)}$ invariant, i.e.,

$$\hat{U}^s V^{(1)} \subseteq V^{(1)} \Rightarrow \hat{U}^s V^{(m)} \subseteq V^{(m)}. \tag{D19}$$

To complete the proof of the theorem, we need to show that this is also a necessary condition.

Suppose that $\hat{U}^s V^{(1)} \not\subseteq V^{(1)}$. Then, there exists a vector v_*^s belonging to $V^{(1)}$ that is mapped out of $V^{(1)}$ under the action of $\hat{U}^s$, i.e.,

$$\hat{U}^s v_*^s \notin V^{(1)}. \tag{D20}$$

This can be rewritten as follows

$$\hat{U}^s (\hat{U}_1^s)^{-1} \hat{U}_1^s v_*^s \notin V^{(1)}, \tag{D21}$$

where $\hat{U}_1^s$ is chosen to satisfy the condition

$$\hat{U}_1^s v_*^s = q_1. \tag{D22}$$

This is always possible since v_*^s is effectively a vector in the three dimensional $q_1 - q_2 - q_3$ space and therefore can be rotated to orient it along the q_1 axis. Since the transformation $\hat{U}_1^s$ that brings about this rotation belongs to the subgroup SO(3), $\hat{U}^s(\hat{U}_1^s)^{-1}$ (or more accurately, the unitary matrix corresponding to this transformation) still belongs to SU(3). In summary, if $\hat{U}^s V^{(1)} \not\subseteq V^{(1)}$, there exists a transformation $\hat{U}_2^s$ [equal to $\hat{U}^s(\hat{U}_1^s)^{-1}$] that maps q_1 out of $V^{(1)}$:

$$\hat{U}_2^s q_1 \notin V^{(1)}. \tag{D23}$$

Now, consider the action of $\hat{U}_2^s$ on the vector q_1^m belonging to $V^{(m)}$:

$$\hat{U}_2^s q_1^m = (\hat{U}_2^s q_1)^m. \tag{D24}$$

Since $\hat{U}_2^s q_1$ does not belong to $V^{(1)}$, it will consist of at least one nonzero term containing p_1, p_2, or p_3. Consequently, from the above equation, even $\hat{U}_2^s q_1^m$ will contain at least one such term. Therefore, the following equation is seen to be true:

$$\hat{U}_2^s q_1^m \notin V^{(m)}. \tag{D25}$$

Since we have produced one vector which leaves $V^{(m)}$ under the action of $\hat{U}_2^s$, we have succeeded in proving the following statement:

$$\hat{U}^s V^{(1)} \not\subseteq V^{(1)} \Rightarrow \hat{U}^s V^{(m)} \not\subseteq V^{(m)}. \tag{D26}$$

Combining Eqs. (D19) and (D26), we see that the condition ''$\hat{U}^s$ leaves $V^{(1)}$ invariant'' is both necessary and sufficient to ensure that $\hat{U}^s$ leaves $V^{(m)}$ invariant. Since SO(3) is the largest subgroup of SU(3) satisfying the first condition, it is also the largest subgroup of SU(3) that leaves $V^{(m)}$ invariant. This completes the proof of the theorem.

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Solution of Nester's gauge conditions

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We give a rigorous proof of the existence of solutions to the nonlinear gauge conditions on orthonormal frames introduced by Nester to prove the positive energy theorem in general relativity. The proof holds in all dimensions $n \geqslant 2$. If the second de Rham cohomology group vanishes one also proves uniqueness. © *1996 American Institute of Physics.* [S0022-2488(96)00208-3]

I. INTRODUCTION

Nester's proof of the positivity of the gravitational energy in general relativity makes use of gauge conditions which must be satisfied by a global orthonormal frame on the initial-value threefold.[1–3] These gauge conditions can be expressed in terms of a nonlinear elliptic operator acting on orthogonal automorphisms of the cotangent bundle. In Ref. 4 Nester generalizes the gauge conditions to Riemannian manifolds of any dimension $n \geqslant 2$, and gives some arguments to support an existence and uniqueness result for the linearized problem which should hold for geometries that in some suitable sense are not too far from the Euclidean geometry.

In this paper we provide a rigorous existence result for the full nonlinear problem, which holds for any parallelizable Riemannian geometry satisfying a suitable condition of asymptotic flatness (cf. Definition 2.3 below), and any $n \geqslant 2$. If the second de Rham cohomology group vanishes, one also has uniqueness.

We consider a connected parallelizable Riemannian manifold (M,g) with a fixed orientation. Let $\{e_i\}$ be a global orthonormal frame, and let $\{\theta^i\}$ be the dual coframe field. We associate with the frame $\{e_i\}$ the differential forms

$$\tilde{q} = i_{e_i} d\theta^i, \quad q = \tfrac{1}{2}\delta_{ik} d\theta^i \wedge \theta^k. \tag{1.1}$$

Nester's gauge conditions are that the forms $\tilde{q}$ and $\star q$ are closed,

$$d\tilde{q} = d\star q = 0,$$

where $\star$ is the Hodge duality operator. One therefore looks for an $SO(n)$-valued function $R^i{}_k$ on M such that the forms $\tilde{\tilde{q}}$ and $\star\overline{q}$ associated with the transformed coframe field $\theta^i = R^i{}_k \theta^k$ are closed. A straightforward computation shows that the gauge conditions amount to

$$d(\tilde{q} + R^c{}_a R^a{}_{k,c}\,\theta^k) = 0, \tag{1.2a}$$

$$d\star(q + \tfrac{1}{2}\delta_{ae} R^a{}_b dR^c{}_b \wedge \theta^e \wedge \theta^b) = 0. \tag{1.2b}$$

The existence and uniqueness result will be proved in four steps. First we prove the existence of solutions to the corresponding linearized problem; we then use Kuranishi's technique to solve the nonlinear problem when the source term in the equations (1.2) (i.e., the forms $\tilde{q}, \star q$) is small enough. The solution of the general nonlinear equation is then reduced to the solution of a finite

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number of equations with small source term. We finally prove the uniqueness of the solutions under the assumption that the second de Rham cohomology group vanishes.

II. STATEMENT OF THE PROBLEM

In this Section we introduce some preliminary definitions and results and give a precise statement of our result.

Definition 2.1: We say that a tensor field T on $\mathbb{R}^n$ falls off as $r^{-\alpha}$ if

$$\lim_{r\to\infty} r^{\beta}T=0$$

uniformly for all $\beta<\alpha$, where r is the radial coordinate.

Definition 2.2: Let γ be a Riemannian metric on $\mathbb{R}^n$, and let γ_0 be the standard Euclidean metric. We say that γ is asymptotically Euclidean if $\gamma-\gamma_0$ falls off as $r^{-\mu}$, with $\mu\geqslant\max\{n/2-2,1\}$.

With this choice of the asymptotic behavior of the metric γ all the differential forms we shall need to consider will be square-summable on M.

We shall assume that the Riemannian manifold (M,g) is asymptotically Euclidean in the following sense (this is related to the definition adopted in Ref. 5).

Definition 2.3: A Riemannian manifold (M,g) is said to be asymptotically Euclidean if there is a compact geodesic ball $X\subset M$ such that $(M-X,g)$ is isometric to the complement of a closed ball in $\mathbb{R}^n$ endowed with an asymptotically Euclidean metric.

Note that since we assume that X is compact, the Riemannian manifold (M,g) is complete (cf. Ref. 6).

We may extend Definition 2.1 to an asymptotically Euclidean Riemannian manifold (M,g) by saying that a (say covariant) tensor field T on M falls off as $r^{-\alpha}$ if ψ^*T does so, where ψ is an isometry realizing the condition of Definition 2.3.

We denote by Ω^p_M the bundle of C^∞ differential p-forms on M, and by $\Omega^p(M)$ the space of its global sections, while $H_k(M,\Omega^p)$ will denote the Sobolev space of index k of differential p-forms on M. Moreover, if Y is a compact manifold with boundary ∂Y and interior Y°, we denote by $H_k(Y^\circ,\Omega^p)$ the space formed by the restrictions to the interior Y° of Y of the elements in $H_k(Y,\Omega^p)$ (for a careful definition of these spaces see Ref. 7, Appendix B.2).

The space V of vertical orthogonal automorphisms of T^*M may be regarded as a Banach-Lie group, modelled on the Banach space $H_2(M,\Omega^2)$. The latter space may also be identified with the Lie algebra of V. The exponential map $\exp: H_2(M,\Omega^2)\to V$ is surjective, i.e., $\phi\in V$ may be written as $\phi=\exp\mathbf{A}$ with $\mathbf{A}\in H_2(M,\Omega^2)$; if a global orthonormal frame has been fixed, this is tantamount to writing the orthogonal point-dependent matrix R representing ϕ as $R=\exp A$, where A is an antisymmetric point-dependent matrix.

Definition 2.4: We say that $\phi\in V$ is asymptotic to the identity if $\phi=\exp\mathbf{A}$, where $\mathbf{A}$ falls off as $r^{-\alpha}$, with $\alpha>n/2$.

We can now state our result. Given an orthonormal coframe θ, let $\tilde{q}$ and q be the associated forms according to (1.1), and set $p=d\tilde{q}+\delta q\in\Omega^2(M)$. The problem (1.2) may be written in the form

$$F_\theta(\phi)=-p, \tag{2.1}$$

where $\phi\in V$ and $F_\theta: V\to H_0(M,\Omega^2)$ is a second-order differential operator. Since the metric g is asymptotically Euclidean, p falls off as $r^{-\mu-2}$, so that it is square-summable [i.e., $p\in H_0(M,\Omega^2)$].

Theorem 2.5: *Let (M,g) be a connected parallelizable asymptotically Euclidean Riemannian manifold, of dimension $n\geqslant 2$, and fix a global orthonormal coframe θ. There is a $\phi\in V$ which satisfies the condition (2.1) and is asymptotic to the identity. Moreover, the automorphism ϕ is C^∞. The automorphism ϕ is unique if $H^2_{DR}(M)=0$.*

III. THE LINEARIZED PROBLEM

We linearize the problem (2.1) by fixing θ and considering an automorphism ϕ which differs ''infinitesimally'' from the identity. We obtain the conditions

$$d[\,\delta\mathbf{A}-\tfrac{1}{2}A_{ab}\delta(\theta^a\wedge\theta^b)]=d\widetilde{q}, \tag{3.1a}$$

$$d\star[d\mathbf{A}-\tfrac{1}{2}A_{ab}d(\theta^a\wedge\theta^b)]=-d\star q, \tag{3.1b}$$

where δ is the operator $\delta=(-1)^k\star d\star$, with k the rank of the form acted upon, and the unknown $\mathbf{A}=\frac{1}{2}A_{ab}\theta^a\wedge\theta^b$ is a 2-form on M.

By taking the Hodge dual of (3.1b) and summing the two equations we get a single condition,

$$\mathfrak{F}_\theta\mathbf{A}=d\widetilde{q}+\delta q; \tag{3.2}$$

here $\mathfrak{F}_\theta$ is the operator,

$$\mathfrak{F}_\theta\mathbf{A}:=\Delta\mathbf{A}-\tfrac{1}{2}d[A_{ab}\delta(\theta^a\wedge\theta^b)]-\tfrac{1}{2}\delta[A_{ab}d(\theta^a\wedge\theta^b)] \tag{3.3}$$

(cf. Ref. 4), where Δ is the Laplace-Beltrami operator $\Delta=d\delta+\delta d$. We regard $\mathfrak{F}_\theta$ as an operator $H_2(M,\Omega^2)\to H_0(M,\Omega^2)$. The problem (3.2) is equivalent to (3.1) due to the orthogonality of the two summands in $\mathfrak{F}_\theta\mathbf{A}$ and in $d\widetilde{q}+\delta q$.

We start by transferring the problem from M to the interior Y^0 of a compact manifold Y with boundary ∂Y diffeomorphic to S^{n-1}. In this way we may use available results on elliptic problems on compact manifolds with boundary (cf. Ref. 7). Let $f:Y^0\to M$ be a diffeomorphism; even though this will be understood in our notation, we shall consider for a while the problem (3.2) on Y^0 endowed with the pullback metric f^*g.

Proposition 3.1: There is a differential form $\mathbf{A}\in\overline{H_2}(Y^\circ,\Omega^2)$ *such that*

$$\mathfrak{F}_\theta\mathbf{A}=p,\quad \mathbf{A}\big|\partial Y=0.$$

Moreover, $\mathbf{A}$ *is* C^∞*, and is unique if* $H^2_{DR}(Y^\circ)=0$.

Proof: The proof of this result is given in the Appendix. □

We consider now the pullback $(f^{-1})^*\mathbf{A}$ of $\mathbf{A}$ to M; we shall denote it by the same letter.

Proposition 3.2: The differential form $\mathbf{A}$ *on* M *solves the problem (3.2) and falls off as* $r^{-\alpha}$*, with* $\alpha>n/2$*. If* $H^2_{DR}(M)=0$, $\mathbf{A}$ *is the unique form in* $H_2(M,\Omega^2)$ *which solves the problem (3.2).*

Proof: The first claim has already been proved. Since $\mathbf{A}$ is square-summable, it has the required asymptotic behavior. The uniqueness follows from the corresponding property proved in Proposition 3.1. □

IV. SOLVING THE NONLINEAR PROBLEM

Provided that the norms of the forms $\widetilde{q}$ and $\star q$ are small enough, we may use a Kuranishi technique to reduce the problem (2.1) to the corresponding linearized problem, which we have solved in Section III. We recall that V is the Banach manifold of vertical orthogonal automorphisms of T^*M. Let F_θ, p be as in Eq. (2.1). The Fréchet differential,

$$((F_\theta)_*)_{id}:T_{id}V\simeq H_2(M,\Omega^2)\to H_0(M,\Omega^2),$$

can be identified with the operator $\mathfrak{F}_\theta$ studied in Section III (id is the point in V corresponding to the identity automorphism).

As usual, by means of the inverse function theorem one shows the existence of
(i) a neighborhood U_0 of id in V;
(ii) a neighborhood U_1 of the origin in $H_2(M,\Omega^2)$;
(iii) a diffeomorphism ρ: $U_1 \to U_0$ such that

$$F_\theta \circ \rho = \mathfrak{F}_\theta \quad \text{and} \quad \rho(0) = id.$$

This, together with Proposition 3.2, implies that the equation (2.1) has a solution ϕ, provided that the L^2 norm of p is small enough, say $\|p\| < \epsilon$. (This implies the existence of solutions whenever the Riemannian metric g is close enough to the Euclidean metric, so that the norm of p is suitably small.) One should also notice that the solution ϕ so found is asymptotic to the identity due to the asymptotic behavior of p.

We may now solve the nonlinear problem by iteration. Fix an initial coframe θ, let N be an integer such that $\|p\| < N\epsilon$ (where ϵ is the same as in the foregoing discussion), and set $p_1 = (1/N)p$. We may solve the problem

$$F_\theta(\phi_1) = -p_1.$$

Let $\theta_1 = \phi_1(\theta)$; a quick computation shows that the corresponding forms q and $\tilde{q}$ are

$$q_1 = \frac{N-1}{N}\, q, \quad \tilde{q}_1 = \frac{N-1}{N}\, \tilde{q}.$$

We may now solve the problem

$$F_{\theta_1}(\phi_2) = -p_1;$$

the forms q and $\tilde{q}$ corresponding to $\theta_2 = \phi_2(\theta_1)$ are

$$q_2 = \frac{N-2}{N}\, q, \quad \tilde{q}_1 = \frac{N-2}{N}\, \tilde{q}.$$

Applying this procedure N times we obtain a coframe,

$$\theta = \phi_N \circ \cdots \circ \phi_1(\theta),$$

which solves the problem (2); since all ϕ_i's are asymptotic to the identity, $\phi = \phi_N \circ \cdots \circ \phi_1$ is asymptotic to the identity as well.

V. UNIQUENESS

Let ϕ_1, ϕ_2 be two orthogonal automorphisms which solve the problem (2) and are asymptotic to the identity, and let $\chi = \phi_2 \circ \phi_1^{-1}$. Then χ is asymptotic to the identity, and solves the problem

$$F_{\theta_1}(\chi) = 0,$$

with $\theta_1 = \phi_1(\theta)$. We may let $\chi = \rho(\mathbf{A})$, with $\mathbf{A} \in H_2(M,\Omega^2)$; $\mathbf{A}$ satisfies the equation $\mathfrak{F}_{\phi_1}\mathbf{A} = 0$. If $H^2_{DR}(M) = 0$, Proposition 3.2 gives $\mathbf{A} = 0$, so that $\chi = \mathrm{id}$.

This proves the uniqueness part of Theorem 2.5, thus concluding its proof.

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APPENDIX: SOLVING THE LINEAR PROBLEM

Let Y be a compact manifold with smooth boundary ∂Y. Let g be a Riemannian metric on Y. We consider the operator $\mathfrak{F}_\theta$ defined by Eq. (3.3), and show an existence and uniqueness result for a homogeneous Dirichlet problem. We shall follow the notation and terminology of Ref. 7. Let F denote the bundle on ∂Y defined as $\Omega^2_Y|\partial Y$, and define the boundary operator,

$$B:\overline{H_2}(Y^\circ,\Omega^2)\to H_{3/2}(F), \quad B(\mathbf{A})=\mathbf{A}|\partial Y.$$

One easily shows that the pairs $\overline{\mathfrak{F}_\theta}=(\mathfrak{F}_\theta,B)$ and $\overline{\Delta}=(\Delta,B)$ define elliptic Fredholm operators (cf. Ref. 7, Chap. XX),

$$\overline{H_2}(Y^\circ,\Omega^2)\to\overline{H_0}(Y^\circ,\Omega^2)\oplus H_{3/2}(F)$$

(Δ is the Laplace-Beltrami operator).

Lemma A.1: $\ker\overline{\mathfrak{F}_\theta}=\ker\Delta$

Proof: Since $\ker\Delta$ is finite-dimensional, by the Hahn-Banach theorem there is a subspace W of $H_2(Y^\circ,\Omega^2)$ such that $H_2(Y^\circ,\Omega^2)=\ker\Delta\oplus W$. We consider the family of operators,

$$\mathfrak{F}_t:W\to\overline{H_0}(Y^\circ,\Omega^2)\oplus H_{3/2}(F)$$

$$\mathfrak{F}_t=\overline{\Delta}+t(\widetilde{\mathfrak{F}_\theta},0), \quad \text{with } t\in[0,1],$$

where

$$\widetilde{\mathfrak{F}_\theta}\mathbf{A}=-\tfrac{1}{2}\,d[A_{ab}\delta(\theta^a\wedge\theta^b)]-\tfrac{1}{2}\,\delta[A_{ab}d(\theta^a\wedge\theta^b)],$$

so that $\mathfrak{F}_1=\overline{\mathfrak{F}_\theta}$ (in this Lemma we consider all operators as defined on W). Let $\epsilon\in\mathbb{R}^+$ be such that

$$\max\left\{\frac{\|\overline{\Delta}\|}{\|\widetilde{\mathfrak{F}_\theta}\|}-2,0\right\}<\epsilon<\frac{\|\overline{\Delta}\|}{\|\widetilde{\mathfrak{F}_\theta}\|}.$$

Since $\overline{\Delta}|W$ is injective, the operator

$$H_1:=\overline{\Delta}+\left(\frac{\|\overline{\Delta}\|}{\|\widetilde{\mathfrak{F}_\theta}\|}-\epsilon\right)(\widetilde{\mathfrak{F}_\theta},0)$$

is injective as well. By iteration we obtain that the operators

$$H_k=\overline{\Delta}+2^{k-1}\left(\frac{\|\overline{\Delta}\|}{\|\widetilde{\mathfrak{F}_\theta}\|}-\epsilon\right)(\widetilde{\mathfrak{F}_\theta},0)$$

are injective for all $k\geqslant 1$. By taking k as the integer part of

$$1-\log_2\left(\frac{\|\overline{\Delta}\|}{\|\widetilde{\mathfrak{F}_\theta}\|}-\epsilon\right),$$

we obtain that $\mathfrak{F}_\theta|W$ is injective; thus $\ker\overline{\mathfrak{F}_\theta}\subset\ker\overline{\Delta}$.

By repeating the argument after exchanging the roles of the operators $\overline{\mathfrak{F}_\theta}$ and $\overline{\Delta}$ we obtain $\ker\overline{\Delta}\subset\ker\overline{\mathfrak{F}_\theta}$. □

Consider now differential forms $\widetilde{q}\in\Omega^1(Y)$ and $q\in\Omega^3(Y)$, and set $p=d\widetilde{q}+\delta q$. The pair

$$(p,0)\in\overline{H_0}(Y^\circ,\Omega^2)\oplus H_{3/2}(F)$$

is orthogonal to the cokernel of $\overline{\mathfrak{F}_\theta}$ (also in view of Lemma A.1). So there is a differential form $\mathbf{A}\in H_2(Y^\circ,\Omega^2)$ such that

$$\mathfrak{F}_\theta\mathbf{A}=p,\quad \mathbf{A}\big|\partial Y=0. \tag{A1}$$

The form $\mathbf{A}$ is actually C^∞ (cf. Ref. 7).

To prove uniqueness we note that any harmonic form $\mathbf{A}\in\overline{H_2}(Y^\circ,\Omega^2)$ which vanishes on the boundary ∂Y is d- and δ-closed. This establishes an injective map $\ker\Delta\to H^2_{DR}(Y^\circ)$.

We may now prove the following result.

Proposition A.2: There is a C^∞ differential from $\mathbf{A}\in\overline{H_2}(Y^\circ,\Omega^2)$ which solves the problem (A.1). If $H^2_{DR}(Y^\circ)=0$, the form $\mathbf{A}$ is unique.

Proof: We need only to note that if $H^2_{DR}(Y^\circ)=0$ we have $\ker\ \overline{\Delta}=0$, and by Lemma A.1 $\ker\overline{\mathfrak{F}_\theta}=0$ as well. □

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The Einstein action for algebras of matrix valued functions—Toy models

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Two toy models are considered within the framework of noncommutative differential geometry. In the first one, the Einstein action of the Levi–Civita connection is computed for the algebra of matrix valued functions on a torus. It is shown that, assuming some constraints on the metric, this action splits into a classical-like, a quantum-like and a mixed term. In the second model, an analogue of the Palatini method of variation is applied to obtain critical points of the Einstein action functional for $M_4(\mathbb{R})$. It is pointed out that a solution to the Palatini variational problem is not necessarily a Levi–Civita connection. In this model, no additional assumptions regarding metrics are made. © *1996 American Institute of Physics.* [S0022-2488(96)00808-0]

I. INTRODUCTION

The goal of this paper is to analyze the behavior of a noncommutative analogue of the Einstein–Hilbert action functional on two toy models. General definitions and constructions employed to study those models are provided in the next section.

In Section III, we present some results regarding the computation of the Einstein action of the Levi–Civita connection for $C^\infty(T^m)\otimes M_n(\mathbb{R})$, the algebra of matrix valued functions on an m-tori. The approach proposed there is analogous to the ''derivation based'' approach to the calculation of the Yang–Mills (Maxwell) action for an algebra of matrix valued functions that was carried out in Ref. 1 (see Section V in Ref. 1, cf. Ref. 2 and the sections 4 and 5 of Ref. 3). We choose our manifold M to be an m-tori because it is a compact Abelian group, and we want integrals over M to be finite, and $\mathrm{Der}(C^\infty(T^m))$ to be commutative as a Lie algebra and free as a $C^\infty(T^m)$-module. We also assume that the metric, understood as a pairing of derivations, has its values in the center of an algebra. Consequently, the results presented there can be interpreted as concerning the ''commutative part'' of noncommutative geometry. [Indeed, the Levi–Civita connections for $M_n(\mathbb{R})$ can be interpreted as the torsion part of the flat connection on $SL(n,\mathbb{R})$ given by the left translations; see Remark 14.]

In Section IV, which is the main part of this work, we study a toy model that is based on the algebra $M_4(\mathbb{R})$ of 4 by 4 real matrices, and the 2-dimensional Lie subalgebra $\mathfrak{so}(2)\oplus\mathfrak{so}(2)$ of $\mathrm{Der}(M_4(\mathbb{R}))$. It is a simple but quite computable model that is presented with the aim of providing hints on how to approach more complicated situations. For this model, we derive an analogue of the Einstein vacuum field equation, and apply the Palatini method of variation to obtain critical points. We find a solution to the Palatini variational problem that is, in general, neither metric nor torsion free. Yet, this solution (a connection ∇^g determined by a metric g) turns out to be Ricci flat for all metrics. Consequently, the Einstein field equation, which depends essentially on the Ricci curvature [see (7)], is automatically satisfied, and (g,∇^g) is a critical point of the Einstein action functional for any metric g. The value of this functional at any critical point is the same (zero). Thus we obtain a result that partially reflects the classical geometric phenomenon

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that, for any Riemannian 2-manifold, the Einstein–Hilbert action computed for a metric g and its Levi–Civita connection does not depend on g (see 9.1.10 in Ref. 4). The key difference between Section IV and the preceding one is that in Section IV we no longer assume that the metric is center valued.

The proofs or calculations are rather straightforward and are often omitted here for the sake of brevity. Except for Proposition 4, the letter k will denote a field, A a unital associative k-algebra, $Z(A)$ its center, and $\Omega(A)$ a differential graded algebra $A \oplus \oplus_{n\geqslant 1}^{\infty} \mathrm{Hom}_{Z(A)}(\wedge^n \mathscr{L}, A)$ with $\mathscr{L}$ as below and the differential defined as in Proposition 4. The Einstein convention of summing over repeating indices is assumed.

II. PRELIMINARIES

Let $\mathscr{L}$ be a $Z(A)$-submodule and Lie subalgebra of $\mathrm{Der}(A)$ such that $\mathscr{L}\otimes_{Z(A)}A$ is a finitely generated projective right A-module. (Compare with the notion of a Lie–Cartan pair introduced in Ref. 5.)

Definition 1: *A linear map* $\nabla:\mathscr{L}\otimes_{Z(A)}\Omega^*(A)\to\mathscr{L}\otimes_{Z(A)}\Omega^{*+1}(A)$ *is called a connection on* $\mathscr{L}$ *iff*

$$\forall X\in\mathscr{L},\ \alpha\in\Omega(A):\ \ \nabla(X\otimes_{Z(A)}\alpha)=(\nabla X)\alpha+X\otimes_{Z(A)}d\alpha.$$

Definition 2: *The endomorphism* $\nabla^2 \in \mathrm{End}_{\Omega(A)}(\mathscr{L}\otimes_{Z(A)}\Omega(A))$ *is called the curvature of a connection* ∇.

Remark 3: The notions of connection and curvature defined above are equivalent to the usual notions of noncommutative connection and curvature on a projective module (e.g., see Section III.B of Ref. 1). In this case, the projective right A-module is $\mathscr{L}\otimes_{Z(A)}A$. ◇

Proposition 4 (cf. p. 369 in Ref. 6): *Let A be an associative unital algebra over a commutative ring k. Let $\mathscr{L}_k$ be a k-Lie subalgebra of the space of all k-derivations of A, and let $\mathscr{E}$ be any right A-module admitting a connection (see Remark 3). If $\Omega(A)$ is a differential graded subalgebra of $A \oplus \oplus_{n\geqslant 1}^{\infty} \mathrm{Hom}_k(\wedge^n\mathscr{L}_k, A)$ with the differential given by (see the first section in Ref. 2):*

$$\begin{aligned}(d\alpha)(X_0,X_1,\cdots,X_n)&\\ =\sum_{0\leqslant i\leqslant n}(-)^i X_i\,\alpha(X_0,\cdots,X_{i-1},X_{i+1},\cdots,X_n)&\\ +\sum_{0\leqslant r<s\leqslant n}(-)^{r+s}\,\alpha([X_r,X_s],X_0,\cdots,X_{r-1},X_{r+1},\cdots,X_{s-1},X_{s+1},\cdots,X_n),&\end{aligned}$$

then

$$\forall\xi\in\mathscr{E},\ \ X,Y\in\mathscr{L}_k:\ \ (\nabla^2\xi)(X,Y)=([\nabla_X,\nabla_Y]-\nabla_{[X,Y]})(\xi),$$

where, as in the classical differential geometry, $\nabla_Z\xi$ *denotes* $(\nabla\xi)(Z)$.

Definition 5: *A map* $g:(\mathscr{L}\otimes_{Z(A)}A)\times(\mathscr{L}\otimes_{Z(A)}A)\to A$ *is called a pseudo-Riemannian metric on* $\mathscr{L}$ *iff it satisfies the following conditions.*

(1) $\forall a,b\in A,\ \xi,\eta\in\mathscr{L}\otimes_{Z(A)}A$: $g(a\xi,\eta b)=ag(\xi,\eta)b$, *where the left module structure on* $\mathscr{L}\otimes_{Z(A)}A$ *is given by* $a(X_i\otimes_{Z(A)}c_i)=X_i\otimes_{Z(A)}ac_i$.

(2) $\forall X,Y\in\mathscr{L}$: $g(X,Y)=g(Y,X)$ *(symmetry condition).*

(3) The induced map $\widetilde{g}:\mathscr{L}\otimes_{Z(A)}A\ni\xi\mapsto g(.,\xi)\in\Omega^1(A)$ *is an isomorphism of right A-modules.*

Definition 6: *A connection on* $\mathscr{L}$ *is said to be compatible with g iff*

$$\forall X,Y,Z\in\mathscr{L}:\ \ Xg(Y,Z)=g(\nabla_XY,Z)+g(Y,\nabla_XZ).$$

Definition 7: The $Z(A)$*-bilinear map,*

$$T_\nabla : \mathscr{L} \times \mathscr{L} \ni (X,Y) \mapsto \nabla_X Y - \nabla_Y X - [X,Y] \otimes_{Z(A)} 1 \in \mathscr{L} \otimes_{Z(A)} A,$$

is called the torsion of ∇.

Definition 8: *Let* $\mathscr{R}_\nabla(X,Y)$ *be the Z(A)-homomorphism given by the formula*

$$\mathscr{L} \ni Z \mapsto \mathscr{R}_\nabla(X,Y)(Z) = (\nabla^2 Y)(Z,X) \in \mathscr{L} \otimes_{Z(A)} A,$$

and let $\mathscr{T}_E \in \mathrm{Hom}_A(\mathrm{Hom}_{Z(A)}(\mathscr{L}, \mathscr{L} \otimes_{Z(A)} A), A)$. *We call the Z(A)-linear map,*

$$Ric_\nabla : \mathscr{L} \ni X \mapsto \mathscr{T}_E(\mathscr{R}_\nabla(X,.)) \in \Omega^1(A),$$

the Ricci curvature of ∇.

Remark 9: When $\mathscr{L}$ or A is a finitely generated projective $Z(A)$-module,

$$\mathrm{Hom}_{Z(A)}(\mathscr{L}, \mathscr{L} \otimes_{Z(A)} A) = \mathrm{End}_{Z(A)}(\mathscr{L}) \otimes_{Z(A)} A$$

(see Proposition 2 in II.4 of Ref. 7), and we can choose $\mathscr{T}_E$ to be a trace on $\mathrm{End}_{Z(A)}(\mathscr{L})$ tensored over $Z(A)$ with id_A. ◇

Definition 10: *Let* $\mathscr{M}(\mathscr{L})$ *and* $\mathscr{C}(\mathscr{L})$ *denote the space of all pseudo-Riemannian metrics on* $\mathscr{L}$, *and the space of all connections on* $\mathscr{L}$, *respectively. The functional* $E : \mathscr{M}(\mathscr{L}) \times \mathscr{C}(\mathscr{L}) \to k$ *given by the formula*

$$E(g,\nabla) = -(\tau_g \circ \mathscr{T}_E)(\tilde{g}^{-1} \circ Ric_\nabla),$$

where $\tau_g : A \to k$ *is a metric dependent trace, is called the Einstein action functional on* $\mathscr{L}$.

Remark 11: With an appropriate choice of τ_g and $\mathscr{T}_E$ (cf. Proposition 15), the functional E coincides for $A = C^\infty(M)$ and $\mathscr{L} = \mathrm{Der}(C^\infty(M))$ with the standard Einstein–Hilbert action functional on M, for any (paracompact) manifold M admitting a (pseudo-)Riemannian metric. ◇

III. THE CASE OF Z(A) VALUED METRICS

One can apply the same reasoning as in the case of classical differential geometry to obtain the following.

Proposition 12 (cf. Section 9 in Ref. 8): *Let* $g(\mathscr{L},\mathscr{L}) \subseteq Z(A)$ *or* $\nabla_{\mathscr{L}} \mathscr{L} \subseteq \mathscr{L}$. *Then there exists at most one metric compatible connection that is torsion free. If it exists, it is given by the formula*

$$\nabla_X Y = \tfrac{1}{2} \tilde{g}^{-1} \Big(Xg(Y,.) + Yg(X,.) - dg(X,Y) + g([X,Y],.) + g([.,X],Y) + g([.,Y],X) \Big). \quad (1)$$

A connection given by (1), will be called the Levi–Civita connection of g, and denoted by ∇_g. For the rest of this section, we work under the assumption that $g(\mathscr{L},\mathscr{L}) \subseteq Z(A)$. The mathematical model considered here is practically identical with a model constructed in Refs. 9 and 10. [Compare (2) with (3.24) in Ref. 9, and Proposition 15 with (3.23), (3.21) in Ref. 9 and (3.26) in Ref. 10.] Note that there is an extra term in $(3.24)^9$ that is absent in Proposition 15 due to our assumption that the classical and the algebraic derivations are orthogonal to each other. Let us also mention that the dual point of view regarding linear connections [i.e., where the space of 1-forms rather than $\mathscr{L} \otimes_{Z(A)} A$ is taken as a starting point] was studied in Refs. 11 and 12 also in the context of ''matrix geometry'' (see Section 4.3 in Ref. 11 and Section 3 in Ref. 12; for duality issues of the aforementioned kind, see Sec. 6 in Ref. 8).

To begin with, let us consider the algebra of matrices $M_n(\mathbb{R})$ and $\mathscr{L} = \mathrm{Der}(M_n(\mathbb{R})) = \mathfrak{sl}(n,\mathbb{R})$. Since $\mathfrak{sl}(n,\mathbb{R})$ is an (n^2-1)-dimensional vector space over $\mathbb{R}$ (the

center of the algebra of matrices), the endomorphisms of this space are simply $(n^2-1)\times(n^2-1)$ matrices, and we can choose $\mathscr{T}_E$ to be the usual matrix trace tensored with $id_{M_n(\mathbb{R})}$ (see Remark 9).

Proposition 13: *Let* $A=M_n(\mathbb{R})$, $\mathscr{L}=\mathrm{Der}(M_n(\mathbb{R}))$, $\tau_g=(1/n)\,|\mathrm{det}g|^{1/2}Tr$, *and* $\mathscr{T}_E=Tr\otimes id_{M_n(\mathbb{R})}$. *Also, let* $\{E_i\}$ *be any basis of* $\mathfrak{sl}(n,\mathbb{R})$. *Then*

$$E(g,\nabla_g)=g^{jp}(K_{jp}+\tfrac{1}{2}g^{il}g_{rk}c^r_{lp}c^k_{ij})\sqrt{|\mathrm{det}g|}, \tag{2}$$

where K is the Killing metric on $SL(n,\mathbb{R})$, *and* $\{K_{jp},g_{ij},g^{kl},c^r_{lp}\}$ *are defined by the formulas* $K_{jp}=g(E_j,E_p)$, $g_{rk}=g(E_r,E_k)$, $g^{pr}g_{rk}=\delta^p_k$, $[E_l,E_p]=c^r_{lp}E_r$, *respectively.*

Proof: A direct computation using the symmetry of a metric and the anti-symmetry of the Lie algebra structure constants. □

Remark 14: Let g be a left invariant metric on $SL(n,\mathbb{R})$. Then g can be identified with a metric on $\mathrm{Der}(M_n(\mathbb{R}))$. The connection on $SL(n,\mathbb{R})$ given by the left translations is compatible with all left invariant metrics. The torsion part of this connection is given by the formula (see (44) in Ref. 13)

$$\mathfrak{T}^i_{jk}:=\tfrac{1}{2}(Q^i_{jk}+g^{il}g_{jn}Q^n_{kl}+g^{il}g_{kn}Q^n_{jl})=\tfrac{1}{2}(c^i_{kj}+g^{il}g_{jn}c^n_{lk}+g^{il}g_{kn}c^n_{lj}).$$

If the coefficients of the $M_n(\mathbb{R})$–Levi–Civita connection of g are defined by the equality $\nabla_{E_j}E_k=\Gamma^i_{kj}E_i$, then $\Gamma^i_{jk}=\mathfrak{T}^i_{jk}\in\mathbb{R}$. (Caution: One often defines the Christoffel symbols by the relation $\nabla_{E_j}E_k=\widetilde{\Gamma}^i_{jk}E_i$. In this notation, which is compatible with the notation used in Ref. 13, the aforementioned relationship between the Christoffel symbols of the noncommutative connection and the torsion part of the classical connection can be equivalently written as $\widetilde{\Gamma}^i_{jk}=\mathfrak{T}^i_{jk}+c^i_{jk}$.) In general, if $\mathrm{Der}(A)$ equals the Lie algebra of some Lie group G, then the noncommutative torsion free g-compatible connection on $\mathrm{Der}(A)$ coincides in the above sense with the torsion part of the flat connection on G given by the left translations. ◇

Our next step is to consider an algebra of matrix valued functions. The module of derivations of such an algebra splits into two direct sum components in the following way (cf. Lemma 2.1 in Ref. 1):

$$\mathrm{Der}\,(C^\infty(M)\otimes M_n(\mathbb{R})\,)=\mathrm{Der}\,(C^\infty(M)\,)\otimes\mathbb{R}\,\oplus\,C^\infty(M)\otimes\mathrm{Der}\,(M_n(\mathbb{R})\,).$$

For $M=T^m$, this module is a free $C^\infty(T^m)$-module of dimension $m+n^2-1$. Consequently, its algebra of endomorphisms is simply the algebra of matrices $M_{m+n^2-1}(C^\infty(T^m))$, and, again, we can choose $\mathscr{T}_E$ to be the usual matrix trace [with values in $C^\infty(T^m)$] tensored with $id_{M_n(\mathbb{R})}$ (see Remark 9).

Proposition 15: *Let* $A=C^\infty(T^m)\otimes M_n(\mathbb{R})$, $\mathscr{L}=\mathrm{Der}(A)$, $\tau_g=(1/n)\int_{T^m}|\mathrm{det}g|^{1/2}Tr$, *and* $\mathscr{T}_E=Tr\otimes id_{M_n(\mathbb{R})}$. *Assume also that there exists a basis* $\{E_i\}_{i\in\{1,\cdots,m\}}$ *of* $\mathrm{Der}(C^\infty(T^m))$, *and a basis* $\{E_j\}_{j\in\{m+1,\cdots m+n^2-1\}}$ *of* $\mathrm{Der}(M_n(\mathbb{R}))$ *such that*

$$g_{ij}=\begin{cases}0, & \text{for } i\leqslant m \text{ and } j>m,\\ g_c(E_i,E_j), & \text{for } i,j\leqslant m,\\ g_q(E_i,E_j), & \text{for } i,j>m,\end{cases}$$

where g_c *is a classical (pseudo-)Riemannian metric on* T^m, *and* g_q *is a function that to each point of* T^m *assigns a metric on* $\mathrm{Der}(M_n(\mathbb{R}))$. *Then*

$$E(g,\nabla_g)=\int_{T^m}R_c\sqrt{|\mathrm{det}g_c|}\sqrt{|\mathrm{det}g_q|}+\int_{T^m}R_q\sqrt{|\mathrm{det}g_q|}\sqrt{|\mathrm{det}g_c|}+\int_{T^m}R_{\,\mathrm{mixed}}\sqrt{|\mathrm{det}g|}, \tag{3}$$

where R_c is the classical scalar curvature of g_c, R_q is a (point dependent) scalar curvature of ∇_{g_q} [i.e., $R_q=\mathscr{T}_E(\tilde{g}_q^{-1}\circ Ric_{\nabla_{g_q}})$], and R_{mixed} is a function on T^m that is a sum of mixed terms of the kind

$$g^{AB}\frac{\partial}{\partial x^\mu}\left(g^{\mu\nu}\frac{\partial g_{AB}}{\partial x^\nu}\right),\quad \mu,\nu\leqslant m,\quad A,B>m.$$

Proof: Very much like the proof of Proposition 13. □

As we see from Proposition 15, the assumption that the metric g is block-diagonal allows us to split the Einstein action of the Levi–Civita connection into the following three terms.

(1) A classical-like term that differs from the usual Einstein–Hilbert action on T^m only by the ''quantum volume element'' $\sqrt{|\det g_q|}$.
(2) A quantum-like term that is equal to the integral over T^m of the (point dependent) Einstein action of the Levi–Civita connection on $M_n(\mathbb{R})$.
(3) A mixed term that involves the derivatives of g_q.

If g_q is constant over T^m, then $R_{\text{mixed}}=0$, and the expression (3) simplifies to

$$E(g,\nabla_g)=\sqrt{|\det g_q|}E(g_c)+E(g_q)\ \text{vol}(T^m,g_c),$$

where $E(g_c)$ is the usual Einstein–Hilbert action, $E(g_q)$ is the action computed in Proposition 13, and $\text{vol}(T^m,g_c)$ is the volume of T^m with respect to the metric g_c.

Finally, let us remark that the Yang–Mills (Maxwell) action calculated in Ref. 1 for a similar algebra also splits into a classical-like, a quantum-like and a mixed term.

IV. THE CASE OF *A* VALUED METRICS

Let us now lift the assumption that $g(\mathscr{S},\mathscr{S})\subseteq Z(A)$, and consider a toy model based on the following data:

$$A=M_4(\mathbb{R}),\quad \mathscr{S}=\mathfrak{so}(2)\oplus\mathfrak{so}(2),\quad \tau_g=\tfrac{1}{4}\sqrt{|\det g|}Tr_{M_4(\mathbb{R})}\ \text{and}\ \mathscr{T}_E=Tr\otimes id_{M_4(\mathbb{R})}.$$

We view $\mathscr{S}$ as a Lie subalgebra of $\text{Der}(M_4(\mathbb{R}))$ generated by $\hat{F}_1:=[F_1,.]$, $\hat{F}_2:=[F_2,.]$, where $F_1:=\left(\begin{smallmatrix}F&0\\0&0\end{smallmatrix}\right)$, $F_2:=\left(\begin{smallmatrix}0&0\\0&F\end{smallmatrix}\right)$, $F:=\left(\begin{smallmatrix}0&1\\-1&0\end{smallmatrix}\right)$. A metric g is treated as an element of $GL_2(M_4(\mathbb{R}))=GL_8(\mathbb{R})$. An assumption that g is symmetric reads $g(\hat{F}_i,\hat{F}_j)=:g_{ij}=g_{ji}:=g(\hat{F}_j,\hat{F}_i)$, or equivalently $g=g^T$, where ^{T} is the transpose in the algebra of 2×2 matrices. As to the inverse of g, denoted by $g^{-1}=:\left(\begin{smallmatrix}g^{11}&g^{12}\\g^{21}&g^{22}\end{smallmatrix}\right)$, in general we do not have $g^{12}=g^{21}$. For instance, if

$$g=\begin{pmatrix}2I_2&0&I_2&I_2\\0&I_2&I_2&0\\I_2&I_2&I_2&0\\I_2&0&0&I_2\end{pmatrix},$$

where $I_2=\left(\begin{smallmatrix}1&0\\0&1\end{smallmatrix}\right)$, then $g^{12}\neq g^{21}$. Very much as we did before, we define the Christoffel symbols by $\nabla_{\hat{F}_i}\hat{F}_j=\hat{F}_k\otimes\Gamma^k_{ji}$, the curvature coefficients by $(\nabla^2\hat{F}_k)(\hat{F}_i,\hat{F}_j)=\hat{F}_m\otimes R^m_{kij}$, and the Ricci curvature coefficients by $(Ric_\nabla\hat{F}_i)(\hat{F}_j)=R_{ji}$. It is straightforward to verify that $R^m_{kij}=\Gamma^m_{ni}\Gamma^n_{kj}-\Gamma^m_{nj}\Gamma^n_{ki}+[F_i,\Gamma^m_{kj}]-[F_j,\Gamma^m_{ki}]$ (see Proposition 4), $R_{kj}=R^i_{kij}$, and

$$E(g,\nabla)=-\tfrac{1}{4}\sqrt{|\det g|}Tr_{M_4(\mathbb{R})}(g^{jk}R_{kj})=-\tfrac{1}{4}\sqrt{|\det g|}tr(g^{-1}r),\tag{4}$$

where tr denotes the usual trace on $M_8(\mathbb{R})$, and $r:=\left(\begin{smallmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{smallmatrix}\right)$. In what follows, rather than look for a Levi–Civita connection, we will use an analogue of the Palatini method of variation (see 21.2 in Ref. 14, cf. 5.4–5.5 in Ref. 15) and find critical points of the Einstein action functional. First, let us determine the equation equivalent to the condition that the variation of E with respect to g vanish. At any critical point, for an arbitrary matrix $h \in M_8(\mathbb{R})$ with the coefficients satisfying $h_{12}=h_{21} \in M_4(\mathbb{R})$, we must have

$$\frac{d}{ds}E(g+sh,\nabla)|_{s=0}=0\,. \tag{5}$$

After substituting (4) into (5), and carrying out the differentiation, we obtain

$$\tfrac{1}{2}tr(g^{-1}r)tr(hg^{-1})=tr(hg^{-1}rg^{-1}). \tag{6}$$

Now, since (6) must be true for any matrix h such that $h_{12}=h_{21}$, we can conclude that

$$\forall i,j\in\{1,2\}\colon \tfrac{1}{2}tr(g^{-1}r)(g^{ij}+g^{ji})=g^{ik}R_{kl}g^{lj}+g^{jk}R_{kl}g^{li}.$$

Multiplying both sides by g_{im}, and then taking the trace, we find that

$$8tr(g^{-1}r)=2tr(g^{-1}r).$$

Hence, very much as in the classical general relativity, we have $tr(g^{-1}r)=0$. Consequently,

$$g^{-1}rg^{-1}+(g^{-1}rg^{-1})^T=0\,. \tag{7}$$

The formula (7) is an analogue of the Einstein vacuum field equation. [Observe that the implication (7)$\Rightarrow$(5) is also true.]

Our next step is to find an explicit form of the equations equivalent to the vanishing of the variation of E with respect to ∇. Let $\nabla+sA$ denote a connection on $\mathscr{L}$ whose Christoffel symbols are $\Gamma^k_{ji}+sA^k_{ji}$, where $s \in \mathbb{R}$, $A^k_{ji} \in M_4(\mathbb{R})$, $i,j,k \in \{1,2\}$. Then the condition that

$$\frac{d}{ds}E(g,\nabla+sA)|_{s=0}=0, \quad \text{for any } A,$$

is equivalent to the following 8 equations:

$$g^{11}\,\Gamma^2_{12}+\,\Gamma^1_{22}g^{22}+[\,\Gamma^1_{12}+F_2,g^{21}]=0, \tag{8}$$

$$g^{11}\,\Gamma^2_{11}+\,\Gamma^1_{21}g^{22}+[\,\Gamma^1_{11}+F_1,g^{21}]=0, \tag{9}$$

$$g^{22}\,\Gamma^1_{22}+\,\Gamma^2_{12}g^{11}+[\,\Gamma^2_{22}+F_2,g^{12}]=0, \tag{10}$$

$$g^{22}\,\Gamma^1_{21}+\,\Gamma^2_{11}g^{11}+[\,\Gamma^2_{21}+F_1,g^{12}]=0, \tag{11}$$

$$g^{22}\,\Gamma^1_{12}-\,\Gamma^2_{22}g^{22}-g^{12}\,\Gamma^2_{12}-\,\Gamma^2_{12}g^{21}-[F_2,g^{22}]=0, \tag{12}$$

$$g^{11}\,\Gamma^2_{22}-\,\Gamma^1_{12}g^{11}-g^{21}\,\Gamma^1_{22}-\,\Gamma^1_{22}g^{12}-[F_2,g^{11}]=0, \tag{13}$$

$$g^{22}\,\Gamma^1_{11}-\,\Gamma^2_{21}g^{22}-g^{12}\,\Gamma^2_{11}-\,\Gamma^2_{11}g^{21}-[F_1,g^{22}]=0, \tag{14}$$

$$g^{11}\,\Gamma^2_{21}-\,\Gamma^1_{11}g^{11}-g^{21}\,\Gamma^1_{21}-\,\Gamma^1_{21}g^{12}-[F_1,g^{11}]=0. \tag{15}$$

It is straightforward to verify that a connection ∇^g (not to be confused with the Levi–Civita connection ∇_g) whose Christoffel symbols are given by

$$\Gamma^1_{22}=\Gamma^1_{21}=-g^{11},\quad \Gamma^2_{22}=-F_2-g^{12},\quad \Gamma^1_{12}=-F_2+g^{21},$$

$$\Gamma^2_{12}=\Gamma^2_{11}=g^{22},\quad \Gamma^2_{21}=-F_1-g^{12},\quad \Gamma^1_{11}=-F_1+g^{21},$$

satisfies (8)–(15), and has vanishing Ricci curvature ($Ric_{\nabla^g}=0$). We have thus arrived at the following.

Proposition 16: *Let $A,\mathscr{S},\tau_g$ and $\mathscr{T}_E$ be as above. Then*

$$\forall g\in\mathscr{M}(\mathscr{S})\ \exists\nabla^g\in\mathscr{C}(\mathscr{S})\ \textit{such that}\ (g,\nabla^g)\ \textit{is a critical point of}\ E.$$

Furthermore, the value of E at any critical point is zero.

Remark 17: The value of the functional E calculated at noncritical points is not necessarily zero. For example, take a metric $g_0=g_0^{-1}$ with the components

$$(g_0)_{11}=(g_0)_{22}=0,\quad (g_0)_{12}=(g_0)_{21}=\begin{pmatrix} I_2 & 0\\ 0 & K\end{pmatrix},\quad K:=\begin{pmatrix}0&1\\1&0\end{pmatrix},$$

and take a connection ∇_0 whose only nonvanishing Christoffel symbol is $(\Gamma_0)^1_{11}=\left(\begin{smallmatrix}0&0\\0&J\end{smallmatrix}\right)$, where $J=\left(\begin{smallmatrix}1&0\\0&-1\end{smallmatrix}\right)$. Then $E(g_0,\nabla_0)=-1$. ◇

Remark 18: Note that for τ_g equal to $Tr_{M_4(\mathbb{R})}$ rather than to $\frac{1}{4}|\det g|^{1/2}Tr_{M_4(\mathbb{R})}$ the field equation (7) and the equations (8)–(15) are still satisfied. Also, $tr(g^{-1}r)$ still equals zero at any critical point. Consequently, Proposition 16 remains valid as well, if we replace $\frac{1}{4}|\det g|^{1/2}Tr_{M_4(\mathbb{R})}$ by the usual trace on $M_4(\mathbb{R})$. ◇

Remark 19: The fact that the functional $\widetilde{E}:\mathscr{M}(\mathscr{S})\ni g\mapsto E(g,\nabla^g)\in\mathbb{R}$ equals identically zero is a reflection of the same effect that we observe for the usual 2-torus. We might try to push this analogy even further and say that we think of a circle S^1 as a Lie group generated by $\mathfrak{so}(2)$, and replace $C^\infty(S^1)$ by $M_2(\mathbb{R})$ for which $\mathfrak{so}(2)$ is the space of all derivations satisfying $X(a^T)=(Xa)^T$. Then it is natural to replace $C^\infty(T^2)$ by $M_2(\mathbb{R})\otimes M_2(\mathbb{R})=M_4(\mathbb{R})$. ◇

Observe that although ∇^g functions as if it were a Levi–Civita connection, it is in general neither metric nor torsion free [e.g., take g to be the identity matrix of $GL_8(\mathbb{R})$]. It is perhaps worth emphasizing, however, that the metric compatibility condition, which can be equivalently written as

$$g^{pj}\Gamma^n_{ji}+\Gamma^p_{ji}g^{jn}+[F_i,g^{pn}]=0,\quad i,p,n\in\{1,2\},$$

is not very different from the formulas (8)–(15). It would be interesting to find a functional on $\mathscr{M}(\mathscr{S})\times\mathscr{C}(\mathscr{S})$ that not only would coincide with the usual Einstein–Hilbert functional (or whose equations of motion would agree with the standard ones) in the case of classical geometry, but also would yield, through its variation with respect to connection, the metric compatibility condition.

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Imploding scalar fields

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Static spherically symmetric uncoupled scalar space–times have no event horizon and a divergent Kretschmann singularity at the origin of the coordinates. The singularity is always present so that nonstatic solutions have been sought to see if the singularities can develop from an initially singular free space–time. In flat space–time the Klein–Gordon equation $\Box\varphi=0$ has the nonstatic spherically symmetric solution $\varphi=\sigma(v)/r$, where $\sigma(v)$ is a once differentiable function of the null coordinate v. In particular, the function $\sigma(v)$ can be taken to be initially zero and then grow, thus producing a singularity in the scalar field. A similar situation occurs when the scalar field is coupled to gravity via Einstein's equations; the solution also develops a divergent Kretschmann invariant singularity, but it has no overall energy. To overcome this, Bekenstein's theorems are applied to give two corresponding conformally coupled solutions. One of these has positive ADM mass and has the following properties: (i) it develops a Kretschmann invariant singularity, (ii) it has no event horizon, (iii) it has a well-defined source, (iv) it has well-defined junction condition to Minkowski space–time, and (v) it is asymptotically flat with positive overall energy. This paper presents this solution and several other nonstatic scalar solutions. The properties of these solutions which are studied are limited to the following three: (i) whether the solution can be joined to Minkowski space–time, (ii) whether the solution is asymptotically flat, (iii) and, if so, what the solutions' Bondi and ADM masses are. © *1996 American Institute of Physics.* [S0022-2488(96)02409-7]

I. INTRODUCTION

Singularities appear in many physical theories. A singularity can be defined as a domain where the description provided by the physical theory breaks down. A prime example is the infinite electromagnetic potential of a point particle in Maxwell's theory. A common approach to a theory which has singularities is to produce another theory governed by more general differential equations and then investigate whether the singularities still occur. For example, in electromagnetic theory Born and Infeld investigated a generalization of Maxwell's Lagrangian to see if the infinite potential was still present. In gravitational theory the situation is more complex: for a point particle the Kretschmann invariant $R_{abcd}R^{abcd}_{\ldots\ldots}$ diverges at the position of the particle; also on occasion the particle is surrounded by an event horizon. The event horizon is not singular in the sense defined above because a description of its effects can be made: but the effects are so bizarre that along with singularities they can be called pathological. Vacuum general relativity frequently has both pathologies, an example being the Schwarzschild solution for a point particle. It is sometimes argued that the existence of both pathologies is palatable because the event horizon makes the divergent Kretschmann invariant invisible at infinity. However, the physical description provided is still incomplete because it does not describe what happens at the divergent Kretschmann invariant. Vacuum general relativity does not furnish a good description of many astrophysical phenomena such as gravitational collapse because the pertinent space–time can

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contain many fields and fluids with nonvanishing stress. Astronomical observations purporting to be of ''black holes'' in fact do not directly observe event horizons. The models which describe the situation merely use a steeper potential than that of Newtonian theory; the Newtonian limit of most relativistic theories produces such a potential.

To find exact solutions of gravitational field equations to fit a particular physical requirement is notoriously difficult. An example is the two-body problem: since the inception of general relativity the solution for two-point particles acting only through gravity has been sought. Another example is the Yukawa problem: in the absence of gravitation a massive scalar field has a shorter range than the corresponding massless case; Yukawa's discovery of this lead to the postulation of nuclear forces. How gravitation alters the shape of the potential is unknown, and this would be of experimental interest as the Yukawa potential can be accurately measured in accelerators; also, it is unknown whether the mass of the interacting scalar field is the same as the ADM mass. Scalar fields coupled to gravity produce unusual potentials, complicated by the fact that the luminosity radial coordinate is often of the form $R=r\exp(\varphi)$, where the metric is explicitly expressed in terms of r. Perhaps the simplest modification of vacuum general relativity is to choose a stress with an uncoupled scalar field. When this is done the situation is mitigated; for the static case there is no event horizon. The problem with static space–times is that the Kretschmann invariant is always present; the space–time does not develop so as to produce it. Nonstatic spherically symmetric scalar solutions have been found, one of which is asymptotically flat.[1,2] This solution has unusual energetics; there is no overall energy, the positive energy of the scalar field and the negative energy of the gravitational field cancel out: as the space–time develops energy is just exchanged between them. To overcome this, Bekenstein's theorems are applied to uncoupled scalar field solutions to give two corresponding conformal scalar solutions. One of these is asymptotically flat and has overall positive ADM energy.

In general relativity scalar fields can implode (and explode) like the example in the abstract; the situation here is more pathological than in flat space because not only is it possible to produce a singularity in the scalar field, but in addition, there is a colocational singularity of the gravitational field as indicated by the divergence of the Kretschmann curvature invariant $R^{abcd}_{\ \ \ \ \ \ \ \ }R_{abcd}$. Einstein–scalar space–times are sometimes not covered by theorems concerned with the general global and singular structure of space–time. These often assume the space–time stress tensor is restricted to: vacuum, or electromagnetic stress, or obey energy inequalities. An example of this is the formal definition of asymptotic flat space–times which assumes that there is only an electromagnetic and gravitational field present. Numerical studies show that the rate of decay of scalar fields is between these two;[1] furthermore, many spherical symmetric perfect fluid stresses do not have (in the sense of taking a radial coordinate $r\to\infty$) asymptotically flat space–times.[3] Here a scalar solution is taken to be asymptotically flat if it reduces to Minkowski space–time as $r\to\infty$. The rate of decay of fields seems to be: most fluids and some conformal scalars are not asymptotically flat, then gravitation>uncoupled scalars>uncoupled vectors>interacting fields.

In Sec. II some Robertson–Walker scalar field solutions are given. The examples chosen have scale factors which can be expressed in terms of straightforward functions. Ordinary scalar stresses obey the energy conditions, but conformal scalar stresses sometimes do not. Violation of the energy conditions allow the possibility of a singular free Robertson–Walker space–time; this can happen for conformal scalar fields[4] and when cosmological constant is present.[5] Here the junction conditions of Robertson–Walker space–time are studied, and possible applications mentioned. In Sec. III Penny's[6] solution is presented; this can implode, but is not asymptotically flat. In Sec. IV the solution previously found by the author,[1,2] and also its two conformal scalar extensions as found by Bekenstein's theorems, are presented. These solutions are explicitly dependent on a radial coordinate so that they are more similar to the example in the abstract than the examples in Secs. II and III. The solution and one of its Bekenstein extensions are asymptotically flat, and also have well-defined junction conditions, contrary to what has been stated by Szabodos.[7] The Bondi and ADM masses of the solutions are calculated. In the first two appendices

I derive the Clarke and Dray[8] junction conditions subject to spherical symmetry. In all the specific cases looked at here if a solution has a continuous metric (and hence first fundamental form) across a junction, then its surface stress (which depends on the derivatives of the metric) vanishes and the junction is well defined. In the third appendix I derive the general expression for the ADM mass subject to spherical symmetry.

The field equations considered are Einstein's equations with scalar fields as source. Specifically the ordinary scalar–Einstein equations are

$$R_{ab}=2\varphi_a\varphi_b\,, \tag{1.1}$$

where the coupling constant is taken to be contained in the scalar field φ. On occasion a null radiation field is also taken to be present with

$$R_{ab}=\Phi^2 k_a k_b\,, \tag{1.2}$$

where k_a is a null vector and Φ is a function of x^a. Conformal scalar solutions can be obtained from ordinary scalar solutions by using Bekenstein's[9] theorems. To derive these let barred quantities denote these quantities for an ordinary scalar solution, i.e., $R_{ab}=2\varphi_a\varphi_b$. Then under a conformal transformation

$$\overline{g}_{ab}=\Omega^2 g_{ab}\,; \tag{1.3}$$

the connection is transformed,

$$\overline{\Gamma^a_{bc}}-\Gamma^a_{bc}=\Omega^{-1}(\delta^a_b\Omega_c+\delta^a_c\Omega_b-g_{bc}\Omega^a); \tag{1.4}$$

and the Ricci tensor is transformed,

$$\overline{R}_{ab}-R_{ab}=-2\Omega(\Omega^{-1})_{;ab}+\Omega^{-2}(\Omega^2)^c_{\cdot c}g_{ab}\,, \tag{1.5}$$

where the covariant derivatives ";" are taken in the unbarred system. Now take

$$\begin{aligned}\Omega=\sqrt{\pm(1-\xi^2\varphi^2)}&=\begin{cases}\text{sech}\\ \text{cosech}\end{cases}\quad \xi\varphi,\\ \xi\varphi=\sqrt{1\mp\Omega^2}&=\begin{cases}\tanh\\ \coth\end{cases}\quad \xi\varphi,\end{aligned} \tag{1.6}$$

where ξ is a constant and φ is a function. Then, substituting into the Ricci tensor (1.5), this obeys the equations for a conformal scalar field

$$(1/\xi^2-\psi^2)R_{ab}=4\psi_a\psi_b-2\psi\psi_{;ab}-(\psi\psi^c{}_{\cdot})_c g_{ab}\,. \tag{1.7}$$

Thus given an ordinary scalar field solution (1.1), Bekenstein's theorems give two conformal scalar solutions (1.6); Bekenstein refers to the upper sign conformal solution as type A and the lower sign conformal solution as type B, as no confusion with blood types should occur the ordinary scalar solution is here called type O. In the conventions used here, the coupling constant is taken to be in the scalar field and thus $\xi^2=\frac{1}{3}$. The conformal scalar solutions are traceless and also obey $\psi^a_{\cdot a}=0$. For type A the theorem generalizes for additional stress present; in the case of a null radiation field this must transform as $\Phi^2\to\Omega^{-2}\Phi^2$, c.f. Bekenstein's[9] equation 15; this generalization does not work for type B. Type B solutions are anticipated to have unusual global properties, for example as $\varphi\to 0$: $\Omega^{-1}\to 0$, $\psi\to\infty$; and also as $\varphi\to\infty$: $\Omega^{-1}\to\infty$, $\psi\to 1$; but applying Bekenstein's theorems does not *a priori* produce a maximally extended space–time so that exact

solutions have to be specified before precise pronouncements on their global properties can be made. Examples of static spherically symmetric conformal scalar fields with unusual properties can be found in Ref. 10.

Having presented some of the properties of scalar fields we can now come back to the questions: general relativity and other gravitational theories are primarily macroscopic theories which couple to stresses that have macroscopic effect; such electromagnetism and perfect fluids are natural choices—why choose scalar fields? First, it only takes an infinitesimal scalar field to change the global nature of a space–time. For example, Wyman's solution, which is the general static spherically symmetric O-scalar–Einstein solution, is a two-parameter solution (M,σ) with M the Schwarzschild mass and σ the scalar charge (an infinitesimal σ is sufficient for there to be no event horizon present). Thus microscopic fields, such as those of particle physics, can have a global effect on space–time. Second, for φ_a timelike an O-scalar field is a particular example of a perfect fluid. Perfect fluids which are well behaved and permeate the whole space–time can usually be shown to have no horizons.[3] The fluid conservation equations often allow the fluid index ω to be equated with the fluid vector and hence the metric. Typically this results in equations such as the lapse $N=1/\omega$; thus a well-behaved fluid index ω can often imply a well-behaved metric. In Appendix D an attempt is made to extend to fields the techniques that lead to this result. Third, in microscopic physics hypothetical particles, the Higgs scalars, are used to introduce ''mass'' terms while preserving gauge invariance. Although other mechanisms have been proposed, for example, by using fermion composites, or using fluids Roberts,[11,12] the resulting Lagrangians have terms similar to scalar fields. Fourth, many quantum and unified theories have gravitational actions with terms of higher order. The quadratic action can be split into two independent parts, the traceless part being the Bach tensor and the other part the Pauli tensor. Using a conformal factor solutions to these equations can be found by Barrow and Cotsakis'[13] method. The Bach tensor has several similarities to conformal scalar fields and there might be a theorem connecting their solutions. Vacuum solutions can generate O-scalar solutions by Buchdahl's trick (the analogous theorem for vector gauge theory is called the Julia–Zee correspondence) (see, for example, Ref. 11); O-scalar solutions can generate A and B scalar solutions by Bekenstien's theorems; and perhaps A and B scalar solutions can generate Bach–Einstien solutions. Fifth, O-scalar solutions obey the energy conditions. The energy conditions are inequalities designed to judge whether macroscopic fluids have reasonable energetics: they break down when considering the interacting fields necessary for particle physics (see, for example, Ref. 14, p. 95).

Apart from the above five reasons for investigating scalar fields, they can be viewed as merely a scalar function defined on a region of space, and such a requirement seems to be fairly ubiquitous in physics. Systematic discussion of them is hindered because there is no recognized way of classifying them. Some indications of their properties are given by the following. *Coupling classification*: call scalar fields coupled only to Einstein's equations type O: conformal scalar fields coupled to Einstein's equations type C, scalar fields with mass self-interaction type Y, renormalizable scalar fields with fourth-order self-interaction type L, inflationary scalar fields with potential $V(\varphi)$ type V, scalar fields that can be represented as fluids type F, symmetry breaking scalar fields coupled to vector fields type H, and so on. *Generational classification*: exact scalar field solutions can be generated from exact solutions to simpler differential equations. For a given configuration usually the generated solution is not the most general one. *Stress classification*: stress tensors can be classified by the Segre or Plebanski methods. *Energy classification*: for a space–time with Lorentz signature $(-,+,+,+)$ rather than positive definite signature $(+,+,+,+)$, vectors can be timelike, null, or spacelike. The existence of timelike vectors allows the measurement of the energy to be defined. For a given space–time ψ_a and $\psi_a T^b{}_a$ are vectors that can be timelike, null, or spacelike; the energy conditions can be investigated and on occasion the overall energy measured.

For conformal scalar fields the energy conditions can be complicated; hand calculations of them for the specific solutions presented here are too long to be practicable. Three observations are

now stated which give a rough indication of what energetics to expect. The first observation is that the general stress for conformal scalar fields contains terms of undetermined sign and this remains the case even if the conformal scalar stress has been obtained by using Bekenstein's theorems; this can been seen from (1.6) and (1.7). The second observation is for an O-scalar solution, it is possible to consider whether the vector φ_α is spacelike, timelike, or null: this just depends on the Ricci scalar because $\overset{..}{g}^{ab}\varphi_a\varphi_b=\frac{1}{2}R$; now using Bekensteins' theorems both for types A and B there is the equation $\overset{..}{g}^{ab}\Psi_a\Psi_b=\frac{1}{2}R$. Thus there is no change in the causal direction of the scalar field. The third observation is achieved by direct inspection of the scalar fields. Neglect that the equation for the stress of a conformal scalar field differs from that of the ordinary case and also that Bekenstein's theorems introduce a conformal factor into the metric. Then the energy conditions will just depend on the relative size of the scalar fields involved. The type O scalar field is a negative real scalar quantity. Bekenstein's theorems give that the type A scalar is the tanh of this and that the type B is the coth of this; thus the scalar fields take real values such that $0>A>O>B>-\infty$. Now the type O scalar field on occasion (an example being that of Sec. IV) contains the same quantity of energy but of the opposite sign as the gravitational field; the above inequalities suggest that the type A solution would have total positive energy because the scalar field is not so negative, and also that the type B solution would have total negative energy. This is found to be the case for the type A solution described in the conclusion. The above suggests that it is a reasonable guess that type A solutions have well-defined energy conditions and that type B do not: this is what would be expected from the known exact solutions where it would account for type A having mundane properties whereas those of type B solutions are bizarre.

II. ROBERTSON–WALKER SCALAR SOLUTIONS

The Robertson–Walker line element can be put in the form

$$ds^2=-N(t)^2\,dt^2+R(t)^2d\Sigma^2_{3,k}, \tag{2.1}$$

where

$$d\Sigma^2_{3,k}=d\chi^2+f(\chi)^2(d\theta^2+\sin^2\theta\,d\varphi^2)$$

and

$$f(\chi)=\sin\chi,\chi,\sinh\chi,$$

for $k=+1,0,-1$ respectively. Taking $A=R^2$, $B=R^2f^2$, $C=N^2$, and $\chi=r$ gives the line element in the spherically symmetric form (B1). Here N is called the lapse and R the scale factor. N can be absorbed into the line element; the choice $N=1$ gives the Robertson–Walker line element in proper time. For the choice $N=R$, Robertson–Walker space–time is conformal to the Einstein static universe and by convention the time coordinate is denoted by η. For $N=1$ the scale factor R can be expanded as a Taylor series around a fixed time $t=t_0$, thus

$$R=R_0[1+H_0(t-t_0)-\tfrac{1}{2}q_0H_0^2(t-t_0)^2+O(t-t_0)^3], \tag{2.2}$$

where

$$H\equiv\dot{R}/R \tag{2.3}$$

is called the Hubble parameter and

$$q\equiv-\ddot{R}.R/(\dot{R}^2) \tag{2.4}$$

is called the deceleration parameter, the subscript ''0'' indicates that the parameter is evaluated at $t=t_0$, and $\mathring{R}=\partial_t R$.

The equation of state

$$p=(\gamma-1)\mu \tag{2.5}$$

produces equations equivalent to those of an ordinary scalar field in the particular case of $\gamma=2$ (see Appendix D). Einstein's equations have been solved by Vajk[15] for the metric (2.1) and equation of state (2.5). Specializing to the $\gamma=2$ ordinary scalar field case gives

$$k=0, \quad \Xi=\alpha\eta^{1/2}, \quad \varphi=\frac{\sqrt{3}}{2}\ln\ \eta,$$

$$k=+1, \quad \Xi=\alpha(\sin\ \eta\ \cos\ \eta)^{1/2}, \quad \varphi=\frac{\sqrt{3}}{2}\ln\tan\ \eta, \tag{2.6}$$

$$k=-1, \quad \Xi=\alpha(\sinh\ \eta\ \cosh\ \eta)^{1/2}, \quad \varphi=\frac{\sqrt{3}}{2}\ln\tanh\ \eta,$$

where

$$\alpha=2R_0\sqrt{\frac{H_0^2R_0^2}{c^2}+k},$$

c is the speed of light, and Ξ is equal to both the scale factor and the lapse, i.e., $\Xi=N=R$. The $k=0$ solution is one of the few solutions known to have an exact form for the world function.[16]

Applying Bekenstein's theorems,

$$k=0, \quad \Upsilon=\frac{\alpha}{2}(\eta\pm1), \quad \frac{1}{\sqrt{3}}\psi=\frac{\eta\mp1}{\eta\pm1},$$

$$k=+1, \quad \Upsilon=\frac{\alpha}{2}(\sin\ \eta\pm\cos\ \eta), \quad \frac{1}{\sqrt{3}}\psi=\frac{\sin\ \eta\mp\cos\ \eta}{\sin\ \eta\pm\cos\ \eta}, \tag{2.7}$$

$$k=-1, \quad \Upsilon=\frac{\alpha}{2}\exp(\pm\eta), \quad \frac{1}{\sqrt{3}}\psi=-\exp(\mp\eta),$$

where $\Upsilon=\Xi\Omega^{-1}$. In the $k=0$ case the ±1 can be absorbed into the line element by defining $\eta'=\eta\pm1$, giving a single solution. Transferring the $k=+1$ solution to proper time by defining $t=(\alpha/2)(-\cos\ \eta\pm\sin\ \eta)$ gives

$$ds^2=-dt^2+\left(\frac{\alpha^2}{2}-t^2\right)d\Sigma^2_{3,+1}, \quad \frac{1}{\sqrt{3}}\psi=\left(\frac{\alpha^2}{2t^2}-1\right)^{-1/2}, \tag{2.8}$$

showing that there is only one $k=+1$ metric. In the $k=-1$ case define $t=(\alpha/2)\exp(\pm\eta)$ to give

$$ds^2=-dt^2+t^2d\Sigma^2_{3,-1}, \quad \frac{1}{\sqrt{3}}\psi=-\frac{\alpha^2}{4t^2}. \tag{2.9}$$

This is just the Milne universe, further discussed at Eq. (2.16); the field ψ is a ghost field that does not contribute to the stress. Conformal scalar stresses are traceless; this can be used to reduce the number of equations. In particular the Einstein–conformal scalar equations with Robertson–Walker metric can be quickly reduced to one equation

$$R_{,\eta\eta} = -kR. \tag{2.10}$$

This gives solutions more general than those of (2.7). However, they are particular instances of the conformal scalar and incoherent radiation solutions of Bekenstein (Ref. 9, 1973) #6. Bekenstein's theorems can then be used in reverse to give generalizations of (2.6).

The null junction conditions are studied by defining

$$v = \eta + r. \tag{2.11}$$

Robertson–Walker space–time in the conformal time coordinate η takes the single null form (A1) with $X = S = Yf^{-2} = R(v-r)^2$. The θ and φ components of the surface stress vanish identically. The v and r components are given by

$$\tau_{ab} = -f^{-2}R^{-2}[(R^2f^2)']n_a n_b, \tag{2.12}$$

which do not vanish at a junction with Minkowski space–time.

The non-null junctions are studied by calculating the second fundamental form as in Appendix B. The second fundamental form across the spacelike surface normal to (B3) is

$$K_{rr} = \frac{-R\mathring{R}}{N},$$
$$K_{\theta\theta} = \sin^{-2}\theta K_{\varphi\varphi} = -\frac{f^2R\mathring{R}}{N}, \tag{2.13}$$

which gives no junctions to Minkowski space–time. The surface normal to the radial spacelike vector (B5) has second fundamental form

$$K_{tt} = 0,$$
$$K_{\theta\theta} = \sin^{-2}\theta K_{\varphi\varphi} = ff'R. \tag{2.14}$$

Again there are no junctions to Minkowski space–time. The radial spacelike vector is not well suited to Robertson–Walker geometries. Choosing the isotropic spacelike vector (B7) gives second fundamental form

$$K_{tt} = K_{tr} = 0,$$
$$K_{r\theta} = \frac{K_{t\varphi}}{\sin\theta} = R\,\frac{K_{\theta\varphi}}{\sin\theta} = -\frac{1}{2}fK_{rr} = \frac{-f'R}{3\sqrt{3}}, \tag{2.15}$$
$$K_{\theta\theta} = \frac{K_{r\theta}}{\sin\theta} = \frac{f}{3\sqrt{3}}\{-\cot\theta + 2f'R\}.$$

Again there are no junctions to Minkowski space–time.

Consider Minkowski space–time in the form (2.1) with $k=0$ and $N=R=1$, $f=r$, and apply the coordinate transformation

$$t=\overline{t}\cosh\chi, \quad r=\overline{t}\sinh\chi. \tag{2.16}$$

This transformation gives the Milne universe which has $N=1$, $R=t$, and $f=\sinh r$. The Milne universe is flat and is identical to Minkowski space–time except that there is a point removed at the origin $t=0$. At first sight it might be expected that the Milne universe could be joined to Minkowski space–time across the surface chosen here. The reason that this does not happen is that the space and time coordinates have been ''mixed'' by (2.16) so that if there was a well defined junction it would be across a different surface from those chosen here. A general treatment of redefinitions of space and time coordinates in Robertson–Walker space–time can be found in Ref. 17.

The junction conditions of Robertson–Walker space–time have two further applications. The first is the production of a spherical Minkowski cavity which has implications for Mach's principle (see, for example, Ref. 18, p. 474). A point inside the cavity is an inertial frame if it does not rotate with respect to the reference frame of the rest of the universe, which is taken to be given by the Robertson–Walker space–time surrounding the cavity. A different approach to Mach's principle is discussed in Ref. 19. The second is to the cell universe models. The surface normal to the vectors chosen here do not allow junctions between Robertson–Walker space–time and Schwarzschild space–time. Thus for the Schwarzschild cell universe of Lindquist and Wheeler[20] to work, a different vector has to be chosen or different physical assumptions made.

III. PENNY'S SOLUTION

Penny's solution,[6] and the related solutions of Gurses[21] and Ray,[22] are conformally flat. The conformal factor generating technique used to find these solutions is also to study solutions of higher-order gravity theories, Barrow and Cotsakis (1988). Here attention is restricted to Penny's solution where the conformal factor and the ordinary scalar field are given by

$$\Xi=k_a x^a+a, \quad k_{a,b}=0, \quad \varphi=\sqrt{3}\ln\Xi, \tag{3.1}$$

respectively. Defining

$$K_a=-\Xi k_a, \tag{3.2}$$

K_a is a Killing vector which is null iff k_a is null. The conformal factor can be expressed as

$$\Xi^2=a+bt+cx+dy+ez, \tag{3.3}$$

where a,b,c,d are constants. There is no asymptotically flat solution. For $a=c=d=e=0$, $b=2R_0^2H_0$, this is the $k=0$ solution (2.6).

Using Bekenstein's theorems, conformal scalar solutions are

$$\begin{gathered}\Upsilon=\Omega^{-1}\Xi,\\ 2\Omega=2\begin{cases}\cosh\\ \sinh\end{cases}\quad \xi\varphi=\Xi\pm\Xi^{-1},\\ \xi\psi=\begin{cases}\tanh\\ \coth\end{cases}\quad \xi\varphi=\frac{\Xi^2\mp1}{\Xi^2\pm1},\end{gathered} \tag{3.4}$$

giving

$$\Upsilon=2\Xi^2/(\Xi^2\pm1).$$

Defining

$$K_a = \Upsilon^2 k_a , \tag{3.5}$$

again K_a is a Killing vector which is null iff k_a is null.

IV. THE SOLUTION PREVIOUSLY FOUND BY THE AUTHOR

The solution found in Refs. 1 and 2 is

$$ds^2 = -(1+2\alpha_{,v})dv^2 + 2dv\,dr + r(r-2\alpha)d\Sigma_2^2, \tag{4.1}$$

where $d\Sigma_2^2 = d\theta^2 + \sin^2\theta/d\varphi^2$, and α is a twice differentiable function of v. The stress is given by a scalar field and a null radiation field

$$\varphi = \frac{1}{2}\ln\left(1-\frac{2\alpha}{r}\right), \quad \Phi^2 = \frac{2\alpha\alpha_{,vv}}{r(r-2\alpha)}. \tag{4.2}$$

Defining the luminosity distance $R^2 = r(r-2\alpha)$, and taking the positive sign of the square root, the solution becomes

$$\begin{gathered} ds^2 = \left(-1+\frac{2\alpha\alpha_{,v}}{\lambda}\right)dv^2 + \frac{2R}{\lambda}\,dr\;dv + R^2 d\Sigma_2^2, \\ \varphi = \frac{1}{2}\ln\left(\frac{\lambda-\alpha}{\lambda+\alpha}\right), \quad \Phi^2 = 2\frac{\alpha\alpha_{,v}}{R^2}, \end{gathered} \tag{4.3}$$

where $\lambda^2 = \alpha^2 + R^2$. The Bondi mass $M(v)$ is half the coefficient of the R^{-1} term of g_{vv}. Expanding gives

$$M(v) = \alpha\alpha_{,v}. \tag{4.4}$$

For the null radiation field to vanish, $\alpha_{,vv} = 0$ or $\alpha = \sigma v + \beta$, where σ and β are constants. It is straightforward to show that β can be absorbed into the line element leaving $\alpha = \sigma v$; this can be substituted into (4.3) for a form of the metric using the luminosity radial coordinate; alternatively it can be substituted into (4.1), giving

$$\begin{gathered} ds^2 = -(1+2\sigma)dv^2 + 2dv\,dr + r(r-2\sigma v)d\Sigma_2^2, \\ \varphi = \frac{1}{2}\ln\left(1-\frac{2\sigma v}{r}\right). \end{gathered} \tag{4.5}$$

Defining $v' = \sqrt{1+2\sigma}v$, and $r' = r/\sqrt{1+2\sigma}$, gives

$$\begin{gathered} ds^2 = -dv'^2 + 2dv'dr' + r'((1+2\sigma)r' - 2\sigma v')d\Sigma_2^2, \\ \varphi = \frac{1}{2}\ln\left(1-\frac{2\sigma}{(1+2\sigma)}\frac{v'}{r'}\right) \end{gathered} \tag{4.6}$$

Then defining $t' = v' - r'$ gives

$$\begin{gathered} ds^2 = -dt'^2 + dr'^2 + r'(r' - 2\sigma t')d\Sigma_2^2, \\ \varphi = \ln(R/r). \end{gathered} \tag{4.7}$$

Also defining $t = t'/1+2\sigma$ the solution can be put in the form

$$ds^2=-(1+2\sigma)dt^2+\frac{dr^2}{(1+2\sigma)}+r\left(\frac{r}{(1+2\sigma)}-2\sigma t\right)d\Sigma_2^2,$$
$$\varphi=\frac{1}{2}\ln\left(\frac{1}{(1+2\sigma)}-\frac{2\sigma t}{r}\right), \tag{4.8}$$

and from this form using (C5) the ADM mass is seen to vanish identically.

Using Bekenstein's theorems to find conformal scalar solutions (4.3) gives

$$R=\overline{R}\Omega^{-1}=\overline{R}\begin{cases}\cosh\\ \sinh\end{cases}\quad \xi\varphi=\tfrac{1}{2}\overline{R}^{1-\xi}[(\lambda-\alpha)^{\xi}\pm(\lambda+\alpha)^{\xi}],$$
$$\xi\psi=\frac{(\lambda-\alpha)^{\xi}\mp(\lambda+\alpha)^{\xi}}{(\lambda-\alpha)^{\xi}\pm(\lambda+\alpha)^{\xi}}, \tag{4.9}$$

where $\lambda^2=\overline{R^2}+\alpha^2$ and $\overline{R}$ denotes the luminosity coordinate for the O-scalar solution, and R denotes it for the conformal scalar solution. For the type A solution general can be retained if the null radiation field is transformed, but for the type B solution α must equal σv. Inspecting (4.9) gives limiting behavior of the conformal scalar solution in terms of the luminosity coordinate for the ordinary solution,

$$\overline{R}\uparrow\infty,\quad \text{Type A:}\quad R\uparrow\infty,\psi\uparrow 0,\quad \text{Type B:}\quad R\downarrow-\xi,\psi\downarrow-\infty,$$
$$\overline{R}\downarrow 0,\quad \text{Type A:}\quad R\downarrow 0,\psi\downarrow-1,\quad \text{Type B:}\quad R\downarrow-0,\psi\uparrow-1. \tag{4.10}$$

The type B solution does not have an asymptotically flat region, so that attention is restricted to the type A solution. Expanding (4.9) for large R gives

$$R=\overline{R}\left(1+\frac{\xi^2\alpha^2}{2\overline{R^2}}+O\left(\frac{\alpha}{\overline{R}}\right)^3\right). \tag{4.11}$$

Solving this quadratic

$$\overline{R}=\frac{R}{2}\left(1\pm\sqrt{1-\frac{2\xi^2\alpha^2}{R^2}}\right), \tag{4.12}$$

the upper sign is taken so that $R=\overline{R}$ when $\xi=0$.

Differentiating

$$d\overline{R}=\frac{1}{2}\left(1+\frac{2}{\sqrt{1-2\xi^2\alpha^2/R^2}}\right)dR-\frac{2\xi^2\alpha\alpha_{,v}dv}{R\sqrt{1-2\xi^2\alpha^2/R^2}}, \tag{4.13}$$

inserting into the line element, and using (4.3), (4.12), (4.13) and that $\lambda^2=\alpha^2+\overline{R^2}$ gives

$$g_{vv}=-1+\frac{2(1-\xi^2)}{R}\,\alpha\alpha_{,v}+O(R^{-2}). \tag{4.14}$$

Thus the Bondi mass is given by

$$M(v)=(1-\xi^2)\alpha\alpha_{,v}, \tag{4.15}$$

which is two-thirds of (4.4). To calculate the ADM mass note that the conformal factor can be used:

$$A^t_{\cdot}=\overline{A^t_{\cdot}}+\lim_{r\to\infty}\left[-\frac{1\overline{B}}{2r}(\Omega^{-2})'\right], \tag{4.16}$$

where $\overline{B},\overline{A}$ are the values of these quantities in the O-scalar solution. Using the metric in the form (4.8) and noting that A vanishes,

$$A^t_{\cdot}=\lim_{r\to\infty}-\frac{\overline{B}\overline{\xi}}{2}\sinh(2\xi\varphi)\cdot\varphi'=\lim_{r\to\infty}-\frac{\xi\sigma}{2}\sinh(2\xi\varphi)\cdot t. \tag{4.17}$$

Expanding $\sinh(2\xi\varphi)$ for $r\to\infty$ gives

$$A^t_{\cdot}=\begin{cases}\xi^2\sigma^2 t, & \text{for } -1<2\sigma<1,\\ 2\xi^{\xi-2}\sigma^{-\xi+1}t, & \text{for } 2\sigma\geqslant 1,\end{cases} \tag{4.18}$$

for $2\sigma\leqslant -1$ the signature of the metric is not retained.

The surface stress (A6) must vanish at any null junction; this implies $[Y']$ must vanish if τ_{vv}, τ_{vr}, τ_{rv}, and τ_{rr} are to vanish, and $[(X/S)'/2S]$ must vanish if $\tau_{\theta\theta}$ and $\tau_{\varphi\varphi}$ are to vanish. For the type O solution take the line element (4.3); $[Y']$ vanishes as this line element is expressed in terms of the luminosity radial coordinate already and

$$\frac{1}{2S}\left(\frac{X}{S}\right)'=\frac{\alpha}{2R^{\xi}}(\alpha-2\lambda\alpha_{,v}). \tag{4.19}$$

Now the metric can be chosen to continuously join to Minkowski space–time by taking α to continuously increase from (or decrease to) $\alpha=0$; (4.19) shows that there is no surface stress at the join $\alpha=0$ so that the field equations are obeyed throughout the space–time. For the type A and B solutions (4.9) gives

$$Y=\tfrac{1}{4}\overline{R^{2-2\xi}}\{(\lambda-\alpha)^{\xi}\pm(\lambda+\alpha)^{\xi}\},$$

$$\begin{aligned}Y'=&\frac{1}{2}\overline{R^{1-2\xi}}\{(\lambda-\alpha)^{\xi}\pm(\lambda+\alpha)^{\xi}\}\\ &\times\left\{(1-\xi)((\lambda-\alpha)^{\xi}\pm(\lambda+\alpha)^{\xi})+\frac{\xi}{\alpha}\overline{R^2}((\lambda-\alpha)^{\xi-1}\pm(\lambda+\alpha)^{\xi-1})\right\},\end{aligned} \tag{4.20}$$

$$\frac{1}{2S}\left(\frac{X}{S}\right)'=\frac{4\alpha(\alpha-\lambda\alpha_{,v})}{\overline{R^{3-2\xi}}\{(\lambda-\alpha)^{\xi}\pm(\lambda+\alpha)^{\xi}\}}.$$

For the type B solution the metric is not continuous at $\alpha=0$ as would be anticipated from the general remarks in the Introduction. The type A solution again has a metric which can be chosen to continuously join to Minkowski space–time by taking α to behave as before.

At any junction across a timelike surface the limits (B7) of the second fundamental form either side of the junction must coincide. For the type O solution, dropping the primes on the metric (4.7) gives the second fundamental form (B6)

$$K_{\theta\theta}=\sin^{-2}\theta K_{\varphi\varphi}=r-\sigma t, \tag{4.21}$$

which gives a junction where the field equations are defined with Minkowski space–time at $t=0$. For type A and B conformal solutions the extension of the metric (4.7) has second fundamental form (B6):

$$K_{tt}=-\tfrac{1}{2}\xi\sigma t(r(r-2\sigma t))^{-\xi/2-1}\cdot\{(r-2\sigma t)^{\xi}\mp r^{\xi}\},$$
$$K_{\theta\theta}=\sin^{-2}\theta K_{\varphi\varphi}=\tfrac{1}{2}(r(r-2\sigma t))^{-\xi/2}\{(r+(\xi-1)\sigma t)(r-2\sigma t)^{\xi}\pm(r-(\xi+1)\sigma t)r^{\xi}\}. \tag{4.22}$$

Again there is a junction at $t=0$.

V. CONCLUSION

Solutions to the Einstein–scalar equations which can represent an imploding scalar field were presented. Bekenstein's theorems were used to generate the corresponding Einstein–conformal scalar solutions. The Robertson–Walker solutions presented here are examples of solutions previously found by Vajk and Bekenstein; they are not asymptotically flat and cannot be joined to Minkowski space–time by the methods used here. Penny's solution also can represent an imploding scalar field but it is not asymptotically flat, and only when it reduces to a Robertson–Walker metric is it spherically symmetric. The solution previously found by the author and its' Bekenstein type A extension are asymptotically flat and have well-defined junctions with Minkowski space–time, and therefore can represent a scalar field imploding from nothing, thus generalizing the example in the abstract. This solution has Bondi mass $\alpha\alpha_{,v}$, and zero ADM mass. The zero ADM mass is because the energy of the gravitational field is negative and equals the positive energy of the scalar field. The type A extension has Bondi mass $(1\text{-}\xi^2)\alpha\alpha_{,v}$, and ADM mass $\xi^2\sigma^2 t$, ($|2\sigma|<1$). Assuming that the null radiation field vanishes, so that there is only the conformal scalar field present, the Type A solution has $\alpha=\sigma v$, therefore

$$\text{Type O:}\quad M(v)=\sigma^2 v,\quad A^t_{\cdot}=0,$$

$$\text{Type A:}\quad M(v)=\tfrac{2}{3}\sigma^2 v,\quad A^t_{\cdot}=\tfrac{1}{3}\sigma^2 t.$$

The type A solution might violate the energy conditions, but subject to this provision it is possible to start with Minkowski space–time and join the type A solution at $t=0$ generating nonzero ADM mass. This only goes to show that you can get something (as measured by ADM mass) from nothing.

APPENDIX A: JUNCTION CONDITIONS ACROSS A NULL SURFACE

In single null coordinates a spherically symmetric line element can be written as

$$ds^2=-X\,dv^2+2S\,dv\,dr+Y(d\theta^2+\sin^2\theta\,d\varphi^2). \tag{A1}$$

A suitable null tetrad is

$$l_a=(S,0,0,0),\quad n_a=(X/2S,-1,0,0),\quad m_a=(0,0,1,i\sin\theta)\sqrt{Y/2}. \tag{A2}$$

The projection tensor is defined by $q_{ab}=g_{ab}+2l_{(a}n_{b)}$ and has nonvanishing components $q_{\theta\cdot}^{\ \theta}=q_{\varphi\cdot}^{\ \varphi}=1$. The internal second fundamental form, $\chi_{ab}=n_{d;c}q^{d}_{\ \cdot a}q^{c}_{\ \cdot b}$, involves covariant derivatives of n_a which can be calculated using the Christoffel symbols in Ref. 2, and it has nonvanishing components

$$\chi_{\theta\theta}=\sin^{-2}\theta\,\chi_{\varphi\varphi}=-(XY'/2S+Y_{,v})/2S. \tag{A3}$$

The external second fundamental form $\psi_{ab}=l_{d;c}q^{c}_{\ \cdot a}q^{d}_{\ \cdot b}$ is

$$\psi_{\theta\theta}=\sin^{-2}\theta\psi_{\varphi\varphi}=Y'/2, \tag{A4}$$

and the normal fundamental form $\eta_a=l_{d;c}q^c_{\cdot a}n^d_{\cdot}$ vanishes. The surface gravity $\omega=-l_d n^c_{\cdot} n^d_{\cdot;c}$ is

$$\omega=-(X/S)'/2S. \tag{A5}$$

The surface stress $\tau_{ab}=-[\mathrm{Tr}\ \psi]n_a n_b-2[\eta_{(a}]_{b)}-[\omega]q_{ab}$ is

$$\tau_{ab}=-[Y']n_a n_b/Y+[(X/S)'/2S]q_{ab}, \tag{A6}$$

with n_a and q_{ab} given by (A2) and where the bracket ''[ ]'' is defined by

$$[Q]|_y=\lim_{x\to y^+} Q-\lim_{x\to y^-} Q \tag{A7}$$

for a point y in the surface.

APPENDIX B: JUNCTION CONDITIONS ACROSS SPACELIKE AND TIMELIKE SURFACES

The line element can be taken in the form

$$ds^2=-C\,dt^2+A\,dr^2+B(d\theta^2+\sin^2\theta\,d\varphi^2). \tag{B1}$$

For a non-null surface, the surface stress vanishes iff the second fundamental form obeys

$$[K_{ab}]=0, \tag{B2}$$

where the bracket ''[ ]'' is defined by (A7). A suitable unit timelike vector field

$$U_\theta=(\sqrt{C},0,0,0). \tag{B3}$$

The projection tensor $h_{a\cdot}^{\ b}=g_{a\cdot}^{\ b}+U_a U^b_{\cdot}$ has three components $h_{r\cdot}^{\ r}=h_{\theta\cdot}^{\ \theta}=h_{\varphi\cdot}^{\ \varphi}=1$. The second fundamental form is $K_{ab}=U_{c;d}h^c_a h^d_{\cdot b}$. It involves covariant derivatives of U_a which can be calculated using the Christoffel symbols in Ref. 2. The nonvanishing components are

$$K_{rr}=-\mathring{A}/(2\sqrt{C}),\quad K_{\theta\theta}=\sin^{-2}\theta\,K_{\varphi\varphi}=-\mathring{B}/(2\sqrt{C}), \tag{B4}$$

where $\mathring{A}=\partial_t A$. The radial unit spacelike vector is

$$U_a=(0,\sqrt{A},0,0). \tag{B5}$$

The spacelike projection tensor $h_{a\cdot}^{\ b}=g_{a\cdot}^{\ b}-U_a U^b_{\cdot}$ has three components $h_{t\cdot}^{\ t}=h_{\theta\cdot}^{\ \theta}=h_{\varphi\cdot}^{\ \varphi}=1$. The second fundamental form for the corresponding timelike surface is

$$K_{tt}=-C'/(2\sqrt{A}),\quad K_{\theta\theta}=\sin^{-2}\theta\,K_{\varphi\varphi}=B'/(2\sqrt{A}), \tag{B6}$$

where $C'=\partial_r C$. Choosing the isotropic unit spacelike vector

$$U_a=\frac{1}{\sqrt{3}}(0,\sqrt{A},\sqrt{B},\sqrt{B}\sin\theta); \tag{B7}$$

similarly the nonvanishing components of the second fundamental form are

$$K_{tt}=-C'/(2\sqrt{3}A),$$

$$K_{tr}=-2\sqrt{\frac{A}{B}}\quad K_{t\theta}=\frac{-2}{\sin\,\theta}\sqrt{\frac{A}{B}}\quad K_{t\varphi}=\frac{-\dot{A}}{3\sqrt{3A}}+\frac{\dot{B}}{3B}\sqrt{\frac{A}{3}},$$
$$K_{r\theta}=\frac{K_{r\varphi}}{\sin\,\theta}=\frac{\sqrt{A}K_{\theta\varphi}}{\sin\,\theta}=\frac{-1}{2}\sqrt{\frac{B}{A}}\quad K_{rr}=\frac{-B'}{6\sqrt{3B}},\tag{B8}$$
$$K_{\theta\theta}=\frac{K_{r\theta}}{\sin\,\theta}=\frac{1}{3\sqrt{3A}}\{-B\,\cot\,\theta+B'\}.$$

The above three vectors (B3), (B5), and (B7) are suitable for the majority of purposes; but, for example, if there is ''Mixing'' between the space and time coordinates, like that of Eq. (2.16), then other vectors have to be used.

APPENDIX C: THE ADM ENERGY

The ADM energy for a spherically symmetric space–time is found by generalizing Weinberg's[20] derivation for the Schwarzschild solution. Define the rectilinear coordinates

$$x_1=r\,\sin\,\theta\,\cos\,\varphi,\quad x_2=r\,\sin\,\theta\,\sin\,\varphi,\quad x_3=r\,\cos\,\theta;\tag{C1}$$

the line element (B1) becomes

$$ds^2=-C\,dt^2+(A/r^2-B/r^4)(\underline{dx.x})^2+(B/r^2)\underline{dx}^2.\tag{C2}$$

Defining $h_{ij}=g_{ij}-\eta_{ij}$, and $n^i_{\cdot}=x^i_{\cdot}/r$, $i,j=1,2,3$, gives

$$h_{ij}=(A-B/r^2)n_in_j+(B/r^2-1)\,\delta_{ij}.\tag{C3}$$

The ADM mass is given by

$$A^t_{\cdot}=\oint dS^i_{\cdot}(h^j_{\cdot\,i,j}-h^j_{\cdot\,j,i}).\tag{C4}$$

Using (C3) this is

$$A^t_{\cdot}=\frac{-1}{2}\,r\left(\frac{-A}{r}+\left(\frac{B}{r^2}\right)'+\frac{B}{r^3}\right).\tag{C5}$$

The remaining components of the ADM vector are given by

$$8\pi A_j=\lim_{r\to\infty}\oint dS^i_{\cdot}(K_{ij}-\delta_{ij}K)$$

using the fundamental form (B5) gives

$$8\pi A_j=\lim_{r\to\infty}(B/(B\sqrt{C}),0,0)$$

and this vanishes in all the cases considered here.

APPENDIX D: A FIELD INDEX

A perfect fluid has Lagrangian $L_d=p$ (the pressure) (see, for example, Ref. 10) and Hamiltonian density $H_d=\mu$ (the density). Taking metric variations of the Lagrangian produces the metric stress

$$T_{ab}=(\mu+p)V_aV_b+pg_{ab}, \quad V_aV^a_{\cdot}=-1. \tag{D1}$$

The absolute derivative is defined by

$$\mathring{X}_{abc\ldots}=V_{\cdot}X_{abc\ldots}. \tag{D2}$$

The Bianchi identities give

$$-V_aT^{ab}_{\cdot\cdot;b}=\mathring{\mu}+(\mu+p)\breve{\Theta}, \quad \breve{\Theta}=V^a_{\cdot;a}$$

$$h_{ab}T^{bc}_{\cdot\cdot;c}=(\mu+p)_a+h_{a\cdot}{}^bp_b. \tag{D3}$$

The Eisenhart–Synge fluid index is

$$\omega=\ln I=\int \frac{dp}{\mu+p}, \tag{D4}$$

in the literature sometime I is called the index and sometimes ω. Assuming an equation of state

$$p=f(\mu), \quad \mu=f^{-1}(p), \tag{D5}$$

the Bianchi identities can be expressed as

$$\breve{\Theta}=\mathring{\omega}\,\frac{df^{-1}}{dp}, \quad \mathring{V}_a=-h_{a\cdot}{}^b\omega_b. \tag{D6}$$

For the equation of state (2.5) the index is $\omega=[(\gamma-1)/\gamma]\ln\mu$. An O-scalar field has this equation of state with $\gamma=2$ and $V_a=\varphi_a/\sqrt{-\varphi_c{}^2}$, $p=\mu=-\varphi_c{}^2$. Taking a timelike vector field, say

$$V_a=(N,0,0,0), \quad V^a_{\cdot}=(-1/N,0,0,0), \tag{D7}$$

it is possible to relate the behavior of the lapse N to the fluid index. For many configurations they can be equated $N=g(\omega)$, typically $N=1/\omega$. Thus if the fluid index is well behaved throughout the space, it is possible, without recourse to field equations, to discuss whether the metric is. Other choices of timelike vector field can be made; for example, for an asymptotically flat space–time there is the normal vector to the three-sphere at infinity.

There is no direct analog of the preceding for fields with infinite degrees of freedom. This is because the stress for fields does not have an explicit dependence on vector fields. It is possible to introduce vector fields into an action and vary it to produce an extreme configuration between the metric, fields, and vector field, in the following manner. Let the fields be describable by a Lagrangian

$$I_l=\int \sqrt{-g}\; d^4x\; L(\varphi,\varphi_a). \tag{D8}$$

Under infinitesimal coordinate variations this gives

$$\frac{\delta I}{\delta x^a_{\cdot}}: \int \sqrt{-g}\; d^4x \nabla_b \Theta^{ab}_c , \tag{D9}$$

where Θ^{ab}_c is the canonical stress

$$\Theta^{ab}_c = \frac{\partial \mathscr{L}}{\partial \varphi_a}\, \partial^b \varphi - g^{ab}_{\cdot\cdot} L_d . \tag{D10}$$

The Hamiltonian density is usually defined in terms of components $H_d = \Theta_{c\cdot 0}^{\;\;0}$. More generally it can be defined as

$$H_d = V_a V_b \Theta^{ab}_c , \tag{D11}$$

where V_a is a unit timelike vector field. Variations of I_l with respect to the metric produce the stress

$$T_{ab} = D_{ab} + L g_{ab} , \tag{D12}$$

where D_{ab} is given by $\delta I_d / \delta g_{ab}$. Applying the timelike vector field and using (D11) gives

$$H_d + L_d = V^a_{\cdot} V^b_{\cdot} D_{ab} . \tag{D13}$$

Variations of actions corresponding to H_d and L_d give dynamical equations. This suggests considering a new action I_n which is a sum of the Hamiltonian and Lagrangian actions

$$I_n = \int \sqrt{-g}\; d^4x (H_d + L_d) = \int \sqrt{-g}\; d^4x V^a_{\cdot} V^b_{\cdot} D_{ab} , \tag{D14}$$

which will give extremeal (maximally stable or unstable) configurations. Another possible way of producing further equations between the fields is to consider higher-order variations. For example, in Ref. 23, the second covariant variation of the point particle action gives the geodesic deviation equations.

A scalar-electrodynamic Lagrangian for a complex scalar field ψ and a vector field A_a is

$$\begin{gathered}\mathscr{L} = -\tfrac{1}{4}F^2 + \tfrac{1}{2}\mu^2 A^2 - \lambda (A^a_{\cdot a})^2 + J_a A^a_{\cdot} - \mathscr{D}_a \psi \mathscr{D}^a \overline{\psi} - V(\psi^2) + 2\beta \psi^2 R, \\ \mathscr{D}_a \psi = \partial_a \psi + ie \psi A_a , \quad \psi^2 = \psi \overline{\psi}, \\ \mathscr{D}_a \overline{\psi} = \partial_a \overline{\psi} - ie \overline{\psi} A_a .\end{gathered} \tag{D15}$$

Varying with respect to the metric gives

$$D_{ab} = F_{ac} F_{b\cdot}^{\;\;c} - \mu^2 A_a A_b - 2 J_a A_b + 4\lambda^2 A_{ab} A_{c\cdot}^{\;\;c} + 2 \mathscr{D}_{(a} \psi \mathscr{D}_{b)} \overline{\psi} - 2\beta (\psi^2)_{ab} - 2\beta \psi^2 R. \tag{D16}$$

Setting up the new action I_n and varying with respect to the fields gives

$$\begin{gathered}\frac{\delta I_n}{\delta \psi}: = -2 (V^a_{\cdot} V^a_{\cdot} \mathscr{D}_b \overline{\psi})_a + 2ie A_a V^a_{\cdot} V^a_{\cdot} \mathscr{D}_b \overline{\psi} + 2\beta \overline{\psi} [(V^a_{\cdot} V^a_{\cdot})_{ab} - R_{ab} V^a_{\cdot} V^b_{\cdot}], \\ \frac{\delta I_n}{\delta A_a}: = -2 (V_a V^b_{\cdot} F_{b\cdot}^{\;\;c} + V^c_{\cdot} V^b_{\cdot} F_{ba})_a + 2 V_a (-\mu^2 V^b_{\cdot} A_b - J_b A^b_{\cdot}) + ie V^a_{\cdot} (\psi \mathscr{D}_c \overline{\psi} - \overline{\psi} \mathscr{D}_c \psi).\end{gathered} \tag{D17}$$

It is also possible to vary with respect to $\mathring{\psi}$, $\mathring{A}_a$, g_{ab}, and V_a. Variations with respect to V_a are best done using velocity potentials (see Ref. 10). Varying with respect to g_{ab} a new ''stress'' tensor can be created. Applying the Bianchi identities to it the equations (D17) are not recovered, because the conservation equations as derived from (D9) are also changed. Choosing $D_{ab}=R_{a\mathring{b}}$ and varying with respect to g_{ab} does not reproduce Raychaudhuri's equations, but instead $\Theta = R_{ab}V^a_{\cdot}V^b_{\cdot} + \Theta^2 - \mathring{V}^a_{\cdot;a} + 1/2\Box V^2$. For the Reissner–Nordstrom solution with vector field (D7), and the null vector field l_a, (D17) becomes

$$\omega_t = -\frac{4\sqrt{2}}{r^3N^3}\, e\left[1+\frac{2m}{r}-\frac{3e^2}{r}\right],$$
$$\omega_v = 4\sqrt{2}\,\frac{e}{r^3}. \tag{D18}$$

For static O-scalar fields the field index vanishes everywhere, for nonstatic O-scalar fields using l_a gives

$$\omega = -2\left(\frac{2S'}{S}+\frac{Y'}{Y}\right)\varphi'. \tag{D19}$$

In the solution (4.5) this is

$$\omega = -\frac{4\sigma v}{Y^2}\,(r-\sigma v). \tag{D20}$$

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Axially symmetric solutions for SU(2) Yang–Mills theory

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By casting the Yang–Mills–Higgs equations of an SU(2) theory in the form of the Ernst equations of general relativity, it is shown how the known exact solutions of general relativity can be used to give similar solutions for Yang–Mills theory. Thus all the known exact solutions of general relativity with axial symmetry (e.g., the Kerr metric, the Tomimatsu–Sato metric) have Yang–Mills equivalents. In this paper we only examine in detail the Kerr-like solution. It will be seen that this solution has surfaces where the gauge and scalar fields become infinite, which correspond to the infinite redshift surfaces of the normal Kerr solution. Unlike the Kerr solution, our solution apparently does not have any intrinsic angular momentum, but rather appears to give the non-Abelian field configuration associated with concentric shells of color charge. Several possible physical consequences of these axial symmetric Yang–Mills field configurations are discussed. © *1996 American Institute of Physics.* [S0022-2488(96)00709-8]

I. INTRODUCTION

Recently, using the long known connection between general relativity and Yang–Mills theories,[1] we found exact Schwarzschild-like solutions for Yang–Mills theories.[2,3] Our results were conceptually similar to several other recent papers[4,5] which discussed related solutions. A natural question which arises from this is if there are other exact solutions of general relativity which have corresponding exact Yang–Mills solutions. Of particular interest is the Kerr solution which has an intrinsic angular momentum. In this paper we show that there are such solutions by considering an SU(2) gauge theory coupled to a scalar field in the adjoint representation. The solutions are found by first transforming the Yang–Mills field equations into the Ernst equations[6] of general relativity, and then applying the form of the general relativistic solution in terms of the gauge and scalar fields. Even though we specialize in this paper to the Kerr-like solution, it is in principle possible to use this same procedure to map over any axially symmetric solutions to Einstein's equations into an equivalent Yang–Mills solution. However, as we will show, even the Kerr-like solution has a very complex structure, which makes it difficult to deal with. In addition it may be possible to reverse the above method and use known exact solution of Yang–Mills theory (e.g., the BPS dyon solution[7,8] and multimonopole solutions[9]) to write down undiscovered solutions to Einstein's equations. One interesting feature of our previous Schwarzschild-like solution was the existence of a spherical shell surrounding the origin, on which the gauge and scalar fields became infinite, implying the presence of a spherical distribution of color charge. The Yang–Mills Kerr-like solution, in contrast, generally has two concentric shells of SU(2) charge (these shells are the equivalent of the infinite redshift surfaces of the normal Kerr solution). Just as the the Kerr solution of general relativity can permanently trap particles which carry the gravitational ''charge'' (i.e., mass-energy) behind its event horizons, so too does the Yang–Mills Kerr-like solution if it is treated as a fixed background field in which a color charged test particle is placed via minimal coupling. This gives a semi-classical type of confinement which has some similiarities with phenomenological bag models. It is not clear whether this is in any way connected with the physical confinement mechanism, which is thought to be a quantum field theoretic effect. Actually, what we call the color event horizon of our solution corresponds to the infinite redshift surfaces rather than the true event horizons of the normal Kerr metric. The reason for

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calling these surfaces the color event horizons is that the physical quantities of our theory (the gauge and scalar fields) develop real singularities on these surfaces. These infinite values of the fields imply, at least classically, that a particle carrying a color charge would either be strongly repelled or strongly attracted by these surfaces. For general relativity the corresponding singular surfaces are coordinate singularities which arise because of the particular coordinates that one chooses. This can best be seen for the normal Schwarzschild solution where one can eliminate the singularity in the metric at the Schwarzschild radius by transforming to Kruskal coordinates. In addition to this difference in the nature of the singularities, it is shown that while the regular Kerr solution has some angular momentum, our Yang–Mills version does not. These differences arise because the symmetries of general relativity are space-time symmetries, while the Yang–Mills symmetries are internal Lie symmetries.

II. THE KERR-LIKE SOLUTION

The theory which we consider is an SU(2) gauge field which is coupled to a scalar field in the adjoint representation, which has no self-interaction or mass terms. The Lagrangian for this theory is

$$\mathscr{L}=-\tfrac{1}{4}F^{\mu\nu a}F^{a}_{\mu\nu}+\tfrac{1}{2}D_{\mu}(\phi^{a})D^{\mu}(\phi^{a}), \tag{1}$$

where

$$F^{a}_{\mu\nu}=\partial_{\mu}W^{a}_{\nu}-\partial_{\nu}W^{a}_{\mu}+g\epsilon^{abc}W^{b}_{\mu}W^{c}_{\nu} \tag{2}$$

and

$$D_{\mu}\phi^{a}=\partial_{\mu}\phi^{a}+g\epsilon^{abc}W^{b}_{\mu}\phi^{c}. \tag{3}$$

To obtain the Bogomolny field equations associated with this theory one finds the field configuration which produces an extremum in the canonical Hamiltonian:

$$\mathscr{H}=\int d^{3}x[\tfrac{1}{4}F^{a}_{ij}F^{aij}-\tfrac{1}{2}F^{a}_{0i}F^{a0i}+\tfrac{1}{2}D_{i}\phi^{a}D^{i}\phi^{a}-\tfrac{1}{2}D_{0}\phi^{a}D^{0}\phi^{a}]. \tag{4}$$

We now introduce an explicit scale factor for the scalar field (i.e., $\phi^{a}\rightarrow A\phi^{a}$) so that we can study the special case with no scalar field by simply taking $A=0$. Next we require that all the fields are time independent and that the time components of the gauge fields are proportional to the scalar fields (i.e., $W^{a}_{0}=C\phi^{a}$, where ϕ^{a} is the rescaled field). Thus W^{a}_{0} acts like an additional Higgs field except that its kinetic term appears with the opposite sign in Eq. (4). Using all these conditions and the antisymmetry of ϵ^{abc} we find that $D_{0}\phi^{a}=0$ and $F^{a}_{0i}=C(D_{i}\phi^{a})$, so that the Hamiltonian becomes

$$\mathscr{H}=\int d^{3}x[\tfrac{1}{4}(F^{a}_{ij}-\epsilon_{ijk}\sqrt{A^{2}-C^{2}}D^{k}\phi^{a})(F^{aij}-\epsilon_{ijl}\sqrt{A^{2}-C^{2}}D^{l}\phi^{a})+\tfrac{1}{2}\epsilon_{ijk}\sqrt{A^{2}-C^{2}}F^{aij}D^{k}\phi^{a}]. \tag{5}$$

Using the relationship $\epsilon_{ijk}F^{aij}D^{k}\phi^{a}=\partial^{i}(\epsilon_{ijk}F^{ajk}\phi^{a})$ the last term in Eq. (5) can be turned into a surface integral, which in the usual development[7] is proportional to the magnetic charge carried by the fields due to the topology of the Higgs field at infinity.[10] The lower limit of the above Hamiltonian can be found be requiring

$$F_{ij}^a = \sqrt{A^2 - C^2}\,\epsilon_{ijk} D^k \phi^a,$$
$$B_k^a = \sqrt{A^2 - C^2} D_k \phi^a. \tag{6}$$

These are the usual Bogomolny field equations, with the presence of the scalar and time component of the gauge fields explicitly displayed through the constants A and C.

Several exact solutions to the field equations of this theory have been found which possess spherical symmetry: the Bogomolny–Prasad–Sommerfield dyon solution,[7,8] and more recently a Schwarzschild-like solution.[2] In this paper we are looking for an axially symmetric solution. Several authors[11,12] have already given an axially symmetric ansatz for the guage and scalar fields

$$\Phi^a = (0, \phi_1, \phi_2), \quad W_\phi^a = -(0, \eta_1, \eta_2),$$
$$W_z^a = (W_1, 0, 0), \quad W_\rho^a = -(W_2, 0, 0), \tag{7}$$

where φ, z, ρ are the usual polar coordinates and ϕ_i, η_i, W_i are functions of ρ, z only. With this ansatz the Bogomolny equations of Eq. (6) become[11]

$$\sqrt{A^2 - C^2}(\partial_\rho \phi_1 - W_2 \phi_2) = -(\partial_z \eta_1 - W_1 \eta_2)/\rho,$$
$$\sqrt{A^2 - C^2}(\partial_\rho \phi_2 + W_2 \phi_1) = -(\partial_z \eta_2 + W_1 \eta_1)/\rho,$$
$$\sqrt{A^2 - C^2}(\phi_1 \eta_2 - \phi_2 \eta_1) = \rho(\partial_\rho W_1 - \partial_z W_2), \tag{8}$$
$$\sqrt{A^2 - C^2}(\partial_z \phi_1 - W_1 \phi_2) = (\partial_\rho \eta_1 - W_2 \eta_2)/\rho,$$
$$\sqrt{A^2 - C^2}(\partial_z \phi_2 + W_1 \phi_1) = (\partial_\rho \eta_2 + W_2 \eta_1)/\rho.$$

These axially symmetric versions of the Bogomolny equations remain invariant under the following Abelian gauge transformation:

$$W_i' \to W_i + \partial_i \Lambda,$$
$$(\phi_1', \eta_1') \to (\phi_1, \eta_1)\cos(\Lambda) + (\phi_2, \eta_2)\sin(\Lambda), \tag{9}$$
$$(\phi_2', \eta_2') \to (\phi_2, \eta_2)\cos(\Lambda) - (\phi_1, \eta_1)\sin(\Lambda).$$

If one defines two new functions, $f(\rho, z)$ and $\psi(\rho, z)$, such that the fields, η_i, ϕ_i, and W_i are written as

$$\sqrt{A^2 - C^2}\,\phi_1 = -W_1 = \frac{1}{f}\frac{\partial \psi}{\partial z}, \quad \eta_1 = \rho W_2 = -\frac{\rho}{f}\frac{\partial \psi}{\partial \rho},$$
$$\sqrt{A^2 - C^2}\,\phi_2 = -\frac{1}{f}\frac{\partial f}{\partial z}, \quad \eta_2 = \frac{\rho}{f}\frac{\partial f}{\partial \rho}, \tag{10}$$

then the Bogomolny equations of Eq. (8) become[9]

$$\mathrm{Re}(\epsilon)\nabla^2 \epsilon = \boldsymbol{\nabla}\epsilon \cdot \boldsymbol{\nabla}\epsilon, \tag{11}$$

where $\epsilon = f + i\psi$, and ∇^2 and $\boldsymbol{\nabla}$ are the Laplacian and gradient in cylinderical coordinates.

Equation (11) is the Ernst equation[6] of general relativity. This form of the Bogomolny equations has been used to find exact, nonsingular, multimonopole solutions for the fields through the

use of the Bäcklund transformations of Harrison.[13] Since the axial Bogomolny equations can be written in the form of the Ernst equations, it should be possible to use the known exact solutions of general relativity to find exact solutions for SU(2) Yang–Mills–Higgs theory. That this link between the general relativistic solutions and their Yang–Mills counterparts has not been exploited before can perhaps be attributed to the singularities which exist in these solutions. Here it is conjectured that these singularities might actually be a desired feature in that they may provide a confinement mechanism for non-Abelian gauge theories. Previously,[2,3] using a different approach we have found exact Schwarzschild-like solutions for SU(2) and SU(N) Yang–Mills–Higgs theories. Here we use the well known Kerr solution, written in terms of variables of the Ernst equation, to give an equivalent solution for the Yang–Mills theory. There are actually several other exact, axially symmetric solutions in general relativity which could be mapped over into Yang–Mills theory (e.g., the Tomimatsu–Sato metric[14] and the NUT-Taub metric[15]). However, the Kerr metric is the simplest axially symmetric solution, and is of physical interest since it gives the exterior gravitational field for a central mass with angular momentum. However, our axial Yang–Mills solution apparently does not possess any angular momentum, but rather seems to represent the non-Abelian field configuration due to an axial symmetric distribution of SU(2) charge. Thus although the Kerr-like solution is found using the general relativistic solution, they appear to have some different physical characteristics.

To find the Kerr solution from the Ernst equation one first introduces the complex potential ζ such that

$$\epsilon = f + i\psi = \frac{\zeta - 1}{\zeta + 1} \tag{12}$$

so that f and ψ are the real and imaginary parts, respectively, of $(\zeta-1)/(\zeta+1)$. Substituting this expression for ϵ into Eq. (11), the Ernst equation becomes

$$(\zeta\overline{\zeta} - 1)\nabla^2\zeta = 2\overline{\zeta}\overline{\boldsymbol{\nabla}}\zeta\cdot\boldsymbol{\nabla}\zeta, \tag{13}$$

where $\overline{\zeta}$ is the complex conjugate of ζ. For this form of the equations the Kerr solution is most easily found using prolate spheroidal coordinates, which can be written in terms of the cylinderical coordinates, ρ and z, as

$$\begin{aligned} x &= \frac{1}{2k}\left[\sqrt{(z+k)^2+\rho^2} + \sqrt{(z-k)^2+\rho^2}\right], \\ y &= \frac{1}{2k}\left[\sqrt{(z+k)^2+\rho^2} - \sqrt{(z-k)^2+\rho^2}\right], \end{aligned} \tag{14}$$

where the ranges of these prolate spheroidal coordinates are $|x|\geqslant 1$ and $|y|\leqslant 1$. The inverse transformation is given by

$$\rho = k\sqrt{x^2-1}\sqrt{1-y^2}, \quad z = kxy, \tag{15}$$

with k, p, and q are arbitrary constants. In these prolate spheroidal coordinates the gradient and Laplacian become

$$\begin{aligned} \boldsymbol{\nabla} &= \frac{k}{\sqrt{x^2-y^2}}\left[\hat{\mathbf{x}}\sqrt{x^2-1}\,\frac{\partial}{\partial x} + \hat{\mathbf{y}}\sqrt{1-y^2}\,\frac{\partial}{\partial y}\right], \\ \nabla^2 &= \frac{k^2}{x^2-y^2}\left[\frac{\partial}{\partial x}(x^2-1)\,\frac{\partial}{\partial x} + \frac{\partial}{\partial y}(1-y^2)\,\frac{\partial}{\partial y}\right], \end{aligned} \tag{16}$$

where $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ are unit vectors. Using these expressions it is easy to see that a solution to the second form of the Ernst equation, Eq. (13), is

$$\zeta = px - iqy, \tag{17}$$

where the constants p,q must satisfy the condition $p^2+q^2=1$. The above solution can be transformed into the standard form of the Kerr solution by doing a transformation from the prolate spheroidal coordinates to Boyer–Lindquist coordinates.[6] The special case when $q=0$, $p=1$, and $\zeta=x$ gives (after a transformation to Schwarzschild coordinates) the usual Schwarzschild metric for general relativity. However, using the solution $\zeta=x$ in the Yang–Mills case to write down the expressions for the gauge and scalar fields, we find that we do not recover our previous Schwarzschild-like solution for SU(2), but obtain a different solution. The reason for this lies in the fact that the ansätze we used in each case were different, and in the previous work we found our solution directly from the Euler–Lagrange field equations, while here we employed the Bogomolny formalism. A field configuration that satisfies the Bogomolny equations will also satisfy the Euler–Lagrange equations, but the reverse is not necessarily true. Nevertheless $\zeta=x$ does give a solution to the Yang–Mills–Higgs equations, which is a special case of the general solution (i.e., $p,q\neq 0$) that we are considering. In general relativity p, q, and k are related to the mass and angular momentum of the central mass which produces the gravitational field. Here p, q, and k will be related to the shape of the axially symmetric SU(2) charge configuration of our solution. In order to find expressions for the fields ϕ_i, η_i, W_i it is first necessary to determine the functions f and ψ. From Eqs. (12) and (17) we find that

$$f = \frac{p^2x^2+q^2y^2-1}{(px+1)^2+q^2y^2}, \quad \psi = \frac{-2qy}{(px+1)^2+q^2y^2}. \tag{18}$$

To get the gauge and scalar fields one simply inserts these expressions for f and ψ into Eq. (10). This is a straightforward but tedious procedure which yields very complicated expressions for the fields. The explicit expressions for the fields are

$$\begin{aligned}
\sqrt{A^2-C^2}\phi_1 = -W_1 &= \frac{-2q[x(1-y^2)((px+1)^2-q^2y^2)-2py^2(px+1)(x^2-1)]}{k[(px+1)^2+q^2y^2](p^2x^2+q^2y^2-1)(x^2-y^2)},\\
\eta_1 = \rho W_2 &= \frac{-2qy[(px+1)^2-q^2y^2+2px(px+1)](x^2-1)(1-y^2)}{(x^2-y^2)[(px+1)^2+q^2y^2](p^2x^2+q^2y^2-1)},\\
\sqrt{A^2-C^2}\phi_2 &= \frac{-2y[p(x^2-1)((px+1)^2-q^2y^2)+2q^2x(px+1)(1-y^2)]}{k(x^2-y^2)(p^2x^2+q^2y^2-1)[(px+1)^2+q^2y^2]},\\
\eta_2 &= \frac{-2(x^2-1)(1-y^2)[px(3q^2y^2-(px+1)^2)+2q^2y^2]}{(x^2-y^2)(p^2x^2+q^2y^2-1)[(px+1)^2+q^2y^2]},
\end{aligned} \tag{19}$$

where the partial derivatives like, $\partial\psi/\partial z$ were determined using the chain rule (e.g., $\partial_x\psi\partial_z x+\partial_y\psi\partial_z y$) and Eq. (14). Notice that in general relativity the physical quantities one usually deals with are the components of the metric tensor. Here the physical quantities are the gauge fields which correspond to the Christoffel symbols in general relativity. This partly explains the complexity of the expressions in Eq. (19), since even in Boyer–Lindquist coordinates, the Christoffel coefficients for the Kerr metric are somewhat involved. If one wanted to have the expressions for the fields in terms of the original coordinates, it would be necessary to use Eq. (14) to replace x,y with ρ,z, making an already complicated expression even more intractible. However, by looking at certain aspects of the expressions of the fields one can still make some interesting comments about this solution.

One feature that can be looked for are regions where the fields become singular. In analogy with Maxwell's equations, where singularities in the electromagnetic field indicate the presence of electric charge, we interpret these singularities as the location of color charge. The shape of these SU(2) charge distributions is much more involved than in electromagnetism. All of the fields from Eq. (19) have three similar terms in their denominators, so the fields can be made to approach infinity if any one of the three factors goes to zero. First, by setting $p^2x^2+q^2y^2-1=0$ it can be seen that all the fields become infinite. This factor is common to all the fields, since from Eq. (10) they all have a factor of f^{-1}. In cylinderical coordinates this condition becomes

$$|pq|(z^2+\rho^2-k^2)=\pm|q^2-p^2|\rho k. \tag{20}$$

By setting $q=\cos\theta$ and $p=\sin\theta$ we replace the two parameters p,q with one parameter, and Eq. (20) becomes

$$z^2+\rho^2-k^2=\pm 2|\cot(2\theta)|\rho k. \tag{21}$$

Solving the above condition for z as a function of ρ allows one to take a vertical slice through the two axially symmetric surfaces defined by Eq. (21). One needs only to look in the range $0°\leqslant\theta\leqslant 45°$ to cover all the possibilities. What one finds are two concentric surfaces which touch each other on the z-axis at $\pm k$. The outer surface is given by the positive solution to Eq. (21). It has a toroidal shape, without the central hole of a normal torus. The inner surface is given by the negative solution, and has an ellipsoidal shape which runs along the z axis. In the special case when $\theta=45°$ (i.e., $p=q$) the two surfaces merge into a single sphere with a radius of k. Second, the fields can become infinite if $x^2-y^2=0$. However, this condition gives two points ($\rho=0$, $z=\pm k$) which are already included in the first condition of Eq. (20). Finally some of the fields become singular when $y=0$ and $px+1=0$ (since x is positive definite this condition only has a solution when $p<0$). The condition $y=0$ implies $z=0$ so that the singularity resides in the plane perpendicular to the z axis, and then $px+1=0$ gives $\rho=k|q|/|p|=k|\cot\theta|$. This corresponds to a ring singularity of radius $k|\cot\theta|$ centered at the origin in the plane perpendicular to the z axis. However, this singularity, produced by the condition $y=0$ and $px+1=0$, duplicates that from the condition of Eq. (21). Thus the singularity produced by the third term in the denominators of the gauge fields does not produce an independent singularity. The geometrical structure of the singular surfaces is different from that of the similar Schwarzschild-like solution. For the Schwarzschild solution we obtained a spherical shell singularity surrounding a point singularity at the origin. In the present case we find concentric toroidal and ellipsoidal surfaces on which the gauge and scalar fields become infinite, with no apparent singularities in the interior of these surfaces.

One of the most interesting features of other Yang–Mills solutions, such as the 't Hooft–Polyakov monopole or the Prasad–Sommerfield dyon, was the topological nature of the magnetic charge carried by these solutions. By examining the far-field behavior of the magnetic field of a special case of the Kerr-like solution we will find that it does not carry any net topological magnetic charge, but behaves like a configuration of two opposite magnetic charge sitting on the z axis, separated by a distance $2k$ (i.e., it acts like a magnetic dipole). The special case we consider is $q=0$ and $p=1$. In this case the only non-zero fields are ϕ_2 and η_2, which become

$$\phi_2=\frac{-2y}{k(x^2-y^2)},\quad \eta_2=\frac{2x(1-y^2)}{(x^2-y^2)}. \tag{22}$$

(We are also taking $A=1$ and $C=0$ here so that the time part of the gauge field is absent.) These fields only become singular at two points $-x=\pm y$, or $\rho=0$, $z=\pm k$. They do not have the singular surfaces of the more general $q\neq 0$ case. Looking back at Eq. (8) to obtain the components of the non-Abelian magnetic field we find that $B_z=-\partial_\rho\eta_2/\rho$ and $B_\rho=\partial_z\eta_2/\rho$. Inserting the fields of Eq. (22) and applying the chain rule we find

$$B_z=\frac{2x[x^2(1-3y^2)+y^2(3-y^2)]}{k^2(x^2-y^2)^3},$$
$$B_\rho=\frac{-2y\sqrt{x^2-1}\sqrt{1-y^2}(3x^2+y^2)}{k^2(x^2-y^2)^3}, \tag{23}$$

where the group index has been dropped since the magnetic fields all point in the same direction in iso-space.[11] If one looks at these fields along the z axis (i.e., $\rho=0$) where $x\to z/k$ and $y\to 1$, then $B_z\to -4zk/(z^2-k^2)^2$ and $B_\rho\to 0$. Now the magnetic field on the z axis of two magnetic point charges $+g$ and $-g$ located at $z=-a$ and $z=+a$, respectively, is $-4agz/(z^2-a^2)^2$. Thus this special case of our solution carries no net topological magnetic charge, but behaves similar to the magnetic dipole field surrounding two point magnetic charges of opposite sign. The magnetic charges of this special case solution can be taken to be located at the two singularities on the z axis at $z=\pm k$. For the general case with $q\neq 0$ one can again take the solutions of Eq. (19) and insert them into the right-hand side of Eq. (8) to get the components of the magnetic field. After a tedious calculation, restricting ourselves to the z axis and taking the limit $z\to\infty$ one finds that all the components of the magnetic field fall off faster than $1/r^2$. Thus none of the Kerr-like solutions carry a net topological magnetic charge. One can also look at the gauge and scalar fields of Eq. (19) and see that as $\rho\to\infty$ and $z\to\infty$ that they fall off as $1/r^2$ or faster, rather than the $1/r$ falloff one would expect for a radial Coulomb field from a net charge.

Just as the Kerr and Schwarzschild solutions of general relativity confine particles behind event horizons, so one may hope that the present solutions will trap color charged particles behind the singularities in the gauge fields. If these axial Yang–Mills solutions are treated as background fields in which a test particle is placed via minimal coupling, one finds that the singular surfaces act as impenetrable barriers, and the test particle does become trapped. A similar result is obtained for the spherically symmetric Schwarzschild-like solutions considered in Refs. 4, 5, and 16. In the present solution there are in general two concentric singular surfaces so the test particle may be trapped either within the inner surface or between the inner and outer surface. The special case, $q=0$ and $p=1$, which was just considered, does not trap test particles in this manner since it only has singular points, not singular surfaces that act as barriers to the test particle. This type of semi-classical confinement is similar to the behavior of phenomenological bag models. In a fully rigorous quantum field theory approach one could argue against these solutions being connected with the physical confinement mechanism. Due to the singularities one gets an infinite action contribution from these field configurations to the path integral. This implies that these solutions are not physically important. This conclusion can be evaded if there is an infinity of neighboring solutions whose infinite entropy contribution can offset the infinite action. This occurs, for example, with the meron solutions considered by Callan, Dashen, and Gross.[17] There the logarithmic divergence of the action was compensated for by the logarithmic increase of the entropy. It is not clear whether a similar result occurs for these axial symmetric solutions, but there is an infinite set of related solutions which are obtained by varying the free parameters k and q (p is not a free parameter because of the constraint $p^2+q^2=1$). The parameter k can vary from 0 to ∞, while q can range from -1 to 1.

The exact expressions for the energy and angular momentum of the Kerr-like solution presented here are rather complicated due to the involved nature of the scalar and gauge fields [see Eq. (19)]. Still some interesting general conclusions can be made about these quantities. To find the energy and angular momentum in the fields it is necessary to calculate the energy-momentum tensor of the Lagrangian of Eq. (1):

$$T^{\mu\nu}=\frac{2}{\sqrt{-g}}\frac{\alpha(\mathscr{L}\sqrt{-g})}{\partial g_{\mu\nu}}=F^{\mu\rho a}F^{\nu a}_{\rho}+D^\mu\phi^a D^\nu\phi^a+g^{\mu\nu}\mathscr{L}. \tag{24}$$

The energy of the field configuration is then

$$E=\int d^3xT^{00}=\int d^3x\left[\frac{1}{4}F^a_{ij}F^{aij}+\frac{1}{2}F^a_{0i}F^{a0i}+\frac{A^2}{2}D_i\phi^aD^i\phi^a+\frac{A^2}{2}D_0\phi^aD^0\phi^a\right]. \quad (25)$$

This is equivalent to the Hamiltonian except the signs are all positive. Now using $D^0\phi^a=0$, $F^a_{0i}=C(D_i\phi_a)$, and $F^a_{ij}=\sqrt{A^2-C^2}\epsilon_{ijk}D^k\phi^a$, the energy becomes

$$E=A^2\int d^3xD_i\phi^aD^i\phi^a=\frac{A^2}{A^2-C^2}\int d^3xB^a_iB^{ia}, \quad (26)$$

where the Bogomolny equations ($B^a_i=\sqrt{A^2-C^2}D_i\phi^a$) were used to obtain the last expression. The constant A is the multiplicative factor that we put in front of the scalar fields in order that we could easily examine the case when there were no scalar fields by taking $A=0$. From Eq. (26) it can be seen that for this special case the energy in the fields of the Kerr-like solution is zero. In addition when $A=0$ either the time components or the space components of the gauge fields are pure imaginary. These results were the same for the Schwarzschild Yang–Mills solution, and we believe that this calls into question the physical relevance of the pure gauge case even though it is mathematically a solution. Taking this view then requires the presence of a scalar field in order to get a physically ''reasonable'' solution. The angular momentum of the field configuration is given by

$$L_i=\int d^3x\epsilon_{ijk}x^jT^{0k}. \quad (27)$$

Using the expression for $T^{\mu\nu}$ from Eq. (24), the condition $F^a_{0i}=C(D_i\phi^a)$, and the Bogomolny field equations, Eq. (6), we find

$$T^{0k}=\epsilon^{klm}C\sqrt{A^2-C^2}(D_l\phi^a)(D_m\phi^a). \quad (28)$$

The antisymmetry of ϵ^{klm} makes $T^{0k}=0$, so that there is no angular momentum in this non-Abelian field configuration. This shows that while our Yang–Mills solution is similar in many ways to its general relativistic counterpart, there are some important distinctions. Part of the reason for this stems from the fact that the symmetries of general relativity are space-time symmetries, while those of Yang–Mills theories are internal Lie symmetries. These differences showed up even in the Yang–Mills Schwarzschild-like solution where the sphere singularity was a true singularity, while for general relativity the event horizon is a coordinate singularity, as can be seen by looking at the Schwarzschild solution in Kruskal coordinates.

Finally, one may wonder if the singularities of our Kerr-like solution might not be gauge artifacts. For example, Arafune *et al.*[10] have shown that the 't Hooft–Polyakov monopole can be formulated either with singularity-free gauge fields and a ''hedgehog'' configuration scalar field, or with gauge fields with a Dirac string singularity and a scalar field in an ''Abelian'' gauge. These two formulations are connected via a singular gauge transformation. In order to show that the singularities of the Kerr-like solution are real features of the solution rather than gauge artifacts one needs to show that these singularities occur in a gauge invariant quantity. (In a certain respect it would be better if these singularities where gauge artifacts, since—leaving aside the speculation about the possible connection to the confinement phenomenon—field configurations with true singularities are often considered unphysical. Even in such cases as the Coulomb potential of electrodynamics one usually expects that the singularity is an unphysical feature.) To show that the singularities are a real feature of the Kerr-like solution one can consider the gauge invariant field energy density, which is the integrand of Eq. (26). To obtain the explicit expressions for $D_i\phi^a$ or B^a_i, which are necessary to obtain the energy density in Eq. (26), one inserts the

solutions of Eq. (19) into Eq. (8) [the left-hand side of Eq. (8) gives $D_i\phi^a$ while the right-hand side gives B_i^a]. Again considering the special case when $p=1$, $q=0$, $A=1$, and $C=0$ [where the magnetic fields are given by Eq. (23)], one finds that the field energy density in the integrand of Eq. (26) becomes

$$B_i^a B^{ia} = B_z^2 + B_\rho^2 = \frac{4(x^2 - y^2 + 3x^2y^2 + y^4)}{k^4(x^2 - y^2)^4}. \tag{29}$$

Thus the energy density develops a singularity at $x = \pm y$, and the total field energy becomes infinite if one integrates through these singularities. The general case when $p,q \neq 0$ follows in the same way, but the final expressions for the energy density are extremely long and cumbersome. In the general case one also finds singularities in the gauge invariant energy density at the locations of the gauge field singularities. A computationally simplier method of showing the gauge invariant nature of the singularities is to examine the length of the Higgs field, $\mathbf{\Phi}_a^\dagger \mathbf{\Phi}_a = \phi_1^2 + \phi_2^2$. In order to calculate this gauge invariant quantity one simply squares ϕ_1 and ϕ_2 from Eq. (19) and takes their sum. This involves much less work than is necessary to obtain the energy density, where one must not only take products of the various fields, but also compute their derivatives with respect to ρ and z. Once the general expression for $\mathbf{\Phi}_a^\dagger \mathbf{\Phi}_a$ is found, one imposes the condition $p^2x^2 + q^2y^2 - 1 = 0$, which is where the gauge and scalar fields become singular. On doing this it is seen that the denominator of $\phi_1^2 + \phi_2^2$ goes to zero while the numerator remains finite. Thus the singularities in the fields of Eq. (19) also occur in the gauge invariant quantities, $\mathbf{\Phi}_a^\dagger \mathbf{\Phi}_a$ and the energy density.

III. DISCUSSION AND CONCLUSION

Extending our previous work on the Schwarzschild-like solution for Yang–Mills–Higgs theories, we have written down the Yang–Mills equivalent of the Kerr solution. By writing the Yang–Mills field equations in the form of the Ernst equation[12] of general relativity,[6] it is straightforward to use any known axially symmetric solution of general relativity to write down similar solutions in terms of the non-Abelian gauge fields. One disadvantage of these general relativistic inspired solutions is that they contain singularities in the fields, which lead to infinite field energies at the classical level. These singularities are of the same character as the singularities which are found in other classical field theory solutions such as the singularity at the origin in the normal Schwarzschild solution, the point singularity in the Wu–Yang solution for SU(2),[18] and the singularity at $r=0$ in the Coulomb potential in electromagnetism. Since our solutions are classical field theory solutions it may be conjectured, as is the case with general relativity, that a proper quantum treatment of the problem might modify these singularities. Fortunately, unlike the case of general relativity, there do exist methods for quantizing such classical solutions.[19,20] In one sense, however, these singularities (particularly the surface singularities) could be a desirable feature in that they may yield a possible confinement mechanism for non-Abelian gauge theories, which would be analogous to the confinement mechanism of general relativistic black holes. By treating these solutions as background fields in which test particles are placed via minimal coupling, one can show that these surface singularities act as impenetrable barriers to the test particle. This procedure was outlined in Refs. 4 and 16 where color charged test particles were placed in a spherically symmetric Yang–Mills field configuration, which had some of the characteristics of the Schwarzschild solution of general relativity. It was found that the wavefunction of the test particle was confined to the region around the origin, inside the spherical singular surface. The singular surfaces of the present axially symmetric solutions should also act as barriers when treated as a background potential.

While this semi-classical type of confinement is suggestive, and shares some common features with phenomenological bag models, it does have shortcomings. First, it ignores the interaction between the color field of the test particle and the field configuration in which it is placed. Since

the field equations of Yang–Mills theories are non-linear, one is not justified in using superposition, and the color field of the test particle could significantly alter the color field of the solution. Second, from a rigorous quantum field theory point of view the existence of singularities in the solutions implies that they will give an infinite action contribution to the path integral, which means that they should have no physical effect. This line of reasoning can be circumvented if there are an infinite set of neighboring solutions in function space whose infinite entropy contribution can offset the infinite action contribution. This in fact happens for the meron solutions considered in Ref. 17. Whether a similar thing occurs for the present solutions is not clear, although there are an infinite number of neighboring solutions which are found by varying the arbitrary parameters k and q.

The very direct link, via the Ernst equations, between general relativity and Yang–Mills–Higgs theories can be used to map over any of the known axially symmetric solutions from general relativity into non-Abelian gauge theories. In this paper we examined in detail only the Kerr solution in the hope of finding a field configuration, which contained an internal angular momentum, so that quantizing this angular momentum to $\hbar/2$ one would be able to have a fermion-like object from an initial theory with only gauge and scalar fields. Explicitly carrying out the calculation of the field angular momentum showed that even though the Kerr-like solution was axially symmetric, it did not carry any angular momentum in its fields. This shows that not all the features of the general relativistic solution carry over into Yang–Mills theory. So far we have used this parallel between the two theories to find solutions for Yang–Mills theories from the known solutions of general relativity. An interesting exercise might be to see if some of the exact solutions of Yang–Mills theory (e.g., the Prasad–Sommerfield solution or the multimonopole solutions)[9] could be used to give unknown exact solutions in general relativity.

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Exact solutions of the Einstein equations with sources from linearized solutions

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It is shown that if $(g_{\mu\nu},F_{\mu\nu})$ is an exact solution of the Einstein–Maxwell equations and l_μ is a principal null direction of $F_{\mu\nu}$ then $(g_{\mu\nu}+2Hl_\mu l_\nu,F_{\mu\nu})$ is also an exact solution of the Einstein–Maxwell equations if and only if $(2Hl_\mu l_\nu,0)$ satisfies the Einstein–Maxwell equations linearized about $(g_{\mu\nu},F_{\mu\nu})$. It is also shown that an analogous result applies in the case of the Einstein–Weyl equations if l_μ is parallel to the flux vector of the neutrino field. © *1996 American Institute of Physics.* [S0022-2488(96)00508-7]

I. INTRODUCTION

It is known that, despite the nonlinear nature of the Einstein field equations, there exist classes of metrics (e.g., those of the Kerr–Schild form[1]) for which the Einstein equations, written in an appropriate basis, reduce to linear differential equations (see also Refs. 2–4). A general result, obtained by Xanthopoulos,[5] states that if $g_{\mu\nu}$ is an exact solution of the Einstein vacuum field equations and l_μ is a null vector, then $g_{\mu\nu}+l_\mu l_\nu$ is also an exact vacuum solution, provided that $l_\mu l_\nu$ satisfies the Einstein vacuum field equations linearized about $g_{\mu\nu}$. The occurrence of linear equations only, simplifies the search for explicit solutions and allows the superposition of solutions.

The aim of this paper is to present a generalization of the Xanthopoulos theorem,[5] showing that if $g_{\mu\nu}$ satisfies the Einstein field equations with an electromagnetic or a neutrino field and l_μ is a principal null direction of the matter field, then $g_{\mu\nu}+l_\mu l_\nu$ is also an exact solution of the Einstein equations with the *same* matter field if and only if the metric perturbation $l_\mu l_\nu$ satisfies the Einstein field equations linearized about the background solution corresponding to $g_{\mu\nu}$. The proof consists of introducing a null tetrad for the perturbed metric related in a simple way with a null tetrad for the background metric and expressing the Einstein equations in these tetrads. We find that, with the assumed alignment of l_μ to the matter field, the Einstein equations only contain linear terms in the metric perturbation. The formulas obtained in the proof of our main result are also useful in the search for metric perturbations and a simple example is also given here. Throughout this paper we make use of the Newman–Penrose notation.[6]

II. THE FIELD EQUATIONS

We shall consider two metrics, $g_{\mu\nu}$ and $\widetilde{g}_{\mu\nu}$, related according to

$$\widetilde{g}_{\mu\nu}=g_{\mu\nu}+2Hl_\mu l_\nu, \tag{1}$$

where H is a real function and l_μ is a null vector with respect to the metric $g_{\mu\nu}$. When $g_{\mu\nu}$ is flat, $\widetilde{g}_{\mu\nu}$ is said to have a Kerr–Schild form. If l^μ, n^μ, m^μ, and $\overline{m^\mu}$ form a null tetrad for the metric $g_{\mu\nu}$, with $l^\mu:=g^{\mu\nu}l_\nu$, then it follows from Eq. (1) that

$$\widetilde{l}^\mu:=l^\mu,\quad \widetilde{n}^\mu:=n^\mu-Hl^\mu,\quad \widetilde{m}^\mu:=m^\mu,\quad \widetilde{\overline{m^\mu}}:=\overline{m^\mu}, \tag{2}$$

or, equivalently,

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$$\widetilde{D}:=D,\quad \widetilde{\Delta}:=\Delta-HD,\quad \widetilde{\delta}:=\delta,\quad \widetilde{\overline{\delta}}:=\overline{\delta}, \tag{3}$$

is a null tetrad for the metric $\widetilde{g}_{\mu\nu}$. (Note that l^μ is also null with respect to the metric $\widetilde{g}_{\mu\nu}$ and that $\widetilde{\overline{\delta}}=\overline{\widetilde{\delta}}$.)

The spin coefficients for the tetrad $\widetilde{D}$, $\widetilde{\Delta}$, $\widetilde{\delta}$, $\widetilde{\overline{\delta}}$ can be related with those corresponding to the tetrad D, Δ, δ, $\overline{\delta}$ by calculating the Lie brackets $[\widetilde{\Delta},\widetilde{D}]$, $[\widetilde{\delta},\widetilde{D}]$, $[\widetilde{\delta},\widetilde{\Delta}]$, and $[\widetilde{\delta},\widetilde{\overline{\delta}}]$. For instance,

$$[\widetilde{\Delta},\widetilde{D}]=[\Delta-HD,D]=[\Delta,D]+(DH)D=(\gamma+\overline{\gamma})D+(\epsilon+\overline{\epsilon})\Delta-(\overline{\tau}+\pi)\delta-(\tau+\overline{\pi})\overline{\delta}+(DH)D$$
$$=(\gamma+\overline{\gamma}+DH+(\epsilon+\overline{\epsilon})H)\widetilde{D}+(\epsilon+\overline{\epsilon})\widetilde{\Delta}-(\overline{\tau}+\pi)\widetilde{\delta}-(\tau+\overline{\pi})\widetilde{\overline{\delta}},$$

which must be equal to

$$(\widetilde{\gamma}+\overline{\widetilde{\gamma}})\widetilde{D}+(\widetilde{\epsilon}+\overline{\widetilde{\epsilon}})\widetilde{\Delta}-(\overline{\widetilde{\tau}}+\widetilde{\pi})\widetilde{\delta}-(\widetilde{\tau}+\overline{\widetilde{\pi}})\widetilde{\overline{\delta}}.$$

In this manner, one readily finds that

$$\widetilde{\kappa}=\kappa,\quad \widetilde{\sigma}=\sigma,\quad \widetilde{\rho}=\rho,\quad \widetilde{\tau}=\tau,\quad \widetilde{\epsilon}=\epsilon,\quad \widetilde{\pi}=\pi,$$
$$\widetilde{\alpha}=\alpha+\tfrac{1}{2}\overline{\kappa}H,\quad \widetilde{\beta}=\beta+\tfrac{1}{2}\kappa H,\quad \widetilde{\gamma}=\gamma+\tfrac{1}{2}(D+2\overline{\epsilon}+\rho-\overline{\rho})H, \tag{4}$$
$$\widetilde{\mu}=\mu+\rho H,\quad \widetilde{\lambda}=\lambda+\overline{\sigma}H,\quad \widetilde{\nu}=\nu+(\overline{\delta}+2\alpha+2\overline{\beta}-\pi-\overline{\tau})H+\overline{\kappa}H^2.$$

Making use of Eqs. (3) and (4), from the Ricci identities we find that the components of the curvature of the metric $\widetilde{g}_{\mu\nu}$, with respect to the null tetrad $\widetilde{D}$, $\widetilde{\Delta}$, $\widetilde{\delta}$, $\widetilde{\overline{\delta}}$, are related to the components of the curvature of $g_{\mu\nu}$, with respect to the null tetrad D, Δ, δ, $\overline{\delta}$, by

$$\widetilde{\Phi}_{00}=\Phi_{00}+2\overline{\kappa}\kappa H,$$
$$\widetilde{\Phi}_{01}=\Phi_{01}+\tfrac{1}{2}\{H\,D\kappa+\kappa(2D+\epsilon+3\overline{\epsilon}-\rho)H+\overline{\kappa}\sigma H\},$$
$$\widetilde{\Phi}_{02}=\Phi_{02}+(D-\epsilon+3\overline{\epsilon}-2\overline{\rho})\sigma H+\kappa(\delta+2\beta+2\overline{\alpha}-\tau-\overline{\pi})H+\kappa^2H^2,$$
$$2\widetilde{\Phi}_{11}=2\Phi_{11}+\tfrac{1}{2}(D+\epsilon+\overline{\epsilon}-\rho+\overline{\rho})(D+2\epsilon+2\overline{\epsilon}+\rho-\overline{\rho})H-(\rho^2-\overline{\sigma}\sigma)H \tag{5}$$
$$+(\text{linear operators acting on }\kappa\text{ or }\overline{\kappa}),$$
$$\widetilde{\Phi}_{12}=\Phi_{12}+\tfrac{1}{2}(\delta+\beta+\overline{\alpha}-\tau)(D+2\overline{\epsilon}+\rho-\overline{\rho})H+\epsilon(\delta+2\beta+2\overline{\alpha}-\tau-\overline{\pi})H+\sigma(\overline{\delta}+\alpha+2\overline{\beta}-\pi$$
$$-\overline{\tau})H+H(D-\epsilon+\overline{\epsilon}-\overline{\rho})\beta-\tau\rho H+(\text{linear operators acting on }\kappa\text{ or }\overline{\kappa}),$$
$$\widetilde{\Phi}_{22}=\Phi_{22}+\Phi_{00}H^2+(\delta+3\beta+\overline{\alpha}-\tau)(\overline{\delta}+2\alpha+2\overline{\beta}-\pi-\overline{\tau})H-(\Delta+\gamma+\overline{\gamma}+\mu)\rho H$$
$$-\mu(D+\epsilon+\overline{\epsilon}+\rho)H+HD\mu-(\lambda\sigma+\overline{\lambda\sigma})H+\pi(\delta+2\beta+2\overline{\alpha}-\tau-\overline{\pi})H$$
$$+(\text{linear operators acting on }\kappa\text{ or }\overline{\kappa}),$$

together with

$$6\widetilde{\Lambda}=6\Lambda-\tfrac{1}{2}(D+\epsilon+\overline{\epsilon}+\rho-\overline{\rho})(D+2\epsilon+2\overline{\epsilon}+\rho-\overline{\rho})H+2(D+\epsilon+\overline{\epsilon}-\overline{\rho})\rho H-(\rho^2+\overline{\sigma}\sigma)H$$
$$+(\text{linear operators acting on }\kappa\text{ or }\overline{\kappa}), \tag{6}$$

and

$$
\begin{aligned}
\widetilde{\Psi}_0 &= \Psi_0 + 2\kappa^2 H,\\
\widetilde{\Psi}_1 &= \Psi_1 + \tfrac{1}{2}\{HD\kappa + \kappa(2D + \epsilon + 3\overline{\epsilon} + 3\rho - 2\overline{\rho})H - \overline{\kappa\sigma}H\},\\
3\widetilde{\Psi}_2 &= 3\Psi_2 + \tfrac{1}{2}(D + \epsilon + \overline{\epsilon} + \rho - \overline{\rho})(D + 2\epsilon + 2\overline{\epsilon} + 3\rho - \overline{\rho})H - 2\overline{\sigma}\sigma H\\
&\quad + (\text{linear operators acting on } \kappa \text{ or } \overline{\kappa}),\\
\widetilde{\Psi}_3 &= \Psi_3 + \tfrac{1}{2}(\overline{\delta} + \alpha + \overline{\beta} - \overline{\tau})(D + 2\overline{\epsilon} + \rho - \overline{\rho})H + (\rho + \epsilon)(\overline{\delta} + 2\alpha + 2\overline{\beta} - \pi - \overline{\tau})H\\
&\quad + H(D + \epsilon - \overline{\epsilon} - \rho)\alpha - \overline{\sigma}(\beta + \tau)H + (\text{linear operators acting on } \kappa \text{ or } \overline{\kappa}),\\
\widetilde{\Psi}_4 &= \Psi_4 + (\overline{\delta} + 3\alpha + \overline{\beta} + \pi - \overline{\tau})(\overline{\delta} + 2\alpha + 2\overline{\beta} - \pi - \overline{\tau})H - (\Delta + 3\gamma - \overline{\gamma} + \mu + \overline{\mu})\overline{\sigma}H - (\lambda + \overline{\sigma}H)\\
&\quad \times (D - \epsilon + 3\overline{\epsilon} + 3\rho - \overline{\rho})H + HD(\lambda + \overline{\sigma}H) + (\text{linear operators acting on } \kappa \text{ or } \overline{\kappa}).
\end{aligned}
\tag{7}
$$

[Equations (1)–(7) are invariant under the simultaneous interchange of the tilded quantities by the untilded ones, and of H by $-H$.]

Before we consider the Einstein equations with sources, we shall give a proof of the Xanthopoulos theorem,[5] allowing the presence of a nonzero cosmological constant.

A. Vacuum case

If $g_{\mu\nu}$ and $\widetilde{g}_{\mu\nu}$ satisfy the Einstein vacuum field equations, possibly with (different) nonzero cosmological constants λ_0 and $\widetilde{\lambda}_0$, respectively, from the first equation in (5) it follows that $\kappa=0$ (excluding the trivial case $H=0$), which means that l^μ is geodetic. Then, setting $\widetilde{\Phi}_{ij}=0=\Phi_{ij}$, $6\Lambda=\lambda_0$, $6\widetilde{\Lambda}=\widetilde{\lambda}_0$, and $\kappa=0$ in Eqs. (5) and (6), the quadratic terms in H disappear, and one obtains

$$
\begin{aligned}
&\kappa = 0,\\
&(D - \epsilon + 3\overline{\epsilon} - 2\overline{\rho})\sigma H = 0,\\
&\tfrac{1}{2}(D + \epsilon + \overline{\epsilon} - \rho + \overline{\rho})(D + 2\epsilon + 2\overline{\epsilon} + \rho - \overline{\rho})H - (\rho^2 - \overline{\sigma}\sigma)H = 0,\\
&\tfrac{1}{2}(\delta + \beta + \overline{\alpha} - \tau)(D + 2\overline{\epsilon} + \rho - \overline{\rho})H + \epsilon(\delta + 2\beta + 2\overline{\alpha} - \tau - \overline{\pi})H\\
&\quad + \sigma(\overline{\delta} + \alpha + 2\overline{\beta} - \pi - \overline{\tau})H + H(D - \epsilon + \overline{\epsilon} - \overline{\rho})\beta - \tau\rho H = 0,\\
&(\delta + 3\beta + \overline{\alpha} - \tau)(\overline{\delta} + 2\alpha + 2\overline{\beta} - \pi - \overline{\tau})H - (\Delta + \gamma + \overline{\gamma} + \mu)\rho H\\
&\quad - \mu(D + \epsilon + \overline{\epsilon} + \rho)H + HD\mu + \pi(\delta + 2\beta + 2\overline{\alpha} - \tau - \overline{\pi})H - (\lambda\sigma + \overline{\lambda}\overline{\sigma})H = 0,\\
&\tfrac{1}{2}(D + \epsilon + \overline{\epsilon} + \rho - \overline{\rho})(D + 2\epsilon + 2\overline{\epsilon} + \rho - \overline{\rho})H - 2(D + \epsilon + \overline{\epsilon} - \overline{\rho})\rho H\\
&\quad + (\rho^2 + \overline{\sigma}\sigma)H = \lambda_0 - \widetilde{\lambda}_0,
\end{aligned}
\tag{8}
$$

which means that $h_{\mu\nu} := 2Hl_\mu l_\nu$ satisfies the Einstein vacuum field equations linearized about $g_{\mu\nu}$.

Conversely, if $2Hl_\mu l_\nu$ satisfies the linearized Einstein vacuum field equations, with or without cosmological constant, Eqs. (8) are fulfilled; then, assuming that $g_{\mu\nu}$ satisfies the Einstein vacuum field equations with or without a cosmological constant (i.e., $\Phi_{ij}=0$, $6\Lambda=\lambda_0$), Eqs. (5) and (6) yield $\widetilde{\Phi}_{ij}=0$, $\widetilde{\Lambda}=$const, which means that $\widetilde{g}_{\mu\nu}$ is also an exact vacuum solution.

If $g_{\mu\nu}$ and $\tilde{g}_{\mu\nu}$ are exact vacuum solutions, from Eqs. (7) it follows that l^μ is a principal null direction of the Weyl tensor of $g_{\mu\nu}$ if and only if it is a principal null direction of the Weyl tensor of $\tilde{g}_{\mu\nu}$ (compare Ref. 5), and that l^μ is a double principal null direction of the Weyl tensor of $g_{\mu\nu}$ if and only if is a double principal null direction of the Weyl tensor of $\tilde{g}_{\mu\nu}$. (Note that these conclusions apply whenever $\tilde{\Phi}_{\mu\nu}l^\mu l^\nu=\Phi_{\mu\nu}l^\mu l^\nu$.)

B. Einstein–Maxwell case

Let $F_{\mu\nu}$ be an electromagnetic field that satisfies the source-free Maxwell equations in the background metric $g_{\mu\nu}$, such that l^μ is a principal null direction of $F_{\mu\nu}$. This means that

$$\varphi_0=0, \tag{9}$$

and the remaining components of $F_{\mu\nu}$ satisfy the equations

$$\begin{gathered}(D-2\rho)\varphi_1+\kappa\varphi_2=0, \quad (\delta-2\tau)\varphi_1+\sigma\varphi_2=0,\\ (\overline{\delta}+2\pi)\varphi_1-(D+2\epsilon-\rho)\varphi_2=0,\\ (\Delta+2\mu)\varphi_1-(\delta+2\beta-\tau)\varphi_2=0.\end{gathered} \tag{10}$$

From Eqs. (2) and (9) it follows that the components of $F_{\mu\nu}$ with respect to the tetrad $\tilde{l}^\mu$, $\tilde{n}^\mu$, $\tilde{m}^\mu$, $\overline{\tilde{m}^\mu}$ are given by

$$\tilde{\varphi}_0=0, \quad \tilde{\varphi}_1=\varphi_1, \quad \tilde{\varphi}_2=\varphi_2. \tag{11}$$

Then, using Eqs. (3), (4), (10), and (11) one finds that $F_{\mu\nu}$ also satisfies the source-free Maxwell equations in the background metric $\tilde{g}_{\mu\nu}$ if and only if

$$\kappa\varphi_2=0. \tag{12}$$

(An alternative proof of this fact can be given using the connection tensor that relates the covariant derivative operators $\boldsymbol{\nabla}_\mu$ and $\tilde{\boldsymbol{\nabla}}_\mu$, as in Ref. 5.)

If $(g_{\mu\nu},F_{\mu\nu})$ and $(\tilde{g}_{\mu\nu},F_{\mu\nu})$ are exact solutions of the Einstein–Maxwell equations (possibly with nonzero cosmological constants), with l^μ being a principal null direction of $F_{\mu\nu}$, using the fact that $\Phi_{ij}=2\varphi_i\overline{\varphi_j}$ $(i,j=0,1,2)$ and Eqs. (5), (9), and (11), it follows that $\kappa=0$ and all the nonlinear terms in H contained in Eqs. (5) and (6) disappear. Hence, $(2Hl_\mu l_\nu,0)$ satisfies the Einstein–Maxwell equations linearized about $(g_{\mu\nu},F_{\mu\nu})$. It must be noticed that the equalities $\Phi_{ij}=\tilde{\Phi}_{ij}$, which follow from Eq. (11), *do not* mean that the energy-momentum tensors of the electromagnetic field $F_{\mu\nu}$ in the backgrounds $g_{\mu\nu}$ and $\tilde{g}_{\mu\nu}$ necessarily coincide. Even though $F_{\mu\nu}$ is left unchanged, the energy-momentum tensors of $F_{\mu\nu}$ in the backgrounds $g_{\mu\nu}$ and $\tilde{g}_{\mu\nu}$ may be different, owing to the presence of the metric in the expression for the energy-momentum tensor of the electromagnetic field.

Conversely, if $(g_{\mu\nu},F_{\mu\nu})$ is an exact solution of the Einstein–Maxwell equations and $(2Hl_\mu l_\nu,0)$ satisfies the Einstein–Maxwell equations linearized about $(g_{\mu\nu},F_{\mu\nu})$, with l_μ being a principal null direction of $F_{\mu\nu}$ [Eqs. (8)], then $(\tilde{g}_{\mu\nu},F_{\mu\nu})$ is an exact solution of the Einstein–Maxwell equations.

C. Einstein–Weyl case

Let η_A be a spinor field that satisfies the Weyl neutrino equation in the background metric $g_{\mu\nu}$, such that the flux vector of the neutrino field is proportional to l^μ; thus,

$$\eta_0=0 \tag{13}$$

and the Weyl equation reduces to

$$(D+\epsilon-\rho)\,\eta_1=0, \quad (\delta+\beta-\tau)\,\eta_1=0. \tag{14}$$

The components of the neutrino field with respect to the null tetrad $\tilde{l}^\mu$, $\tilde{n}^\mu$, $\tilde{m}^\mu$, $\overline{\tilde{m}^\mu}$ are given by

$$\tilde{\eta}_0=0, \quad \tilde{\eta}_1=\eta_1 \tag{15}$$

[i.e., the tensorial objects (the ''flags'') defined by the components (15) with respect to the corresponding tetrads coincide] and from Eqs. (3), (4), and (14) it follows that η_A also satisfies the Weyl equation in the background metric $\tilde{g}_{\mu\nu}$.

The tetrad components of the Einstein field equations with a neutrino field such that $\eta_0=0$, are explicitly given by

$$\begin{gathered}
\Phi_{00}=0, \quad \Phi_{01}=-ik\kappa\overline{\eta_1}\eta_1, \quad \Phi_{02}=-2ik\sigma\overline{\eta_1}\eta_1, \\
\Phi_{11}=ik[\eta_1 D\overline{\eta_1}-\overline{\eta_1}D\eta_1+(\overline{\epsilon}-\epsilon)\overline{\eta_1}\eta_1], \\
\Phi_{12}=ik[\eta_1 \delta\overline{\eta_1}-\overline{\eta_1}\delta\eta_1+(\overline{\alpha}-\beta-\tau)\overline{\eta_1}\eta_1], \\
\Phi_{22}=2ik[\eta_1 \Delta\overline{\eta_1}-\overline{\eta_1}\Delta\eta_1+(\overline{\gamma}-\gamma)\overline{\eta_1}\eta_1], \\
\Lambda=0,
\end{gathered} \tag{16}$$

where k is a real constant. Making use of Eqs. (3), (4), (14), and (15) one finds that the right-hand sides of Eqs. (16) are left unchanged by the substitution of $g_{\mu\nu}$ by $\tilde{g}_{\mu\nu}$. Therefore, if $(g_{\mu\nu},\eta_A)$ and $(\tilde{g}_{\mu\nu},\eta_A)$ are exact solutions of the Einstein–Weyl equations (possibly with nonzero cosmological constants), with l^μ being parallel to the flux vector of the neutrino field, from Eqs. (5) and (16), it follows that $\kappa=0$ and, again, the nonlinear terms in H contained in Eqs. (5) and (6) disappear, which means that $(2Hl_\mu l_\nu,0)$ satisfies the Einstein–Weyl equations linearized about $(g_{\mu\nu},\eta_A)$.

It is easy to see that, conversely, if $(g_{\mu\nu},\eta_A)$ is an exact solution of the Einstein–Weyl equations and $(2Hl_\mu l_\nu,0)$ satisfies the Einstein–Weyl equations linearized about $(g_{\mu\nu},\eta_A)$, with l_μ being parallel to the flux vector of the neutrino field, then $(g_{\mu\nu}+2Hl_\mu l_\nu,\eta_A)$ is also an exact solution of the Einstein–Weyl equations.

D. An example

The Bell–Szekeres solution represents the collision of two plane electromagnetic waves. In each region before the collision, the space-time can be described by the null tetrad,[7]

$$\begin{gathered}
D=-\frac{1}{\sqrt{2}}\,\partial_u, \quad \Delta=-\frac{1}{\sqrt{2}}\,(1-v^2)^{1/2}\partial_v, \\
\delta=(1-v^2)^{-1/2}\partial_z, \quad \overline{\delta}=(1-v^2)^{-1/2}\partial_{\overline{z}},
\end{gathered} \tag{17}$$

where u and v are real coordinates, z is a complex coordinate, and $\overline{z}$ denotes its complex conjugate. The only nonvanishing spin coefficient is

$$\mu=\frac{1}{\sqrt{2}}\,(1-v^2)^{-1/2}v, \tag{18}$$

and the only nonvanishing component of the curvature is

$$\Phi_{22}=\tfrac{1}{2}. \tag{19}$$

Therefore, the electromagnetic field can be taken as

$$\varphi_0=0=\varphi_1, \quad \varphi_2=\tfrac{1}{2}. \tag{20}$$

Since Eqs. (9) and (12) are satisfied, making use of Eqs. (17) and (18), one finds that the perturbed metric $\tilde{g}_{\mu\nu}$ with the electromagnetic field given by Eq. (20) is a solution of the Einstein–Maxwell equations, provided that the function H satisfies Eqs. (8), which reduce to

$$\partial_u^2 H=0, \quad \partial_z\,\partial_u H=0, \quad 2\partial_z\,\partial_{\bar{z}} H+v\sqrt{1-v^2}\,\partial_u H=0. \tag{21}$$

Thus,

$$H=uf(v)-\tfrac{1}{2}\,v\sqrt{1-v^2}f(v)z\overline{z}+g(z,v)+\overline{g(z,v)}, \tag{22}$$

where f is an arbitrary real function and g is an arbitrary function of two variables. Then, from Eqs. (7), it follows that $\tilde{g}_{\mu\nu}$ is of type N or conformally flat.

III. DISCUSSION

The validity of the results presented in this paper depends crucially on the insensitivity of the Maxwell and the Weyl equations to the change of the background metric $g_{\mu\nu}$ by $g_{\mu\nu}+2Hl_\mu l_\nu$ if l_μ is a principal null direction of the electromagnetic or the neutrino field, respectively, which allows us to consider metric perturbations alone (see also Ref. 4). Thus, not only it is possible to consider gravitational perturbations without perturbing the matter field, but they may correspond to exact solutions.

The results of Sec. II B can also be derived, albeit by lengthier computations, making use of the tensor formalism, as in Ref. 5. However, the null tetrad formalism employed here allows us to treat also the Einstein–Weyl equations very easily. It may be pointed out that the perturbation equations (8) possess the gauge freedom corresponding to the null tetrad rotations that preserve the direction of l^μ.

Another remarkable fact is that, owing to the invariance of Eqs. (1)–(7) under the interchange of H by $-H$ and of the tilded quantities by the untilded ones, in the perturbation equations (8), one can equivalently substitute either the tetrad and spin coefficients corresponding to $g_{\mu\nu}$ or to $\tilde{g}_{\mu\nu}$.

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Irreducible tensor operators in the regular coaction formalisms of compact quantum group algebras

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The defining conditions for the irreducible tensor operators associated with the unitary irreducible corepresentations of compact quantum group algebras are deduced first in both the right and left regular coaction formalisms. In each case it is shown that there are *two* types of irreducible tensor operator, which may be called ''ordinary'' and ''twisted.'' The consistency of the definitions is demonstrated, and various consequences are deduced, including generalizations of the Wigner–Eckart theorem for both the ordinary and twisted operators. Also included are discussions (within the regular coaction formalisms for compact quantum group algebras) of inner-products, basis functions, projection operators, Clebsch–Gordan coefficients, and two types of tensor product of corepresentations. The formulation of quantum homogeneous spaces for compact quantum group algebras is discussed, and the defining conditions for the irreducible tensor operators associated with such quantum homogeneous spaces and with the unitary irreducible corepresentations of the compact quantum group algebras are then deduced. There are two versions, which correspond to restrictions of the right and left regular coactions. In each case it is again shown that there are ordinary and twisted irreducible tensor operators. Various consequences are deduced, including the corresponding generalizations of the Wigner–Eckart theorem.
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I. INTRODUCTION

It is well known that most of the applications to physics of the theories of groups and Lie algebras depend on the Wigner–Eckart theorem. It is therefore not surprising that the question of the generalization of this theorem to Hopf algebras having the structure of a deformation of a Lie algebra has also been the subject of a number of studies.[1–15] The present paper is intended to complement and extend these investigations in various important respects. Its detailed relationship to previous work will be indicated in the appropriate places.

The perspective of the present communication is best introduced by considering matters first in the very well established and familiar context of a compact Lie group $\mathscr{G}$ (cf. Refs. 16,17). Even in this context, one can distinguish *three* distinct forms of the Wigner–Eckart theorem.

1. The original form[18] involves the situation in which $\mathscr{G}$ is a group of transformations that act on an external manifold $\mathscr{M}$, the classic example being the case in which $\mathscr{M}$ is three-dimensional Euclidean space $\mathfrak{R}^3$, and $\mathscr{G}$ is the group of all rotations in this space about some fixed point, which may be taken to be the origin O of $\mathfrak{R}^3$. Associated with every such rotation T there exists a 3×3 real orthogonal matrix $\mathbf{R}(T)$, so that the effect of T is to transform each position vector $\mathbf{r}$ into another position vector $\mathbf{r}'$, where

$$\mathbf{r}' = \mathbf{R}(T)\mathbf{r}. \tag{1}$$

Also associated with every rotation T is a unitary operator $P(T)$ whose effect on any function $f(\mathbf{r})$ is defined by

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$$P(T)f(\mathbf{r})=f[\mathbf{R}(T)^{-1}\mathbf{r}]). \tag{2}$$

Let $\mathbf{\Gamma}^p$ be a unitary irreducible representation of dimension d_p of the group $\mathcal{G}$. If there exists a set of functions $\psi_1^p(\mathbf{r}),\psi_2^p(\mathbf{r}),\ldots,\psi_{d_p}^p(\mathbf{r})$ such that

$$P(T)\psi_n^p(\mathbf{r})=\sum_{m=1}^{d_p}\Gamma^p(T)_{mn}\psi_m^p(\mathbf{r}), \tag{3}$$

for all $T\in\mathcal{G}$ and all $n=1,2,\ldots,d_p$, then these are said to form a set of basis functions for $\mathbf{\Gamma}^p$. Similarly, if there exists a set of d_p operators $Q_1^p,Q_2^p,\ldots,Q_{d_p}^p$ that act on functions $f(\mathbf{r})$ in such a way that

$$P(T)Q_n^pP(T)^{-1}=\sum_{m=1}^{d_p}\Gamma^p(T)_{mn}Q_m^p, \tag{4}$$

for all $T\in\mathcal{G}$ and all $n=1,2,\ldots,d_p$, then these are said to form a set of irreducible tensor operators for $\mathbf{\Gamma}^p$. Finally, if the inner product for the Hilbert space of functions $f(\mathbf{r})$ is defined by

$$(f,g)=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\overline{f(\mathbf{r})}\,dx\,dy\,dz, \tag{5}$$

where $\overline{f(\mathbf{r})}$ denotes the complex conjugate of $f(\mathbf{r})$, then the Wigner–Eckart theorem for this situation states that the j,k, and ℓ dependence of $[\psi_\ell^r,Q_k^q(\phi_j^p)]$ depends only on Clebsch–Gordan coefficients for the reduction of the tensor product $\mathbf{\Gamma}^p\otimes\mathbf{\Gamma}^q$ into its irreducible constituents $\mathbf{\Gamma}^r$.

2. In this form the role of the manifold $\mathcal{M}$ is played by $\mathcal{G}$ itself, so that one is concerned with the space of complex-valued continuous functions defined on $\mathcal{G}$. Let this be denoted by $C(\mathcal{G})$. The inner product of $C(\mathcal{G})$ may be taken to be

$$(f,g)=\int_{\mathcal{G}}\overline{f(T)}g(T)\,dT, \tag{6}$$

where the integral is the left and right invariant normalized Haar integral of $\mathcal{G}$, and $\overline{f(T)}$ is the complex conjugate of $f(T)$. In the *right regular formalism*, for each $T\in\mathcal{G}$ there exists an operator $\hat{R}(T)$ that is defined by $\hat{R}(T)f(T')=f(T'T)$ for all f and for all $T,T'\in\mathcal{G}$. If f is a member of $C(\mathcal{G})$ such that $\hat{R}(T)f$ spans a finite- dimensional subspace of $C(\mathcal{G})$, then f is said to be a *representative function* on $\mathcal{G}$. The subspace of $C(\mathcal{G})$ consisting of representative functions will be denoted by $R(\mathcal{G})$. If there exists a set of functions $\psi_1^p(T),\psi_2^p(T),\ldots,\psi_{d_p}^p(T)$ such that $\hat{R}(T)\psi_n^p(T')=\Sigma_{m=1}^{d_q}\Gamma^p(T)_{mn}\psi_m^p(T')$ for all $T,T'\in\mathcal{G}$ and all $n=1,2,\ldots,d_p$, then these are said to form a set of basis functions for $\mathbf{\Gamma}^p$. Similarly, if there exists a set of d_p operators $Q_1^p,Q_2^p,\ldots,Q_{d_p}^p$ that act on functions $f(T)$ in such a way that $\hat{R}(T)Q_n^p\hat{R}(T)^{-1}=\Sigma_{m=1}^{d_q}\Gamma^p(T)_{mn}Q_m^p$ for all $T\in\mathcal{G}$ and all $n=1,2,\ldots,d_p$, then this set is said to form a set of irreducible tensor operators for $\mathbf{\Gamma}^p$. The Wigner–Eckart theorem for this case states that the j,k, and ℓ dependence of $[\psi_\ell^r,Q_k^q(\phi_j^p)]$ again depends only on Clebsch–Gordan coefficients for the reduction of the tensor product $\mathbf{\Gamma}^p\otimes\mathbf{\Gamma}^q$ into its irreducible constituents $\mathbf{\Gamma}^r$. In the *left regular formalism* the situation is the same, except only that the operators $\hat{R}(T)$ are replaced by operators $\hat{L}(T)$ that are defined by $\hat{L}(T)f(T')=f(T^{-1}T')$ for all f and for all $T,T'\in\mathcal{G}$.

3. The final form involves using the abstract carrier spaces of the unitary irreducible representations of $\mathcal{G}$. Let V^p be such a carrier space for $\mathbf{\Gamma}^p$, with ortho-normal basis $\psi_1^p,\psi_2^p,\ldots,\psi_{d_p}^p$, and define for each $T\in\mathcal{G}$ a linear operator $\Phi^p(T)$ that acts on V^p by the

requirement that $\Phi^p(T)\psi_n^p=\Sigma_{m=1}^{d_p}\Gamma^p(T)_{mn}\psi_m^p$ for all $T\in\mathscr{G}$ and all $n=1,2,\ldots,d_p$. Let $\mathbf{\Gamma}^p$, $\mathbf{\Gamma}^q$, and $\mathbf{\Gamma}^r$ be any three unitary irreducible resentations of $\mathscr{G}$. Then one can consider a set of irreducible tensor operators $Q_1^q,Q_2^q,\ldots,Q_{d_q}^q$ that each map V^p into V^r and which are such that $\Phi^r(T)Q_n^q\Phi^p(T)^{-1}=\Sigma_{m=1}^{d_q}\Gamma^q(T)_{mn}Q_m^q$ for all $T\in\mathscr{G}$ and all $n=1,2,\ldots,d_q$. In this case the Wigner–Eckart theorem deals with inner products $\langle,\rangle$ defined on V^r and states that the j,k, and ℓ dependence of $\langle\psi_\ell^r,Q_k^q(\phi_j^p)\rangle$ also depends only on Clebsch–Gordan coefficients for the reduction of the tensor product $\mathbf{\Gamma}^p\otimes\mathbf{\Gamma}^q$ into its irreducible constituents $\mathbf{\Gamma}^r$. In a minor extension of this formalism, one could introduce an inner product space V that is a direct sum of carrier spaces of certain unitary irreducible representations of $\mathscr{G}$ and which contains at least $V^p\oplus V^r$ (and which, in the extreme case, may contain one carrier space for every inequivalent irreducible representation of $\mathscr{G}$). Then, for each $T\in\mathscr{G}$ an operator $\Phi(T)$ can be defined which maps elements of V into V, and which acts as $\Phi^p(T)$ on V^p, as $\Phi^r(T)$ on V^r, and so on. The irreducible tensor operators are then required to each map V into V and to be such that $\Phi(T)Q_n^q\Phi(T)^{-1}=\Sigma_{m=1}^{d_q}\Gamma^q(T)_{mn}Q_m^q$ for all $T\in\mathscr{G}$ and all $n=1,2,\ldots,d_q$. In this case the Wigner–Eckart theorem deals with inner products $\langle,\rangle$ defined on V, but is otherwise the same as above.

The developments that will be described in the present paper up to and including Section VIII are essentially within the spirit of the second of these formulations, but deal with a more general Hopf algebra structure. The generalization of the first formulation in terms of quantum homogeneous spaces then follows in Section IX. (It is intended to extend this analysis to the remaining formulation in a subsequent paper.)

One most important lesson that can be drawn from these simple group theoretical considerations concerns the *consistency* of the definitions of the basis functions (or basis vectors) *and* of the irreducible tensor operators. The essential point will be illustrated in the first of the above formulations, but similar considerations apply in the others. As $P(T)P(T')=P(TT')$ and $\mathbf{\Gamma}^p(T)\mathbf{\Gamma}^p(T')=\mathbf{\Gamma}^p(TT')$ for all $T,T'\in\mathscr{G}$, it follows that if (3) is valid for T and for T', then it is also valid for their product TT'. Similarly, and very significantly, by defining for each $T\in\mathscr{G}$ an operator $\Psi(T)$ by $\Psi(T)Q=P(T)QP(T)^{-1}$ for every operator Q that acts on functions $f(\mathbf{r})$, the definition (4) can be recast as

$$\Psi(T)(Q_n^p)=\sum_{m=1}^{d_p}\Gamma^p(T)_{mn}Q_m^p, \tag{7}$$

for all $T\in\mathscr{G}$ and all $n=1,2,\ldots,d_p$. As $\Psi(T)\Psi(T')=\Psi(TT')$ for all $T,T'\in\mathscr{G}$, it follows that if (7) is valid for T and for T', then it is also valid for their product TT'. Put another way, because of the similarity in form between (3) and (7), the *consistency* of the definition (4) of the irreducible tensor operators Q_n^p is ensured by the fact that they too form a basis for a carrier space of $\mathbf{\Gamma}^p$. In the analysis that follows (cf. Section VI), essentially this argument will be used to justify the definitions that will be given for the irreducible tensor operators of the compact quantum group algebras in the regular corepresentation formalisms, the only essential difference being that the argument has to be cast in terms of *co*representations instead of representations.

It is well known that the set of functions defined on a Lie group $\mathscr{G}$ form a Hopf algebra, $\mathscr{A}$, and that the dual $\mathscr{A}'$ of $\mathscr{A}$ is the universal enveloping algebra of the Lie algebra $\mathscr{L}$ of $\mathscr{G}$. Moreover, the structure of $\mathscr{G}$ can be encoded into the structure of $\mathscr{A}$, and, in particular, $\mathscr{A}$ is commutative. A ''deformation'' (or ''quantization'') of $\mathscr{A}'$ induces a corresponding deformation of $\mathscr{A}$, and will make $\mathscr{A}$ non-commutative as well as being non-cocommutative. Most of the previous work on irreducible tensor operators has been focused on the deformed Hopf algebras $\mathscr{A}'$, with $su_q(2)$ receiving the most attention. However, as has been demonstrated by the pioneering work of Woronowicz,[19–21] which itself has been refined and developed by Dijkhuizen and Koornwinder,[22–26] it is of very great interest to produce a self-contained and direct study of

generalizations of the Hopf algebras $\mathscr{A}$, which can be done by assuming that they have certain characteristic properties. The resulting structures have been called *compact matrix pseudogroups* by Woronowicz,[19–21] and *compact quantum group algebras* by Dijkhuizen and Koornwinder.[22–26] These provide the framework for the present paper, which is devoted to the study of the irreducible tensor operators for compact quantum group algebras. As explained above, this analysis will be given in the regular corepresentation formalisms. [The only previous investigation of irreducible tensor operators within the general compact matrix pseudogroup theory has been by Bragiel,[5] who looked at the analogue of the carrier space formalism (3) above, but with certain restrictive assumptions on multiplicities, though some of the work of Klimyk[9] involves a discussion of special cases, again in the carrier space formalism.]

The structure of the present paper is as follows. Section II contains a brief summary of the essential preliminaries, starting in Section II A with the properties of Hopf *-algebras, and continuing in Section II B with the main features of their right comodules. The definition and relevant properties of a compact quantum group algebra $\mathscr{A}$ follow in Section II C. (Of course the developments of Woronowicz and of Dijkhuizen and Koornwinder extend far beyond what is mentioned here, particularly in their invocation of quantum Tannaka–Krein duality.) This section is concluded in Section II D with some new lemmas concerning the Haar functional of $\mathscr{A}$. The right and left regular comodules of $\mathscr{A}$ are described in Section III, and these are employed in Section IV to introduce and develop the concept of basis functions for right corepresentations of $\mathscr{A}$. In Section V the tensor products (both ''ordinary'' and ''twisted'') of corepresentations of $\mathscr{A}$ are discussed, along with their associated Clebsch–Gordan coefficients. The heart of the paper is reached in Section VI, where the irreducible tensor operators are defined and some of their immediate properties are deduced. In particular, it will be shown there that in both the right and left regular coaction formulations there are *two* types of irreducible tensor operators, which will be described as being *ordinary* and *twisted*, respectively. The motivations for the definitions of Section VI are deliberately relegated to Appendix B in order to emphasize that the treatment given for the compact quantum group algebras in Sections II to IX is entirely self-contained. In Section VII it is shown that there are *two* theorems of the Wigner–Eckart type, one for ''ordinary'' and one for the ''twisted'' irreducible tensor operators. Likewise, in Section VIII, it is demonstrated that these two types of irreducible tensor operator behave differently under multiplication. Finally, in Section IX it is shown how all developments generalize when one considers operators associated with the corresponding homogeneous spaces. In particular, it emerges that there are again two formulations, one associated with the right regular representation and the other with the left regular representation. The vital algebraic quantity that appears in each version is a $\star$-subalgebra $\mathscr{B}$ of $\mathscr{A}$, which is a right coideal of $\mathscr{A}$ in the right regular formulation, but is a left coideal of $\mathscr{A}$ in the left regular formulation. In Section IX B attention is focused on the right coactions $\pi_{\mathscr{B}}^{R}$ and $\pi_{\mathscr{B}}^{L}$ of $\mathscr{A}$ that are obtained by restricting the right and left regular coactions of $\mathscr{A}$ to its subalgebra $\mathscr{B}$. As these are the *transitive* $\star$*-coactions* that correspond to the transitive action of a quantum group on a quantum homogeneous space in the sense of Dijkhuizen and Koornwinder,[23,24] they play the key role in the analysis. In particular the properties of basis functions, as defined in terms of these restricted coactions, are presented in Section IX C, and in Section IX D the irreducible tensor operators are also defined in terms of these coactions. It is shown there that, associated with both $\pi_{\mathscr{B}}^{R}$ and $\pi_{\mathscr{B}}^{L}$ there are two types of irreducible tensor operator, which are again called *ordinary* and *twisted*, and the immediate properties of all these irreducible tensor operators are described. In Section IX E it is shown that the irreducible tensor operators satisfy theorems of the Wigner–Eckart type, and the analysis is concluded in Section IX F with a demonstration that the products of these irreducible tensor operators are themselves expressible as linear combinations of irreducible tensor operators that involve the relevant Clebsch–Gordan coefficients.

Because the space of functions defined on a compact Lie group $\mathscr{G}$ is a special example of a compact quantum group algebra, all the well-known results for compact Lie groups naturally

reappear in this particular case. However, as the detailed analysis shows, the theory in the general situation is rather more subtle, and exhibits various complications.

II. PROPERTIES OF COMPACT QUANTUM GROUP ALGEBRAS

A. Hopf *-algebras

The purpose of this section is mainly to establish notations, and summarize the essential properties. For further details see, for example, Sweedler,[27] Majid,[28] and Chari and Pressley.[29]

A *Hopf algebra* $\mathscr{A}$ over the field of complex numbers $\mathbb{C}$ is a complex vector space with an identity element $1_{\mathscr{A}}$ that possesses a multiplication operator M (which maps $\mathscr{A}\otimes\mathscr{A}$ into $\mathscr{A}$), a unit operator u (which maps $\mathbb{C}$ into $\mathscr{A}$), a comultiplication operator Δ (which maps $\mathscr{A}$ into $\mathscr{A}\otimes\mathscr{A}$), a counit operator ϵ (which maps $\mathscr{A}$ into $\mathbb{C}$), and an antipode operator S (which maps $\mathscr{A}$ into $\mathscr{A}$). These are assumed to be linear in all their arguments and to have the following properties:

$$M\circ(M\otimes id)=M\circ(id\otimes M), \tag{8}$$

$$(\Delta\otimes id)\circ\Delta=(id\otimes\Delta)\circ\Delta, \tag{9}$$

$$\Delta\circ M=(M\otimes M)\circ(id\otimes\sigma\otimes id)\circ(\Delta\otimes\Delta), \tag{10}$$

$$\epsilon\circ M=M_{\mathbb{C}}\circ(\epsilon\otimes\epsilon), \tag{11}$$

$$M_{\mathbb{C},\mathscr{A}}\circ(\epsilon\otimes id)\circ\Delta=M_{\mathscr{A},\mathbb{C}}\circ(id\otimes\epsilon)\circ\Delta=id, \tag{12}$$

$$u(1_{\mathbb{C}})=1_{\mathscr{A}},\quad \epsilon(1_{\mathscr{A}})=1_{\mathbb{C}},\quad S(1_{\mathscr{A}})=1_{\mathscr{A}}, \tag{13}$$

$$M(a\otimes 1_{\mathscr{A}})=M(1_{\mathscr{A}}\otimes a)=a,\quad \text{for all}\quad a\in\mathscr{A}, \tag{14}$$

$$\Delta(1_{\mathscr{A}})=1_{\mathscr{A}}\otimes 1_{\mathscr{A}}, \tag{15}$$

$$S\circ M=M\circ\sigma\circ(S\otimes S), \tag{16}$$

$$\Delta\circ S=(S\otimes S)\circ\sigma\circ\Delta, \tag{17}$$

$$M\circ(S\otimes id)\circ\Delta=M\circ(id\otimes S)\circ\Delta=u\circ\epsilon, \tag{18}$$

$$\epsilon\circ S=\epsilon. \tag{19}$$

Here σ is the transposition operator which interchanges the order of its arguments, so that, for example, when acting on $\mathscr{A}\otimes\mathscr{A}$, $\sigma(a\otimes b)=b\otimes a$ for all $a,b\in\mathscr{A}$. Also $M_{\mathbb{C}}$, $M_{\mathscr{A},\mathbb{C}}$, and $M_{\mathbb{C},\mathscr{A}}$ are the multiplication operators defined by $M_{\mathbb{C}}(w\otimes z)=wz$ for all $w,z\in\mathbb{C}$, and $M_{\mathscr{A},\mathbb{C}}(a\otimes z)=M_{\mathbb{C},\mathscr{A}}(z\otimes a)=za$ for all $z\in\mathbb{C}$ and all $a\in\mathscr{A}$. The product $M(a\otimes b)$ will sometimes be written more concisely as ab, and the coproduct Δ will sometimes be expressed as

$$\Delta(a)=\sum_{(a)} a_{(1)}\otimes a_{(2)}. \tag{20}$$

If $\mathscr{A}$ is finite-dimensional, with basis elements $a_1,a_2,\ldots$, the structure constants m_{jk}^{ℓ}, μ_{ℓ}^{jk}, s_j^k, ϵ_j, and ϵ^j may be defined by $M(a_j\otimes a_k)=\Sigma_{\ell}m_{jk}^{\ell}a_{\ell}$, $\Delta(a_{\ell})=\Sigma_{j,k}\mu_{\ell}^{jk}a_j\otimes a_k$, $S(a_j)=\Sigma_k s_j^k a_k$, $\epsilon(a_j)=\epsilon_j$, and $1_{\mathscr{A}}=\Sigma_j\epsilon^j a_j$. Then (8) to (19) imply that

$$\sum_s m_{jk}^s m_{s\ell}^t = \sum_s m_{js}^t m_{k\ell}^s, \tag{21}$$

$$\sum_j \mu_\ell^{jk} \mu_j^{st} = \sum_j \mu_\ell^{sj} \mu_j^{tk}, \tag{22}$$

$$\sum_{p,q,s,t} \mu_j^{pq} \mu_k^{st} m_{ps}^r m_{qt}^u = \sum_p m_{jk}^p \mu_p^{ru}, \tag{23}$$

$$\sum_\ell m_{jk}^\ell \epsilon_\ell = \epsilon_j \epsilon_k, \tag{24}$$

$$\sum_j \mu_\ell^{jk} \epsilon_j = \sum_j \mu_\ell^{kj} \epsilon_j = \delta_\ell^k, \tag{25}$$

$$\sum_j \epsilon^j s_j^k = \epsilon^k, \quad \sum_j \epsilon^j \epsilon_j = 1_{\mathbb{C}}, \tag{26}$$

$$\sum_k \epsilon^k m_{jk}^\ell = \sum_k \epsilon^k m_{kj}^\ell = \delta_j^\ell, \tag{27}$$

$$\sum_j \epsilon^j \mu_j^{k\ell} = \epsilon^k \epsilon^\ell, \tag{28}$$

$$\sum_q m_{jk}^q s_q^p = \sum_{q,r} m_{rq}^p s_j^q s_k^r, \tag{29}$$

$$\sum_k \mu_k^{pq} s_j^k = \sum_{k,\ell} \mu_j^{k\ell} s_\ell^p s_k^q, \tag{30}$$

$$\sum_{k,\ell,r} \mu_j^{k\ell} s_k^r m_{r\ell}^t = \sum_{k,\ell,r} \mu_j^{k\ell} s_\ell^r m_{kr}^t = \epsilon_j \epsilon^t, \tag{31}$$

and

$$\sum_j \epsilon_j s_k^j = \epsilon_k. \tag{32}$$

A *Hopf *-algebra* $\mathscr{A}$ is defined to be a Hopf algebra that possesses an additional *-operation that maps $\mathscr{A}$ into $\mathscr{A}$. The effect of the * operation on $a \in \mathscr{A}$ will sometimes be denoted by a^*. In particular

$$1_{\mathscr{A}}^* = 1_{\mathscr{A}}. \tag{33}$$

The other properties are

$$(*\circ M_{\mathbb{C},\mathscr{A}})(z\otimes a) = M_{\mathbb{C},\mathscr{A}}(\overline{z}\otimes a^*) = (*\circ M_{\mathscr{A},\mathbb{C}})(a\otimes z) = M_{\mathscr{A},\mathbb{C}}(a^*\otimes\overline{z}) = \overline{z}a^* \tag{34}$$

(for all $z \in \mathbb{C}$ and all $a \in \mathscr{A}$, where $\overline{z}$ denotes the complex conjugate of z),

$$*\circ *=id, \tag{35}$$

$$*\circ M=M\circ(*\otimes *)\circ\sigma, \tag{36}$$

$$\Delta\circ *=(*\otimes *)\circ\Delta, \tag{37}$$

$$(\epsilon\circ *)(a)=\overline{\epsilon(a)}, \quad \text{for all} \quad a\in\mathscr{A}, \tag{38}$$

$$S\circ *\circ S\circ *=id, \tag{39}$$

which implies that S is invertible with inverse given by

$$S^{-1}=*\circ S\circ *. \tag{40}$$

If $\mathscr{A}$ is finite-dimensional, its linear dual will be denoted by $\mathscr{A}'$, the prime being used instead of the usual star to avoid any confusion with the *-operation that has just been defined. The effect of $a'\in\mathscr{A}'$ on $a\in\mathscr{A}$ will be denoted by $\langle a',a\rangle$, and the evaluation map ev (from $\mathscr{A}'\otimes\mathscr{A}$ to $\mathbb{C}$) will be defined by

$$ev(a'\otimes a)=\langle a',a\rangle, \tag{41}$$

for all $a'\in\mathscr{A}'$ and all $a\in\mathscr{A}$. In the case in which $\mathscr{A}$ is of finite dimension n, the dual basis of $\mathscr{A}'$ will be denoted by $a^1,a^2,\ldots,a^n$, and will be assumed to be such that

$$\langle a^j,a_k\rangle=\delta^j_k, \tag{42}$$

for all $j,k=1,2,\ldots,n$.

B. Right comodules of Hopf *-algebras

A *right $\mathscr{A}$-comodule* consists of a vector space V and a linear mapping π_V from V to $V\otimes\mathscr{A}$ such that

$$(\pi_V\otimes id)\circ\pi_V=(id\otimes\Delta)\circ\pi_V \tag{43}$$

and

$$M_{V,\mathbb{C}}\circ(id\otimes\epsilon)\circ\pi_V=id, \tag{44}$$

where $M_{V,\mathbb{C}}(v\otimes z)=zv$ for all $v\in V$ and all $z\in\mathbb{C}$. The operation π_V is then said to be a *right coaction* and provides a *corepresentation* of $\mathscr{A}$ with carrier space V. The present section will be devoted to a very brief account of the essential features of the corepresentations of $\mathscr{A}$. (For the intimate connection between the *corepresentation* theory of $\mathscr{A}$ and the *representation* theory of $\mathscr{A}'$, see Appendix A.)

If V is of finite dimension d, with basis $v_1,v_2,\ldots,v_d$, then there exists a uniquely determined set of elements π^V_{jk} of $\mathscr{A}$ (for $j,k=1,2,\ldots,d$), called the *matrix coefficients* of π_V, which are such that

$$\pi_V(v_j)=\sum_{k=1}^{d} v_k\otimes\pi^V_{kj}, \tag{45}$$

for all $j=1,2,\ldots,d$. (In this situation the corepresentation is said to have dimension d.) The requirements (43) and (44) then imply that

$$\Delta(\pi^V_{jk}) = \sum_{\ell=1}^{d} \pi^V_{j\ell} \otimes \pi^V_{\ell k} \tag{46}$$

and

$$\epsilon(\pi^V_{jk}) = \delta_{jk} \tag{47}$$

(for $j,k = 1,2,\ldots,d$). It is sometimes convenient to write

$$\pi_V(v) = \sum_{[v]} v_{[1]} \otimes v_{[2]}, \tag{48}$$

where $v_{[1]} \in V$ and $v_{[2]} \in \mathscr{A}$.

Two right $\mathscr{A}$-comodules, with carrier spaces V and W, coactions π_V and π_W, and matrix coefficients π^V_{jk} and π^W_{jk} are said to be *equivalent* if there exists a one-to-mapping Φ from V to W such that

$$\pi_W \circ \Phi = (\Phi \otimes id) \circ \pi_V. \tag{49}$$

If V and W have bases $v_1, v_2, \ldots, v_d$ and $w_1, w_2, \ldots, w_d$, respectively, then to the mapping Φ there corresponds a $d \times d$ non-singular matrix $\mathbf{\Phi}$ such that

$$\sum_{\ell=1}^{d} \Phi_{j\ell} \pi^V_{\ell k} = \sum_{\ell=1}^{d} \pi^W_{j\ell} \Phi_{\ell k}, \tag{50}$$

for all $j,k = 1,2,\ldots,d$.

A subspace $W \subset V$ is said to be *invariant* under π_V if $\pi_V(w) \subset W \otimes \mathscr{A}$ for all $w \in W$, and a corepresentation is described as being *irreducible* if V and 0 are the only invariant subspaces of V. If V is the direct sum of two invariant subspaces of V, then the corepresentation π_V is said to be *completely reducible*.

If V is endowed with an inner product $\langle , \rangle_V$ (such that $\langle zw, z'v \rangle_V = \overline{z}z' \langle w, v \rangle_V$ for all z, $z' \in \mathbb{C}$ and all v, $w \in V$), then π_V is said to give a *unitary* corepresentation if

$$\sum_{[v]} \langle w, v_{[1]} \rangle_V S(v_{[2]}) = \sum_{[w]} \langle w_{[1]}, v \rangle_V w^*_{[2]}, \tag{51}$$

for all $v, w \in V$. It can be shown[22–26] that if $v_1, v_2, \ldots, v_d$ is an ortho-normal basis of V then

$$S(\pi^V_{jk}) = \pi^{V*}_{kj}, \tag{52}$$

$$\sum_{\ell=1}^{d} M(\pi^{V*}_{\ell j} \otimes \pi^V_{\ell k}) = \delta_{jk} 1_{\mathscr{A}}, \tag{53}$$

and

$$\sum_{\ell=1}^{d} M(\pi^V_{j\ell} \otimes \pi^{V*}_{k\ell}) = \delta_{jk} 1_{\mathscr{A}} \tag{54}$$

(for all $j,k = 1,2,\ldots,d$).

Corresponding to a right $\mathscr{A}$-comodule with carrier space V and coaction π_V from V to $V\otimes\mathscr{A}$ there exist two other right $\mathscr{A}$-comodules formed from the same carrier space. Firstly, there is the coaction $\pi_V^{\ddagger}$ which is said to be *doubly contragredient* to π_V, and which is defined (as a mapping from V to $V\otimes\mathscr{A}$) by

$$\pi_V^{\ddagger}=(id\otimes S^2)\circ\pi_V. \tag{55}$$

With the matrix coefficients $\pi_{jk}^{V\ddagger}$ of $\pi_V^{\ddagger}$ being defined by

$$\pi_V^{\ddagger}(v_j)=\sum_{k=1}^{d} v_k\otimes\pi_{kj}^{V\ddagger}, \tag{56}$$

for all $j=1,2,\ldots,d$, it follows from (45) that

$$\pi_{jk}^{V\ddagger}=S^2(\pi_{jk}^{V}), \tag{57}$$

for all $j,k=1,2,\ldots,d$. Secondly, let $\overline{V}$ be the conjugate space to V [so that as an Abelian group V is isomorphic to V, but the scalar multiplication operator $M_{\mathbb{C},\overline{V}}$ for V is defined in terms of the corresponding operator $M_{\mathbb{C},V}$ for V by $M_{\mathbb{C},\overline{V}}(z\otimes v)=M_{\mathbb{C},V}(\overline{z}\otimes v)$]. Then the coaction $\overline{\pi_V}$, which is said to be *conjugate* to π_V, is defined (as a mapping from V to $V\otimes\mathscr{A}$) by

$$\overline{\pi_V}=(id\otimes *)\circ\pi_V, \tag{58}$$

so its matrix coefficients $\overline{\pi_{jk}^{V}}$ are given by

$$\overline{\pi_{jk}^{V}}=\pi_{jk}^{V*}, \tag{59}$$

for all $j,k=1,2,\ldots,d$.

C. Compact quantum group algebras

A *compact quantum group algebra* (or *CQG algebra* for short) may be defined[22–26] as a Hopf *-algebra that is spanned by the matrix coefficients of its non- equivalent finite-dimensional unitary irreducible corepresentations. Koornwinder and Dijkhuizen[22–26] have shown that if $\mathscr{A}$ is a CQG algebra then every finite-dimensional corepresentation of $\mathscr{A}$ is equivalent to a unitary corepresentation, and that every finite-dimensional reducible corepresentation of $\mathscr{A}$ is completely reducible. Moreover[22–26] if $\mathscr{A}$ is a CQG algebra then $\mathscr{A}$ possesses a *Haar functional*, h, which is a mapping of $\mathscr{A}$ into $\mathbb{C}$ such that

$$h(1_{\mathscr{A}})=1_{\mathbb{C}}, \tag{60}$$

$$h[M(a^*\otimes a)]>0, \tag{61}$$

$$h(a^*)=\overline{h(a)}, \tag{62}$$

$$h[S(a)]=h(a), \tag{63}$$

and

$$[M_{\mathbb{C},\mathscr{A}}\circ(h\otimes id)\circ\Delta](a)=[M_{\mathscr{A},\mathbb{C}}\circ(id\otimes h)\circ\Delta](a)=h(a)\,1_{\mathscr{A}}, \tag{64}$$

for all $a\in\mathscr{A}$.

Koornwinder and Dijkhuizen[22–26] have also shown that if π^p and π^q are two non-equivalent irreducible corepresentations of a CQG algebra $\mathscr{A}$ with dimensions d_p and d_q and matrix coefficients π^p_{jk} and π^q_{mn}, respectively, then

$$h[M(\pi^p_{jk}\otimes S(\pi^q_{mn})]=0, \quad h[M(S(\pi^p_{jk})\otimes\pi^q_{mn})]=0 \tag{65}$$

(for all $j,k=1,2,\ldots,d_p$ and for all $m,n=1,2,\ldots,d_q$). Moreover every π^p irreducible corepresentation of $\mathscr{A}$ is equivalent to its doubly contragredient partner $\pi^{p\ddagger}$, so in each such case there exists a non-singular $d_p\times d_p$ matrix $\mathbf{F}^p$ such that

$$\sum_{k=1}^{d_p} F^p_{jk}\pi^p_{k\ell}=\sum_{k=1}^{d_p}\pi^{p\ddagger}_{jk}F^p_{k\ell} \tag{66}$$

(for all $j,\ell=1,2,\ldots,d_p$). Then, if π^p is a unitary irreducible corepresentation of $\mathscr{A}$,

$$h[M(\pi^p_{jk}\otimes S(\pi^p_{mn}))]=\delta_{jn}F^p_{mk}/tr(\mathbf{F}^p) \tag{67}$$

and

$$h[M(S(\pi^p_{jk})\otimes\pi^p_{mn})]=\delta_{jn}[(\mathbf{F}^p)^{-1}]_{mk}/tr[(\mathbf{F}^p)^{-1}] \tag{68}$$

(for all $j,k,m,n=1,2,\ldots,d_p$).

Of course in the special case in which $\mathscr{A}$ is the space of functions defined on a compact group $\mathscr{G}$, $\mathscr{A}$ is commutative (i.e., $M=M\circ\sigma$), $S^2=id$, h is the Haar integral,

$$h(a)=\int_{\mathscr{G}} a(x)\,dx, \tag{69}$$

and (64) expresses the invariance properties

$$\int_{\mathscr{G}} a(yx)\,dx=\int_{\mathscr{G}} a(x)\,dx=\int_{\mathscr{G}} a(xy)\,dx \tag{70}$$

(for all $y\in\mathscr{G}$). Moreover in this case each corepresentation of $\mathscr{A}$ is *identical* to its doubly contragredient partner, and (65), (67), and (68) correspond to the orthogonality theorems for the unitary irreducible representations of $\mathscr{G}$.

D. Lemmas concerning the Haar functional

It will now be shown that

$$\sum_{(b)} h[M(a\otimes b_{(1)})]S(b_{(2)})=\sum_{(a)} h[M(a_{(1)}\otimes b)]a_{(2)}, \tag{71}$$

for all $a,b\in\mathscr{A}$.

To prove this consider the operation $u\circ h\circ M$. As the left-hand equality of (64) can be re-expressed as

$$M_{\mathbb{C},\mathscr{A}}\circ(h\otimes id)\circ\Delta=u\circ h, \tag{72}$$

it follows from (10) that

$$u\circ h\circ M=M_{\mathbb{C},\mathscr{A}}\circ(h\otimes id)\circ(M\otimes M)\circ(id\otimes\sigma\otimes id)\circ(\Delta\otimes\Delta). \tag{73}$$

However, by (12), (18), and (9), it also follows that

$$u\circ h\circ M = M_{\mathbb{C},\mathscr{A}}\circ(h\otimes M)\circ(M\otimes S\otimes id)\circ(id\otimes\Delta\otimes id)\circ(id\otimes\Delta). \tag{74}$$

Comparing (73) and (74) then gives

$$\begin{aligned} &M_{\mathbb{C},\mathscr{A}}\circ(h\otimes M)\circ(M\otimes S\otimes id)\circ(id\otimes\Delta\otimes id)\circ(id\otimes\Delta)\\ &\quad = M_{\mathbb{C},\mathscr{A}}\circ(h\otimes id)\circ(M\otimes M)\circ(id\otimes\sigma\otimes id)\circ(\Delta\otimes\Delta), \end{aligned}$$

which can be re-expressed as

$$M\circ(U\otimes id)\circ(id\otimes\Delta) = M\circ(V\otimes id)\circ(id\otimes\Delta), \tag{75}$$

where

$$U = M_{\mathbb{C},\mathscr{A}}\circ(h\otimes id)\circ(M\otimes id)\circ(id\otimes\sigma)\circ(\Delta\otimes id) \tag{76}$$

and

$$V = M_{\mathbb{C},\mathscr{A}}\circ(h\otimes S)\circ(M\otimes id)\circ(id\otimes\Delta). \tag{77}$$

However, (75) implies that

$$\begin{aligned} &M\circ(M\otimes id)\circ(U\otimes id\otimes S)\circ(id\otimes\Delta\otimes id)\circ(id\otimes\Delta)\\ &\quad = M\circ(M\otimes id)\circ(V\otimes id\otimes S)\circ(id\otimes\Delta\otimes id)\circ(id\otimes\Delta). \end{aligned} \tag{78}$$

But

$$\begin{aligned} &M\circ(M\otimes id)\circ(U\otimes id\otimes S)\circ(id\otimes\Delta\otimes id)\circ(id\otimes\Delta)\\ &\quad = M\circ(U\otimes\{M\circ(id\otimes S)\circ\Delta\})\circ(id\otimes\Delta)\\ &\quad = M\circ(U\otimes\{u\circ\epsilon\})\circ(id\otimes\Delta) = U. \end{aligned}$$

As a similar result is true with U replace by V, it follows from (78) that $U=V$, which is an equivalent way of expressing (71).

It can shown by a similar argument that

$$\sum_{(b)} h[M(b_{(2)}\otimes a)]S(b_{(1)}) = \sum_{(a)} h[M(b\otimes a_{(2)})]a_{(1)}, \tag{79}$$

for all $a,b\in\mathscr{A}$.

III. THE RIGHT AND LEFT REGULAR COMODULES

The *right regular comodule* of $\mathscr{A}$ is defined to have $\mathscr{A}$ itself as its carrier space, with Δ providing the coaction $\pi^R_{\mathscr{A}}$. That is

$$V=\mathscr{A}, \quad \pi^R_{\mathscr{A}}=\Delta. \tag{80}$$

In this case the conditions (43) and (44) for $\pi^R_{\mathscr{A}}$ to be a right coaction are immediately satisfied by virtue of the assumptions (9) and (12).

The *left regular comodule* of $\mathscr{A}$ is also defined to have $\mathscr{A}$ itself as its carrier space, but has $\sigma\circ(S\otimes id)\circ\Delta$ as its coaction $\pi^L_{\mathscr{A}}$. That is

$$V=\mathscr{A}, \quad \pi^L_{\mathscr{A}}=\sigma\circ(S\otimes id)\circ\Delta. \tag{81}$$

For this case the condition (43) for $\pi^L_{\mathscr{A}}$ to be a right coaction is satisfied by the assumptions (9) and (17), while the condition (44) is again satisfied as a result of the assumption (12). It should be noted that $\pi^R_{\mathscr{A}}$ and $\pi^L_{\mathscr{A}}$ are both *right* coactions, for, as discussed in Appendix A, the designation ''left'' of $\pi^L_{\mathscr{A}}$ comes from its relation to the left regular action of a group in the special case in which the dual $\mathscr{A}'$ is a group algebra. It is also useful to note that (81) implies that

$$\Delta=(S^{-1}\otimes id)\circ\sigma\circ\pi^L_{\mathscr{A}}. \tag{82}$$

The notation of (48) can be developed further by writing

$$\pi^X_{\mathscr{A}}(a)=\sum_{[a]} a^X_{[1]}\otimes a^X_{[2]}, \tag{83}$$

for $X=R$ and $X=L$, where $a^X_{[1]}$ and $a^X_{[1]}$ are elements of $\mathscr{A}$. Then (20) and (80) imply that

$$a^R_{[1]}=a_{(1)}, \quad a^R_{[2]}=a_{(2)}, \tag{84}$$

but (20) and (81) give

$$a^L_{[1]}=a_{(2)}, \quad a^L_{[2]}=S(a_{(1)}). \tag{85}$$

The right and left regular corepresentations are both *unitary*, provided that the inner products on the carrier space $\mathscr{A}$ are chosen in the following way.

1. For the *right* regular corepresentation take

$$\langle a,b\rangle_{\mathscr{A}}=(a,b)^R=h[M(a^*\otimes b)], \quad \text{for all} \quad a,b\in\mathscr{A}; \tag{86}$$

2. for the *left* regular corepresentation take

$$\langle a,b\rangle_{\mathscr{A}}=(a,b)^L=h\{M[b\otimes(S^2(a))^*]\}, \quad \text{for all} \quad a,b\in\mathscr{A}. \tag{87}$$

In outline the proofs of these statements are as follows. For the *right* regular corepresentation, the unitary condition (51) with the choice (86) for the inner product and with (84) becomes

$$\sum_{(v)} h[M(w^*\otimes v_{(1)})]S(v_{(2)})=\sum_{(w)} h[M(w^*_{(1)}\otimes v)]w^*_{(2)},$$

which in turn reduces to (71) with the substitutions $w=a^*$ and $v=b$. Similarly, for the *left* regular corepresentation, the unitary condition (51) with the choice (87) for inner product and with (85) becomes

$$\sum_{(v)} h\{M[v_{(2)}\otimes(S^2(w))^*]\}S^2(v_{(1)})=\sum_{(w)} h\{M[v\otimes(S^2(w_{(2)}))^*]\}[S(w_{(1)})]^*.$$

With the substitutions $w=S^{-1}(a^*)$ and $v=S^{-1}(b)$, and the application of (17), (37), and (39), this reduces again to (71).

With the choices (86) and (87), both $(a,a)^R$ and $(a,a)^L$ are real and positive for all non-zero $a\in\mathscr{A}$. For $(a,a)^R$ this is an immediate consequence of (61), while for $(a,a)^L$ the demonstration requires (63), (16), (62), and (39) as well.

The inner products (86) and (87) will be used throughout this paper. In the special case in which $\mathscr{A}$ is the space of functions defined on a compact group $\mathscr{G}$, both $(a,b)^R$ and $(a,b)^L$ reduce to the usual inner product,

$$\int_{\mathscr{G}} \overline{a(x)} b(x)\, dx.$$

It is worth noting at this stage that the invariance properties (64) imply that

$$[M_{\mathbb{C},\mathscr{A}} \circ (h \otimes id) \circ \pi^R_{\mathscr{A}}](a) = [M_{\mathscr{A},\mathbb{C}} \circ (id \otimes h) \circ \pi^R_{\mathscr{A}}](a) = h(a)\, 1_{\mathscr{A}} \tag{88}$$

and

$$[M_{\mathbb{C},\mathscr{A}} \circ (h \otimes id) \circ \pi^L_{\mathscr{A}}](a) = [M_{\mathscr{A},\mathbb{C}} \circ (id \otimes h) \circ \pi^L_{\mathscr{A}}](a) = h(a)\, 1_{\mathscr{A}}, \tag{89}$$

for all $a \in \mathscr{A}$. Acting with h again in (88) and (89), and using (60), gives

$$[M_{\mathbb{C}} \circ (h \otimes h) \circ \pi^X_{\mathscr{A}}](a) = h(a), \tag{90}$$

for both $X = R$ and L and for all $a \in \mathscr{A}$. In terms of the notation of (83), this can be re-expressed as

$$h(a) = \sum_{[a]} h(a^X_{[1]}) h(a^X_{[2]}), \tag{91}$$

for $X = R$ and L and for all $a \in \mathscr{A}$.

The effects of the right and left regular coactions on products are quite different. For the right regular coaction, (80) and (10) imply immediately that

$$\pi^R_{\mathscr{A}} \circ M = (M \otimes M) \circ (id \otimes \sigma \otimes id) \circ (\pi^R_{\mathscr{A}} \otimes \pi^R_{\mathscr{A}}), \tag{92}$$

whereas for the left regular coaction, (81), (10), and (16) show that

$$\pi^L_{\mathscr{A}} \circ M = (M \otimes M) \circ (id \otimes id \otimes \sigma) \circ (id \otimes \sigma \otimes id) \circ (\pi^L_{\mathscr{A}} \otimes \pi^L_{\mathscr{A}}), \tag{93}$$

which contains an extra twist factor σ.

IV. BASIS FUNCTIONS

A. Definitions and properties

Suppose that π^p_{jk} are the matrix coefficients of a corepresentation π^p of $\mathscr{A}$ of finite dimension d_p. Then the *basis functions* ψ^{pR}_j *of* π^p *with respect to the right regular coaction* may be defined to be a set of d_p elements of $\mathscr{A}$ that have the property that

$$\pi^R_{\mathscr{A}}(\psi^{pR}_j) = \sum_{k=1}^{d_p} \psi^{pR}_k \otimes \pi^p_{kj}, \tag{94}$$

for all $j = 1,2,\ldots,d_p$. Similarly the *basis functions* ψ^{pL}_j *of* π^p *with respect to the left regular coaction* may be defined as a set of d_p elements of $\mathscr{A}$ that have the property that

$$\pi^L_{\mathscr{A}}(\psi^{pL}_j) = \sum_{k=1}^{d_p} \psi^{pL}_k \otimes \pi^p_{kj}, \tag{95}$$

for all $j = 1,2,\ldots,d_p$.

In the right regular coaction case, an example of a set of basis functions is provided (for any fixed choice of $\ell = 1,2,\ldots$) by

$$\psi_j^{pR} = \pi^p_{\ell j}, \tag{96}$$

for all $j = 1,2,\ldots,d_p$. Likewise, in the left regular coaction case, an example is provided (for any fixed choice of $\ell = 1,2,\ldots$) by

$$\psi_j^{pL} = S^{-2}(\pi^{p*}_{j\ell}), \tag{97}$$

for all $j = 1,2,\ldots,d_p$ (provided that the corepresentation π^p is unitary).

One very useful result, which comes from applying (95), (82), (17), (37), and (39), is that

$$\pi^L_{\mathscr{A}}[(S^2(\psi_k^{qL}))^*] = \sum_{t=1}^{d_p} [S^2(\psi_t^{qL})]^* \otimes \pi^{q*}_{tk}, \tag{98}$$

for all $k = 1,2,\ldots,d_p$.

In spite of the fact that the inner products (86) and (87) for the right and left regular coactions are different, in both the cases the basis functions possess the *same* orthogonality properties, which are as follows: If ψ_k^{qX} and ϕ_j^{pX} are basis functions of the unitary irreducible corepresentations π^q and π^p of $\mathscr{A}$, then

$$(\psi_k^{qX}, \phi_j^{pX})^X = 0, \quad \text{unless} \quad p = q \quad \text{and} \quad j = k, \tag{99}$$

and

$$(\psi_j^{pX}, \phi_j^{pX})^X \text{ is independent of } j, \quad \text{for} \quad j = 1,2,\ldots,d_p. \tag{100}$$

Here X denotes both R and L, and in (100) ψ_j^{pX} and ϕ_j^{pX} need not be identical sets. Indeed, with $X = R$, if the functions ψ_j^{pR} and ϕ_j^{pR} are defined by

$$\psi_j^{pR} = \pi^p_{sj}, \quad \phi_j^{pR} = \pi^p_{tj}, \tag{101}$$

and with $X = L$, if the functions ψ_j^{pL} and ϕ_j^{pL} are similarly defined by

$$\psi_j^{pL} = S^{-2}(\pi^{p*}_{js}), \quad \phi_j^{pL} = S^{-2}(\pi^{p*}_{jt}), \tag{102}$$

then in *both* cases

$$(\psi_j^{pX}, \phi_j^{pX})^X = [(\mathbf{F}^p)^{-1}]_{ts} / tr[(\mathbf{F}^p)^{-1}], \tag{103}$$

for $j = 1,2,\ldots,d_p$.

The proofs of (99), (100), and (103) will now be outlined. Applying (92) and (88) to $M(\psi_k^{qR*} \otimes \phi_j^{pR})$ gives

$$h[M(\psi_k^{qR*} \otimes \phi_j^{pR})]1_{\mathscr{A}} = \sum_{s,t} h[M(\psi_t^{qR*} \otimes \phi_s^{pR})]M(\pi^{q*}_{tk} \otimes \pi^p_{sj}).$$

A further application of h to both sides gives

$$(\psi_k^{qX}, \phi_j^{pX})^X = \sum_{s,t} (\psi_t^{qX}, \phi_s^{pX})^X h[M(\pi^{q*}_{tk} \otimes \pi^p_{sj})], \tag{104}$$

with $X = R$, where (86) and (60) have been invoked. Similarly, applying (93) and (98) to $M[\phi_j^{pL} \otimes (S^2(\psi_k^{qL}))^*]$, and then applying (89) to the result gives

$$h\{M[\phi_j^{pL}\otimes(S^2(\psi_k^{qL}))^*]\}1_{\mathscr{A}}=\sum_{s,t} h\{M[\phi_s^{pL}\otimes(S^2(\psi_t^{qL}))^*]\}M(\pi_{tk}^{q*}\otimes\pi_{sj}^{p}).$$

A further application of h to both sides gives (104) with $X=L$, where this time (87) and (60) have been used. Thus, in both cases, it follows from (104), (52), (65), and (68) that

$$(\psi_k^{qX},\phi_j^{pX})^X=\sum_{s,t}\frac{(\psi_t^{qX},\phi_s^{pX})^X\delta^{qp}\delta_{kj}[(\mathbf{F}^p)^{-1}]_{st}}{tr[(\mathbf{F}^p)^{-1}]}. \tag{105}$$

This implies that (99) is true, and if $j=k$ and $p=q$, then (105) and (99) together give

$$(\psi_j^{pX},\phi_j^{pX})^X=\sum_{s}\frac{(\psi_s^{pX},\phi_s^{pX})^X[(\mathbf{F}^p)^{-1}]_{ss}}{tr[(\mathbf{F}^p)^{-1}]}. \tag{106}$$

As the right-hand side of (106) is independent of j, so too must be the left-hand side, which thereby establishes (100). Finally the combination of (86) and (101) and the combination of (87) and (102) both produce the result

$$(\psi_j^{pX},\phi_j^{pX})^X=h\{M[S(\pi_{js}^{p})\otimes\pi_{tj}^{p}]\},$$

for $X=R$ and for $X=L$, which gives (103) when (68) is used.

B. Projection operators

The argument in Appendix C suggests the following definition. Let π^p be a unitary irreducible corepresentation of $\mathscr{A}$ of dimension d_p with matrix coefficients π_{mn}^{p}. Then the projection operators $\mathscr{P}_{mn}^{pR}$ and $\mathscr{P}_{mn}^{pL}$ are defined by

$$\mathscr{P}_{mn}^{pX}(a)=d_p\sum_{[a]} a_{[1]}^X h[M(\pi_{mn}^{p*}\otimes a_{[2]}^X], \tag{107}$$

for $X=R$ and $X=L$, for all $m,n=1,2,\ldots,d_p$, and all $a\in\mathscr{A}$.

These projection operators have the following two useful properties: Let π^p and π^q be two unitary irreducible corepresentations of $\mathscr{A}$ of dimensions d_p and d_q with matrix coefficients π_{mn}^{p} and π_{jk}^{q}

1. Then

$$\mathscr{P}_{mn}^{pX}\mathscr{P}_{jk}^{qX}=d_p\delta^{pq}\{[(\mathbf{F}^p)^{-1}]_{nj}/tr[(\mathbf{F}^p)^{-1}]\}\mathscr{P}_{mk}^{pX}, \tag{108}$$

for $X=R$ and $X=L$, for all $m,n=1,2,\ldots,d_p$, and for all $j,k=1,2,\ldots,d_q$.

2. Also, if ψ_k^{qX} are basis functions for π^q, then

$$\mathscr{P}_{mn}^{pX}(\psi_k^{qX})=d_p\delta^{pq}\delta_{nk}\sum_{\ell=1}^{d_p}\frac{\psi_\ell^{qX}[(\mathbf{F}^p)^{-1}]_{\ell m}}{tr[(\mathbf{F}^p)^{-1}]}, \tag{109}$$

for $X=R$ and $X=L$, for all $m,n=1,2,\ldots,d_p$, and for all $k=1,2,\ldots,d_q$.

The proof of (108) is as follows. For any $f\in\mathscr{A}$, (107) and (9) imply that

$$\mathscr{P}_{mn}^{pX}[\mathscr{P}_{jk}^{qX}(f)]=d_pd_q\sum_{[f]} f_{[1]}^X h[M(\pi_{jk}^{q*}\otimes(f_{[2]}^X)_{(1)})]h[M(\pi_{mn}^{p*}\otimes(f_{[2]}^X)_{(2)})].$$

On applying (79) with $a=f_{[2]}^X$ and $b=\pi_{jk}^{q*}$ this reduces to

$$\mathscr{P}^{pX}_{mn}[\mathscr{P}^{qX}_{jk}(f)]=d_p d_q \sum_{[f]} \sum_{\ell=1}^{d_q} f^X_{[1]} h[M(\pi^{q*}_{\ell k}\otimes f^X_{[2]})]h[M(\pi^{p*}_{mn}\otimes S(\pi^{q*}_{j\ell}))],$$

so

$$\mathscr{P}^{pX}_{mn}[\mathscr{P}^{qX}_{jk}(f)]=d_p \sum_{\ell=1}^{d_q} \mathscr{P}^{qX}_{\ell k}(f)h[M(\pi^{p*}_{mn}\otimes S(\pi^{q*}_{j\ell}))],$$

which, by (52), (16), and (68) gives (108).

To prove (109) it suffices to note that (107), (94), and (87) imply that

$$\mathscr{P}^{pX}_{mn}(\psi^{qX}_k)=d_p \sum_{\ell=1}^{d_p} \psi^{qX}_\ell h[M(\pi^{p*}_{mn}\otimes \pi^{q}_{\ell k})],$$

which, by (68), leads immediately to (108).

V. TENSOR PRODUCTS AND CLEBSCH–GORDAN COEFFICIENTS

A. Ordinary and twisted tensor products

The *tensor product* of two corepresentations π_V and π_W of $\mathscr{A}$ (with carrier spaces V and W, respectively) is the mapping $\pi_V \boxtimes \pi_W$ from $V\otimes W$ to $V\otimes W\otimes \mathscr{A}$ that is defined by

$$(\pi_V\boxtimes\pi_W)(v\otimes w)=[(id\otimes id\otimes M)\circ(id\otimes\sigma\otimes id)\circ(\pi_V\otimes\pi_W)](v\otimes w), \tag{110}$$

for all $v\in V$ and all $w\in W$. It is easily checked that the conditions (43) and (44) are satisfied with π_V replaced by $\pi_V\boxtimes\pi_W$ and V replaced by $V\otimes W$, so $\pi_V\boxtimes\pi_W$ is indeed a coaction of $\mathscr{A}$ with carrier space $V\otimes W$. If V and W are of finite dimensions d_V and d_W, with bases $v_1,v_2,\ldots,v_{d_V}$, and $w_1,w_2,\ldots,w_{d_W}$, then (45) and (110) give

$$(\pi_V\boxtimes\pi_W)(v_j\otimes w_k)=\sum_{s=1}^{d_V}\sum_{t=1}^{d_W}(v_s\otimes w_t)\otimes[M(\pi^V_{sj}\otimes\pi^W_{tk})], \tag{111}$$

which implies that the matrix coefficients of $\pi_V\boxtimes\pi_W$ are given by

$$(\pi_V\boxtimes\pi_W)_{st,jk}=M(\pi^V_{sj}\otimes\pi^W_{tk}). \tag{112}$$

Henceforth it will always be assumed that in tensor product matrices such as $\pi_V\boxtimes\pi_W$ the pair of indices that specify the columns have the ordering:

$$(j,k)=(1,1),(1,2),\ldots,(1,d_W),(2,1),(2,2),\ldots, \tag{113}$$

and that the same ordering applies to the rows.

There exists a second tensor product of π_V and π_W that has the same carrier space $V\otimes W$. This will be called the *twisted tensor product*, and is defined as the mapping $\pi_V\widetilde{\boxtimes}\pi_W$ from $V\otimes W$ to $V\otimes W\otimes\mathscr{A}$ that is given by

$$(\pi_V\widetilde{\boxtimes}\pi_W)(v\otimes w)=[(id\otimes id\otimes M)\circ(id\otimes id\otimes\sigma)\circ(id\otimes\sigma\otimes id)\circ(\pi_V\otimes\pi_W)](v\otimes w), \tag{114}$$

for all $v\in V$ and all $w\in W$. It is again easily checked that the conditions (43) and (44) are satisfied with π_V replaced by $\pi_V\widetilde{\boxtimes}\pi_W$ and V replaced by $V\otimes W$, so $\pi_V\widetilde{\boxtimes}\pi_W$ is also a coaction of $\mathscr{A}$ with carrier space $V\otimes W$. Then (45) and (114) give

$$(\pi_V \widetilde{\boxtimes} \pi_W)(v_j \otimes w_k) = \sum_{s=1}^{d_V} \sum_{t=1}^{d_W} (v_s \otimes w_t) \otimes [M(\pi_{tk}^W \otimes \pi_{sj}^V)], \tag{115}$$

which implies that the matrix coefficients of $\pi_V \widetilde{\boxtimes} \pi_W$ are given by

$$(\pi_V \widetilde{\boxtimes} \pi_W)_{st,jk} = M(\pi_{tk}^W \otimes \pi_{sj}^V). \tag{116}$$

The tensor product $\pi_W \boxtimes \pi_V$, whose carrier space is $\pi_W \otimes \pi_V$, has matrix coefficients that are given [according to (112)] by

$$(\pi_W \boxtimes \pi_V)_{ts,kj} = M(\pi_{tk}^W \otimes \pi_{sj}^V). \tag{117}$$

As the matrix coefficients of (116) and (117) differ only in their ordering of the pairs of indices that label their rows (and, in the corresponding manner, their columns), it follows that $\pi_V \widetilde{\boxtimes} \pi_W$ and $\pi_W \boxtimes \pi_V$ are *equivalent* corepresentations. If $\mathscr{A}$ is *coquasitriangular* [that is, if $\mathscr{A}'$ is quasitriangular (cf. Drinfel'd[30])], then $\pi_V \boxtimes \pi_W$ and $\pi_W \boxtimes \pi_V$ are equivalent, so in this case $\pi_V \boxtimes \pi_W$ and $\pi_V \widetilde{\boxtimes} \pi_W$ are equivalent. (Of course, in the special case in which $\mathscr{A}$ is *commutative*, the corepresentations $\pi_V \widetilde{\boxtimes} \pi_W$ and $\pi_V \widetilde{\boxtimes} \pi_W$ are *identical*.)

Applying these considerations to the special case in which $\pi_V = \pi^p$ and $\pi_W = \pi^q$ are two irreducible unitary corepresentations of $\mathscr{A}$, (112) and (116) become

$$(\pi^p \boxtimes \pi^q)_{st,jk} = M(\pi_{sj}^p \otimes \pi_{tk}^q) \tag{118}$$

and

$$(\pi^p \widetilde{\boxtimes} \pi^q)_{st,jk} = M(\pi_{tk}^q \otimes \pi_{sj}^p), \tag{119}$$

respectively.

B. Characters

The *character* of a corepresentation π_V of $\mathscr{A}$ of dimension d_V is defined in terms of its matrix coefficients by

$$\chi^V = \sum_{j=1}^{d_V} \pi_{jj}^V, \tag{120}$$

so χ^V is also an element of $\mathscr{A}$. Clearly equivalent corepresentations have identical characters.

If π^p and π^q are two irreducible unitary corepresentations of $\mathscr{A}$ (assumed to be inequivalent if $p \neq q$) and if χ^p and χ^q are their corresponding characters, then (67) and (68) imply that

$$h[M(\chi^{p*} \otimes \chi^q)] = h[M(\chi^q \otimes \chi^{p*})] = \delta^{pq}. \tag{121}$$

If π_V is a (completely) reducible corepresentation of $\mathscr{A}$ that is equivalent to the direct sum $\Sigma \oplus n^p \pi^p$, then the number of times n^p that the irreducible corepresentation π^p (or a corepresentation equivalent to π^p) appears in the reduction of π_V is given by

$$\chi^V = \sum_p n^p \chi^p, \tag{122}$$

so, by (121),

$$n^p = h[M(\chi^V \otimes \chi^{p*})] = h[M(\chi^{p*} \otimes \chi^V)]. \tag{123}$$

For the tensor product $\pi^p \boxtimes \pi^q$ of two irreducible unitary corepresentations π^p and π^q the character is just $\chi^p \chi^q [= M(\chi^p \otimes \chi^q)]$, so the number of times n_{pq}^r that the irreducible corepresentation π^r (or a corepresentation equivalent to π^r) appears in the reduction of $\pi^p \boxtimes \pi^q$ is given by

$$n_{pq}^r = h(\chi^p \chi^q \chi^{r*}) = h(\chi^{r*} \chi^p \chi^q). \tag{124}$$

If $\overline{\pi^p}$ is the irreducible unitary corepresentation that is *conjugate* to π^p, then (59) and (62) show that

$$n_{pq}^r = n_{\overline{p}r}^q, \quad n_{r\overline{p}}^q = n_{qp}^r, \tag{125}$$

where $n_{\overline{p}r}^q$ is the number of times that π^q (or its equivalent) appears in the reduction of $\overline{\pi^p} \boxtimes \pi^r$, and $n_{r\overline{p}}^q$ is the number of times that π^q (or its equivalent) appears in the reduction of $\pi^r \boxtimes \overline{\pi^p}$.

C. Clebsch–Gordan coefficients

As above, suppose that the tensor product $\pi^p \boxtimes \pi^q$ of two irreducible unitary corepresentations π^p and π^q is reducible, and that n_{pq}^r is the number of times that the irreducible corepresentation π^r (or a corepresentation equivalent to it) appears in the reduction of $\pi^p \boxtimes \pi^q$. If π^p has carrier space V^p with basis elements $v_1^p, v_1^p, \ldots, v_{d_p}^p$ and π^q has carrier space V^q with basis elements $v_1^q, v_1^q, \ldots, v_{d_q}^q$, then the set of elements $v_j^p \otimes v_k^q$ form a basis for $V^p \otimes V^q$, the carrier space of $\pi^p \boxtimes \pi^q$, and consequently appropriate linear combinations form bases for all the irreducible corepresentations π^r that appear in the reduction of the tensor product. Let $w_{\ell}^{r,\alpha}$ be such a combination, so that

$$w_{\ell}^{r,\alpha} = \sum_{j=1}^{d_p} \sum_{k=1}^{d_q} \left(\begin{matrix} p & q \\ j & k \end{matrix} \middle| \begin{matrix} r & , & \alpha \\ \ell & & \end{matrix} \right) v_j^p \otimes v_k^q, \tag{126}$$

for $\ell = 1,2,\ldots,d_r$, and $\alpha = 1,2,\ldots,n_{pq}^r$, and

$$(\pi^p \boxtimes \pi^q)(w_{\ell}^{r,\alpha}) = \sum_{u=1}^{d_r} w_u^{r,\alpha} \otimes \pi_{ul}^r, \tag{127}$$

for $u = 1,2,\ldots,d_r$, and $\alpha = 1,2,\ldots,n_{pq}^r$. The inverse of (126) is

$$v_j^p \otimes v_k^q = \sum_r \sum_{\alpha=1}^{n_{pq}^r} \sum_{\ell=1}^{d_r} \left(\begin{matrix} r & , & \alpha \\ \ell & & \end{matrix} \middle| \begin{matrix} p & q \\ j & k \end{matrix} \right) w_{\ell}^{r,\alpha}, \tag{128}$$

for $j = 1,2,\ldots,d_p$ and $k = 1,2,\ldots,d_q$. The *Clebsch–Gordan coefficients* defined in (126) form the elements of a $d_p \times d_q$ matrix $\mathbf{C}$, while the inverse coefficients defined in (128) form the elements of $\mathbf{C}^{-1}$, where

$$\mathbf{C}^{-1}(\pi^p \boxtimes \pi^q)\mathbf{C} = \sum_r \oplus n_{pq}^r \pi^r. \tag{129}$$

That is,

$$\sum_{j=1}^{d_p}\sum_{t=1}^{d_q}(\pi^p\boxtimes\pi^q)_{is,jt}\left(\begin{matrix}p & q\\ j & t\end{matrix}\middle|\begin{matrix}r & , & \alpha\\ \ell & & \end{matrix}\right)=\sum_{u=1}^{d_r}\left(\begin{matrix}p & q\\ i & s\end{matrix}\middle|\begin{matrix}r & , & \alpha\\ u & & \end{matrix}\right)\pi^r_{u\ell}, \tag{130}$$

for $i=1,2,\ldots,d_p$, $s=1,2,\ldots,d_q$, $\ell=1,2,\ldots,d_r$, and $\alpha=1,2,\ldots,n^r_{pq}$.

D. Products of basis functions and Clebsch–Gordan coefficients

Consider first the *right* regular corepresentation. If ϕ^{pR}_j and ψ^{qR}_k are basis functions of the unitary irreducible corepresentations π^p and π^q of $\mathscr{A}$, then (92) and (118) imply that

$$\pi^R_{\mathscr{A}}[M(\phi^{pR}_j\otimes\psi^{qR}_k)]=\sum_{s=1}^{d_p}\sum_{t=1}^{d_q}M(\phi^{pR}_s\otimes\psi^{qR}_t)\otimes(\pi^p\boxtimes\pi^q)_{st,jk}, \tag{131}$$

so that if the set of products $M(\phi^{pR}_j\otimes\psi^{qR}_k)$ (for $j=1,2,\ldots,d_p$, and $k=1,2,\ldots,d_q$) form a linearly independent set, then they form a basis for the tensor product corepresentation $\pi^p\boxtimes\pi^q$. Thus, by (126) and (127), there exists a set of elements $\theta^{r,\alpha R}_\ell$, all members of $\mathscr{A}$, that are defined by

$$\theta^{r,\alpha R}_\ell=\sum_{j=1}^{d_p}\sum_{k=1}^{d_q}\left(\begin{matrix}p & q\\ j & k\end{matrix}\middle|\begin{matrix}r & , & \alpha\\ \ell & & \end{matrix}\right)M(\phi^{pR}_j\otimes\psi^{qR}_k), \tag{132}$$

for $\ell=1,2,\ldots,d_r$, and $\alpha=1,2,\ldots,n^r_{pq}$, and which have the property that

$$\pi^R_{\mathscr{A}}(\theta^{r,\alpha R}_\ell)=\sum_{u=1}^{d_r}\theta^{r,\alpha R}_u\otimes\pi^r_{ul}, \tag{133}$$

for $u=1,2,\ldots,d_r$, and $\alpha=1,2,\ldots,n^r_{pq}$. By (128), the inverse of (132) is then

$$M(\phi^{pR}_j\otimes\psi^{qR}_k)=\sum_r\sum_{\alpha=1}^{n^r_{pq}}\sum_{\ell=1}^{d_r}\left(\begin{matrix}r & , & \alpha\\ \ell & & \end{matrix}\middle|\begin{matrix}p & q\\ j & k\end{matrix}\right)\theta^{r,\alpha R}_\ell, \tag{134}$$

for $j=1,2,\ldots,d_p$ and $k=1,2,\ldots,d_q$. On applying the projection operator $\mathscr{P}^{rR}_{ul}$ of (107) to $M(\phi^{pR}_j\otimes\psi^{qR}_k)$, and using (109), (134), and (132), it follows that

$$\begin{aligned}&\mathscr{P}^{rR}_{ul}[M(\phi^{pR}_j\otimes\psi^{qR}_k)]\\ &\quad=\sum_{\alpha=1}^{n^r_{pq}}\sum_{v=1}^{d_r}\sum_{s=1}^{d_p}\sum_{t=1}^{d_q}\left(\begin{matrix}r & , & \alpha\\ \ell & & \end{matrix}\middle|\begin{matrix}p & q\\ j & k\end{matrix}\right)\left(\begin{matrix}p & q\\ s & t\end{matrix}\middle|\begin{matrix}r & , & \alpha\\ v & & \end{matrix}\right)\\ &\qquad\times d_r\{((\mathbf{F}^r)^{-1})_{vu}/tr[(\mathbf{F}^r)^{-1}]\}M(\phi^{pR}_s\otimes\psi^{qR}_t),\end{aligned} \tag{135}$$

for $j=1,2,\ldots,d_p$ and $k=1,2,\ldots,d_q$. However, the definition (107) taken in conjunction with (131) and (118) gives

$$\mathscr{P}^{rR}_{ul}[M(\phi^{pR}_j\otimes\psi^{qR}_k)]=d_r\sum_{s=1}^{d_p}\sum_{t=1}^{d_q}M(\phi^{pR}_s\otimes\psi^{qR}_t)h(\pi^r_{ul}{}^*\pi^p_{sj}\pi^q_{tk}), \tag{136}$$

so equating coefficients of $M(\phi^{pR}_s\otimes\psi^{qR}_t)$ in (135) and (136) yields

$$h(\pi^r_{ul}{}^{*}\pi^p_{sj}\pi^q_{tk}) = \sum_{\alpha=1}^{n^r_{pq}}\sum_{v=1}^{d_r}\begin{pmatrix} r & , & \alpha \\ \ell & & \end{vmatrix} \begin{matrix} p & q \\ j & k \end{vmatrix} \begin{matrix} p & q \\ s & t \end{vmatrix} \begin{matrix} r & , & \alpha \\ v & & \end{pmatrix} \times\{[(\mathbf{F}^r)^{-1}]_{vu}/tr[(\mathbf{F}^r)^{-1}]\} \tag{137}$$

for all $j=1,2,\ldots,d_p$, $k=1,2,\ldots,d_q$, and $l=1,2,\ldots,d_r$. Of course, this implies that

$$h(\pi^r_{ul}{}^{*}\pi^q_{tk}\pi^p_{sj}) = \sum_{\alpha=1}^{n^r_{qp}}\sum_{v=1}^{d_r}\begin{pmatrix} r & , & \alpha \\ \ell & & \end{vmatrix} \begin{matrix} q & p \\ k & j \end{vmatrix} \begin{matrix} q & p \\ t & s \end{vmatrix} \begin{matrix} r & , & \alpha \\ v & & \end{pmatrix} \times\{[(\mathbf{F}^r)^{-1}]_{vu}/tr[(\mathbf{F}^r)^{-1}]\}, \tag{138}$$

for all $j=1,2,\ldots,d_p$, $k=1,2,\ldots,d_q$, and $l=1,2,\ldots,d_r$.

Although the conclusions (137) and (138) also follow from consideration of the *left* regular coaction, some of the intermediate results are significantly different in this case. Firstly (93) implies that

$$\pi^L_{\mathscr{A}}[M(\phi^{pL}_j\otimes\psi^{qL}_k)]=\sum_{s=1}^{d_p}\sum_{t=1}^{d_q} M(\phi^{pL}_s\otimes\psi^{qL}_t)\otimes M(\pi^q_{tk}\otimes\pi^p_{sj}), \tag{139}$$

so, by (119),

$$\pi^L_{\mathscr{A}}[M(\phi^{pL}_j\otimes\psi^{qL}_k)]=\sum_{s=1}^{d_p}\sum_{t=1}^{d_q} M(\phi^{pL}_s\otimes\psi^{qL}_t)\otimes(\pi^p\widetilde{\boxtimes}\pi^q)_{st,jk}, \tag{140}$$

so that if the set of products $M(\phi^{pL}_j\otimes\psi^{qL}_k)$ (for $j=1,2,\ldots,d_p$, and $k=1,2,\ldots,d_q$) form a linearly independent set, then they form a basis for the *twisted* tensor product corepresentation $\pi^p\widetilde{\boxtimes}\pi^q$. However, on writing $\Phi^{qp}_{kj}=M(\phi^{pL}_j\otimes\psi^{qL}_k)$, (140) can be re-expressed as

$$\pi^L_{\mathscr{A}}(\Phi^{qp}_{kj})=\sum_{s=1}^{d_p}\sum_{t=1}^{d_q}\Phi^{qp}_{ts}\otimes(\pi^q\boxtimes\pi^p)_{ts,kj}. \tag{141}$$

That is, the set Φ^{qp}_{kj} (for $k=1,2,\ldots,d_q$ and $j=1,2,\ldots,d_p$) form a basis for the *ordinary* tensor product corepresentation $\pi^q\boxtimes\pi^p$. Consequently, there exists a set of elements $\theta^{r,\alpha L}_{\ell}$, all members of $\mathscr{A}$, that are defined by

$$\theta^{r,\alpha L}_{\ell}=\sum_{j=1}^{d_p}\sum_{k=1}^{d_q}\begin{pmatrix} q & p \\ k & j \end{vmatrix} \begin{matrix} r & , & \alpha \\ \ell & & \end{pmatrix}\Phi^{qp}_{kj}, \tag{142}$$

for $\ell=1,2,\ldots,d_r$, and $\alpha=1,2,\ldots,n^r_{qp}$, and which have the property that

$$\pi^R_{\mathscr{A}}(\theta^{r,\alpha L}_{\ell})=\sum_{u=1}^{d_r}\theta^{r,\alpha L}_u\otimes\pi^r_{ul}, \tag{143}$$

for $u=1,2,\ldots,d_r$, and $\alpha=1,2,\ldots,n^r_{qp}$. Thus

$$\theta^{r,\alpha L}_{\ell}=\sum_{j=1}^{d_p}\sum_{k=1}^{d_q}\begin{pmatrix} q & p \\ k & j \end{vmatrix} \begin{matrix} r & , & \alpha \\ \ell & & \end{pmatrix} M(\phi^{pL}_j\otimes\psi^{qL}_k), \tag{144}$$

whose inverse is

$$M(\phi_j^{pL}\otimes\psi_k^{qL})=\sum_r\sum_{\alpha=1}^{n_{qp}^r}\sum_{\ell=1}^{d_r}\left(\begin{matrix} r & , & \alpha \\ \ell & & \end{matrix}\middle|\begin{matrix} q & p \\ k & j \end{matrix}\right)\theta_\ell^{r,\alpha L}, \tag{145}$$

for $j=1,2,\ldots,d_p$ and $k=1,2,\ldots,d_q$. Applying the projection operator $\mathscr{P}_{ul}^{rL}$ of (107) to $M(\phi_j^{pL}\otimes\psi_k^{qL})$, and using (109), (145), and (144), it follows that

$$\begin{aligned}&\mathscr{P}_{ul}^{rL}[M(\phi_j^{pL}\otimes\psi_k^{qL})]\\&\quad=\sum_{\alpha=1}^{n_{qp}^r}\sum_{v=1}^{d_r}\sum_{s=1}^{d_p}\sum_{t=1}^{d_q}\left(\begin{matrix} r & , & \alpha \\ \ell & & \end{matrix}\middle|\begin{matrix} q & p \\ k & j \end{matrix}\right)\left(\begin{matrix} q & p \\ t & s \end{matrix}\middle|\begin{matrix} r & , & \alpha \\ v & & \end{matrix}\right)\\&\qquad\times d_r\{[(\mathbf{F}^r)^{-1}]_{vu}/tr[(\mathbf{F}^r)^{-1}]\}M(\phi_s^{pL}\otimes\psi_t^{qL}),\end{aligned} \tag{146}$$

for $j=1,2,\ldots,d_p$ and $k=1,2,\ldots,d_q$. However, the definition (107) taken in conjunction with (139) gives

$$\mathscr{P}_{ul}^{rL}[M(\phi_j^{pL}\otimes\psi_k^{qL})]=d_r\sum_{s=1}^{d_p}\sum_{t=1}^{d_q}M(\phi_s^{pL}\otimes\psi_t^{qL})h(\pi_{ul}^{r*}\pi_{tk}^q\pi_{sj}^p), \tag{147}$$

so equating coefficients of $M(\phi_s^{pL}\otimes\psi_t^{qL})$ in (146) and (147) yields (138) again.

It is also possible to obtain (137) [and hence (138)] *without* making any linear independence assumptions about the set of products $M(\phi_j^{pR}\otimes\psi_k^{qR})$, for by (111), (126), (127), and (128),

$$\begin{aligned}&\sum_r\sum_{\alpha=1}^{n_{pq}^r}\sum_{s=1}^{d_p}\sum_{t=1}^{d_q}\sum_{v,w=1}^{d_r}\left(\begin{matrix} r & , & \alpha \\ w & & \end{matrix}\middle|\begin{matrix} p & q \\ j & k \end{matrix}\right)\left(\begin{matrix} p & q \\ s & t \end{matrix}\middle|\begin{matrix} r & , & \alpha \\ v & & \end{matrix}\right)v_s^p\otimes v_t^q\otimes\pi_{vw}^r\\&\quad=\sum_{s=1}^{d_p}\sum_{t=1}^{d_q}v_s^p\otimes v_t^q\otimes M(\pi_{sj}^p\otimes\pi_{tk}^q),\end{aligned}$$

for all $j=1,2,\ldots,d_p$, and $k=1,2,\ldots,d_q$. As the set $v_s^p\otimes v_t^q$ (for $s=1,2,\ldots,d_p$, and $t=1,2,\ldots,d_q$) is certainly linearly independent, it follows that

$$\sum_r\sum_{\alpha=1}^{n_{pq}^r}\sum_{v,w=1}^{d_r}\left(\begin{matrix} r & , & \alpha \\ w & & \end{matrix}\middle|\begin{matrix} p & q \\ j & k \end{matrix}\right)\left(\begin{matrix} p & q \\ s & t \end{matrix}\middle|\begin{matrix} r & , & \alpha \\ v & & \end{matrix}\right)\pi_{vw}^r=M(\pi_{sj}^p\otimes\pi_{tk}^q)$$

(for $j,s=1,2,\ldots,d_p$, and $k,t=1,2,\ldots,d_q$). On replacing r by r' in the sums of on the left-hand side, multiplying through by $\pi_{u\ell}^{r*}$ from the left, applying the Haar functional h, and using (65) and (68), one regains (137).

VI. THE IRREDUCIBLE TENSOR OPERATORS

A. Introduction

Let π^q be a unitary irreducible right coaction of $\mathscr{A}$ of dimension d_q with matrix coefficients π_{jk}^q It will be shown that within both the right and the left regular corepresentation formalisms there exist two types of irreducible tensor operators that both belong to this corepresentation π^q. These will be denoted by Q_j^{qX} and $\widetilde{Q}_j^{qX}$ (for $j=1,2,\ldots,d_q$ and for $X=R$ or L), and will be called *ordinary* and *twisted* irreducible tensor operators, respectively. Naturally the two types of irreducible tensor operators coincide in the special case in which $\mathscr{A}$ is commutative. Moreover, it should be noted that if $\mathscr{A}^{op}$ is the Hopf algebra in which the multiplication operator M and antipode S of $\mathscr{A}$ are replaced by $M\circ\sigma$ and S^{-1}, respectively, then the ''twisted'' irreducible

tensor operators for $\mathscr{A}$ are the ''ordinary'' irreducible tensor operators for $\mathscr{A}^{op}$ and the ''ordinary'' irreducible tensor operators for $\mathscr{A}$ are the ''twisted'' irreducible tensor operators for $\mathscr{A}^{op}$.

B. Definitions in the right regular corepresentation formalism

1. Definition of the ordinary irreducible tensor operators Q_j^{qR}

The *ordinary irreducible tensor operators* Q_j^{qR} belonging to the unitary irreducible right coaction π^q of $\mathscr{A}$ are *defined* to be members of $\mathscr{L}(\mathscr{A})$ that satisfy the condition

$$((id\otimes M)\circ(\Delta\otimes id)\circ(Q_j^{qR}\otimes S)\circ\Delta)(a)=\sum_{k=1}^{d_q} Q_k^{qR}(a)\otimes\pi_{kj}^q, \tag{148}$$

for all $a\in\mathscr{A}$ and all $j=1,2,\ldots,d_q$. Hereafter $\mathscr{L}(\mathscr{A})$ denotes the set of linear operators that map $\mathscr{A}$ into $\mathscr{A}$.

Clearly this definition involves *only* quantities defined on $\mathscr{A}$, for the right-hand side is a member of $\mathscr{A}\otimes\mathscr{A}$. By virtues of (80) this definition can be written equivalently in terms of the right regular coaction $\pi_{\mathscr{A}}^R$ as

$$[(id\otimes M)\circ(\pi_{\mathscr{A}}^R\otimes id)\circ(Q_j^{qR}\otimes S)\circ\pi_{\mathscr{A}}^R](a)=\sum_{k=1}^{d_q} Q_k^{qR}(a)\otimes\pi_{kj}^q, \tag{149}$$

for all $a\in\mathscr{A}$ and all $j=1,2,\ldots,d_q$. [The motivation behind the definition (148) is explained in Appendix B 2 a].

It will now be shown that (148) provides a *consistent* definition, in that it can be re-expressed by saying that the operators Q_j^{qR} (for $j=1,2,\ldots,d_q$) form the basis of a carrier space for a certain right coaction of $\mathscr{A}$. The motivation for this definition is given in Appendix B 2 b, where the special case in which $\mathscr{A}$ is finite-dimensional is considered in detail, but for the general case it is necessary to apply additional conditions to the domain of this coaction. The analysis of Appendix B 2 b implies that if $\mathscr{A}$ is *finite*-dimensional then, for *every* operator $Q\in\mathscr{L}(\mathscr{A})$, there exist operators $Q_i\in\mathscr{L}(\mathscr{A})$ and elements q_i, both indexed by the same *finite* index set I, such that

$$\sum_{i\in I} Q_i(a)\otimes q_i=[(id\otimes M)\circ(\Delta\otimes id)\circ(Q\otimes S)\circ\Delta](a), \tag{150}$$

for all $a\in\mathscr{A}$, but this is not necessarily true for every $Q\in\mathscr{L}(\mathscr{A})$ if $\mathscr{A}$ is infinite-dimensional. However, one can always define a subspace $\mathscr{T}(\mathscr{A})$ of $\mathscr{L}(\mathscr{A})$ by the requirement that $Q\in\mathscr{T}(\mathscr{A})$ if (i) $Q\in\mathscr{L}(\mathscr{A})$, (ii) Q satisfies (150) with I finite, and (iii) each Q_i appearing on the left-hand side of (150) also satisfies a condition of the same form. This subspace $\mathscr{T}(\mathscr{A})$ is certainly not empty, for the identity operator belongs to it [cf. (170)], as does every irreducible tensor operator Q_j^{qR} [cf. (148)], and, as just noted, if $\mathscr{A}$ is finite-dimensional then $\mathscr{T}(\mathscr{A})$ is identical to $\mathscr{L}(\mathscr{A})$. The *definition* of the required right coaction, which will be denoted by $\pi_{\mathscr{T}(\mathscr{A})}^R$, is then that it is the mapping of $\mathscr{T}(\mathscr{A})$ into $\mathscr{T}(\mathscr{A})\otimes\mathscr{A}$ that given by

$$\pi_{\mathscr{T}(\mathscr{A})}^R(Q)=\sum_{[Q]} Q_{[1]}\otimes Q_{[2]}, \tag{151}$$

where $Q_{[1]}\in\mathscr{T}(\mathscr{A})$ and $Q_{[1]}\in\mathscr{A}$ are such that

$$\sum_{[Q]} Q_{[1]}(a)\otimes Q_{[2]}=[(id\otimes M)\circ(\Delta\otimes id)\circ(Q\otimes S)\circ\Delta](a), \tag{152}$$

for all $Q \in \mathscr{T}(\mathscr{A})$ and all $a \in \mathscr{A}$. It is then quite easily shown [using the identities (8) to (19)] that $\pi^R_{\mathscr{T}(\mathscr{A})}$ satisfies (43) and (44) [with π_V and V replaced by $\pi^R_{\mathscr{T}(\mathscr{A})}$ and $\mathscr{T}(\mathscr{A})$, respectively, and with all operators of $\mathscr{T}(\mathscr{A})$ acting on any member of $\mathscr{A}$ according to the prescription of (152)]. That is,

$$\sum_{[Q]} \sum_{[Q_{[1]}]} (Q_{[1]})_{[1]}(a) \otimes (Q_{[1]})_{[2]} \otimes Q_{[2]} = \sum_{[Q]} Q_{[1]}(a) \otimes \Delta(Q_{[2]}) \tag{153}$$

and

$$\sum_{[Q]} (Q_{[1]})(a) \epsilon(Q_{[2]}) = Q(a),$$

for all $Q \in \mathscr{T}(\mathscr{A})$ and all $a \in \mathscr{A}$. Hence $\pi^R_{\mathscr{T}(\mathscr{A})}$ is indeed a right coaction with carrier space $\mathscr{T}(\mathscr{A})$. Thus (151) and (152) imply that the definition (148) can be written equivalently as

$$\pi^R_{\mathscr{T}(\mathscr{A})}(Q^{qR}_j) = \sum_{k=1}^{d_q} Q^{qR}_k \otimes \pi^q_{kj} \tag{154}$$

(for all $j = 1,2, \ldots$). Because (154) is similar in form to (45), and as $\pi^R_{\mathscr{T}(\mathscr{A})}$ is a right coaction with carrier space $\mathscr{T}(\mathscr{A})$, the consistency of the definition (148) is now ensured.

2. Definition of the twisted irreducible tensor operators $\tilde{Q}^{qR}_j$

The *twisted irreducible tensor operators* $\widetilde{Q}^{qR}_j$ belonging to the unitary irreducible right coaction π^q of $\mathscr{A}$ are *defined* to be members of $\mathscr{L}(\mathscr{A})$ that satisfy the condition

$$[(id \otimes M) \circ (id \otimes \sigma) \circ (\Delta \otimes id) \circ (\widetilde{Q}^{qR}_j \otimes S^{-1}) \circ \Delta](a) = \sum_{k=1}^{d_q} \widetilde{Q}^{qR}_k(a) \otimes \pi^q_{kj}, \tag{155}$$

for all $a \in \mathscr{A}$ and all $j = 1,2, \ldots, d_q$. This can be written equivalently in terms of the right regular coaction $\pi^R_{\mathscr{A}}$ as

$$[(id \otimes M) \circ (id \otimes \sigma) \circ (\pi^R_{\mathscr{A}} \otimes id) \circ (\widetilde{Q}^{qR}_j \otimes S^{-1}) \circ \pi^R_{\mathscr{A}}](a) = \sum_{k=1}^{d_q} \widetilde{Q}^{qR}_k(a) \otimes \pi^q_{kj}, \tag{156}$$

for all $a \in \mathscr{A}$ and all $j = 1,2, \ldots, d_q$. Both (155) and (156) differ from the corresponding definitions (148) and (149) only in the replacement of M by $M \circ \sigma$ *and* S by S^{-1} (neither of which have any effect in the special case in which $\mathscr{A}$ is commutative). (See Appendix B 2 a for further discussion of this pair of substitutions. It should be recorded that Rittenberg and Scheunert[8] noted previously, in the context of what was essentially the ''abstract carrier space formalism'' [form (3) of Section I] as generalized to irreducible *representations* of $\mathscr{A}'$, that these substitutions do produce another type of irreducible tensor operator, but they did not pursue this observation at all.)

The demonstration that (155) provides a *consistent* definition again involves showing that it can be re-expressed by saying that the operators $\widetilde{Q}^{qR}_j$ (for $j = 1,2, \ldots, d_q$) form the basis of a carrier space for a right coaction of $\mathscr{A}$. This right coaction $\widetilde{\pi}^R_{\mathscr{T}(\mathscr{A})}$ [and its associated space $\mathscr{T}(\mathscr{A})$] are essentially obtained from $\pi^R_{\mathscr{T}(\mathscr{A})}$ by replacing M by $M \circ \sigma$ and S by S^{-1}, so $\widetilde{\pi}^R_{\mathscr{T}(\mathscr{A})}$ is *defined* as the mapping of $\mathscr{T}(\mathscr{A})$ into $\mathscr{T}(\mathscr{A}) \otimes \mathscr{A}$ that given by

$$\widetilde{\pi}^R_{\mathscr{T}(\mathscr{A})}(Q) = \sum_{[Q]} Q_{[1]} \otimes Q_{[2]}, \tag{157}$$

where $Q_{[1]} \in \mathscr{T}(\mathscr{A})$ and $Q_{[1]} \in \mathscr{A}$ are such that

$$\sum_{[Q]} Q_{[1]}(a) \otimes Q_{[2]} = [(id \otimes (M \circ \sigma)) \circ (\Delta \otimes id) \circ (Q \otimes S^{-1}) \circ \Delta](a), \tag{158}$$

for all $Q \in \mathscr{T}(\mathscr{A})$ and all $a \in \mathscr{A}$. Then (157) and (158) imply that the definition (155) can be written equivalently as

$$\tilde{\pi}^{R}_{\mathscr{T}(\mathscr{A})}(\tilde{Q}^{qR}_{j}) = \sum_{k=1}^{d_q} \tilde{Q}^{qR}_{k} \otimes \pi^{q}_{kj} \tag{159}$$

(for all $j = 1,2, \ldots$), which then ensures the consistency of the definition (155).

C. Definitions in the left regular corepresentation formalism

1. Definition of the ordinary irreducible tensor operators Q^{qL}_j

The *ordinary irreducible tensor operators* Q^{qL}_j belonging to the unitary irreducible right coaction π^{q} of $\mathscr{A}$ are *defined* to be members of $\mathscr{L}(\mathscr{A})$ that satisfy the condition

$$[(id \otimes M) \circ (\pi^{L}_{\mathscr{A}} \otimes id) \circ (Q^{qL}_{j} \otimes S) \circ \pi^{L}_{\mathscr{A}}](a) = \sum_{k=1}^{d_q} Q^{qL}_{k}(a) \otimes \pi^{q}_{kj}, \tag{160}$$

for all $a \in \mathscr{A}$ and all $j = 1,2, \ldots, d_q$. [This is can be obtained from (149) by replacing $X = R$ by $X = L$, the justification being discussed in more detail in Appendix B 3 a.] In terms of the elementary operations of $\mathscr{A}$, (160) can be re-expressed using (81) as

$$[\sigma \circ (S \otimes id) \circ (M \otimes id) \circ (id \otimes \Delta) \circ (S \otimes Q^{qL}_{j}) \circ \Delta](a) = \sum_{k=1}^{d_q} Q^{qL}_{k}(a) \otimes \pi^{q}_{kj}, \tag{161}$$

for all $a \in \mathscr{A}$ and all $j = 1,2, \ldots, d_q$.

The demonstration that (160) provides a *consistent* definition proceeds in the same way as above. In this case the appropriate right coaction will be denoted by $\pi^{L}_{\mathscr{T}(\mathscr{A})}$, and will be *defined* as the mapping of $\mathscr{T}(\mathscr{A})$ into $\mathscr{T}(\mathscr{A}) \otimes \mathscr{A}$ that given by

$$\pi^{L}_{\mathscr{T}(\mathscr{A})}(Q) = \sum_{[Q]} Q_{[1]} \otimes Q_{[2]}, \tag{162}$$

where $Q_{[1]} \in \mathscr{T}(\mathscr{A})$ and $Q_{[1]} \in \mathscr{A}$ are such that

$$\sum_{[Q]} Q_{[1]}(a) \otimes Q_{[2]} = (\sigma \circ (S \otimes id) \circ (M \otimes id) \circ (id \otimes \Delta) \circ (S \otimes Q) \circ \Delta)(a), \tag{163}$$

for all $Q \in \mathscr{T}(\mathscr{A})$ and all $a \in \mathscr{A}$. [Here the subspace $\mathscr{T}(\mathscr{A})$ of $\mathscr{L}(\mathscr{A})$ is defined as in Section VI B 1, but with the right-hand side of (163) replacing the right-hand side of (152) in (150). The motivation for this definition is given in Appendix B 3 b.] Then the definition (160) can be written equivalently as

$$\pi^{L}_{\mathscr{T}(\mathscr{A})}(Q^{qL}_{j}) = \sum_{k=1}^{d_q} Q^{qL}_{k} \otimes \pi^{q}_{kj} \tag{164}$$

(for all $j = 1,2, \ldots$), which then guarantees its consistency.

2. Definition of the twisted irreducible tensor operators $\tilde{Q}_j^{qL}$

The *twisted irreducible tensor operators* $\tilde{Q}_j^{qL}$ belonging π^q of $\mathscr{A}$ are *defined* to be members of $\mathscr{L}(\mathscr{A})$ that satisfy the condition

$$[(id\otimes M)\circ(id\otimes\sigma)\circ(\pi^L_{\mathscr{A}}\otimes id)\circ(\tilde{Q}_j^{qL}\otimes S^{-1})\circ\pi^L_{\mathscr{A}}](a)=\sum_{k=1}^{d_q}\tilde{Q}_k^{qL}(a)\otimes\pi^q_{kj}, \tag{165}$$

for all $a\in\mathscr{A}$ and all $j=1,2,\ldots,d_q$. In terms of the elementary operations of $\mathscr{A}$, (165) can be re-expressed using (81) as

$$[(id\otimes M)\circ(\sigma\otimes S)\circ(id\otimes\sigma)\circ(id\otimes\Delta)\circ(id\otimes\tilde{Q}_j^{qL})\circ\Delta](a)=\sum_{k=1}^{d_q}\tilde{Q}_k^{qL}(a)\otimes\pi^q_{kj}, \tag{166}$$

for all $a\in\mathscr{A}$ and all $j=1,2,\ldots,d_q$. The definition (165) differs from the corresponding definition (160) only in the replacement of M by $M\circ\sigma$ *and* S by S^{-1} (neither of which have any effect in the special case in which $\mathscr{A}$ is commutative). However, because the two S factors in (161) have different origins, these substitutions do *not* convert (161) into (166). (See Appendix B 3 a for a further discussion of this point.)

The consistency of the definition (165) is again shown in the same way as above. In this case the appropriate right coaction will be denoted by $\tilde{\pi}^L_{\mathscr{T}(\mathscr{A})}$, and will be *defined* as the mapping of $\mathscr{T}(\mathscr{A})$ into $\mathscr{T}(\mathscr{A})\otimes\mathscr{A}$ that given by

$$\tilde{\pi}^L_{\mathscr{T}(\mathscr{A})}(Q)=\sum_{[Q]}Q_{[1]}\otimes Q_{[2]}, \tag{167}$$

where $Q_{[1]}\in\mathscr{T}(\mathscr{A})$ and $Q_{[1]}\in\mathscr{A}$ are such that

$$\sum_{[Q]}Q_{[1]}(a)\otimes Q_{[2]}=[(id\otimes M)\circ(\sigma\otimes S)\circ(id\otimes\sigma)\circ(id\otimes\Delta)\circ(id\otimes Q)\circ\Delta](a), \tag{168}$$

for all $Q\in\mathscr{T}(\mathscr{A})$ and all $a\in\mathscr{A}$. [Here the subspace $\mathscr{T}(\mathscr{A})$ of $\mathscr{L}(\mathscr{A})$ is defined as in Section VI B 1, but with the right-hand side of (168) replacing the right-hand side of (152) in (150). The motivation for this definition is given in Appendix B 3 b.] Then the definition (165) can be written equivalently as

$$\tilde{\pi}^L_{\mathscr{T}(\mathscr{A})}(\tilde{Q}_j^{qL})=\sum_{k=1}^{d_q}\tilde{Q}_k^{qL}\otimes\pi^q_{kj} \tag{169}$$

(for all $j=1,2,\ldots$), which then implies the consistency of (165).

D. The identity operator as an irreducible tensor operator

Suppose that Q is the *identity operator* id of $\mathscr{L}(\mathscr{A})$ [so that $Q(a)=a$ for all $a\in\mathscr{A}$]. Then, on using (9) and (18), it follows that

$$(id\otimes M)\circ(\Delta\otimes id)\circ(id\otimes S)\circ\Delta=id\otimes 1_{\mathscr{A}}, \tag{170}$$

which, by (148), leads to the agreeable conclusion that the identity operator id is an *ordinary* irreducible tensor operator in the *right* regular corepresentation formalism for the one-dimensional *identity* corepresentation whose sole matrix coefficient is $1_{\mathscr{A}}$.

It is easily checked [using (155), (161), and (166) in place of (148)], that id is also a *twisted* irreducible tensor operator for the identity corepresentation in the *right* regular corepresentation formalism , as well as being a both an *ordinary* and a *twisted* irreducible tensor operator for the identity corepresentation in the *left* regular corepresentation formalism.

In fact, if one were to adopt the view that these results concerning the identity operator are an *essential* requirement of any sensible definition of irreducible tensor operators, the fact that they are not true if M is replaced by $M \circ \sigma$ but S is left unchanged, nor if M is left unchanged but S is replaced by S^{-1}, then precludes further consideration of these possibilities.

E. Products as irreducible tensor operators

Suppose now that ψ_j^{qR} and ψ_j^{qL} are sets of basis functions for π^q [as defined in (94) and (95), respectively] and that the operators Q_j^{qX} and $\widetilde{Q}_j^{qX}$ are *defined* by

$$\begin{aligned} Q_j^{qR}(a) &= M(\psi_j^{qR} \otimes a), \\ \widetilde{Q}_j^{qR}(a) &= M(a \otimes \psi_j^{qR}), \\ Q_j^{qL}(a) &= M(a \otimes \psi_j^{qL}), \\ \widetilde{Q}_j^{qL}(a) &= M(\psi_j^{qL} \otimes a), \end{aligned} \tag{171}$$

for all $a \in \mathscr{A}$. Then the identities (21) to (32) imply that the operators Q_j^{qR}, $\widetilde{Q}_j^{qR}$, Q_j^{qL}, and $\widetilde{Q}_j^{qL}$ do indeed satisfy (148), (155), (161), and (166), respectively, and so are irreducible tensor operators belonging to π^q.

F. Two useful identities for the ordinary irreducible tensor operators Q_j^{qX} and $\tilde{Q}_j^{qX}$

If Q_k^{qX} is an *ordinary* irreducible tensor operator belonging to the unitary irreducible right coaction π^q of $\mathscr{A}$ and ψ_j^{pX} is a set of basis functions for the unitary irreducible right coaction π^p of $\mathscr{A}$, then

$$\pi_{\mathscr{A}}^X[Q_k^{qX}(\psi_j^{pX})] = \sum_{s=1}^{d_p} \sum_{t=1}^{d_q} [Q_t^{qX}(\psi_s^{pX})] \otimes [M(\pi_{tk}^q \otimes \pi_{sj}^p)], \tag{172}$$

for $X = R$ and L, for all $j = 1,2, \ldots, d_p$, and $k = 1,2, \ldots, d_q$. That is, by (118),

$$\pi_{\mathscr{A}}^X[Q_k^{qX}(\psi_j^{pX})] = \sum_{s=1}^{d_p} \sum_{t=1}^{d_q} [Q_t^{qX}(\psi_s^{pX})] \otimes (\pi^q \boxtimes \pi^p)_{ts,kj}, \tag{173}$$

for $X = R$ and L, for all $j = 1,2, \ldots, d_p$ and $k = 1,2, \ldots, d_q$.

By contrast, if $\widetilde{Q}_k^{qX}$ is a *twisted* irreducible tensor operator belonging π^q, then

$$\pi_{\mathscr{A}}^X[\widetilde{Q}_k^{qX}(\psi_j^{pX})] = \sum_{s=1}^{d_p} \sum_{t=1}^{d_q} [\widetilde{Q}_t^{qX}(\psi_s^{pX})] \otimes [M(\pi_{sj}^p \otimes \pi_{tk}^q)], \tag{174}$$

for $X = R$ and L, for all $j = 1,2, \ldots, d_p$ and $k = 1,2, \ldots, d_q$. It should be noted that the factors in the second term of the right-hand side of (174) are interchanged relative to those of (172), which implies, by (119), that

$$\pi_{\mathscr{A}}^X[\widetilde{Q}_k^{qX}(\psi_j^{pX})] = \sum_{s=1}^{d_p} \sum_{t=1}^{d_q} [\widetilde{Q}_t^{qX}(\psi_s^{pX})] \otimes (\pi^q \widetilde{\boxtimes} \pi^p)_{ts,kj}, \tag{175}$$

for $X=R$ and L, for all $j=1,2,\ldots,d_p$, and $k=1,2,\ldots,d_q$, which involves the *twisted* tensor product.

The proof of (172) is as follows. Applying (94) or (95) to the case $a=\psi_u^{pX}$ and invoking (149) or (160) (as appropriate) gives

$$\sum_{v=1}^{d_p}(id\otimes M)[\pi^X_{\mathscr{A}}(Q_j^{qX}(\psi_v^{pX}))\otimes S(\pi^p_{vu})]=\sum_{k=1}^{d_q}[Q_k^{qX}(\psi_u^{pX})]\otimes\pi^q_{kj}. \tag{176}$$

However, for any $a\in\mathscr{A}$,

$$(id\otimes M)[\pi^X_{\mathscr{A}}(a)\otimes S(\pi^p_{vu})]=\sum_{[a]}a_{[1]}\otimes M[a_{[2]}\otimes S(\pi^p_{vu})],$$

the right-hand side of which, on multiplication from the right with $1_{\mathscr{A}}\otimes\pi^p_{ui}$, and summing over u, and using (52) and (53), reduces to $\delta_{iv}\pi^X_{\mathscr{A}}(a)$. The desired result (172) is then obtained by multiplying both sides of (176) from the right with $1_{\mathscr{A}}\otimes\pi^p_{ui}$ and summing over u. The line of proof for (174) is similar.

G. Products of operators

If Q and Q' are any two members of $\mathscr{T}(\mathscr{A})$ and $\pi^X_{\mathscr{T}(\mathscr{A})}$ is the *ordinary* right coaction defined in (151) and (152) (for $X=R$) and (162) and (163) (for $X=L$), then

$$\pi^X_{\mathscr{T}(\mathscr{A})}(QQ')=\pi^X_{\mathscr{T}(\mathscr{A})}(Q)\,\pi^X_{\mathscr{T}(\mathscr{A})}(Q'), \tag{177}$$

for $X=R$ and L. This can be re-expressed as

$$(\pi^X_{\mathscr{T}(\mathscr{A})}\circ\hat{M})(Q\otimes Q')=[(\hat{M}\otimes M)\circ(id\otimes\sigma\otimes id)\circ(\pi^X_{\mathscr{T}(\mathscr{A})}\otimes\pi^X_{\mathscr{T}(\mathscr{A})})](Q\otimes Q'), \tag{178}$$

for $X=R$ and L, where the operator multiplication operation $\hat{M}$ is defined by

$$\hat{M}(Q\otimes Q')=Q\circ Q', \tag{179}$$

for all $Q,Q'\in\mathscr{T}(\mathscr{A})$.

By contrast, if $\tilde{\pi}^X_{\mathscr{T}(\mathscr{A})}$ is the *twisted* right coaction defined in (157) and (158) (for $X=R$) and (167) and (168) (for $X=L$), then

$$\begin{aligned}&(\tilde{\pi}^X_{\mathscr{T}(\mathscr{A})}\circ\hat{M})(Q\otimes Q')\\&\quad=[(\hat{M}\otimes M)\circ(id\otimes id\otimes\sigma)\circ(id\otimes\sigma\otimes id)\circ(\tilde{\pi}^X_{\mathscr{T}(\mathscr{A})}\otimes\tilde{\pi}^X_{\mathscr{T}(\mathscr{A})})](Q\otimes Q'),\end{aligned} \tag{180}$$

for $X=R$ and L, whose righthand side involves an extra twist factor $(id\otimes id\otimes\sigma)$ relative to the corresponding result (178).

The proofs of these statements just involve a straightforward application of the identities (8) to (19).

VII. THEOREMS OF THE WIGNER–ECKART TYPE

If π^p, π^q, and π^r are unitary irreducible corepresentations of $\mathscr{A}$ of dimensions d_p, d_q, and d_r, respectively, ϕ_j^{pX} and ψ_ℓ^{rX} are basis functions belonging to π^p and π^r, and Q_k^{qX} is an *ordinary* irreducible tensor operator belonging to π^q, then

$$[\psi_{\ell}^{rX},Q_k^{qX}(\phi_j^{pX})]^X=\sum_{\alpha=1}^{n_{qp}^r}\left(\begin{array}{ccc|cc} r & , & \alpha & q & p \\ \ell & & & k & j \end{array}\right)(r|Q^{qX}|p)_\alpha, \tag{181}$$

for $X=R$ and L, all $j=1,2,\ldots,d_p$, all $k=1,2,\ldots,d_q$, and all $\ell=1,2,\ldots,d_r$. Here the *reduced matrix elements* $(r|Q^{qX}|p)_\alpha$ are given by

$$(r|Q^{qX}|p)_\alpha=\sum_{s=1}^{d_p}\sum_{t=1}^{d_q}\sum_{u,v=1}^{d_r}[\psi_u^{rX},Q_t^{qX}(\phi_s^{pX})]^X\left(\begin{array}{cc|ccc} q & p & r & , & \alpha \\ t & s & v & & \end{array}\right)$$
$$\times\{[(\mathbf{F}^r)^{-1}]_{vu}/tr[(\mathbf{F}^r)^{-1}]\}, \tag{182}$$

for $\alpha=1,2,\ldots,n_{qp}^r$, and the inner products $(,)^R$ and $(,)^L$ are defined in (86) and (87).

On the other hand, if $\tilde{Q}_k^{qX}$ is a *twisted* irreducible tensor operator belonging to π^q, then

$$[\psi_{\ell}^{rX},\tilde{Q}_k^{qX}(\phi_j^{pX})]^X=\sum_{\alpha=1}^{n_{pq}^r}\left(\begin{array}{ccc|cc} r & , & \alpha & p & q \\ \ell & & & j & k \end{array}\right)(r|\tilde{Q}^{qX}|p)_\alpha, \tag{183}$$

for $X=R$ and L, all $j=1,2,\ldots,d_p$, all $k=1,2,\ldots,d_q$, and all $\ell=1,2,\ldots,d_r$, where the reduced matrix elements $(r|\tilde{Q}^{qX}|p)_\alpha$ are given by

$$(r|\tilde{Q}^{qX}|p)_\alpha=\sum_{s=1}^{d_p}\sum_{t=1}^{d_q}\sum_{u,v=1}^{d_r}[\psi_u^{rX},\tilde{Q}_t^{qX}(\phi_s^{pX})]^X\left(\begin{array}{cc|ccc} p & q & r & , & \alpha \\ s & t & v & & \end{array}\right)$$
$$\times\{[(\mathbf{F}^r)^{-1})_{vu}/tr((\mathbf{F}^r)^{-1}]\}, \tag{184}$$

for $\alpha=1,2,\ldots,n_{pq}^r$.

The results (181) and (183) exhibit the classic Wigner–Eckart theorem behaviour, in that they show that the j, k, and ℓ dependences of the inner products $(\psi_{\ell}^{rX},Q_k^{qX}\phi_j^{pX})^X$ and $(\psi_{\ell}^{rX},\tilde{Q}_k^{qX}\phi_j^{pX})^X$ are determined only by Clebsch–Gordan coefficients, but it should be noted that in the general case in which $\mathscr{A}$ is non–commutative, the inner products for the *ordinary* and *twisted* irreducible tensor operators involve *different* sets of Clebsch–Gordan coefficients.

The proof of (181) in the case $X=R$ is as follows. By (92) and (172),

$$\pi_{\mathscr{A}}^R[\psi_{\ell}^{rR*}Q_k^{qR}(\phi_j^{pR})]=\sum_{s=1}^{d_p}\sum_{t=1}^{d_q}\sum_{u=1}^{d_r}[\psi_u^{rR*}Q_t^{qR}(\phi_s^{pR})]\otimes(\pi_{u\ell}^{r*}\pi_{tk}^q\pi_{sj}^p),$$

for all $j=1,2,\ldots,d_p$, $k=1,2,\ldots,d_q$, and $\ell=1,2,\ldots,d_r$. Then, by (91),

$$h[\psi_{\ell}^{rR*}Q_k^{qR}(\phi_j^{pR})]=\sum_{s=1}^{d_p}\sum_{t=1}^{d_q}\sum_{u=1}^{d_r}h[\psi_u^{rR*}Q_t^{qR}(\phi_s^{pR})]h(\pi_{u\ell}^{r*}\pi_{tk}^q\pi_{sj}^p),$$

for all $j=1,2,\ldots,d_p$, $k=1,2,\ldots,d_q$, and $\ell=1,2,\ldots,d_r$. Invoking (86) and (138) then immediately gives (181) and (182).

The proof of (181) in the case $X=L$ is similar. By (172), (93), and (98),

$$\pi_{\mathscr{A}}^L[Q_k^{qL}(\phi_j^{pL})(S^2(\psi_{\ell}^{rL}))^*]=\sum_{s=1}^{d_p}\sum_{t=1}^{d_q}\sum_{u=1}^{d_r}[Q_t^{qL}(\phi_s^{pL})(S^2(\psi_u^{rL}))^*]\otimes(\pi_{u\ell}^{r*}\pi_{tk}^q\pi_{sj}^p),$$

for all $j=1,2,\ldots,d_p$, $k=1,2,\ldots,d_q$, and $\ell=1,2,\ldots,d_r$. On applying (91), (87), and (138), the results (181) and (182) are obtained for this case as well.

The proof of (183) follows the same lines, but employs (174) and (137) in place of (172) and (138).

VIII. PRODUCTS OF IRREDUCIBLE TENSOR OPERATORS

If π^p and π^q are unitary irreducible corepresentations of $\mathscr{A}$ of dimensions d_p and d_q, respectively, and Q_j^{pX} and Q_k^{qX} are *ordinary* irreducible tensor operators belonging to π^p and π^q, then

$$\pi^X_{\mathscr{T}(\mathscr{A})}(Q_j^{pX}Q_k^{qX})=\sum_{s=1}^{d_p}\sum_{t=1}^{d_q}(Q_s^{pX}Q_t^{qX})\otimes(\pi^p\boxtimes\pi^q)_{st,jk}, \tag{185}$$

for $X=R$ and L and for all $j=1,2,\ldots,d_p$, and $k=1,2,\ldots,d_q$. Here the coactions $\pi^R_{\mathscr{T}(\mathscr{A})}$ and $\pi^L_{\mathscr{T}(\mathscr{A})}$ are as defined in (151), (152), (162), and (163), and the matrix coefficients of the tensor product $\pi^p\boxtimes\pi^q$ are given in (118). [The proof of (185) just involves applying (178), (154), (164), and (179).]

Because of the similarity in form between (185) and (131), it follows immediately that

$$Q_\ell^{rX,\alpha}=\sum_{j=1}^{d_p}\sum_{k=1}^{d_q}\left(\begin{array}{cc|ccc} p & q & r & , & \alpha \\ j & k & \ell & & \end{array}\right)Q_j^{pX}Q_k^{qX}, \tag{186}$$

for $\ell=1,2,\ldots,d_r$ and $\alpha=1,2,\ldots,n_{pq}^r$. Here $Q_\ell^{rX,\alpha}$ (for $\alpha=1,2,\ldots,n_{pq}^r$) are n_{pq}^r ordinary irreducible tensor operators belonging to π^r that are, in general, all different.

By contrast, if $\widetilde{Q}_j^{pX}$ and $\widetilde{Q}_k^{qX}$ are *twisted* irreducible tensor operators belonging to π^p and π^q, then

$$\widetilde{\pi}^X_{\mathscr{T}(\mathscr{A})}(\widetilde{Q}_j^{pX}\widetilde{Q}_k^{qX})=\sum_{s=1}^{d_p}\sum_{t=1}^{d_q}(\widetilde{Q}_s^{pX}\widetilde{Q}_t^{qX})\otimes(\pi^p\widetilde{\boxtimes}\pi^q)_{st,jk}, \tag{187}$$

for $X=R$ and L and for all $j=1,2,\ldots,d_p$, and $k=1,2,\ldots,d_q$. Here the right coactions $\widetilde{\pi}^R_{\mathscr{T}(\mathscr{A})}$ and $\widetilde{\pi}^L_{\mathscr{T}(\mathscr{A})}$ are as defined in (157), (158), (167), and (168), and the matrix coefficients of the *twisted* tensor product $\pi^p\widetilde{\boxtimes}\pi^q$ are given in (119). [This result (187) is proved using (180), (159), (169), and (179).]

The analogue of (186) for the *twisted* case is

$$\widetilde{Q}_\ell^{rX,\alpha}=\sum_{j=1}^{d_p}\sum_{k=1}^{d_q}\left(\begin{array}{cc|ccc} q & p & r & , & \alpha \\ k & j & \ell & & \end{array}\right)\widetilde{Q}_j^{pX}\widetilde{Q}_k^{qX}, \tag{188}$$

for $\ell=1,2,\ldots,d_r$ and $\alpha=1,2,\ldots,n_{qp}^r$. Here $\widetilde{Q}_\ell^{rX,\alpha}$ (for $\alpha=1,2,\ldots,n_{qp}^r$) are n_{qp}^r twisted irreducible tensor operators belonging to π^r that are, in general, all different.

IX. GENERALIZATION TO QUANTUM HOMOGENEOUS SPACES

A. Quantum homogeneous spaces

The definition and role of quantum homogeneous spaces are best introduced by considering the situation first in the very well established and familiar context of a compact Lie group $\mathscr{G}$. The homogeneous space formalism for $\mathscr{G}$ has two essential features. Firstly, it is equivalent to the theory in which $\mathscr{G}$ acts as a transformation group on an external manifold $\mathscr{M}$, and, secondly, it is closely related to the regular representation formalisms. Both of these aspects were reviewed briefly in Section I.

With $\mathscr{G}$ taken to be a group of transformations that act on an external manifold $\mathscr{M}$, select some typical point of $\mathscr{M}$. Let $\mathscr{H}$ be the *isotropy subgroup* of $\mathscr{G}$, which consists of all transformations of $\mathscr{G}$ that send this point into itself, and let $\mathscr{M}_0$ be the *orbit* of points of $\mathscr{M}$ that are obtained by acting on this typical point with every transformation of $\mathscr{G}$. In the case in which $\mathscr{G}$ is the rotation group about O and $\mathscr{M}$ is $\mathfrak{R}^3$, let $\mathbf{r}_0$ of $\mathfrak{R}^3$ be this typical point. Then $\mathscr{H}$ is the subgroup of all rotations about the axis from O to the point $\mathbf{r}_0$, and $\mathscr{M}_0$ is the sphere centered on O that contains the point $\mathbf{r}_0$. With an appropriate choice of $\mathbf{r}_0$, $\mathscr{M}_0$ can be parametrized by the spherical polar coordinates θ and ϕ. Effectively it is only the functional dependence on θ and ϕ that comes into symmetry arguments, the dependence on the radial distance r being immaterial. That is, only the subspace $\mathscr{M}_0$ is actually relevant in the group theoretical calculations. However, it is easily demonstrated that there is a one-to-one correspondence between the points of $\mathscr{M}_0$ and the set of *left* cosets $T.\mathscr{H}$ of $\mathscr{G}$ with respect to $\mathscr{H}$. Thus the quantities of interest are the subset $\mathscr{B}$ of $R(\mathscr{G})$ that consists of those members of $R(\mathscr{G})$ which are *constant* on each left coset $T.\mathscr{H}$. Then the operators acting on the members of $\mathscr{B}$ that correspond to the operators $P(T)$ of (2) may be identified with the left regular operators $\hat{L}(T)$ of (A18), as *restricted* to act *only* on $\mathscr{B}$. Moreover the only part of the integral (5) that is relevant to symmetry arguments is the part involving θ and ϕ, which is an integral over $\mathscr{M}_0$, and hence is equivalent to the Haar integral of (6) applied to the functions of $\mathscr{B}$. Finally, in the homogeneous space version, the irreducible tensor operators of (4) become mappings of $\mathscr{B}$ into $\mathscr{B}$.

Henceforth the $\star$-Hopf algebra $R(\mathscr{G})$ will be denoted by $\mathscr{A}$. Then $\mathscr{B}$ becomes a $\star$-subalgebra of $\mathscr{A}$ and a *left* coideal of $\mathscr{A}$. [The convention adopted here is that $\mathscr{B}$ is said to be a left coideal of $\mathscr{A}$ if $\Delta(f) \in \mathscr{A}\otimes\mathscr{B}$ for all $f \in \mathscr{B}$, and $\mathscr{B}$ is said to be a right coideal of $\mathscr{A}$ if $\Delta(f) \in \mathscr{B}\otimes\mathscr{A}$ for all $f \in \mathscr{B}$.] It is also trivially true that $\mathscr{B}$ is S^2-invariant.

There also exists a parallel version of this theory associated with the *right* regular representation of $\mathscr{G}$, the operators $\hat{R}(T)$ of which are defined by $\hat{R}(T)f(T') = f(T'T)$ for all f and for all $T, T' \in \mathscr{G}$. Then, for example, if $\mathscr{G}$ is the group of all rotations in this space about O and $\mathscr{M}$ is $\mathfrak{R}^3$, in place of the transformations of (1) one could define another set in which

$$(\mathbf{r}')^T = \mathbf{r}^T\mathbf{R}(T), \tag{189}$$

where $\mathbf{r}^T$ denotes the transpose of $\mathbf{r}$. Then, for a typical point $\mathbf{r}_0$, there is a one-to-one correspondence between the points of the orbit $\mathscr{M}_0$ of $\mathbf{r}_0$ and the set of *right* cosets $\mathscr{H}T$ of $\mathscr{G}$ with respect to the corresponding isotropy subgroup $\mathscr{H}$ of $\mathbf{r}_0$. In this case the quantity of interest is the set $\mathscr{B}$ of representative functions of $\mathscr{G}$ which are constant on each *right* coset $\mathscr{H}T$. Then $\mathscr{B}$ is a $\star$-subalgebra of $\mathscr{A}$ and a *right* coideal of $\mathscr{A}$, and the analogues of operators $P(T)$ of (2) are the $\hat{R}(T)$ restricted to $\mathscr{B}$. It is again trivially true that $\mathscr{B}$ is S^2-invariant.

There are various ways in which these ideas can be generalized to produce quantum homogeneous spaces,[23–26,31–36] but the present development follows the work of Dijkhuizen and Koornwinder.[23–26] In this formulation one works with a $\star$- Hopf algebra $\mathscr{A}$ (which is in general both non-commutative and non-cocommutative), and with a $\star$-subalgebra $\mathscr{B}$ of $\mathscr{A}$ that is either a right coideal of $\mathscr{A}$ or is a left coideal of $\mathscr{A}$. (The explicit discussion in Refs. 23–26 is actually given for the former situation, but clearly the formulation can also be re-expressed for the latter situation.) Dijkhuizen and Koornwinder[23–26] have discussed various other algebraic objects that are associated with $\mathscr{B}$, and have shown that in the case of the quantum SU(2) group there exists a one-parameter family of such spaces (called ''quantum 2-spheres'') which are mutually non-isomorphic, and they have related these to the work of Podleś.[31]

For the case in which $\mathscr{B}$ is a *left* coideal of $\mathscr{A}$ it will be assumed, for reasons that will become clear in due course, that $\mathscr{B}$ is S^2-invariant. However, when $\mathscr{B}$ is a *right* coideal of $\mathscr{A}$ there is no need to make this assumption when investigating the irreducible tensor operators. Whether this assumption is needed in this case for other purposes is a matter that has been discussed by Dijkhuizen and Koornwinder.[23,24]

B. The restricted right and left regular coactions

In the special case in which $\mathscr{A}$ is the dual of a group algebra, the operations of $\mathscr{A}$ corresponding to the right and left regular actions of the group algebra are the right and left regular *coactions* of $\mathscr{A}$. Consequently the restrictions of right and left regular actions of the group algebra to $\mathscr{B}$ correspond to the right and left regular coactions of $\mathscr{A}$ restricted to $\mathscr{B}$. These are not only the relevant operations of the classical homogeneous space formulation but they are also the basic operations of the *quantum* homogeneous space formulation.

Explicitly, the right regular coaction $\pi^R_{\mathscr{A}}$ and the left regular coaction $\pi^L_{\mathscr{A}}$ for a general compact quantum group algebra $\mathscr{A}$ are defined [in (43) and (81)] by

$$\pi^R_{\mathscr{A}}=\Delta, \quad \pi^L_{\mathscr{A}}=\sigma\circ(S\otimes id)\circ\Delta.$$

Both are *right* coactions of $\mathscr{A}$ with carrier space $\mathscr{A}$. The corresponding *restricted right regular coaction* $\pi^R_{\mathscr{B}}$ and *restricted left regular coaction* $\pi^L_{\mathscr{B}}$ may then be defined by

$$\pi^R_{\mathscr{B}}=\pi^R_{\mathscr{A}|\mathscr{B}}=\Delta_{|\mathscr{B}}, \quad \pi^L_{\mathscr{B}}=\pi^L_{\mathscr{A}|\mathscr{B}}=\sigma\circ(S\otimes id)\circ\Delta_{|\mathscr{B}}. \tag{190}$$

In the context of the restricted right regular coaction it is being assumed that $\mathscr{B}$ is a right coideal of $\mathscr{A}$, whereas in the restricted left regular coaction context $\mathscr{B}$ is assumed to be a left coideal of $\mathscr{A}$. Because of the extra twist factor σ in the definition of $\pi^L_{\mathscr{B}}$, it follows that *both* $\pi^R_{\mathscr{B}}$ *and* $\pi^L_{\mathscr{B}}$ are *right* coactions of $\mathscr{A}$ with carrier space $\mathscr{B}$. (The role of $\pi^R_{\mathscr{B}}$ as a transitive $\star$-coaction corresponding to the transitive action of the quantum group associated with $\mathscr{A}$ on the quantum homogeneous space associated with $\mathscr{B}$ has been described by Dijkhuizen and Koornwinder.[23,24])

The restriction of the Haar functional h of $\mathscr{A}$ to $\mathscr{B}$ provides a positive definite integral for $\mathscr{B}$ with the invariance properties

$$[M_{\mathbb{C},\mathscr{A}}\circ(h\otimes id)\circ\pi^X_{\mathscr{B}}](b)=[M_{\mathscr{A},\mathbb{C}}\circ(id\otimes h)\circ\pi^X_{\mathscr{B}}](b)=h(b)\,1_{\mathscr{A}}, \tag{191}$$

for all $b\in\mathscr{B}$ and for both $X=R$ and $X=L$ [cf. (88) and (89)].

The restricted right and left regular corepresentations are both *unitary*, provided that the inner products on the carrier space $\mathscr{B}$ are chosen in the following way.

1. for the restricted *right* regular corepresentation take

$$\langle b,b'\rangle_{\mathscr{B}}=(b,b')^R=h[M(b^\star\otimes b')], \quad \text{for all} \quad b,b'\in\mathscr{B}; \tag{192}$$

2. for the restricted *left* regular corepresentation take

$$\langle b,b'\rangle_{\mathscr{B}}=(b,b')^L=h\{M[b\otimes(S^2(b'))^\star]\} \quad \text{for all} \quad b,b'\in\mathscr{B}. \tag{193}$$

It should be noted that $(S^2(b'))^\star\in\mathscr{B}$ if $\mathscr{B}$ is S^2-invariant. [The proofs of these unitary properties are essentially the same as for the corresponding results (86) and (87) for the unrestricted regular coactions.]

The effects of the restricted right and left regular coactions on products are also essentially the same as for the unrestricted coactions [cf. (92) and (93)].

C. Basis functions for the restricted right and left regular coactions

Suppose that π^p_{jk} are the matrix coefficients of a corepresentation π^p of $\mathscr{A}$ of finite dimension d_p. Then the *basis functions* ψ^{pR}_j *of* π^p *with respect to the restricted right regular coaction* may be defined to be a set of d_p elements of $\mathscr{B}$ that have the property that

$$\pi^R_{\mathscr{B}}(\psi^{pR}_j)=\sum_{k=1}^{d_p}\psi^{pR}_k\otimes\pi^p_{kj}, \tag{194}$$

for all $j=1,2,\ldots,d_p$. Similarly the *basis functions* ψ_j^{pL} *of* π^p *with respect to the restricted left regular coaction* may be defined as a set of d_p elements of $\mathscr{B}$ that have the property that

$$\pi^L_{\mathscr{B}}(\psi_j^{pL})=\sum_{k=1}^{d_p}\psi_k^{pL}\otimes\pi^p_{kj}, \tag{195}$$

for all $j=1,2,\ldots,d_p$. In both cases the matrix coefficients π^p_{kj} are elements of $\mathscr{A}$, and need not be members of $\mathscr{B}$.

By contrast with the unrestricted coaction situation, in neither case is there any guarantee that for a given corepresentation π^p there actually exist basis functions for restricted coactions. For example, in the restricted right regular coaction case, a set of basis functions is provided (for any fixed choice of $\ell=1,2,\ldots$) by

$$\psi_j^{pR}=\pi^p_{\ell j}, \tag{196}$$

for all $j=1,2,\ldots,d_p$ *only if* $\pi^p_{\ell j}$ is an element of $\mathscr{B}$ for *some* $j=1,2,\ldots,d_p$. [Then (I.43) and the fact that $\mathscr{B}$ is assumed in this context to be a right coideal of $\mathscr{A}$ imply that $\pi^p_{\ell j}\in\mathscr{B}$ for *all* $j=1,2,\ldots,d_p$.] Similarly, in the restricted left regular coaction case, an example is provided (for any fixed choice of $\ell=1,2,\ldots$) by

$$\psi_j^{pL}=S^{-2}(\pi^{p\star}_{j\ell}), \tag{197}$$

for all $j=1,2,\ldots,d_p$ *only if* $\pi^p_{j\ell}$ is an element of $\mathscr{B}$ for *some* $j=1,2,\ldots,d_p$. [Then (I.43) and the fact that $\mathscr{B}$ is assumed in this context to be a S^2-invariant left coideal and $\star$-subalgebra of $\mathscr{A}$ imply that $S^{-2}(\pi^{p\star}_{j\ell})\in\mathscr{B}$ for *all* $j=1,2,\ldots,d_p$.]

One very useful result, proved in the same way as the corresponding unrestricted identity (98), is that if ψ_k^{qL} exists then

$$\pi^L_{\mathscr{B}}[(S^2(\psi_k^{qL}))^\star]=\sum_{t=1}^{d_p}(S^2(\psi_t^{qL}))^\star\otimes\pi^{q\star}_{tk}, \tag{198}$$

for all $k=1,2,\ldots,d_p$.

The orthogonality properties of basis functions are the essentially the same as for those for the unrestricted case that have been given in (99), (100), and (103). (The only qualification is that now it has to be assumed that the relevant matrix corepresentation coefficients are members of $\mathscr{B}$.)

If the basis functions ψ_k^{qX} and ϕ_j^{pX} are members of $\mathscr{B}$ (so that they are basis functions for the restricted coactions), then their products $M(\psi_k^{qX}\otimes\phi_j^{pX})$ are also members of $\mathscr{B}$. Consequently the analysis of Section V D goes through without modification, except that all basis functions involved (including the $\theta^{r,\alpha X}_{\ell}$) are in $\mathscr{B}$ and one can always replace the unrestricted coactions $\pi^X_{\mathscr{A}}$ by the restricted coactions $\pi^X_{\mathscr{B}}$ The rest of the discussion of Section V on tensor products and Clebsch–Gordan coefficients still applies in its entirety.

D. The irreducible tensor operators in the restricted corepresentation formalisms

1. Introduction

Let π^q be a unitary irreducible right coaction of $\mathscr{A}$ of dimension d_q with matrix coefficients π^q_{jk}. It will be shown that within both the restricted right and the restricted left regular corepresentation formalisms there exist two types of irreducible tensor operators that both belong to this corepresentation π^q. These will be denoted by $Q^{qX}_{j,\mathscr{B}}$ and $\widetilde{Q}^{qX}_{j,\mathscr{B}}$ (for $j=1,2,\ldots,d_q$ and for $X=R$ or L), and will be called *ordinary* and *twisted* irreducible tensor operators associated with $\mathscr{B}$, respectively. These operators are members of $\mathscr{L}(\mathscr{B})$, which is the set of linear operators that map

$\mathscr{B}$ into $\mathscr{B}$. Naturally the two types of irreducible tensor operators coincide in the special case in which $\mathscr{A}$ is commutative. As much of the analysis is the same as for the unrestricted case, all the proofs will be omitted.

2. Definition of the ordinary irreducible tensor operators $Q_{j,\mathscr{B}}^{qX}$ and twisted irreducible tensor operators $\tilde{Q}_{j,\mathscr{B}}^{qX}$

The *ordinary irreducible tensor operators* $Q_{j,\mathscr{B}}^{qX}$ belonging to the unitary irreducible right coaction π^q of $\mathscr{A}$ are *defined* (for $X=L,R$) to be members of $\mathscr{L}(\mathscr{B})$ that satisfy the condition

$$[(id\otimes M)\circ(\pi_{\mathscr{B}}^{X}\otimes id)\circ(Q_{j,\mathscr{B}}^{qX}\otimes S)\circ\pi_{\mathscr{B}}^{X}](b)=\sum_{k=1}^{d_q} Q_{k,\mathscr{B}}^{qX}(b)\otimes\pi_{kj}^{q}, \tag{199}$$

for all $b\in\mathscr{B}$ and all $j=1,2,\ldots,d_q$.

The *twisted irreducible tensor operators* $\tilde{Q}_{j,\mathscr{B}}^{qX}$ belonging to the unitary irreducible right coaction π^q of $\mathscr{A}$ are *defined* (for $X=L,R$) to be members of $\mathscr{L}(\mathscr{B})$ that satisfy the condition

$$[(id\otimes M)\circ(id\otimes\sigma)\circ(\pi_{\mathscr{B}}^{X}\otimes id)\circ(\tilde{Q}_{j,\mathscr{B}}^{qX}\otimes S^{-1})\circ\pi_{\mathscr{B}}^{X}](b)=\sum_{k=1}^{d_q}\tilde{Q}_{k,\mathscr{B}}^{qX}(b)\otimes\pi_{kj}^{q}, \tag{200}$$

for all $b\in\mathscr{B}$ and all $j=1,2,\ldots,d_q$. [This definition (200) differs from the corresponding definition (199) only in the replacement of M by $M\circ\sigma$ *and* S by S^{-1} (neither of which have any effect in the special case in which $\mathscr{A}$ is commutative).]

3. Properties of the irreducible tensor operators associated with quantum homogeneous spaces

(1) Suppose that Q is the *identity operator* id of $\mathscr{L}(\mathscr{B})$ [so that $Q(b)=b$ for all $b\in\mathscr{B}$]. Then id is both an *ordinary* and a *twisted* irreducible tensor operator for the one-dimensional *identity* corepresentation of $\mathscr{A}$ (whose sole matrix coefficient is $1_{\mathscr{A}}$) in the restricted *right* regular corepresentation formalism, as well as being a both an *ordinary* and a *twisted* irreducible tensor operator for this identity corepresentation in the restricted *left* regular corepresentation formalism.

(2) Suppose now that ψ_j^{qR} and ψ_j^{qL} are sets of basis functions for π^q, as defined in (194) and (195), respectively (so that they are members of $\mathscr{B}$), and suppose that the operators $Q_{j,\mathscr{B}}^{qX}$ and $\tilde{Q}_{j,\mathscr{B}}^{qX}$ are *defined* by

$$\begin{aligned} Q_{j,\mathscr{B}}^{qR}(b) &= M(\psi_j^{qR}\otimes b),\\ \tilde{Q}_{j,\mathscr{B}}^{qR}(b) &= M(b\otimes\psi_j^{qR}),\\ Q_{j,\mathscr{B}}^{qL}(b) &= M(b\otimes\psi_j^{qL}),\\ \tilde{Q}_{j,\mathscr{B}}^{qL}(b) &= M(\psi_j^{qL}\otimes b), \end{aligned} \tag{201}$$

for all $b\in\mathscr{B}$. Then $Q_{j,\mathscr{B}}^{qR}$, $\tilde{Q}_{j,\mathscr{B}}^{qR}$, $Q_{j,\mathscr{B}}^{qL}$, and $\tilde{Q}_{j,\mathscr{B}}^{qL}$ are irreducible tensor operators belonging to π^q.

E. Wigner–Eckart type theorems associated with quantum homogeneous spaces

If π^p, π^q, and π^r are unitary irreducible corepresentations of $\mathscr{A}$ of dimensions d_p, d_q, and d_r, respectively, ϕ_j^{pX} and ψ_ℓ^{rX} are basis functions belonging π^p and π^r (with ϕ_j^{pX} and ψ_ℓ^{rX} being assumed here to be members of $\mathscr{B}$), and $Q_{k,\mathscr{B}}^{qX}$ is an *ordinary* irreducible tensor operator belonging to π^q (with respect to the relevant restricted regular coaction), then

$$[\psi_{\ell}^{rX},Q_{k\mathscr{B}}^{qX}(\phi_j^{pX})]^X=\sum_{\alpha=1}^{n_{qp}^r}\begin{pmatrix} r & , & \alpha \\ \ell & & \end{vmatrix} \begin{matrix} q & p \\ k & j \end{matrix}\end{pmatrix}(r|Q_{\mathscr{B}}^{qX}|p)_\alpha, \tag{202}$$

for $X=R$ and L, all $j=1,2,\ldots,d_p$, all $k=1,2,\ldots,d_q$, and all $\ell=1,2,\ldots,d_r$. Here the *reduced matrix elements* $(r|Q_{\mathscr{B}}^{qX}|p)_\alpha$ are given by

$$(r|Q_{\mathscr{B}}^{qX}|p)_\alpha=\sum_{s=1}^{d_p}\sum_{t=1}^{d_q}\sum_{u,v=1}^{d_r}[\psi_u^{rX},Q_{t\mathscr{B}}^{qX}(\phi_s^{pX})]^X\begin{pmatrix} q & p & r & , & \alpha \\ t & s & v & & \end{pmatrix}$$
$$\times\{[(\mathbf{F}^r)^{-1}]_{vu}/tr[(\mathbf{F}^r)^{-1}]\}, \tag{203}$$

for $\alpha=1,2,\ldots,n_{qp}^r$, the inner products $(,)^R$ and $(,)^L$ are defined in (192) and (193), and $\mathbf{F}^r$ is defined in (66).

On the other hand, if $\widetilde{Q}_{k\mathscr{B}}^{qX}$ is a *twisted* irreducible tensor operator belonging to π^q (with respect to the relevant restricted regular coaction), then

$$[\psi_{\ell}^{rX},\widetilde{Q}_{k\mathscr{B}}^{qX}(\phi_j^{pX})]^X=\sum_{\alpha=1}^{n_{pq}^r}\begin{pmatrix} r & , & \alpha \\ \ell & & \end{vmatrix} \begin{matrix} p & q \\ j & k \end{matrix}\end{pmatrix}(r|\widetilde{Q}_{\mathscr{B}}^{qX}|p)_\alpha, \tag{204}$$

for $X=R$ and L, all $j=1,2,\ldots,d_p$, all $k=1,2,\ldots,d_q$, and all $\ell=1,2,\ldots,d_r$, where the reduced matrix elements $(r|\widetilde{Q}_{\mathscr{B}}^{qX}|p)_\alpha$ are given by

$$(r|\widetilde{Q}_{\mathscr{B}}^{qX}|p)_\alpha=\sum_{s=1}^{d_p}\sum_{t=1}^{d_q}\sum_{u,v=1}^{d_r}[\psi_u^{rX},\widetilde{Q}_{t\mathscr{B}}^{qX}(\phi_s^{pX})]^X\begin{pmatrix} p & q & r & , & \alpha \\ s & t & v & & \end{pmatrix}$$
$$\times\{[(\mathbf{F}^r)^{-1}]_{vu}/tr[(\mathbf{F}^r)^{-1}]\}, \tag{205}$$

for $\alpha=1,2,\ldots,n_{pq}^r$.

These results (202) and (204) demonstrate that again the j, k, and ℓ dependences of the inner products $(\psi_{\ell}^{rX},Q_{k\mathscr{B}}^{qX}\phi_j^{pX})^X$ and $(\psi_{\ell}^{rX},\widetilde{Q}_{k\mathscr{B}}^{qX}\phi_j^{pX})^X$ are determined only by Clebsch–Gordan coefficients, and so they have the same form as in the classic Wigner–Eckart theorem. (However, it should be noted that in the general case in which $\mathscr{A}$ is non–commutative, the inner products for the *ordinary* and *twisted* irreducible tensor operators involve *different* sets of Clebsch–Gordan coefficients.)

As the proofs of (202) and (204) follow the same lines as in the unrestricted case considered in Section VII, they will be omitted here.

F. Products of irreducible tensor operators associated with quantum homogeneous spaces

The arguments of Section VIII can be applied (with $\mathscr{A}$ replaced by $\mathscr{B}$) to show that

$$Q_{\ell\mathscr{B}}^{rX,\alpha}=\sum_{j=1}^{d_p}\sum_{k=1}^{d_q}\begin{pmatrix} p & q & r & , & \alpha \\ j & k & \ell & & \end{pmatrix}Q_{j\mathscr{B}}^{pX}Q_{k\mathscr{B}}^{qX}, \tag{206}$$

for $\ell=1,2,\ldots,d_r$, and $\alpha=1,2,\ldots,n_{pq}^r$. Here $Q_{\ell\mathscr{B}}^{rX,\alpha}$ (for $\alpha=1,2,\ldots,n_{pq}^r$) are n_{pq}^r ordinary irreducible tensor operators belonging to π^r that are, in general, all different. Moreover,

$$\widetilde{Q}_{\ell\mathscr{B}}^{rX,\alpha}=\sum_{j=1}^{d_p}\sum_{k=1}^{d_q}\begin{pmatrix} q & p & r & , & \alpha \\ k & j & \ell & & \end{pmatrix}\widetilde{Q}_{j\mathscr{B}}^{pX}\widetilde{Q}_{k\mathscr{B}}^{qX}, \tag{207}$$

for $\ell = 1,2,\ldots,d_r$, and $\alpha = 1,2,\ldots,n_{qp}^r$, where $\tilde{Q}_{\ell\mathscr{B}}^{rX,\alpha}$ (for $\alpha = 1,2,\ldots,n_{qp}^r$) are n_{qp}^r twisted irreducible tensor operators belonging to π^r that are, in general, all different.

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APPENDIX A: INTRODUCTION

The purpose of this appendix is to *motivate* the definitions that are given in the main body of the paper for the irreducible tensor operators and the projection operators. This will be done by considering the simple special case in which the Hopf algebra $\mathscr{A}$ is the set of functions defined on a *finite* group $\mathscr{G}$ of order g, so that the dual $\mathscr{A}'$ of $\mathscr{A}$ is the group algebra of $\mathscr{G}$. In this situation both $\mathscr{A}$ and $\mathscr{A}'$ are of finite dimension g. Of course, as $\mathscr{A}$ is commutative in this special case, the resulting expressions are to some extent ambiguous, in that in this special case M is indistinguishable from $M \circ \sigma$ and S is indistinguishable from S^{-1}. The demonstration of the correctness, consistency, and usefulness of the definitions that are actually employed for the *general* case are the subject matter of the self-contained arguments of the main body of this paper.

To proceed with this motivation, it is necessary to start with some well- known facts concerning the relationship of $\mathscr{A}$ and $\mathscr{A}'$. It is easily shown that $\mathscr{A}'$ is also a Hopf algebra, whose multiplication operation $M_{\mathscr{A}'}$, comultiplication operation $\Delta_{\mathscr{A}'}$, and antipode $S_{\mathscr{A}'}$ are related to those of $\mathscr{A}$ by

$$\langle M_{\mathscr{A}'}(a' \otimes b'), a \rangle = \langle (a' \otimes b'), \Delta(a) \rangle, \tag{A1}$$

for all $a \in \mathscr{A}$ and all $a', b' \in \mathscr{A}'$,

$$\langle \Delta_{\mathscr{A}'}(a'), (a \otimes b) \rangle = \langle a', M(a \otimes b) \rangle, \tag{A2}$$

for all $a, b \in \mathscr{A}$ and all $a' \in \mathscr{A}'$, and

$$\langle S_{\mathscr{A}'}(a'), a \rangle = \langle a', S(a) \rangle, \tag{A3}$$

for all $a \in \mathscr{A}$ and all $a' \in \mathscr{A}'$.

Now suppose that π_V is a right coaction of $\mathscr{A}$ with carrier space V. Then there exists a corresponding *left action* π_V' of $\mathscr{A}'$ with the *same* carrier space V. This is a linear mapping from $\mathscr{A}' \otimes \mathscr{V}$ to V such that

$$\pi_V' \circ (id \otimes \pi_V') = \pi_V' \circ (M_{\mathscr{A}'} \otimes id) \tag{A4}$$

and

$$\pi_V' \circ (u_{\mathscr{A}'} \otimes id) = M_{\mathbb{C},V}, \tag{A5}$$

where $u_{\mathscr{A}'}$ is the unit operator of $\mathscr{A}'$, and $M_{\mathbb{C},V}(z \otimes v) = zv$ for all $v \in V$ and all $z \in \mathbb{C}$. The relationship between π_V and π_V' can be expressed as

$$\pi_V'(a' \otimes v) = \sum_{[v]} v_{[1]} \langle a', v_{[2]} \rangle, \tag{A6}$$

for all $a' \in \mathscr{A}'$ and all $v \in V$, where the notation of (48) has been employed, or equivalently as

$$\pi'_V(a'\otimes v)=[M_{V,\mathbb{C}}\circ(id\otimes ev)\circ(\sigma\otimes id)\circ(id\otimes\pi_V)](a'\otimes v), \tag{A7}$$

for all $a'\in\mathscr{A}'$ and all $v\in V$, where the evaluation map ev of (41) has been used. The inverse of these is

$$\pi_V(v)=\sum_j \pi'_V(a^j\otimes v)\otimes a_j, \tag{A8}$$

for all $v\in V$, where the basis of $\mathscr{A}$ and the dual basis of $\mathscr{A}'$ appear, and are assumed to be such that (42) holds. If V is of dimension d with basis elements $v_1,v_2,\ldots,v_d$, the matrix elements $\pi'(a')_{jk}$ of the representation are such that

$$\pi'_V(a'\otimes v_j)=\sum_{k=1}^{d}\pi'(a')_{kj}v_k, \tag{A9}$$

for all $a'\in\mathscr{A}'$ and $j=1,2,\ldots,d$. It then follows from (A8) that these representation matrix elements $\pi'(a')_{jk}$ are related to the corepresentation matrix coefficients of π^V_{jk} of (45) by

$$\pi'(a')_{jk}=\langle a',\pi^V_{jk}\rangle, \tag{A10}$$

for all $a'\in\mathscr{A}'$ and $j,k=1,2,\ldots,d$.

The *right regular action* R of $\mathscr{G}$ is defined by

$$[R(x\otimes f\,)](y)=f(yx), \tag{A11}$$

for all elements $x,y\in\mathscr{G}$ and all functions f defined on $\mathscr{G}$, where yx is evaluated using the group multiplication operation of $\mathscr{G}$. This definition (A11) can be immediately extended to all $x,y\in\mathscr{A}'$, with f being any element of $\mathscr{A}$. It is then easy to verify that R is a *left* action of $\mathscr{A}'$ with carrier space $\mathscr{A}$, and, using (A6) (or its equivalents), that it is the left action that corresponds to the right regular coaction $\pi^R_{\mathscr{A}}$ of $\mathscr{A}$ that was defined in (80). Then, by (A7),

$$R(x\otimes f\,)=[M_{\mathscr{A},\mathbb{C}}\circ(id\otimes ev)\circ(\sigma\otimes id)\circ(id\otimes\Delta)](x\otimes f\,), \tag{A12}$$

for all $x\in\mathscr{A}'$ and all $f\in\mathscr{A}$, and also, by (80) and (A6),

$$\langle y,R(x\otimes f\,)\rangle=\langle y\otimes x,\Delta(\,f\,)\rangle=\langle y\otimes x,\pi^R_{\mathscr{A}}(\,f\,)\rangle, \tag{A13}$$

for all $x,y\in\mathscr{A}'$ and all $f\in\mathscr{A}$. The content of (A11) can usefully be re-expressed as

$$\hat{R}(x)f(y)=f(yx), \tag{A14}$$

by introducing an operator $\hat{R}(x)$ for each $x\in\mathscr{A}'$.

Similarly, the *left regular action* L of $\mathscr{G}$ is defined by

$$[L(x\otimes f\,)](y)=f(x^{-1}y), \tag{A15}$$

for all elements $x,y\in\mathscr{G}$ and all functions f defined on $\mathscr{G}$, which immediately extends to all $x,y\in\mathscr{A}'$ and all $f\in\mathscr{A}$. Then L is the left action of $\mathscr{A}'$ that corresponds to the left regular coaction $\pi^L_{\mathscr{A}}$ of $\mathscr{A}$ that was defined in (81). Thus, by (A7),

$$L(x\otimes f\,)=[M_{\mathscr{A},\mathbb{C}}\circ(id\otimes ev)\circ(\sigma\otimes id)\circ(id\otimes\pi^L_{\mathscr{A}})](x\otimes f\,), \tag{A16}$$

for all $x\in\mathscr{A}'$ and all $f\in\mathscr{A}$, and also, by (81) and (A6),

$$\langle y, L(x\otimes f\ )\rangle = \langle y\otimes x, [\sigma\circ(S\otimes id)\circ\Delta](\ f\ )\rangle = \langle y\otimes x, \pi^{L}_{\mathscr{A}}(\ f\ )\rangle, \tag{A17}$$

for all $x,y \in \mathscr{A}'$ and all $f \in \mathscr{A}$. Moreover, (A15) can be re-written as

$$\hat{L}(x)f(y) = f[S_{\mathscr{A}'}(x)y], \tag{A18}$$

by introducing an operator $\hat{L}(x)$ for each $x \in \mathscr{A}'$.

APPENDIX B: IRREDUCIBLE TENSOR OPERATORS

1. Outline of argument

The first stage is to recall the definition of irreducible tensor operators in the group theoretical context. The next stage is to cast these considerations into the language of Hopf algebras, and the final stage is to put them into a form in which they involve quantities belonging *only* to $\mathscr{A}$. The argument will be given first for the *right* regular situation, and then for the *left* regular situation. In each case the *definitions* of irreducible tensor operators will be deduced first, and motivation for the *right coactions* that appear in the consistency arguments will follow. (The diagrammatic method that is described, for example, by Majid,[37] was employed to deduce the proofs that follow, but for typographical convenience these proofs have been transcribed here into the usual purely symbolic form.)

2. Irreducible tensor operators in the group theoretical right regular representation formalism

a. Derivations of the conditions for the Q_j^{qR} and $\tilde{Q}_j^{qR}$

Let $\mathbf{\Gamma}^q$ be a d_q dimensional representation of $\mathscr{G}$. Then the irreducible tensor operators Q_j^{qR} may be defined to act on functions defined on $\mathscr{G}$ in such a way that

$$\hat{R}(x)Q_j^{qR}\hat{R}(x^{-1}) = \sum_{k=1}^{d_q} \Gamma^q_{kj}(x)Q_k^{qR}, \tag{B1}$$

for all $x \in \mathscr{G}$ and $j = 1,2,\ldots,d_q$, or, more explicitly, such that

$$[\hat{R}(x)Q_j^{qR}\hat{R}(x^{-1})][\ f(y)] = \sum_{k=1}^{d_q} \Gamma^q_{kj}(x)[Q_k^{qR}(\ f\ )](y), \tag{B2}$$

for all $x,y \in \mathscr{G}$, for all functions f defined on $\mathscr{G}$, and $j = 1,2,\ldots,d_q$. Now define $\hat{\pi}^{R\prime}_{\mathscr{L}(\mathscr{A})}(x)$ by

$$\hat{\pi}^{R\prime}_{\mathscr{L}(\mathscr{A})}(x)(Q) = \hat{R}(x)Q\hat{R}(x^{-1}), \tag{B3}$$

for all $x \in \mathscr{G}$ and for all linear operators Q that act on functions defined on $\mathscr{G}$, so that (B1) becomes

$$\hat{\pi}^{R\prime}_{\mathscr{L}(\mathscr{A})}(x)(Q_j^{qR}) = \sum_{k=1}^{d_q} \Gamma^q_{kj}(x)Q_k^{qR}, \tag{B4}$$

for all $x \in \mathscr{G}$ and $j = 1,2,\ldots,d_q$. As discussed previously in Section I (in only a slightly different context), the consistency of the definition (B4) is consequence of the assumption that $\mathbf{\Gamma}^q$ is a representation of $\mathscr{G}$ and the fact that

$$\hat{\pi}^{R\prime}_{\mathscr{L}(\mathscr{A})}(xy) = \hat{\pi}^{R\prime}_{\mathscr{L}(\mathscr{A})}(x)\,\hat{\pi}^{R\prime}_{\mathscr{L}(\mathscr{A})}(y), \tag{B5}$$

for all $x,y \in \mathscr{G}$.

As

$$\Delta_{\mathscr{A}'}(x)=x\otimes x,\quad S_{\mathscr{A}'}(x)=x^{-1}, \tag{B6}$$

for all $x\in\mathscr{G}$, it follows from (A14) and (A11) that

$$(\hat{\pi}^{R\prime}_{\mathscr{L}(\mathscr{A})}(x)(Q_j^{qR}))f(y)=[ev\circ(id\otimes R)\circ(id\otimes id\otimes Q_j^{qR})\circ(id\otimes id\otimes R)$$
$$\circ(id\otimes id\otimes S_{\mathscr{A}'}\otimes id)\circ(id\otimes\Delta_{\mathscr{A}'}\otimes id)](y\otimes x\otimes f), \tag{B7}$$

which is now well-defined for all $x,y\in\mathscr{A}'$, for all $f\in\mathscr{A}$, and $Q_j^{qR}\in\mathscr{L}(\mathscr{A})$. Thus, by (A12),

$$[\hat{\pi}^{R\prime}_{\mathscr{L}(\mathscr{A})}(x)(Q_j^{qR})]f(y)=[ev\circ(id\otimes M_{\mathscr{A},\mathbb{C}})\circ(id\otimes id\otimes ev)\circ(id\otimes\sigma\otimes id)\circ(id\otimes id\otimes\Delta)$$
$$\circ(id\otimes id\otimes Q_j^{qR})\circ(id\otimes id\otimes M_{\mathscr{A},\mathbb{C}})\circ(id\otimes id\otimes id\otimes ev)\circ(id\otimes id\otimes\sigma\otimes id)$$
$$\circ(id\otimes id\otimes id\otimes\Delta)$$
$$\circ(id\otimes id\otimes S_{\mathscr{A}'}\otimes id)\circ(id\otimes\Delta_{\mathscr{A}'}\otimes id)](y\otimes x\otimes f), \tag{B8}$$

which reduces, by (A3), to

$$[\hat{\pi}^{R\prime}_{\mathscr{L}(\mathscr{A})}(x)(Q_j^{qR})]f(y)=[M_{\mathbb{C}}\circ(ev\otimes M_{\mathbb{C}})\circ(id\otimes\sigma\otimes id)\circ(id\otimes ev\otimes id\otimes id)$$
$$\circ\{id\otimes id\otimes(\sigma\circ\Delta\circ Q_j^{qR})\otimes id\}\circ(id\otimes id\otimes\sigma)$$
$$\circ(id\otimes id\otimes ev\otimes id)\circ(id\otimes id\otimes id\otimes S\otimes id)\circ(id\otimes\Delta_{\mathscr{A}'}\otimes\sigma)$$
$$\circ(id\otimes id\otimes\Delta)](y\otimes x\otimes f), \tag{B9}$$

However, (A2) implies that

$$(ev\circ(id\otimes M)\circ(id\otimes\sigma))(x\otimes a\otimes b)=(M_{\mathbb{C}}\circ(ev\otimes ev)\circ(\Delta_{\mathscr{A}'}\otimes id\otimes id])(x\otimes a\otimes b), \tag{B10}$$

for all $a,b\in\mathscr{A}$ and all $x\in\mathscr{A}'$, so (B9) reduces to

$$(\hat{\pi}^{R\prime}_{\mathscr{L}(\mathscr{A})}(x)(Q_j^{qR}))f(y)=[M_{\mathbb{C}}\circ(ev\otimes ev)\circ(id\otimes\sigma\otimes M)\circ(id\otimes id\otimes\Delta\otimes id)$$
$$\circ(id\otimes id\otimes Q_j^{qR}\otimes S)\circ(id\otimes id\otimes\Delta)](y\otimes x\otimes f), \tag{B11}$$

and hence

$$(\hat{\pi}^{R\prime}_{\mathscr{L}(\mathscr{A})}(x)(Q_j^{qR}))f(y)=[M_{\mathbb{C}}\circ(ev\otimes ev)\circ(id\otimes\sigma\otimes id)\circ(id\otimes id\otimes id\otimes M)$$
$$\circ(id\otimes id\otimes\Delta\otimes id)\circ(id\otimes id\otimes Q_j^{qR}\otimes S)\circ(id\otimes id\otimes\Delta)\circ(id\otimes id\otimes M_{\mathscr{A},\mathbb{C}})]$$
$$\times(y\otimes x\otimes f\otimes z), \tag{B12}$$

for all $x,y\in\mathscr{A}'$, all $f\in\mathscr{A}$, $Q_j^{qR}\in\mathscr{L}(\mathscr{A})$, and all $z\in\mathbb{C}$.

Turning to the right-hand side of (B4), by (A10),

$$\sum_{k=1}^{d_q}\Gamma^q_{kj}(x)(Q_k^{qR}(f))(y)=\sum_{k=1}^{d_q}\langle x,\pi^q_{kj}\rangle\langle y,Q_k^{qR}\rangle,$$

for all $x,y\in\mathscr{A}'$, and $j=1,2,\ldots,d_q$, and hence

$$\sum_{k=1}^{d_q} \Gamma_{kj}^{q}(x)(Q_k^{qR}(\ f\ ))(y)=\sum_{k=1}^{d_q} [M_{\mathbb{C}}\circ(ev\otimes ev)\circ(id\otimes\sigma\otimes id)$$

$$\circ(id\otimes id\otimes Q_k^{qR}\otimes\pi_{kj}^{q})\circ(id\otimes id\otimes id\otimes u)](y\otimes x\otimes f\otimes z), \quad \text{(B13)}$$

for all $x,y\in\mathscr{A}'$, all $f\in\mathscr{A}$, $Q_k^{qR}\in\mathscr{L}(\mathscr{A})$, and all $z\in\mathbb{C}$.

Now (B4) implies that the expressions on the right-hand sides of (B12) and (B13) may be equated. As the first three factors of each, namely $M_{\mathbb{C}}\circ(ev\otimes ev)\circ(id\otimes\sigma\otimes id)$, are the same, the equality holds with these removed. However, on both sides of this new equality, the factor $y\otimes x$ is only acted on by a succession of identity operators of the form $id\otimes id$. Consequently both $y\otimes x$ and these identity operators can be removed, leaving the result that (B1) is equivalent to the condition

$$[(id\otimes M)\circ(\Delta\otimes id)\circ(Q_j^{qR}\otimes S)\circ\Delta\circ M_{\mathscr{A},\mathbb{C}}](\ f\otimes z)$$

$$=\sum_{k=1}^{d_q} [(Q_k^{qR}\otimes\pi_{kj}^{q})\circ(id\otimes u)](\ f\otimes z), \quad \text{(B14)}$$

for all $f\in\mathscr{A}$, all $j=1,2,\ldots,d_q$, and all $z\in\mathbb{C}$. This can be rewritten as

$$((id\otimes M)\circ(\Delta\otimes id)\circ(Q_j^{qR}\otimes S)\circ\Delta)(\ f\ )=\sum_{k=1}^{d_q} Q_k^{qR}(\ f\ )\otimes\pi_{kj}^{q}, \quad \text{(B15)}$$

for all $f\in\mathscr{A}$ and all $j=1,2,\ldots,d_q$, which is the condition (148).

Because M is indistinguishable from $M\circ\sigma$ and S is indistinguishable from S^{-1} in the situation being considered here, the above arguments would equally well apply with each of the following 3 substitutions.

(1) Replace M by $M\circ\sigma$, but leave S unchanged;
(2) leave M unchanged, but replace S by S^{-1};
(3) replace M by $M\circ\sigma$ *and* replace S by S^{-1}.

However, in the general case in which $\mathscr{A}$ is non- commutative, the possibilities (1) and (2) are *excluded* because with them the identity operator would not be an irreducible tensor operator belonging to the identity corepresentation. Of course, with the substitution (3), (148) changes into (155), which is the defining condition for a *twisted* irreducible tensor operator $\widetilde{Q}_j^{qR}$.

b. Derivations of the right coactions $\pi^{R}_{\mathscr{L}(\mathscr{A})}$ and $\tilde{\pi}^{R}_{\mathscr{L}(\mathscr{A})}$

First recast (B3) as

$$\pi^{R\prime}_{\mathscr{L}(\mathscr{A})}(x\otimes Q)=\hat{R}(x)Q\hat{R}(x^{-1}), \quad \text{(B16)}$$

for all $x\in\mathscr{G}$ and for all linear operators Q that act on functions defined on $\mathscr{G}$, where $\pi^{R\prime}_{\mathscr{L}(\mathscr{A})}$ is a mapping from $\mathscr{A}'\otimes\mathscr{L}(\mathscr{A})$ into $\mathscr{L}(\mathscr{A})$. In Hopf algebra language, this can be re-expressed as

$$\pi^{R\prime}_{\mathscr{L}(\mathscr{A})}(x\otimes Q)=[\hat{M}\circ(id\otimes\hat{M})\circ(\hat{R}\otimes id\otimes\hat{R})\circ(id\otimes\sigma)\circ(id\otimes S_{\mathscr{A}'}\otimes id)\circ(\Delta_{\mathscr{A}'}\otimes id)](x\otimes Q), \quad \text{(B17)}$$

where $\hat{M}$ is the operator multiplication operator defined in (179). It is then easily shown that $\pi^{R\prime}_{\mathscr{L}(\mathscr{A})}$ is a left action of $\mathscr{A}'$ with carrier space $\mathscr{L}(\mathscr{A})$.

This expression for $\pi^{R\prime}_{\mathscr{L}(\mathscr{A})}$ can be re- expressed in terms of the structure constants introduced in Section II with respect to the basis $a_1, a_2, \ldots$ of $\mathscr{A}$, and the basis $a^1, a^2, \ldots$ of its dual $\mathscr{A}'$. First define the operators $\mathscr{P}^k_j$ by

$$\mathscr{P}^k_j(a) = \langle a^k, a\rangle a_j \tag{B18}$$

(for all $a \in \mathscr{A}$ and all $j,k = 1,2,\ldots$), and then define the matrix elements q^k_j of Q by

$$q^k_j = \langle a^k, Q(a_j)\rangle \tag{B19}$$

(for all $j,k = 1,2,\ldots$). Clearly the operators $\mathscr{P}^k_j$ are members of $\mathscr{L}(\mathscr{A})$, and any operator Q of $\mathscr{L}(\mathscr{A})$ can be expressed as $Q = \Sigma_{j,k} Q^j_k \mathscr{P}^k_j$. Then, by (A13) and (B18),

$$\hat{R}(a^m) = \sum_{j,k=1}^{g} \mu_k^{jm} \mathscr{P}^k_j, \tag{B20}$$

for all $m = 1,2,\ldots,g$. On substituting (B20) into (B17), and using (A2) and (A3), it follows that

$$\pi^{R\prime}_{\mathscr{L}(\mathscr{A})}(a^m \otimes Q) = \sum_{i,j,k,\ell,u,v,w=1}^{g} (m^m_{uv} s^v_w \mu_i^{ju} \mu_k^{\ell w} q^i_\ell) \mathscr{P}^k_j, \tag{B21}$$

for all $Q \in \mathscr{L}(\mathscr{A})$ and all $m = 1,2,\ldots,g$.

Using (A8), the corresponding right coaction $\pi^R_{\mathscr{L}(\mathscr{A})}$ of $\mathscr{A}$ with the same carrier space $\mathscr{L}(\mathscr{A})$ is given by

$$\pi^R_{\mathscr{L}(\mathscr{A})}(Q) = \sum_{m=1}^{g} \pi^{R\prime}_{\mathscr{L}(\mathscr{A})}(a^m \otimes Q) \otimes a_m, \tag{B22}$$

for all $Q \in \mathscr{L}(\mathscr{A})$. Thus

$$\pi^R_{\mathscr{L}(\mathscr{A})}(Q) = \sum_{i,j,k,\ell,m,u,v,w=1}^{g} (m^m_{uv} s^v_w \mu_i^{ju} \mu_k^{\ell w} q^i_\ell)(\mathscr{P}^k_j \otimes a_m),$$

for all $Q \in \mathscr{L}(\mathscr{A})$. The final stage is to re-express this in a basis free form. This can be done by writing

$$\pi^R_{\mathscr{L}(\mathscr{A})}(Q) = \sum_{[Q]} Q_{[1]} \otimes Q_{[2]},$$

where $Q_{[1]} \in \mathscr{L}(\mathscr{A})$ and $Q_{[1]} \in \mathscr{A}$ are such that

$$\sum_{[Q]} Q_{[1]}(a) \otimes Q_{[2]} = [(id \otimes M) \circ (\Delta \otimes id) \circ (Q \otimes S) \circ \Delta](a),$$

for all $Q \in \mathscr{L}(\mathscr{A})$ and all $a \in \mathscr{A}$.

The right coaction $\tilde{\pi}^R_{\mathscr{L}(\mathscr{A})}$ is obtained from $\pi^R_{\mathscr{L}(\mathscr{A})}$ by replacing M by $M \circ \sigma$ and replacing S by S^{-1}. The right coactions $\pi^R_{\mathscr{T}(\mathscr{A})}$ and $\tilde{\pi}^R_{\mathscr{T}(\mathscr{A})}$ of Sections VI B 1 and VI B 2 have essentially the same definitions as $\pi^R_{\mathscr{L}(\mathscr{A})}$ and $\tilde{\pi}^R_{\mathscr{L}(\mathscr{A})}$, except that their domains are restricted to the appropriate subspaces $\mathscr{T}(\mathscr{A})$.

3. Irreducible tensor operators in the group theoretical left regular representation formalism

a. Derivations of the conditions for the Q_j^{qL} and $\tilde{Q}_j^{qL}$

The argument for the *left* regular formalism follows exactly the same line as that for the right regular case given above up to (B7), the only differences being that the operators $\hat{R}(x)$ must be replaced by the operators $\hat{L}(x)$, the left action R must be replaced by the left action L, and the label R must be replaced by L on the irreducible tensor operators Q_j^{qR} on the left action $\pi^{R\prime}_{\mathscr{L}(\mathscr{A})}$, and on the corresponding right coaction $\pi^{R}_{\mathscr{L}(\mathscr{A})}$. Thus, by (A16), the analogue of (B8) is

$$\begin{aligned}(\hat{\pi}^{L\prime}_{\mathscr{L}(\mathscr{A})}(x)(Q_j^{qL}))f(y)(=\hat{L}(x)Q_j^{qL}\hat{L}(x^{-1}))&\\ =[ev\circ(id\otimes M_{\mathscr{A},\mathbb{C}})\circ(id\otimes id\otimes ev)&\\ \circ(id\otimes\sigma\otimes id)\circ(id\otimes id\otimes\sigma)\circ(id\otimes id\otimes S\otimes id)&\\ \circ(id\otimes id\otimes\Delta)\circ(id\otimes id\otimes Q_j^{qL})\circ(id\otimes id\otimes M_{\mathscr{A},\mathbb{C}})&\\ \circ(id\otimes id\otimes id\otimes ev)\circ(id\otimes id\otimes\sigma\otimes id)\circ(id\otimes id\otimes id\otimes\sigma)&\\ \circ(id\otimes id\otimes id\otimes S\otimes id)\circ(id\otimes id\otimes id\otimes\Delta)&\\ \circ(id\otimes id\otimes S_{\mathscr{A}'}\otimes id)\circ(id\otimes\Delta_{\mathscr{A}'}\otimes id)](y\otimes x\otimes f\ ),&\end{aligned}\tag{B23}$$

which reduces, by (A3), (B10), and (16) to

$$\begin{aligned}(\hat{\pi}^{L\prime}_{\mathscr{L}(\mathscr{A})}(x)(Q_j^{qL}))f(y)=[M_{\mathbb{C}}\circ(ev\otimes ev)\circ(id\otimes\sigma\otimes id)\circ(id\otimes id\otimes\sigma)\circ(id\otimes id\otimes S\otimes id)&\\ \circ(id\otimes id\otimes M\otimes id)&\\ \circ(id\otimes id\otimes id\otimes\Delta)\circ(id\otimes id\otimes S\otimes Q_j^{qL})&\\ \circ(id\otimes id\otimes\Delta)\circ(id\otimes id\otimes M_{\mathscr{A},\mathbb{C}})](y\otimes x\otimes f\otimes z),&\end{aligned}\tag{B24}$$

for all $x,y\in\mathscr{A}'$, all $f\in\mathscr{A}$, $Q_j^{qL}\in\mathscr{L}(\mathscr{A})$, and all $z\in\mathbb{C}$.

The right-hand side of the irreducible tensor operator definition that corresponds to this is

$$\begin{aligned}\sum_{k=1}^{d_q}\Gamma^q_{kj}(x)(Q_k^{qL}(\ f\ ))(y)=\sum_{k=1}^{d_q}[M_{\mathbb{C}}\circ(ev\otimes ev)\circ(id\otimes\sigma\otimes id)\circ(id\otimes id\otimes Q_k^{qL}\otimes\pi^q_{kj})&\\ \circ(id\otimes id\otimes id\otimes u)](y\otimes x\otimes f\otimes z),&\end{aligned}\tag{B25}$$

for all $x,y\in\mathscr{A}'$, all $f\in\mathscr{A}$, $Q_k^{qL}\in\mathscr{L}(\mathscr{A})$, and all $z\in\mathbb{C}$.

Equating the right-hand sides (B24) and(B25), removing the common first three factors $[M_{\mathbb{C}}\circ(ev\otimes ev)\circ(id\otimes\sigma\otimes id)]$ of each, and removing the factor $y\otimes x$ and the succession of identity operators of the form $id\otimes id$ that act on $y\otimes x$, it follows that the defining condition becomes

$$\begin{aligned}[\sigma\circ(S\otimes id)\circ(M\otimes id)\circ(id\otimes\Delta)\circ(S\otimes Q_j^{qL})\circ\Delta\circ M_{\mathscr{A},\mathbb{C}}](\ f\otimes z)&\\ =\sum_{k=1}^{d_q}[(Q_k^{qL}\otimes\pi^q_{kj})\circ(id\otimes u)](\ f\otimes z),&\end{aligned}\tag{B26}$$

for all $f\in\mathscr{A}$, all $j=1,2,\ldots,d_q$, and all $z\in\mathbb{C}$. This can be rewritten as

$$[\sigma\circ(S\otimes id)\circ(M\otimes id)\circ(id\otimes\Delta)\circ(S\otimes Q_j^{qL})\circ\Delta](\ f\ )=\sum_{k=1}^{d_q}Q_k^{qL}(\ f\ )\otimes\pi^q_{kj},\tag{B27}$$

for all $f \in \mathscr{A}$ and all $j=1,2,\ldots,d_q$, which is the condition (161).

Because $\Delta_{\mathscr{A}'}$ is indistinguishable from $\sigma \circ \Delta_{\mathscr{A}'}$ and $S_{\mathscr{A}'}$ is indistinguishable from $S^{-1}_{\mathscr{A}'}$ in the situation being considered here, the above arguments would equally well apply to (B23) with each of the following 3 substitutions.

(1) Replace $\Delta_{\mathscr{A}'}$ by $\sigma \circ \Delta_{\mathscr{A}'}$, but leave $S_{\mathscr{A}'}$ unchanged;
(2) leave $\Delta_{\mathscr{A}'}$ unchanged, but replace $S_{\mathscr{A}'}$ by $S^{-1}_{\mathscr{A}'}$;
(3) (c) replace $\Delta_{\mathscr{A}'}$ by $\sigma \circ \Delta_{\mathscr{A}'}$ *and* replace $S_{\mathscr{A}'}$ by $S^{-1}_{\mathscr{A}'}$.

In each case the S factor in (B23) should be left unchanged because it comes from the definition (81) of the left regular (right) coaction. [Replacing S by S^{-1} in (81) would give another right coaction, but the original one is merely the double contragredient of this.] In the general case in which $\mathscr{A}$ is non-commutative, the possibilities (1) and (2) are again *excluded* because with them the identity operator would not be an irreducible tensor operator belonging to the identity corepresentation. However, with the substitution (3), the analogue of (161) is (166), which is the defining condition for a *twisted* irreducible tensor operator $\tilde{Q}^{qL}_j$.

b. Derivations of the right coactions $\pi^L_{\mathscr{L}(\mathscr{A})}$ and $\tilde{\pi}^L_{\mathscr{L}(\mathscr{A})}$

The *left* regular analogues of (B16) and (B17) are

$$\pi^{L\prime}_{\mathscr{L}(\mathscr{A})}(x\otimes Q)=\hat{L}(x)Q\hat{L}(x^{-1})$$

and

$$\pi^{L\prime}_{\mathscr{L}(\mathscr{A})}(x\otimes Q)=[\hat{M}\circ(id\otimes\hat{M})\circ(\hat{L}\otimes id\otimes\hat{L})\circ(id\otimes\sigma)\circ(id\otimes S_{\mathscr{A}'}\otimes id)\circ(\Delta_{\mathscr{A}'}\otimes id)](x\otimes Q), \tag{B28}$$

where $\pi^{L\prime}_{\mathscr{L}(\mathscr{A})}$ is a left action of $\mathscr{A}'$ with carrier space $\mathscr{L}(\mathscr{A})$. However, by (A17) and (B18), and with the basis of $\mathscr{A}'$ defined above,

$$\hat{L}(a^m)=\sum_{j,k,\ell=1}^{g}\mu^{\ell j}_k s^m_\ell \mathscr{P}^k_j, \tag{B29}$$

for all $m=1,2,\ldots,g$. On substituting (B29) into (B28), and using (A2) and (A3), it follows that

$$\pi^{L\prime}_{\mathscr{L}(\mathscr{A})}(a^m\otimes Q)=\sum_{i,j,k,\ell,n,u,v,w=1}^{g}(m^v_{wu}s^m_v s^w_n \mu^{uj}_i \mu^{n\ell}_k q^i_\ell)\mathscr{P}^k_j,$$

for all $Q \in \mathscr{L}(\mathscr{A})$ and all $m=1,2,\ldots,g$.

Then, using (A8), the corresponding right coaction $\pi^L_{\mathscr{L}(\mathscr{A})}$ of $\mathscr{A}$ with the same carrier space $\mathscr{L}(\mathscr{A})$ is given by

$$\pi^L_{\mathscr{L}(\mathscr{A})}(Q)=\sum_{m=1}^{g}\pi^{L\prime}_{\mathscr{L}(\mathscr{A})}(a^m\otimes Q)\otimes a_m,$$

for all $Q \in \mathscr{L}(\mathscr{A})$. Thus

$$\pi^L_{\mathscr{L}(\mathscr{A})}(Q)=\sum_{i,j,k,\ell,m,n,u,v,w=1}^{g}(m^v_{wu}s^m_v s^w_n \mu^{uj}_i \mu^{n\ell}_k q^i_\ell)(\mathscr{P}^k_j\otimes a_m),$$

for all $Q \in \mathscr{L}(\mathscr{A})$. The final stage is to re-express this in a basis free form, which can be done by writing

$$\pi^{L}_{\mathscr{L}(\mathscr{A})}(Q)=\sum_{[Q]} Q_{[1]}\otimes Q_{[2]},$$

where $Q_{[1]} \in \mathscr{L}(\mathscr{A})$ and $Q_{[1]} \in \mathscr{A}$ are such that

$$\sum_{[Q]} Q_{[1]}(a)\otimes Q_{[2]}=[\sigma\circ(S\otimes id)\circ(M\otimes id)\circ(id\otimes\Delta)\circ(S\otimes Q)\circ\Delta](a),$$

for all $Q \in \mathscr{L}(\mathscr{A})$ and all $a \in \mathscr{A}$.

For the corresponding twisted coaction $\tilde{\pi}^{L}_{\mathscr{L}(\mathscr{A})}$ the argument is similar. With the substitutions $\Delta_{\mathscr{A}'}\rightarrow\sigma\circ\Delta_{\mathscr{A}'}$ and $S_{\mathscr{A}'}\rightarrow S^{-1}_{\mathscr{A}'}$, (B28) gives

$$\tilde{\pi}^{L\prime}_{\mathscr{L}(\mathscr{A})}(x\otimes Q)=[\hat{M}\circ(id\otimes\hat{M})\circ(\hat{L}\otimes id\otimes\hat{L})\circ(id\otimes\sigma)\circ(id\otimes S^{-1}_{\mathscr{A}'}\otimes id)\circ((\sigma\otimes\Delta_{\mathscr{A}'})\otimes id)](x\otimes Q), \tag{B30}$$

where $\tilde{\pi}^{L\prime}_{\mathscr{L}(\mathscr{A})}$ is another left action of $\mathscr{A}'$ with carrier space $\mathscr{L}(\mathscr{A})$. By (B29) and (29), this gives

$$\tilde{\pi}^{L\prime}_{\mathscr{L}(\mathscr{A})}(a^{m}\otimes Q)=\sum_{i,j,k,\ell,n,u,v=1}^{g}(m^{m}_{nv}s^{v}_{u}\mu^{uj}_{i}\mu^{n\ell}_{k}q^{i}_{\ell})\mathscr{P}^{k}_{j},$$

for all $Q \in \mathscr{L}(\mathscr{A})$ and all $m=1,2,\ldots,g$. Using (A8), the corresponding right coaction $\tilde{\pi}^{L}_{\mathscr{L}(\mathscr{A})}$ of $\mathscr{A}$ with the same carrier space $\mathscr{L}(\mathscr{A})$ is given by

$$\tilde{\pi}^{L}_{\mathscr{L}(\mathscr{A})}(Q)=\sum_{m=1}^{g}\tilde{\pi}^{L\prime}_{\mathscr{L}(\mathscr{A})}(a^{m}\otimes Q)\otimes a_{m},$$

for all $Q \in \mathscr{L}(\mathscr{A})$. Thus

$$\tilde{\pi}^{L}_{\mathscr{L}(\mathscr{A})}(Q)=\sum_{i,j,k,\ell,m,n,u,v=1}^{g}(m^{m}_{nv}s^{v}_{u}\mu^{uj}_{i}\mu^{n\ell}_{k}q^{i}_{\ell})(\mathscr{P}^{k}_{j}\otimes a_{m}),$$

for all $Q \in \mathscr{L}(\mathscr{A})$. This can be re-expressed in a basis free form by writing

$$\tilde{\pi}^{L}_{\mathscr{L}(\mathscr{A})}(Q)=\sum_{[Q]} Q_{[1]}\otimes Q_{[2]},$$

where $Q_{[1]} \in \mathscr{L}(\mathscr{A})$ and $Q_{[1]} \in \mathscr{A}$ are such that

$$\sum_{[Q]} Q_{[1]}(a)\otimes Q_{[2]}=[(id\otimes M)\circ(\sigma\otimes S)\circ(id\otimes\sigma)\circ(id\otimes\Delta)\circ(id\otimes Q)\circ\Delta](a),$$

for all $Q \in \mathscr{L}(\mathscr{A})$ and all $a \in \mathscr{A}$.

The right coactions $\pi^{L}_{\mathscr{T}(\mathscr{A})}$ and $\tilde{\pi}^{L}_{\mathscr{T}(\mathscr{A})}$ of Sections VI C 1 and VI C 2 have essentially the same definitions as $\pi^{L}_{\mathscr{L}(\mathscr{A})}$ and $\tilde{\pi}^{L}_{\mathscr{L}(\mathscr{A})}$, except that their domains are restricted to the appropriate subspaces $\mathscr{T}(\mathscr{A})$.

APPENDIX C: PROJECTION OPERATORS

The *right* regular formalism will be considered first. If $\mathbf{\Gamma}^p$ is a unitary irreducible representation of dimension d_p of a finite group $\mathscr{G}$ of order g, the projection operators in the right regular formalism are defined by

$$\mathscr{P}^{pR}_{mn}=\left(\frac{d_p}{g}\right)\sum_{x\in\mathscr{G}}\Gamma^p(x)^*_{mn}\hat{R}(x),$$

for all $m,n=1,2,\ldots,d_p$. This can be re-written as

$$\mathscr{P}^{pR}_{mn}=\left(\frac{d_p}{g}\right)\sum_{x\in\mathscr{G}}\Gamma^p(x^{-1})^*_{nm}\hat{R}(x),$$

and hence, by (A10), (A14), (A11), and (B6),

$$\langle y,\mathscr{P}^{pR}_{mn}f\rangle=\left(\frac{d_p}{g}\right)\sum_{x\in\mathscr{G}}\langle S_{\mathscr{A}'}(x),\pi^p_{nm}\rangle\langle y,R(x\otimes f\ )\rangle,$$

for all $m,n=1,2,\ldots,d_p$. Here the π^p_{nm} are the matrix coefficients of the corepresentation π^p of $\mathscr{A}$ that is dual to $\mathbf{\Gamma}^p$. Then, by (A13), for all $x,y\in\mathscr{A}'$ and all $f\in\mathscr{A}$,

$$\langle y,\mathscr{P}^{pR}_{mn}f\rangle=\left(\frac{d_p}{g}\right)\sum_{x\in\mathscr{G}}\langle[(id\otimes id\otimes S_{\mathscr{A}'})\circ(id\otimes\Delta_{\mathscr{A}'})](y\otimes x),(\pi^R_{\mathscr{A}}(\ f\ )\otimes\pi^p_{nm})\rangle,$$

and so, by (52) and (72),

$$\langle y,\mathscr{P}^{pR}_{mn}f\rangle=\left(\frac{d_p}{g}\right)\sum_{x\in\mathscr{G}}\langle(y\otimes x),[(id\otimes M)\circ(id\otimes id\otimes S)](\pi^R_{\mathscr{A}}(\ f\ )\otimes\pi^p_{nm})\rangle. \tag{C1}$$

But the Haar functional is such that

$$h(a)=\left(\frac{1}{g}\right)\sum_{x\in\mathscr{G}}\langle x,a\rangle,$$

for all $a\in\mathscr{A}$, so (C1), (83), and (52) imply that

$$\mathscr{P}^{pR}_{mn}\ f=d_p\sum_{[\ f\ ]}f^R_{[1]}h[M(\ f^R_{[2]}\otimes\pi^{p*}_{mn})]. \tag{C2}$$

As multiplication is commutative in this special case, this could equally well be written as

$$\mathscr{P}^{pR}_{mn}\ f=d_p\sum_{[\ f\ ]}f^R_{[1]}h[M(\pi^{p*}_{mn}\otimes f^R_{[2]})], \tag{C3}$$

for all $m,n=1,2,\ldots,d_p$. In the general case the two formulae (C2) and (C3) are different, but the arguments given in Section IV B show that (C3) [i.e., (107)] is actually the correct choice.

The argument in the *left* regular formalism follows exactly the same line, and can be obtained by merely replacing the label R by L at each stage.

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Metrics and pairs of left and right connections on bimodules

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Properties of metrics and pairs consisting of left and right connections are studied on the bimodules of differential 1-forms. Those bimodules are obtained from the derivation based calculus of an algebra of matrix valued functions, and an $SL_q(2,\mathbb{C})$-covariant calculus of the quantum plane at a generic q and the cubic root of unity. It is shown that, in the aforementioned examples, giving up the middle-linearity of metrics significantly enlarges the space of metrics. A metric compatibility condition for the pairs of left and right connections is defined. Also, a compatibility condition between a left and right connection is discussed. Consequences entailed by reducing to the center of a bimodule the domain of those conditions are investigated in detail. Alternative ways of relating left and right connections are considered. © *1996 American Institute of Physics.* [S0022-2488(96)00408-2]

I. INTRODUCTION

Motivated to a great extent by the need to reconcile the geometric theory of gravity with the (noncommutative) operator algebraic theory of quantum physics, there is considerable interest in generalizing the formalism of General Relativity to the realm of Noncommutative Differential Geometry.[1] In this paper, we study three concepts that are apparently needed for such a generalization: metric, linear connection and metric compatibility condition.

We define a metric $g:E\times E\to A$ as a τ-symmetric A-bilinear pairing on an A-bimodule E, where τ is some generalized permutation. Then we argue that giving up the (often postulated) requirement that a metric factor to a map defined on $E\otimes_A E$ one can obtain an essentially bigger space of metrics. In particular, we provide an example with an ample supply of τ-symmetric metrics but where the requirement that a τ-symmetric metric g descend to $E\otimes_A E$ amounts to demanding that $g=0$ (see Remark 1).

Inspired by Ref. 2 on the one hand and by Ref. 3 on the other, we consider a pair of mutually compatible connections on a bimodule. The first connection of such a compatible pair is a left connection in the sense that it satisfies the Leibniz rule with respect to the left module structure. Similarly, the second connection is a right connection in the sense that it fulfills the Leibniz rule

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on the right. The compatibility condition is simply a requirement that the left and the right connection agree on the center of a bimodule up to a bimodule isomorphism σ (e.g., braiding). This bimodule isomorphism is, again, a generalized permutation. Restricting the domain of the aforementioned left-right compatibility condition to the center of a bimodule permits, at least in the considered examples, a significantly bigger space of solutions to this condition. (This seems desired at least from the point of view of developing variational calculus on the space of connections.)

As to the compatibility between metrics and pairs of left and right connections, we define a 2-parameter family of compatibility conditions, but then restrict ourselves to the one that seems the most natural.

In the first section, we provide the general formalism and fix the notation. Then we proceed to the first example, where A is the algebra of matrix valued functions on a parallelizable manifold, and $E=A^1$ is the bimodule of 1-forms of the derivation based differential calculus equipped with the pullback-of-permutation automorphism. Next we pass on to the quantum plane and the differential calculus with the braiding employed in Ref. 2. First we consider the case of a generic q, and then the case of the cubic root of unity. To obtain a nonzero τ-symmetric metric on the quantum plane we have to ''rescale'' the braiding σ used in Ref. 2 by q^2. The thus obtained automorphism τ appears to be in better agreement with the theory presented in Ref. 4. (Even though in this case both automorphisms can be considered over the same domain, they are different deformations of the usual tensor product permutation.)

In what follows, Einstein's convention of summing over repeating indices is assumed, and the unadorned tensor product stands for the tensor product over a field.

II. GENERAL DEFINITIONS

Let A be a unital associative algebra over a field k, and E be a left and right projective A-bimodule. We begin with a definition of a linear pairing $g:E\times E\to A$, which, for the sake of simplicity (neglecting the nondegeneracy and reality conditions), we call a metric on E (cf. Section 8 and Section 9 in Ref. 5).

Definition 1: *Let $\tau:E\otimes E\to E\otimes E$ be a bimodule automorphism. A linear map g from $E\otimes E$ to A is called a* τ-symmetric metric *on E* (*or simply* metric, *if no confusion arises*) *iff it is*

(1) bilinear over A, i.e., $g(a\zeta,\rho b)=ag(\zeta,\rho)b$, $\forall\zeta,\rho\in E$, $a,b\in A$;

(2) τ-symmetric, i.e., $g\circ\tau=g$.

Note that if E is a central bimodule,[6,5] that is, if the left and right multiplications by the elements of $Z(A)$ coincide on any element of E (which is always the case in the examples considered in this article), then any metric g can be regarded as a map from $E\otimes_{Z(A)}E$ to A. We would like to emphasize here that, contrary to many other papers (e.g., see (10) in Ref. 7), we do not require g to be well-defined on $E\otimes_A E$. As we show in our three examples, a requirement like this (which goes under the name of middle-linearity) can be considered too restrictive (see Proposition 1, Remark 1 and Proposition 5). Giving up the middle-linearity condition allows us to get rid of those restrictions.

Another structure on a bimodule E that we wish to discuss is a pair of compatible left and right connections.

Definition 2: *Let (A^1,d) be a first order differential calculus on A, and*

$$\sigma:E\otimes_A A^1\to A^1\otimes_A E$$

be a bimodule isomorphism. Also, let ∇^L be a left connection, i.e., a linear map from E to $A^1\otimes_A E$ satisfying the left Leibniz rule,

$$\nabla^L(a\zeta)=da\otimes_A\zeta+a\nabla^L\zeta,\quad\forall a\in A,\zeta\in E,$$

and let ∇^R *be a right connection, i.e. a linear map from* E *to* $E\otimes_A A^1$ *fulfilling the right Leibniz rule,*

$$\nabla^R(\zeta a)=(\nabla^R\zeta)a+\zeta\otimes_A da,\quad \forall a\in A,\zeta\in E.$$

A pair (∇^L,∇^R) *is called* σ-compatible *iff*

$$\forall\zeta\in Z(E):\quad \nabla^L\zeta=(\sigma\circ\nabla^R)\zeta, \tag{1}$$

where $Z(E):=\{\zeta\in E\,|\,a\zeta=\zeta a,\quad \forall a\in A\}$ *is the center of* E.

Let us recall that in Section 8 of Ref. 3 a connection on a bimodule is also defined as a pair consisting of a left and right connection. There, however, instead of σ-compatibility condition (1), the condition of ∇^L being a right A-homomorphism and ∇^R being a left A-homomorphism is imposed. The latter condition, albeit it permits for an interesting algebraic theory, cannot be directly transferred to the commutative case $Z(E)=E$. On the other hand, defining a connection on a bimodule by requiring, much as in Definition 3.2 in Ref. 8, that the σ-compatibility condition is fulfilled on the whole bimodule E rather than just its center $Z(E)$, automatically yields, for the appropriate σ (i.e., the usual tensor product flip), the standard definition of a connection in the classical case, but entails essential restrictions on the space of connections in noncommutative examples (see (10), (19), (32),[9] and Theorem 5.6 in Ref. 8; cf. Lemma 1 in Ref. 5). If we demand that the equality $\nabla^L=\sigma\circ\nabla^R$be satisfied on the whole bimodule E, we can equivalently think of a pair (∇^L,∇^R) as a left connection ∇^L fulfilling an additional (right) Leibniz rule of the form

$$\nabla^L(\zeta a)=(\nabla^L\zeta)a+\sigma(\zeta\otimes_A da),\quad \forall a\in A,\zeta\in E$$

(cf. the Introduction in Ref. 10). In the classical differential geometry, with the help of the tensor product flip, any left connection uniquely determines the corresponding right connection, and vice-versa, without imposing any limitations on either of the connections. As we demonstrate in the next section, this is precisely what happens with pairs of σ-compatible connections in the noncommutative example of a ''matrix geometry'' (see Proposition 2). A very similar result (Proposition 6) is obtained for a bimodule of differential 1-forms on the quantum plane (see Proposition 2 in Ref. 11) at the cubic root of unity. (In fact, in all examples presented in this paper, we put $E=A^1$, so that the pairs of σ-compatible connections studied here can be thought of as linear connections.) When dealing with connections and metrics, it seems that in both cases we have the same mechanism at work: solving constraints over just the commutative part allows solutions to be parametrized by a whole noncommutative algebra, whereas solving them over an entire noncommutative space renders the solutions parametrized by the center of an algebra. The examples of subsequent sections allow us to explore this mechanism in some detail.

Let us now consider possible compatibility conditions between a pair of connections (∇^L,∇^R) and a metric g. In order to do so, first we must define two extensions of g:

$$\check{g}:A^1\otimes_A E\otimes E\to A^1 \text{ and } \hat{g}:E\otimes E\otimes_A A^1\to A^1.$$

It appears natural to choose

$$\check{g}(\alpha\otimes_A\zeta,\rho)=\alpha g(\zeta,\rho),\quad \forall\alpha\in A^1,\zeta,\rho\in E; \tag{2}$$

$$\hat{g}(\zeta,\rho\otimes_A\alpha)=g(\zeta,\rho)\alpha,\quad \forall\alpha\in A^1,\zeta,\rho\in E. \tag{3}$$

In principle, one can formulate the class of metric compatibility conditions by requiring the diagram

$$\begin{array}{ccccc} E\otimes E & \xrightarrow{f_L(t)\otimes id\oplus id\otimes f_R(s)} & (A^1\otimes_A E\otimes E)\oplus(E\otimes E\otimes_A A^1) & & \\ \downarrow g & & \downarrow \check{g}\oplus\hat{g}, & & \\ A & \xrightarrow{d} & A^1 & \xleftarrow{+} & A^1\oplus A^1, \end{array} \tag{4}$$

where $f_L(t):=(1-t)\nabla^L+t(\sigma\circ\nabla^R)$, $f_R(s):=s(\sigma^{-1}\circ\nabla^L)+(1-s)\nabla^R$, $t,s\in k$, to commute. Here, however, in order to ensure that $f_L(t)$ and $f_R(s)$ are connections, we settle for the particular case $t=0=s$.

Definition 3: *We say that a pair of connections* (∇^L,∇^R) is compatible with g *iff*

$$dg(\zeta,\rho)=\check{g}(\nabla^L\zeta,\rho)+\hat{g}(\zeta,\nabla^R\rho),\quad \forall\zeta,\rho\in E. \tag{5}$$

As we show in Proposition 7, formula (5) is not always sensitive to whether we consider it over E or only over $Z(E)$. Observe that, if (1) is satisfied, then on the center of a bimodule we have $f_L(t)=\nabla^L$ and $f_R(s)=\nabla^R$ for any values of $t,s\in k$, and, consequently, all metric compatibility conditions for a pair of σ-compatible connections are equivalent when considered over $Z(E)$. Finally, let us remark that the metric compatibility condition for a pair of connections related by $\nabla^L=\sigma\circ\nabla^R$ (on the whole bimodule) that is given by (1.21) and (1.26) in Ref. 2 seems inappropriate for the cases when the metric is not middle-linear.

Next, we apply the above definitions in some quantum geometric models.

III. ALGEBRAS OF MATRIX VALUED FUNCTIONS

Let us choose $A=C^\infty(M)\otimes M_n(\mathbb{C})$, $E=A^1=\mathrm{Hom}_{Z(A)}(\mathrm{Der}A,A)$,

$$\tau(\alpha\otimes\beta)(X,Y)=(\alpha\otimes\beta)(Y,X),\quad \forall X,Y\in \mathrm{Der}A,$$

and σ equal to τ factored to an automorphism of $A^1\otimes_A A^1$. Here M is a parallelizable manifold of dimension m, and the ground field of A is the field of complex numbers. Now, let $\{\theta^i\}_{i\in\{1,\ldots,m+n^2-1\}}$ be the basis of A^1 as defined in Section 3 of Ref. 10. An important property of this basis is that

$$a\,\theta^i=\theta^i a,\quad \forall a\in A,\quad i\in\{1,\ldots,m+n^2-1\}, \tag{6}$$

$$\tau(\theta^i\otimes\theta^j)=\theta^j\otimes\theta^i,\quad \forall a\in A,\quad i,j\in\{1,\ldots,m+n^2-1\}. \tag{7}$$

In this setting, one can immediately verify the following claim (cf. Section 9 in Ref. 5 and p. 5861 in Ref. 10).

Proposition 1: *Let* g^{ij} *denote* $g(\theta^i\otimes\theta^j)$, *where* $i,j\in\{1,\ldots,m+n^2-1\}$. *The map* $\psi:g\mapsto(g^{ij})$ *provides a one-to-one correspondence between the metrics (the middle-linear metrics) on* A^1 *and the symmetric matrices of* $M_{m+n^2-1}(A)$ [*the symmetric matrices of* $M_{m+n^2-1}(Z(A))$, *respectively*].

In the same basis, let us define the Christoffel symbols of ∇^L and ∇^R by

$$\nabla^L\theta^i=\theta^j\otimes_A\theta^k\Gamma^i_{jk},\quad \nabla^R\theta^i=\theta^j\otimes_A\theta^k\widetilde{\Gamma}^i_{jk}. \tag{8}$$

Taking into account (6) and (7) and noticing that $\{\theta^i\}_{i\in\{1,\ldots,m+n^2-1\}}$ is also a basis of the $Z(A)$-module $Z(A^1)$, it is straightforward to prove the following.

Proposition 2: *A pair of connections* (∇^L,∇^R) *is* σ*-compatible if and only if its Christoffel symbols satisfy the equation*

$$\widetilde{\Gamma}^i_{kj}=\Gamma^i_{jk}. \tag{9}$$

Similarly, a pair of connections is σ-compatible on the whole bimodule if and only if [*(3.9) in Ref. 10*]

$$\widetilde{\Gamma}^i_{kj}=\Gamma^i_{jk}\in C^\infty(M). \tag{10}$$

Thus the σ-compatibility condition [over $Z(E)$] allows ∇^L to uniquely determine ∇^R and vice-versa. This is not unexpected since (in this set-up)

$$A^1=AZ(A^1)=Z(A^1)A, \tag{11}$$

and ∇^L and ∇^R satisfy the left and right Leibniz rule, respectively. On the other hand, as we shall see in Section IV (Remark 3) ∇^L and ∇^R can mutually determine each other even if (11) is not satisfied.

Concerning the metric compatibility of (∇^L,∇^R), we can again take an advantage of (6) to show that (5) is equivalent to

$$dg^{ij}=(\Gamma^i_{kl}g^{lj}+g^{il}\widetilde{\Gamma}^j_{lk})\,\theta^k, \quad \forall i,j\in\{1,\ldots,m+n^2-1\}. \tag{12}$$

To end this section, let us observe that, if (∇^L,∇^R) is σ-compatible, then (12) coincides with (3.13) in Ref. 10. One should bear in mind, however, that the latter has been obtained from a different starting point [(1.9) in Ref. 10] and only for middle-linear metrics.

IV. GENERIC QUANTUM PLANE

The next example that we study regards a bimodule of differential 1-forms ($E=A^1$) on the quantum plane. We choose as our space of differential 1-forms the grade one of the differential algebra $\Omega(A)=A\oplus A^1\oplus A^2$ (e.g., see Ref. 2) that is given by the generators $1,x,y,\xi,\eta$, where $\xi=\theta^1=dx$, $\eta=\theta^2=dy$, and relations

$$\begin{gathered} xy=qyx, \quad x\xi=q^2\xi x, \quad x\eta=q\eta x+(q^2-1)\xi y, \quad y\xi=q\xi y, \quad y\eta=q^2\eta y, \\ \eta\xi+q\xi\eta=0, \quad \xi^2=0, \quad \eta^2=0. \end{gathered} \tag{13}$$

For our bimodule automorphism σ it is natural [see the paragraph between (2.11) and (2.12) in Ref. 2] to take the map defined by

$$\begin{gathered} \sigma(\xi\otimes_A\xi)=q^{-2}\xi\otimes_A\xi, \quad \sigma(\xi\otimes_A\eta)=q^{-1}\eta\otimes_A\xi, \\ \sigma(\eta\otimes_A\xi)=q^{-1}\xi\otimes_A\eta-(1-q^{-2})\eta\otimes_A\xi, \quad \sigma(\eta\otimes_A\eta)=q^{-2}\eta\otimes_A\eta. \end{gathered} \tag{14}$$

First we consider the case of a generic q. Then the center of A is $\mathbb{C}$ and, as can be checked by a direct computation, the center of A^1 is zero. If we choose τ equal to σ (modulo the tensor product over A, as was done in the previous section), we can immediately see that, unless $q=1$, there exists no nonzero metric.[2] To remedy this problem, we ''rescale'' σ by q^2. More precisely, we put

$$\begin{gathered} \tau(\xi\otimes\xi)=\xi\otimes\xi, \quad \tau(\xi\otimes\eta)=q\eta\otimes\xi, \\ \tau(\eta\otimes\xi)=q\xi\otimes\eta-(q^2-1)\eta\otimes\xi, \quad \tau(\eta\otimes\eta)=\eta\otimes\eta. \end{gathered} \tag{15}$$

It turns out that this τ is quite natural from the point of view of Ref. 4—it factors to an automorphism of $A^1\otimes_A A^1$ and preserves $\theta\otimes_A\theta$, where $\theta=x\eta-qy\xi$ is the only (up to a multiplication by a complex number) left and right $SL_q(2,\mathbb{C})$-coinvariant 1-form (see Section 2 in Ref. 2).

[Recall that if A is a Hopf algebra, then there exists a unique bimodule homomorphism τ such that $\tau(\alpha_L \otimes_A \alpha_R) = \alpha_R \otimes_A \alpha_L$ for any left coinvariant 1-form α_L and right coinvariant 1-form α_R — see Proposition 3.1 in Ref. 4.]

It is obvious that with τ specified as above, the only constraints that the coefficients of a metric g have to satisfy is

$$g(\xi,\eta) = qg(\eta,\xi). \tag{16}$$

On the other hand, it can be computed that the middle-linearity of g is equivalent to the following equations:

$$\begin{gathered}
xg(\xi,\xi) = q^4 g(\xi,\xi)x, \\
yg(\xi,\xi) = q^2 g(\xi,\xi)y, \\
xg(\xi,\eta) = q^3 g(\xi,\eta)x + q^2(q^2-1)g(\xi,\xi)y, \\
yg(\xi,\eta) = q^3 g(\xi,\eta)y, \\
xg(\eta,\xi) = q^3 g(\eta,\xi)x + q(q^2-1)g(\xi,\xi)y, \\
yg(\eta,\xi) = q^3 g(\eta,\xi)y, \\
xg(\eta,\eta) = q^2 g(\eta,\eta)x + q^2(q^2-1)g(\xi,\eta)y + q(q^2-1)g(\eta,\xi)y, \\
yg(\eta,\eta) = q^4 g(\eta,\eta)y.
\end{gathered} \tag{17}$$

Notice that, due to the commutation relation $xy = qyx$, as long as q is generic and no negative powers of x and y are allowed, there is no nonzero solution to (17) (look at the equations with y). Consequently, we obtain the following.

Remark 1: If q is not a root of unity, there is no (τ-symmetric) middle-linear metric on A^1 (see Ref. 12). ◇

Proposition 3: *If we admit negative powers of x and y, the solutions of (17) form the following three-parameter family:*

$$\begin{gathered}
g(\xi,\xi) = ax^{-2}y^4, \\
g(\xi,\eta) = qx^{-3}(by^3 + q^3 ay^5), \\
g(\eta,\xi) = x^{-3}(by^3 + q^3 ay^5), \\
g(\eta,\eta) = x^{-4}(cy^2 + q^3(q^2+1)by^4 + q^8 ay^6),
\end{gathered} \tag{18}$$

where a, b, c are complex parameters.

Since the center of A^1 is zero, we can immediately conclude that

Proposition 4: *If q is not a root of unity, any pair (∇^L, ∇^R) of σ-compatible connections on A^1 is a pair of independent and unrestricted left and right connections.*

On the other hand, there exists only a one-parameter family of solutions of the σ-compatibility condition considered over the whole A^1 (see (2.13) in Ref. 2). Defining Christoffel symbols $\{F^i_{jk}, \widetilde{F}^i_{jk}\}_{i,j,k\in\{1,2\}}$ of such a compatible pair of connections as in (8), we can write the aforementioned solutions in the following way:

$$\begin{gathered}
F^1_{11} = \nu q x y^2, \quad F^1_{12} = -\nu q^3 x^2 y, \quad F^1_{21} = -\nu q^2 x^2 y, \quad F^1_{22} = \nu q^5 x^3, \\
F^2_{11} = \nu q^3 y^3, \quad F^2_{12} = -\nu q^4 x y^2, \quad F^2_{21} = -\nu q^3 x y^2, \quad F^2_{22} = \nu q^5 x^2 y,
\end{gathered} \tag{19}$$

where ν is a complex parameter. The Christoffel symbols $\{\widetilde{F}^i_{jk}\}_{i,j,k\in\{1,2\}}$ can be expressed in a similar fashion.

As to the metric compatibility condition, formula (5) reads as

$$a_i\Big(dg(\theta^i,\theta^j)-\theta^k g(\theta^l\Gamma^i_{kl},\theta^j)-g(\theta^i,\theta^k)\theta^l\widetilde{\Gamma}^j_{kl}\Big)\widetilde{a}_j=0,\quad \forall a_i,\widetilde{a}_j\in A, i,j\in\{1,2\}. \tag{20}$$

Clearly, (20) is satisfied if and only if the expression in the large parentheses vanishes for any i and j.

V. QUANTUM PLANE AT THE CUBIC ROOT OF UNITY

The setting of this section is identical with the setting of the previous one except that now we take $q=e^{2\pi i/3}$ rather than generic q. (For the sake of simplicity, we call $e^{2\pi i/3}$ *the* cubic root of unity.) Long but rather straightforward reasoning enables one to prove the following lemma.

Lemma 1: *Let q be the cubic root of unity. Then*

$$Z(A)=\{a_{ij}x^{3i}y^{3j}|a_{ij}\in\mathbb{C}\}, \tag{21}$$

$$dZ(A)=0, \tag{22}$$

$$\forall a\in Z(A),\alpha\in A^1:\ a\alpha=\alpha a, \tag{23}$$

$$Z(A^1)=\{c_i\theta^i\in A^1|c_1=axy-bxy^3,\ c_2=bx^2y^2,\ a,b\in Z(A)\}, \tag{24}$$

$$c_i\theta^i=\theta^j\widetilde{c}_j,\ \text{where}\ c_1=axy-bxy^3,\ c_2=bx^2y^2,$$

$$\widetilde{c}_1=axy-qbxy^3,\ \widetilde{c}_2=c_2,\ a,b\in Z(A)\ [\text{see (38)}]. \tag{25}$$

Changing q from generic to $q=e^{2\pi i/3}$ entails no consequence as far as the (general τ-symmetric) metric is concerned. However, regarding middle-linear metrics, with the help of commutation formulas provided in the Appendix, one can prove the following

Proposition 5: *If q is the cubic root of unity and g is middle-linear (but not necessarily τ-symmetric), then (17) is equivalent to*

$$\begin{gathered} g(\xi,\xi)=x^3Zxy,\quad g(\xi,\eta)=qx^3Zy^2+x^3Y,\\ g(\eta,\xi)=x^3Zy^2+x^3W,\ \ g(\eta,\eta)=Ux^2y^2+(qY+W)x^2y+q^2Zx^2y^3,\end{gathered} \tag{26}$$

where Z, Y, W, U are arbitrary elements of $Z(A)$. Furthermore, g is τ-symmetric if and only if $Y=qW$.

Thus, much as in Proposition 1, the space of middle-linear metrics is three-dimensional over $Z(A)$. This is not unexpected, if one remembers that the quantum plane at the n-th root of unity is nothing but $\mathbb{C}[x,y]\otimes M_n(\mathbb{C})$ (cf. Section IV.D.15 of Ref. 13).

Our next step is to determine the space of pairs of σ-compatible connections. In order to make our reasoning more transparent, we introduce *formal* inverses of x and y. (It is simply more convenient, for instance, to write $\widetilde{\Gamma}=xy\Gamma x^{-1}y^{-1}$ as the solution of the equation $\widetilde{\Gamma}xy=xy\Gamma$ rather than consider $\widetilde{\Gamma}$ and Γ as power series in x and y and then express the complex coefficients of $\widetilde{\Gamma}$ in terms of the complex coefficients of Γ. However, we neither need nor assume the existence of x^{-1} and y^{-1} in our algebra.) Treating $\{\theta^i\otimes_A\theta^j\}_{i,j\in\{1,2\}}$ as a basis of the right A-module $A^1\otimes_A A^1$ and taking advantage of Lemma 1, one can carry out lengthy but straightforward calculations that show that the σ-compatibility condition (1) is equivalent to

$$
\begin{aligned}
\widetilde{\Gamma}^1_{11} &= q^2xy\Gamma^1_{11}y^{-1}x^{-1}+(1-q)y^2\Gamma^1_{12}y^{-1}x^{-1}+(q^2-1)y^2\Gamma^1_{21}y^{-1}x^{-1},\\
\widetilde{\Gamma}^1_{12} &= (q^2-1)xy\Gamma^1_{12}y^{-1}x^{-1}+qxy\Gamma^1_{21}y^{-1}x^{-1}+(q-q^2)y^2\Gamma^1_{22}y^{-1}x^{-1},\\
\widetilde{\Gamma}^1_{21} &= qxy\Gamma^1_{12}y^{-1}x^{-1}+(1-q)y^2\Gamma^1_{22}y^{-1}x^{-1},\\
\widetilde{\Gamma}^1_{22} &= q^2xy\Gamma^1_{22}y^{-1}x^{-1},\\
\widetilde{\Gamma}^2_{11} &= xy\Gamma^1_{11}x^{-2}-x\Gamma^1_{11}yx^{-2}+(q-1)y\Gamma^1_{12}yx^{-2}+(q-q^2)y^2\Gamma^1_{12}x^{-2}+(1-q^2)y\Gamma^1_{21}yx^{-2}\\
&\quad +(1-q)y^2\Gamma^1_{21}x^{-2}+q^2x^2y^2\Gamma^2_{11}y^{-2}x^{-2}+(q-1)x\Gamma^2_{12}yx^{-2}\\
&\quad +(1-q^2)x\Gamma^2_{21}yx^{-2}+3y\Gamma^2_{22}yx^{-2},\\
\widetilde{\Gamma}^2_{12} &= (1-q^2)x\Gamma^1_{12}yx^{-2}+(q^2-1)y^2\Gamma^1_{22}x^{-2}+(1-q)xy\Gamma^1_{12}x^{-2}+q^2xy\Gamma^1_{21}x^{-2}-qx\Gamma^1_{21}yx^{-2}\\
&\quad +(q-1)y\Gamma^1_{22}yx^{-2}+(q^2-1)x^2y^2\Gamma^2_{12}y^{-2}x^{-2}+qx^2y^2\Gamma^2_{21}y^{-2}x^{-2}+(q^2-q)x\Gamma^2_{22}yx^{-2},\\
\widetilde{\Gamma}^2_{21} &= q^2xy\Gamma^1_{12}x^{-2}-qx\Gamma^1_{12}yx^{-2}+(1-q^2)y\Gamma^1_{22}yx^{-2}+(q-q^2)y^2\Gamma^1_{22}x^{-2}+qx^2y^2\Gamma^2_{12}y^{-2}x^{-2}\\
&\quad +(q-1)x\Gamma^2_{22}yx^{-2},\\
\widetilde{\Gamma}^2_{22} &= xy\Gamma^1_{22}x^{-2}-qx\Gamma^1_{22}yx^{-2}+q^2x^2y^2\Gamma^2_{22}y^{-2}x^{-2},
\end{aligned}
\tag{27}
$$

where the Christoffel symbols are defined as in (8). The above system of equations allows one to determine uniquely ∇^R through ∇^L, but, as can be seen from the powers of x and y, it cannot be done for an arbitrary left connection ∇^L. [The total power of x and the total power of y in each term of the right hand side of (27) have to be non-negative in order for (27) to make sense.] Since only total powers of x turn negative in (27), it is convenient to think of an element of A as a polynomial in x with coefficients in polynomials in y:

$$
\Gamma^i_{jk} = x^l\Gamma^i_{jkl}, \quad i,j,k \in \{1,2\}. \tag{28}
$$

To determine the necessary and sufficient conditions that $\{\Gamma^i_{jk}\}_{i,j,k\in\{1,2\}}$ have to satisfy in order to make (27) well-defined on the quantum plane, we substitute (28) to (27) and conclude that the necessary and sufficient conditions for $\{\Gamma^i_{jk}\}_{i,j,k\in\{1,2\}}$ are fully given by

$$
\begin{aligned}
&(1-q)y^2\Gamma^1_{120}+(q^2-1)y^2\Gamma^1_{210}=0,\\
&(q-q^2)y^2\Gamma^1_{220}=0, \quad (1-q)y^2\Gamma^1_{220}=0,\\
&xy\Gamma^1_{110}-x\Gamma^1_{110}y+(q-1)y\Gamma^1_{120}y+(q-1)yx\Gamma^1_{121}y+(q-q^2)y^2\Gamma^1_{120}+(q-q^2)y^2x\Gamma^1_{121}\\
&\quad +(1-q^2)y\Gamma^1_{210}y+(1-q^2)yx\Gamma^1_{211}y+(1-q)y^2\Gamma^1_{210}+(1-q)y^2x\Gamma^1_{211}+(q-1)x\Gamma^2_{120}y\\
&\quad +(1-q^2)x\Gamma^2_{210}y+3y\Gamma^2_{220}y+3yx\Gamma^2_{221}y=0,\\
&(1-q^2)x\Gamma^1_{120}y+(q^2-1)y^2\Gamma^1_{220}+(q^2-1)y^2x\Gamma^1_{221}+(1-q)xy\Gamma^1_{120}+q^2xy\Gamma^1_{210}-qx\Gamma^1_{210}y\\
&\quad +(q-1)y\Gamma^1_{220}y+(q-1)yx\Gamma^1_{221}y+(q^2-q)x\Gamma^2_{220}y=0,\\
&q^2xy\Gamma^1_{120}-qx\Gamma^1_{120}y+(1-q^2)y\Gamma^1_{220}y+(1-q^2)yx\Gamma^1_{221}y+(q-q^2)y^2\Gamma^1_{220}\\
&\quad +(q-q^2)y^2x\Gamma^1_{221}+(q-1)x\Gamma^2_{220}y=0,\\
&xy\Gamma^1_{220}-qx\Gamma^1_{220}y=0.
\end{aligned}
\tag{29}
$$

Those equations are equivalent to

$$\Gamma^1_{210}=\Gamma^1_{120}=\Gamma^1_{220}=\Gamma^1_{221}=\Gamma^2_{220}=0$$
$$(q-1)\Gamma^2_{120}+(1-q^2)\Gamma^2_{210}+3q^2y\Gamma^2_{221}=0. \tag{30}$$

Thus we have obtained the following.

Proposition 6: *The σ-compatibility condition (1) has a solution if and only if*

$$\Gamma^1_{11}\in A,\ \ \Gamma^1_{12}\in xA,\ \ \Gamma^1_{21}\in xA,\ \ \Gamma^1_{22}\in x^2A,$$
$$\Gamma^2_{11}\in A,\ \ (q-1)\Gamma^2_{12}+(1-q^2)\Gamma^2_{21}+3q^2yx^{-1}\Gamma^2_{22}\in xA,\ \ \Gamma^2_{22}\in xA. \tag{31}$$

Moreover, if (31) is satisfied, then the general solution of (1) is given by (27).

Remark 2: Expressing $\{\Gamma^i_{jk}\}_{i,j,k\in\{1,2\}}$ in terms of $\{\tilde{\Gamma}^i_{jk}\}_{i,j,k\in\{1,2\}}$ would yield conditions for $\{\tilde{\Gamma}^i_{jk}\}_{i,j,k\in\{1,2\}}$ similar to these in Proposition 6. Only this time y would play the role of x. Let us also observe that, if we replaced σ by $q^2\sigma$ in (1), then (1) would have no solutions whatsoever as long as the negative powers of x and y are disallowed. ◇

Remark 3: As in Section II, equations (27) uniquely determine ∇^L from ∇^R, and vice-versa. Here, however, it happens despite the fact that formula (11) is not fulfilled. [It follows from (24) that $AZ(A^1)\subseteq xyA^1$.] ◇

Notice that, had we required the σ-compatibility condition to be satisfied on the whole bimodule A^1, then, in contrast with Proposition 6, we would obtain that the Christoffel symbols of a left connection have to fulfill the following equations:

$$F^1_{11}=x(y^3(-qf^1_{12}+f^1_{21})+yf^1_{11}-qy^2f^1_{22}),$$
$$F^1_{12}=x^2(yf^1_{22}+y^2f^1_{12}),\quad F^1_{21}=x^2(q^2yf^1_{22}+y^2f^1_{21}),$$
$$F^1_{22}=-q^2x^3f^1_{22},$$
$$F^2_{11}=f^2_{11}+qy^4\left(f^2_{22}-f^1_{12}-\frac{3q}{1-q}f^1_{21}\right)+qy^2(f^1_{11}-f^2_{21}-qf^2_{12}), \tag{32}$$
$$F^2_{12}=x(q^2y^3(-f^2_{22}+f^1_{12})+yf^2_{12}+qy^2f^1_{22})$$
$$F^2_{21}=x(qy^3(-f^2_{22}+qf^1_{21})+yf^2_{21}+y^2f^1_{22}),$$
$$F^2_{22}=x^2(-q^2yf^1_{22}+y^2f^2_{22}),$$

where $f^i_{jk}\in Z(A), i,j,k\in\{1,2\}$.

The metric compatibility condition (5) can again be written in the form of formula (20). This time, however, the center of A^1 is nontrivial and it makes sense to ask what would happen if we imposed the metric compatibility condition only over $Z(A^1)$. It turns out that we have the following.

Proposition 7: *Requiring that the metric compatibility condition (5) be satisfied only over $Z(A^1)$ is equivalent to demanding that it be fulfilled over the whole A^1.*

Proof. Let $\mathbf{P}^{ij}$ denote the expression in the large parentheses in (20). Furthermore, let us put $\mathbf{P}^{ij}=\theta^k\mathbf{P}_k^{ij}$, $a_1=axy-bxy^3$, $a_2=bx^2y^2$, $\tilde{a}_1=a'xy-qb'xy^3$, $\tilde{a}_2=b'x^2y^2$, where a,b,a',b' are arbitrary elements of $Z(A)$. Thanks to (24), substituting those terms to (20) yields an equation that expresses the metric compatibility condition over $Z(A^1)$:

$$(axy-bxy^3)\,\theta^k\mathbf{P}_k^{11}(a'xy-qb'xy^3)+(axy-bxy^3)\,\theta^k\mathbf{P}_k^{12}b'x^2y^2+bx^2y^2\,\theta^k\mathbf{P}_k^{21}(a'xy-qb'xy^3)$$
$$+bx^2y^2\,\theta^k\mathbf{P}_k^{21}b'x^2y^2=0. \tag{33}$$

Commuting everything to the right of $\{\theta^i\}_{i\in\{1,2\}}$ and taking advantage of the fact that $\{\theta^i\}_{i\in\{1,2\}}$ is a basis, one can reduce (33) to

$$\Big((xy\mathbf{P}_1^{11}+(q-q^2)y^2\mathbf{P}_2^{11})a \;+\; (-q^2x\mathbf{P}_1^{11}y^3-(q^2-1)y\mathbf{P}_2^{11}y^3+x^2y^2\mathbf{P}_1^{21}+(q^2-q)xy^3\mathbf{P}_2^{21})b\Big)$$
$$\times(a'xy-qb'xy^3) \;+\; \Big((xy\mathbf{P}_1^{12}+(q-q^2)y^2\mathbf{P}_2^{12})a \;+\; (-q^2x\mathbf{P}_1^{12}y^3-(q^2-1)y\mathbf{P}_2^{12}y^3$$
$$+x^2y^2\mathbf{P}_1^{22}+(q^2-q)xy^3\mathbf{P}_2^{22})b\Big)b'x^2y^2=0$$
$$\Big(xy\mathbf{P}_2^{11}a-(qx\mathbf{P}_2^{11}y^3-x^2y^2\mathbf{P}_2^{21})b\Big)a'xy-qb'xy^3$$
$$+\Big(xy\mathbf{P}_2^{12}a-(qx\mathbf{P}_2^{12}y^3-x^2y^2\mathbf{P}_2^{22})b\Big)b'x^2y^2=0. \tag{34}$$

Now, since a, b, a', b' are arbitrary elements of $Z(A)$, the above two equations boil down to

$$\begin{gathered}
xy\mathbf{P}_2^{11}xy=0,\\
xy\mathbf{P}_1^{11}xy+(q-q^2)y^2\mathbf{P}_2^{11}xy=0,\\
-qxy\mathbf{P}_2^{11}xy^3+xy\mathbf{P}_2^{12}x^2y^2=0,\\
-qxy\mathbf{P}_1^{11}xy^3+(1-q^2)y^2\mathbf{P}_2^{11}xy^3+xy\mathbf{P}_1^{12}x^2y^2+(q-q^2)y^2\mathbf{P}_2^{12}x^2y^2=0,\\
-qx\mathbf{P}_2^{11}xy^4+x^2y^2\mathbf{P}_2^{21}xy=0,\\
-q^2x\mathbf{P}_1^{11}xy^4-(q^2-1)y\mathbf{P}_2^{11}xy^4+x^2y^2\mathbf{P}_1^{21}xy+(q^2-q)xy^3\mathbf{P}_2^{21}xy=0,\\
q^2x\mathbf{P}_2^{11}xy^4-qx^2y^2\mathbf{P}_2^{21}xy^3-qx\mathbf{P}_2^{12}x^2y^5+x^2y^2\mathbf{P}_2^{22}x^2y^2=0,\\
x\mathbf{P}_1^{11}xy^6+(1-q)y\mathbf{P}_2^{11}xy^6-qx^2y^2\mathbf{P}_1^{21}xy^3-(1-q^2)xy^3\mathbf{P}_2^{21}xy^3-q^2x\mathbf{P}_1^{12}x^2y^5+(1-q^2)y\mathbf{P}_2^{12}x^2y^5\\
+x^2y^2\mathbf{P}_1^{22}x^2y^2+(q^2-q)xy^3\mathbf{P}_2^{22}x^2y^2=0.
\end{gathered} \tag{35}$$

Hence $\mathbf{P}_k^{ij}=0$ for any $i,j,k\in\{1,2\}$. Consequently, $\mathbf{P}^{ij}=0$ for any $i,j\in\{1,2\}$, and (5) follows, as claimed. □

The same effect, though in a more trivial way, occurs in the setting of Section II.

VI. CONCLUSIONS

As we have demonstrated, restricting the domain of the σ-compatibility condition $\nabla^L=\sigma\circ\nabla^R$ to $Z(A^1)$ yields a theory of noncommutative linear connections that coincides with the classical theory in the commutative case, does not discriminate against the left or right structure of a bimodule and appears to be rich in the noncommutative set-up. It is easy to check, however, that this σ-compatibility equation is not, in general, gauge covariant, either when considering it over the whole bimodule,[2] or when considering it only over the center of a bimodule. To provide a simple example, let us assume the setting of Section IV and choose our gauge

transformation to be $\theta^i \mapsto U^i_j \theta^j, U=\left(\begin{smallmatrix}1 & x\\ 0 & 1\end{smallmatrix}\right)$. Its action on ∇^L is given by the formula (cf. p. 547 and p. 559 in Ref. 1) $N \mapsto dU.U^{-1}+UNU^{-1}$, where $\nabla^L\theta^i=N^i_k\otimes_A\theta^k$, $N=(N^i_k)\in M_2(A^1)$. It is clear that, although the pure gauge connections ($\Gamma^i_{jk}=0=\tilde{\Gamma}^i_{jk}$, $i,j,k\in\{1,2\}$) satisfy $\nabla^L=\sigma\circ\nabla^R$, the Christoffel symbol Γ^1_{12} of the connection obtained by the action of U on the left pure gauge connection does not fulfill (31). More precisely, $\Gamma^1_{12}=1\notin xA$. [This can be obtained from equation $(dU.U^{-1})^i_k\otimes_A\theta^k=\theta^j\otimes_A\theta^k\Gamma^i_{jk}$, $i\in\{1,2\}$.]

A different approach to the generalized permutation σ has been suggested in Ref. 14. In the set-up of Section 5 in Ref. 14, σ is a function of the connection. Consequently, to determine the space of connections one needs to take into account all possible bimodule homomorphisms σ. Allowing σ to vary makes it possible to change it under the action of a gauge transformation. If we take as a gauge transformation a bimodule automorphism $f:E\to E$ and define its action by the formula

$$(\nabla^L,\nabla^R,\sigma)\ \mapsto\ ((id\otimes_A f^{-1})\circ\nabla^L\circ f,\ (f^{-1}\otimes_A id)\circ\nabla^R\circ f,\ (id\otimes_A f^{-1})\circ\sigma\circ(f\otimes_A id)), \quad (36)$$

then the σ-compatibility condition $\nabla^L=\sigma\circ\nabla^R$ is gauge covariant. Furthermore, since the center of a bimodule is preserved by the bimodule automorphisms, the σ-compatibility condition is also gauge covariant when considered only over $Z(E)$. (We owe noticing this point to Michel Dubois-Violette.) One should bear in mind, however, that, roughly speaking, the bimodule automorphisms correspond to the ''commutative sector'' of the space of gauge transformations.

A more radical point of view that might deserve a detailed investigation relies on employing the metric compatibility condition (5) rather than the equation $\nabla^L=\sigma\circ\nabla^R$ to relate ∇^L and ∇^R uniquely and without (undesirable) restrictions on (∇^L,∇^R). Clearly, for nondegenerate metrics, formulas (12) and (20) provide this kind of mutual dependence of ∇^L and ∇^R. [In those cases, the nondegeneracy of a metric g simply means that (g^{ij}) is an invertible matrix.]

Finally, let us remark that it is plausible that in order to obtain a satisfactory definition of a bimodule connection, one needs to use the language of quantum principal bundles, and, having understood and thoroughly worked out the left-right relationship in this context (see Theorem 4.13 and Remark 4.14 in Ref. 15 and Appendix B in Ref. 16), translate the solution(s) to bimodule terms.

APPENDIX: COMMUTATION FORMULAS

Here we provide commutation formulas for the differential algebra $\Omega(A)$ that is defined with the help of (13). Let $Q_{-1}=Q_0=0$ and, for $n>0$, let $Q_n=\Sigma_{k=1}^n q^{2(k-1)}$. For any natural $n\geqslant 0$, we have

$$x^n\xi=q^{2n}\xi x^n,\ \ x^n\eta=q^n\eta x^n+(q^2-1)Q_n\xi x^{n-1}y,\ \ y^n\xi=q^n\xi y^n,\ \ y^n\eta=q^{2n}\eta y^n;$$

$$x^n\xi\otimes_A\xi=q^{4n}\xi\otimes_A\xi x^n,$$

$$x^n\xi\otimes_A\eta=q^{3n}\xi\otimes_A\eta x^n+(q^2-1)q^{2n}Q_n\xi\otimes_A\xi x^{n-1}y,$$

$$x^n\eta\otimes_A\xi=q^{3n}\eta\otimes_A\xi x^n+(q^2-1)q^{2n-1}Q_n\xi\otimes_A\xi x^{n-1}y, \quad (A1)$$

$$x^n\eta\otimes_A\eta=q^{2n}\eta\otimes_A\eta x^n+(q^2-1)q^nQ_n\eta\otimes_A\xi x^{n-1}y+(q^2-1)q^{n+1}Q_n\xi\otimes_A\eta x^{n-1}y$$
$$+q^2(q^2-1)^2Q_nQ_{n-1}\xi\otimes_A\xi x^{n-2}y^2;$$

$$y^n\xi\otimes_A\xi=q^{2n}\xi\otimes_A\xi y^n,\quad y^n\xi\otimes_A\eta=q^{3n}\xi\otimes_A\eta y^n,$$

$$y^n\eta\otimes_A\xi=q^{3n}\eta\otimes_A\xi y^n,\quad y^n\eta\otimes_A\eta=q^{4n}\eta\otimes_A\eta y^n.$$

One also has

$$
\begin{aligned}
a\xi + b\eta &:= a_{pr}x^p y^r \xi + b_{st}x^s y^t \eta \\
&= \xi\ (q^{2p+r}a_{pr}x^p y^r + q^{2t}(q^2-1)Q_s b_{st}x^{s-1}y^{t+1}) + \eta\ (q^{2t+s}b_{st}x^s y^t) \\
&= \xi((q^{2p+r}a_{pr} + q^{2r-2}(q^2-1)Q_{p+1}b_{p+1\,r-1}\ )x^p y^r + q^{2p}a_{p0}x^p) + \eta\ (q^{2t+s}b_{st}x^s y^t) \\
&=: \xi\tilde{a} + \eta\tilde{b}, \qquad \text{(A2)}
\end{aligned}
$$

where $a_{pr}, b_{st} \in \mathbb{C}$, $p,r,s,t \in \{0,1,\dots\}$.

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Differential calculi and linear connections

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A method is proposed for defining an arbitrary number of differential calculi over a given noncommutative associative algebra. As an example the generalized quantum plane is studied. It is found that there is a strong correlation, but not a one-to-one correspondence, between the module structure of the 1-forms and the metric torsion-free connections on it. In the commutative limit the connection remains as a shadow of the algebraic structure of the 1-forms. © *1996 American Institute of Physics.* [S0022-2488(96)01609-X]

I. INTRODUCTION

We propose a method of defining an arbitrary number of differential calculi over a given noncommutative associative algebra. We shall especially be interested in the generalized quantum plane, an algebra which has a commutative limit which one can identify with the algebra of rational functions on the 2-plane minus the axes. We shall see that the commutation relations between the elements of the algebra and the 1-forms determine a set of torsion-free metric connections which remain non-trivial in the commutative limit. It is to be expected that the converse is true, that every torsion-free metric connection on the 2-plane determines a set of commutation relations. This would mean that in particular the covariant calculus of Wess and Zumino[1] is determined by a geometry on the 2-plane.

The differential calculi we introduce here are based on derivations and are similar to those introduced by Dubois-Violette[2] and Dubois-Violette *et al.*[3] to construct differential calculi over matrix algebras. We refer to Madore[4,5] for a detailed description of how to use this method to construct a sequence of differential calculi over a given matrix algebra. In this previous work the set of derivations was chosen to form an irreducible representation of the Lie algebra of a special linear group SL_m. With this restriction the number of differential calculi which can be put on a matrix algebra of dimension n is equal to the number of integers m such that SL_m has an irreducible representation on a space of dimension n. There are always of course at least two, $m=2$ and $m=n$, but for large n there are in general many more.

In Section II we present a general method for constructing differential calculi, based on a set of derivations which do not necessarily close to form a Lie algebra. In Sections III and IV we present some examples using as algebra the generalized quantum plane. In Section V we investigate linear connections and show how they depend on the choice of differential calculus as well as, of course, the algebra. By $\mathscr{A}$ we designate an arbitrary associative algebra with unit element and with center $\mathscr{Z}(\mathscr{A})$.

II. GENERAL FORMALISM

Of the many differential calculi which can be constructed over an algebra $\mathscr{A}$ the largest is the differential envelope or universal differential calculus $(\Omega_u^*(\mathscr{A}), d_u)$. Every other differential calculus can be considered as a quotient of it. For the definitions we refer, for example, to the book by Connes.[6] Let $(\Omega^*(\mathscr{A}), d)$ be another differential calculus over $\mathscr{A}$. Then there exists a unique d_u-homomorphism ϕ

$$\begin{array}{ccccccc} \mathscr{A} & \overset{d_u}{\rightarrow} & \Omega_u^1(\mathscr{A}) & \overset{d_u}{\rightarrow} & \Omega_u^2(\mathscr{A}) & \overset{d_u}{\rightarrow} & \cdots \\ \| & & \phi_1\downarrow & & \phi_2\downarrow & & \\ \mathscr{A} & \overset{d}{\rightarrow} & \Omega^1(\mathscr{A}) & \overset{d}{\rightarrow} & \Omega^2(\mathscr{A}) & \overset{d}{\rightarrow} & \cdots \end{array} \tag{2.1}$$

of $\Omega_u^*(\mathscr{A})$ onto $\Omega^*(\mathscr{A})$. It is given by

$$\phi(d_u f\,) = df. \tag{2.2}$$

The restriction ϕ_p of ϕ to each Ω_u^p is defined by

$$\phi_p(f_0 d_u f_1 \cdots d_u f_p) = f_0 df_1 \cdots df_p\,.$$

Consider a given algebra $\mathscr{A}$ and suppose that we know how to construct an $\mathscr{A}$-module $\Omega^1(\mathscr{A})$ and an application

$$\mathscr{A} \overset{d}{\rightarrow} \Omega^1(\mathscr{A}). \tag{2.3}$$

Then using (2.1) there is a method of constructing $\Omega^p(\mathscr{A})$ for $p \geqslant 2$ as well as the extension of the differential. Since we know $\Omega_u^1(\mathscr{A})$ and $\Omega^1(\mathscr{A})$ we can suppose that ϕ_1 is given. We must construct $\Omega^2(\mathscr{A})$. The simplest consistent choice would be to set

$$\Omega^2(\mathscr{A}) = \Omega_u^2(\mathscr{A}) / \overline{d_u \mathrm{Ker}\phi_1}, \tag{2.4}$$

where $\overline{d_u \mathrm{Ker}\phi_1}$ is the bimodule generated by $d_u \mathrm{Ker}\phi_1$. The product of two elements ξ and η in $\Omega^1(\mathscr{A})$ is defined by choosing two inverse images ξ_u and η_u in $\Omega_u^1(\mathscr{A})$ and projecting their product onto $\Omega^2(\mathscr{A})$:

$$\xi\eta = \phi_2(\xi_u \otimes \eta_u).$$

This is well-defined because of the equality

$$\overline{d_u \mathrm{Ker}\phi_1} = d_u \mathrm{Ker}\phi_1 + (\Omega_u^1(\mathscr{A}) \otimes \mathrm{Ker}\phi_1) + (\mathrm{Ker}\phi_1 \otimes \Omega_u^1(\mathscr{A})),$$

which in turn follows from the identities

$$f d_u \xi = d_u(f\xi) - (d_u f\,)\xi, \quad (d_u \xi) f = d_u(\xi f\,) - \xi d_u f.$$

Equation (2.4) defines the largest set of 2-forms consistent with the constraints on $\Omega^1(\mathscr{A})$. The map ϕ_2 is defined to be the projection of $\Omega_u^2(\mathscr{A})$ onto $\Omega^2(\mathscr{A})$ so defined and d is defined by $d(fdg) = dfdg$. This procedure can be continued by iteration to arbitrary order in p. See, for example, Baehr *et al.*[7]

To initiate the above construction we shall define the 1-forms using a set of derivations. We shall suppose that they are interior and exclude therefore the case where $\mathscr{A}$ is commutative. For each integer n let λ_a be a set of n linearly independent elements of $\mathscr{A}$ and introduce the derivations $e_a = ad\lambda_a$. In general the e_a do not form a Lie algebra but they do however satisfy commutation relations as a consequence of the commutation relations of $\mathscr{A}$. Define the map (2.3) by

$$df(e_a) = e_a f. \tag{2.5}$$

We shall suppose that there exists a set of n elements θ^a of $\Omega^1(\mathscr{A})$ such that

$$\theta^a(e_b)=\delta^a_b. \tag{2.6}$$

In the examples which we consider we shall show that the θ^a exist by explicit construction. We shall refer to the set of θ^a as a frame or Stehbein. It commutes with the elements $f\in\mathscr{A}$,

$$f\theta^a=\theta^a f. \tag{2.7}$$

The construction of the θ^a from the derivations did not really use the fact that they were inner. For example, if the e_a are n linearly independent vector fields on a manifold V of dimension n, that is, n linearly independent outer derivations of the algebra $\mathscr{A}=\mathscr{C}(V)$ of smooth functions on V, then $\Omega^*(\mathscr{A})$ is the algebra of de Rham forms.

The $\mathscr{A}$-bimodule $\Omega^1(\mathscr{A})$ is generated by all elements of the form fdg or of the form $(df\,)g$. Because of the Leibniz rule these conditions are equivalent. Define $\theta=-\lambda_a\theta^a$. Then one sees that

$$df=-[\theta,f] \tag{2.8}$$

and it follows that as a bimodule $\Omega^1(\mathscr{A})$ is generated by one element. It follows also that the 2-form $d\theta+\theta^2$ can be written in the form

$$d\theta+\theta^2=-\frac{1}{2}K_{ab}\theta^a\theta^b \tag{2.9}$$

with coefficients K_{ab} which lie in $\mathscr{Z}(\mathscr{A})$. By definition

$$fdg(e_a)=fe_ag,\quad (dg)f(e_a)=(e_ag)f.$$

Using the frame we can write these as

$$fdg=(fe_ag)\theta^a,\quad (dg)f=(e_ag)f\theta^a. \tag{2.10}$$

The commutation relations of the algebra constrain the relations between fdg and $(dg)f$ for all f and g.

As a left or right module, $\Omega^1(\mathscr{A})$ is free of rank n. Because of the commutation relations of the algebra, or equivalently, because of the kernel of ϕ_1 in the quotient (2.4), the θ^a satisfy commutation relations. We shall suppose that they can be written in the form

$$\theta^a\theta^b+C^{ad}{}_{cb}\theta^c\theta^d=0. \tag{2.11}$$

The associativity law in $\Omega^*(\mathscr{A})$ will place constraints on the $C^{ab}{}_{cd}$ which will be satisfied in the cases which we consider in detail. If $C^{ad}{}_{cd}=\delta^a_c\delta^b_d$, then one sees that $\Omega^2(\mathscr{A})=0$. It follows from (2.11) that for an arbitrary element f of the algebra

$$[f,C^{ab}{}_{cd}]\theta^c\theta^d=0.$$

We shall suppose that

$$C^{ab}{}_{ef}C^{ef}{}_{cd}=\delta^a_c\delta^b_d$$

and that the relations (2.11) are complete in the sense that if $A_{ab}\theta^a\theta^b=0$ we can conclude that

$$A_{ab}-C^{cd}{}_{ab}A_{cd}=0. \tag{2.12}$$

This will be the case for all the differential calculi which we shall consider on the generalized quantum plane in the next sections. We can conclude then that the $C^{ab}{}_{cd}$ are elements of $\mathscr{Z}(\mathscr{A})$. In ordinary geometry one can choose

$$C^{ab}{}_{cd} = \delta^b_c \delta^a_d$$

and the relation (2.11) expresses the fact that the 1-forms anticommute. Let $\wedge^*_C$ be the twisted exterior algebra determined by the relations (2.11). Then the differential algebra $\Omega^*(\mathscr{A})$ can be factorized as the tensor product

$$\Omega^*(\mathscr{A}) = \mathscr{A} \otimes_{\mathbb{C}} \wedge^*_C .$$

Because the 2-forms are generated by products of the θ^a one has

$$d\theta^a = -\tfrac{1}{2} C^a{}_{bc} \theta^b \theta^c . \tag{2.13}$$

Without loss of generality we can suppose that the structure elements $C^a{}_{bc}$ satisfy the identities

$$C^a{}_{bc} + C^a{}_{de} C^{de}{}_{bc} = 0. \tag{2.14}$$

It is to be noticed that they do not in general lie in $\mathscr{Z}(\mathscr{A})$. In fact from the identity $d(f\theta^a) = d(\theta^a f)$ one sees that

$$(\tfrac{1}{2}[C^a{}_{bc}, f] + e_{(b} f \delta^a_{c)}) \theta^b \theta^c = 0. \tag{2.15}$$

Using the definition of the derivations one can write this in the form

$$(\tfrac{1}{2} C^a{}_{bc} + \lambda_{(b} \delta^a_{c)} - \tfrac{1}{2} F^a{}_{bc}) \theta^b \theta^c = 0 \tag{2.16}$$

with $F^a{}_{bc} \in \mathscr{Z}(\mathscr{A})$. We can suppose that the $F^a{}_{bc}$ satisfy (2.14):

$$F^a{}_{bc} + F^a{}_{de} C^{de}{}_{bc} = 0. \tag{2.17}$$

Using this and the relations (2.11) and (2.14) as well as the completeness assumption (2.12) we can conclude from (2.16) that

$$C^a{}_{bc} - F^a{}_{bc} + \lambda_{(b} \delta^a_{c)} - \lambda_{(d} \delta^a_{e)} C^{de}{}_{bc} = 0. \tag{2.18}$$

The equation (2.16) can also be written in the form

$$d\theta^a = -[\theta, \theta^a] - \tfrac{1}{2} F^a{}_{bc} \theta^b \theta^c \tag{2.19}$$

with a graded commutator. If $F^a{}_{bc} = 0$, the form (2.8) for the exterior derivative is valid for all elements of $\Omega^*(\mathscr{A})$ and the element θ plays the role of the phase of a generalized Dirac operator in the sense of Connes.[8]

From (2.19) we find that

$$d\theta = -2\theta^2 + \tfrac{1}{2} \lambda_a F^a{}_{bc} \theta^b \theta^c .$$

Comparing this with (2.9) we conclude that

$$\theta^2 = \tfrac{1}{2} (\lambda_a F^a{}_{bc} + K_{bc}) \theta^b \theta^c . \tag{2.20}$$

If we suppose that K_{bc} satisfies (2.14),

$$K_{ab} + K_{cd} C^{cd}{}_{ab} = 0,$$

then we can conclude that

$$(\lambda_b\lambda_c - C^{de}{}_{bc}\lambda_d\lambda_e - \lambda_a F^a{}_{bc} - K_{bc})\,\theta^b\theta^c = 0. \tag{2.21}$$

Using again the completeness assumption (2.12) we find

$$\lambda_b\lambda_c - C^{de}{}_{bc}\lambda_d\lambda_e = \lambda_a F^a{}_{bc} + K_{bc}\,. \tag{2.22}$$

If we introduce the twisted bracket

$$[\lambda_a,\lambda_b]_C = \lambda_a\lambda_b - C^{cd}{}_{ab}\lambda_c\lambda_d\,,$$

we can rewrite (2.22) in the form

$$[\lambda_b,\lambda_c]_C = \lambda_a F^a{}_{bc} + K_{bc}\,. \tag{2.23}$$

If we write out in detail the equation $d^2 f = 0$, using (2.12)–(2.14) we find that

$$[e_b,e_c]_C f = e_a f C^a{}_{bc}\,. \tag{2.24}$$

This is the dual relation to the 'Maurer–Cartan' equation (2.13).

The constraint (2.23) follows from the commutation relations (2.11) we have supposed for the frame as well as from the conditions we have imposed on the coefficients $C^{ab}{}_{cd}$. In the matrix case the general formalism simplifies considerably. The elements of the frame anticommute and one can choose $C^{ab}{}_{cd} = \delta^b_c\delta^a_d$. In Equation (2.19) the first term on the right-hand side vanishes and $F^a{}_{bc} = C^a{}_{bc}$. On the right-hand side of Equations (2.9) and (2.23) we have $K_{ab} = 0$.

III. CALCULI BASED ON 2 DERIVATIONS

Using the construction of the previous section one can construct an infinite sequence of differential calculi over the generalized quantum plane $\mathscr{A}$, the algebra generated by four elements (x,y,x^{-1},y^{-1}) subject to the relation $xy = qyx$ as well as the usual relations between an element and its inverse. Here q is an arbitrary complex number. The subalgebra generated by (x,y) alone with the covariant differential calculus of Wess and Zumino is called the quantum plane. In this section we shall consider the case $n = 2$. Define, for $q \neq 1$,

$$\lambda_1 = \frac{q}{q-1}\,y, \quad \lambda_2 = \frac{q}{q-1}\,x. \tag{3.1}$$

The normalization has been chosen here so that the structure elements $C^a{}_{12}$ contain no factors q. The λ_a are singular in the limit $q \to 1$ for the same reason as the limit from quantum mechanics:

$$\frac{1}{\hbar}\,\mathrm{ad}\,p \to \frac{1}{i}\,\frac{\partial}{\partial q}.$$

We find that

$$e_1 x = -xy, \quad e_1 y = 0, \quad e_2 x = 0, \quad e_2 y = xy. \tag{3.2}$$

These rather unusual derivations are extended to arbitrary polynomials in the generators by the Leibniz rule. From (3.2) we conclude that the commutation relations which follow from (2.10) are

$$\begin{aligned} xdx &= qdxx, \quad ydx = q^{-1}dxy, \\ xdy &= qdyx, \quad ydy = q^{-1}dyy. \end{aligned} \tag{3.3}$$

From these relations, if $q \neq -1$, we deduce

$$(dx)^2=0, \quad (dy)^2=0, \quad dxdy+qdydx=0. \tag{3.4}$$

Using the relations (3.2) we find

$$dx=-xy\theta^1, \quad dy=xy\theta^2, \tag{3.5}$$

and solving for the θ^a we obtain

$$\theta^1=-q^{-1}x^{-1}y^{-1}dx, \quad \theta^2=q^{-1}x^{-1}y^{-1}dy. \tag{3.6}$$

The θ^a satisfy the commutation relations

$$(\theta^1)^2=0, \quad (\theta^2)^2=0, \quad \theta^1\theta^2+q\theta^2\theta^1=0. \tag{3.7}$$

This is of the form (2.11). If we reorder the indices (11,12,21,22)=(1,2,3,4), then the matrix $C^{ab}{}_{cd}$ can be written in the form of a 4×4 matrix

$$C=\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & q & 0 \\ 0 & q^{-1} & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{3.8}$$

That is, $C^{12}{}_{21}=q$ and $C^{21}{}_{12}=q^{-1}$. The structure elements $C^a{}_{bc}$ are given by

$$C^1{}_{12}=-x, \quad C^2{}_{12}=-y, \tag{3.9}$$

and the condition (2.14). Equation (2.18) is satisfied. For θ we find the expression

$$\theta=\frac{1}{q-1}(qx^{-1}dx-y^{-1}dy). \tag{3.10}$$

It is a closed form.

As a second example with $n=2$ we define, for $q^4\neq 1$,

$$\lambda_1=\frac{1}{q^4-1}x^{-2}y^2, \quad \lambda_2=\frac{1}{q^4-1}x^{-2}. \tag{3.11}$$

The normalization has been chosen here again so that the structure elements $C^a{}_{12}$ contain no factors q. We find then that for $q^2\neq -1$

$$e_1x=-\frac{1}{q^2(q^2+1)}x^{-1}y^2, \quad e_1y=-\frac{1}{q^2+1}x^{-2}y^3,$$

$$e_2x=0, \quad e_2y=-\frac{1}{q^2+1}x^{-2}y. \tag{3.12}$$

From these we conclude that the commutation relations which follow from (2.10) are

$$xdx=q^2dxx, \quad xdy=qdyx+(q^2-1)dxy,$$

$$ydx=qdxy, \quad ydy=q^2dyy. \tag{3.13}$$

We have then in this case the covariant differential calculus of Wess and Zumino. It has been encoded in the functional form of the λ_a. If $q^2 \neq -1$, from (3.13) we deduce

$$(dx)^2 = 0, \quad (dy)^2 = 0, \quad dydx + qdxdy = 0. \tag{3.14}$$

Using the relation (2.6) we find

$$dx = -\frac{1}{q^2(q^2+1)} x^{-1} y^2 \theta^1, \quad dy = -\frac{1}{q^2+1} x^{-2} y(y^2\theta^1 + \theta^2), \tag{3.15}$$

and solving for the θ^a we obtain

$$\theta^1 = -q^4(q^2+1)xy^{-2}dx, \quad \theta^2 = -q^2(q^2+1)x(xy^{-1}dy - dx). \tag{3.16}$$

The θ^a satisfy the commutation relations

$$(\theta^1)^2 = 0, \quad (\theta^2)^2 = 0, \quad q^4\theta^1\theta^2 + \theta^2\theta^1 = 0. \tag{3.17}$$

This is of the form (2.11) if the matrix $C^{ab}{}_{cd}$ is given by the 4×4 matrix

$$C = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & q^{-4} & 0 \\ 0 & q^4 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{3.18}$$

That is, $C^{12}{}_{21} = q^{-4}$ and $C^{21}{}_{12} = q^4$. The structure elements $C^a{}_{bc}$ are given by

$$C^1{}_{12} = -x^{-2}, \quad C^2{}_{12} = -x^{-2}y^2, \tag{3.19}$$

and the condition (2.14). Equation (2.18) is again satisfied.

For θ we find the expression

$$\theta = \frac{q^2}{q^2-1} y^{-1} dy. \tag{3.20}$$

It is again a closed form.

From these two examples we see that each choice of two elements λ_1 and λ_2 gives rise to a differential calculus on the generalized quantum plane and we shall see in the Section V that each choice gives rise to a linear connection.

IV. CALCULI BASED ON 3 DERIVATIONS

In this section we shall consider the case $n=3$. There is an essential difference with the previous case in that relations of the form (3.3) or (3.13) which allow one to pass from one side of the differential to the other no longer hold. The difference is given in fact in terms of the extra elements of the frame. What we do is extend the definition of dx and dy to another derivation and the extension satisfies quite naturally less relations. The left (or right) module $\Omega^1(\mathcal{A})$ is now of rank 3 instead of 2. As an example we extend the λ_a defined in (3.1) by the addition of a λ_3:

$$\lambda_1 = \frac{q}{q-1} y, \quad \lambda_2 = \frac{q}{q-1} x, \quad \lambda_3 = \frac{q}{q-1} \alpha xy. \tag{4.1}$$

The α is an arbitrary complex number. We have then $[\lambda_1,\lambda_2]=-\alpha^{-1}\lambda_3$, but of course the set of λ_a do not form a Lie algebra. To the relations (3.2) we must add two additional ones,

$$e_3x=-\alpha x^2y, \quad e_3y=\alpha xy^2, \tag{4.2}$$

and so we find

$$dx=-xy\,\theta^1-\alpha x^2y\,\theta^3, \quad dy=xy\,\theta^2+\alpha xy^2\,\theta^3 \tag{4.3}$$

instead of (3.5). Define

$$\tau=x\,dy-q\,dy\,x. \tag{4.4}$$

Then one of the commutation relations (3.3) becomes an expression for θ^3 in terms of τ:

$$\tau=\alpha q^{-1}(q-1)x^2y^2\,\theta^3. \tag{4.5}$$

We can solve then (4.3) for the θ^a and we obtain

$$\begin{aligned}
\theta^1&=-q^{-1}x^{-1}y^{-1}dx-\frac{1}{q^2(q-1)}\,x^{-1}y^{-2}\tau,\\
\theta^2&=q^{-1}x^{-1}y^{-1}dy-\frac{1}{q(q-1)}\,x^{-2}y^{-1}\tau,\\
\theta^3&=\frac{1}{\alpha q^3(q-1)}\,x^{-2}y^{-2}\tau
\end{aligned} \tag{4.6}$$

instead of (3.6). This frame is singular in the limit $q\to1$ as it must be. The differential calculus, expressed in terms of dx and dy, has however a well-defined limit which lies somewhere between the de Rham calculus and the universal one. For a discussion of this point we refer to Dimakis and Müller-Hoissen,[9] Dimakis and Tzanakis,[10] and Baehr *et al.*[7]

If $q\neq-1$, we can deduce the first two of the relations (3.4) and we can conclude that

$$\begin{aligned}
&q(\theta^1)^2+\alpha x(\theta^1\theta^3+q\,\theta^3\theta^1)+\alpha^2x^2(\theta^3)^2=0,\\
&q(\theta^2)^2+\alpha y(\theta^3\theta^2+q\,\theta^2\theta^3)+\alpha^2y^2(\theta^3)^2=0.
\end{aligned} \tag{4.7}$$

Multiply the first equation by y and the second by x and commute through. One deduces then that each of the coefficients must vanish:

$$(\theta^1)^2=0, \quad (\theta^2)^2=0, \quad (\theta^3)^2=0,$$

and

$$\theta^1\theta^3+q\,\theta^3\theta^1=0, \quad \theta^3\theta^2+q\,\theta^2\theta^3=0. \tag{4.8}$$

There is missing a relation between $\theta^1\theta^2$ and $\theta^2\theta^1$. We must therefore rather artificially complete the coefficients in (2.11) by setting $C^{12}{}_{12}=-1$ and $C^{12}{}_{21}=0$. From (2.23) we find then that $K_{ab}=0$ and the $F^a{}_{bc}$ vanish except for the values

$$F^3{}_{12}=\frac{2}{\alpha(q-1)}, \quad F^3{}_{21}=qF^3{}_{12}. \tag{4.9}$$

The form θ is given by

$$\theta = -\frac{q}{q-1}\,(y\,\theta^1 + x\,\theta^2 + \alpha xy\,\theta^3).$$

It follows then immediately from (2.19) that

$$\begin{aligned} d\theta^1 &= \frac{q}{q-1}\,x(\theta^1\theta^2 + \theta^2\theta^1) + \alpha xy\,\theta^1\theta^3, \\ d\theta^2 &= \frac{q}{q-1}\,y(\theta^1\theta^2 + \theta^2\theta^1) + \alpha xy\,\theta^3\theta^2, \\ d\theta^3 &= y\,\theta^1\theta^3 + x\,\theta^3\theta^2 - \frac{1}{\alpha(q-1)}\,(\theta^1\theta^2 + q\,\theta^2\theta^1), \end{aligned} \tag{4.10}$$

from which one can read off the expressions for the structure elements which extend (3.9). The third of the relations (3.4) becomes

$$d\tau = -x^2y^2((\theta^1\theta^2 + q\,\theta^2\theta^1) + \alpha x(\theta^2\theta^3 + \theta^3\theta^2) + \alpha y(\theta^3\theta^1 + \theta^1\theta^3)).$$

Using (4.10) one finds

$$d\tau = -x^2y^2((\theta^1\theta^2 + q\,\theta^2\theta^1) - \alpha q^{-1}(q-1)\,d\theta^3). \tag{4.11}$$

If one adds to (4.8) the supplementary relation

$$\theta^1\theta^2 + q\,\theta^2\theta^1 = 0, \tag{4.12}$$

then $\Omega^2(\mathscr{A})$ becomes a quotient of the right-hand side of (2.4). We can set $C^{12}{}_{21} = q$ and $C^{12}{}_{12} = 0$ as in (3.8). Now we have $K_{ab} = 0$ and $F^a{}_{bc} = 0$ and Equations (4.10) reduce to

$$d\theta^1 = x\,\theta^1\theta^2 + \alpha xy\,\theta^1\theta^3, \quad d\theta^2 = y\,\theta^1\theta^2 + \alpha xy\,\theta^3\theta^2, \quad d\theta^3 = y\,\theta^1\theta^3 + x\,\theta^3\theta^2.$$

Equation (4.11) simplifies to

$$d\tau = \alpha x^2y^2q^{-1}(q-1)\,d\theta^3. \tag{4.13}$$

A similar extension of the second example of the previous section can be given, again by introducing a third derivation. As before this yields an extension of the module of forms as a left (or right) module.

V. LINEAR CONNECTIONS

For each of the differential calculi defined in the previous section one can define a set of linear connections. The definition of a connection as a covariant derivative was given an algebraic form in the Tata lectures by Koszul[11] and generalized to noncommutative geometry by Karoubi[12] and Connes.[8,6] We shall often use here the expressions 'connection' and 'covariant derivative' synonymously. In fact one can distinguish three different types of connections. A 'left $\mathscr{A}$-connection' is a connection on a left $\mathscr{A}$-module; it satisfies a left Leibniz rule. A 'bimodule $\mathscr{A}$-connection' is a connection on a general bimodule $\mathscr{M}$ which satisfies a left and right Leibniz rule. In the particular case where $\mathscr{M}$ is the module of 1-forms we shall speak of a 'linear connection.' A bimodule over an algebra $\mathscr{A}$ is also a left module over the tensor product $\mathscr{A}^e = \mathscr{A}\otimes_{\mathbb{C}}\mathscr{A}^{op}$ of the

algebra with its 'opposite.' Such a bimodule can have a bimodule $\mathscr{A}$-connection as well as a left $\mathscr{A}^e$-connection.[13,14] These two definitions are compared in Dubois-Violette *et al.*[15]

Let $\mathscr{A}$ be an arbitrary algebra and $(\Omega^*(\mathscr{A}),d)$ a differential calculus over $\mathscr{A}$. One defines a left $\mathscr{A}$-connection on a left $\mathscr{A}$-module $\mathscr{H}$ as a covariant derivative

$$\mathscr{H}\overset{D}{\to}\Omega^1(\mathscr{A})\otimes_{\mathscr{A}}\mathscr{H} \tag{5.1}$$

which satisfies the left Leibniz rule

$$D(f\psi)=df\otimes\psi+fD\psi \tag{5.2}$$

for arbitrary $f\in\mathscr{A}$. This map has a natural extension

$$\Omega^*(\mathscr{A})\otimes_{\mathscr{A}}\mathscr{H}\overset{\nabla}{\to}\Omega^*(\mathscr{A})\otimes_{\mathscr{A}}\mathscr{H} \tag{5.3}$$

given, for $\psi\in\mathscr{H}$ and $\alpha\in\Omega^n(\mathscr{A})$, by $\nabla\psi=D\psi$ and

$$\nabla(\alpha\psi)=d\alpha\otimes\psi+(-1)^n\alpha\nabla\psi.$$

The operator ∇^2 is necessarily left-linear. However, when $\mathscr{H}$ is a bimodule it is not, in general, right-linear.

A covariant derivative on the module $\Omega^1(\mathscr{A})$ must satisfy (5.2). But $\Omega^1(\mathscr{A})$ has also a natural structure as a right $\mathscr{A}$-module and one must be able to write a corresponding right Leibniz rule in order to construct a bilinear curvature. Quite generally let $\mathscr{M}$ be an arbitrary bimodule. Consider a covariant derivative

$$\mathscr{M}\overset{D}{\to}\Omega^1(\mathscr{A})\otimes_{\mathscr{A}}\mathscr{M} \tag{5.4}$$

which satisfies both a left and a right Leibniz rule. In order to define a right Leibniz rule which is consistent with the left one, it was proposed by Mourad,[16] by Dubois-Violette and Michor[17] and by Dubois-Violette and Masson[18] to introduce a generalized permutation

$$\mathscr{M}\otimes_{\mathscr{A}}\Omega^1(\mathscr{A})\overset{\sigma}{\to}\Omega^1(\mathscr{A})\otimes_{\mathscr{A}}\mathscr{M}.$$

The right Leibniz rule is given then as

$$D(\xi f\ )=\sigma(\xi\otimes df\ )+(D\xi)f \tag{5.5}$$

for arbitrary $f\in\mathscr{A}$ and $\xi\in\mathscr{M}$. The purpose of the map σ is to bring the differential to the left while respecting the order of the factors. It is necessarily bilinear.[19] Let π be the product in the algebra of forms. It was argued by Mourad[16] and others[19] that a necessary as well as sufficient condition for torsion to be right-linear is that σ satisfy the consistency condition

$$\pi\circ(\sigma+1)=0. \tag{5.6}$$

We define a bimodule $\mathscr{A}$-connection to be the couple (D,σ). We shall make no mention of curvature. There is at the moment no general consensus of the correct definition of the curvature of a bimodule connection. The problem is that the operator ∇^2 is not, in general, right-linear. We refer to Dubois-Violette *et al.*[15] for a recent discussion.

This general formalism can be applied in particular to the differential calculi which we have constructed in Section II. Since $\Omega^1(\mathscr{A})$ is a free module the map σ can be defined by the action on the basis elements:

$$\sigma(\theta^a\otimes\theta^b)=S^{ab}{}_{cd}\theta^c\otimes\theta^d. \tag{5.7}$$

By the sequence of identities

$$fS^{ab}{}_{cd}\theta^c\otimes\theta^d=\sigma(f\theta^a\otimes\theta^b)=\sigma(\theta^a\otimes\theta^b f\ )=S^{ab}{}_{cd}f\theta^c\otimes\theta^d$$

we conclude that the coefficients S^{ab}_{cd} must lie in $\mathscr{Z}(\mathscr{A})$. From (2.12) we see that the condition (5.6) can be written

$$(\delta^a_e\delta^b_f+S^{ab}{}_{ef})(\delta^e_c\delta^f_d-C^{ef}{}_{cd})=0. \tag{5.8}$$

A natural, but certainly not the unique, choice of σ is given by $S^{ab}{}_{cd}=C^{ab}{}_{cd}$.

Since $\Omega^1(\mathscr{A})$ is a free module a covariant derivative can be defined by its action on the basis elements:

$$D\theta^a=-\omega^a_{bc}\theta^b\otimes\theta^c. \tag{5.9}$$

The coefficients here are elements of the algebra. Because of the identity $D(f\theta^a)=D(\theta^a f\ )$ there are very stringent compatibility conditions, which using (5.7) can be written out as

$$[\omega^a_{bc},f]=e_d f(S^{ad}{}_{bc}-\delta^d_b\delta^a_c).$$

The general solution to this equation is of the form $\omega^a{}_{bc}=\omega_{(0)}{}^a{}_{bc}+\chi^a{}_{bc}$ where

$$\omega(0)^a_{bc}=\lambda_d(S^{ad}{}_{bc}-\delta^d_b\delta^a_c) \tag{5.10}$$

and $\chi^a{}_{bc}\in\mathscr{Z}(\mathscr{A})$. One can also express $D_{(0)}$ in the form[19,20]

$$D_{(0)}\theta^a=-\theta\otimes\theta^a+\sigma(\theta^a\otimes\theta).$$

The torsion 2-form is defined as usual as

$$\Theta^a=d\theta^a-\pi\circ D\theta^a.$$

Comparing (5.10) with (2.19), we see that the torsion $\Theta^a_{(0)}$ of $D_{(0)}$ is given by

$$\Theta^a_{(0)}=-\tfrac{1}{2}F^a{}_{bc}\theta^b\theta^c. \tag{5.11}$$

In general a covariant derivative is torsion free provided the condition

$$\omega^a{}_{bc}-\omega^a{}_{de}C^{de}{}_{bc}=C^a{}_{bc}$$

is satisfied. The covariant derivative (5.9) is torsion free if and only if

$$\chi^a{}_{de}(\delta^d_b\delta^e_c-C^{de}{}_{bc})=F^a{}_{bc}.$$

On the ordinary quantum plane one can show that there is there is a unique 1-parameter family of linear connections[19] and that this connection is torsion free. We find here a different result; there is an ambiguity which depends on elements of $\mathscr{Z}(\mathscr{A})$. An interesting limit case is given by

$$S^{ab}{}_{cd}=C^{ab}{}_{cd}=\delta^b_c\delta^a_d. \tag{5.12}$$

In this case from (2.18) one sees that $F^a{}_{bc}=C^a{}_{bc}\neq 0$. From (2.22) one sees that $K_{ab}=0$ and the λ_a form a Lie algebra. The matrix case is a typical example. From (5.10) if follows that $D_{(0)}\theta^a=0$ and so $D_{(0)}$ has torsion but no curvature. The connection corresponds to the canonical flat connection on a parallelizable manifold.

One can define a metric by the condition

$$g(\theta^a\otimes\theta^b)=g^{ab}, \tag{5.13}$$

where the coefficients g^{ab} are elements of the algebra. To be well defined on all elements of the tensor product $\Omega^1(\mathscr{A})\otimes_{\mathscr{A}}\Omega^1(\mathscr{A})$ the metric must be bilinear, and by the sequence of identities

$$f^{ab}_g=g(f\theta^a\otimes\theta^b)=g(\theta^a\otimes\theta^b f\ )=g^{ab}f \tag{5.14}$$

we conclude that the coefficients must lie in $\mathscr{Z}(\mathscr{A})$. The covariant derivative (5.9) is compatible with the metric[19] if and only if

$$\omega^a{}_{bc}+\omega^f{}_{ce}S^{ae}{}_{bf}=0. \tag{5.15}$$

The condition that (5.10) be metric compatible can be written as

$$S^{ae}{}_{dh}g^{hf}S^{cb}{}_{ef}=g^{ac}\delta^b_d. \tag{5.16}$$

Consider now the first differential calculus of Section III, defined by (3.1). On the right-hand side of (2.23) we have $K_{ab}=0$ and $F^a{}_{bc}=0$. The torsion of $D_{(0)}$ vanishes. The coefficients g^{ab} are complex numbers. With the convention of (3.8) they can be written as (g^1,g^2,g^3,g^4). Using the $GL(2,\mathbb{C})$-invariance one can impose that

$$g^4=g^1,\quad g^2=-g^2.$$

If we suppose that $g^2=0$, there is no restriction in supposing that $g^1=1$; the g^{ab} are the components of the Euclidean metric in two dimensions. With the convention of (3.8) the condition (5.16) can be written in the matrix form

$$\begin{pmatrix} S^1_1 & S^1_2 & S^1_3 & S^1_4\\ S^2_1 & S^2_2 & S^2_3 & S^2_4\\ S^3_1 & S^3_2 & S^3_3 & S^3_4\\ S^4_1 & S^4_2 & S^4_3 & S^4_4 \end{pmatrix}\begin{pmatrix} S^1_1 & S^1_3 & S^3_1 & S^3_3\\ S^1_2 & S^1_4 & S^3_2 & S^3_4\\ S^2_1 & S^2_3 & S^4_1 & S^4_3\\ S^2_2 & S^2_4 & S^4_2 & S^4_4 \end{pmatrix}=1. \tag{5.17}$$

From the approximation linear in $q-1$ one sees that the solution must be of the form

$$S=\begin{pmatrix} S^1_1 & 0 & 0 & S^1_4\\ 0 & S^2_2 & S^2_3 & 0\\ 0 & S^3_2 & S^3_3 & 0\\ S^4_1 & 0 & 0 & S^4_4 \end{pmatrix}. \tag{5.18}$$

The consistency conditions (5.8) become

$$1+S^2_2=q^{-1}S^2_3,\quad 1+S^3_3=qS^3_2. \tag{5.19}$$

In general $S^{ab}{}_{cd} = C^{ab}{}_{cd}$ does not yield a metric-compatible covariant derivative. There is a solution, however, to (5.17) and (5.19) given by

$$S=\frac{1}{q^2+1}\begin{pmatrix} 2q & 0 & 0 & 1-q^2 \\ 0 & 1-q^2 & 2q & 0 \\ 0 & 2q & q^2-1 & 0 \\ q^2-1 & 0 & 0 & 2q \end{pmatrix}. \tag{5.20}$$

That is, for example,

$$S^{12}{}_{21}=S^{21}{}_{12}=\frac{2q}{q^2+1}.$$

The expression (5.20) has the same limit as (3.8) when $q\to 1$, as it must for the right-hand side of (5.10) to exist. With σ given by (5.7), the covariant derivative is compatible with the metric (5.13) and torsion free. Comparing (3.18) with (3.8) one sees that one obtains for the second example (3.11) a covariant derivative compatible with the metric (5.13) by the replacement $q\mapsto q^{-4}$ in (5.20). The dependence on q comes through the conditions (5.19). Since $S(q)=-S(-q^{-1})$ the same matrix serves two different values of the parameter q.

The metric we have chosen is not symmetric with respect to σ. That is

$$g^{ab}\neq S^{ab}{}_{cd}g^{cd}$$

in general. If one wishes to find a metric symmetric in the above sense, then one must consider (5.16) as an equation for S and the metric and add the additional equation

$$g^{ab}=S^{ab}{}_{cd}g^{cd}. \tag{5.21}$$

The system (5.16) and (5.21), without the restriction we have placed on the coefficients g^{ab}, if it has a solution, would yield a symmetric metric with a compatible connection.

Restricting one's attention to Hermitian x and y and real q, in the limit $q\to 1$ one obtains on the ordinary 2-plane a metric whose Gaussian curvature K is given by

$$K_1=x^2+y^2, \quad K_2=x^{-4}(1+y^4), \tag{5.22}$$

respectively, for the two examples of Section III. This can be calculated using the $q\to 1$ limit of (5.10). It is easy to characterize all metrics which can be obtained in this way. In the limit $q\to 1$ the commutator determines a Poisson bracket on the 2-plane, given as usual by

$$\{f,g\}=\lim_{q\to 1}\frac{1}{i(q-1)}[f,g]. \tag{5.23}$$

Define

$$p_a=\lim_{q\to 1} i(q-1)\lambda_a .$$

In the limit the differential can be written then in the form

$$df=\{p_a,f\}\theta^a. \tag{5.24}$$

If we write $\theta^a=\theta^a_b dx^b$ in terms of dx^a, from this it follows that the equation

$$\{p_c, x^a\}\theta^c_b = \delta^a_b \tag{5.25}$$

must have a solution for p_a polynomial in the variables. This is not always the case. That is, not all metrics with polynomial curvature can be obtained as were those given by (5.22). For example consider the flat metric $\theta^a_b = \delta^a_b$. The equations (5.25) become the equations $\{p_a, x^b\} = \delta^a_b$. Using the expression for the Poisson bracket for the generalized quantum plane, $\{x,y\} = xy$, one sees immediately that there is no solution for the p_a.

The generalized quantum plane has two outer derivations defined by

$$e^{(0)}_1 x = x, \quad e^{(0)}_1 y = 0, \quad \epsilon^{(0)}_2 x = 0, \quad e^{(0)}_2 y = y. \tag{5.26}$$

The corresponding θ^a are given by

$$\theta^1 = x^{-1}dx, \quad \theta^2 = y^{-1}dy. \tag{5.27}$$

Our construction yields then the ordinary flat metric. If one were to extend the algebra to the Heisenberg algebra, then these derivations would become interior. To obtain a metric which is almost flat one can add to (5.26) a 'small' inner derivation of the form given in Section II, but using λ_a which are 'small' of the order of some expansion parameter ϵ. One defines

$$e_a = e^{(0)}_a + \epsilon \mathrm{ad}\lambda_a \tag{5.28}$$

and proceeds as above but retaining only corrections of first order in ϵ. A problem closely related to this has been examined in another context by one of the authors.[5]

The equations (5.17) and (5.19) admit also the solution

$$S = \frac{1}{q^2+1}\begin{pmatrix} -2q & 0 & 0 & 1-q^2 \\ 0 & 1-q^2 & 2q & 0 \\ 0 & 2q & q^2-1 & 0 \\ q^2-1 & 0 & 0 & -2q \end{pmatrix}. \tag{5.29}$$

but the corresponding covariant derivative defined by (5.10) is singular in the limit $q \to 1$.

A complete study of the matrix case has not been made. However, for the particular case (5.12) it is easy to see that the unique torsion free covariant derivative compatible with the metric (5.13) is given by

$$D\theta^a = -\tfrac{1}{2} C^a{}_{bc}\theta^b \otimes \theta^c. \tag{5.30}$$

The ordinary quantum plane with the differential calculus given by (3.13) has no metric connection but it possesses a unique 1-parameter family of linear connections whose curvature is polynomial in the variables x and y.[19] The precise property of the curvature K_2 in (5.22) which associates the corresponding metric to the $GL_q(2)$-invariant differential calculus (3.13) is not clear. We refer to Madore and Mourad[21] for a description of the possible relevance to the theory of gravity of the relation between linear connections on the one hand and commutation relations on the other.

VI. CONCLUSIONS

We have shown that each differential calculus and set of commutation relations between the 1-forms and the elements of the algebra gives rise in the case of the generalized quantum plane to a metric connection which remains regular in the limit $q \to 1$. Not all metrics with polynomial curvature can be obtained in this way.

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A non-commutative central limit theorem

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We prove a non-commutative version of the Central Limit Theorem for spin-1/2 variables. The non-commutative spins satisfy Bose–Einstein statistics. The proof involves the Feynman–Kac formula for a hopping process and an explicit calculation of the Fourier transform of the corresponding measure. The limit process is a modification of the Ornstein–Uhlenbeck process, the Fourier transform of which was essentially already calculated by Feynman. However, his derivation is not rigorous and we therefore present an alternative derivation here. © *1996 American Institute of Physics.* [S0022-2488(96)03009-5]

I. MOTIVATION AND THE MAIN RESULTS

The usual Central Limit Theorem in the case of Bernoulli variables states that if a particle can take on two states + and − with probabilities 1/2 then the average value of the sum of n particle states has a normal distribution in the limit $n\to\infty$. To be precise:

$$\lim_{n\to\infty} \mathbb{E}\left[f\left(\frac{1}{\sqrt{n}} \sum_{k=1}^{n} x_k \right) \right] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) \exp\left[-\frac{1}{2} x^2 \right] dx \tag{1.1}$$

for any continuous bounded function f. This result can be interpreted as a result in classical statistical mechanics, giving the asymptotic distribution of the total spin of an assembly of independent classical spins x_i. One may then wonder about the behavior of quantum spins.

Quantum spins differ from classical spins in that they are described by non-commuting operators. We introduce annihilation operators a_+ and a_- and creation operators a_+^* and a_-^* which annihilate and create particles with spin + and − respectively. They obey the commutation relations

$$[a_\pm, a_\pm^*] = 1, \quad [a_\pm, a_\mp^*] = 0, \tag{1.2}$$

while creation and annihilation operators commute among themselves. The products $N_\pm = a_\pm^* a_\pm$ count the number of particles with spin + and − respectively. $a_\pm^*$ and $a_\pm$ can be represented on the Hilbert space $\mathscr{H}_\pm$ which is spanned by the eigenstates $|n\rangle_\pm$ of the number operators $N_\pm$. The total Hilbert space is the direct sum of these two: $\mathscr{H} = \mathscr{H}_+ \oplus \mathscr{H}_-$.

We now consider the operators $c_\pm$ and $c_\pm^*$ and Δ defined by

$$c_\pm = \frac{1}{\sqrt{2}} (a_+ \pm a_-) \quad \text{and} \quad \Delta = a_+^* a_+ - a_-^* a_- . \tag{1.3}$$

Notice that $c_\pm$ and $c_\pm^*$ are also annihilation and creation operators in that they satisfy commutation relations analogous to (1.2). Therefore $c_\pm^* c_\pm$ is also a number operator, giving the number of particles in the state $(1/\sqrt{2})(|+\rangle \pm |-\rangle)$. We shall write $c = c_-$ in the following. The corresponding number operator can be written as follows:

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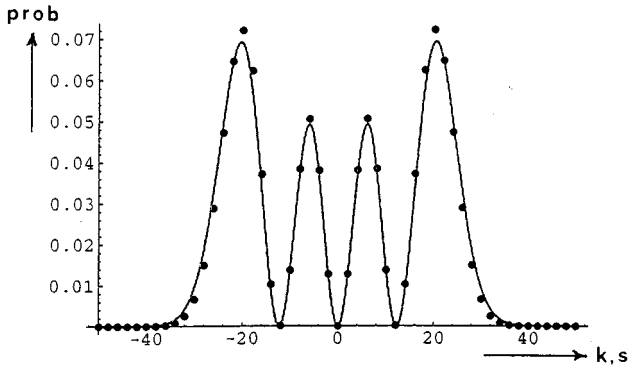

FIG. 1. The probability distribution of the eigenvalues of Δ (heavy dots) and the limiting distribution (grey curve).

$$c^*c = \tfrac{1}{2}(N_- + N_-) - \tfrac{1}{2}(a_+^* a_- + a_-^* a_+). \tag{1.4}$$

The total number operator $N = N_+ + N_-$ commutes with c^*c and also with Δ. We can therefore restrict the system to the n-particle subspace, that is, the subspace of $\mathscr{H}$ where N has the eigenvalue n. The second part of the operator c^*c is a hopping term: it annihilates a particle with one spin and creates a particle with the opposite spin. The operator Δ measures the net spin of all particles. That is similar to the expression $\Sigma_{k=1}^n x_k$ in (1.1). We now prove the following noncommutative analogue of (1.1):

Theorem 1.1: For any $n,m \in \mathbb{N}$ with $0 \leqslant m \leqslant n$, denote by $|n;m\rangle$ the eigenstate of c^*c in the n-particle subspace $\mathscr{H}_n$ with eigenvalue m. Then, for any bounded continuous function $f:\mathbb{R}\to\mathbb{R}$,

$$\lim_{n\to\infty} \langle n;m|f(\Delta/\sqrt{n})|n;m\rangle = \frac{1}{m!\sqrt{2\pi}} \int_{-\infty}^{\infty} H_m(x)^2 e^{-x^2/2} f(x)\,dx, \tag{1.5}$$

where $H_m(x)$ $(m=0,1,2,...)$ are the Hermite polynomials defined by

$$H_m(x) = (-1)^m e^{x^2/2}\left(\frac{d}{dx}\right)^m e^{-x^2/2}. \tag{1.6}$$

Before we prove this simple result, let us consider the graph of the probability distribution of the eigenvalue k of the operator Δ in the case $n=50$ and $m=3$ (see Figure 1). In the same graph the rescaled distribution function

$$\frac{1}{m!\sqrt{2\pi}} H_m\left(\frac{s}{\sqrt{n}}\right)^2 \exp[-s^2/2n]$$

is plotted as a function of the continuous variable s corresponding to k. It is clear that the graphs are already reasonably close. Notice also that the quantum nature of the system does not disappear in the limit! One could say that fluctuations of a quantum system still have a quantum nature in that interference effects remain. A similar phenomenon, but in a different setting was noted by Goderis *et al.*[1,2]

Proof: We prove that the corresponding Fourier transforms converge. This proves the theorem: see, e.g., Refs. 3, 4 or 5. We first compute the characteristic function of the limiting distribution. We use the generating function for the Hermite polynomials:

$$\sum_{m=0}^{\infty} H_m(x)\,\frac{\alpha^m}{m!} = e^{\alpha x-\alpha^2/2}. \tag{1.7}$$

This yields easily

$$\sum_{m_1=0}^{\infty} \frac{\alpha_1^m}{m_1!} \sum_{m_2=0}^{\infty} \frac{\alpha_2^{m_2}}{m_2!} \int_{-\infty}^{\infty} H_{m_1}(x)H_{m_2}(x)e^{itx}e^{-x^2/2}\,\frac{dx}{\sqrt{2\pi}} = e^{-t^2/2}e^{i(\alpha_1+\alpha_2)t+\alpha_1\alpha_2}. \tag{1.8}$$

Expanding the exponential factor we have

$$e^{i(\alpha_1+\alpha_2)t+\alpha_1\alpha_2} = \sum_{m_1=0}^{\infty}\sum_{m_2=0}^{\infty}\left(\sum_{l=0}^{m_1\wedge m_2} \frac{(it)^{m_1+m_2-2l}}{l!(m_1-l)!(m_2-l)!}\right)\alpha_1^{m_1}\alpha_2^{m_2}. \tag{1.9}$$

Extracting the terms $m_1=m_2=m$ we find that

$$\frac{1}{m!}\int_{-\infty}^{\infty} H_m(x)^2e^{itx}e^{-x^2/2}\,\frac{dx}{\sqrt{2\pi}} = \sum_{k=0}^{m}\binom{m}{k}(-1)^k\,\frac{t^{2k}}{k!}\,e^{-t^2/2}. \tag{1.10}$$

To compute the characteristic function of the discrete distribution of the eigenvalues of Δ we use the fact that

$$|n;m\rangle = \frac{1}{\sqrt{m!(n-m)!}}\,c_+^{*(n-m)}c^{*m}|0\rangle \tag{1.11}$$

and hence

$$\begin{aligned}\sum_{m=0}^{n}\binom{n}{m}^{1/2}\alpha^m|n;m\rangle &= \frac{1}{\sqrt{2^n n!}}\sum_{m=0}^{n}\binom{n}{m}\alpha^m(\alpha_+^*+a_-^*)^{n-m}(a_+^*-a_-^*)^m|0\rangle\\ &= \frac{1}{\sqrt{2^n n!}}[(1+\alpha)a_+^*+(1-\alpha)a_-^*]^n|0\rangle\\ &= 2^{-n/2}\sum_{k=0}^{n}\binom{n}{k}^{1/2}(1+\alpha)^k(1-\alpha)^{n-k}|k,n-k\rangle,\end{aligned} \tag{1.12}$$

where $|n_+,n_-\rangle$ denotes an eigenstate of the operators $N_\pm$. Inserting this identity one easily finds that

$$\begin{aligned}&\sum_{m_1=0}^{n}\binom{n}{m_1}^{1/2}\sum_{m_2=0}^{n}\binom{n}{m_2}^{1/2}\langle n;m_1|e^{it\Delta}|n;m_2\rangle\alpha_1^{m_1}\alpha_2^{m_2}\\ &\quad= 2^{-n}[(1+\alpha_1)(1+\alpha_2)e^{it}+(1-\alpha_1)(1-\alpha_2)e^{-it}]^n\\ &\quad= [(1+\alpha_1\alpha_2)\cos t + i(\alpha_1+\alpha_2)\sin t]^n.\end{aligned} \tag{1.13}$$

It follows that

$$\langle n;m|e^{it\Delta}|n;m\rangle=\binom{n}{m}^{-1}\sum_{k=0}^{[n/2]\wedge m}\binom{n}{2k}\binom{2k}{k}\binom{n-2k}{m-k}(-1)^k(\sin t)^{2k}(\cos t)^{n-2k}$$

$$=\sum_{k=0}^{[n/2]\wedge m}\frac{(-1)^k}{k!}\binom{m}{k}\frac{(n-m)!}{(n-m-k)!}(\sin t)^{2k}(\cos t)^{n-2k}. \tag{1.14}$$

Replacing t by $t/\sqrt{n}$ and taking $n\to\infty$ it is now easy to see that this tends to (1.10). Q.E.D.

The above theorem gives a way of computing expressions of the form

$$\mathrm{Trace}_n(e^{-\beta c^*c}f(\Delta/\sqrt{n}))$$

in the limit $n\to\infty$. However, in quantum statistical mechanics one is rather more interested in computing quantities of the form Trace $e^{-\beta H}$, where in our case, $H=c^*c+f(\Delta/\sqrt{n})$. This is not the same as the above because the operators c^*c and Δ do not commute. To compute the latter expression, we could try to use the Trotter product formula (Theorem 1.1 of Ref. 6):

$$e^{A+B}=\lim_{M\to\infty}(e^{A/M}e^{B/M})^M. \tag{1.15}$$

This yields:

$$\mathrm{Trace}_n\ \exp[-\beta c^*c+f(\Delta/\sqrt{n})]$$

$$=\sum_{m=0}^{n}\langle n;m|\exp[-\beta c^*c+f(\Delta/\sqrt{n})]|n;m\rangle$$

$$=\lim_{M\to\infty}\sum_{m_1,\ldots,m_M=0}^{n}\prod_{i=1}^{M}\langle n;m_{i-1}|e^{f(\Delta/\sqrt{n})/M}|n;m_i\rangle\prod_{i=1}^{M}e^{-\beta m_i/M}, \tag{1.16}$$

where $m_0=m_M$. Using a simple generalization of Theorem 1 we can now conjecture that the limit $n\to\infty$ yields

$$\lim_{n\to\infty}\mathrm{Trace}_n\ \exp[-\beta c^*c+f(\Delta/\sqrt{n})]$$

$$=\lim_{M\to\infty}\sum_{m_1,\ldots,m_M=0}^{\infty}\prod_{i=1}^{M}e^{-\beta m_i/M}\times\prod_{i=1}^{M}\left[\frac{1}{\sqrt{2\pi m_{i-1}!m_i!}}\right.$$

$$\left.\times\int_{-\infty}^{\infty}H_{m_{i-1}}(x)H_{m_i}(x)e^{f(x)/M}e^{-x^2/2}dx\right]. \tag{1.17}$$

Now,

$$\psi_m(x)=\frac{1}{\sqrt{m!}}H_m(x)\Omega_0(x) \tag{1.18}$$

is the m-th eigenfunction of the harmonic oscillator Hamiltonian

$$H_0=-\frac{d^2}{dx^2}+\frac{1}{4}x^2-\frac{1}{2}, \tag{1.19}$$

with

$$\Omega_0(x)=(2\pi)^{-1/4}e^{-x^2/4} \tag{1.20}$$

being the ground state: $H_0\Omega_0=0$ and $H_0\psi_m=m\psi_m$. Putting

$$a=\frac{1}{2}x+\frac{d}{dx} \quad \text{and} \quad a^*=\frac{1}{2}x-\frac{d}{dx} \tag{1.21}$$

as usual, we have $[a,a^*]=1$ and

$$H_0=a^*a \quad \text{and} \quad x=a+a^*. \tag{1.22}$$

This means that we can write

$$\begin{aligned}\lim_{n\to\infty}\text{Trace}_n\ \exp[-\beta c^*c+f(\Delta/\sqrt{n})]&=\lim_{M\to\infty}\sum_{m_1,\ldots,m_M=0}^{\infty}\prod_{i=1}^{M}(\psi_{m_{i-1}}|e^{-\beta H_0/M}e^{f(a+a^*)/M}\psi_{m_i})\\&=\lim_{M\to\infty}\sum_{m=0}^{\infty}(\psi_m|(e^{-\beta H_0/M}e^{f(a+a^*)/M})^M\psi_m)\\&=\text{Trace}\ \ e^{-\beta H_0+f(a+a^*)}.\end{aligned} \tag{1.23}$$

Thus we conjecture the following theorem:

Theorem 1.2. For any bounded continuous function f: $\mathbb{R}\to\mathbb{R}$,

$$\lim_{n\to\infty}\text{Trace}_n\ e^{-\beta c^*c+f(\Delta/\sqrt{n})}=\text{Trace}\ \ e^{-\beta a^*a+f(a+a^*)}. \tag{1.24}$$

It should be realized that the above derivation does not constitute a proof since the limits $n\to\infty$ and $M\to\infty$ were interchanged without justification. (Professor Zagrebnov suggested that it may in fact be possible to make the argument rigorous using trace-norm convergence proved in his paper.[7]) The remaining sections of this paper are dedicated to a proof of this last theorem using the Feynman–Kac representation.

Remark. Several versions of the non-commutative central limit theorem were also derived by Hudson.[8–10] Let us briefly comment on the main differences. In Theorem 1.1 we keep the eigenvalue m of the operator c^*c fixed while taking the number of particles n to infinity. Also, the spins are assumed to commute as opposed to anti-commute as in the case of Clifford algebra version considered in Refs. 9 and 10. Notice that we consider only two pairs of creation and annihilation operators whereas in Ref. 8 Hudson considers in effect a sequence of creation and annihilation operators. In Theorem 1.2 the eigenvalue m is not fixed as such but it is implicit in the proof that the main contribution still comes from the subspaces where m is bounded. This is a rudimentary kind of boson condensation and was in fact the main motivation for this work. In both the above theorems it is the number of particles that tends to infinity as opposed to the number of creation and annihilation operators.

II. THE FEYNMAN–KAC FORMULA

In this section we derive a Feynman-Kac formula in the spirit of Ginibre.[11] (However, the derivation is self-contained and does not assume familiarity with Ginibre's work.) We work with eigenstates of Δ instead of c^*c. Let $|x_1,\ldots,x_n\rangle$ denote the state where the k-th spin is given by $x_k(=\pm1)$. (For the moment we assume the individual spins to be distinguishable.) Then we can define individual particle creation and annihilation operators:

$$a_{k,s}|x_1,\ldots,x_n\rangle=\delta_{x_k,s}|x_1,\ldots,\hat{x}_k,\ldots,x_n\rangle,$$
$$a^*_{k,s}|x_1,\ldots,x_n\rangle=|x_1,\ldots,x_{k-1},s,x_k,\ldots,x_n\rangle. \tag{2.1}$$

(The hat above x_k in the first formula indicates that this element is to be omitted.) The states $|x_1,\ldots,x_n\rangle$ form an orthonormal basis of a 2^n-dimensional Hilbert space of distinguishable particles. We can reduce the space to one spanned by distinguishable elements given by symmetric combinations:

$$|n_+,n_-\rangle=\binom{n_++n_-}{n_+}^{-1/2}\sum_{\substack{x_1,\ldots,x_n=\pm\\ \#\{x_k=\pm\}=n_\pm}}|x_1,\ldots,x_n\rangle. \tag{2.2}$$

Let $\mathscr{F}_n$ be the space spanned by all states $|n_+,n_-\rangle$ with $n_++n_-=n$:

$$\mathscr{F}_n=[\![|n_+,n_-\rangle:n_++n_-=n]\!]. \tag{2.3}$$

It is then easy to see that the operators $a_\pm$ and $a^*_\pm$ defined previously can be represented operating on $\mathscr{F}_n$ as follows:

$$a_\pm|_{\mathscr{F}_n}=\frac{1}{\sqrt{n}}\sum_{k=1}^{n}a_{k,\pm}\Big|_{\mathscr{F}_n},\quad a^*_\pm|_{\mathscr{F}_n}=\frac{1}{\sqrt{n+1}}\sum_{k=1}^{n+1}a^*_{k,\pm}\Big|_{\mathscr{F}_n}. \tag{2.4}$$

Inserting these formulas we can now write

$$\begin{aligned}&\langle n'_+,n'_-|e^{-\beta c^*c+f(\Delta)}|n_+,n_-\rangle\\ &\quad=\binom{n}{n'_+}^{-1/2}\binom{n}{n_+}^{-1/2}\\ &\quad\times\sum_{\substack{x'_1,\ldots,x'_n\\ \#\{x'_k=\pm\}=n'_\pm}}\ \sum_{\substack{x_1,\ldots,x_n\\ \#\{x_k=\pm\}=n_\pm}}\langle x'_1,\ldots,x'_n|\exp\Bigg[-\frac{\beta}{2}\sum_{k=1}^{n}(a^*_{k,+}-a^*_{k,-})\\ &\quad\times(a_{k,+}-a_{k,-})+f\Bigg(\sum_{k=1}^{n}(a^*_{k,+}a_{k,+}-a^*_{k,-}a_{k,-})\Bigg)\Bigg]|x_1,\ldots,x_n\rangle.\end{aligned} \tag{2.5}$$

The latter scalar products can be written in terms of a stochastic process. Heuristically, we can define a simple jump process ξ with continuous time and values ±1 by the infinitesimal transition probabilities

$$\mathbb{P}_\beta[\xi(t+\delta t)=x'|\xi(t)=x]=\begin{cases}1-\dfrac{\beta}{2}\,\delta t, & \text{if } x'=x;\\[2mm] \dfrac{\beta}{2}\,\delta t, & \text{if } x'=-x.\end{cases} \tag{2.6}$$

This is the so-called *telegraph process*. It is well-known that this process can be defined rigorously as a measure $\mathbb{P}_{\beta,x}$, where $x=\pm1$ is the starting point of the process, on the space $D[0,1]$ of

functions $\xi:[0,1]\to\mathbb{R}$ which are right-continuous and have limits on the left, the so-called Cadlag space in French terminology. Thus, $\xi\in D[0,1]$ if and only if, for all $t_0\in(0,1)$,

$$\lim_{t\downarrow t_0}\xi(t)=\xi(t_0)\quad\text{and}\quad\lim_{t\uparrow t_0}\xi(t)=\xi(t_0^-)\ \text{exist},\tag{2.7}$$

and, moreover, $\xi(0)=\lim_{t\downarrow 0}\xi(t)$ and $\xi(1)=\lim_{t\uparrow 1}\xi(t)$. On this space one can introduce a metric, the Skorokhod metric, by

$$\rho(\xi,\xi')=\inf_{\lambda\in H}[\sup_{t\in\mathbb{R}}|\xi(\lambda(t))-\xi'(t)|+\sup_{t\in[0,1]}|\lambda(t)-t|].\tag{2.8}$$

Here H is the space of increasing functions $\lambda\colon[0,1]\to[0,1]$. One has the following characterization of compact subsets of $D[0,1]$:

Lemma 2.1: In order that a subset $K\subset D[0,1]$ be compact under the Skorokhod topology it is necessary and sufficient that K be bounded and closed and satisfy the condition

$$\limsup_{\delta\downarrow 0}\sup_{\xi\in K}\omega_\xi(\delta)=0,\tag{2.9}$$

where $\omega_\xi(\delta)$ is defined by

$$\begin{aligned}\omega_\xi(\delta)=&\sup_{t-\delta\le t'\le t\le t''\le t+\delta}\{|\xi(t')-\xi(t)|\wedge|\xi(t'')-\xi(t)|\}\\&+\sup_{0\le t\le\delta}|\xi(t)-\xi(0)|+\sup_{1-\delta\le t\le 1}|\xi(t)-\xi(1)|.\end{aligned}\tag{2.10}$$

(For a proof, see Ref. 12, Chapter 9, Sec. 5, Theorem 1, or Ref. 13, Chapter 7, Theorem 6.2.)

We now use Prokhorov's Theorem to extend the finite-dimensional distributions of $\mathbb{P}_{\beta,x}$ to a measure on $D[0,1]$. These finite-dimensional distributions are easily obtained by integrating the infinitesimal transition probabilities (2.6):

$$\mathbb{P}_{\beta,x}(\xi(t_1)=x_1,\ldots,\xi(t_n)=x_n)=p_{t_1}(x,x_1)p_{t_2-t_1}(x_1,x_2),\ldots,p_{t_n-t_{n-1}}(x_{n-1},x_n),\tag{2.11}$$

where the transition probabilities p_t are given by

$$p_t(x,x')=\tfrac{1}{2}(1+xx'e^{-\beta t}).\tag{2.12}$$

Lemma 2.2: There exists a unique Radon measure $\mathbb{P}_{\beta,x}$ on $D[0,1]$ (for $\beta>0$ and $x=\pm1$) with finite-dimensional distributions given by (2.11) for any finite set of points $0<t_1<\ldots<t_n\le 1$ and any corresponding set of values $x_i=\pm1$, $i=1,\ldots,n$.

Proof: According to Prokhorov's Theorem [see Ref. 14, Theorem 22 of Part I, Chapter I (p. 81)] it suffices to prove that, for all $\epsilon>0$ there exists a compact set $K\subset D[0,1]$ such that $\mu_{(t_1,\ldots,t_n)}[\pi_{(t_1,\ldots,t_n)}(K)]\geqslant 1-\epsilon$ for all finite sets $0<t_1<\ldots<t_n\le 1$, where $\mu_{(t_1,\ldots,t_n)}$ is the measure on $\mathbb{R}^n$ defined by $\mu_{(t_1,\ldots,t_n)}[A]=\mathbb{P}_{\beta,x}[(\xi(t_1),\ldots,\xi(t_n))\in A]$ and $\pi_{(t_1,\ldots,t_n)}$ is the projection given by $\pi_{(t_1,\ldots,t_n)}(\xi)=(\xi(t_1),\ldots,\xi(t_n))$.
(Indeed, it is easy to verify that the measures $\mu_{(t_1,\ldots,t_n)}$ form an exact projective system.) The uniqueness of $\mathbb{P}_{\beta,x}$ then follows from the fact that the projections $\pi_{(t_1,\ldots,t_n)}$ separate the points of $D[0,1]$.

We define the set K_N as follows:

$$K_N=\{\xi\in D[0,1]\,|\,\xi(t)=\pm 1 \text{ for all } t\in[0,1] \text{ and, for all } t_0\in(0,1):$$

$$\text{if } \xi(t_0)\neq\xi(t_0^-) \text{ then } \xi(t)=\xi(t_0)\forall t\in[t_0,t_0+1/N)$$

$$\text{and } \xi(t)=\xi(t_0^-)\forall t\in(t_0-1/N,t_0)\}.$$

The latter condition in the definition of K_N means that all jumps in ξ should be at least $1/N$ apart. It is now easy to see that

$$\mathbb{P}_{\beta,x}[K_N^c]<\frac{\beta^2}{2N}\to 0 \text{ as } N\to\infty. \tag{2.14}$$

One simply divides the interval $[0,1]$ into subintervals $[(m-1)/N,m/N]$. There must then be at least 2 jumps inside two adjacent subintervals. Since there are $N-1$ pairs of such subintervals this occurs with probability bounded by

$$(1-(1+\beta/N)e^{-\beta/N})(N-1)<\beta^2/2N.$$

(In fact this argument has to be done after projection by $\pi_{(t_1,\ldots,t_n)}$. This slightly complicates matters and will be omitted here.)

The sets K_N are obviously compact by the criterion of Lemma 2.1. Indeed, K_N is clearly bounded and it is easy to see that it is also closed (this is not essential). Moreover, $\omega_\xi(\delta)=0$ for all $\xi\in K_N$ whenever $\delta<1/2N$. Q.E.D.

We will need the following technical result:

Lemma 2.3: Given $\xi\in D[0,1]$ the step functions

$$\xi^{(n)}(t)=\sum_{i=0}^{n-2}\xi\left(\frac{i}{n}\right)1_{[(i-1)/n,i/n)}+\xi\left(\frac{n-1}{n}\right)1_{[(n-1)/n,1]}$$

tend to ξ in the ρ-topology as $n\to\infty$. Moreover, if $\xi_n\in D[0,1]$ is an arbitrary sequence tending to ξ for the ρ-topology then $\|\xi_n-\xi\|_2\to 0$, that is, the inclusion of $D[0,1]$ into $L^2[0,1]$ is continuous.

Proof: The first part of this lemma is proved in Ref. 15 (Theorem 1 of Chapter V, Sec. 3). We repeat this proof here for convenience as the second part follows the same lines. Fix $\xi\in D[0,1]$ and $\epsilon>0$. Let $\Gamma(\epsilon)$ denote the set of points τ where ξ has a jump $>\epsilon$, that is $|\xi(\tau)-\xi(\tau^-)|>\epsilon$. Then there is $\delta>0$ such that $\omega_\xi(\delta)<\epsilon/2$ by (2.9). This implies that $\Gamma(\epsilon)$ is a finite set and $\inf_{\tau,\tau'\in\Gamma(\epsilon)}|\tau-\tau'|\geqslant\delta$. Now choose $n>3/\delta$. Then, if $\tau,\tau'\in\Gamma(\epsilon)$, $\tau'\neq\tau$ and $i/n<\tau\leqslant(i+1)/n$, $(i-2)/n\geqslant\tau'$ or $(i+3)/n<\tau'$. We can thus define $\lambda_n\in H$ on the interval of length $3/n$ surrounding $\tau\in\Gamma(\epsilon)$ by

$$\lambda_n(t)=\begin{cases}\dfrac{i-1}{n}+\dfrac{n}{2}\left(t-\dfrac{i-1}{n}\right)\left(\tau-\dfrac{i-1}{n}\right) & \text{if } \dfrac{i-1}{n}\leqslant t\leqslant\dfrac{i+1}{n}\\[2ex] \tau+n\left(t-\dfrac{i-1}{n}\right)\left(\dfrac{i+2}{n}-\tau\right) & \text{if } \dfrac{i+1}{n}\leqslant t\leqslant\dfrac{i+2}{n}.\end{cases}$$

Everywhere else we define $\lambda_n(t)=t$. It is now easy to see that $|\lambda_n(t)-t|\leqslant\delta$ and $|\xi(\lambda_n(t))-\xi(t)|\leqslant 2\omega_\xi(\delta)+\epsilon<2\epsilon$. (Assuming $\omega_\xi(\delta)<\epsilon/2$.) This uses Lemma 3 of Ref. 12 (Chapter IX, Sec. 5) or Lemma 6.4 of Ref. 13 (Chapter 7), which says that if ξ has no jumps of magnitude $>\epsilon$ in an interval $[\alpha,\beta]$ then $|\xi(t')-\xi(t'')|\leqslant 2\omega_\xi(\delta)+\epsilon$ for all $t',t''\in[\alpha,\beta]$ with $|t'-t''|\leqslant\delta$. This proves the first part of the lemma.

For the second part of the lemma, let $\eta>0$ be given and choose $\epsilon>0$ such that $4\epsilon^2<\eta^2/2$. Let $\Gamma(\epsilon)$ and δ be as above and assume in addition that $8M^2\delta<\eta^2/2$, where $M=\sup_{t\in[0,1]}|\xi(t)|$. Then, if $|\lambda(t)-t|<\delta^2$ and $|t-\tau|\geq\delta^2$ for all $\tau\in\Gamma(\epsilon)$, $|\xi(\lambda(t))-\xi(t)|\leq 2\omega_\xi(\delta)+\epsilon<2\epsilon$ by the above quoted lemma, and hence

$$\begin{aligned}\|\xi\circ\lambda-\xi\|_2^2 &\leq \int_{\Gamma_{\delta^2}(\epsilon)}|\xi(\lambda(t))-\xi(t)|^2dt+\int_{\Gamma_{\delta^2}(\epsilon)^c}|\xi(\lambda(t))-\xi(t)|^2dt\\ &\leq (2M)^2\cdot 2\,\delta^2(1/\delta)+(2\epsilon)^2<\eta^2\end{aligned}$$

with $\Gamma_{\delta^2}(\epsilon)=\{t:\exists\,\tau\in\Gamma(\epsilon):|t-\tau|<\delta^2\}$, since there are at most $1/\delta$ points $\tau\in\Gamma(\epsilon)$.

Now assume $\rho(\xi_n,\xi)\to 0$. Then, given $\delta>0$, there exists n_0 such that for all $n\geq n_0$ there exists $\lambda\in H$ with $|\lambda(t)-t|\leq\delta^2$ and $|\xi(\lambda(t))-\xi_n(t)|\leq\delta^2$ for all $t\in[0,1]$. Taking δ as above, and moreover such that $\delta^2<\eta$ then

$$\|\xi_n-\xi\|_2\leq\|\xi_n-\xi\circ\lambda\|_2+\|\xi\circ\lambda-\xi\|_2\leq\delta^2+\eta<2\,\eta.$$

This proves the second part of the lemma. Q.E.D.

Having defined the measure $\mathbb{P}_{\beta,x}$ we can now formulate the Feynman-Kac formula. In the proof we need one more technical lemma, however.

Lemma 2.4: If $f:\mathbb{R}^n\to\mathbb{R}$ is a bounded continuous function then the map $\xi\mapsto\int_0^1 f(\xi(t))dt$ is continuous on $L^2([0,1],\mathbb{R}^n)$.

Proof: Suppose that $(\xi_k)_{k=1}^\infty$ is a sequence in $L^2([0,1],\mathbb{R}^n)$ tending to ξ. Then every subsequence $(\xi_k^{(1)})$ has itself a subsequence $(\xi_k^{(2)})$ converging almost everywhere to ξ. It follows that $f\circ\xi_k^{(2)}$ converges almost everywhere to $f\circ\xi$ and since it is also bounded, $\int_0^1 f(\xi_k^{(2)}(t))dt$ converges to $\int_0^1 f(\xi(t))dt$. Since the limit does not depend on the original subsequence $\xi_k^{(1)}$ chosen, this means that $\int_0^1 f(\xi_k(t))dt$ must converge to $\int_0^1 f(\xi(t))dt$. Q.E.D.

Now notice that the operator $(a_{k,+}^*-a_{k,-}^*)(a_{k,+}-a_{k,-})$ occurring in the expression (2.5) acting on the 1-particle space (at position k) acts exactly as $(1-\sigma^{(x)})$, where $\sigma^{(x)}$ is the usual Pauli matrix and, similarly, the operator $a_{k,+}^*a_{k,+}-a_{k,-}^*a_{k,-}$ acts like $\sigma^{(z)}$. We now have:

Theorem 2.1: Let $\mathbb{P}_{\beta,x}$ be the measure defined in Lemma 2.2. Then, for $x_1,\ldots,x_n$, $x_1',\ldots,x_n'\in\{-1,1\}$ and any continuous function $f:\mathbb{R}^n\to\mathbb{R}$, we have the following integral representation:

$$\langle x_1',\ldots,x_n'|\exp\left[-\frac{\beta}{2}\sum_{k=1}^n(1-\sigma_k^{(x)})+f(\sigma_1^{(z)},\ldots,\sigma_n^{(z)})\right]|x_1,\ldots,x_n\rangle$$

$$=\mathbb{E}_{\beta,x}\left[\exp\left[\int_0^1 f(\xi(t))dt\right]1_{\{\xi:\xi_k(1)=x_k'\,\forall\,k=1,\ldots,n\}}\right],\tag{2.15}$$

where $\mathbb{E}_{\beta,x}$ is the expectation w.r.t. the product measure $\Pi_{k=1}^n\mathbb{P}_{\beta,x_k}$.

Proof: We can follow the first proof of [Ref. 6 (Theorem 6.1)]. First note that

$$\langle x'|\exp\left[-\frac{\beta\delta t}{2}(1-\sigma^{(x)})\right]|x\rangle=p_{\delta t}(x,x')\tag{2.16}$$

[see (2.12)]. Now, by the Trotter product formula (1.15) we have

$$\langle x_1',\ldots,x_n'|\exp\left[-\frac{\beta}{2}\sum_{k=1}^{n}(1-\sigma_k^{(x)})+f(\sigma_1^{(z)},\ldots,\sigma_n^{(z)})\right]|x_1,\ldots,x_n\rangle$$

$$=\lim_{M\to\infty}\langle x_1',\ldots,x_n'|\left\{e^{f(\sigma_1^{(z)},\ldots,\sigma_n^{(z)})/M}\prod_{k=1}^{n}e^{-\beta(1-\sigma_k^{(z)})/2M}\right\}^M|x_1,\ldots,x_n\rangle$$

$$=\lim_{M\to\infty}\sum_{x_1^{(1)},\ldots,x_1^{(M-1)}=\pm1}\cdots\sum_{x_n^{(1)},\ldots,x_n^{(M-1)}=\pm1}\prod_{i=1}^{M}\left\{e^{f(x_1^{(i)},\ldots,x_n^{(i)})/M}\prod_{k=1}^{n}p_{1/M}(x_k^{(i-1)},x_k^{(i)})\right\}$$

$$=\lim_{M\to\infty}\mathbb{E}_{\beta,(x_1,\ldots,x_n)}\left[\exp\left[\frac{1}{M}\sum_{i=1}^{M}f\left(\xi\left(\frac{i}{M}\right)\right)\right]1_{\{\xi:\xi_k(1)=x_k'\forall k\}}\right]. \tag{2.17}$$

But

$$\frac{1}{M}\sum_{i=1}^{M}f\left(\xi\left(\frac{i}{M}\right)\right)=\int_0^1 f(\xi_1^{(M)}(t),\ldots,\xi_n^{(M)}(t))dt$$

if $\xi_k^{(M)}$ is the function defined in Lemma 2.3 and hence $\int f(\xi^{(M)}(t))dt\to\int f(\xi(t))dt$ for all $\xi\in D[0,1]$ by Lemma 2.4 since $\xi_k^{(M)}\to\xi_k$ in ρ-topology, $\xi_k^{(M)}\to\xi_k$ in L^2 by Lemma 2.3. Moreover, the integrand in (2.17) is dominated by $\exp[\sup_{|x|\leqslant\|\xi\|_\infty}|f(x)|]$, so by the dominated convergence theorem, (2.15) holds. Q.E.D.

Inserting this formula into (2.5) we obtain immediately

Corollary: Define the measure $\mathbb{K}_\beta^{(n)}$ on $D[0,1]$ by

$$\mathbb{K}_\beta^{(n)}[F]=\frac{1}{Z_n(\beta)}\sum_{k=0}^{n}\binom{n}{k}^{-1}\sum_{\substack{x_1,\ldots,x_n=\pm1\\ \#\{i:x_i=+1\}=k}}\sum_{\substack{x_1',\ldots,x_n'=\pm1\\ \#\{i:x_i'=+1\}=k}}\mathbb{E}^{(n)}_{\beta,(x_1,\ldots,x_n)}\left[F\left(\sum_{i=1}^{n}\xi_i(t)\right)\prod_{i=1}^{n}1_{\{\xi:\xi_i(1)=x_i'\}}\right] \tag{2.18}$$

for any continuous function $F:\mathbb{R}\to\mathbb{R}$, where $\mathbb{E}^{(n)}_{\beta,(x_1,\ldots,x_n)}$ is the expectation with respect to the n-fold product measure $\Pi_{i=1}^n\mathbb{P}_{\beta,x_i}(d\xi_i)$ on $D[0,1]^n$, and $Z_n(\beta)$ is a normalization factor:

$$Z_n(\beta)=\sum_{k=0}^{n}e^{-\beta n}=\frac{1-e^{-\beta(n+1)}}{1-e^{-\beta}}. \tag{2.19}$$

Then the expression in the left-hand side of (1.24), normalized to 1 for $f=0$, is given by

$$\frac{\mathrm{Trace}_n\ e^{-\beta c^*c+f(\Delta)}}{\mathrm{Trace}_n\ e^{-\beta c^*c}}=\mathbb{K}_\beta^{(n)}\left[\exp\left(\int_0^1 f(\xi(t))dt\right)\right]. \tag{2.20}$$

There is an analogous formula for the limiting expression in (1.24):

Theorem 2.2: Let $\mathbb{E}_0$ denote the expectation with respect to the Ornstein–Uhlenbeck process measure on the continuous functions $C[0,1]$ with generator given by H_0 [see (1.19)]. Then the right-hand side expression of (1.24), normalized to 1 for $f=0$ is given by

$$\frac{\mathrm{Trace}\ e^{-\beta a^*a+f(a+a^*)}}{\mathrm{Trace}\ e^{-\beta a^*a}}=\mathbb{K}_\beta\left[\exp\left(\int_0^1 f(q(\beta t))dt\right)\right], \tag{2.21}$$

where the measure $\mathbb{K}_\beta$ is defined by

$$\mathbb{K}_\beta[F]=\frac{1}{Z(\beta)}\sum_{m=0}^{\infty}\mathbb{E}_0[\psi_m(q(0))\Omega_0(q(0))^{-1}F[q(\cdot)]\psi_m(q(\beta))\Omega_0(q(\beta))^{-1}], \quad (2.22)$$

and where $Z(\beta)$ is the normalization constant given by

$$Z(\beta)=\text{Trace } e^{-\beta a^*a}=\frac{1}{1-e^{-\beta}}. \quad (2.23)$$

[The ground state function Ω_0 and the excited-state wave functions ψ_m are defined by (1.20) and (1.18) respectively.]

Proof: Since f is a bounded function, $\beta H_0 - f(a+a^*)$ is a bounded perturbation of βH_0 and therefore self-adjoint on the domain of H_0. We choose the particular representation for a and a^* given by (1.21). We can then apply the Trotter product formula and write

$$\begin{aligned}(\phi|e^{-\beta H_0+f(a+a^*)}|\psi)&=\lim_{M\to\infty}(\phi|(e^{-\beta H_0/M}e^{f(a+a^*)/M})^M|\psi)\\&=\lim_{M\to\infty}(\Omega_0|\overline{\phi}(x)\Omega_0^{-1}(x)e^{-\beta H_0/M}e^{f(x)/M}\ldots e^{f(x)/M}\psi(x)\Omega_0^{-1}(x)|\Omega_0)\\&=\lim_{M\to\infty}\mathbb{E}\left[\left[\overline{\phi}(q(0))\Omega_0^{-1}(q(0))\exp\left(\sum_{i=1}^{M}f(q(\beta i/M))/M\right)\psi(q(\beta))\Omega_0^{-1}(q(\beta))\right]\right]\\&=\mathbb{E}\left[\overline{\phi}(q(0))\Omega_0^{-1}(q(0))\exp\left(\int_0^1 f(q(\beta s))ds\right)\psi(q(\beta))\Omega_0^{-1}(q(\beta))\right].\end{aligned} \quad (2.24)$$

Here, the first identity is the Trotter product formula, the second uses the particular representation, the third uses the fact that H_0 is the generator of the Ornstein–Uhlenbeck process (see Ref. 6, Theorem 4.7 of Chapter II) and the fourth uses the fact that this process has continuous sample paths (Ref. 6 Theorem 5.2 of Chapter II) and that f is continuous and bounded.

To prove (2.21) it remains to insert the orthonormal basis $\{\psi_m\}_{m=0}^{\infty}$. Q.E.D.

We next prove that the rescaled measures $\mathbb{K}_\beta^{(n)}[d\xi/\sqrt{n}]$ converge to $\mathbb{K}_\beta$. For this we compute the respective Fourier transforms as before. This is done in the next section.

III. THE FOURIER TRANSFORMS

The Fourier transform of $\mathbb{K}_\beta$ has already been computed by Feynman [Ref. 16, Sec. 3.2, formula (3.43)]. We shall prove his formula here in a different way:

Theorem 3.1: The characteristic function of the measure $\mathbb{K}_\beta$ defined by (2.22) is given by

$$\mathbb{K}_\beta\left[\exp\left(i\int_0^1 u(t)q(\beta t)dt\right)\right]=\exp\left\{-\frac{1}{1-e^{-\beta}}\int_0^1 dt_1\int_0^1 dt_2\,\frac{1}{2}\,(e^{-\beta|t_1-t_2|}+e^{-\beta(1-|t_1-t_2|)})u(t_1)u(t_2)\right\}, \quad (3.1)$$

for any (real-valued) function $u\in L^2[0,1]$.

Proof: We first show that it suffices to prove this theorem for $u\in C[0,1]$. Indeed, both the right-hand side and the left-hand side are continuous in $L^2[0,1]$. In the case of the right-hand side this is obvious. For the left-hand side this follows from the fact that $D[0,1]\subset L^2[0,1]$ and the bounded convergence theorem. We can now write

$$\mathbb{K}_\beta\left[\exp\left(i\int_0^1 u(t)q(\beta t)dt\right)\right]=\frac{1}{Z(\beta)}\sum_{m=0}^{\infty}\frac{1}{m!}\,\mathbb{E}_0\left[H_m(q(0))\exp\left[i\int_0^1 u(t)q(\beta t)dt\right]H_m(q(\beta))\right]. \tag{3.2}$$

To compute this we use the generating function for the Hermite polynomials: formula (1.7). Using the fact that $(q(0),q(\beta t_1),\ldots,q(\beta t_{M-1}),q(\beta))$ is Gaussian with mean zero and covariance matrix $C_{i,j}=\exp[-\beta|t_i-t_j|]$ we have, for continuous functions u,

$$\begin{aligned}
&\mathbb{E}_0\left[e^{\alpha_1 q(0)}\exp\left[i\int_0^1 u(t)q(\beta t)dt\right]e^{\alpha_2 q(\beta)}\right]\\
&\quad=\lim_{M\to\infty}\mathbb{E}_0\left[e^{\alpha_1 q(0)}\prod_{i=1}^{M}e^{iu(t_i)q(\beta t_i)/M}e^{\alpha_2 q(\beta)}\right]\\
&\quad=\lim_{M\to\infty}\exp\left\{i\alpha_1\frac{1}{M}\sum_{i=1}^{M}e^{-\beta t_i}u(t_i)-\frac{1}{2M^2}\sum_{i,j=1}^{M}e^{-\beta|t_i-t_j|}u(t_i)u(t_j)\right.\\
&\qquad\left.+i\alpha_2\frac{1}{M}\sum_{i=1}^{M}e^{-\beta(1-t_i)}u(t_i)+\alpha_1\alpha_2e^{-\beta}+\frac{1}{2}(\alpha_1^2+\alpha_2^2)\right\}\\
&\quad=\exp\left\{i\alpha_1\int_0^1 e^{-\beta t}u(t)dt-\frac{1}{2}\int_0^1 dt\int_0^1 dt'e^{-\beta|t-t'|}u(t)u(t')\right.\\
&\qquad\left.+i\alpha_2\int_0^1 e^{-\beta(1-t)}u(t)dt+\alpha_1\alpha_2e^{-\beta}+\frac{1}{2}(\alpha_1^2+\alpha_2^2)\right\}.
\end{aligned}\tag{3.3}$$

Inserting (1.7) we get

$$\begin{aligned}
&\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{1}{n!m!}\,\alpha_1^m\alpha_2^n\mathbb{E}_0\left[H_m(q(0))\exp\left[i\int_0^1 u(t)q(\beta t)dt\right]H_n(q(\beta))\right]\\
&\quad=\exp\left\{i\alpha_1\int_0^1 e^{-\beta t}u(t)dt-\frac{1}{2}\int_0^1 dt\int_0^1 dt'e^{-\beta|t-t'|}u(t)u(t')\right.\\
&\qquad\left.+i\alpha_2\int_0^1 e^{-\beta(1-t)}u(t)dt+\alpha_1\alpha_2e^{-\beta}\right\}.
\end{aligned}\tag{3.4}$$

Finally, we have to extract the terms $m=n$. First notice that

$$\frac{1}{1-e^{-\beta}}\exp\left\{\frac{z}{1-e^{-\beta}}\right\}=\sum_{k=0}^{\infty}\sum_{n=0}^{\infty}\binom{n+k}{k}\frac{z^n}{n!}\,e^{-\beta k}. \tag{3.5}$$

With the shorthand $u_1=\int_0^1 e^{-\beta t}u(t)dt$ and $u_2=\int_0^1 e^{-\beta(1-t)}u(t)dt$ we have

$$\begin{aligned}
\exp[i\alpha_1u_1+i\alpha_2u_2+\alpha_1\alpha_2e^{-\beta}]&=\left(\sum_{n_1=0}^{\infty}\frac{(iu_1)^{n_1}}{n_1!}\,\alpha_1^{n_1}\right)\left(\sum_{n_2=0}^{\infty}\frac{(iu_2)^{n_2}}{n_2!}\,\alpha_2^{n_2}\right)\\
&\quad\times\left(\sum_{k=0}^{\infty}\frac{(\alpha_1\alpha_2)^k}{k!}\,e^{-\beta k}\right).
\end{aligned}\tag{3.6}$$

With $A = 1/2\int_0^1 dt_1 \int_0^1 dt_2 e^{-\beta|t_1-t_2|} u(t_1)u(t_2)$ this yields

$$\sum_{m=0}^{\infty} \frac{1}{m!}\, \mathbb{E}_0\left[H_m(q(0)) \exp\left[i\int_0^1 u(t)q(\beta t)dt \right] H_m(q(\beta)) \right]$$
$$= e^{-A} \sum_{n=0}^{\infty} \sum_{k=0}^{\infty} \frac{(n+k)!}{(n!)^2 k!} (-u_1u_2)^n e^{-\beta k} = \frac{1}{1-e^{-\beta}}\, e^{-A} \exp\left[-\frac{u_1u_2}{1-e^{-\beta}} \right], \qquad (3.7)$$

which is (3.1). Q.E.D.

Next, we would like to find a formula for the characteristic function of the measure $\mathbb{K}_\beta^{(n)}$. To get an idea about the difficulty, consider the case that $u(t)=u$ is a constant. In that case we can work backward and write

$$\mathbb{K}_\beta^{(n)}\left[\exp\left[iu\int_0^1 \xi(t)dt \right] \right] = \frac{\mathrm{Trace}_n\, e^{-\beta c^*c + iu\Delta}}{\mathrm{Trace}_n\, e^{-\beta c^*c}}. \qquad (3.8)$$

The operator $-\beta c^*c + iu\Delta$ is quadratic in the creation and annihilation operators and can be diagonalised by means of a Bogoliubov transformation. The result is

$$\mathbb{K}_\beta^{(n)}\left[\exp\left[iu\int_0^1 \xi(t)dt \right] \right] = \frac{\sinh(\sqrt{(\beta/2)^2-u^2}(n+1))}{\sinh(\beta(n+1)/2)} \frac{\sinh(\beta/2)}{\sinh\sqrt{(\beta/2)^2-u^2}}. \qquad (3.9)$$

In a sense, the general case can be reduced to this case. The result is not such a nice explicit expression, but rather an expression involving series expansions:

Theorem 3.2: The characteristic function of the measures $\mathbb{K}_\beta^{(n)}$ defined by (2.18) is given by

$$\mathbb{K}_\beta^{(n)}\left[\exp\left[i\int_0^1 u(t)\xi(t)dt \right] \right] = \frac{1}{Z_n(\beta)} \frac{\lambda_+^{n+1} - \lambda_-^{n+1}}{\lambda_+ - \lambda_-}, \qquad (3.10)$$

where the $\lambda_\pm$ are the eigenvalues of a 2×2-matrix $A[u]=(A_{mm'}[u])_{m,m'=0,1}$:

$$\lambda_\pm = \frac{1}{2}\left[A_{00} + A_{11} \pm \sqrt{(A_{00}-A_{11})^2 + 4A_{01}A_{10}} \right] \qquad (3.11)$$

and where the matrix elements are given by

$$A_{00} = 1 + \sum_{k=1}^{\infty} (-1)^k \int_0^1 dt_1 \int_{t_1}^1 dt_2 \cdots \int_{t_{2k-1}}^1 dt_{2k} u(t_1)\ldots u(t_{2k}) e^{-\beta(t_{2k}-t_{2k-1}+\cdots+t_2-t_1)}, \qquad (3.12)$$

$$A_{11} = e^{-\beta} + \sum_{k=1}^{\infty} (-1)^k \int_0^1 dt_1 \int_{t_1}^1 dt_2 \cdots \int_{t_{2k-1}}^1 dt_{2k} u(t_1)\ldots u(t_{2k}) e^{-\beta(1-t_{2k}+t_{2k-1}-\cdots-t_2+t_1)}, \qquad (3.13)$$

$$A_{01} = i\sum_{k=0}^{\infty} (-1)^k \int_0^1 dt_1 \int_{t_1}^1 dt_2 \cdots \int_{t_{2k}}^1 dt_{2k+1} u(t_1)\ldots u(t_{2k+1}) e^{-\beta(1-t_{2k+1}+t_{2k}-\cdots+t_2-t_1)}, \qquad (3.14)$$

and

$$A_{10}=i\sum_{k=0}^{\infty}(-1)^k\int_0^1 dt_1\int_{t_1}^1 dt_2\cdots\int_{t_{2k}}^1 dt_{2k+1}u(t_1)\ldots u(t_{2k+1})e^{-\beta(t_{2k+1}-t_{2k}+\cdots+t_3-t_2+t_1)}. \tag{3.15}$$

Proof: With $F(\xi(\cdot))=\exp[i\int_0^1 u(t)\xi(t)dt]$ the expectation in formula (2.18) splits into single-particle expectations

$$\mathbb{E}_{\beta,x}\left[\exp\left(i\int_0^1 u(t)\xi(t)dt\right)1_{\{\xi:\xi(1)=x'\}}\right].$$

This is in fact more easily computed in the c-representation. We first write, assuming that u is continuous,

$$\begin{aligned}&\mathbb{E}_{\beta,x}\left[\exp\left(i\int_0^1 u(t)\xi(t)dt\right)1_{\{\xi:\xi(1)=x'\}}\right]\\&\quad=\lim_{M\to\infty}\sum_{x^{(1)},\ldots,x^{(M-1)}}\prod_{i=1}^{M}\langle x^{(i)}|\exp\left[-\frac{\beta}{2M}(1-\sigma^{(x)})\right]\exp\left[\frac{i}{M}u\left(\frac{i}{M}\right)\sigma^{(z)}\right]|x^{(i-1)}\rangle.\end{aligned} \tag{3.16}$$

Next we change basis in this expression from $|x\rangle$ to $|1;m\rangle$ $(m=0,1)$:

$$|x\rangle=\frac{1}{\sqrt{2}}(|1;0\rangle+x|1;1\rangle)=\frac{1}{\sqrt{2}}\sum_{m=0,1}((1-x)m+x)|1;m\rangle. \tag{3.17}$$

We therefore put

$$\begin{aligned}&\mathbb{E}_{\beta,x}\left[\exp\left(i\int_0^1 u(t)\xi(t)dt\right)1_{\{\xi:\xi(1)=x'\}}\right]\\&\quad=\langle x'|A|x\rangle=\frac{1}{2}\sum_{m,m'=0,1}((1-x)m+x)((1-x')m'+x')\langle 1;m'|A|1;m\rangle\end{aligned} \tag{3.18}$$

and compute

$$\begin{aligned}\langle 1;m'|A|1;m\rangle=\lim_{M\to\infty}\sum_{m^{(1)},\ldots,m^{(M-1)}=0,1}\prod_{i=1}^{M}&\langle 1;m^{(i)}|\exp\left[-\frac{\beta}{2M}(1-\sigma^{(x)})\right]\\&\times\exp\left[\frac{i}{M}u\left(\frac{i}{M}\right)\sigma^{(z)}\right]|1;m^{(i-1)}\rangle.\end{aligned} \tag{3.19}$$

(As usual, $m^{(0)}=m$ and $m^{(M)}=m'$.) Now,

$$\exp\left[\frac{i}{M}u_i\sigma^{(z)}\right]|1;m\rangle\approx\left(1+\frac{i}{M}u_i\sigma^{(z)}\right)|1;m\rangle=|1;m\rangle+\frac{i}{M}u_i|1;1-m\rangle. \tag{3.20}$$

First suppose $m=m'=0$. Then we must have an even number of jumps, i.e. i-values where we choose the second term in the right-hand side of (3.35). Thus,

$$A_{00}=\langle 1;0|A|1;0\rangle$$
$$=\lim_{M\to\infty}\left\{1-\frac{1}{M^2}\sum_{1\leqslant i_1<i_2\leqslant M}e^{-\beta(i_2-i_1)/M}u\left(\frac{i_1}{M}\right)u\left(\frac{i_2}{M}\right)\right.$$
$$\left.+\frac{1}{M^4}\sum_{1\leqslant i_1<i_2<i_3<i_4\leqslant M}e^{-\beta(i_4-i_3+i_2-i_1)/M}u\left(\frac{i_1}{M}\right)u\left(\frac{i_2}{M}\right)u\left(\frac{i_3}{M}\right)u\left(\frac{i_4}{M}\right)+\cdots\right\}. \quad (3.21)$$

This is just (3.12). Notice that the series converges for $u\in L^2[0,1]$ since $|A_{00}|\leqslant\Sigma_{k=0}^{\infty}[\|u\|_2^{2k}/(2k)!]=\cosh\|u\|_2$. The other expressions are derived in a similar manner.

It is easy to see, either by direct transformation or by redoing the derivation of (1.16) in the new basis, that

$$\mathbb{K}_\beta^{(n)}\left[\exp\left[i\int_0^1 u(t)\xi(t)dt\right]\right]=\frac{1}{Z_n(\beta)}\sum_{k=0}^{n}\binom{n}{k}^{-1}\sum_{\substack{m_1,\ldots,m_n=0,1\\ \Sigma m_i=k}}\sum_{\substack{m_1',\ldots,m_n'=0,1\\ \Sigma m_i'=k}}\prod_{i=1}^{n}A_{m_i,m_i'}. \quad (3.22)$$

We can transform A to Jordan normal form (see Ref. 17. Theorem 6.4.7 or Ref. 18, Sec. 7.3)

$$A=SJS^{-1},\ \text{where}\ J=\begin{pmatrix}\lambda_+ & 0\\ 1 & \lambda_-\end{pmatrix} \quad (3.23)$$

and then transform (3.22) again to obtain

$$\mathbb{K}_\beta^{(n)}\left[\exp\left[i\int_0^1 u(t)\xi(t)dt\right]\right]=\frac{1}{Z_n(\beta)}\sum_{k=0}^{n}\binom{n}{k}^{-1}\sum_{\substack{m_1,\ldots,m_n=0,1\\ \Sigma m_i=k}}\sum_{\substack{m_1',\ldots,m_n'=0,1\\ \Sigma m_i'=k}}\prod_{i=1}^{n}J_{m_i,m_i'}$$
$$=\frac{1}{Z_n(\beta)}\sum_{k=0}^{n}\lambda_+^k\lambda_-^{n-k}, \quad (3.24)$$

which is just (3.10) since $\lambda_\pm$ are the eigenvalues of the matrix A given by (3.11). Q.E.D.

Remark: This theorem gives rise to some interesting integral identities. For example, notice that by (3.18),

$$\text{Trace}\ A[u]=\sum_{x=\pm 1}\mathbb{E}_{\beta,x}\left[\exp\left(iu\int_0^1\xi(t)dt\right)1_{\{\xi;\xi(1)=x\}}\right] \quad (3.25)$$

and by (2.15),

$$\text{Trace}\ A[u]=\text{Trace}\ e^{-(\beta/2)(1-\sigma^{(x)})+iu\sigma^{(z)}}=2e^{-\beta/2}\cosh\sqrt{\left(\frac{\beta}{2}\right)^2-u^2}. \quad (3.26)$$

Inserting the expressions for A_{00} and A_{11} we obtain

$$\cosh\sqrt{\left(\frac{\beta}{2}\right)^2-u^2}=\sum_{k=0}^{\infty}(-1)^k\int_0^1 dt_1\int_{t_1}^1 dt_2\cdots\int_{t_{2k-1}}^1 dt_k$$
$$\times\cosh[\beta(\tfrac{1}{2}+t_1-t_2+\cdots+t_{2k-1}-t_{2k})]. \quad (3.27)$$

Replacing $\beta/2$ by β and taking the k-th term in the Taylor expansion in u^2 we get

$$\int_0^1 dt_1 \int_{t_1}^1 dt_2 \cdots \int_{t_{2k-1}}^1 dt_{2k} \cosh[\beta(1+2(t_1-t_2+\cdots+t_{2k-1}-t_{2k}))] = \frac{1}{k!}\left(\frac{d}{d\beta^2}\right)^k \cosh\beta. \tag{3.28}$$

[This can also be derived by means of the Dyson expansion of the second trace in (3.26).]

IV. PROOF OF THE MAIN THEOREM

To complete the proof of Theorem 1.2 we shall show that it suffices to show that the Fourier transforms of the measures $\mathbb{K}_\beta^{(n)}$ converge to those of $\mathbb{K}_\beta$ after replacing u and by $u/\sqrt{n}$. The convergence of the Fourier transforms is easy to see since, for large n,the revised matrix $\widetilde{A}[u] = A[u/\sqrt{n}]$ behaves as follows:

$$\widetilde{A}_{00} \sim 1 - \frac{1}{n}\int_0^1 dt_1 \int_{t_1}^1 dt_2 e^{-\beta(t_2-t_1)} u(t_1)u(t_2) + \mathcal{O}(n^{-2}), \tag{4.1}$$

$$\widetilde{A}_{11} \sim e^{-\beta} - \frac{1}{n}\int_0^1 dt_1 \int_{t_1}^1 dt_2 e^{-\beta+\beta(t_2-t_1)} u(t_1)u(t_2) + \mathcal{O}(n^{-2}), \tag{4.2}$$

$$\widetilde{A}_{01} \sim \frac{i}{\sqrt{n}}\int_0^1 dt e^{-\beta+\beta t} u(t) + \mathcal{O}(n^{-3/2}), \tag{4.3}$$

and

$$\widetilde{A}_{10} \sim \frac{i}{\sqrt{n}}\int_0^1 dt e^{-\beta t} u(t) + \mathcal{O}(n^{-3/2}). \tag{4.4}$$

This leads to

$$\widetilde{\lambda}_+ \sim 1 - \frac{1}{n}\frac{1}{1-e^{-\beta}}\int_0^1 dt_1 \int_{t_1}^1 dt_2 u(t_1)u(t_2)[e^{-\beta(t_2-t_1)} + e^{-\beta+\beta(t_2-t_1)}] \tag{4.5}$$

and

$$\widetilde{\lambda}_- \sim e^{-\beta}\left\{1 + \frac{1}{n}\frac{1}{1-e^{-\beta}}\int_0^1 dt_1 \int_{t_1}^1 dt_2 u(t_1)u(t_2)[e^{-\beta(t_2-t_1)} + e^{-\beta+\beta(t_2-t_1)}]\right\}. \tag{4.6}$$

If we put

$$R = \int_0^1 dt_1 \int_{t_1}^1 dt_2 u(t_1)u(t_2)[e^{-\beta(t_2-t_1)} + e^{-\beta+\beta(t_2-t_1)}], \tag{4.7}$$

then we have

$$\widetilde{\lambda}_+^{n+1} \sim \left(1 - \frac{1}{n}\frac{1}{1-e^{-\beta}}R\right)^{n+1} \to \exp\left[\frac{1}{1-e^{-\beta}}R\right],$$

$$\widetilde{\lambda}_- \sim e^{-\beta(n+1)} \to 0, \tag{4.8}$$

and $\tilde{\lambda}_+ - \tilde{\lambda}_- \to 1 - \mathrm{e}^{-\beta}$ and therefore

$$\frac{\tilde{\lambda}_+^{n+1} - \tilde{\lambda}_-^{n+1}}{\tilde{\lambda}_+ - \tilde{\lambda}_-} \to \frac{1}{1-e^{-\beta}} \exp\left[-\frac{1}{1-e^{-\beta}} R \right]. \tag{4.9}$$

As, moreover, $Z_n(\beta) \to (1-e^{-\beta})^{-1}$, this proves the convergence of the Fourier transforms.

To prove that the weak convergence of the measures follows from the convergence of the corresponding Fourier transforms we need some detailed estimates. A sufficient condition was formulated by Smolyanov and Fomin.[19] According to this condition it suffices that the Fourier transforms are equicontinuous with respect to the so-called Sazonov topology. In the present Hilbert space context this means that for all $\epsilon > 0$ there should exist a sequence $\{\lambda_k\}_{k=0}^{\infty} \in l^2$ such that

$$\sum_{k=0}^{\infty} \lambda_k^2 u_k^2 < 1 \Rightarrow \left| 1 - \mathbb{K}_\beta^{(n)} \left[\exp\left[i \int_0^1 u(t) \xi(t) dt \right] \right] \right| < \epsilon, \tag{4.10}$$

where $\{u_k\}_{k=0}^{\infty}$ are the components of u with respect to some orthonormal basis of $L^2[0,1]$. Unfortunately, this condition seems hard to check in the present case. We therefore use a more direct approach, starting from one of their main lemmas (Ref. 19, Lemma 2 of Sec. 4). We repeat the proof here for completeness:

Lemma 4.1: Suppose that μ is a Radon probability measure on $\mathbb{R}^M$ and assume that, given $\epsilon > 0$, there exists $\lambda \in \mathbb{R}^M$ such that

$$\sum_{i=1}^{M} \lambda_i^2 u_i^2 \leqslant 1 \Rightarrow |1 - \mathrm{Re}\ \tilde{\mu}[u]| \leqslant \epsilon \tag{4.11}$$

where $\tilde{\mu}$ denotes the characteristic function of μ. Then, for all $\eta > 0$ and with $c = (1-e^{-1/2})^{-1}$,

$$\mu\{\xi : \|\xi\|_2 \geqslant \eta\} \leqslant c \left(\epsilon + \frac{2}{\eta^2} \|\lambda\|_2^2 \right). \tag{4.12}$$

Proof: Notice first that if $\|\xi\| \geqslant \eta$ then $c(1 - \exp[-1/2\|\xi\|^2/\eta^2]) \geqslant 1$. It follows that if ν_η is the Gaussian measure on $\mathbb{R}^M$ with covariance $\eta^{-2}1$,

$$\begin{aligned} \mu\{\xi : \|\xi\| \geqslant \eta\} &\leqslant c \int_{\mathbb{R}^M} \left(1 - \exp\left[-\frac{1}{2} \|\xi\|^2 / \eta^2 \right] \right) \mu(d\xi) \\ &= c \int_{\mathbb{R}^M} \nu_\eta(du) \int_{\mathbb{R}^M} [1 - e^{i(\xi,u)}] \mu(d\xi) \\ &= c \int_{\mathbb{R}^M} \nu_\eta(du) [1 - \mathrm{Re}\ \tilde{\mu}[u]]. \end{aligned} \tag{4.13}$$

The latter integral can be split into one over the region where $\Sigma_{i=1}^M \lambda_i^2 u_i^2 \leqslant 1$ and one over the complementary region. The first is bounded by ϵ by the assumption (4.11). In the second we simply bound $1 - \mathrm{Re}\ \tilde{\mu}[u]$ by 2. The integral over the region where $\Sigma_{i=1}^M \lambda_i^2 u_i^2 > 1$ is thus bounded by

$$2 \nu_\eta \left\{ u \in \mathbb{R}^M : \sum_{i=1}^{M} \lambda_i^2 u_i^2 > 1 \right\} \leqslant 2 \sum_{i=1}^{M} \lambda_i^2 \int u_i^2 \nu_\eta(du) = 2 \eta^{-2} \sum_{i=1}^{M} \lambda_i^2. \tag{4.14}$$

This proves the lemma. Q.E.D.

We now use this lemma directly to prove Prokhorov's condition for the weak convergence of measures. This condition holds quite generally but is particularly easy to prove on Hilbert spaces:

Lemma 4.2: In order that the measures $\mathbb{K}_\beta^{(n)}$ converge weakly to $\mathbb{K}_\beta$ it suffices that for all $\epsilon>0$, there exists a compact set $K\subset L^2[0,1]$ such that $\mathbb{K}_\beta^{(n)}[K]>1-\epsilon$ uniformly in n.

Proof: Suppose that this condition is fulfilled. Then, given $F\in\mathscr{C}^b(L^2[0,1])$ and $\epsilon>0$, let K be compact such that $\mathbb{K}_\beta^{(n)}[K^c]\leqslant\epsilon/12\|F\|_\infty$ and the same for $\mathbb{K}_\beta$. Now, F is uniformly continuous on K so there exists $\delta>0$ such that if $\|\xi-\xi'\|_2<\delta$ then $|F(\xi)-F(\xi')|<\epsilon/6$. Moreover, a set $K\subset L^2[0,1]$ is compact if and only if it is bounded and closed and, in a given orthonormal basis $\{h_p\}_{p=0}^\infty$, for any given $\delta>0$ there exists an integer M such that $\Sigma_{r=M}^\infty|(\xi,h_p)|^2<\delta^2$ for all $\xi\in K$. Now let π_M be the projection $\pi_M:L^2[0,1]\to\mathbb{R}^M$ given by $\pi_M(\xi)=((\xi,h_0),\ldots,(\xi,h_{M-1}))$ and let $\pi_M(\mathbb{K}_\beta^{(n)})$ be the image measure. Then $\pi_M(\mathbb{K}_\beta^{(n)})\to\pi_M(\mathbb{K}_\beta)$ because the corresponding characteristic functions converge. It follows that there is n_0 such that for $n\geqslant n_0$,

$$\left|\int F\circ\pi_M d\mathbb{K}_\beta^{(n)}-\int F\circ\pi_M d\mathbb{K}_\beta\right|<\epsilon/3.$$

Also, $\|\pi_M(\xi)-\xi\|_2<\delta$ and hence $|F(\pi_M(\xi))-F(\xi)|<\epsilon/6$ for all $\xi\in K$. Thus, for $n\geqslant n_0$,

$$\begin{aligned}\left|\int Fd\mathbb{K}_\beta^{(n)}-\int Fd\mathbb{K}_\beta\right|&\leqslant\left|\int_K Fd\mathbb{K}_\beta^{(n)}-\int_K Fd\mathbb{K}_\beta\right|+\left|\int_{K^c}Fd\mathbb{K}_\beta^{(n)}\right|+\left|\int_{K^c}Fd\mathbb{K}_\beta\right|\\&\leqslant\left|\int_K F\circ\pi_M d\mathbb{K}_\beta^{(n)}-\int_K F\circ\pi_M d\mathbb{K}_\beta\right|+\frac{\epsilon}{3}+2\|F\|_\infty\frac{\epsilon}{12\|F\|_\infty}\leqslant\left|\int F\circ\pi_M d\mathbb{K}_\beta^{(n)}-\int F\circ\pi_M d\mathbb{K}_\beta\right|\\&\quad+2\|F\|_\infty\frac{\epsilon}{12\|F\|_\infty}+\frac{\epsilon}{3}+\frac{\epsilon}{6}<\epsilon.\end{aligned}\tag{4.15}$$

This proves the lemma. Q.E.D.

Theorem 4.1: The measures $\mathbb{K}_\beta^{(n)}$ converge weakly to $\mathbb{K}_\beta$ as measures on $L^2[0,1]$.

Proof: According to the previous lemma it suffices to prove that, for any $\epsilon>0$, there exists a compact set $K\subset L^2[0,1]$ such that $\mathbb{K}_\beta^{(n)}[K]>1-\epsilon$ uniformly in n. We shall define this set in terms of the Haar basis $h_p\in L^2[0,1]$ $(p=0,1,2,\ldots)$ defined by: $h_0(t)=1$ and

$$h_p(t)=\begin{cases}2^{m/2}, & \text{if } p2^{-m}-1\leqslant t<\left(p+\frac{1}{2}\right)2^{-m}-1;\\ -2^{m/2}, & \text{if } \left(p+\frac{1}{2}\right)2^{-m}-1\leqslant t\leqslant(p+1)2^{-m}-1;\\ 0, & \text{otherwise.}\end{cases}\tag{4.16}$$

We now define the set K as follows:

$$K_\delta=\left\{\xi\in L^2[0,1]\,\middle|\,\sum_{p=2^m}^{2^{m+1}-1}|(\xi,h_p)|^2\leqslant\eta_m\,\forall m\geqslant 0\quad\text{and}\quad|(\xi,h_0)|\leqslant C\right\},\tag{4.17}$$

where $\eta_m=\delta^{-3/2}2^{-m/8}$ and C is a constant depending on ϵ and where $\delta(\epsilon)$ will be determined later. It is easy to see that this set is compact in $L^2[0,1]$. To prove that the complement of this set has small measure we shall use Lemma 4.1 above for each value of m individually. We therefore need to estimate the characteristic functions of the image measures $\mu_m^{(n)}=\pi^{(m)}(\mathbb{K}_\beta^{(n)})$, where $\pi^{(m)}$ is the projection of $L^2[0,1]$ onto the span of $\{h_p;p=2^m,\ldots,2^{m+1}-1\}$. We first estimate $\widetilde{A}_{00}[u]$ with $u\in\pi^{(m)}$ $(L^2[0,1])$. Introducing new variables

$$s_i=2^{m+1}\left\{t_i-\left(p+\frac{1}{2}\right)2^{-m}-1\right\} \tag{4.18}$$

and defining $\beta_m=2^{-m-1}\beta$ we have

$$\widetilde{A}_{00}[u]=1+\sum_{k=1}^{\infty}\frac{(-1)^k}{n^k}2^{mk}2^{-2k(m+1)}\sum_{l=1}^{2k\wedge 2^m}\sum_{\substack{r_1,\dots,r_l\geqslant 1\\ \Sigma r_i=2k}}\sum_{2^m\leqslant p_1<\cdots<p_l<2^{m+1}}\prod_{i=1}^{l}\{u_{p_i}^{r_i}I_{m,r_i}^{\pm}\}, \tag{4.19}$$

where $u_p=(h_p,u)$ and

$$I_{m,r}^{\pm}=(-1)^r\int_{-1}^{1}ds_1\int_{s_1}^{1}ds_2\cdots\int_{s_{r-1}}^{1}ds_r\prod_{i=1}^{r}\operatorname{sgn}(s_i)\exp[\pm\beta_m(s_r-s_{r-1}+\cdots+(-1)^{r-1}s_1)] \tag{4.20}$$

and where the + or − sign is chosen according as to whether $\Sigma_{j=1}^{i}r_j$ is odd or even. We estimate $I_{m,r}^{\pm}$ simply as follows. First note that if $g_i, i=1,\dots,r$, are odd functions then

$$\int_{-1}^{1}ds_1\int_{s_1}^{1}ds_2\cdots\int_{s_{r-1}}^{1}ds_r\prod_{i=1}^{r}g_i(s_i)=0. \tag{4.21}$$

[This follows from the fact that if $g(s)$ is odd then $G(s)=\int_s^1 g(s')ds'$ is even.] With $g_i(s)=\operatorname{sgn}(s)$ we have that $I_{m,r}^{\pm}|_{\beta=0}=0$ and subtracting this from $I_{m,r}^{\pm}$ and using the estimates $|e^{\beta_m s}-1|<\beta_m|s|e^{\beta_m|s|}$ and $|s_r-s_{r-1}+\cdots+(-1)^{r-1}s_1|\leqslant 2$ we have

$$|I_{m,r}^{\pm}|\leqslant 2\beta_m e^{2\beta_m}\int_{-1}^{1}ds_1\int_{s_1}^{1}ds_2\cdots\int_{s_{r-1}}^{1}ds_r 1=\frac{2^{r+1}\beta_m e^{2\beta_m}}{r!}. \tag{4.22}$$

Inserting this into (4.16) we obtain

$$|\widetilde{A}_{00}[u]-1|\leqslant\sum_{k=1}^{\infty}\frac{1}{n^k}2^{-(m+2)k}\sum_{l=1}^{2k\wedge 2^m}\sum_{\substack{r_1,\dots,r_l\geqslant 1\\ \Sigma r_i=2k}}\prod_{i=1}^{l}\frac{2^{r_i+1}\beta_m e^{2\beta_m}}{r_i!}\sum_{2^m\leqslant p_1<\cdots<p_l<2^{m+1}}\prod_{i=1}^{l}|u_{p_i}|. \tag{4.23}$$

Next we use the fact that, for $r\geqslant 2$, $\Sigma_p|u_p|^r\leqslant(\Sigma_p|u_p|^2)^{r/2}=\|u\|_2^r$ and $2^{-m/2}\Sigma_p|u_p|\leqslant(\Sigma_p|u_p|^2)^{1/2}=\|u\|_2$ to bound this by

$$|\widetilde{A}_{00}[u]-1|\leqslant\sum_{k=1}^{\infty}\frac{1}{n^k}2^{-mk}e^{\beta}\beta^{2k}\sum_{l=1}^{2k\wedge 2^m}2^{-ml/2}\sum_{\substack{r_1,\dots,r_l\geqslant 1\\ \Sigma r_i=2k}}\left(\prod_{i=1}^{l}r_i!\right)^{-1}\frac{1}{l!}\|u\|^{2k}. \tag{4.24}$$

Extending the sum over l to infinity this yields

$$\begin{aligned}|\widetilde{A}_{00}[u]-1|&\leqslant e^{\beta}\sum_{k=1}^{\infty}\frac{2^{-mk}\beta^{2k}}{n^k}\sum_{l=1}^{\infty}\frac{2^{-ml/2}l^{2k}}{(2k)!l!}\|u\|_2^{2k}\leqslant e^{\beta}\sum_{l=1}^{\infty}\frac{1}{l!}\left\{\cosh\left(\frac{\beta}{\sqrt{n}}2^{-m/2}\|u\|_2 l\right)-1\right\}\\ &\leqslant\tfrac{1}{2}e^{\beta}\{\exp(e^{\beta n^{-1/2}2^{-m/2}\|u\|_2})+\exp(e^{-\beta n^{-1/2}2^{-m/2}\|u\|_2})-2e\}.\end{aligned} \tag{4.25}$$

In Lemma 4.1 we shall take λ to be the vector with components $\delta^{-1}2^{-m/4}$ with respect to the h_p with $2^m \leq p \leq 2^{m+1}-1$ and 0 with respect to the others. Thus $\|u\|_2 \leq \delta 2^{m/4}$ and hence

$$|\widetilde{A}_{00}[u]-1| \sim \mathcal{O}\left(\frac{1}{n}2^{-m}\|u\|_2^2\right) = \mathcal{O}(2^{-m/2})\,\delta^2 \tag{4.26}$$

uniformly in n. In the same way we find that

$$|\widetilde{A}_{11}[u]-e^{-\beta}| \sim \mathcal{O}\left(\frac{1}{n}2^{-m}\|u\|_2^2\right) = \mathcal{O}(2^{-m/2})\,\delta^2. \tag{4.27}$$

An analogous calculation also yields

$$\begin{aligned}|\widetilde{A}_{01}[u]| &\leq \frac{1}{2\sqrt{n}}\,e^{\beta}\{\exp(e^{\beta n^{-1/2}2^{-m/2}\|u\|_2}) - \exp(e^{-\beta n^{-1/2}2^{-m/2}\|u\|_2})\} \\ &\sim \mathcal{O}\left(\frac{1}{n}2^{-m/2}\|u\|_2\right) \leq \mathcal{O}(2^{-m/4})\,\delta\end{aligned} \tag{4.28}$$

and similarly

$$\widetilde{A}_{10}[u] \sim \mathcal{O}\left(\frac{1}{n}2^{-m/2}\|u\|_2\right) \leq \mathcal{O}(2^{-m/4})\,\delta. \tag{4.29}$$

Inserting in the expression for the eigenvalues $\widetilde{\lambda}_{\pm}$ it follows that

$$\widetilde{\lambda}_{+} \sim 1 + \mathcal{O}(\delta 2^{-m/2}) \tag{4.30}$$

and

$$\widetilde{\lambda}_{-} \sim e^{-\beta} + \mathcal{O}(\delta 2^{-m/2}) \tag{4.31}$$

and hence

$$\psi_m[u] = \pi^{(m)}(\mathbb{K}_\beta^{(n)})[\exp[i(\xi,u)]] \sim 1 + \mathcal{O}(\delta 2^{-m/2}), \tag{4.32}$$

uniformly in n.

Using Lemma 4.1 above with $\eta_m = \delta^{-3/2}2^{-m/8}$ and $\epsilon_m = \delta\mathcal{O}(2^{-m/2})$ we have

$$\mathbb{K}_\beta^{(n)}[\|\pi^{(m)}(\xi)\|_2 > \eta_m] \leq c(\delta_m + 2\eta_m^{-2}\lambda_m^2) \sim \delta\{\mathcal{O}(2^{-m/2}) + \mathcal{O}(2^{-m/4})\}. \tag{4.33}$$

Adding probabilities we now have that

$$\mathbb{K}_\beta^{(n)}[K_\delta] \leq \delta \sum_{m=0}^{\infty} \mathcal{O}(2^{-m/4}) < \epsilon \tag{4.34}$$

for δ small enough. Q.E.D.

To complete the proof of Theorem 1.2 it now suffices to remark that the weak convergence of measures means that the expectation of bounded continuous functions converges and $\int_0^1 f(\xi(t))dt$ is continuous as a function of $\xi \in L^2[0,1]$ because of Lemma 2.4. [Notice also that the denominator of (2.20) converges trivially to that of (2.21).]

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The limit transition $q\to 1$ of the q-Fourier transform

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The behavior of the q-Fourier transformation as $q\to 1$ is investigated. It is shown that the q-Fourier transformation converges to the classical Fourier transformation in the strong operator topology. © *1996 American Institute of Physics.* [S0022-2488(96)02608-4]

I. INTRODUCTION

The q-Fourier transformation is regarded as the q analog of the classical Fourier transformation. It arises as a special case in the context of q-hypergeometric functions and was defined in a paper by Koornwinder and Swarttouw.[1] As it can be inferred from its name, the q-Fourier transformation reduces to the usual Fourier transformation as $q\to 1$. The rigorous proof is of interest both from a mathematical as well as from a physical point of view. The physical importance of the limit transition is due to the fact that the q-Fourier transformation turns out to be the appropriate object when dealing with q-deformed quantum mechanics. In a paper of Hebecker *et al.*[2] the representations of a q-deformed Heisenberg algebra were investigated. The transition from momentum to position eigenstates and vice versa is carried out by means of the q-Fourier transformation. Thus, the analysis of the limit transition of the q-Fourier transformation is strongly related to the question of compatibility of the q-deformed theory with the classical quantum mechanics.

In the second section of this paper, the q-Fourier transformation is introduced in a slightly modified version with respect to Ref. 1. The q-Fourier transformation is defined on a particular space of functions, the space L^2_{q,π_0} of square-summable functions on the set $\{\pi_0 q^n | n\in\mathbb{Z}\}$. In the third section, a possibility of defining the q-Fourier transformation on $L^2(\mathbb{R}^+)$ is presented. This will enable a rigorous limit transition $q\to 1$, which is the subject of the fourth section.

II. DEFINITION OF THE q-FOURIER TRANSFORMATION

To start, some definitions and results of Koornwinder and Swarttouw[1] are stated. In their paper, the following q-deformed cosine and sine functions were defined:

$$\cos(z;q^2)=\sum_{k=0}^{\infty}\frac{(-1)^k q^{k(k+1)} z^{2k}}{(q;q)_{2k}},$$
$$\sin(z;q^2)=\sum_{k=0}^{\infty}\frac{(-1)^k q^{k(k+1)} z^{2k+1}}{(q;q)_{2k+1}}, \tag{2.1}$$

where $q\in\mathbb{R}^+$, $0<q<1$, is the parameter of deformation, and

$$(a;q)_k=\prod_{n=0}^{k-1}(1-aq^n),\quad (a;q)_0=1,\quad (a;q)_\infty=\prod_{n=0}^{\infty}(1-aq^n).$$

As $q\to 1$, the limits

$$\lim_{q\to 1}\cos((1-q)z;q^2)=\cos z,\quad \lim_{q\to 1}\sin((1-q)z;q^2)=\sin z, \tag{2.2}$$

hold pointwise, uniformly on compacta. In the sequel, the discussion is restricted to the cosine function, the results being analogous for the sine function. The q-deformed cosine function satisfies the orthogonality relation,

$$\sum_{n=-\infty}^{\infty} q^n \cos(q^n q^k;q^2)\cos(q^n q^l;q^2)=\frac{(q^2;q^2)_\infty^2}{(q;q^2)_\infty^2}\frac{1}{q^l}\,\delta_{kl}. \tag{2.3}$$

The goal is now to define a q-deformed Fourier transformation that formally tends to its classical analog as $q\to 1$. According to the limit transitions (2.2), the q-Fourier transformation has to be based on the function

$$\mathrm{Cos}(q^k;q^2):=\cos((1-q)q^k;q^2)=\sum_{k=0}^{\infty}\frac{(-1)^k q^{k(k+1)}(1-q)^{2k}z^{2k}}{(q;q)_{2k}}. \tag{2.4}$$

This function obeys an orthogonality relation similar to (2.3), but only if the range of the parameter q is seriously restricted.

Lemma 2.1: For $q\in\{q|(1-q)=q^j,\ j\in\mathbb{Z}\}$ the following identity holds:

$$\sum_{n=-\infty}^{\infty} q^n \,\mathrm{Cos}(q^n q^k;q^2)\mathrm{Cos}(q^n q^l;q^2)=\frac{(1-q)(q^2;q^2)_\infty^2}{(q;q^2)_\infty^2}\frac{1}{q^l}\,\delta_{kl}. \tag{2.5}$$

Proof: The relation is obtained from (2.3) by replacing $m+j$ for n. The restriction on the allowed values of q is due to the fact that the sum $\Sigma_{n=-\infty}^{\infty} q^n \cos(q^\alpha q^n;q^2)\cos(q^\alpha q^n;q^2)$ diverges for $\alpha\notin\mathbb{Z}$ (see Ref. 3). □

The q-deformed Fourier transformation will now be defined.

Definition 2.2: Let f be a function in the space L^2_{q,π_0}, with $\pi_0\in\mathbb{R}^+$ and

$$L^2_{q,\pi_0}:=\{f|\|f\|_{q,\pi_0}<\infty\},\quad \|f\|_{q,\pi_0}:=\sqrt{\sum_{n=-\infty}^{\infty} q^n|f(\pi_0 q^n)|^2}.$$

For q in $\{q|(1-q)=q^j,\ j\in\mathbb{Z}\}$, the q-Fourier transformation $\mathscr{F}_{q,\pi_0}$ is given through the transform pair

$$g(\pi_0^{-1}q^k)=(\mathscr{F}_{q,\pi_0}f)(\pi_0^{-1}q^k)=\mathscr{N}_q\sum_{n=-\infty}^{\infty}(1-q)\pi_0 q^n\,\mathrm{Cos}(q^n q^k;q^2)f(\pi_0 q^n),$$

$$f(\pi_0 q^n)=(\mathscr{F}_{q,\pi_0^{-1}}g)(\pi_0 q^n)=\mathscr{N}_q\sum_{k=-\infty}^{\infty}(1-q)\pi_0^{-1}q^k\,\mathrm{Cos}(q^n q^k;q^2)g(\pi_0^{-1}q^k),$$

where

$$\mathscr{N}_q=\frac{(q;q^2)_\infty}{\sqrt{(1-q)}(q^2;q^2)_\infty}.$$

$\mathscr{F}_{q,\pi_0}$ is an isomorphy between L^2_{q,π_0} and $L^2_{q,\pi_0^{-1}}$:

$$\sum_{k=-\infty}^{\infty} q^k|g(\pi_0^{-1}q^k)|^2=\pi_0^2\sum_{n=-\infty}^{\infty} q^n|f(\pi_0 q^n)|^2. \tag{2.6}$$

III. THE DIRECT FIBER INTEGRAL OF L^2_{q,π_0}

The problem in trying to carry out a rigorous limit transition is obvious. The metrics of L^2_{q,π_0} and $L^2(\mathbb{R}^+,dx)$ are essentially different. Furthermore, the metrics of all the spaces L^2_{q,π_0} are not equivalent for different values of q. The only way to consistently overcome this difficulty is provided by the direct fiber integral. The continuous direct sum of the spaces L^2_{q,π_0} for a fixed value of q will be seen to be the space $L^2(\mathbb{R}^+,dx)$. The q-Fourier transformation is then extended to $L^2(\mathbb{R}^+,dx)$ in a natural way.

Definition 3.1: The direct fiber integral[4,5] is defined through

$$\mathscr{H}_q := \int_{(q,1]}^{\oplus} L^2_{q,m}\, dm,$$

that is

$\mathscr{H}_q = \{f \mid f_m \in L^2_{q,m}$ f.a.e. m, f Lebesgue-meas. and $\|f\|_{\mathscr{H}_q} := (\int_q^1 \|f_m\|^2_{q,m}\, dm)^{1/2} < \infty\}$. f_m (or $\mathbf{f}$) is the restriction of f to the corresponding lattice points.

Lemma 3.2: $\mathscr{H}_q = L^2(\mathbb{R}^+,dx)$.

Proof: Let f be a function in $L^2(\mathbb{R}^+,dx)$. Then the identities

$$\|f\|^2_{L^2} = \int_0^\infty |f(x)|^2\, dx = \sum_{n=-\infty}^{+\infty} \int_{q^{n+1}}^{q^n} |f(x)|^2\, dx = \sum_{n=-\infty}^{+\infty} q^n \int_q^1 |f(mq^n)|^2\, dm$$

$$= \int_q^1 \sum_{n=-\infty}^{+\infty} q^n |f(mq^n)|^2\, dm = \int_q^1 \|\mathbf{f}\|^2_{q,m}\, dm = \|f\|^2_{\mathscr{H}_q},$$

hold and thus $f \in \mathscr{H}_q$ as well. From the second to the third line, a simple substitution is made and from the third to the fourth line Fubini's theorem applied [Σq^n is an integral with the discrete measure $\sigma(q^n) = q^n$, and for f to be Lebesgue measurable is equivalent to being measurable with respect to $(q,1]\times\{q^n \mid n \in \mathbb{Z}\}$]. If f is a function in $\mathscr{H}_q$, then all the identities can be reversed and therefore $f \in L^2(\mathbb{R}^+,dx)$. □

Definition 3.3: The q-Fourier transformation $\mathscr{F}_q$ is defined on $L^2(\mathbb{R}^+,dx)$ through the direct fiber integral of the transformations $\mathscr{F}_{q,\pi_0}$:

$$\mathscr{F}_q = \int_{(q,1]}^{\oplus} \mathscr{F}_{q,m}\, dm, \quad (\mathscr{F}_q f)_{m^{-1}} = \mathscr{F}_{q,m} f_m .$$

Lemma 3.4: $\mathscr{F}_q$ is unitary.

Proof: This is a consequence of (2.6),

$$\|\mathbf{g}\|_{q,\pi_0^{-1}} = \pi_0 \|\mathbf{f}\|_{q,\pi_0}.$$

Therefore

$$\|g_q\|^2_{\mathscr{H}_q} = \int_q^1 \|\mathbf{g_q}\|^2_{q,m}\, dm = \int_1^{q^{-1}} \frac{1}{s^2} \|\mathbf{g_q}\|^2_{q,s^{-1}}\, ds = \int_1^{q^{-1}} \|\mathbf{f}\|^2_{q,s}\, ds = \int_q^1 \frac{1}{q} \|\mathbf{f}\|^2_{q,q^{-1}t}\, dt$$

$$\overset{(*)}{=} \int_q^1 \|\mathbf{f}\|^2_{q,t}\, dt = \|f\|^2_{\mathscr{H}_q}.$$

Equation $(*)$ is due to

$$\frac{1}{q}\,\|\mathbf{f}\|^2_{q,q^{-1}t}=\sum_{k=-\infty}^{\infty} q^{k-1}|\mathbf{f}(tq^{k-1})|^2=\|\mathbf{f}\|^2_{q,t}.$$

□

IV. THE LIMIT TRANSITION $q\to 1$

Our goal is to prove the convergence of the q-Fourier transformation $\mathscr{F}_q$ to the classical Fourier transformation $\mathscr{F}$ in the strong operator topology,

$$\mathscr{F}_q \underset{s}{\to} \mathscr{F}, \tag{4.1}$$

that is for any function $f\in L^2$,

$$\|\mathscr{F}f-\mathscr{F}_q f\|\to 0, \quad \text{as } q\to 1. \tag{4.2}$$

In other words, it has to be shown that the q-deformed Fourier transform converges to the classical Fourier transform in the L^2 norm. We denote the classical Fourier transform by

$$g(\lambda):=(\mathscr{F}f)(\lambda)=\sqrt{\frac{2}{\pi}}\int \cos(\lambda x)f(x)dx,$$

and the q-deformed transform by

$$g_q(\lambda):=(\mathscr{F}_q f)(\lambda)=(\mathscr{F}_{q,m(\lambda)}\mathbf{f})(\lambda)=\mathscr{N}_q\sum_{n=-\infty}^{\infty}(1-q)m(\lambda)q^n\ \mathrm{Cos}(q^{k(\lambda)}q^n;q^2)\mathbf{f}(m(\lambda)q^n)$$

$$=g_q(m(\lambda)^{-1}q^{k(\lambda)}).$$

As enforced by the direct fiber integral, all functions are considered to be defined on $\mathbb{R}^+$, the corresponding lattice for each λ is determined through $\lambda=[1/m(\lambda)]q^{k(\lambda)}$, with $q<m(\lambda)\leqslant 1$ and $k(\lambda)\in\mathbb{Z}$. The proof is carried out in two steps. First, the uniform convergence on compacta is proven for functions in $C_c(\mathbb{R}^+)$, the set of continuous functions with compact support. This implies convergence on compacta in the L^2 norm. Second, the convergence on $\mathbb{R}^+$ for functions in $C_c(\mathbb{R}^+)$ is proven. This implies the convergence for any function in L^2, $C_c(\mathbb{R}^+)$ being dense in L^2.

A. Uniform convergence on compacta

Let f be in the sequel a function in $C_c(\mathbb{R}^+)$, the support being contained in the interval $[0,K]$. The convergence will be investigated on a compactum that is bounded by $M>1$. The series $(q_j)_{j\in\mathbb{N}}$ is fixed through the condition $(1-q)=q^j$. It is observed that

$$\lim_{j\to\infty} q_j=1.$$

It has to be proven that

$$|g(\lambda)-g_{q_j}(\lambda)|\to 0, \quad \text{for } j\to\infty, \tag{4.3}$$

uniformly for $\lambda<M$. The normalization factor $\mathscr{N}_q$ is known to converge to $\sqrt{2/\pi}$ as $q\to 1$ (see Ref. 1). Using the triangle inequality, the Jackson integral of $\cos(\lambda x)f(x)$ is inserted to obtain

$$|\mathcal{M}_{q_j}^{-1} g_{q_j}(\lambda) - \sqrt{\pi/2}\, g(\lambda)|$$

$$= \left| \int \cos(\lambda x) f(x)\, dx - \sum_{n=-\infty}^{\infty} (1--q_j) m(\lambda) q_j^n \operatorname{Cos}(q_j^n q_j^{k(\lambda)}; q_j^2) \mathbf{f}(m(\lambda) q_j^n) \right|$$

$$\leqslant \left| \int \cos(\lambda x) f(x)\, dx - m(\lambda) \int \cos(\lambda m(\lambda) x) \mathbf{f}(m(\lambda) x)\, d_{q_j} x \right|$$

$$+ \left| \sum_{n=-\infty}^{\infty} (1-q_j) m(\lambda) q_j^n \{\operatorname{Cos}(q_j^n q_j^{k(\lambda)}; q_j^2) - \cos(q_j^n q_j^{k(\lambda)})\} \mathbf{f}(m(\lambda) q_j^n) \right|. \quad (4.4)$$

Regarding the second term of the right side of (4.4), it is noted that the support of the cosine functions is bounded by $M \cdot K := K'$, since the support of f is in $[0,K]$. From (2.2) follows that for each positive number ϵ there is an integer N_ϵ, such that

$$\max_{z \leqslant K'} |\operatorname{Cos}(z; q_j^2) - \cos(z)| < \epsilon, \quad \text{for all } j > N_\epsilon,$$

and the whole term is bounded by

$$\epsilon m(\lambda) \int_{[0,K]} \mathbf{f}(m(\lambda) x)\, d_{q_j} x.$$

Because of $f \in C_c(\mathbb{R}^+)$, there is a constant C, such that $|f(x)| < C$ for all $x \in \mathbb{R}^+$, thus

$$\epsilon m(\lambda) \int_{[0,K]} \mathbf{f}(m(\lambda) x)\, d_{q_j} x \leqslant \epsilon C m(\lambda) \int_{[0,K]} d_{q_j} x = \epsilon C K.$$

ϵ was an arbitrary number and the term under consideration converges uniformly to zero as j becomes infinite.

The uniform convergence of the first term is proven, if for each $\epsilon > 0$ there is a $\delta > 0$ such that $|\int \cos(\lambda x) f(x)\, dx - m(\lambda) \int \cos(\lambda m(\lambda) x) \mathbf{f}(m(\lambda) x)\, d_q x| < \epsilon$ for $\lambda \leqslant M$ and $1 - \delta < q < 1$. The integral $\int \cos(\lambda x) f(x)\, dx$ is written as $\Sigma_{n=-\infty}^{\infty} q^n \int_{qm(\lambda)}^{m(\lambda)} \cos(\lambda s q^n) \mathbf{f}(s q^n)\, ds$. According to the mean value theorem of integration there are values $s'(n) \in (qm(\lambda), m(\lambda))$, such that

$$\int_{qm(\lambda)}^{m(\lambda)} \cos(\lambda s q^n) \mathbf{f}(s q^n)\, ds = m(\lambda)(1-q) \cos(\lambda s'(n) q^n) f(s'(n) q^n).$$

The continuous functions cos and f are uniformly continuous on the compactum $[0,K']$. Thus there is for each number $\epsilon > 0$ a number $\delta > 0$ such that $|\cos x - \cos y| < \epsilon$ and $|f(x) - f(y)| < \epsilon$ if $x, y \in [0,K']$ and $|x - y| < \delta K'$. Observe that $|\lambda s'(n) q^n - \lambda m(\lambda) q^n| < \delta K'$ and $|s'(n) q^n - m(\lambda) q^n| < \delta K'$ if $1 - \delta < q < 1$. Put $\epsilon > 0$ and find a $\delta > 0$ as described above. For $1 - \delta < q < 1$, the inequalities

$$\begin{aligned}
&\left| \int \cos(\lambda x) f(x) dx - m(\lambda) \int \cos(\lambda m(\lambda) x) \mathbf{f}(m(\lambda) x) d_q x \right| \\
&= \left| \sum_{n=-\infty}^{\infty} m(\lambda)(1-q) q^n (\cos(\lambda s'(n) q^n) f(s'(n) q^n) - \cos(\lambda m(\lambda) q^n) f(m(\lambda) q^n)) \right| \\
&\leqslant \sum_{n=-\infty}^{\infty} m(\lambda)(1-q) q^n \{ |(\cos(\lambda s'(n) q^n) - \cos(\lambda m(\lambda) q^n)) f(s'(n) q^n)| \\
&\quad + |\cos(\lambda m(\lambda) q^n)(f(s'(n) q^n) - f(m(\lambda) q^n))| \} \\
&\leqslant \sum_{n=-\infty}^{\infty} m(\lambda)(1-q) q^n \{ \epsilon |f(s'(n) q^n)| + \epsilon |\cos(\lambda m(\lambda) q^n)| \} \\
&\leqslant \epsilon K(C+1),
\end{aligned}$$

follow and the proof of uniform convergence is completed.

B. Convergence in the strong operator topology

Of course, L^2 convergence on compacta does not in general imply L^2 convergence on $\mathbb{R}^+$. In the present case, an additional condition is satisfied, namely that all the functions in the series have the same norm as the function they are converging to on compacta. This feature is due to the unitarity of both the classical and the q-deformed Fourier transformation:

$$\|g\|_{L^2} = \|f\|_{L^2} = \|g_{q_j}\|_{L^2}, \quad \forall j \in \mathbb{N}. \tag{4.5}$$

Proposition 4.1: Let $(g_n)_{n\in\mathbb{N}}$ be a series of functions in $L^2(\mathbb{R})$, such that for every compactum K $\|g - g_n\|_{L^2(K)} \to 0$ as $n\to\infty$. Let $\|g_n\|_{L^2(\mathbb{R})} = \|g\|_{L^2(\mathbb{R})}$, $\forall n \in \mathbb{N}$. Then

$$\|g - g_n\|_{L^2(\mathbb{R})} \to 0, \quad \text{as } n\to\infty. \tag{4.6}$$

Proof: Put $1>\epsilon>0$ and $\|g\|=1$. Then there is a compactum B_ϵ, such that

$$\|g\|_{L^2(B_\epsilon)} = \left(\int_{B_\epsilon} |g(p)|^2 \, dp \right)^{1/2} \geqslant 1 - \frac{\epsilon^2}{36}. \tag{4.7}$$

In addition, there is a number N_ϵ, so that

$$\|g - g_n\|_{L^2(B_\epsilon)} \leqslant \frac{\epsilon^2}{36}, \quad \forall n \geqslant N_\epsilon. \tag{4.8}$$

Because of (4.8), the norm of g_n over B_ϵ is bounded from below for each $n \geqslant N_\epsilon$:

$$\|g\|_{L^2(B_\epsilon)} \leqslant \|g - g_n\|_{L^2(B_\epsilon)} + \|g_n\|_{L^2(B_\epsilon)} \leqslant \|g_n\|_{L^2(B_\epsilon)} + \frac{\epsilon^2}{36},$$

$$\Rightarrow \|g_n\|_{L^2(B_\epsilon)} \geqslant \|g\|_{L^2(B_\epsilon)} - \frac{\epsilon^2}{36} \overset{(4.7)}{\geqslant} 1 - \frac{\epsilon^2}{18} \tag{4.9}$$

($\mathscr{C}B_\epsilon$ is the complement of B_ϵ in $\mathbb{R}^+$). Since $\|g_n\|^2_{L^2(B_\epsilon)} + \|g_n\|^2_{L^2(\mathscr{C}B_\epsilon)} = 1$, it follows that

$$\|g_n\|_{L^2(\complement B_\epsilon)} = \sqrt{1-\|g_n\|^2_{L^2(B_\epsilon)}} \leqslant \sqrt{1-\left(1-\frac{\epsilon^2}{18}\right)^2} \leqslant \frac{\epsilon}{3}. \tag{4.10}$$

From (4.7), the analogous relation for g is

$$\|g\|_{L^2(\complement B_\epsilon)} = \sqrt{1-\|g\|^2_{L^2(B_\epsilon)}} \leqslant \sqrt{1-\left(1-\frac{\epsilon^2}{36}\right)^2} \leqslant \frac{\epsilon}{3}, \tag{4.11}$$

and finally

$$\begin{aligned}\|g-g_n\|_{L^2(\mathbb{R}^+)} &\leqslant \|g-g_n\|_{L^2(B_\epsilon)} + \|g-g_n\|_{L^2(\complement B_\epsilon)} \\ &\leqslant \|g-g_n\|_{L^2(B_\epsilon)} + \|g\|_{L^2(\complement B_\epsilon)} + \|g_n\|_{L^2(\complement B_\epsilon)} \\ &\leqslant \underset{(4.8)}{\frac{\epsilon^2}{36}} + \underset{(4.11)}{\frac{\epsilon}{3}} + \underset{(4.10)}{\frac{\epsilon}{3}} \leqslant \epsilon \quad \text{for all } n \geqslant N_\epsilon. \end{aligned} \tag{4.12}$$

Since ϵ was arbitrary, the proof is completed. □

Applying the above proposition to the present case, where f is still restricted to be in $C_c(\mathbb{R}^+)$, results in

$$\|(\mathscr{F}-\mathscr{F}_{q_j})f\|_{L^2} = \|g-g_{q_j}\|_{L^2} \to 0, \quad \text{as } j\to\infty. \tag{4.13}$$

To show that the same holds for f in $L^2(\mathbb{R}^+)$, let $(f_n)_n \subset C_c(\mathbb{R}^+)$ be a series with $\|f-f_n\|_{L^2}\to 0$ as $n\to\infty$. Put $\epsilon>0$. There is an integer n, such that $\|(f-f_n)\|_{L^2} < \epsilon/3$. Due to (4.13), there is an integer N, such that $\|(\mathscr{F}-\mathscr{F}_{qN})f_n\|_{L^2} < \epsilon/3$. Therefore,

$$\begin{aligned}\|(\mathscr{F}-\mathscr{F}_{q_N})f\|_{L^2} &\leqslant \|(\mathscr{F}-\mathscr{F}_{q_N})(f-f_n)\|_{L^2} + \|(\mathscr{F}-\mathscr{F}_{q_N})f_n\|_{L^2} \\ &\leqslant \|\mathscr{F}-\mathscr{F}_{q_N}\|\|(f-f_n)\|_{L^2} + \|(\mathscr{F}-\mathscr{F}_{q_N})f_n\|_{L^2} \\ &\leqslant 2\|(f-f_n)\|_{L^2} + \|(\mathscr{F}-\mathscr{F}_{q_N})f_n\|_{L^2} \\ &< \epsilon. \end{aligned} \tag{4.14}$$

Thus, the proof of the strong convergence of the q-Fourier transformation to the classical Fourier transformation is complete. In the strong operator topology, the q-Fourier transformation emerges as a ''continuous'' deformation of the classical Fourier transformation. It is emphasized that the deformation is not continuous in the proper sense, since the allowed values of q were restricted to a discrete set.

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On the inversion formula of the half-Hartley transform

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The Hartley transform (HT) of a function $g(x)\in L_2[-\infty,\infty]$ is given by

$$g_{\mathrm{H}}(y)=\int_{-\infty}^{\infty} g(x)(\cos(xy)+\sin(xy))dx,\quad y\in[-\infty,\infty]. \tag{1}$$

The properties and applications of this transform can be found in Ref. 1. In particular, the inversion formula takes the form of the simple reciprocity relation,

$$g(x)=\int_{-\infty}^{\infty} g_{\mathrm{H}}(y)(\cos(xy)+\sin(xy))dy. \tag{2}$$

Actually, we are concerned about the inversion formula for the half-Hartley transform (h-HT), which is defined as

$$g_h(y)=\int_{0}^{\infty} g(x)(\cos(xy)+\sin(xy))dx,\quad y\in[0,\infty]. \tag{3}$$

The reciprocity relation, Eq. (2), is no longer satisfactory in this case, since its use requires us to know the function $g_h(y)$ in the whole interval $[-\infty,\infty]$.

Recently, Paveri-Fontana and Zweifel[2] have obtained an inversion formula for the h-HT by reducing the problem to invert the half-Hilbert transform. This last problem involves, in its turn, the solution of the homogeneous Riemann–Hilbert problem. With relation to the method of Paveri-Fontana and Zweifel, also see the work by Pagani.[3]

In this paper we solve the integral equation (3) by following a different way. Multiplying both terms of Eq. (3) by $1/\sqrt{2}$, it can be rewritten as

$$\frac{1}{\sqrt{2}}\,g_h(y)=\int_{0}^{\infty} g(x)\sin\left(xy+\frac{\pi}{4}\right)dx, \tag{4}$$

which, recalling the integral representation,[4]

$$\sin\left(xy+\frac{\pi}{4}\right)=\sqrt{\frac{y}{\pi}}\int_{x}^{\infty}\frac{\sin(uy)}{\sqrt{u-x}}\,du,\quad x,y>0, \tag{5}$$

yields

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$$g_h(y)=\sqrt{\frac{2y}{\pi}}\int_0^\infty g(x)dx\int_x^\infty \frac{\sin(uy)}{\sqrt{u-x}}\,du \tag{6}$$

or

$$\sqrt{\frac{\pi}{2y}}g_h(y)=\int_0^\infty \sin(uy)du\int_0^u \frac{g(x)}{\sqrt{u-x}}\,dx. \tag{7}$$

By Fourier inverting this equation, we get an Abel integral equation:

$$\int_0^u \frac{g(x)}{\sqrt{u-x}}\,dx=\mathscr{F}_s\left[\frac{g_h(y)}{\sqrt{y}}\right], \tag{8}$$

where

$$\mathscr{F}_s[f(y)](u)\equiv\sqrt{\frac{2}{\pi}}\int_0^\infty f(y)\sin(uy)dy. \tag{9}$$

The solution of (8) yields (see, for example, Ref. 5):

$$g(x)=\frac{1}{\pi}\frac{d}{dx}\int_0^x \frac{\mathscr{F}_s[g_h(y)/\sqrt{y}]}{\sqrt{x-u}}\,du, \tag{10}$$

which is a formally simple expression for the inversion formula of the half-Hartley transform.

We apply formula (10) to invert a couple of functions. First we consider $g_h(y)=(2\pi/y)^{1/2}(y>0)$, which is the half-Hartley transform of $g(x)=x^{-1/2}$. In fact, we have[6] $\mathscr{F}_s[g_h(y)/\sqrt{y}]=\pi$ and hence $\int_0^x g(u)du=\int_0^x(x-u)^{-1/2}\,du=2x^{1/2}$. The second example is that given in Sec. V of Ref. 2. The function to half-Hartley invert is $g_h(y)=e^{-\alpha y}$, $\alpha>0$, $y>0$. The Fourier sine transform in the integral of Eq. (10) can be written as

$$\mathscr{F}_s\left[\frac{g_h(y)}{\sqrt{y}}\right]=-\frac{i}{\sqrt{2}}\left[\frac{1}{\sqrt{z}}-\frac{1}{\sqrt{\bar{z}}}\right], \tag{11}$$

where i is the imaginary unity, $z=\alpha-iy$, and $\bar{z}$ denotes the complex conjugate of z. Thus, the integral yields the difference between two hypergeometric functions:[7]

$$\begin{aligned}\int_0^x \frac{\mathscr{F}_s[g_h(y)/\sqrt{y}]}{\sqrt{x-u}}\,du&=-\frac{i^{1/2}}{\sqrt{2}}\,s\left\{{}_2F_1\left(\frac{1}{2},1;\frac{3}{2};s^2\right)-{}_2F_1\left(\frac{1}{2},1;\frac{3}{2};-s^2\right)\right\}\\&=-\frac{i^{1/2}}{\sqrt{2}}\left\{\ln\left[\frac{(1+s)}{(1-s)}\right]^{1/2}-\arctan(s)\right\},\end{aligned} \tag{12}$$

with $s^2=ix/\alpha$. By derivating this equation we recover the result of Ref. 2:

$$g(x)=\frac{1}{\pi}\frac{\sqrt{2\alpha x}}{\alpha^2+x^2},\quad x>0. \tag{13}$$

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Determinant structure of the rational solutions for the Painlevé II equation

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Two types of determinant representations of the rational solutions for the Painlevé II equation are discussed by using the bilinear formalism. One of them is a representation by the Devisme polynomials, and another one is Hankel determinant representation. They are derived from the determinant solutions of the KP hierarchy and Toda lattice, respectively. © *1996 American Institute of Physics.* [S0022-2488(96)04209-0]

I. INTRODUCTION

The six Painlevé transcendents are now regarded as the nonlinear version of the special functions and hence the Painlevé equations are the most fundamental integrable systems in some sense. It is known that the Painlevé transcendents cannot be expressed by the solutions of linear equations, except for two classes of solutions, namely, special function solutions and rational solutions. The Painlevé II equation (P_{II})

$$\frac{d^2}{dz^2}v = 2v^3 - 4zv + 4\alpha, \tag{1}$$

is the simplest equation that admits such solutions among the Painlevé equations. In fact, it is known that it admits one parameter family of Airy function solutions for α being half odd integers, and only one rational solutions for each integer α[1] and it has no other classical solution.[2]

It is well known that the Painlevé equations can be derived from the similarity reduction of various soliton equations.[3] In particular, P_{II} can be reduced from the modified KdV equation. A systematic study of the rational solutions was done by Airault,[4] who constructed the Bäcklund transformation of P_{II} from the similarity reduction of the modified KdV equation. On the other hand, Okamoto revealed that the Bäcklund transformations of Painlevé equations are given by the Toda lattice equation. For the KP and Toda lattice hierarchies, the solutions are described by the Wronski determinants. The Painlevé equations are deeply connected with the KP and Toda, therefore a question naturally arising is what is the structure of the solutions of Painlevé equations. Actually for the special function type solutions of Painlevé equations, it is known that they are expressed by Wronskians whose entries are given by special functions. Such Wronskians are called the τ function. Here, we note that τ functions are originally defined for arbitrary values of parameters through the Hamiltonians of the Painlevé equations.[1,5] This Wronskian structure of the solutions is quite similar to that for the soliton equations. Hence we expect that the rational solutions also have such a structure. Many studies have been done for the rational solutions, but curiously, it seems that the determinant structure of solutions itself has not been well discussed. This situation motivates us for studying the relationship of the solutions of the Painlevé equations and integrable PDE.

In this article, we present the determinant representations for the rational solutions of P_{II} and clarify how those solutions are reduced from the τ functions of the KP hierarchy and Toda lattice.

We present two types of determinant representations. One is directly derived from the Schur polynomials, namely the algebraic solutions for the KP hierarchy, by applying a reduction procedure. Entries of the determinant are expressed by the Devisme polynomials.[6,7] This reduction exactly corresponds to the derivation of P_{II} from the modified KdV equation. The bilinear form for P_{II} is nothing but the bilinear first Bäcklund transformations of the KP hierarchy. Another one is a Hankel determinant representation which is derived from the Hankel determinant solution of the B-type Toda lattice equation.[8] In this case, the Toda lattice is corresponding to the Bäcklund transformation ladder of the solutions of P_{II}.

In Sec. II, the bilinearization of P_{II} is presented. We give a brief review of the algebraic solutions for KP and KdV hierarchies in Sec. III. In Sec. IV, we give the derivation of the rational solutions for P_{II} from the Schur polynomials. In Sec. V, we briefly summarize the determinant solution for the B-type Toda lattice equation. The Hankel determinant representation of the rational solutions is presented in Sec. VI. Section VII is devoted to concluding remarks.

II. BILINEAR FORM FOR P_{II}

By using the dependent variable transformation,

$$v = \frac{d}{dz} \log \frac{g}{f}, \tag{2}$$

Eq. (1) is decomposed into the following bilinear equations:[5,9]

$$(D_z^2 - \lambda) g \cdot f = 0, \tag{3}$$

$$(D_z^3 + (4z - 3\lambda) D_z - 4\alpha) g \cdot f = 0, \tag{4}$$

where D_z^n is the Hirota bilinear differential operator and λ is an arbitrary function of z. Dividing Eqs. (3) and (4) by gf, we obtain

$$s + v^2 = \lambda,$$

$$v_{zz} + 3sv + v^3 + (4z - 3\lambda) v - 4\alpha = 0,$$

where $s = (\log gf)_{zz}$. Eliminating s from above equations, we get $P_{II}(1)$, therefore Eqs. (3) and (4) actually give the bilinear form for P_{II}.

Using the gauge transformation, we can take λ as we like. In the case of the rational solutions of P_{II}, taking λ to be 0 is convenient as is shown in the later. On the other hand, for the Airy function type solutions of P_{II}, λ is taken to be $2z$.[1] If we fix λ to be equal 0, the bilinear equations for P_{II} are

$$D_z^2 g \cdot f = 0, \tag{5}$$

$$(D_z^3 + 4z D_z - 4\alpha) q \cdot f = 0. \tag{6}$$

In this gauge, these equations allow polynomial solutions for f and g which give the rational solutions v for $P_{II}(1)$ through the variable transformation (2). In the following sections, we will show how the rational solutions are constructed from the τ functions of KP hierarchy and Toda lattice equation.

III. ALGEBRAIC SOLUTIONS FOR KP AND KdV HIERARCHIES

We first give a brief review on the algebraic solutions of KP and KdV hierarchies.[10]

Definition 3.1: Let $p_j(y)$, $j = 0,1,2,...$, be polynomials in $y = (y_1, y_2, y_3, \ldots)$ defined by

$$\sum_{k=0}^{\infty} p_k(y)\lambda^k = \exp\sum_{n=1}^{\infty} y_n\lambda^n, \quad \text{and } p_k(y)=0, \quad \text{for } k<0. \tag{7}$$

Then a set of infinitely many bilinear equations for $\tau(x)=\tau(x_1,x_2,x_3,\ldots)$ generated by

$$\left(\sum_{j=0}^{\infty} p_j(-2y)p_{j+1}(\tilde{D})\exp\left(\sum_{n=1}^{\infty} y_n D_{x_n}\right)\right)\tau\cdot\tau=0, \tag{8}$$

where

$$\tilde{D}=(D_{x_1},\tfrac{1}{2}D_{x_2},\tfrac{1}{3}D_{x_3},\ldots),$$

is called the KP hierarchy and τ is called the τ function.

The simplest bilinear equation included in this hierarchy is

$$(D_{x_1}^4-4D_{x_1}D_{x_3}+3D_{x_2}^2)\tau\cdot\tau=0, \tag{9}$$

which yields the KP equation in nonlinear form,

$$(-4u_{x_3}+6uu_{x_1}+u_{x_1x_1x_1})_{x_1}+3u_{x_2}=0, \tag{10}$$

by the dependent variable transformation,

$$u=2(\log\ \tau)_{x_1x_1}. \tag{11}$$

Proposition 3.2: The following Wronskian,

$$\tau_{N,\mathrm{KP}}=\begin{vmatrix} \partial_{x_1}^{N-1}f_1 & \cdots & \partial_{x_1}f_1 & f_1 \\ \partial_{x_1}^{N-1}f_2 & \cdots & \partial_{x_1}f_2 & f_2 \\ \vdots & \cdots & \vdots & \vdots \\ \partial_{x_1}^{N-1}f_N & \cdots & \partial_{x_1}f_N & f_N \end{vmatrix}, \tag{12}$$

solves the KP hierarchy, where f_k, $k=1,2,\ldots,N$ are arbitrary functions in infinitely many independent variables $x=(x_1,x_2,\ldots)$ satisfying

$$\partial_{x_n}f_k=\partial_{x_1}^n f_k, \quad k=1,2,\ldots,N, \quad n=1,2,\ldots\ . \tag{13}$$

The crucial point is that all the bilinear equations in the KP hierarchy for the τ function (12) are reduced to the identities of determinant which are called the Plücker relations.

Definition 3.3: A set of infinitely many bilinear equations in $\tau(x)$ and $\tau'(x)$ generated by

$$\left(\sum_{j=0}^{\infty} p_j(-2y)p_{j+2}(\tilde{D})\exp\left(\sum_{n=1}^{\infty} y_n D_{x_n}\right)\right)\tau\cdot\tau'=0, \tag{14}$$

is called the first modified KP hierarchy.

In particular, $\tau=\tau_{N+1,\mathrm{KP}}$, $\tau'=\tau_{N,\mathrm{KP}}$ solves the first modified KP hierarchy. Hence, this is regarded as the hierarchy of the first Bäcklund transformations. Moreover, the bilinear equations in this hierarchy are regarded as the identities of $(N+1)\times(N+1)$ determinant and $N\times N$ determinant, which are also the Plücker relations. First two equations of this hierarchy are given by

$$(D_{x_1}^2 - D_{x_2})\,\tau_{N+1\mathrm{KP}} \cdot \tau_{N,\mathrm{KP}} = 0, \tag{15}$$

$$(D_{x_1}^3 - 4D_{x_3} + 3D_{x_1}D_{x_2})\,\tau_{N+1,\mathrm{KP}} \cdot \tau_{N,\mathrm{KP}} = 0. \tag{16}$$

Now we discuss the algebraic solutions for the KP hierarchy. We can easily verify that the polynomials $p_k(x)$ defined by Eq. (7) satisfy

$$\partial_{x_n} p_k(x) = p_{k-n}(x), \tag{17}$$

and hence Eq. (13). Taking f_k in the τ function (12) as $p_{i_k+N-k}(x)$, we have,

Proposition 3.4: Let $Y=(i_1,i_2,\ldots,i_N)$, where $i_1 \geqslant i_2 \geqslant \ldots \geqslant i_N > 0$ are integers, be a Young diagram. Then

$$\tau_{Y,\mathrm{KP}} = \begin{vmatrix} p_{i_1}(x) & p_{i_1+1}(x) & \cdots & p_{i_1+N-1}(x) \\ p_{i_2-1}(x) & p_{i_2}(x) & \cdots & p_{i_2+N-2}(x) \\ \vdots & \vdots & \ddots & \vdots \\ p_{i_N-N+1}(x) & p_{i_N-N+2}(x) & \cdots & p_{i_N}(x) \end{vmatrix} \tag{18}$$

gives the algebraic solution for the KP hierarchy.

The polynomial $\tau_{Y,\mathrm{KP}}$ is called the Schur polynomial attached to the Young diagram Y. We note that if we define the weight of x_n as n, then $p_k(x)$ is a polynomial with homogeneous weight k and $\tau_{Y,\mathrm{KP}}$ is also homogeneous with the weight $|Y| = i_1 + i_2 + \ldots + i_N$. This τ function gives the rational solution of Eq. (10) by the dependent variable transformation (11).

Let us apply the reduction to the KdV hierarchy. This is achieved by dropping the dependence of $x_2, x_4, \ldots$, in the τ functions of KP hierarchy. In order to realize this condition, it is sufficient to choose Y as $(N, N-1, \ldots, 1)$ in the algebraic solution for the KP hierarchy (18).

Proposition 3.5:

$$\tau_{N,\mathrm{KdV}} = \begin{vmatrix} p_N(x) & p_{N+1}(x) & \cdots & p_{2N-1}(x) \\ p_{N-2}(x) & p_{N-1}(x) & \cdots & p_{2N-3}(x) \\ \vdots & \vdots & \ddots & \vdots \\ p_{-N+2}(x) & p_{-N+3}(x) & \cdots & p_1(x) \end{vmatrix}. \tag{19}$$

gives the algebraic solution of the KdV hierarchy.

Proposition 3.5 can be easily verified noticing that

$$\frac{\partial \tau_{N,\mathrm{KdV}}}{\partial x_{2j}} = 0, \quad j = 1,2,3,\ldots, \tag{20}$$

which directly follows from Eq. (17). From Eqs. (15), (16), and (20), it is clear that the τ function (19) satisfies the following bilinear equations:

$$D_{x_1}^2 \tau_{N+1,\mathrm{KdV}} \cdot \tau_{N,\mathrm{KdV}} = 0, \tag{21}$$

$$(D_{x_1}^3 - 4D_{x_3})\,\tau_{N+1,\mathrm{KdV}} \cdot \tau_{N,\mathrm{KdV}} = 0. \tag{22}$$

The modified KdV equation,

$$v_{x_3}+\tfrac{3}{2}\,v^2 v_{x_1}-\tfrac{1}{4}\,v_{x_1x_1x_1}=0, \tag{23}$$

is obtained from Eqs. (21) and (22) by the dependent variable transformation,

$$v=\frac{\partial}{\partial x_1}\log\frac{\tau_{N+1,\mathrm{KdV}}}{\tau_{N,\mathrm{KdV}}}. \tag{24}$$

IV. RATIONAL SOLUTIONS FOR P_{II}: DEVISME POLYNOMIAL REPRESENTATION

Now we give a determinant representation for the rational solutions of P_{II}. We first give the definition of the Devisme polynomials.[6,7]

Definition 4.1: The Devisme polynomials $q_k(x_1,x_2,\ldots,x_m)$, $k=0,1,2,\ldots$, are polynomials in $x_1,\ldots,x_m$ defined by

$$\sum_{k=0}^{\infty} q_k(x_1,x_2,\ldots,x_m)\lambda^k=\exp\left(x_1\lambda+x_2\lambda^2+\cdots+x_m\lambda^m+\frac{1}{m+1}\,\lambda^{m+1}\right). \tag{25}$$

Then one of our main results is stated as follows.

Theorem 4.2: Let $q_k(z,t)$, $k=0,1,2,\ldots$, be the Devisme polynomials and τ_N be an $N\times N$ determinant defined by

$$\tau_N=\begin{vmatrix} q_N(z,t) & q_{N+1}(z,t) & \cdots & q_{2N-1}(z,t)\\ q_{N-2}(z,t) & q_{N-1}(z,t) & \cdots & q_{2N-3}(z,t)\\ \vdots & \vdots & \ddots & \vdots\\ q_{-N+2}(z,t) & q_{-N+3}(z,t) & \cdots & q_1(z,t)\end{vmatrix},\quad q_k(z,t)=0\quad \text{for } k<0. \tag{26}$$

Then

$$v=\frac{d}{dz}\log\frac{\tau_{N+1}}{\tau_N}, \tag{27}$$

gives a rational solution for P_{II} (1) with $\alpha=N+1$.

Remark 4.3: (1) The τ function (26) is derived only by putting

$$x_1=z,\quad x_2=t,\quad x_3=\tfrac{1}{3},\quad x_4=x_5=\cdots=0, \tag{28}$$

in Eq. (19). Namely, the rational solutions of P_{II} are given in terms of the special case of the Schur polynomials.

(2) The τ function (26) itself does not depend on t, but we have left t dependence in the entries in order to relate the solutions with the Devisme polynomials.

Theorem 4.2 is a direct consequence of the following proposition.

Proposition 4.4: The τ function τ_N (26) satisfies the bilinear equations (5) and (6) with $\alpha=N+1$.

Proof: Putting $x_5=x_7=\cdots=0$ in the rational solutions of KdV hierarchy (19), it is readily seen that $\tau_{N,\mathrm{KdV}}$ is a homogeneous weight polynomial in x_1 and x_3 with weight $[N(N+1)]/[2]$. Hence, if we put

$$f_N=\frac{1}{x_3^{N(N+1)/6}}\,\tau_{N,\mathrm{KdV}}, \tag{29}$$

then f_N depends only on $t=(x_1)/(x_3^{1/3})$. Thus we have

$$\partial_{x_3} f_N = \frac{\partial t}{\partial x_3} \frac{d}{dt} f_N, \quad \partial_{x_1} f_N = \frac{\partial t}{\partial x_1} \frac{d}{dt} f_N, \tag{30}$$

which yield

$$\partial_{x_3} \tau_{N,\mathrm{KdV}} = \frac{1}{3x_3} \left(\frac{N(N+1)}{2} \tau_{N,\mathrm{KdV}} - x_1 \partial_{x_1} \tau_{N,\mathrm{KdV}} \right). \tag{31}$$

Substituting Eq. (31) into Eq. (22), we get

$$\left(D_{x_1}^3 + \frac{4}{3x_3} x_1 D_{x_1} - \frac{4}{3x_3} (N+1) \right) \tau_{N+1,\mathrm{KdV}} \cdot \tau_{N,\mathrm{KdV}} = 0. \tag{32}$$

Moreover, by putting $z = x_1$ and $x_3 = \frac{1}{3}$, $\tau_{N,\mathrm{KdV}}$ reduces to τ_N in Eq. (26) and Eqs. (5) and (6) with $f = \tau_N$, $g = \tau_{N+1}$ and $\alpha = N+1$ are obtained from Eqs. (21) and (32). □

V. HANKEL DETERMINANT SOLUTION FOR TODA LATTICE

Let us consider the Toda lattice equation,

$$\frac{d^2 u_N}{dz^2} = e^{u_{N-1} - u_N} - e^{u_N - u_{N+1}}, \tag{33}$$

with the symmetric lattice condition,

$$u_N = u_{-N-1}. \tag{34}$$

It is easy to see that Eq. (33) is bilinearized through the dependent variable transformation,

$$u_N = \log \frac{\tau_{N-1}}{\tau_N}, \tag{35}$$

from which we get

$$D_z^2 f_N \cdot f_N = 2(f_{N+1} f_{N-1} - f_N f_N), \quad f_N = f_{-N-1}. \tag{36}$$

Here, we call this type of symmetric lattice as B-type Toda lattice because it concerns the BKP hierarchy.[8,10] Using the gauge freedom, we can translate the above B-type Toda lattice equation in the following form:

$$(D_z^2 + 2a_0) \sigma_N \cdot \sigma_N = 2 \sigma_{N+1} \sigma_{N-1}, \tag{37}$$

where $\sigma_N = f_N / f_0$ and $a_0 = f_1 / f_0$. It is clear that σ_N satisfies

$$\sigma_N = \sigma_{-N-1}, \tag{38}$$

$$\sigma_0 = 1, \quad \sigma_1 = a_0. \tag{39}$$

It is possible to express the general solution of Eqs. (37)–(39) in determinant form.[11]

Proposition 5.1: The general solution for Eqs. (37)–(39) for an arbitrary a_0 is given in the Hankel determinant form

$$\sigma_N=\begin{vmatrix} a_0 & a_1 & \cdots & a_{N-1} \\ a_1 & a_2 & \cdots & a_N \\ \vdots & \vdots & \ddots & \vdots \\ a_{N-1} & a_N & \cdots & a_{2N-2} \end{vmatrix}, \quad N\geqslant 0, \tag{40}$$

where a_n, $n=1,2,3,...$ are recursively defined by

$$a_{n+1}=\frac{da_n}{dz}+\sum_{k=0}^{n-1} a_k a_{n-k-1}, \quad n\geqslant 0. \tag{41}$$

This contains one arbitrary function a_0, hence it gives the general solution for the B-type Toda lattice equation.

VI. RATIONAL SOLUTIONS FOR P_{II}: HANKEL DETERMINANT REPRESENTATION

The rational solutions for P_{II} are derived only by putting

$$a_0=z, \tag{42}$$

in the above σ_N.

Theorem 6.1: Let a_n, $n=0,1,2,...$, be polynomials defined by

$$a_{n+1}=\frac{da_n}{dz}+\sum_{k=0}^{n-1} a_k a_{n-k-1}, \quad n\geqslant 0, \quad a_0=z, \tag{43}$$

and let σ_N be an $N\times N$ determinant given by Eq. (40). Then

$$v=\frac{d}{dz}\log\frac{\sigma_{N+1}}{\sigma_N}, \tag{44}$$

gives a rational solution for P_{II} (1) with $\alpha=N+1$.

Similar to the previous section, Theorem 6.1 is a direct consequence of the following proposition.

Proposition 6.2: $f=\sigma_N$ and $g=\sigma_{N+1}$ satisfies the bilinear equations (5) and (6) with $\alpha=N+1$.

To prove proposition 6.2, let us first introduce the notation σ_{NY}:

Definition 6.3: Let $Y=(i_1,i_2,\ldots,i_h)$ be a Young diagram. Then we define an $N\times N$ determinant σ_{NY} by

$$\sigma_{NY}=\begin{vmatrix} a_0 & a_1 & \cdots & a_{N-h-1} & a_{N-h+i_h} & \cdots & a_{N-2+i_2} & a_{N-1+i_1} \\ a_1 & a_2 & \cdots & a_{N-h} & a_{N-h+1+i_h} & \cdots & a_{N-1+i_2} & a_{N+i_1} \\ \vdots & \vdots & \cdots & \vdots & \vdots & \cdots & \vdots & \vdots \\ a_{N-1} & a_N & \cdots & a_{2N-h-2} & a_{2N-h-1+i_h} & \cdots & a_{2N-3+i_2} & a_{2N-2+i_1} \end{vmatrix}. \tag{45}$$

We first construct the shift operators which are differential operators generating σ_{NY} from σ_N. If entries of the determinant satisfy simple equations like Eq. (13), then construction of the shift operators is straightforward. But when we have to work on more complicated relations among the entries like Eq. (41), it is useful to apply the technique developed in Ref. 12.

We can prove the following lemma.

Lemma 6.4:

$$\sigma_{N\square}=\frac{d}{dz}\,\sigma_N. \tag{46}$$

Proof: Notice that $\sigma_{N\square}$ is expressed by

$$\sigma_{N\square}=\begin{pmatrix} a_1 & a_2 & \cdots & a_N \\ a_2 & a_3 & \cdots & a_{N+1} \\ \vdots & \vdots & \ddots & \vdots \\ a_N & a_{N+1} & \cdots & a_{2N-1} \end{pmatrix}\cdot\begin{pmatrix} \Delta_{11} & \Delta_{12} & \cdots & \Delta_{1N} \\ \Delta_{21} & \Delta_{22} & \cdots & \Delta_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ \Delta_{N1} & \Delta_{N2} & \cdots & \Delta_{NN} \end{pmatrix}, \tag{47}$$

where Δ_{ij} is the (i,j)-cofactor of σ_N and $A\cdot B$ denotes a standard scalar product for $N\times N$ matrices $A=(a_{ij})$ and $B=(b_{ij})$ which is defined as

$$A\cdot B=\sum_{i,j=1}^{N} a_{ij}b_{ij}=\text{trace } A^tB. \tag{48}$$

The first matrix of Eq. (47) is rewritten by using the recursion relation (41) as

$$\begin{pmatrix} \partial_z a_0 & \partial_z a_1 & \cdots & \partial_z a_{N-1} \\ \partial_z a_1 & \partial_z a_2 & \cdots & \partial_z a_N \\ \vdots & \vdots & \ddots & \vdots \\ \partial_z a_{N-1} & \partial_z a_N & \cdots & \partial_z a_{2N-2} \end{pmatrix}$$
$$+\begin{pmatrix} 0 & a_0^2 & \cdots & \displaystyle\sum_{k=0}^{N-2} a_k a_{N-k-2} \\ a_0^2 & a_0a_1+a_1a_0 & \cdots & \displaystyle\sum_{k=0}^{N-1} a_k a_{N-k-1} \\ \displaystyle\sum_{k=0}^{N-2} a_k a_{N-k-2} & \displaystyle\sum_{k=0}^{N-1} a_k a_{N-k-1} & \cdots & \displaystyle\sum_{k=0}^{2N-3} a_k a_{2N-k-3} \end{pmatrix}. \tag{49}$$

The above second term is separated as

$$\begin{pmatrix} 0 & a_0^2 & \cdots & \displaystyle\sum_{k=0}^{N-2} a_k N_{-k-2} \\ 0 & a_0a_1 & \cdots & \displaystyle\sum_{k=0}^{N-2} a_k a_{N-k-1} \\ \vdots & \vdots & \vdots & \vdots \\ 0 & a_0a_{N-1} & \cdots & \displaystyle\sum_{k=0}^{N-2} a_k a_{2N-k-3} \end{pmatrix}$$
$$+\begin{pmatrix} 0 & 0 & \cdots & 0 \\ a_0^2 & a_1a_0 & \cdots & a_{N-1}a_0 \\ \vdots & \vdots & \cdots & \vdots \\ \displaystyle\sum_{k=0}^{N-2} a_k a_{N-k-2} & \displaystyle\sum_{k=1}^{N-1} a_k a_{N-k-1} & \cdots & \displaystyle\sum_{k=N-1}^{2N-3} a_k a_{2N-k-3} \end{pmatrix}. \tag{50}$$

Each of these terms gives zero contribution in Eq. (47). Hence we have proved lemma 6.4. □

Next we have:

Lemma 6.5:

$$\sigma_{N\square\square}+\sigma_{N\square}=\left(\frac{d^2}{dz^2}+z\right)\sigma_N, \tag{51}$$

$$\sigma_{N\square\square}-\sigma_{N\square}=(2N-1)z\sigma_N. \tag{52}$$

Proof: We consider

$$\sigma_{N\square\square}+\sigma_{N\square}=\begin{pmatrix} a_1 & a_2 & \cdots & a_{N-1} & a_{N+1} \\ a_2 & a_3 & \cdots & a_N & a_{N+2} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ a_N & a_{N+1} & \cdots & a_{2N-2} & a_{2N} \end{pmatrix}\cdot\begin{pmatrix} \Delta_{\square 11} & \Delta_{\square 12} & \cdots & \Delta_{\square 1N} \\ \Delta_{\square 21} & \Delta_{\square 22} & \cdots & \Delta_{\square 2N} \\ \vdots & \vdots & \ddots & \vdots \\ \Delta_{\square N1} & \Delta_{\square N2} & \cdots & \Delta_{\square NN} \end{pmatrix}, \tag{53}$$

where $\Delta_{\square ij}$ is (i,j) cofactor of $\sigma_{N\square}$. The first matrix in the right-hand side is equal to

$$\begin{pmatrix} \partial_z a_0 & \partial_z a_1 & \cdots & \partial_z a_{N-2} & \partial_z a_N \\ \partial_z a_1 & \partial_z a_2 & \cdots & \partial_z a_{N-1} & \partial_z a_{N+1} \\ \vdots & \vdots & \vdots & \vdots & \\ \partial_z a_{N-1} & \partial_z a_N & \cdots & \partial_z a_{2N-3} & \partial_z a_{2N-1} \end{pmatrix}$$
$$+\begin{pmatrix} 0 & a_0^2 & \cdots & \sum_{k=0}^{N-3} a_k a_{N-k-3} & \sum_{k=0}^{N-1} a_k a_{N-k-1} \\ 0 & a_0 a_1 & \cdots & \sum_{k=0}^{N-3} a_k a_{N-k-2} & \sum_{k=0}^{N-1} a_k a_{N-k} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & a_0 a_{N-1} & \cdots & \sum_{k=0}^{N-3} a_k a_{2N-k-4} & \sum_{k=0}^{N-1} a_k a_{2N-k-2} \end{pmatrix}$$
$$+\begin{pmatrix} 0 & 0 & \cdots & 0 & 0 \\ a_0^2 & a_1 a_0 & \cdots & a_{N-2} a_0 & a_N a_0 \\ \vdots & \vdots & \cdots & \vdots & \vdots \\ \sum_{k=0}^{N-2} a_k a_{N-k-2} & \sum_{k=1}^{N-1} a_k a_{N-k-1} & \cdots & \sum_{k=N-2}^{2N-4} a_k a_{2N-k-4} & \sum_{k=N}^{2N-2} a_k a_{2N-k-2} \end{pmatrix}. \tag{54}$$

Taking the scalar product, the first and second terms give $\partial_z \sigma_{N\square}$ and $a_0\sigma_N$, respectively, and the third term vanishes. Hence we have

$$\sigma_{N\square\square}+\sigma_{N\square}=\left(\frac{d^2}{dz^2}+z\right)\sigma_N. \tag{55}$$

Next we consider the following equality:

$$\sigma_{N\square\square}-\sigma_{N\square}=\begin{pmatrix} a_2 & a_3 & \cdots & a_{N+1} \\ a_3 & a_4 & \cdots & a_{N+2} \\ \vdots & \vdots & \ddots & \vdots \\ a_{N+1} & a_{N+2} & \cdots & a_{2N} \end{pmatrix}\cdot\begin{pmatrix} \Delta_{11} & \Delta_{12} & \cdots & \Delta_{1N} \\ \Delta_{21} & \Delta_{22} & \cdots & \Delta_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ \Delta_{N1} & \Delta_{N2} & \cdots & \Delta_{NN} \end{pmatrix}. \tag{56}$$

The first matrix of the right-hand side of Eq. (56) is rewritten as

$$\begin{pmatrix} \partial_z a_1 & \partial_z a_2 & \cdots & \partial_z a_N \\ \partial_z a_2 & \partial_z a_3 & \cdots & \partial_z a_{N+1} \\ \vdots & \vdots & \ddots & \vdots \\ \partial_z a_N & \partial_z a_{N+1} & \cdots & \partial_z a_{2N-1} \end{pmatrix}+\begin{pmatrix} a_0^2 & a_0a_1+a_1a_0 & \cdots & \sum_{k=0}^{N-1} a_k a_{N-k-1} \\ a_0a_1 & a_0a_2+a_1a_1 & \cdots & \sum_{k=0}^{N-1} a_k a_{N-k} \\ \vdots & \vdots & \vdots & \vdots \\ a_0a_{N-1} & a_0a_N+a_1a_{N-1} & \cdots & \sum_{k=0}^{N-1} a_k a_{2N-k-2} \end{pmatrix}$$

$$+\begin{pmatrix} 0 & 0 & \cdots & 0 \\ a_1a_0 & a_2a_0 & \cdots & a_Na_0 \\ \vdots & \vdots & \cdots & \vdots \\ \sum_{k=1}^{N-1} a_k a_{N-k-1} & \sum_{k=2}^{N} a_k a_{N-k} & \cdots & \sum_{k=N}^{2N-2} a_k a_{2N-k-2} \end{pmatrix}. \tag{57}$$

Here, we note that a_n's also satisfy

$$\partial_z a_{n+1}=2na_{n-1}, \tag{58}$$

which is proved by induction from Eqs. (41) and (42). The first term of the right hand side of Eq. (57) is rewritten by using Eq. (58) as

$$\begin{pmatrix} 0 & 2a_0 & \cdots & 2(N-1)a_{N-2} \\ 0 & 2a_1 & \cdots & 2(N-1)a_{N-1} \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 2a_{N-1} & \cdots & 2(N-1)a_{2N-3} \end{pmatrix}$$

$$+\begin{pmatrix} 0 & 0 & \cdots & 0 \\ 2a_0 & 2a_1 & \cdots & 2a_{N-1} \\ \vdots & \vdots & \cdots & \vdots \\ 2(N-1)a_{N-2} & 2(N-1)a_{N-1} & \cdots & 2(N-1)a_{2N-3} \end{pmatrix}. \tag{59}$$

Applying the scalar product on these terms, we obtain

$$\sigma_{N\square\square}-\sigma_{N\square}=(2N-1)z\sigma_N. \tag{60}$$

Hence we have proved lemma 6.5.

Continuing the similar argument, we get the following shift operators.

Lemma 6.6:

$$\sigma_{N\square\square\square}+2\sigma_{N\square\square}+\sigma_{N\begin{smallmatrix}\square\\\square\end{smallmatrix}}=\left(\frac{d^3}{dz^3}+3z\frac{d}{dz}+1\right)\sigma_N, \tag{61}$$

$$\sigma_{N\square\square\square}-\sigma_{N\begin{smallmatrix}\square\\\square\end{smallmatrix}}=\left((2N-1)z\frac{d}{dz}+(2N+1)\right)\sigma_N, \tag{62}$$

$$\sigma_{N\square\square\square}-\sigma_{N\square\square}+\sigma_{N\begin{smallmatrix}\square\\\square\end{smallmatrix}}=\left(2z\frac{d}{dz}+2(N^2+N-1)\right)\sigma_N. \tag{63}$$

Finally, we prove proposition 6.2. From the Plücker relations, we have

$$\sigma_{N+1\begin{smallmatrix}\square\\\square\end{smallmatrix}}\sigma_N-\sigma_{N+1\square}\sigma_{N\square}+\sigma_{N+1}\sigma_{N\square\square}=0, \tag{64}$$

$$\sigma_{N+1\square\square}\sigma_N-\sigma_{N+1\square\square}\sigma_{N\square}+\sigma_{N+1}\sigma_{N\square\square\square}=0, \tag{65}$$

which are essentially the same as the bilinear equations (15) and (16) for $\tau_{N,\mathrm{KP}}$. By using lemmas 6.4, 6.5, and 6.6, we get

$$D_z^2\sigma_{N+1}\cdot\sigma_N=0, \tag{66}$$

$$(D_z^3+4zD_z-4(N+1))\sigma_{N+1}\cdot\sigma_N=0, \tag{67}$$

which are the desired result. Thus we have proved proposition 6.2.

VII. CONCLUDING REMARKS

In this article, we have presented two types of determinant representations for the rational solutions of $\mathrm{P_{II}}$. The Devisme polynomial representation follows from the reduction procedure of modified KdV equation and the Hankel determinant representation is obtained from the Toda lattice equation, namely the Bäcklund transformation of the solution of $\mathrm{P_{II}}$. These determinant structures of the rational solutions of $\mathrm{P_{II}}$ exactly reflect the Wronskian structure of the solution of KP hierarchy and Toda lattice equation. The relationship between those two representations is not clear yet. At least, it seems that there is no simple transformation relating the two representations.

It is known that the Airy function type solutions of $\mathrm{P_{II}}$ are expressed as[1]

$$v=\frac{d}{dz}\log\frac{\rho_{N+1}}{\rho_N}, \tag{68}$$

$$\rho_N=\begin{vmatrix} \mathrm{Ai} & \frac{d}{dz}\mathrm{Ai} & \cdots & \frac{d^{N-1}}{dz^{N-1}}\mathrm{Ai} \\ \frac{d}{dz}\mathrm{Ai} & \frac{d^2}{dz^2}\mathrm{Ai} & \cdots & \frac{d^N}{dz^N}\mathrm{Ai} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{d^{N-1}}{dz^{N-1}}\mathrm{Ai} & \frac{d^N}{dz^N}\mathrm{Ai} & \cdots & \frac{d^{2N-2}}{dz^{2N-2}}\mathrm{Ai} \end{vmatrix}, \tag{69}$$

where Ai is the Airy function satisfying

$$\frac{d^2}{dz^2}\mathrm{Ai}=z\,\mathrm{Ai}. \tag{70}$$

Then v satisfies P_{II},

$$\frac{d^2v}{dz^2} = 2v^3 - 2zv + (2N+1). \tag{71}$$

In Ref. 12, it was shown that the τ function (69) can be reduced from that of the KP hierarchy (12).

In the theory of KP hierarchy, an important fact is that we can introduce the τ function which is expressed in terms of determinant. Based on this fact, we can identify the solution space, and the KP hierarchy is regarded as the dynamical system on the infinite dimensional Grassmann manifold. P_{II} is obtained from the similarity reduction of the modified KdV equation, but the parameter of the equation appears as the integration constant, which means that P_{II} has the information of various boundary conditions of the modified KdV equation. From this observation, it looks that one cannot expect such beautiful structures in the solution space of P_{II}. Nevertheless, the results in this article may imply that at least for the special function type solutions and the rational solutions, such structures in the solutions of KP hierarchy may survive through the reduction. It may be an interesting problem to investigate the determinant structures for other Painlevé equations. So far, this is completely an open problem.

Recently, discrete versions of the Painlevé equations have been proposed through the singularity confinement test.[13] As for the solutions, some of them admit discrete or q-difference analog of special function type solutions expressed by determinants.[14,15] Moreover, it was reported that the discrete Painlevé II equation admits rational solutions with determinant structure.[16] We might expect that through such determinant structures of solutions, similarity reductions[17] deriving the discrete Painlevé equations from discrete KP (or Toda) would become more transparent, as we have seen in the continuous P_{II} case.

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The separability ''theorem'' in terms of distributions with discussion of electromagnetic scattering theory

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The separability theorem states that, given a linear partial differential equation and special coordinates allowing to find a family of separated solutions, all solutions of physical interest of the equations can be obtained from linear combinations of the separated solutions. In developing the theory of interaction between an infinite cylinder and a Gaussian beam, it has been recently observed that the theorem may fail in terms of functions. In this paper, it is shown that the separability theorem is recovered if solutions are expressed in terms of distributions instead of in terms of functions. Relevance to light scattering theory is discussed. © *1996 American Institute of Physics.* [S0022-2488(96)02709-0]

I. INTRODUCTION

In many fields of physics and, in particular in light scattering theory, we have to deal with linear partial differential equations of the form

$$A\psi = F \tag{1}$$

in which ψ is a scalar (or a vector) field depending on coordinates and time, A is a differential operator, and F a function. The quantities A and F are known, and the field ψ is unknown.

Let us restrict our attention to homogeneous equations defined by $F=0$. Then, if we possess a set $\{\psi_i\}$, $i=1,\ldots,N$ of solutions of the equation, it appears that any linear combination ψ of the solutions is also a solution

$$\psi = \sum_{i=1}^{N} \alpha_i \psi_i . \tag{2}$$

For convenience, let us focus our attention to 3D spaces spanned by coordinates $\{x_i\}$, $i=1,2,3$. In some cases, i.e., for some equations, it is possible to find so-called separable coordinate systems in which there exists a family of separated solutions reading as

$$\psi = X_1(x_1)X_2(x_2)X_3(x_3). \tag{3}$$

Let ψ_i be a member of the family. Then the separability theorem states[1] that ''all solutions of the partial differential equation can be built up out of linear combinations of the members of the family of separated solutions,'' i.e., ''once we have computed the separated solutions, we can obtain the rest.'' Notice that no condition on the solutions is stated, so that one should not understand this statement as a theorem in the usual meaning but as a property shared by all solutions of interest in theoretical physics; this is why we may write down ''theorem'' instead of theorem.

In this paper, we deal with the theory of interaction between shaped electromagnetic beams (for example Gaussian laser beams) and regular particles (emphasizing the case of infinite cylinders). Under these circumstances, the equation to consider is the Bromwich scalar potential equation. The interaction between shaped beams and spheres (generalized Lorenz–Mie theory, GLMT, Refs. 2–3 and references therein) or stratified spheres[4] has been successfully derived by using the separability theorem in terms of functions. In developing the theory of interaction between shaped beams and infinite cylinders, it has, however, been observed that the same mathematical framework could not be used. In particular, the description of the incident Gaussian beam introduced scalar potentials which, in terms of functions, did not satisfy the separability theorem.[5] This fact induced considerable difficulties in building a complete theory, in particular when handling electromagnetic boundary conditions at the surface of the cylinder.[6] Revisiting the separability theorem, many solutions which do not satisfy the separability theorem in terms of functions have been exhibited for the Bromwich scalar potential and for the scalar wave equations, in both spherical and cylindrical coordinate systems.[7] Let us call them exotic solutions.

In this paper, it is shown that the separability theorem may, however, be recovered if the class of admissible solutions is extended from functions to distributions.[8,9] As a consequence, the theory of interaction between shaped beams and infinite cylinders has been afterward successfully developed by using this extended framework.[10–13]

The paper is organized as follows. Section II presents the Bromwich scalar potentials and their general solutions in terms of functions, relying on the separability theorem, in cylindrical coordinates. A counterexample in terms of functions is given. Section III discusses general solutions in terms of distributions and the aforementioned counterexample is shown to satisfy the separability theorem in that extended framework. Relevance to light scattering is discussed. Section IV is a conclusion.

II. THE SEPARABILITY THEOREM IN TERMS OF FUNCTIONS FOR THE BROMWICH SCALAR POTENTIAL EQUATION

A. Bromwich scalar potentials

Let us consider orthogonal curvilinear coordinates $\{x_i\}$ such as the infinitesimal Riemannian distance ds between two points $[x_i(P)]$ and $[x_i(P)+dx_i]$ reads as

$$ds^2=\sum_{n=1}^{3} e_n^2 (dx_n)^2 \tag{4}$$

in which coefficients e_n are called scale factors.

Let us furthermore assume that the scale factors satisfy the following conditions:

$$e_1=1, \tag{5}$$

$$\frac{\partial}{\partial x_1}\left(\frac{e_1}{e_3}\right)=0. \tag{6}$$

Then we may define Bromwich scalar potentials (BSP), denoted by U, which are solutions of the partial derivative equation[14–16]

$$\frac{\partial^2 U}{\partial x_1^2}+\frac{1}{e_2 e_3}\left[\frac{\partial}{\partial x_2}\left(\frac{e_3}{e_2}\frac{\partial U}{\partial x_2}\right)+\frac{\partial}{\partial x_3}\left(\frac{e_2}{e_3}\frac{\partial U}{\partial x_3}\right)\right]+k^2 U=0. \tag{7}$$

In light scattering theory, BSPs play a dominant role because, once they are known, they allow the determination of electric E_i and magnetic fields H_i by using a set of derivative operators,

here symbolically written as $\hat{d}U \rightarrow (E_i, H_i)$. Maxwell's equations are equivalent to Rel. (7) supplemented by the set $\hat{d}U$. Let us note that, within the set of 11 separable coordinate systems for the wave equation, there are only 6 coordinate systems satisfying conditions (5) and (6), including spherical and cylindrical coordinates (Ref. 1).

B. Cylindrical coordinates

In cylindrical coordinates

$$\{x_i\} = \{z, \rho, \varphi\}, \tag{8}$$

$$ds^2 = dz^2 + d\rho^2 + \rho^2 \, d\varphi^2, \tag{9}$$

the BSP equation reads as

$$\frac{\partial^2 U}{\partial z^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} \rho \frac{\partial U}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2 U}{\partial \varphi^2} + k^2 U = 0 \tag{10}$$

which, in contrast with the case of spherical coordinates, identifies with the wave equation.[7] Separability is achieved by setting

$$U(z, \rho, \varphi) = U_1(z) U_2(\rho) U_3(\varphi). \tag{11}$$

Assuming a 2π periodicity with respect to φ, looking for solutions which are finite in whole space, and considering the description of shaped beams propagating in free space (i.e., the solutions must be defined at $\rho = 0$), it is then found that, in terms of functions, the general solution of Rel. (11) is the summation over all separated solutions reading as[5–7]

$$U = e^{ik\gamma z} \sum_{m=-\infty}^{+\infty} A_m J_m(k\rho\sqrt{1-\gamma^2}) e^{im\varphi} \tag{12}$$

in which $(k\gamma)$ pertains to the real field. Actually, the form of Rel. (12) is general enough to our purpose but is not the most general form in terms of functions. First, we may add a γ spectrum made of a combination of a discrete and of a continuous contribution. Physically, however, in studying the interaction between a Gaussian beam and an infinite cylinder, it is found that the γ spectrum contains one single peak. In particular, if the Gaussian beam is perpendicularly incident on the cylinder, we have $\gamma = 0$.[5,6] Therefore, we shall be content with Rel. (12) in this paper.

Second it is also interesting to note what would happen if we relaxed the condition that solutions should be finite in whole space. Then, we would have to accept solutions diverging exponentially or linearly with respect to z when $z \rightarrow \pm\infty$.[7]

For $\gamma = 0$, i.e., in the case of a Gaussian beam perpendicularly incident on an infinite cylinder, Rel. (12) reduces to

$$U = \sum_{m=-\infty}^{+\infty} A_m J_m(R) e^{im\varphi} \tag{13}$$

in which we use the rescaled coordinate $R = k\rho$. However, the structure given by Rel. (13) is not sufficient to describe the Gaussian beam. Instead, it is found that we may have to deal with BSPs of the form[5,6]

$$U = (Z^2 + iR \cos \varphi) e^{iR \cos \varphi} \tag{14}$$

which is equivalent to

$$U=(Z^2+iR\ \cos\ \varphi)\sum_{m=-\infty}^{+\infty} i^m J_m(R)e^{im\varphi} \tag{15}$$

in which $Z=kz$ is a rescaled coordinate. The BSP U is then equal to a Σ-separable BSP of the form given by Rel. (13) multiplied by a modulation prefactor $(Z^2+iR\ \cos\ \varphi)$. The BSP given by Rel. (15) is a non-Σ-separable solution in terms of functions. Let us note that U diverges quadratically with respect to Z when $z\to\pm\infty$. Such a behavior cannot be recovered by relaxing the condition that solutions are finite in whole space because this would lead to exponential or linear divergence when $z\to\pm\infty$ [see comments following Rel. (12)], not to quadratic divergence.

III. THE SEPARABILITY THEOREM IN TERMS OF DISTRIBUTIONS

We now show that the separability theorem is recovered if we extend the class of solutions from functions to distributions.

Let us again consider the BSP equation (10) in cylindrical coordinates and look for solutions which are temperated distributions with respect to z.

Because any temperated distribution possesses a Fourier transform which is a temperated distribution too,[8,9] we may evaluate the Fourier transform of Rel. (10). For convenience, the Fourier transform of the distribution U is here defined by

$$\hat{U}(\gamma,\rho,\varphi)=\mathscr{F}_z[U](\gamma) \tag{16}$$

in which, for a function $U(z,\rho,\varphi)$, we have

$$\mathscr{F}_z[U](\gamma)=\int U(z,\rho,\varphi)e^{-ik\gamma z}\ dz. \tag{17}$$

Then the Fourier transform $\hat{U}$ satisfies the equation

$$\frac{1}{\rho}\frac{\partial}{\partial\rho}\ \rho\ \frac{\partial\hat{U}}{\partial\rho}+\frac{1}{\rho^2}\frac{\partial^2\hat{U}}{\partial\varphi^2}+k^2(1-\gamma^2)\hat{U}=0. \tag{18}$$

Demanding that U be 2π periodic with respect to φ, we then have

$$\hat{U}(\gamma,\rho,\varphi)=\sum_m\ C_m(\gamma,\rho)e^{im\varphi} \tag{19}$$

in which $C_m(\gamma,\rho)$ is a distribution.

Inserting Rel. (19) in Rel. (18) shows that the distribution $C_m(\gamma,\rho)$ must satisfy

$$\rho^2\ \frac{\partial^2 C_m}{\partial\rho^2}+\rho\ \frac{\partial C_m}{\partial\rho}+[k^2(1-\gamma^2)\rho^2-m^2]C_m=0,\quad \forall_m \tag{20}$$

which is the Bessel equation whose solutions are taken as

$$C_m(\gamma,\rho)=a_m(\gamma)J_m(k\rho\sqrt{1-\gamma^2}) \tag{21}$$

in which $a_m(\gamma)$ is a distribution.

Therefore,

$$\hat{U}(\gamma,\rho,\varphi)=\sum_m\ a_m(\gamma)J_m(k\rho\sqrt{1-\gamma^2})e^{im\varphi} \tag{22}$$

which is Σ-separable in terms of distributions. The distribution U is, therefore, Σ-separable too and reads as

$$U(z,\rho,\varphi)=\sum_m \mathscr{F}_\gamma^{-1}[a_m(\gamma)J_m(k\rho\sqrt{1-\gamma^2})](z)e^{im\varphi}. \tag{23}$$

As an example, let us consider the BSP given by Rel. (15). The cos φ term may be rewritten as

$$U_{\cos}=\frac{1}{2}R\sum_{m=-\infty}^{+\infty} i^m e^{im\varphi}[J_{m-1}(R)-J_{m+1}(R)]=R\sum_{m=-\infty}^{+\infty} i^m e^{im\varphi}J'_m(R), \tag{24}$$

leading to

$$U=\sum_{m=-\infty}^{+\infty} i^m e^{im\varphi}[Z^2J_m(R)+RJ'_m(R)]. \tag{25}$$

On the other hand, Rel. (12) generalizes in terms of distributions to

$$U=\sum_m e^{im\varphi}\langle A_m(\gamma),J_m(R\sqrt{1-\gamma^2})e^{i\gamma Z}\rangle. \tag{26}$$

From Rels. (25) and (26), the distribution $A_m(\gamma)$ is the solution of the equation

$$\langle A_m(\gamma),J_m(R\sqrt{1-\gamma^2})e^{i\gamma Z}\rangle=i^m[Z^2J_m(R)+RJ'_m(R)]. \tag{27}$$

Now, the fact that γ is equal to 0 in terms of functions means that the γ spectrum is $\{0\}$, i.e., that the support of the distribution $A_m(\gamma)$ is $\{0\}$. However, we possess the following theorem: A distribution of support $\{0\}$ reads as

$$T=\sum_{k=0}^{N} a_k\delta^{(k)} \tag{28}$$

in which $a_k\in C$ and $\delta^{(k)}$ is the kth derivative of the Dirac distribution (the reciprocal statement is also true). It is then found that the distribution $A_m(\gamma)$ is of the form given by Rel. (28) and reads as

$$A_m(\gamma)=-i^m\delta''(\gamma). \tag{29}$$

Indeed, we check that

$$\begin{aligned}\langle A_m(\gamma),J_m(R\sqrt{1-\gamma^2})e^{i\gamma Z}\rangle&=-i^m\langle\delta''(\gamma),J_m(R\sqrt{1-\gamma^2})e^{i\gamma Z}\rangle\\&=-i^m(J_m(R\sqrt{1-\gamma^2})e^{i\gamma Z})''_{\gamma=0}\\&=i^m[Z^2J_m(R)+RJ'_m(R)].\end{aligned} \tag{30}$$

Therefore, the separability theorem is recovered in terms of distributions.

IV. CONCLUSION

We examined the Bromwich scalar equation and the wave equation in cylindrical coordinates, in which case both equations identify, and demonstrated that the separability theorem is always

satisfied if solutions are expressed in terms of distributions rather than in terms of functions. In light scattering theory, we then obtain an extended framework allowing to study the interaction between an infinite cylinder and a Gaussian beam,[10–12] more generally an arbitrary shaped beam.[13]

In Ref. 7, we also exhibited exotic solutions in spherical coordinates. The effort required to understand the nature of these solutions appears to be significantly more important than in cylindrical coordinates, an issue which is therefore not clarified at the present time. However, from the point of view of light scattering, exotic solutions in spherical coordinates are of dubious interest in so far as the theory of interaction between spheres and shaped beams can be fully developed by using only nonexotic solutions.[2–4]

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Remarks on the universal central extension of sdiff(T^2)$_{loc}$

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In a paper by C. N. Pope and K. S. Stelle [Phys. Lett. B **226**, 257–263 (1989)], it was shown that the algebra of local area-preserving diffeomorphisms on the torus is equivalent to su(∞). In this paper we present a few remarks on the universal central extension of this infinite dimensional Lie algebra, and construct, for this case, in analogy to the situation in which the affine Lie algebra has an underlying finite-dimensional Lie algebra, the nontrivial universal central extension. © *1996 American Institute of Physics.* [S0022-2488(96)01608-8]

I. INTRODUCTION

Let **I** be the closed unit interval [0,1], and **I**×**I** a topological space lying in the first quadrant of the $x-y$ plane so that two of its adjacent sides lie on the x and y axes of a two-dimensional coordinates system. Then the torus $S^1\times S^1=T^2$ (where $S^1=\{x\in\mathbb{R}^2 \| \|x\|=1\}$ is the one-sphere) is the quotient topological space obtained by making two identifications, i.e., by using an equivalence relation.[1] This involves first identifying the two parallel horizontal edges and subsequently the two vertical edges. We note that the first identification results in a space homeomorphic to the cylinder $S^1\times$**I**, while the second, which is the glueing of two circular edges together, results in the torus. Thus the torus is a polyhedron because of the existence of a triangulation, i.e., an ordered pair consisting of a simplicial complex (whose vertex set consists of the corners of **I**×**I**, i.e., the zero-simplices) and a homeomorphism from the underlying space of the complex to the topological space, the torus. We may note that other triangulations of **I**×**I** result in spaces of physical interest such as the real projective plane $\mathbb{R}P^2$ and the Klein bottle.

We may note that if M and N are C^∞ manifolds and f is a mapping of M into N, then f is called a diffeomorphism of M onto N if f is a one–one differentiable onto mapping and f^{-1} is also differentiable. The group of diffeomorphisms SDiff(D) on a compact Riemannian manifold D, such as the torus, has a subgroup S_0 Diff(D) consisting of volume-preserving diffeomorphisms leaving, for example, the center of mass of the torus fixed. This infinite-dimensional group, S_0 Diff(T^2) to be specific, was first studied by Arnold[2] in his research in hydrodynamics in which the aforementioned group is the configuration space of an ideal fluid filling the torus. This group corresponds to the Lie algebra on the torus of vector fields having zero divergence and such that the stream function is single valued. If one thinks of the elements of the Lie algebra as real-valued functions having zero as average value on the torus, and denotes, for simplicity, the Lie algebra of local area-preserving diffeomorphisms by sdiff(T^2)$_{\rm loc}$, such functions can be specified by their Fourier components.

Central extensions will be discussed in Sec. II. However, it was Schur[3] who first investigated the notion of a universal central extension when he was working on finite groups. After the pioneering work of Arnold, SDiff(T^2) manifested itself as the residual symmetry on relativistic two-dimensional membrane surfaces.[4] This residual symmetry of an extended object manifests itself in the light cone guage. The group has as its elements time-independent reparametrizations (with unit Jacobian) of the spatial coordinates φ^a, $a=1,2$, having the form[5,6]

$$\delta\varphi^a=\xi^a$$

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with

$$\partial\xi^a = 0.$$

One of the two classes of solutions of the latter equation comprises local exact solutions having the form

$$\xi^a = \epsilon^{ab}\partial_b\Lambda$$

while the other class consists of global harmonic solutions which correspond to simultaneously closed and coclosed one-forms, and whose finite number is given by the first Betti number b_1 of the manifold. The term Betti number will be explained in Sec. II.

The real functions (modulo a constant), for example, $f(\underline{\varphi}), g(\underline{\varphi})$ where $\underline{\varphi} = (\varphi_1, \varphi_2)$, identified with sdiff($T^2$) on the torus have the Poisson bracket as their Lie bracket:[4,7,8]

$$[f(\underline{\varphi}),\, g(\underline{\varphi})] = \frac{\partial f}{\partial\varphi_1}\frac{\partial g}{\partial\varphi_2} - \frac{\partial f}{\partial\varphi_2}\frac{\partial g}{\partial\varphi_1}.$$

The Lie algebra also has closed forms whose properties are given in Ref. 5. The formulation of a guage theory on SDiff(T^2) involves the introduction of guage fields $A_\mu^{\varphi_1\varphi_2}$, which takes values in sdiff(T^2). If $\mathbf{m} \in \mathbb{Z}^2\backslash\{0\}$, where $\mathbb{Z}$ is the set of all integers, and we employ the basis functions, $Y_m = -i\exp(i\mathbf{m}\underline{\varphi})$, then the commutation relation above involving the Poisson bracket becomes

$$[Y_m,\, Y_n] = \mathbf{m}\times\mathbf{n}Y_{m+n},$$

where $0 \neq \mathbf{m} = (m_1, m_2)$, $\mathbf{m}\times\mathbf{n} = m_1n_2 - n_1m_2$, $Y_m^\dagger = -Y_{-m}$, and $\underline{\varphi} = (\varphi_1, \varphi_2) \in [0, 2\pi]^2$. This new form of the Lie bracket can be viewed as a representation of the unextended Lie algebra.

Since the problem of the universal central extension of the sdiff(T^2) Lie algebra, i.e., of the Lie algebra connected with the two-brane, was solved essentially about six years ago, it is appropriate to mention, albeit in a very terse manner, the direction in which membrane theory has been propagating since then. The group manifold approach to the description of supersymmetric theories pioneered by T. Regge, Y. Ne'eman, R. D'Auria, and P. Frè, among others, exploits the advantages of both the superspace and the x-component formulation to supersymmetry while endeavouring to shy away from their disadvantages.

In Ref. 9 the parallel between superstrings and higher super p-membranes in d dimensions for $d \leqslant 11$ and $p \leqslant 5$ is highlighted. Here a geometric formulation of p-membrane theories results in a manifestly covariant Wess–Zumino term because this term is $(p+1)$-th order in the supersymmetric currents. Thus it was possible to generalize Siegle's reformulation[10] of the Green–Schwartz superstring to higher super p-membranes. Consequently, a super p-membrane theory is found to be associated with every new space–time superalgebra.

In Ref. 11, which parallels the approach in Ref. 12, the consideration of super p-branes is based on a generalized action principle. This approach derives its impetus from the need to unravel the origin and the geometrical meaning of the local fermionic κ-symmetry of super p-branes in the Green–Schwartz formulation, with the ultimate aim of being able to solve the problem of the covariant quantization of superstrings. One of the attempts at finding a solution to this problem is a variant of the twistorlike approach based on a superfield formulation of super p-branes in world superspace. One may also mention that in Ref. 9 extensions are based on the same gamma matrix theories underlying super p-brane theories. In Sec. II, we construct for su(∞), in analogy to the situation in which the affine Lie algebra has an underlying finite-dimensional algebra,[13] the nontrivial universal central extension.

II. THE UNIVERSAL CENTRAL EXTENSION

Central extensions of Lie algebras are discussed in a mathematical language in which such terms as (co)chains, (co)cycles, (co)boundaries, and (co)homology groups keep on recurring. Hence, we will first discuss the concepts from the point of view of singular homology theory,[1] which provides a graphic manner of perceiving these entities. One starts by defining the standard n-simplex Δ^n as the following subset of $\mathbb{R}^{n+1}$

$$\Delta^n=\left\{(x_1,x_2,\ldots,x_{n+1})\in\mathbb{R}^{n+1}\middle|\text{each } x_i\geqslant 0 \quad \text{and } \sum x_i=1\right\}.$$

It is then clear, for example, that Δ^0 is a point, Δ^1 is a closed interval, Δ^2 is a triangle (with interior), while Δ^3 is a (solid) tetrahedron. Linearly ordering the vertices is synonymous with an orientation of $\Delta^n=[e_0,e_1,\ldots,e_n]$. Suppose X is a topological space and Δ^n is the standard n-simplex. Then a singular n-simplex in X is a continuous mapping $\sigma:\Delta^n\to X$. Since Δ^1 is a closed interval which is homeomorphic to $\mathbf{I}$, a one-simplex is essentially a path in X, while Δ^0 is a point in X.

Suppose B is a subset of an additive Abelian group F. Then F is said to be free Abelian with B as basis if the cyclic group generated by each element $b\in B$ is infinite cyclic and F is a direct sum of these infinite cyclic groups for all $b\in B$. Let X be a topological space. Then for $n\geqslant 0$, $S_n(X)$ is defined as the free Abelian group having as basis all singular n-simplices in X, with $S_{-1}(X)\equiv 0$. We call the elements of $S_n(X)$ the singular n-chains in X. For $n>0$, let $\sigma:\Delta^n\to X$ be a continuous mapping. Then its boundary is denoted by $\partial_n\sigma\in S_{n-1}(X)$. Hence, for each $n\geqslant 0$, there exists a unique homomorphism $\partial_n:S_n(X)\to S_{n-1}(X)$ called a boundary operator.

For each topological space X, the following sequence of free Abelian groups and homomorphisms,

$$\cdots\to S_n(X)\overset{\partial_n}{\to}S_{n-1}(X)\to\cdots\to S_1(X)\overset{\partial_1}{\to}S_0(X)\overset{\partial_0}{\to}0,$$

is called a singular complex of X and is denoted by $S_*(X)$. For all $n\geqslant 0$, $\partial_n\partial_{n+1}=0$. The kernel of ∂_n, $\ker\partial_n$, is called the group of all singular n-cycles in X and is denoted by $Z_n(X)$, while the image of ∂_{n+1}, $\operatorname{im}\partial_{n+1}$, is called the group of singular n-boundaries and is denoted by $B_n(X)$. For every $n\geqslant 0$,

$$B_n(X)\subset Z_n(X)\subset S_n(X).$$

By definition, for each $n\geqslant 0$, the nth singular homology group, $H_n(X)$, of a space X is the quotient of the group $Z_n(X)$ by the group $B_n(X)$, i.e.,

$$H_n(X)=Z_n(X)/B_n(X)=\ker\partial_n/\operatorname{im}\partial_{n+1}$$

In the language of categories and functors, each homology group $H_n(X)$ is, in fact, the (homology) functor from the category of all topological spaces to the category of all Abelian groups. Suppose X and Y are homeomorphic topological spaces. Then $H_n(X)$ is isomorphic to $H_n(Y)$ as groups for all $n\geqslant 0$. Since $H_n(X)$ is now an invariant of the topological space X, the rank of $H_n(X)$, i.e., the cardinality of $H_n(X)$, becomes an invariant of X for each $n\geqslant 0$, and is called the nth Betti number of X.

It was shown in Ref. 14 that there are only two inequivalent su(∞) algebras, to which the local area-preserving algebras on the sphere and on the torus were shown in Ref. 5 to correspond. The Lie algebra sdiff(T^2) corresponds to letting the Dynkin diagram of A_l, whose compact real form is su$(l+1)$, simultaneously approach infinity at both ends. The corresponding Lie algebra su(∞),

unlike $\mathrm{su}_+(\infty)$ which corresponds to sdiff(S^2) where S^2 is the two-sphere, admits a central extension. In the theory of completely integrable systems, central extensions of affine Lie algebras of infinite rank play a prominent role.

If $\mathscr{G}$ is a Lie algebra, a central extension $\mathbf{E}$ of $\mathscr{G}$ by M is the short exact sequence[13]

$$0 \to M \xrightarrow{i} \mathbf{E} \xrightarrow{\pi} \mathscr{G} \to 0$$

such that M is in the center of $\mathbf{E}$. By the definition of a short exact sequence, the image of the mapping i (which is an injection) equals the kernel of the mapping π (which is a surjection). We note that in the extension of $\mathscr{G}$ by a $\mathscr{G}$-module M given by the above short exact sequence, M becomes a $\mathscr{G}$-module by setting, for each $g \in \mathscr{G}$ and $m \in M$,

$$gm = [\tilde{g}, m],$$

which is an element of $\mathscr{G}$ such that $\pi(\tilde{g}) = g$

In defining the universal central extension of a Lie algebra $\mathscr{G}$ one first notes that if

$$0 \to M' \xrightarrow{i'} \mathbf{E}' \xrightarrow{\pi'} \mathscr{G} \to 0$$

is another central extension, then a homomorphism over $\mathscr{G}$ from $\mathbf{E}$ to this second extension is a mapping $f: \mathbf{E} \to \mathbf{E}'$ such that $\pi = \pi' f$. Then $\mathbf{E}$ is a universal central extension if a unique homomorphism $f: \mathbf{E} \to \mathbf{E}'$ exists for every central extension $\mathbf{E}'$ of $\mathscr{G}$.

A Lie algebra is said to be perfect if it is equal to its derived algebra. In the finite-dimensional situation, it is well known that the classical Lie algebras A, B, C, D are perfect in this sense. If $K[t, t^{-1}]$ is the associative algebra of finite linear combinations of integral powers of t, and $\mathscr{G}$ is a finite-dimensional Lie algebra, the space $\mathscr{G} \otimes_K K[t, t^{-1}]$ is given a Lie algebra structure by the Lie bracket

$$[x \otimes t^m, y \otimes t^n] = [x, y] \otimes t^{m+n}, \quad x, y \in \mathscr{G}, \quad m, n \in \mathbb{Z}.$$

Hence the elements of this algebra are the Laurent polynomials $\Sigma x_i t^i$ with $x_i \in \mathscr{G}$, $m, n \in \mathbb{Z}$. If $U\mathscr{G}'$ is the universal enveloping algebra of $\mathscr{G}'$ (i.e., the tensor algebra quotiented by a two-sided ideal), the Chevalley–Eilenberg complex is $V_*(\mathscr{G}' \otimes_K K[t, t^{-1}])$ and equals $V_*(\mathscr{G}') \otimes_K K[t, t^{-1}]$. In the untwisted affine Lie algebra $\mathscr{G}$ corresponding to the limit as $l \to \infty$ of $\mathrm{su}(l+1)$ that we are considering, the Chevalley–Eilenberg complex still decomposes as

$$V_*(\mathscr{G}' \otimes_K K[t, t^{-1}]) = V_*(\mathscr{G}') \otimes_K K[t, t^{-1}].$$

If the sequence of homology groups similarly decomposes, i.e., if we have $H_*(\mathscr{G}' \otimes_K K[t, t^{-1}]) = H_*(\mathscr{G}', K) \otimes_K K[t, t^{-1}]$, we will be able to prove that the affine Lie algebra is perfect.

With $\kappa: \mathscr{G}' \times \mathscr{G}' \to K$ being the Killing form on $\mathscr{G}'$, the form

$$\beta\left(\sum x_i t^i, \sum x_j t^j \right) = \sum i \kappa(x_i, y_i)$$

is bilinear and alternating and therefore a cochain. If δ is the cohomology boundary operator, we have to show that the corresponding three-cochain is mapped to zero by δ by using the invariance $\beta(x, [yz]) = \beta([xy], z)$ of the Killing form. In fact, by substituting $x = \Sigma x_i t^i$, $y = \Sigma y_j t^j$, and $z = \Sigma z_k t^k$, one finds that

$$\delta\beta(x, y, z) = -\beta([xy], z) + \beta([xz], y) - \beta([yz], x) = 0.$$

This implies that the class $[\beta]$ of all two-cocycles is an element of $H^2(\mathscr{G}'\otimes_K K[t,t^{-1}],K)$ with the following corresponding central extension:

$$0\to K\to \hat{\mathscr{G}}'\overset{\pi}{\to}\mathscr{G}'\otimes_K K[t,t^{-1}]\to 0.$$

To show that $\hat{\mathscr{G}}'$ is perfect, one starts with the exact sequence immediately above, and considers the vector space splitting σ of π corresponding to the two-cocycle β. Thus π has a Lie algebra section σ such that $\mathscr{G}'\otimes_K K[t,t^{-1}]\overset{\sigma}{\to}\hat{\mathscr{G}}'$. This vector space splitting enables us to show that $\hat{\mathscr{G}}'$ is perfect, by showing that $[\hat{\mathscr{G}}',\hat{\mathscr{G}}']$ maps onto $\hat{\mathscr{G}}'$, which itself is perfect.

If $K=\mathbb{C}$, there is an element $c\in\mathbb{C}$, such that the short exact sequence immediately above is an extension of $\mathscr{G}'\otimes_K K[t,t^{-1}]$. The universal central extension is the direct sum of $c\mathbb{C}$ and $\mathscr{G}'\otimes_K K[t,t^{-1}]$, and corresponds to the central extension which is a sum of simple coroots in Ref. 14.

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Identifying conical singularities

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A method based upon the concept of holonomy of a metric space–time (M,g), in order to identify the presence of conical singularities in M is proposed. The validity and usefulness of this so-called holonomy method is proven by applying it to a set of four-dimensional space–times and one three-dimensional space–time. The holonomy method predictions are confirmed by the comparison with the predictions obtained after coordinate transformations which take the metrics g, to a new basis where the global properties of conical singularities are explicitly seen. © *1996 American Institute of Physics.* [S0022-2488(96)03209-4]

I. INTRODUCTION

Conical singularities have been known to physicists for a long time.[1] During the 60's and 70's, when a great deal of work was done to understand and classify all types of singularities, the properties and geometrical nature of the conical singularities became better understood (for a review on the results in singularities see Ref. 2).

From these works, we learned that for a space–time M with a metric tensor $g(M,g)$, if there is a conical singularity in M, all scalars formed out of the Riemann tensor are bounded in M, and the presence of this singularity can only be revealed by means of a global procedure.[2] Because of the good behavior of the scalars mentioned above, the conical singularities belong to a type of singularities called quasiregular singularities.[2,3] A more recent interest in conical space–times developed after two important results; the first due to Kibble, and the second to Vilenkin.

Kibble showed in Ref. 4, that the mechanisms of symmetry breaking and symmetry restoration in gauge theories, necessarily, led to the formation of topological defects in the early universe. Among the possible types of defects are the cosmic strings. Inspired by Kibble's ideas Vilenkin demonstrated, among other things in Ref. 5, that the space–time geometry due to a static, infinite, unidimensional string, with a finite linear energy density, in the weak field approximation, is a conical space–time.

Cosmic strings have attracted greater attention than the other types of defects not only because the others have some undesirable properties,[6] but by their own observable effects.[7] Among these effects one may mention the gravitational lensing of light from distant galaxies or quasars, a significant effect on the motion of massive particles, frequency shifts of photons passing by the string and its possible role in the mechanism of galaxy formation (see Ref. 7 for a complete list of observable effects).

From the above discussion one can conclude that conical singularities are very important either on a more formal study of the space–time structure as well as in processes in the early universe leading to presently observable phenomena. One very proper question, at this stage, would be how to identify the presence of conical singularities in a given metric space–time. In fact, there is not a general method of determining whether a metric space–time (M,g), has a conical singularity or not.

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What one usually does, in order to identify the conical singularity in (M,g), is determining whether one of the angular variables, in g, which by definition would vary in the range $[0,2\pi]$ has its range reduced.[8] The amount which is missing to complete 2π is called deficit angle. If a given space–time has a singular point and all the properties of a conical space–time, as described above,[2] but all the relevant angular variables have their normal range, one may try to find a coordinate transformation which reveals the presence of a deficit angle in one of these angular variables range,[9] or construct a particular demonstration of the regularity, or not, of the metric space–time under investigation.[10]

In this paper we would like to propose a method of identifying if a given metric space–time, singular in one point, and with all the properties of a conical space–time, is indeed a conical space–time. This method will use the concept of holonomy group of a space–time (therefore we shall call it holonomy method), and the global and local properties of a conical singularity.

In the next section, Sec. II, we shall introduce the holonomy method. Sec. III is devoted to the application of the holonomy method to four-dimensional space–times which are known to be conical space–times. In Sec. IV, we investigate a three-dimensional metric space–time with a conical singularity which cannot be trivially identified unless we use the holonomy method. Finally, in Sec. V, we conclude by outlining the main results of the paper and commenting on other applications of the holonomy method.

II. DESCRIPTION OF THE HOLONOMY METHOD

Our method will be based in the application of the concept of holonomy,[11] to the space–time being studied. The holonomy group of a space–time M, equipped with a metric g, (M,g) (therefore with an affine connection Γ), is defined as the linear transformations from the tangent space at the point p, T_pM, to itself, constructed by taking a fiducial vector v and parallel transporting it along all closed curves starting and finishing at p. For a space–time, the set of all linear transformations generated by the parallel transport of v along all possible closed curves from p, is called the holonomy group of M at p. In fact, we shall not be interested in computing the holonomy group of the given space–time but we shall use this concept in a related way.

Suppose that the metric g of M is apparently singular at a point s, and all scalars formed out of the Riemann curvature are well behaved in M. Then, for a fiducial vector v in M, we shall evaluate the transformation generated by the parallel transport of v around closed loops. This transformation is a matrix which we call holonomy matrix (H), its elements are functions of the coordinates. For a point p belonging to a closed loop C, both in M, the holonomy matrix at p, and around C, relates the initial value of v at T_p with the value of v, again at T_p, but now after it has completed a full loop around C. The closed loops are defined in order to converge to the apparently singular point s, of M. The convergence of the loops to s is specified by a certain limit of the coordinates describing these loops.

Now, after having computed the holonomy matrix we apply to it the same limit of the coordinates which cause the closed loops to converge to the apparently singular point s. Then, if the point s is regular, the limit of the holonomy matrix defined by the parallel transport of the fiducial vector v around closed loops must be the identity matrix. In other words, the limit of the initial and final values of the vector v at s must be the same. If this is not the case, the space–time is non-regular at s, or it has a conical singularity.

Let us now apply this method to two different types of space–times: The first is composed of space–times where one may trivially identify the presence of conical singularities; the second is a space–time with a conical singularity which cannot be trivially identified unless we use the holonomy method.

III. APPLICATION TO CONICAL SPACE–TIMES

We shall consider here a set of three four-dimensional space–times with a conical singularity. Although we shall treat them together because of their similar metric expressions, they have distinct topologies and curvature scalars **R**. The general metric expression is

$$ds^2=\eta\, dt^2+dz^2+dr^2+\mu^2F^2(r)d\theta^2, \tag{1}$$

where $-\infty<t<\infty$, $-\infty<z<\infty$, $r_{\min}<r<r_{\max}$, $0\leqslant\theta\leqslant 2\pi$; μ is a number which is in the range, $0<\mu\leqslant 1$; $F(r)$ is a function of r without numerical coefficients with the property that, $F(r=r_0)=0$ for a $r_0\in[r_{\min},r_{\max}]$; η may be either -1, which means a Lorentzian signature, or $+1$, which means an Euclidean signature; and the range of r depends on which space–time we are considering. Some remarks are now in order.

It is important to note that the angular variable must vary over the full range $[0,2\pi]$, otherwise we would identify the presence of a conical singularity by inspection. If μ was allowed to be greater than one, after a coordinate transformation of the type

$$\mu\theta\rightarrow\tilde{\theta}, \tag{2}$$

the new angular variable $\tilde{\theta}$ would vary in the range

$$0<\tilde{\theta}<2\pi\mu. \tag{3}$$

This means that we would not be able to talk about deficit angle in a natural way, besides that for this case the space changes character and the description becomes more complicated.[9]

The three distinct space–times will be characterized by different values of the function $F(r)$.[12] We shall compute for each of them the curvature scalar **R**, which for the generic form of the metric (1) is

$$\mathbf{R}=-\frac{F''(r)}{F(r)}, \tag{4}$$

where $'$ means derivation in respect to r.

For each space–time we may list the relevant properties in the following way:
Space–time (a): Topology $\Re^2\times S^2$; $F(r)=\sin r$; $0<r<2\pi$; $\mathbf{R}=1$,
Space–time (b): Topology $\Re^3\times S^1$; $F(r)=r$; $0<r<\infty$; $\mathbf{R}=0$,
Space–time (c): Topology $\Re^2\times H^2$; $F(r)=\sinh r$; $-\infty<r<\infty$; $\mathbf{R}=-1$.

One may note by the above properties of (a), (b), and (c), that they have well behaved scalar curvatures **R** (it is easy to verify that the same is true for other scalars formed out of the Riemann tensor) and an apparent singularity at $r=0$. Indeed, by means of the transformation (2) it is very easy to identify the presence of conical singularities in these space–times. By eq. (3) it is clear that, if $\mu=1$ the space–times are regular, otherwise they have conical singularities with deficit angles $2\pi(1-\mu)$. Let us see, now, how to apply the holonomy method to the above space–times (1).

We start by computing the holonomy matrix H, which can only be done when we have the parallel transport equations. The easiest way to derive them, from Eq. (1), is by working on the orthonormal basis, defined by the transformations

$$w^i=dx_i;\quad w^{\hat{\theta}}=\mu F(r)d\theta, \tag{5}$$

where $x_{0,1,2}=t,z,r$. The non-vanishing connection coefficient components in this basis are

$$-\Gamma^{\hat{r}}_{\hat{\theta}\hat{\theta}}=\frac{F'(r)}{F(r)}=\Gamma^{\hat{\theta}}_{\hat{r}\hat{\theta}}. \tag{6}$$

The general expression for the parallel transport equations of a fiducial vector v, along a given curve is[13]

$$\frac{dv^{\alpha}}{d\lambda}+v^{\beta}\Gamma^{\alpha}_{\beta\gamma}\frac{dx^{\gamma}}{d\lambda}=0, \tag{7}$$

where λ is an affine parameter describing the curve; and the Greek indices vary over all the coordinates.

We must define, now, the closed loops for these cases, as well as the limit which will make them collapsing to the apparently singular point $r=0$. Since the t and z directions do not play important roles in the present cases (the singular point is in the r axis and θ is the unique angular variable), we set them to be constants, independent of λ. For an apparently singular point in r, the simplest closed loops have constant and different values of r, and θ is a non-constant function of λ. These loops will collapse to $r=0$ when we take the limit $r\to 0$. As a matter of simplicity, we choose θ to depend linearly on λ.

Our curves may be written as

$$x_i=C_i, \quad \theta=\lambda+\lambda_0, \tag{8}$$

where λ_0 is a constant and λ varies in the range $[-\lambda_0,-\lambda_0+2\pi]$; C_i are constants and i varies as in eq. (5).

A final remark before writing down the parallel transport equations, is that the set of eqs. (7), for the non-coordinate basis, must be modified such that we may use the closed loops (8) given in the coordinate basis. Then, the new set of equations is written

$$\frac{dv^{\alpha}}{d\lambda}+v^{\beta}\Gamma^{\alpha}_{\beta\gamma}\Lambda^{\gamma}_{\delta}\frac{dx^{\delta}}{d\lambda}=0, \tag{9}$$

where Λ is the basis one-form transformation matrix, also responsible for the transformation of vector components.

We may now write the parallel transport equations (9), for the fiducial vector v, around the closed loop (8), with the aid of eq. (6). They are

$$\frac{dv^{\hat{t}}}{d\lambda}=0=\frac{dv^{\hat{z}}}{d\lambda}, \tag{10}$$

$$\frac{dv^{\hat{r}}}{d\lambda}-\mu F' v^{\hat{\theta}}=0, \tag{11}$$

$$\frac{dv^{\hat{\theta}}}{d\lambda}+\mu F' v^{\hat{r}}=0. \tag{12}$$

The general solution for the system of coupled, linear, homogeneous, first order differential equations (10)–(12), is given by

$$v^{j}(\lambda)=\widetilde{C}_j, \tag{13}$$

$$v^{\hat{r}}(\lambda)=A\ \sin(\alpha\lambda+\delta_0), \tag{14}$$

$$v^{\hat{\theta}}(\lambda)=A\ \cos(\alpha\lambda+\delta_0), \tag{15}$$

where $j=\hat{t},\hat{z}$; $\widetilde{C}_j$, A, δ_0 are constants to be determined by the initial conditions; and $\alpha\equiv\mu F'(r)$.

The initial conditions will be given by

$$v^{\alpha}(\lambda=-\lambda_0)=v_0^{\alpha}, \tag{16}$$

where α varies as in eq. (7); and v_0^{α} are constants. If one imposes these conditions (16) in the eqs. (13)–(15), after some calculations one finds

$$v^{j}(\lambda)=v_0^{j}, \tag{17}$$

$$v^{\hat{r}}(\lambda)=\cos[\alpha(\lambda+\lambda_0)]v_0^{\hat{r}}+\sin[\alpha(\lambda+\lambda_0)]v_0^{\hat{\theta}}, \tag{18}$$

$$v^{\hat{\theta}}(\lambda)=-\sin[\alpha(\lambda+\lambda_0)]v_0^{\hat{r}}+\cos[\alpha(\lambda+\lambda_0)]v_0^{\hat{\theta}}, \tag{19}$$

where j varies as in eq. (13). We may now write the holonomy matrix which relates the initial value of the fiducial vector v, with its value after a complete loop around the closed loop. It is achieved by setting $\lambda=-\lambda_0+2\pi$ in eqs. (17)–(19)

$$v(-\lambda_0+2\pi,\alpha)=H(\alpha)v_0, \tag{20}$$

where

$$H(\alpha)=\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \cos(2\pi\alpha) & \sin(2\pi\alpha) \\ 0 & 0 & -\sin(2\pi\alpha) & \cos(2\pi\alpha) \end{pmatrix}. \tag{21}$$

Before we proceed, it is important to note that H is independent of η, or in other words, it is independent of the metric signature. One may use, then, this method for Lorentzian or Euclidean space–times.

It is clear from eq. (21) that $H(\alpha)$ is not, in general, the identity transformation, not even in the case of a regular space–time. This fact is only a verification that the space–time has a non-vanishing curvature. For space–times (a) and (c) one may verify this fact, for they have constant positive and negative scalars of curvature, but not for space–time (b) which is flat. The final step in our present analysis, is the evaluation of $H(\alpha)$ (21) in the limit when r goes to 0.

The relevant components of the holonomy matrix to be analyzed are

$$\cos(2\pi\alpha) \quad \text{and} \quad \sin(2\pi\alpha). \tag{22}$$

We must, now, take the limit of these quantities (22), when r goes to 0. It is not difficult because for all three space–times (a), (b) and (c), the desired limit of the first derivative of $F(r)$ is the same

$$\lim_{r\to 0} F'(r)=1. \tag{23}$$

So, once $\alpha=\mu F'(r)$, we obtain the following limit as $r\to 0$ to the relevant quantities (22):

$$\cos(2\pi\mu) \quad \text{and} \quad \sin(2\pi\mu). \tag{24}$$

We may conclude that the space–time is regular, or in other words the holonomy matrix goes to the 4×4 identity in this limit, if and only if $\mu=1$, otherwise there is a conical singularity in these space–times. This is the same result stated above and derived by a trivial coordinate transformation in the angular coordinate θ.

IV. APPLICATION TO THE DJH CONICAL SPACE–TIME

This space–time was introduced by Deser, Jackiw, and 't Hooft (DJH), as a solution of Einstein's equations for a single, massive, spinless point-particle, at rest, at the origin of the coordinate system, in three-dimensions (time+2 spatial dimensions).[9] Its metric is given by

$$ds^2=-dt^2+\frac{1}{R^{2\rho}}\,(dR^2+R^2d\Theta^2), \tag{25}$$

where $0\leqslant t\leqslant\infty$, $0\leqslant R\leqslant\infty$, $0\leqslant\Theta\leqslant2\pi$; and ρ is proportional to the mass of the particle and varies in the range $0\leqslant\rho<1$.

It is easy to see from eq. (25) that $R=0$ is an apparent singularity of this space–time, and after a brief calculation one finds that its scalar of curvature **R** is nil. Gathering together these two results we conclude that it is very likely that the apparent singularity at $R=0$ is of a conical type. How can we know beyond any doubt? In what follows we shall apply the holonomy method to this space–time (25), and compare its result with the one derived in Ref. 9 from a non-trivial coordinate transformation.

We start the application of the holonomy method by rewriting eq. (25) in a non-coordinate basis, which coordinate transformations read

$$w^{\hat{t}}=dt;\quad w^{\hat{R}}=R^{-\rho}dR;\quad w^{\hat{\theta}}=R^{1-\rho}d\Theta. \tag{26}$$

The non-vanishing connection coefficient components in this basis are

$$\Gamma^{\hat{t}}_{\hat{\phi}\hat{\phi}}=\frac{-(1-\rho)}{t^{1-\rho}}=-\Gamma^{\hat{\phi}}_{\hat{t}\hat{\phi}}. \tag{27}$$

From here onward the calculations will be a repetition of the previous case, discounting the obvious fact that we have, now, one less spatial coordinate. The closed loops will be defined by constant values of t and R and a linear function of Θ, which may be written as

$$x_i=C_i,\quad \Theta=\lambda+\lambda_0, \tag{28}$$

where $x_{0,1}=t,R$; C_i and λ_0 are constants; and λ is an affine parameter describing the closed loop, which varies in the range $[-\lambda_0,-\lambda_0+2\pi]$. These loops will collapse to the apparently singular point when we take the limit $R\to0$.

The initial conditions for the fiducial vector v, which will be parallel transported around the closed loops, are given by eq. (16) (where here $\alpha=t,R,\Theta$). With these conditions eq. (16), and the aid of eq. (28), we may write and solve the parallel transport equations for v, derived from eq. (9). After some calculations we may write the holonomy matrix $H(\rho)$, for the present case, in the following way:

$$H(\rho)=\begin{pmatrix}1 & 0 & 0\\ 0 & \cos[2\pi(1-\rho)] & \sin[2\pi(1-\rho)]\\ 0 & -\sin[2\pi(1-\rho)] & \cos[2\pi(1-\rho)]\end{pmatrix}. \tag{29}$$

Observing eq. (29) carefully, we note that it is already the final result we were looking for because $H(\rho)$ does not depend upon R. Therefore, the limit of $H(\rho)$ when R goes to zero does not modify eq. (29).

The holonomy method predicts, then, that if $\rho=0$ the space–time (25) is regular, otherwise there is a conical singularity in it. Let us compare, now, this prediction with the one derived from a non-trivial coordinate transformation.

In Ref. 9, Deser, Jackiw, and 't Hooft, proposed the following coordinate transformation for the metric (25)

$$r=\frac{R^{1-\rho}}{1-\rho}, \quad \theta=(1-\rho)\Theta. \tag{30}$$

In terms of r and θ the metric (25) becomes flat

$$ds^2=-dt^2+dr^2+r^2d\theta^2. \tag{31}$$

The ranges of the new variables may be derived by eq. (30), with the aid of the ranges of the old ones, which were given after eq. (25). They are

$$0\leqslant r\leqslant\infty, \quad 0\leqslant\theta\leqslant 2\pi(1-\rho). \tag{32}$$

V. CONCLUSIONS

In the present paper we have introduced what we have called the holonomy method. It is a systematic way, based upon the concept of holonomy, of determining the presence of conical singularities in a given metric space–time (M,g). In Sec. II, we have introduced the holonomy method. Subsequently, in Secs. III and IV, we have demonstrated the validity and usefulness of the method by means of its application in two examples.

It is important to mention that the results derived from the application of the holonomy method for a given metric space–time (M,g), may be used to analyze another metric space–time $(\widetilde{M},\widetilde{g})$. This can be done only and if only g and $\widetilde{g}$ are related by a non-singular basis one-form transformation S, because the old and new holonomy matrices (H and $\widetilde{H}$ respectively) will have the following transformation relation:

$$\widetilde{H}=SHS^{-1}. \tag{33}$$

Therefore, knowing the value of H for a given one-form basis one has only to determine the values of the transformation S, and its inverse S^{-1}, in order to derive the holonomy matrix in the new one-form basis $\widetilde{H}$.

Finally, there is yet another type of metric space–times where the use of the holonomy method greatly simplifies the identification of conical singularities. These d-dimensional space–times have the topology $\mathfrak{R}$ (time) times a flat or negatively curved, $d-1$-dimensional, compact spatial sector. The compactification of the spatial sector is done via the identification of opposite $d-2$-dimensional ''sides'' of a chosen figure.[10,12,14] It is possible that such identifications introduce a singularity of a conical, or even more complicate nature in the resulting space–time.[10,14] Therefore, applying the holonomy method to space–times constructed in this way, one may identify the presence of conical singularities there.

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Quasitriangularity and enveloping algebras for inhomogeneous quantum groups

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Coquasitriangular universal $\mathscr{R}$ matrices on quantum Lorentz and quantum Poincaré groups are classified. The results are extended (under certain assumptions) to inhomogeneous quantum groups. Enveloping algebras on those objects are described. © *1996 American Institute of Physics.* [S0022-2488(96)01508-3]

I. INTRODUCTION

Possible R-matrices for the fundamental representations of inhomogeneous quantum groups were found in Proposition 3.14 of Ref. 1. In the present paper we describe universal $\mathscr{R}$ matrices for those objects (under certain assumptions which are fulfilled in the case of quantum Poincaré groups[2]). Our study will be useful in developing a simple physical model[3] of free particles on a quantum Minkowski space.[2]

In Section II we show how to construct co(quasi)triangular (*-)bialgebras and Hopf (*-)algebras whose relations are given by means of intertwiners: we simplify and extend results of Ref. 4. Next, in Section III we classify co(quasi)triangular (*-)structures $\mathscr{R}$ on quantum Lorentz groups.[5] Using the results of Sections II and III, in Section IV we classify such structures on quantum Poincaré groups[2] and also, more generally, on inhomogeneous quantum groups[1] (certain natural assumptions regarding mainly restriction of those structures to the homogeneous quantum group are made). In Section V we use $\mathscr{R}$ to define enveloping algebras for inhomogeneous quantum groups.

We sum over repeated indices (Einstein's convention). We work over the field $\mathbf{C}$. We write $a\sim b$ if $a=\lambda b$ for $\lambda\in\mathbf{C}\backslash\{0\}$. If V,W are vector spaces, then τ: $V\otimes W\to W\otimes V$ is given by $\tau(x\otimes y)=y\otimes x$, $x\in V$, $y\in W$. If $\mathscr{A}$ is an algebra, $v\in M_N(\mathscr{A})$, $w\in M_K(\mathscr{A})$, then the tensor product $v\otimes w\in M_{NK}(\mathscr{A})$ is defined by $(v\otimes w)_{ij,kl}=v_{ik}w_{jl}$, $i,k=1,\ldots,N$, $j,l=1,\ldots,K$. We set $\dim v=N$. If $\mathscr{A}$ is a *-algebra, then the conjugate of v is defined as $\overline{v}\in M_N(\mathscr{A})$ where $\overline{v}_{ij}=v_{ij}{}^*$, $i,j=1,\ldots,N$.

Throughout the paper quantum groups H are abstract objects described by the corresponding (*-)bialgebras $\mathrm{Poly}(H)=(\mathscr{A},\Delta)$. We denote by Δ,ε,S the comultiplication, counit and (if exists) coinverse of $\mathrm{Poly}(H)$. We say that v is a representation of H (i.e., $v\in\mathrm{Rep}\,H$) if $v\in M_N(\mathscr{A})$, $N\in\mathbf{N}$, and $\Delta v_{ij}=v_{ik}\otimes v_{kj}$, $\varepsilon(v_{ij})=\delta_{ij}$, $i,j=1,\ldots,N$. The conjugate of a representation and tensor product of representations are also representations. Matrix elements of representations of H span $\mathscr{A}$ as a linear space. The set of nonequivalent irreducible representations of H is denoted by $\mathrm{Irr}\,H$. If v, $w\in\mathrm{Rep}\,H$, then we say that $A\in M_{\dim w\times\dim v}(\mathbf{C})$ intertwines v with w [i.e., $A\in\mathrm{Mor}(v,w)$] if $Av=wA$. The dual vector space $\mathscr{A}'$ is an algebra wrt the convolution defined by $\rho*\rho'=(\rho\otimes\rho')\Delta$. It has a unit $I_{\mathscr{A}'}=\varepsilon$. For $\rho\in\mathscr{A}'$, $a\in\mathscr{A}$, we set $\rho*a=(id\otimes\rho)\Delta a$, $a*\rho=(\rho\otimes id)\Delta a$.

II. COQUASITRIANGULAR BIALGEBRAS

In this section we discuss bialgebras $\mathrm{Poly}(G)=(\mathscr{B},\Delta)$ defined by several fundamental representations of G and intertwiners among them. We provide necessary and sufficient conditions for

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the existence of coquasitriangular structure $\mathscr{R}$ for G. Hopf and $*$ structures are also investigated. The results generalize results of Theorem 1.4 of Ref. 4 (see also Theorem 1.1 of Ref. 5).

Proposition 1: Let $\mathscr{B}$ be the universal algebra generated by w^{α}_{mn}, $m,n=1,\ldots,d_{\alpha}$, $\alpha\in\mathscr{J}$, and relations ($0\in\mathscr{J}$, $d_0=1$)

$$w^{\alpha}\otimes w^{0}=w^{0}\otimes w^{\alpha}=w^{\alpha},\quad \alpha\in\mathscr{J}, \tag{II.1}$$

$$W_m(w^{\alpha_{m1}}\otimes w^{\alpha_{m2}}\otimes\cdots\otimes w^{\alpha_{ms_m}})=(w^{\beta_{m1}}\otimes\cdots\otimes w^{\beta_{mt_m}})W_m,\quad m\in K \tag{II.2}$$

(we fix sets $\mathscr{J}$, K, positive integers d_{α}, and matrices W_m of suitable dimensions).

Then $w^{0}=(I_{\mathscr{B}})$ and there exists a unique Δ such that $\mathrm{Poly}(G)=(\mathscr{B},\Delta)$ is a bialgebra and w^{α}, $\alpha\in\mathscr{J}$ are representations of G.

Proof: The proof is the same as in Theorem 1.4 of Ref. 4. □

Let us recall

Definition 1: (cf. Refs. 6–8) We say that $(\mathscr{B},\Delta,\mathscr{R})$ is a coquasitriangular (CQT) bialgebra if $(\mathscr{B},\Delta)$ is a bialgebra and $\mathscr{R}\in(\mathscr{B}\otimes\mathscr{B})'$ satisfies

$$\mathscr{R}(I\otimes x)=\mathscr{R}(x\otimes I)=\varepsilon(x), \tag{II.3}$$

$$\mathscr{R}(xy\otimes z)=\mathscr{R}(x\otimes z^{(1)})\mathscr{R}(y\otimes z^{(2)}), \tag{II.4}$$

$$\mathscr{R}(x\otimes yz)=\mathscr{R}(x^{(1)}\otimes z)\mathscr{R}(x^{(2)}\otimes y), \tag{II.5}$$

$$y^{(1)}x^{(1)}\mathscr{R}(x^{(2)}\otimes y^{(2)})=\mathscr{R}(x^{(1)}\otimes y^{(1)})x^{(2)}y^{(2)}, \tag{II.6}$$

where we have used the Sweedler's notation $\Delta(x)=x^{(1)}_i\otimes x^{(2)}_i\equiv x^{(1)}\otimes x^{(2)}$.

Remark 1: (cf. Refs. 9, 8, and Proposition 1.3 of Ref. 4) Let $\mathrm{Poly}(G)=(\mathscr{B},\Delta)$ be a bialgebra and $\mathscr{R}\in(\mathscr{B}\otimes\mathscr{B})'$. For each v, $w\in\mathrm{Rep}\,G$ one can define $R^{vw}\in\mathrm{Lin}(\mathbf{C}^{\dim v}\otimes\mathbf{C}^{\dim w},\mathbf{C}^{\dim w}\otimes\mathbf{C}^{\dim v})$ by

$$(R^{vw})_{ij,kl}=\mathscr{R}(v_{jk}\otimes w_{il}),\quad j,k=1,\ldots,\dim v,\quad i,l=1,\ldots,\dim w. \tag{II.7}$$

Then

$$(\mathbb{1}\otimes S)R^{v_1w}=R^{v_2w}(S\otimes\mathbb{1})\quad \text{if } S\in\mathrm{Mor}(v_1,v_2), \tag{II.8}$$

$$(S\otimes\mathbb{1})R^{vw_1}=R^{vw_2}(\mathbb{1}\otimes S)\quad \text{if } S\in\mathrm{Mor}(w_1,w_2), \tag{II.9}$$

v,w,v_1, $w_1\in\mathrm{Rep}\,G$. Suppose that $L\subset\mathrm{Rep}\,G$ is such that the matrix elements of representations $v\in L$ linearly span $\mathscr{B}$ (e.g., $L=\mathrm{Rep}\,G$). Consider the conditions

$$R^{0v}=R^{v0}=\mathbb{1},\quad v\in L, \tag{II.10}$$

$$R^{v_1\otimes v_2,w}=(R^{v_1w}\otimes\mathbb{1})(\mathbb{1}\otimes R^{v_2w}),\quad v_1,v_2,w\in L, \tag{II.11}$$

$$R^{v,w_1\otimes w_2}=(\mathbb{1}\otimes R^{vw_2})(R^{vw_1}\otimes\mathbb{1}),\quad v,w_1,w_2\in L, \tag{II.12}$$

$$R^{vw}\in\mathrm{Mor}(v\otimes w,w\otimes v),\quad v,w\in L. \tag{II.13}$$

Then (II.10)⇔(II.3), (II.11)⇔(II.4), (II.12)⇔(II.5), and (II.13)⇔(II.6).

Theorem 1: Let $\mathrm{Poly}\,(G)=(\mathscr{B},\Delta)$ be a bialgebra defined in Proposition 1 and $R^{\alpha\beta}\in\mathrm{Lin}(\mathbf{C}^{d_\alpha}\otimes\mathbf{C}^{d_\beta},\mathbf{C}^{d_\beta}\otimes\mathbf{C}^{d_\alpha}),\alpha,\beta\in\mathscr{J}$.

The following are equivalent:

(1) There exists $\mathscr{R}\in(\mathscr{B}\otimes\mathscr{B})'$ such that $(\mathscr{B},\Delta,\mathscr{R})$ is a CQT bialgebra and $R^{\alpha\beta}=R^{w^{\alpha}w^{\beta}}$.

(2)

$$R^{0\alpha}=R^{\alpha 0}=\mathbb{1}, \quad \alpha\in\mathscr{J}, \tag{II.14}$$

$$(\mathbb{1}\otimes W_m)R^{\alpha_{m1}\cdot\ldots\cdot\alpha_{ms_m},\gamma}=R^{\beta_{m1}\cdot\ldots\cdot\beta_{mt_m},\gamma}(W_m\otimes\mathbb{1}), \quad m\in K,\gamma\in\mathscr{J}\backslash\{0\}, \tag{II.15}$$

$$R^{\gamma,\beta_{m1}\cdot\ldots\cdot\beta_{mt_m}}(\mathbb{1}\otimes W_m)=(W_m\otimes\mathbb{1})R^{\gamma,\alpha_{m1}\cdot\ldots\cdot\alpha_{ms_m}}, \quad m\in K,\gamma\in\mathscr{J}\backslash\{0\}, \tag{II.16}$$

$$R^{\alpha\beta}\in \mathrm{Mor}(w^\alpha\otimes w^\beta, w^\beta\otimes w^\alpha), \quad \alpha,\beta\in\mathscr{J}\backslash\{0\}, \tag{II.17}$$

where $R^{\delta_1\cdot\ldots\cdot\delta_{k+1},\gamma}=(R^{\delta_1\cdot\ldots\cdot\delta_k,\gamma}\otimes\mathbb{1})(\mathbb{1}\otimes R^{\delta_{k+1}\gamma}), R^{\gamma,\delta_1\cdot\ldots\cdot\delta_{k+1}}=(\mathbb{1}\otimes R^{\gamma\delta_{k+1}})(R^{\gamma,\delta_1\cdot\ldots\cdot\delta_k}\otimes\mathbb{1}), \gamma, \delta_1,\ldots,\delta_{k+1}\in\mathscr{J}$, $k=1,2,\ldots$.

Moreover, such $\mathscr{R}$ is unique.

Remark: In special cases related statements can be found in Refs. 10, 8, 7, and Theorem 1.4 of Ref. 4 (cf. Ref. 9).

Proof: Assume condition (1). According to Remark 1, (II.10)–(II.13) follow. Thus we get (II.14) and (II.17). Using (II.8) and (II.9) for $S=W_m$ [see (II.2)] and (II.11) and (II.12), one obtains (II.15) and (II.16) and the condition (2) is proved.

Moreover, $R^{w^\alpha w^\beta}=R^{\alpha\beta}$ uniquely determine R^{vw}, where $v, w\in L_0$,

$$L_0=\{\text{tensor products of some number of copies of representations } w^\alpha, \quad \alpha\in\mathscr{J}\}.$$

Using (II.7) and the fact that the matrix elements of representations from L_0 linearly span $\mathscr{B}$, the uniqueness of $\mathscr{R}$ follows. It remains to prove

(2)⇒(1): Assume condition (2). Using (II.14), we can replace $\mathscr{J}\backslash\{0\}$ by $\mathscr{J}$ in (II.15)–(II.17). We define the homomorphisms $\mathscr{R}^\beta\colon \mathscr{B}\to M_{d_\beta}(\mathbf{C})$, $\beta\in\mathscr{J}$, by

$$[\mathscr{R}^\beta(w^\alpha_{ij})]_{kl}=R^{\alpha\beta}_{ki,jl}, \quad \alpha\in\mathscr{J} \tag{II.18}$$

[later on we will have $\mathscr{R}^\beta_{kl}=\mathscr{R}(\cdot\otimes w^\beta_{kl})$]. They preserve the relations (II.1) and (II.2) due to (II.14) and (II.15). Setting $\alpha=0$ in (II.18), we show that $\mathscr{R}^\beta$ are unital. Setting $\beta=0$ in (II.18), one gets $\mathscr{R}^0_{11}=\varepsilon$ (it is true on the generators w^α_{ij}). Hence $\mathscr{R}^0_{11}*\mathscr{R}^\beta_{kl}=\mathscr{R}^\beta_{kl}*\mathscr{R}^0_{11}=\mathscr{R}^\beta_{kl}$. Let

$$X=\{x\in\mathscr{B}\colon W_{b_1\ldots b_{t_m},a_1\ldots a_{s_m}}(\mathscr{R}^{\alpha_{ms_m}}_{a_{s_m}c_{s_m}}*\cdots*\mathscr{R}^{\alpha_{m1}}_{a_1c_1})(x)$$

$$=(\mathscr{R}^{\beta_{mt_m}}_{b_{t_m}d_{t_m}}*\cdots*\mathscr{R}^{\beta_{1t_1}}_{b_1d_1})(x)W_{d_1\ldots d_{t_m},c_1\ldots c_{s_m}}, \quad m\in K\}.$$

It is straightforward to show that X is an algebra. According to (II.16), $u^\gamma_{kl}\in X (k,l=1,\ldots,d_\gamma$, $\gamma\in\mathscr{J})$. Thus $X=\mathscr{B}$. Hence there exists a linear antihomomorphism $\theta\colon \mathscr{B}\to\mathscr{B}'$ such that $\theta(w^\beta_{kl})=\mathscr{R}^\beta_{kl}$, $k,l=1,\ldots,d_\beta$, $\beta\in\mathscr{J}$ [θ preserves (II.1) and (II.2)]. Setting $\mathscr{R}(x\otimes y)=[\theta(y)](x)$, $x,y\in\mathscr{B}$, we obtain an $\mathscr{R}\in(\mathscr{B}\otimes\mathscr{B})'$ which satisfies (II.5) and (II.3). Moreover, (II.18) yields $R^{\alpha\beta}=R^{w^\alpha w^\beta}$. Let $Y=\{z\in\mathscr{B}\colon\forall x,y\in\mathscr{B}\ \mathscr{R}(xy\otimes z)=\mathscr{R}(x\otimes z^{(1)})\mathscr{R}(y\otimes z^{(2)})\}$. Then Y is an algebra [we use (II.5)] and $w^\beta_{kl}\in Y$. Hence, $Y=\mathscr{B}$ and (II.4) follows. Thus (Remark 1) we get (II.10)–(II.12) for $L=L_0$. That and (II.13) for $v, w\in\{w^\alpha\colon\alpha\in\mathscr{J}\}$ [see (II.17)] give (II.13) for $L=L_0$, hence (Remark 1) (II.6) and the condition (1) is satisfied. □

Remark 2: The unital antihomomorphism $\theta\colon\mathscr{B}\to\mathscr{B}'$ introduced in the above proof exists for each CQT bialgebra (cf. Ref. 9) and satisfies $(\theta\otimes\theta)\Delta=\Delta'\theta$ where $\Delta'\colon\mathscr{B}'\to(\mathscr{B}\otimes\mathscr{B})'$ is defined by $\Delta'(\varphi)=\varphi\circ m$, $\varphi\in\mathscr{B}'$, cf. Appendix of Ref. 4.

Let us now pass to the Hopf algebra structure.

Proposition 2: (cf. Ref. 11 and Proof of Theorem 1.4.1 of Ref. 4) Let $\mathrm{Poly}(G)=(\mathscr{B},\Delta)$ be a bialgebra and w,w',w'' be representations of G. Suppose there exist $E\in\mathrm{Mor}(I,w\otimes w')$,

$E' \in \mathrm{Mor}(w'' \otimes w, I)$ such that E is left nondegenerate, i.e., $E_{i-} = (E_{ij})_{j=1}^{\dim w'}$, $i=1,\ldots,\dim w$, are linearly independent and E' is right nondegenerate, i.e., $E'_{-k} = (E'_{mk})_{m=1}^{\dim w''}$, $k=1,\ldots,\dim w$, are linearly independent. Then w^{-1} exists.

Proposition 3: (cf. Ref. 11 and Proof of Theorem 1.4.1 of Ref. 4) Let $(\mathscr{B},\Delta)$ be the bialgebra defined in Proposition 1. Suppose $(u^{\alpha})^{-1}$ exist, $\alpha \in \mathscr{J}$. Then $(\mathscr{B},\Delta)$ is a Hopf algebra.

A CQT bialgebra $(\mathscr{B},\Delta,\mathscr{R})$ such that $(\mathscr{B},\Delta)$ is a Hopf algebra is called CQT Hopf algebra.

Proposition 4: (cf. Proposition 1.3.1.b of Ref. 4) Let $\mathrm{Poly}(G)=(\mathscr{B},\Delta)$ and $(\mathscr{B},\Delta,\mathscr{R})$ be a CQT Hopf algebra. Then $(R^{vw})^{-1}$ exist for any $v, w \in \mathrm{Rep}\, G$. Moreover, $\mathscr{R}'=\mathscr{R}(S\otimes id)$ satisfies

$$\mathscr{R}'(x^{(1)}\otimes y^{(1)})\mathscr{R}(x^{(2)}\otimes y^{(2)})=\mathscr{R}(x^{(1)}\otimes y^{(1)})\mathscr{R}'(x^{(2)}\otimes y^{(2)})=(\varepsilon\otimes\varepsilon)(x\otimes y)$$

(i.e., $\mathscr{R}'=\mathscr{R}^{-1}$) and

$$\mathscr{R}'(v_{il}\otimes w_{jk})=(R^{vw})^{-1}_{ij,kl}, \quad i,l=1,\ldots,\dim v, \quad j,k=1,\ldots,\dim w.$$

We say that $(\mathscr{B},\Delta)$ is a *-bialgebra if $(\mathscr{B},\Delta)$ is a bialgebra, $\mathscr{B}$ is a *-algebra and

$$(*\otimes *)\Delta(x)=\Delta(x^*) \tag{II.19}$$

for $x \in \mathscr{B}$. A Hopf algebra which is a *-bialgebra is called Hopf *-algebra.

Proposition 5: Let $(\mathscr{B},\Delta)$ be the bialgebra defined in Proposition 1. Suppose there exists an involution $\sim: \mathscr{J}\to\mathscr{J}$ such that $\widetilde{0}=0$, $d_{\widetilde{\alpha}} = d_{\alpha}$ and $\widetilde{W}_m \in \mathrm{Mor}(w^{\widetilde{\alpha}_{ms_m}}\otimes\cdots\otimes w^{\widetilde{\alpha}_{m1}}, w^{\widetilde{\beta}_{mt_m}}\otimes\cdots\otimes w^{\widetilde{\beta}_{m1}})$ where $(\widetilde{W}_m)_{i_{t_m}\ldots i_1, j_{s_m}\ldots j_1} = \overline{(W_m)_{i_1\ldots i_{t_m}, j_1\ldots j_{s_m}}}$. Then there exists a unique $*: \mathscr{B}\to\mathscr{B}$ such that $(\mathscr{B},\Delta)$ is a *-bialgebra and $\overline{w^{\alpha}} = w^{\widetilde{\alpha}}$, $\alpha \in \mathscr{J}$ ($\overline{\ }$ was defined in the Introduction).

Proof: Uniqueness is trivial. Our assumptions imply that $z^{\alpha}_{ij} = w^{\widetilde{\alpha}}_{ij}$ satisfy (II.1) and (II.2) in the conjugate algebra $\mathscr{B}^j$ (conjugate vector space and opposite multiplication). Therefore the desired $*$ exists [we check $*^2=id$ and (II.19) on the generators w^{α}_{ij}]. □

Proposition 6: (cf. the proofs of Proposition 1.3.d.ii and Theorem 1.4.6 of Ref. 4) Let $(\mathscr{B},\Delta,\mathscr{R})$ be a CQT bialgebra and $\mathrm{Poly}(G)=(\mathscr{B},\Delta)$ be a *-bialgebra. Suppose $M\subset\mathrm{Rep}\, G$ is such that the matrix elements of representations from M generate $\mathscr{B}$ as unital algebra. The following are equivalent:

(1) $\overline{\mathscr{R}(y^*\otimes x^*)}=\mathscr{R}(x\otimes y), \quad x,y\in\mathscr{B}$

(2)

$$\overline{(R^{\overline{vw}})_{ji,lk}}=R^{vw}_{ij,kl}, \quad j,k=1,\ldots,\dim v, \quad i,l=1,\ldots,\dim w, \quad v,w\in M. \tag{II.20}$$

If one of the above conditions is satisfied, $(\mathscr{B},\Delta,\mathscr{R})$ is called CQT *-bialgebra. If, moreover, $(\mathscr{B},\Delta)$ is a Hopf algebra, $(\mathscr{B},\Delta,\mathscr{R})$ is called CQT Hopf *-algebra (see Definition 1.1 of Ref. 4).

Proposition 7: (cf. Ref. 9) Let $\mathrm{Poly}(G)=(\mathscr{B},\Delta)$ be a bialgebra and $\mathscr{R}\in(\mathscr{B}\otimes\mathscr{B})'$. Suppose $M\subset\mathrm{Rep}\, G$ is such that the matrix elements of representations from M generate $\mathscr{B}$ as unital algebra. The following are equivalent:

(1) $\mathscr{R}(x^{(1)}\otimes y^{(1)})\mathscr{R}(y^{(2)}\otimes x^{(2)})=(\varepsilon\otimes\varepsilon)(x\otimes y), \quad x,y\in\mathscr{B}$ (i.e., $\mathscr{R}_{21}=\mathscr{R}^{-1}$).

(2)

$$(R^{vw})^{-1}=R^{wv}, \quad v,w\in M. \tag{II.21}$$

If one of the above conditions is satisfied, we replace CQT by CT (cotriangular) in all definitions (cf. Ref. 6).

Proof: Using (II.10)–(II.12), one can assume that [in the condition (2)] matrix elements of representations from M linearly span $\mathscr{B}$. Then in (1) it is enough to consider $x=v_{ij}$, $y=w_{kl}$, $i,j=1,\ldots,\dim v$, $k,l=1,\ldots,\dim w$, $v, w\in M$. Then (1) is equivalent to (II.21). □

III. QUASITRIANGULAR STRUCTURES ON QUANTUM LORENTZ GROUPS

In this section we classify coquasitriangular (*-) structures on quantum Lorentz groups of Ref. 5. For the quantum Lorentz group of Ref. 12 examples of such structures were given in Ref. 13 and Remark 7 of Section 3 of Ref. 4. We also classify (cf. Ref. 14) coquasitriangular (*-) structures on (complex) $\mathrm{SL}_q(2)$ groups and their real forms.

We first recall the definition of Hopf *-algebra corresponding to a quantum Lorentz group[5] essentially repeating the arguments of Theorem 1.1 of Ref. 5. The bialgebra structure of $(\mathscr{A},\Delta)$ is obtained by the construction of Proposition 1 with $\{w^\alpha:\alpha\in\mathscr{I}\}=\{w^0,w,\widetilde{w}\}$. Here the relations (II.1) mean that $w^0=(I_{\mathscr{H}})$ and the relations (II.2) are given by

$$(w\otimes w)E=Ew^0, \tag{III.1}$$

$$(\widetilde{w}\otimes\widetilde{w})\widetilde{E}=\widetilde{E}w^0, \tag{III.2}$$

$$E'(w\otimes w)=w^0E', \tag{III.3}$$

$$\widetilde{E}'(\widetilde{w}\otimes\widetilde{w})=w^0\widetilde{E}', \tag{III.4}$$

$$X(w\otimes\widetilde{w})=(\widetilde{w}\otimes w)X, \tag{III.5}$$

where

$$\widetilde{E}=\tau\overline{E},\quad \widetilde{E}'=\overline{E'}\tau, \tag{III.6}$$

$E\in\mathrm{Lin}(\mathbf{C},\mathbf{C}^2\otimes\mathbf{C}^2)$, $E'\in\mathrm{Lin}(\mathbf{C}^2\otimes\mathbf{C}^2,\mathbf{C})$, $X\in\mathrm{Lin}(\mathbf{C}^2\otimes\mathbf{C}^2,\mathbf{C}^2\otimes\mathbf{C}^2)$ satisfy

$$(E'\otimes 1\!\!1)(1\!\!1\otimes E)=1\!\!1, \tag{III.7}$$

$$(X\otimes 1\!\!1)(1\!\!1\otimes X)(E\otimes 1\!\!1)=1\!\!1\otimes E, \tag{III.8}$$

$$\tau\overline{X}\tau=\beta^{-1}X, \tag{III.9}$$

$E'E\neq 0$, X is invertible, and $\beta\in\mathbf{C}\backslash\{0\}$.

Warning: Our choice of X may differ from the choice of Ref. 5 by a multiplicative nonzero constant.

Moreover, (III.7) implies that E and E' are inverse one to another as matrices,

$$(1\!\!1\otimes E')(E\otimes 1\!\!1)=1\!\!1. \tag{III.10}$$

Hence, E is left nondegenerate, E' is right nondegenerate, and w^{-1} exists (see Proposition 2). Similarly, $(1\!\!1\otimes\widetilde{E}')(\widetilde{E}\otimes 1\!\!1)=1\!\!1$, $\widetilde{E}$ is left nondegenerate, $\widetilde{E}'$ is right nondenegerate, and $\widetilde{w}^{-1}$ exists. But $(w^0)^{-1}=w^0$ and Proposition 3 implies that $(\mathscr{A},\Delta)$ is a Hopf algebra.

Setting $w^{\sim}=\widetilde{w}$, $\widetilde{w}^{\sim}=w$, $w^{0\sim}=w^0$, the assumptions of Proposition 5 are satisfied and $(\mathscr{A},\Delta)$ becomes a *-bialgebra where $*$ is defined by $\overline{w}=\widetilde{w}$. It has the same Poincaré series as the classical $\mathrm{SL}(2,\mathbf{C})$ group (Theorem 1.2 of Ref. 5). We may assume that

(1) $E=e_1\otimes e_2-qe_2\otimes e_1$, $q\in\mathbf{C}\backslash\{0,i,-i\}$, $X=\alpha\tau Q$, Q is given by (13)–(19) of Ref. 5 [$q=-1$ in (17)–(19)], $\alpha=t^{-1/2}$ for (13), $\alpha=(-t)^{-1/2}$ for (14), $\alpha=q^{1/2}$ for (15), $\alpha=(-q)^{1/2}$ for (16), $\alpha=(s^2-1)^{-1/2}$ for (17), $q=(p^2-1)^{-1/2}$ for (18), $\alpha=\frac{1}{2}$ for (19), or

(2) $E=e_1\otimes e_2-e_2\otimes e_1+e_1\otimes e_1$ (in that case we set $q=1$), $X=\tau Q$, Q is given by (20)–(21) of Ref. 5,

e_1,e_2 is the canonical basis of $\mathbf{C}^2$. Moreover, $\beta=t/|t|$ for (13) and (14), $\beta=q/|q|$ for (15), $\beta=-q/|q|$ for (16), $\beta=-i\ \mathrm{sgn}\ \mathrm{Im}(s)$ for (17), $\beta=\mathrm{sgn}(|p|-1)$ for (18), and $\beta=1$ for (19)–(21). In all cases, $\beta^4=1$.

We shall find all $\mathscr{R}\in(\mathscr{A}\otimes\mathscr{A})'$ such that $(\mathscr{A},\Delta,\mathscr{R})$ is a CQT Hopf algebra. So (cf. Theorem 1) we need to determine R^{ww}, $R^{\overline{w}\,\overline{w}}$, $R^{\overline{w}w}$, $R^{w\overline{w}}$ such that 20 relations (II.15) and (II.16) and 4 relations (II.17) are satisfied [we assume (II.14)]. We shall use them in the following. Irreducibility of $w\otimes\overline{w}$ (see Ref. 5) and (III.5) give $R^{w\overline{w}}=\varepsilon_X X$, $R^{\overline{w}w}=\varepsilon'_X X^{-1}$, where $\varepsilon_X,\varepsilon'_X\in\mathbf{C}\backslash\{0\}$ (cf. Proposition II.4). Moreover, $D=R^{ww}$ and $\widetilde{D}=\beta R^{\overline{w}\overline{w}}$ must satisfy (2.11) and (2.17)–(2.20) of Ref. 2 (with $L,\widetilde{L}$ replaced by $D,\widetilde{D}$), hence they are given by (2.21) and (2.22) of Ref. 2, i.e., $R^{ww}=L_i$, $R^{\overline{w}\,\overline{w}}=\tau\overline{L_j^{-1}}\tau$, $i,j=1,2,3,4$, $L_i=q_i(\mathbb{1}+q_i^{-2}EE')$, $q_{1,2}=\pm q^{1/2}$, and $q_{3,4}=\pm q^{-1/2}$. Using (2.1), (2.3) and (2.4) of Ref. 2, we obtain $\varepsilon_X=\pm1$, $\varepsilon'_X=\pm1$, and $\beta=\pm1$. After some calculations one gets that the 24 relations are satisfied. So we get $4\cdot4\cdot4$ $\mathscr{R}$ for $q\neq\pm1$, $\beta=\pm1$; $2\cdot2\cdot4$ $\mathscr{R}$ for $q=\pm1$, $\beta=\pm1$; and no $\mathscr{R}$ for $\beta=\pm i$.

Set $M=\{w,\overline{w}\}$. According to Proposition 6, we get a CQT Hopf *-algebra iff four relations (II.20) are satisfied iff $\beta=1$ and $q_j=q_i^{-1}$ ($4\cdot4$ $\mathscr{R}$ for $q\neq\pm1$, $\beta=1$; $2\cdot4$ $\mathscr{R}$ for $q=\pm1$, $\beta=1$; no $\mathscr{R}$ for $\beta\neq1$). According to Proposition 7, we get CT Hopf algebra iff four relations (II.21) are satisfied iff $q=1$, $\varepsilon'_X=\varepsilon_X$ ($2\cdot2\cdot2$ $\mathscr{R}$ for $q=1$, $\beta=\pm1$; no $\mathscr{R}$ otherwise). Clearly, we get CT Hopf *-algebra iff $q=\beta=1$ and $q_j=q_i^{-1}$, $\varepsilon'_X=\varepsilon_X$ ($2\cdot2$ $\mathscr{R}$ for $q=\beta=1$; no $\mathscr{R}$ otherwise).

Let us also recall $\mathrm{SL}_q(2)$ groups.[15,6] The bialgebra structure is obtained by the construction of Proposition 1 with $\{w^\alpha:\alpha\in\mathscr{J}\}=\{w^0,w\}$; the relations (II.1) mean that $w^0=(I_{\mathscr{H}})$ and those of (II.2) are given by (III.1) and (III.3), where E,E' are as above with $q\in\mathbf{C}\backslash\{0\}$ (only the case 1.). One gets that $(\mathscr{A},\Delta)$ is a Hopf algebra.

We shall describe (cf. Ref. 14) all $\mathscr{R}\in(\mathscr{A}\otimes\mathscr{A})'$ such that $(\mathscr{A},\Delta,\mathscr{R})$ is a CQT Hopf algebra. Due to Theorem 1 we should find $D=R^{ww}\in\mathrm{Mor}(w\otimes w,w\otimes w)$ satisfying four relations (II.15) and (II.16). This means $D=L_i$, $i=1,2,3,4$, so we get 4 $\mathscr{R}$ for $q\neq\pm1$, 0, and 2 $\mathscr{R}$ for $q=\pm1$. In other words, $R^{ww}=\pm L_1^{\pm1}$ where $L_1=q^{1/2}(\mathbb{1}+q^{-1}EE')$. We get CT Hopf algebras iff $L_1^2=\mathbb{1}$ (see Proposition 7 with $M=\{w\}$) iff $q=1$.

Let us pass to real forms. Then $(\mathscr{A},\Delta)$ becomes a Hopf *-algebra where * is defined by $\overline{w}=v^c$, $v=BwB^{-1}$, $B=\mathbb{1}$ for $\mathrm{SU}_q(2)$, $B=\mathrm{diag}(1,-1)$ for $\mathrm{SU}_q(1,1)$, $q\in\mathbf{R}\backslash\{0\}$ (cf. Refs. 15, 16, and 4); $\overline{w}=w$ for $\mathrm{SL}_q(2,\mathbf{R})$, $|q|=1$ (cf. Ref. 16 and Proposition 5). For $\mathrm{SU}_q(2)$, $\mathrm{SU}_q(1,1)$ we get CQT Hopf *-algebras iff L_1 is Hermitian wrt the canonical scalar product in $\mathbf{C}^2$ (see Proposition 6.2 with $M=\{w\}$ and the proof of Theorem 1.4.6 of Ref. 4) iff $q>0$. For $\mathrm{SL}_q(2,\mathbf{R})$ we get CQT Hopf*-algebras iff $\tau L_1\tau=L_1$ (see Proposition 6.2 with $M=\{w\}$) iff $q=1$. So we have CT Hopf*-algebras iff $q=1$ (for each real form).

IV. QUASITRIANGULAR STRUCTURES ON INHOMOGENEOUS QUANTUM GROUPS

For any Hopf algebra $\mathrm{Poly}(H)=(\mathscr{A},\Delta)$ satisfying certain properties one can construct[1] a Hopf algebra $\mathrm{Poly}(G)=(\mathscr{B},\Delta)$ which describes an inhomogeneous quantum group. For certain CQT Hopf algebra structures $(\mathscr{A},\Delta,\mathscr{R}_{\mathscr{A}})$ we find all CQT Hopf algebra structures $(\mathscr{B},\Delta,\mathscr{R})$ such that $\mathscr{R}_{|\mathscr{A}\otimes\mathscr{A}}=\mathscr{R}_{\mathscr{A}}$. The *-structures and cotriangularity are studied as well. In particular, we find all C(Q)T Hopf (*-) algebra structures on quantum Poincaré groups.

Throughout this section $\mathrm{Poly}(H)=(\mathscr{A},\Delta)$ is any bialgebra such that

(a) each representation of H is completely reducible,
(b) Λ is an irreducible representation of H,
(c) $\mathrm{Mor}(v\otimes w,\Lambda\otimes v\otimes w)=\{0\}$ for any two irreducible representations v,w of H.

Moreover, we assume that f_{ij}, $\eta_i\in\mathscr{A}'$, $T_{ij}\in\mathbf{C}$, $i,j=1,\ldots,N=\dim\Lambda$, are given and satisfy

(1) $\mathscr{A}\ni a\to\rho(a)=\begin{pmatrix}f(a) & \eta(a)\\ 0 & \varepsilon(a)\end{pmatrix}\in M_{N+1}(\mathbf{C})$ is a unital homomorphism,
(2) $\Lambda_{st}(f_{tr}*a)=(a*f_{st})\Lambda_{tr}$ for $a\in\mathscr{A}$,
(3) $R^2=\mathbb{1}$, where $R_{ij,sm}=f_{im}(\Lambda_{js})$,
(4) $(\Lambda\otimes\Lambda)_{kl,ij}(\tau^{ij}*a)=a*\tau^{kl}$ for $a\in\mathscr{A}$ where $\tau^{jj}=(R-\mathbb{1})_{\mathrm{ij,mn}}(\eta_n*\eta_m-\eta_m(\Lambda_{ns})\eta_s+T_{mn}\varepsilon-f_{nb}*f_{ma}T_{ab})$,

(5) $A_3\widetilde{F}=0$ where $A_3=1\otimes 1\otimes 1-R\otimes 1-1\otimes R+(R\otimes 1)(1\otimes R)+(1\otimes R)(R\otimes 1)-(R\otimes 1)(1\otimes R)(R\otimes 1)$, $\widetilde{F}_{ijk,m}=\tau^{ij}(\Lambda_{km})$,
(6) $A_3(Z\otimes 1-1\otimes Z)T=0$, $RT=-T$ where $Z_{ij,k}=\eta_i(\Lambda_{jk})$.

In particular, (4) and (5) are satisfied if $\tau^{ij}=0$.

The inhomogeneous quantum group G corresponds to the bialgebra $\mathrm{Poly}(G)=(\mathscr{B},\Delta)$ defined (cf. Corollary 3.8.*a* of Ref. 1) as follows: $\mathscr{B}$ is the universal unital algebra generated by $\mathscr{A}$ and y_i, $i=1,\ldots,N$, with the relations $I_{\mathscr{B}}=I_{\mathscr{A}}$,

$$y_s a=(a*f_{st})y_t+a*\eta_s-\Lambda_{st}(\eta_t*a),\quad a\in\mathscr{A}, \tag{IV.1}$$

$$(R-1)_{kl,ij}(y_i y_j-\eta_i(\Lambda_{js})y_s+T_{ij}-\Lambda_{im}\Lambda_{jn}T_{mn})=0. \tag{IV.2}$$

Moreover, $(\mathscr{A},\Delta)$ is a subbialgebra of $(\mathscr{B},\Delta)$ and $\Delta y_i=\Lambda_{ij}\otimes y_j+y_i\otimes I$ (y_i were denoted by p_i in Ref. 1). In particular, $\mathscr{P}=\left(\begin{smallmatrix}\Lambda & y\\ 0 & 1\end{smallmatrix}\right)$ is a representation of G.

Remark 3: If H is a matrix group, Λ its fundamental representation, and $(\mathscr{A},\Delta)$ its corresponding Hopf algebra (generated by Λ_{ij}, Λ_{ij}^{-1}), then, assuming (a)–(c) above and setting $f_{ij}=\delta_{ij}\varepsilon$, $\eta_i=0$, and $T=0$, $(\mathscr{B},\Delta)$ corresponds to

$$G=H\ltimes\mathbf{R}^N=\left\{g=\begin{pmatrix}h & a\\ 0 & 1\end{pmatrix}\in M_{N+1}(\mathbf{C}):h\in H,a\in\mathbf{R}^N\right\},$$

$f(g)=f(h)$, $y_i(g)=a_i$, $f\in\mathscr{A}$, $i=1,\ldots,N$, $g\in G$.

According to Corollary 3.8.*b* and the proof of Proposition 3.12 of Ref. 1, the bialgebra $(\mathscr{B},\Delta)$ can be obtained by the construction of Proposition 1 with $\{w^\alpha:\alpha\in\mathscr{I}\}=\mathrm{Irr}\,H\cup\{\mathscr{P}\}$. Here the relations (II.1) mean that $w^0\equiv(I_{\mathscr{A}})=(I_{\mathscr{B}})$ and the relations (II.2) are given by

$$(\mathscr{P}\otimes\mathscr{P})R_P=R_P(\mathscr{P}\otimes\mathscr{P}), \tag{IV.3}$$

$$(\mathscr{P}\otimes w)N_w=N_w(w\otimes\mathscr{P}),\quad w\in\mathrm{Irr}\,H, \tag{IV.4}$$

$$(w\otimes w')S^{\alpha}_{ww'w''}=S^{\alpha}_{ww'w''}w'',\quad w,w',w''\in\mathrm{Irr}\,H,\ \ \alpha=1,\ldots,c^{w''}_{ww'}, \tag{IV.5}$$

$$\mathscr{P}i=i\Lambda, \tag{IV.6}$$

$$s\mathscr{P}=w^0 s, \tag{IV.7}$$

where

$$R_P=\begin{pmatrix}R & Z & -R\cdot Z & (R-1)T\\ 0 & 0 & 1 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 0 & 1\end{pmatrix},\quad N_w=\begin{pmatrix}G_w, & H_w\\ 0 & 1\end{pmatrix}, \tag{IV.8}$$

$(G_w)_{iC,Dj}=f_{ij}(w_{CD})$, $(H_w)_{iC,D}=\eta_i(w_{CD})$, $w\in\mathrm{Rep}\,H$, $R=G_\Lambda$, $Z=H_\Lambda$, $S^{\alpha}_{ww'w''}(\alpha=1,\ldots,c^{w''}_{ww'})$ form a basis of $\mathrm{Mor}(w'',w\otimes w')$, $i:\mathbf{C}^N\to\mathbf{C}^N\oplus\mathbf{C}$, $s:\mathbf{C}^N\oplus\mathbf{C}\to\mathbf{C}$ are the canonical mappings. In the following we assume that $(\mathscr{A},\Delta)$ is a Hopf algebra. Then (Proposition 3.12 of Ref. 1) $(\mathscr{B},\Delta)$ is also a Hopf algebra and G_w^{-1} exist:

$$(G_w^{-1})_{Ak,lB}=f_{kl}(w^{-1}_{AB}). \tag{IV.9}$$

If $(\mathscr{A},\Delta)$ is a Hopf*-algebra, then we also assume $\overline{\Lambda}=\Lambda$,

$$f_{ij}(S(a^*))=\overline{f_{ij}(a)},\ \eta_i(S(a^*))=\overline{\eta_i(a)},\quad i,j=1,\ldots,N,a\in\mathscr{A}, \tag{IV.10}$$

$\widetilde{T}-T\in\mathrm{Mor}(w^0,\Lambda\otimes\Lambda)$, where $\widetilde{T}_{ij}=\overline{T_{ji}}$. Then [1] $(\mathscr{B},\Delta)$ has a unique Hopf*-algebra structure such that $(\mathscr{A},\Delta)$ is its Hopf*-subalgebra and $y_i^*=y_i$.

In the following we assume $\mathrm{Mor}(I,\Lambda\otimes\Lambda)\cap\ker(R+\mathbb{1})=\{0\}$, i.e., $\mathrm{Mor}(I,\Lambda\otimes\Lambda)\subset\ker(R-\mathbb{1})$. Then [using (4.14) of Ref. 1] $\widetilde{T}=T$. The main result of the present paper is contained in the following.

Theorem 2: Let $\mathrm{Poly}(H)=(\mathscr{A},\Delta)$ and $\mathrm{Poly}(G)=(\mathscr{B},\Delta)$ be as above, $(\mathscr{A},\Delta,\mathscr{R}_{\mathscr{A}})$ be a CQT Hopf algebra such that

$$R^{v\Lambda}=c_vG_v,\quad R^{\Lambda v}=c_v'G_v^{-1},\quad v\in\mathrm{Irr}\,H, \tag{IV.11}$$

$c_v,c_v'\in\mathbf{C}\setminus\{0\}$. We are interested in CQT Hopf algebra structures $(\mathscr{B},\Delta,\mathscr{R})$ such that

$$\mathscr{R}_{|\mathscr{A}\otimes\mathscr{A}}=\mathscr{R}_{\mathscr{A}}. \tag{IV.12}$$

One has the following.

(1) Such a structure exists iff

$$\tau^{ij}=0,\quad i,j=1,\ldots,N, \tag{IV.13}$$

$$R^{v\Lambda}=G_v,\quad R^{\Lambda v}=G_v^{-1},\quad v\in\mathrm{Irr}\,H. \tag{IV.14}$$

(2) Suppose (IV.13) and (IV.14). Then such structures are in one-to-one correspondence with $m\in\mathrm{Mor}(w^0,\Lambda\otimes\Lambda)$ satisfying

$$(f_{jb}*f_{ia})m_{ab}=m_{ij}\varepsilon,\quad i,j=1,\ldots,N, \tag{IV.15}$$

and are determined by

$$R^{vw}=R^{vw}\ \text{ for }\ \mathscr{R}_{\mathscr{A}},\quad v,w\in\mathrm{Irr}\,H, \tag{IV.16}$$

$$R^{v\mathscr{P}}=N_v,\quad R^{\mathscr{P}v}=N_v^{-1},\quad v\in\mathrm{Irr}\,H, \tag{IV.17}$$

$$R^{\mathscr{P}\mathscr{P}}=R_P+m_P, \tag{IV.18}$$

where

$$m_P=\begin{pmatrix}0&0&0&m\\0&0&0&0\\0&0&0&0\\0&0&0&0\end{pmatrix}. \tag{IV.19}$$

(3) Let $\mathscr{R}$ be as in (2) and let $(\mathscr{A},\Delta)$ and $(\mathscr{B},\Delta)$ be Hopf*-algebras as in the text before the Theorem. Then $(\mathscr{B},\Delta,\mathscr{R})$ is a CQT Hopf*-algebra iff $(\mathscr{A},\Delta,\mathscr{R}_{\mathscr{A}})$ is a CQT Hopf*-algebra and

$$m_{ij}=\overline{m_{ji}},\quad i,j=1,\ldots,N. \tag{IV.20}$$

(4) Let $\mathscr{R}$ be as in (2). Then $(\mathscr{B},\Delta,\mathscr{R})$ is a CT Hopf algebra iff $(\mathscr{A},\Delta,\mathscr{R}_{\mathscr{A}})$ is a CT Hopf algebra and $m=0$.

Proof: Ad 1 and 2: Each such structure is (see Theorem 1) uniquely determined by R^{vw}, $R^{v\mathscr{P}}$, $R^{\mathscr{P}v}$, and $R^{\mathscr{P}\mathscr{P}}$ satisfying (II.15)–(II.17) [we assume (II.14)], $v,w\in\mathrm{Irr}\,H$. Using (IV.12), we

get (IV.16). In virtue of the properties of $\mathscr{R}_{\mathscr{A}}$ the formula (II.17) for R^{vw} follows. Moreover, (II.15) and (II.16) for (IV.6) and $w^\gamma = v \in \mathrm{Irr}\, H$ mean $R^{v\mathscr{P}}(1 \otimes i) = (i \otimes 1)R^{v\Lambda}$, $R^{\mathscr{P}v}(i \otimes 1) = (1 \otimes i)R^{\Lambda v}$. That and (IV.11) give

$$R^{v\mathscr{P}} = c_v \begin{pmatrix} G_v, & ? \\ 0, & ? \end{pmatrix} = c_v N_v, \quad R^{\mathscr{P}v} = c_v' \begin{pmatrix} G_v^{-1} & ? \\ 0 & ? \end{pmatrix} = c_v' N_v^{-1},$$

where the second equalities follow from (II.17) for $R^{v\mathscr{P}}, R^{\mathscr{P}v}$, (IV.4), the independence of I, $y_i (i = 1,\ldots,N)$ over $\mathscr{A}$ [in left and also in right module, see Corollary 3.6 and (1.4) of Ref. 1] and the condition (c). Using (II.15) and (II.16) for (IV.7) and $w^\gamma = v \in \mathrm{Irr}\, H$, one obtains $c_v = c_v' = 1$; we get (IV.14), (IV.17). In virtue of (II.15) and (II.16) for (IV.6) and (IV.7) and $w^\gamma = \mathscr{P}$,

$$R^{\mathscr{P}\mathscr{P}} = \begin{pmatrix} R & Z & -R \cdot Z & ? \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = R_P + m_P$$

for some $m \in \mathrm{Mor}(w^0, \Lambda \otimes \Lambda)$ where the second equality uses (II.17) for $R^{\mathscr{P}\mathscr{P}}$, (IV.3), and (IV.19). Thus (IV.18) follows. We set $R_Q = R_P + m_P = R^{\mathscr{P}\mathscr{P}}$ and replace (IV.3) by equivalent [assuming (IV.5)] relation

$$(\mathscr{P} \otimes \mathscr{P}) R_Q = R_Q (\mathscr{P} \otimes \mathscr{P}). \tag{IV.21}$$

The relations (II.15) and (II.16) for (IV.21), (IV.4), and any $w^\gamma \in \mathrm{Irr}\, H \cup \{\mathscr{P}\}$ are equivalent to

$$(R_Q \otimes 1)(1 \otimes R_Q)(R_Q \otimes 1) = (1 \otimes R_Q)(R_Q \otimes 1)(1 \otimes R_Q), \tag{IV.22}$$

$$(1 \otimes N_v)(N_v \otimes 1)(1 \otimes R_Q) = (R_Q \otimes 1)(1 \otimes N_v)(N_v \otimes 1), \quad v \in \mathrm{Irr}\, H, \tag{IV.23}$$

$$(1 \otimes R^{vw})(N_v \otimes 1)(1 \otimes N_w) = (N_w \otimes 1)(1 \otimes N_v)(R^{vw} \otimes 1), \quad v, w \in \mathrm{Irr}\, H. \tag{IV.24}$$

According to Proposition 3.14 of Ref. 1 and its proof, (IV.22) is equivalent to $\widetilde{F} = 0$. Let us denote the standard basis elements in $\mathbf{C}^{\dim v}$, $v \in \mathrm{Irr}\, H$, by h_i^v, $i = 1,\ldots,\dim v$, $e_i = h_i^\Lambda$, and in $\mathbf{C}$ by $f = 1$. Using (3.65) of Ref. 1 and

$$N_v(h_i^v \otimes e_j) = (G_v)_{kl,ij} e_k \otimes h_l^v,$$

$$N_v(h_i^v \otimes f) = f \otimes h_i^v + (H_v)_{kl,i} e_k \otimes h_l^v,$$

we find that (IV.23) on $h_i^v \otimes e_j \otimes e_k$ follows from the last formula before Proposition 3.14 in Ref. 1; on $h_i^v \otimes e_j \otimes f$, $h_i^v \otimes f \otimes e_j$ follows from (2.18) of Ref. 1; on $h_i^v \otimes f \otimes f$ is equivalent (using $Rm = m$) to $\tau^{ij}(v_{AB}) = 0$ and (IV.15) applied to v_{AB} for all i,j,A,B. So (IV.23) is equivalent to (IV.13) (which implies $\widetilde{F} = 0$) and (IV.15). We also get that (IV.24) on $h_i^v \otimes h_j^w \otimes e_k$ follows from $(1 \otimes R^{vw})(R^{v\Lambda} \otimes 1)(1 \otimes R^{w\Lambda}) = (R^{w\Lambda} \otimes 1)(1 \otimes R^{v\Lambda})(R^{vw} \otimes 1)$ [it can be obtained using (II.13) and (II.8) for $\mathscr{R}_{\mathscr{A}}$; cf. Refs. 6, 8, and (1.14) of Ref. 4]; on $h_i^v \otimes h_j^w \otimes f$ follows from the equality obtained by acting η_i on (II.17) for R^{vw} and using condition (1) (see the beginning of the Section).

The relations (II.15) and (II.16) for (IV.5) and $w^\gamma \in \mathrm{Irr}\, H$ follow from (II.8) and (II.11) for $\mathscr{R}_{\mathscr{A}}$ while for $w^\gamma = \mathscr{P}$ they are equivalent to

$$(N_w \otimes 1)(1 \otimes N_{w'})(S^\alpha_{ww'w''} \otimes 1) = (1 \otimes S^\alpha_{ww'w''}) N_{w''}.$$

That on $h_i^{w''} \otimes e_j$ follows from (II.8) and (II.11) for $\mathscr{R}_{\mathscr{A}}$ and on $h_i^{w''} \otimes f$ that follows from the equality obtained by acting η_i on (IV.5).

Ad 3: We need to check (II.20) for $M=\mathrm{Irr}\,H\cup\{\mathscr{P}\}$. For R^{vw}, $v,w\in\mathrm{Irr}\,H$, it is equivalent to the fact that $(\mathscr{A},\Delta,\mathscr{R}_{\mathscr{A}})$ is a CQT Hopf*-algebra; for $R^{\mathscr{P}v}$ and $R^{v\mathscr{P}}$ follows from (IV.9), (IV.10), and the properties of η_i; for $R^{\mathscr{P}\mathscr{P}}$ it is equivalent [using (4.14) and the next formula of Ref. 1, $Rm=m$, $RT=-T$] to (IV.20).

Ad 4: We need to check (II.21) for $M=\mathrm{Irr}\,H\cup\{\mathscr{P}\}$. For R^{vw}, $v,w\in\mathrm{Irr}\,H$, it is equivalent to the fact that $(\mathscr{A},\Delta,\mathscr{R}_{\mathscr{A}})$ is a CT Hopf algebra; for $R^{\mathscr{P}v}$ and $R^{v\mathscr{P}}$ follows from (IV.17); for $R^{\mathscr{P}\mathscr{P}}$ it is equivalent (using $R_P^2=1$) to $m=0$. □

Remark: If the first formula of the condition (6) is replaced by $0\neq A_3(Z\otimes 1-1\otimes Z)T\in\mathrm{Mor}(I,\Lambda\otimes\Lambda\otimes\Lambda)$ (this is allowed by Ref. 1), then (IV.22) is not satisfied and there is no CQT Hopf algebra structure on $(\mathscr{B},\Delta)$.

As an application we shall consider $(\mathscr{A},\Delta)=\mathrm{Poly}(L)$ where L is a quantum Lorentz group. The corresponding inhomogeneous quantum groups are called quantum Poincaré groups and are (almost) classified in Ref. 2. The classification of C(Q)T Hopf (*-) algebra structures on them is given in the following.

Theorem 3: Let $\mathrm{Poly}(P)=(\mathscr{B},\Delta)$ be the Hopf *-algebra corresponding to a quantum Poincaré group P (Ref. 2) described by an admissible choice of quantum Lorentz group [cases (1)–(7)], $s=\pm 1$, H and T.

(1) Let us consider CQT Hopf algebra structures $(\mathscr{B},\Delta,\mathscr{R})$ on P. One has:
(a)In the cases (1) (except $s=1$, $t=1$, $t_0\neq 0$, see Remark 1.8 of Ref. 2), (2), (3), (4) (except $s=1$, $b\neq 0$), (5) (except $s=\pm 1$, $t=1$, $t_0\neq 0$), (6), and (7) each such structure is uniquely determined by

$$R^{ww}=kL,\quad R^{w\overline{w}}=kX,\quad R^{\overline{w}w}=qkX^{-1},\quad R^{\overline{w}\overline{w}}=qk\widetilde{L}$$

and (IV. 17)–(IV.19), where

$$m=cm_0,\quad m_0=(V^{-1}\otimes V^{-1})(1\otimes X\otimes 1)(E\otimes\tau E),\quad L=sq^{1/2}(1+q^{-1}EE'),\quad \widetilde{L}=q\tau L\tau,$$

where $s=\pm 1$, E,E' are fixed for fixed P and given in Ref. 2, and $k=\pm 1$ (two possible $\mathscr{R}$ for each $c\in\mathbf{C}$).
(b) In the other cases there is no such structure.

(2) Let $\mathscr{R}$ be as in (1). We get CQT Hopf*-algebra iff $q=1$ [which excludes the cases (5)–(7)] and $c\in\mathbf{R}$.

(3) Let $\mathscr{R}$ be as in (1). We get CT Hopf algebra iff $q=1$ [which excludes the cases (5)–(7)] and $c=0$ (then it is also CT Hopf*-algebra).

Proof: Ad 1: We shall use Theorem 2, the results of Ref. 2, and Section III. Thus H is a quantum Lorentz group, $\Lambda=V^{-1}(w\otimes\overline{w})V$ with $V_{CD,i}=(\sigma_i)_{CD}$ ($\sigma_0=1,\sigma_1,\sigma_2,\sigma_3$ are the Pauli matrices), $q=\beta=\pm 1$, and the assumptions about H and G are satisfied. Moreover, $G_w=(V^{-1}\otimes 1)(1\otimes X)(L\otimes 1)(1\otimes V)$ and $G_{\overline{w}}=(V^{-1}\otimes 1)(1\otimes\widetilde{L})(X^{-1}\otimes 1)(1\otimes V)$, where $L=sq^{1/2}(1+q^{-1}EE')$ and $\widetilde{L}=q\tau\overline{L^{-1}}\tau=q\tau L\tau$. The possible η and T are described in Ref. 2. According to the results of Section III, each CQT Hopf algebra structure on $(\mathscr{A},\Delta)$ is uniquely characterized by $R^{ww}=\epsilon_L L$, $R^{\overline{w}\overline{w}}=\epsilon_L'\widetilde{L}$, $R^{w\overline{w}}=\epsilon_X X$, and $R^{\overline{w}w}=\epsilon_X' X^{-1}$, where $\epsilon_L^2=\epsilon_L'^2=\epsilon_X^2=\epsilon_X'^2=1$ (16 possible $\mathscr{R}_{\mathscr{A}}$). Using (II.8), (II.9), (II.11), and (II.12), one gets (IV.11) for $v=w,\overline{w}$ with $c_w=\epsilon_L\epsilon_X$, $c_{\overline{w}}=\epsilon_L'\epsilon_X'$, $c_w'=q\epsilon_L\epsilon_X'$, and $c_{\overline{w}}'=q\epsilon_X\epsilon_L'$. In virtue of Proposition 2.1 of Ref. 2 and (II.8), (II.9), (II.11) and (II.12), the condition (IV.11) is satisfied for all $v\in\mathrm{Irr}\,H$.

Due to Proposition 3.13.2 and Proposition 4.8 of Ref. 1, (IV. 13) is equivalent to $\tau^{ij}(w_{AB})=0$, $i,j=0,1,2,3$, $A,B=1,2$, which means (cf. the proof of Theorem 1.6 of Ref. 2) $\lambda=0$, which excludes the case (4), $s=1$, $b\neq 0$, the case (1), $s=1$, $t=1$, $t_0\neq 0$, and the case (5), $s=\pm 1$, $t=1$, $t_0\neq 0$, where $t_0\in\mathbf{R}$ is introduced in Remark 1.8 of Ref. 2. Moreover, (IV.14) means that $\epsilon_X'=\epsilon_L'$

$=qk$, $\epsilon_X=\epsilon_L=k$ for some $k=\pm 1$. Using Theorem 2.1–2, $\mathrm{Mor}(w^0,\Lambda\otimes\Lambda)=\mathbf{C}m_0$ and (IV.15) for $m=m_0$ (it is enough to prove it on w_{AB}, w_{AB}^* when it follows from the 20 relations considered in Section III), we get (1).

Ad 2: We use $q=\beta=1$ (which implies $q_j=q_i^{-1}$), $(m_0)_{ij}=\overline{(m_0)_{ji}}$ and Theorem 2.3.

Ad 3: We use $q=1$ (which implies $\epsilon_X'=\epsilon_X$) and Theorem 2.4. ■

V. ENVELOPING ALGEBRAS

In this section we study enveloping algebras of inhomogeneous quantum groups. We assume that $(\mathscr{A},\Delta,\mathscr{R}_{\mathscr{A}})$ and $(\mathscr{B},\Delta,\mathscr{R})$ are CQT Hopf algebras as in Theorem 2.1–2 (e.g., as in Theorem 3.1).

We essentially follow the scheme of Refs. 16 and 17, but now we do not assume $Z=T=0$. We define $l_{jl}\in\mathscr{B}'$, $j,l=1,\ldots,N,+$, by

$$l_{jl}(x)=\mathscr{R}(x\otimes\mathscr{P}_{jl}) \tag{V.1}$$

(in the CT case l corresponds to $L^{\pm}$ of Ref. 16 on the subalgebra generated by $\mathscr{P}_{ac}$). According to (II.5) and (II.13) for $v=w=\mathscr{P}$,

$$\begin{aligned}R^{\mathscr{P}\mathscr{P}}_{ab,cd}l_{df}(x^{(1)})l_{ce}(x^{(2)})&=R^{\mathscr{P}\mathscr{P}}_{ab,cd}\mathscr{R}(x^{(1)}\otimes\mathscr{P}_{df})\mathscr{R}(x^{(2)}\otimes\mathscr{P}_{ce})\\&=\mathscr{R}(x\otimes R^{\mathscr{P}\mathscr{P}}_{ab,cd}\mathscr{P}_{ce}\mathscr{P}_{df})\\&=\mathscr{R}(x\otimes\mathscr{P}_{ac}\mathscr{P}_{bd}R^{\mathscr{P}\mathscr{P}}_{cd,ef})\\&=\mathscr{R}(x^{(1)}\otimes\mathscr{P}_{bd})\mathscr{R}(x^{(2)}\otimes\mathscr{P}_{ac})R^{\mathscr{P}\mathscr{P}}_{cd,ef}\\&=l_{bd}(x^{(1)})l_{ac}(x^{(2)})R^{\mathscr{P}\mathscr{P}}_{cd,ef},\end{aligned}$$

hence

$$R^{\mathscr{P}\mathscr{P}}_{ab,cd}(l_{df}*l_{ce})=(l_{bd}*l_{ac})R^{\mathscr{P}\mathscr{P}}_{cd,ef},\quad a,b,e,f=1,\ldots,N,+. \tag{V.2}$$

Setting $l_{ab}=L_{ab}$, $l_{a+}=M_a$, and using $l_{+a}=0$, $l_{++}=\epsilon$, $a,b=1,\ldots,N$, and (IV.18), (V.2) is equivalent to

$$R_{ab,cd}(L_{df}*L_{ce})=(L_{bd}*L_{ac})R_{cd,ef}, \tag{V.3}$$

$$R_{ab,cd}(M_d*L_{ce})+Z_{ab,c}L_{ce}=(L_{bd}*L_{ac})Z_{cd,e}+L_{be}*M_a, \tag{V.4}$$

$$R_{ab,cd}(L_{df}*M_c)-(RZ)_{ab,d}L_{df}=-(L_{bd}*L_{ac})(RZ)_{cd,f}+M_b*L_{af}, \tag{V.5}$$

$$R_{ab,cd}M_d*M_c+Z_{ab,c}M_c-(RZ)_{ab,d}M_d+s_{ab}\epsilon=(L_{bd}*L_{ac})s_{cd}+M_b*M_a, \tag{V.6}$$

$a,b,e,f=1,\ldots,N$, where $s=(R-1)T+m$. Let us notice that (V.5) follows from (V.3) and (V.4). Moreover, using (II.4), (II.3), $l_{ac}(xy)=l_{ab}(x)l_{bc}(y)$, $l_{ac}(I)=\delta_{ac}$, $a,c=1,\ldots,N,+,x,y\in\mathscr{B}$. Thus $L_{ac}(I)=\delta_{ac}$, $M_a(I)=0$,

$$L_{ac}(xy)=L_{ab}(x)L_{bc}(y), \tag{V.7}$$

$$M_a(xy)=L_{ab}(x)M_b(y)+M_a(x)\epsilon(y), \tag{V.8}$$

$a,b=1,\ldots,N,x,y\in\mathscr{B}$. Also $l_{jl}(\mathscr{P}_{ab})=\mathscr{R}(\mathscr{P}_{ab}\otimes\mathscr{P}_{jl})=R^{\mathscr{P}\mathscr{P}}_{ja,bl}$, $l_{jl}(w_{AB})=\mathscr{R}(w_{AB}\otimes\mathscr{P}_{jl})=R^{w\mathscr{P}}_{jA,Bl}=(N_w)_{jA,Bl}$ [see (V.1), (II.7), (IV.17), and (IV.8)], $a,b,j,l=1,\ldots,N,+,A,B=1,\ldots,\dim w, w\in\mathrm{Rep}\,H$. Therefore

$$L_{jl}(\Lambda_{ab})=R_{ja,bl}, \tag{V.9}$$

$$L_{jl}(y_a)=-(RZ)_{ja,l}, \tag{V.10}$$

$$L_{jl}(w_{AB})=(G_w)_{jA,Bl}, \tag{V.11}$$

$$M_j(\Lambda_{ab})=Z_{ja,b}, \tag{V.12}$$

$$M_j(y_a)=s_{ja}, \tag{V.13}$$

$$M_j(w_{AB})=(H_w)_{jA,B}, \tag{V.14}$$

$a,b,j,l=1,\ldots,N, A,B=1,...,$ dim $w, w\in \mathrm{Rep}\, H$. It is clear that l_{jl} generate a unital subalgebra of $\mathscr{B}'$(wrt convolution $*$). Endowing it with Δ' of Remark 2, we get a bialgebra U with l as its corepresentation. Adding $l^{(m)}_{ij}=l_{ij}\circ S^m$, one obtains a Hopf algebra $\hat{U}$ with coinverse $S'(l^{(m)})=l^{(m+1)}$ and corepresentations $l^{(2k)}$, $(l^{(2k+1)})^T$, $k=0,1,2,\ldots$. Acting S'^m on (V.2), one obtains

$$R^{\mathscr{P}\mathscr{P}}_{ab,cd}(l^{(2k)}_{df}*l^{(2k)}_{ce})=(l^{(2k)}_{bd}*l^{(2k)}_{ac})R^{\mathscr{P}\mathscr{P}}_{cd,ef},$$

$$R^{\mathscr{P}\mathscr{P}}_{ab,cd}(l^{(2k+1)}_{ce}*l^{(2k+1)}_{df})=(l^{(2k+1)}_{ac}*l^{(2k+1)}_{bd})R^{\mathscr{P}\mathscr{P}}_{cd,ef}.$$

Here $\hat{U}$ is called enveloping algebra of $(\mathscr{B},\Delta)$. It can be sometimes too small. It happens, e.g., in the classical case (see Remark 3) with $\mathscr{R}=\epsilon\otimes\epsilon$ when $\hat{U}=\mathbf{C}\epsilon$ (cf. also Ref. 18).

Notice that $L_{jl}|_{\mathscr{A}}=f_{jl}$, $M_j|_{\mathscr{A}}=\eta_a$, $l_{|\mathscr{A}}=\rho$. According to the proof of Theorem 1, there exists antihomomorphism $\theta:\mathscr{B}\to\mathscr{B}'$ (given by $\mathscr{R}$) such that $\theta(\Lambda_{jl})=L_{jl}$, $\theta(y_j)=M_j$, $\theta(I)=\epsilon$. Therefore the formulas (3.60), (3.46), and (1.12) of Ref. 1 yield (V.4), (V.6) [with s replaced by $(R-1)T$], and (V.3) which give

$$f_{be}*\eta_a=R_{ab,cd}\eta_d*f_{ce}+Z_{ab,c}f_{ce}-(f_{bd}*f_{ac})Z_{cd,e}$$

[cf. (2.18) of Ref. 1], the condition $\tau^{jj}=0$, and the last formula before Proposition 3.14 in Ref. 1. Suppose $(\Lambda\otimes\Lambda)k=kw^0$, $n(\Lambda\otimes\Lambda)=w^0n$ $[w^0=(I_{\mathscr{B}})]$. Applying θ, we get

$$(L_{bd}*L_{ac})k_{cd}=k_{ab}\epsilon,\quad n_{ab}(L_{bd}*L_{ac})=n_{cd}\epsilon,\quad a,b,c,d=1,\ldots,N. \tag{V.15}$$

Let us set $X_{lj}=L_{jl}\circ S\in\hat{U}$, $j,l=1,\ldots,N$. Then

$$X_{ik}(xy)=X_{ij}(x)X_{jk}(y),\quad X_{ik}(I)=\delta_{ik}, x,y\in\mathscr{B}, \tag{V.16}$$

$$X_{ik}(a)=f_{ki}(S(a)),\quad a\in\mathscr{A}, i,k=1,\ldots,N. \tag{V.17}$$

Using the last equation in the proof of Proposition 3.12 of Ref. 1, (V.7), (IV.9), and (V.10), we obtain

$$X_{ik}(y_l)=Z_{lk,i}. \tag{V.18}$$

Moreover, (V.15) yields

$$k_{ab}(X_{ac}*X_{bd})=k_{cd}\epsilon,\quad (X_{ac}*X_{bd})n_{cd}=n_{ab}\epsilon. \tag{V.19}$$

As in the proof of Proposition 3.1.2 of Ref. 3, there exists a unital homomorphism $X:\mathscr{B}\to M_{N+1}(\mathbf{C})$ such that

$$X=\begin{pmatrix} (X_{jl})_{j,l=1}^{N} & (Y_j)_{j=1}^{N} \\ 0 & \epsilon \end{pmatrix}$$

for some $Y_j \in \mathscr{B}'$ satisfying $Y_j(a)=0$, $a \in \mathscr{A}$, $Y_j(y_k)=\delta_{jk}$, $j,k=1,\ldots,N$. Setting $X_{j+}=Y_j$, $X_{+j}=0$, $X_{++}=\epsilon$, $j=1,\ldots,N$, the commutation relations among X_{ij}, $i,j=1,\ldots,N,+$, are the same as in (3.7) of Ref. 3, i.e.,

$$(X_{ab}*X_{cd})K_{bd,st}=K_{ac,bd}(X_{bs}*X_{dt}), \quad a,c,s,t=1,\ldots,N,+, \tag{V.20}$$

where

$$K=\begin{pmatrix} R^T & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

[it is also possible to replace K in (V.20) by $K+n_P$, where $n \in \mathrm{Mor}(\Lambda\otimes\Lambda, w^0)$; see (IV.19) and (V.19)].

Defining $X_{ij}^{(m)}=X_{ij}\circ S^m$, $i,j=1,\ldots,N,+$, $m=0,1,2,\ldots$, one gets a Hopf algebra $\hat{V}$ generated (as a unital algebra) by $1_{ij}^{(m)}$ and $X_{ij}^{(m)}$. Clearly $S'(X^{(m)})=X^{(m+1)}$; $X^{(2k)}$, $[X^{(2k+1)}]^T$, $k=0,1,\ldots$, are corepresentations of $\hat{V}$. Letting S' act on (V.20), one obtains

$$(X_{ab}^{(2k)}*X_{cd}^{(2k)})K_{bd,st}=K_{ac,bd}(X_{bs}^{(2k)}*X_{dt}^{(2k)}),$$

$$(X_{cd}^{(2k+1)}*X_{ab}^{(2k+1)})K_{bd,st}=K_{ac,bd}(X_{dt}^{(2k+1)}*X_{bs}^{(2k+1)}).$$

Here $\hat{V}$ is called enlarged enveloping algebra of $(\mathscr{B},\Delta)$. It would be interesting to find the commutation relations between M_i and Y_j.

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Integration on quantum Euclidean space and sphere

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Invariant integrals of functions and forms over q-deformed Euclidean space and spheres in N dimensions are defined and shown to be positive definite, compatible with the star structure and to satisfy a cyclic property involving the D matrix of $SO_q(N)$. The definition is based on spherical and radial integration. Stokes theorem is proved with and without spherical boundary terms, as well as on the sphere. © *1996 American Institute of Physics.* [S0022-2488(96)03409-3]

I. INTRODUCTION

In recent years, there has been much interest in formulating physics and, in particular, field theory on quantized, i.e., noncommutative space–time. One of the motivations is that if there are no more ''points'' in space–time, such a theory should be well behaved in the UV. The concept of integration on such a space can certainly be expected to be an essential ingredient. In the simplest case of the quantum plane, such an integral was first introduced by Wess and Zumino;[1] also see Ref. 2. In the presumably more physical case of quantum Euclidean space,[3] the Gaussian integration method was proposed by a number of authors.[4,6] However, it is tedious to calculate, except in the simplest cases, and its properties have never been investigated thoroughly; in particular, we point out that determining the class of integrable functions is a rather subtle issue.

In this paper, we will give a different definition based on spherical integration in N dimensions and investigate its properties in detail. Although this idea has already appeared in the literature,[7] it has not been developed very far. We first show that there is a unique invariant integral over the quantum Euclidean sphere, and prove that it is positive definite and satisfies a cyclic property involving the D matrix of $SO_q(N)$. The integral over quantum Euclidean space is then defined by radial integration, both for functions and N forms. One naturally obtains a large class of integrable functions. It turns out not to be determined uniquely by rotation and translation invariance (=Stokes theorem) alone; it is unique after, e.g., imposing a general scaling law. It is positive definite as well and thus allows us to define a Hilbert space of square-integrable functions, and satisfies the same cyclic property. The cyclic property also holds for the integral of N and $N-1$-forms over spheres, which leads to a simple, truly noncommutative proof of Stokes theorem on Euclidean space with and without spherical boundary terms, as well as on the sphere. These proofs only work for $q\neq 1$, nevertheless, they reduce to the classical Stokes theorem for $q\to 1$. This shows the power of noncommutative geometry. Obviously one would like to use this integral to define actions for field theories on such noncommutative spaces; this is work in progress.

Although only the case of quantum Euclidean space is considered, the general approach is clearly applicable to, e.g., quantum Minkowski space as well.

II. INTEGRAL ON THE QUANTUM SPHERE S_q^{N-1}

To establish the notation, we briefly summarize the definitions used in this paper, following Faddeev, Reshetikhin, and Takhtadjan.[3]

The (function algebra on the) quantum orthogonal group $O_q(N)$ [which is called $SO_q(N)$ in Ref. 3] is the algebra generated by A^i_j modulo the relations

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$$\hat{R}^{ik}_{mn} A^m_j A^n_l = A^i_n A^k_m \hat{R}^{nm}_{jl}\,, \tag{1}$$

$$g_{ij} A^i_k A^j_l = g_{kl}\,. \tag{2}$$

$\mathrm{SO}_q(N)$ is obtained by further imposing

$$A^{i_1}_{j_1} \cdots A^{i_N}_{j_N} \epsilon^{j_1 \cdots j_N}_q = \epsilon^{i_1 \cdots i_N}_q, \tag{3}$$

using the fact that the quantum determinant is central; see, e.g., Ref. 8.

The $\hat{R}$ matrix decomposes into three projectors, $R^{ij}_{kl} = (qP^+ - q^{-1}P^- + q^{1-N}P^0)^{ij}_{kl}$. The metric is determined by $(P^0)^{ij}_{kl} = [(q^2-1)/(q^N-1)(q^{2-N}+1)]g^{ij}g_{kl}$, where $g_{ik}g^{kj} = \delta^j_i$. In this paper, we assume q is real and positive. Then there is a star structure (involution),

$$\overline{A^i_j} = g^{jm} A^l_m g_{li}\,, \tag{4}$$

so that we really have $(\mathrm{S})\mathrm{O}_q(N,\mathbb{R})$, and the antipode can be written as

$$S(A^i_j) = \overline{A^j_i}. \tag{5}$$

Quantum Euclidean space[3] is generated by x^i with commutation relations

$$(P^-)^{ij}_{kl} x^k x^l = 0, \tag{6}$$

and the center is generated by 1 and $r^2 = g_{ij}x^i x^j$. The associated differentials satisfy $(P^+)^{ij}_{kl}\, dx^k\, dx^l = 0$ and $g_{ij}\, dx^i\, dx^j = 0$, i.e.,

$$dx^i\, dx^j = -q\hat{R}^{ij}_{kl}\, dx^k\, dx^l. \tag{7}$$

The epsilon tensor is then determined by the unique top (N) form,

$$dx^{i_1} \cdots dx^{i_N} = \epsilon^{i_1 \cdots i_N}_q\, dx^1 \cdots dx^N \equiv \epsilon^{i_1 \cdots i_N}_q\, d^N x. \tag{8}$$

The above relations are preserved under the coaction of $(\mathrm{S})\mathrm{O}_q(N)$,

$$\Delta(x^i) = A^i_j \otimes x^j \equiv x^i_{(1)} \otimes x^i_{(2)}\,, \tag{9}$$

in Sweedler notation. The involution $\overline{x^i} = x^j g_{ji}$ is compatible with the left coaction of $(\mathrm{S})\mathrm{O}_q(N,\mathbb{R})$. One can also introduce derivatives that satisfy

$$(P^-)^{ij}_{kl} \partial^k \partial^l = 0, \tag{10}$$

$$\partial^i x^j = g^{ij} + q(\hat{R}^{-1})^{ij}_{kl} x^k \partial^l, \tag{11}$$

and

$$\partial^i\, dx^j = q^{-1}\hat{R}^{ij}_{kl}\, dx^k\, \partial^l, \quad x^i\, dx^j = q\hat{R}^{ij}_{kl}\, dx^k\, x^l. \tag{12}$$

This represents one possible choice. For more details, see, e.g., Ref. 9. Finally, the quantum sphere S^{N-1}_q is generated by $t^i = x^i/r$, which satisfies $g_{ij}t^i t^j = 1$.

We first define a (complex-valued) integral $\langle f(t)\rangle_t$ of a function $f(t)$ over S^{N-1}_q. It should certainly be invariant under $\mathrm{O}_q(N)$, which means

$$A^{i_1}_{j_1} \cdots A^{i_n}_{j_n} \langle t^{j_1} \cdots t^{j_n}\rangle_t = \langle t^{i_1} \cdots t^{i_n}\rangle_t\,. \tag{13}$$

Of course, it has to satisfy

$$g_{i_l i_{l+1}}\langle t^{i_1}\cdots t^{i_n}\rangle_t=\langle t^{i_1}\cdots t^{i_{l-1}}t^{i_{l+2}}\cdots t^{i_n}\rangle_t \quad \text{and} \quad (P^-)^{i_l i_{l+1}}_{j_l j_{l+1}}\langle t^{j_1}\cdots t^{j_n}\rangle_t=0. \tag{14}$$

We require one more property, namely that $I^{i_1\cdots i_n}\equiv\langle t^{i_1}\cdots t^{i_n}\rangle_t$ is analytic in $(q-1)$, i.e. its Laurent series in $(q-1)$ has no negative terms (we can then assume that the classical limit $q=1$ is nonzero). These properties, in fact, determine the spherical integral uniquely: for n odd, one should define $\langle t^{i_1}\cdots t^{i_n}\rangle_t=0$, and the following occurs.

Proposition 1: For even n, there exists (up to normalization) one and only one tensor $I^{i_1\cdots i_n}=I^{i_1\cdots i_n}(q)$ analytic in $(q-1)$ that is invariant under $\mathrm{O}_q(N)$,

$$A^{i_1}_{j_1}\cdots A^{i_n}_{j_n}I^{j_1\cdots j_n}=I^{i_1\cdots i_n}, \tag{15}$$

and symmetric,

$$(P^-)^{i_l i_{l+1}}_{j_l j_{l+1}}I^{j_1\cdots j_n}=0, \tag{16}$$

for any l. It can be normalized such that

$$g_{i_l i_{l+1}}I^{i_1\cdots i_n}=I^{i_1\cdots i_{l-1}i_{l+2}\cdots i_n}, \tag{17}$$

for any l. $I^{ij}\propto g^{ij}$.

An explicit form is, e.g., $I^{i_1\cdots i_n}=\lambda_n(\Delta^{n/2}x^{i_1}\cdots x^{i_n})$, where $\Delta=g_{ij}\partial^i\partial^j$ is the Laplacian (in either of the two possible calculi), and λ_n is analytic in $(q-1)$. For $q=1$, they reduce to the classical symmetric invariant tensors.

Proof: The proof is by induction on n. For $n=2$, g^{ij} is in fact the only invariant symmetric (and analytic) such tensor.

Assume the statement is true for n, and suppose I_{n+2} and I'_{n+2} satisfy the above conditions. Using the uniqueness of I_n, we have (in shorthand notation)

$$g_{12}I_{n+2}=f(q-1)I_n, \tag{18}$$

$$g_{12}I'_{n+2}=f'(q-1)I_n, \tag{19}$$

where the $f(q-1)$ are analytic, because the left-hand sides are invariant, symmetric, and analytic. Then $J_{n+2}=f'I_{n+2}-f'I'_{n+2}$ is symmetric, analytic, and satisfies $g_{12}\,J_{n+2}=0$. It remains to show that $J=0$.

Since J is analytic, we can write

$$J^{i_1\cdots i_n}=\sum_{k=n_0}^{\infty}(q-1)^k J^{i_1\cdots i_n}_{(k)}. \tag{20}$$

$(q-1)^{-n_0}J^{i_1\cdots i_n}$ has all the properties of J and has a well-defined, nonzero limit as $q\to 1$; so we may assume $J_{(0)}\neq 0$.

Now consider invariance,

$$J^{i_1\cdots i_n}=A^{i_1}_{j_1}\cdots A^{i_n}_{j_n}J^{j_1\cdots j_n}. \tag{21}$$

This equation is valid for all q, and we can take the limit $q\to 1$. Then A^i_j generate the commutative algebra of functions on the classical Lie group $O(N)$, and J becomes $J_{(0)}$, which is just a classical tensor. Now $(P^-)^{i_l i_{l+1}}_{j_l j_{l+1}}J^{j_1\cdots j_n}=0$ implies that $J_{(0)}$ is symmetric for neighboring indices, and

therefore it is completely symmetric. With $g_{12}J=0$, this implies that $J_{(0)}$ is totally traceless (classically!). But there exists no totally symmetric traceless invariant tensor for $O(N)$. This proves uniqueness. In particular, $I^{i_1\cdots i_n} = \lambda_n(\Delta^{n/2}x^{i_1}\cdots x^{i_n})$ obviously satisfies the assumptions of the proposition; it is analytic, because in evaluating the Laplacians, only the metric and the $\hat{R}$ matrix are involved, which are both analytic. Statement (17) now follows because x^2 is central. □

Such invariant tensors have also been considered in Ref. 4 (where they are called S), as well as the explicit form involving the Laplacian. Our contribution is a self-contained proof of their uniqueness. So $\langle t^{i_1}\cdots t^{i_n}\rangle_t \equiv I^{i_1\cdots i_n}$ for even n (and 0 for odd n) defines the unique invariant integral over S_q^{N-1}, which thus coincides with the definition given in Ref. 7.

From now on we only consider $N\geqslant 3$ since for $N=1,2$, Euclidean space is undeformed. The following lemma is the origin of the cyclic properties of invariant tensors. For quantum groups, the square of the antipode is usually not 1. For $(S)O_q(N)$, it is generated by the D matrix: $S^2A^i_j=D^i_lA^l_k(D^{-1})^k_j$, where $D^i_l=g^{ik}g_{lk}$ (note that D also defines the quantum trace). Then

Lemma 1: For any invariant tensor $J^{i_1\cdots i_n} = A^{i_1}_{j_1}\cdots A^{i_n}_{j_n}J^{j_1\cdots j_n}$, $D^{i_1}_{l_1}J^{i_2\cdots l_1}$ *is invariant too:*

$$A^{i_1}_{j_1}\cdots A^{i_n}_{j_n}D^{j_1}_{l_1}J^{j_2\cdots l_1}=D^{i_1}_{l_1}J^{i_2\cdots l_1}. \tag{22}$$

Proof: From the above, (22) amounts to

$$(S^{-2}A^{i_1}_{j_1})A^{i_2}_{j_2}\cdots A^{i_n}_{j_n}J^{j_2\cdots j_nj_1}=J^{i_2\cdots i_ni_1}. \tag{23}$$

Multiplying with $S^{-1}A^{i_0}_{i_1}$ from the left and using $S^{-1}(ab)=(S^{-1}b)(S^{-1}a)$ and $(S^{-1}A^{i_1}_{j_1})A^{i_0}_{i_1} = \delta^{i_0}_{j_1}$, this becomes

$$A^{i_2}_{j_2}\cdots A^{i_n}_{j_n}J^{j_2\cdots j_ni_0}=S^{-1}A^{i_0}_{i_1}J^{i_2\cdots i_ni_1}. \tag{24}$$

Now multiplying with $A^{l_0}_{i_0}$ from the right, we get

$$A^{i_2}_{j_2}\cdots A^{i_n}_{j_n}A^{l_0}_{i_0}J^{j_2\cdots j_ni_0}=\delta^{l_0}_{i_1}J^{i_2\cdots i_ni_1}. \tag{25}$$

But the (lhs) is just $J^{i_2\cdots i_nl_0}$ by invariance and thus equal to the (rhs). □

We can now show a number of properties of the integral over the sphere.

Theorem 1:

$$\overline{\langle f(t)\rangle_t}=\langle\overline{f(t)}\rangle_t, \tag{26}$$

$$\langle\overline{f(t)}f(t)\rangle_t\geqslant 0, \tag{27}$$

$$\langle f(t)g(t)\rangle_t=\langle g(t)f(Dt)\rangle_t, \tag{28}$$

where $(Dt)^i=D^i_jt^j$. *The last statement follows from*

$$I^{i_1\cdots i_n}=D^{i_1}_{j_1}I^{i_2\cdots i_nj_1}. \tag{29}$$

Proof: For (26), we have to show that $I^{j_n\cdots j_1}g_{j_ni_n}\cdots g_{j_1i_1} = I^{i_1\cdots i_n}$. Using the uniqueness of I, it is enough to show that $I^{j_n\cdots j_1}g_{j_ni_n}\cdots g_{j_1i_1}$ is invariant, symmetric, and normalized as I. So first,

$$A^{i_1}_{j_1}\cdots A^{i_n}_{j_n}(I^{k_n\cdots k_1}g_{k_nj_n}\cdots g_{k_1j_1})=g_{l_1i_1}\cdots g_{l_ni_n}\overline{A^{l_n}_{k_n}\cdots A^{l_1}_{k_1}}I^{k_n\cdots k_1}=\overline{A^{l_n}_{k_n}\cdots A^{l_1}_{k_1}I^{k_n\cdots k_1}}g_{l_1i_1}\cdots g_{l_ni_n}$$
$$=(I^{l_n\cdots l_1}g_{l_ni_n}\cdots g_{l_1i_1}). \tag{30}$$

We have used that I is real (since g^{ij} and $\hat{R}$ are real), and $A^{i_1}_{j_1}g_{k_1j_1}=g_{l_1i_1}\overline{A^{l_1}_{k_1}}$. The symmetry condition (16) follows from standard compatibility conditions between $\hat{R}$ and g^{ij}, and the fact that $\hat{R}$ is symmetric. The correct normalization can be seen easily using $g^{ij}=g_{ij}$ for q—Euclidean space.

To show positive definiteness (27), we use the observation made by Ref. 3 that

$$t^i\to A^i_j u^j, \tag{31}$$

with $u^j=u_1\delta^j_1+u_N\delta^j_N$ is an embedding $S^{N-1}_q\to Fun(O_q(N))$ for $u_1u_N=(q^{(N-2)/2}+q^{(2-N)/2})^{-1}$, since $(P^-)^{ij}_{kl}u^ku^l=0$ and $g_{ij}u^iu^j=1$. In fact, this embedding also respects the star structure if one chooses $u_N=u_1q^{1-N/2}$ and real. Now one can write the integral over S^{N-1}_q in terms of the Haar measure on the compact quantum group $O_q(N,\mathbb{R})$.[10,11] Namely,

$$\langle t^{i_1}\cdots t^{i_n}\rangle_t=\langle A^{i_1}_{j_1}\cdots A^{i_n}_{j_n}\rangle_A u^{j_1}\cdots u^{j_n}\equiv\langle A^i_{\underline{j}}\rangle_A u^{\underline{j}}, \tag{32}$$

(in short notation) since the Haar measure $\langle\,\rangle_A$ is left (and right) invariant $\langle A^i_{\underline{j}}\rangle_A=A^i_{\underline{k}}\langle A^k_{\underline{j}}\rangle_A=\langle A^i_{\underline{k}}\rangle_A A^k_{\underline{j}}$ and analytic, and the normalization condition is satisfied as well. Then $\langle\overline{t^{\underline{i}}}t^{\underline{j}}\rangle_t=\langle\overline{A^{\underline{i}}_{\underline{k}}}A^{\underline{j}}_{\underline{r}}\rangle_A u^{\underline{k}}u^{\underline{r}}$ and for $f(t)=\Sigma f_{\underline{i}}t^{\underline{i}}$, etc.,

$$\langle\overline{f(t)}g(t)\rangle_t=\overline{f_{\underline{i}}}g_{\underline{j}}\langle\overline{A^{\underline{i}}_{\underline{k}}}A^{\underline{j}}_{\underline{r}}\rangle_A u^{\underline{k}}u^{\underline{r}}=\langle\overline{(f_{\underline{i}}A^{\underline{i}}_{\underline{k}}u^{\underline{k}})}(g_{\underline{j}}A^{\underline{j}}_{\underline{r}}u^{\underline{r}})\rangle_A=\langle\overline{f(Au)}g(Au)\rangle_A\,. \tag{33}$$

This shows that the integral over S^{N-1}_q is positive definite, because the Haar measure over compact quantum groups is positive definite,[10] cf. Ref. 12.

Finally we show the cyclic property (29). (28) then follows immediately. For $n=2$, the statement is obvious: $g^{ij}=D^i_k g^{jk}$.

Again using a shorthand notation, define

$$J^{12\cdots n}=D_1I^{23\cdots n1}. \tag{34}$$

Using the previous proposition, we only have to show that J is symmetric, invariant, analytic, and properly normalized. Analyticity is obvious. The normalization follows immediately by induction, using the property shown in proposition (1). Invariance of J follows from the above lemma. It remains to show that J is symmetric, and the only nontrivial part of that is $(P^-)_{12}J^{12\cdots n}=0$. Define

$$\widetilde{J}^{12\cdots n}=(P^-)_{12}\,J^{12\cdots n}, \tag{35}$$

so $\widetilde{J}$ is invariant, antisymmetric, and traceless in the first two indices (12), symmetric in the remaining indices (we will say that such a tensor has the ISAT property), and analytic. It is shown below that there is no such $\widetilde{J}$ for $q=1$ (and $N\geqslant 3$). Then as in Proposition 1, the leading term of the expansion of $\widetilde{J}$ in $(q-1)$ is classical and therefore vanishes, which proves that $\widetilde{J}=0$ for any q.

So from now on $q=1$. We show by induction that $\widetilde{J}=0$. This is true for $n=2$: there is no invariant antisymmetric traceless tensor with two indices (for $N\geqslant 3$). Now assume the statement is true for n even, and that $\widetilde{J}^{12\cdots(n+2)}$ has the ISAT property. Define

$$K^{12\cdots n}=g_{(n+1),(n+2)}\widetilde{J}^{12\cdots(n+2)}. \tag{36}$$

K has the ISAT property, so by the induction assumption

$$K=0. \tag{37}$$

Define

$$M^{145\cdots(n+2)}=g_{23}\widetilde{J}^{12\cdots(n+2)}=\mathscr{S}_{14}M^{145\cdots(n+2)}+\mathscr{A}_{14}M^{145\cdots(n+2)}, \tag{38}$$

where $\mathscr{S}$ and $\mathscr{A}$ are the classical symmetrizer and antisymmetrizer. Again by the induction assumption, $\mathscr{A}_{14}M^{145\cdots(n+2)}=0$ (it satisfies the ISAT property). This shows that M is symmetric in the first two indices (1,4). Together with the definition of M, this implies that M is totally symmetric. Further, $g_{14}M^{145\cdots(n+2)}=g_{14}g_{23}\widetilde{J}^{12\cdots(n+2)}=0$ because $\widetilde{J}$ is antisymmetric in (1,2). But then M is totally traceless, and as in proposition (1) this implies $M=0$. Together with (37) and the ISAT property of $\widetilde{J}$, it follows that $\widetilde{J}$ is totally traceless. So $\widetilde{J}$ corresponds to a certain Young tableaux, describing a larger-than-one-dimensional irreducible representation of O(N). However, $\widetilde{J}$ being invariant means that it is a trivial one-dimensional representation. This is a contradiction and proves $\widetilde{J}=0$. □

Property (27) (which is also implied by results in Ref. 4, once the uniqueness of the invariant tensors is established) in particular means that one can now define the Hilbert space of square-integrable functions on S_q^{N-1}. The same will be true for the integral on the entire Quantum Euclidean space.

The cyclic property (28) is a strong constraint on $I^{i_1\cdots i_n}$ and could actually be used to calculate it recursively, besides its obvious interest in its own. An immediate consequence of (28) is $\langle f(Dt)\rangle_t=\langle f(t)\rangle_t$, which also follows from rotation invariance of the integral, because D is essentially the representation of the (exponential of the) Weyl vector of $\mathscr{U}_q(\mathrm{SO}(N))$.

Notice that although it may not look like it, (28) is consistent with conjugation: even though the D matrix is real, we have

$$\overline{\overline{f(Dt)}}=f(D^{-1}t). \tag{39}$$

To see this, take $f(t)=t^i$; then the (lhs) becomes

$$\overline{D(\overline{t^i})}=\overline{D(t^jg_{ji})}=\overline{D^j_kt^kg_{ji}} \tag{40}$$

$$=D^j_kt^lg_{lk}g_{ji}=t^lg_{jl}g_{ji}=(D^{-1})^i_lt^l, \tag{41}$$

using the cyclic property of g and $D^i_l=g_{ik}g_{lk}$, which is the (rhs) of the above.

III. INTEGRAL OVER QUANTUM EUCLIDEAN SPACE

It is now easy to define an integral over quantum Euclidean space. Since the invariant length $r^2=g_{ij}x^ix^j$ is central, we can use its square root r as well, and write any function on quantum Euclidean space in the form $f(x^i)=f(t^i,r)$. We then define its integral to be

$$\langle f(x)\rangle_x=\langle\langle f(t,r)\rangle_t(r)\cdot r^{N-1}\rangle_r, \tag{42}$$

where $\langle f(t,r)\rangle_t(r)$ is a classical, analytic function in r, and $\langle g(r)\rangle_r$ is some linear functional in r, to be determined by requiring the Stokes theorem. It is essential that this radial integral $\langle g(r)\rangle_r$ is really a functional of the *analytic continuation of* $g(r)$ to a function on the (positive) real line. Only then one obtains a large class of integrable functions, and this concept of integration over the entire space agrees with the classical one.

It will turn out that the Stokes theorem, e.g., in the form $\langle\partial_if(x)\rangle_x=0$ holds if and only if the radial integral satisfies the scaling property

$$\langle g(qr)\rangle_r = q^{-1}\langle g(r)\rangle_r . \tag{43}$$

This can be shown directly; we will instead give a more elegant proof later. This scaling property is obviously satisfied by an arbitrary superposition of Jackson sums,

$$\langle f(r)\rangle_r = \int_1^q dr_0\ \mu(r_0) \sum_{n=-\infty}^{\infty} f(q^n r_0) q^n, \tag{44}$$

with arbitrary (positive) ''weight'' function $\mu(r)>0$. The normalization can be fixed such that, e.g., $\langle e^{-r^2}\rangle_r$ the classical result. If $\mu(r)$ is a delta function, this is simply a Jackson sum; for $\mu(r)=1$, one obtains the classical radial integration,

$$\langle f(r) r^{N-1}\rangle_r = \int_1^q dr_0 \sum_{n=-\infty}^{\infty} q^n (q^n r_0)^{N-1} f(q^n r_0) = \int_0^{\infty} dr\ r^{N-1} f(r). \tag{45}$$

This is the unique choice of $\mu(r)$ for which the scaling property (43) holds for any positive real number, not just for powers of q. We define $f(x^i)$ to be integrable [with respect to $\mu(r)$] if the corresponding radial integral in (42) is finite. We therefore obtain generally inequivalent integrals for different choices of $\mu(r)$, all of which satisfy the Stokes theorem.

Let us try to compare the above definitions with the Gaussian approach. In that case, one does not resort to a classical integral, and determining the class of integrable functions seems to be rather subtle. The Gaussian integration procedure is based on the observation that the integral of functions of the type (polynomial)·(Gaussian) is uniquely determined by the Stokes theorem [and therefore agrees with our definition for any normalized $\mu(r)$]; one would then like to extend it to more general functions by a limiting process. Lacking a natural topology on the space of functions (i.e., formal power series), this limiting process is, however, quite problematic. One way to see this is because there are actually many different inequivalent integrals labeled by $\mu(r)$, such a limiting process can only be unique on the (presumably small) class of functions on which the integral is independent of $\mu(r)$. Furthermore, even classically, although one can calculate, e.g., $\int[1/(r^2+1)]e^{-r^2}$ by expanding it ''properly'' (i.e., using pointwise or L^2 convergence) in terms of Hermite functions, if one tries to expand it formally, e.g., in terms of $\{r^n e^{-r^2}\}$, one obtains a divergent sum of integrals. Thus the result may depend on the choice of basis and limiting procedure. It is not clear to the author how to properly integrate functions other than (polynomial)·(Gaussian) in the Gaussian sense, which would be very desirable, because that approach may be applied to some quantum spaces that do not have a central length element.[6]

The properties of the integral over S_q^{N-1} generalize immediately to the Euclidean case, for any positive $\mu(r)$.

Theorem 2:

$$\overline{\langle f(x)\rangle_x} = \langle \overline{f(x)}\rangle_x , \tag{46}$$

$$\langle \overline{f(x)} f(x)\rangle_x \geqslant 0, \tag{47}$$

$$\langle f(x) g(x)\rangle_x = \langle g(x) f(Dx)\rangle_x , \tag{48}$$

and

$$\langle f(qx)\rangle_x = q^{-N}\langle f(x)\rangle_x , \tag{49}$$

if and only if (43) holds.

Proof: Immediately from theorem (1), (43), and (42), using $Dr=r$ and $\mu(r_0)>0$. □

(46) and (49) were already known for the special case of the Gaussian integral.[4] It was pointed out to me by Fiore that in this case, positivity was also shown in Ref. 5.

IV. INTEGRATION OF FORMS

It turns out to be very useful to consider not only integrals over functions, but also over forms, just like classically. As was mentioned before, there exists a unique N form $dx^{i_1}\cdots dx^{i_N} = \epsilon_q^{i_1\cdots i_N} d^N x$, and we define

$$\int_x d^N x f(x) = \langle f(x)\rangle_x , \tag{50}$$

i.e., we first commute $d^N x$ to the left, and then take the integral over the function on the right. Then the two statements of the Stokes theorem $\langle \partial_i f(x)\rangle_x = 0$ and $\int_x d\omega_{N-1} = 0$ are equivalent.

The following observation by Zumino[13] will be very useful: there is a one-form,

$$\omega = \frac{q^2}{(q+1)r^2}\, d(r^2) = q\,\frac{1}{r}\,dr = dr\,\frac{1}{r}, \tag{51}$$

where $r\ dx^i = q\ dx^i\ r$, which generates the calculus on quantum Euclidean space by

$$[\omega, f]_{\pm} = (1-q)df, \tag{52}$$

for any form f with the appropriate grading. It satisfies

$$d\omega = \omega^2 = 0. \tag{53}$$

We define the integral of an N form over the sphere $r\cdot S_q^{N-1}$ with radius r by

$$\int_{r\cdot S_q^{N-1}} d^N x f(x) = \omega r^N \langle f(x)\rangle_t = dr\ r^{N-1}\langle f(x)\rangle_t , \tag{54}$$

which is a one form in r, as classically. It satisfies

$$\int_{r\cdot S_q^{N-1}} q^N\ d^N x\ f(qx) = \int_{qr\cdot S_q^{N-1}} d^N x\ f(x), \tag{55}$$

where $(drf(r))(qr) = q\ dr\ f(qr)$. Now, defining $\int_r dr\ g(r) = \langle g(r)\rangle_r$, (50) can be written as

$$\int_x d^N x\ f(x) = \int_r \left(\int_{r\cdot S_q^{N-1}} d^N x f(x) \right). \tag{56}$$

The scaling property (43), i.e. $\int_x d^N x\ f(qx) = q^{-N}\int_x d^N x\ f(x)$ holds if and only if the radial integrals satisfy

$$\int_r dr\ f(qr) = q^{-1}\int_r dr\ f(r). \tag{57}$$

We can also define the integral of an $(N-1)$-form $\alpha_{N-1}(x)$ over the sphere with radius r:

$$\int_{r\cdot S_q^{N-1}} \alpha_{N-1} = \omega^{-1}\left(\int_{r\cdot S_q^{N-1}} \omega\alpha_{N-1} \right). \tag{58}$$

The ω^{-1} simply cancels the explicit ω in (54), and it reduces to the correct classical limit for $q=1$.

The epsilon tensor satisfies the cylic property:

Proposition 2:

$$\epsilon_q^{i_1\cdots i_N}=(-1)^{N-1}D^{i_i}_{j_1}\epsilon_q^{i_2\cdots i_N j_1}. \tag{59}$$

Proof: Define

$$\kappa^{12\cdots N}=(-1)^{N-1}D^1\epsilon_q^{23\cdots N1}, \tag{60}$$

in shorthand notation again. Lemma 1 shows that κ is invariant. $\kappa^{12\cdots N}$ is traceless and (q) antisymmetric in $(23\cdots N)$. Now $g_{12}\kappa^{12\cdots N}=0$ because there exists no invariant, totally antisymmetric traceless tensor with $(N-2)$ indices for $q=1$, so by analyticity there is none for arbitrary q. Similarly from the theory of irreducible representations of $SO(N)$,[14] $P^+{}_{12}\kappa^{12\cdots N}=0$, where P^+ is the q symmetrizer, $1=P^++P^-+P^0$. Therefore $\kappa^{12\cdots N}$ is totally antisymmetric and traceless (for neighboring indices), invariant, and analytic. But there exists only one such tensor up to normalization (which can be proved similarly), so $\kappa^{12\cdots N}=f(q)\epsilon_q^{12\cdots N}$. It remains to show $f(q)=1$. By repeating the above, one gets $\epsilon_q^{12\cdots N}=(f(q))^N(\det D)\epsilon_q^{12\cdots N}$ (here $12\cdots N$ stands for the *numbers* 1,2,...,N), and since $\det D=1$, it follows $f(q)=1$ (times an Nth root of unity, which is fixed by the classical limit). □

Now consider a k form $\alpha_k(x)=dx^{i_1}\cdots dx^{i_k}f_{i_1\cdots i_k}(x)$ and an $(N-k)$ form $\beta_{N-k}(x)$. Then the following cyclic property for the integral over forms holds.

Theorem 3:

$$\int_{r\cdot S_q^{N-1}}\alpha_k(x)\beta_{N-k}(x)=(-1)^{k(N-k)}\int_{q^{-k}r\cdot S_q^{N-1}}\beta_{N-k}(x)\alpha_k(q^N\,Dx), \tag{61}$$

where $\alpha_k(q^N\,Dx)=(q^N D\,dx)^{i_1}\cdots(q^N D\,dx)^{i_k}f_{i_1\cdots i_k}(q^N\,Dx)$.

In particular, when α_k and β_{N-k} are forms on S_q^{N-1}, i.e. they involve only $dx^i(1/r)$ and t^i, then

$$\int_{S_q^{N-1}}\alpha_k(t)\beta_{N-k}(t)=(-1)^{k(N-k)}\int_{S_q^{N-1}}\beta_{N-k}(t)\alpha_k(Dt). \tag{62}$$

On Euclidean space,

$$\int_x\alpha_k(x)\beta_{N-k}(x)=(-1)^{k(N-k)}\int_x\beta_{N-k}(x)\alpha_k(q^N\,Dx), \tag{63}$$

if and only if (57) holds.

Notice that on the sphere, $d^Nxf(t)=f(t)d^Nx$.

Proof: We only have to show that

$$\int_{r\cdot S_q^{N-1}}f(x)d^Nx\;g(x)=\int_{r\cdot S_q^{N-1}}d^Nx\;g(x)f(q^N\,Dx) \tag{64}$$

and

$$\int_{r\cdot S_q^{N-1}}dx^i\;\beta_{N-1}(x)=(-1)^{N-1}\int_{q^{-1}r\cdot S_q^{N-1}}\beta_{N-1}(x)(q^N D\,dx)^i. \tag{65}$$

(64) follows immediately from (28) and $x^i\,d^Nx=d^Nx\;q^Nx^i$.

To see (65), we can assume that $\beta_{N-1}(x) = dx^{i_2}\cdots dx^{i_n} f(x)$. The commutation relations $x^i\, dx^j = q\hat{R}^{ij}_{kl}\, dx^k\, x^l$ are equivalent to

$$\begin{aligned} f(q^{-1}x)dx^j &= \mathscr{R}((dx^j)_{(a)}\otimes f_{(1)})(dx^j)_{(b)}(f(x))_{(2)} \\ &= (dx^j \triangleleft \mathscr{R}^1)(f(x)\triangleleft \mathscr{R}^2), \end{aligned} \tag{66}$$

where $\mathscr{R}=\mathscr{R}^1\otimes\mathscr{R}^2$ is the universal $\mathscr{R}$ for $SO_q(N)$, using its quasitriangular property and $\mathscr{R}(A^j_k\otimes {}^i_l) = \hat{R}^{ij}_{kl}$. $f\triangleleft Y = \langle Y, f_{(1)}\rangle f_{(2)}$ is the right action induced by the left coaction (9) of an element $Y\in \mathscr{U}_q(SO(N))$. Now invariance of the integral implies

$$(dx^j\triangleleft\mathscr{R}^1)\langle f(x)\triangleleft\mathscr{R}^2\rangle_t = dx^j\langle f(x)\rangle_t, \tag{67}$$

because $\mathscr{R}^1\otimes\epsilon(\mathscr{R}^2)=1$. Using this, (66), (55), and (54), the (rhs) of (65) becomes

$$\begin{aligned} (-1)^{N-1}\int_{q^{-1}r\cdot S^{N-1}_q}\beta_{N-1}(x)q^N D^i_j\, dx^j &= (-1)^{N-1}D^i_j\int_{r\cdot S^{N-1}_q} dx^{i_2}\cdots dx^{i_N}\, f(q^{-1}x)dx^j \\ &= (-1)^{N-1}\, D^i_j\epsilon^{i_2\cdots i_N j}\omega r^N\langle f(x)\rangle_t \\ &= \epsilon^{ii_2\cdots i_N}\omega r^N\langle f(x)\rangle_t = \int_{r\cdot S^{N-1}_q} dx^i\ \beta_{N-1}(x), \end{aligned} \tag{68}$$

using (59). This shows (65), and (62) follows immediately. (63) then follows from (57). □

Another way to show (65) following an idea of Jurco[15] is to use

$$\int_{r\cdot S^{N-1}_q}(\alpha_k\triangleleft SY)\beta_{N-k} = \int_{r\cdot S^{N-1}_q}\alpha_k(\beta_{N-k}\triangleleft Y) \tag{69}$$

to move the action of $\mathscr{R}^2$ in (66) to the left picking up $\mathscr{R}^1 S\mathscr{R}^2$, which generates the inverse square of the antipode and thus corresponds to the D^{-1} matrix. This approach, however, cannot show (28) or (48), because the commutation relations of functions are more complicated.

(61) shows in particular that the definition (58) is natural, i.e. it essentially does not matter on which side one multiplies with ω. Now we immediately obtain the Stokes theorem for the integral over quantum Euclidean space, if and only if (57) holds. Noticing that $\omega(q^N\, Dx) = \omega(x)$, (63) implies

$$\begin{aligned} \int_x d\alpha_{N-1}(x) &= \frac{1}{1-q}\int_x [\omega,\alpha_{N-1}]_\pm \\ &\propto \int_x \omega\alpha_{N-1} - (-1)^{N-1}\alpha_{N-1}\omega \\ &= \int_x (-1)^{N-1}\alpha_{N-1}\omega - (-1)^{N-1}\alpha_{N-1}\omega = 0. \end{aligned} \tag{70}$$

On the sphere, we get as easily

$$\int_{S^{N-1}_q} d\alpha_{N-2}(t) \propto \int_{S^{N-1}_q}[\omega,\alpha_{N-2}]_\pm = \omega^{-1}\int_{S^{N-1}_q}\omega(\omega\alpha_{N-2} - (-1)^{N-2}\alpha_{N-2}\omega)) = 0, \tag{71}$$

using (62) and $\omega^2=0$.

It is remarkable that these simple proofs only work for $q \neq 1$, nevertheless the statements reduce to the classical Stokes theorem for $q \to 1$. This shows the power of the q-deformation technique.

One can actually obtain a version of the Stokes theorem with spherical boundary terms. Define

$$\int_{q^k r_0}^{q^l r_0} \omega f(r) = \int_{q^k r_0}^{q^l r_0} dr \, \frac{1}{r} \, f(r) = (q-1) \sum_{n=k}^{l-1} f(r_0 q^n), \tag{72}$$

which reduces to the correct classical limit, because the (rhs) is a Riemann sum. Define

$$\int_{q^k r_0 \cdot S_q^{N-1}}^{q^l r_0 \cdot S_q^{N-1}} \alpha_N(x) = \int_{q^k r_0}^{q^l r_0} \left(\int_{r \cdot S_q^{N-1}} \alpha_N(x) \right), \tag{73}$$

For $l \to \infty$ and $k \to -\infty$, this becomes an integral over Euclidean space, as defined before. Then

$$\begin{aligned} \int_{q^k r_0 \cdot S_q^{N-1}}^{q^l r_0 \cdot S_q^{N-1}} d\alpha_{N-1} &= \frac{1}{1-q} \int_{q^k r_0}^{q^l r_0} \left(\int_{r \cdot S_q^{N-1}} \omega \alpha_{N-1} - (-1)^{N-1} \alpha_{N-1} \omega \right) \\ &= \frac{1}{1-q} \int_{q^k r_0}^{q^l r_0} \left(\int_{r \cdot S_q^{N-1}} \omega \alpha_{N-1} - \int_{qr \cdot S_q^{N-1}} \omega \alpha_{N-1} \right) \\ &= \int_{q^l r_0 \cdot S_q^{N-1}} \alpha_{N-1} - \int_{q^k r_0 \cdot S_q^{N-1}} \alpha_{N-1}. \end{aligned} \tag{74}$$

In the last line, (54), (58), and (72) were used.

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Orbit–orbit branching rules for families of classical Lie algebra–subalgebra pairs

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Complete orbit–orbit branching rules are derived for each classical algebra–maximal-subalgebra pair $C_{m+n}\supset C_m\oplus C_n$, $B_{m+n}\supset D_m\oplus B_n$, $D_{m+n}\supset D_m\oplus D_n$. Since each pair is equal rank, and algebra and subalgebra Weyl sectors line up, the integrity basis in each case consists of the subalgebra orbits contained in the fundamental orbits of the algebra. © *1996 American Institute of Physics.* [S0022-2488(96)00109-0]

I. INTRODUCTION

In physics it is generally useful, when possible, to reduce an object of interest to smaller ''building blocks.'' We are thinking of the reduction of irreducible representations (IRs) of a simple, or semisimple, Lie algebra to Weyl orbits (W-orbits, or simply orbits), a device which has seen little exploitation so far in applications of group theory.

A particular use of W-orbits is as an intermediate stage in finding branching rules between IRs of algebra and subalgebra. The procedure consists of three steps.

(i) Reduction of the algebra IR into algebra W-orbits; this can be done by a recursive routine[1,2] or better by a procedure described later in this paragraph under step (iii); extensive tables exist.[3]

(ii) Reduction of algebra W-orbits to subalgebra W-orbits, the subject of this paper, which treats algebra–subalgebra pairs listed in the abstract.

(iii) Assembling subalgebra orbits into subalgebra IRs; the W-orbits of the subalgebra IRs may be lifted, one IR at a time, starting with the highest, from the collection of subalgebra orbits. Alternatively, each subalgebra orbit can be written directly as a superposition of subalgebra IRs.[4] The relevant orbit–IR triangular matrix (for the algebra) can be inverted for a solution of step (i) above.

These steps have been applied to a few low-rank Kac–Moody algebras to obtain IR–IR branching rules.[5]

Usually, in representation theory, it is simplest to use a fundamental weights basis in weight space. In the present context we find it more convenient to use an orthonormal weights basis for the most part; it is easier then to recognize to which algebra W-orbit a given subalgebra W-orbit belongs.

We complete this section with some information from recent papers which give orbit–orbit branching rules for some low-rank algebras:[5,6] the three families to be considered here have the properties that algebra and subalgebra have the same rank and that Weyl sectors of algebra and subalgebra line up, that is, each subalgebra Weyl sector contains only complete algebra sectors. Then the elementary subalgebra orbits consist of the subalgebra orbits lying in the fundamental orbits of the algebra; they form the integrity basis from which all subalgebra orbits are formed by taking stretched products (orbit labels all additive). We then have only to find which pairs of elementary orbits are compatible and which are incompatible to complete the solution of the problem.

II. THE ALGEBRA–SUBALGEBRA PAIR $C_{m+n}\supset C_m\oplus C_n$

We treat this family first because it is simplest.

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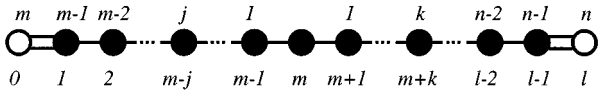

FIG. 1. The Dynkin–Coxeter diagram for $C_{m+n} \supset C_m \oplus C_n$. The numbers below the diagram label the simple roots of C_l ($l=m+n$). Those to the left above label those of C_m, and those to the right above label those of C_n.

As basis vectors in weight space we use the $l=m+n$ orthonormal vectors e_i $(i=1,\ldots l)$. Weyl reflections of C_l consist of sign reversals $e_i \rightarrow -e_i$ and interchanges $e_i \leftrightarrow e_j$.

The simple roots are $\alpha_i = e_i - e_{i+1}$ $(i=1,\ldots,l-1)$ and $\alpha_l = 2e_l$; the extended simple root is $\alpha_0 = -2e_1$ (for simplicity we have multiplied the simple roots, and the fundamental weights below, by $2^{1/2}$). The fundamental weights ω_i are given in terms of the simple roots by the inverse Cartan matrix,

$$\omega_i = \sum_{h=1}^{l} (C^{-1})_{ih} \alpha_h \quad (i=1,\ldots,l), \tag{1}$$

and thus in terms of the orthonormal basis we find

$$\omega_i = \sum_{h=1}^{i} e_h \quad (i=1,\ldots,l). \tag{2}$$

We label a W-orbit by the components λ_j of its highest weight in a fundamental weights basis. The fundamental orbit $[i]$ $[\lambda_j = \delta_{ij}$ (the Kronecker delta)] has highest weight ω_i. According to (2) the weights of the orbit $[i]$ consist of all linear combinations of i distinct e_h, each with coefficient ± 1.

The simple roots of $C_l = C_{m+n}$, C_m, and C_n are shown in Fig. 1. The simple roots α'_j of C_m and α''_k of C_n are given in terms of those of C_l by

$$\begin{aligned} \alpha'_j &= \alpha_{m-j}, \quad (j=1,\ldots,m), \\ \alpha''_k &= \alpha_{m+k}, \quad (k=1,\ldots,n). \end{aligned} \tag{3}$$

Hence the fundamental weights of C_m and C_n are, respectively,

$$\omega'_j = -\sum_{h=1}^{j} e_{m-h+1}, \quad \omega''_k = \sum_{h=1}^{k} e_{m+h}. \tag{4}$$

The elementary $C_m \oplus C_n$ W-orbits are those contained in the fundamental orbits $[i]$ of C_l. We denote one of them by $[j;k]$, the direct product of the fundamental orbits $[j]$ of C_m and $[k]$ of C_n; the ranges of j and of $k=i-j$ are specified below [in (5)]. We may write

$$[i] \supset \sum_{j=\max(i-n,0)}^{\min(i,m)} [j;i-j], \quad i=1,\ldots,l; \tag{5}$$

j is the number of e_h in a weight of $[i]$ for which $1 \leqslant h \leqslant m$ and k is the number in the range $m+1 \leqslant h \leqslant l$; for $j=0$, $[j]$ is the zero or point orbit of C_m and for $k=0$, $[k]$ is the zero orbit of C_n. The elementary orbits $[j;k]$ are shown in tabular form in Fig. 2.

The elementary orbits constitute the integrity basis for all subalgebra orbits: higher orbits are stretched (orbit labels additive) products of powers of the elementary ones.

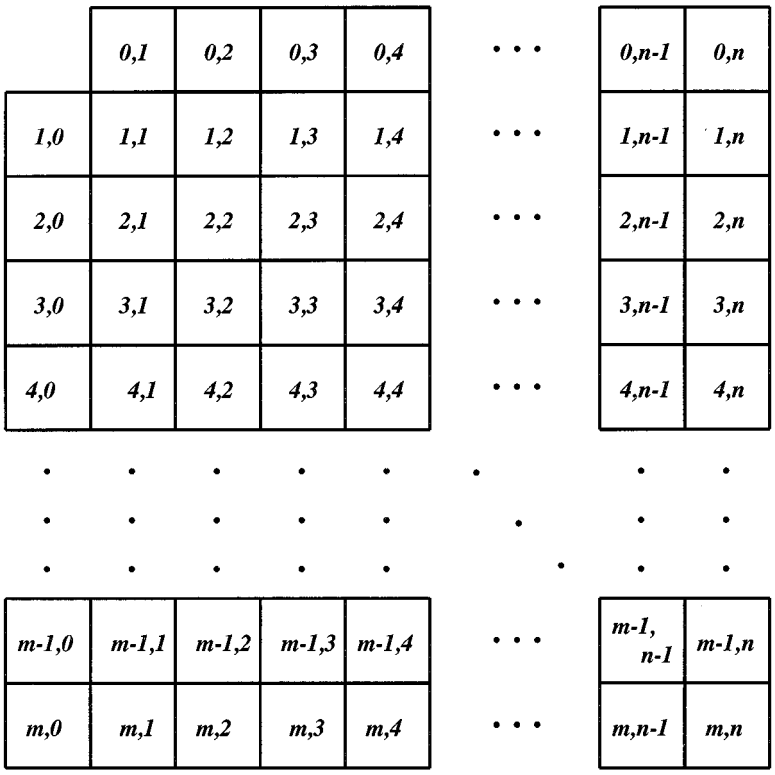

FIG. 2. The elementary $C_{m+n} \supset C_m \oplus C_n$ W-orbits. The elementary orbit $[j;k]$ belongs to the $(j+k)$th fundamental W-orbit of C_{m+n}. The elementary orbits $[j;k]$ and $[j';k']$ are compatible if $j' \geqslant j$, $k' \geqslant k$ (we suppose $j'+k' \geqslant j+k$).

It remains to find the compatibility rules, i.e., the answer to the question ''Which pairs of elementary orbits can appear together in a product yielding a higher orbit?'' Consider the stretched product of the elementary orbits $[j;k]$ and $[j';k']$ which belong respectively to the C_l orbits $[i]$ and $[i']$ with $i=j+k$ and $i'=j'+k'$. We may suppose $i'>i$ (two elementary orbits in the same fundamental orbit are known to be incompatible). Our product must belong to the C_l orbit $[i,i']$ which has labels $\lambda_h=\delta_{hi}+\delta_{hi'}$ (ith and i'th labels unity, other labels zero); each weight of $[i,i']$ has i e_h with coefficient ± 2 and $i'-i$ with coefficient ± 1; the other $l-i'$ e_h have coefficient 0. The stretched product $[j;k]\cdot[j';k']$ belongs to the $C_m \oplus C_n$ orbit $[j,j',k,k']$ with C_m labels $\lambda'_h = \delta_{hj} + \delta_{hj'}$ and C_n labels $\lambda''_h = \delta_{hk} + \delta_{hk'}$. We may suppose $j' \geqslant j$ (otherwise interchange the roles of C_m and C_n); among the first m e_hs there are then j with coefficient ± 2 and $j'-j$ with coefficient ± 1. In the last n e_hs there are thus $i-j=k$ with coefficient ± 2 and $i'-i-j'+j=k'-k$ with coefficient ± 1. It follows that $k' \geqslant k$; two elementary orbits are incompatible if one lies above and to the right of the other in Fig. 2.

Our solution for the $C_{m+n} \supset C_m \oplus C_n$ orbit–orbit branching rules is now complete. For the subalgebra orbit content of the general C_l orbit $[\lambda_1,...,\lambda_l]$ select a sequence of elementary orbits, one $[j_{i'},k_{i'}]$ from each diagonal $j_{i'}+k_{i'}=i'=\text{const}$ for which $\lambda_{i'} \neq 0$. Each one chosen must be compatible with the preceding one $[j_i;k_i]$ in the list, i.e., $j_{i'} \geqslant j_i$, $k_{i'} \geqslant k_i$. Each such sequence corresponds to one subalgebra orbit $[\lambda'_1,\ldots,\lambda'_m;\lambda''_1,\ldots,\lambda''_n]$ with $\lambda'_h = \Sigma_i \lambda_i \delta_{hj_i}$, $\lambda''_h = \Sigma_i \lambda_i \delta_{hk_i}$ (the stretched product of the chosen mutually compatible elementary orbits, the ith one used λ_i times).

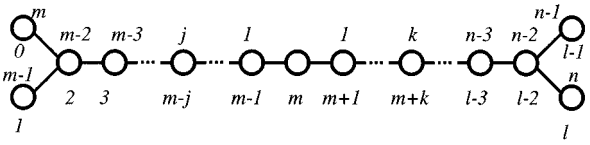

FIG. 3. The Dynkin–Coxeter diagram for $D_{m+n}\supset D_m\oplus D_n$. The numbers below the nodes label the simple roots of D_l $(l=m+n)$. Those to the left above label those of D_m, and those to the right above label those of D_n.

III. THE ALGEBRA–SUBALGEBRA PAIR $D_{m+n}\supset D_m\oplus D_n$

In this section and the next ($B_{m+n}\supset D_m\oplus B_n$), to save space, we state our results without detailed proofs; the proofs are very similar to those given in Sec. II for $C_{m+n}\supset C_m\oplus C_n$, and only slightly more complicated.

We assume here that m and n are both greater than 1. Otherwise we would have to take D_m and/or D_n to be $u(1)$ and the details would be rather different; we hope to treat $D_{m+1}\supset D_m\oplus u(1)$ in a later paper.

As basis vectors in weight space we use $l=m+n$ orthonormal vectors e_i $(i=1,\ldots,l)$. Weyl reflections for D_l consist of interchanges $e_i\leftrightarrow e_j$ and two sign reversals at a time $e_i\rightarrow -e_i$, $e_j\rightarrow -e_j$.

The simple roots are $\alpha_i=e_i-e_{i+1}$ $(i=1,\ldots,l-1)$ and $\alpha_l=e_{l-1}+e_l$. The extended simple root is $\alpha_0=-e_1-e_2$. The fundamental weights ω_i are given in terms of the simple roots by the inverse Cartan matrix [see Eq. (1)] and thus in terms of the orthonormal basis we find

$$\omega_i=\sum_{h=1}^{i} e_h, \quad i=1,\ldots,l-2,$$
$$\omega_{l-1}=\frac{1}{2}\left[\sum_{h=1}^{l-1} e_h-e_l\right], \quad \omega_l=\frac{1}{2}\sum_{h=1}^{l} e_h. \tag{6}$$

The W-orbit labels are defined as in Sec. II following Eq. (1). According to (6) the weights of the fundamental orbit $[i]$, $i=1,\ldots,l-2$, consist of all linear combinations of i distinct e_h with coefficients ± 1; the weights of $[l-1]$ and $[l]$ consist of linear combinations of all e_h, an odd number with coefficient $-\frac{1}{2}$ and the rest with coefficient $+\frac{1}{2}$ for $[l-1]$, an even number with coefficient $-\frac{1}{2}$ and the rest with coefficient $+\frac{1}{2}$ for $[l]$.

The simple roots of D_l, D_m, and D_n are shown in Fig. 3. The simple roots α'_j of D_m and α''_k of D_n are given in terms of D_l simple roots by

$$\alpha'_j=\alpha_{m-j}, \quad j=1,\ldots,m,$$
$$\alpha''_k=\alpha_{m+k}, \quad k=1,\ldots,n. \tag{7}$$

Then the fundamental weights ω'_j of D_m and ω''_k of D_n are respectively

$$\omega'_j=-\sum_{h=m-j+1}^{m} e_h, \quad j=1,\ldots,m-2,$$
$$\omega'_{m-1}=\frac{1}{2}\left[-\sum_{h=2}^{m} e_h+e_1\right], \quad \omega'_m=-\frac{1}{2}\sum_{h=1}^{m} e_h, \tag{8}$$

$$\omega_k''=\sum_{h=m+1}^{m+k} e_h\,,\quad k=1,\ldots,n-2,$$

$$\omega_{n-1}''=\frac{1}{2}\left[\sum_{h=m+1}^{l-1} e_h-e_l\right],\quad \omega_n''=\frac{1}{2}\sum_{h=m+1}^{l} e_h\,.$$

The elementary $D_m\oplus D_n$ orbits are those contained in the fundamental orbits $[i]$ of D_l. We denote one of them by $[j;k]$, the direct product of the orbit $[j]$ of D_m and $[k]$ of D_n, to be specified below. We may write

$$[i]\supset\sum_{j=\max(0,i-n)}^{\min(i,m)}[j;i-j],\quad i=1,\ldots,l-2,$$

$$[l-1]\supset[m;n']+[m';n],\tag{9}$$

$$[l]\supset[m;n]+[m';n'].$$

In the first of Eqs. (9), j is the number of e_h in a weight of $[i]$ for which $1\leqslant h\leqslant m$ and $k=i-j$ is the number in the range $m+1\leqslant h\leqslant l$; for $j=0$ $[j]$ is the zero orbit of D_m and for $j=1,\ldots,m-2$ it is jth fundamental orbit; for $j=m-1$ it is the D_m orbit for which the last two labels, the $(m-1)$th and mth, are unity and the rest zero; for $j=m$ there are two D_m orbits: $[m]$ and $[m']$. The first, $[m]$, has the mth label 2 and the rest 0, while the second, $[m']$, has the $(m-1)$th label 2 and the rest 0. The statements in the preceding sentence are all valid with the replacements $j\to k$, $m\leftrightarrow n$. For $i=l-1$ [the second of Eqs. (9)] there are two elementary orbits, $[m;n']$ and $[m';n]$; for $i=l$ [the third of Eqs. (9)] there are also two, $[m;n]$ and $[m';n']$; here $[m]$ means the mth fundamental orbit of D_m and $[m']$ is the $(m-1)$th; similarly with the replacement $m\leftrightarrow n$.

Figure 4 shows the elementary subalgebra orbits described above. Except for the four in the lower right-hand corner, those for which $j+k=i$ belong to the orbit $[i]$ of D_l. The two at the bottom of the nth column belong to $[l-1]$ while the two at the right of the mth row belong to $[l]$.

To complete the description of our solution we must now give the compatibility rules.

Consider a pair of elementary orbits in Fig. 4, of which neither is in the lower right corner, i.e., belongs to the $(l-1)$th or lth fundamental orbit of D_l and not both of which lie in the bottom row with $j=m$ or m' nor both in the right column with $k=n$ or n'. Then they are incompatible if and only if one lies above and to the right of the other. If both are in the right column and at most one in the lower right corner, they are compatible if and only if both are labeled n or both labeled n'. Similarly if both are in the bottom row and at most one in the lower right corner, they are compatible if and only if both are labeled m or both labeled m'. Those in the lower corner are compatible with all those for which $j\leqslant m-1$ and $k\leqslant n-1$. Finally both in the $(l-1)$th fundamental orbit of D_l are compatible with both in the lth fundamental orbit.

For the complete orbit–orbit branching rules, consider a D_l orbit. For each nonzero label λ_i select one elementary subalgebra orbit from the ith fundamental orbit of D_l so that all the elementary orbits chosen are mutually compatible. Then form the stretched product (orbit labels additive) of the elementary orbits chosen, the ith one used λ_i times. Each such choice of elementary orbits gives one $D_m\oplus D_n$ orbit in the D_l orbit $[\lambda_1,\ldots,\lambda_l]$.

IV. THE ALGEBRA–SUBALGEBRA PAIR $B_{m+n}\supset D_m\oplus B_n$

We suppose that $m>1$ since D_1 would be $u(1)$ and the details different. We hope to deal with $B_{m+1}\supset B_m\oplus u(1)$ in a future paper.

As basis vectors in weight space we use $l=m+n$ orthonormal vectors e_h $(h=1,\ldots,l)$. Weyl reflections for B_l consist of sign reversals $e_i\to -e_i$ and interchanges $e_i\leftrightarrow e_j$.

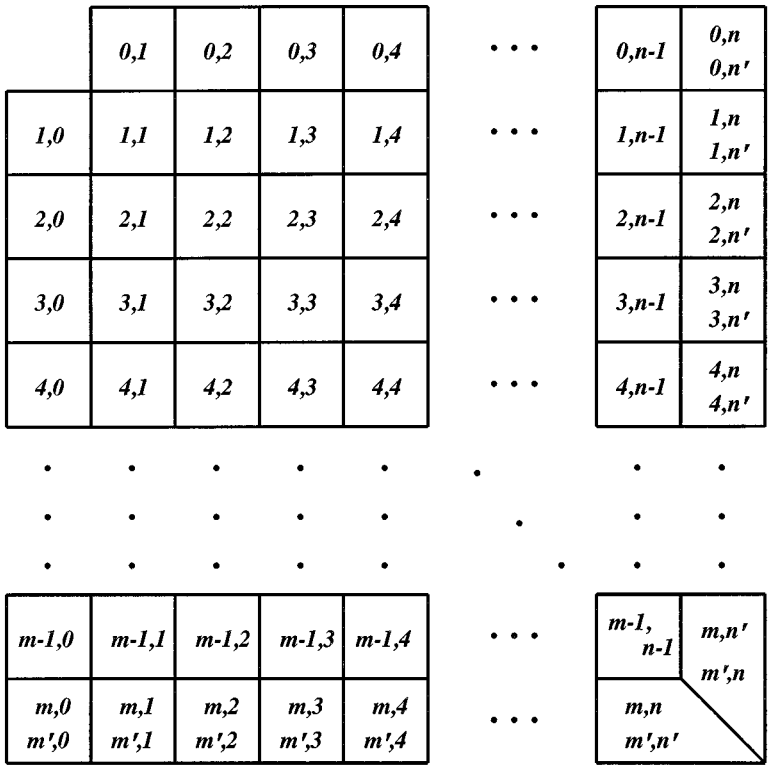

FIG. 4. The elementary $D_{m+n}\supset D_m\oplus D_n$ W-orbits. Which ones belong to a D_{m+n} orbit $[i]$ and which pairs are compatible are stated in the text.

The simple roots are $\alpha_i=e_i-e_{i+1}$ $(i=1,\ldots,l-1)$ and $\alpha_l=e_l$; the extended simple root is $\alpha_0=-e_1-e_2$. The fundamental weights are given in terms of the simple roots by means of the inverse Cartan matrix, and in terms of the orthonormal basis we have

$$\omega_i=\sum_{h=1}^{i} e_h \quad (i=1,\ldots,l-1),$$
$$\omega_l=\frac{1}{2}\sum_{h=1}^{l} e_h . \tag{10}$$

The W-orbit labels are the components λ_i of the highest weight of the orbit in a fundamental weights basis. According to (10) the weights of the fundamental orbit $[i]$, $i=1,\ldots,l-1$, consist of all linear combinations of i distinct e_h with coefficients ±1; the weights of the last fundamental orbit $[l]$ consist of linear combinations of all e_h with coefficients $\pm\frac{1}{2}$.

The simple roots of B_l, D_m, and B_n are shown in Fig. 5. The simple roots α'_j of D_m and α''_j of B_n are given in terms of the B_l simple roots by

$$\alpha'_j=\alpha_{m-j}, \quad j=1,\ldots,m,$$
$$\alpha''_k=\alpha_{m+k}, \quad k=1,\ldots,n. \tag{11}$$

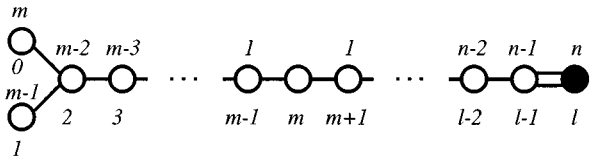

FIG. 5. The Dynkin–Coxeter diagram for $B_{m+n}\supset D_m\oplus B_n$. The numbers below the nodes label the simple roots of B_l ($l=m+n$). Those to the left above label those of D_m, and those to the right above label those of B_n.

Then the fundamental weights ω_j' of D_m and ω_j'' of B_n are respectively

$$\begin{gathered}\omega_j'=-\sum_{h=m-j+1}^{m} e_h, \quad j=1,\ldots,m-2,\\ \omega_{m-1}'=\frac{1}{2}\left(e_1-\sum_{h=2}^{m} e_h\right), \quad \omega_m'=-\frac{1}{2}\sum_{h=1}^{m} e_h,\\ \omega_k''=\sum_{h=m+1}^{m+k} e_h, \quad k=1,\ldots,n-1,\\ \omega_n''=\frac{1}{2}\sum_{h=m+1}^{l} e_h.\end{gathered} \tag{12}$$

The elementary $D_m\oplus B_n$ orbits are those contained in the fundamental orbits $[i]$ of B_l. They may be written $[j;k]$, the direct product of a D_m orbit $[j]$ and a B_n orbit $[k]$. Explicitly we have

$$\begin{gathered}[i]\supset\sum_{j=\max(0,i-n)}^{\min(i,m)}[j;i-j], \quad i=1,\ldots,l-1,\\ [l]\supset[m;n]+[m';n].\end{gathered} \tag{13}$$

Here j is the number of e_h in a weight of $[i]$ for which $1\leqslant h\leqslant m$ and $k=i-j$ is the number in the range $m+1\leqslant k\leqslant l$. For $j=0$, $[j]$ is the zero orbit of D_m and for $k=0$, $[k]$ is the zero orbit of B_n. For $j=1,\ldots,m-2$, $[j]$ is the jth fundamental orbit of D_m and for $k=1,\ldots,n-1$, $[k]$ is the kth fundamental orbit of B_n. For $j=m-1$ $[j]$ is the D_m orbit with the $(m-1)$th and mth labels unity and the rest zero; for $j=m$ there are two D_m orbits, $[m]$, which has the mth label 2 and the rest 0, and $[m']$, which has the $(m-1)$th label 2 and the rest 0. For $k=n$, the B_n orbit $[n]$ has the nth label 2 and the rest 0. For $i=l$, there are two $D_m\oplus B_n$ orbits $[m;n]$ and $[m';n]$ where $[m]$ and $[m']$ are, respectively, the mth and $(m-1)$th fundamental orbits of D_m and $[n]$ is the nth fundamental orbit of B_n.

It remains to give the compatibility rules for $B_l\supset D_m\oplus B_n$; they are very similar to those for $C_l\supset C_m\oplus C_n$ and $D_l\supset D_m\oplus D_n$.

If not more than one of a pair lies in the bottom row of Fig. 6, i.e., if $j\neq m$ for one of the pair, then they are incompatible if either lies above and to the right of the other, otherwise they are compatible. If both lie in the bottom row they are compatible if both are labelled m or both labelled m'; otherwise they are incompatible.

The instructions for finding a complete set of compatible orbits and hence the complete orbit–orbit branching rules are the same as those for $C_l\supset C_m\oplus C_n$ in Sec. II and for $D_l\supset D_m\oplus D_n$ in Sec. III.

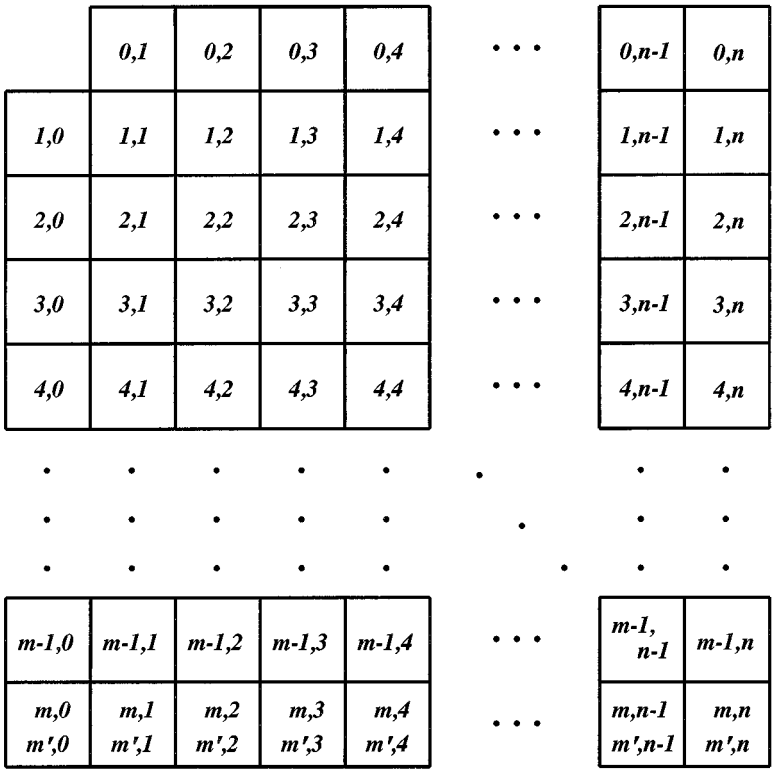

FIG. 6. The elementary $B_{m+n} \supset D_m \oplus B_n$ W-orbits. The elementary orbit $[j;k]$ belongs to the $(j+k)$th fundamental W-orbit of B_{m+n} (two of them when $k=m$).

V. CONCLUDING REMARKS

We hope in the near future to publish orbit–orbit branching rules for compact algebra–subalgebra families in which the subalgebra is reductive but not semisimple, i.e., contains a $u(1)$ factor. We are thinking of $A_{m+n+1} \supset A_m \oplus A_n \oplus u(1)$, $C_{m+1} \supset A_m \oplus u(1)$, and $D_{m+1} \supset A_m \oplus u(1)$. Then we hope to deal with families of Kac–Moody algebra–subalgebras; we had started on this problem when we noticed that the classical problem had never been solved and decided it should be dealt with first.

ACKNOWLEDGMENTS

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A group analysis approach for a nonlinear differential system arising in diffusion phenomena

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We consider a class of second-order partial differential equations which arises in diffusion phenomena and, following a new approach, we look for a Lie invariance classification via equivalence transformations. A class of exact invariant solutions containing an arbitrary function is obtained. © *1996 American Institute of Physics.* [S0022-2488(96)00909-7]

I. INTRODUCTION

Lie point symmetries approach is a systematic way to construct exact solutions for partial differential equations (PDEs).[1–3] The looking for symmetries via the Lie infinitesimal criterion leads to the so-called ''determining system'', which is a linear PDEs system in the unknown coordinates of the invariance operator. The determining system, in general, is an overdetermined system which becomes very difficult to solve when arbitrary functions appear. In fact, quite often in these cases the general solution of the determining system is a wasteful venture. In these cases an effective way which gives a group classification is based on equivalence transformations.

In some recent papers[4–9] it was shown that it is possible to obtain subalgebras of the Lie algebra of PDEs, starting from equivalence algebra. Of course, this fact allows, quite often, only a partial classification, but this approach offers a systematic way to get solutions of the determining system.

In this framework we consider the system

$$u_t = h(u,v), \quad v_t = [g(v)v_x + f(v)u_x]_x, \tag{1.1}$$

where we assume $g' \neq 0$ and $f' \neq 0$. Moreover, we denote with $(\ )_t$ and $(\ )_x$ the partial derivatives with respect to the independent variables t and x, respectively, while the prime denotes the derivative of the functions with respect to their argument.

The equations (1.1), apart from their own theoretical interest, can describe the diffusion of a solvent into a polymer slab, which is characterized by a sharp front that moves into the medium and lasts for long time.

The stress in the polymer increases because of the intrusion of the solvent which deforms the polymer. On the contrary this stress reacts back on the penetrant and tries to push it from regions of high stress to regions of low stress.

So the model equations proposed include solvent flux due to stress gradients in the polymer in addition to the fickian flux (see, e.g., Refs. 10 and 11).

We give a group classification of system (1.1) by means of continuous equivalence transformations.

As is well known, the equivalence transformations change a system into a system belonging to the same class.[9,12] Generally speaking, the system (1.1) is mapped into a system of the same form but with different $h(u,v)$, $g(v)$, and $f(v)$.

In the classical approach for finding equivalence transformations of system (1.1) in agreement with Ref. 12, by using the Lie infinitesimal criterion, the infinitesimal equivalence generator of our system is obtained by requiring in the space of (t,x,u,v,h,f,g) the invariance of (1.1) and the invariance of the auxiliary conditions

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TABLE I. f, g arbitrary.

No.	h	Extensions of L_P
1	$\hat{h}(v)e^{au}$	$X_3=2t\frac{\partial}{\partial t}+x\frac{\partial}{\partial x}-\frac{2}{a}\frac{\partial}{\partial u}$
	$a\neq 0$	
2	$h_0u+\hat{h}(v)$	$X_3=e^{h_0t}\frac{\partial}{\partial u}$
3	h_0	$X_3=2t\frac{\partial}{\partial t}+x\frac{\partial}{\partial x}+2h_0t\frac{\partial}{\partial u}$
		$X_4=\frac{\partial}{\partial u}$

$$f_t=g_t=h_t=f_x=\cdots=0, \tag{1.2}$$

which characterize the functional dependence of the functions f, g, and h.

Nevertheless, in this paper we leave the classical approach and we behave as follows:[8,9]

(a) we do not work in the space (t,x,u,v,h,f,g), but in the space (t,x,u,v,h), in order to obtain an *equivalence classification* with respect to f and g;

(b) we consider the function h at first depending on t, x, u, and v.

The plan of the paper is the following:

In Sec. II we give an *equivalence classification* of system (1.1) without taking auxiliary conditions into account (we show, at the end of Sec. III, how the auxiliary conditions restrict the equivalence algebra).

In Sec. III we obtain the Lie classification for a function $h(u,v)$ (in Tables I–IV the final results are summarized).

In Sec. IV we find a class of exact invariant solutions for the system of equations which describe the behavior of a solvent penetrating in a polymer. In this class an arbitrary function of x appears which could be determined by the initial conditions.

II. AN EQUIVALENCE CLASSIFICATION

We consider the class of second-order partial differential equation systems

$$u_t=h(t,x,u,v), \quad v_t=[g(v)v_x+f(v)u_x)]_x, \tag{2.1}$$

and look for continuous equivalence transformations which map system (2.1) into a system of the same form but with different $h(t,x,u,v)$, so we consider the function h as a dependent variable. Having in mind to apply the infinitesimal invariance criterion,[12] the infinitesimal equivalence operator Y works in the space (t,x,u,v,h), so it is chosen of the following form:

$$Y=\xi^1\frac{\partial}{\partial t}+\xi^2\frac{\partial}{\partial x}+\eta^1\frac{\partial}{\partial u}+\eta^2\frac{\partial}{\partial v}+\mu\frac{\partial}{\partial h}, \tag{2.2}$$

where the coordinates ξ^i, η^i are sought as functions of t, x, u and v, while μ may depend on t, x, u, v, and h.

The prolongation of Y, which we need, is

TABLE II. $f=f_0e^{pv}$, $g=g_0e^{qv}$, $p\neq 0$, $q\neq 0$.

No.	h	Extensions of L_P
1	$\hat{h}(\lambda)e^{av}$ $\lambda=(u+\delta)e^{(p-q)v}$ $q\neq p$	$X_3=(q-p-a)t\dfrac{\partial}{\partial t}+\dfrac{(2q-p-a)x}{2}\dfrac{\partial}{\partial x}+(q-p)(u+\delta)\dfrac{\partial}{\partial u}+\dfrac{\partial}{\partial v}$
2	$\hat{h}(\lambda)e^{av}$ $\lambda=\delta v-u$	$X_3=-at\dfrac{\partial}{\partial t}+\dfrac{q-a}{2}x\dfrac{\partial}{\partial x}+\delta\dfrac{\partial}{\partial u}+\dfrac{\partial}{\partial v}$
3	$h_0u+h_1e^{(q-p)v}+h_2$ $h_0\neq 0,\ q\neq p$	$X_3=\dfrac{q}{2}x\dfrac{\partial}{\partial x}+(q-p)\left(u+\dfrac{h_2}{h_0}\right)\dfrac{\partial}{\partial u}+\dfrac{\partial}{\partial v}$ $X_4=e^{h_0t}\dfrac{\partial}{\partial u}$
4	$h_0u+h_1v+h_2$ $h_0\neq 0,\ q=p$	$X_3=\dfrac{q}{2}x\dfrac{\partial}{\partial x}-\dfrac{h_1}{h_0}\dfrac{\partial}{\partial u}+\dfrac{\partial}{\partial v}$ $X_4=e^{h_0t}\dfrac{\partial}{\partial u}$
5	$h(v)$	$X_3=\dfrac{\partial}{\partial u}$
6	h_0v+h_1	$X_3=\dfrac{\partial}{\partial u}$ $X_4=(q-p)t\dfrac{\partial}{\partial t}+\dfrac{2q-p}{2}x\dfrac{\partial}{\partial x}+[(q-p)u+h_0t]\dfrac{\partial}{\partial u}+\dfrac{\partial}{\partial v}$
7	h_1	$X_3=\dfrac{\partial}{\partial u}$ $X_4=-qt\dfrac{\partial}{\partial t}+[(q-p)u+h_1(p-2q)t]\dfrac{\partial}{\partial u}+\dfrac{\partial}{\partial v}$ $X_5=2t\dfrac{\partial}{\partial t}+x\dfrac{\partial}{\partial x}+2h_1t\dfrac{\partial}{\partial u}$

$$\widetilde{Y}=Y+\zeta_1^1\frac{\partial}{\partial u_t}+\zeta_2^1\frac{\partial}{\partial u_x}+\zeta_1^2\frac{\partial}{\partial v_t}+\zeta_2^2\frac{\partial}{\partial v_x}+\zeta_{22}^1\frac{\partial}{\partial u_{xx}}+\zeta_{22}^2\frac{\partial}{\partial v_{xx}},\tag{2.3}$$

where the coefficients ζ_i^j and ζ_{22}^i, after putting

$$(x^1,x^2)\equiv(t,x),\quad (y^1,y^2)\equiv(u,v),$$

$$y_j^i=\frac{\partial y^i}{\partial x^j},\quad y_{jk}^i=\frac{\partial y^i}{\partial x^j x^k},\quad D_j=\frac{\partial}{\partial x^j}+y_j^i\frac{\partial}{\partial y^i}+y_{jk}^i\frac{\partial}{\partial y_k^i}\cdots,\tag{2.4}$$

are given by

TABLE III. $f=f_0(v+\nu_0)^p$, $g=g_0(v+\nu_0)^q$; $p\neq 0,\ -1$; $q\neq 0,\ -2$.

No.	h	Extensions of L_P
1	$\hat{h}(\lambda)(v+\nu 0)a$ $\lambda=(u+\delta)(u+\nu 0)p-q-1$ $1+q-p\neq 0$	$X_3=(1+q-p-a)t\frac{\partial}{\partial t}+\frac{(1+2q-p-a)x}{2}\frac{\partial}{\partial x}$ $+(1+q-p)(u+\delta)\frac{\partial}{\partial u}+(v+\nu_0)\frac{\partial}{\partial v}$
2	$\hat{h}(\lambda)(v+\nu_0)^a$ $\lambda=\delta lg(v+\nu_0)-u$ $p=1+q$	$X_3=-at\frac{\partial}{\partial t}+\frac{(q-a)x}{2}\frac{\partial}{\partial x}+\delta\frac{\partial}{\partial u}+(v+\nu_0)\frac{\partial}{\partial v}$
3	$h_0u+(v+\nu_0)^{1+q-p}h_1+h_2$ $h_0\neq 0,\ 1+q-p\neq 0$	$X_3=\frac{qx}{2}\frac{\partial}{\partial x}+(1+q-p)\left(u+\frac{h_2}{h_0}\right)\frac{\partial}{\partial u}+(v+\nu_0)\frac{\partial}{\partial v}$ $X_4=e^{h_0t}\frac{\partial}{\partial u}$
4	$h_0u+h_1lg(v+\nu_0)+h_2$ $h_0\neq 0,\ p=1+q$	$X_3=\frac{qx}{2}\frac{\partial}{\partial x}-\frac{h_1}{h_0}\frac{\partial}{\partial u}+(v+\nu_0)\frac{\partial}{\partial v}$ $X_4=e^{h_0t}\frac{\partial}{\partial u}$
5	$\hat{h}(v)$	$X_3=\frac{\partial}{\partial u}$
6	$h_0(v+\nu_0)^a+h_1$ $a\neq 0$	$X_3=\frac{\partial}{\partial u}$ $X_4=(1-p-a+q)t\frac{\partial}{\partial t}+\frac{1-p+2q-a}{2}x\frac{\partial}{\partial x}$ $+[(1+q-p)u-ah_1t]\frac{\partial}{\partial u}+(v+\nu_0)\frac{\partial}{\partial v}$
7	$h_0lg(v+\nu_0)+h_1$	$X_3=\frac{\partial}{\partial u}$ $X_4=(1-p+q)t\frac{\partial}{\partial t}+\frac{1-p+2q}{2}x\frac{\partial}{\partial x}+[h_0t+(1+q-p)u]\frac{\partial}{\partial u}$ $+(v+\nu_0)\frac{\partial}{\partial v}$
8	h_0	$X_3=\frac{\partial}{\partial u}$ $X_4=-qt\frac{\partial}{\partial t}+[(1+q-p)u+h_0(p-2q-1)t]\frac{\partial}{\partial u}+(v+\nu_0)\frac{\partial}{\partial v}$ $X_5=2t\frac{\partial}{\partial t}+x\frac{\partial}{\partial x}+2h_0t\frac{\partial}{\partial u}$

$$\zeta_j^i=D_j\eta^i-y_t^iD_j\xi^1-y_x^iD_j\xi^2,\quad \zeta_{22}^i=D_2\zeta_2^i-y_{tx}^iD_2\xi^1-y_{xx}^iD_2\xi^2. \tag{2.5}$$

Requiring the invariance of (2.1) with respect the operator $\tilde{Y}$ by following the well-known procedure,[5,9,13] we obtain the determining system which leads to the following conditions:

TABLE IV. $f=f_0(v+\nu_0)^{-1}$, $g=g_0(v+\nu_0)^{-2}$.

No.	h	Extensions of L_P
1	$h_0(v+\nu_0)^{ag_0/f_0}e^{au}$	$X_3=2t\frac{\partial}{\partial t}-\left(\frac{g_0}{f_0}+\frac{2}{a}\right)\frac{\partial}{\partial u}+(v+\nu_0)\frac{\partial}{\partial v}$
	$a\neq 0$	$X_\psi=\psi(x)\frac{\partial}{\partial x}+\frac{g_0}{f_0}\psi'\frac{\partial}{\partial u}-(v+\nu_0)\psi'\frac{\partial}{\partial v}$
2	$\hat{h}(\lambda)$	$X_\psi=\psi(x)\frac{\partial}{\partial x}+\frac{g_0}{f_0}\psi'\frac{\partial}{\partial u}-(v+\nu_0)\psi'\frac{\partial}{\partial v}$
	$\lambda=\frac{f_0}{g_0}u+lg(v+\nu_0)$	
3	$h_0(u+\frac{g_0}{f_0}lg(v+\nu_0))+h_1$	$X_\psi=\psi(x)\frac{\partial}{\partial x}+\frac{g_0}{f_0}\psi'\frac{\partial}{\partial u}-(v+\nu_0)\psi'\frac{\partial}{\partial v}$
		$X_3=e^{h_0t}\frac{\partial}{\partial u}$
4	$h_0u+h_1lg(v+\nu_0)+h_2$	$X_3=x\frac{\partial}{\partial x}+\frac{h_1}{h_0}\frac{\partial}{\partial u}-(v+\nu_0)\frac{\partial}{\partial v}$
		$X_4=e^{h_0t}\frac{\partial}{\partial u}$
5	$\hat{h}(v)$	$X_3=\frac{\partial}{\partial u}$
6	$h_0(v+\nu_0)^a+h_1$	$X_3=\frac{\partial}{\partial u}$
	$a\neq 0$	$X_4=2t\frac{\partial}{\partial t}+\frac{2+a}{a}x\frac{\partial}{\partial x}+\left(\frac{g_0}{f_0}\frac{2+a}{a}+2h_1t\right)\frac{\partial}{\partial u}-\frac{2}{a}(v+\nu_0)\frac{\partial}{\partial v}$
7	$h_0lg(v+\nu_0)+h_1$	$X_3=\frac{\partial}{\partial u}$
		$X_4=x\frac{\partial}{\partial x}+\left(\frac{g_0}{f_0}-h_0t\right)\frac{\partial}{\partial u}-(v+\nu_0)\frac{\partial}{\partial v}$
8	h_0	$X_3=\frac{\partial}{\partial u}$
		$X_4=2t\frac{\partial}{\partial t}+2h_0t\frac{\partial}{\partial u}+(v+\nu_0)\frac{\partial}{\partial v}$
		$X_\psi=\psi(x)\frac{\partial}{\partial x}+\frac{g_0}{f_0}\psi'\frac{\partial}{\partial u}-(v+\nu_0)\psi'\frac{\partial}{\partial v}$

$$
\begin{gathered}
f'\eta_x^2=f\xi_{xx}^2,\quad g'\eta^2+g(\xi_t^1-2\xi_x^2)=0,\\
f'\eta_x^1+2g'\eta_x^2+g(2\eta_{xv}^2-\xi_{xx}^2)=0,\\
f'\eta^2+f(\xi_t^1-\eta_v^2+\eta_u^1-2\xi_x^2)=0,\quad f\eta_{xx}^1+g\eta_{xx}^2-\eta_t^2=0,
\end{gathered}
\tag{2.6}
$$

for the functions

$$
\begin{gathered}
\xi^1=\xi^1(t),\quad \xi^2=\xi^2(x),\\
\eta^1=\alpha(t)u+\beta(x,t),\quad \eta^2=\gamma(x,t)v+\pi(x,t),
\end{gathered}
\tag{2.7}
$$

while μ is given from

$$\mu = h(\eta_u^1 - \xi_t^1) + \eta_t^1. \tag{2.8}$$

After some calculations we obtain the following *equivalence classification* of system (2.1):
(a) f,g arbitrary:

$$\xi^1 = 2c_3 t + c_1, \quad \xi^2 = c_3 x + c_2, \quad \eta^1 = \phi(t), \quad \eta^2 = 0, \quad \mu = \phi' - 2c_3 h, \tag{2.9}$$

where c_1, c_2, c_3 are arbitrary constants and ϕ is an arbitrary function of t.
(b) $f = f_0 e^{pv}$, $g = g_0 e^{qv}$, $p \neq 0$, $q \neq 0$:

$$\begin{gathered} \xi^1 = (2c_1 - qc_3)t + c_4, \quad \xi^2 = c_1 x + c_2, \\ \eta^1 = c_3(q-p)u + \phi(t), \quad \eta^2 = c_3, \\ \mu = \phi' + [c_3(2q-p) - 2c_1]h, \end{gathered} \tag{2.10}$$

with f_0, g_0, p, and q constitutive constants, while c_1, c_2, c_3, c_4 are arbitrary constants and ϕ is an arbitrary function of t.
(c) $f = f_0(v+\nu_0)^p$, $g = g_0(v+\nu_0)^q$, $p \neq 0,-1$; $q \neq 0,-2$:

$$\begin{gathered} \xi^1 = (2c_1 - qc_3)t + c_4, \quad \xi^2 = c_1 x + c_2, \\ \eta^1 = c_3(1+q-p)u + \phi(t), \quad \eta^2 = c_3(v+\nu_0), \\ \mu = \phi' + [c_3(1+2q-p) - 2c_1]h, \end{gathered} \tag{2.11}$$

with f_0, g_0, ν_0, p, and q constitutive constants, while c_1, c_2, c_3, c_4 are arbitrary constants and ϕ is an arbitrary function of t.
(d) $f = f_0(v+\nu_0)^{-1}$, $g = g_0(v+\nu_0)^{-2}$:

$$\begin{gathered} \xi^1 = 2c_1 t + c_2, \quad \xi^2 = \psi(x), \quad \eta^1 = \frac{g_0}{f_0}\psi' + \phi(t), \\ \eta^2 = (v+\nu_0)(c_1 - \psi'), \quad \mu = \phi' - 2c_1 h, \end{gathered} \tag{2.12}$$

with f_0, g_0, and ν_0 constitutive constants, while c_1, c_2 are arbitrary constants, ψ is an arbitrary function of x, and ϕ is an arbitrary function of t.

III. LIE SYMMETRIES VIA EQUIVALENCE TRANSFORMATIONS

In this section we will show how it is possible to obtain a symmetry classification of system (1.1), starting from the equivalence classifications obtained in Sec. II.

First of all it must be stressed that the projection of operator Y in the space (t,x,u,v), i.e.,

$$X = \xi^1 \frac{\partial}{\partial t} + \xi^2 \frac{\partial}{\partial x} + \eta^1 \frac{\partial}{\partial u} + \eta^2 \frac{\partial}{\partial v}, \tag{3.1}$$

is a symmetry operator.

Then, starting from the equivalence classification of system (2.1), we obtain some invariance algebras, applying the following theorem:[7,9,13]

Theorem 3.1: Let Y be an equivalence operator for the system (2.1). The operator X is an invariance operator for the system (2.1) where $h=\hat{h}(t,x,u,v)$ if and only if $\hat{h}$ is invariant with respect to Y.

The proof of this theorem follows immediately from the analogous theorems given in Refs. 6 and 9.

Now, we shall give some symmetry operators of systems (1.1) applying the following corollary of previous theorem:

Corollary: By choosing $\hat{h}\equiv h(u,v)$, the operator X is an invariance operator of systems (1.1).

The invariance of the function $\hat{h}$ with respect to the operator Y of the system (2.1), requested by Theorem 3.1, leads to

$$\eta^1 h_u+\eta^2 h_v=h(\eta^1_u-\xi^1_t)+\eta^1_t. \tag{3.2}$$

Specializing the form of η^1, η^2, and ξ^1 for each of the equivalence classes obtained in Sec. II, we obtain a Lie invariance classification with respect to $\hat{h}\equiv h(u,v)$.

We begin by showing the results for the equivalence class (a). With this class we have f and g as arbitrary functions and the equivalence operator Y given by

$$Y=(2c_3t+c_1)\frac{\partial}{\partial t}+(c_3x+c_2)\frac{\partial}{\partial x}+\phi(t)\frac{\partial}{\partial u}+(\phi'-2c_3h)\frac{\partial}{\partial h}. \tag{3.3}$$

So the condition (3.2) becomes

$$\phi(t)h_u=-2c_3h+\phi'. \tag{3.4}$$

This equation is the classifying equation for h in the equivalence class (a). Of course for h arbitrary, from (3.4) we obtain the principal Lie algebra $L_{\mathscr{P}}$ spanned by

$$X_1=\frac{\partial}{\partial t},\quad X_2=\frac{\partial}{\partial x}. \tag{3.5}$$

The classification of h and the corresponding extensions of $L_{\mathscr{P}}$ can be obtained solving (3.4) with respect to h, taking into account that h is independent of t and x. So by deriving with respect to t we obtain

$$\phi' h_u=\phi''. \tag{3.6}$$

From (3.6) and (3.4) three cases arise which lead, after easy calculations, to the following results:

(1) $h=\hat{h}(v)e^{au}$, $a\neq 0$, $\phi=-2c_3/a$,

$$X_3=2t\frac{\partial}{\partial t}+x\frac{\partial}{\partial x}-\frac{2}{a}\frac{\partial}{\partial u}; \tag{3.7}$$

(2) $h=h_0u+\hat{h}(v)$, $\phi=c_4e^{h_0t}$, $c_3=0$,

$$X_3=e^{h_0t}\frac{\partial}{\partial u}; \tag{3.8}$$

(3) $h=h_0$, $\phi=2c_3h_0t+c_4$,

$$X_3=2t\frac{\partial}{\partial t}+x\frac{\partial}{\partial x}+2h_0t\frac{\partial}{\partial u};\quad X_4=\frac{\partial}{\partial u}, \tag{3.9}$$

where h_0 and a are constitutive constants and $\hat{h}(v)$ is a constitutive function of v, while c_3 and c_4 are arbitrary constants.

The results concerning the other equivalence classes (b)–(d) can be obtained following a similar procedure.

The final results are summarized in Tables I–IV, which correspond to equivalence classes (a)–(d), respectively.

Remark: We have a symmetry classification of system (1.1) starting from the equivalence classifications of system (2.1). It is worthwhile remarking that the symmetry classification obtained is larger than the one which could be obtained following the procedures introduced in Ref. 6. In fact, if we look for equivalence transformations which map the system (1.1) into a system of the same form but with a function h depending only on u and v, by following the procedures introduced in Ref. 6, we must take into consideration the restrictions on the equivalence generator given from the auxiliary conditions

$$h_t = h_x = 0, \tag{3.10}$$

which characterize the functional dependence of the function h. So, the prolongation of Y, which now we need, is

$$Y^* = \widetilde{Y} + \omega_1 \frac{\partial}{\partial h_t} + \omega_2 \frac{\partial}{\partial h_x}, \tag{3.11}$$

where the coefficients ω_i, after recalling the notation introduced in (2.4), and after putting

$$\widetilde{D}_i = \frac{\partial}{\partial x^i} + h_{x^i} \frac{\partial}{\partial h}, \tag{3.12}$$

are given by

$$\omega_i = \widetilde{D}_i \mu - h_{x^k} \widetilde{D}_i \xi^k - h_{y^k} \widetilde{D}_i \eta^k. \tag{3.13}$$

Then requiring[9] the invariance of (3.10), with respect to Y^*, we obtain

$$\mu_t = \mu_x = 0, \quad \eta^1_t = \eta^1_x = 0, \quad \eta^2_t = \eta^2_x = 0. \tag{3.14}$$

After observing that the additional restrictions (3.14) are decoupled from conditions (2.6), we can obtain the equivalence transformations of systems (1.1) for the cases (a)–(d) of the previous section by substituting

$$\phi(t) = c_5, \quad \psi(x) = c_6 x + c_7, \tag{3.15}$$

where c_5, c_6, and c_7 are arbitrary constants.

It is a simple matter to verify that if we look for a symmetry classification of systems (1.1), by projection in the space (t,x,u,v), starting from the equivalence transformations of systems (1.1), some extensions of the principal Lie algebra $L_{\mathscr{P}}$ in Tables I–IV cannot be obtained because of (3.15). To ascertain this, it is enough to consider in Table IV the case Nos. 1, 2, 3, and 8 where the symmetry algebras are infinite dimensional.

IV. A CLASS OF INVARIANT SOLUTIONS

As said in Sec. I, the system of equations (1.1) can describe the diffusion of a solvent in a polymer slab. The behavior of the diffusion of the solvent in the polymer cannot be explained by the usual diffusion equation. The introduction of the stress as a dependent variable involves an evolution equation for it. A general formulation of this equation is

$$u_t = r(v)[s(v) - u], \tag{4.1}$$

which is an amalgamation of the Maxwell viscoelastic model and the Kelvin–Voigt elastic model.[10,11]

Starting from some results of previous sections, here we give a class of invariant solutions which involves an arbitrary function of the independent variable x.

After observing that in this case from (4.1) it follows that

$$h = r(v)[s(v) - u], \tag{4.2}$$

it is easy to see that such a class of solutions could be obtained from the case No. 3 in Table IV. Then the system (1.1) is specialized as follows:

$$\begin{aligned} u_t &= h_0 u + \frac{h_0 g_0}{f_0}\, lg(v+\nu_0) + h_1, \\ v_t &= [f_0 (v+\nu_0)^{-1} u_x + g_0 (v+\nu_0)^{-2} v_x]_x. \end{aligned} \tag{4.3}$$

We look for solutions invariant with respect to the generator given by a linear combination of X_1 and X_ψ, that is

$$X = c_1 \frac{\partial}{\partial t} + c_2 \left[\psi(x) \frac{\partial}{\partial x} + \frac{g_0}{f_0}\, \psi' \frac{\partial}{\partial u} - (v+\nu_0)\psi' \frac{\partial}{\partial v} \right]. \tag{4.4}$$

The invariant surface conditions lead to the following equations:

$$\begin{aligned} c_1 \frac{\partial u}{\partial t} + c_2 \psi(x) \frac{\partial u}{\partial x} &= \frac{c_2 g_0}{f_0}\, \psi', \\ c_1 \frac{\partial v}{\partial t} + c_2 \psi(x) \frac{\partial v}{\partial x} &= -c_2 (v+\nu_0)\psi', \end{aligned} \tag{4.5}$$

from which we obtain

$$u = U(\sigma) + \frac{g_0}{f_0}\, lg\, \psi(x), \quad v = V(\sigma)\psi^{-1}(x) - \nu_0, \tag{4.6}$$

where

$$\sigma := c_2 t - c_1 \Gamma(x), \quad \Gamma(x) := \int \frac{1}{\psi(x)}\, dx, \tag{4.7}$$

while U and V are solutions of the following reduced system:

$$\begin{aligned} c_2 U' &= h_0 U + \frac{h_0 g_0}{f_0}\, lgV + h_1, \\ c_2 V^3 V' &= -2 g_0 c_1^2 V'^2 + g_0 c_1^2 V V'' - f_0 c_1^2 V V' U' + f_0 c_1^2 V^2 U'', \end{aligned} \tag{4.8}$$

obtained after substituting (4.6) in (4.3). Looking for solutions of the form

$$V = e^{\mu_1 \sigma + \mu_0} \tag{4.9}$$

after some calculations from (4.8) we obtain

$$U=e^{(h_0/c_2)\sigma+2\mu_0}-\frac{h_0g_0}{2c_2f_0}\,\sigma+\gamma_0,\quad V=e^{(h_0/2c_2)\sigma+\mu_0},\tag{4.10}$$

with μ_0 arbitrary constant,

$$\gamma_0=-\frac{h_0g_0(2\mu_0+1)+2h_1f_0}{2h_0f_0},\tag{4.11}$$

and provided that

$$c_1=\frac{c_2}{\sqrt{h_0f_0}}.\tag{4.12}$$

Going back to (4.6) we obtain

$$\begin{aligned}u&=e^{(h_0/c_2)\sigma+2\mu_0}-\frac{h_0g_0}{2c_2f_0}\,\sigma+\frac{g_0}{f_0}\,lg\,\psi(x)+\gamma_0,\\ v&=\psi(x)^{-1}e^{(h_0/2c_2)\sigma+\mu_0}-\nu_0,\end{aligned}\tag{4.13}$$

where $\psi(x)$ is an arbitrary function which will determined, together with μ_0 and c_2, from suitable initial conditions.

V. CONCLUSIONS

The method proposed in this paper gives a Lie classification of the system (1.1) via equivalence transformations which is larger than that which can be obtained following the classical equivalence approach.[4–9] We showed that the auxiliary conditions restrict the equivalence algebra and then the symmetry algebras.

Moreover, it is interesting to note that, in a physical case, we get a class of invariant solutions which contain an arbitrary function of x. Often, in the nonlinear cases, the invariant solutions contain only arbitrary constants. This implies that such a type of solution cannot satisfy arbitrary initial boundary conditions. In our case, the presence of an arbitrary function of x adds more possibilities in assigning suitable initial conditions.

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Erratum: On the integrability of the inhomogeneous spherically symmetric Heisenberg ferromagnet in arbitrary dimensions [J. Math. Phys. 35, 6498–6510 (1994)]

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There are a few misprints in some of the equations in Sec. V of the paper. The following are the corrected versions of them.

1. Eq. (49b)

The expressions for $\rho(t)$ and $\zeta(t)$ given in Eqs. (49b) should read as

$$\rho(t)=\frac{\rho(0)+2n\varepsilon_2(\rho^2(0)+\zeta^2(0))t}{(1+2n\varepsilon_2\rho(0)t)^2+4n^2\varepsilon_2^2\zeta^2(0)t^2}\,, \quad \zeta(t)=\frac{\zeta(0)}{(1+2n\varepsilon_2\rho(0)t)^2+4n^2\varepsilon_2^2\zeta^2(0)t^2}\,.$$

2. Eqs. (51) and (52)

In the terms proportional to ε_1, $\lambda^2(t)t$ should be replaced by $\int_0^t\lambda^2(t')dt'$.

3. Eq. (55b)

The term $4\varepsilon_1\rho t$ must be replaced by $4\varepsilon_1\int_0^t\rho\ dt'$.

4. Eq. (55a)

The correct form of the solution given in Eq. (55a) must be read as follows.

$$\begin{aligned}S^{\pm}\equiv S^x\pm iS^y=\frac{2\zeta}{\rho^2+\zeta^2}&\left\{\rho\pm i\zeta\,\tanh\left[2\left(\frac{\zeta r^n}{n}-4\varepsilon_1\int_0^t\zeta\rho dt'\right)-\Delta_1\right]\right\}\\&\times\operatorname{sech}\left[2\zeta\left\{\frac{r^n}{n}-4\varepsilon_1\int_0^t\rho\ dt'-\Delta_1\right\}\right]\\&\times\exp\left[\pm 2i\left\{\frac{\rho r^n}{n}-2\varepsilon_1\int_0^t(\rho^2-\zeta^2)dt'+\delta_1\right\}\right].\end{aligned}$$

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Erratum: Markov diffusions in comoving coordinates and stochastic quantization of the free relativistic spinless particle [J. Math. Phys. 36, 4691–4710 (1995)]

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Corollary 2 (and therefore $2'$) is incorrect. The correct statement should read as follows: *Corollary 2:* The global coordinate transformation $\Phi: x \mapsto \xi := \Phi(x)$, $x \in \mathbb{R}^{1+n}$, transforms the Euclidean metric tensor $\delta_{\mu\nu}$ into the tensor $g^E_{\mu\nu}$ with components

$$g^E_{\mu\nu}(\xi) := \begin{cases} g_{00}(\xi), & \mu = \nu = 0, \\ 0, & \mu = 0, \nu = 1,\ldots,n; \quad \nu = 0, \mu = 1,\ldots,n, \\ g_{ij}(\xi), & \text{otherwise.} \end{cases}$$

In case $\|V\| = \text{const.}$, then $g_{00}(\xi) = f(\xi^0)$.

Corollary 3 should be understood under the assumption $g_{ij}(\xi) = \sigma_{ij}(\xi^1,\ldots,\xi^n)$.

In Sec. IV, the parameter t should be understood as belonging to a time interval $[-\Delta,\Delta]$, $\Delta \in \mathbb{R}^+$, where Δ is chosen on an appropriate scale, so that $g_{ij}(\xi^0,\xi^1,\xi^2,\xi^3) \simeq g_{ij}(\xi^0 = 0,\xi^1,\xi^2,\xi^3) \equiv \sigma_{ij}(q^1,q^2,q^3)$. Such a scale is infinite if the field V is constant.

Introduction

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This issue is devoted to mesoscopic physics and related topics. Mesoscopic physics is a subject whose development was led to a large extent by technology in the search of a progressive miniaturization of electronic devices. The opportunity to fabricate devices with characteristic dimensions significantly below 1 μm has stimulated the investigation of a whole range of novel physical phenomena.

It is an area of condensed matter still very young with great experimental achievements. From a conceptual point of view mesoscopic physics provides direct verifications of the fundamental laws of quantum mechanics on scales inaccessible only a few years ago. This is a leading thread that unifies the many facets of this area whose boundaries are not yet well defined.

It was clear from the beginning that this special issue could not cover all the aspects involved and choices would have to be made in view of the possible mathematical developments. It was also necessary to make guesses about the directions in which progress may be expected in the near future. After consultation with several experts I decided to take as a leitmotiv of the issue *transport properties in heterostructures*. It is a hard core of mesoscopic physics which, beside its practical importance, involves in several ways an aspect of quantum mechanics of great conceptual and mathematical interest. This is quantum chaos, a theme which appears in many articles of this issue.

The issue contains 21 original contributions and a reprint of an article by R. Landauer of considerable historical interest not easily available today. Let me describe briefly the contents of the articles and their connections.

The first article by F. Capasso, J. Faist, and C. Sirtori provides an overview on heterostructures with interesting physical properties arising from quantum confinement, tunneling and quantum coherence on a mesoscopic scale. It gives an idea of the great possibilities of quantum design.

We then have a series of six articles focused on transport in mesoscopic conductors. M. Büttiker discusses conductance and quantum noise phenomena in a unified theoretical framework. C. Presilla and J. Sjöstrand include the effect of electron–electron interaction in time-dependent transport. L. S. Levitov, H. Lee, and G. B. Lesovik consider statistical prob-lems in connection to measurements of mesoscopic currents. Ballistic transport in coupled quantum waveguides is studied in a rigorous way to P. Exner, P. Sěba, M. Tater, and D. Vaněk while S-matrix, resonances, and wave functions are exactly calculated for simple models of billiards with leads by S. Albeverio, F. Haake, P. Kurasov, M. Kus, and P. Sěba. P. W. Brouwer and C. W. J. Beenakker develop a diagrammatic method for averaging over the circular ensemble of random matrix theory and apply it to chaotic billiards and other systems.

Random matrix theory is dominant in the next group of five articles. Originally proposed in the framework of nuclear physics, this topic has become a central tool in mesoscopic physics in connection with two different aspects: complex behavior due to the presence of impurities or due to chaoticity of the corresponding classical system. Both aspects are present in the article by V. I. Fal'ko and K. B. Efetov in the study of the statistics of wave functions in the more general framework of the supersymmetric nonlinear σ model. A. V. Andreev, B. D. Simons, and B. L. Altshuler are concerned with energy level statistics in disordered systems and how these statistics deviate from the universal ones. The mathematical structures underlying the connection between random matrix theory and the supersymmetric formalism is the subject of the article by M. R. Zirnbauer. P. N. Walker, M. J. Sanchez, and M. Wilkinson discuss singularities of the energy

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levels of a system depending on a set of parameters and described by a random matrix model. A. M. Khorunzhy, B. A. Khoruzhenko, and L. A. Pastur develop a rigorous method for studying the normalized trace of the resolvent of large random matrices.

An alternative approach for studying the spectral statistics in disordered conductors in a regime where random matrix theory is not applicable is proposed in the article by J. T. Chalker, I. V. Lerner, and R. A. Smith.

The article by K. Richter, D. Ullmo, and R. A. Jalabert studies the response to a magnetic field of an integrable billiard in presence of disorder.

Mesoscopic physics offers, in perspective, the possibility of studying chaotic phenomena at the many-particle level when the size of heterostructures and the number of particles are such that a thermodynamic limit represents a natural first approximation. In this limit a quantum system can be chaotic in its time evolution and not simply show signatures of classical chaos as is the case with confined finite systems. One then feels the need for a systematic development of a quantum ergodic theory. The next two articles by S. Graffi and A. Martinez and by M. Lenci take an explicit step in this direction and provide, for the first time, a rigorous analytic proof of ergodicity and mixing for the infinite quantum harmonic crystal and the Volkovisky–Sinai model of an ideal gas quantized according to Boltzmann statistics, respectively.

Arrays of heterostructures represent a new challenge for experimentalists and theorists and presumably will be an important direction for development for mesoscopic physics. The articles by G. Parisi and by V. A. Geyler, B. S. Pavlov, and I. Yu. Popov provide different examples of theoretical problems arising in such a context. Parisi considers the statistical properties of arrays of Josephson junctions while Geyler, Pavlov, and Popov study the spectral properties of lattices of billiards.

Schrödinger operators with singular continuous spectrum have attracted considerable attention on the part of mathematical physicists in recent years. Mesoscopic physics with its wide possibilities of quantum design presents situations which can be modeled by such operators. The next two articles must be read in this perspective. I. Guarneri studies the relationship between quantum dynamics and fractal properties of the spectrum. C. H. Kreft and R. Seiler analyze quantum mechanical models for transport phenomena in two dimensions with fractal spectra.

The last article by F. Benatti deals with quantum information theory. He compares the concept of accessible information of quantum communication channels with the entropy of a subalgebra with respect to a quantum state. Strictly speaking it is a subject which does not belong to the main theme of the issue. It is however a topic of wide interest which in my opinion should become relevant in some applications of mesoscopic physics.

The paper by R. Landauer reprinted in the issue is put in perspective by a comment of the author.

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I wish to express my gratitude to all the authors who responded with great enthusiasm to the project by contributing articles of very high quality. I must acknowledge conversations with B. Altshuler, F. Capasso, and L. Levitov and correspondence with H. Baranger and L. Pastur which were useful in planning the issue. My greatest debt is with C. Presilla who collaborated with me in all phases of the realization of the project. He has been a very wise counselor and a constant source of scientific insight. Last but not least I wish to thank the editor of the *Journal of Mathematical Physics*, Roger Newton, for proposing this project. I was reluctant to accept the role of guest editor for this issue, but he insisted and I am grateful to him for involving me in a very interesting enterprise.

Mesoscopic phenomena in semiconductor nanostructures by quantum design

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The energy levels, wave functions, optical matrix elements, and scattering rates of electrons can be tailored at will using semiconductor nanostructures as building blocks for practically any kind of potential. This allows the design and experimental realization of new artificial materials and devices, with interesting optical and transport properties arising from quantum confinement, tunneling, and quantum coherence on a mesoscopic scale ranging typically from 1 to 100 nm. This approach is illustrated with a number of recent examples based on experiments and calculations, such as resonant tunneling through double barriers, quantum interference phenomena in transport and optical absorption, bound states in the continuum, quantum well ''pseudomolecules'' with giant nonlinear optical susceptibilities, and quantum cascade lasers. © *1996 American Institute of Physics.* [S0022-2488(96)00210-1]

I. INTRODUCTION

Quantum engineering of the electronic energy levels, wave functions and band structure, matrix elements, and scattering rates using ultrathin semiconductor layers[1,2] grown by molecular beam epitaxy (MBE)[3] allows one to design and observe quantum phenomena on a mesoscopic scale (typically 1–100 nm), much larger than the atomic one.[4–7] This approach is the basis for modifying and tailoring in unprecedented ways the electronic, transport, and optical properties, which has led in many cases to altogether new materials (materials by design) and useful device applications.[2,5–8]

Essential to the emergence of this field of research has been MBE.[3] This epitaxial growth technique allows multilayer heterojunction structures to be grown with atomically abrupt interfaces and precisely controlled material composition over distances as short as a few nanometers. Such structures include quantum wells. These potential energy wells are formed by sandwiching a material such as gallium arsenide (of thickness comparable or smaller than the carrier thermal de Broglie wavelength, which is $\sim$25 nm for electrons in gallium arsenide at room temperature) between two wider energy bandgap semiconductors (for example, aluminum gallium arsenide). The energy spacings of the discrete states of the well arising from quantum confinement depend on the well thickness and depth.

If many quantum wells are grown on top of one another and the barriers are made so thin (typically$<$5 nm) that tunneling between the coupled wells becomes important, a superlattice is formed and the energy levels broaden into energy bands called minibands separated by minigaps.[1] Superlattices are artificial materials with novel optical and transport properties introduced by the artificial periodicity.[2,6,7]

In this paper we shall review our recent work on mesoscopic quantum phenomena based on tunneling and on electronic transitions between quantized states of the same band (intersubband transitions[8]) in semiconductor nanostructures.

Several of the structures considered in this paper should also appeal to mathematicians and mathematical-physicists since this approach allows one to design, synthesize, and experimentally investigate potentials of significant mathematical interest that cannot be found in nature. We shall limit ourselves to one-dimensional potentials, i.e., structures based on quantum wells. For struc-

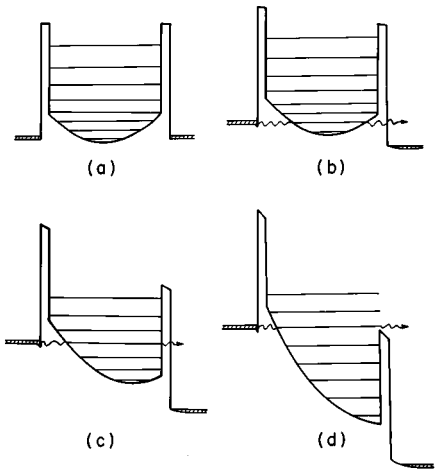

FIG. 1. Energy diagram of resonant tunneling structure under different conditions of applied electric field. (a) Zero field; (b),(c) the electric field is such that electrons resonantly tunnel through the parabolic portion of the well; (d) the applied field is high enough that electrons probe the continuum resonances. The wells are drawn to scale; however, for sake of clarity only half the number of levels in an energy interval are shown.

tures based on quantum wires and dots, i.e., relying on quantum confinement along two and three dimensions, respectively, the reader is referred to Ref. 4.

II. RESONANT TUNNELING AND QUANTUM INTERFERENCE IN ELECTRONIC TRANSPORT

The resonant tunneling double barrier consists of two potential barriers in series separated by a potential well.[9] This well can, of course, have various shapes (Fig. 1).

The kinetic energy of an electron's motion perpendicular to the layers is quantized, just as one would expect for a particle in a box. In the plane of the layers, however, the electron is free, and it behaves semiclassically. As a result, two-dimensional energy subbands $E_n(k)$ are formed:

$$E_n(k)=E_n+\frac{\hbar^2k^2}{2m^*}, \tag{1}$$

where E_n is the nth energy level given by the quantization of the perpendicular kinetic energy, and the second term is the kinetic energy of the electron's free motion parallel to the layers, with wave number k and effective mass m^*.

The energy levels E_n correspond to a half-integer number of electron de Broglie wavelengths across the width of the quantum well. The barriers are thin enough that electrons can tunnel through them into and out of the quantum well. This structure is often compared to a Fabry–Perot optical interferometer: the two barriers play the role of partially transparent mirrors through which light is coupled into and out of a resonant cavity.

As we might expect, the transmissivity for electrons through the double barrier shows resonant peaks when the perpendicular kinetic energy of the incident electrons equals E_n. At these resonant energies the transmissivity for a symmetric double barrier reaches 100%, even though the transmissivity for a single barrier might be less than 1%. This striking resonant enhancement of electron transmission is easily understood in terms of constructive interference between multiply reflected waves. But it cannot be understood within the semiclassical framework, which forbids tunneling through even a single barrier.

This description in terms of Fabry–Perot interferometry is somewhat idealized. In many realistic devices the resonant enhancement of the transmission is considerably weakened by scat-

tering processes because scattering events destroy the phase coherence of multiply reflected waves. One way to estimate the role of scattering is to compare the intrinsic energy width Γ_R of the resonance peak with the collisional broadening Γ_C of the resonance. Γ_R is determined by the degree of transmission through the individual barriers, that is, by the degree of external coupling to the cavity; it is approximately equal to $E_n T_B$, where T_B is the transmissivity of one barrier. Γ_C is determined by the scattering rate, that is, by the internal Q of the cavity. Γ_C is roughly $\hbar/\tau$, where τ is the average time between successive collisions and $\hbar$ is Planck's constant divided by 2π. If Γ_R is much larger than Γ_C, the Fabry–Perot description is appropriate. On the other hand, if Γ_C is much larger than Γ_R, the process can be viewed as sequential rather than coherent: the electrons tunnel into the well, scatter, and tunnel out the opposite side. Devices usually operate somewhere in between these extremes. The scattering reduces the peak transmissivity and broadens the resonance. The area under the transmissivity curve, however, stays constant.

A very important factor in the operation of resonant tunneling structures is the role of space-charge buildup within the well, which gives rise to an electrostatic potential that shifts the resonant energy of the well E_n relative to the energy of incident electrons in the emitter. This is analogous to the shift in the resonant frequency of a nonlinear Fabry–Perot interferometer due to light-intensity buildup, which is known to lead to optical bistability. This effect can give rise to interesting nonlinear oscillations or even chaotic behavior of the charge accumulating in the well.[10,11] Other interesting dynamical phenomena associated with charge accumulation in the well in resonant tunneling structures are discussed in the paper of Presilla and Siostrand of this issue.

In most experiments one measures the current through a resonant tunneling diode when a voltage is applied across the double barrier through the heavily doped contact layers. The applied bias voltage lowers the resonant energy of the cavity relative to the energy of the incident electrons. Once the resonant energy has fallen below the range of incident energies—below the conduction-band edge in the emitter—there is a sharp drop in the current as the applied voltage is increased further. This negative differential resistance is a useful feature for device applications such as high-frequency oscillators and multistate transistors.[5,6,12] Oscillators have operated up to frequencies in excess of 700 GHz.[12]

One can design and implement by MBE the electronic potential and the wave functions of a resonant tunneling structure in a nearly arbitrary way. This is illustrated by the energy diagram (Fig. 1) of a parabolic well between rectangular barriers under different conditions of applied electric fields.[13] This structure was grown by MBE. The 44 nm wide well is bound by 3.5 nm thick aluminum arsenide (AlAs) barriers and its chemical composition is varied from $Al_{0.30}Ga_{0.7}As$ (an alloy) at the edges and gallium arsenide (GaAs) at the center. The subscripts indicate the molar fractions of AlAs and GaAs in the alloy. This double barrier is sandwiched between two high conductivity semiconductor layers to allow application of a voltage. Figure 2 shows the measured current as a function of applied voltage for opposite polarities and the corresponding conductance (i.e., the derivative of the current with respect to voltage). The latter is plotted to enhance the features corresponding to resonant tunneling through the quantum states.

The overall features of the current voltage curve ($I-V$) can be interpreted physically by means of the energy diagrams of Fig. 1. At zero bias, [Fig. 1(a)], the first six energy levels of the well are confined by a parabolic well 225 meV deep, corresponding to the grading from $x=0$ to $x=0.30$, and their spacing is $\simeq$35 meV. When the voltage is increased from 0 to 0.3 V the first four energy levels probed by resonant tunneling [Fig. 1(b)] remain confined by the parabolic portion of the well, and their spacing is practically independent of the electric field, since it is primarily controlled by the curvature of the potential. This gives rise to the calculated and observed equal spacing of the first four resonances in the $I-V$ characteristic (Fig. 2). Consider now the higher-energy levels confined by the rectangular part of the well ($>$230 meV) at zero bias. When the voltage is raised above 0.3 V these levels become increasingly confined on the emitter side by the parabolic portion of the well and on the opposite side by a rectangular barrier, thus becoming progressively more separated, although retaining the nearly equal spacing [Fig. 1(c)].

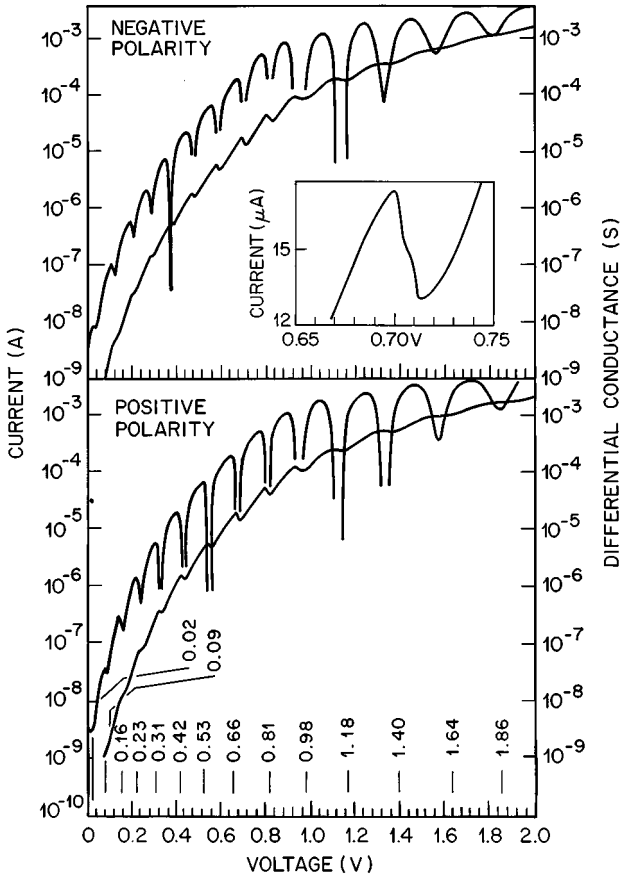

FIG. 2. Current versus applied voltage at 10 K temperature and corresponding differential conductance (dI/dV) for a double barrier structure (Fig. 1) under opposite voltage polarity conditions. The inset shows the eight resonance on a linear scale. The vertical segments near the horizontal axis indicate the calculated positions of the resonances.

This leads to the observed gradual increase in the voltage separation of the resonances as the bias is increased from 0.3 to 1.0 V. Above 1 V the electrons injected from the emitter probe the virtual levels in the quasicontinuum above the collector barrier [Fig. 1(d)]. These resonances result from electron interference effects associated with multiple quantum mechanical reflections at the well–barrier interface for energies above the barrier height. These reflections give rise to the features observed above 1 V in the current–voltage characteristic (Fig. 2), and must be clearly distinguished from the ones occurring at lower voltages, which are due to tunneling through two barriers. It should be noted that in the latter case the reflection from the second barrier is associated with an imaginary wave number in the barrier. In the case of the continuum resonances shown in Fig. 1(d) instead, the reflections from the second barrier are associated with a real wave number since the incident electron energy is greater than the barrier height.

III. QUANTUM INTERFERENCE IN OPTICAL ABSORPTION

Quantum interference effects in the absorption of atoms and molecules have been known since the classic work of Fano.[14] The development of MBE and quantum engineering of semiconductor heterostructures has made possible the observation of new optical absorption phenomena. In particular, in this section, we shall focus on intersubband absorption effects.[15] Intersubband transitions are those where the initial and final quantized states are in the same band, e.g. the

conduction band.[8] In an intersubband transition electrons in a lower state characterized by an eigenvalue (energy level) E_i with a dispersion of the type shown in Eq. (1) make a transition to a higher-energy final state (in the case of optical absorption) characterized by an eigenvalue E_f. Conservation of energy and momentum require $E_i+\hbar\omega=E_f$, where $\hbar\omega$ is the photon energy and $k_i=k_f$. The latter equality comes about because of the negligible momentum of the photon compared to that of the electron $\hbar k$. It should be noted that in such a transition the envelope function of the electron, determined by the one-dimensional heterostructure potential, changes while the rapidly oscillating Bloch function associated with the atomical level periodicity of the underlying crystal is approximately the same for the final and initial states. The latter approximation is correct under the assumptions that band nonparabolicities[15] associated with the effective mass being energy dependent are small, a condition verified in many absorption experiments.

The matrix element of the $i\rightarrow f$ transition is $\langle i|z|f\ )\rangle$, where z is the coordinate normal to the layers. In order to couple to this matrix element the incident radiation must be polarized or at least have a component of the polarization normal to the plane of the layers, i.e., along z. Electrons in the quantum well structures are introduced during crystal growth by the well-known process of doping, i.e., through impurities such as silicon atoms that release an electron. The infrared transmission spectrum can then be measured using standard techniques such as Fourier transform interferometry.

A. Suppression of optical absorption by electric-field-induced quantum interference

Recently the design and demonstration of coupled quantum well structures exhibiting a striking interference effect in the matrix element for intersubband absorption has been reported.[16] The potential and a specific optical transition (1–3) are designed [Fig. 3(a)] so that under application of an appropriate electric field the corresponding matrix element has a null [Fig. 3(b)].

The sample, grown by MBE, comprises 50 coupled quantum wells. Each period consists of two GaAs wells, respectively, 62 and 72 nm thick, separated by a 2 nm $Al_{0.33}Ga_{0.67}As$ barrier. The coupled well periods are separated by a 145 nm $Al_{0.33}Ga_{0.67}As$ spacer layer. To supply the electron charge in the wells an atomically thin layer of silicon dopant ($1\times10^{12}/cm^2$) is inserted in the spacer layers to ensure a symmetric charge transfer. Figure 3(a) shows the energy diagram of the coupled quantum well structure with no applied voltage. Indicated are the energy levels and the moduli squared of the wave functions. The energy levels and wave functions are computed by solving Schrödinger's and Poisson's equations in the envelope function formalism.[1,15]

To get a better insight into the behavior of the coupled well system as a function of the applied electric field, let us first consider the two quantum wells, denoted here as wells a and b, coupled by the barrier in a tight-binding approach.[1] In such a model, the calculated wave functions ψ_i ($i=1,...,4$) of this system are expanded in terms of the eigenfunctions $\phi_{1,2}^{a,b}$ of the first two bound states 1,2 of the two isolated wells. In the tight-binding approximation, the dipole matrix element $z_{1i}=\langle\psi_1|z|\psi_i\rangle$ ($i=3,4$) between the first and the third or fourth state of the coupled well system can now be written as the sum of the contribution from the two wells a and b,

$$z_{1i}=\langle\psi_1|\phi_1^a\rangle\langle\psi_i|\phi_2^a\rangle z_{12}^a+\langle\psi_1|\phi_1^b\rangle\langle\psi_i|\phi_2^b\rangle z_{12}^b, \tag{3}$$

where z_{12}^a and z_{12}^b are the transition matrix elements computed for the isolated wells. As ψ_1 is the ground state of the system, $\langle\psi_1|\phi_1^a\rangle$ and $\langle\psi_1|\phi_1^b\rangle$ have the same sign. On the contrary, since the second excited state ψ_3 crosses zero twice and is constructed from the antisymmetric wave functions $\phi_2^{a,b}$, $\langle\psi_3|\phi_2^a\rangle$ and $\langle\psi_3|\phi_2^b\rangle$ have opposite signs. Therefore, if we consider a transition between the first and third state of the coupled well system, the two terms of Eq. (3) have opposite signs. One thus expects large values of z_{13} for large absolute values of the electric field, where both wave functions are localized in either well a or b [the first or last term of Eq. (3) dominates] and a null for some intermediate value of the electric field. At this field the absorption will be suppressed. This behavior is clearly apparent in Fig. 3(b), where we display the calculated $|z_{13}|^2$. The absorp-

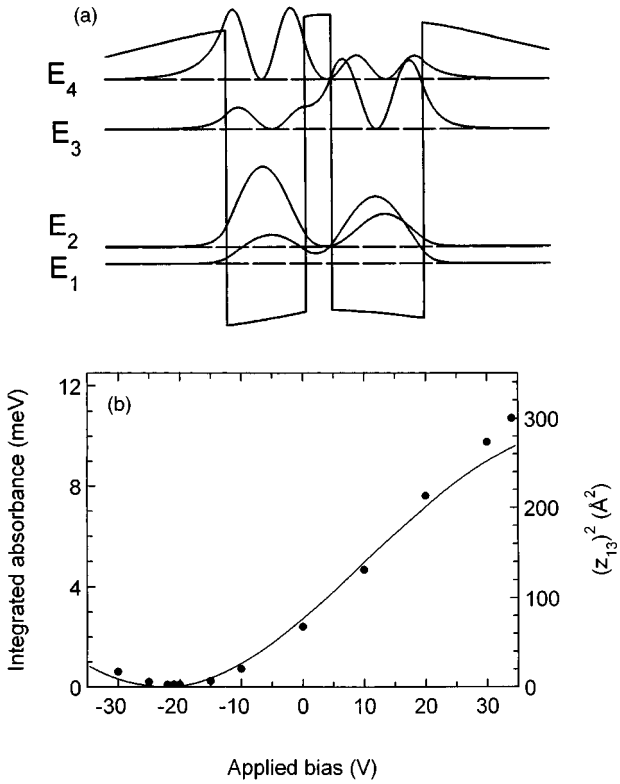

FIG. 3. (a) Energy diagram of an GaAs/$Al_{0.33}Ga_{0.67}As$ coupled-quantum-well structure used to investigate quantum interference in optical absorption. Shown are the positions of the calculated energy subbands and the corresponding modulus squared of the wave functions. We computed E_1=63 meV, E_2=80 meV, E_3=198 meV, and E_4=250 meV. (b) Square of the transition matrix element $(z_{13})^2$ (right axis), as derived experimentally from the integrated absorbance below the (1–3) absorption peak (left axis). The solid line is the calculated value.

tion spectra showed very clearly this effect as the applied electric field was varied.[16] The experimental $|z_{13}|^2$ is derived from a measurement of the area under the 1–3 absorption peak (in units of photon energy), and taking the nominal electron sheet density in the wells (5×10^{11} cm^{-2}). The experimental points in Fig. 3(b) are in good agreement with the calculation.

B. Fano quantum interference

When the excited state $|\phi\rangle$ of a quantum system is coupled to a continuum $|\psi\rangle$ at the same energy it broadens due to the finite lifetime τ introduced by the coupling to the continuum. The absorption spectrum from the ground state $|1\rangle$ to this excited state will be Lorentzian with a full width at half-maximum $\Gamma=\hbar/\tau$. However, a peculiar situation arises when the matrix element $\langle 1|z|\psi\rangle$ from the ground state to the continuum is nonvanishing: the absorption lineshape changes dramatically, becoming asymmetric, and displaying a zero within a few Γ from the absorption peak. This phenomenon, called Fano interference,[14] has been observed in many atomic, molecular, or solid-state systems.

Recently, we have reported the observation of Fano interference in a heterostructure, where all the relevant parameters, i.e., the escape rate Γ and the matrix element to the continuum $\langle 1|z|\psi\rangle$, are tailorable and controlled by design.[17]

The structures are grown by MBE and consist of ten periods. As shown in Fig. 4, each period consists of a GaAs coupled well confined by a high, 40 nm thick $Al_{0.33}Ga_{0.67}As$ barrier on the right

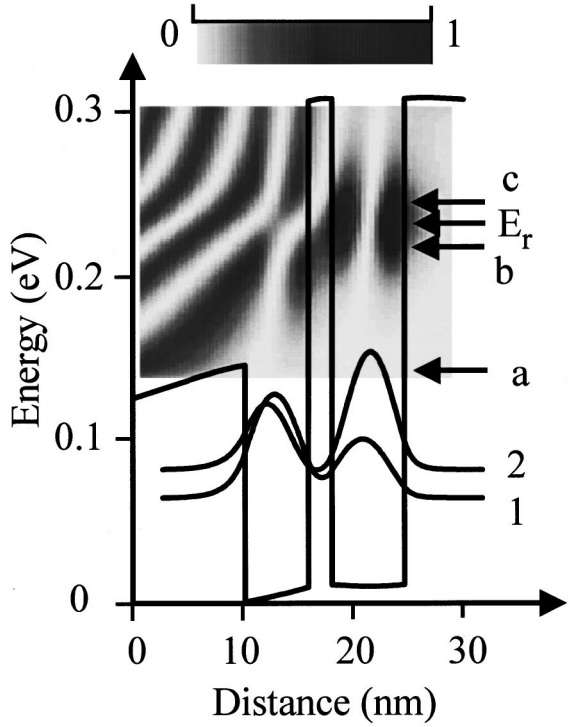

FIG. 4. Energy diagram of a portion of the structure used to study Fano quantum interference in absorption. The thicknesses and doping used in this self-consistent calculation correspond to sample A (see the text). The moduli squared of the wave functions of the $n=1$ and $n=2$ states are displayed. The modulo squared of the wave function in the continuum $|\Psi\rangle$ is represented as a gray-scale density plot. Points a, b, and c represent the final state energies corresponding to the onset of the continuum, the zero, and the maximum of the absorption spectrum (see Fig. 5). The shift between the maximum of the absorption and the position of the resonance E_r is a feature characteristic of Fano interference.

and a thick low $Al_{0.165}Ga_{0.835}As$ barrier on the left. The thickness $L=200$ nm of the $Al_{0.165}Ga_{0.835}As$ barrier is chosen such that it is much longer than the electron's coherence length $\lambda_c \sim 20-50$ nm, and therefore the states of this region behave as a continuum. Two structures with different quantum well thicknesses were grown. Sample A had the strongest coupling due to the relatively thin 2.0 nm $Al_{0.33}Ga_{0.67}As$ barrier coupling the 5.2 nm left well to the 6.4 nm right well. A doping sheet in the $Al_{0.165}Ga_{0.855}As$, separated from the quantum wells by a 25 nm spacer layer provides the 2.5×10^{11} cm^{-2} electron sheet density in the coupled well region. Sample B had a weaker coupling due to the thicker 2.5 nm barrier coupling the 5.5 nm left well to the 6.5 nm well. The electron sheet density was $n_s=5\times10^{10}$ cm^{-2} and the spacer layer 50 nm.

In these samples, the individual ground states of the two wells couple through the thin intermediate barrier to form a doublet with a splitting of about 20 meV. The same barrier also couples the excited state of the right well $|\phi\rangle$ with energy E_r to the energetically degenerate continuum that broadens the state $|\phi\rangle$ by $\Gamma\cong12$ meV for sample A and $\Gamma\cong6$ meV for sample B. In both cases, we have the condition $\Gamma \gg \Gamma_d$, where $\Gamma_d \sim 1-2$ meV is the broadening of $|\phi\rangle$ (homogenous and inhomogeneous) caused by interface roughness and optical phonon scattering. Since the ground state wave function spans both wells and therefore has a strong dipole coupling to both state $|\phi\rangle$ and the continuum state $|\psi\rangle$ above the left well, the structure fulfills the requirements for the observation of Fano interference.[14] In a tight-binding picture,[1] we are coupling a bound-to-bound transition in the right well to a bound-to-continuum in the left well. Note that one would not observe this interference in a sample having only the right well, since the matrix element $\langle 1|z|\psi\rangle \approx 0$ in this case. The features associated with Fano interference are also clearly

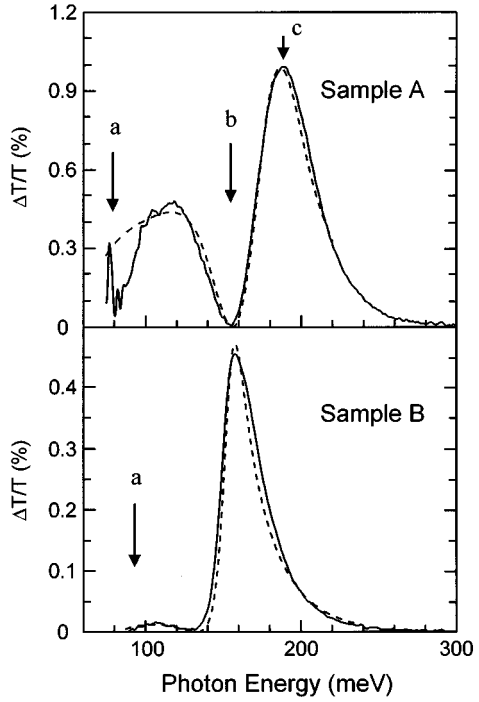

FIG. 5. Absorption spectra of structures exhibiting Fano quantum interference. (a) The solid curve is the measured absorption spectrum for sample A with strong coupling and asymmetry. Points a, b, and c refer to the onset of the continuum, the zero, and the maximum of the absorption (see Fig. 4). The dashed curve is the calculated spectrum. (b) The same for sample B. Note the shift between the absorption peak and the onset of the continuum, which is a feature specific to these samples exhibiting Fano interference.

apparent in the plot of the modulus squared of the eigenfunctions $|\psi\rangle$ of the whole system (consisting of the continuum plus the quantum wells) displayed as a gray scale plot in Fig. 4. As predicted for Fano interference, the calculated maximum and zero of the absorption (points c and b in Fig. 5) lie above and below E_r, respectively. This occurs because $\langle 1|z|\phi\rangle$ and $\langle 1|z|\psi\rangle$ interfere with *opposite phase* on the two sides of the resonance.[14] The expected energy-dependent phase shift experienced by the wave function $|\psi\rangle$ is evident in Fig. 5 as an abrupt shift of the position of the minimum of the modulus squared of the wave functions as the energy crosses the resonant energy. The absorption for both samples is reported in Fig. 5 along with the calculated spectra.[17] The Fano interference is contained in the calculated spectra automatically, since the absorption is computed using the wave function $|\psi\rangle$, which is an eigenfunction of the whole system, coupled well plus continuum. Thus the agreement between the measured and calculated spectra is the proof that these samples exhibit Fano interference. However, note that these experimental lines cannot be fitted in satisfactory fashion with the original Fano lineshape[14] because the same important assumptions used to derive that expression (invariance of both the matrix element and the coupling strength as a function of energy) do not hold in our case. Both spectra also show the qualitative features of the Fano lineshapes with a zero close to the asymmetric absorption peak. The shift ($\sim$100 meV) between the absorption peak and the onset of the continuum is another feature that is specific of these structures exhibiting Fano resonance. An absorption spectrum from a bound-to-continuum single quantum well would peak very close (20 meV) to the onset of the continuum. As expected, the main peak is broader for sample A (50 meV) than for sample B (30 meV) due to its stronger coupling to the continuum.

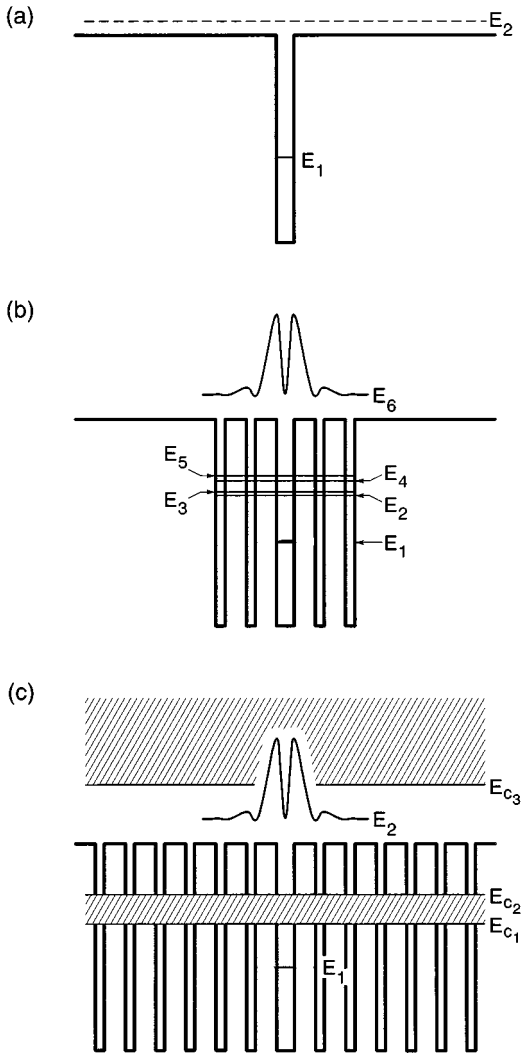

FIG. 6. Energy diagrams of potentials used to study highly localized states in the continuum. (a) Reference sample. Shown are the ground state of the well (E_1=204 meV) and the position (dashed line) of the first transmission resonance in the continuum (E_2=560 meV). (b) Quantum well cladded by two-period quarter-wave stacks. Shown is $|\Psi|^2$ of the localized quasibound state (E_6=560 meV) formed in correspondence to the transmission resonance and the positions of new states created at lower energies (E_2=320 meV, E_3=322 meV, E_4=356 meV, E_5=359 meV). (c) In the superlattice limit the $\lambda/4$ stacks behave as Bragg reflectors. The state above the well now becomes a bound state localized by the superlattice minigap (=266 meV). The low-energy miniband extends from 307 to 379 meV.

IV. CONTINUUM RESONANCES: ELECTRON WAVE INTERFERENCE AND BOUND STATES ABOVE A POTENTIAL WELL

In the previous section we have seen how confined states of quantum wells are central in a number of tunneling and optical phenomena. Highly localized states and even bound states can also be created at energies above the barrier height in a potential well using constructive interference phenomena.[18,19]

Consider first a conventional rectangular well [Fig. 6(a)]. At energies greater than the barrier height one has a continuum of scattering states. For discrete energies corresponding to a semi-integer number of electron wavelengths across the well, one finds transmission resonances. Al-

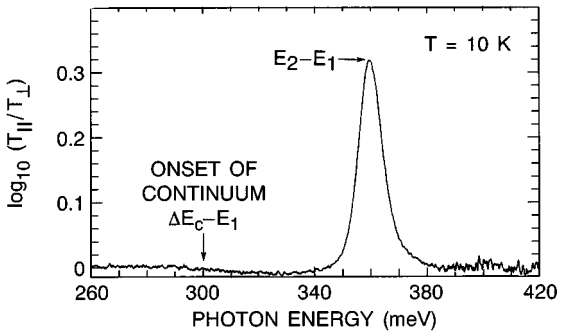

FIG. 7. Absorption spectra at cryogenic temperature for the structure with superlattice Bragg reflectors of Fig. 6(c) (bottom). The transition to the confined state above the well [E_2 in Fig. 6(c)] corresponds to the peak at 360 meV, in excellent agreement with the calculated value for E_2-E_1.

though at these energies the electron amplitude in the well layer is enhanced, the wave functions do not decay exponentially in the barrier, unlike the confined states of the well, but are plane-wave-like. These states can be localized in the well using as barriers stacks of layers of thickness $\lambda/4$ each, where λ is the de Broglie wavelength in the layer (at an energy comparable to that of the selected transmission resonance) [Figs. 6(b)–6(c)]. The net effect is that the reflection coefficient of electrons acquires a high value (near unity) for a significant range of energies (typically 0.1–0.2 eV) above the barrier height. This high value of the reflectivity is the result of interference between the waves partially reflected by the heterointerfaces of the $\lambda/4$ stacks, which leads to the formation of a quasibound state above the center well [Fig. 6(b)]. This strongly narrows the transmission resonance in analogy with a Fabry–Perot optical filter, where sharp optical resonances are produced using as high reflectivity mirrors dielectric quarter-wave stacks. The degree of localization increases with the number of periods; in the structure with just two-period stacks, the wave function is already highly confined [Fig. 6(b)]. In the superlattice limit and at low temperatures, to minimize scattering, the stacks behave as Bragg reflectors; a minigap opens up [Fig. 6(c)] and the localized state becomes a bound state at energies greater than the barrier height. The prediction that certain oscillatory potentials support bound states in the continuum, due to quantum interference, was first put forth by von Neumann and Wigner in 1929.[20]

The reference sample [Fig. 6(a)] had 20 3.2 nm InGaAs doped quantum wells separated by 15 nm undoped AlInAs barriers. In the other three structures the 3.2 nm wells, doped to the same level were cladded, respectively, by one-period, two-period [Fig. 6(b)], and six-period [Fig. 6(c)] $\lambda/4$ stacks consisting of 3.9 nm AlInAs barriers and 1.6 nm GaInAs wells, designed as discussed above. The phase coherence length in the superlattice structure of Fig. 6(c) is estimated to be $\sim$30 nm at 10 K.

The room temperature absorption spectra of the reference sample is broad with a long-wavelength cutoff determined by the height of the barrier.[18] In the structure with one $\lambda/4$ period the peak is considerably narrower and centered at an energy corresponding to the transition between the ground state of the well and the localized resonant state at the energy E_6.[18] As the number of quarter-wave stacks is doubled the absorption peak does not shift and considerably narrows, precisely the behavior expected for an interference filter. In fact, the observed narrowing (16 meV) can be quantitatively explained in terms of the reflectivity increase of the $\lambda/4$ stacks.[18] In the structure with six periods at cryogenic temperatures, the highly localized state becomes effectively a bound state confined by Bragg reflectors from the superlattice.[19] The absorption spectrum (Fig. 7) shows an isolated peak at 360 meV of width $\sim$10 meV corresponding to the transition from the state E_1 to the state E_2 in Fig. 6(c).[19] It is worth noting that the width of the transition to the confined state above the well in the two- and six-period structures is identical to that of the bound-to-bound state transition measured in a conventional 5.5 nm thick GaInAs well

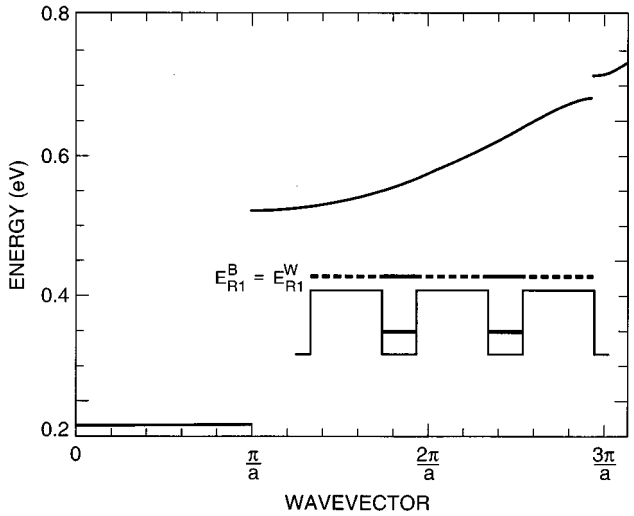

FIG. 8. Energy dispersion along the superlattice axis for a structure (inset) where the first barrier resonance E^B_{R1} is degenerate with second well resonance E^W_{R1}. The resulting mixing of these states produces a very broad miniband from π/a to $\pi/3a$ and suppression of the energy gap at $\pi/2a$. The barriers (AlInAs) and the wells (GaInAs) are, respectively, 8.8 and 3 nm thick.

with 30 nm thick barriers, thus demonstrating the highly localized nature of the state above the well.

Other intriguing phenomena arise when, for example, the first continuum resonances of quantum wells are at the same energy of the first barrier resonance.[21] This can be achieved by suitable adjustment of the layer thicknesses in a superlattice. In this case a very broad miniband is formed that extends in k space from π/a to $3\pi/a$ (where a is the superlattice period), with a minigap suppression at $2\pi/a$ (see Fig. 8). This effect has been confirmed experimentally.[21]

V. COUPLED QUANTUM WELL PSEUDOMOLECULES WITH GIANT NONLINEAR OPTICAL SUSCEPTIBILITIES

Consider an electromagnetic field at frequency ω, propagating through a material. Optical phenomena such as dispersion, absorption, and stimulated emission are described in Maxwell's equations by a linear polarization $P(\omega)=\epsilon_0\chi(\omega)E(\omega)$ proportional to the electric field of the wave $E(\omega)$ via a coefficient $\chi(\omega)$ called susceptibility, where ϵ_0 is the vacuum permittivity. More generally, the polarization contains higher-order but smaller terms at frequencies such as 2ω and 3ω. These nonlinear terms are proportional to powers of the field via nonlinear susceptibilities such as $\chi^{(2)}$ (2ω) and $\chi^{(3)}(3\omega)$, and are responsible for phenomena such as second harmonic generation (SHG) at 2ω and third harmonic generation THG 3ω. The polarizations for these two phenomena can be written as $P(2\omega)=\epsilon_0\chi^{(2)}_{(2\omega)}E^2(\omega)$ and $P(3\omega)=\epsilon_0\chi^{(3)}_{(3\omega)}E^3(\omega)$. More generally, when two beams at frequencies ω_1 and ω_2 are present, nonlinear phenomena such as sum or difference frequency generation at $\omega_1\pm\omega_2$ are possible.

The structures discussed in this section can be viewed as ''pseudomolecules'' with giant dipole matrix elements and nearly equally spaced energy levels (Fig. 9). These characteristics lead to a large enhancement of their nonlinear optical susceptibilities.[22] Physically these susceptibilities in our structures arise from the interaction of light with the quantized anharmonic oscillations of electrons in the potentials of Fig. 10. The latter are grown in the AlInAs/GaInAs system lattice matched to InP, and only the thickest well is doped n-type to provide electrons. The choice of this material system facilitates the tunnel coupling between the layers due to the low effective mass $(0.07\ m_0)$ of the barrier region and provides a large potential barrier (0.5 eV) essential for con-

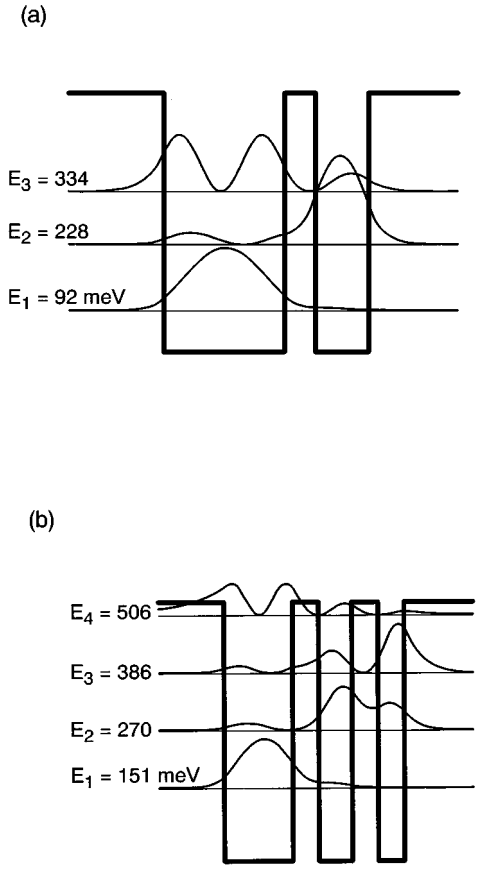

FIG. 9. Energy diagrams of the AlInAs/GaInAs coupled-quantum-well nonlinear optical structures. Shown are the positions of the calculated energy levels and the corresponding moduli squared of the wave functions. (a) The structure used for resonant second harmonic generation. The GaInAs wells have thicknesses of 6.4 and 2.8 nm and are separated by a 1.6 nm AlInAs barrier. (b) The structure used for triply resonant third harmonic generation. The GaInAs wells have thicknesses of 4.2, 2.0, and 1.8 nm, respectively, and are separated by 1.6 nm AlInAs barriers.

fining four states in the three-well structure separated by an energy corresponding to that of the photon from a carbon dioxide (CO_2) laser ($\approx$120 meV). To optically excite the quantized motion normal to the layer interfaces, one must use light with a component of the polarization normal to the layers. In our experiments this was done using linearly polarized light in a multipass waveguide structure wedged at 45°. In our SHG experiment a coherent polarization is created at double the frequency ω of the pump wave (a CO_2 laser beam) due to the lack of reflection symmetry of our two-well structure [Fig. 9(a)]. This coherent polarization radiates a wave of frequency 2ω colinear with the pump. The vicinity of the pump photon energy to E_2-E_1 and of 2ω to E_3-E_1 produces a strong resonant enhancement of the nonlinear susceptibility $\chi^{(2)}_{2\omega}$ associated with SHG.[22] The maximum susceptibility ($\chi^{(2)}_{2\omega}$) corresponds to exact matching, i.e. $\hbar\omega=E_2-E_1=E_3-E_2$. This can be achieved using the large linear Stark effect typical of this structure by applying an electric field of suitable polarity normal to the layers. In these conditions a $|\chi^{(2)}_{2\omega}|=10^{-7}$ m/V was measured, approximately 300 times the value of $|\chi^{(2)}_{2\omega}|$ in bulk GaAs at $\lambda=10$ μm.[22]

The three-well structure [Fig. 9(b)] with the near equal separation of its four energy levels is suitable for triply resonant THG. In this process a pump wave at frequency ω sets up a nonlinear polarization at 3ω that coherently radiates a wave at this frequency.[22] The nonlinear susceptibility $\chi^{(3)}_{3\omega}$ that enters the expression for the polarization is strongly enhanced when the condition

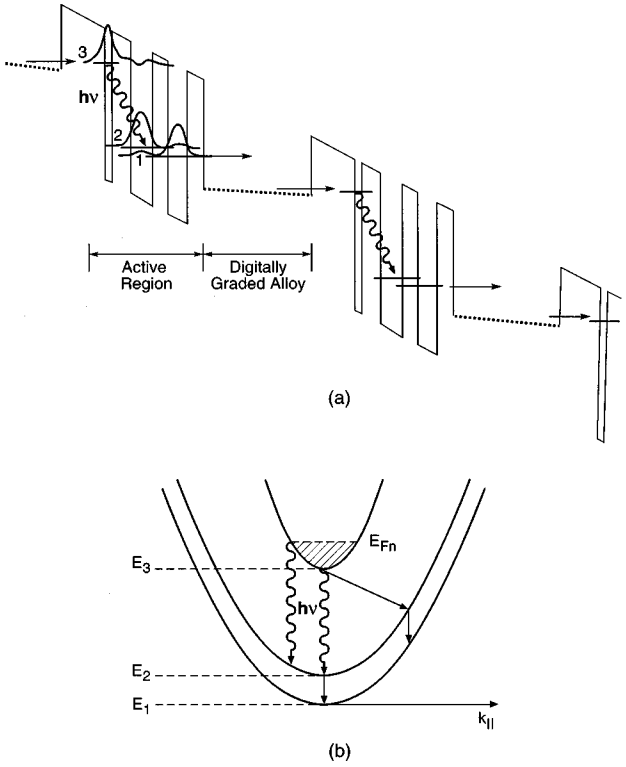

FIG. 10. (a) Energy diagram of a quantum cascade laser showing also the moduli squared of the wave functions. (b) Schematic representation of the dispersion of the $n=1$, 2, and 3 states parallel to the layers; $k_{\|}$ is the corresponding wave number. The wavy lines represent the laser transition.

$\hbar\omega \simeq E_2-E_1 \simeq E_3-E_2 \simeq E_4-E_3$ is met. It is important to note that a parabolic well (i.e., a harmonic oscillator potential) is unsuitable for this purpose, since in such a system the electron oscillations are linear (in quantum mechanical terms the transition matrix elements between nonadjacent states are zero, a property of Hermite polynomials). THG experiments in the structure of Fig. 10(b) have found a $|\chi^{(3)}_{3\omega}|=10^{-14}$ (m/V)^2 at 300 K.[22] At cryogenic temperatures $|\chi^{(3)}_{3\omega}|$ is four times larger. These are the highest third-order susceptibility of any known material system. The three-coupled well structure was also used to study multiphoton electron escape from a well under an applied electric field, the analog of multiphoton ionization of an atom.[23] In this process electrons are photoexcited into the continuum via a CO_2 laser using a three photon transition, giving rise to a photocurrent. The cross section for this process is found to be many orders of magnitude larger than in atoms and molecules.

Consider now the nonlinear optical phenomenon of difference frequency mixing in which two incident waves at frequencies ω_1 and ω_2 interact in a suitable asymmetric medium to set up a polarization at the difference frequency $\omega_1-\omega_2$.[24] This polarization is responsible for the generation of radiation at $\omega=\omega_1-\omega_2$. Quantum nanostructures can be designed to exhibit a very large $\chi^{(2)}(\omega=\omega_1-\omega_2)$ when the incident photons and their energy difference are resonant with optical transitions of the structure. The asymmetric structure of Fig. 3(a) was in fact used for infrared ($\lambda\simeq 60$ μm) difference frequency generation near the energy difference between states $n=2$ and $n=1$, i.e., $\omega_3 \simeq (E_2-E_1)/\hbar$.[24] The photons at ω_1 and ω_2 are chosen to be near resonance with the (1–3) and (3–2) transitions, respectively. As the photon energy difference $\hbar(\omega_1-\omega_2)$ of the two incident CO_2 lasers was tuned near E_2-E_1, the measured far infrared radiation (at $\lambda\sim 60$ μm) exhibited the typical resonant behavior of this process.[24]

VI. QUANTUM CASCADE LASERS

The quantum cascade (QC) laser is an excellent example of how quantum engineering can be used to design new laser materials and related light sources. It is based on intersubband transitions between excited states of coupled quantum wells and on resonant tunneling as the pumping mechanism (Fig. 10). The population inversion between the states of the laser transition is designed by tailoring the electron intersubband scattering times. This tailoring of scattering adds an important dimension to quantum engineering of mesoscopic structures. In QC lasers, unlike all other laser sources, the wavelength is determined by quantum confinement, i.e., by the layer thicknesses of the active region rather than by the chemical properties of the material. As such, it can be tailored over a very wide range using the same heterostructure material. Since the initial report of QC lasers in 1994 (Ref. 25), we have demonstrated emission wavelengths in the 4–8.5 μm range using AlInAs/GaInAs heterostructures lattice matched to InP.[26–29] Figure 10(a) illustrates the conduction band energy diagram of a portion of the 25-period (active region plus injector) section of the quantum cascade laser under an applied electric field normal to the layers $\sim 10^5$ V/cm corresponding to lasing conditions. The dashed lines are the effective conduction band edges of the digitally graded electron-injecting regions, where electrons relax their energy before being injected in the next region. These injectors are short period superlattices (Fig. 11). The population inversion between the states of the laser transition ($n=3$ and $n=2$ in Fig. 10) is obtained by ensuring, by suitable design, that the scattering time from the upper state ($n=3$) to the lower one ($n=2$) is larger than the lifetime of the latter. At the same time one must reduce as much as possible the tunneling escape rate from the $n=3$ state to the continuum, since this process in steady state tends to reduce the population of the upper level. Finally, tunneling out of the lowest state ($n=1$) should be fast enough to avoid a buildup of electrons in that subband. As described below, these requirements are met by a suitable choice of layer thicknesses, number of quantum wells, and electric field in the active region. More specifically, the latter is designed to have a laser transition that is ''diagonal in real space'' (Fig. 10) and an energy separation between the $n=2$ and $n=1$ states resonant with the optical phonon. Electrons are injected through a 4.5 nm AlInAs barrier into the $n=3$ energy level of the active region. The latter includes 0.8 and 3.5 nm thick GaInAs wells separated by a 3.5 nm AlInAs barrier. Note the reduced spatial overlap between the $n=3$ and $n=2$ states (''diagonal'' or photon-assisted tunneling transition) and the strong coupling to an adjacent 2.8 nm GaInAs well through a 3.0 nm AlInAs barrier. Electrons escape from this well through a 3.0 nm AlInAs barrier. The calculated energy differences are $E_3-E_2=295$ meV and $E_2-E_1=30$ meV. The wavy arrow indicates the laser transition. Figure 10(b) shows a schematic representation of the dispersion of the $n=1,2$, and 3 states parallel to the layers; $k_{\|}$ is the corresponding wave number. The bottom of these subbands correspond to energy levels $n=1$, 2, and 3 indicated in (a). The wavy arrows indicate that all radiative transitions originating from the electron population (shown as shaded) in the $n=3$ state have essentially the same wavelength. The quasi-Fermi energy E_{Fn} corresponding to the population inversion at threshold ($n_s=1.7\times10^{11}$ cm^{-2}) is $\sim$8 meV, measured from the bottom of the $n=3$ subband. The straight arrows represent the intersubband scattering processes by optical phonons.

The tunneling rate through the trapezoidal injection barrier is extremely fast ($\sim$0.2 ps)$^{-1}$, ensuring the efficient filling of level 3. The coupled-well region is essentially a four-level laser system, where a population inversion is achieved between the two excited states $n=3$ and $n=2$. The intersubband optical-phonon-limited relaxation time,[25] τ_{32}, between these states is estimated to be $\sim$4.3 ps at $\sim 10^5$ V/cm; this process is between states of reduced spatial overlap and accompanied by a large momentum transfer [Fig. 10(b)] associated with the large intersubband separation; as such, τ_{32} is relatively long. This ensures population inversion between the two states because the lower of the two empties with a relaxation time estimated around 0.6 ps. Strong inelastic relaxation by means of optical phonons with nearly zero momentum transfer occurs between the strongly overlapped and closely spaced $n=2$ and $n=1$ subbands [Fig. 11(b)]. Finally,

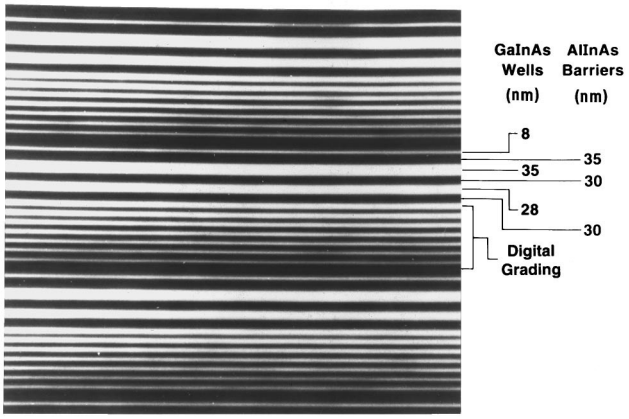

FIG. 11. Transmission electron micrograph of a portion of the cleaved cross section of the quantum cascade laser of Fig. 10. Three periods of the 25 stage structure are shown. The superlattice period of the digitally graded regions is 3 nm and the duty cycle of the AlInAs barrier layers varies from 40% to 77% top-to-bottom, creating a compositionally graded pseudoquarternary alloy in these regions. This is used for injecting electrons from top-to-bottom into the 0.8 nm GaInAs well. The wells and barriers of the digitally graded regions are doped n-type to 1.5×10^{17} cm^{-3} to avoid space-charge buildup under injection, while the other layers are undoped.

the tunneling escape time out of the $n=1$ state is extremely short ($\lesssim$0.5 ps), further facilitating population inversion. The ''diagonal'' nature of the laser transition increases the escape time into the continuum from the $n=3$ level ($\tau_{\text{escp}}\simeq$6 ps), thus enhancing the injection efficiency. Figure 11 is a transmission electron microscope photograph of a cleaved section of the QC laser, showing three periods of the active region.

The 25-period active region is sandwiched between thick AlInAs cladding layers to provide an optical waveguide parallel to the layers. The optical cavity is obtained by cleaving 0.5–3 mm long bars normal to the layers. The crystalline cleavage planes serve as mirrors. With the design of Fig. 10 laser action was obtained in pulsed mode at $\lambda=4.3$ μm with several tens of mW of peak powers and up to $\sim$100 K operating temperatures, but with relatively high thresholds. In this design, the width of the luminescence transition is relatively broad [full width at half-maximum (FWHM)=22 meV] since a diagonal transition is more sensitive to interface roughness associated with thickness fluctuations ($\sim$ one atomic layer) in the plane of the layers. As a consequence, the peak gain is reduced. To circumvent this problem we designed the structure of Fig. 12, where electrons make a vertical radiative transition essentially in the same well.[26] This reduces considerably the width of the gain spectrum (FWHM$\approx$10 meV), and therefore the laser threshold current density. To prevent electron escape in the continuum, which is greatly reduced in the case of the diagonal transition, the superlattice of the digitally graded injector is now designed as an effective Bragg reflector for electrons in the higher excited state and to simultaneously ensure swift electron escape from the lower states via a miniband facing of the latter (Fig. 12).[26] The active region consists of 4.5 mm InGaAs quantum well coupled to a 3.6 nm well by a 2.8 nm AlInAs barrier. Tunneling injection from the superlattice into the active region is through a 6.5 nm AlInAs barrier and electrons escape out of the $n=1$ state through a 3.0 nm AlInAs barrier. As in the other structure, the lower state of the laser transition is separated by an optical phonon ($\approx$30 meV) from the $n=1$ state. The calculated relaxation time is $\tau_{21}\simeq$0.6 ps, which is considerably less than that between the $n=3$ and $n=2$ state (1.8 ps), thus creating population inversion condition between these energy levels. Electrons can, in turn, tunnel out of the $n=1$ state in a subpicosecond time to prevent electron buildup.

Dramatic performance improvements have been obtained with vertical transition QC lasers.[26] The threshold current density is considerably reduced ($\sim$ a factor of 2) leading to higher operating

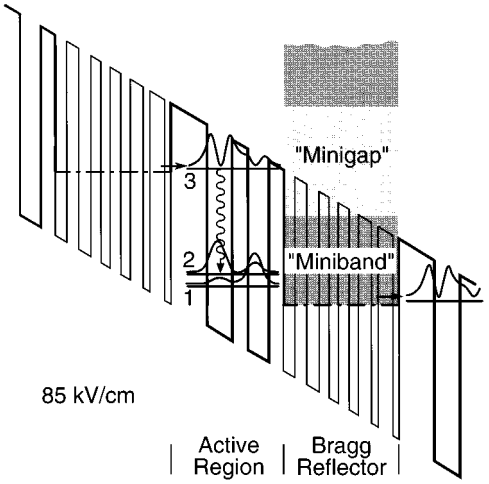

FIG. 12. The schematic energy diagram of a portion of the $Ga_{0.47}In_{0.53}As/Al_{0.48}In_{0.52}As$ quantum cascade laser with vertical transition under positive bias condition and an electric field of 8.5×10^4 V/cm. The dashed lines are the effective conduction band edges of the 20.8 nm thick superlattice electron injector. As shown, this superlattice is also designed as to create a minigap that blocks electron escape from level 3. The wavy line indicates the transition responsible for laser action. The moduli squared of the relevant wave functions are shown.

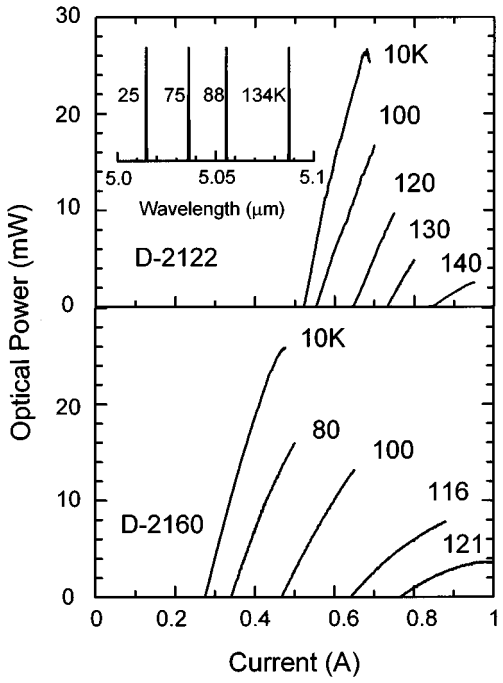

FIG. 13. Continuous optical output power from a single facet versus injection current for various temperatures of a quantum cascade laser (Ref. 30). (a) Sample D-2122, with a device 2.9 mm long and 7 μm wide. (b) Sample D-2160, with a device 3 mm long and 9 μm wide. Single mode high resolution spectra are shown in the inset at various temperatures. The lasers operated in pulsed mode up to room temperature and above (320 K).

temperatures. In addition, the peak optical power is also greatly enhanced and the lasers can operate in continuous wave.[27,28]

More recently, the design of vertical transition QC lasers has been further improved by adding a thin quantum well between the graded injector layer and the double-well active region.[29] This increases the tunneling injection efficiency. The above features, together with the substitution of the AlInAs cladding layers with InP regions of much higher thermal conductivity, has led to the room-temperature high peak power ($\sim$200 mW) pulsed operation of QC lasers at $\lambda=5.2$ μm.[30] Continuous wave single mode operation has also been achieved up to 140 K (Fig. 13). These are the first semiconductor lasers operating at room temperature in the mid-infrared. Their overall performance makes them excellent candidates for many applications such as environmental sensing and pollution monitoring in the 3–5 μm and 8–13 μm atmospheric windows.

VII. CONCLUSIONS

This review has highlighted the range of interesting transport and optical mesoscopic phenomena made possible by wave function engineering in semiconductor nanostructures grown by MBE. By controlling the phase of the electronic envelope function states and of their transition matrix elements, a number of interesting quantum interference effects have been observed in double-barrier transport and optical absorption. This quantum engineering approach has also led to the design and demonstration of new materials with giant nonlinear optical coefficients. Finally, not only the electronic states but also the scattering rates can be tailored. This adds a new dimension to quantum design and has allowed us to demonstrate new light sources (quantum cascade lasers), where the population inversion is designed rather than determined by relaxation times intrinsic to the laser material.

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Dynamic conductance and quantum noise in mesoscopic conductors

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We present results for the dc conductance, the ac conductance, and the current–current fluctuation spectra of mesoscopic, phase-coherent conductors based on a second quantization approach to scattering and a self-consistent potential approach. A second quantization approach permits an investigation of statistical effects due to the symmetry of the wave functions under exchange of particles. A self-consistent approach is needed to enforce overall charge conservation and to obtain current conserving expressions for frequency-dependent conductances and fluctuation spectra. For the particular example of a mesoscopic capacitor we present microscopic expressions for the electrochemical capacitance and the charge relaxation resistance. © *1996 American Institute of Physics.* [S0022-2488(96)00810-9]

I. INTRODUCTION

Electrical transport in conductors which are so small that carrier transport from one contact of the sample to an other contact of the sample is phase coherent is a subject of considerable interest. Much of what has been learned about samples so small that the wave nature of electrons matters has been achieved through the theoretical and experimental investigation of dc conductances.[1–3] Electrical transport can, however, not only be characterized by its steady state average behavior but also by dynamical fluctuations away from its average behavior. Therefore, it is desirable to characterize also the fluctuation, the noise, of such conductors. Moreover, the conductor can, by application of time-dependent perturbations be brought into a dynamical state and, therefore, it is useful to characterize the conductor through its ac-conductances. The growing interest in these subjects is illustrated by a series of recent clever experiments on ac conductances[4–7] and quantum shot noise.[8–11] Both noise measurements and dynamic conductance measurements can reveal properties of a conductor which cannot be tested by a dc experiment.

The purpose of this work is to show that there exists a common theoretical framework to address dc conductances, quantum noise and the ac conductance of mesoscopic conductors. We present first a scattering theory of dc-conductance[12–17] and the low frequency noise[18–24] carried out in a second quantization framework.[19,20,22,23] The derivation of the dc-conductances uses in an essential manner the coherent transmission from one electron reservoir to another and represents a rederivation of results by Büttiker[15,16] and Imry[14] and Landauer.[17] For the discussion of the noise our interest is focused on the statistical effects which arise due to the fact that an electrical conductor is made up of indistinguishable carriers. The quantum statistical effects of such a system are a property of the wave functions under exchange of two of its particles. Basically under such an exchange the wave functions must either remain invariant (Bose statistics) or the wave function changes sign (Fermi statistics). For multiprobe conductors[22,23] this gives a generalized Johnson–Nyquist formula relating the equilibrium fluctuations to transmission probabilities of the conductor. We discuss the current–current fluctuations in the presence of transport. We relate the low-frequency current fluctuations and correlations to products of four scattering matrices.[22,23] The discussions by Khlus,[18] Lesovik,[19] and Yurke and Kochanski[20] and Martin and Landauer[24] are essentially single channel discussions or assume that the scattering matrix is diagonal. The second quantization approach of Refs. 22 and 23 permits to carry out such a discussion *at every stage* in an arbitrary basis, for an arbitrary scattering matrix. To highlight the role of statistics we compare

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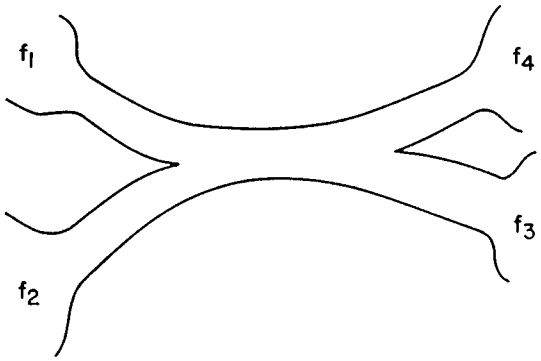

FIG. 1. Conductor connected to four contacts with equilibrium Fermi distributions f_α, $\alpha=1,2,3,4$. After Ref. 23.

a system subject to Fermi statistics with a system subject to Bose statistics. We extend this approach to ac transport for the case that a sample is brought into a dynamical state by application of frequency-dependent voltages to the contacts of the sample.[25,26] For this discussion the displacement of charge in response to the perturbations is central: to conserve charge the charge deviation from the equilibrium state must be of dipolar or higher order multipolar form. To achieve such a charge distribution an independent electron approach[27,28] is insufficient. As a consequence results for the ac conductance must include the effects of the long range Coulomb interaction. The leading coefficient proportional to frequency which describes the displacement currents measured at the contacts of the sample is called the emittance.[26] The emittance describes a capacitive current response if carrier transmission plays no role but describes an inductivelike, kinetic current response if transmission of carriers is important. An extension of this theory to frequency-dependent noise spectra is discussed for the case of a mesoscopic capacitor.

This work is not a review of these topics but is focused on demonstrating the unity of this approach as it is applied to these diverse but interrelated subjects. We only motivate and discuss the results and refer the reader to the original literature for detailed derivations. The conceptual points we make can be made for normal conductors: the dc conductance[29] and the zero-frequency noise[30,31] of hybrid normal and superconducting structures can be formulated in close analogy. We also emphasize only coherent transport. In the frame work presented here incoherence can be introduced by the addition of ''fictitious'' voltage probes.[32] We emphasize expressions in terms of the local density of states and the local, continuous potential. Much insight can be gained by using piecewise constant potentials[33–35,41] instead of the continuous potential distribution.

II. SECOND QUANTIZATION FORMULATION OF THE SCATTERING APPROACH

We present a brief outline of the second quantization approach to scattering theory. First, it is necessary to discuss the formulation of electron transport in the form of a scattering problem.[12,14–16]

A. Quantum channels

We envision a mesoscopic conductor (see Fig. 1) connected to an arbitrary number of contacts[15,16] labeled $\alpha=1,2,\ldots$. Each contact, far away from the connection to the conductor will be viewed as a perfect, translationally invariant conductor. For contact α, let x_α be the coordinate along the conductor and y_α and z_α the orthogonal transverse coordinates. The single-electron Hamiltonian for a carrier with effective mass m in such a lead is given by

$$H=-\frac{\hbar^2}{2m}\Delta_\alpha+eU(y_\alpha,z_\alpha), \tag{1}$$

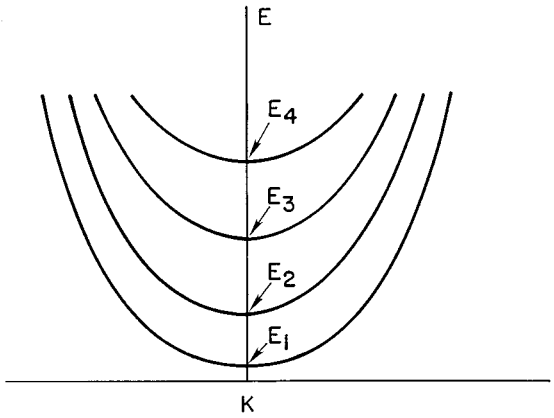

FIG. 2. Energy dispersions $E_n(k)$ of quantum channels of a perfect wire. $E_n(0)$ is the energy of the nth transverse state.

with a potential $eU(y_\alpha,z_\alpha)$ that might be an arbitrary function of the transverse coordinates but is independent of x_α. This Hamiltonian is separable. The transverse motion is described by a ladder of states with eigenfunctions[36,37] $\phi_{\alpha n}(y_\alpha,z_\alpha)$ and energies $E_{\alpha n}(0)$, labeled by the index $n=1,2,3,\ldots$. The eigenfunctions of the Hamiltonian H are of the form $\chi_{\alpha n}(k_{\alpha n},x_\alpha,y_\alpha,z_\alpha)=\exp(ik_{\alpha n}x_\alpha)\phi_{\alpha n}(y_\alpha,z_\alpha)$ with an energy

$$E_{\alpha n}(k_{\alpha n})=E_{\alpha n}(0)+\hbar^2k_{\alpha n}^2/2m \tag{2}$$

shown in Fig. 2. For a given energy E there are two solutions $k_{\pm,\alpha n}(E)$ of the equation $E=E_{\alpha n}(k_{\alpha n})$. If the energy E exceeds the channel threshold $E_{\alpha n}(0)$ the two solutions are real and describe an in-going state with velocity $v_{\alpha n}(E)$ and an out-coming state with velocity $-v_{\alpha n}(E)$. We call these two states a quantum channel. In general for a given energy E we will have N transverse states with energy $E_{\alpha n}$ below E. In this case we have $2N$ real wave vectors which characterize in and out-going states. Below such a contact is called an N channel contact. It is not necessary to have a simple dispersion of the form of Eq. (2). For a lattice Hamiltonian or in the presence of a magnetic field the transverse wave functions also depend on the longitudinal wave vector. The scattering approach to conductance is powerful because none of the results given below depends on the precise nature of the dispersion in the contacts.

B. Scattering states

The quantum channels defined above can now be used to describe in and out-going states and can thus be used to define a scattering problem. A scattering state[16] $\Psi_{\alpha n}(E,\mathbf{r})$ is a wave function with unit incident amplitude in channel n in lead α and reflected waves in typically all the other channels in the same contact and transmitted waves in typically all other contacts. The scattering states together with possible bound states form a complete set. For simplicity we assume here that all states are extended (no bound states). The amplitudes of the reflected waves and the transmitted waves are determined by the elements $s_{\beta\alpha mn}$ of the scattering matrix. The scattering matrix is the ratio of the out-going current amplitude in contact β in channel m and the incident current amplitude in contact α in channel n. An elegant description of scattering in second quantization can be given in terms of two sets of annihilation operators[22,23,38] $\hat{a}_{\alpha n}(E)$ and $\hat{b}_{\alpha n}(E)$. The operator $\hat{a}_{\alpha n}(E)$ annihilates a carrier in an incoming state in probe α in channel n with energy E. The operator $\hat{b}_{\alpha n}(E)$ annihilates a carrier in an out-going state in probe α in channel n with energy E. It is useful to group these operators for each probe together in a vector $\hat{\mathbf{a}}_\alpha(E)$ and $\hat{\mathbf{b}}_\alpha(E)$ and to

introduce the submatrice $\mathbf{s}_{\beta\alpha}$ which relates all the current amplitudes incident in probe α to the current amplitudes transmitted into probe β. The $\hat{\mathbf{a}}_\alpha(E)$ and $\hat{\mathbf{b}}_\alpha(E)$ operators are related by a unitary transformation which is given by the scattering matrix[23,38]

$$\hat{\mathbf{b}}_\beta = \sum_\alpha \mathbf{s}_{\beta\alpha}\hat{\mathbf{a}}_\alpha . \tag{3}$$

Thus the $\hat{b}_{\alpha n}$ operators obey exactly the same commutation (anticommutation) relations as the $\hat{a}_{\alpha n}$ operators.

C. Self-consistent scattering states

The scattering matrices introduced in Eq. (3) are not only a function of energy but also a functional of the electrostatic potential $U(\mathbf{r})$. The electrostatic potential depends via a Poisson equation on the charge distribution in the sample. The charge distribution in the sample depends on the voltages applied to the sample. At equilibrium when all electrochemical potentials μ_α at all contacts are identical, this potential is the equilibrium electrostatic potential $U_{\rm eq}(\mathbf{r})$. In steady-state stationary transport the charge distribution and hence the potential depends on the electrochemical potentials at the contacts. Consequently the nonequilibrium potential is also a function of the electrochemical potentials at the contacts $U([\mu_\alpha],\mathbf{r})$. Hence the scattering matrix in an electric conductor is never truly a single particle matrix but is a function both of the energy of the carriers and implicitly via the electrostatic potential a function of the electrochemical potentials,

$$\mathbf{s}_{\beta\alpha}(E, U([\mu_\alpha],\mathbf{r})). \tag{4}$$

The situation is even more complex, when we deal with quantum noise. The fluctuations in the charge density inside the conductor lead then to a potential that is also fluctuating. In the following discussion we will now present results which are correct for a fixed given potential. Later on when we discuss the ac conductance and frequency-dependent noise spectra we will also discuss the consequence of the time-dependent potential and its fluctuations.

D. The current operator

We now want to express the operator of the total current in probe α in terms of the annihilation (and creation) operators introduced above. A derivation can be found in Ref. 22 and 23. The result is simple and can be motivated as follows: Consider first the current dI incident in a fully occupied quantum channel in a small energy interval dE at energy E. In channel n in probe α this current is[37] $dI_{\alpha n} = e v_{\alpha n} dn_{\alpha n}$. Here $v_{\alpha n}$ is the velocity of this channel at energy E and $dn_{\alpha n}$ is the carrier density in this energy interval in this channel. This density is $(dn_{\alpha n}/dE)dE$. But $dn_{\alpha n}/dE = (dn_{\alpha n}/dk_{\alpha n})dk_{\alpha n}/dE_{\alpha n}$ is equal to the density of states of a uniform wire in k space which is $1/2\pi$ multiplied by $1/\hbar v_{\alpha n}$. Thus $dn_{\alpha n}/dE = 1/h v_{\alpha n}$. As a consequence the incident current $dI_{\alpha n} = (e/h)dE$ is independent of any properties of the quantum channel. This is a central result of the scattering approach to electrical conductance and is deeply connected to the fact that the conductance of quantum point contacts[39] and in Hall conductors[3] can be quantized. Now we take into account that the channel needs not always to be full. We introduce the occupation probability $n^+_{\alpha n}$ of the incoming branch of quantum channel αn. Similarly, we introduce the occupation probability $n^-_{\alpha n}$ of the outcoming branch of quantum channel αn. The net current on both the incoming and outgoing branch of quantum channel n is $dI_{\alpha n}(E) = (e/h)dE(n^+_{\alpha n}(E) - n^-_{\alpha n}(E))$. We generalize this result in two ways. First, we assume that it is valid even if the occupation probabilities are not stationary but are functions of time, $n^\pm_{\alpha n}(E,t)$. Second, we express the occupation probabilities in terms of the annihilation (creation) operators introduced above. We have $\hat{n}^+_{\alpha n}(E,t) = \int d(\hbar\omega)\hat{a}^\dagger_{\alpha n}(E)\hat{a}_{\alpha n}(E + \hbar\omega)\exp(-i\omega t)$ and

$\hat{n}^{-}_{\alpha n}(E,t) = \int d(\hbar\omega)\hat{b}^{\dagger}_{\alpha n}(E)\hat{b}_{\alpha n}(E+\hbar\omega)\exp(-i\omega t)$. Finally, to obtain the operator for the total current, we must sum over all channels in probe α and integrate the resulting expression over energy. Consequently, the operator for the total current in probe α is[23]

$$I_\alpha(t) = \frac{e}{h}\int dE dE' [\hat{\mathbf{a}}^{\dagger}_{\alpha}(E)\hat{\mathbf{a}}_{\alpha}(E') - \hat{\mathbf{b}}^{\dagger}_{\alpha n}(E)\hat{\mathbf{b}}_{\alpha}(E')]\exp(i(E-E')t/\hbar). \tag{5}$$

Clearly, this is an intuitively appealing result. Before proceeding, we remark that this expression contains no detailed spatial information on the location of the carriers but only takes into account whether a carrier is in an incoming or outgoing channel in a given reservoir. A formal derivation of Eq. (5) proceeds by constructing the Fermi field operator. This is carried out in Ref. 23 in detail. The Fourier transform of Eq. (5) is exact to first order in frequency. For larger frequencies it is an approximation to the actual space-dependent expression of the current operator (see the discussions in Refs. 40 and 41).

To proceed we use Eq. (3) to eliminate the $\hat{b}$ operators in Eq. (5) to find an expression for the current operator in terms of the $\hat{a}$ operators alone. The resulting current operator can be written in a compact form with the help of the matrix[22,23]

$$\mathbf{A}_{\beta\gamma}(\alpha,E,E+\hbar\omega) = \mathbf{1}_\alpha\delta_{\alpha\beta}\delta_{\alpha\gamma} - \mathbf{s}^{\dagger}_{\alpha\beta}(E)\mathbf{s}_{\alpha\gamma}(E+\hbar\omega). \tag{6}$$

Here $\mathbf{1}_\alpha$ is a unit matrix with dimensions N_α equal to the number of quantum channels in lead α. The elements of this matrix are the current matrix elements calculated not with the asymptotic states but with the full scattering states $\Psi_{\beta n}(E;\mathbf{r})$ and $\Psi_{\gamma n}(E;\mathbf{r})$ evaluated in lead α and divided by $(hv_{\alpha n}(E)hv_{\alpha m}(E))^{1/2}$. With the help of this matrix we obtain the desired expression for the current operator,[22]

$$I_\alpha(t) = \frac{e}{h}\sum_{\beta\gamma}\int dE dE' \hat{\mathbf{a}}^{\dagger}_{\beta}(E)\mathbf{A}_{\beta\gamma}(\alpha,E,E')\hat{\mathbf{a}}_{\gamma}(E')\exp(i(E-E')t/\hbar). \tag{7}$$

Below we will use this expression to derive the conductane coefficients, the equilibrium and transport noise of mesoscopic conductors and expressions for the ac conductance.

III. AVERAGE CURRENTS AND CONDUCTANCE

First, we now use Eq. (7) to find the average currents and conductance of an arbitrary multichannel[37,42] multilead[15,16,43] structure. The key assumption of our discussion is that the wide portion of the leads can be assumed to be reservoirs which are in an equilibrium state. Thus the $\hat{a}_\alpha$ operators which act on the incident state in reservoir α obey the equilibrium statistical mechanics of reservoir α. In principle one first finds the quantum average of $\hat{a}^{\dagger}_{\beta m}(E)\hat{a}_{\gamma n}(E')$ and then computes the statistical average. To simplify our notation we will use the symbol $\langle\ \rangle$ to denote both of these averages. With this notation we have

$$\langle \hat{a}^{\dagger}_{\beta m}(E)\hat{a}_{\gamma}(E')\rangle = \delta_{\alpha\beta}\delta_{mn}\delta(E-E')f_\alpha(E). \tag{8}$$

Here $f_\alpha(E)$ is the Fermi (Bose) function of reservoir α. Note that on the average it is only the product in which both $\hat{a}$ operators have the same reservoir and channel index and the same energy which is non-vanishing. Using Eq. (8) gives for the average currents[23]

$$\langle I_\alpha\rangle = \frac{e}{h}\sum_{\beta}\int dE\ \mathrm{Tr}[A_{\beta\beta}(\alpha,E,E)]f_\beta(E). \tag{9}$$

Here the trace Tr is over channel indices. Since $\mathrm{Tr}(\mathbf{s}^{\dagger}_{\alpha\alpha}(E)\mathbf{s}_{\alpha\alpha}(E)) = R_{\alpha\alpha}(E)$ is the total reflection probability of waves incident from lead α back into lead α and $\mathrm{Tr}(\mathbf{s}^{\dagger}_{\alpha\beta}(E)\mathbf{s}_{\alpha\beta}(E)) = T_{\alpha\beta}(E)$ is the total transmission probability of particles incident from reservoir β into reservoir α we find,[23]

$$\langle I_\alpha\rangle = \frac{e}{h}\int dE\left[(N_\alpha - R_{\alpha\alpha}(E))f_\alpha(E) - \sum_\beta T_{\alpha\beta}(E)f_\beta(E)\right]. \tag{10}$$

Equation (10) is a nonlinear result which depends on the applied voltages not only through the Fermi functions but as discussed in Sec. II C implicitly through the electrostatic potential. A more detailed discussion is given in Ref. 26 and in a work by Christen and the author.[44] Now we assume that the electrochemical potentials of the reservoirs μ_α differ only by a small amount from the equilibrium chemical potential μ_0. We can expand the Fermi functions away from this equilibrium potential, $f_\alpha(E) = f_0 - (df/dE)(\mu_\alpha - \mu_0) + \cdots$. Similarly the potential $U([\mu_\alpha],\mathbf{r})$ is expanded away from the equilibrium potential $U_{\mathrm{eq}}(\mathbf{r})$. Inserting this into Eq. (10) gives

$$\langle I_\alpha\rangle = \frac{e}{h}\int dE(-df/dE)\left[(N_\alpha - R_{\alpha\alpha}(E))\mu_\alpha - \sum_\beta T_{\alpha\beta}(E)\mu_\beta\right]. \tag{11}$$

That is the central result found in Ref. 15. In this expression the scattering matrix and the transmission and reflection probabilities are functions of the *equilibrium* electrostatic potential $U_{\mathrm{eq}}(\mathbf{r})$. The equilibrium electrochemical potential μ_0 does not appear since the unitarity of the scattering matrix gives

$$N_\alpha = R_{\alpha\alpha}(E) + \sum_\beta T_{\alpha\beta}(E) = R_{\alpha\alpha}(E) + \sum_\beta T_{\beta\alpha}(E). \tag{12}$$

From Eq. (11) we obtain the conductance coefficients at zero bias. The conductance coefficients $G_{\alpha\beta}$ are the derivatives of the current in probe α with respect to electrochemical potentials of probe β, $G_{\alpha\beta} = e d\langle I_\alpha\rangle/d\mu_\beta|_{[\mu_\alpha]=\mu_0}$. We obtain

$$G_{\alpha\alpha} = \frac{e^2}{h}\int dE(-df/dE)(N_\alpha - R_{\alpha\alpha}(E)), \tag{13}$$

and for the off-diagonal conductances obtain

$$G_{\alpha\beta} = -\frac{e^2}{h}\int dE(-df/dE)T_{\alpha\beta}(E). \tag{14}$$

Note that the unitarity of the scattering matrix (current conservation) also implies

$$\sum_\beta G_{\alpha\beta} = \sum_\beta G_{\beta\alpha} = 0. \tag{15}$$

We will later discuss what the equivalent sum rules are for ac conductances. Typically, in experiments, it is not the conductance coefficients which are measured but resistances.[45,46] In the typical setup only two probes are used to drive a current through the conductor and all other probes are connected to voltmeters. Since voltmeters have ideally an infinite impedance this implies that at a voltage probe the average current is zero. The electrochemical potential of this probe floats to a value which gives zero-current in that probe. Imposing the current on two of the probes and imposing the zero-current condition on all other probes in Eq. (11) yields rational functions for the resistances in terms of the conductance coefficients (transmission probabilities) given by Eq. (13)

and Eq. (14). It is the wide range of applicability to all possible geometries which has made Eq. (11) a very useful result. Another important aspect of these results is their symmetry under magnetic field reversal.[15,16,45,47–49]

IV. CURRENT–CURRENT FLUCTUATIONS

Electric conduction is not only characterized by its average behavior but also by its fluctuations away from the average. There are typically many sources of fluctuations. Here we are interested in the fluctuations that are fundamental in the sense that they are unavoidable. There are two such fundamental sources of fluctuations. First, at equilibrium we have Nyquist–Johnson noise. At equilibrium such thermal noise is the only unavoidable noise. As is well known, this noise is related via the fluctuation dissipation theorem to the equilibrium transport coefficients, Eqs. (13) and (14). In the presence of transport a second more interesting noise comes to the forefront: a quantum statistical partition noise.[18–20,22,50,51]

On a single particle level the origin of this noise lies in the fact that a particle can only be detected at one place and must be detected in its entirety. Consider for a moment a simple scattering problem with transmission T and reflection probability R. If we consider a series of events, each with a single particle incident from the left, the average occupation number of the transmitted beam is $\langle n_T\rangle = T$. But the actual occupation number in each event is either $n_T=1$, if the particle has been transmitted or is $n_T=0$, if the particle has been reflected. This leads to a mean square fluctuation in the occupation number which is $\langle(\Delta n_T)^2\rangle = T(1-T)$. This noise peaks when the uncertainty for the particle to arrive in this channel is maximal, i.e., when $T=1/2$. In a conductor we deal not with single particles nor with particles that arrive at the scatterer in a sequence of events that are separated in time and space. We must allow for states which carry more then one particle. As a consequence this noise depends on the symmetry of the wave function under exchange of particles. Concern with such effects in optics goes back to the midel fifties when Hanbury Brown and Twiss[50] carried out a number of experiments which revealed quantum statistical effects in beams of light from stars or man made light sources. In solid state physics, partition noise has also been discussed a long time ago, but to our knowledge only as a purely classical phenomena.[52] Text books mostly emphasize the limit of small transmission, and the resulting noise is called shot noise and given by Shottky, $\langle(\Delta I)^2\rangle = 2e\Delta\nu\langle I\rangle$. Here $\Delta\nu$ is the band width over which the noise is measured and $\langle I\rangle$ is the average current. According to this expression the noise is a consequence of carriers arriving and being transmitted with a Poisson distribution. The quantum statistical partition noise can be much smaller then the Shottky noise.

A. Spectral densities of current fluctuations

The spectral densities $S_{\alpha\beta}(\omega)$ of current fluctuations for a quantum mechanical problem are given by

$$(1/2)\langle\Delta\hat{I}_\alpha(\omega)\Delta\hat{I}_\beta(\omega')+\Delta\hat{I}_\beta(\omega')\Delta\hat{I}_\alpha(\omega)\rangle = 2\pi S_{\alpha\beta}(\omega)\,\delta(\omega-\omega'). \tag{16}$$

Here $\Delta\hat{I}_\alpha(\omega)$ stands for the Fourier transform of Eq. (7) with the average current (zero-frequency component) subtracted. Below we will use a somewhat more transparent notation. Instead of $S_{\alpha\beta}(\omega)$ we write

$$\langle\Delta I_\alpha\Delta I_\beta\rangle = 2\Delta\nu S_{\alpha\beta}(\omega) \tag{17}$$

with $\Delta\nu$ the experimental band width in which the noise is measured.

The spectral densities, Eqs. (16) or (17), are defined by expectation values of products of four operators.[53,23] These expectation values for a system at equilibrium are known and given by

$$\langle \hat{a}^{\dagger}_{\alpha m}(E_1)\hat{a}_{\beta n}(E_2)\hat{a}^{\dagger}_{\gamma k}(E_3)\hat{a}_{\delta l}(E_4)\rangle - \langle \hat{a}^{\dagger}_{\alpha m}(E_1)\hat{a}_{\beta n}(E_2)\rangle\langle a^{\dagger}_{\gamma k}(E_3)\hat{a}_{\delta l}(E_4)\rangle$$
$$= \delta_{\alpha\delta}\delta_{\beta\gamma}\delta_{ml}\delta_{nk}\delta(E_1-E_4)\,\delta(E_2-E_3)f_{\alpha}(E_1)(1-f_{\beta}(E_2)). \tag{18}$$

The statistical average of only two $\hat{a}$ operators is local in the sense that only products with the same quantum channel index and the same reservoir index are nonvanishing. However, Eq. (18) is not local: it correlates average occupation factors of different quantum channels in the same reservoir and even in different reservoirs!

Using Eq. (18) and the Fourier transform of the current operator Eq. (7) gives for the current-current correlations the expression[40,23]

$$\langle \Delta I_{\alpha}\Delta I_{\beta}\rangle = \frac{e^2}{h}\,\Delta\nu \sum_{\gamma\delta} \int dE\ \mathrm{Tr}[\mathbf{A}_{\gamma\delta}(\alpha,E,E+\hbar\omega)\mathbf{A}_{\gamma\delta}(\beta,E+\hbar\omega,E)]F_{\gamma\delta}(E,E+\hbar\omega), \tag{19}$$

where

$$F_{\gamma\delta}(E,E+\hbar\omega) = f_{\gamma}(E)(1-f_{\delta}(E+\hbar\omega)) + f_{\delta}(E+\hbar\omega)(1-f_{\gamma}(E)). \tag{20}$$

First, our interest will be in the zero-frequency limit. In this case it can be shown that Eq. (19) reduces to the following expression:[54,23]

$$\langle \Delta I_{\alpha}\Delta I_{\beta}\rangle = 2\,\frac{e^2}{h}\,\Delta\nu \sum_{\gamma\delta} \int dE\ \mathrm{Tr}[\mathbf{A}_{\gamma\delta}(\alpha,E,E)\mathbf{A}_{\gamma\delta}(\beta,E,E)]f_{\gamma}(E)(1-f_{\delta}(E)) \tag{21}$$

This is obvious for the case $\alpha=\beta$ but requires some consideration for the case that $\alpha\neq\beta$. We will discuss Eq. (21) in various limiting cases.

B. Equilibrium current fluctuations

At equilibrium our expression Eq. (21) can be simplified still further since all distribution functions f_{α} are the same and given by the distribution function f with an electrochemical potential μ_0. Only terms which are bilinear in the scattering matrices survive. Using that $f(1-f) = kT(-df/dE)$ and using $\mathrm{Tr}(\mathbf{s}_{\alpha\alpha}(E)\mathbf{s}^{\dagger}_{\alpha\alpha}(E)) = R_{\alpha\alpha}(E)$ and $\mathrm{Tr}(\mathbf{s}_{\alpha\beta}(E)\mathbf{s}^{\dagger}_{\alpha\beta}(E)) = T_{\alpha\beta}(E)$ we find for the mean square fluctuations ($\alpha=\beta$)

$$\langle (\Delta I_{\alpha})^2\rangle = 4\Delta\nu kT\,\frac{e^2}{h}\int dE(-df/dE)[N_{\alpha}-R_{\alpha\alpha}(E)] = 4\Delta\nu kT G_{\alpha\alpha} \tag{22}$$

and the correlations ($\alpha\neq\beta$)

$$\langle \Delta I_{\alpha}\Delta I_{\beta}\rangle = -2\Delta\nu kT\,\frac{e^2}{h}\int dE(-df/dE)[T_{\alpha\beta}(E)+T_{\beta\alpha}(E)] = 2\Delta\nu kT[G_{\alpha\beta}+G_{\beta\alpha}]. \tag{23}$$

Therefore, as we expect it, the equilibrium mean square fluctuations are related to the diagonal conductances and the correlations are related to the *symmetrized* off-diagonal conductances.[22,23] The equilibrium fluctuations are not without interest. They can serve to calibrate noise measurements.[10,11] The equilibrium fluctuations are also particularly interesting in the quantized Hall regime since in this case the conductances either vanish or are quantized (at least if the contacts to the sample behave ideal). If the contacts along the perimeter of the sample are labeled clock-wise only conductances between consecutive contacts $G_{\alpha+1,\alpha}$ are nonvanishing and quantized.[22] As a consequence only the correlations between currents of two next nearest neighbor

contacts are nonzero. For the voltage fluctuations this implies the absence of correlations between Hall voltage fluctuations and longitudinal voltage fluctuations. This has been observed by Kil *et al.*[55]

C. Zero temperature transport fluctuations

We have seen that at equilibrium only expressions survive which are quadratic in the scattering matrices. In fact, only transmission probabilities matter. In the presence of transport, and in the zero temperature limit, it is the products of four scattering matrices which count. In Eq. (21) all terms in the sum for which $\gamma=\delta$ vanish, since $f_\alpha(1-f_\alpha)$ is zero at zero temperature. But for the terms for which $\gamma\neq\delta$ the A matrices are of the form. $\mathbf{A}_{\gamma\delta}(\alpha)(E,E) = -\mathbf{s}^\dagger_{\alpha\gamma}(E)\mathbf{s}_{\alpha\delta}(E)$ and consequently we find from Eq. (21),

$$\langle \Delta I_\alpha \Delta I_\beta\rangle = 2\frac{e^2}{h}\Delta\nu \sum_{\gamma\delta,\,\gamma\neq\delta}\int dE\ \mathrm{Tr}[\mathbf{s}^\dagger_{\alpha\gamma}(E)\mathbf{s}_{\alpha\delta}(E)\mathbf{s}^\dagger_{\beta\delta}(E)\mathbf{s}_{\beta\gamma}(E)]f_\gamma(E)(1-f_\delta(E)), \tag{24}$$

where $f\alpha(E)=\Theta(E-\mu_\alpha(E))$ with Θ the step function.[22,24]

Let us discuss this result for the case of a two-terminal conductor. Using the notation $\mathbf{s}_{11}\equiv\mathbf{r}_{11}$, $\mathbf{s}_{22}\equiv\mathbf{r}_{22}$, $\mathbf{s}_{21}\equiv\mathbf{t}_{21}$, and $\mathbf{s}_{12}\equiv\mathbf{t}_{12}$, which more explicitly emphasizes reflection r and transmission t the conductance $G\equiv G_{11}=G_{22}=-G_{12}=-G_{21}$ is $G=(e^2/h)\mathrm{Tr}(\mathbf{t}^\dagger_{21}\mathbf{t}_{21})=(e^2/h)\mathrm{Tr}(\mathbf{t}^\dagger_{12}\mathbf{t}_{12})$. The average current driven through the sample is thus $\langle I\rangle=GV$ with $eV=\mu_1-\mu_2$. Form Eq. (24) the mean square current fluctuations are determined by a single term $\mathrm{Tr}[\mathbf{s}^\dagger_{11}\mathbf{s}_{12}\mathbf{s}^\dagger_{12}\mathbf{s}_{11}]$ $=\mathrm{Tr}[\mathbf{r}_{11}\mathbf{r}^\dagger_{11}\mathbf{t}_{12}\mathbf{t}^\dagger_{12}]$. Thus we find[22]

$$\langle(\Delta I)^2\rangle = 2\frac{e^2}{h}\Delta\nu|eV|\mathrm{Tr}[\mathbf{r}_{11}\mathbf{r}^\dagger_{11}\mathbf{t}_{12}\mathbf{t}^\dagger_{12}]. \tag{25}$$

The matrices $\mathbf{r}_{11}\mathbf{r}^\dagger_{11}$ and $\mathbf{t}_{12}\mathbf{t}^\dagger_{12}$ are hermitian and commute and can, therefore, be diagonalized simultaneously. Let us denote the eigenvalues of $\mathbf{t}_{12}\mathbf{t}^\dagger_{12}$ by T_n and the eigenvalues of $\mathbf{r}_{11}\mathbf{r}^\dagger_{11}$ by R_n. In terms of the transmission eigenvalues T_n the conductance is simply $G=(e^2/h)\Sigma_n T_n$. Our result Eq. (25) can be written in the form

$$\langle(\Delta I)^2\rangle = 2e\Delta\nu|V|\ \frac{e^2}{h}\sum_n T_n(1-T_n). \tag{26}$$

This result can now be connected with the results obtained by Khlus[18] and by Lesovik.[19] In these works it was assumed from the outset that the transmission matrix is diagonal. Thus the results given in these works are in fact general, if the diagonal elements are identified with the eigenvalues of $\mathrm{Tr}[\mathbf{tt}^\dagger]$. This result seems natural, but it is not as obvious as one might think at first! Below we illustrate this with a discussion that starts from slightly different assumptions and indeed does not lead to Eq. (25) even so for a diagonal transmission matrix it leads to the result of Khlus and Lesovik.

First, we like to discuss the interesting properties of this result. Eq. (26) leads to the standard Shottky noise formula only and only if all transmission eigenvalues T_n are small compared to 1. Then we can neglect terms quadratic in T_n in Eq. (26) and find $\langle(\Delta I)^2\rangle=2e\Delta\nu|\langle I\rangle|$. Like the partition noise Eq. (25) has the property that an eigenmode gives a maximum contribution when T_n is equal to 1/2 and gives no contribution if the channel is completely closed $T_n=0$ or completely open $T_n=1$. Conductors in which situations of completely open or completely closed eigen channels can be realized are quantum point contacts,[39] quantized Hall conductors[3] and perhaps ballistic conductors. Thus at a conductance plateau of a quantum point contact or in the quantized Hall regime in the range of a Hall plateau the noise given by Eq. (26) vanishes completely.

Initial experiments on quantum point contacts[56] and in quantized Hall conductors[57] provided only an indication of the expected noise reduction in the plateau regions. But the more recent experiments by Kumar *et al.*[10] and Reznikov *et al.*[9] provide strikingly clear data which makes even a quantitative comparison with theory possible. This advance is even more striking when one considers the often wide ranging gap of theory and experiment on noise in physical systems.[58]

We mention two results to indicate the wide range of problems to which this theory can be applied. A metallic diffusive conductor (distance between impurities small compared to the sample width and length) has transmission probabilities T_{12mn} which are very small compared to 1 when averaged over an ensemble. Thus one might expect that a mesoscopic metallic diffusive conductor exhibits full shot noise. However, the eigenvalues T_n of such an ensemble are distributed in a bi-modal manner with a concentration at $T_n=1$ and a concentration at $T_n=0$. As a consequence it is found that a mesoscopic metallic diffusive conductor exhibits a shot noise which is 1/3 of the full shot noise[59]

$$\langle(\Delta I)^2\rangle_e = \tfrac{2}{3} e \Delta\nu |V| \langle I\rangle. \tag{27}$$

Here the index e indicates not only a quantum and statistical average but also an ensemble average. A recent experimental work by Steinbach *et al.*[11] provides a more complete discussion and additional references. For a chaotic cavity connected to two leads it is found that the ensemble averaged shot noise is 1/4 of the full shot noise[60]

$$\langle(\Delta I)^2\rangle_e = \tfrac{2}{4} e \Delta\nu |V| \langle I\rangle. \tag{28}$$

It is possible to discuss not only the ensemble average but also the mean square deviations away from this average.[61]

D. Single particle versus many particle quantum shot noise

It would be deceiving if we tried to understand the result, Eq. (25) only in the special basis of eigen channels. If we write out the trace of the product of the four scattering matrices in terms of the transmission and reflection matrix elements, we find

$$\mathrm{Tr}[\mathbf{r}\mathbf{r}^\dagger\mathbf{t}\mathbf{t}^\dagger] = \sum_{klmn} r_{ml} r^*_{ml} t_{mn} t^*_{kn}. \tag{29}$$

In a general basis only a few terms in this expression are products of the transmission and reflection probabilities. Most of the terms in Eq. (29) consist of products of four scattering amplitudes which are not real valued. If we attribute a transmission probability with the transfer of one electron (a product of two hermitian conjugate) amplitudes, then we should associate a two-electron process with products of four scattering amplitudes. We should be able to demonstrate that if only one electron at the time is incident on the conductor such complex products are in fact not present. The following considerations show that this is indeed the case.

Assume for a moment that we have an electron source which injects single electrons into a definite quantum channel in events that are well separated in time and space. As above, we consider the case of vanishing temperature. First let us assume that the current source at contact η injects carriers into channel o with probability 1. For this experiment the right hand side of Eq. (18) is replaced by the quantum expectation value

$$\delta_{\alpha\delta}\delta_{\beta\gamma}\delta_{ml}\delta_{nk}\delta(E_1-E_4)\delta(E_2-E_3)n_{\alpha n}(E_1)(1-n_{\beta m}(E_2)) \tag{30}$$

with $n_{\alpha n}=\delta_{\eta\alpha}\delta_{on}$. The resulting partition noise can then be expressed in terms of the probabilities $S_{\alpha\eta o}=\Sigma_m |s_{\alpha\eta mo}|^2$. Instead of Eq. (25) we find a shot noise proportional to $S_{\alpha\eta o}[\delta_{\alpha\beta}-S_{\beta\eta o}]$. If

we now consider a series of successive experiments in which the channel o eventually can be any of the incident channels in probe η and consider the total noise, the current-current correlations are

$$\langle \Delta I_\alpha \Delta I_\beta \rangle = 2\frac{e^2}{h}\Delta\nu|eV|\sum_o S_{\alpha\eta o}[\delta_{\alpha\beta} - S_{\beta\eta o}]. \tag{31}$$

It can be shown that these expressions are current conserving, $\Sigma_\alpha \langle \Delta I_\alpha \Delta I_\beta \rangle = \Sigma_\beta \langle \Delta I_\alpha \Delta I_\beta \rangle = 0$. For the mean squared current $\langle (\Delta I)^2 \rangle$ we obtain, therefore, $\langle (\Delta I)^2 \rangle = e^2/h\Delta\nu|eV|\Sigma_o T_{21o} R_{11o}$ where $T_{21o} = S_{21o}$ and $R_{11o} = S_{11o}$. Evidently, if the transmission and reflection matrices t and r are diagonal, Eq. (31) is identical with Eq. (26). But in contrast to Eq. (25), Eq. (31) for the case of a general scattering matrix is expressed in terms of probabilities only. It contains no exchange terms.

From this exercise we can conclude that it is not possible, without ad hoc assumptions, to derive a many-channel result simply by deriving first the result in the eigen channel basis. Experimentally, it will be difficult to distinguish between Eq. (25) and Eq. (31). Thus in Ref. 54 we have proposed an experiment on a multipole conductor to directly detect the exchange terms. We will briefly restate this proposal below. But first we proceed with the discussion of noise in a two probe conductor.

E. Quantum statistical shot noise

At elevated temperatures, Eq. (21) predicts a combined thermal and shot noise, which when expressed in terms of the transmission probabilities T_n of the eigen channels is given by

$$\langle (\Delta I)^2 \rangle = 2e\Delta\nu\frac{e^2}{h}\sum_n \int dE[f_1(E)(1 \pm f_1(E))T_n + f_2(E)(1 \pm f_2(E))T_n \pm T_n(1-T_n)(f_1 - f_2)^2]. \tag{32}$$

Here we have compared a system subject to Fermi statistics (upper signs) with a system subject to Bose statistics (lower signs). The result for Fermions was obtained by Lesovik[19] and the result for Bose statistics was given in Ref. 54. Clearly, the first two terms in this expression represent thermal contributions to the noise. The last term which is quadratic in the difference of the distribution function and has an amplitude $T_n(1-T_n)$ is the quantum partition noise. This contribution to the noise is quadratic in the intensity of the incident electron (photon) flux and most significantly, changes sign as we change statistics. In comparison to the first two terms quantum statistical partition increases the overall noise for Fermions but quantum statistical partition decreases the shot noise for Bosons. The reduction of noise in the bosonic case can be understood as follows: the scattering obstacle can break up incident multiquanta states $n\hbar\omega$ and transmit a portion and reflect a portion. As a consequence the transmitted stream will on the average contain particles with fewer quanta and thus produce a reduced noise.[62]

F. Making exchange effects visible

It is illuminating to consider the following thought experiment:[23,54] Consider a conductor with four probes (see for example Fig. 1). In experiment A, contact 1 is described by a distribution function f and all other contacts by a distribution function f_0. The correlation function between the fluxes at the contacts 3 and 4 is measured and denoted by $\langle \Delta I_3 \Delta I_4 \rangle_A$. In a second experiment B, contact 2 is described by a distribution function f and all other contacts by a distribution function f_0. Again the correlation function between the fluxes at contacts 3 and 4 is measured and denoted by $\langle \Delta I_3 \Delta I_4 \rangle_B$. In a third experiment *both* contacts 1 and 2 are described by the distribution function f and only contacts 3 and 4 are determined by the distribution function f_0. The correlation function measured in the third experiment is denoted by $\langle \Delta I_3 \Delta I_4 \rangle_C$. For a classical

system, we would expect that experiment C is simply determined by the sum of the correlation functions measured in experiments A and B, $\langle \Delta I_3 \Delta I_4 \rangle_C = \langle \Delta I_3 \Delta I_4 \rangle_A + \langle \Delta I_3 \Delta I_4 \rangle_B$. The quantum mechanical result, however, is different, and is given by

$$\langle \Delta I_3 \Delta I_4 \rangle_C = \langle \Delta I_3 \Delta I_4 \rangle_A + \langle \Delta I_3 \Delta I_4 \rangle_B \pm 2\Delta\nu \frac{e^2}{h} \times \int dE (f - f_0)^2 [\mathrm{Tr}(\mathbf{s}_{31}\mathbf{s}_{32}^\dagger \mathbf{s}_{41}\mathbf{s}_{42}^\dagger) + \mathrm{Tr}(\mathbf{s}_{32}\mathbf{s}_{31}^\dagger \mathbf{s}_{42}\mathbf{s}_{41}^\dagger)]. \quad (33)$$

This contribution to the correlation function is an exchange term. It is a consequence of the fact that we deal with a quantum mechanical problem of many indistinguishable particles. Interestingly the individual terms in Eq. (33) are not real and thus have a phase associated with them. A more detailed interpretation and discussion of this phase is presented in Refs. 23 and 54.

G. Frequency-dependent noise spectra

So far we have focused only on the zero-frequency limit of the noise spectra. Let us briefly consider the equilibrium frequency-dependent spectrum. At equilibrium the function $F_{\gamma\delta}(E, E+\hbar\omega)$, given by Eq. (20), simplifies. It is independent of the indices $\gamma\delta$ and given by $F(E, E+\hbar\omega) = (f(E) - f(E+\hbar\omega))\epsilon(\hbar\omega)/\hbar\omega$, where $\epsilon(\hbar\omega)$ is the energy of a harmonic quantum oscillator with frequency ω at temperature T. As in the zero-frequency limit, it can be shown that all products of four scattering matrices vanish identically. The equilibrium frequency-dependent spectrum can be expressed as a *sum* of two **A** matrices. It is proportional to $\mathrm{Tr}[\mathbf{A}_{\beta\beta}(\alpha, E, E+\hbar\omega) + \mathbf{A}_{\alpha\alpha}(\beta, E+\hbar\omega, E)]$ and in terms of the *s* matrices the frequency-dependent equilibrium spectrum is[40]

$$\langle \Delta I_\alpha \Delta I_\beta \rangle = 2\frac{e^2}{h} \Delta\nu \int dE\ \mathrm{Tr}[2\mathbf{1}_\alpha \delta_{\alpha\beta} - \mathbf{s}_{\alpha\beta}^\dagger(E)\mathbf{s}_{\alpha\beta}(E+\hbar\omega) - \mathbf{s}_{\beta\alpha}^\dagger(E+\hbar\omega)\mathbf{s}_{\beta\alpha}(E)] \frac{(f(E) - f(E+\hbar\omega))}{\hbar\omega} \epsilon(\hbar\omega). \quad (34)$$

Now on general grounds we know that their must exist a frequency-dependent conductance $G_{\alpha\beta}(\omega)$ whose real part $G'_{\alpha\beta}(\omega) = (1/2)[G_{\alpha\beta}(\omega) + G^*_{\beta\alpha}(\omega)]$ is related to this spectrum via a fluctuation dissipation theorem,

$$\langle \Delta I_\alpha \Delta I_\beta \rangle = 4\Delta\nu\epsilon(\hbar\omega) G'_{\alpha\beta}(\omega). \quad (35)$$

The task is to find the conductance $G_{\alpha\beta}(\omega)$.

V. DYNAMIC CONDUCTANCE

The standard procedure to derive a dynamical conductance is to use linear response theory. The current density is calculated in response to an electric field. But which electric field? Most discussions use without qualification a uniform electric field. But even if we are more ambitious and calculate the dynamical conductance to a non-uniform field, we will still obtain a frequency-dependent current response that depends on the particular field configuration. In reality, the field that counts is not arbitrary but is determined by the distribution of charges inside the sample.

Against this back-ground, the immediate task we have at hand, namely deriving the $G_{\alpha\beta}(\omega)$ which belongs to the noise-spectrum Eq. (34), is puzzling. Clearly, the spectrum Eq. (34) contains *no* information on the electric field configuration. In deriving the fluctuation spectra we have made explicitly the assumption that the electric potential is fixed and given by the equilibrium potential.

To derive $G_{\alpha\beta}(\omega)$ which belongs to Eq. (34) we need thus to find perturbations (driving forces) which are not given by the frequency-dependent nonequilibrium electric field.

Of course the response to the self-consistent electric field exists and must be part of a complete answer. Therefore, we adopt a two step strategy. First, we find the conductance which belongs to Eq. (34). We call this the *external* response or the *external* conductance. In a second step we find the charges, which as a consequence of our dynamical perturbation are injected into the sample. A self-consistent scheme is then used to find the total charge (injected charge and induced charges) and the electrical-potential belonging to this charge distribution. In the next step the current response to this internal potential is calculated. The total current response is then determined by both the external conductance and an internal conductance in response to the internal electric potential.

A. External response

In collaboration with Thomas,[63] and Pretre and Thomas[25] we have found two different perturbations which give rise to the conductance which obeys the fluctuation dissipation theorem, stated in Eq. (35). The first perturbation has an energy

$$H_1^{\phi} = \sum_{\alpha} \hat{I}_{\alpha} \phi_{\alpha}. \tag{36}$$

Here $\hat{I}_{\alpha}$ is the current operator given by Eq. (5). The fluxes ϕ_{α} have the property that they act only on the carriers in reservoir α. The fluxes ϕ_{α} are linearly related to the fluxes penetrating the loops of the external circuit to which the mesoscopic sample is connected.[25] It is assumed that the mesoscopic sample itself is shielded from any effect of these fluxes. A second energy which also gives the desired response corresponds to a sample connected to an external circuit with infinite impedance. In this case each reservoir is taken to be a macroscopic entity which is closed, except for a narrow opening through which it connects to a lead of the sample. We can then define the charge $\hat{Q}_{\alpha}$ on such a reservoir. The voltage V_{α} of the reservoir can be made to oscillate by coupling capacitively to an external circuit. In this case the energy of the perturbation is

$$H_1^{V} = \sum_{\alpha} \hat{Q}_{\alpha} V_{\alpha}. \tag{37}$$

A linear response calculation using the analytic properties of the scattering matrices leads to $G_{\alpha\beta}(\omega) = \langle \delta I_{\alpha}(\omega) \rangle / \delta V_{\alpha}(\omega)$ given by[25]

$$G_{\alpha\beta}(\omega) = \frac{e^2}{h} \int dE \ \mathrm{Tr}[\mathbf{1}_{\alpha} - \mathbf{s}_{\alpha\beta}^{\dagger}(E)\mathbf{s}_{\alpha\beta}(E+\hbar\omega)] \frac{(f(E) - f(E+\hbar\omega))}{\hbar\omega}. \tag{38}$$

The real part of this conductance obeys the fluctuation dissipation theorem stated above. In the zero-frequency limit Eq. (38) leads to the dc-conductances Eqs. (13) and (14). This clearly shows that the dc-conductances are not a consequence of acceleration of carriers due to an electric field inside the sample.

Let us next discuss the low-frequency expansion of this result. To first order in frequency we find from Eq. (38)

$$G_{\alpha\beta}(\omega) = G_{\alpha\beta}(0) - i\omega e^2 \int dE (dN_{\alpha\beta}/dE)(-df/dE) \tag{39}$$

where

$$\frac{dN_{\alpha\beta}}{dE}=\frac{1}{4\pi i}\,\mathrm{Tr}\left[\mathbf{s}^{\dagger}_{\alpha\beta}(E)\,\frac{d\mathbf{s}_{\alpha\beta}(E)}{dE}-\frac{d\mathbf{s}^{\dagger}_{\alpha\beta}(E)}{dE}\,\mathbf{s}_{\alpha\beta}(E)\right] \tag{40}$$

is called a *global partial* density of states. It is called global since it relates to a density of states in an entire volume Ω that encloses the mesoscopic conductor and a large portion of the reservoirs. Later we will also introduce local densities of states. It is called a partial density of states since the total global density of states inside Ω is given by the sum of all partial densities of states, $dN/dE=\Sigma_{\alpha\beta}dN_{\alpha\beta}/dE$. The global partial density of states $dN_{\alpha\beta}/dE$ is obviously the change of charge in the sample brought about by the perturbation in contact β which contributes to the ac-current in contact α. Thus like the scattering matrix $\mathbf{s}_{\alpha\beta}$ represents a preselection of carriers (incident from β) and a post selection (exiting into contact α) so similarly the global partial density of states represent both a pre- and postselection. We should emphasize that the partial densities of states are not density of states in the usual sense. In fact $dN_{\alpha\beta}/dE$, unlike dN/dE is not necessarily a positive quantity.

The total charge injected into the volume Ω by the perturbation in probe β is $\Sigma_{\alpha}dN_{\alpha\beta}/dE$. In a metallic sample which likes to be locally charge neutral, such an addition of charge is unrealistic. Below we discuss systems with interactions, which make charge accumulation or depletion energetically costly. Before discussing such a self-consistent scheme, we discuss now the response to an oscillating electrostatic potential.

B. Internal response

Consider a time-dependent electric potential $U(\mathbf{r},t)$ which represents a small deviation away from the equilibrium electrostatic potential $U_{\mathrm{eq}}(\mathbf{r})$ of the conductor. We assume that the total potential is of the form $U(\mathbf{r},t)=U_{\mathrm{eq}}(\mathbf{r})+u(\mathbf{r})(U_{+\omega}\exp(-i\omega t)+U_{-\omega}\exp(i\omega t))$ where $u(\mathbf{r})$ is a dimensionless function which determines the spatial distribution of the potential away from its equilibrium value. Since the potential is real we have $U_{+\omega}=U^{*}_{-\omega}$. Scattering theory now leads to the following picture. Particles which are incident from a reservoir at energy E in the presence of such an oscillating potential can absorb a modulation quantum $\hbar\omega$ or emit a modulation quantum $\hbar\omega$ or can have their energy unchanged. Thus the reflected and transmitted carriers will emerge not only at the energy E but also with energies $E\pm\hbar\omega$. We cannot describe this scattering problem with the scattering matrix which we have used so far. Now we must introduce the scattering amplitudes $s_{\pm\alpha\beta mn}(E\pm\hbar\omega,E)U_{\pm\omega}$ which give the probability amplitude that a carrier incident in probe β in channel n with energy E leaves the conductor in probe α in channel m with energy $E\pm\hbar\omega$. In the next step we express the operators $\hat{b}(E)$ which annihilate outcoming carriers in terms of the $\hat{a}$ operators at energy $E,E+\hbar\omega$ and $E-\hbar\omega$ with the help of the original scattering matrix and with the help of the scattering amplitudes $s_{\pm\alpha\beta}(E\pm\hbar\omega,E)U_{\pm\omega}$. We use again the current operator Eq. (5) and use the statistical properties of the a operators valid for an equilibrium reservoir. This gives rise to a current at contact α which is given by an internal conductance $G^{i}_{\alpha}(\omega)=\langle dI_{\alpha}(\omega)\rangle/dU_{+\omega}$,

$$G^{i}_{\alpha}(\omega)=-\frac{e^2}{h}\int dE\sum_{\beta}\;\mathrm{Tr}[\mathbf{s}^{\dagger}_{\alpha\beta}(E)\mathbf{s}_{+\alpha\beta}(E+\hbar\omega,E)](f(E)-f(E+\hbar\omega)). \tag{41}$$

To proceed, we need to specify the amplitude $\mathbf{s}_{+\alpha\beta}(E+\hbar\omega,E)$. Unfortunately, little is known about this scattering matrix, except some solutions for particularly simple problems. However, in the limit of small frequencies, on which we concentrate below, the general solution is known. For small frequencies the particles see the instantaneous potential. Therefore, this amplitude can be found by replacing in the ordinary scattering matrix $\mathbf{s}_{\alpha\beta}(E,U_{\mathrm{eq}}(\mathbf{r}))$ the equilibrium potential by the actual potential $U(\mathbf{r},t)$ and by expanding the time-dependent matrix in the deviations away from the equilibrium potential. This gives

$$\lim_{\omega\to 0} \mathbf{s}_{+\,\alpha\beta}(E+\hbar\omega,E) = \int d^3r(\delta\mathbf{s}_{\alpha\beta}(E,U(\mathbf{r}))/\delta U(\mathbf{r}))u(\mathbf{r}). \tag{42}$$

Consequently, to first order in ω the low frequency response to an nonuniform potential is determined by[64]

$$G^i_\alpha(\omega) = ie^2\omega \int d^3r(dn(\alpha,\mathbf{r})/dE)u(\mathbf{r}). \tag{43}$$

Here $dn(\alpha,\mathbf{r})dE$ is a *local partial* density of states which we call the emissivity of point $\mathbf{r}$ into contact α,

$$dn(\alpha,\mathbf{r})/dE = -\frac{1}{4\pi i}\sum_\beta \mathrm{Tr}\left[\mathbf{s}^\dagger_{\alpha\beta}\frac{\delta\mathbf{s}_{\alpha\beta}}{e\,\delta U(\mathbf{r})} - \frac{\delta\mathbf{s}^\dagger_{\alpha\beta}}{e\,\delta U(\mathbf{r})}\mathbf{s}_{\alpha\beta}\right]. \tag{44}$$

Note that the emissivity is obtained by finding the variation of the scattering matrix in response to small changes of the (equilibrium) potential. Note also that the emissivity only invokes a postselection. The contact through which carriers enter is immaterial, only the contact through which the carriers leave the sample matters.

Evidently, there is a closely related local partial density of states, which we call the *injectivity* of contact β into point $\mathbf{r}$. The injectivity[26] is obtained by summing over the first index of the scattering matrices and is given by

$$dn(\mathbf{r},\beta)/dE = -\frac{1}{4\pi i}\sum_\alpha \mathrm{Tr}\left[\mathbf{s}^\dagger_{\alpha\beta}\frac{\delta\mathbf{s}_{\alpha\beta}}{e\,\delta U(\mathbf{r})} - \frac{\delta\mathbf{s}^\dagger_{\alpha\beta}}{e\,\delta U(\mathbf{r})}\mathbf{s}_{\alpha\beta}\right]. \tag{45}$$

The sum over either all the injectivities or all the emissivities is equal to the local density of states, $dn(\mathbf{r})/dE = \Sigma_\alpha dn(\mathbf{r},\alpha)/dE = \Sigma_\alpha dn(\omega,\mathbf{r})/dE$. In contrast to the partial density of states with both a pre- and post-selection the injectivities and emissivities are positive. In fact the injectivity is related to the time a carrier dwells[65] in a small region around the point $\mathbf{r}$. The dwell time $d\tau(\mathbf{r},\alpha)$ near $\mathbf{r}$ for carriers incident from contact α is given by $d\tau(\mathbf{r},\alpha) = \hbar(dn(\mathbf{r},\alpha)/dE)d^3r$. But the dwell time is directly related to the absolute square of the wave functions at point $\mathbf{r}$. Hence the injectivity can also be expressed in terms of the scattering states as[64,66]

$$dn(\mathbf{r},\alpha)/dE = \sum_{\alpha m}(1/hv_{\alpha m})|\Psi_{\alpha m}(\mathbf{r})|^2. \tag{46}$$

Using the microreversibility of the scattering matrix, we see that there is a connection between the injectivity and emissivity, $dn_{+B}(\mathbf{r},\alpha)/dE = dn_{-B}(\alpha,\mathbf{r})/dE$. The injectivity from contact α into point $\mathbf{r}$ in positive a magnetic field B is equal to the emissivity from $\mathbf{r}$ into contact α in a magnetic field pointing into the opposite direction. A detailed discussion of possible decompositions of the local density of states and their relationship to Green's functions is presented elsewhere.[66]

To complete the discussion of the ac-conductance, we must next develop a self-consistent theory of the potential $U(\mathbf{r},\omega)$. We notice that to liner order in ω it is sufficient to develop a self-consistent theory of the potential to the zero-th order in frequency for the potential $U(\mathbf{r},\omega)$ since the response given by Eq. (43) is already proportional to ω.

C. Self-consistent potentials

The electrostatic potential $U([\mu_\alpha],\mathbf{r})$ for mesoscopic conductors is a function of the electrochemical potentials $[\mu_\alpha]$ of the contacts, and a complicated function of position. Small increases in the electrochemical potentials $\delta\mu_\alpha$ bring the conductor to a new state (see Fig. 4) with an elec-

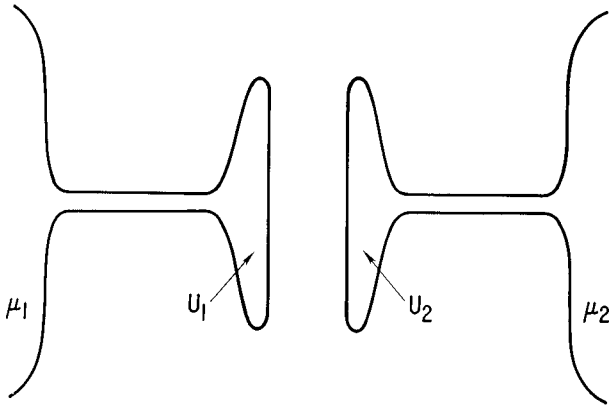

FIG. 3. Mesoscopic capacitor: Two small plates are via leads connected to electron reservoirs at electrochemical potentials μ_1 and μ_2. After Ref. 34.

trostatic potential $U([\mu_\alpha+\delta\mu_\alpha],\mathbf{r})$. The difference δU between these two potentials can be expanded in powers of the increment in the electrochemical potential. To linear order we have

$$e\,\delta U([|\mu_\alpha],\mathbf{r})=\sum_\alpha u_\alpha(\mathbf{r})\,\delta\mu_\alpha. \tag{47}$$

Here, $u_\alpha(\mathbf{r}) = e\partial U([\mu_\alpha],\mathbf{r})/\partial\mu_\alpha|_{\mu_\alpha=\mu_0}$ are the *characteristic potentials*[26] which determine the electrostatic potential inside the sample in response to a variation of an electrochemical potential μ_α at a contact. For the case of a mesoscopic capacitor [see Fig. 3] the electrochemical and the electrostatic potentials and the characteristic function u_1 are shown in Fig. 4.

Suppose for a moment that we increase all electrochemical potentials simultaneously and by the same amount, $\delta\mu_\alpha\equiv\delta\mu$. Both before and after the change the conductor is at equilibrium, hence the physical properties of the conductor remain unchanged. Consequently, the shift of the electrochemical potentials must be accompanied by a shift $e\,\delta U\equiv\delta\mu$ of the electrical potential. This implies that the sum of all characteristic potentials is equal to one at every space point,[26]

$$\sum_\alpha u_\alpha(\mathbf{r})\equiv 1. \tag{48}$$

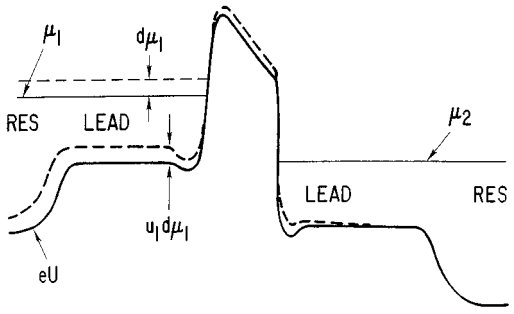

FIG. 4. Electrochemical potentials and electrostatic potentials of the mesoscopic capacitor at μ_1 and μ_2 (solid lines) and at $\mu_1+d\mu_1$ and μ_2 (broken lines). u_1 is the characteristic potential function of contact 1. After Ref. 26.

Equation (48) is a consequence of the long-range Coulomb interaction. The conservation of charge under the application of a dc or ac bias and the conservation of current are a consequence of Eq. (48).

Let us now return to our original problem and consider what happens if we increase just one electrochemical potential, say in reservoir α, by $\delta\mu_\alpha$. Obviously, the condition that the electrochemical potential and the electrostatic potential move in synchronism deep inside reservoir α implies that the characteristic function $u_\alpha(\mathbf{r})=1$ for $\mathbf{r}$ deep inside reservoir α. This implies that Eqs. (13) and (14) are valid if and only if the characteristic potentials have the property that $u_\alpha(\mathbf{r})=1$ for $\mathbf{r}$ deep in contact α and $u_\alpha(\mathbf{r})=0$ for $\mathbf{r}$ deep in any other contact.

The electrostatic potentials are determined by the charge distribution in the sample. As we increase the chemical potential of contact α *keeping the electrostatic potentials fixed*, the additional charge $\delta n(\mathbf{r})=(dn(\mathbf{r},\alpha)/dE)\,\delta\mu_\alpha$ enters the conductor. Here, $dn(\mathbf{r},\alpha)/dE$ is the *injectivity* of contact α into point $\mathbf{r}$ of the sample. The injected charges induce a change in the electrostatic potential which in turn implies an induced contribution $\delta n_{\rm ind}$ to the density. The total charge density is

$$\delta n(\mathbf{r})=(dn(\mathbf{r},\alpha)/dE)\,\delta\mu_\alpha+\delta n_{\rm ind}(\mathbf{r}). \tag{49}$$

The induced charge density is connected to the electrostatic potential via the response function $\Pi(\mathbf{r},\mathbf{r}')$ (Lindhard function or polarization function), $\delta n_{\rm ind}(\mathbf{r})=-\int d^3r'\,\Pi(\mathbf{r},\mathbf{r}')e\,\delta U(\mathbf{r}')$. The response function can be expressed in terms of the scattering states[67] (Green's function of the Schrödinger equation). For the purpose of our discussion we simply assume that this response has been calculated and is known. By inserting Eq. (49) into Poisson's equation and using $e\,\delta U(\mathbf{r})=u_\alpha(\mathbf{r})\,\delta\mu_\alpha$, we find that the characteristic potential $u_\alpha(\mathbf{r})$ is the solution of a field equation with a non-local screening kernel and a source term given by the *injectivity* of contact α,

$$-\Delta u_\alpha(\mathbf{r})+4\pi e^2\int d^3r'\,\Pi(\mathbf{r},\mathbf{r}')u_\alpha(\mathbf{r}')=4\pi e^2(dn(\mathbf{r},\alpha)/dE). \tag{50}$$

We define the Green's function $g(\mathbf{r},\mathbf{r}_0)$ as the solution of Eq. (50) with the source term $e\,dn(\mathbf{r},\alpha)/dE$ replaced by a localized test charge $e\,\delta(\mathbf{r}-\mathbf{r}_0)$ at point $\mathbf{r}_0$. The characteristic potential $u_\alpha(\mathbf{r})$ can then be written in the form

$$u_\alpha(\mathbf{r})=\int d^3r'\,g(\mathbf{r},\mathbf{r}')(dn(\mathbf{r}',\alpha)/dE). \tag{51}$$

Using Eq. (48) a summation over α implies for Green's function the property[26]

$$\int d^3r'\,g(\mathbf{r},\mathbf{r}')\sum_\alpha\,(dn(\mathbf{r}',\alpha)/dE)=\int d^3r'\,g(\mathbf{r},\mathbf{r}')(dn(\mathbf{r}')/dE)\equiv 1. \tag{52}$$

The same relationship follows from the condition that the sum of all induced charge densities plus the test charge is zero.

Now we find the condition for the electrical self-consistency of Eqs. (13) and (14). According to Eq. (52) the characteristic potential is equal to unity if the Green's function is convoluted with the total local density of states. Therefore, in order that the characteristic function $u_\alpha(\mathbf{r})$ is equal to one in reservoir α, we must have that the injectivity $dn(\mathbf{r},\alpha)/dE$ deep in contact α is equal to the local density of states $dn(\mathbf{r})/dE$. This requires that nearly all (in a thermodynamic sense) electrons approaching the contact α are reflected back into the reservoir. If the conductor and the reservoir consist of the same material then the reservoir, as emphasized by Landauer[68] must be wide compared to the mesoscopic conductor. In semiconductor samples with metallic contacts, on the other hand, the contact might be actually narrow compared to the dimensions of the semiconductor

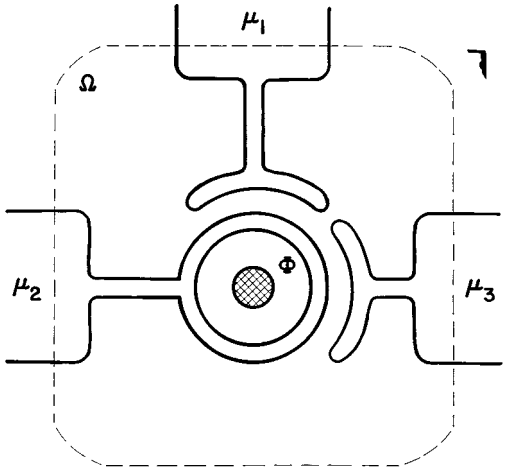

FIG. 5. Purely capacitive arrangement of conductors. The Aharonov–Bohm flux Φ threading the ring leads to oscillations in the capacitance coefficients. After Ref. 69.

since the density of states at the Fermi energy of the metal is much larger then that of the semiconductor. This is the case, for instance, in Ga/As samples used to measure the quantized Hall effect.[3] In any case, this discussion clearly implies, that one cannot attribute a conductance to a one-dimensional wire without contacts.

D. Capacitance and emittance of mesoscopic conductors

The total response is the sum of the external response Eq. (39) and the internal response Eq. (43), $G_{\alpha\beta}(\omega)=G^e_{\alpha\beta}(\omega)+G^i_{\alpha\beta}$. We express it in the form

$$G_{\alpha\beta}(\omega)=G_{\alpha\beta}(0)-i\omega E_{\alpha\beta}+O(\omega^2) \tag{53}$$

and call $E_{\alpha\beta}$ the (screened) *emittance* of the conductor. It is given by[26]

$$E_{\alpha\beta}=e^2\frac{dN_{\alpha\beta}}{dE}-e^2\int d^3r\int d^3r'\,\frac{dn(\alpha,\mathbf{r})}{dE}\,g(\mathbf{r},\mathbf{r}')\,\frac{dn(\mathbf{r}',\beta)}{dE}. \tag{54}$$

It is important to notice that Eq. (54) applies not only to one conductor but in fact also applies if there are several nearby conductors which interact via long-range Coulomb forces. The variable α then runs not only over the contacts of one conductor but over all contacts of all nearby electrical conductors. In particular it also applies if we bring two (or more) conductors near each other without any transmission between them (see Fig. 3 and Fig. 5). In this case, the scattering matrix consists only of reflection matrices $\mathbf{s}_{\alpha\alpha}$. The transmission matrices $\mathbf{s}_{\alpha\beta}$ with $\alpha\neq\beta$ vanish and all emittance coefficients are capacitive $E_{\alpha\beta}\equiv C_{\alpha\beta}$. All capacitance coefficients are even functions of the Aharonov–Bohm flux.[26,69] In contrast to the expressions for the capacitance we know from text books, the microscopic expression given here takes into account that the electric field penetrates the distance of a screening length into the two conductors. As a consequence the capacitance is not a purely geometrical quantity but depends on the physical properties of the conductors. The field penetration into the conductor gives rise to quantum corrections to the capacitance. In models in which the potential is taken to be piecewise constant[33–35,41] these corrections are determined by the density of states at the surfaces of the two conductors. This has interesting consequences: For the case were one of the plates has the form of a ring with an Aharonov–Bohm flux

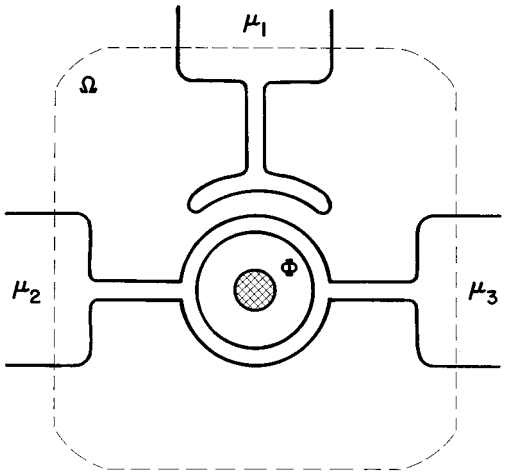

FIG. 6. An Aharonov–Bohm ring connected to two contacts, and capacitively coupled to an other nearby conductor. For a ballistic ring some emittance elements are not capacitive but inductive. After Ref. 69.

through the hole of the ring the density of states is a periodic function of flux and consequently also the capacitance is a periodic function of the Aharonov–Bohm flux.[69,70]

If one of the conductors is connected to two or more contacts (see Fig. 6) the emittance tensor is not purely capacitive. If the conductor permits good transmission, some elements of the emittance acquire a sign that is opposite to that expected for a capacitance tensor. This is reminiscent of inductive behavior. Furthermore, it can be shown[26] and has been experimentally verified[5] that for such a general arrangement the emittance tensor elements are not even functions of flux (magnetic field) but obey the reciprocity relation $E_{\alpha\beta}(\Phi)=E_{\beta\alpha}(-\Phi)$.

We emphasize that the emittance tensor is current and charge conserving. The rows and columns of the emittance matrix add up to zero. Consider the case of a conductor with two contacts. Consider the first column. If we add E_{11} and E_{21} the first terms in the emittance give the total charge $dN_{11}/dE+dN_{21}/dE$ injected from contact 1. In the second term the two emissivities add to give the local density of states. Now Eq. (52) is used. What remains is the integral over the entire volume of the injectivity which is just the total injected charge. Thus for a two terminal conductor in electrical isolation the emittance matrix satisfies $E_\mu \equiv E_{11}=-E_{12}=-E_{21}=E_{22}$. Thus the dynamical conductance matrix $G_{\alpha\beta}$ where the two indices now run over all contacts of all nearby conductors obeys the same ''sum rules,'' Eq. (15), that we found for the dc conductance. We conclude by giving two examples. Consider a uniform ballistic conductor connecting two reservoirs. Assume that contact effects can be neglected and determine the potential from a condition of local charge neutrality. It is found that the emittance is inductive (negative). The emittance is 1/4 of the density of states of the ballistic wire,[35]

$$E_\mu=-(1/4)e^2 dN/dE. \tag{55}$$

In contrast, the ensemble averaged emittance of a metallic diffusive wire is found to be capacitive and is determined by 1/6 of the total density of states,[35]

$$\langle E_\mu\rangle_e=(1/6)e^2\langle dN/dE\rangle_e. \tag{56}$$

Since the total unscreened density of states which is available to carriers from one contact is $1/2\langle dN/dE\rangle$ this corresponds (in magnitude) to a reduction factor of 1/3 similar to the reduction of the shot noise below the full Poisson result.

VI. FLUCTUATIONS OF A MESOSCOPIC CAPACITOR

In this section we derive an expression for the conductance of a mesoscopic capacitor (see Fig. 3) valid up to second order in frequency. To linear order in frequency the current response is $\langle I(\omega)\rangle = -i\omega C_\mu$, where C_μ is the electrochemical capacitance. To second order in frequency the response of a capacitor with resistances in series[34,71] is determined by the product of the capacitance and a relaxation time $R_q C_\mu$. Since we know the electrochemical capacitance the second order term determines the charge relaxation resistance R_q. With the electrochemical capacitance and the charge relaxation resistance the conductance of the capacitor is to second order in frequency

$$G(\omega) = -i\omega C_\mu + \omega^2 C_\mu^2 R_q . \tag{57}$$

We want to determine the charge relaxation resistance. One way to proceed is to generalize the discussion of the conductance. This requires us to determine the potential $U(\mathbf{r},\omega)$ to first order in frequency. Thus a dynamic screening theory is needed. An alternative way to determine this resistance is to find the current-current fluctuations to second order in frequency, and to use the fluctuation–dissipation theorem. This, as we will show, permits us to use again the (fluctuating) quasistatic potential. We chose this second approach.

The key point of our discussion is again to achieve a current and charge conserving result. A thermally induced fluctuation which leads to an increase of the charge on one capacitor plate must lead to a decrease of an equal amount of charge on the other capacitor plate. The long range Coulomb interaction completely correlates the charge fluctuations on the two plates. Consider first the charge fluctuations of the capacitor with the potential held fixed at its equilibrium value. These charge fluctuations can be found from the Fermi field operator.[23] For the local density operator we find quite generally,

$$\hat{n}(\mathbf{r},\omega) = \sum_{\alpha\beta nm} dE (h v_{\alpha n}(E))^{-1/2} (h v_{\beta m}(E+\hbar\omega))^{-1/2} \Psi^*_{\alpha n}(\mathbf{r},E)\Psi_{\beta m}(\mathbf{r},E+\hbar\omega)\hat{a}^\dagger_{\alpha n}(E) \times \hat{a}_{\beta m}(E+h\omega). \tag{58}$$

Now what counts are the deviation of this ''density'' away from the equilibrium value. Therefore, we substitute this density into the Poisson equation. The Poisson equation is now an operator equation. For each pair $\hat{a}^\dagger_{\alpha n}(E)\hat{a}_{\beta m}(E+\hbar\omega)$ there exists a potential operator $\hat{u}_{\alpha\beta nm}$. We introduce a potential operator $\hat{u}_{\alpha\beta}$ which is the sum of $\hat{u}_{\alpha\beta nm}$ over all channels in contact α and β. We can write this operator with the help of a nondiagonal density of states matrix. In the zero-frequency limit which is of interest here, this matrix is

$$d\mathbf{n}_{\gamma\delta}(\mathbf{r})/dE = -(1/4\pi i)\sum_\beta (\mathbf{s}^\dagger_{\beta\gamma}(\delta\mathbf{s}_{\beta\delta}/e\,\delta U(x)) - (\delta\mathbf{s}^\dagger_{\beta\gamma}/e\,\delta U(x))\mathbf{s}_{\beta\delta}) \tag{59}$$

with elements

$$dn_{\gamma\delta mn}(\mathbf{r})/dE = \sum_{mn} (h v_{\gamma n}(E))^{-1/2} (h v_{\delta m}(E))^{-1/2} \Psi^*_{\gamma n}(\mathbf{r},E)\Psi_{\delta m}(\mathbf{r},E). \tag{60}$$

Thus the potential operator is given by

$$\hat{u}_{\alpha\beta}(\mathbf{r}) = \int d^3r'\, g(\mathbf{r},\mathbf{r}')\hat{\mathbf{a}}^\dagger_\alpha(E)[d\mathbf{n}_{\alpha\beta}(\mathbf{r}')/dE]\hat{\mathbf{a}}_\beta(E). \tag{61}$$

So far we have been completely general. Now we consider the mesoscopic capacitor shown in Fig. 3. There is no transmission. We have only two contacts α=1,2. Thus it is only the diagonal

matrices $d\mathbf{n}_{\alpha\alpha}(\mathbf{r})/dE$ which are non-vanishing. Since the scattering matrix is unitary for each conductor separately, the expression for this matrix can be simplified, $d\mathbf{n}_{\gamma\gamma}(\mathbf{r})/dE = -(1/2\pi i)\mathbf{s}^{\dagger}_{\gamma\gamma}(\delta\mathbf{s}_{\gamma\gamma}/e\,\delta U(x))$. Next we expand the particle–current operator to first order in frequency. We find

$$\hat{I}_{\alpha}(\omega) = -ie\omega \int dE \hat{\mathbf{a}}^{\dagger}_{\alpha}(E)(d\mathbf{N}_{\alpha\alpha}(\alpha)/dE)\hat{\mathbf{a}}_{\alpha}(E), \tag{62}$$

$$d\mathbf{N}_{\alpha\alpha}(\alpha)/dE = (1/2\pi i)\mathbf{s}^{\dagger}_{\alpha\alpha}(E)(d\mathbf{s}_{\alpha\alpha}/dE). \tag{63}$$

The fluctuations in the potential give rise to an induced current. In response to a classical potential we found $I_{\alpha}(\omega) = ie^2\omega\int d^3r(dn(\alpha,\mathbf{r})/dE)u(\mathbf{r})$ [see Eq. (43)]. Now we need an operator expression. In the Hartree approach treated here we can replace the classical potential by the quantum operator potential. Thus the induced current is now

$$\hat{I}_{\alpha}(\omega) = ie^2\omega \int d^3r(dn(\alpha,\mathbf{r})/dE)\sum_{\gamma} \hat{u}_{\gamma\gamma}(\mathbf{r}). \tag{64}$$

The total current can be expressed with the help of a screened density of states matrix

$$\mathbf{D}_{\gamma\gamma}(\alpha) = \left[\delta_{\alpha\gamma}(d\mathbf{N}_{\gamma\gamma}/dE) - \int d^3r d^3r'(dn(\alpha,\mathbf{r})/dE)g(\mathbf{r},\mathbf{r}')(d\mathbf{n}_{\gamma\gamma}(\mathbf{r}')/dE)\right], \tag{65}$$

in the following simple form

$$\hat{I}_{\alpha}(\omega) = -ie\omega \int dE \sum_{\gamma} \hat{\mathbf{a}}^{\dagger}_{\gamma}(E)\mathbf{D}_{\gamma\gamma}(\alpha)\hat{\mathbf{a}}_{\gamma}(E). \tag{66}$$

It is seen immediately that we have achieved current conservation. The sum $\hat{I}_1(\omega)+\hat{I}_2(\omega)$ vanishes identically since $\int d^3r(dn(\mathbf{r})/dE)g(\mathbf{r},\mathbf{r}')$ is one at every point $\mathbf{r}'$ and since $\int d^3r'(\delta s_{\beta\delta}/e\,\delta U(x)) = -(ds_{\beta\delta}/dE)$. As a consequence we have $\mathbf{D}_{\gamma\gamma}(1)+\mathbf{D}_{\gamma\gamma}(2)=0$. Evaluating the fluctuations and writing the result in the form

$$\langle(\Delta I)^2\rangle = 2kT\Delta\nu\omega^2 C_{\mu}^2 R_q \tag{67}$$

determines the charge relaxation resistance. The electrochemical capacitance is the trace of the effective screened density of states operator,

$$C_{\mu} = e^2 \int dE(-df/dE)\mathrm{Tr}[\mathbf{D}], \tag{68}$$

where $\mathrm{Tr}[\mathbf{D}]=\mathrm{Tr}[\mathbf{D}_{11}(1)]=\mathrm{Tr}[\mathbf{D}_{22}(2)]=-\mathrm{Tr}[\mathbf{D}_{11}(2)]=-\mathrm{Tr}[\mathbf{D}_{22}(1)]$. The charge relaxation resistance is

$$R_q = \left(\frac{h}{e^2}\right)\frac{\int dE(-df/dE)\Sigma_{\gamma}\,\mathrm{Tr}[\mathbf{D}^{\dagger}_{\gamma\gamma}(\alpha)\mathbf{D}_{\gamma\gamma}(\alpha)]}{(\int dE(-df/dE)\mathrm{Tr}[\mathbf{D}])^2}. \tag{69}$$

Note that in the expression for the charge relaxation resistance α can be taken to be either 1 or 2. Equation (69) which expresses the capacitance as a trace of an effective density of states is identical to the result that one obtains from the emittance matrix Eq. (54). Equation (69) is a microscopic expression of the charge relaxation resistance given in Ref. 34 for the case of a discrete potential model. The charge relaxation resistance is inversely proportional to the number of channels which contribute to the density of states. Thus a measurement of this resistance can be carried out best by changing the number of channels for instance with the help of a magnetic field.

We can also understand the capacitance and the charge relaxation resistance in terms of the time a carrier is *dwelling* in the region of the surface over which the electric field penetrates into the conductors. For noninteracting carriers the dwell time in a volume is the integrated particle

density in this volume divided by the incident current.[65] Here we extend this consideration and take the dwell time to be the integrated charge density on a capacitor plate divided by the current at the contact of that plate. The average time a carrier dwells on either one of the plates (at $kT=0$) is $\langle\tau\rangle=h\ \mathrm{Tr}[\mathbf{D}]$. Thus the capacitance is simply $C_\mu=e^2\langle\tau\rangle/h$. Now we see that the charge relaxation resistance is related to the mean square dwell time divided by the average dwell time squared, $R_q=(e^2/h)\langle\tau^2\rangle/\langle\tau\rangle^2$. Note that these times are ultimately determined by functional derivatives (potential derivatives) of the scattering matrix rather then energy derivatives. We also note that the dwell time is the same on either plate, in contrast to the dwell times one obtains by analyzing an unscreened free electron problem. This shows clearly that one cannot apply uncritically concepts of dwell or tunneling times obtained for noninteracting particles to electrical conductors. The electrical relaxation time is the RC time. From the definition of the dwell time given above we find that the RC time is the ratio of the mean square dwell time divided by the mean dwell time, $\tau_{\mathrm{RC}}=\langle\tau^2\rangle/\langle\tau\rangle$.

VII. CONCLUSION

In this article we have discussed expressions for the dc conductance, the ac conductance and the spectral densities for the current and charge fluctuations. We have used a common mathematical framework. Starting from expressions in which the internal potential is held fixed, we have used a self-consistent scheme to obtain ac conductance and frequency-dependent noise spectra which are charge and current conserving. In fact the structure of these results suggests that a self-consistent ac-theory or frequency-dependent spectrum has exactly the same form as that found for the case of a fixed internal potential, except that the current matrix A needs to be replaced by a more complicated self-consistent expression A^{eff}. To show this with more generality then was done here, is clearly a worthwhile task.

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Transport properties in resonant tunneling heterostructures

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An adiabatic approximation in terms of instantaneous resonances to study the steady-state and time-dependent transport properties of interacting electrons in biased resonant tunneling heterostructures is used. This approach leads, in a natural way, to a transport model of large applicability consisting of reservoirs coupled to regions where the system is described by a nonlinear Schrödinger equation. From the mathematical point of view, this work is nonrigorous but may offer some fresh and interesting problems involving semiclassical approximation, adiabatic theory, nonlinear Schrödinger equations, and dynamical systems. © *1996 American Institute of Physics.* [S0022-2488(96)00510-5]

I. INTRODUCTION

Man-tailored semiconductor heterostructures[1] offer, for the first time, the possibility to test quantum mechanics at a mesoscopic level.[2] The scenario of systems which can be investigated is so rich that the art of their realization deserves the name of quantum design.

In the simplest case, a quantum designer can grow sandwiches of different semiconductor alloys by choosing the number of atomic layers for each kind of alloy. In the resulting heterostructure, the conduction band profile along the growth direction forms steps whose height can be continuously varied by a proper choice of the alloy composition. Typical widths and heights are of the order of tens of Å and tenths of eV, respectively.

At low temperature, the mean free path of carriers for scattering from crystal impurities is of the order of 10^4 Å, and for heterostructures smaller than this size the electric transport along the growth direction is phase coherent quantum scattering from the conduction band discontinuities.[3] Due to the translational invariance in the plane orthogonal to the growth direction, the problem is one-dimensional. Moreover, the carriers are described by an effective mass which accounts for the microscopic scattering with the periodic crystal sites, and their wave function is an envelope wave function.[4]

In a homogeneous neutral conductor, the electron–electron interaction can be taken into account by a renormalization of the carrier effective masses[5] and one deals with a transport problem like in a noninteracting case. In a heterostructure, even as simple as that described above, the breaking of translational invariance in the transport direction allows the electric neutrality to be locally violated. The corresponding interaction potential, obtained, at Hartree level, by solving a proper Poisson equation, can strongly modify the transport properties. The example of a double barrier heterostructure with the exterior regions doped with donors is illuminating.[6] Due to tunneling, electrons populate the resonance(s) created by the double barrier and the region between the barriers becomes negatively charged. This generates an electric potential which decreases the

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tunneling probability of electrons in the double barrier region. As a consequence, current oscillations on the picosecond scale[7,8] and chaotic behavior without classical counterpart[9] have been predicted in a ballistic configuration in which electrons are injected at some chosen energy.

Experiments with ballistic electrons are difficult, and measurements became available only recently.[10] Technologically simpler is the case of biased heterostructures where transport is due to the presence of reservoirs at thermal equilibrium with different chemical potentials. Manifestations of the electron–electron interaction are known also in this configuration. For example, hysteresis in the current–voltage characteristics of double barrier heterostructures have been observed[11] and recognized as a consequence of the accumulation of electrons in the resonance.[11–15] In this case, however, one has the theoretical problem of attaching reservoirs at thermal equilibrium to a piece of conductor where quantum coherent transport takes place.

In the recent paper[16] we proposed an approach to this problem based on a mathematical method earlier applied in the framework of ballistic transport.[17] We showed that for heterostructures with a single resonance our approach allows one (i) to obtain steady-state voltage–current characteristics having hysteresis or not in agreement with the experimental results[18] and (ii) to predict time-dependent properties analogous to those studied in optically bistable systems.[19] Here, we develop the general mathematical scheme of this approach and discuss the case with several resonances where multistability phenomena can take place as in superlattices.[20,21]

For simplicity, consider the one-dimensional double barrier heterostructure discussed above. The idea is that due to the presence of resonances the corresponding Schrödinger problem can be divided in two parts: a Schrödinger equation for the barrier region and one for the exterior space, the two being weakly coupled by tunneling. This decomposition corresponds to the schematization of the transport process as a coherent process fed by reservoirs. In the exterior space (reservoirs), homogeneous and neutral, the electron–electron interaction is neglected and thermal equilibrium is taken into account by considering a continuous set of energy eigenstates distributed according to Fermi statistics. In the barrier region (coherent conductor), the Coulomb interaction is included in a self-consistent potential obtained by solving the Poisson equation associated with the local charge density. Under the assumption that the barriers are wide enough, the corresponding nonlinear Schrödinger problem is discussed in two steps. In the first step we eliminate the potential well between the two barriers by artificially increasing the potential there, and we solve the Schrödinger equation asymptotically for the new potential by means of WKB-expansions. The resulting solution is then very small near the (filled) potential well, so we get only a small error in the Schrödinger equation when we go back to the true potential. In the second step we correct for this small error by adding a wave function concentrated near the potential well. Assuming *a priori* that the charge in the well changes slowly with time, the correcting wave function can be expected to be large only at energies close to the resonances, and be well approximated by some linear combination of the resonant states.

In most of the article we discuss the case in which only one resonance participates. The validity of this one-mode approximation has been tested numerically with excellent results in the ballistic configuration of Ref. 17. Here, the coefficient of the one-mode approximation obeys an ordinary differential equation with respect to time in the infinite-dimensional space of square integrable functions of energy. We study the stationary points of the corresponding vector field and their nature, whether they are attractive or not, and arrive at quite neat answers. For solutions of the dynamical system which have existed as bounded solutions for a long time and in a suitable asymptotic limit (of wide barriers) we derive a simplified scalar differential equation for the evolution of the sheet density of electrons trapped in the well, which gives a good global understanding of the more complete dynamical system. Using these results, we are able to discuss the phenomenon of hysteresis and we support and illustrate the discussion with several numerical results. The discussion includes the evolution of solutions away from fixed points which necessarily appears when there is hysteresis. We also discuss the case of several resonances and get analogous results.

From the mathematical point of view, the present article could be a starting point for rigorous work on some fresh problems, involving semiclassical analysis, adiabatic theory, nonlinear Schrödinger equations, and dynamical systems. A strong motivation for such an enterprise is the fact that the theory of electric transport in semiconductor devices offers many problems similar to the one we illustrate here.[22]

The plan of the article is as follows. In Sec. II we define the model. In Sec. III we review the WKB expansion for slowly varying potentials. In Secs. IV and V we determine the driving term and the ground resonant state, respectively, within the WKB approximation. The central equation of our article is derived in Sec. VI, and the general properties of the associated fixed points and linearizations are discussed in Sec. VII. In Sec. VIII we introduce an approximation valid in the limit of small resonance width and discuss the corresponding fixed-point solutions and linearizations. In Sec. IX we obtain a simplified differential equation describing the dynamics of the electron density in the well. A qualitative discussion of the hysteresis phenomenon in comparison with numerical results is given in Sec. X. In Sec. XI we finally consider the case with several resonances.

II. DEFINITION OF THE MODEL

Let us consider a heterostructure whose conduction band profile consists of two barriers of height V_0 located in $[a,b]$ and $[c,d]$,

$$V_{\mathrm{cb}}(x)=\begin{cases}0, & x<a\\ V_0, & a<x<b\\ 0, & b<x<c\\ V_0, & c<x<d\\ 0, & x>d\end{cases} \tag{2.1}$$

with $a<b<c<d$ along the growth direction x. We wish to evaluate the transport properties of this device when a bias energy ΔV is applied between the emitter ($x<a$) and collector ($x>d$) regions uniformly doped. Due to doping, the band of conduction electrons formed in the emitter and collector regions is characterized by a Fermi energy $E_F=(3\pi^2 n_D)^{2/3}$, where n_D is the net donor concentration. We will use everywhere effective atomic units $\hbar=2m^*=1$ and $e^2/\epsilon=2a_B^{-1}$, where m^* is the electron effective mass and ϵ the dielectric constant. In these units, every physical quantity is expressed in terms of the effective Bohr radius $a_B=\hbar^2\epsilon/(m^*e^2)$. Assuming an ideal heterostructure homogeneous in the plane yz parallel to the junctions (and orthogonal to the growth direction x), the single-electron momenta k_y and k_z are conserved quantities. As a consequence, the single-electron wave function at energy $E+E_\parallel$, where $E_\parallel=k_y^2+k_z^2$, can be factorized as $\phi(x,t,E)\chi(y,z,t,E_\parallel)$ with

$$\chi(y,z,t,E_\parallel)=\frac{1}{\sqrt{A}}\,e^{i(k_y y+k_z z)}e^{-iE_\parallel t}. \tag{2.2}$$

We will assume periodic boundary conditions in a two-dimensional region A so that the momenta k_y and k_z are quantized as in a real device having finite lateral area of size A. The time-dependent Schrödinger equation for the single-electron wave function at energy E along the x direction is

$$[-i\partial_t-\partial_x^2+V_{\mathrm{cb}}(x)+U(\phi,x)]\phi(x,t,E)=0, \tag{2.3}$$

where $U(\phi,x)$ takes into account the applied bias and, at Hartree level, the electron–electron interaction. Assuming ideal metallic behavior in the emitter and collector regions, i.e., neglecting the formation of accumulation and depletion layers, $U(\phi,x)$ can be obtained as the solution of the Poisson equation

$$\partial_x^2 U(\phi,x) = -8\pi a_B^{-1}\rho(\phi) \tag{2.4}$$

with Dirichlet boundary conditions $U(\phi,a)=0$ and $U(\phi,d)=-\Delta V$. The density ρ takes into account all the electrons in the occupied energy states and depends only on the wave-function component ϕ. Indeed, if the emitter and collector regions are at thermal equilibrium with temperature T we have

$$\rho = 2\int_0^\infty dE \sum_{E_\parallel} |\phi(x,t,E)\chi(y,z,t,E_\parallel)|^2 (1+e^{(E+E_\parallel-E_F)/k_BT})^{-1} = \int dE\ g(E)|\phi(x,t,E)|^2, \tag{2.5}$$

where the factor 2 takes into account the spin degeneracy. Energies are measured from the bottom of the emitter conduction band, and the lower integration bound $E=0$ in the first line of Eq. (2.5) stems from the fact that for $E_F \ll \Delta V$, as we will assume, only electrons from the emitter conduction band can penetrate the region $[a,d]$ where the electron density is of interest. In the second line of Eq. (2.5) this lower bound is absorbed in the definition of $g(E)$ by a Heaviside function $\theta(E)$. The function $g(E)$ can be explicitly evaluated by approximating the sum over the parallel degrees of freedom with an integral

$$\begin{aligned} g(E) &= \theta(E) 2\int_0^\infty dE_\parallel \frac{A}{4\pi}\left|\frac{1}{\sqrt{A}}\right|^2 (1+e^{(E+E_\parallel-E_F)/k_BT})^{-1} \\ &= \theta(E)\,\frac{1}{2\pi}\,[k_BT\,\ln(1+e^{(E-E_F)/k_BT})+E_F-E]. \end{aligned} \tag{2.6}$$

Note that the chemical potential at temperature T in the Fermi function has been approximated with its value at $T=0$, i.e., the Fermi energy determined by the net donor concentration.

In general, the solution of Eq. (2.4) cannot be handled analytically. We will suppose that, due to the accumulation of electrons in the well with sheet density

$$s(\phi) = \int dE\ g(E) \int_{(a+b)/2}^{(c+d)/2} dx |\phi(x,t,E)|^2, \tag{2.7}$$

ideal metallic behavior in the well $[b,c]$ and ideal insulating behavior in the barriers $[a,b]$ and $[c,d]$ hold. This is equivalent to approximate Eq. (2.4) with

$$\partial_x^2 U(\phi,x) = -8\pi a_B^{-1} s(\phi)[B\delta(x-b)+C\delta(x-c)], \quad B+C=1 \tag{2.8}$$

and the condition that $\partial_x U(\phi,x)=0$ for $b<x<c$. In this case $U(\phi,x)$ becomes a piecewise linear function of x with $\partial_x U(\phi,x)$ having jump discontinuities at $x=b$ and $x=c$. The total potential $V_{\rm cb}+U$ in Eq. (2.3) is better rewritten as $V+W$, where

$$V(x) = \begin{cases} 0, & x<a \\ V_0 - \Delta V(x-a)/l, & a<x<b \\ -\Delta V(b-a)/l, & b<x<c \\ V_0 - \Delta V(b-a+x-c)/l, & c<x<d \\ -\Delta V, & x>d \end{cases} \tag{2.9}$$

gives the band profile modified by the external bias and

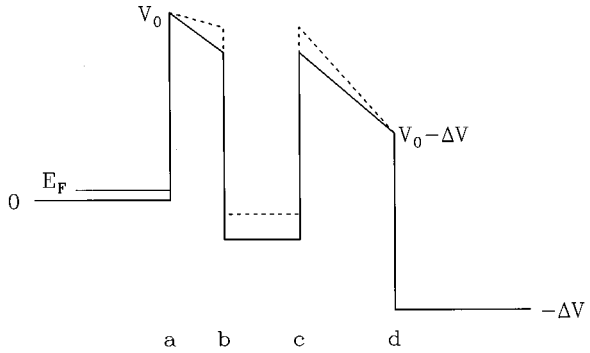

FIG. 1. Potential $V(x)$ representing the band profile modified by the external bias energy ΔV (solid line) and total potential $V(x)+W(s,x)$ including the electrostatic contribution due to electrons trapped in the well with sheet density s (dashed line).

$$W(s,x)=8\pi a_B^{-1}s(\phi)\times\begin{cases}0, & x<a\\ (x-a)(d-c)/l, & a<x<b\\ (b-a)(d-c)/l, & b<x<c\\ (b-a)(d-x)/l, & c<x<d\\ 0, & x>d\end{cases} \tag{2.10}$$

depends on the wave function ϕ through the sheet density of electrons in the well $s(\phi)$. Here $l=b-a+d-c$. The potentials $V(x)$ and $W(s,x)$ are shown in Fig. 1.

We will try to solve the nonlinear partial differential equation

$$[-i\partial_t-\partial_x^2+V(x)+W(s,x)]\phi(x,t,E)=0, \tag{2.11}$$

where $s(\phi)$ is given by Eq. (2.7), in two steps. Let $V_{\text{fill}}(x)=V(x)+V_0 1_{[b,c]}(x)$ be the potential obtained by filling the well $[b,c]$. Here $1_{[b,c]}(x)$ is the characteristic function of the interval $[b,c]$. First we solve

$$[-i\partial_t-\partial_x^2+V_{\text{fill}}(x)+W(s,x)]\tilde{\mu}(x,t,E)=0 \tag{2.12}$$

and then we look for ϕ in the form $\phi=\tilde{\mu}+\tilde{\nu}$, where $\tilde{\nu}$ should solve

$$[-i\partial_t-\partial_x^2+V(x)+W(s,x)]\tilde{\nu}(x,t,E)=V_0 1_{[b,c]}(x)\tilde{\mu}(x,t,E). \tag{2.13}$$

The wave function $\tilde{\mu}$ describes an electron at energy E which is delocalized in the emitter and collector regions and has an exponentially small probability to be found in the forbidden region $[a,d]$. The wave function $\tilde{\nu}$ describes the localization, driven by $\tilde{\mu}$, of the same electron in the well $[b,c]$. The wave function ϕ of the original problem (2.11) can be approximated by $\tilde{\nu}$ or $\tilde{\mu}$ inside or outside the two barriers, respectively, with an error which is exponentially small in the limit of wide barriers.[17]

To evaluate $\tilde{\mu}$ we will use a WKB approximation in the forbidden region $[a,d]$. Equation (2.13) will be treated with a one-mode approximation in which $\tilde{\nu}$ is assumed proportional to a resonant state corresponding to the potential $V+W$. To evaluate this resonant state and the corresponding resonance, we will again use a WKB approximation. In both cases, the justification of using a WKB approximation stems from the fact that $V_{\text{fill}}+W$ and $V+W$ are slowly varying potentials in the barriers regions if $b-a$ and $d-c$ are large while ΔV and s remain bounded.

III. WKB EXPANSION FOR SLOWLY VARYING POTENTIALS

Let $\mathscr{U}=\mathscr{U}_h(x)$ be a real valued potential on some interval, with $\partial_x\mathscr{U}=\mathscr{O}(|h|)$ and $\partial_x^2\mathscr{U}=\mathscr{O}(h^2)$, where $|h|\ll 1$ is a parameter. Let $\mathscr{E}$ be a real energy and assume that $\mathscr{U}_h(x)-\mathscr{E}$ is bounded from above and from below by some strictly positive constants that are independent of h. This means that we are in the classically forbidden region. Then

$$\begin{aligned}&[-\partial_x^2+\mathscr{U}-\mathscr{E}](\mathscr{U}-\mathscr{E})^{-1/4}\exp\left(-\int^x dx'(\mathscr{U}-\mathscr{E})^{1/2}\right)\\&\quad=\left[-\frac{5}{16}(\mathscr{U}-\mathscr{E})^{-9/4}(\partial_x\mathscr{U})^2+\frac{1}{4}(\mathscr{U}-\mathscr{E})^{-5/4}\partial_x^2\mathscr{U}\right]\exp\left(-\int^x dx'(\mathscr{U}-\mathscr{E})^{1/2}\right)\\&\quad=e^{-\int^x dx'(\mathscr{U}-\mathscr{E})^{1/2}}\mathscr{O}(h^2),\end{aligned}\tag{3.1}$$

and therefore

$$(\mathscr{U}-\mathscr{E})^{-1/4}\exp\left(-\int^x dx'(\mathscr{U}-\mathscr{E})^{1/2}\right)\tag{3.2}$$

is a good approximation to a corresponding exact eigenfunction, even over intervals of length $\mathscr{O}(|h|^{-1})$.

In the following sections, we will apply the above approximation in the barrier regions $[a,b]$ and $[c,d]$ with h equal to the x derivative of $V+W$ in these intervals.

IV. THE DRIVING TERM

Equation (2.12) can be solved by evaluating the instantaneous eigenstates of the potential $V_{\text{fill}}+W$. We set $\tilde{\mu}(x,t,E)=\exp(-iEt)\mu(x,t,E)$ and suppose that ΔV and s are slowly varying functions of time so that also $\mu(x,t,E)$ is slowly varying in time. Thus in the equation

$$[-i\partial_t-\partial_x^2+V_{\text{fill}}(x)+W(s,x)-E]\mu(x,t,E)=0,\tag{4.1}$$

we make a very small error if we neglect the term $-i\partial_t\mu$, as we shall do in the following. In the emitter region $x<a$, we take $\mu(x,t,E)$ as the sum of a left- and a right-going plane wave at energy E,

$$\mu(x,t,E)=\frac{1}{\sqrt{4\pi\sqrt{E}}}[e^{i\sqrt{E}(x-a)}+r(E)e^{-i\sqrt{E}(x-a)}],\tag{4.2}$$

where $r(E)$ is a reflection amplitude to be computed. Note that the normalization factor in Eq. (4.2) is chosen in order to have $\int dx\mu(x,t,E)\overline{\mu(x,t,E')}=\delta(E-E')$, in agreement with the expression of the electron density (2.5) in terms of an integral over the energy E. We propagate the expression (4.2) to the adjacent regions by requiring μ to be of class C^1 and applying the WKB approximation described in Sec. III. In the interval $[a,b]$ the potential is $V_{\text{fill}}+W=V_0+\alpha(x-a)$, where

$$\alpha=\frac{8\pi a_B^{-1}s(d-c)-\Delta V}{b-a+d-c}\tag{4.3}$$

plays the role of the small parameter h of Sec. III. For $a<x<b$ we can then use the WKB approximation

$$\mu(x,t,E)=\frac{1}{\sqrt{4\pi\sqrt{E}}}\frac{(V_0-E)^{1/4}}{[V_0+\alpha(x-a)-E]^{1/4}}\,t(E)\exp\left(-\int_a^x dx'[V_0+\alpha(x'-a)-E]^{1/2}\right), \tag{4.4}$$

where $t(E)$ is a transmission amplitude to be determined with $r(E)$ from the C^1 condition at $x=a$

$$1+r(E)=t(E), \tag{4.5a}$$

$$i\sqrt{E}-i\sqrt{E}r(E)=t(E)[(V_0-E)^{1/2}-\tfrac{1}{4}(V_0-E)^{-5/4}\alpha]. \tag{4.5b}$$

Neglecting the last term in the square brackets, which is $\mathcal{O}(|\alpha|)$, we get

$$r(E)=\frac{1+i(V_0/E-1)^{1/2}}{1-i(V_0/E-1)^{1/2}}, \tag{4.6a}$$

$$t(E)=\frac{2}{1-i(V_0/E-1)^{1/2}}. \tag{4.6b}$$

Note that the neglected term would give correction factors $1+\mathcal{O}(|\alpha|)$ to $r(E)$ and $t(E)$.

At $x=b$ we can set up a similar transition problem but here $V_{\text{fill}}+W$ is continuous and the corresponding transmission amplitude is $1+\mathcal{O}(|\alpha|)$. Neglecting again a factor $1+\mathcal{O}(|\alpha|)$, for $b<x<c$ we get

$$\mu(x,t,E)=\mu_0(t,E)e^{-[V_0+\alpha(b-a)-E]^{1/2}(x-b)}, \tag{4.7}$$

where

$$\mu_0(t,E)=\frac{1}{\sqrt{4\pi\sqrt{E}}}\frac{(V_0-E)^{1/4}}{(V_0+\alpha(x-a)-E)^{1/4}}\frac{2e^{\{(V_0-E)^{3/2}-[V_0+\alpha(b-a)-E]^{3/2}\}2/3\alpha}}{1+i(V_0/E-1)^{1/2}}. \tag{4.8}$$

Only this expression of μ in the region $[b,c]$ will be used in the following as driving term of Eq. (2.13).

V. RESONANCE AND RESONANT STATE

In this section we will obtain a WKB approximate expression for the ground-state resonance $\lambda(s)=E_R(s)-i\Gamma(s)/2$ and the corresponding resonant state $e(s,x)$ for the potential $V+W$. We will assume that $c-b$ is bounded from below and from above by positive constants, while $b-a$ and $d-c$ are large enough.

To start with, we recall the construction of the ground state eigenvalue E_0^w of the potential $V_w(x)=V_0[1_{]-\infty,b]}(x)+1_{[c,+\infty[}(x)]$ which coincides, up to the constant shift

$$\Delta E=\frac{8\pi a_B^{-1}s(b-a)(d-c)-\Delta V(b-a)}{b-a+d-c}, \tag{5.1}$$

with the potential $V+W$ in the well region $[b,c]$. The corresponding ground eigenstate is

$$e_0^w(x)=C_0^w\times\begin{cases}\cos[\sqrt{E_0^w}(c-b)/2]e^{-(V_0-E_0^w)^{1/2}(b-x)}, & x<b\\ \cos\{\sqrt{E_0^w}[x-(b+c)/2]\}, & b<x<c\\ \cos[\sqrt{E_0^w}(c-b)/2]e^{-(V_0-E_0^w)^{1/2}(x-c)}, & x>c\end{cases} \tag{5.2}$$

where $0<E_0^w<\min(V_0,\pi^2/(c-b)^2)$ is determined by the requirement that $e_0^w(x)$ is of class C^1,

$$\tan[\sqrt{E_0^w}(c-b)/2]=(V_0/E_0^w-1)^{1/2}, \tag{5.3}$$

and the normalization constant is

$$C_0^w=\left[\frac{E_0^w}{V_0(V_0-E_0^w)^{1/2}}+\frac{c-b}{2}+\frac{(V_0-E_0^w)^{1/2}}{V_0}\right]^{-1/2}, \tag{5.4}$$

where we used the identities $\cos^2 u=(1+\tan^2 u)^{-1}$, $(\sin 2u)/2=\sin u\cos u=\tan u(1+\tan^2 u)^{-1}$. In the following we will assume that $E_0^w+\Delta E<V_0-\Delta V$.

Next we look at the ground state of the potential

$$V_b(x)=\begin{cases} V_0+\alpha(a-b), & x<a \\ V_0+\alpha(x-b), & a<x<b \\ 0, \quad b<x<c & \\ V_0+\beta(x-c), & c<x<d \\ V_0+\beta(d-c), & x>d \end{cases} \tag{5.5}$$

which coincides, up to the constant shift ΔE, with $V+W$ on the larger region $[a,d]$ which includes the barriers. In Eq. (5.5) α is given by Eq. (4.3) and

$$\beta=\frac{-8\pi a_B^{-1}s(b-a)-\Delta V}{b-a+d-c}. \tag{5.6}$$

Note that the potential V_b has been obtained by bending the barriers of V_w in the intervals $[a,b]$ and $[c,d]$ proportionally to α and β, respectively. Let E_0^b be the ground state of V_b and $e_0^b(x)$ the corresponding eigenfunction. Since $|\alpha|$ and $|\beta|$ are small, from the same WKB considerations of Sec. III we have $E_0^b=E_0^w+\mathcal{O}(|\alpha|+|\beta|)$ and $e_0^b(x)=e_0^w(x)+\mathcal{O}(|\alpha|+|\beta|)$. To get the leading asymptotics of the resonance width, we need to determine the linear contribution to $\mathcal{O}(|\alpha|+|\beta|)$ in E_0^b. By differentiating the eigenvalue equation for the potential V_b, we have

$$\partial_\alpha E_0^b|_{\alpha=\beta=0}=\int_{-\infty}^{+\infty}dx\overline{e_0^b(x)}\partial_\alpha V_b(x)|_{\alpha=\beta=0}e_0^b(x)\simeq\int_{-\infty}^{b}dx(x-b)|e_0^w(x)|^2, \tag{5.7}$$

$$\partial_\beta E_0^b|_{\alpha=\beta=0}=\int_{-\infty}^{+\infty}dx\overline{e_0^b(x)}\partial_\beta V_b(x)|_{\alpha=\beta=0}e_0^b(x)\simeq\int_{c}^{+\infty}dx(x-c)|e_0^w(x)|^2, \tag{5.8}$$

and using Eq. (5.2) we get

$$\begin{aligned}\partial_\alpha E_0^b|_{\alpha=\beta=0}&=-\partial_\beta E_0^b|_{\alpha=\beta=0}=(C_0^w)^2\cos^2[\sqrt{E_0^w}(c-b)/2]\int_{-\infty}^{0}dx\ xe^{2(V_0-E_0^w)^{1/2}x}\\&=-\frac{(C_0^w)^2E_0^w}{4V_0(V_0-E_0^w)}.\end{aligned} \tag{5.9}$$

Observing that $\alpha-\beta=8\pi a_B^{-1}s$, we finally get

$$E_0^b=E_0^w-8\pi a_B^{-1}s\,\frac{(C_0^w)^2E_0^w}{4V_0(V_0-E_0^w)}+\mathcal{O}(\alpha^2+\beta^2). \tag{5.10}$$

The real part $E_R(s)$ of the shape resonance of $-\partial_x^2+V+W$ which is close to the ground-state eigenvalue of $-\partial_x^2+V_b+\Delta E$ is very well approximated by the above calculated $E_0^b+\Delta E$ which can be rewritten as

$$E_R(s)=E_R(0)+\eta s, \tag{5.11}$$

where

$$E_R(0)=E_0^w-\Delta V(b-a)/l \tag{5.12}$$

and

$$\eta=\frac{8\pi a_B^{-1}(b-a)(d-c)}{b-a+d-c}-\frac{8\pi a_B^{-1}(C_0^w)^2E_0^w}{4V_0(V_0-E_0^w)}. \tag{5.13}$$

Now we discuss the determination of the imaginary part $\Gamma(s)$ of the resonance. In the interval $[a,d]$ the ground state of V_b is

$$e_0^b(x)=C_0^b \times\begin{cases}\dfrac{\cos[\sqrt{E_0^b}(c-b)/2](V_0-E_0^b)^{1/4}}{[V_0+\alpha(x-b)-E_0^b]^{1/4}}\exp\left(-\displaystyle\int_x^b dx'[V_0+\alpha(x'-b)-E_0^b]^{1/2}\right), & a<x<b\\ \cos\{\sqrt{E_0^b}[x-(b+c)/2]\}, & b<x<c\\ \dfrac{\cos[\sqrt{E_0^b}(c-b)/2](V_0-E_0^b)^{1/4}}{[V_0+\beta(x-c)-E_0^b]^{1/4}}\exp\left(-\displaystyle\int_c^x dx'[V_0+\beta(x'-c)-E_0^b]^{1/2}\right), & c<x<d\end{cases} \tag{5.14}$$

where $C_0^b=C_0^w+\mathcal{O}(|\alpha|+|\beta|)$. In the interval $[a,d]$, the resonant state $e(s,x)$ can be approximated by adding to Eq. (5.14) terms due to reflections at $x=a$ and $x=d$. For $x\lesssim d$ we try with

$$e(s,x)=\frac{C_0^w\cos[\sqrt{E_0^b}(c-b)/2](V_0-E_0^b)^{1/4}}{[V_0+\beta(x-c)-E_0^b]^{1/4}}\exp\left(-\int_c^d dx'[V_0+\beta(x'-c)-E_0^b]^{1/2}\right)$$
$$\times(e^{-[V_0+\beta(d-c)-E_0^b]^{1/2}(x-d)}+re^{[V_0+\beta(d-c)-E_0^b]^{1/2}(x-d)}), \tag{5.15}$$

where we have also replaced the exponent with its linear approximation at $x=d$. For $x\gtrsim d$ we try the right-going plane wave

$$e(s,x)=\frac{C_0^w\cos[\sqrt{E_0^b}(c-b)/2](V_0-E_0^b)^{1/4}}{[V_0+\beta(d-c)-E_0^b]^{1/4}}$$
$$\times\exp\left(-\int_c^d dx'[V_0+\beta(x'-c)-E_0^b]^{1/2}\right)te^{i[E_0^b-\beta(d-c)]^{1/2}(x-d)}. \tag{5.16}$$

The C^1 condition at $x=d$ gives, up to terms $\mathcal{O}(|\beta|)$,

$$1+r=t, \tag{5.17a}$$

$$-[V_0+\beta(d-c)-E_0^b]^{1/2}+[V_0+\beta(d-c)-E_0^b]^{1/2}r=i[E_0^b-\beta(d-c)]^{1/2}t, \tag{5.17b}$$

which determines r and t so that for $x\gtrsim d$ we have

$$e(s,x)=\frac{C_0^w\cos[\sqrt{E_0^b}(c-b)/2](V_0-E_0^b)^{1/4}}{[V_0+\beta(d-c)-E_0^b]^{1/4}}2\left[1-i\frac{[E_0^b-\beta(d-c)]^{1/2}}{[V_0+\beta(d-c)-E_0^b]^{1/2}}\right]^{-1}\times\exp\left\{\frac{2}{3\beta}\{(V_0-E_0^b)^{3/2}-[V_0+\beta(d-c)-E_0^b]^{3/2}\}+i[E_0^b-\beta(d-c)]^{1/2}(x-d)\right\}. \tag{5.18}$$

In these calculations we have assumed that $E_0^b-\beta(d-c)>0$, $V_0+\beta(d-c)-E_0^b>0$. The first inequality is always fulfilled in experimentally relevant situations, while the second one, equivalent to $E_R(s)<V_0-\Delta V$ may be more critical and, possibly, one should replace Eq. (5.18) by a more complicated formula.

The same calculation can be repeated for $x=a$. For $x\gtrsim a$ we try with

$$e(s,x)=\frac{C_0^w\cos[\sqrt{E_0^b}(c-b)/2](V_0-E_0^b)^{1/4}}{[V_0+\alpha(x-b)-E_0^b]^{1/4}}\exp\left(-\int_a^b dx'[V_0+\alpha(x'-b)-E_0^b]^{1/2}\right)\times(e^{[V_0+\alpha(a-b)-E_0^b]^{1/2}(x-a)}+re^{-[V_0+\alpha(a-b)-E_0^b]^{1/2}(x-a)}), \tag{5.19}$$

with a new reflection amplitude r. For $x\lesssim a$ we try the left-going plane wave

$$e(s,x)=\frac{C_0^w\cos[\sqrt{E_0^b}(c-b)/2](V_0-E_0^b)^{1/4}}{[V_0+\alpha(a-b)-E_0^b]^{1/4}}\exp\left(-\int_a^b dx'(V_0+\alpha(x'-b)-E_0^b)^{1/2}\right)\times te^{-i[E_0^b+\alpha(b-a)]^{1/2}(x-a)} \tag{5.20}$$

with a new transmission amplitude t. The C^1 condition at $x=a$ gives, up to terms $\mathcal{O}(|\alpha|)$,

$$1+r=t, \tag{5.21a}$$

$$[V_0+\alpha(a-b)-E_0^b]^{1/2}-[V_0+\alpha(a-b)-E_0^b]^{1/2}r=-i[E_0^b-\alpha(a-b)]^{1/2}t, \tag{5.21b}$$

which determines r and t so that for $x\lesssim a$ we have

$$e(s,x)=\frac{C_0^w\cos[\sqrt{E_0^b}(c-b)/2](V_0-E_0^b)^{1/4}}{[V_0-\alpha(b-a)-E_0^b]^{1/4}}2\left[1-i\frac{[E_0^b+\alpha(b-a)]^{1/2}}{[V_0-\alpha(b-a)-E_0^b]^{1/2}}\right]^{-1}\times\exp\left\{\frac{2}{3\alpha}\{[V_0-\alpha(b-a)-E_0^b]^{3/2}-(V_0-E_0^b)^{3/2}\}-i[E_0^b+\alpha(b-a)]^{1/2}(x-a)\right\}. \tag{5.22}$$

Note that for $x\lesssim a$, $e(s,x)$ is a true left-going plane wave only for ΔV not too large when $E_0^b+\alpha(b-a)>0$. If $E_0^b+\alpha(b-a)<0$, Eq. (5.22) becomes an exponentially decaying function whose corresponding probability current density vanishes. Since $E_0^b+\alpha(b-a)=E_R(s)$, this case corresponds to $E_R(s)<0$. In Eq. (5.22), we also assumed that $V_0-\alpha(b-a)-E_0^b>0$, i.e., $E_R(s)<V_0$.

The resonance width can be now computed by means of the Green formula

$$\Gamma(s)\int_{a'}^{d'}dx|e(s,x)|^2=2\,\mathrm{Im}[\overline{e(s,x)}\partial_x e(s,x)]\Big|_{a'}^{d'}, \tag{5.23}$$

where $a'<a$ and $d'>d$. The integral in the left-hand side (lhs) of Eq. (5.23) is $1+\mathcal{O}(|\alpha|+|\beta|)$ and using Eqs. (5.18) and (5.22) we get, up to such a factor,

$$\Gamma(s)=8(C_0^w)^2E_0^b(V_0-E_0^b)^{1/2}V_0^{-2}\{[V_0+\beta(d-c)-E_0^b]^{1/2}[E_0^b-\beta(d-c)]^{1/2}$$
$$\times e^{\{(V_0-E_0^b)^{3/2}-[V_0+\beta(d-c)-E_0^b]^{3/2}\}4/3\beta}+[V_0-\alpha(b-a)-E_0^b]^{1/2}$$
$$\times[E_0^b+\alpha(b-a)]_+^{1/2}e^{\{[V_0-\alpha(b-a)-E_0^b]^{3/2}-(V_0-E_0^b)^{3/2}\}4/3\alpha}\}, \tag{5.24}$$

where we used $u_+=\theta(u)\ u$.

VI. ONE-MODE APPROXIMATION

Equation (2.13) can be simplified by developing $\tilde{\nu}$ into the instantaneous eigenstates of the potential $V+W$ and keeping only the contributions from the discrete resonant states, i.e., neglecting the contributions from the continuous spectrum.[17] For the moment, we will suppose there is only one resonant state and set $\tilde{\nu}(x,t,E)=\exp(-iEt)z(t,E)e(s,x)$ where $e(s,x)$ is the (ground) resonant state of the potential $V+W$,

$$[-\lambda(s)-\partial_x^2+V(x)+W(s,x)]e(s,x)=0, \tag{6.1}$$

with complex eigenvalue $\lambda(s)=E_R(s)-i\Gamma(s)/2$. The eigenfunction $e(s,x)$ is of class L^2 on the contour $\gamma\equiv(e^{i\theta}]-\infty,0]+a)\cup[a,d]\cup(d+e^{i\theta}[0,+\infty[$ for θ conveniently chosen[23] and satisfies

$$\int_\gamma dx\ e(s,x)^2=1, \quad \int_\gamma dx\ e(s,x)\partial_s e(s,x)=0. \tag{6.2}$$

Multiplying Eq. (2.13) with $e(s,x)$ and integrating over γ, we get

$$\partial_t z(t,E)=i[E-\lambda(s)]z(t,E)+\mathscr{B}(t,s,E) \tag{6.3}$$

with the driving term given by

$$\mathscr{B}(t,s,E)=iV_0\int_b^c dx\ \mu(x,t,E)e(s,x) \tag{6.4}$$

and the sheet density (2.7) reduced, with small error, to

$$s(t)=\int dE\ g(E)|z(t,E)|^2\equiv\|z(t)\|^2. \tag{6.5}$$

VII. FIXED POINTS AND LINEARIZATIONS: GENERAL RESULTS

We consider the vector field in the lhs of Eq. (6.3),

$$\mathscr{V}(z,E)=\mathscr{A}(\|z\|^2,E)z(E)+\mathscr{B}(\|z\|^2,E), \tag{7.1}$$

where

$$\mathscr{A}(s,E)=-\Gamma(s)/2+i\{E-[E_R(0)+\eta s]\}, \tag{7.2}$$

is a nonvanishing function. For simplicity, we assume that $\mathscr{B}$ is independent of t. When $\mathscr{B}$ varies slowly with t, the discussion below should be applied to each such fixed value of t.

We first look for fixed points of $\mathscr{V}$, i.e., functions $z=z(E)$ in $L^2(g(E)dE)$ with $\mathscr{V}(z(E),E)=0$. Clearly $z=z(E)$ is a fixed point iff

$$z(E)=-\frac{\mathscr{B}(\|z\|^2,E)}{\mathscr{A}(\|z\|^2,E)}, \tag{7.3}$$

so the L^2-norm $s=\|z\|^2$ has to satisfy

$$s=\int dE\ g(E)\ \frac{|.\mathscr{B}(s,E)|^2}{|.\mathscr{A}(s,E)|^2}. \tag{7.4}$$

Conversely, if $s\geqslant 0$ is a solution of Eq. (7.4), then

$$z(E)=-\frac{\mathscr{B}(s,E)}{\mathscr{A}(s,E)} \tag{7.5}$$

gives the unique fixed point of $\mathscr{V}$ with $\|z\|^2=s$.

Assuming that we have found a fixed point $z=z(E)$, we look for the linearization of the vector field $\mathscr{V}$ at that point. By giving an infinitesimal increment $\delta z(E)$ to $z(E)$, the corresponding increment $\delta\mathscr{V}$ to $\mathscr{V}$ is

$$\delta\mathscr{V}(z,E)=\mathscr{A}(s,E)\,\delta z(E)+(\langle\delta z|z\rangle+\langle\overline{\delta z}|\overline{z}\rangle)[\partial_s.\mathscr{A}(s,E)z(E)+\partial_s.\mathscr{B}(s,E)], \tag{7.6}$$

where $s=\|z\|^2$ is the corresponding solution of Eq. (7.4) and $\langle u|v\rangle=\int dE\ g(E)u(E)\overline{v(E)}$. Hence,

$$\overline{\delta\mathscr{V}}(z,E)=\overline{\mathscr{A}}(s,E)\,\overline{\delta z}(E)+(\langle\delta z|z\rangle+\langle\overline{\delta z}|\overline{z}\rangle)[\overline{\partial_s.\mathscr{A}}(s,E)\overline{z(E)}+\overline{\partial_s.\mathscr{B}}(s,E)], \tag{7.7}$$

so with $u(E)=\delta z(E)$ and $v(E)=\overline{\delta z}(E)$, we get the complexification of the linearization,

$$\mathscr{L}\begin{pmatrix}u\\v\end{pmatrix}=\begin{pmatrix}\mathscr{A} & 0\\ 0 & \overline{\mathscr{A}}\end{pmatrix}\begin{pmatrix}u\\v\end{pmatrix}+\begin{pmatrix}(\langle u|z\rangle+\langle v|\overline{z}\rangle)(\partial_s.\mathscr{A}z+\partial_s.\mathscr{B})\\ (\langle u|z\rangle+\langle v|\overline{z}\rangle)(\partial_s.\overline{\mathscr{A}}\overline{z}+\partial_s.\overline{\mathscr{B}})\end{pmatrix}. \tag{7.8}$$

The matrix in the first term of the rhs has a continuous spectrum contained in $-\Gamma(s)/2+i\mathbf{R}$ and the second term appears as a rank one perturbation. If $\lambda\in\mathbf{C}$ is an eigenvalue of $\mathscr{L}$ with a real part different from $-\Gamma(s)/2$, we get

$$[.\mathscr{A}(s,E)-\lambda]u+(\langle u|z\rangle+\langle v|\overline{z}\rangle)[\partial_s.\mathscr{A}(s,E)z+\partial_s.\mathscr{B}(s,E)]=0, \tag{7.9a}$$

$$[.\overline{\mathscr{A}}(s,E)-\lambda]v+(\langle u|z\rangle+\langle v|\overline{z}\rangle)[\overline{\partial_s.\mathscr{A}}(s,E)\overline{z}+\overline{\partial_s.\mathscr{B}}(s,E)]=0. \tag{7.9b}$$

We must then have

$$u(E)=\kappa\,\frac{\partial_s.\mathscr{A}(s,E)z+\partial_s.\mathscr{B}(s,E)}{\mathscr{A}(s,E)-\lambda}, \tag{7.10a}$$

$$v(E)=\kappa\,\frac{\overline{\partial_s.\mathscr{A}}(s,E)\overline{z}+\overline{\partial_s.\mathscr{B}}(s,E)}{\overline{\mathscr{A}}(s,E)-\lambda}, \tag{7.10b}$$

where $\kappa=\langle u|z\rangle+\langle v|\overline{z}\rangle$. In order to have a nontrivial solution $\kappa\neq 0$, it is necessary and sufficient that

$$1+\int dE\ g(E)\ \frac{\partial_s[(\mathscr{A}-\lambda)(\overline{\mathscr{A}}-\lambda)]|.\mathscr{B}|^2-\mathscr{A}(\overline{\mathscr{A}}-\lambda).\overline{\mathscr{B}}\partial_s.\mathscr{B}-\overline{\mathscr{A}}(\mathscr{A}-\lambda).\mathscr{B}\partial_s.\overline{\mathscr{B}}}{[(\mathrm{Re}\,.\mathscr{A}-\lambda)^2+(\mathrm{Im}\,.\mathscr{A})^2]|.\mathscr{A}|^2}=0. \tag{7.11}$$

Here, the lhs is real for real λ, and tends to 1, when $\lambda \to +\infty$.

On the other hand, the s-derivative of the lhs minus the rhs of Eq. (7.4) is

$$1+\int dE\ g(E)\ \frac{|\mathscr{B}(s,E)|^2\partial_s|\mathscr{A}(s,E)|^2-|\mathscr{A}(s,E)|^2\partial_s|\mathscr{B}(s,E)|^2}{|\mathscr{A}(s,E)|^4}, \tag{7.12}$$

which coincides with the lhs of Eq. (7.11) for $\lambda=0$. So if the expression (7.12) is <0, we see that Eq. (7.11) must have a solution $\lambda>0$. Let us say that the fixed point is stable if the spectrum of the linearization $\mathscr{L}$ is contained in the open left half-plane and unstable otherwise. The discussion above then gives the following.

Proposition VII.1: Let z be a fixed point of $\mathscr{V}$ so that Eqs. (7.4) and (7.5) hold. If the s-derivative of the lhs *minus the* rhs *of Eq. (7.4) is <0, then z is an unstable fixed point. More precisely, the linearization $\mathscr{L}$ then has an eigenvalue which is >0.*

VIII. FIXED POINTS AND LINEARIZATIONS: THE SMALL-Γ LIMIT

In this section we assume that the driving term $\mathscr{B}(s,E)$ is a sufficiently smooth function of E, at least near the point $E_R(0)+\eta s$, where s solves Eq. (7.4). When the barriers are very wide, $\Gamma(s)$ will be very small and

$$\frac{1}{|\mathscr{A}(s,E)|^2}=\frac{1}{[\Gamma(s)/2]^2+[E_R(0)+\eta s-E]^2}$$

is a function of E which is sharply peaked at $E_R(s)=E_R(0)+\eta s$. In Eq. (7.4) it is therefore justified to replace $g(E)|\mathscr{B}(s,E)|^2$ by the constant value $g(E_R(0)+\eta s)|\mathscr{B}(s,E_R(0)+\eta s)|^2$. Then Eq. (7.4) is well approximated by

$$s=2\pi\,\frac{g(E_R(s))|\mathscr{B}(s,E_R(s))|^2}{\Gamma(s)}. \tag{8.1}$$

We shall next apply a similar argument to Eq. (7.11) for the eigenvalues of the linearization $\mathscr{L}$ and, for more transparency, we start with a simplified case, in which

$$\mathscr{B} \quad \text{and} \quad \Gamma \quad \text{are independent of} \quad s. \tag{8.2}$$

In this case, Eq. (7.11) reduces to

$$1-2\eta\int dE\ \frac{[E-E_R(0)-\eta s]g(E)|\mathscr{B}(E)|^2}{\{(\Gamma/2+\lambda)^2+[E-E_R(0)-\eta s]^2\}\{(\Gamma/2)^2+[E-E_R(0)-\eta s]^2\}}=0. \tag{8.3}$$

We shall use

$$\int_{-\infty}^{+\infty}dt\ \frac{t^2}{(q^2+t^2)(p^2+t^2)}=\begin{cases}\dfrac{\pi}{p+q}, & \text{Re } p>0, \quad \text{Re } q>0\\[2ex] \dfrac{\pi}{p-q}, & \text{Re } p>0, \quad \text{Re } q<0\end{cases} \tag{8.4}$$

$$\int_{-\infty}^{+\infty}dt\ \frac{1}{(q^2+t^2)(p^2+t^2)}=\begin{cases}\dfrac{\pi}{qp(p+q)}, & \text{Re } p>0, \quad \text{Re } q>0\\[2ex] \dfrac{-\pi}{qp(p-q)}, & \text{Re } p>0, \quad \text{Re } q<0.\end{cases} \tag{8.5}$$

If we replace $g(E)|\mathscr{B}(E)|^2$ in the integral in Eq. (8.3) with its value at $E=E_R(0)+\eta s$, that integral vanishes since the integrand becomes an odd function of $E-E_R(0)-\eta s$. Instead, we get an approximation of the integral in Eq. (8.3) by replacing $g(E)|\mathscr{B}(E)|^2$ with the linear term in its Taylor expansion at $E=E_R(0)+\eta s$. Using Eq. (8.4), we then get from Eq. (8.3)

$$1-2\eta\,\frac{(g|\mathscr{B}|^2)'[E_R(0)+\eta s]\pi}{\Gamma+\lambda}=0 \quad \text{when } \Gamma/2+\mathrm{Re}\,\lambda>0, \tag{8.6}$$

$$1+2\eta\,\frac{(g|\mathscr{B}|^2)'[E_R(0)+\eta s]\pi}{\lambda}=0 \quad \text{when } \Gamma/2+\mathrm{Re}\,\lambda<0, \tag{8.7}$$

where $(g|\mathscr{B}|^2)'=\partial_E(g|\mathscr{B}|^2)$. The solution of Eq. (8.6) is

$$\lambda=2\pi\eta(g|\mathscr{B}|^2)'[E_R(0)+\eta s]-\Gamma, \tag{8.8}$$

and this is an eigenvalue of the linearization $\mathscr{L}$ as long as

$$2\pi\eta(g|\mathscr{B}|^2)'[E_R(0)+\eta s]>\frac{\Gamma}{2}. \tag{8.9}$$

The solution of Eq. (8.7) is

$$\lambda=-2\pi\eta(g|\mathscr{B}|^2)'[E_R(0)+\eta s] \tag{8.10}$$

and describes an eigenvalue of $\mathscr{L}$ precisely when Eq. (8.9) is fulfilled. We then have the following conclusion under the simplifying assumption (8.2) and in the small-Γ limit.

When $2\pi\eta(g|\mathscr{B}|^2)'[E_R(0)+\eta s]\leqslant\Gamma/2$*: no eigenvalues of* $\mathscr{L}$ and hence an attractive fixed point.

When $\Gamma/2<2\pi\eta(g|\mathscr{B}|^2)'[E_R(0)+\eta s]<\Gamma$*: two eigenvalues of* $\mathscr{L}$ and still an attractive fixed point.

When $2\pi\eta(g|\mathscr{B}|^2)'[E_R(0)+\eta s]\geqslant\Gamma$*: two eigenvalues and a nonattractive fixed point.*

The main conclusion under the same assumptions is then the following.

Proposition VIII.1: We have an attractive fixed point precisely when the s-derivative of the difference of the lhs *and the* rhs *in Eq. (8.1) is* >0.

Now we drop the simplifying assumption (8.2) and see that the preceding proposition still holds in the small-Γ limit. Let z be a fixed point, so that $s=\|z\|^2$ (approximately) solves Eq. (8.1). In view of Eq. (7.2), Eq. (7.11) can be written as

$$1+\int dE\; g(E)\,\frac{\partial_s[(\mathscr{A}-\lambda)(\overline{\mathscr{A}}-\lambda)]|\mathscr{B}|^2-\mathscr{A}(\overline{\mathscr{A}}-\lambda)\partial_s\mathscr{B}\overline{\mathscr{B}}-\overline{\mathscr{A}}(\mathscr{A}-\lambda)\mathscr{B}\partial_s\overline{\mathscr{B}}}{\{[\Gamma(s)/2+\lambda]^2+[E-E_R(0)-\eta s]^2\}\{[\Gamma(s)/2]^2+[E-E_R(0)-\eta s]^2\}}=0. \tag{8.11}$$

Here, the numerator of the integrand can be simplified to

$$\begin{aligned}&[\partial_s\Gamma(\Gamma/2+\lambda)|\mathscr{B}|^2-(\Gamma/2)(\Gamma/2+\lambda)\partial_s|\mathscr{B}|^2]+\{[E-E_R(0)-\eta s][-2\eta|\mathscr{B}|^2\\&\quad+i\lambda(\partial_s\mathscr{B}\overline{\mathscr{B}}-\mathscr{B}\partial_s\overline{\mathscr{B}})]\}-\{[E-E_R(0)-\eta s]^2\partial_s|\mathscr{B}|^2\}.\end{aligned} \tag{8.12}$$

Accordingly, we split the integral into three pieces and apply the small-Γ approximation to each one. If we assume, for simplicity, that $\Gamma/2+\mathrm{Re}\,\lambda>0$ (which is necessarily the case if the eigenvalue λ is to ruin attractiveness), we get

$$1+\frac{[\partial_s\Gamma(\Gamma/2+\lambda)|.\mathscr{B}|^2-(\Gamma/2)(\Gamma/2+\lambda)\partial_s|.\mathscr{B}|^2]\pi g}{(\Gamma/2)(\Gamma/2+\lambda)(\Gamma+\lambda)}$$
$$+\frac{(\partial_E\{g[-2\eta|.\mathscr{B}|^2+i\lambda(\partial_s.\mathscr{B}.\overline{\mathscr{B}}-.\mathscr{B}\partial_s.\overline{\mathscr{B}})]\}-g\partial_s|.\mathscr{B}|^2)\pi}{\Gamma+\lambda}=0 \tag{8.13}$$

at $E=E_R(0)+\eta s$. This can be rewritten as

$$1+\frac{2\pi(\partial_s\Gamma/\Gamma)g|.\mathscr{B}|^2}{\Gamma+\lambda}-\frac{2\pi\partial_s(g|.\mathscr{B}|^2)}{\Gamma+\lambda}-\frac{2\pi\eta\partial_E(g|.\mathscr{B}|^2)}{\Gamma+\lambda}+\frac{i\lambda\pi\partial_E[g(\partial_s.\mathscr{B}.\overline{\mathscr{B}}-.\mathscr{B}\partial_s.\overline{\mathscr{B}})]}{\Gamma+\lambda}=0, \tag{8.14}$$

again at $E=E_R(0)+\eta s$. Noticing that

$$\frac{d}{ds}[(g|.\mathscr{B}|^2)(s,E_R(0)+\eta s)]=(\eta\partial_E+\partial_s)(g|.\mathscr{B}|^2)(s,E_R(0)+\eta s),$$

and multiplying with $\Gamma+\lambda$, we get the following approximation of Eq. (7.11)

$$\lambda\{1+i\pi\partial_E[g(\partial_s.\mathscr{B}.\overline{\mathscr{B}}-.\mathscr{B}\partial_s.\overline{\mathscr{B}})]\}=-\Gamma(s)-2\pi\frac{(g|.\mathscr{B}|^2)(s,E_R(0)+\eta s)}{\Gamma(s)}\partial_s\Gamma(s)$$
$$+2\pi\frac{d}{ds}[(g|.\mathscr{B}|^2)(s,E_R(0)+\eta s)]. \tag{8.15}$$

We assume that $1+i\pi\partial_E[g(\partial_s.\mathscr{B}.\overline{\mathscr{B}}-.\mathscr{B}\partial_s.\overline{\mathscr{B}})]>0$, so that the solution λ of Eq. (8.15) is real and has the same sign as the rhs of Eq. (8.15).

On the other hand, the s-derivative of the lhs minus the rhs of Eq. (8.1) is

$$1-\frac{2\pi}{\Gamma(s)}\frac{d}{ds}[(g|.\mathscr{B}|^2)(s,E_R(0)+\eta s)]+2\pi(g|.\mathscr{B}|^2)(s,E_R(0)+\eta s)\frac{\partial_s\Gamma(s)}{\Gamma(s)^2}$$
$$=-\frac{1}{\Gamma(s)}\left(-\Gamma(s)+2\pi\frac{d}{ds}[(g|.\mathscr{B}|^2)(s,E_R(0)+\eta s)]\right.$$
$$\left.-2\pi\frac{(g|.\mathscr{B}|^2)(s,E_R(0)+\eta s)}{\Gamma(s)}\partial_s\Gamma(s)\right),$$

which is of the opposite sign to the rhs in Eq. (8.15). We then have the following.

Proposition VIII.2: Under the weaker assumptions above and in the small-Γ *limit, we still have an attractive fixed point precisely when the s-derivative of the* lhs *minus the* rhs *of Eq. (8.1) is* >0.

IX. A SIMPLIFIED DIFFERENTIAL EQUATION FOR THE SHEET DENSITY

Consider the differential equation (6.3)

$$\partial_t z(t,E)=(-\Gamma(s(t))/2+i\{E-[E_R(0)+\eta s(t)]\})z(t,E)+\mathscr{B}(s(t),E), \tag{9.1}$$

where $s(t)=\|z(t,\cdot)\|^2$, and where we could also let $\mathscr{B}$ be a slowly varying function of t through $s(t)$. Assuming $s(t)$ to be a known function, the solution of Eq. (9.1) with a prescribed initial value at time t_0 is

$$z(t,E)=\int_{t_0}^{t}dt'\ \exp\left(i[E-E_R(0)](t-t')-\int_{t'}^{t}dt''\Gamma(s(t''))/2-i\eta\int_{t'}^{t}dt''s(t'')\right).\mathscr{B}(s(t'),E)$$
$$+\exp\left(i[E-E_R(0)](t-t_0)-\int_{t_0}^{t}dt'\Gamma(s(t'))/2-i\eta\int_{t_0}^{t}dt's(t')\right)z(t_0,E).$$

Assuming that the solution has existed as a bounded solution for a very long time, say from the time $-\infty$, we can let t_0 tend to $-\infty$ in the formula above and get

$$z(t,E)=\int_{-\infty}^{t}dt'\ \exp\left(i[E-E_R(0)](t-t')-\int_{t'}^{t}dt''\Gamma(s(t''))/2-i\eta\int_{t'}^{t}dt''s(t'')\right).\mathscr{B}(s(t'),E). \tag{9.2}$$

Taking the scalar product of Eq. (9.1) and z gives the following equation for the derivative of the sheet density

$$\frac{d}{dt}s(t)=2\ \mathrm{Re}\langle z|\partial_t z\rangle=-\Gamma(s(t))s(t)+2\ \mathrm{Re}\langle z|.\mathscr{B}\rangle, \tag{9.3}$$

where

$$2\ \mathrm{Re}\langle z|.\mathscr{B}\rangle=2\ \mathrm{Re}\int dE\ g(E)\int_{-\infty}^{t}dt'\ \exp\left(i[E-E_R(0)](t-t')-\int_{t'}^{t}dt''\Gamma(s(t''))/2\right.$$
$$\left.-i\eta\int_{t'}^{t}dt''s(t'')\right).\mathscr{B}(s(t'),E).\overline{\mathscr{B}(s(t),E)}. \tag{9.4}$$

We now assume that $s(t)$ varies slowly with t and replace $\mathscr{B}(s(t'),E)$ in the above integral by $\mathscr{B}(s(t),E)$. Making the E-integration first, we get

$$2\ \mathrm{Re}\langle z|.\mathscr{B}\rangle=2\ \mathrm{Re}\int_{-\infty}^{t}dt'\ \exp\left(-iE_R(0)(t-t')-\int_{t'}^{t}dt''\Gamma(s(t''))/2-i\eta\int_{t'}^{t}dt''s(t'')\right)$$
$$\times\mathscr{F}(g|.\mathscr{B}|^2)(s(t),t'-t), \tag{9.5}$$

where $\mathscr{F}$ denotes the Fourier transform with respect to E. Assuming that $g(E)|.\mathscr{B}(s(t),E)|^2$ is sufficiently smooth as a function of E, we see that $\mathscr{F}(g|.\mathscr{B}|^2)(s(t),t'-t)$ is sufficiently rapidly decreasing as a function of $t'-t$ for the following approximations to be made: (i) since $\Gamma(s)$ is small, we may assume that $\exp\{-\int_{t'}^{t}dt''\Gamma(t'')/2\}\simeq 1$ and (ii) since $s(t'')$ varies slowly, we may replace $\int_{t'}^{t}dt''s(t'')$ by $s(t)(t-t')$. We then get

$$2\ \mathrm{Re}\langle z|.\mathscr{B}\rangle\simeq 2\ \mathrm{Re}\int_{-\infty}^{t}dt'e^{-i[E_R(0)+\eta s(t)](t-t')}\mathscr{F}(g|.\mathscr{B}|^2)(s(t),t'-t)$$
$$=2\ \mathrm{Re}\int_{-\infty}^{0}dt'e^{i[E_R(0)+\eta s(t)]t'}\mathscr{F}(g|.\mathscr{B}|^2)(s(t),t').$$

Using the property $\mathscr{F}(u)(-t)=\overline{\mathscr{F}(u)(t)}$, valid for any real valued function $u(E)$, we obtain

$$2\ \mathrm{Re}\langle s|.\mathscr{B}\rangle=\int_{-\infty}^{+\infty}dt'e^{i[E_R(0)+\eta s(t)]t'}.\mathscr{F}(g|.\mathscr{B}|^2)(s(t),t')=2\pi(g|.\mathscr{B}|^2)(s(t),E_R(0)+\eta s(t)). \tag{9.6}$$

Inserting this in Eq. (9.3), we get the approximate differential equation for the sheet density $s(t)=\|z(t,\cdot)\|^2$

$$\frac{d}{dt}\,s(t)=-\Gamma(s(t))\left[s(t)-2\pi\,\frac{(g|\mathscr{B}|^2)(s(t),E_R(0)+\eta s(t))}{\Gamma(s(t))}\right]. \tag{9.7}$$

This equation is valid for slowly varying solutions which have evolved for a time much longer than Γ^{-1}.

X. QUALITATIVE DISCUSSION AND NUMERICAL RESULTS

We start by examining the simplified fixed-point equation (8.1). For $0\leqslant E\lesssim E_F$ with $E_F\ll V_0$, we have $V_0-E\sim V_0$ (of the same order of magnitude). By evaluating the integral in Eq. (6.4) with $e(s,x)$ approximated by Eq. (5.2) and the driving term given by Eq. (4.7), we have

$$|\mathscr{B}(s,E)|^2\sim(C_0^w)^2V_0^{-1}E_0^wE^{1/2}e^{\{(V_0-E)^{3/2}-[V_0+\alpha(b-a)-E]^{3/2}\}4/3\alpha}.$$

Assuming for simplicity zero temperature, so that $g(E)=\theta(E)(E_F-E)_+/2\pi$, we get

$$g(E_R(s))|\mathscr{B}(s,E_R(s))|^2\sim(C_0^w)^2V_0^{-1}E_0^wE_R(s)_+^{1/2}[E_F-E_R(s)]_+ \times e^{\{[V_0-E_R(s)]^{3/2}-[V_0-E_R(s)+\alpha(b-a)]^{3/2}\}4/3\alpha}.$$

Recalling that $E_R(s)=E_R(0)+\eta s=E_0^b+\alpha(b-a)=E_0^b-\beta(d-c)-\Delta V$, where α and β are given by Eqs. (4.3) and (5.6), respectively, from Eq. (5.24) we get

$$\Gamma(s)\sim(C_0^w)^2E_0^bV_0^{-3/2}\{[V_0-E_R(s)]^{1/2}E_R(s)_+^{1/2}e^{\{[V_0-E_R(s)]^{3/2}-[V_0-E_R(s)+\alpha(b-a)]^{3/2}\}4/3\alpha} +[V_0-\Delta V-E_R(s)]^{1/2}[E_R(s)+\Delta V]^{1/2}e^{\{[V_0-\Delta V-E_R(s)-\beta(d-c)]^{3/2}-[V_0-\Delta V-E_R(s)]^{3/2}\}4/3\beta}\}.$$

We will consider the following two cases:

(1) The barrier $[c,d]$ is more opaque than $[a,b]$ in the sense that the exponential factor in the second term of the above expression for $\Gamma(s)$ is much smaller than the exponential factor in the first term.

(2) The barrier $[a,b]$ is more opaque than $[c,d]$.

In the intermediate case when the two barriers have opacity of the same order, the discussion of case (1) will roughly apply. Notice that opacity depends not only on the relative sizes of $b-a$ and $d-c$, but also on s and ΔV. Therefore, we may have transitions between the two cases when these parameters vary. Interesting phenomena appear when case (1) is possible and we start with that case, recalling that $E_R(s)=E_R(0)+\eta s=E_0^w-\Delta V(b-a)/l+\eta s$. In this case [and neglecting, to start with, the possibility of a transition to the case (2)] the first term in the expression for $\Gamma(s)$ dominates, except when $E_R(s)$ is negative or very small and positive. The function

$$f(s)=2\pi\,\frac{g(E_R(s))|\mathscr{B}(s,E_R(s))|^2}{\Gamma(s)} \tag{10.1}$$

vanishes for $E_R(s)\leqslant 0$ and rises very sharply [with a square root singularity at $E_R(s)=0$] from 0 to

$$f_{\max}\sim E_F \tag{10.2}$$

when $E_R(s)$ is increased from 0 to a small positive value. When $E_R(s)$ is further increased, the function $f(s)$ decreases roughly linearly and vanishes for $E_R(s)\geqslant E_F$. The values $E_R(s)=0$, $E_R(s)=E_F$ correspond to

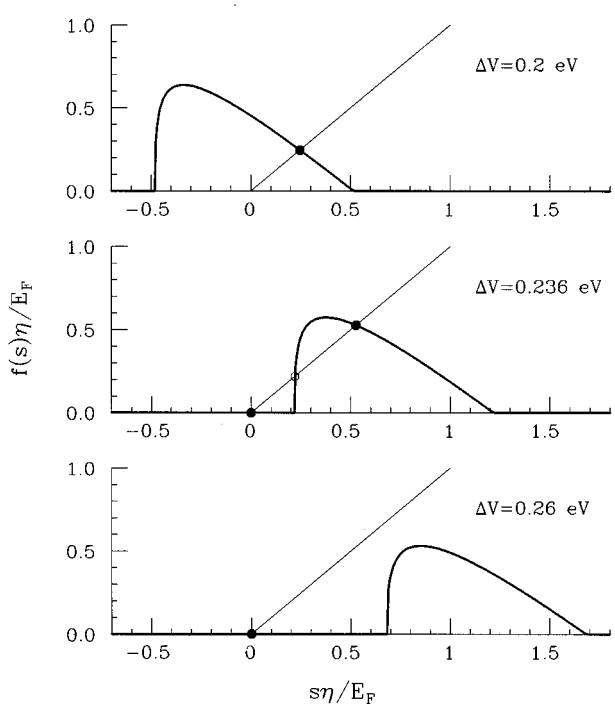

FIG. 2. Graphical solution of the equation $s=f(s)$ for different values of the bias energy ΔV. Note that the support of $f(s)$ has width $\Delta s \simeq E_F/\eta$ (equality strictly holds at zero temperature). The example shown here corresponds to a typical GaAs–AlGaAs heterostructure in which the parameters described in the text have the following values: $n_D=2\times10^{17}$ cm^{-3}, $T=1$ K, $b-a=40$ Å, $c-b=56$ Å, $d-c=70$ Å, $V_0=0.34$ eV, $\epsilon=11.44$, and $m^*=0.067m$, where m is the free electron mass.

$$s=[\Delta V(b-a)/l-E_0^w]/\eta, \quad s=[\Delta V(b-a)/l-E_0^w+E_F]/\eta, \tag{10.3}$$

and describe the boundary points of the support of the function (10.1). When ΔV is increased, these two points move to the right with the same speed as shown in the example of Fig. 2. In Fig. 2 we also see the graphical solution of Eq. (8.1), $s=f(s)$, for different values of ΔV. It is clear that Eq. (8.1) will first have only one solution when $\Delta V(b-a)/l-E_0^w \leqslant 0$, then three solutions for ΔV in some interval, until $\Delta V(b-a)/l-E_0^w \sim \eta f_{\max}$, and again only one solution for even larger values of ΔV. According to the results of Sec. VIII, we see that in the case in which Eq. (8.1) has only one solution, this solution corresponds to an attractive fixed point, and when there are three solutions, the smallest and the largest of these correspond to attractive fixed points, while the intermediate solution corresponds to an unstable fixed point.

For many experimentally relevant situations the resonance width is much smaller than the other energy scales (essentially E_F). In this case we may expect the simplified fixed-point equation (8.1) to be a very good approximation of the more correct equation (7.4), except near the boundary points of the support of the function (10.1). This is confirmed by Fig. 3 where we show the numerical solutions (stable and unstable) of both Eqs. (7.4) and (8.1) for a system having $\Gamma(0)/E_F \simeq 0.01$ at $\Delta V=0.2$ eV. In the case of Eq. (7.4), the corresponding energy integral has been evaluated on a uniform energy mesh having a density of points $\gg \Gamma(0)^{-1}$.

The solutions of the simplified differential equation (9.7) converge to one of the solutions of Eq. (8.1), associated with an attractive fixed point. The phenomenon of hysteresis then becomes clear. We let ΔV increase very slowly from some sufficiently small value up to some sufficiently large positive value and subsequently decrease it very slowly, back to its initial value. Consider a

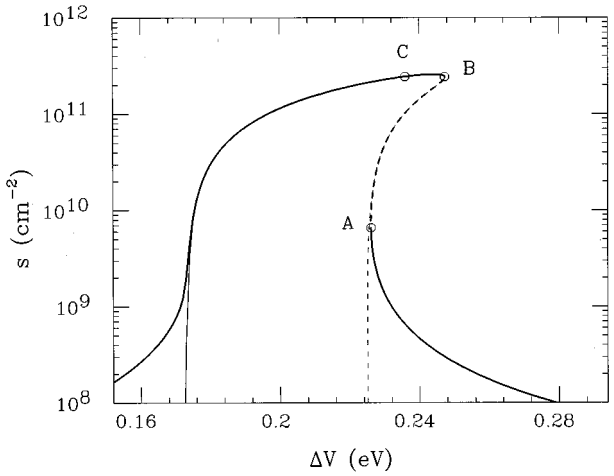

FIG. 3. Fixed point solutions of the sheet density of electrons in the well s as a function of the bias energy ΔV in the same case of Fig. 2. The thick line is the exact case (7.4) and the thin line the small-Γ approximation (8.1). Unstable solutions are represented by dashed lines (both thick and thin).

corresponding solution of the time-dependent Schrödinger equation (2.3) so that we expect the corresponding evolution of the sheet density to be well approximated by the solution of Eq. (9.7), where $\mathscr{B}$ varies slowly with time. First, there is only one (attractive) fixed point and the time-dependent solution has to stay close to that fixed point. Then we have creation of a pair of fixed points (one stable and one unstable) away from the solution, but the solution continues to stay close to the old (stable) fixed point. When ΔV reaches a sufficiently large value, the unstable fixed point runs into the old stable one and they both disappear. At this point, the time-dependent solution has no other choice than to converge to the only remaining fixed point (which is stable). When decreasing ΔV back to its initial value, we have the same behavior, in the sense that the solution stays close to the initially unique fixed point as long as it exists and converges to the new unique fixed point after the old one has collapsed with the unstable one. The bias energy ΔV at which this collapse happens depends on the value of the time-dependent solution and therefore is different when ΔV is increased or decreased.

The phenomenon of hysteresis is clearly seen in Fig. 3, where the collapse points for ΔV decreased from large values and ΔV increased from small values have been marked with A and B, respectively. We have $\Delta V_A < \Delta V_B$. We can estimate the order of magnitude of the hysteresis width $\Delta V_B - \Delta V_A$ by considering that ΔV_A is determined by the condition $E_R(s=0)=0$ and ΔV_B by the condition $E_R(s \simeq f_{\max}) \simeq 0$. We have

$$\Delta V_B - \Delta V_A \sim \eta f_{\max} l (b-a)^{-1} \sim a_B^{-1} E_F (d-c). \tag{10.4}$$

In Figs. 4 and 5 we show the time-dependent evolution of the sheet density $s(t)$ when we start from a fixed point solution corresponding to the point A or B and give an instantaneous small decrement or increment δV to ΔV_A or ΔV_B, respectively. In these figures, the thick lines are the solutions of the full equations (6.3) and (6.5) and the thin lines the solution of the simplified differential equation (9.7). In Fig. 4 the solutions corresponding to the small-Γ limit and the full Schrödinger equation start, as shown in Fig. 3, from different fixed point values, $s(0)$, and converge to the same (approximatively) values. On the other hand, when the starting point is B (Fig. 5) the small-Γ approximation is close to the solution of the full equation except for the value which $s(t)$ has to converge to, again in agreement with Fig. 3.

As a third example of time evolution of the sheet density of electrons in the well, in Fig. 6 we show the behavior of the $s(t)$ solution of the full equations (6.3) and (6.5) after an instantaneous

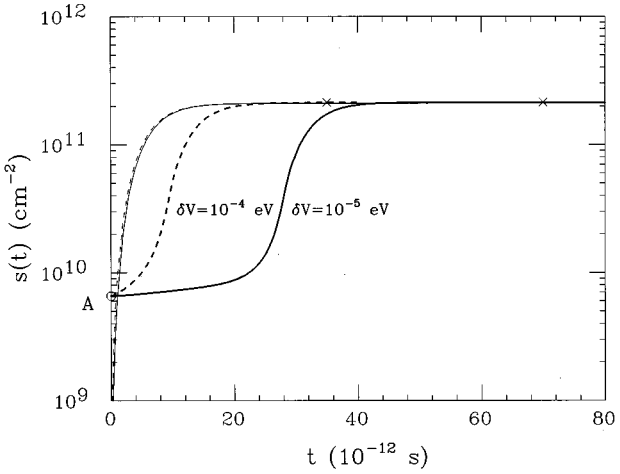

FIG. 4. Sheet density of electrons in the well $s(t)$ as a function of time after an instantaneous decrease δV of the bias energy from the point A of Fig. 3 (thick lines). The crosses are the fixed point solutions at bias $\Delta V_A - \delta V$ where $s(t)$ is expected to converge. The thin lines are the corresponding small-Γ approximation starting from $s(0)=0$.

change δV of the bias energy corresponding to the point C of Fig. 3 well inside the hysteresis region. If $|\delta V|$ is chosen sufficiently large, we observe oscillations of $s(t)$ on the picosecond time scale. Contrary to the claim of Ref. 14, these oscillations are damped since $s(t)$ has to converge to the fixed point solution corresponding the bias energy $\Delta V_C + \delta V$.

In case (2), when the barrier $[a,b]$ is more opaque than the barrier $[c,d]$, the function (10.1) is very small, and for solutions of Eq. (8.1) we can observe only a microscopical hysteresis effect, due to the square root singularity at $E_R(s)=0$, which is likely to be completely absent in the more correct equation (7.4). The absence of the hysteresis effect in this case is in agreement with the experimental results of Ref. 18 and is discussed in Ref. 16.

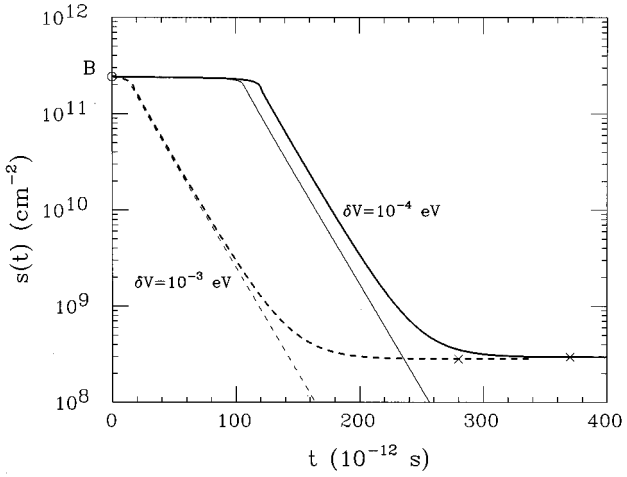

FIG. 5. Sheet density of electrons in the well $s(t)$ as a function of time after an instantaneous increase δV of the bias energy from the point B of Fig. 3 (thick lines). The crosses are the fixed point solutions at bias $\Delta V_B + \delta V$ where $s(t)$ is expected to converge. The thin lines are the corresponding small-Γ approximation. For δV not too large a ghost fixed-point solution is observed with $s(t)$ decaying linearly for $t \leq t_g$ and t_g defined by the condition $E_R(s(t_g))=0$.

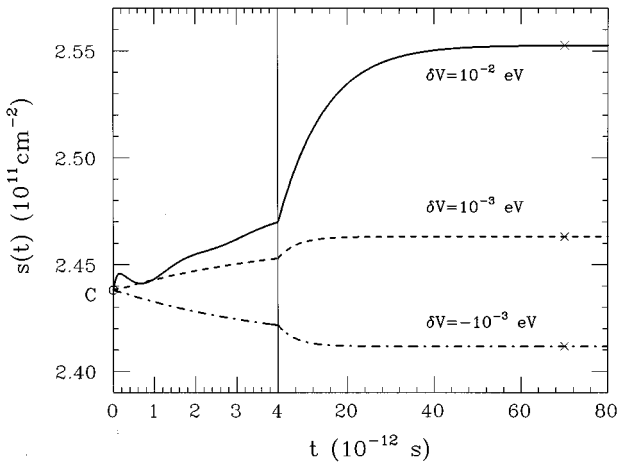

FIG. 6. Sheet density of electrons in the well $s(t)$ as a function of time after an instantaneous change δV of the bias energy from the point C of Fig. 3. The crosses are the fixed-point solutions at bias $\Delta V_C+\delta V$ where $s(t)$ is expected to converge. For $|\delta V|$ not too small damped oscillations are seen at the picosecond scale.

Let us finally consider the case of very wide barriers and see that a transition between cases (1) and (2) has to take place in the hysteresis region. Let $c-b=$const, $(b-a)/(d-c)$ $=$const<1, and $b-a\to\infty$. In this limit, $\eta\sim a_B^{-1}(b-a)$, and the values in Eq. (10.3) are the end points of a short interval of length $\sim E_F a_B/(b-a)$. Let us consider Eq. (8.1) when ΔV is increased from the initial value $(E_0^w-E_F)l/(b-a)$ for which the right end point in Eq. (10.3) is 0. If the constant $(b-a)/(d-c)$ is sufficiently small, we are in case (1). For $(E_0^w-E_F)l/(b-a)\leqslant\Delta V\leqslant E_0^w l/(b-a)$, we remain in case (1), provided that $(b-a)/(d-c)$ is sufficiently small, and Eq. (8.1) has a unique solution. At $\Delta V=E_0^w l/(b-a)$ we have the creation of two new fixed points. If we follow the old fixed point, we cannot remain in case (1) until it disappears. Indeed, if we did, the disappearance would take place when $s\sim f_{\max}$ and at a bias energy $\Delta V\sim a_B^{-1}(d-c)f_{\max}$ obtained by the condition $E_R(s\simeq f_{\max})\simeq 0$. Since $E_R(s)=E_0^b+\alpha(b-a)$ is between 0 and E_F, the inclination α of the first barrier would have to be very small, and we get a finite inclination $\beta\sim -a_B^{-1}f_{\max}$ for the barrier $[c,d]$. Therefore, when $b-a\to\infty$ only the opacity of the first barrier would diverge and, at some point, we would be no longer in case (1). What will actually happen is that when ΔV reaches some value which is bounded independently of $b-a$, we have a transition from case (1) to case (2), and $f_{\max}$ decreases to some value which is much smaller than the rhs in Eq. (10.2). This will cause the disappearance of the fixed point for a much smaller value of s. When a transition from case (1) to case (2) happens, we still observe a hysteresis phenomenon, but this is now caused not only by the *translation* of $f(s)$ as a function of ΔV but also by a *variation* of its height. This effect is already apparent in Fig. 3 where we see a decreasing height of $f(s)$ when increasing ΔV.

XI. THE CASE OF SEVERAL RESONANCES

In this section we discuss very briefly the case with several shape resonances. Much of the discussion is similar to the case of one resonance and we shall assume that we are in a parameter range where all the WKB considerations apply.

First we review the approximation for the shape resonances. We start with the potential V_w and consider its eigenstates $e_j^w(x)$, $j=0,1,\ldots,N-1$ and the corresponding eigenvalues $0<E_0^w<E_1^w<\cdots<E_{N-1}^w<V_0$. Since $e_j^w(x)$ is even as a function of $x-(b+c)/2$ for even j and odd for odd j, we have

$$e_j^w(x)=C_j^w\times\begin{cases}\sin[(j+1)\pi/2-\sqrt{E_j^w}(c-b)/2]e^{-(V_0-E_j^w)^{1/2}(b-x)}, & x<b\\ \sin\{(j+1)\pi/2+\sqrt{E_j^w}[x-(b+c)/2]\}, & b<x<c\\ \sin[(j+1)\pi/2+\sqrt{E_j^w}(c-b)/2]e^{-(V_0-E_j^w)^{1/2}(x-c)}, & x>c.\end{cases}$$

The C^1 condition at $x=b$, or equivalently at $x=c$, gives the quantization condition

$$\tan[(j+1)\pi/2+\sqrt{E_j^w}(c-b)/2]=-(V_0/E_j^w-1)^{-1/2},$$

which can also be written as

$$\tan[\sqrt{E_j^w}(c-b)/2-j\pi/2]=(V_0/E_j^w-1)^{1/2}. \tag{11.1}$$

Representing this equation graphically, we see that $N-1$ is the largest integer $\geqslant 1$ with $\sqrt{V_0}(c-b)/2>(N-1)\pi/2$. The functions $e_j^w(x)$ are normalized, if we choose

$$C_j^w=\left(\frac{E_j^w}{V_0(V_0-E_j^w)^{1/2}}+\frac{(c-b)}{2}+\frac{(V_0-E_j^w)^{1/2}}{V_0}\right)^{-1/2}. \tag{11.2}$$

The eigenvalues E_j^b associated with the potential V_b in Eq. (5.5) can be studied as before, and we get

$$E_j^b=E_j^w-8\pi a_B^{-1}s\,\frac{(C_j^w)^2E_j^w}{4V_0(V_0-E_j^w)}+\mathcal{O}(\alpha^2+\beta^2). \tag{11.3}$$

In the following, we neglect the error $\mathcal{O}(\alpha^2+\beta^2)$. The shape resonances $\lambda_j(s)=E_{R,j}(s)-i\Gamma_j(s)/2$ for the potential $V+W$ are then given by

$$E_{R,j}(s)=E_{R,j}(0)+\eta_j s, \tag{11.4}$$

where

$$E_{R,j}(0)=E_j^w-\Delta V(b-a)/l,\qquad \eta_j=\frac{8\pi a_B^{-1}(b-a)(d-c)}{b-a+d-c}-\frac{8\pi a_B^{-1}(C_j^w)^2E_j^w}{4V_0(V_0-E_j^w)}, \tag{11.5}$$

and

$$\begin{aligned}\Gamma_j(s)=8(C_j^w)^2E_j^b(V_0-E_j^b)^{1/2}V_0^{-2}\{&[V_0+\beta(d-c)-E_j^b]^{1/2}[E_j^b-\beta(d-c)]^{1/2}\\ &\times e^{\{(V_0-E_j^b)^{3/2}-[V_0+\beta(d-c)-E_j^b]^{3/2}\}4/3\beta}+[V_0-\alpha(b-a)-E_j^b]^{1/2}\\ &\times[E_j^b+\alpha(b-a)]_+^{1/2}e^{\{[V_0-\alpha(b-a)-E_j^b]^{3/2}-(V_0-E_j^b)^{3/2}\}4/3\alpha}\}.\end{aligned} \tag{11.6}$$

The corresponding resonant state $e_j(s,x)$, satisfying Eq. (6.2), can be described as in Sec. V.

We still try to solve Eq. (2.11) in two steps. Equation (2.12) is treated as before, while Eq. (2.13) is now handled by letting $\tilde{\nu}$ be a linear combination of the N resonant states $e_0(s,x),\ldots,e_{N-1}(s,x)$. More precisely, we write $\tilde{\nu}(x,t,E)=\exp(-iEt)\nu(x,t,E)$ and $\tilde{\mu}(x,t,E)=\exp(-iEt)\mu(x,t,E)$, so that Eq. (2.13) becomes

$$[-i\partial_t-\partial_x^2+V(x)+W(s,x)-E]\nu(x,t,E)=V_0 1_{[b,c]}(x)\mu(x,t,E). \tag{11.7}$$

Assume,

$$\nu(x,t,E)=\sum_{k=0}^{N-1} z_k(t,E)e_k(s,x), \tag{11.8}$$

where s is defined in Eq. (2.7) and hence will be time dependent. The functions $e_0(s,x),\ldots,e_{N-1}(s,x)$ approximately form an orthonormal family in $L^2([(a+b)/2,(c+d)/2])$, and if we assume that ν dominates over μ in $[(a+b)/2,(c+d)/2]$ then, with a small error, we have

$$s(t)=\sum_{k=0}^{N-1} \|z_k(t,\cdot)\|^2=\|z(t,\cdot)\|^2, \tag{11.9}$$

where the norms are in $L^2(g(E)dE)$ and in $L^2(g(E)dE)^N$, respectively.

Substituting Eq. (11.8) into Eq. (11.7), multiplying by $e_j(s,x)$, and integrating over the contour γ, we get

$$\sum_{k=0}^{N-1} \int_\gamma dx[-i\partial_t+\lambda_k(s)-E][z_k(t,E)e_k(s,x)]e_j(s,x)=V_0\int_b^c dx\ \mu(x,t,E)e_j(s,x). \tag{11.10}$$

From the relations $\int_\gamma dx\ e_k(s,x)e_j(s,x)=\delta_{k,j}$, we conclude that $\int_\gamma dx[\partial_s e_k(s,x)]e_j(s,x)$ is an antisymmetric matrix, and since $e_k(s,x)$ are approximately real functions near $[b,c]$, this matrix is also very close to a real one. Equation (11.10) can be written as

$$[-i\partial_t+\lambda_j(s)-E]z_j(t,E)-i\partial_t(s(t))\sum_{k=0}^{N-1}\int_\gamma dx[\partial_s e_k(s,x)]e_j(s,x)$$
$$=V_0\int_b^c dx\ \mu(x,t,E)e_j(s,x). \tag{11.11}$$

Due to the facts that (i) $\partial_t s(t)$ can be expected to be very small and (ii) $e_k(s,x)$ is roughly independent of s near $[b,c]$ so that the integral $\int_\gamma dx[\partial_s e_k(s,x)]e_j(s,x)$ can be expected to be very small, we will neglect the sum in the lhs of Eq. (11.11). In this case, we have

$$\partial_t z_j(t,E)=\{-\Gamma_j(s)/2+i[E-E_{R,j}(s)]\}z_j(t,E)+\mathscr{B}_j(t,s,E), \tag{11.12}$$

where $\mathscr{B}_j(t,s,E)=iV_0\int_b^c dx\ \mu(x,t,E)e_j(s,x)$.

We assume that $\mathscr{B}_j$ vary slowly with t, so it is meaningful to look at instantaneous fixed points of the vector field defined by the rhs of Eq. (11.12) in $L^2(g(E)dE)^N$. Assuming, for simplicity, that $\mathscr{B}_j$ are independent of t we see that $z(E)=(z_0(E),\ldots,z_{N-1}(E))$ is a fixed point precisely when

$$z_j(E)=\frac{-\mathscr{B}_j(s,E)}{-\Gamma_j(s)/2+i[E-E_{R,j}(s)]},\quad j=0,\ldots,N-1 \tag{11.13}$$

from which we get the compatibility condition for $s=\|z\|^2$:

$$s-\sum_{j=0}^{N-1}\int dE\ \frac{g(E)|\mathscr{B}_j(s,E)|^2}{[\Gamma_j(s)/2]^2+[E-E_{R,j}(s)]^2}=0. \tag{11.14}$$

Conversely, if s is a solution of Eq. (11.14), then Eq. (11.13) defines the unique fixed point with $\|z\|^2=s$.

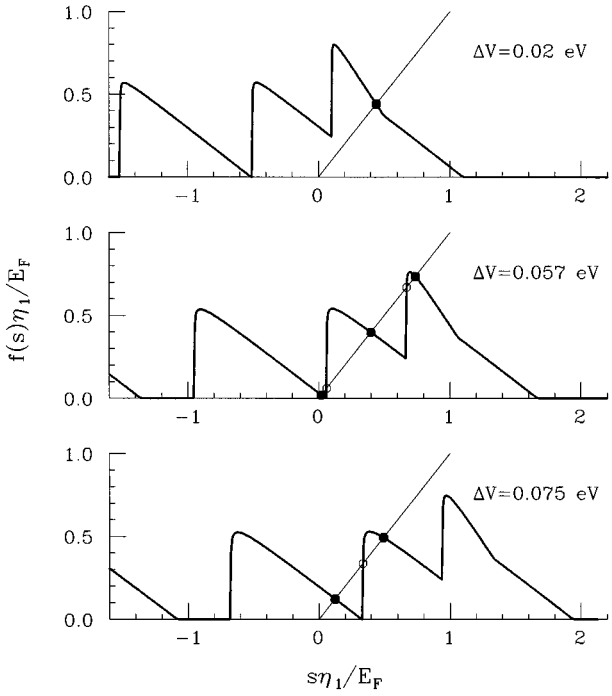

FIG. 7. Graphical solution of the equation $s=f(s)$ for different values of the bias energy ΔV in a multiple-resonance case. We used the same parameters of Fig. 2 except $b-a=20$ Å, $c-b=360$ Å, $d-c=50$ Å.

In the small-Γ limit, as in Sec. VIII we get the simplified fixed-point equation

$$s-\sum_{j=0}^{N-1} 2\pi \frac{(g|\mathscr{B}_j|^2)(s,E_{R,j}(s))}{\Gamma_j(s)}=0. \tag{11.15}$$

In view of Eq. (11.4), the term of index j in Eq. (11.15) is a function of s with support in the interval

$$[\Delta V(b-a)/l-E_j^{\mathrm{w}}]/\eta_j \leqslant s \leqslant [\Delta V(b-a)/l-E_j^{\mathrm{w}}+E_F]/\eta_j\,, \tag{11.16}$$

and when ΔV increases this interval moves to the right with speed $(b-a)/(l\eta_j)$ as shown in the example of Fig. 7.

In Fig. 8 we compare the corresponding fixed point solutions obtained by solving Eq. (11.14) with those obtained in the small-Γ limit (11.15) as a function of the bias energy ΔV. Between the points marked as A and B we observe five fixed points. Below we give some results about the nature of fixed points, which are more complicated than those in the case of a single resonance, and it is not clear that those results are applicable in the situation of Fig. 8. If we assume that they are applicable, then three fixed points are stable and two unstable. The existence of more than three fixed points, i.e., the maximum number allowed for $N=1$, is related to the possibility that the intervals (11.16) are not disjoint, as clearly understood by Fig. 7.

It is interesting to study the evolution of the sheet density $s(t)$ away from a point like B in Fig. 8 where a (presumably) stable fixed point and an unstable one collapse while two other fixed points survive. In Fig. 9 we show the behavior of $s(t)$ obtained by numerically integrating Eq. (11.12) after an instantaneous increase ΔV of the initial bias ΔV_B. If the total bias $\Delta V_B+\delta V<\Delta V_C$, where C is the next point where a new couple of fixed points collapse, $s(t)$

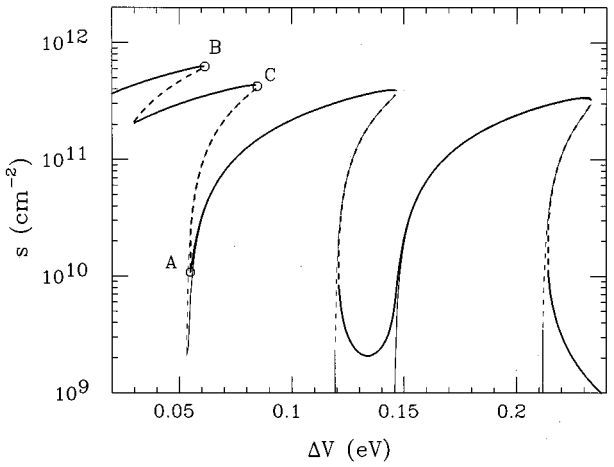

FIG. 8. Fixed-point solutions of the sheet density of electrons in the well s as a function of the bias energy ΔV in the same case of Fig. 7. The thick line is the solution of Eq. (11.14) and the thin line the small-Γ limit (11.15). Possibly unstable solutions are represented by dashed lines (both thick and thin).

converges to the fixed point closest to its initial value $s(0)$. When $\Delta V_B+\delta V>\Delta V_C$, $s(t)$ first approaches the value corresponding to the collapse point C but finally has to converge to the lower unique fixed point corresponding to the chosen bias.

Next we study the linearization of the vector field defined by the rhs of Eq. (11.12) at a fixed point under the following simplifying assumption:

$$\begin{gathered}\Gamma_j \text{ is independent of } s, \quad \mathscr{B}_j=\mathscr{B}_j(E) \text{ is independent of } t \text{ and } s,\\ \eta_j=\eta \text{ is independent of } j.\end{gathered} \tag{11.17}$$

Then Eq. (11.12) becomes,

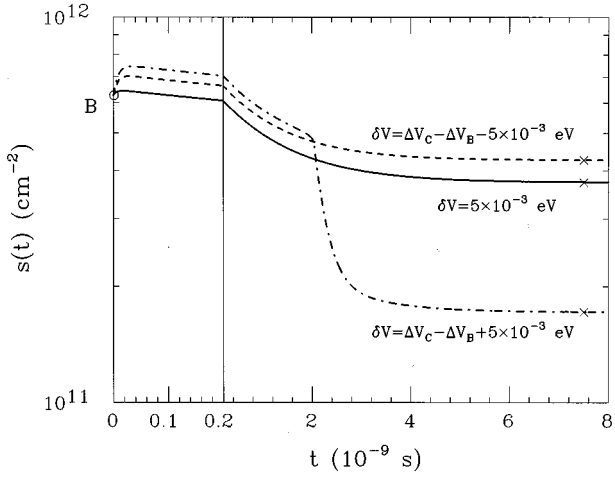

FIG. 9. Sheet density of electrons in the well $s(t)$ as a function of time after an instantaneous increase δV of the bias energy from the point B of Fig. 8. The crosses are the fixed-point solutions at bias $\Delta V_B+\delta V$ where $s(t)$ is expected to converge.

$$\partial_t z_j(t,E)=[-\Gamma_j/2+i[E-E_{R,j}(0)-\eta s]]z_j(t,E)+\mathscr{B}_j(E). \tag{11.18}$$

The same calculations as in Sec. VIII show that the complexification $\mathscr{L}$ of the linearization of the vector field defined by the rhs of Eq. (11.18) at a fixed point is given by

$$\mathscr{L}\begin{pmatrix} u_0 \\ \vdots \\ u_{N-1} \\ v_0 \\ \vdots \\ v_{N-1} \end{pmatrix} = \begin{pmatrix} \{-\Gamma_0/2+i[E-E_{R,0}(0)-\eta s]\}u_0 - i\,\eta(\langle u|z\rangle+\langle v|\overline{z}\rangle)z_0 \\ \vdots \\ \{-\Gamma_{N-1}/2+i[E-E_{R,N-1}(0)-\eta s]\}u_{N-1} - i\,\eta(\langle u|z\rangle+\langle v|\overline{z}\rangle)z_{N-1} \\ \{-\Gamma_0/2-i[E-E_{R,0}(0)-\eta s]\}v_0 + i\,\eta(\langle u|z\rangle+\langle v|\overline{z}\rangle)\overline{z_0} \\ \vdots \\ \{-\Gamma_{N-1}/2-i[E-E_{R,N-1}(0)-\eta s]\}v_{N-1} + i\,\eta(\langle u|z\rangle+\langle v|\overline{z}\rangle)\overline{z_{N-1}} \end{pmatrix}. \tag{11.19}$$

Here, $\langle u|z\rangle = \Sigma_{j=0}^{N-1}\langle u_j|z_j\rangle_{L^2(g(E)dE)}$. The operator $\mathscr{L}$ is a rank one perturbation of an operator with essential spectrum contained in $\cup_{j=0}^{N-1}(-\Gamma_j/2+i\mathbf{R})$. We look for eigenvalues $\lambda\in\mathbf{C}$ with $\mathrm{Re}\,\lambda\neq-\Gamma_j/2$ for all j. If $(u_0,\ldots,u_{N-1},v_0,\ldots,v_{N-1})$ is a corresponding eigenvector, we get as in Sec. VIII

$$u_j=\frac{\kappa z_j(E)}{-\Gamma_j/2+i[E-E_{R,j}(0)-\eta s]-\lambda}, \quad v_j=\frac{-\kappa\overline{z_j}(E)}{-\Gamma_j/2-i[E-E_{R,j}(0)-\eta s]-\lambda}, \tag{11.20}$$

where

$$\kappa=i\,\eta(\langle u|z\rangle+\langle v|\overline{z}\rangle). \tag{11.21}$$

Using Eqs. (11.13) and (11.20) in Eq. (11.21), we see that λ is an eigenvector precisely when

$$1-2\,\eta\sum_{k=0}^{N-1}\int dE\,\frac{[E-E_{R,k}(0)-\eta s]g(E)|\mathscr{B}_k(E)|^2}{\{(\Gamma_k/2+\lambda)^2+[E-E_{R,k}(0)-\eta s]^2\}\{(\Gamma_k/2)^2+[E-E_{R,k}(0)-\eta s]^2\}}=0. \tag{11.22}$$

As in the case $N=1$, we observe that the lhs of Eq. (11.22) for $\lambda=0$ is equal to the s-derivative of the lhs of Eq. (11.14). Moreover, when $\lambda\to+\infty$, the lhs of Eq. (11.22) converges to 1, so if it is <0 for $\lambda=0$, it has to vanish for some $\lambda>0$. Hence, as in the case $N=1$, we get the following:

Proposition XI.1: Let z be a fixed point of Eq. (11.18), so that $s=\|z\|^2$ solves Eq. (11.14). If the s-derivative of the lhs *of Eq. (11.14) is <0, then z is not an attractive fixed point.*

We now pass to the small-Γ limit, where Eq. (11.14) is replaced by Eq. (11.15) and we keep the simplifying assumption (11.17).

Proposition XI.2 (small-Γ limit): Assume that the intervals (11.16) are disjoint and let z be a fixed point of Eq. (11.18). Then z is attractive precisely when the s-derivative of the lhs of Eq. (11.15) is >0.

Proof: The s-derivative of the lhs of Eq. (11.15) is

$$1-\sum_{j=0}^{N-1}\frac{2\pi\eta(g|\mathscr{B}_j|^2)'[E_{R,j}(0)+\eta s]}{\Gamma_j}, \tag{11.23}$$

where $(g|\mathscr{B}_j|^2)'=\partial_E(g|\mathscr{B}_j|^2)$. On the other hand, in the small-Γ limit, Eq. (11.22) for the eigenvalues of the linearization becomes as in Sec. VIII

$$1-2\eta\sum_{k;\Gamma_k/2+\mathrm{Re}\,\lambda>0}\frac{\pi(g|\mathscr{B}_k|^2)'(E_{R,k}(0)+\eta s)}{\Gamma_k+\lambda}$$
$$+2\eta\sum_{k;\Gamma_k/2+\mathrm{Re}\,\lambda<0}\frac{\pi(g|\mathscr{B}_k|^2)'(E_{R,k}(0)+\eta s)}{\lambda}=0. \tag{11.24}$$

We are only interested in the possible existence of solutions to this equation with $\mathrm{Re}\,\lambda\geqslant 0$, and for such λ Eq. (11.24) reduces to

$$1-2\eta\sum_{k=0}^{N-1}\frac{\pi(g|\mathscr{B}_k|^2)'[E_{R,k}(0)+\eta s]}{\Gamma_k+\lambda}=0. \tag{11.25}$$

If λ is a solution, then by the condition that the intervals (11.16) are disjoint, only one term in the last sum, say for $k=m$, is $\neq 0$, so that Eq. (11.25) becomes

$$1-2\eta\,\frac{\pi(g|\mathscr{B}_m|^2)'[E_{R,m}(0)+\eta s]}{\Gamma_m+\lambda}=0, \tag{11.26}$$

while expression (11.23) becomes

$$1-2\eta\,\frac{\pi(g|\mathscr{B}_m|^2)'[E_{R,m}(0)+\eta s]}{\Gamma_m}. \tag{11.27}$$

It is then easy to see that the solution of Eq. (11.26) has a negative real part precisely when expression (11.27) is positive, and this concludes the proof of the last proposition.

When the intervals (11.16) have nonempty intersections, the situation is more complicated, and the following example is an indication that the last proposition may be false.

Example: There exist $\Gamma_1,\Gamma_2>0$, $a_1,a_2\in\mathbf{R}$, such that $1-(a_1/\Gamma_1+a_2/\Gamma_2)>0$, while $1-[a_1/(\Gamma_1+\lambda)+a_2/(\Gamma_2+\lambda)]=0$ for some positive λ. Indeed, choose $\Gamma_1=1$, $a_1=2$, $\Gamma_2=\delta>0$ very small, $a_2=-2\delta$. Then $1-a_1/\Gamma_1-a_2/\Gamma_2=1>0$. If $\delta\ll\lambda_0\ll 1$, we have

$$1-\frac{a_1}{\Gamma_1+\lambda_0}-\frac{a_2}{\Gamma_2+\lambda_0}\approx -1.$$

Hence $1-[a_1/(\Gamma_1+\lambda)+a_2/(\Gamma_2+\lambda)]$ must vanish for some λ between 0 and λ_0.

As in Sec. IX, we can derive a simplified differential equation for $(s_0(t),\ldots,s_{N-1}(t))$, where $s_j(t)=\|z_j(t,\cdot)\|^2$, so that $s(t)=\Sigma_{j=0}^{N-1}s_j(t)$. We drop the simplifying assumption (11.17), but keep, for simplicity, the assumption that $\mathscr{B}_j$ are independent of t. Assume that $z(t,E)=(z_0(t,E),\ldots,z_{N-1}(t,E))$ is a solution of Eq. (11.12) which has existed for a long time with a uniformly bounded norm. As in Sec. IX, we take the scalar product of Eq. (11.12) with z_j and get

$$\frac{d}{dt}s_j(t)=-\Gamma_j(s)+2\,\mathrm{Re}\langle z_j|\mathscr{B}_j\rangle. \tag{11.28}$$

Using

$$z_j(t,E)=\int_{-\infty}^{t}dt'\,e^{i[E-E_{R,j}(0)](t-t')-\int_{t'}^{t}dt''\Gamma_j(s(t''))/2-i\eta_j\int_{t'}^{t}dt''s(t'')}\mathscr{B}_j(s(t'),E), \tag{11.29}$$

and, under the assumption that $s(t')$ is slowly varying, we get as in Sec. IX

$$2\,\mathrm{Re}\langle z_j|\mathscr{B}_j\rangle \simeq 2\pi(g|\mathscr{B}_j|^2)(s(t),E_{R,j}(0)+\eta_j s(t)), \tag{11.30}$$

and the simplified equations

$$\frac{d}{dt}\,s_j(t) = -\Gamma_j(s(t))\left[s_j(t) - 2\pi\,\frac{(g|\mathscr{B}_j|^2)(s(t),E_{R,j}(0)+\eta_j s(t))}{\Gamma_j(s(t))}\right], \tag{11.31}$$

for $j=0,1,\ldots,N-1$, and $s=\Sigma_{j=0}^{N-1}s_j$. We notice that the region defined by $s_j\geqslant 0$ for $0\leqslant j\leqslant N-1$ is stable under the forward flow associated with the system (11.31). Moreover, if $(s_0,\ldots,s_{N-1})$ is a fixed point of this system, then we get precisely Eq. (11.15). Conversely, if s is a solution of Eq. (11.15), then

$$s_j = 2\pi\,\frac{(g|\mathscr{B}_j|^2)(s,E_{R,j}(0)+\eta_j s)}{\Gamma_j(s)} \tag{11.32}$$

defines the corresponding unique fixed point solution with $s=\Sigma_{j=0}^{N-1}s_j$.

We end this section by investigating the linearization of Eq. (11.31) at a fixed-point solution, under the simplifying assumption (11.17). An easy calculation shows that the linearization is given by

$$\mathscr{M}\begin{pmatrix} v_0 \\ \vdots \\ v_{N-1}\end{pmatrix} = \begin{pmatrix} -\Gamma_0 v_0 + 2\pi\eta s(g|\mathscr{B}_0|^2)'[E_{R,0}(0)+\eta s]\Sigma_{k=0}^{N-1}v_k \\ \vdots \\ -\Gamma_{N-1}v_{N-1} + 2\pi\eta s(g|\mathscr{B}_{N-1}|^2)'[E_{R,N-1}(0)+\eta s]\Sigma_{k=0}^{N-1}v_k\end{pmatrix}. \tag{11.33}$$

If λ is an eigenvalue of $\mathscr{M}$ with $\Gamma_j+\lambda\neq 0$ for every j, and ${}^t(v_0,\ldots,v_{N-1})$ a corresponding nontrivial eigenvector, we have

$$v_j = 2\pi\eta\,\frac{(g(|\mathscr{B}_j|^2)'[E_{R,j}(0)+\eta s]}{\Gamma_j+\lambda}\sum_{k=0}^{N-1}v_k.$$

Then necessarily the sum is $\neq 0$, and by summing these N relations, we see that λ is an eigenvalue precisely when Eq. (11.25) holds. We finally get:

Proposition XI.3: Under the simplifying assumption (11.17) and in the small-Γ limit, let z be a fixed point of Eq. (11.18) and let $(s_0,\ldots,s_{N-1})$ be the corresponding fixed-point solution of Eq. (11.31). Then the linearizations of Eqs. (11.18) and (11.31) at the corresponding fixed points have the same eigenvalues in the right half plane $\mathrm{Re}\,\lambda\geqslant 0$ *[given by Eq. (11.25)]. In particular, z is an attractive fixed point for Eq. (11.18) precisely when $(s_0,\ldots,s_{N-1})$ is an attractive fixed point for Eq. (11.31).*

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Electron counting statistics and coherent states of electric current

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A theory of electron counting statistics in quantum transport is presented. It involves an idealized scheme of current measurement using a spin 1/2 coupled to the current so that it precesses at the rate proportional to the current. Within such an approach, counting charge without breaking the circuit is possible. As an application, we derive the counting statistics in a single channel conductor at finite temperature and bias. For a perfectly transmitting channel the counting distribution is Gaussian, both for zero-point fluctuations and at finite temperature. At constant bias and low temperature the distribution is binomial, i.e., it arises from Bernoulli statistics. Another application considered is the noise due to short current pulses that involve few electrons. We find the time-dependence of the driving potential that produces coherent noise-minimizing current pulses, and display analogies of such current states with quantum-mechanical coherent states. © *1996 American Institute of Physics.* [S0022-2488(96)01610-6]

I. INTRODUCTION

Quantum transport in nanostructures has been a subject of many recent studies.[1] Transport properties like Ohmic conductivity can be understood in terms of the quantum scattering problem in the conductor, which provides a theory of quantum coherence of transport.[2] An interesting topic emerging from this theory is that of fluctuations of electric current due to the discreteness of electric charge, a property intrinsic to quantum transport.[3–5] It has been found that current fluctuations have properties reflecting profound aspects of underlying quantum dynamics.[6–9] For example, the quantum noise caused by a dc current is reduced below classical shot noise level.[3–9] This suppression has been understood as an effect of enhanced regularity of transmission events due to Fermi statistics.[10] Besides theoretical interest, such phenomena may lead to applications. Given the development of nano-technologies, the transmission of signals by single- or few-electron pulses will become common, and then one will see the quantum statistics of current working.

In this paper we update the theory of quantum measurement of electric current.[11] Our goal is a complete description of charge fluctuations, rather than developing measurement theory (see Secs. II, III). We shall derive a microscopic formula for electron counting distribution [see Sec. III, Eq. (11), and Sec. IV, Eq. (26)] that can be used for any system, e.g., with an interaction or with a time-dependent potential.[12] As an application, we test the method on the statistics in a single channel ideal conductor for non-equilibrium and equilibrium noise at finite temperature, and for zero-point equilibrium fluctuations (Secs. IV, V). In particular, the fluctuations of a dc current at zero temperature are found to obey binomial statistics (Sec. VI) with the probabilities of outcomes related to transmission coefficients of elastic scattering in the system, and with the number of attempts $N=eVt/h$, where V is applied voltage, and t is the time of measurement.

Another property of quantum noise that does not have a classical analog is its phase sensitivity.[13,14] For the current correlator $\langle\langle j(t_1)j(t_2)\rangle\rangle_+$ it results in a periodic sinusoidal dependence on Faraday's flux due to applied voltage, $\Phi=c\int_{t_1}^{t_2}V(t)dt$, with the period $\Phi_0=hc/e$. The

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phase sensitivity manifests itself in singularities of the low frequency noise power in a junction driven by ac and dc signals together.[15]

Even more remarkable is the behavior of current fluctuations induced by a short pulse of voltage.[13,16] Total charge that flows through the conductor due to a voltage pulse fluctuates in such a way that the mean square fluctuation diverges whenever the flux of the pulse is not an integer: $\varphi = e/\hbar \int_{-\infty}^{\infty} V(t)dt \neq 2\pi n$. On the other hand, for $\varphi = 2\pi n$ the fluctuation of the transmitted charge is finite (Sec. VII). This result has a simple interpretation in terms of the Anderson orthogonality catastrophe theory, since the flux φ enters the time-dependent scattering matrix of the conductor through the forward scattering amplitude.

With this, one is led to address the issue of current states that minimize the current fluctuations at fixed mean transmitted charge.[16,17] It is found in Sec. VIII that such states are produced by time-dependent voltage of the form

$$V(t) = \pm \frac{h}{\pi e} \sum_{k=1}^{n} \frac{\tau_k}{(t-t_k)^2 + \tau_k^2}, \quad \tau_k > 0, \tag{1}$$

a sum of Lorentzian pulses of unit flux each. It is remarkable that the minimal noise due to such sequence of pulses is independent of the pulse positions t_k and widths τ_k, which leads to obvious parallels with solitons in the theory of non-linear integrable systems. The noise minimizing current states can be compared to the coherent states that minimize the quantum-mechanical uncertainty. Apart from the obvious similarity, there is a difference: the coherent current states are many-body time-dependent scattering states. Their role in transport is an interesting subject of future work: one expects that representing many-body states as a superposition of these coherent states has an advantage similar to that provided by coherent states of one particle.

II. MEASURING ELECTRIC CURRENT

Instantaneous measurement is described in quantum mechanics by wavepacket reduction that involves projecting on eigenstates of an observable, represented by a Hermitian operator. A different kind of measurement, extended in the time domain, is realized in detectors and other counting devices. It is known that in such cases a certain revision of the measurement description is necessary. A famous example is the theory of photon detectors[18] in quantum optics. Due to Bose statistics, photons entering a photo-counter are correlated in time, and this makes the theory of photon detection a problem of many-particle statistics. For a single normal mode of radiation field the probability P_m to count m photons over time t is given by

$$P_m = \frac{(\eta t)^m}{m!} \langle :(a^+ a)^m e^{-\eta t a^+ a}: \rangle, \tag{2}$$

where a^+ and a are Bose operators of the mode, η is the counter efficiency parameter, and $\langle \cdots \rangle$ stands for the average over a quantum state. The normal ordering $:\cdots:$ is an important element of the formalism. Physically, it means that, after having been detected, each photon is destroyed, e.g., it is absorbed in the detector. Instead of the probabilities (2), it is more convenient to deal with the generating function

$$\chi(\lambda) = \sum_m P_m e^{i\lambda m}. \tag{3}$$

For the single normal mode Eq. (2) leads to

$$\chi(\lambda) = \langle :\exp\ \eta t (e^{i\lambda} - 1) a^+ a: \rangle. \tag{4}$$

Eqs. (2), (3), and (4) account very well for numerous experimental situations.[19] Particularly interesting is the case of a coherent state $|z\rangle$, $a|z\rangle = z|z\rangle$, where z is a complex number. It corresponds to the radiation field of an ideal laser, and with Eq. (4) one easily gets Poisson counting distribution,

$$P_m = \frac{(Jt)^m}{m!} e^{-Jt}, \quad J = \eta |z|^2, \tag{5}$$

which describes the so-called minimally bunched light source.

Similar to the photon detection, electric measurement is performed on a system containing an enormous number of particles—in this case fermions—and thus one expects the effects of Fermi statistics to be important. Also, the duration of electric measurement is typically much longer than the time it takes the system to transmit one electron by microscopic tunneling, scattering, or diffusion. Apart from these similarities, there is, however, a crucial difference from the photon counting: the number of electrons is not changed by the current measurement, since electric charge is conserved. This has to be contrasted with absorption of photons in photo-counters. Related to this, there is another important difference: at every detection of a photon, its energy $\hbar\omega$ is taken from the radiation field, which makes plain photodetectors insensitive to zero-point fluctuations of electromagnetic field. On the contrary, the measurement of current fluctuation is usually performed without changing energy of the system, which makes the zero-point noise an unavoidable component of any electric measurement.[20] (Let us emphasize that the difference has nothing to do with the type of quantum statistics, Fermi or Bose. Rather it is the difference between the two kinds of measurement, e.g., see Ref. 21, where counting of fermions was discussed using an optical-like counter that has to capture an electron in order to detect it.)

In the classical picture, the measurement gives the charge $Q(t) = \int_0^t j(t')dt'$ transmitted during the measurement time t. The probabilities P_m of counting m electrons can then be obtained by averaging $\delta(Q(t) - me)$ over the state of the system. In a quantum problem electric current is an operator, and since currents at different moments do not commute, the operator of transmitted charge $\hat{Q}(t) = \int_0^t \hat{j}(t')dt'$ generally does not make any sense. Instead, since we are interested in higher-order statistics of current fluctuations, beyond $\langle \hat{j}(t) \rangle$ and $\langle\langle j(t_1) j(t_2) \rangle\rangle_+$, in order to compute electron counting distribution, we have to include the measuring system in the quantum Hamiltonian. Our approach is motivated by the example of the quantum mechanical systems with strong coupling to macroscopic environment, introduced by Leggett, that can be treated consistently only by adding the ''measuring environment'' to the quantum problem.[22]

For that we introduce a model quantum galvanometer, a spin 1/2 that precesses in the magnetic field B of the current. For a classical system, the rate of precession is proportional to $B(t)$, and $B(t)$ is proportional to the current $I(t)$: $B(t) = \text{const}\, I(t)$. Therefore, the precession angle of the spin directly measures transmitted charge $\delta Q = \int_0^t I(t')dt'$. We adopt the same measurement procedure for the quantum circuit, i.e., we include in the electron Hamiltonian the Ampère's vector potential due to the spin:

$$\vec{A}(r) = -\mu \vec{\sigma} \times \vec{\nabla} \frac{1}{|r|}, \tag{6}$$

where $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are Pauli matrices. Thus we obtain a Hamiltonian describing the motion of electrons, the measuring spin, and their coupling. Now, according to what has been said, we have to solve dynamics of the spin in the presence of the fluctuating current, find the distribution of precession angles, and then interpret it as a distribution of transmitted charge. Of course, a question remains about the back effect of the spin on the system, as in any other problem of quantum measurement. However, as we find below in (18) and (19), only the phase of an electron state is affected by the presence of the spin, not the amplitude. Moreover, the phase will change

only for the transmitted, but not for the reflected wave. As a result, the probabilities we obtain do not depend on the coupling constant of the spin. This justifies the assumption that the spin measures charge transfer in a non-invasive way.

It is worth remarking that our scheme resembles the ''Larmor clock'' approach[23] to the problem of traversal time for motion through a classically forbidden region. In this problem one is interested, e.g., in the time spent by a particle tunneling through a barrier. The Larmor clock approach involves an auxiliary constant magnetic field B added in the classically forbidden region, and a spin 1/2 carried by the particle that interacts with the field: $\mathscr{H}_{int}=-\hat{\sigma}_z B$. The precession angle of the spin measures traversal time. Comparing the two approaches is very tutorial: see Appendix A, where the Larmor clock is reviewed.

III. SPIN 1/2 AS A GALVANOMETER

Having clarified our motivation, we proceed semi-phenomenologically and choose a new vector potential in the spin-current interaction $-(1/c)\vec{j}\vec{A}$. We replace the Ampère's long-range form (6) by a model vector potential,

$$\hat{A}_i(r)=\frac{\lambda\Phi_0}{4\pi}\hat{\sigma}_z\nabla_i\theta(f(r)-f_0), \tag{7}$$

concentrated on some surface S defined by the equation $f(r)=f_0$. Here $\Phi_0=hc/e$, λ is a coupling constant, $f(r)$ is an arbitrary function, and, as usual, the step-function $\theta(x)=1$ for $x>0$, 0 for $x<0$. The surface S defines a section of the conductor on which the interaction is localized:

$$\mathscr{H}_{int}=\int -\frac{1}{c}\hat{\vec{j}}\vec{\hat{A}}d^3r=-\frac{\lambda\hbar}{2e}\hat{\sigma}_z\hat{I}_S, \tag{8}$$

where $\hat{I}_S=\int_S\hat{\vec{j}}\,\vec{ds}$, i.e., the spin now is coupled to the total current through the section S. With the choice (7) of the vector potential one can study current fluctuations in an arbitrary section of the conductor. Another advantage of the phenomenological Equation (7) is that it involves only one Pauli matrix, which makes the spin dynamics essentially trivial. The choice of the quantization axis of the spin is arbitrary since (8) will be the only spin-dependent part of the Hamiltonian. Finally, another advantage of the form (8) is that by switching from the smooth function (6) to the singular form (7) we enforce integer values of counted charge. To understand this, let us note that in the ''fuzzy'' case (6) the measurement can start at the moment when one of the electrons is located somewhere in the middle of the volume where $A\neq 0$, and then a fractional part of the electron charge will be counted. On the contrary, in the ''sharp'' case (7), the spin responds to the presence of an electron only when it crosses the section S. We shall see below in a microscopic calculation that integer values of charge follow automatically from gauge invariance, since the form (7) is a gradient of a scalar.

Thus we come to the Hamiltonian,

$$\hat{\mathscr{H}}_\sigma=\hat{\mathscr{H}}(\tilde{p},r),\quad \tilde{p}_i=p_i-\frac{e}{c}\hat{A}_i, \tag{9}$$

where the spin-dependent $\vec{\hat{A}}$ is taken in the form (7). An essential feature of our approach is that we treat the constant λ of coupling between the spin and the current as a *variable*, i.e., we consider the spin precession as a function of the parameter λ. The reason is that, unlike the photon counting problem, our measurement scheme directly generates the function $\chi(\lambda)$, and then the counting probabilities P_m are obtained by reading Eq. (3) backwards.

At this point we are able to formulate our main result. Let us define a new Hamiltonian,

$$\hat{\mathscr{H}}_\lambda = \hat{\mathscr{H}}(\tilde{p}, r), \quad \tilde{p}_i = p_i - \tfrac{1}{2}\lambda\hbar\nabla_i\theta(f(r) - f_0), \tag{10}$$

simply by supressing $\hat{\sigma}_z$ in Eq. (7). The Hamiltonian $\hat{\mathscr{H}}_\lambda$ involves only quantities of the electron subsystem. Below we show that by measuring precession of the spin coupled to the current, one obtains the quantity

$$\chi(\lambda) = \langle e^{i\hat{\mathscr{H}}_{-\lambda}t} e^{-i\hat{\mathscr{H}}_\lambda t}\rangle. \tag{11}$$

Here the brackets $\langle\cdots\rangle$ stand for averaging over the initial state of electrons. Note that $\chi(\lambda)$ is written in terms of a purely electron problem, not involving spin variables. We shall find that the function $\chi(\lambda)$ defines the result of any measurement of the spin polarization after the time t when the spin-current coupling is turned off. Moreover, we shall see that the function (11) has the meaning of a generating function of electron counting distribution, i.e., the Fourier transform of $\chi(\lambda)$ gives counting probabilities, entirely analogous to (3).

Our goal now will be to express evolution of the spin in terms of quantities corresponding to the electron system. The interaction is given by Eqs. (7), (9). Suppose that the measurement started at the moment 0 and stopped at the time t, i.e., the spin-current interaction is turned on during the time interval $0 < \tau < t$. Let us evaluate the density matrix $\hat{\rho}_s(t)$ of the spin, right after it is disconnected from the circuit. We have

$$\hat{\rho}_s(t) = \mathrm{tr}_e(e^{-i\hat{\mathscr{H}}_\sigma t}\hat{\rho}e^{i\hat{\mathscr{H}}_\sigma t}), \tag{12}$$

where $\hat{\rho}$ is the initial density matrix $\hat{\rho}_e \otimes \hat{\rho}_s$ at $t = 0$, $\hat{\rho}_e$ is the initial density matrix of electrons, and $\mathrm{tr}_e(\cdots)$ means the partial trace taken over electron states, the spin indices left free. In terms of the spin variables, the operator $e^{-i\hat{\mathscr{H}}_\sigma t}$ is a function only of $\hat{\sigma}_z$, and hence it is diagonal in spin: $\langle\uparrow|e^{-i\hat{\mathscr{H}}_\sigma t}|\downarrow\rangle = \langle\downarrow|e^{-i\hat{\mathscr{H}}_\sigma t}|\uparrow\rangle = 0$. In other words, if initially the spin is in a pure state, up or down, it will not precess. For $\hat{\rho}_s(t)$ this remark yields

$$\hat{\rho}_s(t) = \begin{bmatrix} \hat{\rho}_{\uparrow\uparrow}(0) & \chi(\lambda)\hat{\rho}_{\uparrow\downarrow}(0) \\ \chi(-\lambda)\hat{\rho}_{\downarrow\uparrow}(0) & \hat{\rho}_{\downarrow\downarrow}(0) \end{bmatrix}. \tag{13}$$

Here $\chi(\lambda) = \mathrm{tr}_e(e^{-i\hat{\mathscr{H}}_\lambda t}\hat{\rho}_e e^{i\hat{\mathscr{H}}_{-\lambda}t})$, where $e^{-i\hat{\mathscr{H}}_\lambda t}$ is the evolution operator for the problem (10). Now, after the spin degrees of freedom are taken care of by (13), we are left with a purely electron problem, that involves only electron degrees of freedom, but not the spin. By using the cyclic property of the trace $\mathrm{tr}_e(\cdots)$, one can show that $\chi(\lambda)$ in Eq. (13) is identical to (11).

In principle, any entry of a density matrix can be measured, and therefore the quantity $\chi(\lambda)$ is also measurable. In order to make clear the relation of $\chi(\lambda)$ with the distribution of precession angles, let us recall the transformation rule for the spin 1/2 density matrix under rotation by an angle θ around the $z-$axis:

$$\mathscr{R}_\theta(\hat{\rho}) = \begin{bmatrix} \hat{\rho}_{\uparrow\uparrow} & e^{-i\theta}\hat{\rho}_{\uparrow\downarrow} \\ e^{i\theta}\hat{\rho}_{\downarrow\uparrow} & \hat{\rho}_{\downarrow\downarrow} \end{bmatrix}. \tag{14}$$

By combining this with Eq. (3) we write $\hat{\rho}_s(t)$ as

$$\hat{\rho}_s(t) = \sum_m P_m \mathscr{R}_{\theta = m\lambda}(\hat{\rho}), \tag{15}$$

which assigns to P_m the meaning of the probability to observe precession angle $m\lambda$. Let us finally note that such an interpretation of P_m is consistent with what one expects on classical grounds,

because for a *classical* magnetic moment $\vec{\sigma}$ interacting with the current according to (7), the angle $\theta=\lambda$ corresponds to the precession due to a current pulse carrying the charge of one electron.

IV. SINGLE-CHANNEL CONDUCTOR. GENERAL FORMALISM

In order to see Eq. (11) working, let us consider an ideal single channel conductor, i.e., the Schrödinger equation,

$$i\frac{\partial\psi}{\partial t}=\left[\frac{1}{2}\left(-i\frac{\partial}{\partial x}-\frac{\lambda}{2}\delta(x)\right)^2+U(x)\right]\psi, \tag{16}$$

in one dimension, where the potential $U(x)$ represents the scattering region and the vector potential is inserted according to (7) at the $x=0$ section. In order to describe transport, we shall use scattering states, left and right. Their energy distributions $n_{L(R)}(E)$ are equilibrium Fermi functions with temperature T and chemical potentials shifted by eV, $\mu_L-\mu_R=eV$, representing a dc voltage.

For the problem (16) one can write time-dependent scattering states as

$$\begin{aligned}\psi_{L,k}(x,t)&=e^{-iE_kt}\begin{cases}e^{ikx}+B_Le^{-ikx}, & x<-a/2,\\ e^{i\lambda/2}A_Le^{ikx}, & x>a/2,\end{cases}\\ \psi_{R,k}(x,t)&=e^{-iE_kt}\begin{cases}e^{-i\lambda/2}A_Re^{-ikx}, & x<-a/2,\\ e^{-ikx}+B_Re^{ikx}, & x>a/2,\end{cases}\end{aligned} \tag{17}$$

where a is the width of the barrier, and $A_{L,R}$ and $B_{L,R}$ are the transmission and reflection amplitudes in the absence of the spin vector potential. To make expressions less heavy, we supress electron spin. The phase factors $e^{\pm i\lambda/2}$ in (17) are found immediately by observing that the vector potential in the Schrödinger equation can be eliminated by the gauge transformation $\psi(x)\to\exp(i\lambda/2\,\theta(x))\,\psi(x)$. The scattering amplitudes form a unitary matrix:

$$\hat{S}_\lambda=\begin{bmatrix}e^{i\lambda/2}A_L & B_R\\ B_L & e^{-i\lambda/2}A_R\end{bmatrix}. \tag{18}$$

We will study the range of small $T,eV\ll E_F$, when only the states close to the Fermi level are important. In this case, there is an additional simplification because the states near Fermi energy have almost linear dispersion, and thus all wavepackets travel with the speed v_F without changing shape. Then, following Landauer and Martin,[8] instead of the usual scattering states (17), it is convenient to use their Fourier transform. By ignoring the energy-dependence of $A_{L,R}$ and $B_{L,R}$, which is equivalent to saying that the scattering time is negligible, and assuming that the dispersion is strictly linear, one obtains the representation of scattering in terms of time-dependent scattering wavepackets,

$$\begin{aligned}\psi_{L,\tau}(x,t)&=\begin{cases}\delta(x_-), & t<\tau,\\ e^{i\lambda/2}A_L\,\delta(x_-)+B_L\,\delta(x_+), & t>\tau,\end{cases}\\ \psi_{R,\tau}(x,t)&=\begin{cases}\delta(x_+), & t<\tau,\\ e^{-i\lambda/2}A_R\,\delta(x_+)+B_R\,\delta(x_-), & t>\tau,\end{cases}\end{aligned} \tag{19}$$

where $x_\pm=x\pm v_F(t-\tau)$. Here τ is the packet arrival moment, at which it is scattered. It is straightforward to verify orthogonality of the states (19). Any time-dependent electron state can be written as a superposition of the states (19), with the arrival time τ serving in this representation as a label in the continuum of states, like k in (17). The assumption that the scattering amplitudes

are energy-independent (and thus the scattering takes no time) is equivalent to replacing the barrier $U(x)$ of finite width by $U_0\delta(x)$ and is consistent with the closeness of relevant energies to E_F.

Second-quantized, electron states (19) lead to $\hat{\psi}(x,t)=\hat{\psi}_L(x,t)+\hat{\psi}_R(x,t)$ with

$$\hat{\psi}_{L(R)}(x,t)=\sum_{\tau}\ \psi_{L(R),\tau}(x,t)\hat{c}_{1(2),\tau}, \tag{20}$$

where $c_{1,\tau}$ and $c_{2,\tau}$ are canonical Fermi operators corresponding to the states (19), the left and the right, respectively. One checks that fermionic commutation relations for $c_{1(2),\tau}$,

$$c^{+}_{i,\tau}c_{j,\tau'}+c_{j,\tau'}c^{+}_{i,\tau}=\delta_{ij}\delta(\tau-\tau'), \tag{21}$$

$$c_{i,\tau}c_{j,\tau'}+c_{j,\tau'}c_{i,\tau}=0,\quad c^{+}_{i,\tau}c^{+}_{j,\tau'}+c^{+}_{j,\tau'}c^{+}_{i,\tau}=0, \tag{22}$$

yield the usual commutation relations for $\psi_{L(R)}(x,t)$. From that one finds the meaning of the summation in (20): $\Sigma_{\tau}\cdots=\int_{-\infty}^{\infty}\cdots d\tau$. Mathematically, in this paragraph we defined the second-quantized $\psi(x)$ in (16).

The advantage of introducing the basis of the wavepackets (19),(20) is that now it is straightforward to write the many-particle evolution operator through the single-particle scattering matrix $\hat{S}_{\lambda}$:

$$e^{-i\hat{\mathscr{H}}_{\lambda}t}=\exp\ \int_0^t d\tau\sum_{ij}\ \ln[\hat{S}_{\lambda}]_{ij}c^{+}_{i,\tau}c_{j,\tau}, \tag{23}$$

where $\hat{S}_{\lambda}$ is given by (18). To verify (23), let us note that in the wavepacket representation (19), according to Eqs. (21), Fermi correlations occur only for the pairs of left and right states that scatter at the same instant of time. For each of such pairs the evolution operator $e^{-i\hat{\mathscr{H}}_{\lambda}t}$ is $\hat{1}$ if both states are occupied or both are empty, otherwise it is given by the single-particle scattering matrix (18).

Using similar arguments, we compute

$$e^{i\hat{\mathscr{H}}_{-\lambda}t}e^{-i\hat{\mathscr{H}}_{\lambda}t}=\exp\int_0^t d\tau\sum_{ij}\ \hat{W}_{ij}c^{+}_{i,\tau}c_{j,\tau}, \tag{24}$$

where $e^{\hat{W}}=\hat{S}^{-1}_{-\lambda}\hat{S}_{\lambda}$ is readily obtained from (18):

$$e^{\hat{W}}=\begin{bmatrix} e^{i\lambda}|A_L|^2+|B_L|^2 & 2i\ \sin\lambda\overline{A_L}B_R \\ 2i\ \sin\lambda\overline{B_R}A_L & e^{-i\lambda}|A_R|^2+|B_R|^2 \end{bmatrix}. \tag{25}$$

Using unitarity of $e^{\hat{W}}$ and commutation rules for $c_{\alpha,\tau}$ one can rewrite (24) in terms of normal ordering:

$$e^{i\hat{\mathscr{H}}_{-\lambda}t}e^{-i\hat{\mathscr{H}}_{\lambda}t}=:\exp\int_0^t d\tau\sum_{ij}\ [e^{\hat{W}}-1]_{ij}c^{+}_{i,\tau}c_{j,\tau}: \tag{26}$$

This form is ready to be plugged into Eq. (11) and averaged over the initial state. Let us note the striking similarity of two formulas obtained by different means: the fermionic Equation (26) and the bosonic Equation (4).

Also, let us mention that the periodicity of the matrix (25) in λ ensures periodicity of $\chi(\lambda)$, and thus guarantees integer values of charge.

V. EQUILIBRIUM FLUCTUATIONS

Let us start with a simple one-particle example. Consider a particle in the state $c^+_{1,\tau}|\text{vac}\rangle$, which corresponds to scattering at the moment τ. In this case, from (26) and (11) one gets

$$\chi(\lambda)=\begin{cases} e^{i\lambda}|A|^2+|B|^2, & \text{for } 0<\tau<t; \\ 1 \quad \text{otherwise;} \end{cases} \tag{27}$$

$|A|=|A_L|=|A_R|$, $|B|=|B_L|=|B_R|$. Evidently, according to Eq. (3), this simply means that for the scattering occurring during operation of the detector, the counting probabilities are identical to the one-particle scattering probabilities, as it should be expected.

Now, we consider current fluctuations in an equilibrium Fermi gas. First, let us assume perfect transmission: $B_{L(R)}=0$. Then Eq. (25) gives $\hat{W}=i\lambda\sigma_z$, and thus Eq. (24) becomes

$$e^{i\hat{\mathscr{H}}_{-\lambda}t}e^{-i\hat{\mathscr{H}}_{\lambda}t}=\exp\, i\lambda\int_0^t (c^+_{1,\tau}c_{1,\tau}-c^+_{2,\tau}c_{2,\tau})\,d\tau, \tag{28}$$

i.e., the right and the left states separate.

We observe that averaging of (28) over the Fermi ground state is identical to that performed in the orthogonality catastrophe calculation.[24,25] Hence, averaging of (28) can be done by using the bosonization method[26] that replaces the fermionic Hamiltonian by a bosonic one. (The calculation is described in Appendix B.) In the bosonized representation one has to do a simple Gaussian average, which gives

$$\chi(\lambda)=e^{-\tilde{\lambda}^2 f(t,T)}, \tag{29}$$

where $\tilde{\lambda}/2\pi+1/2=\lfloor\lambda/2\pi+1/2\rfloor$, with $\lfloor\cdots\rfloor$ being the fractional part. The function

$$f(t,T)=\left\langle\left\langle\left(\int_0^t c^+_{1,\tau}c_{1,\tau}\,d\tau\right)^2\right\rangle\right\rangle=-\text{Re}\frac{1}{4}\int_0^t\int_0^t\frac{T^2\,dt_1\,dt_2}{\sinh^2(\pi T(t_1-t_2-i\delta))} \tag{30}$$

$$=\frac{1}{2\pi^2}\ln\left(\frac{1}{\pi T\delta}\sinh\,\pi Tt\right)=\begin{cases} \dfrac{1}{2\pi^2}\ln\dfrac{t}{\delta}, & \delta\ll t\ll\dfrac{\hbar}{T}, \\ \dfrac{Tt}{h}-\dfrac{1}{2\pi^2}\ln 2\pi T\delta, & t\gg\dfrac{\hbar}{T}, \end{cases} \tag{31}$$

where δ is an ultraviolet cutoff time, of the order of $\hbar/E_F$. At long times, according to (3), this leads to Gaussian counting statistics.

As a side remark, the distribution given by Eq. (29) also gives a solution to another problem: the statistics of the number of fermions inside a segment of fixed length in one dimension. The relation is immediately obvious after one assigns to τ in Eq. (28) the meaning of a coordinate on a line. Thus, in this problem the statistics are Gaussian as well.

Now, it turns out that the general case of non-vanishing reflection, $B\neq 0$, can be reduced to (28) by a canonical Bogoliubov transformation of $c_{\alpha,\tau}$ making the quadratic form in (24) diagonal. The transformation is related in the usual way with the eigenvectors of the matrix $\hat{W}$. Thus, we come to Eqs. (28),(29) with λ replaced by λ_*:

$$\sin\frac{\lambda_*}{2}=|A|\sin\frac{\lambda}{2}. \tag{32}$$

The counting statistics in this case are non-Gaussian:

$$\chi(\lambda)=e^{-\lambda *^2 f(t,T)}. \tag{33}$$

One checks that the second moment of the distribution,

$$\langle\langle m^2\rangle\rangle=-\left.\frac{\partial^2\chi(\lambda)}{\partial\lambda^2}\right|_{\lambda=0}=2|A|^2 f(t,T), \tag{34}$$

agrees with the Johnson-Nyquist formula for the equilibrium noise.

VI. STATISTICS OF A DC CURRENT: QUANTUM SHOT NOISE

Let us consider nonequilibrium noise. In this case, due to the asymmetry in the distributions, $n_{L(R)}(E)=(\exp(E\pm\frac{1}{2}eV)/T+1)^{-1}$, generally one cannot uncouple the two channels by a canonical transformation. We calculate the statistics within an approximation that ignores the effect of switching at $\tau=0$ and $\tau=t$. Let us close the axis τ into a circle of length t, which amounts to restricting on periodic states:

$$\psi(\tau)=\psi(\tau\pm t). \tag{35}$$

For the $t-$periodic problem, by going to the Fourier space, one has

$$\chi(\lambda)=\prod_{k\in Z}\left[1+|A|^2(e^{-i\lambda}-1)n_L(E_k)(1-n_R(E_k))+|A|^2(e^{i\lambda}-1)n_R(E_k)(1-n_L(E_k))\right], \tag{36}$$

where $E_k=2\pi\hbar k/t$, k is an integer. For large t, $t\gg\hbar/T$ or $t\gg\hbar/eV$, the product is converted to an integral:

$$\ln(\chi(\lambda))=\frac{t}{2\pi\hbar}\int_{-\infty}^{+\infty}dE\ \ln(1+|A|^2(e^{-i\lambda}-1)\times n_L(1-n_R)+|A|^2(e^{i\lambda}-1)n_R(1-n_L)). \tag{37}$$

We evaluate it analytically, and get

$$\chi(\lambda)=\exp(-tTu_+u_-/h), \tag{38}$$

where

$$u_\pm=v\pm\cosh^{-1}(|A|^2\ \cosh(v+i\lambda)+|B|^2\ \cosh\ v), \tag{39}$$

$v=eV/2T$. The answer simplifies in the two limits: $T\gg eV$ and $eV\gg T$. In the first case we return to the equilibrium result (33). In the second case, corresponding to the recently discussed quantum shot noise,[3–5] we have

$$\chi(\lambda)=(e^{i\epsilon\lambda}|A|^2+|B|^2)^{e|V|t/h},\quad \epsilon=\text{sgn}\ V, \tag{40}$$

Analyzed according to Eq. (3), this $\chi(\lambda)$ leads to the binomial distribution

$$P_N(m)=p^m q^{N-m}C_N^m,$$

$p=|A|^2$, $q=|B|^2$, $N=e|V|t/h$. One checks that the moments $\langle m\rangle=pN$ and $\langle\langle m^2\rangle\rangle=pqN$ correspond directly to the Landauer formula and to the formula for the intensity of the quantum shot noise.[3–5] The correction to the statistics due to the switching effects is insignificant.[10]

VII. NOISE DUE TO A VOLTAGE PULSE: ORTHOGONALITY CATASTROPHE

Here we consider the fluctuations of current in a single-channel conductor induced by a voltage pulse. The result will be that the dependence of the fluctuations on Faraday's flux $\Phi=-c\int V(t)dt$ contains a logarithmically divergent term periodic in Φ with the period $\Phi_0=hc/e$. The fluctuation is smallest near $\Phi=n\Phi_0$. The divergence is explained by a comparison with the orthogonality catastrophe problem. The Φ_0-periodicity is related with the discreteness of ''attempts'' in the binomial statistics picture of charge fluctuations presented above.

Initially, the orthogonality catastrophe problem emerged from the observation that the ground state of a Fermi system with a localized perturbation is orthogonal to the nonperturbed ground state, no matter how weak the perturbation.[27] Originally, the discussion was focused on the purely static effect of Fermi correlations on the ground state that leads to the orthogonality, but then it shifted to dynamical effects. When a sudden localized perturbation is turned on in a Fermi gas, the number of excited particle-hole pairs detected over a large time interval t diverges as $\ln t/\tau$, where τ is the time of switching of the perturbation. This effect leads to power law singularities in transition rates involving collective response of fermions, such as x-ray absorption in metals.[28,24] In this section we present an application of the orthogonality catastrophe picture to the electric current noise.

Let us consider a single channel conductor in an external field described by the one-dimensional Schrödinger equation,

$$i\frac{\partial}{\partial t}\psi(x,t)=\hat{\mathscr{H}}\psi(x,t),$$
$$\hat{\mathscr{H}}=\frac{1}{2}\left(-i\frac{\partial}{\partial x}-\frac{e}{c}A(x,t)\right)^2+U(x), \tag{41}$$

where the potential $U(x)$ represents the scattering region and $A(x,t)$ is the vector potential corresponding to the applied pulse of electric field. Since the pulse duration τ is assumed to be much longer than the time of scattering, one can treat the vector potential as static and apply a gauge transformation in order to accumulate the flux $\varphi(t)=e/\hbar\int_{-\infty}^{t}V(t')dt'$ in the phases of the transmission amplitudes, thus making them time dependent. By going through the argument presented in Sec. IV, one obtains the scattering states (17) and (19) with time-dependent forward scattering amplitudes:

$$A_{L(R)}\rightarrow A_{L(R)}e^{\pm i\varphi(t_r)}, \tag{42}$$

where the time $t_r=t-|x|/v_F$ is taken retarded in order to account for the finite speed of motion after scattering. As before, here we assume that scattering by the potential as well as traversing the region where the voltage is applied takes negligible time compared to the duration of the voltage pulse. In this approximation the amplitudes of backward scattering $B_{L(R)}$ are time-independent constants.

To draw a relation with the orthogonality catastrophe problem, let us study the effect of the voltage pulse on the scattering phases δ_1, δ_2. They can be found by diagonalizing the scattering matrix,

$$\hat{\mathscr{S}}(t)=\begin{bmatrix} A_L e^{i\varphi(t)+i\lambda/2} & B_R \\ B_L & A_R e^{-i\varphi(t)-i\lambda/2}\end{bmatrix}, \tag{43}$$

and writing its eigenvalues as $e^{i\delta_1},e^{i\delta_2}$. The relation between the phases $\delta_{1,2}$ before and after the pulse is written conveniently through $\delta_\pm=(\delta_1\pm\delta_2)/2$. The phase δ_+ does not change at any time, and the phase δ_- changes according to

$$\cos^2\ \delta_-(t')+\cos^2\ \delta_-(t)-2\cos\ \delta_-(t')\cos\ \delta_-(t)\cos\ \Delta\varphi=|A_L|^2\ \sin^2\ \Delta\varphi, \tag{44}$$

where $\Delta\varphi=\varphi(t')-\varphi(t)$. Now, let us compare the situation to the orthogonality catastrophe in the Fermi system subjected to a time-dependent perturbation (43). Change of the flux induces the shift of the phases $\delta_\pm\to\delta'_\pm$ and makes the new ground state orthogonal to the old one:

$$\langle 0'|0\rangle=\exp\left(-2\frac{\delta_*^2}{\pi^2}\ln\frac{L}{\lambda_F}\right), \tag{45}$$

where L is the system size, λ_F is Fermi wavelength, and $e^{i\delta_*}$ is an eigenvalue of the matrix $\hat{\mathscr{S}}^{-1}(t=\infty)\hat{\mathscr{S}}(t=-\infty)$:

$$\sin\frac{\delta_*}{2}=|A_L|\sin\frac{\Delta\varphi}{2}. \tag{46}$$

In terms of dynamics, this implies that the old ground state is shaken up so that infinitely many particle-hole pairs are excited.[24] It should lead to a logarithmically diverging contribution to noise, since for each of the particle-hole pairs there is a finite probability (equal to $|A_LB_R|^2$) that the particle and the hole will go to different terminals of the conductor, thus resulting in a current fluctuation. The periodicity in Faraday's flux $\Phi=-c\int V(t)dt$ follows from the gauge invariance and is explicit in Eqs. (44),(46) for $\delta'_\pm$. The logarithmic divergence vanishes at $\Phi=n\Phi_0$, as expected, since at integer Φ there is no long-term change of the scattering.

Let us calculate the mean square fluctuation of the charge $\langle\langle Q^2\rangle\rangle$ transmitted through the system due to the pulse. For that, one can use the formula (26) with the time-dependent scattering matrix (43). To get the second cumulant $\langle\langle Q^2\rangle\rangle$ one expands the exponent (26) up to second order terms in λ, and takes an irreducible average using Wick theorem. The averages of $c_{i,\tau}$ have the usual form:

$$\begin{aligned}\langle c^+_{i,\tau}c_{j,\tau'}\rangle&=\delta_{ij}\int n(E)e^{iE(\tau-\tau')}\frac{dE}{2\pi},\\ \langle c_{i,\tau}c^+_{j,\tau'}\rangle&=\delta_{ij}\int\ (1-n(E))e^{-iE(\tau-\tau')}\frac{dE}{2\pi},\end{aligned} \tag{47}$$

where $n(E)=(e^{E/T}+1)^{-1}$ is the Fermi distribution. The result reads as

$$\langle\langle Q^2\rangle\rangle=\frac{ge^2}{2\pi}\int\left(|A|^4\left|\int_0^t e^{i\omega t'}\ dt'\right|^2+|AB|^2\times\left|\int_0^t e^{i\varphi(t')+i\omega t'}\ dt'\right|^2\right)\omega\ \coth\frac{\hbar\omega}{2T}\ \frac{d\omega}{2\pi}, \tag{48}$$

where g is spin degeneracy. The first term in (48) is a part of equilibrium noise since it does not depend on φ. To analyze the second term, let us take a step-like time-dependence of φ resulting from an abrupt voltage pulse applied at the time t_0, $0<t_0<t$, the pulse duration τ being much shorter than t. Taking the integral and keeping only the terms diverging at $t\to\infty$, we find

$$\frac{ge^2}{2\pi}\int\left|\frac{e^{i\omega t_0}-1}{i\omega}+e^{2\pi i\Phi/\Phi_0}\frac{e^{i\omega t}-e^{i\omega t_0}}{i\omega}\right|^2|\omega|\frac{d\omega}{2\pi}=\frac{ge^2}{\pi^2}\left(\ln\frac{tE_F}{\hbar}+2\sin^2\frac{\pi\Phi}{\Phi_0}\ln\frac{t}{\tau}\right), \tag{49}$$

where the ultraviolet-diveregent integrals are cut at frequency $\sim E_F/\hbar$. By subtracting the result for $\Phi=0$ as corresponding to equilibrium, one obtains a logarithmic contribution to the non-equilibrium noise:

$$\langle\langle Q^2\rangle\rangle = ge^2|AB|^2\left[\frac{2}{\pi^2}\sin^2\frac{\pi\Phi}{\Phi_0}\ln\frac{t_0}{\tau}+\frac{\Phi}{\Phi_0}\right]+\cdots+\langle\langle Q\rangle\rangle_{eq}. \tag{50}$$

The origin of the non-diverging term in Eq. (50) proportional to Φ/Φ_0 will be discussed below. The dots in Eq. (50) represent corrections higher order in Φ_0/Φ, and the equilibrium noise,

$$\langle\langle Q^2\rangle\rangle_{eq}=\frac{e^2G}{\pi^2}\ln\frac{tE_F}{\hbar}, \quad G=g\frac{e^2}{\hbar}|A|^2, \tag{51}$$

is obtained by repeating the calculation for $\Phi=0$. The expression (51) agrees with the Nyquist formula,

$$\langle\langle j_\omega j_{-\omega}\rangle\rangle = e^2G\omega\ \coth\frac{\omega}{2T}, \tag{52}$$

taken at $T=0$, Fourier transformed, and combined with the relation $Q=\int_0^t j(t')dt'$.

The term in Eq. (50) proportional to Φ/Φ_0 is obtained by rewriting the integral in the second term of (48) as

$$\int\int\int\frac{d\omega}{2\pi}|\omega|dt_1\ dt_2\ e^{i(\varphi(t_1)-\varphi(t_2)+\omega(t_1-t_2))}, \tag{53}$$

and extracting the contribution of almost coinciding times t_1 and t_2 by going to new variables $t=(t_1+t_2)/2$, $t'=t_1-t_2$, and changing the order of integrations:

$$\int dt\int\frac{d\omega}{2\pi}|\omega|\int dt'\ e^{i\varphi(t_1)-i\varphi(t_2)+i\omega t'}=\int|\dot\varphi|dt, \tag{54}$$

where we replaced $\varphi(t_1)-\varphi(t_2)=\varphi(t+t'/2)-\varphi(t-t'/2)$ by $\dot\varphi t'$. The result (54) is approximate: it does not give the log-term because the transformation (54) properly takes care of the integral (53) only in the domain $t_1\simeq t_2$, under the restriction that $\Phi(t)$ is varying sufficiently smoothly. When $\Phi(t)$ is a monotonous function, $\dot\varphi>0$, the integral in the right hand side of (54) equals $2\pi\Phi/\Phi_0$ and thus produces the term of Eq. (50) proportional to Φ/Φ_0.

It is clear from the derivation that the two terms in the brackets in Eq. (50) arise from different integration domains in the t_1-t_2 space: the first term corresponds to $|t_{1,2}|\geqslant\tau, t_1t_2<0$, while the second one is due to almost coinciding moments, $|t_1-t_2|\ll\tau$. Since these domains are almost non-overlapping, the two contributions to the noise (50) do not interfere (cross terms are small).

In order to estimate the correction to the result (50), let us derive it by another method that allows to trace out the higher order terms. For that, let us take the flux in the form $\varphi(t)=N\lambda(t)$, where $\lambda(t)$ is a smooth monotonous function, $\lambda(-\infty)=0$, $\lambda(\infty)=2\pi$. For integer $N\gg1$ the Fourier component of $e^{iN\lambda(t)}$ entering Eq. (54) in the stationary phase approximation is given by

$$\int_{-\infty}^{\infty}e^{iN\lambda(t)+i\omega t}\ dt=\sum_k\ \sqrt{\frac{2\pi i}{N\ddot\lambda(t_k)}}e^{iN\lambda(t_k)+i\omega t_k}+\cdots, \tag{55}$$

where the dots indicate terms $\sim O(N^{-3/2})$, and t_k's are real solutions of the equation $N\dot\lambda(t)+\omega=0$. Then we can write

$$\left|\int_{-\infty}^{\infty}e^{iN\lambda(t)+i\omega t}\ dt\right|^2=\sum_k\ \frac{2\pi}{N\ddot\lambda(t_k)}+O(N^{-2}), \tag{56}$$

and thus obtain

$$\langle\langle Q^2\rangle\rangle = A\int_{-\infty}^{\infty}\sum_k \frac{|\omega|d\omega}{N\ddot{\lambda}(t_k)} + \cdots, \tag{57}$$

where the dots represent higher order terms. By differentiating both sides of the equation $N\dot{\lambda}(t) = -\omega$ one finds the relation $d\omega = -N\ddot{\lambda}(t_k)dt_k$, which means that $|\omega|d\omega/\ddot{\lambda}(t_k) = -|\dot{\lambda}(t_k)|dt_k$, and therefore the integral in Eq. (57) equals $N\int_{-\infty}^{\infty}d\lambda = 2\pi N$. Since $|\omega|d\omega$ scales as N^2, the correction to Eq. (57) can be evaluated as $O(1)$, i.e., it is of the order of one for any N. This means that Eq. (77) has relative accuracy of $O(1/N)$.

The term in (50) proportional to Φ/Φ_0 is interesting in connection with the picture of binomial statistics presented in Sec. VI. In the dc bias case, the distribution of charge for a single channel situation was found to be binomial with the frequency of attempts equal to eV/h and the probabilities of outcomes $p = |A|^2$, $q = |B|^2$. Taken literally, this means that the attempts to transfer charge are repeated regularly in time, almost periodic with the period h/eV, with each attempt having two outcomes–transmission or reflection–occurring with the probabilities p and q. However, the regularity of the attempts does not lead to an ac component in the current, rather it appears just as a part of statistical description of charge fluctuations. Still, the presence of a non-zero frequency in a noninteracting system requires interpretation.

Let us suppose that the flux varies linearly with time, $\Phi(t) = -cVt$. Since the e.m.f.$= -\partial\Phi/c\,\partial t$, the linear dependence of $\Phi(t)$ is equivalent in its effect on the noise to constant voltage V. In accordance with one's expectation, the second term in the brackets in Eq. (50) for a single channel is $\langle\langle Q^2\rangle\rangle = ge^2|AB|^2\Phi/\Phi_0$, i.e., it is precisely of the form arising from the binomial distribution with probabilities of outcomes p and q, and the number of attempts $N = \Phi/\Phi_0$. (Let us recall that the second moment of the binomial distribution equals pqN.) Taking into account that the time during which the flux changes by Φ_0 is h/eV, we can interpret the number of attempts in the statistical picture as the number of flux quanta by which the flux is changed. Such a conclusion suggests an interesting generalization of the picture of binomial statistics by attributing the meaning of the number of attempts to the flux change measured in the units of Φ_0, regardless of the linear or non-linear character of the flux dependence on time.

It is appealing to put the special role of integer fluxes in connection with the binomial statistics of current, where the flux quanta are naturally interpreted as discrete attempts to transmit charge. Although this picture is yet to be confirmed by analytic treatment, it receives some support from the property of the Φ_0-periodic term in (50) to vanish at every integer Φ. One may conjecture that the statistics are close to binomial only when the flux change is an integer, and have diverging logarithmic corrections otherwise. The distinction that Eq. (50) makes between integer and non-integer values of the flux and the relation of integer flux change to the number of attempts in the binomial distribution, gives another perspective to the statistical picture of a current pulse.

To summarize, the fluctuations caused by a voltage pulse, in contrast to the average transmitted charge, distinguish between integer and non-integer flux change. As a result, the dependence of noise on the flux is non-monotonous and has minima at integer values of the flux.

VIII. COHERENT STATES OF CURRENT

The question we address in this section is about the optimal way of changing flux that minimizes induced noise. It is clear from what has been said that to achieve minimum of the noise one should change the flux by an integer amount,

$$\Delta\varphi = \varphi(t=\infty) - \varphi(t=-\infty) = 2\pi n, \tag{58}$$

in order to suppress the logarithmically divergent term. However, since for a given $\Delta\varphi$ the noise depends on the actual function $\varphi(t)$, not just on $\Delta\varphi$, we have a variational problem to solve for the noise as a functional of the time dependence of the flux. This functional was derived in Sec. VII. At zero temperature it is given by

$$\langle\langle Q^2\rangle\rangle = \frac{ge^2}{2\pi}|AB|^2 \int \left| \int e^{i\varphi(t)+i\omega t}\, dt \right|^2 |\omega| \frac{d\omega}{2\pi}, \tag{59}$$

where A and B are transmission and reflection amplitudes, and g is spin degeneracy. We shall study the variational problem (49) with the boundary condition (58) and show that its general solution has the form of a sum of soliton-like functions:

$$\Phi(t) = \pm\frac{\Phi_0}{\pi}\sum_{k=1}^{n} \tan^{-1}\left(\frac{t-t_k}{\tau_k}\right), \quad \tau_k > 0, \tag{60}$$

where t_k and τ_k are arbitrary constants. Under the condition (58), any time dependence of the form (60) gives absolute minimum to the noise:

$$\min[\langle\langle Q^2\rangle\rangle] = ge^2|AB|^2|n|. \tag{61}$$

For an optimal time dependence of the voltage $V = -\partial\Phi/c\ \partial t$, therefore, one has a sum of Lorentzian peaks:

$$V(t) = \mp\frac{\Phi_0}{c\pi}\sum_{k=1}^{n} \frac{\tau_k}{(t-t_k)^2+\tau_k^2}. \tag{62}$$

In order to compare quantum noise with conductance, let us mention that the average transmitted charge,

$$\langle\langle Q\rangle\rangle = ge|A|^2\frac{\Delta\varphi}{2\pi} = g\frac{e^2}{h}|A|^2\int V(t)dt, \tag{63}$$

simply obeys the Ohm's law, i.e., there is no particular dependence on the way the flux change $\Delta\varphi$ is realized.

The results (60),(61) have a simple interpretation in terms of the binomial statistics picture of charge fluctuations. For the binomial distribution with probabilities of outcomes p and q, $p+q=1$, and with the number of attempts N, the second moment is known to be equal to pqN. The comparison with Eq. (61) suggests that we attribute to $n=\Delta\Phi/\Phi_0$ the meaning of the *number of attempts*. This interpretation is supported by the structure of the function (60) consisting of n terms, each corresponding to a unit change of flux. A remarkable property of the function (60) is its separability, manifest both in the form of the terms and in the way the parameters t_k, τ_k enter the expression. Let us note that by making some of the t_k's close to each other one can have an overlap in time of different ''attempts.'' The overlap, however, does not change the fluctuations (61). The situation reminds us of the one with solitons in integrable non-linear systems, or with non-interacting instantons in integrable field theories. Also, the absence of interference is interesting in the context of coherent nature of transport in this system: after all, we simply have scattering by a time-dependent potential. Perhaps, proper interpretation of this effect should be sought in establishing a relation with the theory of coherent states, known to eliminate to some extent the quantum mechanical interference.

Let us now turn to the variational problem. It is convenient to do the integral over ω first and to rewrite (49) as

$$\langle\langle Q^2\rangle\rangle = -\frac{D}{\pi}\int\int \frac{e^{i\varphi(t)-i\varphi(t')}}{(t-t')^2}dt\ dt', \tag{64}$$

where $D=(ge^2/2\pi)\,|AB|^2$. In order to avoid divergence at $t=t'$ the denominator in (64) should be understood as

$$\frac{1}{2}\left[\frac{1}{(t-t'+i\delta)^2}+\frac{1}{(t-t'-i\delta)^2}\right], \quad \delta\to 0, \tag{65}$$

the condition that one obtains by introducing regularization in (49): $|\omega|\to|\omega|e^{-|\omega|\delta}$. By considering variation of the functional (64) we have the equation for an extremum:

$$\mathrm{Im}\left[e^{i\varphi(t)}\int\frac{e^{-i\varphi(t')}}{(t-t')^2}dt\right]=0. \tag{66}$$

By using the Cauchy formula one checks that the functions

$$e^{i\varphi(t)}=\prod_{k=1}^{n}\frac{t-\lambda_k}{t-\overline{\lambda}_k}, \quad \lambda_k=t_k+i\tau_k, \tag{67}$$

satisfy (66) provided that τ_k's are all of the same sign. Obviously, the functions (67) are just another form of (60).

It remains to be shown that the functional reaches its minimum on the solutions (67). To prove it we proceed in the following steps. Let us write $e^{i\varphi(t)}$ as

$$e^{i\varphi(t)}=f_+(t)+f_-(t), \tag{68}$$

where $f_+(t)$ and $f_-(t)$ are bounded analytic functions in the upper and lower complex t half-plane, respectively. Representation (68) exists for any non-singular function and defines the functions f_+ and f_- up to a constant. Then we substitute Eq. (68) in (64), and apply the Cauchy formula for the derivative,

$$\dot{f}_\pm(t)=\pm\frac{i}{2\pi}\oint\frac{f_\pm(t')dt'}{(t-t'\pm i0)^2}, \tag{69}$$

where the contour of integration is chosen in the half-plane of analyticity of f_+ or f_-, respectively. Thus one gets

$$\langle\langle Q^2\rangle\rangle=-iD\int(\overline{f_+}\dot{f}_+-\overline{f_-}\dot{f}_-)dt. \tag{70}$$

On the other hand,

$$n=\frac{1}{2\pi i}\int e^{-i\varphi(t)}\frac{d}{dt}e^{i\varphi(t)}\,dt=-\frac{i}{2\pi}\int(\overline{f_+}\dot{f}_++\overline{f_-}\dot{f}_-)dt, \tag{71}$$

where the last equality is a result of substituting (68) and using the relations

$$\int\overline{f_+}\dot{f}_-=\int\overline{f_-}\dot{f}_+=0, \tag{72}$$

which follow from the Cauchy theorem. Now, Eq. (70) can be rewritten through Fourier components of f_+ and f_- as

$$\langle\langle Q^2\rangle\rangle = D\int_0^\infty (|f_+(\omega)|^2 + |f_-(-\omega)|^2)\,\omega\,\frac{d\omega}{2\pi}, \tag{73}$$

thus demonstrating positivity of both terms in (70). [It is used that $f_+(\omega)=f_-(-\omega)=0$ for $\omega<0$.] With this, by comparing (70) and (71) we obtain

$$\langle\langle Q^2\rangle\rangle \geqslant 2\pi D|n|. \tag{74}$$

Equality in (74) is reached only when either $f_+(t)$ or $f_-(t)$ vanishes. Therefore, to obtain the minimum one has to take the functions $e^{i\varphi(t)}$ that are regular in one of the half-planes. This remark is sufficient to see that the functions (67) form a complete family of solutions.

It is worth mentioning that the method used to derive (74) copies almost entirely the procedure of derivation of the duality condition in the theory of instantons. Like in other situations where the duality condition holds, our ''solitons'' do not interact: $\langle\langle Q^2\rangle\rangle$ shows no dependence on the parameters λ_k of the solution (67). Among numerous field theories that allow for an exact solution of the instanton problem the one most similar to our case is the theory of the classical Heisenberg ferromagnet in two dimensions. For this problem the instantons were found by mapping the order parameter space (i.e., the unit sphere) on the complex plane.[29] The duality condition was shown to take the form of the constraint of analyticity or anti-analyticity of the mapped order parameter function (compare with the condition $f_+=0$ or $f_-=0$ derived above). Multi-instanton solutions were given as products of single instanton solutions [cf. Eq. (67)]. This analogy obviously deserves more attention.

At this point let us examine an interesting nonoptimal time dependence of the flux, the sum of two solitons with opposite charge:

$$\varphi(t) = 2\left[\tan^{-1}\left(\frac{t-t_1}{\tau_1}\right) - \tan^{-1}\left(\frac{t-t_2}{\tau_2}\right)\right], \tag{75}$$

$\tau_{1,2}>0$. This function corresponds to $e^{i\varphi(t)}$ of the form (67) but with the poles in both half-planes. In this case $\Delta\varphi=0$, and thus $\langle\langle Q\rangle\rangle=0$, so $\min[\langle\langle Q^2\rangle\rangle]=0$. With the function (75), however, one finds

$$\langle\langle Q^2\rangle\rangle = 4\pi D\left|\frac{\lambda_1-\lambda_2}{\lambda_1-\lambda_2}\right|^2, \tag{76}$$

where $\lambda_{1,2}=t_{1,2}+i\tau_{1,2}$. For different values of the parameters $t_{1,2}$, $\tau_{1,2}$, Eq. (76) interpolates between two trivial limiting cases: (i) $\langle\langle Q^2\rangle\rangle\to 0$, when the two flux steps in (75) have nearly the same duration and almost overlap; (ii) $\langle\langle Q^2\rangle\rangle\to 4\pi A$, when the flux steps either differ strongly in their duration or do not overlap. In the case (ii) the noise is two times bigger than the noise due to a single step, as it should be.

We see that when $\Delta\varphi/2\pi$ is of the order of one a non-optimal time dependence $\varphi(t)$ can considerably enhance the noise. It is not the case, however, for $\Delta\varphi/2\pi\gg 1$. This limit was studied in Sec. VII, where it was found that when $\varphi(t)$ is a monotonous function the result

$$\langle\langle Q^2\rangle\rangle = ge^2|AB|^2|\Delta\varphi/2\pi| \tag{77}$$

is rather accurate, even if the time dependence $\varphi(t)$ is not optimal.[13]

A more intuitive way to understand the accuracy of Eq. (77) is to note that for a given n the number of parameters in the optimal flux dependence (53) is $2n$, which means that half of them

are in some sense redundant. Because of that any smooth monotonous function with sufficiently large variation $\Delta\varphi$ can be rather accurately approximated by a function of the form (53), and therefore the noise exceeds the lower bound just slightly.

An implication of this result for the binomial statistics picture is as follows. As it was discussed above there is a (conjectured) correspondence of the terms of Eq. (60) and of the attempts. The deviation from the binomial distribution, that of course should exist for a non-optimal flux function $\varphi(t)$, will remain bounded in the case of a smooth $\varphi(t)$, as $\Delta\varphi$ increases taking integer values. More precisely, the distribution will be written as a mixture of binomial distributions with different numbers N of attempts, $P(m)=\Sigma_N \rho_N P_N(m)$, where $P_N(m)=p^m q^{N-m} C_N^m$. The estimated correction implies that the distribution of attempts ρ_N has finite variance in the limit $N=\Delta\varphi/2\pi\to\infty$.

Before closing, let us mention that in order to apply the results of Secs. VII, VIII to transport in a mesoscopic metallic conductor with disorder, described by many conducting channels with transmission constants T_n, one just needs to replace $|AB|^2$ by $\Sigma_n T_n(1-T_n)$, since different scattering channels contribute to the noise independently. The condition of validity of our treatment then is that the variation of the flux is sufficiently slow, so that $\min[\tau_k]\gg\hbar/E_c$, the time of diffusion across the sample. However, at non-zero temperature one also has to satisfy the condition $\tau_k\ll\hbar/T$, the time of phase breaking. So, the temperature interval where our estimate of the noise holds is $T\leqslant E_c$.

IX. CONCLUSIONS

We introduced a quantum-mechanical scheme that gives complete statistical description of electron transport. It involves a spin 1/2 coupled to the current so that the spin precession measures transmitted charge. The off-diagonal part of the spin density matrix, taken as a function of the coupling constant, gives the generating function for the electron counting statistics. We find the statistics in a single-channel ideal conductor for arbitrary relation between temperature and voltage. In equilibrium, the counting statistics are Gaussian, both for zero-point fluctuations and at finite temperature. At constant voltage and low temperature the statistics are Bernoullian and the distribution is binomial.

The theory leads to interesting conclusions applied to the current fluctuations produced by a voltage pulse. In this case, the noise has phase sensitivity: it oscillates as a function of Faraday's flux, $c\int V(t)dt$, reaching minimum at integer fluxes. We studied the noise as a function of the shape of the voltage pulse and found optimal time dependence that provides an absolute minimum of the noise for a given average transmitted charge. The solution displays an interesting analogy with the problem of instantons in the field theories obeying duality symmetry. Optimal time dependence is a sum of Lorentzian peaks of voltage, each corresponding to a soliton of flux. The change of flux for a soliton is equal to the flux quantum Φ_0. The solitons are interpreted in terms of the binomial statistics picture of charge fluctuations as attempts to transmit electrons, one electron per soliton.

APPENDIX A: LARMOR CLOCK MEASUREMENT OF TUNNELING TIME

How long does it take a particle to tunnel under a barrier? More precisely, suppose a particle of energy E is moving in one dimension, and is scatterred on a potential barrier:

$$i\frac{\partial}{\partial t}\psi(x,t)=\left[-\frac{1}{2}\frac{\partial^2}{\partial x^2}+U(x)\right]\psi(x,t). \tag{A1}$$

What is the probability that during the scattering the particle spends time τ within the region $a<x<b$ under the barrier? Questions of that kind arise naturally in discussion of any quantum-mechanical process that takes finite time, like nuclear or chemical reactions, resonance scattering, or tunneling.

There have been several attempts to treat such problems[23] that resulted in the formulation of a very interesting concept of a Larmor clock. It has various analogies with the spin galvanometer discussed above, and it seems useful to review the Larmor clock here using the same language. The Larmor clock uses an auxiliary spin 1/2 attached to the scattering particle, and an auxiliary constant magnetic field ω localized within the region of interest, $a<x<b$,

$$\hat{\mathscr{H}}_{int}=-\frac{1}{2}\omega\sigma_z\int_a^b \psi^+(x)\psi(x)dx. \tag{A2}$$

The choice of coupling is such that the spin precession angle is proportional to the time spent in the region $a<x<b$. The difference from our spin-galvanometer is that the spin is not stationary, but travels with the particle, and also that the spin is coupled to the particle density, rather than to the current.

To find the distribution of times one has to write down the system density matrix evolved in time, and take partial trace over the particle outgoing states. (We assume that one does not have to distinguish between different results of scattering, and is interested in the tunneling time only, regardless of whether the particle went through the barrier, or has been reflected.) Then, by following the argument of Sec. III one obtains the spin density matrix:

$$\hat{\rho}_s(t)=\begin{bmatrix} \hat{\rho}_{\uparrow\uparrow}(0) & \chi(\omega)\hat{\rho}_{\uparrow\downarrow}(0) \\ \chi(-\omega)\hat{\rho}_{\downarrow\uparrow}(0) & \hat{\rho}_{\downarrow\downarrow}(0) \end{bmatrix}. \tag{A3}$$

Here

$$\chi(\omega)=\mathrm{tr}_e(e^{-i.\hat{\mathscr{H}}_\omega t}\hat{\rho}_e e^{i.\hat{\mathscr{H}}_{-\omega}t}), \tag{A4}$$

where $e^{-i.\hat{\mathscr{H}}_\omega t}$ is the evolution operator for the one-particle problem with no spin:

$$i\frac{\partial}{\partial t}\psi(x,t)=\left[-\frac{1}{2}\frac{\partial^2}{\partial x^2}+U(x)-\frac{1}{2}\omega\theta_{ab}(x)\right]\psi(x,t), \tag{A5}$$

where $\theta_{ab}=\theta(x-a)\theta(b-x)$. The auxiliary magnetic field ω now turns into a constant potential within the region $a<x<b$, and zero outside. Here again, with the spin degrees of freedom taken care of by (A3), we are left with a single particle problem. By using cyclic property of the trace one finds

$$\chi(\omega)=\langle e^{i.\hat{\mathscr{H}}_{-\omega}t}e^{-i.\hat{\mathscr{H}}_\omega t}\rangle. \tag{A6}$$

Here the brackets $\langle\cdots\rangle$ mean averaging over the particle initial state. Note that $\chi(\omega)$ is written in terms of a purely single particle problem, not involving spin variables.

The quantity $\chi(\omega)$ obtained by measuring precession of the spin is a generating function for the distribution of times, which is clear from the Fourier transform

$$\chi(\omega)=\int P(\tau)e^{i\omega\tau}\,d\tau. \tag{A7}$$

The probabilities $P(\tau)$ of different precession angles of the spin should be interpreted as the scattering time distribution.

The probabilities $P(\tau)$ defined by (A5), (A6), and (A7) have several interesting properties: *(a)* $\int P(\tau)d\tau=1$; *(b)* $P(\tau)$ are real numbers; *(c)* $P(\tau)$ vanish at negative times $\tau<0$. The normalization property *(a)* is derived from (A6) by setting $\omega=0$. Property *(b)* (real valuedness) is derived from $\chi(-\omega)=\overline{\chi(\omega)}$ which follows from (A6). The causality property *c)* follows from considering

the evolution in the problem (A5) with ω continued to complex values. One notes that both the solution $\psi(x,t)$ of Eq. (A5) and the evolution operator $e^{-i\hat{\mathscr{H}}_\omega t}$ are regular in the upper half-plane $\mathrm{Im}\omega>0$, which means that the same is true for $\chi(\omega)$. From that, the causality property *(c)* follows by the usual argument using the Cauchy theorem in the integral

$$P(\tau)=\int_{-\infty}^{\infty}\chi(\omega)e^{-i\omega\tau}\frac{d\omega}{2\pi}, \tag{A8}$$

by closing the integration contour in the upper half-plane.

The properties *(a)*, *(b)* and *(c)* suggest that $P(\tau)$, so far defined formally as the Fourier spectrum of $\chi(\omega)$, can have a meaning of probability. However, generally the sign of $P(\tau)$ can be either positive or negative, which makes the probabilistic interpretation problematic.

For the one particle problem one can write the generating function $\chi(\omega)$ in terms of the scattering amplitudes A and B. For that, it is convenient to use the expressions (23), (24) for the evolution operator in terms of the scattering matrix $\hat{\mathscr{S}}$, written using the wavepacket scattering states (19). Specializing to one particle and taking partial trace, one finds

$$\chi(\omega)=\overline{A}_{-\omega}(E)A_\omega(E)+\overline{B}_{-\omega}(E)B_\omega(E), \tag{A9}$$

where $A(\omega)$ and $B(\omega)$ are the transmission and reflection amplitudes of the problem (A5) taken at the energy E of incident particle.

To see the Larmor clock working, let us consider an example of resonance scattering, where a particle is scattered on a potential forming a quasibound state of life-time Γ. Using the method described above one can find the distribution of times it takes the particle to scatter. For simplicity, suppose that the particle can be only reflected, but not transmitted ($A=0$). Then the reflection amplitude as function of energy is given by the Breit–Wigner formula:

$$B(E)=\frac{E-E_0-i\Gamma/2}{E-E_0+i\Gamma/2}. \tag{A10}$$

Turning on the field ω in the quasibound state region is equivalent to shifting the resonance energy: $E_0\to E_0-\omega/2$. Thus, the generating function of the time distribution is

$$\chi(\omega)=\frac{\varepsilon-\omega+i\Gamma}{\varepsilon-\omega-i\Gamma}\,\frac{\varepsilon+\omega-i\Gamma}{\varepsilon+\omega+i\Gamma}, \tag{A11}$$

where $\varepsilon=2(E-E_0)$. The distribution $P(\tau)$ is found by Fourier transform:

$$P(\tau)=\int\chi(\omega)e^{-i\omega\tau}\frac{d\omega}{2\pi}=\delta(\tau)-\frac{4\Gamma}{\varepsilon}(\Gamma\,\sin\,\varepsilon\tau-\varepsilon\,\cos\,\varepsilon\tau)e^{-\Gamma\tau}=\frac{\partial}{\partial\tau}\left(\theta(\tau)-\frac{4\Gamma}{\varepsilon}\sin\,\varepsilon\tau\,e^{-\Gamma\tau}\right). \tag{A12}$$

The δ-function term corresponds to the nonresonance scattering channel. Other terms describe dwelling in the quasi-bound state. In this example $P(\tau)$ is changing sign, which makes the probabilistic interpretation ambiguous.

The paradox arising due to negative $P(\tau)$ is only an apparent one. Really, the measurement of time performed by the Larmor clock is not the usual quantum-mechanical measurement, since the time is not an operator, and thus it cannot be measured in the same sense as other quantum-mechanical observables. This should be contrasted with the measurement of charge described above. Although the spin precession measurement scheme we use looks quite similar to the

Larmor clock, there is a difference: Electric charge is an observable in the usual quantum-mechanical sense, it takes quantized integer values, and the probabilities of those values resulting from our calculation are non-negative.

APPENDIX B: BOSONIZATION CALCULATION OF COUNTING STATISTICS

In order to find generating function of counting statistics for a single channel conductor, we have to evaluate

$$\chi(\lambda)=\langle \exp i\lambda \hat{N}_t\rangle, \tag{B1}$$

where $\hat{N}_t=\int (c^+_{1,\tau}c_{1,\tau}-c^+_{2,\tau}c_{2,\tau})d\tau$, and $c_{i,\tau}$, $c^+_{i,\tau}$ are canonical Fermi operators.

In one dimension, there is an equivalence between an ideal Fermi gas and a harmonic Bose chain, which provides a representation of the Fermi problem in terms of free bosons, known as the bosonization transformation.[24–26] This representation facilitates calculting averages like (B1), since they are being transformed to the form of a Gaussian average.[25]

According to the bosonization method, the bosonic Hamiltonian representing the fermionic problem is written as

$$\hat{\mathscr{H}}_{\text{Bose}}=\frac{\hbar v_F}{4\pi}\int :(\nabla\theta_L)^2:+:(\nabla\theta_R)^2:dx, \tag{B2}$$

where $\theta_{L(R)}(x)$ are Bose operators,

$$[\nabla\theta_{L(R)}(x),\theta_{L(R)}(y)]=\pm 2\pi i\,\delta(x-y). \tag{B3}$$

Connection to the fermionic problem is given as a relation between the densities of the left- and right-moving fermions, $\hat{\rho}_i(x)=c^+_{i,x}c_{i,x}$, $i=1,2$, and the bosonic variables $\theta_{L(R)}(x)$, written as

$$\hat{\rho}_{1(2)}(x)=\frac{1}{2\pi}\nabla\theta_{L(R)}(x). \tag{B4}$$

One notes that the operator $\hat{N}_t$ in (B1) is linear in the densities $\hat{\rho}_i$, and thus it is represented by an expression linear in the bosonic variables,

$$\hat{N}_t=\frac{1}{2\pi}(\theta_L(t)-\theta_L(0)-\theta_R(t)+\theta_R(0)), \tag{B5}$$

which turns the average in (B1) into a Gaussian type.

Therefore, the average of (28) is equal to the product of averages,

$$\chi(\lambda)=\left\langle \exp\frac{i\lambda}{2\pi}(\theta_L(t)-\theta_L(0))\right\rangle\left\langle \exp\frac{-i\lambda}{2\pi}(\theta_R(t)-\theta_R(0))\right\rangle, \tag{B6}$$

taken over the ground state of the Hamiltonian (B2). To perform the average in (B6), it is sufficient to deal with the average over θ_L's, because of the left-right symmetry of the problem.

Let us write $\theta_L(x)$ in terms of bosonic operators of plane waves:

$$\begin{aligned}\theta_L(x)&=\sum_{k>0}\left(\frac{2\pi}{k}\right)^{1/2}[e^{ikx}b_k+e^{-ikx}b^+_k];\\ \nabla\theta_L(x)&=\sum_{k>0}(2\pi k)^{1/2}i[e^{ikx}b_k-e^{-ikx}b^+_k].\end{aligned} \tag{B7}$$

One checks that the commutation relations (B3) are consistent with canonical commutation relations between b_k and $b_{k'}^+$. (The Hamiltonian of the left-moving fermions is represented by $\hat{\mathscr{H}}_L = \Sigma_{k>0} v k b_k^+ b_k$.) Then the quantity $\theta_L(t) - \theta_L(0)$ appearing in the average (B6) is written as

$$\sum_{k>0} \left(\frac{2\pi}{k}\right)^{1/2} [(e^{ikvt}-1)b_k + (e^{-ikvt}-1)b_k^+]. \tag{B8}$$

We evaluate the average

$$\begin{aligned}\langle\langle(\theta_L(t)-\theta_L(0))^2\rangle\rangle &= \sum_{k>0} \frac{2\pi}{k} |e^{ikvt}-1|^2 (2N_{\text{Bose}}(kv)+1) \\ &= 4\int_{-\infty}^{\infty} \frac{dk}{|k|} \sin^2\left(\frac{vkt}{2}\right) \coth\left(\frac{vk}{2T}\right) \\ &= 2\ln\left(\frac{1}{\pi T\delta}\sinh(\pi T t)\right),\end{aligned} \tag{B9}$$

where δ is an ultraviolet cutoff. This expression equals $(2\pi)^2$ times the function $f(t,T)$ computed in (30). From that, we find the average (B6) to be

$$\chi(\lambda) = \left\langle \exp\frac{i\lambda}{2\pi}(\theta_L(t)-\theta_L(0)) \right\rangle^2 = \exp\left[-\left(\frac{\lambda}{2\pi}\right)^2 \langle\langle(\theta_L(t)-\theta_L(0))^2\rangle\rangle\right] = \exp(-\lambda^2 f(t,T)), \tag{B10}$$

which is the desired result.

Periodicity of $\chi(\lambda)$ in λ, corresponding to the charge quantization, is recovered if one corrects the relation between $\hat{\rho}_i(x)$ and $\theta_i(x)$, in order to take into account the integer-valuedness of the particle number $\hat{N}_t$. Using the relation, $\hat{\rho}_i(x) = \Sigma_n e^{in\theta(x)}$, and performing the average, one arrives at the result (29).

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Bound states and scattering in quantum waveguides coupled laterally through a boundary window

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We consider a pair of parallel straight quantum waveguides coupled laterally through a window of a width l in the common boundary. We show that such a system has at least one bound state for any $l>0$. We find the corresponding eigenvalues and eigenfunctions numerically using the mode-matching method, and discuss their behavior in several situations. We also discuss the scattering problem in this setup, in particular, the turbulent behavior of the probability flow associated with resonances. The level and phase-shift spacing statistics shows that in distinction to closed pseudo-integrable billiards, the present system is essentially nonchaotic. Finally, we illustrate time evolution of wave packets in the present model. © *1996 American Institute of Physics.* [S0022-2488(96)00310-6]

I. INTRODUCTION

Spectral and scattering properties of quantum particles whose motion is confined to nontrivial subsets of $\mathbb{R}^n$ represented until recently rather textbook examples or technical tools used in proofs. There are several reasons why these problems attracted a wave of interest in a last few years. The most mathematical among them stems from the observation that, roughly speaking, one can choose the region in such a way that the spectrum of the corresponding Neumann Laplacian coincides with a chosen set;[1,2] of course, the boundary of such a region may be in general rather complicated.

On the other hand, even regions with nice boundaries may exhibit various unexpected properties manifested, for instance, in spectra of the corresponding Dirichlet Laplacians. A prominent example is the existence of bound states, i.e., localized solutions to the free Schrödinger equation, in infinitely stretched regions such as bent, branched, or crossed tubes of a constant cross section—see, e.g., Refs. 3–7; more references are given in the review paper.[8]

A. Quantum wire systems

A strong motivation to study such bound states and related resonance effects[9–11] comes from recent developments in semiconductor physics, because they can be used as models of electron motion in so-called *quantum wires*, i.e., tiny strips of a very pure semiconductor material, and similar structures. Let us briefly recall key features of such systems; more details and a guide to the physical literature can be found in Ref. 8.

Characteristic properties of the semiconductor microstructures under consideration are of small size, typically from tens to hundreds of nanometers, high purity, which means that the electron mean free path can be a few μm or even larger, and crystalline structure. In addition,

boundaries of the microstructures consist usually of an interface between two different semiconductor materials; the electron wave functions are known to be suppressed there.

Behavior of an electron in such a ''mesoscopic'' system structure is, of course, governed by the many-body Schrödinger equation describing its interaction with the lattice atoms including the boundary, external fields, and possible impurities. The mentioned properties allow us, however, to adopt several simplifying assumptions. As we have said, the mean free path is typically two or three orders of magnitude larger than the size of the structure; hence the electron motion can be assumed in a reasonable approximation as ballistic, i.e., undisturbed by impurity scattering.

The most important simplification comes from the crystalline structure. The one-electron Hamiltonian as a Schrödinger operator with a periodic potential exhibits an absolutely continuous spectrum (see Ref. 12, Sec. XIII.16); in the solid-state physics language one says that the electron moves in the lattice as *free* with some effective mass m^*. The latter changes, of course, along the spectrum but one can regard it as a constant when we restrict our attention to the physically interesting part of the valence band; recall that its value may differ substantially from the true electron mass, for instance, one has $m^* = 0.067 m_e$ for GaAs, which is the most common semiconductor material used in mesoscopic devices.

This property together with the wave function suppression at the interfaces makes it natural to model electrons in a quantum wire system as free (spinless) particles living in the corresponding spatial region with the Dirichlet condition on its boundary; an interaction term must be added only if the whole structure is placed into an external field. This is the framework in which the mentioned curvature-induced bound states and resonances were studied. However, the physical conclusions one can draw from it are not restricted to mesoscopic devices: the results are useful for description of other ''new'' quantum systems[13] and provide fresh insights into the classical theory of electromagnetic waveguides.[14–16]

B. Motivation of the present work

Apart from these practical reasons, the curvature-induced bound states provide at the same time a warning example showing that an intuition based on semiclassical concepts may fail when dealing with quantum systems. It is well known, for instance, that low-dimensional Schrödinger operators have bound states for an arbitrarily small coupling constant as long as the potential is not repulsive in the mean and decays sufficiently fast at infinity.[17,18] A common wisdom, however, is that this is rather an exception, and that the number of bound states of a quantum system is at least *roughly* proportional to the classically allowed volume of the phase space. The waveguide systems in question illustrate that this is not true, because they can exhibit in principle *any* number of bound states, while having *no* closed classical trajectories with the exception of an obvious zero-measure set.

In this article we are going to consider another example of that kind, this time consisting of two straight parallel quantum waveguides. We suppose that they have a common boundary which has a window of a width l allowing the particle to leak from one duct to the other. This an idealized setup for several recently studied quantum-wire systems (see Refs. 19–22). Using a variational argument we shall show that such a system has always at least one bound state, i.e., an isolated eigenvalue below the threshold of the continuous spectrum. Moreover, the system can have any prescribed number of bound states provided the window width is chosen large enough. These conclusions follow from simple estimates; however, they tell us nothing about the corresponding wave functions and more detailed dependence of the bound-state energies on the parameters. To this aim, we shall formulate in Sec. IV a method to solve the problem numerically using the mode-matching technique. In particular, we shall discuss how the first eigenvalue emerges from the continuum as the window opens.

Interesting properties of the system are not exhausted by this. The coupling between the wave functions in the ''arms'' and the connecting region allows the particle to tunnel between different transverse modes, so the scattering matrix is nontrivial; one naturally expects it to have resonances

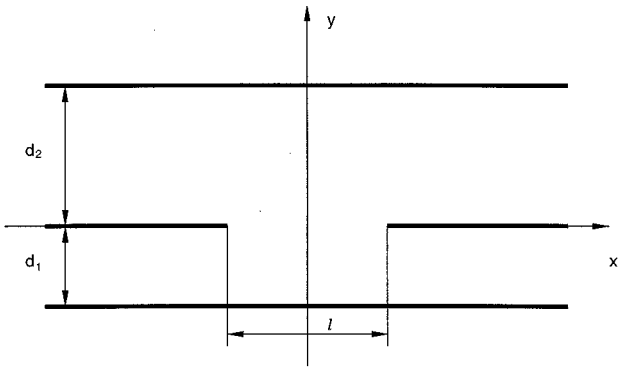


FIG. 1. Laterally coupled quantum waveguides.

with properties similar to those of the bound states below the first transverse-mode energy. It is not easy to prove the existence of such resonances, because there is no natural parameter in the problem which would make it possible to tune the intermode coupling. Neither the window width l nor the replacement of the ''empty'' window by an ''opaque'' one with a suitable point interaction as in Ref. 23 allow for a sensible perturbation theory, because in both cases the unperturbed bound state disappears as the coupling is switched out. Hence we rely again on a numerical analysis based on the mode-matching technique; the results confirm our expectation about the resonance character of the scattering and its dependence on parameters of the problem.

There is one more interesting aspect. The corresponding classical system of coupled ducts is pseudo-integrable, its phase space being of genus three. Other systems of that type have been recently studied;[24,25] it was shown that their quantum couterparts exhibit a chaotic behavior. One asks naturally whether a similar effect can be observed here. To find the level-spacing distribution of the bound states, a very wide window is needed to produce a large number of eigenvalues. At the same time, the spectrum has to be unfolded, i.e., rescaled so that the mean spacing does not change along it. The result suggests that the spacing distribution is then sharply localized around a fixed value; hence there is no chaos. This is not surprising, since all the bound-state wave functions have transversally the shape of the first mode; so effectively they correspond to a one-dimensional system. What is less trivial is that the spacing distribution of the scattering phase shifts also does not witness a fully developed chaos; this suggests that repeated reflections are an essential ingredient of the chaotic behavior of particles in bounded pseudo-integrable billiards.

The above mentioned scattering analysis relies on the stationary approach. The time evolution of wave packets deserves a separate study. In this article we limit ourselves to a single example: in the concluding section we present a numerical method to solve the corresponding time-dependent Schrödinger equation, which allows us to draw some qualitative conclusions about time delay in the scattering on the connecting window.

II. PRELIMINARIES

The system we are going to study is sketched in Fig. 1. We consider a Schrödinger particle whose motion is confined to a pair of parallel strips of widths d_1 and d_2, respectively. For definiteness we assume that they are placed to both sides of the x-axis, and they are separated by the Dirichlet boundary everywhere except in the interval $(-a,a)$; we shall denote this configuration space by Ω and $l:=2a$. Setting $\hbar^2/2m=1$, we may identify the particle Hamiltonian with the Dirichlet Laplacian,

$$H\equiv H(d_1,d_2;l):=-\Delta_D^{\Omega}, \tag{2.1}$$

on $L^2(\Omega)$ defined in the standard way (see Ref. 12, Sec. XIII.15). Since the boundary of Ω has the segment property, it acts as the usual Laplace operator with the Dirichlet condition at the boundary.

A simple bracketing argument[12] shows that H has bound states for all l large enough. Let us first introduce some notation. Set $d:=\max\{d_1,d_2\}$ and $D:=d_1+d_2$, and furthermore

$$\nu:=\frac{\min\{d_1,d_2\}}{\max\{d_1,d_2\}}.$$

We shall also use $\mu_d:=(\pi/d)^2$, with μ_D and μ_l corresponding in the same way to D and l, respectively. Cutting now Ω by the additional Neumann or Dirichlet boundaries parallel to the y-axis at $x=\pm a$, we get $H_t^{(N)}\oplus H_c^{(N)}\leqslant H\leqslant H_t^{(D)}\oplus H_c^{(D)}$, where the ''tail'' part corresponds to the four half strips and the rest to the central part with the Neumann and Dirichlet condition on the vertical boundaries, respectively.

Since $\sigma_{\rm ess}(H_t^{(j)})=[\mu_d,\infty)$, $j=N,D$, the same is by the minimax principle true for H, and possible isolated eigenvalues of H are squeezed between those of $H_c^{(j)}$, $j=N,D$. The Neumann estimate tells us that

$$\inf\,\sigma(H(d_1,d_2;l))\geqslant\mu_D=\mu_d(1+\nu)^{-2}. \tag{2.2}$$

On the other hand, H has an eigenvalue below μ_D provided $H_c^{(D)}$ does, which is true if $\mu_D+\mu_l\leqslant\mu_d$; this shows that a sufficient condition for $H(d_1,d_2;l)$ to have at least a bound state is that the length of the opening satisfies the inequality

$$l\geqslant\frac{d(1+\nu)}{\sqrt{\nu(\nu+2)}}. \tag{2.3}$$

If $\nu=1$, the coefficient on the right side is $2/\sqrt{3}\approx 1.155$; it grows as Ω becomes more asymmetric.

More generally, the number of eigenvalues of $H_c^{(D)}$ is $N_D:=[\sqrt{(\mu_d-\mu_D)/\mu_l}]$, where $[\cdot]$ denotes the entire part (recall that since $D\leqslant 2d$, the first transversally excited state is already above μ_d), while the number of ''Neumann'' eigenvalues is $N_N:=1+N_D$; this means that the number of bound states of $H(d_1,d_2;l)$ satisfies the inequality

$$\left[\frac{l}{d}\,\frac{\sqrt{\nu(\nu+2)}}{1+\nu}\right]\leqslant N\leqslant 1+\left[\frac{l}{d}\,\frac{\sqrt{\nu(\nu+2)}}{1+\nu}\right]. \tag{2.4}$$

We see that $H(d_1,d_2;l)$ has isolated eigenvalues, at least for l large enough, despite the absence of (a nonzero-measure set of) closed classical trajectories mentioned in the Introduction. In heuristic terms, this may be understood as a manifestation of the fact that the semi-infinite ''spikes'' of the open barrier between the two ducts are capable of reflecting a quantum particle due to a finite smearing of the wave packet. In the same way, one finds that the mth eigenvalue μ_m of $H(d_1,d_2;l)$ is estimated by

$$\left(\frac{m-1}{\lambda}\right)^2\leqslant\frac{\mu_m}{\mu_d}-\frac{1}{(1+\nu)^2}\leqslant\left(\frac{m}{\lambda}\right)^2, \tag{2.5}$$

where $\lambda:=l/d$, and that the critical value $\lambda_m\equiv l_m/d$ at which mth eigenvalue appears satisfies the bounds

$$\frac{(m-1)(1+\nu)}{\sqrt{\nu(\nu+2)}}\leqslant\lambda_m\leqslant\frac{m(1+\nu)}{\sqrt{\nu(\nu+2)}}. \tag{2.6}$$

To learn more about the dependence of the eigenvalues and the corresponding eigenfunctions on λ and ν, we have to use a different technique.

III. EXISTENCE OF BOUND STATES

The above existence argument giving Eq. (2.3) is a crude one; in fact, there is no lower bound on the window width as the following result shows:

Theorem: $H(d_1,d_2;l)$ has an isolated eigenvalue in $[\mu_D,\mu_d)$ for any $l>0$.

Proof: We modify for the present purpose the variational argument of Ref. 6; see also Ref. 8, Sec. 2. Without loss of generality we may assume that $d_2 \leqslant d_1 = d$. The transverse ground-state wave function is then

$$\chi_1(y) := \begin{cases} \sqrt{\dfrac{2}{d_1}} \sin(\kappa_1 y), & y \in (0,d_1), \\ 0, \quad \text{otherwise}, \end{cases}$$

where $\kappa_1 := \sqrt{\mu_d}$; similarly we define the transverse ground state in the opening,

$$\eta_1(y) := \sqrt{\frac{2}{D}} \sin[K_1(d_1-y)]$$

with $K_1 := \sqrt{\mu_D}$. For any $\Phi \in D(H)$ we set

$$q[\Phi] := \|H\Phi\|^2 - \mu_d \|\Phi\|^2$$

[if not marked explicitly, the norms always refer to $L^2(\Omega)$].

Since the essential spectrum of H starts at μ_d, we have to find a trial function Φ such that $q[\Phi]<0$; it has to belong to the form domain $Q(H)$, which means, in particular, that it must be continuous inside Ω but not necessarily smooth. Notice first that if $\Phi(x,y)=\varphi(x)\chi_1(y)$, we have

$$q[\Phi] = \|\varphi'\|^2_{L^2(\mathbb{R})}. \tag{3.1}$$

To make the longitudinal contribution to the kinetic energy small, we use an external scaling. We choose an interval $J := [-b,b]$ for a positive $b>a$ and a function $\varphi \in \mathcal{S}(\mathbb{R})$ such that $\varphi(x)=1$ if $x \in J$; then we define the family $\{\varphi_\sigma : \sigma>0\}$ by

$$\varphi_\sigma(x) := \begin{cases} \varphi(x), & |x| \leqslant b, \\ \varphi(\pm b + \sigma(x \mp b)), & |x| \geqslant b. \end{cases}$$

Finally, let us choose a localization function $j \in C_0^\infty((-a,a))$ and define

$$\Phi_{\sigma,\epsilon}(x,y) := \varphi_\sigma(x)[\chi_1(y) + \epsilon j(x)^2 \eta_1(y)] \tag{3.2}$$

for any $\sigma,\epsilon>0$. The main point of the construction is that we modify the factorized function we started with in two mutually disjoint regions, outside and inside the rectangle $J\times(-d_2,d_1)$. Hence the functions φ'_σ and j^2 have disjoint supports. Using this together with the identity

$$\|\varphi'_\sigma\|^2_{L^2(\mathbb{R})} = \sigma \|\varphi'\|^2_{L^2(\mathbb{R})}$$

and the explicit forms of the functions χ_1,η_1, we substitute Eq. (3.2) into Eq. (3.1) and find after a tedious but straightforward computation

$$q[\Phi_{\sigma,\epsilon}] = \sigma\|\varphi'\|^2_{L^2(\mathbb{R})} - 4\pi\epsilon d_1^{-3/2} D^{-1/2} \|j^2\|^2_{L^2(\mathbb{R})} \sin\left(\frac{\pi}{1+\nu}\right)$$

$$+ \epsilon^2 \{\|2jj'\|^2_{L^2(\mathbb{R})} - (\mu_d^2 - \mu_D^2)\|j^2\|^2_{L^2(\mathbb{R})}\}. \tag{3.3}$$

By construction, the last two terms on the right side of Eq. (3.3) are independent of σ. Moreover, the term linear in ϵ is negative (recall that $\nu \in (0,1]$), so choosing ϵ sufficiently small, we can make it dominate over the quadratic one. Finally, we fix this ϵ and choose a small enough σ to make the right side of Eq. (3.3) negative. ■

Remark: Though it is not the subject of the present article, we want to note that the same argument demonstrates existence of a bound state in a straight Dirichlet strip with an arbitrarily small protrusion; one has only to replace $J \times [-d_2, 0]$ by a rectangle contained in the protruded part. An alternative proof of this result has been given recently in Ref. 26; these authors also derived an asymptotic formula for the eigenvalue in terms of the protrusion volume.

IV. MODE MATCHING

To learn more about the eigenvalues and eigenfunctions in question, we shall now solve the corresponding Schrödinger equation numerically. Since Ω consists of several rectangular regions, the easiest way to do that is by the mode-matching method.

A. Symmetric case

Consider first the situation when $d_1 = d_2 = d$. The Hamiltonian (2.1) then decouples into an orthogonal sum of the even and the odd part, the spectrum of the latter being clearly trivial, i.e., the same as in the case $l = 0$. At the same time, the mirror symmetry with respect to the y-axis allows us to consider separately the symmetric and antisymmetric solutions.

We may therefore restrict ourselves to the part of Ω in the first quadrant, with the Neumann boundary condition in the segment $(0,a)$ of the x-axis, and Neumann or Dirichlet condition in the segment $(0,d)$ of the y-axis. We expand the sought solutions in terms of corresponding transverse eigenfunctions

$$\chi_j(y) := \sqrt{\frac{2}{d}} \sin(\kappa_j y), \quad j = 1,2,\ldots, \tag{4.1}$$

$$\phi_j(y) := \sqrt{2}\,\eta_{2j-1}(y) = \sqrt{\frac{2}{d}} \sin[K_{2j-1}(d-y)], \quad j = 1,2,\ldots, \tag{4.2}$$

where $\kappa_j := j\kappa_1$ and $K_{2j-1} := (2j-1)K_1$. A natural Ansatz for the solution of an energy $\epsilon\mu_d$, $\frac{1}{4} \leqslant \epsilon < 1$, is

$$\psi(x,y) = \sum_{j=1}^{\infty} b_j e^{q_j(a-x)} \chi_j(y) \tag{4.3}$$

for $x \geqslant a$, where $q_j := \kappa_1 \sqrt{j^2 - \epsilon}$, and

$$\psi_{\mathrm{s}}(x,y) = \sum_{j=1}^{\infty} a_j \frac{\cosh(p_j x)}{\cosh(p_j a)} \phi_j(y), \quad \psi_{\mathrm{as}}(x,y) = \sum_{j=1}^{\infty} a_j \frac{\sinh(p_j x)}{\sinh(p_j a)} \phi_j(y) \tag{4.4}$$

for $0 \leqslant x \leqslant a$ and the symmetric and antisymmetric cases, respectively, where the longitudinal momentum is defined by $p_j := \kappa_1 \sqrt{(j-\frac{1}{2})^2 - \epsilon}$. It is straightforward to compute the norms of the functions (4.3) and (4.4); since $j^{-1}q_j$ and $j^{-1}p_j$ tend to μ_d as $j \to \infty$, the square integrability of ψ requires the sequences $\{a_j\}$ and $\{b_j\}$ to belong to the space $l^2(j^{-1})$.

As an element of the domain of H, the function ψ should be continuous together with its normal derivative at the segment dividing the two regions, $x = a$. Let us first solve this condition formally. The continuity means $\Sigma_{k=1}^{\infty} a_k \phi_k(y) = \Sigma_{k=1}^{\infty} b_k \chi_k(y)$; using the orthonormality of $\{\chi_j\}$ we get from here

$$b_j = \sum_{k=1}^{\infty} a_k (\chi_j, \phi_k). \tag{4.5}$$

In the same way, the normal-derivative continuity at $x = a$ yields

$$q_j b_j + \sum_{k=1}^{\infty} a_k p_k \tanh(p_k a)(\chi_j, \phi_k) = 0 \tag{4.6}$$

in the Neumann case, and the analogous relation with tanh replaced by coth for Dirichlet. Substituting from Eq. (4.5) to Eq. (4.6), we can write the equation as

$$Ca = 0, \tag{4.7}$$

where

$$C_{jk} := \left(q_j + p_k \left\{ \begin{matrix} \tanh \\ \coth \end{matrix} \right\} (p_k a) \right) (\chi_j, \phi_k) \tag{4.8}$$

in the Neumann and Dirichlet case, respectively, with the two orthonormal bases related by

$$(\chi_j, \phi_k) = \frac{(-1)^{j-k}}{\pi} \frac{2j}{j^2 - (k-\frac{1}{2})^2}. \tag{4.9}$$

One has to make sure, of course, that Eq. (4.8) makes sense, and that one can solve it by a sequence of truncations. It is possible to follow the procedure formulated in Ref. 4. A more direct way, however, is to notice that if ψ is an eigenvector of H, it must belong to the domain of any integer power of this operator. It is easy to check that $\psi \in D(H^n)$ iff $\{a_j\}, \{b_j\} \in l^2(j^{2n-1})$; hence the sought sequences should belong to $l^2(j^s)$ for all $s \geqslant -1$. This fact also justifies *a posteriori* the interchange of summation and differentiation we have made in the matching procedure.

Consider now the diagonal operator S_r on $l^2(j^{-1})$, $(S_r a)_j := j^{-r} a_j$. If C has zero eigenvalue with a fast decaying eigenvector, the same is true for $C^{(s,r)} := S_s C S_r$ with arbitrary non-negative s, r. The last named operator is represented by the matrix

$$C_{jk}^{(s,r)} := [q_j + p_k \tanh(p_k a)] \frac{(-1)^{j-k}}{\pi} \frac{2 j^{1-s} k^{-r}}{j^2 - (k-\frac{1}{2})^2}$$

(for the sake of brevity, we speak about the Neumann case only), so it is Hilbert–Schmidt case for r, s large enough, and its eigenvalues can therefore be obtained from a sequence of truncated operators. Since finite matrices pose no convergence problems, the truncation procedure may be applied to the operator C directly.

Of course, $C^{(r,s)}$ may have eigenvectors to which no square-summable eigenvector of C corresponds, because S_r^{-1} is unbounded for $r>0$. Fortunately, the search for solutions may be terminated once we find the number of them which saturates the upper bound derived in Sec. II.

B. Alternative method

A natural modification of the above described procedure is to express $\{a_k\}$ from Eq. (4.5) using the orthonormality of $\{\phi_k\}$, and to substitute it into Eq. (4.6); then the spectral condition acquires the form

$$b + Kb = 0, \tag{4.10}$$

where

$$K_{jm} := \frac{1}{q_j} \sum_{k=1}^{\infty} (\chi_j, \phi_k) p_k \tanh(p_k a)(\phi_k, \chi_m), \tag{4.11}$$

and the same with $\coth(p_k a)$ in the Dirichlet case.

The two approaches are, of course, equivalent. Solving the equation numerically, however, we truncate not only the matrices but also the series in Eq. (4.11). The sequences approximating a given eigenvalue are therefore different. Moreover, in the examples given below we find them monotonous in the opposite sense. The sequences coming from Eq. (4.7) were approaching the limiting values from above, while those obtained from Eq. (4.10) were increasing; in combination this gives a good idea about the numerical stability of the solution.

C. Asymmetric case

Let us pass now to the case when the widths of the ducts are nonequal, $d_1 \neq d_2$. Without loss of generality, we may again suppose that $d_2 \leqslant d_1 = d$. With the mirror symmetry with respect to the y-axis in mind, we shall consider the right-halfplane part of Ω only with the Neumann and Dirichlet condition on the segment $\mathscr{W} := [-d_2, d_1]$ of the y-axis.

To expand the sought solution, we need again suitable transverse bases. In the ''connecting part,'' $0 \leqslant x \leqslant a$, we use

$$\eta_k(y) = \sqrt{\frac{2}{D}} \sin[K_k(d_1 - y)], \quad k = 1,2,\ldots, \tag{4.12}$$

where $K_k := kK_1 = k\kappa_1(1+\nu)^{-1}$. On the other hand, for the ducts we choose

$$\chi_j^{(+)}(y) := \sqrt{\frac{2}{d_1}} \sin(\kappa_j y) i_+(y), \quad j = 1,2,\ldots, \tag{4.13}$$

$$\chi_j^{(-)}(y) := -\sqrt{\frac{2}{d_2}} \sin(\kappa_j \nu^{-1} y) i_-(y), \quad j = 1,2,\ldots, \tag{4.14}$$

where $\kappa_j := j\kappa_1$ and $i_\pm$ are the indicator functions of the intervals $\mathscr{D}_+ := [0, d_1]$ and $\mathscr{D}_- := [-d_2, 0]$, respectively.

The union of the two bases is, of course, an orthonormal basis in $L^2(\mathscr{W})$. Since the numerical computation involves a truncation procedure, we need to introduce a proper ordering. For that we arrange the eigenvalues corresponding to Eq. (4.13) to a single nondecreasing sequence. Equivalently, we arrange the numbers $j, k\nu^{-1}$ with $j,k = 1,2,\ldots$ into a nondecreasing sequence (if ν is rational and there is a coincidence, any order can be chosen in the pair); we denote its elements by θ_m,

$$\theta_1 := 1, \quad \theta_2 := \min\{2, \nu^{-1}\}, \quad \text{etc.}$$

The corresponding ordered basis in $L^2(\mathscr{W})$ is

$$\xi_m: \ \xi_m(y) = \begin{cases} \chi_j^{(+)}(y), & \theta_m = j, \\ \chi_j^{(-)}(y), & \theta_m = j\nu^{-1} \end{cases}. \tag{4.15}$$

Consider first the even solutions, i.e., the Neumann condition at $x=0$. A natural Ansatz for a solution of an energy $\epsilon\mu_d$, $(1+\nu)^{-2} \leqslant \epsilon < 1$, is

$$\psi(x,y) := \sum_{k=1}^{\infty} a_k \frac{\cosh(p_k x)}{\cosh(p_k a)} \eta_k(y), \quad 0 \leqslant x \leqslant a,$$

where

$$\psi(x,y) := \sum_{j=1}^{\infty} b_j^{(\pm)} e^{q_j^{(\pm)}(a-x)} \chi_j^{(\pm)}(y), \quad x \geqslant a, \quad y \in \mathscr{D}_{\pm}, \tag{4.16}$$

where

$$p_j := \kappa_1 \sqrt{\left(\frac{j}{1+\nu}\right)^2 - \epsilon}$$

and

$$q_j^{(+)} := \kappa_1 \sqrt{j^2 - \epsilon}, \quad q_j^{(-)} := \kappa_1 \sqrt{\left(\frac{j}{\nu}\right)^2 - \epsilon}.$$

The duct part of Eq. (4.16) can be also written in a unified way as

$$\psi(x,y) = \sum_{m=1}^{\infty} c_m e^{r_m(a-x)} \xi_m(y), \tag{4.17}$$

where

$$c_m := \begin{cases} b_j^{(+)}, & \theta_m = j \\ b_j^{(-)}, & \theta_m = j\nu^{-1}, \end{cases} \quad r_m := \begin{cases} q_j^{(+)}, & \theta_m = j, \\ q_j^{(-)}, & \theta_m = j\nu^{-1}. \end{cases}$$

Using the continuity of the function and its normal derivative at $x=a$ together with the orthonormality of $\{\chi_j^{\pm}\}$, we find conditions for the coefficient sequences,

$$b_j^{(\pm)} = \sum_{k=1}^{\infty} a_k (\chi_j^{(\pm)}, \eta_k), \tag{4.18}$$

$$q_j^{(\pm)} b_j^{(\pm)} + \sum_{k=1}^{\infty} a_k p_k \tanh(p_k a)(\chi_j^{(\pm)}, \eta_k) = 0. \tag{4.19}$$

This can be also written as

$$c_m = \sum_{k=1}^{\infty} a_k (\xi_m, \eta_k), \quad r_m c_m + \sum_{k=1}^{\infty} a_k p_k \tanh(p_k a)(\xi_m, \eta_k) = 0;$$

substituting from the first equation to the second one, we obtain the spectral condition in the form (4.7) with

$$C_{mk} := [r_m + p_k \tanh(p_k a)](\xi_m, \eta_k), \tag{4.20}$$

where the overlap integrals are given by

$$(\chi_j^{(+)}, \eta_k) = \frac{2j}{\pi\sqrt{1+\nu}} \frac{\sin(\pi k/(1+\nu))}{j^2 - (k/(1+\nu))^2},$$

$$(\chi_j^{(-)}, \eta_k) = \frac{2j}{\pi} \sqrt{\frac{\nu}{1+\nu}} \frac{\sin(\pi k/(1+\nu))}{j^2 - (k\nu/(1+\nu))^2}. \tag{4.21}$$

In the odd case, i.e., Dirichlet condition at $x=0$, we get the same equation with tanh replaced by coth in Eq. (4.20).

By a straightforward modification of the above argument, one can check that the coefficient sequences have a faster-than-powerlike decay and the spectral condition can be solved by a sequence of truncations. One can also rewrite the condition in the form analogous to Eq. (4.10), $c + Kc = 0$, where

$$K_{jm} := \frac{1}{r_j} \sum_{k=1}^{\infty} (\xi_j, \eta_k) p_k \tanh(p_k a)(\eta_k, \xi_m). \tag{4.22}$$

V. SCATTERING

The analysis is similar to that of the previous section. The incident wave is supposed to be of the form $\chi_j^{(+)}(y) e^{-ik_j^{(+)}x}$ in the upper channel, where we have introduced

$$k_j^{(+)} := \kappa_1 \sqrt{k^2 - j^2}, \quad k_j^{(-)} := \kappa_1 \sqrt{k^2 - \left(\frac{j}{\nu}\right)^2};$$

we denote by $r_{jj'}^{(\pm)}, t_{jj'}^{(\pm)}$, respectively, the corresponding reflection and transmission amplitudes to the j'th transverse mode in the upper/lower guide. Due to the mirror symmetry, we can again separate the symmetric and antisymmetric situation with respect $x=0$ and to write

$$r_{jj'}^{(\pm)} = \tfrac{1}{2}(\rho_{jj'}^{(s,\pm)} + \rho_{jj'}^{(a,\pm)}), \quad t_{jj'}^{(\pm)} = \tfrac{1}{2}(\rho_{jj'}^{(s,\pm)} - \rho_{jj'}^{(a,\pm)}), \tag{5.1}$$

where $\rho_{jj'}^{(\sigma,\pm)}$, $\sigma = s,a$, are the appropriate reflection amplitudes. In the symmetric case we have the following Ansatz for the solution

$$\psi(x,y) := \sum_{l=1}^{\infty} a_l \frac{\cos(p_l x)}{\cos(p_l a)} \eta_l(y), \quad 0 \leqslant x \leqslant a,$$

$$\psi(x,y) := \sum_{j'=1}^{\infty} (\delta_{jj'} e^{-ik_j^{(+)}(x-a)} + \rho_{jj'}^{(+)} e^{ik_{j'}^{(+)}(x-a)}) \chi_{j'}^{(+)}(y), \quad x \geqslant a, \quad y \in \mathscr{D}_+,$$

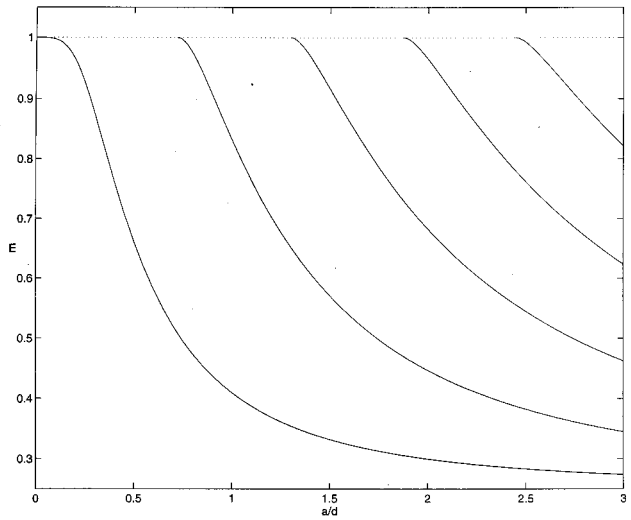


FIG. 2. Bound-state energies vs the window width l in the symmetric case.

$$\psi(x,y) := \sum_{j'=1}^{\infty} \rho_{jj'}^{(-)} e^{ik_{j'}^{(-)}(x-a)} \chi_{j'}^{(-)}(y), \quad x \geqslant a, \quad y \in \mathscr{D}_- . \tag{5.2}$$

The last two relations can be written also as

$$\psi(x,y) = \sum_{m'=1}^{\infty} (\delta_{mm'} e^{-ik_m(x-a)} + \rho_{mm'} e^{ik_{m'}(x-a)}) \xi_{m'}(y),$$

where

$$\rho_{mm'} := \begin{cases} \rho_{jj'}^{(+)}, & \theta_m = j, \quad \theta_{m'} = j', \\ \rho_{jj'}^{(-)}, & \theta_m = j, \quad \theta_{m'} = j' \nu,^{-1} \end{cases} \qquad k_m := \begin{cases} k_j^{(+)}, & \theta_m = j, \\ k_j^{(-)}, & \theta_m = j \nu^{-1}. \end{cases}$$

Matching the functions (5.2) smoothly at $x = a$ we arrive in the same way as above at the equation

$$\sum_{m'=1}^{\infty} [ik_l + p_{m'} \tan(p_{m'} a)](\xi_l, \eta_{m'}) a_{m'} = 2ik_l \delta_{ml}, \tag{5.3}$$

where the index m corresponds to the incident wave and the overlap integrals are given again by Eq. (4.21); in the antisymmetric case one has to replace tan by $-\cot$. The reflection amplitudes are given then by

$$\rho_{ml}^{(\pm)} = -\delta_{ml} + \sum_{m'=1}^{\infty} a_{m'}^{(\pm)}(\xi_l, \eta_{m'}); \tag{5.4}$$

they determine the full S-matrix via Eq. (5.1).

VI. RESULTS

A. Bound states

The results of the mode-matching computation are illustrated on Figs. 2–4. In accordance

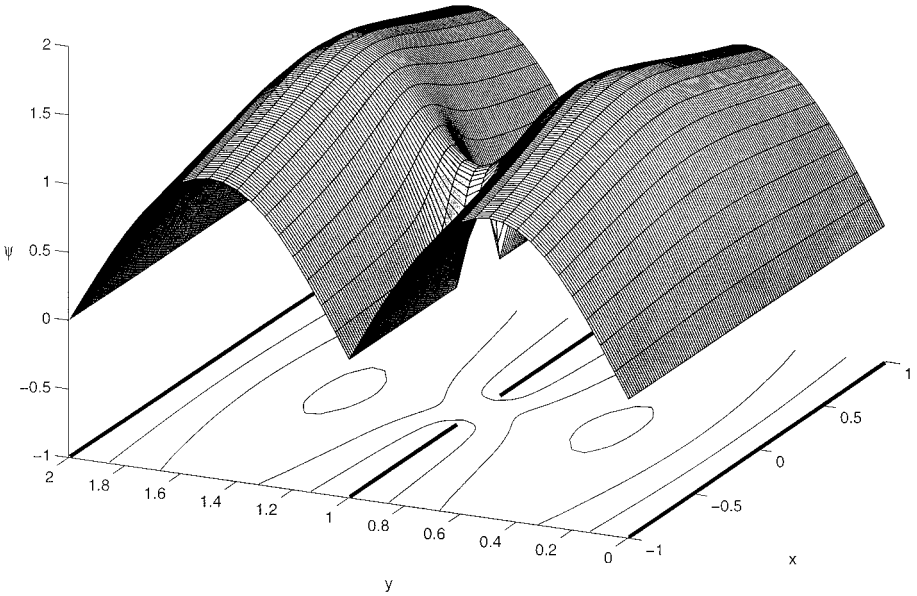


FIG. 3. The ground-state eigenfunction in the symmetric case for $l/d=0.3$.

with the general results of Sec. II the eigenvalues decrease monotonously with the increasing window width and one can sandwich them between the estimates, Eq. (2.5). The eigenfunctions decay exponentially out of the ''interaction'' region. The ground-state wave function is, of course, positive up to a phase factor; the nodal lines of the excited states are parallel to the y-axis. The last feature illustrates once more that apart of the exponential tails in the ducts, the quantum particle ''feels'' the window part as a closed rectangular resonator.

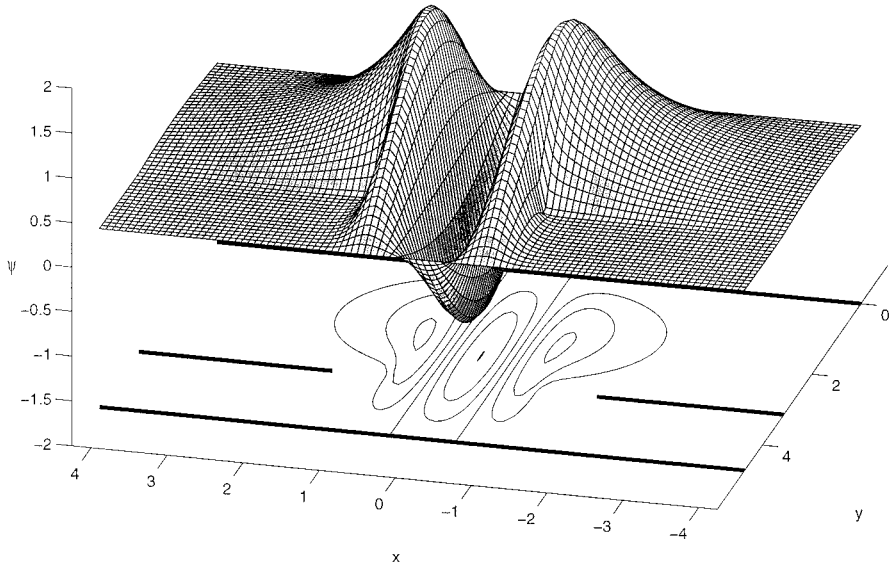


FIG. 4. The eigenfunction of the second excited state in the unsymmetric case, $\nu=1/2$, for $l/d_1=1.08$.

It is also interesting to estimate the rate at which the eigenvalues emerge from the continuum. The results of the mentioned paper[26] together with the Dirichlet bracketing allow us to find a simple upper bound for the ground-state energy by means of a single strip with a ''blister'' whose volume is squeezed to zero. Since the asymptotic formula derived in Ref. 26 applies to ''gentle'' protrusions, it may be employed if the power with which the bump is scaled transversally is larger than the longitudinal one. Hence the gap between the eigenvalue and the continuum for a narrow window is bound from below by $C(\epsilon)l^{4+\epsilon}+\mathcal{O}(l^5)$ for any $\epsilon>0$.

This can be compared with the numerical results. Redrawing the first eigenvalue curve of Fig. 2 and analogous results for $\nu\neq 1$ in the logarithmic scale, we find that the asymptotic behavior is powerlike. The convergence of our method for small l is rather slow; nevertheless, using cutoff dimensions of order 10^3 we get for the power values witnessing clearly that the above bound is saturated,

$$\mu_1(l)=\mu_d-c(\nu)l^4+\mathcal{O}(l^5). \tag{6.1}$$

The numerically found coefficient $c(\nu)$ is monotonous and reaches its maximum value for $\nu=1$; this is the expected behavior as can be seen from a simple bracketing argument. Proving the conjecture (6.1) and finding an analytical expression for $c(\nu)$ remains an open problem; the same can be said about the ''coupling-constant thresholds,'' i.e., the way the other eigenvalues emerge from the continuum.

B. Scattering

The passage of the particle through the window region is determined by the transmission and reflection amplitudes, Eq. (5.1). The physically interesting quantity is the conductivity. If we suppose, for instance, that the particle comes from the upper right guide and leaves through the upper left one, then the conductivity (denoted conventionally as TP and measured in the standard units $2e^2/h$) is given by

$$G(k)=\sum_{j,j'=1}^{[k]} \frac{k_{j'}^{(+)}}{k_j^{(+)}}\,|t_{jj'}^{(+)}(k)|^2, \tag{6.2}$$

and similarly for the other combinations; the summation runs over all open channels. The resonance structure is visible on Fig. 5.

Another insight can be obtained by investigating the probability flow distribution associated with the generalized eigenvector (5.2), which is defined in the standard way,

$$\mathbf{j}(\mathbf{x}):=-i\,\overline{\psi(\mathbf{x})}\,\boldsymbol{\nabla}\psi(\mathbf{x}). \tag{6.3}$$

The flow patterns change with the momentum of the incident particle. They exhibit conspicuous vortices at the resonance energies which represent the ''trapped part'' of the wave function; this phenomenon is illustrated on Fig. 6. It has been argued in the literature that leaky wires similar to those studied here may serve as switching devices.[22] The vortices which emerge in resonance situations lead to the appearance of a magnetic dipole moment, which might be in principle measured experimentally. In this respect situations with a single well developed vortex such as the one illustrated on Fig. 7 are particularly promising.

C. Chaos

Discussing a chaotic behavior of a quantum system, it is useful to start with its classical counterpart, and in particular, its phase space. In the present case of an infinite two-strip ''billiard'' there are no closed classical trajectories with the exception of the obvious zero-measure set;

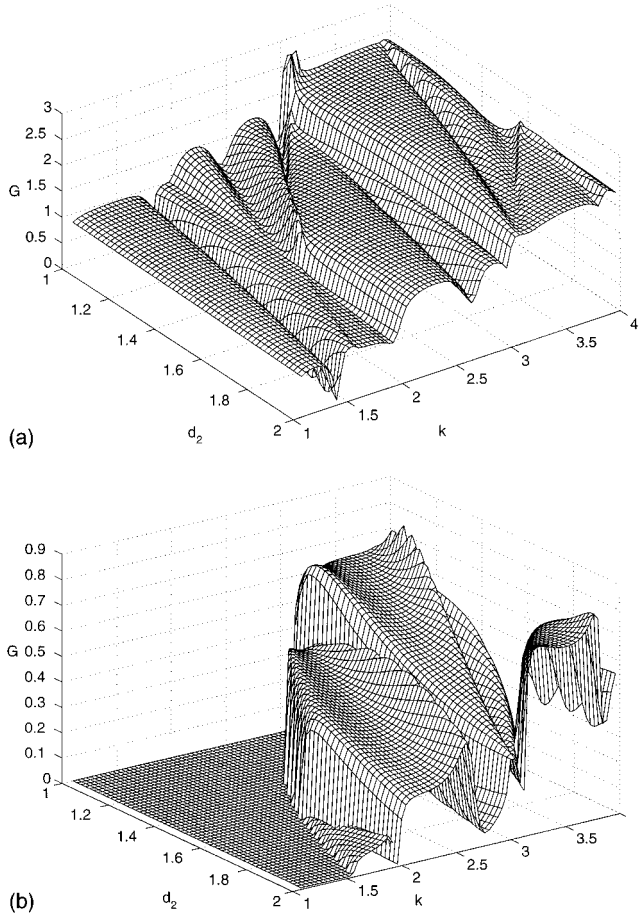


FIG. 5. The conductivity for the particle coming from the right in the upper duct as a function of the momentum k and the width d_2 of the lower tube for $d_1=\pi$, $l=2$. (a) The particle leaves through the upper left channel. A deep resonance is clearly visible. (b) The particle leaves through the lower left channel. The conductivity is zero when there are no propagating modes in the lower part.

hence one has to consider the scattering, i.e., motion of a point particle bouncing its way through the system. The reflection from the walls is supposed be perfectly elastic.

There are two integrals of motion: the longitudinal component of the momentum, $I_1=p_x$, and the modulus of its transverse part, $I_2=|p_y|$. Hence the phase space trajectory of the system is restricted to a two-dimensional manifold (invariant surface) in the four-dimensional phase space. However, due to the singularity of corresponding classical flow at the edges of the connecting window, the topology of this surface is not equivalent to that of a two-dimensional cylinder, but rather of a pair of mutually crossed cylinders; similar systems are usually dubbed pseudo-integrable.[27] The topological structure of the invariant surface has a consequence for the quantum counterpart: the system cannot be quantized semiclassically.

On the other hand, the quantum system of coupled waveguides has in view of our previous arguments bound states, even many of them iff $l\sqrt{\nu}\gg d$. Then one can plot the distribution of the eigenvalue spacing as shown on Fig. 8 for a particular values of ν and l; the character of the distribution does not change as they are varied.

A few comments are due. Since the level statistics depends, in general, on symmetry properties of the corresponding eigenfunction,[28] we have to consider separately bound states of even and

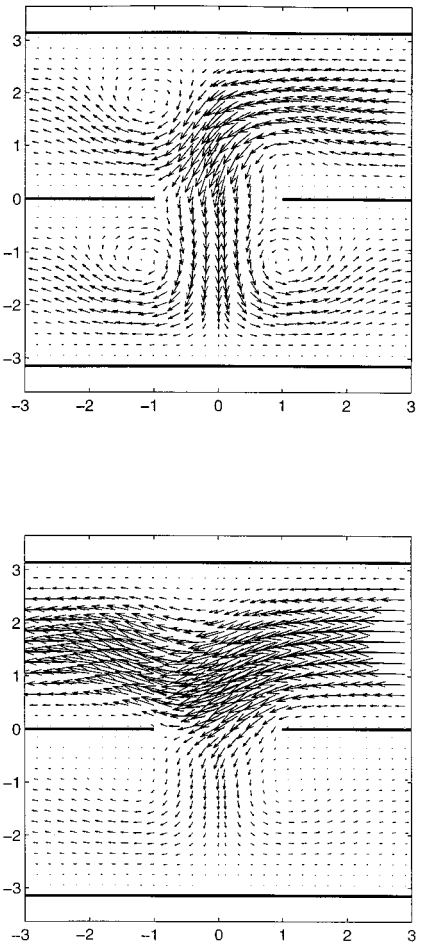


FIG. 6. The quantum probability flow Eq. (6.3), for the symmetric situation, $\nu=1$, in the resonance and nonresonance situation, respectively. The appearance of vortices associated with the resonance scattering is obvious.

odd parity. Furthermore, the inequalities (2.5) show that the energy levels have the same mean spacing if plotted on the scale given by the momentum value $ip_1=\sqrt{\mu_d[\epsilon-(1+\nu)^{-2}]}$. This represents a natural unfolding of our problem; the mean spacing between levels of the same parity then equals $2\pi^2/dl$.

The distributions shown on Fig. 8 differ from typical (unfolded) eigenvalue distributions in billiards, both integrable and chaotic, in the first place due to the existence of the sharp localization around the mean-spacing value. The used statistics (over a thousand eigenvalues in each case) does not allow us to tell what is the behavior around zero; we see, however, that the decay off the peak is at least exponential. This differs substantially from a typical behavior of chaotic systems; however, one should not be surprised because all the corresponding eigenfunctions are dominated transversally by the lowest mode, so the bound-state family in our ''billiard'' is effectively one-dimensional.

It is less trivial whether a chaotic behavior may be manifested in the scattering; recall that spatially restricted pseudo-integrable billiards are known to exhibit the so-called wave chaos.[24] To decide whether a quantum scattering system is chaotic or not, one has to study eigenvalue distribution of the corresponding S-matrix, again properly unfolded, which is expected to conform with that of the Dyson circular ensemble of random matrices[29] in the former case. We have performed

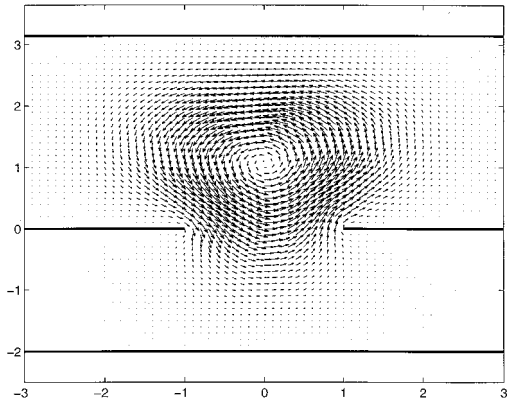


FIG. 7. A single vortex corresponding to the sharp stopping resonance of Fig. 5(a). The conductivity is small in this situation so the waveguide system is closed for the electron transport.

this task for the system under consideration numerically, analyzing the distribution of the spacing between two neighboring eigenvalues of the S-matrix. The result is plotted on Fig. 9; they are compared with the Wigner and the Poissonian distributions peculiar for the chaotic and nonchaotic situation, respectively. It can be seen that the overall shape of this distribution matches the Poissonian distribution for all spacings large enough; on the other hand, the deformation of the distribution near the origin provides a clear sign of nonintegrability of the system. The fact that this nonintegrability differs from a typical chaotic behavior can be attributed to the fact that the scattered particle passes the window region ''only once'' without being bounced to and fro as it is the case of finite billiards.

The absence of the fully developed chaos in the coupled waveguides can also be seen when plotting the coefficients a_l which determine the wave function in the interaction region by Eq. (5.2) as illustrated in Fig. 10. Their distribution remains well localized even for higher energies of

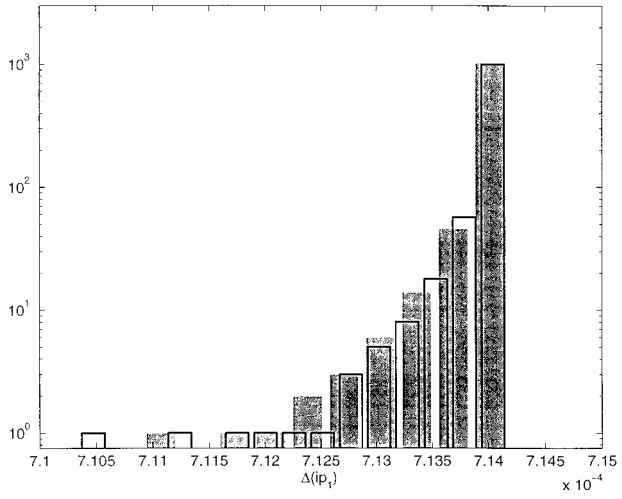


FIG. 8. The unfolded level-spacing distribution of the symmetric and antisymmetric bound states for $d=\pi$, $l=8800$, and $\nu=2(1+\sqrt{5})^{-1}$. The mean momentum distance between eigenvalues of the same parity is 7.1399×10^{-4}. The white and grey boxes correspond to even and odd levels, respectively.

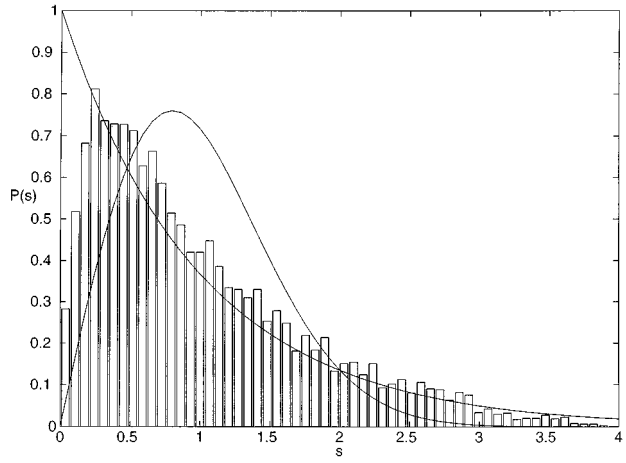


FIG. 9. The unfolded level-spacing distribution for the S-matrix corresponding to $\nu=2/\pi$ and averaged over momentum, in comparison with the Poisson and Wigner distribution.

the incoming particle, its tail being approximately exponential, while in case of an irregular scattering one would expect a slower decay.

VII. TIME EVOLUTION

Up to now we have discussed the coupled waveguide system from the stationary point of view only. Let us look briefly how the window coupling can affect propagation of wave packets in the ducts. This problem has a natural motivation: it has been suggested recently[22,30,31] that coupled electron waveguides provide an analog of the optical directional coupler in the sense that they may switch electrons from one quantum wire to another. Moreover, the authors of Ref. 22 conjectured that the electron switching process should be rather fast due to the direct character of the corresponding resonance, since the electron is not trapped in the interaction region during the resonant switching.

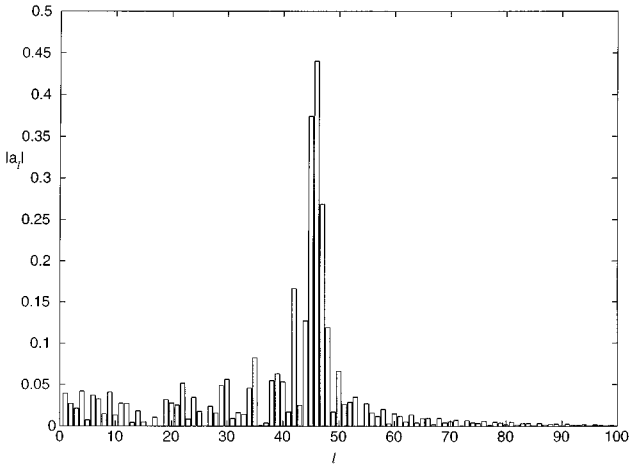
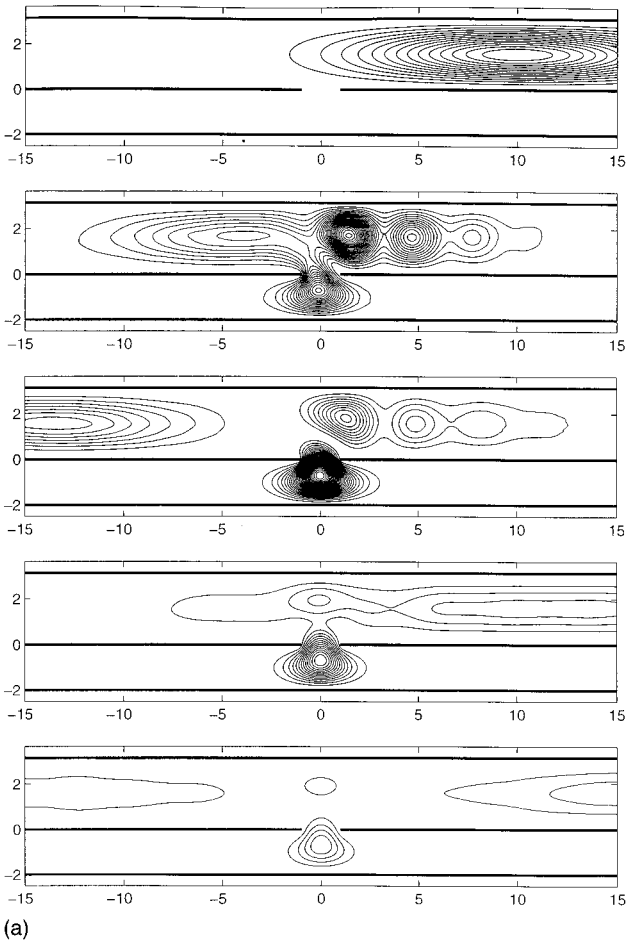


FIG. 10. The absolute value of the coefficients a_l of Eq. (5.2) in the symmetric case for $\nu=2/\pi$ and $k=28.432$; the particle is supposed to be initially in the eighteenth transverse mode.

The existence of probability-flow vortices discussed above in the interaction region indicates that this might not be the case, i.e., that the electron dwelling time in the junction may not be generally neglected. To get a better insight we have investigated time evolution of wave packets numerically. This can be achieved by approximating the evolution operator by a Trotter-formula product (see Ref. 12, Sec. VIII.8) with the Dirichlet boundary condition replaced by a very steep and narrow potential barrier localized along the boundary; the latter has been chosen in such a way that the dynamics of the system was equivalent to the dynamics of the true Dirichlet problem for all times taken into account, i.e., that the tunneling leak was negligible during that period.

The kinetic- and potential-part factors of the evolution operator are then multiplication operators in the momentum and coordinate representation, respectively; the passage between the two representations has been realized by means of the two-dimensional fast Fourier transform method[32] with a grid of $2^9\times 2^7$ points. The time evolution of a wave packet approaching the junction through the upper right arm of the structure is plotted on Fig. 11. The incoming wave function was chosen as $\psi(x,y):=g(x)\chi_1^{(+)}(y)$, where $g(x):=\exp\{-a(x-x_0)^2+ikx\}$ with suitably chosen parameters a,x_0.

The difference between the resonant and nonresonant situation is clearly visible. In the first case the electron stays in the junction region and escapes only slowly, while the electron whose



(a)

FIG. 11. The time evolution of the wavepacket inside the junction with $\nu=2/\pi$ plotted for times $t=0$, 5, 10, 15, and 20, respectively. (a) The resonance case with $k=1.4242$, (b) the near-to-resonance situation, $k=1.48$.

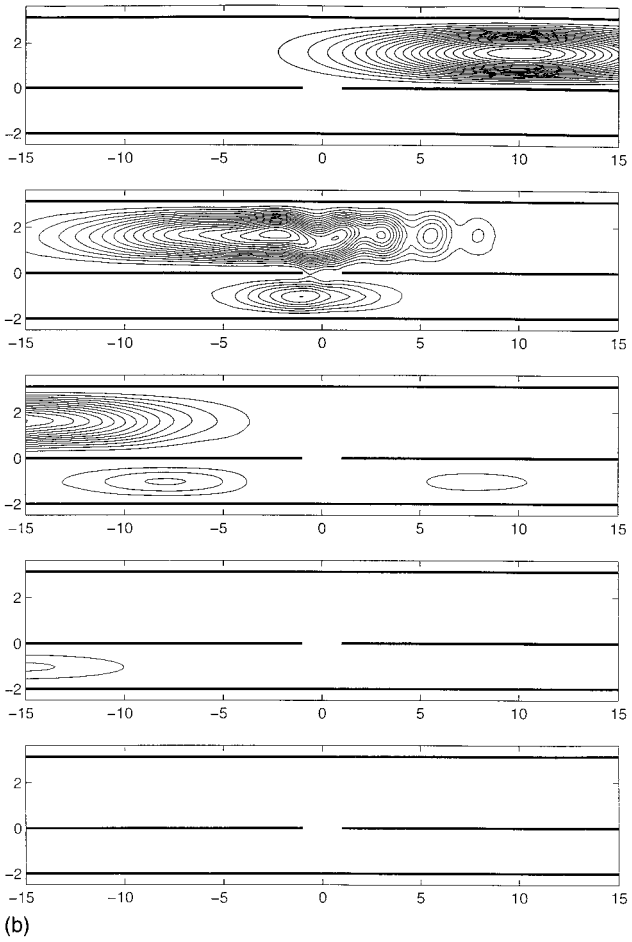


FIG. 11 (*Continued.*)

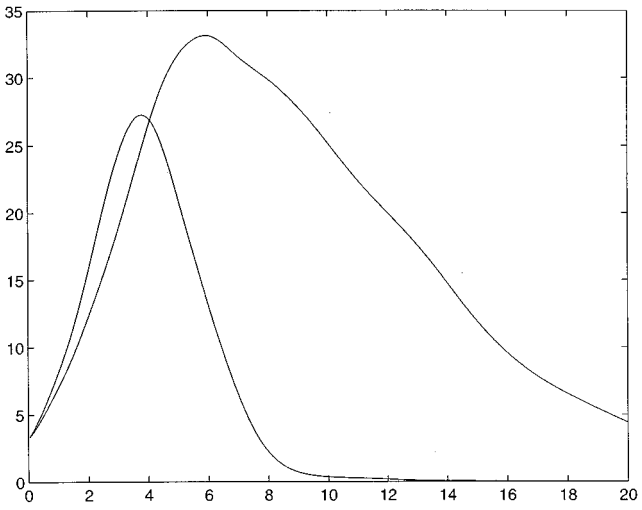


FIG. 12. The probability that the electron will be found within the junction as a function of time evaluated for the same parameters as on Fig. 11.

momentum is localized around a slightly different but nonresonant value of momentum passes the junction ''ballistically.'' Wang and Guo[22] based the mentioned conjecture—which in a realistic situation would lead to ultrashort switching times of a few picoseconds only—on a concept of transmitivity of coupled waveguides leaning on a classical intuition. As we have said in the introduction and demonstrated in the previous sections, this may be a false guide when quantum systems are considered. The example of time evolution offers another illustration. During the resonance-scattering process the evanescent-mode amplitudes inside the quantum wire are considerably enhanced; as a result the electron is trapped temporarily inside the junction. The probability of finding it there in the resonant and nonresonant case, respectively, is shown on Fig. 12. It is desirable to perform the time-delay analysis for the present model, in particular, to confirm that the ''switching time'' of the coupler is inversely proportional to the resonance width.

ACKNOWLEDGMENTS

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S-matrix, resonances, and wave functions for transport through billiards with leads

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For a simple model describing the *S*-matrices of open resonators the statistical properties of the resonances are investigated, as well as the wave functions inside the resonator. © *1996 American Institute of Physics.* [S0022-2488(96)00610-X]

I. INTRODUCTION

The properties of ballistic electron transport through a mesoscopic quantum dot are of considerable interest both experimentally and theoretically.[1,2] For the character of the electron motion the shape of the quantum dot is of particular importance. The transport characteristics—such as the conductance fluctuations—are different for shapes which correspond to integrable and chaotic classical motion inside the dot.[3] Similar results have been obtained also in experiments with microwave resonators.[4,5]

The theory accounting for this phenomena is usually based on the so-called stochastic approach, which is able to reproduce the scattering characteristics of the system[6] employing the theory of random matrices. Our aim here is to develop a simple model which will be able to describe not only the corresponding *S*-matrix but also give information about the structure of the wave function inside the cavity.

The system we would like to investigate consists of a cavity (quantum dot, electromagnetic resonator) with attached leads (antenna). The cavity is assumed to be either integrable or fully chaotic. In particular the following characteristics of the system will be of interest for us:

(1) The structure of the *S*-matrix.

(2) Statistical properties of the resonances, including the spacing distribution of the resonance positions and the distribution of the resonance widths.

(3) Statistical properties of the wave function, which is excited inside the cavity by a wave incoming through the waveguide.

We assume that the whole device consists of two different parts. The first part includes ideal leads (waveguides) which couple the device to the measuring apparatus and/or serve as a power

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supply. The electron/wave moves freely inside these leads, i.e., without scattering by impurities, etc. The second part contains the ''randomizing'' part of the device. Inside this part the electron acquires chaotic features, for instance, through multiple scattering on the boundary of the sample and/or impurities. We shall assume that the dynamics inside this part of the system is chaotic so that its Hamiltonian can be considered as a member of an appropriate random matrix ensemble. We shall also investigate integrable cavities (like a rectangular resonator) and show that the wave transport through it also acquires chaotic features since by connecting such a system to continua one destroys integrability. In the integrable case we shall assume that the internal Hamiltonian is described by a Poisson ensemble.

II. THE MODEL

In this section we shall construct a Hamiltonian describing a resonator coupled to waveguides. Starting with the description of the leads we assume these to support M open channels which are described by one-dimensional Hamiltonians

$$H_l = -\frac{d^2}{dx^2} + \lambda_l, \quad l = 1,\ldots,M. \tag{1}$$

Here λ_l is the threshold energy of the lth channel. Combining these operators into a Hamiltonian H_{ex} for the ''external'' part of the system, i.e., the leads, we get

$$H_{\mathrm{ex}} = -\bigoplus_{l=1}^{M} \frac{d^2}{dx_l^2} + \Lambda. \tag{2}$$

Here Λ is a diagonal matrix describing the threshold energies of the channels,

$$\Lambda = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_M). \tag{3}$$

The resonator is described by a Hermitian matrix H_{in} of size $N \times N$, with N much larger than the number of open channels, $N \gg M$. The matrix H_{in} is assumed to belong to the Gaussian orthogonal/unitary ensemble (GOE/GUE) for chaotic resonators and to a Poisson ensemble for integrable ones (see, e.g., Ref. 7 for these concepts). To describe the scattering we couple the resonator and leads by defining the Hamiltonian H of the whole system as

$$H\begin{pmatrix} u \\ u_{\mathrm{in}} \end{pmatrix} = \begin{pmatrix} H_{\mathrm{ex}} u \\ H_{\mathrm{in}} u_{\mathrm{in}} + A u'(0) \end{pmatrix}, \tag{4}$$

where $u = (u_1, \ldots, u_M)$ stands for the wave function inside the leads and u_{in} describes the wave function within the resonator; $u'(0)$ denotes the derivative of the wave functions of the leads at the points of contact with the resonator which are taken as the zeros of the waveguide coordinates, and A is an $N \times M$ coupling matrix. The local character of the coupling in Eq. (4) (a point contact) is justified whenever the diameter of the junction of lead and resonator is smaller than a typical wavelength inside the resonator. The differential operator H_{ex} can be defined on the Sobolev space $W_2^2(R_+, C^M)$ of all complex vector valued square integrable functions on R_+ having two generalized square integrable derivatives. Then the operator H is defined in the Hilbert space $\mathscr{H} = L^2(R^+, C^M) \oplus C^N$ with the scalar product

$$(U, V) = \int_0^\infty \langle u(x), v(x) \rangle_{C^M} dx + \langle u_{\mathrm{in}}, v_{\mathrm{in}} \rangle_{C^N},$$

$\langle \cdot, \cdot \rangle_{C^N}$ denotes the scalar product in the N-dimensional Hilbert space. The domain of the operator H should contain the domain $W_2^2(R_+, C^M) \oplus C^N$ but H is not self-adjoint on the latter domain.

Theorem 1: The operator H defined by formula (4) is self-adjoint on the domain of functions from $W_2^2(R_+,C^M)\oplus C^N$ satisfying the boundary conditions

$$A^\dagger u_{\rm in}=-u(0). \tag{5}$$

Proof: The boundary form of the linear operator H evaluated on the functions $U,V\in W_2^2(R_+,C^M)\oplus C^N$ is given by the following expression

$$\begin{aligned} b[U,V]&=(U,HV)-(HU,V)\\ &=\int_0^\infty \left\langle u(x),-\frac{d^2}{dx^2}\,v(x)+\Lambda v(x)\right\rangle_{C^M} dx+\langle u_{\rm in},H_{\rm in}v_{\rm in}\rangle_{C^N}\\ &\quad+\langle u_{\rm in},Av'(0)\rangle_{C^N}-\int_0^\infty \left\langle -\frac{d^2}{dx^2}\,u(x)+\Lambda u(x),v(x)\right\rangle_{C^M} dx-\langle H_{\rm in}u_{\rm in},v_{\rm in}\rangle_{C^N}\\ &\quad-\langle Au'(0),v_{\rm in}\rangle_{C^N}\\ &=\langle u(0),v'(0)\rangle_{C^M}-\langle u'(0),v(0)\rangle_{C^M}+\langle u_{\rm in},Av'(0)\rangle_{C^N}\\ &\quad-\langle Au'(0),v_{\rm in}\rangle_{C^N}. \end{aligned} \tag{6}$$

The boundary form vanishes if both elements U, V satisfy the boundary conditions (5)

$$\begin{aligned} b[U,V]&=\langle u(0),v'(0)\rangle_{C^M}-\langle u'(0),v(0)\rangle_{C^M}+\langle A^\dagger u_{\rm in},v'(0)\rangle_{C^N}-\langle u'(0),A^\dagger v_{\rm in}\rangle_{C^N}\\ &=\langle u(0),v'(0)\rangle_{C^M}-\langle u'(0),v(0)\rangle_{C^M}-\langle u(0),v'(0)\rangle_{C^M}+\langle u'(0),v(0)\rangle_{C^M}\\ &=0, \end{aligned}$$

where the dagger denotes the adjoint of an operator. This proves that the operator H is symmetric. The self-adjointness of the operator follows from the fact that the range of $H-i$ coincides with the whole Hilbert space $\mathscr{H}$. □

Note: In what follows we shall denote by H the self-adjoint operator defined by formula (4) and the boundary condition (5). The domain of the operator will be denoted by $D(H)$.

Similar models were suggested first in Refs. 8–11. Their main appeal is that they allow for a spectral analysis of the operator H in terms of elementary functions. Moreover, by calculating the eigenfunctions pertaining to the continuous spectrum one may obtain the scattering matrix in terms of the internal Hamiltonian $H_{\rm in}$ and the coupling matrix A. The eigenfunctions

$$\Psi(E)=\begin{pmatrix}\psi(E,x)\\ \psi_{\rm in}\end{pmatrix}$$

corresponding to the energy E solve the equations

$$\begin{pmatrix}-\dfrac{d^2}{dx^2}\,\psi(E,x)+\Lambda\psi(E,x)\\ H_{\rm in}\psi_{\rm in}(E)+A\psi'(E,0)\end{pmatrix}=E\begin{pmatrix}\psi(E,x)\\ \psi_{\rm in}\end{pmatrix}. \tag{7}$$

The second of the foregoing equations leads, together with the boundary condition (5), to the following energy-dependent condition for the external component of the wave function,

$$\psi(E,0)=A^\dagger\,\frac{1}{H_{\rm in}-E}\,A\psi'(E,0). \tag{8}$$

Moreover, the external component is a solution of the free Schrödinger equation. For the energy $E \neq \lambda_j$, $j=1,\ldots,M$, it can be presented in the form

$$\psi(E,x)=\frac{e^{-i\sqrt{E-\Lambda}x}}{\sqrt[4]{E-\Lambda}}\,\mathscr{A}_{\rm inc}-\frac{e^{i\sqrt{E-\Lambda}x}}{\sqrt[4]{E-\Lambda}}\,\mathscr{A}_{\rm out}, \tag{9}$$

where $\mathscr{A}_{\rm inc}$ and $\mathscr{A}_{\rm out}$ are the amplitudes of the incoming and outgoing wave, respectively. For all $E>\max\{\lambda_j\}$ every solution is bounded and the scattering matrix $S(E)$ can easily be defined. The normalization used in Eq. (9) ensures that the S-matrix relates the amplitudes of the incoming and outgoing waves as

$$\mathscr{A}_{\rm out}=S(E).\mathscr{A}_{\rm inc}.$$

The scattering matrix can be calculated substituting the external component of the wave function into the energy-dependent boundary condition (8). The boundary values of the external component at the ''origin,'' i.e., at the coupling points, are equal to

$$\psi(0)=Q(1-S).\mathscr{A}_{\rm inc}, \quad \psi'(0)=iQ^{-1}(-1-S).\mathscr{A}_{\rm inc},$$

where $Q\equiv Q(E)$ denotes the $M\times M$ matrix $Q(E)=(E-\Lambda)^{-1/4}$. For energies above the thresholds the S-matrix can be determined through the following:

Lemma 1: The stationary scattering matrix for the operator H is equal to

$$S(E)=\frac{i+\widetilde{W}^{\dagger}(E-H_{\rm in})^{-1}\widetilde{W}}{i-\widetilde{W}^{\dagger}(E-H_{\rm in})^{-1}\widetilde{W}}, \tag{10}$$

where $E>\max\{\lambda_j\}$ and $\widetilde{W}=AQ^{-1}$.

Similar results were obtained earlier in Ref. 11.

The knowledge of the Hamiltonian of the system enables us to go beyond the standard scattering characteristics and to solve Eq. (7) for the internal-component of the wave function,

$$\psi_{\rm in}=\frac{2}{E-H_{\rm in}}\,\widetilde{W}\,\frac{1}{i-\widetilde{W}^{\dagger}(E-H_{\rm in})^{-1}\widetilde{W}}\,\mathscr{A}_{\rm inc}. \tag{11}$$

In Sec. IV we shall use this formula to evaluate the structure of the wave function in the internal (interaction) part of the system.

Before proceeding further let us shortly comment on the properties of the S-matrix (10). First, we show that the S-matrix (10) can be rewritten in the more familiar form[12]

$$S=I-2\pi i W^{\dagger}\,\frac{1}{E-H_{\rm in}+i\pi WW^{\dagger}}\,W. \tag{12}$$

To prove the equivalence of Eqs. (10) and (12) we use the resolvent equation

$$R(E)=R_0(E)-i\pi R_0(E)P[1+i\pi PR_0(E)P]^{-1}PR_0(E) \tag{13}$$

with $R(E)=(E-H_{\rm in}+i\pi WW^{\dagger})^{-1}$, $R_0(E)=(E-H_{\rm in})^{-1}$, and $P=WW^{\dagger}$. Inserting this into Eq. (12) we obtain after a simple calculation

$$S=\frac{i+\pi W^{\dagger}R_0(E)W}{i-\pi W^{\dagger}R_0(E)W},$$

which is fully equivalent to Eq. (10) provided we identify $\widetilde{W}$ and $\sqrt{\pi}W$. There is, however, one important difference: The coupling matrix $\widetilde{W}$ is energy dependent. This dependence takes into account the threshold effects which are often disregarded in the stochastic approach; it has, however, measurable consequences and leads to the correct high-energy behavior of the S-matrix.[13] We shall come back to this point in Sec. V when we use the model to describe the experimental results obtained for rectangular electromagnetic resonators.

III. RESONANCE DISTRIBUTION

We now propose to study how the distribution of nearest-neighbor spacings between the resonances of our open system differs from the distribution of spacings between eigenenergies of the closed resonator. For simplicity we confine ourselves to the simplest case, that of a single open channel, $M=1$. The original $N\times M$ matrix A becomes then an N-component vector. We shall focus on an integrable resonator rather than a chaotic one since in this case the differences in question turn out to be most drastic: roughly speaking, the opening of the resonator by waveguides destroys the usual spectral signatures of integrability. In what follows we assume that the coupling vector A is normalized as

$$A=ga, \quad \|a\|=1,$$

and that the coupling constant g is large, $g\gg 1$. The resonances of the whole system are the eigenvalues of the effective ''Hamiltonian''

$$H_{\text{eff}}=H_{\text{in}}-i\widetilde{W}\widetilde{W}^{\dagger}=H_{\text{in}}-ig^2aQ^2a^{\dagger}.$$

The ''perturbation'' $-i\widetilde{W}\widetilde{W}^{\dagger}$ of H_{in} is negative imaginary and has rank one. Every eigenfunction of the effective Hamiltonian H_{eff} is a solution to the equation

$$(H_{\text{in}}-ig^2aQ^2a^{\dagger})\psi_{\text{in}}=E\psi_{\text{in}},$$

and comes with a certain resonance energy $E\in\mathbb{C}$. Applying the resolvent of the internal Hamiltonian to the latter equality we get a ''dispersion equation'' for the resonance energy,

$$\frac{1}{g^2\sqrt{\lambda-E}}=a^{\dagger}\,\frac{1}{H_{\text{in}}-E}\,a. \tag{14}$$

Denoting by $F(E)$ the right-hand side (rhs) of Eq. (14) and expressing it in the eigenrepresentation of H_{in} we have

$$F(E)=\sum_{n=1}^{N}\frac{|a_n|^2}{E_n-E}, \tag{15}$$

where E_n are the eigenvalues of the internal Hamiltonian. The function $F(E)$ has a positive imaginary part in the upper half plane and is real on the real axis. Therefore all solutions of Eq. (14) are localized in the lower complex half plane. Consider the case of strong coupling, $g\to\infty$. Then all solutions of the dispersion equation (14) are situated at the zeros of the function $F(E)$. Our aim here is to investigate the distribution of spacings between such zeros (following a method similar to that used in Ref. 14).

It is clear that between two poles there is exactly one zero of $F(E)$. Moreover, two neighboring zeros are locked between three neighboring poles. Since we are interested in the distribution of resonance spacings for small spacings, it suffices to restrict the sum $F(E)$ in Eq. (15) to three terms only, namely, to those whose poles lock up the two colliding zeros of $F(E)$. Let us

label those poles by E_1, E_2, E_3. In order to simplify the expressions (but without loss of generality) we shift the origin of the energy scale to the central pole such that $E_2=0$, whereupon E_1 is negative, $E_1<0$. Then the eigenvalue equation (14) simplifies to

$$\frac{w_1}{E_1-E}-\frac{w_2}{E}+\frac{w_3}{E_3-E}=0 \tag{16}$$

with $w_i=|a_i|^2$, $i=1,2,3$. The two zeros in discussion solve the quadratic equation

$$(w_1+w_2+w_3)E^2-[(w_1+w_2)E_3+(w_2+w_3)E_1]E+w_2E_1E_3=0, \tag{17}$$

and their squared distance $D=s^2$ is given by

$$D=\frac{[(w_1+w_2)E_3+(w_2+w_3)E_1]^2}{(w_1+w_2+w_3)^2}-\frac{w_2E_1E_3}{w_1+w_2+w_3}. \tag{18}$$

Our aim here is to investigate the cumulative probability of these squared spacings, $P(D)=P((z_1-z_2)^2\leqslant D)$, where z_1 and z_2 are the two solutions of Eq. (17) in the case when the internal Hamiltonian H_{in} belongs to the Poisson ensemble, i.e., corresponds to an integrable system. As already announced above that distribution will reveal level repulsion due to the attached waveguides, even though the internal Hamiltonian H_{in} belongs to the Poisson ensemble, i.e., corresponds to an integrable system. Before proceeding further we shall need the following.

Lemma 2: (a) $f(t)\equiv t^\alpha \exp(-t)\leqslant a^\alpha e^{-\alpha}\ \forall t\geqslant 0$, $\alpha>0$. (b) Let $0<\alpha<1$, $b>0$; *then the following estimate is valid*:

$$\int_0^\infty \frac{e^{-br}}{r^{1-\alpha}}\,dr\leqslant\frac{1}{\alpha}+\frac{1}{b}.$$

Proof: (a) holds because f is continuous with maximum at $t=\alpha$. (b) follows from

$$\int_0^\infty \frac{e^{-br}}{r^{1-\alpha}}\,dr=\int_0^1 \frac{e^{-br}}{r^{1-\alpha}}\,dr+\int_1^\infty \frac{e^{-br}}{r^{1-\alpha}}\,dr\leqslant\int_0^1 \frac{1}{r^{1-\alpha}}\,dr+\int_1^\infty e^{-br}dr\leqslant\frac{1}{\alpha}+\frac{1}{b}.$$

□

A. Estimates from above

It follows from Eq. (18) that one can use the following lower estimate for D,

$$D\geqslant -4\,\frac{w_2}{w_1+w_2+w_3}\,E_1E_3. \tag{19}$$

This inequality implies

$$P(D)\leqslant P(X) \tag{20}$$

with $X=-4[w_2/(w_1+w_2+w_3)]E_1E_3$.

Case 1. Constant coupling $w_1=w_2=w_3=1$

Let us assume first that the coefficients w_i are constant and equal, as is not unreasonable when the antenna is attached to a ''symmetry point'' of the resonator and when we restrict ourselves to resonances belonging to one parity class only. For a rectangular resonator this means that we couple the antenna to the geometric center and investigate only resonances which have even–even parity. The probability can be estimated as follows,

$$P(D) \leqslant \int_0^D da \int_{-\infty}^0 dE_1 e^{E_1} \int_0^\infty dE_3 e^{-E_3} \delta(-\tfrac{4}{3} E_1 E_3 - a)$$

$$= -\int_0^D da \int_{-\infty}^0 dE_1 \frac{3}{4E_1} \exp(E_1) \exp\left\{ \frac{3a}{4E_1} \right\}.$$

Thus for any $0<\alpha<1$ we have using Lemmas 2 and 3

$$P(D) \leqslant -\int_0^D da \frac{3}{4} \int_{-\infty}^0 dE_1 \frac{e^{E_1}}{E_1} \left(-\frac{3a}{4E_1} \right)^{-\alpha} \left(-\frac{3a}{4E_1} \right)^{\alpha} \exp\left\{ \frac{3a}{4E_1} \right\}$$

$$\leqslant \left(\frac{3}{4} \right)^{1-\alpha} \int_0^D da \frac{\alpha^\alpha}{a^\alpha} \left(1 + \frac{1}{\alpha} \right) e^{-\alpha}$$

$$= \left(\frac{3}{4} \right)^{1-\alpha} \frac{\alpha^\alpha}{1-\alpha} \left(1 + \frac{1}{\alpha} \right) e^{-\alpha} D^{1-\alpha}$$

$$= C_1(\alpha) D^{1-\alpha}.$$

We note that the latter estimate is valid for any positive value of the parameter α, but the constant $C_1(\alpha)$ tends to infinity when α tends to zero.

Case 2. Poisson distribution of w_i

Another physically relevant case we discuss here is the case when the coupling vector a is complex with coefficients whose real and imaginary parts are independent and normally distributed. Then the w_i are independent random numbers with a χ^2 distribution with two degrees of freedom. Moreover, the sum $w_1+w_2+w_3$ has a χ^2 distribution with 6 degrees of freedom. Having this in mind we obtain that $y=w_2/(w_1+w_2+w_3)$ has a distribution with a density given by $p(y)=2(1-y)$, $y \in [0,1]$. Using Lemma 2 we can estimate $P(D)$ as follows, given by

$$P(D) \leqslant \int_0^D da \int_{-\infty}^0 dE_1 e^{E_1} \int_0^\infty dE_3 e^{-E_3} \int_0^1 dy 2(1-y) \delta(-4yE_1E_3 - a)$$

$$= -\int_0^D da \int_{-\infty}^0 dE_1 e^{E_1} \int_0^1 dy e^{a/4yE_1} \frac{1}{4yE_1} 2(1-y)$$

$$= \int_0^D \frac{da}{a^\alpha} \int_{-\infty}^0 dE_1 e^{E_1} \int_0^1 dy e^{a/4yE_1} \left(-\frac{1}{4yE_1} \right)^{1-\alpha} \left(-\frac{a}{4yE_1} \right)^{\alpha} 2(1-y)$$

$$\leqslant \int_0^D \frac{da}{a^\alpha} \int_0^1 dy 2(1-y) \frac{\alpha^\alpha e^{-\alpha}}{(4y)^{1-\alpha}} \left(\frac{1}{\alpha} + 1 \right) \leqslant C_2(\alpha) D^{1-\alpha}$$

for any $1>\alpha>0$. Similarly as in the previous case $C_2(\alpha)$ is some function of α with $\lim_{\alpha \to 0} C_2(\alpha) = \infty$. Thus we got the same estimate as in the case 1.

A similar estimate is also valid in the case where the components of the vector w are real independent random numbers equally distributed in the interval $[0,1]$.

B. Lower estimates

To obtain a lower estimate for $P(D)$ we use first following upper estimate for the distance between the two zeros:

$$(z_1 - z_2)^2 \leqslant (-E_1 + E_3)^2.$$

Then

$$P(D)\geqslant\int_0^D da\int_{-\infty}^0 dE_1 e^{E_1}\int_0^\infty dE_3 e^{-E_3}\delta((-E_1+E_3)^2-a)$$

$$=\int\int_{-E_1+E_3\leqslant\sqrt{D}} dE_1 dE_3 e^{-(-E_1+E_3)}$$

$$=\frac{1}{2}\int_0^{\sqrt{D}} dx e^{-x}\int_{-x}^{x} dy$$

$$=\int_0^{\sqrt{D}} dx e^{-x}x=1-e^{-\sqrt{D}}(1+\sqrt{D}).$$

Thus the probability $P(D)$ can be approximated from below by a linear function for small values of D,

$$P(D)\geqslant D+o(D)\geqslant BD,$$

where $B\leqslant 1$, $o(D)/D\to 0$ as $D\to 0$.

C. Asymptotic behavior at small spacings

Combining together lower and upper estimates for the probability we can write

$$BD\leqslant P(D)\leqslant C(\alpha)D^{1-\alpha}. \tag{21}$$

A similar estimate can be obtained also for the probability of resonance spacings $\tilde{P}(s)$, $s^2=D$:

$$Bs^2\leqslant\tilde{P}(s)\leqslant C(\alpha)s^{2-2\alpha}. \tag{22}$$

The physically relevant quantity is, however, not the distribution $\tilde{P}(s)$ but the corresponding probability density $p(s)$:

$$\tilde{P}(s)=\int_0^s p(t)dt.$$

Suppose that for small s the probability density has the behavior

$$p(s)\sim ks^\beta+o(s^\beta),$$

with some real constants k and β. Substituting the last asymptotic expansion into the estimate (22) we get for the constants k and β

$$\beta=1,\quad k\geqslant 2B.$$

It follows that the probability density of the spacing s is approximately linear for small values of s. This estimate shows that the presence of the antenna changes the character of the resonance spacing distribution from Poisson to a distribution which displays linear repulsion for small s. For the slope k of the distribution we find $k\geqslant 2$ for small s. This means that the slope k is always larger than the slope of the spacing probability density in a fully chaotic system, which is given by the Wigner distribution with a slope equal to $\pi/2$. The resonance repulsion is therefore always weaker than the level repulsion for a typical GOE matrix.

IV. INTERNAL WAVE FUNCTION

Let us now discuss the properties of the internal wave function (11). To investigate the structure of ψ_{in} in a more detailed way we introduce a coupling constant g and will write $g\widetilde{W}$ for the coupling matrix. The complicated part of this expression is contained in the term

$$\frac{1}{i-g^2T(E)} \tag{23}$$

with the $M\times M$ matrix $T(E)=\widetilde{W}^{\dagger}(E-H_{\text{in}})^{-1}\widetilde{W}$. We solve the spectral problem for the latter matrix:

$$T(E)f_n=\lambda_n(E)f_n \tag{24}$$

[note that for E real $T(E)$ is a symmetric matrix and hence the eigenvalues $\lambda_n(E)$ are real numbers] and use the eigenvectors f_n to define the M vectors ψ_n living in the N-dimensional internal space:

$$\psi_n=(E-H_{\text{in}})^{-1}\widetilde{W}f_n\,. \tag{25}$$

(We shall normalize the vectors f_n, so that $\|f_n\|=1$. This means that the vectors ψ_n are not normalized.)

The vector ψ_n is a solution of the equation

$$\left(H_{\text{in}}+\frac{1}{\lambda_n(E)}\,\widetilde{W}\widetilde{W}^{\dagger}\right)\psi_n=E\psi_n\,. \tag{26}$$

To reveal the usefulness of these vectors we employ the spectral decomposition of the operator (23):

$$\frac{1}{i-g^2T(E)}=\sum_{n=1}^{M}\ \frac{f_nf_n^{\dagger}}{i-g^2\lambda_n(E)} \tag{27}$$

(where $f_nf_n^{\dagger}$ is the projector onto the one-dimensional subspace spanned by the vector f_n). Inserting this into the internal wave function (11) we finally obtain

$$\psi_{\text{in}}=2g\sum_{n=1}^{M}\ \frac{\langle f_n\,,\mathscr{A}_{\text{inc}}\rangle_{C^M}}{i-g^2\lambda_n(E)}\,\psi_n\,. \tag{28}$$

It is most interesting to realize, thus, that internal wave functions (each with N components) can be linearly composed from only M (fewer!) N-component vectors ψ_n.

It can be easily seen that for real energies E the vectors ψ_n are real provided H_{in} and $\widetilde{W}$ are real matrices. The properties of the internal wave function ψ_{in} depend substantially on the structure of these vectors and on the number of terms which contribute to the sum (28). In what follows we shall investigate the structure of ψ_{in} for resonances.

Resonances are defined as poles of the S-matrix in the complex energy plane. Using the above notation the resonances $E_{\text{reson}}=E_r-i\Gamma$ are nothing but the solutions of the following sequence of equations:

$$\lambda_n(E_{\text{reson}})=\frac{i}{g^2},\quad n=1,\ldots,M. \tag{29}$$

(E_r describes the position of the resonance peak, while Γ gives its width.) We shall now assume that the energy E in the incoming wave coincides with the position of some resonance: $E=E_r$. To obtain information about ψ_{in} we insert Eq. (29) into Eq. (26) obtaining for ψ_n

$$(H_{\text{in}}-ig^2\tilde{W}\tilde{W}^{\dagger})\psi_n=E_{\text{reson}}\psi_n\,. \tag{30}$$

It follows therefore that in the resonance case ψ_n are identical with the eigenvectors of the effective Hamiltonian $H_{\text{eff}}=H_{\text{in}}-ig^2\tilde{W}\tilde{W}^{\dagger}$.

For weak coupling ($g\ll 1$) the resonances are localized near the eigenvalues of H_{in} and the resonance widths are small ($\Gamma\ll 1$). Moreover, it follows from Eq. (30) that the vectors ψ_n practically coincide with the eigenvectors of H_{in}. Using the relation $i-g^2\lambda_n(E_r)=-ig^2\Gamma\Lambda_n'(E_r)+O(g^4)$ we obtain from Eq. (28)

$$\psi_{\text{in}}=2i\,\frac{\langle f_{n_0}|\mathscr{A}_{\text{inc}}\rangle_{C^M}}{g\Gamma\lambda_n'(E_r)}\,\psi_{n_0}+O(g)\,, \tag{31}$$

where ψ_{n_0} refers to the appropriate solution of Eq. (30). Consequently, the structure of ψ_{in} coincides with the structure of ψ_{n_0}, which is [up to terms of the order $O(g)$] identical with the corresponding eigenvector of H_{in}.

A similar analysis can be done also for strong coupling ($g\gg 1$). Since $\tilde{W}\tilde{W}^{\dagger}$ is a matrix of rank M the family of resonances can be split into two parts: M resonances are localized deep in the lower complex half plane and have widths $\Gamma\approx g^2$, and the remaining $N-M$ resonances approach the real axis and have widths $\Gamma\approx 1/g^2$. We are interested in the second group of resonances, since they form sharp resonance peaks and are hence easily measurable. A similar analysis as in the weak coupling case gives

$$\psi_{\text{in}}=2i\,\frac{\langle f_{n_0}|\mathscr{A}_{\text{inc}}\rangle_{C^M}}{g\Gamma\lambda_n'(E_r)}\,\psi_{n_0}+O\left(\frac{1}{g}\right). \tag{32}$$

This formula seems to be nearly the same as for weak coupling. There is, however, one deep difference: the position of the resonance E_r does not tend as $g\to\infty$ to some eigenvalue of the internal Hamiltonian H_{in}. This in turn means that the corresponding vector ψ_{n_0} does not coincide with an eigenvector of H_{in}. In fact, for a generic coupling matrix W the vector ψ_{n_0} is a real superposition of all eigenvectors of H_{in}.

For intermediate coupling the resonances overlap and one has to take all terms in Eq. (28) into account. ψ_{in} is in this case a superposition of the vectors ψ_n with complex coefficients.

Let us now discuss the consequences of the above analysis for the statistical properties of the internal wave function ψ_{in}. For weak coupling the properties of ψ_{in} coincide with those of the corresponding eigenfunction of H_{in}. This means that in the GOE case $|\psi_{\text{in}}|^2$ has a Porter–Thomas distribution, similarly for strong coupling. In this case ψ_{in} is proportional to a *real* superposition of the eigenvectors of H_{in}. This means again a Porter–Thomas distribution in the GOE case.

The structure of ψ_{in} becomes interesting in particular for H_{in} describing an integrable system. We know that ψ_{in} becomes a *superposition* of the (integrable) eigenvectors of H_{in}. Hence the internal wave function acquires a structure other than an eigenvector of integrable system. We shall show in the next section that ψ_{in} has features which are similar to the properties of eigenvectors of chaotic quantum systems. This fact supports the finding of the preceding section that opening an integrable system leads to a level repulsion which is typical for the behavior of quantum nonintegrable systems.

It remains to discuss the moderate-coupling case. Here, as already mentioned, the internal vector ψ_{in} becomes a superposition of vectors ψ_n with *complex* coefficients. The consequence is that the statistical properties of ψ_{in} differ from the standard predictions of the random-matrix

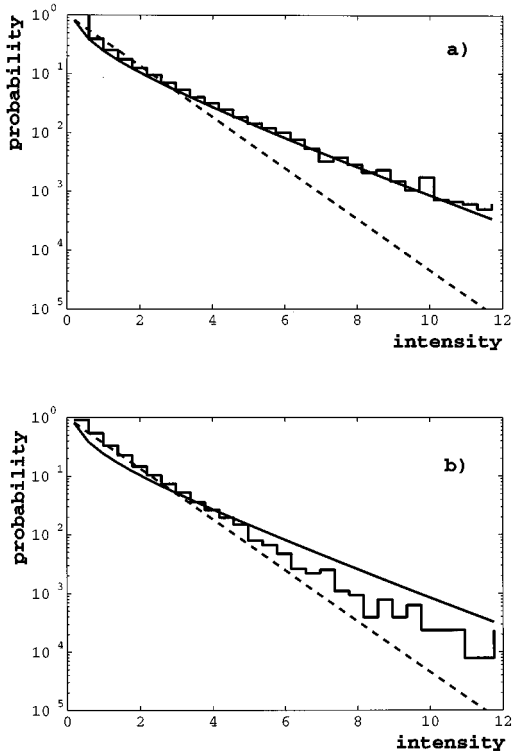

FIG. 1. The intensity distribution $|\psi|^2$ of the internal wave function (11) excited inside the resonator cavity is plotted in a semilogarithmic plot and compared with the Porter–Thomas (dashed line) and the Poisson (Rayleigh) distribution (full line). (a) pertains to one open channel ($M=1$). Good agreement with the Porter–Thomas distribution is visible. (b) shows the result for $M=10$ with a clear shift towards the Poisson distribution.

theory. The complex nature of ψ_{in} moves its statistical properties from a GOE prediction (Porter–Thomas distribution) toward a GUE prediction (Poisson distribution). (Note that ψ_{in} will display a Poisson distribution if its real and imaginary parts are statistically independent and of the same magnitude.) Such a distribution (also known as Rayleigh distribution in the literature[15]) is usually observed when waves excited by a monochromatic source propagate through a random medium—see also Ref. 16. In our case the randomizing effect is due solely to the multiple reflection of the waves inside the resonator. Numerical estimates show that already for $M=3$ the Rayleigh intensity pattern inside the resonator is well developed (see Fig. 1).

V. EXAMPLE

Let us now discuss a rectangular resonator attached to two microwave cables each of which supports one open channel. We assume that the channel threshold energies are set to zero, $\lambda_1=\lambda_2=0$. This system has recently been experimentally investigated in Refs. 4, 5, and 17. The Hamiltonian H_{reson} describing the resonator is given by the two-dimensional Laplace operator

$$H_{\text{reson}}=-\Delta$$

defined on a bounded domain Ω with Dirichlet boundary conditions $f=0$ on the boundary $\partial\Omega$. We shall investigate the statistical properties of the resonances and the structure of the field intensity inside the resonator as excited by waves entering through the microwave cable. Let E_n $[f_n(\mathbf{r}),\mathbf{r}\in\mathbb{R}^2]$ be the eigenvalues [eigenfunctions] of H_{reson}:

$$H_{\text{reson}} f_n(\mathbf{r}) = E_n f_n(\mathbf{r}). \tag{33}$$

Using these solutions let us define the finite-dimensional internal Hamiltonian acting on the space spanned by the first N eigenstates of H_{reson},

$$H_{\text{in}} = \sum_{n=1}^{N} E_n f_n f_n^{\dagger}. \tag{34}$$

The coupling operator A maps the two-dimensional vector

$$\begin{pmatrix} u_1'(0) \\ u_2'(0) \end{pmatrix}$$

into a certain function belonging to the N-dimensional internal space. Let $u_1(x)$ $[u_2(x)]$ denote the first, [second] component of the wave function in the cable. Applying the matrix A to the incoming vector we get

$$A\begin{pmatrix} u_1'(0) \\ u_2'(0) \end{pmatrix} = \alpha_1 d_1^N(\mathbf{r}) u_1'(0) + \alpha_2 d_2^N(\mathbf{r}) u_2'(0),$$

where α_1 and α_2 are the coupling constants and d_l^N, $l=1,2$ are functions spanned by the vectors f_n, $n=1,\ldots,N$. In the experiment the two antennas are coupled to the resonator at the points $\mathbf{r}_1$ and $\mathbf{r}_2$. In order to mimic this local coupling we choose the functions $d_l^N(\mathbf{r})$, $l=1,2$, in a special way, namely, such that they converge to $\delta^2(\mathbf{r}-\mathbf{r}_l)$ when $N\to\infty$, i.e.,

$$d_l^N(\mathbf{r}) = \sum_{i=1}^{N} f_i(\mathbf{r}_l) f_i(\mathbf{r}) \tag{35}$$

such that $\lim_{N\to\infty} d_l^N(\mathbf{r}) = \delta^2(\mathbf{r}-\mathbf{r}_l)$ (in the sense of generalized functions with $\mathbf{r}\in\mathbb{R}^2$).

The Hamiltonian H describing the whole system is self-adjoint on the domain determined by the boundary conditions

$$\langle d_l^N, u_{\text{in}} \rangle = -u_l(0).$$

In the limit $N\to\infty$ the boundary conditions are given by the formula

$$\alpha_l u_{\text{in}}(\mathbf{r}_l) = -u_l(0).$$

For N large enough the S-matrix reads

$$S = \frac{i + T(E)}{i - T(E)} \tag{36}$$

where $T(E)$ is a 2×2 matrix with elements

$$T(E)_{l,m} = \alpha_l \alpha_m \sqrt{E} \sum_{n=1}^{N} \frac{f_n(\mathbf{r}_l) f_m(\mathbf{r}_m)}{E_n - E}. \tag{37}$$

(Implicitly a similar formula has already been used in Ref. 18 in order to evaluate the conductance fluctuation for electrons passing a quantum dot.)

Let us start with the simplest case with one attached antenna only. (The second antenna is easily excluded by choosing the coupling $\alpha_2=0$.) In what follows we shall focus on the statistical properties of the resonances inside such a resonator.

The resonances are identified with the poles of the corresponding S-matrix. In the case of one coupled antenna the resonances are just the solutions of the algebraic equation $T(E)=i$, which is equivalent to

$$\sum_{n=1}^{N} \frac{|f_n(\mathbf{r}_1)|^2}{E_n-E} = \frac{i}{\alpha_1^2\sqrt{E}}. \tag{38}$$

This is an algebraic equation for E which has solutions on the lower complex half plane only. The solutions coincide with the zeros of a certain polynomial of order $2N+1$. One can solve this equation directly using some appropriate numerical method. But before doing this it seems to be helpful to investigate this equation by decoupling it into real and imaginary parts. Let $E=E_r-i\Gamma$ denote a solution with E_r and Γ the position and the width of the resonance, respectively. Assuming that $\Gamma \ll E_r$ we can approximate Eq. (38) by

$$\sum_{n=1}^{N} \frac{|f_n(\mathbf{r}_1)|^2}{E_n-E_r} = 0, \tag{39}$$

whereby the corresponding resonance widths are given by

$$\Gamma = 1 \Big/ \alpha_1^2\sqrt{E_r}\sum_{n=1}^{N} \frac{|f_n(\mathbf{r}_1)|^2}{(E_n-E_r)^2}. \tag{40}$$

This approximation is well justified in particular in the case of strong coupling ($\alpha_1 \gg 1$). In the numerical tests we used this approximate solution as a starting point for a routine searching for the complex roots of Eq. (38).

For the wave function ψ excited inside the resonator we find

$$\psi(\mathbf{r}) = \sum_{k=1}^{2}\sum_{l=1}^{2} 2(E)^{1/4}\alpha_k G(\mathbf{r},\mathbf{r}_k,E)\left(\frac{1}{i-T(E)}\right)_{k,l} \mathscr{A}_{\mathrm{inc},l}, \tag{41}$$

where

$$G(\mathbf{x},\mathbf{x}_k,E) = \sum_{n=1}^{N} \frac{f_n(\mathbf{x})\overline{f_n(\mathbf{x}_k)}}{E_n-E}$$

and $\mathscr{A}_{\mathrm{inc},l}$ denotes the amplitude of the incoming wave in the channel l. It is clear that in the case of a strong coupling to the antenna the structure of the resonance wave function differs substantially from the structure of the original resonator eigenfunction $f_n(x)$.

Let us now apply the above theory to the description of a rectangular resonator with one attached antenna. In the case of a rectangular resonator the eigenvalues E_n and the eigenfunctions f_n are explicitly known. Inserting these solutions into the formulas above we obtain an explicit solution of the perturbed resonator problem. As already mentioned, the resonances of such a system have been measured systematically.[19] In order to enhance the number of measured resonances the results for various rectangular billiards have been combined. In order to reproduce the experimental results we have evaluated resonances for 40 different rectangular billiards. In each billiard we evaluated the first 350 resonances which roughly correspond with the number of experimentally accessible ones. The obtained results have been rescaled (to obtain a mean resonance spacing equal to 1) and divided into three groups: the first group corresponds to resonances

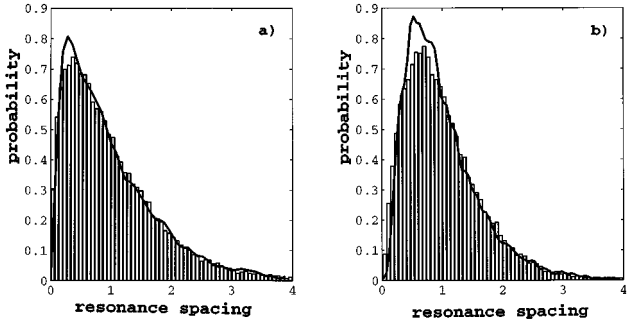

FIG. 2. The distribution of resonance spacings evaluated for a rectangular billiard is plotted (bins) and compared with the experimental results obtained in Ref. 19 (full line). The frequency range used was (a) 5–10 GHz; (b) 10–15 GHz.

measured within the frequency range 5–10 GHz, the second group corresponds to 10–15 GHz, and the third to a frequency range 15–18 GHz. The resonance spacing statistics have been evaluated for each group separately. The coupling constant α_1 has been taken to be equal to 2 in all three cases. The obtained results are plotted in Fig. 2 and compared with the experimental finding. It is worth noting that the theory predicts the effective coupling of the antenna to the resonator to become stronger for higher frequencies. This follows from the fact that the effective coupling of the antenna depends on $\alpha_1^2\sqrt{E}$ and hence on the wave frequency ω. (Note that the energy E and the microwave frequency ω are related by $E \approx \omega^2$.)

The distribution of the corresponding resonance widths is plotted in Fig. 3. We have compared this distribution with the recent prediction by Fyodorov and Sommers[20] for fully chaotic systems (resonators) with one open channel. It is interesting to remark that even though the rectangular resonator is originally integrable the distribution of resonance widths resembles closely that of a fully chaotic system. Clearly, then, the antenna represents a strong perturbation of the original integrable system. This perturbation is also responsible for the observed linear resonance repulsion visible in Fig. 2.

The influence of the antenna on the structure of the corresponding resonance function (i.e., on the structure of the electromagnetic field excited inside the resonator) is demonstrated in Fig. 4.

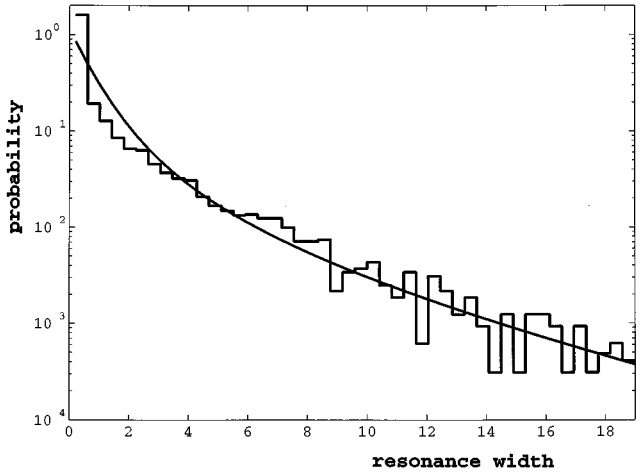

FIG. 3. The distribution of resonance widths evaluated for the frequency range 10–15 GHz is compared with the theoretical prediction for a fully chaotic system with one open channel (Ref. 20).

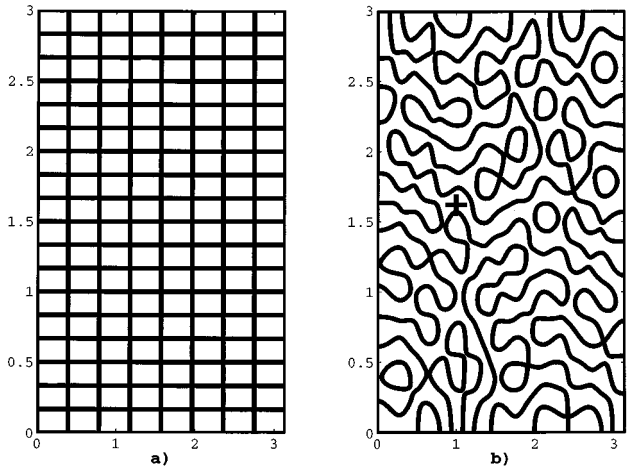

FIG. 4. Nodal lines of the electric field intensity inside a rectangular resonator with sides of lengths π and 3. (a) pertains to the unperturbed 187th state. (b) shows how this nodal line pattern changes after an antenna has been attached at the point marked by a cross.

The figure shows that the structure of the original eigenfunction f_n of the resonator is destroyed.

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APPENDIX: PERTURBATION OF THE NEUMANN BOUNDARY CONDITION

The interaction between the external and internal channels can be introduced in a different way. Consider, for example, the operator

$$H_B\begin{pmatrix} u \\ u_{\text{in}} \end{pmatrix} = \begin{pmatrix} H_{\text{ex}}u \\ H_{\text{in}}u_{\text{in}} + Bu(0) \end{pmatrix} \tag{A1}$$

with B being a self-adjoint operator. H_B is self-adjoint on the domain of functions from $W_2^2(R_+, C^M) \oplus C^N$ satisfying the boundary conditions

$$B^\dagger u_{\text{in}} = u'(0).$$

We arrive at the following energy-dependent boundary conditions for the eigenfunctions of the operator H_B:

$$\psi'(E,0) = -B^\dagger (H_{\text{in}} - E)^{-1} B\psi(E,0).$$

Then the scattering matrix above the thresholds is given by

$$S(E) = -\frac{i + \widetilde{W}_B^\dagger (E - H_{\text{in}})^{-1} \widetilde{W}_B}{i - \widetilde{W}_B^\dagger (E - H_{\text{in}})^{-1} \widetilde{W}_B},$$

where $\widetilde{W}_B = BQ$. For the small coupling, $\widetilde{W}_B \to 0$, the scattering matrix tends to -1 and this shows that the model operator constructed here can be considered as a perturbation of the operator H_{ex} with the Neumann boundary conditions at the origin.

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Diagrammatic method of integration over the unitary group, with applications to quantum transport in mesoscopic systems

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A diagrammatic method is presented for averaging over the circular ensemble of random-matrix theory. The method is applied to phase-coherent conduction through a chaotic cavity (a ''quantum dot'') and through the interface between a normal metal and a superconductor. © *1996 American Institute of Physics.* [S0022-2488(96)01510-1]

I. INTRODUCTION

The random-matrix theory of quantum transport describes the statistics of transport properties of phase-coherent (mesoscopic) systems in terms of the statistics of random matrices (for reviews, see Refs. 1–4). There exist two separate (but equivalent) approaches: Either the random matrix is used to model the Hamiltonian of the closed system, or it is used to model the scattering matrix of the open system. The second approach is more direct than the first, because the scattering matrix directly determines the conductance through the Landauer formula,

$$G=\frac{2e^2}{h}\,\mathrm{tr}\; tt^\dagger. \tag{1.1}$$

(The transmission matrix t is a submatrix of the scattering matrix.)

Random-matrix theory has been applied successfully to two types of mesoscopic systems: chaotic cavities and disordered wires. Baranger and Mello[5] and Jalabert, Pichard, and Beenakker[6] studied conduction through a chaotic cavity on the assumption that the scattering matrix S is uniformly distributed in the unitary group, restricted only by symmetry. This is the circular ensemble, introduced by Dyson,[7] and shown to apply to a chaotic cavity by Blümel and Smilansky.[8] The symmetry restriction is that $SS^*=1$ in the presence of time-reversal symmetry. (The superscript $*$ indicates complex conjugation if the elements of S are complex numbers; in the presence of spin-orbit scattering, S is a matrix of quaternions, and S^* denotes the quaternion complex conjugate.) For the disordered wire, the circular ensemble applies not to the scattering matrix itself, but to the unitary matrices v, w, v', and w' in the polar decomposition,

$$S=\begin{pmatrix} v & 0 \\ 0 & w \end{pmatrix}\begin{pmatrix} \sqrt{1-T} & i\sqrt{T} \\ i\sqrt{T} & \sqrt{1-T} \end{pmatrix}\begin{pmatrix} v' & 0 \\ 0 & w' \end{pmatrix}. \tag{1.2}$$

The matrix T is a diagonal matrix containing the transmission eigenvalues $T_n \in [0,1]$ on the diagonal. (The T_n's are the eigenvalues of the matrix product $tt^\dagger$.) The distribution of the transmission eigenvalues is governed by a Fokker–Planck equation, the Dorokhov–Mello–Pereyra–Kumar (DMPK) equation.[9,10] The isotropy assumption[10] states that v, v', w, and w' are uniformly and independently distributed in the unitary group, with the restriction $v^*v'=1$, $w^*w'=1$ in the presence of time-reversal symmetry.

The role of the circular ensemble of unitary matrices in the scattering matrix approach is comparable to the role of the Gaussian ensemble of Hermitian matrices in the Hamiltonian approach. However, whereas many computational techniques have been developed for averaging over the Gaussian ensemble,[11–18] the circular ensemble has received less attention. If the dimension N of the unitary matrices is small, the average over the circular ensemble can be done

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exactly.[19,20] For some applications in the regime of large N, one may regard the elements of the unitary matrix as independent Gaussian variables,[21] and then use the known diagrammatic perturbation theory for the Gaussian ensemble.[12,17] In other applications the Gaussian approximation breaks down.

In this paper we present a diagrammatic technique for integration over the unitary group, which is not restricted to the Gaussian approximation. We discuss two applications: a chaotic cavity coupled to the outside via a tunnel barrier, and a disordered wire attached to a superconductor. In both cases, we calculate the mean and variance of the conductance up to and including terms of order 1. We point out the analogy between the diagrams contributing to the average over the circular ensemble and the diffuson and cooperon diagrams which appear in the theory of weak localization[22,23] and universal conductance fluctuations[24,25] in disordered metals. In the presence of the superconductor a third type of diagrams shows up, which gives rise to the coexistence of weak localization with a magnetic field,[26,27] and to anomalous conductance fluctuations.[28]

The paper starts in Sec. II with a summary of known results[29–31] for the integration over the unitary group of a polynomial function of matrix elements. The diagrammatic technique is explained in Sec. III. Generalizations to unitary symmetric matrices and to unitary quaternion matrices are given in Secs. IV and V, respectively. We then apply the technique to the chaotic cavity (Sec. VI) and the normal-metal–superconductor junction (Sec. VII). Some of the results of Sec. VI have been obtained previously by Iida, Weidenmüller, and Zuk,[1,15] and by Efetov,[32] who used the Hamiltonian approach to quantum transport and the supersymmetry technique. The results of Sec. VII have been published in Refs. 26 and 28, without the detailed derivation presented here. There is some overlap between Sec. VII and a recent work by Argaman and Zee.[33]

II. INTEGRATION OF POLYNOMIALS OF UNITARY MATRICES

In this section we summarize known results[29–31] for the integration of a polynomial function $f(U)$ of the matrix elements of an $N\times N$ unitary matrix U over the unitary group $\mathscr{U}(N)$. We refer to the integration as an ''average,'' which we denote by brackets $\langle\cdots\rangle$,

$$\langle f\rangle \equiv \int dU f(U). \tag{2.1}$$

Here dU is the invariant measure (Haar measure) on $\mathscr{U}(N)$, normalized to unity ($\int dU = 1$). The ensemble of unitary matrices that corresponds to this average is known as the circular unitary ensemble (CUE).[7,34]

We consider a polynomial function $f(U) = U_{a_1 b_1}\ldots U_{a_n b_n} U^*_{\alpha_1\beta_1}\ldots U^*_{\alpha_m\beta_m}$. The average $\langle f(U)\rangle$ is zero unless $n=m$, $\alpha_1,\ldots,\alpha_n$ is a permutation P of $a_1,\ldots,a_n$, and $\beta_1,\ldots,\beta_n$ is a permutation P' of $b_1,\ldots,b_n$. The general structure of the average is

$$\langle U_{a_1 b_1}\ldots U_{a_m b_m} U^*_{\alpha_1\beta_1}\ldots U^*_{\alpha_n\beta_n}\rangle = \delta_{nm}\sum_{P,P'} V_{P,P'}\prod_{j=1}^{n}\delta_{a_j\alpha_{P(j)}}\delta_{b_j\beta_{P'(j)}}, \tag{2.2}$$

where the summation is over all permutations P and P' of the numbers $1,\ldots,n$. The coefficients $V_{P,P'}$ depend only on the *cycle structure* of the permutation $P^{-1}P'$.[30] Recall that each permutation of $1,\ldots,n$ has a unique factorization in disjoint cyclic permutations (''cycles'') of lengths $c_1,\ \ldots\ ,c_k$ (where $n=\sum_{j=1}^{k} c_k$). The statement that $V_{P,P'}$ depends only on the cycle structure of $P^{-1}P'$ means that $V_{P,P'}$ depends only on the lengths $c_1,\ldots,c_k$ of the cycles in the factorization of $P^{-1}P'$. One may therefore write $V_{c_1,\ldots,c_k}$ instead of $V_{P,P'}$.

As an example, we consider the case $n=m=2$ explicitly. The summation over the permutations P and P' extends over the identity permutation $\mathrm{id}=[(1,2)\to(1,2)]$ and the exchange permutation $\mathrm{ex}=[(1,2)\to(2,1)]$. Hence Eq. (2.2) reads

$$\langle U_{a_1b_1}U_{a_2b_2}U^*_{\alpha_1\beta_1}U^*_{\alpha_2\beta_2}\rangle = V_{\mathrm{id,id}}\delta_{a_1\alpha_1}\delta_{b_1\beta_1}\delta_{a_2\alpha_2}\delta_{b_2\beta_2} + V_{\mathrm{ex,id}}\delta_{a_1\alpha_2}\delta_{b_1\beta_1}\delta_{a_2\alpha_1}\delta_{b_2\beta_2} + V_{\mathrm{id,ex}}\delta_{a_1\alpha_1}\delta_{b_1\beta_2}\delta_{a_2\alpha_2}\delta_{b_2\beta_1} + V_{\mathrm{ex,ex}}\delta_{a_1\alpha_2}\delta_{b_1\beta_2}\delta_{a_2\alpha_1}\delta_{b_2\beta_1}. \tag{2.3}$$

The permutation $P^{-1}P'$ that corresponds to $P=P'=\mathrm{id}$ [the first term on the r.h.s. of Eq. (2.3)] is again the identity permutation: $P^{-1}P'=\mathrm{id}=[(1,2)\to(1,2)]$. Its factorization in cyclic permutations is $\mathrm{id}=(1\to1)(2\to2)$, so that $P^{-1}P'$ factorizes in two cyclic permutations of unit length. Hence the cycle structure of $P^{-1}P'$ is $\{1,1\}$, and $V_{\mathrm{id,id}}=V_{1,1}$. The second term on the r.h.s. of Eq. (2.3), corresponding to $P=\mathrm{ex}$, $P'=\mathrm{id}$, has $P^{-1}P'=\mathrm{ex}=[(1,2)\to(2,1)]$, which factorizes in a single cyclic permutation of length two, $\mathrm{ex}=(1\to2\to1)$. Hence the cycle structure of $P^{-1}P'$ is $\{2\}$, and $V_{\mathrm{ex,id}}=V_2$. Treating the remaining two terms of Eq. (2.3) similarly, we obtain

$$\langle U_{a_1b_1}U_{a_2b_2}U^*_{\alpha_1\beta_1}U^*_{\alpha_2\beta_2}\rangle = V_{1,1}\delta_{a_1\alpha_1}\delta_{b_1\beta_1}\delta_{a_2\alpha_2}\delta_{b_2\beta_2} + V_2\delta_{a_1\alpha_2}\delta_{b_1\beta_1}\delta_{a_2\alpha_1}\delta_{b_2\beta_2} + V_2\delta_{a_1\alpha_1}\delta_{b_1\beta_2}\delta_{a_2\alpha_2}\delta_{b_2\beta_1} + V_{1,1}\delta_{a_1\alpha_2}\delta_{b_1\beta_2}\delta_{a_2\alpha_1}\delta_{b_2\beta_1}. \tag{2.4}$$

In general, the coefficient $V_{1,\ldots,1}$ refers to equal permutations $P=P'$, corresponding to a pairwise (Gaussian) contraction of the matrices U and U^*. Coefficients $V_{c_1,\ldots,c_k}$ with some $c_j\neq1$ give non-Gaussian contributions.

The coefficients V are determined by the recursion relation[30]

$$NV_{c_1,\ldots,c_k} + \sum_{p+q=c_1} V_{p,q,c_2,\ldots,c_k} + \sum_{j=2}^{k} c_j V_{c_1+c_j,c_2,\ldots,c_{j-1},c_{j+1},\ldots,c_k} = \delta_{c_1,1}V_{c_2,\ldots,c_k}, \tag{2.5}$$

with $V_0\equiv1$. One can show that the solution $V_{c_1,\ldots,c_k}$ does not depend on the order of the indices $c_1,\ldots,c_k$. Results for V up to $n=5$ are given in the Appendix. The large-N expansion of V is

$$V_{c_1,\ldots,c_k} = \prod_{j=1}^{k} V_{c_j} + \mathcal{O}(N^{k-2n-2}), \tag{2.6a}$$

$$V_c = \frac{1}{c}N^{1-2c}(-1)^{c-1}\binom{2c-2}{c-1} + \mathcal{O}(N^{-1-2c}). \tag{2.6b}$$

(The numbers $c^{-1}\binom{2c-2}{c-1}$ are the Catalan numbers.) For example, $V_{1,\ldots,1}=N^{-n}+\mathcal{O}(N^{-n-2})$. The Gaussian approximation amounts to setting all V's equal to zero except $V_{1,\ldots,1}$, which is set to N^{-n}.

The coefficients $V_{c_1,\ldots,c_k}$ determine the moments of U. Similarly, the coefficients $W_{c_1,\ldots,c_k}$ determine the cumulants of U. The cumulants are obtained from the moments by subsequent subtraction of all possible factorizations in cumulants of lower degree. For example,

$$W_{c_1} = V_{c_1}, \tag{2.7a}$$

$$W_{c_1,c_2} = V_{c_1,c_2} - W_{c_1}W_{c_2}, \tag{2.7b}$$

$$W_{c_1,c_2,c_3} = V_{c_1,c_2,c_3} - W_{c_1}W_{c_2,c_3} - W_{c_2}W_{c_1,c_3} - W_{c_3}W_{c_1,c_2} - W_{c_1}W_{c_2}W_{c_3}. \tag{2.7c}$$

The recursion relation (2.5) for V implies a recursion relation for W,

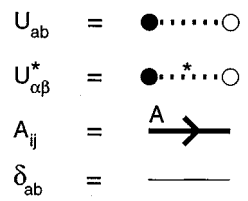

FIG. 1. Substitution rules for the unitary matrices U and U^*, the fixed matrix A and the Kronecker delta.

$$NW_{c_1,\ldots,c_k}+\sum_{p+q=c_1} W_{p,q,c_2,\ldots,c_k}+\sum_{j=2}^{k} c_j W_{c_1+c_j,c_2,\ldots,c_{j-1},c_{j+1},\ldots,c_k}$$
$$+\sum_{p+q=c_1}\sum_{l=1}^{k}\frac{1}{(l-1)!(k-l)!}\sum_{P} W_{p,c_{P(2)},\ldots,c_{P(l)}}W_{q,c_{P(l+1)},c_{P(k)}}=0, \tag{2.8}$$

with $W_0\equiv 1$ and P a permutation of $2,\ldots,k$. To leading order in $1/N$ this equation has the solution,

$$W_{c_1,\ldots,c_k}=2^k N^{-2n-k+2}(-1)^{n+k}\frac{(2n+k-3)!}{(2n)!}\prod_{j=1}^{k}\frac{(2c_j-1)!}{(c_j-1)!^2}+\mathcal{O}(N^{-2n-k}). \tag{2.9}$$

Notice that $W_{c_1,\ldots,c_k}$ decreases with increasing number of cycles k, opposite to the behavior of $V_{c_1,\ldots,c_k}$.

In principle, the recursion relations permit an exact evaluation of the average of any polynomial function of U. In practice, as the number of U's and U^*'s increases, keeping track of the indices and of the Kronecker delta's which connect them becomes more and more cumbersome. It is by the introduction of a diagrammatic technique that one can carry out this bookkeeping problem in a controlled and systematic way.

III. DIAGRAMMATIC TECHNIQUE

The usefulness of diagrams for the bookkeeping problem is well-established for averages over the Gaussian ensemble of Hermitian matrices.[12] Brézin and Zee[17] have developed a diagrammatic method which can be applied to non-Gaussian ensembles as well, as a perturbation expansion in a small parameter multiplying the non-Gaussian terms in the distribution. No such small parameter exists for the circular ensemble. The method presented here deals with non-Gaussian contributions to all orders. Creutz[29] has given a diagrammatic algorithm for integrals over SU(N). Because of the more complicated structure of SU(N), we could not effectively apply his method to integrals over $\mathcal{U}(N)$ in the case of a large number of U's.

The diagrams consist of the building blocks shown in Fig. 1. We represent matrix elements U_{ab} or $U^*_{\alpha\beta}$ by thick dotted lines. The first index (a or α) is a black dot, the second index (b or β) a white dot. A fixed matrix A_{ij} is represented by a directed thick solid line, pointed from the first to the second index. Summation over an index is indicated by attachment of the solid line to a dot. As an example, the functions $f(U)=\mathrm{tr}\,AUBU^\dagger$ and $g(U)=\mathrm{tr}\,AUBUCU^\dagger DU^\dagger$ are represented in Fig. 2.

The average over the matrix U consists of summing over all permutations P and P' in Eq. (2.2). Permutations are generated by drawing thin lines (representing Kronecker deltas) between all black dots attached to U and black dots attached to U^* (one line per dot). Black dots connect

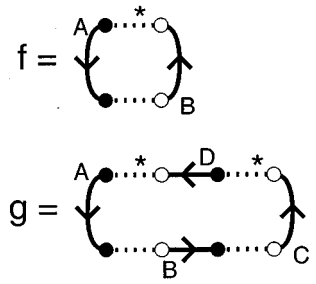

FIG. 2. Diagrammatic representation of the functions $f(U)=\mathrm{tr}\,AUBU^\dagger$ and $g(U)=\mathrm{tr}\,AUBUCU^\dagger DU^\dagger$.

to black dots and white dots to white dots. To find the contribution of the permutations P and P' to $\langle f(U)\rangle$, we need (i) to determine the cycle structure of the permutation $P^{-1}P'$, and (ii) to sum over the indices of the fixed matrices A.

(i) The cycle structure can be read off from the diagrams. A cycle of the permutation $P^{-1}P'$ gives rise to a closed circuit in the diagram consisting of alternating dotted and thin lines. The length c_k of the cycle is half the number of dotted lines contained in the circuit. We call such circuits U-cycles of length c_k.

(ii) The trace over the elements of A is done by inspection of the closed circuits in the diagram which consist of alternating thick and thin lines. We call such circuits T-cycles. A T-cycle containing the matrices $A^{(1)},A^{(2)},\ \ldots\ ,A^{(k)}$ (in this order) gives rise to $\mathrm{tr}\,A^{(1)}A^{(2)}\ldots A^{(k)}$. If the thick line corresponding to a matrix A is traversed opposite to its direction, the matrix should be replaced by its transpose A^{T}.

As an example, let us consider the average of the functions $f(U)=\mathrm{tr}\,AUBU^\dagger$ and $g(U)=\mathrm{tr}\,AUBUCU^\dagger DU^\dagger$. Connecting the dots by thin lines, we arrive at the diagrams of Fig. 3. For f, there is only one diagram. It contains a single U-cycle of length 1 (weight V_1) and two T-cycles (which generate tr A and tr B). We look up the value of $V_1=1/N$ in the Appendix, and find

$$\langle f(U)\rangle = V_1\,\mathrm{tr}\,A\,\mathrm{tr}\,B = N^{-1}\,\mathrm{tr}\,A\,\mathrm{tr}\,B, \tag{3.1}$$

Four diagrams contribute to g. The first diagram contains two U-cycles of length 1, and three T-cycles. Its contribution is $V_{1,1}\,\mathrm{tr}\,A\,\mathrm{tr}\,BD\,\mathrm{tr}\,C$. The second diagram contains two U-cycles of

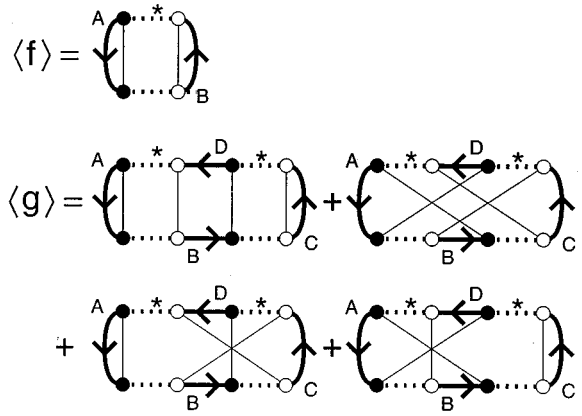

FIG. 3. Diagrammatic representation of the averages of the functions f and g in Fig. 2.

length 1 and a single T-cycle. Its contribution is $V_{1,1}$ tr $ADCB$. The third and fourth diagram each contain a single U-cycle of length 2 and two T-cycles. Their contributions are V_2 tr A tr BDC and V_2 tr ADB tr C. In total we find

$$\begin{aligned}\langle g(U)\rangle &= V_{1,1}(\text{tr } A \text{ tr } BD \text{ tr } C + \text{tr } ADCB) + V_2(\text{tr} A \text{ tr } BDC + \text{tr } ADB \text{ tr } C)\\ &= (N^2-1)^{-1}(\text{tr } A \text{ tr } BD \text{ tr } C + \text{tr } ADCB)\\ &\quad -[N(N^2-1)]^{-1}(\text{tr } A \text{ tr } BDC + \text{tr } ADB \text{tr } C).\end{aligned} \tag{3.2}$$

Whereas each individual T-cycle gives rise to a trace of matrices, it is only the combination of *all* U-cycles together that determines the coefficient $V_{c_1,\ldots,c_k}$. The evaluation of a diagram would be more efficient, if we could attribute a weight to an *individual* U-cycle. We introduced the cumulant expansion of the coefficients V in the coefficients W for this purpose. The leading term $V_{c_1,\ldots,c_k}=\Pi_{p=1}^k W_{c_p}$ of the cumulant expansion attributes a weight W_{c_p} to each individual U-cycle of length c_p. This is sufficient for the calculation of the large-N limit of the average $\langle f\rangle$. The next term $\Sigma_{i<j}^k W_{c_i,c_j}\Pi_{p\neq i,j}^k W_{c_p}$ attributes a weight W_{c_i,c_j} to the pair (i,j) of U-cycles, and the weight W_{c_p} to all others individually. This is sufficient for the variance of f. The general rule is that the jth order cumulant of f in the large-N limit requires the jth order term in the cumulant expansion of the coefficients V, and hence requires consideration of groups of j U-cycles.

Let us summarize the diagrammatic rules:

(1) Draw the diagrams according to the substitution rules of Fig. 1.
(2) Draw thin lines to pair black dots attached to U to black dots attached to U^*. Do the same for the white dots.
(3) Every closed circuit of alternating thick solid lines and thin solid lines (a T-cycle) corresponds to a trace of the matrices A appearing in the circuit. If a thick line is traversed opposite to its direction, the transpose of the matrix appears in the trace.
(4) Every closed circuit of alternating dotted and thin solid lines (a U-cycle) corresponds to a cycle of length c_k equal to half the number of dotted lines. The set of U-cycles in a diagram defines the coefficient $V_{c_1,\ldots,c_k}$, which is the weight of the diagram. The coefficient V can be factorized into cumulants. To determine the cumulant coefficients W, partition the U-cycles into groups. Every group of p U-cycles of lengths $c_1,\ldots,c_p$ contributes a weight $W_{c_1,\ldots,c_p}$.

The diagrammatic rules are exact. In the large-N limit, we may reduce the number of diagrams and partitions that is involved. Let us determine the order in N of a diagram with l T-cycles and k U-cycles of total length n partitioned into g groups. Counting every trace as an order N and using the large-N result (2.9) for the coefficients W, we find a contribution of order $N^{2g+l-k-2n}$. Since $g\leqslant k$, the order is maximal if $g=k$ and the total number of cycles $k+l$ is maximal. Thus, for large N, we may restrict ourselves to diagrams with as many cycles as possible and with a partition of the U-cycles in groups of a single cycle (i.e., we may approximate $V_{c_1,\ldots,c_k}\approx W_{c_1}\cdots W_{c_k}$).

We conclude this section with one more example, which is the calculation of the variance var $f=\langle f^2\rangle-\langle f\rangle^2$ of the function $f(U)=$ tr $AUBU^\dagger$. Diagrammatically, we calculate $\langle f^2\rangle$ as in Fig. 4(a), resulting in

$$\langle f^2\rangle = V_{1,1}[(\text{tr } A)^2(\text{tr } B)^2 + \text{tr } A^2 \text{ tr } B^2] + W_2[\text{tr } A^2(\text{tr } B)^2 + (\text{tr } A)^2 \text{ tr } B^2], \tag{3.3a}$$

$$\begin{aligned}\Rightarrow \text{var } f &= W_{1,1}[(\text{tr } A)^2(\text{tr } B)^2 + \text{tr } A^2 \text{ tr } B^2] + W_1^2 \text{ tr } A^2 \text{ tr } B^2\\ &\quad + W_2[\text{tr } A^2(\text{tr } B)^2 + (\text{tr } A)^2 \text{ tr } B^2].\end{aligned} \tag{3.3b}$$

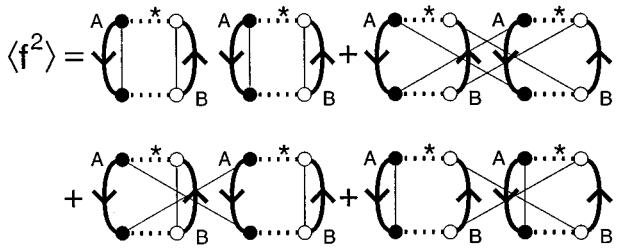

FIG. 4. Diagrammatic representation of $\langle f^2\rangle$.

If we now consider the order in N of the various contributions, we see that the leading $\mathcal{O}(N^2)$ term of $\langle f^2\rangle$ ($l=4$, $g=k=2$, corresponding to 6 cycles and a partition of the U-cycles into two groups of a single cycle), is exactly canceled by $\langle f\rangle^2$. This exact cancelation is possible because the leading contribution of $\langle f^2\rangle$ is *disconnected*: Each T-cycle, and each group of U-cycles belongs entirely to one of the two factors $\mathrm{tr}\, AUBU^\dagger$ of f^2. Only connected diagrams contribute to the variance of f. The connected diagrams are of order 1 ($k+l=4$ and $g=k$ or $k+l=6$ and $g=k-1$). They give the variance

$$\mathrm{var}\, f = W_{1,1}(\mathrm{tr}\, A)^2(\mathrm{tr}\, B)^2 + W_1^2\, \mathrm{tr}\, A^2\, \mathrm{tr}\, B^2 + W_2[\mathrm{tr}\, A^2(\mathrm{tr}\, B)^2 + (\mathrm{tr}\, A)^2\, \mathrm{tr}\, B^2] + \mathcal{O}(N^{-1}). \tag{3.4}$$

IV. INTEGRATION OF UNITARY SYMMETRIC MATRICES

In the presence of time-reversal symmetry the scattering matrix S is both unitary and symmetric: $SS^\dagger=1$, $S=S^{\mathrm{T}}$. The elements of S are complex numbers. (The case of a quaternion S, corresponding to spin-orbit scattering, is treated in the next section.) The ensemble of uniformly distributed unitary symmetric matrices is known as the circular orthogonal ensemble (COE).[7,34] Averages of the unitary symmetric matrix U over the COE can be computed in two ways. One way is to substitute $U=VV^{\mathrm{T}}$, with the matrix V uniformly distributed over the unitary group. This has the advantage that one can use the same formulas as for averages over the CUE, but the disadvantage that the number of unitary matrices is doubled. A more efficient way is to use specific formulas for the COE, as we now discuss.

The average of a polynomial in U and U^* over the COE has the general structure

$$\langle U_{a_1a_2}\cdots U_{a_{2n-1}a_{2n}} U^*_{\alpha_1\alpha_2}\cdots U^*_{\alpha_{2m-1}\alpha_{2m}}\rangle = \delta_{nm}\sum_P V_P \prod_{j=1}^{2n} \delta_{a_j\alpha_{P(j)}}. \tag{4.1}$$

The summation is over permutations P of the numbers $1,\ldots,2n$. We can decompose P as

$$P = \left(\prod_{j=1}^{n} T_j\right) P_{\mathrm{e}} P_{\mathrm{o}} \left(\prod_{j=1}^{n} T'_j\right), \tag{4.2}$$

where T_j and T'_j permute the numbers $2j-1$ and $2j$, and P_{e} (P_{o}) permutes n even (odd) numbers. Because $U_{ab}=U_{ba}$, the moment coefficient V_P depends only on the cycle structure $\{c_1,\ldots,c_k\}$ of $P_{\mathrm{e}}^{-1}P_{\mathrm{o}}$,[35] so that we may write $V_{c_1,\ldots,c_k}$ instead of V_P.

The moment coefficients obey the recursion relation

$$(N+c_1)V_{c_1,\ldots,c_k} + \sum_{p+q=c_1} V_{p,q,c_2,\ldots,c_k} + 2\sum_{j=2}^{k} c_j V_{c_1+c_j,c_2,\ldots,c_{j-1},c_{j+1},\ldots,c_k} = \delta_{c_1 1} V_{c_2,\ldots,c_k}, \tag{4.3}$$

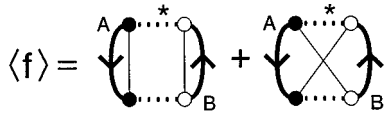

FIG. 5. Diagrammatic representation of $\langle f(U)\rangle$ for $f(U)=\mathrm{tr}\,AUBU^{\dagger}$, where U is a unitary symmetric matrix. The second term arises because of the symmetry constraint.

with $V_0\equiv 1$. The large-N expansion of V is

$$V_{c_1,\ldots,c_k}=\prod_{j=1}^{k} V_{c_j}+\mathcal{O}(N^{k-2n-2}), \tag{4.4a}$$

$$V_c=\frac{1}{c}N^{1-2c}(-1)^{c-1}\binom{2c-2}{c-1}-N^{-2c}(-4)^{c-1}+\mathcal{O}(N^{-1-2c}). \tag{4.4b}$$

Compared with Eq. (2.6) an extra term of order N^{-2c} appears in V_c because of the symmetry restriction. The recursion relation for the cumulant coefficients W is

$$\begin{aligned}(N+c_1)W_{c_1,\ldots,c_k}&+\sum_{p+q=c_1} W_{p,q,c_2,\ldots,c_k}+2\sum_{j=2}^{k} c_j W_{c_1+c_j,c_2,\ldots,c_{j-1},c_{j+1},\ldots,c_k}\\ &+\sum_{p+q=c_1}\sum_{l=1}^{k}\frac{1}{(l-1)!(k-l)!}\sum_{P} W_{p,c_{P(2)},\ldots,c_{P(l)}}W_{q,c_{P(l+1)},c_{P(k)}}=0,\end{aligned} \tag{4.5}$$

with $W_0\equiv 1$ and P a permutation of the numbers $2,\ldots,k$. The solution for large N is

$$W_{c_1,\ldots,c_k}=2^{2k-1}N^{-2n-k+2}(-1)^{n+k}\frac{(2n+k-3)!}{(2n)!}\prod_{j=1}^{k}\frac{(2c_j-1)!}{(c_j-1)!^2}+\mathcal{O}(N^{-2n-k+1}). \tag{4.6}$$

The coefficients $V_{c_1,\ldots,c_k}$ and $W_{c_1,\ldots,c_k}$ are listed in the Appendix for $n=c_1+\cdots+c_k\leqslant 5$.

For the diagrammatic representation, we again use the substitution rules of Fig. 1. The symmetry of U is taken into account by allowing thin lines between black and white dots. Therefore, rule (2) is replaced by

(2) Pair the dots attached to U to the dots attached to U^* by connecting them with thin lines.

As examples, we compute the averages of $f(U)=\mathrm{tr}\,AUBU^{\dagger}$ and $g(U)=\mathrm{tr}\,AUBUCU^{\dagger}DU^{\dagger}$ over the COE. The diagrams for $\langle f(U)\rangle$ are shown in Fig. 5, with the result

$$\langle f(U)\rangle=V_1(\mathrm{tr}\,A\,\mathrm{tr}\,B+\mathrm{tr}\,A^{\mathrm{T}}B)=(N+1)^{-1}(\mathrm{tr}\,A\,\mathrm{tr}\,B+\mathrm{tr}\,A^{\mathrm{T}}B). \tag{4.7a}$$

Similarly, we find that

$$\begin{aligned}\langle g(U)\rangle=&[(N+1)(N+3)]^{-1}(\mathrm{tr}\,A\mathrm{tr}\,BD\,\mathrm{tr}\,C+\mathrm{tr}\,AD^{\mathrm{T}}B^{\mathrm{T}}\,\mathrm{tr}\,C+\mathrm{tr}\,A\,\mathrm{tr}\,BC^{\mathrm{T}}D+\mathrm{tr}\,AD^{\mathrm{T}}CB^{\mathrm{T}}\\ &+\mathrm{tr}\,ADCB+\mathrm{tr}\,AC^{\mathrm{T}}D^{\mathrm{T}}B+\mathrm{tr}\,ADB^{\mathrm{T}}C^{\mathrm{T}}+\mathrm{tr}\,AC^{\mathrm{T}}\,\mathrm{tr}\,BD^{\mathrm{T}})-[(N(N+1)(N+3)]^{-1}\\ &\times(\mathrm{tr}\,A\,\mathrm{tr}\,BDC+\mathrm{tr}\,AC^{\mathrm{T}}D^{\mathrm{T}}B^{\mathrm{T}}+\mathrm{tr}\,A\,\mathrm{tr}\,BD^{\mathrm{T}}C+\mathrm{tr}\,AC^{\mathrm{T}}\,DB^{\mathrm{T}}+\mathrm{tr}\,ADB\,\mathrm{tr}\,C\\ &+\mathrm{tr}\,AD^{\mathrm{T}}B\,\mathrm{tr}\,C+\mathrm{tr}\,ADBC^{\mathrm{T}}+\mathrm{tr}\,AD^{\mathrm{T}}BC^{\mathrm{T}}+\mathrm{tr}\,AD^{\mathrm{T}}B^{\mathrm{T}}C^{\mathrm{T}}+\mathrm{tr}\,AC^{\mathrm{T}}\,\mathrm{tr}\,BD\\ &+\mathrm{tr}\,AD^{\mathrm{T}}\,CB+\mathrm{tr}\,AC^{\mathrm{T}}DB+\mathrm{tr}\,A\,\mathrm{tr}\,BC^{\mathrm{T}}D^{\mathrm{T}}+\mathrm{tr}\,ADCB^{\mathrm{T}}+\mathrm{tr}\,A\,\mathrm{tr}\,BD^{\mathrm{T}}\,\mathrm{tr}\,C\\ &+\mathrm{tr}\,ADB^{\mathrm{T}}\,\mathrm{tr}\,C).\end{aligned} \tag{4.7b}$$

V. INTEGRATION OF MATRICES OF QUATERNIONS

We extend the results of the previous sections for integrals over unitary matrices of complex numbers to integrals over unitary matrices of quaternions. This is relevant to the case that spin-rotation symmetry is broken by spin-orbit scattering.

Let us first recall the definition and basic properties of quaternions.[34] A quaternion q is represented by a 2×2 matrix,

$$q=a_0\mathbb{1}+ia_1\sigma_1+ia_2\sigma_2+ia_3\sigma_3, \tag{5.1}$$

where $\mathbb{1}$ is the 2×2 unit matrix and σ_i is a Pauli matrix,

$$\sigma_1=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},\quad \sigma_2=\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix},\quad \sigma_3=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}. \tag{5.2}$$

The coefficients a_j are complex numbers. The complex conjugate q^* and Hermitian conjugate $q^\dagger$ of a quaternion q are defined as

$$q^*=a_0^*\mathbb{1}+ia_1^*\sigma_1+ia_2^*\sigma_2+ia_3^*\sigma_3,\quad q^\dagger=a_0^*\mathbb{1}-ia_1^*\sigma_1-ia_2^*\sigma_2-ia_3^*\sigma_3. \tag{5.3}$$

The complex conjugate of a quaternion differs from the complex conjugate of a 2×2 matrix, whereas the Hermitian conjugate equals the Hermitian conjugate of a 2×2 matrix. Let Q be an $N\times N$ matrix of quaternions with elements $Q_{kl}=Q_{kl}^{(0)}\mathbb{1}+iQ_{kl}^{(1)}\sigma_1+iQ_{kl}^{(2)}\sigma_2+iQ_{kl}^{(3)}\sigma_3$. The complex conjugate Q^* and Hermitian conjugate $Q^\dagger$ are defined by $(Q^*)_{kl}=Q_{kl}^*$ and $(Q^\dagger)_{kl}=Q_{lk}^\dagger$. The dual matrix Q^{R} is defined by $Q^{\mathrm{R}}=(Q^\dagger)^*=(Q^*)^\dagger$. We call Q unitary if $QQ^\dagger=1$ and self-dual if $Q=Q^{\mathrm{R}}$. A unitary self-dual matrix is defined by $QQ^\dagger=QQ^*=1$. The trace tr Q is defined by tr $Q=\Sigma_j Q_{jj}^{(0)}$, which equals 1/2 the trace of the $2N\times 2N$ complex matrix corresponding to Q. The scattering matrix in zero magnetic field is a unitary self-dual matrix, because of time-reversal symmetry. The ensemble of quaternion matrices which is uniformly distributed over the unitary group is called the circular unitary ensemble (CUE). If the ensemble is restricted to self-dual matrices it is called the circular symplectic ensemble (CSE).[7,34]

The integration of a polynomial function $f(U)$ of an $N\times N$ quaternion matrix U over the CUE or CSE can be related to the integration of a function $\hat{f}(U)$ of an $N\times N$ complex matrix U over the CUE or COE. The translation rule is as follows (a similar rule has been formulated for Gaussian ensembles in Refs. 36 and 37):

(1) $\hat{f}(U)$ is constructed from $f(U)$ by replacing, respectively, the complex conjugates, Hermitian conjugates, and duals of quaternion matrices by complex conjugates, Hermitian conjugates, and transposes of complex matrices. Furthermore, every trace is replaced by $-\frac{1}{2}$ tr, and numerical factors N are replaced by $-\frac{1}{2}N$.
(2) The average $\langle\hat{f}(U)\rangle$ is calculated using the rules for integration of $N\times N$ complex matrices over the CUE or COE.
(3) The average $\langle f(U)\rangle$ over the CUE or CSE is found by replacing, respectively, the complex conjugates, Hermitian conjugates, and transposes of complex matrices by the complex conjugates, Hermitian conjugates, and duals of quaternion matrices. Traces are replaced by -2 tr and numerical factors N by $-2N$.

As examples, we compute the averages of the functions $f(U)=\mathrm{tr}\,AUBU^\dagger$ and $g(U)=\mathrm{tr}\,AUBUCU^\dagger DU^\dagger$ of $N\times N$ quaternion matrices over the CUE and CSE. The first step is to construct the functions $\hat{f}(U)$ and $\hat{g}(U)$ of $N\times N$ complex matrices,

$$\hat{f}(U)=-\tfrac{1}{2}\,\mathrm{tr}\,AUBU^\dagger,\quad \hat{g}(U)=-\tfrac{1}{2}\,\mathrm{tr}\,AUBUCU^\dagger DU^\dagger. \tag{5.4}$$

The second step is to average $\hat{f}$ and $\hat{g}$ over the CUE. The result is in Eqs. (3.1) and (3.2),

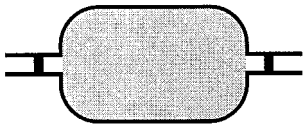

FIG. 6. Chaotic cavity (grey) connected to two leads containing tunnel barriers (black).

$$\langle \hat{f} \rangle_{\rm CUE} = -\tfrac{1}{2} N^{-1} \,{\rm tr}\, A \,{\rm tr}\, B, \tag{5.5a}$$

$$\langle \hat{g} \rangle_{\rm CUE} = -\tfrac{1}{2}(N^2-1)^{-1}({\rm tr}\, A \,{\rm tr}\, BD \,{\rm tr}\, C + {\rm tr}\, ADCB) + \tfrac{1}{2}[N(N^2-1)]^{-1}({\rm tr}\, A \,{\rm tr}\, BDC + {\rm tr}\, ADB \,{\rm tr}\, C). \tag{5.5b}$$

The third step is to translate back to quaternion matrices,

$$\langle f \rangle_{\rm CUE} = N^{-1} \,{\rm tr}\, A \,{\rm tr}\, B, \tag{5.6a}$$

$$\langle g \rangle_{\rm CUE} = (4N^2-1)^{-1}(4\,{\rm tr}\, A \,{\rm tr}\, BD \,{\rm tr}\, C + {\rm tr}\, ADCB) - [N(4N^2-1)]^{-1}({\rm tr}\, A \,{\rm tr}\, BDC + {\rm tr}\, ADB \,{\rm tr}\, C). \tag{5.6b}$$

Similarly, to average of f and g over the CSE we need the average of $\hat{f}$ and $\hat{g}$ over the COE given by Eq. (4.7a), and then translate back to quaternion matrices. For $\langle f(U) \rangle$ we find

$$\langle \hat{f} \rangle_{\rm COE} = -\tfrac{1}{2}(N+1)^{-1}({\rm tr}\, A \,{\rm tr}\, B + {\rm tr}\, A^{\rm T} B),$$

$$\Rightarrow \langle f \rangle_{\rm CSE} = (2N-1)^{-1}(2{\rm tr}\, A \,{\rm tr}\, B - {\rm tr}\, A^{\rm R} B). \tag{5.7a}$$

Similarly, we find for $\langle g(U) \rangle$ the final result

$$\begin{aligned}\langle g \rangle_{\rm CSE} = {} & [(2N-1)(2N-3)]^{-1}(4{\rm tr}\, A \,{\rm tr}\, BD \,{\rm tr}\, C - 2\,{\rm tr}\, AD^{\rm R}B^{\rm R} \,{\rm tr}\, C - 2\,{\rm tr}\, A \,{\rm tr}\, BC^{\rm R}D \\ & + {\rm tr}\, AD^{\rm R}CB^{\rm R} + {\rm tr}\, ADCB + {\rm tr}\, AC^{\rm R}D^{\rm R}B + {\rm tr}\, ADB^{\rm R}C^{\rm R} - 2\,{\rm tr}\, AC^{\rm R} \,{\rm tr}\, BD^{\rm R}) \\ & - [(2N(2N-1)(2N-3)]^{-1}(2\,{\rm tr}\, A \,{\rm tr}\, BDC - {\rm tr}\, AC^{\rm R}D^{\rm R}B^{\rm R} + 2\,{\rm tr}\, A \,{\rm tr}\, BD^{\rm R}C \\ & - {\rm tr}\, AC^{\rm R}DB^{\rm R} + 2\ {\rm tr}\, ADB \,{\rm tr}\, C + 2\,{\rm tr}\, AD^{\rm R}B \,{\rm tr}\, C - {\rm tr}\, ADBC^{\rm R} - {\rm tr}\, AD^{\rm R}BC^{\rm R} \\ & + 2\,{\rm tr}\, A \,{\rm tr}\, BC^{\rm R}D^{\rm R} - {\rm tr}\, ADCB^{\rm R} - 4\,{\rm tr}\, A \,{\rm tr}\, BD^{\rm R} \,{\rm tr}\, C + 2\ {\rm tr}\, ADB^{\rm R} \,{\rm tr}\, C - {\rm tr}\, AD^{\rm R}B^{\rm R}C^{\rm R} \\ & + 2\,{\rm tr}\, AC^{\rm R} \,{\rm tr}\, BD - {\rm tr}\, AD^{\rm R}CB - {\rm tr}\, AC^{\rm R}DB).\end{aligned} \tag{5.7b}$$

VI. APPLICATION TO A CHAOTIC CAVITY

We consider the system shown in Fig. 6, consisting of a chaotic cavity attached to two leads, containing tunnel barriers. The $M \times M$ scattering matrix S is decomposed into $N_i \times N_j$ submatrices s_{ij},

$$S = \begin{pmatrix} s_{11} & s_{12} \\ s_{21} & s_{22} \end{pmatrix}, \tag{6.1}$$

which describe scattering from lead j into lead i ($M = N_i + N_j$). The conductance G is given by the Landauer formula,

$$G/G_0 = {\rm tr}\, s_{12} s_{12}^{\dagger} = {\rm tr}\, C_1 S C_2 S^{\dagger}, \quad G_0 = 2e^2/h. \tag{6.2}$$

The projection matrices C_1 and $C_2=1-C_1$ are defined by $(C_1)_{ij}=1$ if $i=j\leqslant N_1$ and 0 otherwise.

In the absence of tunnel barriers in the leads, S is distributed according to the circular ensemble. The symmetry index $\beta \in \{1,2,4\}$ distinguishes the COE ($\beta=1$), CUE ($\beta=2$), and CSE ($\beta=4$). Calculation of the average and variance of G is straightforward,[5,6]

$$\langle G/G_0\rangle = \frac{\beta N_1 N_2}{\beta M+2-\beta}, \tag{6.3}$$

$$\text{var } G/G_0 = \frac{2\beta N_1 N_2(\beta N_1+2-\beta)(\beta N_2+2-\beta)}{(\beta M+2-2\beta)(\beta M+2-\beta)^2(\beta M+4-\beta)}. \tag{6.4}$$

In the presence of a tunnel barrier in lead i with reflection matrix r_i, the distribution of S is given by the Poisson kernel,[38–41]

$$P(S)\propto \left|\det(1-\overline{S}^{\dagger}S)\right|^{-(\beta M+2-\beta)}, \quad \overline{S}=\begin{pmatrix} r_1 & 0 \\ 0 & r_2 \end{pmatrix}. \tag{6.5}$$

The sub-unitary matrix $\overline{S}$ is the ensemble average of S: $\int dS P(S) S=\overline{S}$. The eigenvalues Γ_j of $1-S\overline{S}^{\dagger}$ are the transmission eigenvalues of the tunnel barriers. The fluctuating part $\delta S\equiv S-\overline{S}$ of S can be parametrized as

$$\delta S = T'(1-UR')^{-1}UT, \tag{6.6}$$

where T, T', and R' are $M\times M$ matrices such that the $2M\times 2M$ matrix

$$\Sigma=\begin{pmatrix} \overline{S} & T' \\ T & R' \end{pmatrix} \tag{6.7}$$

is unitary. The usefulness of the parametrization (6.6) is that U is distributed according the circular ensemble.[21,38,41] In the presence of time-reversal symmetry, we further have $\overline{S}=\overline{S}^{\rm T}$, $T'=T^{\rm T}$, $R'=R'^{\rm T}$, and $U=U^{\rm T}$. Physically, U corresponds to the scattering matrix of the cavity without the tunnel barriers in the leads and Σ corresponds to the scattering matrix of the tunnel barriers in the absence of the cavity.[19,41]

The parametrization (6.6) reduces the problem of averaging S with the Poisson kernel to integrating U over the unitary group. Because the conductance G is a rational function of U, this average cannot be done in closed form for all M. For $N_1, N_2\gg 1$ a perturbative calculation is possible. In this section we will compute the mean and variance of the conductance in the large-N limit, using the diagrammatic technique of the previous sections.

A. Average conductance

According to the Landauer formula (6.2) the average conductance is given by

$$\langle G/G_0\rangle = \langle \text{tr } C_1\delta S C_2 \delta S^{\dagger}\rangle, \tag{6.8}$$

where we have used that $\langle \delta S\rangle=0$. Expansion of the denominator in the parametrization (6.6) of δS yields the series

$$\langle G/G_0\rangle = \sum_{n=1}^{\infty}\langle f_n(U)\rangle, \tag{6.9a}$$

$$f_n(U)=\text{tr } C_1 T'(UR')^{n-1}UTC_2T^{\dagger}U^{\dagger}(R'^{\dagger}U^{\dagger})^{n-1}T'^{\dagger}. \tag{6.9b}$$

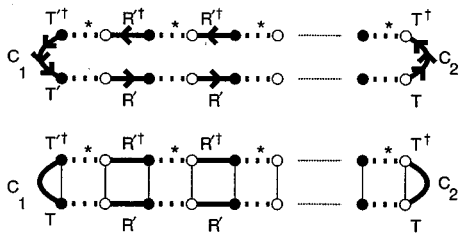

FIG. 7. Top: Diagrammatic representation of the function $f_n(U)$ in Eq. (6.9); Bottom: Ladder diagram with the largest number of cycles, which gives the $\mathcal{O}(N)$ contribution to the average conductance. The arrows are omitted if the direction of the diagram is not ambiguous.

The average of the polynomial function $f_n(U)$ can be calculated diagrammatically. We represent $f_n(U)$ by the top diagram in Fig. 7. The average over the matrix U is done as follows.

The leading contribution, which is of order M, comes from the diagrams with the largest number of T- and U-cycles. For a polynomial of the type (6.8) (all U's are on one side of the $U^\dagger$'s), these diagrams have a ''ladder'' structure (see bottom diagram in Fig. 7). The ladder diagrams contain n U-cycles and $n+1$ T-cycles. Their weight is $W_1^n = M^{-n} + \mathcal{O}(M^{-n-1})$, resulting in

$$\langle f_n(U)\rangle = M^{-n}\,\mathrm{tr}\; T'^{\dagger} C_1 T' (\mathrm{tr}\; R' R'^{\dagger})^{n-1}\,\mathrm{tr}\; T C_2 T^{\dagger} + \mathcal{O}(1). \tag{6.10}$$

Summation of the series (6.9) yields $\langle G\rangle$ to leading order in M,

$$\langle G/G_0\rangle = \frac{(\mathrm{tr}\; T'^{\dagger} C_1 T')(\mathrm{tr}\; T C_2 T^{\dagger})}{M - \mathrm{tr}\; R' R'^{\dagger}} + \mathcal{O}(1) = \frac{(N_1 - \mathrm{tr}\; \overline{S^{\dagger}} C_1 \overline{S})(N_2 - \mathrm{tr}\; \overline{S} C_2 \overline{S^{\dagger}})}{M - \mathrm{tr}\; \overline{S S^{\dagger}}} + \mathcal{O}(1). \tag{6.11}$$

In the second equality we have used the unitarity of the matrix Σ defined in Eq. (6.7).

The weak-localization correction is the $\mathcal{O}(1)$ contribution to $\langle G\rangle$. In general, an $\mathcal{O}(1)$ contribution to the average conductance can have two sources: (i) a higher order contribution to the weight $W_{c_1,\ldots,c_k}$ of the leading-order diagrams, and (ii) higher order diagrams. In the absence of time-reversal symmetry both contributions are absent: (i) $W_1 = M^{-1}$ has no $\mathcal{O}(M^{-2})$ term, and (ii) there are no diagrams of order 1.

The situation is different in the presence of time-reversal symmetry. We discuss the case $\beta = 1$ in which there is no spin-orbit scattering. The case $\beta = 4$ then follows from the translation rule of Sec. V. In the presence of time-reversal symmetry, (i) the coefficient $W_1 = M^{-1} - M^{-2} + \cdots$ has an $\mathcal{O}(M^{-2})$ term, and (ii) there are diagrams of order 1. The first contribution is a correction nM^{-n-1} to the weight M^{-n} in Eq. (6.10). Summation over n yields the first correction to Eq. (6.11),

$$\delta G_1 = -\frac{(\mathrm{tr}\; T'^{\dagger} C_1 T')(\mathrm{tr}\; T C_2 T^{\dagger})}{(M - \mathrm{tr}\; R' R'^{\dagger})^2}. \tag{6.12}$$

The second contribution is from diagrams which are obtained from the ladder diagrams by reversing the order of the contractions in a part of the diagram. The central part of the diagram is ''maximally crossed,'' the left and right ends are ladders (see Fig. 8). In disordered systems, the ladder diagrams are known as diffusons, while the maximally crossed diagrams are known as cooperons. The maximally crossed diagrams are not allowed in the absence of time-reversal

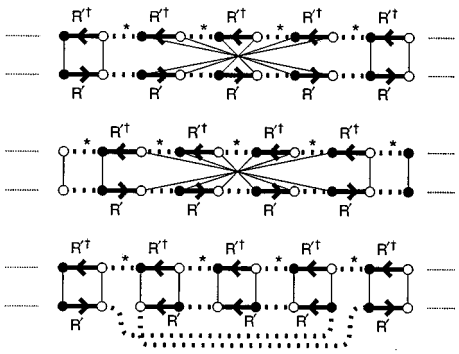

FIG. 8. Top and middle: Two maximally crossed diagrams contributing to the weak-localization correction to the average conductance. The right and left parts of the diagram have a ladder structure; Bottom: The maximally crossed part of the top diagram redrawn as a ladder diagram.

symmetry, because dots of different color are connected by thin lines [violating rule (2) in Sec. III]. A maximally crossed diagram can be redrawn as a ladder diagram by flipping one of the horizontal lines along a vertical axis (bottom diagram in Fig. 8).

In the maximally crossed diagrams all cycles but one have minimum length. The cycle with the exceptional length can be a U-cycle (top diagram in Fig. 8), or a T-cycle (middle diagram). To evaluate these diagrams, we need to introduce some more notation (see Fig. 9). We denote the left and right ladder diagrams by matrices $F_{\rm L}$ and $F_{\rm R}$,

$$F_{\rm L}=T'^{\dagger}C_1T'+\sum_{n=1}^{\infty}M^{-n}(\mathrm{tr}\ T'^{\dagger}C_1T')(\mathrm{tr}\ R'^{\dagger}R')^{n-1}R'^{\dagger}R'$$

$$=T'^{\dagger}C_1T'+\left(\frac{\mathrm{tr}\ T'^{\dagger}C_1T'}{M-\mathrm{tr}\ R'R'^{\dagger}}\right)R'^{\dagger}R', \tag{6.13a}$$

$$F_{\rm R}=TC_2T^{\dagger}+\sum_{n=1}^{\infty}M^{-n}R'R'^{\dagger}(\mathrm{tr}\ R'R'^{\dagger})^{n-1}(\mathrm{tr}\ TC_2T^{\dagger})$$

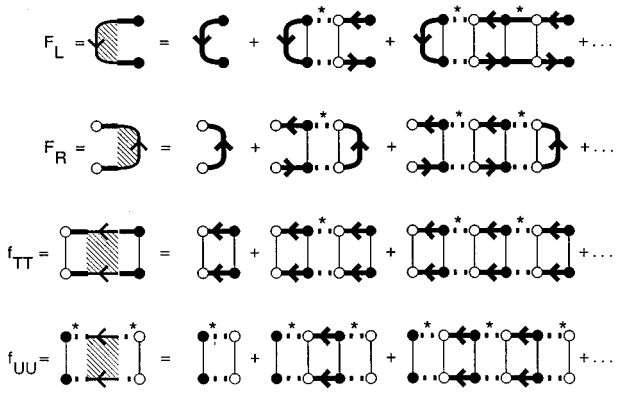

FIG. 9. Diagrammatic representation of Eqs. (6.13) and (6.14).

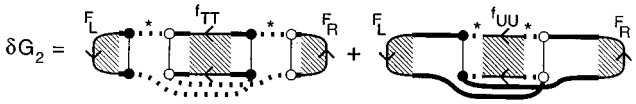

FIG. 10. Diagrammatic representation of the weak-localization correction δG_2 from the maximally crossed diagrams. The total correction $\delta G=\delta G_1+\delta G_2$ contains also a contribution δG_1 from the weight factors [Eq. (6.12)].

$$=TC_2T^\dagger+R'R'^\dagger\left(\frac{\text{tr } TC_2T^\dagger}{M-\text{tr } R'R'^\dagger}\right). \tag{6.13b}$$

The scalars f_{UU} and f_{TT} represent the maximally crossed part of the diagram,

$$f_{TT}=\sum_{n=0}^{\infty} M^{-n}(\text{tr } R'R'^\dagger)^{n+1}=\frac{M \text{ tr } RR'^\dagger}{M-\text{tr } R'R'^\dagger}, \tag{6.14a}$$

$$f_{UU}=\sum_{n=0}^{\infty} M^{-n-1}(\text{tr } R'R'^\dagger)^{n}=\frac{1}{M-\text{tr } R'R'^\dagger}. \tag{6.14b}$$

We used the symmetry of R' to replace R'^{T} by R'. With this notation we may draw the contribution δG_2 to the weak-localization correction from the maximally crossed diagrams as in Fig. 10. It evaluates to

$$\delta G_2=-M^{-3}\,\text{tr } F_{\mathrm{L}}f_{TT}\,\text{tr } F_{\mathrm{R}}+\text{ tr } F_{\mathrm{L}}f_{UU}F_{\mathrm{R}}^{\mathrm{T}}. \tag{6.15}$$

The total weak-localization correction $\delta G=\delta G_1+\delta G_2$ becomes

$$\delta G=-(\text{tr } T^\dagger T)^{-3}[(\text{tr } C_2T^\dagger T)^2\,\text{tr } C_1(T^\dagger T)^2+(\text{tr } C_1T^\dagger T)^2\,\text{tr } C_2(T^\dagger T)^2]. \tag{6.16}$$

Since $T^\dagger T=1-\overline{S^\dagger S}$ has eigenvalues Γ_n, we may write the final result for the average conductance in the form

$$\langle G/G_0\rangle=\frac{g_1g_1'}{g_1+g_1'}+\left(1-\frac{2}{\beta}\right)\frac{g_2g_1'^2+g_2'g_1^2}{(g_1+g_1')^3}+\mathcal{O}(M^{-1}), \tag{6.17}$$

$$g_p=\sum_{n=1}^{N_1}\Gamma_n^p,\quad g_p'=\sum_{n=1+N_1}^{M}\Gamma_n^p. \tag{6.18}$$

(The $\beta=4$ result follows from the translation rule of Sec. V.) The first term in Eq. (6.17) is the series conductance of the two tunnel conductances G_0g_1 and G_0g_1'. The term proportional to $1-2/\beta$ is the weak-localization correction. In the absence of tunnel barriers one has $g_p=N_1$, $g_p'=N_2$, and the large-M limit of Eq. (6.3) is recovered. In the case of two identical tunnel barriers ($N_1=N_2=M/2\equiv N$, $\Gamma_n=\Gamma_{n+N}$ for $n=1,\ldots,N$), Eq. (6.17) simplifies to

$$\langle G/G_0\rangle=\tfrac{1}{2}g_1+\left(1-\frac{2}{\beta}\right)\frac{g_2}{4g_1}+\mathcal{O}(M^{-1}). \tag{6.19}$$

Eq. (6.19) was previously obtained by Iida, Weidenmüller and Zuk[15]. If all Γ_n's are equal to Γ, Eq. (6.19) simplifies further to $\langle G/G_0\rangle=\frac{1}{2}N\Gamma+\frac{1}{4}(1-2/\beta)\Gamma$.

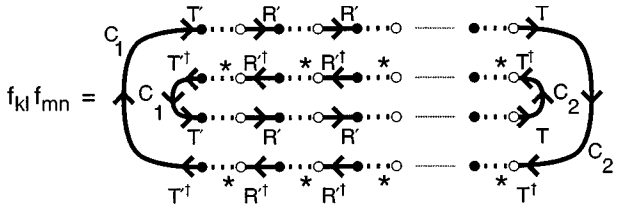

FIG. 11. Diagrammatic representation of a term contributing to G^2, and hence to the variance (6.20) of the conductance.

B. Conductance fluctuations

We seek the effect of tunnel barriers on the variance of the conductance, var $G=\langle G^2\rangle-\langle G\rangle^2$. We consider $\beta=1$ and 2 first, and translate to $\beta=4$ in the end. Using the parametrization (6.6) we write the variance in the form

$$\text{var } G/G_0=\text{var}(\text{tr } C_1\delta S C_2\delta S^\dagger)=\sum_{k,l,m,n\geqslant 1}\text{covar}(f_{kl},f_{mn}), \tag{6.20a}$$

$$f_{kl}=\text{tr } C_1T'(UR')^{k-1}UTC_2T^\dagger U^\dagger(R'^\dagger U^\dagger)^{l-1}T'^\dagger. \tag{6.20b}$$

Since the number U's and U^*'s must be equal for a non-zero average, $\text{covar}(f_{kl},f_{mn})\equiv\langle f_{kl}f_{mn}\rangle-\langle f_{kl}\rangle\langle f_{mn}\rangle=0$ unless $k+m=l+n$. Diagrammatically, we represent $f_{kl}f_{mn}$ by Fig. 11. The diagram consists of an inner loop, corresponding to f_{kl}, and an outer loop, corresponding to f_{mn}. The covariance of f_{kl} and f_{mn} is given by the connected diagrams. We call a diagram ''connected'' if (i) the partition of the U-cycles contains a group which consists of U-cycles from the inner and the outer part, or (ii) the diagram contains a cycle (a U-cycle or a T-cycle) connecting the inner and outer loops.

We first compute the contribution from diagrams which are connected only because of (i), i.e., diagrams in which all U-cycles and T-cycles belong either to the inner or outer loop. The contribution from such a diagram is maximal, if the U-cycles are partitioned in groups which are as small as possible. The optimal partition consists of groups of size 1, except for a single group of size 2, which contains one U-cycle from the inner and one from the outer loop. Furthermore, the total number of cycles is maximal if both the inner and outer loops are ladder diagrams. This requires $k=l$ and $m=n$. The covariance from this diagram is

$$\text{covariance}=km\,\delta_{kl}\delta_{mn}W_{1,1}W_1^{k+m-2}(\text{tr } T'^\dagger C_1T')^2(\text{tr } R'R'^\dagger)^{k+m-2}(\text{tr } TC_2T^\dagger)^2+\mathcal{O}(M^{-1}). \tag{6.21}$$

Summing over k and m we obtain the first contribution to var G/G_0,

$$\text{variance }=M^{-4}(\text{tr } F_{\rm L}\,\text{tr } F_{\rm R})^2. \tag{6.22}$$

The second contribution, consisting of diagrams in which the inner and outer loops are connected by T- or U-cycles, is of maximal order if the partition of the U-cycles involves only groups of size 1. For $\beta=2$ there are 16 connected diagrams of maximal order. They are shown in Fig. 12, and their contribution to var G/G_0 is tabulated in Table I. The shaded areas indicate ladder parts of the diagram (see Figs. 9 and 13). The matrices $F_{\rm L}$ and $F_{\rm R}$, and the scalars f_{UU} and f_{TT} are defined in Eqs. (6.13) and (6.14). The definitions of the matrix H and of the scalars f_{UT} and f_{TU} are

$$f_{UT}=f_{TU}=\sum_{n=0}^{\infty}M^{-n}(\text{tr } R'R'^\dagger)^n=\frac{M}{M-\text{tr } R'R'^\dagger}, \tag{6.23a}$$

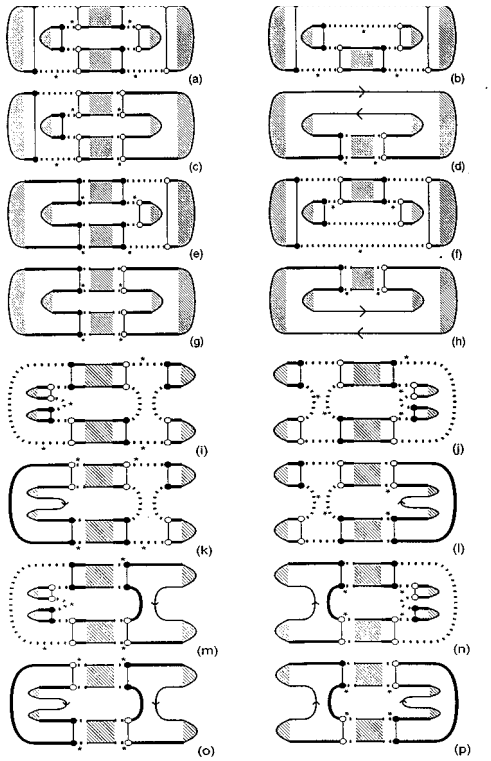

FIG. 12. The 16 connected diagrams which contribute to the variance of the conductance. The shaded parts are defined in Figs. 9 and 13. These diagrams contribute for $\beta=1$ and 2. For $\beta=1$ there are 16 more diagrams, obtained by flipping the inner loop around a vertical axis (diagram a–h) or around a horizontal axis (i–p), so that ladders become maximally crossed.

$$H=M^{-1}(\mathrm{tr}\,F_{\mathrm{R}})R'T'^{\dagger}C_1T'+M^{-1}(\mathrm{tr}\,F_{\mathrm{L}})TC_2T^{\dagger}R'+M^{-2}(\mathrm{tr}\,F_{\mathrm{L}})(\mathrm{tr}\,F_{\mathrm{R}})R'R'^{\dagger}R'. \tag{6.23b}$$

In the presence of time-reversal symmetry ($\beta=1$), the matrix U is symmetric. Diagrammatically, this means that no distinction is made between black and white dots. In addition to the 16 diffuson-like diagrams of Fig. 12, 16 more cooperon-like diagrams contribute. These are obtained from the diagrams of Fig. 12 by flipping the inner loop around a vertical (Figs. 12a–h) or horizontal (Figs. 12i–p) axis, so that segments with a ladder structure become maximally crossed. Their contributions are listed in Table I. The contributions from the individual diffuson-like and cooperon-like diagrams are different. The total contribution to var G from diffuson-like and cooperon-like diagrams is the same.

The final result for the variance of G is

$$\begin{aligned}\mathrm{var}\,G/G_0=2\beta^{-1}(g_1+g_1')^{-6}(&2g_1^4g_1'^2+4g_1^3g_1'^3-4g_1^2g_2g_1'^3+2g_1^2g_1'^4\\&-2g_1g_2g_1'^4+3g_2^2g_1'^4-2g_1g_3g_1'^4+2g_2g_1'^5-2g_3g_1'^5+2g_1^5g_2'-2g_1^4g_1'g_2'\\&-4g_1^3g_1'^2g_2'+6g_1^2g_2g_1'^2g_2'+3g_1^4g_2'^2-2g_1^5g_3'-2g_1^4g_1'g_3').\end{aligned} \tag{6.24}$$

Eq. (6.24) was previously obtained by Efetov.[32] One verifies that the large-N limit of Eq. (6.4) is recovered in the absence of tunnel barriers. For the special case of identical tunnel barriers ($g_p=g_p'$), this simplifies to

TABLE I. Contribution to var G/G_0 from the connected diagrams of Fig. 12.

Diagram	$\beta=1,2$	$\beta=1$
a	$W_2^2(\mathrm{tr}\, F_L)^2 f_{TT}^2(\mathrm{tr}\, F_R)^2$	$W_2^2\,\mathrm{tr}\, F_R\,\mathrm{tr}\, R_L f_{TT}^2\,\mathrm{tr}\, F_L\,\mathrm{tr}\, F_R$
b	$W_3(\mathrm{tr}\, F_L)^2 f_{TT}(\mathrm{tr}\, F_R)^2$	$W_3\,\mathrm{tr}\, F_R\,\mathrm{tr}\, F_L f_{TT}\,\mathrm{tr}\, F_L\,\mathrm{tr}\, F_R$
c	$W_2(\mathrm{tr}\, F_L)^2 f_{TU}^2\,\mathrm{tr}\, F_R^2$	$W_2\,\mathrm{tr}\, F_R\,\mathrm{tr}\, F_L f_{TU}^2\,\mathrm{tr}\, F_L^{\mathrm{T}} F_R$
d	$\mathrm{tr}\, HH^\dagger f_{UU}$	$\mathrm{tr}\, H^{\mathrm{T}} H^\dagger f_{UU}$
e	$W_2\,\mathrm{tr}\, F_L^2 f_{UT}^2(\mathrm{tr}\, F_R)^2$	$W_2\,\mathrm{tr}\, F_R^{\mathrm{T}} F_L f_{UT}^2\,\mathrm{tr}\, F_L\,\mathrm{tr}\, F_R$
f	$W_3(\mathrm{tr}\, F_L)^2 f_{TT}(\mathrm{tr}\, F_R)^2$	$W_3\,\mathrm{tr}\, F_R\,\mathrm{tr}\, F_L f_{TT}\,\mathrm{tr}\, F_L\,\mathrm{tr}\, F_R$
g	$\mathrm{tr}\, F_L^2 f_{UU}^2\,\mathrm{tr}\, F_R^2$	$\mathrm{tr}\, F_R^{\mathrm{T}} F_L f_{UU}^2\,\mathrm{tr}\, F_L^{\mathrm{T}} F_R$
h	$\mathrm{tr}\, H^\dagger H f_{UU}$	$\mathrm{tr}\, H^* H f_{UU}$
i	$W_2^2\,\mathrm{tr}\, F_L\,\mathrm{tr}\, F_R f_{TT}^2\,\mathrm{tr}\, F_L\,\mathrm{tr}\, F_R$	$W_2^2\,\mathrm{tr}\, F_R\,\mathrm{tr}\, F_L f_{TT}^2\,\mathrm{tr}\, F_L\,\mathrm{tr}\, F_R$
j	$W_2^2\,\mathrm{tr}\, F_L\,\mathrm{tr}\, F_R f_{TT}^2\,\mathrm{tr}\, F_L\,\mathrm{tr}\, F_R$	$W_2^2\,\mathrm{tr}\, F_L\,\mathrm{tr}\, F_R f_{TT}^2\,\mathrm{tr}\, F_R\,\mathrm{tr}\, F_L$
k	$W_2\,\mathrm{tr}\, HR'^\dagger f_{TU} f_{UT}\,\mathrm{tr}\, F_L\,\mathrm{tr}\, F_R$	$W_2\,\mathrm{tr}\, H^{\mathrm{T}} R'^\dagger f_{TU} f_{UT}\,\mathrm{tr}\, F_L\,\mathrm{tr}\, F_R$
l	$W_2\,\mathrm{tr}\, F_L\,\mathrm{tr}\, F_R f_{TU} f_{UT}\,\mathrm{tr}\, H^\dagger R'$	$W_2\,\mathrm{tr}\, F_L\,\mathrm{tr}\, F_R f_{TU} f_{UT}\,\mathrm{tr}\, H^* R'$
m	$W_2\,\mathrm{tr}\, F_L\,\mathrm{tr}\, F_R f_{TU} f_{UT}\,\mathrm{tr}\, R' H^\dagger$	$W_2\,\mathrm{tr}\, F_R\,\mathrm{tr}\, F_L f_{TU} f_{UT}\,\mathrm{tr}\, R'^{\mathrm{T}} H^\dagger$
n	$W_2\,\mathrm{tr}\, R'^\dagger H f_{TU} f_{UT}\,\mathrm{tr}\, F_L\,\mathrm{tr}\, F_R$	$W_2\,\mathrm{tr}\, R'^* H f_{TU} f_{UT}\,\mathrm{tr}\, F_L\,\mathrm{tr}\, F_R$
o	$\mathrm{tr}\, HR'^\dagger f_{UU}^2\,\mathrm{tr}\, R' H^\dagger$	$\mathrm{tr}\, H^{\mathrm{T}} R'^\dagger f_{UU}^2\,\mathrm{tr}\, R'^{\mathrm{T}} H^\dagger$
p	$\mathrm{tr}\, R'^\dagger H f_{UU}^2\,\mathrm{tr}\, H^\dagger R'$	$\mathrm{tr}\, R'^* H f_{UU}^2\,\mathrm{tr}\, H^* R'$

$$\mathrm{var}\, G/G_0=(8\beta g_1^2)^{-1}(2g_1^2-2g_1g_2+3g_2^2-2g_1g_3), \tag{6.25}$$

in agreement with Ref. 15. Another special case is that of high tunnel barriers, $\Gamma_n \ll 1$ for all n, when Eq. (6.24) simplifies to[42]

$$\mathrm{var}\, G/G_0=4\beta^{-1}(g_1+g_1')^{-4}g_1^2 g_1'^2. \tag{6.26}$$

If all transmission eigenvalues $\Gamma_n \equiv \Gamma$ are equal, one has var $G/G_0=(8\beta)^{-1}[1+(1-\Gamma)^2]$. A high tunnel barrier ($\Gamma \ll 1$) thus doubles the variance.

C. Density of transmission eigenvalues

The transmission eigenvalues $T_n \in [0,1]$ are the N_1 eigenvalues of the matrix product $s_{12}s_{12}^\dagger$. Without loss of generality we may assume that $N_1 \leq N_2$. The matrix product $s_{21}s_{21}^\dagger$ then

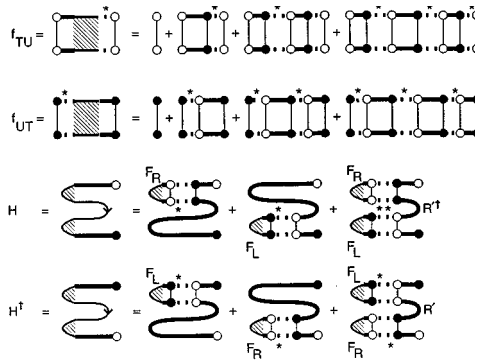

FIG. 13. Diagrammatic representation of Eq. (6.23).

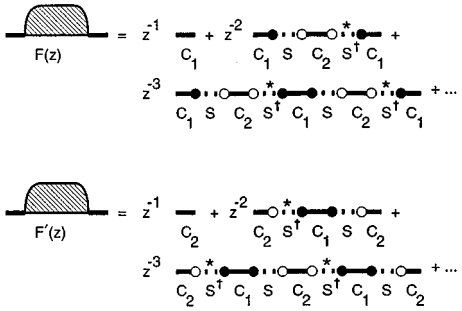

FIG. 14. Diagrammatic representation of the Green functions for the density of transmission eigenvalues.

has the same N_1 eigenvalues as $s_{12}s_{12}^\dagger$, plus N_2-N_1 eigenvalues equal to zero. The N_1 non-zero transmission eigenvalues appear as the diagonal elements of the diagonal matrix T in the polar decomposition of the scattering matrix

$$S=\begin{pmatrix} s_{11} & s_{12} \\ s_{21} & s_{22} \end{pmatrix}=\begin{pmatrix} v & 0 \\ 0 & w \end{pmatrix}\begin{pmatrix} \sqrt{1-T} & 0 & i\sqrt{T} \\ 0 & \mathbb{1} & 0 \\ i\sqrt{T} & 0 & \sqrt{1-T} \end{pmatrix}\begin{pmatrix} v' & 0 \\ 0 & w' \end{pmatrix}. \tag{6.27}$$

Here v and v' (w and w') are $N_1\times N_1$ ($N_2\times N_2$) unitary matrices and $\mathbb{1}$ is the N_2-N_1 dimensional unit matrix. If $N_1=N_2$, Eq. (6.27) simplifies to Eq. (1.2).

So far we have only studied the conductance $G=G_0\Sigma_n T_n$. The leading contribution to the average conductance comes from ladder diagrams. If we wish to average transport properties of the form $A=\Sigma_n a(T_n)$ (so-called linear statistics on the transmission eigenvalues), we need to know the density $\rho(T)$ of the transmission eigenvalues T_n. The leading-order contribution to the transmission-eigenvalue density is given by a larger class of diagrams, as we now discuss.

The density $\rho(T)=\langle\Sigma_{n=1}^{N_1}\delta(T-T_n)\rangle$ of the transmission eigenvalues follows from the matrix Green function $F(z)$:

$$F(z)=\langle C_1(z-SC_2S^\dagger C_1)^{-1}\rangle, \tag{6.28a}$$

$$\rho(T)=-\pi^{-1}\,\mathrm{Im\ tr}\,F(T+i\epsilon), \tag{6.28b}$$

where ϵ is a positive infinitesimal. We first compute $\rho(T)$ in the absence of tunnel barriers, when the result is known from other methods.[4–6,43] Then we include the tunnel barriers, when the result is not known.

In the absence of tunnel barriers, the scattering matrix S is distributed according to the circular ensemble, so that averaging amounts to integrating over the unitary group. We compute $F(z)$ as an expansion in powers of $1/z$,

$$F(z)=\sum_{n=0}^{\infty}\langle C_1 z^{-1}(SC_2S^\dagger C_1 z^{-1})^n\rangle. \tag{6.29}$$

We will also need the Green function

$$F'(z)=\langle C_2(z-S^\dagger C_1 SC_2)^{-1}\rangle=\sum_{n=0}^{\infty}\langle C_2 z^{-1}(S^\dagger C_1 SC_2 z^{-1})^n\rangle. \tag{6.30}$$

The two Green functions F and F' are represented diagrammatically in Fig. 14. A diagram

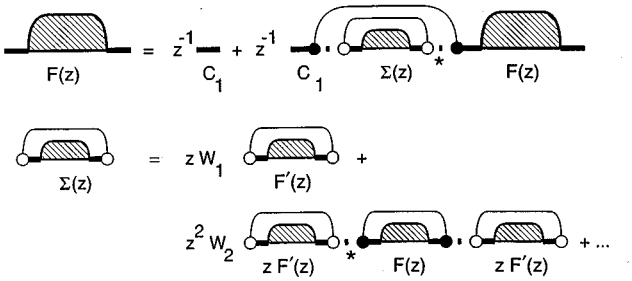

FIG. 15. Diagrammatic representation of the Dyson equation (6.31) for $F(z)$.

contributes to leading order [which is $\mathcal{O}(1)$] if the number of T- and U-cycles is maximal. That is the case if the diagram is *planar*, meaning that the thin lines do not cross. The ladder diagrams are a subset of the planar diagrams. Planar diagrams have been studied in the context of the diagrammatic evaluation of integrals over Hermitian matrices, in particular for the Gaussian ensemble.[12,17] For the Gaussian ensemble, only planar diagrams with U-cycles of unit length have to be taken into account. Summation over all these diagrams results in a self-consistency or Dyson equation for $F(z)$, which solves the problem.[17] For an integral of unitary matrices, U-cycles of arbitrary length need to be taken into account, as is shown diagrammatically in Fig. 15. The corresponding Dyson equation is

$$F(z)=z^{-1}C_1+z^{-1}C_1\Sigma(z)F(z),\quad \Sigma(z)=\sum_{n=1}^{\infty} W_n[z\ \mathrm{tr}\ F'(z)]^n[\mathrm{tr}\ F(z)]^{n-1}, \tag{6.31a}$$

$$F'(z)=z^{-1}C_2+z^{-1}C_2\Sigma'(z)F'(z),\quad \Sigma'(z)=\sum_{n=1}^{\infty} W_n[z\ \mathrm{tr}\ F(z)]^n[\mathrm{tr}\ F'(z)]^{n-1}. \tag{6.31b}$$

In terms of the generating function

$$h(z)=\sum_{n=1}^{\infty} W_n z^{n-1}=\frac{1}{2z}(\sqrt{M^2+4z}-M), \tag{6.32}$$

we may rewrite Eq. (6.31) as

$$F(z)=C_1(z-\Sigma(z)C_1)^{-1},\quad \Sigma(z)=hb(z\ \mathrm{tr}\ F(z)\ \mathrm{tr}\ F'(z)b)z\ \mathrm{tr}\ F'(z), \tag{6.33a}$$

$$F'(z)=C_2(z-\Sigma(z)C_2)^{-1},\quad \Sigma'(z)=hb(z\ \mathrm{tr}\ F(z)\ \mathrm{tr}\ F'(z))z\ \mathrm{tr}\ F(z). \tag{6.33b}$$

In the derivation of Eq. (6.33) we did not use the particular form of the matrices C_1 and C_2. As a check we may choose $C_1=C_2=1$, so that $F(z)=F'(z)=(z-1)^{-1}$, and verify that Eq. (6.33) holds.

The solution of Eq. (6.33) is

$$\mathrm{tr}\ F(z)=\frac{N_1-N_2}{2z}+\frac{\sqrt{M^2z-(N_1-N_2)^2}}{2z\sqrt{z-1}}, \tag{6.34a}$$

$$\mathrm{tr}\, F'(z) = \frac{N_2 - N_1}{2z} + \frac{\sqrt{M^2 z - (N_2 - N_1)^2}}{2z\sqrt{z-1}}. \tag{6.34b}$$

The resulting density of transmission eigenvalues is

$$\rho(T) = \frac{M\sqrt{T - T_{\min}}}{2\pi T\sqrt{1-T}}\,\theta(T - T_{\min}), \quad T_{\min} = \frac{(N_1 - N_2)^2}{M^2}, \tag{6.35}$$

in agreement with Refs. 5, 6, and 43. (The function $\theta(x) = 1$ if $x > 0$ and 0 if $x < 0$.)

The weak-localization correction to $\rho(T)$ follows from the $\mathcal{O}(M^{-1})$ term in the large-M expansion of $F(z)$. As in Sec. VI A, it has two contributions: $\delta F_1(z)$, which is due to the sub-leading order term in the large-M expansion of W_n, and $\delta F_2(z)$, which is due to diagrams of order $\mathcal{O}(M^{-1})$. In the absence of time-reversal symmetry, both contributions are absent. In the presence of time-reversal symmetry, the sub-leading order term $\delta W_n = -M^{-2n}(-4)^{n-1}$ in the large-M expansion of W_n [cf. Eq. (4.4)] yields a sub-leading order contribution δh to the generating function h,

$$\delta h(z) = \sum_{n=1}^{\infty} \delta W_n z^{n-1} = -(M^2 + 4z)^{-1}, \tag{6.36}$$

from which we obtain

$$\mathrm{tr}\ \delta F_1(z) = \tfrac{1}{4}(z - T_{\min})^{-1} - \tfrac{1}{4}(z-1)^{-1}. \tag{6.37}$$

The contribution $\delta F_2(z)$ comes from diagrams in which thin lines connect black and white dots. Each such diagram contains the product $C_1 C_2$, which vanishes. Hence, the $\mathcal{O}(M^{-1})$ contribution to $F(z)$ consists of $\delta F_1(z)$ only. The resulting weak-localization correction to the transmission eigenvalue density is

$$\delta\rho(T) = \frac{2-\beta}{4\beta}[\,\delta(T - T_{\min} - \epsilon) - \delta(T - 1 + \epsilon)], \tag{6.38}$$

in agreement with Refs. 4 and 6.

We now include tunnel barriers in the leads. Motivated by Nazarov's calculation of the density of transmission eigenvalues in a disordered metal,[44] we introduce the $2M \times 2M$ matrices

$$\mathbf{S} = \begin{pmatrix} S & 0 \\ 0 & S^\dagger \end{pmatrix}, \quad \mathbf{C} = \begin{pmatrix} 0 & C_2 \\ C_1 & 0 \end{pmatrix}, \quad \mathbf{F}(z) = \begin{pmatrix} 0 & F'(z) \\ F(z) & 0 \end{pmatrix}, \tag{6.39a}$$

$$\mathbf{T} = \begin{pmatrix} T & 0 \\ 0 & T^\dagger \end{pmatrix}, \quad \mathbf{T}' = \begin{pmatrix} T' & 0 \\ 0 & T'^\dagger \end{pmatrix}, \quad \mathbf{R}' = \begin{pmatrix} R' & 0 \\ 0 & R'^\dagger \end{pmatrix}. \tag{6.39b}$$

Analogous to Eq. (6.6), we decompose $\mathbf{S} = \overline{\mathbf{S}} + \delta\mathbf{S}$, where $\overline{\mathbf{S}} = \langle \mathbf{S} \rangle$ and

$$\delta\mathbf{S} = \mathbf{T}'(1 - \mathbf{U}\mathbf{R}')^{-1}\mathbf{U}\mathbf{T}, \quad \mathbf{U} = \begin{pmatrix} U & 0 \\ 0 & U^\dagger \end{pmatrix} \tag{6.40}$$

is given in terms of a matrix U which is distributed according to the circular ensemble. Because S, C_1, and C_2 commute and $C_1 C_2 = 0$, we may replace S by δS in the expression (6.28a) for $F(z)$. The result for the matrix Green function $\mathbf{F}(z)$ is

$$\mathbf{F}(z)=(2z)^{-1}\sum_{\pm}\langle \mathbf{C}\pm\mathbf{C}\mathbf{T}'[1-\mathbf{U}(\mathbf{R}'\pm\mathbf{T}\mathbf{C}\mathbf{T}'z^{-1/2})]^{-1}\mathbf{U}\mathbf{T}\mathbf{C}z^{-1/2}\rangle$$

$$=(2z)^{-1}\sum_{\pm}[\mathbf{C}\pm\mathbf{A}_{\pm}(\mathbf{F}_{\pm}-\mathbf{X}_{\pm})\mathbf{B}_{\pm}]. \tag{6.41}$$

In the second equation we abbreviated $\mathbf{X}_{\pm}=\mathbf{R}'\pm\mathbf{T}\mathbf{C}\mathbf{T}'z^{-1/2}$, $\mathbf{F}_{\pm}=\langle\mathbf{X}_{\pm}(1-\mathbf{U}\mathbf{X}_{\pm})^{-1}\rangle$, and defined $\mathbf{A}_{\pm}$ and $\mathbf{B}_{\pm}$ such that $\mathbf{A}_{\pm}\mathbf{X}_{\pm}=\mathbf{C}\mathbf{T}'$, $\mathbf{X}_{\pm}\mathbf{B}_{\pm}=\mathbf{T}\mathbf{C}z^{-1/2}$.

After these algebraic manipulations we are ready to compute $\mathbf{F}_{\pm}$ by expanding in planar diagrams. The result is a Dyson equation similar to Eq. (6.31),

$$\mathbf{F}_{\pm}=\mathbf{X}_{\pm}(1+\mathbf{\Sigma}_{\pm}\mathbf{F}_{\pm}),\quad \mathbf{\Sigma}_{\pm}=\sum_{n=1}^{\infty}W_n(\mathscr{P}\mathbf{F}_{\pm})^{2n-1}, \tag{6.42}$$

where the projection operator $\mathscr{P}$ acts on a $2M\times 2M$ matrix $\mathbf{A}$ as

$$\mathbf{A}=\begin{pmatrix}A_{11} & A_{12}\\ A_{21} & A_{22}\end{pmatrix},\quad \mathscr{P}\mathbf{A}=\begin{pmatrix}0 & \mathbb{1}_M\,\mathrm{tr}A_{12}\\ \mathbb{1}_M\,\mathrm{tr}A_{21} & 0\end{pmatrix}, \tag{6.43}$$

$\mathbb{1}_M$ being the $M\times M$ unit matrix. The presence of the projection operator $\mathscr{P}$ in Eq. (6.42) ensures that the planar diagrams contain only contractions between U (the 1,1 block of $\mathbf{U}$) and $U^{\dagger}$ (the 2,2 block of $\mathbf{U}$). In terms of the generating function h we obtain the result

$$\mathbf{F}=(2z)^{-1}\sum_{\pm}(\mathbf{C}\pm\mathbf{C}\mathbf{T}'(1-\mathbf{\Sigma}_{\pm}\mathbf{X}_{\pm})^{-1}\mathbf{\Sigma}_{\pm}\mathbf{T}\mathbf{C}z^{-1/2}), \tag{6.44}$$

$$\mathbf{\Sigma}_{\pm}=(\mathscr{P}\mathbf{X}_{\pm}(1-\mathbf{\Sigma}_{\pm}\mathbf{X}_{\pm})^{-1})h((\mathscr{P}\mathbf{X}_{\pm}(1-\mathbf{\Sigma}_{\pm}\mathbf{X}_{\pm})^{-1})^2). \tag{6.45}$$

It remains to solve the 2×2 matrix equation (6.45). We could not do this analytically for arbitrary Γ_j, but only for the case of two identical tunnel barriers: $N_1=N_2=\frac{1}{2}M\equiv N$, $\Gamma_j=\Gamma_{j+N}$ ($j=1,2,\ldots,N$). The solution of Eq. (6.45) in that case is

$$\mathbf{\Sigma}_{\pm}=\pm(\sqrt{z}-\sqrt{z-1})\begin{pmatrix}0 & \mathbb{1}_M\\ \mathbb{1}_M & 0\end{pmatrix}, \tag{6.46}$$

independent of the Γ_j's. The trace of the Green function is

$$\mathrm{tr}\,F(z)=\sum_{j=1}^{N}\frac{2(1-\Gamma_j)(\sqrt{z}-\sqrt{z-1})+\Gamma_j/\sqrt{z-1}}{2z(1-\Gamma_j)(\sqrt{z}-\sqrt{z-1})+\Gamma_j\sqrt{z}}, \tag{6.47}$$

and the corresponding density of transmission eigenvalues is

$$\rho(T)=\sum_{j=1}^{N}\frac{\Gamma_j(2-\Gamma_j)}{\pi(\Gamma_j^2-4\Gamma_jT+4T)\sqrt{T(1-T)}}. \tag{6.48}$$

As a check, we note that $\rho(T)\to N\delta(T)$ if $\Gamma_j\to 0$ for all j, and $\rho(T)\to N\pi^{-1}[T(1-T)]^{-1/2}$ if $\Gamma_j\to 1$ for all j [in agreement with Eq. (6.35)].

VII. APPLICATION TO A NORMAL-METAL–SUPERCONDUCTOR JUNCTION

As an altogether different application of the diagrammatic technique, we consider a junction between a normal metal (N) and a superconductor (S) (see Fig. 16). At temperatures and voltages

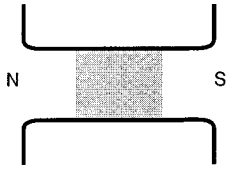

FIG. 16. Conductor consisting of a normal metal (grey) coupled to one normal-metal reservoir (N) and one superconducting reservoir (S). The conductor may consist of a disordered segment or of a quantum dot.

below the excitation gap Δ in S, conduction takes place via the mechanism of Andreev reflection:[45] An electron coming from N with an energy ε (relative to the Fermi energy E_F) is reflected at the NS interface as a hole with energy $-\varepsilon$. The missing charge of $2e$ is absorbed by the superconducting condensate. We calculate the average and variance of the conductance, for the two cases that the NS junction consists of a disordered wire or of a chaotic cavity.

Starting point of the calculation is the relationship between the differential conductance $G_{\rm NS}(eV)=dI/dV$ of the NS junction and the transmission and reflection matrices of the normal region,[46]

$$G_{\rm NS}(\varepsilon)=\frac{4e^2}{h}\,{\rm tr}(t'(\varepsilon)[1+r'(-\varepsilon)^*r'(\varepsilon)]^{-1}t(-\varepsilon)^*)\times(t'(\varepsilon)[1+r'(-\varepsilon)^*r'(\varepsilon)]^{-1}t(-\varepsilon)^*)^\dagger. \tag{7.1}$$

This formula requires $eV\ll\Delta\ll E_F$ and zero temperature. The reflection and transmission matrices are $N\times N$ matrices, which together constitute the $2N\times 2N$ scattering matrix S. Using the polar decomposition (1.2) we may rewrite the conductance formula (7.1) as

$$G_{\rm NS}(\varepsilon)=\frac{4e^2}{h}\,{\rm tr}[T_+(1+u_+\sqrt{1-T_-}u_-^*\sqrt{1-T_+})^{-1}\times u_+T_-u_+^\dagger(1+\sqrt{1-T_+}u_-^{\rm T}\sqrt{1-T_-}u_+^\dagger)^{-1}], \tag{7.2}$$

where $T_\pm=T(\pm\varepsilon)$ and $u_\pm=w'(\pm\varepsilon)w(\mp\varepsilon)^*$. In the presence of spin-orbit scattering, S is a matrix of quaternions, and the transpose should be replaced by the dual. In what follows, we will consider the case of no spin-orbit scattering. Spin-orbit scattering (considered by Slevin, Pichard, and Mello[47]) will be included at the end by means of the translation rule of Sec. V.

Averages are computed in two steps: first over the unitary matrix u, then over the matrix of transmission eigenvalues T. Four cases can be distinguished, depending on the magnitude of the magnetic field B and voltage V relative to the characteristic field B_c for breaking time-reversal symmetry ($\mathscr{T}$) and characteristic voltage E_c/e for breaking electron-hole degeneracy ($\mathscr{D}$):[48]

(1) $eV\ll E_c$, $B\ll B_c\Leftrightarrow\mathscr{T}$ and $\mathscr{D}$ are both present: Then $u_\pm$ may be approximated by the unit matrix, so that one only needs to average over the transmission eigenvalues. This case has been studied extensively[49] and does not concern us here.

(2) $eV\ll E_c$, $B\gg B_c\Leftrightarrow\mathscr{D}$ is present, but $\mathscr{T}$ is broken: Then we may neglect the ε-dependence of S, so that $u_+=u_-\equiv u$. According to the isotropy assumption, u is uniformly distributed in $\mathscr{U}(N)$.

(3) $eV\gg E_c$, $B\ll B_c\Leftrightarrow.\mathscr{T}$ is present, but $\mathscr{D}$ is broken: Then we may consider $S(\varepsilon)$ and $S(-\varepsilon)$ as independent unitary symmetric matrices. Hence $u_+=u_-^\dagger\equiv u$ is uniformly distributed in $\mathscr{U}(N)$.

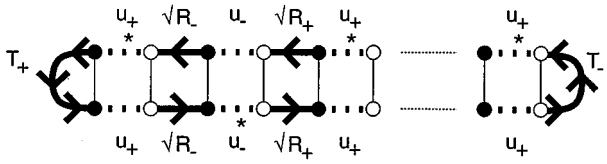

FIG. 17. Ladder diagram for the $\mathcal{O}(N)$ contribution to $\langle G_{\rm NS}\rangle$. We defined $R_\pm = 1 - T_\pm$.

(4) $eV \gg E_c$, $B \gg B_c \Leftrightarrow$ both $\mathcal{T}$ and $\mathcal{D}$ are broken: Then u_+ and u_- are independent, both uniformly distributed in $\mathcal{U}(N)$.

We compute the average and variance of the conductance for cases (2), (3), and (4).

A. Average conductance

We start with the computation of the average conductance $\langle G_{\rm NS}\rangle$. We first perform the average $\langle\cdots\rangle_u$ over $u_\pm$ and then over $T_\pm$. To leading order only ladder diagrams contribute, see Fig. 17. The result is the same for cases (2), (3) and (4):

$$\langle G_{\rm NS}/G_0\rangle_u = 2N \frac{\tau_{1+}\tau_{1-}}{\tau_{1+}+\tau_{1-}-\tau_{1+}\tau_{1-}} + \mathcal{O}(1), \tag{7.3a}$$

$$\tau_{k\pm} = \frac{1}{N}\,\mathrm{tr}\; T_\pm^k = \frac{1}{N}\sum_{j=1}^{N} T_j^k(\pm\varepsilon). \tag{7.3b}$$

The $\mathcal{O}(1)$ contribution $\delta G_{\rm NS}$ is different for the three cases.

Case (2), absence of $\mathcal{T}$ and presence of $\mathcal{D}$. We put $u_\pm = u$, $\tau_{k\pm} = \tau_k$. For normal metals, the $\mathcal{O}(1)$ contribution δG to $\langle G\rangle$ vanishes if $\mathcal{T}$ is broken. However, in the NS junction an $\mathcal{O}(1)$ contribution remains.[26] The diagrams which contribute to $\delta G_{\rm NS}$ have a maximally crossed central part, with contractions between U's and U^*'s on the same side of the diagram (Fig. 18, top). The left and right ends have a ladder structure. In the Hamiltonian approach, a similar maximally crossed diagram has been studied by Altland and Zirnbauer.[27] In total four diagrams contribute to $\delta G_{\rm NS}$, see Fig. 19. The building blocks of the diagram have the algebraic expressions

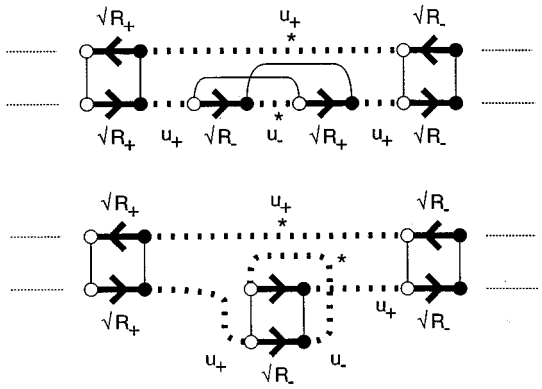

FIG. 18. Maximally crossed diagram for the $\mathcal{O}(1)$ correction to $\langle G_{\rm NS}\rangle$ in the absence of time-reversal symmetry and presence of electron-hole degeneracy (top). The right and left parts of the diagram have a ladder structure. The central part may be redrawn as a ladder diagram (bottom).

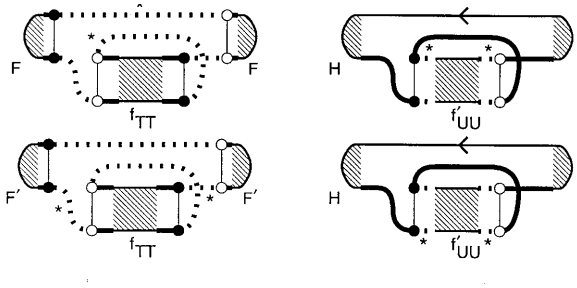

FIG. 19. Diagrams for the $\mathcal{O}(1)$ correction to $\langle G_{\rm NS}\rangle$ in the absence of time-reversal symmetry and presence of electron-hole degeneracy.

$$F_\pm = T_\pm + (1-T_\pm)\ \mathrm{tr}\ T_\pm\ \mathrm{tr}(1-T_\mp)\sum_{j=0}^{\infty} N^{-2j-2}[\ \mathrm{tr}(1-T_+)\ \mathrm{tr}(1-T_-)]^j$$

$$= (\tau_{1\pm} + T_\pm \tau_{1\mp} - \tau_{1+}\tau_{1-})(\tau_{1+} + \tau_{1-} - \tau_{1+}\tau_{1-})^{-1}, \tag{7.4a}$$

$$F'_\pm = -(1-T_\mp)\ \mathrm{tr}\ T_\pm \sum_{j=0}^{\infty} N^{-2j-1}[\ \mathrm{tr}(1-T_+)\ \mathrm{tr}(1-T_-)]^j$$

$$= -(\tau_{1\pm} - \tau_{1\pm}T_\mp)(\tau_{1+} + \tau_{1-} - \tau_{1+}\tau_{1-})^{-1}, \tag{7.4b}$$

$$H_\pm = iN^{-1}T_\pm\sqrt{1-T_\pm}\ \mathrm{tr}\ F_\mp - iN^{-2}(1-T_\pm)\sqrt{1-T_\pm}\ \mathrm{tr}\ F_\mp\ \mathrm{tr}\ F'_\pm, \tag{7.4c}$$

$$f_{TT\pm} = -\ \mathrm{tr}(1-T_\pm)\sum_{j=0}^{\infty} N^{-2j}[\ \mathrm{tr}(1-T_+)\ \mathrm{tr}(1-T_-)]^j = -N(1-\tau_{1\pm})(\tau_{1+} + \tau_{1-} - \tau_{1+}\tau_{1-})^{-1}, \tag{7.4d}$$

$$f_{UU\pm} = -\ \mathrm{tr}(1-T_\pm)\sum_{j=0}^{\infty} N^{-2j-2}[\ \mathrm{tr}(1-T_+)\ \mathrm{tr}(1-T_-)]^j$$

$$= -N^{-1}(1-\tau_{1\pm})[\tau_{1+} + \tau_{1-} - \tau_{1+}\tau_{1-}]^{-1}, \tag{7.4e}$$

$$f'_{UU\pm} = \sum_{j=0}^{\infty} N^{-2j-1}[\ \mathrm{tr}(1-T_+)\ \mathrm{tr}(1-T_-)]^j = N^{-1}(\tau_{1+} + \tau_{1-} - \tau_{1+}\tau_{1-})^{-1}. \tag{7.4f}$$

Capital letters indicate matrices, lower-case letters indicate scalars. The subscripts $\pm$ are omitted from Fig. 19 because of electron-hole degeneracy. The $\mathcal{O}(1)$ correction $\delta G_{\rm NS}$ represented in Fig. 19 equals

$$\delta G_{\rm NS}/G_0 = 8 f'_{UU}\ \mathrm{tr}\ iH\sqrt{1-T} + 4W_2 f_{TT}[(\ \mathrm{tr}\ F)^2 + (\ \mathrm{tr}\ F')^2] = -\frac{8\tau_1 - 4\tau_1^2 + 4\tau_1^3 - 8\tau_2}{\tau_1(2-\tau_1)^3}. \tag{7.5}$$

We still have to average over the transmission eigenvalues. We use that the sample-to-sample fluctuations $\tau_k - \langle\tau_k\rangle$ are an order $1/N$ smaller than the average. (This is a general property of a linear statistics, i.e. of quantities of the form $A = \Sigma_n a(T_n)$, see Ref. 4.) Hence

$$\langle f(\tau_k)\rangle = f(\langle\tau_k\rangle)[1 + \mathcal{O}(N^{-2})], \tag{7.6}$$

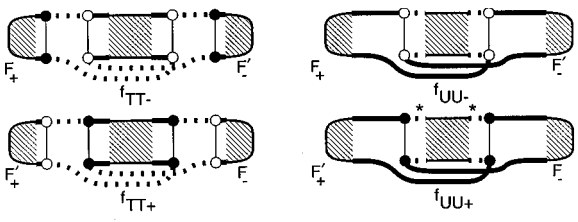

FIG. 20. Diagrams for the $\mathcal{O}(1)$ correction to $\langle G_{\rm NS}\rangle$ in the absence of electron-hole degeneracy and presence of time-reversal symmetry.

which implies that we may replace the average of the rational functions (7.3) and (7.5) of the τ_k's by the rational functions of the average $\langle\tau_k\rangle$. This average has the $1/N$ expansion

$$\langle\tau_k\rangle=\langle\tau_k\rangle_0+\mathcal{O}(N^{-2}), \tag{7.7}$$

where $\langle\tau_k\rangle_0$ is $\mathcal{O}(N^0)$. There is no term of order N^{-1} in the absence of $\mathscr{T}$. The average over T of Eqs. (7.3) and (7.5) becomes

$$\langle G_{\rm NS}/G_0\rangle=\frac{2N\langle\tau_1\rangle_0}{2-\langle\tau_1\rangle_0}-\frac{8\langle\tau_1\rangle_0-4\langle\tau_1\rangle_0^2+4\langle\tau_1\rangle_0^3-8\langle\tau_2\rangle_0}{\langle\tau_1\rangle_0(2-\langle\tau_1\rangle_0)^3}+\mathcal{O}(N^{-1}). \tag{7.8}$$

Case (3), presence of $\mathscr{T}$ and absence of $\mathscr{D}$. We put $u_+=u_-^\dagger\equiv u$. The $\mathcal{O}(1)$ correction comes from the maximally crossed diagrams of Fig. 20,

$$\begin{aligned}\delta G_{\rm NS}/G_0=&\,2W_2\ \mathrm{tr}\ F_+f_{TT-}\ \mathrm{tr}\ F'_-+2W_2\ \mathrm{tr}\ F'_+f_{TT+}\ \mathrm{tr}\ F_-\\&+2\ \mathrm{tr}\ F_+f_{UU-}F'^{\,\mathrm{T}}_-+2\ \mathrm{tr}\ F'_+f_{UU+}F^{\mathrm{T}}_-.\end{aligned} \tag{7.9}$$

Averaging over the transmission eigenvalues amounts to replacing $\tau_{k\pm}$ by its average, $\tau_{k\pm}\to\langle\tau_k\rangle_0+N^{-1}\delta\tau_k+\mathcal{O}(N^{-2})$. (The average of $\tau_{k\pm}$ is the same for $+\varepsilon$ and $-\varepsilon$.) Because $\mathscr{T}$ is not broken there is a term of $\mathcal{O}(N^{-1})$ in this expression. We find for the average conductance

$$\langle G_{\rm NS}/G_0\rangle=\frac{2N\langle\tau_1\rangle_0}{2-\langle\tau_1\rangle_0}+\frac{4\delta\tau_1}{(2-\langle\tau_1\rangle_0)^2}+\frac{4\langle\tau_1\rangle_0^2-4\langle\tau_1\rangle_0^3-4\langle\tau_2\rangle_0+4\langle\tau_1\rangle_0\langle\tau_2\rangle_0}{\langle\tau_1\rangle_0(2-\langle\tau_1\rangle_0)^3}+\mathcal{O}(N^{-1}). \tag{7.10}$$

Case (4), both $\mathscr{T}$ and $\mathscr{D}$ broken. Because u_+ and u_- are independent, there are no diagrams which contribute to order 1. The average conductance is obtained by averaging Eq. (7.3) over the transmission eigenvalues,

$$\langle G_{\rm NS}/G_0\rangle=\frac{2N\langle\tau_1\rangle_0}{2-\langle\tau_1\rangle_0}+\mathcal{O}(N^{-1}). \tag{7.11}$$

From the translation rule of Sec. V one deduces that in the presence of spin-orbit scattering, the leading $\mathcal{O}(N)$ term of the average conductance is unchanged, while the $\mathcal{O}(1)$ correction is multiplied by $-1/2$, in agreement with what was found by Slevin, Pichard and Mello.[47]

The formulas given above apply to any system for which the isotropy assumption holds. We discuss two examples:

(a) A disordered wire (length L, mean free path ℓ, number of transverse modes N), connected to a superconductor. We use the results[50]

$$\langle \tau_1 \rangle_0 = (1+L/\ell)^{-1}, \tag{7.12a}$$

$$\langle \tau_2 \rangle_0 = \tfrac{2}{3}(1+L/\ell)^{-1} + \tfrac{1}{3}(1+L/\ell)^{-4}, \tag{7.12b}$$

$$\delta\tau_1 = -\tfrac{1}{3}(1+\ell/L)^{-3}. \tag{7.12c}$$

We assume $\ell \ll L \ll N\ell$ and neglect terms of order $L/N\ell$ and ℓ/L but retain terms of order 1 and $N\ell^p/L^p (p \geq 1)$. Substitution of Eq. (7.12) into Eqs. (7.8), (7.10), and (7.11) yields

$$\langle G_{\rm NS}/G_0 \rangle = \begin{cases} N(1+L/\ell)^{-1} - 1 + 4/\pi^2 & (\mathscr{D},\mathscr{T}), \\ N(1/2+L/\ell)^{-1} - 1/3 & (\mathscr{D},\ \text{no}\ \mathscr{T}), \\ N(1/2+L/\ell)^{-1} - 2/3 & (\ \text{no}\ \mathscr{D},\mathscr{T}), \\ N(1/2+L/\ell)^{-1} & (\ \text{no}\ \mathscr{D},\ \text{no}\ \mathscr{T}). \end{cases} \tag{7.13}$$

The result in the presence of both $\mathscr{T}$ and $\mathscr{D}$ has been taken from Refs. 51 and 52. In the presence of spin-orbit scattering, the $\mathscr{O}(N)$ term is unchanged, while the $\mathscr{O}(1)$ term is multiplied by $-1/2$.

(b) A chaotic cavity without tunnel barriers in the leads. Lead 1 (with N_1 modes) is connected to a normal metal, lead 2 (with N_2 modes) to a superconductor. An asymmetry between N_1 and N_2 appears because the dimension of u_+ in the polar decomposition (6.27) is $N_2 \times N_2$. The $N_2 \times N_2$ matrix T_+ contains the $\min(N_1,N_2)$ non-zero transmission eigenvalues on the diagonal (remaining diagonal elements being zero). We denote $N_{\rm tot} = N_1 + N_2$ and $N_A = (N_1^2 + 6N_1N_2 + N_2^2)^{1/2}$. The averages $\langle \tau_1 \rangle_0$ and $\langle \tau_2 \rangle_0$ and the correction $\delta\tau_1$ can be computed from the density of transmission eigenvalues [Eqs. (6.35) and (6.38)]. The results are

$$\delta\tau_1 = -N_1N_2N_{\rm tot}^{-2}, \quad \langle \tau_1 \rangle_0 = N_1N_{\rm tot}^{-1}, \quad \langle \tau_2 \rangle_0 = N_1(N_{\rm tot}^2 - N_1N_2)N_{\rm tot}^{-3}. \tag{7.14}$$

Substitution into Eqs. (7.8), (7.10), and (7.11) gives

$$\langle G_{\rm NS}/G_0 \rangle = \begin{cases} N_{\rm tot}(1-N_{\rm tot}/N_A) - 8N_1N_2N_{\rm tot}^2/N_A^4 & (\mathscr{D},\mathscr{T}), \\ 2N_1N_2/(N_{\rm tot}+N_2) - 4N_1N_2N_{\rm tot}/(N_{\rm tot}+N_2)^3 & (\mathscr{D},\ \text{no}\ \mathscr{T}), \\ 2N_1N_2/(N_{\rm tot}+N_2) - 4N_2N_{\rm tot}^2/(N_{\rm tot}+N_2)^3 & (\ \text{no}\ \mathscr{D},\mathscr{T}), \\ 2N_1N_2/(N_{\rm tot}+N_2) & (\ \text{no}\ \mathscr{D},\ \text{no}\ \mathscr{T}). \end{cases} \tag{7.15}$$

The leading order term in Eq. (7.15) has also been obtained by Argaman and Zee.[33] (The case $N_1 = N_2$ was given in Ref. 6).

B. Conductance fluctuations

To compute the variance of the conductance, we average in two steps: $\langle \cdots \rangle = \langle \langle \cdots \rangle_u \rangle_T$, where $\langle \cdots \rangle_u$ and $\langle \cdots \rangle_T$ are, respectively, the average over the unitary matrices u_+ and over the matrices of transmission eigenvalues T_+. It is convenient to add and subtract $\langle \langle G_{\rm NS} \rangle_u^2 \rangle_T$, so that the variance splits up into two parts,

$$\text{var}\, G_{\rm NS} = \langle \langle G_{\rm NS} \rangle_u^2 \rangle_T - \langle \langle G_{\rm NS} \rangle_u \rangle_T^2 + \langle \langle G_{\rm NS}^2 \rangle_u - \langle G_{\rm NS} \rangle_u^2 \rangle_T, \tag{7.16}$$

which we evaluate separately.

The first two terms of Eqs. (7.16) give the variance of $\langle G_{\rm NS} \rangle_u$ over the distribution of transmission eigenvalues. We calculated $\langle G_{\rm NS} \rangle_u$ in Eq. (7.3). Since $\langle G_{\rm NS} \rangle_u$ is a function of the linear statistic τ_{1+} only, we know that its fluctuations are an order $1/N$ smaller than the average. This implies that, to leading order in $1/N$,

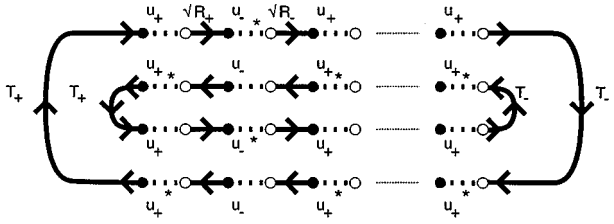

FIG. 21. Diagrammatic representation of $G_{\rm NS}^2$.

$$\langle\langle G_{\rm NS}\rangle_u^2\rangle_T-\langle\langle G_{\rm NS}\rangle_u\rangle_T^2=\sum_{\sigma,\sigma'=\pm}\left\langle\frac{\partial\langle G_{\rm NS}\rangle_u}{\partial\tau_{1\sigma}}\right\rangle_T\left\langle\frac{\partial\langle G_{\rm NS}\rangle_u}{\partial\tau_{1\sigma'}}\right\rangle_T \mathrm{covar}(\tau_{1\sigma},\tau_{1\sigma'})$$
$$=8G_0^2N^2(2-\langle\tau_1\rangle_0)^{-4}\ \mathrm{var}\ \tau_1\times\begin{cases}1 & (\text{without }\mathscr{D}),\\ 2 & (\text{with }\mathscr{D}).\end{cases} \tag{7.17}$$

We now turn to the third and fourth term of Eq. (7.16). These terms involve the variance $\langle G_{\rm NS}^2\rangle_u-\langle G_{\rm NS}\rangle_u^2$ of $G_{\rm NS}$ over $\mathscr{U}(N)$ and subsequently an average over the T_n's. The calculation is similar to that of Sec. VI B. We represent $G_{\rm NS}^2$ by the diagram in Fig. 21. The variance with respect to $u_\pm$ is given by the connected diagrams. We distinguish between two types of connected diagrams: (i) diagrams in which the inner and the outer loop are connected by a T-cycle or by a U-cycle, and (ii) diagrams in which the partition of the U-cycles involves a group which consists of a U-cycle from the inner loop and a U-cycle from the outer loop. The diagrams are similar to those of Fig. 12, and are omitted. The final result is

$$\langle\langle G_{\rm NS}^2\rangle_u-\langle G_{\rm NS}\rangle_u^2\rangle_T=8\,G_0^2(2-\langle\tau_1\rangle_0)^{-6}\langle\tau_1\rangle_0^{-2}(4\langle\tau_1\rangle_0^2-8\langle\tau_1\rangle_0^3+9\langle\tau_1\rangle_0^4-4\langle\tau_1\rangle_0^5+2\langle\tau_1\rangle_0^6$$
$$-4\langle\tau_1\rangle_0\langle\tau_2\rangle_0+2\langle\tau_1\rangle_0^2\langle\tau_2\rangle_0-2\langle\tau_1\rangle_0^3\langle\tau_2\rangle_0-2\langle\tau_1\rangle_0^4\langle\tau_2\rangle_0+6\langle\tau_2\rangle_0^2$$
$$-6\langle\tau_1\rangle_0\langle\tau_2\rangle_0^2+3\langle\tau_1\rangle_0^2\langle\tau_2\rangle_0^2-4\langle\tau_1\rangle_0\langle\tau_3\rangle_0+6\langle\tau_1\rangle^2\langle\tau_3\rangle_0-2\langle\tau_1\rangle_0^3\langle\tau_3\rangle_0)$$
$$\times\begin{cases}2 & (\mathscr{D},\text{ no }\mathscr{T}),\\ 2 & (\mathscr{T},\text{ no }\mathscr{D}),\\ 1 & (\text{ no }\mathscr{D},\text{ no }\mathscr{T}).\end{cases} \tag{7.18}$$

The sum of Eqs. (7.17) and (7.18) equals var $G_{\rm NS}$, according to Eq. (7.16).

In the presence of spin-orbit scattering var $G_{\rm NS}$ is four times as small, according to the translation rule of Sec. V.

We give explicit results for the disordered wire and the chaotic cavity.

(a) For the disordered wire one has[50,53] var $\tau_1=\frac{1}{15}N^{-2}$, $\langle\tau_k\rangle_0=\frac{1}{2}(\ell/L)\Gamma(\frac{1}{2})\Gamma(k)/\Gamma(k+\frac{1}{2}$. Substitution into Eqs. (7.17) and (7.18) yields the variance

$$\mathrm{var}\ G_{\rm NS}/G_0=\begin{cases}16/15-48/\pi^4\approx0.574 & (\mathscr{D},\mathscr{T}),\\ 8/15\approx0.533 & (\mathscr{D},\text{ no }\mathscr{T}),\\ 8/15\approx0.533 & (\mathscr{T},\text{ no }\mathscr{D}),\\ 4/15\approx0.267 & (\text{ no }\mathscr{D},\text{ no }\mathscr{T}).\end{cases} \tag{7.19}$$

The result in the presence of both $\mathscr{T}$ and $\mathscr{D}$ has been taken from Ref. 52 and 54. If both $\mathscr{D}$ and $\mathscr{T}$ are present, breaking $\mathscr{T}$ (or $\mathscr{D}$) reduces the variance by less than 10%.[28,55]

TABLE II. Denominators A_n of the coefficients $V_{c_1,\ldots,c_k}$ for $n=c_1+\ldots+c_k\leqslant 5$.

n	A_n (CUE)	A_n (COE)
1	N	$N+1$
2	$N(N^2-1)$	$N(N+1)(N+3)$
3	$N(N^2-1)(N^2-4)$	$(N-1)N(N+1)(N+3)(N+5)$
4	$N^2(N^2-1)(N^2-4)(N^2-9)$	$(N-2)(N-1)N(N+1)(N+2)(N+3)$ $\times(N+5)(N+7)$
5	$N^2(N^2-1)(N^2-4)(N^2-9)(N^2-16)$	$(N-3)(N-2)(N-1)N(N+1)(N+2)$ $\times(N+3)(N+5)(N+7)(N+9)$

(b) For the chaotic cavity one has var $\tau_1=2N_1^2/\beta N_{\rm tot}^4$ and $\langle\tau_3\rangle_0=N_1(N_{\rm tot}^4-2N_{\rm tot}^2N_1N_2+2N_1^2N_2^2)/N_{\rm tot}^5$ [see Eqs. (6.4) and (6.35)]. In combination with Eq. (7.14) this gives

$$\text{var } G_{\rm NS}/G_0=\begin{cases}128N_1^2N_2^2(N_{\rm tot}^4+2N_1^2N_2^2)(N_{\rm tot}^2+4N_1N_2)^{-4} & (\mathscr{D},\mathscr{T}),\\ 32N_2^2N_{\rm tot}^2(N_{\rm tot}^2-N_1N_2)(N_{\rm tot}+N_2)^{-6} & (\mathscr{D},\text{no }\mathscr{T}),\\ 32N_2^2N_{\rm tot}^2(N_{\rm tot}^2-N_1N_2)(N_{\rm tot}+N_2)^{-6} & (\mathscr{T},\text{no }\mathscr{D}),\\ 16N_2^2N_{\rm tot}^2(N_{\rm tot}^2-N_1N_2)(N_{\rm tot}+N_2)^{-6} & (\text{no }\mathscr{D},\text{no }\mathscr{T}).\end{cases}\tag{7.20}$$

If the coupling between the cavity and the normal metal is weak compared to the coupling to the superconductor ($N_2\gg N_1$), one finds var $G_{\rm NS}(\mathscr{D},\mathscr{T})$/var $G_{\rm NS}(\mathscr{D},\text{no}\,\mathscr{T})=\mathscr{O}(N_1/N_2)^2$. In this case breaking $\mathscr{T}$ greatly enhances the conductance fluctuations. In the opposite case, if the couplings are equal ($N_1=N_2$), one finds var $G_{\rm NS}(\mathscr{D},\mathscr{T})$/var $G_{\rm NS}(\mathscr{D},\text{no}\,\mathscr{T})=2187/2084\approx 1.07$. In this case breaking $\mathscr{T}$ has almost no effect on the conductance fluctuations.

VIII. SUMMARY

We developed a diagrammatic technique for the evaluation of integrals of polynomial functions of unitary matrices over the unitary group $\mathscr{U}(N)$. In the large-N limit the number of relevant diagrams is restricted, which allows for the evaluation of integrals over rational functions. We also considered integrals of unitary symmetric matrices, by means of a slight modification of the diagrammatic rules. A translation rule was given to relate integrals of (self-dual) unitary matrices of quaternions to integrals over (symmetric) unitary matrices of complex numbers.

We discussed two applications: a chaotic cavity (quantum dot) with tunnel barriers in the leads and a normal-metal–superconductor (NS) junction. In both cases, the conductance is a rational function of a unitary matrix. In the large-N limit the average conductance is given by a series of ladder diagrams. The weak-localization correction consists of maximally-crossed diagrams. These two types of diagrams are analogous to the diffuson and cooperon diagrams in the diagrammatic perturbation theory for disordered systems.[22,23] We computed the density of trans-

TABLE III. Denominators B_n of the coefficients $W_{c_1,\ldots,c_k}$ for $n=c_1+\ldots+c_k\leqslant 5$.

n	B_n (CUE)	B_n (COE)
1	N	$N+1$
2	$N^2(N^2-1)$	$N(N+1)^2(N+3)$
3	$N^3(N^2-1)(N^2-4)$	$(N-1)N(N+1)^3(N+3)(N+5)$
4	$N^4(N^2-1)^2(N^2-4)(N^2-9)$	$(N-2)(N-1)N^2(N+1)^4(N+2)$ $\times(N+3)^2(N+5)(N+7)$
5	$N^5(N^2-1)^2(N^2-4)(N^2-9)(N^2-16)$	$(N-3)(N-2)(N-1)N^2(N+1)^5(N+2)$ $\times(N+3)^2(N+5)(N+7)(N+9)$

TABLE IV. Numerators $A_n V_{c_1,\ldots,c_k}$ of the coefficients $V_{c_1,\ldots,c_k}$ for $n=c_1+\ldots+c_k\leqslant 5$. The denominators A_n are given Table II.

$c_1,\ldots,c_k$	$A_n V_{c_1,\ldots,c_k}$ (CUE)	$A_n V_{c_1,\ldots,c_k}$ (COE)
1	1	1
1,1	N	$2+N$
2	-1	-1
1,1,1	$-2+N^2$	$2+5N+N^2$
2,1	$-N$	$-3-N$
3	2	2
1,1,1,1	$6-8N^2+N^4$	$-32-8N+28N^2+11N^3+N^4$
2,1,1	$4N-N^3$	$-4-18N-9N^2-N^3$
2,2	$6+N^2$	$24+7N+N^2$
3,1	$-3+2N^2$	$10+12N+2N^2$
4	$-5N$	$-11-5N$
1,1,1,1,1	$78N-20N^3+N^5$	$128-408N-84N^2+59N^3+16N^4+N^5$
2,1,1,1	$-24+14N^2-N^4$	$92+38N-43N^2-14N^3-N^4$
2,2,1	$-2N+N^3$	$56+43N+12N^2+N^3$
3,1,1	$-18N+2N^3$	$-52+40N+22N^2+2N^3$
3,2	$-24-2N^2$	$-88-18N-2N^2$
4,1	$24-5N^2$	$-7-36N-5N^2$
5	$14N$	$38+14N$

TABLE V. Numerators $B_n W_{c_1,\ldots,c_k}$ of the coefficients $W_{c_1,\ldots,c_k}$ for $n=c_1+\ldots+c_k\leqslant 5$. The denominators B_n are given in Table III.

$c_1,\ldots,c_k$	$B_n W_{c_1,\ldots,c_k}$ (CUE)	$B_n W_{c_1,\ldots,c_k}$ (COE)
1	1	1
1,1	1	2
2	$-N$	$-1-N$
1,1,1	8	32
2,1	$-4N$	$-8-8N$
3	$2N^2$	$2+4N+2N^2$
1,1,1,1	$-216+144N^2$	$-1680+6720N+6096N^2+1152N^3$
2,1,1	$72N-48N^3$	$280-840N-2136N^2-1208N^3-192N^4$
2,2	$-42N^2+18N^4$	$-140-116N+384N^2+592N^3+268N^4+36N^5$
3,1	$-15N^2+15N^4$	$198N+552N^2+540N^3+216N^4+30N^5$
4	$5N^3-5N^5$	$-33N-125N^2-182N^3-126N^4-41N^5-5N^6$
1,1,1,1,1	$-13824+4224N^2$	$-483840+297984N+407040N^2+67584N^3$
2,1,1,1	$3456N-1056N^3$	$60480+23232N-88128N^2-59328N^3-8448N^4$
2,2,1	$-1248N^2+288N^4$	$-12096-21120N+1152N^2+18432N^3+9408N^4+1152N^5$
3,1,1	$-480N^2+240N^4$	$-3024+192N+15072N^2+18432N^3+7536N^4+960N^5$
3,2	$312N^3-72N^5$	$1512+4152N+2496N^2-2448N^3-3480N^4-1320N^5-144N^6$
4,1	$56N^3-56N^5$	$-912N-3376N^2-4768N^3-3168N^4-976N^5-112N^6$
5	$-14N^4+14N^6$	$114N+536N^2+1018N^3+992N^4+518N^5+136N^6+14N^7$

mission eigenvalues, where the leading order term is given by planar diagrams. Resummation of the diagrams leads to a Dyson equation for the Green function, similar to that encountered in the theory of integrals over Hermitian matrices.[12,17]

For the NS junction, the $\mathcal{O}(1)$ correction to the average conductance is non-zero in the presence of a magnetic field, because of a different type of maximally crossed diagrams. These diagrams are suppressed by a sufficiently large voltage to break electron-hole degeneracy. The new type of maximally crossed diagrams explains the coexistence of weak localization with a magnetic field[26] and the insensitivity of the conductance fluctuations to a magnetic field.[28,55]

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APPENDIX: WEIGHT FACTORS FOR POLYNOMIAL INTEGRALS

In Tables II–V we list the weight factors $V_{c_1,\ldots,c_k}$ and $W_{c_1,\ldots,c_k}$ for $n=c_1+\ldots+c_k\leqslant 5$ for the CUE and the COE. (tables of V are also given in Refs. 30, and 31 for the CUE and in Ref. 35 for the COE.) The weight factors are rational functions of the dimension N of the unitary matrix. The denominators A_n and B_n of, respectively, $V_{c_1,\ldots,c_k}$ and $W_{c_1,\ldots,c_k}$ depend only on n. They are tabulated in Tables II and III. The numerators $A_nV_{c_1,\ldots,c_k}$ and $B_nW_{c_1,\ldots,c_k}$ are tabulated in Tables IV and V.

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Statistics of wave functions in mesoscopic systems

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We review the results of a recent study of fluctuations of wave functions in confined chaotic systems. The fluctuations can be due to a random potential or be a consequence of a chaotic scattering by the walls. The entire distribution function of the local amplitudes of the wave functions, f_1, and the joint two-point distribution are calculated in various situations. The computation is performed using the supersymmetry technique and employs the studies of a reduced version of the non-linear supersymmetric σ-model developed especially for investigating the properties of a single eigenstate in a discrete spectrum of a chaotic quantum system. For not very large amplitudes, the complete description can be achieved using the zero-dimensional approximation of the σ-model. The distribution function calculated in the limit of various symmetry classes shows the universal behavior known as the Porter-Thomas statistics, and fluctuations at distant points do not correlate. In the crossover regime between the ensembles, the distribution of local amplitudes shows a somewhat more sophisticated behavior: the fluctuations in this case are correlated over distances exceeding the mean free path. For large amplitudes generated by the states the most affected by the localization (we call them prelocalized), the zero-dimensional approximation is no longer valid. Instead, the statistics of their wave functions is determined by nontrivial vacua of the reduced σ-model which is quite similar to the Liouville model known in conformal field theory. In particular, the vacuum state of the reduced σ-model obeys the Liouville equation, which indicates that in two dimensions the prelocalized states have nearly critical properties: we prove their multifractality and power-law statistically averaged envelope $|\varphi(r)|^2 \propto r^{-2\mu}$ at the intermediate range of distances below the localization length with a spectrum of exponents $\mu<1$, as well as obtain a logarithmically-normal tail of the distribution function f_1. We also find an evidence of prelocalized states in quasi-one-dimensional wires with the length shorter than the localization length: their statistically averaged envelope has power-law asymptotics, $|\varphi(x)|^2 \propto x^{-2}$, and the tail of the distribution function is similar to that describing localized states in the infinite wires. [S0022-2488(96)02110-X]

I. INTRODUCTION

The recent progress in semiconductor technology has given an access to the experimental studies of the physics of nanoscale electronic systems. This, in its turn, has generated a number of theoretical problems which did not previously call close enough attention, such as the problem of statistical properties of a single quantum state in a confined chaotic quantum system. Being studied at low temperatures, the small electronic devices are the objects in which the electron motion is coherent and the quantum nature of carriers evidences in many experimental data.[1,2] During the previous decade, the quantum effects in transport have been mainly explored in the

systems where they give small—but nevertheless observable—features in addition to the conductance (inverse resistance) values expected on the basis of a purely classical mechanics analysis. Weak localization effects[3] and mesoscopic conductance fluctuations[1,4,5] are the best known and, maybe, the most spectacular examples of them which can be understood and successfully described on the basis of a semiclassical analysis of quantum mechanics.[4,6,7]

In more recent studies[8] of smaller structures put into a weak (tunneling) contact to the bulk electrodes and cooled down to the temperatures of the order of tens of mK, the resonant tunneling regime of the transport through a single discrete level in a quantum dot has been achieved. Since the value of the resonance tunneling conductance is determined by the amplitudes of the resonance state wave functions in the vicinity of contact, fluctuations and spatial structure of the single-particle eigenstates in a dot become important observables, especially regarding a rich experimental information which is already available in the literature.[9,10]

In small semiconductor structures the capacitance of the dot (filled by a large number of electrons, $N \gg 1$) is so small that the dot charging energy becomes larger than other relevant energy scales in the system. Therefore, if the resistance of contacts of a dot to the external world are much higher than the resistance quantum, h/e^2, the system occurs in the Coulomb blockade regime and the transport through the dot is only possible when a single electron added to the dot does not change its total energy: $E_{N+1}=E_N$, where N is the number of excess electrons. In the semiconductor structures, the condition of such resonance can be controlled by an external gate voltage U_g applied to the dot. Experimentally, this produces a set of conductance peaks at voltages $U_g(N)\approx(N+1/2)e/C$ at which the destruction of the Coulomb blockade makes the transport possible.

Therefore, an important quantity that has become a subject of statistical analysis is the height of the Coulomb blockade peaks. Although the positions of these peaks are periodic, their strengths are quite different depending on current-carrying abilities of those states in the dot that should be filled by the tunneling electrons. Assuming that the level width and the temperature are smaller than the mean-level spacing Δ one may consider only a single single-particle level contribution to each resonance.[11,12] This means that one can use a Breit-Wigner type formula to describe the resonance conductance. Taking into account temperature smearing of the Fermi distribution and assuming that temperature T much exceeds the typical level width γ,[13] one can write the resonance conductance in the form[14,15]

$$g=\frac{e^2}{h}\,\frac{1}{4\pi T}\,\frac{\gamma_L\gamma_R}{\gamma_L+\gamma_R}. \tag{1}$$

In Eq. (1), the level widths $\gamma_{L,R}=A_{L,R}|\varphi_\alpha(\mathbf{r}_{L,R})|^2$ are determined by the wave function amplitudes $|\varphi_\alpha(\mathbf{r}_{L,R})|$ of the resonant state at the coordinates $\mathbf{r}_{L,R}$ of tunnel links to the current leads. The coefficients $A_{L,R}$ depend only on the properties of contacts and, together with temperature T determine the typical conductance values in a specific device, whereas statistics of the heights of conductance peaks are completely controlled by statistics of amplitudes of the electron waves of the confined system near the contact.

At present, it is quite clear that the character of the fluctuations in the conductance peaks series depends on whether the corresponding classical motion of a carrier in quantum dot is chaotic or regular. In the latter case calculation of the wave functions should follow a straightforward procedure, whereas a description of the wave functions in the regime of chaotic dynamics demands considerable effort. By studying experimentally the conductance fluctuations for ''chaotic'' dots, one can check theoretical results for statistics of the amplitudes of the chaotic electron

waves in mesoscopic dots—at least, would a single-particle description work being applied to the system of interacting electrons.

Besides the measurements on the quantum dots, a series of experiments on a completely different object is worth mentioning. These are the experiments on microwave scattering in metallic cavities in which the local amplitudes of electromagnetic waves were measured and their statistics were analyzed.[16,17] Being confined to a thin slab, the electromagnetic waves are strongly polarized and obey the same equation as the Schrödinger equation for the electron. One can make either ballistic cavities where the electromagnetic waves are scattered by the walls or add into the cavity small pieces of a good metal which models impurities. Changing an impurity configuration or sweeping the frequency and passing from one resonance to another, one can collect statistics of the eigenmodes intensities at some fixed point of a sample. In some sense, the microwave cavities represent convenient toy systems for modelling various regimes of quantum chaos, since they have a much higher degree of freedom in changing the parameters (as compared to the experiments on the electronic devices), e.g., the level of disorder, they operate with much better statististics and deliver the direct information about the density distributions of the chaotic electromagnetic waves. At the same time, the single-particle description is completely adequate in this case.

Both types of experiments mentioned above (which can be classified as mesoscopic) provide a good reason for studying in great detail fluctuations of wave functions in chaotic or disordered confined systems. At this point we have to note that the simplest way to produce chaos in a quantum or classical billiard is to fill it with impurities, so that one would expect that all the generic features of quantum chaos may be understood by studying the disordered conductors. Although this expectation is partly true, the physics of disordered systems is even more rich than that. The structure and statistics of eigenstates in the systems where chaos is generated by a large number of impurities is strongly affected by the localization effects, especially in low-dimensional systems. From this point of view, the issue which we intend to answer below is what are the properties of wave functions in disordered systems where localization is expected at long distances that they show being confined by external boundaries below the localization length scale. In the cases when the mean free path is determined mainly by scattering by walls, the localization effects can be ignored, it is reasonable to speak of ''ballistic chaos.''

II. CHOICE OF THE MODEL

Below wave functions of models with disorder will be studied. In all cases consideration is restricted to systems of non-interacting particles in a finite volume. The assumption that the particles do not interact means that, in fact, a one-particle problem is considered. The assumption is very well justified if we consider electromagnetic or sound waves in a box. At the same time, the validity of it is less clear for electrons in a quantum dot where both electron-electron and electron-phonon interactions can be quite important. Nevertheless, at low temperatures the inelastic mean free path can be large and very often the one-particle approximation serves as a good description of interesting physical problems.

To simplify the discussion we will speak about electrons in a box and study solutions of the Schrödinger equation although most of the results obtained below are also applicable to electromagnetic and sound waves.

So, we start with the Schrödinger equation for an electron moving in a limited volume V in the presence of an external potential $U_{dis}(\mathbf{r})$. The potential $U_{dis}(\mathbf{r})$ describes an interaction with impurities. In principle, an external magnetic field H can be applied and the potential $U_{dis}(\mathbf{r})$ can include magnetic and spin-orbit interactions. In the presence of the magnetic and spin-orbit impurities one should take into account electron spin and write two-component wave functions. To avoid complicated formulae, from the beginning we consider first a system without spin interactions. Then, the Schrödinger equation can be written in the form

$$\hat{H}\varphi_\alpha(\mathbf{r})=\epsilon_\alpha\varphi_\alpha(\mathbf{r}), \quad \hat{H}=\hat{H}_0+U_{dis}(\mathbf{r}), \tag{2}$$

where ϵ_α are the eigenenergies of the spectral problem in the dot, Eq. (2), measured off the energy ϵ fixed by an external observer (e.g., the Fermi energy in the bulk electrodes attached to the quantum dot to make an electric measurement); $\varphi_\alpha(\mathbf{r})$ are the corresponding eigenfunctions, and

$$\hat{H}_0 = E_K\left(-i\hbar\nabla - \frac{e}{c}\mathbf{A}\right) - \epsilon, \tag{3}$$

with $E_K(\mathbf{p})$ being the energy of free motion and $\mathbf{A}$ being the vector potential corresponding to the magnetic field $\mathbf{H}=\mathrm{rot}\mathbf{A}$; for the sake of convenience, we use such a gauge that $\mathrm{div}\mathbf{A}=0$ and $\mathbf{An}=0$ at the surface (edge) of the sample. We also assume that fluctuations of U_{dis} are Gaussian and satisfy the following relations:

$$\langle U_{dis}(\mathbf{r})\rangle = 0, \quad \langle U_{dis}(\mathbf{r})U_{dis}(\mathbf{r}')\rangle = \frac{1}{2\pi\nu\tau}\delta(\mathbf{r}-\mathbf{r}'), \tag{4}$$

where τ is the mean free path time and ν is the density of states at the energy ϵ, which are usual notations of condensed matter physics. The angular brackets stand for the averaging procedure.

In principle, the eigenstates problem Eq. (2) should be complemented by the boundary conditions for the wave functions. The fact that the electron is confined in a finite region means that it is located in a quantum well. For our consideration the explicit form of the confining potential is not important. This can be a hard wall model and then the wave functions turn to zero at the boundary or it can be a more general potential resulting in a fast decay of the wave functions at infinity. For calculations presented below it is only important that the spectrum of the eigenenergies is discrete.

The description of quantum chaos by modelling it using the electron motion in a confined disordered system seems to be, in principle, very attractive because of a number of powerful techniques developed during the past two decades in the theory of metals.[1,3] Nevertheless, it remains a non-trivial theoretical problem. This is because the most standard calculational tool—the diagrammatic perturbation theory— fails to work when it is applied to the description of properties of a single discrete quantum level. The perturbation theory calculation consists of the summation of certain classes of diagrams corresponding to terms of an expansion in the impurity concentration. By now, it is well known that the quantum interference is properly described in terms of so called ''cooperons'' and ''diffusons'' which appear as a result of the summation of certain ladder diagrams. To use the perturbation theory, one should start with a ''good metal'' and to assume that the length of the mean free path l is much longer than the electron wavelength λ. But this is only one necessary condition. The reason for a limited power of the perturbation theory with respect to disorder lies in the equivalence of the constraints made for its applicability and those of the semiclassical approximation.[7,18] The semiclassics, in its turn, is able to describe only wave packets composed of a large number of quantum levels, which require any kind of a discrete level broadening γ to be larger than the mean level spacing Δ in the confined quantum dot. The origin of the broadening may be different. It can result from a strong coupling of the dot to external leads, so that the broadening γ is caused by the fast decay of the state due to the particle escape to the bulk electrodes, or this may be a ''homogeneous'' inelastic broadening of the level due to any other relaxation process. That is why the perturbation theory analysis gives reliable results in systems where the contacts of a dot to massive reservoirs have conductances g_c that can be relatively small, as compared to the ''intrinsic'' conductance of the dot, but should be larger than the conductance quantum e^2/h.[19–22] At the same time, the perturbation theory is not an adequate tool to study the properties of a single level in a dot where conductances of contacts are much less than the conductance quantum and where the inelastic broadening γ is much smaller than the mean level spacing.

Another approach to the quantum chaos in disordered conductors is based on the Gorkov and Eliashberg idea[23] to replace the randomness of an impurity configuration in a small piece of metal

by a randomness of a matrix Hamiltonian that describes the specral single-particle problem in it. This enables one to reformulate the issue of statistics of spectra and wave functions in a disordered system in terms of random matrix theory (RMT) the apparatus of which has been developed in many details in nuclear physics.[24,25]

The random matrix theory proved to be a very convenient method and has brought to light some important features of the statistics of conductance fluctuations in chaotic billiards.[14] In particular, depending on the presence or absence of the time reversal invariance in the systems (i.e., of a magnetic field), the eigenstates of the RMT Hamiltonian can be described as either real or complex vectors and have a purely Gaussian distribution of the amplitudes of their projections onto some arbitrarily chosen direction in the basis (Porter-Thomas distribution in the RMT), which is equivalent to the universal distribution of local densities of single-particle wave functions in the ergodic regime of a chaos. The intensive numerical studies of a large number of high-lying eigenstates of confined systems, such as ''quantum billiards'',[26,27] have confirmed the Gaussian distribution of local wave functions amplitudes,[27] and this has been observed directly in the microwave experiments.[16]

On the other hand, although the random matrix theory enables one to catch some part of the physics of quantum chaotic systems, it remains to be a phenomological method which has to be modified each time when broader classes of chaotic systems are involved. The use of the RMT[28] in the studies of the eigenstates problem becomes rather complicated when the crossover regime between different universality classes is studied[29] and is helpless when spatial correlations of the wave functions are called in question.

Another phenomenological approach related to the RMT which also confirms the Gaussian distribution of the wave functions amplitudes has been proposed by Berry. It is based on the assumption that the local structure of the eigenstates can be represented as a superposition of an infinite number of plane waves with random phases and equal wave number.[30] Originally, the applicability of such a conjecture has been justified by classical ergodicity of chaotic systems. For ergodic systems one can assume that relevant classical orbits are the typical ones that pass close to all points on the energy surface corresponding to the energy ϵ of the state with the wave function φ and, in the semiclassical approximation, this leads to random phases. Using this approach, one can describe spatial correlations of the amplitudes of the wave functions of a chaotic billiard[31] which show behavior similar to that of the Friedel oscillations.[32]

However, both the advantage and the disadvantage of this phenomenology are related to the statistical equivalence of eigenstates which is built into the construction of the random matrix substituting the real dynamics, or stands behind Berry's conjecture. This reveals the set of universal features of chaos in the limits where they do exist but hides peculiarities of physically different systems in the cases when universality is broken. In particular, the phenomenolgy can be helpful in the limiting cases of the orthogonal and unitary ensembles corresponding to time reversal invariant systems or to systems where this invariance is completely broken, but not in the crossover regime (quantum billiard in a weak magnetic field). Moreover, they cannot be used in situations where localization effects due to a real disorder become important and the statistical equivalence of the eigenstates is no longer valid.

As a result of the disadvantages of the phenomenological approaches, a derivation of statistics of amplitudes of the wave functions directly from a well defined model without using additional hypotheses (i.e., from the first principles) is desirable, and this requires development of other analytical methods. Fortunately, this goal can be achieved by a modification of the supersymmetry technique originally proposed by one of the present authors (see, e.g., Refs. 33 and 34) for studying the Anderson localization. Within this method, calculation of different physical quantities characterizing, e.g., localization or mesoscopic fluctuations is reduced to the study of a non-linear supermatrix σ-model. At present, this method is well developed and has been used for solving a broad spectrum of quite different problems.[34,35] Models with disorder were the first ones studied by the supersymmetry technique. The zero-dimensional (0D) version of the model corresponds to

the Wigner-Dyson random matrix theory, and, in the simplest cases recovers the RMT results (see Section V). Later on, other versions of the σ-model have been derived from the RMT,[36] from models of random band and sparse matrices[37] and from some models of a ''ballistic chaos''.[38,39]

Below, we demonstrate how the supersymmetry technique can be applied to the problem of the statistics of wave functions in disordered and chaotic confined two-dimensional (2D) and quasi-one-dimensional (Q1D) systems. In this article, we give a complete account of the results[15,40–46] obtained for the disordered models. Most of the methodical part of it (see Sections VI and VII) is devoted to the derivation of a reduced σ-model[41,44] that is adapted for describing the properties of a single eigenstate in the discrete spectrum of a confined chaotic system. The formal derivation we do here is restricted to the usual potential disorder in Eq. (4), but the analysis can also be extended to a broader variety of systems, for example, to the models involving a random gauge or magnetic field.[47] Skipping the details, these models give the same as the analysis of the unitary ensemble, both on the level of perturbation theory analysis[48] and using the nonlinear σ-model approach.[47] Most of the results presented below for the distribution functions of the wave functions have been obtained by the supersymmetry technique and, by now, we know no other way to reproduce them.

III. DEFINITIONS OF THE EIGENSTATES STATISTICS

The most complete information about statistical and correlation properties of the wave functions is implicit to the N-point *joint distribution functions* $f_N(p_1,\ldots,p_N)$ defined as

$$f_N(p_1,\ldots,p_N;\mathbf{r}_1,\ldots,\mathbf{r}_N)=\Delta\left\langle \sum_{\alpha}\ \delta(\epsilon-\epsilon_\alpha)\prod_{n=1}^{N}\ \delta(p_n-|\varphi_\alpha(\mathbf{r}_n)|^2)\right\rangle_{dis}. \tag{5}$$

In Eq. (5) $\Delta=(\nu V)^{-1}$ is the mean level spacing which is finite in a confined system, and $\langle\ldots\rangle_{dis}$ stands for averaging over the random potential configurations. In this definition, we do not take into account spin degrees of freedom. One can find some details on the definition of statistics of a local spin desntity of eigenstates in Ref. 45.

The function $f_N(p_1,\ldots,p_N)$ measures the probability of given amplitudes of the wave function corresponding to the energy ϵ at N different coordinates $\mathbf{r}_n$. When speaking about the problem of a distribution of irradiation in a chaotic cavity, this function describes a probability to detect a given configuration of local electromagnetic field intensities in any resonance. In principle, using the supersymmetry technique one can try to compute the function $f_N(p_1,\ldots,p_N)$ for arbitrary N, but we restrict the analysis below to the functions f_1 and f_2 that are of special importance for physical applications. For example, the conductance g, Eq. (2), and its distribution function can be directly related to f_2, whereas $f_1(p)$ has been directly measured in the microwave experiments.[16] In addition, since f_1 and f_2 can be related as follows:

$$f_1(p,\mathbf{r}_1)=\int_{-\infty}^{\infty} f_2(p,p';\mathbf{r}_1,\mathbf{r}')dp', \tag{6}$$

it would be enough to calculate f_2 alone. Nevertheless, in some cases, it is much easier to analyze f_1, so that below we shall deal with both of them. Knowledge of the distribution function f_1 makes it possible to calculate its moments, the so-called inverse participation numbers (IPN),

$$P_m=\left\langle \sum_{\alpha}\ |\varphi_\alpha(\mathbf{r}_1)|^{2m}\delta(\epsilon-\epsilon_\alpha)\right\rangle_{dis}\equiv\int_0^{\infty} p^m f_1(p,\mathbf{r}_1)dp. \tag{7}$$

A similar definition can be used for introducing the correlation functions

$$K_{nm}(r)=\int_0^\infty dp_1 dp_2 p_1^n p_2^m f_2(p_1,p_2;|\mathbf{r}_1-\mathbf{r}_2|=r)-P_m P_n;$$
$$R(p,r)=\int_0^\infty dp' p' f_2(p,p';|\mathbf{r}_1-\mathbf{r}_2|=r), \tag{8}$$

describing spatial correlations of the wave functions $\varphi_\alpha(\mathbf{r})$. Because of the normalization of wave functions in confined systems, one obtains $P_1\equiv V^{-1}$, and in many cases the correlator K_{22} is the simplest non-trivial one.

To apply the supersymmetry technique to the calculation of physical quantities, one has to express these quantities in terms of retarded G_ϵ^R and advanced G_ϵ^A Green functions. These functions are solutions of equations

$$\left[\hat{H}\pm i\frac{\gamma}{2}\right]G_\epsilon^{R,A}(\mathbf{r},\mathbf{r}')=\delta(\mathbf{r}-\mathbf{r}'). \tag{9}$$

Each of the functions $G_\epsilon^{R,A}(\mathbf{r},\mathbf{r}')$ are analytical in the upper (lower) half plane of complex ϵ, which is controlled by the presence of a finite width of each level γ. The *broadening* γ is introduced here artificially and is assumed to be the same for all quantum levels ϵ_α. The parameter γ allows us to relate the properties of a single quantum state to the Green functions $G^{R,A}$. Indeed, the latter can be represented as

$$G_\epsilon^{R,A}(\mathbf{r},\mathbf{r}')=\sum_\alpha \frac{\varphi_\alpha(\mathbf{r})\varphi_\alpha^*(\mathbf{r}')}{\epsilon-\epsilon_\alpha\pm i\gamma/2}, \tag{10}$$

so that the procedure of taking the *elastic quantum limit* $\gamma\to 0$ becomes a way to pick up a contribution to any expression containing some number of Green functions $G_\epsilon^{R,A}$ taken at the same energy ϵ from a single quantum level in order to study statistical and correlation properties of an individual eigenstate.

The algebraic exercise which shows how one can do this consists in the proof of the following equality:

$$\lim_{\gamma\to 0,\beta\to 1}\int_0^1 dt\frac{d}{d\beta}\left[\beta\frac{(i\gamma\beta t)^m}{(x+i\gamma/2)^m}\frac{(-i\gamma\beta(1-t))^n}{(x-i\gamma/2)^n}\frac{\gamma}{x^2+(\gamma/2)^2}\right]=2\pi\delta(x). \tag{11}$$

To prove Eq. (11), we integrate, first, over t which gives

$$\int_0^1 t^m(1-t)^n dt=\frac{m!n!}{(m+n+1)!}, \tag{12}$$

and then over x, using the formula

$$\gamma^{m+n+1}i^{m-n}\int_{-\infty}^\infty \frac{dx}{(x+i\gamma/2)^{m+1}(x-i\gamma/2)^{n+1}}=2\pi\frac{(m+n)!}{m!n!}. \tag{13}$$

Therefore, recalling the definition of the Green functions $G_\epsilon^{R,A}(\mathbf{r},\mathbf{r}')$, Eq. (10), one can rewrite the distribution function f_2 in the form

$$f_2(p_1,p_2;\mathbf{r}_1,\mathbf{r}_2)=\frac{\Delta}{\pi}\lim_{\gamma\to 0,\beta\to 1}\frac{d}{d\beta}\Big\langle \beta\int_0^1 dt\int d\mathbf{r}\,\mathrm{Im}[G^A_\epsilon(\mathbf{r},\mathbf{r})]$$
$$\times\delta(p_1+iY_AG^A_\epsilon(\mathbf{r}_1,\mathbf{r}_1))\,\delta(p_2-iY_RG^R_\epsilon(\mathbf{r}_2,\mathbf{r}_2))\Big\rangle_{dis}, \tag{14}$$

where $Y_A=\gamma\beta Vt$ and $Y_R=\gamma\beta V(1-t)$.

IV. STATISTICS OF WAVE FUNCTIONS AND NON-LINEAR SUPERMATRIX σ-MODEL

The goal of the manipulations with the distribution functions in the preceding section was to represent these quantities in a form suitable for application of the supersymmetry technique. Following the scheme of calculations developed in Refs. 33 and 34, one should express the function f_N, Eq. (14), in terms of an integral over supervectors ψ containing both commuting s and anticommuting χ elements. To rewrite Eq. (14) in such a form, we expand the δ-functions as a series in the Green functions $G^{R,A}$ and use the representation of the latter in terms of supersymmetric functional integrals. To do this, one can use a 4-component supervector for each of retarded and advanced Green functions, so that the minimal size of the superspace in the theory is 8, Refs. 33 and 34:

$$\psi=\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix},\quad \psi_m=\begin{pmatrix}\lambda_m\\ S_m\end{pmatrix},\quad \lambda_m=\frac{1}{\sqrt{2}}\begin{pmatrix}\chi^*_m\\ \chi_m\end{pmatrix},\quad S_m=\frac{1}{\sqrt{2}}\begin{pmatrix}s^*_m\\ s_m\end{pmatrix},$$
$$\overline{\psi}=(\overline{\psi_1},-\overline{\psi_2}),\quad \overline{\lambda_m}=\frac{1}{\sqrt{2}}(\chi_m,\chi^*_m),\quad \overline{S_m}=\frac{1}{\sqrt{2}}(s_m,s^*_m),\quad m=1,2. \tag{15}$$

In Eq. (15), the superscripts 1 and 2 relate to the advanced and retarded Green functions, respectively. The components χ and χ^* are anticommuting Grassmann variables whereas s and s^* are conventional complex numbers conjugate with respect to each other.

In principle, to obtain a proper expression for a product of a large number of Green functions related to different energies, one would have to increase the size of the superspace, which would make any further computation extremely difficult. Fortunately, the distribution functions f_N which describe the properties of a single quantum level are all expressed in terms of $G^{R,A}_\epsilon$ taken at exactly the same energy. This enables us to operate in the superspace ψ in Eq. (15) without increasing its dimensions. Within the supersymmetry technique, one uses the Lagrangian L in the form

$$L[\psi]=-\int d\mathbf{r}\,\overline{\psi}(\mathbf{r})\left[\hat{H}_0+U(\mathbf{r})+\frac{i\gamma}{2}\Lambda\right]\psi(\mathbf{r}), \tag{16}$$

where 8×8 supermatrix Λ is

$$\Lambda=\begin{pmatrix}\mathbf{1}_4 & 0\\ 0 & -\mathbf{1}_4\end{pmatrix},\quad \mathbf{1}_4=\mathrm{diag}(1,1,1,1), \tag{17}$$

and represents any product of Green functions which would appear in a formal series expansion of Eq. (14),

$$B_{mn}=\langle G^A_\epsilon(\mathbf{r},\mathbf{r})[G^A_\epsilon(\mathbf{r}_1,\mathbf{r}_1)]^m[G^R_\epsilon(\mathbf{r}_2,\mathbf{r}_2)]^n\rangle_{dis} \tag{18}$$

as

$$m!n!i^{n-m-1}B_{mn}=\left\langle \int \chi_1(\mathbf{r})\chi_1^*(\mathbf{r})|s_1(\mathbf{r}_1)|^{2n}|s_2(\mathbf{r}_2)|^{2m}e^{-iL[\psi]}\mathrm{D}\psi\right\rangle_{dis}, \tag{19}$$

Due to the absence of a weight denominator, the averaging in Eq. (19) can be immediately performed and it leads to the appearance of an effective ''interaction'' $(\psi\psi)^2$ in the Lagrangian. Then, one decouples the interaction using Gaussian integration over 8×8 supermatrices Q with indices $Q^{ij}_{\alpha\beta}$ slowly varying in space. In accordance to the notations of the projections in the supervector space, we distinguish the pair of upper indices $i(j)=1,2$ which indicate from which Green function (advanced or retarded) the corresponding matrix element of Q was originated, and down indices $\alpha,\beta=1.4$ which distinguish between commuting (3,4) and anticommuting (1,2) components of $\psi_{1,2}$. After this, we integrate over ψ with the quadratic (after decoupling) effective Lagrangian

$$L_{\mathrm{eff}}[\psi,Q]=-\int\left[\overline{\psi}(\mathbf{r})\left(\hat{H}_0+\frac{i\gamma}{2}\Lambda+\frac{i}{2\tau}Q\right)\psi(\mathbf{r})\right]d\mathbf{r}. \tag{20}$$

As usual, one can perform the Gaussian integration using the Wick theorem. In principle, not only pairing of the type $\langle\psi_\alpha(\mathbf{r}_n)\underline{\psi}_\alpha(\mathbf{r}_n)\rangle$, such that both ψ's are taken at the same point is possible, but also pairings like $\langle\psi_\alpha(\mathbf{r}_n)\psi_\alpha(\mathbf{r}_m)\rangle$, $n\neq m$, should be taken into account. The latter pairing determines spatial dependence of the correlations of the wave functions. They decay already at distances of the order of wave length and are even exponentially suppressed at distances longer than the mean free path l. As soon as one studies correlations at distances $|\mathbf{r}_1-\mathbf{r}_2|>l$ only the pairings at coinciding points need to be considered and now let us restrict ourselves to this case. Of course, this limits the applicability of this theory to the effects determined by the long-range behavior of the diffusive waves and washes out all features of an electron motion at the short range scale where the specific character of a random potential starts playing an important role. To anticipate a little, the approach we use below enables us to work with zero-dimensional, 2D and quasi-1D systems where the long enough diffusive electron trajectories dominate in forming the structure of quantum states and in localization effects, whereas we cannot use it for studying the localization in three-dimensional (3D) systems.

After these remarks, the Gaussian integration over ψ in Eq. (19) with the Lagrangian L_{eff}, Eq. (20) can be easily performed, and, after collecting all terms B_{nm}, one reduces the function f_2 to the form

$$f_2(p_1,p_2,;|\mathbf{r}_1-\mathbf{r}_2|\gg l)=\lim_{\gamma\to 0,\beta\to 1}\frac{d}{d\beta}\left\langle\frac{\beta}{2V}\int\frac{d\zeta_1 d\zeta_2}{(2\pi)^2}\int_0^1 dt\int d\mathbf{r}(Q^{11}_{11}(\mathbf{r})-Q^{22}_{11}(\mathbf{r}))\right.$$
$$\left.\times\delta\left(p_1-\frac{t\gamma\beta}{2V\Delta}\overline{z_1}Q(\mathbf{r}_1)z_1\right)\delta\left(p_2+\frac{(1-t)\gamma\beta}{2V\Delta}\overline{z_2}Q(\mathbf{r}_2)z_2\right)\right\rangle_Q, \tag{21}$$

where $\langle\cdots\rangle_Q$ stands for the integration[33] over the supermatrices Q with the free energy functional $F[Q]$,

$$F[Q]=\frac{\pi\nu}{8}\mathrm{Str}\int\left[D\left(\nabla Q-\frac{ie}{c\hbar}\mathbf{A}[Q,\tau_3]\right)^2-\gamma\Lambda Q\right]d\mathbf{r},\langle\cdots\rangle_Q=\int DQ\cdots e^{-F[Q]}. \tag{22}$$

Str is supertrace and D is the classical diffusion coefficients. The supermatrix Q obeys the constraint $Q^2=1$ and can be represented in the form

$$Q=U\Lambda\overline{U}, \tag{23}$$

where U is a transformation generating the degeneracy space of graded symmetry group.[49] This field-theoretical model is essentially non-linear, since the matrix U satisfies the condition $\overline{U}U=1$, where an overbar indicates the operation of conjugation defined in Ref. 33 as

$$\overline{U}=CU^TC^T; \quad C=\begin{pmatrix} C_0 & 0 \\ 0 & -C_0 \end{pmatrix}; \quad C_0=\begin{pmatrix} -i\tau_2 & 0 \\ 0 & \tau_1 \end{pmatrix}, \tag{24}$$

where τ_α are the ordinary Pauli matrices and T means the transposition operation.

The transformation U can be imagined as a pseudo-unitary ''rotation'',

$$U=\begin{pmatrix} u_1 & 0 \\ 0 & v \end{pmatrix}\exp\begin{pmatrix} 0 & -iu_2\dfrac{\hat{\theta}}{2} \\ -i\dfrac{\hat{\theta}}{2}\overline{u_2} & 0 \end{pmatrix}, \tag{25}$$

and can be parametrized with an equal number of commuting and anticommuting variables. The second matrix in the product in Eq. (25) is composed only of commuting variables with u_2 an ordinary unitary matrix. All anticommuting variables are collected into matrices u_1 and v_1. The vectors $z_{1,2}$ and $\overline{z_{1,2}}$ have the form determined by

$$\overline{z_1}=(0,0,e^{i\zeta_1},e^{-i\zeta_1},0,0,0,0), \quad \overline{z_2}=(0,0,0,0,0,0,e^{i\zeta_2},e^{-i\zeta_2}). \tag{26}$$

Equations (21–25) completely reduce the problem of computation of the distribution function f_N to functional integration over supermatrices Q within the non-linear σ-model.

The reduction of quantum mechanics of a particle in a disorder medium to the non-linear σ-model has several approximations implicit in the above derivation. First of all, by introducing smoothly varying fields Q, we make a separation between ''fast'' and ''slow'' variables, where the ''fast'' variables have sense only if the particle motion can be everywhere considered as a semiclassical one, that is, the action it takes should be large and real. This excludes from the theory below the effects related to the tunneling through potential barriers—the rare configuration of a random potential which are, nevertheless, possible within the Gaussian model of disorder (but not allowed in the case of the box distribution, for example). At the same time, the procedure[33] which leads to the conjecture $Q^2=1$ and the following gradient expansion we use in determining the effective free energy functional prevents us from discussing features of the wave functions at the length scales shorter than l, and what we are able to describe within the σ-model approach is the structure of quantum states smeared over the volume of a ''Hikami-box'' which is (for the models with short-range scatterers) $\sim\lambda^{d-1}l$. As a result, the localization effects in 3D systems which are dominated by the short-range dynamics of a particle[60] cannot be treated consistently by the σ-model approach we use: they would be systematically underestimated. In 2D and quasi-1D systems, the long-range diffusive trajectories of a particle are important, so that the σ-model approach works, but we cannot speak about densities p higher than $(\lambda^{d-1}l)^{-1}$, and we also cannot anticipate the form of specific configurations of a random potential responsible for forming prelocalized states. We make the latter remark since at short distance (in small volumes) it is possible to imagine rare configurations of scatterers (whose probability to be found strongly depends on the model of disorder) which would appear more efficient being studied beyond the Born approximation.

The same should be repeated concerning the analysis of a somewhat more simple function f_1 which can be expressed in terms of an integral over the supermatrices Q in a similar way starting from Eq. (5):

$$f_1(p,\mathbf{r}_1)=\frac{1}{4V}\int\frac{d\zeta_1 d\zeta_2}{(2\pi)^2}\lim_{\gamma\to 0}\left\langle\int d\mathbf{r}(\overline{z_1}(Q(\mathbf{r})-\Lambda)z_1)\right.$$

$$\left.\times\delta\left(p-\frac{\gamma}{2V\Delta}\overline{z_2}Q(\mathbf{r}_1)z_2\right)\right\rangle_Q. \tag{27}$$

Computation of this function is easier to follow, so that we start the next section from the analysis of this function and study a situation where the σ-model results can be easily compared to those of the RMT.[24]

V. UNIVERSAL EIGENSTATE STATISTICS AND 0D σ-MODEL FOR SYSTEMS WITH BROKEN TIME-REVERSAL SYMMETRY

Disordered systems with the broken time-reversal symmetry represent the simplest ones where the supersymmetric σ-model can be applied and where the results obtained by using this method can be compared with the predictions of the phenomenological approaches. The RMT predicts that the function f_1 describes the Gaussian distribution of wave function amplitudes which, in the case of a broken time-reversal symmetry (unitary ensemble) corresponds to

$$f_1(p;\mathbf{r})=V\exp\{-Vp\}\quad\text{and}\quad P_n=n!V^{-n}. \tag{28}$$

Such a distribution has universal form in the sense that it contains no information about any dynamical parameter such as a mean free path, shape of a cavity or position of the observation point inside it, but only manifests the fact that the density of all eigenstates in the system is normalized by its volume (or area in 2D).

The goal of the analysis presented in this section is to reproduce the result of Eq. (28) using the σ-model calculations. In other words, we have to find an approximation of the complete field theory which would give us the universal statistics. From the explicit form of the free energy functional $F[Q]$ in Eq. (22), it is clear that the only way to omit such a dynamical parameter as the diffusion coefficient D would be to consider the so called zero-dimensional (0D) version of a model, that is, to assume that the only relevant degree of freedom of the field $Q(\mathbf{r})$ is its zero space harmonics $Q(\mathbf{r})=\text{const}=Q_0\equiv Q(\mathbf{r}_1)$.

Physically, the 0D approximation described above neglects any localization effect, which indicates that each wave function is sensitive to boundaries of the sample. The 0D approximation bridges the σ-model to the RMT and, at the same time, drastically simplifies calculations since the functional integration in it is replaced by a definite integral over superspace with a simplified free energy,

$$\langle\ldots\rangle_Q=\int dQ_0 e^{-F_{0D}},\quad F_{0D}[Q]=-\frac{\pi\gamma}{8\Delta}\text{Str}(\Lambda Q). \tag{29}$$

The choice of the unitary ensemble is also motivated by its simplicity. In a strong magnetic field, so called ''cooperon'' degrees of freedom are ''frozen'', and only the part of the supermatrix Q commuting with matrix τ_3 (see the notations in Refs. 33 and 34) gives a contribution. That is why, in the unitary case, the number of independent components of the supermatrix Q is two times smaller than, e.g., in the orthogonal case when the time-reversal symmetry is not broken. The parametrization of the superspace can be made using the invariant representation of Eq. (25), $Q=U_d\Lambda\overline{U_d}$, with group transformations U_d in the form of Eq. (25) where

$$\hat{\theta}=\begin{pmatrix}\theta_d\mathbf{1}_2 & 0\\ 0 & i\theta_{1d}\mathbf{1}_2\end{pmatrix},\quad\begin{matrix}0<\theta_d<\pi,\\ 0<\theta_{1d}<\infty;\end{matrix}\quad\mathbf{1}_2=\begin{pmatrix}1&0\\0&1\end{pmatrix},\quad u_2=\exp\begin{pmatrix}i\varphi_1\tau_3 & 0\\ 0 & i\varphi_2\tau_3\end{pmatrix}, \tag{30}$$

and

$$u_1=\begin{pmatrix} 1-2\hat{\eta}_d\hat{\eta}_d^\dagger & 2\hat{\eta}_d \\ -2\hat{\eta}_d^\dagger & 1+2\hat{\eta}_d\hat{\eta}_d^\dagger \end{pmatrix}, \quad v=\begin{pmatrix} 1+2\hat{\kappa}_d\hat{\kappa}_d^\dagger & 2i\hat{\kappa}_d \\ -2i\hat{\kappa}_d^\dagger & 1-2\hat{\kappa}_d\hat{\kappa}_d^\dagger \end{pmatrix},$$
$$\hat{\eta}_d=\begin{pmatrix} \eta_d & 0 \\ 0 & \eta_d^* \end{pmatrix}, \quad \hat{\kappa}_d=\begin{pmatrix} \kappa_d & 0 \\ 0 & -\kappa_d^* \end{pmatrix}. \tag{31}$$

In this parametrization, the $\theta_{d,1d}$ and $\varphi_{1,2}$ are commuting variables, whereas $\eta_d, \eta_d^*, \kappa_d, \kappa_d^*$ are Grassmann variables. The integration over the superspace in the parametrization Eqs. (30), (31), implies the knowledge of the Jacobian,[33,34]

$$J_d=\frac{d\lambda_{1d}d\lambda_d}{(\lambda_{1d}-\lambda_d)^2}\,\frac{d\eta_d d\eta_d^* d\kappa_d d\kappa_d^*}{16}\,\frac{d\varphi_1 d\varphi_2}{(2\pi)^2}; \quad \lambda_{1d}=\cosh(\theta_{1d}), \quad \lambda_d=\cos(\theta_d). \tag{32}$$

In terms of the variables λ_{1d} and λ_d, the free energy F_{0D} can be reduced to the form

$$F_{0D}=\frac{\pi\gamma}{\Delta}[\lambda_{1d}-\lambda_d]. \tag{33}$$

The pre-exponential factor in Eq. (27) can be simplified as well, since vectors z_1 and z_2 commute with Q, and the integration over the variables ζ_1 and ζ_2 is trivial. As a result, Eq. (27) can be rewritten as

$$f_1(p)=\frac{V}{2}\lim_{\gamma\to 0}\int (Q_{33}^{11}-1)\,\delta\left(p-\frac{\gamma}{\Delta}Q_{33}^{22}\right)e^{-F_{0D}[Q]}dQ, \tag{34}$$

where Q_{33}^{11} and Q_{33}^{22} are matrix elements (the superscripts denote the blocks originating from the presence of both advanced and retarded Green functions and the subscripts—the elements in these blocks).

Note that the combination entering the δ-function in Eq. (34) contains the broadening γ which has to be put to 0. When $\gamma\to 0$, the only possibility to have a finite value of the product $(\gamma/\Delta)Q_{33}^{22}$, which is necessary since p is a finite wave function density in a finite volume, is to take into account the values of Q_{33}^{22} as large as $\Delta/\gamma\to\infty$. We can do it since the degeneracy space of the supersymmetric field theory is non-compact. To be more precise, one has to deal with that part of the superspace where $\lambda_{1d}\sim\Delta/\gamma\to\infty$.

This argument simplifies dramatically our calculus. Indeed, in the leading approximation with respect to γ, it is enough to keep only the pseudo-unitary part in the matrix U_d and even to replace it by an asymptotical expression

$$U_d\to U_\infty=\frac{\sqrt{\lambda_{1d}}}{2}\begin{pmatrix} u_1u_2 & 0 \\ 0 & v \end{pmatrix}\Pi, \quad \overline{U_d}\to\overline{U_\infty}=\frac{\sqrt{\lambda_{1d}}}{2}\overline{\Pi}\begin{pmatrix} \overline{u_2u_1} & 0 \\ 0 & \overline{v} \end{pmatrix},$$
$$\Pi=\begin{pmatrix} \pi_b & \pi_b \\ \pi_b & \pi_b \end{pmatrix}, \quad \overline{\Pi}=\begin{pmatrix} \pi_b & -\pi_b \\ -\pi_b & \pi_b \end{pmatrix}\equiv\Lambda\Pi\Lambda, \quad \pi_b=\begin{pmatrix} 0 & 0 \\ 0 & \mathbf{1}_2 \end{pmatrix}. \tag{35}$$

The matrix U_∞ in Eq. (35) does not belong to the graded symmetry group. It has a sense only as an asymptotical form of parametrization of the ''infinities'' of the superspace in the integrals like in Eq. (21,29,34). Both the Jacobian in Eq. (32) and free energy in Eq. (33) can also be simplified by neglecting a finite $\lambda_d\leqslant 1$ in comparison to infinitely large $\lambda_{1d}\sim\Delta/\gamma$, which finally results in the distribution function in the form of Eq. (28).

Computation of the function $f_2(p_1,p_2;\mathbf{r_1},\mathbf{r_2})$ in the limit of large distances $|\mathbf{r}_1-\mathbf{r}_2|\gg l)$, Eq. (21), can be performed in the same way. At large distances, the distribution function f_2 in the unitary ensemble no longer depends on the coordinates, so they can be omitted. Starting with the expression from Eq. (21), we find that the distribution function has a separable form,

$$f_2(p_1,p_2;|\mathbf{r}_1-\mathbf{r}_2|\gg l)=V^2\ \exp\{-V(p_1+p_2)\}. \tag{36}$$

The separability of the joint density distribution function indicates that, at large distances, the correlations between amplitudes of the wave function are suppressed. To find the law describing their decay with increase of the distance $|\mathbf{r}_1-\mathbf{r}_2|$ (starting from the wavelength scale $\lambda=2\pi k^{-1}$, $\mathbf{k}$ being the wave vector), one has to take into account pairing $\langle\psi_\alpha(\mathbf{r}_n)\psi_\alpha(\mathbf{r}_m)\rangle$ in the derivation of the σ-model in Eqs. (18)–(21). This analysis has been performed by Prigodin.[42] Here we mention the final result re-addressing the reader to Refs. 42 and 43 for technical details. The joint distribution function f_2 in the unitary symmetry class at short distances has the form

$$f_2(p_1,p_2;|\mathbf{r}_1-\mathbf{r}_2|)=\frac{V^2}{1-g^2}\ \exp\left(-\frac{V(p_1+p_2)}{1-g^2}\right)\mathrm{I}_0\left(\frac{2V\sqrt{g^2p_1p_2}}{1-g^2}\right), \tag{37}$$

where $\mathrm{I}_0(x)$ is the modified Bessel function and $g^2(r)$ is the Friedel function[32] ($r=|\mathbf{r}_1-\mathbf{r}_2|$):

$$g=\begin{cases}\mathrm{J}_0(kr)e^{-r/l}, & \text{2D},\\ \sin(kr)e^{-r/l}/(kr), & \text{3D}\cdot\end{cases} \tag{38}$$

From Eqs. (36)–(38) we see that the correlations decay at distances of the order of the wavelength. Absence of distant correlations in wave functions is in so good agreement with a naive expectation coming from the phenomenological models, that one may think that it is the general result which is valid for any chaotic system. However, this is not the case. The suppression of correlations at large distances occurs in the limiting cases of unitary and orthogonal symmetry classes, but does not work in the crossover regime of weak magnetic fields. The correlation of wave functions in the crossover regime will be discussed in detail in the next section.

VI. REDUCED σ-MODEL AND EIGENSTATE STATISTICS BEYOND THE UNIVERSALITY REGIMES: CROSSOVER BETWEEN ORTHOGONAL AND UNITARY ENSEMBLES

Note that the procedure of integration over the ''diffusion'' degrees of freedom in the 0D approximation of the previous section together with the necessity to take the limit $\gamma\to 0$ gives us a result that is free of any level broadening and describes the statistics of a single chaotic eigenstate. Moreover, integration over the zero ''diffusion'' mode in the limit $\gamma\to 0$ can be a good move for any particular realization of the σ-model (e.g., in the case where the magnetic field H is so weak that the magnetic flux through the sample area is small, or when the sample is large enough to expect that the localization effects play an important role). What we obtain after such a manipulation is a *reduced σ-model* which directly describes the statistical properties and spatial structure of a single state in the discrete spectrum of a confined quantum system.

In the general case, the field Q depends on the coordinates and contains more variables. In the crossover regime between the unitary and orthogonal symmetry classes, the presence of the ''cooperon'' degrees of freedom doubles the number of independent parameters, and the transformation U in Eq. (27) can be represented[50] as the product

$$U=U_dU_c;\quad U_c=\begin{pmatrix} u_{1c} & 0\\ 0 & v_c\end{pmatrix}\exp\begin{pmatrix} 0 & -u_{2c}C_0\dfrac{\hat{i}\theta_c}{2}\\ -\dfrac{\hat{i}\theta_c}{2}C_0^{\dagger}\overline{u_{2c}} & 0\end{pmatrix},$$
$$\hat{\theta}_c=\begin{pmatrix}\theta_c\mathbf{1}_2 & 0\\ 0 & i\theta_{1c}\mathbf{1}_2\end{pmatrix},\quad \text{where}\quad \begin{matrix}0<\theta_c<\pi/2,\\ 0<\theta_{1c}<\infty,\end{matrix}. \tag{39}$$

In Eq. (39), C_0 is defined as in Eq. (24), and the matrices $u_{1c,2c}$ and v_c are similar to those in the parametrization of V_d in Eq. (34). The measure of the integration over the ''cooperon'' variables described above is given by

$$dQ_c=\left(\frac{2\lambda_c}{\lambda_{1c}^2-\lambda_c^2}\right)^2\frac{d\lambda_c d\lambda_{1c}}{16}\frac{d\varphi_1' d\varphi_2'}{(2\pi)^2}dR_c,\quad dR_c=d\eta_c d\eta_c^* d\kappa_c^* d\kappa_c, \tag{40}$$

where $\eta_c,\eta_c^*,\kappa_c,\kappa_c^*$ are Grassmann variables.

To derive the reduced σ-model, we represent the supermatrix field $Q(\mathbf{r})$ at any point $\mathbf{r}$ inside the sample in the form

$$Q(\mathbf{r})=U_d(\mathbf{r}_1)\widetilde{Q}(\mathbf{r})\overline{U_d}(\mathbf{r}_1), \tag{41}$$

where $U_d(\mathbf{r}_1)$ is parametrized by Eqs. (33) and (34) and describes the values of the full set of ''diffusion'' variables of the field Q at the observation point $\mathbf{r}_1$. The integration over the zero diffusion mode is equivalent to integration of Eq. (21) over all possible ''directions'' U_d of the superfield in the sample ''as a whole.'' Because of the δ-functional form of the pre-exponential part of the expressions involved, only large $\theta_d(\mathbf{r}_1)$, such that $e^{\theta_d}\sim\Delta/\gamma\to\infty$, contribute to the integrals in Eqs. (21) and (29). So, we use Eq. (35) in the same way as in the previous section.

As a result, the general σ-model transforms into the reduced one with a modified free energy functional. It is easier to follow the derivation calculating the distribution function f_1. In particular, the second term in $F[Q]$ in Eq. (22) containing infinitely small γ, after the integration of $\delta(p-(\gamma/2V\Delta)\overline{z_1}Q(\mathbf{r}_1)z_1)$ over all the variables of $V_d(\mathbf{r}_0)$ converts it into

$$F_2[Q]\to F_2[\widetilde{Q}]=\frac{p}{2\overline{z_1}\Lambda\Pi\widetilde{Q}(\mathbf{r}_1)z_1}\int d\mathbf{r}\,\mathrm{Str}(\Lambda\Pi\widetilde{Q}(\mathbf{r})). \tag{42}$$

The term of Eq. (42) plays the role of an ''external field'' (introduced by the procedure of measurement of the local wave function density) breaking the symmetry between bosonic and fermionic degrees of freedom of the field Q. Note that the above procedure suggests that, the field $\widetilde{Q}(\mathbf{r})$ parametrized as $\widetilde{Q}=\widetilde{U}_d\widetilde{U}_c\Lambda\tilde{\tilde{U}}_c\tilde{\tilde{U}}_d$, corresponds to boundary conditions $U_d(\mathbf{r}_1)=\mathbf{1}$.

On the contrary, the gradient term of the free energy $F[Q]$ in Eq. (22) does not change its form:

$$F_1[Q]\to F_1[\widetilde{Q}]=\frac{D\pi\nu}{8}\int d\mathbf{r}\,\mathrm{Str}\left(\nabla\widetilde{Q}-\frac{ie}{\hbar c}\mathbf{A}[\widetilde{Q},\tau_3]\right)^2. \tag{43}$$

As to the form of the pre-exponential factor in the generating functional of the reduced σ-model, it depends on the index N of the joint distribution and can be sufficiently simplified in several special cases, in particular, when studying the crossover regime between the orthogonal and unitary symmetry classes. Analogously to the derivation of the universal statistics in the

previous section, in a relatively small system we can neglect spatial variations of the field $\widetilde{Q}$, so that $\widetilde{Q}(\mathbf{r})\equiv\widetilde{Q}(\mathbf{r}_1)$. Then the lowest ''cooperon'' mode is described by the expression for the free energy,

$$F_1=-\left(\frac{X}{4}\right)^2\mathrm{Str}([\widetilde{Q},\tau_3]^2)=X^2(\lambda_{1c}^2-\lambda_c^2)X^2=(2\pi)^3\frac{D}{\Delta}\int\frac{d\mathbf{r}}{V}\left(\frac{\mathbf{A}(\mathbf{r})}{\phi_0}\right)^2=\alpha_g\frac{\phi^2}{\phi_0^2}\frac{E_c}{\Delta},$$

where $\phi_0=hc/e$ is the flux quantum, α_g is the sample geometry dependent factor, D is the classical diffusion coefficient, E_c is the Thouless energy equivalent to the inverse time of flight through the system, L^2/D.

The physical meaning of this term arising in the 0D σ-model is that it is related to distribution of the magnetic fluxes encircled by a semiclassical electron trajectory. Due to the Aharonov-Bohm effect,[51] the encircled fluxes determine the phases of the electron wave in a magnetic field,

$$\frac{e}{c\hbar}\oint(\mathbf{A}d\mathbf{r})=\frac{2\pi}{\phi_0}\int\mathbf{H}d\mathbf{S}.$$

In a classical picture of chaos, these phases, as well as the magnetic fluxes, can be arbitrarily large. This is in contrast to the correct semiclassical picture of quantum mechanics where they cannot. The lengths of geometrical paths attributed to classical trajectories in semiclassics should be limited, since the trajectorial description breaks down at the time scale longer than the Heisenberg time, $t_H\sim h/\Delta$. Hence, the values of the encircled magnetic flux are also limited, so that the classical ergodicity does not always lead to the complete randomness of the wave function phases. That is why the crossover between the two limiting symmetry classes extends over a finite region of magnetic fluxes through the sample cross-sectional area, which indicates that there can exist long-range correlations in the chaotic wave function in the entire crossover regime. On the other hand, in classically non-integrable systems, the Heisenberg time is usually much longer than the time flight L^2/D, so that crossover between time-reversal and no-time-reversal symmetry limits occurs at fairly weak magnetic fields.[33,52,53]

In order to establish the presence or absence of the correlations, we study the joint distribution function $f_2(p_1,p_2;\mathbf{r}_1,\mathbf{r}_2)$ at two points separated by the distance $|\mathbf{r}_1-\mathbf{r}_2|$ much larger than the mean free path l and compare it with the single-point distribution function f_1. As discussed in the previous section, the Friedel-type oscillations are dead at these distances, so that the presence of correlations means the non-separability of the joint function $f_2(p_1,p_2)$ into the product $f_1(p_1)f_1(p_2)$.

After some necessary algebra,[41,45] the joint distribution function f_2 and the distribution function f_1 can be represented as

$$f_N(p_1,\ldots,p_N)=V^N\int_0^1 d\lambda_c\int_1^\infty d\lambda_{1c}\exp(-F_\phi)\times\frac{\lambda_c^2}{(\lambda_{1c}^2-\lambda_c^2)^2}$$
$$\times\int\int P\prod_{n=1}^{N}\frac{d\zeta_n}{2\pi}\frac{\exp(-Vp_n/A_n)}{A_n}dR_c, \tag{44}$$

which is a parametrized representation of the reduced σ-model. In Eq. (44), $N=1,2$, and functions P and A_n are defined as

$$P=\lambda_{1c}+2(\eta_c\eta_c^*-\kappa_c\kappa_c^*)(\lambda_{1c}-\lambda_c),\quad A_n=1+\mathrm{Re}\,\frac{Le^{i\zeta_n}}{P},$$

$$L=\sqrt{\lambda_{1c}^2-1}(1+2\eta_c\eta_c^*)(1-2\kappa_c\kappa_c^*)+4\sqrt{1-\lambda_c^2}\eta_c\kappa_c.$$

Skipping further technical details of the algebraic manipulations with Eq. (44), we are able to represent the joint distribution function f_N, $N=1,2$ in the form

$$f_N = V^N \int_1^\infty B(X,x) \prod_{n=1}^{N} M(Vp_n,x)\,dx, \tag{45}$$

where

$$B(X,x) = X^2[(xX^2-1)\Phi_2(X)+\Phi_1(X)]e^{-X^2(x-1)},$$

$$M(q,x) = \sqrt{x}\,\exp(-qx)\mathrm{I}_0(q\sqrt{x^2-x}),$$

Here, $\mathrm{I}_0(z)$ is the modified Bessel function, and

$$\Phi_1(X) = \frac{e^{-X^2}}{X}\int_0^X e^{y^2}dy, \quad \Phi_2(X) = \frac{1-\Phi_1(X)}{X^2}.$$

First of all, let us compare the result obtained by using the σ-model and the predictions of the random matrix theory for the universal statistics. The comparison with the unitary case, $X\to\infty$, may serve as a check of the algebra, since it coincides with the results of Eqs. (30) and (36). In the orthogonal ensemble, $X\to 0$, we also find from Eq. (45) that the joint distribution function is separable at large distances,

$$f_2(p_1,p_2)\to \prod_{n=1,2}\frac{Ve^{-Vp_n/2}}{\sqrt{2\pi Vp_n}}; \quad f_1(p)\to\sqrt{\frac{V}{2\pi p}}\exp\left(-\frac{1}{2}Vp\right). \tag{46}$$

However, the joint distribution function is not separable at any finite magnetic field, which indicates that, even in the limit of large distances between the points $\mathbf{r}_1$ and $\mathbf{r}_2$, the correlations do not vanish. To demonstrate the *existence of a long-range correlation in each individual wave function* in a quantum billiard subjected to a weak magnetic field, we calculate the correlation function $K_{22}(r\gg l)$ defined in Eq. (8). Fig. 1(a) illustrates how the correlations evolve as function of a normalized flux through the sample area. As one can see from Fig. 1(a), the correlations are present all over the crossover regime: from the smallest to the highest values of the normalized flux. Numerically, these correlations are never strong (of the order of one percent), since the maximal value of the correlator $\max(K_{22})\approx 0.05$ has to be compared to the square of the second moment P_2 varying from the value of 3 to 2 between the orthogonal and unitary symmetry classes. The distant correlations in the wave functions can also be traced in the joint probability to find simultaneously two zeros of the wave function $\varphi(\mathbf{r}_{1,2})=0$. At small fluxes corresponding to $X\ll 1$, $[f_1(0)]^2\approx(4\pi/9)X^{-2}$ whereas $f_2(0,0)\approx\frac{5}{3}X^{-2}$, and Fig. 1(b) illustrates the evolution of the distribution function $\varphi(\tau)=2\tau f_1(\tau^2)$ of local amplitudes $\tau=\sqrt{(p)}$ following the variation of a magnetic flux.

Since the pioneering work by Berry,[30] it has been believed that in classically ergodic systems the local wave function density can be imagined as a result of superposition of an infinite number of plane waves with random phases and equal momenta. In the unitary case, this is a complete randomness. In the orthogonal ensemble, the pairs of time-reversed plane waves with wave vectors $\pm\mathbf{k}$ enter this representation with conjugate phases. The randomness of the phases results in the Gaussian randomness of the amplitude φ_α and vanishing of correlations at large distances. Our result in Eq. (45) means that a weak magnetic flux through the sample area introduces some non-local correlations in $\varphi_\alpha(\mathbf{r})$ related to the fact that the Aharonov-Bohm phases taken by an electron moving in a quantum billiard cannot be arbitrarily large and that the phases of the ''plane waves'' in the phenomenological picture are slightly correlated at each point, which has not been

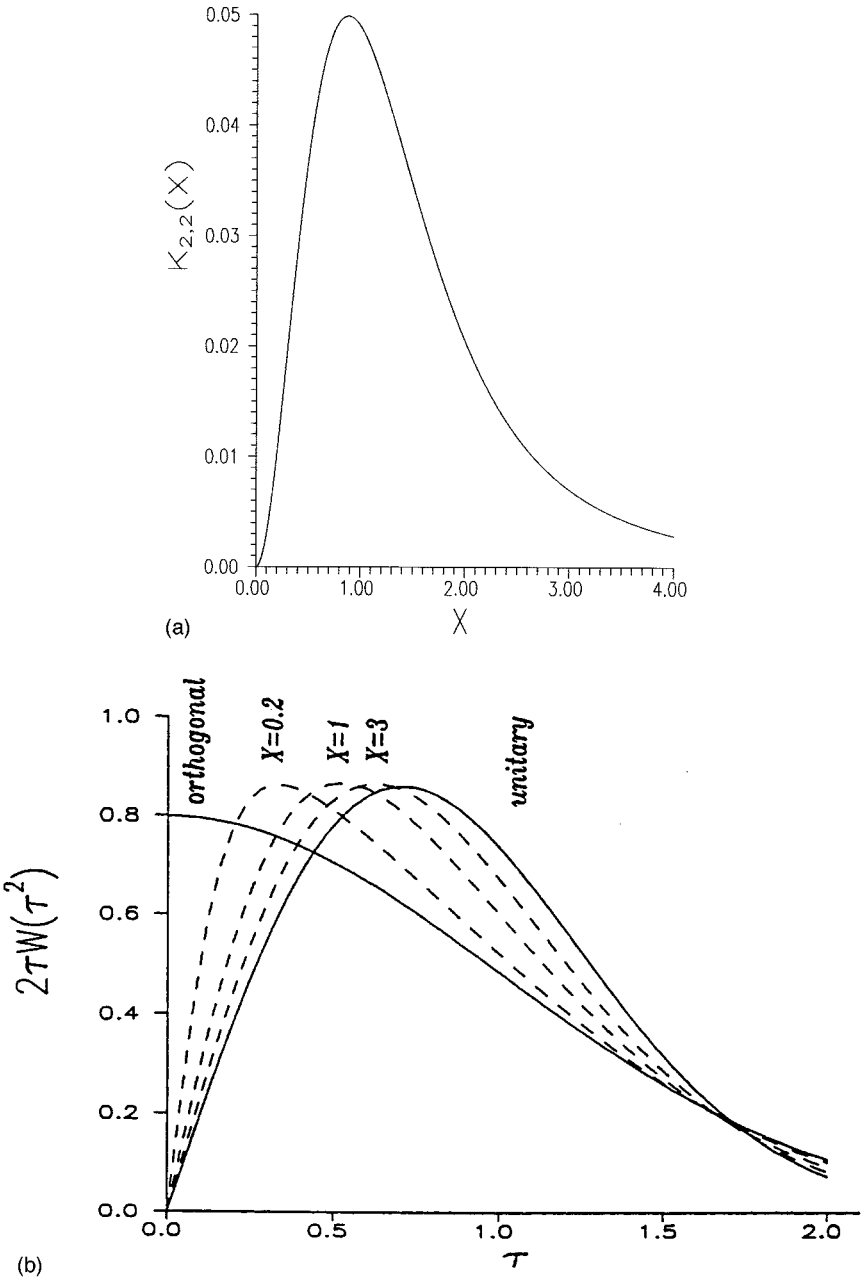

FIG. 1. (a) Two-point correlation function at distant points as a function of a normalized flux. (b) Distribution function of local amplitudes of wave functions (as described in the text) for various values of a normalized magnetic flux through the system.

anticipated in previous semiclassical theories. These correlations are present in the entire crossover regime and can be diminished only by the localization effects which have not been taken into account, yet, but will be considered in the next section.

VII. LOCALIZATION EFFECTS IN THE WAVE FUNCTIONS STATISTICS AND NON-TRIVIAL VACUUM OF THE REDUCED σ-MODEL

To study the localization effects in the wave functions statistics, one has to go beyond the 0D approximation of the σ-model.[33,54–59,44,45] Depending on the system to be studied and problem to be considered, the inhomogeneous field $Q(\mathbf{r})$ can be treated in different ways. In the perturbation theory calculation in the weak localization regime, they appear as non-zero spatial ''cooperon'' modes.[3] In quasi-1D wires, the account for the inhomogeneous $Q(x)$ using the transfer matrix method gives an exact solution of the localization problem in the limit of a weak disorder.[56] Recently, in revising the perturbative results of Ref. 60 on the long-living current relaxation in mesoscopic conductors, Muzykantskii and Khmelnitskii[59] have suggested that an adequate description of anomalous events in the weak localization regime may involve the treatment of the supersymmetric σ-model by using a saddle-point method.

In the studies of the eigenstates statistics in weakly disordered conductors with a size smaller than the localization length,[44,45] the inhomogeneous supermatrix fields appear as a *non-trivial vacuum state of the reduced σ-model.* In this Section, we present all details of the calculus for the unitary symmetry class. That is, regarding to the discussion in Section VI, we assume that the magnetic field applied to the system is large enough (though the classical cyclotron radius is still longer than the mean free path) and formally require that $l/\lambda \gg Hl^2/\phi_0 \gg \sqrt{\lambda/l}$. The unitary symmetry class can be also modeled by a random magnetic or gauge field disorder.[47,48] This allows us to suppress completely the ''cooperon'' degrees of freedom of the Q-field and to deal only with the ''diffusion'' ones. The content of the next few paragraphs repeats the derivation earlier from Ref. 44, and one can find in Ref. 45 its generalization to other fundamental symmetry classes. We also restrict the analysis to the calculation of the single-point distribution function $f_1(p)$ which contains enough information to indicate the existence of *prelocalized states* in a disordered system (the states with an anomalously high local density), and to the correlation function $R(p,r)$ defined in Eq. (8) which tells us about their statistically averaged envelopes. The generating functional of the reduced σ-model equals

$$\Phi_u(p) = \int_{\widetilde{Q}(\mathbf{r}_1)=\Lambda} \mathrm{D}\widetilde{Q}(\mathbf{r}) e^{-F[\widetilde{Q}]}, \tag{47}$$

where the free energy has the form

$$F[\widetilde{Q}] = \int d\mathbf{r} \mathrm{Str}\left[\frac{\pi\nu D}{8}(\nabla\widetilde{Q})^2 - \frac{p}{4}\Lambda\Pi\widetilde{Q}(\mathbf{r})\right], \tag{48}$$

and we are reminded that $\widetilde{Q}(\mathbf{r}_o)=\Lambda$ at the origin and projector Π is that defined in Eq. (35). At the same time, the distribution function f_1 and its moments P_n can be represented (in terms of the generating functional Φ_u) as

$$f_1(p) = \frac{1}{V}\frac{d^2\Phi_u(p)}{dp^2}, \quad P_n = \frac{n(n-1)}{V}\int_0^\infty p^{n-2}\Phi_u(p)dp. \tag{49}$$

As far as other fundamental symmetry classes are concerned, this relation may take various forms (see Ref. 45).

The generating functional in Eq. (47) has several funny features. First, at $p=0$, it has a completely invariant form, and therefore is equal to unity, which corresponds to the normalization of all wave functions,

$$VP_1 = \Phi_u(0) \equiv 1. \tag{50}$$

On the other hand, for any finite p the reduced σ-model has broken symmetry, so that the minimum of the free energy in Eqs. (47) and (48) corresponds to an inhomogeneous $\widetilde{Q}_p(\mathbf{r})$. Indeed, $(p/4)\Lambda\Pi$ in the second term in Eq. (48) resembles a field tending to align the matrix $\widetilde{Q}$ along the non-compact ''direction'' of the Q-space (related to the parameter θ_{1d}), whereas the boundary condition at $\mathbf{r}_0$ together with the gradient term can be viewed as a rigidity attempting to prevent that. The competition between these two tendencies results in a non-trivial minimum configuration of $\widetilde{Q}$. To find this non-trivial vacuum state (saddle-point), we use again the invariance of the Q-space with respect to rotations $\widetilde{U}$ and represent Q as

$$\widetilde{Q}(\mathbf{r})=U_{\mathrm{vac}}(\mathbf{r})\Lambda\frac{1+iP}{1-iP}\overline{U}_{\mathrm{vac}}(\mathbf{r}),\quad P=\begin{pmatrix}0 & B\\ \overline{B} & 0\end{pmatrix}\otimes\mathbf{1}_2, \tag{51}$$

where a weak perturbation P stands for fluctuations around the saddle-point, and the matrices $B,\overline{B}$ can be decomposed into blocks as follows:

$$B=\begin{pmatrix}s_{1,1}\tau_0+is_{1,2}\tau_3 & \hat{\sigma}_1\\ \hat{\sigma}_2^{+} & s_{2,1}\tau_0+is_{2,2}\tau_3\end{pmatrix},\quad \hat{\sigma}_\alpha=\begin{pmatrix}\sigma_\alpha & 0\\ 0 & -\sigma_\alpha^{*}\end{pmatrix}. \tag{52}$$

The parametrization of fluctuation using Eq. (52) is especially convenient from the point of view of the perturbative analysis, since it has a unit value of the Jacobian (Berezian).[34] The form of the saddle-point $\widetilde{Q}_{\mathrm{vac}}=U_{\mathrm{vac}}\Lambda\overline{U}_{\mathrm{vac}}$ follows from the requirement of the absence of linear terms in the expansion of F into the series

$$F[\widetilde{Q}]=F_p+F^{(2)}+F^{(3)}+F^{(4)}+\ldots, \tag{53}$$

in the perturbation $B,\overline{B}$. This selects

$$U_{\mathrm{vac}}=\exp\begin{pmatrix}0 & \frac{1}{2}\theta_p e^{i\chi\tau_3}\pi_b\\ \frac{1}{2}\theta_p e^{-i\chi\tau_3}\pi_b & 0\end{pmatrix}, \tag{54}$$

where the parameter $\theta_t(\mathbf{r})$ satisfies the equation

$$\nabla^2\theta_p(\mathbf{r})=-\frac{p}{\pi\nu D}e^{-\theta_p},\quad \chi=\pi, \tag{55}$$

with the boundary conditions $\theta_p(\mathbf{r}_1)=0$ in the origin and $(\mathbf{n}\nabla)\theta_p=0$ at the surface of the sample. In Eqs. (55) and (54), ∇^2 stands for the Laplacian in the real d-dimensional space, and projection matrix π_b is that defined in Eq. (35).

A similar analysis of the reduced σ-model can also be performed for other symmetry classes and leads us to the same saddle-point equation as in Eq. (55). The difference between the unitary, orthogonal and symplectic (including spin-orbit scattering) ensembles leads only to different values of the coefficient β,

$$\beta_o=\frac{1}{2},\quad \beta_u=1,\quad \beta_s=2, \tag{56}$$

in the expression describing the minimal free energy,

$$F_p = \beta \int d\mathbf{r} \left\{ \frac{\pi \nu D}{2} (\nabla \theta_p)^2 + p e^{-\theta_p} \right\}, \tag{57}$$

and in the higher order terms of the expansion of $F[\widetilde{Q}]$ in the vicinity of the vacuum state $Q_{\rm vac} = U_{\rm vac} \Lambda U_{\rm vac}$.

The optimum (saddle-point) equation in Eqs. (54) and (55) is analogous to the saddle-point equation derived by Muzykantskii and Khmelnitskii[59] when revising the problem of long-living current relaxation in open conductors.[60] Nevertheless, the fact that we started from the reduced σ-model which describes properties of a single quantum state in a confined system results in a different non-linearity in it and different boundary conditions. The *non-trivial vacuum of the reduced σ-model* from Eqs. (51)–(55) *satisfies the Liouville equation*. For those familiar with the conformal theory of quantum gravity,[61] this fact immediately points to the critical properties of the wave functions in two dimensions. The issue of peculiar properties of prelocalized states in 2D conductors will be discussed in more detail in the next section; here we only mention the general difference between the purely conformal quantum Liouville theory[61] and the localization problem. The Liouville equation (55) describes the ''mean field'' distribution of the length scales in the system and is invariant under rescaling $r \to ar$ and $\theta_p \to \theta_p - 2\ln(a)$. Without the above-mentioned boundary conditions, this would give us an infinitely broad distribution of length scales in the structure of the wave functions in two dimensions, and there exist several examples[62–66] when the critical wave functions can be constructed starting from very special models of disorder (e.g., 2D-electrons with g-factor 2 living in a random magnetic field,[62] or 2D relativistic spin-$\frac{1}{2}$ particles in a randon Abelian gauge field).[63] It is amusing to note that the f_1-statistics and some simple correlation functions in the above-mentioned models of disorder may be calculated using the saddle-point method applied to the generating functional analogous to that in Eq. (47).[67]

Although the similarity of the optimum equation, Eq. (55), describing the vacuum state of the reduced σ-model to the Liouville equation and conformal field theory may call helpful analogies,[66] the answers which can be anticipated in this way might be used only as intermediate asymptotics. In conventional models of disorder, there are several relevant length scales in the problem, such as the mean free path l which we keep much smaller than the size of the system L. In our theory, the latter comes to the play through the boundary condition at the edge; the former - through the condition at the origin which has to be replaced by the ''smoothed'' requirement $\theta_p(r_0 \sim l) = 0$. This restricts applicability of the saddle-point calculations by the domain of validity of the σ-model in its standard form: to systems with dimensions lower than three. In 3D systems, the free energy of the non-trivial vacuum state of reduced σ-model is sensitive to the singular behavior of Q-fields at distances shorter than l,[45] and the application of our method to dimension three cannot give an adequate quantitative description of statistics of anomalously high splashes of wave functions and would systematically underestimate the probability of their appearance: As we recently learned from Shklovskii, at short distance (in small volumes), it is possible to construct rare configurations of a random potential which would become more efficient would one go beyond the Born approximation with respect to the random potential implicit to the σ-model approach.

Another difference between precisely conformally invariant Liouville theory and the σ-model description of localization consists in a number of additional degrees of freedom which are present in the supersymmetric order parameter $\widetilde{Q}$. Playing no role in forming the vacuum state, these degrees of freedom become crucially important if the *fluctuations around the non-trivial vacuum* are taken into account. In a complete theoretical construction, they would result in the localized behavior at long distances of all the states we are studying. At present, we are not able to provide a rigorous theoretical treatment of this problem, which seems to require some kind of a functional renormalization group approach. But what we can do here, that is to account for fluctuations perturbatively and to get the lowest order estimation and to control the regime of applicability of the saddle-point method and check the stability of the vacuum.

Since now, we represent the generating functional $\Phi_u(p)$ in the form

$$\Phi_u(p)=J(p)\exp(-F_p). \tag{58}$$

In the conducting regime, the value of the minimal free energy determines the leading term in the exponential of the generating functional, whereas the effect of fluctuations around the non-trivial vacuum is included into the function $J(p)$,

$$J(p)=\int DB\ \exp\{-F^{(2)}-F^{(3)}-F^{(4)}\dots\}. \tag{59}$$

Because of the normalization condition in Eq. (50), the relation $J(0)=1$ holds exactly. The contribution from the fluctuations B at $p=0$ can be calculated by expanding the exponential in the integrand in Eq. (59) in a series in higher order terms $F^{(3,4,\dots)}$ and performing Gaussian integrations over B with the weight $\exp\{-F^{(2)}\}$ determined by the second order correction to the free energy.

The applicability of such a perturbation theory is justified by the fact that the contribution of the higher order terms to the free energy are, at least, by the factor of $(2\pi\nu D)^{-1}\ll 1$ smaller, as compared to what is given by

$$J(p)\approx\int DB\ \exp\{-F^{(2)}[B]\}. \tag{60}$$

The $J(p)$ is the superdeterminant of the Hamiltonian related to the fluctuations around the saddle-point. The value of $J(p)$ differs from unity merely because the symmetry between fermionic and bosonic degrees of freedom is broken by a vacuum state. Since not all projections of the infinitesimal B to the generators of the Lie algebra of the graded symmetry group are equivalently affected by the symmetry breaking, it is convenient to separate in $F^{(2)}$ the terms that perceive the existence of the minimal solution from those that do not. Depending on the physical symmetry class, this involves different sets of variables. Nevertheless, after an appropriate diagonalization, the quadratic form $F^{(2)}$ can be represented uniquely for all symmetry classes:[45]

$$F^{(2)}=F_p^{(2)}+\mathfrak{s}F_0^{(2)},\quad \begin{matrix}\mathfrak{s}_u=0,\\ \mathfrak{s}_{o,s}=1.\end{matrix} \tag{61}$$

The term $F_0^{(2)}$ in Eq. (61) is composed of fields which are not affected by the symmetry breaking,

$$F_0^{(2)}=2\pi\nu D\sum_{\alpha=1,2}\int d\mathbf{r}\{\vec{\nabla}\sigma_\alpha^-\vec{\nabla}(\sigma_\alpha^-)^*+\vec{\nabla}s_\alpha^-\vec{\nabla}(s_\alpha^-)^*\}.$$

This term does not contribute to the function J in the Gaussian approximation, due to the symmetry between boson (s) and fermion σ degrees of freedom incorporated. On the contrary, the first term in Eq.(61) is the sum over those four pairs of dynamical variables which are sensitive to the violation of the boson-fermion symmetry,

$$F_p^{(2)}=2\pi\nu D\int d\mathbf{r}\left\{\sum_{\alpha=1,2}[\nabla\sigma_\alpha\nabla\sigma_\alpha^*+U_\sigma\sigma_\alpha\sigma_\alpha^*]+\sum_{\beta,\alpha=1,2}[(\nabla s_{\alpha,\beta})^2+U_s^{\alpha\beta}s_{\alpha,\beta}^2]\right\}.$$

Therefore, the pre-exponential J can be represented as

$$J=\exp\left\{\frac{1}{2}\sum_n\ln\left(\frac{(\chi_\sigma(n))^4}{\Pi_{\alpha,\beta}\chi_s^{\alpha\beta}(n)}\right)\right\}, \tag{62}$$

where the sum is extended over all eigenvalues $\{\chi\}$ of the spectral problem,

$$[-\Delta+U-\chi]\phi=0, \quad \phi(\mathbf{r}_1)=0, \quad \mathbf{n}\nabla\phi=0|_{edge}. \tag{63}$$

As mentioned, any difference of J from unity is due to the broken symmetry between fermionic and bosonic degrees of freedom in B. The broken symmetry in the Hamiltonian $F_p^{(2)}$ is a consequence of the difference between the effective potentials U_σ and U_s,

$$U_\sigma=\frac{1}{4}(\nabla\theta_p)^2+\frac{p}{2\pi\nu D}e^{-\theta_p}, \quad U_s^{\alpha\beta}=\frac{k_{\alpha,\beta}}{4}(\nabla\theta_p)^2+\frac{pq_{\alpha,\beta}}{2\pi\nu D}e^{-\theta_p}, \tag{64}$$

in the Hamiltonian $F_p^{(2)}$ In Eq. (64), $k_{\alpha,1}=q_{\alpha,1}=0$ and $k_{1,2}=4$, $k_{2,2}=0$, $q_{\alpha,2}=2$. The spectra $\{\chi_\sigma(n)\}$ and $\{\chi_s^{\alpha\beta}(n)\}$ of modes remain gapfull, since all $U>0$. Moreover, because of the sum rule

$$\sum_{\alpha\beta} U_s^{\alpha\beta}=4\sum U_\sigma, \tag{65}$$

their main contribution to J comes from low-lying eigenvalues of Eq. (63). Since the set of U's in Eq. (64) depends on the vacuum state only, the calculation of the correction to the exponent in this order in $(2\pi\nu D)^{-1}$ can be performed for all symmetry classes at once and is small, if the size of the system is shorter than the localization length.

The existence of a non-trivial vacuum of the reduced σ-model and a relatively small contribution from fluctuations in the metallic regime makes it easy to find the form of the cross-correlation function $R(p,r)$ from Eq. (8), too. If we study the envelope of the wave function at sufficiently large distances $r\gg l$ from the position of a high amplitude splash, the reasoning used above can be repeated for $R(p,r)$ with minor modifications, and we arrive at

$$|\varphi_p(r)|^2\sim R(p,r)/f_1(p)\propto pe^{-\theta_p(r)}, \tag{66}$$

so that one can say that the envelope of $|\varphi(r)|^2$ follows the form of the saddle-point configuration of the reduced σ-model.[44,45]

VIII. MULTIFRACTALITY OF EIGENSTATES IN WEAKLY DISORDERED 2D CONDUCTORS

The form of the vacuum state of the reduced σ-model depends on the real dimensionality of the system. In 3D systems, the localization effects are known to be the weakest. Although the distribution function f_1 acquires a broader distribution than the universal one, all its moments P_n (IPN) scale with the inverse integer power of the volume of the system. We, therefore, omit the 3D case, since it gives the results the most resembling the universal ones.[45]

On the contrary, the statistics of eigenstates in quasi-1D wires are the most affected by the localization, and show a clear evidence of prelocalized states. The properties of wires will be discussed in the Section IX, whereas the present chapter is devoted to the most intriguing issue: the statistics of prelocalized wave functions in disordered 2D systems.

The fact is that the 2D disordered systems are very close to the critical ones and, as it has been anticipated by Wegner[54,55] and by Altshuler, Kravtsov and Lerner[60] and confirmed by extensive numerical simulations,[68–73] they possess nearly critical properties in a broad range of distances between the mean free path and the exponentially long localization length. In our calculations, we are after manifestations of very peculiar states which show the behavior similar to that of percolating states at the metal-insulator transition point,[73,74] and it is already commonly believed that the criticality is directly related to the logarithmically-normal statistics and multifractal structure of the objects under investigation.[75,74] Of course, the localization problem in two dimensions is not

really a critical one. The possibility to detect multifractality in the calculations presented below is only because we study finite systems with a size smaller than 2D localization length, and it appears as an approximate intermediate asymptotical result, since the wave functions of critical type are strongly affected by the presence of boundaries, and the evidence about their existence is hidden in the large p tails of the distribution function $f_1(p)$.

To find the distribution function f_1 and the full set of IPN's in a large ($L \gg l$) weakly disordered ($L_c \gg l$) 2D system, one has to solve the optimum equation in Eq. (55) and find the free energy F_p of the vacuum state. For the sake of simplicity, we consider the sample in the form of a disk (with the radius L) and place the observation point $\mathbf{r}_1$ exactly in its center. This choice will be approved by the logarithmic dependences $\ln(L/l)$ we get on the end of calculations. Therefore, we seek a symmetric solution $\theta_p(r)$ of the equation

$$(r^{-1}\partial_r r \partial_r)\theta_p = -\frac{p}{\pi\nu D} e^{-\theta_p}, \quad \theta_p(r_0 \sim l) = 0, \quad \partial_r \theta_p(L) = 0; \quad \rho = \sqrt{\frac{2\pi\nu D}{p l^2}}. \tag{67}$$

This can be done exactly.[76] The solution has the form

$$e^{-\theta_p} = \left[\frac{2(l/r)^{1-A}[\sqrt{(1/A\rho)^2+1}+1]}{[\sqrt{(1/A\rho)^2+1}+1]^2 - (1/A\rho)^2 \left(\frac{r}{l}\right)^{2A}} \right]^2, \tag{68}$$

where A should be found from the boundary condition at the sample edge $r = L$,

$$\sqrt{A^2+\rho^{-2}} + A = \frac{(L/l)^A}{\rho}\sqrt{\frac{1+A}{1-A}}. \tag{69}$$

Substituting the saddle-point solution $\theta_p(r)$ from Eqs. (68) to Eq. (57), we find the minimal free energy,

$$F_p = \beta 4\pi^2 \nu D \left\{ \ln\left(\frac{(L/l)^{(1+A^2)}}{\rho^2[1-A^2]} \right) + 2(1 - \sqrt{A^2+\rho^{-2}}) \right\}.$$

Together with Eq. (69), this can be used for the numerical analysis of the exponential in the distribution function.

The numerical analysis shows that the consistency equation, Eq. (69), has positive roots only if $\rho > \ln(L/l) \gg 1$, which provides a reasonable limitation to the wave function amplitudes we can study using this method. It limits the density p of a splash by the value $\sim(\lambda l)^{-1}$ related to the density of an electron state bound to the forward-and-backward scattered trajectory between two impurities [in fact, we have the restriction $p < p_{\max} \approx (\lambda l)^{-1}/\ln(L/l)$, where λ is the wavelength]. At the same time, in the limit of $\rho > 1$, the roots of Eq. (69) can be approximated by $A = 1 - \mu$, where $\mu < 1$. The same conditions enable us to replace the exact solution in Eq. (68) by

$$e^{-\theta_p} \approx (l/r)^{2\mu}. \tag{70}$$

Prelocalized states which are responsible for the logarithmically-normal tails do not decay exponentially. The statistically averaged envelope of the density of such states can be anticipated from the form of the correlation function $R(p,r)$ in Eqs. (8) and (66) and has power-law asymptotic tails,

$$|\varphi_p(\mathbf{r})|^2 \sim \frac{R(p,r)}{f_1(p)} = e^{-\theta_p(r)} \approx \left(\frac{l}{r}\right)^{2\mu}, \tag{71}$$

with the spectrum of exponents $\{\mu(p)\}$ described by the equation

$$\mu=\frac{(L/l)^{2-2\mu}}{2(1-\mu)\rho^2}\approx\frac{z(T)}{2\ln(L/l)},\quad \text{where } ze^z=T\equiv\frac{pV\ln(L/l)}{2\pi^2\nu D}. \tag{72}$$

For small values of p, $\mu\to 0$, when p grows up to $p_{\max}\sim(l\lambda_F)^{-1}/\ln(L/l)$, μ approaches the limiting value $\mu\approx 1$ which corresponds to $|\varphi_p(r)|^2\propto r^{-2}$. With the same accuracy, the free energy of the vacuum state can be approximated by

$$F_p\approx\beta 4\pi^2\nu D\left\{\mu+\mu^2\ln\frac{L}{l}\right\}, \tag{73}$$

and the applicability of the saddle-point method can be now checked by comparing F_p to the effect of the fluctuations in the lowest order.

The contribution of fluctuations in the environs of the vacuum state can be calculated[45] following the way described in the Section VII. To find the lowest (second) order corrections to the minimal free energy, one has to know the spectrum of fluctuations described by Eqs. (61)–above, this spectrum $\{\chi(n,m)\}$ can be classified by the orbital and radial quantum numbers m and n, respectively, and can be found from the eigenvalues of the Hamiltonian,

$$\hat{H}=-r^{-1}\partial_r(r\partial_r)+m^2r^{-2}+U,$$

where U is determined by Eqs. (64) and (65).

When $U=0$, the spectrum of χ's can be approximated by

$$\chi(0,0)\approx\frac{2L^{-2}}{\ln(L/l)};\quad \chi(n,m)\approx\left(\frac{\pi}{L}\right)^2\left[n+\frac{1}{4}+\frac{m}{2}\right]^2. \tag{74}$$

In the non-trivial vacuum, the fermion-boson symmetry is broken, which induces effective potentials in fermionic sectors and some of bosonic sectors, too. The latter are composed of two terms,

$$\frac{1}{4}k(\partial\theta_p)^2\approx\frac{k\mu^2}{r^2}\quad\text{and}\quad q\frac{p}{2\pi\nu D}e^{-\theta_p}\approx q\mu L^{-2}\left(\frac{L}{r}\right)^{2\mu}.$$

In the above equations, the approximate values are given for the most important range of distances $r\leqslant L\sqrt{z(T)/T}$, and one has to remember that $\mu<1$.

For any $m\neq 0$, the potential U is relatively small, $U\ll m^2/r^2$, and could be treated perturbatively. Due to the sum rule in Eq. (64), the modes with $m\neq 0$ contribute only in the second order in U, and what they give to the exponential of J is of the order of either $\mu^4\ln(L/l)$ or μ^2. With the accuracy we need here regarding the leading terms in F_p, this contribution can be neglected. The spectrum of low-lying modes $\{\chi(n>0,0)\}$ is given by the expression

$$\chi(n,0)\sim\left(\frac{\pi}{L}\right)^2\left[n+\frac{1}{4}+\sqrt{k}\frac{\mu}{2}\right]^2,\quad 0<n\leqslant\frac{L}{\pi l}. \tag{75}$$

The lesson we learn from the above calculated spectrum of fluctuation is that all the eigenvalues χ are positive and increase as compared to what one would get starting from the trivial vacuum ($\widetilde{Q}=\Lambda$), so that we conclude that the vacuum state Q_{vac} is, at least, locally stable. However, the account for the fluctuations $B,\bar{B}$ in the quadratic approximation does not tell us more than that and is not informative from the point of view of manifestation of real localization expected in 2D systems at larger distances.[77] This would need a higher order perturbation theory

with respect to $B,\overline{B}$ in Eq. (53). The second order terms give just corrections to the minimal free energy which are small, as compared to F_p, when $g \gg 1$. This can be checked by substituting the eigenvalues from Eqs. (74)–(75) to the general equation in Eq. (62):

$$J = 1 + 0(T^2), \quad T \ll 1$$
$$J \propto \mu \exp\left(\mu \ln \frac{L}{l}\right) \sim T, \quad T \gg 1.$$

All this enables us to analyze the distribution function f_1. Below, we extend this analysis up to the leading orders in the exponents. For small amplitudes $p < 2\pi\nu D/[L^2 \ln L/l]$, one obtains

$$f_1 \approx \exp\left(-\beta V p\left[1 - \frac{T}{2} + \ldots\right]\right) \times \begin{cases} \sqrt{\frac{V}{2\pi p}}, o, \\ V, u, \\ 2V, s, \end{cases} . \tag{76}$$

where T and β are defined in Eqs. (72) and (56), respectively.

In the opposite limit, $p > 2\pi\nu D/[L^2 \ln L/l]$, the distribution function takes the form

$$f_1 \sim V \exp\left(-\frac{\beta \pi^2 \nu D}{\ln(L/l)} \ln^2 T\right). \tag{77}$$

Equation (77) demonstrates that for all fundamental symmetries, - orthogonal, symplectic and unitary, - disorder makes the appearance of high-amplitude splashes of wave functions much more probable than one would expect from the Porter-Thomas formula and, as concerns the most extra-ordinary events, the tails take the logarithmically-normal form. When written for the orthogonal ensemble, the logarithmically-normal law in Eq. (77) coincides with the form of the asymptotics of the distribution of the local density of states in open systems found in Ref. 60, although our theory is developed for closed systems and is based on a completely different scheme of calculations.

Inverse participation numbers P_n derived on the basis of Eq. (49) show such a scaling with the size of a system which implies a multifractal structure. To find the moments P_n accurately enough, we have to take into account that although the crossover to the 0D case looks like the formal limit $T(p) \to 0$, the Porter-Thomas statistics fail unless the condition $pV \ll \sqrt{2\pi\nu D}$ is satisfied [see Eq. (63)]. Figure 2 illustrates how the large amplitude tail of the distribution function f_1 develops at higher values of p, and the exponentially large deviation from the Porter-Thomas distribution, we find, an indication that only the first few ratios P_n, $2 \leqslant n \ll \sqrt{2\pi\nu D}$, can be estimated using a finite polynomial expansion of $f_1(p)$ in a series in T. Having been treated in such a way, we reproduce corrections to the universal statistics found pertubatively in Ref. 78. Alternatively, we derive the higher order IPN's from Eqs. (49) using the saddle-point method. The moments P_n calculated in both ways are in a good agreement with each other and, in the leading order, can be represented as

$$P_n \approx \frac{\min\{c(n), [2\pi\nu D/\ln L/l]^n\}}{l^{2\delta} V} \left(\frac{1}{V}\right)^{\tau(n)/2}, \tag{78}$$

where

$$\tau(n) = (n-1) d^*(n), \quad d^*(n) \approx 2 - \frac{\beta^{-1} n}{4\pi^2 \nu D}. \tag{79}$$

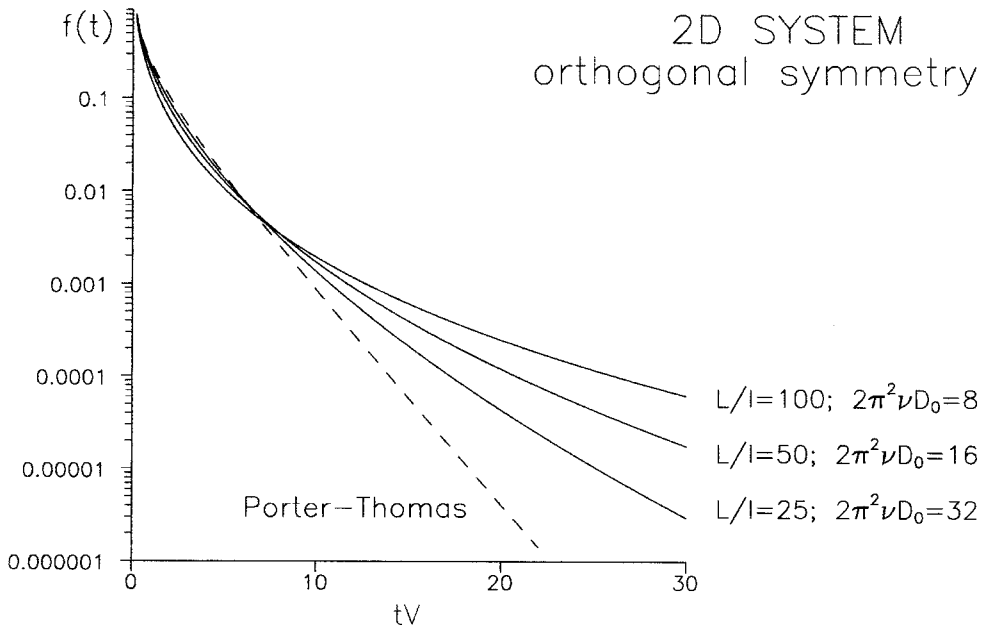

FIG. 2. Distribution function of a local density for 2D disordered system with time reversal symmetry (orthogonal ensemble) calculated for various levels of disorder.

In Eq. (78), $c_u(n)=n!$ in the unitary and $c_o(n)=(2n-1)!!$ in the orthogonal case; β is specified in Eq. (56).

The intermediate asymptotical scaling laws we end up with in Eqs. (78) and (79) manifest the multifractal behavior of quantum states. The set of indices $\tau(n)$ determines the spectrum of fractal (Reny) dimensions $d^*(n)$. In a full agreement with its name, the multifractality indicates that the density of a wave function may be imagined as distributed over some tree whose Hausdorf dimension decreases with increasing the length scale. In truly conformally invariant theories,[66] this property might be traced both by enlarging the system size L for a fixed amplitude of the wave function, or by looking at increasingly growing density peaks for a fixed L. Both ways of moving through the increasing density (p) or length scale (L) would lead to the selection of a ''current'' value of fractal dimension $d^*(n_*)$ determined by a typical n_* which corresponds to the typical wave functions living at this scale. In disordered systems we study in this article, the process of moving along the n-axis of the function $\tau(n)$ cannot last indefinitely, since we should meet one of two obstacles: the limiting value of the density, $p_{\max}\sim(l\lambda)^{-1}/\ln^2 L/l$, or the localization length, and the effective dimensions at large n's should start saturating in order to remain positive, $d^*>0$.

IX. SEMICLASSICAL SOLUTION OF THE TRANSFER-MATRIX METHOD AND PRELOCALIZED STATES IN A SHORT DISORDERED WIRE

The models of disorder in one dimension are explored the most, and there is a lot known about the localization effects in one-dimensional and quasi-one-dimensional (Q1D) wires. In particular, it is well known[79,80] that all quantum states of a particle in a disordered Q1D system are localized, even when disorder is weak. In really one-dimensional objects, the localization length is hardly distinguishable from the classically determined mean free path l. In wires with cross-sectional width w (or area w^2) which is much larger than the wavelength λ (or λ^2), the localization length, L_c, is as large as the number of ''transverse channels'' $N=(w/\lambda)^{d-1}$,[80,56]

$$L_c = \beta 2\pi\nu D \sim (w/\lambda)^{d-1} l \sim Nl, \tag{80}$$

where β is specified by Eq. (56) and the effective 1D density of states ν is determined as the local density of states integrated over the cross-section. In the following, we also redefine the variable p as integrated over the wire cross-section, $p \to w^{d-1}p$, so that it is measured in units of the inverse length. When $w \gg \lambda$, the localization length in Eq. (80) can be much longer than the mean free path l, and the typical (mean value) of the conductance of such a wire, $g = L_c/L$, is large, $g \gg 1$. This allows us to consider short Q1D wires with the length $l < L < L_c$ as typically metallic, and apply to their studies the non-linear σ-model approach. To avoid discussions of a dimensional crossover, we also assume that $w < l$.

It would be a straightforward procedure to use the transfer-matrix method[81] for solving the σ-model in one dimension.[56] It consists in projecting the one-dimensional field theory of the supermatrix $Q(x)$ onto the quantum-mechanical problem of calculation of the Green function of a ''particle'' living on the degeneracy space of the σ-model and an imaginary time ix. To solve such a problem comprehensively, one has to find the full spectrum of ''energies'' and ''eigenstates'' of the corresponding Schrödinger equation determined on the Q-space. Its lowest ''energy'' is nothing but the inverse localization length, L_c^{-1} and the knowledge of the low-lying modes in such a ''quantum mechanics'' is necessary when studying the long-range properties of the system. The problem of statistics of wave functions in disordered quasi-1D wires has been treated in this context by Mirlin and Fyodorov[58] and solved in two asymptotical regimes: of fluctuations with relatively small amplitudes in short wires, and finite-amplitude fluctuations in infinitely long wires. As regarding the statistics of densities $p \sim V^{-1}$ in wires which are much shorter than the localization length, it occurs very close to the universal Porter-Thomas distribution discussed in Eqs. (28) and (46), which is natural to expect for typical states in the metallic regime. For long wires with $L \gg L_c$ and $g \ll 1$, Ref. 58 gives the distribution $f_1(p)$ in the unitary ensemble which is described by the function of a density p normalized by the localization length,

$$f_1(p) \propto \mathrm{K}_1^2(4\sqrt{pL_c}) + \mathrm{K}_0^2(4\sqrt{pL_c}) \propto \sqrt{\frac{L_c}{p}}\,\exp(-4\sqrt{pL_c}), \tag{81}$$

where K_n are modified Bessel functions. Such a scaling law is also naively expected, since it describes behaviour of the states which live at the length scale L_c and have a normalizable density.

What is not that obvious in the problem of statistics of quantum states in disordered wires, is that there exist a small number of prelocalized states even in the metallic regime, when $L \ll L_c$ and $g \gg 1$, which have an anomalously large local amplitude of wave functions. These are described by the asymptotical form of the distribution function which resembles that in the infinite wire: It is dominated by the exponential term in which the density p scales with the localization length and which is independent of the wire length L. In this section, we use the saddle-point method to derive the statistics of such prelocalized states and to describe their spatial structure. Reciting the discussion of two previous paragraphs, the saddle-point calculation in Q1D is nothing but the *''quasiclassical'' solution* of the effective Schrödinger equation on the Q-space[33,56] which appears in the *transfer-matrix method*, and the calculational procedure consists of the steps described by Eqs. (55)–(58),(62) and (66) in Section VII.

First of all, we have to solve the Liouville equation on the vacuum state,

$$\partial_x^2 \theta_p(x) = -\frac{p}{\pi\nu D}\,\exp\{-\theta_p\}, \tag{82}$$

and use its solution $\theta_p(x)$ when calculating the minimal free energy F_p. Due to the condition $\theta_p(x_1) = 0$ at the observation point x_1, the latter splits the wire with the length L into two (not

necessarily equal) intervals $0<x<L_{i=L,R}$. The form of $\theta_p(x)$ can be found separately in each of them. In one dimension, the differential equation in Eq. (82) can be solved exactly,[76] and we represent its general solution in the form

$$e^{-\theta_p}=\left[\frac{A_i}{\cos\{A_i\sqrt{T_i}(1-x/L_i)\}}\right]^2, \quad x>0; i=L,R. \tag{83}$$

The general form of this solution formally contains a singularity at $x_\infty=-L_i[\pi/(2A_i\sqrt{T_i})-1]$ located in the non-physical region $x<0$ which plays a role when one formulates the limitations to our theory. The requirement $x_\infty \gg l$ is related to the limitations on maximal values of gradients permitted by the use of only the lowest order gradient expansion in the free energy functional in Eq. (20). We shall discuss the consequences of this condition at the end of this chapter, assuming for a while that it is satisfied. If so, the consistency equations on the parameters A_i come from the boundary conditions $\partial_x\theta_p(L_i)=0$ at the edges and have the form

$$A_i=\cos(A_i\sqrt{T_i}), \tag{84}$$

where T_i are defined as

$$T_i=\frac{pL_i^2}{2\pi\nu D}. \tag{85}$$

The minimal value of the free energy can be found, in its turn, as

$$F_p=\beta\sum_{i=L,R}\frac{L_i p}{\sqrt{T_i}}[2\sqrt{1-A_i^2}-A_i^2\sqrt{T_i}]. \tag{86}$$

The pre-exponential factor J arising from the fluctuations in the vicinity of the vacuum state can be taken into account as well. As far as the condition $\theta_p=0$ at $x=x_1$ splits the interval $[0,L]$ into two pieces, the spectrum $\{\chi(n)\}$ of fluctuations in Eqs. (63)–(64) can be found in each interval separately, and we represent $J=J_LJ_R$ as a product of contributions from the left- and right-hand-side intervals with lengths $L_{L,R}$. Each of $J_{L,R}$ is determined by the eigenvalues of the Schrödinger equation in Eqs. (63),(64) with the symmetry-breaking potentials

$$U_i=\left[kT_i+q\left(\left[\frac{\sqrt{T_i}\pi/2}{1+\sqrt{T_i}}\right]\Big/\sin\left\{\frac{\sqrt{T_i}\pi/2}{1+\sqrt{T_i}}\frac{x}{L_i}\right\}\right)^2\right]L_i^{-2},$$

where $i=L,R$. When $T\ll 1$ (in the paragraph below, we omit indices L and R), these potentials can be treated perturbatively. Their first order corrections cancel due to the sum rule from Eq. (65), so that $J\approx 1+T^2\approx 1$. When $T\gg 1$, the same cancellation eliminates contributions from the high-excitation eigenvalues $\chi>(\pi/2L)^2T$, so that the important contribution comes from the low-energy part of the spectrum, $\chi<(\pi/2L)^2T$, where one can approximate

$$U\approx(\pi/2L)^2[k+k'/\sin^2(\pi x/2L)], \quad k'=k+q,$$

and the spectral problem can be solved exactly. To find the exact solution, one has to change variables from x to $y=\cot(\pi x/2L)$ and then seek for the eigenstates in the form $P_n(y^2)/(1+y^2)^{\delta(n)}$, where $P_n(y^2)$ are polynomials. This results in the set of eigenvalues $\chi(n)$, $0\leqslant n<T$,

$$\chi(n)=(\pi/2L)^2\{[2n+1/2+\sqrt{k'+1/4}]^2-k\}.$$

Being substituted into Eq. (62), this gives the pre-exponential factor J in the main order in $T_{L,R}$:

$$J \approx \exp\left(\sum_{i=L,R} \frac{1}{4} \ln T_i + \text{ const} \right) \approx C(T_L T_R)^{1/4}. \tag{87}$$

In general, the exact form of F_p in Eq. (86) based on the closed set of equations in Eqs. (83)–(85) can be studied numerically at any value of the parameters included, but a somewhat simpler analytical expression can be written in the asymptotical regions, also because we are able to analyze the effect of fluctuation around the saddle-point mainly for small and large amplitudes separately. First of all, we examine the limit of small amplitudes, $T_i < 1$, where the exact distribution has to match the random matrix theory results. At $T_i < 1$, the results of Eqs. ((84)–(86)) can be expanded into the series in T_i, which gives $A_i \approx 1 - \frac{1}{2} T_i + \frac{13}{24} T_i^2 + \ldots$ and

$$F_p \approx Vp\left(1 - \sum_{i=L,R} \frac{T_i L_i}{3L} + \ldots \right),$$

whereas the contribution from fluctuations can be neglected,[45] and we find that

$$f_1(p) \approx e^{-\beta F_p} \times \begin{cases} V, & u, \\ \sqrt{\dfrac{V}{2\pi p}}, & o. \end{cases} \tag{88}$$

Therefore, the Porter-Thomas formula which describes those amplitudes p which are $p < L^{-1}\sqrt{L_c/L}$. Otherwise, the second term of this expansion, VpT_i, becomes larger than unity and strongly affects the probability to detect a very high splash of the wave function attributed to the prelocalized state.

When

$$T = \frac{pL^2}{2\pi\nu D} \gg 1, \quad \text{i.e.,} \quad p > \frac{2\pi\nu D}{L^2} \sim \frac{g}{L}, \tag{89}$$

$e^{-\theta_p}$ develops at the length scale of $\xi = \sqrt{2\pi\nu D/p} \sim \sqrt{L_c/p}$, where it can be approximated as

$$e^{-\theta_p(x)} \sim (\xi/x)^2, \tag{90}$$

and becomes less sensitive to the presence of the boundaries. Indeed, being an image of a statistically averaged *envelope of the density of the prelocalized wave functions* $\varphi_p(x)$, the vacuum of the σ-model described by Eq. (90) is related to the quantum states with the density integrable at the short range scale,

$$|\varphi_p(x)|^2 \sim \frac{p}{w^{d-1}} e^{-\theta_p} \sim \frac{L_c/w^{d-1}}{x^2} \sim \frac{l/\lambda^2}{x^2}. \tag{91}$$

This behavior very much resembles the localization, with an important difference: It is not a conventional localization with exponential decay $\varphi(x) \propto \exp(-|x|/L_c)$ of the wave functions at large distances $x > L_c$, but only the power-law one.

The asymptotical regime of the distribution function in the limit of $T_i \gg 1$, i.e., of $p > g/L$, is thus described by the minimal free energy

$$F_p = 4\sqrt{\beta L_c p}\{1 - \delta_L - \delta_R\}, \quad \delta_{L(R)} \sim \frac{\pi^2}{8}\left[T_{L(R)}^{-1/2} - \frac{1}{2} T_{L(R)}^{-1} + \ldots \right], \tag{92}$$

and by the pre-exponential factor in Eq. (87). The applicability of the saddle-point method requires that the value of minimal free energy in Eq. (92) dominates over the contribution from fluctuation in Eq. (87), which is satisfied when the conductance of the wire is large, $g \approx L_c/L \gg 1$.

Another limitation to the applicability of the analysis presented above emerges from the requirement of a smoothness of the saddle-point solution, so that its characteristic length scale ξ should be longer than the mean free path, $\xi > l$. Otherwise, the singularity x_∞ of the equation in Eq. (83) comes too close to the physical part of the space. After taking into account that the variable p describes the wave function density integrated over the wire cross-section, we find that $\max[|\varphi_p|^2] \sim p/w^{d-1} < 1/l\lambda^{d-1}$. This restriction is quite natural[45] and is similar to what we wrote about the 2D systems: It limits the density of the wave function by the density of a state bound to a forward and backward scattered trajectory at the length scale of the mean free path (i.e., the inverse volume of the Hikami-box).

Finally, the probability to find an anomalously high splash of a wave function $p > g/L$ related to the power-law prelocalized states has the form

$$f_1(p) \approx C \frac{\sqrt{L_L L_R}}{L} \sqrt{\frac{L_c}{p}} \exp[-4\sqrt{\beta L_c p}\{1-\delta_L-\delta_R\}]. \tag{93}$$

In this asymptotical regime, the distribution function depends on the density normalized by localization length and is insensitive to the systems size, as one gets in the infinite wires.[58] Because of such a coincidence, one may aim to get the asymptotical functional form of f_1 using a less formal heuristic argumentation. We have made this attempt together with Kravtsov and Lerner[82] in the spirit of interpretation of localization results in disordered wires.[80] First of all, we assume that the high splash of the density at the coordinate x_1 is due to a prelocalized state located within the interval $[x_1-\xi, x_1+\xi]$ near this observation point. If so, we describe it as typically metallic in a shorter wire with the length ξ, with a typical occurrence obeying the Porter-Thomas law $A(p,\xi) \sim \exp(-p\xi)$ in such a reduced geometry. On the other hand, the chance to find such a state is very small. To estimate it, we can try to follow the evolution of a locally created wave packet which starts to spread diffusively all over the sample. At the short time scale, its spreading is dominated by the laws of classical random walks, so that the probability of finding a particle inside an interval $[x_1-\xi, x_1+\xi]$ after time $t > \xi^2/D$ passes is $\sim \exp(-tD/\xi^2)$. If a prelocalized state is formed within this interval, it can show up in the wave packet evolution at the time scale of about the Heisenberg time $t_H(\xi) \sim \alpha\hbar/\Delta(\xi) \sim \hbar\nu\xi$ (inverse mean level spacing) related to the length scale ξ, since this is when the classical regime of a progressively spreading particle density changes into quantum limit where the states are already formed in a finite volume ξ. Coming from the classical side, we estimate the expectation value to find a particle inside the interval as $B(\xi) \sim \exp(-t_H(\xi)D/\xi^2)$, which gives us the probability $A(p,\xi)B(\xi)$ to find a high density splash p.

When speaking about typical states in an infinite wire, we take $p \sim \xi^{-1}$ and find that the length scale ξ which we have to choose by assuming that $B \sim 1$ is the localization length $L_c \sim 2\pi\nu D$: that is where the classical diffusion is typically blocked by the quantum interference.[80]

If we study the anomalously dense states in a short wire with the length $L < L_c$, we have to find such a length scale $l \ll \xi < L$ that provides an optimum between two competing exponentially small factors A and B. The optimum corresponds to $\xi = \sqrt{\alpha\nu D/p} \sim \sqrt{L_c/p}$. Since it has any sense only when $\xi < L$, the above reasoning results in the functional form of f_1[82] similar to that in Eq. (93),

$$f_1(p) \sim \min_\xi \left[\exp\left\{ -p\xi - \alpha\frac{D\nu}{\xi} \right\} \right] \sim \exp(-2\sqrt{\alpha p D \nu}), \tag{94}$$

and which is valid in the same asymptotical regime as desribed by Eq. (89).

Note that both in the above-presented scenario of formation of prelocalized states and in the σ-model treatment of the eigenstates statistics, the high amplitude splashes of the density p are produced by the states which extend over the distances $\xi \sim \sqrt{L_c/p}$ larger than $1/p$. This means that, although we are speaking of the localization effects, the localization is not the only reason for the high amplitudes of the wave function. It is quite plausible that the statistics in Eq. (93) detect the rare events of caustics of randomly focused electron waves, whereas the role of localization is to ''return'' the wave ''back'' and to increase the probability of these caustics being formed. This is also the reason that the wire would be linked to bulk ''electrodes'', the statistics of the amplitudes would sufficiently change and take the logarithmically-normal asymptotics[83] with much more suppressed tails of a distribution.

X. CONCLUSIONS

In summary, we review the recent results on the statistical properties and spatial structure of chaotic wave functions in disordered systems obtained using the supersymmetric nonlinear σ-model approach. The use of the σ-model allows us not only to revise and recover the universal statistics of wave functions previously obtained by means of such a phenomenology as the random matrix theory, but also to go far beyond the universality limit. In particular, we give a full account of the properties of chaotic wave functions in the crossover regime between the fundamental symmetry classes (orthogonal and unitary) and in the regime when the localization effects become important. Concerning the latter case, our calculation enables us to find indications of prelocalized states (among the eigenstates of disordered cavities) which exist at any weak disorder and manifest themselves via deformed large-amplitude tails of the distribution function of the local wave functions density, as compared to the universal Porter-Thomas distributions. According to the cross-correlation functions we calculated above, at the short distances below the localization length, the prelocalized states in quasi-one-dimensional wires can be associated with a power-law localization (in contrast to the conventional one which is exponential), whereas in two dimensions they have nearly critical properties and possess all the accessories of multifractal behavior.

The common feature of all the effects discussed in the present article is that they have behind them large random semiclassical phases taken by a particle moving along a chaotic trajectory or undergoing a random walk. On one hand, the ability of a chaotic trajectory to fill the entire isoenergetic surface in the classical phase space predetermines some part of the answers. In unitary or orthogonal fundamental symmetry classes they may be digested just by using the knowledge that the classical counterpart of quantum dynamics is chaotic, whereas the account for localization effects is in many aspects based on the statistical properties of diffusive paths. On the other hand, the deviations from the universal statistics, such as the long-range correlation of the wave functions at low magnetic fields, as well as prelocalized states and multifractality, give us the examples where the application of conventional semiclassics meets restrictions from the discreteness of the spectrum of quantum object. The use of the supersymmetry method enables us to overcome this difficulty and to match the description of a quantum chaos and localization within a unified theoretical approach.

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Energy level correlations in disordered metals: Beyond universality

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This short review is concerned with energy level statistics in weakly disordered metallic grains. In particular, we concentrate on how these statistics deviate from the universal ones. Using a nonperturbative approach we evaluate the large frequency asymptotics of the two-point correlator of the density of states. This allows us to describe the behavior of the system at arbitrary times. © *1996 American Institute of Physics.* [S0022-2488(96)02010-5]

I. INTRODUCTION

A great variety of systems exhibit the phenomenon of quantum chaos. Amongst those most commonly studied are the neutron resonances of atomic nuclei,[1] Rydberg atoms in strong magnetic fields,[2] and electrons in weakly disordered metallic grains (quantum dots).[3] The energy spectrum as a whole is specific for each individual chaotic system. However, in contrast to integrable systems, each eigenstate is characterized only by its energy, rather than by a set of quantum numbers.[4] The variables in the corresponding Schroedinger equation do not separate, which prohibits its analytical solution. Therefore, the only reasonable description of highly excited eigenstates in chaotic systems is a statistical one.

The statistical approach assumes certain averaging. Sometimes, as with disorder, one can think about an ensemble of chaotic systems. In such cases ensemble averaging is sufficient. For an individual chaotic system, such as Rydberg atoms in a magnetic field averaging over a wide energy interval, is the only choice.

The quantities studied in the statistical approach to quantum spectra are various correlators of the density of states (DoS),

$$\nu(E)=\mathrm{Tr}\,\delta(E-H), \tag{1}$$

where H is the Hamiltonian of the system. It is natural to measure the energy difference in units of the mean level spacing Δ. Perhaps the most frequently studied is the dimensionless two-point DoS correlator,

$$R_2(s)=\Delta^2\left\langle \nu\left(E+\frac{s}{2}\Delta\right)\nu\left(E-\frac{s}{2}\Delta\right)\right\rangle -1, \tag{2}$$

where s is the dimensionless energy difference. As has already been mentioned, for disordered

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metals the statistical average denoted by $\langle \cdots \rangle$ can be performed over different realizations of the random Hamiltonian, while in general, the average can be taken over a wide energy band.

Associated with each particular chaotic system, there are typically two relevant energy scales. The first, E_c, is associated with the *classical* time scale $t_c = 1/E_c$ on which a density distribution in phase space becomes ergodic, i.e. spreads uniformly over the constant energy shell.[5] On these time scales time averages over a classical trajectory can be substituted by microcanonical averages. In a cavity in which a quantum particle scatters ballistically from a boundary, known as a chaotic billiard, the energy scale E_c is typically set by the frequency of the shortest periodic orbit, or the inverse flight time across the system. In a weakly disordered metallic grain, on the other hand, the classical energy scale is set by the inverse transport time, or Thouless energy $E_c = D/L^2$, where D denotes the classical diffusion constant, and L represents the system size.

The second energy scale is set by the mean energy level spacing $\Delta = 1/t_H$ and defines the Heisenberg time t_H. These energy scales can be combined into the dimensionless ratio,

$$g = E_c/\Delta \gg 1, \tag{3}$$

which represents the ''dimensionless conductance''[6] of a chaotic system. The ergodic time $t_c = 1/E_c$ sets the scale beyond which the details of the classical dynamics of the system become irrelevant (as long as the system is chaotic). Correspondingly for energy scales $s \ll E_c/\Delta = g$ the spectral statistics become universal, independent of the details of the underlying classical dynamics. To a very good approximation they are determined only by the global symmetries of the system, such as T-invariance, and coincide with the universal Wigner–Dyson level statistics of the corresponding random matrix ensembles:[7] Unitary (broken T-invariance), Orthogonal (spinless T-invariant systems), or Symplectic (T-invariant systems with spin-orbit interaction).[8,9] In the semiclassical limit, and in dimensions greater than one, the dimensionless conductance is large, $g \gg 1$, and universal statistics apply in a wide energy interval.

In metals, where the mean free path is much longer than the electron wavelength, the electronic motion can be considered semiclassically, and $g \gg 1$. Thus, the energy interval where the statistics are universal is indeed wide.

The first application of random matrix theory to disordered metals was made by Gorkov and Eliashberg.[10] More than a decade later Efetov[11] provided a microscopic justification for the use of random matrices by showing that spectral statistics in an ensemble of disordered metallic grains in the limit $g \to \infty$ are described by the zero dimensional supersymmetric nonlinear σ-model. The latter has been shown by Verbaarschot, Weidenmueller, and Zirnbauer[12] to be equivalent to random matrix theory.

Remarkably, even with no ensemble averaging (i.e., only energy averaging) spectral statistics of chaotic systems for small energy differences also become universal. This is supported by strong numerical[13,14] as well as recent analytical evidence.[15,16] Thus, universal spectral statistics are a ubiquitous feature of quantum chaos.

For random matrix ensembles, analytic expressions for $R_2(s)$ were obtained for all three ensembles by Dyson:[7]

$$R_2^U(s) = \delta(s) - \frac{1-\cos(2\pi s)}{2\pi^2 s^2}, \tag{4a}$$

$$R_2^O(s) = \delta(s) - \frac{1-\cos(2\pi s)}{2\pi^2 s^2} - \frac{d}{ds}\left(\frac{\sin \pi s}{\pi^2 s}\right)\int_1^\infty \frac{\sin \pi s t}{t}\,dt, \tag{4b}$$

$$R_2^S(s) = \delta(s) - \frac{1-\cos(2\pi s)}{2\pi^2 s^2} + \frac{d}{ds}\left(\frac{\sin \pi s}{\pi^2 s}\right)\int_0^1 \frac{\sin \pi s t}{t}\,dt. \tag{4c}$$

We would like to recall a formal but beautiful connection between energy spectra with universal Wigner–Dyson statistics and one dimensional fermions with interaction inversely proportional to the square of the distance.[17] These models are known as the Calogero–Sutherland models.[18,19] It was shown by Sutherland[18] that each of the two-point correlation functions $R_2(s)$ shown in Eq. (4) coincide with the density-density correlation function of one of the Calogero–Sutherland models if the energy separation s is associated with the spatial separation between quantum particles r. In the Unitary case, after such a substitution, $R_2(s)$ gives the density correlator of noninteracting particles, while the Orthogonal (Symplectic) correlators correspond to those of the fermions that attract (repel) each other with a certain strength. Indeed a similar analogy extends even beyond universality (see the discussion in Sec. VII).

The robust feature of the universal (Wigner–Dyson) level statistics is the rigidity of the energy spectrum which leads to the following characteristic properties:

1 The probability of finding two energy levels separated by a distance $s \ll 1$ vanishes in the limit $s \to 0$.
2 The typical fluctuation of the number of levels inside some window of width $N\Delta$ as measured by the variance scales in proportion to $\ln N$. This contrasts with a linear dependence on N expected for systems in which neighboring levels are uncorrelated.
3 Both the monotonic and the oscillatory parts in the two-point correlator $R_2(s)$ shown in Eq. (4) decay only algebraically.

Spectral rigidity in the dimensionless two level structure factor,

$$S(\tau) = \int_{-\infty}^{\infty} ds e^{is\tau} R_2(s), \tag{5}$$

is manifest in the vanishing of $S(\tau)$ in the limit $\tau \to 0$, while the algebraic decay of the oscillations in $R_2(s)$ leads to a singularity in $S(\tau)$ which appears at the (dimensionless) Heisenberg time, $t_H\Delta$. In the unitary case

$$S(\tau) = \begin{cases} |\tau|/(2\pi), & |\tau| \leqslant 2\pi, \\ 1, & |\tau| > 2\pi; \end{cases} \tag{6}$$

i.e., the derivative of $S(\tau)$ shows a discontinuity at $\tau = 0$ and $\tau = 2\pi$. In the symplectic case $S(\tau)$ itself diverges logarithmically as $\tau \to \pi$, while in the orthogonal case its third derivative is discontinuous at $\tau = 2\pi$.

Note that $S(\tau)$ determines the time evolution in quantum systems. For example, the probability of finding a quantum particle at the original point at a time τ after the start of the evolution is completely determined by $S(\tau)$.[20]

The universal description of spectral statistics of a given chaotic system is far from being exact. Features specific to a given system become more pronounced for large energy separations (which correspond to the short time dynamics). Universality of spectral statistics as well as deviations from it at short times have been the subject of numerous investigations.[13,14,21,22]

In order to understand short time $t \ll t_H$ dynamics one can consider spectral statistics smoothed over a frequency interval of order t^{-1}. For example the structure factor $S(\tau)$ is related to the two-point DoS correlation function $R_2(s)$ averaged over a frequency interval of width $\propto \tau^{-1}$. These smoothed correlation functions were studied in Ref. 23 by making use of a perturbation theory in $1/g$ (see, for example, Refs. 24 and 25). The zeroth order of this perturbation theory was found to coincide with the random matrix theory results of Eqs. (4) when rapidly oscillating terms like $\cos(2\pi s)$ are omitted. The corrections to the universal form of $R_2(s)$, though small in $1/g$, turned out to exceed the universal part for $s > g$.

Recently Kravtsov and Mirlin[26] obtained the corrections, leading order in s/g, to both the smooth and rapidly oscillating part of the two point correlation function at $s \ll g$. In this interval the nonuniversal corrections are small as compared to the universal results of Eqs. (4) [see Eq. (14) below].

In order to understand both the universal and system specific features of level statistics, not only at short times but also at times of the order of t_H, one has to evaluate $R_2(s)$ at arbitrary s without making additional smoothing. This however can not be done in the framework of the perturbation theory [for example, note that $\cos(2\pi s)$ can not be expanded in series in $1/s$].

Here we discuss the field-theoretical scheme that allows an evaluation of the nonperturbative contributions to $R_2(s)$ together with the perturbative ones, as well as a description of the dependence of the two level structure factor on g, and on the geometry of the grains at arbitrary times. This approach allows a generalization to the case of specific quantum systems without disorder. We will discuss this generalization very briefly at the end of the paper.

We would like to mention that Bogomolny and Keating[27] are developing an interesting alternative approach to the energy level statistics beyond universality which is based on the periodic orbit theory. However since this approach is not directly related with the statistics in disordered systems we will not discuss it here.

II. MAIN RESULTS

Here we study the high frequency $s \gg 1$ behavior of $R_2(s)$ retaining the oscillatory terms and monitor how the singularity in $S(\tau)$ that develops at the Heisenberg time is modified by the finite conductance g. To do so we will make use of the nonperturbative field theoretic approach to disordered metals based on the supersymmetric nonlinear σ-model introduced by Efetov.[11] For $s \gg 1$ (the relation between s and g can be arbitrary) we evaluate the σ-model functional integral by a stationary phase approximation. The oscillatory contribution to $R_2(s)$ is associated with a nontrivial saddle-point of the field theory.[28] Associated with this nonperturbative saddle-point are fluctuations which can be treated perturbatively. Their dependence on the same operator that controls the diagrammatic perturbation theory suggests a generality of the results which will be discussed in Sec. VIII.

For $s \gg 1$, $R_2(s)$ separates into a sum of the monotonic perturbative contribution, $R_{\rm p}(s)$ and the oscillatory nonperturbative contribution, $R_{\rm osc}(s)$,

$$R_2(s) = R_{\rm p}(s) + R_{\rm osc}(s). \tag{7}$$

Here the perturbative contribution is given by

$$R_{\rm p}(s,x) = \frac{1}{\alpha \pi^2} \Re \ \mathrm{Tr}\ P(s)^2, \tag{8}$$

where

$$P(s) = \frac{1}{-is - (D/\Delta)\nabla^2} \tag{9}$$

denotes the resolvent of the classical diffuson (Laplace) operator in the grain (D is the classical diffusion constant). The constant α is equal to 1, 2, and 1 for the Orthogonal, Unitary, Symplectic ensembles, respectively.[29]

We will show that the oscillatory terms for the three ensembles are given by[30]

$$R^U_{\rm osc}(s) = -\frac{\cos(2\pi s)}{2\pi^2 s^2} D(s), \tag{10a}$$

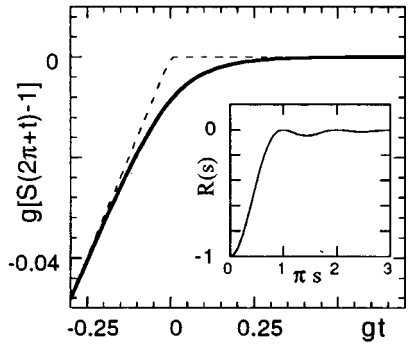

FIG. 1. Structure factor in the quasi-1D case for unitary symmetry (solid line) and the universal structure factor (dashed line). Inset: the two level correlator as a function of level separation.

$$R^{O}_{\mathrm{osc}}(s) = -\frac{\cos(2\pi s)}{2\pi^4 s^4} D^2(s,x), \tag{10b}$$

$$R^{S}_{\mathrm{osc}}(s) = \frac{\cos(\pi s)}{2s} D(s) + \frac{\cos(2\pi s)}{2\pi^4 s^4} D^2(s), \tag{10c}$$

$$D(s) = \prod_{\mu,\epsilon_\mu \neq 0} \left[1 + \left(\frac{s}{\epsilon_\mu} \right)^2 \right]^{-1}, \tag{10d}$$

where ϵ_μ denote the eigenvalues of the dimensionless diffusion operator $(D/\Delta)\nabla^2$. $D(s)$ can be expressed through the regularized determinant of $P(s)$ defined in Eq. (9):

$$D(s) = \left| \frac{\det' P(s)}{\det' P(0)} \right|^2. \tag{11}$$

Here $\det'$ denotes the determinant of the operator, from which the zero eigenvalue has been excluded.[31]

The perturbative part of $R_2(s)$ given by Eq. (8) can be expressed through the spectral determinant $D(s)$ by use of the formula

$$R_{\mathrm{p}}(s) = -\frac{1}{\alpha\pi^2 s^2} - \Re \frac{1}{2\alpha\pi^2} \frac{\partial^2 \ln[D(s)]}{\partial s^2}. \tag{12}$$

For a cubic sample in dimension $d<4$, with closed boundary conditions and $s \gg g$, we obtain the asymptotics

$$D(s) \to \exp\left[-\frac{\pi (s/\pi g)^{d/2}}{\Gamma(d/2) d \sin(\pi d/4)} \right]. \tag{13}$$

This shows that the amplitude of oscillations in $R_2(s)$ decays exponentially as a function of s in contrast to the universal algebraic behavior. This decay removes the singularity in $S(\tau)$ at the Heisenberg time $\tau_H = 2\pi$ and renders the function everywhere *analytic*. The scale of smoothening of the singularity is the inverse dimensionless conductance $1/g$. In real units it is the Thouless time $t_c = L^2/D$. In Figs. 1 and 2 we plot the structure factor around the Heisenberg time for a quasi-one dimensional sample in the unitary and symplectic cases, respectively.

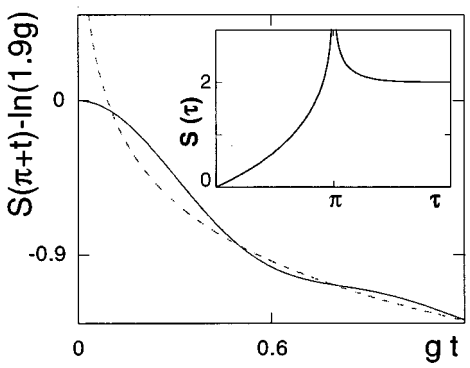

FIG. 2. The structure factor for the symplectic case in quasi-1D (solid line) and the universal result (dashed line). Inset: the universal structure factor.

For $1 \ll s \ll g$ the sums of Eqs. (10) and Eq. (8) provide the leading high frequency asymptotics of the universal result. For $s \gg g$ we recover the perturbative result $R_{\mathrm{p}}(s)$ in Eq. (8) found in Ref. 23.

Taking a closed cubic sample (Dirichlet boundary conditions), the eigenvalues of the dimensionless diffusion operator are given by $\epsilon_\mu = g\pi^2 \vec{n}^2$, where $\vec{n} = (n_1, \ldots, n_d)$ and n_i are nonnegative integers. Then, for frequencies smaller that the dimensionless conductance $1 \ll s \ll g$, the unitary ensemble yields the expression

$$R_2^U(s) = -\frac{\sin^2(\pi s)}{(\pi s)^2}\left[1 - \frac{s^2}{g^2}\sum_{\vec{n}} \frac{1}{(\pi^2\vec{n}^2)^2}\right]. \tag{14}$$

This coincides with the result of Kravtsov and Mirlin[26] who considered nonuniversal corrections to the Wigner-Dyson result of Eq. (4) for $s \ll 1$. In the common domain of applicability, $1 \ll s \ll g$, the two approaches lead to the same results for all three ensembles. These differ from the universal results shown in Eq. (4) by a correction which is as small as $(s/g)^2$. It is interesting to note that Eq. (14) for the unitary case seems to coincide with the result of Ref. 26 even at $s < 1$.

This completes the survey of the main results discussed in more detail below. The rest of paper is organised as follows. In Sec. III we will define the field theoretic construction which describes the statistical properties of weakly disordered metallic grains. We will identify the stationary points of the theory—one generates the standard diagrammatic perturbation theory while others control the dominant nonperturbative contributions. A general scheme to study the fluctuations around each point will be described. In Secs. IV, V, and VI we will obtain the high frequency asymptotics of $R_2(s)$ for the unitary, orthogonal, and symplectic ensembles, respectively. This will allow us to study the behavior of the structure factor near the Heisenberg time. In Sec. VII we make some remarks on our results. Finally, in Sec. VIII we will discuss what implications these results offer to the problem of general quantum chaotic systems.

III. FIELD THEORY OF DISORDERED METALS

As a model to describe the low energy degrees of freedom of electrons propagating in disordered conductors, the functional nonlinear σ-model was first proposed by Wegner.[32] A subsequent generalization by Efetov introduced superfields which obviated the need for replicas.[11] This development was not just convenient but proved to be necessary for describing correlations in the ergodic limit.[33] In this section we will review the microscopic derivation of the nonlinear

σ-model which will serve as the starting point for our investigation of level correlations. Since our aim is not to supplement the many reviews on the foundation of this method but rather to emphasize results that can be obtained from it we will keep the discussion brief and refer to Refs. 11,12, and 34 for a more detailed description.

The model describing a single electron moving in a random impurity potential $V(\vec{r})$ is described by the Hamiltonian

$$H=\frac{1}{2m}\left(\vec{p}-\frac{e}{c}\vec{A}\right)^2+V(\vec{r}), \tag{15}$$

where $\vec{A}(\vec{r})$ denotes the vector potential. For simplicity, we will assume the impurity potential to be δ-correlated and Gaussian distributed with a mean free time τ_{imp}:

$$\langle V(\vec{r})\rangle=0, \quad \langle V(\vec{r})V(\vec{r'})\rangle=\frac{1}{2\pi\nu\tau_{\mathrm{imp}}}\delta(\vec{r}-\vec{r'}). \tag{16}$$

The dimensions of the grain L are assumed to be much larger than the elastic mean free path $\ell\equiv v_F\tau_{\mathrm{imp}}\ll L$ so that the motion of the electron is diffusive.

The starting point is the representation of the generating function of Green functions as a functional integral over the 8-component superfields corresponding to advanced (A) and retarded (R) Green functions,

$$\Psi^p_{gd}(\vec{r})=\begin{pmatrix}\Psi^A_{gd}\\ \Psi^R_{gd}\end{pmatrix}, \quad \Psi^p_{g=1,d}=\begin{pmatrix}\chi^p_d\\ \chi^{p*}_d\end{pmatrix}, \quad \Psi^p_{g=2,d}=\begin{pmatrix}S^p_d\\ S^{p*}_d\end{pmatrix}. \tag{17}$$

Here, following Ref. 35 we introduced block notations. Superscript p refers to retarded/advanced components, subscript g refers to fermionic (F) components $\chi(\vec{r})$ and bosonic (B) components $S(\vec{r})$, and subscript d refers to time-reversal (complex conjugated) components. The introduction of equal numbers of bosonic and fermionic fields is a standard trick which obviates the need to introduce replicas and normalizes the generating function to unity. Expressed as a field integral, the generating function for two-point correlators takes the form

$$\mathcal{Z}(\hat{J})=\int D\Psi\ \exp\left[-\frac{i}{2}\int d\vec{r}\Psi^\dagger(\vec{r})\Lambda\left(\hat{G}^{-1}(\epsilon)-\frac{\hat{J}}{4\Delta}k\Lambda\right)\Psi(\vec{r})\right], \tag{18}$$

where

$$\hat{G}^{-1}(\epsilon)=\epsilon-\frac{s^+\Lambda}{2}-\frac{1}{\Delta}\hat{H}\left(\vec{p}-\frac{e}{c}\tau_3\vec{A}\right), \tag{19}$$

denotes the dimensionless matrix Green function with energy difference s between retarded (R) and advanced (A) blocks and $\hat{J}k\Lambda$ represents the source. Matrices

$$\Lambda=\begin{pmatrix}1&0\\0&-1\end{pmatrix}^p\otimes 1_g\otimes 1_d, \quad k=1^p\otimes\begin{pmatrix}1&0\\0&-1\end{pmatrix}_g\otimes 1_d, \quad \tau_3=1^p\otimes 1_g\otimes\begin{pmatrix}1&0\\0&-1\end{pmatrix}_d, \tag{20}$$

break the symmetry between the advanced/retarded, graded, and conjugate components, respectively. The operations of complex conjugation and transposition of supervectors are defined following Efetov,[11] while STr denotes the trace operation for supermatrices,

$$\mathrm{STr}\ M=\mathrm{Tr}\ M_{FF}-\mathrm{Tr}\ M_{BB}. \tag{21}$$

Equation (18) can be used to represent the two-point correlator of DoS fluctuations. If we choose the source to be a constant $\hat{J}=J$ and perform the ensemble averaging of Eq. (16) we obtain

$$R_2(s)=-\frac{\Delta^2}{\pi^2}\,\Re\,\frac{\partial^2}{\partial J^2}\langle\mathcal{Z}(\hat{J})\rangle_{\epsilon_0}\Big|_{J=0}. \tag{22}$$

Averaging over the disorder potential generates a quartic interaction of the fields $\Psi(\vec{r})$. If the disorder potential is weak, the fields vary only slowly in comparison to the electron wavelength, λ, and the problem can be treated within a semi-classical approximation. In this approximation the interaction can be decoupled by means of a Hubbard–Stratonovich transformation with the introduction of 8×8 supermatrix fields $Q(\vec{r})$ with the symmetry similar to that of the dyadic product $\Psi\otimes\Psi^{\dagger}$. As a result the Ψ integration becomes Gaussian and can be performed.

Further progress is possible within a saddle-point approximation. The manifold of saddle-points is defined by $Q=T^{-1}\Lambda T$, where matrices T occupy the symmetric space $\mathbf{H}=\mathbf{G}/\mathbf{K}$. The groups $\mathbf{G}$ and $\mathbf{K}$ depend on the ensemble.[12] For example, in the unitary ensemble $\mathbf{H}=\mathbf{U(1,1/2)}/\mathbf{U(1/1)}\times\mathbf{U(1/1)}$.[36] Allowing for slow spatial fluctuations of T and expanding to leading order in ℓ/L and $s\Delta\tau_{\rm imp}$, we obtain[11]

$$\langle\mathcal{Z}\rangle=\int d[Q]\exp(-S[Q]), \tag{23a}$$

$$S[Q]=\frac{\pi\nu}{8}\int d\vec{r}\,\mathrm{STr}\left[D\left(\nabla Q+i\frac{e\vec{A}}{c}[\tau_3,Q]\right)^2+2is^{+}\Delta\Lambda Q+iJ\Lambda kQ-\frac{x^2\Delta}{2}(\Lambda Q)^2\right], \tag{23b}$$

where Q matrices obey the nonlinear constraint $Q(\vec{r})^2=1$. Here, we have introduced an additional term containing x^2 into the action which plays the role of a regulator. Its effect will be to stabilise the stationary points which will arise in the evaluation of the integral in Eq. (23b). Ultimately, only after all the integrals have been performed, x^2 should be taken to zero. The integration measure for Q in the functional integral is the invariant measure on $\mathbf{H}$.

The large frequency asymptotics of $R_2(s)$ can be obtained from Eq. (23a) by use of the stationary phase method. Conventional diagrammatic perturbation theory corresponds to integrating over the small fluctuations of Q around Λ.[11] A systematic expansion can be obtained from the explicit parametrisation of the saddle-point manifold,

$$Q=\Lambda(1+iP)(1-iP)^{-1},\quad P=\begin{pmatrix}0 & B\\ \overline{B} & 0\end{pmatrix}, \tag{24}$$

where the matrix P describes deviations of Q from Λ. However, in Ref. 28 two of us showed that $Q=\Lambda$ is not the only stationary point on $\mathbf{H}$. In fact, it is possible to parameterize fluctuations around a general stationary point Q_0, where $Q=Q_0(1+iP_0)(1-iP_0)^{-1}$. Expanding the free energy in Eq. (23b) in powers of P_0 we would obtain the stationarity condition $\partial S/\partial P_0=0$.

This route however is inconvenient since the parameterization of P_0 will depend explicitly on Q_0. Instead it is convenient to perform a global coordinate transformation on $\mathbf{H}$ that maps Q_0 to Λ, $Q_0\to T_0^{-1}Q_0T_0=\Lambda$. Since all points on a symmetric space are equivalent by definition, this coordinate transformation preserves the invariant measure. In particular, let us concentrate on the matrices Λ and $-\Lambda k$ which both belong to $\mathbf{H}$. The corresponding terms in Eq. (23b) can be viewed as symmetry breaking sources. This transformation maps Λ to $Q_\Lambda=T_0^{-1}\Lambda T_0$ and Λk to $Q_{\Lambda k}=T_0^{-1}\Lambda kT_0$. Thus we can employ the parameterization of Eq. (24) with the *same* invariant measure but simply change the sources. As a result, using Eq. (22), we find

$$R_2(s)=\frac{1}{64V^2}\,\Re\int d[Q]\left[\int d\vec{r}\ \mathrm{STr}(Q_{\Lambda k}Q)\right]^2\exp(-S_{Q_\Lambda}[Q]), \tag{25a}$$

$$S_{Q_\Lambda}[Q]=\frac{\pi\nu}{8}\int d\vec{r}\ \mathrm{STr}\left[D\left(\nabla Q+i\frac{e\vec{A}}{c}[\tau_3,Q]\right)^2+2is^+\Delta Q_\Lambda Q-\frac{x^2\Delta}{2}(Q_\Lambda Q)^2\right]. \tag{25b}$$

The stationarity condition,

$$\frac{\partial}{\partial P}S_{Q_\Lambda}[Q]|_{P=0}=0, \tag{26}$$

implies that all the elements of Q_Λ in the AR and RA blocks should vanish [as can be seen from Eq. (24)].

This completes our formulation of the model. For each symmetry class we will find the stationary points of the effective action and generate a perturbative expansion around each point. In principle we could study the transition interval between different universality classes. However, for simplicity we will focus on the ''pure'' symmetry classes. We will begin by studying the Unitary case in some detail.

IV. UNITARY ENSEMBLE

In a strong magnetic field, the components of the $Q(\vec{r})$ matrices that do not commute with τ_3 acquire a mass—the Cooperon gap. For a strong enough field those modes with energies smaller than this gap are frozen out and can be neglected. In the pure unitary ensemble $[\tau_3,Q]=0$ and the magnetic field dependence is removed. In this case we can write an explicit parametrisation for the 4×4 supermatrices B and $\overline{B}$ in the form

$$B=\begin{pmatrix} a & 0 & i\sigma_1 & 0\\ 0 & a^* & 0 & -i\sigma_1^*\\ \sigma_2^* & 0 & ib & 0\\ 0 & \sigma_2 & 0 & ib^*\end{pmatrix},\quad \overline{B}=\begin{pmatrix} a^* & 0 & -\sigma_2 & 0\\ 0 & a & 0 & \sigma_2^*\\ -i\sigma_1^* & 0 & ib^* & 0\\ 0 & -i\sigma_1 & 0 & ib\end{pmatrix}. \tag{27}$$

The zeros in the ''off-diagonal'' elements reflect the absence of the Cooperonic degrees of freedom.

Besides the conventional saddle-point Λ, there is only one other $Q_\Lambda\equiv\widetilde{\Lambda}=-k\Lambda$ ($Q_{k\Lambda}=-\Lambda$) that satisfies the stationarity condition of Eq. (26). All other matrices from the saddle-point manifold contain nonzero elements in the AR and RA blocks. To obtain the high frequency asymptotics of $R_2(s)$ we must take into account both saddle points. Let us first consider the contribution of the usual saddle-point $Q_\Lambda=\Lambda$.

A. Λ point

Instead of calculating the generating function explicitly, we will consider the direct contribution of this point to the two-point correlator of DoS. The stationary point $Q_\Lambda=\Lambda$ is stable, and we set x^2 to zero before taking the integrals over B. Expanding the effective action Eq. (25b) to second order in B we obtain

$$S_\Lambda[Q]=\frac{\pi\nu}{8}\int d\vec{r}\ \mathrm{STr}[D\nabla\overline{B}\nabla B+i2s^+\Delta\overline{B}B]. \tag{28}$$

Employing the parametrisation above and performing the Gaussian integrals we obtain the expression previously found in Ref. 23,

$$R_{\mathrm{p}}(s)=\frac{1}{2\pi^2}\,\Re\ \mathrm{Tr}\ P(s)^2, \tag{29}$$

where $P(s)$ is defined in Eq. (9). For a cubic sample of size L the eigenvalues of the diffusion equation are given by $\epsilon_{\vec{n}}=g\pi^2\vec{n}^2$, where $\vec{n}=(n_1,\ldots,n_d)$, and n_i are non-negative integers.

At large frequencies $s\gg g$ one can substitute the sum by the integral, which gives the result

$$R_{\mathrm{p}}^{U}(s)\propto s^{d/2-2}. \tag{30}$$

B. $\tilde{\Lambda}$ point

Having obtained the contribution to R_2 from the conventional perturbation theory, let us now consider that from the second saddle-point. Substituting $Q_\Lambda=-k\Lambda$ and $Q_{k\Lambda}=\underline{-}\Lambda$ into Eq. (25), expanding both the action and the pre-exponent to the second order in B and $\bar{B}$, and introducing the Fourier components $B_{\vec{q}}$,

$$B(\vec{r})=\sum_{\vec{q}}\ e^{i\vec{q}\vec{r}}B_{\vec{q}}, \tag{31}$$

we obtain

$$\begin{aligned}R_{\mathrm{osc}}^{U}(s)=e^{2\pi i s}\Re\int d[B_{\vec{q}}]\Bigg[\sum_{\vec{q}}\ [a_{\vec{q}}a^{*}_{-\vec{q}}+b_{\vec{q}}b^{*}_{-\vec{q}}-\sigma^{*}_{1,-\vec{q}}\sigma_{1,\vec{q}}+\sigma^{*}_{2,-\vec{q}}\sigma_{2,\vec{q}}]\Bigg]^2\\ \times\exp\Bigg[-2\pi\sum_{\vec{q}}\ (P^{-1}_{\vec{q}}(-s,x^2)a_{\vec{q}}a^{*}_{-\vec{q}}+P^{-1}_{\vec{q}}(s,x^2)b_{\vec{q}}b^{*}_{-\vec{q}}-P^{-1}_{\vec{q}}(0,0)\\ \times[\sigma^{*}_{1,-\vec{q}}\sigma_{1,\vec{q}}-\sigma^{*}_{2,-\vec{q}}\sigma_{2,\vec{q}}])\Bigg].\end{aligned} \tag{32}$$

where $P^{-1}_{\vec{q}}(s,x^2)$ is given by

$$P^{-1}_{\vec{q}}(s,x^2)=-is+2x^2+g(\vec{q}L)^2, \tag{33}$$

and x is the regulator that we introduced in Eq. (23b) to ensure the convergence of the integrations.[37]

Since the action in Eq. (32) contains no Grassmann variables in the zero mode they must come from the pre-exponent. Therefore, out of the whole square of the sum in the pre-exponent only the terms containing all four zero mode Grassmann variables contribute. There are only two such terms. The evaluation of the Gaussian integrals is straightforward and generates products of the determinants of the diffusion operator.

Since the supersymmetry around $\tilde{\Lambda}$ is broken by s, integration over nonuniform modes yields a superdeterminant which differs from unity. The integration measure for Grassmann variables should be defined as

$$\prod_{\vec{q}}\ d\sigma_{1\vec{q}}d\sigma^{*}_{1\vec{q}}d\sigma^{*}_{2\vec{q}}d\sigma_{2\vec{q}}, \tag{34}$$

to enforce the correct sign. (One should keep in mind that the Fourier components with opposite $\vec{q}$ are not independent, and $\vec{q}$ in the product ranges over one half of the total vector space only.) In

an isolated sample the derivative of Q normal to the boundary must vanish, $\nabla Q_{\perp}=0$. For a d-dimensional cubic sample of size L with these boundary conditions we can write $\vec{q}=\pi\vec{n}/L$.

After integration we set x to zero and obtain

$$R^{U}_{\rm osc}(s)=\frac{\cos(2\pi s)}{2\pi^2 s^2}\widetilde{\prod_{\vec{n}\neq\vec{0}}}\left(1+\left(\frac{s}{\pi^2 g\vec{n}^2}\right)^2\right)^{-1}, \tag{35}$$

where the tilde signifies that the product should be taken over one half of the vector space. The product in Eq. (35) can be expressed through the spectral determinant of the diffusion operator.

In the contribution of the conventional saddle-point $Q_{\Lambda}=\Lambda$ the Green function of the same operator appears [see Eq. (29)]. The product (sum) over $\vec{n}$ should be interpreted as the product (sum) over the eigenvalues of the diffusion operator for more complicated boundary conditions.

In quasi-1D the product over momenta can be evaluated exactly.

$$R^{U}_{\rm osc}(s)=\frac{\cos(2\pi s)}{2\pi^2 s^2}\,\frac{s/g}{\sinh^2(\sqrt{s/2g})+\sin^2(\sqrt{s/2g})}. \tag{36}$$

In arbitrary dimensions the product can be evaluated in the limit of high frequency $s\gg g$ and expressed as the sum of logarithms. In the limit $s\gg g$ the sum can be substituted by an integral and we obtain

$$R^{U}_{\rm osc}(s)\to\frac{\cos(2\pi s)}{2\pi^2 s^2}\exp\left(-\frac{1}{2}\left[\frac{s}{\pi^2 g}\right]^{d/2}\int d\vec{t}\ln[1+\vec{t}^{-4}]\right), \tag{37}$$

where $\vec{t}=\pi\vec{n}\sqrt{g/s}$.

The full function $R_2(s)$ is given by the sum of contributions from both saddle-points, Eq. (35) and Eq. (29). At small frequencies $s\ll g$ we can expand the product in Eq. (35) in powers of s/g. Expanding to second order we obtain Eq. (14) which coincides with the result of Ref. 26.

C. Structure factor

The dimensionless two-level structure factor $S^{U}(\tau)$, defined in Eq. (5), has singularities at $|\tau|=2\pi$ and $|\tau|=0$, which are related to the large frequency asymptotics of $R^{U}_{2}(s)$. The former is related to $R^{U}_{\rm osc}(s)$ and the latter to $R^{U}_{\rm p}(s)$. We will address the singularity in $S^{U}(\tau)$ at the Heisenberg time $\tau=2\pi$.

For closed boundary conditions in quasi-1D the contribution to the structure factor from the Λ-point is given by

$$\begin{aligned}S^{U}(\tau)_{\rm p}&=\int_{-\infty}^{+\infty}\sum_{n=0}^{\infty}\frac{ds\ \exp(is\tau)}{(2\pi)^2}\left(\frac{1}{(-is+g\pi^2n^2)^2}+\frac{1}{(is+g\pi^2n^2)^2}\right)\\&=\frac{|\tau|}{2\pi}\sum_{n=0}^{\infty}\exp(-g\pi^2n^2|\tau|).\end{aligned} \tag{38}$$

The contribution from the nonperturbative saddle-point $\widetilde{\Lambda}$-point is given by

$$S^{U}(\tau)_{\rm osc}=\int_{-\infty}^{+\infty}\frac{ds\ \cos(2\pi s)\exp(is\tau)}{2\pi^2 s^2}\,\frac{s/g}{\sin(\sqrt{is/g})\sin(\sqrt{-is/g})}. \tag{39}$$

The integrand has simple poles at $s=\pm ig\pi^2n^2$ for $n=1,2,\ldots$ and a second order pole at $s=0$. Since the expansion of

$$\frac{s/g}{\sin(\sqrt{is/g})\sin(\sqrt{-is/g})} \tag{40}$$

begins at second order in s, the residue of the pole at $s=0$ is unaffected by the fact that g is finite. Therefore this pole always gives the contribution $-|t|/4\pi$, where $t=\tau-2\pi$. The contribution of the other poles can be evaluated straightforwardly and gives

$$\sum_{n=1}^{\infty} \frac{(-1)^n \exp(-\pi^2 n^2 g|t|)}{\pi^2 g n \sinh(\pi n)}. \tag{41}$$

Therefore the structure factor is given by

$$S^U(2\pi+t)_{\rm osc} = -\frac{|t|}{4\pi} + \sum_{n=1}^{\infty} \frac{(-1)^n \exp(-\pi^2 n^2 g|t|)}{\pi^2 g n \sinh(\pi n)}, \tag{42}$$

and is plotted in Fig. 1.

Even though Eq. (42) seems to depend on $|t|$, $S^U(2\pi+t)_{\rm osc}$ depends only on t^2 and is regular at $t=0$.

We can also estimate $S^U(2\pi)_{\rm osc}$ in any dimension. It is proportional to $1/g$ and is given by

$$S^U(2\pi)_{\rm osc} = \frac{1}{g}\int_{-\infty}^{+\infty} \frac{dz}{2\pi^2 z^2} \prod_{\vec{n}\neq\vec{0}} \left(1+\frac{z^2}{\pi^4 n^4}\right)^{-1}. \tag{43}$$

At large times we can keep only the first exponentials in the sums in Eq. (42) and Eq. (38) and obtain the asymptotic expression for the complete structure factor,

$$S(\tau) \approx \frac{|\tau|}{2\pi}\exp(-g\pi^2\tau) - \frac{1}{\pi^2 g \sinh(n)}\exp(-g\pi^2[\tau-2\pi]), \tag{44}$$

which shows the contribution of the $\tilde{\Lambda}$-point to be dominant.

V. ORTHOGONAL ENSEMBLE

Consider now ensembles which respect T-invariance—Orthogonal symmetry. In this case it is necessary to account for both Cooperon as well as diffuson degrees of freedom. However, there are still only two stationary points on the saddle-point manifold: Λ and $\tilde{\Lambda}=-k\Lambda$. To obtain the contribution of the $\tilde{\Lambda}$-point we can use the formula in Eq. (25b) with $Q_\Lambda=\tilde{\Lambda}$ and $Q_{k\Lambda}=-\Lambda$ as well as the parametrization of Efetov for the perturbation theory.[11] The matrices B and $\bar{B}$ are now given by

$$B=\begin{pmatrix} a_1 & a_2 & i\sigma_1 & i\sigma_2 \\ -a_2^* & a_1^* & -i\sigma_2^* & -i\sigma_1^* \\ \sigma_3^* & \sigma_4 & ib_1 & ib_2 \\ \sigma_4^* & \sigma_3 & ib_2^* & ib_1^* \end{pmatrix}, \quad \bar{B}=\begin{pmatrix} a_1^* & -a_2 & -\sigma_3 & -\sigma_4 \\ a_2^* & a_1 & \sigma_4^* & \sigma_3^* \\ -i\sigma_1^* & -i\sigma_2 & ib_1^* & ib_2 \\ -i\sigma_2^* & -i\sigma_1 & ib_2^* & ib_1 \end{pmatrix}. \tag{45}$$

This parametrization implies the following expansion of the action in Eq. (25b),

$$S_{\tilde{\Lambda}}[Q] = -2\pi i s + 2\pi \sum_{\vec{q}} \{P_{\vec{q}}^{-1}(-s,x^2)(a_{1,\vec{q}}a_{1,-\vec{q}}^* + a_{2,\vec{q}}a_{2,-\vec{q}}^*) + P_{\vec{q}}^{-1}(s,x^2)(b_{1,\vec{q}}b_{1,-\vec{q}}^* + b_{2,\vec{q}}b_{2,-\vec{q}}^*)$$

$$+P_{\vec{q}}^{-1}(0,0)(-\sigma^*_{1,-\vec{q}}\sigma_{1,\vec{q}}-\sigma^*_{2,-\vec{q}}\sigma_{2,\vec{q}}+\sigma^*_{3,-\vec{q}}\sigma_{3,\vec{q}}+\sigma^*_{4,-\vec{q}}\sigma_{4,\vec{q}})\}. \tag{46}$$

Once again, since there are no zero mode Grassmann variables in the action, they must come from the prefactor in Eq. (25a). Even though an expansion of the action to higher orders in B will generate Grassmann variables in the zero mode, these terms will contain higher powers of $1/s$ and are smaller than the leading terms at $s \gg 1$. To obtain all eight zero mode Grassmann variables in the prefactor in Eq. (25a) it is necessary to expand it to eighth order in B and $\overline{B}$,

$$[\mathrm{Str}(\Lambda Q)]^2 \approx 16[(\mathrm{STr}(\overline{B}B)^2)^2+2\mathrm{STr}(\overline{B}B)\mathrm{STr}(\overline{B}B)^3]. \tag{47}$$

The second term in this expression does not contribute to the highest weight term in Grassmann variables (it gives only the sixth order) and can be omitted. Then we obtain for the $\widetilde{\Lambda}$-point contribution to the two-point correlator of DoS,

$$R^O_{\mathrm{osc}}(s)=-\frac{\cos(2\pi s)}{2\pi^4 s^4}\widetilde{\prod_{\vec{n}\neq\vec{0}}}\left(1+\left(\frac{s}{\pi^2 g\vec{n}^2}\right)^2\right)^{-2}, \tag{48}$$

where, as before, the product goes over one-half of the total space.

VI. SYMPLECTIC ENSEMBLE

Finally, in the case of the symplectic ensemble there are three types of stationary points which correspond to singularities at $\tau=0$, π, and 2π in the structure factor. The singularity at $\tau=2\pi$ corresponds to $Q_\Lambda=\widetilde{\Lambda}=-k\Lambda$, and its contribution to $R_2(s)$ differs from the one for the Orthogonal case in Eq. (48) only by a minus sign.

The parametrization of the matrices B is and $\overline{B}$ is now given by

$$B=\begin{pmatrix} a_1 & a_2 & i\sigma_1 & i\sigma_2 \\ a_2^* & a_1^* & -i\sigma_2 & i\sigma_1 \\ \sigma_3 & \sigma_4 & ib_1 & -ib_2 \\ -\sigma_4 & \sigma_3 & ib_2^* & ib_1^* \end{pmatrix}, \quad \overline{B}=\begin{pmatrix} a_1^* & a_2 & \sigma_3^* & -\sigma_4^* \\ a_2^* & a_1 & \sigma_4^* & \sigma_3^* \\ -i\sigma_1^* & i\sigma_2^* & ib_1^* & ib_2 \\ -i\sigma_2^* & -i\sigma_1^* & -ib_2^* & ib_1 \end{pmatrix}. \tag{49}$$

Below we concentrate on the singularity at $\tau=\pi$. As we will show, it corresponds to a degenerate set on the saddle-point manifold.

Using Efetov's parametrization[11] we can represent Q_Λ as

$$Q_\Lambda=\hat{U}\begin{pmatrix} \cos\hat{\theta} & i\sin\hat{\theta} \\ -i\sin\hat{\theta} & -\cos\hat{\theta} \end{pmatrix}\widetilde{U},$$
$$\hat{\theta}=\begin{pmatrix} \theta_{11} & 0 \\ 0 & \theta_{22} \end{pmatrix}_g, \quad \theta_{11}=\begin{pmatrix} \theta_1 & \theta_2 \\ \theta_2 & \theta_1 \end{pmatrix}_d, \quad \theta_{22}=\begin{pmatrix} \theta & 0 \\ 0 & \theta \end{pmatrix}_d, \tag{50}$$

and the explicit form of $\hat{U}$ is not important for the present discussion.

The stationarity condition Eq. (26) implies $\sin\hat{\theta}=0$ for Q_Λ, so that terms linear in B in the effective action in Eq. (25b) vanish. It is satisfied if $\theta=0$ and $\theta_1=\pm\pi/2$, $\theta_2=\pm\pi/2$. The matrices $\hat{U}$ in Eq. (50) generate a continuous manifold of stationary points. One such matrix is

$$Q_\Lambda=\widetilde{\Lambda}_1=\Lambda\otimes\begin{pmatrix} \tau_1 & 0 \\ 0 & \mathbb{1} \end{pmatrix}_g, \quad [\tau_1]_d=\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}_d. \tag{51}$$

In Efetov's parametrization it corresponds to $\theta_1=\theta_2=\pi/2$ and all other variables equal to zero. With this source the expression for the effective action, Eq. (25b), becomes

$$S_{\tilde{\Lambda}_1}[Q]=\frac{\pi\nu}{8}\int d\vec{r}\ \mathrm{STr}\left[D(\nabla Q)^2+2is^+\Delta\tilde{\Lambda}_1 Q-\frac{x^2\Delta}{2}(\tilde{\Lambda}_1 Q)^2\right]. \tag{52}$$

In perturbation theory the expression for this effective action can be made more compact by rewriting B and $\bar{B}$ in Eq. (49) in terms of the vectors

$$\begin{gathered}\vec{a}^{\,T}=(a_1,a_1^*,a_2,a_2^*),\ \vec{a}^{\,T}=(b_1,b_1^*,b_2,b_2^*),\\ \vec{\sigma}_{12}^{T}=(\sigma_1,\sigma_1^*,\sigma_2,\sigma_2^*),\quad \vec{\sigma}_{34}^{T}=(\sigma_3,\sigma_3^*,\sigma_4,\sigma_4^*),\end{gathered} \tag{53}$$

and introducing Fourier components as in Eq. (31).

To second order in B, Eq. (52) has the form

$$S_{\tilde{\Lambda}_1}[Q]=-\pi is+\pi\sum_{\vec{q}}\left[\vec{a}_{\vec{q}}^{\dagger}T_{a,\vec{q}}\vec{a}_{\vec{q}}+\vec{b}_{\vec{q}}^{\dagger}T_{b,\vec{q}}\vec{b}_{\vec{q}}+\vec{\sigma}_{12,\vec{q}}^{\dagger}T_{\sigma_{12},\vec{q}}\vec{\sigma}_{12,\vec{q}}+\vec{\sigma}_{34,\vec{q}}^{\dagger}T_{\sigma_{34},\vec{q}}\vec{\sigma}_{34,\vec{q}}\right], \tag{54}$$

where

$$T_{a,\vec{q}}=\begin{pmatrix} P_{\vec{q}}^{-1}(0,x^2/2) & x^2 & -is/2 & -is/2\\ x^2 & P_{\vec{q}}^{-1}(0,x^2/2) & -is/2 & -is/2\\ -is/2 & -is/2 & P_{\vec{q}}^{-1}(0,x^2/2) & x^2\\ -is/2 & -is/2 & x^2 & P_{\vec{q}}^{-1}(0,x^2/2)\end{pmatrix},$$

$$T_{\sigma_{12},\vec{q}}=\begin{pmatrix} P_{\vec{q}}^{-1}(s/2,x^2/2) & 0 & 0 & -is/2-x^2\\ 0 & -P_{\vec{q}}^{-1}(s,x^2/2) & -is/2-x^2 & 0\\ 0 & is/2+x^2 & P_{\vec{q}}^{-1}(s,x^2/2) & 0\\ is/2+x^2 & 0 & 0 & -P_{\vec{q}}^{-1}(s/2,x^2/2)\end{pmatrix},$$

$$T_{b,\vec{q}}=P_{\vec{q}}^{-1}(s,x^2)\otimes\mathrm{diag}(1,1,1,1),\quad T_{\sigma_{34},\vec{q}}=-T_{\sigma_{12},\vec{q}}. \tag{55}$$

The integral over the variables Eq. (53) for each $\vec{q}$ yields

$$\sqrt{\frac{\det T_{\sigma_{12},\vec{q}}\det T_{\sigma_{34},\vec{q}}}{\det T_{a,\vec{q}}\det T_{b,\vec{q}}}}. \tag{56}$$

Evaluating the determinants we obtain

$$\begin{gathered}\det T_{a,\vec{q}}=P_{\vec{q}}^{-1}(s/2,x^2)P_{\vec{q}}^{-1}(-s/2,x^2)(P_{\vec{q}}^{-1}(0,0))^2,\\ \det T_{b,\vec{q}}=(P_{\vec{q}}^{-1}(s/2,x^2))^4,\\ \det T_{\sigma_{12},\vec{q}}=\det T_{\sigma_{34},\vec{q}}=(P_{\vec{q}}^{-1}(s/2,x^2))^2(P_{\vec{q}}^{-1}(0,0))^2.\end{gathered} \tag{57}$$

The integration over the nonuniform modes generates the product of expressions in Eq. (56) for different $\vec{q}$. Taking the limit $x^2 \to 0$ we obtain for this product

$$\prod_{\vec{q}\neq 0} \left[1 + \left(\frac{s\Delta}{D\vec{q}^2} \right)^2 \right]^{-1/2}. \tag{58}$$

The integration over the zero mode variables gives the factor $1/2|s|$. Since $\Im a_1$ and $\Im a_2$ do not enter the the effective action of Eq. (54) in the zero mode,[38] it might appear that the perturbative expansion will diverge. However, this is not so. The degenerate manifold of saddle-points of this type is compact, and the integration over $\Im a_1$ and $\Im a_2$ yields a finite result. The simplest way to obtain it is by making a comparison with the large frequency asymptotics of the Wigner-Dyson distribution. For a cubic sample $\vec{q} = \pi\vec{n}/L$, and we obtain the expression

$$R^S(s)_{\Lambda_1} = \frac{\cos(\pi s)}{2|s|} \widetilde{\prod}_{\vec{n}\neq\vec{0}} \left[1 + \left(\frac{s}{\pi^2 g n^2} \right)^2 \right]^{-1}, \tag{59}$$

where the tilde signifies that the product goes over $\vec{n}$ with non-negative entries only.

In quasi-1D we can obtain the leading contribution to the structure factor $S(\tau)$ around $\tau = \pi$,

$$S^s(t+\pi,0) = \int_0^\infty \frac{-4\sin^2(g|t|z)dz}{\sinh^2\sqrt{z} + \sin^2\sqrt{z}} + \ln(1.9g) + O\left(\frac{1}{g}\right). \tag{60}$$

The result is plotted in Fig. 2. In all dimensions the logarithmic divergence in the zero mode result is now cut off by finite g, and $S^S(\pi,0) \propto \ln g$.

VII. SOME REMARKS

To conclude, let us mention several remarks about these results.

1. The classification of physical systems into the three universality classes (Unitary, Orthogonal, and Symplectic) is, of course, an oversimplification. In practice there is always a time scale which determines the crossover from one ensemble to another. For example if a system is subject to a magnetic field the short time dynamics will appear Orthogonal while the long time behavior is Unitary. The characteristic time is set by the strength of the magnetic field.
   For a disordered metallic grain in a magnetic field this characteristic time is given by ℓ_H^2/D. For frequencies larger than D/ℓ_H^2 the system effectively becomes Orthogonal. This implies that even if we neglect the spatially nonuniform fluctuations of the Q-matrix the cusp in $S(\tau)$ at $\tau = 2\pi$ will be washed out on the scale of $\Delta\ell_H^2/D$ [although there will still remain a jump in the third derivative of $S(\tau)$]. For the system to behave as Unitary for frequencies of order g the magnetic length ℓ_H must be shorter than the size of the system. Spin-orbit interaction that causes the Orthogonal to Symplectic crossover can be considered in a similar way.
2. A rounding off of the singularity in $S(2\pi)$ is also present in the random matrix model with preferred basis.[39,40] However, our results differ from those in Ref. 40 substantially. This means that finite g is not equivalent to finite temperature for the corresponding Calogero-Sutherland model.[17] In fact, the relation of Eq. (12) between the smooth and the oscillatory parts of the two-point correlation function is similar to the one for the density-density correlation function of the Calogero-Sutherland model in a smooth potential $U(E)$ (such that one can neglect back-scattering). Equation (10) can be recovered if the random potential is determined by the correlation function $\langle U(E)U(E+s\Delta)\rangle \propto \Re\Sigma_{\mu\neq 0}(-is+\epsilon_\mu)^{-2}$.

This can be checked from the bosonization of the Calogero-Sutherland Hamiltonian where, in the limit $\epsilon_\mu \gg 1$, the assumption that back-scattering is absent is justified.

VIII. CONCLUSIONS AND PERSPECTIVES

We have described in some detail the calculation of nonuniversal corrections to the two-point density correlation function $R_2(s)$ for an ensemble of disordered metallic grains with the same conductance g and the same geometry. Using ensemble averaging we have evaluated this function for large s: $s \gg 1$. This enabled us to describe the rounding off of the singularity in the structure factor $S(\tau)$ present in the universal limit at $\tau \to 0$ and $\tau \to \tau_H$.

The main conclusion is that this nonuniversal behavior is determined by the spectral properties of the diffusion (Laplace) operator for a given geometry. In particular, the non-oscillatory part of the two-point correlation function is determined by the trace of the resolvent of this operator, while the part that oscillates as $\cos(2\pi s)$ is given by its spectral determinant. As a result, the two parts of $R_2(s)$ are connected by the relation shown in Eq. (12).

The diffusion operator is a purely classical one. Nevertheless, the structure of the supersymmetric σ-model allows us to take into account quantum mechanical interference to some extent. This can be seen from the consideration of T-invariance. The latter is violated by a magnetic field. The magnetic field manifests itself in quantum dynamics through two effects: (1) through the Aharonov-Bohm effect which affects the interference of different Feynman paths and does not alter the classical dynamics, and (2) through the Lorentz force. At weak fields the first effect dominates and governs the crossover of spectral statistics from the orthogonal to unitary ensemble, although classically they are equivalent. In the σ-model formalism T-invariance manifests itself through the additional diffusion mode—the Cooperon. From the semiclassical point of view this difference is due to the fact that, given a trajectory in phase space, the inversion of time transforms it to a different trajectory which in the orthogonal case is characterized by the same Feynman amplitude. This multiplicity of equivalent trajectories can therefore be taken into account by the field theoretic approach.

In general, the σ-model approach seems to be capable of describing systems where the classical limit exists modulo constant degeneracy of Feynman amplitudes. To understand what we mean consider a quantum mechanical return probability. It is given by the double sum over the Feynman paths $\Sigma_{i,j} A_i A_j^*$ where A_i is the Feynman amplitude of the ith path. If the classical limit exists, in the limit when actions are large as compared to $\hbar$ this sum can be substituted by the sum of probabilities $\Sigma_i |A_i|^2$. Discrete symmetries of the system, such as T-invariance, can lead to the fact that the Feynman amplitudes of different paths are degenerate. If this degeneracy is finite and constant for different orbits, like in the case of T-invariance, it could be incorporated into the σ-model.

The results which have been derived here are correct only in the leading order in g^{-1}. There definitely exist quantum corrections which may be referred to as weak localization corrections. It should be mentioned, however, that the sum of these corrections does not reduce to the renormalization of the diffusion constant D.

Here we discussed only the case of an ensemble of disordered quantum dots. Recently it became clear that a similar analysis based on a σ-model approach can be made for individual chaotic systems with a given Hamiltonian H.[28,15,41,16,42] As mentioned earlier, for a given chaotic systems one can use only energy averaging for constructing statistics of energy levels. Nevertheless, a σ-model can be derived for each individual system,[15,16] and results similar to Eq. (10) and Eq. (12) can be obtained.[16,42] The main difference between the general case and that of disorder is that the diffusion operator is substituted by the classical time evolution operator of the system

$$\hat{\mathscr{L}} = \sum_i \left(\frac{\partial H}{\partial p_i} \frac{\partial}{\partial q_i} - \frac{\partial H}{\partial q_i} \frac{\partial}{\partial p_i} \right), \tag{61}$$

where q_i and p_i are, respectively, canonical coordinates and canonical momenta of the system. The eigenvalues of this operator determine the spectral determinant $D(s)$ in Eq. (10d) in the same way as the eigenvalues of the diffusion operator do for a disordered grain.

In common with the diffusion operator in a closed grain, $\hat{\mathscr{L}}$ has a zero eigenvalue which corresponds to the ergodic state and manifests the conservation of the total probability. The nonuniversal part of the two point correlation function R_2 is given by the other (nontrivial) eigenvalues of $\hat{\mathscr{L}}$.

In contrast to the diffusion operator, the operator $\hat{\mathscr{L}}$ acts on the functions defined in phase space rather than in just coordinate space. Moreover, it is very important to realise that $\hat{\mathscr{L}}$ describes *time irreversible* dynamics and its nontrivial eigenvalues acquire a finite real part. This real part appears as a result of the regularization of the operator $\hat{\mathscr{L}}$. Further details of this generalization can be found elsewhere.[42]

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Riemannian symmetric superspaces and their origin in random-matrix theory

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Gaussian random-matrix ensembles defined over the tangent spaces of the large families of Cartan's symmetric spaces are considered. Such ensembles play a central role in mesoscopic physics, as they describe the universal ergodic limit of disordered and chaotic single-particle systems. The generating function for the spectral correlations of each ensemble is reduced to an integral over a Riemannian symmetric superspace in the limit of large matrix dimension. Such a space is defined as a pair $(G/H, M_r)$, where G/H is a complex-analytic graded manifold homogeneous with respect to the action of a complex Lie supergroup G, and M_r is a maximal Riemannian submanifold of the support of G/H. © *1996 American Institute of Physics.* [S0022-2488(96)00710-4]

I. INTRODUCTION

The mathematics of supersymmetry, though conceived and developed in elementary particle theory, has been applied extensively to the physics of disordered metals during the past decade. Improving on earlier work by Wegner,[1,2] Efetov[3] showed how to approximately map the problem of calculating disorder averages of products of the energy Green's functions for a single electron in a random potential, on a supersymmetric nonlinear σ model. Later it was shown[4] that the same nonlinear σ model describes the large-N limit of a random-matrix ensemble of the Wigner–Dyson[5] type. Since then, Efetov's method has evolved into a prime analytical tool in the theory of disordered or chaotic mesoscopic single-particle systems. Competing methods are limited either to the diffusive regime (the impurity diagram technique), or to isolated systems in the ergodic regime (the Dyson–Mehta orthogonal polynomial method), or to quasi-one-dimensional systems (the DMPK equation). In contrast, Efetov's method is applicable to isolated and to open systems in the diffusive, ergodic, localized, and even ballistic regime, to both spectral correlations and transport properties, and it can, in principle, be used in any dimension. This versatility has engendered a large body of nontrivial applications, many of which are outside the range of other methods. Of these, let me mention (i) the Anderson transition on a Bethe lattice,[6–8] (ii) localization in disordered wires,[9–13] (iii) multifractality of energy eigenstates in two dimensions,[14–16] (iv) weak localization and conductance fluctuations of chaotic billiards strongly coupled to a small number of scattering channels,[17,18] and, most recently, (v) a theoretical physicist's proof of the Bohigas–Giannoni–Schmit conjecture for chaotic Hamiltonian systems.[19,20]

In spite of these manifest successes, Efetov's supersymmetry method has been ignored (for all that I know) by mathematical physicists. This is rather unfortunate for several reasons. First, an infusion of mathematical expertise is needed to sort out some matters of principle and promote the method to a rigorous tool. Second, various extensions of currently available results seem possible but have been hindered by the lack of mathematical training on the part of the condensed matter theorists applying the method. And third, the geometric structures underlying Efetov's nonlinear σ models are of exquisite beauty and deserve to be studied in their own right. Part of the reason why neither mathematicians nor mathematical physicists have monitored or contributed to the devel-

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opment, may be that there does not exist a concise status report that would appeal to a mind striving for clarity and rigor. Hence the first, and very ambitious, motivation for getting started on the present paper was to make an attempt and partially fill the gap.

Another objective is to report on a recent extension of the supersymmetry method to random-matrix theories beyond the standard Wigner–Dyson ones. In her study of Anderson localization in the presence of an A–B sublattice symmetry, Gade[21] noticed that the manifold of the nonlinear σ model is promoted to a larger manifold at zero energy. The same phenomenon occurs in the chiral limit of the QCD Dirac operator at zero virtuality.[22] For several years it remained unclear how to handle this enlargement of the manifold in the supersymmetric scheme. (Gade used the replica trick instead of supersymmetry.) The key to solving the problem can be found in a paper by Andreev, Simons, and Taniguchi,[23] who observed that what one needs to do is to avoid complex conjugation of the anticommuting variables. In the present paper I will elaborate on this observation and cast it in a concise mathematical language. Moreover, I will show that the same technical innovation allows one to treat the random-matrix theories that arose[24,25] in the stochastic modeling of mesoscopic metallic systems in contact with a superconductor.

An outline of the basic mathematical structure is as follows. Consider a homogeneous space G/H, where G and H are complex Lie supergroups, and regard G/H as a complex-analytic (p,q)-dimensional supermanifold in the sense of Berezin–Kostant–Leites.[26,27] To integrate its holomorphic sections, select a closed, oriented, and real p-manifold M_r contained in the support $M=G_0/H_0$ of the supermanifold. The natural (invariant) supergeometry of G/H induces a geometry on M_r by restriction. If this geometry is Riemann and M_r is a symmetric space, the pair $(G/H,M_r)$ is called a Riemannian symmetric superspace. This definition will be shown to be the one needed for the extension of the supersymmetry method beyond Wigner–Dyson. The difficulties disordered single-particle theorists had been battling with were caused by the fact that the exact sequence

$$0\rightarrow \text{nilpotents}\rightarrow G/H\rightarrow M\rightarrow 0,$$

does not, in general, reduce to an exact sequence of sheaves of *real-analytic* sections terminating at the Riemannian submanifold M_r.

When integrating the invariant holomorphic Berezin superform on G/H, one must pay careful attention to its coordinate ambiguity. This subtle point is reviewed in Sec. II A. After a brief reminder of the procedure of Grassmann-analytic continuation (in Sec. II B), the complex Lie supergroups $\mathrm{Gl}(m|n)$ and $\mathrm{Osp}(m|2n)$ (in Sec. II C), and Cartan's symmetric spaces (in Sec. II E), the details of the definition of Riemannian symmetric superspaces are given in Sec. II F. Table II lists the large families of these spaces.

Section III, the largest of the paper, treats the Gaussian random-matrix ensemble defined over the symplectic Lie algebra $\mathrm{sp}(N)$, by an adaptation of Efetov's method. A simple example (Sec. III A) illustrates the general strategy. Details of the method, including a complete justification of all manipulations involved, are presented in Secs. III B–III F. Theorem 3.3 expresses the Gaussian ensemble average of a product of n ratios of spectral determinants as a superintegral. Theorem 3.4 reduces this expression to an integral over the Riemannian symmetric superspace $\mathrm{Osp}(2n|2n)/\mathrm{Gl}(n|n)$ with $M_r=(\mathrm{SO}^*(2n)/\mathrm{U}(n))\times(\mathrm{Sp}(n)/\mathrm{U}(n))$, in the limit $N\rightarrow\infty$.

According to Cartan's list, there exists 11 large families of symmetric spaces. Ten of these correspond to universality classes that are known to describe disordered single-particle systems in the ergodic regime.[24,25] The class singled out for detailed treatment in Sec. III describes mesoscopic normal-superconducting hybrid systems with time-reversal symmetry broken by a weak magnetic field. The remaining nine classes are briefly discussed in Sec. IV. Each of them is related, by the supersymmetry method, to one of the large families of Riemannian symmetric superspaces of Table II. A summary is given in Sec. V.

II. RIEMANNIAN SYMMETRIC SUPERSPACES

A. The Berezin integral on analytic supermanifolds

Let $A(U)$ denote the algebra of analytic functions on an open subset U of p-dimensional real space. By taking the tensor product with the Grassmann algebra with q generators one obtains $A(U)\otimes\Lambda(\mathbb{R}^q)$, the algebra of analytic functions on U with values in $\Lambda(\mathbb{R}^q)$. Multiplication on $\Lambda(\mathbb{R}^q)$ is the exterior one, so the algebra is supercommutative (or graded commutative). The object at hand serves as a model for what is called a real-analytic (p,q)-dimensional supermanifold (or graded manifold[28]) in the sense of Berezin, Kostant, and Leites (BKL);[26,27] which, precisely speaking, is a sheaf of supercommutative algebras $\mathscr{A}$ with an ideal $\mathscr{N}$ (the nilpotents), such that $M\simeq\mathscr{A}/\mathscr{N}$ is an analytic p-manifold and on a domain $U\subset M$, $\mathscr{A}$ splits as $A(U)\otimes\Lambda(\mathbb{R}^q)$. The global sections of the bundle $\mathscr{A}\to M$ are called superfunctions, or functions for short. M is called the underlying space, or base, or support, of the supermanifold. M will be assumed to be orientable and closed ($\partial M=0$).

The calculus on analytic supermanifolds is a natural extension of the calculus on analytic manifolds. Functions are locally expressed in terms of (super-)coordinates $(x;\xi):=(x^1,\ldots,x^p;\xi^1,\ldots,\xi^q)$, where $x^i(\xi^j)$ are even (resp., odd) local sections of $\mathscr{A}$. If $(x;\xi)$ and $(y;\eta)$ are two sets of local coordinates on domains that overlap, the transition functions $y^i=f^i(x;\xi)$ and $\eta^j=\varphi^j(x;\xi)$ are analytic functions of their arguments and are consistent with the $\mathbb{Z}_2$ grading of $\mathscr{A}$.

In what follows the focus is on the theory of integration on analytic supermanifolds. Recall that on p-manifolds the objects one integrates are p-forms and their transformation law is given by

$$dy^1\wedge\cdots\wedge dy^p=dx^1\wedge\cdots\wedge dx^p\,\mathrm{Det}\left(\frac{\partial y^i}{\partial x^j}\right).$$

The obvious (super-)generalization of the Jacobian $\mathrm{Det}(\partial y^i/\partial x^j)$ is the Berezinian[29]

$$\mathrm{Ber}\left(\frac{y,\eta}{x,\xi}\right):=\mathrm{SDet}\begin{pmatrix}\dfrac{\partial y^i}{\partial x^j} & \dfrac{\partial y^i}{\partial \xi^j}\\[2ex] \dfrac{\partial \eta_i}{\partial x^j} & \dfrac{\partial \eta_i}{\partial \xi^j}\end{pmatrix},$$

where SDet is the symbol for superdeterminant. Guided by analogy, one postulates that an integral superform ought to be an object $\widetilde{D}$ transforming according to the law

$$\widetilde{D}(y,\eta)=\widetilde{D}(x,\xi)\mathrm{Ber}(y,\eta/x,\xi). \tag{1}$$

A natural candidate would seem to be

$$D(x,\xi):=dx^1\wedge\cdots\wedge dx^p\otimes\partial_{\xi^1}\cdots\partial_{\xi^q},$$

which is a linear differential operator taking superfunctions f into p-forms $D[f]$ (∂_{ξ^i} denotes the partial derivative with respect to the anticommuting coordinate ξ^i). The p-form $D[f]$ can be integrated in the usual sense to produce a number. However, the transformation law for $D(x,\xi)$ turns out to be not quite (1), but rather

$$D(y,\eta)=D(x,\xi)\mathrm{Ber}(y,\eta/x,\xi)+\beta. \tag{2}$$

An explicit description of the term β on the right-hand side, here referred to as the *anomaly*, was first given by Rothstein.[30] It is nonzero whenever some even coordinate functions are shifted by nilpotent terms. Its main characteristic is that on applying it to a superfunction f, one gets a p-form that is *exact*: $\beta[f]=d(\alpha[f])$.

The existence of an anomaly in the transformation law for $D(x,\xi)$ leads one to consider a larger class of objects, namely, $\Lambda^p(M)\otimes_{\mathscr{A}}\mathscr{D}$, the sheaf of linear differential operators on $\mathscr{A}$ with values in the p-forms on M. [$\Lambda^p(M)\otimes_{\mathscr{A}}\mathscr{D}$ naturally is a right $\mathscr{A}$-module.] To rescue the simple transformation law (1) one usually passes from $\Lambda^p(M)\otimes_{\mathscr{A}}\mathscr{D}$ to its quotient by the anomalies.[30] In order for the integral to be well-defined over the quotient, one must take the functions one integrates to be compactly supported.

Sadly, this last option *is not available to us*. The functions that will be encountered in the applications worked out below, do not ever have compact support but are *analytic* functions instead. When integrating such functions, we need to work with the full transformation law (2), which includes the anomaly.

Another way of avoiding the anomaly is to arrange for the transition functions never to shift the even coordinates by nilpotents, by constructing a restricted subatlas.[31] However, because the concept of a restricted subatlas is somewhat contrived, this approach has been found to be of limited use in the type of problem that is of interest here.

To arrive at a definition of superintegration that is useful in practice, we proceed as follows. The supermanifold is covered by a set of charts with domains U_i and coordinates $(x_{(i)},\xi_{(i)})$ $(i=1,\ldots,n)$. On chart i let $\omega_i:=D(x_{(i)},\xi_{(i)})\circ\widetilde{\omega}_i$ with $\widetilde{\omega}_i$ a local section of $\mathscr{A}$, and let $\alpha_i \in \Lambda^{p-1}(M)\otimes_{\mathscr{A}}\mathscr{D}|_{U_i}$. Partition M into a number of consistently oriented p-cells $D_1,\ldots,D_n$, with D_i contained in U_i. For $i<j$ put $D_{ij}:=\partial D_i\cap\partial D_j$ and, if D_{ij} is nonempty and is a $(p-1)$-cell, fix its orientation by $\partial D_i=+D_{ij}+\cdots$.

Definition 2.1: A collection $\{\omega_i,\alpha_i\}_{i=1,\ldots,n}$ is called a *Berezin measure* ω if the conditions

$$\widetilde{\omega}_i/\widetilde{\omega}_j=\mathrm{Ber}(i/j), \tag{3}$$

$$\omega_i+d\alpha_i=\omega_j+d\alpha_j, \tag{4}$$

are satisfied on overlapping domains. The Berezin integral $f\mapsto\int_M\omega[f]$ is defined as

$$\int_M\omega[f]=\sum_{i=1}^{n}\int_{D_i}\omega_i[f]+\sum_{i<j}\int_{D_{ij}}\alpha_{ij}[f], \tag{5}$$

where $\alpha_{ij}=\alpha_i-\alpha_j$. The quantities ω_i and α_i are called the principal term and the anomaly of the Berezin measure on chart i.

Remark 2.2: The conditions (3) and (4) ensure the existence of a global section $\omega\in\Lambda^p(M)\otimes_{\mathscr{A}}\mathscr{D}$, whose local expression in chart i is $\omega_i+d\alpha_i$. The existence of ω means that the distribution (5) is independent of the coordinate systems and the cell partition chosen. Because (5) depends only on the differences $\alpha_i-\alpha_j$, one can gauge the anomaly to zero on one of the charts without changing the Berezin integral.

Example 2.3: Consider the real supersphere $S^{p|2}$, a $(p,2)$-dimensional supermanifold with support S^p, which is the space of solutions in $(p+1,2)$ dimensions of the quadratic equation

$$\widetilde{x}_0^2+\widetilde{x}_1^2+\cdots+\widetilde{x}_p^2+2\widetilde{\xi}_1\widetilde{\xi}_2=1.$$

Cover S^p by two domains 1 and 2 obtained by removing the South $(\widetilde{x}_0=-1)$ or North Pole $(\widetilde{x}_0=+1)$. Introduce stereographic coordinates $(x_1,\ldots,x_p;\xi_1,\xi_2)$ and $(y_1,\ldots,y_p;\eta_1,\eta_2)$ for $S^{p|2}$ on these domains with transition functions

$$y_1=-\frac{x_1}{R^2},\quad y_i=\frac{x_i}{R^2}\quad (i=2,\ldots,p),\quad \eta_j=\frac{\xi_j}{R^2}\quad (j=1,2),$$

where $R^2=\Sigma_{i=1}^{p}x_i^2+2\xi_1\xi_2$. (The minus sign preserves the orientation.) Consider

$$\omega_1=D(x,\xi)\circ\left(1+\sum x_i^2+2\xi_1\xi_2\right)^{-p+2},$$

$$\omega_2=D(y,\eta)\circ\left(1+\sum y_i^2+2\eta_1\eta_2\right)^{-p+2},$$

$$\alpha_{12}=-\Omega\,\frac{(\Sigma x_i^2)^{(p-2)/2}}{(1+\Sigma x_i^2)^{p-2}}\otimes 2\partial_{\xi_1}\partial_{\xi_2}\circ\xi_1\xi_2,$$

where $\Omega=(\Sigma_j x_j^2)^{-p/2}\Sigma_{i=1}^{p}(-1)^i dx_1\wedge\cdots\wedge dx_{i-1}\wedge x_i dx_{i+1}\wedge\cdots\wedge dx_p$ is the solid-angle $(p-1)$ form in p dimensions. It is not difficult to check by direct calculation that ω_1, ω_2 and $\alpha_1=\alpha_{12}$, $\alpha_2\equiv 0$ obey the relations (3) and (4). Hence, they express a globally defined Berezin measure ω in the sense of Definition 2.1. (The geometric meaning of ω will be specified in Sec. II C.) For $p\geqslant 3$, the anomaly α_{12} scales to zero when $\Sigma x_i^2\to\infty$, so we may shrink cell 2 to a single point (a set of measure zero) and compute the Berezin integral simply from

$$\int_{S^p}\omega[f]=\int_{\mathbb{R}^p}D(x,\xi)\left(1+\sum x_i^2+2\xi_1\xi_2\right)^{-p+2}f(x;\xi).$$

In these cases we can get away with using only a single chart. The situation is different for $p=2$ and $p=1$. In the first case the anomaly is scale-invariant (the solid angle is) and by again shrinking cell 2 to one point [the South Pole $(y_1,y_2)=(0,0)$ on S^2] we get

$$\int_{S^2}\omega[f]=\int_{\mathbb{R}^2}D(x,\xi)f(x;\xi)+4\pi f\Big|_{\text{South Pole}}.$$

In particular, $\int_{S^2}\omega[1]=4\pi$. For $p=1$ the anomaly diverges at $x=0$ and $x=\infty$. In this case the general formula (5) must be used, and one finds $\int_{S^1}\omega[1]=0$.

B. Grassmann-analytic continuation

In the formulation of BKL, the vector fields of a supermanifold do not constitute a module over $\mathscr{A}$ but are constrained to be *even* derivations of $\mathscr{A}$, which is to say that their coordinate expression is of the form

$$\hat{X}=f^i(x;\xi)\,\frac{\partial}{\partial x^i}+\varphi^j(x;\xi)\,\frac{\partial}{\partial\xi^j},$$

where f^i and φ^j are even and odd superfunctions, respectively. Unfortunately, this formulation is too narrow for most purposes. The reason is that in applications one typically deals not with a single supermanifold but with many copies thereof (one per lattice site of a lattice-regularized field theory, for example). So, in addition to the anticommuting coordinates of the one supermanifold that is singled out for special consideration, there exist many more anticommuting variables associated with the other copies of the supermanifold. When the focus is on one supermanifold, these can be considered as ''parameters.'' Often one wants to make parameter-dependent coordinate transformations, leading to coefficients $f_{i_1\cdots i_n}(x)$ in the expansion $f(x;\xi)=\Sigma f_{i_1\cdots i_n}(x)\xi^{i_1}\cdots\xi^{i_n}$ that depend on extraneous Grassmann parameters. (For example, when the

supermanifold is a Lie supergroup, it is natural to consider making left and right translations $g \mapsto g_L g g_R$.) The upshot is that one wants to take $\mathscr{A}$ as a sheaf of graded commutative algebras not over $\mathbb{R}$ but over some (large) parameter Grassmann algebra Λ (the Grassmann algebra generated by the anticommuting coordinates of the ''other'' supermanifolds). Making this extension, which is called ''Grassmann-analytic continuation'' in Ref. 29, one is led to consider the more general class of vector fields of the form

$$\hat{X} = f^i(x,\xi;\beta)\,\frac{\partial}{\partial x^i} + \varphi^j(x,\xi;\beta)\,\frac{\partial}{\partial \xi^j}, \tag{6}$$

where the symbol β stands for the extra Grassmann parameters and the dependences on these are such that f^i and φ^j continue to be even and odd, respectively (the $\mathbb{Z}_2$ grading of $\mathscr{A}$ after Grassmann-analytic continuation is the natural one).

The vector fields (6) still are even derivations of the extended algebra. One can go further by demanding that Der $\mathscr{A}$ be free over $\mathscr{A}$ and including the odd ones, too. When that development is followed to its logical conclusion, one arrives at Rothstein's axiomatic definition[32] of supermanifolds, superseding an earlier attempt by Rogers.[33,34] Although there is no denying the elegance and consistency of Rothstein's formulation, we are not going to embrace it here, the main reason being that odd derivations will not really be needed. For the purposes of the present paper we will get away with considering vector fields of the constrained form (6).

C. The complex Lie supergroups Gl($m|n$) and Osp($m|2n$)

The supermanifolds we will encounter all derive from the complex Lie supergroups[29,28] Gl($m|n$) and Osp($m|2n$), by forming cosets. The definition of Gl($m|n$) rests on the notion of an invertible supermatrix

$$g = \begin{pmatrix} g_{00} & g_{01} \\ g_{10} & g_{11} \end{pmatrix},$$

where g_{00}, g_{01}, g_{10}, and g_{11} are matrices of size $m\times m$, $m\times n$, $n\times m$, and $n\times n$. The supermanifold structure of Gl($m|n$) comes from taking the matrix elements of g_{00} and g_{11} (g_{01} and g_{10}) for the even (resp., odd) coordinates on suitable domains of the base $M = \mathrm{Gl}(m,\mathbb{C})\times\mathrm{Gl}(n,\mathbb{C})$. The Lie supergroup structure derives from the usual law of matrix multiplication.

For $m \neq n$, it is common practice to split off from Gl($m|n$) the Gl(1)-ideal generated by the unit matrix, so as to have an irreducible Lie superalgebra.[35,36] For $m = n$, which turns out to be the case of most interest here, one ends up having to remove two Gl(1)'s, one generated by the unit matrix and the other one by the superparity matrix $\sigma = \mathrm{diag}(1_n, -1_n)$. And even then the Lie superalgebra is not irreducible in a sense, for the Killing form $\mathrm{STr}\,\mathrm{ad}(X)\mathrm{ad}(Y)$ vanishes identically. We therefore prefer to take Gl($m|n$) as it stands (with no ideals removed) and replace the Killing form by the invariant quadratic form $\mathrm{B}(X,Y) = \mathrm{STr}\,XY$, which is nondegenerate in all cases (including $m = n$).

The complex orthosymplectic Lie supergroup Osp($m|2n$) is defined as a connected subgroup of Gl($m|2n$) fixed by an involutory automorphism $g \mapsto \hat{\tau}(g) = \tau g^{-1^{\mathrm{T}}} \tau^{-1}$, where τ is supersymmetric ($\tau = \tau^{\mathrm{T}}\sigma = \sigma\tau^{\mathrm{T}}$).[37] The support of Osp($m|2n$) is $\mathrm{SO}(m,\mathbb{C})\times\mathrm{Sp}(n,\mathbb{C})$.

The action of a Lie supergroup on itself by left and right translations gives rise to right- and left-invariant vector fields. A Berezin measure on a Lie supergroup is said to be invariant, and is called a Berezin–Haar measure, if its Lie derivatives[29] with respect to the invariant vector fields vanish.

Given a Lie supergroup G and a subgroup H, the coset superspace G/H is defined by decreeing that the structure sheaf of the coset superspace is a quotient of sheaves. The action of G

on G/H by left translation gives rise to so-called Killing vector fields. A Berezin measure on G/H is called invariant if its Lie derivatives with respect to the Killing vector fields are zero.

If $\mathrm{Osp}_{\mathbb{R}}(m|2n)$ denotes the orthosymplectic supergroup over the reals, the coset space $\mathrm{Osp}_{\mathbb{R}}(m+1|2n)/\mathrm{Osp}_{\mathbb{R}}(m|2n)$ can be identified with the real supersphere $S^{m|2n}$. The Berezin measure discussed in Example 2.3 is invariant with respect to the action of $\mathrm{Osp}_{\mathbb{R}}(p+1|2)$ on $S^{p|2}$ and can be viewed as the ''volume superform'' of $S^{p|2}$. Hence we can restate the results of that example as follows: $\mathrm{vol}(S^{2|2}) := \int_{S^2}\omega[1] = 4\pi$ and $\mathrm{vol}(S^{1|2}) := \int_{S^1}\omega[1] = 0$.

D. Holomorphic Berezin measures on complex-analytic supermanifolds

To go from real-analytic supermanifolds to complex-analytic ones, one replaces the structure sheaf $\mathscr{A}$ by a sheaf of graded commutative algebras $\mathscr{H}$ over $\mathbb{C}$ such that $M \simeq \mathscr{H}/\mathscr{N}$ is a complex manifold and $\mathscr{H}$ is locally modeled by $H(U)\otimes\Lambda(\mathbb{C}^q)$, where $H(U)$ is the algebra of holomorphic functions on $U\subset M$. The natural objects to consider then are holomorphic superfunctions, i.e., global sections of the bundle $\mathscr{H}\to M$. In local coordinates $z^1,\ldots,z^p$; $\zeta^1,\ldots,\zeta^q$ such sections are written as $f(z;\zeta)$. Grassmann-analytic continuation is done as before when needed. A Berezin measure on a complex-analytic (p,q)-dimensional supermanifold is a linear differential operator ω that takes holomorphic superfunctions f into holomorphic p-forms $\omega[f]$ on M. The statements made in Sec. II A about the anomalous transformation behavior of Berezin measures apply here, too (mutatis mutandi).

To define Berezin's integral in the present context, one more piece of data must be supplied, namely a *real* p-dimensional submanifold $M_r\subset M$ over which the holomorphic p-form $\omega[f]$ can be integrated to produce a complex number. Thus, given ω and M_r, Berezin's integral is the distribution

$$f\mapsto \int_{M_r}\omega[f]. \tag{7}$$

Let me digress and mention that this definition, natural and simple as it is, was not ''discovered'' by the random-matrix and mesoscopic physics community (including myself) until quite recently. With one notable exception,[23] all past superanalytic work on disordered single-particle systems employed some operation of ''complex conjugation'' of the Grassmann generators—namely an adjoint of the first or second kind[29]—to make the treatment of the ordinary (''bosonic'') and anticommuting (''fermionic'') degrees of freedom look as much alike as possible. Presumably this was done because it was felt that such egalitarian treatment is what is required by the principle of ''supersymmetry.'' Specifically, a reality constraint was imposed, not just on the underlying space M (fixing M_r) but on the entire structure sheaf to reduce $\mathscr{H}$ to a sheaf of algebras over $\mathbb{R}$. Although this reduction can be done with impunity in some cases (namely, the classic Wigner–Dyson symmetry classes), it has turned out to lead to insurmountable difficulties in others (the chiral and normal-superconducting symmetry classes). A major incentive of the present paper is to demonstrate that the construction (7) is in fact the ''good'' one to use for the application of supermanifold theory to disordered single-particle systems in general. Although that construction may hurt the physicists' aesthetic sense by ''torturing supersymmetry,'' it should be clear that we are not breaking any rules. Recall that according to Berezin, superintegration is a two-step process: first, the Fermi integral (i.e., differentiation with respect to the anticommuting coordinates) is carried out, and it is only *afterward* that the ordinary (Bose) integrals are done. When the sequential nature of the Berezin integral is taken seriously, there is no compelling reason why one should ever want to ''complex conjugate'' a Grassmann variable. In the present paper, we take the radical step of abandoning complex conjugation of Grassmann variables altogether.

Example 2.4: The simplest nontrivial example[23] is given by $\mathrm{Gl}(1|1)$, the Lie supergroup of regular complex 2×2 supermatrices

$$g=\begin{pmatrix} a & \beta \\ \gamma & d \end{pmatrix}$$

with support $M=\mathrm{Gl}(1,\mathbb{C})\times\mathrm{Gl}(1,\mathbb{C})$. The Berezin–Haar measure on $\mathrm{Gl}(1|1)$ is $\omega=(2\pi i)^{-1}D(ad;\beta\gamma)$, where $D(ad;\beta\gamma)=da\wedge dd\otimes\partial_\beta\partial_\gamma$. Solving the regularity conditions $a\neq 0$ and $d\neq 0$ by parametrizing $\mathrm{Gl}(1|1)$ through its Lie algebra,

$$g=\exp\begin{pmatrix} z_1 & \zeta_1 \\ \zeta_2 & z_2 \end{pmatrix},$$

one finds

$$2\pi i\omega=D(z_1z_2;\zeta_1\zeta_2)\circ\frac{(z_1-z_2)^2}{(1-e^{z_1-z_2})(e^{z_2-z_1}-1)}$$
$$-\left(d\,\ln(e^{z_1}-e^{z_2})-\frac{(z_1-z_2)(dz_1-dz_2)}{(1-e^{z_1-z_2})(e^{z_2-z_1}-1)}\right)\otimes\partial_{\zeta_1}\partial_{\zeta_2}\circ\zeta_1\zeta_2. \tag{8}$$

Note that this expression is holomorphic in a neighborhood of the origin $z_1=z_2=0$. The first term on the right-hand side is the principal term, and the second one is the anomaly of ω in these coordinates. To integrate ω, one might be tempted to choose for M_r the $\mathrm{U}(1)\times\mathrm{U}(1)$ subgroup defined by $\mathrm{Re}(z_1)=0=\mathrm{Re}(z_2)$. However, since the rank-two tensor $\mathrm{STr}\,dg\;dg^{-1}=da\;da^{-1}-dd\;dd^{-1}+\text{nilpotents}=-dz_1^2+dz_2^2+\cdots$ is not Riemann on $\mathrm{U}(1)\times\mathrm{U}(1)$, this will not be the best choice. A Riemannian structure is obtained by taking $M_r=\mathbb{R}^+\times S^1$ defined by $\mathrm{Im}(z_1)=0=\mathrm{Re}(z_2)$. To compute $\int_{\mathbb{R}^+\times S^1}\omega[f]$ we may use a single cell,

$$D:-\infty<x<+\infty,\quad -\pi<y<+\pi,$$

where $x=\mathrm{Re}(z_1)$ and $y=\mathrm{Im}(z_2)$. The boundary ∂D consists of the two lines $y=-\pi$ and $y=\pi$ ($x\in\mathbb{R}$). Using (8), paying attention to the orientation of the boundary, and simplifying terms, one finds the following explicit expression for the integral of ω:

$$\int_{\mathbb{R}^+\times S^1}\omega[f]=\frac{1}{4\pi}\int_{-\infty}^{\infty}dx\int_{-\pi}^{\pi}dy\,\frac{(x-iy)^2}{\cosh(x-iy)-1}\,\partial_{\zeta_1}\partial_{\zeta_2}f\left(\exp\begin{pmatrix} x & \zeta_1 \\ \zeta_2 & iy \end{pmatrix}\right)$$
$$+\frac{1}{2}\int_{-\infty}^{\infty}\frac{dx}{\cosh x+1}\,f\left(\begin{pmatrix} e^x & 0 \\ 0 & -1 \end{pmatrix}\right).$$

By construction, this Berezin integral is invariant under left and right translations $f(g)\mapsto f(g_Lgg_R)$. Evaluation gives $\int_{\mathbb{R}^+\times S^1}\omega[1]=1\neq 0$. The naive guess would have been $\int\omega[1]=(2\pi i)^{-1}\int da\wedge dd\;\partial_\beta\partial_\gamma=0$ due to $\partial_\beta\partial_\gamma\cdot 1=0$. Such reasoning is false because $\int_{\mathbb{R}^+}da=\infty$.

E. Symmetric spaces: A reminder

A Riemannian (globally) symmetric space is a Riemannian manifold M, such that every $p\in M$ is an isolated fixed point of an involutive isometry. (In normal coordinates x^i centered around p, this isometry is given by $x^i\mapsto -x^i$.) This definition implies (cf. Ref. 38) that the Riemann curvature tensor is covariantly constant, so that ''the geometry is the same everywhere.'' The curvature can be positive, negative, or zero, and the symmetric space is said to be of compact, noncompact, or Euclidean type correspondingly.

According to Cartan's complete classification scheme, there exist ten[39] large classes of symmetric spaces. Apart from some minor modifications these are the entries of Table I. The differ-

TABLE I. The large families of symmetry spaces.

Class	Noncompact type	Compact type
A	$\mathrm{Gl}(N,\mathbb{C})/\mathrm{U}(N)$	$\mathrm{U}(N)$
AI	$\mathrm{Gl}(N,\mathbb{R})/\mathrm{O}(N)$	$\mathrm{U}(N)/\mathrm{O}(N)$
AII	$\mathrm{U}^*(2N)/\mathrm{Sp}(N)$	$\mathrm{U}(2N)/\mathrm{Sp}(N)$
$AIII$	$\mathrm{U}(p,q)/\mathrm{U}(p)\times\mathrm{U}(q)$	$\mathrm{U}(p+q)/\mathrm{U}(p)\times\mathrm{U}(q)$
BDI	$\mathrm{SO}(p,q)/\mathrm{SO}(p)\times\mathrm{SO}(q)$	$\mathrm{SO}(p+q)/\mathrm{SO}(p)\times\mathrm{SO}(q)$
CII	$\mathrm{Sp}(p,q)/\mathrm{Sp}(p)\times\mathrm{Sp}(q)$	$\mathrm{Sp}(p+q)/\mathrm{Sp}(p)\times\mathrm{Sp}(q)$
BD	$\mathrm{SO}(N,\mathbb{C})/\mathrm{SO}(N)$	$\mathrm{SO}(N)$
C	$\mathrm{Sp}(N,\mathbb{C})/\mathrm{Sp}(N)$	$\mathrm{Sp}(N)$
CI	$\mathrm{Sp}(N,\mathbb{R})/\mathrm{U}(N)$	$\mathrm{Sp}(N)/\mathrm{U}(N)$
$DIII$	$\mathrm{SO}^*(2N)/\mathrm{U}(N)$	$\mathrm{SO}(2N)/\mathrm{U}(N)$

ence from the standard table[38] is that some of the entries of Table I, namely, the spaces of type A, AI, and AII, are not irreducible. They can be made so by dividing out a factor U(1) ($\mathbb{R}^+$) in the compact (resp., noncompact) cases. Division by such a factor is analogous to removing the center of mass motion from a mechanical system with translational invariance. It turns out that, with a view to superanalytic extensions (cf. Example 2.4), it is preferable not to insist on irreducibility but to ''retain the center of mass motion.''

The next section introduces supergeneralizations of Cartan's symmetric spaces, which have appeared in the theory of mesoscopic and disordered single-particle systems and have come to play an important role in that field.

F. Riemannian symmetric superspaces (definition)

Let G_Λ be a complex Lie supergroup that is realized as a group of supermatrices

$$g=\begin{pmatrix} g_{00} & g_{01} \\ g_{10} & g_{11} \end{pmatrix},$$

with matrix elements that take values in a (sufficiently large) parameter Grassmann algebra $\Lambda=\Lambda_0+\Lambda_1$. If $\mathscr{G}_\mathbb{C}=\mathscr{G}_\mathbb{C}^0+\mathscr{G}_\mathbb{C}^1$ is the Lie superalgebra of G_Λ, the Lie algebra of G_Λ is obtained by taking the even part of the tensor product with Λ: $\mathrm{Lie}\,(G_\Lambda)=\Lambda_0\otimes\mathscr{G}_\mathbb{C}^0+\Lambda_1\otimes\mathscr{G}_\mathbb{C}^1=(\Lambda\otimes\mathscr{G}_\mathbb{C})_0$. Thus, if $\{e_i,\epsilon_j\}$ is a homogeneous basis of complex matrices in $\mathscr{G}_\mathbb{C}$, an element $X\in\mathrm{Lie}(G_\Lambda)$ is expressed by $X=z^ie_i+\zeta^j\epsilon_j$ with $z^i\in\Lambda_0$ and $\zeta^j\in\Lambda_1$.

Let $\theta:G_\Lambda\to G_\Lambda$ be an involutory automorphism and let $H_\Lambda\subset G_\Lambda$ be the subgroup fixed by θ. The decomposition into even and odd eigenspaces of $\theta_*:\mathrm{Lie}(G_\Lambda)\to\mathrm{Lie}(G_\Lambda)$ is written as $\mathrm{Lie}(G_\Lambda)=\mathrm{Lie}(H_\Lambda)+\mathscr{M}_\Lambda$. This decomposition is orthogonal with respect to the $\mathrm{Ad}(G_\Lambda)$-invariant quadratic form $\mathrm{B}:\mathrm{Lie}(G_\Lambda)\times\mathrm{Lie}(G_\Lambda)\to\Lambda_0$, $\mathrm{B}(X,Y):=\mathrm{STr}\,XY$.

Both G_Λ and H_Λ are supermanifolds with underlying spaces that are Lie groups and are denoted by $G_\mathbb{C}$ and $H_\mathbb{C}$. Passing to the coset spaces one obtains a graded commutative algebra $\mathscr{H}=\mathscr{H}_0+\mathscr{H}_1$ of (Grassmann-analytically continued) holomorphic sections of the bundle $G_\Lambda/H_\Lambda\to G_\mathbb{C}/H_\mathbb{C}$. These sections are called (super-)functions (on G_Λ/H_Λ) for short. In local complex coordinates $z^1,\ldots,z^p;\ \zeta^1,\ldots,\zeta^q$ they are written as $f(z^1,\ldots,z^p;\zeta^1,\ldots,\zeta^q)=\Sigma f_{i_1\cdots i_n}(z^1,\ldots,z^p)\zeta^{i_1}\cdots\zeta^{i_n}$, where the coefficients $f_{i_1\cdots i_n}(z^1,\ldots,z^p)$ take values in Λ after Grassmann-analytic continuation. For coordinate-independent calculations the alternative notation $f(gH_\Lambda)$ or $f(g\cdot o)$ is used. In the following $G_\mathbb{C}/H_\mathbb{C}$ is assumed to be connected.

Every $X\in\mathrm{Lie}(G_\Lambda)$ is associated with a vector field (or even derivation) $\hat{X}:\mathscr{H}\to\mathscr{H}$ by

$$(\hat{X}f)(g\cdot o)=\left.\frac{d}{ds}\right|_{s=0} f(e^{-sX}g\cdot o). \tag{9}$$

Here $e^{sX}g$ means the usual product of supermatrices, and the function $f(e^{sX}g\cdot o)$ is determined from $f(g\cdot o)$ by Grassmann-analytic continuation. The Lie algebra of even derivations of $\mathscr{H}$ is a left $\mathscr{H}_0$-module denoted by $\mathrm{Der}_0\,\mathscr{H}$.[40]

A notion of supergeometry on G_Λ/H_Λ is introduced via a left-invariant tensor field $\langle\bullet,\bullet\rangle:\mathrm{Der}_0\,\mathscr{H}\times\mathrm{Der}_0\,\mathscr{H}\to\mathscr{H}_0$. The details are as follows. G_Λ acts on G_Λ/H_Λ by left translation, $T_h^*:f(g\cdot o)\mapsto f((hg)\cdot o)$. The left-translate $dT_h(\hat{X})$ of a vector field $\hat{X}$ is defined by the equation $T_h^*(dT_h(\hat{X})f)=\hat{X}(T_h^*f)$, and one requires

$$T_h^*\langle dT_h(\hat{X}),dT_h(\hat{Y})\rangle=\langle\hat{X},\hat{Y}\rangle.$$

This equation determines $\langle\bullet,\bullet\rangle$ uniquely within a multiplicative constant. For vector fields of the special form (9), one obtains

$$\langle\hat{X},\hat{Y}\rangle(g\cdot o)=c_0\times\mathrm{B}((\mathrm{Ad}(g)^{-1}X)_{\mathscr{M}_\Lambda},(\mathrm{Ad}(g)^{-1}Y)_{\mathscr{M}_\Lambda}),$$

where the subscript $\mathscr{M}_\Lambda$ means projection on the odd eigenspace of θ_*. Note that since $(\mathrm{Ad}(gh)^{-1}X)_{\mathscr{M}_\Lambda}=\mathrm{Ad}(h)^{-1}(\mathrm{Ad}(g)^{-1}X)_{\mathscr{M}_\Lambda}$ for $h\in H_\Lambda$, this is well-defined as a function on G_Λ/H_Λ. The normalization is fixed by choosing $c_0=1$.

The metric tensor $\langle\bullet,\bullet\rangle$ induces a geometry on the ordinary manifold $G_{\mathrm{C}}/H_{\mathrm{C}}$ by restriction (i.e., by setting all anticommuting variables equal to zero). Of course, since the groups G_{C} and H_{C} are complex, this geometry is never Riemann. However, there exist submanifolds in $G_{\mathrm{C}}/H_{\mathrm{C}}$ that are Riemannian symmetric spaces and can be constructed by selecting from the tangent space $T_o(G_{\mathrm{C}}/H_{\mathrm{C}})$ a Lie-triple subsystem $\mathscr{M}$ (i.e., $[\mathscr{M},[\mathscr{M},\mathscr{M}]]\subset\mathscr{M}$), such that the quadratic form B restricted to $\mathscr{M}$ is of definite sign. It is then not hard to show[38] that the image of $\mathscr{M}$ under the exponential map $X\mapsto e^XH_\Lambda$ is Riemann in the geometry given by restriction of $\langle\bullet,\bullet\rangle$. Its completion is a symmetric space.

Definition 2.5: A Riemannian symmetric superspace is a pair $(G_\Lambda/H_\Lambda;M)$, where M is a maximal Riemannian submanifold of the base $G_{\mathrm{C}}/H_{\mathrm{C}}$.

Remark 2.6: The merit of this definition is that it avoids any use of an adjoint (or ''complex conjugation'') of the Grassmann variables. ■

By the complex structure of $G_{\mathrm{C}}/H_{\mathrm{C}}$, the tangent space $\mathscr{M}_{\mathrm{C}}:=T_o(G_{\mathrm{C}}/H_{\mathrm{C}})$ decomposes as $\mathscr{M}_{\mathrm{C}}=\mathscr{M}+i\mathscr{M}$, where $\mathscr{M}$ is taken to be the subspace of $\mathscr{M}_{\mathrm{C}}$ on which the quadratic form B is strictly positive. Now observe that, since an element $g\in G_{\mathrm{C}}$ is of the form $g=\mathrm{diag}(g_{00},g_{11})$, the group G_{C} is a Cartesian product of two factors, and the same is true for H_{C}. Hence, $G_{\mathrm{C}}/H_{\mathrm{C}}$ factors as $G_{\mathrm{C}}/H_{\mathrm{C}}=M_{\mathrm{C}}^0\times M_{\mathrm{C}}^1$, and $\mathscr{M}$ is a sum of two spaces: $\mathscr{M}=\mathscr{M}_0\oplus\mathscr{M}_1$, which are orthogonal with respect to the quadratic form B. (It may happen, of course, that one of these spaces is trivial.) For $Z\in\mathscr{M}$, let the corresponding orthogonal decomposition be written as $Z=X+Y$. Then B restricted to $\mathscr{M}$ is evaluated as

$$\mathrm{B}(Z,Z)=\mathrm{Tr}_0\,X^2-\mathrm{Tr}_1\,Y^2,$$

where the relative minus sign between traces is due to supersymmetry ($\mathrm{STr}=\mathrm{Tr}_0-\mathrm{Tr}_1$). The positivity of B on $\mathscr{M}$ is seen to imply $X=X^\dagger$ and $Y=-Y^\dagger$ (the dagger denotes Hermitian conjugation, i.e. transposition in conjunction with complex conjugation).

Given G_Λ/H_Λ, the condition that M be Riemann and maximal in $G_{\mathrm{C}}/H_{\mathrm{C}}$, fixes M uniquely up to two possibilities: either $T_o(M)=\mathscr{M}$, or $T_o(M)=i\mathscr{M}$. In either case, M is a product of two factors, $M=M_0\times M_1$, both of which are Riemannian symmetric spaces. In the first case, M_0 is of the noncompact type and M_1 is of the compact type, while in the second case it is the other way around. We adopt the convention of denoting the compact space by M_{F} and the noncompact one by M_{B}.

In view of Cartan's list of symmetric spaces (Table I), we arrive at Table II listing the large families of Riemannian symmetric superspaces. Although the entries $A|A$, $BD|C$, and $C|BD$ look

TABLE II. The large families of Riemannian symmetric superspaces.

Class	G_Λ/H_Λ	M_B	M_F
$A\|A$	$\mathrm{Gl}(m\|n)$	A	A
$AI\|AII$	$\mathrm{Gl}(m\|2n)/\mathrm{Osp}(m\|2n)$	AI	AII
$AII\|AI$	$\mathrm{Gl}(m\|2n)/\mathrm{Osp}(m\|2n)$	AII	AI
$AIII\|AIII$	$\mathrm{Gl}(m_1+m_2\|n_1+n_2)/\mathrm{Gl}(m_1\|n_1)\times\mathrm{Gl}(m_2\|n_2)$	$AIII$	$AIII$
$BD\|C$	$\mathrm{Osp}(m\|2n)$	BD	C
$C\|BD$	$\mathrm{Osp}(m\|2n)$	C	BD
$CI\|DIII$	$\mathrm{Osp}(2m\|2n)/\mathrm{Gl}(m\|n)$	CI	$DIII$
$DIII\|CI$	$\mathrm{Osp}(2m\|2n)/\mathrm{Gl}(m\|n)$	$DIII$	CI
$BDI\|CII$	$\mathrm{Osp}(m_1+m_2\|2n_1+2n_2)/\mathrm{Osp}(m_1\|2n_1)\times\mathrm{Osp}(m_2\|2n_2)$	BDI	CII
$CII\|BDI$	$\mathrm{Osp}(m_1+m_2\|2n_1+2n_2)/\mathrm{Osp}(m_1\|2n_1)\times\mathrm{Osp}(m_2\|2n_2)$	CII	BDI

extraneous because they are groups rather than coset spaces, they fit in the same framework by putting by $G_\Lambda = G\times G$ and $\theta(g_1,g_2)=(g_2,g_1)$, so $H_\Lambda=\mathrm{diag}(G\times G)\simeq G$ and $G_\Lambda/H_\Lambda\simeq G$.

As far as applications to random-matrix theory and disordered single-particle systems are concerned, the most important structure carried by Riemannian symmetric superspaces is their G_Λ-invariant Berezin measure. Such a measure always exists by Definition 2.1 and the existence of local coordinates. To describe it in explicit terms, one introduces a local coordinate system by the exponential map $\mathscr{M}_\Lambda\to G_\Lambda/H_\Lambda$, $Z\mapsto\exp(Z)H_\Lambda$. By straightforward generalization (replace the Jacobian by the Berezinian) of a corresponding calculation (cf. Ref. 38) for ordinary symmetric spaces, one obtains for the principal term of the invariant Berezin measure the expression $DZ\circ J(Z)$, where $DZ = dz^1\wedge\cdots\wedge dz^p\otimes\partial_{\zeta^1}\cdots\partial_{\zeta^q}$ denotes the flat Berezin measure on $\mathscr{M}_\Lambda$, and if $T_Z:\mathscr{M}_\Lambda\to\mathscr{M}_\Lambda$ is the linear operator defined by

$$T_Z=\sum_{n=0}^{\infty}\frac{\mathrm{ad}^{2n}(Z)}{(2n+1)!},$$

the function $J(Z)=\mathrm{SDet}T_Z$. [Note $\Sigma_{n=0}^{\infty}x^{2n}/(2n+1)!=x^{-1}\sinh x$]. A universally valid expression for the anomaly in these coordinates is not available at present.

III. SUPERSYMMETRY APPLIED TO THE GAUSSIAN RANDOM-MATRIX ENSEMBLE OF CLASS *C*

The goal of the remainder of this paper will be to demonstrate that Riemannian symmetric superspaces, as defined in Sec. II F, arise in a compelling way when Gaussian ensemble averages of ratios of spectral determinants for random matrices are considered in the large-N limit. The example to be discussed in detail will be the Gaussian ensemble defined over the symplectic Lie algebra $\mathrm{sp}(N)$, which has recently been identified[24] as a model for the ergodic limit of normal-superconducting mesoscopic systems with broken time-reversal symmetry.

A. The supersymmetry method: A simple example

The pedagogical purpose of this section is to illustrate our strategy at a simple example.[41] If $\mathrm{u}(N)$ is the Lie algebra of the unitary group in N dimensions, consider on $i\mathrm{u}(N)$ (the Hermitian $N\times N$ matrices) the Gaussian probability measure with width $v/\sqrt{N}$. Denoting by H the elements of $i\mathrm{u}(N)$ and by dH a Euclidean measure, we write the Gaussian probability measure in the form $d\mu(H)=\exp(-N\,\mathrm{Tr}\,H^2/2v^2)dH$, $\int d\mu(H)=1$. This measure is called the Gaussian unitary ensemble (GUE) in random-matrix theory. The object of illustration will be the average ratio of spectral determinants,

$$Z(\alpha,\beta)=\int_{iu(N)}\mathrm{Det}\left(\frac{H-\beta}{H-\alpha}\right)d\mu(H),$$

where α,β are complex numbers and α is not in the spectrum of H. Given the generating function Z, the GUE average resolvent is obtained by

$$\int_{iu(N)}\mathrm{Tr}(H-z)^{-1}d\mu(H)=\frac{\partial}{\partial\alpha}\,Z(\alpha,\beta)\bigg|_{\alpha=\beta=z}.$$

We will now show how to compute Z using a formalism that readily generalizes to more complicated situations.

To avoid the introduction of indices and have a basis-independent formulation, we choose to interpret H as a self-adjoint endomorphism $H\in\mathrm{End}(V)$ of N-dimensional complex space $V:=\mathbb{C}^N$ with a Hermitian quadratic form $(x,y)\mapsto\langle\overline{x},y\rangle_V$.

The supersymmetry method starts by introducing ''bosonic space'' $W_\mathrm{B}=W_0=\mathbb{C}$ and ''fermionic space'' $W_\mathrm{F}=W_1=\mathbb{C}$. Auxiliary space is the $\mathbb{Z}_2$-graded sum $W=W_\mathrm{B}\oplus W_\mathrm{F}=\mathbb{C}^{1|1}$. The Cartesian basis of W is denoted by $e_\mathrm{B}=(1,0)$ and $e_\mathrm{F}=(0,1)$. Let $\mathrm{Hom}_\lambda(W,V):=\lambda_0\otimes\mathrm{Hom}(W_\mathrm{B},V)+\lambda_1\otimes\mathrm{Hom}(W_\mathrm{F},V)$, where $\lambda=\lambda_0+\lambda_1$ is the Grassmann algebra with $\dim_\mathbb{C}\mathrm{Hom}(W_\mathrm{F},V)=N$ generators. (Grassmann-analytic continuation will not be needed here.) $\mathrm{Hom}_{\tilde\lambda}(V,W)$ is defined similarly, with another Grassmann algebra $\tilde\lambda$. The key idea is to utilize the Gaussian Berezin integral over the complex-analytic superspace $\mathrm{Hom}_\lambda(W,V)\times\mathrm{Hom}_{\tilde\lambda}(V,W)$. Let $D(\psi,\tilde\psi)$ [with $\psi\in\mathrm{Hom}_\lambda(W,V)$ and $\tilde\psi\in\mathrm{Hom}_{\tilde\lambda}(V,W)$] denote a translation-invariant holomorphic Berezin measure on this linear space. If $\psi_\mathrm{B}(\tilde\psi_\mathrm{B})$ is the restriction of $\psi(\tilde\psi)$ to a map $W_\mathrm{B}\to V$ (resp., $V\to W_\mathrm{B}$), fix a Berezin integral $f\mapsto\int D(\psi,\tilde\psi)f(\psi,\tilde\psi)$ by choosing for the domain of integration the subspace M_r selected by the linear condition $\tilde\psi_\mathrm{B}=\psi_\mathrm{B}$ (the adjoint $\psi_\mathrm{B}^\dagger:\mathbb{C}^N\to\mathbb{C}$ being defined by $\overline{\psi_\mathrm{B}^\dagger z}=\langle\overline{z},\psi_\mathrm{B}\cdot 1\rangle_V$). Because $\mathrm{Hom}_\lambda(W,V)\times\mathrm{Hom}_{\tilde\lambda}(V,W)$ has complex dimension $(2N,2N)$, the integral $\int D(\psi,\tilde\psi)f(\psi,\tilde\psi)$ does not change its value when f is replaced by the rescaled function $f^s(\psi,\tilde\psi)=f(s\psi,s\tilde\psi)$ $(s\in\mathbb{R})$. Now with $\mathrm{End}_0(W)=\mathrm{End}(W_\mathrm{B})\oplus\mathrm{End}(W_\mathrm{F})$ and $\mathrm{End}_1(W)=\mathrm{Hom}(W_\mathrm{B},W_\mathrm{F})\oplus\mathrm{Hom}(W_\mathrm{F},W_\mathrm{B})$, let

$$\mathrm{End}_\Lambda(W):=\Lambda_0\otimes\mathrm{End}_0(W)+\Lambda_1\otimes\mathrm{End}_1(W),$$

where $\Lambda=\Lambda_0+\Lambda_1$ is the Grassmann algebra with $\dim_\mathbb{C}\mathrm{End}_1(W)=2$ generators, and pick $A\in\mathrm{End}(V)$, $B\in\mathrm{End}_\Lambda(W)$. B corresponds to what is called a 2×2 supermatrix in physics. An elementary but useful result is that, if we normalize $D(\psi,\tilde\psi)$ by $\int D(\psi,\tilde\psi)\exp(-s^2\,\mathrm{Tr}\,\tilde\psi\psi)=1$, the identity

$$\int D(\psi,\tilde\psi)\exp(i\,\mathrm{Tr}_V\,A\psi\tilde\psi-i\,\mathrm{STr}_W\,B\tilde\psi\psi)=\mathrm{SDet}_{V\otimes W}(A\otimes 1-1\otimes B)^{-c},\tag{10}$$

holds with $c=1$ provided that the integral exists. (The parameter c is introduced for later convenience.) When A and B are represented by diagonal matrices, verification of (10) is a simple matter of doing one-dimensional Gaussian integrals. The general case follows by the invariance of $D(\psi,\tilde\psi)$ under unitary transformations of V and ''super-rotations'' in W.

Now introduce elements E_BB and E_FF of $\mathrm{End}_0(W)$ by $E_\mathrm{BB}e_\mathrm{B}=e_\mathrm{B}$, $E_\mathrm{FF}e_\mathrm{F}=e_\mathrm{F}$, and $E_\mathrm{BB}e_\mathrm{F}=E_\mathrm{FF}e_\mathrm{B}=0$. By setting $A:=H$ and $B:=\alpha E_\mathrm{BB}+\beta E_\mathrm{FF}=:\omega$, and using

$$\mathrm{SDet}_{V\otimes W}(H\otimes 1-1\otimes\omega)=\mathrm{Det}(H-\alpha)/\mathrm{Det}(H-\beta),$$

we get a Gaussian integral representation of Z:

$$Z(\omega) := Z(\alpha,\beta) = \int \mathrm{SDet}_{V\otimes W}(H\otimes 1 - 1\otimes\omega)^{-c} d\mu(H)$$

$$= \int D(\psi,\tilde{\psi}) \int \exp(i\ \mathrm{Tr}_V\ H\psi\tilde{\psi} - i\ \mathrm{STr}_W\ \omega\tilde{\psi}\psi) d\mu(H). \tag{11}$$

In the next step, the GUE ensemble average is subjected to the following manipulations:

$$\int \exp(i\ \mathrm{Tr}\ H\psi\tilde{\psi}) d\mu(H) = \int_{iu(N)} \exp\left(i\ \mathrm{Tr}\ H\psi\tilde{\psi} - \frac{N\ \mathrm{Tr}\ H^2}{2v^2}\right) dH$$

$$= \exp - \frac{v^2}{2N}\ \mathrm{Tr}_V(\psi\tilde{\psi})^2$$

$$= \exp - \frac{v^2}{2N}\ \mathrm{STr}_W(\tilde{\psi}\psi)^2$$

$$= \int_{\mathbb{R}\times i\mathbb{R}} DQ\ \exp\left(i\ \mathrm{STr}\ Q\tilde{\psi}\psi - \frac{N\ \mathrm{STr}\ Q^2}{2v^2}\right)$$

$$=: \int D\mu(Q) \exp(i\ \mathrm{STr}\ Q\tilde{\psi}\psi). \tag{12}$$

The fourth equality sign decouples the quartic term $\mathrm{STr}_W(\tilde{\psi}\psi)^2$ by introducing an auxiliary integration over $Q \in \mathrm{End}_\Lambda(W)$. In order for this Gaussian integral to converge, the integration domain for the BB part $Q_{\mathrm{BB}}: W_{\mathrm{B}} \to W_{\mathrm{B}}$ (FF part, $Q_{\mathrm{FF}}: W_{\mathrm{F}} \to W_{\mathrm{F}}$), is taken to be the real (resp., imaginary) numbers. By using the relations (10)–(12), we obtain

$$Z(\omega) = \int D(\psi,\tilde{\psi}) \left(\int \exp(i\ \mathrm{Tr}_V\ H\psi\tilde{\psi}) d\mu(H)\right) \exp - i\ \mathrm{STr}_W\ \omega\tilde{\psi}\psi$$

$$= \int D\mu(Q) \int D(\psi,\tilde{\psi}) \exp\ i\ \mathrm{Tr}_V\ \psi(Q-\omega)\tilde{\psi}$$

$$= \int D\mu(Q)\, \mathrm{SDet}_{V\otimes W}(1_N \otimes (Q-\omega))^{-c}$$

$$= \int D\mu(Q)\, \mathrm{SDet}_W(Q-\omega)^{-N}$$

$$= \int_{\mathbb{R}\times i\mathbb{R}} DQ\ \exp - N\ \mathrm{STr}\left(\frac{Q^2}{2v^2} + \ln(Q-\omega)\right). \tag{13}$$

These steps reduce an integral over the $N\times N$ matrix H to an integral over the 2×2 supermatrix Q. The large parameter N now appears in the exponent of the integrand, so that the Q integral can be evaluated by a saddle-point approximation that becomes exact in the limit $N\to\infty$. By solving the saddle-point equation $-Q/v^2 = (Q-\omega)^{-1}$ and doing an elementary calculation, one obtains Wigner's semicircle law for the GUE density of states:[42]

$$\int \mathrm{Tr}\ \delta(E-H) d\mu(H) = \frac{N}{\pi v}\ \sqrt{1 - \left(\frac{E}{2v}\right)^2}, \tag{14}$$

which will be of use later.

B. Definition of the Gaussian ensemble of type *C*

Having run through a simple and well-known example, we now treat in detail a less trivial case where the reduction to a Q-integral representation requires more care.

The ''physical space'' of our model is $V=\mathbb{C}^2\otimes\mathbb{C}^N$. As before, let $x\mapsto\overline{x}$ denote complex conjugation, and fix a symmetric quadratic form $\langle\bullet,\bullet\rangle_V: V\times V\to\mathbb{C}$, such that the corresponding Hermitian quadratic form $\langle\overline{x},y\rangle_V = \overline{\langle\overline{y},x\rangle}_V$ is strictly positive. The transpose and the adjoint of a linear transformation $L\in\mathrm{End}(V)$ are defined by $\langle x,L^{\mathrm{T}}y\rangle_V=\langle Lx,y\rangle_V$ and $\langle\overline{x},L^{\dagger}y\rangle_V = \overline{\langle Lx,y\rangle}_V$, as usual.

Consider now the space, P, of self-adjoint Hamiltonians $H\in\mathrm{End}(V)$ subject to the linear condition

$$H=-\mathscr{C}H^{\mathrm{T}}\mathscr{C}^{-1}, \tag{15}$$

where $\mathscr{C}$ is skew and $\mathscr{C}^2=-1$. Clearly, iP is isomorphic to $\mathrm{sp}(N)=C_N$ (the symplectic Lie algebra in $2N$ dimensions). Introducing an orthonormal real basis of V we can represent H by a $2N\times 2N$ matrix. The explicit form of such a matrix is

$$H=\begin{pmatrix} a & b \\ b^{\dagger} & -a^{\mathrm{T}}\end{pmatrix}, \quad \text{if } \mathscr{C}=\begin{pmatrix} 0 & 1_N \\ -1_N & 0\end{pmatrix},$$

where $a(b)$ is a complex Hermitian (resp., symmetric) $N\times N$ matrix. The Gaussian ensemble to be studied is defined by the probability measure $d\mu(H)=\exp(-N\ \mathrm{Tr}\,H^2/2v^2)dH$, $\int d\mu(H)=1$. For any two $A,B\in\mathrm{End}(V)$,

$$\int_{i\times\mathrm{sp}(N)}\mathrm{Tr}(AH)\mathrm{Tr}(BH)d\mu(H)=\frac{v^2}{2N}\,\mathrm{Tr}(AB-A\mathscr{C}B^{\mathrm{T}}\mathscr{C}^{-1}). \tag{16}$$

The joint probability density for the eigenvalues of H has been given in Ref. 24.

The physical motivation for considering a Gaussian random-matrix ensemble of the above type (type C) comes from the fact[24] that it describes the ergodic limit of mesoscopic normal-superconducting hybrid systems with time-reversal symmetry broken by the presence of a weak magnetic field. To deal with such systems, the Bogoliubov–deGennes (BdG) independent-quasiparticle formalism is used. The first factor in the tensor product $V=\mathbb{C}^2\otimes\mathbb{C}^N$ accounts for the BdG particle-hole degree of freedom, which is introduced for the purpose of treating the pairing field of the superconductor within the formalism of first quantization. The second factor represents the orbital degrees of freedom of the electron. H is the Hamiltonian that enters into the BdG equations, and the relation (15) expresses the particle-hole symmetry of the BdG formalism.

Our goal is to compute the following ensemble average:

$$Z_n(\alpha_1,\ldots,\alpha_n;\beta_1,\ldots,\beta_n)=\int_{i\ \mathrm{sp}(N)}\prod_{i=1}^{n}\mathrm{Det}\left(\frac{H-\beta_i}{H-\alpha_i}\right)d\mu(H). \tag{17}$$

By the particle-hole symmetry of H, Z_n is invariant under a reversal of sign for any pair (α_i,β_j), so no information is lost by restricting all α_i to one-half of the complex plane. For definiteness, we require

$$\mathrm{Im}\ \alpha_i<0 \quad (i=1,\ldots,n). \tag{18}$$

All information about the statistical correlations between the eigenvalues of H can be extracted from Z_n. For example, the probability that, given there is an eigenvalue at E_1, there exist $n-1$ eigenvalues at $E_2,\ldots,E_n$ (regardless of the positions of all other eigenvalues) is equal to

$$R_n(E_1,\ldots,E_n)=\lim_{\epsilon\to 0}\left(\frac{-\epsilon}{\pi}\right)^n \prod_{l=1}^{n}\frac{\partial}{\partial\alpha_{2l}}\bigg|_{\alpha_{2l}=E_l-i\epsilon}\prod_{l=1}^{n}\frac{\partial}{\partial\alpha_{2l-1}}\bigg|_{\alpha_{2l-1}=-E_l-i\epsilon}$$
$$\times Z_{2n}(\alpha_1,\ldots,\alpha_{2n};E_1-i\epsilon,-E_1-i\epsilon,\ldots,E_n-i\epsilon,-E_n-i\epsilon). \tag{19}$$

The function $R_n(E_1,\ldots,E_n)$ is called the n-level correlation function in random-matrix theory.[42]

C. Symmetries of the auxiliary space

To transcribe the supersymmetry method of Sec. III A to the computation of Z_n (which involves n ratios of spectral determinants), a simple and natural procedure would be to enlarge the auxiliary space W by taking the tensor product with $\mathbb{C}^n$. However, on using the formula

$$\int \exp(i\ \mathrm{Tr}\ H\psi\widetilde{\psi})\,d\mu(H)=\exp\left(-\frac{1}{2}\int_{i\ \mathrm{sp}(N)}(\mathrm{Tr}\ H\psi\widetilde{\psi})^2\ d\mu(H)\right),$$

one faces the complication that the second moment $\int(\mathrm{Tr}\,H\psi\widetilde{\psi})^2\,d\mu(H)$ then is a sum of two terms, see the right-hand side of (16). Consequently, one needs *two* decoupling supermatrices Q (one for each term). Although this presents no difficulty of a principal nature, it does lead to rather complicated notations. An elegant remedy is to modify the definition of ψ and $\widetilde{\psi}$ so that $\psi\widetilde{\psi}$ shares the symmetry (15) of the BdG Hamiltonian H. The two terms then combine into a single one:

$$\int (\mathrm{Tr}\ H\psi\widetilde{\psi})^2\ d\mu(H)=\frac{v^2}{N}\,\mathrm{STr}_W(\widetilde{\psi}\psi)^2,$$

which can again be decoupled by a single supermatrix Q. To implement the symmetry (15), we proceed as follows.

We enlarge the auxiliary space $W=W_{\mathrm{B}}\oplus W_{\mathrm{F}}$ in some way (left unspecified for the moment) and fix a rule of supertransposition $\mathrm{Hom}_\lambda(W,V)\to\mathrm{Hom}_\lambda(V,W)$, $\psi\mapsto\psi^{\mathrm{T}}$, and $\mathrm{Hom}_\lambda(V,W)\to\mathrm{Hom}_\lambda(W,V)$, $\widetilde{\psi}\mapsto\widetilde{\psi}^{\,\mathrm{T}}$. Such a rule obeys $\psi^{\mathrm{T}\,\mathrm{T}}=\psi\sigma$ and $\widetilde{\psi}^{\,\mathrm{T}\,\mathrm{T}}=\sigma\widetilde{\psi}$, where $\sigma\in\mathrm{End}_0(W)$ is the operator for superparity, i.e. $\sigma(x+y)=x-y$ for $x+y\in W_{\mathrm{B}}\oplus W_{\mathrm{F}}=W$. It induces a rule of supertransposition $\mathrm{End}_\Lambda(W)\to\mathrm{End}_\Lambda(W)$, $Q\mapsto Q^{\mathrm{T}}$ (no separate symbol is introduced). Combination with complex conjugation gives a rule of Hermitian conjugation $\dagger:\mathrm{End}_0(W)\to\mathrm{End}_0(W)$. Now impose on $\psi\in\mathrm{Hom}_\lambda(W,V)$, $\widetilde{\psi}\in\mathrm{Hom}_\lambda(V,W)$ the linear conditions

$$\psi=\mathscr{C}\widetilde{\psi}^{\mathrm{T}}\gamma^{-1},\quad \widetilde{\psi}=-\gamma\psi^{\mathrm{T}}\mathscr{C}^{-1}, \tag{20}$$

with some invertible even element γ of $\mathrm{End}_0(W)$. The mutual consistency of these equations requires

$$\gamma=\gamma^{\mathrm{T}}\sigma. \tag{21}$$

To see that, insert the transpose of the second equation in (20) into the first one. Using $\psi^{\mathrm{TT}}=\psi\sigma$ you obtain $\psi=-\mathscr{C}\mathscr{C}^{-1^{\mathrm{T}}}\psi\sigma\gamma^{\mathrm{T}}\gamma^{-1}$. Since $\mathscr{C}\mathscr{C}^{-1^{\mathrm{T}}}=-1$ and $\sigma\gamma^{\mathrm{T}}=\gamma^{\mathrm{T}}\sigma$, Eq. (21) follows. The consistency condition can be implemented by taking $W_{\mathrm{B}}=W_{\mathrm{F}}=\mathbb{C}^2\otimes\mathbb{C}^n$, see below. By multiplying the equations (20) we obtain

$$\psi\widetilde{\psi}=-\mathscr{C}(\psi\widetilde{\psi})^{\mathrm{T}}\mathscr{C}^{-1},\quad \widetilde{\psi}\psi=-\gamma(\widetilde{\psi}\psi)^{\mathrm{T}}\gamma^{-1}. \tag{22}$$

The first equation is the desired symmetry relation allowing us to combine terms. To appreciate the consequences of the second equation, note that by the fourth step in (12) the symmetries of $\widetilde{\psi}\psi$ get transferred onto Q, so that the latter is subject to

$$Q = -\gamma Q^{\mathrm{T}} \gamma^{-1}. \tag{23}$$

This symmetry reflects that of the BdG Hamiltonian H, see (15). The linear space $\mathrm{End}_{\Lambda}(W)$, when given a Lie bracket by the commutator, can be identified with $\mathrm{gl}(2n|2n) = \mathrm{Lie}(\mathrm{Gl}(2n|2n))$. As γ is supersymmetric ($\gamma = \gamma^{\mathrm{T}}\sigma$), (23) fixes an $\mathrm{osp}(2n|2n)$ subalgebra.

γ is not unique. For definiteness we choose it as follows. Let $\{E_{ij}\}_{i,j=1,\ldots,M}$ be a canonical basis of $\mathrm{End}(\mathbb{C}^M)$ satisfying $E_{ij}E_{kl} = \delta_{jk}E_{il}$ (here $M=2$ or $M=n$). For $M=2$ define the Pauli spin operators $\sigma_x = E_{12} + E_{21}$, $\sigma_y = -iE_{12} + iE_{21}$, and $\sigma_z = E_{11} - E_{22}$. The usual rule of supertransposition on $\mathrm{End}_{\Lambda}(W)$ is given by ($\mu,\nu = 1,2$ and $i,j = 1,\ldots,n$)

$$\begin{aligned} &(E_{\mathrm{BB}} \otimes E_{\mu\nu} \otimes E_{ij})^{\mathrm{T}} = E_{\mathrm{BB}} \otimes E_{\nu\mu} \otimes E_{ji}, \quad (E_{\mathrm{BF}} \otimes E_{\mu\nu} \otimes E_{ij})^{\mathrm{T}} = -E_{\mathrm{FB}} \otimes E_{\nu\mu} \otimes E_{ji}, \\ &(E_{\mathrm{FB}} \otimes E_{\mu\nu} \otimes E_{ij})^{\mathrm{T}} = E_{\mathrm{BF}} \otimes E_{\nu\mu} \otimes E_{ji}, \quad (E_{\mathrm{FF}} \otimes E_{\mu\nu} \otimes E_{ij})^{\mathrm{T}} = E_{\mathrm{FF}} \otimes E_{\nu\mu} \otimes E_{ji}. \end{aligned}$$

With these conventions, one possible choice for γ is

$$\gamma = E_{\mathrm{BB}} \otimes \gamma_{\mathrm{B}} + E_{\mathrm{FF}} \otimes \gamma_{\mathrm{F}}, \quad \text{where} \quad \gamma_{\mathrm{B}} = \sigma_x \otimes 1_n, \quad \gamma_{\mathrm{F}} = i\sigma_y \otimes 1_n. \tag{24}$$

This is the choice we make.

D. Gaussian Berezin integral

To repeat the steps of Sec. III A and derive a Q-integral representation for the generating function Z_n, we must first generalize the basic identity (10), whose left-hand side is

$$\int D(\psi,\widetilde{\psi}) \exp(i\ \mathrm{Tr}_V\, A\psi\widetilde{\psi} - i\ \mathrm{STr}_W\, B\widetilde{\psi}\psi). \tag{25}$$

By (22) we have

$$\mathrm{Tr}\ A\psi\widetilde{\psi} = \mathrm{Tr}(\psi\widetilde{\psi})^{\mathrm{T}} A^{\mathrm{T}} = \tfrac{1}{2}\mathrm{Tr}(A - \mathscr{C}A^{\mathrm{T}}\mathscr{C}^{-1})\psi\widetilde{\psi},$$

$$\mathrm{STr}\ B\widetilde{\psi}\psi = \mathrm{STr}(\widetilde{\psi}\psi)^{\mathrm{T}} B^{\mathrm{T}} = \tfrac{1}{2}\mathrm{Tr}(B - \gamma B^{\mathrm{T}}\gamma^{-1})\widetilde{\psi}\psi.$$

In view of this we demand that A and B satisfy

$$A = -\mathscr{C}A^{\mathrm{T}}\mathscr{C}^{-1}, \quad B = -\gamma B^{\mathrm{T}}\gamma^{-1}. \tag{26}$$

When carrying out the calculation (11)–(13) we need to apply the identity (10) twice, the first time with $A = H$, $B = \omega$, and the second time with $A = 0$, $B = \omega - Q$. In order for (26) to be satisfied with these identifications, we choose to set

$$\omega = E_{\mathrm{BB}} \otimes \sigma_z \otimes \sum_{i=1}^{n} \alpha_i E_{ii} + E_{\mathrm{FF}} \otimes \sigma_z \otimes \sum_{j=1}^{n} \beta_j E_{jj}.$$

The presence of the factor $\sigma_z = \mathrm{diag}(+1,-1)$ reverses the sign of the α_i and β_j on that subspace where σ_z acts by multiplication with -1. As the imaginary parts of the α_i control the convergence of the integral, this sign reversal affects the correct choice of integration domain for ψ_{B} and $\widetilde{\psi}_{\mathrm{B}}$. To ensure convergence of the integral (25), we require $\mathrm{Im\,STr}\ \omega\widetilde{\psi}\psi \leqslant 0$. This inequality is achieved by imposing the condition $\widetilde{\psi}_{\mathrm{B}} = (\sigma_z \otimes 1_n)\psi_{\mathrm{B}}^{\dagger}$, which is compatible with $\mathscr{C} = i\sigma_y \otimes 1_N$, $\psi_{\mathrm{B}} = \mathscr{C}\widetilde{\psi}_{\mathrm{B}}^{\mathrm{T}}\gamma_{\mathrm{B}}^{-1}$, and $\gamma_{\mathrm{B}} = \sigma_x \otimes 1_n$.

Lemma 3.1: Let $D(\psi,\widetilde{\psi})$ denote a translation-invariant holomorphic Berezin measure on the subspace of $\mathrm{Hom}_\Lambda(W,V)\times\mathrm{Hom}_\Lambda(V,W)$ defined by (20). Fix the integration domain by $\widetilde{\psi}_{\mathrm{B}} = (\sigma_z \otimes 1_n)\psi_{\mathrm{B}}^\dagger$, and normalize $D(\psi,\widetilde{\psi})$ so that $\int D(\psi,\widetilde{\psi})\exp(-s^2\,\mathrm{Tr}\,\psi\widetilde{\psi})=1$ $(s\in\mathbb{R})$. Then if $A\in\mathrm{End}(V)$ and $B\in\mathrm{End}_\Lambda(W)$ are diagonalizable and satisfy the linear conditions (26), the identity (10) holds with $c=1/2$ provided that the integral exists.

Proof: Assume that A and B are represented by diagonal matrices,

$$A=\sigma_z\otimes\sum_{i=1}^{N} x_i E_{ii}\,,\quad B=E_{\mathrm{BB}}\otimes\sigma_z\otimes\sum_{j=1}^{n} z_j E_{jj}+E_{\mathrm{FF}}\otimes\sigma_z\otimes\sum_{j=1}^{n} y_j E_{jj}\,,$$

which conforms with (26). The right-hand side of (10) then reduces to

$$\mathrm{SDet}_{V\otimes W}(A\otimes 1-1\otimes B)^{-1/2}=\prod_{i=1}^{N}\prod_{j=1}^{n}\frac{(x_i-y_j)(x_i+y_j)}{(x_i-z_j)(x_i+z_j)}. \tag{27}$$

To evaluate the left-hand side, write

$$\psi_{\mathrm{B}}=\begin{pmatrix} a & b\\ c & d\end{pmatrix},\quad \psi_{\mathrm{F}}=\begin{pmatrix}\alpha & \beta\\ \gamma & \delta\end{pmatrix},$$

where $a,b,c,d(\alpha,\beta,\gamma,\delta)$ are complex $N\times n$ matrices with commuting (resp., anticommuting) matrix elements. The constraint $\widetilde{\psi}=-\gamma\psi^{\mathrm{T}}\mathscr{C}^{-1}$ results in

$$\widetilde{\psi}_{\mathrm{B}}=\begin{pmatrix}-d^{\mathrm{T}} & b^{\mathrm{T}}\\ -c^{\mathrm{T}} & a^{\mathrm{T}}\end{pmatrix},\quad \widetilde{\psi}_{\mathrm{F}}=\begin{pmatrix}-\delta^{\mathrm{T}} & \beta^{\mathrm{T}}\\ \gamma^{\mathrm{T}} & -\alpha^{\mathrm{T}}\end{pmatrix},$$

and the reality condition $\widetilde{\psi}_{\mathrm{B}} = (\sigma_z\otimes 1_n)\psi_{\mathrm{B}}^\dagger$ means $d=-\overline{a}$ and $c=\overline{b}$. The exponent of the integrand is expressed by

$$\frac{1}{2}\,\mathrm{Tr}\,A\psi\widetilde{\psi}-\frac{1}{2}\,\mathrm{Tr}\,B\widetilde{\psi}\psi=\sum_{i=1}^{N}\sum_{j=1}^{n}\big((x_i-z_j)a_{ij}\overline{a_{ij}}-(x_i+z_j)b_{ij}\overline{b_{ij}}$$
$$+(x_i+y_j)\alpha_{ij}\delta_{ij}-(x_i-y_j)\beta_{ij}\gamma_{ij}\big).$$

Doing the Gaussian integrals one gets a result that is identical to (27), which proves the Lemma for diagonal A and B. The general case follows by the invariance properties of $D(\psi,\widetilde{\psi})$.

Remark: The condition of diagonalizability can of course be weakened but we will not need that here. ∎

To apply Lemma 3.1 to our problem, note

$$\mathrm{SDet}_{V\otimes W}(H\otimes 1-1\otimes\omega)^{1/2}=\prod_{i=1}^{n}\mathrm{Det}_V\left(\frac{(H-\alpha_i)(H+\alpha_i)}{(H-\beta_i)(H+\beta_i)}\right)^{1/2}=\prod_{i=1}^{n}\mathrm{Det}\left(\frac{H-\alpha_i}{H-\beta_i}\right),$$

where in the second step we used the invariance of the ratio of determinants under $H\mapsto -H$, which is due to the particle-hole symmetry $H=-\mathscr{C}H^{\mathrm{T}}\mathscr{C}^{-1}$. Moreover, note

$$\mathrm{SDet}_{V\otimes W}(1\otimes(Q-\omega))^{-1/2}=\mathrm{SDet}_W(Q-\omega)^{-N}.$$

The previous calculation (11)–(13) thus *formally* goes through with $c=1/2$, and $i\mathrm{sp}(N)$ for $i\mathrm{u}(N)$, and we arrive at the following representation of the generating function:

$$Z_n(\omega)=\int DQ\ \exp -N\ \mathrm{STr}\left(\frac{Q^2}{2v^2}+\ln(Q-\omega)\right), \tag{28}$$

where the supermatrix

$$Q=\begin{pmatrix} Q_{\mathrm{BB}} & Q_{\mathrm{BF}} \\ Q_{\mathrm{FB}} & Q_{\mathrm{FF}} \end{pmatrix}$$

is subject to (23). To make this rigorous, we have to specify the integration domain for Q and show that the interchange of the $(\psi,\tilde{\psi})$- and Q-integrations is permitted.

E. Choice of integration domain

If the steps (11)–(13) are to be valid, we must arrange for all integrals to be convergent, at least. This is easily achieved for Q_{FF}, the FF component of Q, but requires substantial labor for ψ_{B}, $\tilde{\psi}_{\mathrm{B}}$, and Q_{BB}. Consider Q_{FF} first. Since $-\mathrm{STr}\,Q^2=-\mathrm{Tr}\,Q_{\mathrm{BB}}^2+\mathrm{Tr}\,Q_{\mathrm{FF}}^2+\text{nilpotents}$, we want $\mathrm{Tr}\,Q_{\mathrm{FF}}Q_{\mathrm{FF}}\leqslant 0$, which leads us to require that Q_{FF} be anti-Hermitian. Combining this with (23) we get

$$Q_{\mathrm{FF}}=-\gamma_{\mathrm{F}}Q_{\mathrm{FF}}^{\mathrm{T}}\gamma_{\mathrm{F}}^{-1}=-Q_{\mathrm{FF}}^{\dagger},$$

where $\gamma_{\mathrm{F}}=i\sigma_y\otimes 1_n$; see (24). The solution space of these equations is $\mathrm{sp}(n)$, the symplectic Lie algebra in $2n$ dimensions. Thus we choose $\mathscr{U}:=\mathrm{sp}(n)$ for the integration domain of Q_{FF}, and, of course, the integration measure is taken to be the flat one.

The choice of integration domain for Q_{BB} is a much more delicate matter and will occupy us for the remainder of this section. Recall, first of all, that the convergence of

$$\int D(\psi,\tilde{\psi})\exp(i\ \mathrm{Tr}\ H\psi\tilde{\psi}-i\ \mathrm{STr}\ \omega\tilde{\psi}\psi)$$

requires taking $\tilde{\psi}_{\mathrm{B}}=\beta\psi_{\mathrm{B}}^{\dagger}$, where $\beta:=\sigma_z\otimes 1_n$ cancels the minus signs that multiply the imaginary parts of the parameters α_i in ω. To ensure the convergence of

$$\int D(\psi,\tilde{\psi})\exp\ i\ \mathrm{Tr}\ \psi(Q-\omega)\tilde{\psi},$$

one is tempted to choose Q_{BB} in such a way that $\mathrm{Re}\,\mathrm{Tr}\,\psi Q\tilde{\psi}=0$. Unfortunately, when this condition is adopted one gets $Q_{\mathrm{BB}}=\beta Q_{\mathrm{BB}}^{\dagger}\beta$, which causes $\mathrm{Tr}\,Q_{\mathrm{BB}}^2=\mathrm{Tr}\,Q_{\mathrm{BB}}\beta Q_{\mathrm{BB}}^{\dagger}\beta$, to be of *indefinite sign*, so that the integral over Q does not exist.

A way out of this difficulty was first described by Schäfer and Wegner[2] in a related context. We are now going to formulate their prescription in a language that anticipates the geometric structure emerging in the large-N limit. To simplify the notation, we put $Q_{\mathrm{BB}}=iZ$. What we need to do is investigate the expression

$$\exp(-N\ \mathrm{Tr}\ Q_{\mathrm{BB}}^2/2v^2+i\ \mathrm{Tr}\ Q_{\mathrm{BB}}\tilde{\psi}_{\mathrm{B}}\psi_{\mathrm{B}})=\exp(N\ \mathrm{Tr}\ Z^2/2v^2-\mathrm{Tr}\ Z\tilde{\psi}_{\mathrm{B}}\psi_{\mathrm{B}}). \tag{29}$$

The conditions on Q_{BB} translate into

$$Z=-\gamma_{\mathrm{B}}Z^{\mathrm{T}}\gamma_{\mathrm{B}}^{-1}=-\beta Z^{\dagger}\beta^{-1}.$$

Because $\gamma_{\mathrm{B}}=\sigma_x\otimes 1_n$ is symmetric, the solution space of the first equation is a complex Lie algebra $\mathscr{G}_{\mathbb{C}}\simeq\mathrm{so}(2n,\mathbb{C})$. The matrix representation of an element $Z\in\mathscr{G}_{\mathbb{C}}$ is of the form

$$\begin{pmatrix} A & B \\ C & -A^{\mathrm{T}} \end{pmatrix},$$

where B and C are skew. The second equation ($Z=-\beta Z^{\dagger}\beta^{-1}$) means $A=-A^{\dagger}$ and $C=B^{\dagger}$, which fixes a real form $\mathcal{G}=\mathrm{so}^*(2n)$ of $\mathcal{G}_{\mathbb{C}}=\mathrm{so}(2n,\mathbb{C})$. This real form is *noncompact* [i.e., $\mathcal{G}=\mathrm{Lie}(G)$ with G a noncompact Lie group], which is what causes all the trouble and is forcing us to work hard. Its maximal compact subalgebra $\mathcal{K}$ is the set of solutions of $X=\beta X\beta^{-1}$ in $\mathcal{G}$. From

$$X=\begin{pmatrix} A & 0 \\ 0 & -A^{\mathrm{T}} \end{pmatrix}$$

and $A=-A^{\dagger}$ we see that $\mathcal{K}\simeq u(n)$.

To display clearly the general nature of the following construction, we introduce a symmetric quadratic form $\mathrm{B}:\mathcal{G}_{\mathbb{C}}\times\mathcal{G}_{\mathbb{C}}\to\mathbb{C}$ by $\mathrm{B}(X,Y)=\mathrm{Tr}\,XY$. The Cartan (orthogonal) decomposition of $\mathcal{G}$ with respect to this quadratic form is written as $\mathcal{G}=\mathcal{K}\oplus\mathcal{M}$. An element Y of $\mathcal{M}$ satisfies $Y=-\beta Y\beta^{-1}$. From this, in conjunction with the equation fixing $\mathcal{K}$ ($X=+\beta X\beta^{-1}$), one deduces the commutation relations

$$[\mathcal{M},\mathcal{M}]\subset\mathcal{K},\quad [\mathcal{K},\mathcal{M}]\subset\mathcal{M},\quad [\mathcal{K},\mathcal{K}]\subset\mathcal{K}. \tag{30}$$

Note that the elements of $\mathcal{M}$ are Hermitian while those of $\mathcal{K}$ are anti-Hermitian. We will also encounter the complexified spaces $\mathcal{K}_{\mathbb{C}}=\mathcal{K}+i\mathcal{K}$ and $\mathcal{M}_{\mathbb{C}}=\mathcal{M}+i\mathcal{M}$. They, too, are orthogonal with respect to B and satisfy the commutation relations (30). The element $\beta=\sigma_z\otimes 1_n$ satisfies $\beta=-\gamma_{\mathrm{B}}\beta^{\mathrm{T}}\gamma_{\mathrm{B}}^{-1}$ and can therefore be regarded as an element of $\mathcal{G}_{\mathbb{C}}$. Moreover, $\beta\in i\mathcal{K}\subset\mathcal{G}_{\mathbb{C}}$.

Now we embed $\mathcal{G}=\mathcal{K}\oplus\mathcal{M}$ into $\mathcal{G}_{\mathbb{C}}$ by a map ϕ_b,

$$\phi_b:\mathcal{K}\times\mathcal{M}\to\mathcal{G}_{\mathbb{C}},$$

$$(X,Y)\mapsto\phi_b(X,Y)=b\times(X+e^{Y}\beta e^{-Y}),$$

where $b\neq 0$ is some constant that will be specified later.

Lemma 3.2: $\phi_b(\mathcal{K}\times\mathcal{M})$ is an analytic manifold without boundary, and is diffeomorphic to $\mathcal{G}$.

Proof: Analyticity is clear. To prove the other properties, we first establish that ϕ_b is injective. For that purpose, we write $e^{Y}\beta e^{-Y}=e^{\mathrm{ad}(Y)}\beta$, where $\mathrm{ad}(Y)\beta=[Y,\beta]$ is the adjoint action on $\mathcal{G}_{\mathbb{C}}$. Decomposing the exponential function according to $\exp=\cosh+\sinh$, we write $\phi_b=\phi_+ +\phi_-$, where

$$\phi_+(X,Y)=b\times(X+\cosh\,\mathrm{ad}(Y)\beta),$$

$$\phi_-(X,Y)=b\times\sinh\,\mathrm{ad}(Y)\beta.$$

From the commutation relations (30) and $\beta\in i\mathcal{K}$, we see that $\phi_{\pm}$ takes values $\phi_+(X,Y)\in\mathcal{K}_{\mathbb{C}}$ and $\phi_-(X,Y)\in\mathcal{M}_{\mathbb{C}}$. Since $\mathcal{G}_{\mathbb{C}}=\mathcal{K}_{\mathbb{C}}\oplus\mathcal{M}_{\mathbb{C}}$ (direct sum), injectivity is equivalent to the regularity of the maps $X\mapsto\phi_+(X,Y)$ (with Y viewed as a parameter) and $Y\mapsto\phi_-(X,Y)$. The function $\phi_+(X,\cdot)=X+\mathrm{const}$ is obviously regular. By $Y=Y^{\dagger}$ the element Y is diagonalizable with real eigenvalues. The regularity of ϕ_- then follows from $\sinh:\mathbb{R}\to\mathbb{R}$ being monotonic and $Y\mapsto\mathrm{ad}(Y)\beta$ being regular. This completes the proof that ϕ_b is injective. The injectivity of ϕ_b means that $\phi_b(\mathcal{K}\times\mathcal{M})$ is diffeomorphic to $\mathcal{G}=\mathcal{K}\oplus\mathcal{M}$. This in turn means that, since $\mathcal{G}$ has no boundary, $\phi_b(\mathcal{K}\times\mathcal{M})$ has no boundary either. ■

We are now going to demonstrate that $\phi_b(\mathscr{K}\times\mathscr{M})$ for any $b>0$ may serve as a mathematically satisfactory domain of integration for the variable Z in (29). We begin by investigating the quadratic form $\mathrm{Tr}\, Z^2=\mathrm{B}(Z,Z)$ on $\phi_b(\mathscr{K}\times\mathscr{M})$. For this we set $Z=Z_+ + Z_-$ with $Z_\pm=\phi_\pm(X,Y)$. Using $\mathrm{B}(Z_+,Z_-)=0$ (recall $\mathscr{K}_\mathbb{C}\perp\mathscr{M}_\mathbb{C}$), $\mathrm{B}(\mathrm{ad}(Y)A,B)=-\mathrm{B}(A,\mathrm{ad}(Y)B)$ and $\cosh^2-\sinh^2=1$, we obtain

$$\mathrm{B}(Z,Z)/b^2=\mathrm{B}(X,X)+2\mathrm{B}(X,\cosh\,\mathrm{ad}(Y)\beta)+\mathrm{B}(\beta,\beta).$$

The antihermiticity of $X\in\mathscr{K}$ gives $\mathrm{B}(X,X)\leqslant 0$. In contrast, $\cosh\,\mathrm{ad}(Y)\beta\in i\mathscr{K}$ is Hermitian, so $\mathrm{B}(X,\cosh\,\mathrm{ad}(Y)\beta)\in i\mathbb{R}$. It follows that $\exp(N\,\mathrm{Tr}\,Z^2/2v^2)=\exp(N\,\mathrm{Tr}\,\phi_b(X,Y)^2/2v^2)$ is decaying with respect to X and oscillatory with respect to Y.

We have not yet made any use of $b>0$ yet. This inequality comes into play when the coupling term

$$-\mathrm{Tr}\, Z\widetilde{\psi}_\mathrm{B}\psi_\mathrm{B}=-\mathrm{B}(Z,\widetilde{\psi}_\mathrm{B}\psi_\mathrm{B})=-b\mathrm{B}(X,\widetilde{\psi}_\mathrm{B}\psi_\mathrm{B})-b\mathrm{B}(e^Y\beta e^{-Y},\widetilde{\psi}_\mathrm{B}\psi_\mathrm{B})$$

is considered. From (22) and $\widetilde{\psi}_\mathrm{B}=\beta\psi_\mathrm{B}^\dagger$ we see that $\widetilde{\psi}_\mathrm{B}\psi_\mathrm{B}$ satisfies

$$\widetilde{\psi}_\mathrm{B}\psi_\mathrm{B}=-\gamma_\mathrm{B}(\widetilde{\psi}_\mathrm{B}\psi_\mathrm{B})^\mathrm{T}\gamma_\mathrm{B}^{-1}=+\beta(\widetilde{\psi}_\mathrm{B}\psi_\mathrm{B})^\dagger\beta^{-1},$$

so $\widetilde{\psi}_\mathrm{B}\psi_\mathrm{B}\in i\mathscr{G}$. Since B is real valued on $\mathscr{G}\times\mathscr{G}$, the term $\mathrm{B}(X,\widetilde{\psi}_\mathrm{B}\psi_\mathrm{B})$ is purely imaginary. The other term,

$$-b\mathrm{B}(e^Y\beta e^{-Y},\widetilde{\psi}_\mathrm{B}\psi_\mathrm{B})=-b\ \mathrm{Tr}(\psi_\mathrm{B}e^{2Y}\psi_\mathrm{B}^\dagger)\leqslant 0,$$

is never positive if $b>0$. Hence the real part of the exponential in (29) is negative semidefinite for $Q=iZ\in i\,\phi_b(\mathscr{K}\times\mathscr{M})$ and $b>0$. As a result, the integrals over Q and $\psi,\widetilde{\psi}$ converge if the integration domain for Q is taken to be $i\,\phi_b(\mathscr{K}\times\mathscr{M})\times\mathscr{U}$ $(b>0)$. Because $i\,\phi_b(\mathscr{K}\times\mathscr{M})\times\mathscr{U}$ is an analytic manifold without boundary and Cauchy's theorem applies, we may perform the shift of integration variables that is implied by the fourth equality sign in (12). Moreover, the presence of the nonvanishing imaginary parts of the parameters α_i in ω ensures *uniform convergence* of the $(\psi,\widetilde{\psi})$ integral with respect to Q, so that we may interchange the order of integration [the second equality sign in (13)]. And finally, any breakdown of diagonalizability of $Q-\omega$ occurs on a set of measure zero, so that the identity (10) (Lemma 3.1) may be used, and all steps leading to (28) are rigorous. In summary, we have proved the following result.

Theorem 3.3: For $V=\mathbb{C}^2\otimes\mathbb{C}^N$ and $W=\mathbb{C}^{1|1}\otimes\mathbb{C}^2\otimes\mathbb{C}^n$ define the generating function

$$Z_{n,N}(\omega)=\int_{i\times\mathrm{sp}(N)}\mathrm{SDet}_{V\otimes W}(H\otimes 1-1\otimes\omega)^{-1/2}\exp\left(-\frac{N\ \mathrm{Tr}\ H^2}{2v^2}\right)dH,$$

$$\omega=E_\mathrm{BB}\otimes\sigma_z\otimes\sum_{i=1}^n\alpha_iE_{ii}+E_\mathrm{FF}\otimes\sigma_z\otimes\sum_{j=1}^n\beta_jE_{jj}\quad(\mathrm{Im}\ \alpha_i<0).$$

Let DQ denote a translation-invariant holomorphic Berezin measure of the complex-analytic superspace $\mathrm{osp}(2n|2n)$. Then for all $N\in\mathbb{N}$, $n\in\mathbb{N}$ and $b>0$, DQ can be normalized so that

$$Z_{n,N}(\omega)=\int_{i\,\phi_b(\mathscr{K}\times\mathscr{M})\times\mathscr{U}}DQ\ \exp-N\ \mathrm{STr}\left(\frac{Q^2}{2v^2}+\ln(Q-\omega)\right),\tag{31}$$

where $\mathscr{U}=\mathrm{sp}(n)$, $\mathscr{K}\simeq u(n)$, $\mathscr{M}$ is determined by $\mathscr{K}\oplus\mathscr{M}=\mathrm{so}^*(2n)$, and $\phi_b(X,Y)=b(X+\mathrm{Ad}(e^Y)(\sigma_z\otimes 1_n))$. ■

We conclude this section with a comment. In the literature a parametrization of the form $Q=TPT^{-1}$ (cf. Ref. 43) has been very popular. In our language, this factorization amounts to choosing for the integration domain of Q_{BB} the image of $\varphi:\mathscr{G}=\mathscr{K}\oplus\mathscr{M}\to\mathscr{G}$, $X+Y\mapsto e^{Y}Xe^{-Y}$. This is *not* a valid choice as $\varphi(\mathscr{G})$ *does have a boundary*, namely the light cone $\{Z|\mathrm{B}(Z,Z)=0\}$ in $\mathscr{G}$, so that shifting of integration variables is not permitted. (However, it turns out that the error made becomes negligible in the limit $N\to\infty$, so that the final results remain valid if that limit is assumed.)

F. Saddle-point supermanifold

The result (31) holds for all $N\in\mathbb{N}$. We are now going to use the method of steepest descent to show that in the limit $N\to\infty$, the integral on the right-hand side reduces to an integral over a Riemannian symmetric superspace of type $D\mathrm{III}|C\mathrm{I}$.

With our choice of normalization, the mean spacing between the eigenvalues of H scales as N^{-1} for $N\to\infty$; see (14). We are most interested in the eigenvalues close to zero, as their statistical properties describe those of the low-lying Bogoliubov independent-quasiparticle energy levels of mesoscopic normal-superconducting systems.[24] To probe their statistical behavior, what we need to do is keep $\hat{\omega}=N\omega/\pi v$ (i.e., ω scaled by the mean level spacing) fixed as N goes to infinity. In this limit $\omega\sim\mathscr{O}(1/N)$ can be treated as a small perturbation and we may expand $N\ \mathrm{STr}\ln(Q-\omega)=N\ \mathrm{STr}\ln Q-\pi v\ \mathrm{STr}\,Q^{-1}\hat{\omega}+\mathscr{O}(1/N)$ if Q^{-1} exists.

To evaluate the integral (31) by the method of steepest descent, we first look for the critical points of the function $NF(Q)=N\ \mathrm{STr}(Q^2/2v^2+\ln Q)$. These are the solutions of

$$F'(Q)=Q/v^2+Q^{-1}=0,$$

or $Q^2=-v^2$. The solution spaces, the so-called ''saddle-point supermanifolds,'' are nonlinear subspaces of $\mathrm{osp}(2n|2n)$, which can be distinguished by the eigenvalues of Q. Of these supermanifolds, which are the ones to select for the steepest-descent evaluation of the integral (31)?

To tackle this question, we start out by setting all Grassmann variables to zero. The BB part of the saddle-point manifold(s) is uniquely determined by the forced choice of integration domain $i\phi_b(\mathscr{K}\times\mathscr{M})$ and by analyticity. This is because the saddle-point manifold must be deformable (using Cauchy's theorem) into the integration domain without crossing any of the singularities of $\mathrm{SDet}(Q-\omega)^{-N}$; and by inspection one finds that this condition rules out all saddle-point manifolds except for one, which is $i\phi_v(0\times\mathscr{M})$, the subspace of the integration domain $i\phi_b(\mathscr{K}\times\mathscr{M})|_{b=v}$ obtained by dropping from $\mathscr{G}=\mathscr{K}\oplus\mathscr{M}$ the $\mathscr{K}$ degrees of freedom (these are the directions of steepest descent). By an argument given in the proof of Lemma 3.2 we know that $i\phi_v(0\times\mathscr{M})$ is diffeomorphic to $\mathscr{M}$. On general grounds the latter is diffeomorphic to a coset space G/K by the exponential map $\mathscr{M}\to G/K$, $Y\mapsto e^{Y}K$; where in the present case $G=\{g\in\mathrm{Gl}(2n,\mathbb{C})|g=\gamma_{\mathrm{B}}g^{-1^{\mathrm{T}}}\gamma_{\mathrm{B}}^{-1}=\beta g^{-1^{\dagger}}\beta^{-1}\}$, and $K=\{k\in G|k=\beta k\beta^{-1}\}$ (on setting $g=\exp Z$, $k=\exp X$ and linearizing, we recover the conditions $Z=-\gamma_{\mathrm{B}}Z^{\mathrm{T}}\gamma_{\mathrm{B}}^{-1}=-\beta Z^{\dagger}\beta^{-1}$ defining $\mathscr{G}$ and the condition $X=\beta X\beta^{-1}$ fixing the subalgebra $\mathscr{K}$). We already know $\mathscr{G}=\mathrm{so}^*(2n)$ and $\mathscr{K}\simeq\mathrm{u}(n)$, so $G=\exp\mathscr{G}=\mathrm{SO}^*(2n)$ and $K=\exp\mathscr{K}=\mathrm{U}(n)$. Because K is a maximal compact subgroup, the coset space G/K is a Riemannian symmetric space of the noncompact type. In Cartan's notation, $G/K=\mathrm{SO}^*(2n)/U(n)$ is called type $D\mathrm{III}$. For better distinction from its FF analog, we will henceforth denote G/K by G/K_{B}.

We turn to the FF sector. Since $\mathrm{SDet}(Q-\omega)^{-N}$ does not have poles but only has *zeros* as a function of Q_{FF}, analyticity provides *no* criterion for selecting any specific solution space of the saddle-point equation $Q_{\mathrm{FF}}^2=-v^2$. Instead, the determining agent now is the limit $N\to\infty$. From (31) it is seen that integration over the Gaussian fluctuations around the saddle-point manifold produces one factor of $N^{-1}(N^{+1})$ for every commuting (resp., anticommuting) direction of steepest descent. Therefore, the limit $N\to\infty$ is dominated by the saddle-point manifold that has the minimal transverse (super-)dimension $d_{\mathrm{B}}^{\perp}-d_{\mathrm{F}}^{\perp}$. A little thought shows that the transverse dimen-

sion is minimized by choosing Q_{FF} to possess n eigenvalues $+iv$ and n eigenvalues $-iv$. Thus, the dominant saddle-point manifold is unique and contains the special point $q_0 := iv\beta$ ($\beta = \sigma_z \otimes 1_n$ now acts in the fermionic subspace).

Recall that the integration domain for Q_{FF} is a compact Lie algebra $\mathscr{U} = \mathrm{sp}(n)$. The corresponding Lie group $U = \mathrm{Sp}(n)$ operates on $\mathscr{U}$ by the adjoint action $\mathrm{Ad}(u): \mathscr{U} \to \mathscr{U}$, $X \mapsto uXu^{-1}$. Because the saddle-point equation $Q_{\mathrm{FF}} = -v^2 Q_{\mathrm{FF}}^{-1}$ is invariant under this action, the FF part of the (dominant) saddle-point manifold can be viewed as the orbit of the action of $\mathrm{Ad}(U)$ on the special point $q_0 \in \mathscr{U}$. Let K_{F} be the stability group of q_0, i.e., $K_{\mathrm{F}} = \{k \in U | kq_0k^{-1} = q_0\}$. By $\mathrm{Ad}(K_{\mathrm{F}})q_0 = q_0$ the orbit $\mathrm{Ad}(U)q_0$ is diffeomorphic to the coset space U/K_{F}. Arguing in the same way as for the BB sector, one shows that $K_{\mathrm{F}} \simeq K_{\mathrm{B}} \simeq \mathrm{U}(n)$. Hence $U/K_{\mathrm{F}} = \mathrm{Sp}(n)/U(n)$, which in Cartan's notation is a compact Riemannian symmetric space of type CI.

We are finally in a position to construct the full saddle-point *super*manifold. Recall, first of all, that Q is subject to the condition $Q = -\gamma Q^{\mathrm{T}} \gamma^{-1}$, which defines an orthosymplectic complex Lie algebra $\mathscr{G}_\Lambda := \mathrm{osp}(2n|2n)$ in $\mathrm{End}_\Lambda(W)$. The solution spaces in $\mathscr{G}_\Lambda$ of the equation $Q/v^2 + Q^{-1} = 0$ are complex-analytic supermanifolds that are invariant under the adjoint action of the complex Lie supergroup $G_\Lambda := \mathrm{Osp}(2n|2n)$. They can be regarded as $\mathrm{Ad}(G_\Lambda)$ orbits of elements $Q_0 \in \mathrm{Lie}(G_\Lambda)$ that are solutions of $(Q_0)^2 = -v^2$. From the above analysis of the BB and FF sectors, we know that the saddle-point supermanifold that dominates in the large-N limit is obtained by setting $Q_0 = iv\Sigma_z$ where $\Sigma_z = 1_{\mathrm{B|F}} \otimes \beta = (E_{\mathrm{BB}} + E_{\mathrm{FF}}) \otimes \sigma_z \otimes 1_n$. If H_Λ is the stability group of Q_0, the orbit $\mathrm{Ad}(G_\Lambda)Q_0$ is diffeomorphic to the coset space G_Λ/H_Λ. From $\gamma\Sigma_z + \Sigma_z\gamma = 0$ and the equation $h\Sigma_z h^{-1} = \Sigma_z$ (or, equivalently, $h = \Sigma_z h \Sigma_z$) for $h \in H_\Lambda$ one infers $H_\Lambda \simeq \mathrm{Gl}(n|n)$. Hence the unique complex-analytic saddle-point supermanifold that dominates the large-N limit is $G_\Lambda/H_\Lambda \simeq \mathrm{Osp}(2n|2n)/\mathrm{Gl}(n|n)$.

Turning to the integral (31) we note the relations $\mathrm{STr}\, Q_0^2 = -v^2\, \mathrm{STr}\, 1 = 0$ and $\ln \mathrm{SDet} Q_0 = \ln 1 = 0$. These imply that the function $F(Q) = \mathrm{STr}(Q^2/2v^2 + \ln Q)$ vanishes identically on $\mathrm{Ad}(G_\Lambda)Q_0$. Hence the exponent of the integrand in (31) restricted to G_Λ/H_Λ is

$$\pi v\ \mathrm{STr}\ Q^{-1}\hat{\omega}\big|_{G_\Lambda/H_\Lambda} + \mathscr{O}(1/N) = -i\pi \mathrm{B}(\hat{\omega}, \mathrm{Ad}(g)\Sigma_z) + \mathscr{O}(1/N).$$

To complete the steepest-descent evaluation of (31) we need to Taylor expand the exponent of the integrand up to second order and do a Gaussian integral. By the $\mathrm{Ad}(G_\Lambda)$ invariance of the function $NF(Q)$ it is sufficient to do this calculation for one element of the saddle-point supermanifold, say $Q = Q_0$. Putting $Q = Q_0 + Z$ ($Z \in \mathscr{G}_\Lambda$) we get

$$NF(Q_0 + Z) = \frac{N}{2v^2}\, \mathrm{STr}(Z^2 + Z\Sigma_z Z \Sigma_z) + \mathscr{O}(Z^3).$$

Now we make the orthogonal decomposition $\mathscr{G}_\Lambda = \mathrm{Lie}(H_\Lambda) + \mathscr{M}_\Lambda$, $Z = X + Y$, where $Y = -\Sigma_z Y \Sigma_z$ are the degrees of freedom tangent to the saddle-point supermanifold, and $X = +\Sigma_z X \Sigma_z$ are the degrees of freedom transverse to it. The translation-invariant Berezin measure DZ of $\mathscr{G}_\Lambda$ factors as $DZ = DY\ DX$. We thus obtain the transverse Gaussian integral

$$\int DX\ \exp\left(-\frac{N}{v^2}\, \mathrm{STr}\, X^2 + \mathscr{O}(N^0) \right).$$

The integration domain for X is $i\mathscr{K}_{\mathrm{B}} \times \mathscr{K}_{\mathrm{F}} \simeq i\mathrm{u}(n) \times \mathrm{u}(n)$. By $\dim \mathrm{Lie}(H_\Lambda) = (p,q)$ and $p = q$, this integral reduces to a constant independent of N in the limit $N \to \infty$.

What remains is an integral over the saddle-point supermanifold itself. Since DY is the local expression of the invariant Berezin measure of G_Λ/H_Λ at $\mathrm{Ad}(e^Y)Q_0|_{Y=0} = Q_0$ we arrive at the following result.

Theorem 3.4: If Dg_H is a suitably normalized invariant holomorphic Berezin measure of the complex-analytic supermanifold $G_\Lambda/H_\Lambda \simeq \mathrm{Osp}(2n|2n)/\mathrm{Gl}(n|n)$,

$$\lim_{N\to\infty} Z_{n,N}\left(\frac{\pi v\,\hat{\omega}}{N}\right) = \int_{M_{\mathrm{B}}\times M_{\mathrm{F}}} Dg_H \,\exp -i\pi \mathrm{B}(\hat{\omega},\mathrm{Ad}(g)\Sigma_z), \tag{32}$$

where $\Sigma_z = 1_{\mathrm{B|F}}\otimes\sigma_z\otimes 1_n$, $M_{\mathrm{B}}\simeq \mathrm{SO}^*(2n)/\mathrm{U}(n)$, and $M_{\mathrm{F}}\simeq \mathrm{Sp}(n)/\mathrm{U}(n)$.

Remark 3.5: This result expresses the generating function for $N\to\infty$ as an integral over a Riemannian symmetric superspace of type $D\mathrm{III}|C\mathrm{I}$ (see Tables I and II) with $m=n$.

In Ref. 44 the n-level correlation function R_n is calculated exactly from (32) for all n.

IV. OTHER SYMMETRY CLASSES

There exist ten known universality classes of ergodic disordered single-particle systems. These are the three classic Wigner-Dyson classes (GOE, GUE, GSE), the three ''chiral'' ones describing a Dirac particle in a random gauge field (chGUE, chGOE, chGSE), and the four classes that can be realized in mesoscopic normal-superconducting (NS) hybrid systems. In Ref. 25 it was noted that there exists a one-to-one correspondence between these universality classes and the large families of symmetric spaces (with the exception of the orthogonal group in odd dimensions). Specifically, the Gaussian random-matrix ensemble over the tangent space of the symmetric space describes the corresponding universality class, in the limit $N\to\infty$. In the notation of Table I the correspondences are $A\leftrightarrow$GUE, $A\mathrm{I}\leftrightarrow$GOE, $A\mathrm{II}\leftrightarrow$GSE, $A\mathrm{III}\leftrightarrow$chGUE, $BD\mathrm{I}\leftrightarrow$chGOE, $C\mathrm{II}\leftrightarrow$chGSE, and the four NS classes correspond to C, D, $C\mathrm{I}$, and $D\mathrm{III}$.

We have shown in detail how to use the supersymmetry method for the Gaussian ensemble over $C_N=\mathrm{sp}(N)$, the tangent space of the symplectic Lie group. There are nine more ensembles to study. We will now briefly run through all these cases, giving only a summary of the essential changes.

A. Class *D*

Recall the definitions given at the beginning of Sec. III B and replace the symplectic unit by $\mathscr{C}=\sigma_x\otimes 1_N$. What you get is a Gaussian random-matrix ensemble over $D_N=\mathrm{so}(2N)$, the orthogonal Lie algebra in $2N$ dimensions. The explicit form of the Hamiltonian is

$$H=\begin{pmatrix} a & b \\ b^\dagger & -a^{\mathrm{T}} \end{pmatrix},$$

where $a(b)$ is complex Hermitian (resp., skew). The treatment of this ensemble closely parallels that of type C. A change first occurs in the consistency condition for γ, which now reads as $\gamma=-\gamma^{\mathrm{T}}\sigma$ (instead of $\gamma=+\gamma^{\mathrm{T}}\sigma$) by $\mathscr{C}\mathscr{C}^{-1^{\mathrm{T}}}=+1$. The extra minus sign can be accommodated by simply exchanging the BB and FF sectors ($\gamma_{\mathrm{B}}\leftrightarrow\gamma_{\mathrm{F}}$). The linear constraint $Q=-\gamma Q^{\mathrm{T}}\gamma^{-1}$ again defines an $\mathrm{osp}(2n|2n)$ Lie algebra, the only difference being that the BB sector is now ''symplectic'' while the FF sector has turned ''orthogonal.'' Everything else goes through as before and we arrive at the statement of Theorem 3.3 with $\mathscr{U}\simeq\mathrm{so}(2n)$, $\mathscr{K}\simeq\mathrm{u}(n)$, and $\mathscr{K}\oplus\mathscr{M}\simeq\mathrm{sp}(n,\mathbb{R})$.

A novel feature arises in the large-N limit, where instead of one dominant saddle-point supermanifold there now emerge *two*. One of them is the orbit with respect to the adjoint action of $\mathrm{Osp}(2n|2n)$ on $Q_0=iv1_{\mathrm{B|F}}\otimes\sigma_z\otimes 1_n$ as before, and the other one is the orbit of

$$Q_1 = ivE_{\mathrm{BB}}\otimes\sigma_z\otimes 1_n + ivE_{\mathrm{FF}}\otimes\sigma_z\otimes\left(E_{11}-\sum_{i=2}^{n}E_{ii}\right).$$

[The orbits of Q_0 and Q_1 are disconnected because the Weyl group of $\mathrm{so}(2n)$ is ''too small.''] Consequently, the right-hand side of Theorem 3.4 is replaced by a sum of two terms, one for each of the two saddle-point supermanifolds. The integral is over a Riemannian symmetric superspace of type $C\mathrm{I}|D\mathrm{III}$ ($m=n$) in both cases.

B. Class *CI*

Let $V=\mathbb{C}^2\otimes\mathbb{C}^N$ carry a Hermitian inner product (as always), and consider the space, P, of self-adjoint Hamiltonians $H\in\mathrm{End}(V)$ of the form

$$H=H^{\mathrm{T}}=-\mathscr{C}H^{\mathrm{T}}\mathscr{C}^{-1}=\begin{pmatrix} a & b \\ b & -a \end{pmatrix}, \quad \text{where } \mathscr{C}=i\sigma_y\otimes 1_N=\begin{pmatrix} 0 & 1_N \\ -1_N & 0 \end{pmatrix}.$$

The $N\times N$ matrices a and b are real symmetric. It is easy to see[25] that P is isomorphic to the tangent space of the symmetric space $\mathrm{Sp}(N)/\mathrm{U}(N)$ (type CI). A Gaussian measure $d\mu(H)$ on P is completely specified by its first two moments, $\int_P \mathrm{Tr}(AH)d\mu(H)=0$ and

$$\int_P \mathrm{Tr}(AH)\mathrm{Tr}(BH)d\mu(H)=\frac{v^2}{4N}\,\mathrm{Tr}(A(B+B^{\mathrm{T}})-A\mathscr{C}(B+B^{\mathrm{T}})\mathscr{C}^{-1}).$$

To deal with the random-matrix ensemble defined by this measure, we take $W=\mathbb{C}^{1|1}\otimes\mathbb{C}^2\otimes\mathbb{C}^2\otimes\mathbb{C}^n$. Recall $\psi\in\mathrm{Hom}_\Lambda(W,V)$ and $\widetilde{\psi}\in\mathrm{Hom}_{\tilde{\Lambda}}(V,W)$. The symmetries of H are copied to $\psi\widetilde{\psi}$ by imposing the linear conditions

$$\psi=\mathscr{C}\widetilde{\psi}^{\mathrm{T}}\gamma^{-1}, \quad \widetilde{\psi}=-\gamma\psi^{\mathrm{T}}\mathscr{C}^{-1}; \quad \psi=\widetilde{\psi}^{\mathrm{T}}\tau^{-1}, \quad \widetilde{\psi}=\tau\psi^{\mathrm{T}}.$$

In order for these conditions to be mutually consistent, $\tau,\ \gamma\in\mathrm{End}_0(W)$ must satisfy

$$\gamma=\gamma^{\mathrm{T}}\sigma, \quad \tau=\tau^{\mathrm{T}}\sigma, \quad \gamma\tau^{-1}=-\tau\gamma^{-1}.$$

Without loss, we take γ and τ to be orthogonal. The consistency conditions can then be written in the form

$$\gamma^2=\sigma=\tau^2, \quad \gamma\tau+\tau\gamma=0.$$

If $\mathrm{Gl}(W)\simeq\mathrm{Gl}(4n|4n)$ is the Lie supergroup of regular elements in $\mathrm{End}_\Lambda(W)$, the equation $\gamma^2=\sigma$ in conjunction with $g^{\mathrm{TT}}=\sigma g\sigma$ means that the automorphism $\hat{\gamma}:\mathrm{Gl}(W)\to\mathrm{Gl}(W)$ defined by $\hat{\gamma}(g)=\gamma g^{-1^{\mathrm{T}}}\gamma^{-1}$ is involutory. The same is true for $\hat{\tau}$ defined by $\hat{\tau}(g)=\tau g^{-1^{\mathrm{T}}}\tau^{-1}$ and, moreover, $\hat{\gamma}$ and $\hat{\tau}$ commute by $\gamma\tau+\tau\gamma=0$. For definiteness we take

$$\begin{aligned} \gamma&=E_{\mathrm{BB}}\otimes\gamma_{\mathrm{B}}+E_{\mathrm{FF}}\otimes\gamma_{\mathrm{F}}, \quad \gamma_{\mathrm{B}}=\sigma_x\otimes\sigma_z\otimes 1_n, \quad \gamma_{\mathrm{F}}=i\sigma_y\otimes 1_2\otimes 1_n, \\ \tau&=E_{\mathrm{BB}}\otimes\tau_{\mathrm{B}}+E_{\mathrm{FF}}\otimes\tau_{\mathrm{F}}, \quad \tau_{\mathrm{B}}=1_2\otimes\sigma_x\otimes 1_n, \quad \tau_{\mathrm{F}}=\sigma_z\otimes i\sigma_y\otimes 1_n. \end{aligned}$$

(This choice is consistent with $\widetilde{\psi}_B=\beta\psi_B^\dagger$, $\beta=\sigma_z\otimes 1_2\otimes 1_n$.) Let

$$\mathscr{Q}:=\{Q\in\mathrm{End}_\Lambda(W)\,|\,Q=-\gamma Q^{\mathrm{T}}\gamma^{-1}=+\tau Q^{\mathrm{T}}\tau^{-1}\}$$

be the subspace distinguished by the symmetry properties of $\widetilde{\psi}\psi$. The group $\mathrm{Gl}(W)$ acts on $\mathscr{Q}$ by $Q\mapsto gQg^{-1}$. We now ask what is the subgroup G_Λ of $\mathrm{Gl}(W)$ that leaves the symmetries of Q invariant [the normalizer of $\mathscr{Q}$ in $\mathrm{Gl}(W)$].

Lemma 4.1: G_Λ is isomorphic to $\mathrm{Osp}(2n|2n)\times\mathrm{Osp}(2n|2n)$.

Proof: The conditions on $g\in G_\Lambda$ can be phrased as follows:

$$\gamma=g\gamma g^{\mathrm{T}}, \quad \tau=g\tau g^{\mathrm{T}}.$$

Equivalently, G_Λ can be described as the simultaneous ''fixed point set''[45] of the involutory automorphisms $\hat{\gamma}$ and $\hat{\tau}$. We first describe the fixed point set of $\hat{\gamma}\circ\hat{\tau}$, which acts by $(\hat{\gamma}\circ\hat{\tau})(g)=\epsilon g\epsilon^{-1}$, where $\epsilon=-i\gamma\tau^{-1}$. From the explicit expression $\epsilon=1_{B|F}\otimes\sigma_x\otimes\sigma_y\otimes 1_n$ we see that ϵ has $4n$ eigenvalues equal to $+1$, $4n$ eigenvalues equal to -1, and these are equally

distributed over the bosonic and fermionic subspaces. Hence the subgroup of $\mathrm{Gl}(W)$ fixed by $\hat{\gamma}\circ\hat{\tau}$ is isomorphic to $G_+\times G_-$, where $G_+\simeq\mathrm{Gl}(2n|2n)\simeq G_-$. Denote the embedding $G_+\times G_-\to\mathrm{Gl}(W)$ by $\varphi(g_+,g_-)=g$. The group G_Λ is the fixed point set of $\hat{\tau}$ (or, equivalently, of $\hat{\gamma}$) in $\varphi(G_+\times G_-)$ [$\hat{\tau}$ commutes with $\hat{\gamma}\circ\hat{\tau}$ and therefore takes $\varphi(G_+\times G_-)$ into itself]. Note $\epsilon\tau=-\tau\epsilon$, $\epsilon^{-1^{\mathrm{T}}}=-\epsilon$, and for $g\in\varphi(G_+\times G_-)$ do the following little calculation:

$$\epsilon\hat{\tau}(g)=\epsilon\tau g^{-1^{\mathrm{T}}}\tau^{-1}=-\tau\epsilon g^{-1^{\mathrm{T}}}\tau^{-1}=\tau(\epsilon g)^{-1^{\mathrm{T}}}\tau^{-1}=\hat{\tau}(\epsilon g).$$

Combining this with $\epsilon\varphi(g_+,g_-)=\varphi(g_+,-g_-)$ one infers that $\hat{\tau}$ acting on $\varphi(G_+\times G_-)$ is of the form $\hat{\tau}\varphi(g_+,g_-)=\varphi(\hat{\tau}_+(g_+),\hat{\tau}_-(g_-))$. By a short calculation (work in an eigenbasis of ϵ) one sees that the involutory automorphisms $\hat{\tau}_i$: $\mathrm{Gl}(2n|2n)\to\mathrm{Gl}(2n|2n)$ $(i=\pm)$ are expressed by $\hat{\tau}_i(g)=\tau_i g^{-1^{\mathrm{T}}}\tau_i^{-1}$ with supersymmetric $\tau_i(\tau_i=\tau_i^{\mathrm{T}}\sigma)$. It follows that $\hat{\tau}_i$ fixes an orthosymplectic subgroup of $G_i\simeq\mathrm{Gl}(2n|2n)$, so $G_\Lambda\simeq\mathrm{Osp}(2n|2n)\times\mathrm{Osp}(2n|2n)$, as claimed.

Corollary 4.2: The space $\mathscr{Q}$ is isomorphic to the complement of $\mathrm{osp}(2n|2n)\oplus\mathrm{osp}(2n|2n)$ in $\mathrm{osp}(4n|4n)$.

Proof: The solution space in $\mathrm{End}_\Lambda(W)$ of $Q=-\gamma Q^{\mathrm{T}}\gamma^{-1}$ is an $\mathrm{osp}(4n|4n)$ algebra. Implementing the second condition $Q=+\tau Q^{\mathrm{T}}\tau^{-1}$ amounts to removing from $\mathrm{osp}(4n|4n)$ the subalgebra fixed by $X=-\tau X^{\mathrm{T}}\tau^{-1}$. By linearization of the conditions $g=\hat{\gamma}(g)=\hat{\tau}(g)$, this subalgebra is identified as $\mathrm{Lie}(G_\Lambda)\simeq\mathrm{osp}(2n|2n)\oplus\mathrm{osp}(2n|2n)$. ■

The Gaussian integral identity (10) continues to hold, albeit with a different value of $c=1/4$. The proof is essentially the same as before.

Since $\mathscr{Q}$ is not a Lie algebra, the description of the correct choice of integration domain for the auxiliary variable Q is more complicated than before. In the FF sector we take $\mathscr{U}:=\{Q_{\mathrm{FF}}\in\mathscr{Q}_{\mathrm{FF}}|Q_{\mathrm{FF}}=-Q_{\mathrm{FF}}^\dagger\}$. By Corollary 4.2, $\mathrm{sp}(2n)\simeq(\mathrm{sp}(n)\oplus\mathrm{sp}(n))\oplus\mathscr{U}$. To deal with the BB sector we introduce the spaces

$$\mathscr{G}=\{X\in\mathrm{gl}(2n,\mathbb{C})|X=-\gamma_{\mathrm{B}}X^{\mathrm{T}}\gamma_{\mathrm{B}}^{-1}=-\tau_{\mathrm{B}}X^{\mathrm{T}}\tau_{\mathrm{B}}^{-1}=-\beta X^\dagger\beta^{-1}\},$$

$$\mathscr{M}=\{Y\in\mathscr{G}|Y=-\beta Y\beta^{-1}\},\quad \mathscr{P}^\pm=\{X\in\mathscr{Q}_{\mathrm{BB}}|X=-\beta X^\dagger\beta^{-1}=\pm\beta X\beta^{-1}\},$$

where $\beta=\sigma_z\otimes 1_2\otimes 1_n$. The Lie algebra $\mathscr{G}$ is a noncompact real form of the BB part of $\mathrm{Lie}(G_\Lambda)$. By $\beta\in i\mathscr{P}^+$ and the commutation relations $[\mathscr{M},\mathscr{P}^+]\subset\mathscr{P}^-$ and $[\mathscr{M},\mathscr{P}^-]\subset\mathscr{P}^+$, we have an embedding,

$$\phi_b:\mathscr{P}^+\times\mathscr{M}\to\mathscr{Q}_{\mathrm{BB}}=\mathscr{P}^+_{\mathrm{C}}+\mathscr{P}^-_{\mathrm{C}},$$

$$(X,Y)\mapsto b\times(X+e^{\mathrm{ad}(Y)}\beta).$$

Similar considerations as in Sec. III E show that all integrals are rendered convergent by the choice of integration domain $\phi_b(\mathscr{P}^+\times\mathscr{M})\times\mathscr{U}$ $(b>0)$ for Q. With this choice we again arrive at Theorem 3.3.

The large-N limit is dominated by a single saddle-point supermanifold, which can be taken as the orbit of $Q_0=iv\Sigma_z$ (here $\Sigma_z=1_{\mathrm{B|F}}\otimes\sigma_z\otimes 1_2\otimes 1_n$) under the adjoint action of G_Λ. This orbit is diffeomorphic to G_Λ/H_Λ, where $H_\Lambda=\{h\in G_\Lambda|h\Sigma_z h^{-1}=\Sigma_z\}$. The stability group H_Λ can equivalently be described as the fixed point set of $\hat{\Sigma}_z:G_\Lambda\to G_\Lambda$, $\hat{\Sigma}_z(g)=\Sigma_z g\Sigma_z$. By the relations $\Sigma_z=\Sigma_z^{\mathrm{T}}=-\gamma\Sigma_z\gamma^{-1}=\tau\Sigma_z\tau^{-1}$ $(\Sigma_z\in\mathscr{Q})$, the element Σ_z anticommutes with $\epsilon=-i\gamma\tau^{-1}$, and $\hat{\Sigma}_z$ commutes with $\hat{\gamma}\circ\hat{\tau}$. These relations are compatible with the existence of an embedding ϕ: $\mathrm{Osp}(2n|2n)\times\mathrm{Osp}(2n|2n)\to\mathrm{Gl}(W)$, such that $(\hat{\Sigma}_z\circ\phi)(g_+,g_-)=\phi(g_-,g_+)$. (Such an embedding is easily constructed.) Hence $H_\Lambda\simeq\mathrm{diag}(\mathrm{Osp}(2n|2n)\times\mathrm{Osp}(2n|2n))\simeq\mathrm{Osp}(2n|2n)$. In this way we arrive at Theorem 3.4 with $G_\Lambda/H_\Lambda\simeq\mathrm{Osp}(2n|2n)$, and the maximal Riemannian submanifold $M_{\mathrm{B}}\times M_{\mathrm{F}}$, where $M_{\mathrm{B}}\simeq\mathrm{SO}(2n,\mathbb{C})/\mathrm{SO}(2n)$ and $M_{\mathrm{F}}\simeq\mathrm{Sp}(n)$ (type $D|C$).[47]

C. Class *D*III

Consider for $V=\mathbb{C}^2\otimes\mathbb{C}^2\otimes\mathbb{C}^N$ the linear space

$$P=\{H\in\mathrm{End}(V)\,|\,H=H^\dagger=-\mathscr{C}H^{\mathrm{T}}\mathscr{C}^{-1}=+\mathscr{T}H^{\mathrm{T}}\mathscr{T}^{-1}\},$$

where $\mathscr{C}=\sigma_x\otimes 1_2\otimes 1_N$ and $\mathscr{T}=1_2\otimes i\sigma_y\otimes 1_N$. It has been shown[25] that P is isomorphic to the tangent space of $\mathrm{SO}(4N)/\mathrm{U}(2N)$ (a symmetric space of type *D*III). Introducing an orthonormal real basis of V, we can represent H by a $4N\times 4N$ matrix. If $\mathscr{C}$ and $\mathscr{T}$ are given by

$$\mathscr{C}=\begin{pmatrix} 0 & 0 & 1_N & 0\\ 0 & 0 & 0 & 1_N\\ 1_N & 0 & 0 & 0\\ 0 & 1_N & 0 & 0\end{pmatrix},\quad \mathscr{T}=\begin{pmatrix} 0 & 1_N & 0 & 0\\ -1_N & 0 & 0 & 0\\ 0 & 0 & 0 & 1_N\\ 0 & 0 & -1_N & 0\end{pmatrix},$$

the explicit form of such a matrix is

$$H=\begin{pmatrix} a & b & c & d\\ b^\dagger & a^{\mathrm{T}} & -d^{\mathrm{T}} & -c^\dagger\\ c^\dagger & -d^{\mathrm{T}} & -a^{\mathrm{T}} & b^\dagger\\ d & -c & b & -a\end{pmatrix},$$

where all entries are complex $N\times N$ matrices and $a,d(b,c)$ are Hermitian (skew).

The Gaussian random-matrix ensemble on P is defined by the Gaussian measure $d\mu(H)$ with vanishing first moment, and second moment,

$$\int_P \mathrm{Tr}(AH)\mathrm{Tr}(BH)d\mu(H)=\frac{v^2}{4N}\,\mathrm{Tr}(AB-A\mathscr{C}B^{\mathrm{T}}\mathscr{C}^{-1}+A\mathscr{T}B^{\mathrm{T}}\mathscr{T}^{-1}-A(\mathscr{C}\mathscr{T})B(\mathscr{C}\mathscr{T})^{-1}).$$

Given the auxiliary space $W:=\mathbb{C}^{1|1}\otimes\mathbb{C}^2\otimes\mathbb{C}^2\otimes\mathbb{C}^n$, we impose on $\psi\in\mathrm{Hom}_\lambda(W,V)$, $\tilde{\psi}\in\mathrm{Hom}_{\tilde{\lambda}}(V,W)$ the linear conditions

$$\psi=\gamma\tilde{\psi}^{\mathrm{T}}\mathscr{C}^{-1},\quad \tilde{\psi}=-\mathscr{C}\psi^{\mathrm{T}}\gamma^{-1},$$
$$\psi=\tau\tilde{\psi}^{\mathrm{T}}\mathscr{T}^{-1},\quad \tilde{\psi}=\mathscr{T}\psi^{\mathrm{T}}\tau^{-1},$$

with some invertible orthogonal elements γ,τ of $\mathrm{End}_0(W)$. Consistency requires $\gamma^2=-\sigma=\tau^2$ and $\gamma\tau+\tau\gamma=0$. A possible choice is

$$\gamma=(E_{\mathrm{BB}}\otimes i\sigma_y\otimes 1_2+E_{\mathrm{FF}}\otimes\sigma_x\otimes\sigma_z)\otimes 1_n,$$

$$\tau=(E_{\mathrm{BB}}\otimes\sigma_z\otimes i\sigma_y+E_{\mathrm{FF}}\otimes 1_2\otimes\sigma_x)\otimes 1_n.$$

Because this differs from class *C*I only by the exchange of the bosonic and fermionic subspaces, the following development closely parallels that for *C*I, and we arrive at another variant of Theorem 3.3.

The large-N limit is dominated by a pair of complex-analytic saddle-point supermanifolds, each being isomorphic to $\mathrm{Osp}(2n|2n)$. [The reason why there are two is that $\mathrm{O}(2n,\mathbb{C})$ has two connected components.] The first one is the orbit under $\mathrm{Ad}(G_\Lambda)$ of $Q_0=iv1_{\mathrm{B|F}}\otimes\sigma_z\otimes 1_2\otimes 1_n$, and the second one is the orbit of

$$Q_1 = iv\left(E_{\mathrm{BB}} \otimes \sigma_z \otimes 1_2 \otimes 1_n + E_{\mathrm{FF}} \otimes \left(1_2 \otimes \sigma_x \otimes E_{11} + \sigma_z \otimes 1_2 \otimes \sum_{i=2}^{n} E_{ii} \right) \right).$$

Both saddle-point supermanifolds are Riemannian symmetric superspaces of type $C|D$ with dimensionality $m=2n$ (Table II).[47]

D. Class *AIII*

The tangent space at the origin of $\mathrm{U}(p,q)/\mathrm{U}(p)\times\mathrm{U}(q)$ consists of the matrices of the form

$$H = \begin{pmatrix} 0 & Z \\ Z^\dagger & 0 \end{pmatrix},$$

where Z is complex and has dimension $p\times q$. Such matrices are equivalently described by $H^\dagger = H = -\mathscr{P}H\mathscr{P}^{-1}$, where $\mathscr{P}=\mathrm{diag}(1_p,-1_q)$. For simplicity, we will consider only the case $p=q$ (the general case has not yet been analyzed in the present formalism). The Gaussian ensemble of random matrices H is taken to have second moment

$$\int \mathrm{Tr}(AH)\mathrm{Tr}(BH)\,d\mu(H) = \frac{v^2}{2N}\,\mathrm{Tr}(AB - A\mathscr{P}B\mathscr{P}^{-1}).$$

The physical space is $V=\mathbb{C}^2\otimes\mathbb{C}^p$, and the auxiliary space is $W=\mathbb{C}^{1|1}\otimes\mathbb{C}^2\otimes\mathbb{C}^n$. The definition of ω is unchanged from class C. To implement the symmetry condition $\psi\widetilde{\psi} = -\mathscr{P}\psi\widetilde{\psi}\mathscr{P}^{-1}$ we set

$$\psi = i\mathscr{P}\psi\pi^{-1}, \quad \widetilde{\psi} = i\pi\widetilde{\psi}\mathscr{P}^{-1},$$

where $\pi = 1_{\mathrm{B|F}}\otimes i\sigma_y\otimes 1_{\mathcal{L}}$. This choice is consistent with the relation $\widetilde{\psi}_{\mathrm{B}} = \beta\psi_{\mathrm{B}}^\dagger$ which ensures convergence of the $(\psi,\widetilde{\psi})$ integration. The auxiliary variable Q ranges over the complex-analytic superspace

$$\mathscr{Q} = \{Q \in \mathrm{End}_\Lambda(W) \,|\, Q = -\pi Q \pi^{-1}\},$$

and the normalizer of $\mathscr{Q}$ in $\mathrm{Gl}(W)$ is

$$G_\Lambda = \{g \in \mathrm{Gl}(W) \,|\, g = \pi g \pi^{-1}\} \simeq \mathrm{Gl}(n|n)\times\mathrm{Gl}(n|n).$$

For the integration domain $\mathscr{M}$ in the FF sector we again take the anti-Hermitian matrices in $\mathscr{Q}_{\mathrm{FF}}$. In the BB sector we set

$$\mathscr{M} = \{Y \in \mathrm{End}_{\mathbb{C}}(W_{\mathrm{B}}) \,|\, Y = \pi Y \pi^{-1} = -\beta Y \beta^{-1} = Y^\dagger\},$$

$$\mathscr{P}^{\pm} = \{X \in \mathrm{End}_{\mathbb{C}}(W_{\mathrm{B}}) \,|\, X = -\pi X \pi^{-1} = \pm\beta X \beta^{-1} = \mp X^\dagger\}.$$

The treatment of Sec. III E then goes through as before, leading again to Theorem 3.3.

There is a single dominant saddle-point supermanifold, which is the $\mathrm{Ad}(G_\Lambda)$ orbit of $Q_0 = iv\,1_{\mathrm{B|F}}\otimes\sigma_z\otimes 1_n$ and is diffeomorphic to $G_\Lambda/H_\Lambda \simeq \mathrm{Gl}(n|n)$. The integration domain $M_{\mathrm{B}}\times M_{\mathrm{F}}$ is given by $M_{\mathrm{B}}\simeq\mathrm{Gl}(n,\mathbb{C})/\mathrm{U}(n)$ and $M_{\mathrm{F}}=\mathrm{U}(n)$. The invariant Berezin measure of this Riemannian symmetric superspace of type $A|A$ was discussed for $n=1$ in Example 2.4.

E. Class *BD*I

The form of the random-matrix Hamiltonian H for class BDI can be obtained from the preceding case by taking the $p\times q$ matrix Z to be real. Put in formulas, H is subject to $H^\dagger = H = H^{\mathrm{T}} = -\mathscr{P}H\mathscr{P}^{-1}$. We again make the restriction to $p=q$. The basic correlation law of the Gaussian ensemble is

$$\int \mathrm{Tr}(AH)\mathrm{Tr}(BH)\,d\mu(H) = \frac{v^2}{4N}\,\mathrm{Tr}(A(B+B^{\mathrm{T}}) - A\mathscr{P}(B+B^{\mathrm{T}})\mathscr{P}^{-1}).$$

To accommodate the extra symmetry $H=H^{\mathrm{T}}$, auxiliary space is extended to $W=\mathbb{C}^{1|1}\otimes\mathbb{C}^2\otimes\mathbb{C}^2\otimes\mathbb{C}^n$. The symmetry conditions on ψ, $\widetilde{\psi}$ are

$$\psi = i\mathscr{P}\psi\pi^{-1}, \quad \widetilde{\psi} = i\pi\widetilde{\psi}\mathscr{P}^{-1}; \quad \psi = \widetilde{\psi}^{\mathrm{T}}\tau^{-1}, \quad \widetilde{\psi} = \tau\psi^{\mathrm{T}},$$

where $\pi = 1_{\mathrm{B|F}}\otimes i\sigma_y\otimes 1_2\otimes 1_n$ and $\tau = (E_{\mathrm{BB}}\otimes 1_2\otimes\sigma_x + E_{\mathrm{FF}}\otimes 1_2\otimes i\sigma_y)\otimes 1_n$. The auxiliary integration space,

$$\mathscr{Q} = \{Q\in \mathrm{End}_\Lambda(W) \,|\, Q = -\pi Q\pi^{-1} = +\tau Q^{\mathrm{T}}\tau^{-1}\},$$

has the symmetry group (or normalizer)

$$G_\Lambda = \{g\in \mathrm{Gl}(W) \,|\, g = \pi g\pi^{-1} = \tau {g^{-1}}^{\mathrm{T}}\tau^{-1}\} \simeq \mathrm{Gl}(2n|2n).$$

For the integration domain $\mathscr{U}$ in the FF sector we once again take the anti-Hermitian matrices in $\mathscr{Q}_{\mathrm{FF}}$. In the BB sector we set

$$\mathscr{M} = \{Y\in \mathrm{End}_{\mathbb{C}}(W_{\mathrm{B}}) \,|\, Y = \pi Y\pi^{-1} = -\tau Y^{\mathrm{T}}\tau^{-1} = -\beta Y\beta^{-1} = Y^\dagger\},$$

$$\mathscr{P}^{\pm} = \{X\in \mathrm{End}_{\mathbb{C}}(W_{\mathrm{B}}) \,|\, X = -\pi X\pi^{-1} = +\tau X^{\mathrm{T}}\tau^{-1} = \pm\beta X\beta^{-1} = \mp X^\dagger\}.$$

The treatment of Sec. III E then goes through with modifications as in Sec. IV B.

There is a single dominant saddle-point supermanifold, which is the $\mathrm{Ad}(G_\Lambda)$ orbit of $Q_0 = iv\,1_{\mathrm{B|F}}\otimes\sigma_z\otimes 1_2\otimes 1_n$ and is diffeomorphic to $G_\Lambda/H_\Lambda \simeq \mathrm{Gl}(2n|2n)/\mathrm{Osp}(2n|2n)$. The integration domain $M_{\mathrm{B}}\times M_{\mathrm{F}}$ is given by $M_{\mathrm{B}}\simeq \mathrm{Gl}(2n,\mathbb{R})/\mathrm{O}(2n)$ and $M_{\mathrm{F}} = \mathrm{U}(2n)/\mathrm{Sp}(n)$. This is a Riemannian symmetric superspace of type $AI|AII$ with $m=2n$ (Table II).

F. Class *C*II

The tangent space at the origin of $\mathrm{Sp}(N,N)/\mathrm{Sp}(N)\times\mathrm{Sp}(N)$ (a noncompact symmetric space of type CII) can be described by the equations

$$H^\dagger = H = -\mathscr{P}H\mathscr{P}^{-1} = -\mathscr{T}H^{\mathrm{T}}\mathscr{T}^{-1},$$

where $\mathscr{P} = \sigma_z\otimes 1_2\otimes 1_N$ and $\mathscr{T} = 1_2\otimes i\sigma_y\otimes 1_N$ (the physical space is $V=\mathbb{C}^2\otimes\mathbb{C}^2\otimes\mathbb{C}^N$). The explicit form of the matrices is

$$H = \begin{pmatrix} 0 & 0 & a & b \\ 0 & 0 & -\overline{b} & \overline{a} \\ a^\dagger & -b^{\mathrm{T}} & 0 & 0 \\ b^\dagger & a^{\mathrm{T}} & 0 & 0 \end{pmatrix},$$

if

$$\mathscr{P}=\begin{pmatrix} 1_N & 0 & 0 & 0 \\ 0 & 1_N & 0 & 0 \\ 0 & 0 & -1_N & 0 \\ 0 & 0 & 0 & -1_N \end{pmatrix}$$

and

$$\mathscr{T}=\begin{pmatrix} 0 & 1_N & 0 & 0 \\ -1_N & 0 & 0 & 0 \\ 0 & 0 & 0 & 1_N \\ 0 & 0 & -1_N & 0 \end{pmatrix},$$

where a and b are complex and have dimension $N\times N$. The correlation law of the Gaussian random-matrix ensemble of type CII is

$$\int \mathrm{Tr}(AH)\mathrm{Tr}(BH)d\mu(H)=\frac{v^2}{4N}\,\mathrm{Tr}(A-\mathscr{P}A\mathscr{P}^{-1})(B-\mathscr{T}B^{\mathrm{T}}\mathscr{T}^{-1}).$$

As before, $W=\mathbb{C}^{1|1}\otimes\mathbb{C}^2\otimes\mathbb{C}^2\otimes\mathbb{C}^n$. The symmetry conditions on ψ, $\widetilde{\psi}$ are

$$\psi=i\mathscr{P}\psi\pi^{-1},\quad \widetilde{\psi}=i\pi\widetilde{\psi}\mathscr{P}^{-1};\quad \psi=\mathscr{T}\widetilde{\psi}^{\mathrm{T}}\tau^{-1},\quad \widetilde{\psi}=\tau\psi^{\mathrm{T}}\mathscr{T}^{-1},$$

where $\pi=1_{\mathrm{B|F}}\otimes i\sigma_y\otimes 1_2\otimes 1_n$ and $\tau=(E_{\mathrm{BB}}\otimes 1_2\otimes i\sigma_y+E_{\mathrm{FF}}\otimes 1_2\otimes\sigma_x)\otimes 1_n$. This differs from class BDI only by the exchange of the bosonic and fermionic subspaces. Once more we arrive at another version of Theorem 3.3.

There is only one complex-analytic supermanifold of saddle-points that dominates for $N\to\infty$. It is isomorphic to that for class BDI. The integration domain $M_{\mathrm{B}}\times M_{\mathrm{F}}$ changes to $M_{\mathrm{B}}\simeq \mathrm{U}^*(2n)/\mathrm{Sp}(n)$ and $M_{\mathrm{F}}\simeq \mathrm{U}(2n)/\mathrm{O}(2n)$ [not $\mathrm{U}(2n)/\mathrm{SO}(2n)$]. This is a Riemannian symmetric superspace of type AII$|A$I with $m=2n$ (Table II). The group $\mathrm{U}^*(2n)$ is defined as the noncompact real subgroup of $\mathrm{Gl}(2n,\mathbb{C})$ fixed by $g=\mathscr{C}\overline{g}\mathscr{C}^{-1}$, where $\mathscr{C}=i\sigma_y\otimes 1_n$.

G. Class A

This class for $n=1$ was used to illustrate our general strategy in Sec. III A. Let us now do the case of arbitrary n,

$$Z_n(\alpha_1,\ldots,\alpha_n;\beta_1,\ldots,\beta_n)=\int_{i\,\mathrm{u}(N)}\prod_{i=1}^{n}\mathrm{Det}\left(\frac{H-\beta_i}{H-\alpha_i}\right)d\mu(H).$$

The classes treated so far (C,D,CI,DIII,AIII,BDI,CII) all share one feature, namely the existence of a particle-hole type of symmetry ($H=-\mathscr{P}H\mathscr{P}^{-1}$ or $H=-\mathscr{C}H^{\mathrm{T}}\mathscr{C}^{-1}$), which allows us to restrict all α_i to one-half of the complex plane. Such a symmetry is absent for the Wigner–Dyson symmetry classes A, AI, and AII, which results in a somewhat different scenario, as it now matters how many α_i lie above or below the real axis. For definiteness let

$$\mathrm{Im}\ \alpha_i<0\quad (i=1,\ldots,n_A),\quad \mathrm{Im}\ \alpha_j>0\quad (j=n_A+1,\ldots,n),$$

and set $n_R=n-n_A$.

Auxiliary space is taken to be $W=\mathbb{C}^{1|1}\otimes\mathbb{C}^n$. The definition of ω changes to

$$\omega = E_{\mathrm{BB}} \otimes \sum_{i=1}^{n} \alpha_i E_{ii} + E_{\mathrm{FF}} \otimes \sum_{j=1}^{n} \beta_j E_{jj} .$$

Recall that the imaginary parts of the α_i steer the convergence of the $(\psi, \widetilde{\psi})$ integration. Since ω couples to $\psi, \widetilde{\psi}$ by $\exp -i\ \mathrm{STr}_W\ \omega \widetilde{\psi} \psi$, convergence forces us to take $\widetilde{\psi}_{\mathrm{B}} = \beta \psi_{\mathrm{B}}^{\dagger}$, where

$$\beta = \sum_{i=1}^{n_A} E_{ii} - \sum_{j=n_A+1}^{n} E_{jj} .$$

There are no further constraints on ψ, $\widetilde{\psi}$, or Q. Thus the complex-analytic auxiliary integration space is $\mathcal{Q} = \mathrm{End}_{\Lambda}(W)$, and $G_{\Lambda} = \mathrm{Gl}(W) \simeq \mathrm{Gl}(n|n)$.

The integration domain for Q in the FF sector is taken to be the anti-Hermitian matrices $\mathcal{U} = \mathrm{u}(n)$. In the BB sector we introduce

$$\mathcal{G} = \{X \in \mathrm{gl}(n, \mathbb{C}) | X = -\beta X^{\dagger} \beta^{-1}\}, \quad \mathcal{K} = \{X \in \mathcal{G} | X = \beta X \beta^{-1}\}.$$

The Lie algebra $\mathcal{G}$ is a noncompact real form $\mathrm{u}(n_A, n_R)$ of $\mathrm{gl}(n, \mathbb{C})$, and $\mathcal{K} = \mathrm{u}(n_A) \oplus \mathrm{u}(n_R)$ is a maximal compact subalgebra. The space $\mathcal{M}$ is defined by the Cartan decomposition $\mathcal{G} = \mathcal{K} \oplus \mathcal{M}$. The integration domain for Q_{BB} is taken to be $i\phi_b(\mathcal{K} \times \mathcal{M})$, where $\phi_b(X, Y) = b(X + e^{\mathrm{ad}(Y)} \beta)$ $(b > 0)$. This gives Theorem 3.3.

By simple power counting, the limit $N \to \infty$ is again dominated by a single complex-analytic saddle-point supermanifold, which is the $\mathrm{Ad}(G_{\Lambda})$-orbit of $Q_0 = iv 1_{\mathrm{B|F}} \otimes \beta$. The stability group H_{Λ} of Q_0 is $H_{\Lambda} = \mathrm{Gl}(n_A|n_A) \times \mathrm{Gl}(n_R|n_R)$, so

$$\mathrm{Ad}(G_{\Lambda}) Q_0 \simeq G_{\Lambda} / H_{\Lambda} = \mathrm{Gl}(n|n) / \mathrm{Gl}(n_A|n_A) \times \mathrm{Gl}(n_R|n_R).$$

The intersection of $\mathrm{Ad}(G_{\Lambda}) Q_0$ with $i\phi_v(\mathcal{K} \times \mathcal{M}) \times \mathcal{U}$ is $M_{\mathrm{B}} \times M_{\mathrm{F}}$, where $M_{\mathrm{B}} \simeq \mathrm{U}(n_A, n_R)/\mathrm{U}(n_A) \times \mathrm{U}(n_R)$ and $M_{\mathrm{F}} \simeq \mathrm{U}(n_A + n_R)/\mathrm{U}(n_A) \times \mathrm{U}(n_R)$. This is a Riemannian symmetric superspace of type $A\mathrm{III}|A\mathrm{III}$ with $m_1 = n_1 = n_A$ and $m_2 = n_2 = n_R$ (see Table II).

H. Class *AI*

The tangent space of $\mathrm{U}(N)/\mathrm{O}(N)$ is the same as (i times) the real symmetric matrices $H^{\dagger} = H = H^{\mathrm{T}}$. It differs from the tangent space of $\mathrm{SU}(N)/\mathrm{SO}(N)$, a symmetric space of type $A\mathrm{I}$ in an inessential way (just remove the multiples of the unit matrix). The Gaussian ensemble over the real symmetric matrices has its second moment given by

$$\int \mathrm{Tr}(AH)\mathrm{Tr}(BH) d\mu(H) = \frac{v^2}{2N} \mathrm{Tr}(AB + AB^{\mathrm{T}}).$$

This ensemble is related to type A in the same way that type $C\mathrm{I}$ is related to type C.

To implement the symmetry $H = H^{\mathrm{T}}$ we set $W = \mathbb{C}^{1|1} \otimes \mathbb{C}^2 \otimes \mathbb{C}^n$ and require $\psi = \widetilde{\psi}^{\mathrm{T}} \tau^{-1}$, $\widetilde{\psi} = \tau \psi^{\mathrm{T}}$, where $\tau = (E_{\mathrm{BB}} \otimes \sigma_x + E_{\mathrm{FF}} \otimes i\sigma_y) \otimes 1_n$. The auxiliary integration space,

$$\mathcal{Q} = \{Q \in \mathrm{End}_{\Lambda}(W) | Q = \tau Q^{\mathrm{T}} \tau^{-1}\},$$

has the symmetry group

$$G_{\Lambda} = \{g \in \mathrm{Gl}(W) | g = \tau g^{-1^{\mathrm{T}}} \tau^{-1}\} \simeq \mathrm{Osp}(2n|2n).$$

The intersection $\mathcal{U}$ of the FF sector $\mathcal{Q}_{\mathrm{FF}}$ with the anti-Hermitian matrices is given by $\mathrm{sp}(n) \oplus \mathcal{U} = \mathrm{u}(2n)$. In the *BB* sector we put

$$\mathscr{M}=\{Y\in \mathrm{End}_{\mathbb{C}}(W_{\mathrm{B}})\,|\,Y=-\tau Y^{T}\tau^{-1}=-\beta Y\beta^{-1}=Y^{\dagger}\},$$

$$\mathscr{P}^{\pm}=\{X\in \mathrm{End}_{\mathbb{C}}(W_{\mathrm{B}})\,|\,X=+\tau X^{T}\tau^{-1}=\pm\beta X\beta^{-1}=\mp X^{\dagger}\},$$

which leads to yet another version of Theorem 3.3.

The large-N limit is controlled by a single complex-analytic saddle-point supermanifold $\mathrm{Ad}(G_{\Lambda})Q_0\simeq G_{\Lambda}/H_{\Lambda}$, where $H_{\Lambda}\simeq \mathrm{Osp}(2n_A|2n_A)\times\mathrm{Osp}(2n_R|2n_R)$ is the stability group of $Q_0=iv1_{\mathrm{B|F}}\otimes(\Sigma_{i=1}^{n_A}E_{ii}-\Sigma_{j=n_A+1}^{n}E_{jj})$. The intersection of $\mathrm{Ad}(G_{\Lambda})Q_0$ with the integration domain $\phi_v(\mathscr{P}^{+}\times\mathscr{M})\times\mathscr{U}$ is $M_{\mathrm{B}}\times M_{\mathrm{F}}$, where $M_{\mathrm{B}}\simeq \mathrm{SO}(2n_A,2n_R)/\mathrm{SO}(2n_A)\times\mathrm{SO}(2n_R)$ and $M_{\mathrm{F}}\simeq \mathrm{Sp}(n_A+n_R)/\mathrm{Sp}(n_A)\times\mathrm{Sp}(n_R)$. This is a Riemannian symmetric superspace of type $BD\mathrm{I}|C\mathrm{II}$ (Table II) with $m_1=2n_1=2n_A$ and $m_2=2n_2=2n_R$.

I. Class *A*II

Finally, the tangent space of $\mathrm{U}(2N)/\mathrm{Sp}(N)$ [a symmetric space of type *A*II, except for the substitution $\mathrm{SU}(2N)\to\mathrm{U}(2N)$] can be described as ($i$ times) the subspace of $\mathrm{End}(\mathbb{C}^2\otimes\mathbb{C}^N)$ fixed by the linear equations $H^{\dagger}=H=\mathscr{T}H^{\mathrm{T}}\mathscr{T}^{-1}$, $\mathscr{T}=i\sigma_y\otimes 1_N$. The explicit matrix form of H is

$$H=\begin{pmatrix} a & b \\ b^{\dagger} & a^{\mathrm{T}}\end{pmatrix},$$

where b is skew and a is Hermitian.

The conditions $\psi=\mathscr{T}\tilde{\psi}^{\mathrm{T}}\tau^{-1}$ and $\tilde{\psi}=\tau\psi^{\mathrm{T}}\mathscr{T}^{-1}$ are mutually consistent if, say, $\tau=(E_{\mathrm{BB}}\otimes i\sigma_y+E_{\mathrm{FF}}\otimes\sigma_x)\otimes 1_n$. The rest of the manipulations leading up to Theorem 3.3 are the same as for class *A*I, except for the exchange of the bosonic and fermionic subspaces ($\tau_{\mathrm{B}}\leftrightarrow\tau_{\mathrm{F}}$). The large-$N$ limit is controlled by a single saddle-point supermanifold $(G_{\Lambda}/H_{\Lambda},M_{\mathrm{B}}\times M_{\mathrm{F}})$, where

$$G_{\Lambda}/H_{\Lambda}=\mathrm{Osp}(2n|2n)/\mathrm{Osp}(2n_A|2n_A)\times\mathrm{Osp}(2n_R|2n_R),$$

$$M_{\mathrm{B}}=\mathrm{Sp}(n_A,n_R)/\mathrm{Sp}(n_A)\times\mathrm{Sp}(n_R),$$

$$M_{\mathrm{F}}=\mathrm{SO}(2n_A+2n_R)/\mathrm{SO}(2n_A)\times\mathrm{SO}(2n_R),$$

which is a Riemannian symmetric superspace of type $C\mathrm{II}|BD\mathrm{I}$ (Table II) with $m_1=2n_1=2n_A$ and $m_2=2n_2=2n_R$.

V. SUMMARY

When Dyson realized[46] that the random-matrix ensembles he had introduced were based on the symmetric spaces of type *A*, *A*I, and *A*II, he wrote: ''The proof of (the) Theorem... is a mere verification. It would be highly desirable to find a more illuminating proof, in which the appearance of the (final result) might be related directly to the structure of the symmetric space...''. The advent of the supersymmetry method of Efetov and others has improved the situation lamented by Dyson. The present work takes the Gaussian random-matrix ensembles defined over Cartan's large families of symmetric spaces and, going to the limit of large matrix dimension, expresses their spectral correlation functions as integrals over the corresponding Riemannian symmetric superspaces. These correspondences are summarized in Table III. The Riemannian symmetric superspaces that appear there all have superdimension (p,q) with $p=q$. We say that they are ''perfectly graded'' or ''supersymmetric.'' An interesting question for future mathematical research is whether our procedure can be optimized by reducing it to a computation involving no more than the root system of the symmetric space, thereby obviating the space- and time-consuming need to distinguish cases. (Although I have treated all ten cases separately, it is possible, following Efetov,[3] to shorten the derivation by starting from a large ''master ensemble'' of highest symme-

TABLE III. The symmetric-space based random-matrix theories of the first column map onto the Riemannian symmetric superspaces listed in the third column. The notation for the dimensions is taken from Table II.

RMT	Comments	RSS	Dimensions
A	Wigner–Dyson (GUE)	$A\mathrm{III}\vert A\mathrm{III}$	$m_1=n_1=n_A$, $m_2=n_2=n_R$
$A\mathrm{I}$	Wigner–Dyson (GOE)	$BD\mathrm{I}\vert C\mathrm{II}$	$m_1=2n_1=2n_A$, $m_2=2n_2=2n_R$
$A\mathrm{II}$	Wigner–Dyson (GSE)	$C\mathrm{II}\vert BD\mathrm{I}$	$m_1=2n_1=2n_A$, $m_2=2n_2=2n_R$
$A\mathrm{III}$ $(p=q)$	chiral GUE	$A\vert A$	$m=n$
$BD\mathrm{I}$ $(p=q)$	chiral GOE	$A\mathrm{I}\vert A\mathrm{II}$	$m=n$
$C\mathrm{II}$ $(p=q)$	chiral GSE	$A\mathrm{II}\vert A\mathrm{I}$	$m=n$
C	NS	$D\mathrm{III}\vert C\mathrm{I}$	$m=n$
$C\mathrm{I}$	NS	$D\vert C$	$m=2n$
D	NS	$C\mathrm{I}\vert D\mathrm{III}$	$m=n$
$D\mathrm{III}$	NS	$C\vert D$	$m=2n$

try and then reducing it by the addition of symmetry-breaking terms. I chose not to follow this route as it involves handling large tensor products, which makes the computations less transparent and the identification of the spaces involved more difficult.)

The great strength of the supersymmetry method, as compared to other methods of mesoscopic physics, stems from the fact that it easily extends beyond the universal random-matrix limit to diffusive and localized systems. What one obtains for these more general systems are field theories of the nonlinear σ model type, with fields that take values in a Riemannian symmetric superspace. The method also extends beyond spectral correlations and allows the calculation of wave function statistics and of transport coefficients such as the electrical conductance (see the literature cited in the Introduction).

Let me end on a provocative note. Mathematicians and mathematical physicists working on supermanifold theory have taken much guidance from developments in such esoteric subjects as supergravity and superstring theory. Would it not be just as worthwhile to investigate the beautiful structures outlined in the present paper, whose physical basis is not speculative but firmly established, and which are of direct relevance to experiments that are currently being performed in physics laboratories all over the world?

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Singularities in the spectra of random matrices

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We consider singularities of the set of energy levels $E_n(\mathbf{X})$ of a quantum Hamiltonian, obtained by varying a set of d parameters $\mathbf{X}=(X_1,..,X_d)$. Singularities such as minima, degeneracies, branch points, and avoided crossings can play an important role in physical applications. We discuss a general method for counting these singularities, and apply it to a random matrix model for the parameter dependence of energy levels. We also show how the density of avoided crossing singularities is related to a non-analyticity of a correlation function describing the energy levels. © *1996 American Institute of Physics.* [S0022-2488(96)01810-5]

I. INTRODUCTION

It is now widely accepted that random matrices provide an excellent model for statistical properties of the spectra of quantum systems for which the energy levels cannot be determined analytically:[1,2] random matrix models have been successfully applied to disordered solids, classically chaotic systems, and many body problems. There are many contexts in which families of Hamiltonians depending smoothly on a set of parameters are of physical importance, for example the parameters could represent the positions of atomic nuclei in the Hamiltonian for the electrons in a molecule, or the Bloch wavevectors of an electron in a periodic potential. Recently the random matrix approach has been extended to describe statistics which characterize the parameter dependence of energy levels.[3–9] One approach to analyzing the parameter dependence is to consider correlation functions; an example which has received attention[6–8] is the correlation function $C(X)$ of the derivatives of energy levels $E_n'=dE_n/dX$:

$$C(X)=\langle E_n'(X+X_0)E_n'(X_0)\rangle. \tag{1.1}$$

An alternative approach is to examine various types of singularity in the spectrum, such as degeneracies[9,10] (where a pair of energy levels become equal at some real valued point in the parameter space), branch points[8] (where energy levels become degenerate at complex parameter values), and avoided crossings[3] (characteristic structures where energy levels come close to degeneracy). These singularities can have direct physical consequences, in determining various aspects of the breakdown of the adiabatic theorem,[11–14,3] and discontinuities of the quantized Hall conductance.[15,16,10]

This paper has two objectives. The first is to explain the strategy for calculating the density of singularities in the parameter space; we will present some new calculations of the density of singularities, as well as reviewing existing results. The second objective is to discuss the implications of these results for the calculation of correlation functions such as (1.1). Guaneri *et al.*[8]

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demonstrated that the existence of branch point singularities in the spectrum implies that correlation functions such as $C(X)$ have a non-analytic behavior at $X=0$. We will show how the leading order non-analytic part of this function is obtained from the density of singularities.

This paper is organized as follows. In Sec. II we discuss parameter dependent generalizations of the standard random matrix models. In Sec. III we describe the approach to counting densities of singularities of random functions, using the density of minima as an example. In Sec. IV we review the known results on the density of various types of singularity, and their physical applications. Some of the results in Sec. IV are new, and of these the density of degeneracies for the GUE and GSE ensembles are not easily obtained; these calculations are explained in Sec. V and in an Appendix. Finally in Sec. VI we discuss the implications of the results given in Sec. IV for correlation functions such as (1.1).

In this paper we will discuss a variety of different probability distributions. To avoid naming a multiplicity of different functions describing these distributions, we will introduce the notational convention that $dP=P[X]dX$ is a probability measure for the quantity X.

II. PARAMETER DEPENDENT RANDOM MATRICES

The most fundamental random matrix models are the Gaussian ensembles introduced by Porter and Dyson. These are constructed from real symmetric matrices $\tilde{H}^{(S)}$ and real antisymmetric matrices $\tilde{H}_k^{(A)}$ with independent Gaussian distributed elements; the variance of the ijth element of these matrices is, respectively, $1\pm\delta_{ij}$. There are three Gaussian ensembles, invariant under orthogonal, general unitary, and ''symplectic'' unitary transformations,[1,2] which are constructed from combinations of the symmetric and antisymmetric matrices as follows:

$$[\tilde{H}]_{ij}=\frac{1}{\sqrt{\beta}}\left\{[\tilde{H}^{(S)}]_{ij}\mathbf{e}_0+\sum_{k=1}^{\beta-1}[\tilde{H}_k^{(A)}]_{ij}\mathbf{e}_k\right\}. \tag{2.1}$$

Here $\beta=1,2,4$ for the orthogonal, unitary and symplectic ensembles, respectively, $\mathbf{e}_0$, $\mathbf{e}_1$ are 1, $\sqrt{-1}$, respectively, and the other $\mathbf{e}_k$ are the other bases for the quaternion algebra. In order for these to be useful models for energy level statistics, the dimension N of the matrix should be large.

In order to study singularities of the spectrum, it is necessary to construct a parameter dependent version of these random matrix models. It is convenient to do this in such a way that $\partial\hat{H}/\partial X$ is an independent realization of the same ensemble as $\hat{H}$, and that the distribution of both of these quantities is stationary: this is achieved by writing

$$\hat{H}(X)=\cos X\hat{H}_1+\sin X\hat{H}_2, \tag{2.2}$$

where $\hat{H}_1$ and $\hat{H}_2$ are Hermitean operators represented by independent samples from the same Gaussian symmetry-invariant ensemble defined above. Reference 5 discusses theoretical arguments and numerical results which support the use of (2.2) as a model for parameter dependencies of spectra. In the calculations below, we will require the matrix elements of $d\hat{H}/dX$ in the basis formed by the eigenstates of $\hat{H}$: this is simply an arbitrary unitary transformation of $d\hat{H}/dX$ within the appropriate symmetry class (orthogonal, unitary, or symplectic). Because the Gaussian invariant ensembles are invariant under these unitary transformations, the matrix elements $\partial H_{nm}\equiv\langle\phi_n|d\hat{H}/dX|\phi_m\rangle$ have the same statistical properties as those of the matrix $d\hat{H}/dX$.

In order to compare a random matrix model with the spectrum of a ''real'' physical system in the neighborhood of energy E, we must scale energy levels of the system so that the density of states $\rho(E)$ corresponds to that of the random matrix model. In a parameter dependent system, it is also necessary to adjust another parameter, describing the sensitivity of the energy levels of the system to perturbations: the natural choice is to use either the variance of the off-diagonal matrix elements of $d\hat{H}/dX$ in the eigenbasis,

$$\sigma^2(E)=\langle|\partial H_{nm}|^2\rangle_{\substack{E_n\sim E_m\sim E\\ n\neq m}}, \tag{2.3}$$

or the variance of dE_n/dX: these are related by

$$\mathrm{var}\left[\frac{dE_n}{dX}\right]=\frac{2}{\beta}\sigma^2. \tag{2.4}$$

Equation (2.4) follows from the definition (2.1) for the Gaussian random matrix models, and there are several arguments suggesting that it should also hold for complex quantum systems.[17,18] For the random matrix ensemble (2.2), we have $\sigma=1$.

The model (2.2) can be extended to systems with d parameters in several ways; the simplest is to use $2d$ independent realizations of the random matrices, and write

$$\hat{H}(\mathbf{X})=\sum_{i=1}^{d}\ \cos X_i\hat{H}_{2i-1}+\ \sin X_i\hat{H}_{2i}. \tag{2.5}$$

Now the sensitivity of energy levels to the parameters X_i can be characterized by defining a set of parameters C_{ij} which generalize (2.3):

$$C_{ij}=\langle\partial_i H^*_{nm}\partial_j H_{nm}\rangle_{\substack{E_n\sim E_m\sim E\\ n\neq m}}, \tag{2.6}$$

where $\partial_i H_{nm}\equiv\langle\phi_n|\partial\hat{H}/\partial X_i|\phi_m\rangle$. A change of variables makes the parameter dependence of the energy levels resemble that of the model (2.5). In the many-parameter case the parameter σ characterizing the sensitivity of energy levels is naturally defined in terms of the Jacobean of this transformation: noting that for (2.5) we have $C_{ij}=\delta_{ij}$, the natural definition is

$$\sigma^2=(\det[\widetilde{C}])^{1/d}, \tag{2.7}$$

where $\widetilde{C}$ is a matrix with elements C_{ij}. In order to use the parametrized random matrix models, both the density of states ρ and the sensitivity parameter σ must be estimated. This can always be done numerically calculating an average over energy levels. For systems which exhibit semiclassical behavior, ρ can be estimated using the Weyl formula,[19] and σ^2 can be estimated from the classical correlation function of $\partial H/\partial X$.[20]

III. COUNTING SINGULARITIES

The method which we use for calculating the density of singularities can be viewed as an extension of one described by Rice,[21] who gives an expression for the frequency of zero crossings of a random function $f(x)$, for which the joint probability density of the function and its derivative f' is known. If $\mathscr{D}^{(0)}$ is the density of zeros of the function, the probability of finding a zero in a short interval of length $[x_0,x_0+\delta x]$ at a randomly chosen point x_0 is $\delta P=\mathscr{D}^{(0)}\delta x$. If the point x_0 happens to be close to a zero, the distance from x_0 to this zero crossing is approximately $-f(x_0)/f'(x_0)$, and the probability of the zero crossing lying within δx of x_0 is

$$\delta P\sim\int_{-\infty}^{\infty}df\int_{-\infty}^{\infty}df'\,P[f,f']\chi\left(\frac{-f}{f'\delta x}\right),$$
$$\chi(x)=\begin{cases}1, & 0<x<1,\\ 0, & 0>x>1.\end{cases} \tag{3.1}$$

Dividing by δx and taking the limit $\delta x\to 0$ gives

$$\mathscr{D}^{(0)}=\int_{-\infty}^{\infty}df\int_{-\infty}^{\infty}df'\,P[f,f']\delta\left(\frac{f}{f'}\right)=\int_{-\infty}^{\infty}df'|f'|P[0,f']. \tag{3.2}$$

The same approach is used to determine the density of any point singularity: we use the known statistics of the function to calculate the probability of finding a singularity in a small element centered on a randomly chosen test point, and equate this to the density of singularities multiplied by the volume of the element.

As an elementary example, we can use (3.2) to determine the density of minima $\mathscr{D}^{(\min)}$ of $E_n(X)$ for the random matrix model (2.2). The density of minima might find physical applications, for example in determining the number of possible energetically stable configurations of complex molecules which can be obtained by varying configuration of the nuclei.

The first and second derivatives of $E_n(X)$,

$$E_n'=\frac{dE_n}{dX}=\partial H_{nn}, \quad E_n''=\frac{d^2E_n}{dX^2}=2\sum_{m\neq n}\frac{|\partial H_{nm}|^2}{(E_n-E_m)}-2E_n, \tag{3.3}$$

are independent, because they depend upon different matrix elements. We denote the distributions of the first two derivatives by $P[E']$ and $P[E'']$, respectively. The first derivative E' is Gaussian distributed with variance $2\sigma^2/\beta$, and with a mean value which is zero for the model (2.2), but which may have a non-zero value $\langle E'\rangle$ in physical applications. The distribution of the second derivative is difficult to calculate: when the matrix dimension N is large, an excellent approximation[22] is

$$P[E'']=\frac{C_\beta}{[a_\beta^2+E''^2]^{(\beta+2)/2}}, \tag{3.4}$$

which is also an exact result for the GUE in the limit $N\to\infty$.[23] The constants C_β are given in Refs. 4,5,

$$C_1=2\pi^2\rho^2\sigma^4, \quad C_2=2^4\pi^2\rho^3\sigma^6, \quad C_4=2^8\pi^4\rho^5\sigma^{10}/3, \tag{3.5}$$

and the a_β are then determined by normalizing the distribution: we find $a_1=2\pi\rho\sigma^2$ and $a_1=a_2=a_4$. The density of minima can now be calculated by using (3.2) to calculate the density of zeros of $E_n'(X)$, and dividing by two because half of the extrema of $E_n(X)$ are maxima:

$$\mathscr{D}_\beta^{(\min)}=P[E'=0]\int_0^\infty dE''|E''|P[E'']=C_\beta^{(\min)}\rho\sigma\,\exp\left[\frac{-\beta\langle E'\rangle^2}{4\sigma^2}\right], \tag{3.6}$$

with dimensionless constants

$$C_1^{(\min)}=\frac{\sqrt{\pi}}{2}, \quad C_2^{(\min)}=\sqrt{\frac{2}{\pi}}, \quad C_4^{(\min)}=\frac{4}{3\sqrt{\pi}}. \tag{3.7}$$

These results are exact for the GUE in the limit $N\to\infty$, and at least a very good approximation for the GOE and GSE.

IV. REVIEW OF RESULTS ON DENSITY OF SINGULARITIES

Below we discuss the various other types of singularity of the spectrum which are of interest and their physical significance, and review the existing results on their density. All of the results are exact for the random matrix models introduced in Sec. II in the limit $N\to\infty$.

A. Degeneracies

A degeneracy occurs when two or more energy levels are equal for some real valued point in parameter space; in practice we will only be interested in degeneracies between pairs of levels, because higher order degeneracies have a higher codimension. Generically, two parameters must be varied in a family of real symmetric matrices to create a degeneracy, three parameters in a family of Hermitean matrices, and five parameters in a family of quaternion symmetric matrices.[24] We will therefore consider the density of degeneracies in the model (2.5) with $d=2,3,5$ for the GOE, GUE and GSE versions, respectively.

An interesting example of the importance of degeneracies is given by Simon,[15] who shows that the Chern integers describing the quantized Hall conductance[16] change, typically by ± 1, at degeneracies. Degeneracies can also enable other invariant quantities to change; for example the center of symmetry associated with Wannier functions of a Bloch band can change discontinuously when the band touches a neighboring band at some point in the Brillouin zone.

The density of degeneracies for the parametrized ensembles is defined in a space of $\beta+1$ parameters, and their density is

$$\mathscr{D}_\beta^{(\mathrm{deg})} = C_\beta^{(\mathrm{deg})} (\rho\sigma)^{\beta+1}, \tag{4.1}$$

with dimensionless prefactors

$$C_1^{(\mathrm{deg})} = \frac{\pi}{3}, \quad C_2^{(\mathrm{deg})} = \frac{2\sqrt{\pi}}{3}, \quad C_4^{(\mathrm{deg})} = \frac{16\sqrt{2}\,\pi^{3/2}}{45}; \tag{4.2}$$

$C_1^{(\mathrm{deg})}$ was derived in Ref. 9 and $C_2^{(\mathrm{deg})}$ was quoted in Ref. 10 without a full derivation. An estimate consistent with (4.1) was given in an earlier paper[25] for the special case of billiards, without an accurate value of the prefactor. The derivations of $C_2^{(\mathrm{deg})}$ and $C_4^{(\mathrm{deg})}$ will be given in Sec. V and in an Appendix, respectively.

In the neighborhood of a degeneracy, the separation $\Delta = E_{n+1} - E_n$ of the degenerating levels is given by the square root of a quadratic form; for example in the case of a system such as the GOE, where the Hamiltonian is real, we can write

$$\Delta^2 = A_{11}\delta X_1^2 + A_{22}\delta X_2^2 + 2A_{12}\delta X_1 \delta X_2 + O(\delta X^3). \tag{4.3}$$

This quadratic form can be defined by the orientation, eccentricity, and size of the elliptical level curves of Δ. For the model (2.5), the orientation of the ellipses is random, and the other parameters are defined by the trace $t = A_{11} + A_{22}$ and determinant $d = A_{11}A_{22} - A_{12}^2$ of the matrix which represents the quadratic form. The joint distribution of the trace and determinant has been calculated:[9] it is

$$P[t,d] = \frac{d}{256\sigma^6} \exp\left(\frac{-t}{8\sigma^2} \right), \tag{4.4}$$

within the physically allowed region $t>0$, $d>0$, $d \leqslant \frac{1}{2}t^2$. Other statistics describing the elliptical contours of Δ can be obtained directly from this simple result; for example the distribution of eccentricity e of the ellipses is

$$P[e] = \left(\frac{2e}{2-e^2} \right)^3. \tag{4.5}$$

The distribution of parameters of the quadratic form for the unitary and symplectic ensembles is not known.

B. Avoided crossings

When a single parameter is varied, energy levels of systems without symmetries never cross,[26] but they can approach each other very closely at events called avoided crossings. When the separation of a pair of energy levels is very small compared to their separation from all of the other levels, the structure of these avoided crossings can be understood using degenerate perturbation theory for a two level system: provided the Hamiltonian is a regular function of parameter in the neighborhood of the near-degeneracy, the levels have a hyperbolic form,

$$E_{\pm}(X) \sim B(X-X_0) \pm \frac{1}{2}\sqrt{\epsilon^2 + A^2(X-X_0)^2}. \tag{4.6}$$

The avoided crossing is characterized by four parameters, the gap ϵ, the difference of the asymptotic slopes A, the mean of the asymptotic slopes B, and the position X_0.

Avoided crossings are physically important because they mediate the breakdown of the adiabatic theorem by Landau-Zener transitions,[11,12,3] and in Sec. VI we will show that they determine the form of singular terms in the expansion of correlation functions such as (1.1).

The density of avoided crossings can be defined as follows: $\mathscr{D}_\beta^{(\mathrm{ac})}(A,B,\epsilon)dAdBd\epsilon dX$ is the expected number of avoided crossings between a given pair of successive levels, in an interval of length dX, for which the slope difference, mean slope, and gap parameters all lie in intervals of widths, respectively, dA, dB, $d\epsilon$, centered on the values A, B, ϵ. This statistic is only meaningful for small values of ϵ, because A and B are only defined for avoided crossings with gaps which are very small compared to the mean level separation $1/\rho$. The avoided crossing density is calculated by exactly the same approach as for the density of degeneracies, although the calculation is somewhat more difficult: the result, obtained in Refs. 3 and 5 is

$$\mathscr{D}_\beta^{(\mathrm{ac})}(A,B,\epsilon)dAdBd\epsilon = P[B]dBC_\beta^{(\mathrm{ac})}(\rho/\sigma)^{\beta+1}\epsilon^{\beta-1}d\epsilon A^{\beta+1}\ \exp[-\beta A^2/8\sigma^2]dA, \tag{4.7}$$

where $P[B]dB$ is a Gaussian distribution, with variance σ^2/β, and

$$C_1^{(\mathrm{ac})} = \frac{\pi}{24}, \quad C_2^{(\mathrm{ac})} = \frac{\pi^{3/2}}{12}, \quad C_4^{(\mathrm{ac})} = \frac{8\pi^{7/2}}{135\sqrt{2}}. \tag{4.8}$$

C. Branch points

Degeneracies between levels of the one parameter model (2.2) can occur for complex values of X; these degeneracies have a branch point structure. The branch points are important because they are used to determine the exponents describing the probability of non-adiabatic transitions.[13,14] Branch points can be identified with a particular pair of levels by considering a closed path in the complex X plane which leaves the real axis and loops around one, and only one, branch point. For all but one of the levels indices n, the energy level $E_n(X)$ is single valued when traced around this path, but one level, E_m say, is continuously transformed into another level $E_{m'}$ when traced around this path. The levels with indices m, m' are connected by the branch point.

We define $\mathscr{D}_\beta^{(\mathrm{br})}(Y,N)dY$ to be the frequency with which we encounter branch points involving the nth level and the level $n+N$, with the imaginary part of the parameter X in an interval of width dY centered on Y.

We have only been able to find the density of branch points for $N=1$ and small Y. Branch points very close to the real axis are associated with avoided crossings with very small values of ϵ: the distance of the branch point from the real axis is ϵ/A. The density of these branch points is obtained immediately from (4.7) and (4.8):

$$\mathscr{D}_\beta^{(\mathrm{br})}(Y,1)=\int_0^\infty dA\int_{-\infty}^\infty dB\int_0^\infty d\epsilon\,\mathscr{D}^{(\mathrm{ac})}(A,B,\epsilon)\,\delta\left(\ Y-\frac{\epsilon}{A}\ \right)$$

$$=C_\beta^{(\mathrm{br})}(\rho\sigma)^{\beta+1}Y^{\beta-1}, \tag{4.9}$$

with dimensionless constants

$$C_1^{(\mathrm{br})}=\frac{4\pi}{3},\quad C_2^{(\mathrm{br})}=\frac{16\pi^{3/2}}{3},\quad C_4^{(\mathrm{br})}=\frac{2^{10}\pi^{7/2}}{45\sqrt{2}}. \tag{4.10}$$

Guarneri *et al.*[8] gave an argument for an expression of the form (4.9), but did not obtain the prefactors (4.10).

V. DENSITY OF DEGENERACIES

We now discuss how to determine the density of degeneracies. This has already been described in detail for the Gaussian orthogonal ensemble,[9] and the result for the Gaussian unitary ensemble has also been quoted in an earlier paper.[10] Here we discuss the GUE case in detail, presenting details of the calculation which were omitted in Ref. 10; the calculation for the GSE case is similar, and is discussed in an Appendix.

Following the approach introduced in Sec. III, we select an arbitrary point in parameter space $\mathbf{X}_0$. We assume that this point is close to a degeneracy between levels with indices n and $n+1$. In the neighborhood of this point we represent the Hamiltonian in the basis formed by the eigenfunctions $|\psi_n(\mathbf{X}_0)\rangle$ at $\mathbf{X}_0$, and apply two-state degenerate perturbation theory. The separation of the nearly degenerate levels at a nearby position $\mathbf{X}=\mathbf{X}_0+\delta\mathbf{X}$ is

$$E_{n+1}-E_n\sim\sqrt{\left[\Delta+\sum_i\ (\partial_i H_{n+1\,n+1}-\partial_i H_{nn})\,\delta X_i\right]^2+4\left|\sum_i\ \partial_i H_{nn+1}\delta X_i\right|^2}\quad , \tag{5.1}$$

where $\Delta=E_{n+1}(\mathbf{X}_0)-E_n(\mathbf{X}_0)$. Within this approximation the degeneracy occurs when the discriminant (5.1) vanishes, at a displacement $\delta\mathbf{X}$ from $\mathbf{X}_0$. The components δX_i of this displacement are given by solving a system of linear equations:

$$\sum_{j=1}^3 M_{ij}\delta X_j=\Delta\,\delta_{1j}\,, \tag{5.2}$$

where the elements of the 3×3 matrix $\widetilde{M}=\{M_{ij}\}$ are

$$\begin{aligned} M_{1j}&=\partial_j H_{n+1\,n+1}-\partial_j H_{nn}\,,\\ M_{2j}&=2\ \mathrm{Re}[\partial_j H_{nn+1}],\quad M_{3j}=2\ \mathrm{Im}[\partial_j H_{nn+1}]. \end{aligned} \tag{5.3}$$

Note that the M_{ij} are elements of a real, non-symmetric, random matrix $\widetilde{M}$ with statistically independent elements, all of which are identically Gaussian distributed, with variance $2\sigma^2$ and mean 0.

The distance from the reference point to the degeneracy, $R=|\delta\mathbf{X}|$, is proportional to Δ: we write $R=\Delta f$ where

$$f^2=\sum_{i=1}^3\ [(\widetilde{M}^{-1})_{i1}]^2. \tag{5.4}$$

The probability $P[R]$ that the nearest degeneracy exists at a small distance R can then be written, by analogy with (3.2),

$$P[R]=\int_0^\infty df\int_0^\infty d\Delta P[f]P[\Delta]\delta(R-f\Delta), \tag{5.5}$$

where $P[f]$ is the probability distribution for f, and $P[\Delta]$ is the distribution of neighboring energy level separations: these quantities are independent because of the statistical independence of $\hat{H}$ and $\partial_i\hat{H}$ (note that Δ depends only upon $\hat{H}$ whereas f depends only upon the matrix elements $\partial_i H_{nm}$). The distribution $P[\Delta]$ is the well known level spacing distribution.[1,2] When R is small, the Dirac delta function only supports small values of Δ, for which the level spacing distribution is known analytically[2] in the limit $N\to\infty$:

$$P[\Delta]d\Delta=\left[\frac{1}{3}\pi^2\rho^3\Delta^2+O(\Delta^3)\right]d\Delta, \tag{5.6}$$

where ρ is the density of states. Performing the integrals in (5.5) gives

$$P[R]=\left[\frac{1}{3}\pi^2\rho^3\langle f^{-3}\rangle R^2+O(R^3)\right]dR. \tag{5.7}$$

The expected number of degeneracies in a spherical shell of radius R and thickness dR is $4\pi\mathscr{D}_2^{(\mathrm{deg})}R^2dR$; comparing this with (5.7) gives

$$\mathscr{D}_2^{(\mathrm{deg})}=\frac{1}{12}\pi\rho^3\langle f^{-3}\rangle. \tag{5.8}$$

It remains to evaluate the integral $I=\langle f^{-3}\rangle$, by averaging over the probability density

$$dP=P[\tilde{M}]d\tilde{M}=P[M_{11},M_{12},\ldots,M_{33}]\prod_{ij}dM_{ij}=A\exp\left[-\frac{\mathrm{tr}(\tilde{M}^T\tilde{M})}{4\sigma^2}\right]d\tilde{M}, \tag{5.9}$$

where A is a normalization factor. To facilitate the calculation of the average, the non-symmetric real matrix $\tilde{M}$ is decomposed into a product of two orthogonal matrices $\tilde{O}_1$, $\tilde{O}_2$, and a diagonal matrix $\tilde{D}$:

$$\tilde{M}=\tilde{O}_1^T\tilde{D}\tilde{O}_2. \tag{5.10}$$

This gives a useful simplification of the expression for f:

$$f^2=\sum_{i=1}^3[(\tilde{O}_1^T\tilde{D}\tilde{O}_2)^{-1}]_{i1}^2=\sum_{i=1}^3[\tilde{O}_2^T\tilde{D}^{-1}\tilde{O}_1)_{i1}]^2=\sum_{i=1}^3\lambda_i^{-2}(\tilde{O}_1)_{i1}^2, \tag{5.11}$$

where λ_i is the ith diagonal element of $\tilde{D}$. Also, the trace in (5.9) takes on a simple form when we use (5.10):

$$\mathrm{tr}(\tilde{M}^T\tilde{M})=\mathrm{tr}(\tilde{D}^2)=\sum_{i=1}^3\lambda_i^2. \tag{5.12}$$

We can now calculate $\langle f^{-3}\rangle$ by transforming from the coordinates $\{M_{ij}\}$ to a set of coordinates consisting of the three diagonal elements of $\tilde{D}$, and two sets of three coordinates

$\alpha=\{\alpha_1,\alpha_2,\alpha_3\}$ and $\beta=\{\beta_1,\beta_2,\beta_3\}$ which parametrize the orthogonal matrices $\widetilde{O}_1$ and $\widetilde{O}_2$, respectively. The Jacobian J of the coordinate transformation is defined by

$$d\widetilde{M}=Jd\alpha_1 d\alpha_2 d\alpha_3 d\beta_1 d\beta_2 d\beta_3 d\lambda_1 d\lambda_2 d\lambda_3, \tag{5.13}$$

where $J=|\det\widetilde{j}\,|$ and $\widetilde{j}$ is composed of three, 9×3 blocks:

$$\widetilde{j}=\left(\frac{\partial\widetilde{M}}{\partial\lambda}\,\middle|\,\frac{\partial\widetilde{M}}{\partial\alpha}\,\middle|\,\frac{\partial\widetilde{M}}{\partial\beta}\right). \tag{5.14}$$

In the first block, the elements of the type $\partial M_{ij}/\partial\lambda_k$ are independent of the λ_i. In the second block the elements $\partial M_{ij}/\partial\alpha_k$ are linear in the λ_i; the same applies for the third block. Expanding out the determinant, we find that all the terms which contribute to J are 6th degree polynomials in the λ_i. Furthermore, If $\lambda_i=\pm\lambda_j$ for any i,j, then there exists at least one coordinate for the orthogonal matrices $\widetilde{O}_1$, $\widetilde{O}_2$ which does not affect the matrix $\widetilde{M}$. This implies that the Jacobian J must vanish whenever $\lambda_i=\pm\lambda_j$. These observations lead to a unique form for the Jacobian,

$$J=g(\alpha)g(\beta)\prod_{\substack{i,j=1\\ i>j}}^{3}|\lambda_i^2-\lambda_j^2|, \tag{5.15}$$

where $g(\alpha)d\alpha_1 d\alpha_2 d\alpha_3$ is an invariant measure for the orthogonal group. The probability measure in the transformed coordinates is therefore

$$dP=Ag(\alpha)g(\beta)\prod_{\substack{i,j=1\\ i>j}}^{3}|\lambda_i^2-\lambda_j^2|\exp\left[-\frac{1}{4\sigma^2}\sum_{k=1}^{3}\lambda_k^2\right]\prod_{i=1}^{3}d\alpha_i d\beta_i d\lambda_i. \tag{5.16}$$

We can now use (5.11) and (5.16) to evaluate $\langle f^{-3}\rangle$. The three elements $(\widetilde{O}_1)_{i1}$ in (5.11) are components of a unit vector with random direction, and can easily be represented using polar coordinates θ, ϕ. The required average is then

$$\langle f^{-3}\rangle=I_1/I_2,$$

$$I_1=\int d\lambda P[\lambda]\int_0^{\pi}d\theta\,\sin\,\theta\int_0^{2\pi}d\phi(\lambda_1^{-2}\cos^2\,\theta+\lambda_2^{-2}\sin^2\,\theta\sin^2\,\phi+\lambda_3^{-2}\sin^2\,\theta\cos^2\,\phi)^{-3/2} \tag{5.17}$$

$$I_2=\int d\lambda P[\lambda]\int_0^{\pi}d\theta\,\sin\,\theta\int_0^{2\pi}d\phi,$$

where $P[\lambda]$ is the product of the polynomial and exponential in (5.16). After performing the integrals over θ and ϕ, we find

$$\langle f^{-3}\rangle=\frac{\sqrt{8}\sigma^3\mathscr{I}(1,\frac{1}{2},3)}{\mathscr{I}(\frac{1}{2},\frac{1}{2},3)}, \tag{5.18}$$

where the $\mathscr{I}(\alpha,\gamma,n)$ are integrals obtained from results derived by Selberg[27] and Aomoto,[28] quoted by Mehta,[2]

$$\mathscr{I}(\alpha,\gamma,n)=\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\prod_{i=1}^{n}|x_i|^{2\alpha-1}\prod_{1\leqslant j<i\leqslant n}|x_i^2-x_j^2|^{2\gamma}\exp\left[\frac{-x_i^2}{2}\right]dx_i$$

$$=2^{\alpha n+\gamma n(n-1)}\prod_{j=1}^{n}\frac{\Gamma(1+\gamma j)\Gamma(\alpha+\gamma(j-1))}{\Gamma(1+\gamma)}. \tag{4.29}$$

We find $\mathscr{I}(1,\frac{1}{2},3)=96$, $\mathscr{I}(\frac{1}{2},\frac{1}{2},3)=24\sqrt{2\pi}$, so that $\langle f^{-3}\rangle=8\sigma^3/\sqrt{\pi}$. The density of degeneracies is therefore $\mathscr{D}_2^{(\mathrm{deg})}=\frac{2}{3}\sqrt{\pi}\rho^3\sigma^3$.

VI. SINGULARITIES OF CORRELATION FUNCTIONS

Now we discuss how the singularities of the energy levels are related to singularities of the correlation function $C(X)$ defined in (1.1). Our contribution builds upon work of Guarneri *et al.*,[8] who showed that the Fourier transform of $C(X)$ has a power law decay as $|k|\to\infty$:

$$\widetilde{C}(k)\sim\frac{\alpha_\beta\sigma}{\rho}\left(\frac{\rho\sigma}{|k|}\right)^{\beta+2}, \tag{6.1}$$

where we will define the Fourier transform $\widetilde{f}(k)$ of $f(x)$ as follows:

$$\widetilde{f}(k)=\int_{-\infty}^{\infty}dx f(x)\exp[ikx]. \tag{6.2}$$

Guarneri *et al.* were not able to determine the coefficients α_β; we will show how they can be obtained using the results of Sec. IV B. They showed that the power law decay is caused by avoided crossings with small values of the gap parameter ϵ, and deduced that the algebraic decay of $\widetilde{C}(k)$ implies that $C(X)$ has a non-analytic behavior at $X=0$. Using the generalized Fourier transform pairs,[29]

$$\widetilde{f}(k)=\frac{1}{|k|^3}\Leftrightarrow f(x)=\frac{1}{2\pi}x^2\left(\log|x|+\gamma-\frac{3}{2}\right), \tag{6.3a}$$

$$\widetilde{f}(k)=\frac{1}{k^4}\Leftrightarrow f(x)=\frac{1}{12}|x|^3, \tag{6.3b}$$

$$\widetilde{f}(k)=\frac{1}{k^6}\Leftrightarrow f(x)=-\frac{1}{240}|x|^5, \tag{6.3c}$$

it can be seen that (6.1) implies the existence of non-analytic terms in the expansion of the correlation function about $X=0$. Expressed in terms of the natural dimensionless variable $x=\rho\sigma X$, the behaviour of $C(x)$ up to and including the leading non-analytic term is

$$C(x)=2\sigma^2[1+\gamma_1|x|^2\log|x|+\cdots]\quad(\mathrm{GOE}), \tag{6.4a}$$

$$C(x)=\sigma^2[1+C_2^{(2)}x^2+\gamma_2|x|^3+\cdots]\quad(\mathrm{GUE}), \tag{6.4b}$$

$$C(x)=\tfrac{1}{2}\sigma^2[1+C_4^{(2)}x^2+C_4^{(4)}x^4+\gamma_4|x|^5+\cdots]\quad(\mathrm{GSE}). \tag{6.4c}$$

The coefficients of the power series expansion are obtained by a straightforward application of perturbation theory: the quadratic terms were calculated by Simons and Altshuler,[6] and take the values $C_2^{(2)}=-2\pi^2$ and $C_4^{(2)}=-\frac{4}{3}\pi^2$, respectively; the coefficient $C_4^{(4)}$ could also be determined by the same method. The higher order coefficients of the power series expansion diverge because of the effects of small denominators. We will now calculate the coefficients α_β in (6.1), enabling the coefficients γ_β of the singular terms to be identified.

We will find it convenient to assume that the energy levels are periodic in X, with period L, so that the energy level $E_n(X)$ can be expanded as a Fourier series:

$$E_n(X)=\sum_{m=-\infty}^{\infty} a_m \exp\left[\frac{2\pi i m X}{L}\right]. \tag{6.5}$$

Later we will consider the limit $L\to\infty$. The correlation function $C(X)$ will be defined in terms of an average over the length L, which is conveniently expressed in terms of the Fourier coefficients a_m:

$$C(X)=\frac{1}{L}\int_0^L dX' E_n'(X+X')E_n'(X')=\sum_{m=-\infty}^{\infty}\left(\frac{2\pi m}{L}\right)^2 |a_m|^2 \exp\left[\frac{2\pi i m X}{L}\right]. \tag{6.6}$$

For large m, the Fourier coefficients are determined by singularities of $E_n(X)$ closest to the real axis. These are branch points associated with the avoided crossings with small values of the gap parameter ϵ. In order to calculate the effect of these singularities on the Fourier coefficients, we will assume that the second derivative of the energy can be approximated by a sum of contributions from the avoided crossings:

$$E_n''(X)\sim\sum_j (-1)^{P_j} f(X-X_j,A_j,\epsilon_j), \tag{6.7}$$

where A_j, ϵ_j, and X_j are the parameters of the jth avoided crossing. (It is more convenient to use the second derivative, since this approaches zero at $\pm\infty$.) Here the sum runs over all avoided crossings between 0 and L, P_j is zero if the avoided crossing is with a level below, unity for crossing with a level above, and $f(X,A,\epsilon)$ is the second derivative of the energy associated with a single avoided crossing with slope and gap parameters (A,ϵ) at position $X=0$:

$$f(X,A,\epsilon)=\frac{A^2\epsilon^2}{2(A^2X^2+\epsilon^2)^{3/2}}. \tag{6.8}$$

Using (6.7) to estimate the Fourier coefficients a_m, and we find

$$\begin{aligned} a_m &= -\left(\frac{2\pi m}{L}\right)^{-2}\frac{1}{L}\sum_j (-1)^{P_j}\int_0^L dx f(x-X_j,A_j,\epsilon_j) \\ &\sim -\frac{1}{k^2 L}\sum_j (-1)^{P_j}\exp[ikX_j]\tilde{f}(k,A_j,\epsilon_j), \end{aligned} \tag{6.9}$$

where $k=2\pi m/L$, and $\tilde{f}(k,A,\epsilon)$ is the Fourier transform of $f(X,A,\epsilon)$ with respect to X: in the second relation we have assumed that L is sufficiently large that, for all the avoided crossings except those close to $X_j=0$ or $X_j=L$, the errors associated with taking the limits of integration to infinity can be neglected. Using (6.9) to estimate $|a_m|^2$ gives an expression involving a double sum over pairs of avoided crossings. The positions X_j of the narrowly avoided crossings can be

assumed to be random, implying that the average over off-diagonal terms of the double sum containing the phase factor $\exp[ik(X_j - X_{j'})]$ vanishes. We can therefore write

$$|a_m|^2 \sim \frac{1}{k^4 L^2} \sum_j |\tilde{f}(k, A_j, \epsilon_j)|^2$$

$$\sim \frac{2}{k^4 L} \int_0^\infty dA \int_\infty^\infty dB \int_0^\infty d\epsilon \, \mathscr{D}_\beta^{(\mathrm{deg})}(A,B,\epsilon) |\tilde{f}(k,A,\epsilon)|^2, \tag{6.10}$$

where $\mathscr{D}_\beta^{(\mathrm{deg})}$ is the density of avoided crossings defined in Sec. IV B, and the factor of 2 is included because avoided crossings with both the levels above and below must be considered.

The Fourier transform of (6.8) is

$$\tilde{f}(k,A,\epsilon) = k\epsilon K_1(k\epsilon/A), \tag{6.11}$$

where $K_1(x)$ is the Bessel function with imaginary argument.[30,31] In the limit $L \to \infty$ we can approximate the sum in (6.6) as an integral, and using (6.10) we write

$$C(X) = \frac{1}{2\pi} \int_{-\infty}^\infty dk \, \exp[-ikX] \tilde{C}(k), \tag{6.12}$$

$$\tilde{C}(k) = \frac{2}{k^2} \int_0^\infty dA \int_{-\infty}^\infty dB \int_0^\infty d\epsilon \, \mathscr{D}_\beta^{(\mathrm{deg})}(A,B,\epsilon) |\tilde{f}(k,A,\epsilon)|^2$$

$$= \frac{2 C_\beta^{(\mathrm{ac})}}{k^{(\beta+2)}} \left(\frac{\rho}{\sigma} \right)^{\beta+1} \int_0^\infty dA A^{2\beta+3} \exp\left[\frac{-\beta A^2}{8\sigma^2} \right] \int_0^\infty dx x^{\beta+1} |K_1(x)|^2,$$

where we have used (4.7). Using the integral identity[31]

$$\int_0^\infty dx \, x^\nu |K_1(x)|^2 = \frac{2^{\nu-6}(\nu+1)(\nu-1)^3 [\Gamma(\frac{1}{2}(\nu-1))]^4}{\Gamma(\nu+1)}, \tag{6.13}$$

we find that $\tilde{C}(k)$ is in the form (6.1), with dimensionless constants

$$\alpha_1 = 4\pi^3, \quad \alpha_2 = \frac{256\pi^{3/2}}{3}, \quad \alpha_4 = \frac{2^{14}\sqrt{2}\pi^{7/2}}{45}. \tag{6.14}$$

Expressed in terms of the dimensionless variable $x = \rho\sigma X$, the correlation function, up to and including the first singular term, is therefore

$$C(x) = 2\sigma^2 [1 - \pi^2 x^2 \log|x| + \cdots] \quad \text{(GOE)},$$

$$C(x) = \sigma^2 \left[1 - 2\pi^2 x^2 - \frac{64\pi^{3/2}}{9} |x|^3 + \cdots \right] \quad \text{(GUE)}, \tag{6.15}$$

$$C(x) = \tfrac{1}{2}\sigma^2 \left[1 - \frac{4\pi^2}{3} x^2 + C_4^{(4)} x^4 + \frac{2048\sqrt{2}\pi^{7/2}}{675} |x|^5 + \ldots \right] \quad \text{(GSE)}.$$

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APPENDIX: THE DENSITY OF DEGENERACIES FOR THE GSE

Here we discuss the density of degeneracies $\mathscr{D}_4^{(\mathrm{deg})}$ for a parametrized Gaussian symplectic ensemble. The method employed is the same as that for the GUE, and so can be presented briefly.

The quaternion elements $\mathbf{e}_k$ can be represented by the 2×2 matrices:

$$\mathbf{e}_0=\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix},\quad \mathbf{e}_1=\begin{pmatrix}i & 0\\ 0 & -i\end{pmatrix},\quad \mathbf{e}_2=\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix},\quad \mathbf{e}_3=\begin{pmatrix}0 & i\\ i & 0\end{pmatrix}, \tag{A1}$$

enabling the GSE matrix to be represented by a $2N\times 2N$ real matrix, which has N, 2–fold degenerate eigenvalues: this (Kramer's) degeneracy will be neglected, and we will calculate the density of degeneracies between pairs of these double levels. Five parameters must be varied in order to create these degeneracies.

The condition for a degeneracy between levels n and $n+1$ to be at a distance $\delta\mathbf{X}$ from an arbitrary point can be written in a form analogous to (5.2), where $\widetilde{M}$ is now a 5×5 matrix with elements

$$\begin{aligned} M_{1j}&=[\partial_j\widetilde{H}^{(S)}]_{nn}-[\partial_j\widetilde{H}^{(S)}]_{n+1\,n+1},\\ M_{2j}&=2[\partial_j\widetilde{H}^{(S)}]_{nn+1},\\ M_{ij}&=2[\partial_j\widetilde{H}^{(A)}_{i-2}]_{nn+1},\quad i=3,4,5. \end{aligned} \tag{A2}$$

Again $\widetilde{M}=\{M_{ij}\}$ is a non-symmetric real matrix with independent, Gaussian distributed elements, with mean value zero; the variance is σ^2 in this case.

The Euclidean length of the vector which solves (5.2) is again written $R=\Delta f$, and following the GUE analysis we find the probability $P[R]dR$ that the nearest degeneracy lies in a shell of thickness dR at distance R. Using the fact that for the GSE, the level spacing distribution is $P[\Delta]d\Delta\sim\frac{16}{135}\pi^4\rho^5\Delta^4 d\Delta$ for $\Delta\rho\ll 1$, $N\gg 1$, we find

$$P[R]\sim\frac{16}{135}\pi^4\rho^5R^4\langle f^{-5}\rangle, \tag{A3}$$

which is valid for small R. The expected number of degeneracies in this shell is $P[R]dR=\frac{8}{3}\pi^2R^4\mathscr{D}_4^{(\mathrm{deg})}dR$ implying that the density of degeneracies for the parameterized GSE is

$$\mathscr{D}_4^{(\mathrm{deg})}=\frac{2}{45}\pi^2\rho^5\langle f^{-5}\rangle. \tag{A4}$$

The integral $I=\langle f^{-5}\rangle$ can be evaluated using the same approach as that used for $\langle f^{-3}\rangle$ in Sec. V, using the decomposition of $\widetilde{M}$ given by (5.10). After some algebra, the original 25 dimensional integral over the M_{ij} is reduced to the quotient of two five dimensional integrals:

$$\langle f^{-5}\rangle = \frac{\sigma^5 \mathscr{I}(1,\frac{1}{2},5)}{\mathscr{I}(\frac{1}{2},\frac{1}{2},5)} = \frac{16\sigma^5}{\sqrt{2\pi}}, \tag{A5}$$

where $\mathscr{I}(\alpha,\gamma,n)$ is the integral (5.19). Combining (A4) and (A5), we then find $\mathscr{D}_4^{(\mathrm{deg})} = (16\sqrt{2}\pi^{3/2}/45)\rho^5\sigma^5$.

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Asymptotic properties of large random matrices with independent entries

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We study the normalized trace $g_n(z)=n^{-1}\,\mathrm{tr}(H-zI)^{-1}$ of the resolvent of $n\times n$ real symmetric matrices $H=[(1+\delta_{jk})W_{jk}\sqrt{n}]_{j,k=1}^{n}$ assuming that their entries are independent but not necessarily identically distributed random variables. We develop a rigorous method of asymptotic analysis of moments of $g_n(z)$ for $|\Im z|\geqslant\eta_0$ where η_0 is determined by the second moment of W_{jk}. By using this method we find the asymptotic form of the expectation $\mathbf{E}\{g_n(z)\}$ and of the connected correlator $\mathbf{E}\{g_n(z_1)g_n(z_2)\}-\mathbf{E}\{g_n(z_1)\}\mathbf{E}\{g_n(z_2)\}$. We also prove that the centralized trace $ng_n(z)-\mathbf{E}\{ng_n(z)\}$ has the Gaussian distribution in the limit $n=\infty$. Based on these results we present heuristic arguments supporting the universality property of the local eigenvalue statistics for this class of random matrix ensembles. © *1996 American Institute of Physics.* [S0022-2488(96)01210-8]

I. INTRODUCTION

Since the pioneer works of Wigner and Dyson random matrix theory (RMT) has been successfully used to describe the energy levels of complex quantum systems: heavy nuclei, quantum chaotic systems, mesoscopic samples, etc. (see, e.g., Refs. 1–5). Another rather broad field of the RMT applications is related to quantum field theory: the large colour limit of QCD, two-dimensional (2D) quantum gravity and bosonic strings (see, e.g., Refs. 6–8).

The phenomenological nature of the RMT approach that may be regarded as its certain drawback on the one hand, provides, on the other hand, the model independent frameworks, that make the approach applicable to a wide variety of systems having different microscopic natures and origins. These frameworks assume a certain amount of ''robustness'' of the RMT models and results. In other words, it is believed that a ''sufficiently large'' number of them should have no dependence or a rather weak one on the random matrix ensemble used. This belief partly explains the fact that the majority of RMT ideas and applications are based on results obtained for the archetype Gaussian ensembles (GE's) and the circular ensembles (CE's). On the other hand, this belief requires a certain justification, in particular extending the results known for the GE's and for the CE's to other classes of ensembles.

The most frequently referred to are the Gaussian orthogonal ensemble (GOE) of random $n\times n$ symmetric matrices and the Gaussian Unitary Ensemble (GUE) of random $n\times n$ Hermitian matrices. The density of the probability distribution in these ensembles has the form

$$P_n(H)=Z_n^{-1}\,\exp[-n\,\mathrm{tr}\,F(H)], \tag{I.1}$$

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where $F(x)=x^2/4w^2$ and Z_n is the normalization constant.

The probability distribution (I.1) possesses two important properties: (i) it is invariant with respect to either orthogonal or unitary transformations of $\mathbf{R}^n$ or $\mathbf{C}^n$, respectively; and (ii) the matrix elements are independent random variables (modulo the obvious symmetry conditions).

These properties of the GE's determine them uniquely and motivate two classes of generalizations of the GE's.

The first class consists of ensembles having an orthogonal or unitary invariant but not necessarily matrix-element-independent probability distribution. The typical representatives are the ensembles with the probability distribution of the form (I.1) in which $F(x)$ is an arbitrary bounded below and growing fast enough on infinity function. These invariant ensembles can be used to describe physical systems having no preferential basis. They also arose in studying the large-n limit in quantum field theory[6–8] and later found other applications.[3,9,10]

Random matrices with invariant distributions show remarkable ''robustness'' (known as the universality) of spectral properties in the microscopic regime. In this regime one scales the energy so that the mean distance between nearest eigenvalues remains of the order of unity as the dimension of matrices increases.[1,11] Thus one is able to study properties of a finite number of eigenvalues. The universality of the level spacing distribution and other microscopic (local) spectral characteristics has been extensively discussed in recent theoretical physics and mathematical literature. We refer the reader to a number of publications: Refs. 11–16.

The second class consists of ensembles whose matrix elements in a certain basis are independent random variables, i.e., the ensemble probability distribution factorizes into a product of distributions of the matrix elements in this basis. The corresponding random matrices can be associated with physical systems having a preferential basis and appear, in particular, in condensed matter physics and theory of disordered systems. This second class goes back to Wigner[17] and we shall refer to the corresponding ensembles as Wigner ensembles (or Wigner matrices).

The subject of the present paper is the Wigner ensemble of $n\times n$ real symmetric matrices of the form

$$H=[H_{jk}]_{j,k=1}^{n}, \quad H_{jk}=(1+\delta_{jk})W_{jk}/\sqrt{n}, \tag{I.2}$$

where $W_{jk}, j\leqslant k$ are independent random variables such that

$$\mathbf{E}\{W_{jk}\}=0, \quad \mathbf{E}\{W_{jk}^2\}=w^2. \tag{I.3}$$

Here and thereafter $\mathbf{E}\{\cdot\}$ denotes averaging over all $W_{jk}, j\leqslant k$.

The distributions of W_{jk}'s may depend on (j,k), but we assume that they are independent of n. We make the latter assumption mainly for the sake of technical simplicity. On the other hand, this assumption allows one to consider all W_{jk} on the same probability space and to find an optimal form of a number of important facts related to the Wigner ensembles (for example, the convergence with probability 1 in formulae (I.7) and (I.11) below). If W_{jk}'s are independent Gaussian random variables, then the ensemble (I.2)–(I.3) coincides with the GOE. This justifies the presence of the term with δ_{jk} in Eq. (I.2).

Macroscopic properties of Wigner ensembles are more or less well understood. We call macroscopic the asymptotic regime in which the number of eigenvalues in unit energy interval is proportional to n. Discussing macroscopic properties of random matrices we have to mention first of all the density of states (DOS) which is the simplest macroscopic characteristic of the ensemble eigenvalue statistics. It turns out that under rather natural and mild conditions on the distributions of W_{jk} the DOS in the Wigner ensemble (I.2)–(I.3) does not depend on the form of the distributions of W_{jk}. This DOS is known as the Wigner semi-circle law (see Eq. (I.5) below). Other macroscopic spectral quantities such as the conductivity and the interband light absorption coefficient show the same ''robustness.''[18–20] Definition of these quantities requires some care for Wigner matrices. However, the conductivity and the interband light absorption coefficient can be

defined and computed for the so-called band random matrices and random operators with independent matrix elements that are quite close to the Wigner ensemble (I.2)–(I.3) in their macroscopic properties both technically and by results (see, e.g., Ref. 21). As for the microscopic scale, supersymmetry calculations[22] suggest ''robustness'' (universality) of spectral properties of the Wigner ensemble (I.2)–(I.3) as well but evidence of this has not been rigorously established so far.

Introduce the normalized eigenvalue counting function

$$N_n(E)=n^{-1}\#\{E_j:\ E_j \quad \text{is an eigenvalue of } H \text{ and } E_j\leqslant E\}. \tag{I.4}$$

Wigner at the end of the 1950s proved[17] that in the case of identically distributed W_{jk} having all moments $N_n(E)$ converges in probability as $n\to\infty$ to a non-decreasing function $N_{sc}(E)$ (the semi-circle law) whose derivative (DOS) is

$$\rho(E)=\begin{cases}\dfrac{1}{2\pi w^2}\sqrt{4w^2-E^2}, & |E|\leqslant 2w\\ 0, & |E|>2w.\end{cases} \tag{I.5}$$

The modern formulation of Wigner's result is as follows. Let us consider random matrices (I.2)–(I.3) with mutually independent arbitrary distributed entries defined on a common probability space. Then the condition (the matrix analogue of the Lindeberg condition of probability theory)

$$\lim_{n\to\infty}\frac{1}{n^2}\sum_{j\leqslant k}\int_{|x|>\nu n^{1/2}}x^2\ d\ \mathrm{Prob}[W_{jk}\leqslant x]=0, \quad \text{for any} \quad \nu>0, \tag{I.6}$$

is sufficient[23] and necessary[24] for the following limiting relation

$$\lim_{n\to\infty}N_n(E)=N_{sc}(E) \tag{I.7}$$

to hold for every E with probability 1.[25] If we will not assume that W_{jk} are defined on the same probability space or if their probability distributions depend on n, then the same condition (I.6) will imply the convergence in probability in Eq. (I.7)

As is usual in spectral theory, this result admits a natural reformulation in terms of the resolvent (Green's function). Indeed, the normalized trace of the resolvent

$$g_n(z)=n^{-1}\ \mathrm{tr}\ (H-zI)^{-1} \tag{I.8}$$

is simply the Stieltjes transform of $N_n(E)$:

$$g_n(z)=\frac{1}{n}\sum_{j=1}^{n}\frac{1}{E_j-z}=\int\frac{dN_n(E)}{E-z}. \tag{I.9}$$

Denote the Stieltjes transform of the Wigner law (I.5) by $r(z)$,

$$r(z)=\int\frac{N_{sc}(dE)}{E-z}=\frac{-z+\sqrt{z^2-4w^2}}{2w^2}. \tag{I.10}$$

The obvious condition $\Im r(z)\Im z\geqslant 0$ determines the branch of the square root in Eq. (I.10). Due to the one-to-one correspondence between non-decreasing functions and their Stieltjes transforms[26] Eq. (I.7) is equivalent to the following limiting relation

$$\lim_{n\to\infty} g_n(z)=r(z), \tag{I.11}$$

which holds with probability 1 for any non-real z.

The relation (I.11) and the obvious bound $|g_n(z)|\leqslant|\Im z|^{-1}$ imply that the variance of $g_n(z)$ vanishes as $n\to\infty$ and hence the moments

$$m_n^{(p)}(z_1,\ldots,z_p)=\mathbf{E}\left\{\prod_{l=1}^{p} g_n(z_l)\right\} \tag{I.12}$$

factorize:

$$m_n^{(p)}(z_1,\ldots,z_p)=\prod_{l=1}^{p} m_n^{(1)}(z_l)+o(1), \quad n\to\infty \tag{I.13}$$

This factorization, which follows already from the convergence in probability in Eq. (I.7) or in Eq. (I.11) , is typical for the macroscopic regime and can be found hidden behind many calculations in this regime. It has been known in fact since Refs. 17, 27, 23 and 28.

Since according to Eq. (I.11) $m_n^{(1)}(z)=\mathbf{E}\{g_n(z)\}=r(z)+o(1)$, the leading term of $m_n^{(p)}(z_1,\ldots,z_p)$ is $\Pi_{l=1}^{p} r(z_l)$. It seems interesting from a number of points of view to also find sub-leading terms and their dependence on the probability distributions of matrix elements. For instance these sub-leading terms are important when we would like to go beyond the macroscopic regime, when we are computing connected correlators of $g_n(z)$, etc.

For the Gaussian entries respective corrections were studied in Ref. 29 where the formal perturbation theory with respect to H_{jk} and the respective diagrammatic technique were applied. This approach is an adaptation of the technique developed in Ref. 30 in order to construct the $1/n$ expansion for the random operator describing disordered systems on $\mathbf{Z}^d$ with n orbitals per site.

In Ref. 31 we suggested an approach that allows for the rigorous treatment of this problem in the general case of independent and arbitrary but not necessarily identically distributed matrix elements. Our approach allows us to estimate remainders in respective asymptotic formulae and we show that these estimates are in a sense optimal. The approach is also free to a large extent from the cumbersome combinatorial problem of rearranging diagrams which is necessary in order to carry out various ''dressing'' procedures. In particular, the dressing procedure that replaces the ''bare'' Green function $-1/z$ by $\lim_{n\to\infty}\mathbf{E}\{g_n(z)\}$ is automatic in our approach. Following Ref. 31 one is able to find as many terms in the asymptotic expansion of $m_n^{(p)}(z_1,\ldots,z_p)$ as needed, though the technical difficulties increase with the order.

In the present paper we use the general scheme of Ref. 31 in order to compute first terms in the asymptotic expansion of $\mathbf{E}\{g_n(z)\}$. We also prove that if the distributions of W_{jk} satisfy the Lindeberg condition (I.6) with x^2 in the integral replaced by x^4, and if in addition to Eq. (I.3) the fourth moments of W_{jk} do not depend on (j,k), then

$$F_n(z_1,z_2)=m_n^{(2)}(z_1,z_2)-m_n^{(1)}(z_1)m_n^{(1)}(z_2)=n^{-2}f(z_1,z_2)+o(n^{-2}), \tag{I.14}$$

where

$$f(z_1,z_2)=\frac{2w^2}{[1-w^2r^2(z_1)][1-w^2r^2(z_2)]}\left[\frac{r(z_1)-r(z_2)}{z_1-z_2}\right]^2+\frac{2\sigma r^3(z_1)r^3(z_2)}{[1-w^2r^2(z_1)][1-w^2r^2(z_2)]} \tag{I.15}$$

and $\sigma=\mathbf{E}\{W_{jk}^4\}-3\mathbf{E}^2\{W_{jk}^2\}$ is the excess of W_{jk}. We also establish a limit theorem for the centralized trace $ng_n(z)-\mathbf{E}\{ng_n(z)\}$ of the resolvent.

Unfortunately, our approach gives an estimate for the remainder term in Eq. (I.14) containing a power of $|\Im z_1 \Im z_2|^{-1}$ as a factor. Thus we cannot treat rigorously the microscopic regime which requires $\Im z \propto 1/n$. On the other hand, the first term [Eq. (I.15)] of the asymptotic formula (I.14) is well defined in this regime and coincides with the respective exact expression known for the GOE, provided that the latter is considered for large level spacings and is smoothed over an interval Δ such that $1/n \ll |\Delta| \ll 1$ in proper units (see Section VI). We feel therefore, that by using our procedure of computing corrections, i.e., keeping the imaginary part of energy fixed when n goes to infinity and then letting $\Im z$ go to zero , one may treat energy intervals that are very large on the microscopic scale. On this intermediate scale the second term on the right-hand side (rhs) of Eq. (I.15) which contains the probability distribution excess σ vanishes and the above mentioned universality is restored.

Our article is organized as follows. In Section II we present our basic tools. In Section III we calculate first terms of the asymptotic expansion for $\mathbf{E}\{g_n(z)\}$. In Section IV we give a simple proof of Eqs. (I.14)–(I.15) with $o(n^{-2})$ replaced by $O(n^{-5/2})$ provided that the fifth absolute moment of W_{jk} is uniformly bounded. This result was cited without proof in Ref. 31. In Section V we treat the general case of W_{jk} satisfying the higher order Lindeberg condition mentioned above. We prove that the fluctuations of $ng_n(z)$ around its mean value become Gaussian in the limit $n \to \infty$ and that the covariance of the limiting Gaussian function is $f(z_1, z_2)$, thus proving Eqs. (I.14)–(I.15) in the general case. Section VI contains a discussion of some implications of our results.

II. PRELIMINARIES

In this section we present our basic technical tools.

(i) If ξ is a real-valued random variable such that $\mathbf{E}\{|\xi|^{p+2}\} < \infty$ and if $f(t)$ is a complex-valued function of a real variable such that its first $p+1$ derivatives are continuous and bounded, then

$$\mathbf{E}\{\xi f(\xi)\} = \sum_{a=0}^{p} \frac{\kappa_{a+1}}{a!} \mathbf{E}\{f^{(a)}(\xi)\} + \varepsilon, \tag{II.16}$$

where κ_a are the semi-invariants (cumulants) of ξ, $|\varepsilon| \leqslant C \sup_t |f^{(p+1)}(t)| \mathbf{E}\{|\xi|^{p+2}\}$ and the quantity C depends on p only.

The semi-invariants can be expressed in terms of the moments. If $\mathbf{E}\{\xi\} = 0$ (the case we shall deal with) and $\mu_a = \mathbf{E}\{\xi^a\}$, then a few such first relations are: $\kappa_1 = \mu_1 = 0$, $\kappa_2 = \mu_2$, $\kappa_3 = \mu_3$, $\kappa_4 = \mu_4 - 3\mu_2^2$, $\kappa_5 = \mu_5 - 10\mu_3\mu_2$, $\kappa_6 = \mu_6 - 15\mu_4\mu_2 - 10\mu_3^2 - 30\mu_2^3$, etc. For a Gaussian random variable with zero mean, all semi-invariants but κ_2 vanish and Eq. (II.16) reduces to the exact relation

$$\mathbf{E}\{\xi f(\xi)\} = \mathbf{E}\{\xi^2\} \mathbf{E}\{f'(\xi)\}, \tag{II.17}$$

which can directly be checked integrating the left-hand side (lhs) of Eq. (II.17) by parts. This is only the case when formula (II.16) contains a finite number of terms for non-polynomial f's. Indeed, according to the Marcynkiewicz theorem[32] if all but a finite number of cumulants are zero, then only the first and second can be non-zero.

(ii) For any matrix $A = [A_{\alpha\beta}]_{\alpha,\beta=1}^{n}$

$$\frac{\partial}{\partial A_{jk}} (A^{-1})_{\alpha\beta} = -(A^{-1})_{\alpha j} (A^{-1})_{k\beta}$$

provided A^{-1} exists. For the resolvent G of a real symmetric matrix H this becomes

$$\frac{\partial G_{\alpha\beta}}{\partial H_{jk}}=\begin{cases}-G_{\alpha j}G_{k\beta}, & j=k\\ -G_{\alpha j}G_{k\beta}-G_{\alpha k}G_{j\beta}, & j\neq k.\end{cases} \tag{II.18}$$

(iii) For any two real symmetric matrices and any non-real z the resolvent identity

$$(H_2-zI)^{-1}=(H_1-zI)^{-1}-(H_1-zI)^{-1}(H_2-H_1)(H_2-zI)^{-1} \tag{II.19}$$

is valid. In particular, if $H_2=H$, $H_1=0$ and $G=(H-zI)^{-1}$, then

$$G_{jm}=z^{-1}\delta_{jm}+z^{-1}\sum_{k=1}^{n} G_{jk}H_{km}. \tag{II.20}$$

Let H belong to the Wigner ensemble (I.2)–(I.3). For a fixed complex z consider complex-valued random variable $g_n(z)=n^{-1}\,\mathrm{tr}(H-zI)^{-1}$. Define its variance as

$$\mathbf{E}\{|g_n(z)-\mathbf{E}\{g_n(z)\}|^2\}=F_n(z,z^{\dagger}) \tag{II.21}$$

and define also the domain in the complex plane as follows

$$U_0=\{z\in\mathbf{C}_{\pm}:|\Im z|\geqslant 2w\}. \tag{II.22}$$

We use an asterisk to denote complex conjugate and the sub-index C to indicate centering to zero mean. For instance, $g_n^C(z)=g_n(z)-\mathbf{E}\{g_n(z)\}$ and thus we can rewrite Eq. (II.21) as

$$F_n(z,z^{\dagger})=\mathbf{E}\{|g_n^C(z)|^2\}=\mathbf{E}\{g_n(z)g_n^C(z^{\dagger})\}. \tag{II.23}$$

We will write $O(n^{-p})$ in asymptotic formulae for the remainders having a uniform (with respect $z\in U_0$) upper bound of the form Cn^{-p} where C does not depend on n. In fact the bounds we are able to derive contain $1/(1-|\Im z|^2/2w^2)$ (see, e.g., formula (II.29) below for the simplest case). Thus C is finite for any fixed z satisfying $|\Im z|>\sqrt{2}w$. But we prefer to use $|\Im z|\geqslant 2w$ in favor of uniformity of the bounds with respect to $z\in U_0$.

(iv) Let H belong to the Wigner ensemble (I.2)–(I.3). Assume that the fifth absolute moment of the random variables W_{jk} is uniformly bounded, i.e. $\sup_{j\leqslant k}\mathbf{E}\{|W_{jk}|^5\}<+\infty$, and that $z\in U_0$. Then

$$\mathbf{E}\{|g_n(z)-\mathbf{E}\{g_n(z)\}|^2\}=\mathbf{E}\{|g_n^C(z)|^2\}=O(n^{-2}),\quad \text{as } n\to\infty. \tag{II.24}$$

Let us comment on (i)–(iv). Facts (ii) and (iii) are well known. The ''decoupling'' formula (II.16) is simple to understand in the case when ξ has all moments and $f(x)$ belongs to the Schwartz space. Indeed, by using the Parseval relation for the Fourier transforms we can rewrite the lhs of Eq. (II.16) as

$$\frac{i}{2\pi}\int_{-\infty}^{\infty}\frac{d}{dt}F^{\dagger}(t)\Pi(t)dt=-\frac{i}{2\pi}\int_{-\infty}^{\infty}F^{\dagger}(t)\frac{d}{dt}\Pi(t)dt \tag{II.25}$$

where

$$F(t)=\int_{-\infty}^{\infty}e^{i\xi t}f(\xi)d\xi \quad\text{and}\quad \Pi(t)=\int_{-\infty}^{\infty}e^{i\xi t}dP(\xi)$$

are the Fourier transforms of $f(\xi)$ and of the probability distribution $P(\cdot)$ of ξ, respectively. Now, if we take into account that

$$\Pi(t)=\sum_{a=0}^{\infty}\frac{(it)^a\mu_a}{a!}\quad\text{and}\quad u(t)\equiv\log\,\Pi(t)=\sum_{a=1}^{\infty}\frac{(it)^a\kappa_a}{a!}$$

we can rewrite the rhs of Eq. (II.25) as

$$-\frac{i}{2\pi}\int_{-\infty}^{\infty}F^{\dagger}(t)u'(t)e^{u(t)}dt=-\frac{i}{2\pi}\sum_{a=0}^{\infty}\frac{\kappa_{a+1}}{a!}\int_{-\infty}^{\infty}(it)^{a+1}F^{\dagger}(t)\Pi(t)dt=\sum_{a=0}^{\infty}\frac{\kappa_{a+1}}{a!}\mathbf{E}\{f^{(a)}(\xi)\},$$

where we again used the Parseval relation. The latter formula is obviously Eq. (II.16) for $p=\infty$. The case when ξ has a finite number of moments and $f(\xi)$ has a respective number of derivatives requires certain technicalities which we will not discuss here.

The bound (iv) plays an important role in many questions of random matrix theory and its applications. In fact, it is the simplest of bounds for connected correlators (cumulants) of $g_n(z)$ or, more generally, for cumulants of linear statistics of the eigenvalues (i.e., sums $n^{-1}\Sigma_{j=0}^{n}\,\phi(E_j)$ where $\phi(E)$ is smooth enough). We are going to present a detailed derivation of these bounds and asymptotics (both for the Wigner ensembles and unitary invariant ensembles) in a subsequent publication.

Here we only outline the scheme of the derivation of the bound (iv) considering the simplest case of the GOE and treating it as a representative of the Wigner ensembles, i.e. ensembles with independent entries. Set $r_n(z)=\mathbf{E}\{g_n(z)\}$. Then, according to Eqs. (II.17), (II.18) and (II.20) we have the relation

$$r_n(z)=-\frac{1}{z}-\frac{w^2}{z}\mathbf{E}\{g_n^2(z)\}+\frac{w^2}{n^2z}\mathbf{E}\{\text{ tr }G^2\}. \tag{II.26}$$

Applying similar arguments to $\mathbf{E}\{|g_n^2(z)|\}$ and using Eq. (II.26) we obtain the analogous relation for the variance (II.23)

$$F_n=-\frac{w^2}{z}E\{g_n^2(z)g_n^C(z^{\dagger})\}-\frac{w^2}{n^2z}\mathbf{E}\{[g_n^C(z)]^{\dagger}\text{ tr }G^2\}-\frac{2w^2}{n^3z}\mathbf{E}\{\text{ tr }G(G^*)^2\}, \tag{II.27}$$

where $G^*=(H-z^{\dagger}I)^{-1}$. By using the identity $E\{g_n^2(z)g_n^C(z^{\dagger})\}=E\{(g_n(z)+E\{g_n(z)\})\times|\,g_n^C(z)|^2\}$, the Cauchy–Schwarz inequality and the inequality (III.33) below we can show that the first term on the rhs of Eq. (II.27) is bounded above by $2w^2\eta^{-2}F_n$, where $\eta=|\Im z|$, the second is bounded by $w^2(n\eta^2)^{-1}F_n^{1/2}$ and the third is bounded by $2w^2(n^2\eta^4)^{-1}$. As a result we obtain the following inequality for $\eta^2>2w^2$

$$\left(1-\frac{2w^2}{\eta^2}\right)F_n-\frac{w^2}{n\eta^2}F_n^{1/2}-\frac{2w^2}{n^2\eta^4}\leqslant 0, \tag{II.28}$$

which implies that

$$F_n=\mathbf{E}\{|g_n^C(z)|^2\}\equiv\mathbf{E}\{|g_n(z)-\mathbf{E}\{g_n(z)\}|^2\}\leqslant\frac{C_1}{n^2}, \tag{II.29}$$

where $C_1=\eta^{-2}(\epsilon-1)^{-2}C_1(\epsilon)$, $\epsilon=\eta^2/2w^2$, $1<\epsilon<\infty$ and $C_1(\epsilon)$ is finite for $1\leqslant\epsilon<\infty$ Thus we have obtained Eq. (II.24) for the GOE. This is the simplest but typical bound that can be obtained by our method. In the general case of non-Gaussian W_{jk}'s one has to iterate the resolvent identity (I.20) and use Eq. (I.16) instead of Eq. (I.17), truncating this procedure on the proper step and estimating remainders by variants of arguments presented above.

The bounds (II.29) and (II.26) allow us to prove Eqs. (I.7) and (I.11) for the GOE. Indeed, combining Eq. (II.26) and (II.29) we obtain

$$\left| r_n(z) + \frac{1}{z} + \frac{w^2}{z} r_n^2(z) \right| \leqslant \frac{C_2}{n},$$

where C_2 has same properties as C_1 in Eq. (II.29). The bound and standard compactness arguments show that any limit point $r(z)$ of the sequence $\{r_n(z)\}$ satisfies the equation

$$w^2 r^2(z) + z r(z) + 1 = 0 \tag{II.30}$$

for $|\Im z| \geqslant \eta_0 > 0$. Since this equation has the unique solution (I.10) satisfying $\Im r(z) \Im z \geqslant 0$, we conclude that uniformly in $|\Im z| \geqslant \eta_0 > 0$ $\lim_{n\to\infty} r_n(z) = r(z)$ where $r(z)$ is given by Eq. (I.10). Besides, since the Gaussian W_{jk} satisfying Eq. (I.3) can be defined on the same probability space we conclude from Eq. (II.29) and the Borel–Cantelli lemma that Eqs. (I.11) and (I.7) and are valid.

III. ASYMPTOTIC EXPANSION FOR $E\{g_n(z)\}$

We recall our notation $m_n^{(1)}(z)$ for the mean value of $g_n(z) = n^{-1} \operatorname{tr} (H - zI)^{-1}$. In this section we prove the following

Theorem 1: *Consider the Wigner ensemble of random real symmetric matrices with independent entries defined by Eqs. (I.2)–(I.3). Assume additionally that the third and fourth moments of W_{jk} do not depend on j and k and that $\hat{\mu}_5 = \sup_{j \leqslant k} \mathbf{E}\{|W_{jk}|^5\} < +\infty$.*

Then the following asymptotic formula

$$m_n^{(1)}(z) = r(z) \left\{ 1 + \frac{1}{n} \left[\frac{w^2 r^2(z)}{[1 - w^2 r^2(z)]^2} + \frac{\sigma r^4(z)}{1 - w^2 r^2(z)} \right] \right\} + O(n^{-3/2}) \tag{III.31}$$

holds for any $z \in U_0$ (U_0 is defined in Eq. (II.22)).

Proof: By the resolvent identity (II.19)–(II.20),

$$m_n^{(1)}(z) = -z^{-1} + (zn)^{-1} \sum_{j,m=1}^{n} \mathbf{E}\{G_{jm} H_{mj}\}. \tag{III.32}$$

If we were following the conventional perturbational-diagrammatic approach trying to develop the asymptotic expansion for $\mathbf{E}\{g_n(z)\}$, we would repeatedly iterate the resolvent identity selecting on each step the terms that contribute to the leading and sub-leading terms. The obvious drawback of such an approach is that infinitely many iterations are needed and in the non-Gaussian case, when there is no analogue of the Wick theorem, the diagrammatic approach is rather complicated.

We propose making use of Eq. (II.16) instead of iterating the resolvent identity. For each pair (j,m), G_{jm} is a smooth function of H_{mj} and its derivatives are bounded because of Eq. (II.18) and the inequality

$$|G_{jm}| \leqslant \|G\| \leqslant |\Im z|^{-1}, \tag{III.33}$$

which holds for the resolvent of any real symmetric matrix. In particular, $|D_{mj}^4 G_{jm}| \leqslant C |\Im z|^{-5}$ where C is an absolute constant. Here and thereafter we use the notation D_{mj} for $\partial / \partial H_{mj}$.

According to Eqs. (I.2)–(I.3) and our assumptions, the fifth absolute moment of H_{mj} is of the order $n^{-5/2}$. Thus applying Eq. (II.16) (with $p = 3$) to each of the summands in the rhs of Eq. (III.32) one finds that

$$zm_n^{(1)}(z) = -1 + \sum_{a=1}^{3} \frac{1}{n^{(a+3)/2}} \sum_{j,m=1}^{n} \frac{\kappa_{a+1}(1+\delta_{jm})^{(a+1)/2}}{a!} \mathbf{E}\{D_{mj}^a G_{jm}\} + \varepsilon_n, \qquad \text{(III.34)}$$

where κ_a are the semi-invariants of W_{mj} and

$$|\varepsilon_n| \leqslant \frac{C}{n^{3/2}} \frac{\hat{\mu}_5}{|\Im z|^5}.$$

Obviously, G is a complex symmetric matrix, i.e. $G_{jm} = G_{mj}$. By Eq. (II.18), $D_{mm}^a G_{mm} = a! G_{mm}^{a+1}$ and

$$-D_{mj}^1 G_{jm} = G_{jm}^2 + G_{jj} G_{mm}, \qquad \text{(III.35)}$$

$$D_{mj}^2 G_{jm} = 2G_{jm}^3 + 6G_{jm} G_{jj} G_{mm}, \qquad \text{(III.36)}$$

$$-D_{mj}^3 G_{jm} = 6G_{jm}^4 + 36G_{jm}^2 G_{jj} G_{mm} + 6G_{jj}^2 G_{mm}^2 \qquad \text{(III.37)}$$

for distinct j and m. Let us set $\kappa_2 = w^2$ and $\kappa_4 = \sigma$ in Eq. (III.34). Then, as a consequence of Eqs. (III.35)–(III.37),

$$zm_n^{(1)}(z) = -1 - w^2 m_n^{(2)}(z,z) - n^{-1}[w^2 \mathbf{E}\{c_n(z)\} + \sigma \mathbf{E}\{d_n^2(z)\}] + \varepsilon_n, \qquad \text{(III.38)}$$

where

$$c_n(z) = \frac{1}{n} \sum_{j,m=1}^{n} G_{jm}^2, \quad d_n(z) = \frac{1}{n} \sum_{m=1}^{n} G_{mm}^2 \qquad \text{(III.39)}$$

and

$$|\varepsilon_n| \leqslant \frac{C}{n^{3/2}} \left(\frac{|\kappa_3|}{|\Im z|^3} + \frac{|\kappa_4|}{|\Im z|^4} + \frac{\hat{\mu}_5}{|\Im z|^5} \right). \qquad \text{(III.40)}$$

provided $|\Im z| \geqslant 2w$ and n is large enough.

To infer Eqs. (III.38)–(III.40) from Eq. (III.34), notice first that for the sum over $j = m$ on the rhs of Eq. (III.34) we have the bound

$$\frac{1}{n^{(a+3)/2}} \left| \sum_{m=1}^{n} D_{mm}^a G_{mm} \right| \leqslant \frac{C}{n^{(a+1)/2} |\Im z|^{a+1}} \propto \frac{1}{n^{(a+1)/2}} \leqslant \frac{1}{n^{3/2}}, \quad a = 2,3$$

for all realizations of W_{jk}. Therefore, being interested in the leading-order and $1/n$-order terms of $m_n^{(1)}(z)$ we can omit δ_{jm} from the factor in front of the second and third derivatives. As for the first derivatives, it follows from Eq. (III.35), that for all j and m $(1+\delta_{jm}) D_{jm}^1 G_{jm} = G_{jm}^2 + G_{jj} G_{mm}$ and the term arising from δ_{jm} contributes to $1/n$-order term in the asymptotic expansion of $m_n^{(1)}(z)$.

Now, G_{jm}^2 in the rhs of Eq. (III.35) makes $\mathbf{E}\{c_n(z)\}$ in Eq. (III.38) and $G_{jj} G_{mm}$ does $m_n^{(2)}(z,z)$. The term containing $G_{jj}^2 G_{mm}^2$ in the rhs of Eq. (III.37) leads to $\mathbf{E}\{d_n^2(z)\}$ in Eq. (III.38) and the rest in the rhs of Eqs. (III.36) and (III.37) contributes to ε_n in Eq. (III.38). Corresponding bounds for the terms coming from G_{jm}^3 in Eq. (III.36) and from G_{jm}^4 and $G_{jm}^2 G_{jj} G_{mm}$ in Eq. (III.37) result from the simple inequality

$$n^{-1}\sum_{j,m=1}^{n}|G_{jm}|^p\leqslant|\Im z|^{-p},\quad p\geqslant 2 \tag{III.41}$$

which holds for the resolvent of any real symmetric matrix. Estimating the term coming from $G_{jm}G_{jj}G_{mm}$ in the rhs of Eq. (III.36) requires a longer calculation. Set

$$h_n(z)=\frac{1}{n}\sum_{j,m=1}^{n}G_{jm}G_{jj}G_{mm}. \tag{III.42}$$

Substitute the rhs of Eq. (II.20) for G_{jm} in $h_n(z)$. Then

$$z\mathbf{E}\{h_n(z)\}=-\frac{1}{n}\sum_{m=1}^{n}\mathbf{E}\{G_{mm}^2\}-w^2\mathbf{E}\{g_n(z)h_n(z)\}+O(n^{-1/2}) \tag{III.43}$$

as follows from Eqs. (II.16), (III.35)–(III.37) and simple resolvent bounds like Eq. (III.33) or Eq. (III.41). Here and below we use the notation $O(n^{-p})$ for remainders admitting the upper bound Cn^{-p}, where C does not depend on n for $|\Im z|\geqslant 2w$.

According to Eq. (II.24) the variance of $g_n(z)$ is of order n^{-2} under our assumptions. In other words

$$m_n^{(2)}(z,z)=[m_n^{(1)}(z)]^2+O(n^{-2}) \tag{III.44}$$

if $z\in U_0$. Obviously,

$$\mathbf{E}\{h_n(z)g_n(z)\}-\mathbf{E}\{h_n(z)\}\mathbf{E}\{g_n(z)\}=\mathbf{E}\{h_n(z)[g_n(z)-\mathbf{E}\{g_n(z)\}]\}$$

and by the Cauchy–Schwarz inequality

$$\mathbf{E}\{h_n(z)g_n(z)\}=\mathbf{E}\{h_n(z)\}m_n^{(1)}(z)+O(n^{-1}).$$

Therefore by Eq. (III.43),

$$[z-w^2m_n^{(1)}(z)]\mathbf{E}\{h_n(z)\}=-\frac{1}{n}\sum_{m=1}^{n}\mathbf{E}\{G_{mm}^2\}+O(n^{-1/2}) \tag{III.45}$$

and $\mathbf{E}\{h_n(z)\}$ is of the order of unity. The term we wish to estimate is

$$\frac{2\kappa_3}{n^{5/2}}\sum_{j,m=1}^{n}\mathbf{E}\{G_{jm}G_{jj}G_{mm}\}=\frac{2\kappa_3}{n^{3/2}}\mathbf{E}\{h_n(z)\}$$

and from Eq. (III.45) we see it is of the order of $n^{-3/2}$. This proves Eqs. (III.38)–(III.40).

The calculation above is typical of our approach and uses Eqs. (II.16) and (II.20) combined with simple resolvent bounds on different stages. In what follows we shall often use similar calculations omitting details.

Equations (III.38)–(III.40) and Eq. (III.44) imply that

$$m_n^{(1)}(z)=r(z)+O(n^{-1}), \tag{III.46}$$

where $r(z)$ solves Eq. (II.30). Because of Eq. (I.9) $m_n^1(z)$ as a function of z must satisfy the inequality $\Im r(z)\Im z\geqslant 0$. This restriction fix the branch of the square root in the expression for the solutions of Eq. (II.30). Thus $r(z)$ coincides with the Stieltjes transform (I.10) of the semi-circle law (I.5), as expected.

Once the leading term of $m_n^{(1)}(z)$ is found, we can proceed with finding the sub-leading term. From Eq. (III.38) it is clear that performing this task requires calculating the leading-order terms of $\mathbf{E}\{c_n(z)\}$ and $\mathbf{E}\{d_n^2(z)\}$. Substitute the rhs of Eq. (II.20) for one of G_{jm} in $c_n(z)$ and apply Eq. (II.16). As a result,

$$z\mathbf{E}\{c_n(z)\} = -m_n^{(1)}(z) - 2w^2\mathbf{E}\{c_n(z)g_n(z)\} + O(n^{-1}).$$

By Eq. (II.24),

$$z\mathbf{E}\{c_n(z)\} = -m_n^{(1)}(z) - 2w^2 m_n^{(1)}(z)\mathbf{E}\{c_n(z)\} + O(n^{-1}) \tag{III.47}$$

and in the leading order

$$\mathbf{E}\{c_n(z)\} = -m_n^{(1)}(z)[z + 2w^2 m_n^{(1)}(z)]^{-1}.$$

Taking into account Eqs. (III.46)–(II.30) we conclude that

$$\mathbf{E}\{c_n(z)\} = r^2(z)[1 - w^2 r^2(z)]^{-1} + O(n^{-1}). \tag{III.48}$$

Now, calculate the leading-order term of $\mathbf{E}\{d_n^2(z)\}$. Recall that according to Eq. (II.24) the variance of $g_n(z)$ is of the order of n^{-2}. By Eq. (I.11), $g_n(z) = n^{-1}\Sigma_{m=1}{}^n G_{mm}$ converges almost surely to $r(z)$ as $n \to \infty$. Or, put another way, the Cesaro limit of G_{mm} is $r(z)$. This suggests that the Cesaro limit of G_{mm}^2 should be equal to $r^2(z)$, or in other words $d_n(z)$ should converge almost surely to $r^2(z)$. Therefore $\mathbf{E}\{d_n^2(z)\}$ should converge to $r^2(z)$.

To prove the convergence rigorously and to estimate its rate, we first note that the variance of $d_n(z)$ is of order n^{-1} if $z \in U_0$ (this can be proved following the calculations of Appendix B). Therefore

$$\mathbf{E}\{d_n^2(z)\} = \mathbf{E}\{d_n(z)\}^2 + O(n^{-2}). \tag{III.49}$$

Thus, it suffices to find the leading-order term of $\mathbf{E}\{d_n(z)\}$.

Again, as in the case of $c_n(z)$, substitute the rhs of Eq. (II.20) ($j = m$) for one of G_{mm} in $d_n(z)$ and apply Eq. (II.16). As a result,

$$z\mathbf{E}\{d_n(z)\} = -m_n^{(1)}(z) - w^2\mathbf{E}\{d_n(z)g_n(z)\} + O(n^{-1/2}).$$

By Eq. (II.24),

$$z\mathbf{E}\{d_n(z)\} = -m_n^{(1)}(z) - w^2 m_n^{(1)}(z)\mathbf{E}\{d_n(z)\} + O(n^{-1/2})$$

and

$$\mathbf{E}\{d_n(z)\} = -m_n^{(1)}(z)[z + w^2 m_n^{(1)}(z)]^{-1} + O(n^{-1/2}).$$

Finally by Eqs. (III.46) and (II.30),

$$\mathbf{E}\{d_n(z)\} = r^2(z) + O(n^{-1/2}) \tag{III.50}$$

and by Eq. (III.49),

$$\mathbf{E}\{d_n^2(z)\} = r^4(z) + O(n^{-1/2}). \tag{III.51}$$

Now we are in a position to find the sub-leading term of $m_n^{(1)}(z)$. Collect Eqs. (III.38), (III.44), (III.48) and (III.51) and write

$$zm_n^{(1)}(z) = -1 - w^2[m_n^{(1)}(z)]^2 - \frac{1}{n}\left[\frac{w^2r^2(z)}{1-w^2r^2(z)} + \sigma r^4(z)\right] + O(n^{-3/2}).$$

In view of Eqs. (III.46) and (II.30) this relation is obviously equivalent to the statement of the theorem, i.e. to the asymptotic formula (III.16). The theorem is proved.

Remarks:

1. Our bound for the remainder in Eq. (III.31) is an optimal one. By assuming the sixth absolute moment of W_{jk} to be uniformly bounded and keeping one more term when applying Eq. (II.16), we can find a term of the order of $n^{-3/2}$ in the asymptotic expansion of $m_n^{(1)}(z)$. This term is proportional to $\kappa_3 = \mathbf{E}\{W_{jk}^3\}$

2. If the distributions of W_{jk} are such that $\mathbf{E}\{W_{jk}^3\} = 0$, then the bound $O(n^{-3/2})$ for the remainder in Eq. (III.31) can be strengthened to $O(n^{-2})$. For terms of the order of $n^{-3/2}$ appear in Eq. (III.31) due to the contribution of $\kappa_3 n^{-3/2}\mathbf{E}\{h_n(z)\}$ to ε_n in Eq. (III.38) and also because of Eq. (III.51). If $\mathbf{E}\{W_{jk}^3\} = 0$, then $\kappa_3 = 0$ and we can prove that the remainder in Eq. (III.51) is of the order of n^{-1} (terms of order $n^{-1/2}$ in the rhs of Eq. (III.51) are proportional to κ_3).

3. For Gaussian W_{jk} the excess σ is zero and Eq. (III.31) reduces to the asymptotic formula

$$\mathbf{E}\{g_n(z)\} = r(z)\left[1 + \frac{1}{n}\frac{w^2r^2(z)}{[1-w^2r^2(z)]^2}\right] + O(n^{-2}),$$

which has been derived earlier by the formal diagrammatic approach.[29]

IV. LEADING ORDER OF $F_n(z_1, z_2)$

Let us recall our notation $F_n(z_1, z_2)$ (see Eq. (I.14)) for the covariance function of $g_n(z) = n^{-1}\,\mathrm{tr}(H - zI)^{-1}$,

$$F_n(z_1, z_2) = \mathbf{E}\{g_n^C(z_1)g_n^C(z_2)\} = \mathbf{E}\{g_n(z_1)g_n^C(z_2)\}.$$

In this section we prove the following

Theorem 2: *Consider the Wigner ensemble of random real symmetric matrices with independent entries defined by Eqs. (I.2)–(I.3). Assume additionally that the third and fourth moments of W_{jk} do not depend on j and k and that $\hat{\mu}_5 = \sup_{j \leqslant k}\mathbf{E}\{|W_{jk}|^5\} < +\infty$.*

Let $f(z_1, z_2)$ be the function given by Eqs. (I.15). If z_1 and z_2 belong to U_0 Eq. (II.22), then the following asymptotic relation

$$F_n(z_1, z_2) = n^{-2}f(z_1, z_2) + O(n^{-5/2}) \tag{IV.52}$$

is valid.

Proof: Let us first prove Eq. (IV.52) under the assumption

$$\hat{\mu}_7 = \sup_{j \leqslant k}\mathbf{E}\{|W_{jk}|^7\} < +\infty. \tag{IV.53}$$

Let $G_{jm}(z)$ denote a matrix element of $(H - zI)^{-1}$. By Eq. (II.20),

$$z_1F_n(z_1, z_2) = \frac{1}{n}\sum_{j,m=1}^{n}\mathbf{E}\{H_{mj}G_{jm}(z_1)g_n^C(z_2)\}.$$

For each pair (j, m) $G_{jm}(z_1)g_n^C(z_2)$ is a smooth function of H_{mj} and its derivatives are bounded because of Eq. (III.33). In particular, $|D_{mj}^6[G_{jm}(z_1)g_n^C(z_2)]| \leqslant C(|\Im z_1|^{-1} + (|\Im z_2|^{-1})^8$. Therefore by Eq. (II.16),

$$zF_n(z_1,z_2)=\sum_{a=1}^{5}\frac{1}{n^{(a+3)/2}}\sum_{j,m=1}^{n}\frac{\kappa_{a+1}(1+\delta_{jm})^{(a+1)/2}}{a!}\mathbf{E}\{D_{mj}^{a}[G_{jm}(z_1)g_n^C(z_2)]\}+\varepsilon_n,\tag{IV.54}$$

where κ_a are semi-invariants of W_{mj}, as in Eq. (III.34), and

$$|\varepsilon_n|\leqslant n^{-5/2}C\hat{\mu}_7(|\Im z_1|^{-1}+(|\Im z_2|^{-1})^8.$$

Performing differentiation on the rhs of Eq. (IV.54) one finds that the sums of the fifth, fourth and second derivatives in the rhs of Eq. (IV.54) contribute to $z_1F_n(z_1,z_2)$ terms of order $n^{-9/2}$, $n^{-7/2}$ and $n^{-5/2}$, respectively (corresponding bounds can be obtained using Eqs. (II.24), (III.33) and (III.41)). So, these derivatives give no contribution to the leading-order term of $F_n(z_1,z_2)$. It remains to estimate the contributions coming from the first and third derivatives.

The contribution of third derivatives to $z_1F_n(z_1,z_2)$ consists of several terms which we shall label by integer a and b satisfying $0\leqslant a,b\leqslant 3$ and $a+b=3$. These terms are

$$s_n^{(a,b)}(z_1,z_2)=\frac{\kappa_4}{6n^3}\sum_{j,m=1}^{n}\mathbf{E}\{D_{mj}^{a}G_{jm}(z_1)D_{mj}^{b}g_n^C(z_2)\}.$$

First estimate $s_n^{(3,0)}(z_1,z_2)$. After differentiating it takes the form

$$s_n^{(3,0)}(z_1,z_2)=-n^{-2}\kappa_4\mathbf{E}\left\{n^{-1}\sum_{j,m=1}^{n}G_{jm}^4(z_1)g_n^C(z_2)+6h_n(z_1)g_n^C(z_2)\right\}-n^{-1}\kappa_4\mathbf{E}\{d_n^2(z_1)g_n^C(z_2)\}.\tag{IV.55}$$

($h_n(z)$ and $d_n(z)$ are defined in Eqs. (III.42) and (III.39), respectively). As follows from Eqs. (II.24) and (III.41), the mean value in the rhs of the equation above is $O(n^{-1})$, so

$$s_n^{(3,0)}(z_1,z_2)=-n^{-1}\kappa_4\mathbf{E}\{d_n^2(z_1)g_n^C(z_2)\}+O(n^{-3}).$$

Now we employ the obvious algebraic relation (in the below sub-index C indicates the subtracted mean value)

$$\mathbf{E}\{\eta^2\xi^C\}=2\mathbf{E}\{\eta^C\xi^C\}\mathbf{E}\{\eta\}+\mathbf{E}\{(\eta^C)^2\xi^C\}\tag{IV.56}$$

and write $\mathbf{E}\{d_n^2(z_1)g_n^C(z_2)\}$ as

$$2\mathbf{E}\{d_n^C(z_1)g_n^C(z_2)\}\mathbf{E}\{d_n(z_1)\}+\mathbf{E}\{[d_n^C(z_1)]^2g_n^C(z_2)\}.$$

If $z\in U_0$, variances of $g_n(z)$ and $d_n(z)$ are of order n^{-2}. In addition to this, $d_n(z)$ is bounded in absolute value by $C|\Im z|^{-2}$ for all realizations of W_{jk}. Therefore by the Cauchy–Schwarz inequality, $\mathbf{E}\{d_n^2(z_1)g_n^C(z_2)\}=O(n^{-2})$, provided $z_1,z_2\in U_0$. Thus we have proved that $s_n^{(3,0)}(z_1,z_2)=O(n^{-3})$. A similar argument shows that $s_n^{(0,3)}(z_1,z_2)$ and $s_n^{(2,1)}(z_1,z_2)$ are $O(n^{-3})$, too. The last term we need to estimate is $s_n^{(1,2)}(z_1,z_2)$. It is easy to see that

$$s_n^{(1,2)}(z_1,z_2)=n^{-1}2\kappa_4\mathbf{E}\left\{n^{-1}\sum_{m=1}^{n}G_{mm}(z_1)G_{mm}(z_2)\right\}\mathbf{E}\left\{n^{-1}\sum_{j,m=1}^{n}G_{mm}(z_1)G_{jm}^2(z_2)\right\}+O(n^{-3}).$$

Mean values in the above are calculated in exactly the same way as $\mathbf{E}\{c_n(z)\}$ and $\mathbf{E}\{d_n(z)\}$ have been done. For large n:

$$n^{-1}2\kappa_4\mathbf{E}\left\{n^{-1}\sum_{m=1}^{n}G_{mm}(z_1)G_{mm}(z_2)\right\}=r(z_1)r(z_2)+O(n^{-1/2})$$

and

$$\mathbf{E}\left\{n^{-1}\sum_{j,m=1}^{n}G_{mm}(z_1)G_{jm}^2(z_2)\right\}=r(z_1)r^2(z_2)+O(n^{-1})$$

(compare with Eqs. (III.48) and (III.50)). Thus we conclude that the contribution of third derivatives is

$$-\frac{1}{n^2}\frac{\sigma r^2(z_1)r^3(z_2)}{1-w^2r^2(z_2)}, \tag{IV.57}$$

Eq. (II.17) (we recall using σ for κ_4).

First derivatives in the rhs of Eq. (IV.54) contribute to $z_1F_n(z_1,z_2)$ the term

$$\begin{aligned}t_n(z_1,z_2)=&-w^2\mathbf{E}\{g_n^2(z_1)g_n^C(z_2)\}-n^{-1}w^2\mathbf{E}\{c_n(z_1)g_n^C(z_2)\}\\&-n^{-2}2w^2\mathbf{E}\{n^{-1}\operatorname{tr}(H-z_1I)^{-1}(H-z_2I)^{-2}\}.\end{aligned} \tag{IV.58}$$

By the resolvent identity (II.19)

$$(H-z_1I)^{-1}(H-z_2I)^{-1}=(z_1-z_2)^{-1}[(H-z_1I)^{-1}-(H-z_2I)^{-1}].$$

Thus one reduces $\mathbf{E}\{n^{-1}\operatorname{tr}(H-z_1I)^{-1}(H-z_2I)^{-2}\}$ to

$$(z_1-z_2)^{-1}[(z_1-z_2)^{-1}\mathbf{E}\{g_n(z_1)-g_n(z_2)\}-\mathbf{E}\{c_n(z_2)\}].$$

Now recalling Eqs. (III.46), (III.48) and (II.30),

$$\mathbf{E}\{n^{-1}\operatorname{tr}(H-z_1I)^{-1}(H-z_2I)^{-2}\}=\frac{1}{r(z_1)[1-w^2r^2(z_2)]}\left[\frac{r(z_1)-r(z_2)}{z_1-z_2}\right]^2+O(n^{-1}). \tag{IV.59}$$

Clearly, $\mathbf{E}\{c_n(z_1)g_n^C(z_2)\}=\mathbf{E}\{c_n^C(z_1)g_n^C(z_2)\}$ and the corresponding summand on the rhs of Eq. (IV.58) is $O(n^{-3})$. So it remains to find $\mathbf{E}\{g_n^2(z_1)g_n^C(z_2)\}$.

Use Eq. (IV.56) to write

$$\mathbf{E}\{g_n^2(z_1)g_n^C(z_2)\}=2F_n(z_1,z_2)m_n^{(1)}(z_1)+\mathbf{E}\{[g_n^C(z_1)]^2g_n^C(z_2)\}=2F_n(z_1,z_2)m_n^{(1)}(z_1)+O(n^{-5/2}). \tag{IV.60}$$

The latter equality uses $\mathbf{E}\{[g_n^C(z_1)]^2g_n^C(z_2)\}=O(n^{-5/2})$, the bound which can be obtained following calculations of Appendix B.

Now we are in a position to find the leading order of $F_n(z_1,z_2)$. Collecting Eqs. (IV.57)–(IV.60), we find that

$$\begin{aligned}z_1F_n(z_1,z_2)=&-2w^2F_n(z_1,z_2)m_n^{(1)}(z_1)-\frac{1}{n^2}\frac{\sigma r^2(z_1)r^3(z_2)}{1-w^2r^2(z_2)}\\&-\frac{2w^2}{r(z_1)[1-w^2r^2(z_2)]}\left[\frac{r(z_1)-r(z_2)}{z_1-z_2}\right]^2+O(n^{-5/2}).\end{aligned}$$

As it is clear from Eqs. (III.46) and (II.30),

$$[z_1+2w^2m_n^{(1)}(z_1)]^{-1}=-r(z_1)[1-w^2r^2(z_1)]^{-1}+O(n^{-1})$$

and we end up with Eq. (IV.52).

The standard truncation technique of probability theory allows us to prove Eq. (IV.52) in the case when only the fifth absolute moment of the random variables W_{jk} is uniformly bounded. Calculations using the truncation technique are similar to those used in next section in proof of Theorem 3 and we omit them. Theorem 2 is proved.

One can consider the covariance function $F_n(z_1,z_2)$ for the Wigner ensemble of random Hermitian matrices (see remark 3 after the statement in Theorem 3 in the next section). Repeating almost literally calculations used in the proof of Theorem 2, one can prove that for the Wigner ensemble of Hermitian matrices Eq. (IV.52) is still valid. The only difference is that now $f(z_1,z_2)$ is given by the rhs of Eq. (I.15) multiplied by factor 1/2.

V. GAUSSIAN FLUCTUATIONS OF THE CENTRALIZED TRACE OF THE RESOLVENT

In this section we prove the statement which is analogous to the central limit theorem in the same sense in which the result Eq. (I.11) is analogous to the law of large numbers. Indeed, we can rewrite (I.11) as following limiting relation

$$\lim_{n\to\infty}\frac{1}{n}\sum_{m=1}^{n}G_{mm}=r(z) \tag{V.61}$$

valid with probability 1. Since the lhs here has the form of the arithmetic (Cesaro) mean, this relation is obviously similar to the strong law of large numbers (or more generally to the ergodic theorem). Common wisdom of probability and ergodic theory suggests that Eq. (V.61) should imply that the probability distribution of the random variable

$$n^{1/2}\left[n^{-1}\sum_{m=1}^{n}(G_{mm}-\mathbf{E}\{G_{mm}\})\right]=n^{1/2}[g_n(z)-\mathbf{E}\{g_n(z)\}] \tag{V.62}$$

has the Gaussian form in the limit $n=\infty$. We prove that under rather natural conditions on W_{jk} this is indeed the case provided that we use non-standard normalization, replacing $n^{1/2}$ in Eq. (V.62) by n, i.e., we consider just the centralized trace of the resolvent

$$\gamma^{(n)}(z)=\sum_{m=1}^{n}(G_{mm}-\mathbf{E}\{G_{mm}\})=ng_n(z)-\mathbf{E}\{ng_n(z)\} \tag{V.63}$$

instead of $n^{1/2}\gamma^{(n)}(z)$. This normalization can of course be anticipated from the formula (I.14) giving the order of magnitude (in fact, the asymptotics) of the variance of $g_n(z)$. This decay of the variance, which is ''twice'' as strong than in the standard central limit theorem setting, is rather typical for a number of problems of the theory of disordered systems with non-local interaction and is known as the strong self-averaging property (see e. g. Refs. 28 and 33).

Theorem 3: *Consider the Wigner ensemble of random real symmetric matrices with independent entries defined by Eqs. (I.2)–(I.3) assuming additionally that the fourth moments of W_{jk} exist and are independent of j and k and that the probability distribution functions $P_{jk}(w)$ of W_{jk} satisfy the condition: for any fixed $\nu>0$*

$$\lim_{n\to\infty}\frac{1}{n^2}\sum_{j\leqslant k}\int_{|x|>\nu n^{1/2}}x^4d\ \mathrm{Prob}[W_{jk}\leqslant x]=0. \tag{V.64}$$

Then for any z from $U_0=\{z \in \mathbf{C}_\pm : |\Im z| \geqslant 2w\}$ *the random function* $\gamma^{(n)}(z)$ *[Eq. (V.63)] converges in distribution as* $n\to\infty$ *to the Gaussian random function* $\gamma(z)$ *with zero mean and the covariance function* $f(z_1,z_2)$ *given by Eq. (I.15). In other words, for any integer q and arbitrary collection* $z_1,\ldots,z_q$ *of complex numbers from* U_0 *the joint probability distribution of random variables* $\gamma^{(n)}(z_1),\ldots,\gamma^{(n)}(z_q)$ *converges as* $n\to\infty$ *to the q-dimensional Gaussian distribution with zero mean and the covariance matrix* $[f(z_s,z_t)]_{s,t=1}^q$.

Remarks:

1. Limit theorems concerning $\gamma^{(n)}(z)$ for the Wigner ensemble were established for the first time by Girko (see Ref. 24 and references therein) under the assumption that there exist a positive δ such that

$$\sup_{j\leqslant k}\mathbf{E}|W_{jk}|^{4+\delta}<\infty, \tag{V.65}$$

which is slightly more restrictive than Eq. (V.64). For example in the case of identically distributed W_{jk}, Eq. (V.64) is obviously satisfied if $w_4\equiv\mathbf{E}\{W_{jk}^4\}$ is finite. However, in our opinion, the more important improvement of the result of Ref. 24 is that we calculate the covariance matrix of the limiting Gaussian process in the explicit form while in Ref. 24 this matrix was given in the implicit form as a solution of a system of cumbersome partial differential equations.

2. For the random variables W_{jk} satisfying Eq. (V.65) we can estimate the rate of convergence:

$$\sup_{z_1,z_2\in U_0}|\mathbf{E}\{\gamma^{(n)}(z_1)\gamma^{(n)}(z_2)\}-f(z_1,z_2)|=O(n^{-\delta/2}). \tag{V.66}$$

3. Consider the Wigner ensemble of the $n\times n$ random Hermitian matrices defined as in Eq. (I.2) with $W_{jk}=A_{jk}+iB_{jk}, j\leqslant k$, $W_{jk}=W_{kj}^\dagger$ where A_{jk} and B_{jk} are mutually independent random variables with zero mean, variance $w^2/2$ and excess $\sigma/2$. It can be proved by analogous technique that in this ensemble the fluctuations of the trace of the resolvent around its mean become Gaussian in the limit $n\to\infty$. The corresponding covariance function is given by Eq. (I.15) in which the factor 2 is replaced by 1 in the denominator of both terms.

Proof: We shall work with real-valued variables $\alpha^{(n)}(z)=\Re\gamma^{(n)}(z)$ and $\beta^{(n)}(z)=\Im\gamma^{(n)}(z)$. Then we have to prove that the limiting random functions $\alpha(z)$ and $\beta(z)$ are jointly Gaussian, i.e. if

$$X(z,c)=\begin{cases}\alpha(z) & \text{if } c=\alpha;\\ \beta(z) & \text{if } c=\beta,\end{cases}$$

and

$$(a(c),b(c))=\begin{cases}(1/2,1/2) & \text{if } c=\alpha;\\ (1/2i,1/2i) & \text{if } c=\beta,\end{cases}$$

then $\mathbf{E}\{X(z,c)\}=0$ and for any integer q and arbitrary collections $z_s, s=1,\ldots,q$, $z_s\in U_0$ and $c_s, s=1,\ldots,q$, $c_s\in\{\alpha,\beta\}$ the joint probability distribution of random variables $X(z_1,c_1),\ldots,X(z_q,c_q)$ is the q-dimensional Caussian distribution with zero mean and covariance matrix

$$\begin{aligned}\mathbf{E}\{X(z_s,c_s)X(z_t,c_t)\}=&a(c_s)a(c_t)f(z_s,z_t)+a(c_s)b(c_t)f(z_s,z_t^\dagger)\\&+a(c_t)b(c_s)f(z_s^\dagger,z_t)+b(c_s)b(c_t)f(z_s^\dagger,z_t^\dagger),\end{aligned} \tag{V.67}$$

Let us consider the characteristic function of random variables $X(z_1,c_1),..,X(z_q,c_q)$ which we shall write in the form

$$e_q^{(n)}(T_q,C_q,Z_q)=\mathbf{E}\prod_{s=1}^{q}\exp\{i\tau_s[a(c_s)\gamma^{(n)}(z_s)+b(c_s)\gamma^{(n)}(z_s^\dagger)]\},$$

where $T_q=(\tau_1,\ldots,\tau_q)$, $C_q=(c_1,\ldots,c_q)$, $Z_q=(z_1,\ldots,z_q)$

Recall that we designate the complex conjugate by the symbol an asterisk. Also writing the characteristic function we shall often omit indices indicating its dependence on n and some other variables provided no confusion will arise.

Obviously

$$\frac{\partial}{\partial\tau_s}\mathbf{E}\{e_q(T_q)\}=i\mathbf{E}\{e_q[a(c_s)\gamma^{(n)}(z_s)+b(c_s)\gamma^{(n)}(z_s^\dagger)]\}.$$

Our aim is to show that there exists a set of ''covariance'' coefficients $A_{st}^{(n)}$ $s,t=1,\ldots,q$ such that for each fixed T_q

$$\lim_{n\to\infty}\left|\mathbf{E}\{e_q^{(n)}[a_s\gamma^{(n)}(z_s)+b_s\gamma^{(n)}(z_s^\dagger)]\}-i\sum_{t=1}^{q}\tau_sA_{st}^{(n)}\mathbf{E}\{e_q^{(n)}\}\right|=0,\quad z\in U_0,$$

to show that limits of all these coefficients exist

$$A_{st}=\lim_{n\to\infty}A_{st}^{(n)},\tag{V.68}$$

and correspond to the rhs of Eq. (V.67). Then standard arguments will allow us to prove that the limit characteristic function has the Gaussian form $\exp(-1/2\Sigma_{s,t=1}^{q}A_{st}\tau_s\tau_t)$.

Thus, we have to compute

$$\mathbf{E}\{e_q\gamma^{(n)}(z)\}=\sum_{j=1}^{n}\mathbf{E}\{e_q^C(Z_q)G_{jj}\},$$

for large n (we recall that the sub-index C indicates centering to zero mean). Then putting one of $z_1,\ldots,z_q$ or one of their conjugates in place of z we calculate the limits in Eq. (V.68).

We have complex energies $z,z_1,\ldots,z_q$ and we introduce the notation $G(z_s)$ for the resolvent corresponding to z_s keeping the notation G for the resolvent corresponding to z.

By the resolvent identity Eq. (II.20),

$$\sum_{j=1}^{n}\mathbf{E}\{e_q^CG_{jj}\}=z^{-1}\sum_{j,m=1}^{n}\mathbf{E}\{e_q^CG_{jm}H_{mj}\}.\tag{V.69}$$

We compute the average in the rhs of Eq. (V.69) following the scheme described in Section II. However its direct application requires too strong conditions on the distribution of W_{jk}. Thus, we modify slightly the general scheme and carry out more accurate estimates.

Denote by $\mathbf{E}_{mj}$ the conditional expectation $\mathbf{E}\{\cdot\,|W_{mj}=w\}$ and rewrite the right-hand side of Eq. (V.69) in the form

$$z^{-1}n^{-1/2}\sum_{j,m=1}^{n}\int\mathbf{E}_{mj}\{e_q^CG_{jm}\}w\,dP_{mj}(w).$$

We split the integral into the two ones over sets $\Gamma_1(n)=\{\omega:|W_{mj}|\leqslant\delta n^{1/2}\}$ and $\Gamma_2(n)=\{\omega:|W_{mj}|>\delta n^{1/2}\}$. Now the inequalities

$$\left|n^{-1/2}\sum_{j,m=1}^{n}\int_{\Gamma_2(n)}\mathbf{E}_{mj}\{e_q^C G_{jm}\}wP_{mj}(w)\right|\leqslant\eta^{-1}n^{-1/2}\sum_{j,m=1}^{n}\int_{\Gamma_2(n)}|w|dP_{mj}(w)$$
$$\leqslant\eta^{-1}\nu^{-3}n^{-2}\sum_{j,m=1}^{n}\int_{\Gamma_2(n)}w^4dP_{mj}(w)$$

and the assumption (V.64) imply that only the integrals over $\Gamma_1(n)$ give a non-vanishing contribution to Eq. (V.69).

Following our general scheme, we expand the function $e_q^C G_{jm}$ in powers of random variable $H_{mj}=n^{-1/2}W_{mj}$ restricted to $\Gamma_1(n)$. Since it is bounded by absolute value by ν we can write the relation

$$n^{-1/2}\sum_{j,m=1}^{n}\int_{\Gamma_1}\mathbf{E}_{mj}\{e_q^C G_{jm}\}wdP_{mj}(w)=\sum_{k=1}^{5}S_k(n),\tag{V.70}$$

where

$$S_k(n)=n^{k/2}\sum_{j,m=1}^{n}\mathbf{E}[e_q^C G_{jm}]_{mj}^{(k-1)}\int_{\Gamma_1}w^kdP_{mj}(w),$$

and $[\ldots]_{mj}^{(k)}$ denotes that the kth derivatives with respect to H_{mj} are taken and then H_{mj} is replaced by zero. Let us note also that in S_5 the expression in square brackets is taken at some point $\widetilde{H}_{mj}\in(0,\nu)$.

The term $S_1(n)$ vanishes as $n\to\infty$ due to our assumption [Eq. (V.64)]:

$$|S_1(n)|\leqslant\left|n^{-1/2}\sum_{j,m=1}^{n}\mathbf{E}[e_q^C G_{jm}]_{mj}\int_{\Gamma_1}wdP_{mj}(w)\right|\leqslant\eta^{-1}\nu^{-3}n^{-2}\sum_{j,m=1}^{n}\int_{\Gamma_1}w^4dP_{mj}(w),$$

where $\eta\equiv|\Im z|$.

The term $S_5(n)$ vanishes as $n\to\infty$ because it can be estimated by

$$\frac{B_4(T_p)}{\eta^6n^{5/2}}\sum_{j,m=1}^{n}\int_{\Gamma_1}|w|^5dP_{mj}(w)\leqslant\frac{B_4(T_p)\nu}{\eta^6n^2}\sum_{j,m=1}^{n}\int_{\Gamma_1}w^4dP_{mj}(w),$$

where $B_4(T_p)$ is the upper bound of absolute value of the fourth derivative in Eq. (V.70). For any fixed T_p, $B_4(T_p)$ is finite and recalling Eq. (V.64) we see that $S_5(n)$ goes to zero as $n\to\infty$.

The term $S_3(n)$ also vanishes as $n\to\infty$. We establish this fact at the end of the proof.

The terms $S_2(n)$ and $S_4(n)$ give main contributions to Eq. (V.69). Let us first consider $S_2(n)$. The resolvents $G(z_s)$ and G are complex symmetric matrices and we have:

$$-\sum_{j,m=1}^{n}[e_q^C G_{jm}]_{mj}^{(1)}=[e_q^C G_{jj}G_{mm}]_{mj}+\sum_{j,m=1}^{n}[e_q^C G_{jm}^2]_{mj}+i\sum_{j,m=1}^{n}\left[\sum_{s=1}^{q}2\tau_s(a_s[G^2(z_s)]_{jm}\right.$$
$$\left.+b_s[G^2(z_s^\dagger)]_{jm})G_{jm}e_q\right]_{mj}.\tag{V.71}$$

Each term of the right-hand side of this relation is a function of H in which H_{mj} is replaced by zero and we have to come ''back'' to expressions dependent on the whole matrix H. To this end, we again use the resolvent identity but now in the ''opposite '' direction. We obtain for the first term of Eq. (V.71)

$$w^2 n^{-1} \sum_{j,m=1}^{n} \mathbf{E}\{[e_q^C G_{jj} G_{mm}]_{mj}\} = v^2 n^{-1} \sum_{j,m=1}^{n} \mathbf{E}\{e_q^C G_{jj} G_{mm}\} - w^2 \Psi^{(n)},$$

where

$$\begin{aligned}\Psi^{(n)} = {} & n^{-3/2} \sum_{j,m=1}^{n} \mathbf{E}\{[e_q^C G_{jj} G_{mm}]_{mj}^{(1)}\} \int_{\Gamma_1} w dP_{mj}(w) \\ & - 2^{-1} n^{-2} \sum_{j,m=1}^{n} \mathbf{E}\{[e_q^C G_{jj} G_{mm}]_{mj}^{(2)}\} \int_{\Gamma_1} w^2 dP_{mj}(w) \\ & - 6^{-1} n^{-5/2} \sum_{j,m=1}^{n} \mathbf{E}\{[e_q^C G_{jj} G_{mm}]^{(3)} W_{mj}^3\}.\end{aligned}$$

It is easy to see that the first and the last terms of $\Psi^{(n)}$ vanish as $n \to \infty$ due to our assumption (V.64).

Using Eqs. (V.64) and (III.37), we can rewrite the second term of $\Psi^{(n)}$ in the form

$$\frac{-2iw^2}{n^2} \sum_{j,m=1}^{n} \mathbf{E}\left[e_q \sum_{s=1}^{q} \tau_s (a_s [G^2(z_s)]_{mm} [G(z_s)]_{jj} + b_s [G^2(z_s^\dagger)]_{mm} [G(z_s^\dagger)]_{jj}) G_{jj} G_{mm} \right]_{mj} + \Phi^{(n)},$$

where the remainder $\Phi^{(n)}$ includes terms which have one or more factors G_{jm} or terms of the form

$$n^{-2} \sum_{j,m=1}^{n} \mathbf{E}\{[e_q^C [G(z_s)_{jj}]^2 [G(z_j)_{jj}]^2]_{mj}\}.$$

It is clear that in all these expressions we can remove square brackets $[\ldots]_{mj}$ because this procedure will add terms of order $O(n^{-1/2})$ to the sums under consideration. Using the estimate (III.41), taking into account the self-averaging property

$$\mathbf{E}|g_n^C(z)|^2 = o(n^{-1}), \text{ as } n \to \infty \tag{V.72}$$

(see Lemma 1 of Appendix B for the proof), and the relation

$$\lim_{n\to\infty} \mathbf{E} \left| \left(n^{-1} \sum_j G_{jj}^{\alpha} G_{jj}^{\beta} n^{-1} \sum_j G_{mm}^{\mu} G_{mm}^{\nu} \right)^C \right| = 0 \tag{V.73}$$

with some $\alpha, \beta, \mu, \nu = 0,1,2$ (Lemma 2 of Appendix B), it is easy to prove that $\Phi^{(n)}$ also vanishes as $n \to \infty$.

We finally obtain that among terms coming from the first summand in the right-hand side of Eq. (V.71) only the following

$$w^2 z^{-1}\mathbf{E}\left\{ e_q^C \sum_{j=1}^{n} G_{jj} \right\} g_n(z) - \frac{-2iw_4}{n^2}\mathbf{E}\{e_q\}\sum_{s=1}^{q} \tau_s \mathbf{E}\left\{ \sum_{j,k=1}^{n} (a_s [G^2(z_s)]_{mm}[G(z_s)]_{jj} \right.$$

$$\left. + b_s [G^2(z_s^\dagger)]_{mm}[G(z_s^\dagger)]_{jj}) G_{jj} G_{mm} \right\} \tag{V.74}$$

does not vanish as $n \to \infty$.

The second summand in the rhs of Eq. (V.71) vanishes as $n \to \infty$. This becomes clear after applying the same procedure of removing square brackets $[\dots]_{mj}$ to the expression $n^{-2}\Sigma_{j,m=1}^{n}[e_q^C (G_{jm})^2]_{mj}^{(k)}$ and using the estimates (III.41) and (V.73).

Let us consider the contribution of the last summand in the rhs of Eq. (V.71) for a fixed parameter $z_s, s=1,\dots,q$. Taking into account Eq. (V.64) and repeating the ''returning'' procedure, we obtain for this term

$$\begin{aligned} n^{-1}\sum_{j,m=1}^{n} [[G^2(z_s)]_{jm} G_{mj} e_q]_{mj} = n^{-1}\sum_{j,m=1}^{n} [G^2(z_s)]_{jm} G_{mj} e_q \\ - n^{-3/2}\sum_{j,m=1}^{n} [[G^2(z_s)]_{jm} G_{mj} e_q]_{mj}^{(1)} \int_{\Gamma_1} w dP_{mj}(w) \\ - n^{-2}\sum_{j,m=1}^{n} [[G^2(z_s)]_{jm} G_{mj} e_q]_{mj}^{(2)} \int_{\Gamma_1} w^2 dP_{mj}(w) \\ - n^{-5/2}\sum_{j,m=1}^{n} \mathbf{E}\{[[G^2(z_s)]_{jm} G_{mj} e_q]^{(3)} W_{mj}^3\}. \end{aligned}$$

It is easy to see that in this equality terms with the first and the third derivatives vanish as $n \to \infty$. The second derivative gives

$$2[\{[G^2(z_s)]_{jj} G_{jj} G_{mm} G_{mm} + [G^2(z_s)]_{mm} G_{mm} [G(z_s)]_{jj} G_{jj}\} e_q]_{mj}$$

and 24 terms having a factor of the form $(G^\alpha)_{jm}, \alpha = 1,2$. Omitting brackets $[\dots]_{mj}$ and using Eqs. (V.72)–(V.73), we see that the last term of Eq. (V.71) gives the leading contribution

$$\begin{aligned} \mathbf{E}\{e_q^C\}\sum_{s=1}^{q} \tau_s \mathbf{E}\{a_s n^{-1} \operatorname{tr} G^2(z_s) G + b_s n^{-1} \operatorname{tr} G^2(z_s^\dagger) G\} - iw_4 \mathbf{E}\{e_q^C\} \\ \times \sum_{s=1}^{q} \tau_s \mathbf{E}\left\{ n^{-2}\sum_{j,m=1}^{n} (a_s [G^2(z_s)]_{jj}[G(z_s)]_{mm} + b_s [G(z_s)]_{jj}[G^2(z_s)]_{mm}) G_{jj} G_{mm} \right\}. \end{aligned} \tag{V.75}$$

Consider now the term $S_4(n)$ of Eq. (V.70). The third derivative $[e_q^C G_{jm}]_{mj}'''$ consists of 140 terms. One part of them vanishes as $n \to \infty$ due to the properties (V.72)–(V.73), another part — due to the presence of the factor of the form $(G^\alpha)_{jm}, \alpha = 1,2,3$. Only six terms of the form

$$iw_4 \sum_{s=1}^{q} \mathbf{E}\{e_q^C\}\mathbf{E}\left\{ n^{-2}\sum_{j,m=1}^{n} (a_s [G^2(z_s)]_{jj}[G(z_s)]_{mm} + b_s [G(z_s)]_{jj}[G(z_s)^2]_{mm}) G_{jj} G_{mm} \right\}$$

are non-vanishing in the limit $n\to\infty$. These terms arise when we differentiate G_{jm} once and e_q twice with respect to H_{mj}. Combining these terms with Eqs. (V.74) and (V.75), we finally obtain that

$$\mathbf{E}\{e_q^C \text{ tr } G\} = i\frac{1}{z-2w^2 g_n(z)}\mathbf{E}\{e_q^C\}\sum_{s=1}^{q}\tau_s\Bigg(2w^2 n^{-1}\mathbf{E}\{\text{ tr }(a_s G(z_s)^2 + b_s G(z_s^\dagger)^2)G\} + 2\sigma\mathbf{E}\Bigg\{n^{-2}\sum_{j,m=1}(a_s G^2(z_s)_{jj}G(z_s)_{mm} + b_s G^2(z_s^\dagger)_{jj}G(z_s^\dagger)_{mm})G_{jj}G_{mm}\Bigg\}\Bigg). \tag{V.76}$$

Notice, that the denominator in the first term of the rhs of this expression is bounded away from zero because z belongs to the domain (II.22). Now, combining Eqs. (I.11) and (I.10) with relations

$$\lim_{n\to\infty}\mathbf{E}\Bigg\{n^{-1}\sum_{j=1}^{m}[G^2(z_s)]_{jj}G_{jj}\Bigg\} = r^2(z_s)[1-w^2 r^2(z_s)]^{-1}r(z), \tag{V.77}$$

we derive from Eq. (V.76) the final form of the covariance.

Relation (V.77) can be easily deduced from our proof of Eqs. (V.72)–(V.73).

Let us briefly discuss now the proof of the fact that $S_3(n)$ of Eq. (V.70) vanishes as $n\to\infty$. The second derivative $[e_q^C G_{jm}]_{mj}^{(2)}$ gives terms each having the factor of the form $[(G^\alpha)_{jj}(G^k)_{jm}(G^\beta)_{mm}]_{mj}$. The brackets can be simply omitted because the ''returning'' procedure adds terms of order $O(n^{-1/2})$. Now, regarding $n^{-1/2}(G^\alpha)_{jj}$ as vectors and $(G^m)_{mj}$ as the kernel, we can write inequality

$$\Bigg|n^{-3/2}\sum_{j,m=1}^{n}(G^\alpha)_{jj}(G^m)_{mj}(G^\beta)_{mm}\Bigg| \leqslant \eta^{-\alpha-\beta-m}n^{-1/2}$$

which completes the proof of Theorem 3.

VI. SCALING LIMIT AND UNIVERSALITY CONJECTURE

We have presented above the rigorous derivation of asymptotic corrections (in fact expansions) for moments and more complex quantities constructed from the traces of the Green functions of the Wigner random matrix ensembles. Now we use our result to draw certain non-rigorous conclusions on the form of the leading term of the correlation function $S_n(E_1,E_2)$ of the formal level density $\rho_n(E)=n^{-1}\text{ tr }\delta(H-EI)$. Since $\rho_n(E)=N_n'(E)$ where $N_n(E)$ is defined in Eq. (I.4), then based on the relation (I.7) one can conclude that the number of eigenvalues lying inside the interval (E_1,E_2) with the center at E will be $N(E_2)-N(E_1)\sim n\rho_n(E)(E_2-E_1)$, i.e. that the mean distance between levels is $[n\rho_n(E)]^{-1}$. Thus the scaling $E_2-E_1=O(n^{-1})$ defines the microscopic or local regime in which one deals with a finite numbers of eigenvalues.[1,11]

Consider the density–density correlation function

$$S_n(E_1,E_2)=\mathbf{E}\{\rho_n(E_1)\rho_n(E_2)\}-\mathbf{E}\{\rho_n(E_1)\}\mathbf{E}\{\rho_n(E_2)\}. \tag{VI.78}$$

By using Eqs. (I.8) and (I.9) we obtain from Eqs. (I.14) and (V.63) that the Stieltjes transform of $S_n(E_1,E_2)$

$$F_n(z_1,z_2)=\int\int\frac{S_n(E_1,E_2)}{(E_1-z_1)(E_2-z_2)}dE_1dE_2, \quad \Im z_i\neq 0$$

is

$$F_n(z_1,z_2)=n^{-2}\mathbf{E}\{\gamma^{(n)}(z_1)\gamma^{(n)}(z_2)\}.$$

It follows from the inversion formula for the Stieltjes transform $f(z)=\int(E-z)^{-1}\rho(E)dE$

$$\rho(E)=\pi^{-1}\lim_{\epsilon\downarrow 0}\Im f(E+i\epsilon)\equiv I_{E_1}\{f(z)\} \tag{VI.79}$$

that to find $S_n(E_1,E_2)$, one has to know $F_n(z_1,z_2)$ up to the real axis in both variables because

$$S_n(E_1,E_2)=I_{E_1}\circ I_{E_2}\{F_n(z_1,z_2)\}. \tag{VI.80}$$

On the other hand, we have found the form (I.14) and (I.15) of $F_n(z_1,z_2)$ only in the domain $|\Im z|\geqslant 2w$. However, since the function $f(z_1,z_2)$ given by Eq. (I.15) can obviously be continued up to the real axis with respect to the both variables z_1 and z_2 we can apply to the first term of Eq. (I.14) the operation $I_{E_1}I_{E_2}$, $E_1\neq E_2$ to compute formally the ''leading'' term of the density–density correlation function. This means that we perform first the limit $n\to\infty$ and then the limits $\epsilon_1,\epsilon_2\downarrow 0$. This order of limiting transitions is inverse with respect to that prescribed by the definition of this correlation function.

To make these computations, we use the identity

$$\frac{r_1-r_2}{z_1-z_2}=\frac{r_1r_2}{1-w^2r_1r_2}$$

which follows from Eq. (I.10) or Eq. (II.30). The identity yields the relations $\varepsilon|r(E+i\varepsilon)|^2=\Im r(E+i\varepsilon)(1-w^2|r(E+i\varepsilon)|^2)$ and $|r(E+i0)|^2=w^{-2}$ for E such that $\Im r(E+i0)>0$. Combining these relations with Eq. (I.5), we obtain that

$$w^2[\Re r(E+i0)]^2=\frac{E^2}{4w^2}\quad\text{and}\quad w^2[\Im r(E+i0)]^2=1-\frac{E^2}{4w^2}.$$

Using these equalities, we derive from our results (I.14) and (I.15) and from Eqs. (VI.79) and (VI.80) that

$$\begin{aligned}S_n(E_1,E_2)=&-\frac{1}{\beta\pi^2[n(E_1-E_2)]^2}\,\frac{4w^2-E_1E_2}{(4w^2-E_1^2)^{1/2}(4w^2-E_2^2)^{1/2}}\\&+\frac{\sigma}{2n^2\pi^2w^8}\,\frac{(2w^2-E_1^2)(2w^2-E_2^2)}{(4w^2-E_1^2)^{1/2}(4w^2-E_2^2)^{1/2}}\end{aligned} \tag{VI.81}$$

with $\beta=1$. It can be shown that for the Hermitian matrices with independent entries (see Remark 3 to Theorem 3) the density–density correlator has the same form with $\beta=2$. For the Gaussian orthogonal and unitary ensembles (GOE and GUE) $\sigma=0$, and we recover the result

$$S_n(E_1,E_2)=-\frac{1}{\beta\pi^2[n(E_1-E_2)]^2}\,\frac{4w^2-E_1E_2}{(4w^2-E_1^2)^{1/2}(4w^2-E_2^2)^{1/2}}$$

obtained in Ref. 34 and Ref. 35.

We see that in a general non-Gaussian case the respective expression depends not only on the second moment of entries, but also on their fourth moment via the excess σ.

The remarkable fact is that this dependence vanishes in the microscopic (also called the scaling) limit

$$E_1, E_2 \to E, \quad n(E_2 - E_1) \to s. \tag{VI.82}$$

Indeed, it easy to see that in this limit we obtain from Eq. (VI.81) a very simple expression:

$$\lim_{n(E_2-E_1)\to s} S_n(E_1, E_2) = -\frac{1}{\beta \pi^2 s^2}. \tag{VI.83}$$

According to Wigner and Dyson (see, e.g., Ref. 1), the exact large-s asymptotics for the limiting correlation function of the Gaussian ensembles are: $-1/(\pi^2 s^2)$ (GOE) and $-\sin^2 \pi\rho(E)s/(\pi^2 s^2)$ (GUE). Comparing these expressions with our results, we see that the procedure of computing the correlation function yields for the general case the expression coinciding with the large-s asymptotics of the Gaussian ensembles correlation function smoothed over energy intervals whose length is much smaller than the macroscopic scale $w = \mathbf{E}\{W^2\}^{1/2}$ but much bigger than the microscopic scale given by the mean level spacing $[n\rho(E)]^{-1}$. It is natural to think that in our computations the smoothing has been implemented ''automatically'' due to the non-zero imaginary part of the spectral parameter $\Im z_j$. We notice that the same procedure is widely used in the mesocsopic calculations based on the Kubo formula, weak disorder perturbation theory, etc.

The independence of the scaling limit expressions (VI.83) on the excess σ can be regarded as a support of the universality conjecture for the Wigner ensembles. Let us mention supports of this conjecture for other ensembles.

The first one[22] concerns the so-called sparse (or diluted) random matrices whose entries are independently distributed random variables such that $\Pr\{H_{k,l} = 0\} = p/n$. The authors of Ref. 22 used the Grassman integral technique and found the Wigner–Dyson universal form of the density–density correlator if p is large enough.

The second[36] concerns the ensemble $H = \Sigma_{\mu=1}^{p} \tau_\mu(\cdot, \xi^\mu)\xi^\mu$, where τ_μ and $\xi^\mu = \{\xi_1^\mu, \ldots, \xi_n^\mu\}$ are independent identically distributed random variables (the ensemble was introduced in Ref. 27). For this ensemble, whose entries are dependent random variables, the analogue of Eq. (VI.81) is obtained and it is shown that its scaling limit is the same as above.

The third follows from Appendix A below. We consider there the case of the deformed GOE (see definitions below). For this ensemble the analog of Theorem 3 was proved in Ref. 37. In the appendix we present a short derivation of the density–density correlator and show that in the scaling limit it has the form (VI.83).

We mention also that for the unitary invariant ensembles of the form (I.1) the universality conjecture is rigorously proved in Ref. 16 for a rather broad class of functions $F(x)$.

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APPENDIX A: SCALING LIMIT FOR THE DEFORMED GOE

In this Appendix we find the exact form of the leading term of the covariance function $F_n(z_1, z_2)$ [Eq. (I.14)] for the ensemble $H_d = H^{(0)} + H$, where $H^{(0)}$ are $n \times n$ nonrandom matrices such that there exists the ''unperturbed'' IDS

$$N^{(0)}(E) = \lim_{n\to\infty} n^{-1} \#\{e_j : e_j \text{ is an eigenvalue of } H^{(0)} \text{ and } e_j \leqslant E\}$$

and H belongs to the GOE (Eq. (I.1) with $F=x^2/4w^2$). This ensemble is called[2] the deformed GOE. Because of the orthogonal invariance of the GOE distribution, we can restrict our consideration to the case of diagonal $H^{(0)}$. So we assume that $H^{(0)}=[\delta_{jk}e_j]_{j,k=1}^n$ and real numbers e_j are such that the limit

$$g^{(0)}(z)=\lim_{n\to\infty}\frac{1}{n}\sum_{j=1}^{n}\frac{1}{e_j-z} \tag{A1}$$

exists for all non-real z. The function $g^{(0)}(z)$ is the Stieltjes transform of $N^{(0)}(E)$. We shall use the notation $d_j(z)$ for $(e_j-z)^{-1}$ and $g_n(z)$ for the normalized trace of the resolvent of H_d.

Subsequent arguments are quite similar to those used in derivation of Eqs. (II.24) and (II.26) –(II.29) for the GOE. By using Eqs. (II.17) and (II.19) for $H_1=H^{(0)}$ and $H_2=H_d$ one can derive the following two relations (analogues of Eqs. (II.26) and (II.27)) :

$$\mathbf{E}\{G_{jk}(z)\}=d_j(z)\,\delta_{jk}+\mathbf{E}\{g_n(z)G_{jk}(z)\}d_k(z)+n^{-1}\sum_m\mathbf{E}\{G_{jm}(z)G_{km}(z)\}d_k(z), \tag{A2}$$

and

$$\begin{aligned}\mathbf{E}\{g_n^C(z_1)G_{jj}(z_2)\}=&\,w^2\mathbf{E}\{g_n^C(z_1)G_{jj}(z_2)\}\mathbf{E}\{g_n(z_2)\}d_j(z_2)+w^2\mathbf{E}\{g_n^C(z_1)g_n^C(z_2)G_{jj}(z_2)\}d_j(z_2)\\&+w^2n^{-1}\mathbf{E}\{g_n^C(z_1)[G^2(z_2)]_{jj}\}d_j(z_2)\\&+2w^2n^{-2}\sum_m\mathbf{E}\{[G^2(z_1)]_{jm}G_{mj}(z_2)\}d_j(z_2).\end{aligned} \tag{A3}$$

It follows from Eq. (A2) that if for $z\in U_0$ where U_0 is defined in Eq. (II.22)

$$\lim_{n\to\infty}\mathbf{E}\{|g_n(z)-\mathbf{E}\{g_n(z)\}|\}=0, \tag{A4}$$

then $\lim_{n\to\infty}\mathbf{E}\{g_n(z)\}=g(z)$, where $g(z)$ is the unique solution of the functional equation[23]

$$g(z)=g^{(0)}(z+w^2g(z)) \tag{A5}$$

satisfying $\Im g(z)\Im z\geqslant 0$. In the equation above, $g^{(0)}(z)$ is given by Eq. (A1).

It is easy to show that Eqs. (A2) and (A4) imply the relation

$$\sup_{j=1,\ldots,n}|\mathbf{E}\{G_{jj}(z)\}-g_j^{(n)}(z)|=O(n^{-1}),\quad z\in U_0, \tag{A6}$$

where $g_j^{(n)}(z)$ solves the equations

$$g_j^{(n)}(z)=\frac{1}{e_j-z-w^2g^{(n)}(z)},\quad j=1,\ldots,n\quad g^{(n)}(z)=n^{-1}\sum_{m=1}^{n}g_m^{(n)}(z). \tag{A7}$$

Indeed, if $V_j^{(n)}=\mathbf{E}\{g_n^C(z_1)G_{jj}(z_2)\}$ then by Eq. (A3),

$$V_j^{(n)} = w^2 V_j^{(n)} \mathbf{E}\{g_n(z_2) d_j(z_2)\} + n^{-1} \sum_j V_j^{(n)} \mathbf{E}\{g_n(z_2) d_j(z_2)\}$$
$$+ 2w^2 n^{-2} \mathbf{E}\left\{ \sum_j [G^2(z_2)]_{jm} G_{mj}(z_2) d_j(z_2) \right\} + w^2 n^{-1} \mathbf{E}\{g_n^C(z_1)[G^2(z_2)]_{jj}\} d_j(z_2)$$
$$+ w^2 \mathbf{E}\{g_n^C(z_1) g_n^C(z_2)[G_{jj}(z_2)]^C\} d_j(z_2). \tag{A8}$$

Now, repeating arguments used at the end of Section II, we can easily obtain the estimate $n^{-1}\Sigma_j V_j^{(n)} = O(n^{-2})$ which proves Eq. (A6). Using this estimate and considering Eq. (A8) once more, we obtain the estimate

$$\sup_j |V_j^{(n)}| = O(n^{-2}). \tag{A9}$$

It follows from the resolvent identity (II.19) that

$$\sum_j [G^2(z_1)]_{jm} [G(z_2)]_{mj} = \frac{[G^2(z_1)]_{jj}}{z_1 - z_2} - \frac{[G(z_1)]_{jj} - [G(z_2)]_{jj}}{(z_1 - z_2)^2}.$$

Taking into account this relation, Eq. (A6), and Eq. (A9), we obtain that if

$$f_d(z_1, z_2) = \lim_{n \to \infty} n^2 \mathbf{E}\{g^C(z_1) g^C(z_2)\},$$

then

$$\left| n^{-1} \sum_j V_m^{(n)} - f_d(z_1, z_2) \right| = o(n^{-2}), \quad z \in U_0,$$

and as the result

$$f_d(z_1, z_2) = -\frac{2w^2}{(z_1 - z_2)^2} \lim_{n \to \infty} \frac{n^{-1} \Sigma_m [g_m^{(n)}(z_1) - g_m^{(n)}(z_2)] g_m^{(n)}(z_2)}{1 - w^2 n^{-1} \Sigma_j g_m^{(n)}(z_2)^2}$$
$$+ \frac{1}{z_1 - z_2} \lim_{n \to \infty} \frac{n^{-1} \Sigma_j [G^2(z_1)](z_1) g_m^{(n)}(z_2)}{(1 - w^2 n^{-1} \Sigma_j g_m^{(n)}(z_1)^2)(1 - w^2 n^{-1} \Sigma_j g_m^{(n)}(z_2)^2)}. \tag{A10}$$

Since $\lim_{n \to \infty} n^{-1} \Sigma_m \, g_m^{(n)}(z)^2 = \int (E - z - w^2 g_0(z))^{-2} dN_0(E) \equiv \Phi_2$, then the second fraction of the last term of Eq. (A10) is not singular for $z_i = E \pm i0$ with E such that $\Im g(E + i0) > 0$. Thus, this term vanishes in the scaling limit (VI.82).

Consider now the first term of the right-hand side of Eq. (A10). A simple computation shows that

$$n^{-1} \sum_m g_m^{(n)}(z_1) g_m^{(n)}(z_2) = \frac{g^{(n)}(z_1) - g^{(n)}(z_2)}{z_1 - z_2 + w^2 [g^{(n)}(z_1) - g^{(n)}(z_2)]}.$$

Since, according to Eqs. (A4)–(A7) $\lim_{n \to \infty} g^{(n)}(z) = g(z)$ we find for this term

$$-\frac{2w^2}{(z_1 - z_2)^2} \left(\frac{g_0(z_1) - g_0(z_2)}{z_1 - z_2 + w^2 [g_0(z_1) - g_0(z_2)]} - \Phi_2 \right) (1 - w^2 \Phi_2)^{-1} + O(|z_1 - z_2|^{-1}).$$

This relation implies that in the scaling limit (VI.82) we obtain again the simple universal expression (VI.83) .

APPENDIX B: AUXILIARY FACTS

Lemma 1: *Self-averageness property (V.72) holds under assumptions of Theorem 3.*
Proof: We denote

$$F_n(z,z')=\mathbf{E}\{g^C(g')^C\}\equiv\mathbf{E}\{g^Cg'\}, \tag{B1}$$

where $g\equiv g_n(z)$ and $g'\equiv g_n(z')$, $g_n(z)=n^{-1}\,\mathrm{tr}\,(H-zI)^{-1}$ and $g^C=g-\mathbf{E}\{g\}$.

Obviously, $G_{jj}(z^\dagger)=G^\dagger_{jj}(z)$ and $F_n(z,z^\dagger)=\mathbf{E}\{|g^C(z)|^2\}$.

Let us apply the resolvent identity (II.20) to the last factor g' on the right-hand side of Eq. (B1). We obtain the relation

$$F_n(z,z')=\frac{1}{z'n}\sum_{jm}\mathbf{E}\{g^CG'_{jm}H_{mj}\}, \tag{B2}$$

where $G'\equiv G(z')$. Comparing relations (B2) and (V.69), we see that their right-hand sides are similar. The only difference is that the sum in Eq. (B2) has an extra factor n^{-1} and e_q of Eq. (V.69) is replaced by g. Hence, one can compute the average in Eq. (B2) in the same way as it was done for the right-hand side of Eq. (V.69) and come to the expression $F_n(z,z')=\Sigma_{k=1}^5\,T_k(n)$, where $T_k(n)$ are similar to $S_k(n)$, $k=1,..,5$ in Eq. (V.70).

Thus we find that $T_1(n)$ and $T_3(n)$ are of order $o(n^{-1})$, as $n\to\infty$ just as in the case of $S_1(n)$ and $S_3(n)$.

Consider $T_5(n)$ which is analogous to $S_5(n)$ in Eq. (V.70). It contains four derivatives of $G_{kk}G_{jm}$ by H_{mj}. It follows from Eq. (III.37) that the result of differentiating includes at least one factor G_{jm}. Combining Eq. (III.41) with inequalities used to estimate $S_5(n)$, we easily derive that $T_5(n)$ is a quantity of order $O(n^{-3/2})$.

Let us estimate $T_4(n)$ acting in the same way as in the case of $S_4(n)$. As mentioned in Sec. V, the non-vanishing contribution to $S_4(n)$ comes from terms arising from one derivative of G'_{jm} and two derivatives of e_q. The rest of the terms are of order $o(1)$. Thus, in the corresponding terms of $T_4(n)$ we have to take into account only terms with factors G or G' having coincident arguments. It is easy to see that due to extra factor n^{-1} in front of the whole sum and factor n^{-1} in $g(z)$, these terms are of order n^{-2}. Thus, $T_4(n)$ is of order $o(n^{-1})$.

Turning to $T_2(n)$ and taking into account previous arguments, we arrive at the relation

$$F_n(z,z')=-\frac{w^2}{z'n^2}\sum_{j,m}\mathbf{E}\{g^CG'_{jj}G'_{mm}\}-\frac{w^2}{z'n^2}\sum_{j,m}\mathbf{E}\{g^CG'_{jm}G'_{jm}\}+\Phi'(z,z'), \tag{B3}$$

where $\Phi'(z,z')=o(n^{-1})$. Using Eq. (III.41), we easily obtain that

$$\frac{w^2}{n^2}\left|\sum_{j,m}\mathbf{E}\{g^CG'_{jm}G'_{jm}\}\right|\leqslant\frac{w^2}{n^2}\sum_j\mathbf{E}\left\{|g^C|\sum_m|G'_{jm}|^2\right\}\leqslant\frac{w^2}{n|\Im z'|^2}\mathbf{E}^{1/2}\{|g^C|^2\}.$$

Observing that

$$\mathbf{E}\{g^Cg'g'\}=2\mathbf{E}\{g^Cg'\}\mathbf{E}\{g'\}+\mathbf{E}\{g^C[g']^Cg'\},$$

we derive from Eq. (B3) that for $z'=z^\dagger$ and $z\in U_0$ [Eq. (II.22)]:

$$C_1F_n(z,z^\dagger)-C_2n^{-1}|F_n(z,z^\dagger)|^{1/2}-|\Phi'_n|\leqslant O,$$

where C_1 and C_2 are absolute constants (cf. Eq. (II.28)). This inequality implies Eq. (V.72). Lemma proved

Lemma 2: *Under assumptions of Theorem 3 the relation Eq. (V.73) is true.*

Proof: It suffices to show that

$$R_n \equiv \mathbf{E}\{|G_2^C|^2\} = o(1), \quad n \to \infty, \tag{B4}$$

where $G_2 \equiv n^{-1}\Sigma_j G_{jj}^2$. Repeating computations of previous proof, we obtain the following relation

$$R_n = \frac{1}{z'n}\sum_{j,m} \mathbf{E}\{G_2^C G'_{jj} G'_{jm} H_{mj}\}.$$

Comparing again the right-hand side of this equality with those of Eqs. (B2) and (V.69) and repeating the corresponding computation, we conclude that

$$R_n = -\frac{w^2}{z'n^2}\sum_{j,m} \mathbf{E}\{G_2^C G'_{jj} G'_{jj} G'_{mm}\} + \frac{w^2}{z'n^2}\sum_{j,m} \mathbf{E}\{G_2^C G'_{jj} G'_{jm} G'_{mm}\} + \Phi''_n, \tag{B5}$$

where $\Phi''_n = o(1)$ as $n \to \infty$ for $z' = z^\dagger$ and $|\Im z| > 0$. Taking into account Eq. (V.72), we derive from Eq. (B5) that for $z \in U_0$

$$C_3 R_n - C_3 R_n - n^{-1} C_4 |R_n|^{1/2} + o(1) \leqslant 0,$$

where C_3 and C_4 are some absolute constants (cf. Eq. (II.28)). This inequality implies Eq. (B4). Lemma is proved.

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Fictitious level dynamics: A novel approach to spectral statistics in disordered conductors

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We establish a new approach to calculating spectral statistics in disordered conductors, by considering how energy levels move in response to changes in the impurity potential. We use this fictitious dynamics to calculate the spectral form factor in two ways. First, describing the dynamics using a Fokker–Planck equation, we make a physically motivated decoupling, obtaining the spectral correlations in terms of the quantum return probability. Second, from an identity which we derive between two- and three-particle correlation functions, we make a mathematically controlled decoupling to obtain the same result. We also calculate weak localization corrections to this result, and show for two dimensional systems (which are of most interest) that corrections vanish to three-loop order. © *1996 American Institute of Physics.* [S0022-2488(96)01110-3]

I. INTRODUCTION

Numerous properties of quantum systems can be described in terms of their energy spectra. For complex systems an exact determination of energy levels is not feasible, and a statistical description becomes necessary. It turns out that the Wigner–Dyson (WD) statistics[1,2] of eigenvalues of random Hermitian matrices describes energy levels in a wide variety of different systems.[3] The joint distribution of eigenvalues is dominated by level repulsion and is universal in the sense that level correlations depend only upon the symmetry of the Hamiltonian while all specific properties of the system are absorbed into the mean level spacing, Δ. A very important feature of WD statistics is that — by construction of invariant ensembles of random matrices — spectral properties are independent of eigenstate correlations. In real systems such an independence can at best be approximate. It holds, however, in the ergodic regime where the entire phase space of a system is explored. If a non-ergodic regime is of interest, not only is WD statistics inapplicable but the whole concept of the independence of spectral and eigenstate correlations should be re-examined.

Disordered mesoscopic conductors present a natural ensemble for a statistical description - the ensemble of impurity configurations. In this case spectral statistics in the non-ergodic regime are very important for both transport and thermodynamic properties of electrons. Different regimes in disordered conductors are determined by the energy or time scale, as shown in Fig. 1. The ergodic regime involves energy level separations $\varepsilon \lesssim E_c \equiv \hbar/t_{\rm erg}$ where E_c is called the Thouless energy, and $t_{\rm erg} \sim D/L^2$ is the time required for the electronic diffusive motion, with diffusion constant D, to fill all phase space, in a sample of size L. The quantum limit of this regime corresponds to smaller energy separations, $\varepsilon \lesssim \Delta$, where Δ is the mean level spacing, and to longer times $t \gtrsim t_H$, where $t_H \equiv \hbar/\Delta$ is the Heisenberg time. Note that the ratio E_c/Δ is proportional to the dimensionless conductance g (i.e., the conductance measured in the units of $e^2/\hbar$), and is large in the metallic phase. The diffusive regime involves energies $\hbar/t_{\rm erg} \lesssim \varepsilon \lesssim \hbar/t_{\rm el}$, where $t_{\rm el}$ is the mean

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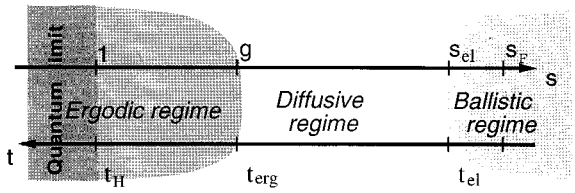

FIG. 1. Regimes of energy and time in a disordered metal; here $s_{\rm el}=\hbar/t_{\rm el}\Delta$ and $s_{_F}=\varepsilon_{_F}/\Delta$.

elastic-scattering time. The largest energies, $\hbar/t_{\rm el}\lesssim\varepsilon\lesssim\varepsilon_{_F}$, (where $\varepsilon_{_F}$ is the Fermi energy) and the shortest times, $t\lesssim t_{\rm el}$, correspond to the ballistic regime in which multiple scattering by impurities is irrelevant.

It was first conjectured by Gor'kov and Eliashberg[4] and then shown by Efetov[5] that spectral correlations in the ergodic regime are described by the random matrix theory (RMT) of Wigner and Dyson. Correlations in the non-ergodic diffusive regime which are important, in particular, for universal conductance fluctuations were analyzed by Altshuler and Shklovskii[6] at leading order in diagrammatic perturbation theory. Their results were later reproduced by Argaman *et al.*[7] within the semiclassical approach, using the diagonal approximation.

We have recently developed[8] an alternative approach to level statistics in the non-ergodic regime which takes into account the inevitable coupling between eigenvalue and eigenstate correlations, and can be extended beyond the region of validity of the perturbative technique. Our approach is based on the idea of parametric motion through the ensemble of disordered Hamiltonians: we treat the energy eigenvalues as particles with fictitious dynamics induced by changing some parameter of the Hamiltonian. This dynamics takes the form of Brownian motion in a fictitious time τ related to the parameter being changed. Originally, this idea was employed by Dyson[9] in the context of RMT. Later, in the context of the semiclassical description, Pechukas[10] used motion along a smooth path in the space of Hamiltonians to generate fictitious dynamics of a different kind. Both Dyson and Pechukas were interested in level dynamics primarily as a way of generating the level distribution. In contrast, a number of recent authors,[11] notably Szafer, Simons and Altshuler,[12,13] have investigated the dynamical problem in its own right, calculating parametric statistics: eigenvalue correlations as a function of position in the space of Hamiltonians.[14] In distinction to our approach, eigenfunction correlations have played no role in previous work,[11–15] an assumption justified only for the ergodic regime.

We have found[8] that a treatment based on Brownian motion through the ensemble of Hamiltonians provides a unified description of all regimes in disordered conductors, except the quantum limit ($t\gtrsim t_{_H}$, or $E\lesssim\Delta$), which is also beyond the scope of diagrammatic and semiclassical approaches. The main result is a new relation explicitly linking the spectral correlation function to the quantum return probability for an expanding wavepacket which, in turn, is related to a certain eigenfuction correlator. The derivation given in Ref. 8 has a limitation: when obtaining a closed Langevin equation describing the Brownian motion, we make use of an uncontrolled, although physically transparent assumption. Thus, within the framework of that calculation it is not possible to establish exactly the region of validity and accuracy.

In this paper, we re-derive the relation between spectral and eigenstate correlation functions using a more explicit procedure: we decouple a certain exact relation between two- and three-level correlation functions using the Kirkwood superposition approximation. Then we examine the accuracy of this decoupling using perturbative diagrammatic techniques. Remarkably, it not only reproduces the results of the diagonal approximation[6,7] but holds well beyond it. We show this to third order in a perturbative expansion in g^{-1}, for two-dimensional systems with or without time-reversal symmetry. We are therefore encouraged to believe that the connection between spectral and eigenstate correlation functions should be useful rather generally, and especially for

problems where the usual diagrammatic technique cannot straightforwardly be applied, such as spectral statistics in the critical regime near the Anderson transition.

II. DEFINITIONS AND MAIN RESULTS

A convenient way to consider spectral correlations is to introduce fictitious level dynamics in response to changing some parameter λ of the Hamiltonian. Thus we parametrize the ensemble of Hamiltonians as follows;

$$H(\lambda)=H_0+\lambda W(\boldsymbol{r}). \tag{2.1}$$

Here both H_0 and $H(\lambda)$ belong to the same symmetry class, and the point $\lambda=0$ corresponds to some arbitrary choice of one of the many members of the same ensemble. We will specify the choice of H_0 and W in the next section.

We consider in this paper the two-level correlation function (TLCF) and its Fourier transform, the spectral form factor, in a disordered conductor described by the Hamiltonian equation (2.1). Let $E_n(\lambda)$ be the energy levels of $H(\lambda)$. We introduce the density of states per unit volume (DoS) as

$$\rho(E,\lambda)=\frac{1}{L^d}\sum_n \delta(E-E_n(\lambda)). \tag{2.2}$$

The mean level spacing, Δ, is then related to the mean DoS, $\rho\equiv\langle\rho\rangle$, by $\Delta=(\rho L^d)^{-1}$. The TLCF is defined as

$$R(s,\lambda)=\rho^{-2}\langle\rho(E+s\Delta,\lambda)\rho(E,0)\rangle-1\,, \tag{2.3}$$

where $\omega=s\Delta$ is the energy difference between two levels. The mean DoS is practically a constant in the entire energy region of interest (as it changes only at scale of order ε_F while we consider energy windows centered at ε_F of width not exceeding $\hbar/t_{\rm el}\ll\varepsilon_F$). We consider only values of λ small enough so that the statistical regime does not change and neither does the mean DoS (for large enough L this nevertheless allows arbitrarily large λ on the scale relevant for parametric correlations). Because of this the TLCF cannot depend on either E, or on the choice of the point H_0 in the ensemble (2.1). We define the (dimensionless) spectral form factor as

$$K(t,\lambda)=\int_{-\infty}^{\infty} e^{-ist/t_H}R(s,\lambda)ds. \tag{2.4}$$

Our main result relates the spectral form factor to the quantum return probability $p(t)$ of a diffusing electron as follows:

$$K(t)=\frac{(2\pi\hbar\rho)^{-1}|t|p(t)}{1+(\pi\hbar\rho)^{-1}\int_{0^+}^{|t|}p(t')dt'}. \tag{2.5}$$

We have obtained this expression for times shorter than the Heisenberg time $t_H\equiv\hbar/\Delta$. Here we define $p(t)$ as the probability density for the wavepacket, originally created in a small volume $V_0\sim\ell^d$, to remain in this volume at the time t (ℓ is the elastic mean free path which is a natural coarse-graining size for the disordered metal; however, we could choose V_0 arbitrarily, provided that $\ell^d\gtrsim V_0\gtrsim\lambda_F^d$ where λ_F is the Fermi wavelength). The ensemble-averaged return probability is related, as we will show later, to the following wave-function correlations:

$$p(t)=\int d^d r\left\langle \sum_l |\psi_n(r)|^2|\psi_{n+l}(r)|^2 e^{-i(E_n-E_{n+l})t/\hbar}\right\rangle. \tag{2.6}$$

It is important to note that, by definition of the wave packet above, the summation here is limited to the number of levels $\mathcal{N}\sim L^d/V_0$ with energies lying within the energy band of width $E_0\sim 1/\rho V_0$.

Equation (2.5) relates the spectral and wave-function correlations. Let us analyze this relation in the metallic phase. In the diffusive regime, $t_{\rm el}\lesssim t\lesssim t_{\rm erg}$, the quantum return probability $p(t)$ reduces at leading order to the *classical* return probability for random walks, multiplied by a symmetry factor $2/\beta$, where $\beta=1, 2$ or 4 is the usual index[3] corresponding to the orthogonal, unitary, and symplectic symmetry ensembles, respectively:

$$p_0(t)=\frac{2}{\beta(4\pi Dt)^{d/2}}. \tag{2.7}$$

Noting that in the ballistic regime, $t\lesssim t_{\rm el}$, $p(t)$ saturates at $p_0(t_{\rm el})\sim 1/\ell^d$, one sees that the integral in the denominator of Eq. (2.5) is of order $(t_{\rm el}/\hbar\rho\ell^d)\sim g_0^{-1}$ for $d>2$, and of order $g_0^{-1}\ln(t/t_{\rm el})$ for $d=2$, where $g_0\gg 1$ is the dimensionless conductance at scale ℓ. It is well known that such an integral describes a weak localization correction to conductance and other physical quantities.[16] On the other hand, the quantum return probability $p(t)$ contains weak localization corrections itself. Neglecting these corrections in both the numerator and denominator of Eq. (2.5), we reduce it to

$$K_0(t)=(2\pi\hbar\rho)^{-1}|t|p_0(t). \tag{2.8}$$

To leading order, this expression is also valid in the ergodic regime, $t_{\rm erg}\lesssim t\ll t_H$, where the classical return probability saturates at $(2/\beta)L^d$ so that the second term in the denominator in Eq. (2.5) is of order $t/t_H\ll 1$ and may be neglected. We should not expect Eq. (2.5) to be correct in the quantum limit, $t\gg t_H$, as we have derived it under the assumption that the opposite inequality holds, as will be seen later. Indeed, in this regime Eq. (2.5) gives the saturation of $K(t)$ at 1/2 instead of the correct limiting value $K(t)=1$.

Equation (2.8) coincides with the result obtained by Argaman *et al.*[7] using the diagonal approximation in semiclassical periodic-orbit theory. The Fourier transform of this expression corresponds to the TLCF obtained originally by Altshuler and Shklovskii.[6] In the diffusive regime, $R(s,0)\sim A_d g^{-d/2}s^{d/2-2}$, where A_d is a numerical coefficient which is zero[17] for $d=2$; and in the ergodic regime,[18] $R(s,0)\sim -1/s^2$.

We also obtain a second relation between $K(t)$ and $p(t)$

$$K(t)+(\pi\hbar\rho)^{-1}\int_{0+}^{|t|}K(t-t')p(t')dt'=(2\pi\hbar\rho)^{-1}|t|p(t), \tag{2.9}$$

which we can see is very similar to Eq. (2.5). The latter is obtained from a diagrammatic analysis discussed in section VI. The new feature is that we have a convolution of $K(t)$ and $p(t)$ which occurs because the decoupling is in ω-space rather than t-space. In 2d, up to 3-loop order in perturbation theory, both these relations correctly reproduce the TLCF. It seems to us quite remarkable that a relation derived from a phenomenological model of energy level dynamics could be exact to 3-loop order. We note that the 2d case is expected to be a good model for the behavior of the system for $d>2$ at the mobility edge. From the point of view of a power-counting analysis of the properties of $K(t)$ at the mobility edge, both Eq. (2.5) and Eq. (2.9) should work equally well.

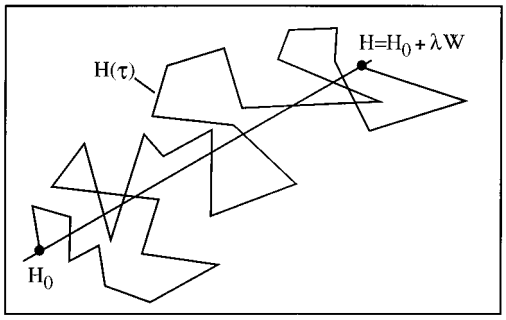

FIG. 2. Smooth $[H(\lambda)]$ and Brownian $[H(\tau)]$ paths through the space of Hamiltonians.

III. RANDOM WALKS THROUGH THE ENSEMBLE OF HAMILTONIANS

We have established elsewhere[8] the relation (2.5), using a Langevin equation to describe the motion of levels on the energy axis in response to a random walk through the ensemble of Hamiltonians. In contrast to eigenvalue statistics in RMT where the Brownian motion ideas were originally applied,[9,15] the Langevin equation for level motion is not closed, and certain assumptions are required to solve it. In the following section, we will re-derive Eq. (2.5) with the help of a different approach based on the decoupling of a certain exact relation between two- and three-level correlation functions. Before doing this, however, it is useful to analyze the Brownian motion picture within the Fokker–Planck scheme. Although the Langevin and Fokker–Planck schemes are in principle equivalent, the assumptions required in order to make the description closed are different. The Langevin scheme of Ref. 8 is physically more transparent. The advantage of the Fokker–Planck scheme which we develop here is that the approximations made are more closely related to those analyzed in subsequent sections.

We consider paths of two types through the ensemble of Hamiltonians (2.1) which, for free electrons in a random potential, have the form

$$H(\lambda) = -\frac{\hbar^2}{2m}\nabla^2 + U(\boldsymbol{r}) + \lambda W(\boldsymbol{r}). \tag{3.1}$$

Here both $U(r)$ and $W(r)$ are chosen to be of Gaussian white-noise form with zero average and

$$\begin{aligned} \langle U(\boldsymbol{r})U(\boldsymbol{r}')\rangle &= \frac{\hbar}{2\pi\rho t_{\mathrm{el}}}\delta(\boldsymbol{r}-\boldsymbol{r}'), \\ \langle W(\boldsymbol{r})W(\boldsymbol{r}')\rangle &= v^2 L^d \delta(\boldsymbol{r}-\boldsymbol{r}'). \end{aligned} \tag{3.2}$$

The first type of path is a straight line through the ensemble, and is generated by varying λ in Eq. (3.1). The second type is a Brownian path through the ensemble, parameterized by the fictitious time τ, generated in the following way:

$$H(\tau) = H_0 + \int_0^\tau d\tau' V(\tau', \boldsymbol{r}). \tag{3.3}$$

We take $V(\tau,\boldsymbol{r})$ to be Gaussian distributed with zero average and

$$\langle V(\tau,\boldsymbol{r})V(\tau',\boldsymbol{r}')\rangle = v^2 L^d \delta(\tau-\tau')\delta(\boldsymbol{r}-\boldsymbol{r}'). \tag{3.4}$$

Referring to Fig 2, one sees that the two ways of exploring the ensemble are equivalent if one

makes the identification $\tau=\lambda^2$.

In our derivation we will use averages over both W or, equivalently, V and then over H_0, and we must here discuss the role of each. The average over all possible perturbations, W, will be necessary to derive the equation of motion of the energy levels, and thence the density of states. We can then obtain correlation functions for energy levels of the system at different parameter values by averaging over the starting point H_0. Such functions should then depend only upon energy and parameter differences by homogeneity.

The first step in our derivation is to obtain the equation of motion for the joint probability density function (JPDF) of energy levels, $P(\{E_n\},\tau)$. We use perturbation theory to second order to calculate the change of $E_n(\tau)$ in response to the evolution from τ to $\tau+\delta\tau$. After averaging over W we obtain

$$\langle \delta E_n(\tau)\rangle=(\delta\tau)v^2\sum_{m\neq n}\frac{c_{nm}(\tau)}{E_n(\tau)-E_m(\tau)}, \tag{3.5a}$$

$$\langle \delta E_n(\tau)\,\delta E_m(\tau)\rangle=(\delta\tau)v^2 c_{nm}(\tau), \tag{3.5b}$$

where

$$c_{nm}(\tau)=L^d\int d^dr\,|\psi_n(\tau,r)|^2|\psi_m(\tau,\mathbf{r})|^2, \tag{3.6}$$

and $\psi_n(\tau,\mathbf{r})$ are the corresponding eigenfunctions of $H(\tau)$. Before we can use the above equations to derive a Fokker–Planck equation for the JPDF, $P(\{E_n\},\tau)$, we must make an assumption. We replace $c_{nm}(\tau)$ by its average over the ensemble of H_0. This amounts to ignoring correlations between eigenvalues and eigenvectors. We take the disorder average to be a function only of the energy difference, $\omega=E_n-E_m$, within the window of interest:

$$\langle c_{nm}(\tau)\rangle\equiv c(\omega). \tag{3.7}$$

Furthermore, we assume that in the Fourier transform of the wavefunction correlator $c(\omega)$ we may neglect the correlations between the eigenvectors and eigenvalues so that

$$C(t)=\left\langle\frac{\Delta}{2\pi\hbar}\sum_l c_{n,n+l}e^{-i\Delta lt/\hbar}\right\rangle=\int_{-\infty}^{\infty}c(\omega)e^{-i\omega t/\hbar}\frac{d\omega}{2\pi\hbar}. \tag{3.8}$$

We can relate $C(t)$ to the return probability of a diffusing electron, Eq. (2.6). To this end, consider a wavepacket made from the eigenstates of $H(\tau)$ and concentrated initially in a volume V_0 of order ℓ^d near the origin (since τ plays no role, we suppress it as a label in the following):

$$\Psi(\mathbf{r},t)=A\sum_n \psi_n(\mathbf{0})^*\psi_n(\mathbf{r})e^{-iE_nt/\hbar}.$$

Here the summation is limited to $\mathcal{N}\sim(L/\ell)^d$ levels with energies $|E_n|\lesssim 1/\rho\ell^d$, and the normalization constant is $A^2=L^d/\mathcal{N}$. The ensemble-averaged return probability $p(t)=\langle|\Psi(\mathbf{0},t)|^2\rangle$ is given by

$$p(t)=A^2\sum_{nm}\langle|\psi_n(0)|^2|\psi_m(0)|^2e^{-i(E_n-E_m)t/\hbar}\rangle=\left\langle\sum_l|\psi_n(0)|^2|\psi_{n+l}(0)|^2e^{-i(E_n-E_{n+l})t/\hbar}\right\rangle,$$

where we have used the fact that the first sum above depends only on the difference $|n-m|$. Noticing also that the ensemble-averaged quantity is spatially homogeneous, we reduce this expression to that given in Eq. (2.6). Comparing this to the definition of c_{nm}, Eq. (3.6), we obtain for $t>0$,

$$p(t)=\frac{1}{L^d}\left\langle \sum_l c_{n,n+l}e^{-i(E_n-E_{n+l})t/\hbar}\right\rangle. \tag{3.9}$$

On the face of it, this coincides, up to a constant factor, with $C(t)$, the Fourier transform of $c_{n,n+l}$, introduced in Eq. (3.8). There is, however, an essential difference: $C(t)$ is defined by the Fourier sum containing all the levels (say, up to ε_F), while the Fourier sum for $p(t)$ contains only the levels within the bandwidth $E_0 \ll \varepsilon_F$. When $|E_n-E_{n+l}| \gtrsim E_0$ the two levels are practically uncorrelated, and $c(\omega)=1$ for $\omega \gtrsim E_0$, so that $C(t)$ contains a δ-like function for t near zero. As we are not interested in an exact description at the ballistic time scale, we can represent the relation between $C(t)$ and $p(t)$ as follows:

$$\begin{aligned} &p(t)=2\pi\hbar\rho C(t), \quad t>0\,; \\ &\int_0^t C(t')dt'=\frac{1}{2}+\frac{1}{2\pi\hbar\rho}\int_{0^+}^t p(t')dt'. \end{aligned} \tag{3.10}$$

We also note that the definition of $H(\tau)$ in Eq. (3.3) causes the energy levels to move away from each other indefinitely as parametric time increases. To overcome this problem we introduce a rescaling term, $-\delta\tau U(E_n)$; to the r.h.s. of Eq. (3.5a). This $U(E_n)$ can be thought of as a Lagrange multiplier, and it will be set later on by the condition that correlation functions can depend only on differences in parametric time.

With these considerations, starting with Eqs. (3.5) we end up with the Fokker–Planck equation for the JPDF:

$$\frac{1}{v^2}\frac{\partial P}{\partial \tau}=-\sum_n \frac{\partial}{\partial E_n}\left(\frac{\partial \mathscr{U}}{\partial E_n}P\right)+\sum_{nm}\frac{\partial^2}{\partial E_n \partial E_m}(c_{nm}P), \tag{3.11}$$

where the drift potential term $\mathscr{U}$ is the sum of one-particle and two-particle potentials,

$$\mathscr{U}(\{E_n\})=\sum_n U(E_n)+\frac{1}{2}\sum_{m\neq n} f(E_n-E_m). \tag{3.12}$$

The one-particle potential arises from the energy rescaling described above, and may be considered as a confinement potential for a one-dimensional gas of fictitious particles interacting via the two-particle potential, $f(\omega)$, which is related to $c(\omega)$ by

$$\frac{\partial f(\omega)}{\partial \omega}=\frac{c(\omega)}{\omega}. \tag{3.13}$$

We see that both the drift potential and the diffusion term in the Fokker–Planck equation are expressed in terms of the function $c(\omega)$, which we have shown to be related to the return probability $p(t)$. The off-diagonal diffusion terms in Eq. (3.11), which are due to eigenfunction correlations, mean that the static solution does not have a simple Gibbs form. In fact we cannot write down its solution in closed form at all. The absence of a simple static solution to the Fokker–Planck equation (3.11) is an important difference between the current problem and the Brownian motion approach to RMT where such a solution yields[9] the exact JPDF. However, the

JPDF contains much more information than we require; for our purposes it is sufficient to study the equation of motion for the density of states, which can be written in the form

$$\rho(E,\tau)=L^{-d}\overline{\sum_n \delta(E-E_n)}, \tag{3.14}$$

where $\overline{\ldots}$ means averaging over the JPDF $P(\{E_n\},\tau)$. Following the procedure of Dyson[19] and Pastur[20] we obtain

$$\frac{1}{v^2}\frac{\partial\rho(E,\tau)}{\partial\tau}=\frac{\partial^2}{\partial E^2}[c(0)\rho(E,\tau)]+\frac{\partial}{\partial E}\left[\frac{\partial U}{\partial E}+L^d\int dE'\rho_2(E,E',\tau)\frac{\partial f(|E-E'|)}{\partial E'}\right], \tag{3.15}$$

where

$$\rho_2(E,E',\tau)=L^{-2d}\overline{\sum_{n\neq m}\delta(E-E_n)\delta(E-E_m)}. \tag{3.16}$$

Since we are only interested in level correlations in energy windows small compared to the scale at which ρ varies, the first term in Eq. (3.15) is negligible. We rewrite the last term in Eq. (3.15) in terms of the static TLCF, $R(E-E')$,

$$\rho_2(E,E',\tau)=\rho(E,\tau)\rho(E',\tau)[1+R(E-E')]. \tag{3.17}$$

After substitution into Eq. (3.15) we see that the integral over $\rho\rho R$ is dominated by a region of relatively small energy differences since the product Rf' falls off rapidly. In this region ρ is roughly constant, and the integral vanishes by oddness of the integrand. We have therefore arrived at the equation

$$\frac{1}{v^2}\frac{\partial\rho(E,\tau)}{\partial\tau}=\frac{\partial}{\partial E}\left[\rho(E,\tau)\frac{\partial}{\partial E}\left(U(E)+L^d\int dE'\rho(E',\tau)f(|E-E'|)\right)\right]. \tag{3.18}$$

This is a non-linear equation, and to proceed further we must linearize it. The static solution of Eq. (3.18) is just the equilibrium density of states, $\rho_{eq}(E)$, and we perform our linearization around by expanding around $\rho_{eq}(E)$, to give the following equation for $\tilde{\rho}(E,\tau)=\rho(E,\tau)-\rho_{eq}(E)$:

$$\frac{1}{v^2}\frac{\partial\tilde{\rho}(E,\tau)}{\partial\tau}=\frac{1}{\Delta}\frac{\partial}{\partial E}\int dE' f(|E-E'|)\frac{\partial}{\partial E'}\,\tilde{\rho}(E',\tau),$$

where we have approximated $\rho_{eq}(E)$ by ρ. Multiplying both sides of this equation by $\rho(E'',0)$ and averaging over the starting point H_0 gives us the evolution equation for the TLCF, $R(E,\tau)$,

$$\frac{\partial}{\partial\tau}R(\omega,\tau)=\frac{\partial}{\partial\omega}\int\frac{d\omega'}{2\pi\hbar}\,f(|\omega-\omega'|)\frac{\partial}{\partial\omega'}\,R(\omega',\tau), \tag{3.19}$$

where we have fixed the units of τ by setting $v^2=\Delta/\pi\hbar$. Equation (3.19) can then be solved by taking the Fourier transform to yield the result for the spectral form factor

$$K(t,\tau)=K(t,0)\exp\left[-\frac{M(t)}{2\hbar^2}|t\tau|\right], \tag{3.20}$$

where $M(t)=2tf(t)$. From the definition of $f(\omega)$, Eq. (3.13), we see that $M(t)$ is related to $C(t)$, the Fourier transform of $c(\omega)$, by

$$M(t)=2\int_0^t C(t')dt'=1+\frac{1}{\pi\hbar\rho}\int_{0^+}^{|t|} p(t')dt. \tag{3.21}$$

Although Eq. (3.20) gives the parametric dependence of $K(t,\tau)$ in terms of a function $M(t)$ related to eigenfunction correlations, we still do not know $K(t,0)$. To relate $K(t,0)$ to eigenfunction correlations we introduce a Ward identity as follows. Similarly to the TLCF, Eq. (2.3), we define the current–current correlation function:

$$\mathscr{C}(s,\lambda)=\Delta^2\sum_{n,m}\langle \dot{E}_n(\lambda)\dot{E}_m(0)\,\delta(E+s\Delta-E_n(\lambda))\,\delta(E-E_m(0))\rangle. \tag{3.22}$$

The assumption that both the correlation functions depend only upon energy and parameter differences leads to the Ward identity

$$\frac{\partial^2\mathscr{C}(\omega,\lambda)}{\partial\omega^2}=\frac{\partial^2 R(\omega,\lambda)}{\partial\lambda^2}, \tag{3.23}$$

and thence to the relation

$$\frac{\partial K(t,\tau)}{\partial\tau}=-\frac{\Delta}{2}\int d\omega\,\mathscr{C}(\omega,0)e^{-i\omega t/\hbar}. \tag{3.24}$$

Finally we can relate $\mathscr{C}(\omega,0)$ to eigenstate correlations assuming, as above, that we can ignore higher order correlations between eigenvalues and eigenstates:

$$\mathscr{C}(\omega,0)=\Delta^2\sum_{n\neq m}\langle W_{nn}W_{mm}\delta(\omega-E_n)\,\delta(E_m)\rangle\approx v^2 c(\omega), \tag{3.25}$$

from which it follows that

$$K(t,0)=\frac{1}{2}\left(\frac{t}{\hbar}\right)^2\frac{C(t)}{M(t)}. \tag{3.26}$$

With allowance for Eqs. (3.10) and (3.21), this is equivalent to the relation (2.5) obtained within the Langevin picture of Ref. 8.

The crucial assumptions used in the Brownian motion approach were in the linearization of appropriate equations, and in the neglection of higher order correlations between eigenvalues and eigenstates. We believe that these assumptions are reasonable provided that one considers only behavior at energy scales much larger than the mean level spacing. However, it is not possible to establish exactly their region of validity and accuracy within the Brownian-motion approach developed here and in Ref. 8. This we will do in the next section using an alternative approach.

IV. EXACT RELATIONS BETWEEN THE RETURN PROBABILITY AND HIGHER ORDER CORRELATION FUNCTIONS

Our aim now is to re-derive Eq. (2.5) using some exact relations which involve the return probability by making only *explicit* assumptions whose region of validity can later be verified. We again consider the ensemble of Hamiltonians, each describing a particular realization of the impurity potential. Now it will be more convenient to use the representation of Eq. (2.1) where the path through the ensemble is a straight line. We define the Fourier transform of the DoS as follows:

$$\mathscr{R}(t,\lambda)=L^d\int_{-\infty}^{\infty}\rho(E,\lambda)e^{-iEt/\hbar}dE=\sum_n\ e^{-iE_n(\lambda)t/\hbar}. \tag{4.1}$$

As all members of the ensemble are statistically equivalent, averaging over realizations should give the same result whatever point along the path has been chosen. Thus one should have

$$\langle\mathscr{R}(t,\lambda).\mathscr{R}(t',\lambda)\rangle=\langle\mathscr{R}(t,0).\mathscr{R}(t',0)\rangle. \tag{4.2}$$

Now we write for small λ;

$$\mathscr{R}(t,\lambda)=\mathscr{R}(t,0)+\lambda.\dot{\mathscr{R}}(t,0)+\frac{1}{2}\lambda^2.\ddot{\mathscr{R}}(t,0)+O(\lambda^3),$$

and substitute this expansion into Eq. (4.2) to obtain

$$2\langle\dot{\mathscr{R}}(t,0).\dot{\mathscr{R}}(t',0)\rangle+\langle\ddot{\mathscr{R}}(t,0).\mathscr{R}(t',0)\rangle+\langle\ddot{\mathscr{R}}(t',0).\mathscr{R}(t,0)\rangle=0\ . \tag{4.3}$$

We will use this identity to derive exact relations between spectral correlation functions. It follows from the definition (4.1) that

$$\begin{aligned}\dot{\mathscr{R}}(t,0)&=-\frac{it}{\hbar}\sum_n\ \dot{E}_n e^{-iE_nt/\hbar},\\ \ddot{\mathscr{R}}(t,0)&=-\frac{it}{\hbar}\sum_n\ \left(\ddot{E}_n-\frac{it}{\hbar}\dot{E}_n^2\right)e^{-iE_nt/\hbar},\end{aligned} \tag{4.4}$$

where

$$\dot{E}_n=\langle n|W|n\rangle,\ddot{E}_n=\sum_m{}'\ \frac{|\langle n|W|m\rangle|^2}{E_n-E_m}.$$

First consider $\langle\dot{\mathscr{R}}(t).\dot{\mathscr{R}}(t')\rangle$. Averaging over W only, we have $\langle\dot{E}_n\dot{E}_{n+l}\rangle_W=v^2c_{n,n+l}$. Hence, averaging also over H_0, we obtain

$$\langle\dot{\mathscr{R}}(t).\dot{\mathscr{R}}(t')\rangle=\frac{2\pi v^2t^2}{\hbar\Delta}\delta(t+t')\left\langle\frac{1}{L^d}\sum_l\ c_{n,n+l}e^{-i(E_n-E_{n+l})t/\hbar}\right\rangle=\frac{2\pi v^2t^2}{\hbar\Delta}p(t), \tag{4.5}$$

where we have used Eqs. (3.9) and (3.10) to relate the average above to the return probability $p(t)$. The crucial assumption in the derivation of Eq. (4.5) was that of homogeneity in energy space which means that $\langle c_{n,n+l}\rangle$ does not depend on n. We expect this assumption to be valid in the whole energy range of interest since the mean density of states is a disorder-independent constant in the energy window centered near ε_F of width $E_0\ll\varepsilon_F$.

Next, consider $\langle\ddot{\mathscr{R}}(t).\mathscr{R}(t')\rangle$, initially averaging only over W. Noting that $\langle\ddot{\mathscr{R}}(t).\mathscr{R}(t')\rangle_W=.\mathscr{R}(t')\langle\ddot{\mathscr{R}}(t)\rangle_W$, as $\mathscr{R}(t')\equiv\mathscr{R}(t',0)$ does not depend on W, and

$$\langle\ddot{E}_n\rangle_W=\frac{2v^2}{L^d}\sum_{l\neq0}\frac{c_{n,n+l}}{E_n-E_{n+l}},$$

we obtain from Eq. (4.4) after rearranging the terms in the summation

$$\langle \ddot{\mathscr{R}}(t)\rangle_W = -\frac{itv^2}{\hbar L^d}\sum_n \left\{ \sum_{l\neq 0} \frac{1-e^{i(E_n-E_{n+l})t/\hbar}}{E_n-E_{n+l}} c_{n,n+l} - \frac{it}{\hbar} c_{nn} \right\} e^{-iE_n t/\hbar}$$

$$= -\frac{tv^2}{\hbar^2 L^d}\sum_{nl} e^{-iE_n t/\hbar} \int_0^t dt'' e^{i(E_n-E_{n+l})t''/\hbar} c_{n,n+l}.$$

Hence, averaging on H_0 as well and using the same assumption as in the derivation of Eq. (4.5), we have

$$\langle \ddot{\mathscr{R}}(t,0).\mathscr{R}(t',0)\rangle = -\frac{2\pi v^2 t}{\hbar\Delta}\delta(t+t')\int_0^t dt'' \left\langle \frac{1}{L^d}\sum_{lm} c_{n,n+l} e^{i(E_n-E_{n+l})t''/\hbar} e^{-i(E_n-E_{n+m})t/\hbar} \right\rangle. \tag{4.6}$$

On exchanging t and t', one gets the same expression.

Now, substituting Eqs. (4.5) and (4.6) into Eq. (4.3), we obtain the following exact relation:

$$tp(t) = Q(t) \equiv \int_0^t dt' \left\langle \frac{1}{L^d}\sum_{lm} c_{n,n+l} e^{i(E_n-E_{n+l})t'/\hbar} e^{-i(E_n-E_{n+m})t/\hbar} \right\rangle, \tag{4.7}$$

where $p(t)$ is the return probability, defined by Eq. (2.6). This exact relation is a starting point to investigate the nature of the approximations needed to obtain our Brownian motion formula, Eq. (2.5). The exact relation involves the higher order correlations, and we need to construct some decoupling procedure. This will be done in the next section. Then we will use the diagrammatic technique to analyze the accuracy of the decoupling.

V. DECOUPLING OF THE HIGHER ORDER CORRELATIONS IN ω-SPACE AND t-SPACE

It is seen from Eq. (2.6) that $p(t)$ involves correlations of two energy levels, whereas, from Eq. (4.7), $Q(t)$ involves correlations of three energy levels. We should therefore assume that $Q(t)$ can be factorized in terms of two-level correlations. In order to see how to factorize Eq. (4.7), let us note that, using homogeneity of the energy space and the definitions of the DoS and TLCF, Eqs. (2.2) and (2.3), one can represent the TLCF (at $\lambda = 0$) as

$$R(\omega) \equiv R(s\Delta) = \Delta \left\langle \sum_m \delta(\omega - E_n + E_{n+m}) \right\rangle - 1 .$$

Then, from the definition (2.4) one obtains the following representation for the form factor:

$$K(t) = \left\langle \sum_m e^{-i(E_n-E_{n+m})t/\hbar} \right\rangle - \frac{2\pi\hbar}{\Delta}\delta(t). \tag{5.1}$$

The δ function above cancels that arising from summation over high levels in Eq. (5.1). Naturally, $K(t)$ defined by Eq. (2.4) as the form factor for the irreducible TLCF, Eq. (2.3), is regular at $t=0$. It is seen now that the natural factorization of Eq. (4.7) is

$$Q(t) \approx 2\int_0^t dt' \left\langle \frac{1}{L^d}\sum_l c_{n,n+l} e^{i(E_n-E_{n+l})t'/\hbar} \right\rangle \left\langle \sum_m e^{-i(E_n-E_{n+m})t/\hbar} \right\rangle. \tag{5.2}$$

The only feature that deserves comment is the factor of 2 on the r.h.s. of Eq. (5.2). To see how this arises we rewrite Eq. (4.7) using the definition of $c_{n,n+l}$,

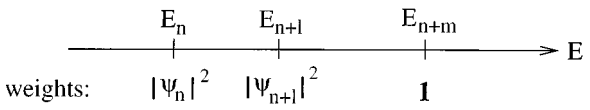

FIG. 3. Structure of the three-level correlation function $Q(t)$. We see that if in factorization we consider the correlation between E_n and E_{n+m}, we must also consider that between E_{n+l} and E_{n+m}.

$$Q(t)=\int_0^t dt' \int d^d r \left\langle \sum_{l,m} |\psi_n(\mathbf{r})|^2 |\psi_{n+l}(\mathbf{r})|^2 e^{i(E_n-E_{n+l})t'/\hbar} e^{i(E_{n+m}-E_n)t/\hbar} \right\rangle .$$

This can be represented on the energy axis in the schematic form shown in Fig. 3. We should allow both for correlations of E_{n+m} with E_n and E_{n+m} with E_{n+l}, since these are equivalent. This is made manifest by changing variable in the integral from t' to $t''=t-t'$,

$$Q(t)=\int_0^t dt'' \int d^d r \left\langle \sum_{l,m} |\psi_n(\mathbf{r})|^2 |\psi_{n+l}(\mathbf{r})|^2 e^{i(E_{n+l}-E_n)t''/\hbar} e^{i(E_{n+m}-E_{n+l})t/\hbar} \right\rangle .$$

We rewrite Eq. (5.2), taking into account that (i) $Q(t)=tp(t)$; (ii) the first average in Eq. (5.2) equals $2\pi\hbar\rho C(t')$, Eq. (3.8); and (iii) the second average is equal to $K(t)$, Eq. (5.1):

$$K(t)=\frac{1}{4\pi\hbar\rho}\frac{tp(t)}{\int_0^t dt' C(t')}, \tag{5.3}$$

which is, with allowance for Eq. (3.10), exactly equivalent to the Brownian motion result of Eq. (2.5). Now it is clear that the assumptions we have made to derive Eq. (2.5) are equivalent to neglecting three-level correlations and keeping only two-level correlations. In the above derivation, we have disregarded the δ function coming from Eq. (5.1), as the exact relation (4.7) has been actually derived from Eqs. (4.5) and (4.6) as $t^2p(t)=tQ(t)$, and this δ function enters in the combination $t\delta(t)$.

For further analysis of the accuracy of Eq. (2.5), it will be useful to see how the factorization (5.2) arises in the energy representation. We begin by representing $Q(t)$ in Eq. (4.7) as follows:

$$Q(t)=\int_0^t dt' \int d\omega \int d\omega' e^{-i\omega' t'/\hbar} e^{i\omega t/\hbar} Q(\omega',\omega), \tag{5.4a}$$

$$Q(\omega',\omega)=L^{-d}\left\langle \sum_{l,m} \delta(E_{n+l}-E_n-\omega')\,\delta(E_{n+m}-E_n-\omega)\,c_{n,n+l} \right\rangle . \tag{5.4b}$$

The function $Q(\omega',\omega)$ can now be related to the three-level correlation function $\mathcal{Q}(E'',E',E)$ defined by

$$\mathcal{Q}(E'',E',E)=L^{-d}\left\langle \sum_{n,l,m} \delta(E''-E_n)\,\delta(E'-E_{n+l})\,\delta(E-E_{n+m})\,c_{n,n+l} \right\rangle , \tag{5.5a}$$

$$=L^d \int d^d r \langle \rho(E'',\mathbf{r})\rho(E',\mathbf{r})\rho(E)\rangle \equiv L^d \int d^d r \mathcal{Q}(E'',E',E;\mathbf{r}), \tag{5.5b}$$

where

$$\rho(E',\mathbf{r}) \equiv \sum_n |\psi_n(\mathbf{r})|^2 \delta(E-E_n) \tag{5.6}$$

is the local density of states (LDoS). Thus the correlation function involves, by definition, correlations of eigenvalues and eigenstates. By the assumption of homogeneity of energy space we see that $\mathcal{Q}(E'',E',E)$ is a function only of energy differences $\omega = E-E''$ and $\omega' = E'-E''$, so that we can put $E''=0$ without loss of generality. Integrating Eq. (5.5a) over E'' prior to and after putting E'' to 0 then yields the following identity:

$$\mathcal{N} Q(\omega',\omega) = E_0 \mathcal{Q}(0,\omega',\omega),$$

where E_0 is energy bandwidth and $\mathcal{N}$ is the total number of energy levels. From this identity and Eq. (5.4b) we obtain the following representation for $Q(\omega',\omega)$:

$$Q(\omega',\omega) = \frac{\Delta}{L^d}\left\langle \sum_{n,l,m} \delta(E_n)\delta(E_{n+l}-E_n-\omega')\delta(E_{n+m}-E_n-\omega)c_{n,n+l}\right\rangle \equiv \Delta \mathcal{Q}(0,\omega',\omega). \tag{5.7}$$

We now apply the Kirkwood approximation[21] to the correlation function, Eq. (5.5b), in the following form:

$$\mathcal{Q}(0,\omega',\omega;\mathbf{r}) = \frac{\langle\rho(0,\mathbf{r})\rho(\omega',\mathbf{r})\rangle\langle\rho(0,\mathbf{r})\rho(\omega)\rangle\langle\rho(\omega',\mathbf{r})\rho(\omega)\rangle}{\rho^3} + B(0,\omega',\omega;\mathbf{r}), \tag{5.8}$$

where the numerator is chosen to incorporate all pairwise correlations, and the denominator ensures the correct limiting value as each energy difference tends to infinity. The correction B is small if the approximation is good, which is expected to be the case unless E'', $E' \equiv E''+\omega'$ and $E \equiv E''+\omega$ are all close together. Now from the definitions of $\rho(E)$ and $\rho(E,r)$, Eqs. (2.2) and (5.6), the averages in Eq. (5.8) can be expressed via the TLCF, $R(\omega)$,

$$\langle\rho(E+\omega,\mathbf{r})\rho(E)\rangle = \langle\rho(E+\omega)\rho(E)\rangle = \rho^2(1+R(\omega)),$$

and the Fourier transform of the return probability, $p(\omega)$,

$$\int d^d r \langle\rho(E+\omega,\mathbf{r})\rho(E,\mathbf{r})\rangle = \frac{1}{2\pi\hbar\Delta}[p(\omega)+2\pi\hbar\rho] = \frac{\rho}{\Delta}c(\omega),$$

where we have taken into account that $p(\omega)$ is expressed via the irreducible part of the LDoS correlation function, and used the relation (3.10).

Thus the Kirkwood approximation of Eq. (5.8) yields the expression

$$Q(\omega',\omega) = \frac{\rho}{\Delta}\{c(\omega')[1+R(\omega)+R(\omega'-\omega)]\} + \frac{\rho}{\Delta}c(\omega')R(\omega)R(\omega'-\omega)$$
$$+ \Delta\int d^d r B(0,\omega',\omega;\mathbf{r}). \tag{5.9}$$

The first line of the above equation represents the terms included in the Brownian motion formula, and the second line is the correction. We can now rewrite the exact relation Eq. (4.7) using Eq. (5.4) and the factorization given by the first line of Eq. (5.9) to obtain

$$K(t) = \left(\frac{1}{4\pi\hbar\rho}\right)\frac{tp(t)-A(t)}{\int_0^t dt'\ C(t')}, \tag{5.10}$$

where the remainder $A(t)$ is given by the Fourier transform in the form (5.4a) of the second line of Eq. (5.9). Note that in deriving Eq. (5.10), we have again neglected a non-integrated $\delta(t)$ function which does not contribute to the final result.

If we ignore the remainder $A(t)$, Eq. (5.10) is equivalent to Eq. (5.3) and thus to the Brownian motion result, Eq. (2.5). We see that the use of the Kirkwood approximation is just a more formal way of doing the factorization discussed previously. The factor of 2 that occurs in Eq. (5.2) emerges naturally, as the two equivalent two-level correlations are automatically taken into account. It is obvious that the second line of Eq. (5.9) could be small only if $|\omega|,|\omega'|,|\omega-\omega'| \gg \Delta$. Thus we could expect $A(t)$ to be small, and Eq. (2.5) to be valid, only outside of the quantum regime, i.e. for $t \lesssim t_H$.

What we would like to be able to do is to find out how big the remainder term $A(t)$ actually is in this non-quantum limit. We can see that $A(t)$ consists of two parts: the first involves a product of three two-level correlation functions, and is the Kirkwood approximation's attempt to represent three-level correlations in terms of two-level correlations; the second is the correction to the approximation itself. To proceed we will introduce diagrammatic perturbation theory in the next section, rewrite our factorization in this language and hence discover what is left over.

VI. DIAGRAMMATIC ANALYSIS

Our aim now is to check the validity of Eq. (2.5) beyond the trivial diagonal approximation in which one can just neglect the t-dependence of the denominator, and substitute the classical limit of $p(t)$ into the numerator of this expression. The simplest way of doing this is to calculate both $K(t)$ and $p(t)$ to higher order in perturbation theory, and to compare directly the r.h.s. and l.h.s. of Eq. (2.5). It is more instructive, however, to analyze diagrammatically the exact relation (4.7) and the decoupling procedure based on Eqs. (5.4) and (5.9). In this way we will not only check the accuracy of Eq. (2.5), but arrive at an alternative factorization given by Eq. (2.9).

Let us note that the role of higher order corrections is different in $d=2$ and $d>2$. In the $2d$ case they are universal in the sense that they are due to diffusive motion of electrons throughout the whole sample and almost insensitive to details of motion at the ballistic scale. In $d>2$, corrections are mainly due to the motion at the ballistic scale, and proportional to powers of an additional small parameter $(t/t_{\mathrm{el}})^{d/2-1}$ (as well as to powers of the standard weak disorder parameter, inverse dimensionless conductance g^{-1}). These corrections are not only small but of no particular interest as they do not drive the system from weak to strong-disorder regime. In contrast to this, the $2d$ corrections do describe crossover from weak to strong disorder, and are widely believed to be more relevant in the vicinity of the metal-insulator transition for $d>2$ than those calculated in the metallic limit directly in $d>2$ dimensions. Moreover, since in the diagonal approximation $K(t) \propto tp(t) \sim$ const for $t \lesssim t_{\mathrm{erg}}$ at $d=2$, the TLCF vanishes in this approximation in the diffusive regime ($E \gtrsim E_c$). Therefore, in this regime the first non-vanishing higher-order contribution governs the main effect rather than describing some correction. For all these reasons, we will consider mainly the $2d$ case in this section.

A. General relations

To be able to work in complete generality we will rewrite the exact equation (4.7) in terms of Green's functions that can then be expanded using standard diagrammatic methods. The form of the diagrams for $K(t)$ is by now well known, but those for $p(t)$ and the three-level correlator $Q(t)$ are less familiar.

We start with the standard expression for DoS in terms of exact Green's functions where, as well as elsewhere in this section, we use the units $\hbar=1$:

$$\rho(E,\boldsymbol{r}) = \frac{i}{2\pi}[G^R(E;\boldsymbol{r},\boldsymbol{r}) - G^A(E;\boldsymbol{r},\boldsymbol{r})]. \tag{6.1}$$

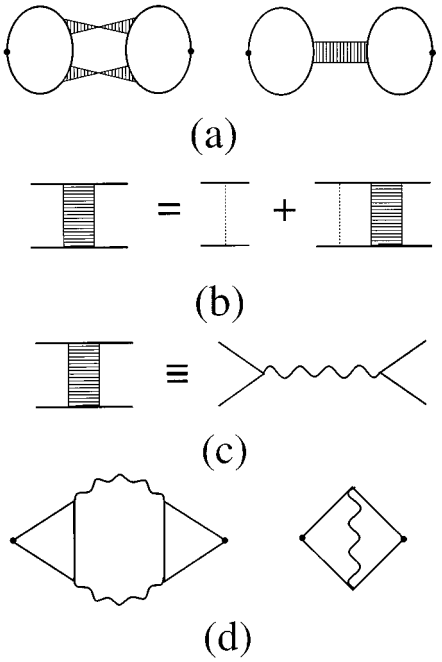

FIG. 4. (a) The two one-loop diagrams for $R(\omega)$ in a disordered metal. The diagram on the left gives the (dominant) Altshuler–Shklovskii contribution; that on the right is smaller by a factor $\Delta t_{\rm el}$, and is usually ignored. (b) Definition of the impurity ladders occurring in (a). (c) Rewriting the impurity ladder as an effective propagator. (d) Rewriting the diagrams in (a) using the notation of (c). The electron Green's function lines end up in the so-called Hikami boxes.

Here the retarded, G^R and advanced G^A Green's functions are defined by

$$G^{R,A}(E;\boldsymbol{r},\boldsymbol{r}')=\sum_n \frac{\psi_n(\boldsymbol{r})\psi_n(\boldsymbol{r}')}{E-E_n\pm i0}. \tag{6.2}$$

For the density–density correlation function we get the formula

$$R(\omega)=\left(\frac{i\Delta}{2\pi}\right)^2\int d^dr\int d^dr'\langle \mathscr{G}(0;\boldsymbol{r},\boldsymbol{r})\mathscr{G}(\omega;\boldsymbol{r}',\boldsymbol{r}')\rangle, \tag{6.3}$$

where $\mathscr{G}=G^R-G^A$. The diagrams for this then consist of two loops, each with an external vertex (with coordinates $\boldsymbol{r}$ and $\boldsymbol{r}'$), as shown in Fig. 4(a). Averaging over the disorder ensemble then leads to the presence of impurity lines both within a loop and across loops. Only the connected diagrams contribute to $R(\omega)$, while the trivial unconnected diagrams are cancelled by the -1 in the definition of $R(\omega)$, Eq. (2.3).

Similarly, $p(\omega)$ is given by

$$p(\omega)=\frac{2\pi}{\rho L^d}\int d^dr\langle\rho(E+\omega,\boldsymbol{r})\rho(E,\boldsymbol{r})\rangle=-\frac{\Delta}{2\pi}\int d^dr\langle\mathscr{G}(\omega;\boldsymbol{r},\boldsymbol{r})\mathscr{G}(0;\boldsymbol{r},\boldsymbol{r})\rangle. \tag{6.4}$$

The difference between the formulae (6.3) and (6.4) is that in the latter the densities of states are evaluated at the same point $\boldsymbol{r}$ in space rather than at different points. In diagrammatic terms this means that $p(\omega)$ consists of two loops connected to a single external point $\boldsymbol{r}$, as shown in Fig. 5.

In the diffusive regime of the disordered metal it is impurity ladders describing diffusive motion which give the important energy dependent contributions. They must have both a R and

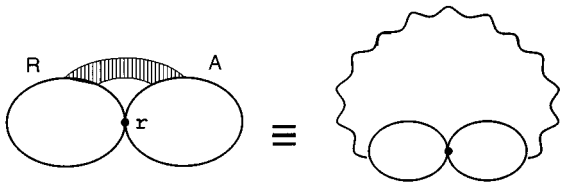

FIG. 5. The one-loop diagram for the quantum return probability $p(\omega)$ in the ladder and Hikami-box representations.

A line – so only RA and AR diagrams can contribute. Since the latter are complex conjugates of each other it follows that we can write the expressions for $R(\omega)$ and $p(\omega)$ in the following form:

$$R(\omega)=\frac{\Delta^2}{2\pi^2}\,\mathfrak{Re}\int d^dr\int d^dr'\langle G^R(\omega;\mathbf{r},\mathbf{r})G^A(0;\mathbf{r}',\mathbf{r}')\rangle, \tag{6.5}$$

$$p(\omega)=\frac{\Delta}{\pi}\,\mathfrak{Re}\int d^dr\langle G^R(\omega;\mathbf{r},\mathbf{r})G^A(0;\mathbf{r},\mathbf{r})\rangle. \tag{6.6}$$

The impurity ladders [Fig. 4(b)] which connect the two loops describe either diffusion or Cooperon propagators and are given in momentum space by

$$D(q;\omega)=\frac{1}{2\pi\rho t_{el}^2}\,\frac{1}{Dq^2-i\omega}. \tag{6.7}$$

We will consider both the cases with and without time-reversal symmetry, referring to them as the orthogonal case ($\beta=1$) and the unitary case ($\beta=2$). Diagrammatically, the latter differs from the former by the absence of the Cooperon contributions which differ from the diffusions by the relative direction of arrows in impurity ladders.

The loops can be connected by an arbitrary number of the ladders. In the lowest order there are the two contributions to $R(\omega)$ shown in Fig. 4(a), and one contribution to $p(\omega)$ (Fig. 5). The dominant contribution to $R(\omega)$ – which is called Altshuler-Shklovskii diagram – has two impurity ladders; the diagram with only one ladder gives a much smaller contribution.

Thus the perturbation order of a diagram is not determined by the number of ladders. A standard way[22,23] to determine this order, and to make the calculation of diagrams more straightforward, is to rewrite them in the form where impurity ladders are represented as propagators [a wavy line in Fig. 4(c)]; this is convenient since the ladders involve small momentum, $q\ell\ll 1$, and energy, $\omega t_{el}\ll 1$. All other Green's function lines are absorbed into effective interactions between propagators (as shown in Figs. 4 and 5) known as Hikami boxes. Then the order of a diagram is the number of independent momenta occurring in the propagators, which is just the number of loops made of the wavy lines. (Each box can be thought of as being contracted into a single node which corresponds to a spatial region of size ℓ; any diagram would then consist of a number of wavy lines joined together at such nodes.) The loop-expansion parameter here is $1/g$ where g is the dimensionless conductance of the sample.

The one-loop diagrams for $R(\omega)$ are shown in Fig. 4(d). The two external vertices may be in separate (odd) boxes, or the same (even) box; we ignore the latter since they are smaller than the former by factor $\Delta t_{\mathrm{el}}\sim(\ell/L)^d$ in the same order of perturbation theory. The remaining Hikami boxes that do not contain an external vertex have an even number of sides.

Rewriting diagrams for $p(\omega)$ in terms of Hikami boxes we find that the external vertex [corresponding to the point $\mathbf{r}$ in Eq. (6.6)] has two boxes connected to it – these can either both be odd boxes, or both be ''2-gons'' (larger even boxes are not allowed since one can always string impurity ladders across them to recover the ''2-gon'' structure). All other boxes have no external

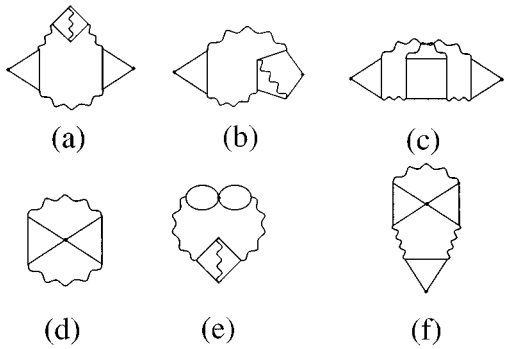

FIG. 6. Two-loop order diagrams to $R(\omega)$ [(a), (b), (c)]; $\tilde{p}(\omega)$ [(d), (e)]; and $\tilde{Q}(\omega)$ (f). All diagrams contribute in the orthogonal case, while only (d) and (f) contribute in the unitary case.

vertex and so have an even number of sides. Note that all the Hikami boxes must be ''dressed,'' i.e. single-impurity lines should connect (without mutual intersection) those *non-adjacent* sides of the boxes which have the same analyticity (both R, or both A).[23] In all diagrams below the boxes are assumed to be dressed. The one-loop contribution to $p(\omega)$ is given in Fig. 5 in both the ladder and Hikami representations. All the two-loop contributions to $p(\omega)$ and $R(\omega)$ are given in the Hikami representation in Fig. 6.

Before comparing the higher order contributions made to Eq. (2.5) by the diagrams for $R(\omega)$ and $p(\omega)$, we consider the three-level correlator $Q(\omega',\omega)$. Starting from Eq. (5.7), and rewriting the densities of states via Eq. (6.1) we get

$$Q(\omega',\omega)=\Delta\left(\frac{i}{2\pi}\right)^3\int d^dr\int d^dr'\langle\mathscr{G}(0;\mathbf{r},\mathbf{r})\mathscr{G}(\omega';\mathbf{r},\mathbf{r})\mathscr{G}(\omega;\mathbf{r}',\mathbf{r}')\rangle. \tag{6.8}$$

Following the procedure used for $R(\omega)$ and $p(\omega)$ above we see that in the ladder representation the diagrams for $Q(\omega',\omega)$ consist of three loops, two of which are joined at the external vertex $\mathbf{r}$, and the third having the external vertex $\mathbf{r}'$. There are now several classes of diagrams that are not fully connected, as shown in Fig. 7(a). (The shaded strips there include symbolically all possible combinations of impurity ladders.) The most trivial has all loops unconnected and yields a constant term. The two others are reducible as they have only two out of the three loops connected by impurity ladders, and contribute terms proportional to $\rho^3R(\omega)$, $\rho^3R(\omega'-\omega)$ and $\rho p(\omega')$. These reducible contributions add up to give

$$Q_{uc}(\omega',\omega)=\left(\frac{\rho L^d}{2\pi}\right)\{2\pi\rho[1+R(\omega)+R(\omega'-\omega)]+p(\omega')\}. \tag{6.9}$$

We see that the r.h.s. of the above is similar , but not identical to, the first line of the r.h.s. of Eq. (5.9). The difference is that the is no $p(\omega')$ multiplying the $R(\omega)$ and $R(\omega'-\omega)$ in Eq. (6.9), only its constant part $2\pi\rho$. If we substitute this term into Eq. (4.7) we obtain $K(t)=(2\pi\hbar)^{-1}tp(t)$. In other words, the reducible diagrams of the three-level correlator Q are enough to reproduce the diagonal approximation of semi-classics. In order to recover our formula, Eq. (2.5), we will need to analyze the irreducible contributions to Q given schematically in Fig. 7(b).

If we look at the irreducible contributions the first thing to note is that each diagram can only have ladders between two of the three *pairs* of loops. This is because ladders are always between an R and an A line, and so in an irreducible diagram either two loops are R and the third A or vice

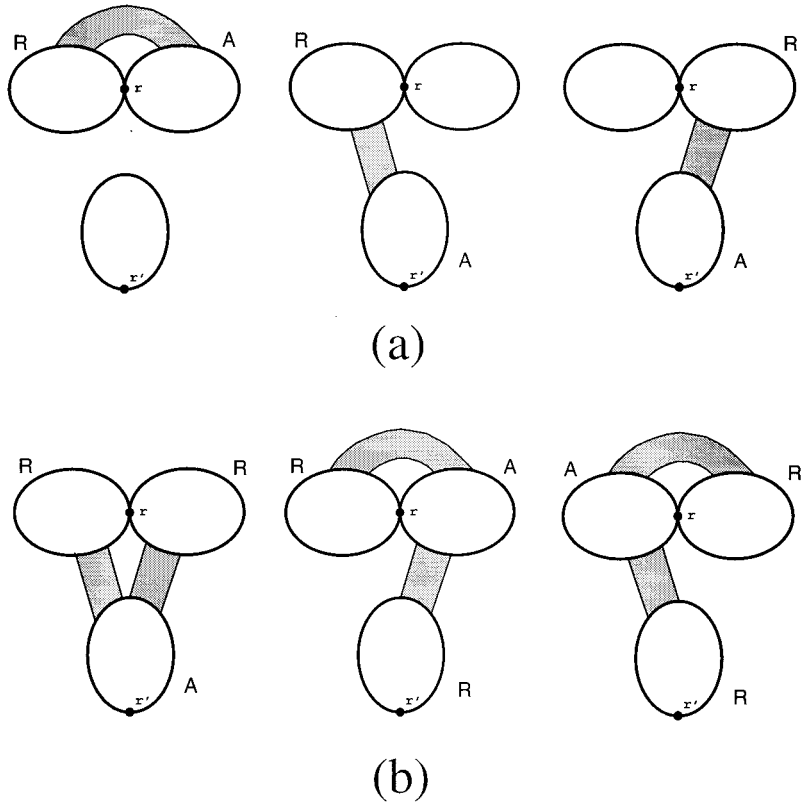

FIG. 7. (a) The reducible contributions to the three-level correlator $Q(\omega',\omega)$. The first diagram yields no contribution to the function $Q(t)$, while the other two yield equal contributions to $Q(t)$ that are proportional to $K(t)$. (b) The irreducible contributions to the three-level correlator $Q(\omega',\omega)$. For analyticity reasons the last two diagrams give no contribution to the function $Q(t)$, so we need consider only diagrams of the first type.

versa. There are therefore 6 possibilities which come in complex conjugate pairs: AAR and RRA; ARA and RAR; RAA and ARR. The irreducible part of $Q(\omega',\omega)$ can then be written in the form

$$Q_c(\omega',\omega)=\frac{1}{4\pi^3\rho L^d}\int d^dr\int d^dr'\,\mathrm{Im}\{\langle G^A(0;\mathbf{r},\mathbf{r})G^A(\omega;\mathbf{r},\mathbf{r})G^R(\omega';\mathbf{r}',\mathbf{r}')\rangle$$
$$+\langle G^A(0;\mathbf{r},\mathbf{r})G^R(\omega;\mathbf{r},\mathbf{r})G^A(\omega';\mathbf{r}',\mathbf{r}')\rangle+\langle G^R(0;\mathbf{r},\mathbf{r})G^A(\omega;\mathbf{r},\mathbf{r})G^A(\omega';\mathbf{r}',\mathbf{r}')\rangle\}. \tag{6.10}$$

When rewritten in the Hikami-box representation the diagrams for Q consist of the two boxes connected to external vertex $\mathbf{r}$ found in $p(\omega)$ diagrams, plus a single odd box connected to external point $\mathbf{r}'$ as found in $R(\omega)$ diagrams; these are then held together by wavy lines and even boxes with no external vertices. Q_{AAR} diagrams cannot have the ''2-gon'' structure in the part connected to external point $\mathbf{r}$ since such a structure ends in ladders, which cannot happen here as both lines of the ladder would be A. Q_{ARA} and Q_{RAA} diagrams can have this ''2-gon'' structure.

If we are to re-derive our main result Eq. (2.5) diagrammatically we will need to show that the connected part of $Q(\omega',\omega)$ factors into a product of R and p. This can be seen by recalling the derivation of Eq. (2.5) via the Kirkwood approximation, where such factorization occurs in the first line of Eq. (5.9). The fact that only two pairs of loops can have ladders between them suggests

a possible reason for this to occur. At this point we note that we are interested not in $Q(\omega',\omega)$ itself but rather in $Q(t)$ which is derived from it by Fourier transforms as in Eq. (5.4a). The analyticity properties of $Q(\omega',\omega)$ diagrams will lead to some types giving no contribution to $Q(t)$. Eventually, a factorization emerges from this analysis which is different to that suggested in Eq. (5.9), but which, remarkably, yields the same spectral form factor in two dimensions, to third-loop order.

B. Analytical properties of the three-level correlation function

First let us prove that only the Q_{AAR} diagrams survive, starting with the formula for $Q(t)$ given by Eq. (5.4),

$$Q(t)=\int_0^t dt' \int d\omega' \int d\omega e^{-i\omega' t'} e^{i\omega t} Q(\omega',\omega)=\int d\omega' \int d\omega \frac{e^{i\omega t}-e^{i(\omega-\omega')t}}{i\omega'} Q(\omega',\omega). \tag{6.11}$$

Taking the Fourier transform of $Q(t)$ then yields

$$\begin{aligned}
&\int dt e^{i\overline{\omega} t} \int d\omega' \int d\omega \frac{e^{i\omega t}-e^{i(\omega-\omega')t}}{i\omega'} Q(\omega',\omega) \\
&\quad = 2\pi \int d\omega' \int d\omega \frac{1}{i\omega'} [\delta(\overline{\omega}+\omega)-\delta(\overline{\omega}+\omega-\omega')] Q(\omega',\omega) \\
&\quad = -2\pi i \int \frac{d\omega'}{\omega'} [Q(\omega',-\overline{\omega})-Q(\omega',\omega'-\overline{\omega})].
\end{aligned} \tag{6.12}$$

Now consider the analyticity properties of the ARR, ARA and AAR, respectively. They can be written in the form

$$\begin{aligned}
Q_{RAA}(\omega',\omega) &= f(-\omega',-\omega), \\
Q_{ARA}(\omega',\omega) &= f(\omega',\omega'-\omega), \\
Q_{AAR}(\omega',\omega) &= f(\omega,\omega-\omega'),
\end{aligned} \tag{6.13}$$

where in each case $f(\omega_1,\omega_2)$ is a function analytic in the u.h.p. for both arguments. For Q_{RAA} Eq. (6.12) gives

$$-2\pi i \int \frac{d\omega'}{\omega'} [f(-\omega',\overline{\omega})-f(-\omega',-\omega'+\overline{\omega})] = -2\pi^2 [f(0,-\overline{\omega})-f(0,-\overline{\omega})] = 0\,, \tag{6.14}$$

since upon closing each term in l.h.p. we only get contributions from the pole at $\omega'=0$, and these cancel. Similarly for Q_{ARA} we get upon closing in the u.h.p.,

$$-2\pi i \int \frac{d\omega'}{\omega'} [f(\omega',\omega'+\overline{\omega})-f(\omega',\overline{\omega})] = 2\pi^2 [f(0,\overline{\omega})-f(0,\overline{\omega})] = 0\,. \tag{6.15}$$

Finally for Q_{AAR} we get

$$-2\pi i \int \frac{d\omega'}{\omega'} [f(-\overline{\omega},-\omega'-\overline{\omega})-f(\omega'-\overline{\omega},-\overline{\omega})] = -(2\pi)^2 f(-\overline{\omega},-\overline{\omega}), \tag{6.16}$$

where we closed first term in l.h.p., second in u.h.p. to yield contributions that add up. The above term can be rewritten in the form $-(2\pi)^2 Q_{AAR}(\omega'=0,-\overline{\omega})$, so it follows that diagrams for Q_{AAR} can yield Fourier transform of $Q(t)$ directly. We have therefore verified our previous assertion, and moreover have derived the contribution to the Fourier transform of $Q(t)$ coming from the Q_{AAR} diagrams. Diagrammatically the above means that all ladders in Q_{AAR} diagrams will have the same energy dependence.

Let us discuss what the above means for our factorization hypothesis. The reason we expected that it would be the Q_{RAR} and Q_{ARR} diagrams that survived is that we can envisage a natural factorization into terms with energy dependence of the form $R(\omega)p(\omega')$ and $R(\omega'-\omega)p(\omega')$, which are exactly what is needed to reproduce Eq. (2.5). The fact that it is Q_{AAR} which survives means that our factorization hypothesis must be altered to have an energy dependence $R(\omega)p(\omega)$, which leads to a convolution in t-space. More precisely, we expect the ω-space factorization to have the form

$$\widetilde{Q}(\omega)=-\frac{(2\pi)^2 i}{\Delta}\widetilde{p}(\omega)\widetilde{R}(\omega). \tag{6.17}$$

Here we have introduced the analytical functions $\widetilde{Q}(\omega),\widetilde{p}(\omega)$ and $\widetilde{R}(\omega)$ as follows:

$$\widetilde{Q}(\omega)\equiv Q_{AAR}(0,\omega);\quad p(\omega)\equiv 2\Re\mathrm{e}\widetilde{p}(\omega);\quad R(\omega)\equiv 2\Re\mathrm{e}\widetilde{R}(\omega). \tag{6.18}$$

Note that diagrammatically we calculate exactly these analytical functions. Before giving the results for higher-loop contributions, note that calculations of $\widetilde{R}(\omega)$ are considerably simplified due to the fact that it can be obtained as the second derivative of ''free energy'' $F(\omega)$:

$$\widetilde{R}(\omega)=-\left(\frac{\Delta}{2\pi}\right)^2\frac{\partial^2}{\partial\omega^2}\,\widetilde{F}(\omega). \tag{6.19}$$

Here $F(\omega)$ is given by the sum of all diagrams that have no external vertices, and the coefficient of proportionality is chosen so as to make $F(\omega)$ dimensionless.

C. Calculation of diagrams up to three-loop order

As a result of the above discussion we can now lay out the diagrammatic program ahead. First, we will calculate the contributions to $\widetilde{F}(\omega)$, $\widetilde{p}(\omega)$ and $\widetilde{Q}(\omega)$ up to three-loop order. Then, we will verify that the exact relation (4.7) is fulfilled with these contributions and check the factorization scheme of Eq. (6.17) which is dictated by the analytical structure described above. This factorization is equivalent to that given by Eq. (2.9). Finally, we will, having verified this factorization up to the three-loop order, check the factorization that comes out of the Kirkwood approximation, Eq. (5.9), and is equivalent to the result of the Brownian-motion model, Eq. (2.5). We will show that up to the third-loop order both the factorizations are identical and exact in $d=2$. Therefore, Eq. (2.5) obtained within the Brownian motion picture turn out to be correct to quite a non-trivial order of perturbation theory.

Let us introduce a notation that is convenient for further analysis:

$$\mathscr{P}_{1\ldots n}\equiv D(\boldsymbol{q}_1+\cdots+\boldsymbol{q}_n)^2-i\omega, \tag{6.20}$$

In particular, $\mathscr{P}_1\equiv Dq_1^2-i\omega$.

Now, two-loop order contributions corresponding to the diagrams in Fig. 8(a) (equivalent to those in Figs. 6(a)–6(c)] and in Figs. 6(d)–6(f) may be written as

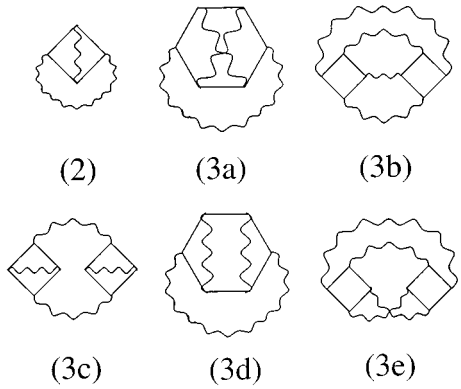

FIG. 8. Two- and three-loop order diagrams for the function $\widetilde{F}(\omega)$. The two-loop diagram is equivalent to those in Figs. 6a–c, and contributes only to the orthogonal case. All 5 three-loop diagrams contribute to the orthogonal case, while only 3a and 3b contribute to the unitary case.

$$\widetilde{F}_2(\omega)=\left(\frac{2-\beta}{\beta}\right)\frac{\Delta}{2\pi}\sum_{q_1,q_2}\frac{\mathscr{P}_1+\mathscr{P}_2+i\omega}{\mathscr{P}_1\mathscr{P}_2};$$

$$\widetilde{p}_2(\omega)=\left(\frac{2}{\beta}\right)\frac{\Delta}{2\pi L^d}\,\mathfrak{Re}\sum_{q_1,q_2}\left\{\frac{1}{\mathscr{P}_1\mathscr{P}_2}+2(2-\beta)\frac{\mathscr{P}_1+\mathscr{P}_2+i\omega}{(\mathscr{P}_1)^2\mathscr{P}_2}\right\}; \tag{6.21}$$

$$\widetilde{Q}_2(\omega)=-i\left(\frac{2}{\beta}\right)^2\frac{\Delta}{L^d}\sum_{q_1,q_2}\frac{1}{(\mathscr{P}_1)^2\mathscr{P}_2}.$$

Here we note the following. The diagrammatic approach could be used both in the diffusive regime, $\omega\gg E_c$, where all the sums above should be replaced by integrals, and in the ergodic regime, $E_c\gg\omega\gg\Delta$, where only the contribution of the zero mode (all $\boldsymbol{q}=0$) survives. In the diffusive regime, regularization of divergent integrals is required. Although we do not explicitly calculate contributions of all diagrams below, in all algebraic manipulations we use dimensional regularization near $d=2$. These manipulations involve dealing with large $q\sim\ell^{-1}$, and so all diagrammatic expressions we give here are not directly valid in the ergodic regime. However, it is straightforward to verify the accuracy of our factorization scheme in the zero-mode regime as well.

The three-loop contributions to $F(\omega)$, $p(\omega)$ and $Q(\omega)$ are shown in Figs. 8, 9 and 10,

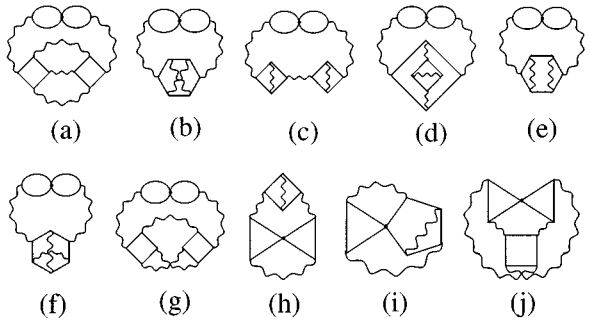

FIG. 9. Three-loop order diagrams for the quantum return probability $\widetilde{p}(\omega)$. All 10 diagrams contribute in the orthogonal case, while only the first 2 contribute in the unitary case.

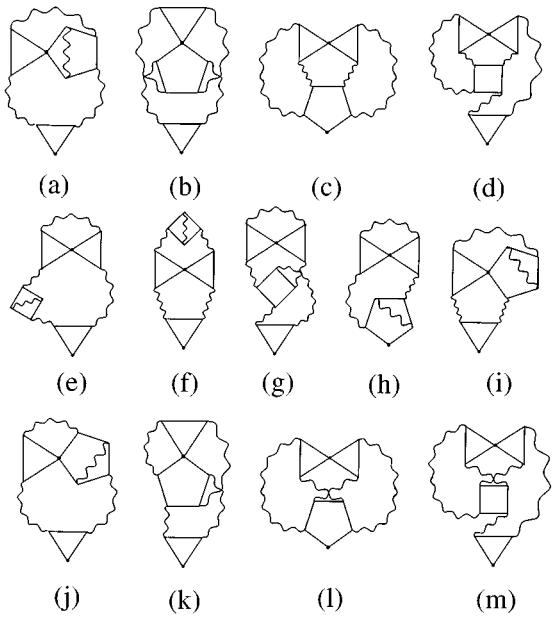

FIG. 10. Three-loop order diagrams for the function $\widetilde{Q}(\omega)$. All 13 diagrams contribute in the orthogonal case, while only the first 4 contribute in the unitary case.

respectively. In Fig. 8(a) we have also drawn the two-loop contribution to $F(\omega)$ which is equivalent to the three two-loop contributions to $R(\omega)$ shown in Fig. 6. Note that in the three-loop order there are 41 diagrams that contribute directly to $R(\omega)$, so that to have instead only the 5 diagrams for $F(\omega)$, as in Fig. 8, is a considerable simplification. Nevertheless, these three-loop results are quite bulky, and we list contributions of each diagram Tables I–III below.

The labels in the tables correspond to those in Figs. 8–10, and in the figure captions we describe which diagrams are made of diffusions only and thus contribute in the unitary ($\beta=2$) case. Obviously, all the diagrams contribute in the orthogonal ($\beta=1$) case. Results for the symplectic symmetry class ($\beta=4$) are practically the same as for the orthogonal case but we do not list them here to avoid complications with the coefficients.

The starting point for our diagrammatic analysis is Eq. (4.7) which we now rewrite as follows. The Fourier transform, Eq. (5.4), of the function $Q(t)$ is split into the reducible and irreducible

TABLE I. Three-loop order contributions to $\widetilde{F}(\omega)$: an overall factor of $(\Delta/2\pi)^2$ should be attached to each contribution.

$3F_a=F_d=-2\Sigma_{q_1,q_2,q_3}\dfrac{2(\mathscr{P}_1+\mathscr{P}_2+\mathscr{P}_3)+3i\omega}{\mathscr{P}_1\mathscr{P}_2\mathscr{P}_3}$
$F_b=\frac{1}{4}\Sigma_{q_1,q_2,q_3}\dfrac{(\mathscr{P}_{12}+\mathscr{P}_{23})^2}{\mathscr{P}_1\mathscr{P}_2\mathscr{P}_3\mathscr{P}_{123}}$
$F_c=2\Sigma_{q_1,q_2,q_3}\dfrac{(\mathscr{P}_1+\mathscr{P}_2+i\omega)(\mathscr{P}_1+\mathscr{P}_3+i\omega)}{\mathscr{P}_1^2\mathscr{P}_2\mathscr{P}_3}$
$F_e=\frac{1}{2}\Sigma_{q_1,q_2,q_3}\dfrac{(\mathscr{P}_{12}+\mathscr{P}_{23})(\mathscr{P}_{13}+\mathscr{P}_{32})}{\mathscr{P}_1\mathscr{P}_2\mathscr{P}_3\mathscr{P}_{123}}$

TABLE II. Three-loop order contributions to $\tilde{p}(\omega)$: an overall factor of $L^{-d}(\Delta/2\pi)^2$ should be attached to each contribution.

$$p_a=\tfrac{1}{2}p_e=p_f=-2\Sigma_{q_1,q_2,q_3}\frac{2(\mathscr{P}_1+\mathscr{P}_2+\mathscr{P}_3)+3i\omega)}{\mathscr{P}_1^2\mathscr{P}_2\mathscr{P}_3}$$

$$p_b=\Sigma_{q_1,q_2,q_3}\frac{(\mathscr{P}_{12}+\mathscr{P}_{23})^2}{\mathscr{P}_1^2\mathscr{P}_2\mathscr{P}_3\mathscr{P}_{123}}$$

$$p_c=4\Sigma_{q_1,q_2,q_3}\frac{(\mathscr{P}_1+\mathscr{P}_2+i\omega)(\mathscr{P}_1+\mathscr{P}_3+i\omega)}{\mathscr{P}_1^3\mathscr{P}_2\mathscr{P}_3}$$

$$p_d=4\Sigma_{q_1,q_2,q_3}\frac{(\mathscr{P}_1+\mathscr{P}_2+i\omega)(\mathscr{P}_2+\mathscr{P}_3+i\omega)}{\mathscr{P}_1^2\mathscr{P}_2^2\mathscr{P}_3}$$

$$p_g=2\Sigma_{q_1,q_2,q_3}\frac{(\mathscr{P}_{12}+\mathscr{P}_{23})(\mathscr{P}_{13}+\mathscr{P}_{32})}{\mathscr{P}_1^2\mathscr{P}_2\mathscr{P}_3\mathscr{P}_{123}}$$

$$p_h=4\Sigma_{q_1,q_2,q_3}\frac{(\mathscr{P}_1+\mathscr{P}_2+i\omega)}{\mathscr{P}_1^2\mathscr{P}_2\mathscr{P}_3}$$

$$p_i=-4\Sigma_{q_1,q_2,q_3}\frac{1}{\mathscr{P}_1\mathscr{P}_2\mathscr{P}_3}$$

$$p_j=\Sigma_{q_1,q_2,q_3}\frac{(\mathscr{P}_{12}+\mathscr{P}_{23})}{\mathscr{P}_1\mathscr{P}_2\mathscr{P}_3\mathscr{P}_{123}}$$

parts [Eqs. (6.9) and (6.10), respectively]. As only $\tilde{Q}(\omega)$, Eq. (6.18), contributes to the irreducible part, we obtain

$$\frac{\partial}{\partial(i\omega)}\left[\frac{1}{L^d}\frac{\partial}{\partial(i\omega)}F(\omega)-\tilde{p}(\omega)\right]=\frac{i}{\pi}\tilde{Q}(\omega). \tag{6.22}$$

This is the exact relation which holds to all orders in perturbation theory. It allows us to check the accuracy of our diagrammatics up to three-loop order for both the unitary and orthogonal cases. We do this by first substituting the two-loop results of Eq. (6.21—which is quite straightforward, and then the three-loop data from the tables which requires some significant algebra. We verify that this identity holds with our diagrammatic results which gives us confidence in their accuracy.

TABLE III. Three-loop order contributions to $\tilde{Q}(\omega)$: an overall factor of $(\Delta^2/2\pi L^d)$ should be attached to each contribution.

$$Q_a=2Q_b=Q_h=Q_i=Q_j=Q_k=2i\Sigma_{q_1,q_2,q_3}\frac{1}{\mathscr{P}_1^2\mathscr{P}_2\mathscr{P}_3}$$

$$Q_c=Q_l=i\Sigma_{q_1,q_2,q_3}\frac{1}{\mathscr{P}_1\mathscr{P}_2\mathscr{P}_3\mathscr{P}_{123}}$$

$$Q_d=Q_m=-2i\Sigma_{q_1,q_2,q_3}\frac{(\mathscr{P}_{12}+\mathscr{P}_{23})}{\mathscr{P}_1^2\mathscr{P}_2\mathscr{P}_3\mathscr{P}_{123}}$$

$$Q_e=-4i\Sigma_{q_1,q_2,q_3}\frac{(\mathscr{P}_1+\mathscr{P}_2+i\omega)}{\mathscr{P}_1^3\mathscr{P}_2\mathscr{P}_3}$$

$$Q_f=-2i\Sigma_{q_1,q_2,q_3}\frac{(\mathscr{P}_1+\mathscr{P}_3+i\omega)}{\mathscr{P}_1^2\mathscr{P}_2^2\mathscr{P}_3}$$

$$Q_g=-2i\Sigma_{q_1,q_2,q_3}\frac{(\mathscr{P}_1+\mathscr{P}_2+i\omega)}{\mathscr{P}_1^2\mathscr{P}_2^2\mathscr{P}_3}$$

The next step is to see whether our projected ω-space factorization occurs to two- and three-loop order in both the orthogonal and unitary cases. To check Eq. (6.17) up to two-loop order, we calculate both factors in the r.h.s. to the first order only. This is simple and yields

$$\tilde{Q}_2(\omega) = -i\left(\frac{2}{\beta}\right)^2 \sum_{q_1,q_2} \frac{1}{(\mathscr{P}_1)^2 \mathscr{P}_2} = -\frac{i(2\pi)^2}{\Delta} \tilde{p}_1(\omega)\tilde{R}_1(\omega),$$

so that the factorization (6.17) is exact in this order. The reason why this is so simple is that with only two momenta q_1 and q_2 there is no way for the momenta to become ''entangled,'' and so there is only really one possible functional form. The fact that the numerical coefficients match up exactly is the important thing. The three loop case is more involved because now the entanglement can occur, and this leads to the factorization not being exact. For both the unitary and orthogonal cases, however, we get the same functional form in the remainder,

$$Q_3(\omega) + \frac{i(2\pi)^2}{\Delta}[\tilde{R}_1(\omega)\tilde{p}_2(\omega) + \tilde{R}_2(\omega)\tilde{p}_1(\omega)]$$
$$= -\frac{2i\Delta^2}{\pi\beta^2 L^d} \sum_{q_1,q_2,q_3} \left\{ \frac{4}{(\mathscr{P}_1)^2 \mathscr{P}_2 \mathscr{P}_3} - \frac{2(\mathscr{P}_{12}+\mathscr{P}_{23})}{(\mathscr{P}_1)^2 \mathscr{P}_2 \mathscr{P}_3 \mathscr{P}_{123}} + \frac{1}{\mathscr{P}_1 \mathscr{P}_2 \mathscr{P}_3 \mathscr{P}_{123}} \right\}.$$

The remainder can then be algebraically manipulated to give

$$\frac{2\Delta^2}{3\pi\beta^2 L^d} \frac{\partial}{\partial(i\omega)} \sum_{q_1,q_2,q_3} \left\{ \frac{i\omega}{\mathscr{P}_1 \mathscr{P}_2 \mathscr{P}_3 \mathscr{P}_{123}} \right\}. \tag{6.23}$$

At the three-loop level we see that the factorization is not exact, but that the remainder term is simple and its momentum integrals are fully convergent. Certainly for the orthogonal case many terms have been removed to yield this remainder. We next note that in the special case of two dimensions this remainder is zero, and the factorization is exact. This is because for $d=2$ dimensional analysis shows that the term inside the derivative is a constant – it is of the form $(-i\omega)^0$, and no logarithmic singularities are present – and so one gets zero upon taking derivative. Even if the remainder were not able to be written as a derivative, but just as a sum of terms with no logarithmic singularities, it would yield zero. This is because dimensional analysis shows that the result is of the form $a/(-i\omega)$, where a is a real constant. Since we have to take the real part of this to get $R(\omega)$ this would give zero. However in this case there would be a constant contribution to the Fourier transform $K(t)$, because $a/(-i\omega)$ does actually have a real part proportional to $\delta(\omega)$ – this is exactly what happens in the case of the 1-loop contribution in $d=2$. We note that our factorization is exact to 3-loop order in $d=2$ even in the sense of getting the constant term in $K(t)$ correct.

It seems to us that the exactness of factorization up to three-loop order in $d=2$ for both orthogonal and unitary cases is no accident, and we conjecture that this result persists to all orders in perturbation theory. Obviously such a conjecture cannot be proved using order-by-order analysis (although, of course, it could be disproved this way), so any attempt to verify this will require analysis of the structure of $R(\omega)$, $p(\omega)$ and $Q(\omega)$ diagrams.

D. Comparison of the two factorization schemes

In this section we will compare the two factorization schemes that we have introduced in this paper: the t-space scheme that arose from consideration of the Brownian motion model of section III, and the ω-space scheme that arose in the diagrammatic analysis of section VI. We have shown that the ω-space scheme is exact to 2-loop order in all dimensions, and to 3-loop order in the 2d case. We will now examine the validity of the t-space scheme. This involves very little extra work

because most of the algebraic manipulation has already been performed in the ω-space analysis. We first compare the two relations by writing both of them in t-space to yield

$$K(t)-(2\pi\hbar\rho)^{-1}tp(t)=-(\pi\hbar\rho)^{-1}\int_{0+}^{t}dt'K(t')p(t-t'), \tag{6.24a}$$

$$K(t)-(2\pi\hbar\rho)^{-1}tp(t)=-(\pi\hbar\rho)^{-1}K(t)\int_{0}^{t}p(t'), \tag{6.24b}$$

where, of course, we know the region of validity of the first formula. To investigate the t-space factorization we need only compare the r.h.s. of the above equations. In the 2-loop case the $K(t)$ and $p(t)$ in the r.h.s. will both be of 1-loop order, and we know that $p_1(t) \propto t^{-d/2}$ and $K_1(t) \propto t^{1-d/2}$. We find that the two equations above only agree for $d=2$, where $K_1(t)=1$. The t-space factorization is therefore exact to 2-loops only in 2d, and we restrict ourselves to the 2d case from now on.

To look at the t-space scheme to 3-loop order in 2d we note that we can have the combinations K_1, p_2 and K_2, p_1. For the unitary case $K_2(t)=0$, so this leaves only the first contribution, and since $K_1(t)=1$ the two factorizations become the same. For the orthogonal case we have to look at the second contribution. We find that the two equations differ by a constant. For the purpose of calculating the asymptotic behavior of $R(\omega)$, constant terms in $K(t)$ have no effect, so that the t-space factorization works up to 3-loop order in 2d for both orthogonal and unitary cases.

At this point it seems that the ω-space scheme may be perturbatively slightly more accurate than the t-space scheme in that it is correct in 2-loops for all dimensions, and at 3-loop order it gets the constant term in $K(t)$ correct in the orthogonal case. However we are still justified in saying that both schemes are correct to 3-loop order in 2d.

VII. SUMMARY

In this paper we have examined spectral correlations in disordered conductors, starting from the idea [Eq. 4.2] that two samples with impurity configurations differing by an infinitesimal amount should be statistically equivalent. In the first instance, this equivalence yields an identity relating two-point to three-point correlation functions; it is useful only if one can decouple the latter. We argue that a decoupling based on the Kirkwood superposition approximation is physically reasonable provided one is interested only in correlations at scales large compared to the mean level spacing. Within this approximation, we express [Eq. 2.5] both the non-parametric and the parametric spectral form factor in terms of the quantum return probability for a spreading wavepacket. We test the decoupling by calculating corrections, using the standard diagrammatic perturbation theory for disordered conductors to expand about the metallic limit in inverse powers of the dimensionless conductance, g. We show that in two-dimensional systems, the case of greatest interest, there are no corrections to order g^{-3}. We believe that the results we obtain from this approach should be useful rather generally, and especially when a diagrammatic analysis is not straightforward, as at the Anderson transition; the implications of our work in that regime will be discussed elsewhere.

Note added: Since completing this work, we have become aware of an earlier discussion by Wilkinson,[24] in which the effects of eigenfunction correlations on Brownian level dynamics are investigated, using periodic orbit theory to treat the semiclassical limit.

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Integrability and disorder in mesoscopic systems: Application to orbital magnetism

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We present a semiclassical theory of weak disorder effects in small structures and apply it to the magnetic response of non-interacting electrons confined in integrable geometries. We discuss the various averaging procedures describing different experimental situations in terms of one- and two-particle Green functions. We demonstrate that the anomalously large zero-field susceptibility characteristic of clean integrable structures is only weakly suppressed by disorder. This damping depends on the ratio of the typical size of the structure with the two characteristic length scales describing the disorder (elastic mean-free-path and correlation length of the potential) in a power-law form for the experimentally relevant parameter region. We establish the comparison with the available experimental data and we extend the study of the interplay between disorder and integrability to finite magnetic fields. © *1996 American Institute of Physics.* [S0022-2488(96)01310-2]

I. INTRODUCTION

Electronic mesoscopic systems offer nowadays the possibility of being used as a laboratory for studying quantum chaos. The main question of this novel discipline — the quantum signatures of the underlying classical dynamics — can be addressed in microstructures defined on high mobility semiconductor heterojunctions. This connection presents a considerable challenge to experimentalists since it implies complicated fabrication processes and delicate measurements. The challenge for theoreticians is not any less complicated since semiconductor microstructures are very rich condensed matter systems (involving effects of temperature, confinement, disorder, electron-electron and electron-phonon interactions, etc.) where the applicability and validity of simple models has to be clearly established.

Within the simple model of a particle-in-a-billiard, important differences have been predicted,[1] and later measured,[2,3] in the transport through chaotic and integrable geometries. In the former nearby trajectories diverge exponentially and periodic orbits are usually isolated; the latter are characterized by having as many constants of motion in involution as degrees of freedom, and periodic orbits are organized in families on invariant tori.[4] Chaotic cavities exhibit a universal behavior for the conductance fluctuations and weak-localization, characterized by a single scale. On the contrary, integrable cavities do not show generic behavior presenting more fine-scale fluctuations and a non-Lorentzian line-shape of the low-field magneto resistance. In the case of thermodynamical properties like the magnetic susceptibility, the differences between chaotic and integrable billiards are more spectacular since they involve an order-of-magnitude enhancement of

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the low-field susceptibility of integrable geometries compared to that of chaotic ones.[5–7] Unlike the transport problem, the predicted different behavior according to the integrability of the underlying classical mechanics, has not been experimentally confirmed.

The residual disorder present in actual microstructures plays a special role in the quantum chaos studies. Indeed, any perturbing potential, such as the one provided by the disorder, immediately breaks the integrable character of the classical dynamics. Since small amounts of disorder are unavoidable in actual microstructures, the question of whether or not integrable behavior should be observed, naturally arises. It is then of foremost importance to establish if the differences between chaotic and integrable geometries persist when we go beyond the particle-in-a-box model. This interplay between integrability and disorder is the main subject of this paper.

We start by characterizing the disorder. One limiting case is the absence of it, where the dynamics is determined by the non-random confinement potential (particle-in-a-box or *clean* models). On the other extreme we have the *diffusive* limit where the electron motion is a random walk between the impurities and the confining effects are not important. The strength of the disorder in the diffusive case is characterized by the transport mean free path l_T: the mean distance over which the electron momentum is randomized. When l_T becomes of the order of the typical size a of the microstructure, confinement *and* disorder are relevant. For $l_T > a$ we arrive at the *ballistic* regime where electrons can traverse the structure with a small drift in their momentum (going along almost straight lines), and their dynamics is mainly given by the bounces off the walls of the confining potential. In the ballistic regime the underlying classical mechanics still depends on the geometry and we would like to understand the different role of disorder in integrable and chaotic geometries.

For short range impurity potentials (as typically found in metallic samples) the scattering is isotropic (s-type) and the momentum is randomized after each collision with an impurity. There is therefore only one length scale, namely l_T, characterizing the disorder. For smooth impurity potentials (as typically realized in high-mobility microstructures) the scattering is forward directed and l_T may be significantly larger than the elastic mean free path l associated to the total amplitude diffracted by the disorder.[8] The regime $l_T > a > l$ is particularly interesting because it is ballistic (since the classical mechanics is hardly affected by disorder), but the single particle eigenstates are short lived. In a more technical language that we will precise in the sequel, we have l given by a single-particle Green function and l_T by a two-particle Green function.[9] We will study the interplay between disorder and confinement for physical observables that depend on one- and two-particle Green functions, concentrating on the magnetic susceptibility of individual and ensembles of ballistic microstructures.

The natural tools to attack the interplay between disorder and confinement are semiclassical expansions since they transparently convey at the quantum level the information about the classical mechanics. Supersymmetry[10] and random matrix theories are quite powerful methods that have been widely used in recent studies of quantum chaos and disordered systems,[11–14] but are not applicable to our regime of interest since they deal with the ergodic universal (long time) properties of completely chaotic systems. Diagrammatic perturbation theory for the disorder can describe the diffusive regime,[15] but calculations become exceedingly complicated when the confinement and the detailed nature of the impurity potential has to be considered.

In our semiclassical approach we emphasize the dependence of disorder effects on the ratio between the finite system size a and the disorder correlation length ξ, showing that confined systems exhibit strong deviations from the bulk-behavior. In particular we demonstrate that for integrable geometries the effect of smooth disorder results in a power-law damping of the two-particle Green function properties, and we compare this behavior with that expected in chaotic systems. For completeness of the presentation we first briefly review in Sec. II our work on the magnetic response of clean systems.[5,6] We then develop in detail a treatment of disorder in ballistic microstructures extending some preliminary work.[16] In Sec. III we present the disorder model and some general implications at the level of one- and two-particle Green functions. In

Secs. IV and V we focus on the impurity averaged magnetic susceptibility for individual and ensembles of microstructures.

II. ORBITAL MAGNETISM IN CLEAN SYSTEMS: A BRIEF REVIEW

A. Thermodynamic formalism

In this section we present the basic thermodynamical formalism for obtaining the orbital magnetism within a semiclassical approach. We indicate the main ideas for its application to clean microstructures[5,6] which will be further developed in Secs. IV and V in order to allow for the treatment of static disorder. The principle is to derive thermodynamical expressions for the free energy and the grand potential using a semiclassical approximation for the density of states. This allows us to calculate physical observables such as the magnetic susceptibility for the canonical and grand canonical ensembles.

For a system of electrons confined to an area A at temperature T and subject to a perpendicular magnetic field H, the free energy $F(T,H,\mathbf{N})$ for a fixed number $\mathbf{N}$ of electrons and the grand potential $\Omega(T,H,\mu)$ (representing the coupling to a particle reservoir with chemical potential μ) are related by means of the Legendre transform

$$F(T,H,\mathbf{N})=\mu\mathbf{N}+\Omega(T,H,\mu). \tag{2.1}$$

The canonical (χ) and grand canonical (χ^{GC}) susceptibilities of a confined electron gas are given by

$$\chi=-\frac{1}{A}\left(\frac{\partial^2 F}{\partial H^2}\right)_{T,\mathbf{N}}, \quad \chi^{\mathrm{GC}}=-\frac{1}{A}\left(\frac{\partial^2 \Omega}{\partial H^2}\right)_{T,\mu}. \tag{2.2}$$

The grand potential can be expressed in the form

$$\Omega(T,H,\mu)=-\frac{1}{\beta}\int \mathrm{d}E\, d(E)\, \ln[1+\exp(\beta(\mu-E))] \tag{2.3}$$

(with $\beta=1/k_B T$) in terms of the single-particle density of states $d(E)$ which we decompose into a smooth mean and oscillating part according to

$$d(E)=\overline{d}(E)+d^{\mathrm{osc}}(E). \tag{2.4}$$

As has first been noticed in the context of persistent currents in disordered rings,[17] a distinction between χ and χ^{GC} may be of crucial importance in mesoscopic thermodynamics: Although the number of electrons can be large for a mesoscopic system, the fact that $\mathbf{N}$ is fixed must be taken into account (by working in the canonical formalism) if a disorder or energy averaged magnetic response of an *ensemble* of isolated microsystems is examined. According to Imry[18] a convenient representation for the canonical free energy in terms of grand canonical quantities is obtained by expanding the relationship (2.1) to second order in $\mu-\overline{\mu}$ with a mean chemical potential $\overline{\mu}$ being implicitly defined by accommodating $\mathbf{N}$ charge carriers with the mean number of states

$$\mathbf{N}=N(\mu)=\overline{N}(\overline{\mu}). \tag{2.5}$$

Here

$$N(\mu)=\int_0^\infty \mathrm{d}E\, d(E) f(E-\mu) \tag{2.6}$$

with the Fermi distribution function

$$f(E-\mu)=\frac{1}{1+\exp[\beta(E-\mu)]}. \tag{2.7}$$

$\overline{N}$ is obtained in Eq. (2.5) by replacing $d(E)$ by $\overline{d}(E)$. This finally allows an expansion of the free energy as[17]

$$F(\mathbf{N})\simeq F^0+\Delta F^{(1)}+\Delta F^{(2)}, \tag{2.8}$$

with

$$F^0=\overline{\mu}\mathbf{N}+\overline{\Omega}(\overline{\mu}), \tag{2.9a}$$

$$\Delta F^{(1)}=\Omega^{\mathrm{osc}}(\overline{\mu}), \tag{2.9b}$$

$$\Delta F^{(2)}=\frac{1}{2\overline{d}(\overline{\mu})}(N^{\mathrm{osc}}(\overline{\mu}))^2. \tag{2.9c}$$

The functions $\Omega^{\mathrm{osc}}(\overline{\mu})$ and $N^{\mathrm{osc}}(\overline{\mu})$ are expressed by means of Eqs. (2.3) and (2.6), respectively, upon inserting the oscillating part $d^{\mathrm{osc}}(E)$ of the density of states (2.4). The leading order contribution to F is given by the first two terms $F^0+\Delta F^{(1)}$ yielding the susceptibility calculated in the *grand* canonical case. F^0 gives rise to the (two-dimensional) diamagnetic Landau-susceptibility which for billiard-like systems is expressed as for the bulk as

$$-\chi_L=-\frac{g_s e^2}{24\pi mc^2} \tag{2.10}$$

with $g_s=2$ the spin degeneracy.

B. Semiclassical treatment of susceptibilities

For a semiclassical computation of $\Delta F^{(1)}$ and $\Delta F^{(2)}$ and their derivatives with respect to H we calculate $d^{\mathrm{osc}}(E,H)$ from the trace

$$d(E,H)=-\frac{g_s}{\pi}\,\mathrm{Im}\int d\mathbf{r}\; G_E(\mathbf{r},\mathbf{r}) \tag{2.11}$$

of the semiclassical one-particle Green function. Its contribution to $d^{\mathrm{osc}}(E)$ is given by[4]

$$G_E(\mathbf{r}',\mathbf{r})=\sum_t D_t \exp\left[i\left(\frac{S_t}{\hbar}-\eta_t\frac{\pi}{2}\right)\right], \tag{2.12}$$

as the sum over all classical paths t (of non-zero length) joining $\mathbf{r}$ to $\mathbf{r}'$ at energy E.

$$S_t=\int_{\mathscr{C}_t}\mathbf{p}d\mathbf{q} \tag{2.13}$$

is the classical action integral along the path $\mathscr{C}_t$. The amplitude D_t takes care of the classical probability conservation, and η_t is the Maslov index.

The evaluation of the trace integral (2.11) for chaotic and integrable systems leads to the Gutzwiller[4] and Berry–Tabor[19] periodic-orbit trace formulas, respectively. In order to calculate the magnetic susceptibility at small fields one has to carefully distinguish[6] between the three

possibilities of a chaotic billiard, the special case of an integrable billiard remaining integrable upon inclusion of the H-field, and the more general case where the field acts as a perturbation breaking the integrability of a regular structure.

Since our main interest in Secs. III, IV and V will be devoted to disorder effects on the susceptibility of billiards being integrable at zero H-field we will focus here on the last case. There neither Gutzwiller nor Berry–Tabor-trace formulas are directly applicable and, following Ozorio de Almeida,[20] a uniform treatment of the perturbing H-field is necessary. In the integrable zero-field limit each closed trajectory belongs to a torus $I_{\mathbf{M}}$ and we can replace $\mathbf{r}$ in the trace integral (2.11) by angle coordinates Θ_1 specifying the trajectory within the (one-parameter) family and by the position Θ_2 on the trajectory. For small magnetic field the classical orbits can be treated as essentially unaffected while the field acts merely on the phases in the Green function in terms of the magnetic flux through the area $\mathscr{A}_{\mathbf{M}}(\Theta_1)$ enclosed by each orbit of family $\mathbf{M}$. Evaluating the trace integral (2.11) along Θ_2 for the semiclassical Green function of an integrable system leads in this approximation to a factorization of the density of states

$$d^{\mathrm{osc}}(E)=\sum_{\mathbf{M}\neq 0}\mathscr{C}_{\mathbf{M}}(H)\,d^0_{\mathbf{M}}(E) \tag{2.14}$$

into the contribution from the integrable zero-field limit

$$d^0_{\mathbf{M}}(E)=\widetilde{D}_{\mathbf{M}}\cos\left(k_F L_{\mathbf{M}}-\eta_{\mathbf{M}}\frac{\pi}{2}-\frac{\pi}{4}\right) \tag{2.15}$$

($L_{\mathbf{M}}$ is the length of the orbits of family $\mathbf{M}$ and $\widetilde{D}_{\mathbf{M}}$ the semiclassical weight[19]) and the function

$$\mathscr{C}_{\mathbf{M}}(H)=\frac{1}{2\pi}\int_0^{2\pi}\mathrm{d}\Theta_1\cos\left[2\pi\frac{H.\mathscr{A}_{\mathbf{M}}(\Theta_1)}{\Phi_0}\right] \tag{2.16}$$

containing the H-field dependence ($\Phi_0=hc/e$). Calculating $\Delta F^{(1)}$ from Eq. (2.9b) and taking the derivatives with respect to H gives the grand canonical contribution to the susceptibility at small magnetic field

$$\frac{\chi^{(1)}}{\chi_L}=-\frac{24\pi}{g_s}mA\left(\frac{\Phi_0}{2\pi A}\right)^2\sum_{\mathbf{M}}\frac{R_T(\tau_{\mathbf{M}})}{\tau^2_{\mathbf{M}}}d^0_{\mathbf{M}}(\mu)\frac{d^2\mathscr{C}_{\mathbf{M}}}{dH^2}. \tag{2.17}$$

Here, $\tau_{\mathbf{M}}$ is the period of a closed orbit of family $\mathbf{M}$ and

$$R_T(\tau)=\frac{\tau/\tau_c}{\sinh(\tau/\tau_c)};\quad \tau_c=\frac{\hbar\beta}{\pi} \tag{2.18}$$

is a temperature damping factor which arises from the convolution integral in Eq. (2.3) and gives an exponential suppression of long orbits. This is important from a physical as well as computational point of view, as conceptual difficulties associated with the questions of absolute convergence of semiclassical expansions at zero temperature do not arise.

Eq. (2.17) is the basic equation for the susceptibility of an individual microstructure. When considering ensembles of ballistic microstructures however, an average $\overline{(\cdot)}$ over energy (i.e., k_F) or over the system size a usually has to be performed and leads to variations in the phases (actions $S/\hbar=k_F L_{\mathbf{M}}$) of the density of states (2.15) which are much larger than 2π. Therefore, $\chi^{(1)}$ vanishes upon ensemble average. In order to characterize the orbital magnetism of ensembles we introduce the *typical* susceptibility $\chi^{(\mathrm{t})}=(\overline{\chi^2})^{1/2}$ (the width of the distribution) and the ensemble average $\overline{\chi}$ [its mean value, which is non-zero because of the term $\Delta F^{(2)}$ in the expansion

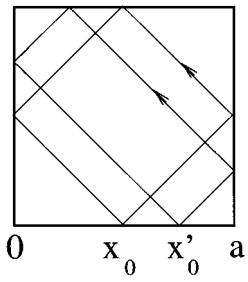

FIG. 1. Two representative periodic orbits characterized by x_0 and x_0' belonging to the family $\mathbf{M}=(1,1)$ (denoting one bounce with each wall) of a square billiard of length a.

Eq. (2.8)]. The typical and ensemble average susceptibilities are of theoretical interest since they are based on two-particle Green functions and are relevant for the description of experiments on ensembles of mesoscopic systems.

If we assume that there are no degeneracies in the lengths of orbits from different families $\mathbf{M}$ we obtain for $\chi^{(t)}$

$$\left(\frac{\chi^{(t)}}{\chi_L}\right)^2=\left(\frac{24\pi}{g_s}mA\right)^2\left(\frac{\Phi_0}{2\pi A}\right)^4\sum_{\mathbf{M}}\frac{R_T^2(\tau_{\mathbf{M}})}{\tau_{\mathbf{M}}^4}\,\overline{d_{\mathbf{M}}^0(\mu)^2}\left(\frac{d^2\mathscr{C}_{\mathbf{M}}}{dH^2}\right)^2. \tag{2.19}$$

In calculating $\overline{\chi}$, the grand canonical contribution $\chi^{(1)}$ from $\Delta F^{(1)}$ vanishes under energy average and the canonical correction $\Delta F^{(2)}$ in Eq. (2.8) gives in semiclassical approximation using Eq. (2.9c)

$$\frac{\overline{\chi}}{\chi_L}\simeq\frac{\overline{\chi^{(2)}}}{\chi_L}=-\frac{24\pi^2}{g_s^2}\hbar^2\left(\frac{\Phi_0}{2\pi A}\right)^2\sum_{\mathbf{M}}\frac{R_T^2(\tau_{\mathbf{M}})}{\tau_{\mathbf{M}}^2}\,\overline{d_{\mathbf{M}}^0(\mu)^2}\,\frac{d^2\mathscr{C}_{\mathbf{M}}^2}{dH^2}. \tag{2.20}$$

Eqs. (2.17)–(2.20) provide the general starting point for a computation of the susceptibility of integrable billiards at small fields.

As an important example, which is also of experimental relevance,[21] we will apply the results to square billiards. At finite temperature χ is essentially given by the family $\mathbf{M}=(1,1)$ of the shortest, flux-enclosing periodic orbits depicted in Fig. 1. A complete treatment including families of longer orbits is given in Ref. 6. Instead of Θ_1 we use the lower reflection point x_0 as orbit parameterization within the family. The orbits (1,1) have the unique length $L_{11}=2\sqrt{2}a$ and enclose a normalized area $\mathscr{A}(x_0)=4\pi x_0(a-x_0)/a^2$. Computation of $d_{11}^0(\mu)$ for the square geometry gives for $\chi^{(1)}$ [Eq. (2.17)]

$$\frac{\chi^{(1)}}{\chi^0}=\int_0^a\frac{dx_0}{a}\,\mathscr{A}^2(x_0)\cos(\varphi\mathscr{A}(x_0))\sin\left(k_FL_{11}+\frac{\pi}{4}\right) \tag{2.21}$$

as a function of the total flux $\varphi=Ha^2/\Phi_0$ with $\Phi_0=hc/e$. The prefactor

$$\chi^0=\chi_L\frac{3}{(\sqrt{2}\pi)^{5/2}}(k_Fa)^{3/2}R_T(L_{11}). \tag{2.22}$$

shows the $(k_Fa)^{3/2}$-dependence typical for (nearly-) integrable systems.

For the square geometry Eqs. (2.19) and (2.20) for the susceptibilities $\chi^{(t)}$ and $\overline{\chi}$ (characterizing different ensemble averages) can be reduced to [including only the dominant contributions from the family (1,1)]

$$\frac{\chi^{(t)}}{\chi^0} \simeq \frac{\sqrt{\overline{\chi^{(1)^2}}}}{\chi^0} = \frac{1}{\sqrt{2}} \int_0^a \frac{dx_0}{a} \mathscr{A}^2(x_0) \cos(\varphi.\mathscr{A}(x_0)) \tag{2.23}$$

and

$$\frac{\overline{\chi}}{\overline{\chi^0}} = \frac{1}{2} \int_0^a \frac{dx_0}{a} \int_0^a \frac{dx_0'}{a} [\mathscr{A}_-^2 \cos(\varphi.\mathscr{A}_-) + \mathscr{A}_+^2 \cos(\varphi.\mathscr{A}_+)] \tag{2.24}$$

with

$$\frac{\overline{\chi^0}}{\chi_L} = \frac{3}{(\sqrt{2}\pi)^3} (k_F a) R_T^2(L_{11}) \tag{2.25}$$

and $\mathscr{A}_\pm = \mathscr{A}(x_0) \pm \mathscr{A}(x_0')$. Although the integrals (2.21), (2.23), and (2.24) can be evaluated analytically in the clean case (leading to Fresnel functions of the magnetic flux[5]), the above expressions serve as suitable starting points for the study of disorder effects on ensembles of microstructures discussed in Secs. IV and V.

III. SEMICLASSICAL APPROACH TO WEAK DISORDER

Disorder is usually studied in terms of the ensemble average over impurity realizations, since it is a perturbation of an electrostatic potential whose detailed nature is unknown. Typically, quantum perturbation theory is followed by the average over the strengths and positions of the impurities. This approach is suited for macroscopic metallic samples (which are self-averaging) or ensembles of mesoscopic samples (where different samples present different impurity configurations). The possibility of measuring a single disordered mesoscopic sample poses a conceptual difficulty since there is not an average process involved. When discussing the effect of disorder on the orbital magnetism of microstructures, it is therefore necessary to distinguish between the behavior of an individual sample and an ensemble.[22]

Moreover, we have to consider the cases where the Fermi energy and size of the microstructures are kept fixed under impurity average and the cases where these parameters change with the different impurity realizations. These various averages, that will be thoroughly discussed in the remainder of the paper, can be expressed in terms of the impurity average of one- and two-particle Green functions. Therefore we perform in this section a general treatment of disorder effects on the basis of semiclassical expansions of Green functions. The Green function formalism, which is useful for a wide range of physical problems, can be applied to thermodynamical quantities like the magnetic susceptibility (Secs. IV and V) as well as to quantum transport problems.

1. Disorder models

Our basic assumptions for the treatment of disorder are the following: We study a spatially random potential $V(\mathbf{r})$ characterized by a correlation function

$$C(|\mathbf{r}-\mathbf{r}'|) = \langle V(\mathbf{r}) V(\mathbf{r}') \rangle \tag{3.1}$$

with a typical correlation length ξ and a mean disorder strength $C^0 = C(0)$. We will make use of a Gaussian correlation

$$C(|\mathbf{r}-\mathbf{r}'|) = C^0 \exp\left(-\frac{(\mathbf{r}-\mathbf{r}')^2}{4\xi^2} \right) \tag{3.2}$$

which allows us to derive analytical expressions for the disorder averages considered below.[23] The disorder correlation function (3.2) can be viewed as being generated by means of a realization i of a two-dimensional Gaussian disorder potential given by the sum

$$V(\mathbf{r})=\sum_{j}^{N_i}\frac{u_j}{2\pi\xi^2}\exp\left\{-\frac{(\mathbf{r}-\mathbf{R}_j)^2}{2\xi^2}\right\} \tag{3.3}$$

of the potentials of N_i *independent* impurities located at points $\mathbf{R}_j$ with uniform probability on an area V. The strengths u_j obey $\langle u_j u_{j'}\rangle = u^2\delta_{jj'}$.The disorder strength [as defined in Eq. (3.2)] is

$$C^0=\frac{u^2 n_i}{4\pi\xi^2} \tag{3.4}$$

with $n_i=N_i/\mathsf{V}$. For $\xi\to 0$ this model yields the white noise case of δ-function scatterers $V(\mathbf{r})=\Sigma_j^{N_i}u_j\delta(\mathbf{r}-\mathbf{R}_j)$. We will use the model of Gaussian disorder for some analytical calculations and for numerical quantum simulations. However, the general results expressed in terms of the correlation function $C(|\mathbf{r}-\mathbf{r}'|)$ will be valid for any kind of disorder.

As we will show, disorder effects depend on several length scales: the elastic mean free path, the Fermi-wavelength λ_F of the electrons, the disorder correlation length ξ and the size a of the microstructure. In the bulk case of an unconstrained two-dimensional electron gas (2DEG) we will distinguish between short range ($\xi<\lambda_F$) and finite range ($\xi>\lambda_F$) disorder potentials. In the case of a microstructure a third, long range regime for $\xi>a>\lambda_F$ has to be considered. The cleanest samples used in today experiments are in the finite range regime $a>\xi>\lambda_F$.[24]

2. Single-particle Green function

If we assume a microstructure with size $a\gg\lambda_F$ (a condition which is always met in lithographically defined samples) and work in the finite range or long range regime, where the disorder potential is smooth on the scale of λ_F, a semiclassical treatment is well justified. A natural starting point is the semiclassical expression (2.12) for the single-particle Green function $G_E(\mathbf{r}',\mathbf{r})$ as a sum over the contributions from classical paths. The classical mechanics of trajectories with length $L_t\ll l_T$ (the transport mean free path) is essentially unaffected by disorder. Therefore the dominant effect on the Green function in Eq. (2.12) results from shifts in the semiclassical phases due to the modification of the actions while the amplitudes D_t and topological indices η_t are nearly unchanged. The first-order approximation to the classical action (2.13) along a path $\mathscr{C}_t$ in a system with weak disorder potential is

$$S_t^d\simeq S_t^c+\delta S_t, \tag{3.5}$$

where the clean action S_t^c is obtained by integrating along the *unperturbed* trajectory $\mathscr{C}_t^c$ without disorder (i.e., $S_t^c=k_F L_t$ in the case of billiards without magnetic field) instead of the actual path $\mathscr{C}_t$. The correction term δS_t is obtained, after expanding $\mathbf{p}=\sqrt{2m[E-V(\mathbf{q})]}$ for small V/E, by the integral

$$\delta S_t=-\frac{1}{v_F}\int_{\mathscr{C}_t^c}V(\mathbf{q})\mathrm{d}q. \tag{3.6}$$

In this approximation an impurity average $\langle\ldots\rangle$ acts only on δS_t and the disorder averaged Green function reads

$$\langle G_E(\mathbf{r}',\mathbf{r})\rangle=\sum_t G_{E,t}^c(\mathbf{r}',\mathbf{r})\left\langle\exp\left[\frac{i}{\hbar}\delta S_t\right]\right\rangle. \tag{3.7}$$

Here $G^c_{E,t}$ is the contribution of the trajectory t to the zero-disorder Green function G^c_E.

For trajectories of length $L_t \gg \xi$ the contributions to δS according to Eq. (3.6) from the disorder potential at trajectory segments separated by a distance larger than ξ are uncorrelated. The related stochastic accumulation of action along the path can therefore be interpreted as determined by a random-walk process, resulting in a Gaussian distribution of $\delta S_t(L_t)$. For larger ξ or shorter trajectories ($L_t \not\gg \xi$), one can still think of a Gaussian distribution of the de-phasing δS_t provided $V(\mathbf{r})$ is generated by a sum of a large number of independent impurity potentials. As a consequence of the Gaussian character of the distribution of $\delta S_t(L_t)$, the disorder contribution involved in Eq. (3.7) is given by

$$\left\langle \exp\left[\frac{i}{\hbar}\delta S_t\right]\right\rangle = \exp\left[-\frac{\langle \delta S_t^2\rangle}{2\hbar^2}\right] \tag{3.8}$$

and therefore entirely specified by the variance

$$\langle \delta S_t^2\rangle = \frac{1}{v_F^2}\int_{\mathscr{C}_t^c} dq \int_{\mathscr{C}_t^c} dq' \langle V(\mathbf{q})V(\mathbf{q}')\rangle, \tag{3.9}$$

which is expressed as the mean of the disorder correlation function $C(|\mathbf{q}-\mathbf{q}'|)$ when the unperturbed orbit is traversed.

If we consider, to start with, an unconstrained 2DEG the sum in Eq. (3.7) is reduced to the direct trajectory joining $\mathbf{r}$ and $\mathbf{r}'$. If $L=|\mathbf{r}-\mathbf{r}'| \gg \xi$ the inner integral in Eq. (3.9) can be extended to infinity and we obtain

$$\langle \delta S^2\rangle = \frac{L}{v_F^2}\int dq\ C(\mathbf{q}). \tag{3.10}$$

The semiclassical average Green function for the bulk exhibits therefore an exponential behavior[16,25] (on a length scale $l_T > L \gg \xi$)

$$\langle G_E(\mathbf{r}',\mathbf{r})\rangle = G^c_E(\mathbf{r}',\mathbf{r})\exp\left(-\frac{L}{2l}\right), \tag{3.11}$$

with the damping governed by an inverse *elastic* mean free path

$$\frac{1}{l} = \frac{1}{\hbar^2 v_F^2}\int dq\ C(\mathbf{q}). \tag{3.12}$$

In the case of Gaussian correlation $C(\mathbf{q})$ is given by Eq. (3.2) and we get

$$l = \frac{\hbar^2 v_F^2}{\xi\sqrt{\pi}C^0}. \tag{3.13}$$

Using the disorder strength (3.4) we have

$$l = \frac{4\sqrt{\pi}\hbar^2 v_F^2 \xi}{u^2 n_i}. \tag{3.14}$$

In the Appendix we discuss the relation between the semiclassical elastic MFPs [Eqs. (3.12)–(3.14)] and the MFP obtained from quantum diagrammatic perturbation theory for the bulk for the disorder model (3.3). The semiclassical and the quantum result [Eq. (A5)] agree asymptotically to

leading order in $k_F\xi$. In the limit of small ξ, especially $\xi<\lambda_F$, our semiclassical approach is no longer applicable.[26] However, Eq. (3.11) still holds, but with l replaced by l_δ given in Eq. (A4).

We now turn from the semiclassical treatment of the bulk to that of a confined system. In the constrained case in the limit $l_T \ll a$ impurity scattering is the dominant process.[27] This gives rise to diffusive motion, and thus there is no essential difference to the bulk for the damping of the Green function. We will treat the ballistic regime $l_T > a$ where both, the confinement *and* the impurities have to be considered. The calculation of l_T in the Appendix shows that for finite ξ the transport MFP l is considerably larger than the elastic one and a ballistic treatment is therefore well justified, even if l is of the order of the system size.

In contrast to the bulk case a disorder averaged confined system is no longer translationally invariant and one has to impose in quantum calculations the correct boundary conditions of the geometry. Confinement implies semi-classically that $G_E^c(\mathbf{r}',\mathbf{r})$ is given as a sum over all direct and multiply reflected paths connecting $\mathbf{r}$ and $\mathbf{r}'$; disorder modifies the corresponding actions according to Eq. (3.6).

In the regimes of short- and finite-range scatterers, the damping of each contribution $\langle G_{E,t}\rangle$ to $\langle G_E\rangle$ is given, analogous to the bulk expression (3.11), [using Eq. (3.10)] by

$$\langle G_E(\mathbf{r}',\mathbf{r})\rangle = \sum_t G_{E,t}^c(\mathbf{r}',\mathbf{r}) \exp\left(-\frac{L_t}{2l}\right). \tag{3.15}$$

Here, L is now replaced by the trajectory length $L_t > a \gg \xi$. This gives an individual damping $\exp(-L_t/2l)$ for each geometry-affected path contributing to $\langle G_E\rangle$.

In the long range regime and for $\xi \sim a$ the correlation integral (3.9) can no longer be approximated (as for $\xi \ll L_t$) by $L\int_{-\infty}^{+\infty} dq\ C(\mathbf{q})$ due to correlations across different sectors of an orbit (with distance smaller ξ). Therefore, the orbit-geometry enters into the correlation integral. For $\xi \gg a$ we can, however, expand $C(|\mathbf{r}-\mathbf{r}'|)$ and obtain in the case of Gaussian disorder (up to first order in ξ^{-2}) $C(|\mathbf{r}-\mathbf{r}'|) \simeq C^0[1-(\mathbf{r}-\mathbf{r}')^2/(4\xi^2)]$. In this approximation the integral (3.9) gives for the Green function damping an exponent

$$\frac{\langle \delta S_t^2\rangle}{2\hbar^2} = \frac{1}{4\sqrt{\pi}} \frac{L_t^2}{l\xi}\left(1-\frac{1}{2}\frac{I_t}{\xi^2}\right). \tag{3.16}$$

$I_t = (1/L_t)\int_{\mathscr{C}_t} \mathbf{r}^2(q)\mathrm{d}q$ can be regarded as the ''moment of inertia'' of the unperturbed trajectory $\mathscr{C}_t$ with respect to its ''center of mass'' $(1/L_t)\int_{\mathscr{C}_t} \mathbf{r}(q)\mathrm{d}q$. Eq. (3.16) shows that the damping in the long range regime depends quadratically on L_t (in contrast to linear behavior in the finite range case or bulk). The length scale of damping is now given by the geometrical mean of the bulk MFP l *and* ξ. The leading damping term does not depend on the specific orbit geometry since it essentially reflects the fluctuation in the mean of the (smooth) potentials of different impurity configurations. Inclusion of higher powers of ξ^{-2} leads to additional contributions from higher moments $\int_{\mathscr{C}_t} r^n(q)\mathrm{d}q$ on the RHS of Eq. (3.16).

3. Two-particle Green function

Density correlation functions in general or the typical [Eq. (2.19)] and ensemble averaged susceptibility [Eq. (2.20)], which will be treated in the subsequent sections, involve the square of the density of states. Writing the latter, Eq. (2.11), in terms of the difference between advanced and retarded Green functions $(G^+ - G^-)$ we are left with products of one-particle Green functions. The terms of most interest are the cross products $G^+(r,r') \times G^-(r,r') = G^+(r,r')G^{+*}(r',r)$, because they survive the energy average and are sensitive to changes in the magnetic field.

Since, in the non-interacting approach we are using, the two-particle Green function factorizes into a product of one-particle Green function[28] we will use the former as a synonym for the latter. The semiclassical average for products of single-particle Green functions will be quantitatively performed for the susceptibility of confined integrable systems in Sec. V, and we discuss here the underlying ideas for the general case.

Considering for instance the product $G(r_1,r_2)G^*(r_1',r_2')$, the effect of the disorder potential can be taken into account perturbatively for each realization of the disorder in the same way as before by Eqs. (3.5)–(3.6). Using the same kind of argument, one can therefore write the disorder average as a double sum over the averaged contributions from trajectories t and t'

$$\langle G_E G_E^* \rangle = \sum_t \sum_{t'} \langle G_{E,t} G_{E,t'}^* \rangle = \sum_t \sum_{t'} G_{E,t}^c G_{E,t'}^{c*} \langle e^{(i/\hbar)(\delta S_t - \delta S_{t'})} \rangle$$
$$= \sum_t \sum_{t'} G_{E,t}^c G_{E,t'}^{c*} \exp\left[- \frac{\langle (\delta S_t - \delta S_{t'})^2 \rangle}{2\hbar^2} \right]. \tag{3.17}$$

It is necessary here, however, to take into account the correlation of the disorder potential between points on trajectories t and t'. One limiting case for instance would be that t and t' are either the same trajectory or the time reversal one of each other. In these cases their contribution acquires exactly the same phase shift and $\langle G_{E,t} G_{E,t}^* \rangle = |G_{E,t}^c|^2$. Within our approximation the diagonal contributions $t=t'$, which, e.g., are responsible for the classical part of the conductivity, remain thus disorder-unaffected, since we assume the trajectories have a length much smaller than l_T. (A semiclassical consideration of these effects for trajectories of length of the order of l_T or larger was performed in Ref. 25 for the bulk, giving a damping of the two-point Green function on the scale of l_T.) At the opposite extreme, if trajectories t,t' are completely uncorrelated, i.e., for long trajectories in classical chaotic systems or trajectories in integrable systems with a spatial distance larger than ξ, the average in Eq. (3.17) factorizes: $\langle G_{E,t} G_{E,t'}^* \rangle = \langle G_{E,t} \rangle \cdot \langle G_{E,t'}^* \rangle$ and lead to single-particle damping behavior.

The double sum Eq. (3.17) may however involve pairs of trajectories which stay within a distance of the order of ξ (as for nearby paths on a torus of an integrable system). In this case the behavior of $\langle G_{E,t} G_{E,t'}^* \rangle$ is more complicated and depends of the confinement geometry of the system under consideration. As a simple illustration of the interplay between disorder correlation and families of orbits, let us consider for the case of the bulk the product of $G(r_1,r_2)$ joining $r_1=(0,0)$ to $r_2=(L,0)$ with $G^*(r_1',r_2')$ joining $r_1=(0,y)$ to $r_2=(L,y)$, with $L \gg \xi$ but y possibly of the order of ξ. Introducing the function

$$K(y) = \int_{-\infty}^{+\infty} C(x,y)\mathrm{d}x \tag{3.18}$$

[for Gaussian correlations Eq. (3.2), $K(y)/K(0) = \exp(-y^2/(4\xi^2))$], the variance of the de-phasing is obtained as

$$\langle (\delta S_t - \delta S_{t'})^2 \rangle = 2L \frac{(K(0)-K(y))}{v_F^2} \tag{3.19}$$

and therefore $\langle G_E G_E^* \rangle = G_E^c G_E^{c*} \tilde{f}(y)$ with

$$\tilde{f}(y) = \exp\left[- \frac{L}{l} \left(1 - \frac{K(y)}{K(0)} \right) \right]. \tag{3.20}$$

The function $\tilde{f}(y)$ expresses in a very simple way that as $y \to 0$, the effect of disorder disappears ($\tilde{f}(0)=1$) while for $y \gg \xi$ the function $\tilde{f}(y)$ behaves as the square of single particle Green function damping.

IV. FIXED-SIZE IMPURITY AVERAGE OF THE MAGNETIC SUSCEPTIBILITY

We consider here a disorder average (which will henceforth be called a fixed-size impurity average) of an ensemble of structures for which the parameters of the corresponding clean system (geometry, size, chemical potential) remain fixed under the change of impurity realizations. In Sec. V, we will then treat the more realistic case of the orbital magnetic response of a *combined* energy (or size) and disorder average.

As shown in the previous section, averages over weak disorder exponentially damp, but do not completely suppress oscillatory contributions (with phase $k_F L_t$) to the single-particle Green function from geometrical paths in confined systems. An observable quantity dependent on these contributions is the disorder averaged susceptibility of an ensemble of billiards of the same size or same clean-system Fermi energy, which will be studied first.

We will treat regular billiards at zero or small magnetic fields, where the integrability is approximately maintained and the density of states has the H-dependence of the formulae (2.14)–(2.16). The general result for $\chi^{(1)}$, Eq. (2.17), formally persists with the replacement of $\mathscr{C}_{\mathrm{M}}$ by

$$\langle \mathscr{C}_{\mathbf{M}}(H) \rangle = \frac{1}{2\pi} \int_0^{2\pi} \mathrm{d}\Theta_1 \, \cos\left[2\pi \frac{H \mathscr{A}_{\mathbf{M}}(\Theta_1)}{\Phi_0} \right] \exp\left[- \frac{\langle (\delta S_{\mathrm{M}}(\Theta_1))^2 \rangle}{2\hbar^2} \right], \tag{4.1}$$

where $\langle \delta S_{\mathrm{M}}^2(\Theta_1) \rangle$ is given by Eq. (3.9) with the integrals performed along the orbits of the family **M** parameterized by Θ_1. In the finite range case (if all orbits of a family **M** are of the same length as in billiards) each family exhibits a unique disorder damping giving a contribution

$$\langle \chi_{\mathrm{M}}^{(1)} \rangle = \chi_{\mathrm{M}}^{(1)} \cdot \exp\left(- \frac{\langle \delta S_{\mathrm{M}}^2 \rangle}{2\hbar^2} \right) \tag{4.2}$$

to the ballistic susceptibility. $\chi_{\mathbf{M}}^{(1)}$ is the contribution of family **M** to the clean susceptibility [Eq. (2.17)] and $\langle \delta S_{\mathrm{M}}^2 \rangle / 2\hbar^2 = L_{\mathrm{M}}/2l$.

In the case of square billiards, where the dominant contribution stems from the family (1,1), we obtain, in analogy with Eq. (2.21),

$$\frac{\langle \chi \rangle}{\chi^0} \simeq \frac{\langle \chi^{(1)} \rangle}{\chi^0} = \int_0^a \frac{\mathrm{d}x_0}{a} \mathscr{A}^2(x_0) \cos(\varphi_{\mathscr{A}}(x_0)) \left\langle \sin\left(k_F L_{11} + \frac{\pi}{4} + \frac{\delta S(x_0)}{\hbar} \right) \right\rangle \tag{4.3}$$

with χ^0 given by Eq. (2.22). For a square billiard $\delta S(x_0)$ is independent of x_0 for the finite- as well as for the long-range regime since $I_{11} = a^2/12$ [entering into Eq. (3.16)] is the same for all orbits (11). Therefore Eq. (4.2) with $\mathbf{M}=(1,1)$ holds for both limiting cases. In the same way as for the damping of the one-particle Green function [Eq. (3.15)] we obtain for square billiards at finite temperature in the finite range regime

$$\langle \chi \rangle \simeq \langle \chi^{(1)} \rangle = \chi_{\mathrm{cl}}^{(1)} \cdot \exp\left(- \frac{L_{11}}{2l} \right), \tag{4.4}$$

where $\chi_{\mathrm{cl}}^{(1)}$ denotes the susceptibility of the system without disorder.

In order to control the validity of our analytical semiclassical approximations we performed numerical quantum calculations by diagonalizing the Hamiltonian for non-interacting particles in a square billiard subject to a uniform perpendicular magnetic field and a random disorder potential of the form of Eq. (3.3). For a given selected correlation length ξ a quantum mechanically

calculated elastic MFP l_{qm} and a fixed Fermi momentum k_F the product of the impurity density and squared mean impurity potential, $n_i u^2$, is determined by Eqs. (A3) and (A4). We found that our numerical results are essentially independent of the choice of n_i (with u^2 adjusted accordingly) for $n_i \geqslant 200$ and used this value for the calculations presented here. The positions $\mathbf{R}_j$ of the impurities were chosen as independently distributed and for the u_j we used a box distribution.

Each impurity configuration α has a self-averaging effect for an *individual* square billiard (for $\xi < a$) due to the differences of the impurity potential $V_\alpha(\mathbf{r})$ across the structure. In an *average* over an ensemble of square billiards, differences in the mean impurity potential $\overline{V_\alpha} = (1/a^2)\int \mathrm{d}\mathbf{r} V_\alpha(\mathbf{r})$ (the integral is taken over the area of the billiard) between different squares lead to an additional damping. It is characterized by the variance

$$\langle \overline{V^2} \rangle = \frac{u^2 n_i}{a^2 \eta^2}\left[\eta\ \mathrm{erf}(\eta) + \frac{1}{\sqrt{\pi}}(e^{-\eta^2} - 1)\right]^2; \quad \eta = \frac{a}{2\xi} \tag{4.5}$$

$$\rightarrow \frac{u^2 n_i}{4\pi\xi^2} \quad \text{for } \xi/a \rightarrow \infty \tag{4.6}$$

$$\rightarrow \frac{u^2 n_i}{a^2} \quad \text{for } \xi \rightarrow 0. \tag{4.7}$$

In the limit of $\xi \gg a$ our numerical calculations showed that the self-averaging effect is negligible (since the impurity potential is essentially flat across the square) and the clean susceptibility of an *individual* structure remains practically unaffected by disorder. In this limit variations in the mean potential V of an ensemble [Eq. (4.6)] dominate the damping. In the limit of short range disorder, fluctuations in the mean V of different samples play a minor role and self-averaging is the predominant process for an integrable system: In semi-classical terms different trajectories of a family of closed orbits are perturbed by white noise disorder in an uncorrelated manner. Therefore we do not observe considerable differences between the susceptibility of a single disordered billiard of integrable geometry and the corresponding ensemble for $\xi \ll a$. In a chaotic billiard this self-averaging effect does not exist (for not too small ξ, see end of Sec. V), since orbits are isolated. Therefore distinct differences between an individual disordered sample and an ensemble of disordered billiards are expected.

To improve the statistics of our numerical ensemble average for square billiards we performed an average over disorder configurations with the same mean V and in addition averaged over V according to Eq. (4.5).[29] Fig. 2 shows results of the numerical quantum simulations for the average susceptibility $\langle \chi \rangle$ of an ensemble of squares with fixed size but different disorder realizations at a temperature $k_B T = 3\mathrm{g}_\mathrm{s}\Delta$, where Δ is the mean level spacing. The characteristic oscillations in $k_F a$ show an interchange between para- and dia-magnetic behavior on a scale $k_F L_{11}$. This indicates that they are dominated by contributions from the shortest flux-enclosing orbits of the family (1,1) [according to Eqs. (2.17) and (4.3)], as has been already shown for the *clean* case in Refs. 5 and 6. Fig. 2 demonstrates the damping of the clean susceptibility (dotted line) with decreasing elastic MFP $l/a = 4, 2, 1, 0.5$ for fixed $\xi/a = 0.1$ (which represents a typical disorder correlation length in experimental realizations). Variations in the mean V lead to a de-phasing of the oscillations in the finite range case on a scale $(\delta k)a \sim (4\pi)^{1/4}\sqrt{\xi/l_{\mathrm{qm}}(\xi)}$ which is, as discussed above, small compared to the self-averaging effect in this regime.

Figure 3 depicts the quantitative comparison between numerical and analytical results: It shows the logarithm of $\langle \chi \rangle$ normalized to the corresponding zero-disorder susceptibility as a function of the inverse MFP for different correlation lengths ξ. The semi-classically predicted exponential damping [Eq. (4.2)] is shown as straight lines for the short range [$\xi \ll a$, Eq. (3.11),

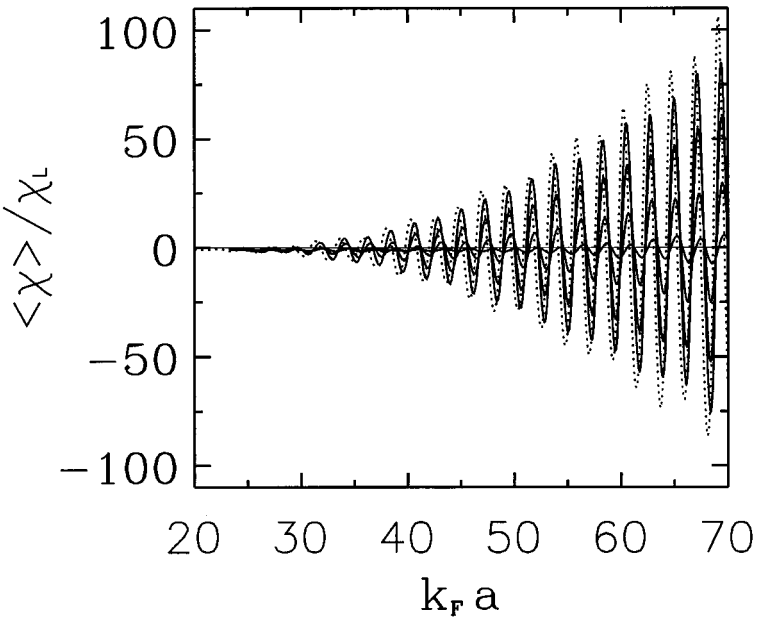

FIG. 2. Magnetic susceptibility $\langle\chi\rangle$ (normalized with respect to the Landau susceptibility χ_L) of a square billiard as a function of $k_F a$ for the clean case (dotted) and for the ensemble average of billiards of fixed size with increasing Gaussian disorder ($\xi/a=0.1$) according to an elastic mean free-path $l/a=4$, 2, 1, 0.5 (solid lines in the order of decreasing amplitude). The susceptibility is calculated for zero magnetic field and at a temperature equal to 6 level spacings.

full line for $\xi=0$] and long range [$\xi>a$, Eq. (3.16), dotted lines for $\xi/a=4$, 2, 1 from the top]. The semiclassical predictions accurately agree with the corresponding quantum results (symbols) for $\xi/a=4$, 2, 1, 0 and fail for intermediate values $\xi/a=0.5$, 0.2 (squares and diamonds) which are off the range of validity of the approximations. The transition from self-averaging dominated ($\xi\to 0$) suppression to damping according to fluctuations in the floor V (for $\xi/a\to\infty$) turns out to be non-monotonic.

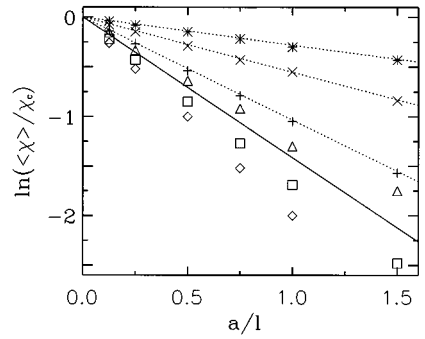

FIG. 3. Logarithm of the ratio $\langle\chi\rangle/\chi_{cl}$ as a function of the inverse elastic MFP a/l. The symbols indicate the numerical quantum results (from the top for $\xi/a=4$, 2, 1, 0, 0.5 and 0.2. The dotted lines show the semiclassical analytical results for $\xi/a=4$, 2, 1 (from above) according to Eq. (3.16). The full line is the semiclassical result for $\xi=0$ [Eq. (3.11)]. The quantum results for $\xi=0.5$ (squares) and 0.2 (diamonds) are beyond the regime of validity of the analytical limits $\xi/a\gg 1$ and $\xi/a\ll 1$.

V. COMBINED IMPURITY- AND ENERGY-AVERAGE OF THE SUSCEPTIBILITY

In currently experimentally realizable structures disorder averages cannot be performed independently from size-averages since the detailed features of the confining potential do not remain unchanged for different impurity configurations. From the basic expressions (2.21) and (4.3) for the susceptibility we see that changes in size a give rise to rapid variations in the phase $k_F a$ (on a quantum scale) and a much slower secular variation through the geometrical factors $\mathscr{A}$. Thus, the effect of small size variations is equivalent to an energy (k_F) average. As discussed in Sec. II for the clean case, variations in k_F lead to vanishing $\chi^{(1)}$. Therefore we have to use the typical and energy averaged susceptibilities [see Eqs. (2.19) and (2.20) for their definition in the clean case]. When disorder is introduced we must consider energy- *and* disorder averages. The typical susceptibility is now defined by $\chi^{(t)}=\langle\overline{\chi^2}\rangle^{1/2}$. It applies to the case of repeated measurements on a given microstructure when different impurity realizations (and simultaneous changes in k_F) are obtained by some kind of perturbation (e.g., cycling to room temperature). From now on we will reserve the term $\chi_{\rm cl}^{(t)}$ for the clean typical susceptibility $(\overline{\chi^2})^{1/2}$. The energy and impurity averaged susceptibility $\langle\overline{\chi}\rangle$ describes the magnetic response of an ensemble of a large number of microstructures with different impurity realizations and variations in size. This is the situation of the experiment of Ref. 21 that we discuss in the sequel.

A. Integrable systems: The square billiard

The semiclassical results for $\chi^{(t)}$ and $\langle\overline{\chi}\rangle$ for a system of integrable geometry are obtained in an analogous way as we proceeded for $\langle\chi\rangle$ in Sec. IV, that is by including in the integral (2.16) for $\mathscr{C}_{\mathbf{M}}$ a Θ_1-dependent disorder-induced phase $\exp(i\delta S(\Theta_1)/\hbar)$ [see Eq. (4.1)]. However, now we have to take the square of $\mathscr{C}_{\mathbf{M}}$ (respectively, $\partial^2\mathscr{C}_{\mathbf{M}}/\partial H^2$) before the impurity average and cross correlations between different paths Θ and Θ' on a torus $\mathbf{M}$ or between different tori have to be considered. We discuss this effect, typical of integrable systems, for the case of a square billiard. For sake of clarity we assume moreover a temperature range such that only the contribution of the shortest closed orbit has to be taken into account. Instead of Eqs. (2.23) and (2.24) which hold for the clean case, the contribution of orbits of topology $\mathbf{M}=(1,1)$ for the typical susceptibility now reads

$$\left(\frac{\chi^{(t)}}{\chi^0}\right)^2=\frac{1}{2}\int_0^a\frac{dx_0}{a}\int_0^a\frac{dx_0'}{a}\mathscr{A}^2(x_0)\mathscr{A}^2(x_0')\cos(\varphi\mathscr{A}(x_0))\cos(\varphi\mathscr{A}(x_0'))f(x_0,x_0'),\tag{5.1}$$

with χ^0 defined as in Eq. (2.22). The function

$$f(x_0,x_0')=\left\langle\exp\left\{\frac{i}{\hbar}(\delta S(x_0)-\delta S(x_0'))\right\}\right\rangle\tag{5.2}$$

$$=\exp\left\{-\frac{1}{2\hbar^2}[\langle\delta S^2(x_0)\rangle+\langle\delta S^2(x_0')\rangle-2\langle\delta S(x_0)\delta S(x_0')\rangle]\right\}\tag{5.3}$$

accounts for the effect of disorder on pairs of orbits x_0 and x_0'. [See Eq. (3.20) for the treatment in the general case]. For the magnetic response of an energy- and disorder-averaged ensemble we find correspondingly

$$\frac{\langle\overline{\chi}\rangle}{\overline{\chi^0}}=\frac{1}{2}\int_0^a\frac{dx_0}{a}\int_0^a\frac{dx_0'}{a}[\mathscr{A}_-^2\cos(\varphi\mathscr{A}_-)+\mathscr{A}_+^2\cos(\varphi\mathscr{A}_+)]f(x_0,x_0')\tag{5.4}$$

with $\overline{\chi^0}$ defined in Eq. (2.25) and $\mathscr{A}_\pm$ as in Eq. (2.24).

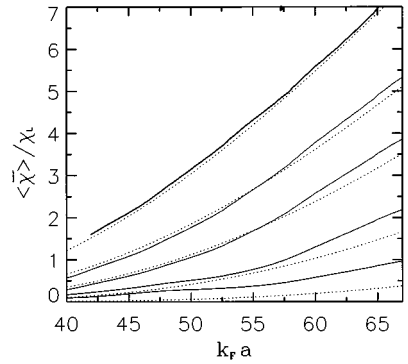

FIG. 4. Averaged magnetic susceptibility (at $H\approx 0$ of an ensemble of square billiards with variations in the size and impurity potential ($\xi=0$) for different disorder strength, i.e., elastic mean free path l_δ. The full curves show the numerical quantum results and the dotted lines the semiclassical predictions from Eq. (5.6) taking into account the variations of l_δ with k_F [see Eq. (A4)]. The two sets of curves correspond to an elastic MFP $l_\delta/a=\infty$, 8, 4, 2, 1 (at $k_F a=65$), (from the top).

1. Short range case

We begin with the discussion of the short range case: Although we reach the border of applicability of our semiclassical approximation for $\xi\to 0$, it shows us that in this limit orbits with $x_0 \neq x_0'$ are disorder-uncorrelated and all such pair contributions are exponentially damped. Using exclusively the family (1,1), one obtains an overall suppression of the typical and average susceptibility at finite temperature according to

$$\lim_{\xi\to 0}\chi^{(t)}=\chi_{\mathrm{cl}}^{(t)}e^{-L_{11}/2l_\delta}, \tag{5.5}$$

$$\lim_{\xi\to 0}\langle\overline{\chi}\rangle=\overline{\chi e}^{-L_{11}/l_\delta}. \tag{5.6}$$

Note that the exponent for $\langle\overline{\chi}\rangle$ differs by a factor 1/2 from that for $\langle\chi\rangle$ [see Eq. (4.2) and subsequent text].

Figure 4 depicts the $k_F a$ dependence of the ensemble averaged susceptibility $\langle\overline{\chi}\rangle$ in the short range case $\xi=0$. The dotted curves showing the semiclassical analytical formula (5.6) are compared with a direct quantum mechanical calculation of $\langle\chi^{(2)}\rangle$ [using the numerically obtained $N^{\mathrm{osc}}(\overline{\mu})$ in Eq. (2.9c)] for disorder ensembles of different impurity strength equivalent to an elastic MFP $l_\delta/a=\infty$, 8, 4, and 1 at $k_F a\sim 65$ (from the top). Note, that the effective MFP decreases along the curves with decreasing k_F [see Eq. (A4)] and the localized regime may eventually be reached for small $k_F a$. At the limit of the ballistic regime at small $l\sim a$ the semiclassical result begins to differ from the quantum one although the functional behavior remains the same. This arising difference may be related to non-ballistic scattering from impurities which is not included here.

2. Finite range case

In the finite range $\lambda_F<\xi\ll a$, the phase shifts $\delta S(x_0)$ and $\delta S(x_0')$ in $f(x_0,x_0')$ are accumulated in a correlated way, if the spatial distance of two orbits x_0 and x_0' is smaller than ξ. To evaluate the product term $2\langle\delta S(x_0)\,\delta S(x_0')\rangle$ in the exponent of $f(x_0,x_0')$ in this regime the integrations are performed as in Eq. (3.9) but with $\mathbf{q}$ and $\mathbf{q}'$ running along paths starting at x_0, respectively, x_0'. Ignoring the additional correlations occuring near the bounces off the boundaries of the billiard, the trajectories x_0 and x_0' (see Fig. 1) can be regarded as straight lines remaining at a

constant distance $y=|x_0-x_0'|/\sqrt{2}$ from another. We can therefore approximate $f(x_0,x_0')$ by $\tilde{f}(|x_0-x_0'|/\sqrt{2})$ with the function $\tilde{f}$ given by Eq. (3.20). For Gaussian correlation we thus have

$$f(x_0,x_0')=\exp\left\{-\frac{L_{11}}{l}\left[1-\exp\left(-\frac{(x_0-x_0')^2}{8\xi^2}\right)\right]\right\}. \tag{5.7}$$

Orbits separated by $|x_0-x_0'|\gg\xi$ are disorder-uncorrelated and exponentially suppressed: $f(x_0,x_0')\simeq\exp(-L_{11}/l)$. For those orbits the random disorder leads to an uncorrelated detuning of the phases. In contrast to that, disorder only weakly affects trajectories separated by $|x_0-x_0'|<\xi$.

The disorder averages in the finite range regime lead, by means of the function f, to a non-exponential damping of the susceptibilities for systems with families of periodic orbits. This behavior becomes obvious for the case of square billiards where at $H=0$ the integrals (5.1) and (5.4) can be evaluated analytically in the limits of $L_{11}\ll l$ (extreme ballistic) and $L_{11}\gg l$ (deep ballistic). We find for the typical and average susceptibility at $H=0$ in the finite range case for $L_{11}\ll l$

$$\left(\frac{\chi^{(t)}}{\chi_{\rm cl}^{(t)}}\right)^2\simeq 1-\frac{L_{11}}{l}\left(1-c_t\frac{\xi}{a}\right), \tag{5.8a}$$

$$\frac{\langle\overline{\chi}\rangle}{\overline{\chi}}\simeq 1-\frac{L_{11}}{l}\left(1-c_a\frac{\xi}{a}\right), \tag{5.8b}$$

and for $L_{11}\gg l$ (by steepest descent)

$$\left(\frac{\chi^{(t)}}{\chi_{\rm cl}^{(t)}}\right)^2\simeq c_t\left(\frac{\xi}{a}\right)\left(\frac{l}{L_{11}}\right)^{1/2}, \tag{5.9a}$$

$$\frac{\langle\overline{\chi}\rangle}{\overline{\chi}}\simeq c_a\left(\frac{\xi}{a}\right)\left(\frac{l}{L_{11}}\right)^{1/2}. \tag{5.9b}$$

The constants in the above equations are $c_t=(20/7)\sqrt{2\pi}$ and $c_a=2\sqrt{2\pi}$. Eqs. (5.8) express the limit of very weak disorder, showing that the small disorder effect is further reduced due to the correlation of the disorder potential. The other limit, Eqs. (5.9), is noticeably more interesting since it shows that disorder correlation effects lead to a replacement of the exponential disorder damping by a power law.

Figure 5 depicts in logarithmic representation our collected results for the disorder averaged typical (a) and averaged (b) susceptibility for square billiards (at $H=0$ and $k_BT=2g_s\Delta$) as a function of the inverse elastic MFP for different disorder correlation lengths. The symbols denote results from numerical quantum simulations described in the previous section and the full curves semiclassical results from numerical integration of the Eqs. (5.1) and (5.4). For the short range case $\xi=0$ they reduce to Eq. (5.6) predicting an exponential decrease with exponent L_{11}/l which is in line with the quantum calculations (circles). The semiclassical results for the finite range are on the whole in agreement with the numerical results for $\xi/a=0.1$ (diamonds), $\xi/a=0.2$ (triangles) and $\xi/a=0.5$ (squares). The semiclassical curves seem to overestimate the damping of the typical susceptibility. The dotted curves (shown for $a/l\geqslant 1$) depict the analytical expressions (5.9) in the regime $L_{11}>l$. Since for finite ξ the transport MFP $l_T>l$ [see Eq. (A6)], this regime can still be considered as (deep) ballistic and our semiclassical assumptions being based on straight-line trajectories remain valid.

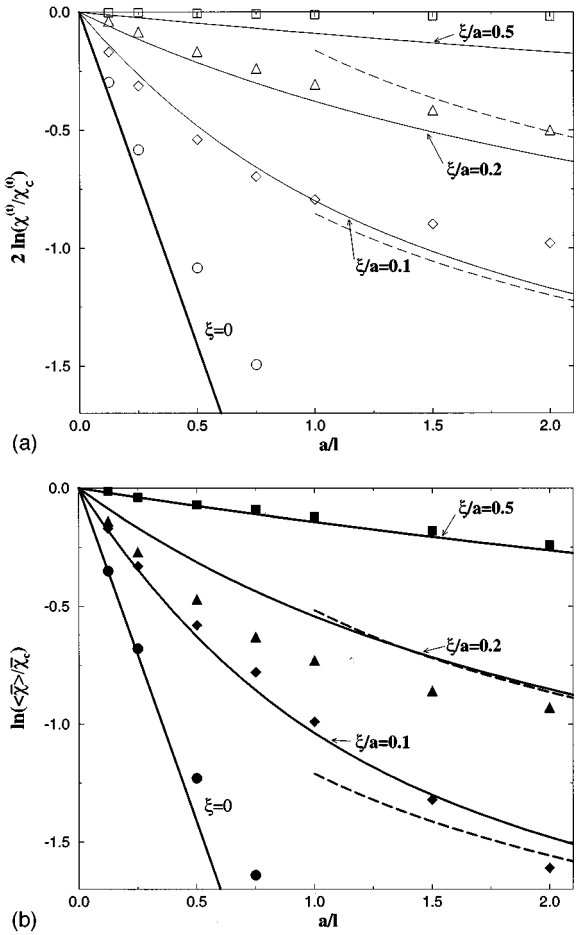

FIG. 5. Logarithm of the ratio between disorder averaged and clean results for (a) typical $\chi^{(t)}$ (b) ensemble averaged $\langle\overline{\chi}\rangle$ susceptibilities as a function of increasing inverse elastic MFP a/l for different values of ξ/a. The symbols denote the numerical quantum results, the solid lines (for $\xi>0$) the semiclassical integrals (5.1) (a) and (5.4) (b) and the dashed lines asymptotic expansions (5.9) of the integrals for large a/l.

As the semiclassical formulae already indicate, the overall disorder behavior of $\langle\overline{\chi}\rangle$ and $\chi^{(t)}$ is quite similar.

3. Long range case

For completeness, we will consider the effect of the disorder for the long range regime: We can use the Eqs. (5.1) and (5.4) but cannot calculate the disorder function $f(x_0,x_0')$ in the same way as for the finite range. We can however, similar as for $\langle\chi\rangle$ in Sec. IV, expand the exponent $-\langle(\delta S(x_0)-\delta S(x_0'))^2\rangle$ of $f(x_0,x_0')$ in Eq. (5.2) for small a/ξ. In the case of the square all orders up to $(a/\xi)^8$ vanish and we find a *very* small overall reduction of the clean averaged susceptibilities [from family (11)] given by

$$\left(\frac{\chi^{(t)}}{\chi_{\mathrm{cl}}^{(t)}}\right)^2 \simeq 1-6.5\cdot 10^{-5}\frac{a}{l}\left(\frac{a}{\xi}\right)^9. \tag{5.10}$$

For square billiards this leading order contribution no longer depends on x_0. The energy- and disorder-average $\langle\overline{\chi}\rangle$ exhibits the same damping as $(\chi^{(t)})^2$. Note that besides the high order in

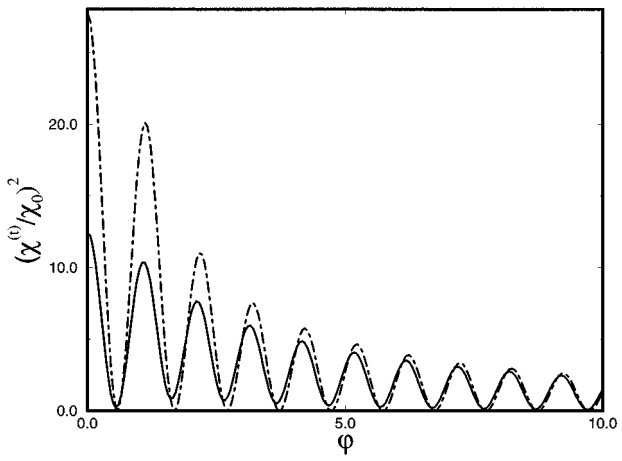

FIG. 6. Typical susceptibility as predicted by Eq. (5.1) as a function of the dimensionless flux $\varphi = Ha^2/\Phi_0$. Dash line: clean case; solid line: $l = a$ and $\xi = 0.1$.

(a/ξ) the prefactor is rather small. This weak suppression of the averaged susceptibilities can be related to the fact that in the long range case, different sectors of the contributing periodic orbits are highly correlated. As seen in Fig. 5(a), the quantum mechanical results (squares) for $\chi^{(t)}$ at $\xi/a = 0.5$, which are closest to the long range case, exhibit already a very weak damping.

B. Disorder effects at finite *H*-field: From integrable to chaotic behavior

In Fig. 6 we compare the ratio $(\chi^{(t)}/\chi^0)^2$ [obtained from calculating the integral in Eq. (5.1)] as a function of the dimensionless flux $\varphi = Ha^2/\Phi_0$ for the clean case and for disorder characterized by $l = a$ and $\xi = 0.1$. This figure shows that the damping due to disorder is maximal at zero field, but that already for $\varphi = 5$ the disorder seems not to affect the magnetic response any further.

The origin of this behavior can be understood readily by observing that as soon as φ is larger than one, the integral Eq. (5.1) is correctly approximated by a stationary phase approximation.[5] The stationary point $x_0^s = a/2$ corresponds to the two periodic orbits of the *perturbed* system, and only the trajectories such that

$$(x_0 - x_0^s)^2 \varphi < 1 \tag{5.11}$$

actually contribute to the integral. The magnetic field causes a de-phasing of the contributions of the various trajectories of the family, thus breaking the integrability of the system. This effect is responsible for the overall decrease of the typical susceptibility as the field increases. In this respect clean and disordered square billiards are not equivalent. In the disordered case, trajectories separated by a distance larger than ξ are already not contributing in phase. Therefore the additional magnetic field affects the magnitude of the susceptibility much less. This remains true up to the point where the condition (5.11) implies $|x_0 - x_0^s| < \xi$ in which case the disorder is not effective anymore, and the two curves coincide.

Therefore the behavior of the disorder damping we discussed in the previous subsection is characteristic for integrable geometries. For chaotic systems diagonal contributions (pair products of the same periodic orbit) are barely affected by disorder. This behavior is similar to that of integrable systems at finite field. When evaluating the contribution to the trace of the Green function in the neighborhood of a periodic orbit by stationary phase approximation, (as for the

derivation of the Gutzwiller trace formula) only orbits extremely close to the periodic orbit under consideration actually contribute. Unless ξ is exceedingly small, all these trajectories will see the same disorder potential.

As a final remark, note that *non-diagonal* contributions (pairs of different paths) are fully damped upon impurity average for chaotic as well as integrable systems, since the disorder potential along two different trajectories is usually not correlated [see also the discussion of the averaged Green function product after Eq. (3.17)]. Therefore non-diagonal contributions, which may be necessary to consider in the clean case,[30] are exponentially suppressed in the presence of disorder. On the contrary, *diagonal* terms which contain orbit correlations on distances ξ, exhibit non-exponential behavior [Eq. (5.7)] as a function of the inverse MFP $1/l$ for integrable geometries and are not affected (within our approximations) by disorder in the chaotic case.

C. Relation to experiment and other theories

Measurements of the orbital magnetism of small microstructures are still rare today. The only experiment on ensembles of ballistic billiards that we are aware of, was performed by Lévy *et al.*[21] and investigated the magnetic susceptibility of an array of about 10^5 ballistic square-like cavities. The size of the squares is on average $a=4.5\mu$m, with a large dispersion (estimated between 10% and 30%) along the array. Each individual square is a mesoscopic ballistic system since the phase-coherence length is estimated to be $L_\Phi=15-40$ μm and the elastic mean-free-path $l=4.5-10$ μm. The potential correlation length can be estimated[24] to be of the order of $\xi/a\simeq 0.1$. Taking the most unfavourable case of $l\simeq a\simeq 4.5$ μm we obtain, with respect to the clean case, a disorder reduction for the averaged susceptibility of $\langle\overline{\chi}\rangle/\overline{\chi}\simeq 0.37$, showing that the features of the clean integrable systems (strong paramagnetic susceptibility at $H=0$) persist upon inclusion of disorder. Since $\overline{\chi}\simeq 100\chi_L$,[5–7] our calculations for the paramagnetic response of the ballistic squares agree quantitatively with the experimental findings (given the experimental uncertainties).

Persistent currents in individual quasi-ballistic rings have recently been measured.[31] A similar setup would be needed for measuring the magnetic response of singly connected geometries, where our typical susceptibility (5.1) should be measured for the integrable case. Since modern lithographic techniques allow one to design chaotic as well as integrable cavities[2,3] and since we have demonstrated that disorder does not mask this difference, an order-of-magnitude effect is expected in the susceptibility according to the shape (chaotic vs. integrable) of the cavity.

In a related theoretical work Gefen *et al.*[32] followed a complementary approach to ours and calculated the disorder-averaged susceptibility for an ensemble of ballistic squares based on long trajectories (strongly) affected by scattering from δ-like impurities. They found that the average susceptibility does not depend on the elastic MFP. These results are not borne out by either our analytical or our semiclassical calculations at temperatures relevant for the experiment, where the exponential damping from Eq. (2.18) makes very long trajectories irrelevant.

VI. SUMMARY

In this work we have studied the interplay between integrability and disorder in the ballistic regime. The integrable property of the confining potential of a microstructure implies a peculiar behavior of its thermodynamical response functions, like the magnetic susceptibility. The disorder effects provided by remote impurity scattering tend to weaken the importance of the boundary scattering (and therefore the relevance of the underlying classical mechanics). Using a semiclassical approach we quantify this damping and show it to be much weaker than previously estimated (power-law suppression instead of exponential damping for the typical and average susceptibility). The disorder damping is decisively affected by finite-size effects since it depends not only on bulk-like characteristics of the disorder (like the elastic mean-free-path), but also on the ratio between the size of the structure and the correlation length of the potential.

TABLE I. Summary of the different average susceptibilities (at $H=0$) considered in the short range ($\xi<\lambda_F<a$), finite range ($\lambda_F<\xi<a$) and long range ($\lambda_F<a<\xi$) regimes. The fixed-size impurity averaged susceptibility $\langle\chi\rangle$ is given by the one-particle Green function, while the typical $\chi^{(t)}$ and average $\langle\overline{\chi}\rangle$ susceptibilities are given by two-particle Green functions and involve impurity and energy averages. The different average susceptibilities are normalized with respect to the corresponding clean counterparts. L_{11} is the length of the shortest flux-enclosing periodic trajectories in the square. In the short range regime the damping is governed by the elastic mean-free-path l_δ given by the quantum mechanical expression (A4). The damping in the finite and long range regimes is governed by the elastic MFP l [whose semiclassical expression is given in Eq. (3.14)], the correlation length ξ of the impurity potential and the size a of the structure. I_t is the moment of inertia of the (11) trajectories [Eq. (3.16)]. The finite-range expressions for $\chi^{(t)}$ and $\langle\overline{\chi}\rangle$ showing a power-law damping hold in the deep ballistic limit $l<L_{11}$. The numerical factors are $c_t=(20/7)\sqrt{2\pi}, c_a=2\sqrt{2\pi}, d_1=1/4\sqrt{\pi}$, and $d_2=6.5\cdot 10^{-5}$.

	Short range	Finite range	Long range
$\langle\chi\rangle/\chi_{cl}$	$\exp(-L_{11}/2l_\delta)$	$\exp(-L_{11}/2l)$	$\exp\{-d_1(L^2/l\xi)[1-I_t/(2\xi^2)]\}$
$(\chi^{(t)}/\chi_{cl}^{(t)})^2$	$\exp(-L_{11}/l_\delta)$	$c_t(\xi/a)(l/L_{11})^{1/2}$	$1-d_2 a/l(a/\xi)^9$
$\langle\overline{\chi}\rangle/\overline{\chi}$	$\exp(-L_{11}/l_\delta)$	$c_a(\xi/a)(l/L_{11})^{1/2}$	$1-d_2 a/l(a/\xi)^9$

Our finding for the weak disorder damping is particularly important due to the large phase coherence effects found for clean integrable structures and to the fact that the difference in the magnetic response between integrable and chaotic geometries has not yet been experimentally demonstrated.

Our calculational tools have been semiclassical expansions, which naturally convey at the quantum level information about the underlying classical mechanics and its sensitivity with respect to disorder. For the weak disorder that we have considered in this work, the lowest order approximation consists of the perturbative modification of the classical actions by the impurity potential. Averages over impurity configurations following our semiclassical calculations, allow us to obtain various ensemble susceptibilities. Our analytical calculations have been checked against numerical quantum simulations performing exact diagonalizations of the corresponding Hamiltonian.

The need to consider different averages is inherent to ballistic nanostructures, which are sufficiently small to be non-self-averaging. These various types of impurity-averaged susceptibilities for integrable systems are summarized in Table I for the three regimes defined by the correlation length of the impurity potential. We have first studied the fixed-size averaged susceptibility, directly obtainable from the disorder average of one-particle Green functions. It corresponds to the case where different impurity configurations of a given sample with a fixed Fermi energy are considered. For the short range regime, where the disorder correlation length $\xi<\lambda_F$, we have an exponential suppression of the clean results governed by the short-range elastic mean-free-path l_δ and the length of the most relevant trajectories. This result also holds in the finite-range ($\lambda_F<\xi\ll a$), but with an elastic mean-free-path that we have evaluated semi-classically. In the long-range regime ($\xi>a$) the fixed-size averaged susceptibility depends exponentially on the product $(L/l)\cdot(L/\xi)$ (where L denotes the typical orbit length) and a correction taking into account the geometry of the periodic trajectories.

For comparison with actual experiments we have to take into account that different impurity realizations are obtained together with a change in the Fermi energy and the size of the structures. We are then led to consider impurity and size averaged susceptibilities, which are expressed in terms of two-particle Green functions. The typical susceptibility is appropriate when considering the magnetic response of an individual sample which is thermally cycled in order to obtain different realizations of the potential. The average susceptibility is obtained from the measurement of an array of microscopically different samples. For the short-range case the only difference between one- and two-point Green function quantities is the factor 1/2 of the exponential damping of the former. In the finite-range regime there appear important differences when considering two-point Green function quantities with respect to the one-particle case. Closed trajectories that

remain closer than the correlation length of the potential result in a weak damping with a power-law dependence on l/L and ξ/a. This is the experimentally relevant situation, and the use of standard parameters led us to conclude that disorder damping in currently realizable microstructures is sufficiently weak in order not to mask the large effects due to integrability. In the long-range case the damping due to disorder is extremely small.

We have further considered the interplay between disorder and magnetic field in integrable geometries. It is interesting to note that both have a similar effect since they produce de-phasing between nearby trajectories. Since the two sources of de-phasing do not superpose, we find that disorder is less effective at finite fields, and reciprocally, disordered samples are less sensitive to magnetic field.

In chaotic geometries periodic trajectories are usually isolated, resulting in smaller oscillations of the density of states and a much smaller magnetic response than integrable systems. Introduction of disorder in chaotic geometries is therefore less dramatic than in integrable systems, since it merely changes the action of the relevant periodic trajectories instead of producing de-phasing within a family. The transition from the ballistic regime (where classical trajectories are essentially unaffected by disorder) to the diffusive regime will be considered in a subsequent publication.

In this work we have started from a system that is physically realizable using modern technology and we have developed a theoretical model with some key ingredients involving integrability and disorder. These are deep theoretical issues that need to be complemented by the consideration of other effects, like interactions, in order to obtain a complete description of the thermodynamics of mesoscopic systems.

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APPENDIX: RELATION BETWEEN SEMICLASSICAL AND QUANTUM MECHANICAL RESULTS FOR BULK MEAN FREE PATHS

It is instructive to compare the semiclassical results of Eqs. (3.12)–(3.14) for the ballistic regime with their counterparts obtained from quantum mechanical scattering theory.

In a perturbative diagrammatic approach (treating the related Dyson-equation for scattering within a self-consistent Born approximation) the damping of the disorder-averaged one-particle Green function in a random potential is of the same exponential form as in Eq. (3.11).[9] This is usually obtained by replacing the imaginary part of the self-energy in the Green function after impurity average by the product of the density of states of the unperturbed system and $n{:}u^2$. The resulting quantum mechanical inverse elastic MFP l_{qm}, which appears in Eq. (3.11), is related to the total cross section σ by means of

$$\frac{1}{l_{\mathrm{qm}}} = n_i \sigma, \tag{A1}$$

where n_i is the impurity density and

$$\sigma = \int \mathrm{d}\Theta \, \sigma(\Theta) \tag{A2}$$

with $\sigma(\Theta)$ being the partial cross section for scattering with an angle Θ.

For a Gaussian disorder potential of the form of Eq. (3.3) a calculation of the cross section can be performed analytically and the corresponding inverse MFP gives

$$\frac{1}{l_{\rm qm}}=\frac{1}{l_\delta}I_0[2(k\xi)^2]e^{-2(k\xi)^2}. \tag{A3}$$

Here, I_0 is a modified Bessel function and

$$\frac{1}{l_\delta}=\frac{2\pi}{\hbar}\frac{n_i u^2}{v_{\rm F}}d(\mu)=\frac{n_i u^2}{v_{\rm F}}\frac{m}{\hbar^3} \tag{A4}$$

is the inverse MFP for the white noise case of δ-like scatterers of mean strength u. The $v_{\rm F}$ is the Fermi velocity and $d(\mu)=m/(2\pi\hbar^2)$ the density of states at the Fermi energy of a 2DEG.[9]

In order to compare $l_{\rm qm}$ with our semiclassical result we expand $l_{\rm qm}(k\xi)$ for large $k\xi$ which gives

$$l_{\rm qm}(k\xi)\simeq\sqrt{4\pi}(k\xi)l_\delta\left[1-\frac{1}{16(k\xi)^2}\right]\quad\text{for}\quad k\xi\to\infty. \tag{A5}$$

The leading order term is exactly the semiclassical MFP Eq. (3.14) for the Gaussian disorder model (3.3). The agreement between the semiclassical and diagrammatic approaches for the bulk can be related to the fact that our semiclassical treatment of disorder corresponds to the use of the Eikonal approximation (for each single scattering event) which is known to give the same results as Born approximation for large $k\xi$.

In the limit of $\xi<\lambda_F$ where our semiclassical description is no longer applicable, the mean free path $l_{\rm qm}$ approaches l_δ, which means that Eq. (3.11) can further be used, but with the semiclassical l replaced by l_δ.

The quantum mechanical transport mean free path $l_{\rm T}$ is calculated by including a factor $(1-\cos\Theta)$ in the integral (A2) for the scattering amplitude. It reads for Gaussian disorder

$$\frac{1}{l_{\rm T}}=\frac{1}{l_\delta}(I_0[2(k\xi)^2]-I_1[2(k\xi)^2])e^{-2(k\xi)^2} \tag{A6}$$

$$\simeq\frac{1}{l_{\rm qm}}\frac{1}{4(k\xi)^2}\quad\text{for}\quad k\xi\to\infty. \tag{A7}$$

This relation shows that $l_{\rm T}$ can be considerably larger than $l_{\rm qm}$ for $\lambda_F<\xi$. This shows that in the case of a confined system and smooth disorder, the system may behave ballistically although the elastic MFP l state might be considerably smaller than the system size.

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Ergodic properties of infinite quantum harmonic crystals: An analytic approach

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We prove that the quantum dynamics of a class of infinite harmonic crystals becomes ergodic and mixing in the following sense: if H_m is the m-particle Schrödinger operator, $\omega_{\beta,m}(A)=\mathrm{Tr}(A\exp-\beta H_m)/\mathrm{Tr}(\exp-\beta H_m)$ the corresponding quantum Gibbs distribution over the observables $A,B,\psi_{m,\lambda}$ the coherent states in the mth particle Hilbert space, $g_{m,\lambda}=(\exp-\beta H_m)\psi_{m,\lambda}$ then $\lim_{t\to\infty}\lim_{n\to\infty}\lim_{m\to\infty}(1/T)\int_0^T\langle e^{iH_nt}Ae^{-iH_nt}\psi_{m,\lambda},\psi_{m,\lambda}\rangle dt=\lim_{m\to\infty}\omega_{\beta,m}(A)$ if the classical infinite dynamics is ergodic, and $\lim_{t\to\infty}\lim_{n\to\infty}\lim_{m\to\infty}\omega_{\beta,m}(e^{iH_nt}Ae^{-iH_nt}B)=\lim_{m\to\infty}\omega_{\beta,m}(A)\lim_{m\to\infty}\omega_{\beta,m}(B)$ if it is in addition mixing. The classical ergodicity and mixing properties are recovered as $\hbar\to0$, and $\lim_{m\to\infty}\omega_{\beta,m}(A)$ turns out to be the average over a classical Gibbs measure of the symbol generating A under Weyl quantization. © *1996 American Institute of Physics.* [S0022-2488(96)01710-0]

I. INTRODUCTION

This paper deals with the ergodic theory of a class of infinite quantum systems, the harmonic crystals. In this introduction we review the relevance of the infinitely many particle limit in detecting chaotic behavior of quantum systems, state the results, and relate why in our opinion it is convenient to examine the problem via pseudodifferential operators.

Let H be the quantization of a Hamiltonian generating a flow S_t on a constant energy manifold $M_E\subset R^m$, $A, B\in\mathscr{L}(\mathscr{H})$ any suitable quantum observable in $\mathscr{H}=L^2(\mathbb{R}^m)$, and let $\sigma(H)$ be discrete and simple, with projections P_n on the eigenvectors $\{u_n: n=0,1,...\}$. If quantum chaotic behavior (if any) is to be characterized in terms of ergodicity and mixing, we have to consider the quantum microcanonical ensemble at energy E, i.e., the application $\omega_{\Delta,E}$ mapping any $A\in\mathscr{L}(\mathscr{H})$ into:

$$\omega_{\Delta,E}(A)=\frac{\mathrm{Tr}\,A\Sigma_{n:E-\Delta<E_n<E}P_n}{\mathrm{Tr}\,\Sigma_{n:E-\Delta<E_n<E}P_n}\equiv\frac{\mathrm{Tr}\,A\delta(H-E)}{\mathrm{Tr}\,\delta(H-E)} \tag{I.1}$$

(see Ref. 1, Sec. 1.3; $\Delta>0$ is arbitrarily small). The quantum evolution $A_H(t)=e^{iHt}Ae^{-iHt}$ of A leaves $\omega_{\Delta,E}(A)$ invariant. Hence the consequent definition of mixing is (see Appendix B for details)

$$\lim_{t\to\infty}\omega_{\Delta,E}(A_H(t)B)=\omega_{\Delta,E}(A)\cdot\omega_{\Delta,E}(B). \tag{I.2}$$

We can always find in $\mathscr{H}$ (see Appendix B for easy verification) a family of normalized vectors $(\psi_\lambda)_{\lambda\in\Lambda},\Lambda=\mathbb{R}^{2m}$ complete for $\omega_{\Delta,E}$, namely,

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$$\omega_{\Delta,E}(A)=\int_{\Lambda}\langle A\psi_{\lambda},\psi_{\lambda}\rangle_{\mathscr{H}}d\nu_{\Delta,E}(\lambda),\quad \forall A\in\mathscr{L}(\mathscr{H}) \tag{I.3}$$

for a well-determined probability measure $\nu_{\Delta,E}(\lambda)$ on Λ.[1]
Then Eq. (I.2) becomes

$$\int_{\Lambda}\langle A_H(t)B\psi_{\lambda},\psi_{\lambda}\rangle_{\mathscr{H}}d\nu_{\Delta,E}(\lambda)\to\int_{\Lambda}\langle A\psi_{\lambda},\psi_{\lambda}\rangle_{\mathscr{H}}d\nu_{\Delta,E}(\lambda)\int_{\Lambda}\langle B\psi_{\lambda},\psi_{\lambda}\rangle_{\mathscr{H}}d\nu_{\Delta,E}(\lambda) \tag{I.4}$$

as $|t|\to\infty$. This entails the following representation of the quantum ergodicity notion (again see Appendix B): for any $A\in\mathscr{L}(\mathscr{H})$ and for $d\nu$-almost all $\lambda\in\mathbb{R}^{2m}$,

$$\frac{1}{T}\int_0^T\langle A_H(t)\psi_{\lambda},\psi_{\lambda}\rangle_{\mathscr{H}}dt\to\int_{\Lambda}\langle A\psi_{\lambda},\psi_{\lambda}\rangle_{\mathscr{H}}d\nu_{\Delta,E}(\lambda)=\omega_{\Delta,E}(A)\quad\text{as}\quad|T|\to\infty. \tag{I.5}$$

On the other hand it is well known (and easy to verify) that

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T\langle\psi,A_H(t)\psi\rangle dt=\sum_{n=0}^{\infty}|\lambda_n|^2\langle u_n,Au_n\rangle. \tag{I.6}$$

Here $\psi=\Sigma_{n=0}^{\infty}\lambda_n u_n$ is any normalized quantum state expanded on the eigenvector basis (u_n). Equation (I.6) is the Von Neumann definition of quantum ergodicity[2] on the microcanonical ensemble. Now the verification of Eq. (I.5) requires H to have a continuous spectrum (Ref. 1, Sec. 1.3), and Eq. (I.6) shows that the time average cannot eliminate the dependence on the initial datum $\psi\equiv\{\lambda_n\}_{n=0}^{\infty}$.

This *a priori* lack of ergodicity, and *a fortiori* of mixing, looks like a manifestation of the so-called ''quantum suppression of classical chaos,'' which however can disappear when the number of particles tends to infinity. This has been noted in different contexts and within different approaches in Refs. 3–6. Hence the quantum counterparts of chaotic systems with infinitely many degrees of freedom (for a recent review see Ref. 6) are the best candidates to look for chaotic behavior. The simplest one is the infinite linear harmonic system

$$\ddot{q}_i=-2\sum_{i,j\in\mathbb{Z}}V_{ij}q_j. \tag{I.7}$$

We prove that, when the couplings V_{ij} generate an infinite dimensional dynamics ϕ_t ergodic with *respect to the (infinite dimensional) Gibbs measure* $d\mu_G(\beta)$,[7–9] the quantum evolution is ergodic, and mixing if ϕ_t is in addition mixing. The averages are now to be computed on the quantum canonical ensemble (the Gibbs state at an inverse temperature β), i.e., the application ω_β mapping any $A\in\mathscr{L}(\mathscr{H})$ into $\omega_\beta(A)=\mathrm{Tr}\,Ae^{-\beta H}/\mathrm{Tr}\,e^{-\beta H}$. More precisely, denote:

$$q_m(x,\xi)=\tfrac{1}{2}|\xi|^2+\langle V_m x,x\rangle,\quad V_m=(V_{i,j})_{\substack{|i|\le m\\|j|\le m}} \tag{I.8}$$

the $(2m+1)$ dimensional Hamiltonian defined on $\Lambda_m=(\mathbb{R}^{2m+1})^2$; $H_m=\mathrm{Op}^W(q_m)$ the operator on $L_m^2\equiv L^2(\mathbb{R}^{2m+1})$ defined by its Weyl quantization, $A=\mathrm{Op}^W(a)$ the operator on L_m^2 quantizing $a\circ\Pi_{m_1}(x,\xi)$ (m_1 fixed) where a is any smooth classical observable on Λ_{m_1}. Here $\Pi_{m_1}(x,\xi)\equiv(x,\xi)_{|i|\le m_1}$.

Then the present results are (see Theorems 2.2, 2.3 and Proposition 5.1 for a sharper version): $\forall\beta>0$ and $m_1\in\mathbb{N}$

$$\lim_{T\to\infty}\lim_{n\to\infty}\lim_{m\to\infty}\frac{1}{T}\int_0^T\langle A_n(t)\psi_{\lambda,m},\psi_{\lambda,m}\rangle_{L^2_m}dt=\lim_{m\to\infty}\int_{\Lambda_\infty}\langle A\psi_{\lambda,m},\psi_{\lambda,m}\rangle_{L^2_m}d\nu_m(\lambda) \tag{I.9}$$

for ν-almost any λ, and

$$\lim_{t\to\infty}\lim_{n\to\infty}\lim_{m\to\infty}\omega_{\beta,m}(A_n(t)B)=\lim_{m\to\infty}\omega_{\beta,m}(A)\cdot\lim_{m\to\infty}\omega_{\beta,m}(B). \tag{I.10}$$

Here

$$\omega_{\beta,m}(A)=\frac{\mathrm{Tr}\,Ae^{-\beta H_m}}{\mathrm{Tr}\,e^{-\beta H_m}};\quad \omega_{\beta,m}(A_n(t)B)=\frac{\mathrm{Tr}\,A_n(t)Be^{-\beta H_m}}{\mathrm{Tr}\,e^{-\beta H_m}}; \tag{I.11}$$

$A_n(t)$ is the Heisenberg observable corresponding to A under the quantum evolution of H_n;

$$\psi_{\lambda,m}=\frac{\exp(-\beta H_m/2)f_{\lambda,m}}{\|\exp(-\beta H_m/2)f_{\lambda,m}\|},\quad \nu_m(\lambda)=\frac{\|\exp(-\beta H_m/2)f_{\lambda,m}\|^2d\lambda}{\int_{\Lambda_m}\|\exp(-\beta H_m/2)f_{\lambda,m}\|^2d\lambda},$$

with $f_{\lambda,m}$ being the Bargmann coherent states (a set of vectors in $L^2(\mathbb{R}^{2m+1})$ indexed by $\lambda\in\Lambda_m$ whose definition is recalled in Appendix B); $\nu(\lambda)=\lim_{m\to\infty}\nu_m(\lambda)$.

Remark 1: The mixing property with respect to the KMS states in the CCR algebra of the infinite harmonic crystal (which has the same W^* closure of the pseudodifferential algebra we use) is proved in Ref. 6, Example 4.46, through the asymptotic abelianess of the Weyl algebra automorphism generated by the dynamics of the infinite crystal, when $\sigma(V)$ is purely absolutely continuous so that classical mixing holds.[7] The asymptotic abelianess may however fail if $\sigma(V)$ is only continuous and the classical system only ergodic. Hence the ergodicity result (I.9) requires in general an independent proof.

Remark 2: The main reason why, in our opinion, an ''analytic'' proof, based on pseudodifferential calculus, is in any case useful is that the notion (I.4) is proved to have the expected classical limit (Appendix B).

Additional reasons are as follows.

(1) One finds the right-hand sides (rhs) of Eqs. (I.9) and (I.10) to be the relevant classical averages:

$$\lim_{m\to\infty}\int_{\Lambda_\infty}\langle A_{m_1}\psi_{\lambda,m},\psi_{\lambda,m}\rangle d\nu_m(\lambda)=\int_{\Lambda_\infty}a\circ\Pi_{m_1}d\hat{\mu}_\beta, \tag{I.12}$$

$$\lim_{m\to\infty}\frac{\mathrm{Tr}\,A_{m_1}e^{-\beta H_m}}{\mathrm{Tr}\,e^{-\beta H_m}}\cdot\frac{\mathrm{Tr}\,B_{m_1}e^{-\beta H_m}}{\mathrm{Tr}\,e^{-\beta H_m}}=\int_{\Lambda_\infty}a\circ\Pi_{m_1}d\hat{\mu}_\beta\cdot\int_{\Lambda_\infty}b\circ\Pi_{m_1}d\hat{\mu}_\beta. \tag{I.13}$$

Here $\hat{\mu}_\beta=\lim_{m\to\infty}\hat{\mu}_{\beta,m}$, where $\hat{\mu}_{\beta,m}$ is the (explicitly constructed) Gibbs measure on Λ whose Weyl quantization yields $e^{-\beta H_m}$. It turns out that $\hat{\mu}_\beta$ depends on $\hbar$ to reduce to $\mu_G(\beta)$ as $\hbar\to 0$, because $e^{-\beta g_m}$ is just the principal symbol of $e^{-\beta H_m}$ realized as a pseudodifferential operator.

(2) If the initial states $\psi_{m,\lambda}$ belong to an explicitly constructed set (the image under $e^{-\beta H_m}$ of ''almost all'' coherent states on Λ_m), the $m\to\infty$ limit can actually eliminate the dependence of the rhs of Eq. (I.9) on the particular state in the set.

(3) Unlike the algebraic proof, the analytic one can, in principle, be extended to systems quantizing nonlinear classical equations. Work in this direction is in progress: it can be proved[10] that in some nonlinear cases the above results are still true in the sense of the formal power series in $\hbar$.

We conclude Sec. I with the remark that the dynamical mechanism generating chaotic behavior, in

the classical case and in the quantum one as well, is but free propagation of the chaotic initial condition: the infinite harmonic crystal indeed goes over (when the spacing goes to zero, and for special choices of V) to the free wave equation (equivalently, there exist coordinates in which the particle motions are free) and the chaotic initial condition is selected by the invariant Gibbs measure. This situation is referred to as kinematic chaos.[11]

The paper is organized as follows: in Sec. II we state assumptions and results, after a brief review of the infinite dimensional classical harmonic dynamics; in Secs. III and IV we prove the quantum ergodicity and the quantum mixing, respectively, in the most general formulation. In Secs. V and VI we prove a sharper formulation of the above results when $\exp-\beta H_m$ is replaced by $\mathrm{Op}^W(\exp-\beta q_m)$ and the family of vectors in L^2_m is specialized to the coherent states. Appendix A contains the proof of some technical lemmas, and Appendix B contains the discussion of our results in light of the existing notions of quantum ergodicity and mixing, together with the verification that they have the expected classical limit.

II. ASSUMPTIONS AND STATEMENT OF THE RESULTS

In the notation of Ref. 7, to which we refer the reader for any further detail on the system of infinitely many oscillators, let $V=(V_{i,j})_{i,j\in\mathbb{z}}$ be an infinite real-symmetric matrix; q_m and V_m are as in Eq. (II.8) and $\Lambda_m=(\mathbb{R}^{2m+1})^2$.

We write $S_m(1)$ for the set of C^∞ functions on Λ_m which are bounded together with all their derivatives, and for $a\in S_m(1)$ we denote $\mathrm{Op}^W(a)$ the Weyl quantization (with $\hbar=1$) of the symbol (equivalently, classical observable) a, explicitly given by the oscillatory integral:

$$\mathrm{Op}^W(a)u(x)=(2\pi)^{-(2m+1)}\int_{\Lambda_m} e^{i\langle (x-y),\xi\rangle}a\left(\frac{x+y}{2},\xi\right)u(y)dy\,d\xi \tag{II.1}$$

for all $u\in\mathscr{S}(\mathbb{R}^{2m+1})$. In particular the Schrödinger operator H_m on $L^2(\mathbb{R}^{2m+1})$

$$H_m:=\mathrm{Op}^W(q_m)=\frac{1}{2}\left(\sum_{j=1}^{2m+1}D_{x_j}^2\right)+\langle V_m x,x\rangle,\quad D_{x_j}=-i\,\frac{\partial}{\partial x_j} \tag{II.2}$$

quantizes the Hamiltonian q_m describing m oscillators coupled through V_m.

We assume from now on

(H1) $$|V_{ij}|=\mathscr{O}(|i-j|^{-\infty}),\quad |i-j|\to+\infty$$

and $\exists 0<\epsilon<M<\infty$ such that $\forall\geqslant 0$, $\sigma(V_m)\subset[\epsilon,M]$.
In particular, $V:l^2(\mathbb{z})\to l^2(\mathbb{Z})$ is bounded and strictly positive, with $\sigma(V)\subset[\epsilon,M]$.
(H2) The operator V acting on $l^2(\mathbb{Z})$ has no point spectrum.
Denote

$$\Lambda_\infty:=\bigcup_{k\in\mathbb{N}}\{(x_j,\xi_j)\};\quad |x_j|+|\xi_j|=\mathscr{O}(|j|^k),\ |j|\to\infty\}:=\bigcup_{k\in\mathbb{N}}\mathscr{H}_k. \tag{II.3}$$

It is proved in Ref. 7 that under condition (H1), Λ_∞ is invariant under the classical evolution of infinitely many degrees of freedom defined as follows:

$$\phi_t(x,\xi)\equiv\phi(t,x,\xi)=e^{tB}(x,\xi),\quad \forall(x,\xi)\in\Lambda_\infty,\quad \forall t\in\mathbb{R}, \tag{II.4}$$

where $B(x,\xi)$ is the infinite-dimensional Hamiltonian vector field generated by q_m when $m\to\infty$

$$B(x,\xi)=\left(\xi_j,-2\sum_{k\in\mathbb{Z}}V_{jk}x_k\right)_{j\in\mathbb{Z}}. \tag{II.5}$$

Moreover, if $\Pi_m:\Lambda_\infty\to\Lambda_m$ denotes the projection

$$\Pi_m(x,\xi)=(x_j,\xi_j)_{|j|\leqslant m} \tag{II.6}$$

for any $(x,\xi)\in\mathscr{H}_k$ one has

$$\phi(t,x,\xi)=\lim_{m\to\infty}\ \phi_{m,t}(\Pi_m(x,\xi))\in\mathscr{H}_k, \tag{II.7}$$

where

$$\phi_{m,t}=\exp\ tH_{q_m},\ \ H_{q_m}=\left(\frac{\partial q_m}{\partial\xi},-\frac{\partial q_m}{\partial x}\right)$$

is the vector field generated by q_m, and the limit is taken with respect to the natural Banach space topology of $\mathscr{H}_k$.

Now by condition (H1) the operator $V^{-1/2}$ exists and is continuous on $l^2(\mathbb{Z})$. This assumption and (H2) allow Lanford and Lebowitz[7] to prove the existence of the infinite dimensional, ergodic Gibbs measure $d\mu_G(\beta)$ on Λ_∞, namely

(1)

$$\int_{\Lambda_\infty}\varphi\circ\Pi_{m_1}d\mu_G(\beta)=\lim_{m\to\infty}\int_{\Lambda_m}\varphi\circ\Pi_{m_1}(x,\xi)e^{-\beta q_m(x,\xi)}\frac{dx\,d\xi}{Z_m},\quad\forall\varphi\in C_b^0(\mathbb{R}^{2m_1+1}) \tag{II.8}$$

where

$$Z_m(\beta)=\int_{\Lambda_m}e^{-\beta q_m(x,\xi)}dx\,d\xi \tag{II.9}$$

is the m-particle partition function

(2) The Gibbs measure is invariant and ergodic with respect to the flow $\phi(t;x,\xi)$, namely the continuous dynamical system $(\Lambda_\infty,\phi_t,d\mu_G(\beta))$ is ergodic.

An example of an infinite matrix satisfying (H1)–(H2) is given by $V=W$ where

$$W_{ij}=0,\quad |i-j|\geqslant 2,\quad W_{ii}=1,\quad W_{i,i+1}=W_{i,i-1}=\alpha \tag{II.10}$$

with $|\alpha|<\frac{1}{2}$, $\alpha\in\mathbb{R}$. The properties (H1), (H2) are proved, e.g., in Ref. 12.

To state our result we need to establish some further notation. For $f\in L^2(\mathbb{R}^{2m+1})$ and $(x,\xi)\in\Lambda_m$, we introduce the Wigner function of f

$$w_f(x,\xi)=\int_{\mathbb{R}^{2m+1}}e^{iu\xi}f\left(x-\frac{u}{2}\right)\overline{f\left(x+\frac{u}{2}\right)}du \tag{II.11}$$

and we restrict our attention to a random set of states f in the following sense: for all $m\in\mathbb{N}$, we consider a measure space (X_m,θ_m) with positive measure θ_m, and a family $(f_\lambda)_{\lambda\in X_m}$ of functions in $L^2(\mathbb{R}^{2m+1})$ such that:

(H3) For $dxd\xi$-almost all $(x,\xi)\in\Lambda_m$ the application $X_m\ni\lambda\mapsto w_{f_\lambda}(x,\xi)$ is in $L^1(X_m,d\theta_m)$ with non-negative values, and the quantity $\int_{X_m}w_{f_\lambda}(x,\xi)d\theta_m(\lambda)$ is ($dxd\xi$-almost everywhere) constant with respect to (x,ξ).

Here we can notice that, at least formally, condition (H3) is implied by the property [to be compared with Eq. (B10)]:

$$\mathrm{Tr}(A)=\int \langle Af_\lambda, f_\lambda\rangle d\theta_m(\lambda)$$

for any trace-class operator A. Indeed we have $w_{f_\lambda}(x,\xi) = \langle A_{x,\xi}f_\lambda, f_\lambda\rangle$ with $A_{x,\xi}f(y) = e^{2i(y-x)\xi}f(2x-y)$, which actually is not trace-class, but whose distributional kernel $K_{x,\xi}(y,y') = e^{2i(y-x)\xi}\delta(y'+y=2x)$ formally satisfies: $\int K_{x,\xi}(y,y)dy=1$.

In the last section we develop an example (the so-called coherent states) where condition (H3) is satisfied. Note that in any case, $w_f(x,\xi)$ is real and satisfies: $\int w_f(x,\xi)dxd\xi=(2\pi)^{2m+1}\|f\|^2$.

As we shall see, condition (H3) implies among other things that

$$\int_{X_m} \|e^{-\beta H_m/2}f_\lambda\|^2 d\theta_m(\lambda)<+\infty \tag{II.12}$$

so that we can consider the following probability measure on X_m:

$$d\nu_m(\lambda)=\frac{\|e^{-\beta H_m/2}f_\lambda\|^2 d\theta_m(\lambda)}{\int_{X_m}\|e^{-\beta H_m/2}f_\lambda\|^2 d\theta_m(\lambda)}. \tag{II.13}$$

Now let

$$W_\beta=\sqrt{2}V^{-1/2}\tanh\frac{\beta V^{1/2}}{\sqrt{2}} \tag{II.14}$$

(which is well-defined on $l^2(\mathbb{Z})$), and for $\beta>0$, denote $\hat{\mu}_\beta$ the Gaussian probability measure on Λ_∞ with mean zero and covariance given by

$$E[x_ix_j]=\langle(2VW_\beta)^{-1}e_i,e_j\rangle_{l^2(\mathbb{Z})},$$

$$E[\xi_i\xi_j]=\langle W_\beta^{-1}e_i,e_j\rangle_{l^2(\mathbb{Z})},$$

$$E[x_i\xi_j]=0, \tag{II.15}$$

where $e_i = (\delta_{ij})_{j\in\mathbb{Z}}$. Then our first main result is as follows:

Theorem II.1: Assume (H1)–(H3). Then:

(i) *For any $\beta>0$, the dynamical system $(\Lambda_\infty,\phi_t,\hat{\mu}_\beta)$ is ergodic*;

(ii) *For $m_1\in\mathbb{N}$ fixed and $a \in S_{m_1}(1)$, denote*

$$g_{m,\beta,\lambda}=\frac{e^{-1/2\beta H_m}f_\lambda}{\|e^{-1/2\beta H_m}f_\lambda\|}$$

and

$$A(m,n,T,\lambda)=\frac{1}{T}\int_0^T\langle e^{itH_n}\,\mathrm{Op}^W(a\circ\Pi_{m_1})e^{-itH_n}g_{m,\beta,\lambda},g_{m,\beta,\lambda}\rangle_{L^2(\mathbb{R}^{2m+1})}dt.$$

Then one has

$$\lim_{T\to\infty}\limsup_{n\to\infty}\limsup_{m\to\infty}\int_{X_m}\left|A(m,n,T,\lambda)-\int_{\Lambda_\infty}a\circ\Pi_{m_1}d\hat{\mu}_\beta\right|d\nu_m(\lambda)=0.$$

Remarks:

(1) $A(m,n,T,\lambda)$ can be made arbitrarily close to $\int a \circ \Pi_{m_1} d\hat{\mu}_\beta$ in $L^1(X_m, d\nu_m(\lambda))$ by first choosing T, then $n=n(T)$, and finally $m=m(n,T)$ large enough. The *pointwise* convergence of $A(m,n,T,\lambda)$ is proved in Proposition 5.1 below, choosing for f_λ a particular set of coherent states.

(2) Note that $A(m,n,T,\lambda)$ is well-defined since the action of $e^{itH_n}\mathrm{Op}^W(a \circ \Pi_{m_1})e^{-itH_n}$ on $g_{m,\beta,\lambda}$ which is a C^∞ function on $\mathbb{R}^{2m+1}$ is well-defined for $n \leqslant m$.

(3) For small β, we have $W_\beta = \beta I + \mathcal{O}(\beta^3)$ and therefore the covariance of $\hat{\mu}_\beta$ coincides with the one of the usual Gibbs measures $\mu_G(\beta)$ up to a $\mathcal{O}(\beta^3)$-error term. In this sense, we can say that $\hat{\mu}_\beta$ and $\mu_G(\beta)$ are asymptotically equal for small β's (that is for large temperatures).

(4) The measure $\hat{\mu}_\beta$ can be seen as the limit when $m \to +\infty$ of the probability measure on Λ_m obtained by normalizing $e^{-q_{\beta,m}(x,\xi)}dx\,d\xi$, where

$$q_{\beta,m}(x,\xi) = q_m(W_{\beta,m}^{1/2}x, W_{\beta,m}^{1/2}\xi) \tag{II.16}$$

and

$$W_{\beta,m} = \sqrt{2}V_m^{-1/2} \tanh \frac{\beta V_m^{1/2}}{\sqrt{2}}. \tag{II.17}$$

(In fact, one can prove that condition (H1) and the spectral theorem imply that for any continuous function f on $\mathbb{R}$, $\langle f(V_m)e_i, e_j\rangle$ tends to $\langle f(V)e_i, e_j\rangle$ as $m \to \infty$.) This relation between $\hat{\mu}_\beta$ and the usual Gibbs measure reflects the relation between the usual quantum Gibbs measure $e^{-\beta H_m}$ and the Weyl quantization of the classical Gibbs measure $e^{-\beta q_m}$, namely (see Lemma III.1 below):

$$e^{-\beta H_m} = C_{\beta,m}\ \mathrm{Op}^W(e^{-q_{\beta,m}}),$$

where $C_{\beta,m}$ is a constant. In particular, if we denote by # the Weyl composition of symbols, we get (with some other constant $C'_{\beta,m}$):

$$e^{-q_{\beta,m}} \# e^{-q_{\beta,m}} = C'_{\beta,m} e^{-q_{2\beta,m}}, \tag{II.18}$$

which also explains the fact that $\hat{\mu}_\beta$ appears in the result given the above choice of $g_{m,\beta,\lambda}$, dictated by the standard requirement $\mathrm{Tr}\ e^{-\beta H_m} < +\infty$.

To state the mixing property we need two additional assumptions

(H4) The spectrum of V on $l^2(\mathbb{Z})$ is absolutely continuous.

(H5) The matrix $W_{\beta,m} = \sqrt{2}V_m^{-1/2} \tanh \beta V_m^{1/2}/\sqrt{2}$ satisfies:

$$(W_{\beta,m})_{i,j} = \mathcal{O}(|i-j|^{-\infty})$$

uniformly with respect to m, i, and j.

Note that (H5) is satisfied, e.g., for V of the form $V = I + \alpha J$ where J admits only a finite number of nonzero diagonals and $\alpha \in \mathbb{R}$ is chosen small enough. In particular, the example given in Eq. (II.10) satisfies assumption (H1) and assumptions (H4)–(H5) if $|\alpha|$ is small enough. Note also that the absolute continuity of $\sigma(V)$ implies (Ref. 7) that the continuous dynamical system $(\Lambda_\infty, \phi_t, \mu_G)$ enjoys the mixing property. For $m_1 \in \mathbb{N}$ and $a \in S_{m_1}(1)$, we denote $\hat{a} \in \mathcal{S}'(\Lambda_{m_1})$ the usual Fourier transform of a formally given by the integral:

$$\hat{a}(x^*,\xi^*) = \int_{\Lambda_{m_1}} e^{-i\langle (x,\xi),(x^*,\xi^*)\rangle} a(x,\xi)\,dx\,d\xi. \tag{II.19}$$

Then the result is

Theorem II.2: *Assume* (H1) *and* (H4)–(H5). *For* $m_1 \in \mathbb{N}$ *fixed,* $a, b \in S_{m_1}(1)$, *and* $n \geqslant m_1$ *denote*

$$A = \mathrm{Op}^W(a \circ \Pi_{m_1}),$$

$$A_n(t) = e^{itH_n} A e^{-itH_n} = \mathrm{Op}^W(a \circ \Pi_{m_1} \circ \phi_{n,t}) := \mathrm{Op}^W(a_{n,t}),$$

$$B = \mathrm{Op}^W(b \circ \Pi_{m_1}).$$

Then we have

$$\lim_{m\to\infty} \frac{\mathrm{Tr}(Ae^{-\beta H_m})}{\mathrm{Tr}(e^{-\beta H_m})} = \int_{\Lambda_\infty} a \circ \Pi_{m_1} d\hat{\mu}_\beta := \omega_\beta(A) \tag{II.20}$$

and if moreover $\hat{a}$ *and* $\hat{b}$ *are bounded measures on* Λ_{m_1}, *one has:*

$$\lim_{t\to\infty} \lim_{n\to\infty} \omega_\beta(A_n(t)B) = \omega_\beta(A) \cdot \omega_\beta(B). \tag{II.21}$$

Remark: Although this corresponds to the notion of quantum mixing already existing in the framework of W^* dynamical systems, our procedure permits us to completely avoid to realize any algebra of operators on an infinite dimensional space.

Under an additional assumption on V the results of Theorems 2.1 and 2.2 admit a less cumbersome formulation which eliminates the necessity of the double limit with respect to m and n. The further assumption is

(H6) For all $m \geqslant 0$ there exists a $(2m+1)\times(2m+1)$ real-symmetric matrix $\tilde{V}_m$ satisfying the same assumption (H1) as V_m, and such that:

(i) $\forall i,j \in \mathbb{Z}$, $\langle \tilde{V}_m^{-1} e_i, e_j \rangle$ tends to $\langle V^{-1} e_i, e_j \rangle_{l^2}$ as $m \to +\infty$;
(ii) $\forall m,n \in \mathbb{Z}$, the operator $\Pi_m \tilde{V}_n^{-1/2} \Pi_n$ becomes independent of n for $\ddot{n}$ sufficiently large;
(iii) The operator $\tilde{V}_m^{-1/2} \Pi_m \tilde{V}_n^{-1/2} \Pi_n$ tends strongly to the identity on each $\mathscr{H}_k$ ($k \in \mathbb{N}$) as $m \to +\infty$.

It is not very difficult to verify that an example of such V satisfying (H4) (in addition to (H1)–(H2)) is given by $V = W^2$ where W is as in the example (II.10): in this case one can take $\tilde{V}_m = (W_m)^2$ where W_m is extracted from W as in Eq. (I.8).

Under assumption (H6), we define for $0 < \beta < (2M)^{-1/2}$:

$$\tilde{q}_{\beta,m}(x,\xi) = \langle F_{\beta,m}\xi, \xi \rangle + \langle G_{\beta,m}x, x \rangle, \tag{II.22}$$

where (denoting I_m the identity on $\mathbb{R}^{2m+1}$):

$$F_{\beta,m} = \frac{1}{2\beta} \tilde{V}_m^{-1} (I_m - (I_m - 2\beta^2 \tilde{V}_m)^{1/2}), \tag{II.23}$$

$$G_{\beta,m} = 2\tilde{V}_m F_{\beta,m}. \tag{II.24}$$

We also consider on X_m the probability measure:

$$d\tilde{\nu}_m(\lambda) = \frac{\|\mathrm{Op}^W(e^{-\tilde{q}_{\beta,m}}) f_\lambda\|^2 d\theta_m(\lambda)}{\int_{X_m} \|\mathrm{Op}^W(e^{-\tilde{q}_{\beta,m}}) f_\lambda\|^2 d\theta_m(\lambda)}. \tag{II.25}$$

Then the result is:

Theorem II.3: *Assume* (H1)–(H3) *and,* (H6), *and, for* $m_1 \in \mathbb{N}$ *fixed,* $a \in S_{m_1}(1)$ *and* $0 < \beta < (2M)^{-1/2}$, *denote*

$$\widetilde{g}_{m,\beta,\lambda}=\frac{\mathrm{Op}^W(e^{-\widetilde{q}_{\beta/2,m}})f_\lambda}{\|\mathrm{Op}^W(e^{-\widetilde{q}_{\beta/2,m}})f_\lambda\|}$$

and

$$\widetilde{A}(m,T,\lambda)=\frac{1}{T}\int_0^T\langle e^{itH_m}\,\mathrm{Op}^W(a\circ\Pi_{m_1})e^{-itH_m}\widetilde{g}_{m,\beta,\lambda},\widetilde{g}_{m,\beta,\lambda}\rangle_{L^2(\mathbb{R}^{2m+1})}dt.$$

Then one has

(i)

$$\lim_{T\to\infty}\limsup_{m\to\infty}\int_{X_m}\left|\widetilde{A}(m,T,\lambda)-\int_{\Lambda_\infty}a\circ\Pi_{m_1}d\mu_G(\beta)\right|d\widetilde{\nu}_m(\lambda)=0.$$

(ii) *Assume furthermore* (H4). *Then Eq.* (II.20) *becomes*

$$\lim_{m\to\infty}\frac{\mathrm{Tr}\,A\,\mathrm{Op}^W(e^{-\beta q_m})}{\mathrm{Tr}\,\mathrm{Op}^W(e^{-\beta q_m})}=\int_{\Lambda_\infty}a\circ\Pi_{m_1}d\mu_G\beta:=\widetilde{\omega}_\beta(A)\tag{II.26}$$

and if moreover $\hat{a}$ *and* $\hat{b}$ *are bounded measures on* Λ_{m_1}, *Eq.* (II.21) *becomes*:

$$\lim_{t\to\infty}\lim_{m\to\infty}\widetilde{\omega}_\beta(A_m(t)B)=\widetilde{\omega}_\beta(A)\cdot\widetilde{\omega}_\beta(B).\tag{II.27}$$

Remarks:

(1) Here, the choice of the quadratic form $\widetilde{q}_{\beta,m}$ is dictated from the fact that we have (see Lemma V.2 below):

$$e^{-\widetilde{q}_{\beta,m}}\#e^{-\widetilde{q}_{\beta,m}}=C''_{\beta,m}e^{-2\beta\widetilde{q}_m},\tag{II.28}$$

where

$$\widetilde{q}_m(x,\xi)=\tfrac{1}{2}|\xi|^2+\langle\widetilde{V}_m x,x\rangle.$$

In view of assumption (H6) (i), this explains why we get the usual Gibbs measure in the limit $m\to+\infty$. Note that we also have $F_{\beta,m}=\beta/2I_m+\mathcal{O}(\beta^3)$ and $G_{\beta,m}=\beta V_m+\mathcal{O}(\beta^3)$, so that $\widetilde{q}_{\beta,m}$ is asymptotically equal to $\beta\widetilde{q}_m$ as $\beta\to0_+$.

(2) For small β it is possible to compare $\mathrm{Op}^W(e^{-\widetilde{q}_{\beta,m}})$ with $e^{-\beta\widetilde{H}_m}$, where $\widetilde{H}_m=\mathrm{Op}^W(\widetilde{q}_m)=2/1(\Sigma_{j=1}^{2m+1}D_{x_j}^2)+\langle\widetilde{V}_m x,x\rangle$. Actually, denoting $\widetilde{\lambda}_1,\ldots,\lambda_{2m+1}$ the eigenvalues of $\widetilde{V}_m$, we get by standard formulas (see Eq. (III.3) below) that $\mathrm{Op}^W(e^{-\widetilde{q}_{\beta,m}})$ is unitarily equivalent to

$$\bigotimes_{j=1}^{2m+1}\frac{1}{\sqrt{1-\beta^2\widetilde{\lambda}_j/2}}\exp\left[-\frac{1}{2}\left(\ln\frac{1+\beta\sqrt{\widetilde{\lambda}_j/2}}{1-\beta\sqrt{\widetilde{\lambda}_j/2}}\right)(D_{x_j}^2+x_j^2)\right]\tag{II.29}$$

while under the same unitary transformation $e^{-\beta\widetilde{H}_m}$ becomes

$$\bigotimes_{j=1}^{2m+1}e^{-\beta\sqrt{\widetilde{\lambda}_j/2}(D_{x_j}^2+x_j^2)}.\tag{II.30}$$

Since for small β we have:

$$\frac{1}{2}\ln\frac{1+\beta\sqrt{\tilde{\lambda}_j/2}}{1-\beta\sqrt{\tilde{\lambda}_j/2}}=\beta\sqrt{\frac{\tilde{\lambda}_j}{2}}\,(1+\mathcal{O}(\beta))$$

we get from Eqs. (II.29) and (II.30):

$$\mathrm{Op}^W(e^{-\tilde{q}_{\beta,m}})=e^{-\beta\tilde{H}_m(1+\beta R_{\beta,m})}, \tag{II.31}$$

where $[R_{\beta,m},\tilde{H}_m]=0$ and $1/(2m+1)R_{\beta,m}$ is uniformly bounded in (β,m).

(3) The previous remark proves that for small β, $[\mathrm{Op}^W(e^{-\tilde{q}_{\beta,m}}),\tilde{H}_m]=0$. This is true for all positive β, by formula (III.4) below, and the fact that

$$e^{-\tilde{q}_{\beta,m}}\circ\exp tH_{\tilde{q}_m}(x,\xi)=e^{-\tilde{q}_{\beta,m}}\circ\exp tH_{\tilde{q}_{\beta,m}}((2F_{\beta,m})^{-1/2}x,(2F_{\beta,m})^{-1/2}\xi)$$

is constant with respect to $t\in\mathbb{R}$.

(4) Since the choice of the lattice $\mathbb{Z}$ does not play any role at all in our proofs, it can be replaced without modification by any lattice $\Gamma\subset\mathbb{R}^d$ $(d\geqslant 1)$ of the type considered in Ref. 7, in which case the model describes an infinite harmonic crystal in $\mathbb{R}^d$. Also the choice of Λ_m is nonssential, in the sense that any other choice $\Lambda_m'\to\Lambda_\infty$ in a reasonable way leads to the same results.

III. PROOF OF THEOREM 2.1

Now we turn to the proof of Theorem 2.1. The fact that $(\lambda_\infty,\phi_t,\hat{\mu}_\beta)$ is ergodic essentially follows from the arguments of Ref. 7, but, for the sake of completeness, we give a sketch of the proof. First, the invariance of $\hat{\mu}_\beta$ under ϕ_t is a consequence of the commutativity between the operator B defined in Eq. (II.5) and the operator $l^2(\mathbb{Z})\oplus l^2(\mathbb{Z})\ni(x,\xi)\mapsto(W_\beta^{1/2}x,W_\beta^{1/2}\xi)$. Now, denote $\hat{h}_1$ the closure in $L^2(\Lambda_\infty,d\hat{\mu}_\beta)$ of the set of all finite sums of $(a_jx_j+b_j\xi_j)$'s, $(a_j,b_j\in\mathbb{C};j\in\mathbb{Z})$. Then, denoting $d(\mathbb{Z})$ the elements of $l^2(\mathbb{Z})$ with finite support, the application

$$\Theta: d(\mathbb{Z})\oplus d(\mathbb{Z})\to\hat{h}_1,$$

$$a\oplus b\mapsto\sum_j\,(a_jx_j+b_j\xi_j),$$

can be extended into an isomorphism from $D((2VW_\beta)^{-1/2})\oplus D(W_\beta^{-1/2})$ to $\hat{h}_1$ (where $D(A)$ denotes the domain of the operator A). Moreover, identifying $D((2VW_\beta)^{-1/2})\oplus D(W_\beta^{-1/2})$ with $l^2(\mathbb{Z})\oplus l^2(\mathbb{Z})$ in an obvious way, we see that the action of ϕ_t on $\hat{h}_1$ is represented on $l^2(\mathbb{Z})\oplus l^2(\mathbb{Z})$ (via the two previous identifications) by its infinitesimal generator

$$U=\begin{pmatrix}0 & -V^{-1/2}\\ V^{1/2} & 0\end{pmatrix}.$$

Since, by assumption (H2), U has no point spectrum the result (i) follows by an abstract argument (see Ref. 7, Proposition 4.2).

To prove (ii) we first show:

Lemma III.1: There exists a constant $C_{\beta,m}$ such that:

$$e^{-\beta H_m}=C_{\beta,m}\mathrm{Op}^W(e^{-q_{\beta,m}}).$$

Proof: Let $\lambda_1,\ldots,\lambda_{2m+1}$ be the eigenvalues of V_m, and denote $y=(y_1,\ldots,y_{2m+1})$ the coordinates in $\mathbb{R}^{2m+1}$ corresponding to an orthonormal basis of eigenvectors of V_m. Then H_m becomes:

$$H'_m = -\frac{1}{2}\,\Delta_y + \sum_j \lambda_j y_j^2$$

while the operator $K_m = \mathrm{Op}^W(e^{-q_{\beta,m}})$ is transformed into

$$K'_m = \bigotimes_{j=1}^{2m+1} \mathrm{Op}^W\left(\exp -\left(\frac{1}{\sqrt{2\lambda_j}}\tanh\left(\beta\sqrt{\frac{\lambda_j}{2}}\right)\eta_j^2 + \sqrt{2\lambda_j}\tanh\left(\beta\sqrt{\frac{\lambda_j}{2}}\right)y_j^2\right)\right).$$

[Here η is the dual variable of y, and $\xi = ({}^tM)^{-1}\eta = M\eta$ since $x = My$ with M orthogonal.] Then the change of variables

$$y_j \mapsto z_j = (2\lambda_j)^{1/4} y_j$$

transforms H'_m into

$$H''_m = \sum_j \sqrt{\frac{\lambda_j}{2}}\,(D_{z_j}^2 + z_j^2) \tag{III.1}$$

and K'_m into

$$K''_m = \bigotimes_{j=1}^{2m+1} \mathrm{Op}^W\left(\exp\left[\tanh\left(\beta\sqrt{\frac{\lambda_j}{2}}\right)(\zeta_j^2 + z_j^2)\right]\right). \tag{III.2}$$

Next, consider the well known one-dimensional identity valid for $0<a<1$

$$\mathrm{Op}^W(e^{-a(x^2+\xi^2)}) = \frac{1}{\sqrt{1-a^2}}\exp\left(-\frac{a}{2}\,x^2\right)\exp\left(-\frac{a}{1-a^2}\,D_x^2\right)\exp\left(-\frac{a}{2}\,x^2\right),$$

which can be for instance verified by explicit computation of the Weyl symbol on the right-hand side. Then, using the formula (see, e.g., Ref. 13)

$$\exp\left(-\frac{x^2}{2}\right)\exp(-tD_x^2)\exp\left(-\frac{x^2}{2}\right) = \exp\left[-\frac{\ln(z+\sqrt{z^2-1})}{4k\sqrt{z^2-1}}\,(D_x^2 + 4k^2(z^2-1)x^2)\right]$$

with $k = 1/4t$, $z = 2t+1$ $(t>0)$, we get in particular for $0<a<1$:

$$\mathrm{Op}^W(e^{-a(x^2+\xi^2)}) = \frac{1}{\sqrt{1-a^2}}\exp\left[-\frac{1}{2}\left(\ln\frac{1+a}{1-a}\right)(D_x^2 + x^2)\right] \tag{III.3}$$

Taking $a = \tanh(\beta\sqrt{\lambda_j/2})$, the Lemma follows from Eqs. (III.1)–(III.3). □

Now, since the flow generated by q_n defines a linear canonical transformation on Λ_n, we have

$$e^{itH_n}\mathrm{Op}^W(a)e^{itH_n} = \mathrm{Op}^W(a\circ\exp tH_{q_n}), \quad \forall a \in S_n(1). \tag{III.4}$$

This relation [an ''exact Egorov theorem,'' going back at least to Van Hove (see, e.g., Ref. 14)] holds only in the Weyl quantization[15] (Sec. 5.2).

For $n \leqslant m$ and $(x,\xi) \in \Lambda_m$, denote

$$\rho(m,\lambda) = \|e^{-1/2\beta H_m} f_\lambda\|^2, \tag{III.5}$$

$$a_{n,T}(x,\xi)=\frac{1}{T}\int_0^T (a\circ\Pi_{m_1}\circ\exp\, tH_{q_n}\circ\Pi_n)(x,\xi))dt. \tag{III.6}$$

Using Lemma (III.1), (III.4), and (II.11), we get

$$A(m,n,T,\lambda)=\frac{C_{\beta,m}^2}{\rho(m,\lambda)}\int_{\Lambda_m}(e^{-q_{\beta,m}}\#a_{n,T}\#e^{-q_{\beta,m}})(x,\xi)w_{f_\lambda}(x,\xi)dxd\xi, \tag{III.7}$$

where # is the Weyl composition of symbols on Λ_m:

$$(a\#b)(x,\xi)=\pi^{-2(2m+1)}\int_{\Lambda_m^2}a(x+y,\xi+\eta)b(x+z,\xi+\zeta)e^{2i(\zeta y-z\eta)}dyd\eta dzd\zeta. \tag{III.8}$$

Taking advantage of assumption (H3), we get from Eq. (III.7)

$$\int_{X_m}A(m,n,T,\lambda)\rho(m,\lambda)d\theta_m(\lambda)=C_0\int_{\Lambda_m}(e^{-q_{\beta,m}}\#a_{n,T}\#e^{-q_{\beta,m}})(x,\xi)dxd\xi, \tag{III.9}$$

$$\int_{X_m}|A(m,n,T,\lambda)|\rho(m,\lambda)d\theta_m(\lambda)\leqslant C_0\int_{\Lambda_m}|(e^{-q_{\beta,m}}\#a_{n,T}\#e^{-q_{\beta,m}})(x,\xi)|dxd\xi, \tag{III.10}$$

where $C_0=C_0(\beta,m)$ is a constant, which can be computed by taking $a\equiv 1$ in (III.9):

$$C_0=\left(\int e^{-q_{\beta,m}}\#e^{-q_{\beta,m}}dxd\xi\right)^{-1}\int_{X_m}\rho(m,\lambda)d\theta_m(\lambda). \tag{III.11}$$

This also proves Eq. (II.12) so that, using the notation (II.13) we can rewrite Eqs. (III.9)–(III.10) as:

$$\int_{X_m}A(m,n,T,\lambda)d\nu_m(\lambda)=C_1\int_{\Lambda_m}(e^{-q_{\beta,m}}\#a_{n,T}\#e^{-q_{\beta,m}})(x,\xi)dxd\xi, \tag{III.12}$$

$$\int_{X_m}|A(m,n,T,\lambda)|d\nu_m(\lambda)\leqslant C_1\int_{\Lambda_m}|(e^{-q_{\beta,m}}\#a_{n,T}\#e^{-q_{\beta,m}})(x,\xi)|dxd\xi \tag{III.13}$$

with

$$C_1=\left(\int e^{-q_{\beta,m}}\#e^{-q_{\beta,m}}dxd\xi\right)^{-1}.$$

Now we make use of the two following properties of the operation # (valid, e.g., for any a,b,c in $\mathcal{S}(\Lambda_m)$):

$$\int_{\Lambda_m}(a\#b\#c)(x,\xi)dxd\xi=\int_{\Lambda_m}(b\#c\#a)(x,\xi)dxd\xi, \tag{III.14}$$

$$\int_{\Lambda_m}(a\#b)(x,\xi)dxd\xi=\int_{\Lambda_m}a(x,\xi)b(x,\xi)dxd\xi. \tag{III.15}$$

The property (III.14) is just a consequence of the cyclicity of the trace of operators, and Eq. (III.15) comes from a direct computation using Eq. (III.8).

Here our symbol a is not supposed to be in $\mathscr{S}(\Lambda_m)$, but an easy argument of density allows us to deduce from Eq. (III.12) and Eqs. (III.14)–(III.15) [using also Eq. (II.18)]:

$$\int_{X_m} A(m,n,T,\lambda)\,d\nu_m(\lambda) = \int_{\Lambda_m} a_{n,T}(x,\xi)[e^{-q_{\beta,m}(x,\xi)}dx\,d\xi]_N, \tag{III.16}$$

where we have used the notation:

$$\int_E f[d\mu]_N = \frac{1}{\mu(E)} \int_E f\,d\mu \tag{III.17}$$

for any finite positive measure μ on a set E.

Now the problem is to rewrite also Eq. (III.13) in this way, despite the appearance of the modulus. The argument to do this is based upon the following:

Lemma III.2: There exists a positive definite quadratic form $Q_{\beta,m}(x,\xi,y,\eta)$ on Λ_m^2 such that for all $a \in S_m(1)$:

$$e^{-q_{\beta,m}} \# a \# e^{-q_{\beta,m}} = C'_{\beta,m} \tilde{a} e^{-q_{2\beta,m}},$$

where $C'_{\beta,m}$ is the constant appearing in Eq. (II.18), and

$$\tilde{a}(x,\xi) = \int_{\Lambda_m} a(y,\eta)[e^{-Q_{\beta,m}(x,\xi,y,\eta)}dy\,d\eta]_N.$$

Proof: See Appendix A.

We deduce in particular from Lemma III.2 the existence of a positive C^∞ function $\gamma(x,\xi)$ on Λ_m such that for all $a \in S_m(1)$:

$$\int_{\Lambda_m} (e^{-q_{\beta,m}} \# a \# e^{-q_{\beta,m}})dx\,d\xi = \int_{\Lambda_m} a(x,\xi)\,\gamma(x,\xi)dx\,d\xi, \tag{III.18}$$

$$\int_{\Lambda_m} |e^{-q_{\beta,m}} \# a \# e^{-q_{\beta,m}}|dx\,d\xi \leqslant \int_{\Lambda_m} |a(x,\xi)|\,\gamma(x,\xi)dx\,d\xi. \tag{III.19}$$

By Eqs. (III.12), (III.16), and (III.18) we get that γ equals a constant times $e^{-q_{2\beta,m}}$, which by Eqs. (III.13) and (III.19) allows us to conclude that:

$$\int_{X_m} |A(m,n,T,\lambda)|\,d\nu_m(\lambda) \leqslant \int_{\Lambda_m} |a_{n,T}(x,\xi)|[e^{-q_{\beta,m}(x,\xi)}dx\,d\xi]_N. \tag{III.20}$$

Without loss of generality, we can assume from now on that $\int_{\Lambda_\infty} (a \circ \Pi_{m_1})\,d\hat{\mu}_\beta = 0$, and then it remains to estimate the rhs of Eq. (III.20). Since $a_{n,T}(x,\xi)$ depends only on $\Pi_n(x,\xi)$, we can let m go to $+\infty$ in Eq. (III.20) and we get

$$\limsup_{m\to\infty} \int_{X_m} |A(m,n,T,\lambda)|\,d\nu_m(\lambda) \leqslant \int_{\Lambda_\infty} |a_{n,T}(x,\xi)|\,d\hat{\mu}_\beta. \tag{III.21}$$

Then we use Eq. (II.7) to let n go to $+\infty$ in Eq. (III.22). By the dominated convergence theorem, we then obtain

$$\limsup_{n\to\infty}\limsup_{m\to\infty}\int_{X_m}|A(m,n,T,\lambda)|d\nu_m(\lambda)\leqslant\int_{\Lambda_\infty}\left|\frac{1}{T}\int_0^T(a\circ\Pi_{m_1}\circ\phi_t)(x,\xi)dt\right|d\hat{\mu}_\beta. \tag{III.22}$$

Finally, we let T go to $+\infty$. By the ergodicity property, we have that

$$\frac{1}{T}\int_0^T(a\circ\Pi_{m_1}\circ\phi_t)(x,\xi)dt\to\int_{\Lambda_\infty}(a\circ\Pi_{m_1})d\hat{\mu}_\beta=0$$

for $\hat{\mu}_\beta$—almost all (x,ξ) in Λ_∞. Therefore, again applying the dominated convergence theorem, we get from Eq. (III.22):

$$\lim_{T\to+\infty}\limsup_{n\to\infty}\limsup_{m\to\infty}\int_{X_m}|A(m,n,T,\lambda)|d\nu_m(\lambda)\leqslant 0 \tag{III.23}$$

and this completes the proof of Theorem 2.1. □

IV. PROOF OF THEOREM 2.2

Let us now proceed to the proof of Theorem 2.2. Denote

$$\omega_{\beta,m}(A)=\frac{\mathrm{Tr}(Ae^{-\beta H_m})}{\mathrm{Tr}(e^{-\beta H_m})}. \tag{IV.1}$$

Using Lemma III.1 and Eq. (III.15) we see that

$$\omega_{\beta,m}(A)=\int_{\Lambda_m}a\circ\Pi_{m_1}(x,\xi)[e^{-q_{\beta,m}(x,\xi)}dxd\xi]_N \tag{IV.2}$$

so that the first assertion (II.20) of the theorem is obvious.

For $m\geqslant n\geqslant m_1$ we also have:

$$\omega_{\beta,m}(A_n(t)B)=\int_{\Lambda_m}a_{n,t}\#(b\circ\Pi_{m_1})(x,\xi)[e^{-q_{\beta,m}(x,\xi)}dxd\xi]_N. \tag{IV.3}$$

For $X=(x,\xi)$ and $Y=(y,\eta)\in\Lambda_m$, we denote

$$\sigma(X,Y)=\xi y-x\eta \tag{IV.4}$$

the canonical symplectic form on Λ_m. Then by Eq. (III.8) we have:

$$a_{n,t}\#(b\circ\Pi_{m_1})(X)=\pi^{-2(2m+1)}\int_{\Lambda_n^2}(a_{n,t}\circ\Pi_n)(Y)(b\circ\Pi_{m_1})(Z)e^{2i[\sigma(Y,X)+\sigma(Z,Y-X)]}dYdZ. \tag{IV.5}$$

By the Fourier inversion formula and the assumption on a,b, we can write for any $Y_1\in\Lambda_{m_1}$:

$$a(Y_1)=(2\pi)^{-2(2m_1+1)}\int_{\Lambda_{m_1}}e^{\langle Y_1,Y^*\rangle}\hat{a}(Y^*)dY^* \tag{IV.6}$$

and a similar formula for b. Here we have used an abuse of notation by writing $\hat{a}(Y^*)dY^*$ for the (not necessarily Lebesgue absolutely continuous) measure defined by the Fourier transform of a.

In particular, taking $Y_1 = \Pi_{m_1}\phi_{n,t}\Pi_n(Y)$ in Eq. (IV.6) and substituting in Eq. (IV.5), we get

$$a_{n,t}\#(b\circ\Pi_{m_1})(X) = \pi^{-2(2m+1)}(2\pi)^{-4(2m_1+1)} \times \int e^{2i[\sigma(Y,X)+\sigma(Z,Y-X)]+i\langle\phi_{n,t}\Pi_n(Y),Y^*\rangle+i\langle Z,Z^*\rangle} \times \hat{a}(Y^*)dY^*\hat{b}(Z^*)dZ^*dYdZ,$$

where the integration runs over $(Y^*,Z^*,Y,Z) \in \Lambda_{m_1}\times\Lambda_{m_1}\times\Lambda_m\times\Lambda_m$, and Λ_{m_1} has been identified in an obvious way with a subspace of Λ_n and of Λ_m.

Interpreting the integration over (Y,Z) as an oscillatory one, we can first integrate with respect to Z, and we obtain (using the well-known identity $\int_{\mathbb{R}^d} e^{2i(x-y)\xi}d\xi = \pi^d\delta(y=x)$):

$$a_{n,t}\#(b\circ\Pi_{m_1})(X) = (2\pi)^{-4(2m_1+1)}\int e^{i\langle Z^*,X\rangle+i\langle\phi_{n,t}\Pi_n(X+\tilde{Z}^*/2),Y^*\rangle}\hat{a}(Y^*)dY^*\hat{b}(Z^*)dZ^*, \tag{IV.7}$$

where we have denoted $\tilde{Z}^* = (-\zeta^*, z^*)$ if $Z^* = (z^*,\zeta^*)$.

Now, inserting Eq. (IV.7) into Eq. (IV.3), and making the change of variables $X \mapsto X - \tilde{Z}^*/2$, this gives:

$$\omega_{\beta,m}(A_n(t)B) = (2\pi)^{-4(2m_1+1)}\int_{\Lambda_m\times\Lambda_{m_1}^2} e^{i\langle Z^*,X\rangle+i\langle\phi_{n,t}\Pi_n(X),Y^*\rangle} \times [e^{-q_{\beta,m}(X-\tilde{Z}^*/2)}dX]_N\hat{a}(Y^*)dY^*\hat{b}(Z^*)dZ^*$$

and therefore, writing $q_{\beta,m}(X) = \langle Q_{\beta,m}X,X\rangle$ with $Q_{\beta,m}(x,\xi) = (V_mW_{\beta,m}x, W_{\beta,m}\xi)$:

$$\omega_{\beta,m}(A_n(t)B) = (2\pi)^{-4(2m_1+1)}\int_{\Lambda_{m_1}^2}\Gamma_{m,n,t}(Y^*,Z^*)e^{-q_{\beta,m}(\tilde{Z}^*)/4}\hat{a}(Y^*)dY^*\hat{b}(Z^*)dZ^*, \tag{IV.8}$$

where

$$\Gamma_{m,n,t}(Y^*,Z^*) = \int_{\Lambda_m} e^{i\langle Z^*,X\rangle+\langle\tilde{Z}^*,Q_{\beta,m}X\rangle+i\langle\phi_{n,t}\Pi_n(X),Y^*\rangle}[e^{-q_{\beta,m}(X)}dX]_N \tag{IV.9}$$

is of the form

$$\Gamma_{m,n,t}(Y^*,Z^*) = \int_{\Lambda_m} F_{n,t,Y^*,\tilde{Z}^*}(\Pi_{m_1}Q_{\beta,m}X,\Pi_nX))[e^{-q_{\beta,m}(X)}dX]_N \tag{IV.10}$$

with F_{n,t,Y^*,Z^*} smooth and uniformly bounded together with all its derivatives on $\Lambda_{m_1}\times\Lambda_n$. To let m tend to infinity in Eq. (IV.10), we use the following lemma (which is the point where (H5) is used):

Lemma IV.1: Let $F \in C^\infty(\Lambda_{m_1}\times\Lambda_n)$ be uniformly bounded with all its derivatives. Then

$$\int_{\Lambda_m} F(\Pi_{m_1}Q_{\beta,m}X,\Pi_nX))[e^{-q_{\beta,m}(X)}dX]_N \to \int_{\Lambda_\infty} F(\Pi_{m_1}Q_\beta X,\Pi_nX))d\hat{\mu}_\beta \quad (m\to\infty),$$

where $\hat{\mu}_\beta$ is defined in Eq. (II.15), *and Q_β is defined on Λ_∞ by*

$$Q_\beta(x,\xi)=(VW_\beta x, W_\beta \xi), \quad W_\beta=\sqrt{2}V^{-1/2}\tanh\frac{\beta V^{1/2}}{\sqrt{2}}.$$

Proof: See Appendix A.

Now, for any fixed (n,t,Y^*,Z^*), we see on Eqs. (IV.9)–(IV.10) that, as $m\to\infty$, $\Gamma_{m,n,t}(Y^*,Z^*)$ tends to

$$\Gamma_{n,t}(Y^*,Z^*)=\int_{\Lambda_\infty} e^{i\langle Z^*,X\rangle+\langle \tilde{Z}^*,Q_\beta X\rangle+i\langle \phi_{n,t}\Pi_n(X),Y^*\rangle}d\hat{\mu}_\beta \tag{IV.11}$$

which in turn is of the form:

$$\Gamma_{n,t}(Y^*,Z^*)=\int_{\Lambda_\infty} f_{Z^*}(X)g_{Y^*}(\Pi_{m_1}\phi_{n,t}\Pi_n X)d\hat{\mu}_\beta \tag{IV.12}$$

with f_{Z^*} and g_{Y^*} uniformly bounded, and g_{Y^*} continuous on Λ_{m_1}. Then, using Eq. (II.7) and the dominated convergence theorem, we see on Eq. (IV.12) that, as $n\to\infty$, $\Gamma_{n,t}(Y^*,Z^*)$ tends to

$$\Gamma_t(Y^*,Z^*)=\int_{\Lambda_\infty} f_{Z^*}(X)g_{Y^*}(\Pi_{m_1}\phi_t X)d\hat{\mu}_\beta. \tag{IV.13}$$

Now, the same arguments used in the proof of Theorem 2.1 (i) (see the beginning of Sec. III) lead to the fact that under (H4) the classical dynamical system $(\Lambda_\infty,\phi_t,\hat{\mu}_\beta)$ is mixing. As a consequence, we get from Eq. (IV.13)

$$\Gamma_t(Y^*,Z^*)\to\int f_{Z^*}(X)d\hat{\mu}_\beta\cdot\int g_{Y^*}(\Pi_{m_1}X)d\hat{\mu}_\beta \quad \text{as} \quad t\to\infty. \tag{IV.14}$$

Summing up Eqs. (IV.9)–(IV.14), we have proved that for any fixed $(Y^*,Z^*)\in\Lambda_{m_1}^2$, we have

$$\lim_{t\to\infty}\lim_{n\to\infty}\lim_{m\to\infty}\Gamma_{m,n,t}(Y^*,Z^*)=\int_{\Lambda_\infty} e^{i\langle Z^*,X\rangle+\langle\tilde{Z}^*,Q_\beta X\rangle}d\hat{\mu}_\beta(X)\cdot\int_{\Lambda_\infty} e^{i\langle X,Y^*\rangle}d\hat{\mu}_\beta(X) \tag{IV.15}$$

and because of the translation invariance of the Lebesgue measure on Λ_m, and the fact that $\langle Z^*,\tilde{Z}^*\rangle=0$, it is also easy to verify that

$$\int_{\Lambda_\infty} e^{i\langle Z^*,X\rangle+\langle\tilde{Z}^*,Q_\beta X\rangle}d\hat{\mu}_\beta(X)=e^{\langle Q_\beta\tilde{Z}^*,\tilde{Z}^*\rangle/4}\int_{\Lambda_\infty} e^{i\langle Z^*,X\rangle}d\hat{\mu}_\beta(X). \tag{IV.16}$$

Since by assumption $\hat{a}(Y^*)dY^*$ and $\hat{b}(Z^*)dZ^*$ are bounded measures on Λ_{m_1} and $|\Gamma_{m,n,t}(Y^*,Z^*)e^{-q_{\beta,m}(\tilde{Z}^*)/4}|=1$, we can use the dominated convergence theorem in Eq. (IV.8) and conclude from Eqs. (IV.15)–(IV.16) (using also the obvious fact that $q_{\beta,m}(\tilde{Z}^*)$ tends to $\langle Q_\beta\tilde{Z}^*,\tilde{Z}^*\rangle$ as $m\to\infty$) that

$$\lim_{t\to\infty}\lim_{n\to\infty}\lim_{m\to\infty}\omega_{\beta,m}(A_n(t)B)=(2\pi)^{-4(2m_1+1)}\int_{\Lambda_{m_1}\times\Lambda_\infty}e^{i\langle X,Y^*\rangle}\hat{a}(Y^*)dY^*d\hat{\mu}_\beta(X)$$

$$\cdot\int_{\Lambda_{m_1}\times\Lambda_\infty}e^{i\langle Z^*,X\rangle}\hat{b}(Z^*)dZ^*d\hat{\mu}_\beta(X)$$

$$=\int_{\Lambda_\infty}a\circ\Pi_{m_1}d\hat{\mu}_\beta\cdot\int_{\Lambda_\infty}b\circ\Pi_{m_1}d\hat{\mu}_\beta,$$

where the last equality comes again from the Fourier-inversion formula. □

V. PROOF OF THEOREM 2.3

Lemma V.2: For any pair of positive definite real-symmetric matrices F and G on Λ_m, there exists a constant C=C(F,G,m) such that:

$$e^{-(\langle F\xi,\xi\rangle+\langle Gx,x\rangle)}\#e^{-(\langle F\xi,\xi\rangle+\langle Gx,x\rangle)}=Ce^{-2(\langle F(F+G^{-1})^{-1}G^{-1}\xi,\xi\rangle+\langle(F+G^{-1})^{-1}x,x\rangle)}.$$

Proof: See Appendix A.

In particular, taking $F=F_{\beta,m}$ and $G=G_{\beta,m}$ defined in Eqs. (II.23) and (II.24) we easily get Eq. (II.28) from Lemma V.2. Then computations analogous to those of the previous section [Eqs. (III.7)–(III.20)] lead to

$$\int_{X_m}|\widetilde{A}(m,T,\lambda)|d\tilde{\nu}_m(\lambda)\leqslant\int_{\Lambda_m}|a_{m,T}(x,\xi)|[e^{-\beta\tilde{q}_m(x,\xi)}dxd\xi]_N. \tag{V.1}$$

Now on the rhs of Eq. (V.1) we make the change of variables:

$$x=\widetilde{V}_m^{-1/2}y,\quad \xi=\eta,$$

which gives

$$\int_{\Lambda_m}|a_{m,T}(x,\xi)|[e^{-\beta\tilde{q}_m(x,\xi)}dxd\xi]_N=\int_{\Lambda_m}|a_{m,T}(\widetilde{V}_m^{-1/2}y,\eta)|[e^{-\beta(\eta^2+y^2)}dyd\eta]_N. \tag{V.2}$$

Since the quadratic form in the exponent is now diagonal, we can integrate over $n\geqslant m$ variables so that

$$\int_{\Lambda_m}|a_{m,T}(x,\xi)|[e^{-\beta\tilde{q}_m(x,\xi)}dxd\xi]_N=\int_{\Lambda_n}|a_{m,T}(\widetilde{V}_m^{-1/2}\Pi_m y,\Pi_m\eta)|[e^{-\beta(\eta^2+y^2)}dyd\eta]_N \tag{V.3}$$

for any $n\geqslant m$. Coming back to the old variables on Λ_n, this gives

$$\int_{\Lambda_m}|a_{m,T}(x,\xi)|[e^{-\beta\tilde{q}_m(x,\xi)}dxd\xi]_N=\int_{\Lambda_n}|a_{m,T}(\widetilde{V}_m^{-1/2}\Pi_m\widetilde{V}_n^{1/2}x,\Pi_m\xi)|[e^{-\beta\tilde{q}_n(x,\xi)}dxd\xi]_N. \tag{V.4}$$

Now, by assumption (H4) (ii), for n large enough, the function $a_{m,T}(\widetilde{V}_m^{-1/2}\Pi_m V_n^{-1/2}x,\Pi_m\xi)$ depends only on a fixed number of variables independent of n. Then, by assumption (H4) (i) and standard results on the Gaussian measures (see, e.g., Ref. 7), letting n tend to $+\infty$ in Eq. (V.4), we get

$$\int_{\Lambda_m} |a_{m,T}(x,\xi)|[e^{-\beta \tilde{q}_m(x,\xi)} dx d\xi]_N = \int_{\Lambda_\infty} |a_{m,T}(\tilde{V}_m^{-1/2}\Pi_m \tilde{V}_n^{1/2}\Pi_n x, \Pi_m \xi)| d\mu_G(\beta). \quad \text{(V.5)}$$

Finally, using assumption (H4) (iii), Eq. (II.7), and the uniform (with respect to $m \geqslant 0$) continuity of $\exp tH_{q_m} \circ \Pi_m$ on each $\mathscr{K}_k$, we see that for all $(x,\xi) \in \Lambda_\infty$ and $t \in \mathbb{R}$:

$$(a \circ \Pi_{m_1} \circ \exp\, tH_{q_m})(\tilde{V}_m^{-1/2}\Pi_m \tilde{V}_n^{1/2}\Pi_n x, \Pi_m \xi) \to (a \circ \Pi_{m_1} \circ \phi_t)(x,\xi) \quad \text{as} \quad m \to +\infty. \quad \text{(V.6)}$$

It follows from Eqs. (V.6), (V.5), and (V.1) and the dominated convergence theorem that

$$\limsup_{m \to +\infty} \int_{X_m} |\tilde{A}(m,T,\lambda)| d\tilde{\nu}_m(\lambda) \leqslant \int_{\Lambda_\infty} \left| \frac{1}{T} \int_0^T (a \circ \Pi_{m_1} \circ \phi_t)(x,\xi) dt \right| d\mu_G(\beta). \quad \text{(V.7)}$$

Letting T tend to infinity in Eq. (V.7), the ergodicity of the system $[\Lambda_\infty, \phi_t, \mu_G(\beta)]$ and the fact that we can restrict to the case $\int a \circ \Pi_{m_1} d\mu_G(2\beta) = 0$ yield the assertion. □

VI. COHERENT STATES: SHARPENING THE ERGODICITY RESULT

Now we take $X_m = \Lambda_m$, $d\theta_m(\lambda) = d\lambda$, and for $\lambda = (\lambda_x, \lambda_\xi) \in \Lambda_m$ the corehent states defined by

$$f_\lambda(x,\xi) = e^{ix\lambda_\xi - (x-\lambda_x)^2/2}. \quad \text{(VI.1)}$$

Then a direct computation gives

$$w_{f_\lambda}(x,\xi) = 2^{2m+1}\pi^{m+1/2} e^{-(\xi-\lambda_\xi)^2 - (x-\lambda_x)^2} \quad \text{(VI.2)}$$

so that (H3) is obviously satisfied. Therefore the results of Theorems 2.1 and 2.2 hold for V satisfying assumptions (H1)–(H2) [respectively, assumptions (H1), (H2), and (H6)]. The new fact which appears in this situation is

Lemma VI.1: Under Eq. (VI.1), *the two measures* $d\nu_m(\lambda)$ *and* $d\tilde{\nu}_m(\lambda)$, *defined, respectively, by Eqs.* (II.13) *and* (II.25), *are Gaussian probability measures on* $X_m = \Lambda_m$.

Proof: In each case, the measure is of the form $C\|\mathrm{Op}^W(e^{-q}) f_\lambda\|^2 d\lambda$ where C is a constant and q is a positive definite quadratic form on Λ_m. Moreover, by computations analogous, e.g., to those for Eq. (III.7) we have

$$\|\mathrm{Op}^W(e^{-q}) f_\lambda\|^2 = C' \int_{\Lambda_m} (e^{-q} \# e^{-q})(x,\xi) w_{f_\lambda}(x,\xi) dx d\xi, \quad \text{(VI.3)}$$

where C' is another constant. Then the result follows immediately by Eq. (VI.2) and the fact that $e^{-q} \# e^{-q} = C'' e^{-q'}$ where q' is a positive definite quadratic form on Λ_m and C'' is a constant. □

Now denote L_m and $\tilde{L}_m$ the two real-symmetric positive definite $(4m+2) \times (4m+2)$ matrices defined by

$$d\nu_m(\lambda) = [e^{-\langle L_m \lambda, \lambda \rangle} d\lambda]_N, \quad \text{(VI.4)}$$

$$d\tilde{\nu}_m(\lambda) = [e^{-\langle \tilde{L}_m \lambda, \lambda \rangle} d\lambda]_N. \quad \text{(VI.5)}$$

Then for any bounded function $A(\lambda)$ we have

$$\int_{\Lambda_m} A(\lambda) d\nu_m(\lambda) = \int_{\Lambda_m} A(L_m^{-1/2}\lambda)[e^{-|\lambda|^2} d\lambda]_N \quad \text{(VI.6)}$$

and therefore, by an argument similar to the one leading to Eq. (V.21):

$$\int_{\Lambda_m} A(\lambda)d\nu_m(\lambda)=\int_{\Lambda_\infty} A(L_m^{-1/2}\Pi_m\lambda)d\nu_G(\lambda), \tag{VI.7}$$

where $d\nu_G(\lambda)$ is the finite dimensional Gibbs measure obtained by taking the limit of $[e^{-|\lambda|^2}d\lambda]_N$ on Λ_n as $n\to+\infty$. A formula analogous to Eq. (VI.7) is also true for $d\tilde{\nu}_m(\lambda)$, and therefore it follows from Theorems 2.1 and 2.2 that we have in this situation:

$$\lim_{T\to\infty}\ \limsup_{n\to\infty}\ \limsup_{m\to\infty}\int_{\Lambda_\infty}\left|A(m,n,T,L_m^{-1/2}\Pi_m\lambda)-\int_{\Lambda_\infty} a\circ\Pi_{m_1}d\hat{\mu}_\beta\right|d\nu_G(\lambda)=0, \tag{VI.8}$$

$$\lim_{T\to\infty}\ \limsup_{m\to\infty}\int_{\Lambda_\infty}\left|\tilde{A}(m,T,\tilde{L}_m^{-1/2}\Pi_m\lambda)-\int_{\Lambda_\infty} a\circ\Pi_{m_1}d\mu_G(\beta)\right|d\nu_G(\lambda)=0. \tag{VI.9}$$

Finally, using a very standard argument of measure theory, we easily deduce from Eqs. (VI.8) and (VI.9) the following:

Proposition VI.1: Assume (H1)–(H2) *and choose the set of coherent states* (VI.1). *Then there exist sequences* $(T_k)_{k\in\mathbb{N}}$, $(m_k)_{k\in\mathbb{N}}$, $(n_k)_{k\in\mathbb{N}}$ *simultaneously tending to* $+\infty$ *such that for* ν_G*—almost all* $\lambda\in\Lambda_\infty$:

$$\lim_{k\to+\infty} A(m_k,n_k,T_k,L_{m_k}^{-1/2}\Pi_{m_k}\lambda)=\int_{\Lambda_\infty} a\circ\Pi_{m_1}d\hat{\mu}_\beta.$$

If moreover assumption (H3) *is satisfied, there exist sequences* $(T_k)_{k\in\mathbb{N}}$, $(m_k)_{k\in\mathbb{N}}$ *both tending to* $+\infty$ *such that for* ν_G*—almost all* $\lambda\in\Lambda_\infty$:

$$\lim_{k\to+\infty}\tilde{A}(m_k,T_k,\tilde{L}_{m_k}^{-1/2}\Pi_{m_k}\lambda)=\int_{\Lambda_\infty} a\circ\Pi_{m_1}d\mu_G(\beta).$$

Remarks:

(1) An analogous result holds if Eq. (VI.1) is replaced by the more general case $f_\lambda(x,\xi)=e^{ix\lambda_\xi-\langle F_m(x-\lambda_x),x-\lambda_x\rangle}$, F_m being any positive definite symmetric matrix.

(2) Actually, one can replace L_m by any other symmetric matrix L_m' such that $K_m=(L_m')^{-1/2}L_m(L_m')^{-1/2}$ is a diagonal matrix and the measure $[e^{-\langle K_m\lambda,\lambda\rangle}d\lambda]_N$ on Λ_m admits a limit $d\nu_\infty$ as $m\to+\infty$. In this case the ''ν_G—almost all λ'' of the Proposition must be replaced by ''ν_∞—almost all λ.''

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APPENDIX A: PROOF OF THE LEMMAS

Proof of Lemma III.2

Using Eq. (III.8), we see that $e^{-q_{\beta,m}}\#a\#e^{-q_{\beta,m}}$ can be put under the form:

$$(e^{-q_{\beta,m}}\#a\#e^{-q_{\beta,m}})(x,\xi)=C_1\int_{\Lambda_m^4} a(Y_1)e^{-q_1(x,\xi,Y_1,Y_2,Y_3,Y_4)}dY_1dY_2dY_3dY_4, \tag{A1}$$

where all along this proof C_j $(j=1,2...)$ will denote complex constants, q_1 is a complex quadratic form on Λ_m^5, and the integral (A1) is oscillatory. Moreover, a direct computation gives:

$$\int_{\Lambda_m^3} e^{-q_1(x,\xi,Y_1,Y_2,Y_3,Y_4)} dY_2 dY_3 dY_4 = C_2 e^{-Q(x,\xi,Y_1)}, \tag{A2}$$

where $C_2 \in \mathbb{R}$ and Q is a positive definite quadratic form. Actually, this can also be seen without computation in the following way: the existence of the complex constant C_2 and the complex quadratic form Q such that Eq. (A2) holds is clear, and if a is real then $\mathrm{Op}^W(e^{-q_{\beta,m}} \# a \# e^{-q_{\beta,m}}) = \mathrm{Op}^W(e^{-q_{\beta,m}})\mathrm{Op}^W(a)\mathrm{Op}^W(e^{-q_{\beta,m}})$ is a symmetric operator. As a consequence $e^{-q_{\beta,m}} \# a \# e^{-q_{\beta,m}}$ must be real for a real, which implies that Ce^{-Q} is real (and hence both C and Q are). Moreover, one can show easily that the application $S_m(1) \ni a \mapsto e^{-q_{\beta,m}} \# a \# e^{-q_{\beta,m}}$ maps continuously $S_m(1)$ into $\mathscr{S}(\Lambda_m)$, so that Q is necessarily positive definite.

When $a \equiv 1$, we get from Eqs. (II.8), (A1), and (A2):

$$C_1 C_2 \int_{\Lambda_m} e^{-Q(x,\xi,Y_1)} dY_1 = e^{-\tilde{q}_{2\beta,m}}. \tag{A3}$$

Then the result follows from Eqs. (A1), (A2), and (A3) by writing:

$$(e^{-q_{\beta,m}} \# a \# e^{-q_{\beta,m}})(x,\xi) = \left(C_1 C_2 \int_{\Lambda_m} e^{-Q(x,\xi,Y_1)} dY_1 \right) \int_{\Lambda_m} a(Y_1) [e^{-Q(x,\xi,Y_1)} dY_1]_N .$$

□

Proof of Lemma IV.1

Denote $\Delta(m)$ the difference between the two expressions. For any $p,q \in \mathbb{N}$, we write:

$$\Delta(m) = \Delta_1(m,p,q) + \Delta_2(m,p,q) + \Delta_3(m,p) + \Delta_4(p,q) \tag{A4}$$

with

$$\Delta_1(m,p,q) = \int_{\Lambda_m} F(\Pi_{m_1} Q_{\beta,q} \Pi_p X, \Pi_n X)[e^{-q_{\beta,m}(X)} dX]_N - \int_{\Lambda_\infty} F(\Pi_{m_1} Q_{\beta,q} \Pi_p X, \Pi_n X) d\hat{\mu}_\beta ,$$

$$\Delta_2(m,p,q) = \int_{\Lambda_m} (F(\Pi_{m_1} Q_{\beta,m} \Pi_p X, \Pi_n X) - F(\Pi_{m_1} Q_{\beta,q} \Pi_p X, \Pi_n X))[e^{-q_{\beta,m}(X)} dX]_N ,$$

$$\Delta_3(m,p) = \int_{\Lambda_m} (F(\Pi_{m_1} Q_{\beta,m} X, \Pi_n X) - F(\Pi_{m_1} Q_{\beta,m} \Pi_p X, \Pi_n X))[e^{-q_{\beta,m}(X)} dX]_N ,$$

$$\Delta_4(p,q) = \int_{\Lambda_\infty} (F(\Pi_{m_1} Q_{\beta,q} \Pi_p X, \Pi_n X) - F(\Pi_{m_1} Q_\beta X, \Pi_n X)) d\hat{\mu}_\beta .$$

Now, by assumption on F, there exists a positive constant C such that for any m and p:

$$|\Delta_3(m,p)| \leq C \int_{\Lambda_m} \| \Pi_{m_1} Q_{\beta,m} (X - \Pi_p X) \|_{l^\infty} [e^{-q_{\beta,m}(X)} dX]_N \tag{A5}$$

and we have (with obvious notations)

$$\|\Pi_{m_1} Q_{\beta,m}(X-\Pi_p X)\|_{l^\infty} \leqslant \sup_{|i|\leqslant m_1} \sum_{|j|>p} |(Q_{\beta,m})_{i,j} X_j|$$

$$\leqslant \sup_{|i|\leqslant m_1} \left(\sum_{|j|>p} j^2 |(Q_{\beta,m})_{i,j}|^2 \right)^{1/2} \left(1+\sum_{j\neq 0} \frac{X_j^2}{j^2} \right)^{1/2}$$

and therefore, using assumption (H5):

$$\|\Pi_{m_1} Q_{\beta,m}(X-\Pi_p X)\|_{l^\infty} \leqslant \frac{C'}{p} \left(1+\sum_{j\neq 0} \frac{X_j^2}{j^2} \right) \tag{A6}$$

with a constant C' independent of m and p. Since also

$$\int_{\Lambda_m} X_j^2 [e^{-q_{\beta,m}(X)} dX]_N = (Q_{\beta,m}^{-1})_{j,j} \leqslant \|Q_{\beta,m}^{-1}\|_{\mathscr{L}(l^2)} = \mathscr{O}(1) \tag{A7}$$

uniformly with respect to m, we deduce from Eqs. (A5) and (A6):

$$|\Delta_3(m,p)| = \mathscr{O}(p^{-1}) \tag{A8}$$

uniformly with respect to m and p.

In a similar way, using the fact that for fixed p, both finite dimensional matrices $\Pi_{m_1} Q_{\beta,m} \Pi_p$ and $\Pi_{m_1} Q_{\beta,q} \Pi_p$ tend to $\Pi_{m_1} Q_\beta \Pi_p$ as m and q tend to infinity, one can prove that:

$$\Delta_2(m,p,q) \to 0 \quad \text{as} \quad m \quad \text{and} \quad q \to \infty. \tag{A9}$$

Moreover, for any fixed (p,q) we see that

$$\Delta_1(m,p,q) \to 0 \quad \text{as} \quad m \to \infty. \tag{A10}$$

The same arguments also give, substituting Q_β for $Q_{\beta,m}$, that

$$\Delta_4(p,q) \to 0 \quad \text{as} \quad p \quad \text{and} \quad q \to \infty. \tag{A11}$$

Then, choosing $\epsilon > 0$ arbitrarily small, one can first fix p large enough so that $|\Delta_3(m,p)| \leqslant \epsilon$ for all (m,q) and $|\Delta_4(p,q)| \leqslant \epsilon$ for all q sufficiently large, then fix q large enough so that $|\Delta_2(m,p,q)| \leqslant \epsilon$ for all sufficiently large m, and finally get $|\Delta_1(m,p,q)| \leqslant \epsilon$, and thus $|\Delta(m)| \leqslant 4\epsilon$, by taking m large enough. □

Proof of Lemma V.2

From Eq. (III.8) we get easily:

$$e^{-(\langle F\xi,\xi\rangle+\langle Gx,x\rangle)} \# e^{-(\langle F\xi,\xi\rangle+\langle Gx,x\rangle)} = \pi^{-2(2m+1)} \left| \int_{\Lambda_m} e^{2i\zeta y - \langle G(x+y),x+y\rangle - \langle F(\xi+\zeta),\xi+\zeta\rangle} dy d\zeta \right|^2$$

$$= \pi^{-2(2m+1)} |I|^2, \tag{A12}$$

where

$$I = e^{-\langle Gx,x\rangle - \langle F\xi,\xi\rangle} \int e^{iy(2\zeta+2iGx) - \langle Gy,y\rangle - 2\langle F\xi,\zeta\rangle - \langle F\zeta,\zeta\rangle} dy d\zeta. \tag{A13}$$

Making the change of variables $y' = \sqrt{2} G^{1/2} y$ and integrating first with respect to y' we get:

$$I = Ce^{-\langle Gx,x\rangle - \langle F\xi,\xi\rangle} \int e^{-\langle G^{-1}(\zeta + iGx),\zeta + iGx\rangle - 2\langle F\xi,\zeta\rangle - \langle F\zeta,\zeta\rangle} d\zeta, \tag{A14}$$

where C is a constant, and therefore, setting $\zeta' = \sqrt{2}(F + G^{-1})^{1/2}\zeta$, this gives:

$$I = C' e^{-\langle F\xi,\xi\rangle - \langle (F+G^{-1})^{-1}(x - iF\xi),x - iF\xi\rangle}, \tag{A15}$$

where C' is a constant. Then Eqs. (A12) and (A15) yield the result. □

APPENDIX B: REMARKS ON QUANTUM MIXING AND ERGODICITY

The elementary remarks collected here, useful to clarify the subsequent statements, are presumably known but we were unable to locate a precise reference.

We first formulate into an abstract setting the definitions recalled in the introduction. Let H be a positive self-adjoint operator on a separable Hilbert space $\mathscr{H}$ such that $\sigma(H)$ is discrete and simple and $e^{-\beta H}$ is trace class for any positive β. Given $A \in \mathscr{L}(\mathscr{H})$ let $\omega(A)$ be the quantum microcanonical measure defined as in Eq. (I.1) or the corresponding quantum Gibbs measure at inverse temperature β

$$\omega(A) = \frac{\mathrm{Tr}(Ae^{-\beta H})}{\mathrm{Tr}(e^{-\beta H})} \tag{B1}$$

indifferently. Let also $\mathscr{A}$ be a weakly closed sub-algebra of $\mathscr{L}(\mathscr{H})$ invariant under the action of e^{itH}. In this general context we assume (and verify below in our specific case) the existence of a family of normalized states $(\psi_\lambda)_{\lambda \in \Lambda}$ complete for ω on $\mathscr{A}$, in the sense that there is a probability measure $d\nu(\lambda)$ on the set Λ such that

$$\omega(A) = \int_\Lambda \langle A\psi_\lambda, \psi_\lambda\rangle_{\mathscr{H}} d\nu(\lambda), \quad \forall A \in \mathscr{A}. \tag{B2}$$

Then the quantum mixing property on $\mathscr{A}$, defined as

$$\omega(A_H(t)B) \to \omega(A)\omega(B) \quad \text{as} \quad |t| \to \infty \tag{B3}$$

for any operators $A, B \in \mathscr{A}$ can be rewritten as

$$\int_\Lambda \langle A_H(t)B\psi_\lambda, \psi_\lambda\rangle_{\mathscr{H}} d\nu(\lambda) \to \int_\Lambda \langle A\psi_\lambda, \psi_\lambda\rangle_{\mathscr{H}} d\nu(\lambda) \int_\Lambda \langle B\psi_\lambda, \psi_\lambda\rangle_{\mathscr{H}} d\nu(\lambda). \tag{B4}$$

Remark that Eqs. (I.1), (B1), and (B2) imply the invariance property

$$\int_\Lambda \langle A_H(t)\psi_\lambda, \psi_\lambda\rangle_{\mathscr{H}} d\nu(\lambda) = \int_\Lambda \langle A\psi_\lambda, \psi_\lambda\rangle_{\mathscr{H}} d\nu(\lambda) \tag{B5}$$

and by analogy with the classical dynamical systems, a natural possible definition of quantum ergodicity is that for any $A \in \mathscr{A}$:

$$\frac{1}{T}\int_0^T \langle A_H(t)\psi_\lambda, \psi_\lambda\rangle_{\mathscr{H}} dt \to \omega(A) \quad \nu(\lambda) - a.e. \quad \text{as} \quad T \to \infty. \tag{B6}$$

This definition is also motivated from the fact that in most situations the quantum mixing property (B4) implies Eq. (B6). Indeed, still assuming that $\sigma(H)$ is discrete and simple, we see in Eq. (I.6) that for any $A \in \mathscr{A}$ the limit

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T\langle A_H(t)\varphi,\psi\rangle_{\mathscr{H}}dt:=\langle\overline{A}\varphi,\psi\rangle_{\mathscr{H}} \tag{B7}$$

exists for all φ, $\psi\in\mathscr{H}$, and the operator $\overline{A}\in\mathscr{A}$ is invariant under the action of e^{itH}. As a consequence, the definition (B6) of quantum ergodicity is equivalent to the fact that for any $A\in\mathscr{A}$ we have the identity

$$\langle\overline{A}\psi_\lambda,\psi_\lambda\rangle=\omega(A) \tag{B8}$$

for ν—almost every λ. Now it is easy to see that the quantum mixing property implies that for any $A,B\in\mathscr{A}$, $\omega(AB)=\omega(A)\omega(B)$. Therefore, if we assume moreover (which is obviously true in the concrete example discussed below) that for any $A\in\mathscr{A}$, the family $(\omega(AB))_{B\in\mathscr{A}}$ determines $\langle A\psi_\lambda,\psi_\lambda\rangle$ for ν-almost every λ, we deduce immediately that the quantum mixing implies Eq. (B8), and hence quantum ergodicity. Concerning this definition of quantum ergodicity, we remark that it is trivially included in the notion of ergodicity of the W^* dynamical systems[6,16] with respect to the triple $(\mathscr{A},\Theta,\phi)$ where Θ is the automorphism of $\mathscr{A}$ generated by the unitary group e^{iHt} and ϕ is the state defined by the microcanonical or canonical measure.

Let us now turn to an explicit construction, in the particular case $\mathscr{H}=L^2(\mathbb{R}^m)$ ($m<+\infty$ fixed) mentioned in Sec. I of the measures $d\nu(\lambda)$, both in the microcanonical case and in the canonical one as well, through some natural choice of the set $\{\psi_\lambda:\lambda\in\Lambda\}$. This will also enable us to recover the classical definitions of mixing and ergodicity out of Eqs. (B3) and (B6) at the classical limit $h\to 0$.

More precisely, for $\lambda=(\lambda_x,\lambda_\xi)\in\mathbb{R}^{2m}$ consider the Bargmann coherent states defined on $\mathbb{R}^{2m}$:

$$f_\lambda(x)=(\pi h)^{-m/4}e^{ix\lambda_\xi/h-(x-\lambda_x)^2/2h}. \tag{B9}$$

Then it is well known (see, e.g., Ref. 15, Chap. 5) that for any trace class operator A on $L^2(\mathbb{R}^m)$, one has:

$$\int_{\mathbb{R}^{2m}}\langle Af_\lambda,f_\lambda\rangle_{L^2(\mathbb{R}^m)}d\lambda=\mathrm{Tr}(A). \tag{B10}$$

In particular, since $e^{-\beta H}$ is trace class on $L^2(\mathbb{R}^m)$, then

$$\int\|e^{-\beta H/2}f_\lambda\|^2d\lambda=\int\langle e^{-\beta H}f_\lambda,f_\lambda\rangle d\lambda=\mathrm{Tr}(e^{-\beta H})<+\infty.$$

Hence we can consider the following probability measures on $\mathbb{R}^{2m}$:

$$d\nu_m(\lambda)=\frac{\|e^{-\beta H/2}f_\lambda\|^2d\lambda}{\int\|e^{-\beta H/2}f_\lambda\|^2d\lambda},\quad d\nu_{\Delta,E}(\lambda)=\frac{\|\delta(H-E)f_\lambda\|^2d\lambda}{\int\|\delta(H-E)f_\lambda\|^2d\lambda}, \tag{B11}$$

whereas in Sec. I, $\delta(H-E)=\Sigma_{n:E-\Delta<E_n<E}P_n$ with $\Delta>0$ fixed. If we also set

$$\psi_\lambda^c=\frac{e^{-\beta H/2}f_\lambda}{\|e^{-\beta H/2}f_\lambda\|},\quad \psi_\lambda^{mc}=\frac{\delta(H-E)f_\lambda}{\|\delta(H-E)f_\lambda\|}. \tag{B12}$$

then we have the following result [to be compared with Eq. (B2)]:

Lemma B.1: For any bounded operator A on $L^2(\mathbb{R}^m)$, the following identities hold:

$$\frac{\mathrm{Tr}(Ae^{-\beta H})}{\mathrm{Tr}(e^{-\beta H})}=\int\langle A\psi_\lambda^c,\psi_\lambda^c\rangle d\nu_m(\lambda),\quad \frac{\mathrm{Tr}(A\delta(H-E))}{\mathrm{Tr}(\delta(H-E))}=\int\langle A\psi_\lambda^{mc},\psi_\lambda^{mc}\rangle d\nu_{\Delta,E}(\lambda).$$

Proof: Just write

$$\mathrm{Tr}(Ae^{-\beta H}) = \mathrm{Tr}(e^{-\beta H/2} A e^{-\beta H/2}),$$

$$\mathrm{Tr}(A\,\delta(H-E)) = \mathrm{Tr}(\,\delta(H-E) A\,\delta(H-E))$$

and use Eq. (B10). □.

Consider now the particular case where A is the h-Weyl quantization of a classical observable $a = a(x,\xi) \in \mathscr{S}(\mathbb{R}^{2m})$, namely the operator $\mathrm{Op}_h^W(a)$ defined by the oscillatory integral:

$$\mathrm{Op}_h^W(a)u(x) = (2\pi h)^{-m} \int e^{i(x-y)\xi/h} a\left(\frac{x+y}{2}, \xi\right) u(y)\,dy\,d\xi. \tag{B13}$$

A well-known direct application of the stationary phase method yields[16]

$$\lim_{h\to 0} \langle \mathrm{Op}_h^W(a) f_\lambda, f_\lambda \rangle = a(\lambda).$$

As a consequence, if we also have

$$H = \mathrm{Op}_h^W(q)$$

for some symbol $q \in C^\infty(\mathbb{R}^{2m})$, then the semiclassical symbolic and functional calculus of pseudodifferential operators (see Ref. 17) immediately implies:

Lemma B.2: For any $\lambda \in \mathbb{R}^{2m}$,

$$\lim_{h\to 0} \langle \mathrm{Op}_h^W(a) \psi_\lambda, \psi_\lambda \rangle = a(\lambda).$$

Moreover,

$$\lim_{h\to 0} \int_{\mathbb{R}^{2m}} \langle \mathrm{Op}_h^W(a) \psi_\lambda^c, \psi_\lambda^c \rangle d\nu_m(\lambda) = \int a(\lambda) d\mu^c(\lambda),$$

$$d\mu^c(\lambda) = \frac{e^{-\beta q} d\lambda}{\int_{\mathbb{R}^{2m}} e^{-\beta q} d\lambda}$$

and

$$\lim_{h\to 0} \int_{\mathbb{R}^{2m}} \langle \mathrm{Op}_h^W(a) \psi_\lambda^{mc}, \psi_\lambda^{mc} \rangle d\nu_{\Delta,E}(\lambda) = \int_{\mathbb{R}^{2m}} a(\lambda) d\mu^{mc}(\lambda),$$

$$d\mu^{mc}(\lambda) = \frac{\delta(q-E)d\lambda}{\int_{\mathbb{R}^{2m}} \delta(q-E)d\lambda}.$$

Since, by the semiclassical Egorov theorem (Ref. 17, Sec. 5.4) the principal symbol of $e^{itH/h}\mathrm{Op}_h^W(a)e^{-itH/h}$ is given by

$$a_t(x,\xi) = a(\phi_t(x,\xi))$$

where ϕ_t is the Hamiltonian flow generated by q, it follows that for any $a, b \in \mathscr{S}(\mathbb{R}^{2m})$:

$$\lim_{h\to 0} \langle e^{itH/h}\ \mathrm{Op}_h^W(a) e^{-itH/h}\ \mathrm{Op}_h^W(b) \psi_\lambda, \psi_\lambda \rangle = a(\phi_t(\lambda)) b(\lambda). \tag{B14}$$

It has now become clear out of Lemma A.2 and Eq. (A14) that the quantum notions of mixing and ergodicity given by Eqs. (A3) and (A6) formally yield the corresponding classical notions as $h \to 0$.

As a final remark let us mention that if A is a pseudodifferential operator also the Von Neumann definition (I.6) reproduces the classical one at the classical limit if $\langle u_n, Au_n \rangle$ tends to the phase average of the symbol of A, as verified in many instances (see, e.g., Refs. 18–23), in which H is the quantization of a Hamiltonian generating an ergodic flow. Some authors (Refs. 24 and 22) assume this limiting property as the very definition of quantum ergodicity.

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Ergodic properties of the quantum ideal gas in the Maxwell–Boltzmann statistics

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It is proved that the quantization of the Volkovyski–Sinai model of ideal gas (in the Maxwell–Boltzmann statistics) enjoys at the thermodynamical limit the property of quantum mixing in the following sense: $\lim_{|t|\to\infty} \lim_{\substack{m,L\to\infty \\ m/L\to\rho}} \omega^m_{\beta,L}(e^{iH_m t/\hbar} \times A e^{-iH_m t/\hbar} B) = \lim_{\substack{m,L\to\infty \\ m/L\to\rho}} \omega^m_{\beta,L}(A) \cdot \lim_{\substack{m,L\to\infty \\ m/L\to\rho}} \omega^m_{\beta,L}(B)$. Here H_m is the Schrödinger operator of m free particles moving on a circle of length L; A and B are the Weyl quantization of two classical observables a and b; $\omega^m_{\beta,L}(A)$ is the corresponding quantum Gibbs state. Moreover, one has $\lim_{\substack{m,L\to\infty \\ m/L\to\rho}} \omega_{\beta,m}(A) = P_{\rho,\beta}(a)$, where $P_{\rho,\beta}(a)$ is the classical Gibbs measure. The consequent notion of quantum ergodicity is also independently proven. © *1996 American Institute of Physics.* [S0022-2488(96)00910-3]

I. INTRODUCTION

The purpose of the present paper is to analyze the quantum ergodic properties of the Volkovyski–Sinai model of ideal gas,[1] quantized according to a Maxwell–Boltzmann statistics (i.e., all particles are distinguishable). This paper represents the companion paper of Ref. 2, where the same result is proved for a strongly analogous system, namely the infinite harmonic chain with suitable restrictions on the normal mode frequencies.

These two systems provide examples of *kinematic quantum chaos*. We borrow the expression *kinematic chaos* from the enlightening paper by Jona-Lasinio and Presilla.[3] By that we mean trivial motion whose chaotic behavior is due to the randomness of the infinite-dimensional initial condition (see, besides Ref. 3 itself, the remark after Theorem III.3). For both the ideal gas and the harmonic chain, this is a classical feature of the system, which works on the quantum level as well because of the *exact Egorov Theorem* (Lemma IV.1). The latter is a fundamental fact here, since it allows us to treat the quantum time evolution as the classical one.

A clear explanation of the motivations for the investigation of the quantum behavior of infinite systems is given in Ref. 2, as well as further references. Here we just sketch what the immediate problems are, concerning the search for *quantum chaos*.

To fix the ideas, let H be a self-adjoint operator acting on $L^2(\Omega)$, $\Omega \in \mathbb{R}^m$, resulting from the quantization of some classical Hamiltonian function $\mathscr{H}$ over $\mathbb{R}^m \times \Omega$. Suppose, as it happens in all interesting cases, that $\sigma(H)$ is discrete. Consider two operators A, $B \in \mathscr{L}(L^2(\Omega))$, which is regarded as our set of observables, and define $\Theta[t](A) := e^{iHt/\hbar} A e^{-iHt/\hbar}$, the Heisenberg evolution. All the physical experiments one can do on such a system imply a certain ''measure'' on the observables is used. In quantum mechanics such measures are *states* over the algebra of the operators. These *quantum ensembles* (see Ref. 4, Sec. 1.3) are typically described as

$$\omega_\varrho(A) = \frac{\operatorname{Tr} A\varrho}{\operatorname{Tr} \varrho}, \tag{I.1}$$

with ϱ a suitable trace-class operator. A suitable definition of mixing would be, then[5,6]

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$$\lim_{|t|\to\infty} \omega_\varrho(\Theta[t](A),B)=\omega_\varrho(A)\omega_\varrho(B), \quad \forall A,B\in\mathscr{L}(L^2(\Omega)). \tag{I.2}$$

It is easily realized, writing ω_ϱ by means of the matrix elements of the operators, w.r.t. the eigenbasis of H, that such a property can never be verified, *for each underlying classical dynamics*. The same is true for any reasonable definition of ergodicity, as von Neumann's formula[7] shows (see Ref. 2 for details). This is a consequence of the quasiperiodicity of the classical evolution—as long as we have finite degrees of freedom—and it is called ''quantum suppression of classical chaos.''[8,3] Hence the idea of taking the number of degrees of freedom to infinity.

The system we consider is the quantization of the ideal gas in the formulation found in Sinai's book:[9] i.e., m noninteracting particles moving freely on a circle of length L, when m and L are taken to infinity, subject to the finite density requirement $m/L\to\rho$.

For an outline of the ''analytic approach'' we will follow in studying the quantum infinite system in question, the reader is definitely referred to the introduction of Ref. 2, due to the similarities of the two works. There the consequences of such a study are also properly emphasized. In the next paragraph we just point out the structural differences, between the two models, which require nonobvious modifications of the arguments of Graffi and Martinez[2] valid for the harmonic chain. Specifically the following.

(i) The other important classical mechanism which provides the unpredictability (mixing) of the time evolution here, besides the mentioned kinematic effect, is the *symmetry* of the observables under particle exchange. This corresponds to the physical fact that one is not able to distinguish between the particles in a gas. Actually, such a restriction on the observables also has the noticeable outcome to allow the interchange of the time average limit with the thermodynamical limit [see Theorem III.3, Corollary III.4, and relation (III.19)]. The remark after Theorem III.3 will contain more comments. On the quantum side, the symmetry of the observables would entail for a Bose–Einsten or a Fermi–Dirac statistics. Nevertheless, we use Maxwell–Boltzmann for the sake of convenience: see remark 2 in Sec. II B.

(ii) The phase space of any m-particle subsystem is $\mathbb{R}^m\times(LS^1)^m$, with LS^1 denoting henceforth the circle of length L. In other words, the phase space has a cylindrical structure. This has the effect of making necessary a Bloch decomposition of $L^2(\mathbb{R}^m)$, and consequently a direct fiber decomposition of operators, if we want to consider functions on phase space as symbols of operators on a one-to-one correspondence under quantization. Equivalently, $\mathbb{R}^m\times(LS^1)^m$ generates a cylindrical Heisenberg group (see Ref. 10 and Sec. II B) and its only faithful unitary representation is given by a fibered L^2 space.

(iii) The coherent states we use are those adapted to the cylindrical phase space, as presented in the Appendix, Sec. 1 (refer also to Refs. 10 and 11).

(iv) The infinite-particle limit is a true thermodynamic limit, because here not only do we have $m\to\infty$, but also $L\to\infty$ under the constraint of finite density $m/L\to\rho,\rho>0$.

(v) On the other hand, in this model the classical dynamics is just free motion. This entails a simplification: the Weyl symbol of the quantum m-particle Schrödinger operator H_m is obviously the classical Hamiltonian $\mathscr{H}_m=(\frac{1}{2})\Sigma_{i=1}^m p_i^2$, namely $H_m=Op(\mathscr{H}_m)$. Then the Weyl symbol of the (unnormalized here) quantum Gibbs measure is

$$e^{-\beta H_m}=Op(e^{-\beta\mathscr{H}_m}),$$

where, here and above, $Op:=Op^W$ denotes the operation of Weyl quantization of a symbol, whose definition in the present context is recalled in Sec. II B.

Now, as it will be explained in sharper detail in Sec. III A, consider the normalized quantum Gibbs state at inverse temperature β (for a system of m free particles in LS^1), namely the functional

$$\omega^m_{\beta,L}(A) := \frac{\mathrm{Tr}\, A e^{-\beta H_m}}{\mathrm{Tr}\, e^{-\beta H_m}}, \tag{I.3}$$

defined, for instance, over the class of bounded operators A that are ''L-periodic in the coordinate variable'' (refer to Sec. II B). The application Tr is practically the trace over $L^2(\mathbb{R}^m)$ (see Sec. III A for details). Then the main result of the present work, in analogy with Ref. 2, can be stated as

$$\lim_{|t|\to\infty} \lim_{\substack{m,L\to\infty \\ m/L\to\rho}} \omega^m_{\beta,L}(\Theta^m[t](A)B) = \lim_{\substack{m,L\to\infty \\ m/L\to\rho}} \omega^m_{\beta,L}(A) \cdot \lim_{\substack{m,L\to\infty \\ m/L\to\rho}} \omega^m_{\beta,L}(B) \tag{I.4}$$

[see also Theorem III.2 and (III.18)]. Here A and B are actually dependent on L and m and represent the operators quantizing two classical observables, a and b, over the Hilbert spaces for m particles in a L circle (square integrable Bloch functions). Also $\Theta^m[t](A) := e^{iH_m t/\hbar} A e^{-iH_m t/\hbar}$. Moreover,

$$\lim_{\substack{m,L\to\infty \\ m/L\to\rho}} \omega_{\beta,m}(A) = P_{\rho,\beta}(a). \tag{I.5}$$

Formula (I.4) is the quantum mixing property and induces a consistent formulation of the quantum ergodicity: for instance,

$$\lim_{T\to\infty} \lim_{\substack{m,L\to\infty \\ m/L\to\rho}} \omega^m_{\beta,L}((\Xi^m[T](A))^2) = \lim_{\substack{m,L\to\infty \\ m/L\to\rho}} (\omega^m_{\beta,L}(A))^2, \tag{I.6}$$

if $\Xi^m[T](A) = (1/2T)\int_{-T}^{T} \Theta^m[t](A)\,dt$.

The present model of quantum ideal gas is structurally different from the free Bose gas or the free Fermi gas in the grand canonical ensemble, discussed, e.g., in Ref. 5, Sec. 5.2. The arguments[5,6] yielding the mixing property with respect to the KMS states through the asymptotic abelianess of the CCR (or CAR) automorphisms generated by free dynamics do not apply in this context.

The paper is organized as follows: in the next section we briefly recall the ideal gas model and construct its quantization; in Sec. III we state the results, whose proofs are given in Sec. IV. Finally, in the Appendix we recall the construction of the coherent states on the cylinder[10] with some additional details; we collect two technical lemmas; and we exploit the properties of the convolution over LS^1, as $L\to\infty$, which are crucially used in the proofs.

II. THE CLASSICAL IDEAL GAS AND ITS QUANTIZATION

A. The Volkovyski–Sinai model

To make the exposition self-contained, a brief reminder is here given of the Volkovyski–Sinai model of ideal gas. The reader is referred to Ref. 9, Lecture 8, for details.

Consider a system of m free particles of unit mass constrained to move on a circle of length L. Its Hamiltonian function is

$$\mathscr{H}_m(p,q) = \frac{1}{2}\sum_{j=1}^{m} p_j^2 = \frac{p^2}{2}, \tag{II.1}$$

defined on the phase space $\Lambda_L^m := \mathbb{R}^m \times (LS^1)^m$, which, with a view to the limiting case $L \to \infty$ to be considered below, will be identified with $\mathbb{R}^m \times T_L^m$, $T_L^m := [-L/2, L/2)^m$. The physical intuition is to stretch the circle LS^1 more and more toward a straight line, namely $\mathbb{R}$.

On Λ_L^m the motion is given by the flow map: $\phi_L^m[t](p,q) := (p, q+pt)$. The dynamical system is completely integrable and Λ_L^m is decomposed in a noncountable family of invariant tori: all motions are quasiperiodic. Introducing any ''reasonable'' measure on Λ_L^m (in Ref. 9 the microcanonical measure is used; for reasons that will become clear when quantizing, the natural measure to introduce here is the canonical one) the system is, of course, not even ergodic.

But a suitable thermodynamical limit of it might be. The construction of the infinite dynamical system is based on the idea that the particles should be ''unlabeled.'' More precisely, the phase space for the infinite system is defined as follows:

$$\Lambda_\infty := \{(p,q);\ q \text{ countable subset of } \mathbb{R},\ p: q \to \mathbb{R}\}, \tag{II.2}$$

with the interpretation that $q = \{x_1, x_2, \ldots, x_j, \ldots\}$ contains the positions of the particles, now undistinguishable, and p is a function such that $p(x_j)$ gives the velocity of the particle located at x_j. It may occur that more than one particle—say n—are located at x_j: in this case, with an abuse of notation with respect to definition (II.2), $p(x_j)$ is an n-tuple of velocities. The flow $\phi_\infty[t]: \Lambda_\infty \to \Lambda_\infty$ is defined accordingly: $\phi_\infty[t](p,q) = (p', q')$, where $q' := \{x + p(x)t; x \in q\}$ and $p': q' \to \mathbb{R}$ is $p'(x + p(x)t) := p(x)$.

What we have introduced is the natural limiting object of the spaces $\Lambda_L^m/\mathbb{S}^m$, $\mathbb{S}^m$ being the group of permutations of m coordinates and momenta. Such spaces are expressly defined in Ref. 9 in a way completely analogous to (II.2), i.e., as the collection of all couples (p,q) with $q \subset LS^1$, $\#q \leqslant m$ and $p: q \to \mathbb{R}$ having m values, in the sense specified above. They can be regarded as belonging to Λ_∞, since $q \subset LS^1 \simeq [-L/2, L/2)$. This motivates the above identification.

This remark enables us to consider functions defined on Λ_∞ as having a natural restriction on $\Lambda_L^m/\mathbb{S}^m$. And a function f on $\Lambda_L^m/\mathbb{S}^m$ is simply a totally symmetric function on Λ_L^m, namely $f \circ \Pi_L^m$, where Π_L^m is the natural immersion $\Lambda_L^m \to \Lambda_\infty$:

$$\Pi_L^m(p_1, \ldots, p_m, q_1, \ldots, q_m) := (p: q \to \mathbb{R}, q := \{q_1, \ldots, q_m\}), \tag{II.3}$$

p taking values $p(q_1) = p_1, \ldots, p(q_m) = p_m$. It will be useful in the remainder to notice that

$$\phi_\infty[t] \circ \Pi_L^m = \Pi_L^m \circ \phi_L^m[t]. \tag{II.4}$$

To complete the definition of our infinite dynamical system, we need to specify the measurable functions, i.e., to fix a σ-algebra $\mathscr{A}$ and—after that—a probability measure on it. The answer in Ref. 1 is $\mathscr{A} := \sigma(\gamma(\Delta))_{\Delta \in \mathscr{B}(\mathbb{R})}$. Here Δ runs among the Borel sets in $\mathbb{R}$ and $\gamma(\Delta)$ is the σ-algebra of all subsets of Λ_∞, depending only on the positions and momenta of the *unlabeled* particles in Δ.[12] For the sake of simplicity, we just restrict ourselves to real functions.

Examples of measurable functions are $f_\Delta(p,q) := \#(q \cap \Delta)$, the number of particles of the configuration q located in Δ; or $g_\Delta(p,q) := \Sigma_{x \in \Delta}\, p(x)$, the total momentum of the particles in Δ.

We endow $\mathscr{A}$ with the measure $P_{\rho,\beta}$ defined by the following properties.

(1) The distribution of particles in the configuration space is Poissonian with parameter ρ; that is

$$P_{\rho,\beta}(\{(p,q); f_\Delta(p,q) = n\}) = e^{-\rho|\Delta|}\, \frac{(\rho|\Delta|)^n}{n!}; \tag{II.5}$$

for every $\Delta \in \mathscr{B}(\mathbb{R})$. This implies that the distributions over two disjoint Borel sets Δ_1 and Δ_2 are independent.

(2) The momenta are independent centered Gaussian variables with variance $1/\beta$. This means that, fixed $A \in \mathscr{B}(\mathbb{R}^n)$ and a vector $(x_1,\dots,x_n) \in \mathbb{R}^n$, we have

$$P_{\rho,\beta}(\{(p(x_1),\dots,p(x_n)) \in A\} | \{\{x_1,\dots,x_n\} \subset q\}) = \int_A [e^{-\beta p^2/2}\, dp]_N, \tag{II.6}$$

$[\cdots]_N$ being the normalized measure. This is a Maxwell distribution with inverse temperature β.

This measure has been chosen intentionally as the limit of the canonical measures over the phase spaces of finite numbers of particles.

Proposition II.1: Let a measurable in $\mathscr{A}$. At the thermodynamical limit, i.e., $m,L \to \infty$; $m/L \to \rho$,

$$\int_{\Lambda_L^m} (a \circ \Pi_L^m)(p,q) [e^{-\beta p^2/2}\, dp\ dq]_N \to P_{\rho,\beta}(a).$$

As regards the proof, the statement concerning the distribution of the positions is clearly explained in Ref. 9, while (II.6) trivially holds since the distributions over the momentum spaces for a finite number of particles are given as Maxwellian with inverse temperature β.

We conclude this section formulating the key theorem.

Theorem II.2: *(Ref. 1) The measure $P_{\rho,\beta}$ is invariant under $\phi_\infty[t]$ and the dynamical system $(\Lambda_\infty, \mathscr{A}, P_{\rho,\beta}, \phi_\infty[t])$ is a K flow.*

It may be worth noticing here that the infinite dynamical system just recalled has a nice abstract construction, which is described in Ref. 13 (and shortly in Ref. 6, Example 2.34). It is called the *Poisson system* constructed for a one-dimensional free particle with a Maxwell velocity distribution. Its ergodic properties follow via a general technique, namely the *Bernoulli construction*. This viewpoint shows clearly that $\mathscr{A}$ is generated by the following sets:

$$B^{(n)}_{\Delta,\Gamma} := \{(p,q) \in \Lambda_\infty | \#\{x \in q | x \in \Delta, p(x) \in \Gamma\} = n\}, \tag{II.7}$$

where $\Delta,\Gamma \in \mathscr{B}(\mathbb{R})$. Such a remark will be useful while proving the statements.

Nonetheless, the approach we have chosen has the advantage of constructing the infinite-particle dynamical system through a thermodynamical limit (see above, and in particular Proposition II.1). This fact will be crucial throughout this paper.

B. The quantization

The Hilbert spaces associated to a quantum system of m particles on a circle of length L are denoted by $L^2_{(k)}(T_L^m), k \in [0,1/L)^m$. Each of these is defined as

$$L^2_{(k)}(T_L^m) := \left\{ f \ \text{ on } \ \mathbb{R}^m | \forall j \in \mathbb{Z}^m, f(q+Lj) = e^{2\pi i L k \cdot j} f(q), \int_{T_L^m} |f|^2 < \infty \right\}, \tag{II.8}$$

that is the space of the Bloch functions of parameter k that are square-integrable on a given fundamental domain. Concerning this definition, we remark the following.

(1) The above family of spaces is the familiar one for Schrödinger operators with periodic potential (Ref. 14, Sec. XIII.16). They have to be simultaneously considered for all values of $k \in [0,1/L)^m$, otherwise the quantization application is not well defined since the Schrödinger representation of the Heisenberg group is not faithful: e.g., in one dimension, if we selected only $k=0$, then $T(L,0) = T(0,0) = 1$ (see below).

As a matter of fact, the whole Hilbert space $L^2(\mathbb{R}^m)$ is recovered through the standard direct integral formula[14]

$$\int_{[0,1/L)^m}^{\oplus} L^2_{(k)}(T^m_L)\,dk \simeq L^2(\mathbb{R}^m). \tag{II.9}$$

More details are given in Sec. 1 in the Appendix and in Ref. 10. A basis for $L^2_{(k)}(T^m_L)$ is obviously $e^{(k)}_\alpha := L^{-m/2} e^{2\pi i(\alpha+k)\cdot x}$, with $\alpha \in (\mathbb{Z}/L)^m$.

(2) The choice of the Hilbert spaces in (II.8) corresponds to Maxwell–Boltzmann statistics, since we ask for no wave function symmetry with respect to particle permutations. One could also think of quantizing this system according to Bose–Einstein or Fermi–Dirac statistics. To give a physical explanation, we are considering particles that are, in principle, enumerable, but our observables do not see this enumeration. This approximation makes sense in the semiclassical realm.[15]

A further step toward the definition of the quantization application is the introduction of the Fourier transform and antitransform in Λ^m_L. We define first the dual of the phase space: $(\Lambda^m_L)^* := \mathbb{R}^m \times (T^m_L)^*$, where $(T^m_L)^* := (\mathbb{Z}/L)^m$. Now, if $b \in \mathscr{S}(\Lambda^m_L)$, that is the Schwartz class of functions in Λ^m_L; then for $(\eta,\xi) \in (\Lambda^m_L)^*$, the Fourier transform of b is

$$\hat{b}(\eta,\xi) := \int_{\mathbb{R}^m} \int_{T^m_L} b(p,q) e^{-2\pi i(\eta\cdot p + \xi\cdot q)}\, dq\, dp. \tag{II.10}$$

Correspondingly, the antitransformation is given by

$$b(p,q) := \frac{1}{L^m} \sum_{\xi \in (T^m_L)^*} \int_{\mathbb{R}^m} \hat{b}(\eta,\xi) e^{2\pi i(p\cdot\eta + q\cdot\xi)}\, d\eta. \tag{II.11}$$

The Heisenberg group to be considered in this situation is the naturally induced *cylinder subgroup* of the Heisenberg group on $\mathbb{R}^{2m}\times\mathbb{R}$, namely, $(\Lambda^m_L)^*\times\mathbb{R}$ endowed with the product law

$$(\eta,\xi,\tau)(\eta',\xi',\tau') = (\eta+\eta, \xi+\xi', \tau+\tau' + \tfrac{1}{2}(\eta\cdot\xi' - \xi\cdot\eta')). \tag{II.12}$$

Accordingly,[16] its unitary Schrödinger representation in $L^2(\mathbb{R}^m)$ is defined in the following way:

$$(T(\eta,\xi) f\,)(x) = e^{2\pi i \xi\cdot(\eta/2 + x)} f(x+\eta). \tag{II.13}$$

This can be formally written as $T(\eta,\xi) = e^{2\pi i(\eta\cdot P + \xi\cdot Q)}$, where Q corresponds to the multiplication operator by q, and $P = (2\pi i)^{-1}\nabla_x$. We have therefore taken $\hbar = (2\pi)^{-1}$. It is evident that $T(\eta,\xi)$ preserves $L^2_{(k)}(T^m_L)$: we denote by $T^{(k)}(\eta,\xi)$ its restriction to that space.

We are now in a position to define the quantization application. If b is a pseudodifferential symbol of a given finite order[16,17] on Λ^m_L, then

$$Op(b) := \frac{1}{L^m} \sum_{\xi \in (T^m_L)^*} \int_{\mathbb{R}^m} \hat{b}(\eta,\xi) T(\eta,\xi)\, d\eta; \tag{II.14}$$

with $\hat{b}$ possibly interpreted in a distributional sense.

The restriction of this operator to the invariant space $L^2_{(k)}(T^m_L)$ will be once more denoted by $Op(b)^{(k)}$. The above definition is nothing else than the standard Weyl quantization induced by the cylindrical Heisenberg group and subject to our choice of inverse Fourier transform (II.11). As a matter of fact, elementary algebraic manipulations yield the following explicit formula: for $f^{(k)} \in L^2_{(k)}(T^m_L)$,

$$(Op(b)^{(k)} f^{(k)})(x) = \int_{\mathbb{R}^m} \int_{\mathbb{R}^m} b\left(\frac{x+y}{2}, p\right) e^{2\pi i p\cdot(x-y)} f^{(k)}(y)\, dy\, dp. \tag{II.15}$$

Remark that, since $f^{(k)} \in \mathscr{S}(\mathbb{R}^{2m})$, *a priori* this makes no sense, even as an oscillatory integral. The sense we can give it is, again, distributional, as we know[17] that for pseudodifferential symbols, $Op(b): \mathscr{S}' \to \mathscr{S}'$. Notice also that, as usual, (II.15) implies that if b depends only on one canonical variable, for instance p, then $Op(b) = b(P)$ in the spectral-theoretic sense. In particular, if the quantum Hamiltonian is $H_m := -(1/8\pi^2)\Delta_x = Op(\mathscr{H}_m)$, we have $Op(e^{-\beta \mathscr{H}_m}) = e^{-\beta H_m}$.

We can now calculate the *Weyl composition* $a\#b$ of two symbols a and b, i.e., the (unique) symbol such that $Op(a\#b) = Op(a)Op(b)$. This is done by means of (II.14), remembering that $T(\eta,\xi)$ obeys the multiplication law of the Heisenberg group and that a symbol is obtained by its correspondent operator by substituting $e^{2\pi i(p\cdot\eta + q\cdot\xi)}$ to $T(\eta,\xi)$ when the operator is in the form (II.14)–compare (II.11) with (II.14). The result, after some manipulations of the integrals, is—not surprisingly—an adaptation of the corresponding formula for the Euclidean space case (Ref. 16, Sec. 2.1):

$$\begin{aligned}(a\sharp b)(p,q) &= \frac{1}{L^{2m}} \sum_{\xi_1,\xi_2} \int \hat{a}(\eta_1,\xi_1)\hat{b}(\eta_2,\xi_2) e^{\pi i(\eta_1\cdot\xi_2 - \xi_1\cdot\eta_2)} e^{2\pi i[(\eta_1+\eta_2)\cdot p + (\xi_1+\xi_2)\cdot q]}\, d\eta_1\, d\eta_2 \\ &= \frac{1}{L^{2m}} \sum_{\xi_1,\xi_2} \int a\left(p+\frac{\xi_1}{2}, q+q_1\right) b\left(p+\frac{\xi_2}{2}, q+q_2\right) e^{2\pi i(\xi_2\cdot q_1 - \xi_1\cdot q_2)}\, dq_1\, dq_2 .\end{aligned} \tag{II.16}$$

Notice that the sum is carried over $\xi_1, \xi_2 \in (T_L^m)^*$ and the integration over $q_1, q_2 \in T_L^m$.

By the above formula we deduce that the Weyl composition has a property that may be called the *quasitracial property:*

$$\int_{\Lambda_L^m} (a\#b)(p,q)\,dp\,dq = \int_{\Lambda_L^m} a(p,q)b(p,q)\,dp\,dq, \tag{II.17}$$

even though we cannot hope to have the tracial property for some $L^2_{(k)}(T_L^m)$, i.e., (II.17) with $\mathrm{Tr}_{L^2_{(k)}(T_L^m)} Op(a)Op(b)$ on the lhs, as explained in Ref. 10. Actually, as it will be clear in Sec. III A, what appears on the lhs is something resembling $\mathrm{Tr}_{L^2(\mathbb{R}^m)}$.

Given $f^{(k)}, g^{(k)} \in L^2_{(k)}(T_L^m)$, we define the Fourier–Wigner function relative to those two vectors as $V_{f^{(k)},g^{(k)}}(\eta,\xi) := \langle f^{(k)}, T(\eta,\xi) g^{(k)} \rangle$. This is completely analogous to what is found in Ref. 16. The Wigner function $W_{f^{(k)},g^{(k)}}$ is defined to be the (possibly distributional) Fourier transform of $V_{f^{(k)},g^{(k)}}$ and thus, from (II.14),

$$\langle f^{(k)}, Op(b) g^{(k)} \rangle_{L^2_{(k)}(T_L^m)} = \int_{\Lambda_L^m} b(p,q) W_{f^{(k)},g^{(k)}}(p,q)\,dp\,dq; \tag{II.18}$$

to be understood as $W_{f^{(k)},g^{(k)}}$ being the distribution kernel of $b \mapsto \langle f^{(k)}, Op(b) g^{(k)} \rangle$. Again the standard form for this ''function,''[16] calculated from (II.15) or from its very definition,

$$W_{f^{(k)},g^{(k)}}(p,q) := \int_{\mathbb{R}^m} e^{-2\pi i p\cdot z} \overline{f^{(k)}\left(q - \frac{z}{2}\right)} g^{(k)}\left(q + \frac{z}{2}\right) dz, \tag{II.19}$$

has to be interpreted in the weak sense.

III. STATEMENT OF THE RESULTS

Suppose we have, $\forall L > 0$; $m \in \mathbb{Z}$, $m \geqslant 1$ a measure space $(X_L^m, d\theta)$[18] and a family of states

$$\{f_\lambda\}_{\lambda \in X_L^m} \subset \bigcup_{k \in [0,1/L)^m} L^2_{(k)}(T_L^m), \tag{III.1}$$

labeled by the index λ ranging in X_L^m. Call $w_\lambda(p,q) := W_{f_\lambda,f_\lambda}(p,q)$, the Wigner function corresponding to f_λ.

Hypothesis: We suppose that

$$\int_{X_L^m} w_\lambda(p,q)\,d\theta(\lambda) \equiv 1, \tag{III.2}$$

as a distribution on Λ_L^m.

Remark: Such a family of states represents in this context the quantum substitute for the classical phase space. As a matter of fact, (III.2) says that the $\{f_\lambda\}$ are evenly distributed, as a whole, over Λ_L^m. Hence they play the role of ''points.'' This is clearly seen in the case of the *coherent states*, perhaps the most remarkable example of states fulfilling the above hypothesis. They are introduced in the Appendix, Sec. 1. However, (III.2) can be restated by saying that we are given a set of states complete over all $L^2_{(k)}(T_L^m)$, $k \in [0,1/L)^m$—see Sec. III A.

Since $\|e^{-\beta H_m} f_\lambda\|^2 = \langle f_\lambda, e^{-2\beta H_m} f_\lambda\rangle$,[19] then (III.2) immediately implies

$$\int_{X_L^m} \|e^{-\beta H_m} f_\lambda\|^2 \, d\theta(\lambda) = \int_{\Lambda_L^m} e^{-2\beta \mathscr{H}_m(p)} \, dp \, dq = L^m \left(\frac{\pi}{\beta}\right)^{m/2}. \tag{III.3}$$

We define

$$d\nu(\lambda) := \frac{\|e^{-\beta H_m} f_\lambda\|^2 \, d\theta(\lambda)}{\int_{X_L^m} \|e^{-\beta H_m} f_{\lambda'}\|^2 \, d\theta(\lambda')} \tag{III.4}$$

and

$$g_\lambda := \frac{e^{-\beta H_m} f_\lambda}{\|e^{-\beta H_m} f_\lambda\|} \tag{III.5}$$

be the image under the quantum Gibbs measure of each of our states.

Definition III.1: $a \in \mathscr{A}$ *is said to be an* asymptotic symbol *if* $\exists m_0 \in \mathbb{N}$, $L_0 > 0$ *such that* $\forall m \geqslant m_0$, $L \geqslant L_0$, $a \circ \Pi_L^m$ *is a pseudodifferential symbol over* Λ_L^m.

Remark: Notice that with such a definition, asymptotic symbols are rather rigid objects. In fact, fixed an $m \geqslant m_0$, take $L_0 \leqslant L \leqslant L_1$. Now $\mathrm{Im}(\Pi_L^m) \subseteq \mathrm{Im}(\Pi_{L_1}^m) \subseteq \Lambda_\infty$. So $a \circ \Pi_L^m$ is just the restriction of $a \circ \Pi_{L_1}^m$ to Λ_L^m. But also $a \circ \Pi_L^m$, in order to be a symbol must be C^∞ and T_L^m-periodic. This means that $\forall i = 1,\ldots,m$,

$$(a \circ \Pi_{L_1}^m)(\ldots, -L/2, \ldots) = (a \circ \Pi_{L_1}^m)(\ldots, +L/2, \ldots); \tag{III.6}$$

$$\frac{d}{dq_i}(a \circ \Pi_{L_1}^m)(\ldots, -L/2, \ldots) = \frac{d}{dq_i}(a \circ \Pi_{L_1}^m)(\ldots, +L/2, \ldots), \tag{III.7}$$

where $(\ldots, \pm L/2, \ldots)$ stands for $(p_1,\ldots,p_m,q_1,\ldots,q_{i-1},\pm L/2,q_{i+1},\ldots,q_m)$. Thus, parity arguments imply that for every $|q_i| \geqslant L_0/2$,

$$\frac{d}{dq_i}(a \circ \Pi_{L_1}^m)(\ldots, q_i, \ldots) = 0. \tag{III.8}$$

Hence, for a fixed large m, $(a \circ \Pi^m_{L_1})$ is a constantwise continuation of $(a \circ \Pi^m_{L_0})$, and the former is completely determined by the latter. This also explains why we had to ask for *asymptotic* symbols: one could not request the above property to hold $\forall m \geqslant 0$, $L \geqslant 0$. Examples of such functions are to be found in the families $\mathscr{B}^{(n)}$ defined after Lemma IV.2 in Sec. IV.

We are now ready to state the theorems. For any operator A acting over $L^2(\mathbb{R}^m)$, define

$$\Theta^m[t](A) := e^{2\pi i t H_m} A e^{-2\pi i t H_m}; \tag{III.9}$$

$$\Xi^m[T](A) := \frac{1}{2T} \int_{-T}^{T} \Theta^m[t](A)\, dt. \tag{III.10}$$

The quantum mixing property reads as follows.

Theorem III.2: *Suppose a, b are asymptotic symbols in $L^2(\Lambda_\infty, P_{\rho,2\beta})$ and denote*

$$I(t,L,m) := \int_{X^m_L} \langle g_\lambda, \Theta^m[t](Op(a \circ \Pi^m_L))\, Op(b \circ \Pi^m_L) g_\lambda \rangle\, d\nu(\lambda).$$

Then

$$\lim_{|t|\to\infty} \lim_{\substack{m,L\to\infty \\ m/L\to\rho}} I(t,L,m) = P_{\rho,2\beta}(a) P_{\rho,2\beta}(b).$$

As regards the quantum ergodicity the following is true.

Theorem III.3: *Let a be an asymptotic symbol in $L^2(\Lambda_\infty, P_{\rho,2\beta})$. Let*

$$J(T,L,m) := \int_{X^m_L} \| (\Xi^m[T](Op(a \circ \Pi^m_L)) - P_{\rho,2\beta}(a)) g_\lambda \|^2\, d\nu(\lambda).$$

Then, for all L, m, the operator

$$\Xi^m[\infty](Op(a \circ \Pi^m_L)) := \lim_{T\to\infty} \Xi^m[T](Op(a \circ \Pi^m_L))$$

exists in the domain of $Op(a \circ \Pi^m_L)$ and

$$\lim_{\substack{m,L\to\infty \\ m/L\to\rho}} J(\infty,L,m) = 0.$$

Furthermore, if a is also bounded, then the two limits can be inverted:

$$\lim_{T\to\infty} \lim_{\substack{m,L\to\infty \\ m/L\to\rho}} J(T,L,m) = 0.$$

Remark: The interchange of the time limit with the thermodynamical limit, in the above theorem, is remarkable. The fact that the time average can be taken before the thermodynamical limit can be described saying that the finite-particle system (the ''real'' one) is *quasiergodic*, for very large L and m; that is, the time average of any *decent* function is close, in measure, to a constant. This is a feature of the classical ideal gas, which has nothing to do with quantum mechanics. It is rather a consequence of the kinematic chaos and the restriction to symmetric observables, as anticipated in the Introduction, remark (i). This can be seen quite easily, due to the

integrability of the motion: time averaging means almost averaging everywhere over a torus. The invariant tori here are the sets $\{p\}\times T_L^m \in \Lambda_L^m$, and so the time average of $a(p,q)$ is simply $\int a(p,q)dq$; the invariant functions would depend on p only. Those functions, however, are requested to be symmetric and thus they cannot concentrate around a torus if they do not concentrate around all ''symmetric tori'' as well. An example is

$$a(p_1,\ldots,p_m)=\begin{cases}1 & \text{if } p_i\in\Gamma,\ \forall i=1,\ldots,m;\\ 0, & \text{otherwise,}\end{cases} \tag{III.11}$$

where Γ is a Borel set of $\mathbb{R}$. Now the kinematic chaos effect comes: at the thermodynamical limit, the support of this function, which is the probability to find all the particles having momenta in Γ, is exponentially small.

We can compare this to the situation one has for the harmonic chain, as shown in the companion paper.[2] In that case, there is no requirement on the observables. The fact that they cannot concentrate over invariant tori is due instead to the assumptions on the coupling matrix, which shuffles the tori at the infinite-particle limit.

An even clearer reason for referring to Theorem III.3 as quantum ergodicity comes from the following.

Corollary III.4: Assume a bounded asymptotic symbol. Then, $\forall\epsilon>0$*; set*

$$K(\epsilon,T,L,m):=\nu(\{\lambda\in X_L^m \,|\, |\langle g_\lambda, \Xi^m[T](Op(a\circ\Pi_L^m))g_\lambda\rangle - P_{\rho,2\beta}(a)|>\epsilon\}).$$

Then

$$\lim_{T\to\infty}\ \lim_{\substack{m,L\to\infty\\ m/L\to\rho}} K(\epsilon,T,L,m)=\lim_{\substack{m,L\to\infty\\ m/L\to\rho}}\ \lim_{T\to\infty} K(\epsilon,T,L,m)=0.$$

This can be phrased as follows. Call (T,ϵ)-*exceptional initial states* those states g_λ for which the quantum expectation of the T-time average differs more than ϵ from the classical phase average. Then the claim is that the measure of the (T,ϵ)-exceptional initial states vanishes when the thermodynamical limit and the time limit are performed.

Proof of Corollary III.4: An easy consequence of Theorem III.3, using a Cauchy–Schwartz inequality. Q.E.D.

A. The quantum Gibbs state

The results just formulated can be given a compact form, within the realm of the C^*-dynamical systems theory. It is beyond the purpose of this paper to go deep into that, so we do not outline the main notions of such a theory, hoping that the statements in this section are self-explanatory. However, a brief survey is given in Ref. 2, Appendix 2. Here we just observe that the relations we will write are included in such a general frame. The interested reader is referred to Ref. 5 for complete details, and to Ref. 6 for a recent well-organized review.

Consider $\mathscr{L}_L^m$, the space of all operators on $L^2(\mathbb{R}^m)$ that are invariant and bounded over all the fibers $L^2_{(k)}(T_L^m)$. This is a C^*-algebra when endowed with the usual operator norm. Associated to this algebra we define the Heisenberg dynamics given by $\Theta^m[t](A)$ as in (III.9), and the quantum Gibbs state expressed by

$$\omega_{\beta,L}^m(A):=\frac{\int_{[0,1/L)^m}\mathrm{Tr}_{L,m,k}(Ae^{-\beta H_m})dk}{\int_{[0,1/L)^m}\mathrm{Tr}_{L,m,k}(e^{-\beta H_m})dk}, \tag{III.12}$$

where $\mathrm{Tr}_{L,m,k}$ denotes the trace over $L^2_{(k)}(T_L^m)$. This functional is clearly normalized[20] and invariant for the *-automorphism $\Theta^m[t]$. Actually, it turns out to be a KMS state with parameter β over the W^*-dynamical system $(\mathscr{L}_L^m,\Theta^m[t],\omega_{\beta,L}^m)$.

Now consider, for each value of $k \in [0,1/L)^m$, the standard Fourier basis $\{e_\alpha^{(k)}\}$, as defined in Sec. II A. Next, consider the family of all such vectors, labeled by the index $\lambda := (\alpha,k) \in X_L^m := (T_L^m)^* \times [0,1/L)^m$. Endow X_L^m with the measure

$$d\theta(\alpha,k) := L^m \sum_{\xi \in (T_L^m)^*} \delta(\alpha-\xi)\, d\alpha\, dk. \tag{III.13}$$

Such a family satisfies hypothesis (III.2). In fact, calling $w_{\alpha,k}$ the Wigner function relative to $e_\alpha^{(k)}$, a straightforward computation from (II.19) yields

$$w_{\alpha,k}(p,q) = \frac{1}{L^m}\, \delta(p-(\alpha+k)). \tag{III.14}$$

Integrating this in $d\theta(\alpha,k)$ we obtain (III.2). Thus, define, as it is done in at the beginning of this section, $g_{\alpha,k} := e^{-\beta H_m} e_\alpha^{(k)} / \| e^{-\beta H_m} e_\alpha^{(k)} \|$. By definition (III.12), if $A \in \mathscr{L}_L^m$, we have[21]

$$\omega_{2\beta,L}^m(A) = \frac{\int dk \Sigma_\alpha \langle e^{-\beta H_m} e_\alpha^{(k)}, A e^{-\beta H_m} e_\alpha^{(k)} \rangle}{\int dk \Sigma_\alpha \| e^{-\beta H_m} e_\alpha^{(k)} \|^2} = \int_{X_L^m} \langle g_{\alpha,k}, A g_{\alpha,k} \rangle\, d\nu(\alpha,k), \tag{III.15}$$

with $d\nu$ defined as in (III.4). On the other hand, if one calls in a natural way $A_L^m := Op(a \circ \Pi_L^m)$, then a simple argument that is better explained in the following [see formulas (IV.2) and (IV.3)] gives

$$\omega_{2\beta,L}^m(A_L^m) = \int_{\Lambda_L^m} (a \circ \Pi_L^m)(p,q) [e^{-2\beta \mathscr{H}_m(p)}\, dp\, dq]_N. \tag{III.16}$$

Proposition II.1 immediately yields

$$\lim_{\substack{m,L\to\infty \\ m/L\to\rho}} \omega_{2\beta,L}^m(A_L^m) = P_{\rho,2\beta}(a). \tag{III.17}$$

Hence, if a,b are asymptotic symbols, we have just proved that Theorem III.2 can be rewritten as

$$\lim_{|t|\to\infty} \lim_{\substack{m,L\to\infty \\ m/L\to\rho}} \omega_{2\beta,L}^m(\Theta^m[t](A_L^m) B_L^m) = \lim_{\substack{m,L\to\infty \\ m/L\to\rho}} \omega_{2\beta,L}^m(A_L^m) \cdot \lim_{\substack{m,L\to\infty \\ m/L\to\rho}} \omega_{2\beta,L}^m(B_L^m). \tag{III.18}$$

In the same spirit, Theorem III.3 becomes

$$\lim_{T\to\infty} \lim_{\substack{m,L\to\infty \\ m/L\to\rho}} \omega_{2\beta,L}^m((\Xi^m[T](A_L^m))^2) = \lim_{\substack{m,L\to\infty \\ m/L\to\rho}} \omega_{2\beta,L}^m((\Xi^m[\infty](A_L^m))^2) = \lim_{\substack{m,L\to\infty \\ m/L\to\rho}} (\omega_{2\beta,L}^m(A_L^m))^2. \tag{III.19}$$

Remark: We have not defined an algebra of quantum observables for the infinite-particle system, limiting ourselves to deal with finite dimensions and to take a thermodynamical limit afterward (also see Comment 3 below). Had we introduced such a mathematical framework, then relations (III.18) and (III.19), for the state $\lim_{\substack{m,L\to\infty \\ m/L\to\rho}} \omega_{2\beta,L}^m$, would be contained in the general set of chaoticity notions in C^*-dynamical system theory (see Ref. 6, Definitions 4.42, 4.43).[22]

Some comments concerning the above reformulation of the theorems as compared to the paper by Graffi and Martinez follow.[2]

(1) (III.18) is completely analogous to statement (1.10) in Ref. 2. That is, the quantum mixing, forbidden in the finite-particle frame by the quasiperiodicity of the Heisenberg evolution, regardless of the dynamics of the classical flow (see the Introduction), is restored at the thermodynamical limit.

(2) A formulation of the ergodicity similar to (1.9) in Ref. 2 has not been chosen in this context because of the technicalities it would require. The coherent states we have here (see the Appendix, Sec. 1) are indexed by $\lambda \in T_L^m \times \mathbb{R}^m \times [0,1/L)_m =: X_L^m$, which is not exactly the classical phase space Λ_L^m. However, one could explicitly calculate $d\nu$ over X_L^m, for particular choices of the coherent states, and find a limit measure space—say—$(X, d\nu)$, but this turns out to be rather cumbersome and possibly misleading. Understandably, though, (III.19) and especially Corollary III.4 carry the same physical meaning as the mentioned result.

(3) As already exploited, we are able to state the ergodicity results here with a commutation of the limits.

(4) As emphasized in Ref. 2, Sec. 1, Remark 2, the techniques we use to prove the quantum ergodic properties at the thermodynamical limit, have the useful outcome to show that the rhs of (III.18) and (III.19) are the expected classical Gibbs averages. This is why we have formulated Theorems III.2 and III.3 in the first place.

(5) More importantly, here, results (III.18) and (III.19) were not known, at least to us.

IV. THE PROOFS

The first key fact is the following.

Lemma IV.1: For every symbol c defined on Λ_L^m,

$$e^{2\pi i t H_m}\, Op(c)\, e^{-2\pi i t H_m} = Op(c \circ \phi_L^m[t]).$$

This is true since we are dealing with a linear flow. This property of linear flows—sometimes referred to as the *exact Egorov Theorem* for the evolution canonical transformation—dates back at least to Van Hove and is valid only for Weyl quantization, whose restriction to L-periodic symbols we are now using. Anyway, for the sake of convenience, a direct proof is found in the Appendix, Sec. 2.

In our case, applying this lemma to $a \circ \Pi_L^m$ and using the remark in formula (II.4), we have

$$e^{2\pi i t H_m}\, Op(a \circ \Pi_L^m)\, e^{-2\pi i t H_m} = Op(a \circ \phi_\infty[t] \circ \Pi_L^m). \tag{IV.1}$$

A. Proof of Theorem III.2

In view of the above relation we call $a_t := a \circ \phi_\infty[t]$. In the rest of this proof, whenever there is no confusion, we denote by a quote the immersion application from Λ_L^m to Λ_∞. Hence $a' := a \circ \Pi_L^m$, and so on. In other words, a' is just our observable a looked at in the finite-dimensional phase space Λ_L^m. By (III.2) and (III.4), the definition of I, in the statement of the theorem, yields

$$I(t,L,m) = \frac{\int_{\Lambda_L^m} (e^{-\beta \mathscr{H}_m} \# a_t' \# b' \# e^{-\beta \mathscr{H}_m})\, dp\, dq}{\int_{\Lambda_L^m} e^{-2\beta \mathscr{H}_m}\, dp\, dq}. \tag{IV.2}$$

Using twice (II.17)—once to permutate cyclically the factors in (IV.2) and once to remove one of the # signs—leads to

$$I(t,L,m) = \int_{\Lambda_L^m} (a_t' \# b')(p,q)\, [e^{-2\beta \mathscr{H}_m(p)}\, dp\, dq]_N, \tag{IV.3}$$

since obviously $e^{-\beta\mathscr{H}_m}\#e^{-\beta\mathscr{H}_m}=e^{-2\beta\mathscr{H}_m}$. We further denote by μ_L^m the classical Gibbs measure (at inverse temperature 2β) over Λ_L^m: $\mu_L^m(p,q):=L^{-m}(\pi/\beta)^{-m/2}e^{-\beta p^2}$, and by $\breve{\mu}^m$ its component in the p space: $\breve{\mu}^m(p):=(\pi/\beta)^{-m/2}e^{-\beta p^2}$.

In view of (II.16), (IV.3) becomes, after some elementary but tedious rearrangements of the nested integrals,

$$I(t,L,m)=\int_{\Lambda_L^m}[a_t'(b'*_L\Phi_L^m)](p,q)\,d\mu_L^m(p,q), \tag{IV.4}$$

where

$$\Phi_L^m(p,q)=e^{\beta p^2}\frac{1}{L^m}\sum_{\xi\in(T_L^m)^*}e^{-\beta(p-\xi/2)^2}e^{2\pi i\xi\cdot q}, \tag{IV.5}$$

and $*_L$ means convolution in the q variable on T_L^m. Particular care must be taken here about this convolution *on a torus*, in order to prevent mistakes: see the Appendix, Sec. 3.

Thus Φ_L^m is completely factorizable, with Φ_L being a natural symbol for each of his factors: if $f(p_1,\ldots,p_m,q_1,\ldots,q_m)=f_1(p_1,q_1)\cdots f_m(p_m,q_m)$, then

$$(f*_L\Phi_L^m)(p,q)=(f_1*_L\Phi_L)(p_1,q_1)\cdots(f_m*_L\Phi_L)(p_m,q_m). \tag{IV.6}$$

This property will be useful in the following. Also, if 1 is the function on Λ_L^m identically equal to 1,

$$1*_L\Phi_L^m=1. \tag{IV.7}$$

We are going to prove the statement of the theorem, starting from (IV.4), for b in a dense subspace of $L^2(\Lambda_\infty,P_{\rho,2\beta})$. To accomplish that we need to make the following construction.

Fix a positive integer n and consider the function $\beta(p,q)\in C_0^\infty(\mathbb{R}^{2n})$,[23] that is, infinitely differentiable functions with compact support. For $m>n$ define the application

$$N_{L,m}^{(n)}(\beta)(p_1,\ldots,p_m,q_1,\ldots,q_m):=\sum_{j_1=1}^m\cdots\sum_{j_n=1}^m\beta(p_{j_1},\ldots,p_{j_n},q_{j_1},\ldots,q_{j_n}). \tag{IV.8}$$

So $N_{L,m}^{(n)}(\beta)$ is a function defined on $\mathbb{R}^{2m}$, and thus, in particular, on Λ_L^m. The use of this application is explained by the following lemma.

Lemma IV.2: If $\beta(p,q)\in\mathscr{S}(\mathbb{R}^{2n})$[24] then there exists a function $b\in L^2(\Lambda_\infty,P_{\rho,2\beta})$ *s.t.* $N_{L,m}^{(n)}(\beta)=b\circ\Pi_L^m$. *Plus, the following properties hold:*

$$\int_{\Lambda_L^m}|(b\circ\Pi_L^m)(p,q)|^2\,d\mu_L^m(p,q)\leqslant m^{2n}\Big(\sup_{(p',q')\in\Lambda_L^n}|\beta(p',q')|\Big)^2; \tag{IV.9}$$

$$\int_{\Lambda_L^m}(b\circ\Pi_L^m)(p,q)\,d\mu_L^m(p,q)=\frac{m!}{L^n(m-n)!}\int_{\Lambda_L^n}\beta(p',q')\,d\breve{\mu}^n(p')\,dq'. \tag{IV.10}$$

Proof of Lemma IV.2: The first inequality simply follows by definition (IV.8), since μ_L^m is a probability measure.

To prove the rest we approximate β with suitably chosen indicator functions over $\mathbb{R}^{2n}$. More precisely, take two sufficiently fine partitions of $\mathbb{R}$, $\{\Gamma_j\},\{\Delta_l\}\subset\mathscr{B}(\mathbb{R})$ with $\sup_{j,l}\{\breve{\mu}(\beta_j),|\Delta_l|\}$ small.[25] Let $\chi_{j_1,\ldots,j_n,l_1,\ldots,l_n}(p',q')$ be the indicator function of the set $\Gamma_{j_1}\times\cdots\times\Gamma_{j_n}\times\Delta_{l_1}\times\cdots\times\Delta_{l_1}$ and approximate β with $\beta_a:=\Sigma c_{j_1,\ldots,l_n}\chi_{j_1,\ldots,l_n}$. So

$$N^{(n)}_{L,m}(\beta_a)(p,q)=\sum_{j_1,\dots,l_n} c_{j_1,\dots,l_n} N^{(n)}_{L,m}(\chi_{j_1,\dots,l_n})(p,q). \tag{IV.11}$$

Since $\chi_{j_1,\dots,l_n}$ is completely factorizable, then it is easy to realize, by definition (IV.8), that $N^{(n)}_{L,m}(\chi_{j_1,\dots,l_n})(p,q) = N^{(1)}_{L,m}(\chi_{\Gamma_{j_1}\times\Delta_{l_1}})\cdots N^{(1)}_{L,m}(\chi_{\Gamma_{j_n}\times\Delta_{l_n}})$. We see that $N^{(1)}_{L,m}(\chi_{\Gamma\times\Delta})(p,q)$ takes integer values between 0 and m. Specifically, it counts the number of particles in the configuration $(p,q)\in\Lambda^m_L$ whose momentum is contained in Γ and whose coordinate in Δ.[26] So $N^{(1)}_{L,m}(\chi_{\Gamma\times\Delta})=N_{\Gamma\times\Delta}\circ\Pi^m_L$, where $N_{\Gamma\times\Delta}:\Lambda_\infty\to\mathbb{N}$ is defined by

$$N_{\Gamma\times\Delta}(p,q):=\#\{x\in q\cap\Delta \,|\, p(x)\in\Gamma\}, \tag{IV.12}$$

where, with sloppy notation, (p,q) denotes a point in Λ_∞. Recalling what we said in Sec. II A, this function obviously belongs to $\mathscr{A}$: see, in particular, (II.7) and comments thereby. Therefore so does every finite product of similar functions. Looking at (IV.11), and subsequent comments, this proves that there exists a $b_a\in\mathbb{A}$, such that $\beta_a=b_a\circ\Pi^m_L$. The analogous statement holds for β as well, by density.

Let us go over to the proof of (IV.10). Fix a sequence $(j,l):=(j_1,\dots,l_n)$ like those we have in formula (IV.11) and fix n integers $k:=(k_1,\dots,k_n)$, such that $k_1+\cdots+k_n\leqslant m$. Now consider the set $A^{(k)}_{j,l}:=\{N^{(1)}_{L,m}(\chi_{\Gamma_{j_i}\times\Delta_{l_i}})=k_i;\forall i=1,\dots,n\}\in\Lambda^m_L$, i.e., the set of the configurations having k_1 particles in $\Gamma_{j_1}\times\Delta_{l_1}$, k_2 particles in $\Gamma_{j_2}\times\Delta_{l_2}$, and so on. Notice that (use some combinatorics)

$$\mu^m_L(A^{(k)}_{j,l})=\frac{m!}{(m-\Sigma k_i)!}\left[\prod_{i=1}^n \frac{1}{k_i!}\left(\frac{|\Delta_{l_i}|}{L}\,\breve{\mu}(\Gamma_{j_i})\right)^{k_i}\right]\left(1-\sum_{i=1}^n \frac{|\Delta_{l_i}|}{L}\,\breve{\mu}(\Gamma_{j_i})\right)^{m-\Sigma k_i}. \tag{IV.13}$$

We have seen that $N^{(n)}_{L,m}(\chi_{j_1,\dots,l_n}) = \Sigma_k k_1\cdots k_n A^{(k)}_{j,l}$. So, when the initially chosen partition is fine, $\mu^m_L(\chi_{j_1,\dots,l_n}) = m!/(L^n(m-n)!)\Pi_i|\Delta_{l_i}|\breve{\mu}(\Gamma_{j_i}) + o(|\Delta_{l_i}|,\breve{\mu}(\Gamma_{j_i}))$. Looking back at (IV.11) this proves that (IV.10) holds with negligible errors for β_a, and thus is exact for β. Q.E.D.

Let us call $\mathscr{B}^{(n)}\in\mathscr{A}$ the space of functions b granted by Lemma IV.2 when $\beta\in C^\infty_0(\mathbb{R}^{2n})$. From now on we will suppose $b\in\mathscr{B}^{(n)}$, so that $b':=b\circ\Pi^m_L=N^{(n)}_{L,m}(\beta)$. In so doing we will be proving Theorem III.2 for $b\in\oplus_{\text{finite}}\mathscr{B}^{(n)}$. But this is dense in $L^2(\Gamma_\infty,P_{\rho,2\beta})$ since, looking at the proof of Lemma IV.2, the closure of $\mathscr{B}^{(n)}$ contains the product of n functions like $N_{\Gamma\times\Delta}$. This means that in the algebra $\overline{(\oplus\mathscr{B}^{(n)})}$ we are able to find the indicator functions of the sets $N^{-1}_{\Gamma\times\Delta}(n),\forall n\in\mathbb{N}$. But these generate $\mathscr{A}$ [look at (II.7) and refer to Refs. 13 and 6].

Under the above assumption, we go back to (IV.4): since $b'=N^{(n)}_{L,m}(\beta)$, then $b'*_L\Phi^m_L=N^{(n)}_{L,m}(\beta*_L\Phi^n_L)$[27] because of the mentioned properties of Φ^m_L [see (IV.5)–(IV.7)]. If we denote by $\gamma_L:=\beta*_L\Phi^n_L$, it is obvious that $\gamma_L\in\mathscr{S}(\mathbb{R}^{2n})$, and so $N^{(n)}_{L,m}(\gamma_L) = c'_L$ for some $c_L\in L^2(\Lambda_\infty,P_{\rho,2\beta})$, by Lemma IV.2. This allows us to rewrite (IV.4) as

$$I(t,L,m)=\langle a'_t,c'_L\rangle_{L^2(\Lambda^m_L,\mu^m_L)}. \tag{IV.14}$$

If we are able to find a limit for c_L then we are done with the cumbersome part of this proof. To this goal, we formulate the following.

Lemma IV.3: There exists a $\gamma_\infty\in\mathscr{S}(\mathbb{R}^{2n})$ such that

$$\sup_{\Lambda^n_L}|\gamma_\infty-\gamma_L|=\mathscr{O}(L^{-\infty}). \tag{IV.15}$$

Furthermore,

$$\int_{\mathbb{R}^{2n}} \gamma_\infty(p',q')d\check{\mu}^n(p')dq' = \int_{\mathbb{R}^{2n}} \beta(p',q')d\check{\mu}^n(p')dq'. \tag{IV.16}$$

The proof of this lemma is found in the Appendix, Sec. 4.

In analogy with the above notations we call c_∞ the observable in $L^2(\Lambda_\infty, P_{\rho,2\beta})$ obtained applying Lemma IV.2 to γ_∞. Comparing now (IV.15) in Lemma IV.3 with (IV.9), we deduce that

$$\lim_{\substack{m,L\to\infty \\ m/L\to\rho}} \|c'_\infty - c'_L\|^2_{L^2(\Lambda_L^m,\mu_L^m)} = 0. \tag{IV.17}$$

Dropping for the sake of simplicity the subscript in the scalar product notation, this means that, when $m, L\to\infty$, $m/L\to\rho$,

$$|\langle a'_t, c'_L\rangle - P_{\rho,2\beta}(a_t c_\infty)| \leqslant \|a'_t\|^2\|c'_L - c'_\infty\|^2 + |\mu_L^m(a'_t c'_\infty) - P_{\rho,2\beta}(a_t c_\infty)| \to 0, \tag{IV.18}$$

because of Proposition II.1. Now we use the other main ingredient of this proof, i.e., the classical result, Theorem II.2. We obtain

$$\lim_{|t|\to\infty} \lim_{\substack{m,L\to\infty \\ m/L\to\rho}} I(t,L,m) = P_{\rho,2\beta}(a)P_{\rho,2\beta}(c_\infty). \tag{IV.19}$$

Now, using the integrals of γ_∞ and β to compare the integrals of c_∞ and b [apply (IV.16) into (IV.10)], we see that $\mu_L^m(c'_\infty) = \mu_L^m(b')$. Taking the limits, $P_{\rho,2\beta}(c_\infty) = P_{\rho.2\beta}(b)$, which, together with the last relation, completes the proof.

B. Proof of Theorem III.3

First of all, it has to be noticed that both statements of Theorem III.3 [respectively, relation (III.19)] cannot be derived so trivially from Theorem III.2 [resp., (III.18)]. This will be seen below in each case.

We borrow the notation from the previous proof: so, for example, $a'_t := a \circ \phi_\infty[t] \circ \Pi_L^m$. Also, let $a'_T := (1/2T)\int_{-T}^{T} a'_t \, dt$. Formula (IV.1) proves that

$$\Xi^m[T](A_L^m) = Op(a'_T), \tag{IV.20}$$

where, as in Sec. III A, we call $A_L^m := Op(a')$.

The existence of $\Xi^m[\infty](A_L^m)$ is a trivial consequence of the Heisenberg evolution: we can easily figure it out looking at its matrix elements wrt the bases $\{e_\alpha^{(k)}\} \subset L^2_{(k)}(T_L^m)$. These bases diagonalize the Hamiltonian H_m, as well as any operator function of P only. We call such eigenvalues

$$E_\alpha^{(k)} = \frac{1}{2}(\alpha + k)^2 = \frac{1}{2}\sum_{i=1}^{n}(\alpha_i + k_i)^2. \tag{IV.21}$$

Now it is easy to see that, $\forall k \in [0,1/L)^m, \alpha, \gamma \in (T_L^m)^*$,

$$\langle e_\alpha^{(k)}, \Xi^m[\infty](A_L^m) e_\gamma^{(k)}\rangle = \langle e_\alpha^{(k)}, A_L^m e_\gamma^{(k)}\rangle \delta_{E_\alpha^{(k)}, E_\gamma^{(k)}}, \tag{IV.22}$$

where δ is the Kronecker δ-function. This formula shows that $\Xi^m[\infty](A_L^m)$ is well defined on all vectors in $D(A_L^m)$.

One might think to prove now the statement regarding $J(\infty,L,m)$ by simply substituting the Heisenberg invariant operator $\Xi^m[\infty](A_L^m)$ to $Op(a')$ and $Op(b')$ in Theorem III.2. We cannot quite do this, since such operator is not, in general, pseudodifferential. It is obvious, though, that

it can be approximated to any extent by pseudodifferential operators, and the result would follow by density. However, as remarked in Sec. III A, we have not defined a proper C^*-algebra for the infinite-particle system. Thus, we cannot talk of any density and have to prove the theorem directly.

$\Xi^m[\infty](A_L^m)$, roughly speaking, represents the quantization of $a'_\infty := \lim_{T\to\infty} a'_T$, which is not, in general, a symbol, being possibly not even continuous. But simple considerations based upon the trivial dynamics over Λ_L^m (also see the remark after the statement of this theorem) show that it is almost everywhere [namely, for $p=(p_1,\dots,p_m)$ having rationally independent components] equal to

$$c'(p,q)=c'(p):=\frac{1}{L^m}\int_{T_L^m} a'(p,q)\,dq, \tag{IV.23}$$

which is a symbol. Moreover, we denote it c' since one can straightforwardly find a $c\in\mathscr{A}$ such that $c'=c\circ\Pi_L^m$. The whole idea of this proof is exactly to show that, in some sense, $Op(c')$ is a.e. equal to $\Xi^m[\infty](A_L^m)$, so that the former can be substituted to the latter in the definition of $J(\infty,L,m)$ in order to apply Theorem III.2 [also compare (III.19) and (III.18)].

We first remark some basic properties of $Op(c')$. Since $c'(p,q)=c'(p)$ then $Op(c')$ is diagonal wrt $\{e_\alpha^{(k)}\}$. Its diagonal matrix elements, using (III.14), are found to be

$$\langle e_\alpha^{(k)}, Op(c')e_\alpha^{(k)}\rangle=\frac{c'(\alpha+k)}{\omega t}=\frac{1}{L^m}\int_{T_L^m} a'(\alpha+k,q)\,dq=\langle e_\alpha^{(k)}, A_L^m e_\alpha^{(k)}\rangle. \tag{IV.24}$$

Also (IV.24), together with (IV.22), implies that $Op(c')^{(k)}=(\Xi^m[\infty](A_L^m))^{(k)}$ [28] for those $k\in[0,1/L)^m$ for which $H_m^{(k)}$ is diagonal.

Using (II.19) over a generic f_λ picked up from the set of states satisfying (III.2), one can see that $w_\lambda(p,q)$ contains a (possibly countable) sum of δ-functions in p. This simple argument shows that, in order for $\{f_\lambda\}$ to verify (III.2), a factor of the measure space $(X_L^m, d\theta)$ must be $([0,1/L)^m, d\tau(k))$, with $d\tau$ absolutely continuous wrt the Lebesgue measure.[29] So if we prove that $\sigma(H_m^{(k)})$ is simple for Lebesgue—almost all k's then

$$J(\infty,L,m):=\int_{X_l^m}\|(Op(c')-P_{\rho,2\beta}(a))g\lambda\|^2\,d\nu(\lambda), \tag{IV.25}$$

and we can apply Theorem III.2 with $a=b=c-P_{\rho,2\beta}(a)$, which is time invariant. This would complete the proof of the first claim.

Rescaling (IV.21) by a factor L^m, what we need is equivalent to the following lemma.

Lemma IV.4:

$$|\{k\in[0,1)^m \mid \exists j,n\in\mathbb{Z}^m s.t.(j+k)^2=(n+k)^2\}|=0.$$

Proof of Lemma IV.4:[30] Thinking of it as a geometric problem in $\mathbb{R}^m$, when such j,n exist, then $-k$ lies in the axial hyperplane of the segment joining j to n, i.e., the set of points in the space equally distant from j and n. By their very construction there is only a countable number of such hyperplanes. Q.E.D.

As far as the last statement of Theorem III.3 is concerned, we see again that it cannot be derived as a corollary of the mixing theorem, since we are taking time limits of both operators. But we can give a direct proof using the techniques of Sec. IV A and the classical ergodicity result contained in Theorem II.2.

Exactly as in (IV.2) and (IV.3) we can write

$$J(T,L,m)=\int_{\Lambda_L^m}[(a'_T-P_{\rho,2\beta}(a))\#(a'_T-P_{\rho,2\beta}(a))](p,q)[e^{-2\beta\mathscr{H}_m(p)}\,dp\,dq]_N, \quad \text{(IV.26)}$$

having used (IV.20). We have become familiar with this object in Sec. IV A, and we have seen that integrating—wrt the Gibbs measure—the Weyl composition of two functions means integrating the product of the two functions, one of which is scrambled by a convolution [see (IV.3), (IV.4), and (IV.14)]. At the thermodynamic limit, this amounts to saying that

$$\lim_{\substack{m,L\to\infty\\ m/L\to\rho}} J(T,L,m)=P_{\rho,2\beta}((a_T-P_{\rho,2\beta}(a))c^{(T)}), \quad \text{(IV.27)}$$

where $c^{(T)}$ is the limit of the ''scrambled functions'' constructed upon $(a_T-P_{\rho,2\beta}(a))$. Its existence is granted by Lemmas IV.3 and IV.2, which yielded (IV.17). From the construction we have just recalled it can be seen that if $(a_T-P_{\rho,2\beta}(a))$ is bounded then $c^{(T)}$ is as well.

A remark is in order here: in Sec. IV A we have worked with symbols belonging to $\mathscr{B}^{(n)}$, and those are unbounded by definition, being the limits of functions like $N_{L,m}^{(n)}(\beta)$ defined in (IV.8). But a simple argument shows that a bounded $a\in\mathscr{A}=\sigma(\oplus\mathscr{B}^{(n)})$ remains bounded after the above procedure, since, roughly speaking, it gets deformed in the same way in each of its $\mathscr{B}^{(n)}$-components.

Finally, we can apply Lebesgue dominated convergence in (IV.27) since the integrand function is bounded and tends pointwise to zero as $T\to\infty$. Thus, the T-limit of (IV.27) gives the last statement in Theorem III.3, whence the end of the proof. Q.E.D.

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APPENDIX

1. Coherent states for the cylinder

We begin this section by recalling some notions about the Bloch decomposition (II.9), following Refs. 14 and 10. The idea is very simple: given a function $f\in L^2(\mathbb{R}^m)$, and therefore its Fourier transform $\hat{f}(p)$, we pick up from the latter only the terms at $p=\xi+k$, $(\xi\in(T_L^m)^*)$ to construct $f^{(k)}$, which clearly lies in $L^2_{(k)}(T_L^m)$.

In formula:

$$f^{(k)}(x):=\frac{1}{L^m}\sum_{\xi\in(T_L^m)^*}\hat{f}(\xi+k)e^{2\pi i(\xi+k)\cdot x}. \quad \text{(A1)}$$

Considering the scalar products in the dual spaces [respectively, $L^2(\mathbb{R}^m)$ and $l^2((\mathbb{Z}/L)^m+k)$], it is easy to see the decomposition property that justifies (II.9):

$$\langle f,g\rangle_{L^2(\mathbb{R}^m)}=\int_{[0,1/L)^m}\langle f^{(k)},g^{(k)}\rangle_{L^2_{(k)}(T_L^m)}\,dk. \quad \text{(A2)}$$

An explicit formula for $f^{(k)}$, more direct than (A1), is also computable with the aid of the Poisson summation formula:

$$f^{(k)}(x)=\sum_{n\in\mathbb{Z}^m}e^{-2\pi iLn\cdot k}f(x+Ln). \quad \text{(A3)}$$

We can now proceed to the construction of a remarkable example of states satisfying the assumptions of the theorems. Let a family of generalized coherent states for the Euclidean $2m$-dimensional phase space be given,

$$f_{(u,v)} := T(-u,v) f_0, \tag{A4}$$

as constructed in Ref. 11, where $(u,v) \in \mathbb{R}^{2m}$ and $f_0 \in L^2(\mathbb{R}^m)$, usually a Gaussian centered at the origin. According to our preparatory remark, we give the following definition.

Definition A.1:[10] *The family* $f^{(k)}_{(u,v)}$ *where* $(u,v,k) \in X^m_L := T^m_L \times \mathbb{R}^m \times [0,1/L)^m$ *constructed as above is called a set of* coherent states on Λ^m_L.

We endow X^m_L with the measure $d\theta(u,v,k) := du\ dv\ dk$ and check that they verify the hypothesis of the theorem.

We shall work on the Fourier antitransform of w_λ, i.e., on the Fourier–Wigner function relative to the state f_λ,

$$\begin{aligned}
&\int_{\Lambda^m_L} du\ dv \int_{[0,1/L)^m} dk \langle f^{(k)}_{(u,v)}, T^{(k)}(\eta,\xi) f^{(k)}_{(u,v)} \rangle_{L^2_{(k)}(T^m_L)} \\
&\quad = \int_{\Lambda^m_L} du\ dv \langle f_{(u,v)}, T(\eta,\xi) f_{(u,v)} \rangle_{L^2(\mathbb{R}^m)} \\
&\quad = \int_{\Lambda^m_L} du\ dv \langle T(-u,v) f_0, T(-u,v) T(\eta,\xi) f_0 \rangle_{L^2(\mathbb{R}^m)} e^{2\pi i(\eta\cdot v + \xi\cdot u)} \\
&\quad = \int_{\Lambda^m_L} du\ dv \langle f_0, T(\eta,\xi) f_0 \rangle_{L^2(\mathbb{R}^m)}\ e^{2\pi i(\eta\cdot v + \xi\cdot u)} = \langle f_0, T(\eta,\xi) f_0 \rangle_{L^2(\mathbb{R}^m)}\ \delta_\xi \delta(\eta) = \delta_\xi \delta(\eta),
\end{aligned} \tag{A5}$$

which is another way to state (III.2). The first step is justified by (A2) and the third by the commutation relations in the Heisenberg group.

Finally, this set of coherent states is perhaps the most important among the possible collections one could choose. As a matter of fact, such states are indeed introduced to be as *localized* as the Heisenberg principle permits.[10] Had we performed a limit $\hbar \to 0$, exploiting the Wigner function as a measure of the degree of localization of a state, we would have seen that

$$W_{f^{(k)}_{(u,v)}, f^{(k)}_{(u,v)}}(p,q) \to \delta(p-u)\,\delta(q-v), \quad \text{as } \hbar \to 0; \tag{A6}$$

where the dependence on $\hbar$ is implicit in the construction of $f^{(k)}_{(u,v)}$. This is why one can say that such a state is a good analog of a point in the phase space. Therefore we see that the physical meaning of our quantum ergodic properties gets clearer and more classical, of course, in the semiclassical regime.

2. Proof of Lemma IV.1

Let us check that equality on all the matrix elements with respect to the standard basis of $L^2_{(k)}(T^m_L), \{e^{(k)}_\alpha\}_{\alpha \in (T^m_L)^*}$ introduced in Sec. II B. It is easily computed that

$$T^{(k)}(\eta,\xi) e^{(k)}_\alpha = e^{2\pi i \eta\cdot(\xi/2 + \alpha + k)} e^{(k)}_{\alpha+\xi}. \tag{A7}$$

If we now denote $c^t(p,q) := (c \circ \phi^m_L[t]) = c(p, q+pt)$, we can compute its Fourier transform, which turns out to be $\hat{c}^t(\eta,\xi) = \hat{c}(\eta - \xi t, \xi)$. Thus, substituting into (II.14) and changing the variable

$$Op(c^t) := \frac{1}{L^m} \sum_{\xi \in (T_L^m)^*} \int_{\mathbb{R}^m} \hat{c}(\eta, \xi) T(\eta + \xi t, \xi) d\eta. \tag{A8}$$

In order for the statement to hold for every c, it is a necessary and sufficient condition that $\forall \alpha, \gamma \in (T_L^m)^*$,

$$\langle e_\alpha^{(k)}, T(\eta + \xi t, \xi) e_\gamma^{(k)} \rangle = \langle e_\alpha^{(k)}, e^{2\pi i t H_m} T(\eta, \xi) e^{-2\pi i t H_m} e_\gamma^{(k)} \rangle. \tag{A9}$$

Using (A7) we find on the rhs,

$$\langle e_\alpha^{(k)}, T(\eta + \xi t, \xi) e_\gamma^{(k)} \rangle = e^{2\pi i (\eta + \xi t) \cdot (\xi/2 + \gamma + k)} \delta_{\alpha, \gamma + \xi}. \tag{A10}$$

Since $P^{(k)} e_\alpha^{(k)} = (\alpha + k) e_\alpha^{(k)}$, on the lhs, we have

$$\begin{aligned} \langle e_\alpha^{(k)}, e^{2\pi i t H_m} T(\eta, \xi) e^{-2\pi i t H_m} e_\gamma^{(k)} \rangle &= e^{\pi i (\alpha + k)^2 t} e^{-\pi i (\gamma + k)^2 t} e^{2\pi i \eta \cdot (\xi/2 + \gamma + k)} \delta_{\alpha, \gamma + \xi} \\ &= e^{2\pi i ((\xi/2 + \gamma + k) \xi t + (\xi/2 + \gamma + k) \eta)} \delta_{\alpha, \gamma + \xi}, \end{aligned} \tag{A11}$$

where we have substituted for α its value $\gamma + \xi$. This relation finally verifies (A9). Q.E.D.

3. Convolutions over tori and over Euclidean spaces

The purpose of this section is to clarify the meaning of the symbol $*_L$, indicating q-convolution over T_L^m, when applied to functions that are, in principle, defined over larger sets, like the functions $b \circ \Pi_L^m$, for instance. Also, we want to understand how this is related to $*_\infty$, the ordinary convolution on $\mathbb{R}^m$, when $L \to \infty$.

Since the arguments here are essentially descriptive, we specialize to one dimension, without loss of generality. If f is a nice function defined on $\mathbb{R}$, denote by $f^{(L)}$ its *periodic restriction*, i.e., the function, *defined again on* $\mathbb{R}$, which is L-periodic and coincides with f on $[-L/2, L/2)$. Then if g is also a nice function on $\mathbb{R}$, we define

$$(f *_L g)(x) := (f^{(L)} * g^{(L)})(x) = \int_{-L/2}^{L/2} f^{(L)}(y) g^{(L)}(x - y) dy = \int_{-L/2}^{L/2} f(y) g^{(L)}(x - y) dy. \tag{A12}$$

Thus, for instance, $(f *_L g)(x) \neq \int_{-L/2}^{L/2} f(y) g(x - y) dy$. As $L \to \infty$, however, we expect this to be approximately true, at least for a fixed $x \in \mathbb{R}$. As a matter of fact, requiring some properties of f and g, one can prove a useful lemma. Call $S_R := [-R, R]$.

Lemma A.2: Suppose $f \in C_0^\infty(\mathbb{R})$ *and* supp $f \subseteq S_R$. *Assume also that* $|g|$ *vanishes monotonically at infinity. Defining*

$$h(x) = (f *_L g - f *_\infty g)(x),$$

then one has, for sufficiently large L,

$$h(x) \begin{cases} \leq M(|g(-L/2)| + |g(L/2 - R)|), & \text{for } x \in [-L/2, -L/2 + R), \\ = 0, & \text{for } x \in [-L/2 + R, L/2 - R], \\ \leq M(|g(L/2)| + |g(-L/2 + R)|), & \text{for } x \in (L/2 - R, L/2], \end{cases}$$

where $M := R \max |f|$.

Proof of Lemma A.2: Take L so large that $L/2 > R$ and $|g|$ is increasing in $(-\infty, -L/2 + R]$ and decreasing in $[L/2 - R, +\infty)$.

Looking at (A12) and recalling the hypothesis on f, we can write

$$(f*_L g)(x)=\int_{S_R} f(y)g^{(L)}(x-y)dy. \tag{A13}$$

Hence

$$h(x)=\int_{S_R} f(y)(g^{(L)}-g)(x-y)dy. \tag{A14}$$

Now, $g^{(L)}(x-y)$ coincides with $g(x-y)$ when $x-y\in S_{L/2}$, that is, when $y\in[x-L/2,x+L/2]$. So (A14) is rewritten as

$$h(x)=\int_{S_R\setminus(x+S_{L/2})} f(y)(g^{(L)}-g)(x-y)dy. \tag{A15}$$

It is easily seen that if $x\in[-L/2+R,L/2-R]$, then $S_R\subseteq(x+S_{L/2})$, such that $h(x)=0$ and part of the claim is proved. If $x\in[-L/2,-L/2+R]$, making the change of variable $z=x-y$, (A14) gives

$$|h(x)|=\left|\int_{x-R}^{-L/2} f(x-z)(g^{(L)}-g)(z)dz\right|\leqslant\max|f|\int_{-L/2-R}^{-L/2}(|g^{(L)}(z)|+|g(z)|)dz. \tag{A16}$$

Since by definition, for $z<-L/2$, $g^{(L)}(z)=g(z+L)$, the monotonicity property of g gives the first case in the statement of the lemma. The third case is, of course, analogous. Q.E.D

4. Proof of Lemma IV.3

Before even getting started, let us agree upon denoting, throughout this proof, by (p,q) all momentum-coordinate variables, be they defined on Λ_L^m or on $\mathbb{R}^{2n}$ or on Λ_L^1. Notice that, in the proof of Theorem III.2, we referred to n-dimensional variables as (p',q').

The whole idea here is to realize that, if n is fixed, the function Φ_L^n defined as in (IV.5), gets closer and closer, in Λ_L^n, to

$$\Phi_\infty^n(p,q)=e^{\beta p^2}\int_{\mathbb{R}^n} d\xi e^{-\beta(p-\xi/2)^2}e^{2\pi i\xi\cdot q}=e^{\beta p^2}e^{4\pi ip\cdot q}\left(\frac{4\pi}{\beta}\right)^{n/2}e^{-(4\pi^2/\beta)q^2}=e^{\beta p^2}e^{4\pi ip\cdot q}v^n(q), \tag{A17}$$

where $v(q):=\sqrt{4\pi/\beta}e^{-(4\pi^2/\beta)q^2}$. In the following we will use repeatedly the asymptotic estimate $v(L/2)=\mathcal{O}(L^{-\infty})$.

Anyway, Φ_∞^n is defined by the fact that it has the same Fourier spectrum of Φ_L^n, suitably extended to all of $\mathbb{R}^n$. If we denote by $\tilde{\cdot}$ the q-Fourier transform over T_L^n, then this amounts to saying that, for $\xi\in(T_L^n)^*=(\mathbb{Z}/L)^n$,

$$\int_{\mathbb{R}^n}\Phi_\infty^n(p,q)e^{-2\pi i\xi\cdot q}dq=e^{\beta p^2}e^{-\beta(p-\xi/2)^2}=:\tilde{\Phi}_L^n(p,\xi). \tag{A18}$$

So the best candidate for γ_∞ is $\beta*_\infty\Phi_\infty^n$. The symbol $*_\infty$ designates the q convolution over $\mathbb{R}^n$, as explained in Sec. 3 of this appendix. First of all, such a γ_∞ verifies (IV.16): this is a consequence of the fact that $\int_{\mathbb{R}^n}\Phi_\infty^n=1$, which is easily verified. Let us proceed to the proof of (IV.15).

Recalling the warning in Sec. 3 of this appendix, the main inequality will be

$$\sup_{\Lambda_L^n}|\gamma_L-\gamma_\infty|=\sup_{\Lambda_L^n}|\beta*_L\Phi_L^n-\beta*_\infty\Phi_\infty^n|\leqslant\sup_{\Lambda_L^n}|\beta*_L(\Phi_L^n-\Phi_\infty^n)|+\sup_{\Lambda_L^n}|\beta*_L\Phi_\infty^n-\beta*_\infty\Phi_\infty^n|. \tag{A19}$$

The rightmost term can be worked out easily, using (A17) and Lemma A.2 of Sec. 3 of this appendix. If $(p,q)\in\Lambda_L^n$,

$$|(\beta *_L \Phi_\infty^n - \beta *_\infty \Phi_\infty^n)(p,q)| \leqslant M v^n\left(\frac{L}{2}-R\right) = \mathscr{O}(L^{-\infty}), \tag{A20}$$

where $M \simeq \max(|\beta(p,q)|e^{\beta p^2})$ and R is the radius of the ball containing supp β. To work out the other term in (A19) we employ the ideas stated at the beginning of this section about Φ_∞^n. We start by noticing that $\|\cdot\|_{L^1(T_L^n,dq)} \leqslant L^{n/2}\|\cdot\|_{L^2(T_L^n,dq)}$. We have

$$\sup_{q\in T_L^n} |\beta *_L (\Phi_L^n - \Phi_\infty^n)(p,q)| \leqslant \sup_{q\in T_L^n} |\beta(p,q)| L^{n/2} \|(\Phi_L^n - \Phi_\infty^n)(p,\cdot)\|_{L^2(T_L^n,dq)}. \tag{A21}$$

Notice that β is compactly supported. We also see that

$$\|(\Phi_L^n - \Phi_\infty^n)(p_1,\ldots,p_n,\cdot)\|^2_{L^2(T_L^n,d)} = \prod_{i=1}^n \|(\Phi_L - \Phi_\infty)(p_i,\cdot)\|^2_{L^2(T_L,dq_i)}, \tag{A22}$$

since Φ_L^n and Φ_∞^n are completely factorizable: we call, obviously, Φ_L and Φ_∞ their one-dimensional versions, on which we are immediately going to work. As anticipated at the beginning of this section, we will be a little imprecise and use again the label (p,q) for (p_i,q_i). Now

$$\|(\Phi_L - \Phi_\infty)(p,\cdot)\|^2_{L^2(T_L)} = \frac{1}{L}\sum_{\xi\in(\mathbb{Z}/L)} |\tilde{\Phi}_L(p,\xi) - \tilde{\Phi}_\infty(p,\xi)|^2, \tag{A23}$$

with $\tilde{\Phi}_\infty(p,\xi) = \int_{-L/2}^{L/2} \Phi_\infty(p,q) e^{-2\pi i\xi q}\, dq$. Looking back at (A18) and using definition (A17), we can write

$$\begin{aligned}
|\tilde{\Phi}_L(p,\xi) - \tilde{\Phi}_\infty(p,\xi)| &= \left| \int_{\mathbb{R}\setminus T_L} \Phi_\infty(p,q) e^{-2\pi i\xi q}\, dq \right| \\
&= 2e^{\beta p^2} \left| \int_{L/2}^{+\infty} v(q)\cos(2\pi(\xi-2p)q) dq \right| \\
&= 2e^{\beta p^2} \left| \left[\frac{v(q)\sin(2\pi(\xi-2p)q)}{2\pi(\xi-2p)} \right]_{L/2}^{+\infty} - \int_{L/2}^{+\infty} \frac{v'(q)\sin(2\pi(\xi-2p)q)}{2\pi(\xi-2p)}\, dq \right| \\
&\leqslant e^{\beta p^2} g(\xi-2p) v(L/2),
\end{aligned} \tag{A24}$$

where $g(x)$ is a continuous function defined on $\mathbb{R}$ behaving like $|x|^{-1}$ for large values of $|x|$. Note that, as $L\to\infty$, $(1/L)\Sigma_{\xi\in(\mathbb{Z}/L)} g^2(\xi - 2p) \to \int_{\mathbb{R}} g^2(\xi) d\xi =: K$, *uniformly* for p in a compact set. So, looking at (A21), and merging up (A22), (A23), and (A24), we have

$$\begin{aligned}
\sup_{(p,q)\in\Lambda_L^n} |\beta *_L (\Phi_L^n - \Phi_\infty^n)(p,q)| &\leqslant L^{n/2} \sup_{(p,q)\in\Lambda_L^n} |\beta| \sup_{|p|<R} \|(\Phi_L^n - \Phi_\infty^n)(p,\cdot)\|_{L^2(T_L^n,dq)} \\
&\leqslant (e^{2\beta R^2}(K+1) v^2(L/2) L)^{n/2} \sup|\beta| = \mathscr{O}(L^{-\infty}),
\end{aligned} \tag{A25}$$

since β has compact support. Inserting (A20) and (A25) into the fundamental inequality (A19) the proof is completed.

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[18] We are intentionally a little informal here, in order to keep the notation not to be cumbersome. A better label for $d\theta$ would be $d\theta_L^m$. The same for $d\nu$ in the following.
[19] Again a remark about the notation. A more formal symbol for the scalar product would be $\langle \cdot\,, \cdot \rangle_{L^2_{(k)}(T_L^m)}$, where $k = k(\lambda)$ is the uniquely determined $k \in [0,1/L)^m$, such that the arguments are in $L^2_{(k)}(T_L^m)$. Since the scalar products have the same structure on each $L^2_{(k)}(T_L^m)$ we will drop that subscript.
[20] Here normalized means $\omega^m_{\beta,L}(1) = 1$.
[21] Notice that we are using 2β instead of β in the remainder.
[22] We are not granted, in principle, all the equivalent ergodicity and mixing properties recalled in that reference, since we have not proved asymptotic commutativity.
[23] Not to be confused with the inverse temperature β, a fixed parameter throughout this paper.
[24] $\mathscr{S}(\cdot)$ denotes the Schwartz class.
[25] $|\cdot|$ denotes the Lebesgue measure.
[26] This explains why we have chosen such a notation for $N^{(n)}_{L,m}$.
[27] This time $*_L$ means convolution in the q-variable over T_L^n. We warn the reader again about the possible confusion arising from the fact that $\beta(p,q)$ is defined on $\mathbb{R}^{2n}$. When in a $*_L$-convolution, it has to be considered as restricted to $[-L/2, L/2)^n$ and periodic according to the identification $[-L/2, L/2)^n \simeq T_L^n$. See again Sec. 3 of the Appendix.
[28] Remember that with $A^{(k)}$ we denote $A_{|L^2_{(k)}(T_L^m)}$ as explained in Sec. II B.
[29] This is a manifestation of the fact that all fibers $L^2_{(k)}(T_L^m)$ need to be taken into account, as mentioned in Sec. II B, Remark 1. We can convince ourselves of this also looking at the two examples of $\{f_\lambda\}$ we have explicitly written: the Fourier basis in Sec. III A and the coherent states in the appendix, Sec. 1. In both cases $(X_L^m, d\theta) = ([0,1/L)^m, dk)) \times$some measure.
[30] I thank D. Dolgopyat for this simple proof.

A mean field theory for arrays of Josephson junctions

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I present here some results on the mean field theory approach to the statistical mechanics of a D-dimensional array of Josephson junctions in the presence of a magnetic field. The mean field theory equations are obtained by computing the thermodynamical properties. In the high temperature region in the limit $D\to\infty$, where the problem is simplified, this limit defines the mean field approximation. Close to the transition point the system behaves very similar to a particular form of spin glasses, i.e., to gauge glasses. We have noticed that in this limit the evaluation of the coefficients of the high temperature expansion may be mapped onto the computation of some matrix elements for the q-deformed harmonic oscillator. The same arguments can be used to predict the thermodynamical properties in the mean field limit. These results can be extended to the low temperature phase using a conjecture on the equivalence of some system without disorder with appropriate random systems.
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I. INTRODUCTION

In this article I am interested to study the statistical mechanics of arrays of Josephson junctions in D-dimensions in the limit where $D\to\infty$. Here I will show how to obtain the results for the thermodynamics in the framework of the mean field approximation. In order to obtain a consistent mean field theory approach I will show how to perform the limit of infinite dimension.

The main motivation for this enterprise would be to have a starting point which could be used as a starting point to predict the behavior of the system in more realistic situations. Here I will report mainly the results of Refs. 1 and 2, which are an extension to these systems of previous results obtained in Ref. 3.

The model has been extensively studied in two dimensions, especially in the low temperature region.[4,5] It is possible that something has been done to study the three-dimensional extension of the model, but no results are known in very high dimensions.

The article is organized as follows. After this introduction I will describe in detail the model. In Sec. III will describe the computation of the high temperature expansion in the mean field limit for the Gaussian model. In Sec. IV I will show how to extend these results to real spins. In Sec. V I will present the general conjecture which allows us to extend these results to the lower temperature region. In Sec. VI I will discuss the correctness of this conjecture on the equivalence of some system without disorder with appropriate random systems. In Sec. VI I will show how to apply the general conjecture to this case. In Sec. VII I will present a comparison with the numerical simulations.

II. THE MODEL

The model we consider is described by the Hamiltonian:

$$H=-c(D)\sum_{j,k}\ \overline{\phi_j}U_{j,k}\phi_k+\text{h.c.} \tag{1}$$

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Here $c(D)\equiv(2D)^{-1}$ is a normalization constant, which will be useful later to rescale the Hamiltonian in order to obtain a nontrivial limit when D goes to infinity. The spins ϕ_j are defined on a D-dimensional hypercubic lattice.

We will consider three possibilities:

• The spins ϕ_j are constrained to be of modulus one.

• The spins ϕ_j have modulus one in the average at $\beta=0$: in this limit they have a Gaussian distribution.

• The spins satisfy the constraint $\Sigma_i\,|\phi_i|^2=N$. This is the spherical model which is intermediate among the two previous models.[6]

In the limit where the dimension D goes to infinity the properties of the first model and of the third model can be obtained from that of the Gaussian model. We will concentrate our attention on the Gaussian case and we will later study the other cases.

The couplings U are nonzero only for nearest neighbor sites. They are complex numbers of modulus one and they satisfy the relation

$$U_{k,j}=\overline{U_{j,k}}. \tag{2}$$

In other words the couplings U are the links variables of an $U(1)$ lattice gauge field.

We will select the couplings U to give a constant magnetic field. Many different orientations of the magnetic field can be chosen. For simplicity we restrict our computation to the case where the flux through each elementary plaquette is given by B (or $-B$) independently from the plane to which the plaquette belongs. This corresponds to constant uniform frustration on all the plaquettes. In the extreme case ($B=\pi$) we obtain a fully frustrated model, while for $B=0$ we recover the ferromagnetic case. Random point dependent B values corresponds to a particular form of spin glasses, i.e., to gauge glasses.[7–10]

More precisely we set

$$B_{\alpha,\beta}=S_{\alpha,\beta}B, \tag{3}$$

where $S_{\alpha,\beta}$ may take the values 1 or -1, $B_{\alpha,\beta}$ is the antisymmetric tensor corresponding to the magnetic field, which in the continuum limit is given by $\partial_\alpha A_\beta-\partial_\beta A_\alpha$. The ordered product of the four links of a plaquette in the α,β plane is equal to $\exp(iB_{\alpha,\beta})$.

We must now specify $S_{\alpha,\beta}$, i.e., the sign of $B_{\alpha,\beta}$. A possible choice would be to take

$$S_{\alpha,\beta}=1 \quad \text{for } \alpha>\beta, \tag{4}$$

which implies $B_{\alpha,\beta}=B$ for $\alpha>\beta$.

In two and in three dimensions this choice is equivalent to any other possible choice of the sign. In three dimensions the magnetic field is a vector and all the vectors corresponding to different choices of the sign may be obtained one from the other with a rotation. The choice of S does not influence the thermodynamics.

In more than three dimensions different choices of the matrix S are not equivalent and we must select one among all the possible ones. In this note we consider the case in which the matrix S is a generic one, i.e., the signs of B are randomly chosen. The system is translation invariant and the randomness appears in only in the relative orientation of the magnetic field with the crystal axis.

In the two-dimensional case we recover the usual description for an XY system (or equivalently an array of Josephson junctions) in constant magnetic field.

In order to compute the statistical properties of this model in the mean field approximation in the high temperature region we must find the spectral properties of the lattice discretized Laplacian in presence of a magnetic field. The lattice Laplacian is defined as

$$(\Delta f)_j = \sum_k U_{j,k} f_k . \tag{5}$$

The spectral properties of the lattice Laplacian in two dimension have been carefully studied. They depend on the arithmetic properties of the B/π, i.e., different results are obtained for rational and irrational B/π.[5]

The study of the lattice Laplacian in higher dimensions is much less developed. In any dimension the explicit construction of the field U shows that for rational B/π, of the form $B=2\pi r/s$, with both r and s integers, there is a gauge in which the U couplings are periodic functions of the position, with period s. In this case the spectrum of the Laplacian has the typical band form, the edges of the bands being related to the eigenvalues of a $s^D \times s^D$ matrix. When both s and D are large, a direct study of the eigenvalues is rather complex.

We will study this problem in the limit of an infinite number of dimensions. We will find some unexpected relations with the properties of the q-deformed harmonic oscillator. At the end the behavior of the model will come out very similar to that of spin glasses. The reader should notice that the properties of the model in high dimensions may be quite different from that of the two-dimensional model.

A simplified model (the *single cell* model) can be constructed if we restrict the spins to belong to a single hypercubic cell of size $L=2$ and volume $N=2^D$. The advantage of this simplified model is to allow a simpler computation of the behavior of the system in the low temperature phase. Moreover it is the only case in which numerical simulations can be done for high values of D. The difference of the two models should be small when the dimension of the space D goes to infinity. Indeed in many cases the infinite dimensions limit does not depend on the size (L) of the box, provided that $L>1$.

III. ON THE HIGH TEMPERATURE EXPANSION

A. General considerations

There are two extreme cases for the U which are very well studied for the Hamiltonian (1):

• We set

$$U_{j,k}=1. \tag{6}$$

In this way we obtain the usual ferromagnetic XY model. There is a ferromagnetic transition at $\beta=1$ in the limit $D\to\infty$, if we set $c(D)=1/2D$, i.e., $c(D)$ has to be equal to the inverse of the coordination number of the hypercubic lattice.

• We set

$$U_{j,k}=\exp(i r_{j,k}), \tag{7}$$

where r are random numbers belonging to the interval $0-2\pi$, such that the symmetry condition Eq. (2) is satisfied.

In this way be obtain a spin glass model of the XY type, which is called a gauge glass. The transition temperature is $\beta=1$ in the limit $D\to\infty$, if we set $c(D)=(2D)^{-1/2}$, i.e., $c(D)$ is equal to the inverse of the square root of the coordination number.

The model we study is intermediate among the previous two problems. In order to define it properly, it is convenient to introduce the so-called Wilson loop. Let us consider a closed oriented circuit (C) on the lattice, which goes from the point j to the same point j and let us define $W(C)$ as the product of the U's along the circuit. The Wilson loop $W(C)$ is a gauge invariant. The knowledge of $W(C)$ for any C gives all gauge invariant information concerning the gauge field.

In the continuum limit we have

$$W(C)=\exp\left(i\int_C dx^\mu\, A_\mu(x)\right)=\exp(i\Phi(C)), \tag{8}$$

where $\Phi(C)$ is the magnetic flux entangled within C.

In 2 dimensions in presence of a constant magnetic field the Wilson loop is given by

$$W(C)=\exp(iBS(C)). \tag{9}$$

where $S(C)$ is the signed area of the loop C.

In D dimensions there are $D(D-1)/2$ planes oriented in the directions of the lattice. The choice of the magnetic field we study here is

$$W(C)=\exp(i\Phi(C)),$$

$$\Phi(C)=\sum_{\nu,\mu=\nu<\mu} S_{\nu,\mu}(C)B_{\nu,\mu}, \tag{10}$$

where the indices ν and μ denote one of the D possible different directions and $S_{\nu,\mu}$ is the signed area of the projection of the curve C on the ν, μ plane.

As a consequence of gauge invariance there are infinite many choices of the U which correspond to these Wilson loops. All these choice are physically equivalent. In two dimensions we could set

$$U_1(j)=1, \quad U_2(j)=\exp(iBj_1),$$

where j_ν is the νth component of the vector j and we have introduced the short-hand notation

$$U_\nu(j)=U(j,j+n_\nu), \tag{11}$$

n_ν being the unit vector in the ν direction.

This construction can be generalized to the D-dimensional case. For example in 4 dimensions one obtains

$$U_1(j)=1, \quad U_2(j)=\exp(iB_{2,1}j_1),$$

$$U_3(j)=\exp(i(B_{3,1}j_1+B_{3,2}j_2)), \quad U_4(j)=\exp(i(B_{4,1}j_1+B_{4,2}j_2+B_{4,3}j_3)). \tag{12}$$

Our main task will be the study of the associated Gaussian model, where the Hamiltonian is given

$$H=-c(D)\sum_{j,k}\ \overline{\phi_j}U_{j,k}\phi_k+\text{h.c.}-1/2\sum_k\ |\phi_k|^2. \tag{13}$$

The solution of this associated Gaussian model is a crucial step in the computation of the properties of the high temperature expansion.

B. The high temperature expansion for the Gaussian model

In the case of the Gaussian model the free-energy density can be written as

$$\beta F(\beta)=\sum_C\ W(C)(\beta c(D))^{L/(C)}/L(C), \tag{14}$$

where the sum is done over all the closed lattice circuits with given starting point; $L(C)$ is the length of the circuit.[10]

In a model (like the present one) where gauge invariant quantities are translational invariant, we can chose the origin (and the end) of the circuit at an arbitrary point of the lattice. In other cases, like spin glasses, we must average over all the possible starting points.[11,12]

The previous formula can also be written as

$$\beta F(\beta)=\mathrm{tr}\,\ln(1+c(D)\beta\Delta)=\sum_n \frac{(\beta c(D))^n}{n}\mathcal{N}(n)\langle W(C)\rangle_n, \tag{15}$$

where by $\langle W(C)\rangle_n$ we denote the average over all the circuits of length n and by $\mathcal{N}(n)$ the number of (rooted) closed circuits.

Differentiating the previous formulas we obtain a similar result for the internal energy density:

$$2\beta c(D)U(\beta)=\sum_n (\beta c(D))^n \mathcal{N}(n)\langle W(C)\rangle_n. \tag{16}$$

Here the factor $1/n$ has disappeared. It is easy to show that the coefficients of the high temperature expansions remain finite when $D\to\infty$ if $C(D)=(2D)^{-1}$. From now on we will follow this choice.

C. The results for gauge glasses

In this case we will compute the spectrum of the random Laplacian. This can be done in the infinite dimensions limit since we recover the old problem of computing the spectrum of a random matrix, which is given by a semicircle law.

In this case the U's have zero average and are random elements of the $U(1)$ group. After the average over all the possible starting points. $W(C)$ gets contributions only from those circuits for which for any step going from i to k there is a step going from k to i. In other words we must sum only over *backtracking* circuits.

Let us count the number of these circuits in infinite dimensions. We must to compute

$$G_{2n}=\lim_{D\to\infty}(2D)^{-n}\mathcal{N}(2n)\langle W\rangle_{2n}. \tag{17}$$

The computation of G_n can be thus cast under a graphical form. For each given word, we put its $2n$ letters (two by two equal), on a circle starting from a given point, in the same order of the letters of the corresponding word. We connect those points which have an identical letter by a line and we count the number of intersections of the lines. This number is topological invariant and it does not depend on the point where the letters have been put on the circle, but only on their order.

We can associate to each word the number of intersections. Let us call $I_n(m)$ the number of words which have m intersections ($m\leqslant n(n-1)/2$). It is easy to check that

$$I_n(0)=G_n. \tag{18}$$

Indeed only in the case in which the resulting diagram is planar, the diagram may be reduced to zero by removing consecutively equal letters.

The combinatorial problem of computing $I_n(0)$ has been solved[13] in the past. After a short computation one finds

$$I_n(0)=4^n\frac{\Gamma(n+1/2)}{\Gamma(1/2)\Gamma(n+2)}. \tag{19}$$

We finally find that

$$1+\beta U(\beta)=\sum_n (4\beta^2)^n \frac{\Gamma(n+1/2)}{\Gamma(1/2)\Gamma(n+2)}=\frac{2}{\pi}\int_{-2}^{2} d\lambda \frac{(1-\lambda^2/4)^{1/2}}{(1+\beta\lambda)}. \tag{20}$$

There is a transition at $\beta=1/2$, which is characterized by a singularity of the specific heat of the form $(\beta_c-\beta)^{-1/2}$. In other words the critical exponent α is equal to 1/2.

Equation (20) gives the result for spin glasses in the Gaussian approximation. Starting from it one can obtain the more familiar results for the Ising spin glass or for the spherical spin glass.

D. Josephson junctions in magnetic field

In this case we need at first to compute the function

$$G_n(B)=\lim_{D\to\infty}(2D)^{-n}\mathcal{N}(2n)\langle W\rangle_n. \tag{21}$$

We will follow the strategy of first dividing the circuits into classes corresponding to different words of $2n$ letters (as in the previous case) and to evaluate the contribution of each class.

Let us start by computing $G_2(B)$ (it is trivial that $G_1(B)=1$). The backtracking circuits which correspond to the *planar* diagrams, (the corresponding words are $aabb$ and $abba$) give a contribution 1 each. More generally we can define the area of a circuit as the minimal area of a surface of lattice plaquettes which have that circuit as boundary. Backtracking circuits can be characterized as area zero circuits.

We finally find

$$G_4(B)=2+q, \tag{22}$$

where

$$q=\cos(B). \tag{23}$$

Generally speaking each different word of length $2n$ is associated to $(2D)^n$ circuits having the same area. The signed area of these circuits having the same area (A) is different. In a large number of dimensions (in the generic case where all the independent steps are done in different directions) the projected signed areas $S_{\mu,\nu}$ take only the values 0 or ± 1 and

$$\sum |S_{\mu,\nu}|=A. \tag{24}$$

If we average over all the possible orientations of the lattice the contribution coming from the circuits having the same word, we find that the average value of $\langle W(C)\rangle$ depends only on A and it is given by

$$\langle W(C)\rangle_A=\left(\frac{\exp(iB)+\exp(-iB)}{2}\right)^A=q^A. \tag{25}$$

We finally find that

$$G_n(B)=\sum_w q^{A(w)}, \tag{26}$$

where the sum is taken over all words of $2n$ letters and $A(w)$ is the area associated to each of these words.

It is possible to prove that the area of a of the circuit is exactly equal to the number of intersections of the lines connecting equal letters in the corresponding diagram. In this way we

have transformed the problem of computing the high temperature expansion into a combinatorial problem, although not very easy, which generalize the computation of planar diagrams. The solution of this problem will be presented in the next section.

E. The q-deformed harmonic oscillator plays a role

We have reduced the problem of evaluating the high temperature expansion of the Gaussian model in the presence of a magnetic field to the computation of the number of words of $2n$ letters, two by two equal, such that the number of intersections in the corresponding diagram is equal to a given number.

A detailed recursive combinatorial analysis show that

$$G_n(B)=\sum_w q^{A(w)}=\langle 0|X^{2n}|0\rangle, \tag{27}$$

where

$$X=\mathscr{R}_q+\mathscr{L}_q, \tag{28}$$

and the operators $\mathscr{L}$ and $\mathscr{R}$ satisfy the commutation relation of a q-deformed harmonic oscillator:

$$\mathscr{L}_q\mathscr{R}_q-q.\mathscr{R}_q\mathscr{L}_q=1. \tag{29}$$

[In the case $q=1$ we have Bosonic commutation relations, for $q=1$ we have Fermionic commutation relations and for $q=\exp(i\theta)$ anyonic commutation relations. For $q=0$ we recover the so-called Kunz algebra. Some applications of the anyonic commutation relations can be found in Refs. 14 and 15 and references therein.]

Therefore $\mathscr{L}_q$ may be identified with the destruction operator and R_q with the creation operator for a q-deformed harmonic oscillator. For $q=1$ we recover the ferromagnetic case, for $q=-1$ the fully frustrated case and for $q=0$ the spin glass case.

These operators may be represented as

$$\mathscr{R}_q|m\rangle=[m]_q^{1/2}|m+1\rangle, \quad \mathscr{L}_q|m\rangle=[m-1]_1^{1/2}|m-1\rangle, \tag{30}$$

where

$$[m]_q=(1-q^{m+1})/(1-q), \tag{31}$$

and m ranges in the interval $[0-\infty]$. In the limit $q\to 1$ we obtain the usual Bosonic oscillator and we recover the usual formulas.

Intuitively Eq. (27) tells us that when we use the Wick theorem for q-deformed harmonic oscillators, we must bring together the different terms we contract and for each term we get a factor q to the power of the number of object we have to cross.

If we use this result, we finally find the quite simple formula:

$$1+\beta U(\beta)=\langle 0|\,\frac{1}{1+\beta X}\,|0\rangle_q, \tag{32}$$

which gives a remarkable connection among the high temperature behavior of the Gaussian model and the q-deformed harmonic oscillator.

In this way we have reduced the combinatorial problem of computing the high temperature expansion to an algebraic problem.

F. Near the critical point

The problem now is reduced to the computation of the spectrum of the operator X of the q-deformed harmonic oscillator. The computation is apparently nontrivial. We are however interested to the computation of the spectral density near the largest eigenvalues.

A simple case is $q=1$, where the operator X_q is not bounded and the high temperature expansion is divergent. In this case X has a continuum spectrum and the highest eigenvalues of X are concentrated in the large m region. Let us assume that this feature is valid for q inside the interval $[-1,1]$. One finds that

$$\mathscr{L}_q \sim (1-q)^{-1/2}\mathscr{L}, \quad \mathscr{R}\sim(1-q)^{-1/2}\mathscr{R}. \tag{33}$$

when the operator is applied to a state $|m\rangle$ in the region of large m. ($\mathscr{L}$ and $\mathscr{R}$ are the two shift operators for $q=0$ which are used in the planar case.)

The difference among $\mathscr{L}_q$ and $(1-q)^{-1/2}\mathscr{L}$ can be seen only when the two operators act on a state of low m. It is very reasonable to assume that the spectral radius and the spectral density near the maximum eigenvalues is the same in the two case. We have verified numerically that this conjecture is consistent (at least for q not too close to 1) by estimating the spectral density of X_q in subspaces of various size ($m<M$, with M up to 300).

We find therefore that the critical temperature is given by

$$\beta_c=(1-q)^{1/2}/2, \tag{34}$$

which is the inverse of the spectral value of X, i.e.,

$$|X|^2=4/(1-q). \tag{35}$$

The behavior of the spectral density near the edge is the same as for the random matrix model, i.e., in spin glass. In this way we find the same critical exponents as in spin glasses in the Gaussian approximation.

A possible physical interpretation is the following. In computing the internal energy one has to sum over all the closed circuits. Circuits with large physical area average to zero and only fattened backtracking circuits survive. The situation is very similar to spin glasses, where only backtracking circuits contribute, the only effect being a renormalization of the temperature.

IV. THE HIGH TEMPERATURE EXPANSION

We have explained that we will construct the model based on the random couplings $\hat{U}$ by requiring that the high T expansion is the same than in the original model with complex frustration (and no disorder). Let us remark that both these models, the random one and the deterministic one, are *regular*, i.e., there are no couplings of $O(1)$ when $D\to\infty$. In other words all the U couplings and the $\hat{U}$ ones, after being multiplied times the appropriate $c(D)$ factor, go to zero in this limit. Under this condition the high temperature expansion for the XY model is equal to the one of the spherical model. One can verify this statement by checking that in the two cases (i.e., for the spherical for the XY model) the same diagrams survive in the $D\to\infty$ limit. This condition guarantees the absence of couplings of $O(1)$ which could break the equivalence.

Thanks to this result we will be able to start from computing the high T expansion of the spherical model, in order to work out results valid for the XY model. That will make our task far easier.

We denote the spectral density of the Laplacian operator by $\rho_\Delta(\lambda)$, and we express the trace of its nth moment as

$$2^{-D}\ \mathrm{Tr}(\Delta^n)=\int d\lambda\ \rho_\Delta(\lambda)\lambda^n. \tag{36}$$

Here the trace is taken over a space of dimensionality 2^D, and the normalizing factor 2^{-D} is such that the spectral density of the identity operator $\rho_1(\lambda)$ is $\delta(\lambda-1)$.

We start by remarking that the internal energy density of the Gaussian model is given in terms of $\rho_\Delta(\lambda)$ by

$$E_G=\int d\lambda\ \rho_\Delta(\lambda)\ \frac{\lambda}{1-\beta\lambda}. \tag{37}$$

By using the expression of the Hamiltonian which includes the spherical constraint, we find

$$E_S=\int d\lambda\ \rho_\Delta(\lambda)\ \frac{\lambda}{\mu(\beta)-\beta\lambda}, \tag{38}$$

where μ is a function of β. It is fixed by the condition

$$\int\ d\lambda\ \rho_\Delta(\lambda)\ \frac{1}{\mu(\beta)-\beta\lambda}=1, \tag{39}$$

which tells that $\langle\Sigma_i|\sigma_i|^2\rangle=N$, i.e., that the σ variables satisfy the spherical constraint.

Equations (38) and (39) can be written in a more compact form as

$$\mu(\beta)=R\left(\frac{\beta}{\mu(\beta)}\right), \tag{40}$$

$$E(\beta)=\frac{\mu-1}{\beta}, \tag{41}$$

where the function R is given by

$$R(z)=\int d\lambda\ \rho_\Delta(\lambda)\ \frac{1}{1-z\lambda}. \tag{42}$$

One uses (40) to determine μ, and inserting it in (41) one determines the internal energy density of the system.

The critical temperature β_c^{-1} is fixed by the condition that Eq. (40) does not admit a solution for $\beta>\beta_c$, i.e., is such that

$$z_c R(z_c)=\beta_c, \tag{43}$$

where z_c is the inverse of the largest eigenvalue of Δ.

In the limit $D\to\infty$, the function $R(z)$ has been defined in the previous section:

$$R(z)=\langle 0|\ \frac{1}{1-zX}\ |0\rangle. \tag{44}$$

It can be shown[10] that the function, $R(z)$ has a singularity of the form

$$R(z)=A(z_c^2-z^2)^{1/2}, \tag{45}$$

where

$$z_c=\sqrt{1-q}/2. \tag{46}$$

The critical behavior does not depend on q.

The critical temperature can be found from Eq. (43). A simple computation shows that the specific heat remains finite at the critical temperature.

V. OUR STRATEGY AND THE DEFINITION OF THE RANDOM MODEL

We will use here a strategy we have introduced in Refs. 1 and 2. We start with a model which does not contain quenched disorder, but that is complex enough to make us suspicious of the possible presence of a spin glass like phase for temperatures T low enough. We look for a model which contains quenched disorder, and that is similar enough to the original model to have potentially the same behavior (even in the low T phase, if we are very ambitious). Replica theory allows us to solve the random model, and to try and get information about the deterministic model. Reference 2 discusses successful examples of the use of this strategy.

Here we will adopt the same approach. We will introduce a model containing random quenched disorder. In this new model the new $\hat{U}$ couplings will be chosen at random [as opposed to the original U couplings which are determined by the deterministic equation (12) such to give us the needed complex frustration]. The random values of the $\hat{U}$ will be selected, following Ref. 2, such that the new free energy will have the same high temperature expansion than the original model. We will have a model where the couplings $\hat{U}$ will be distributed according to a probability distribution, determined from the request of finding the same high T expansion than in the original frustrated model. The original model will be this way by construction, a given (hopefully typical) realization of the coupling constants constructed according to this probability distribution.

Because of these remarks, and of our constructive procedure, the deterministic model and the random one coincide in the high T phase. We hope to learn as much as possible about the low T phase, and that the two models are also in this phase very similar.

We will have to start by computing the high temperature expansion for our model with complex frustration. Knowing that we will use a reverse engineering procedure in order to find out the probability distribution of random couplings $\hat{U}$ that have the same high temperature expansion. Finally we will use the replica theory to compute the low temperature behavior of the random model. For sake of simplicity we will present here the computation done under the hypothesis of no replica symmetry breaking. We will compare these analytic results to numerical simulations of the frustrated model.

We will consider a model containing quenched disorder that has the same form of the original model with complex deterministic frustration. In the random model the couplings $\hat{U}$ will be taken randomly among all matrices having the same spectral distribution of the deterministic model. More precisely for finite D we extract a set of 2^D values of the eigenvalues λ, such that

$$2^{-D} \sum_{j=1,2^D} \lambda_j^n \simeq \int d\lambda \ \rho_\Delta(\lambda)\lambda^n, \tag{47}$$

where ρ_Δ is the spectral density of the Laplacian operator, and will be discussed in more detail in next section. We finally set

$$\hat{U}_{i,k} = \sum_{j=1,2^D} V^*_{i,j}\lambda_j V_{j,k}, \tag{48}$$

where V is a random unitary matrix i a 2^D dimensional space.

VI. THE LOW TEMPERATURE REGION

In Sec. V we have discussed the high T region of the deterministic model with complex frustration. Monte Carlo has been done in this region and the data reproduce well (as expected) the

series obtained by computing the Green functions of the q-deformed harmonic oscillator. We also know that in the high T phase the model with quenched disorder coincides by construction with the deterministic model, but we will see that better in the following.

In order to get information about the low T phase we have to use the random model, which we have defined in Eqs. (47) and (48). We will use replica theory to solve it both in the high T phase (where we will find again the same high T series) and in the low T phase. We will try to understand how much the replica formulation of the system is connected to the Monte Carlo data which we will get directly from the deterministic model with complex frustration. This task will be achieved for the *single cell* model, where the computations are much simpler. It is quite possible that similar results can be obtained for the infinite volume model.

Let us solve the random model by using the techniques introduced in Ref. 2. The computation follows quite closely the one of Ref. 2, and we will give here only the main details. One introduces n replicas, where n has to be sent to zero at the end of the computation. The n-dependent free energy is given by

$$f^{(n)}(\beta)\equiv -\lim_{N\to\infty}\frac{1}{\beta N}\frac{\ln\overline{Z_U^n}}{n}, \tag{49}$$

where the bar denotes the average over the random couplings and the replicated partition function Z_U^n depends over the noise and can be written as

$$Z_U^n\equiv\int [d\sigma]\exp\left(-\beta\sum_{a=1}^{n} H_U^a\right). \tag{50}$$

The integration over the unitary group (i.e., the matrix V) can be done explicitly. After some algebra one finds that one has to evaluate the stationary points of the following free energy:

$$A[Q,\Lambda]=-\mathrm{Tr}\ G(\beta Q)+\mathrm{Tr}(\Lambda Q)-F(\Lambda), \tag{51}$$

where Q and Λ are $n\times n$ matrices, the function G is related to the one defined in Eq. (41) by

$$\frac{dG}{dz}\equiv E(z), \tag{52}$$

and

$$F(\Lambda)\equiv\ln\int d[\sigma]\exp\left(\sum_{a,b}\Lambda_{a,b}\sigma^a\sigma^b\right). \tag{53}$$

In the high temperature phase the off-diagonal terms of the two matrices Q and Λ are zero. If we set

$$Q_{a,b}=\delta_{a,b}q,$$

$$\Lambda_{a,b}=\delta_{a,b}\lambda, \tag{54}$$

we find that the stationary equations imply that

$$q=1 \quad \text{and} \quad \lambda=E(\beta). \tag{55}$$

We finally find that in the high temperature phase

$$\frac{\partial F}{\partial \beta} = E(\beta), \tag{56}$$

where $E(\beta)$ is the function defined in (52). In this way we have derived again the equivalence of the model with quenched disorder and the deterministic model with complex frustration in the high temperature phase.

In the low temperature region the off-diagonal terms of the two matrices are nonzero. If we assume that replica symmetry is unbroken, we have that the off-diagonal terms are given by

$$Q_{a,b} = q, \quad \Lambda_{a,b} = \lambda. \tag{57}$$

(We set $Q_{a,a}=1$. The value we choose for $\Lambda_{a,a}$ is irrelevant, and does not change the results.) In this way we find that we have to minimize the free energy

$$G(\beta(1-q)) + \beta q E(\beta(1-q)) - \lambda q + f(\lambda), \tag{58}$$

where the function f is given by

$$\ln\left(\int dh \, \exp(-h^2/2) \right) \ln\left(\int d\sigma_r \, d\sigma_i \, \delta(\sigma_r^2 + \sigma_i^2 - 1) \exp(-\lambda^{1/2} h \sigma_r) \right). \tag{59}$$

The energy turns out to be

$$E(\beta) = G'(\beta(1-q)) - \beta q (1-q) G''(\beta(1-q)). \tag{60}$$

By deriving this expression and evaluating it for $\beta=\beta_c$ we find that

$$C_V(\beta_c^+) = C_V(\beta_c^-) = 1. \tag{61}$$

The critical temperature can also be determined through the relation

$$\beta_c^2 G''(\beta_c) = 1. \tag{62}$$

One also finds that at zero temperature

$$C_V(\infty) = \tfrac{1}{2}, \tag{63}$$

in agreement with the equipartition theorem.

The equations which determine the minimum of such free energy can be solved numerically.

We will show and discuss their solution in Sec. VII, for different q values, together with the Monte Carlo results in the low T phase.

We expect the unbroken replica solution to give rather accurate values for the free energy. In the SK model the error over the correct, replica broken result is smaller than 3%, and it is likely to be even smaller in the present case. It is interesting to note that the replica symmetric solution normally gives a lower bound to the true free energy and to the true internal energy of the system. Numerical simulations show that when we compare numerical simulations of the deterministic model to the replica symmetric solution of the disordered model in the cold phase this is not always the case in our system, pointing to a non complete coincidence of the two models.

VII. COMPUTER SIMULATIONS

We will describe here the numerical simulations of the model with complex frustration, defined with the couplings of Eq. (12), and compare them with the analytic solution of the model with quenched disorder that we have discussed in Sec. III. Here we will mainly focus on the low T phase.

In Ref. 2, systems of size 2 have simulated with D going from 3 to 16, i.e., containing from 8 to 65 536 sites. In the high temperature phase everything is in reasonable agreement with the theoretical predictions.

In the low T phase we will compare the analytic solution of the random model (47) with the numerical simulation of the deterministic model. We will use the replica symmetric solution, which we believe is not too wrong. We shall see that the data are indicative of a strong similarity, but maybe not of a complete equivalence of the two models.

The agreement of Monte Carlo data for the deterministic model and replica symmetric solution of the random model is quite good also in the broken phase, for $T<T_c$. We expect that the solution with broken replica symmetry will have an energy slightly higher than the unbroken one (as we already said, in the general case the replica symmetric energy is a lower bound to the true energy of the physical system). Very small residual finite size effect and this small energy drift to the the breaking of replica symmetry should explain the small discrepancy between the numerical data and the analytic curve. So in the case of the $q=0$ model things seem to go smoothly.

When moving on the side of negative q values things do not change much, and if there is a discrepancy it is very small. This is completely in agreement with the discussion of the behavior of the coefficients of the high T expansion of Sec. VI.

In conclusion, it seems that for $q<0$ and even for small q positive values the replica theory describes the deterministic model with very high accuracy. On the contrary for $q<0$ not so small there is a clear, even if quite small discrepancy between the two models. It is quite possible, although it looks strange, that the discrepancy is due to finite volume effects and to a very slow convergence of the $1/D$ expansion. The computation of the $1/D$ corrections in the low temperature phase would be quite useful to resolve this dilemma.

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Spectral properties of a charged particle in antidot array: A limiting case of quantum billiard

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A model of the periodic array of quantum antidots in the presence of a uniform magnetic field is suggested. The model can be conceived as a periodic lattice of resonators (curvilinear triangles) connected through ''infinitely small'' openings at the vertices of the triangles. The model Hamiltonian is obtained by means of operator extension theory in indefinite metric spaces. In the case of rational magnetic flux through an elementary cell of the lattice, the dispersion equation is found in an explicit form with the help of harmonic analysis on the magnetic translation group. It is proved, at least in the case of integer flux, that the spectrum of the model Hamiltonian consists of three parts: (1) Landau levels (they correspond to the classical orbits lying between antidots); (2) extended states that correspond to the classical propagation trajectories; and (3) bound states satisfying the dispersion equation; they correspond to the classical chaotic orbits rotating around single antidots. Among other things, methods of finding the Green's function for some planar domains with curvilinear boundaries are derived. © *1996 American Institute of Physics.* [S0022-2488(96)01410-7]

I. INTRODUCTION

Beginning with the works of Azbel,[1] Hofstadter,[2] and Wannier,[3] unusual spectral properties of two-dimensional periodic systems in a quantizing magnetic field **B** attract ever increasing attention. The most interesting properties of these systems are connected with the presence of two natural geometric scales, namely, the magnetic length and the size of the unit cell of the period lattice. The commensurability (or incommensurability) of the scales leads to such a pecularity of the systems as the transition from the band structure of the spectrum to the fractal one (Hofstadter butterfly).[4,5] This pecularity is important in the theory of the quantum Hall effect (see Refs. 6, 7, and references therein). Nevertheless, because the number η of flux quanta through a unit cell of a crystal lattice is very small for the experimentally accessible values of $B(\eta \sim 10^{-3})$, no energy spectrum of the Hofstadter type is observable in usual quantum Hall systems. Advances in micropatterning of two-dimensional electron systems at semiconductor interfaces have rendered it possible to fabricate a so-called periodic dot array, which is obtained by a laterally periodic modulation of the confining potential of electrons in the system. In the periodic dot array the above-mentioned geometric scales are comparable, and, in consequence, an experimental observation of the Hofstadter butterfly has been made possible.[8] Curiously, Hofstadter himself wrote in 1979 that he ''would be the most surprized person in the world if the butterfly came out of any experiment.'' [9]

A reversed structure to a dot array, i.e., periodic ''antidot'' array is obtained by inducing an periodic array of voids in a two-dimensional electron gas.[10,11] The magnetotransport experiments

with the antidot array show that such a structure can be considered the solide-state realization of a Sinai billiard.[12–16] The experiments unveiled a series of low-B resistance peaks at commensurate B, for which the classical cyclotron orbit encompasses a particular number of antidots. A detailed semiclassical analysis of the transport anomalies in the antidot lattice leads to the conclusion that they stem from electrons trapped on classically chaotic trajectories for commensurate B.[17] The presence of such trajectories should lead to the appearance of bound states in the quantum-mechanical energy spectrum of the system. A numerical investigation of the propagator of a charged particle in a periodic antidot array has been performed by Stratford and Beeby,[18] their results suggest that bound states appear at the condition of the commensurability of the cell size and the magnetic length.

Up to the present there is no complete quantum-mechanical theory of billiard phenomena in the antidot array. In this connection various approximate models are of special interest. The aim of the paper is to construct and study an explicitly solvable model of a periodic antidot array by means of operator extension theory.

Let us describe the basic idea of the construction, introducing simultaneously some notations. Let Γ be a two-dimensional crystal lattice, i.e., $\Gamma=K+\Lambda\equiv\{\kappa+\lambda:\kappa\in K,\ \lambda\in\Lambda\}$, where Λ is a Bravais lattice (a discrete additive subgroup of $\mathbf{R}^2$ with two generators $\mathbf{a}_1$, $\mathbf{a}_2$), and K is a finite subset of the elementary cell $C_\Lambda=\{t_1\mathbf{a}_1+t_2\mathbf{a}_2\colon\ 0\leqslant t_1,\ t_2<1\}$ of Λ; we assume without loss of generality that $0\in K$. We can represent the collection of the voids in the array in the form $V+\Gamma$, where V is a bounded domain in $\mathbf{R}^2$ with the picewise smooth boundary such that $0\in V$ and $(V+\gamma)\cap(V+\gamma')=\varnothing$ if $\gamma,\ \gamma'\in\Gamma,\ \gamma\neq\gamma'$. A realistic quantum-mechanical Hamiltonian of the system should be the operator

$$\hat{H}=(-i\boldsymbol{\nabla}-\mathbf{A})^2, \tag{1}$$

in the domain $G=\mathbf{R}^2\backslash(V+\Gamma)$ with the Dirichlet boundary conditions on ∂G; here $\mathbf{A}$ is the vector potential of the magnetic field. In spite of seeming simplicity, the model with the Hamiltonian $\hat{H}$ is far from being explicitly soluble. It is reasonable in this connection to consider two limiting cases.

(1) *V is small enough.*

In the limit of ''infinitesimal'' V we get the model of periodic point interactions.[19,20] It is known that the energy spectrum of the model contains bound states (namely, unbroadened Landau levels) if η is greater than the number of elements in K. This fact was discovered in numerical experiments by Ando[21] and rigorously proved in Refs. 22 and 23; also see Ref. 24. Nevertheless, it seems likely that the point interaction model is not relevant to the problem in question. The appearance of the bound states in the spectrum of the model is connected with the number of points in K rather than with the sizes of C_Λ and V.

Now let us take up another limiting case.

(2) *V is so large that $V+\gamma$ and $V+\gamma'$ touch one another.*

We restrict our attention to the most interesting case of the honeycomb lattice Γ; in this case $|\mathbf{a}_1|=|\mathbf{a}_2|$, $\widehat{\mathbf{a}_1\mathbf{a}_2}=60°$, $K=\{0,\mathbf{b}\}$, where $\mathbf{b}=2(\mathbf{a}_1+\mathbf{a}_2)/3$ (Fig. 1). At first we suppose that V is a circle, therefore the collection of the voids in the considered array is the densest packing of equal disks (Fig. 2). Hence, $G=\Omega+\Gamma$, where Ω is a curvilinear equilateral triangle with zero angles (Fig. 3). We shall denote in the course of the paper $\Omega_\gamma=\Omega+\gamma$, hence $G=\cup_{\gamma\in\Gamma}\Omega_\gamma$. Obviously, the state space $\mathscr{H}^0$ is isomorphic to the direct sum $\mathscr{H}^0=\Sigma_{\gamma\in\Gamma}\oplus\mathscr{H}^0_\gamma$, where $\mathscr{H}^0_\gamma=L^2(\Omega_\gamma)$, and the Hamiltonian H^0 of the model has the form $H^0=\Sigma_{\gamma\in\Gamma}\oplus H^0_\gamma$, where H^0_γ is defined by the differential expression (1) in the domain Ω_γ and the Dirichlet boundary conditions on $\partial\Omega_\gamma$. The obtained operator corresponds to the absence of any charge transport between domains Ω_γ. To get a nontrivial model Hamiltonian we employ the ''restriction-extension'' procedure.[19,25] Notice that this procedure found use in constructing and studying of explicitly soluble models of crystals[26] and quantum dot arrays.[27,28] Intuitively, we puncture the boundary $\partial\Omega_\gamma$ of every curvilinear tri-

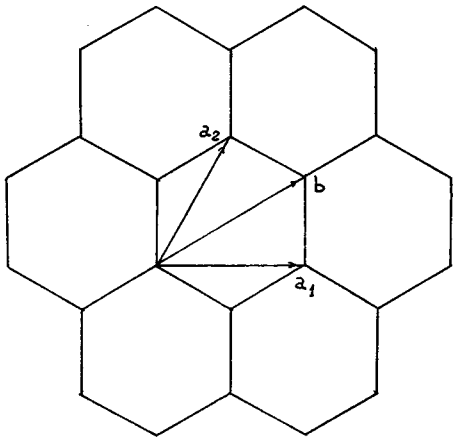

FIG. 1. Honeycomb lattice; $\mathbf{a}_1$, $\mathbf{a}_2$ are basic vectors, $b=2(\mathbf{a}_1+\mathbf{a}_2)/3$.

angle Ω_γ in each vertex to connect the domains Ω_γ with each other.[29,30] From the mathematical point of view we restrict the operator H^0 to the set of smooth functions that vanish near the vertices of the triangles Ω_γ. Nontrivial (i.e., different from H^0) self-adjoint extensions of such a restriction S_0 can be considered as a model Hamiltonian H of the antidot array. Nevertheless, the operator S_0 is essentially self-adjoint, therefore it has no nontrivial self-adjoint extensions in the space $L^2(G)$. Beginning with the Berezin[31] paper on the Lee model of the quantum field theory self-adjoint extensions in Pontryagin or Krein spaces containing $L^2(G)$ are common. A general mathematical formalism for such extensions is elaborated by Shondin,[32] in an easy-to-use form; the formalism is explained in Ref. 33. In Refs. 34 and 35 this method has been used to solve some problems that are similar to those of the present paper. In the cited papers the method of operator extensions in indefinite inner product spaces is developed for Pontryagin spaces only, but in our

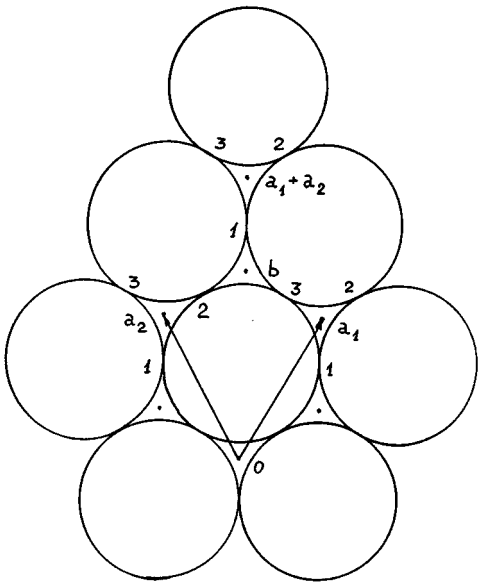

FIG. 2. Periodic system of curvilinear triangles. The centers $\mathbf{0}$, $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{b}$, $\mathbf{a}_1+\mathbf{a}_2$ of the triangles are marked.

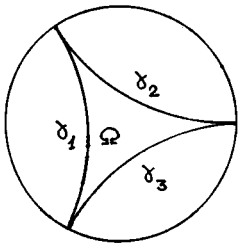

FIG. 3. Curvilinear triangle Ω.

situation we can use this method mutatis mutandis for Krein spaces also.[36] We do not consider the physical status of the state spaces with an indefinite metric, but, seemingly, some comments are necessary. Dirac[37] and Pauli[38] are the first to use the indefinite inner product spaces in some problems of quantum mechanics; also see Ref. 39 and references therein. In Refs. 32, 33, and 40, the physical meaning of the state spaces with indefinite metric and self-adjoint operators in them are discussed in the context of point perturbations.

The paper is organized as follows. To have an explicitly soluble model, we need a description of the Green's function for the domain Ω. Such a description is given in the first part of Sec. II for the case of a curvilinear triangle with zero angles and for the Hamiltonian with zero magnetic field. The description is represented in a convenient form for numerical analysis; such an analysis of our periodic model will be explained elsewhere. Two last parts of Sec. III are devoted to an auxiliary (with relation to our main goal) problem, namely, we show how ''to switch on'' the tunneling between two curvilinear triangles. In this part we offer a method to construct the indefinite inner product space in question. The results of Sec. II are of independent interest also; they describe a model of two coupled quantum dots of a complicated form and generalize some results of Ref. 35.

In Sec. III we present the above-mentioned quantum-mechanical lattice model of a periodic antidot array. The Hamiltonian of the model is invariant with respect to the magnetic translation group.[41] In the case of the rational flux, as it is called, we use the harmonic analysis on the magnetic translation group to represent the model Hamiltonian as a direct integral of finite-dimensional operators. Hence we reduce the spectral problem for the Hamiltonian to an eigenvalue problem of linear algebra, and what is more, in the case of rational flux we obtain the dispersion equation in an explicit form. The formalism used in Sec. III is a generalization of that in Ref. 23 and employs an appropriate modification of the Krein resolvent formula.[42] In conclusion, we prove a main result of the paper, namely, the existence of bound states in the model spectrum that are different from levels of the unperturbed operator H^0. Such states may be considered as quantum-mechanical counterparts of above-mentioned chaotic trajectories. As the final result, we obtain that the spectrum of the model Hamiltonian H_A in the presence of a strong magnetic field consists of three parts: (1) Landau levels that correspond to the classical orbits lying between antidots; (2) extended states that are solutions of the dispersion equation (45); they correspond to the classical propagation trajectories; and (3) bound states that are solutions of Eq. (45) also and correspond to the classical chaotic orbits rotating around a single antidot. The described structure of the spectrum coinsides with that obtained by numerical calculation.[43]

It should be especially stressed that the results of Sec. III do not depend on a particular form of the Green's function of the unperturbed operator H^0, therefore the zero-field restriction of Sec. II does not obstruct the proof of our main result.

II. THE MODEL OF TWO COUPLED TRIANGLES

In this section we show how to find the Green's function of the Laplace–Dirichlet operator in a curvilinear equilateral triangle with zero angles. Then we construct an explicitly soluble model

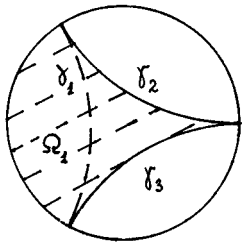

FIG. 4. The auxiliary domain $\hat{\Omega}_1$; γ_i $(i=1,2,3)$ are arcs of a circle (the boundary of the curvilinear triangle Ω).

of two ''quantum dots'' coupled with each other by a small opening; the dots are two curvilinear triangles having only one common point, which is a common vertex of the triangles. The role of such a model in the context of the model of an antidot array is described in the Introduction.

A. Green's function for a curvilinear triangle

Here we consider the most complicated case of a curvilinear triangle with zero angles. At first, we describe the Green's function for the Dirichlet problem in the auxiliary domain $\hat{\Omega}_1$ shown in Fig. 4. Let us map this domain onto a semistrip $\tilde{\Omega}_1$ by a linear-fractional transformation $z=f(\zeta)$. Then the equation for the desired Green's function G_1,

$$-\Delta_z G_1(z,z';\lambda)=\delta(z-z')+\lambda G_1(z,z';\lambda),$$

takes the following form:

$$-\Delta_\zeta \tilde{G}_1(\zeta,\zeta';\lambda)=|f(\zeta)|^{-2}\delta(\zeta-\zeta')+\lambda|f(\zeta)|^{-2}\tilde{G}_1(\zeta,\zeta';\lambda).$$

For the case $\lambda=0$,

$$\tilde{G}_1(\zeta,\zeta';0)=G_{\text{strip}}(\zeta,\zeta';0)-G_{\text{strip}}(\zeta,\zeta'';0),$$

where G_{strip} is the Green's function for the strip, ζ'' is the mirror image of the point ζ' with respect to the end of the semistrip $\tilde{\Omega}_1$.

In the case of nonzero λ we obtain the Lippmann–Shwinger equation for the function $\tilde{G}_1(\zeta,\zeta';\lambda)$:

$$\tilde{G}_1(\zeta,\zeta';\lambda)=\tilde{G}_1(\zeta,\zeta';0)+\lambda|f(\zeta)|^{-2}\int_{\tilde{\Omega}_1}|f(\xi)|^{-2}\tilde{G}_1(\xi,\zeta';0)d\xi.$$

It is essentially a one-dimensional integral equation that can be solved by ordinary methods. In a similar way we can describe the Green's functions for the domains $\tilde{\Omega}_2$ and $\tilde{\Omega}_3$ obtained by the cyclic permutation of γ_1, γ_2, and γ_3. The corresponding Green's functions we denote as G_2 and G_3.

Now we consider the Green's function for the curvilinear triangle Ω (Fig. 2). Let G_0 be the Green's function for the circumscribed circle, v_i $(i=1,2,3)$ be some functions defined on γ_i (densities). We seek the Green's function for Ω in the form

$$G=G_0+P_1(v_2\dot{+}v_3)+P_2(v_3\dot{+}v_1)+P_3(v_1\dot{+}v_2).$$

Here P_i is an integral operator with the Poisson kernel $P_i(x,s)=\partial G_i(x,s)/\partial n_s$, and $v_i \dot{+} v_j$ is the function coinciding with v_i on γ_i and with v_j on γ_j. Bearing in mind the Dirichlet boundary condition, one comes to the following system of integral equations:

$$G|_{\gamma_1}=0=G_0|_{\gamma_1}+P_1(v_2\dot{+}v_3)|_{\gamma_1}+2v_1,$$

$$G|_{\gamma_2}=0=G_0|_{\gamma_2}+P_2(v_3\dot{+}v_1)|_{\gamma_2}+2v_2,$$

$$G|_{\gamma_3}=0=G_0|_{\gamma_3}+P_1(v_1\dot{+}v_2)|_{\gamma_3}+2v_3. \tag{2}$$

Here we take into account that

$$P_2(v_3\dot{+}v_1)|_{\gamma_1}=P_2(v_3)|_{\gamma_1}+P_2(v_1)|_{\gamma_1}=0+v_1,$$

and analogously,

$$P_i(v_j)|_{\gamma_k}=0, \quad \text{if } i,j,k, \text{ are three different indices,}$$
$$P_i(v_j)|_{\gamma_j}=v_j, \quad i\neq j,$$
$$P_i(v_j\dot{+}v_k)|_{\gamma_i}=K_{ij}v_j+K_{ik}v_k, \quad i\neq j,$$

where K_{ij} are integral operators.

Consider the problem of solvability of the system (2). If $\lambda<0$, then one has, in accordance with the maximum principle:

$$|P_i(v_j\dot{+}v_k)|_{\gamma_i}|\leqslant\max\{\|v_j\|_{C(\gamma_j)},\|v_k\|_{C(\gamma_k)}\}. \tag{3}$$

Here $C(\gamma_j)$ is the space of continuous functions on γ_j. The system (2) takes the form

$$G_0|_{\gamma_1}+2v_1+K_{12}v_2+K_{13}v_3=0,$$

$$G_0|_{\gamma_2}+2v_2+K_{23}v_3+K_{21}v_1=0, \tag{4}$$

$$G_0|_{\gamma_3}+2v_3+K_{31}v_1+K_{32}v_2=0.$$

The equations are considered in the space $\widetilde{C}=C(\gamma_1\cup\gamma_2\cup\gamma_3)$. Let K denote the matrix with the elements K_{ij}, where we put $K_{ii}=0$, and let $V=(v_1,v_2,v_3)$. Then the system (4) can be rewritten in the form

$$2^{-1}G_0+V+2^{-1}KV=0, \tag{5}$$

where, in accordance with (3), one get $\|K\|_{\widetilde{C}}\leqslant 1$. Hence it is possible to solve the system by iterations:

$$V=-2^{-1}G_0+2^{-2}KG_0-2^{-3}K^2G_0+\cdots.$$

For $\lambda>0$ the situation is more complicated because there are eigenvalues in this case. Write G_j in the form

$$G_j(\lambda)=G_j(0)+\sum_{k=0}^{n}\lambda^k(G_j(0))^{k+1}+\lambda^{n+1}(G_j(0))^{n+1}G_j(\lambda)$$

(this relation is the iterated Hilbert identity, see, for example, Popov[34]). Let n be so large that the series

$$\sum_{l=1}^{\infty} \frac{|\phi_l\rangle\langle\phi_l|}{\lambda_l^{n+1}(\lambda_l-\lambda)},$$

converges for each λ outside the spectrum of the Dirichlet problem for $\hat{\Omega}_j$. Let λ range over a bounded set. Then this set contains only a finite number of eigenvalues, e.g., $\lambda_1,...,\lambda_N$. Hence the representation of the Green's function G_j takes the form

$$G_j(\lambda)=G_j(0)+\sum_{k=0}^{n}\lambda^k(G_j(0))^{k+1}+\lambda^{n+1}\sum_{l=1}^{N}\frac{|\phi_l\rangle\langle\phi_l|}{\lambda_l^{n+1}(\lambda_l-\lambda)}+\lambda^{n+1}\sum_{l=N+1}^{\infty}\frac{|\phi_l\langle\phi_l|}{\lambda_l^{n+1}(\lambda_l-\lambda)}.$$

We obtain the similar expression for the Poisson kernel:

$$P_j(\lambda)=P_j(0)+\sum_{k=0}^{n}\lambda^k\left(\frac{\partial}{\partial n}G_j(0)\right)^{k+1}+\lambda^{n+1}\sum_{l=1}^{N}\frac{|\phi_l\rangle\langle(\partial/\partial n)\phi_l|}{\lambda_l^{n+1}(\lambda_l-\lambda)}$$
$$+\lambda^{n+1}\sum_{l=N+1}^{\infty}\frac{|\phi_l\langle(\partial/\partial n)\phi_l|}{\lambda_l^{n+1}(\lambda_l-\lambda)}.$$

Note that in this expression $P_j(0)$ is a contracting operator, the second term is smooth with respect to λ, the third term is finite dimensional, and the fourth one is small for an appropriate choice of n and N. Substituting this expression into (4), we represent the operator K in the form

$$K=K_0+K_1+K_2+K_3,$$

where the operator K_0 is a contraction, K_1 is a finite-dimensional operator, K_2 is smooth, and K_3 is an operator with a small norm. Taking into account the character of singularity of the two-dimensional Green's function, one can see that it is possible to choose $n=0$, consequently, there is no smooth term K_2 in the expression

$$K=K_0+K_1+K_3.$$

Hence the equation (5) takes the form

$$2^{-1}G_0+V+2^{-1}K_0V+2^{-1}K_1V+2^{-1}K_3V=0.$$

Since $\|2^{-1}K_0\|\leqslant 2^{-1}$, we have $\|2^{-1}K_0+2^{-1}K_3\|<1$ for an appropriate choice of N. Consequently, the operator $I+2^{-1}K_0+2^{-1}K_3$ is a reversible one. Then we have

$$V+(2I+K_0+K_3)^{-1}K_1V+(2I+K_0+K_3)^{-1}G_0=0.$$

The operator $(2I+K_0+K_3)^{-1}K_1$ is finite dimensional, hence it is reversible for λ different from eigenvalues. Thus we prove that the system (2) is solvable if λ range over a bounded set of half-line containing no eigenvalues.

B. Two coupled curvilinear triangles with nonzero angles

To explain the basic idea of this part we consider at first a planar domain Ω^{in} with the smooth boundary $\partial\Omega^{\text{in}}$. Let $\Omega^{\text{ex}}=\mathbf{R}^2\backslash\overline{\Omega^{\text{in}}}$, $x_0\in\partial\Omega^{\text{in}}$. We shall consider the operator $-\Delta=-(\Delta^{\text{in}}\oplus\Delta^{\text{ex}})$, where Δ^{in} and Δ^{ex} are the Laplace operators with the Neumann boundary conditions in domains Ω^{in} and Ω^{ex}, respectively.

Let us restrict this operator to the set of smooth functions vanishing near the point x_0, then we obtain a symmetric operator S_0 with the deficiency indices (2,2). Therefore S_0 has self-adjoint extensions that are different from $-\Delta$. Each such extension may be considered as a model of an

obstacle Ω^{in} with very small opening around the point x_0. It was shown that one can choose the parameters of the extension in such a way that its Green's function coincides with the leading term of the asymptotics of the Green's function for the obstacle with an opening of small but finite diameter, as the diameter tends to zero.[35] It means that the suggested model of an opening in the obstacle is rather realistic. Furthermore, this model is a solvable one in the following sense: if the solutions of the spectral or scattering problems in the domains Ω^{in} and Ω^{ex} without opening are known, one can obtain the corresponding solutions for the model operator in an explicit form. The described model has also another advantage: the model Green's function and the model solution of scattering problem have the same analytical properties as the corresponding ''realistic'' Green's function and the solution of a ''realistic'' scattering problem.

In a similar way we can proceed in the case of two planar domain Ω^i, $i=1,2$, with the smooth boundaries, having no common interior points but a common point x_0 of their boundaries. The situation changes radicaly in the case of Dirichlet boundary conditions because the singular solutions with the singularity at the point x_0 do not belong to the space L^2 in this case (the singularity is too strong). If Ω^i are curvilinear triangles with a common vertex x_0, some additional obstacles arise connected with singularities of boundaries at the point x_0. We overcome all this difficulties by using operator extension theory in indefinite inner product spaces (see the Introduction).

Let us consider two equal nonoverlapping curvilinear equilateral triangles Ω^1 and Ω^2 having only one common vertex x_0. We shall distinguish two cases: (i) *the angles are equal to* π/p, $p\in\mathbf{N}$; (ii) *the angles are equal to zero.*

The case of zero angles will be discussed in the final part of the section; in what follows we assume that angles are equal to π/p, $p\in\mathbf{N}$. In this case the principal singularity of the Green's function has the order r^p. To construct the nontrivial self-adjoint extensions of the operator S_0 it is necessary to extend the initial state space $L^2(\Omega^1\cup\Omega^2)$ by adding the corresponding pth multipole. More precisely, let $G_p^j(x,k) = Q_p(-\nabla_y)G_D^j(x,y;k)|_{y=x_0}$, where G_D^j is the Green's function for the Dirichlet problem in Ω^j and $Q_p(x)$ is the harmonic polynomial corresponding to the singularity. Let A_p^j be the following set of functions:

$$A_p^j=\left\{ f\in L^2(\Omega^i)\colon \int_{\Omega^j}|f(x)||x-x_0|^{-p-1}\,dx<\infty\right\}.$$

Introduce the chain of functions,

$$h^j_{-p,p}(x)=G_p^j(x,k_0),\quad h^j_{-p+2,p}(x)=(-\Delta^j-\lambda_0)^{-1}h^j_{-p,p},\ldots,$$

$$h^j_{p,p}(x)=(-\Delta^j-\lambda_0)^{-p}h^j_{-p,p}.$$

Here k_0 is a fixed imaginary number such that $\lambda_0=k_0^2$ is a regular point of the Laplace–Dirichlet operator $H_j=-\Delta^j$. Consider the set $\mathscr{H}_p^j$:

$$\mathscr{H}_p^j=\{f^j\colon f^j=f_p^j+C^j_{p,p}h^j_{p,p}+\cdots+C^j_{-p,p}h^j_{-p,p}\},$$

where $f_p^j\in A_p^j$. We define the scalar product in the space $\mathscr{H}_p^j$ in the following way:

$$(f,g)_{\mathscr{H}_p^j}=(f_p,g_p)_{L^2}+\sum_{r=-p}^{p-2}\int_{\Omega^j}f_p(x)\overline{C^j_{r,p}(g)h^j_{r,p}(x)}dx+\sum_{r=-p}^{p-2}\int_{\Omega^j}C^j_{r,p}(f)h^j_{r,p}(x)\overline{g_p(x)}dx$$
$$+\sum_{r,q=-p}^{p-2}C^j_{r,p}(f)\overline{C^j_{q,p}(g)}[h^j_{r,p},h^j_{q,p}],\tag{6}$$

where

$$[h^j_{r,p},h^j_{q,p}]=\begin{cases}\int_{\Omega^j} h^j_{r,p}(x)\overline{h^j_{q,p}(x)}dx, & \text{if the integral converges,}\\ 0, & \text{otherwise.}\end{cases} \tag{7}$$

The set $\mathscr{H}^j_p$ is imbedded as a linear set into the Pontryagin space Π_κ [$\kappa=p/2$ for even p, and $\kappa=(p+1)/2$ for odd p] by the standard way.[31,44]

Define an operator $\widetilde{S}_{p,j}$ in the following way. The domain of the operator is

$$\mathscr{D}(\widetilde{S}_{p,j})=\{f^j\in\mathscr{H}^j_p: f^j_p\in W^2_{2,\mathrm{loc}}(\Omega^j),\quad f_p=f^j_{p+1}+Ch^j_{p,p}\},$$

where f^j_{p+1} belongs to A^j_{p+1} and $(-\widetilde{S}_{p,j}-\lambda_0)f^j_{p+1}\in A^j_p$. On the set A^j_p the operator $\widetilde{S}_{p,j}$ acts by definition as the Laplacian, and on the chain $\{h^j_{r,p}\}$ the operator $(-\widetilde{S}_{p,j}-\lambda_0)$ is the shift operator:

$$(-\widetilde{S}_{p,j}-\lambda_0)h^j_{r,p}=h^j_{r-2,p}.$$

Lemma 2.1: The operator $\widetilde{S}_{p,j}$ is self-adjoint.

Proof: It is easy to check by direct calculations that $\widetilde{S}_{p,j}$ is symmetric. The relation,

$$(-\widetilde{S}_{p,j}-\lambda_0)\mathscr{D}(\widetilde{S}_{p,j})=\mathscr{H}^j_p,$$

implies that it is self-adjoint. ■

Remark: It is worth noting that not only λ_0, but the whole negative half-line, belongs also to the set of regular points of the operator $-\widetilde{S}_{p,j}$. It is simple to show that the space $\mathscr{H}^j_p$ does not depend on the choice of λ_0.

Consider the functional χ_j, defined on the space $\mathscr{D}(\widetilde{S}_{p,j})$ by the relation

$$(f,\chi_j)=((-\widetilde{S}_{p,j}-\lambda_0)f,h^j_{-p,p});$$

this functional is called the generalized deficiency element of the operator $-\widetilde{S}_{p,j}$.[31] Formally we can write

$$\chi_j=(-\widetilde{S}_{p,j}-\lambda_0)h^j_{-p,p}.$$

Restrict the operator $\widetilde{S}_{p,j}$ onto the following set:

$$\mathscr{D}(S^0_{p,j})=\{f\in\mathscr{D}(\widetilde{S}_{p,j}):(f,\chi_j)=0\}.$$

We denote the obtained operator as $S^0_{p,j}$.

Lemma 2.2: The operator $S^0_{p,j}$ is symmetric and has the deficiency indices (1,1).

Proof: Really, for each function f from $\mathscr{D}(S^0_{p,j})$ one has

$$((-\widetilde{S}_{p,j}-\lambda_0)f,h^j_{-p,p})=0.$$

Since $\mathscr{H}^j_p$ is densely imbedded into Π_κ, $S^0_{p,j}$ has no other deficiency elements. ■

Thus the operator $\widetilde{S}_p=\widetilde{S}_{p,j}\oplus\widetilde{S}_{p,2}$ is a self-adjoint one and the operator $S_p=S^0_{p,1}\oplus S^0_{p,2}$ is symmetric with the deficiency indices (2,2). Therefore the operator S_p has self-adjoint extensions. The domain of such an extension is an annihilator subspace of the following ''boundary form'' on $\mathscr{D}(S^*_p)$:

$$J(f,\phi)=((-S^*_p-\lambda_0)f,\phi)-(f;(-S^*_p-\lambda_0)\phi).$$

Now let us describe $\mathscr{D}(S^*_p)$.

Lemma 2.3: The set $\mathscr{D}(S_P^*)$ *consists of all elements* f *from* $\mathscr{D}(\widetilde{S}_p)$ *satisfying the condition* $C^1_{p,p}(f)=C^2_{p,p}(f)=0$.

Proof: Remark that in accordance with the definition (6) of the inner product in the space $\mathscr{H}^j_p$, the relations

$$((-\widetilde{S}_{p,j}-\lambda_0)h^j_{r,p},h^j_{-p,p})=0,\quad j=1,2,$$

hold for each $h^j_{r,p}$, $-p<r<p$. In virtue of the Green's formula we have for each f^j_p from $\mathscr{D}(\widetilde{S}_{p,j})$, $j=1,2$:

$$\int_{\Omega^j}(-\widetilde{S}_{p,j}-\lambda_0)f^j_p(x)\overline{h^j_{-p,p}(x)}dx=\lim_{\epsilon\to 0}\int_{\Sigma^j_\epsilon}\left(f^j_p\frac{\partial\overline{h^j_{-p,p}}}{\partial n}-\overline{h^j_{-p,p}}\frac{\partial f^j_p}{\partial n}\right)dx=C^j_{p,p}(f).$$

Hence

$$((-\widetilde{S}_{p,j}-\lambda_0)f^j_p,h^j_{-p,p})=C^j_{p,p}(f),$$

and the lemma follows from this equality. ■

Note that $C^j_{p,p}(f)$ are the corresponding coefficients of the asymptotics (of the order r^p) of the function f_p near the point x_0 multiplied by a constant that is independent of f.

Lemma 2.3 leads immediately to the following statement.

Lemma 2.4: $\mathscr{D}(S_p^*)=\{f\in\mathscr{H}_p: f_p=f_{p+1}+\alpha h_{p,p},\alpha\in\mathbf{C}\}$. ■

Remark: Lemma 2.4 is equivalent to the assertion

$$\mathscr{D}(S_p^*)=\mathscr{D}(S_p)+\mathscr{N}_{\lambda_0},$$

where $\mathscr{N}_{\lambda_0}$ is the deficiency subspace corresponding to λ_0.

Let us consider the boundary form $J(f,\phi)$ thoroughly:

$$J(f,\phi)=J^1(f,\phi)+J^2(f,\phi),$$

$$\begin{aligned}J^j(f,\phi)=&((-S_p^*-\lambda_0)f^{(0),j},\phi^{(0),j})+((-S_p^*-\lambda_0)f^{(0),j},C^i_{-p,p}(\phi)h^j_{-p,p})\\&-(C^i_{-p,p}(f)h^j_{-p,p},(-S_p^*-\lambda_0)\phi^{(0),j})-(f^{(0),j},(-S_p^*-\lambda_0)\phi^{(0),j}),\end{aligned}$$

where $f^{(0),j},\phi^{(0),j}\in\mathscr{D}(\widetilde{S}_{p,j})$, $j=1,2$. Taking into account the self-adjointness of the operator $\widetilde{S}_{p,j}$, one gets

$$\begin{aligned}J(f,\phi)=&((-S_p^*-\lambda_0)f^{(0),1},C^1_{-p,p}(\phi)h^1_{-p,p})-(C^1_{-p,p}(f)h^1_{-p,p},(-S_p^*-\lambda_0)\phi^{(0),1})\\&+((-S_p^*-\lambda_0)f^{(0),2},C^2_{-p,p}(\phi)h^2_{-p,p})-(C^2_{-p,p}(f)h^2_{-p,p},(-S_p^*-\lambda_0)\phi^{(0),2}).\end{aligned}$$

After brief calculations one obtains

$$J(f,\phi)=C^1_{p,p}(f)\overline{C^1_{-p,p}(\phi)}-C^1_{-p,p}(f)\overline{C^1_{p,p}(\phi)}+C^2_{p,p}(f)\overline{C^2_{-p,p}(\phi)}-C^2_{-p,p}(f)\overline{C^2_{p,p}(\phi)}.$$

To construct a self-adjoint extension it is necessary to study the condition of annihilation of the boundary form. Let us note that the algebraic structure of the form is the same as for conventional zero-width slit model,[35] that is why its analysis is similar to one in the cited paper (the problem now reduces to the problem of linear algebra). The result is the following description of all self-adjoint extensions $H_{A(p)},H_{B(p)}$ of the operator S_p.

Theorem 2.1: *There exist two families* $\{H_{A(p)}\},\{H_{B(p)}\}$ *of self-adjoint extensions of the operator* S_p *which domains consist of all elements from* $\mathscr{D}(S_p^*)$ *satisfying the conditions*

$$\begin{pmatrix} C^1_{p,p} \\ C^2_{p,p} \end{pmatrix} = \begin{pmatrix} a^{(p)}_{11} & a^{(p)}_{12} \\ a^{(p)}_{21} & a^{(p)}_{22} \end{pmatrix} \begin{pmatrix} C^1_{-p,p} \\ C^2_{-p,p} \end{pmatrix} \tag{8}$$

or

$$\begin{pmatrix} C^1_{-p,p} \\ -C^2_{p,p} \end{pmatrix} = \begin{pmatrix} b^{(p)}_{11} & b^{(p)}_{12} \\ b^{(p)}_{21} & b^{(p)}_{22} \end{pmatrix} \begin{pmatrix} C^1_{p,p} \\ C^2_{-p,p} \end{pmatrix}. \tag{9}$$

■

Let us construct the Green's function with the source at the point $Y \in \Omega^2$ for the extended operator (for example, for $-H_{B^{(p)}}$). We seek the function in the form

$$G^p(x,Y;k) = \begin{cases} a^1_p Q_{p-1}(-\nabla_y) \dfrac{\partial}{\partial n} G^1_D(x,y;k)\Big|_{y=x_0}, & x \in \Omega^1, \\ G^{2,p}(x,Y;k) + a^2_p Q_{p-1}(-\nabla_y) \dfrac{\partial}{\partial n} G^2_D(x,y;k)\Big|_{y=x_0}, & x \in \Omega^2, \end{cases}$$

where $G^{2,p}(x,Y;k)$ has the following form in a neighborhood of the point x_0:

$$G^{2,p}(x,Y;k) = Q_{p-1}(-\nabla_y) \frac{\partial}{\partial n} G^2_D(x_0,y;k)\Big|_{y=x_0} Q_p(x-x_0) + o(|x-x_0|^p).$$

Here

$$Q_p(\nabla_y) = Q_{p-1}(-\nabla_y) \frac{\partial}{\partial n}.$$

To satisfy (9) it is necessary to determine $C^1_{-p,p}, C^2_{-p,p}, C^1_{p,p}, C^2_{p,p}$. It is simple to show that

$$C^1_{-p,p} = a^1_p, \quad C^2_{-p,p} = a^2_p.$$

There exist two ways to determine $C^1_{p,p}, C^2_{p,p}$: to investigate the asymptotic expansions of the Green's functions for the operators H_1 and H_2 or to use some operator relations. Let us choose the second way. We start from the Hilbert identity,

$$(H_j - \lambda)^{-1} - (H_j - \lambda_0)^{-1} = (\lambda - \lambda_0)(H_j - \lambda_0)^{-1}(H_j - \lambda)^{-1}.$$

Iterating this identity p times, we obtain

$$\begin{aligned}(H_j - \lambda)^{-1} = (H_j - \lambda_0)^{-1} &+ (\lambda - \lambda_0)(H_j - \lambda_0)^{-1}(H_j - \lambda)^{-1} + \cdots + (\lambda - \lambda_0)^{p-1} \\ &\times (H_j - \lambda_0)^{-p+1}(H_j - \lambda)^{-1} + (\lambda - \lambda_0)^p (H_j - \lambda_0)^{-p}(H_j - \lambda)^{-1}.\end{aligned}$$

After differentiation with respect to y we get

$$\begin{aligned}Q_p(-\nabla_y) G^j_D(x_0,y;k) = Q_p(-\nabla_y) G^j_D(x_0,y;k_0) &+ (\lambda - \lambda_0)(H_j - \lambda_0)^{-1} Q_p(-\nabla_y) G^j_D(x_0,y;k) \\ &+ \cdots + (\lambda - \lambda_0)^{p-1}(H_j - \lambda_0)^{-p+1} Q_p(-\nabla_y) G^j_D(x_0,y;k) \\ &+ (\lambda - \lambda_0)^p (H_j - \lambda_0)^{-p} Q_p(-\nabla_y) G^j_D(x_0,y;k). \end{aligned} \tag{10}$$

It is significant that each iteration of the Hilbert identity rises the smoothness of the last term. Particularly,

$$(H_j-\lambda_0)^{-p}Q_p(-\nabla_y)G_D^j(x_0,y;k)\big|_{y=x_0}\in C^p.$$

The remarkable fact is that the other terms in (10) are elements of the chain $\{h_{r,p}^j\}$. That is why the corresponding coefficient can be simply determined:

$$C_{p,p}^1=\widetilde{C}_{p,p}^1 a_p^1,\quad C_{p,p}^2=\widetilde{C}_{p,p}^2+G_p^2,$$

where

$$\widetilde{C}_{p,p}^j=\lim_{\epsilon\to 0}\int_{\Sigma_\epsilon^j}(\lambda-\lambda_0)^p\left(F_j\,\frac{\partial\overline{h_{-p,p}^j}}{\partial n}-\overline{h_{-p,p}^j}\,\frac{\partial F_j}{\partial n}\right)dx,$$

$$F_j=Q_p(-\nabla_x)(H_j-\lambda_0)^{-p}Q_p(-\nabla_y)G_D^j(x_0,y;k)\big|_{x=x_0,y=x_0},$$

$$G_p^2=\lim_{\epsilon\to 0}\int_{\Sigma_\epsilon^j}\Bigg(Q_p(-\nabla_y)G_D^2(x_0,y;k)\Big|_{y=x_0}Q_p(x-x_0)$$
$$\times\frac{\partial\overline{h_{-p,p}^2}}{\partial n}-\overline{h_{-p,p}^2}\,\frac{\partial}{\partial n}\,(Q_p(-\nabla_y)G_D^2(x_0,y;k)\Big|_{y=x_0}Q_p(x-x_0))\Bigg)dx.$$

C. Two coupled curvilinear triangles with zero angles

Now we consider how to ''switch on'' the interaction through the vertex of a zero angle. In this case the Green's function with the source at the vertex would be a deficiency element. But this function, as has been mentioned above, has an essential singularity at the vertex. Hence there is no finite number n such that nth power of the resolvent maps the function into L^2. Consequently, we cannot realize the above construction of the model in a Pontryagin space. We need to construct a new extension of the initial space such that the determined earlier Green's function belongs to the extended spaces. Let us outline a variant of this procedure. We shall use the following result concerning the asymptotics of the W_2^2 solution of the Dirichlet problem near a vertex of zero angles.[45] Choose Cartesian coordinates (x,y) in the curvilinear triangle Ω^i with zero angles in such a way that the x axis is the common tangent line of two circles forming the zero angle and that the triangle lies in the half-plane $x\geqslant 0$. Then the equation of the boundary line has the asymptotic form $y=cx^2$. The asymptotics of the solution $u(x,y)$ of the Dirichlet problem for the equation $(H_i-\lambda)u=0$ is the following:

$$u(x,y)=C\,\exp(-i\xi_0 x^{-1})\sum_{j=0}^{\infty}\phi_j(x^{-2}y)x^j,$$

where ϕ_j are smooth functions on the cross section θ of the domain by the line $x=1$, ξ_0 is an eigenvalue of the operator $A(\xi)=H_i(d/dy,\xi)$ with the domain $W_2^2(\theta)\cup\mathring{W}_1^2(\theta)$. Here $H_i(\partial/\partial y,\partial/\partial x)$ is the initial operator for the domain Ω^i (see Sec. II B).

In spite of the fact that the described properties of the Green's function are more complicated than ones for the case of nonzero angles, the construction of nontrivial extensions of the operator S_0 is developed formally by the same procedure. Here we start from the set A_∞^i of functions tending exponentially to zero at the vertex, more precisely,

$$A_\infty^i=\{u\in L^2(\Omega^i):\Delta u\in L^2(\Omega^i),\quad u(x,y)\exp(i\xi_0 x^{-1})\to\text{const},\quad \text{as}\ \ x\to 0\}.$$

Then we construct a chain of subspaces, adding step-by-step elements with determined behavior near the vertex $(\phi_j(x^{-2}y)x^j\eta(x,y))$, where $\eta(x,y)$ is a smooth cut-off function, i.e. $\eta(x,y)=1$ for $x^2+y^2<1$ and $\eta(x,y)=0$ for $x^2+y^2>2$. Finally, as above, we add elements χ_i that is proportional to the Green's function for our domain. In the constructed space $\mathscr{H}^i_\infty$ we introduce an inner product $(\cdot,\cdot)_{\mathscr{H}^i_\infty}$. There is some nonessential freedom in the choice of the product. To avoid the ambiguity, we adapt the usual L^2 product on each step of the construction if the corresponding integral converges and suppose the inner product is equal to zero otherwise [see, e.g., Eqs. (7)]. Completing the obtained indefinite metric space, we obtain a Krein space $\mathscr{K}^i$. In this space the considered operators act formally as the corresponding differential expressions. Restrict such an operator on the set of all elements ϕ obeying $(\phi,\chi_i)_{\mathscr{H}^i_\infty}=0$; then we get a symmetric operator $S^0_{\infty,i}$, having self-adjoint extensions, and can introduce the symmetric operator $S_\infty=S^0_{\infty,1}\oplus S^0_{\infty,2}$. In the considered case, the Krein resolvent formula[33,36,42] is a more convenient tool to describe self-adjoint extensions of S_∞ in the Krein space $\mathscr{K}=\mathscr{K}^1\oplus\mathscr{K}^2$. Let us denote by $H_0=H_1\oplus H_2$ the unperturbed operator in the space $L^2(\Omega^1\cup\Omega^2)$ and by $R_0(z)$, $R_0(z)=(H_0-z)^{-1}$, its resolvent. Let $\overline{R_0(z)}$ be the continuous extension of $R_0(z)$ on the space $\mathscr{K}$. In what follows we restrict ourselves to so-called ''transversal'' to H_0 self-adjoint extensions,[46] they are sufficient to our purposes. According to the Krein approach, the resolvent $R(z)$ of a transversal self-adjoint extension of S_∞ has the form

$$R(z)=\overline{R_0(z)}-\sum_{i,j=1}^{2}[Q(z)-A]^{-1}_{ij}\overline{R_0(z)}|\chi_i\rangle\langle\chi_j|\overline{R_0(z)}. \tag{11}$$

Here A is a Hermitian 2×2-matrix that parametrize the extension, and $Q(z)$ is the so-called Krein $\mathscr{Q}$ matrix that has the elements

$$q_{ij}(z)=\tfrac{1}{2}(z-z_0)\langle\chi_i|\overline{R_0(z)R_0(z_0)}|\chi_j\rangle+\tfrac{1}{2}(z-\overline{z_0})\langle\chi_i|\overline{R_0(z)R_0(\overline{z_0})}|\chi_j\rangle, \tag{12}$$

where $z_0\in\mathbf{C}\backslash\sigma(H_0)$ is fixed.

III. MODEL OF A PERIODIC ANTIDOT ARRAY

In this section we consider a periodic system of curvilinear triangles $\Omega_\gamma=\Omega+\gamma$, $\gamma\in\Gamma$; here Ω is a fixed curvilinear equilateral triangle with zero angles or with angles equal to π/p, where $p\geqslant3$ is a fixed positive integer (of course, if $p=3$, this is an ordinary triangle). Thus the typical void V is a circle in the first case and a (in general, curvilinear) triangle in the second one. Instead of condition $0\in V$ it is convenient now to suppose that 0 is the center of the triangle $\Omega=\Omega_0$. (Fig. 2).

As before, the symbol G denotes the domain $\Omega+\Gamma$; remember that $\mathscr{H}^0$ denotes the initial state space $L^2(G)=\Sigma_{\gamma\in\Gamma}{}^{\oplus}\mathscr{H}^0_\gamma$ and $H^0=\Sigma_{\gamma\in\Gamma}{}^{\oplus}H^0_\gamma$ is the unperturbed Hamiltonian of the model (see the Introduction). This Hamiltonian describes a charge carrier in the set of isolated triangles Ω_γ. To switch on the tunneling between the triangles through their vertices by means of operator extension theory, we need three deficiency elements $\chi^{(\gamma)}_i$ in $\mathscr{H}_\gamma$ $(i=1,2,3)$, corresponding to each vertex of the triangle Ω_γ. As a result we obtain an indefinite metric state space containing the space $\mathscr{H}^0_\gamma$ (see Sec. II). It is convenient to proceed in the space $\mathscr{H}^0_0=L^2(\Omega)$ only; this is possible because $\mathscr{H}^0_\gamma$ and $\mathscr{H}^0_0$ are isomorphic. In the absence of magnetic fields an isomorphism is established via translations by vectors from Γ, but in the presence of a magnetic field we must deal with the magnetic translation group.[41] In this connection we begin with some basic concepts related to this group.

A. Magnetic translation group and its lattice representations

Choose some basis vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ of the lattice Λ; if $\mathbf{v}$ is any vector from $\mathbf{R}^2$ we denote by v_1,v_2 the coordinates of $\mathbf{v}$ with respect to the basis $\mathbf{a}_1$, $\mathbf{a}_2$: $\mathbf{v}=v_1\mathbf{a}_1+v_2\mathbf{a}_2$. If $\mathbf{v}$, $\mathbf{v}'\in\mathbf{R}^2$, then the symbol $\mathbf{v}\wedge\mathbf{v}'$ will denote the number $v_1v'_2-v_2v'_1$. It is obvious that $\mathbf{v}\wedge\mathbf{v}'=\mathbf{v}\times\mathbf{v}'/S_\Lambda$, where

$\mathbf{v}\times\mathbf{v}'$ is the standard symplectic product in $\mathbf{R}^2$, and $S_\Lambda=\mathbf{a}_1\times\mathbf{a}_2$ is the oriented area of the elementary cell C_Λ (see the Introduction). Remember that η denotes the number of magnetic flux quanta through the cell C_Λ: $\eta=|S_\lambda(Be/2\pi\hbar c)|$. Let G_η be a subgroup of the multiplicative group $\mathbf{S}^1(\mathbf{S}^1=\{\zeta\in C:|\zeta|=1\})$, consisting of all elements of the form $\exp(\pi i\eta n)$, $n\in\mathbf{Z}$. The symbol W_η will be denote the set $\Lambda\times G_\eta$; W_η become a group structure by defining the multiplication as follows:

$$(\lambda,\zeta)(\lambda',\zeta')=(\lambda+\lambda',\zeta\zeta'\ \exp[\pi i\eta(\lambda\wedge\lambda')]); \tag{13}$$

this group is called the magnetic translation group. It is evident that the definition of W_η does not depend on a choice of basis vectors $\mathbf{a}_1$, $\mathbf{a}_2$.

If a magnetic field is absent, then a quantum-mechanical Hamiltonian H of a charged particle in the lattice system of triangles is invariant with respect to the translations by vectors from Λ. The presence of a magnetic field violates the translation symmetry of the Hamiltonian. Instead of the Λ invariance the Hamiltonian H is invariant under the composition of the translation by a vector $\lambda\in\Lambda$, and the gauge transformation of the vector potential of the magnetic field: $\mathbf{A}\mapsto\mathbf{A}-(\mathbf{B}\times\lambda)/2$. From the mathematical point of view the operator H is invariant with respect to a unitary representation of the group W_η. Under this representation an element $(\lambda,\zeta)\in W_\eta$ corresponds to the unitary operator $[\lambda,\zeta]$, which acts on any function $f\in L^2(G)$ according to the formula

$$([\lambda,\zeta]f\ )(x)=\zeta\ \exp[-\pi i\eta(x\wedge\lambda)]f(x-\lambda). \tag{14}$$

Let us introduce a lattice counterpart of the representation (14). Consider a family $(\mathcal{G}_\gamma)_{\gamma\in\Gamma}$ of complete inner product spaces (Hilbert spaces, Pontryagin spaces, or Krein spaces), such that $\mathcal{G}_{\gamma_1}=\mathcal{G}_{\gamma_2}$ if $\gamma_1\equiv\lambda_2$ (mod Λ). We shall denote

$$\mathcal{G}=\sum_{\gamma\in\Gamma}\oplus\mathcal{G}_\gamma,\quad \mathcal{G}_K=\sum_{\gamma\in K}\oplus\mathcal{G}_\gamma,$$

hence $\mathcal{G}=\Sigma_{\gamma\in\Lambda}\ \oplus\mathcal{G}'_\lambda$, where $\mathcal{G}'_\lambda\simeq\mathcal{G}_K$ for each $\lambda\in\Lambda$. In other words, $\mathcal{G}=\mathcal{G}_K\otimes l^2(\Lambda)$. We shall consider an element $g=(g_\gamma)_{\gamma\in\Gamma}$ of the space $\mathcal{G}$ as a function $g:\Gamma\to\cup_{\gamma\in\Gamma}\mathcal{G}_\lambda$ and write $g(\gamma)$ instead of g_γ. Equation (14) requires that we should define the unitary representation $(\lambda,\zeta)\mapsto[\lambda,\zeta]$ of the group W_η in the space $\mathcal{G}$ in the following way:

$$([\lambda,\zeta]g)(\gamma)=\zeta\ \exp[-\pi i\eta(\gamma\wedge\lambda)]g(\gamma-\lambda). \tag{15}$$

We shall denote the representation (15) as $D^{\mathcal{G}}_\eta$.

We recall that each bounded operator A in the direct sum $\mathcal{G}=\Sigma_{\gamma\in\Gamma}\oplus\mathcal{G}_\gamma$ is represented by the corresponding matrix $(A(\gamma,\gamma'))_{\gamma,\gamma'\in\Gamma}$, where $A(\gamma,\gamma')$ is a bounded operator acting from $\mathcal{G}_{\gamma'}$ into $\mathcal{G}_\gamma$. Namely, let J_γ be the canonical imbedding operator, $J_\gamma:\mathcal{G}_\gamma\hookrightarrow\mathcal{G}$, and let P_γ be the canonical projection, $P_\gamma:\mathcal{G}\to\mathcal{G}_\gamma$. Then $A(\gamma,\gamma')=P_\gamma AJ_{\gamma'}$, and for every $\phi\in\mathcal{G}$ we have

$$(A\phi)(\gamma)=\sum_{\gamma'\in\Gamma}A(\gamma,\gamma')\phi(\gamma'), \tag{16}$$

where the series converges unconditionally in the space $\mathcal{G}$.

Proposition 3.1: The operator A in the space $\mathcal{G}$ is $D^{\mathcal{G}}_\eta$-invariant iff its matrix $(A(\gamma,\gamma'))_{\gamma,\gamma'\in\Gamma}$ satisfies the condition

$$A(\gamma-\lambda,\gamma'-\lambda)=\exp[\pi i\eta((\gamma-\gamma')\wedge\lambda)]A(\gamma,\gamma'), \tag{17}$$

where, γ, $\gamma'\in\Gamma$, $\lambda\in\Lambda$.

Proof: We have from definitions that the relation

$$A[\lambda,1]\phi(\gamma)=[\lambda,1]A(\gamma)$$

($\gamma\in\Gamma$) is equivalent to the following one:

$$\sum_{\gamma'\in\Gamma}A(\gamma,\gamma')\exp[\pi i\,\eta(\lambda\wedge\gamma')]\phi(\gamma'-\lambda)=\sum_{\gamma'\in\Gamma}A(\gamma-\lambda,\gamma')\exp[\pi i\,\eta(\lambda\wedge\gamma)]\phi(\gamma').$$

We can rewrite the relation (17) in the form

$$\sum_{\gamma'\in\Gamma}A(\gamma,\gamma'+\lambda)\exp[\pi i\,\eta(\lambda\wedge(\gamma'-\gamma))]\phi(\gamma')=\sum_{\gamma'\in\Gamma}A(\gamma-\lambda,\gamma')\phi(\gamma'). \tag{18}$$

Taking into account that the linear hull of the set $\cup_{\gamma\in\Gamma}\mathscr{G}_\gamma$ is dense in the space $\mathscr{G}$, we conclude that the validity of the equality (18) is equivalent to the validity of the condition

$$A(\gamma,\gamma'+\lambda)=\exp[\pi i\,\eta((\gamma'-\gamma)\wedge\lambda)]A(\gamma-\lambda,\gamma'),$$

for every $\gamma,\ \gamma'\in\Gamma$ and $\lambda\in\Lambda$. Replacing $\gamma'+\lambda$ by γ', we finish the proof of the proposition. ■

Corollary: The $D^{\mathscr{G}}_\eta$-invariant operator A is fully determined only by the matrix elements $A(\gamma,\kappa')$ ($\gamma\in\Gamma,\ \kappa'\in K$) by the formula

$$A(\gamma,\gamma')=\exp[\pi i\,\eta((\gamma'-\gamma)\wedge\lambda')]A(\gamma-\lambda',\kappa'), \tag{19}$$

where $\lambda'=\gamma'-\kappa',\ \kappa'\in K$. More precisely, let $A(\lambda,\kappa'):\mathscr{G}_{\kappa'}\to\mathscr{G}_\gamma$ ($\gamma\in\Gamma,\ \kappa'\in K$) be a family of bounded operators such that for every $\phi\in\mathscr{G}$ the series (16) unconditionally converges if the operators $A(\gamma,\gamma')$ are defined by the formula (19); then the formula (16) defines a bounded $D^{\mathscr{G}}_\eta$-invariant operator A. ■

Proposition 3.2: In order that the formula (19) gives us a self-adjoint operator A it is necessary and sufficient that the operator family $A(\gamma,\kappa')$ ($\gamma\in\Gamma,\ \kappa'\in K$) satisfies the condition

$$A(\kappa+\lambda,\kappa')=\exp[\pi i\,\eta((\kappa'-\kappa)\wedge\lambda)]A^*(\kappa'-\lambda,\kappa), \tag{20}$$

where $\lambda\in\Lambda,\ \kappa,\ \kappa'\in K$.

Proof: In accordance with (19),

$$A(\gamma,\gamma')=\exp[\pi i\,\eta((\gamma-\gamma')\wedge\mu)]A(\gamma'-\mu,\kappa), \tag{21}$$

where $\gamma,\ \gamma'\in\Gamma,\ \kappa\in K,\ \mu=\gamma-\kappa$. Hence the equality

$$A(\gamma,\gamma')=A^*(\gamma',\gamma), \tag{22}$$

which is equivalent to the self-adjointness of the operator A, takes the form

$$\exp[\pi i\,\eta((\gamma'-\gamma)\wedge\lambda)]A(\gamma-\lambda,\kappa')=\exp[\pi i\,\eta((\gamma'-\gamma)\wedge\mu)]A^*(\gamma'-\mu,\kappa),$$

where $\mu=\gamma-\kappa,\ \lambda=\gamma'-\kappa'$. In the other words, the relation (22) is equivalent to the following one:

$$A(\gamma-\lambda,\kappa')=\exp[\pi i\,\eta((\gamma'-\gamma)\wedge(\mu-\lambda))]A^*(\gamma'-\mu,\kappa),$$

or

$$\begin{aligned}A(\kappa+\mu-\lambda,\kappa')&=\exp[\pi i\,\eta((\kappa'-\kappa+\lambda-\mu)\wedge(\mu-\lambda))]A^*(\kappa'+\lambda-\mu,\kappa)\\&=\exp[\pi i\,\eta((\kappa'-\kappa)\wedge(\mu-\lambda))]A^*(\kappa'+\lambda-\mu,\kappa).\end{aligned}$$

Replacing $\mu-\lambda$ by λ, we obtain (20). ■

The propositions 3.1 and 3.2 allow us to simplify the construction of a model Hamiltonian.

B. Construction of the model

We return to the construction of the model state space and the model Hamiltonian. In our case $K=\{0,\mathbf{b}\}$, where $\mathbf{b}=2(\mathbf{a}_1+\mathbf{a}_2)/3$. We shall identify the space $\mathscr{H}_\gamma^0=L^2(\Omega_\gamma)$ with the space $\mathscr{H}_0^0=L^2(\Omega_0)$ using magnetic translations $[\gamma,1]$ defined in accordance with (14). More precisely, let $\mathscr{H}_\gamma=\mathscr{H}_0$ for every $\gamma\in\Gamma$. We shall identify a function $f\in L^2(G)=L^2(\Omega_0+\Gamma)$ with the family $(f_\gamma)_{\gamma\in\Gamma}\in\mathscr{H}=[|\mathrm{M}|\mathrm{s}_{\gamma\in\Gamma}.\mathscr{H}_\gamma$ by the relation

$$f_\gamma(x)=\exp[\pi i\,\eta x\wedge\gamma]f(x+\gamma),\quad x\in\Omega_0.$$

It is a straightforward matter to establish that the isomorphism $f\mapsto(f_\gamma)_{\gamma\in\Gamma}$ intertwines the unitary representations (13) and (15), i.e., $[\lambda,\zeta](f_\gamma)_{\gamma\in\Gamma}=(([\lambda,\zeta]f_\gamma)_\gamma)_{\gamma\in\Gamma}$ for every $(\lambda,\zeta)\in W_\eta$.

Let us consider now the unperturbed Hamiltonian $H^0=\Sigma_{\gamma\in\Gamma}\oplus H_\gamma^0$, where $H_\gamma^0=H_0^0$ is the operator defined in $L^2(\Omega_0)=\mathscr{H}_0^0$ by the differential expression (1) and Dirichlet boundary conditions. Let S_0^0 be the restriction of H_0^0 to the set of functions from $\mathscr{H}_0^0$ vanishing near of the vertices of the curvilinear triangle Ω_0. We shall denote by χ_i $(i=1,\,2,\,3)$ the generalized deficiency elements of S_0^0 corresponding to the vertices (see Secs. II B and II C). In accordance with the results of Sec. II the operator S_0^0 has nontrivial self-adjoint extensions in an inner product space $\mathscr{H}_0$, which is a Pontryagin or Krein space. Let $R_0(z)$ be the resolvent of the operator H_0^0 in the space $\mathscr{H}_0^0$; as in Sec. II we denote by $\overline{R_0(z)}$ its continuous extension on the space $\mathscr{H}_0$. Let $R^0(z)=\Sigma_{\gamma\in\Gamma}\oplus R^{(\gamma)}(z)$, where $R^{(\gamma)}(z)=\overline{R_0(z)}$ for each $\gamma\in\Gamma$. Now we are able to introduce the state space $\mathscr{H}$ of our model, this is the direct sum $\mathscr{H}=\Sigma_{\gamma\in\Gamma}\oplus\mathscr{H}_\gamma$, where $\mathscr{H}_\gamma=\mathscr{H}_0$ for each $\gamma\in\Gamma$. Let $S^0=\Sigma_{\gamma\in\Gamma}\oplus S_\gamma^0$, where $S_\gamma^0=S_0^0\ \forall\gamma\in\Gamma$. We shall seek the Hamiltonian of our model among self-adjoint extensions of the operator S^0 in the space $\mathscr{H}$. At first, we describe the required extensions using the Krein resolvent formula. To do this, we need three auxiliary objects:[42] the typical deficiency space $\mathscr{G}$, the Krein Γ function $K(z):\mathscr{G}\to\mathscr{H}$, and the Krein $\mathscr{Q}$ function $Q(z):\mathscr{G}\to\mathscr{G}(z\in\mathbf{C}\backslash\sigma(H^0))$. Let us describe them. In our case, the Hilbert space $\mathscr{G}$ is the direct sum $\mathscr{G}=\Sigma_{\gamma\in\Gamma}\oplus\mathscr{G}_\gamma$, where $\mathscr{G}_\gamma$ is the standard three-dimensional Hilbert space $\mathbf{C}^3$ for each $\gamma\in\Gamma$. We shall denote by $Q_\gamma(z)$ $(\gamma\in\Gamma)$ the linear mapping in $\mathbf{C}^3$ with the matrix $q(z)=\|q_{ij}(z)\|$, where the elements $q_{ij}(z)$ are defined by Eq. (12) (now $i,j=1,2,3$). The symbol $Q(z)$ will denote the direct sum $Q(z)=\Sigma_{\gamma\in\Gamma}\oplus\mathscr{Q}_\gamma(z)$. The operator-valued function $Q(z)$ defined on $\mathbf{C}\backslash\sigma(H^0)$ is just the Krein $\mathscr{Q}$ function. Further, denote by $K_\gamma(z)$ the linear mapping from $\mathscr{G}_\gamma=\mathbf{C}^3$ into the space $\mathscr{H}_\gamma=\mathscr{H}_0$ defined on the standard basis vectors $\mathbf{e}_j$ by the formula

$$K_\gamma(z)\mathbf{e}_j=\overline{R_0(z)|\chi_j\rangle}.$$

In our case the Krein Γ function $K(z)$ is the direct sum $K(z)=\Sigma_{\gamma\in\Gamma}\oplus K_\gamma(z)$. Now all the required self-adjoint extensions of the unperturbed Hamiltonian are given by the Krein resolvent formula. Namely, let A be a bounded self-adjoint operator in $\mathscr{G}$ such that the bounded inverse operator exists. Then the operator $R_A(z)$,

$$R_A(z)=R^0(z)-K(z)[Q(z)-A]^{-1}K^*(z),\tag{23}$$

is the resolvent of a self-adjoint extension H_A of the operator H^0 [see Refs. 33 and 36].

The Hamiltonian of our model should be invariant with respect to magnetic translations from W_η. The proposition below provides a condition of the invariance of H_A.

Proposition 3.3: The operator H_A is $D_\eta^{\mathscr{H}}$ invariant-iff the operator A is $D_\eta^{\mathscr{G}}$ invariant.

Proof: We shall use the standard definition of commutation of a bounded operator B with a densely defined closed operator A (see, e.g., Ref. 47): B commutes with A iff $BA\subset AB$, i.e. iff for each $\phi\in\mathscr{D}(A)$ we have $B\phi\in\mathscr{D}(A)$ and $AB\phi=BA\phi$. Taking into account that the operator $R^0(z)$

is $D_\eta^{\mathscr{H}}$ invariant and the operator $Q(z)$ is $D_\eta^{\mathscr{G}}$ invariant, we can finish the proof by reference to Ref. 47, Part III.5.6. ■

We can decompose the operator A into two parts: $A=B+T$, where a bounded self-adjoint operator B parametrizes those extensions H_B which are the model Hamiltonians of arrays consisting of isolated domains Ω_γ, like the operator H^0. The operator T turn on a tunneling between regions Ω_γ. On the one hand, the physical meaning of the operators B and T and on the other the propositions 3.1, 3.2, and 3.3 impose very strong restrictions to the matrices of the operators B and T. Namely, the matrix $B(\gamma,\gamma')$ must be of the form $B(\gamma,\gamma')=B_0\delta_{\gamma,\gamma'}$, where B_0 is a self-adjoint operator in $\mathbf{C}^3$; in other words, B_0 is a Hermitian 3×3 matrix. A detailed physical motivation how to choice the matrix T is presented in Refs. 27 and 28; here we follow the line of the cited papers. To identify an acting in the space $\mathbf{C}^3$ operator $T(\gamma,\gamma')$ with a 3×3 matrix, we enumerate the vertices of the triangle Ω_0 with the numbers 1, 2, 3 in an arbitrary way. Then each triangle Ω_γ acquires the uniquely determined enumeration of vertices by means of the translation of Ω_0 on the vector γ. If Ω_γ and $\Omega_{\gamma'}$ have no common vertex, then, evidently, the equality $T(\gamma,\gamma')=0$ should be valid. Otherwise, the magnitude $|T_{ij}(\gamma,\gamma')|^2$ is proportional to the tunneling probability from a ''infinitesimal neighborhood'' of the ith vertex in Ω_γ to a ''infinitesimal neighborhood'' of the jth vertex in $\Omega_{\gamma'}$. By symmetry, all the nonzero elements T_{ij} must be mutually equal; we shall denote their common value as τ. In virtue of Proposition 3.1 it is sufficient to find the matrices of the form $T(\gamma,0)$ and $T(\gamma,\mathbf{b})$ only. The above arguments show that only the elements of the kind $T(\lambda,\mathbf{b})$ and $T(\mathbf{b}+\lambda,0)$ $(\lambda\in\Lambda)$ may be nonzero. Using Fig. 2 we obtain

$$T(\lambda,\mathbf{b})=\begin{cases}\begin{pmatrix}0&0&\tau\\0&0&0\\0&0&0\end{pmatrix}, & \lambda=\mathbf{a}_1,\\ \begin{pmatrix}0&0&0\\0&0&0\\0&\tau&0\end{pmatrix}, & \alpha=\mathbf{a}_2,\\ \begin{pmatrix}0&0&0\\\tau&0&0\\0&0&0\end{pmatrix}, & \lambda=\mathbf{a}_1+\mathbf{s}_2,\\ \begin{pmatrix}0&0&0\\0&0&0\\0&0&0\end{pmatrix}, & \text{in other cases.}\end{cases} \tag{24}$$

Proposition 3.2 implies that

$$T(\mathbf{b}+\lambda,0)=\exp[\tfrac{2}{3}\pi i\,\eta(\lambda_1-\lambda_2)]T^*(-\lambda,\mathbf{b}). \tag{25}$$

Finally, the operator T is determined by (19) and (20). The construction of the model Hamiltonian is completed, it is the operator H_A with the parametric matrix $A=B+T$ described above. The ''fitting parameters'' of our model are the elements β_{ij} of the Hermitian matrix B and the number τ.

C. Dispersion equation for the model Hamiltonian H_A—the bound states

If the flux η is a rational number: $\eta=N/M$, where N and M are coprime integers, we can use harmonic analysis on the group W_η to reduce the spectral problem for the operator H_A to the eigenvalue problem of linear algebra. Further, we shall write D instead of $D_\eta^{\mathscr{G}}$ for simplicity. The symbol $\mathbf{T}_\eta^2$ will denote the torus,

$$\mathbf{T}^2_\eta=[0,M^{-1})\times[0,1),$$

and we abbreviate $\mathbf{T}^2=\mathbf{T}^2_1=[0,1)\times[0,1)$.

Let us denote by $\widetilde{\mathscr{G}}$ the direct integral,

$$\widetilde{\mathscr{G}}=\int_{\mathbf{T}^2_\eta}\oplus\,\widetilde{\mathscr{G}}(\mathbf{p})d\mathbf{p},$$

where each fiber $\widetilde{\mathscr{G}}(\mathbf{p})$ coincides with the space $\mathbf{C}^M\otimes\mathbf{C}^M\otimes\mathscr{G}_K$. It is evident that

$$\widetilde{\mathscr{G}}=L^2(\mathbf{T}^2_\eta)\otimes\mathbf{C}^M\otimes\mathbf{C}^M\otimes\mathscr{G}_K. \tag{26}$$

Thus, we shall consider the elements ϕ of the space $\widetilde{\mathscr{G}}$ as functions of five variables:

$$\phi=\phi(p_1,p_2,j,m,\kappa)=\phi(\mathbf{p},j,m,\kappa),$$

where $p_1\in[0,M^{-1})$, $p_2\in[0,1)$, $j,\ m\in\{0,\ldots,M-1\}$, $\kappa\in K$.

We define an isomorphism $\mathscr{T}_\eta:\mathscr{G}\to\widetilde{\mathscr{G}}$ in accordance with the formula

$$(\mathscr{T}_\eta\phi)(\mathbf{p};j,m,\kappa)=\sum_{\lambda_1,\lambda_2\in\mathbf{Z}}\phi(\lambda_1\mathbf{a}_1+(\lambda_2M+m)\mathbf{a}_2+\kappa)\exp[\,\pi i\,\eta\kappa\wedge(\lambda_1\mathbf{a}_1+(\lambda_2M+m)\mathbf{a}_2)$$
$$-2\pi i(\lambda_1p_1+\lambda_2p_2+(\lambda_1\eta/2)(M\lambda_2+m+2j))]. \tag{27}$$

Proposition 3.4: The operator $\mathscr{T}_\eta$ *is a well-defined Hilbert isomorphism.*

Proof: It is easy to prove that the operator $\mathscr{T}_\eta$ is a superposition of the following four operators $\mathscr{T}^{(i)}_\eta$ $(i=1,2,3,4)$.

(1) $\mathscr{T}^{(1)}_\eta$ maps the sequence $\phi\in\mathscr{G}=l^2(\Lambda)\otimes\mathscr{G}_K$ to the sequence $\phi'\in\mathscr{G}=l^2(\mathbf{Z}^2)\otimes\mathbf{C}^M\otimes\mathscr{G}_K$ in accordance with the formula

$$\phi'(\lambda_1,\lambda_2,m,\kappa)=\phi(\lambda_1\mathbf{a}_1+(\lambda_2M+m)\mathbf{a}_2+\kappa).$$

(2) $\mathscr{T}^{(2)}_\eta$ maps the sequence $\phi'\in\mathscr{G}=l^2(\mathbf{Z}^2)\otimes\mathbf{C}^M\otimes\mathscr{G}_K$ to the sequence $\phi''\in\mathscr{G}=l^2(\mathbf{Z}^2)\otimes\mathbf{C}^M\otimes\mathscr{G}_K$ according to the formula

$$\phi''(\lambda_1,\lambda_2,m,\kappa)=\exp[\,\pi i\,\eta\kappa\wedge(\lambda_1\mathbf{a}_1+(\lambda_2M+m)\mathbf{a}_2)-\pi i\lambda_1\eta(\lambda_2M+m)]\phi'(\lambda_1,\lambda_2,m,\kappa)$$
$$=\exp[\,\pi i\,\eta(\kappa+m\mathbf{a}_2)\wedge(\lambda_1\mathbf{a}_1+(\lambda_2M+m)\mathbf{a})-\pi iN\lambda_1\lambda_2]\phi'(\lambda_1,\lambda_2,m,\kappa).$$

(3) $\mathscr{T}^{(3)}_{\mathrm{gh}}$ is the Fourier transform with respect to the variables from $\mathbf{Z}^2$, i.e., $\mathscr{T}^{(3)}_\eta$ maps the sequence $\phi''\in\mathscr{G}=l^2(\mathbf{Z}^2)\otimes\mathbf{C}^M\otimes\mathscr{G}_K$ to the function $\hat{\phi}$ from the space $L^2(\mathbf{T}^2_\eta)\oplus\mathbf{C}^M\oplus\mathscr{G}_K$:

$$\hat{\phi}(\mathbf{p},m,\kappa)=\sum_{\lambda_1,\lambda_2\in\mathbf{Z}}\phi''(\lambda_1,\lambda_2,m,\kappa)\exp[-2\pi i(\lambda_1p_1+\lambda_2p)].$$

(4) $\mathscr{T}^{(4)}_\eta$ has the form $F\otimes I_{\mathbf{C}^M\oplus\mathscr{G}_K}$, where the operator F maps a function $f\in L^2(\mathbf{T}^2)$, to the function $\widetilde{f}\in L^2(\mathbf{T}^2_\eta)\oplus\mathbf{C}^M$ in accordance with the formula

$$\widetilde{f}(p_1,p_2,j)=f(p_1+\{\eta j\},p_2).$$

Here $\{x\}$ is the integer part of the real number x.

Obviously, all the operators $\mathscr{T}^{(i)}_\eta$ $(i=1,\ 2,\ 3,\ 4)$ are Hilbert isomorphisms, hence the operator $\mathscr{T}_\eta$ is an isomorphism too. ∎

Let F be an bounded D-invariant operator in the space $\mathscr{G}$ with the matrix $F(\gamma,\gamma')$, and let $\widetilde{F}$ be the operator $\mathscr{T}_\eta F\mathscr{T}_\eta^{-1}$. Since the operator F is D invariant, the operator $\widetilde{F}$ acts fiberwise. By direct calculation we can obtain that the operator $\widetilde{F}$ in the fiber over a point $\mathbf{p}\in\mathbf{T}^2_\eta$ has the following matrix:

$$\widetilde{F}(\mathbf{p};j,m,\kappa;j',m',\kappa')=\delta_{jj'}\ \exp[-\pi i\,\eta m'\kappa/\!\!\wedge\mathbf{a}_2]\sum_{\lambda_1,\lambda_2\in\mathbf{Z}}F(\lambda_1\mathbf{a}_1+(\lambda_2M+m)\mathbf{a}_2+\kappa;m'\mathbf{a}_2+\kappa')\exp[\pi i\,\eta\kappa/\!\!\wedge(\lambda_1\mathbf{a}_1+(\lambda_2M+m)\mathbf{a}_2)-2\pi i(\lambda_1p_1+\lambda_2p_2+(\lambda_1\eta/2)(M\lambda_2+m+2j))]. \tag{28}$$

The formula (28) is equivalent to the following one:

$$\widetilde{F}(\mathbf{p};j,m,\kappa;j',m',\kappa')=\delta_{jj'}\ \exp[-\pi i\,\eta m'\kappa/\!\!\wedge\mathbf{a}_2]\sum_{\lambda_1,\lambda_2\in\mathbf{Z}}F(\lambda_1\mathbf{a}_1+(\lambda_2M+m-m')\mathbf{a}_2+\kappa;\kappa')\exp[\pi i\,\eta\kappa/\!\!\wedge(\lambda_1\mathbf{a}_1+(\lambda_2M+m)\mathbf{a}_2)-2\pi i(\lambda_1p_1+\lambda_2p_2+(\lambda_1\eta/2)(M\lambda_2+m+m'+2j))]. \tag{29}$$

Really, in virtue of (17),

$$\begin{aligned}F(\lambda_1\mathbf{a}_1+(\lambda_2M+m)\mathbf{a}_2+\kappa;m'\mathbf{a}_2+\kappa')&=F(\lambda_1\mathbf{a}_1+(\lambda_2M+m-m')\mathbf{a}_2+\kappa;\kappa')\\&\quad\times\exp[-\pi i\,\eta(\lambda_1\mathbf{a}_1+(\lambda_2M+m-m')\mathbf{a}_2+\kappa-\kappa')\\&\quad/\!\!\wedge m'\mathbf{a}_2]\\&=F(\lambda_1\mathbf{a}_1+(\lambda_2M+m-m')\mathbf{a}_2+\kappa;\kappa')\\&\quad\times\exp(-\pi i\,\eta\lambda_1m')\exp[-\pi i\,\eta m'(\kappa-\kappa')/\!\!\wedge\mathbf{a}_2].\end{aligned}$$

Fix a point $\mathbf{p}\in\mathbf{T}^2_\eta$ and consider the operator $\widetilde{F}(\mathbf{p})$ acting in the space $\mathbf{C}^M\otimes\mathbf{C}^M\otimes\mathscr{G}_K$ and having the matrix kernel $\widetilde{F}(\mathbf{p};j,m,\kappa;j',m',\kappa')$. In virtue of (28) the operator $\widetilde{F}(\mathbf{p})$ has a block-diagonal structure with respect to the index j. In other words, let $(\widetilde{F}_{jj'}(\mathbf{p}))$ be the matrix representation of the operator $\widetilde{F}(\mathbf{p})$ [all operators $\widetilde{F}_{jj'}(\mathbf{p})$ act in the space $\mathbf{C}^M\otimes\mathscr{G}_K$], then the matrix $\widetilde{F}_{jj'}(\mathbf{p})$ is a diagonal one:

$$\widetilde{F}_{jj'}(\mathbf{p})=\delta_{jj'}\widetilde{F}_j(\mathbf{p}). \tag{30}$$

Each operator in (30) is defined in an obvious way according to the formula (26).

Let V be a unitary operator in the space $\mathbf{C}^M\otimes\mathscr{G}_K$ having the form

$$V=U\otimes I_{\mathscr{G}_K}, \tag{31}$$

where U is a unitary operator in the space $\mathbf{C}^M$ with a matrix of the form

$$\begin{pmatrix}0 & I_{M-1}\\ \exp(2\pi ip2) & 0\end{pmatrix}$$

(here I_n denotes the $n\times n$ identity matrix). It is evident that U acts onto the vectors $\mathbf{e}_m$ of a standard basis as follows:

$$U\mathbf{e}_m=\exp[2\pi i\,\delta_{m0}p_2]\mathbf{e}_{m\ominus1}, \tag{32}$$

hence

$$U^*\mathbf{e}_m=\exp[-2\pi i\,\delta_{m,M-1}p_2]\mathbf{e}_{m\oplus1}; \tag{33}$$

here $n\oplus m$ and $n\ominus m$ are addition and subtraction modulo M, respectively.

Proposition 3.5: The following relation is valid for each $\mathbf{p}\in\mathbf{T}^2_\eta$:

$$V\widetilde{F}_j(\mathbf{p})V^*=\widetilde{F}_{j\oplus 1}(\mathbf{p}). \tag{34}$$

Proof: In virtue of (32) and (33), we get

$$\begin{aligned}(V\widetilde{F}_jV^*)&(\mathbf{p};m,\kappa;m',\kappa')\\ &=\langle\mathbf{e}_m|U\widetilde{F}_j(\mathbf{p};\kappa,\kappa')U^*\mathbf{e}_{m'}\rangle\\ &=\langle U^*\mathbf{e}_m|\widetilde{F}_j(\mathbf{p};\kappa,\kappa')U^*\mathbf{e}_{m'}\rangle\\ &=\exp[2\pi ip_2(\delta_{m,M-1}-\delta_{m',M-1})]\langle\mathbf{e}_{m\oplus 1}|\widetilde{F}_j(\mathbf{p};\kappa,\kappa')\mathbf{e}_{m'\oplus 1}\rangle\\ &=\exp[2\pi ip_2(\delta_{m,M-1}-\delta_{m',M-1})]\widetilde{F}_j(\mathbf{p};m\oplus 1\kappa;m'\oplus 1,\kappa').\end{aligned}$$

Let us prove that

$$\exp[2\pi ip_2(\delta_{m,M-1}-\delta_{m',M-1})]\widetilde{F}_j(\mathbf{p};m\oplus 1\kappa;m'\oplus 1,\kappa')=\widetilde{F}_{j\oplus 1}(\mathbf{p};m,\kappa;m',\kappa'). \tag{35}$$

This is evident for $m\neq M-1$ and $m'\neq M-1$ [see (29)]. Let $m=M-1$, but $m'\neq M-1$. Then

$$\begin{aligned}\widetilde{F}_j(\mathbf{p};m\oplus 1,\kappa;m'\oplus 1,\kappa')&=\exp[-\pi i\,\eta(m'+1)\kappa\wedge\mathbf{a}_2]\sum_{\lambda_1,\lambda_2\in\mathbf{Z}}F(\lambda_1\mathbf{a}_1+(\lambda_2M-m'-1)\mathbf{a}_2\\ &\quad+\kappa;\kappa')\exp[\pi i\,\eta\kappa\wedge(\lambda_1\mathbf{a}_1+\lambda_2M\mathbf{a}_2)-2\pi i(\lambda_1p_1+\lambda_2p_2+(\lambda_1\eta/2)\\ &\quad\times(M\lambda_2+m'+1+2j))]\\ &=\exp[-\pi i\,\eta m'\kappa\wedge\mathbf{a}_2]\sum_{\lambda_1,\lambda_2\in\mathbf{Z}}F(\lambda_1\mathbf{a}_1+((\lambda_2-1)M+m-m')\mathbf{a}_2\\ &\quad+\kappa;\kappa')\exp[\pi i\,\eta\kappa\wedge(\lambda_1\mathbf{a}_1+((\lambda_2-1)M+m)\mathbf{a}_2)-2\pi i(\lambda_1p_1+\lambda_2p_2\\ &\quad+(\lambda_1\eta/2)(M(\lambda_2-1)+m'+m+2j+2))]\\ &=\exp(-2\pi ip_2)\widetilde{F}_{j\oplus 1}(\mathbf{p};m,\kappa;m',\kappa').\end{aligned}$$

Thus, in this case the equality (34) is proved. Let now $m'=M-1$, but $m\neq M-1$. Then

$$\begin{aligned}\widetilde{F}_j(\mathbf{p};m\oplus 1,\kappa;m'\oplus 1,\kappa')&=\sum_{\lambda_1,\lambda_2\in\mathbf{Z}}F(\lambda_1\mathbf{a}_1+(\lambda_2M+m+1)\mathbf{a}_2+\kappa;\kappa')\\ &\quad\times\exp[\pi i\,\eta\kappa\wedge(\lambda_1\mathbf{a}_1+(\lambda_2M+m+1)\mathbf{a}_2)-2\pi i(\lambda_1p_1+\lambda_2p_2\\ &\quad+(\lambda_1\eta/2)(M\lambda_2+m+1+2j))]\\ &=\exp[-\pi i\,\eta m'\kappa\wedge\mathbf{a}_2]\sum_{\lambda_1,\lambda_2\in\mathbf{Z}}F(\lambda_1\mathbf{a}_1+((\lambda_2+1)M+m-m')\mathbf{a}_2\\ &\quad+\kappa;\kappa')\\ &\quad\times\exp[\pi i\,\eta\kappa\wedge(\lambda_1\mathbf{a}_1+((\lambda_2+1)M+m)\mathbf{a}_2)-2\pi i(\lambda_1p_1+\lambda_2p_2\\ &\quad+(\lambda_1\eta/2)(M(\lambda_2+1)+m+m'+2+2j-2M))]\\ &=\exp(2\pi ip_2)\widetilde{F}_{j\oplus 1}(\mathbf{p};m,\kappa;m',\kappa').\end{aligned}$$

Hence, in this case the equality (34) is also valid. If last $m=m'=M-1$, then we get

$$\begin{aligned}\widetilde{F}_j(\mathbf{p};m\oplus 1,\kappa;m'\oplus 1,\kappa')&=\sum_{\lambda_1,\lambda_2\in Z}F(\lambda_1\mathbf{a}_1+\lambda_2 M\mathbf{a}_2+\kappa;\kappa')\exp[\pi i\eta\kappa/\!\backslash(\lambda_1\mathbf{a}_1+\lambda_2 M\mathbf{a}_2)\\&\quad-2\pi i(\lambda_1 p_1+\lambda_2 p_2+(\lambda_1\eta/2)(M\lambda_2+2j))]\\&=\exp[-\pi i\eta m'\kappa/\!\backslash\mathbf{a}_2]\sum_{\lambda_1,\lambda_2\in\mathbf{Z}}F(\lambda_1\mathbf{a}_1+(\lambda_2 M+m-m')\mathbf{a}_2+\kappa;\kappa')\\&\quad\times\exp[\pi i\eta\kappa/\!\backslash(\lambda_1\mathbf{a}_1+(\lambda_2 M+m)\mathbf{a}_2)-2\pi i(\lambda_1 p_1+\lambda_2 p_2\\&\quad+(\lambda_1\eta/2)(M\lambda_2+m+m'+2+2j-2M))]\\&=\widetilde{F}_{j\oplus 1}(\mathbf{p};m,\kappa;m',\kappa').\end{aligned}$$

The proof is complete. ■

Corollary: Let $\mathbf{p}\in\mathbf{T}^2_\eta$ *be fixed. Then the operators* $\widetilde{F}_j(\mathbf{p})$ $(j=0,\ldots,M-1)$ *are mutually unitarily equivalent.* ■

Now we find the matrix $\widetilde{F}(\mathbf{p};j,m,\kappa;j',m',\kappa')$, where $F=Q(z)-A=Q(z)-(B+T)$. In virtue of Proposition 3.5, it is sufficient to determine the matrices $\widetilde{F}_0(\mathbf{p};m,\kappa;m',\kappa')=\widetilde{F}(\mathbf{p};0,m,\kappa;0,m',\kappa')$ only. It is simple to show that

$$\widetilde{Q}_0(\mathbf{p};m,\kappa;m',\kappa')=\begin{cases}q(z), & \text{if } m=m' \text{ and } \kappa=\kappa';\\ 0, & \text{otherwise.}\end{cases}\tag{36}$$

Similarly,

$$\widetilde{B}_0(\mathbf{p};m,\kappa;m',\kappa')=\begin{cases}B_0, & \text{if } m=m' \text{ and } \kappa=\kappa',\\ 0, & \text{otherwise.}\end{cases}\tag{37}$$

To determine the matrix $\widetilde{T}_0$ let us introduce the following notations:

$$L_1=\begin{pmatrix}0&0&\tau\\0&0&0\\0&0&0\end{pmatrix},\quad L_2=\begin{pmatrix}0&0&0\\0&0&0\\0&\tau&0\end{pmatrix},\quad L_3=\begin{pmatrix}0&0&0\\\tau&0&0\\0&0&0\end{pmatrix}.\tag{38}$$

Using (25), we obtain

$$\widetilde{T}_0(\mathbf{p};m,0;m',0)=\widetilde{T}_0(\mathbf{p};m,\mathbf{b};m',\mathbf{b})=0,\quad\forall m,m'.\tag{39}$$

Moreover, the Hermitian symmetry gives us

$$\widetilde{T}_0(\mathbf{p};m,\mathbf{b};m',0)=\widetilde{T}_0^*(\mathbf{p};m',0;m,\mathbf{b}),\quad\forall m,m'.\tag{40}$$

To calculate the nonzero elements of the matrix $\widetilde{T}_0(\mathbf{p})$, we shall deal with three cases.

1. Case M=1

In this case the indices m,m' are equal to zero, and may be omitted from the notations. Simple calculations give us

$$\widetilde{T}_0(\mathbf{p};0,\mathbf{b})=\exp(-2\pi i p_1)L_1+\exp(-2\pi i p_2)L_2+\exp[-2\pi i(p_1+p_2+N/2)]L_3,\tag{41}$$

$$\widetilde{T}_0(\mathbf{p};\mathbf{b},0)=\exp(2\pi i p_1)L_1^*+\exp(2\pi i p_2)L_2^*+\exp[2\pi i(p_1+p_2+N/2)]L_3^*.\tag{42}$$

Considering cases 2 and 3, we shall write $\widetilde{T}^{(0)}_{\kappa\kappa'}(\mathbf{p};m,m')$ instead of $\widetilde{T}^{(0)}(\mathbf{p};m,\kappa;m',\kappa')$. In virtue of (39) and (40), it is sufficient to find the matrix elements $\widetilde{T}^{(0)}_{0\mathbf{b}}(\mathbf{p}m,m')$ only.

2. Case $M=2$

Simple calculations give us

$$\begin{gathered}\widetilde{T}^{(0)}_{0\mathbf{b}}(\mathbf{p};0,0)=\exp(-2\pi i p_1)L_1,\\ \widetilde{T}^{(0)}_{0\mathbf{b}}(\mathbf{p};1,1)=\exp[-2\pi i(p_1+\eta)]L_1,\\ \widetilde{T}^{(0)}_{0\mathbf{b}}(\mathbf{p};1,0)=L_2+\exp[-2\pi i(p_1+\eta/2)]L_3,\\ \widetilde{T}^{(0)}_{0\mathbf{b}}(\mathbf{p};0,1)=\exp(-2\pi i p_2)L_2+\exp[-2\pi i(p_1+p_2+3\eta/2)]L_3.\end{gathered} \tag{43}$$

3. Case $M>2$

Only the following three subcases are possible:

$$\text{(i)}\quad \lambda_1=\pm 1, M\lambda_2+m-m'=0;$$

$$\text{(ii)}\quad \lambda_1=0,\quad M\lambda_2+m-m'=1;$$

$$\text{(iii)}\quad \lambda_1=0,\quad M\lambda_2+m-m'=-1.$$

In subcase (i) the number $\lambda_2=(m-m)/M$ should be an integer. Since $0\leqslant m,m'<M$, then $-(M-1)\leqslant m'-m\leqslant M-1$, hence λ_2 is an integer iff $m-m'=0$. Thus the condition (i) may be rewritten in the form

$$\text{(i}')\quad \lambda_1=\pm 1,\quad \lambda_2=0,\quad m=m'.$$

In subcase (ii) the number $\lambda_2=(1+m-m')/M$ should be an integer. Since $-M+2\leqslant 1+m+m'\leqslant M$, then $1+m-m'=0$ or $1+m-m'=M$. Thus we have two possibilities:

$$\begin{aligned}&\text{(ii}')\quad \lambda_1=0,\quad \lambda_2=0,\quad m'=m-1,\\ &\text{(ii}'')\quad \lambda_1=0,\quad \lambda_2=1,\quad m'=M+m-1.\end{aligned}$$

In virtue of the inequality $0\leqslant m'\leqslant M-1$ subcase (ii″) may be reformulated in the following manner:

$$\text{(ii}'')\quad \lambda_1=0,\quad \lambda_2=1,\quad m=0,\quad m'=M-1.$$

The condition (iii) divides into the following two subcases by an analogous way:

$$\begin{aligned}&\text{(iii}')\quad \lambda_1=0,\quad \lambda_2=0,\quad m=m'-,\\ &\text{(iii}'')\quad \lambda_1=0,\quad \lambda_2=-1,\quad m'=0,\quad m=M-1.\end{aligned}$$

Using the relations (i′),...,(iii″), it is easy to find all nonzero elements of the matrix $\widetilde{T}_0(\mathbf{p})$. As a result, we obtain for $M>2$:

$$\widetilde{T}^{(0)}_{0\mathbf{b}}(\mathbf{p};m,m)=\exp[-2\pi i(p_1+\eta m)]L_1,$$

$$\widetilde{T}^{(0)}_{0\mathbf{b}}(\mathbf{p};m,m-1)=L_2+\exp[-2\pi i(p_1+\eta(2m-1)/2)]L_3,\quad 1\leqslant m\leqslant M-1,$$

$$\widetilde{T}^{(0)}_{0\mathbf{b}}(\mathbf{p};0,M-1)=\exp(-2\pi i p_2)L_2+\exp[-2\pi i(\mathbf{p}_1+p_2+\eta(2M-1)/2)]L_3. \tag{44}$$

Now we describe the spectrum of the Hamiltonian H_A. First, we note that the spectrum of the unperturbed Hamiltonian H_0 coincides (as a set) with the spectrum of H_0^0, which is a discrete one. Hence, the spectrum of H_0 is pure point and consists of infinitely degenerate eigenvalues (Landau levels). A point $E\in\sigma(H_0)$ is contained in the spectrum of H_A as an eigenvalue, if $\eta>1$ (Refs. 23, 27, and 28). Other points of the spectrum $\sigma(H_A)$ are defined by the dispersion equation

$$\det(\widetilde{Q}(E)-\widetilde{T}(\mathbf{p}))=0. \tag{45}$$

The equation (45) determines a multivalued function $E(\mathbf{p})$. The continuous single-valued branches $E_j(\mathbf{p})$ of the function $E(\mathbf{p})$ are called the dispersion laws. The images of the functions $E_j(\mathbf{p})$ are segments that form bands of the spectrum. In virtue of the corollary of Proposition 3.5, each band is M-fold degenerate. As in Ref. 23, the following picture of the spectrum $\sigma(H_A)$ can be established: an eigenvalue of the operator H_0 broadens into a band that lies below the eigenvalue; each band divides into M subbands. It should be emphasized that the bands and the subbands may overlap.

The origin of an eigenvalue $E\in\sigma(H_A)$ that is simultaneously an eigenvalue of the unperturbed operator H_0 is clear: it corresponds to the classical trajectory lying in an area Ω_γ, wholly.[43] The following theorem, which is the main result of the section, shows that there is another possibility of appearance of bound states in the spectrum $\sigma(H_A)$. Namely, a bound state may be arise as a constant solution (independent of the quasimomentum $\mathbf{p}$) of the dispersion equation (45).

Theorem 3.1: *If η is an integer: $\eta=N$, then elements of the ''fitting matrix'' B can be chosen in such a way that the dispersion equation has a solution independent of a quasimomentum $\mathbf{p}\in\mathbf{T}^2$ and the tunneling parameter τ.*

Proof: Let $E_0\in\mathbf{R}\backslash\sigma(H_0)$; we put

$$\beta_{ij}=\begin{cases} q_{ij}(E_0), & \text{if } i=j,\\ q_{ij}(E_0)-1, & \text{if } i\neq j.\end{cases}$$

Evidently, $B=\|\beta_{ij}\|$ is a Hermitian matrix. If τ is not an eigenvalue of $-B$, then the Hamiltonian H_A is well defined. By symmetry, $q_{jj}(z)$ does not depend on j; denote $p(z)=q_{jj}(z)-\beta_{jj}$. After cumbersome algebra, we bring the left-hand side of Eq. (45) for $z=E_0$ to the form

$$p^6+9\tau p^4-4\tau^2p^3+a_2\tau^3p^2+a_1\tau^4p=0, \tag{46}$$

where

$$a_2=-18+2[\cos 2\pi(p_1+N/2)+\cos 2\pi(p_2+N/2)+\cos 2\pi(p_1-p_2)],$$

$$a_1=4[3-\cos 2\pi(p_1+N/2)+\cos 2\pi(p_2+N/2)+\cos 2\pi(p_1-p_2)].$$

The theorem follows from Eq. (46). ■

Remark: The hypothesis of Theorem 3.1 does not exclude the case $N=0$ as well.

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Singular continuous spectra and discrete wave packet dynamics

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Asymptotic estimates which relate the diffusion of wave packets on discrete lattices to Hausdorff dimensions of the local density of states are discussed. © *1996 American Institute of Physics.* [S0022-2488(96)01010-9]

I. INTRODUCTION

The basic mathematical objects of this article are a discrete unitary group $\{U^t\}_{t\in\mathbf{Z}}$ in an infinite-dimensional separable Hilbert space $\mathscr{H}$, and a complete Hilbert basis $B=\{e_n\}_{n\in\mathbf{Z}}$. The discrete-time evolution of vectors $\psi\in\mathscr{H}$ is obtained by repeated application of the generator U. Upon expanding vectors $U^t\psi$ on the basis B, vectors in $l^2(\mathbf{Z})$ are obtained, which can be physically depicted as quantum wave packets propagating on a discrete one-dimensional lattice, the sites of which are in one-to-one correspondence to the basis vectors. According to conventional wisdom, long-time wave packet dynamics and spectral structure are qualitatively connected: wave packets will remain essentially confined within a finite region, or will propagate unboundedly, depending on the discrete or continuous nature of the spectrum. The intuitive idea, that the motion of wave packets will be more ''delocalized,'' the more ''continuous'' the spectrum, turns out to have a validity at all points between the extreme cases of discrete and absolutely continuous spectra. It has in fact been turned into rigorous estimates, which relate the asymptotical (in time) wave packet dynamics, to ''spectral'' dimensions of the Hausdorff type, which describe how continuous the spectral measure (local density of states) associated with the vector ψ is. Estimates of this kind make up the subject of this article.

Physical motivation is provided by the increasingly frequent apparition of singular continuous spectra in quantum mechanical models for electron dynamics in solids, where such spectra may have a great influence on quantum transport. This issue has been numerically investigated on several quasiperiodic, incommensurate models. Fractal dimensions which are somehow related to the singular continuous structure of the spectrum have been numerically obtained from a scaling analysis of the band spectra of periodic approximants.[1–4] The results obtained in this way suggest a connection between ''band-scaling'' fractal dimensions and (anomalous) wave packet diffusion. Recourse to more sophisticated concepts of fractal analysis[5,6] now appears necessary, in order to further pursue this line of investigation; a theoretical approach has been proposed.[5]

Further numerical works have investigated the multifractal structure of the spectral measure itself, on different models.[6–8] A comparison of such data with data from numerical simulation of the quantum evolution in time[7,8] confirms a qualitative connection, but at the same time indicates that no simple exact relation exists between diffusion exponents and dimensions of the local density of states.

Rigorous results available to date concern the decay in time of the time-averaged probability of survival in the initial state,[3,9–11] and the algebraic growth of the ''width'' of wave packets, as measured, e.g., by the moments of the associated probability distribution. In the latter case, through successive generalizations the result has been obtained[12–16] that the exponent of growth is bounded from below by the information dimension D_1 of the spectral measure, independently of the choice of the basis B.

No such general *upper* bound is to be expected. The very definition of moments depends on the labeling of the basis vectors, and so do the corresponding growth exponents, independently of

the properties of spectral measures. Thus, although the growth exponents are in all cases subject to the above mentioned lower bound, they do actually depend on the choice of a basis; therefore the ''spatial'' structure of the operator U on the basis B has to be taken into account in order to get upper bounds on growth exponents. For instance, it will be shown in sec. V that a ballistic upper bound is valid as soon as the operator U satisfies a certain ''analyticity'' property with respect to the basis B.

According to empirical evidence, the actual growth exponents can be

significantly different from both the ballistic upper bound and the D_1 lower bound. Getting precise asymptotic estimates on the long-time behavior of wave packets is an open problem that may not be solvable on the level of generality attained by the existing bounds.

In this article a different dynamical characterization of singular continuous spectra is given, based on the growth with time of the dimension of the Hilbert subspace explored by the trajectory of a state ψ. By refining and extending results of Ref. 15, it will be shown that the corresponding growth exponents are related by upper and lower estimates to the fractal and Hausdorff dimensions, respectively, of the spectral measure. These results are presented in sec. IV below. In secs. II and III a survey of some basic definitions and of previous results, which are needed for the elaborations in sec. IV and VI, is given.

Finally, in this article some steps are taken towards a multifractal analysis of the spatial structure of the wave packet, following an idea of Evangelou and Katsanos.[17] Such an analysis is suggested by numerical evidence[15,17] that growth exponents of moments do not scale in a simple way with the order of the moments (*multiscaling*), and so give rise to a nontrivial spectrum of growth exponents. This can be taken as an indication that wave packets develop a sort of multifractal structure in space, which may in turn reflect an analogous structure of eigenfunctions.[1,18] From this viewpoint, estimating growth exponents is but a special aspect of a more general problem: how is this structure related to the multifractal structure of the spectral measures? Some results in this direction, which follow from general lower bound on growth exponents, are presented in sec. VI.

Multiscaling is also a justification for an aspect of the present article, which may appear disturbing to the reader: the proliferation of different quantities, all of which somehow measure the growth of wave packets, but still may behave differently in time. Establishing precise connections between these different definitions would enable reducing their number; however, this as yet unsolved problem is closely related to the problem of upper bounds. Previous general remarks about the latter problem are valid in this case, too.

II. SPECTRAL DIMENSIONS

In the following, the set $\{\lambda \in [0,2\pi]: e^{i\lambda} \in \mathrm{Spec}(U)\}$ will be called ''spectrum.'' The spectral measure of the vector ψ will be supported in this set and is denoted μ_ψ; the label ψ will be usually omitted. The spectral measure μ_ψ is uniquely defined by

$$(\psi, U^t\psi) = \int_0^{2\pi} e^{it\lambda} d\mu_\psi(\lambda)$$

valid at all times t. The distribution of the spectral measure is also called (integrated) *local density of states*, at least in concrete cases in which ψ is an eigenvector of a position operator. In this section we assume $\mu_\psi([0,2\pi]) = \|\psi\|^2 = 1$.

By $d_\mu^-(x), d_\mu^+(x)$ we will denote the lower and upper pointwise dimensions of μ at the point x of the spectrum, defined by

$$d_\mu^-(x) = \lim \inf_{\delta \searrow 0} \frac{\log\, \mu(I_\delta(x))}{\log\, \delta}, \quad d_\mu^+(x) = \lim \sup_{\delta \searrow 0} \frac{\log\, \mu(I_\delta(x))}{\log\, \delta}$$

where $I_\delta(x)$ is an interval of size δ centered at x. If $d_\mu^-(x)=d_\mu^+(x)$, then their common value defines the *local*, or *pointwise*, dimension of the measure μ at the point x. Upper and lower global dimensions of μ will be defined by

$$\dim_H^+(\mu)=\mu\text{-ess sup}d_\mu^-(x)$$
$$\dim_H^-(\mu)=\mu\text{-ess inf}d_\mu^-(x).$$

Note that both definitions involve the *lower* local dimension only. The subscript H stands for Hausdorff; the connection to Hausdorff dimensions is clarified by the following result, where $d_H(A)$ denotes the Hausdorff dimension of a set A.

Theorem 1:

$$\dim_H^+(\mu):=\inf\{d_H(A):\mu(A)=1\};$$
$$\dim_H^-(\mu)=\sup\{\alpha:\mu(A)=0 \quad \text{if} \quad d_H(A)<\alpha\}$$

Proof: These equalities follow from general results of Rodgers and Taylor,[19] compactly reviewed in Refs. 16 and 20. Let $\beta>\mu$ -ess sup$d_\mu^-(x)$; then μ is supported by a set of dimension β,[20] so $\beta\geqslant\dim_H^+(\mu)$ by definition; hence, μ-ess sup$d_\mu^-(x)\geqslant\dim_H^+(\mu)$. Conversely, let $\beta<\mu$-ess sup$d_\mu^-(x)$, and let S be any set supporting μ. Then $d_\mu^-(x)>\beta$ for all x in a set $B\subseteq S$ of positive measure. If χ_B is the characteristic function of B, and $d\mu_B:=\chi_B d\mu$, then the measure μ_B is supported by B, and satisfies $d_{\mu_B}^-(x)\geqslant d_\mu^-(x)>\beta$ for μ_B—almost all x. Any set of Hausdorff dimension less than β must have zero μ_B measure,[20] which entails $d_H(B)\geqslant\beta$, and also $d_H(S)\geqslant\beta$. This holds for any S supporting μ, therefore $\dim_H^+(\mu)\geqslant\beta$; it follows that μ-ess sup$d_\mu^-(x)\leqslant\dim_H^+(\mu)$.

The proof of the second equality is similar. Let $\gamma=\mu$-ess inf$d_\mu^-(x)$. Let us prove $\gamma\leqslant\dim_H^-(\mu)$. If $\gamma=0$ this is obvious. If $\gamma>0$, let $\beta<\gamma$; then $d_\mu{}^-(x)>\beta$ for μ—almost all x, so μ gives zero weight to any set of dimension less than β, which means $\beta\leqslant\dim_H^-(\mu)$. Conversely, if $\beta>\gamma$, then $d_\mu^-(x)<\beta$ on a set S of positive measure. This set S is a subset of the set T_β, defined as

$$T_\beta=\left\{x:\lim\sup_{\delta\searrow 0}\frac{\mu(I_\delta(x))}{\delta^\beta}=+\infty\right\}. \tag{2.1}$$

It is a known result[20] that a set T'_β exists, with $d_H(T'_\beta)\leqslant\beta$, and $\mu(T'_\beta\cap T_\beta)=\mu(T_\beta)$. Therefore, if $S'=S\cap T'_\beta$, then $\mu(S')=\mu(S)>0$, and $d_H(S')\leqslant d_H(T'_\beta)\leqslant\beta$. Hence, $\beta>\dim_H^-(\mu)$. □

If $\dim_H^-(\mu)=\dim_H^+(\mu)=d$ [that is, if $d_\mu{}^-(x)=d$, μ-*a.e.*], the measure is said to have *exact* dimension d. This denomination is not universally agreed upon; for instance, a measure is sometimes[21] said to have exact dimension d if $d_\mu{}^-(x)=d_\mu^+(x)=d$, μ-*a.e.*, that is, if the measure has a well defined constant local dimension μ-*a.e.* A measure with this property will be called here an *exactly scaling* (ES) measure. ES measures also have exact dimension in the sense used here, but the converse is not true—in Ref. 20 examples are given of measures with exact dimension 0 which have $d_\mu^+(x)=1$ μ-*a.e.* Although exceptional on mathematical grounds, in the physical literature the ES property is often assumed of ''smooth multifractal'' measures. On purely empirical grounds, and on the present level of numerical accuracy, this assumption has not shown, so far, any serious inconsistency with numerical data, at least in a few test cases which are relevant to the subject of this article, and which were mentioned in the Introduction. On the other hand, there are certain non generic features in these cases, which enforce great caution in assuming that a likewise smooth structure of spectral measures will be typical, even within the class of quasi-periodic Schrödinger operators.

$\dim_H^+(\mu)$ is known as the Hausdorff dimension of the measure μ. It is also sometimes called the *information dimension* $D_I(\mu)$ of μ,[22] although the latter name is more often given to a

generalized fractal dimension, usually denoted $D_1(\mu)$ [which corresponds to $q=1$ in the set of generalized fractal (box-counting) dimensions $D_q(\mu)$]. For ''smooth'' multifractal measures (as discussed, e.g., in Ref. 23) $D_I(\mu)=D_1(\mu)$, but this is not true in general, not even of exactly dimensional measures.

The *fractal* dimension of μ will instead be defined as

$$\dim_F(\mu)=\sup_{0<\epsilon<1}\inf_K\{d_F(K):\ K\ \text{ compact},\ \ \mu(K)>1-\epsilon\} \tag{2.2}$$

where the fractal dimension $d_F(K)$ of a compact set K is defined by[24]

$$d_F(K)=\lim\ \sup_{\delta\searrow 0}\frac{\log\ N_K(\delta)}{\log(1/\delta)}.$$

Here, $N_K(\delta)$ is the minimum number of closed intervals of size $\leqslant\delta$ which are needed to cover K.

Theorem 2: $\dim_F(\mu)\leqslant\mu$-ess sup $\ d^+_\mu(x)$.

Proof: Let $d^+_\mu(x)<\alpha$ for μ—almost all x; we have to show that $\dim_F(\mu)\leqslant\alpha$. Because

$$\lim_{\delta_0\to 0}\ \sup_{\delta<\delta_0}\frac{\log\ \mu(I_\delta(x))}{\log\ \delta}<\alpha \tag{2.3}$$

for all x in a set of full measure, then, on the strength of the Egorov theorem, we can find a set $J_\epsilon\subset(0,2\pi)$, of measure $\mu(J_\epsilon)>1-\epsilon/2$, in which the monotonic limit on the lhs of (2.3) is uniform, so there is a $\overline{\delta_{\epsilon,\alpha}}$ such that

$$\mu(I_\delta(x))>\delta^\alpha\quad\forall x\in J_\epsilon,\quad\forall\,\delta<\overline{\delta_{\epsilon,\alpha}}. \tag{2.4}$$

Let us fix δ so small that (2.4) holds. The family $\{I_\delta(x)\}_{x\in J_\epsilon}$ is a covering of J_ϵ, from which we can extract a finite or countable covering of the same set with no more than c overlaps, with c a fixed integer (this comes, e.g., from the Besicovitch covering lemma, as formulated in Ref. 25). Denote by $I_1,\ldots$ the intervals in this covering, and let M be their number. From $m\,\delta^\alpha\leqslant\Sigma_1^m\mu(I_j)\leqslant c\,\mu(\cup_1^m I_j)\leqslant c$, which holds for any positive integer $m<M$, it follows that M is finite, $M\leqslant c\,\delta^{-\alpha}$. Finally, choose a compact $K\subset J_\epsilon$, with $\mu(J_\epsilon\backslash K)<\epsilon/2$. For all sufficiently small δ, $N_K(\delta)\leqslant M$, so $d_F(K)\leqslant\alpha$; moreover, $\mu(K)>1-\epsilon$, so, from (2.2), we conclude $\dim_F(\mu)\leqslant\alpha$. □

Remark: Theorem 2 shows that the Hausdorff and the fractal dimensions of ES measures coincide.

III. SPREADING OF WAVE PACKETS

Let $B\equiv\{e_n\}_{n\in\mathbf{Z}}$ an orthonormal set. For any positive integer time t let

$$p_n(t):=\frac{1}{t}\sum_{s=0}^{t-1}|\psi_n(s)|^2 \tag{3.1}$$

where $\psi_n(t):=(e_n,U^t\psi)$. Since time averages like the one in (3.1) appear frequently in the following, the shorthand notation $\langle\cdot\rangle_{t_1}^{t_2}$ will be used for time averages from time t_1 to time t_2-1.

Equation (3.1) defines a finite measure $\mathscr{P}_{t,\psi}$ on subsets A of $\mathbf{Z}$, via $\mathscr{P}_{t,\psi}(A)=\Sigma_{k\in A}p_k(t)$. If B is complete, then the total mass of this measure is just $\|\psi\|^2$. A *minimal ϵ-support* of the measure $\mathscr{P}_{t,\psi}$ will be any finite family $\mathscr{T}_\epsilon\subset\mathbf{Z}$ such that (i) $\mathscr{P}_{t,\psi}(\mathscr{T}_\epsilon)>(1-\epsilon^2)\mathscr{P}_{t,\psi}(\mathbf{Z})$, and (ii)

$\mathscr{P}_{t,\psi}(\mathscr{F}') \leqslant (1-\epsilon^2)\mathscr{P}_{t,\psi}(\mathbf{Z})$ for any other finite family of indices $\mathscr{F}'$ such that $\sharp(\mathscr{F}') < \sharp(\mathscr{F}_\epsilon)$, where $\sharp$ denotes cardinality. The distribution (3.1) may have different minimal ϵ-supports, but they must have the same ''size'' $\sharp(\mathscr{F}_\epsilon)$, which will be denoted by $n_\epsilon(\psi,t,B)$. For simplicity's sake, in the following we shall often omit the complete list of parameters on which n_ϵ, and other quantities, depend, leaving understood those whose specification is not strictly necessary.

If μ_ψ is a purely continuous measure, then it is a classical result that $p_k(t) \to 0$ as $t \to \infty$, $\forall k$, so $\mathscr{P}_{t,\psi}$ gives smaller and smaller weight to any finite set $A \subset \mathbf{Z}$. Thus, if the total mass is constant, or at least bounded away from zero at all times, then n_ϵ diverges in the limit $t \to \infty$. This is true, in particular, when B is complete. It will be shown below that, in the latter case, n_ϵ diverges as soon as μ_ψ has a continuous component. Our aim here is to describe asymptotic bounds on the growth of n_ϵ, in terms of spectral dimensions of μ_ψ, defined in sec. II.

The asymptotic spreading of $\mathscr{P}_{t,\psi}$ can also be quantitatively described by other quantities, e.g. by the moments $m^{(\alpha)}(t)$, which are defined, for $\alpha > 0$, by

$$m^{(\alpha)}(t) := \sum_{k \in \mathbf{Z}} |k|^\alpha p_k(t).$$

The growth of n_ϵ as $t \to \infty$ bounds the growth of $(m^{(\alpha)})^{1/\alpha}$ from below, via a Chebyshev-like inequality. Instead, from the divergence of moments nothing can be inferred about the behavior of n_ϵ; examples are known, in which μ_ψ is pure-point, n_ϵ is bounded in time, but moments diverge algebraically.

A description of the asymptotical growth in time of quantities which in one way or another measure the ''size'' of wave packets is provided by upper and lower growth exponents, which, for a given positive sequence $c \equiv \{c_t\}$, labelled by the discrete time t, will be defined and denoted as follows:

$$\beta^-(c) = \lim \inf_{t \to \infty} \frac{\log c_t}{\log t}, \quad \beta^+(c) = \lim \sup_{t \to \infty} \frac{\log c_t}{\log t}. \tag{3.2}$$

Previous results by the present author[14,15] can be cast in the form of theorem 3 below. These results can be significantly strengthened (see remark 1 below), but the version used here is convenient for the purposes of this article.

Theorem 3: *Let* $\|\psi\| = 1$, $0 < \epsilon < 1$, *and suppose that* B *is complete. Then* $\beta^-(\{n_\epsilon(\psi,t)\}) \geqslant \dim_H^-(\mu)$.

Remark 1: An immediate corollary is $\beta^-(\{m^{(\alpha)}(t)\}) \geqslant \alpha \dim_H^-(\mu)$, because the growth of $n_\epsilon(\psi,t)$ bounds the growth of moments from below. Last[16] has strengthened this result, proving that $m^{(\alpha)}(t) > \text{const} \times t^{\alpha \dim_H^+(\mu)}$ for *any* spectral measure μ (Last's formulation is somewhat different, as it is given in terms of Hausdorff decompositions of μ). A similar generalization of Theorem 3 is also possible, yielding

$$\sup_\epsilon \beta^-(\{n_\epsilon\}) \geqslant \dim_H^+(\mu) \tag{3.3}$$

This step will be explained later.

Remark 2: The result is also true if B is not complete, still $\langle \|P_B \psi(t)\|^2 \rangle_0^t \geqslant \Delta^2 > 0$, $\forall t > 0$, P_B being the projection onto the subspace spanned by B. In this case Theorem 3 holds for $0 < \epsilon < \Delta$. The same is *not* true of the generalization mentioned in remark 1, though.

Remark 3: In Refs. 14 and 15 Theorem 3 was formulated for the case of exactly scaling measures μ. The proof given there is also valid for the present version, without any modification. Other minor differences require no special comment.

Remark 4: Combes and co-workers[13,11] and Last[16] generalize similar results to continuous unitary groups, generated by Schrödinger operators in $L^2(R^n)$.

The following form of Theorem 3 is proven in the same way, and will be used later, in the proof of Proposition 2.

Theorem 3a: *If B is an orthonormal (not necessarily complete) set, and there is a sequence of times $t_k \to \infty$ such that, $\forall k$*

$$\langle \| P_B U^s \psi \|^2 \rangle_{t_k}^{t_{k+1}} \geqslant \Delta^2, \tag{3.4}$$

then, for all sufficiently small positive $\epsilon < \Delta$,

$$\lim \inf_{k \to \infty} \frac{\log n_\epsilon(\psi, t_k)}{\log t_k} \geqslant \dim_H^-(\mu). \tag{3.5}$$

IV. EFFECTIVE DIMENSIONS

For $\psi \neq 0$ consider finite strings $\sigma_{s,t}(\psi) = \{U^s\psi, U^{s+1}\psi, \ldots, U^{s+t-1}\psi\}$ of the orbit of ψ. If μ_ψ has a continuous component, then, $\forall s,t$, $\sigma_{s,t}$ spans a subspace $\Sigma_{s,t}$ of $\mathscr{H}$, of dimension t. Nevertheless it may happen that the ''effective dimension'' of $\sigma_{s,t}$ is significantly smaller, in the sense that some subspace of $\Sigma_{s,t}$, of dimension $\ll t$, exists, such that $U^s\psi, U^{s+1}\psi, \ldots, U^{s+t-1}\psi$ have but a small component outside it. This raises the question, how does the effective dimension of the subspace spanned by a string of length t increase with t?

This question will be formalized as follows. Given $\epsilon \in (0,1)$, let $\theta_\epsilon(\sigma_{s,t}(\psi))$ be the minimum dimension of an orthogonal projector P in $\mathscr{H}$ such that $\|P^\perp U^j \psi\| < \epsilon$ for $s \leqslant j \leqslant s+t-1$. In other words, $\theta_\epsilon(\sigma_{s,t}(\psi))$ is the minimum dimension of a subspace such that the string $\sigma_{s,t}(\psi)$ lies within a distance ϵ of it. Moreover, let $\underline{\theta}_\epsilon(\sigma_{s,t}(\psi))$ be the minimum dimension of a subspace such that the same string lies within ϵ of it *in the average*, that is, $\langle \| P^\perp U^j \psi \|^2 \rangle_s^{s+t} < \epsilon^2$. The mentioned minimal subspaces can be assumed to be subspaces of the subspace spanned by $\sigma_{s,t}(\psi)$. Moreover, since $\sigma_{s,t}(\psi) = U^s(\sigma_{0,t}(\psi))$, all the strings of a given length are unitary images of one another, so $\underline{\theta}_\epsilon(\sigma_{s,t}(\psi))$ and $\theta_\epsilon(\sigma_{s,t}(\psi))$ only depend on t, and will therefore be denoted $\theta_\epsilon(\psi,t)$ and $\underline{\theta}_\epsilon(\psi,t)$. If $\epsilon > \|\psi\|$, then $\theta_\epsilon(\psi,t) = 0$.

Immediate consequences of these definitions are as follows.

Proposition 1:

(i) $\underline{\theta}_\epsilon(\psi,t) \leqslant \theta_\epsilon(\psi,t) \leqslant t$,

(ii) $\theta_\epsilon(\psi, t+s) \leqslant \theta_\epsilon(\psi,t) + \theta_\epsilon(\psi,s)$,

(iii) *if $\psi_1 \in \mathscr{H}_1, \psi_2 \in \mathscr{H}_2$ where $\mathscr{H}_1, \mathscr{H}_2$ are mutually orthogonal subspaces, invariant under U, then*

$$\theta_\epsilon(\psi_1 + \psi_2, t) \geqslant max[\,\theta_\epsilon(\psi_1,t), \theta_\epsilon(\psi_2,t)\,]. \tag{4.1}$$

Moreover, (ii and iii) also hold for $\overline{\theta_\epsilon}$.

Proof: (i) is obvious. (ii) follows from $\theta_\epsilon(\sigma_{0,t} \cup \sigma_{t,s}) \leqslant \theta_\epsilon(\sigma_{0,t}) + \theta_\epsilon(\sigma_{t,s})$. As to (iii), note that $\sigma_{0,t}(\psi_i) \subset \mathscr{H}_i$, and that vectors $\xi_1, \ldots, \xi_t$ exist, which span a subspace of dimension $\theta_\epsilon(\psi_1 + \psi_2, t)$, and satisfy $\|\xi_j - U^j(\psi_1 + \psi_2)\| < \epsilon$ for $j = 0, \ldots, t-1$. Now let projections $P_i \xi_j$ on $\mathscr{H}_i$ span a subspace $\mathscr{S}_i$ of $\mathscr{H}_i$, with $i = 1,2$. On one hand, $\dim(\mathscr{S}_i)$ cannot be larger than $\theta_\epsilon(\psi_1 + \psi_2, t)$, and on the other it cannot be less than $\underline{\theta}_\epsilon(\psi_i, t)$, because $\|P_i \xi_j - U^j \psi_i\| < \epsilon$ for $j = 0, \ldots t-1$. Thus $\theta_\epsilon(\psi_1 + \psi_2, t) \geqslant \underline{\theta}_\epsilon(\psi_i, t)$. For $\overline{\theta_\epsilon}$ the proof proceeds in a similar way. □

At given ϵ, ψ, both $\theta_\epsilon(\psi,t)$ and $\underline{\theta}_\epsilon(\psi,t)$ are positive nondecreasing sequences. Their growth exponents will be presently investigated.

Proposition 2: *If $d_\mu^-(x) > \alpha$, μ-a.e., then, for sufficiently small positive ϵ, $\beta^-(\overline{\theta_\epsilon}) \geqslant \alpha$.*

Proof: Given a sequence of times $t_k \to \infty$, such that

$$\beta^-(\overline{\theta_\epsilon}) = \lim_{k\to\infty} \frac{\log\, \overline{\theta_\epsilon}(\psi, t_k)}{\log\, t_k},$$

let us recursively construct a subsequence $\{t_{k_j}\}$, with $k_1 = 1$, and

$$k_{j+1} = \min\{k: \quad t_k > 2^{l_j}\},$$

where $l_j = \Sigma_{s=1}{}^{j} t_{k_s}$. Let us partition the orbit of ψ into segments $\sigma_j \equiv \{\psi(s), l_j \leqslant s < l_{j+1}\}$; the length of σ_j is thus t_{k_j}. According to the definition of $\overline{\theta_\epsilon}(\psi, t)$ we can find a sequence $\{\varphi_t\}$ of vectors such that, $\forall j$,

$$\langle \| \varphi_s - U^s \psi \|^2 \rangle_{l_j}^{l_{j+1}} < \epsilon^2 \tag{4.2}$$

(so that σ_j lies within an average distance ϵ of the subspace spanned by $\{\varphi_s,\ l_j \leqslant s < l_{j+1}\}$), and, moreover, the subspace spanned by $\{\varphi_s, l_j \leqslant s < l_{j+1}\}$ has exactly dimension $\theta_\epsilon(\psi, t_{k_j})$. On orthonormalizing the sequence $\{\varphi_t\}$ we obtain an orthonormal set B_ϵ with the property that, $\forall j$

$$\langle \| P_{B_\epsilon} U^s \psi \|^2 \rangle_{l_j}^{l_{j+1}} > \| \psi \|^2 - \epsilon^2. \tag{4.3}$$

Therefore we can use Theorem 3a to the effect that, if ϵ is small enough,

$$\lim\ \inf_{j\to\infty} \frac{\log\, n_\epsilon(\psi, B_\epsilon, l_j)}{\log\, l_j} \geqslant \alpha. \tag{4.4}$$

On the other hand, $\psi(0), \ldots, \psi(l_j)$ lie within an average distance ϵ of the subspace spanned by the first l_j vectors φ_t. This subspace has dimension $N(l_j) \leqslant \Sigma_{s=1}^{j} \overline{\theta_\epsilon}(\psi, t_{k_s})$, and is also spanned by the first $N(l_j)$ vectors in B_ϵ. From the definition of a minimal ϵ- support it follows that $n_\epsilon(\psi, B_\epsilon, l_j) \leqslant N(l_j) \leqslant \Sigma_{s=1}{}^{j} \theta_\epsilon(\psi, t_{k_s})$; therefore, using Proposition 1,

$$\frac{\log_2 n_\epsilon(\psi, B_\epsilon, l_j)}{\log_2 l_j} \leqslant \frac{\log_2 \Sigma_{s=1}^{j} \overline{\theta_\epsilon}(\psi, t_{k_s})}{\log_2 l_j} \leqslant \frac{\log_2 \Sigma_{s=1}^{j-1} t_{k_s}}{\log_2 t_{k_j}} + \frac{\log_2 \overline{\theta_\epsilon}(\psi, t_{k_j})}{\log_2 t_{k_j}}$$

$$\leqslant \frac{\log_2 l_{j-1}}{l_{j-1}} + \frac{\log_2 \overline{\theta_\epsilon}(\psi, t_{k_j})}{\log_2 t_{k_j}}$$

Taking the limit $j \to \infty$ and using (4.4) the required result is obtained. □

One further step can be taken, in the spirit of Last's extension of Theorem 3.[16] Recall that $\dim_H^+(\mu) = \mu$-ess $\sup d_\mu^-(x)$. For any small η, let $A_\eta = \{x: d_\mu^-(x) > \dim_H^+(\mu) - \eta\}$; then $\mu(A_\eta) > 0$, and one can write $\psi = \psi_1 + \psi_2$, the spectral decomposition of ψ according to the set A_η and its complement. Then $d\mu_{\psi_1} = \chi_{A_\eta} d\mu$, so $d_{\mu_{\psi_1}}^-(x) \geqslant d_\mu^-(x)$, and $\dim_H^-(\mu_{\psi_1}) \geqslant \dim_H^+ \times (\mu) - \eta$. On account of Proposition 2 and of Proposition 1(iii), $\beta^-(\overline{\theta_\epsilon}) \geqslant \dim_H^+(\mu) - \eta$ if ϵ is smaller than some ϵ_0. The latter depends in general on η, so we can conclude the following.

Proposition 3: *For any $\psi \neq 0$, and for sufficiently small ϵ, $\beta^-(\overline{\theta_\epsilon}(\psi, t)) \geqslant \dim_H^-(\mu)$. Moreover,*

$$\sup_\epsilon \beta^-(\overline{\theta_\epsilon}(\psi, t)) \geqslant \dim_H{}^+(\mu).$$

Remark: This result includes all the versions of Theorem 3 discussed in Remarks 1–3, and inequality (3.3) in particular.

Proposition 4: $\forall \epsilon>0$, $\beta^+(\theta_\epsilon)\leqslant \dim_F(\mu)$ (*the fractal dimension of* μ).

Proof: By spectral equivalence, we can work in the space $\mathscr{L}^2([0,2\pi],\mu)$, where $\psi(t)\equiv e^{itx}$ μ-*a.e.* Choose $\epsilon>0$ and define, for all integer times t, $\delta_t=\epsilon/t\sqrt{2}$. Then, if $\alpha>\dim_F(\mu)$, we can find a compact K with $\mu(K)>1-\epsilon^2/2$, and with a fractal dimension $d_F(K)<\alpha$. For all sufficiently large t, K can be covered by N_t closed intervals I_j of width $\leqslant\delta_t$, with $N_t\leqslant\delta_t^{-\alpha}$. We can assume that the intervals I_j have no more than 2 overlaps; therefore, using their endpoints we can define a covering of K with a number $M_t\leqslant 2N_t\leqslant 2\delta_t^{-\alpha}$ of disjoint intervals of width $\leqslant\delta_t$, which for simplicity will be denoted again by I_j, and which satisfy $\mu(\cup I_j)>1-\epsilon^2/2$. In every interval I_j choose a point x_j and, for $0\leqslant s\leqslant t-1$, define

$$\xi_s(x)\equiv\sum_{j=1}^{M_t} e^{isx_j}\chi_j(x), \quad \text{for } x\in\cup I_j,$$

$$\xi_s(x)\equiv 0, \quad \text{elsewhere},$$

where $\chi_j(x)$ is the characteristic function of I_j. Then

$$\|\psi(s)-\xi_s\|^2=\int_0^{2\pi}|e^{isx}-\xi_s(x)|^2 d\mu(x)\leqslant s^2\delta_t^2+\mu([0,2\pi]\backslash\cup I_j)<t^2\delta_t^2+\frac{\epsilon^2}{2}<\epsilon^2$$

Now ξ_s $(s=0,\ldots,t-1)$ belong by construction in the subspace spanned by $\{\chi_j\}_{1\leqslant j\leqslant M_t}$, which, for sufficiently large t, has dimension $M_t\leqslant 2N_t\leqslant 2(\sqrt{2}t/\epsilon)^\alpha$. Thus, this subspace contains vectors which are $\epsilon-$close to $\psi,\ldots,\psi(t-1)$; therefore, at large times, $\theta_\epsilon(\psi,t)\leqslant 2(\sqrt{2}t/\epsilon)^\alpha$. □

Putting Theorem 2 and propositions 1(i), 2, 3, 4 together, we get

Proposition 5: *If* μ *is exactly scaling, with dimension* d*, then, for sufficiently small* $\epsilon>0$ *the limits*

$$\lim_{t\to\infty}\frac{\log\ \overline{\theta(\epsilon,\psi,t)}}{\log\ t}, \quad \lim_{t\to\infty}\frac{\log\ \theta(\epsilon,\psi,t)}{\log\ t} \tag{4.5}$$

exist, and have the same value $d=\dim_H(\mu)$.

Remark: One may speculate whether Proposition 3, too (hence, Theorem 3 itself) can be proven by a ''box counting'' argument of the kind used in the proof of Proposition 4.

V. A BALLISTIC UPPER BOUND

It is not possible to extract from the above results upper bounds for moments, and not even for the growth of the size of minimal ϵ-supports. Further assumptions are needed, which concern the ''spatial'' structure of the operator U on the basis B. Here a result in this vein is presented. For convenience, we'll say that the spread is *not faster than ballistic* if $[m^{(\alpha)}(t)]^{1/\alpha}$ does not increase faster than linearly with t, $\forall\alpha>0$. In this case, it is easily seen that $n_\epsilon(\psi,t,B)$, too, does not increase faster than linearly.

Proposition 6: *For* $\alpha\geqslant 0$ *let*

$$X_\alpha:=\{\psi\in\mathscr{H} \quad \text{such that} \quad \|\psi\|_\alpha:=\sup_{n\in\mathbf{Z}}|(e_n,\psi)\exp\alpha|n||<\infty\}$$

and suppose that $U(X_\alpha)\subseteq X_\alpha$ for some $\alpha>0$. Then, if $\psi\in X_\alpha$, *the spread is not faster than ballistic. Moreover,* $\forall\psi\in\mathscr{H}$, $n_\epsilon(\psi,t,B)$ *does not increase faster than linearly.*

Proof: Under the stated hypothesis , $U]X_\alpha$ is an everywhere defined linear operator in X_α, which is a Banach space under the norm $\|\cdot\|_\alpha$. Let $\{\psi_n\}$ be a convergent sequence in the

X_α-norm, such that $\{U\psi_n\}$ also converges in that norm, and let $\psi_\infty, \psi'_\infty$ be the corresponding limits. Then $\psi_n \to \psi_\infty$ and $U\psi_n \to \psi'_\infty$ in the weaker Hilbert norm, too; therefore $U\psi_n \to U\psi_\infty$ in the Hilbert norm because U is unitary. It follows that $\psi_\infty{}' = U\psi_\infty$, so $U \restriction X_\alpha$ is a closed operator in X_α. By the Closed Graph Theorem, it must be bounded. Therefore, if $\psi \in X_\alpha$, then $\forall t, n$

$$|\psi_n(t)| \leqslant \|U^t\psi\|_\alpha e^{-\alpha|n|} \leqslant \|U\|_\alpha^t \|\psi\|_\alpha e^{-\alpha|n|}. \tag{5.1}$$

Using (5.1) for $n \geqslant n_t := \alpha^{-1} t \log \|U\|_\alpha + \alpha^{-1} \log \|\psi\|_\alpha$, and $|\psi_n(t)| \leqslant 1$ for $n < n_t$, the announced bound on the growth of moments is immediately obtained. Finally, given any $\psi \in \mathscr{H}$, there is a $\psi' \in X_\alpha$ with $\|\psi - \psi'\| < \epsilon/2$; at any time t, any $\epsilon/2$- support for $U^t\psi'$ is also a ϵ-support for $U^t\psi$. □

Remark 1: Under the hypotheses of Proposition 6, the spread of wave packets in the presence of an absolutely continuous component is exactly ballistic.

Remark 2: Proposition 6 applies in several cases of concrete interest, including tight-binding discrete models and quantum maps like the kicked rotor[26] or the kicked Harper model.[4]

VI. DYNAMICAL DIMENSIONS

In this section, we shall discuss a different characterization of the structure of wave packets, which still makes reference to a specific basis, but, unlike moments, does not depend on the labelling of the basis vectors, or sites. On formal grounds, the construction to be presently described looks like a multifractal analysis of the measure $\mathscr{P}_{t,\psi}$, with the scaling limit defined by $t \to \infty$. It has been proposed, and numerically implemented, on the critical Harper model, in Ref. 17. In the following, $\|\psi\| = 1$, and completeness of B, are always assumed. Let us define the family of *partition functions*

$$Z_q(\psi, t) := \sum_{k \in \mathbf{Z}} p_k^q(t), \tag{6.1}$$

for all values of q such that the series converges at all times t. Such values include a half line $q > q_0$, with $0 \leqslant q_0 \leqslant 1$; for instance, under the assumptions of Proposition 6, Z_q is finite $\forall t$, $\forall\ q > 0$. In the following $q_0 < 1$ is assumed. Generalized entropies are defined, for $q \neq 1$, by

$$S_q := \frac{1}{1-q} \log Z_q$$

and for $q = 1$ by

$$S_1 = \sum_{k \in \mathbf{Z}} \Theta((p_k(t)), \tag{6.2}$$

where $\Theta(x) = -x \log x$ for $0 < x \leqslant 1$, $\Theta(0) = 1$. S_1 is the Shannon entropy of the distribution (3.1). With such definitions, S_q is a continuous function of q. Finally, define the *number of states*

$$\mathscr{N}_q(t) := e^{S_q(t)} = Z_q^{1/(1-q)}(t) \tag{6.3}$$

(the 2nd equality for $q \neq 1$) which, at fixed t, is a nonincreasing function of q.

The growth exponents $\beta^\pm(\mathscr{N}_q) = \mathscr{D}_q^\pm$ will be called here *dynamical dimensions*. From their very definition it follows that

Proposition 7: *$\mathscr{D}_q^\pm$ are nonincreasing functions of q, and $(1-q)\mathscr{D}_q^\pm$ are convex functions of q. Therefore, $\mathscr{D}_q^\pm$ are continuous functions of q, except possibly at $q = 1$.*

Proposition 8: (i) $\mathscr{D}_q^- \geqslant \dim_H^+(\mu)$ for $q < 1$, (ii) $\mathscr{D}_1^- \geqslant \dim_H^-(\mu)$.

Proof: Given $\epsilon>0$, $q<1$, define $\mathscr{A}_{\epsilon,q,t}:=\{k \in \mathbf{Z}: p_k(t)<\epsilon^{1/(1-q)}\mathscr{N}_q(t)^{-1}\}$ and $\mathscr{B}_{\epsilon,q,t}:=\mathbf{Z}\setminus\mathscr{A}_{\epsilon,q,t}$. Then $p_k^{q-1}>\epsilon^{-1}Z_q(t)$ if $k \in A_{\epsilon,q,t}$. From

$$Z_q(t)\geqslant\sum_{k\in\mathscr{A}_{\epsilon,q,t}} p_k(t)p_k^{q-1}(t)\geqslant\epsilon^{-1}Z_q(t)\mathscr{P}_{\psi,t}(\mathscr{A}_{\epsilon,q,t})$$

we obtain $\mathscr{P}_{\psi,t}(\mathscr{B}_{\epsilon,q,t})\geqslant 1-\epsilon$. From the definition of a minimal-support of $\mathscr{P}_{\psi,t}$ it follows that $\sharp(\mathscr{B}_{\epsilon,q,t})\geqslant n_\epsilon(\psi,t)$; therefore,

$$\begin{aligned} Z_q(t)&\geqslant\sum_{k\in\mathscr{B}_{\epsilon,q,t}} p_k^q(t)\\ &\geqslant n_\epsilon(\psi,t)\epsilon^{\frac{q}{1-q}}\mathscr{N}_q(t)^{-q}\\ &= n_\epsilon(\psi,t)\epsilon^{\frac{q}{1-q}}Z_q(t)^{-\frac{q}{1-q}}\end{aligned}$$

which entails $\mathscr{N}_q(t)=Z_q(t)^{1/(1-q)}\geqslant\epsilon^{q/(1-q)}n_\epsilon(\psi,t)$. Since this holds for arbitrarily small ϵ, part (i) of the thesis follows from inequality (3.3).

If $q=1$, let $\mathscr{A}_{\epsilon,t}:=\{k \in Z: p_k(t)<e^{-S_1(t)/\epsilon}\}$, and $\mathscr{B}_{\epsilon,t}=\mathbf{Z}\setminus\mathscr{A}_{\epsilon,t}$. If $k \in \mathscr{A}_{\epsilon,t}$, then $\log\frac{1}{p_k(t)}>[S_1(t)/\epsilon]$, which implies $\mathscr{P}_{\psi,t}(\mathscr{B}_{\epsilon,t})\geqslant 1-\epsilon$, so $\sharp(\mathscr{B}_{\epsilon,t})\geqslant n_\epsilon(\psi,t)$. Now let $\overline{\mathscr{B}}_{\epsilon,t}:=\mathscr{B}_{\epsilon,t}\cap\{k\in\mathbf{Z}: p_k(t)<e^{-1}\}$. Then $\sharp(\overline{\mathscr{B}}_{\epsilon,t})\geqslant n_\epsilon(\psi,t)-3$. Consequently,

$$S_1(t)\geqslant\sum_{k\in\mathscr{B}_{\epsilon,q,t}}\Theta(p_k(t))\geqslant(n_\epsilon(\psi,t)-3)\epsilon^{-1}S_1(t)e^{-S_1(t)/\epsilon}$$

because $\Theta(x)$ is increasing in $(0,e^{-1})$. Now, if $\beta^-(n_\epsilon)=0$, then also $\dim^-(\mu)=0$ by Theorem 3, so (ii) is obvious; if, instead, $\beta^-(n_\epsilon)>0$, then $n_\epsilon>3$ eventually, so, $\mathscr{N}_1\geqslant\epsilon^{-\epsilon}(n_\epsilon(\psi,t)-3)^\epsilon$, and finally $\mathscr{D}_1^-\geqslant\epsilon\beta^-(n_\epsilon)\geqslant\epsilon\dim_H^-(\mu)$ by Theorem 3. Since $\epsilon<1$ is arbitrary, (ii) is proved. □

Remark 1: $\mathscr{D}_1^-\geqslant\dim_H^+(\mu)$ is false in general. If the ''width'' of the wave packet on the basis B is measured by means of the ''informational'' number of states $\mathscr{N}_1$, then the wave packet does not necessarily spread as fast as its fastest component, contrary to what happens with moments. The following elementary example illustrates this and other peculiarities. Let $Ue_k=e_{k+1}$ for $k\neq 0,-1$, and $Ue_{-1}=e_1$, $Ue_0=e_0$. If $\psi=e_0\cos\alpha+e_1\sin\alpha$, then $d\mu_\psi=(\cos^2\alpha)\delta+(\sin^2\alpha)dx$, with δ, and dx the Dirac and Lebesgue measures respectively; so $\dim_H^+(\mu)=1$. On the other hand, $\mathscr{D}_q^\pm=0,\sin^2\alpha,1$ respectively for $q>1, q=1, q<1$. This example shows that, at fixed $\dim_H^+(\mu)$, the value of $\mathscr{D}_1^\pm$ is affected by the weight of different spectral components, and suggests that a discontinuity of $\mathscr{D}_q^\pm$ at $q=1$ may be typical of non-exactly dimensional spectral measures. In particular, such a discontinuity should always appear, in case of coexistence of both a point and a continuous component of the spectral measure.

Remark 2: Inequalities of ''thermodynamic'' type show that $\mathscr{N}_1$ cannot increase faster than $[m^{(\alpha)}(t)]^{1/\alpha}$.

Remark 3: Like moments, $\mathscr{N}_q$ $(q\leqslant 1)$ can, in principle, diverge as $t\to\infty$, even in the absence of a continuous spectrum.

Remark 4: In case μ_ψ has a point component (and only in that case), some at least of the $p_k(t)$ will not converge to 0 as $t\to\infty$; then Z_q will be bounded away from zero at large times, and $\mathscr{N}_q$ will not diverge in the limit $t\to\infty$ if $q>1$. Therefore the presence of a point component of μ_ψ enforces $\mathscr{D}_q^\pm=0$ for $q>1$.

Finding upper bounds for dynamical dimensions appears difficult in general, except in the limit $q\to\infty$, and in the particular case in which ψ is one of the basis vectors, which without loss of generality we may assume to be e_0. Then let

$$\lim\ \inf_{t\to\infty}\frac{\log\, p_0(t)}{\log\, t}=-c^+;\quad \lim\ \sup_{t\to\infty}\frac{\log\, p_0(t)}{\log\, t}=-c^-$$

Now $c^\pm$ can be exactly identified with certain fractal dimensions of μ. Rigorous reformulations of a result by Ketzmerick, Petschel, and Geisel,[3] due to Holschneider,[9] Barbaroux, Combes, and Motcho,[11] and Guerin and Holschneider,[10] show that $c^\pm=D_2^\pm(\mu)$, the upper and lower *correlation dimensions* of the spectral measure (for the exact definition of which the reader is deferred to the quoted papers). In the case when $D_2^+(\mu)=D_2^-(\mu)$, their common value is just called correlation dimension and denoted $D_2(\mu)$. Then, denoting $\mathscr{D}_\infty^\pm$ the $q\to\infty$ limits of the monotonic functions $\mathscr{D}_q^\pm$, we have

Proposition 8: *If* $\psi\in B$, *then* $\mathscr{D}_\infty^-\leqslant D_2^-(\mu)$, *and* $\mathscr{D}_\infty^+\leqslant D_2^+(\mu)$.

Proof: If $q>1$, from $Z_q(t)\geqslant p_0^q(t)\geqslant t^{-(c^++\eta)q}$, which is eventually true (in t) for any small η, we get $\mathscr{D}_q^+\leqslant[q/(q-1)](c^++\eta)$. Analogously, from $Z_q(t)\geqslant p_0^q(t)\geqslant t^{-(c^-+\eta)q}$, which is frequently true, we get $N_q(t)\leqslant t^{q(c^-+\eta)}$ frequently, that is, $\mathscr{D}_q^-\leqslant[q/(q-1)](c^-+\eta)$. □

The above results intuitively fit in a rough qualitative picture of the role of spectral dimensions. The behavior of $Z_q(t)$ at $q<1$ is mainly determined by that part of the probability distribution, which decays faster. This part corresponds to the fastest component of the wave packet, which, according to Theorem 3 [in the form of inequality (3.2)], probes the ''most continuous'' part of the spectrum; this is the sense of Proposition 8. As $q>1$ increases, instead, the slowly propagating part of the wave packet becomes more and more important. This very part also accounts for the tail in the decay of the probability at the initial site, which is determined by a less continuous region of the spectrum, and is in fact described by the correlation dimension(s).

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Models of the Hofstadter-type

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Spectra and eigenfunctions of discrete Hamiltonians are computed using algebraic, analytic, and numerical tools. In particular, we consider the Hofstadter and the Second Neighbor Square Lattice model, the Triangular Lattice model in an inhomogenous magnetic field, the Doubly-discrete Quantum Pendulum, and the Honeycomb model. Qualitative properties of the spectra are related to symmetries. Semiclassical analysis in the algebraic setting for the Doubly-discrete Quantum Pendulum is shown to match numerical results well. The connection to integrable models is mentioned. © *1996 American Institute of Physics.*
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I. INTRODUCTION

The subject of this paper lies on the edge of physics, mathematics, and computer science. It concerns the analysis of some quantum mechanical models for transport phenomena in two-dimensional solids.

For many decades it has been well known that the transport of electrons shows remarkable properties. The collective behavior of particles often leads to situations where charge transport can be described best in terms of quasiparticles. They can have positive, negative, or even noninteger charge. Of particular interest are phenomena that are seen in two-dimensional systems in the presence of large magnetic fields and at low temperature. It is there where integer or fractional quantum Hall conductance is observed.

Such phenomena can be modeled in part by Hamiltonians of the Hofstadter type. These operators have interesting mathematical properties. Their spectra are typically fractal and charge transport is integral.

There are several computational methods for dealing with Hamiltonians of the Hofstadter type. For the computation of spectra Chambers formula (see Sec. V, Theorem 1) is most useful.[1] Dynamics of wave functions can be visualized best in terms of Husimi functions (see Sec. II and Sec. III).

The elementary objects that underlie the construction of all model Hamiltonians are the discrete magnetic translations.[2] We will give a systematic exposition of these operators in terms of Weyl operators in the following section. At this point let us just adopt a pragmatic point of view and discretize the well-known expressions for a charged particle in a constant magnetic field in the most straightforward way.

Let Ψ be a function on $\mathbb{Z}^2$ with values in $\mathbb{C}$ and $\chi=(\chi_1,\chi_2)$ a discrete and real valued vector potential, such that

$$\text{curl } \chi(n) := \partial_1\chi_2 - \partial_2\chi_1 = \Phi. \tag{1}$$

Discrete derivatives are defined by

$$\partial_j F(n) := F(n) - F(n-e_j) \quad (j=1,2), \tag{2}$$

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and magnetic translations as follows:

$$T_1\Psi(n)=e^{i\chi_1(n)}\Psi(n_1-1,n_2), \tag{3}$$

$$T_2\Psi(n)=e^{i\chi_2(n)}\Psi(n_1,n_2-1). \tag{4}$$

[The magnetic translations can be interpreted as connections on the trivial discrete vector bundle $\mathbb{Z}^2\times\mathbb{C}$. Equation (1) defines χ in terms of Φ up to a discrete gradient $(\partial_1\varphi,\partial_2\varphi)$, where φ denotes a function on $\mathbb{Z}^2$ generating a discrete gauge transformation.] They are unitary on $l^2(\mathbb{Z}^2)$. Due to the phase in their definition they have an elementary holonomy,

$$T_1^{-1}T_2^{-1}T_1T_2=e^{i\Phi}. \tag{5}$$

$(1-T_1)$ and $(1-T_2)$ are discrete magnetic momentum operators and give rise to the magnetic discrete Laplacian,

$$\Delta=\sum_{l=1}^{2}(1-T_l)^*(1-T_l), \tag{6}$$

coinciding with the Hofstadter Hamiltonian up to a sign and an additive constant,

$$H_{\mathrm{Hof}}=T_1+T_2+T_1^*+T_2^*. \tag{7}$$

The Hofstadter model has several physical interpretations. The most prominent one is as a tight-binding approximation for electrons bound to atomic sites in a two-dimensional crystal and in a strong external magnetic field. It is a model with two typical frequencies. The first corresponding to the area of the unit cell in the lattice, the second to the flux through a unit cell, which in our notation is Φ.

The history of the Hofstadter model goes back to the work of Peierls[3] on Bloch electrons in metals under the influence of a magnetic field. In the 1950s and 1960s progress was made by Azbel,[4] Harper,[5] Zak,[2] Chambers,[1] and Langbein.[6] They discovered the role of magnetic translations and began a systematic study of the square lattice model.

In 1976, Hofstadter[7] published the famous Hofstadter butterfly (Fig. 3). He found that the figure of the spectral bands versus the magnetic flux exhibits a complicated yet beautiful fractal structure. A detailed study of the square lattice and other models began thereafter. We just mention work by Wilkinson[8] who related the fractal structure to a WKB analysis of tunneling between different lattice cells. This semiclassical approach was put in a rigorous form by Helffer and Sjöstrand[9–13] using pseudodifferential operator calculus. This work was recently simplified and completed by Buslaev and Fedotov[14–18] by means of a WKB approach for difference equations. Since the Hofstadter model turns into Harper's equation by a Bloch-wave ansatz, the spectral analysis of the two models is the same. About the latter and its generalization, the Discrete Mathieu model, detailed results are known. Let us mention just one, the theorem by Last and Wilkinson about the total length of the band spectrum S for the critical value $\lambda=2$ (Harper's equation) and magnetic flux $\phi=2\pi p/q$:[19,20]

$$\frac{2(\sqrt{5}+1)}{q}<S<\frac{8e}{q}. \tag{8}$$

For more details we refer to the recent articles by Last, Jitomirskaya, and Shubin.[21–23] In parallel, the algebraic study was put forward by Bellissard,[24–26] who related the Hofstadter model to the work of Connes[27] on noncommutative geometry.

It was a big surprise at the beginning of the 1990s when it turned out that the Quantum Discrete Sine–Gordon equation[28,29] leads to the Hofstadter model.[29] Presently, Quantum groups and the Bethe Ansatz in the context of the Hofstadter model receive considerable attention.[30–32]

Hamiltonians of the Hofstadter type like the Hofstadter Hamiltonian, the triangular, the hexagonal model, or the Doubly-discrete Quantum Pendulum are the main objects of analysis in this paper. They are all elements of a C^*-algebra generated by the magnetic translations, the so-called rotation algebra, which is a particular case of a Weyl-Heisenberg algebra. Furthermore, they can be understood as pseudodifferential operators on the circle. In this setup the classical symbol of the Hofstadter Hamiltonian is

$$H_{\mathrm{Hof}}(\xi,x)=\cos\ \xi+\cos\ x. \tag{9}$$

It is defined on phase space $S^1\times S^1$ with the natural symplectic structure. For a list of the Hamiltonians discussed in this paper and their symbols, we refer to Table II.

Many of these Hamiltonians allow for a completely different interpretation: they are quantum integrals of a dynamical automorphism of the rotation algebra. Consider, e.g., the Hamiltonian of the Doubly-discrete Quantum Pendulum for $k\in\mathbb{R}\backslash\{0\}$,

$$H_{\mathrm{QP}}=2(T_1+T_2+T_1^*+T_2^*)+k(e^{-i\Phi/2}T_1T_2+e^{i\Phi/2}T_2^*T_1^*)+(1/k)(e^{-i\Phi/2}T_2T_1^*+e^{i\Phi/2}T_1T_2^*). \tag{10}$$

It is invariant under the automorphism generated by the map

$$\alpha:\langle T_1,T_2\rangle\mapsto\left\langle T_2,T_3=T_1^*\left(\frac{k+e^{i\Phi/2}T_2}{1+ke^{i\Phi/2}T_2}\right)^2\right\rangle. \tag{11}$$

This automorphism appeared first in the doubly discrete integrable sine–Gordon theory.[29,28,33]

[In the continuum case the automorphism is generated by Eq. (12) below. It is a special case of the hyperbolic equation,

$$(\partial_t^2-\partial_x^2)\phi(t,x)+g\ \sin\ \phi(t,x)=0. \tag{12}$$

For space-independent solutions $\phi(t)$, one gets the pendulum equation,

$$\partial_t^2\phi(t)+g\ \sin\ \phi(t)=o.] \tag{13}$$

This paper is structured as follows. In the next section we formulate elementary discrete quantum mechanics. The ground state of the elementary Hofstadter Hamiltonian is shown to be unique and invariant under discrete Fourier transformation. All this lays the basics for the ''Kinematics of the Hofstadter Type Models,'' which is the subject of the third section, where there is some overlap with a recent article by Faddeev[34] on the Discrete Heisenberg–Weyl Group and the Modular Group. The discrete analog of the Landau momentum and the Landau velocity is introduced and combined to form generators of the quantum group SL_q. In the fourth section we describe the models and present numerical results. Symmetries are used to understand some qualitative properties of the spectra. The Husimi functions of the Doubly-discrete Quantum Pendulum are shown to be localized at the classical orbits. In the last section we discuss Chambers relation for the Doubly-discrete Quantum Pendulum and comment on semiclassical methods for the computation of spectra. The semiclassical results are shown to approximate the numerical results well. For details on most of the material presented here we refer to Ref. 35.

Quantum group structures appear naturally in the context of the models of the Hofstadter type. It is hoped that this will eventually lead to a better understanding of the complicated and interesting nested structure of their spectra. This has, however, not yet materialized, although we have worked in this direction for several years.

II. ELEMENTARY DISCRETE QUANTUM MECHANICS

The irreducible state space for a discrete quantum system with one degree of freedom and rational Planck constant $\Phi = p/q$, where p and q are relatively prime, is the complex vector space $\mathbb{C}^q$. The canonical position and momentum operators are

$$t_1 = \begin{pmatrix} 0 & 0 & \dots & \dots & 0 & 1 \\ 1 & 0 & & & 0 & 0 \\ \vdots & \ddots & \ddots & & & \\ \vdots & & \ddots & \ddots & & \\ \vdots & & & \ddots & 0 & 0 \\ 0 & \dots & \dots & \dots & 1 & 0 \end{pmatrix} \tag{14}$$

and

$$t_2 = \mathrm{diag}(e^{i\Phi}, e^{2i\Phi}, \dots, e^{iq\Phi}), \quad \Phi = 2\pi\Phi. \tag{15}$$

The operators t_1 and t_2 have simple and remarkable properties listed below.

(1) t_1 and t_2 satisfy the same commutation relations (5) as the magnetic translations T_1 and T_2 defined in the Introduction, formula (3).

(2) They are, however, idempotent,

$$t_1^q = t_2^q = 1. \tag{16}$$

(3) t_1 can be understood as a shift on the q-periodic doubly infinite sequences (which is naturally identified with $\mathbb{C}^q$).

(4) t_1 and t_2 are related by discrete Fourier transformation,

$$\mathscr{F}: \mathbb{C}^q \to \mathbb{C}^q, \quad f(n) \mapsto \hat{f}(n) = \frac{1}{\sqrt{q}} \sum_m e^{inm\Phi} f(m), \tag{17}$$

$$t_2 = \mathscr{F} t_1 \mathscr{F}^{-1}. \tag{18}$$

Note that $\mathscr{F}$ is unitary, $\mathscr{F}^{-1} = \mathscr{F}^*$ and $\mathscr{F}^4 = 1$. Thus

$$\sigma(\mathscr{F}) \subset \{1, -1, i, -i\}. \tag{19}$$

(5) t_1 and t_2 have the same invariants. Particularly for $q > 1$, one gets the equations

$$\det t_1 = \det t_2 = 1, \quad \mathrm{trace}\ t_1 = \mathrm{trace}\ t_2 = 0. \tag{20}$$

The elementary Hofstadter Hamiltonian is the simplest nontrivial self-adjoint operator made out of t_1 and t_2,

$$h = t_1 + t_2 + t_1^* + t_2^*. \tag{21}$$

It is invariant under Fourier transformation. h is the elementary constituent of the Hofstadter Hamiltonian (see Theorem 3, Sec. III and remark 1 thereafter). Furthermore, h (or rather, $4-h$) is the discrete analog of the harmonic oscillator. Unfortunately, its ground state is not expressible in simple terms. Nevertheless, a partial characterization can be given, as the following theorem shows.

Theorem 1:

(i) $4-h$ has a nondegenerate ground state, ω. There is a strictly positive choice for ω.

(ii) ω is invariant under Fourier transformation.

Proof:

(i) The first statement follows from the Perron–Frobenius theorem.[36] Consider the Hamiltonian $h+3$. It has non-negative entries only. Furthermore, for each entry of the matrices the following inequality holds:

$$((h+3)^q)_{i,j} \geqslant ((t_1+t_1^*+1)^q)_{i,j}. \tag{22}$$

Next we replace t_1 by the nilpotent matrix D,

$$D=\begin{pmatrix} 0 & 0 & \dots & \dots & 0 & 0 \\ 1 & 0 & & & 0 & 0 \\ \vdots & \ddots & \ddots & & & \\ \vdots & & \ddots & \ddots & & \\ \vdots & & & \ddots & 0 & 0 \\ 0 & \dots & \dots & \dots & 1 & 0 \end{pmatrix}, \tag{23}$$

and obtain the inequality

$$(t_1+t_1^*+1)^q \geqslant (D+D^*+1)^q \geqslant \sum_{l=1}^{q} (d^l+d^{*l})+1. \tag{24}$$

Hence each entry of the matrix $(h+3)^q$ is larger than one; therefore, $h+3$ is ergodic.

(ii) Since $\mathscr{F}$ commutes with h, there is a choice of ω that is an eigenvector of $\mathscr{F}$ too:

$$\mathscr{F}\omega=\lambda\omega, \tag{25}$$

for some $\lambda \in \{+1,-1,-i,+i\}$.

Consider now the last component in the equation above,

$$\frac{1}{\sqrt{q}} \sum e^{iql\Phi}\omega(l)=\frac{1}{\sqrt{q}} \sum \omega(l)=\lambda\omega(q). \tag{26}$$

Since $\omega(i)$, $i \in \{1,\dots,q\}$, is strictly positive, this is consistent with $\lambda=1$ only.

So it is well motivated to call the ground state ω of h a discrete version of the Gauss function. This is supported by numerical computations (see Fig. 1).

Discrete quantum mechanics can also be formulated in terms of functions on discrete phase space $\mathbb{C}^q \times \mathbb{C}^q$. The transition from one formulation to the other is given by a discrete Bargmann transformation. This formulation is useful—as in the continuous case—for making contact with the corresponding classical theory.

Discrete position and momentum give rise to the Weyl operators $w(m)$, $m \in \mathbb{Z}^2$, defined by

$$\begin{gathered} w(1,0)=t_1, \quad w(0,1)=t_2, \\ w(m+n)=\exp\left[-\frac{i}{2}\Phi\sigma(m,n)\right]w(m)w(n) \quad (m,n \in \mathbb{Z}^2). \end{gathered} \tag{27}$$

$\sigma(m,n)$ denotes the standard discrete sympletic form,

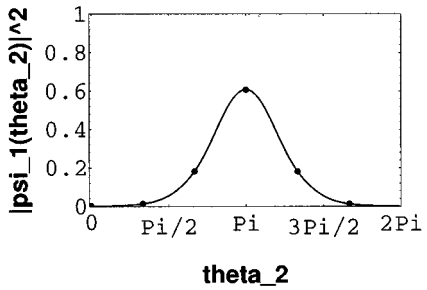

FIG. 1. Ground state of the Discrete Harmonic Oscillator for $q=6$.

$$\sigma(m,n):=m_1n_2-m_2n_1. \tag{28}$$

Note that the discrete Weyl operator w is doubly q-periodic,

$$w(m+qn)=w(m) \quad (m,n\in\mathbb{Z}^2). \tag{29}$$

Fourier transformation acts on w like a rotation by $\pi/2$,

$$\mathscr{F}w(m)\mathscr{F}^{-1}=w(Jm) \quad [m=(m_1,m_2)\in\mathbb{C}^q\times\mathbb{C}^q], \tag{30}$$

where J denotes the discrete complex structure $Jn=(-n_2,n_1)$, $n\in\mathbb{Z}^2$.

In terms of the discrete Weyl operator w and the ground state ω of h, the discrete Bargmann transformation is defined by

$$B:\mathbb{C}^q\to\mathbb{C}^q\times\mathbb{C}^q, \quad \psi\mapsto B_\psi(m):=(\omega,w(Jm)\psi). \tag{31}$$

The action of all relevant operators on the state space $\mathbb{C}^q$ can now easily be transformed to the Bargmann representation.

In order to interpret wave functions in classical terms it is useful to look at the Husimi functions. They are usually defined in terms of Bargmann functions,

$$H_\psi(m)=|B_\psi(m)|^2. \tag{32}$$

Notice, however, that they can also by given in terms of a trace over projectors in the original state space $\mathbb{C}^q$,

$$H_\psi(m)=\mathrm{trace}[p_\psi w(m)p_\omega w^{-1}(m)], \tag{33}$$

where p_ψ and p_ω denote the projectors onto ψ and ω, respectively.

III. KINEMATICS OF HOFSTADTER-TYPE MODELS

Kinematics of the Landau, the Hofstadter model, and their descendents are very close to each other. It is, therefore, natural to develop them in parallel. The basic object in the background of what follows is the Heisenberg group in $2+1$ one dimensions. It gives rise to the following family of unitary Weyl operators on $L^2(\mathbb{C})$:

$$W_\Phi(x)F(y)=\exp\left[\frac{i}{2}\,\Phi\sigma(x,y)\right]F(y-x). \tag{34}$$

σ denotes the natural symplectic quadratic form on $\mathbb{C}$, $\sigma(x,y)=\mathrm{Im}\,\overline{xy}=x_1y_2-x_2y_1$ ($x=x_1+ix_2\in\mathbb{C}$), and Φ is a real parameter that is interpreted to be the magnetic flux through a surface of unit area. Some times it is convenient to identify Φ with a vector $(0,0,\Phi)\in\mathbb{R}^3$.

The Weyl operators W_Φ satisfy the composition law

$$W_\Phi(x)W_\Phi(y)=\exp\left[\frac{i}{2}\,\Phi\sigma(x,y)\right]W_\Phi(x+y), \tag{35}$$

which gives rise to the canonical commutation relation

$$W_\Phi(x)W_\Phi(y)=\exp[i\Phi\sigma(x,y)]W_\Phi(y)W_\Phi(x). \tag{36}$$

Equations (34) and (36) have nice and simple geometric interpretations. [$W_\Phi(x)$ is the integrated connection $\nabla=d+iA$, $dA=\Phi\ dx^1\wedge dx^2$ on $\mathbb{C}\times\mathbb{C}$. Furthermore, W_Φ is a projective representation of the Abelian group $\mathbb{C}$, and at the same time a noncommutative deformation of the characters of $\mathbb{R}^2$.]

The operators $W_{-\Phi}$ commute with the W_Φ's. In fact, it can be proved[23] that the commutand of the von Neumann algebra generated by the W_Φ's is equal to the von Neumann algebra generated by the $W_{-\Phi}$'s and vice versa,

$$\{W_\Phi(x)|x\in\mathbb{C}\}'=\{W_{-\Phi}(x)|x\in\mathbb{C}\}''. \tag{37}$$

The operators W_Φ and $W_{-\Phi}$ form two commuting two-parametric, strongly continuous unitary groups and are, therefore, generated by self-adjoint operators, v and k, as follows:

$$\begin{aligned}
&W_\Phi(x)=\exp\ ix\cdot v, \quad x\cdot v=x_1v_1+x_2v_2,\\
&v_1=i\partial_1-\frac{\Phi}{2}\,y_2, \quad v_2=i\partial_2+\frac{\Phi}{2}\,y_1;\\
&W_{-\Phi}(x)=\exp\ ix\cdot k, \quad x\cdot k=x_1k_1+x_2k_2,\\
&k_1=i\partial_1+\frac{\Phi}{2}\,y_2, \quad k_2=i\partial_2-\frac{\Phi}{2}\,y_1.
\end{aligned} \tag{38}$$

The commutation relations (36) imply

$$[v_1,v_2]=i\Phi, \quad [k_1,k_2]=-i\Phi, \quad [k_m,v_n]=0, \quad m,n\in\{1,2\}. \tag{39}$$

In physical terms, v is the velocity and k the momentum operator. From k, one derives the operator $c=1/\Phi^2\ (k\wedge\Phi)$, which is the operator of the Landau center. (The expectation value of the position operator circles around the expectation value of c according to the dynamics of the Landau Hamiltonian. Furthermore, c is an integral of motion.) It has the commutation relations

$$[c_1,c_2]=-\frac{i}{\Phi}. \tag{40}$$

The magnetic flux Φ plays a role much like Planck's constant in quantum mechanics. This analogy leads naturally to quantization of arbitrary functions on phase space. Let F be an element of the Schwartz test function space and $\hat{F}$ its Fourier transformation. The corresponding quantization is naturally defined by

$$W_\Phi(F)=\left(\frac{1}{2\pi}\right)\int dx\ \hat{F}(x)W_\Phi(x). \tag{41}$$

[The definition below produces a noncommutative Φ-deformation of the algebra of functions on phase space $\mathbb{C}$.] These operators generate a C^* algebra (norm closure) or a von Neumann algebra (weak closure), respectively. According to the von Neumann uniqueness theorem the von Neumann algebra has irreducible constituents that are all equivalent to the standard Schrödinger representation.

Kinematics of the models of the Hofstadter type are a discrete version of the one for the Landau model described above. Consider the discrete phase space $\mathbb{Z}^2$ and the standard discrete symplectic structure σ as defined before (28).

The corresponding Weyl operators on $l^2(\mathbb{Z}^2)$ are defined by

$$W_\Phi(m)F(n)=\exp\left[\frac{i}{2}\,\Phi\sigma(m,n)\right]F(n-m). \tag{42}$$

Again, they satisfy the Weyl relations,

$$W_\Phi(m)W_\Phi(n)=\exp\left[\frac{i}{2}\,\Phi\sigma(m,n)\right]W_\Phi(m+n), \tag{43}$$

$$W_\Phi(m)W_\Phi(n)=\exp[i\Phi\sigma(m,n)]W_\Phi(n)W_\Phi(m) \tag{45}$$

Equations (42) and (43) again have simple geometric interpretations in terms of connections on a discrete complex line bundle over $\mathbb{Z}^2$.

The discrete Weyl operators $W_{-\Phi}$ commute with the W_Φ's and they generate their respective commutant,

$$\{W_\Phi(n)|n\in\mathbb{Z}^2\}'=\{W_{-\Phi}(m)|m\in\mathbb{Z}^2\}''. \tag{46}$$

The operators W_Φ and $W_{-\Phi}$ form 2-parametric, discrete unitary groups. They are generated by the elementary pairs of unitary operators,

$$T_1^{(v)}:=W_\Phi(1,0),\quad T_2^{(v)}:=W_\Phi(0,1), \tag{47}$$

and

$$T_1^{(k)}:=W_{-\Phi}(1,0),\quad T_2^{(k)}:=W_{-\Phi}(0,1), \tag{48}$$

respectively, and satisfy the relations

$$T_1^{(v)}T_2^{(v)}:=e^{i\Phi}T_2^{(v)}T_1^{(v)},\quad T_1^{(k)}T_2^{(k)}=e^{-i\Phi}T_2^{(k)}T_1^{(k)}. \tag{49}$$

In physical terms $T^{(v)}$ is the discrete velocity and $T^{(k)}$ the discrete momenum operator.

Each pair $(T_1^{(v)},T_2^{(v)})$, $(T_1^{(k)},T_2^{(k)})$ generates a rotation algebra. Together they have a natural structure as a quantum group SL_q, $q=e^{i\Phi}$. [Each pair forms a degenerate representation of a quantum group SL_q with the L operators

$$L^{(v)}=\begin{pmatrix} T_1^{(v)} & T_2^{(v)} \\ 0 & T_1^{(v)*}\end{pmatrix},\quad L^{(k)}=\begin{pmatrix} T_2^{(k)} & 0 \\ T_1^{(k)} & T_2^{(k)*}\end{pmatrix}. \tag{50}$$

Since $L^{(v)}$ and $L^{(k)}$ satisfy the Yang–Baxter equation,

$$R_{12}L_1^{(\sigma)}L_2^{(\sigma)}=L_2^{(\sigma)}L_2^{(\sigma)}R_{12} \quad (\sigma\in\{v,k\}), \tag{51}$$

the same is true for their tensor product,

$$L^{(v)}\otimes L^{(k)}=\begin{pmatrix} T_1^{(v)}T_2^{(k)}+T_2^{(v)}T_1^{(k)} & T_2^{(v)}T_2^{(k)*} \\ T_1^{(v)*}T_1^{(k)} & T_1^{(v)*}T_2^{(k)*} \end{pmatrix}. \tag{52}$$

The R-matrix is the canonical one,

$$R=\begin{pmatrix} q & 0 & 0 & 0 \\ 0 & 1 & q-\dfrac{1}{q} & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & q \end{pmatrix}. \tag{53}$$

By contruction the q determinant is unity.]

In the following we will mostly use the first pair, $T_1^{(v)}$, $T_2^{(v)}$. To simplify notation we drop the upper index from now on and simply write $T_1:=T_1^{(v)}$, $T_2:=T_2^{(v)}$. Furthermore, we replace $W_\Phi(n)$ by $W(n)$.

Quantization of phase space functions, $f\in C^\infty(T^2)$, where T^2 denotes the two-torus, given by

$$W(f)=\sum \hat{f}(m)W(m) \quad \left(f(x)=\sum \hat{f}(m)e^{imx}\right), \tag{54}$$

leads to the C^*-algebra $\mathscr{C}_\Phi$ and the von Neumann algebra $\mathscr{N}_\Phi$ by norm and weak closures, respectively. To fix the notation, let us call $\mathscr{C}_\Phi$ the rotation algebra and $\mathscr{N}_\Phi$ the Weyl–Heisenberg algebra. [The above definition produces a noncommutative Φ-deformation of the algebra of functions on the torus. In the terminology of Connes this is the quantized torus.] f is the classical symbol of the operator $W(f)$. There is a natural trace on the C^*-algebra generated by the Weyl operators $W(f)$,

$$\text{trace } W(f)=\hat{f}(0). \tag{55}$$

The GNS construction with respect to this trace leads back to the representation (42) we started from.

It is well known that all irreducible representations of the Weyl–Heisenberg algebra $\mathscr{N}_\Phi$ for rational $\Phi=\Phi/2\pi$ can explicitly be written in terms of finite-dimensional matrices.

Theorem 2: Let the magnetic flux be rational, $\Phi=2\pi(p/q)$ and p,q relatively prime. Then all irreducible representations of $\mathscr{N}_\Phi$ are labeled by an element of the torus $S^1\times S^1$. The representation π_θ is, up to unitary conjugation, defined by

$$\pi_\theta(T_1)=e^{i\theta_1}t_1, \quad \pi_\theta(T_2)=e^{i\theta_2}t_2, \tag{56}$$

where t_1 and t_2 are the discrete momentum and the discrete position operators introduced in Sec. II, formulas (14) and (15).

The irreducible representations π_θ have several interesting properties that are, in part, just translations from the corresponding properties of t_1 and t_2.

(1) Representations π_θ, $\theta\in S^1\times S^1$ are not injective since T_1^q and $(e^{iq\theta_1}.\ 1)$ have the same image under the map π_θ.

(2) Two representations, π_θ and $\pi_{\theta'}$ for $\theta\neq\theta'$ and $(\theta,\theta')\in[0,2\pi/q)\times[0,2\pi/q)$, are inequivalent because the spectra of $\pi_\theta(T_l)$ and $\pi_{\theta'}(T_l)$, $l=1,2$, are different.

TABLE I. Useful homomorphisms of the rotational algebra.

No.	Description	Matrix	det(M)	Automorphism	Classical
i	Rotation by $\pi/2$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	1	$T_1 \to T_2$ $T_2 \to T_1^*$	$x_1 \to x_2$ $x_2 \to -x_1$
ii	Rotation by π	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$	1	$T_1 \to T_1^*$ $T_2 \to T_2^*$	$x_1 \to -x_1$ $x_2 \to -x_2$
iii	Reflection at $x_1 = x_2$	$\begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$	-1	$T_1 \to T_2$ $T_2 \to T_1$	$x_1 \to x_2$ $x_2 \to x_1$
iv	Reflection at $x_1 = -x_2$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	-1	$T_1 \to T_2^*$ $T_2 \to T_1^*$	$x_1 \to -x_2$ $x_2 \to -x_1$
v	Shear	$\begin{pmatrix} 1 & 0 \\ -1 & 1 \end{pmatrix}$	1	$T_1 \to T_1$ $T_2 \to e^{i(\Phi/2)} T_1 T_2$	$x_1 \to x_1$ $x_2 \to x_1 + x_2$
vi	Rotation and stretch	$\begin{pmatrix} -1 & 1 \\ -1 & -1 \end{pmatrix}$	2	$T_1 \to e^{-i(\Phi/2)} T_1^* T_2^*$ $T_2 \to e^{i(\Phi/2)} T_1 T_2^*$	$x_1 \to x_1 + x_2$ $x_2 \to x_1 - x_2$
vii	Rotation by $\pi/3$	$\begin{pmatrix} -1 & -1 \\ 1 & 0 \end{pmatrix}$	1	$T_1 \to T_2$ $T_2 \to e^{-i(\Phi/2)} T_1^* T_2^*$	$x_1 \to x_2$ $x_2 \to -x_1 - x_2$
viii	Reflection at $x = 0$	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$	-1	$T_1 \to T_1$ $T_2 \to T_2^*$	$x_1 \to x_1$ $x_2 \to -x_2$
No.	Description	(ζ_1, ζ_2)		Automorphism	
ix	Reverse sign of T's	$(-1,-1)$		$T_1 \to -T_1$ $T_2 \to -T_2$	
x	Reverse sign of T_2	$(1,-1)$		$T_1 \to T_1$ $T_2 \to -T_2$	

(3) If however $\theta' = \theta + (2\pi/q)m$ for $m \in \mathbb{Z}^2$, the two representations $\pi_{\theta'}$ and π_θ are equivalent. The unitary intertwining between $\pi_{\theta'}$ and π_θ is constructed as follows: From the commutation relations of the Weyl operators we conclude that for every $n \in \mathbb{Z}^2$ and $A \in \mathscr{N}_\Phi$,

$$\pi_{\theta + \Phi n}(A) = W(Jn)\, \pi_\theta(A)\, W^{-1}(Jn). \tag{57}$$

Since, furthermore, the Diophantine equation for r, s in $\mathbb{Z}$,

$$pr + qs = 1, \tag{58}$$

has a solution—due to the Euclidean algorithm—we find, for every $m \in \mathbb{Z}^2$, an element $n \in \mathbb{Z}^2$ such that

$$\Phi n = \frac{m}{q} \quad \text{modulo } 1. \tag{59}$$

For rational Φ, the von Neumann algebra $\mathscr{N}_\Phi$ is of Type I_q, where $\Phi = p/q$, p and q relatively prime. This situation changes if $\Phi \notin Q$. In this case the center $\mathscr{N}_\Phi \cap \mathscr{N}_\Phi' = \mathbb{C}1$, hence $\mathscr{N}_\Phi$ is a factor. In fact, $\mathscr{N}_\Phi$ is a II_1 factor because the trace defined by (55) is weakly continuous and strictly positive.[23]

The representation of the Weyl algebra $\mathscr{N}_\Phi$ for rational Φ is reducible. In fact, each irreducible representation appears exactly once. This is the content of the following theorem that we cite with no proof.

Theorem 3: For rational $\Phi = p/q$, p and q relatively prime, there exists a unitary transformation,

TABLE II. Models, Hamiltonians, and classical symbols.

Model	Hamiltonian	Classical symbol
Hofstadter	$H_{\mathrm{Hof}}=T_1+T_2+\mathrm{h.c.}$	$2\cos(x_1)+2\cos(x_2)$
Mathieu	$H_\mu=T_1+\mu T_2+\mathrm{h.c.}$	$2\cos(x_1)+2\mu\cos(x_2)$
Second neighbor	$H_\epsilon=T_1+T_2+\epsilon(T_1^2+T_2^2)+\mathrm{h.c.}$	$2\cos(x_1)+2\cos(x_2)$ $+2\epsilon(\cos(2x)+\cos(2x_2))$
Quantum Pendulum	$H_{\epsilon,k}=\epsilon(T_1+T_2)+ke^{-i(\Phi/2)}T_1T_2$ $+\frac{1}{k}e^{i(\Phi/2)}T_1T_2^*+\mathrm{h.c.}$	$\epsilon(2\cos(x_1)+2\cos(x_2))$ $+2k\cos(x_1+x_2)+(2/k)\cos(x_1-x_2)$
Triangular lattice	$H_\eta=T_1+T_2+e^{-i\eta}T_1T_2+\mathrm{h.c.}$	$\cos(x_1)+\cos(x_2)+\cos(x_1+x_2-\eta+\phi/2)$
Honeycomb lattice	$H_{HC}=\begin{pmatrix}0 & T_1+T_2+e^{-i(\Phi/2)}T_1T_2\\ T_{-1}+T^{-2}+e^{i\Phi/2}T_2^{-1}T_1^{-1} & 0\end{pmatrix}$	none

$$U:l^2(\mathbb{Z}^2)\to\frac{1}{|\mathscr{B}|}\int_{\mathscr{B}}^{\oplus}d^2\theta\ \mathbb{C}^q\otimes\mathbb{C}^q, \tag{60}$$

such that

$$T_\alpha^{(v)}\cong\frac{1}{|\mathscr{B}|}\int_{\mathscr{B}}^{\oplus}d^2\theta\ \pi_\theta(T_\alpha)\otimes\mathbb{1},\quad T_\alpha^{(k)}\cong\frac{1}{|\mathscr{B}|}\int_{\mathscr{B}}^{\oplus}d^2\theta\ \mathbb{1}\otimes\pi_\theta(T_{\alpha+1})\quad(\alpha\in\mathbb{Z}_2). \tag{61}$$

Here, $\cong$ denotes equality up to conjugation by U and $\mathscr{B}$ denotes the magnetic Brillouin torus,

$$\mathscr{B}=\mathbb{R}\left(\mathrm{mod}\ \frac{2\pi}{q}\right)\mathbb{R}\left(\mathrm{mod}\ \frac{2\pi}{q}\right). \tag{62}$$

Theorem 3 has several useful consequences.

(1) The spectral analysis of an element A of $\mathscr{N}_\Phi$ can be reduced to the analysis of its restriction to each individual fiber, since

$$A\cong\frac{1}{|\mathscr{B}|}\int_{\mathscr{B}}^{\oplus}d^2\theta A(\theta)\otimes\mathbb{1}, \tag{63}$$

$$\sigma(A)=\bigcup_{\theta\in\mathscr{B}}\sigma(\pi_\theta(A)). \tag{64}$$

TABLE III. Symmetries of the Mathieu model.

Transformation	Description	Symmetry
No. i	Rotation by $\pi/2$ (Aubry duality)	$\sigma(\mu)=\mu\sigma(1/\mu)$
No. x	Reverse sign of T_2	$\sigma(\mu)=\sigma(-\mu)$
No. ix	Reversion of sign infront of T_j	$\sigma(\mu)=-\sigma(\mu)$
No. viii	Reflection at $x=0$	$\sigma(\Phi)=\sigma(-\Phi)$
$\Phi\to\Phi+2\pi$	Flux periodicity	$\sigma(\Phi)=\sigma(\Phi+2\pi n)$
	Parameter space	$\Phi\in[0,\pi]$
		$\mu\in[0,1]$

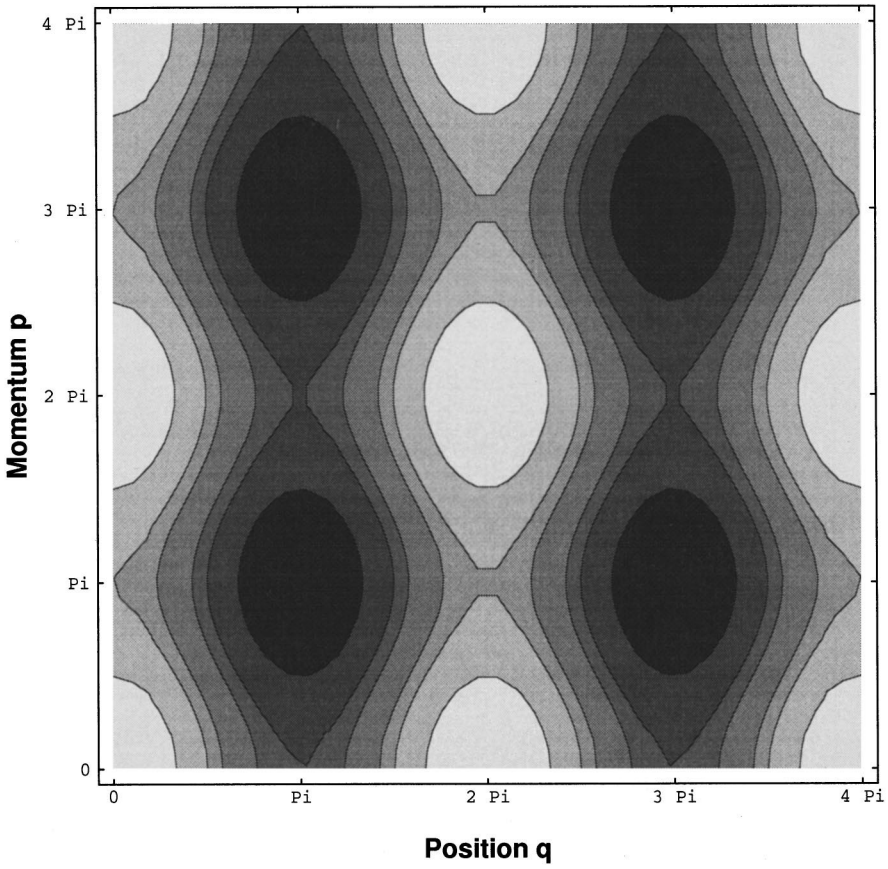

FIG. 2. Classical contour levels the the Discrete Mathieu model for $\mu=0.5$.

This means, in particular, that the spectral analysis of a Hamiltonian of the Hofstadter type is reduced to a matrix problem, e.g.,

$$\sigma(H_{\mathrm{Hof}})=\bigcup_{\theta\in\mathscr{B}}\sigma(H_{\mathrm{Hof}}(\theta)), \tag{65}$$

$$H_{\mathrm{Hof}}(\theta)=e^{i\theta_1}t_1+e^{i\theta_2}t_2+e^{-i\theta_1}t_1^*+e^{-i\theta_2}t_2^*, \tag{66}$$

where we used the notation $H_{\mathrm{Hof}}(\theta)=\pi_\theta(H_{\mathrm{Hof}})$.

(2) The commutand of $\mathscr{N}_\Phi$ is given by the formula

$$\mathscr{N}'_\Phi=\mathrm{End}(L^2(\mathscr{B}))\otimes\mathbb{1}\otimes\mathrm{End}(\mathbb{C}^q), \tag{67}$$

where $\mathrm{End}(L^2(\mathscr{B}))$ and $\mathrm{End}(\mathbb{C}^q)$ denote the spaces of bounded linear operators on $L^2(\mathscr{B})$ and $\mathbb{C}^q$, respectively. [We used the natural identification of $(1/|\mathscr{B}|)\int_{\mathscr{B}}^{\oplus} d^2\theta\ \mathbb{C}^q\otimes\mathbb{C}^q$ with $L^2(\mathscr{B})\otimes\mathbb{C}^q\otimes\mathbb{C}^q$.]

As a last subject in this section we mention a useful property of the Husimi functions. Let $\Psi(\theta)$ be an eigenvector of $H(\theta)=\pi_\theta(H)$, $(\theta\in\mathscr{B})$, where H denotes a Hamiltonian, which by assumption is an element of the von Neumann algebra $\mathscr{N}_\Phi$.

Due to equation (57) one gets for the Husimi function,

$$H_{\Psi(\theta)}(n):=|(w,W(Jn)\Psi(\theta))|^2, \tag{68}$$

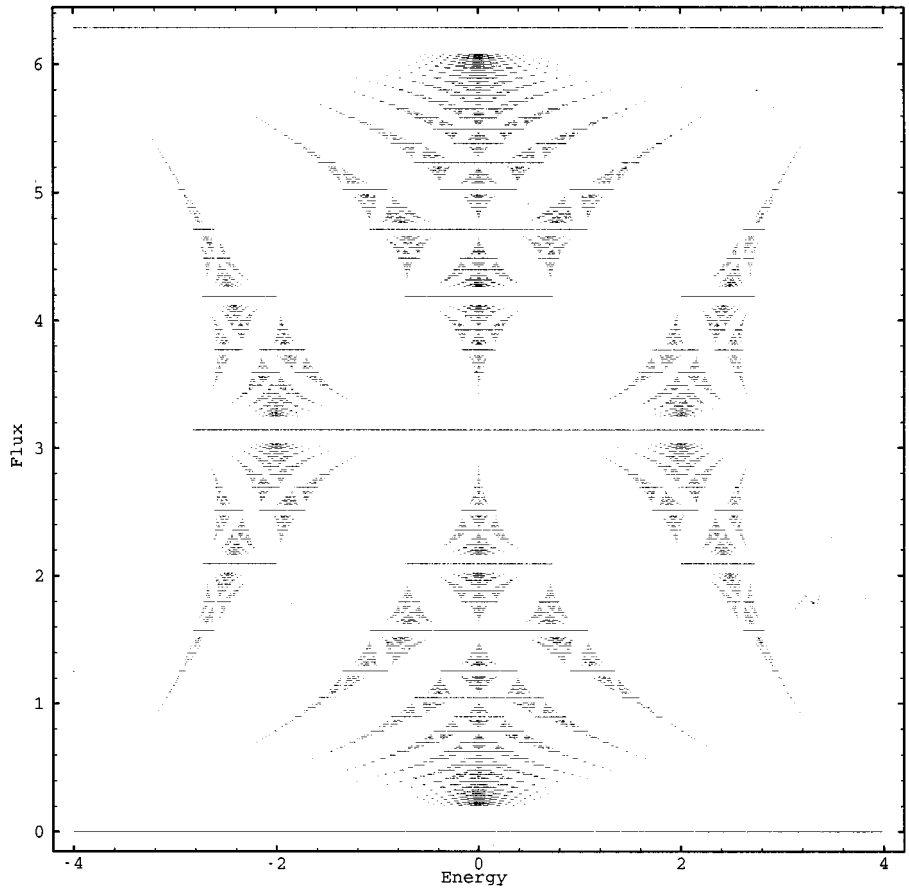

FIG. 3. Hofstadter Butterfly: Spectrum of the Hofstadter Model.

the equation

$$H_{\Psi(\theta)}(n)=H_{\Psi(\theta+\Phi n)}(0) \quad (n\in\mathbb{Z}^2,\theta\in\mathbb{R}^2). \tag{69}$$

It defines a natural interpolation $H_{\Psi(\theta)}(x)$, $x\in\mathbb{R}$, between the discrete values of $H_{\Psi(\theta)}(n)$:

$$H_{\Psi(\theta)}(n)=H_{\Psi(\theta+\Phi n)}(0) \quad (n\in\mathbb{Z}^2,\theta\in\mathbb{R}^2). \tag{70}$$

In particular, one gets the formula

$$H_{\Psi(0)}(\theta)=H_{\Psi(\Phi\theta)}(0) \quad (\theta\in\mathbb{R}^2). \tag{71}$$

IV. THE MODELS

There are many automorphisms of the discrete Weyl–Heisenberg algebra; some are linear others are nonlinear—some are inner others not. We have not studied them systematically. This would be an interesting mathematical problem in itself. However, we will give a list of examples. Many of them will show up later as symmetries of model Hamiltonians.

The simplest class of automorphisms are the linear ones. They may be called discrete Bogoliubov–Valatin transformations.

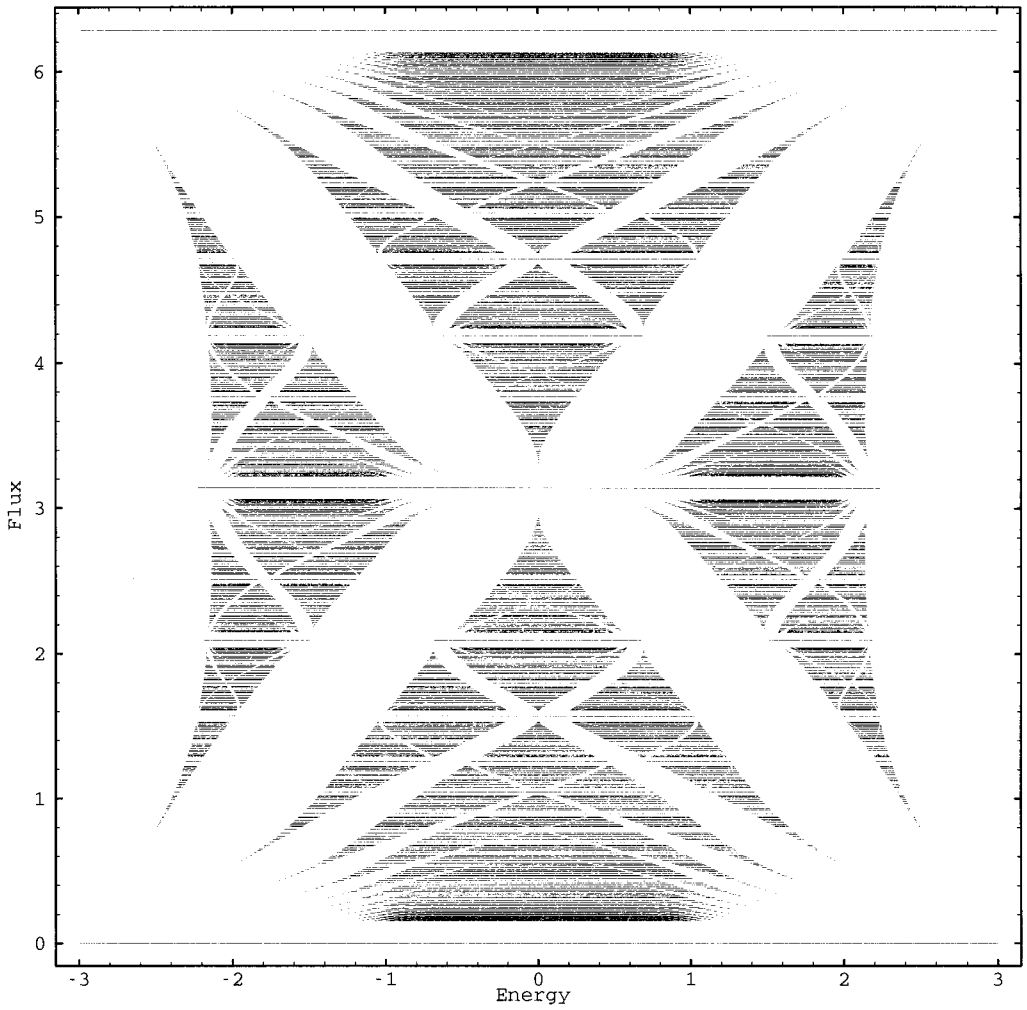

FIG. 4. Spectrum of the Discrete Mathieu Hamiltonian for $\mu=0.5$ and $q<40$.

Proposition: Let M be a 2×2 matrix with integer entries and nonvanishing determinant. Then the map

$$\alpha_M : W(m) \to W(Mm) \quad (m \in \mathbb{Z}^2), \tag{72}$$

generates an algebra homomorphism from $\mathcal{N}_\Phi$ onto $\mathcal{N}_{\det M,\Phi}$.

The statement follows directly from the commutation relations (45). The discrete Fourier transformation implements a special case of a discrete linear automorphism,

$$W(m) = \mathcal{F} W(Jm) \mathcal{F}^{-1}, \tag{73}$$

where J denotes the discrete complex structure introduced before. Others are summarized in Table I.

Nonlinear automorphisms are typically generated by an arbitrary function f that maps the unit circle into itself. In terms of magnetic translations they are defined by the shift

$$\alpha_f : (T_1, T_2) \to (T_2, T_3), \quad T_1 T_3 = f(T_2), \tag{74}$$

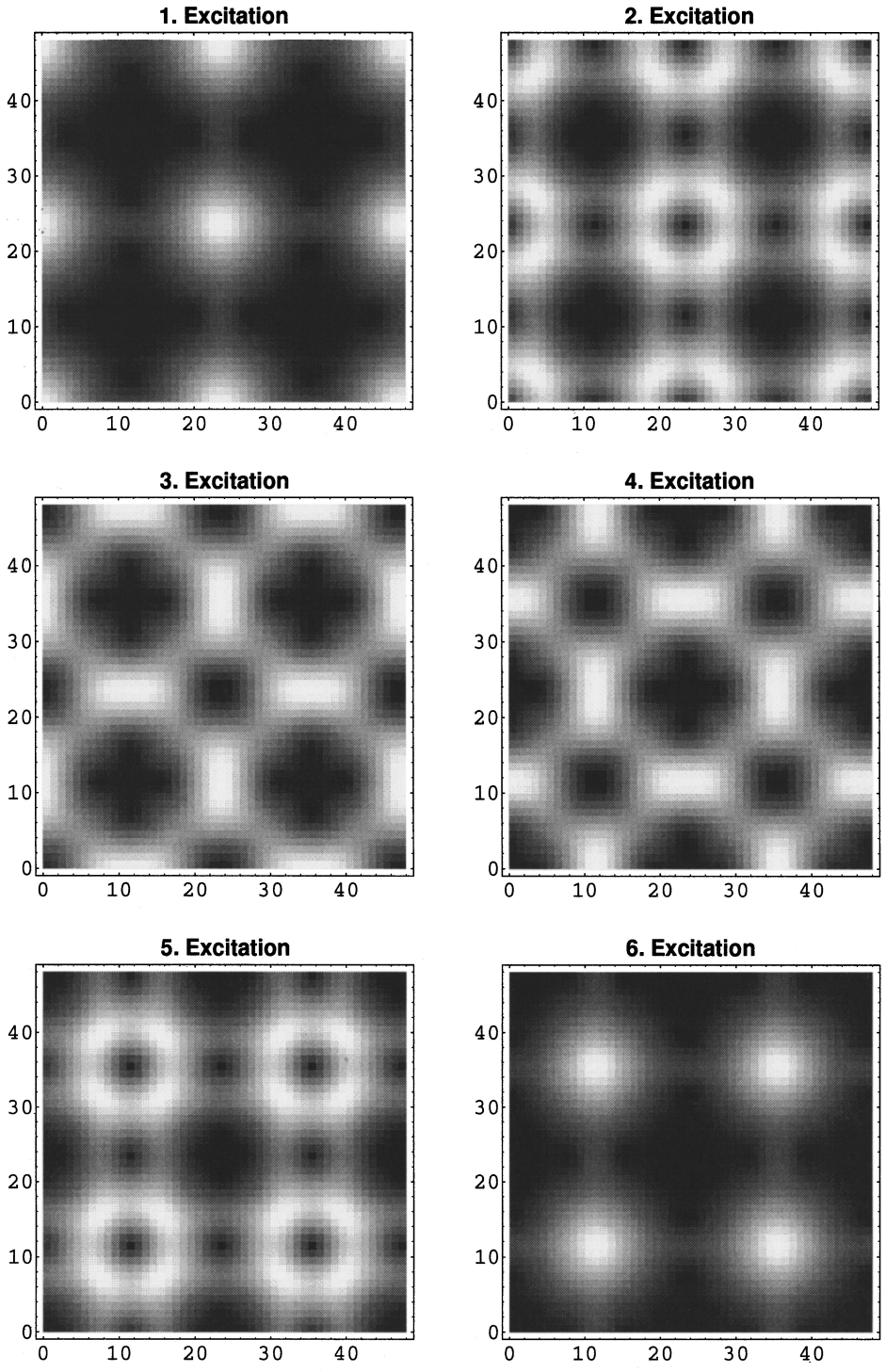

FIG. 5. Continuous Husimi Transformation for Hofstadter model ($p/q=1/6$).

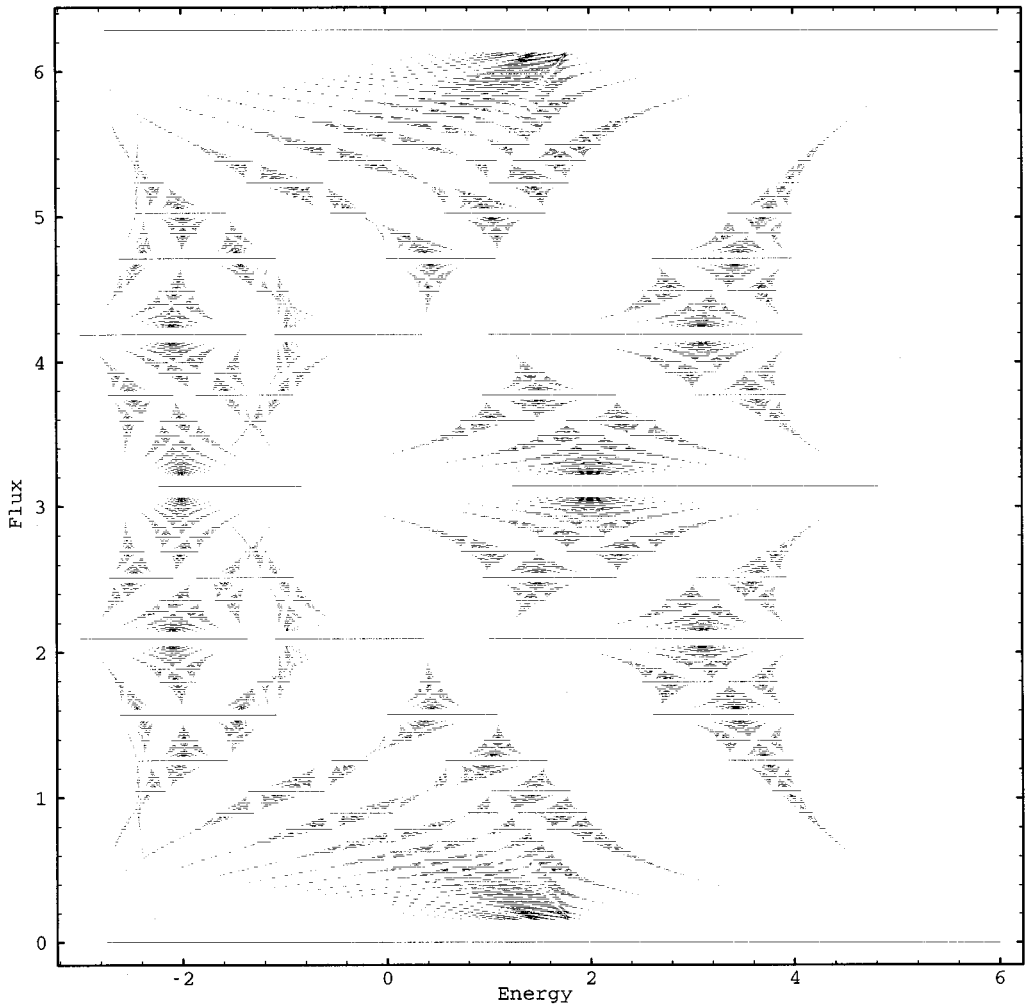

FIG. 6. Spectrum of the Second Neighbor Square Lattice model for $\epsilon=0.25$ and $q<40$.

where T_3 is defined by (74). It is easy to check that α_f is an algebra automorphism as long as all quantities encountered on the way of verification are well defined. (This requires some regularity for f.) A particularly nice example is the one arising from the Doubly-discrete Quantum Pendulum,[29] where

TABLE IV. Symmetries of the second neighbor model.

Transformation	Description	Symmetry
No. iii	Reflection at $x=p$	$\sigma(\Phi)=\sigma(-\Phi)$
No. ix	Reversion of sign infront of T_j	$\sigma(\epsilon)=-\sigma(-\epsilon)$
$\Phi\to\Phi+2\pi$	Flux periodicity	$\sigma(\Phi)=\sigma(\Phi+2\pi n)$
	Parameter space	$\Phi\in[0,\pi]$
		$\epsilon\in[0,\infty)$

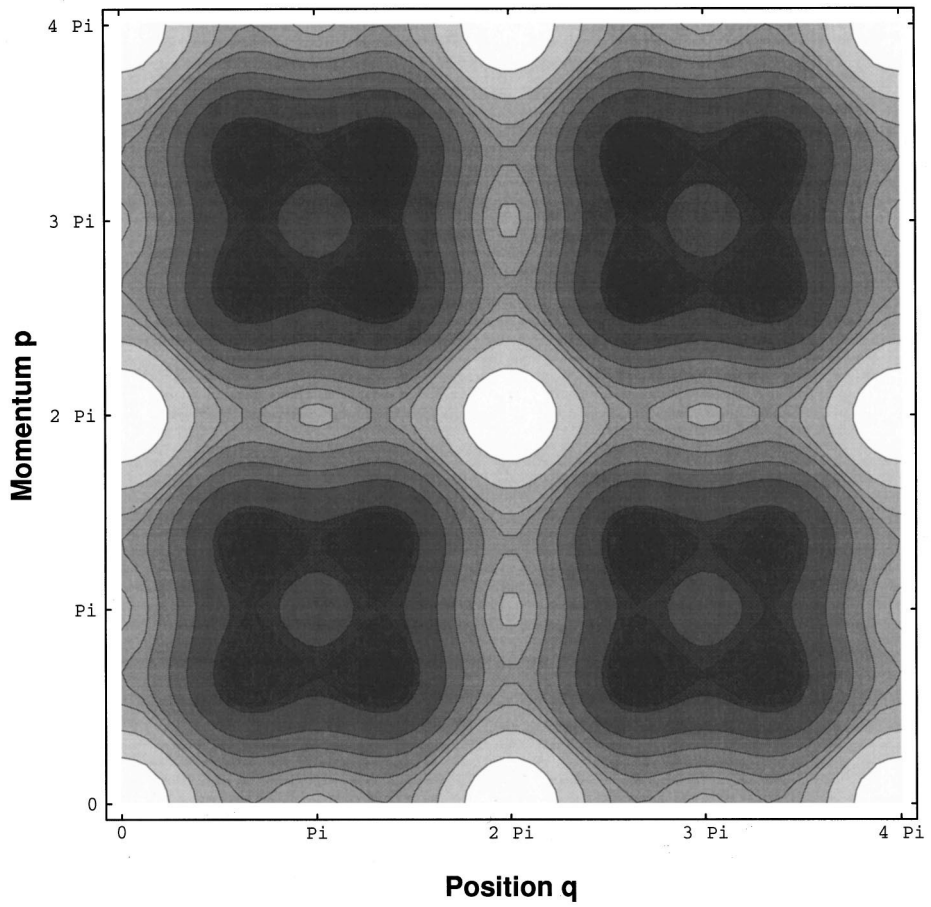

FIG. 7. Classical contour levels in the Second Neighbor Square Lattice model for $\epsilon=0.25$.

$$f_{\mathrm{QP}}(z)=\frac{k+e^{i\phi/2}z}{i+ke^{i\phi/2}z}, \tag{75}$$

k is a real parameter defining the model; it is related to discrete curvature.

The algebra automorphism generated by f_{QP} is a symmetry of the Hamiltonian,

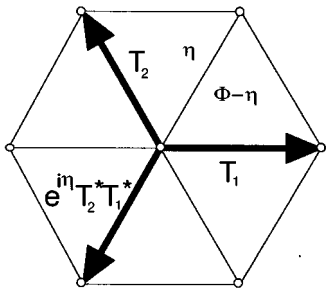

FIG. 8. Hopping interaction in the Triangular Lattice model.

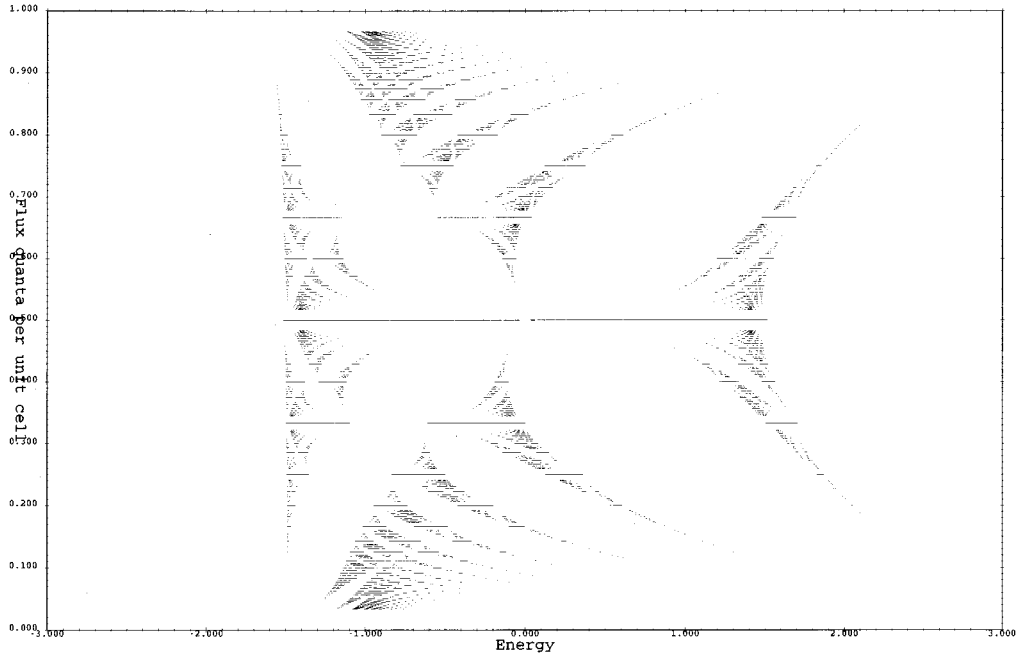

FIG. 9. Spectrum of the Triangular Lattice model for $\eta=0.075$ and $q\leqslant 40$.

$$H_{\mathrm{QP}} := 2\left(W(1,0)+W(1,0)^*+W(0,1)+W(0,1)^*\right)+k\left(W(1,1)+W(1,1)^*\right)+\frac{1}{k}\left(W(1,-1)+W(1,-1)^*\right),$$
$$\alpha_{f_{\mathrm{QP}}}(H_{\mathrm{QP}})=H_{\mathrm{QP}}. \tag{76}$$

Put differently, H_{QP} is a quantum integral of the dynamics generated by $\alpha_{f_{\mathrm{QP}}}$.

In the remaining part of this section we introduce several models of the Hofstadter type and mention their symmetries, from which one can deduce then some qualitative properties of their spectrum and eigenfunctions. Furthermore, we show the results of numerical computations of spectra and eigenfunctions. In Table II the Hamiltonians of all these models are listed, together with their classical symbols.

TABLE V. Symmetries of the triangular lattice model.

Transformation	Description	Symmetry
No. ii	Rotation by π	$\sigma(\eta,\Phi)=\sigma(\eta+\Phi,\Phi)$
No. iii	Reflection at $x_1=x_2$	$\sigma(\eta,\Phi)=\sigma(\eta,-\Phi)$
No. iv	Reflection at $x_1=-x_2$	$\sigma(\eta,\Phi)=\sigma(-\eta,\Phi)$
No. ix	Reversion of sign infront of T_j	$\sigma(\eta)=(-1)^n\sigma(\eta+\pi n)$
$\Phi\to\Phi+2\pi$	Flux periodicity	$\sigma(\Phi)=\sigma(\Phi+2\pi n)$
	Parameter space	$\Phi\in[0,2\pi]$
		$\eta\in[0,\pi]$

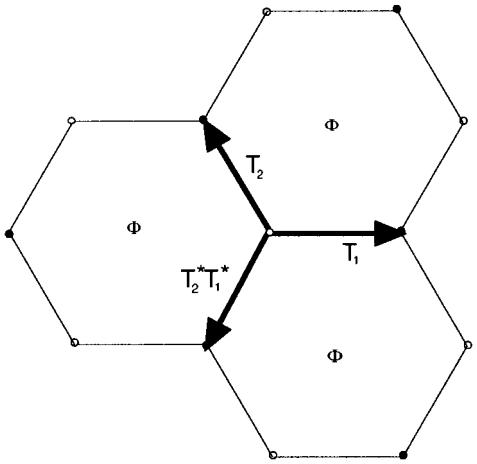

FIG. 10. Interactions in the Honeycomb model.

All numerical computations of the spectra are based on Chamber's relation (see Sec. V). This implies, in particular, that symmetries of classical symbols are reflected in spectral properties [see formula (108) in Sec. V].

A. The discrete Mathieu model

The discrete Mathieu Hamiltonian describes an anisotropic variant of the Hofstadter model. It contains a real parameter μ, which may be interpreted as the relative strength between the hopping interactions in the two lattice directions. The Hamiltonian is given by

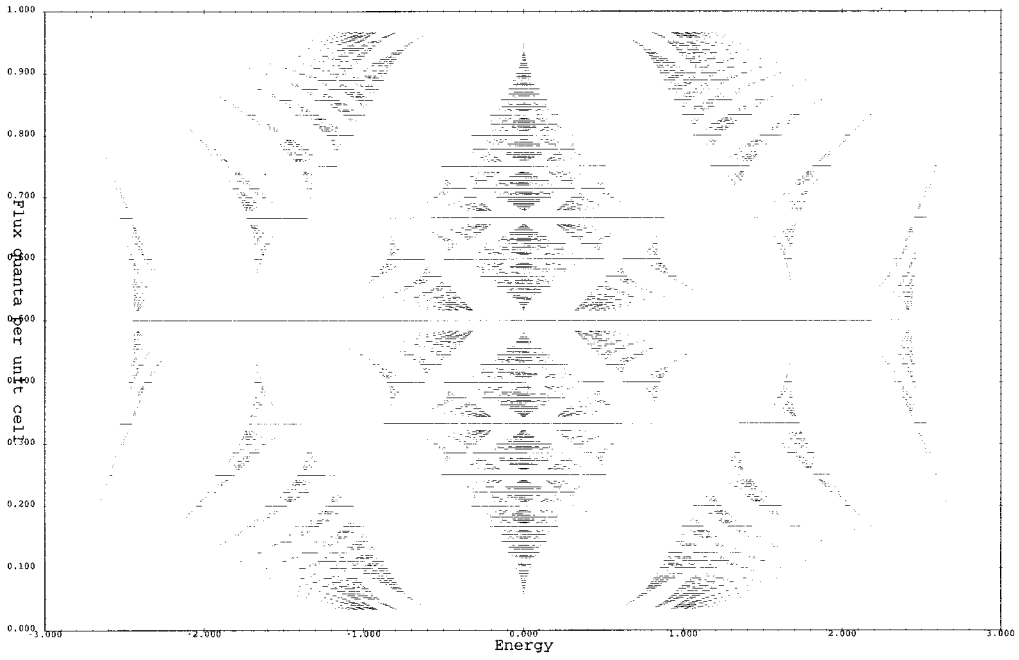

FIG. 11. Spectrum for the Honeycomb model.

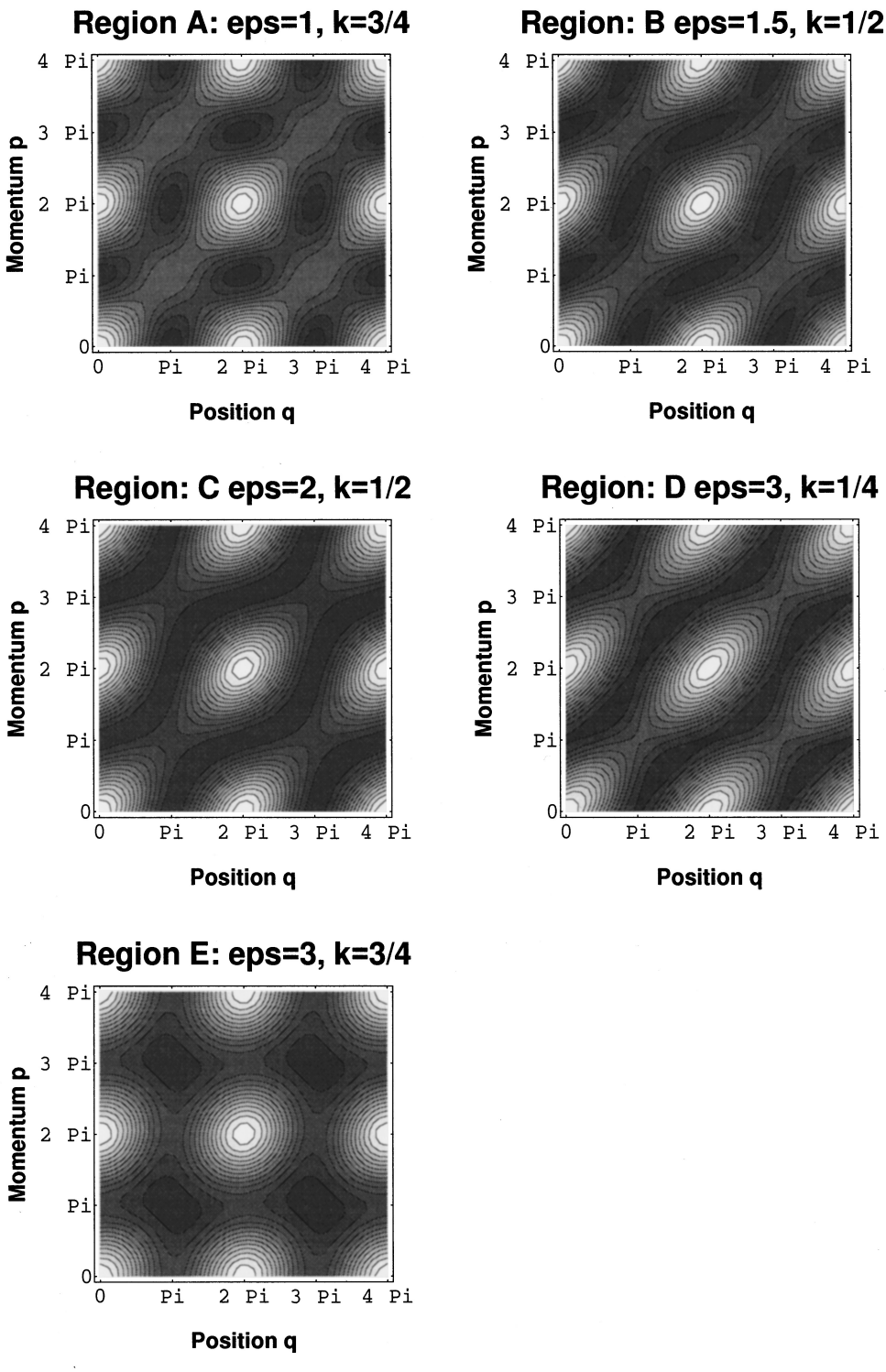

FIG. 12. Examples for classical contour levels in regions A–E for the Doubly-discrete Quantum Pendulum.

TABLE VI. Symmetries of the Doubly-discrete Quantum Pendulum.

Transformation	Description	Symmetry
No. i	Rotation by $\pi/2$	$\sigma(k)=\sigma(1/k)$
No. iii	Reflection at $x_1=x_2$	$\sigma(\Phi)=\sigma(-\Phi)$
No. ix	Reversion of sign infront of T_j	$\sigma(\epsilon)=-\sigma(-\epsilon)$
	Reversion of energy $H\to -H$	$\sigma(\epsilon,k)=-\sigma(-\epsilon,-k)$
	Derived	$\sigma(k)=-\sigma(-k)$
$\Phi\to\Phi+2\pi$	Flux periodicity	$\sigma(\Phi)=(-1)^n\sigma(\Phi+2\pi n)$
	Parameter space	$\Phi\in[0,2\pi]$
		$k\in(0,1]$
		$\epsilon\in[0,\infty)$

$$H(\mu)=T_1+\mu T_2+T_1^*+\mu T_2^*\,. \tag{77}$$

For $\mu=1$, we recover the Hofstadter Hamiltonian and, for $\mu=0$, the one-dimensional discrete Laplacian, which can be diagonalized explicitly. Hence μ interpolates between these limiting cases; therefore the discrete Mathieu model is a tool to derive properties of the Hofstadter model; e.g., in Ref. 37, the Chern number has been computed in this way. Other properties discussed by that method are the gap labeling,[38] the total gap length, and the spectrum for irrational flux (for recent results see Last[20]).

In Table III the symmetries including the automorphism that gives rise to the Aubry duality are put together. (Notice that in our formulation the Aubry duality transformation is simply the linear automorphism generated by a rotation about the angle $\pi/2$. It is implemented by discrete Fourier transformation.) In the last column of the table, their consequence for the spectrum is

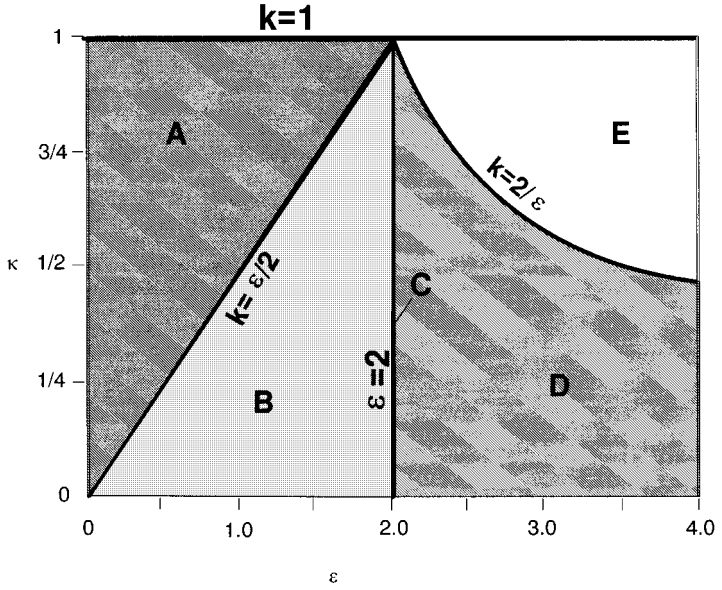

FIG. 13. Regions A–E for critical points in parameter space for the Doubly-discrete Quantum Pendulum.

TABLE VII. Critical points of the classical symbol for the Quantum Pendulum.

	Critical point		Region				
	x,p	Energy	A	B	C	D	E
Ia	$2\pi n,\ 2\pi m$	$2(2\epsilon+k+\frac{1}{k})$	a max.	a max.	a max.	a max.	a max.
Ib	$2\pi n,\ \pi(2m+1)$ or $\pi(2n+1),\ 2\pi m$	$-2(k+\frac{1}{k})$	a min.	a min.	a min.=IV	saddle	saddle
Ic	$\pi(2n+1),\ \pi(2m+1)$	$2(-2\epsilon+k+\frac{1}{k})$	1 max.	saddle	saddle	saddle	a min
II	$\pi n\pm\rightarrow\arccos((-1)^{n+1}\epsilon k/2)$, $\pi n\mp\rightarrow\arccos((-1)^{n+1}\epsilon k/2)$	$2((1-\epsilon^2/2k)-\frac{1}{k}$	saddle	saddle	a min=IV	a min	-
III	$\pi n\pm\rightarrow\arccos((-1)^{n+1})$, $-\pi n\pm\rightarrow\arccos((-1)^{n+1}\frac{\epsilon}{2k})$	$2(-k+(1-\epsilon^2/2)\frac{1}{k})$	saddle	-	-	-	-
IV	$t\pm\rightarrow\arccos(-\frac{\epsilon k}{2}\cos(t))$, $-t\pm\rightarrow\arccos(-\frac{\epsilon k}{2}\cos(t))$	$-2(k+\frac{1}{k})$	-	-	a min.	-	-

shown. These symmetries can also be read off from the contour levels of the classical symbol (Fig. 2). The spectra of the Hofstadter and the discrete Mathieu model are shown in Figs. 3 and 4, respectively. In Fig. 5, the Husimi function $H_{\Psi(0)}(n)$ for eigenstates of the Hofstadter model are shown. Small values are dark and large values white. The interpolation between the discrete values of n here and in the sequel are done using Eq. (71) of Sec. III.

B. The second neighbor square lattice model

The model was discussed by Wilkinson already in 1984.[8] Its Hamiltonian is given by the formula

$$H_{\mathrm{SN}}(\varepsilon)=T_1+T_2+\varepsilon(T_1^2+T_2^2)+\mathrm{h.c.}, \tag{78}$$

where ε denotes the relative strength of the coupling to the second neighbor in the lattice. Some qualitative properties of the spectrum (Fig. 6) follow already from the symmetries of the classical symbol (Table IV). Wilkinson's computation of the spectrum showed a splitting of the lowest subband into a braid-type structure (Fig. 6, focus on the point flux=0 and energy -2.4). This has been investigated in Ref. 39, and it was shown that the braid structure can be understood as a phase space tunneling between the four bottom wells in the Brillouin torus (Fig. 7).

C. The triangular lattice model

The triangular model was introduced by Claro and Wannier[40] and describes a hexagonal crystal. They computed the spectrum nummerically and found a nesting structure similar to the one for the Hofstadter model. A semiclassical analysis was presented in Ref. 41. In Ref. 42 the model was generalized to different fluxes in the two classes of triangles (Fig. 8). Its Hamiltonian is

$$H_{\mathrm{TR}}(\eta)=T_1+T_2+e^{-i\eta}T_1T_2+\mathrm{h.c.}. \tag{79}$$

It is remarkable that also in this case the spectrum can be computed in spite of the spatial inhomogeneity of the flux (Fig. 9). This is possible because Chamber's relation still holds (Sec.

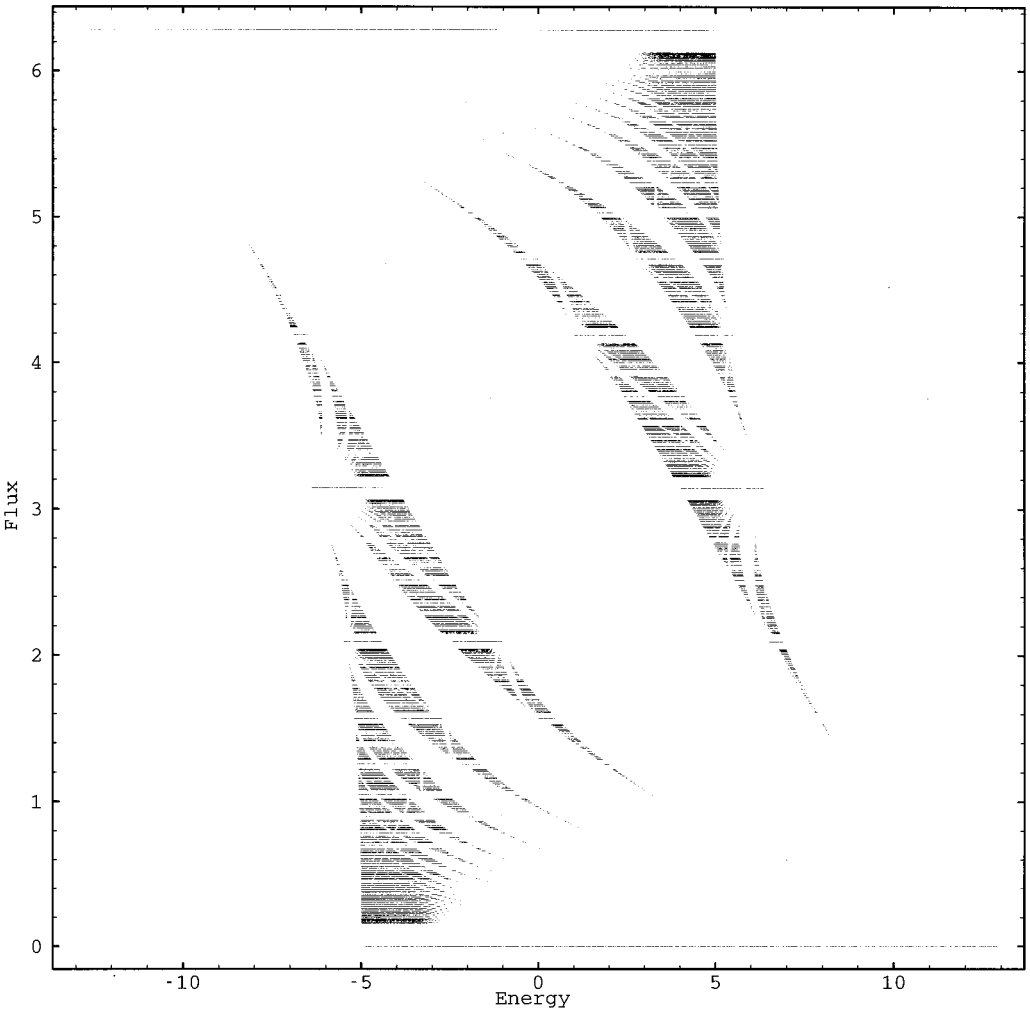

FIG. 14. Spectrum of the Doubly-discrete Quantum Pendulum at $\epsilon=2$ and $k=1/2$ (region C).

V). Numerical computations are in excellent agreement with semiclassical analysis.[42] Several qualitative aspects of the spectrum can already be understood by a simple consideration of symmetries (see Table V).

D. The honeycomb lattice model

This model has been introduced by Rammal[43] and is defined in terms of the Hamiltonian,

$$H_{\mathrm{HC}}=\begin{pmatrix} 0 & T_1+T_2+W(1,1) \\ T_1^*+T_2^*+W(1,1)^* & 0 \end{pmatrix}. \tag{80}$$

He computed the spectrum numerically. The Hamiltonian linkes sites of a bipartite lattice (Fig. 10). This implies that the square of the Hamiltonian is just two independent triangular

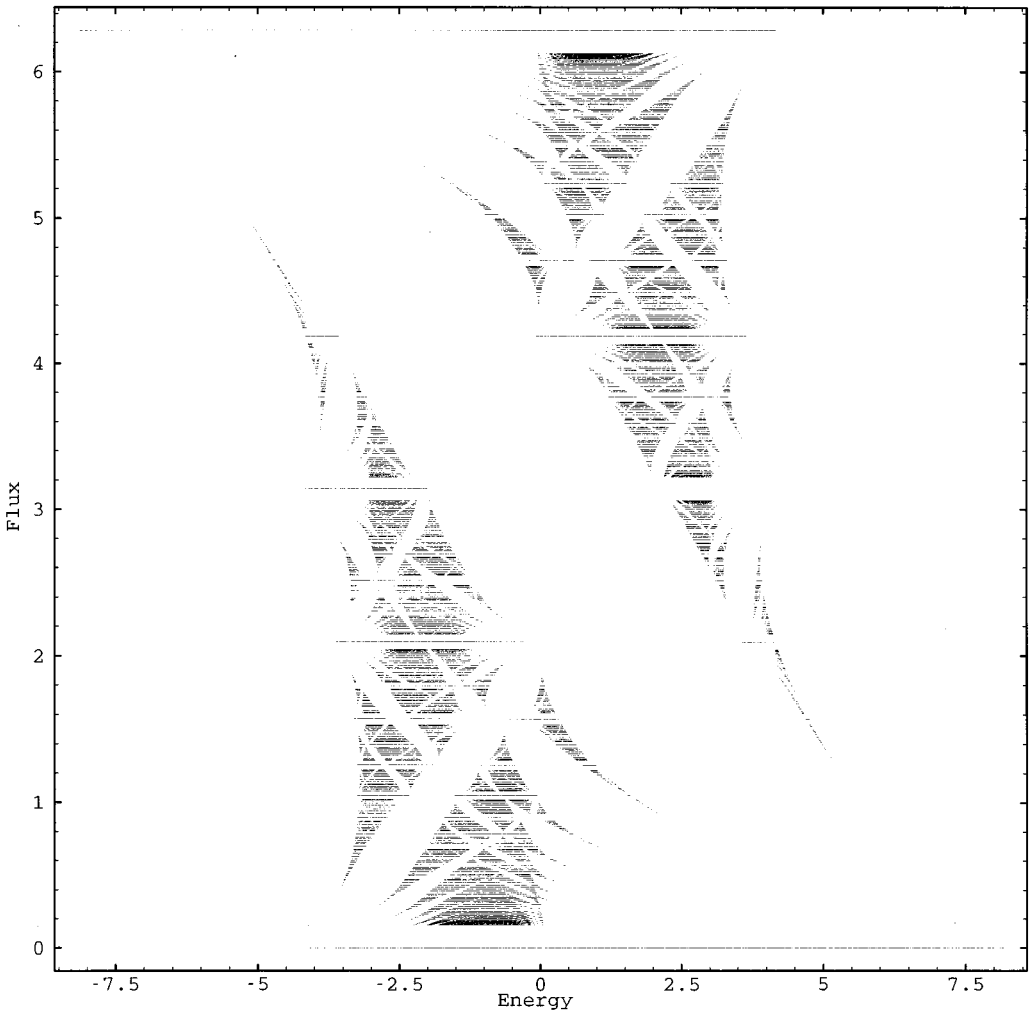

FIG. 15. Spectrum of the Doubly-discrete Quantum Pendulum at $\epsilon=1$ and $k=3/4$ (region A).

lattice models with, as it turns out, flux $\eta=0$. Hence the computation can be reduced to the previous case (Fig. 11).[42]

E. The doubly-discrete quantum pendulum

Recently, Bobenko, Kutz, and Pinkall have introduced a family of Hamiltonians that arises in the analysis of the Doubly-discrete sine-Gordon equation,[29]

$$H_{\mathrm{QP}}(\varepsilon,k)=\varepsilon(T_1+T_2)+kW(1,1)+\frac{1}{k}\,W(1,-1)+\mathrm{h.c.}, \tag{81}$$

where ε and k are real parameters. For $\varepsilon=2$, the Hamiltonian represents a quantum integral with respect to the automorphism defined by the Doubly-discrete sine-Gordon equation in zero spatial dimension [see the Introduction, Eq. (11)]. k is related to curvature.

The Hamiltonian H_{QP} in (81) belongs to the class of the next nearest neighbor Hamiltonians introduced by Hatsugai and Kohomoto.[44]

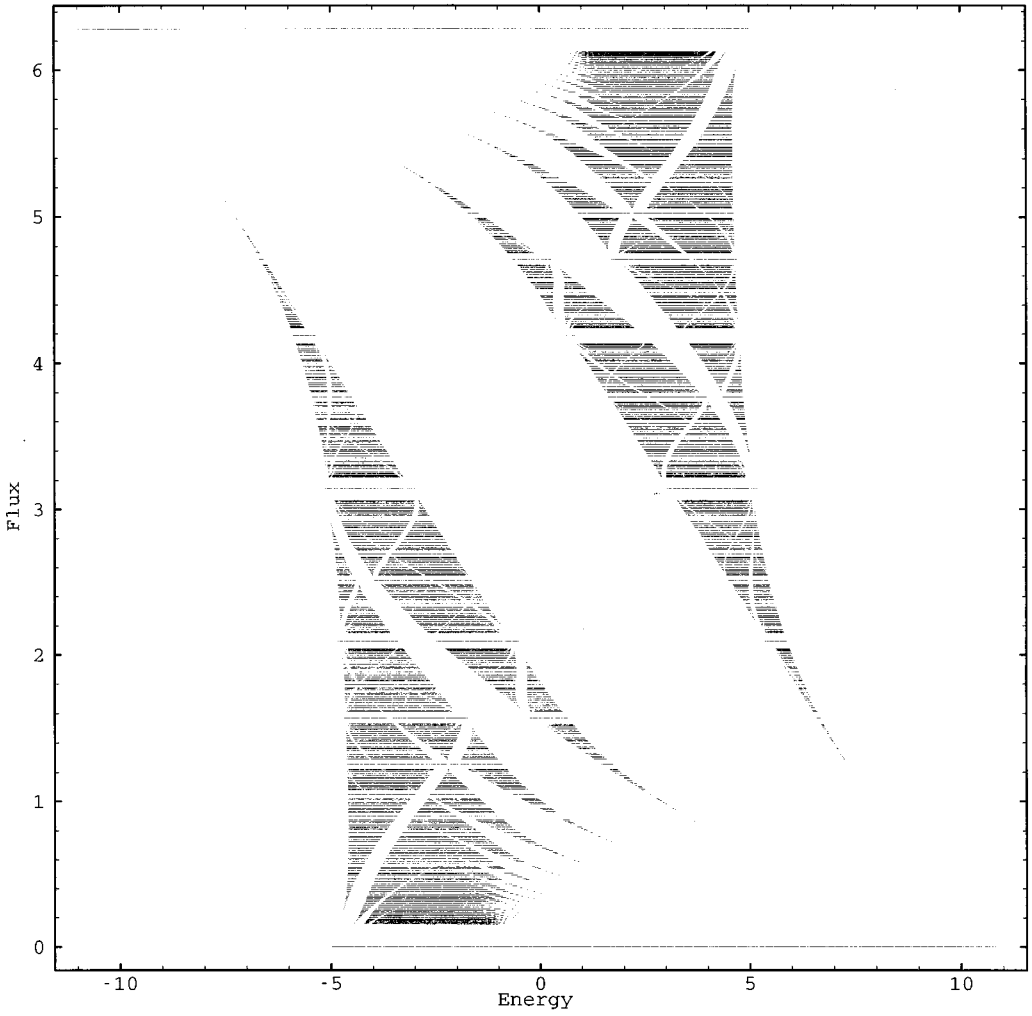

FIG. 16. Spectrum of the Doubly-discrete Quantum Pendulum at $\epsilon=1,5$ and $k=1/2$ (region B).

From the contour levels in classical phase space (Fig. 12), it becomes clear that the model is related to a classical pendulum. In each unit cell of phase space we have closed classical orbits at small energies. At high energies we see extended contours giving rise to rotating solutions. The parameter k is the analog of the gravitational constant in the usual pendulum and controls the onset of rotating solutions. The parameter ε interpolates between the discrete Mathieu model ($\varepsilon=0$) with flux $\Phi'=2\Phi$ and rescaled energy $E'=kE$ and the quantum integral ($\varepsilon=2$). Here, we used the algebra homomorpism

$$\Phi\mapsto 2\Phi, \quad T_1\mapsto e^{i\phi/2}T_2^*T_1^*, \quad T_2\mapsto e^{i\phi/2}T_1T_2^*. \tag{82}$$

In the limit $k\to 0$ the term $1/k$ dominates and the system turns into a discrete Laplacian (up to the factor $1/k$). Finally, if $\varepsilon=k$, the Hamiltonian converges in the limit $\varepsilon\to\infty$ to the Hamiltonian of a triangular lattice model with rescaled energy. Qualitative properties of the spectrum follow again from symmetries of the classical symbol (Table VI) due to the Chambers relation [(108), Sec. V].

The discussion of this model will be continued in the next section.

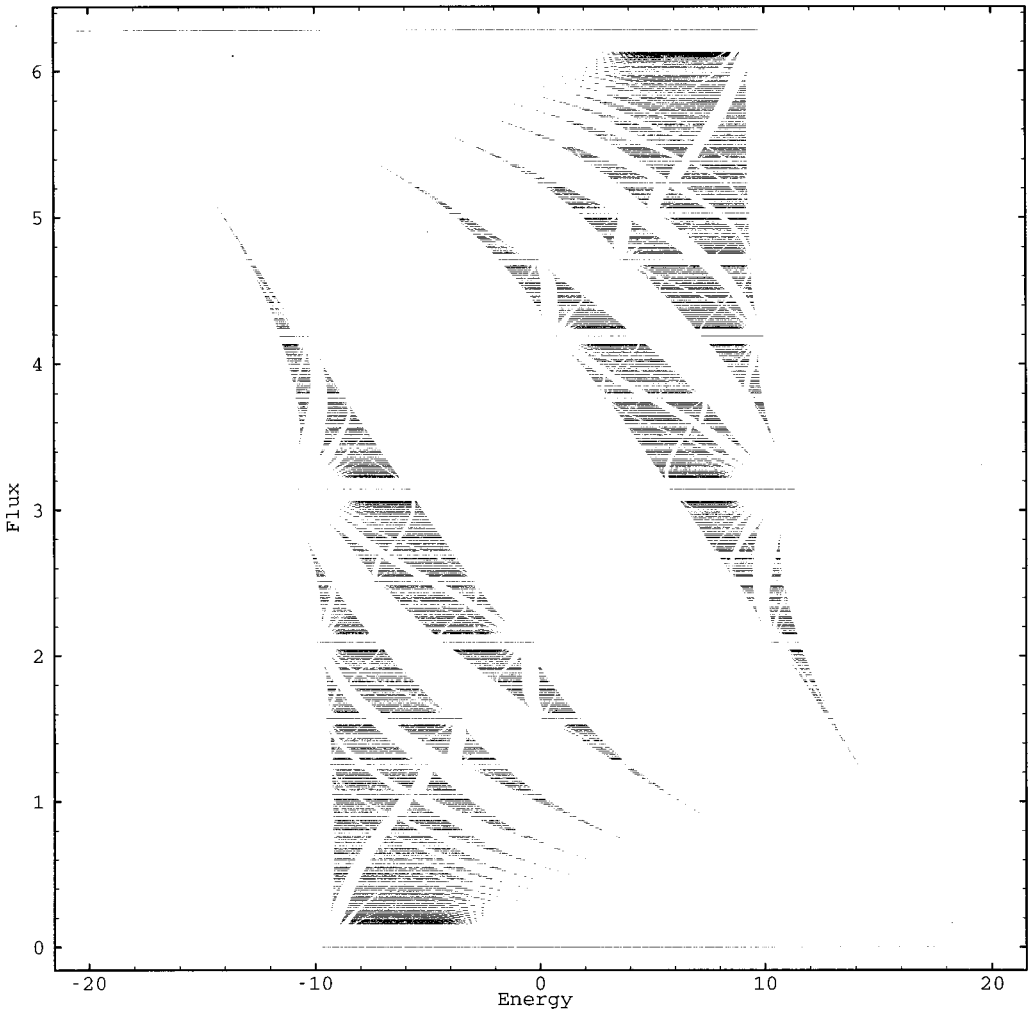

FIG. 17. Spectrum of the Doubly-discrete Quantum Pendulum at $\epsilon=3$ and $k=1/4$ (region D).

V. SPECTRA AND EIGENFUNCTIONS

The analysis of the spectra for Hamiltonians of the Hofstadter-type models is greatly simplified by the Chambers relation. It expresses the fact that the characteristic polynomial of the Hamiltonian restricted to a fiber over the Brillouin torus is the sum of two terms. The first one is a universal polynomial, i.e., it is independent of the coordinate θ of the Brillouin zone, and the second term is the zeroth-order term of the polynomial. It is the only term where the θ dependence enters. This term is furthermore a scaled version of the principal symbol of the Hamiltonian.

We explain Chambers relation for the case of the Doubly-discrete Quantum Pendulum and prove the following result.

Theorem 1: If the flux $\Phi=p/q$ is rational and p,q relatively prime, the secular determinant for the Doubly-discrete Quantum Pendulum is given by Chamber's formula,

$$\det(H_{\mathrm{QP}}(\theta)-z)=p(z)+h_{\mathrm{QP}}(\theta), \tag{83}$$

where $p(z)$ is a polynomial of degree q and

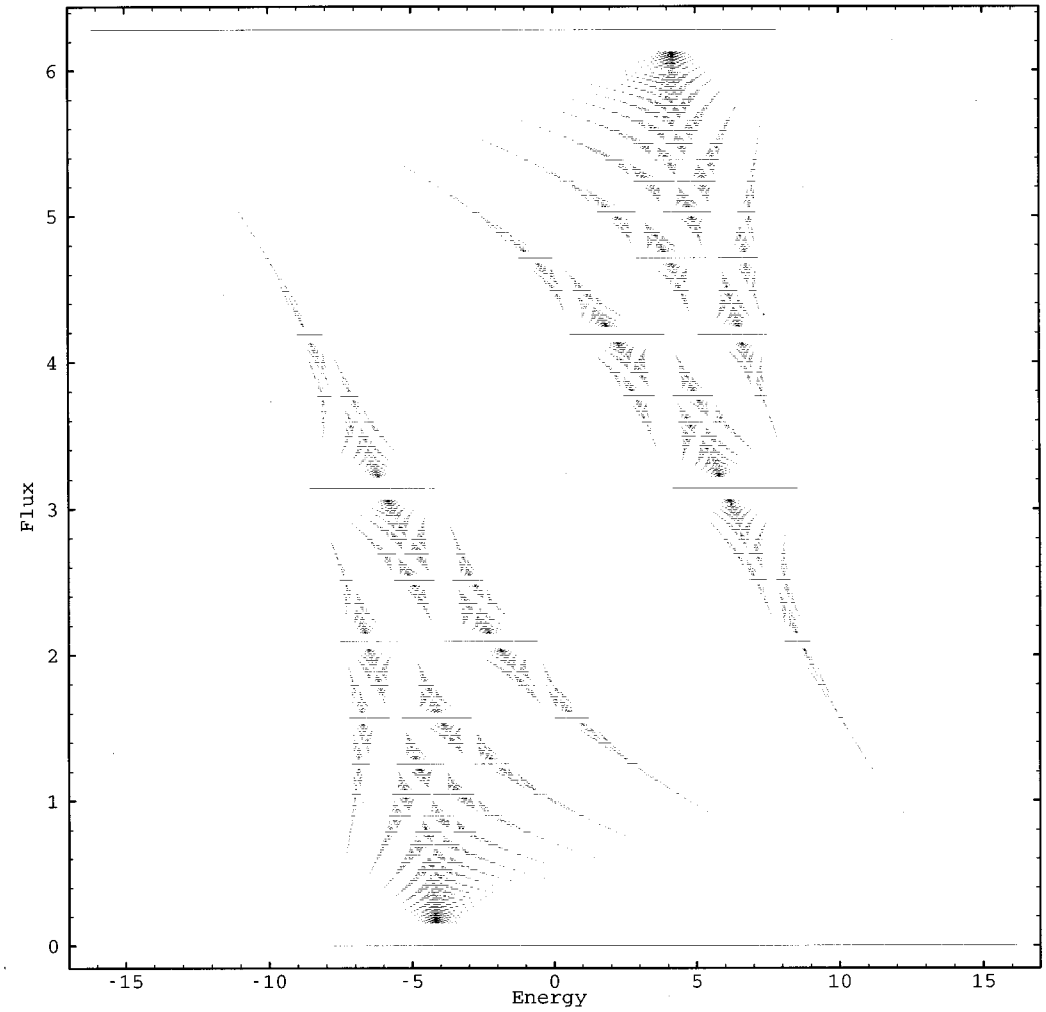

FIG. 18. Spectrum of the Doubly-discrete Quantum Pendulum at $\epsilon=3$ and $k=3/4$ (region E).

$$h_{\mathrm{QP}}(\theta)=-4T_q(-\varepsilon/2)(\cos q\theta_1+\cos q\theta_2)+2(-1)^p\left(k^q\cos q(\theta_1+\theta_2)+\frac{1}{k^q}\cos q(\theta_1-\theta_2)\right). \tag{84}$$

Here T_q denotes the Chebyshev polynomial of degree q, defined by $T_q(\cos x)=\cos qx$ and $T_q(-1)=(-1)^q$.

Chamber's relation is not only very useful to compute spectra. It also shows several conceptually interesting features. The offset function $h_{\mathrm{QP}}(\theta)$—which is almost the classical symbol—generates on the Brillouin torus a Hamiltonian vector field, which gives rise to an isospectral flow.[45] Furthermore, the secular determinant for the Hofstadter model can be factorized at the band edges. This makes it possible to compute the spectral bands algebraically for rather large values of p and q in the field of the cyclotomic extensions of the rationals.[46]

Proof: The characteristic polynomial is a function of $\theta\in\mathscr{B}$ and $z\in\mathbb{C}$,

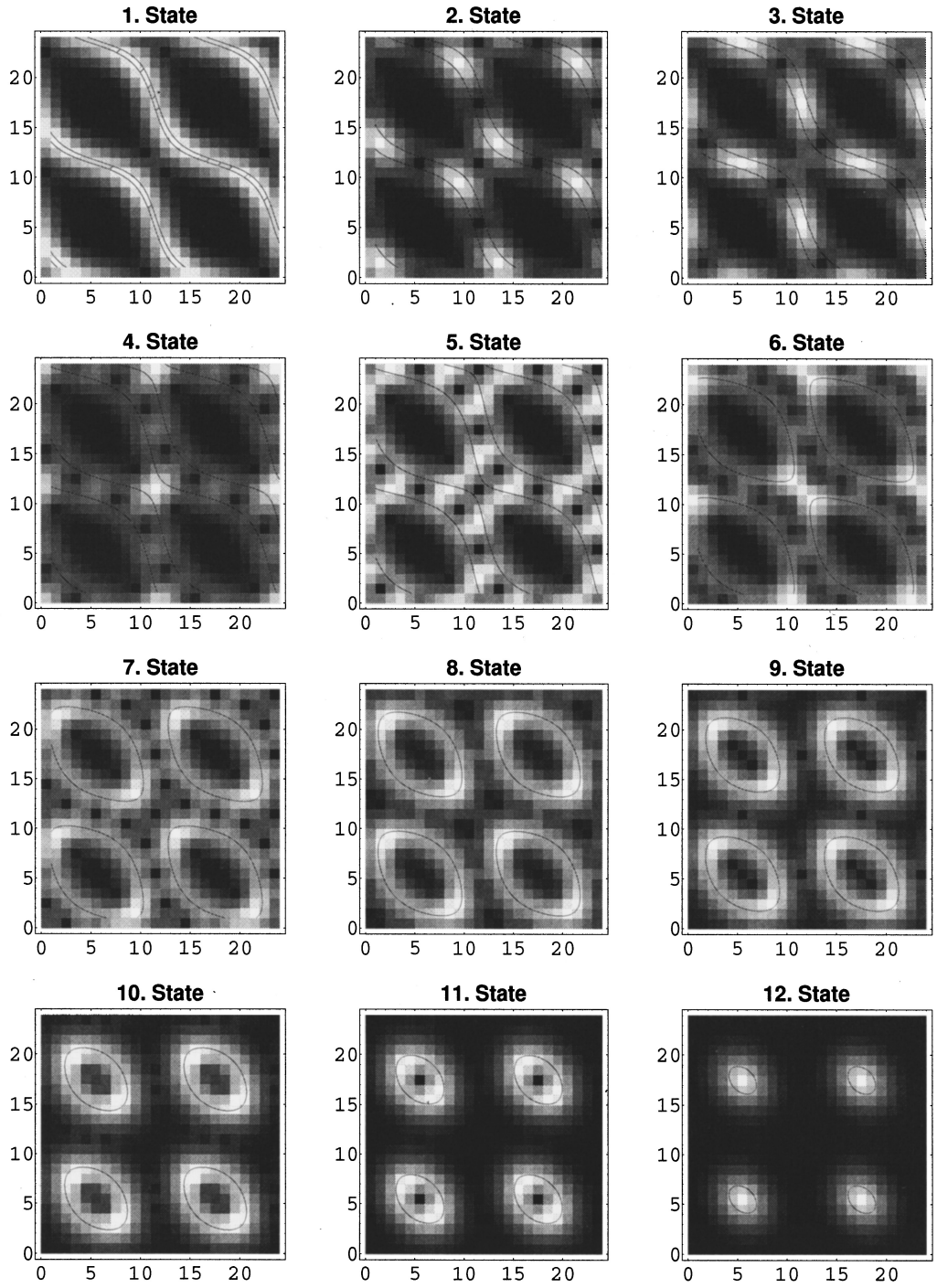

FIG. 19. Husimi transformation for eigenstates of the Quantum Pendulum at $\Phi=2\pi(1/12)$, $\epsilon=2$, $k=1/2$, $\theta=(0,0)$.

$$F(\theta,z):=\det(H_{\mathrm{QP}}(\varepsilon,k,\theta)-z). \tag{85}$$

By definition, it is 2π periodic in the variable θ. Due to Remark 3 after Theorem 2 in Sec. III it is, however, $2\pi/q$-periodic in θ_1 and θ_2. Hence, it can be expressed in terms of a Fourier series as follows:

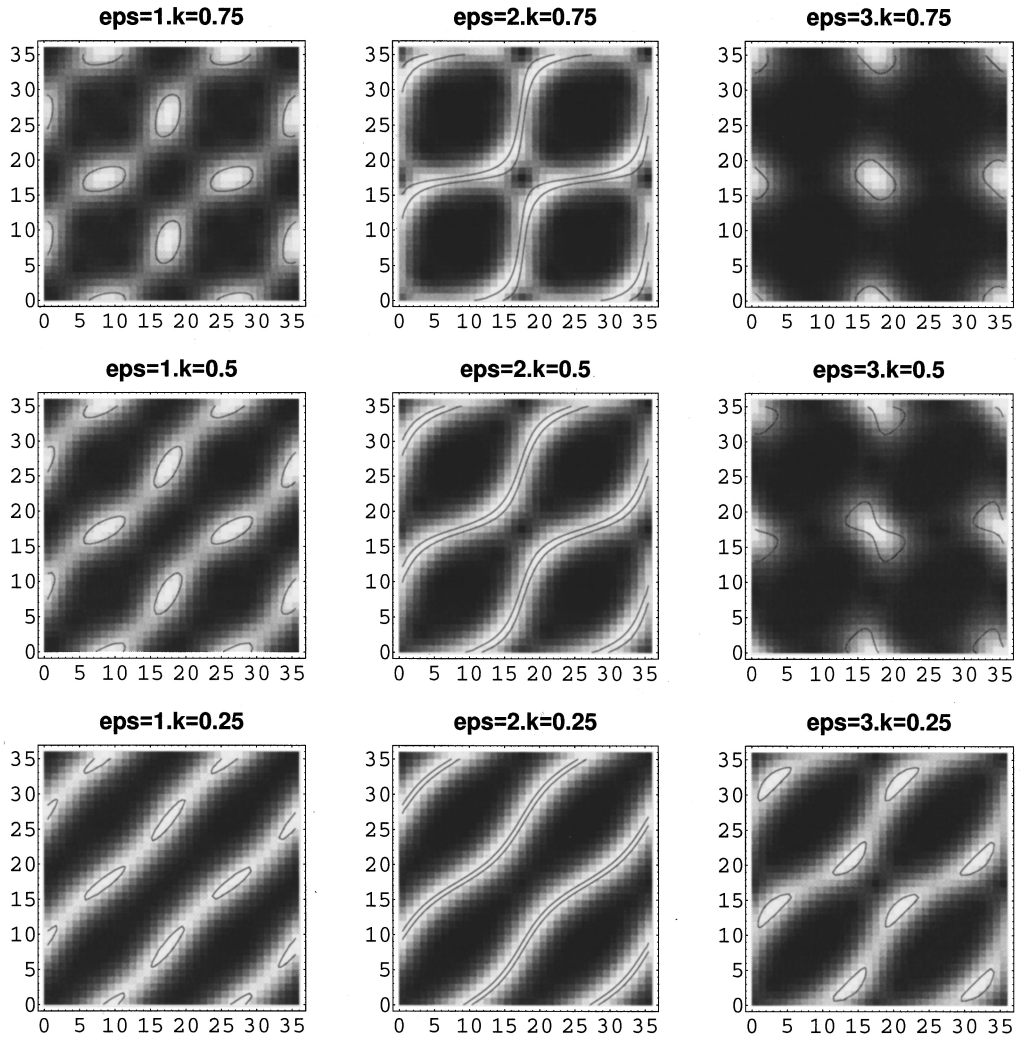

FIG. 20. Husimi transformation of the ground state of the Doubly-discrete Quantum Pendulum for $\Phi=2\pi\frac{1}{9}$.

$$F(\theta,z)=\sum_{n\in\mathbb{Z}^2} F_n(z)\xi_1^{qn_1}\cdot\xi_2^{qn_2}, \tag{86}$$

where we introduced the notation $\xi_1 = e^{i\theta_1}$, $\xi_2 = e^{i\theta_2}$.

Next, we argue that the only nonvanishing terms in the above Fourier series are those for which $|n_1|\leqslant 1$ and $|n_2|\leqslant 1$. This follows from the explicit form of the Hamiltonian,

$$H_{\mathrm{QP}}(\varepsilon,k,\theta)=\varepsilon\left(\xi_1 t_1+\xi_2 t_2+\frac{1}{\xi_1}t_1^*+\frac{1}{\xi_2}t_2^*\right)+k\left(\xi_1\xi_2 W(1,1)+\frac{1}{\xi_1\xi_2}W(1,1)^*\right)$$
$$+\frac{1}{k}\left(\frac{\xi_1}{\xi_2}W(1,-1)+\frac{\xi_2}{\xi_1}W(1,-1)^*\right), \tag{87}$$

and the obvious fact that the determinant is homogeneous of order q in the entries of the $q\times q$ matrix; so we get

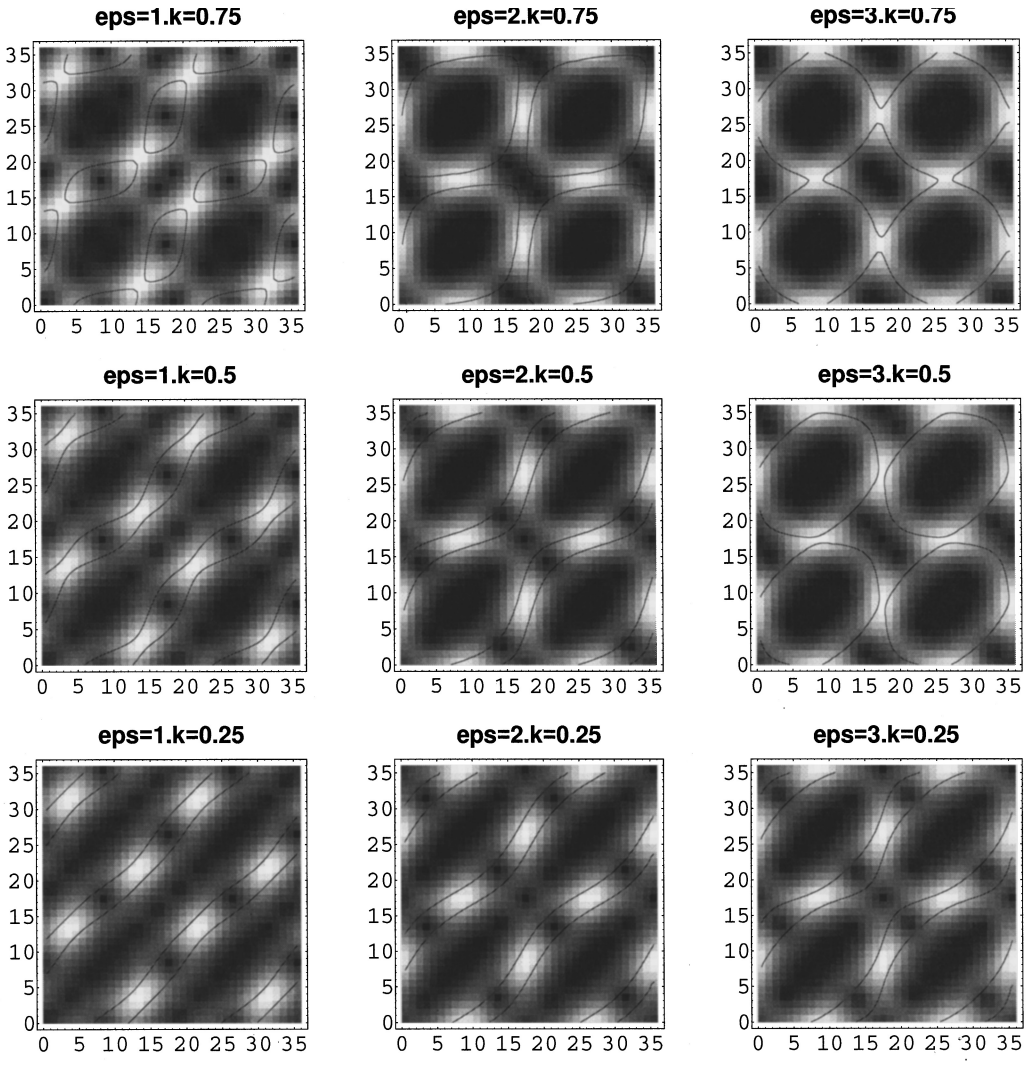

FIG. 21. Husimi transformation of the third state of the Doubly-discrete Quantum Pendulum for $\Phi=2\pi\frac{1}{9}$.

$$F(\theta,z)=\sum_{\substack{|n_1|\leqslant 1\\ |n_2|\leqslant 1}} F_n(z)\xi_1^{qn_1}\xi_2^{qn_2}. \tag{88}$$

The coefficients $F_n(z)$ are now computed by taking limits in this equation to various singular points,

$$\det(H_{\mathrm{QP}}(\varepsilon,k,\theta)-z)=\det\left(\varepsilon\left(\xi_1 t_1+\xi_2 t_2+\frac{1}{\xi_1}t_1^*+\frac{1}{\xi_2}t_2^*\right)+k\left(\xi_1\xi_2 e^{-i\Phi/2}t_1t_2+\frac{1}{\xi_1\xi_2}e^{i\Phi/2}t_2^*t_1^*\right)\right.$$
$$\left.+\frac{1}{k}\left(\frac{\xi_1}{\xi_2}e^{i\Phi/2}t_1t_2^*+\frac{\xi_2}{\xi_1}e^{-i\Phi/2}t_2t_1^*\right)-z\right)=\sum_{\substack{|n_1|\leqslant 1\\ |n_2|\leqslant 1}} F_n(z)\xi_1^{qn_1}\xi_2^{qn_2}. \tag{89}$$

Consider, for instance, the case $\xi_1\to\infty$. It leads to the equation (using $\det t_1=1$)

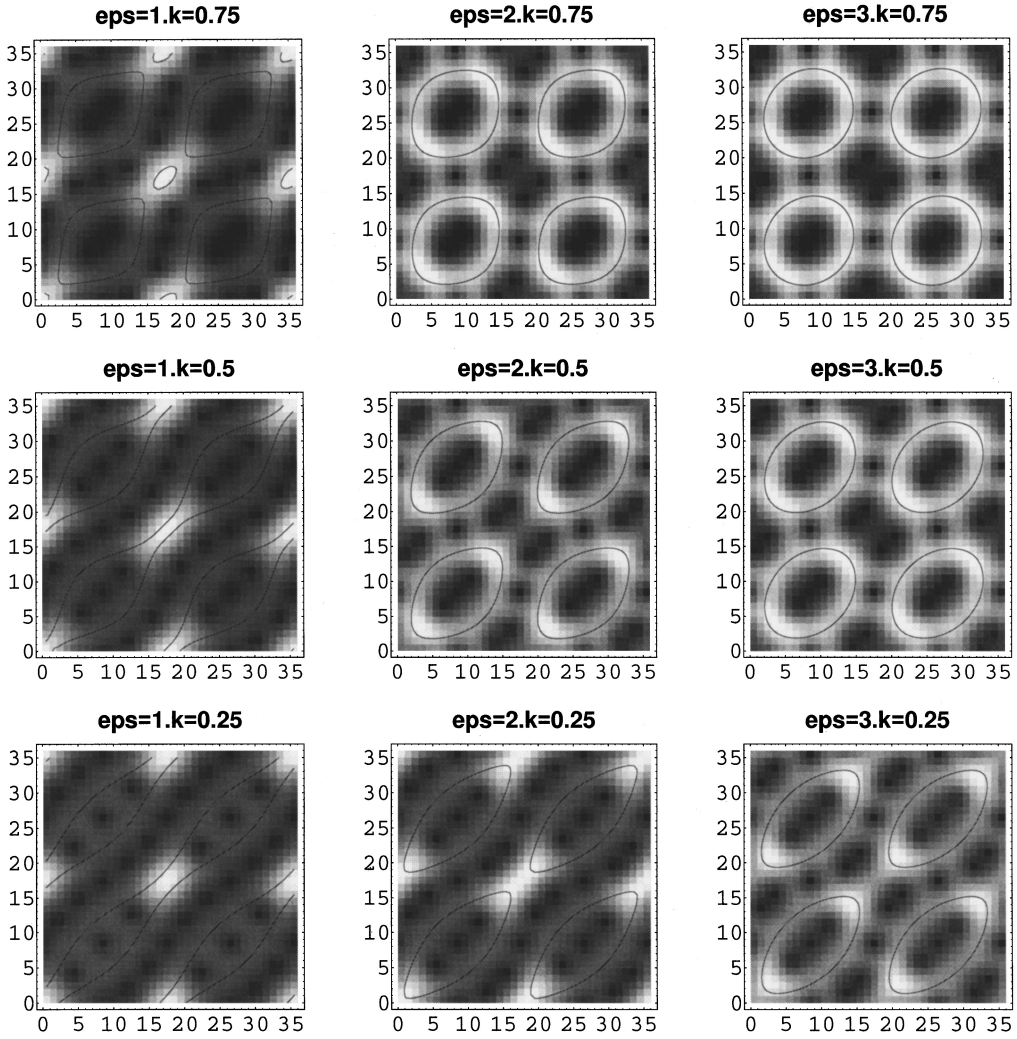

FIG. 22. Husimi transformation of the sixth state excitation of the Doubly-discrete Quantum Pendulum for $\Phi=2\pi\frac{1}{9}$.

$$\det\left(\varepsilon t_1+k\varepsilon_2 e^{-i\Phi/2}t_1t_2+\frac{1}{k\xi_2}\,e^{-i\Phi/2}t_1t_2^*\right)=\det\left(\varepsilon+k\xi_2 e^{-i\Phi/2}t_2+\frac{1}{k\xi_2}\,e^{i\Phi/2}t_2^*\right)$$
$$=F_{1,0}(z)+F_{1,1}(z)\xi_2^q+F_{1,-1}^{(z)}\xi_2^{-q}. \tag{90}$$

A second limiting procedure $\xi_2\to\infty$ leads to

$$\det(ke^{-i\Phi/2}t_2)=F_{1,1}(z). \tag{91}$$

Since $\det(t_1)=\det(t_2)=1$, we get the result

$$F_{1,1}(z)=k^q\cdot e^{-iq\Phi/2}=k^q(-1)^p. \tag{92}$$

If we replace the limit above by $\xi_2\to 0$, we find

$$F_{1,-1}(z)=k^{-q}(-1)^p. \tag{93}$$

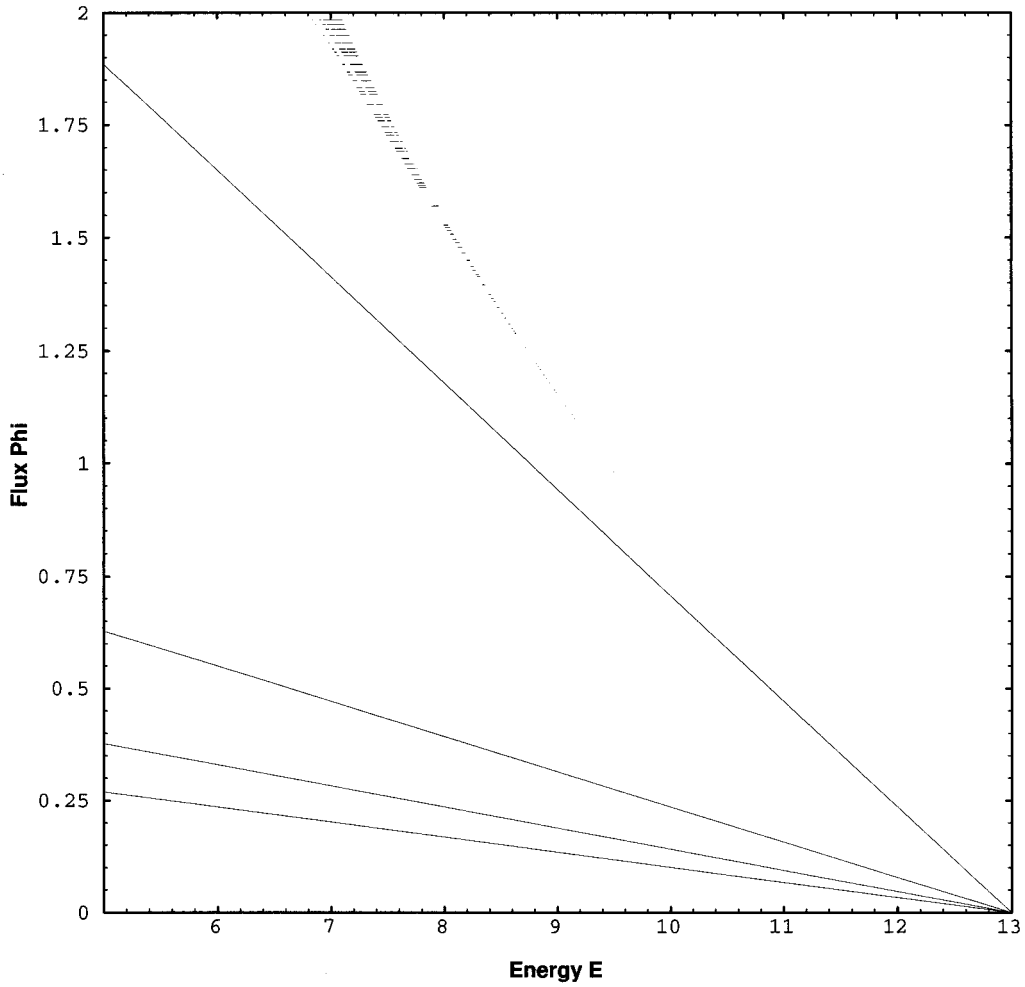

FIG. 23. Exact spectrum and semiclassical Landau levels at $\epsilon=2$, $k=1/2$.

Similarly, we can replace the limit $\xi_1\to\infty$ by $\xi_1\to 0$ followed by $\xi_2\to\infty$ and $\xi_2\to 0$.

This leads to

$$F_{-1,1}(z)=k^{-q}(-1)^p, \quad F_{-1,-1}(z)=k^q(-1)^p. \tag{94}$$

Among the coefficients arising in these equations, only $F_{1,0}(z)$ remains to be computed. This follows easily from the following proposition.

Proposition 2: for any $z\in\mathbb{C}$, $j=1,2$, and $\lambda\in\mathbb{C}\setminus\{0\}$,

$$\det\left(\lambda t_j+\frac{1}{\lambda}\,t_j^*-z\right)=-2T_q\left(\frac{z}{2}\right)+(\lambda^q+\lambda^{-q}), \tag{95}$$

where $T_n(x)=\cos(n\arccos(x))$ is the nth Chebyshev polynomial.

The proof of the proposition uses again the same idea as before. The function $[\lambda t_1 + (1/\lambda)t_1^* - z]$ is a Laurent polynomial in λ of order q and invariant under the substitution $\lambda\to e2\pi i/q\lambda$. Hence, it can be expressed in terms of a Fourier series with three terms only,

$$\det\left(\lambda t_1+\frac{1}{\lambda}\,t_1^*-z\right)=b_0(z)+b_{+1}(z)\lambda^q+b_{-1}(z)\lambda^{-q}. \tag{96}$$

The terms $b_{\pm 1}(z)$ can be computed through the limits $\lambda\to\pm\infty$, from which we infer that $b_\pm(z)=\det t_1^{\pm 1}=1$. So we are left with the computation of the polynomial $b_0(z)$.

By construction, t_1 has the eigenvalue one and is diagonal. Hence, the left-hand side of (96) vanishes if

$$\lambda+\frac{1}{\lambda}-z=0. \tag{97}$$

From this equation and (96) we conclude that

$$b_0\left(\lambda+\frac{1}{\lambda}\right)+\lambda^q+\lambda^{-q}=0, \tag{98}$$

which up to trivial factors, is the functional equation for the Chebyshev polynomial $T_q(x)$,

$$T_q\left(\frac{1}{2}\,(\lambda+\lambda^{-1})\right)-\frac{1}{2}\,(\lambda^q+\lambda^{-q})=0. \tag{99}$$

So, we finally get the result

$$b_0(x)=-2T_q\left(\frac{x}{2}\right). \tag{100}$$

This proves Proposition 2.

Now we are prepared to compute F_{10} from Eq. (90):

$$F_{10}(z)=\det\left(\varepsilon+k\xi_2 e^{-i\Phi/2}t_2+\frac{1}{k\xi_2}\,e^{i\Phi/2}t_2^*\right)-k^q(-1)^p(\xi_2^q+\xi_2^{-q})=-2T_q\left(-\frac{\varepsilon}{2}\right). \tag{101}$$

Analogously, we obtain

$$F_{-1,0}(z)=-2T_q\left(-\frac{\varepsilon}{2}\right). \tag{102}$$

The only term left is $F_{00}(z)$. The results proved so far show that it is the only coefficient among the F_n's, which possibly has an explicit z dependence. All other terms are independent of z. Summarizing, we obtain

$$F(\theta,z)=F_{(0,0)}(z)+\sum_{\substack{|n_1|=1\\|n_2|=1}}(-1)^p k^{n_1n_2q}\xi_1^{n_1q}\xi_2^{n_2q}-2T_q(-\varepsilon/2)((\xi_1^q+\xi_1^{-q})+(\xi_2^q+\xi_2^{-q})). \tag{103}$$

This finishes the proof of Theorem 1.

Similar results hold for many other Hamiltonians of the Hofstadter type; in particular, for all those that are of the form

$$H=\sum_{\substack{|m_1|\leqslant 1\\|m_2|\leqslant 1}}t(m)W(m). \tag{104}$$

This class contains all the models mentioned so far (except the second neighbor square lattice model).

For rational flux the spectrum of the Hamiltonian is computed in terms of band functions, defined as follows. For $\Phi = p/q$, $p \wedge q = 1$, the Hamiltonian H may be expressed in terms of a direct integral (Sec. III, Theorem 3 and Eq. (63)],

$$H \cong \frac{1}{|\mathscr{B}|} \int_{\mathscr{B}}^{\oplus} d^2\theta \; H(\theta) \otimes \mathbb{1}, \tag{105}$$

where $H(\theta)$ is a $q \times q$ matrix operator. Its spectrum is given in terms of the spectra of the fiber Hamiltonians, $H(\theta)$, by

$$\sigma(H) = \bigcup_{\theta \in \mathscr{B}} \sigma(H(\theta)). \tag{106}$$

The latter is computed as the zero set of the secular determinant:

$$\{z | \det(H(\theta) - z) = 0\} = \{E_1(\theta), \ldots, E_q(\theta)\}. \tag{107}$$

$E_1(\theta), \ldots, E_q(\theta)$ are the band functions. Since $H(\theta) = \overline{H(\theta)}^*$ is analytic in θ_1 and θ_2 the band functions are real analytic in both θ_1 and θ_2 separately and continuous jointly in θ_1 and θ_2.[47]

Due to Chambers relation,

$$\det(H(\theta) - z) = P(z) - h(\theta), \tag{108}$$

the band functions are the branches of the relation $P^{-1} \circ h$.

Each band function $E(\theta)$ gives rise to a band $[E_{\min}, E_{\max}] \subset \sigma(H)$, where the band edges are critical points, $dE(\theta_{\min}) = dE(\theta_{\max}) = 0$.

Chamber's relation has another interesting consequence for the critical points of all band functions. Every critical point of the classical symbol $h(\theta)$ is a joint critical point of all band functions, since

$$P'(E(\theta)) \cdot E'(\theta) = h'(\theta). \tag{109}$$

The converse is slightly more subtle. If $E(\theta)$ describes a band that does not touch another one, i.e., $P'(E(\theta)) \neq 0$, for critical points θ of h, the critical points of $E(\theta)$ coincide with those of $h(\theta)$. Degeneracies of spectra occur generically only on a set of codimension 3, hence for discrete points (θ, Φ) in $\mathscr{B} \times \mathbb{R}$ (Neumann and Wigner[48]).

Notice that the fact just mentioned simplifies the computation of spectra considerably since instead of computing all the band functions one merely needs to compute the band edges, i.e., the zeros of the equation

$$P(z) = h(\theta_{\text{crit}}), \tag{110}$$

for all critical points θ_{crit} of h.

Critical points of band functions or of the corresponding classical symbol, respectively, are relevant for the semiclassical analysis of the spectra (see below). They can have a complicated geometrical structure depending on the parameters of the model.

As an example we consider the case of the Doubly-discrete Quantum Pendulum. The parameter space is decomposed into five regions A–E as shown in Fig. 13. In Table VII we list the critical sets in the Brillouin torus $\mathscr{B}$ of the classical symbol. *a* max and *a* min denote absolute maxima and absolute minima, respectively, while max and min refer to local maxima and minima.

In all five regions, there is just one absolute maximum at $(x_1, x_2) = (0,0)$. In a vicinity of this point the Hamiltonian is parabolic and gives rise to oscillating classical solutions. There is one

absolute minimum in all regions except in case C, where $\varepsilon=2$. This case is the one originating from discrete geometry. The absolute minimum is a loop in $\mathscr{B}$, hence a classical orbit.

In the general case, there is a saddle point between the absolute maximum and the absolute minimum. This is clearly seen from the plot of classical contour levels (see Fig. 12).

We have computed numerically the band spectrum of the Doubly-discrete Quantum Pendulum for rational flux by diagonalizing the fiber Hamiltonian $H(\theta)$ at the critical points of the dilated classical symbol h_{QP} defined in (84). These values can be computed easily from the critical points of the classical symbol (Table VII). In Figs. 14–18 we present typical spectra for the regions A–E. In Figs. 19–22, Husimi functions for various parameters and quantum numbers are shown. The figures contain the classical orbits and show that the Husimi functions are localized at their classical counterparts.

Now we present a semirigorous semiclassical analysis of the spectrum of the Doubly-discrete Quantum Pendulum and apply techniques known from the Hofstadter model[8] to the critical points of the classical symbol. If the critical points are not isolated, as is the case for the Doubly-discrete Quantum Pendulum with $\varepsilon=2$, one has to apply technics that are analytically even more involved.[49,50] They go back in spirit to the reaction path method of quantum chemistry.[51,52]

In the case of an isolated critical point there are classically oscillating orbits nearby, giving rise to quasimodes. Their energy can be computed as follows: Consider, e.g., the absolute maximum of the classical symbol at $(x_1,x_2)=(0,0)$, which is unique for all parameter values. Using a semiclassical representation of the Rotation Algebra, namely,

$$T_1=e^{i(x_1+\sqrt{\Phi}K_1)},\quad T_2=e^{i(x_2+\sqrt{\Phi}K_2)},\quad [K_1,K_2]=i, \tag{111}$$

we expand the Hamiltonian in $\sqrt{\Phi}$ around the critical point up to second order and obtain the formal expression

$$H=H_{\mathrm{QP}}(0,0)\pm|\Phi|\sqrt{\det D^2H_{\mathrm{QP}}(0,0)}(K_1^2+K_2^2)+O(|\Phi|^{3/2}). \tag{112}$$

$D^2H_{\mathrm{QP}}(0,0)$ is the Hessian of the classical symbol at the critical point (0,0) where the equation holds:

$$\omega_{\varepsilon,k}=-\sqrt{\det D^2{}_{\mathrm{QP}}(0,0)}=\sqrt{(\varepsilon+2k)(\varepsilon+2/k)}, \tag{113}$$

and, thus, the semiclassical eigenvalues are given by

$$E_n=2(2\varepsilon+k+1/k)-\omega_{\varepsilon,k}(2n+1),\quad (n\in\mathbb{Z}). \tag{114}$$

In physical terms this corresponds to a Bohr–Sommerfeld quantization of classically oscillating solutions.

This approach is oriented toward energies at the top—respectively for isolated critical values of the classical symbol—and small flux. In this case the bands are very short, so one may refer to them as single numbers. As in other Hofstadter-like, models the results match the exact spectrum very well, even for comparatively large values of magnetic flux Φ [see Fig. 23]. For larger flux and smaller energies this changes—due to tunneling—and the bands get longer.

This semiclassical argument does not hold anymore if the energy is close to a classical saddle point, where there are rotating classical solutions.

Except at $\varepsilon=2$ the classical symbol possesses an absolute minimum in phase space, which, again, gives rise to energy levels of the same type as before. This time, however, they emerge from the minimal classical energy. In Fig. 18 (region E) one can easily spot them since the minimal energy is well separated from the separatrix energy, as in the case of the square lattice.

In each region of the parameter space we find rotating solutions for the classical Hamiltonian. In the covering space of phase space they appear as noncompact contours in an energy range

between two distinct saddle points. Except for the trajectory at minimal energy for $\varepsilon=2$, we always find two different rotating solutions at the same energy level. Their semiclassical analysis is more complicated and will not be discussed here.[49,50]

ACKNOWLEDGMENTS

The idea of proof of Chamber's relation (Sec. V) and much more about the Hofstadter model, we learned from Jean Bellissard many years ago, before the discovery of the Doubly-discrete Quantum Pendulum. In particular, he introduced us into the algebraic setting of the Hofstadter Model. We benefitted, furthermore, much from discussions with Ulrich Pinkall and many other members of the SFB ''Differential Geometry and Quantum Physics.'' In particular, the automorphism relating the Hofstadter model to the Doubly-discrete Quantum Pendulum is due to him (Sec. V). We had many stimulating discussions with Ludwig Faddeev. Volker Bach helped us with scientific and linguistic questions alike.

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Entropy of a subalgebra and quantum estimation

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In this paper we compare the accessible information of quantum communication channels with the entropic content of finite-dimensional matrix algebras with respect to quantum states, as defined by Connes, Narnhofer, and Thirring. In particular, every Abelian $n\times n$ matrix algebra together with a density matrix define the input alphabet of a quantum communication channel whose accessible information equals the entropic content of the algebra with respect to the state. The cases $n=2$ and $n=3$ are concretely examined in connection with the problem of the best estimation. © *1996 American Institute of Physics.* [S0022-2488(96)00110-7]

I. INTRODUCTION

The recent advances in the technology of information transmission[1,2] and the highly stimulating field of quantum computation[3] have greatly enhanced the need of noncommutative generalizations of Shannon's classical information theory.[4]

We will consider idealized communication channels at whose ends Alice is the sender and Bob the receiver. Alice uses quantum means (photons and an optical fiber) to encode a message and to send it to Bob. She might transmit photons in orthogonal, say vertically–horizontally polarized states, each one containing a classical bit of information. Then Bob, by measuring whether the incoming photons are vertically or horizontally polarized, would decode Alice's message.

On the other hand, according to the prescriptions of quantum criptography, possible eavesdroppers will be baffled by Alice using nonorthogonal, say vertical, respectively, 60° right of the vertical, polarized states.[3,5] In this case, however, Bob needs an error correcting code to cope with the fact that he has fixed probabilities of measuring both vertical and horizontal linear polarizations when the incoming photon is not vertically polarized. More photons are to be sent by Alice in order to correct Bob's imperfect distinction between two nonorthogonal photon states, whence the problem of estimating how many *quantum its* in Wheeler's therminology[1] are needed to convey a certain amount of *classical bits*.[6]

In general, Alice might be using a quantum statistical ensemble composed by n quantum (mixed) states $\hat{\rho}_j$ with weights p_j which is thus represented by the density matrix

$$\hat{\rho}=\sum_j p_j\hat{\rho}_j\,. \tag{1}$$

Bob's decoding strategy rests on some set of observables $\hat{e}_k$ he chooses in order to maximize the amount of information he extracts from his measurements. Let the $\hat{e}_k$ be orthogonal, one-dimensional projections such that that $\Sigma_k\hat{e}_k=\hat{1}$. Out of the incoming signal states $\hat{\rho}_j$, Bob will get the $\hat{e}_k$'s eigenstate $|e_k\rangle$ with probability $p_k^e(\hat{\rho}_j):=\mathrm{Tr}\,\hat{\rho}_j\hat{e}_k$, respectively, $p_k^e(\hat{\rho}):=\mathrm{Tr}\,\hat{\rho}\hat{e}_k$ if he happens to measure $\hat{e}_k$ on the whole mixture represented by $\hat{\rho}$. The information content of the (discrete) probability distributions,

$$p^e(\hat{\rho}):=\{p_k^e(\hat{\rho})\},\quad p^e(\hat{\rho}_j):=\{p_k^e(\hat{\rho}_j)\}, \tag{2}$$

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is measured by the Shannon's entropies:

$$S(p^e(\hat{\rho}))=-\sum_k p_k^e(\hat{\rho})\log p_k^e(\hat{\rho}), \tag{3}$$

$$S(p^e(\hat{\rho}_j))=-\sum_k p_k^e(\hat{\rho}_j)\log p_k^e(\hat{\rho}_j). \tag{4}$$

Since we assumed the $\hat{e}_k$ to be orthogonal, one-dimensional projections, $p^e(\hat{\rho})$, respectively $p^e(\hat{\rho}_j)$, are the spectra of the states resulting from $\hat{\rho}$, respectively $\hat{\rho}_j$, after repeated, nonselective measurements of the observables $\hat{e}_k$:

$$\hat{\rho}^e:=\sum_k p_k^e(\hat{\rho})\hat{e}_k, \quad \text{respectively} \quad \hat{\rho}_j^e:=\sum_k p_k^e(\hat{\rho}_j)\hat{e}_k. \tag{5}$$

Then (3) and (4) coincide with the von Neumann entropies,

$$S(\hat{\rho}^e)=-\mathrm{Tr}\ \hat{\rho}^e\ \log\ \hat{\rho}^e=-\sum_k p_k^e(\hat{\rho})\log p_k^e(\hat{\rho}), \tag{6}$$

$$S(\hat{\rho}_j^e)=-\mathrm{Tr}\ \hat{\rho}_j^e\ \log\ \hat{\rho}_j^e=-\sum_k p_k^e(\hat{\rho}_j)\log p_k^e(\hat{\rho}_j). \tag{7}$$

Notice that from (1) and (2) it follows that $\Sigma_j p_j p_k^e(\hat{\rho}_j)=p_k^e(\hat{\rho})$, whence $p^e(\hat{\rho}_j)$ can be interpreted as the probability of the event $\hat{e}_k$ conditioned upon the occurrence of the event $\hat{\rho}_j$ and

$$\sum_j p_j S(p^e(\hat{\rho}_j)), \tag{8}$$

as the corresponding conditional entropy. Then, Shannon's mutual information is defined as the difference,[2]

$$I_{\hat{\rho}}^e:=S(p^e(\hat{\rho}))-\sum_j p_j S(p^e(\hat{\rho}_j)). \tag{9}$$

In the conventional (classical) setting Alice sends signals to Bob by means of orthogonal photon states $\hat{\rho}_{1,2}$ out of, say, a mixture of them with probabilities p_1 and $p_2=1-p_1$. Then, by measuring the orthogonal projections $\hat{\rho}_{1,2}$, Bob will maximize the amount of information he can extract per measurement. In fact, in this case, the conditional probabilities $p_k^e(\hat{\rho}_j)=0,1$ so that the conditional entropy vanishes and $I_{\hat{\rho}}^e=-p_1\log p_1-p_2\log p_2$ is maximal.

In Sec. IV we will address the corresponding quantum problem, namely the question of the best noncommutative decoding strategy.

Dynamical entropies

The Kolmogorov–Sinai dynamical entropy[1] is, in essence, classical information applied to ergodic theory and provides us with powerful methods to characterize the degree of randomness of classical dynamical systems.

Abstractly, the dynamics is represented by the iterations of a map T on a measure space $\mathscr{X}$, equipped with an invariant measure μ (*a priori* state). Information about the system is gained by assigning the phase point representing the system to one of the disjoint atoms P_j, $1\leqslant j\leqslant n$ of a chosen coarse-grained description (partition) $\mathscr{P}$ of $\mathscr{X}$. The atoms have volumes $\mu(P_j)$ that are probabilities, and the entropy

$$H_\mu(\mathscr{P}) = -\sum_j \mu(P_j)\log\,\mu(P_j) \tag{10}$$

measures the *a priori* information relative to $\mathscr{P}$.

If we get information about the system by means of a different partition $\mathscr{Q} := \{Q_k\}_{k=1}^m$, $\mu_{jk}^Q := \mu(P_j \cap Q_k)/\mu(P_j)$ is the probability of finding the system in the atom Q_k if it is in the atom P_j. The uncertainty removed as a consequence of the assignment of the phase point to any of the atoms Q_k is thus given by

$$H_j^Q := -\sum_j \mu_{jk}^Q \log\,\mu_{jk}^Q, \tag{11}$$

and Shannon's mutual information reads as

$$I_\mu^Q = H_\mu(\mathscr{P}) - \sum_j \mu(P_j) H_j^Q. \tag{12}$$

We can identify the triple $(\mu,\mathscr{P},\mathscr{Q})$ with a classical communication channel by simply thinking of $\mathscr{P}$ as providing a decomposition of the state μ and of $\mathscr{Q}$ as of a decoding procedure. Then, I_Q measures the information capacity of the given classical communication channel and attains its maximum $H_\mu(\mathscr{P})$ when $\mathscr{Q}=\mathscr{P}$. This fits very well with the use of $H_\mu(\mathscr{P})$ as the natural measure of the information content of the partition $\mathscr{P}$ with respect to the state μ. The entropy of a partition is indeed the central notion for the dynamical entropy constructed by Kolmogorov and Sinai.[1]

Any attempt at a quantum generalization of the above considerations encounters a major conceptual problem. In fact, quantum states are generally perturbed by measurement processes. For instance, in (5) $\hat{\rho}_j^e \neq \hat{\rho}_j$, unless $\hat{\rho}_j$ commutes with the $\hat{e}_k$'s. In classical contexts the perturbations of the state due to measurements can always be made negligible, at least in the line of the principle. As a matter of exemplification, in the case of the localization of the phase point within one of the atoms of the partition $\mathscr{P}$, what corresponds to the quantum state $\hat{\rho}$ transforming into the new state $\hat{\rho}^e$ in (5) is the following:

$$\mu \mapsto \mu^P := \sum_j \mu(P_j)\chi_{P_j}, \tag{13}$$

where the χ_{P_j} are the index functions of the various (disjoint) atoms. That $\mu^P = \mu$ can be checked by considering the mean values $\mu(f)$ and $\mu^P(f)$ of any μ-integrable function f.

Intuitively, at the core of the notion of dynamical entropy lies the idea that the more we know about the past of an evolving system, the more confident we are on our predictions about its future. If this is not the case then we have a signature of random behavior. The reliability of our predictions also depends on the degree of accuracy of the observations we performed on the system in order to acquire information about it. In a classical context we can always think of carrying them out without altering the regularity or irregularity of the system, the latter being then intrinsic properties. Quantum mechanically instead, one is very likely to introduce randomness into the system by performing measurements on it. Thus, an observer-independent characterization of quantum chaos based on any meaningful notion of quantum information requires that information be gathered without perturbing the physical state. However, the effects of quantum measurements are inherently quantum mechanical and one is not at all sure that these should not be incorporated in any physical theory of quantum chaos.[7]

In the case of a formulation solely based on the dynamics with respect to which the given state of the system is invariant, what is required is, first, a good notion of ''quantum partition'' and, second, a good measure of the amount of information contained in it with respect to a given

quantum state. In the following, we will be dealing with a proposal of quantum dynamical entropy that tries to fulfill the latter needs, while we refer the reader to Ref. 8 for a formulation that allows for external perturbations of the quantum states.

In the noncommutative setting one usually replaces the measure-theoretic description of classical dynamical systems with an algebraic one. That is, one refers to some algebra $\mathscr{A}$ of bounded operators (C^* or von Neumann algebra) equipped with a dynamical automorphism θ that respects the algebraic relations and preserves a state ω, the latter assigning the expectation values of all the observables of the system.

Finite-dimensional subalgebras $\mathbf{N}\subset\mathscr{A}$ offer themselves as natural substitutes for classical partitions. In Ref. 9 the infinitely many decompositions of any nonpure quantum state are used to construct the *entropy of a subalgebra* $H_\omega(\mathbf{N})$, the quantum generalization of the classical entropy of a partition $H_\mu(\mathscr{P})$ in (10) (also see Ref. 10). We will show that the entropy of an Abelian subalgebra $\mathbf{A}\subset\mathbf{M}_n(\mathbb{C})$ coincides with the accessible information of a specific quantum communication channel. Moreover, a temptative information-geometric interpretation of these optimal decompositions is compared with recent results concerning generic states on $\mathbf{M}_2(\mathbb{C})$ and completely symmetric ones on $\mathbf{M}_3(\mathbb{C})$.[11]

II. ENTROPY OF A SUBALGEBRA

We consider the simplest possible quantum mechanical setting, namely an n-level system the observables, respectively the states, of which are Hermitian $n\times n$ matrices in $\mathbf{M}_n(\mathbb{C})$, respectively density matrices $\hat{\rho}$, with positive eigenvalues ρ_l, $l=1,\ldots,n$ such that $\Sigma_l\rho_l=1$. Any density matrix $\hat{\rho}$ for which $\hat{\rho}^2\neq\hat{\rho}$ is a mixed state and can be arbitrarily decomposed into a convex linear combination of other states $\hat{\rho}_j\in\mathbf{M}_n(\mathbb{C})$ as in (1), with given weights $0\leqslant p_j\leqslant 1$, $\Sigma_j p_j=1$. For our purposes, we will be content with finite linear convex combinations that we will call ''decompositions.''

Two observations are in order at this point: the effect of a quantum measurement on a quantum state is usually described as in (5).[12] The latter amounts to a decomposition if and only if the $\hat{e}_k$ (in general, not orthogonal projections) commute with the state itself. Second, any resolution of the identity, $\Sigma_j\hat{x}_j=\hat{\mathbb{1}}$, by means of positive operators $0\leqslant\hat{x}_j\in\mathbf{M}_n(\mathbb{C})$ gives a decomposition of a state $\hat{\rho}\in\mathbf{M}_n(\mathbb{C})$. As follows:

$$\hat{\rho}=\sum_j \operatorname{Tr}\hat{\rho}\hat{x}_j\,\frac{\sqrt{\hat{\rho}}\hat{x}_j\sqrt{\hat{\rho}}}{\operatorname{Tr}\hat{\rho}\hat{x}_j}. \tag{14}$$

Remark 1: The converse is also true: given a decomposition $\hat{\rho}=\Sigma_j\lambda_j\hat{\rho}_j$, *there exists a set of positive operators* $\hat{x}_j\in\mathbf{M}_n(\mathbb{C})$, $\Sigma_j\hat{x}_j=\hat{\mathbb{1}}$, *such that (14) holds. The clue to it is the so-called GNS construction based on* $\hat{\rho}$ *itself, if it is invertible, otherwise upon restricting to its support projection.*[13]

The information content of quantum states is measured by the von Neumann entropy:

$$S(\hat{\rho})=-\operatorname{Tr}\hat{\rho}\,\log\,\hat{\rho}. \tag{15}$$

Let us now consider a maximally Abelian subalgebra $\mathbf{A}\subset\mathbf{M}_n(\mathbb{C})$ generated by n orthogonal one-dimensional (minimal) projections $\hat{a}_j$ such that $\Sigma_j\hat{a}_j=\hat{\mathbb{1}}$. The restriction $\hat{\rho}\restriction\mathbf{A}$ of any state $\hat{\rho}$ to $\mathbf{A}$ provides us with a discrete probability $P^a_{\hat{\rho}}:=\{p^a_j\}$, $j=1,\ldots,n$ and $p^a_j:=\operatorname{Tr}\hat{\rho}\hat{a}_j$. That is,

$$\hat{\rho}\restriction\mathbf{A}=\sum_j \hat{a}_j\hat{\rho}\hat{a}_j=\sum_j\{\operatorname{Tr}\hat{\rho}\hat{a}_j\}\hat{a}_j \tag{16}$$

and

$$S(\hat{\rho}\restriction\mathbf{A}) = -\sum_j p_j^a \log p_j^a . \tag{17}$$

Now, the map $\hat{\rho}\mapsto\Sigma_j \hat{a}_j\hat{\rho}\hat{a}_j$ is such that $S(\hat{\rho})\leqslant S(\hat{\rho}\restriction\mathbf{A})$ (Ref. 14, Chap. 2), and

$$S(\hat{\rho}) = \min\{S(\hat{\rho}\restriction\mathbf{A}) : \mathbf{A}\subset\mathbf{M}_n(\mathbb{C}) \text{maximally Abelian}\}, \tag{18}$$

the minimum being attained at any maximally Abelian $\mathbf{A}$ containing the spectral projections of $\hat{\rho}$.

The above result makes clear that $S(\hat{\rho}\restriction\mathbf{N})$ is useless as a measure of the information content of a subalgebra $\mathbf{N}\subseteq\mathbf{M}_n(\mathbb{C})$ with respect to the state $\hat{\rho}$. Indeed, we expect that, like finer classical partitions have greater entropy, larger subalgebras contain more information. At the core of the fact that there are subalgebras $\mathbf{N}$ and $\mathbf{M}$ with $\mathbf{N}\subset\mathbf{M}$ and, nevertheless, $S(\hat{\rho}\restriction\mathbf{N})>S(\hat{\rho}\restriction\mathbf{M})$, we find purely quantum reasons (state entanglement): the singlet state of two spin $\frac{1}{2}$ particles is pure and has zero entropy, whereas restricted to the single spin algebra it becomes a mixture of equally distributed spin up and down states with von Neumann entropy log 2.

An entropic-like quantity that is always increasing under embedding is the *relative entropy* of two states $\hat{\rho},\hat{\sigma}$:

$$S(\hat{\rho},\hat{\sigma}) := \mathrm{Tr}\,\hat{\sigma}(\log\,\hat{\sigma} - \log\,\hat{\rho}). \tag{19}$$

Among other properties, $S(\hat{\rho},\hat{\sigma})$ is always positive and vanishes if and only if $\hat{\sigma}=\hat{\rho}$. Moreover, it is monotonic (see Ref. 15):

$$S(\hat{\rho}\restriction\mathbf{N}_1,\hat{\sigma}\restriction\mathbf{N}_1)\leqslant S(\hat{\rho}\restriction\mathbf{N}_2,\hat{\sigma}\restriction\mathbf{N}_2), \quad \text{if } \mathbf{N}_1\subseteq\mathbf{N}_2 . \tag{20}$$

Let a state $\hat{\rho}$, a subalgebra $\mathbf{N}\subseteq\mathbf{M}(\mathbb{C})$ and a decomposition $\hat{\rho}=\Sigma_j p_j\hat{\rho}_j$ be given. Then, we construct the functional

$$H_{\hat{\rho}}(\{p_j\hat{\rho}_j\},\mathbf{N}) := \sum_j p_j S(\hat{\rho}\restriction\mathbf{N},\hat{\rho}_j\restriction\mathbf{N}), \tag{21}$$

$$= S(\hat{\rho}\restriction\mathbf{N}) - \sum_j p_j S(\hat{\rho}_j\restriction\mathbf{N}). \tag{22}$$

The latter equality follows from $\hat{\rho}=\Sigma_j p_j\hat{\rho}_j$ and (19).

Definition 1: The entropy of a subalgebra $\mathbf{N}\subseteq\mathbf{M}_n(\mathbb{C})$ *with respect to a state* $\hat{\rho}$ *is defined*[9] *as*

$$H_{\hat{\rho}}(\mathbf{N}) := \sup\left\{ H_{\hat{\rho}}(\{p_j\hat{\rho}_j\},\mathbf{N}) : \hat{\rho}=\sum_j p_j\hat{\rho}_j \right\}, \tag{23}$$

the supremum being computed over all possible decompositions of $\hat{\rho}$. *The decomposition(s) at which it is attained are called ''optimal decomposition(s).''*

The entropy of a subalgebra has the right monotonicity properties and fulfills the following bounds:

$$\mathbf{M}\subseteq\mathbf{N}\Rightarrow 0\leqslant H_{\hat{\rho}}(\mathbf{M})\leqslant H_{\hat{\rho}}(\mathbf{N})\leqslant S(\hat{\rho}\restriction\mathbf{N}). \tag{24}$$

Some concrete results

We now enumerate a series of known results that mainly stem from Refs. 16 and 11. Four of them are easier to discuss than the others: (0) the state $\hat{\rho}$ is pure, that is, it cannot be decomposed; (1) The subalgebra $\mathbf{N}$ coincides with the whole algebra $\mathbf{M}_n(\mathbb{C})$; (2) $\mathbf{N}$ is a maximally Abelian subalgebra $\mathbf{A}$ commuting with the state $\hat{\rho}$; (3) $\mathbf{N}\subseteq\mathbf{M}_n(\mathbb{C})$ is any subalgebra, but the state $\hat{\rho}$ is the so-called ''tracial state'' (denoted by τ), namely $\tau=\hat{\mathbb{1}}/n$.

Case (0): this case is trivial, namely $H_{\hat{\rho}}(\mathbf{N}) = 0$ for all $\mathbf{N}\subseteq\mathbf{M}_n(\mathbb{C})$.

Case (1): one chooses any decomposition of $\hat{\rho}$ as in (14) with the $\hat{x}_j$ to be one-dimensional projections in $\mathbf{M}_n(\mathbb{C})$. The corresponding $\hat{\rho}_j$ are one-dimensional projections and they obviously equal their restrictions $\hat{\rho}_j\restriction\mathbf{M}_n(\mathbb{C})$. Thus, the entropy $S(\hat{\rho}_j\restriction\mathbf{M}_n(\mathbb{C}))=0$ and the functional in (22) attains its maximum $H_{\hat{\rho}}(\mathbf{M}_n(\mathbb{C})) = S(\hat{\rho})$ at infinitely many optimal decompositions.

Case (2): a generic one-dimensional projection is seen as a mixed state when restricted to $\mathbf{A}$. However, using (14) and the choice $\hat{x}_j=\hat{a}_j$, where the $\hat{a}_j$ are the minimal projections that generate $\mathbf{A}$, one sees that the states

$$\hat{\rho}_j\restriction\mathbf{A}=\frac{\sqrt{\hat{\rho}}\hat{a}_j\sqrt{\hat{\rho}}}{\mathrm{Tr}\,\hat{\rho}\hat{a}_j}\restriction\mathbf{A} \tag{25}$$

are orthogonal, one-dimensional projections, whence $S(\hat{\rho}_j\restriction\mathbf{A})=0$. Therefore, the maximum in (23) equals $H_{\hat{\rho}}(\mathbf{A}) = S(\hat{\rho}\restriction\mathbf{A})$ and is attained at the optimal decomposition $\hat{\rho} = \Sigma_j\sqrt{\hat{\rho}}\hat{a}_j\sqrt{\hat{\rho}}$.

Case 3: one considers any maximally Abelian subalgebra $\mathbf{A}\subseteq\mathbf{N}$, with minimal (in $\mathbf{N}$) projections $\hat{a}_k$ of dimension $\mathrm{Tr}\,\hat{a}_k=d_k\geqslant 1$. Then

$$H_\tau(\mathbf{A})\leqslant H_\tau(\mathbf{N})\leqslant S(\tau\restriction\mathbf{N})\leqslant S(\tau\restriction\mathbf{A}), \tag{26}$$

because of (24) and (18). Let τ be decomposed as $\tau=\Sigma_{j=1}^n\hat{p}_j/n$, where the $\hat{p}_j$, $\Sigma_{j=1}^n\hat{p}_j=\hat{\mathbb{1}}$, are minimal [in $M_n(\mathbb{C})$] projections such that either $\hat{p}_j\hat{a}_k=0$ or $\hat{p}_j\hat{a}_k=\hat{p}_j$. It follows that

$$H_\tau(\mathbf{N})=S(\tau\restriction\mathbf{A})=-\sum_k\ \frac{d_k}{n}\log\frac{d_k}{n}. \tag{27}$$

Obviously, the optimal decompositions correspond to the possible refinements of the orthogonal projections $\hat{a}_k$ into one-dimensional orthogonal ones $\hat{p}_j$.

In more general situations than those discussed above, there are general results concerning $\mathbf{M}_2(\mathbb{C})$.[11,16] Hopes for easy generalizations to higher dimensions are somehow frustrated by a result concerning the entropy of a maximally Abelian subalgebra of $\mathbf{M}_3(\mathbb{C})$ with respect to a particularly symmetric state.[11]

By means of the Pauli matrix $(\hat{\sigma}_x,\hat{\sigma}_y,\hat{\sigma}_z)$ a generic state in $\mathbf{M}_2(\mathbb{C})$ can be written by means of a vector $\mathbf{b}\in\mathbb{R}^3$. As follows:

$$\hat{\rho}=\frac{\hat{1}}{2}+\frac{b_x}{1+b^2}\,\hat{\sigma}_x+\frac{b_y}{1+b^2}\,\hat{\sigma}_y+\frac{b_z}{1+b^2}\,\hat{\sigma}_z,\quad b=|\mathbf{b}|. \tag{28}$$

When $b=1$, $\hat{\rho}$ is a pure state (one-dimensional projection), whereas, if $b=0$, $\hat{\rho}$ is the two-dimensional tracial state τ.

Any proper subalgebra $\mathbf{N}$ of $\mathbf{M}_2(\mathbb{C})$ is a maximally Abelian subalgebra $\mathbf{A}$ that is not restrictive to identify with the one generated by the minimal projections $\hat{a}_\pm:=\hat{\mathbb{1}}/2\pm\hat{\sigma}_z/2$. Setting $\mathbf{n}:=2\mathbf{b}/(1+b^2)$ and $\mathbf{k}:=(0,0,1)$, we shall write

$$\hat{\rho}=\frac{\hat{1}+\mathbf{n}\cdot\hat{\sigma}}{2},\quad \hat{a}_\pm=\frac{\hat{1}\pm\mathbf{k}\cdot\hat{\sigma}}{2}. \tag{29}$$

Let $\mathbf{n}_\perp:=(n_x,n_y,0)$, $\mathbf{n}_\pm^*:=\mathbf{n}_\perp\pm\sqrt{1-\mathbf{n}_\perp^2}\mathbf{k}$ and

$$\hat{\rho}_\pm^*:=\frac{\hat{1}+\mathbf{n}_\pm^*\cdot\hat{\sigma}}{2},\quad p_\pm^*:=\frac{1}{2}\pm\frac{b_z}{\sqrt{(1-b^2)^2+4b_z^2}}. \tag{30}$$

As $\mathbf{n}^*_\pm \cdot \mathbf{n}^*_\pm = 1$, the states $\hat{\rho}^*_\pm$ are one-dimensional projections, but, in general, not orthogonal. The weights $p^*_\pm$ are such that $\hat{\rho} = p^*_+\hat{\rho}^*_+ + p^*_-\hat{\rho}^*_-$. It follows[16,11] that the entropy $H_{\hat{\rho}}(\mathbf{A})$ of $\mathbf{A}$ with respect to $\hat{\rho}$ is attained exactly at this decomposition, that is

$$H_{\hat{\rho}}(\mathbf{A}) = S(\hat{\rho}\restriction\mathbf{A}) - p^*_+ S(\hat{\rho}^*_+\restriction\mathbf{A}) - p^*_- S(\hat{\rho}^*_-\restriction\mathbf{A}). \tag{31}$$

It is easy to check that, when $b=0$ or $\mathbf{b}=(0,0,b)$, the results of the previous cases (2) and (3) are reproduced. Moreover, according to Remark 1, there exist ''observables'' $\hat{e}^*_\pm \in \mathbf{M}_2(\mathbb{C})$, $\hat{e}^*_+ + \hat{e}^*_- = \hat{1}$, namely,

$$\hat{e}^*_\pm = \frac{\hat{\mathbb{1}} \pm \mathbf{e}^* \cdot \hat{\sigma}}{2}, \quad \mathbf{e}^* := \frac{(2b_x b_z, 2b_y b_z, 1-b^2+2b_z^2)}{\sqrt{(1-b^2)^2+4b_z^2}}, \tag{32}$$

that allow us to write

$$\hat{\rho}^*_\pm = \frac{\sqrt{\hat{\rho}}\hat{e}^*_\pm\sqrt{\hat{\rho}}}{\mathrm{Tr}\,\hat{\rho}\hat{e}^*_\pm}. \tag{33}$$

We shall call them ''optimal observables.''

Remark 2: There are some peculiar geometrical symmetries in $\mathbf{M}_2(\mathbb{C})$. *For sake of simplicity and of comparison with Ref. 16, let the vector* $\mathbf{b}$ *identifying the state equal* $(z,0,0)$ *so that*

$$\hat{\rho} = \begin{pmatrix} \frac{1}{2} & z \\ z & \frac{1}{2} \end{pmatrix}.$$

Then, the z*-dependent optimal observables* $\hat{e}^*_\pm(z)$ *remain the same,*

$$\hat{e}^*_\pm(z) = \frac{\hat{\mathbb{1}} \pm \mathbf{k}\cdot\hat{\sigma}}{2} = \hat{a}_\pm, \quad \textit{for all } -1/2 < z < 1/2. \tag{34}$$

Vice versa, let us fix $\mathbf{b}=(b,0,0)$ *(hence the optimal decomposers* $\hat{\rho}^*_\pm$*) and construct the state*

$$\hat{\rho}(t) = t\hat{\rho}^*_+ + (1-t)\hat{\rho}^*_- = \frac{\hat{\mathbb{1}}}{2} + \frac{b}{1+b^2}\,\hat{\sigma}_x + \left(t-\frac{1}{2}\right)\frac{1-b^2}{1+b^2}\,\hat{\sigma}_z, \tag{35}$$

where $0<t<1$. *Then, the optimal observables* $\hat{e}^*_\pm(t)$ *vary, while the optimal decomposers* $\hat{\rho}^*_\pm(t)$ *remain the same, namely* $\hat{\rho}^*_\pm$, *for all* $0<t<1$.

The latter observation is a particular instance of the following general result that we quote from Ref. 11.

Proposition 1: Let $\hat{\rho} = \Sigma_{j\in J} p_j \hat{\rho}_j$ *be an optimal decomposition for a subalgebra* $\mathbf{N}\subseteq\mathbf{M}_n(\mathbb{C})$ *with respect to the state* $\hat{\rho}$. *Let* $\hat{\sigma} = \Sigma_{k\in J}\lambda_k\hat{\rho}_k$ *be any other state obtained as a convex linear combination of (some of) the optimal decomposers* $\hat{\rho}_j$. *Then, this is already an optimal decomposition for* $\mathbf{N}$ *with respect to* $\hat{\sigma}$, *namely*

$$H_{\hat{\sigma}}(\mathbf{N}) = S(\hat{\sigma}\restriction\mathbf{N}) - \sum_k \lambda_k S(\hat{\rho}_k\restriction\mathbf{N}). \tag{36}$$

As to the second geometrical symmetry present in the two-dimensional case, one wonders whether that too holds in greater generality. A clue to this problem comes from considering the maximally Abelian subalgebra $\mathbf{A}\subset\mathbf{M}_3(\mathbb{C})$ generated by

$$\hat{a}_1=\begin{pmatrix}1&0&0\\0&0&0\\0&0&0\end{pmatrix},\quad \hat{a}_2=\begin{pmatrix}0&0&0\\0&1&0\\0&0&0\end{pmatrix},\quad \hat{a}_3=\begin{pmatrix}0&0&0\\0&0&0\\0&0&1\end{pmatrix}. \tag{37}$$

The calculation of its entropy with respect to the symmetric state,

$$\hat{\rho}(z):=\begin{pmatrix}\frac{1}{3}&z&z\\z&\frac{1}{3}&z\\z&z&\frac{1}{3}\end{pmatrix},\quad -\tfrac{1}{6}\leqslant z\leqslant\tfrac{1}{3}, \tag{38}$$

leads to a surprising and intriguing departure from the two-dimensional case.

Let $a:=\sqrt{1+6z}$ and $b:=2\sqrt{1-3z}$. It turns out[11] that $\hat{\rho}(z)$ can be decomposed as

$$\hat{\rho}(z)=\tfrac{1}{3}\,[|\phi^{(1)}_{u,z}\rangle\langle\phi^{(1)}_{u,z}|+|\phi^{(2)}_{u,z}\rangle\langle\phi^{(2)}_{u,z}|+|\phi^{(3)}_{u,z}\rangle\langle\phi^{(3)}_{u,z}|], \tag{39}$$

by means of a one-parameter family of vectors and their cyclic permutations:

$$|\phi^{(1)}_{u,z}\rangle:=\begin{pmatrix}\phi_1(u,z)\\\phi_2(u,z)\\\phi_3(u,z)\end{pmatrix},\quad |\phi^{(2)}_{u,z}\rangle:=\begin{pmatrix}\phi_3(u,z)\\\phi_1(u,z)\\\phi_2(u,z)\end{pmatrix},\quad |\phi^{(3)}_{u,z}\rangle:=\begin{pmatrix}\phi_2(u,z)\\\phi_3(u,z)\\\phi_1(u,z)\end{pmatrix}, \tag{40}$$

$$\phi_1(u,z):=\frac{1}{3}\left[a+b\,\cos\left(u-\frac{\pi}{3}\right)\right], \tag{41}$$

$$\phi_2(u,z):=\frac{1}{3}\left[a+b\,\cos\left(u+\frac{\pi}{3}\right)\right], \tag{42}$$

$$\phi_3(u,z):=\frac{1}{3}\,[a-b\,\cos u]. \tag{43}$$

Proposition 2: There exists a value $z^*<0$ of the real parameter z,

$$z^*=\frac{1}{3}\,\frac{(t^*)^2-4t^*+3}{2(t^*)^2-4t^*+3},\quad \textit{where}\ \ \mathbf{e}^{-t^*}=t^*-1, \tag{44}$$

such that, for $z\geqslant z^*$, the angular parameter $u=\pi/3$ renders the decomposition (39) optimal for the maximally Abelian subalgebra $\mathbf{A}\subset\mathbf{M}_3(\mathbb{C})$ with respect to the state $\hat{\rho}(z)$. When $z<z^*$, there are two possible optimal decompositions corresponding to $u_{\pm}(z)=\pi/3\pm\alpha(z)$.

The proof of this result is partly analytic partly numerical.[11] We examine its consequences.

Proposition 3: The optimal observables $\hat{x}_j(z)$ that, according to Remark 1, correspond to the optimal decompositions of the previous proposition are the minimal projections $\hat{a}_j$ of $\mathbf{A}$ when $z^*\leqslant z<1/3$. Whereas, for $-1/6<z<z^*$, they are one-dimensional, but not orthogonal projections.

Proof: The observables $\hat{e}_j(u,z)$ associated with a given decomposition of the form (39) are given by

$$\tfrac{1}{3}\,|\phi^{(j)}_{u,z}\rangle\langle\phi^{(j)}_{u,z}|=\sqrt{\hat{\rho}(z)}\hat{e}_j(u,z)\sqrt{\hat{\rho}(z)}, \tag{45}$$

whence, via inverting $\hat{\rho}(z)$:

$$\hat{e}_1(u,z)=\frac{1}{9}\begin{pmatrix} C_+^2 & C_+C_- & C_+C \\ C_-C_+ & C_-^2 & C_-C \\ CC_+ & CC_- & C^2 \end{pmatrix}, \quad \begin{cases} C_\pm = 1+\cos u \pm \sqrt{3}\,\sin u, \\ C = 1-2\cos u. \end{cases} \tag{46}$$

$\hat{e}_1(u,z)$ projects onto $|1\rangle := 1/3(C_+, C_-, C)$ and $\hat{e}_2(u,z)$, respectively $\hat{e}_3(u,z)$, project onto $|2\rangle = 1/3(C, C_+, C_-)$, respectively $|3\rangle := 1/3(C_-, C, C_+)$.

According to Proposition 2, for $z^* \leqslant z < 1/3$, $u = \pi/3$ fixes an optimal decomposition and one sees that $|1\rangle = (1,0,0)$, hence $\hat{e}_j^*(\pi/3, z) = \hat{a}_j$.

On the other hand, the scalar products $\langle i|j\rangle$, $i \neq j$, $i,j = 1,2,3$, equal $2\cos^2 u + \cos u - 1$ and vanish for $u = \pi/3$, π only. Therefore, the angular values $u_\pm(z) = \pi/3 \pm \alpha(z)$ fixing two optimal decompositions when $-1/6 < z < z^*$, determine two sets of optimal observables $\hat{e}_j^*(u_\pm(z), z)$ that are one-dimensional, but not orthogonal projections. □

Remark 3: For $z^* \leqslant z < 1/3$ the three- and two-dimensional cases agree (compare Remark 2). However, when $-1/6 < z < z^*$ the situation drastically changes and two different optimal decompositions appear. Moreover, every linear convex combination of optimal decompositions of $\hat{\rho}(z)$ with respect to **A** *is again optimal, and thus, below the critical value z^*, we have infinitely many of them.*[11]

III. ACCESSIBLE INFORMATION

In this section we establish a connection between the concept of entropy of a subalgebra with respect to a given quantum state introduced in the previous section and the notion of information capacity briefly touched upon in the Introduction (see Ref. 17 for the classical case, Ref. 18 and Ref. 15 for the quantum one).

Definition 2: We call ''quantum communication channel'' the couple $\{\mathscr{R}, \mathscr{E}\}$, where $\mathscr{R} := \{p_j, \hat{\rho}_j\}$ is a statistical ensemble of quantum states $\hat{\rho}_j$ with weights p_j, $\Sigma_j p_j = 1$, and $\mathscr{E} := \{\hat{e}_k\}$ is a set of operators $0 \leqslant \hat{e}_k$ such that $\Sigma_k \hat{e}_k = \hat{\mathbb{1}}$.

The quantum state $\hat{\rho} = \Sigma_j p_j \hat{\rho}_j$ is Alice's signal source, or ''input alphabet,'' whereas the observables $\mathscr{E} = \{\hat{e}_k\}$ make up Bob's detection scheme or ''output alphabet.''[17] Notice that, unlike in the Introduction, the $\hat{e}_k$ need not be orthogonal projections. More generally, they define a so-called ''Positive Operator Valued (POV) Measure,'' which generalizes (5) to the following completely positive map[12] on quantum states:

$$\hat{\rho} \mapsto \mathscr{E}(\hat{\rho}) = \sum_k \sqrt{\hat{e}_k}\hat{\rho}\sqrt{\hat{e}_k}. \tag{47}$$

The next almost obvious Lemma establishes a natural connection between certain input alphabets $\mathscr{E}$ and the restrictions $\hat{\rho}\restriction\mathbf{A}$ of quantum states to Abelian subalgebras.

Lemma 1: Given a density matrix $\hat{\rho} \in \mathbf{M}_n(\mathbb{C})$, every (not necessarily maximally) Abelian subalgebra $\mathbf{A} \subset \mathbf{M}_n(\mathbb{C})$ identifies an input alphabet $\mathscr{A}_{\hat{\rho}}$.

Proof: We simply use the projections $\hat{a}_j$, $1 \leqslant j \leqslant n$ [not necessarily minimal in $\mathbf{M}_n(\mathbb{C})$] to decompose the state $\hat{\rho}$ as in (14), whence

$$\mathscr{A}_{\hat{\rho}} := \{p_j^a, \hat{\rho}_j^a\}, \quad p_j^a := \mathrm{Tr}\,\hat{\rho}\hat{a}_j, \quad \hat{\rho}_j^a := \frac{\sqrt{\hat{\rho}}\hat{a}_j\sqrt{\hat{\rho}}}{\mathrm{Tr}\,\hat{\rho}\hat{a}_j}. \tag{48}$$

Given an input, respectively output, alphabet $\mathscr{R} = \{p_j, \hat{\rho}_j\}$, respectively $\mathscr{E} = \{\hat{e}_k\}$, the argument developed in the Introduction for Shannon's mutual entropy (9) leads to associating with the probability measures $p_e(\hat{\rho}) := \{\mathrm{Tr}\,\hat{\rho}\hat{e}_k\}$ and $p^e(\hat{\rho}_j) := \{\mathrm{Tr}\,\hat{\rho}_j\hat{e}_k\}$, the information contents,

$$S(p^e(\hat{\rho})) := -\sum_k \text{Tr}\ \hat{\rho}\hat{e}_k \log \text{Tr}\ \hat{\rho}\hat{e}_k, \tag{49}$$

$$S(p^e(\hat{\rho}_j)) := -\sum_k \text{Tr}\ \hat{\rho}_j\hat{e}_k \log \text{Tr}\ \hat{\rho}_j\hat{e}_k, \tag{50}$$

whence the following[18,19] occurs.

Definition 3: Let a quantum communication channel $\{\mathscr{R},\mathscr{E}\}$ *be given, where* $\mathscr{R}=\{p_j,\hat{\rho}_j\}$ *and* $\mathscr{E}=\{\hat{e}_k\}$*, then the mutual information of the channel is*

$$I(\mathscr{R},\mathscr{E}) := S(p^e(\hat{\rho})) - \sum_j p_j S(p^e(\hat{\rho}_j)). \tag{51}$$

For a given input alphabet $\mathscr{R}$*,*

$$I(\mathscr{R}) := \sup_{\mathscr{E}} I(\mathscr{R},\mathscr{E}), \tag{52}$$

represents the maximal information achievable by varying the detection strategy, namely the output alphabet $\mathscr{E}$*.* $I(\mathscr{R})$ *is called ''accessible information.''*

As we have seen in the previous section any mixed state $\hat{\rho}$ can be decomposed as $\hat{\rho}=\Sigma_j p_j\hat{\rho}_j$ by using whatever decomposition of the identity by means of positive operators we might envisage. From a statistical point of view all these possibilities are equivalent: they all are described by the same density matrix. However, the average relative entropy,

$$\sum_j p_j S(\hat{\rho},\hat{\rho}_j) = S(\hat{\rho}) - \sum_j p_j S(\hat{\rho}_j), \tag{53}$$

we have already encountered [see (21)] is a tool to partially distinguish among them. An important relation between the accessible information of a given statistical mixture $\hat{\rho}=\Sigma_j p_j\hat{\rho}_j$, and the average relative entropy is contained in the so-called Holevo bound.[20] If $\mathscr{R}=\{p_j,\hat{\rho}_j\}$ is Alice's input alphabet, Bob's accessible information must fulfill

$$I(\mathscr{E}) \leqslant S(\hat{\rho}) - \sum_j p_j S(\hat{\rho}_j). \tag{54}$$

Notice that if the $\hat{\rho}_j$ are pure states, then the bound reduces to $S(\hat{\rho})$.

The above considerations point to a close connection between the notion of entropy of a subalgebra and the accessible information of an input alphabet. Indeed, the entropy of an Abelian subalgebra $\mathbf{A}\subset\mathbf{M}_n(\mathbb{C})$ with respect to a state $\hat{\rho}\in\mathbf{M}_n(\mathbb{C})$ equals the accessible information of the input alphabet $\mathscr{A}_{\hat{\rho}}$ determined by $\mathbf{A}$ and $\hat{\rho}$.

Proposition 4: Let $\mathbf{A}\subset\mathbf{M}_n(\mathbb{C})$ *be an Abelian subalgebra generated by orthogonal projections* $\hat{a}_j$, $1\leqslant j\leqslant n$*, and* $\hat{\rho}\in\mathbf{M}_n(\mathbb{C})$ *a given state. Then*

$$H_{\hat{\rho}}(\mathbf{A}) = I(\mathscr{A}_{\hat{\rho}}), \tag{55}$$

where the left-hand side is the entropy of $\mathbf{A}$ *with respect to* $\hat{\rho}$ *as defined in Definition 1, while the right-hand side is the accessible information of the input alphabet associated with* $\mathbf{A}$ *and* $\hat{\rho}$ *as in Lemma 1.*

Proof: Let $\mathscr{A}_{\hat{\rho}} = \{p_j^a, \hat{\rho}_j^a\}$ be the input alphabet as in (48), that is $p_j^a = \mathrm{Tr}\,\hat{\rho}\hat{a}_j$ and $\hat{\rho}_j^a = \sqrt{\hat{\rho}}\hat{a}_j\sqrt{\hat{\rho}}/\mathrm{Tr}\,\hat{\rho}\hat{a}_j$. Let $\mathscr{E} = \{\hat{e}_k\}$ be a given output alphabet and use it to decompose $\hat{\rho}$ as in (14), namely $\hat{\rho} = \Sigma_k p_k^e \hat{\rho}_k^e$, $p_k^e = \mathrm{Tr}\,\hat{\rho}\hat{e}_k$, $\hat{\rho}_k^e = \sqrt{\hat{\rho}}\hat{e}_k\sqrt{\hat{\rho}}/\mathrm{Tr}\,\hat{\rho}\hat{e}_k$. Then, from (22) and (17) (the latter holds independently of the $\hat{a}_j$ being minimal projections),

$$H_{\hat{\rho}}(\{p_k^e\hat{\rho}_k^e\}, \mathbf{A}) = S(\hat{\rho}\restriction\mathbf{A}) - \sum_k p_k^e S(\hat{\rho}_k^e\restriction\mathbf{A}) = -\sum_j p_j^a \log p_j^a + \sum_{j,k} p_k^e\, \mathrm{Tr}\,\hat{\rho}_k^e\hat{a}_j \log \mathrm{Tr}\,\hat{\rho}_k^e\hat{a}_j\,. \tag{56}$$

Using the cyclycity of the trace, we write

$$\mathrm{Tr}\,\hat{\rho}_k^e\hat{a}_j = \frac{p_j^a}{p_k^e}\,\mathrm{Tr}\,\hat{\rho}_j^a\hat{e}_k\,, \tag{57}$$

whence (56) reads as

$$H_{\hat{\rho}}(\{p_k^e\hat{\rho}_k^e\}, \mathbf{A}) = \sum_{j,k} p_j^a\, \mathrm{Tr}\,\hat{\rho}_j^a\hat{e}_k \log \mathrm{Tr}\,\hat{\rho}_j^a\hat{e}_k - \sum_j p_j^a \log p_j^a + \sum_{j,k} \{\mathrm{Tr}\sqrt{\hat{\rho}}\hat{a}_j\sqrt{\hat{\rho}}\hat{e}_k\}\log\frac{p_j^a}{p_k^e} \tag{58}$$

$$= -\sum_k p_k^e \log p_k^e + \sum_{j,k} p_j^a\, \mathrm{Tr}\,\hat{\rho}_j^a\hat{e}_k \log \mathrm{Tr}\,\hat{\rho}_j^a\hat{e}_k = I(\mathscr{A}_{\hat{\rho}}, \mathscr{E}). \tag{59}$$

□

Let us now go back to the two-dimensional case where $\mathbf{A}$ is the Abelian subalgebra generated by projections $\hat{a}_\pm$ of (29) and the state is parametrized as in the same (29). The input alphabet $\mathscr{A}_{\hat{\rho}}$ is formed by the statistical mixture of the pure states,

$$\hat{\rho}_\pm^a := \frac{\sqrt{\hat{\rho}}\hat{a}_\pm\sqrt{\hat{\rho}}}{\mathrm{Tr}\,\hat{\rho}\hat{a}_\pm} = \frac{\hat{\mathbb{1}}}{2} + \frac{\mathbf{n}_\pm}{2}\cdot\hat{\sigma}, \quad \mathbf{n}_\pm := \frac{2\mathbf{b}(1\pm b_z) \pm (1-b^2)\mathbf{k}}{1\pm 2b_z + b^2}, \tag{60}$$

with weights

$$p_\pm^a := \mathrm{Tr}\,\hat{\rho}\hat{a}_\pm = \frac{1+b^2\pm 2b_z}{2(1+b^2)}. \tag{61}$$

In Ref. 19 one finds that this is one of the few cases when the accessible information $I(\mathscr{A}_{\hat{\rho}})$ can be explicitly worked out together with the optimal output alphabet $\mathscr{E}$ at which it is attained. The latter, according to the previous proposition, must consist of the two orthogonal projections $\hat{e}_\pm^*$ in (32). Due to interesting connections with the problem of optimal parameter estimation, the proof of this fact will be postponed to the next section.

Remark 4: From the upper bound in (24) and the previous result we deduce that $I(\mathscr{A}_{\hat{\rho}}) = H_{\hat{\rho}}(\mathbf{A}) \leqslant S(\hat{\rho}\restriction\mathbf{A})$. *On the other, when* $\mathbf{A}$ *is maximally Abelian the states* $\hat{\rho}_j^a$ *in the input alphabet* $\mathscr{A}_{\hat{\rho}}$ *are one-dimensional projections so that the Holevo bound (54) gives* $I(\mathscr{A}_{\hat{\rho}}) \leqslant S(\hat{\rho})$. *This is a better bound than the previous one, as follows from (18).*

IV. OPTIMAL ESTIMATION

In this section we address the question of whether there is any operational interpretation behind the optimal observables giving the accessible information $I(\mathscr{A}_{\hat{\rho}})$, or equivalently, the entropy $H_{\hat{\rho}}(\mathbf{A})$ of the Abelian algebra $\mathbf{A}\subset\mathbf{M}_n(\mathbb{C})$ with respect to the state $\hat{\rho}$. Again, it will turn out that the nice picture that emerges in the two-dimensional case is somewhat misleading. Indeed, the

optimal observables $\hat{e}^*_{\pm}$ in (32) maximize the so-called Fisher information. The latter appears in a lower (Cramer–Rao) bound to the variance of any function X that estimates the parameter t when one deals with a one-parameter family (state path) of classical probability distributions $P(t)$ or quantum states $\hat{\rho}(t)$.[21] Quite interesting are the connections, both in the classical and quantum case, between the best estimation problem and the so-called distinguishability metrics on the state space.[22–24] We will adapt the discussion to the context previously developed in this paper by following Ref. 23.

Let $\hat{\rho}(t)$ be a one-parameter family of quantum states in $\mathbf{M}_n(\mathbb{C})$ such that the ''derivative'' $\hat{\rho}'(t) := d\hat{\rho}(t)/dt$ is well defined. Let $\mathscr{E}=\{\hat{e}_k\}_{k\in K}$ be a set of observables (an output alphabet or POV measure as in Definition 2), that when measured give a (finite) set of results $k\in K$ with probabilities $p^e_k(t) := \mathrm{Tr}\,\hat{e}_k\hat{\rho}(t)$. Out of iterated measurements of $\mathscr{E}$ one tries to estimate the parameter t by means of an estimator function $X^e_N(k_1,\ldots,k_N)$. After N measurements one ends up with a joint probability measure $P^e_N(k_1\cdots k_n;t) := \Pi_{j=1}^N p^e_{k_j}(t)$ and with a mean value $\langle X^e_N\rangle(t) := \Sigma_{k_1\cdots k_n} P^e_N(k_1\cdots k_n;t)X^e_N(k_1\cdots k_n)$ for the estimated parameter t. Let $\Delta^e_N X := X^e_N(k_1\cdots k_n) - \langle X^e_N\rangle(t)$. From the obvious equality $\Sigma_{k_1\cdots k_n} P^e_N(k_1\cdots k_n;t)\Delta^e_N X = 0$ one first derives

$$\frac{d\langle X^e_N\rangle(t)}{dt} = \sum_{k_1\cdots k_n} P^e_N(k_1\cdots k_n;t)\sum_{j=1}^N \frac{d\,\log p^e_{k_j}(t)}{dt}\,\Delta^e_N X. \tag{62}$$

Then, the Cauchy–Schwartz inequality gives the Cramér–Rao lower bound,

$$\langle(\Delta^e_N X)^2\rangle_N(t) \geqslant \frac{1}{NF(t)}\left(\frac{d\langle X^e_N\rangle(t)}{dt}\right)^2, \tag{63}$$

to the variance of the estimator function, where

$$F^e(t) := \sum_{k\in k} p^e_k(t)\left(\frac{d\,\log p^e_k(t)}{dt}\right)^2 \tag{64}$$

is the Fisher information relative to the distribution $p^e(t) := \{p^e_k(t)\}$.

Roughly speaking, in order to diminish the error in the estimate of t one tries to maximize

$$F^e(t) = \sum_{k\in K} (p^e_k)^{-1}(t)\left(\frac{dp^e_k(t)}{dt}\right)^2. \tag{65}$$

Of great help is the so-called logarithmic derivative of $\hat{\rho}'(t)$ at $\hat{\rho}(t)$. The latter, denoted by $\mathscr{L}_{\hat{\rho}(t)}[\hat{\rho}'(t)]$, is defined by Refs. 23 and 24 (also see Ref. 22):

$$\tfrac{1}{2}\{\hat{\rho}(t)\mathscr{L}_{\hat{\rho}(t)}[\hat{\rho}'(t)] + \mathscr{L}_{\hat{\rho}(t)}[\hat{\rho}'(t)]\hat{\rho}(t)\} = \hat{\rho}'(t), \tag{66}$$

and allows us to rewrite (65) as follows (Re means real part):

$$F^e(t) = \sum_{k\in K}\{\mathrm{Tr}\,\hat{\rho}\hat{e}_k\}^{-1}[\mathrm{Re}\,\mathrm{Tr}\,\hat{\rho}(t)\mathscr{L}_{\hat{\rho}}[\hat{\rho}(t)]\hat{e}_k]^2. \tag{67}$$

Then, from the cyclicity of the trace and the properties of the Hilbert–Schmidt norm, namely that $|\mathrm{Tr}\,\hat{a}^*\hat{b}|^2 \leqslant \mathrm{Tr}\,\hat{a}^*\hat{a}\,\mathrm{Tr}\,\hat{b}^*\hat{b}$, we get the upper bound,

$$[\mathrm{Re\ Tr}\ \hat{\rho}(t)\mathscr{L}_{\hat{\rho}(t)}[\hat{\rho}(t)]\hat{e}_k]^2=[\mathrm{Re\ Tr}\sqrt{\hat{\rho}(t)}\mathscr{L}_{\hat{\rho}(t)}[\hat{\rho}'(t)]\sqrt{\hat{e}_k}\sqrt{\hat{e}_k}\sqrt{\hat{\rho}(t)}]^2$$
$$\leqslant \mathrm{Tr}\ \hat{\rho}(t)\mathscr{L}_{\hat{\rho}(t)}[\hat{\rho}'(t)]\hat{e}_k\mathscr{L}_{\hat{\rho}(t)}[\hat{\rho}'(t)]\mathrm{Tr}\ \hat{\rho}\hat{e}_k. \tag{68}$$

Finally, since $\Sigma_{k\in K}\hat{e}_k=\hat{\mathbb{1}}$,

$$F^e(t)\leqslant \mathrm{Tr}\ \hat{\rho}'(t)\mathscr{L}_{\hat{\rho}(t)}[\hat{\rho}'(t)]. \tag{69}$$

The upper bound is attained at the input alphabet $\mathscr{E}=\{\hat{e}_k\}$, such that

$$\mathscr{L}_{\hat{\rho}(t)}[\hat{\rho}'(t)]\sqrt{\hat{e}_k}=\lambda_k\sqrt{\hat{e}_k},\quad \lambda_k=\frac{\mathrm{Tr}\ \hat{\rho}(t)\hat{e}_k\mathscr{L}_{\hat{\rho}(t)}[\hat{\rho}'(t)]}{\mathrm{Tr}\ \hat{\rho}(t)\hat{e}_k}\in\mathbb{R}, \tag{70}$$

a condition that can always be met by choosing the $\hat{e}_k$ as the eigenprojections of the (self-adjoint) operator $\mathscr{L}_{\hat{\rho}(t)}[\hat{\rho}'(t)]$.

Concretely, we will consider the two-dimensional case by taking as state path $\hat{\rho}(t)$, $0\leqslant t\leqslant 1$, the one-parameter family of density matrices,

$$\hat{\rho}(t):=t\hat{\rho}_+^a+(1-t)\hat{\rho}_-^a=\frac{\hat{\mathbb{1}}}{2}+\frac{\mathbf{n}(t)}{2}\cdot\hat{\sigma}, \tag{71}$$

where, from (60), $\mathbf{n}(t):=t\mathbf{n}_+ +(1-t)\mathbf{n}_-$. Namely, we will deal with the convex hull of the states corresponding to the input alphabet $\mathscr{A}_{\hat{\rho}}$ defined by the Abelian algebra $\mathbf{A}$ of the projections $\hat{a}_\pm$ in (30) and by the state $\hat{\rho}$ in (29).

In order to arrive at an explicit expression of the logarithmic derivative $\mathscr{L}_{\hat{\rho}(t)}[\hat{\rho}'(t)]$, we notice that

$$\hat{\rho}'(t)=\hat{\rho}_+^a-\hat{\rho}_-^a=\mathbf{n}_{+-}\cdot\hat{\sigma},\quad \mathbf{n}_{+-}:=(1-b^2)\,\frac{(1+b^2)\mathbf{k}-2b_z\mathbf{b}}{(1+b^2)^2-4b_z^2}, \tag{72}$$

is a self-adjoint operator and that its logarithmic derivative at $\hat{\rho}(t)$ is self-adjoint, too. We shall then insert

$$\mathscr{L}_{\hat{\rho}(t)}[\hat{\rho}'(t)]=\lambda_+\hat{x}_+ +\lambda_-\hat{x}_-, \tag{73}$$

in (66) and solve for the orthogonal eigenprojections $\hat{x}_\pm$ and the eigenvalues $\lambda_\pm$. After writing $\hat{x}_\pm=\hat{\mathbb{1}}/2\pm\mathbf{x}/2\cdot\hat{\sigma}$, with $\mathbf{x}\cdot\mathbf{x}=1$ (the projection condition), we obtain

$$\lambda_+ +\lambda_- +(\lambda_+ -\lambda_-)\mathbf{n}(t)\cdot\mathbf{x}=0, \tag{74}$$

$$(\lambda_+ -\lambda_-)\mathbf{x}+(\lambda_+ +\lambda_-)\mathbf{n}(t)=4\mathbf{n}_{+-}. \tag{75}$$

From these equations we calculate the unit vector $\mathbf{x}$:

$$\mathscr{N}(t)\mathbf{x}=2\mathbf{b}[(1-b_z)(1+b^2+2b_z)-2t(1+b^2-2b_z^2)]-\mathbf{k}(1-b^2)(1+b^2+2b_z-4tb_z), \tag{76}$$

$$\mathscr{N}(t):=\sqrt{(1+b^2)^2-4b_z^2-16t(1-t)(b^2-b_z^2)}\,\sqrt{(1+b^2)^2-4b_z^2}. \tag{77}$$

The state $\hat{\rho}$ of (29) corresponds to the choice $t=p_+^a$ [see (61)]. Once inserted in the above expression it gives $\mathbf{x}=\mathbf{e}^*$. Therefore we have the following.

Proposition 5: Let $\mathbf{A}\subset\mathbf{M}_2(\mathbb{C})$ *be the subalgebra generated by the projections* $\hat{a}_\pm$ *of (29) and* $\hat{\rho}$ *a given density matrix. Let* $\hat{\rho}(t)$ *the state path in (71). Then, the eigenprojections of the*

logarithmic derivative at $\hat{\rho}(p_+^a)=\hat{\rho}$ *coincide with the observables at which the entropy* $H_{\hat{\rho}}(\mathbf{A})$, *equivalently the accessible information* $I(\mathscr{A}_{\hat{\rho}})$, *is attained. The same optimal observables maximize the Fisher information* $F^e(p_+^a)$ *in (64).*

The above proposition is in agreement with analogous results in Ref. 19, where a proof of the Holevo bound is given by using the logarithmic derivative and in Ref. 2, where the more general question of the optimal measurements in $\mathbf{M}_2(\mathbb{C})$ is addressed.

Optimizing the Fisher information with respect to all possible generalized quantum measurements is essential in constructing a so-called distinguishability metric on the state space. The idea is to provide density matrices with a distance that reasonably discriminates between neighboring states.[23,24] In the symmetric case of Remark 2, that is, for $\mathbf{b}=(b,0,0)$, the logarithmic derivative at $\hat{\rho}(1/2)$ equals

$$\mathscr{L}_{\hat{\rho}(1/2)}\left[\hat{\rho}'\left(\frac{1}{2}\right)\right]=-2\,\frac{1-b^2}{1+b^2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}. \tag{78}$$

The projections $\hat{a}_\pm$ can thus be interpreted as the observables that optimally distinguish the symmetric state $\hat{\rho}(1/2)$ from neighboring states $\hat{\rho}(t)$ along the state path (35).

A similar argument does not hold in $\mathbf{M}_3(\mathbb{C})$ for the symmetric state $\hat{\rho}(z)$ in (38). Indeed, one can consider, for instance, the state path

$$\hat{\rho}(t,z)=t\hat{\rho}_1(z)+t\hat{\rho}_2(z)+(1-2t)\hat{\rho}_3(z),\quad \hat{\rho}_j(z)=\frac{\sqrt{\hat{\rho}(z)}\hat{a}_j\sqrt{\hat{\rho}(z)}}{\mathrm{Tr}\,\hat{\rho}(z)\hat{a}_j}, \tag{79}$$

where the $\hat{a}_j$ are the projections in (37), $0\leqslant t\leqslant 1/2$, and $\hat{\rho}(1/3,z)=\hat{\rho}(z)$. After some labor, it turns out that, unless $z=0$, that is, unless $\hat{\rho}(z)$ is the three-dimensional tracial state,

$$\mathscr{L}_{\hat{\rho}(z)}\left[\hat{\rho}'\left(\frac{1}{3},z\right)\right]=\begin{pmatrix}L_1 & L_2 & L_3\\ L_2 & L_1 & L_3\\ L_3 & L_3 & -2L_1\end{pmatrix},\quad \begin{cases} L_1=1+4\,\dfrac{\sqrt{1+3z-18z^2}}{2+3z},\\ L_2=2-4\,\dfrac{\sqrt{1+3z-18z^2}}{2+3z},\\ L_3=1-2\,\dfrac{\sqrt{1+3z-18z^2}}{2+3z}, \end{cases} \tag{80}$$

is not diagonal in the basis in which the $\hat{a}_j$ are diagonal.

Actually, according to Proposition 3, the situation is even more troublesome. In fact, when $z^*\leqslant z<1/3$, the possibility still remains of envisaging a suitable state path, such that the corresponding logarithmic derivative at $\hat{\rho}(1/3,z)$ has the $\hat{a}_j$ as eigenprojections. On the contrary, for $-1/6<z<z^*$, not only are there two sets of optimal observables for the entropy $H_{\hat{\rho}(z)}(\mathbf{A})$ of $\mathbf{A}$ with respect to $\hat{\rho}(z)$, but, above all, the $\hat{e}_j^*(u_\pm(z),z)$ are one dimensional, nonorthogonal projections, therefore they cannot be the spectral projections of a nontrivial logarithmic derivative.

V. CONCLUSIONS

In this paper we have compared two concepts: the accessible information of a quantum communication channel and the entropy of a subalgebra with respect to a quantum state. The first is an important tool to investigate the information content of messages transmitted by quantum carriers; the second aims at generalizing the notion of entropy of a partition of classical ergodic theory. Both find a common ground in the increasingly felt necessity of extending to quantum systems the apparatus of Shannon information theory.

We have pointed out the connections between the two notions, showing that the entropy of a subalgebra corresponds to the accessible information of a particular quantum communication channel, thus giving this seemingly abstract concept a nearly operative concreteness.

On the other hand, the fundamental role of the entropy of a subalgebra in generalizing to the noncommutative realm the dynamical entropy of Kolmogorov and Sinai, opens a wider horizon to the accessible information itself.

In the case of the two-dimensional algebra $\mathbf{M}_2(\mathbb{C})$ we have reviewed results common to both contexts, but apparently unknown to each other. The peculiarity of quantum mechanics, however, shows up when working in $\mathbf{M}_3(\mathbb{C})$, where a recent surprising result renders somehow problematic the promising relationships between the optimal observables and the so-called information geometries or distinguishability metrics that hold in the two-dimensional case.

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Spatial variation of currents and fields due to localized scatterers in metallic conduction (and comment)

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Comment by R. Landauer

The paper, published in the first volume of the then newly established IBM Journal of Research and Development, is not all that easily located in 1996. As a result the frequent citations to it often assign content to that paper which does not agree with reality. The primary purpose of the paper, conveyed by its title, was to investigate the spatial variation of the transport field, in the presence of highly localized scatterers, and to show that such scatterers were associated with highly localized transport fields. The viewpoint has, since then, been elaborated by a good many other investigators, but has still not become a part of the material widely reflected in texts, review papers and conferences. A second aim of the 1957 paper was to bring a new view to electron transport theory. To the physicist the applied field has always been the source of transport, and the resulting carrier flow is viewed as the response. Electrical engineers, in circuit theory, have had a broader view, allowing for a duality between current sources and voltage sources. My 1957 paper introduced the notion that we can view the carriers introduced at the boundaries of the sample as the source of transport, and then ask how the resulting build-up of carriers produces fields. My 1957 paper is most often cited in connection with the now widely used expressions which relate conductance to the overall transmissive behavior of a sample which transmits carriers in a quantum mechanically coherent and elastic fashion. That result is, however, not contained in the 1957 paper, which is semi-classical and assumes that scatterers act incoherently. It took me several more years to understand that the relation between conductance and transmission is general, and not only applicable to localized plane barriers. It took about another decade after that to get the material accepted by a journal. That history was presented in the introductory paper of a recent conference volume.[1]

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R. Landauer

Spatial Variation of Currents and Fields Due to Localized Scatterers in Metallic Conduction

Abstract: Localized scatterers can be expected to give rise to spatial variations in the electric field and in the current distribution. The transport equation allowing for spatial variations is solved by first considering the homogeneous transport equation which omits electric fields. The homogeneous solution gives the purely diffusive motion of current carriers and involves large space charges. The electric field is then found, and approximate space charge neutrality is restored, by adding a particular solution of the transport equation in which the electric field is associated only with space charge but not with a current. The presence of point scatterers leads to a dipole field about each scatterer. The spatial average of a number of these dipole fields is the same as that obtained by the usual approach which does not explicitly consider the spatial variation. Infinite plane obstacles with a reflection coefficient r are also considered. These produce a resistance proportional to $r/(1-r)$.

1. Introduction

In the solution of the transport equation in modern treatments of the electrical conductivity process, it is customary to assume that the distribution of electrons in momentum space is the same throughout the specimen (or at best has only a macroscopic variation due to temperature gradients, et cetera). Coupled with this is an assumption that the applied field is uniform. The applied field then produces a motion of the electronic distribution in momentum space. Scattering by lattice waves and obstacles tends to restore the original distribution, and equilibrium is established between the scattering and the accelerating field. The current density is then computed by taking a sum over the states of the undisturbed crystal and weighting the current associated with each state by its probability of occupation. This process ignores the off-diagonal elements of the current matrix. These off-diagonal elements do not contribute to the space average of the current density, but they can represent local fluctuations in the current distribution. The current due to each of the diagonal terms has the periodicity of the crystal. The spatial uniformity of current can, therefore, be regarded as a consequence of the assumed field uniformity and of the neglect of the off-diagonal matrix elements.

We wish to point out that the uniformity of the field and current density are assumptions which may frequently be well justified, but whose validity in general is not apparent. If the intensity of scattering is not uniformly distributed over the material, but is concentrated in well localized scattering centers, as is the case in the residual resistivity caused by impurities at low temperatures, then it seems in fact reasonable that the field should be concentrated near the points where the scattering is actually produced, so as to enable the current to pass around these obstacles. We shall, therefore, in this paper solve the transport equations in two simple cases without neglecting the relevant spatial variations. We shall consider the case of highly localized point scatterers and also the case of scattering by specular reflection at planes of infinite extension.

Despite the fact that the ordinary viewpoint neglects spatial variations it will, in most cases, lead to a correct answer. The quantities which have spatial variations may be characterized by suitably defined average values, which then can be used in the usual formalism. Some care must be exercised in this averaging process. If the averaging is carried out in too naive a manner, incorrect results can be obtained, as will be shown in the case of plane obstacles treated in Section 8.

In constructing our solution we do not wish to assume a uniform field and initially do not know the correct field distribution. It will, instead, be assumed that at the boundaries of the specimen the number of electrons which are moving into the interior of the specimen are so controlled as to maintain the proper current flow in and out of the

material. If there were no scattering in the specimen, the current carriers could move unhampered, and the maintenance of the current at the surfaces of the specimen would not produce a field. An obstacle in the path of the current will result in a pile-up of electrons on one side of the obstacles and a deficit on the other side. This dipole moment will grow until the resultant electric field enables the incident current to pass the obstacle at the same rate at which further charges arrive. It is a superposition of many such dipole fields which will then constitute the electric field associated with the current flow, and it is the space average of these dipole fields which enter into a conductivity measurement.

In the usual discussions of the residual resistivity of metals, the conductivity is evaluated with the aid of the electron acceleration law, $d\mathbf{k}/dt = -e\mathbf{E}/\hbar$. Since the electric field is spatially inhomogeneous and highly concentrated about positions where the periodicity of the lattice potential is disturbed, the use of this relation is questionable. The transport equation, as used in the subsequent discussion, will naturally involve a term closely related to the electron acceleration law. It will be seen, however, that the term can be modified at positions close to the scatterers without affecting our evaluation of the conductivity.

2. General form of treatment

All the complications due to the real crystalline nature of the medium will be neglected in this treatment, and we will assume that our medium is isotropic. Its crystalline nature will be acknowledged only through the fact that the density of states in energy, dn/dU, at the spherical Fermi surface, and the wave number k_0 associated with this Fermi surface, will be taken as independent quantities. Except for the use of Fermi statistics our considerations will be classical, and we shall assume that at each point in space there is a well-defined distribution of electrons in $\mathbf{k}$ space. ($\mathbf{k}$ is the wave vector which determines the wave-function variation in going from cell to cell.) In the presence of a current, the number of electrons per unit volume moving within a solid angle $d\Omega$ about the direction $\boldsymbol{\Omega}$ (a unit vector) will differ from the number that moves in that direction in the undisturbed metal by an amount $N(\boldsymbol{\Omega})d\Omega$. We shall restrict ourselves to sufficiently low temperatures so that the distribution changes represented by $N(\boldsymbol{\Omega})$ are contained in a sufficiently narrow energy range to give all the $N(\boldsymbol{\Omega})$ extra (or deficit) electrons the same velocity and scattering cross sections. The transport equation for the steady state can then be written in the form

$$\partial N(\boldsymbol{\Omega}, r)/\partial t = 0 = -\alpha\boldsymbol{\Omega}\cdot\mathbf{E} - \boldsymbol{\nabla}N\cdot\mathbf{v} + (\partial N/\partial t)_S. \tag{2.1}$$

In this equation the first term on the right-hand side represents the acceleration by the field. In terms of the electronic charge e and the Fermi-surface wave number k_0, we have $\alpha = ek_0^2/4\pi^3\hbar$. The second right-hand term represents spatial gradients, and $\mathbf{v} = \hbar^{-1}\boldsymbol{\Omega}\, dU/dk$. The last term represents the effect of the scatterers which cause the resistance.

Eq. (2.1), considered as an equation for N, is a linear inhomogeneous equation. Such equations can be solved by taking a particular solution and then adding to it solutions of the homogeneous equation to satisfy the boundary conditions. We shall use this procedure and shall use a particularly simple solution of Eq. (2.1) for the particular solution. Eq. (2.1) always has a solution in which the electric field produces spatial variations in electronic density but does not cause a current. This is a solution in which $N(\boldsymbol{\Omega}, \mathbf{r})$ is independent of $\boldsymbol{\Omega}$. In that case, we can expect the term $(\partial N/\partial t)_S$ to vanish. Using $\mathbf{E} = -\boldsymbol{\nabla}V$, we then find for Eq. (2.1) the form

$$\alpha\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}V = v\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}N, \tag{2.2}$$

which has the solution

$$N(\mathbf{r}) = \frac{\alpha}{v}V(\mathbf{r}) + c = \frac{1}{4\pi}\frac{dn}{dU}eV(\mathbf{r}) + c, \tag{2.3}$$

where c is independent of $\mathbf{r}$, and dn/dU is the density of states at the Fermi surface.

The boundary conditions which determine the current entering and leaving the specimen must then be satisfied by a solution of the homogeneous transport equation. The homogeneous equation represents the motion of particles subject only to scattering and therefore gives the purely diffusive motion of the carriers.

3. Neutrality condition

Let $N_D(\boldsymbol{\Omega}, \mathbf{r})$ represent the solution to the homogeneous equation. Let $N_V(\boldsymbol{\Omega}, \mathbf{r})$ be the particular solution as given by Eq. (2.3). N_D will be determined by the boundary conditions and the diffusive motion. To determine N_V and V, we have to use Poisson's equation in addition to Eq. (2.1). This states

$$\nabla^2 V = 4\pi e\int(N_D + N_V)d\boldsymbol{\Omega}. \tag{3.1}$$

Now let

$$n_D = \int N_D d\boldsymbol{\Omega} \quad \text{and} \quad n_V = \int N_V d\boldsymbol{\Omega}. \tag{3.2}$$

If in (2.3) we choose the origin of the potential such that $N(\mathbf{r}) = 0$ where $V(\mathbf{r}) = 0$, it becomes

$$n_V(\mathbf{r}) = \frac{dn}{dU}eV(\mathbf{r}). \tag{3.3}$$

Combining (3.3), (3.2), and (3.1), we find

$$n_V - l^2\nabla^2 n_V = n_D, \tag{3.4}$$

with $1/l^2 = 4\pi e^2 dn/dU$. The distance l is the range to which the electronic screening in this medium permits electric fields to penetrate. In a typical good conductor, if we are concerned with variations existing over a distance of several atomic cells, then we can neglect the term $l^2\nabla^2 n_V$ in Eq. (3.4) and find

$$n_V = -n_D, \tag{3.5}$$

$$(dn/dU)eV = -n_D. \tag{3.6}$$

4. Point scatterer

We shall now analyze in detail the case of a point scatterer embedded in a spatially uniform background scattering. This is immediately suggestive of an impurity embedded in

a material which is scattering thermally. As we shall see later, however, other interpretations are possible.

Before entering into the details of our argument we would like to clear up one frequent misconception concerned with the relative importance of the physical dimensions, e.g., the radius a of a point scatterer and its quantum mechanical scattering cross section σ. We will assume that both a and $\sqrt{\sigma}$ are small compared to the mean free path. The localized obstacle will disturb the otherwise uniform current flow. If we are at a distance several times a from the center of the obstacle, then the disturbances set up there by the obstacle will depend only on the number of electrons that have had their direction changed by the obstacle—i. e., on the differential cross section of the obstacle. The physical size of the obstacle and the potential variation within its physical extension are primarily relevant to an evaluation of the disturbances in the volume of the obstacle itself. These will not concern us, except for some auxiliary discussions.

In solving the problem of the point scatterer, we shall use Eq. (2.1) in the form

$$-\alpha\boldsymbol{\Omega}\cdot\mathbf{E}-\boldsymbol{\nabla}N\cdot\mathbf{v}+(\partial N/\partial t)_B=0, \tag{4.1}$$

where $(\partial N/\partial t)_B$ denotes the background scattering. Eq. (4.1) is then satisfied everywhere except at the obstacle which is taken to be at $\mathbf{r}=0$. We shall satisfy the scattering conditions at $\mathbf{r}=0$ by superposing two solutions of Eq. (4.1). One solution represents the motion of the electrons without the obstacle, and the other represents the corrections due to the changed motion of the carriers after their incidence on the obstacle.

We shall restrict the nature of the scattering, both for the obstacle and for $(\partial N/\partial t)_B$. In both cases the probability of scattering will be taken as a function only of the angle through which the electron is deflected, and not as a function of the incident direction. In that case[1], the usual theory of conductivity which neglects spatial variations permits the background scattering to be characterized by a single conductivity relaxation time τ_B, and also permits the medium which has only a distribution of obstacles to be characterized by a single conductivity relaxation time τ_O. Furthermore, in that case the combined effects of both types of scattering can also be described by a single relaxation time in accordance with Matthiessen's rule.[2]

It is to be particularly noted that the assumption of differential scattering cross sections which are functions only of the angle through which the particle is scattered, leads to a simple timewise exponential relaxation for the disturbance produced by an electric field. For these same scattering cross sections, there will be many other possible disturbances from equilibrium which do not show a relaxation characterized by a single time constant.

In the ensuing discussion we shall use the symbol $\mathbf{i}$ to denote a current measured in numbers of electrons crossing a unit area in unit time. The electrical current $\mathbf{j}$ will then be given by $\mathbf{j}=-e\mathbf{i}$. We shall take the particular situation in which $\mathbf{i}$ far away from the obstacle has only a z component denoted by i_∞. If $v=\hbar^{-1}dU/dk$ is the velocity at the Fermi surface far away from the obstacle, we will have

$$N(\boldsymbol{\Omega})=3i_\infty\cos\theta/4\pi v, \tag{4.2}$$

where θ is the angle between $\boldsymbol{\Omega}$ and the z-axis. This current is accompanied by a field which can be determined from Eq. (4.1). Omitting the second term in Eq. (4.1) gives

$$E_z=-3i_\infty/4\pi v\alpha\tau_B, \tag{4.3}$$

which corresponds to a conductivity

$$\sigma_B=-\frac{ei_\infty}{E_z}=\frac{e^2k_0^2}{3\pi^2\hbar^2}\frac{dU}{dk}\tau_B. \tag{4.4}$$

If $N(\boldsymbol{\Omega})$ and $E(\mathbf{r})$, as given by Eqs. (4.2) and (4.3), are presumed to hold for all $\mathbf{r}$, then Eq. (4.1) is satisfied everywhere. The effect of the localized obstacle will in that case be ignored. Let us assume that the obstacle has a differential scattering cross section, $f^2(\theta)d\Omega$, for scattering through the angle θ into a range $d\Omega$ of solid angle. If Eq. (4.2) is correct in describing the number of electrons incident on the obstacle, then the rate at which electrons are scattered by the obstacle into an angular range $d\Omega$ about the direction $\boldsymbol{\Omega}_f$ is, through the use of (4.2),

$$d\Omega\int f^2(\boldsymbol{\Omega}_f,\boldsymbol{\Omega}_i)N(\boldsymbol{\Omega}_i)v\,d\boldsymbol{\Omega}_i=d\Omega\frac{3i_\infty}{4\pi}\int f^2(\boldsymbol{\Omega}_f,\boldsymbol{\Omega}_i)\cos\theta_i\,d\boldsymbol{\Omega}_i. \tag{4.5}$$

In Eq. (4.5), $f^2(\boldsymbol{\Omega}_f\boldsymbol{\Omega}_i,)$ denotes $f^2(\theta)$ where θ is the angle between the incident direction $\boldsymbol{\Omega}_i$ and the scattered direction $\boldsymbol{\Omega}_f$. θ_i denotes the angle between the direction of incidence and the z-axis. θ_f will similarly locate the scattered direction relative to the z-axis. With a little spherical trigonometry, the right-hand side of Eq. (4.5) can be put into the form

$$d\Omega\frac{3i_\infty}{4\pi}\cos\theta_f\int f^2(\theta)\cos\theta\,d\boldsymbol{\Omega}, \tag{4.6}$$

where the integral is now independent of $\boldsymbol{\Omega}_f$. Expression (4.6) gives the rate at which electrons are scattered into $\boldsymbol{\Omega}_f$, but it has not had subtracted from it the rate at which electrons which were originally moving within a range $d\Omega$ of the direction $\boldsymbol{\Omega}_f$ are scattered out of this range. The latter rate will be

$$d\Omega N(\boldsymbol{\Omega}_f)v\int f^2(\theta)d\boldsymbol{\Omega}=d\Omega\frac{3i_\infty}{4\pi}\cos\theta_f\int f^2(\theta)d\boldsymbol{\Omega}. \tag{4.7}$$

Subtracting the right hand side of Eq. (4.7) from (4.6), we find that the number of electrons per second leaving the obstacle in the range $d\Omega$ exceeds the number specified in Eq. (4.2) by

$$-d\Omega\frac{3i_\infty}{4\pi}(\cos\theta_f)\int f^2(\theta)(1-\cos\theta)d\boldsymbol{\Omega}. \tag{4.8}$$

The integral in (4.8), in which deflections are weighted by the factor $(1-\cos\theta)$, is the scattering cross section found relevant in the usual theory of conductivity and we will label it S_O. Then (4.8) can be written

$$-d\Omega\frac{3i_\infty}{4\pi}(\cos\theta_f)S_O. \tag{4.9}$$

We shall now construct a solution of Eq. (4.1) which has

as its source electrons issuing from the obstacle as specified by (4.9). Furthermore, we shall require that the solution $N_S(\Omega,\mathbf{r})$ generated by this source vanish at infinity. The superposition, then, of N_S on the spatially uniform solution given by Eq. (4.2) and (4.3) satisfies both Eq. (4.1) and the scattering conditions imposed by the obstacle. This is actually not quite correct. The solution N_S contains electrons which can, after some scattering by the background, return again to the obstacle at $\mathbf{r}=0$. Since N_S is a strict solution of Eq. (4.1), it does not take into account scattering by the obstacle when the electron returns to the obstacle a second (or later) time. If, however, the mean free path determined by the background is large compared to the effective dimensions of the scatterer (i. e., the square root of its scattering cross section), the probability of multiple scatterings by the obstacle will be small, and we will therefore restrict our further considerations to this case.

We shall deal with the scattered solution $N_S(\Omega,\mathbf{r})$ by first treating the purely diffusive motion, thus finding $N_{SD}(\Omega,\mathbf{r})$, and then using Eq. (3.6) to find the accompanying field.

5. Diffusive motion about point scatterer

The diffusive motion about a point scatterer is schematized in Fig. 1. Line A shows a direction in which the number of incident carriers exceeds the equilibrium number. Similarly, line B shows a direction in which fewer than the equilibrium number are moving. A and B represent the spatially uniform solution (4.2) which gives the number of electrons incident on the obstacle. Line C shows a direction along which there is an excess of scattered electrons. Along line D there is a deficit. After a number of scatterings by the background the electrons which initially move away from the obstacle along C and D will have their velocity completely randomized. Their motion will then obey the diffusion equation. This diffusion current is schematically indicated by the broad arcs, which finally show the recombination of the electron excess and deficit.

Consider first the diffusion current generated by all the electrons which start their motion away from the scattering center in directions that lie within $d\Omega_f$ of the direction Ω_f. Far away from $\mathbf{r}=0$ at a position in space denoted by (r, ω), where r is the distance from the scattering center and ω is a unit vector pointing from the scatterer to the point involved, the diffusion current will establish a concentration $C(\Omega_f,\omega,r)d\Omega_f$ of electrons, all of which were originally travelling away from $\mathbf{r}=0$ in the direction Ω_f. This concentration obeys the steady state diffusion equation $\nabla^2 C=0$. Up to terms of order $1/r^2$ this has the solution

$$C(\Omega_f,\omega, r)=a/r+\mathbf{p}\cdot\omega/r^2, \tag{5.1}$$

with a and $\mathbf{p}$ arbitrary. The radial current density (in electrons/cm^{2}sec) far from the origin due to the a/r term is $d\Omega_f D_B a/r^2$ where D_B is the diffusion coefficient of electrons in the presence of the background scattering. The integrated flow out of a large sphere is then $4\pi D_B a d\Omega_f$ electrons /sec. The other term $\mathbf{p}\cdot\omega/r^2$ does not contribute to the integrated flow. Equating $4\pi D_B a d\Omega_f$ to (4.9) gives

$$a(\Omega_f)=-\frac{3i_\infty(\cos\theta_f)S_O}{(4\pi)^2 D_B}. \tag{5.2}$$

To terms of order $1/r^2$, the right-hand side of Eq. (5.1) has the form $a/|\mathbf{r}-\mathbf{r}_f|$ with $\mathbf{r}_f=\mathbf{p}/a$. The term $\mathbf{p}\cdot\omega/r^2$ simply serves to displace the effective source away from the origin in the direction of $\mathbf{p}$. The average position of the particles described by Eq. (5.1) is therefore $\mathbf{r}_f=\mathbf{p}/a$. The average position of the particles can also be found by following a beam of particles issuing from $\mathbf{r}=0$ at $t=0$, and initially proceeding along Ω_f. The average position then is:

$$\mathbf{r}_f=\left\langle\int_0^\infty \mathbf{v}dt\right\rangle_{Av}=\int_0^\infty\langle\mathbf{v}\rangle_{Av}dt. \tag{5.3}$$

$\langle\mathbf{v}\rangle_{Av}$ as used in Eq. (5.3) is an average over electrons which initially left $\mathbf{r}=0$ in the direction Ω_f. $\langle\mathbf{v}\rangle_{Av}$ is therefore a function of Ω_f, but for the sake of typographical compactness this will not be explicitly indicated. $\langle\mathbf{v}\rangle_{Av}$ decays with time because of background scattering. The decay is generally not a simple exponential, since the initial velocity distribution, a collimated beam, is not the distribution involved in the usual definition of a relaxation time for the conductivity process. Since $\mathbf{p}=\mathbf{r}_f a$, combining (5.2) and (5.3) gives

$$\mathbf{p}=-\frac{3i_\infty(\cos\theta_f)S_O}{(4\pi)^2 D_B}\int_0^\infty\langle\mathbf{v}\rangle_{Av}dt. \tag{5.4}$$

To find the total concentration of diffused carriers we have to integrate (5.1) over all values of Ω_f. The integration over the a/r terms gives a vanishing result since the total number of carriers emitted at $\mathbf{r}=0$, according to (4.9), is zero. This leaves

$$n_f(\omega, r)=\int d\Omega_f C(\Omega_f,\omega, r)=\int d\Omega_f\mathbf{p}\cdot\omega/r^2$$
$$=-\frac{3i_\infty S_O}{(4\pi)^2 D_B}\frac{1}{r^2}\omega\cdot\int d\Omega_f(\cos\theta_f)\int_0^\infty\langle\mathbf{v}\rangle_{Av}dt. \tag{5.5}$$

After exchange of integrations this becomes

$$n_D(\omega, r)=-\frac{3i_\infty S_O}{(4\pi)^2 D_B}\frac{1}{r^2}\omega\cdot\int_0^\infty dt\int d\Omega_f(\cos\theta_f)\langle\mathbf{v}\rangle_{Av}. \tag{5.6}$$

The values of $\langle\mathbf{v}\rangle_{Av}$ which result from the electrons initially proceeding along Ω_f are now weighted with the factor $\cos\theta_f$. Therefore, Eq. (5.6) represents a timewise integration over a velocity distribution which is initially similar to the distribution produced by an electric field. Hence we can expect $\int d\Omega_f(\cos\theta_f)\langle\mathbf{v}\rangle_{Av}$ to decay as exp $(-t/\tau_B)$, where τ_B is the conductivity relaxation time for the background scattering. At t = 0 we have an initial value

$$d\Omega_f\langle\mathbf{v}\rangle_{Av}\cos\theta_f=\int d\Omega_f\frac{1}{\hbar}\frac{dU}{dk}\Omega_f\cos\theta_f=\frac{4\pi}{3\hbar}\frac{dU}{dk}\mathbf{z}_1, \tag{5.7}$$

with $\mathbf{z}_1$ representing the unit vector in the z-direction. Combining (5.5) with (5.7) gives

$$n_D(\omega,r)=-\frac{i_\infty S_O}{4\pi D_B}\frac{1}{\hbar}\frac{dU}{dk}\frac{1}{r^2}\omega\cdot\mathbf{z}_1\int_0^\infty dte^{-t/\tau_B}$$
$$=-\frac{i_\infty\tau_B}{4\pi D_B}S_O\frac{1}{\hbar}\frac{dU}{dk}\frac{\cos\theta_\omega}{r^2}. \tag{5.8}$$

θ_ω is the angle between ω and the positive z-axis.

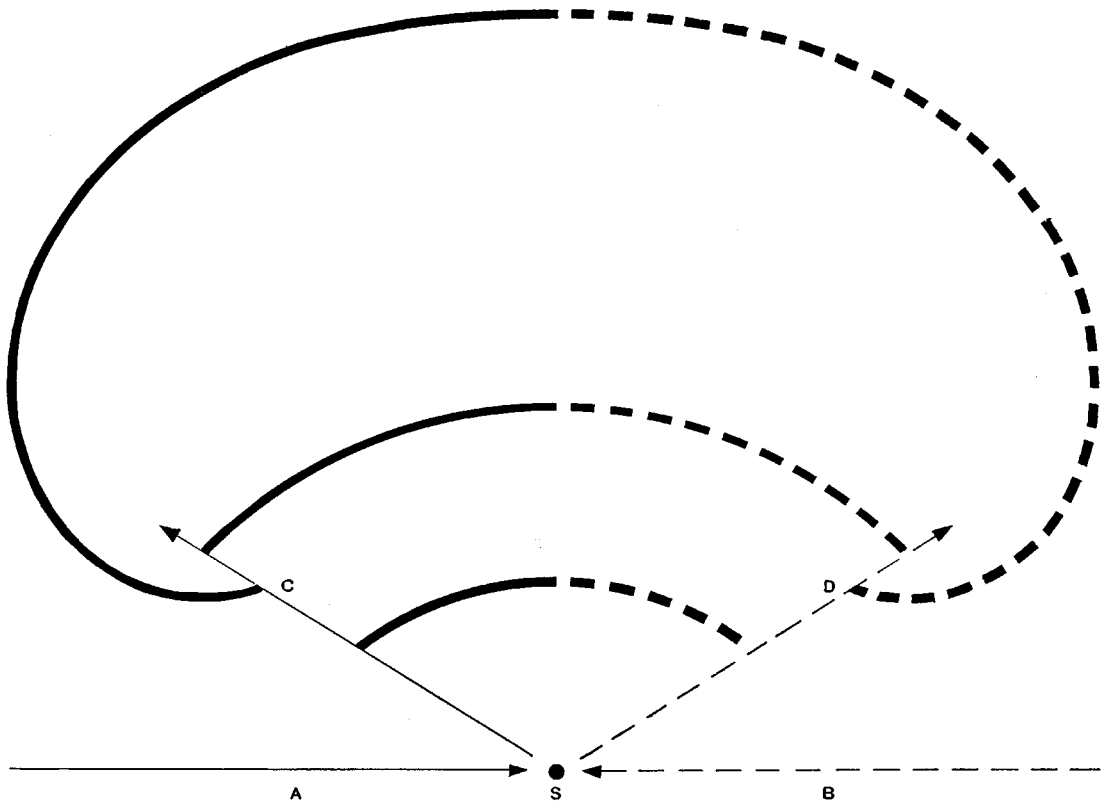

Figure 1 **Schematic representation of current flow disturbed by the scatterer** S.
Electrons in excess numbers are incident along A, then are scattered to C, then scattered by the background. The number of electrons incident along B is less than the equilibrium number. The deficit is scattered to D, then scattered by the background. The excess and deficit diffuse together and recombine along the arcs.

The diffusion coefficient D_B, as determined by the background scattering, and the conductivity σ_B, determined by the same scattering, are not independent. By considering the balance between diffusion currents and conductivity currents, in an equilibrium situation, we arrive at the "Einstein" relation for completely degenerate Fermi statistics in the same way as for semiconductors.[3] The resulting relation is

$$De^2 dn/dU = \sigma. \tag{5.9}$$

For our isotropic band structure and isotropic background scattering the conductivity in (5.9) is given by

$$\sigma_B = \frac{\tau_B}{3\pi^2}\frac{e^2}{\hbar^2}k^2\frac{dU}{dk}. \tag{5.10}$$

Hence we find

$$D_B = \frac{\tau_B}{3\pi^2}\frac{k^2}{\hbar^2}\frac{dU}{dk}\left(\frac{dn}{dU}\right)^{-1}. \tag{5.11}$$

This value for D_B can be introduced into Eq. (5.8) to give

$$n_D(\omega, r) = -\frac{3\pi i_\infty S_0 \hbar}{4k^2}\frac{dn}{dU}\frac{\cos\theta_\omega}{r^2}. \tag{5.12}$$

Eq. (3.6) permits us to go from the above to the potential distribution

$$V = -\frac{n_D}{e}\left(\frac{dn}{dU}\right)^{-1} = \frac{3\pi i_\infty S_0 \hbar}{4k^2 e}\frac{\cos\theta_\omega}{r^2}. \tag{5.13}$$

Eq. (5.1) which we used in the derivation of (5.12) and (5.13) is only an asymptotic expansion, and therefore we cannot on the basis of the above derivation expect (5.13) to be valid close to the scatterer. Consider the electrons close to the scatterer as specified by (4.9) and before they have been appreciably scattered by the background. The density $n_D(\omega, r)$ due to these electrons is easily evaluated and leads again to the expression (5.12). Since (5.12) is correct when we are much closer to the scatterer than a

mean free path, and also when we are many mean free path lengths away from the scatterer, and since furthermore it is easily shown from (4.9) that $n_D(\omega, r)$ must vary as $\cos\theta_\omega$, for all values of r, we can expect that $n_D(\omega, r)$ is closely approximated by (5.12) for all r values. In computing an average field or conductivity, however, it is only the asymptotic behavior of (5.13) that matters, and this has been accurately justified.

Eq. (5.13) gives a potential associated with a dipole of moment

$$p=3\pi i_\infty S_O\hbar/4k^2e. \tag{5.14}$$

If we have a density of $\mathfrak{N}$ obstacles per unit volume which are sufficiently far apart to be non-interacting, there will be a polarization $\mathfrak{N}\mathbf{p}$, and the space average of the dipole fields will be

$$E_z=-4\pi P_z=-3\pi^2 i_\infty S_O\hbar\mathfrak{N}/k^2e. \tag{5.15}$$

The mean free time τ_O as used in the usual conductivity theory, and associated only with scattering by the obstacle is given by

$$\tau_O=1/\mathfrak{N}S_O v. \tag{5.16}$$

This makes the space average field, as given in (5.15), equal to

$$E_z=-3\pi^2 i_\infty\hbar/k^2ev\tau_O. \tag{5.17}$$

In terms of the electric current $j_\infty=-ei_\infty$, we find

$$E_z=\frac{3\pi^2\hbar^2}{k^2e^2\tau_O}\left(\frac{dU}{dk}\right)^{-1}j_\infty, \tag{5.18}$$

which is exactly the field associated with the obstacles, as found by the usual approach [e. g., compare with Eq. (5.10) which gives the connection between σ and τ resulting from the usual considerations]. The field given by (5.18) exists in addition to the background field of Eq. (4.3). Matthiessen's rule is satisfied; (5.18) does not depend on τ_B.

We would like to stress the extreme extent to which these dipole fields are really localized. To do this we must consider how the charges that are responsible for the dipole moment given by (5.14) are actually distributed. Let us assume for the moment that the charge density, in the (spherical) volume of the scatterer is of the form $\rho(r)\cos\theta_\omega$ and vanishes outside the scatterer. In computing an average field for the whole specimen we must evaluate $\int\mathbf{E}d\tau$, where the $\mathbf{E}$ includes the contributions of the particular dipole moment under discussion. Under the conditions specified above, 2/3 of this dipole contribution to $\int\mathbf{E}d\tau$ comes from the volume of the scatterer. Actually, of course, the dipole charges cannot be as well localized as we have assumed. [The screening length l of Eq. (3.4) is finite, the uncertainty principle also prevents an excessively localized charge. Furthermore, Eq. (5.12) is derived from a point model and cannot be expected to hold true up to the actual surface of the scatterer.] Therefore, only perhaps 1/3, instead of 2/3, of the voltage drop associated with the residual resistance is contained in the volume occupied by the impurity atoms.

Since such a large portion of the field is located where the crystalline potential has been disturbed, the use of the usual electron acceleration equation, $d\mathbf{k}/dt=-e\mathbf{E}/\hbar$, becomes questionable. Note that in our arguments the field is found as a result of screening considerations. The exact nature of the screening close to the impurity atom, is not relevant to the evaluation of an average field. That is, the nature of the first term in Eq. (2.1) can be modified, close to the impurity atoms, without appreciably affecting our asymptotic evaluation of the dipole potential. It is only necessary that (dn/dU), in Eq. (3.6) represent the actual density of states, in the dilute alloy, rather than the density in the pure solvent.

6. Interaction of obstacles

The preceding section has been concerned with a localized obstacle of cross section S_O embedded in a medium with a relaxation time τ_B. This is obviously applicable to the case of a single obstacle in a medium which otherwise has only thermal scattering. If we consider a medium which has a density of obstacles such that the obstacle scattering is comparable to the uniform scattering or larger, then we must invoke some supplemental considerations. First of all, the radial current scattered by a particular obstacle, as given by Eq. (4.9), will now be subject to scattering by other obstacles as well as by the uniform background. Let us confine our considerations to the most common case, that in which the mean free path (as determined by the combined scattering) is large compared to the distance between obstacles. Only a small portion of the radial current will then be scattered by any one obstacle and the radial current will therefore see a relaxation time τ_B which depends on both kinds of scattering. Therefore, as the density of obstacles is increased, the effective value of τ_B changes. The value of τ_B, however, does not affect the dipole field brought in with each additional obstacle. As the number of obstacles is increased, therefore, the space average of the electric field changes just as it does in the usual theory.

We have assumed in the preceding section that the electron velocity distribution incident upon the obstacle is equal to the average velocity distribution which exists far away from the obstacle. A localized scatterer disturbs the velocity distribution. Close to the obstacle there are the scattered radial currents as given by Eq. (4.9). Further away there are the diffusion currents. Both of these kinds of currents constitute deviations from the average velocity distribution. A second obstacle placed near the first will be exposed to the deviations caused by the first obstacle. An obstacle, however, will generally see the deviations caused by many obstacles, not just those caused by one. If we add the disturbances due to the many obstacles randomly placed within the vicinity of a given one, then we are doing the same thing as adding the disturbances due to a particular obstacle over many points in its environment, as long as the obstacles are uncorrelated in their positions. The mere fact that the obstacles are finite in extension will give them some correlation. Let us temporarily neglect this. It is easily shown that if we consider the deviations caused by a *single* obstacle, in a *particular* velocity class,

these deviations vanish after integration over all space. Hence, an obstacle which is exposed to the deviations caused by many other obstacles is exposed to the average velocity distribution.

The argument which has just been given relies on an integration which in turn strictly requires a point scatterer, as we have assumed. Let us take a more realistic view and give the scatterer an extension in space. Then the scatterers exclude (or diminish) the current within a small volume, and the average value of the current density at locations which are outside of the excluded regions is larger than the average taken over *all* space. It is this larger current density which an additional scatterer, placed among the previously existing ones, will see. In principle, therefore, one should apply corrections to find the correct "internal" velocity distribution in a manner similar to the use of Lorentz corrections in dielectric theory. If the volume occupied by the scatterers is small, as in a dilute solution, this is presumably a small effect. If the scatterers occupy an appreciable fraction of the volume, these corrections will very likely be overshadowed by the direct effect of the scatterers on the electronic structure of the medium. In the extreme case where the *complete* volume of the metal is occupied by the scatterers, as in the case of high temperature scattering by independently vibrating atoms, then again the incident velocity distribution must be the average velocity distribution.

7. Degree of localization required

The argument we have used in arriving at our dipole field relies upon the localization of the scatterer. Since the quantities entering into the transport equation vary on a scale comparable to the mean free path (associated with the background), it is only necessary that the scatterer be small compared to the mean free path. This condition will generally be satisfied for impurity scattering.

Actually, the localization of the background scattering is as relevant as that of the obstacle scattering. The use of Eq. (4.1) implies that the scattering depends only on the disturbance $N_D(\mathbf{\Omega}, r)$ at the point $\mathbf{r}$ under consideration. Therefore, the obstacle and the background must be "localized" to the same extent. Scattering of electrons by phonons is generally sufficiently localized, since a wave packet of the representative thermally excited phonons is usually short compared to the electronic mean free path. The only apparent exception is the case of electron scattering by phonons at extremely low temperatures in an alloy where the scattering is almost completely determined by the lattice defects. At a sufficiently low temperature, the typical phonon wavelength will then exceed the mean free path. In this case, however, the phonon scattering will be an extremely small portion of the total scattering. Furthermore, this is a case in which any other theory would presumably have difficulties in correctly evaluating the contribution of the phonon scattering.

It might be thought that the spatial variations discussed here must disappear at very low temperatures since the small energy range of the order kT over which the probability of occupation varies from 1 to 0, does not permit the construction of very localized wave packets. This is, however, not relevant. One can, in principle, form stationary states which represent the multiple scattering of electrons by many obstacles, and thus find the probability of directional changes at various points in space. Such a solution specifies the scattered intensity as a function of direction of scattering within a few wavelengths of the scattering center. The relevant dynamic parameters for our theory are thus obtainable from solutions of the time-independent wave equation for a particular energy. (At least this is true for the cases where the time-wise variation of the lattice vibrations is not significant.)

The condition that one can construct highly localized wave packets, small compared to the mean free path, is the condition $\hbar/\tau < kT$, given by Peierls[4] long ago for the validity of the Bloch theory. This criterion was introduced as a consequence of the use of time-dependent perturbation theory and is a criterion only of the validity of time-dependent perturbation theory. If the probability of scattering is known correctly from some other treatment, this criterion has no relevance.

8. Reflecting walls

When there is a current impinging on a reflecting wall one can expect a voltage drop confined to the immediate vicinity of the reflecting plane. This is, in fact, taken for granted in the treatment of the contact resistance at the junction of two metallic conductors.[5] We have in mind a situation in which the current flow is perpendicular to the wall, and assume that the reflection is specular. A density of $\mathfrak{N}$ such planes per cm will be assumed without any additional source of electron scattering. These walls can be considered to be models of grain boundaries or of stacking faults. The reflection coefficient r will be assumed to be a function of the angle, θ, between the wall normal and the direction of incidence. We shall take the wall normal to be in the positive z-direction and θ to be the angle with this direction so that $r(\theta) = r(\pi - \theta)$, and shall first compute the conductivity according to the usual non-local viewpoint.

An electron travelling in a direction at an angle θ with the z-axis will pass $\mathfrak{N}|\cos\theta|$ walls per cm of its travel, and will therefore be incident upon $\mathfrak{N}|\cos\theta|v$ walls per second, where v is the velocity at the Fermi surface. At each of these collisions only a fraction $r(\theta)$ of the electrons are reflected. If there are n_+ electrons per unit volume moving in a certain direction, and n_- electrons in the reflected direction, we can expect that

$$dn_+/dt = -n_+\mathfrak{N}|\cos\theta|r(\theta)|v + n_-\mathfrak{N}|\cos\theta|r(\theta)|v, \tag{8.1}$$

$$dn_-/dt = -n_-\mathfrak{N}|\cos\theta|r(\theta)|v + n_+\mathfrak{N}|\cos\theta|r(\theta)|v. \tag{8.2}$$

If n_0 is the number of electrons travelling in the two directions concerned, in the absence of a current, then symmetry requires

$$n_+ - n_0 = n_0 - n_-. \tag{8.3}$$

If (8.3) is substituted in (8.2) and (8.1), we find

$$\frac{d}{dt}(n_+ - n_0) = -(n_+ - n_0)2\mathfrak{N}|\cos\theta|r(\theta)|v, \tag{8.4}$$

$$\frac{d}{dt}(n_- - n_0) = -(n_- - n_0)2\mathfrak{N}|\cos\theta|r(\theta)|v, \tag{8.5}$$

and therefore a relaxation time $\tau(\theta) = v/2\mathfrak{N}|\cos\theta|r(\theta)$. The usual conductivity theory then gives us a conductivity

$$\sigma = \frac{e^2k^2}{8\pi^3\mathfrak{N}\hbar}\int d\Omega|\cos\theta|r(\theta), \tag{8.6}$$

where the integration is over all directions of motion. Note that this value for the conductivity cannot be exact. As $r(\theta)$ is permitted to approach unity for all θ, all current flow must cease, yet Eq. (8.6) still yields a finite conductivity. This finite conductivity results from a finite relaxation time. The latter, in turn, is a result of the assumption of a uniform field. If the accelerating electric field is taken to be uniform, and the current flow is generated equally at all points in space, then it will take a finite time for portions of this current to reach the nearest reflecting barrier, and this is the relaxation time which can be obtained from (8.4) and (8.5), even if $r = 1$.

Instead of the treatment leading to Eq. (8.6), we can handle the problem by the methods we have already described. This requires that we have an expression for the distribution of electrons incident upon the wall. For any incident velocity distribution we can calculate a scattered current and a compensating charge. In general, however, these will be such that a second plane, parallel to the first, would be exposed to a different incident velocity distribution. We must therefore choose an incident velocity distribution such that the final resultant velocity distribution is the same on both sides of the plane at distances which are more than a screening length away from the plane. This leads, with a little calculation, to a velocity distribution (including incident electrons, reflected electrons, and compensating charge), of the form

$$N(\boldsymbol{\Omega},\mathbf{r}) = \beta\left(\frac{1-r(\theta)}{r(\theta)}\right)\frac{\cos\theta}{|\cos\theta|}, \tag{8.7}$$

where β is independent of θ. The conductivity resulting from the detailed localized treatment is

$$\sigma = \frac{e^2k^2}{8\pi^3\mathfrak{N}\hbar}\int d\Omega|\cos\theta|\frac{1-r(\theta)}{r(\theta)}. \tag{8.8}$$

This differs from (8.6) through the appearance in the integrand of the factor $(1-r(\theta))$. This factor serves to make the conductivity vanish as $r(\theta)$ approaches unity for all θ. The difference between (8.6) and (8.8) is therefore only important if the reflection probability is comparable to unity. In this connection it is interesting to note that some of the calculations for the reflection coefficient of stacking faults predict values for r which are not very small compared to unity.[6]

Note that the velocity distribution (8.7) does not vary with θ as $\cos\theta$. Therefore, there is no single relaxation time for the whole conduction process. If reflecting walls exist simultaneously with thermal scattering, Matthiessen's rule will not be satisfied. Even without thermal scattering, if we have a number of such walls with differing orientations, the scattering probabilities cannot just be added, since each orientation by itself would result in a different shape for the velocity distribution.

9. Multiple reflections by a single obstacle

In the treatment of point obstacles in Sections 4 and 5 we ignored the possibility of repeated reflections by the same localized obstacle, and found that the field associated with the point obstacles was linear in the scattering cross section S_0. In the treatment of plane reflectors in Section 8, our method did not ignore the multiple reflections and the resultant field was not linear in r, but varied as $r/(1-r)$. We shall here give a very rough argument to show that a more careful treatment of the point scatterer, taking into account the possibility of repeated reflection by the same obstacle, also leads to a resistivity which is non-linear in the scattering cross section S_0.

Consider the scattered current as given by Eq. (4.9). The z-component of the scattered current (measured in carriers per sec) is obtained by multiplying (4.9) by $\cos\theta_f$ and integrating over $d\Omega$. The resulting current has only a z-component given by $I_z = -S_0 i_\infty$. This scattered current consists of electrons moving away from the obstacle in a radial direction for a distance of about λ, where λ is the mean free path determined by the background scattering. After moving through this distance λ, the electrons have their velocity randomized and follow a diffusive motion. After this randomization a fraction of them will be scattered again by the original obstacle. This fraction is roughly $S_0/4\pi\lambda^2$.

The total current incident on the obstacle at any one time is due to electrons which are incident for the first time and also due to electrons which have previously been scattered by the obstacle one or more times. The scattered current, integrated over all directions, is therefore of the form

$$\begin{aligned} i_z &= S_0 i_\infty(1 + S_0/4\pi\lambda^2 + (S_0/4\pi\lambda^2)^2 + \ldots) \\ &= S_0 i_\infty/(1 - S_0/4\pi\lambda^2). \end{aligned} \tag{9.1}$$

The diffusion charges, N_D, and the resulting potential will then vary with S_0 as $S_0/(1-S_0/4\pi\lambda^2)$. This is comparable to the factor $r/(1-r)$ in the case of plane reflectors. It seems plausible, then, that in situations in which the mean free path is large enough so that multiple scatterings are negligible, we can expect the resistivity to vary linearly with scattering cross sections and can expect the usual formalism to be applicable. Thus, for example, in the case of highly localized, well separated cylindrical obstacles, we would expect that most of the carriers which are incident upon a given obstacle will be scattered only once by it, and that therefore the usual relations between resistance and scattering cross section are valid.

10. Conclusions

A detailed solution of the transport equation has shown that spatially localized scatterers produce spatially localized electric fields in the presence of current flow. In the case of point scatterers, these localized fields are dipole fields, one for each scatterer. The resistivity calculated on this basis

is the same as that given by the more usual calculations. The resistivity calculation has, however, been put on a more secure footing since the discussion that has been presented does not rely as intimately as the usual theory upon the acceleration law, $d\mathbf{k}/dt = -e\mathbf{E}/\hbar$, which has been proven only for uniform fields in strictly periodic crystals. In the case of a reflecting plane, the resistivity calculated from the localized fields is higher than that calculated from the usual equations, but the difference is significant only if the reflection coefficient is comparable to unity.

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Isomorphisms between the Batalin–Vilkovisky antibracket and the Poisson bracket

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One may introduce at least three different Lie algebras in any Lagrangian field theory: (i) the Lie algebra of local BRST cohomology classes equipped with the odd Batalin–Vilkovisky antibracket, which has attracted considerable interest recently; (ii) the Lie algebra of local conserved currents equipped with the Dickey bracket; and (iii) the Lie algebra of conserved, integrated charges equipped with the Poisson bracket. We show in this paper that the subalgebra of (i) in ghost number -1 and the other two algebras are isomorphic for a field theory without gauge invariance. We also prove that, in the presence of a gauge freedom, (ii) is still isomorphic to the subalgebra of (i) in ghost number -1, while (iii) is isomorphic to the quotient of (ii) by the ideal of currents without charge. In ghost number different from -1, a more detailed analysis of the local BRST cohomology classes in the Hamiltonian formalism allows one to prove an isomorphism theorem between the antibracket and the extended Poisson bracket of Batalin, Fradkin, and Vilkovisky.
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I. INTRODUCTION

The first appearance of an antibracket in the context of Lagrangian field theories can be traced back to the study of the renormalization of Yang–Mills theories when the Ward identities are expressed in terms of the generating functional for one-particle irreducible proper vertices.[1] This antibracket has been developed and generalized in the work of Batalin and Vilkovisky[2] on Lagrangian quantization methods for generic gauge theories. The Batalin–Vilkovisky formalism and the antibracket play, for instance, a fundamental role in the covariant formulation of string field theory.[3] It is therefore of interest to gain a better understanding of the physical significance of this antibracket.

We relate in this paper the Batalin–Vilkovisky antibracket at ghost number -1, both to the bracket introduced by Dickey[4] in the space of local currents, and to the Poisson bracket of conserved charges. More generally, we relate the Batalin–Vilkovisky antibracket for arbitrary values of the ghost number to the extended Poisson bracket appearing in the Hamiltonian formulation of the BRST theory.[5,6]

The paper is organized as follows. In the next section, we review the Batalin–Vilkovisky construction and show that the Batalin–Vilkovisky antibracket naturally induces a well-defined odd Lie bracket $\{\cdot,\cdot\}$ in the cohomolgy classes $H^{*,n}(s|d)$ of the BRST differential s modulo the exterior space–time differential d in form degree n. The algebra $(H^{*,n}(s|d), \{\cdot,\cdot\})$ possesses a subalgebra $\mathscr{S}$, namely $(H^{-1,n}(s|d), \{\cdot,\cdot\})$.

We then define the Dickey algebra of conserved currents j^μ (Sec. III) and show that it

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possesses an ideal, namely the ideal I of nontrivial conserved currents for which the charge $Q=\int d^{n-1}x\ j^0$ is zero on shell. Such currents are trivial (i.e., on shell equal to identically conserved currents) when there is no gauge freedom, so that I is effectively zero in that case. They may, however, be nontrivial otherwise. We introduce furthermore the Lie algebra of integrated conserved charges equipped with the covariant Poisson bracket induced by the Dickey bracket.

Isomorphism theorems between $\mathscr{S}$ and the other two Lie algebras in the case of nondegenerate field theories are proved in Sec. IV. The modification of these theorems for gauge theories are discussed in Sec. V. More precisely, we show that $\mathscr{S}$ is still isomorphic to the Dickey algebra, but this algebra itself is now isomorphic to the Lie algebra of conserved charges only after taking the quotient by the ideal I.

In Sec. VI, we investigate the antibracket map for an arbitrary ghost number. In order to do so, we go to the extended Hamiltonian formalism and use the fact that the local BRST cohomology group and the associated antibracket map are invariant under this change of description of the theory. The advantage of the Hamiltonian formulation is that the equations of motion are in normal form, which allows one to control the antifield dependence of the local BRST cohomology classes. We show that it is always possible to choose representatives that are, at most, linear in the antifields of the Hamiltonian description. This allows one to get the general relationship between the antibracket map and the extended Poisson bracket map of the Hamiltonian BRST formalism.

By applying these results to the case of ghost number -1, we find in particular that I is an Abelian subalgebra and corresponds to a subspace of the characteristic cohomology associated with the Hamiltonian constraint surface.

II. THE ANTIBRACKET MAP INDUCED IN LOCAL BRST COHOMOLOGY

In the Batalin–Vilkovisky formalism for gauge theories, which we consider for notational simplicity to be irreducible, one introduces, besides the original fields ϕ^i of ghost number 0 and the ghosts C^α of ghost number 1 related to the gauge invariance, the corresponding antifields ϕ^*_i and C^*_α of opposite Grassmann parity, and ghost number -1 and -2, respectively.[2,6] It is natural to define an antibracket by declaring that the fields $\phi^A\equiv(\phi^i,C^\alpha)$ and antifields ϕ^*_A are conjugate:

$$(\phi^A(x),\phi^*_B(y))=\delta^A_B\delta^n(x-y). \tag{1}$$

The antibracket is then given for arbitrary functionals A_1 and A_2 by

$$(A_1,A_2)=\int d^nx\left(\frac{\delta^R A_1}{\delta\phi^A(x)}\frac{\delta^L A_2}{\delta\phi^*_A(x)}-\frac{\delta^R A_1}{\delta\phi^*_A(x)}\frac{\delta^L A_2}{\delta\phi^A(x)}\right). \tag{2}$$

The central goal of the formalism is the construction of a proper solution to the master equation,

$$(S,S)=0. \tag{3}$$

The functional S is required to start like the classical action S_0, to which one couples through the antifields the gauge transformations with the gauge parameters replaced by the ghosts:

$$S=\int d^nx\ \hat{\mathscr{L}}=\int d^nx\ \hat{\mathscr{L}}_0+\phi^*_i R^i_\alpha C^\alpha+\cdots. \tag{4}$$

The BRST symmetry is canonically generated in the antibracket through the equation

$$s=(S,\cdot). \tag{5}$$

In order to analyze the properties of the antibracket, it is necessary to have a more precise definition of the functionals to which it applies. We will consider in the following only local functionals. A local functional,

$$A[z^a(x)]=\int_X d^n x\ \hat{a}[z^a], \quad z^a(x)\to 0, \quad \text{for } x\to \partial X, \tag{6}$$

is defined as the integral over an orientable domain X of space–time M^n of a local function $\hat{a}[z^a]$, i.e., a function ^{a} of x^μ, the fields and antifields $z^a \equiv (\phi^A, \phi^*_A)$, and their derivatives up to some finite order, evaluated for field and antifield histories $z^a(x)$, which appropriately vanish at the boundary ∂X. Note that X can be all of Minkowski space M^n, and that a local function corresponds to a function on the finite-dimensional ''jet space'' $M^n \times V^k$ with coordinates $x^\mu, \partial_{(\nu)} z^a, |\nu| \leqslant k$ (see Appendix A for more details). The space of local functionals so defined can be proved (see for instance Refs. 7, 6) to be isomorphic to the space of equivalence classes of local functions $\hat{a}$ modulo total divergences $\partial_\mu j^\mu$, for some arbitrary local current j^μ. The total derivative ∂_μ is defined in multi-index notation by

$$\partial_\mu = \frac{\partial^L}{\partial x^\mu} + \partial_{\mu(\nu)} z^a \frac{\partial^L}{\partial(\partial_{(\nu)} z^a)}. \tag{7}$$

Furthermore one can prove that a local function is a total divergence if and only if its Euler–Lagrange derivatives vanish (see, e.g., Ref. 7).

Turning to form notations, $\hat{a}\to a = d^n x\ \hat{a}$ and introducing the space–time exterior derivative $d = dx^\mu\ \partial_\mu$, the space of local functionals can be identified with the cohomology group $H^n(d)$ of the differential d in form degree n in the space of local, form-valued functions.

It is easy to verify that the antibracket of two local functionals is also a local functional. Thus the antibracket induces a well-defined map in the cohomology group $H^n(d)$,

$$\{\cdot,\cdot\}: H^n(d)\times H^n(d)\to H^n(d). \tag{8}$$

This bilinear map inherits from the antibracket the property of being a true, odd, Lie bracket. If we denote by $[a]$ the cohomological class of the n-form a in $H^n(d)$, one may view the antibracket in $H^n(d)$ as arising from a local antibracket in the space of local functions defined as follows:

$$\{\hat{a}_1, \hat{a}_2\} = \frac{\delta^R \hat{a}_1}{\delta \phi^A}\frac{\delta^L \hat{a}_2}{\delta \phi^*_A} - \frac{\delta^R \hat{a}_1}{\delta \phi^*_A}\frac{\delta^L \hat{a}_2}{\delta \phi^A}, \tag{9}$$

$$\{[a_1],[a_2]\} = [d^n x\{\hat{a}_1, \hat{a}_2\}]. \tag{10}$$

In (9), $\delta/\delta\phi^A$ is the Euler–Lagrange derivative defined by

$$\frac{\delta}{\delta \phi^A} = (-\partial)_{(\nu)} \frac{\partial}{\partial(\partial_{(\nu)}\phi^A)}, \tag{11}$$

with $(-\partial)_{(\nu)} = (-)^{|\nu|}\partial_{(\nu)}$. While the bracket (8) in $H^n(d)$ is a true bracket, the local antibracket (9) in the space of local functions is graded symmetric, but satisfies the graded Leibnitz rule and Jacobi identity only up to total divergences (see Appendix B).

It is clear that the antibracket for the integrands that gives rise to the antibracket in $H^n(d)$ is not unique, but expressions differing from the one in (9) by a total divergence are also admissible. This is the case, for instance, for the following expression (see Appendix B):

$$\{\hat{a}_1,\hat{a}_2\}_{\mathrm{alt}}=\partial_{(\nu)}\left(\frac{\delta^R\hat{a}_1}{\delta\phi^A}\right)\frac{\partial^L\hat{a}_2}{\partial(\partial_{(\nu)}\phi^*_A)}-\partial_{(\nu)}\left(\frac{\delta^R\hat{a}_1}{\delta\phi^*_A}\right)\frac{\partial^L\hat{a}_2}{\partial(\partial_{(\nu)}\phi^A)}, \tag{12}$$

which satisfies a graded Leibnitz rule in the second argument, but is only graded symmetric up to a total divergence.

In the Batalin–Vilkovisky formalism, one introduces additional fields, the ghosts and antifields. Quantities of direct physical interest are recovered by considering the cohomology classes of the BRST differential s. The identification of local functionals with the cohomology group $H^n(d)$ implies that the BRST cohomology for local functionals is given by $H^*(s,H^n(d))$. This last group is isomorphic to the relative cohomology group $H^{*,n}(s|d)$ of s modulo d in form degree n evaluated in the space of form-valued local functions. Due to the fact that the BRST symmetry acting on a local function is canonically generated through the formula

$$s\hat{a}=\{\hat{\mathscr{S}},\hat{a}\}_{\mathrm{alt}}, \tag{13}$$

it is straightforward[b] to verify that the local antibracket induces a well-defined odd Lie bracket in the relative cohomology group of s modulo d:

$$\{\cdot,\cdot\}:H^{g_1,n}(s|d)\times H^{g_2,n}(s|d)\to H^{g_1+g_2+1,n}(s|d),\{[a_1],[a_2]\}=[d^nx\{\hat{a}_1,\hat{a}_2\}]. \tag{14}$$

An inspection of the various possible cases shows that it is only for ghost number -1 that this map associates to two cohomology classes a cohomology class of the same type, i.e., of the same ghost number. The subspace $H^{-1,n}(s|d)$ equipped with the antibracket defines a subalgebra of $H^{*,n}(s|d)$, which we denote by $\mathscr{S}$,

$$\mathscr{S}=(H^{-1,n}(s|d),\{\cdot,\cdot\}). \tag{15}$$

III. THE DICKEY BRACKET

Let Σ_k be the stationary surface, i.e., the surface defined by the equations

$$\partial_{(\lambda)}\frac{\delta\hat{\mathscr{L}}_0}{\delta\phi^i}=0, \tag{16}$$

(with $|\lambda|\leqslant k-2$ for second-order equations) in the spaces $M^n\times F^k$ with coordinates x^μ, $\partial_{(\mu)}\phi^i$, $|\mu|\leqslant k$.

The vector space of (equivalence classes of) inequivalent Lagrangian conservation laws is defined by

$$\{j^\mu,\partial_\mu j^\mu\approx 0,\ \text{modulo the identification}\ j^\mu\sim|_\Sigma\, j^\mu+\partial_\nu S^{[\nu\mu]}\}, \tag{17}$$

where the j^μ are local functions. In form notation, we get equivalence classes $[j]$ of $n-1$ forms whose pullback to the stationary surface is d closed, where two such forms have to be identified if they differ by the exterior derivative of an $n-2$ form on the stationary surface:

$$[j]\in H^{n-1}(d^*,\Omega(\Sigma)). \tag{18}$$

Inequivalent conserved currents belong, by definition, to the so-called characteristic cohomology of the stationary surface in form degree $n-1$.

The standard regularity conditions are that locally in the jet space, the equations $\delta\hat{\mathscr{L}}_0/\delta\phi^i$ and their derivatives can be split into two groups: the ''independent equations,'' which can be taken locally as a new coordinate system on the jet space, replacing some of the fields and their

derivatives; and the ''dependent equations'' which hold as a consequence of the independent ones. One then can prove[7,6] that a function that vanishes on the stationary surface can be written as a linear combination of the equations defining the surface, hence

$$\partial_\mu j^\mu = X^{i(\lambda)} \partial_{(\lambda)} \frac{\delta \hat{\mathscr{L}}_0}{\delta \phi^i}, \tag{19}$$

for some local functions $X^{i(\lambda)}$. This equation does not determine $X^{i(\lambda)}$ completely, one is, for instance, free to add functions of the form

$$Y^{i(\lambda)j(\nu)} \partial_{(\nu)} \frac{\delta \hat{\mathscr{L}}_0}{\delta \phi^j}, \tag{20}$$

with Y antisymmetric under the exchange of the pairs $i(\lambda)$ and $j(\nu)$[c].

The characteristic[7,4] of the equivalence class of conservation laws described by $[j]$ is defined by the equivalence class of local functions of the form $X^i = (-\partial)_{(\lambda)} X^{i(\lambda)}$, where two sets X^i's of local functions have to be identified if they differ by a function of the form

$$(-\partial_{(\lambda)}) \left[Y^{i(\lambda)j(\nu)} \partial_{(\nu)} \frac{\delta \hat{\mathscr{L}}_0}{\delta \phi^j} \right]. \tag{21}$$

It is straightforward to verify that the characteristic does not depend on the choice of the representative for j^μ. Let δ_X be the evolutionary vector field defined by X^i:

$$\delta_X = \partial_{(\lambda)} X^i \frac{\partial}{\partial(\partial_{(\lambda)} \phi^i)}. \tag{22}$$

Note that X^i and δ_X satisfy the equations

$$X^i \frac{\delta \hat{\mathscr{L}}_0}{\delta \phi^i} = \partial_\mu j'^\mu, \quad \delta_X \hat{\mathscr{L}}_0 = \partial_\mu j''^\mu, \tag{23}$$

with j'^μ, j''^μ in the same equivalence class as j. This means that the characteristics define variational symmetries, i.e., symmetries of the action. In the nondegenerate case, one can then prove directly that there is a one to one correspondence between inequivalent symmetries of the action and inequivalent conservation laws (Noether's theorem),[7] but we will not do so here because it is also a direct consequence of our analysis in the next section.

The Dickey bracket in the space of inequivalent conservation laws (17) is defined by[4]

$$\{[j_1],[j_2]\}_D = -[\delta_{X_1} j_2]. \tag{24}$$

By using properties of the Euler–Lagrange derivatives, one finds the following equivalent expressions (see Ref. 4 and Appendix B):

$$\begin{aligned}\{[j_1],[j_2]\}_D = [\delta_{X_2} j_1] &= \frac{1}{2}[\delta_{X_2} j_1 - \delta_{X_1} j_2] \\ &= \left[-\frac{(\tilde{\nu})_{\mu_1}+1}{|\nu|+1} \partial_{(\nu)} \left[\delta_{X_2} \left(\frac{\delta \hat{\mathscr{L}}_0}{\delta(\partial_{(\nu)\mu_1}\phi^i)} \right) X_1^i - \delta_{X_1} \left(\frac{\delta \hat{\mathscr{L}}_0}{\delta(\partial_{(\nu)\mu_1}\phi^i)} \right) X_2^i \right] \right. \\ &\quad \left. \times \frac{1}{(n-1)!} \epsilon_{\mu_1 \cdots \mu_n} dx^{\mu_2} \cdots dx^{\mu_n} \right],\end{aligned} \tag{25}$$

where $(\tilde{\nu})_\mu$ denotes the number of occurrences of μ in the multi-index (ν). This last expression corresponds to the contraction of the horizontal $(n-1)$ and vertical 2 form,

$$\Omega = \frac{1}{(n-1)!}\,\epsilon_{\mu_1\cdots\mu_n}\,dx^{\mu_2}\cdots dx^{\mu_n}\,\frac{(\tilde{\nu})_{\mu_1}+1}{|\nu|+1}\,\partial_{(\nu)}\left[d_V\left(\frac{\delta\hat{\mathscr{L}}_0}{\delta(\partial_{(\nu)\mu_1}\phi^i)}\right)d_V\phi^i\right], \tag{26}$$

with the evolutionary vector fields δ_{X_1} and δ_{X_2}. This formula involves the vertical derivatives and the higher-order Euler operators defined, for instance, in Refs. 7, 4 (see also Appendices A and B).

Again, in the nondegenerate case, one can prove directly that the Dickey bracket is a well-defined Lie bracket in the space of inequivalent conserved currents (see Ref. 4); namely, it is unambiguous in the quotient space, antisymmetric, and satisfies the Jacobi identity. Alternatively, these properties follow from the isomorphism theorem proved in the next section.

Among the conserved currents, one may distinguish those for which j^0 is trivial, i.e. of the form $j^0 \approx \partial_m S^{m0}$. The corresponding Noether charge $Q=\int d^{n-1}x\; j^0$ is zero on the stationary surface. These currents form an ideal for the Dickey bracket since $\delta_X j^0$ is trivial if j^0 is trivial. We call this ideal the ideal of ''conserved currents without charge'' and we denote it by I.

As we shall show in the next section, the ideal I is trivial in the absence of gauge symmetry. That is, if a conserved current has a vanishing Noether charge, then, it is trivial, i.e., on shell equal to an identically conserved current. But this may not be so in the presence of gauge freedom, for which there exist nontrivial currents in I.

The third algebra that we shall introduce is the algebra of conserved, integrated charges, $Q=\int d^{n-1}x\; j^0$, $\partial_0 j^0 \approx -\partial_k j^k$ for some spatial current j^k, with the identification of two such charges if they agree on the stationary surface. By using the Hamiltonian formalism, one may equip this algebra with a well-defined even bracket, namely, the standard Hamiltonian Poisson bracket. We denote this algebra by $\mathscr{Q}$. It is clear that $\mathscr{Q}$ is isomorphic as a vector space to the quotient of the space of conserved currents by the ideal I. We shall prove furthermore that the Poisson bracket is just the corresponding induced Dickey bracket.

IV. ISOMORPHISMS IN THE CASE OF NONDEGENERATE LAGRANGIAN FIELD THEORY

In the absence of gauge invariance, the only additional fields in the Batalin–Vilkovisky construction besides the original ϕ^i, which we assume for simplicity to be bosonic, are the antifields ϕ_i^*. The original action $S[\phi^i]=\int d^n x\;\hat{\mathscr{L}}_0[\phi^i]$ is by itself a proper solution of the master equation generating the BRST symmetry,

$$s\phi_i^* = \frac{\delta\hat{\mathscr{L}}_0}{\delta\phi^i}, \quad s\phi^i = 0, \quad s\partial_\mu = \partial_\mu s, \tag{27}$$

which reduces to the so-called Koszul–Tate differential δ.[6] In the nondegenerate case, the equations of motion and their derivatives can be taken locally as first coordinates in a new coordinate system replacing some of the fields and their derivatives. One can prove[6] that the BRST cohomology in the spaces $C^\infty(\mathbf{R}^n\times F^k)\times\mathbf{R}[\partial_{(\nu)}\phi_i^*]$ (with $|\nu|\leqslant k-2$ for second-order equations) is given by smooth functions defined on the stationary surface[d]: $H^0(\delta)\simeq C^\infty(\mathbf{R}^n\times\Sigma^k)$ and $H^g(\delta)=0$, $g\neq 0$.

In the new coordinate system, where the equations and their derivatives are taken as new coordinates, we denote by $I_0=\{x_a\}$ the set of fields and their derivatives needed to complete the coordinate system. Let us assume that the nondegenerate theory is of Cauchy order 1, meaning that $\partial_k x_a \in I_0$ for $k\geqslant 1$. One can then prove[8] that, apart from $H^{0,n}(s|d)$, which corresponds to local functionals defined on the stationary surface, the only nontrivial local BRST cohomology classes are in ghost number -1 and form degree n.

By integrations by parts, the representatives of $H^{-1,n}(s|d)$ can be assumed to be of the characteristic form

$$a = d^n x \ \phi_i^* X^i[\phi^i], \tag{28}$$

for local functions X^i. The cocycle condition reads as

$$\frac{\delta \hat{\mathscr{L}}_0}{\delta \phi^i} X^i = \partial_\mu j^\mu, \tag{29}$$

and implies that the field variation $\delta\phi^i = X^i$ defines a variational symmetry. Furthermore, to a trivial representative of $H^{-1,n}(s|d)$ corresponds to a variational symmetry that is given by an ''antisymmetric'' combination of the equations of motions as in (21)[e]. The space $H^{-1,n}(s|d)$ is accordingly given by inequivalent variational symmetries or characteristics of inequivalent conservation laws[f].

The local antibracket map for such representatives of $H^{-1,n}(s|d)$ is given by

$$\begin{aligned} &\{[d^n x \ \phi_i^* X_1^i],[d^n x \ \phi_i^* X_2^i]\} = [d^n x \ \phi_i^*[X_1, X_2]_L^i], \\ &[X_1, X_2]_L^i = \frac{\partial X_1^i}{\partial \phi_{(\mu)}^j} \partial_{(\mu)}(X_2^j) - \frac{\partial X_2^i}{\partial \phi_{(\mu)}^j} \partial_{(\mu)}(X_1^j) = \delta_{X_2} X_1^i - \delta_{X_1} X_2^i . \end{aligned} \tag{30}$$

Hence we find that, in ghost number -1, the local antibracket map corresponds to the traditional, even Lie bracket for inequivalent variational symmetries under characteristic form given in Ref. 7. Since the Lie bracket for evolutionary vector fields is induced by the commutator for vector fields, we get the following.

Theorem 1: *The odd Lie algebra* $\mathscr{S} = (H^{-1,n}(s|d), \{\cdot,\cdot\})$ *is isomorphic to the algebra of inequivalent variational symmetries equipped with the bracket induced by the commutator for vector fields.*

Using the acyclicity of $s = \delta$[6] at negative ghost numbers and the triviality of the cohomology of d in form degree $p < n$ [$H^p(d) = \delta_0^p \mathbf{R}$, see, e.g., Ref. 7], we can easily prove the isomorphism

$$H^{-1,n}(\delta|d) \simeq H^{n-1,0}(d|\delta)/\delta_1^n \mathbf{R}. \tag{31}$$

This follows from a general relationship for relative cohomology groups proved in Ref. 9. The last space corresponds to the space of inequivalent conserved currents. Indeed, the cocycle condition implies that representatives must be $n-1$ forms, which restrict to closed forms on the stationary surface, while the coboundary condition requires two such currents to be considered as equivalent if they differ on this surface by the exterior derivative of an $n-2$ form, i.e., the divergence of a ''superpotential'' in dual notation, or by a constant in one dimension.

The above isomorphism is explicitly given by associating to a representative a of the first space the representative j of the second space in the equation $sa + dj = 0$. Furthermore, the antibracket map induces through this isomorphism a well-defined Lie bracket in the space of inequivalent conserved currents. An explicit calculation (Appendix B) shows that the corresponding bracket is just given by the Dickey bracket. Hence the following holds.

Theorem 2: *The odd Lie algebra* $\mathscr{S}$ *is isomorphic to the space of inequivalent conservation laws equipped with the Dickey bracket.*

There is no contradiction in the fact that the isomorphism relates an odd bracket to an even bracket, because there is at the same time a shift in the degree [from odd (-1) to even (0)].

Combining theorems 1 and 2, we get the full Noether theorem.

Corollary 1: There is a Lie algebra isomorphism between inequivalent conservation laws and inequivalent variational symmetries.

The ideal I of currents without charge is trivial. Indeed, the coboundary condition allows us to take all the j^k to depend on the x_a alone. Because $\partial_k x_a$ depends also on x_a and not on equations of motion, one must have $\partial_k j^k=0$ identically, which implies that $j^k=\delta_2^n \mathbf{R}+\partial_m S^{[mk]}$. Hence, the Dickey algebra and the space of inequivalent, integrated conserved charges are isomorphic as vector spaces. That the induced Dickey bracket in the space $\mathcal{Q}$ corresponds to the Poisson bracket in $\mathcal{Q}$ in the Hamiltonian formalism is a consequence of the analysis in Sec. VI. Alternatively, it could be proved directly along the lines of Ref. 10, by taking, furthermore, locality into account. Hence the following is true.

Theorem 3: *In dimensions different from 2, if the theory is of Cauchy order 1, the Dickey algebra of inequivalent conserved currents is isomorphic to the algebra of inequivalent conserved charges equipped with the Poisson bracket.*

V. GAUGE THEORIES. GHOST NUMBER −1

The advantage of the cohomological reformulation of Noether's theorem in Eq. (31) is that one can extend this theorem in a straightforward way to gauge theories, which are not covered by the analysis in Refs. 7, 4. One can prove[8] that the subalgebra $\mathcal{S}$ is isomorphic to the algebra $\mathcal{R}=(H_1^n(\delta|d),\{\cdot,\cdot\}_R)$, where the cohomology group $H_1^n(\delta|d)$ involves only the original fields and the antifields, but no ghosts, δ being the Koszul–Tate part of s and the degree of δ the antighost number, which is minus the ghost number (for a function that does not involve the ghosts). The restricted antibracket map $\{\cdot,\cdot\}_R$ is the antibracket map restricted to the original fields ϕ^i and the antifields ϕ_i^*.

The differential δ acts nontrivially on the antifields of higher order. In the case of irreducible gauge theories, its action on C_a^* is given by

$$\delta\ \partial_{(\lambda)} C_a^* = \partial_{(\lambda)}[R_a^{+i(\nu)}\ \partial_{(\nu)}\phi_i^*], \tag{32}$$

where the operators $R_a^{+i(\nu)}\partial_{(\nu)}$ define the Noether identities of the theory, i.e.,

$$R_a^{+i(\nu)}\partial_{(\nu)}\ \frac{\delta \hat{\mathscr{L}}_0}{\delta \phi^i}=0. \tag{33}$$

This additional piece maintains $\delta^2=0$ and guarantees that δ still defines a homological resolution of the functions defined on the constraint surface, implying for instance that Eq. (31) still holds.

If we still want Theorem 1 to hold, the definition of δ requires that we change the notion of a trivial variational symmetry; they have to correspond to X^i's that are ''antisymmetric'' combinations of the equations of motion up to a gauge transformation, where the gauge parameters are replaced by arbitrary local functions:

$$X^i=(-\partial)_{(\lambda)}\left[Y^{i(\lambda)j(\nu)}\partial_{(\nu)}\ \frac{\delta \hat{\mathscr{L}}_0}{\delta \phi^j}\right]+R_a^{i(\nu)}\ \partial_{(\nu)}f^a. \tag{34}$$

The operators $R_a^{i(\nu)}\partial_{(\nu)}$ are the adjoints of the operators defining the Noether identities and define the gauge transformations.

With this modification of the space of inequivalent variational symmetries, Theorems 1, 2 and Corollary 1 hold, as in the case with no gauge invariance.

The ideal I, however, is not trivial in the case of gauge theories, because the theory is no longer of Cauchy order 1. For instance, the current $j^\mu=F^{0\mu}=(0,F^{0k})$ in free Maxwell's theory belongs to I since $\int j^0\ d^{n-1}x=0$, but $F^{0k}\neq\partial_m S^{[km]}$ (even weakly). Theorem 3 becomes the following.

Theorem 4: *The Dickey algebra of conserved currents modulo the ideal I is isomorphic to the algebra of inequivalent conserved charges equipped with the Poisson bracket*.

The proof that the induced Dickey bracket is, in fact, the ordinary Poisson bracket in the Hamiltonian formalism again follows from the reasoning given in the next section.

VI. GAUGE THEORIES. GENERAL ANALYSIS

The previous theorems relate the antibracket and the Poisson bracket at particular values of the ghost number. In order to fully prove them, we shall first put them in a more general setting. Indeed, these theorems can be extended to arbitrary values of the ghost number.

To relate the antibracket and the Poisson bracket for all values of the ghost number, one first uses the invariance of the local BRST cohomology group with respect to the introduction of auxiliary fields and generalized auxiliary fields, as shown in Ref. 8. One proves by an analoguous reasoning that the same is true for the antibracket map induced in cohomology. This implies that one can go to the total Hamiltonian formalism and then to the extended Hamiltonian formalism, which we will assume to be local,[6] and describe the solution of the master equation in terms of the Batalin–Fradkin–Vilkovisky framework.

Let us recall that in this framework, a central object is the extended Poisson bracket $[\cdot,\cdot]_{\mathrm{P}}$ for which the ghosts C^a and the ghost momenta $\mathscr{P}_b$ are considered as conjugate dynamical variables, in addition to the usual fields and their momenta. One then constructs out of the constraints, which we assume for simplicity to be irreducible and first class, the BRST charge $\Omega=\int d^{n-1}x\ \omega$, which is a local functional in space verifying $[\Omega,\Omega]_{\mathrm{P}}=0$. The Hamiltonian $H=\int d^{n-1}x\ h$ verifying $[\Omega,H]_{\mathrm{P}}=0$ is also a local functional in space and these two functionals depend only on the fields $\tilde{\phi}^A\equiv\phi^i,\pi_j,C^a,\mathscr{P}_b$ and their spatial derivatives.

The functionals in space are replaced by spatial functions in the same way as in the space–time case, which leads to a local extended Poisson bracket $\{\cdot,\cdot\}_{\mathrm{P}}$ defined through spatial Euler Lagrange derivatives. The BRST charge Ω generates the symmetry $s_\omega=\{\omega,\cdot\}_{\mathrm{P,alt}}$, where $\{\cdot,\cdot\}_{\mathrm{P,alt}}$ is defined in a way analoguous to $\{\cdot,\cdot\}_{\mathrm{alt}}$ in (12). The local extended Poisson bracket induces a well-defined even Lie bracket, the Poisson bracket map, in the cohomology group of s_ω modulo the spatial exterior derivative $\tilde{d}$.

The symmetry s_ω is only a part of the BRST symmetry, which is isomorphic to the BRST symmetry of the initial Lagrangian system through the elimination of (generalized) auxiliary fields. The complete BRST symmetry is generated through the solution of the master equation in the extended Hamiltonian formalism given by[11,6]

$$S_{\mathrm{H}}[\tilde{\phi}^A,\tilde{\phi}^*_A]=\int dt\ d^{n-1}x\left(-\frac{1}{2}\,\dot{\tilde{\phi}}^A(\sigma^{-1})_{AB}\tilde{\phi}^B-h-\{\tilde{\phi}^*_A\tilde{\phi}^A,\omega\}_{\mathrm{P,alt}}\right),\tag{35}$$

where we have introduced the notation

$$\sigma^{AB}=\begin{pmatrix}0&0&\delta^i_j&0\\0&0&0&-\delta^a_b\\-\delta^i_j&0&0&0\\0&-\delta^a_b&0&0\end{pmatrix}.\tag{36}$$

Explicitly, the BRST symmetry $s_{\mathrm{H}}=\{S_{\mathrm{H}},\cdot\}_{\mathrm{alt}}$ reads as

$$s_{\mathrm{H}}=\partial_{(\mu)}\left(\frac{\tilde{\delta}^R\omega}{\delta\tilde{\phi}^A}\right)\sigma^{AB}\,\frac{\partial^L}{\partial(\partial_{(\mu)}\tilde{\phi}^B)}+\partial_{(\mu)}\mathscr{L}_A\,\frac{\partial^L}{\partial(\partial_{(\mu)}\tilde{\phi}^*_A)},\tag{37}$$

where the tilded Euler–Lagrange derivatives are restricted to spatial derivatives only and

$$\mathscr{L}_A \equiv -\dot{\widetilde{\phi}}^B (\sigma^{-1})_{BA} - \frac{\widetilde{\delta}^R h}{\delta \widetilde{\phi}^A} - \frac{\widetilde{\delta}^R}{\delta \widetilde{\phi}^A} (\{\widetilde{\phi}^*_B \widetilde{\phi}^B, \omega\}_{\mathrm{P,alt}}). \tag{38}$$

Note that in the proper solution S_{H} to the master equation in the extended Hamiltonian formalism, we have made the identification of minus the antifields $-\lambda^*_a$ of the Lagrange multipliers for the first class constraints with the ghost momenta $\mathscr{P}_a$. This implies that in terms of the new antifields, the Koszul–Tate part is now associated to the surface $\mathscr{L}_A(\widetilde{\phi}^*=0)=0$ and not with the gauge-invariant, original, Hamiltonian equations of motion. The part in resolution degree 0, the resolution degree being the degree associated to the Koszul–Tate differential,[6] with respect to the *new* antifields, is given by

$$\gamma = s^0_\omega - \partial_{(\mu)} \frac{\widetilde{\delta}^R}{\delta \widetilde{\phi}^A} (\{\widetilde{\phi}^*_B \widetilde{\phi}^B, \omega\}_{\mathrm{P,alt}}) \frac{\partial L}{\partial(\partial_{(\mu)} \phi^*_A)}, \tag{39}$$

and the BRST differential has no contributions in higher resolution degree, contrary to what may happen in the old resolution degree. Here, s^0_ω is defined by the first term on the right-hand side of Eq. (37) and coincides with s_ω when acting on a function involving no time derivatives of the fields. Evaluating the action of $s^{(0)}_\omega$ on ϕ^i, π_j and putting to zero the ghost momenta $\mathscr{P}_a$ reproduces the gauge transformations of these fields with gauge parameters replaced by the ghosts C^a.

One then investigates the local BRST cohomology groups $H(s_{\mathrm{H}}|d)$. A first step is the following theorem.

Theorem 5: *The ordinary BRST cohomology depending on the fields ϕ^A, the antifields ϕ^*_A, and their derivatives is isomorphic to the cohomology of s_ω depending on the fields $\widetilde{\phi}^A$ and their spatial derivatives*:

$$H(s, [\phi^A, \phi^*_A]) \simeq H(s_{\mathrm{H}}, [\widetilde{\phi}^A, \widetilde{\phi}^*_A]) \simeq H(s_\omega, [\widetilde{\phi}^A]). \tag{40}$$

In other words, in a s_{H} cocycle, one can get rid of the temporal derivatives and of the antifields through the addition of a s_{H} coboundary. For a proof of this theorem, see Appendix C.

Starting from the bottom of the descent equations, one then proves (see again Appendix C) that a nontrivial cocycle modulo d, a, $s_{\mathrm{H}} a + db = 0$, given by $a = \widetilde{a} + dt\, a^0$, where $\widetilde{a}$ does not involve the differential dt, can be characterized by

$$a = dt(-\{\widetilde{\phi}^*_A \widetilde{\phi}^A, \widetilde{b}_0\}_{\mathrm{P,alt}} + a^0_0) + \widetilde{a}_0, \tag{41}$$

verifying

$$s_\omega \widetilde{a}_0 + \widetilde{d} \widetilde{b}_0 = 0, \tag{42}$$

$$s_\omega a^0_0 + \widetilde{d} b^0_0 - \frac{\partial}{\partial t} \widetilde{b}_0 + \{h, \widetilde{b}_0\}_{\mathrm{P,alt}} = 0. \tag{43}$$

Here, $\widetilde{a}_0$, $\widetilde{b}_0$, a^0_0, and b^0_0 contain no antifields and no time derivatives of the fields, while $\widetilde{b}_0$ and b^0_0 satisfy analoguous equations to $\widetilde{a}_0$ and a^0_0 for some $\widetilde{m}_0$, m^0_0. In maximum form degree n, there is, of course, no $\widetilde{a}$ and at the bottom, say n, of the descent equations, $\widetilde{n}_0$ and n^0_0 are s_ω cocycles[g].

In the coboundary condition for such cocycles $a = s_{\mathrm{H}} c + de$, we have

$$c = dt(-\{\widetilde{\phi}^*_A \widetilde{\phi}^A, \widetilde{e}_0\}_{\mathrm{P,alt}} + e^0_0) + \widetilde{a}_0, \tag{44}$$

giving the conditions

$$\tilde{a}_0 = s_\omega \tilde{c}_0 + \tilde{d}\tilde{e}_0, \tag{45}$$

$$a_0^0 = -s_\omega c_0^0 - \tilde{d}e_0^0 + \frac{\partial}{\partial t}\tilde{e}_0 - \{h, \tilde{e}_0\}_{\mathrm{P,alt}}, \tag{46}$$

where $\tilde{c}_0$, $\tilde{e}_0$, c_0^0, and e_0^0 again contain no antifields and no time derivatives of the fields, with analogous equations holding for $\tilde{b}_0$, b_0^0 in terms of $\tilde{e}_0$, e_0^0, $\tilde{f}_0$, f_0^0. In maximum form degree, there is no $\tilde{a}$, $\tilde{c}$ and Eq. (45) is trivially satisfied.

In order to characterize the local BRST cohomology groups $H^{g,k}(s_{\mathrm{H}}|d)$, one can first find a basis for the vector space $H^{g,k}(s_\omega|\tilde{d})$ in the space of antifield and time derivative-independent local forms with only spatial differentials (the most general nontrivial solution for $\tilde{a}_0$). One then finds a basis for $H^{g+1,k-1}(s_\omega|\tilde{d})$ (the most general nontrivial solution for $\tilde{b}_0$). One finally considers the subspace $l[H^{g+1,k-1}(s_\omega|\tilde{d})]$ for which Eq. (43) admits a particular solution $a_{0\mathrm{P}}^0$. The general nontrivial form for a_0^0 is then given by $a_0^0 = a_{0\mathrm{P}}^0 + \overline{a_0^0}$, where $\overline{a_0^0}$ belongs to $r[H^{g,k-1}(s_\omega|\tilde{d})]$, which is the subspace of $H^{g,k-1}(s_\omega|\tilde{d})$ remaining nontrivial under the more general coboundary condition (46).

We thus get the following result on the relationship between the local BRST cohomology groups in Lagrangian and Hamiltonian formalism.

Theorem 6: *The local BRST cohomology groups are isomorphic to the direct sum of the following three local cohomology groups of the Hamiltonian formalism:*

$$H^{g,k}(s|d) \simeq H^{g,k}(s_{\mathrm{H}}|d) \simeq H^{g,k}(s_\omega|\tilde{d}) \oplus l[H^{g+1,k-1}(s_\omega|\tilde{d})] \oplus r[H^{g,k-1}(s_\omega|\tilde{d})]. \tag{47}$$

Note that in maximal form degree n, the first group of the last expression vanishes. This decomposition is, in general, quite difficult to achieve in practice since it requires the resolution of complicated equations. However, it corresponds to the natural resolution of the spatiotemporal descent equations in the Hamiltonian formalism, and it is useful, in principle, since it enables one to relate the bracket and the antibracket.

Remark: The groups with prefix r and l appear also in the covariant analysis of the descent equations in the following way. The descent equations provide a homomorphism $\mathscr{D}: H^{g,k}(s|d) \to H^{g+1,k-1}(s|d)$ with $\mathscr{D}[a] = [b]$ for $sa + db = 0 (\to sb + dc = 0)$. The kernel of $\mathscr{D}$ can easily be shown to consist of the vector space $H^{g,k}(s)$ seen as a subspace of $H^{g,k}(s|d)$, i.e., the equivalence classes of s-cocycles, with the equivalence relation determined by s modulo d exactness. We denote this kernel by $r[H^{g,k}(s)]$.

The image of $\mathscr{D}$ is given by the classes $[b] \in H^{g+1,k-1}(s|d)$, which can be lifted, i.e., such that there exists a with $sa + db = 0$. We denote this space by $l[H^{g+1,k-1}(s|d)]$.

This implies the isomorphism

$$H^{g,k}(s|d) \simeq l[H^{g+1,k-1}(s|d)] \oplus r[H^{g,k}(s)], \tag{48}$$

and, by iteration,

$$H^{g,k}(s|d) \simeq \oplus_{i=0}^{k} l^i r[H^{g+i,k-i}(s)], \tag{49}$$

where in the last space ($i = k$) one can forget the r, because there are no d exact terms in form degree 0. Note that since $H^0(d) = \mathbf{R}$, if $g = -k$, the last space has to be replaced by the space $\{e, se = c, e \sim e + sf + c'; c, c' \in \mathbf{R}\}$, which is isomorphic to $H^0(s)/\mathbf{R}$.

In the Hamiltonian case above, we consider only the part of the descent equations involving the exterior derivative with respect to time: $d^0 = dt(d/dt)$. □

We now use Theorem 6 to derive information on the antibracket from the Poisson bracket induced in $H(s_\omega|\tilde{d})$. On the representatives of the local BRST cohomology groups determined by Eqs. (41)–(46), the local antibracket gives

$$\{\hat{a}_1,\hat{a}_2\}=\{\widetilde{\phi}^*_A\widetilde{\phi}^A,\{\hat{\widetilde{b}}_1,\hat{\widetilde{b}}_2\}_{\mathrm{P}}\}_{\mathrm{P,alt}}-\{\hat{a}^0_1,\hat{\widetilde{b}}_2\}_{\mathrm{P}}-(-)^{\epsilon_{\hat{\widetilde{b}}_1}}\{\hat{\widetilde{b}}_1,\hat{a}^0_2\}_{\mathrm{P}}. \tag{50}$$

Hence, (i) the antibracket map can be entirely rewritten in terms of the local Poisson bracket; and (ii) it is nontrivial only if $l[H^{*,n-1}(s_\omega|\widetilde{d})]$ is nontrivial.

More precisely, according to the split of $H^{*,n}(s|d)$ in (47) to which corresponds the split of a^0 into a^0_{P} and $\overline{a_0}$, we see that the antibracket map (14) is completely determined by the local Poisson bracket map induced in

$$\{\cdot,\cdot\}_{\mathrm{P}}:l[H^{g_1+1,n-1}(s_\omega|\widetilde{d})]\times l[H^{g_2+1,n-1}(s_\omega|\widetilde{d})]\to l[H^{g_1+g_2+2,n-1}(s_\omega|\widetilde{d})], \tag{51}$$

and by the local Poisson bracket map in

$$\{\cdot,\cdot\}_{\mathrm{P}}:l[H^{g_1+1,n-1}(s_\omega|\widetilde{d})]\times r[H^{g_2,n-1}(s_\omega|\widetilde{d})]\to r[H^{g_1+g_2+1,n-1}(s_\omega|\widetilde{d})]. \tag{52}$$

Hence the antibracket map is determined by the following matrix in maximum spatial form degree $n-1$:

$$\begin{pmatrix} \{l[H^{g_1+1}(s_\omega|\widetilde{d})],l[H^{g_2+1}(s_\omega|\widetilde{d})]\}_{\mathrm{P}} & (-)^{\epsilon_{g_1+1}}\{l[H^{g_1+1}(s_\omega|\widetilde{d})],r[H^{g_2}(s_\omega|\widetilde{d})]\}_{\mathrm{P}} \\ \{r[H^{g_1}(s_\omega|\widetilde{d})],l[H^{g_2+1}(s_\omega|\widetilde{d})]\}_{\mathrm{P}} & 0 \end{pmatrix}. \tag{53}$$

Equations (52) and (53) mean, in particular, that $r[H^{*,n-1}(s_\omega|\widetilde{d})]$ is an abelian subalgebra and an ideal in the odd Lie algebra $(H^{*,n}(s|d),\{\cdot,\cdot\})$. We have thus proved the following.

Theorem 7: *The odd Lie algebra* $(H^{*,n}(s|d),\{\cdot,\cdot\})$ *is isomorphic to the semidirect sum of the Abelian Lie algebra* $r[H^{*,n-1}(s_\omega|d)]$ *and the Lie algebra* $(l[H^{*,n-1}(s_\omega|d)],\{\cdot,\cdot\}_{\mathrm{P}})$, *where the action of* $l[H^{*,n+1}(s_\omega|\widetilde{d})]$ *on* $r[H^{*,n-1}(s_\omega|d)]$ *is determined by the Poisson bracket map from one space to the other. By taking the quotient, the following isomorphism is seen to hold:*

$$(H^{*,n}(s|d)/r[H^{*,n-1}(s_\omega|\widetilde{d})],\{\cdot,\cdot\})\simeq(l[H^{*,n-1}(s_\omega|\widetilde{d})],\{\cdot,\cdot\}_{\mathrm{P}}). \tag{54}$$

The consequences of this result in the particular case of conserved currents, i.e., for $g_1=g_2=-1$, $k=n$ are as follows. Using the results of Ref. 8 in both the Lagrangian and the Hamiltonian context, the isomorphism (47) means:

(i) The space of inequivalent Lagrangian conservation laws not belonging to I is isomorphic to the subspace of spatial local functionals in the coordinates and momenta, defined on the constraint surface $\widetilde{\Sigma}$ and gauge invariant on this surface, whose Poisson bracket with the first class Hamiltonian $\widetilde{H}_0$ plus the explicit time derivative vanishes on the constraint surface,

$$\left\{ Q=\int_{t=t_0}\widetilde{b}_0[\phi^i\pi_j]\equiv\int_{t=t_0}d^1x\cdots d^{n-1}x\ \widetilde{j}^0[\phi^i\pi_j],\right.$$
$$\left.[Q,H_0]_{\mathrm{P}}+\frac{\partial}{\partial t}Q=0|_{\widetilde{\Sigma}},Q\sim Q|_{\widetilde{\Sigma}}\right\}, \tag{55}$$

(ii) The space of inequivalent Lagrangian conservation laws belonging to I is isomorphic to a subspace of the characteristic cohomology of the constraint surface in spatial form degree $(n-1)-1$, the space of conservation laws associated to the constraint surface, where two such conservation laws have to be considered to be equivalent if they differ on the constraint surface by a spatial superpotential and the total time derivative of a spatial current,

$$\left\{\widetilde{j}^k,\partial_k\widetilde{j}^k=0|_{\widetilde{\Sigma}},\widetilde{j}^k\sim|_{\widetilde{\Sigma}}\widetilde{j}^k+\partial_j\widetilde{S}^{[jk]}+\frac{\partial}{\partial t}\widetilde{f}^k-\{h_0,\widetilde{f}^k\}_{\mathrm{P,al}}\right\}. \tag{56}$$

For example, the current corresponding to the Lagrangian current $j^\mu = F^{0\mu}$ is given by the momenta π^k in the case of electromagnetism.

The semidirect sum structure holds also for the Lagrangian Dickey algebra, but furthermore, we get from (53) that (i) the algebra of inequivalent conserved charges $\mathcal{Q}$ equipped with the induced Dickey bracket corresponds to the ordinary Poisson bracket algebra of conserved inequivalent charges in the Hamiltonian formalism; and (ii) that the ideal I of conserved currents without charge forms an Abelian subalgebra.

VII. CONCLUSION

We have shown what is the precise relationship between the antibracket map and various Lie algebras existing for local gauge field theories. In the case of conserved currents, where ''covariant'' Poisson brackets are known, a direct comparison has been given.

In the general case, the antibracket map is related to the Poisson bracket of the canonical formalism. The core of this analysis is the relationship of the local BRST cohomologies in the Lagrangian and the Hamiltonian formalisms (i.e., the cohomologies modulo d in the Lagrangian case and modulo $\tilde{d}$ in the Hamiltonian one). This relationship turns out to be somewhat more subtle than for the ordinary cohomologies, or the cohomologies modulo $\tilde{d}$, which are simply isomorphic.

We have shown, in particular, what is the precise analog of the Lie algebra of inequivalent conserved currents in the Hamiltonian framework, which in turn allows some general statements on the structure of this Lie algebra and could be useful for its actual computation.

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APPENDIX A: JET SPACES, VARIATIONAL BICOMPLEX, AND KOSZUL–TATE RESOLUTION

In this appendix, we recall briefly the construction of jet bundles and of the variational bicomplex. We will construct a tricomplex containing the horizontal, the vertical, and the Koszul–Tate differentials. The construction enhances the cohomological setup of the variational bicomplex associated to possibly degenerate partial differential equations by implementing the pullback from the free bicomplex to the bicomplex of the surface defined by the equations through the homology of the Koszul–Tate differential. (Different considerations on the Batalin–Vilkovisky formalism in the context of the variational bicomplex are given in Ref. 12.)

Let us first recall some of the ingredients of the variational bicomplex relevant for our purpose (for a review see Refs. 7, 13, and 14 and the references to the original literature therein). As we will not be concerned with global properties, we will work in local coordinates throughout. Consider a trivial fiber bundle,

$$\pi: E = \mathbf{M}^n \times F \to \mathbf{M}^n, \tag{A1}$$

with local coordinates

$$\pi: (x^\mu, \phi^i) \to (x^\mu), \tag{A2}$$

where $\mu = 0,\ldots,n-1$ and $i = 1,\ldots,m$, with F a manifold homeomorphic to $\mathbf{R}^m$ parametrized by the ϕ^i. For simplicity, we assume here that all the ϕ^i are even, but all the considerations that follow could also be done in the case where the original bundle is a superbundle.

The induced coordinates on the infinite jet bundle,

$$\pi^{\infty}: J^{\infty}(E) = \mathbf{M}^n \times F^{\infty} \to \mathbf{M}^n \tag{A3}$$

of jets of sections on $\mathbf{M}^n$ are given by

$$(x^{\mu}, \phi^i, \phi^i_{\mu}, \phi^i_{\mu_1\mu_2}, \ldots,). \tag{A4}$$

Let $\Omega^P(J^{\infty}(E))$ be the local differential forms on $J^{\infty}(E)$. The exterior differential d_T is split into horizontal and vertical differentials: $d_T = d_H + d_V$, with

$$d_H = dx^{\mu}\ \partial_{\mu}, \quad \partial_{\mu} = \frac{\partial^L}{\partial x^{\mu}} + \phi^i_{(\nu)\mu}\ \frac{\partial^L}{\partial \phi^i_{(\nu)}} \tag{A5}$$

and

$$d_V \phi^i_{(\nu)} = d\phi^i_{(\nu)} - dx^{\mu}\ \phi^i_{(\nu)\mu}, \quad d_V x^{\mu} = 0. \tag{A6}$$

Note that everywhere else in the paper, we have omitted the subscript H on the horizontal differential and that we have introduced the more compact notation $\phi^i_{(\nu)} \equiv \partial_{(\nu)}\phi^i$ for the independent coordinates corresponding to the derivatives of the fields.

Furthermore, we have

$$d_H d_V + d_V d_H = d_H^2 = d_V^2 = 0. \tag{A7}$$

A local p-form of $\Omega^p(J^{\infty}(E))$ can then be written as a sum of terms of the form $f[\phi]dx^{\mu_1}\cdots dx^{\mu_r}\ d_V\phi^{i_1}_{(\nu_1)}\cdots d_V\phi^{i_s}_{(\nu_s)}$ of horizontal degree r and vertical degree s with $r+s=p$ and $f[\phi]$ a smooth function of x^{μ}, ϕ^i, and a finite number of their derivatives. The free variational bicomplex is the double complex $(\Omega^{*,*}((J^{\infty}(E)), d_H, d_V)$ of differential forms on $(J^{\infty}(E))$,

$$\begin{array}{ccccccccccccc}
 & & & & \vdots & & & & \vdots & & \vdots & & \\
 & & & & d_V\uparrow & & & & d_V\uparrow & & \delta_V\uparrow & & \\
 & & 0 & \to & \Omega^{0,2}(J^{\infty}(E)) & \stackrel{d}{\to} & \cdots & \stackrel{d}{\to} & \Omega^{n,2}(J^{\infty}(E)) & \stackrel{\int}{\to} & \mathscr{F}^2(J^{\infty}(E)) & \to & 0 \\
 & & & & d_V\uparrow & & & & d_V\uparrow & & \delta_V\uparrow & & \\
 & & 0 & \to & \Omega^{0,1}(J^{\infty}(E)) & \stackrel{d}{\to} & \cdots & \stackrel{d}{\to} & \Omega^{n,1}(J^{\infty}(E)) & \stackrel{\int}{\to} & \mathscr{F}^1(J^{\infty}(E)) & \to & 0 \\
 & & & & d_V\uparrow & & & & d_V\uparrow & & \delta_V\uparrow & & \\
0 & \to & \mathbf{R} & \to & \Omega^{0,0}(J^{\infty}(E)) & \stackrel{d}{\to} & \cdots & \stackrel{d}{\to} & \Omega^{n,0}(J^{\infty}(E)) & \stackrel{\int}{\to} & \mathscr{F}^0(J^{\infty}(E)) & \to & 0 \\
 & & & & \uparrow & & & & \uparrow & & \uparrow & & \\
0 & \to & \mathbf{R} & \to & \Lambda^0(\mathbf{M^n}) & \stackrel{d}{\to} & \cdots & \stackrel{d}{\to} & \Lambda^n(\mathbf{M^n}) & \to & 0 & &
\end{array}$$

The important property of this bicomplex is that all the rows and columns of the above diagram are exact.[7,13,4] The integral sign $\int$ denotes the projection, for each vertical degree s, of horizontal n-forms onto the space of local functional forms $\mathscr{F}^s$, i.e., the space of equivalence classes obtained by identifying exact horizontal n-forms with zero: $\mathscr{F}^s = \Omega^{n,s}/d_H\Omega^{n-1,s}$. δ_V is the induced action of the vertical derivative in $\mathscr{F}^s$: $\delta_V \int \omega^{n,s} = \int d_V \omega^{n,s}$. An evolutionary vector field on E is given by $v_Q = Q^i[\phi]\partial^L/\delta\phi^i$. It prolongation is given by $\delta_Q = \partial_{(\nu)}Q^i\partial^L/\partial\phi^i_{(\nu)}$. Because $[\delta_Q, \partial_{\mu}] = 0$, the contraction of a functional form with the prolongation of evolutionary vector fields is well defined.

A system $\mathscr{R}$ of kth-order partial differential equations on E,

$$\mathscr{R}_a(x^\mu, \phi^i, \phi^i_\mu, \ldots, \phi^i_{\mu_1 \cdots \mu_k}) = 0, \quad a = 1, \ldots, l, \tag{A8}$$

defines a sub-bundle $\mathscr{R} \to \mathbf{R}^n$ of $J^k(E) \to \mathbf{R}^n$. We shall assume that the equations $\mathscr{R}_a = 0$, $\partial_\mu \mathscr{R}_a = 0, \ldots, \partial_{\mu_1 \cdots \mu_1} \mathscr{R}_a = 0$ define, for each x^μ, a smooth surface and provide a regular representation of this surface in the vector spaces F^{s+k} for each s, i.e., the equations can be split into independent equations (L_m), which can be locally taken as first coordinates in a new, regular, coordinate system in the vicinity of the surface defined by the equations, and into dependent ones (L_Δ), which hold as a consequence of the independent ones.

This implies that one can split locally the ϕ^i and their derivatives up to order $s+k$ into independent variables x_A not constrained by the equations and dependent variables z_α in such a way that the equations $\mathscr{R}_a = 0, \ldots, \partial_{\mu_1 \cdots \mu_s} \mathscr{R}_a = 0$ are equivalent to $z_\alpha = z_\alpha(x_A, L_m)$. A local coordinate system adapted to the equations is then given by (x^μ, x_A, L_m) in $J^{s+k}(E)$. How this works in detail for Yang–Mills theory, gravity, or two-form fields is discussed in Ref. 8. The infinite prolongation $\mathscr{R}^\infty$ of $\mathscr{R}$, i.e., the given sets of equations and all their total derivatives, define a sub-bundle in $J^\infty(E)$. In the sequel, by ''stationary surface'' or by ''on shell'' we mean that we are on the sub-bundle defined by $\mathscr{R}_a = 0$ and an appropriate number of its derivatives, depending on the space $J^l(E)$ under consideration.

A consequence of the regularity condition is that any function $f[\phi]$ that vanishes on the stationary surface, $f \approx 0$, can be written as a combination of the equations defining this surface.[7,6]

The knowledge of the split of the equations into dependent and independent ones allows one to find a locally complete set of nontrivial local reducibility operators in $J^l(E)$, i.e., operators $R^{+a(\mu)}_{a_1} \partial_{(\mu)}$ for some local functions $R^{+a(\mu)}_{a_1}[\phi]$ on $J^l(E)$, which do not all vanish on shell, such that

$$R^{+a(\mu)} \partial_{(\mu)} \cdot \mathscr{R}_a = 0, \tag{A9}$$

and verifying the property that if $\lambda^{+a(\mu)} \partial_{(\mu)} \cdot \mathscr{R}_a = 0$ for some local functions $\lambda^{+a(\mu)}[\phi]$ on $J^l(E)$, then

$$\lambda^{+a(\rho)} \partial_{(\rho)} = \lambda^{+a_1(\lambda)} \partial_{(\lambda)} (R^{+a(\mu)}_{a_1} \partial_{(\mu)} \cdot) + \mu^{a(\mu)b(\nu)} (\partial_{(\nu)} \cdot \mathscr{R}_b) \partial_{(\mu)}, \tag{A10}$$

for some local functions $\lambda^{+a_1(\lambda)}[\phi]$, and $\mu^{a(\mu)b(\nu)}$ on $J^l(E)$, where $\mu^{a(\mu)b(\nu)} = -\mu^{b(\nu)a(\mu)}$. Furthermore, the first term of the right-hand side of Eq. (A10) can be assumed to be absent if the functions $\lambda^{+a(\mu)}$ vanish on shell.[6] Such reducibility operators will be called trivial because they exist for any gauge theory.

For simplicity, we will assume here that the reducibility operators are themselves irreducible in the sense that if $\lambda^{+a_1(\lambda)} R^{+a(\mu)} \partial_{(\mu)}$ vanishes on the stationary surface, the functions $\lambda^{+a_1(\lambda)}$ vanish on the stationary surface. All the considerations that follow can be generalized to the case with higher-order reducibility operators at the price of increasing the number of additional generators introduced below like in Ref. 6.

The variational bicomplex $(\Omega^{*,*}(\mathscr{R}^\infty), d_H, d_V)$ of the differential equations $\mathscr{R}$ is the pullback of the variational bicomplex from $J^\infty(E)$ to $\mathscr{R}^\infty$. With the previous assumptions, it is straightforward to verify that $\Omega^{*,*}(\mathscr{R}^\infty)$ is locally isomorphic to the forms in dx^μ and $d_V x_A$ with coefficients that are smooth functions in the x^μ, x_A. The columns of this bicomplex remain exact, because the contracting homotopy,[7] which allows us to prove exactness in the free case, still holds when we consider only $d_V x_A$'s. There exist, however, nontrivial cohomology groups along the rows.

The Koszul–Tate resolution of this bicomplex is obtained by a straightforward generalization of the Koszul–Tate resolution of the stationary surface $\mathscr{R}^\infty$.[6] One considers the superbundle

$$\pi: K = M^n \times (F \oplus \Phi^* \oplus C^*) \to M^n, \tag{A11}$$

and the associated free variational bicomplex $(\Omega^{*,*}(J^\infty(K)), d_H, d_V)$. Φ^* is the vector space with coordinates the Grassmann odd ϕ_a^* and is of dimension l, the number of original equations. C^* is the vector space with coordinates, the Grassmann even $C^*_{a_1}$, and its dimension equals the number of nontrivial reducibility operators $R^{+a(\mu)}_{a_1}\partial_{(\mu)}$. The Koszul–Tate differential δ is defined on $\Omega^{*,*}(J^\infty(K))$ by

$$\delta x^\mu = \delta\, dx^\mu = \delta\phi^i = 0,$$

$$\delta\phi_a^* = \mathscr{R}_a, \quad \delta C^*_{a_1} = R^{+a(\mu)}_{a_1}\partial_{(\mu)}\phi_a^*, \tag{A12}$$

$$\delta d_H + d_H\delta = 0 = \delta d_V + d_V\delta,$$

and is extended as a left antiderivation. The associated grading is obtained from the eigenvalues of the antighost number operator defined by

$$\text{antigh} = \phi^*_{a(\mu)}\frac{\partial^L}{\partial\phi^*_{a(\mu)}} + d_V\phi^*_{a(\mu)}\frac{\partial^L}{\partial d_V\,\phi^*_{a(\mu)}} + 2C^*_{a_1(\mu)}\frac{\partial^L}{\partial C^*_{a_1(\mu)}} + 2\,d_V C^*_{a_1(\mu)}\frac{\partial^L}{\partial\, d_V C^*_{a_1(\mu)}}. \tag{A13}$$

As in Ref. 6, one can then prove that

$$H_0(\delta, \Omega_0^{*,*}(J^\infty(K))) \simeq \Omega^{*,*}(J^\infty(E))/\mathscr{N} \simeq \Omega^{*,*}(\mathscr{R}^\infty), \tag{A14}$$

and that

$$H_k(\delta, \Omega_k^{*,*}(J^\infty(K))) = 0, \quad \text{for } k > 0. \tag{A15}$$

Here, $\mathscr{N}$ is the ideal of forms such that each term contains at least one of the terms $\partial_{(\mu)}\mathscr{R}_a$ or $d_V\,\partial_{(\mu)}\mathscr{R}_a$. Hence, locally, the quotient is isomorphic to the forms in dx^μ and $d_V x_A$ with coefficients that are smooth functions in the x^μ, x_A. By using a partition of unity, we then get the last isomorphism in the above equation. This means that the diagram,

$$\cdots \xrightarrow{\delta} \Omega_k^{*,*}(J^\infty(K)) \xrightarrow{\delta} \Omega_{k-1}^{*,*}(J^\infty(K)) \xrightarrow{\delta} \cdots$$

$$\cdots \xrightarrow{\delta} \Omega_1^{*,*}(J^\infty(K)) \xrightarrow{\delta} \Omega^{*,*}(\mathscr{R}^\infty) \to 0,$$

is exact.

In the three-dimensional grid corresponding to the tricomplex,

$$(\Omega_*^{*,*}(J^\infty(K), d_H, d_V, \delta)), \tag{A16}$$

augmented by the projection on local functionals in the d_H direction and by the projection on the bicomplex for the partial differential equations $(\Omega^{*,*}(\mathscr{R}^\infty), d_H, d_V)$ in the δ direction, except for the rows of this last complex, the sequences are exact in all directions.

The advantage of this cohomological resolution of the variational bicomplex for partial differential equations is that the nontrivial cohomology groups $H^{r,*}(d_H, \Omega^{r,*}(\mathscr{R}^\infty))$ are given by relative cohomology groups in the free tricomplex,

$$H^{r,*}(d_H, \Omega^{r,*}(\mathscr{R}^\infty)) \simeq H_0^{r,*}(d_H|\,\delta, \Omega_0^{r,*}(J^\infty(K))). \tag{A17}$$

Since $H_*^{q,*}(d_H,\Omega_*^{q,*}(J^\infty(K)))=0$ for $0<q<n$ and $H_k^{*,*}(\delta,\Omega_k^{*,*}(J^\infty(K)))=0$ for $k>0$, one can, for instance, apply the method of diagram chasing (or ''snake lemma'') in the horizontal and δ directions to get, for $(r,s)\neq(0,0)$,

$$H_0^{r,s}(d_H|\,\delta,\Omega_0^{r,s}(J^\infty(K)))\simeq H_1^{r+1,s}(d_H|\,\delta,\Omega_1^{r,s}(J^\infty(K)))\simeq\cdots\simeq H_{n-r-1}^{n-1,s}(d_H|\,\delta,\Omega_{n-r-1}^{n-1,s}(J^\infty(K))). \tag{A18}$$

For $(r,s)=(0,0)$, the same chain of isomorphisms remain true if one replaces the first element in the chain by $H^{0,0}(d_H|\delta,\Omega_0^{0,0}(J^\infty(K)))/\mathbf{R}$. Furthermore, like in Ref. 9, one proves that

$$\frac{H_k^{r,*}(d_H|\,\delta,\Omega_k^{r,*}(J^\infty(K)))}{p^\sharp H_k^{r,*}(d_H,\Omega_k^{r,*}(J^\infty(K)))}\simeq\frac{H_{k+1}^{r+1,*}(\delta|d_H,\Omega_{k+1}^{r+1,*}(J^\infty(K)))}{p^\sharp H_{k+1}^{r+1,*}(\delta,\Omega_{k+1}^{r+1,*}(J^\infty(K)))}, \tag{A19}$$

where $p^\sharp$ denotes the natural inclusion of an absolute cohomology group as a relative cohomology group. Using the results on the cohomology of d_H and δ, these relations reduce to

$$H_0^{0,0}(d_H|\,\delta,\Omega_0^{0,0}(J^\infty(K)))/\mathbf{R}\simeq H_1^{1,1}(\delta|d_H,\Omega_1^{1,1}(J^\infty(K))), \tag{A20}$$

$$H_k^{r,*}(d_H|\,\delta,\Omega_k^{r,*}(J^\infty(K)))\simeq H_{k+1}^{r+1,*}(\delta|d_H,\Omega_{k+1}^{r+1,*}(J^\infty(K))),\quad (r,s,k)\neq(0,0,0),\quad r<n. \tag{A21}$$

APPENDIX B: LOCAL BRACKETS AND SURFACE TERMS

In the first part of this appendix, we want to calculate explicitly the total divergences that arise in the Jacobi identity for the local (anti)bracket.

Let $z^a=(\phi^A,\phi_A^*)$ and

$$\zeta^{ab}=\begin{pmatrix}0 & \delta_B{}^A\\ -\delta_B{}^A & 0\end{pmatrix}.$$

Let $(\tilde{\nu})_{\mu_1}$ denote the number of times the index μ appears in the multiindex (ν). The higher Euler operators[7] are uniquely defined by the expression

$$\delta_Q f=\partial_{(\nu)}\left(Q^a\,\frac{\delta^L f}{\delta z^a_{(\nu)}}\right). \tag{B1}$$

Let us furthermore define the ''generalized Hamiltonian vector field:''

$$\overline{a^b}=\left(\frac{\delta^R\hat{a}}{\delta z^a}\right)\zeta^{ab}. \tag{B2}$$

Then the local antibracket in the space of integrands (9) can be rewritten as

$$\{a_1,a_2\}=d^nx\left[\partial_{(\mu)}\left(\frac{\delta^R\hat{a}_1}{\delta z^a}\right)\zeta^{ab}\left(\frac{\partial^L\hat{a}_2}{\partial z^b_{(\mu)}}\right)-\frac{(\tilde{\nu})_\mu+1}{|\nu|+1}\,\partial_{\mu(\nu)}\left(\frac{\delta^R\hat{a}_1}{\delta z^a}\,\zeta^{ab}\,\frac{\delta\hat{a}_2}{\delta z^b_{\mu(\nu)}}\right)\right]\equiv\delta\overline{_{a_1}}a_2-dI\overline{_{a_1}}\,a_2. \tag{B3}$$

This expression implies that the graded Leibnitz rule holds up to a total divergence.

We have pointed out in the text that the local antibracket (B3) does not satisfy the graded Jacobi identity strictly, but only up to a total divergence. Similarly, in the Hamiltonian theory, the Poisson bracket among local functions of the fields, their conjugate momenta, and their derivatives,

$$\{\hat{a}_1,\hat{a}_2\}_{\mathrm{P}}=\frac{\widetilde{\delta}^R\hat{a}_1}{\delta\phi^i}\,\sigma^{ij}\,\frac{\widetilde{\delta}^L\hat{a}_2}{\delta\phi^j}, \tag{B4}$$

satisfies the Jacobi identity $\{\hat{a},\{\hat{b},\hat{c}\}\}+cyclic=0$ only up to a (spatial) total divergence. In Eq. (B4), ϕ^i collectively denotes the fields and their conjugate momenta, the tilde superscript denotes the spatial Euler–Lagrange derivatives, and

$$\sigma^{ij}=\begin{pmatrix} 0 & \delta^i_j \\ -\delta^i_j & 0 \end{pmatrix}.$$

For definiteness, we shall evaluate here explicitly the boundary terms in the Jacobi identity in the Hamiltonian case and assume that the fields ϕ^i and the densities $\hat{a}$, $\hat{b}$, and $\hat{c}$ are all even. We will, however, not write explicitly the tilded superscript to indicate the spatial derivatives. The calculation for the local antibracket or the local extended Poisson bracket is simply a matter of taking care of the sign factors.

We will need the following lemma:

$$(-\partial)_{(\alpha)}\left(f\,\frac{\partial}{\partial\phi^i_{(\alpha)}}\,\partial_\beta g\right)=-(-\partial)_{(\alpha)}\left(\partial_\beta f\,\frac{\partial}{\partial\phi^i_{(\alpha)}}\,g\right). \tag{B5}$$

The proof of this lemma follows from a straightforward extension of the proof of $(\delta/\delta\phi^i)(\partial_\beta g)=0$ in Ref. 15.

A direct calculation, using the analog of (B3) for the Poisson bracket and the fact that the Euler–Lagrange derivatives annihilate total divergences, yields

$$\begin{aligned}\{a,\{b,c\}\}+cyclic&=\{a,\{b,c\}\}-\{b,\{a,c\}\}-\{\{a,b\},c\}\\&=\delta_{\bar{a}}\delta_{\bar{b}}c-\delta_{\bar{b}}\delta_{\bar{a}}c-\delta_{\{\overline{a,b}\}}c,\end{aligned} \tag{B6}$$

$$-dI_{\bar{a}}(\delta_{\bar{b}}c)+dI_{\bar{b}}(\delta_{\bar{a}}c)+dI_{\{\overline{a,b}\}}c. \tag{B7}$$

We have

$$(\delta_{\bar{a}}\delta_{\bar{b}}-\delta_{\bar{b}}\delta_{\bar{a}})c=\delta_{\bar{d}}c, \tag{B8}$$

with

$$\begin{aligned}\overline{d^i}&=\delta_{\bar{a}}\left(\frac{\delta\hat{b}}{\delta\phi^j}\right)\sigma^{ji}-(\hat{a}\leftrightarrow\hat{b})\\&=\frac{\delta}{\delta\phi^j}(\delta_{\bar{a}}\hat{b})\sigma^{ji}-(-\partial)_{(\alpha)}\left[\frac{\partial}{\partial\phi^j_{(\alpha)}}\left(\partial_{(\beta)}\,\frac{\delta\hat{a}}{\delta\phi^k}\right)\sigma^{kl}\,\frac{\partial\hat{b}}{\partial\phi^l_{(\beta)}}\right]\sigma^{ji}-(\hat{a}\leftrightarrow\hat{b})\\&=\frac{\delta}{\delta\phi^j}\{\hat{a},\hat{b}\}\sigma^{ji}-(-\partial)_{(\alpha)}\left[\frac{\partial}{\partial\phi^j_{(\alpha)}}\left(\frac{\delta\hat{a}}{\delta\phi^k}\right)\sigma^{kl}\,\frac{\delta\hat{b}}{\delta\phi^l}\right]\sigma^{ji}-(\hat{a}\leftrightarrow\hat{b})\\&=2\,\frac{\delta}{\delta\phi^j}\{\hat{a},\hat{b}\}\sigma^{ji}-(-\partial)_{(\alpha)}\left[\frac{\partial}{\partial\phi^j_{(\alpha)}}\left(\frac{\delta\hat{a}}{\delta\phi^k}\,\sigma^{kl}\,\frac{\delta\hat{b}}{\delta\phi^l}\right)\right]\sigma^{ji}=\frac{\delta}{\delta\phi^j}\{\hat{a},\hat{b}\}\sigma^{ji}=\{\overline{a,b}\}^i.\end{aligned} \tag{B9}$$

To get the line before last, we have used repeatedly the above-mentioned lemma (B5). Hence,

$$\{a,\{b,c\}\}+cyclic=d(-I_{\bar{a}}(\delta_{\bar{b}}c)+I_{\bar{b}}(\delta_{\bar{a}}c)+I_{\{\overline{a,b}\}}c). \tag{B10}$$

This is the desired formula.[h] □

We now prove that the expressions in Eq. (25) for the Dickey bracket are equivalent to the definition in Eq. (24). Let us write terms that vanish on shell by $\delta(\ )$. By applying the lemma (B5), we find that, if X is the characteristic of a variational symmetry, the following equation holds:

$$\delta_X\left(\frac{\delta\hat{\mathscr{L}}_0}{\delta\phi^i}\right)Y^i\ d^nx=-(-\partial)_{(\mu)}\left[\frac{\partial}{\partial\phi^i_{(\mu)}}\,(\partial_{(\nu)}X^j)\,\frac{\partial\hat{\mathscr{L}}_0}{\partial\phi^j_{(\nu)}}\right]Y^i\ d^nx$$
$$=-(-\partial)_{(\mu)}\left[\frac{\partial}{\partial\phi^i_{(\mu)}}\,(X^j)\,\frac{\delta\hat{\mathscr{L}}_0}{\delta\phi^j}\right]Y^i\ d^nx=-\delta_Y(X^j)\,\frac{\delta\hat{\mathscr{L}}_0}{\delta\phi^j}\,d^nx+d\,\delta(\ ). \tag{B11}$$

Let us evaluate $d(-\delta_{X_1}j_2)$. Using (B11) twice, we get,

$$d(-\delta_{X_1}j_2)=-\delta_{X_1}\left(\frac{\delta\hat{\mathscr{L}}_0}{\delta\phi^i}\,X_2^i\right)d^nx+d\,\delta(\ )$$
$$=-\delta_{X_1}(X_2^i)\,\frac{\delta\hat{\mathscr{L}}_0}{\delta\phi^i}\,d^nx+\delta_{X_2}(X_1^j)\,\frac{\delta\hat{\mathscr{L}}_0}{\delta\phi^i}\,d^nx+d\,\delta(\ ), \tag{B12}$$

$$=d(\delta_{X_2}j_1)+d\,\delta(\ ). \tag{B13}$$

From this equation it also follows immediately that

$$d(-\delta_{X_1}j_2)=\tfrac{1}{2}\,d(\delta_{X_2}j_1)-d(\delta_{X_1}j_2)+d\,\delta(\ ). \tag{B14}$$

Using the triviality of the cohomology of d in form degree $n-1(>0)$ implies the first two expressions in Eq. (25).

From Eq. (B12), it follows that

$$d(-\delta_{X_1}j_2)=\left[\delta_{[X_1,X_2]_L}\hat{\mathscr{L}}_0-\frac{(\widetilde{\nu})_\mu+1}{|\nu|+1}\,\partial_{\mu(\nu)}\left(\frac{\delta\hat{\mathscr{L}}_0}{\delta\phi^i_{(\nu)\mu}}\,[X_1,X_2]_L^i\right)\right]d^nx+d\,\delta(\ ). \tag{B15}$$

But we also have

$$\delta_{[X_1,X_2]}\hat{\mathscr{L}}_0=(\delta_{X_2}\delta_{X_1}-\delta_{X_1}\delta_{X_2})\hat{\mathscr{L}}_0$$
$$=\partial_\mu(\delta_{X_2}j_1^\mu-\delta_{X_1}j_2^\mu)+\frac{(\widetilde{\nu})_\mu+1}{|\nu|+1}\,\partial_{\mu(\nu)}\left[\delta_{X_2}\left(\frac{\delta\hat{\mathscr{L}}_0}{\delta\phi^i_{(\nu)\mu}}\,X_1^i\right)-\delta_{X_1}\left(\frac{\delta\hat{\mathscr{L}}_0}{\delta\phi^i_{(\nu)\mu}}\,X_2^i\right)\right]. \tag{B16}$$

This implies

$$d(-\delta_{X_1}j_2)=d(\delta_{X_2}j_1-\delta_{X_1}j_2)+\frac{(\widetilde{\nu})_\mu+1}{|\nu|+1}\,\partial_{\mu(\nu)}\left(\delta_{X_2}\left(\frac{\delta\hat{\mathscr{L}}_0}{\delta\phi^i_{(\nu)\mu}}\right)X_1^i-\delta_{X_1}\left(\frac{\delta\hat{\mathscr{L}}_0}{\delta\phi^i_{(\nu)\mu}}\right)X_2^i\right)d^nx$$
$$+d\,\delta(\ ). \tag{B17}$$

Using (B14), we find the last expression of (25):

$$d(-\delta_{X_1} j_2) = -\frac{(\tilde{\nu})_\mu + 1}{|\nu|+1}\,\partial_{\mu(\nu)}\left(\delta_{X_2}\left(\frac{\delta\hat{\mathscr{L}}_0}{\delta\phi^i_{(\nu)\mu}}\right)X_1^i - \delta_{X_1}\left(\frac{\delta\hat{\mathscr{L}}_0}{\delta\phi^i_{(\nu)\mu}}\right)X_2^i\right)d^n x + d\,\delta(\ ). \quad \text{(B18)}$$

□

In the last part of the appendix, we establish the relationship between the antibracket map and the Dickey bracket. As explained before theorem 2, we have to evaluate $\delta\{a_1,a_2\}$, where $a = d^n x\ \phi_i^* X^i$, with X^i defining a variational symmetry:

$$\delta\{a_1,a_2\} = \left(d^n x\,\frac{\delta X_1^i}{\delta\phi^j}\,X_2^j - \frac{\delta X_2^i}{\delta\phi^j}\,X_1^i\right)\frac{\delta\hat{\mathscr{L}}_0}{\delta\phi^i} = d^n x(\delta_{X_2}X_1^i - \delta_{X_1}X_2^i)\,\frac{\delta\hat{\mathscr{L}}_0}{\delta\phi^i} + d\,\delta(\ )$$
$$= d(-\delta_{X_1} j_2) + d\,\delta(\ ), \quad \text{(B19)}$$

where we have used (B12) in order to get the last equality. This proves that to the antibracket map of two classes in $H_1^n(\delta|d)$ corresponds to the Dickey bracket of the corresponding currents. □

APPENDIX C: DESCENT EQUATIONS IN THE HAMILTONIAN FORMALISM

We analyze in this appendix, first of all, the relationship between the cohomology of s_{H} defined in Eq. (37) and the cohomology of s_ω, thereby proving Theorem 5. Then we analyze the spatiotemporal descent equations of s_{H} by choosing representatives appropriate to the Hamiltonian formalism, proving Eqs. (41)–(46).

1. Cohomology of s_{H} and s_ω

The cocyle n in $s_{\mathrm{H}} n = 0$ depends on the coordinates $x^\mu, \partial_{(\mu)}\tilde{\phi}^A, \partial_{(\mu)}\tilde{\phi}^*_A$. Consider the change of coordinates, which consists in replacing the time derivatives of the fields and all their derivatives by the $\partial_{(\mu)}\mathscr{L}_A$. In the new coordinates, n depends on $x^\mu, \partial_{(k)}\tilde{\phi}^A, \partial_{(\mu)}\tilde{\phi}^*_A, \partial_{(\mu)}\mathscr{L}_A$. Using $s_\omega\Omega = s_\omega H = 0$ and the identity

$$-s_\omega\{\tilde{\phi}^*_A\tilde{\phi}^A,\cdot\}_{\mathrm{P,alt}} + \partial_{(k)}\,\frac{\tilde{\delta}^R}{\delta\tilde{\phi}^C}\,(\sigma^{CA}\{\tilde{\phi}^*_B\tilde{\phi}^B,\omega\}_{\mathrm{P,alt}})\,\frac{\partial^L}{\partial(\partial_{(k)}\tilde{\phi}^A)} = \{\tilde{\phi}^*_A\tilde{\phi}^A, s_\omega\cdot\}_{\mathrm{P,alt}} \quad \text{(C1)}$$

we find that $s_{\mathrm{H}}\mathscr{L}_A = 0$. This means that in the new coordinate system,

$$s_{\mathrm{H}} = s_\omega + \partial_{(\mu)}\mathscr{L}_A\,\frac{\partial^L}{\partial(\partial_{(\mu)}\tilde{\phi}^*_A)}, \quad \text{(C2)}$$

where s_ω is restricted to spatial derivatives. Introducing the contracting homotopy,

$$\rho = \partial_{(\mu)}\tilde{\phi}^*_A\,\frac{\partial^L}{\partial(\partial_{(\mu)}\mathscr{L}_A)}, \quad \text{(C3)}$$

the anticommutator $\{s_{\mathrm{H}},\rho\} = N = z^\alpha(\partial^L/\partial z^\alpha)$ is the operator counting the number of coordinates, $z^\alpha \equiv \partial_{(\mu)}\tilde{\phi}^*_A, \partial_{(\mu)}\mathscr{L}_A$. The standard argument is then that

$$n = n(z^\alpha = 0) + \int_0^1 \frac{d\lambda}{\lambda}\,(Nn)[\lambda z^\alpha], \quad \text{(C4)}$$

$$= n_0 + s_{\mathrm{H}}\left(\int_0^1 \frac{d\lambda}{\lambda}\,(\rho n)[\lambda z^\alpha]\right). \quad \text{(C5)}$$

The cocycle condition now reduces to $s_\omega n_0=0$, and the coboundary condition $n_0=s_{\mathrm{H}}p$ reduces to $n_0=s_\omega p_0$. Indeed, applying N to the coboundary condition implies that $Ns_{\mathrm{H}}p=0$. Using

$$[N,s_{\mathrm{H}}]=0, \tag{C6}$$

and the same decomposition of p as for n in (C4), this equation implies that $s_{\mathrm{H}}p=s_\omega p_0$.

This proves Theorem 5. □

In order to analyze the spatiotemporal descent equations for s_{H}, we start form the bottom, which we can assume to be of the form n_0, as above. We then want to know under what conditions n_0 can be lifted i.e., what are the conditions for the existence of m, such that $s_{\mathrm{H}}m+dn_0=0$. We will now prove, in particular, the crucial lemma that m can be assumed to be independent of the coordinates $\partial_{(\mu)}\mathscr{L}_A$, with a linear dependence in the antifields $\partial_{(k)}\tilde{\phi}^*_A$ only in the terms involving the differential dt.

2. First lift from the bottom of the descent equations

The spatial exterior differential has the same form in the new coordinate system as it had in the old one. The total time derivative, however, is given by

$$\frac{d}{dt}=\frac{\partial}{\partial t}+\partial_{(k)l+1}\tilde{\phi}^*_A\,\frac{\partial^L}{\partial(\partial_{(k)l}\tilde{\phi}^*_A)}+\partial_{(k)l+1}\mathscr{L}_A\,\frac{\partial^L}{\partial(\partial_{(k)l}\mathscr{L}_A)}$$
$$+\partial_{(k)}\sigma^{CA}\left[-\mathscr{L}_C-\frac{\tilde{\delta}^R h}{\delta\tilde{\phi}^C}-\frac{\tilde{\delta}^R}{\delta\tilde{\phi}^C}\{\tilde{\phi}^*_B\tilde{\phi}^B,\omega\}_{\mathrm{P,alt}}\right]\frac{\partial^L}{\partial(\partial_{(k)}\tilde{\phi}^A)}. \tag{C7}$$

We then decompose m and n_0 into pieces, respectively, containing the differential dt or not (m^0, n_0^0, and $\tilde{m},\tilde{n}_0$). The cocycle condition splits into

$$s_{\mathrm{H}}\tilde{m}+\tilde{d}\tilde{n}_0=0,\quad s_{\mathrm{H}}m^0+\tilde{d}n_0^0-\frac{d}{dt}\,\tilde{n}_0=0 \tag{C8}$$

From the homotopy formula (C4) applied to $\tilde{m}$ and the cocycle condition, we get that $\tilde{m}=\tilde{m}_0+s_{\mathrm{H}}(\ )-\tilde{d}(\int_0^1(d\lambda/\lambda)(\rho\tilde{n}_0)[\lambda z^\alpha)$ because ρ (anti)commutes with $\tilde{d}$ and $\tilde{d}$ is homogeneous of degree 0 in z^α. The last expression vanishes since $\rho\tilde{n}_0=0$. Injecting the remaining expression into the cocycle condition, we get

$$s_\omega\tilde{m}_0+\tilde{d}\tilde{n}_0=0. \tag{C9}$$

The homotopy formula (C4) applied to m^0, together with the cocycle condition, implies that

$$m^0=m_0^0+s_{\mathrm{H}}(\ )+\tilde{d}\left(\int_0^1\frac{d\lambda}{\lambda}\,(\rho n_0^0)\right)+\int_0^1\frac{d\lambda}{\lambda}\,\rho\sigma^{CA}\partial_{(k)}\left(-\mathscr{L}_C-\frac{\tilde{\delta}^R h}{\delta\tilde{\phi}^C}\right.$$
$$\left.-\frac{\tilde{\delta}^R}{\delta\tilde{\phi}^C}\{\tilde{\phi}^*_B\tilde{\phi}^B,\omega\}_{\mathrm{P,alt}}\right)\frac{\partial^L}{\partial(\partial_{(k)}\tilde{\phi}^A)}\,\tilde{n}_0[\lambda z^\alpha]$$
$$=m_0^0+s_{\mathrm{H}}(\ )-\{\tilde{\phi}^*_A\tilde{\phi}^A,\tilde{n}_0\}_{\mathrm{P,alt}}, \tag{C10}$$

proving in particular the lemma on the dependence of m on the coordinates z^α. Injecting this last expression in the cocycle condition, using $s_\omega n_0^0=0$ and (C1), implies

$$s_\omega m_0^0 + \tilde{d} n_0^0 - \frac{\partial}{\partial t} \tilde{n}_0 + \{h, \tilde{n}_0\}_{\mathrm{P,alt}} = 0. \tag{C11}$$

3. Next steps in the lifting procedure

We then have to try to lift the equivalent representative of m given by

$$m' = dt(-\{\tilde{\phi}_A^* \tilde{\phi}^A, \tilde{n}_0\}_{\mathrm{P,alt}} + m_0^0) + \tilde{m}_0, \tag{C12}$$

i.e., find $l = dt\ l^0 + \tilde{l}$, such that $s_{\mathrm{H}} l + d m' = 0$. This implies

$$s_{\mathrm{H}} \tilde{l} + \tilde{d} \tilde{m}_0 = 0, \quad s_{\mathrm{H}} l^0 + \tilde{d}(-\{\tilde{\phi}_A^* \tilde{\phi}^A, \tilde{n}_0\}_{\mathrm{P,alt}} + m_0^0) - \frac{d}{dt} \tilde{m}_0 = 0. \tag{C13}$$

By exactly the same reasoning as before, the first equation implies that

$$\tilde{l} = \tilde{l}_0 + s_{\mathrm{H}}(\ ), \quad s_\omega \tilde{l}_0 + \tilde{d} \tilde{m}_0 = 0. \tag{C14}$$

The second equation implies as before that

$$l^0 = l_0^0 + s_{\mathrm{H}}(\ ) - \{\tilde{\phi}_A^* \tilde{\phi}^A, \tilde{m}_0\}_{\mathrm{P,alt}}, \tag{C15}$$

because ρ annihilates the supplementary $\tilde{\phi}_A^*$-dependent term, which does not depend on $\mathscr{S}_A$. Injecting into the cocycle condition, we get

$$s_\omega l_0^0 + \tilde{d} m_0^0 - \frac{\partial}{\partial t} \tilde{m}_0 + \{h, \tilde{m}_0\}_{\mathrm{P,alt}} = 0, \tag{C16}$$

the supplementary antifield-dependent term in m^0 cancelling the term coming from (C1) using the fact that $s_\omega \tilde{m}_0 + \tilde{d} \tilde{n}_0 = 0$. This shows that at every step we get the same dependence on the coordinates z^α, i.e., independence on $\partial_{(\mu)} \mathscr{S}_A$, or by going back to the old coordinate system, on the time derivatives of the fields, with a linear dependence in the antifields and their spatial derivatives $\partial_{(k)} \tilde{\phi}_A^*$ only in the terms involving the differential dt. Furthermore, we have proved the set of equations (41)–(43).

4. Coboundary condition

Let us now consider the coboundary condition for l' defined in an analoguous way as m' in (C12). From $l' = s_{\mathrm{H}} r + d u$, we have, by applying s_{H}, that $s_{\mathrm{H}} u + d p = 0$. Hence, u satisfies the same equation as l above, which implies by (C14) and an appropriate modification of r that we can assume $\tilde{u} = \tilde{u}_0$ and $u^0 = u_0^0 - \{\tilde{\phi}_A^* \tilde{\phi}^A, \tilde{p}_0\}_{\mathrm{P,alt}}$.

We have that $\tilde{l}_0 = s_{\mathrm{H}} \tilde{r} + \tilde{d} \tilde{u}$, which implies, by applying the homotopy formula (C4) to r, that we can assume that $\tilde{r} = \tilde{r}_0$, $\tilde{u} = \tilde{u}_0$. The coboundary condition becomes $\tilde{l}_0 = s_\omega \tilde{r}_0 + \tilde{d} \tilde{u}_0$, proving Eq. (45).

By applying the homotopy formula (C4) to r^0, the coboundary condition,

$$-\{\tilde{\phi}_A^* \tilde{\phi}^A, \tilde{m}_0\}_{\mathrm{P,alt}} + l_0^0 = -s_{\mathrm{H}} r^0 - \tilde{d} u^0 + \frac{d}{dt} \tilde{u}_0, \tag{C17}$$

implies

$$-\{\tilde{\phi}^*_A\tilde{\phi}^A,\tilde{n}_0\}_{\mathrm{P,alt}}+l^0_0=-s_\omega r^0_0-s_{\mathrm{H}}\int_0^1\frac{d\lambda}{\lambda}\left(\rho\left(\{\tilde{\phi}^*_A\tilde{\phi}^A,\tilde{m}_0\}_{\mathrm{P,alt}}-l^0_0-\tilde{d}u^0+\frac{d}{dt}\,\tilde{u}_0\right)\right)[\lambda z^\alpha]-\tilde{d}u^0+\frac{d}{dt}\,\tilde{u}_0. \tag{C18}$$

This gives

$$l^0_0=-s_\omega r^0_0-\tilde{d}u^0_0+\frac{\partial}{\partial t}\,\tilde{u}_0-\{h,\tilde{u}_0\}_{\mathrm{P,alt}}, \tag{C19}$$

proving Eq. (46). These coboundary conditions are satisfied by choosing in the equation $l=s_{\mathrm{H}}r+du$, r to be given by $dt(-\{\tilde{\phi}^*_A\tilde{\phi}^A,\tilde{u}_0\}_{\mathrm{P,alt}}+r^0_0)+\tilde{r}_0$ and a similar equation holding for u. This proves (44). □

NOTES

[a]We will not be too precise about the nature of the field dependence of the local functions (polynomiality or smooth dependence). Similarly, we will not specify whether one should consider polynomials or infinite formal series in the antifields and their derivatives,[8] since most aspects we will consider are really independent of these considerations. For simplicity, we will assume, however, that all the fields live on a star-shaped space.

[b]One uses the facts that (i) $\{\cdot,\cdot\}_{\mathrm{alt}}$ differs from $\{\cdot,\cdot\}$ by a total divergence; (ii) that $\{\cdot,\cdot\}$ satisfies the graded Jacobi up to a total divergence; and (iii) that Euler–Lagrange derivatives annihilate total divergences.

[c]This exhausts the arbitrariness of the functions $X^{i(\lambda)}$ only in the case where the equations and their derivatives are independent;[7,6] in the general case, one has to also take care of the Noether identities, as shown below.

[d]One says that the Koszul–Tate differential δ provides a homological resolution of the functions defined on the stationary surface (also see Appendix A).

[e]A trivial variational symmetry vanishes on the stationary surface. Under certain assumptions,[8] one can prove that *vice versa* every variational symmetry that vanishes on the stationary surface corresponds to a trivial representative of $H^{-1,n}(s|d)$, i.e., an ''antisymmetric'' combination of the equations of motion.

[f]This is the formalization in the appropriate jet space of the idea that functions linear in the antifields define tangent vectors,[16] the physically relevant ones here being those that are ''tangent'' to the stationary surface.

[g]These equations have been first used in Ref. 17 to compare anomalies in the Hamiltonian and the Lagrangian formalism.

[h]It also follows from this proof that the alternative bracket given by $\{a,b\}_{\mathrm{alt}}=\delta_a b$ satisfies a strict Jacobi identity under Leibnitz form [defined by the second expression of (B6)], using, furthermore, the fact that $\{\overline{a,b}\}_{\mathrm{alt}}=\{\overline{a,b}\}$.

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On Green–Cusson Ansätze and deformed supersymmetric quantum mechanics

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Supersymmetric quantum mechanics cannot be deformed when the superposition of only a pair of usual bosons and fermions is considered, but it can if nontrivial parabosons and parafermions of the same order p of paraquantization are superposed. We take the simplest case $p=2$ and exhibit reducibility problems in that context by using Green–Cusson Ansätze following Macfarlane methods. Specific representations of the Lie superalgebra osp $(2|2, \mathbb{R})$ play an interesting role in connection with possible deformations. © *1996 American Institute of Physics.* [S0022-2488(96)01411-9]

I. INTRODUCTION

By revisiting the so-called *Green Ansätze*[1] in parastatistical developments,[2,3] Macfarlane[4] has recently pointed out some *''methods allowing various new results for q-deformed (parabose) oscillators to be derived.''* In particular, Fock bases characterized by bilinear (rather than trilinear) structure relations play a very interesting role in such considerations. Here, we plan to exploit the corresponding *Green–Cusson Ansätze*[5,6] in the study of quantum deformations in a fundamental physical theory such as supersymmetric quantum mechanics (SSQM).[7]

Let us recall that quantum deformations[8] have been investigated, developed, and applied in a large number of fields in quantum physics. More recently, different generalizations[9–13] have also been proposed in order to cover a maximum of information through refined methods.

In particular, a specific question has been asked by Spiridonov[14] in connection with the possible deformation of the standard Witten model[7] of SSQM. A few months later, his answer presented as a q-deformation has been shown[15] as resulting only from ordinary SSQM but including q-dependent superpotentials. It is now evident that SSQM [based on the $D^{(1/2)-}$ representation of su$(2,\mathbb{C})$] cannot be deformed although its super-Hamiltonian can.[16] Let us also mention another recent approach[17] containing investigations on links between high-order derivative supersymmetry and q-deformed SSQM but without direct connections with the point of view we want to develop here.

One of the main purposes of this paper is to circumvent this difficulty by using the above-mentioned Green–Cusson Ansätze and by constructing, in the Macfarlane way, a Fock space exploiting the context of the second-order $(p=2)$ of paraquantization in the so-called relative parabosonic (or relative parafermionic) set characterized by Greenberg and Messiah.[3] Through such developments we will show that SSQM can be deformed by exploiting previous results.[6,18]

The contents of this paper are then distributed as follows. In Sec. II we summarize a few properties[18] resulting from supersymmetric developments in connection with parabosons and parafermions (of order 2, but also valid for arbitrary orders), an important one being the existence of an invariance Lie superalgebra of SSQM, i.e., the orthosymplectic Lie superalgebra osp $(2/2,\mathbb{R})$. Section III is then devoted to the construction of an effective Fock basis in the context of the relative parabosonic set when Green–Cusson Ansätze are exploited. The corresponding state

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vectors will appear as characterized by a family of six (simultaneously measurable) observables associated with two usual bosons and four usual fermions. They will be classified in three irreducible representations of the above orthosymplectic Lie superalgebra and will allow us to determine the energy superspectrum of such a context. In Sec. IV, we construct the pair of deformed parabosonic and parafermionic operators leading to generalized deformed supercharges in particular, but also to the eight deformed generators of the orthosymplectic Lie superalgebra. In Sec. V we discuss possible deformations of the superalgebra sqm (2) seen as a subalgebra of osp $(2/2,\mathbb{R})$. The conclusion will be that, effectively, SSQM can be deformed.

II. SUMMARY OF SOME PRECEDING RESULTS

After Greenberg–Messiah,[3] we have learned that there exist only two different relative sets of *trilinear* structure relations which are respectively called the *parabosonic* (or *para-Bose*) and *parafermionic* (or *para-Fermi*) sets characterized by typical relations as follows. If we denote by a (and $a^\dagger$) the parabosonic annihilation (and creation) operator(s) and by b (and $b^\dagger$) the parafermionic annihilation (and creation) operator(s), we have for the two sets the *common* structure relations (when only one pair of paraparticles are concerned)

$$\begin{gathered}[a,\{a^\dagger,a\}]=2a, \quad [b,[b^\dagger,b]]=2b,\\ [\{a^\dagger,a\},b]=0, \quad [[b^\dagger,b],a]=0,\\ [\{a,a\},b]=0, \quad [\{a^\dagger,a^\dagger\},b]=0.\end{gathered} \tag{2.1a}$$

They are supplemented by the following ones,

$$\begin{gathered}[\{a,b\},a^\dagger]=-[\{a^\dagger,b\},a]=2b,\\ \{\{a,b^\dagger\},b\}=\{\{a,b\},b^\dagger\}=2a,\\ [\{a,b\},a]=\{\{a,b\},b\}=0,\\ [\{a^\dagger,b\},a^\dagger]=\{\{a,b^\dagger\},b^\dagger\}=0,\end{gathered} \tag{2.1b}$$

when the *relative parabosonic set* is concerned, *and* by

$$\begin{gathered}\{a,[a^\dagger,b]\}=\{a^\dagger,[b,a]\}=2b,\\ [b^\dagger,[b,a]]=[b,[b^\dagger,a]]=2a,\\ [b,[a,b]]=\{a,[b,a]\}=0,\\ [b^\dagger,[a,b^\dagger]]=\{a^\dagger,[b,a^\dagger]\}=0,\end{gathered} \tag{2.1c}$$

when the *relative parafermionic set* is concerned.

From the first and second sets, we have shown[18] that it is possible to define two supercharges in each context such that, with the corresponding Hamiltonian H, they generate the superalgebra of ordinary SSQM, i.e., sqm (2) (Ref. 7) characterized by the structure relations

$$H=\{Q,Q^\dagger\}, \quad \{Q,Q\}=\{Q^\dagger,Q^\dagger\}=0, \quad [H,Q]=[H,Q^\dagger]=0, \tag{2.2}$$

where H is the sum of a (para)bosonic part $\frac{1}{2}\{a,a^\dagger\}$ and a (para)fermionic part $\frac{1}{2}[b^\dagger,b]$ as in SSQM. Indeed, we have defined, for the relative *parabosonic* set (2.1a) and (2.1b), the two supercharges

$$Q_{(1)}=\tfrac{1}{2}\{a,b\},\quad Q_{(1)}^{\dagger}=\tfrac{1}{2}\{b^{\dagger},a^{\dagger}\} \tag{2.3a}$$

and, in correspondence with the relativistic *parafermionic* set (2.1a) and (2.1c), the other two supercharges

$$Q_{(2)}=\tfrac{1}{2}[a,b],\quad Q_{(2)}^{\dagger}=\tfrac{1}{2}[b^{\dagger},a^{\dagger}], \tag{2.3b}$$

each context ensuring the relations (2.2). Physically speaking, these results mean that the superposition of parabosons with parafermions of order $p=2$ [but this is also true for *arbitrary* orders p (Ref. 18) iff the *same* orders of paraquantization are considered] leads to the rich concept of supersymmetry pointed out by superposing usual bosons and fermions. As we want to show and to exploit in the following, this property leads to a large number of ''reducibility problems,'' as mentioned in particular by Macfarlane[4] in his disconnected considerations on parabosons and parafermions. In fact, we will use the Green–Cusson Ansätze (as proposed in the next section) for illustrating this reducibility.

In order to shorten and to simplify our paper, let us immediately inform the reader that we plan, in the following, to limit ourselves to the explicit use of the relative parabosonic set with the characteristics (2.3a). In fact, all the corresponding developments can also be realized with the relative parafermionic set and the characteristics (2.3b), but they lead to the same conclusions, the resulting (para)supersymmetric Hamiltonian,

$$H=\tfrac{1}{2}\{a,a^{\dagger}\}+\tfrac{1}{2}[b^{\dagger},b], \tag{2.4}$$

being a common operator whose properties have already been pointed out.[18]

III. THE CONSTRUCTION OF A FOCK BASIS FROM THE GREEN–CUSSON ANSÄTZE

As SSQM cannot be deformed when only a pair of usual bosons and fermions are superposed (i.e., when one paraboson and one parafermion of order $p=1$ are superposed), let us go to the order $p=2$ of paraquantization, the first nontrivial order characterized by *trilinear* structure relations but maintaining the main properties of SSQM as recalled in the preceding section. Moreover, let us introduce the Green–Cusson Ansätze for $p=2$ parabosons as well as for $p=2$ parafermions, in order to construct an *ad hoc* Fock basis. This will help us in the realization of the corresponding operators (annihilation and creation ones, parasupercharges, etc.) when, as already chosen, we will consider operators belonging to the *relative parabosonic set* characterized by the structure relations (2.1a) and (2.1b).

Inside this set, let us denote as already mentioned $a(a^{\dagger})$ and $b(b^{\dagger})$ the corresponding annihilation (creation) operators for the paraboson and the parafermion, respectively, so that the Green–Cusson Ansätze can be expressed in terms of a pair of *two* (independent) bosonic oscillators [let us call them in the following a_1 and a_2, see Eq. (3.3a)] and of *four* (independent) fermionic ones [let us call then b_1, b_2, b_3, and f, see Eq. (3.3b)], the motivations for these last four ones having to be justified as follows. The relations (2.1a) and (2.1b) are satisfied if we realize the parabosonic and the parafermionic annihilation operators through the following Green–Cusson Ansätze.

$$a=\sum_{\alpha=1}^{p=2}A_{\alpha}\xi_{\alpha},\quad b=\sum_{\beta=1}^{p=2}B_{\beta}\xi_{\beta}, \tag{3.1}$$

respectively, with the relations[6]

$$\{\xi_{\alpha},\xi_{\beta}\}=2\,\delta_{\alpha\beta},\quad \xi_{\alpha}^{\dagger}=\xi_{\alpha},\quad \alpha,\beta=1,2, \tag{3.2a}$$

$$[A_\alpha, A_\beta^\dagger] = \delta_{\alpha\beta}, \quad \{B_\alpha, B_\beta^\dagger\} = \delta_{\alpha\beta}. \tag{3.2b}$$

The simultaneous consideration of (3.1) thus asks for a usual fermionic annihilation operator [let us call it f, $f \equiv \frac{1}{2}(\xi_1 - i\xi_2)$, see Eqs. (3.3) and (3.4)] besides the two usual bosonic operators A_1, A_2 implied by a in Eq. (3.1) and the two usual fermionic operators B_1, B_2 implied by b in Eq. (3.1) also. These two anticommuting [see Eq. (3.2b)] operators can be replaced by three commuting sets of fermions [see Eq. (3.46)] with

$$B_1 + iB_2 = \sqrt{2} b_1 (b_3 + b_3^\dagger)$$

and

$$B_1 - iB_2 = \sqrt{2} b_2 (b_3 - b_3^\dagger).$$

The Fock basis vectors will then be characterized by two ''eigenvalues'' n_1 and n_2 of the bosonic number operators N_1 and N_2 supplemented by four ''eigenvalues'' σ of the four fermionic number operators corresponding to the four types of necessary fermions. We evidently know that n_1, $n_2 = 0,1,2,...,\infty$ while σ takes only the values 0 or 1, so that we are interested in basis vectors labelled in the following way: $|n_1, n_2, \sigma_1, \sigma_2, \sigma_3, \sigma_4\rangle$. Due to the fact that the independent fermion f has to deal with the usual bosons as well as with the usual fermions, we have to take care of precise combinations inside the resulting Green–Cusson Ansätze. In fact, we explicitly have

$$a = \sqrt{2}(a_1 f + a_2 f^\dagger), \tag{3.3a}$$

where

$$a_1 \equiv \frac{1}{\sqrt{2}}(A_1 + iA_2), \quad a_2 \equiv \frac{1}{\sqrt{2}}(A_1 - iA_2),$$

and

$$b = \sqrt{2}[b_1 (b_3 + b_3^\dagger) f + b_2 (b_3 - b_3^\dagger) f^\dagger]. \tag{3.3b}$$

Let us remember that the independent character of these sets of bosons and fermions requires the relations

$$[a_\alpha, a_\alpha^\dagger] = 1, \quad [a_1, a_2] = 0, \quad \{f, f^\dagger\} = 1, \quad [a_\alpha, f] = 0, \quad \alpha = 1,2 \tag{3.4a}$$

and

$$\begin{gathered} \{b_j, b_j^\dagger\} = 1, \quad [b_j, b_k^\dagger] = 0 \quad (j \neq k), \\ [b_j, b_k] = 0, \quad [b_j, f] = 0, \quad [a_\alpha, b_j] = 0, \quad j,k = 1,2,3. \end{gathered} \tag{3.4b}$$

With such expressions (3.3) and their Hermitian conjugates, we can show that the relative parabosonic set is correctly realized when these operators act on the above Fock basis. A final useful refinement consists of distinguishing more specifically the subspaces corresponding to the eigenvalues $\sigma_4 = 0$ and $\sigma_4 = 1$ due to the specific role played by the fermion f with respect to the two bosons associated with a_1 and a_2 [see Eq. (3.3a)].

At this stage, we are thus interested in the action of a, $a^\dagger$, b, and $b^\dagger$ on the two kinds of states $|n_1, n_2, \sigma_1, \sigma_2, \sigma_3, 0\rangle$ and $|n_1, n_2; \sigma_1, \sigma_2, \sigma_3, 1\rangle$. If we recall[19] that usual bosonic operators are such that

$$a_\alpha|n_\alpha\rangle=\sqrt{n_\alpha}|n_\alpha-1\rangle,\quad a_\alpha^\dagger|n_\alpha\rangle=\sqrt{n_\alpha+1}|n_\alpha+1\rangle,\quad \alpha=1,2, \tag{3.5a}$$

while usual fermionic operators are characterized by

$$b_j|0\rangle=0,\quad b_j|1\rangle=|0\rangle,\quad b_j^\dagger|0\rangle=|1\rangle,\quad b_j^\dagger|1\rangle=0,\quad j=1,2,3,4, \tag{3.5b}$$

it is straightforward to get the following information by taking account of the definitions (3.3):

$$a|n_1,n_2;\sigma_1,\sigma_2,\sigma_3,0\rangle=\sqrt{2n_2}|n_1,n_2-1;\sigma_1,\sigma_2,\sigma_3 1\rangle, \tag{3.6a}$$

$$a|n_1,n_2;\sigma_1,\sigma_2,\sigma_3,1\rangle=\sqrt{2n_1}|n_1-1,n_2;\sigma_1,\sigma_2,\sigma_3,0\rangle, \tag{3.6b}$$

$$a^\dagger|n_1,n_2;\sigma_1,\sigma_2,\sigma_3,0\rangle=\sqrt{2(n_1+1)}|n_1+1,n_2;\sigma_1,\sigma_2,\sigma_3,1\rangle, \tag{3.6c}$$

$$a^\dagger|n_1,n_2;\sigma_1,\sigma_2,\sigma_3,1\rangle=\sqrt{2(n_2+1)}|n_1,n_2+1;\sigma_1,\sigma_2,\sigma_3,0\rangle, \tag{3.6d}$$

$$\begin{aligned} b|n_1,n_2;\sigma_1,\sigma_2,\sigma_3,0\rangle=&\sqrt{2\sigma_2\sigma_3}|n_1,n_2;\sigma_1,\sigma_2-1,\sigma_3-1,1\rangle\\ &-\sqrt{2\sigma_2(\sigma_3+1)}|n_1,n_2;\sigma_1,\sigma_2-1,\sigma_3+1,1\rangle, \end{aligned} \tag{3.6e}$$

$$\begin{aligned} b|n_1,n_2;\sigma_1,\sigma_2,\sigma_3,1\rangle=&\sqrt{2\sigma_1\sigma_3}|n_1,n_2;\sigma_1-1,\sigma_2,\sigma_3-1,0\rangle\\ &+\sqrt{2\sigma_1(\sigma_3+1)}|n_1,n_2;\sigma_1-1,\sigma_2,\sigma_3+1,0\rangle, \end{aligned} \tag{3.6f}$$

$$\begin{aligned} b^\dagger|n_1,n_2;\sigma_1,\sigma_2,\sigma_3,0\rangle=&\sqrt{2(\sigma_1+1)\sigma_3}|n_1,n_2;\sigma_1+1,\sigma_2,\sigma_3-1,1\rangle\\ &+\sqrt{2(\sigma_1+1)(\sigma_3+1)}|n_1,n_2;\sigma_1+1,\sigma_2,\sigma_3+1,1\rangle \end{aligned} \tag{3.6g}$$

and

$$\begin{aligned} b^\dagger|n_1,n_2;\sigma_1,\sigma_2,\sigma_3,1\rangle=&\sqrt{2(\sigma_2+1)(\sigma_3+1)}|n_1,n_2;\sigma_1,\sigma_2+1,\sigma_3+1,0\rangle\\ &-\sqrt{2(\sigma_2+1)\sigma_3}|n_1,n_2;\sigma_1,\sigma_2+1,\sigma_3-1,0\}. \end{aligned} \tag{3.6h}$$

Having these relations at our disposal, it is then easy to verify that all the trilinear relations (2.1a) and (2.1b) are satisfied on the Fock space characterized by the above basis

$$\{|n_1,n_2;\sigma_1,\sigma_2,\sigma_3,\sigma_4\rangle\}. \tag{3.7}$$

In order to complete the characteristics of SSQM in the context of the relative parabosonic set, we also have to give the action of the two ''supercharges'' (2.3a) and to confirm[6] that this set admits the simple Lie superalgebra osp(2|2,$\mathbb{R}$) as invariance algebra. Here we obtain

$$\begin{aligned} Q_{(1)}|n_1,n_2;\sigma_1,\sigma_2,\sigma_3,\sigma_4\rangle=&\sqrt{\sigma_1\sigma_3 n_2}|n_1,n_2-1;\sigma_1-1,\sigma_2,\sigma_3-1,\sigma_4\rangle+\sqrt{\sigma_1(\sigma_3+1)n_2}|n_1,n_2\\ &-1;\sigma_1-1,\sigma_2,\sigma_3+1,\sigma_4\rangle+\sqrt{\sigma_2\sigma_3 n_1}|n_1-1,n_2;\sigma_1,\sigma_2,-1,\sigma_3\\ &-1,\sigma_4\rangle-\sqrt{\sigma_2(\sigma_3+1)n_1}|n_1-1,n_2;\sigma_1,\sigma_2-1,\sigma_3+1,\sigma_4\rangle \end{aligned} \tag{3.8a}$$

and

$$Q_{(1)}^{\dagger}|n_1,n_2;\sigma_1,\sigma_2,\sigma_3,\sigma_4\rangle=\sqrt{(\sigma_1+1)\sigma_3(n_2+1)}|n_1,n_2+1;\sigma_1+1,\sigma_2,\sigma_3-1,\sigma_4\rangle$$
$$+\sqrt{(\sigma_1+1)(\sigma_3+1)(n_2+1)}|n_1,n_2+1;\sigma_1+1,\sigma_2,\sigma_3+1,\sigma_4\rangle$$
$$+\sqrt{(\sigma_2+1)(\sigma_3+1)(n_1+1)}|n_1+1,n_2;\sigma_1,\sigma_2+1,\sigma_3+1,\sigma_4\rangle$$
$$-\sqrt{(\sigma_2+1)\sigma_3(n_1+1)}|n_1+1,n_2;\sigma_1,\sigma_2+1,\sigma_3-1,\sigma_4\rangle, \quad (3.8b)$$

leading to the supersymmetric Hamiltonian [cf. Eq. (2.4)]

$$H|n_1,n_2;\sigma_1,\sigma_2,\sigma_3,\sigma_4\rangle=\{Q_{(1)},Q_{(1)}^{\dagger}\}|n_1,n_2;\sigma_1,\sigma_2,\sigma_3,\sigma_4\rangle$$
$$=(\tfrac{1}{2}\{a,a^{\dagger}\}+\tfrac{1}{2}[b^{\dagger},b])|n_1,n_2;\sigma_1,\sigma_2,\sigma_3,\sigma_4\rangle$$
$$=(H_{\mathrm{PB}}+H_{\mathrm{PF}})|n_1,n_2;\sigma_1,\sigma_2,\sigma_3,\sigma_4\rangle$$
$$=\{(\sigma_1+1)\sigma_3(n_2+1)+(\sigma_1+1)(\sigma_3+1)(n_2+1)+(\sigma_2+1)(\sigma_3+1)$$
$$\times(n_1+1)+(\sigma_2+1)\sigma_3(n_1+1)+\sigma_1\sigma_3 n_2+\sigma_1(\sigma_3+1)n_2+\sigma_2\sigma_3 n_1$$
$$+\sigma_2(\sigma_3+1)n_1\}|n_1,n_2;\sigma_1,\sigma_2,\sigma_3,\sigma_4\rangle. \quad (3.9)$$

A very simple discussion of the possible values of the four σs leads to 16 sets of eigenvectors labeled by the discrete numbers n_1 and n_2 which can take all non-negative integer values. In correspondence, we also find three parts of the energy spectrum distributed in subspectra characterized by n_1+n_2+2, n_1+n_2+1, and n_1+n_2, the last one ensuring already that we are dealing with an *exact* ''supersymmetry'' due to the possible values $n_1=n_2=0$.

Let us now complete the information on the invariance superalgebra osp$(2|2,\mathbb{R})$ through the five generators complementary to the three above ones called H, $Q_{(1)}$ and $Q_1^{\dagger}$, i.e., the operators

$$H'=\tfrac{1}{2}\{a,a^{\dagger}\}-\tfrac{1}{2}[b^{\dagger},b]=H_{\mathrm{PB}}-H_{\mathrm{PF}}, \quad (3.10a)$$

$$C_{+}=\tfrac{1}{2}\{a^{\dagger},a^{\dagger}\}, \quad C_{-}=\tfrac{1}{2}\{a,a\}, \quad (3.10b)$$

$$S=\tfrac{1}{2}\{b^{\dagger},a\}, \quad S^{\dagger}=\tfrac{1}{2}\{a^{\dagger},b\}, \quad (3.10c)$$

which have also a well-defined action on the basis (3.7). The eight generators of osp$(2|2,\mathbb{R})$ now help us to search for how many of the 16 sets of eigenvectors do survive according also to the well-known typical characteristics of parabosonic[2,20] and parafermionic[2] operators in the $p=2$ context. Effectively, in the parabosonic case, we have to distinguish between even and odd state vectors as follows:

$$a|2n\rangle=\sqrt{2n}|2n-1\rangle, \quad (3.11a)$$

$$a|2n+1\rangle=\sqrt{2n+2}|2n\rangle, \quad (3.11b)$$

while, in the parafermionic case, we have (due to the property $b^3=0$) to point out only three state vectors [remember the $D^{(1)}$ representation of su$(2,\mathbb{C})$]:

$$b|0\rangle=0, \quad b|1\rangle=\sqrt{2}|0\rangle, \quad b|2\rangle=\sqrt{2}|1\rangle. \quad (3.12)$$

Acceptable eigenvectors compatible with Eqs. (3.6e) and (3.12) are, for example, $|n_1,n_2;0,0,0,0\rangle$, $|n_1,n_2;1,0,1,1\rangle$, and $|n_1,n_2;1,1,0,0\rangle$, and the ladder operators Q, $Q^{\dagger}$, S, and $S^{\dagger}$ select *only* five more of the type $|n_1,n_2;1,0,1,0\rangle$, $|n_1,n_2;0,1,1,0\rangle$, $|n_1,n_2;1,1,0,1\rangle$, $|n_1,n_2;0,0,0,1\rangle$, and $|n_1,n_2;0,1,1,1\rangle$, so that such considerations show that there are eight sets of linearly independent

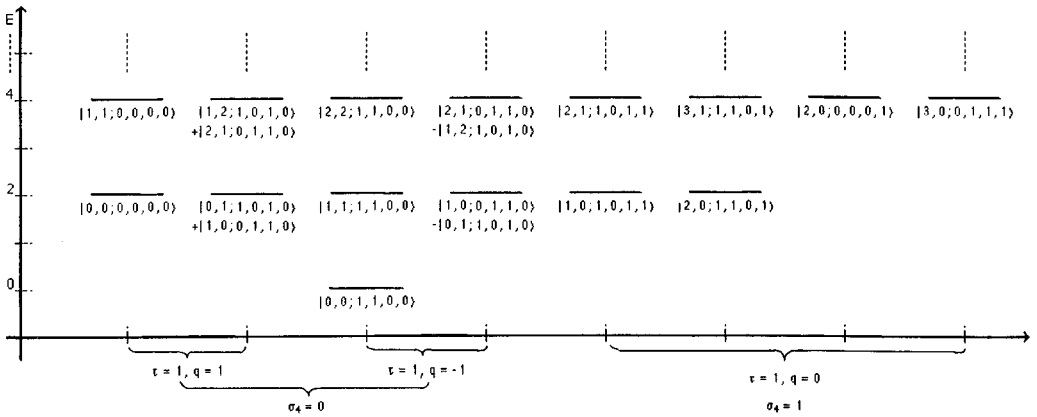

FIG. 1. The three subspectra associated with the three irreducible representations of osp (2/2;$\mathbb{R}$) displayed in our Fock space. The first two columns refer to the atypical ($\tau=1$, $q=1$) representation and the energy eigenvalues $E_n=2n+2$; the third and fourth columns to the atypical ($\tau=1$, $q=-1$) one and $E_n=2n$; the fifth to eighth columns to the typical ($\tau=1$, $q=0$) one and $E_n=2n+2$. The four columns on the left refer to the eigenvalue $\sigma_4=0$ while the four on the right refer to $\sigma_4=1$.

state vectors in the Fock basis (3.7). Moreover, by taking care of the requirements (3.11), we immediately notice that, if $\sigma_4=0$ or 1, the ''even'' vector states always have to be characterized by $n_1=n_2=n$, while the ''odd'' ones are such that $n_1=n+1$ and $n_2=n$.

By collecting all these details, our Fock basis is finally characterized by the following *eight* (families of) vectors ($n=0,1,2,...$),

$$|n,n;0,0,0,0\rangle,|n,n;1,1,0,0\rangle,|n,n+1;1,0,1,0\rangle,|n+1,n;0,1,1,0\rangle,|n+1,n;1,0,1,1\rangle,$$
$$|n+2,n;1,1,0,1\rangle,|n+1,n-1;0,0,0,1\rangle,|n+2,n-1;0,1,1,1\rangle. \tag{3.13}$$

By means of the supercharges (2.3a), the corresponding Hamiltonian (3.9), and its energy eigenvalue problem, it results that there are only three (infinite) irreducible representations of osp(2/2,$\mathbb{R}$) which appear in our Fock space, two of them being *atypical* ones and one being of the *typical* type. These properties are obtained through the study of the Casimir operator of osp(2/2, $\mathbb{R}$) and the well-known properties of the above Lie superalgebra.[16,21] Let us only recall that the Casimir operator here is given by

$$C=H_{\mathrm{PB}}^2-\tfrac{1}{2}\{C_+,C_-\}-H_{\mathrm{PF}}^2-[Q_+,Q_-]+[S_-,S_+] \tag{3.14}$$

and leads to eigenvalues $4(\tau^2-q^2)$. First, we get an *atypical* irreducible representation associated with the values $\tau=1$, $q=1$ (and evidently $C=0$) admitting twofold degeneracies for each energy eigenvalues $E_n=2n+2$, these results being characteristic of the family of eigenvectors $|n,n;0,0,0,0\rangle$. Second, there is another *atypical* one ($\tau=1$, $q=-1$, $C=0$), possible twofold degeneracies, $E_n=2n$ and $|n,n;1,1,0,0\rangle$. Third, there is a *typical* irreducible representation characterized by $\tau=1$, $q=0$ ($C=4$), showing possible fourfold degeneracies, $E_n=2n+2$ and $|n+1,n;1,0,1,1\rangle$. All the states vectors (3.13) are recovered by acting with the ladder operators $Q_{(1)}$ and $Q_{(1)}^{\dagger}$ and the complete spectrum is shown in Fig. 1, pointing out the whole set of eigenvalues and eigenvectors corresponding to $n=0,1,2,...$. Such a spectrum appears as the superposition of the three subspectra: we have only a fundamental state with zero energy (exact supersymmetry), six states with the energy eigenvalue equal to 2, and eight states with energy eigenvalue equal to all the even value 4,6,8,... .

Such results associated with our Fock basis show the reducibility obtained by having realized parabosonic and parafermionic operators through Green–Cusson Ansätze. This reducibility will be exploited in the following sections in order to get possible deformations.

IV. TOWARD DEFORMED PARABOSONIC AND PARAFERMIONIC OPERATORS

Having at our disposal an interesting Fock space, with precise information on its contents with respect to the irreducible representations of the invariance superalgebra osp(2/2, $\mathbb{R}$) of SSQM, let us now polarize our attention on the deformation of the symmetry operators. We notice that we recover here a completely parallel situation with respect to the pioneering contributions[22] for deforming the simple Lie algebra su(2,$\mathbb{C}$).

We want thus to deform more particularly the fundamental operators a and b given by Eqs. (3.1) and, correspondingly, the osp(2/2,$\mathbb{R}$) generators in the relative parabosonic context given by Eqs. (2.3a), (2.4), and (3.10).

Let us first take advantage of the generalized deformed parafermions recently proposed by Quesne.[11] In correspondence with the typical double commutator

$$[b,[b^\dagger,b]]=2b \tag{4.1}$$

contained in the set (2.1a), we propose to associate to the annihilation operator b of parafermion(s) a generalized deformed one—hereafter denoted B—defined by

$$b\rightarrow B=\frac{1}{2\sqrt{2}}\,(\sqrt{F_1}b^\dagger b^2+\sqrt{F_2}b^2b^\dagger), \tag{4.2}$$

where F_1 and F_2 are constants which, except for the particular case $F_1=F_2$, will assign a deformed character to B. We have to remember that, in the $p=2$ context, parafermionic operators are such that

$$b^2b^\dagger+b^\dagger b^2=2b, \quad bb^\dagger b=2b, \tag{4.3}$$

in perfect agreement with Eq. (4.1). When $F_1=F_2$, the two operators b and B are directly proportional and such a case does not interest us.

The second step now consists of the deformation of the parabosonic annihilation operator a. This context is not analogous to the parafermionic one due to the important different behavior of even or odd state vectors as already quoted in Eqs. (3.11). In order to circumvent this difficulty, we propose to introduce functions of the number operator N rather than constants entering into the deformed expression. Here, according to the peculiar relation (2.1a),

$$[a,\{a^\dagger,a\}]=2a, \tag{4.4}$$

and the corresponding $p=2$ property,

$$a^2a^\dagger-a^\dagger a^2=2a, \tag{4.5}$$

we suggest the association

$$a\rightarrow A=\frac{1}{2\sqrt{2}}\,(\sqrt{F_2(N)}a^2a^\dagger-\sqrt{F_1(N)}a^\dagger a^2), \tag{4.6}$$

where the number operator is as usual defined by

$$N=\tfrac{1}{2}\{a,a^\dagger\}-1=H_{\mathrm{PB}}-1 \tag{4.7}$$

characterized in the bosonic context resulting from Sec. III [see Eq. (3.3a), for example] by eigenvalues n_1+n_2 ($n_1,n_2=0,1,2,\ldots$). In passing, let us notice that the case $F_1(N)=F_2(N)$ still corresponds to a deformation in this parabosonic context due to the explicit dependence on N.

By taking care of the specificities introduced in Sec. III for the construction of the Fock basis (3.7), we can apply our new generalized deformed operators A, $A^\dagger$, B, and $B^\dagger$ and obtain the relations corresponding to Eqs. (3.6). By defining the special functions

$$G(n_1,n_2)=[(n_2+1)F_2(n_1+n_2)]^{1/2}(n_1+1)-[(n_2+1)F_1(n_1+n_2)]^{1/2}n_1, \tag{4.8}$$

we get the following information:

$$A|n_1,n_2;\sigma_1,\sigma_2,\sigma_3,0\rangle=G(n_1,n_2-1)|n_1,n_2-1;\sigma_1,\sigma_2,\sigma_3,1\rangle, \tag{4.9a}$$

$$A|n_1,n_2;\sigma_1,\sigma_2,\sigma_3,1\rangle=G(n_2,n_1-1)|n_1-1,n_2;\sigma_1,\sigma_2,\sigma_3,0\rangle, \tag{4.9b}$$

$$A^\dagger|n_1,n_2;\sigma_1,\sigma_2,\sigma_3,0\rangle=G(n_2,n_1)|n_1+1,n_2;\sigma_1,\sigma_2,\sigma_3,1\rangle, \tag{4.9c}$$

$$A^\dagger|n_1,n_2;\sigma_1,\sigma_2,\sigma_3,1\rangle=G(n_1,n_2)|n_1,n_2+1;\sigma_1,\sigma_2,\sigma_3,0\rangle, \tag{4.9d}$$

$$\begin{aligned}B|n_1,n_2;\sigma_1,\sigma_2,\sigma_3,0\rangle=&[\sigma_1\sigma_3\sqrt{F_1}+(\sigma_1+1)\sigma_3\sqrt{F_2}]\sqrt{\sigma_2\sigma_3}|n_1,n_2;\sigma_1,\sigma_2-1,\sigma_3-1,1\rangle\\&-[\sigma_1(\sigma_3+1)\sqrt{F_1}+(\sigma_1+1)(\sigma_3+1)\sqrt{F_2}]\sqrt{\sigma_2(\sigma_3+1)}\\&\times|n_1,n_2;\sigma_1,\sigma_2-1,\sigma_3+1,1\rangle,\end{aligned} \tag{4.9e}$$

$$\begin{aligned}B|n_1,n_2;\sigma_1,\sigma_2,\sigma_3,1\rangle=&[\sigma_2\sigma_3\sqrt{F_1}+(\sigma_2+1)\sigma_3\sqrt{F_2}]\sqrt{\sigma_1\sigma_3}|n_1,n_2;\sigma_1-1,\sigma_2,\sigma_3-1,0\rangle\\&+[\sigma_2(\sigma_3+1)\sqrt{F_1}+(\sigma_2+1)(\sigma_3+1)\sqrt{F_2}]\sqrt{\sigma_1(\sigma_3+1)}\\&\times|n_1,n_2;\sigma_1-1,\sigma_2,\sigma_3+1,0\rangle,\end{aligned} \tag{4.9f}$$

$$\begin{aligned}B^\dagger|n_1,n_2;\sigma_1,\sigma_2,\sigma_3,0\rangle=&[\sigma_2\sigma_3\sqrt{F_1}+(\sigma_2+1)\sigma_3\sqrt{F_2}]\sqrt{(\sigma_1+1)\sigma_3}|n_1,n_2;\sigma_1+1,\sigma_2,\sigma_3-1,1\rangle\\&+[\sigma_2(\sigma_3+1)\sqrt{F_1}+(\sigma_2+1)(\sigma_3+1,\sqrt{F_2}]\\&\times\sqrt{(\sigma_1+1)(\sigma_3+1)}|n_1,n_2;\sigma_1+1,\sigma_2,\sigma_3+1,1\rangle,\end{aligned} \tag{4.9g}$$

and

$$\begin{aligned}B^\dagger|n_1,n_2;\sigma_1,\sigma_2,\sigma_3,1\rangle=&[\sigma_1(\sigma_3+1)\sqrt{F_1}+(\sigma_1+1)(\sigma_3+1)\sqrt{F_2}]\sqrt{(\sigma_2+1)(\sigma_3+1)}\\&\times|n_1,n_2;\sigma_1,\sigma_2+1,\sigma_3+1,0\rangle-[\sigma_1\sigma_3\sqrt{F_1}+(\sigma_1+1)\sigma_3\sqrt{F_2}]\\&\times\sqrt{(\sigma_2+1)\sigma_3}|n_1,n_2;\sigma_1,\sigma_2+1,\sigma_3-1,0\rangle.\end{aligned} \tag{4.9h}$$

Let us insist on the fact that these relations are evidently in correspondence with Eqs. (3.6), the resulting state vectors being unchanged up to factors characterizing the deformation. Moreover, through the new deformed supercharges corresponding, for example, to the definitions (2.3a), i.e.,

$$Q_{(1)}=\tfrac{1}{2}\{A,B\},\quad Q_{(1)}^\dagger=\tfrac{1}{2}\{B^\dagger,A^\dagger\}, \tag{4.10}$$

the above relations (4.9) allow us to deduce constraints on the special functions (4.8) in order to discuss possible or impossible deformations of sqm (2), in particular.

So, by applying the operators (4.10) to the Fock state vectors (3.7), it is easy to test the relations (2.2) of the superalgebra sqm (2). An interesting result comes out immediately: by limiting our developments to the acceptable eigenvectors defined after Eqs. (3.12), we have to

mention that the expected nilpotencies ($Q_{(1)}^2 = Q_{(1)}^{\dagger 2} = 0$) are not true in general. They fail when applied to the families of state vectors $|n_1, n_2; 1,1,0,0\rangle$ and $|n_1, n_2; 1,1,0,1\rangle$, but are such that, on these states, we have (also evidently on the others)

$$Q_{(1)}^3 = 0. \tag{4.11}$$

Such a nilpotency calls for analyzing possible deformations in connection with parasupersymmetric developments[23,24] that will be discussed in the following section.

In order to be as complete as possible, let us go now to the eight explicit families of our Fock space subtended by the Lie superalgebra osp (2/2; $\mathbb{R}$) and its atypical and typical irreducible representations pointed out in the previous section.

V. ON POSSIBLE DEFORMATIONS OF sqm (2)

Let us mainly polarize our attention on the superalgebra sqm (2) seen as a subalgebra of osp (2/2; $\mathbb{R}$) in the above deformed context with the operators (4.2) and (4.6) and their actions (4.9). Explicit calculations lead to the results that $Q_{(1)}$, $Q_{(1)}^{\dagger}$, and H still admit only the eight families of state vectors that we have already mentioned in connection with the Casimir operator (3.14) and the atypical and typical representations associated with the spectrum of Fig. 1.

More precisely, let us mention that, on the states belonging to the atypical representation ($\tau = 1$, $q = 1$, $C = 0$), we have

$$\begin{aligned} Q_{(1)}|n,n;0,0,0,0\rangle &= 0, \\ Q_{(1)}(|n,n+1;1,0,1,0\rangle + |n+1,n;0,1,1,0\rangle) &= \sqrt{F_2}\,G(n,n)|n,n;0,0,0,0\rangle, \\ H|n,n;0,0,0,0\rangle &= \frac{F_2}{2}\,G^2(n,n)|n,n;0,0,0,0\rangle, \end{aligned} \tag{5.1}$$

and

$$H(|n,n+1;1,0,1,0\rangle + |n+1,n;0,1,1,0\rangle) = \frac{F_2}{2}\,G^2(n,n)(|n,n+1;1,0,1,0\rangle + |n+1,n;0,1,1,0,\rangle).$$

Double degeneracies are thus present, corresponding to eigenvalues $E_n \approx G^2(n,n)$ leading to a deformed superspectrum but to an undeformed superalgebra sqm (2) always characterized by the structure relations (2.2).

On the states belonging to the other atypical representation ($\tau = 1$, $q = -1$, $C = 0$), we also get relations similar to Eqs. (5.1), but here we have

$$\begin{aligned} Q_{(1)}|n,n;1,1,0,0\rangle &= -\frac{\sqrt{F_1}}{2}\,G(n,n-1)(|n-1,n;1,0,1,0\rangle - |n,n-1;0,1,1,0\rangle), \\ Q_{(1)}(|n-1;n;1,0,1,0\rangle - |n,n-1;0,1,1,0\rangle) &= 0, \\ H|n,n;1,1,0,0\rangle &= \frac{F_1}{2}\,G(n,n-1)|n;1,1,0,0\rangle \end{aligned} \tag{5.2}$$

and

$$H(|n-1,n;1,0,1,0\rangle - |n,n-1;0,1,1,0\rangle) = \frac{F_1}{2}\,G^2(n,n-1)(|n-1,n;1,0,1,0\rangle - |n,n-1;0,1,1,0\rangle).$$

In this case, we point out the existence of a null energy eigenvalue due to the property (4.9a) when $n_1=n_2=n=0$ and its implication $G(0,-1)=0$. Moreover, the other energy eigenvalues are once again doubly degenerated and are such that $E_{n+1}\approx G^2(n+1,n)$. We thus obtain a new deformed superspectrum but an undeformed superalgebra sqm (2).

The third irreducible representation, i.e., the typical ($\tau=1$, $q=0$) one, will happily give us the opportunity to open some possibilities of deformations of sqm (2). Indeed, if we notice that

$$Q_{(1)}|n+2,n-1;0,1,1,1\rangle=\frac{\sqrt{F_2}}{2}\,G(n-1,n+1)|n+1,n-1;0,0,0,1\rangle,$$

$$Q_{(1)}|n+1,n;1,0,1,1\rangle=\frac{\sqrt{F_2}}{2}\,G(n+1,n-1)|n+1,n-1;0,0,0,1\rangle, \tag{5.3}$$

$$Q_{(1)}|n+2,n;1,1,0,1\rangle=\frac{\sqrt{F_1}}{2}\,[G(n+2,n-1)|n+2,n-1;0,1,1,1\rangle-G(n,n+1)|n+1,n;1,0,1,1\rangle],$$

and

$$Q_{(1)}|n+1,n-1;0,0,0,1\rangle=0,$$

we evidently get

$$Q_{(1)}^2|n+2,n;1,1,0,1\rangle=\frac{\sqrt{F_1F_2}}{4}\,[G(n+2,n-1)G(n-1,n+1)-G(n,n+1)G(n+1,n-1)]$$
$$\times|n+1,n-1;0,0,0,1\rangle \tag{5.4}$$

and

$$Q_{(1)}^3|n+2,n;1,1,0,1\rangle=0. \tag{5.5}$$

The nilpotencies of sqm (2) [see Eqs. (2.2)] are thus only ensured iff

$$G(n+2,n-1)G(n-1,n+1)=G(n,n+1)G(n+1,n-1), \tag{5.6}$$

leading once again to a deformed spectrum but to an undeformed structure. In this case, a convenient choice for the functions G ensuring Eq. (5.6) is, for example,

$$G(x,y)=[(y+1)f(y)F_1]^{1/2}\quad\text{for even}\quad|x-y| \tag{5.7a}$$

and

$$G(x,y)=[(y+1)f(y)F_2]^{1/2}\quad\text{for odd}\quad|x-y|. \tag{5.7b}$$

Then, simple calculations lead to a diagonal super-Hamiltonian whose spectrum has the same configuration as the one contained in the four columns on the right of Fig. 1, *but* with the energy eigenvalues given by

$$E_n^{(d)}=nf(n-1)+(n+2)f(n+1),\quad n=0,1,2,\ldots\ . \tag{5.8}$$

the upper index (d) referring to the deformed spectrum. Remembering that this context corresponds to the undeformed eigenvalues $E_n=2n+2$, we understand their relation by noticing that, within our choice, the undeformed function $f(x)$ has to become one.

Let us end this section by coming back on the only context leading to possible deformations of sqm (2), i.e., when Eq. (5.6) is *not* valid, so that we have the constraints (5.4) and (5.5), the last one looking like a nilpotency typical of $p=2$ parastatistical developments.[2] Within our Fock basis and its typical representation ($\tau=1$, $q=0$, $C\neq 0$), the missing information is now only transferred on the corresponding Hamiltonian. *As an example*, let us require *trilinear* relations defining H as it is the case in the parasupersymmetric quantum context[23] but with three unknown complex constants c_i $(i=1,2,3)$, i.e.,

$$c_1 Q_{(1)}^2 Q_{(1)}^\dagger + c_2 Q_{(1)}^\dagger Q_{(1)}^2 + c_3 Q_{(1)} Q_{(1)}^\dagger Q_{(1)} = H Q_{(1)}, \tag{5.9}$$

besides evidently the necessary relations (4.11) and

$$[Q_{(1)}, H]=0, \quad [Q_{(1)}^\dagger, H]=0. \tag{5.10}$$

Now, by defining

$$G(x,y)=[(y+1)f(x)F_1]^{1/2} \quad \text{for even } |x-y| \tag{5.11a}$$

and

$$G(x,y)=[(y+1)f(x)F_2]^{1/2} \quad \text{for odd } |x-y|, \tag{5.11b}$$

and by asking that

$$f(n+2)f(n-1)\neq f(n)f(n+1) \quad \forall n=0,1,2,\ldots, \tag{5.12}$$

we can search for the corresponding spectrum of H in terms of these functions f and the constants c_i $(i=1,2,3)$. In that way, six constraints are put in evidence and lead to a specific discussion not reproduced here for brevity. Let us only point out that, if we choose $c_1=c_2=0$, $c_3=1$, and the following values,

$$f(4n)=-3n, \quad f(4n+1)=n+1, \quad f(4n+2)=3n+2, \quad f(4n+3)=-n-1, \tag{5.13}$$

we can recover the spectrum of the supersymmetric harmonic oscillator but with further degeneracies in comparison with old results.[25] In that way, we can interpret the Rubakov–Spiridonov structure[23] as a deformation of sqm(2). The other case $c_1=c_2=1$, $c_3=0$, is also interesting: it shows that the Beckers–Debergh structure[24] does not appear as a deformation of sqm(2), this property acting once again the nonequivalence of these two approaches of parasupersymmetric quantum mechanics.[23,24]

As a final comment, let us mention that, if we come back to the relations (5.3), it is not difficult to realize the charge $Q_{(1)}$ as a 4×4 matrix and to realize, for example, the Beckers–Debergh structure[24] by constraining the different functions $G(x,y)$ and constants F_1 and F_2. Applied to the particular context of the harmonic oscillator with angular frequency ω, we get the conditions

$$\begin{aligned}
&F_2^{1/2} G(n+1,n-1)=2\sqrt{n\omega}=F_2^{1/2}[(n+2)\sqrt{nF_2(2n)}-(n+1)\sqrt{nF_1(2n)}],\\
&F_1^{1/2} G(n,n+1)=2\sqrt{n\omega}=F_1^{1/2}[(n+1)\sqrt{(n+2)F_2(2n+1)}-n\sqrt{(n+2)F_1(2n+1)}],\\
&G(n+2,n-1)=-2\sqrt{n\omega}=F_1^{1/2}[(n+3)\sqrt{nF_2(2n+1)}-(n+2)\sqrt{nF_1(2n+1)}],
\end{aligned} \tag{5.14}$$

and

$$F_2^{1/2}G(n-1,n+1)=2\sqrt{n\omega}=F_2^{1/2}[n\sqrt{(n+2)F_2(2n)}-(n-1)\sqrt{(n+2)F_1(2n)}],$$

where, besides the constants F_1 and F_2, we have taken care of the relations (4.8) in terms of the deformed functions $F_1(x)$ and $F_2(x)$. Consistency relations impose

$$\begin{gathered}F_1(0)=0,\quad F_2(0)=\frac{\omega}{F_2},\quad F_1(1)=\frac{\omega}{F_1},\quad F_2(1)=0,\\ [F_1(2n)]^{1/2}\geqslant 0,\quad [F_2(2n)]^{1/2}\geqslant 0,\quad [F_1(2n+1)]^{1/2}\geqslant 0,\quad [F_2(2n+1)]^{1/2}\geqslant 0,\end{gathered}\tag{5.15}$$

and the Beckers–Debergh structure will be a deformation of sqm (2) under the following set of final conditions for each $n=0,1,2,...$:

$$\begin{aligned}[F_1(2n)]^{1/2}&=\sqrt{\frac{\omega n}{F_2}}\,(\sqrt{n+2}-\sqrt{n}),\\ [F_2(2n)]^{1/2}&=\frac{1}{n+2}\,\sqrt{\frac{\omega}{F_2}}\,((n+1)\sqrt{n}(\sqrt{n+2}-\sqrt{n})+2),\\ [F_1(2n+1)]^{1/2}&=\sqrt{\frac{\omega}{F_1}}\left(n+1+(n+3)\sqrt{\frac{n}{n+2}}\right),\\ [F_2(2n+1)]^{1/2}&=\sqrt{\frac{\omega n}{F_1}}\,(\sqrt{n+2}+\sqrt{n}).\end{aligned}\tag{5.16}$$

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Becchi–Rouet–Stora cohomology of zero curvature systems. I. The complete ladder case

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We present here the zero curvature formulation for a wide class of field theory models. This formalism, which relies on the existence of an operator δ which decomposes the exterior space–time derivative as a BRS commutator, turns out to be particularly useful in order to solve the Wess–Zumino consistency condition. The examples of the topological theories and of the $B-C$ string ghost system are considered in detail. © *1996 American Institute of Physics.*
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I. INTRODUCTION

Nowadays it is an established fact that the search for the possible anomalies and for the counterterms which arise at the quantum level in local field theories can be done in a purely algebraic way[1] by identifying the cohomology classes of the nilpotent Becchi–Rouet–Stora (BRS) operator b in the space of the integrated local polynomials in the fields and their derivatives. This means that one has to look at the nontrivial solutions of the equation

$$b\int \omega_D^G = 0, \tag{1}$$

ω_D^G denoting a local polynomial in the fields of ghost number G and form degree D, D being the dimension of the space–time. The cases $G=0,1$ correspond, respectively, to counterterms and anomalies.

The BRS consistency condition (1), when translated at the nonintegrated level, yields a system of equations usually called descent equations (see Ref. 1 and references therein)

$$\begin{gathered} b\omega_D^G + d\omega_{D-1}^{G+1} = 0, \quad b\omega_{D-1}^{G+1} + d\omega_{D-2}^{G+2} = 0, \\ \cdots \\ \cdots \\ b\omega_1^{G+D-1} + d\omega_0^{G+D} = 0, \quad b\omega_0^{G+D} = 0, \end{gathered} \tag{2}$$

$d = dx^\mu \partial_\mu$ being the exterior space–time derivative and ω_j^{G+D-j} $(0 \leqslant j \leqslant D)$ being the local polynomials of ghost number $(G+D-j)$ and form degree j. The operators b and d obey the algebraic relations

$$b^2 = d^2 = bd + db = 0. \tag{3}$$

It should be remarked that at the nonintegrated level one loses the property of making integration by parts. This implies that the fields and their derivatives have to be considered as independent variables.

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The problem of solving the descent equations (2) is a problem of cohomology of b modulo d, the corresponding cohomology classes being given by solutions of (2) which are not of the type

$$\omega_m^{G+D-m} = b\,\hat{\omega}_m^{G+D-m-1} + d\,\hat{\omega}_{m-1}^{G+D-m}, \quad 1 \leqslant m \leqslant D,$$
$$\omega_0^{G+D} = b\,\hat{\omega}_0^{G+D-1}, \tag{4}$$

with $\hat{\omega}$'s being local polynomials.

Recently a new method for finding nontrivial solutions of the tower (2) has been proposed by one of the authors[2] and successfully applied to a large number of field models such as Yang–Mills theories,[3] gravity,[4–6] topological field theories,[7–9] string[10] and superstring[11] theories, as well as W_3-algebras.[12] The method relies on the introduction of an operator δ which allows the decomposition of the exterior derivative as a BRS commutator, i.e.,

$$d = -[b,\ \delta]. \tag{5}$$

It is easily proven that, once the decomposition (5) has been found, repeated applications of the operator δ on the polynomial ω_0^{G+D} which solves the last of the equations (2) will give an explicit nontrivial solution for the higher cocycles ω_j^{G+D-j}.

One has to note that solving the last equation of the tower (2) is a problem of local cohomology instead of a modulo-d one. Moreover, the former can be systematically attacked by using several methods such as, for instance, the spectral sequences technique.[13] It is also worth mentioning that the solutions of the descent equations (2) obtained via the decomposition (5) have been proven to be equivalent to those provided by the transgression procedure based on the so-called *Russian Formula*.[14,15]

The aim of the present work is twofold: first, to improve and extend the results obtained in Ref. 2 and, second, to discuss the deep relation between the existence of the operator δ entering the decomposition (5) and the possibility of encoding all the relevant informations (BRS transformations of the fields, BRS cohomology classes, solutions of the descent equations) into a unique equation which takes the form of a generalized zero curvature condition:

$$\tilde{\mathscr{F}} = \tilde{d}.\tilde{\mathscr{A}} - i.\tilde{\mathscr{A}}^2 = 0. \tag{6}$$

The operator $\tilde{d}$ and the generalized gauge connection $\tilde{\mathscr{A}}$ in Eq. (6) turn out to be respectively the δ-transform of the BRS operator b and of the ghost field c corresponding to the Maurer–Cartan form of the underlying gauge algebra

$$\tilde{d} = e^{\delta} b e^{-\delta} = b + d + \cdots, \quad \tilde{d}^2 = 0,$$
$$\tilde{\mathscr{A}} = e^{\delta} c = c + \cdots\ . \tag{7}$$

The main purpose of this work will be that of clarifying the meaning of the generalized gauge connection $\tilde{\mathscr{A}}$ and of the dots $\cdots$ appearing in Eq. (7) with the help of several examples.

In particular, as we shall see, the zero-curvature condition (6) immediately yields the cohomology classes of the generalized operator $\tilde{d}$,[16] the nilpotency of which being a direct consequence of the zero curvature condition (6). The latter turns out to be naturally related to the solutions of the descent equations (2). In other words, once the zero-curvature condition of the model under consideration has been established, the problem of finding the anomalies and the invariant actions becomes straightforward to be solved.

For the sake of completeness and in order to present several detailed models, the paper has been split in two parts, referred as part I and part II. This division corresponds to two different situations, called, respectively, the *complete* and the *noncomplete* ladder case. In the first case the

components of the generalized gauge connection $\tilde{\mathscr{A}}$ form a ladder of fields which span all possible form degrees compatible with the space–time dimension D, i.e., ordering the components of $\tilde{\mathscr{A}}$ according to their increasing form degree p, the allowed interval $0 \leqslant p \leqslant D$, is fully covered. Instead, in the noncomplete ladder case the maximum form degree reached by the components of $\tilde{\mathscr{A}}$ is strictly lower than the space–time dimension D, i.e., $0 \leqslant p < D$. Examples of models belonging to the first case are, for instance, the topological models of the Schwartz type such as the Chern–Simons and the BF models,[17] and the B-C ghost system of the bosonic string theory.[18] On the other hand, the Yang–Mills-type theories can be accommodated in the noncomplete ladder case.

As we shall see in details in the next sections, this means that we shall deal with a generalized gauge connection $\tilde{\mathscr{A}}$ which takes respectively the following forms:

$$\tilde{\mathscr{A}} = \sum_{j=0}^{D} \varphi_j^{1-j} = \varphi_0^1 + \varphi_1^0 + \varphi_2^{-1} + \cdots + \varphi_D^{1-D}, \quad \text{complete ladder case,} \tag{8}$$

and

$$\tilde{\mathscr{A}} = \sum_{j=0}^{q<D} \varphi_j^{1-j} = \varphi_0^1 + \varphi_1^0 + \varphi_2^{-1} + \cdots + \varphi_q^{1-q}, \quad \text{noncomplete ladder case,} \tag{9}$$

where the set $\{\varphi_j^{1-j}\}$ denotes generically the field content which will be used through the work, the indices $(1-j)$ and j identifying respectively the ghost number and the form degree. One has to note that in writing the expressions (8) and (9) we have tacitly assumed that the class of models which we shall consider can be indeed described in terms of the form-valued fields $\{\varphi_j^{1-j}\}$ appearing in Eqs. (8) and (9) and of their exterior derivatives. In other words, we shall assume that the descent equations (2) will be restricted to the functional space of form-valued polynomials in the fields $\{\varphi_j^{1-j}\}$ and their differentials. Of course, the same assumption holds for the decomposition (5).

It is worthwhile to recall here that in the case of the aforementioned topological models this assumption is in fact realized. As it is well known,[7–9,17,19] this is due to the fact that the topological models turn out to be characterized by a set of fields which can be naturally accommodated in a complete ladder.

For where it concerns the Yang–Mills-type theories, it should also be remarked that the use of the space of the form-valued polynomials is not the most general one. Indeed such a functional space does not allow us to obtain all possible Yang–Mills actions,[20] due to the absence of the space–time metric tensor. However, as proven in Refs. 15 and 21, the space of polynomials of forms turns out to be bigger in half to include the anomalies and the Chern–Simons-type actions which, due to their topological character,[14] can be systematically written in terms of differential forms. Therefore also in the noncomplete ladder case, we shall limit ourselves to the algebraic characterization of topological objects like anomalies and Chern–Simons terms.

Even if many properties of the models covered by the complete ladder case have already been investigated,[8,19] their zero curvature formulation still represents a very elegant and interesting aspect. Moreover, in the noncomplete case, the zero curvature condition (6) requires the existence of a set of new operators $(\mathscr{G}_k^{1-k},\ 2 \leqslant k \leqslant D)$ which are in involution, i.e., the operator $\mathscr{G}_k^{1-k}$ is generated by the commutator between $\mathscr{G}_{k-1}^{2-k}$ and the operator δ of (5), according to the recursive formula

$$\mathscr{G}_2^{-1}=\tfrac{1}{2}[\delta,d],$$
$$\mathscr{G}_k^{1-k}=\frac{1}{k}[\delta,\mathscr{G}_{k-1}^{2-k}],\quad k>2. \tag{10}$$

This structure naturally reminds us of the recursive construction of the Lax pair operators of the integrable systems.[22] This is a quite welcome and attractive feature which may signal a deeper relation between the BRS cohomology techniques and the integrability. Needless to say, the zero-curvature condition represents in fact one of the most important chapters of the integrable systems (see also the recent works of Ref. 23).

This paper (referred to as part I) is organized as follows. In Sec. II the general algebraic setup is presented. In Sec. III we discuss the geometrical meaning of the zero-curvature condition. Sections IV and V are devoted, respectively, to the computation of the BRS cohomology and to characterizing the solution of the descent equations. In Sec. VI we deal with the coupling with matter fields in the context of the BF models. Without entering in details, let us briefly comment that, in analogy with the gauge ladder $\tilde{\mathscr{A}}$, the matter fields can be introduced by means of a second complete ladder $\tilde{\mathscr{B}}$ constrained by the requirement of being covariantly constant with respect to the gauge ladder, i.e.,

$$\tilde{\mathscr{D}}\tilde{\mathscr{B}}=\tilde{d}\tilde{\mathscr{B}}-i[\tilde{\mathscr{A}},\tilde{\mathscr{B}}]=0. \tag{11}$$

As we shall see, condition (11) completely characterizes the BRS transformations of the various components of $\tilde{\mathscr{B}}$.

Finally, Sec. VII contains a detailed discussion of the zero-curvature formulation of the $B-C$ string ghost system.

II. THE GENERAL SETUP

In order to present the general algebraic setup, let us begin by fixing the notations. As already said in the Introduction, we shall work in a space–time of dimension D equipped with a set of fields generically denoted by $\{\varphi_q^p\}$, q and p being, respectively, the form degree and the ghost number. The components φ_q^p will be treated as commuting or anticommuting variables according to the fact that their total degree, i.e., the sum $(q+p)$, is even or odd. Otherwise stated, the φ_q^p are Lie algebra valued, $\varphi_q^p=(\varphi_q^p)^a T^a$, T^a being the Hermitian generators of a compact semisimple Lie group G. Moreover, these fields are assumed to be collected into a unique generalized complete field $\tilde{\mathscr{A}}$ of total degree one, i.e.,

$$\tilde{\mathscr{A}}=\sum_{j=0}^{D}\varphi_j^{1-j}=\varphi_0^1+\varphi_1^0+\varphi_2^{-1}+\cdots+\varphi_D^{1-D}. \tag{12}$$

The name complete is due to the fact that the field content of the expansion (12) spans all possible form degrees. In addition, Eq. (12) shows that the generalized field $\tilde{\mathscr{A}}$ contains a zero form with ghost number one φ_0^1, and a one-form with ghost number zero φ_1^0. These fields will be naturally identified with the Faddeev–Popov ghost field and with the gauge connection of the familiar Yang–Mills gauge transformations. Therefore $\tilde{\mathscr{A}}$ will be called the gauge ladder and the components φ_0^1 and φ_1^0 will be denoted, respectively, by c and A, so that

$$\tilde{\mathscr{A}}=c+A+\varphi_2^{-1}+\cdots+\varphi_D^{1-D}. \tag{13}$$

Finally, as already remarked, the functional space $\mathscr{V}$ the BRS operator b acts upon is the space of the form-valued polynomials in the fields φ_j^{1-j} and their differentials, i.e.,

$$\mathscr{V}=\text{polynomials in } (\varphi_j^{1-j}, d\varphi_j^{1-j}; 0\leqslant j\leqslant D), \tag{14}$$

d being the exterior derivative defined as

$$d\eta_p = dx^\mu \partial_\mu \eta_p \tag{15}$$

for any p-form

$$\eta_p = \frac{1}{p!}\ \eta_{i_1\cdots i_p} dx^{i_1}\cdots dx^{i_p}, \tag{16}$$

where a wedge product has to be understood. Observe also that $d\varphi_D^{1-D}$ automatically vanishes, due to the dimension of the space–time.

In order to obtain the BRS transformations of the fields belonging to the gauge ladder (13), we introduce the generalized operator of total degree one (*we recall here that the operators* b *and* d *raise respectively the ghost number and the form degree by one unit*)

$$\tilde{d} = b + d, \tag{17}$$

and we impose the zero curvature condition

$$\tilde{d}\tilde{\mathscr{A}} = i\tilde{\mathscr{A}}^2 = \frac{i}{2}[\tilde{\mathscr{A}}, \tilde{\mathscr{A}}], \tag{18}$$

where $[a,b]=ab-(-1)^{|a||b|}ba$ denotes the graded commutator and $|a|$ is the total degree of a.

Developing equation (18) in components and identifying the terms with the same ghost number and form degree, we obtain the following transformations:

$$bc = ic^2, \quad bA = -dc + i[c,A], \tag{19}$$

$$b\varphi_j^{1-j} = -d\varphi_{j-1}^{2-j} + \frac{i}{2}\sum_{m=0}^{j}[\varphi_m^{1-m}, \varphi_{j-m}^{1-j+m}], \quad 2\leqslant j\leqslant D,$$

which are easily checked to be nilpotent.

$$b^2 = 0. \tag{20}$$

Notice that, as announced, the transformations of the first two components of the ladder $\tilde{\mathscr{A}}$ are nothing but the familiar BRS transformations of the Faddeev–Popov ghost and of the Yang–Mills gauge connection.

Let us introduce now the operator δ defined by (see also Refs. 1, 4, and 8)

$$\tilde{\mathscr{A}} = e^{\delta} c, \tag{21}$$

i.e.,

$$\delta\varphi_j^{1-j} = (j+1)\varphi_{j+1}^{-j}, \quad 0\leqslant j\leqslant D-1, \quad \delta\varphi_D^{1-D} = 0. \tag{22}$$

Its action extends on the differentials $(d\varphi_j^{1-j},\ 0\leqslant j\leqslant D)$ as

$$\begin{aligned} &\delta d\varphi_j^{1-j} = (j+1)d\varphi_{j+1}^{-j}, \quad 0\leqslant j\leqslant D-2, \\ &\delta d\varphi_{D-1}^{2-D} = 0. \end{aligned} \tag{23}$$

It is easily verified then that, on the functional space $\mathscr{V}$, the operators b and δ obey

$$d=-[b,\delta],\quad [d,\delta]=0, \tag{24}$$

i.e., δ allows the decomposition of the exterior derivative as a BRS commutator.

Equations (22) and (23) show that the operator δ increases the form degree by one unit and decreases the ghost number by the same amount, so that it has total degree zero. In particular from Eq. (24) it follows that

$$\tilde{d}=b+d=e^{\delta}be^{-\delta}. \tag{25}$$

III. THE GEOMETRICAL MEANING OF THE ZERO-CURVATURE CONDITION

In the previous section the BRS transformations of the component fields φ_j^{1-j} have been obtained as a consequence of the zero-curvature condition (18).

Conversely, it is very simple to show that, assuming the BRS transformations (19) hold, the zero-curvature condition can be derived as a consequence of the existence of the operator δ. Indeed, applying e^{δ} to the BRS transformation of the ghost field c, i.e.,

$$e^{\delta}be^{-\delta}e^{\delta}c=ie^{\delta}c^2, \tag{26}$$

and making use of Eq. (21) and (25), one gets the zero-curvature condition

$$\tilde{d}\tilde{\mathscr{A}}=i\tilde{\mathscr{A}}^2. \tag{27}$$

This is not surprising since, as it is well known, the ghost field c identifies the so-called Maurer–Cartan form of the gauge group G, and its BRS transformation is nothing but the corresponding Maurer–Cartan equation,[24] which is in fact a zero-curvature condition. This is the geometrical meaning of Eq. (18).

IV. COHOMOLOGY OF THE BRS OPERATOR

Even if the cohomology of the BRS operator in the case of a complete ladder field has already been studied,[8] let us present here a simple derivation which may be useful for the reader.

In order to compute the cohomology of the BRS operator b on the functional space $\mathscr{V}$, we introduce the filtering operator[1,13] $\mathscr{N}$ defined as

$$\begin{aligned}&\mathscr{N}\varphi_j^{1-j}=\varphi_j^{1-j},\quad 0\leqslant j\leqslant D,\\ &\mathscr{N}d\varphi_j^{1-j}=d\varphi_j^{1-j},\end{aligned} \tag{28}$$

according to which the BRS operator b decomposes as

$$b=b_0+b_1, \tag{29}$$

with

$$b_0c=0,\quad b_0\varphi_m^{1-m}=-d\varphi_{m-1}^{2-m},\quad b_0d\varphi_{m-1}^{2-m}=0,\quad 1\leqslant m\leqslant D, \tag{30}$$

and

$$b_0^2=0. \tag{31}$$

The usefulness of the above decomposition relies on a very general theorem on the BRS cohomology.[13] The latter states that the cohomology of the operator b is isomorphic to a subspace of the cohomology of b_0. We focus then on the study of the cohomology of b_0.

In particular, Eq. (30) shows that all the fields $(\varphi_m^{1-m},\ 1\leqslant m\leqslant D)$ with form degree greater than zero and their differentials are grouped in BRS doublets.[1,13,21] It is known that the cohomology does not depend on such variables. Therefore the cohomology classes of b_0 depend only on the ghost field c undifferentiated, i.e., they are given by elements of the type

$$\omega_{i_1\cdots i_n}c^{i_1}\cdots c^{i_n} \tag{32}$$

with $\omega_{i_1\cdots i_n}$ arbitrary coefficients. Moreover, from the previous theorem it follows that the cohomology of b is also given by elements of the form (32) with, in addition, the restriction that the coefficients $\omega_{i_1\cdots i_n}$ are invariant tensors of the gauge group.[15,20,21,25]

In summary, the cohomology of the BRS operator b in the complete ladder case is spanned by invariant polynomials in the ghost field c built up with monomials of the type

$$\mathrm{Tr}\left(\frac{c^{2n+1}}{(2n+1)!}\right),\quad n\geqslant 1. \tag{33}$$

V. SOLUTION OF THE DESCENT EQUATIONS

Having computed the cohomology of the BRS operator b, let us face now the problem of solving the descent equations

$$\begin{gathered} b\omega_{D-j}^{G+j}+d\omega_{D-j-1}^{G+j+1}=0,\quad 0\leqslant j\leqslant D-1,\\ b\omega_0^{G+D}=0. \end{gathered} \tag{34}$$

Introducing the generalized cocycle of total degree $(G+D)$

$$\tilde{\omega}^{G+D}=\sum_{j=0}^{D}\omega_j^{G+D-j}, \tag{35}$$

the descent equations (34) can be cast in the more compact form

$$\tilde{d}\tilde{\omega}^{G+D}=0, \tag{36}$$

$\tilde{d}$ being the nilpotent generalized differential of Eq. (25). Taking into account the zero-curvature condition

$$\tilde{d}\tilde{\mathscr{A}}=i\tilde{\mathscr{A}}^2 \tag{37}$$

and the previous result (33) on the cohomology of the BRS operator b, it follows that the generalized monomials of the type

$$\mathrm{Tr}\,\frac{\tilde{\mathscr{A}}^{2n+1}}{(2n+1)!},\quad n\geqslant 1, \tag{38}$$

belongs to the cohomology of $\tilde{d}$,

$$\tilde{d}\left(\mathrm{Tr}\,\frac{\tilde{\mathscr{A}}^{2n+1}}{(2n+1)!}\right)=0,\quad \mathrm{Tr}\,\frac{\tilde{\mathscr{A}}^{2n+1}}{(2n+1)!}\neq\tilde{d}\tilde{\mathscr{Q}}^{2n}, \tag{39}$$

for any local polynomial $\tilde{\mathcal{Q}}^{2n}$.

Thus it is apparent that a solution of the descent equations (34) is simply provided by

$$\tilde{\omega}^{G+D}=\mathrm{Tr}\,\frac{\tilde{\mathscr{A}}^{G+D}}{(G+D)!}, \tag{40}$$

which, of course, is nonvanishing only if its total degree $(G+D)$ is odd. In fact, developing $(\mathrm{Tr}\,\tilde{\mathscr{A}}^{G+D})$ according to the form degree and to the ghost number

$$\left(\mathrm{Tr}\,\frac{\tilde{\mathscr{A}}^{G+D}}{(G+D)!}\right)=\sum_{j=0}^{D}\omega_j^{G+D-j}, \tag{41}$$

and recalling that $\tilde{d}\tilde{\omega}^{G+D}=0$, it is easily verified that the ω's in Eq. (41) obey

$$\begin{aligned} b\,\omega_{D-j}^{G+j}+d\,\omega_{D-j-1}^{G+j+1}&=0,\\ b\,\omega_0^{G+D}&=0, \end{aligned} \tag{42}$$

i.e., they solve the descent equations.

In addition, from $(\mathrm{Tr}\,\tilde{\mathscr{A}}^{2n+1}\neq\tilde{d}\tilde{\mathcal{Q}}^{2n})$, it follows that they provide a nontrivial solution

$$\begin{aligned} \omega_j^{G+D-j}&\neq b\mathcal{Q}_j^{G+D-1-j}+d\mathcal{Q}_{j-1}^{G+D-j},\quad 1\leqslant j\leqslant D,\\ \omega_0^{G+D}&\neq b\mathcal{Q}_0^{G+D-1}. \end{aligned} \tag{43}$$

In particular, for the zero form ω_0^{G+D} we obtain

$$\omega_0^{G+D}=\mathrm{Tr}\,\frac{c^{G+D}}{(G+D)!}. \tag{44}$$

Let us remark, finally, that as a consequence of the fact that the generalized ladder $\tilde{\mathscr{A}}$ is the δ-transform of the ghost field c, $\tilde{\mathscr{A}}=e^{\delta}c$, the generalized cocycle (38) is the δ-transform of the corresponding ghost cocycle (44), i.e.,

$$\left(\mathrm{Tr}\,\frac{\tilde{\mathscr{A}}^{2n+1}}{(2n+1)!}\right)=e^{\delta}\,\mathrm{Tr}\left(\frac{c^{2n+1}}{(2n+1)!}\right). \tag{45}$$

A. Example I: The Chern–Simons theory

For a better understanding of the previous construction let us discuss in detail the case of the three-dimensional Chern–Simons theory, corresponding to $G=0$ and $D=3$. This example will give us the possibility of clarifying the meaning of the negative ghost number components $(\varphi_j^{1-j}$, $2\leqslant j\leqslant D)$ of the gauge ladder $\tilde{\mathscr{A}}$. As we shall see, these fields turn out to be the so-called external BRS sources (*called also antifields in the framework of Batalin–Vilkovsky*[26]) needed in order to properly define[1] the nonlinear transformations of the gauge connection A and of the Faddeev–Popov ghost c. The external sources are then naturally included in the zero-curvature formalism.

In a three-dimensional space–time the complete gauge ladder $\tilde{\mathscr{A}}$ of Eq. (13) takes the following form:

$$\tilde{\mathscr{A}} = c + A + \gamma + \tau, \tag{46}$$

γ and τ identifying, respectively, the negative ghost number components φ_2^{-1} and φ_3^{-2}. From the zero curvature condition (18) one obtains the BRS transformations:

$$\begin{gathered} bc = ic^2, \quad bA = -dc + i[c,\ A], \\ b\gamma = -F + i[c,\ \gamma], \quad b\tau = -d\gamma + i[c,\ \tau] + i[A,\ \gamma], \end{gathered} \tag{47}$$

F being the two-form gauge field strength $F = dA - iA^2$. As explained before, in order to find a solution of the descent equations

$$\begin{gathered} b\omega_{3-j}^{j} + d\omega_{2-j}^{j+1} = 0, \quad 0 \leqslant j \leqslant 2, \\ b\omega_0^3 = 0, \end{gathered} \tag{48}$$

it is sufficient to expand the generalized cocycle of total degree three:

$$\tilde{\omega}^3 = \frac{1}{3!}\ \mathrm{Tr}\ \tilde{\mathscr{A}}^3. \tag{49}$$

After an easy computation we get

$$\frac{1}{3!}\ \mathrm{Tr}\ \tilde{\mathscr{A}}^3 = \omega_3^0 + \omega_2^1 + \omega_1^2 + \omega_0^3, \tag{50}$$

with

$$\begin{gathered} \omega_0^3 = \frac{1}{3!}\ \mathrm{Tr}\ c^3, \quad \omega_1^2 = \frac{1}{2}\ \mathrm{Tr}\ c^2 A, \\ \omega_2^1 = \frac{1}{2}\ \mathrm{Tr}(c^2\gamma + cA^2), \\ \omega_3^0 = \frac{1}{2}\ \mathrm{Tr}\left(c^2\tau + cA\gamma + c\gamma A + \frac{A^3}{3} \right). \end{gathered} \tag{51}$$

From

$$-i\ \mathrm{Tr}(c^2\tau + cA\gamma + c\gamma A) = -\mathrm{Tr}\ AF + b\ \mathrm{Tr}(c\tau + A\gamma) + d\ \mathrm{Tr}\ c\gamma, \tag{52}$$

the three-form ω_3^0 can be rewritten as

$$\omega_3^0 = \frac{-i}{2}\ \mathrm{Tr}\left(AF + i\,\frac{A^3}{3} \right) + \frac{i}{2}\ b\ \mathrm{Tr}(c\tau + A\gamma) + \frac{i}{2}\ d\ \mathrm{Tr}\ c\gamma, \tag{53}$$

yielding thus the invariant action

$$S = i\int \omega_3^0 = \frac{1}{2}\int \mathrm{Tr}\left(AF + i\,\frac{A^3}{3} \right) - \frac{1}{2}\ b\int \mathrm{Tr}(c\tau + A\gamma), \tag{54}$$

which is easily recognized to be the so-called truncated action[1] of the fully quantized Chern–Simons gauge theory. In particular, one sees that the components (γ,τ) of the gauge ladder (46) are the BRS external sources corresponding to the nonlinear transformations of the fields A and c.

VI. COUPLING WITH MATTER FIELDS

The zero-curvature formalism can be extended to include the case in which the gauge fields are coupled to matter fields whose quantization requires the introduction of a complete ladder matter multiplet. A typical example of this kind of coupling is given by the topological BF systems[17,27] whose classical action reads

$$\mathrm{Tr}\int_{\mathscr{M}^D}\mathscr{B}^0_{D-2}F, \tag{55}$$

where F is the two-form gauge curvature, $\mathscr{B}^0_{D-2}$ is a $(D-2)$ form with ghost number zero, and $\mathscr{M}^D$ is a D-dimensional manifold without boundaries.

In the next section we shall discuss another example of matter system, namely the B-C ghost system of the string theory, whose action is not directly given in terms of differential forms. Nevertheless we shall see that this model, although different from the BF systems, actually shares many properties of the latters.

The inclusion of the matter fields goes as follows (see also Ref. 19): we introduce a set of fields $(\mathscr{B}^{D-2}_0, \mathscr{B}^{D-3}_1,\ldots, \mathscr{B}^1_{D-3}, \mathscr{B}^{-1}_{D-1}, \mathscr{B}^{-2}_D)$ which together with the matter field $\mathscr{B}^0_{D-2}$ give rise to a complete ladder $\mathscr{B}$ of total degree $(D-2)$, i.e.,

$$\tilde{\mathscr{B}}=\sum_{j=0}^{D}\mathscr{B}^{D-2-j}_j. \tag{56}$$

The BRS transformations of the various components of this ladder are obtained by requiring that $\tilde{\mathscr{B}}$ is covariantly constant with respect to the generalized covariant derivative $\tilde{\mathscr{D}}=\tilde{d}-i[\tilde{\mathscr{A}},]$,

$$\tilde{\mathscr{D}}\tilde{\mathscr{B}}=\tilde{d}\tilde{\mathscr{B}}-i[\tilde{\mathscr{A}},\ \tilde{\mathscr{B}}]=0. \tag{57}$$

This condition, when expanded in terms of the form degree and of the ghost number, gives in fact the following nilpotent transformations:

$$\begin{aligned} b\mathscr{B}^{D-2}_0&=i[c,\ \mathscr{B}^{D-2}_0],\\ b\mathscr{B}^{D-2-j}_j&=-d\mathscr{B}^{D-1-j}_{j-1}+i\sum_{m=0}^{j}[\varphi^{1-m}_m,\ \mathscr{B}^{D-2-j+m}_{j-m}],\quad 1\leqslant j\leqslant D. \end{aligned} \tag{58}$$

Repeating the same procedure of Sec. IV and making use of the general results of Refs. 15, 20, 21, and 25, one easily checks that with the inclusion of the matter ladder the cohomology of the BRS operator is given by polynomials in the undifferentiated zero form ghosts $(c, \mathscr{B}^{D-2}_0)$ built up with factorized monomials of the type

$$\left(\mathrm{Tr}\,\frac{c^{2n+1}}{(2n+1)!}\right)\cdot\mathrm{Tr}(\mathscr{B}^{D-2}_0)^m,\quad m,n\geqslant 1. \tag{59}$$

In much the same way as the gauge ladder $\tilde{\mathscr{A}}$, the operator δ extends to the matter multiplet $\tilde{\mathscr{B}}$ by means of

$$\tilde{\mathscr{B}} = e^{\delta}.\mathscr{B}_0^{D-2}, \tag{60}$$

i.e.,

$$\begin{gathered}\delta.\mathscr{B}_j^{D-2-j} = (j+1).\mathscr{B}_{j+1}^{D-3-j}, \quad 0 \leqslant j \leqslant D-1, \\ \delta.\mathscr{B}_D^{-2} = 0,\end{gathered} \tag{61}$$

and

$$\begin{gathered}\delta d.\mathscr{B}_j^{D-2-j} = (j+1)d.\mathscr{B}_{j+1}^{D-3-j}, \quad 0 \leqslant j \leqslant D-2, \\ \delta d.\mathscr{B}_{D-1}^{-1} = 0,\end{gathered} \tag{62}$$

so that the algebraic relations

$$d = -[b,\ \delta], \quad [\delta,\ d] = 0, \tag{63}$$

are fulfilled.

For what concerns the cohomology of the generalized operator $\tilde{d}$ of Eqs. (37) and (57), it is immediately seen from Eq. (59) that it is spanned by factorized monomials in the ladders $\tilde{\mathscr{A}}$ and $\tilde{\mathscr{B}}$ of the type

$$\left(\mathrm{Tr}\,\frac{\tilde{\mathscr{A}}^{2n+1}}{(2n+1)!}\right)\cdot(\mathrm{Tr}\,\tilde{\mathscr{B}}^{m}). \tag{64}$$

As already discussed in the previous section, the expansion of the above expression (64) in terms of the form degree and of the ghost number yields a solution of the descent equations (34) in the presence of a matter field ladder, reproducing thus the results already established in Ref. 8. Again

$$\left(\mathrm{Tr}\,\frac{\tilde{\mathscr{A}}^{2n+1}}{(2n+1)!}\right)\cdot \mathrm{Tr}\,\tilde{\mathscr{B}}^{m} = e^{\delta}\left(\mathrm{Tr}\,\frac{c^{2n+1}}{(2n+1)!}\right)\cdot(\mathrm{Tr}(.\mathscr{B}_0^{D-2})^{m}), \tag{65}$$

which shows that the cohomology of $\tilde{d}$ is the δ-transform of that of the BRS operator b. Let us conclude this section by remarking that in a space–time of dimension ($D \geqslant 2$) the gauge ladder $\tilde{\mathscr{A}}$ contains $(D-1)$ components of negative ghost number, i.e., $(\varphi_2^{-1},...,\varphi_D^{1-D})$, while the matter ladder $\tilde{\mathscr{B}}$ contains $(D-2)$ components with positive ghost number, i.e., $(\mathscr{B}_0^{D-2}, \mathscr{B}_1^{D-3},...,\mathscr{B}_{D-3}^{1})$, and two components of negative ghost number, namely $(\mathscr{B}_{D-1}^{-1}, \mathscr{B}_D^{-2})$.

These fields turn out to possess the following meaning. The set $(\mathscr{B}_0^{D-2}, \mathscr{B}_1^{D-3},...,\mathscr{B}_{D-3}^{1})$ identifies the well-known tower of ghosts for ghosts needed for the quantization of the *BF* systems. The components $(\varphi_3^{-2},...,\varphi_D^{1-D})$ are then the corresponding $(D-2)$ external sources (or antifields) associated to the nonlinear transformations of the ghosts for ghosts [see Eq. (58)], while φ_2^{-1} is the external source for the $(D-2)$ form $\mathscr{B}_{D-2}^{0}$. Finally $(\mathscr{B}_{D-1}^{-1}, \mathscr{B}_D^{-2})$ are the sources corresponding to the first two components of the gauge ladder, i.e., c and A. We thus see that in the case of the *BF* systems the external sources are exchanged,[8] i.e., the sources for the quantized components of the matter ladder are grouped into the gauge ladder and vice versa.

Let us also recall, for completeness, that the truncated action (including the ghosts for ghosts and the external sources) for the *BF* systems can be cast in the simple form[19]

$$S=\mathrm{Tr}\int_{\mathscr{M}^D}\tilde{\mathscr{B}}(d.\tilde{\mathscr{A}}-i.\tilde{\mathscr{A}}^2)\Big|_D^0=-\mathrm{Tr}\int_{\mathscr{M}^D}\tilde{\mathscr{B}}b.\tilde{\mathscr{A}}\Big|_D^0, \tag{66}$$

where $|_D^0$ means the restriction to terms of ghost number 0 and form degree D. The equality in Eq. (66) stems from the zero-curvature condition (18).

In particular, using Eq. (57), expression (66) is easily proven to be invariant under the action of the operator b,

$$bS=0, \tag{67}$$

this equation expressing the content of the Slavnov–Taylor (or Master Equation) identity.

VII. EXAMPLE II: THE *B*-*C* GHOST SYSTEM

We present here, as another interesting example of matter system, the zero-curvature formulation of the two-dimensional B-C model whose action reads

$$S_{B\text{-}C}=\int dz\, d\bar{z}\, B\, \bar{\partial}C, \tag{68}$$

where the fields $B=B_{zz}$ and $C=C^z$ are anticommuting and carry, respectively, ghost number -1 and $+1$.

It should be noted that, unlike the previous examples, the fields appearing in the action (68) are not naturally associated to differential forms. However, we shall see that, in spite of the fact that these fields do not give rise to a complete ladder structure, this system turns out to possess the same algebraic features of the BF models. The action (68) is recognized to be the ghost part of the quantized bosonic string action which, as it is well known, is left invariant by the following nonlinear BRS transformations

$$\begin{aligned} sC&=C\partial C,\\ sB&=-(\partial B)C-2B\partial C. \end{aligned} \tag{69}$$

The above expression (68) is usually accompanied by its complex conjugate. However, the inclusion of the latter in the present framework does not require any additional difficulty.

In particular, the right-hand side of the BRS transformation of the field B is recognized to be the component T_{zz} of the energy–momentum tensor corresponding to the action (68), this property allowing for a topological interpretation of the model.

Transformations (69) being nonlinear, one needs to introduce two external invariant sources $\mu=\mu_{\bar{z}}^z$ and $L=L_{zz\bar{z}}$ of ghost numbers, respectively, 0 and -2

$$S_{\mathrm{ext}}=\int dz\, d\bar{z}(\mu sB+LsC). \tag{70}$$

The complete action

$$S=S_{B\text{-}C}+S_{\mathrm{ext}} \tag{71}$$

obeys thus the classical Slavnov–Taylor identity

$$\int dz\, d\bar{z}\left(\frac{\delta S}{\delta B}\frac{\delta S}{\delta \mu}+\frac{\delta S}{\delta L}\frac{\delta S}{\delta C}\right)=0=\frac{1}{2}\,bS, \tag{72}$$

b denoting the nilpotent linearized operator

$$b=\int dz\ d\overline{z}\left(\frac{\delta S}{\delta B}\frac{\delta}{\delta\mu}+\frac{\delta S}{\delta\mu}\frac{\delta}{\delta B}+\frac{\delta S}{\delta L}\frac{\delta}{\delta C}+\frac{\delta S}{\delta C}\frac{\delta}{\delta L}\right). \tag{73}$$

The operator b acts on the fields and on the external sources in the following way:

$$bC=sC=C\partial C,\quad b\mu=\overline{\partial C}+(\partial\mu)C-\mu(\partial C), \tag{74}$$

and

$$\begin{aligned} bB&=sB=-(\partial B)C-2B\partial C,\\ bL&=\overline{\partial B}-(2B)\partial\mu-\mu\partial B+(\partial L)C+2L\partial C. \end{aligned} \tag{75}$$

It should be noted that, due to the fact that the BRS transformation of B is the component T_{zz} of the energy-momentum tensor, the differentiation with respect to the external source μ of the Legendre transformation of the complete action (71),

$$Z(j,\mu,L)=S+\int dz\ d\overline{z}(j_C C+j_B B), \tag{76}$$

allows us to obtain the Green's functions with insertion of T_{zz}. In other words, the Slavnov–Taylor identity (72) is the starting point for the algebraic characterization of the energy–momentum current algebra.

Introducing now the two functional operators[10]

$$\mathscr{W}=\int dz\ d\overline{z}\frac{\delta}{\delta C},\quad \overline{\mathscr{W}}=\int dz\ d\overline{z}\left(\mu\frac{\delta}{\delta C}+L\frac{\delta}{\delta B}\right), \tag{77}$$

one easily proves that

$$\delta=dz\mathscr{W}+d\overline{z}\overline{\mathscr{W}} \tag{78}$$

obeys

$$d=-[b,\ \delta],\quad [d,\ \delta]=0, \tag{79}$$

d being the exterior derivative $d=dz\partial+d\overline{z}\overline{\partial}$. We have thus realized the decomposition (24). In order to derive the transformations (74) and (75) from a zero curvature condition we proceed as before and we define the analogue of the gauge ladder (13) as

$$\widetilde{C}^z=e^{\delta}C^z=C^z+dz+d\overline{z}\mu^z_{\overline{z}}. \tag{80}$$

Introducing then the holomorphic generalized vector field $\widetilde{C}=\widetilde{C}^z\partial_z$, it is easily checked that equations (74) can be cast in the form of a zero curvature condition

$$\widetilde{d}\widetilde{C}=\tfrac{1}{2}[\widetilde{C},\ \widetilde{C}]=\mathscr{L}_{\widetilde{C}}\widetilde{C}, \tag{81}$$

where, as usual, $\widetilde{d}$ is the operator

$$\widetilde{d}=e^{\delta}be^{-\delta}=b+d, \tag{82}$$

and $\mathscr{L}_{\widetilde{C}}$ denotes the Lie derivative with respect to the vector field $\widetilde{C}$. Of course, the bracket $[\widetilde{C}, \widetilde{C}]$ in Eq. (82) refers now to the usual Lie bracket of vector fields.

Concerning now the second set of transformations (75), we define the matter ladder $\widetilde{\mathscr{B}}_{zz}$ as

$$\widetilde{\mathscr{B}}_{zz}=e^{\delta}.\mathscr{B}_{zz}=\mathscr{B}_{zz}+d\overline{z}\,L_{zz\overline{z}}. \tag{83}$$

To expression (83) one can naturally associate the generalized holomorphic quadratic differential

$$\widetilde{\mathscr{B}}=\widetilde{\mathscr{B}}_{zz}\,dz\otimes dz. \tag{84}$$

Therefore, transformations (75) can be rewritten as

$$\widetilde{d}.\widetilde{\mathscr{B}}-\mathscr{L}_{\widetilde{C}}\widetilde{\mathscr{B}}=0. \tag{85}$$

This equation is the analogue of the covariantly constant matter condition (57) and together with Eq. (81) completely characterizes the B-C system. One has to remark that, as it happens in the case of the BF models, the external sources (μ, L) are interchanged, i.e., the source μ associated to the nonlinear transformation of B belongs to the gauge ladder $\widetilde{C}$ and vice versa.

Let us consider now the problem of identifying the anomalies which affect the Slavnov–Taylor identity (72) at the quantum level. We look then at the solution of the descent equations

$$b\,\omega_2^1+d\,\omega_1^2=0,\quad b\,\omega_1^2+d\,\omega_0^3=0,\quad b\,\omega_0^3=0. \tag{86}$$

As it has been proven in Refs. 10 and 28, the cohomology of the BRS operator in the sector of the zero forms with ghost number three contains, in the present case, a unique element given by

$$\omega_0^3=C\partial C\partial^2 C. \tag{87}$$

From the zero-curvature condition (81), it follows then that the generalized cocycle of total degree three,

$$\widetilde{\omega}^3=\widetilde{C}\partial\widetilde{C}\partial^2\widetilde{C}, \tag{88}$$

belongs to the cohomology of $\widetilde{d}$. The expansion of $\widetilde{\omega}^3$ will give thus a solution of the ladder (86), i.e.,

$$\widetilde{\omega}^3=\omega_0^3+\omega_1^2+\omega_2^1, \tag{89}$$

with ω_1^2, ω_2^1 given, respectively, by

$$\begin{aligned}\omega_1^2&=(C\partial C\partial^2\mu-C\partial^2 C\partial\mu+\mu\partial C\partial^2 C)d\overline{z}+(\partial C)(\partial^2 C)dz,\\ \omega_2^1&=(-\partial C\partial^2\mu+\partial\mu\partial^2 C)dz\wedge d\overline{z}.\end{aligned} \tag{90}$$

In particular,

$$\int\ \omega_2^1=2\int dz d\overline{z}C\partial^3\mu \tag{91}$$

is recognized to be the well-known two-dimensional diffeomorphism anomaly characterizing the central charge of the energy–momentum current algebra.

Let us conclude by remarking that the complete B-C action (71) can be written, in perfect analogy with Eq. (66) as

$$S=\int \tilde{\mathscr{B}}_{zz}(d\tilde{C}^z-\tilde{C}^z\ \partial\tilde{C}^z)dz\Big|_2^0=-\int \tilde{\mathscr{B}}_{zz}b\tilde{C}^z\ dz\Big|_2^0, \tag{92}$$

showing that the B-C model can be interpreted as a kind of two-dimensional BF system.

VIII. CONCLUSION

The zero curvature formulation of models characterized by means of a complete ladder field can be obtained as a consequence of the existence of the operator δ realizing the decomposition (5). Moreover, the zero curvature condition enables us to encode into a unique equation all the relevant informations concerning the BRS cohomology classes.

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Becchi–Rouet–Stora cohomology of zero curvature systems. II. The noncomplete ladder case

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The Yang–Mills-type theories and their BRS cohomologies are analyzed within the zero curvature formalism. © *1996 American Institute of Physics.*
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I. INTRODUCTION

In the first part of this work[1] (referred to as part I), we have studied the zero-curvature formulation of systems described by means of a complete ladder field, the components of which span all possible form degrees. The present paper is devoted to analyzing the zero-curvature equation in the case in which the completeness condition for the generalized ladder field is relaxed. This means that we shall deal with a gauge ladder $\tilde{\mathscr{A}}$ for which the form degree of the highest component is strictly lower than the space–time dimension D, i.e.,

$$\tilde{\mathscr{A}}=c+A+\varphi_2^{-1}+\cdots+\varphi_q^{1-q}, \quad 1\leqslant q<D. \tag{1}$$

As we shall see in the following, the noncomplete case will display a set of remarkable features which will make it quite different from the previous complete case. The first interesting aspect, as already mentioned in the Introduction of part I, is that the consistency of the zero-curvature condition

$$\tilde{\mathscr{F}}=\tilde{d}.\tilde{\mathscr{A}}-i.\tilde{\mathscr{A}}^2=0 \tag{2}$$

implies now the existence of a set of new operators ($\mathscr{G}_k^{1-k}$, $2\leqslant k\leqslant D$) which are in involution, according to the algebra

$$\begin{aligned}\mathscr{G}_2^{-1}&=\frac{1}{2}[\delta,\ d],\\ \mathscr{G}_k^{1-k}&=\frac{1}{k}[\delta,\ \mathscr{G}_{k-1}^{2-k}], \quad k>2,\end{aligned} \tag{3}$$

δ being the operator which together with the Becchi–Rouet–Stora (BRS) operator b decomposes the exterior space–time derivative d as

$$d=-[b,\ \delta], \tag{4}$$

where, as already remarked in the Introduction of part I, the decomposition (4) has to be understood to hold in the space of form-valued polynomials. This space is in fact the basic functional space of our analysis.

The second interesting feature of the noncomplete case is that the cohomology of the BRS operator b is richer than the corresponding one of the complete case. Indeed, the noncompleteness of $\tilde{\mathscr{A}}$ will allow us to introduce a set of curvatures $(R^{1-m}_{m+1},\ 1\leqslant m\leqslant q)$ which are a generalization of the familiar two-form gauge field strength $F=dA-iA^2$. It follows then that, in addition to the usual ghost cocycles $(\mathrm{Tr}\, c^{2n+1})$ of the complete case (see Sec. IV of part I), the cohomology of b now includes also invariant polynomials in the highest curvature (R^{1-q}_{q+1}).

As a consequence of these new features, the expressions of the polynomials ω^{G+D-j}_j $(0\leqslant j\leqslant D)$ which solve the descent equations

$$\begin{gathered} b\,\omega^{G+j}_{D-j}+d\,\omega^{G+j+1}_{D-j-1}=0, \quad 0\leqslant j\leqslant (D-1), \\ b\,\omega^{G+D}_0=0, \end{gathered} \tag{5}$$

will get modified with respect to the complete case. This modification will result in the appearance of a set of local polynomials Ω^{G+D-j}_j $(q+1\leqslant j\leqslant D)$ in the curvatures (R^{1-m}_{m+1}) which have to be added to the cocycles obtained from the expansion of the generalized terms $(\mathrm{Tr}\,\tilde{\mathscr{A}}^{G+D})$. These polynomials, as already observed in Refs. 2 and 3 in the case of Yang–Mills, turn out to be characterized by a set of consistency conditions involving the operators $\mathscr{G}^{1-k}_k$.

This second part of the work is organized as follows. In Sec. II we present the zero-curvature condition for the noncomplete gauge ladder. Section III is devoted to the study of the cohomology of the BRS operator. In Sec. IV we solve the descent equations. Sections V and VI are finally devoted to the discussion of several examples among which one finds the zero-curvature formulation of the pure Yang–Mills gauge theory.

II. THE ZERO-CURVATURE CONDITION

In part I (cf. Sec. II) the BRS transformations of the various components of the gauge ladder $\tilde{\mathscr{A}}$ have been obtained by constraining the latter to obey a zero-curvature condition. Equivalently, as we have seen in Sec. III of part I, once the BRS transformations of the fields have been given, the zero-curvature condition becomes a consequence of the existence of the operator δ which realizes the decomposition (4). This second procedure will be taken as the starting point for the discussion of the zero-curvature condition in the present noncomplete case. The gauge ladder $\tilde{\mathscr{A}}$ now takes the following form;

$$\tilde{\mathscr{A}}=c+A+\varphi^{-1}_2+\cdots+\varphi^{1-q}_q, \quad 1\leqslant q<D, \tag{6}$$

D being the dimension of the space–time. We will assume therefore that the nilpotent BRS transformations of the components $\varphi^{1-j}_j (0\leqslant j\leqslant q)$ of (6) will be the same as those of the corresponding complete case (see Sec. II of part I), i.e.,

$$\begin{gathered} bc=ic^2, \quad bA=-dc+i[c,\ A], \\ b\varphi^{1-j}_j=-d\varphi^{2-j}_{j-1}+\frac{i}{2}\sum_{m=0}^{j}[\varphi^{1-m}_m,\ \varphi^{1-j+m}_{j-m}], \quad 2\leqslant j\leqslant q, \end{gathered} \tag{7}$$

where, as usual, $[a,\ b]=ab-(-1)^{|a||b|}ba$ denotes the graded commutator and, as done in part I, we shall work in the functional space $\mathscr{V}$ of form-valued polynomials built up with the fields φ^{1-j}_j and their differential $d\varphi^{1-j}_j$, i.e.,

$$\mathscr{V}=\text{polynomials in } (\varphi^{1-j}_j, d\varphi^{1-j}_j; 0\leqslant j\leqslant q). \tag{8}$$

Having assigned the BRS transformations, let us turn to the introduction of the decomposition (4). To this purpose we define the operator δ as

$$\tilde{\mathscr{A}}=e^{\delta}c,$$
$$\delta\varphi_j^{1-j}=(j+1)\varphi_{j+1}^{-j},\quad 0\leqslant j\leqslant q-1, \tag{9}$$
$$\delta\varphi_q^{1-q}=0,$$

and

$$\delta d\varphi_m^{1-m}=(m+1)d\varphi_{m+1}^{-m},\quad 0\leqslant m\leqslant q-2,$$
$$\delta d\varphi_{q-1}^{2-q}=q d\varphi_q^{1-q}-(q+1)\left(d\varphi_q^{1-q}-\frac{i}{2}\sum_{j=1}^{q}[\varphi_j^{1-j},\ \varphi_{q-j+1}^{j-q}]\right), \tag{10}$$
$$\delta d\varphi_q^{1-q}=\frac{i}{2}(q+1)\sum_{j=1}^{q}[\varphi_{q+2-j}^{-1-q+j},\ \varphi_j^{1-j}].$$

One easily checks that, on the functional space $\mathscr{V}$, the operators b and δ realize the decomposition (4), i.e.,

$$d=-[b,\ \delta]. \tag{11}$$

Comparing now Eqs. (9) and (10) the corresponding ones of the complete ladder case (see Sec. II of part I) one sees that, while the action of the operator δ on the components (φ_j^{1-j}) is the same, the transformations of the differentials of higher form degree, i.e., $(d\varphi_{q-1}^{2-q})$ and $(d\varphi_q^{1-q})$, are now nonvanishing. This fact implies that, contrary to the complete case, the operator δ does not commute anymore with the exterior derivative d,

$$[\delta,\ d]\neq 0. \tag{12}$$

In addition, depending on the dimension of the space–time D and on the number q of components of the gauge ladder $\mathscr{A}$, the commutators

$$[\delta,[\delta,[\delta,\ldots,d]]] \tag{13}$$

turn out to be nonvanishing as well.

This algebraic structure, which generalizes that of Refs. 2 and 3, will have important consequences on the zero-curvature condition. The latter, repeating the same argument of Sec. III of part I, is obtained by applying the operator e^{δ} on the BRS transformation of the zero-form ghost field c, i.e.,

$$e^{\delta}be^{-\delta}e^{\delta}c=e^{\delta}ic^2. \tag{14}$$

Recalling now that $\tilde{\mathscr{A}}=e^{\delta}c$ and defining the generalized operator $\tilde{d}$ as

$$\tilde{d}=e^{\delta}be^{-\delta}, \tag{15}$$

we get the zero-curvature condition

$$\tilde{d}\tilde{\mathscr{A}}=i\tilde{\mathscr{A}}^2 \tag{16}$$

for the noncomplete ladder case. Equation (16) is, however, only apparently similar to the corresponding condition of the complete ladder case. In fact, due to Eqs. (12) and (13), the operator $\tilde{d}$ is now given by

$$\tilde{d}=b+d+\sum_{n\geqslant 2}^{D}\frac{1}{n!}\underbrace{[\delta,[\delta,[\delta,\ldots,d]]]}_{(n-1)\text{ times}}, \tag{17}$$

so that, defining the operators

$$\begin{aligned}
\mathcal{G}_2^{\,1}&=\frac{1}{2}[\delta,\,d],\\
\mathcal{G}_3^{\,2}&=\frac{1}{3!}[\delta,[\delta,d]]=\frac{1}{3}[\delta,\,\mathcal{G}_2^{\,1}],\\
\mathcal{G}_4^{\,3}&=\frac{1}{4!}[\delta,[\delta,[\delta,d]]]=\frac{1}{4}[\delta,\mathcal{G}_3^{\,2}],\\
&\cdots,
\end{aligned} \tag{18}$$

we have

$$\tilde{d}=b+d+\sum_{k\geqslant 2}^{D}\mathcal{G}_k^{1-k} \tag{19}$$

with

$$\begin{aligned}
\mathcal{G}_2^{\,1}&=\frac{1}{2}[\delta,\,d],\\
\mathcal{G}_k^{1-k}&=\frac{1}{k}[\delta,\,\mathcal{G}_{k-1}^{2-k}],\quad k>2.
\end{aligned} \tag{20}$$

One thus sees that in the noncomplete case the zero-curvature condition is accompanied by a set of operators $\mathcal{G}_k^{1-k}$ which are in involution, according to Eq. (20). We underline, in particular, that the origin of the operators $\mathcal{G}_k^{1-k}$ actually relies on the noncomplete character of the gauge ladder (6). It is very easy, using Eqs. (9) and (10), to derive the explicit form of the various operators $\mathcal{G}_k^{1-k}$ appearing in Eq. (16). In particular, as we shall show later on in the examples, the number of operators $\mathcal{G}_k^{1-k}$ which do not identically vanish depends both on the dimension D of the space–time and on the number q of components of the gauge ladder $\tilde{\mathcal{A}}$. We also notice that these operators are absent when $q=D$, i.e., they are not present in the case in which the ladder is complete.

Moreover their existence implies that the cohomology of the operator $\tilde{d}$ is no more directly related to that of the operator $(d+b)$. Therefore the cohomology classes of $\tilde{d}$ do not immediately provide solutions of the descent equations (5). It turns out indeed that in order to obtain a solution of the tower (5) we must add to the cohomology classes of $\tilde{d}$, i.e., $\mathrm{Tr}\,\tilde{\mathcal{A}}^{2n+1}$, certain polynomials Ω_j^{G+D-j} $(q+1\leqslant j\leqslant D)$ which obey a set of consistency conditions involving the operator $\mathcal{G}_k^{1-k}$. In other words, the presence of the $\mathcal{G}_k^{1-k}$'s requires a modification of the solution of the descent equations with respect to the complete ladder case (see Sec. V of part I).

Let us conclude this section with the following remark. Instead of having assumed the BRS transformations (7) we could have started directly with the zero-curvature condition (16). It is easily verified then that the introduction of the operators $\mathcal{G}_k^{1-k}$ is needed in order to avoid the appearance of constraints among the components of the noncomplete ladder field $\tilde{\mathcal{A}}$.

III. COHOMOLOGY OF THE BRS OPERATOR

The first step in order to solve the descent equations (5) is that of computing the cohomology of the BRS operator b. This task, due to the noncomplete character of $\mathscr{A}$, will turn out to be simplified by the introduction of the following curvatures R_{m+1}^{1-m} of total degree two:

$$R_{m+1}^{1-m}=d\varphi_m^{1-m}-\frac{i}{2}\sum_{k=1}^{m}[\varphi_k^{1-k},\ \varphi_{m+1-k}^{k-m}];\quad 1\leqslant m\leqslant q. \tag{21}$$

In particular, for $m=1$ the expression (21) reduces to

$$R_2^0=dA-iA^2=F, \tag{22}$$

i.e., one recovers the familiar two-form gauge field strength. We also remark that, for $m>1$, the curvatures R_{m+1}^{1-m} possess the property of having negative ghost number.

The great advantage of working with the curvatures R_{m+1}^{1-m} relies on the fact that they transform covariantly under the action of the BRS operator, i.e.,

$$bR_{m+1}^{1-m}=i[c,\ R_{m+1}^{1-m}]. \tag{23}$$

This feature, following the well-known Yang–Mills case,[4–7] suggests that it is convenient to use the curvatures R_{m+1}^{1-m} as independent variables instead of the differentials $d\varphi_m^{1-m}$, i.e., we replace everywhere the variables $d\varphi_m^{1-m}$ by R_{m+1}^{1-m} making use of Eq. (21). Consequently, for the functional space $\mathscr{V}$ we have

$$\mathscr{V}=\text{polynomials in } (c,A,\varphi_m^{1-m},2\leqslant m\leqslant q;dc,R_{j+1}^{1-j},1\leqslant j\leqslant q), \tag{24}$$

and, for the nilpotent BRS transformations,

$$\begin{aligned}
bc&=ic^2,\\
bA&=-dc+i[c,\ A],\\
b\varphi_m^{1-m}&=i[c,\ \varphi_m^{1-m}]-R_m^{2-m},\quad 2\leqslant m\leqslant q,\\
bdc&=i[c,\ dc],\\
bR_{j+1}^{1-j}&=i[c,\ R_{j+1}^{1-j}],\quad 1\leqslant j\leqslant q.
\end{aligned} \tag{25}$$

Let us turn now to the computation of the cohomology of b. Introducing the filtering operator $\mathscr{N}$

$$\begin{aligned}
&\mathscr{N}c=c,\quad \mathscr{N}A=A,\\
&\mathscr{N}\varphi_m^{1-m}=\varphi_m^{1-m},\quad 2\leqslant m\leqslant q,\\
&\mathscr{N}dc=dc,\quad \mathscr{N}R_{j+1}^{1-j}=R_{j+1}^{1-j},\quad 1\leqslant j\leqslant q,
\end{aligned} \tag{26}$$

the BRS operator decomposes as

$$b=b_0+b_1, \tag{27}$$

with

$$\begin{gathered} b_0 c = 0, \quad b_0 A = -dc, \quad b_0 dc = 0, \\ b_0 \varphi_m^{1-m} = -R_m^{2-m}, \quad b_0 R_m^{2-m} = 0, \quad 2 \leqslant m \leqslant q, \\ b_0 R_{q+1}^{1-q} = 0, \quad b_0^2 = 0. \end{gathered} \tag{28}$$

Equations (28) show that all the variables except the zero-form ghost c and the highest curvature R_{q+1}^{1-q} are grouped in BRS doublets. This implies that the cohomology of b_0 and, in turn, that of the full BRS operator b, depend only on c and R_{q+1}^{1-q}. More precisely, using the general results of Refs. 4–7, it follows that the cohomology of b on the functional space V is spanned by invariant polynomials in the variables (c, R_{q+1}^{1-q}) built up with factorized monomials of the form

$$\left(\mathrm{Tr}\, \frac{c^{2n+1}}{(2n+1)!} \right) \cdot (\mathrm{Tr}(R_{q+1}^{1-q})^m), \quad n, m = 1, 2, \ldots . \tag{29}$$

One sees that in the noncomplete ladder case the cohomology of the BRS operator b, in addition of the usual ghost cocycles $(\mathrm{Tr}\, c^{2n+1})$, includes also polynomials in the highest curvatures R_{q+1}^{1-q}. Notice finally that, being the ghost number of the highest curvature R_{q+1}^{1-q} negative for $q>1$, the cohomology classes of b are nonvanishing in the negative charged sectors.

We conclude this section by remarking that the highest curvature R_{q+1}^{1-q} is actually related to the ghost field c through the action of the operator $\mathscr{G}_{q+1}^{-q}$,

$$\mathscr{G}_{q+1}^{-q} c = (\mathrm{const}) R_{q+1}^{1-q}, \tag{30}$$

the proportionality factor being easily computed by means of Eqs. (9) and (10).

IV. SOLUTION OF THE DESCENT EQUATIONS

Having characterized the cohomology of the BRS operator b, let us focus on the cohomology of b modulo d, i.e., let us try to solve the descent equations

$$\begin{gathered} b\, \omega_{D-j}^{G+j} + d\, \omega_{D-j-1}^{G+j+1} = 0, \quad 0 \leqslant j \leqslant (D-1), \\ b\, \omega_0^{G+D} = 0. \end{gathered} \tag{31}$$

As mentioned before and as already observed in the case of pure Yang–Mills (i.e., $q=1$), the presence of the operators $\mathscr{G}_k^{1-k}$ in the zero-curvature condition (16) requires a slight modification of the climbing procedure presented in the previous complete ladder case (see part I).

Repeating indeed the same argument of Ref. 2, it is easy to convince oneself that, once a solution ω_0^{G+D} of the last equation of (31) has been obtained, an explicit expression for the higher polynomials ω_j^{G+D-j} is provided by the generalized cocycle $\tilde{\omega}^{G+D}$ of total degree $(G+D)$,

$$\begin{gathered} \tilde{\omega}^{G+D} = \sum_{j=0}^{D} \omega_j^{G+D-j}, \\ \tilde{\omega}^{G+D} = e^{\delta} \left(\omega_0^{G+D} + \sum_{j=q+1}^{D} \Omega_j^{G+D-j} \right), \end{gathered} \tag{32}$$

where ω_0^{G+D} is

$$\omega_0^{G+D}=\mathrm{Tr}\,\frac{c^{G+D}}{(G+D)!},\tag{33}$$

and the quantities Ω_j^{G+D-j} are determined recursively by means of the consistency conditions

$$\begin{aligned} b\Omega_j^{G+D-j}&=(j-1)(-1)^j\mathscr{G}_j^{1-j}\omega_0^{G+D}+\sum_{k=2}^{(j-1)}(k-1)(-1)^k\mathscr{G}_k^{1-k}\Omega_{j-k}^{G+D-j+k},\\ \Omega_{j-k}^{G+D-j+k}&=0,\quad \text{if}\quad (j-k)<q+1. \end{aligned}\tag{34}$$

As we shall see, the latter turns out to be easily disentangled by using the results (29) on the BRS cohomology. Moreover, setting $q=1$, Eqs. (34) are seen to reproduce those already met in the pure Yang–Mills case.[1] In particular, from Eqs. (32) and (33), we see that the solution of the tower (31) in the noncomplete case turn out to be deformed with respect to the corresponding solution of the complete ladder case (see Sec. V of part I) by the inclusion of the cocycles Ω_j^{G+D-j}.

V. EXAMPLE I: PURE YANG–MILLS THEORY AS A ZERO-CURVATURE SYSTEM

As a first important example of a noncomplete ladder system, let us present here the zero-curvature formulation of the pure Yang–Mills gauge theory in any space–time dimension, corresponding to a generalized ladder with $q=1$, i.e.,

$$\tilde{\mathscr{A}}=c+A.\tag{35}$$

It is worthwhile to recall that, since the Yang–Mills theories are power-counting nonrenormalizable for space–time dimensions greater than four, the fields A and c, unlike the three-dimensional Chern–Simons case discussed in Part I, are now regarded as unquantized external fields coupled to currents of quantum matter fields. Therefore, the existence of gauge anomalies at the quantum level will correspond to a violation of the conservation law of the matter currents and to the appearance of Schwinger terms in the corresponding current algebra.

It is easily checked that in this case the consistency of the zero-curvature condition (16) requires that only the first operator $\mathscr{G}_2^{-1}$ of Eq. (19) is nonvanishing. Therefore, for the operator $\tilde{d}$ we get

$$\tilde{d}=b+d+\mathscr{G}_2^{-1},\tag{36}$$

and from

$$\tilde{d}.\tilde{\mathscr{A}}=i.\tilde{\mathscr{A}}^2\tag{37}$$

we obtain

$$bc=ic^2,\quad bA=-dc+i[c,\,A],\tag{38}$$

and

$$\begin{aligned} \mathscr{G}_2^{-1}c&=-dA+iA^2=-F,\\ \mathscr{G}_2^{-1}dc&=i[A,\,F],\\ \mathscr{G}_2^{-1}A&=\mathscr{G}_2^{-1}F=0. \end{aligned}\tag{39}$$

From Eqs. (9) and (10), for the operator δ we have

$$\delta c = A, \quad \delta\, dc = -dA + 2iA^2,$$
$$\delta A = 0, \quad \delta dA = 0, \tag{40}$$

and

$$d = -[d,\ \delta], \quad \mathscr{G}_2^{-1} = \tfrac{1}{2}[\delta,\ d],$$
$$[\delta,\ \mathscr{G}_2^{-1}] = [b,\ \mathscr{G}_2^{-1}] = [d,\ \mathscr{G}_2^{-1}] = 0. \tag{41}$$

For what concerns the solutions of the descent equations (31), here we shall limit ourselves only to state the final result, reminding the reader of the detailed discussion and proofs already given in Ref. 2. We underline in particular that, as proven in Ref. 3, the cocycles Ω_j^{G+D-j} appearing in Eq. (32) can be summed up into a unique closed generalized expression which collects both the gauge anomalies and the Chern–Simons terms. The latter are given respectively by

$$\omega_{2n}^1 = \sum_{p=0}^{n} \frac{i^{(n-p)}}{(2n-p+1)!p!} (\mathscr{P}(c, F^p, (A^2)^{n-p}) + i(n-p)\mathscr{P}([c,\ A], F^p, A, (A^2)^{n-p})) \tag{42}$$

and

$$\omega_{2n+1}^0 = \sum_{p=0}^{n} \frac{i^{(n-p)}}{(2n-p+1)!p!} \mathscr{P}(F^p, A, (A^2)^{n-p}), \tag{43}$$

where the integer $n = 1,2,...$ labels the various dimensions of the space–time and $\mathscr{P}(\mathscr{J}_1, \mathscr{J}_2, ..., \mathscr{J}_n)$ denotes the symmetric invariant polynomials defined as

$$\mathscr{P}(\mathscr{J}_1, \mathscr{J}_2, \ldots, \mathscr{J}_n) = \mathscr{J}_1^{a_1} \mathscr{J}_2^{a_2} \cdots \mathscr{J}_n^{a_n} S\ \mathrm{Tr}(T^{a_1} T^{a_2} \cdots T^{a_n}), \tag{44}$$

S Tr being the symmetrized trace[8] and, following Zumino's notations,[9] we have used

$$\mathscr{P}(\mathscr{J}_1, \mathscr{J}_2, \ldots, \mathscr{J}^p) = \mathscr{P}(\mathscr{J}_1, \mathscr{J}_2, \mathscr{J}_3, \underbrace{\mathscr{J}, \ldots, \mathscr{J}}_{p \text{ times}}). \tag{45}$$

It is worthwhile to emphasize that, actually, the formulas (42) and (43) represent one of the most compact expressions for the gauge anomaly and for the Chern–Simons term in any space–time dimension.

VI. EXAMPLE II: THE CASE $D=6$, $G=1$, $q=3$

In order to clarify the role of the operators $\mathscr{G}_k^{1-k}$ and of the generalized curvatures R_{m+1}^{1-m}, let us discuss in this second example the solution of the descent equations (5) in the six-dimensional case $D=6$ with ghost number $G=1$ and a gauge ladder with $q=3$, i.e.,

$$\tilde{\mathscr{A}} = c + A + \varphi_2^{-1} + \varphi_3^{-2}. \tag{46}$$

From Eqs. (25), for the BRS transformations we have

$$\begin{aligned} bc &= ic^2, \\ bA &= -dc + i[c,\ A], \\ b\varphi_2^{-1} &= i[c,\ \varphi_2^{-1}] - R_2^0, \\ b\varphi_3^{-2} &= i[c,\ \varphi_3^{-2}] - R_3^{-1}, \end{aligned} \tag{47}$$

where R_2^0 and R_3^{-1} are the generalized curvatures of Eq. (21) whose expressions are given

$$\begin{aligned} R_2^0 &= F = dA - iA^2, \\ R_3^{-1} &= d\varphi_2^{-1} - i[A,\ \varphi_2^{-1}]. \end{aligned} \tag{48}$$

In particular, for the highest curvature R_4^{-2} we have

$$R_4^{-2} = d\varphi_3^{-2} - i[A,\ \varphi_3^{-2}] - \frac{i}{2}[\varphi_2^{-1},\ \varphi_2^{-1}] \tag{49}$$

and

$$bR_{m+1}^{1-m} = i[c,\ R_{m+1}^{1-m}], \quad 1 \leqslant m \leqslant 3. \tag{50}$$

The curvatures $(R_2^0, R_3^{-1}, R_4^{-2})$ obey the following generalized Bianchi identities:

$$\begin{aligned} dR_2^0 &= i[A,\ R_2^0], \\ dR_3^{-1} &= i[A,\ R_3^{-1}] + i[\varphi_2^{-1},\ R_2^0], \\ dR_4^{-2} &= i[A,\ R_4^{-2}] + i[\varphi_2^{-1},\ R_3^{-1}] + i[\varphi_3^{-2},\ R_2^0]. \end{aligned} \tag{51}$$

They transform under the operator δ of Eqs. (9) and (10) as

$$\begin{aligned} \delta R_2^0 &= 2R_3^{-1}, \\ \delta R_3^{-1} &= -R_4^{-2} - \frac{i}{2}[\varphi_2^{-1},\ \varphi_2^{-1}], \\ \delta R_4^{-2} &= -i\,[\varphi_3^{-2},\ \varphi_2^{-1}]. \end{aligned} \tag{52}$$

For what concerns the operators $\mathscr{G}_k^{1-k}$ of Eq. (20) it is easily seen that in the present example the zero-curvature Equation (16) implies the existence of a set of five nonvanishing operators $(\mathscr{G}_2^{-1}, \mathscr{G}_3^{-2}, \mathscr{G}_4^{3}, \mathscr{G}_5^{4}, \mathscr{G}_6^{5})$. Their action on the fields and on the curvatures is given, respectively, by

$$\begin{aligned} &\mathscr{G}_2^{-1}c = 0, \quad \mathscr{G}_2^{-1}A = 0, \quad \mathscr{G}_2^{-1}\varphi_2^{-1} = -2R_4^{-2}, \\ &\mathscr{G}_2^{-1}\varphi_3^{-2} = 2i[\varphi_3^{-2},\ \varphi_2^{-1}], \\ &\mathscr{G}_2^{-1}dc = 0, \quad \mathscr{G}_2^{-1}R_2^0 = 0, \\ &\mathscr{G}_2^{-1}R_3^{-1} = 2i([\varphi_2^{-1},\ R_3^{-1}] + [\varphi_3^{-2},\ R_2^0]), \\ &\mathscr{G}_2^{-1}R_4^{-2} = 2i[\varphi_3^{-2},\ R_3^{-1}]; \end{aligned} \tag{53}$$

$$\mathcal{G}_3^{-2}c=0,\quad \mathcal{G}_3^{-2}A=\frac{4}{3}R_4^{-2},$$

$$\mathcal{G}_3^{-2}\varphi_2^{-1}=-\frac{4i}{3}[\varphi_3^{-2},\ \varphi_2^{-1}],$$

$$\mathcal{G}_3^{-2}\varphi_3^{-2}=2i[\varphi_3^{-2},\ \varphi_3^{-2}],$$

$$\mathcal{G}_3^{-2}dc=0, \tag{54}$$

$$\mathcal{G}_3^{-2}R_2^0=-\frac{4i}{3}([\varphi_2^{-1},\ R_3^{-1}]+[\varphi_3^{-2},\ R_2^0]),$$

$$\mathcal{G}_3^{-2}R_3^{-1}=4i[\varphi_3^{-2},\ R_3^{-1}],$$

$$\mathcal{G}_3^{-2}R_4^{-2}=0;$$

$$\mathcal{G}_4^{-3}c=-\frac{1}{3}R_4^{-2},\quad \mathcal{G}_4^{-3}A=\frac{i}{3}[\varphi_3^{-2},\ \varphi_2^{-1}],$$

$$\mathcal{G}_4^{-3}\varphi_2^{-1}=-\frac{5i}{2}[\varphi_3^{-2},\ \varphi_3^{-2}],\quad \mathcal{G}_4^{-3}\varphi_3^{-2}=0,$$

$$\mathcal{G}_4^{-3}dc=\frac{i}{3}([A,\ R_4^{-2}]+[\varphi_2^{-1},\ R_3^{-1}]+[\varphi_3^{-2},\ R_2^0]), \tag{55}$$

$$\mathcal{G}_4^{-3}R_2^0=\frac{i}{3}([\varphi_2^{-1},\ R_4^{-2}]-11[\varphi_3^{-2},\ R_3^{-1}]),$$

$$\mathcal{G}_4^{-3}R_3^{-1}=0,\quad \mathcal{G}_4^{-3}R_4^{-2}=0;$$

$$\mathcal{G}_5^{-4}c=0,\quad \mathcal{G}_5^{-4}A=\frac{6i}{5}[\varphi_3^{-2},\ \varphi_3^{-2}],$$

$$\mathcal{G}_5^{-4}\varphi_2^{-1}=0,\quad \mathcal{G}_5^{-4}\varphi_3^{-2}=0,$$

$$\mathcal{G}_5^{-4}dc=\frac{16i}{5}[\varphi_3^{-2},\ R_3^{-1}], \tag{56}$$

$$\mathcal{G}_5^{-4}R_2^0=\mathcal{G}_5^{-4}R_3^{-1}=\mathcal{G}_5^{-4}R_4^{-2}=0;$$

$$\mathcal{G}_6^{-5}c=-\frac{i}{5}[\varphi_3^{-2},\ \varphi_3^{-2}],$$

$$\mathcal{G}_6^{-5}A=\mathcal{G}_6^{-5}\varphi_2^{-1}=\mathcal{G}_6^{-5}\varphi_3^{-2}=0, \tag{57}$$

$$\mathcal{G}_6^{-5}dc=\mathcal{G}_6^{-5}R_2^0=\mathcal{G}_6^{-5}R_3^{-1}=\mathcal{G}_6^{-5}R_4^{-2}=0.$$

Turning now to the descent equations

$$b\omega_{6-j}^{1+j}+d\omega_{5-j}^{2+j}=0, \quad 0\leqslant j\leqslant 5,$$
$$b\omega_0^7=0, \tag{58}$$

we have that, taking into account the result (23) on the cohomology of the BRS operator b and the equation (32), a solution of the ladder (58) is provided by the generalized cocycle of total degree seven

$$\tilde{\omega}^7=e^{\delta}(\omega_0^7+\Omega_4^3+\Omega_5^2+\Omega_6^1) \tag{59}$$

with

$$\omega_0^7=\mathrm{Tr}\,\frac{c^7}{7!}, \tag{60}$$

and $(\Omega_4^3,\Omega_5^2,\Omega_6^1)$ solutions of the equations (34), i.e.,

$$b\Omega_4^3=3\mathscr{I}_4^{-3}\omega_0^7, \tag{61}$$

$$b\Omega_5^2=-4\mathscr{I}_5^{-4}\omega_0^7, \tag{62}$$

$$b\Omega_6^1=\mathscr{I}_2^{-1}\Omega_4^3+5\mathscr{I}_6^{-5}\omega_0^7. \tag{63}$$

This system can be easily solved by using the cohomology of b. Indeed, beginning with the first equation (61), we have from (55)

$$\mathscr{I}_4^{-3}\omega_0^7=-\frac{1}{6!}\,\mathrm{Tr}\,\frac{R_4^{-2}c^6}{3}, \tag{64}$$

so that Ω_4^3 may be identified with

$$\Omega_4^3=-\frac{1}{6!}\,\mathrm{Tr}\,R_4^{-2}c^5. \tag{65}$$

Concerning now the second equation (62), we get from (56) that

$$\mathscr{I}_5^{-4}\omega_0^7=0. \tag{66}$$

Moreover, since the cohomology of b in the sector of form degree five and ghost number two is empty, we may choose Ω_5^2 to be vanishing as well

$$\Omega_5^2=0. \tag{67}$$

Finally for the last equation (63), we get

$$b\Omega_6^1=\frac{2}{6!}\,\mathrm{Tr}([\varphi_3^{-2},\,R_3^{-1}]c^5-i\varphi_3^{-2}\varphi_3^{-2}c^6). \tag{68}$$

However, from

$$b(\mathrm{Tr}\;\varphi_3^{-2}\varphi_3^{-2}c^5)=\mathrm{Tr}([\varphi_3^{-2},\,R_3^{-1}]c^5-i\varphi_3^{-2}\varphi_3^{-2}c^6), \tag{69}$$

we obtain

$$\Omega_6^1=\frac{1}{6!}\,\mathrm{Tr}([\varphi_3^{-2},\varphi_3^{-2}]c^5). \tag{70}$$

Summarizing, an explicit expression for the Ω's is given by

$$\Omega_4^3=-\frac{i}{6!}\,\mathrm{Tr}\,R_4^{-2}c^5,$$

$$\Omega_5^2=0, \tag{71}$$

$$\Omega_6^1=\frac{1}{6!}\,\mathrm{Tr}([\varphi_3^{-2},\varphi_3^{-2}]c^5).$$

Of course, the above expressions are always determined modulo trivial b-cocycles.

Concluding, for the generalized cocycle $\tilde{\omega}^7$ we have

$$\tilde{\omega}^7=\mathrm{Tr}\left(\frac{\tilde{\mathscr{A}}^7}{7!}+\Omega_4^3+\delta\Omega_4^3+\frac{\delta^2}{2}\,\Omega_4^3+\Omega_6^1\right). \tag{72}$$

The expansion of $\tilde{\omega}^7$ in terms of components of different degree and ghost number will give an explicit expression for the cocycles entering the descent equations (58).

VIII. CONCLUSION

We have shown that the Yang–Mills-type theories can be characterized by means of a non-complete gauge ladder field constrained to obey a zero curvature condition, which implies the existence of a set of new operators $\mathscr{F}_k^{1-k}$. These operators give rise together with the BRS operator b to a kind of descent equation which is easily solved using the results on the cohomology of b. These solutions provide a deformation of the cohomology of b modulo d with respect to the corresponding complete ladder case presented in the part I.

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Density conditions for quantum propositions

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As has already been pointed out by Birkhoff and von Neumann, quantum logic can be formulated in terms of projective geometry. In three-dimensional Hilbert space, elementary logical propositions are associated with one-dimensional subspaces, corresponding to points of the projective plane. It is shown that, starting with three such propositions corresponding to some basis $\{\mathbf{u},\mathbf{v},\mathbf{w}\}$, successive application of the binary logical operation $(x,y)\mapsto(x \vee y)^{\perp}$ generates a set of elementary propositions which is countable infinite and dense in the projective plane if and only if no vector of the basis $\{\mathbf{u},\mathbf{v},\mathbf{w}\}$ is orthogonal to the other ones. © *1996 American Institute of Physics.* [S0022-2488(96)00309-X]

I. INTRODUCTION

The geometrization of quantum logic was initiated by Birkhoff and von Neumann.[1] In their ''top-down'' approach, the logical entities are identified with Hilbert space entities as follows. Elementary propositions are identified with one-dimensional subspaces or with the vector spanning that subspace. The binary logical operations ''and'' ($\wedge$) and ''or'' ($\vee$) correspond to the set theoretic intersection and to the linear span, respectively. The unary logical operation ''not'' ($^{\perp}$) corresponds to the orthogonal subspace. The proposition which is always false is identified with the null vector. The proposition which is always true is identified with the entire Hilbert space. In that way, the geometry of Hilbert space induces a logical structure which, if Hilbert space quantum mechanics[2] is an appropriate theory of quantum physics, describes correctly the logical structure of measurements (cf. Refs. 3–7).

In what follows, we concentrate on the following question. Assume we start with a set $\{u,v,w\}$ of three elementary quantum mechanical propositions representable as one-dimensional subspaces (spanned by the vectors $\{\mathbf{u}, \mathbf{v}, \mathbf{w}\}$) of three-dimensional Hilbert space. New propositions can be formed from the old ones by the logical operations ''and, or, not.'' In particular, the operation $(x \vee y)^{\perp}$ corresponding to ''not (x or y)'' is just the subspace spanned by the vector product $\mathbf{x}\times\mathbf{y}$. Suppose this operation is carried out recursively. That is, at each step we form the vector product of all (nonparallel) vectors and add the (nonparallel) results to the previous set of vectors. One may ask, what are the conditions for the resulting set (of intersection points with the unit ball) to be dense? Evidently, the set of one-dimensional subspaces spanned by the recursive application of the vector product can at most be countable (cardinality $\aleph_0$). It is less obvious if there can be any regions or ''holes'' formed by the recursively obtained set of one-dimensional subspaces which are unreachable. An answer is given in Theorem 3.

As has been already pointed out by Birkhoff and von Neumann,[1] the structure obtained for three-dimensional Hilbert space is essentially a projective plane. Points of the projective geometry are identified with elementary propositions, and lines are identified with two-dimensional sub-

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spaces. We emphasize this point of view by reformulating the above problem into the geometric language of the real projective plane endowed with the elliptic metric.

The original motivation for this question originates from the consideration of Kochen-Specker type constructions.[8,9] It has been conjectured that every set of three nonorthogonal one-dimensional subspaces generates a Kochen-Specker paradox.[10] More generally, one could ask if any single elementary proposition (corresponding to a one-dimensional subspace of three-dimensional Hilbert space) can be approximated by a logical construction originating from just three propositions (corresponding to nonorthogonal one-dimensional subspaces of three-dimensional Hilbert space).

It has to be kept in mind, however, that a consistent two-valued measure—serving as a classical truth function—will in general not be definable on the set of recursively generated one-dimensional subspaces identifiable with elementary propositions. Indeed, due to complementarity, even for the generating set of three vectors, such an identification of truth functions will only have an operational (physical) meaning if these vectors were mutually orthogonal—a condition which would yield a trivial orthogonal tripod configuration, for which any recursion does not produce any additional vectors.

II. SUBPLANES OF PROJECTIVE PLANES

A *projective plane* is formally a geometric structure $(\mathscr{P},\mathscr{L},I)$ consisting of a set $\mathscr{P}$ of elements called *points*, a set $\mathscr{L}$ of elements called *lines* and a binary relation $I\subset\mathscr{P}\times\mathscr{L}$ called *incidence* satisfying the following axioms.

(P1) Any two distinct points are incident with exactly one common line.

(P2) Any two distinct lines are incident with a common point.

(P3) There are four points, no three of which are incident with a common line.

Instead of $(p,L)\in I$ we also write pIL and use familiar expressions like ''p is on L,'' ''L is running through p,'' etc. A set of points is said to be *colinear*, if all points are on a common line, a *triangle* is a set of three non-colinear points, a *quadrangle* is a set of four points satisfying the condition of axiom (P3). If we are given two distinct points $p_1,p_2\in\mathscr{P}$ then $p_1\vee p_2$ denotes the unique line joining these two points. By (P1) and (P2), two distinct lines $L_1,L_2\in\mathscr{L}$ meet at a unique point which is written as $L_1\wedge L_2$. For basic properties of projective planes see [Ref. 11, Chap. 4], Ref. 12 or Ref. 13.

Let F be a skewfield (division ring). Then F^3 (regarded as left vector space over F) gives rise to a projective plane as follows: Define $\mathscr{P}$ as set of all one-dimensional subspaces of F^3, viz.

$$\mathscr{P}:=\{F\mathbf{a}\,|\,\mathbf{o}\neq\mathbf{a}\in F^3\}, \tag{1}$$

and $\mathscr{L}$ as the set of all two-dimensional subspaces of F^3. Incidence is defined by

$$I:=\{(F\mathbf{a},\mathbf{L})\in\mathscr{P}\times\mathscr{L}\,|\,F\mathbf{a}\subset L\}. \tag{2}$$

We set $(\mathscr{P},\mathscr{L},I)=:\mathrm{PG}(2,F)$. See, e.g., Ref. 14, p. 29, Ref. 15, p. 222 or the textbooks mentioned above for more details.

We remark that there are also projective planes that are not isomorphic to any plane of the form $\mathrm{PG}(2,F)$. Such projective planes are called *Non-Desarguesian* and will not be of interest in this paper.

Suppose that $(\mathscr{P},\mathscr{L},I)$ is a projective plane and that $\widetilde{\mathscr{P}}$ is any subset of $\mathscr{P}$. Put

$$\widetilde{\mathscr{L}}:=\{p_1\vee p_2\,|\,p_1,p_2\in\widetilde{\mathscr{P}},p_1\neq p_2\}\quad\text{and}\quad\widetilde{I}:=I\cap(\widetilde{\mathscr{P}}\times\widetilde{\mathscr{L}}). \tag{3}$$

The substructure $(\widetilde{\mathscr{P}},\widetilde{\mathscr{L}},\widetilde{I})$ is satisfying axiom (P1), but not necessarily (P2) or (P3). If $(\widetilde{\mathscr{P}},\widetilde{\mathscr{L}},\widetilde{I})$ is a projective plane, then it is called a *projective subplane* of $(\mathscr{P},\mathscr{L},I)$. A *degenerate subplane* $(\widetilde{\mathscr{P}},\widetilde{\mathscr{L}},\widetilde{I})$ is satisfying (P2), but not (P3).

All degenerate subplanes are easily described: If $\#\widetilde{\mathscr{L}} \leqslant 1$, then $\widetilde{\mathscr{P}}$ is a set of colinear points. If $\#\widetilde{\mathscr{L}} \geqslant 2$, then $\widetilde{\mathscr{P}}$ is formed by a set of two or more points on a line, say L, plus one more point, say u, off the line L. This L is the only line in $\widetilde{\mathscr{L}}$ not running through u.

In PG(2,F) we may obtain a projective subplane as follows: Let $\{\mathbf{b}_1,\mathbf{b}_2,\mathbf{b}_3\} \subset F^3$ be a basis and let $\widetilde{F} \subset F$ be a sub-skewfield of F. Then set

$$\widetilde{\mathscr{P}} = \left\{ F\mathbf{a} \,\middle|\, \mathbf{a} = \sum_{i=1}^{3} \xi_i \mathbf{b}_i, (0,0,0) \neq (\xi_1,\xi_2,\xi_3) \in \widetilde{F}^3 \right\}, \tag{4}$$

and define $\widetilde{\mathscr{L}}, \widetilde{I}$ according to (3). The verification of (P2) amounts to solving a homogeneous system of linear equations within the sub-skewfield $\widetilde{F}$. A quadrangle in $\widetilde{\mathscr{P}}$ is given by $\{\mathbb{R}\mathbf{b}_1, \mathbb{R}\mathbf{b}_2, \mathbb{R}\mathbf{b}_3, \mathbb{R}(\mathbf{b}_1+\mathbf{b}_2+\mathbf{b}_3)\}$.

The backbone of this article is the following innocently looking result (Ref. 13, p. 266): Any projective subplane of PG(2,F) is of the form (4). (See also Ref. 16, p. 1008.) This allows us to recover an algebraic structure, namely a sub-skewfield of F, from a projective subplane of PG(2,F). Let us add, for the sake of completeness, the following remark: If in (4) the basis $\{\mathbf{b}_1,\mathbf{b}_2,\mathbf{b}_3\}$ is replaced by $\{\alpha\mathbf{b}_1,\alpha\mathbf{b}_2,\alpha\mathbf{b}_3\}$ for some nonzero $\alpha \in F$ and if $\widetilde{F}$ is modified to the sub-skewfield $\alpha\widetilde{F}\alpha^{-1}$, then $\widetilde{\mathscr{P}}$ remains unchanged. Actually, a projective subplane of PG(2,F) determines ''its'' sub-skewfield of F only to within transformation under inner automorphisms of F. Clearly, for a (commutative) field F this means uniqueness.

We confine our attention to the *real projective plane* PG(2,$\mathbb{R}$). The *elliptic metric* on $\mathscr{P}$ is given by

$$d: \mathscr{P}\times\mathscr{P} \to \mathbb{R}, (\mathbb{R}\mathbf{a}, \mathbb{R}\mathbf{b}) \mapsto \arccos\frac{|\mathbf{a}\cdot\mathbf{b}|}{\|\mathbf{a}\|\|\mathbf{b}\|} \in \left[0, \frac{\pi}{2}\right], \tag{5}$$

where $\cdot$ denotes the standard dot product and $\|\ \|$ stands for the Euclidean norm of $\mathbb{R}^3$. The *elliptic distance* $d(\mathbb{R}\mathbf{a}, \mathbb{R}\mathbf{b})$ of two points of PG(2,$\mathbb{R}$) is just the Euclidean angle of the corresponding one-dimensional subspaces through the origin of $\mathbb{R}^3$. It is invariant under transformations (e.g., rotations) which preserve normality. Besides, a connection can be made between the elliptic distance and the more physically motivated *statistical distance*.[17]

For each point $\mathbb{R}\mathbf{a}$ of PG(2,$\mathbb{R}$) there are exactly two unit vectors in $\mathbb{R}\mathbf{a}$. This gives the well-known alternative description of the real projective plane: The ''points'' may be viewed as unordered pairs of opposite points of the unit sphere, the ''lines'' are the great circles and incidence is defined via inclusion. In this interpretation the elliptic distance is equal to the *spherical distance* (Ref. 18, Chap. VI).

If T is a subset of $\mathbb{R}^3$ then $T^{\perp} := \{\mathbf{a} | \mathbf{a}\cdot\mathbf{t} = 0 \text{ for all } \mathbf{t} \in T\}$ is a subspace. In geometric terms $\perp$ is a *polarity* of the projective plane PG(2,$\mathbb{R}$); cf. (Ref. 11, Chap. 17, Ref. 18, p. 52, Ref. 14, p. 110, or Ref. 12, p. 45). Points and lines are interchanged bijectively subject to the rule $\mathbb{R}\mathbf{a} \times (\in\mathscr{P}) \mapsto \mathbf{a}\perp (\in\mathscr{L})$. *The geometric operations of ''join'' ($\vee$) and ''meet'' ($\wedge$) therefore allow a simple algebraic description*: *Given linearly independent vectors* $\mathbf{a},\mathbf{b} \in \mathbb{R}^3$ then

$$\mathbb{R}\mathbf{a} \vee \mathbb{R}\mathbf{b} = (\mathbf{a}\times\mathbf{b})^{\perp}, \tag{6}$$

$$\mathbf{a}^{\perp} \wedge \mathbf{b}^{\perp} = \mathbb{R}(\mathbf{a}\times\mathbf{b}). \tag{7}$$

The following result is essentially ($\widetilde{F} = \mathbb{Q}$) due to Möbius:

Lemma 1: If $(\widetilde{\mathscr{P}}, \widetilde{\mathscr{L}}, \widetilde{I})$ is a projective subplane of $(\mathscr{P},\mathscr{L},I) =$ PG(2,$\mathbb{R}$), then $\widetilde{\mathscr{P}}$ is dense in $\mathscr{P}$.

Proof: Let $\widetilde{\mathscr{P}}$ be given according to (4) with $\widetilde{F} \subset \mathbb{R}$. The field $\mathbb{Q}$ of rational numbers equals the intersection of all subfields of $\mathbb{R}$, whence $\mathbb{Q} \subset \widetilde{F}$. Given a point $\mathbb{R}\mathbf{a} \in \mathscr{P}$ we obtain

$$\mathbf{a}=\xi_1\mathbf{b}_1+\xi_2\mathbf{b}_2+\xi_3\mathbf{b}_3 \quad \text{with} \quad (\xi_1,\xi_2,\xi_3)\in\mathbb{R}^3. \tag{8}$$

There exist three sequences,

$$(\xi_{j,i})_{i\in\mathbb{N}}, \quad \text{with } \xi_{j,i}\in\mathbb{Q}\backslash\{0\} \quad \text{and} \quad \lim_{i\to\infty}\xi_{j,i}=\xi_j \quad (j\in\{1,2,3\}). \tag{9}$$

Defining

$$\mathbf{a}_i:=\xi_{1,i}\mathbf{b}_1+\xi_{2,i}\mathbf{b}_2+\xi_{3,i}\mathbf{b}_3\neq\mathbf{o} \quad (i\in\mathbb{N}) \tag{10}$$

yields a sequence of points $\mathbb{R}\mathbf{a}_i\in\widetilde{\mathscr{P}}$ with $(\mathbb{R}\mathbf{a}_i)_{i\in\mathbb{N}}\to\mathbb{R}\mathbf{a}$, since, by the continuity of dot product and norm,

$$\lim_{i\to\infty}\frac{\mathbf{a}\cdot\mathbf{a}_i}{\|\mathbf{a}\|\|\mathbf{a}_i\|}=\frac{\mathbf{a}\cdot\mathbf{a}}{\|\mathbf{a}\|\|\mathbf{a}\|}=1. \tag{11}$$

This completes the proof. □

The projective subplanes of PG(2,$\mathbb{R}$) belonging to the rational number field are called *Möbius nets*. They allow a simple recursive geometric construction (Ref. 19, p. 140): Starting with a quadrangle one draws all the lines spanned by these points. Next mark all points of intersection arising from these lines. With this set of points the procedure is repeated, and so on. The set of all points that can be reached in a finite number of steps gives then a projective subplane over $\mathbb{Q}$.

III. MAIN THEOREMS

Theorem 1: Let $V_1=\{\mathbf{u},\mathbf{v},\mathbf{w}\}$ be a basis of $\mathbb{R}^3$. Define subsets V_i, V of $\mathbb{R}^3$ as follows:

$$V_{i+1}:=V_i\cup\{\mathbf{r}\times\mathbf{s}|\mathbf{r},\mathbf{s}\in V_i,\mathbf{r}\times\mathbf{s}\neq\mathbf{o}\} \quad (i\in\mathbb{N}), \quad V:=\bigcup_{i=1}^{\infty}V_i. \tag{12}$$

Then

$$\widetilde{\mathscr{P}}:=\{\mathbb{R}\mathbf{a}|\mathbf{a}\in V\} \tag{13}$$

yields a projective or degenerate subplane $(\widetilde{\mathscr{P}},\widetilde{\mathscr{L}},\widetilde{I})$ of PG(2,$\mathbb{R}$) which is ortho-closed. That is, $\mathbb{R}\mathbf{a}\in\widetilde{\mathscr{P}}$ implies $\mathbf{a}^\perp\in\widetilde{\mathscr{L}}$.

Proof: Let $L_1,L_2\in\widetilde{\mathscr{L}}$ be distinct. By (6) and the definition of $\widetilde{\mathscr{L}}$, there are vectors $\mathbf{p}_1,\mathbf{q}_1,\mathbf{p}_2,\mathbf{q}_2\in V$ with

$$L_1=(\mathbf{p}_1\times\mathbf{q}_1)^\perp, \quad L_2=(\mathbf{p}_2\times\mathbf{q}_2)^\perp. \tag{14}$$

Now (7) yields

$$L_1\wedge L_2=\mathbb{R}((\mathbf{p}_1\times\mathbf{q}_1)\times(\mathbf{p}_2\times\mathbf{q}_2))\in\widetilde{\mathscr{P}}. \tag{15}$$

This establishes (P2).

Given a point $\mathbb{R}\mathbf{a}\in\widetilde{\mathscr{P}}$, there exist two vectors in V_1, say **u,v**, such that {**a,u,v**} is a basis of $\mathbb{R}^3$. Then $u\notin\text{span}\{\mathbf{a},\mathbf{v}\}=(\mathbf{a}\times\mathbf{v})^\perp$, but $\mathbf{u}\in(\mathbf{a}\times\mathbf{u})^\perp$. Thus $\mathbb{R}(\mathbf{a}\times\mathbf{v})$ and $\mathbb{R}(\mathbf{a}\times\mathbf{v})$ are distinct points of $\widetilde{\mathscr{P}}$ on the line $\mathbf{a}^\perp$. □

Observe that axiom (P2) may be derived alternatively from the well-known formula

$$(\mathbf{p}_1\times\mathbf{q}_1)\times(\mathbf{p}_2\times\mathbf{q}_2)=\det(\mathbf{p}_1,\mathbf{q}_1,\mathbf{q}_2)\mathbf{p}_2-\det(\mathbf{p}_1,\mathbf{q}_1,\mathbf{p}_2)\mathbf{q}_2=\det(\mathbf{p}_1,\mathbf{p}_2,\mathbf{q}_2)\mathbf{q}_1-\det(\mathbf{q}_1,\mathbf{p}_2,\mathbf{q}_2)\mathbf{p}_1. \tag{16}$$

since linearly dependent vectors yield colinear points.

Theorem 2: The subplane $(\widetilde{\mathscr{P}},\widetilde{\mathscr{L}},\widetilde{I})$ described in Theorem 1 is degenerate if and only if one vector of the basis $\{\mathbf{u},\mathbf{v},\mathbf{w}\}$ is orthogonal to the other ones.

Proof: Let $(\widetilde{\mathscr{P}},\widetilde{\mathscr{L}},\widetilde{I})$ be degenerate. $\{\mathbb{R}\mathbf{u},\mathbb{R}\mathbf{v},\mathbb{R}\mathbf{w}\}$ being a triangle forces $\#\widetilde{\mathscr{L}}\geqslant 3$. We read off from the description of degenerate subplanes in section II that $\widetilde{\mathscr{P}}$ has to consist of one point of this triangle, say $\mathbb{R}\mathbf{u}$, and a subset of points on the line joining $\mathbb{R}\mathbf{v}$ and $\mathbb{R}\mathbf{w}$. The line $\mathbf{u}^{\perp}$ belongs to $\widetilde{\mathscr{L}}$ by Theorem 1. Now $\mathbf{u}\notin\mathbf{u}^{\perp}$ tells us that the point $\mathbb{R}\mathbf{u}$ is off that line. Since $\mathbb{R}\mathbf{u}$ is on all lines of $\widetilde{\mathscr{L}}$ but one, we obtain $\mathbf{v},\mathbf{w}\in\mathbf{u}^{\perp}$.

Conversely, assume that $\mathbf{v},\mathbf{w}\in\mathbf{u}^{\perp}$. Then

$$\widetilde{\mathscr{P}}=\{\mathbb{R}\mathbf{u},\mathbb{R}\mathbf{v},\mathbb{R}\mathbf{w},\mathbb{R}(\mathbf{u}\times\mathbf{v}),\mathbb{R}(\mathbf{u}\times\mathbf{w})\} \tag{17}$$

is a set of five points if $\mathbf{v}\not\perp\mathbf{w}$, and it is a set of just three points if $\mathbf{u},\mathbf{v},\mathbf{w}$ are mutually orthogonal. Thus $\widetilde{\mathscr{P}}$ yields a degenerate subplane. □

Summing up, gives this final result.

Theorem 3: With the settings of Theorem 1 the following assertions are equivalent.

1. The basis $\{\mathbf{u},\mathbf{v},\mathbf{w}\}$ of $\mathbb{R}^3$ does not contain a vector that is orthogonal to the remaining ones.
2. The point set $\widetilde{\mathscr{P}}$ given by (13) is dense in PG$(2,\mathbb{R})$.
3. The point set $\widetilde{\mathscr{P}}$ given by (13) is infinite.

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Geometrical interpretation of BRST symmetry in topological Yang–Mills–Higgs theory

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We study the topological Yang–Mills–Higgs theories in two and three dimensions and the topological Yang–Mills theory in four dimensions in a unified framework of superconnections. In this framework, we first show that a classical action of topological Yang–Mills type can provide all three classical actions of these theories via appropriate projections. Then we obtain the Becchi–Rouet–Stora–Tyutin (BRST) and anti-BRST transformation rules encompassing these three topological theories from an extended definition of curvature and a geometrical requirement of the Bianchi identity. This is an extension of Perry and Teo's work in the topological Yang–Mills case. Finally, comparing this result with our previous treatment in which we used the ''modified horizontality condition,'' we provide a meaning of the Bianchi identity from the BRST symmetry viewpoint and thus interpret the BRST symmetry in a geometrical setting. © *1996 American Institute of Physics.* [S0022-2488(96)01611-8]

I. INTRODUCTION

Soon after Witten[1] constructed the topological Yang–Mills theory to generate the Donaldson invariants of smooth four-manifolds, Baulieu and Singer[2] showed that Witten's topological quantum action could be obtained by gauge fixing the classical topological action

$$I_4=\int_{M_4} \mathrm{Tr}\, F\wedge F \tag{1}$$

in the Becchi–Rouet–Stora–Tyutin (BRST) quantization scheme. Then Perry and Teo[3] argued that the asymmetry of BRST transformation rules that appeared in Baulieu and Singer's work was caused by treating only the BRST symmetry,[4] and not the anti-BRST symmetry.[5] And they obtained symmetric BRST and anti-BRST transformation rules by treating them on an equal footing. They further identified the difference between the ordinary Yang–Mills theory and the topological Yang–Mills theory as follows. In the ordinary Yang–Mills theory, one can impose the so-called ''horizontality condition'' to find BRST symmetry. This is tantamount to requiring that the unphysical components of Yang–Mills field strength (curvature), which contain ghosts, vanish. In the topological case, one cannot impose this vanishing field strength condition along unphysical directions, and one can only impose the Bianchi identity in the extended space where ghosts are included.

Parallel to this development, topological Yang–Mills–Higgs actions in two and three dimensions were also constructed. Following the Baulieu and Singer's approach, Baulieu and Grossman[6] found a topological action for magnetic monopoles by gauge fixing the following classical action in three dimensions:

$$I_3=\int_{M_3} \mathrm{Tr}\, F\wedge D\phi. \tag{2}$$

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The two-dimensional case was studied by Chapline and Grossman[7] by gauge fixing the following two-dimensional classical action:

$$I_2=\int_{M_2} \mathrm{Tr}(F[\Phi^\dagger,\ \Phi]-D\Phi^\dagger\wedge D\Phi), \tag{3}$$

and the quantized version of this theory turned out to be connected to the theory of vortices and knots.

In our previous work,[8] we investigated the BRST/anti-BRST symmetry of the above topological Yang–Mills–Higgs theory in two and three dimensions by modifying the horizontality condition in a way that it could account for the topological symmetry in addition to the ordinary Yang–Mills gauge symmetry. This work was done in the superconnection framework so that the scalar and vector gauge fields were treated on the same footing as a connection. Thereby we could find the BRST/anti-BRST transformation rules of the scalar and vector gauge fields immediately in one calculation instead of doing additional and separate calculations.

In this paper, we investigate the BRST/anti-BRST symmetry of these theories through the ''Bianchi identity'' in the same superconnection framework that we used in our previous work. This investigation was motivated by the question of whether Perry and Teo's work could be extended to the topological Yang–Mills–Higgs case where additional ghosts for the scalar field appear. The superconnection framework became a very natural testing ground for this idea. The result of the test is affirmative. By comparing these two approaches—the present work and our previous work—we can further provide a meaning for the Bianchi identity in the extended space from the BRST symmetry view point. This in turn allows a geometrical interpretation of the BRST/anti-BRST symmetry in the extended space.

In Sec. II, we show that the classical actions, $I_4,\ I_3,\ I_2$, can be obtained from a classical action of the topological Yang–Mills type written in superconnection language by appropriate projections depending on the dimensions of spaces to which corresponding theories belong. In Sec. III, we find the BRST/anti-BRST transformation rules of the topological Yang–Mills–Higgs theory from the Bianchi identity in the extended space and an extended definition of curvature expressed in superconnection formalism. In Sec. IV, we compare our present work with the ''horizontality condition'' approach which we adopted in our previous work. From the comparison of these two approaches, we provide a geometrical meaning to the BRST symmetry in the topological Yang–Mills–Higgs theory. In Sec. V, we draw our conclusions.

II. CLASSICAL TOPOLOGICAL ACTION WITH SUPERCONNECTIONS

In 1982, while studying a generalized gauge theory possessing an internal supersymmetry, Thierry-Mieg and Ne'eman[9] constructed a generalized system of connections with arbitrary form degrees hinted from the old idea of Cartan's integrable system.[10] In mathematics, a similar concept was introduced by Quillen in 1985[11] under the notion of superconnections, independently of Thierry-Mieg and Ne'eman's work. Then Ne'eman and Sternberg[12] used Quillen's superconnection concept to study the Higgs mechanism where the Higgs field occurred as the zeroth-order part of the superconnection. Ne'eman and Sternberg's work made it easier for physicists to understand the superconnection concept. It has also shown that the superconnection is not much different from Thierry-Mieg and Ne'eman's generalized connection, except for the existence of zeroth-order connection. In this paper, we follow Ne'eman and Sternberg's presentation of superconnections. In general, the superconnection contains all orders. It contains an even part with odd degree forms and an odd part with even degree forms. However, since the theories we are dealing with have scalar and vector gauge fields only, we shall deal with superconnections which only contain zero-forms and one-forms in this paper. Now, we may write down our superconnection as

$$\mathscr{J}=\begin{pmatrix} A & i\Phi \\ i\Phi^{\dagger} & A \end{pmatrix} \tag{4}$$

where A and Φ are Lie-algebra-valued one-form and zero-form, respectively. The multiplication rule among the elements of total Z_2-graded ''superspace'' is given by[12]

$$\begin{pmatrix} A & C \\ D & B \end{pmatrix}\begin{pmatrix} A' & C' \\ D' & B' \end{pmatrix}=\begin{pmatrix} A\wedge A'+(-1)^{|D'|}C\wedge D' & A\wedge C'+(-1)^{|B'|}C\wedge B' \\ (-1)^{|A'|}D\wedge A'+B\wedge D' & (-1)^{|C'|}D\wedge C'+B\wedge B' \end{pmatrix}, \tag{5}$$

where $A,\ldots,A',\ldots$ are matrices of differential forms, and $|A'|$, $|B'|$, $|C'|$, $|D'|$ denote form degrees of A', B', C', D', respectively.

The ''super'' curvature is defined from superconnection as

$$\mathscr{F}=\mathbf{d}\mathscr{J}+\mathscr{J}\mathscr{J}, \tag{6}$$

where $\mathbf{d}$ denotes a one-form differential operator given by $\mathbf{d}=\left(\begin{smallmatrix} d & 0 \\ 0 & d \end{smallmatrix}\right)$ with d denoting the ordinary one-form exterior derivative times a unit matrix. For brevity, we shall use the term curvature instead of ''super'' curvature from now on. Written in the component form, the curvature is given by

$$\mathscr{F}=\begin{pmatrix} F-\Phi\Phi^{\dagger} & iD\Phi \\ iD\Phi^{\dagger} & F-\Phi^{\dagger}\Phi \end{pmatrix}, \tag{7}$$

where $F=dA+A\wedge A$ and $D\Phi=d\Phi+A\Phi-\Phi A$. Now, we claim our classical topological action as

$$I=\int_M \mathrm{G\,Tr}\,\mathscr{F}\mathscr{F}, \tag{8}$$

and explain ''GTr'' below. In general, we can write down $\mathscr{F}$ as

$$\mathscr{F}=\begin{pmatrix} \mathscr{F}_{ev} & (\mathscr{F}_{od})_1 \\ (\mathscr{F}_{od})_2 & \mathscr{F}_{ev} \end{pmatrix},$$

and $\mathscr{F}\mathscr{F}$ can be written as

$$\mathscr{F}\mathscr{F}=\begin{pmatrix} (\mathscr{F}_{ev})^2-(\mathscr{F}_{od})_1(\mathscr{F}_{od})_2 & \mathscr{F}_{ev}(\mathscr{F}_{od})_1+(\mathscr{F}_{od})_1\mathscr{F}_{ev} \\ (\mathscr{F}_{od})_2\mathscr{F}_{ev}+\mathscr{F}_{ev}(\mathscr{F}_{od})_2 & (\mathscr{F}_{ev})^2-(\mathscr{F}_{od})_2(\mathscr{F}_{od})_1 \end{pmatrix}. \tag{9}$$

In four dimensions, only $(\mathscr{F}_{ev})^2$ terms can contribute since $\mathscr{F}_{ev}$ is either a two-form or zero-form. Thus we take the ordinary trace for ''GTr'' in order to get a meaningful result. In three dimensions, only $\mathscr{F}_{od}\mathscr{F}_{ev}$-type terms can contribute since $\mathscr{F}_{od}$ is a one-form. In this case, ''GTr'' becomes taking the ordinary trace after adding the odd parts of $\mathscr{F}\mathscr{F}$. We denote this procedure as ''QTr'' following the notation of the queer trace defined in Ref. 13. In two dimensions, two types of terms can contribute, $(\mathscr{F}_{ev})^2$ and $\mathscr{F}_{od}\mathscr{F}_{od}$. However, only $\mathscr{F}_{od}\mathscr{F}_{od}$-type terms have second derivative terms and we take ''GTr'' in such a way that these terms do not vanish. Thus we take supertrace in the two-dimensional case. Given this rule, the classical topological action (8) becomes

(a) in four dimensions

$$I=\int_{M_4} \mathrm{Tr}\, \mathscr{F}\mathscr{F}=2\int_{M_4} \mathrm{Tr}\, F\wedge F; \tag{10}$$

(b) in three dimensions

$$I=\int_{M_3} \mathrm{Q}\,\mathrm{Tr}\, \mathscr{F}\mathscr{F}=4i\int_{M_3} \mathrm{Tr}\, F\wedge D\phi, \tag{11}$$

where $\phi=\frac{1}{2}(\Phi^{\dagger}+\Phi)$;

(c) in two dimensions

$$I=\int_{M_2} \mathrm{S}\,\mathrm{Tr}\, \mathscr{F}\mathscr{F}=2\int_{M_2} \mathrm{Tr}(F[\Phi^{\dagger},\,\Phi]-D\Phi^{\dagger}\wedge D\Phi), \tag{12}$$

where we used the anticommuting property of one form $D\Phi$. In this way, we retrieve all three classical actions of the topological Yang–Mills–Higgs theory that appeared in Refs. 2, 6, and 7.

III. CURVATURE, BIANCHI IDENTITY, AND BRST/ANTI-BRST SYMMETRY

In the geometrical BRST quantization scheme, the base space is extended to a (double) fiber bundle space so that it contains unphysical (fiber–gauge orbit) directions, as well as physical (space–time) directions. This scheme was first developed by Thierry-Mieg and Ne'eman[14,15] with the principal fiber bundle structure yielding only the BRST symmetry which is related to the ghost (fiber) direction. It was further developed to yield the BRST and anti-BRST symmetry together. This was yielded by including the antighost direction and employing a double fiber bundle structure.[16] In order to have the antighost direction a double fiber bundle structure must be used. In this scheme, the ghost (antighost) field is obtained from the gauge field by replacing its space–time leg dx^{μ} with $dy^{N}(d\overline{y}^{N})$ where $y,\overline{y}$ represent the fiber coordinates in a double fiber bundle.[9,17–19] If one does not like the interpretation of this extended fiber bundle approach, one can take the superspace interpretation given in Refs. 20 and 21, whose view was taken in Perry and Teo's work.[3] In the superspace approach, the fiber coordinates $y,\overline{y}$ are replaced by a set of anticommuting variables θ and $\overline{\theta}$ which represent the coordinates of an abstract superspace extended from the space–time basemanifold. However, the resultant BRST/anti-BRST transformation rules are exactly the same whichever approach one uses. We do not need to distinguish between the subtle differences of the two approaches because they yield the same result. In the ordinary Yang–Mills theory, the BRST/anti-BRST symmetry is obtained from a condition which is to let the ordinary curvature equal the extended curvature. This is tantamount to requiring the curvature components containing vertical (fiber) directions to vanish, thus only the horizontal components of curvature (physical Yang–Mills field strength) in the extended space survive. For this reason, people gave the name ''horizontality condition''[18] to this condition. In this paper, we denote objects in the extended space with tildes.

Following this geometrical BRST scheme, we first extend the superconnection as

$$\tilde{\mathscr{J}}=\mathscr{J}+\mathscr{C}+\overline{\mathscr{C}}, \tag{13}$$

where $\mathscr{C}$ and $\overline{\mathscr{C}}$ are the first generation ghost and antighost for $\mathscr{J}$, which are given by

$$\mathscr{C}=\begin{pmatrix} c & 0 \\ 0 & c \end{pmatrix}, \quad \overline{\mathscr{C}}=\begin{pmatrix} \overline{c} & 0 \\ 0 & \overline{c} \end{pmatrix}. \tag{14}$$

Here c and $\overline{c}$ denote $c=A_N dy^N$ and $\overline{c}=\overline{A_N}d\overline{y}^{N}$, and represent the ghost and antighost fields, respectively. In this extended space, the curvature is given by

$$\tilde{\mathscr{F}}=\tilde{\mathbf{d}}\tilde{\mathscr{J}}+\tilde{\mathscr{J}}\tilde{\mathscr{J}}, \tag{15}$$

where

$$\tilde{\mathbf{d}}=\mathbf{d}+\mathbf{s}+\overline{\mathbf{s}}. \tag{16}$$

Here, $\mathbf{s}$ and $\overline{\mathbf{s}}$ denote one-form exterior derivative operators acting on ghost and antighost directions expressed in superconnection language. They do the role of $\mathbf{d}$ in space–time. Now, following the spirit of Refs. 2 and 3, we identify the curvature components in unphysical directions with new fields. One thing which is different from the previous works[2,3] is that here we have the first generation ghost and antighost fields which are one-forms in the extended space (having only dy or $d\overline{y}$). This difference was caused by the existence of the one-form curvature components due to the zero-form scalar field in superconnection formalism:

$$\tilde{\mathscr{F}}=\begin{pmatrix} F-\Phi\Phi^{\dagger}+\psi+\tilde{\psi}+m+\lambda+\overline{m} & i(D\Phi+\xi+\overline{\xi}) \\ i(D\Phi^{\dagger}+\xi^{\dagger}+\overline{\xi^{\dagger}}) & F-\Phi^{\dagger}\Phi+\psi+\overline{\psi}+m+\lambda+\overline{m} \end{pmatrix}. \tag{17}$$

Here ψ, $\overline{\psi}$, m, λ, and $\overline{m}$ are the first and second generation ghost and antighost fields for the two form curvature F, and ξ, $\bar{\xi}$ are the first generation ghost and antighost fields for the one form curvature $D\Phi$:

$$\begin{gathered} \psi=\mathscr{F}^{\ 1}_{\mu N}\,dx^{\mu}\,dy^{N}, \quad \overline{\psi}=\mathscr{F}^{\ -1}_{\mu N}\,dx^{\mu}\,d\overline{y}^{N}, \\ m=\mathscr{F}^{\ 2}_{MN}\,dy^{M}\,dy^{N}, \quad \lambda=\mathscr{F}^{\ 0}_{MN}\,dy^{M}\,d\overline{y}^{N}, \\ \overline{m}=\mathscr{F}^{\ -2}_{MN}\,d\overline{y}^{M}\,d\overline{y}^{N}, \\ \xi=\mathscr{F}^{\ 1}_{N}\,dy^{N}, \quad \overline{\xi}=\mathscr{F}^{\ -1}_{N}\,d\overline{y}^{N}, \end{gathered} \tag{18}$$

where upper indices $1,-1,2$, etc., represent ghost numbers. For instance, ψ has ghost number 1 and $\overline{\psi}$ has ghost number -1.

The curvature in the extended space should also satisfy the Bianchi identity:

$$\tilde{\mathbf{d}}\,\tilde{\mathscr{F}}+[\tilde{\mathscr{J}},\,\tilde{\mathscr{F}}]=0. \tag{19}$$

We thus have two conditions now:

(a) We have to equate Eq. (15) with Eq. (17), and
(b) the Bianchi identity, Eq. (19).

The rules of BRST/anti-BRST symmetry are obtained from these two conditions. The BRST/anti-BRST transformation rules for the components of the extended superconnection $\tilde{\mathscr{J}}$ are given by the condition (a):

even part:

$$\begin{gathered} sA+dc+cA+Ac=\psi, \\ \overline{sA}+d\overline{c}+\overline{cA}+A\overline{c}=\overline{\psi}, \\ sc+cc=m, \\ \overline{s\,c}+\overline{c\,c}=\overline{m}, \\ s\overline{c}+\overline{sc}+c\overline{c}+\overline{cc}=\lambda, \end{gathered} \tag{20}$$

odd part:

$$\begin{gathered} s\Phi+c\Phi-\Phi c=\xi, \\ \overline{s\Phi}+\overline{c\Phi}-\Phi\overline{c}=\overline{\xi}. \end{gathered}$$

The condition (b), the Bianchi identity, gives the BRST/anti-BRST transformation rules for the components of the extended curvature $\tilde{\mathcal{F}}$:

even part:

$$\begin{aligned}
&s\psi+dm+Am+c\psi-mA-\psi c=0,\\
&s\overline{\psi}+d\overline{m}+A\overline{m}+c\overline{\psi}-\overline{m}A-\overline{\psi}c=0,\\
&s\psi+s\overline{\psi}+d\lambda+A\lambda+c\psi+c\overline{\psi}-\lambda A-\psi\overline{c}-\overline{\psi}c=0,\\
&sm+cm-mc=0,\\
&s\overline{m}+c\overline{m}-\overline{m}c=0,\\
&s\lambda+sm+c\lambda+cm-m\overline{c}-\lambda c=0,\\
&s\overline{m}+s\overline{\lambda}+c\overline{m}+c\overline{\lambda}-\lambda\overline{c}-\overline{m}c=0,
\end{aligned}\tag{21}$$

odd part:

$$\begin{aligned}
&s\xi+c\xi+\Phi m-m\Phi+\xi c=0,\\
&s\overline{\xi}+c\overline{\xi}+\Phi\overline{m}-\overline{m}\Phi+\xi\overline{c}=0,\\
&s\xi+s\overline{\xi}+c\xi+c\overline{\xi}+\Phi\lambda-\lambda\Phi+\xi\overline{c}+\overline{\xi}c=0.
\end{aligned}$$

As usual, we have to introduce auxiliary fields to completely fix the BRST/anti-BRST transformation rules. We define auxiliary fields as

$$s\overline{c}=b,\quad s\overline{\psi}=-\kappa,\quad s\lambda=\eta,\quad s\overline{m}=\overline{\eta},\quad s\overline{\xi}=\zeta,\tag{22}$$

then we get the following from Eqs. (20) and (21):

$$\begin{aligned}
&\overline{sc}=-b-[c,\overline{c}]+\lambda,\quad \overline{s\psi}=\kappa-D\lambda-[c,\overline{\psi}]-[\overline{c},\psi],\\
&\overline{sm}=-\eta-[c,\lambda]-[\overline{c},m],\quad \overline{s\lambda}=-\overline{\eta}-[c,\overline{m}]-[\overline{c},\lambda],\\
&\overline{s\xi}=-\zeta-[\Phi,\lambda]-[c,\overline{\xi}]-[\overline{c},\xi].
\end{aligned}\tag{23}$$

The nilpotency of BRST/anti-BRST transformation operators, $s^2=\overline{s^2}=0$, determines all the rest:

$$\begin{aligned}
&sb=0,\quad \overline{sb}=[b,\overline{c}]-\overline{\eta},\\
&s\kappa=0,\quad \overline{s\kappa}=-[b,\overline{\psi}]+D\overline{\eta}-[\overline{c},\kappa]+[\overline{m},sA],\\
&s\eta=0,\quad \overline{s\eta}=[b,\lambda]-[c,\overline{\eta}]-[\overline{c},\eta]-[\overline{m},sc],\\
&s\overline{\eta}=0,\quad \overline{s\eta}=[b,\overline{m}]-[\overline{c},\overline{\eta}],\\
&s\zeta=0,\quad \overline{s\zeta}=[b,\overline{\xi}]-[\Phi\ \overline{\eta}]-[\overline{c},\zeta]-[\overline{m},s\Phi].
\end{aligned}\tag{24}$$

Here sA, sc, and $s\Phi$ were given in Eq. (20). The square brackets in Eqs. (23) and (24) denote a graded commutator. For instance, $[c,\overline{c}]=c\overline{c}+\overline{c}c$ and $[b,\overline{c}]=b\overline{c}-\overline{c}b$, since c and $\overline{c}$ are anticommuting fields and b is a commuting field. In this way, we obtain all the transformation rules of the BRST/anti-BRST symmetry of the topological Yang–Mills–Higgs theory in Refs. 3, 6, and 7.

IV. COMPARISON WITH THE ''HORIZONTALITY CONDITION'' APPROACH

The BRST symmetry of the ordinary Yang–Mills theory can be obtained from the so-called horizontality condition.[18] On the other hand, the BRST symmetry of the topological Yang–Mills theory cannot be obtained through a direct application of the horizontality condition. However, it can be obtained through a modified definition of extended curvature, and the Bianchi identity in the extended space.[3] In Ref. 8, we modified the horizontality condition in a way that it yielded the complete BRST symmetry of the topological Yang–Mills–Higgs theory, without relying upon the Bianchi identity. The rationale of this modified horizontality condition approach was the following. In the ordinary Yang–Mills case, the curvature in the extended space has vanishing components along the vertical directions which represent the gauge fiber orbits of classical gauge symmetry. This fact can be expressed as the horizontality condition

$$\tilde{F}=\tilde{d}\tilde{A}+\tilde{A}\tilde{A}=dA+AA=F, \tag{25}$$

where $\tilde{d}=d+s+\overline{s}$ and $\tilde{A}=A+c+\overline{c}$. In the topological case, the symmetry is bigger than the gauge symmetry, and the extra symmetry which cannot be included as gauge symmetry also has to be gauge fixed. This means that we need extra ghosts besides the ordinary ones $(c,\overline{c})$ which are originated from the gauge symmetry. Hence one may modify the horizontality condition by adding ''permissible'' ghosts to the extended curvature so that these additional ghosts account for the extra symmetry of topological nature. For this purpose, we take the modified horizontality condition as

$$\tilde{F}_T=F, \quad \text{where } \tilde{F}_T=\tilde{F}+\tilde{F}', \tag{26}$$

where $\tilde{F}'$ consists of ghosts and antighosts only and satisfies the nilpotency of BRST symmetry, $s^2\tilde{F}'(=\overline{s}^2\tilde{F}')=0$. Furthermore, this $\tilde{F}'$ has to be chosen in a way that it respects $s^2\tilde{A}'(=\overline{s}^2\tilde{A})=0$. In this way, we can obtain the correct BRST/anti-BRST symmetry of the topological Yang–Mills theory in Ref. 3. What we have explained so far is for the topological Yang–Mills case, not including the Higgs field. In order to encompass the topological Yang–Mills–Higgs case,[6,7] what we did in our previous work[8] was to carry out the same procedure in the superconnection framework:

$$\tilde{\mathscr{F}}_T=\mathscr{F}, \quad \text{where } \tilde{\mathscr{F}}_T=\tilde{\mathscr{F}}+\tilde{\mathscr{F}}'. \tag{27}$$

Here, $\mathscr{F}$, $\tilde{\mathscr{F}}$ were given by Eqs. (7) and (15), respectively, and $\tilde{\mathscr{F}}'$ was given by

$$\tilde{\mathscr{F}}'=-\begin{pmatrix} \psi+\overline{\psi}+m+\lambda+\overline{m} & i(\xi+\overline{\xi}) \\ i(\xi^\dagger+\overline{\xi^\dagger}) & \psi+\overline{\psi}+m+\lambda+\overline{m} \end{pmatrix}.$$

Comparing the above approach that we used in our previous work with the Bianchi identity approach that we have carried out in this paper, we note two things. First, the newly defined components of the extended curvature in the Bianchi identity approach correspond to the additional curvature $\tilde{F}'$ (or $\tilde{\mathscr{F}}'$) in the modified horizontality condition approach. Second, the Bianchi identity condition for the newly defined curvature in Eq. (17) is replaced with the BRST/anti-BRST nilpotency condition for the additional curvature, $\tilde{F}'$ (or $\tilde{\mathscr{F}}'$), in the modified horizontality condition approach. Now, the first observation tells us that the newly defined curvature components $(\psi,\psi,m,\lambda,\overline{m},\xi,\xi)$ in Eq. (17) in the Bianchi identity approach are necessitated by the existence of extra symmetry of topological nature, since the ordinary gauge symmetry has been accounted for by the ghost sector of the extended connection $\tilde{A}$ (or $\tilde{\mathscr{A}}$). The second observation tells us that the Bianchi identity in the extended space is simply another expression of the BRST/anti-BRST nilpotency condition for the extra ghost/antighost fields appearing in the newly added

piece of curvature, $\tilde{F}'$ (or $\tilde{\mathscr{F}}'$), in the modified horizontality condition approach. In fact, the last point was already implied in the Bianchi identity approach, since the validity of the Bianchi identity, which is given by

$$\tilde{d}\tilde{F}+[\tilde{A},\ \tilde{F}]=0, \quad \text{where } \tilde{F}=\tilde{d}\tilde{A}+\tilde{A}\tilde{A}, \tag{28}$$

depends on the nilpotency property of the extended exterior derivative $\tilde{d}=d+s+\overline{s}$. Also, the nilpotency of $\tilde{d}$ implies the nilpotency of the BRST symmetry, $s^2=\overline{s}^2=0$. Therefore, in the Bianchi identity approach one does not require the nilpotency condition for the newly introduced ghost degrees of freedom, since this condition is taken care of by the Bianchi identity itself.

Now, the above observations can be summed up as follows. Loosening the horizontality condition is necessary in the topological Yang–Mills-type theories so that new ghost degrees of freedom, which take care of the extra symmetry of topological nature, can be introduced. This point can be implemented either by modifying the definition of the extended curvature in the Bianchi identity approach or by adding a new piece of extended curvature, which is solely consisted of (anti) ghost fields, in the modified horizontality condition approach. The correct behavior of these new ghost fields is then insured by the BRST nilpotency condition in the modified horizontality condition approach, and by the nilpotency property of the extended exterior derivative in the Bianchi identity approach. Hence, in the geometrical setting, the BRST symmetry of topological nature can be expressed by the extended curvature containing all ''permissible'' ghosts whose property is dictated by the Bianchi identity in the extended space. In other words, from the BRST symmetry view point only the extended curvature containing all ''permissible'' ghosts is a geometrically meaningful object in the topological Yang–Mills–Higgs theory.

V. CONCLUSIONS

In this paper, we found the rules for the BRST/anti-BRST symmetry encompassing topological Yang–Mills–Higgs theory in two, three, and four dimensions. This was done in the superconnection framework so that the scalar field is regarded as a part of a connection, as is the vector gauge field. Using the superconnection language, we obtain the classical topological actions in two, three, and four dimensions from a classical action of topological Yang–Mills type through appropriate projections depending on the dimensions of space–times to which corresponding theories belong. In this framework, the BRST/anti-BRST rules for the scalar and vector gauge fields are obtained together rather than separately. This also tells us that the usefulness of the superconnection language when dealing with the scalar and vector gauge fields is greater than in the ordinary treatment, because in the ordinary treatment the BRST/anti-BRST rules for these two fields are obtained separately. In the superconnection language these rules are obtained in one calculation. As a result, we extend the work of Perry and Teo[3] in the topological Yang–Mills case to the topological Yang–Mills–Higgs case in two[7] and three[6] dimensions using the Bianchi identity. Comparing the present work with our previous work of the modified horizontality condition approach, we conclude the following in the topological Yang–Mills–Higgs theory. First, new ghost fields appear due to the existence of topological symmetry, and these fields can be identified as the components of the modified extended curvature in Perry and Teo's work.[3] Second, the symmetry property that these new ghosts should obey is constrained by the Bianchi identity in the extended space, and this requirement is nothing but the nilpotency condition of the BRST symmetry in another guise. Thus in theories with topological symmetry, it can be said that if things are expressed in the extended space, a space which contains the ghost directions, then one can treat the BRST symmetry in a geometrical setting. In this geometrical setting the curvature should contain all the ''permissible'' ghosts, and the BRST symmetry due to the topological symmetry is constrained by the Bianchi identity in this extended space.

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Reformulation of QCD in the language of general relativity

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It is shown that there exists such a collection of variables that the standard QCD Lagrangian can be represented as the sum of usual Palatini Lagrangian for Einstein general relativity and the Lagrangian of matter and some other fields where the tetrad fields and the metric are constructed from initial SU(3) Yang–Mills fields.
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I. INTRODUCTION

Unified description of all interactions is one of the main goals of modern physics. Partial unification, namely unification of electromagnetic and weak interactions, is achieved in Salam–Weinberg theory and its numerous modifications. More or less satisfactory unification of electromagnetic, weak and strong interactions is achieved in grand unified theories based on various ''large'' gauge groups (SU(5),SO(10), etc.) But the satisfactory unified description of electromagnetic, weak, strong, and gravity interactions is still an open problem.

The origin of the difficulties is clear. Whereas all realistic theories of strong, weak, and electromagnetic interactions are based on Yang–Mills (YM) action

$$S_{\mathrm{YM}}=\int \mathrm{tr}(dA+A\wedge A)\wedge *(dA+A\wedge A), \tag{1}$$

the general relativity is based on Einstein–Hilbert action

$$S_{\mathrm{EH}}=\int dx\sqrt{g}R \tag{2}$$

or, in Palatini formalism, on the action

$$S_P=\int e^a\wedge e^b\wedge(d\Gamma+\Gamma\wedge\Gamma)^{cd}\varepsilon_{abcd}. \tag{3}$$

[We omit inessential overall factors before actions (1)–(3).]

Obviously, the mathematical structure of action (1) and actions (2) or (3) is very different. So the origination of the theory, that reduces to Eqs. (1) and (2) (or Eq. (3)) in certain limiting cases is a very hard problem.

The most direct way to construct unified theory of all interactions is, of course, to replace action (1) by some gravity-like action, or, vice versa, to replace action (2) or (3) by another one, that is more similar to Eq. (1).

The first possibility is realized, for instance, in tensor dominance (or strong gravity) model[1] (see also Ref. 2 for review and further references). The Lagrangian of this model is very similar to a gravitational one, but until now relation of this model and realistic physical models based on YM action is unclear.

The second possibility is realized, for example, in Poincare gauge theories of gravitation (see Refs. 2 and 3 for review), or in SL(6,C) gauge theory of Salam, Isham, and Strathdee[4] and their

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modifications.[2,5,6] But physical meaning of all above mentioned theories is not quite clear because the corresponding actions are unlike the action of the standard model and it is not obvious that the latter can be considered as some limiting case of the former.

There exist also many other approaches to unification of gravity and YM gauge theories based on different modifications of actions (1)–(3). But, to author's knowledge, all theories proposed are rather far from real physics.

But there exist the third way to unification of general relativity and YM theories. Namely, one can try to find such variables that standard Einstein–Hilbert or Palatini actions written in these variables are transformed in standard YM action (plus, maybe, the action with some supplementary fields), or, vice versa, one can try to transform by change of variables the usual YM action in Einstein–Hilbert or Palatini ones.

During the last 20 years, and especially during last 5 years, the great progress was achieved in both directions.

First of all, the author would like to mention the Ne'eman–Sijacki ''chromogravity'' approach to QCD developed in Ref. 7. Ne'eman and Sijacki showed that there exists the mechanism of appearance of gravity-like forces in infrared limit of QCD. Some speculations in spirit of Ne'eman–Sijacki approach were also given in recent paper of Kuchiev.[8]

But in present paper we will follow another approach, namely the approach proposed in a previous paper.[9]

Let us consider, first, YM theory and general relativity in three dimensional space-time.[10] In this case YM action in the first order formalism can be written in the form

$$S_{\mathrm{YM}}=\int \mathrm{tr}*F\wedge(dA+A\wedge A)+\lambda^2\int \mathrm{tr}*F\wedge F, \tag{4}$$

whereas first order action for gravity is

$$S_{\mathrm{3D}}=\int e^a\wedge(d\Gamma+\Gamma\wedge\Gamma)^{bc}\varepsilon_{abc}. \tag{5}$$

In formula (4) λ means coupling constant and $*$ is the Hodge operator with respect to the space–time metric g_{mn}. (We reserve more usual notations e or g for determinants of the tetrad and the metric, respectively.) Below we will consider the case of Euclidean space–time.

For SU(2) gauge group, forms F and A valued in the space of anti-symmetric 3×3 matrices and so we can write

$$*F^{ab}=-\varepsilon^{abc}*F^c, \tag{6}$$

$$S^{\mathrm{YM}}=\int *F^a\wedge(dA+A\wedge A)^{bc}\varepsilon_{abc}-\lambda^2\int *F^a\wedge F^a. \tag{7}$$

In three dimensions $*F^a$ are 1-forms and so the first term in Eq. (7) coincides with three dimensional Palatini actions (5) up to notations! This fact allows to formulate 3D YM theory in general relativity-like form with the tensor

$$G_{mn}=(*F^a)_m(*F^a)_n \tag{8}$$

as the new space–time metric. In particular, usual YM equations appear to be equivalent to Einstein ones with simple rhs.

The above mentioned results concerning relations between 3D gravity and 3D YM theory were obtained, first, in the author's paper.[9] Independently, analogous results were obtained also in

Ref. 11 in the context of (3+1) dimensional SU(2) YM theory in the gauge $A_0^a=0$. However, in the latter approach YM induced gravity lives only on the three dimensional hyperplanes $x^0=\text{const}$ and so this approach is essentially non-covariant.

Further three dimensional space-time geometry discovered in works 9 and 11 was investigated in Refs. 12–18. In particular, in Ref. 12 solutions of Euclidean 3D YM equations with singularity on the sphere were discovered. These solutions can be also interpreted as stationary solutions of 4D YM equations in the gauge $A_0=0$ and can be considered as analog of Schwarzchild solution in general relativity. Analogous Schwarzchild-like and Kerr-like solutions of Yang–Mills–Higgs equations were recently discovered by Singleton.[19]

It was shown that a quantum particle moving in such a YM field (that is considered as external one) inside this sphere cannot leave it. So, maybe, such solutions can be used for elaborating the black hole or microuniverse (see Ref. 20) mechanism of confinement.

We see that in a three dimensional world, gravity does live inside YM theory. It is easy to understand the origin of such YM induced gravity. Indeed, the usual gravity is described by the triad of covectors e^a defined in each point of the space-time up to SO(3) rotation, and SO(3) connection Γ that defines the parallel transport of tensors in the space-time. All these objects appear naturally in YM theory–1-forms $*F^a$ play the role of the triad and SU(2) YM connection A plays the role of the space-time connection Γ.

But how to generalize this construction for a realistic four dimensional case?[21] Direct generalization is not possible, because, first, $*F$ in four dimensions are 2-forms (rather then 1-forms as in 3D case), and, the second, the structure of 4D Palatini action (3) differs from one of 3D action (5). Nevertheless, such generalization exists. Moreover, this problem was partially solved, in fact, almost 20 years ago in Plebanski's work.[22] But Plebanski obtained his results in absolutely different context (he investigated complex structures in general relativity). Maybe, due to this reason his results have not been used in investigations of YM induced gravity until now.[23]

Let us rewrite the Palatini action (3) in spinor notations

$$S_P=\int e^A_{C'}\wedge e^{BC'}\wedge(d\Gamma_{AB}+\Gamma_{AC}\wedge\Gamma^C_B). \tag{9}$$

(We use the usual isomorphism between the spaces of $O(4)$ vectors and $\mathrm{SU}(2)\times\mathrm{SU}(2)$ spinors.) Sign conventions, normalization factors, etc., are describe in section II below. Further, we omit the part of Palatini action that contains the fields $\Gamma_{A'B'}$. (See, for instance, Refs. 24 and 25, in which it was shown that the using of chiral action (9) is very natural, in particular, in Ashtekar formalism.)

One can note that 1-forms $e^{AA'}$ enter in action only in the combination

$$\Sigma^{AB}=e^A_{C'}\wedge e^{BC'}. \tag{10}$$

So the Palatini action (9) can be represented in the form

$$S_P=\int \Sigma^{AB}\wedge(d\Gamma_{AB}+\Gamma_{AC}\wedge\Gamma^C_B). \tag{11}$$

Of course, the quantities Σ^{AB} in Eq. (11) cannot be considered as the independent dynamical variables. Indeed, due to Eq. (10) the 2-forms Σ^{AB} satisfy the condition

$$\Sigma^{(AB}\wedge\Sigma^{CD)}=0. \tag{12}$$

Further, Plebanski showed that if the conditions (12) are satisfied and

$$\Sigma^{AB}\wedge\Sigma_{AB}\neq 0, \tag{13}$$

then Σ^{AB} can be represented in form (10) with non-degenerate tetrad $e^{AA'}$. So the Palatini action (9) is equivalent to Plebanski action

$$S_{Pl}=\int \Sigma^{AB}\wedge(d\Gamma_{AB}+\Gamma_{AC}\wedge\Gamma^{C}_{B})+\int \phi_{ABCD}\Sigma^{AB}\wedge\Sigma^{CD}. \tag{14}$$

The second term in Eq. (14) with totally symmetric Lagrange multipliers ϕ_{ABCD} is introduced to take into account condition (12).

In action (14) fields Σ^{AB}, Γ_{AB} and ϕ_{ABCD} are independent dynamical variables. The first term in Eq. (14) coincides with the first term in the first order SU(2) YM action

$$S_{\mathrm{YM}}=\int F^{BC}\wedge(dA_{BC}+A_{BD}\wedge A^{D}_{C})+\lambda^{2}\int F^{BC}\wedge *F_{BC} \tag{15}$$

up to notations. But it does not mean that the gravity lives inside SU(2) YM theory as in 3D case, because the analog of the second term in Eq. (14) is absent in Eq. (15) and so we have no analog of Eq. (12) in SU(2) YM theory. But without condition (12) we cannot reconstruct the tetrad $e^{AA'}$.

Let us consider, however, the theory with more large gauge group $G\supset \mathrm{SU}(2)$. One can choose among $N=\dim G$ 2-forms F three forms $F^{AB}=F^{(AB)}$ that are transformed as rank two symmetric spinor under gauge transformations from certain SU(2) subgroup of the group G. Then action (15) will be a piece of the total YM action. Further, if $\dim G\geqslant 8$, then, in general, we can impose, using other gauge degrees of freedom, five SU(2) invariant gauge conditions

$$F^{(AB}\wedge F^{CD)}=0. \tag{16}$$

Conditions (16), that we will call ''the Plebanski gauge,'' coincide with Plebanski conditions (12) up to notations whereas the first term in YM action (15) coincides, up to notations, with the first term in Plebanski action (14). *So we can conclude that gravity lives inside YM theory if the dimension of the gauge group is more or equal to eight.* Indeed, due to Plebanski theorem we can reconstruct the tetrad $e^{AA'}$ and the corresponding metric

$$F^{AB}=e^{A}_{A'}\wedge e^{BA'}, \tag{17}$$

$$G_{mn}=e^{AA'}_{m}e_{AA'n}. \tag{18}$$

After substituting Eq. (17) in the first term of action (15) we obtain the usual Palatini action for gravity (9).

The main idea of the present work is to use of the gauge (16) to reformulate the YM theory in general relativity-like form. Below we will show that the gauge (16) really exists for the gauge group SU(3) and the corresponding gauge theory, the Quantum Chromodynamics, can be formulated in the close analogy with general relativity. But before author would like to give some additional notes concerning 2-forms formalism in general relativity.

Plebanski results allow to use three 2-forms Σ^{AB} instead of metric. In Plebanski's approach these forms satisfy the constraints (12) that play the crucial role in Plebanski's formalism. But later it was shown that this conditions are not necessary. Namely, it appears that, in generic case, any three 2-forms define unique, up to conformal factor, the metric, with respect to which they are (anti)-self-dual. These statement is known now as Urbantke theorem (see Ref. 26. Another proof and some refinements were given in Ref. 27). In particular, in generic case any collection of three 2-forms defined up to SL(3) transformation naturally determine the unique metric. Moreover, later t'Hooft showed[28] that any triple of two forms (with some non-degeneracy condition) natu-

rally defines not only the metric but also certain SL(3) connection and so it is possible to reformulate the general relativity in terms of triples of 2-forms. Similar formalism with GL(3) connection instead of SL(3) ones was proposed also in recent paper.[29]

However, the Lagrangian of t'Hooft and its modifications are reduced to Plebanski's Lagrangian (14) by imposing of gauge conditions that are exactly coincide with Eq. (12). On the other hand, t' Hooft Lagrangian, without the imposing of conditions (12), is quadrilinear and so is not similar to YM one. By these reasons in the present paper we use the old Plebanski formalism rather then its further generalizations.

Clear relations between gravity and YM theory also appear in Ashtekar formalism.[30] An attempt to develop the formalism for unified description of YM and gravity fields in the spirit of Ashtekar phase space approach was done in other works.[31] However, this theory gives the conventional YM theory only in the lowest order in the fields and so it is hard to make consistent its predictions with ones of the Standard Model. Originally discovered,[30] it was very unlike the Plebanski approach. But later it was shown[32] that Ashtekar formalism can be reproduced by (3+1) decomposition of Plebanski Lagrangian.

The paper is organized as follows. In section II we describe our notations. In sections III and IV we formulate QCD in general relativity-like form at classical amd quantum levels respectively. In section V we discuss obtained results.

II. NOTATIONS

Indexes a,b,c,d are frame ones and run over the set $\{0,1,2,3\}$. Indexes m,n,p,q are world ones and run over the same set. Upper case Latin indexes $A,B,C,\ldots$ are SU(2) spinor ones and run over the set $\{0,1\}$. Greek indexes α,β,γ runs over the set $\{1,2,3\}$.

A. SU(2) spinors and O(3) vectors

Lowering and raising of SU(2) spinor indexes are performed by anti-symmetric spinors ε_{AB}, ε^{AB}, $\varepsilon_{01}=\varepsilon^{01}=+1$,

$$\varphi_A=\varphi^B\varepsilon_{BA}, \quad \varphi^B=\varepsilon^{BA}\varphi_A. \tag{19}$$

Hermitian conjugation of SU(2) spinors are defined as

$$(\varphi^\dagger)^{AB\ldots}=\overline{\varphi_{CD\ldots}}\,\varepsilon^{CA}\varepsilon^{DB}\ldots, \tag{20}$$

where quantities $\overline{\varphi_{CD\ldots}}$ are complex conjugated to φ^{CD}. The spaces of symmetric second rank SU(2) spinors and O(3) vectors are isomorphic. The isomorphism is established by the formula

$$S^\alpha\leftrightarrow S^{AB}=-\frac{i}{\sqrt{2}}\,S^\alpha\sigma_\alpha^{AB}, \tag{21}$$

where $\sigma_{\alpha B}^A$ are Pauli matrices. Real vectors correspond to Hermitian spinors,

$$\varepsilon^{\alpha\beta\gamma}U^\alpha V^\beta W^\gamma=\sqrt{2}U^{AB}V_{BC}W_A^C \quad S^\alpha S^\alpha=S^{AB}S_{AB}. \tag{22}$$

Below we will use the convention (21) with one exception: if Γ^α are components of some O(3) connection and

$$R^\alpha=d\Gamma^\alpha+\frac{1}{2}\,\varepsilon^{\alpha\beta\gamma}\Gamma^\beta\wedge\Gamma^\gamma \tag{23}$$

are components of the corresponding curvature form, then

$$\Gamma^{AB}=\frac{1}{2i}\ \sigma_{\alpha}^{AB}\Gamma^{\alpha},\quad R^{AB}=\frac{1}{2i}\ \sigma_{\alpha}^{AB}R^{\alpha}. \tag{24}$$

Using Eq. (24), one can prove that

$$R^{AB}=d\Gamma^{AB}+\Gamma_{C}^{A}\wedge\Gamma^{CB}. \tag{25}$$

B. SU(2)×SU(2) spinors and O(4) vectors

O(4) frame vector indexes are lowered and raised by the tensor δ^{ab}. The spaces of rank (1,1) SU(2)×SU(2) spinors and O(4) vectors are isomorphic. The isomorphism is established by the formula

$$S_{AA'}\leftrightarrow S_a=g_a^{AA'}S_{AA'}, \tag{26}$$

where $g_a^{AA'}$ are Euclidean Infeld–van der Vaerden symbols for flat space

$$(g_a^{AA'})=\left(\frac{1}{\sqrt{2}}\ \delta_{A'}^{A},\ \frac{i}{\sqrt{2}}\ \sigma_{\alpha A'}^{A}\right). \tag{27}$$

Real vectors correspond to Hermitian spinors (Hermitian conjugation of the latter is defined in the previous subsection),

$$S_aS_a=S_{AA'}S^{AA'}. \tag{28}$$

C. O(4) (anti)-self-dual tensors and O(3) vectors

For frame O(4) tensors Hodge operator is defined as usual

$$*M_{ab}=\frac{1}{2}\ \varepsilon_{abcd}M_{cd}. \tag{29}$$

The spaces of the (anti)-self-dual tensors and O(3) vectors are isomorphic. The isomorphism is estublished by the formula

$$^{\pm}M^{\alpha}=\ ^{\pm}\eta_{ab}^{\alpha}\ ^{\pm}M_{ab}, \tag{30}$$

where $^{\pm}\eta_{ab}^{\alpha}$ are t'Hooft symbols

$$^{+}\eta_{ab}^{\alpha}=-\frac{1}{2i}\ \overline{\sigma}_{\alpha B'}^{A'}g_{aAA'}g_{b}^{AB'}, \tag{31}$$

$$^{-}\eta_{ab}^{\alpha}=\frac{1}{2i}\ \sigma_{\alpha B}^{A}g_{aAA'}g_{b}^{BA'}. \tag{32}$$

t'Hooft symbols satisfy the following equations:

$$^{\pm}\eta_{ac}^{\alpha}\ ^{\pm}\eta_{cb}^{\beta}=-\frac{1}{4}\ \delta^{\alpha\beta}\delta_{ab}+\frac{1}{2}\ \varepsilon^{\alpha\beta\gamma}\ ^{\pm}\eta_{ab}^{\gamma} \tag{33}$$

$$^{\pm}\eta^{\gamma}_{ab}\ {}^{\pm}\eta^{\gamma}_{cd}=\frac{1}{4}\ (\delta_{ac}\delta_{bd}-\delta_{ad}\delta_{bc}\pm\varepsilon_{abcd}). \tag{34}$$

Formulas (22), (28), (33), and (34) allow easy translation of any formula from spinor to vector language and vice versa.

III. PLEBANSKI GAUGE IN SU(3) YANG-MILLS THEORY

A. Plebanski theorem for real 2-forms

Plebanski showed that three complex 2-forms Σ^{AB}, satisfying conditions (12) and (13), can be represented in form (10). The ''real'' variant of this theorem can be formulated in the following way:

Let S^{α} be three real 2-forms obeying the conditions

$$S^{\alpha}\wedge S^{\beta}=\frac{1}{3}\ \delta^{\alpha\beta}S^{\gamma}\wedge S^{\gamma}, \tag{35}$$

$$S^{\gamma}\wedge S^{\gamma}\neq 0. \tag{36}$$

Let G_{mn} be the Urbantke metric (our definition of the metric (37) differs from the original definition of Urbantke[26] by inessential factor)

$$G_{mn}=-\frac{4}{3}\ [S^{\delta}_{tu}S^{\delta}_{vw}\varepsilon^{tuvw}]^{-1}\varepsilon_{\alpha\beta\gamma}\varepsilon^{pqrs}S^{\alpha}_{mp}S^{\beta}_{qr}S^{\gamma}_{sn}. \tag{37}$$

Then G_{mn} has definite signature, $(++++)$ or $(----)$, and S^{α} can be represented, respectively, as

$$S^{\alpha}=\pm\ ^{-}\eta^{\alpha}_{ab}e^{a}\wedge e^{b}. \tag{38}$$

One notes, that the equations (35) and (36) are nothing but reformulation of Eqs. (12) and (13) in vector language. The spinor analog of Eq. (38) is

$$S^{AB}=\pm\frac{1}{2}\ e^{AC'}\wedge e^{B}_{C'}, \tag{39}$$

where

$$(S^{\dagger})^{AB}=S^{AB},\quad (e^{\dagger})^{AA'}=e^{AA'}. \tag{40}$$

Equation (39) is the analog of Eq. (10).

Let us prove the theorem formulated above. Let

$$M^{\alpha\beta}=\varepsilon^{mnpq}S^{\alpha}_{mn}S^{\beta}_{pq}. \tag{41}$$

Then the matrix $M^{\alpha\beta}$ has a definite signature [see Eq. (35)]. So, due to results of Urbantke[26] and Harnett,[27] the Urbantke metric (37) is non-degenerate, has a definite signature, and 2-forms S^{α} are self-dual or anti-self-dual with respect to Hodge operator corresponding to this metric. Hence, the Urbantke metric can be written as

$$G_{mn}=\pm e^{a}_{m}e^{a}_{n}, \tag{42}$$

whereas 2-forms S^{α} as

$$S^\alpha = C^\alpha_\beta \, {}^- \eta^\beta_{ab} e^a \wedge e^b \tag{43}$$

or

$$S^\alpha = C^\alpha_\beta \, {}^+ \eta^\beta_{ab} e^a \wedge e^b, \tag{44}$$

because the set of three 2-forms ${}^\pm \eta^\alpha_{ab} e^a \wedge e^b$ is a basis in the space of the (anti)-self-dual forms.

One notes, that Eq. (44) can be transformed in Eq. (43). Indeed, 1-forms e^a are defined by Eq. (42) up to transformation

$$e^a \to O^a_b e^b, \quad O \in O(4). \tag{45}$$

Let $O = \mathrm{diag}\{1,-1,-1,-1\}$. Then

$${}^+ \eta^\alpha_{ab} O^a_c O^b_d = - \, {}^- \eta^\alpha_{cd}. \tag{46}$$

So, redefining e^a and C^α_β according to Eqs. (45) and (46), one can transform Eq. (44) in Eq. (43).

One substitutes Eq. (43) in Eq. (35). Using the formulas of the section II C, one obtains

$$C^\alpha_\gamma C^\beta_\gamma = \frac{1}{3} \, \delta^{\alpha\beta} C^\delta_\gamma C^\delta_\gamma. \tag{47}$$

So

$$C^\alpha_\beta = \pm C O^\alpha_\beta, \tag{48}$$

where

$$O \in \mathrm{SO}(3), \quad C = \sqrt{\frac{1}{3} \, C^\delta_\gamma C^\delta_\gamma} > 0. \tag{49}$$

For given $O \in \mathrm{SO}(3)$ there exists the matrix $\widetilde{O} \in \mathrm{SO}(4)$ such that

$${}^- \eta^\alpha_{ab} \widetilde{O}^a_c \widetilde{O}^b_d = (O^{-1})^\alpha_\beta \, {}^- \eta^\beta_{cd}. \tag{50}$$

So, redefining e^a according to Eq. (45) with $O = \widetilde{O}$, and taking into account Eq. (45), one reduces Eq. (43) to

$$S^\alpha = \pm C \, {}^- \eta^\alpha_{ab} e^a \wedge e^b. \tag{51}$$

Finally, substituting Eq. (51) in Eq. (37), one obtains that $C = 1$. The theorem is proved.

B. SU(3) YM action in Plebanski gauge

We start from the usual SU(3) YM action in the first order formalism,

$$S_{\mathrm{YM}} = \int \mathrm{tr}[F \wedge (dA + A \wedge A) + \lambda^2 F \wedge * F], \tag{52}$$

where F and A are considered as independent variables.

The forms F and A valued in the space of 3×3 anti-Hermitian traceless matrices. So we can write

$$A = \Gamma + i\Phi, \quad F = S + iQ, \tag{53}$$

where Γ, Φ, S, and Q valued in the space of real 3×3 matrices, and

$$\Gamma^T=-\Gamma, \quad S^T=-S,$$
$$\Phi^T=\Phi, \quad Q^T=Q, \tag{54}$$
$$\mathrm{tr}\ \Phi=0, \quad \mathrm{tr}\ Q=0,$$

where the superscript T means transposition.

Substituting Eq. (53) in Eq. (52), one obtains

$$S_{\mathrm{YM}}=\int \mathrm{tr}[S\wedge(R-\Phi\wedge\Phi)+Q\wedge D\Phi+\lambda^2 S\wedge *S-\lambda^2 Q\wedge *Q], \tag{55}$$

where

$$R=d\Gamma+\Gamma\wedge\Gamma, \tag{56}$$

$$D\Phi=d\Phi+\Gamma\wedge\Phi+\Phi\wedge\Gamma. \tag{57}$$

Decomposition (53) corresponds to certain embedding of the algebra $\mathrm{su}(2)\approx\mathrm{o}(3)$ in $\mathrm{su}(3)$. So Γ and R can be considered as the forms of connection and curvature corresponding to the subgroup $\mathrm{SU}(2)$ of the gauge group $\mathrm{SU}(3)$ whereas D is covariant derivative defined by the connection Γ.

Due to Eq. (54), one can write

$$S^{\alpha\beta}=-\varepsilon^{\alpha\beta\gamma}S^{\gamma}$$

and to impose the gauge conditions (35) on the 2-forms S^{α}.

Substituting Eq. (39) in Eq. (55), one obtains the action

$$S=2\int e^{A}_{C'}\wedge e^{BC'}\wedge R_{AB}+2\int e^{AC'}\wedge e^{B}_{C'}\wedge\Phi^{CDE}_{A}\wedge\Phi_{BCDE}+\int Q^{ABCD}\wedge D\Phi_{ABCD}$$
$$-\lambda^2\int e^{AC'}\wedge e^{B}_{C'}\wedge *(e^{D'}_{A}\wedge e_{BD'})-\lambda^2\int Q^{ABCD}\wedge *Q_{ABCD}, \tag{58}$$

where R_{AB} is defined by formula (25), Φ^{ABCD} and Q^{ABCD} are the forms Φ, Q written in the spinor language Here we have wrote the YM action in new variables for the upper sign case in Eq. (39). Below we will show that this is enough to formulate quantum version of the theory under consideration.

The first term in Eq. (58) is the Palatini action. So action (58) can be considered as one for gravity coupled with several matter fields. In particular, first three terms in action (58) are invariant under the action of the group of the general coordinate transformations $\mathrm{Diff}(R^4)$—just as in general relativity. But the total action, of course, is not $\mathrm{Diff}(R^4)$ invariant because the last two terms in Eq. (58) depend on fixed space–time metric via Hodge operator.

Action (58) can be rewritten in several equivalent forms. First, one can represent the connection in the form

$$\Gamma=\hat{\Gamma}+K,$$

where $\hat{\Gamma}$ is unique torsionless metric connection and K is contorsion 1-form. Let $\hat{D}$ and $\hat{R}$ are covariant differential and curvature 2-form corresponding to connection $\hat{\Gamma}$. Then

$$\int e^A_{C'} \wedge e^{BC'} \wedge R_{AB} = \int e^A_{C'} \wedge e^{BC'} \wedge (\hat{R}_{AB} + \hat{D}K_{AB} + K_{AC} \wedge K^C_B). \tag{59}$$

But due to torsionless condition

$$\hat{D}e^{AA'} = 0$$

the second term in the rhs of Eq. (59) is total divergence and so can be omitted. Hence, the action (58) can be rewritten as

$$S = 2\int e^A_{C'} \wedge e^{BC'} \wedge (\hat{R}_{AB} + K_{AC} \wedge K^C_B) + 2\int e^{AC'} \wedge e^B_{C'} \wedge \Phi^{CDE}_A \wedge \Phi_{BCDE} + \int Q^{ABCD}$$
$$\wedge (\hat{D}\Phi_{ABCD} + 4K^E_{(A}\Phi_{|E|BCD)}) - \lambda^2 \int e^{AC'} \wedge e^B_{C'} \wedge *(e^{D'}_A \wedge e_{BD'}) - \lambda^2 \int Q^{ABCD} \wedge *Q_{ABCD}. \tag{60}$$

We see that the first term in Eq. (60) is nothing but usual Einstein–Hilbert action. Further, as in usual theories of gravitation with torsion, action (60) depend on torsion quadratically without derivatives. So torsion can be eliminated from action by solving equations of motion. We return to discussion of this point in the last section.

The ''matter'' terms in the action seem rather strange. But they can be rewritten in more familiar form if one eliminates the field Φ from the action by solving the equations

$$\frac{\delta S}{\delta \Phi} = 0. \tag{61}$$

Substituting the solution of Eq. (61) in Eq. (58), one obtains

$$S = 2\int e^A_{C'} \wedge e^{BC'} \wedge R_{AB} + \frac{1}{2}\int DQ^{ABCD} \wedge \star DQ_{ABCD} - \frac{1}{6}\int e^A_{C'} \wedge e^{BC'} \wedge \star DQ^{CDE}_A \wedge \star DQ_{BCDE}$$
$$- \lambda^2 \int Q^{ABCD} \wedge *Q_{ABCD} - \lambda^2 \int e^{AC'} \wedge e^B_{C'} \wedge *(e^{D'}_A \wedge e_{BD'}), \tag{62}$$

where $\star$ denotes Hodge operator with respect to YM metric G_{mn}.

This form of matter action is more recognizable The second and the third terms in Eq. (62) can be interpreted as ''kinetic'' ones whereas the forth term can be considered as ''mass'' term for field Q. The last term in Eq. (62) can be rewritten as

$$S_2 = \int dx \sqrt{g}[g^{mp}g^{nq}G_{mn}G_{pq} - (g^{mn}G_{mn})^2]$$

and so can be considered as ''mass'' term for chromo-gravity field. Terms of such type in the action are already considered in context of strong gravity approach.[20]

We will continue the investigation of SU(3) YM theory in introduced variables in the next section at quantum level. But before we must prove that Plebanski gauge really fixes the gauge up to SU(2) transformations.

C. Investigation of the Plebanski gauge

Any SU(3) matrix U can be written in the form

$$U = e^{i\omega}, \tag{63}$$

where ω is a traceless Hermitian 3×3 matrix. Pure imaginary matrices ω corresponds to generators of the subgroup SU(2), whereas real matrices can be considered as coordinates on the space SU(3)/SU(2). Obviously, the latter satisfy the equations

$$\omega^{\alpha\beta}=\omega^{\beta\alpha}, \quad \omega^{\alpha\alpha}=0. \tag{64}$$

Let us consider the infinitesimal gauge transformations with parameters obeying Eq. (64)

$$\delta A = i d\omega + i[A,\omega], \tag{65}$$

$$\delta F = i[F,\omega]. \tag{66}$$

Comparing Eqs. (65), (66), and (53), one obtains

$$\delta\Gamma = -[\Phi,\omega], \quad \delta\Phi = D\omega, \tag{67}$$

$$\delta S = -[Q,\omega], \quad \delta Q = [S,\omega]. \tag{68}$$

Let

$$T^{ABCD}=*[S^{(AB}\wedge S^{CD)}]. \tag{69}$$

Using Eq. (68), one finds

$$\delta T^{ABCD}=c\varepsilon^{mnpq}e^{(A}_{A'm}e^{B|A'|}_{n}Q^{C}_{EFGpq}\omega^{D)EFG}, \tag{70}$$

where c is irrelevant numerical constant, $e^{AA'}_{m}$ and Q^{ABCD}_{pq} are components of the forms $e^{AA'}$ and Q^{ABCD}, whereas ω^{ABCD} is SU(2) spinor that corresponds to O(3) tensor $\omega^{\alpha\beta}$.

To prove that Plebanski gauge reduces the initial SU(3) YM theory to the SU(2) one, it is sufficient to prove that the equations

$$\delta T^{ABCD}=0 \tag{71}$$

have the only trivial solution $\omega^{ABCD}=0$ for almost all field configurations.

One notes that due to Eq. (64)

$$\omega^{ABCD}=\omega^{(ABCD)}. \tag{72}$$

So Eqs. (71) are the system of five linear homogeneous equations for five unknown ω^{ABCD}.

The system (71) can be rewritten as

$$G^{(ABC}_{EFG}\delta^{D)}_{H}\omega^{EFGH}=0, \tag{73}$$

where

$$G^{ABCEFG}=\varepsilon^{mnpq}e^{A}_{A'm}e^{BA'}_{n}Q^{CEFG}_{pq}. \tag{74}$$

In generic case, the spinor G^{ABCEFG} satisfies the only constraints

$$G^{ABCDEF}=G^{(AB)CDEF}, \quad G^{ABCDEF}=G^{AB(CDEF)}. \tag{75}$$

Now let us consider the field configuration for which the only non-zero components of G^{ABCDEF} are G^{000000}, G^{111111}, and

$$G^{000111}=G^{001011}=G^{001101}=G^{001110}.$$

For such configuration one obtains from Eq. (73)

$$G^{000000}\omega^{0001}+G^{000111}\omega^{1111}=0,$$

$$G^{000000}\omega^{0000}=0, \quad G^{000111}\omega^{0011}=0, \tag{76}$$

$$G^{111111}\omega^{0111}=0, \quad G^{111111}\omega^{1111}=0.$$

Obviously, that the system (76) has the only trivial solution for non-zero G^{000000}, G^{111111}, and G^{000111}.

Let

$$M^{ABCD}_{EFGH}=G^{(ABC}_{(EFG}\delta^{D)}_{H)} \tag{77}$$

the spinor M^{ABCD}_{EFGH} can be considered as some 5×5 matrix M. We have proved that $\det M \neq 0$ for certain field configuration. But $\det M$ is polynomial with respect to fields $e^{AA'}$ and Q^{ABCD}. So $\det M \neq 0$ for almost all field configuration. This means that the system (73) has the only trivial solution for almost all configurations of fields.

IV. QUANTIZATION

We start from usual expression for Euclidean vacuum expectation value of certain Hermitian gauge invariant functional $\mathcal{O}=\mathcal{O}[A,\Psi,\overline{\Psi}]$:

$$\langle\mathcal{O}\rangle=\int dAd\overline{\Psi}d\Psi\mathcal{O}[A,\overline{\Psi},\Psi]\exp\{-S_{\mathrm{YM}}-S_{\mathrm{mat}}\}, \tag{78}$$

where $\overline{\Psi},\Psi$ are matter fields,

$$S_{\mathrm{YM}}[A]=-\frac{1}{4\lambda^2}\int \mathrm{tr}(dA+A\wedge A)\wedge*(dA+A\wedge A), \tag{79}$$

and

$$S_{\mathrm{mat}}=\int dx\sqrt{g}\left\{\sum_{\mathrm{flavors}}(\overline{\Psi}_f\hat{\nabla}\Psi_f-m_f\overline{\Psi}_f\Psi_f)\right\}. \tag{80}$$

Formula (78) can be written as

$$\langle\mathcal{O}\rangle=\int dFdAd\overline{\Psi}d\Psi\mathcal{O}[A,\overline{\Psi},\Psi]\exp\left\{i\int \mathrm{tr}[F\wedge(dA+A\wedge A)]\right\}\exp\left\{-\lambda^2\int \mathrm{tr}F\wedge*F-S_{\mathrm{mat}}\right\} \tag{81}$$

or, finally, as

$$\langle\mathcal{O}\rangle=\int dSdQd\Gamma d\Phi d\overline{\Psi}d\Psi\mathcal{O}[\Gamma+i\Phi,\overline{\Psi},\Psi]$$
$$\times\exp\left\{i\int \mathrm{tr}[S\wedge(R-\Phi\wedge\Phi)+Q\wedge D\Phi]\right\}\exp\left\{\lambda^2\int \mathrm{tr}[S\wedge*S-Q\wedge*Q]\right\}\exp\{-S_{\mathrm{mat}}\}, \tag{82}$$

where variables S, Q, Γ, and Φ are defined by (53).

We will fix the gauge (namely, Plebanski gauge) by usual Faddeev–Popov trick. We insert in Eq. (82) the unit

$$1=\int_{\mathrm{SU}(3)/\mathrm{SU}(2)} d\mu(\omega)\,\delta(*[(S^{\omega})^{(AB}\wedge(S^{\omega})^{CD)}])\Delta_{\mathrm{FP}} \tag{83}$$

where $d\mu(\omega)$ is invariant measure on SU(3)/SU(2), $(S^{\omega})^{AB}$ is a gauge transformation of S^{AB}, and Δ_{FP} is Faddeev–Popov functional. Then, after usual manipulations, one obtains

$$\begin{aligned}\langle\mathscr{O}\rangle=&\int dSdQd\Gamma d\Phi d\overline{\Psi}d\Psi\mathscr{O}[\Gamma+i\Phi,\overline{\Psi},\Psi]\delta(*[S^{(AB}\wedge S^{CD)}])\det M\\&\times\exp\left\{i\int \mathrm{tr}[S\wedge(R-\Phi\wedge\Phi)+Q\wedge D\Phi]\right\}\exp\left\{\lambda^2\int \mathrm{tr}[S\wedge *S-Q\wedge *Q]\right\}\exp\{-S_{\mathrm{mat}}\}.\end{aligned} \tag{84}$$

Here $\det M$ is Faddeev–Popov determinant, where M is 5×5 matrix

$$M^{ABCD}_{EFGH}=*[S^{(AB}\wedge Q^{C}_{(EFG}\delta^{D)}_{H)}]. \tag{85}$$

This matrix coincides, on the surface

$$S^{(AB}\wedge S^{CD)}=0, \tag{86}$$

with the matrix (77). So $\det M\neq0$ for almost all field configurations (see the section III C).

Let $\mathscr{S}_+(\mathscr{S}_-)$ be the set of all 2-forms S^{α} for which Urbantke metric (37) is positive (negative) definite. We can write the integral (84) as the sum of the integrals over $\mathscr{S}_+$ and $\mathscr{S}_-$.

Obviously, that $\mathscr{S}_-$ is mapped onto $\mathscr{S}_+$ by the transformation $S\to-S$, $Q\to-Q$. But the latter is equivalent to the complex conjugation in the integral over $\mathscr{S}_-$. So the integral over $\mathscr{S}_+$ is equal to complex conjugated integral over $\mathscr{S}_-$. Hence,

$$\begin{aligned}\langle\mathscr{O}\rangle=&\mathrm{Re}\int_{\mathscr{S}_+} dSdQd\Gamma d\Phi d\overline{\Psi}d\Psi\mathscr{O}[\Gamma+i\Phi,\overline{\Psi},\Psi]\delta(*[S^{(AB}\wedge S^{CD)}])\det M\\&\times\exp\left\{i\int \mathrm{tr}[S\wedge(R-\Phi\wedge\Phi)+Q\wedge D\Phi]\right\}\exp\left\{\lambda^2\int \mathrm{tr}[S\wedge *S-Q\wedge *Q]\right\}\exp\{-S_{\mathrm{mat}}\}.\end{aligned} \tag{87}$$

We showed in the section III A that the solution of Plebanski gauge conditions (86) for $S\in\mathscr{S}_+$ is given, in vector language, by the formula

$$S^{\alpha}=\bar{}\,\eta^{\alpha}_{ab}e^{a}\wedge e^{b}. \tag{88}$$

So, for $S\in\mathscr{S}_+$,

$$\int\prod_{a,n}de^{a}_{n}\prod_{\substack{\alpha\\m>n}}\delta(S^{\alpha}_{mn}-\bar{}\,\eta^{\alpha}_{ab}e^{a}_{m}e^{b}_{n})=f(S)\prod_{\substack{\alpha\leqslant\beta\\(\alpha,\beta)\neq(3,3)}}\delta\left(*\left[S^{\alpha}\wedge S^{\beta}-\frac{1}{3}\,\delta^{\alpha\beta}S^{\gamma}\wedge S^{\gamma}\right]\right), \tag{89}$$

where the function $f(S)$ to be determined.

It is easy to prove that

$$f=\mathrm{const}. \tag{90}$$

Indeed, $f(S)$ is scalar density with respect to general coordinate transformations and O(3) gauge transformations. So

$$f=f(\varepsilon^{mnpq}S^{\alpha}_{mn}S^{\alpha}_{pq}). \tag{91}$$

But the dimension of f is zero. So the function (91) is a constant.

Inserting Eqs. (89) and (90) in Eq. (87), one obtains

$$\langle\mathscr{O}\rangle=\mathrm{Re}\int dedQd\Gamma d\Phi d\overline{\Psi}d\Psi\mathscr{O}[\Gamma+i\Phi,\overline{\Psi},\Psi]\det M\ \exp\{iS_1-\lambda^2S_2-S_{\mathrm{mat}}\}, \tag{92}$$

where

$$S_1=\int e^A_{C'}\wedge e^{BC'}\wedge R_{AB}+2\int e^{AC'}\wedge e^B_{C'}\wedge\Phi^{CDE}_A\wedge\Phi_{BCDE}+\int Q^{ABCD}\wedge D\Phi_{ABCD},$$

$$S_2=\int dx\sqrt{g}[g^{mp}g^{nq}G_{mn}G_{pq}-(g^{mn}G_{mn})^2]+\int Q^{ABCD}\wedge *Q_{ABCD}, \tag{93}$$

where

$$G_{mn}=e^a_m e^a_n \tag{94}$$

is YM induced metric, det M is Faddeev–Popov determinant,

$$M^{ABCD}_{EFGH}=*[e^{(A|C'|}\wedge e^B_{C'}\wedge Q^C_{(EFG}\delta^{D)}_{H)}] \tag{95}$$

and

$$S_{\mathrm{mat}}=\sum_{\text{flavors}}\int dx\sqrt{g}\{i\overline{\Psi}_{fAB}{}^{(0)}e^n_a\gamma^a D_n\Psi^{AB}_f+i\overline{\Psi}_{fAB}{}^{(0)}e^n_a\gamma^a\Phi^{ABCD}_n\Psi_{fCD}-m_f\overline{\Psi}_{fAB}\Psi^{AB}_f\}.$$

In the latter formula ${}^{(0)}e^n_a$ means the space–time tetrad (that is, $g^{mn}={}^{(0)}e^{m(0)}_a e^n_a$).

The integrand in Eq. (92) is O(4) gauge invariant. To fix this gauge freedom, it is necessary to impose further gauge conditions. The simplest choice is

$$e_{ma}=e_{am}. \tag{96}$$

This gauge entangles space–time and gauge degrees of freedom and so, after imposing of the gauge (96), they must be considered on the equal footing.

It is easy to prove, that Faddeev–Popov determinant, corresponding to gauge (96), is equal to $|e|^{3/2}$. So formula (92) can be written as

$$\langle\mathscr{O}\rangle=\mathrm{Re}\int_{e_{am}=e_{ma}} dedQd\Gamma d\Phi d\overline{\Psi}d\Psi\mathscr{O}[\Gamma+i\Phi,\overline{\Psi},\Psi]|e|^{\frac{3}{2}}\det M\ \exp\{iS_1-\lambda^2S_2-S_{\mathrm{mat}}\}. \tag{97}$$

(It would be remind, that $e^{AA'}_m$ and e_{am} in (97) are connected, according to rules of the section II B, by relation $e^{AA'}_m=g^{aAA'}e_{am}$).

The formula (92) can be also rewritten in manifestly O(4) invariant variables, such as G_{mn},

$$\Phi_{mnpqr}dx^r\equiv\Phi^{\alpha\beta}_r\eta^{\alpha}_{ab}e^a_m e^b_n\eta^{\beta}_{cd}e^c_p e^d_q dx^r,$$

etc. But in such variables the corresponding action in Eq. (92) contains Einstein–Hilbert term $\sqrt{G}R$ and so is not polynomial. So we prefer to consider formulas (92) and (97) as final results of our investigation.

V. DISCUSSION

We have shown that gravity-like interactions live inside QCD. This conclusion is supported by the results of Ne'eman and Sijacki[7] concerning existence of gravity-like interactions in infrared sector of QCD, and vice versa.

Author hopes that the results presented in this paper will be starting point of various new approaches to QCD. Here we will list only some themes of the further investigations.

• Rescaling fields Q^{ABCD} and G_{mn} in Eq. (92), one can rewrite this formula as

$$\langle \mathcal{O} \rangle = \mathrm{Re} \int dedQd\Gamma d\Phi d\overline{\Psi} d\Psi \mathcal{O}[\Gamma + i\Phi, \overline{\Psi}, \Psi] \det M \exp\left\{ \frac{i}{\lambda} S_1 - S_2 - S_{\mathrm{mat}} \right\}. \tag{98}$$

So it is naturally to apply the stationary phase method for expansion of $\langle \mathcal{O} \rangle$ in power series with respect to λ

Such expansion in our theory is absolutely unlike standard perturbative ones in quantum field theory because in our theory one must expend integrand near some non-perturbative (most likely) solution of Einstein–Cartan equations (99) that corresponds to some non-trivial vacuum of the theory under consideration. So the expansion of path integral in power series in λ doesn't mean that interaction is supposed to be weak. So, in particular, there are no contradictions between our results and Ne'eman–Sijacky ones concerning the appearance of gravity-like interactions in infrared limit of QCD in which interaction is strong.

The stationary points are determined by equations

$$\delta S_1 = 0. \tag{99}$$

But Eqs. (99) are nothing but Euclidean Einstein ones. What is the meaning of known exact solutions of Einstein equations (such as gravitational instantons, wormholes, etc.) in the context of QCD?

• In particular, what is the meaning of the flat space solution

$$G_{mn} = c^2 g_{mn}, \quad c = \mathrm{const} \tag{100}$$

of Eq. (99)? How to construct the expansion of the integrand in Eq. (98) near such solution? Does the existence of the flat solutions (100) leads to appearance the vacuum condensates of the gluon fields?

• The action (92) depends on contorsion 1-form quadratically without derivatives. So the contorsion can be integrated out. Obviously, this leads to four-fermion interaction terms in the action (as in usual theories of gravitation with torsion). Recently such four-fermion interaction are intensively investigated at effective low energy theory in the spirit of Nambu–Jona-Lasinio model.[33] It would be very interesting to try to investigate such effective theory in framework of our approach.

• The actions S_1, S_2, and S_{mat} in Eq. (92) are polynomial. So it is possible to derive the corresponding Schwinger equations. What are the solutions of these equations in the usual approximations? Do the solutions exist that correspond to non-zero vacuum condensate of the field G_{mn}?

• The action S_1 in Eq. (92) is invariant with respect to the group $\mathrm{Diff}(R^4)$ of the general coordinate transformations. It is easy to derive the corresponding Ward identities. Obviously, that these identities express nothing but the energy—momentum conservation. Nevertheless, it is interesting to investigate consequences of such Ward identities because in proposed variables they have very unusual form and, most likely, can lead to new interesting results.

Now let us discuss the shortcomings of the proposed approach. First, our formulation is

essencially chiral because left and right SU(2) subgroups of the total $SU(2)\times SU(2)\approx O(4)$ invariance group of the action (58) play the different roles in our formalism. In itself, it is not a difficulty, but after imposing of the gauge conditions that entangle space–time and internal degrees of freedom [as the gauge (96)], one obtains the theory that is not manifestly parity invariant. It is not convenient.

This left–right asymmetry in our approach is connected with the structure of the group SU(3). Indeed, there is no faithful embedding of the group O(4) in SU(3). So it is needed more large gauge group to originate left–right symmetric general relativity-like formalism. Thus

- it is interesting to develop general relativity-like formalism for the grand unified theories based on the groups SU(5),SO(10), etc. Except left–right symmetric formulation, one may hope to find natural spontaneous parity breaking mechanism in electroweak sector of the theory in this way.

Further, our theory is essentially Euclidean and it is unclear how to develop the general relativity-like formulation of YM theory in which YM induced metric has Lorentzian signature in presented approach. This shortcoming again is connected with the structure of the gauge group SU(3). Indeed, the gauge group SU(3) is compact, and so it is impossible to embed in SU(3) neither the non-compact group SO(3,1) nor any its subgroup in a covariant way.

The existence of the only Euclidean formulation of the theory, per se, is not a difficulty. But the formulation of the theory in the Minkowski space is more visual. In particular, the absence of such formulation hampers the investigation of the confinement in our approach. Meanwhile, the results of the works[12,19] indicates that, may be, there exists black hole like mechanism of the confinement. But black holes live in the Lorentzian space rather then in the Euclidean one.

- The author hopes to overcome the above mentioned difficulties by using the formalism developed in Ref. 34 where it was shown that SU(N) YM theory is equivalent to certain GL(N,C) gauge theory in the following sense: classes of the gauge equivalent solutions of the initial SU(N) YM theory are in one-to-one correspondence to classes of the gauge equivalent solutions of the above mentioned GL(N,C) gauge theory. In the QCD case $N=3$, and so Lorentz group SL(2,C) can be embedded in the QCD gauge group in such GL(3,C) formalism. So it is possible to develop the Lorentzian analog of the Euclidean general relativity like formulation of QCD given in the presented work.

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On the consistent effect histories approach to quantum mechanics

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A formulation of the consistent histories approach to quantum mechanics in terms of generalized observables (POV measures) and effect operators is provided. The usual notion of ''history'' is generalized to the notion of ''effect history.'' The space of effect histories carries the structure of a *D*-poset. Recent results of J. D. Maitland Wright imply that every decoherence functional defined for ordinary histories can be uniquely extended to a bi-additive decoherence functional on the space of effect histories. Omnès' logical interpretation is generalized to the present context. The result of this work considerably generalizes and simplifies the earlier formulation of the consistent effect histories approach to quantum mechanics communicated in a previous work of this author. © *1996 American Institute of Physics.* [S0022-2488(96)00211-3]

I. INTRODUCTION

Nonrelativistic quantum mechanics in its standard formulation is not a theory which describes dynamical processes in time, but it is a theory which gives probabilities to various possible events and measurement outcomes at fixed instants of time. The dynamical law of quantum mechanics, the Schrödinger equation, describes the change of the probability amplitude with time. Quantum mechanics in its usual form does not provide us with a dynamical law which describes the time evolution of events. This can be succinctly summarized by saying that quantum mechanics in its usual form does not provide us with a (naive) model of what is ''actually'' going on on a microscopic level in a quantum system. It is often felt that this is a serious drawback of quantum mechanics. Examples for attempts to modify quantum mechanics to a theory providing us with a model for what is ''actually'' happening are hidden variables theories (see, e.g., Refs. 1–3), the dynamical state vector reduction models (see, e.g., Refs. 4–7), or related models (see, e.g., Ref. 8). The consistent histories formulation of quantum mechanics is another attempt to remedy the situation and to incorporate time sequences of events and—as a special case—sequential measurements into quantum mechanics without providing a naive dynamical model for the microscopic world in the above sense and without altering the basic principles and the basic mathematical structure of Hilbert space quantum mechanics.

The consistent histories approach to nonrelativistic quantum mechanics has been inaugurated in a seminal paper by Griffiths[9] and further developed by Griffiths,[10–12] by Omnès,[13–20] by Isham[21] and Isham and Linden[22,23] and by Isham, Linden, and Schreckenberg[24] and applied to quantum cosmology by Gell-Mann and Hartle[25–30] and Hartle.[31,32] Dowker and Kent have carried out a critical reexamination of the consistent histories approach and particularly of Omnès' notion of truth and of the Gell-Mann–Hartle program (see Refs. 33–35). A critical discussion of the consistent histories approach can also be found in Ref. 36. The consistent histories approach asserts that quantum mechanics provides a realistic description of individual quantum mechanical systems, regardless of whether they are open or closed. The possibility of a quantum mechanical description of single closed systems, which neither interact with their environment nor are exposed to measurements, is denied by the conventional Copenhagen-type interpretations of quantum mechanics.

By contrast, in the logical interpretation developed by Omnès, the notion of measurement is

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not a key concept. Instead one takes the point of view that the aim of an interpretation is generally to provide us with a systematic and unambiguous language specifying the meaning of the objects in the formalism in terms of real physical objects and specifying what can meaningfully be said about the physical systems described by the theory. We will call this attitude the *semantic* approach to interpretation. Clearly the logical interpretation is a realistic interpretation in the sense that it is presupposed that physical systems really exist and have real properties regardless of whether they are measured or not.

A key notion in the formulation of quantum mechanics is the notion of observable. In the spirit of the logical interpretation the term *speakable* would be more appropriate, but we stick to the usual terminology. In usual Hilbert space quantum mechanics the observables are identified with self-adjoint operators on the Hilbert space and propositions about quantum mechanical systems are identified with projection operators on Hilbert space. There is a one-to-one correspondence between self-adjoint operators on Hilbert space and projection valued (PV) measures on the real line $\mathbb{R}$. To every Borel subset $\mathscr{B}$ of $\mathbb{R}$ there corresponds one projection operator representing the proposition that the value of the considered observable is in the set $\mathscr{B}$. More remarks about observables and propositions in ordinary quantum mechanics can be found in Ref. 37.

The question which objects in the formalism have to be identified with observables (or speakables) is clearly a question belonging to the interpretation of quantum mechanics. Reasonableness and mathematical simplicity are the guiding principles to answer this question. The most general notion of observable compatible with the probabilistic structure of quantum mechanics is that of *positive operator valued (POV) measures*, which contains the ordinary observables represented by PV measures on $\mathbb{R}$ as a subclass. Quantum mechanics is totally consistent without POV measures, but POV measures enrich the language of quantum mechanics and enlarge the measurement theoretical possibilities of quantum mechanics.[38,39] On the other hand, the claim that POV measures represent the observables in quantum mechanics is not only consistent with the mathematical structure of Hilbert space quantum mechanics but furthermore is also reasonable. Many examples can be found in the monograph by Busch *et al.*[40]

In this work we take on the view that POV measures are the observables in quantum mechanics and that all POV measures should be treated on the same footing and that all effects should be identified with the general properties (or speakables or beables) of quantum systems. We further consider *every* effect operator as representative of some sort of reality. Some arguments supporting this view can be found in Ref. 37 and references therein. It is perhaps worthwhile to mention a further simple argument which is essentially due to Ludwig.[41] To this end consider a measuring device $\mathscr{M}$ consisting of a detector $\mathscr{D}$ (designed to measure some property E associated with some projection operator) and some scatterer $\mathscr{S}$. An appropriately prepared incident physical system $\mathscr{T}$ (e.g., a particle) is first scattered by $\mathscr{S}$ and then detected by the detector $\mathscr{D}$. To obtain the property F measured by the device $\mathscr{M}$ one has to apply the unitary transformation given by the S-matrix S of $\mathscr{S}$ to the property measured by $\mathscr{D}$. Let $\varrho_{\mathscr{T}}$ denote the initial state of $\mathscr{T}$ and $\varrho_{\mathscr{S}}$ denote the initial state of $\mathscr{S}$. Then the relation between E and F is given by

$$\mathrm{tr}\big(S(\varrho_{\mathscr{T}}\otimes\varrho_{\mathscr{S}})S^{\dagger}(E\otimes 1)\big)=\mathrm{tr}(\varrho_{\mathscr{T}}F),$$

where the trace on the right-hand side is in the Hilbert space $\mathbb{H}_{\mathscr{T}}$ of $\mathscr{T}$ and the trace on the left-hand side is in the tensor product $\mathbb{H}_{\mathscr{T}}\otimes\mathbb{H}_{\mathscr{S}}$ of the Hilbert spaces $\mathbb{H}_{\mathscr{T}}$ of $\mathscr{T}$ and $\mathbb{H}_{\mathscr{S}}$ of $\mathscr{S}$. The operator F is uniquely determined by this equation. However, realistic physical S-matrices S transform projection operators (according to the above equation) in general to effect operators and only the set of effect operators is invariant under this transformations. Therefore whether a measuring device measures an effect or a property associated with some projection operator may depend on an arbitrary cut between the system and the apparatus. This argument can be formalized (see Ref. 42).

In the consistent histories approach it is claimed that all results of measurement theory also *follow* from the consistent histories approach. In the present work we take seriously this claim and

continue our efforts to formulate the consistent histories formalism for general observables represented by POV measures. This program was first formulated and studied in Ref. 37. We will freely use the notation and terminology from Ref. 37 and review only the bare essentials.

This work is organized as follows: In Sec. II we summarize the consistent histories approach to nonrelativistic Hilbert space quantum mechanics and the logical interpretation of quantum mechanics. In Sec. III we recall basic definitions and results from Ref. 37 and we formulate our generalized (effect) history theory and a generalized logical rule of interpretation for effect histories. Our results are based on an important theorem by Wright.[43] This theorem relies heavily on the recent solution of the Mackey–Gleason problem (see Refs. 44 and 45). The results in Sec. III considerably simplify and generalize the results formulated in Ref. 37. In Sec. IV we present our summary.

As in Ref. 37 it must be emphasized that the representation and the interpretation of the consistent histories approach in this work might not be accepted by the authors cited. The present work solely reflects the inclination and the views of this author.

II. CONSISTENT HISTORIES AND THE LOGICAL INTERPRETATION

We consider a quantum mechanical system $\mathscr{S}$ without superselection rules represented by a separable complex Hilbert space $\mathbb{H}$ and a Hamiltonian operator H. Every physical state of the considered system is mathematically represented by a density operator on $\mathbb{H}$, i.e., a linear, positive, trace-class operator on $\mathbb{H}$ with trace 1. The time evolution is governed by the unitary operator $U(t',t)=\exp(-i(t'-t)H/\hbar)$ which maps states at time t into states at time t' and satisfies $U(t'',t')U(t',t)=U(t'',t)$ and $U(t,t)=1$.

In the familiar formulations of quantum mechanics the observables are identified with (and represented by) the self-adjoint operators on $\mathbb{H}$, and according to the spectral theorem observables can be identified with projection operator valued (PV) measures on the real line; that is, there is a one-to-one correspondence between self-adjoint operators on $\mathbb{H}$ and maps $\mathscr{O}$: $\mathscr{B}(\mathbb{R})\to\mathscr{P}(\mathbb{H})$, such that $\mathscr{O}(\mathbb{R})=1$ and $\mathscr{O}(\cup_i K_i)=\Sigma_i\mathscr{O}(K_i)$ for every pairwise disjoint sequence $\{K_i\}_i$ in $\mathscr{B}(\mathbb{R})$ (the series converging in the ultraweak topology). Here $\mathscr{B}(\mathbb{R})$ denotes the Borel σ-algebra of $\mathbb{R}$ and $\mathscr{P}(\mathbb{H})$ denotes the set of projection operators on $\mathbb{H}$, i.e., self-adjoint operators P satisfying $P=PP$.

A meaningful proposition about the system (also called *physical quality*) is a proposition specifying that the value of some observable $\mathscr{O}$ lies in some set $B\in\mathscr{B}(\mathbb{R})$. This means that to every meaningful proposition about the system under consideration there corresponds one projection operator on $\mathbb{H}$.

In the state represented by the density operator ϱ the probability of a proposition represented by the projection operator P is given by $\mathrm{tr}(\varrho P)$, where tr denotes the trace in $\mathbb{H}$.

Positive and bounded operators F on $\mathbb{H}$, satisfying $0\leqslant F\leqslant 1$, are commonly called *effects* and the set of all effects on the Hilbert space $\mathbb{H}$ will be denoted by $\mathfrak{E}(\mathbb{H})$. We further denote the set of all bounded, linear operators on $\mathbb{H}$ by $\mathscr{B}(\mathbb{H})$.

If $\mathbb{H}$ is an infinite-dimensional Hilbert space, then the set of all projection operators $\mathscr{P}(\mathbb{H})$ on $\mathbb{H}$ is weakly dense in $\mathfrak{E}(\mathbb{H})$.[46]

Generalized observables are now identified with positive operator valued (POV) measures on some measurable space $(\Omega,\mathscr{F})$, i.e., maps $O:\mathscr{F}\to\mathfrak{E}(\mathbb{H})$ with the following properties.

(i) $O(A)\geqslant O(\varnothing)$, for all $A\in\mathscr{F}$.
(ii) Let $\{A_i\}$ be a countable set of disjoint sets in $\mathscr{F}$, then $O(\cup_i A_i)=\Sigma_i O(A_i)$, the series converging ultraweakly.
(iii) $O(\Omega)=1$.

Generalized observables are also called *effect valued measures*. Ordinary observables (associated with self-adjoint operators on $\mathbb{H}$) are then identified with the projection valued measures on the real line $\mathbb{R}$. Generalizing our above terminology, we regard all propositions specifying the value of

some generalized observable as generalized physical qualities. In order to discriminate physical qualities corresponding to ordinary observables from physical qualities corresponding to generalized observables, we will call the former ''ordinary physical qualities'' and the latter ''generalized physical qualities.'' In the generalized approach to every physical quality there corresponds one effect operator.

A *homogeneous history* is a map $h:\mathbb{R}\to\mathscr{P}(\mathbb{H})$, $t\mapsto h_t$. We call $t_i(h):=\min(t\in\mathbb{R}|h_t\neq 1)$ the *initial* and $t_f(h):=\max(t\in\mathbb{R}|h_t\neq 1)$ the *final time* of h, respectively. Furthermore, the *support of h* is given by $\mathfrak{s}(h):=\{t\in\mathbb{R}|h_t\neq 1\}$. If $\mathfrak{s}(h)$ is finite, countable, or uncountable, then we say that h is a *finite, countable*, or *uncountable history*, respectively. The space of all homogeneous histories will be denoted by $\mathscr{H}(\mathbb{H})$, the space of all finite homogeneous histories by $\mathscr{H}_{\text{fin}}(\mathbb{H})$, and the space of all finite homogeneous histories with support S by $\mathscr{H}_S(\mathbb{H})$.

By a *history proposition* we mean a proposition about the system specifying which history will be realized. We use the terms history and history proposition synonymously in this work.

In this work we focus attention on finite histories. If a homogeneous history vanishes for some $t_0\in\mathbb{R}$, i.e., $h_{t_0}=0$, then we say that h is a *zero history*. All zero histories are collectively denoted by 0, slightly abusing the notation.

For every finite subset S of $\mathbb{R}$ we can consider the Hilbert tensor product $\otimes_{t\in S}\mathbb{H}$ and the algebra $\mathscr{B}^{\otimes}_S(\mathbb{H}):=\mathscr{B}(\otimes_{t\in S}\mathbb{H})$ of bounded linear operators on $\otimes_{t\in S}\mathbb{H}$. It has been pointed out by Isham[21] that for any fixed S there is an injective (but not surjective) correspondence σ_S between finite histories with support S and elements of $\mathscr{B}^{\otimes}_S(\mathbb{H})$ given by

$$\sigma_S:\mathscr{H}_S(\mathbb{H})\to\mathscr{B}^{\otimes}_S(\mathbb{H}),\quad h\simeq\{h_{t_k}\}_{t_k\in S}\mapsto\otimes_{t_k\in S}h_{t_k}. \tag{1}$$

The finite homogeneous histories with support S can therefore be identified with projection operators on $\otimes_{t\in S}\mathbb{H}$. The set of all projection operators on $\otimes_{t\in S}\mathbb{H}$ will in the sequel be denoted by $\mathscr{P}^{\otimes}_S(\mathbb{H})$. However, not all projection operators in $\mathscr{P}^{\otimes}_S(\mathbb{H})$ have the form $\sigma_S(h)$ with $h\in\mathscr{H}_S(\mathbb{H})$.

The projection operators in $\mathscr{P}^{\otimes}_S(\mathbb{H})$ are called *finite inhomogeneous histories with support S* and the space $\mathscr{K}_S(\mathbb{H}):=\mathscr{P}^{\otimes}_S(\mathbb{H})$ of projection operators on $\otimes_{t\in S}\mathbb{H}$ is called the *space of finite inhomogeneous histories with support S*. The space of all finite inhomogeneous histories with arbitrary support will be denoted by $\mathscr{K}_{\text{fin}}(\mathbb{H})$ or by $\mathscr{P}^{\otimes}{}_{\text{fin}}(\mathbb{H})$. Furthermore, to every finite homogeneous history $h\in\mathscr{H}_{\text{fin}}(\mathbb{H})$ we associate its *class operator with respect to the fiducial time* t_0 by $C_{t_0}(h):=U(t_0,t_n)h_{t_n}U(t_n,t_{n-1})h_{t_{n-1}}\cdots U(t_2,t_1)h_{t_1}U(t_1,t_0)$. The class operators can be unambiguously extended to finite inhomogeneous histories such that C_{t_0} is additive for orthogonal projectors, i.e., $C_{t_0}(h\vee k):=C_{t_0}(h)+C_{t_0}(k)$ for $h\perp k$. The functional $d_\varrho:\mathscr{K}_{\text{fin}}(\mathbb{H})\times\mathscr{K}_{\text{fin}}(\mathbb{H})\to\mathbb{C}$, $(h,k)\mapsto d_\varrho(h,k):=\text{tr}(C_{t_0}(h)\varrho(t_0)C_{t_0}(k)^\dagger)$ will be called the *consistency functional associated with the state* ϱ. The consistency functional d_ϱ satisfies for all $h,h',k\in\mathscr{K}_{\text{fin}}(\mathbb{H})$

(i) $d_\varrho(h,h)\in\mathbb{R}$ and $d_\varrho(h,h)\geqslant 0$;
(ii) $d_\varrho(h,k)=d_\varrho(k,h)^*$;
(iii) $d_\varrho(1,1)=1$;
(iv) $d_\varrho(h\vee h',k)=d_\varrho(h,k)+d_\varrho(h',k)$, whenever $h\perp h'$;
(v) $d_\varrho(0,h)=0$, for all h.

In Ref. 37 we have used a slightly different terminology: the above consistency functional d_ϱ has been called there ''decoherence functional.'' In this work we want to carefully distinguish biadditive functionals on a Boolean lattice from biadditive functionals defined on a D-poset. Thus, the former are called consistency functionals, whereas we reserve the term ''decoherence functional'' for a biadditive functional defined on a D-poset (see below).

Any collection $\mathscr{C}'$ of histories in $\mathscr{P}^{\otimes}_{\text{fin}}(\mathbb{H})$ is said to be *consistent with respect to the state* ϱ if $\mathscr{C}'$ is a Boolean algebra [with respect to the meet, join, and orthocomplementation in $\mathscr{P}^{\otimes}_{\text{fin}}(\mathbb{H})$ and

with unit $1_{\mathscr{C}'}$] and if $\mathrm{Re}\, d_\varrho(h,k)=0$ for every two disjoint histories $h,k\in\mathscr{C}'$. Here two (possibly inhomogeneous) finite histories h and k are said to be *disjoint* if $h\leqslant\neg k$, where $\leqslant$ is the partial order on $\mathscr{K}_{\mathfrak{s}(h)\cup\mathfrak{s}(k)}(\mathbb{H})$.

It is now easy to see that the consistency functional d_ϱ induces an additive probability measure p_ϱ on every consistent Boolean sublattice $\mathscr{C}\subset\mathscr{P}^{\otimes}_{\mathrm{fin}}(\mathbb{H})$. The probability measure p_ϱ is defined by

$$p_\varrho:\mathscr{C}\to\mathbb{R}^+,\quad p_\varrho(h):=\frac{d_\varrho(h,h)}{d_\varrho(1_{\mathscr{C}},1_{\mathscr{C}})}. \tag{2}$$

The probability measure p_ϱ on a consistent Boolean algebra $\mathscr{C}$ of history propositions induced by the consistency functional d_ϱ according to Eq. (2) defines two logical relations in $\mathscr{C}$, namely an implication and an equivalence relation between histories. A history proposition h is said to *imply* a history proposition k if the conditional probability $p_\varrho(k|h)\equiv[p_\varrho(h\wedge_{\mathscr{C}}k)]/p_\varrho(h)$ is well defined and equal to one. Two history propositions h and k are said to be *equivalent* if h implies k and vice versa.

The universal rule of interpretation of quantum mechanics can now be formulated as follows.

Rule 1 (Omnès): Propositions about quantum mechanical systems should solely be expressed in terms of history propositions. Every description of an isolated quantum mechanical system should be expressed in terms of finite history propositions belonging to a common consistent Boolean algebra of histories. Every reasoning relating several propositions should be expressed in terms of the logical relations induced by the probability measure from Eq. (2) in that Boolean algebra.

III. CONSISTENT EFFECT HISTORIES

In Ref. 37 we have motivated and introduced the following notion of homogeneous effect history

Definition 1: A **homogeneous effect history (of the first kind)** *is a map* $u:\mathbb{R}\to\mathfrak{E}(\mathbb{H})$, $t\mapsto u_t$. *The* **support of** u *is given by* $\mathfrak{s}(u):=\{t\in\mathbb{R}|u_t\neq 1\}$. *If* $\mathfrak{s}(u)$ *is finite, countable, or uncountable, then we say that* u *is a* **finite, countable**, or **uncountable effect history**, *respectively. The space of all homogeneous effect histories (of the first kind) will be denoted by* $\mathbb{E}(\mathbb{H})$, *the space of all finite homogeneous effect histories (of the first kind) by* $\mathbb{E}_{\mathrm{fin}}(\mathbb{H})$, *and the space of all finite homogeneous effect histories (of the first kind) with support* S *by* $\mathbb{E}_S(\mathbb{H})$. *All homogeneous effect histories for which there exists at least one* $t\in\mathbb{R}$ *such that* $u_t=0$ *are collectively denoted by* 0, *slightly abusing the notation.*

The class operator C_{t_0} defined above for finite ordinary homogeneous histories can be defined for homogeneous finite effect histories $u\in\mathbb{E}_{\mathrm{fin}}(\mathbb{H})$:

$$C_{t_0}(u):=U(t_0,t_n)\sqrt{u_{t_n}}U(t_n,t_{n-1})\sqrt{u_{t_{n-1}}}\cdots U(t_2,t_1)\sqrt{u_{t_1}}U(t_1,t_0).$$

For every pair u and v of finite homogeneous effect histories (of the first kind) we define the *decoherence weight* of u and v by

$$d_\varrho(u,v):=\mathrm{tr}(C_{t_0}(u)\varrho(t_0)C_{t_0}(v)^\dagger).$$

The functional $d_\varrho:\mathbb{E}_{\mathrm{fin}}(\mathbb{H})\times\mathbb{E}_{\mathrm{fin}}(\mathbb{H})\to\mathbb{C}$, $(u,v)\mapsto d_\varrho(u,v)$, will be called the *decoherence functional associated with the state* ϱ.

The map σ_S given by Eq. (1) can be extended to a map

$$\sigma_{\mathrm{fin}}:\mathbb{E}_{\mathrm{fin}}(\mathbb{H})\to\mathscr{P}^{\otimes}_{\mathrm{fin}}(\mathbb{H}),\quad u\simeq\{u_{t_k}\}_{t_k\in\mathfrak{s}(u)}\mapsto\otimes_{t_k\in\mathfrak{s}(u)}u_{t_k}, \tag{3}$$

where $\mathscr{B}^{\otimes}_{\mathrm{fin}}(\mathbb{H})$ denotes the disjoint union of all $\mathscr{B}^{\otimes}_{S}(\mathbb{H})$, $S\subset\mathbb{R}$ finite. The map σ_{fin} is neither injective nor surjective. However, $d_{\varrho}(u,v)$ depends on u and v only through $\sigma_{\mathrm{fin}}(u)$ and $\sigma_{\mathrm{fin}}(v)$. From a mathematical point of view it thus seems to be natural to define the notion of *inhomogeneous* effect history as follows:

Definition 2: Let S be a finite subset of $\mathbb{R}$. *Then we call the space* $\mathfrak{E}^{\otimes}_{S}(\mathbb{H}):=\mathfrak{E}(\otimes_{t\in S}\mathbb{H})$ *of effect operators on* $\otimes_{t\in S}\mathbb{H}$ *the* **space of finite inhomogeneous effect histories with support** S. *The space of all finite inhomogeneous effect histories with arbitrary support will be denoted by* $\mathfrak{E}^{\otimes}_{\mathrm{fin}}(\mathbb{H})$. *The elements in* $\mathfrak{E}^{\otimes}_{\mathrm{fin}}(\mathbb{H})$ *will also be called* **effect history propositions**.

The homogeneous elements in $\mathfrak{E}^{\otimes}_{\mathrm{fin}}(\mathbb{H})$ represent equivalence classes of homogeneous effect histories. In this work we will carefully distinguish between homogeneous effect histories as defined in Definition 1 and homogeneous elements in $\mathfrak{E}^{\otimes}_{\mathrm{fin}}(\mathbb{H})$. For clarity of exposition we will call the former *homogeneous effect histories of the first kind* or (where no confusion can arise) simply homogeneous effect histories, whereas the latter will be called *homogeneous effect histories of the second kind*.

In technical terms $\mathfrak{E}^{\otimes}_{\mathrm{fin}}(\mathbb{H})$ is the direct limit of the directed system $\{\mathfrak{E}^{\otimes}_{S}(\mathbb{H})|S\subset\mathbb{R}\text{ finite}\}$. All the $\mathfrak{E}^{\otimes}_{S}(\mathbb{H})$, $S\subset\mathbb{R}$, and $\mathfrak{E}^{\otimes}_{\mathrm{fin}}(\mathbb{H})$ carry several distinct D-poset structures, as discussed in Ref. 37. For further literature on D-posets and effect algebras, see Refs. 47–54. As in Ref. 37 we use the terms *D-poset* and *effect algebra* synonymously. We refer to the D-poset structure on $\mathfrak{E}^{\otimes}_{\mathrm{fin}}(\mathbb{H})$ given by the partial addition $\oplus$, where $E_1\oplus E_2$ is defined if $E_1+E_2\leqslant 1$ by $E_1\oplus E_2:=E_1+E_2$, as the *canonical D-poset structure*. We will denote the canonical partial addition on $\mathfrak{E}^{\otimes}_{\mathrm{fin}}(\mathbb{H})$ by $\oplus$ and the canonical partial substraction on $\mathfrak{E}^{\otimes}_{\mathrm{fin}}(\mathbb{H})$ by $\ominus$.

In Ref. 37 we have used a different notion of inhomogeneous effect history, because it was not clear whether the decoherence functional d_{ϱ} defined above on the space of homogeneous effect histories (of the first kind) can be (uniquely) extended to in some appropriate sense a biadditive functional on the space of inhomogeneous effect histories as defined in Definition 2. In Ref. 37 we gave a rather technical definition of the notion of inhomogeneous effect history. Essentially we defined an inhomogeneous effect history to be a member of the free lattice generated by the homogeneous effect histories (of the first kind) by at most finitely many applications of the grammatical connectives ''and'' and ''or,'' to wit, we have viewed inhomogeneous effect histories to be—in essence—propositions in the language of quantum mechanics involving several (but at most finitely many) homogeneous effect histories. In turn only the latter were viewed as the basic *physical* entities in the formalism. We have shown in Ref. 37 that with this definition it is possible to consistently extend the consistent histories formulation of quantum mechanics and to incorporate effect histories. However, this approach involves a rather technical and mathematically by no means canonical definition of the notion of inhomogeneous history. Inhomogeneous effect histories in the sense of Ref. 37 represent only semantical entities without an obvious physical interpretation. In this work the term inhomogeneous effect history is always meant in the sense of Definition 2 unless explicitly otherwise stated.

In this work we use a recent result of J. D. Maitland Wright[43] which implies that the decoherence functional d_{ϱ} as defined above on the space of homogeneous effect histories (of the second kind) can indeed be extended to a functional on the space of inhomogeneous effect histories with the desired properties. We first recall the central result from Ref. 43.

Theorem 1: *Let A be a von Neumann algebra with no type* I_2 *direct summand. Let* $d:\mathscr{P}(A)\times\mathscr{P}(A)\to\mathbb{C}$ *be a decoherence functional. If d is bounded, then d extends to a unique bounded bilinear functional* $\tilde{d}$ *on* $A\times A$. *Furthermore, d is continuous when* $\mathscr{P}(A)$ *is equipped with the topology induced by the norm of A. Also,* $d(u,v)^*=d(v^*,u^*)$.

If A is a von Neumann algebra, let $\mathscr{P}(A)$ denote the set of projectors in A. A function $d:\mathscr{P}(A)\times\mathscr{P}(A)\to\mathbb{C}$ is called a *decoherence functional*, if (i) $d(p_1\oplus p_2,q)=d(p_1,q)+d(p_2,q)$, whenever p_1 and p_2 are mutually orthogonal; (ii) $d(p,q)^*=d(q,p)$; (iii) $d(p,p)\geqslant 0$; and (iv) $d(1,1)=1$.

Since the set $\mathscr{B}(\mathbb{H})$ of bounded operators on a Hilbert space $\mathbb{H}$ with dimension greater than 2

is a von Neumann algebra (of type I), Theorem 1 can be applied to the decoherence functional $d_\varrho : \mathscr{K}_{\text{fin}}(\mathbb{H}) \times \mathscr{K}_{\text{fin}}(\mathbb{H}) \to \mathbb{C}, (h,k) \mapsto d_\varrho(h,k) := \text{tr}(C_{t_0}(h)\varrho(t_0)C_{t_0}(k)^\dagger)$ defined in Sec. II above. Thus for every finite subset $S \subset \mathbb{R}$ there is a unique bounded bilinear functional $\widetilde{d}_{\varrho,S}$ on $\mathscr{B}_S^\otimes(\mathbb{H}) \times \mathscr{B}_S^\otimes(\mathbb{H})$ extending the decoherence functional d_ϱ restricted to $\mathscr{P}_S^\otimes(\mathbb{H}) \times \mathscr{P}_S^\otimes(\mathbb{H})$.

The restriction $\hat{d}_{\varrho,S}$ of $\widetilde{d}_{\varrho,S}$ to $\mathfrak{E}_S^\otimes(\mathbb{H}) \times \mathfrak{E}_S^\otimes(\mathbb{H})$ is a bounded functional which is additive in both arguments with respect to the canonical D-poset structure on $\mathfrak{E}_S^\otimes(\mathbb{H})$. The collection of all such functionals $\hat{d}_{\varrho,S}$ for any finite $S \subset \mathbb{R}$ induces a bounded functional $\hat{d}_\varrho$ on $\mathfrak{E}_{\text{fin}}^\otimes(\mathbb{H}) \times \mathfrak{E}_{\text{fin}}^\otimes(\mathbb{H})$ which is additive in both arguments with respect to the canonical D-poset structure on $\mathfrak{E}_{\text{fin}}^\otimes(\mathbb{H})$. The functional $\hat{d}_\varrho$ will be called the *decoherence functional with respect to the state* ϱ *on* $\mathfrak{E}_{\text{fin}}^\otimes(\mathbb{H})$.

Since $\mathfrak{E}_{\text{fin}}^\otimes(\mathbb{H})$ is a D-poset, $\mathfrak{E}_{\text{fin}}^\otimes(\mathbb{H})$ is in particular a partially ordered set. However, for two elements $e_1, e_2 \in \mathfrak{E}_{\text{fin}}^\otimes(\mathbb{H})$ the supremum $e_1 \vee e_2$ and the infimum $e_1 \wedge e_2$ not necessarily exist, that is, $\mathfrak{E}_{\text{fin}}^\otimes(\mathbb{H})$ is not a lattice. But there exists a partially defined join operation denoted by $\vee$ and a partially defined meet operation denoted by $\wedge$. To every element $e \in \mathfrak{E}_{\text{fin}}^\otimes(\mathbb{H})$ there exists one unique element $e' \in \mathfrak{E}_{\text{fin}}^\otimes(\mathbb{H})$ such that $e \oplus e'$ is well defined and $e \oplus e' = 1$. We refer to $e' = 1 \ominus e$ as to the *complement* of e.

Definition 3: A subset $\mathscr{B} \subset \mathfrak{E}_{\text{fin}}^\otimes(\mathbb{H})$ *is said to be an* **admissible Boolean lattice of (inhomogeneous) effect histories** *if the following conditions are satisfied.*

(i) *There exist two binary operations on* $\mathscr{B}$*, denoted by* $\vee_{\mathscr{B}}$ *and* $\wedge_{\mathscr{B}}$*, respectively, and one unary operation on* $\mathscr{B}$*, denoted by* $\neg_{\mathscr{B}}$*, such that the operations* $\vee_{\mathscr{B}}$*,* $\wedge_{\mathscr{B}}$*, and* $\neg_{\mathscr{B}}$ *are compatible with the partial order on* $\mathscr{B}$ *induced by the partial order on* $\mathfrak{E}_{\text{fin}}^\otimes(\mathbb{H})$ *and such that* $(\mathscr{B}, \vee_{\mathscr{B}}, \wedge_{\mathscr{B}}, \neg_{\mathscr{B}})$ *is a Boolean lattice,* i.e., $\vee_{\mathscr{B}}$ *is the join operation,* $\wedge_{\mathscr{B}}$ *is the meet operation, and* $\neg_{\mathscr{B}}$ *is the complementation operation on* $\mathscr{B}$*. The lattice-operations* $\vee_{\mathscr{B}}$ *and* $\wedge_{\mathscr{B}}$ *coincide with the partially defined meet operation* $\vee$ *and join operation* $\wedge$ *on* $\mathfrak{E}_{\text{fin}}^\otimes(\mathbb{H})$ *whenever the latter are well defined, to wit,* $e_1 \wedge_{\mathscr{B}} e_2 = e_1 \wedge e_2$ *and* $e_3 \vee_{\mathscr{B}} e_4 = e_3 \vee e_4$ *for all* $e_1, e_2, e_3, e_4 \in \mathscr{B}$*, whenever the right-hand sides are well defined in* $\mathfrak{E}_{\text{fin}}^\otimes(\mathbb{H})$*. The lattice operations* $\vee_{\mathscr{B}}$ *and* $\wedge_{\mathscr{B}}$ *are such that a complementation* $\neg_{\mathscr{B}}$ *can be unambiguously defined on* $\mathscr{B}$*.*

(ii) *There exists an injective map* $\mathfrak{M} : \mathscr{B} \to \mathfrak{E}_{\text{fin}}^\otimes(\mathbb{H})$*, which satisfies the following conditions*:

(a) $\mathfrak{M}$ *is a* **positive valuation** *on* $\mathscr{B}$ *with values in* $\mathfrak{E}_{\text{fin}}^\otimes(\mathbb{H})$*, to wit, a map satisfying the valuation condition* $\mathfrak{M}(b_1 \vee_{\mathscr{B}} b_2) \ominus \mathfrak{M}(b_1) = \mathfrak{M}(b_2) \ominus \mathfrak{M}(b_1 \wedge_{\mathscr{B}} b_2)$*, for all* $b_1, b_2 \in \mathscr{B}$*. This condition means in particular that the left-hand side and the right-hand side are well defined for all* $b_1, b_2 \in \mathscr{B}$;

(b) $\mathfrak{M}$ *preserves decoherence weights, i.e.,* $\hat{d}_\varrho(e_1, e_2) = \hat{d}_\varrho(\mathfrak{M}(e_1), \mathfrak{M}(e_2))$*, for all* $e_1, e_2 \in \mathscr{B}$*.*

An admissible Boolean sublattice of $\mathfrak{E}_{\text{fin}}^\otimes(\mathbb{H})$ *will be briefly denoted by* $(\mathscr{B}, \mathfrak{M})$.

Remark 1: Strictly speaking a **sublattice** $\mathscr{L}$ *of* $\mathfrak{E}_{\text{fin}}^\otimes(\mathbb{H})$ *is a subset* $\mathscr{L} \subset \mathfrak{E}_{\text{fin}}^\otimes(\mathbb{H})$ *such that* $\mathscr{L}$ *endowed with the restrictions of* $\vee$ *and* $\wedge$ *to* $\mathscr{L}$ *is a lattice. It makes thus sense to speak of sublattices of* $\mathfrak{E}_{\text{fin}}^\otimes(\mathbb{H})$*. However, it is important to notice that an admissible Boolean sublattice of* $\mathfrak{E}_{\text{fin}}^\otimes(\mathbb{H})$ *is not necessarily a sublattice of* $\mathfrak{E}_{\text{fin}}^\otimes(\mathbb{H})$ *in this sense.*

Remark 2: Let $\mathscr{L}_1, \mathscr{L}_2$ *be lattices. A map* $\nu : \mathscr{L}_1 \to \mathscr{L}_2$ *is called* **positive** *if* $\nu(p) < \nu(q)$*, whenever* $p < q$*. Since any Boolean lattice is relatively complemented, the condition that the map* $\mathfrak{M}$ *in Definition 3 is positive is actually redundant and follows already from the definition of D-posets and from the valuation condition. In particular* $\mathfrak{M}$ *is order preserving.*

Remark 3: The complement $e' = 1 - e$ *in* $\mathfrak{E}_{\text{fin}}^\otimes(\mathbb{H})$ *of some element* $e \in \mathscr{B}$ *does in general not coincide with the complement* $\neg_{\mathscr{B}} e$ *in* $\mathscr{B}$*. The greatest element* $1_{\mathscr{B}}$ *and the least element* $0_{\mathscr{B}}$ *in* $\mathscr{B}$ *do not necessarily coincide with the greatest element* 1 *and the least element* 0 *in* $\mathfrak{E}_{\text{fin}}^\otimes(\mathbb{H})$*, respectively.*

Our target is to generalize Omnès' logical rule and thus to single out the appropriate subsets of $\mathfrak{E}_{\text{fin}}^\otimes(\mathbb{H})$ on which a reasoning involving (inhomogeneous) effect histories compatible with ''common sense'' can be defined. The conditions in Definition 3 are clearly the minimal structure

required. Usually ''common sense'' (compare Ref. 19) is tacitly associated with Boolean lattices. Thus the first condition in Definition 3 that $\mathscr{B}$ is a Boolean lattice is indispensable. We have already mentioned above that the set $\mathfrak{E}_{\mathrm{fin}}^{\otimes}(\mathbb{H})$ carries (among others) a canonical D-poset structure, but no lattice structure, and that the decoherence functional $\hat{d}_{\varrho}$ is additive with respect to the D-poset structure on $\mathfrak{E}_{\mathrm{fin}}^{\otimes}(\mathbb{H})$. In the consistent histories approach, however, reasoning is defined on Boolean lattices $\mathscr{B}$ with the help of consistency functionals which are additive with respect to the lattice structure of $\mathscr{B}$. Thus one has to restrict oneself to Boolean lattices $\mathscr{B}\subset\mathfrak{E}_{\mathrm{fin}}^{\otimes}(\mathbb{H})$ such that the lattice structure of $\mathscr{B}$ is exactly mirrored in the D-poset structure of $\mathfrak{E}_{\mathrm{fin}}^{\otimes}(\mathbb{H})$ (by the map $\mathfrak{M}$). This leads to the condition that there exists a positive valuation $\mathfrak{M}$ as required in the second condition of Definition 3. The reasoning to be defined should be independent of the map $\mathfrak{M}$ chosen. Thus it is necessary to require that $\mathfrak{M}$ preserves decoherence weights.

Remark 4: The decoherence functional $\hat{d}_{\varrho}$ induces a consistency functional $d_{\varrho,\mathscr{B}}$ on $\mathscr{B}\times\mathscr{B}$ by $d_{\varrho,\mathscr{B}}:\mathscr{B}\times\mathscr{B}\to\mathbb{C}, d_{\varrho,\mathscr{B}}(p_1,p_2):=\hat{d}_{\varrho}(\mathfrak{M}(p_1),\mathfrak{M}(p_2))$, which is additive in both arguments with respect to the Boolean lattice structure on $\mathscr{B}$.

Definition 4: An admissible Boolean lattice $(\mathscr{B},\mathfrak{M})$ is called **consistent wrt** *ϱ if for every pair of disjoint elements $b_1,b_2\in\mathscr{B}$ (i.e., elements satisfying $b_1\wedge_{\mathscr{B}} b_2=0$) the* **consistency condition** $\mathrm{Re}\, d_{\varrho,\mathscr{B}}(b_1,b_2)=0$ *is satisfied.*

Theorem 2: *Let $(\mathscr{B},\mathfrak{M})$ be a consistent admissible Boolean lattice of effect histories. Then the consistency functional $d_{\varrho,\mathscr{B}}$ induces a probability functional $p_{\varrho,\mathscr{B}}$ on $\mathscr{B}$ by $b\mapsto p_{\varrho,\mathscr{B}}(b)\equiv[d_{\varrho,\mathscr{B}}(\mathfrak{M}(b),\mathfrak{M}(b))]/d_{\varrho,\mathscr{B}}(\mathfrak{M}(1_{\mathscr{B}}),\mathfrak{M}(1_{\mathscr{B}}))$.*

Definition 5: An effect history proposition $e_1\in\mathfrak{E}_{\mathrm{fin}}^{\otimes}(\mathbb{H})$ is said to **imply** *an effect history proposition $e_2\in\mathfrak{E}_{\mathrm{fin}}^{\otimes}(\mathbb{H})$ in the state ϱ if there exists a consistent admissible Boolean sublattice $\mathscr{B}$ of $\mathfrak{E}_{\mathrm{fin}}^{\otimes}(\mathbb{H})$ containing e_1 and e_2 and if the conditional probability $p_{\varrho,\mathscr{B}}(e_2|e_1)\equiv[p_{\varrho,\mathscr{B}}(e_1\wedge_{\mathscr{B}}e_2)]/p_{\varrho,\mathscr{B}}(e_1)$ is well defined and equal to one. We write $e_{1\Rightarrow\varrho}\,e_2$. Two history propositions e_1 and e_2 are said to be* **equivalent** *if e_1 implies e_2* and *vice versa. We write $e_1\Leftrightarrow_{\varrho}e_2$.*

Remark 5: If $e_1\wedge e_2$ exists in $\mathfrak{E}_{\mathrm{fin}}^{\otimes}(\mathbb{H})$, then it is easy to verify that if $p_{\varrho,\mathscr{B}_0}(e_2|e_1)$ is well defined and equal to one in some consistent admissible Boolean lattice $\mathscr{B}_0$ containing e_1 and e_2, then $p_{\varrho,\mathscr{B}}(e_2|e_1)$ is well defined and equal to one in every consistent admissible Boolean lattice $\mathscr{B}$ containing e_1 and e_2. If $e_1\wedge e_2$ does not exist in $\mathfrak{E}_{\mathrm{fin}}^{\otimes}(\mathbb{H})$, then there may be consistent Boolean lattices $\mathscr{B}_1$ containing e_1 and e_2 such that $p_{\varrho,\mathscr{B}_1}(e_2|e_1)$ is not one or is not well defined. If $e_1\wedge e_2$ does not exist in $\mathfrak{E}_{\mathrm{fin}}^{\otimes}(\mathbb{H})$, then it seems reasonable to define $e_1\Rightarrow_{\varrho}e_2$ if there exists an admissible Boolean lattice $\mathscr{B}$ containing e_1, e_2 and some further element $e_3\in\mathfrak{E}_{\mathrm{fin}}^{\otimes}(\mathbb{H})$ satisfying $e_1\geqslant e_3$ and $e_2\geqslant e_3$ such that $[p_{\varrho,\mathscr{B}}(e_3,e_3)]/p_{\varrho,\mathscr{B}}(e_1,e_1)$ is well defined in $\mathscr{B}$ and equal to one.

The generalized universal rule of interpretation of quantum mechanics can now simply be formulated as follows.

Rule 3: Propositions about quantum mechanical systems should solely be expressed in terms of effect history propositions. Every description of an isolated quantum mechanical system should be expressed in terms of finite effect history propositions belonging to a common consistent admissible Boolean algebra of effect histories. Every reasoning relating several propositions should be expressed in terms of the logical relations induced by the probability measure from Theorem 2 in that Boolean algebra.

(This rule is numbered ''Rule 3'' in order to distinguish it from Rule 2 stated in Ref. 37.) It is instructive to compare Rule 3 with Rule 2 stated in Ref. 37. It is obvious that Rule 1 is contained in Rule 3 as a special case. A more extensive discussion of the motivation and the philosophy underlying the logical interpretation of quantum mechanics can be found in Refs. 17–19 and 37 and will not be repeated here.

Compared with the treatment in Ref. 37 we have achieved a considerable simplification of the logical interpretation in terms of generalized observables and of the formalism of the consistent effect histories approach to generalized quantum mechanics. From a mathematical point of view, the extension of the ordinary consistent histories approach given in this article is a natural one.

Rule 3 asserts that to every meaningful proposition about a quantum mechanical system there

is an inhomogeneous effect history $e \in \mathfrak{E}^{\otimes}_{\mathrm{fin}}(\mathbb{H})$. However, homogeneous effect histories of the first kind, which have a direct physical interpretation, are not contained in $\mathfrak{E}^{\otimes}_{\mathrm{fin}}(\mathbb{H})$. According to Rule 3, homogeneous effect histories of the first kind can only indirectly be included into a description of a quantum mechanical system by representing every homogeneous effect history of the first kind e by its corresponding homogeneous effect history of the second kind $\sigma_{\mathrm{fin}}(e)$.

It remains to determine the connection of Rule 3 stated above and the generalized logical rule (Rule 2) formulated in Ref. 37. In contrast to Rule 3 above, the propositions about a quantum mechanical system permitted by Rule 2 stated in Ref. 37 contain the homogeneous effect histories of the first kind as a subclass and accordingly a description of a quantum mechanical system and reasoning can be done directly in terms of homogeneous effect histories of the first kind. In the next subsection we will see, however, that in an appropriate sense Rule 3 is a generalization of Rule 2 stated in Ref. 37 and that a description and reasoning (permitted by Rule 2) directly in terms of homogeneous effect histories of the first kind can always be lifted to a description and reasoning (permitted by Rule 3) in terms of the corresponding homogeneous effect histories of the second kind.

A. The connection between admissible and allowed Boolean lattices

In this subsection we will show that Rule 3 formulated above is indeed a generalization of the generalized logical rule as formulated in Ref. 37. In this subsection we will use the notation and terminology introduced in Ref. 37 without further notice. In this subsection the term *homogeneous effect history* is always meant to denote homogeneous effect histories of the first kind.

Consider some homogeneous effect history of order $k>0$ denoted by $w^k_{E_1,\ldots,E_m}$, where $E_1,\ldots,E_m \in \mathfrak{E}(\mathbb{H})$. The corresponding history proposition states that first at k successive times $t_{1,1},\ldots,t_{1,k}$ the appropriately time translated effect $E_1(t_{1,j})=U(t_{1,j},t_{1,1})E_1U(t_{1,j},t_{1,1})^{\dagger}$ $(1\leqslant j\leqslant k)$ is realized and then at k successive times $t_{2,1},\ldots,t_{2,k}$ the effect $E_2(t_{2,j})=U(t_{2,j},t_{1,1})E_2U(t_{2,j},t_{1,1})^{\dagger}$ $(1\leqslant j\leqslant k)$ and so on. [We refer the reader to the discussion following Theorem 4 in Ref. 37; for simplicity we assume that the history w_0 appearing there is the unit history, i.e., $(w_0)_t=1$ for all t.]

Now we first observe that the exact times associated with the effects in some homogeneous effect history are inessential. The only thing that physically matters is the order and sequence of the effects in the homogeneous history. The time points associated with the effect operators in some homogeneous effect history can be changed provided the order remains fixed and provided the effect operators associated with the shifted times are appropriately time translated with the unitary evolution operator U. We say that two homogeneous effect histories related in this way to each other are *shift equivalent*.

If we define $F_j := E_j^{k/2}$, for all $1\leqslant j\leqslant k$, then we see that every homogeneous effect history $w^k_{E_1,\ldots,E_m}$ of order k can be mapped to a homogeneous effect history $w^2_{F_1,\ldots,F_m}$ of order 2. This map preserves decoherence weights. The history $w^2_{F_1,\ldots,F_m}$ is unique up to shift equivalence. That the F_j are effect operators follows from Proposition 2 in Ref. 55. We further recall that $F\oplus_1 F'=F\oplus F'=(E\oplus_{2/k}E')^{k/2}$, where $F=E^{k/2}$ and $F'=(E')^{k/2}$ whenever the expressions are well defined. Now it is easy to see that for every allowed Boolean algebra $(\mathscr{B},\mathrm{B})$ of order k (as defined in Ref. 37) there exists an allowed Boolean algebra $(\mathscr{B}',\mathrm{B}')$ of order 2 and a lattice isomorphism $\varphi:\mathscr{B}\to\mathscr{B}'$ such that $\mathrm{B}=\mathrm{B}'\circ\varphi$. Thus, it suffices to consider allowed Boolean algebras of order 2 in the sequel. In Theorem 3 below $\mathfrak{N}$ denotes the canonical map defined in Remark 15 in Ref. 37.

Theorem 3: *Let $(\mathscr{B},\mathfrak{M})$ be an admissible Boolean lattice in the sense of Definition 3 above and let $(\mathscr{A},\mathfrak{J})$ be an allowed Boolean lattice of effect histories of order k as defined in Ref. 37. Let $\mathscr{A}_0$ denote the set of atoms of $\mathscr{A}$. Then there exists a lattice isomorphism $\psi:\mathscr{A}\to\mathscr{B}$ preserving decoherence weights and satisfying $\mathfrak{J}=\mathfrak{M}\circ\psi$ if an only if $\mathscr{B}$ is atomic, $\mathfrak{M}$ maps the set $\mathscr{B}_0$ of atoms of $\mathscr{B}$ bijectively to $\mathfrak{J}(\mathscr{A}_0)$, and $\mathfrak{M}(0_{\mathscr{B}})=\mathfrak{J}(0_{\mathscr{A}})$.*

Proof: ''⇒:'' trivial. ''⇐:'' $\mathfrak{M}^{-1}\circ\mathfrak{J}$ restricted to $\tilde{\mathscr{A}}:=\mathscr{A}_0\cup\{0_{\mathscr{A}}\}$ can in an obvious way be extended to a lattice isomorphism $\psi:\mathscr{A}\to\mathscr{B}$ by requiring $\psi(\bigvee_{\mathscr{A},i\in I}a_i)=\bigvee_{\mathscr{B},i\in I}\psi(a_i)$ for any $\{a_i\}_{i\in I}\subset\mathscr{A}_0$. Then $\tilde{\mathfrak{J}}:=\mathfrak{M}\circ\psi$ is a positive valuation satisfying the valuation condition and extending the map $\mathfrak{N}_{|\tilde{A}}$ as required in the Definition of the allowed Boolean lattice. Since $(\mathscr{A},\tilde{\mathfrak{J}})$ is an allowed Boolean lattice, $\mathfrak{J}$ is the unique positive valuation with this property and thus $\mathfrak{J}=\tilde{\mathfrak{J}}$. That ψ preserves decoherence weights follows immediately: $d_{\varrho,\mathscr{L}}(a_1,a_2):=d_{\varrho,\mathfrak{E},k}(\mathfrak{J}(a_1),\mathfrak{J}(a_2))=\hat{d}_{\varrho}(\mathfrak{M}\circ\psi(a_1),\mathfrak{M}\circ\psi(a_2))=\hat{d}_{\varrho}(\psi(a_1),\psi(a_2))$, for all $a_1,a_2\in\mathscr{A}$, where $d_{\varrho,\mathfrak{E},k}$ denotes the decoherence functional on $\mathfrak{E}(\mathbb{H})_{2/k,\mathfrak{E}}$ (compare Remark 20 in Ref. 37).

Theorem 4: *For every allowed Boolean lattice* $(\mathscr{A},\mathfrak{J})$ *in the sense of Ref. 37 there is an admissible Boolean lattice* $(\mathscr{B},\mathfrak{M})$ *such that there exists an isomorphism* $\psi:\mathscr{A}\to\mathscr{B}$ *satisfying the conditions from Theorem 3.*

Proof: We denote by $\mathscr{A}_0$ the set of atoms of $\mathscr{A}$. We construct $\mathscr{B}$ inductively. We choose $\mathfrak{J}(\mathscr{A}_0)$ to be the set of atoms of $\mathscr{B}$ and $0_{\mathscr{B}}:=\mathfrak{J}(0_{\mathscr{A}})$. We define $\mathfrak{J}(a_1)\vee_{\mathscr{B}}\mathfrak{J}(a_2):=\mathfrak{J}(a_1\vee_{\mathscr{A}}a_2)$ for all $a_1,a_2\in\mathscr{A}_0$. If $\mathscr{A}_0$ contains more than two elements, then $\mathfrak{J}(a_1)\vee_{\mathscr{B}}\mathfrak{J}(a_2)=\mathfrak{J}(a_1)\oplus\mathfrak{J}(a_2)$ for $a_1\neq a_2$. This definition makes sense since $\mathfrak{J}(a_1)\oplus\mathfrak{J}(a_2)$ is well defined for all $a_1,a_2\in\mathscr{A}_0$ with $a_1\neq a_2$ and since $\mathfrak{J}(a_1)\neq\mathfrak{J}(a_2)$ for all $a_1,a_2\in\mathscr{A}_0$ with $a_1\neq a_2$. If $\mathscr{A}_0$ contains exactly two elements, then $\mathfrak{J}(a_1)\vee_{\mathscr{B}}\mathfrak{J}(a_2)=\mathfrak{J}(a_1)\oplus\mathfrak{J}(a_2)\ominus\mathfrak{J}(0_{\mathscr{A}})$ for $a_1\neq a_2$. This definition makes sense since $\mathfrak{J}(a_1)\oplus\mathfrak{J}(a_2)\ominus\mathfrak{J}(0_{\mathscr{A}})$ is well defined for all $a_1,a_2\in\mathscr{A}_0$ with $a_1\neq a_2$ and since $\mathfrak{J}(a_1)\neq\mathfrak{J}(a_2)$ for all $a_1,a_2\in\mathscr{A}_0$ with $a_1\neq a_2$.

The *full D-posets* also discussed in Ref. 37 are trivially contained in the class of admissible Boolean lattices defined in Definition 3.

From Theorem 4 and our Definition 5 of the implication relation between effect histories it follows immediately that if e_1 and e_2 are homogeneous effect histories such that $e_1\Rightarrow_{\varrho}e_2$ in the sense of Ref. 37, then also $e_1\Rightarrow_{\varrho}e_2$ in the sense of Definition 5.

Thus, Theorem 4 clearly shows that Rule 3 is indeed a generalization of Rule 2 stated in Ref. 37.

IV. SUMMARY

We now summarize our discussion by stating the general axioms for a generalized quantum theory based on our generalized history concept. This subsection parallels the discussion in Ref. 21.

(1) The space $\mathfrak{U}$ of general history propositions.
  (a) The space $\mathfrak{U}$ carries a canonical D-poset structure denoted by $\oplus$.
    (i) In this work $\mathfrak{U}$ is given by $\mathfrak{E}^{\otimes}_{\mathrm{fin}}(\mathbb{H})$.

(2) The space $\mathscr{U}$ of history filters or homogeneous histories.
  (a) $\mathscr{U}$ is the space of the basic physical properties of a physical system with a direct physical interpretation. An element of $\mathscr{U}$ is a time-ordered sequence of one-time propositions about the system. There exists a map F mapping the elements of $\mathscr{U}$ to a D-poset $\mathfrak{E}$. Here $\mathfrak{E}$ can be interpreted as the set of (equivalence classes of) one-time propositions.
    (i) In this work $\mathscr{U}$ equals the space of homogeneous effect histories of the first kind $\mathscr{U}=\mathbb{E}_{\mathrm{fin}}(\mathbb{H})$, cf. Definition 1; $\mathfrak{E}$ is given by $\mathfrak{E}(\mathbb{H})$ and F is given by $F(u)=C_{t_0}(u)^{\dagger}C_{t_0}(u)$.
  (b) $\mathscr{U}$ is a partially ordered set with unit history 1 and null history 0.
  (c) There exists an order preserving map $\tau:\mathscr{U}\to\mathfrak{U}$, i.e., $\tau(\mathscr{U})\subset\mathfrak{U}$.
    (i) In this work τ is given by σ_{fin}.
  (d) $\mathscr{U}$ is a partial semigroup with composition law $\circ$, cf. Ref. 21. Here $a\circ b$ is well-defined if $t_f(a)<t_i(b)$. In this case we say that *a proceeds b* or that *b follows a*. Further, $1\circ a=a\circ 1=a$ and $a\circ 0=0\circ a=0$. If $a\circ b$ is defined, then $a\circ b=a\wedge b$, in particular the right-hand side is well defined.
  (e) The partial ordering on $\mathscr{U}$ induces a partial unary operation $\neg$(complementation) and two

partial binary operations $\wedge$ and $\vee$ (meet and join) on $\mathscr{U}$.

(3) The space of decoherence functionals.
   (a) A decoherence functional is a map $d:\mathfrak{U}\times\mathfrak{U}\to\mathbb{C}$ which satisfies for all $\alpha,\alpha',\beta\in\mathfrak{U}$
      (i) $d(\alpha,\alpha)\in\mathbb{R}$ and $d(\alpha,\alpha)\geqslant 0$;
      (ii) $d(\alpha,\beta)=d(\beta,\alpha)^*$;
      (iii) $d(1,1)=1$;
      (iv) $d(0,\alpha)=0$, for all α;
      (v) $d(\alpha_1\oplus\alpha_2,\beta)=d(\alpha_1,\beta)+d(\alpha_2,\beta)$ for all $\alpha_1,\alpha_2,\beta\in\mathfrak{U}$ for which $\alpha_1\oplus\alpha_2$ is well defined.
   (b) In Ref. 37 it was possible to explicitly construct the decoherence functional on all inhomogeneous effect histories considered. In this work we have no explicit construction of the decoherence functional on $\mathfrak{E}^{\otimes}_{\mathrm{fin}}(\mathbb{H})$. Only its existence is known by Theorem 1.

(4) The physical interpretation.
   (a) The physically interesting subsets of $\mathfrak{U}$ are the ''admissible'' Boolean sublattices $\mathscr{B}$ of $\mathfrak{U}$ (see Definition 3) on which a positive valuation $\mathfrak{M}$ can be defined with values in $\mathfrak{U}$ such that for every $u\in\mathscr{B}$ the value $\mathfrak{M}(u)$ does not depend upon the particular ''admissible'' Boolean lattice $\mathscr{B}$ chosen.
   (b) The map $\mathfrak{M}$ ''lifts'' the lattice structure of $\mathscr{B}$ to the D-poset structure of $\mathfrak{U}$ and every decoherence functional on $\mathfrak{U}$ induces a consistency functional on $\mathscr{B}$.
   (c) The decoherence functional induces a probability measure on the consistent (wrt the decoherence functional) ''admissible'' Boolean sublattices of $\mathfrak{U}$.
   (d) On the ''admissible'' Boolean sublattices of $\mathfrak{U}$ decoherence functional defines a partial logical implication which allows us to make logical inferences.
   (e) The description of a physical system and reasoning in terms of elements of $\mathfrak{U}$ (homogeneous effect histories of the first kind) is only indirectly possible by using the map $\tau:\mathscr{U}\to\mathfrak{U}$.
   (f) While homogeneous effect histories have a direct physical interpretation in terms of time sequences of physical properties, inhomogeneous (effect) histories have no such direct interpretation. We tentatively suggest, however, that they may be interpreted as representatives of *unsharp quantum events*, i.e., events which cannot be associated with some fixed time, but which are smeared out in time.

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Greechie diagrams, nonexistence of measures in quantum logics, and Kochen–Specker-type constructions

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We use Greechie diagrams to construct finite orthomodular lattices ''realizable'' in the orthomodular lattice of subspaces in a three-dimensional Hilbert space such that the set of two-valued states is not ''large'' (i.e., full, separating, unital, nonempty, resp.). We discuss the number of elements of such orthomodular lattices, of their sets of (ortho)generators and of their subsets that do not admit a ''large'' set of two-valued states. We show connections with other results of this type. © *1996 American Institute of Physics.* [S0022-2488(96)00409-4]

I. INTRODUCTION

Quantum logic, as it has been pioneered by Birkhoff and von Neumann,[1] is usually derived from Hilbert space. There, the logical primitives, such as propositions and the logical operators ''and,'' ''or,'' and ''not'' are defined by Hilbert space entities. For instance, consider the three-dimensional, real Hilbert space $\mathbf{R}^3$ with the usual scalar product $(v,w):=\Sigma_{i=1}^{3}v_i w_i$, $v,w\in\mathbf{R}^3$. There, any proposition is identified with a subspace of $\mathbf{R}^3$. For instance, the zero vector corresponds to a false statement. Any line spanned by a nonzero vector corresponds to the statement that the physical system is in the pure state associated with the vector. Any plane formed by the linear combination of two (noncolinear) vectors v,w corresponds to the statement that the physical system is either in the pure state v or in the pure state w. The whole Hilbert space $\mathbf{R}^3$ corresponds to the tautology (true propositions). The logical ''and'' operation is identified with the set theoretical intersection of two propositions; e.g., with the intersection of two lines. The logical ''not'' operation, or the ''complement,'' is identified with taking the orthogonal subspace; e.g., the complement of a line is the plane orthogonal to that line.

In this top-down approach, one arrives at a propositional calculus that resembles the classical one, but differs from it in several important aspects. It has a non-Boolean, i.e., nondistributive, algebraic structure. Furthermore, as has first been pointed out by Kochen and Specker in the context of partial algebras,[2–4] there exist certain *finite* sets of lines, such that the associated propositional structure cannot be classically embedded. That is, there does not exist any classical, i.e., two-valued, measure that could be interpreted as the fact that propositions are either ''true'' (≡measure value 1) or ''false'' (≡measure value 0). The Kochen and Specker original construction used 117 lines. The number of lines has been subsequently reduced.[5–8] These constructions are examples of propositional structures without any two-valued measures.

In this paper we shall deal with the following questions: which orthomodular structure—finite or infinite—underlies the Kochen–Specker construction. The question can be approached from two different viewpoints: (i) Which *minimal* set of propositions generates some Kochen–Specker-type configurations? By ''generate'' we mean the construction of the propositional structure con-

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taining it. (ii) What is the *minimal propositional structure* containing some sort of Kochen–Specker-type configuration? In particular, is it finite or infinite?

II. BASIC NOTIONS

The following definition gives two main concepts of a propositional structure.

Definition 2.1: An *orthomodular poset* is a structure $(P,\leqslant,',0,1)$ fulfilling the following conditions.

(1) $(P,\leqslant)$ is a partial ordered set such that $0\leqslant a\leqslant 1$ for every $a\in P$.

(2) $':P\to P$ is an orthocomplementation, i.e., for every $a, b\in P$: (a) $a''=a$; (b) $a\leqslant b$ implies $b'\leqslant a'$; (c) $a\vee a'=1$.

(3) If $a\leqslant b'$ then the supremum $a\vee b$ exists in P.

(4) If $a\leqslant b$ then there is an element $c\in L$ such that $c\leqslant a'$ and $b=a\vee c$ (the orthomodular law).

An *orthomodular lattice* is an orthomodular poset that is a lattice.

Elements a, b of an orthomodular poset are called *orthogonal* (denoted by $a\perp b$) if $a\leqslant b'$. A subset O of an orthomodular poset is called *orthogonal* if every pair of its elements is orthogonal.

Definition 2.2: Let P_1, P_2 be orthomodular posets. P_1 is *orthorepresentable* in P_2 if there is a mapping (called *orthoembedding*) $h: P_1\to P_2$ such that for every $a, b\in P_1$, (1) $h(0)=0$, (2) $h(a')=h(a)'$, (3) $a\leqslant b$ if and only if $h(a)\leqslant h(b)$, and (4) $h(a\vee b)=h(a)\vee h(b)$ whenever $a\perp b$.

P_1 is *representable* in P_2 if there is a mapping (called *embedding*) $h: P_1\to P_2$ such that h is orthoembedding, and for every $a, b\in P_1$, (4′) $h(a\vee b)=h(a)\vee h(b)$.

The set $h(P_1)$ is then called an *(ortho)representation* of P_1 in P_2.

A *suborthoposet* (*subortholattice*, resp.) is a subset such that the identity mapping is orthoembedding (embedding, resp.).

Boolean subalgebra of an orthomodular poset is a suborthoposet that is a Boolean algebra. *Block* is a maximal Boolean subalgebra.

As we will see later, there are lattices L_1, L_2 such that L_1 is a suborthoposet but not a subortholattice of L_2. On the other hand, a suborthoposet of an orthomodular lattice need not be a lattice.

Definition 2.3: Let L be an orthomodular lattice, G, $\overline{L\subseteq P}$ and let us denote by $L(G)$ [$P(G)$, resp.] the least subortholattice (suborthoposet, resp.) of L containing G. We say that G *generates* (*orthogenerates*, resp.) L if $L\subseteq L(G)$ [$L\subseteq P(G)$, resp.].

$P(G)$ and $L(G)$ can be explicitly defined by the following process: $P(G)=\cup_{n=0}^{\infty}P_n(G)$, $L(G)=\cup_{n=0}^{\infty}L_n(G)$, where $P_0(G)=L_0(G)=G$ and, for every natural number, n:

$$L_{n+1}(G)=\{\vee O;\ O \text{ is a finite subset of } L_n(G)\cup L_n(G)'\},$$

$$P_{n+1}(G)=\{\vee O;\ O \text{ is a finite orthogonal subset of } P_n(G)\cup P_n(G)'\}$$

(M' denotes the set $\{a';a\in M\}$). Hence, every countable set G generates a countable subortholattice and orthogenerates a countable suborthoposet.

A very useful tool for constructing and representing some orthomodular posets is the so-called Greechie diagram.

Definition 2.4: A *diagram* is a pair (V,E), where $V\neq\emptyset$ is a set of *vertices* (usually drawn as points) and $E\subseteq\exp V\setminus\{\emptyset\}$ is a set of *edges* (usually drawn as line segments connecting corresponding points).

Let $n\geqslant 2$ be a natural number. A *loop* of order n in a diagram (V,E) is a sequence $(e_1,\ldots,e_n)\in E^n$ of mutually different edges such that there are mutually different vertices $v_1,\ldots,v_n$ with $v_i\in e_i\cap e_{i+1}$ $(i=1,\ldots,n,\ e_{n+1}=e_1)$.

A *Greechie diagram* is a diagram fulfilling the following conditions.

FIG. 1. Examples of diagrams that are not Greechie diagrams.

(1) Every vertex belongs to at least one edge.
(2) If there are at least two vertices then every edge is at least a two-element.
(3) Every edge that intersects with another edge is at least a three-element.
(4) Every pair of different edges intersects in at most one vertex.
(5) There is no loop of order 3.

Some examples of diagrams that are not Greechie diagrams are given in Fig. 1—these examples violate exactly one of conditions (2)–(5) in the above definition. (We usually do not denote one-element edges.) The condition (4) states that in Greechie diagrams there is no loop of order 2.

Before we present the representation theorem let us recall that an *atom* in an orthomodular poset P is a minimal element of $P\setminus\{\emptyset\}$.

Theorem 2.5: *For every Greechie diagram with only finite edges there is exactly one (up to an isomorphism) orthomodular poset, such that there are one-to-one correspondences between vertices and atoms and between edges and blocks that preserve incidence relations. A Greechie diagram does not contain any loop of order 4 if and only if the corresponding orthomodular poset is a lattice.*

The proof can be found, e.g., in Ref. 9. Let us reserve the notion *Greechie logic* for an orthomodular poset that can be represented by a Greechie diagram with only finite edges. It is easy to see that such an orthomodular poset does not contain any infinite chain, hence every element is a supremum of a finite orthogonal set of atoms.

Let us remark that there are finite orthomodular posets not representable by Greechie diagrams—intersections of blocks might be greater than a four-element Boolean subalgebra, and hence the condition (4) of Definition 2.4 cannot be fulfilled. On the other hand, every orthomodular poset with only finite and at most three atomic blocks (the case we are interested about) is a Greechie logic.

We will have a special interest about the following example.

Definition 2.6: The three-dimensional *Hilbert logic* H_3 is the orthomodular lattice of linear subspaces of $\mathbf{R}^3$. The ordering is given by inclusion and the orthocomplementation is given by $a'=\{v\in\mathbf{R}^3;\ v\perp a\}$ for every $a\in H_3$.

The least element of H_3 is $0=\{(0,0,0)\}$, the greatest element of H_3 is $1=\mathbf{R}^3$. Moreover, $a\wedge b=a\cap b$ and $a\vee b=\mathrm{Sp}(a\cup b)$ for every $a,b\in H_3$, where $\mathrm{Sp}(G)$ is the *span* of G in $\mathbf{R}^3$. [We will usually omit unnecessary parentheses, e.g., Sp(1,0,0) denotes Sp({(1,0,0)}).]

Every element of $H_3\setminus\{0,1\}$ is either an atom or a coatom, every block in H_3 is finite and at most a three-element, every suborthoposet P of H_3 is a Greechie logic and is uniquely determined by the set $A_1(P)$ of its one-dimensional atoms (lines):

$$P=\{0,1\}\cup A_1(P)\cup A_1(P)'.$$

(There might be also two-dimensional atoms in P, e.g., if P is a four-element.) Moreover, for every set G of lines in H_3 the set of lines of the orthomodular lattice $L(G)$ [orthomodular poset $P(G)$, resp.] generated (orthogenerated, resp.) by G can be expressed as follows: $A_1(P(G))=\cup_{n=0}^{\infty}P_n$, $A_1(L(G))=\cup_{n=0}^{\infty}L_n$, where $P_0=L_0=G$ and, for every natural number n,

$$L_{n+1}=L_n\cup\{(a\vee b)';a,b\in L_n\},$$

$$P_{n+1}=P_n\cup\{(a\vee b)';a,b\in P_n,\ \text{such that}\ a\perp b\}.$$

III. TWO-VALUED STATES AND GREECHIE DIAGRAMS

Let us present the main definition.

Definition 3.1: Let P be an orthomodular poset and let $G\subset P$. A *state* s on G is a mapping s: $P\rightarrow[0,1]$, such that

(1) $s(0)=0$,

(2) $s(a)\leqslant s(b)$ whenever $a,b\in G$ with $a\leqslant b$;

(3) $\Sigma_{a\in O}s(a)\leqslant 1$ for every orthogonal set $O\subset G$; and

(4) $\Sigma_{a\in O}s(a)=1$ for every orthogonal set $O\subset G$ with $\vee O=1$.

A *two-valued state* is a state with values in $\{0,1\}$.

If $G=P$ then conditions (1)–(2) follow from conditions (3)–(4) and from the orthomodular law and, moreover, $s(a')=1-s(a)$ for every $a\in P$.

The Kochen–Specker construction gives an example of a propositional structure without any two-valued state. We will use a more general attempt and will ask whether there is a propositional structure without ''enough'' two-valued states. Originally, ''enough'' meant ''at least one.'' We will also use the following properties of state space, which are important in quantum logic theories.

Definition 3.2: Let P be an orthomodular poset and let $G\subseteq P$. A set S of states on G is called *unital* if for every $a\in G\backslash\{0\}$ there is a state $s\in S$ such that $s(a)=1$;

separating if for every $a,b\in G$ with $a\neq b$ there is a state $s\in S$ such that $s(a)\neq s(b)$;

full if for every $a,b\in G$ with $a\not\leqslant b$ there is a state $s\in S$ such that $s(a)>s(b)$.

Existence of a unital set of states means that every proposition that is not a tautology is sometimes false. Existence of a separating set of states means that a different propositions are distinguishable. Existence of a full set of two-valued states means that if some proposition does not imply another, then there is such a state that the first is true while the second is not. These properties are largely studied. An orthomodular poset with a full set of two-valued states is called a *concrete logic* (see, e.g., Ref. 10), an orthomodular poset with a separating set of two-valued states is called a *partition logic*—this notion is within orthomodular posets equivalent to the notion of *automaton logic* (see, e.g., Refs. 11–14).

It is easy to see that a full set of states is separating and that a separating set of two-valued states is unital. Before we give examples demonstrating differences in the above-defined notions let us give some criteria, how we can verify whether an orthomodular poset given by a Greechie diagram has ''enough'' two-valued states.

Definition 3.3: Let P be an orthomodular poset and let A be the set of atoms in P. A *weight* w on A is a mapping w: $A\rightarrow[0,1]$, such that $\Sigma_{a\in O}w(a)=1$ for every maximal orthogonal set $O\subseteq P$. A *two-valued* weight is a weight with values in $\{0,1\}$.

Lemma 3.4: Let P be a Greechie logic and let A be the set of atoms in P. Then there is a one-to-one correspondence between two-valued states s on P and two-valued weights w on A given by $w=s|A$.

Proof: Obvious.

Due to this correspondence we may (and will) identify states and weights and study only the values of states on the set of atoms. Since every maximal orthogonal set of atoms corresponds uniquely to a block, we need only to check that the sum of values of a state on every edge in a Greechie diagram is equal to 1.

Proposition 3.5: Let P be a Greechie logic and let A be the set of atoms in P. Then P has a full set of two-valued states (i.e., P is a concrete logic) if and only if for every pair a_1, $a_2\in$P *of different nonorthogonal atoms there is a two-valued weight w on A such that* $w(a_1)=w(a_2)=1$.

Proof⇒: Let $a_1, a_2 \in A$, such that $a_1 \not\perp a_2$. Then $a_1 \leqslant a_2'$ and there is a two-valued state s on P such that $1 = s(a_1) > s(a_2') = 0$. Hence, $s(a_2)=1$ and, according to Lemma 3.4, it suffices to take $w=s|A$.

⇐*:* Let $b_1, b_2 \in P$ such that $b_1 \not\leqslant b_2$, i.e., $b_1 \not\perp b_2'$. There are orthogonal sets $A_1, A_2 \neq \emptyset$ of atoms in P such that $b_1 = \vee A_1$, $b_2' = \vee A_2$. According to Lemma 3.4, it suffices to prove that there are atoms $a_1 \in A_1$, $a_2 \in A_2'$ and a weight w on A such that $w(a_1)=w(a_2)=1$. Let us suppose first that $A_1 \cap A_2 = \emptyset$. Then there are atoms $a_1 \in A_1$ and $a_2 \in A_2$ such that $a_1 \neq a_2$ and $a_1 \not\perp a_2$ and, due to our assumption, a weight w on A such that $w(a_1)=w(a_2)=1$. Let us suppose now that $A_1 \cap A_2 \neq \emptyset$. Then there is an atom $a_1 \leqslant b_1, b_2'$ and either there is an atom $a_2 \neq a_1$ such that $a_1 \not\perp a_2$, or $a_1 \perp a$ for every atom $a \neq a_1$. In both cases there is a two-valued weight w on A such that $w(a_1)=1$; in the first case due to our assumption and in the second case we can put $w(a)=1$ iff $a=a_1$.

The situation for a separating set of states is much more complicated and we will state a criterion in a special case (which is in our interest here).

Proposition 3.6: Let P be a Greechie logic with, at most three atomic blocks and let A be the set of atoms in P. Then the set of two-valued states on P is separating (i.e., P is a partition logic) if and only if the following conditions hold.

(1) *For every atom $a \in P$ there is a two-valued weight w on A such that $w(a)=1$.*

(2) *For every pair $a_1, a_2 \in$ P of different nonorthogonal atoms there are two-valued weights w_+, w_- on A such that $w_+(a_1)=w_+(a_2)$ and $w_-(a_1) \neq w_-(a_2)$.*

Proof ⇒: Let $a \in A$. Then $a \neq 0$ and there is a two-valued state s on P such that $1=s(a) > s(0)=0$. Let $a_1, a_2 \in A$ such that $a_1 \neq a_2$ and $a_1 \not\perp a_2$. Then also $a_1 \neq a_2'$ and there are two-valued states s_-, s_+ on P such that $1=s_-(a_1) > s_-(a_2)=0$, $1 = s_+(a_1) > s_+(a_2') = 0$, i.e., $s_+(a_1)=s_+(a_2)$. The rest follows from Lemma 3.4.

⇐*:* Let $b_1, b_2 \in P$ such that $b_1 \neq b_2$. Since every element of $P \backslash \{0,1\}$ is either an atom or a coatom, there are atoms $a_1, a_2 \in P$ such that $b_1 \in \{0, a_1, a_1', 1\}$ and $b_2 \in \{0, a_2, a_2', 1\}$. If $a_1 = a_2$ then there are two-valued weights w_+, w_- on A such that $w_+(a_1)=1$ and $w_-(a_1)=0$. If $a_1 \neq a_2$ then there are two-valued weights w_+, w_- on A such that $w_+(a_1)=w_+(a_2)$ and $w_-(a_1) \neq w_-(a_2)$. In both cases there are, according to Lemma 3.4, two-valued states s_+, s_- on P such that either $s_+(b_1) \neq s_+(b_2)$ or $s_-(b_1) \neq s_-(b_2)$.

Let us present a lemma, which might simplify to verify criteria in Proposition 3.6.

Lemma 3.7: Let P be a Greechie logic and let A be the set of atoms in P. If W is an at least three-element set of two-valued weights on A such that $\{w^{-1}(1); w \in W\}$ is a partition of A, then

(1) for every atom $a \in A$ there is a weight $w \in W$ such that $w(a)=1$;

(2) for every pair $a_1, a_2 \in A$ there is a weight $w \in W$ such that $w(a_1)=w(a_2)$.

Proof: Obvious.

Let us remark that in Greechie diagrams it suffices to use the above conditions for every connected subdiagram separately (weights behave independently on nonconnected subgraphs). In terms of orthomodular posets we can use the following important notion.

Definition 3.8: Let $\mathscr{P}$ be a set of orthomodular posets such that $P_1 \cap P_2 = \{0,1\}$ for every P_1, $P_2 \in \mathscr{P}$ with $P_1 \neq P_2$. The *horizontal sum* $\Sigma_{P \in \mathscr{P}} P$ is defined as $(\cup_{P \in \mathscr{P}} P, \cup_{P \in \mathscr{P} \leqslant P}, \cup_{P \in \mathscr{P}} {}'^{P}, 0, 1)$.

More generally, we speak about the horizontal sum of P_i, $i \in I$. It is an abbreviation for saying that we take disjoint representations P_i of P_i (e.g., $\{i\} \times P_i$), identify all 0_i ($i \in I$) and all 1_i ($i \in I$), and take $\Sigma_{i \in I} P_i$. It is easy to see that a horizontal sum of orthomodular posets (orthomodular lattices, resp.) is an orthomodular poset (orthomodular lattice, resp.) and that a set of states is nonempty (unital, separating, full, resp.) on a horizontal sum if and only if it is nonempty (unital, separating, full, resp.) on every horizontal summand.

In a Greechie diagram every connected subdiagram corresponds to a horizontal summand. (In particular, every finite two-atomic block is a horizontal summand.) On the other hand, the horizontal sum of Greechie logics is a Greechie logic with the Greechie diagram, which is a (disjoint)

union of summands with only one exception—we lose isolated vertices (these correspond to the trivial orthomodular poset {0,1}).

The notion of a horizontal sum is a special kind of the notion of *pasting*. We are not interested here in a general setting (see, e.g., Ref. 9), thus we describe only special cases showing how we can obtain a new Greechie logic using this process. Greechie diagram of the *pasting of Greechie logics* P_i $(i\in I)$ *for atoms* $a_i\in P_i$ $(i\in I)$ we obtain as follows: we take the disjoint union of Greechie diagrams of $P_i(i\in I)$, identify vertices corresponding to a_i $(i\in I)$ and, if some a_i $(i\in I)$ belong to a two-atomic block, we delete necessary vertices corresponding to such a_i' such that the condition (3) of Definition 2.4 is fulfilled. Greechie diagram of the *pasting of Greechie logics* P_i $(i\in I)$ *for blocks* $B_i\subseteq P_i$ $(i\in I)$ with the same number of atoms we obtain as follows: we take the disjoint union of Greechie diagrams of P_i $(i\in I)$ and identify edges corresponding to B_i $(i\in I)$ (i.e., we identify also atoms in these blocks.) It is easy to see that such pastings of (lattice) Greechie logics are (lattice) Greechie logics.

The notion of a horizontal sum is also related to the following notion.

Definition 3.9: Let P be an orthomodular poset. The *distance* d on P is a mapping d: $P\times P\to\mathbf{N}\cup\{\infty\}$, defined by

$d(a,b)=\inf\{n\in\mathbf{N}$; there are blocks $B_1,\ldots,B_n$ in P such that $B_i\cap B_{i+1}\neq\{0,1\}$ for $i=0,\ldots,n$, $B_0=\{a\}$, $B_{n+1}=\{b\}\}$.

The distance function defines the largest decomposition of P into horizontal summands—the least summands are maximal subsets of $P\setminus\{0,1\}$ of elements with finite distances joined with $\{0,1\}$.

The following result we will use in the sequel.

Proposition 3.10: Every Greechie logic without any loop has a full set of two-valued states.

Proof: The distance function on P decompose P into the horizontal sum $\Sigma_{i\in I}P_i$, such that the distance of every pair of elements in every summand is finite. It suffices to prove fullness for every summand. According to Proposition 3.5, it suffices, for every $i\in I$ and for every pair a_1, a_2 of different nonorthogonal atoms in P_i, to find a weight w on the set A of atoms in P_i, such that $w(a_1)=w(a_2)=1$. Let us put $A_n=\{a\in A;d(a,a_1)=n\}$ for every natural number n and let us define w by induction.

I. $w(a_1)=1$.

II. Let us suppose that there is a natural number $n\geqslant 0$ such that w is defined on $A_0\cup\cdots\cup A_n$. Every element of A_{n+1} belongs to some block B in P_i such that $B\cap A_n\neq\emptyset$. For every such block B we have $B\cap A_n=\{a_B\}$. If $w(a_B)=1$, we put $w|B\cap A\setminus A_n=0$. If $w(a_B)=0$, we can choose (B has at least three atoms) properly a $b_B\in B\cap A\setminus A_n$ and put $w(b_B)=1$, $w|B\cap A\setminus b_B\}=0$. Properly means that if $n=d(a_2,a_1)-2$ then b_B is chosen such that it does not belong to the same block as a_2 and if $n=d(a_2,a_1)-1$ then $b_B=a_2$.

Let us present examples demonstrating differences in properties of state space.

Proposition 3.11: Let us consider the following conditions.

(1) The set of two-valued states is full.

(2) The set of two-valued states is separating but not full.

(3) The set of two-valued states is unital but not separating.

(4) The set of two-valued states is nonempty but not unital.

(5) The set of two-valued states is empty.

For each of the above conditions there is an orthomodular lattice with only finite three-atomic blocks, which fulfills it.

Proof: (1) See Fig. 2.1. It is a Boolean algebra, which obviously has a full set of two-valued states.

(2) See Fig. 2.2. For every two-valued state s we have $s(a)+s(b)\leqslant(1-s(c_a)+1-s(d_a)+1-s(c_b)+1-s(d_b))/2=(2-s(c)-s(d))/2\leqslant 3/2$. Hence $s(a)+s(b)\leqslant 1$ and, according to Proposition 3.5, this orthomodular lattice has not a full set of two-valued states. The set $S_1=\{s_1,s_2,s_3\}$ of states given in Fig. 3 fulfills conditions of Lemma 3.7. It can be checked that the set of all two-valued states ''symmetric'' to some state from S distinguish different nonor-

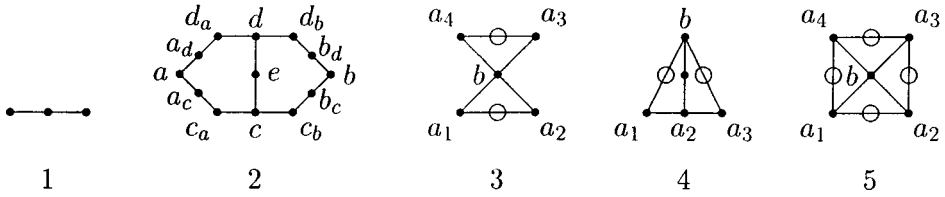

FIG. 2. Greechie diagrams of orthomodular posets with finite three-atomic blocks demonstrating differences of state spaces ($a\!\multimap\!\ominus\!\multimap\!b$ denotes diagram 2).

thogonal atoms. Hence, the set of two-valued states fulfills conditions of Proposition 3.6. A smaller example of a separating set of states is given in Fig. 3. We can express this orthomodular lattice as a partition logic on a six-element set of these states—see Fig. 4.1. (Compare with the representation on the 14-element set of states in Ref. 14).

(3) See Fig. 2.3. Let us use the previous result. For every two-valued state s with $s(a_1)=1$ we obtain $s(a_2)=s(b)=0$, hence $s(a_4)=1$. Using the symmetry we obtain $s(a_1)=s(a_4)$ for every two-valued state, hence the set of two-valued states is not separating. The unitality can be verified routinely.

(4) See Fig. 2.4. For every two-valued state s there is an $i\in\{1,2,3\}$ such that $s(a_i)=1$ and therefore $s(b)=0$. Hence, the set of two-valued states is not unital. Existence of a two-valued state can be verified routinely. (Let us note that if we paste ''sides of the triangle'' not only for b but for the whole block we obtain a smaller example with 25 atoms.)

(5) See Fig. 2.5. According to part (3) of this proof, $s(a_1)=s(a_2)=s(a_3)=s(a_4)$ for every two-valued state s. Hence all these values are equal to 0 and $s(b)=1$. The desired example we obtain by pasting this orthomodular lattice with the orthomodular lattice from Fig. 2.4 for b's or, more effectively, by pasting for blocks containing b's and a_2's.

IV. SUBORTHOLATTICES OF H_3

There are only several types of finite subortholattices of H_3. The following characterization of finite subortholattices of H_3 seems to be in a common knowledge (see, e.g., Ref. 15, Example 1.5.3), but we do not know a proper reference for its proof.

Lemma 4.1: Let L be a subortholattice of H_3 and let lines a_1, a_2, a_3, $b\in L$ be such that a_1, a_2, a_3 are mutually orthogonal and $b\not\perp a_1$, a_2, a_3. Then there is a line $c\in L$ such that $c\not\perp a_3$ and the angle $\angle(c,a_3)$ is greater than $\angle(b,a_3)$.

Proof: Let us choose the system of coordinates such that $a_1=\mathrm{Sp}(1,0,0)$, $a_2=\mathrm{Sp}(0,1,0)$, $a_3=\mathrm{Sp}(0,0,1)$, $b=\mathrm{Sp}(x,y,z)$, such that $x,y,z>0$. Since L is a subortholattice of H_3, the following elements belong to L:

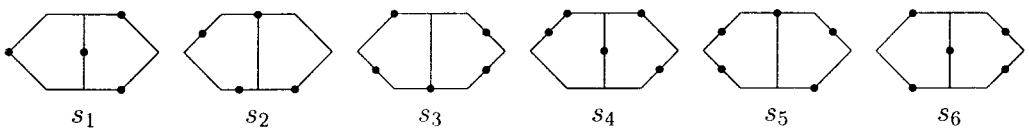

FIG. 3. Separating set of two-valued states on an orthomodular lattice from Fig. 2.2. (only atoms in which the corresponding state is equal to 1 are marked).

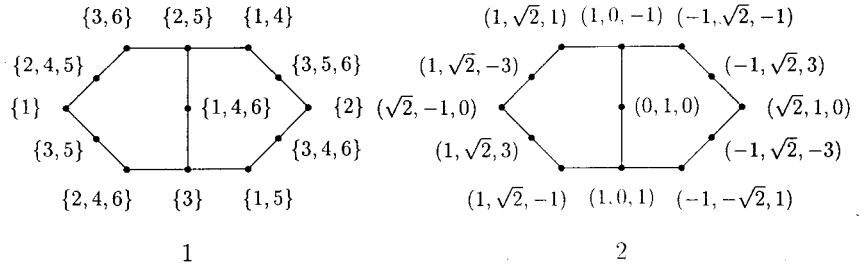

FIG. 4. Various representations of an orthomodular lattice from Fig. 2.2.

$$\overline{b} = (a_1 \vee a_2) \wedge b' = \mathrm{Sp}(y, -x, 0),$$

$$c = (a_1 \vee a_3) \wedge (b \vee \overline{b}) = \mathrm{Sp}(x + y^2/x, 0, z).$$

Hence,

$$0 < \cos\angle(c, a_3) = \frac{z}{\sqrt{(x + y^2/x)^2 + z^2}} < \frac{z}{\sqrt{x^2 + y^2 + z^2}} = \cos\angle(b, a_3).$$

Theorem 4.2: *Let $L \subset H_3$ be a finite orthomodular lattice. Then L is a subortholattice of H_3 if and only if exactly one of the following possibilities is fulfilled.*

(1) *$L = \{0,1\}$, i.e., L is a one-atomic Boolean algebra*;

(2) *$L = \{0, a, a', 1\}$ for some line $a \in H_3$, i.e., L is a two-atomic Boolean algebra.*

(3) *$L = \{0, a_1, a_2, a_3, a_1', a_2', a_3', 1\}$ for some orthogonal set $\{a_1, a_2, a_3\}$ of lines in H_3, i.e., L is a three-atomic Boolean algebra.*

(4) *$L = \{0, a, a', 1\} \cup G \cup G' \cup \{a \vee b; b \in G\} \cup \{a' \wedge b'; b \in G\}$ for some line $a \in H_3$ and some at least two-element set G of mutually nonorthogonal atoms orthogonal to a, i.e., L is a finite pasting of at least two three-atomic Boolean algebras for a given atom.*

Proof: It is easy to see that each of these conditions excludes the others and gives a subortholattice of H_3. Let us suppose that there is a finite subortholattice L of H_3 that fulfills no condition (1)–(4), and seek a contradiction. There are three mutually nonorthogonal lines $a, b, c \in L$. Let $d_3 = (a \vee b)' \in L$. Since L is finite, there is a line $e \in L$ such that $\angle(e, d_3)$ is the greatest among all lines from L nonorthogonal to d_3. Since $a \not\perp b$ there is a $d_1 \in \{a, b\}$ such that $d_1 \not\perp e, e' \wedge d_3'$. Let us put $d_2 = d_1' \wedge d_2' \in L$. Hence, lines d_1, d_2, d_3 are mutually orthogonal and $e \not\perp d_1, d_2, d_3$. According to Lemma 4.1, there is an element $f \in L$ such that $f \not\perp d_3$ and $\angle(f, d_3) < \angle(e, d_3)$—this contradicts the selection of e.

Greechie diagrams of finite subortholattices of H_3 are given in Fig. 5.

Corollary 4.3: Every finite subortholattice of H_3 has a full set of two-valued states.

Proof: It follows from Theorem 4.2 and Proposition 3.10.

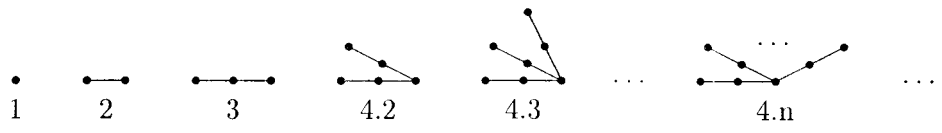

FIG. 5. Greechie diagrams of finite subortholattices of H_3.

As concerns infinite subortholattices of H_3, there is a countable subortholattice of H_3 without any two-valued states (e.g., generated by finite sets without any two-valued state—see Corollary 7.5). On the other hand, there are infinite subortholattices with a full set of two-valued states, e.g. infinite pastings of three-atomic Boolean algebras for a given atom [compare condition (4) of Theorem 4.2]. It seems to be an open problem whether there is an infinite subortholattice of H_3 that is not of this type and that has a two-valued state. Moreover, there might be an interesting connection between the nonexistence of a two-valued state and density in $\mathbf{R}^3$. This might give better insight into the nature of subortholattices of H_3 and the connection with the famous Gleason theorem,[16,10] which (among other things) states that there is no two-valued state on H_3.

It should be noted that Greechie diagrams of subortholattices of H_3 are relatively ''complex''—the distance of every pair of elements is at most 2 (every pair of different lines has a common orthogonal line). Hence, it is usually difficult to give a Greechie diagram of an infinite subortholattice of H_3.

V. REALIZABILITY IN H_3

The study of finite suborthoposets of H_3 is more complicated. We would like to know whether a Greechie logic is orthorepresentable in H_3. The first problem erases with the intrinsic geometrical structure of H_3.

Definition 5.1: Let P be an orthomodular poset. We say that P is *weakly realizable* in H_3 if there is a mapping h: $P\rightarrow H_3$, such that, for every $a,b\in P$,

(1) $h(0)=0$;

(2) $h(a')=h(a)'$,

(3) $h(a)\leqslant h(b)$ whenever $a\leqslant b$; and

(4) $h(a)\neq 0$ whenever $a\neq 0$.

If, moreover, the mapping h fulfills for every $a,b\in P$ the following occurs:

(4′) $h(a)\neq h(b)$ whenever $a\neq b$,

we say that P *is realizable*. The set $h(P)$ is called a (*weak*) *realization* of P in H_3.

Weak realizability means that all orthogonality relations remain true in the images, and, since every nonzero element has a nonzero image, if the set of two-valued states on $G\subseteq P$ is empty (not unital, resp.) then the set of two-valued states on $h(G)$ is empty (not unital., resp.), too. Realizability means that, moreover, the mapping is one to one. Hence, if the set of two-valued states on $G\subseteq P$ is not separating (full, resp.), then the set of two-valued states on $h(G)$ is not separating (full, resp.), too. A realization need not be a suborthoposet because a new orthogonal pairs might appear in the images.

Let us give a characterization of orthomodular posets weakly realizable in H_3.

Lemma 5.2: Let $P_{\mathscr{P}}$ be the pasting of a set $\mathscr{P}$ of orthomodular posets and let there is a mapping h: $P_{\mathscr{P}}\rightarrow H_3$ such that h(P) is a weak realization of P for every $P\in\mathscr{P}$. Then h($P_{\mathscr{P}}$) is a weak realization of $P_{\mathscr{P}}$ in H_3. In particular, every horizontal sum of orthomodular posets weakly realizable in H_3 is weakly realizable in H_3.

Proof: Obvious.

Proposition 5.3: An orthomodular poset is weakly realizable in H_3 if and only if every its block is finite and at most three-atomic.

Proof $\Rightarrow$*:* Every orthogonal set of nonzero elements in an orthomodular poset P corresponds to an orthogonal set of nonzero elements in H_3. Since such a set in H_3 is at most a three-element, every block of P is finite with at most three atoms.

$\Leftarrow$*:* Let P be an orthomodular poset with only finite, at most three-atomic blocks. Let us decompose P into the horizontal sum $\Sigma_{i\in I}P_i$ of minimal horizontal summands. Let us choose a line $l\in H_3$ and let us define a mapping h_i for every $i\in I$ as follows: $h(0)=0$, $h(1)=1$; if P_i is a four element, then let us take an atom $a_i\in P_i$ and put $h(a_i)=l$, $h(a_i')=l'$; if P_i has more than four elements then every block has three atoms, and we put $h(a)=l$, $h(a')=l'$ for every atom

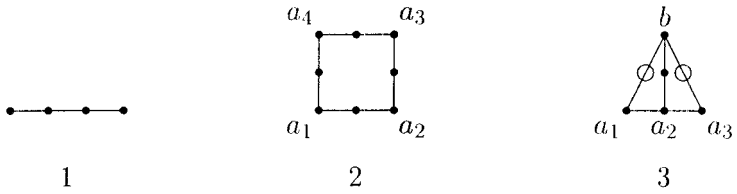

FIG. 6. Greechie diagrams of some orthomodular posets nonrealizable in H_3 (a•⊖•b is an abbreviation of the Greechie diagram in Fig. 2.2).

$a \in P_i$. It is easy to see that $h_i(P_i)$ is a weak realization of P_i in H_3 and that $\cup_{i \in I} h_i(P_i)$ is a weak realization of P in H_3.

The situation with realizability is more difficult and we do not know a characterization of it. Some results we will present in the next section. Let us now present another necessary condition.

Proposition 5.4: Every orthomodular poset realizable in H_3 is a lattice.

Proof: Let us suppose that P is an orthomodular poset with a loop of order 4 realizable in H_3 and seek a contradiction. There are nonzero mutually different elements $a_1 \perp a_2 \perp a_3 \perp a_4 \perp a_1$ in P (see Fig. 6.2). Since for every pair of different nonzero elements there is only one nonzero element in H_3 orthogonal to them, $a_1 = a_3$—a contradiction.

Examples of orthomodular posets nonrealizable in H_3 are given in Fig. 6. The first has a four-atomic block, the second is not a lattice. The third example is much more subtle and depends on the following intrinsic property of H_3.

Lemma 5.5: Let L be a realization of an orthomodular lattice given in Fig. 2.2. *Then $\angle(a,b) \in \langle \arccos 1/3, \pi/2)$. On the other hand, for every $\alpha \in \langle \arccos 1/3, \pi/2)$ there is a realization of L such that $\angle(a,b) = \alpha$.*

Proof [See also Ref. 17]: Let us choose a coordinate system such that $c = \mathrm{Sp}(1,0,0)$, $d = \mathrm{Sp}(0,1,0)$. Hence $e = \mathrm{Sp}(0,0,1)$. Since $c_a \perp c$ and $d_b \perp d$, there are $x, y \in \mathbf{R} \setminus \{0\}$ such that

$$c_a = \mathrm{Sp}(0,y,1), \quad d_b = \mathrm{Sp}(x,0,1).$$

Since $c_b \perp c$, c_a and $d_a \perp d$, d_b, $a \perp c_a$, d_a, and $b \perp c_b$, d_b, we obtain

$$c_b = \mathrm{Sp}(0,-1,y), \quad d_a = \mathrm{Sp}(-1,0,x),$$

$$a = \mathrm{Sp}(xy,-1,y), \quad b = \mathrm{Sp}(-1,xy,x).$$

Thus, using an elementary calculus,

$$\cos\angle(a,b) = \frac{|xy|}{\sqrt{(1+x^2+x^2y^2)(1+y^2+x^2y^2)}} \in \left\langle 0, \frac{1}{3} \right\rangle.$$

For an arbitrary $\alpha \in (\arccos 1/3, \pi/2)$ we can solve this equation and obtain, e.g.,

$$x = y = \sqrt{\frac{1/\cos\,\alpha - 1}{2} - \sqrt{\left(\frac{1/\cos\,\alpha}{2}\right)^2 - 1}}.$$

For $\alpha = \arccos 1/3$ we have exactly one realization (two different solutions given by the symmetry of the Greechie diagram). In Fig. 4.2 there is an example such that symmetries of the

realization are easily seen (with respect to the axis o of a and b and to planes $\mathrm{Sp}\{a,b\}$, $\mathrm{Sp}\{o,a\times b\}$). For $\alpha\in(\arccos 1/3,\pi/2)$ we have two different realizations (each symmetric with respect to the axis of a and b).

The orthomodular lattice given in Fig. 6.3 is not realizable, because for every triple a_1, a_2, $a_3\in H_3$ of mutually orthogonal nonzero elements and for every $b\in H_3$ there is an $i\in\{1,2,3\}$ such that $\angle(b,a_i)\leqslant\arccos 1/\sqrt{3}$.

Let us note that in Ref. 17 the above lemma is also stated for $\alpha=\pi/2$. This is not true, because then either $x=0$ or $y=0$ and we obtain only a weak realization.

VI. SUBORTHOPOSETS OF H_3

We would like to present examples of orthomodular lattices orthorepresentable in H_3. To ensure that an orthomodular lattice is orthorepresentable in H_3 it suffices to find its realization in H_3 such that there are not ordered (orthogonal, resp.) pairs other than it was intended, e.g., it can be easily verified that an orthomodular lattice given in Fig. 2.2 is orthorepresentable in H_3 (see Fig. 4.2). We present partial results that orthomodular lattices are orthorepresentable (realizable, resp.) in H_3. The idea of their proofs is that we can find uncountable many (continuum) weak realizations while only for a countable many of them some images coincide or, in case of orthorepresentability, give a new ordered (orthogonal, resp.) pair.

We show that there is a large class of infinite suborthoposets of H_3 with a full set of two-valued states.

Proposition 6.1: Every horizontal sum of countable many countable orthomodular lattices orthorepresentable (realizable, resp.) in H_3 is orthorepresentable (reliazable, resp.) in H_3.

Proof: It suffices to prove this proposition for two summands (we can proceed by induction). Let L_1, L_2 be their orthorepresentations (realizations, resp.) in H_3. It suffices to prove that we can rotate L_2 to L_2 such that $a_1\not\perp za_2$ and $a_2\not\perp a_1$ for every $a_1\in L_1\backslash\{0,1\}$ and for every $a_2\in L_2\backslash\{0,1\}$, i.e. such that $l\not\perp\cup(L_1\backslash\{1\})$ for every line $l\in L_2$. If $L_2=\{0,1\}$ then the proof is complete. Let us suppose that $L_2\neq\{0,1\}$. Then there is a line $l_0\in L_2$. Since $\cup(L_1\backslash\{1\})\neq\mathbf{R}^3$ there is a line $\overline{l_0}\not\perp\cup(\mathrm{L}_1\backslash\{1\})$ and we can rotate L_2 such that l_0 goes to l_0. Rotating now the image of L_2 around l_0 we obtain an uncountable many possibilities, while for only a countable many of them there is a line $l\in L_2$ such that $l\subseteq\cup(L_1\backslash\{1\})$. Indeed, for every $l\in L_2$ all possible positions of l in a unit sphere $S(0,1)$ in $\mathbf{R}^3$ form a circle C with the center on l_0, while, for every $a\in L_1\backslash\{1\}$, $a\cap S(0,1)$ is either a two-element set (a is a line) or a circle not identical to C; hence $a\cap S(0,1)\cap C$ is at most a two-element.

Proposition 6.2: Every pasting for an atom of a pair of countable orthomodular lattices orthorepresentable (realizable, resp.) in H_3 is orthorepresentable (realizable, resp.) in H_3.

Proof: If we paste for an atom in a two-atomic block then we obtain a horizontal sum and the proof follows from Proposition 6.1. Let us suppose that we paste for atoms in three-atomic blocks. Let L_1, L_2 be orthorepresentations (realizations, resp.) in H_3 of given orthomodular lattices such that $L_1\cap L_2\ni l_0$, where l_0 represents the atom in both L_1, L_2 for which we paste. It suffices to prove that there is a rotation L_2 of L_2 around the line l_0 such that $a_1\not\perp a_2$ and $a_2\not\perp a_1$ for every $a_1\in L_1\backslash\{0,1,l_0,l_0'\}$ and for every $a_2\in L_2\backslash\{0,1,l_0,l_0'\}$, i.e., such that $l\not\perp\cup(L_1\backslash\{1,l_0'\})$ for every line $l\in L_2$. This gives only countable many restrictions to uncountable possible positions of L_2, hence the proof is complete.

Corollary 6.3: Every countable Greechie logic with at most three atomic blocks and without any loop is orthorepresentable in H_3.

Proof: Every countable Greechie logic with only finite at most three atomic blocks is a horizontal sum of subsequent countable pastings of finite three-atomic Boolean algebras for an atom. The rest follows from Theorem 4.2, Proposition 6.2 (using the induction) and Proposition 6.1.

According to Proposition 3.10, Greechie logics from the above Corollary have a full set of two-valued states.

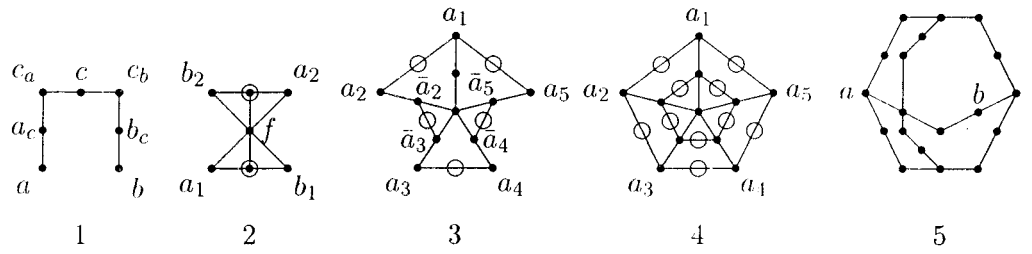

FIG. 7. Greechie diagrams of orthomodular lattices weakly realizable in H_3.

Lemma 6.4: Let L_1 be a countable orthomodular lattice orthorepresentable (realizable, resp.) in H_3 and L_2 be an orthomodular lattice given in Fig. 7.1 such that $L_1 \cap L_2 = \{0,a,b,a',b',1\}$ and $a \neq b$ are nonorthogonal atoms in L_1 (in its realization, resp.). Then the pasting of L_1 and L_2 is orthorepresentable (realizable, resp.) in H_3.

Proof: Let us suppose that L_1 is an orthorepresentation (realization, resp.) in H_3 of a given orthomodular lattice. If a (b, resp.) is a two-dimensional subspace of H_3 then a (b, resp.) is a part of a four-element horizontal summand, and this summand might be considered as a part of L_2. The proof then follows from Proposition 6.2. Let us suppose that a, b are lines. Let us consider all atoms $c_a \leqslant a'$. We have uncountable many possibilities that fill in the unit sphere $S(0,1)$ a circle C_a. Of course, $c_a \leqslant a'$ and $a_c = a' \wedge c_a' \leqslant a'$ but all other ordering of c_a and a_c with elements of $L_1 \backslash \{0,1\}$ can be excluded if we exclude a countable many possibilities. Similarly, if positions of c_a fill a circle C_a then positions of $c_b \perp c_a$, b fill a circle $C_b \subset b'$ ($a \not\perp b$). Again, there is only a countable many positions of c_a for which either c_b or $b_c = b' \wedge c_b'$ is ordered with some element of $L_1 \backslash \{0,1,b'\}$. Finally, it can be shown that positions of c fill a smooth curve on $S(0,1)$, which is not a circle. Hence, there is a possibility to choose c_a such that we obtain the desired orthorepresentation (realization, resp.).

Proposition 6.5: Let $n \geqslant 5$ be a natural number and let $B_1,...,B_n$ be finite three-atomic Boolean algebras such that $B_i \cap B_{i+1} = \{0,a_i,a_i',1\}$ for every $i \in \{1,...,n\}$, where $B_{n+1} = B_1$ and $a_1,...,a_n$ are mutually different atoms. Then the pasting of $\{B_1,...,B_n\}$ (so-called n-cycle) is orthorepresentable in H_3.

Proof: It follows from Proposition 6.2 and from Lemma 6.4.

VII. KOCHEN–SPECKER-TYPE CONFIGURATIONS

We will give several examples of Kochen–Specker-type configurations that arise from Greechie diagrams. Some of these examples has been already used in the literature in the attempt to find a subset of H_3 without a two-valued state. We present the connection to Greechie diagrams (this gives a better geometric insight), show a nonexistence of a ''large'' set of two-valued states for various concepts, and, moreover, we do not stop in proving weak realizability but we discuss the real number of elements.

Proposition 7.1: There is a finite suborthoposet of H_3 such that the set of two-valued states on it is not full.

Proof: Let us consider a suborthoposet L of H_3 given in Fig. 4.2. It is an orthorepresentation of an orthomodular lattice given in Fig. 2.2, it is 28 element (13 atomic), and the set of two-valued states on L is not full [see the proof of Proposition 3.11.(1)]. In fact, in the proof of Proposition 3.11(1) it was shown that there is no two-valued state on the eight-element set $\{a,c_a,d_a,c,d,c_b,d_b,b\}$, such that $s(a)=s(b)=1$ (a reformulation of fullness—see Proposition 3.5). This orthomodular lattice can be orthogenerated, e.g., by the six-element set $\{a,c_a,c_b,b,d_b,d_a\}$ and generated, e.g., by the three-element set $\{a,c_b,d_b\}$.

Proposition 7.2: There is a finite suborthoposet of H_3 such that the set of two-valued states on it is not separating.

Proof: Let us consider an orthomodular lattice given in Fig. 2.3. It is an orthomodular lattice without a separating set of two-valued states [see the proof of Proposition 3.11.(2)]. It has 56 elements (27 atoms) and a 17-element subset without a separating set of states (five marked and six ''hidden'' in every circle). It can be checked that it has the following realization (which forms a suborthoposet of H_3 given in Fig. 7.2—points in the circles denote the middle elements of the diagram from Fig. 2.2): $f=\mathrm{Sp}(0,0,1)$, a_1•⊖•b_1 given by Fig. 4.2; a_2•⊖•b_2 we obtain from the representation on Fig. 4.2 rotating by $\pi/2$ around f. There is a ten-element set of orthogenerators (e.g., $\{a_1,b_1,c_{a1},c_{b1},d_{a1},d_{b1},f,c_2,c_{b2},d_{b2}\}$) and a four-element set of generators (e.g., $\{a_1,c_{b1},d_{b1},c_{b2}\}$).

Let us note that we can take a realization of an orthomodular lattice given in Fig. 2.2, such that we obtain an orthorepresentation of the orthomodular lattice given in Fig. 2.3, but the set of (ortho)generators is larger in this case.

Proposition 7.3: There is a finite suborthoposet of H_3 such that the set of two-valued states on it is not unital.

Proof: Let us consider an orthomodular lattice L given in Fig. 7.3. It is an orthomodular lattice without a unital set of two-valued states. Indeed, for every two-valued state s on L with $s(a_1)=1$ we have $s(f)=s(a_2)=s(a_5)=0$, $s(\overline{a_2})=s(\overline{a_5})=1$, $s(\overline{a_3})=s(\overline{a_4})=0$, $s(a_3)=s(a_4)=1$-a contradiction. It has 132 elements (65 atoms) and a 40-element subset without a unital set of states (six hidden in every circle and all marked a_i's and $\overline{a_i}$'s). Let us find a weak realization of L. It can be done as follows: Put $f=\mathrm{Sp}(0,0,1)$, $a_1=\mathrm{Sp}(1,0,0)$, $\overline{a_1}=\mathrm{Sp}(0,1,0)$, and let $a_k,\overline{a_k}(k=2,\ldots,5)$ be images of $a_1,\overline{a_1}$ in rotations around f about $k\cdot 72°$. Find a realization of the orthomodular lattice given in Fig. 2.2 such that the angle of images of a,b is 72° (see the proof of Lemma 5.5) and rotate this realization to the following pairs of lines: (a_1,a_2), $(\overline{a_2},\overline{a_3})$, (a_3,a_4), $(\overline{a_4},\overline{a_5})$, (a_5,a_1) (i.e., a goes to the first and b to the second line for every pair). It can be checked that an orthomodular poset orthogenerated by this weak realization is finite. (In fact, it is a weak realization of an orthomodular lattice given in Fig. 7.4 by the same way.)

It can be shown that if we take the realization of the orthomodular lattice given in Fig. 2.2 such that the angle between a and b is equal to 72° by the expression given in the proof of Lemma 5.5 as the first copy and if the second and the third copy arise by rotations around the axis of the plane given by a and b such that b coincides with a of the next copy, then some elements coincide:

$$(c_a,c,c_b,b_c,b,b_d,d_b)_1=(d,d_b,d_a,a_d,a,a_c,c_a)_2,$$

$$(c,d_b,d,d_a,e)_1=(c_a,d,c,e,c_b)_3.$$

(The index denotes the number of the copy.) Hence, the weak realization of the orthomodular lattice from the above proof gives a 29-element subset of H_3 without a unital set of two-valued states and the suborthoposet orthogenerated by it has 104 elements (51 atoms), is orthogenerated by a 16-element set and generated by a four-element set (e.g., elements a, c_b, d_b of some $a????b$ and some element from the inner ''pentagon''). The ''almost'' Greechie diagram (20 points that belong to exactly one edge are for simplicity omitted) of this suborthoposet of H_3 (realization of the orthomodular lattice given in Fig. 7.4) is given in Fig. 8, with

$$a_1=\mathrm{Sp}(1,\quad 0,\quad 0),$$

$$a_2=\mathrm{Sp}(\sqrt{3-\sqrt{5}},\quad \sqrt{5+\sqrt{5}},\quad 0),$$

$$a_3=\mathrm{Sp}(-\sqrt{3+\sqrt{5}},\quad \sqrt{5-\sqrt{5}},\quad 0),$$

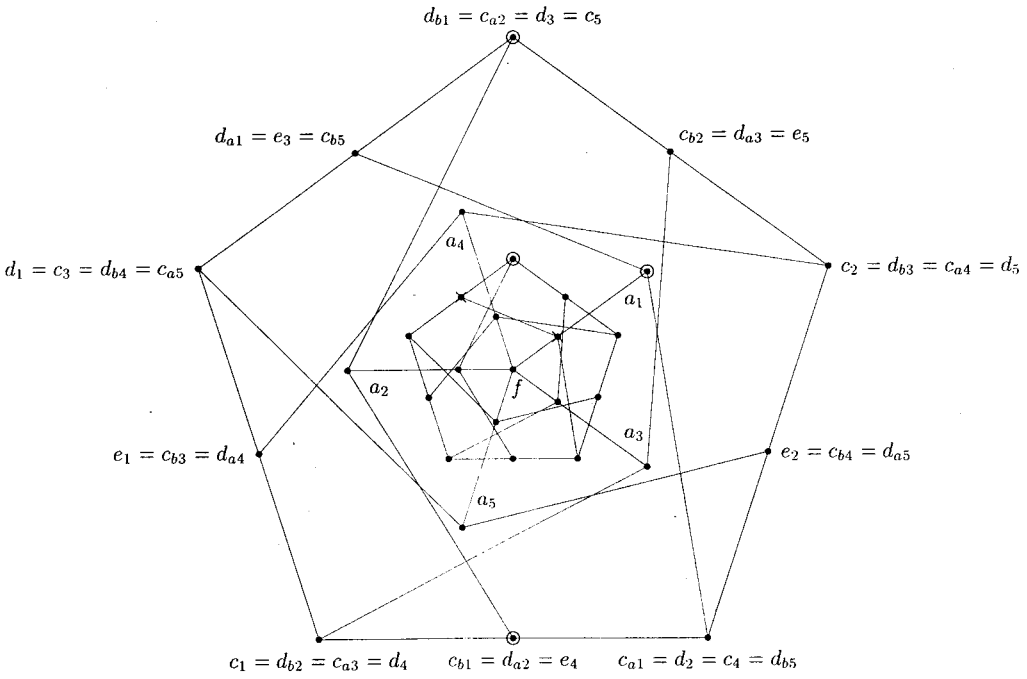

FIG. 8. ''Almost'' Greechie diagram of a suborthoposet of H_3 without a unital set of two-valued states.

$$a_4 = \mathrm{Sp}(-\sqrt{3+\sqrt{5}},\quad -\sqrt{5-\sqrt{5}},\quad 0),$$

$$a_5 = \mathrm{Sp}(\sqrt{3-\sqrt{5}},\quad -\sqrt{5+\sqrt{5}},\quad 0),$$

$$c_{a1} = \mathrm{Sp}(0,-\sqrt{-1+\sqrt{5}},\quad 1),$$

$$d_{a1} = \mathrm{Sp}(0,\quad \sqrt{2},\sqrt{-2+\sqrt{5}}),$$

$$c_1 = \mathrm{Sp}(\sqrt{\sqrt{5}},\quad \sqrt{2+\sqrt{5}},\quad \sqrt{3+\sqrt{5}}),$$

$$d_1 = \mathrm{Sp}(-\sqrt{\sqrt{5}},-\sqrt{-2+\sqrt{5}},\quad \sqrt{2}),$$

$$c_{b1} = \mathrm{Sp}(-\sqrt{5+\sqrt{5}},\quad \sqrt{3-\sqrt{5}},2\sqrt{-2+\sqrt{5}}),$$

$$d_{b1} = \mathrm{Sp}(\sqrt{\sqrt{5}},-\sqrt{-2+\sqrt{5}},\quad \sqrt{2}),$$

$$e_1 = \mathrm{Sp}(\sqrt{\sqrt{5}},\quad -\sqrt{2+\sqrt{5}},\quad \sqrt{3-\sqrt{5}}),$$

$$c_2 = \mathrm{Sp}(-\sqrt{\sqrt{5}},\quad \sqrt{2+\sqrt{5}},\quad \sqrt{3+\sqrt{5}}),$$

$$c_{b2} = \mathrm{Sp}(-\sqrt{\sqrt{5}},\quad -\sqrt{2+\sqrt{5}},\quad \sqrt{3-\sqrt{5}}),$$

$$e_2 = \mathrm{Sp}(\sqrt{5+\sqrt{5}},\quad \sqrt{3-\sqrt{5}},2\sqrt{-2+\sqrt{5}}),$$

$$f = \mathrm{Sp}(0,\quad 0,\quad 1).$$

Elements of the 29-element subset without a unital set of two-valued states are all marked points that are not crossed, a set of orthogenerators is e.g., the set of vertices of both pentagons with a_i's and with the middle point, a set of generators is marked by circles.

It should be noted that in Refs. 8 and 18 there is an example of an 11-element set of lines orthogenerating a 25-element set of lines and a 76-element (37-atomic) suborthoposet of H_3 without a unital set of two-valued states. This suborthoposet is generated by a three-element set. The Greechie diagram of this example does not seem to provide an easy survey, hence we omit it. A more detailed description of this example is given in Sec. VIII.

Proposition 7.4: There is a finite suborthoposet of H_3 such that the set of two-valued states on it is empty.

Proof: Let us consider an orthomodular lattice L, which is the pasting of the orthomodular lattice given in Fig. 7.3 for a_1 and of the orthomodular lattice given in Fig. 7.4 for its middle point. It is an orthomodular lattice without any two-valued state. Indeed, if s is a two-valued state on L then $s(a_1)=0$ (see above). Analogously from the other diagram, $s(a_1)=1$—a contradiction. It has 374 elements (186 atoms) and a 110-element subset without any two-valued state (six ''hidden'' in every circle and all marked except two of them—a_1 and $\overline{a_1}$). According to Proposition 6.2, this orthomodular poset is weakly realizable in H_3.

It can be shown that we can paste for the whole block and obtain a weak realization, which is a union of weak realizations of two copies of an orthomodular lattice given in Fig. 7.4. Hence, this suborthoposet has 200 elements (99 atoms) and a 58-element subset without any two-valued state.

It should be noted that in Ref. 6 there is an example of a 33-element set of lines without any two-valued state. Direction vectors of these lines arise by all permutations of coordinates from (0,0,1), $(0,\pm1,1)$ $(0,\pm1,\sqrt{2})$, and $(\pm1,\pm1,\sqrt{2})$. This set of lines orthogenerates a suborthoposet of H_3 with 116 elements (57 atoms). Direction vectors of remaining lines arise by all permutations of coordinates from $(\pm1,\pm3,\sqrt{2})$. This suborthoposet of H_3 has a 17-element set of orthogenerators (e.g., lines with direction vectors (0,0,1), (0,1,0) and all coordinate permutations from $(0,1,\sqrt{2})$, $(1,\pm1,\sqrt{2})$) and a three-element set of generators [e.g., lines with direction vectors (1,0,0), (1,1,0), $(\sqrt{2},1,1)$]. The ''almost'' Greechie diagram (24 points that belong to exactly one edge are, for simplicity, omitted) of this example is given in Fig. 9 (one edge is denoted by a circle). The above-mentioned three-element set of generators is marked by circles.

Corollary 7.5: There is a three-element set of lines in H_3 such that no subortholattice of H_3 containing it has a two-valued state.

It seems to be an open question whether every three-element set of mutually nonorthogonal lines in H_3 generates a subortholattice without any two-valued state. The least numbers in constructions are given in Table I.

Let us note that the examples in Proposition 7.1 and in Proposition 7.2 appeared in Ref. 17, the example in Fig. 7.4 appeared (not explicitly) in Refs. 17 and 5 as a part of their construction. In Ref. 19 the author uses (not explicitly) the orthomodular lattice given in Fig. 7.3 and paste three copies to distinct atoms of a block obtaining thus an orthomodular lattice without any two-valued state (however, his estimation of lines does not seem to be correct).

In Ref. 7 the author uses weak realizability of an orthomodular lattice in Fig. 7.5 whenever we represent elements a, b by lines in H_3, such that their angle is less than 45°. This leads to the construction of an orthomodular lattice with 392 elements (146 atoms) weakly realizable in H_3 and (at most) 130-element set of lines without any two-valued state.

VIII. DISCUSSION OF PHYSICAL RELEVANCE

In this final section we shall give a brief review of the physical relevance of the above findings. The nonexistence of two-valued measures on certain finite propositional structures in three-dimensional Hilbert spaces has first been explicitly demonstrated by Kochen and Specker.[17] It is strongly recommended that this original account be read. Their result has given rise to a

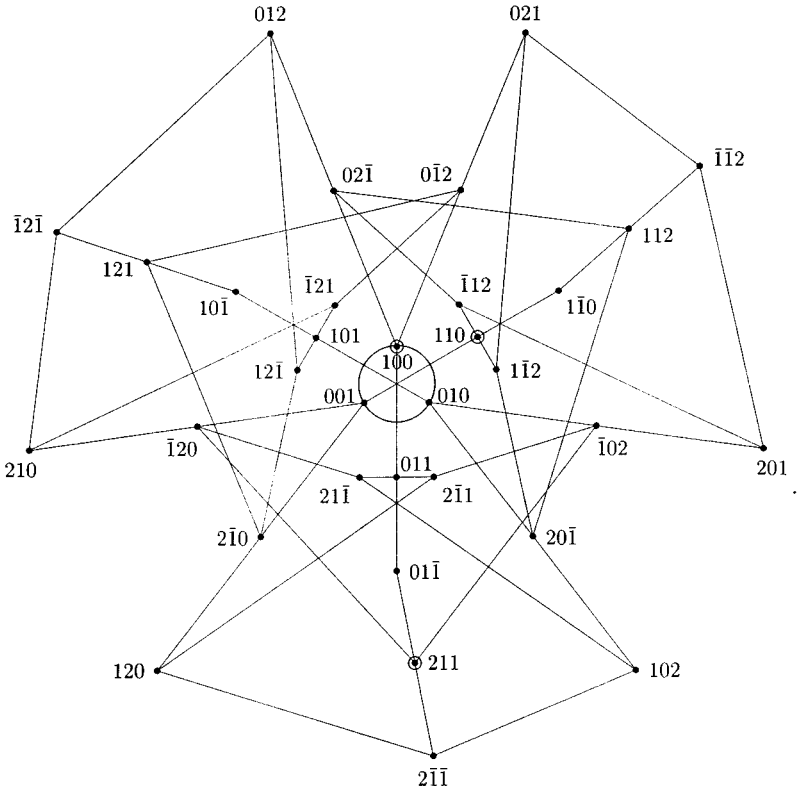

FIG. 9. ''Almost'' Greechie diagram of a suborthoposet of H_3 without any two-valued state [e.g., 1!2 denotes $\mathrm{Sp}(1,-1,\sqrt{2})$].

number of interpretations, by Kochen and Specker and others. A detailed overview of the history of the subject can, for instance, be found in the reviews by Mermin[7] and Brown.[20]

What does it physically mean that *three* nonorthogonal rays in three-dimensional Hilbert space are sufficient to generate a finite system of rays that have no two-valued state? To state the associated Kochen–Specker paradox explicitly, let us associate any one-dimensional subspace $\mathrm{Sp}(v)$ spanned by a nonzero vector v with the proposition that the physical system is in a pure state associated with that subspace. That is,

$$\mathrm{Sp}(1,0,0)=a, \quad \mathrm{Sp}(1,1,0)=b, \quad \mathrm{Sp}(\sqrt{2},1,1)=c,$$

TABLE I. Numbers of elements of constructed propositional structures in H_3 without a ''large'' set of two-valued states.

''Large:''	Full	Separating	Unital		Nonempty
Example (figure)	4.2	7.2	cf. Refs. 8,18	8	9
Elements of a suborthoposet	28	56	76	104	116
Atoms of a suborthoposet	13	27	37	51	57
Lines	8	17	25	29	33
Orthogenerators	6	9	11	16	17
Generators	3	4	3	4	3

where a, b, and c are propositions. If a (similar for b and c) is measured, then we associate the logical value ''true'' or ''false'' with the two-valued state function $s(a)=1$ and $s(a)=0$, respectively. a, b, c generate the propositional structure derived by Peres[6] (cf. also Ref. 21, pp. 186–190). That is, if v and w are two vectors in three-dimensional Hilbert space corresponding to the propositions p_v and p_w, respectively, then the vector product $v\times w$ corresponds to the proposition $(p_v\vee p_w)'$. In particular,

$$\mathrm{Sp}(1,0,0)=a,$$

$$\mathrm{Sp}(1,1,0)=b,$$

$$\mathrm{Sp}(\sqrt{2},1,1)=c,$$

$$\mathrm{Sp}(0,0,1)=(\mathrm{Sp}(1,0,0)\vee\mathrm{Sp}(1,1,0))'=(a\vee b)',$$

$$\mathrm{Sp}(0,1,-1)=(\mathrm{Sp}(1,0,0)\vee\mathrm{Sp}(\sqrt{2},1,1))'=(a\vee c)',$$

$$\mathrm{Sp}(0,1,0)=(\mathrm{Sp}(1,0,0)\vee\mathrm{Sp}(0,0,1))'=(a\vee(a\vee b)')',$$

$$\mathrm{Sp}(0,1,1)=(\mathrm{Sp}(1,0,0)\wedge\mathrm{Sp}(0,1,-1))'=(a\vee(a\vee c)')',$$

$$\mathrm{Sp}(1,-1,0)=(\mathrm{Sp}(1,1,0)\vee\mathrm{Sp}(0,0,1))'=(b\vee(a\vee b)')',$$

$$\mathrm{Sp}(-1,\sqrt{2},0)=(\mathrm{Sp}(\sqrt{2},1,1)\vee\mathrm{Sp}(0,0,1))'=(c\vee(a\vee b)')',$$

$$\mathrm{Sp}(\sqrt{2},-1,-1)=(\mathrm{Sp}(\sqrt{2},1,1)\vee\mathrm{Sp}(0,1,-1))'=(c\vee(a\vee c)')',$$

$$\mathrm{Sp}(-1,0,\sqrt{2})=(\mathrm{Sp}(\sqrt{2},1,1)\vee\mathrm{Sp}(0,1,0))'=(c\vee(a\vee(a\vee b)')')',$$

$$\mathrm{Sp}(\sqrt{2},1,0)=(\mathrm{Sp}(0,0,1)\vee\mathrm{Sp}(-1,\sqrt{2},0))'=((a\vee b)'\vee(c\vee(a\vee b)')')',$$

$$\mathrm{Sp}(1,\sqrt{2},0)=(\mathrm{Sp}(0,0,1)\vee\mathrm{Sp}(\sqrt{2},-1,-1))'=((a\vee b)'\vee(c\vee(a\vee c)'))')',$$

$$\mathrm{Sp}(1,0,\sqrt{2})=(\mathrm{Sp}(0,1,0)\vee\mathrm{Sp}(\sqrt{2},-1,-1))'=((a\vee(a\vee b)')'\vee(c\vee(a\vee c)')')',$$

$$\mathrm{Sp}(\sqrt{2},1,-1)=(\mathrm{Sp}(0,1,1)\vee\mathrm{Sp}(-1,\sqrt{2},0))'=(a\vee(a\vee c)')'\vee(c\vee(a\vee b)'))')',$$

$$\mathrm{Sp}(\sqrt{2},0,1)=(\mathrm{Sp}(0,1,0)\vee\mathrm{Sp}(-1,0,\sqrt{2}))'=((a\vee(a\vee b)')'\vee(c\vee(a\vee(a\vee b)')')')',$$

$$\mathrm{Sp}(\sqrt{2},-1,0)=(\mathrm{Sp}(0,0,1)\vee\mathrm{Sp}(1,\sqrt{2},0))'=((a\vee b)'\vee((a\vee b)'\vee(c\vee(a\vee c)')')')',$$

$$\mathrm{Sp}(\sqrt{2},-1,1)=(\mathrm{Sp}(0,1,1)\vee\mathrm{Sp}(-1,0,\sqrt{2}))'=((a\vee(a\vee c)')'\vee(c\vee(a\vee(a\vee b)')')')',$$

$$\mathrm{Sp}(-1,1,\sqrt{2})=(\mathrm{Sp}(1,1,0)\vee\mathrm{Sp}(\sqrt{2},0,1))'=(b\vee((a\vee(a\vee b)')'\vee(c\vee(a\vee(a\vee b)')')')')',$$

$$\begin{aligned}\mathrm{Sp}(0,\sqrt{2},-1)&=(\mathrm{Sp}(1,0,0)\vee\mathrm{Sp}(-1,1,\sqrt{2}))'\\&=(a\vee(b\vee((a\vee(a\vee b)')'\vee(c\vee(a\vee(a\vee b)')')')')')',\end{aligned}$$

$$\begin{aligned}\mathrm{Sp}(\sqrt{2},0,-1)&=(\mathrm{Sp}(0,1,0)\vee\mathrm{Sp}(1,0,\sqrt{2}))'\\&=((a\vee(a\vee b)')'\vee((a\vee(a\vee b)')'\vee(c\vee(a\vee c)')')')',\end{aligned}$$

$$\mathrm{Sp}(1,-1,\sqrt{2}) = (\mathrm{Sp}(1,1,0) \vee \mathrm{Sp}(-1,1,\sqrt{2}))'$$
$$= (b \vee (b \vee ((a \vee (a \vee b)')' \vee (c \vee (a \vee (a \vee b)')')')')')',$$

$$\mathrm{Sp}(0,1,\sqrt{2}) = (\mathrm{Sp}(1,0,0) \vee \mathrm{Sp}(0,\sqrt{2},-1))'$$
$$= (a \vee (a \vee (b \vee ((a \vee (a \vee b)')' \vee (c \vee (a \vee (a \vee b)')')')')')')',$$

$$\mathrm{Sp}(0,\sqrt{2},1) = (\mathrm{Sp}(1,0,0) \vee \mathrm{Sp}(1,-1,\sqrt{2}))'$$
$$= (a \vee (b \vee (b \vee ((a \vee (a \vee b)')' \vee (c \vee (a \vee (a \vee b)')')')')')')',$$

$$\mathrm{Sp}(-1,-1,\sqrt{2}) = (\mathrm{Sp}(1,-1,0) \vee \mathrm{Sp}(\sqrt{2},0,1))'$$
$$= ((b \vee (a \vee b)')' \vee ((a \vee (a \vee b)')' \vee (c \vee (a \vee (a \vee b)')')')')',$$

$$\mathrm{Sp}(0,-1,\sqrt{2}) = (\mathrm{Sp}(1,0,0) \vee \mathrm{Sp}(0,\sqrt{2},1))'$$
$$= (a \vee (a \vee (b \vee (b \vee ((a \vee (a \vee b)')' \vee (c \vee (a \vee (a \vee b)')')')')')')')',$$

$$\mathrm{Sp}(1,1,\sqrt{2}) = (\mathrm{Sp}(1,-1,0) \vee \mathrm{Sp}(0,\sqrt{2},-1))'$$
$$= ((b \vee (a \vee b)')' \vee (a \vee (b \vee ((a \vee (a \vee b)')' \vee (c \vee (a \vee (a \vee b)')')')')')')',$$

$$\mathrm{Sp}(-1,\sqrt{2},-1) = (\mathrm{Sp}(\sqrt{2},1,0) \vee \mathrm{Sp}(0,1,\sqrt{2}))'$$
$$= (((a \vee b)' \vee (c \vee (a \vee b)')')' (a \vee (a \vee (b \vee ((a \vee (a \vee b)')'$$
$$\vee (c \vee (a \vee (a \vee b)')')')')')')',$$

$$\mathrm{Sp}(-1,\sqrt{2},1) = (\mathrm{Sp}(\sqrt{2},1,0) \vee \mathrm{Sp}(0,-1,\sqrt{2}))'$$
$$= (((a \vee b)' \vee (c \vee (a \vee b)')')' \vee (a \vee (a \vee (b \vee (b \vee ((a \vee (a \vee b)')'$$
$$\vee (c \vee (a \vee (a \vee b)')')')')')')')',$$

$$\mathrm{Sp}(1,\sqrt{2},-1) = (\mathrm{Sp}(\sqrt{2},-1,0) \vee \mathrm{Sp}(0,1,\sqrt{2}))'$$
$$= (((a \vee b)' \vee ((a \vee b)' \vee (c \vee (a \vee c)')')')' \vee (a \vee (a \vee (b \vee ((a \vee (a \vee b)')'$$
$$\vee (c \vee (a \vee (a \vee b)')')')')')')')',$$

$$\mathrm{Sp}(-1,0,1) = (\mathrm{Sp}(0,1,0) \vee \mathrm{Sp}(-1,\sqrt{2},-1))'$$
$$= ((a \vee (a \vee b)')' \vee (((a \vee b)' \vee (\vee (a \vee b)')')'$$
$$\vee (a \vee (a \vee (b \vee ((a \vee (a \vee b)')'$$
$$\vee (c \vee (a \vee (a \vee b)')')')')')')')')',$$

$$\mathrm{Sp}(1,\sqrt{2},1) = (\mathrm{Sp}(\sqrt{2},-1,0) \vee Sp(0,-1,\sqrt{2}))'$$
$$= (((a \vee b)' \vee ((a \vee b)' \vee (c \vee (a \vee c)')')')'$$
$$\vee (a \vee (a \vee (b \vee (b \vee ((a \vee (a \vee b)')'$$
$$\vee (c \vee (a \vee (a \vee b)')')')')')')')',$$

$$\begin{aligned}\mathrm{Sp}(1,0,1) &= (\mathrm{Sp}(0,1,0) \vee \mathrm{Sp}(-1,\sqrt{2},1))' \\ &= ((a \vee (a \vee b)')' \vee (((a \vee b)' \vee (c \vee (a \vee b)')')' \\ &\quad \vee (a \vee (a \vee (b \vee (b \vee ((a \vee (a \vee b)')' \\ &\quad \vee (c \vee (a \vee (a \vee b)')')')')')')')')')'.\end{aligned}$$

Suppose, for the sake of contradiction, that each one of the above 33 propositions corresponds to an ''element of physical reality''.[22] That is, suppose that its value is either ''true'' (exclusive) or ''false,'' irrespective of whether it has been actually measured or just counterfactually inferred. Let us further assume with Peres[6,21] that—provided these ''elements of reality'' exist—$\mathrm{Sp}(0,0,1) = \mathrm{Sp}(1,0,1) = \mathrm{Sp}(0,1,1) = \mathrm{Sp}(1,-1,\sqrt{2}) = \mathrm{Sp}(1,0,\sqrt{2}) = \mathrm{Sp}(\sqrt{2},1,1) = \mathrm{Sp}(\sqrt{2},0,1) = \mathrm{Sp}(1,1,\sqrt{2}) = \mathrm{Sp}(0,1,\sqrt{2}) = \mathrm{Sp}(1,\sqrt{2},1) =$ ''true.'' One can follow Peres' arguments to show that—provided these ''elements of reality'' exist—all other rays belong to triads that are orthogonal to the above rays. Therefore, these latter rays must correspond to propositions whose value is ''false.'' In particular, $\mathrm{Sp}(1,0,0) = \mathrm{Sp}(0,\sqrt{2},1) = \mathrm{Sp}(0,-1,\sqrt{2}) =$ ''false,'' associate with $s(\mathrm{Sp}(1,0,0)) = s(\mathrm{Sp}(0,\sqrt{2},1)) = s(\mathrm{Sp}(0,-1,\sqrt{2})) = 0$. Thus, $s(\mathrm{Sp}(1,0,0)) + s(\mathrm{Sp}(0,\sqrt{2},1)) + s(\mathrm{Sp}(0,-1,\sqrt{2})) = 0+0+0 = 0$. But $\mathrm{Sp}(1,0,0)$, $\mathrm{Sp}(0,\sqrt{2},1)$, and $\mathrm{Sp}(0,-1,\sqrt{2})$ are mutually orthogonal. This is in contradiction to the assumption that for any orthogonal triad spanning the entire Hilbert space, the sum of the measures should be one [cf. Definition 3.1.(4)]. Notice that in order to arrive at this Kochen–Specker paradox, we had to explicitly assume the existence of the ''elements of reality,'' irrespective of whether they have (or could have) actually been measured or not.

What physical use can be a paradox? How can one measure a contradiction? Indeed, what can actually be measured is merely *one* triplet of propositions corresponding to some of the triads of mutually orthogonal rays. Such a measurement can be performed with the operator discussed by Peres, or with an arrangement of beam splitters discussed by Reck *et al.*[23]

For instance, after c is found to be ''true'' [corresponding to $s(c) = 1$], then measurement of the original values of a or b is no longer possible. However, suppose one would be willing to believe in the existence of ''elements of reality,''[22,24] which could merely be *counterfactually* inferred. Then one could for instance—at least in principle—''measure'' all 16 orthogonal triads by the production of a state with 16 entangled subsystems. On each one of the 16 different entangled subsystems one could measure one of the 16 different orthogonal triads. This is similar to a proposal by Greenberger, Horne, and Zeilinger,[25] which use three particles and eight-dimensional Hilbert space. Indeed, only in such a way—namely by (counterfactually) inferring noncomeasurable propositions—one would encounter a complete Kochen–Specker contradiction.

As has been already proven in the Kochen and Specker original work (cf. Ref. 17, pp. 82–85, Theorem 4), the notion of tautology is connected to a classical (Boolean) imbedding of a partial Boolean algebra. Indeed, there exist propositions that are tautologies in the classical (Boolean) algebra but that are not tautologies in the partial Boolean algebra if and only if the partial Boolean algebra does not have a unital set of two-valued states and thus cannot be imbedded into a classical (Boolean) algebra.

This is true for all partial Boolean algebras, in particular for orthomodular posets. Notice that the above result does not imply that every propositional structure giving rise to a (classical) Boolean tautology that is no quantum tautology also has no two-valued measure (cf. below).

Until now, the lowest number of rays necessary to produce a classical tautology that is not always true quantum mechanically is due to Schütte.[8,18] The 11 rays used by Schütte can also be generated by the three vectors (1,0,0), (1,1,0), and $(\sqrt{2},1,1)$ (corresponding to a, b, and c) used before. Indeed, $d = \mathrm{Sp}(0,1,-1) = (\mathrm{Sp}(1,1,0) \vee \mathrm{Sp}(\sqrt{2},1,1))' = (a \vee c)'$ and

$$a_1 = \mathrm{Sp}(1,0,0) = a,$$

$$a_2 = \mathrm{Sp}(0,1,0) = (\mathrm{Sp}(1,0,0) \vee \mathrm{Sp}(0,0,1))' = (a \vee (a \vee b)')',$$

$$b_1=\mathrm{Sp}(0,1,1)=(Sp(1,0,0)\vee Sp(0,1,-1))'=(a\vee d)',$$

$$b_2=\mathrm{Sp}(1,0,1)=(\mathrm{Sp}(0,1,0)\vee\mathrm{Sp}(-1,1,1))'=((a\vee(a\vee b)')'\vee(b\vee d)')',$$

$$b_3=\mathrm{Sp}(1,1,0)=b,$$

$$c_1=\mathrm{Sp}(1,0,2)=(\mathrm{Sp}(0,1,0)\vee\mathrm{Sp}(2,1,-1))'=((a\vee(a\vee b)')'\vee((a\vee d)'\vee(b\vee(a\vee d)')')')',$$

$$c_2=\mathrm{Sp}(2,0,1)=(\mathrm{Sp}(0,1,0)\vee\mathrm{Sp}(-1,0,2))'=((a\vee(a\vee b)')'\vee((a\vee(a\vee b)')'\vee((a\vee d)'\vee((a\vee d)'\vee(b\vee(a\vee b)')')')')',$$

$$d_1=\mathrm{Sp}(-1,1,1)=(\mathrm{Sp}(1,1,0)\vee\mathrm{Sp}(0,1,-1))'=(b\vee d)',$$

$$d_2=\mathrm{Sp}(1,-1,1)=(\mathrm{Sp}(1,1,0)\vee\mathrm{Sp}(0,1,1))'=(b\vee(a\vee d)')',$$

$$d_3=\mathrm{Sp}(1,1,-1)=(\mathrm{Sp}(0,1,1)\vee\mathrm{Sp}(1,-1,0))'=((a\vee d)'\vee(b\vee(a\vee b)')')',$$

$$d_4=\mathrm{Sp}(1,1,1)=(\mathrm{Sp}(0,1,-1)\vee\mathrm{Sp}(1,-1,0))'=(d\vee(b\vee(a\vee b)')')',$$

where

$$\mathrm{Sp}(2,1,-1)=(\mathrm{Sp}(0,1,1)\vee\mathrm{Sp}(1,-1,1))'=((a\vee d)'\vee(b\vee(a\vee d)')')',$$

$$\mathrm{Sp}(-1,0,2)=(\mathrm{Sp}(0,1,0)\vee\mathrm{Sp}(-2,1,-1))'=((a\vee(a\vee b)')'\vee((a\vee d)'\vee((a\vee d)'\vee(b\vee(a\vee b)')')')')',$$

$$\mathrm{Sp}(2,-1,1)=(\mathrm{Sp}(0,1,1)\vee\mathrm{Sp}(1,1,-1))'=((a\vee d)'\vee((a\vee d)'\vee(b\vee(a\vee b)')')')'.$$

As we have mentioned above, there is not a unital set of two-valued states on a suborthoposet orthogenerated by these rays (e.g., there is no two-valued state s with $s(\mathrm{Sp}(1,0,0))=1$). On the other hand, a two-valued can be defined by $s(\mathrm{Sp}(0,1,0))=s(\mathrm{Sp}(0,1,1))=s(\mathrm{Sp}(1,1,0))=s(\mathrm{Sp}(1,1,1))=s(\mathrm{Sp}(1,1,2))=s(\mathrm{Sp}(1,2,1))=s(\mathrm{Sp}(2,1,1))=s(\mathrm{Sp}(1,2,-1))=s(\mathrm{Sp}(-1,2,1))=s(\mathrm{Sp}(1,5,2))=s(\mathrm{Sp}(2,5,1))=s(\mathrm{Sp}(-1,5,2))=s(\mathrm{Sp}(2,5,-1))=s(\mathrm{Sp}(1,5,-2))=s(\mathrm{Sp}(-2,5,1))=1$ and $s(\mathrm{Sp}(1,0,0))=s(\mathrm{Sp}(0,0,1))=s(\mathrm{Sp}(1,0,1))=s(\mathrm{Sp}(0,1,-1))=s(\mathrm{Sp}(1,0,-1))=s(\mathrm{Sp}(1,-1,0))=s(\mathrm{Sp}(1,1,-1))=s(\mathrm{Sp}(1,-1,1))=s(\mathrm{Sp}(-1,1,1))=s(\mathrm{Sp}(-1,-1,2))=s(\mathrm{Sp}(-1,2,-1))=s(\mathrm{Sp}(2,-1,-1))=s(\mathrm{Sp}(1,-1,2))=s(\mathrm{Sp}(-1,1,2))=s(\mathrm{Sp}(2,1,-1))=s(\mathrm{Sp}(2,-1,1))=s(\mathrm{Sp}(1,0,2))=s(\mathrm{Sp}(2,0,1))=s(\mathrm{Sp}(-1,0,2))=s(\mathrm{Sp}(2,0,-1))=s(\mathrm{Sp}(1,-5,2))=s(\mathrm{Sp}(2,-5,1))=0$.

Consider now the following propositions (notice that any binary operation is either performed by orthogonal rays or by a ray and an orthocomplement of another ray, such that these rays are orthogonal):

$$f_1=d_1\rightarrow b_2'=(d_1\wedge b_2)',$$

$$f_2=d_1\rightarrow b_3'=(d_1\wedge b_3)',$$

$$f_3=d_2\rightarrow a_2\vee b_2=(d_2\wedge(a_2\vee b_2)')',$$

$$f_4=d_2\rightarrow b_3'=(d_2\wedge b_3)',$$

$$f_5=d_3\rightarrow b_2'=(d_3\wedge b_2)',$$

$$f_6 = d_3 \rightarrow (a_1 \vee a_2 \rightarrow b_3) = (d_3 \wedge ((a_1 \vee a_2)' \vee b_3)')',$$

$$f_7 = d_4 \rightarrow a_2 \vee b_2 = (d_4 \wedge (a_2 \vee b_2)')',$$

$$f_8 = d_4 \rightarrow (a_1 \vee a_2 \rightarrow b_3) = (d_4 \wedge ((a_1 \vee a_2)' \vee b_3)')',$$

$$f_9 = (a_2 \vee c_1) \vee (b_3 \vee d_1) = ((a_2 \vee c_1)' \wedge (b_3 \vee d_1)')',$$

$$f_{10} = (a_2 \vee c_2) \vee (a_1 \vee b_1 \rightarrow d_1) = ((a_2 \vee c_2)' \wedge ((a_1 \vee b_1)' \vee d_1)')',$$

$$f_{11} = c_1 \rightarrow b_1 \vee d_2 = (c_1 \wedge (b_1 \vee d_2)')',$$

$$f_{12} = c_2 \rightarrow b_3 \vee d_2 = (c_2 \wedge (b_3 \vee d_2)')',$$

$$f_{13} = (a_2 \vee c_1) \vee [(a_1 \vee a_2 \rightarrow b_3) \rightarrow d_3] = ((a_2 \vee c_1)' \wedge (((a_1 \vee a_2)' \vee b_3)' \vee d_3)')',$$

$$f_{14} = (a_2 \vee c_2) \vee (b_1 \vee d_3) = ((a_2 \vee c_2)' \wedge (b_1 \vee d_3)')',$$

$$f_{15} = c_2 \rightarrow [(a_1 \vee a_2 \rightarrow b_3) \rightarrow d_4] = (c_2 \wedge (((a_1 \vee a_2)' \vee b_3)' \vee d_4)')',$$

$$f_{16} = c_1 \rightarrow (a_1 \vee b_1 \rightarrow d_4) = (c_1 \wedge ((a_1 \vee b_1)' \vee d_4)')',$$

$$f_{17} = (a_1 \rightarrow a_2) \vee b_1 = (a_1' \vee a_2) \vee b_1.$$

The ''implication'' relation has been expressed as $x \rightarrow y \equiv x' \vee y \equiv (x \wedge y')'$.

As can be straightforwardly checked, the proposition formed by

$$F: f_1 \wedge f_2 \wedge \cdots \wedge f_{16} \rightarrow f_{17},$$

is a classical tautology. Nevertheless, F is not valid in three-dimensional (real) Hilbert space $\mathbf{R}^3$, since $f_1, f_2, \ldots, f_{16} = \mathbf{R}^3$, whereas $f_{17} = (\mathrm{Sp}(1,0,0))' = \mathrm{Sp}(0,1,0) \vee \mathrm{Sp}(0,0,1) \neq \mathbf{R}^3$.

The three vectors (1,0,0), (1,1,0), and $(\sqrt{2},1,1)$ generating the Schütte rays are not mutually orthogonal. Therefore, the corresponding propositions a, b, and c are not comeasureable. In the sense of partial algebras, they cannot be combined by logical operations ''or'' ($\vee$), ''and'' ($\wedge$), ''not'' ($'$) to form new expressions. Thus, it would be incorrect to state that there exists a classical tautology in the three variables a, b, and c, which is no quantum tautology. Indeed, Coray proved[26] that all classical tautologies in three variables are tautologies in all partial algebras, in particular in the one associated with the logic of quantum observables.

However, also Schütte's example is counterfactual in nature. Although every operation or relation is solely defined on comeasurable propositions, the entire formula F contains 11 non-comeasurable variables (nonorthogonal rays). In order to be able to evaluate this formula, one would have to know the true value of all these 11 variables in parallel. Since they are not comeasurable, this is possible only by counterfactual inference; in very much the same way as discussed before in the case of the original Kochen–Specker paradox. Indeed, Corey's result shows that *any* classical (Boolean) tautology that is no quantum tautology will have to rely on at least four variables that cannot be mutually orthogonal (in $\mathbf{R}^3$), and therefore must be based upon counterfactual inference.

Finally, let us briefly mention the relevance of these findings to the partition logic of automata. Corollary 4.3 states that every finite subortholattice of $\mathbf{R}^3$ has a full (and thus separating) set of two-valued states. Thus, any finite subortholattice of $\mathbf{R}^3$ can be expressed as an automaton logic. The subortholattices of $\mathbf{R}^3$ that have no two-valued state are infinite.

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The canonical form of the Rabi Hamiltonian

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The Rabi Hamiltonian, describing the coupling of a two-level system to a single quantized boson mode, is studied in the Bargmann–Fock representation. The corresponding system of differential equations is transformed into a canonical form in which all regular singularities between zero and infinity have been removed. The canonical or Birkhoff-transformed equations give rise to a two-dimensional eigenvalue problem, involving the energy and a transformational parameter which affects the coupling strength. The known isolated exact solutions of the Rabi Hamiltonian are found to correspond to the uncoupled form of the canonical system. © *1996 American Institute of Physics.* [S0022-2488(96)01211-X]

I. INTRODUCTION

In the study of dynamical problems the harmonic oscillator occupies a prominent place as a prototype of the fundamental unitary symmetry group. The spell of group theory also extends to anharmonic oscillators, which have recently been exposed as mere q-deformations of the unitary group algebra.[1] In contrast dynamical problems which arise in the study of boson–fermion interactions are more reluctant to reveal their hidden symmetries. Such problems are more involved since the actual states of the system are of composite nature with a boson and a fermion part. This results in the appearance of singularities in the corresponding eigenvalue problem. Examples include the Jahn–Teller Hamiltonian in molecular physics and the Rabi Hamiltonian in nuclear physics and quantum optics.

A rather peculiar feature of these systems is the emergence of isolated exact solutions, with eigenvalues that correspond to simple expressions in rational numbers. Such were obtained—in a rather heuristic way—by Judd[2] for the case of the $E\otimes e$ Jahn–Teller Hamiltonian, and by Kuś[3] for the spectrum of a two-level atom coupled to a single quantized mode. It was suggested that the exact solutions probably hint at some dynamical symmetry group, but so far no progress was reported in this direction.

In the present paper we analyze the one-mode Rabi problem in a more rigorous way. First—following Refs. 3 and 4—the dynamical problem is defined in the Bargmann–Fock Hilbert space of entire functions. The resulting system of differential equations is then put into canonical form using a theorem due to Birkhoff. Under this transformation the Kuś exact solutions are found to be mapped onto the levels of a displaced harmonic oscillator. In this way hidden symmetry appears.

II. THE BARGMANN–FOCK REPRESENTATION OF A HILBERT SPACE

Before turning to the actual results we briefly review basic information about the Hilbert space of entire functions introduced by Fock[5] and Bargmann.[6] Let $\mathcal{F}_n$, for n integral, be the set of entire analytic functions $f(z)$, where $z=(z_1,\ldots,z_n)$ and $z_k\in\mathbf{C}$ are complex numbers, $k=1,\ldots,n$. Because $f(z)$ is entire it has an everywhere converging power series

$$f(z)=\sum_{k_1,\ldots,k_n}\alpha_{k_1,\ldots,k_n}z_1^{k_1}\cdot\ \cdots\ \cdot z_n^{k_n}, \tag{1}$$

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where summation extends over the whole set of non-negative integers $k_1,\ldots,k_n$ and $\alpha_{k_1,\ldots,k_n}$ are complex coefficients. We define an inner product of two elements f and g of $\mathscr{F}_n$ by

$$(f,g)=\int \overline{f(z)}\cdot g(z)\,d\mu_n(z), \tag{2}$$

where $\overline{f(z)}\cdot g(z)$ is a usual scalar product in $\mathbf{C}^n$,

$$d\mu_n(z)=\frac{1}{\pi^n}\exp(-\overline{z}\cdot z)\prod_{k=1}^{n} dx_k dy_k, \quad z_k=x_k+iy_k, \tag{3}$$

and the integration extends over the whole space $\mathbf{C}^n$. The Bargmann–Fock space $\mathscr{F}_n$ is a set of all entire functions (1), which have a finite norm $(f,f)<\infty$. This is equivalent to the requirement that

$$|f(z)|\leqslant c\,\exp(\tfrac{1}{2}\gamma\overline{z}\cdot z), \tag{4}$$

where c and γ are positive constants with $\gamma<1$. The Bargmann–Fock space $\mathscr{F}_n$ with the inner product defined by (2) is a Hilbert space.

Let us now consider two operators in $\mathscr{F}_n$: multiplication by z_k and differentiation d/dz_k. Since the functions $f(z)$ of $\mathscr{F}_n$ are analytic, $z_k f$ and $(d/dz_k)f$ always exist. The operators satisfy the commutation rules

$$[z_k,z_l]=0, \quad \left[\frac{d}{dz_k},\frac{d}{dz_l}\right]=0, \quad \left[\frac{d}{dz_k},z_l\right]=\delta_{kl}. \tag{5}$$

Furthermore, with respect to the inner product (2), z_k and d/dz_k are Hermitian conjugate

$$(z_k f,g)=\left(f,\frac{d}{dz_k}g\right) \tag{6}$$

whenever $z_k f$ and $(d/dz_k)f$ belong to $\mathscr{F}_n$.

On the other hand, relations (5) and (6) are well-known algebraic relations defining Hermitian conjugate annihilation a_k and creation a_k^+ operators of boson fields in second quantization:

$$[\alpha_k^+,a_l^+]=0, \quad [a_k,a_l]=0, \quad [a_k,a_l^+]=\delta_{kl}. \tag{7}$$

We conclude therefore that within $\mathscr{F}_n$ the annihilation operator a_k is represented by the operation d/dz_k, and the creation operator a_k^+ corresponds to the multiplication by z_k.

As an instructive example let us take a set of n identical uncoupled harmonic oscillators which are described up to a constant by the Hamiltonian $H=\Sigma_{l=1}^n a_l^+ a_l$. The corresponding operator in the Bargmann–Fock space (denoted by $\mathscr{H}$) is $\mathscr{H}=\Sigma_{l=1}^n z_l d/dz_l$ and the corresponding eigenproblem is the system of differential equations

$$\sum_{l=1}^{n} z_l \frac{d}{dz_l} f_k(z)=E_k\, f_k(z). \tag{8}$$

It is easily verified that the eigenfunctions in this case are functions of the type (1), which are homogeneous polynomials of the order k, i.e., in (1) the sum is over $k_1+\cdots+k_n=k$ and the corresponding eigenvalues are $E_k=k$.

III. THE TRANSFORMATION TO A CANONICAL FORM

In the Bargmann–Fock representation of a Hilbert space, quantum mechanical equations for bosons interacting with a manifold of fermion states are represented by a system of linear differential equations in the complex domain.[3,4] The physical solutions (1) of such a system must belong to $\mathscr{F}_n$, i.e., be entire and obey condition (4). In practice the solution of this equation is complicated due to the occurrence of finite regular singularities.

In this section we describe a transformation, due to Birkhoff,[7] which allows us, for a system of linear equations of the first order in one variable, to find a canonical form. To be in the canonical form the system must be transformed in such a way that all its finite singularities reduce to only one singularity at zero, while at the same time preserving the order of the singularity at infinity. Consequently, the transformed system is more likely to be exactly solvable.

The system of m linear differential equations of the first order has a general form

$$\frac{df_r}{dz}=\sum_{s=1}^{m} p_{rs}(z)f_s, \quad r=1,\ldots,m, \tag{9}$$

and we assume that $p_{rs}(z)$ are analytic functions of a complex variable apart from a finite number of regular singularities (even at infinity). Practically it means that, outside the circle $|z|=R$, which includes all the finite singular points, the coefficients may be expanded in a Laurent series

$$p_{rs}(z)=\sum_{k=-\infty}^{q} p_{rs}^{(k)}z^k, \quad p_{rs}^{(k)}\in \mathbf{C}, \tag{10}$$

where $q\geqslant -1$ and $q+1$ is termed the *rank* of the singular point at infinity. In general the system (9) can have m independent sets of solutions $f_s^{(t)}(z)$, where $s=1,\ldots,m$ denotes different solutions within a set $t=1,\ldots,m$. Now we assume a linear transformation of the form

$$f_r(z)=\sum_{s=1}^{m} a_{rs}(z)F_s(z), \tag{11}$$

where the coefficients $a_{rs}(z)$ are analytic at infinity and reduce at infinity to a unit matrix

$$a_{rs}(z)=\sum_{k=0}^{\infty} \frac{a_{rs}^{(k)}}{z^k}, \quad a_{rs}^{(k)}\in \mathbf{C}, \quad a_{rs}^{(0)}=\delta_{rs}. \tag{12}$$

In a sense this $\{a_{rs}(z)\}$ matrix could be said to contain all the finite singularities of the initial system. Under this transformation the original system (9) turns into a system of a slightly different form:

$$z\,\frac{dF_r(z)}{dz}=\sum_{s=1}^{m} P_{rs}(z)F_s(z), \quad r=1,\ldots,m. \tag{13}$$

The coefficients of the transformed system are given by the equation

$$\{P_{rs}(z)\}=z\left(\{a_{rk}^{-1}(z)\}\{p_{kl}(z)\}\{a_{ls}(z)\}-\{a_{rk}^{-1}(z)\}\left\{\frac{d}{dz}\,a_{ks}(z)\right\}\right), \tag{14}$$

where $\{a_{rk}^{-1}(z)\}$ is the matrix inverse to the matrix $\{a_{rk}(z)\}$ and $\{a_{rk}(z)\}\{p_{ks}(z)\}$ denotes the matrix multiplication. Now we are in the position to formulate the Birkhoff theorem—the crucial result in our analysis.

The Birkhoff theorem states that *for every system of the type (9) there exists a transformation matrix (12) such that the coefficients $P_{rs}(z)$ of the transformed system (13) are polynomials of a degree not exceeding $q+1$.*[7]

There are several properties of the above transformation which should be stated here.

(i) All finite singular points of the initial system (9) coalesce to only one singularity at zero [because $P_{rs}(z)$ are polynomials]. This is the most significant property of the transformation and because of it the system (13) may be termed the *canonical* form of the system (9).

(ii) The ranks of the singular points at infinity for both systems (9) and (13) are equal.

(iii) If a given set of solutions $f_s^{(t)}(z)$, $s=1,\ldots,m$, belongs to the Bargmann–Fock space $\mathscr{F}_1$, then the corresponding transformed solutions $F_s^{(t)}(z)$, which are found due to the Birkhoff theorem, also belong to this space. This can easily be shown by adapting the treatment by Birkhoff to the case of entire functions.

The final property allows us to reject all the solutions of the transformed system which do not belong to the Bargmann–Fock space as being nonphysical. However, the inverse of this property is not automatically true, but requires a proper choice of the transformation matrix. We will come back to this point when discussing the actual solutions of the system under investigation.

A useful test to check if the solutions of the transformed system can be entire is given by the indicial equation of the transformed system[8]

$$\det\{c_{rs}-\rho\delta_{rs}\}=0, \tag{15}$$

where $c_{rs}=P_{rs}(0)$, $r,s=1,\ldots,m$. The solutions of (13) depend on the roots $\rho_1,\ldots,\rho_m$ of the indicial equation. There are several rules connected with this equation which indicate the possibility of existence of entire solutions and their degeneracy.

D_0. If none of the roots is a non-negative integer, the equation (13) has no entire solutions (because they are not analytic in the origin).

D_1. If one of the roots ρ_t is a non-negative integer and the remaining roots are either nonintegers or are equal to ρ_t, then there exists exactly one, up to linear dependence, set of analytic solutions of (13) and it is of the form

$$F_s^{(t)}(z)=z^{\rho_t}u_s(z), \quad s=1,\ldots,m, \tag{16}$$

where the $u_s(z)$ are analytic and $u_s(0)\neq 0$. Functions (16) are entire provided their radii of convergence are infinite.

D_2. In the remaining cases if two or more roots of the indicial equation are integers (at least one of them is non-negative), there exists at least one analytic set of solutions of the form (16), where ρ_t is the maximal integral root of (15). The remaining solutions corresponding to other integral roots are usually singular in the origin, but in exceptional cases may also be analytic.

It should be pointed out that the Birkhoff theorem is an existence theorem, which as such does not provide the actual form of the canonical equation nor the transformation matrix. In practice at least the canonical equation can usually be found relatively easy by the use of (14), keeping in mind that the $P_{rs}(z)$ are polynomials of a given degree. To this aim we invert Eq. (14) and express it in terms of the relevant expansion coefficients. This yields, for every integer $l\geqslant 0$, a system of m^2 equations

$$\sum_{i=0}^{l}\left(\{a_{rk}^{(l-i)}\}\{P_{ks}^{(q+1-i)}\}-\{p_{rk}^{(q-i)}\}\{a_{ks}^{(l-i)}\}\right)=(l-q-1)\{a_{rs}^{(l-q-1)}\}, \tag{17}$$

where expansion coefficients for $\{p_{rk}(z)\}$, $\{a_{rk}(z)\}$, and $\{P_{rs}(z)\}$ are defined by (10), (12), and $P_{rs}(z)=\Sigma_{k=0}^{q+1}P_{rs}^{(k)}z^k$, respectively. We assume also that $\{a_{rk}^{(i)}\}$ and $\{P_{rk}^{(i)}\}$ with negative indices i are zero matrices.

This formula can now be used to find the coefficients $P_{rs}(z)$ of the transformed system. In this case we only need the equations corresponding to $l=0,\ldots,q+1$. Here the trivial case with $l=0$ immediately yields

$$\{P_{rs}^{(q+1)}\}=\{p_{rs}^{(q)}\}. \tag{18}$$

For higher l, $1\leqslant l\leqslant q+1$, the resulting expansion coefficients in the transformed system may also depend on the $a_{ks}^{(1)},\ldots,a_{ks}^{(q+1)}$ coefficients in the expansion of the transformation matrix. These coefficients thus may enter the transformed system as extra degrees of freedom, which we will denote as the *parameters* of the transformed equation. The canonical transformation can only be defined up to these parameters. However, in the context of a physical model, their values will be constrained by the requirement that the solution of the initial system belong to the Bargmann–Fock space.

The remaining equations in the system (17), i.e., the formulas corresponding to $l=q+2$, $q+3$, ..., form a set of recurrence equations for the $\{a_{rs}(z)\}$ matrix. This system determines $\{a_{rs}(z)\}$ as a function of the parameters of the transformed system. The procedure of determining the transformation matrix for a given set of parameters is in general infinite and it may be very difficult to find the parameters that lead to solutions in the Bargmann–Fock space. Hence it is conceivable that we know the initial (9) and the transformed (13) systems of equations, without being able to solve the transformation matrix (12). In some cases this still allows us to draw some important conclusions about features of physical interest, such as degeneracies or symmetries.

A special case arises if we assume that the expansion (12) of $\{a_{rs}(z)\}$ in negative powers of z is finite. In this case confinement to the Bargmann–Fock space can indeed easily be guaranteed. If the highest order in the denominators of (12) is not greater than ρ_t from (16), which is the lowest power in the expansion of the $F_s^{(t)}(z)$, then the corresponding solution of the initial system is automatically analytic in the origin. In this case the system (17) also remains finite and can be solved. This procedure precisely leads to the isolated exact solutions of the initial system.

IV. THE SOLUTION OF A TWO-LEVEL SYSTEM COUPLED TO A SINGLE QUANTIZED MODE

A. The canonical form

In this section we derive the canonical form of the dynamical equations for a two-level system coupled to a single quantized mode. The Hamiltonian of such a system, sometimes called Rabi Hamiltonian,[4] is of the form

$$H=\omega a^+a+\mu\sigma_3+\lambda(\sigma^++\sigma^-)(a^++a), \tag{19}$$

where a^+ and a are boson field (7) creation and annihilation operators, $\sigma^{\pm}=\frac{1}{2}(\sigma_1\pm i\sigma_2)$, and σ_1, σ_2, σ_3 are Pauli matrices. The parameter ω is the boson field frequency, 2μ is the atomic level separation, and λ is the atom–boson field coupling constant. We choose the energy unit in such a way that $\omega=1$, and we assume that λ and μ are not vanishing simultaneously.

The first step to solve the system (19) is to make a unitary transformation which replaces operators $\sigma_1\to\sigma_3$, $\sigma_3\to\sigma_1$, and $\sigma_2\to-\sigma_2$. Then we write the stationary Schrödinger equation for the two-component wavefunction in the position variable $\binom{f_1(\xi)}{f_2(\xi)}$. In the second step, by replacing $a^+\to z$ and $a\to d/dz$, we perform a transition to a Bargmann–Fock space. In this space the Schrödinger equation is equivalent to a system of two first-order differential equations for the Bargmann–Fock space functions $f_1(z)$, $f_2(z)\in\mathscr{F}_1$:

$$\frac{d}{dz} f_1(z) = \frac{E-\lambda z}{z+\lambda} f_1(z) - \frac{\mu}{z+\lambda} f_2(z),$$
$$\frac{d}{dz} f_2(z) = -\frac{\mu}{z-\lambda} f_1(z) + \frac{E+\lambda z}{z-\lambda} f_2(z), \tag{20}$$

where E is an eigenenergy of $\mathscr{H}$. Note that in the Schrödinger representation of creation and annihilation operators we have $a^+ \to (1/\sqrt{2})(\xi - ip_\xi)$, $a \to (1/\sqrt{2})(\xi + ip_\xi)$, where ξ and p_ξ are conjugate position and momentum. The system corresponding to (20) in this representation consist of two second-order differential equations in a real variable ξ.

The present Bargmann–Fock space formulation of the problem has been investigated earlier and approximate solutions have been found.[4,9] In addition Kuś has derived some isolated exact solutions, corresponding to degenerate levels.[3]

For our purposes we point out three properties of the system. First, it is of the form (9) with two finite singularities in $z=\lambda,-\lambda$. Second, expanding coefficients of (20) in a Laurent series (10) we find that $q=0$ and therefore the singular point at infinity is of the first rank. Finally, we note the following symmetry: if $\binom{f_1(z)}{f_2(z)}$ is a solution of (20), then $\binom{f_2(-z)}{f_1(-z)}$ is also a solution, corresponding to the same energy value.

The Birkhoff theorem is found to apply to the system in (20). Hence one can claim the existence of a canonical form. With $q=0$, the coefficients of this form will be polynomials of the first degree! They can be obtained from Eqs. (17) and (18), as explained in the previous section. The linear terms of $P_{rs}(z)$ are inferred at once from (18), i.e., $P_{rs}^{(1)}(z) = (-1)^r \lambda \delta_{rs}$. To calculate the remaining four zeroth-order terms of $P_{rs}(z)$ we use Eq. (17) with $l=1$. The canonical form of the system (20) is therefore

$$z \frac{d}{dz} F_1(z) = (E - \lambda z + \lambda^2) F_1(z) + (-\mu - 2\lambda a_{12}^{(1)}) F_2(z),$$
$$z \frac{d}{dz} F_2(z) = (-\mu + 2\lambda a_{21}^{(1)}) F_1(z) + (E + \lambda z + \lambda^2) F_2(z), \tag{21}$$

where $F_1(z)$ and $F_2(z)$ are linearly transformed $f_1(z)$ and $f_2(z)$ (11), and $a_{12}^{(1)}$ and $a_{21}^{(1)}$ are parameters belonging to the transformation matrix (12).

The main feature of the canonical system is that it has only one singularity at $z=0$, and because of that is exactly solvable. Prior to solving it, however, we exploit the symmetry of solutions $\binom{f_1(z)}{f_2(z)}$ of the initial system (20). To preserve this symmetry in the transformed pair, i.e., if $\binom{F_1(z)}{F_2(z)}$ is a solution of (21), then so is $\binom{F_2(-z)}{F_1(-z)}$, we must impose the following symmetry of the transformation matrix

$$a_{ij}(z) = a_{[i+1][j+1]}(-z), \quad i,j = 1,2, \tag{22}$$

where $[\cdot + \cdot]$ denotes an addition modulo 2.

B. Quantization conditions and canonical solutions

Physical constraints require the solutions of (20) belong to the Bargmann–Fock space, i.e., to converge in the entire plane. This leads to quantization conditions, as we will show in this section.

The canonical system contains four parameters λ, μ, E, and $a_{12}^{(1)}$. In the usual perception of the problem λ and μ are external quantities, describing the physics of the system, while E and $a_{12}^{(1)}$ are essentially free parameters, to be determined by the quantum conditions. The indicial equation (15) corresponding to the system (21) is seen to link E and $a_{12}^{(1)}$:

$$\rho = E + \lambda^2 \pm A, \tag{23}$$

where $A = \mu + 2\lambda a_{12}^{(1)}$. For the system (21) to have solutions in the Bargmann–Fock space, at least one value of ρ must be a non-negative integer. The value of A thus determines the whole energy spectrum, but in turn it is controlled by the $a_{12}^{(1)}$ parameter, from which the transformation matrix can be generated via (17). For the time being we will treat it as a free parameter, delineating classes of solutions in the energy spectrum. As we will see later its value will be fixed by the requirement that the solutions of the original system (20) are in the Bargmann–Fock space.

The general solution of (21) can be obtained by transforming it into a second-order form

$$z^2 F_1''(z) + z[1 - 2(E + \lambda^2)]F_1'(z) + [(E + \lambda^2)^2 - A^2 + \lambda z - \lambda^2 z^2]F_1(z) = 0. \tag{24}$$

This equation can be reduced to a confluent hypergeometric (or Kummer) equation. Its general solution is a combination of two functions

$$\begin{aligned} F_1(z) = {} & C_1 \exp(\lambda z)\, {}_1F_1(1 + A, 1 + 2A; -2\lambda z) z^{E + \lambda^2 + A} \\ & + C_2 \exp(\lambda z)\, {}_1F_1(1 - A, 1 - 2A; -2\lambda z) z^{E + \lambda^2 - A}, \end{aligned} \tag{25}$$

with arbitrary C_1 and C_2. The function ${}_1F_1(a, c; z)$ is called confluent series or Kummer function and is defined for all complex a, z and $c \neq -n$, $n = 0,1,2,...$:

$${}_1F_1(a, c; z) = 1 + \frac{a}{c}\frac{z}{1!} + \frac{a(a+1)}{c(c+1)}\frac{z^2}{2!} + \frac{a(a+1)(a+2)}{c(c+1)(c+2)}\frac{z^3}{3!} + \cdots . \tag{26}$$

The Kummer function is entire. The solutions for $F_2(z)$ are of the same general form (25), with however z replaced by $-z$.

The asymptotic behavior of the solution (25) for $|z| \to \infty$ is restricted by the function $z^{\alpha_1} \exp(\lambda z) + z^{\alpha_2} \exp(-\lambda z)$, where α_1 and α_2 are real numbers[10] and therefore the condition (4) is always obeyed. Consequently the solution (25) belongs to the Bargmann—Fock space $\mathscr{F}_1$, provided at least one of the roots of the indicial equation (23) is a non-negative integer.

A particularly simple case occurs if $\lambda = 0$ because then the transformed system (21) coincides with the initial one (20). The transformation matrix reduces in this case to the unit matrix.

Let us now discuss the solutions (25) and their degeneracy for different values of $E + \lambda^2$.

(i) If $E + \lambda^2$ is neither an integer nor a half-integer, then, to get physical solutions, we should take A such that one of the numbers $\rho_1 = E + \lambda^2 + A$ and $\rho_2 = E + \lambda^2 - A$ is a non-negative integer. In this case, according to the general rule D_1, one of the two functions composing $F_1(z)$ can be entire. The corresponding solution for $F_2(z)$ is also one-dimensional and is given by $F_2(z) = (-1)^{\rho_t + t} F_1(-z)$.

(ii) If $E + \lambda^2$ is a half-integer, then we take A also half-integral. Despite the fact that both $E + \lambda^2 + A$ and $E + \lambda^2 - A$ are now integers (rule D_2), the solutions $F_1(z)$ and $F_2(z)$ are still one-dimensional because in this case one of the numbers $1 + 2A$ or $1 - 2A$ is a non-positive integer and the corresponding Kummer function is not defined.

(iii) If $E + \lambda^2$ is an integer, we can take the simple choice $A = 0$. Then, for $E + \lambda^2 \geqslant 0$, each of the solutions is entire and forms a one-dimensional space (rule D_1), but because the system (21) is diagonal we can always take its two linearly independent solutions of the form $\binom{F_1(z)}{F_2(z)}$ and $\binom{F_1(z)}{-F_2(z)}$. Consequently in this case the solutions are degenerate. This class of solutions will comprise the exact solutions found by Kuś.

(iv) If $E + \lambda^2$ is an integer and $E + \lambda^2 > 0$, we can also take A integral, $0 < |A| \leqslant E + \lambda^2$. In this case, although the system (21) is no more diagonal, solutions $F_1(z)$ and $F_2(z)$ become two-dimensional and lead to degenerate solutions. This represents the rarest case of D_2

when two roots of the indicial equation are integral and both corresponding solutions are analytical.

To summarize we conclude that the only case where solutions are degenerate can occur when $E+\lambda^2$ is a non-negative integer.

C. The isolated exact solutions

In the previous section we have shown that the canonical form of the Rabi Hamiltonian can be solved within Bargmann–Fock conditions. This results in a coupling between A and E parameters, which is interesting in its own right, but does not lead to quantized energies. As we have already mentioned, the true quantization condition stems from the requirement that the solutions of the original system belong to the Bargmann–Fock space. This implies that the transformation of the canonical solutions must act within the Bargmann–Fock space. In this way we fix A and hence E.

In general this procedure is nontrivial since the transformation matrix is generated by an infinite system of equations (17), yielding an infinite series of coefficients $a_{rs}^{(k)}$. In this section we will not be concerned with the general case, but only study the exactly solvable class of solutions, which corresponds to $A=0$. We assume that the transformation is nontrivial, i.e., $\lambda\neq 0$.

Let us first consider the simplest possibility $\mu=0$. With $A=0$, and hence $a_{12}^{(1)}=0$, the indicial equation yields that $\rho=E+\lambda^2$ must be a non-negative integer. It is easy to find that the corresponding transformation matrix is diagonal and reads

$$\{a_{rs}(z)\}=\begin{pmatrix} \left(1+\dfrac{\lambda}{z}\right)^{E+\lambda^2} & 0 \\ 0 & \left(1-\dfrac{\lambda}{z}\right)^{E+\lambda^2} \end{pmatrix}, \tag{27}$$

whereas the solutions are generated by

$$F_1(z)=\exp(-\lambda z)z^{E+\lambda^2}, \qquad F_2(z)=\exp(\lambda z)z^{E+\lambda^2}. \tag{28}$$

Note that in this case the expansion (12) in negative powers of both diagonal terms terminate. The last nonzero coefficients are $a_{rs}^{(E+\lambda^2)}$. On the other hand, the lowest power of z in the expansion of the transformed solution (25) is also $E+\lambda^2$. It is then easily verified that the solution of the initial system, which follows from (11), is of form (1) and thus belongs to the Bargmann–Fock space. The energy spectrum is obtained directly from the indicial equation (23) and reads $E_\rho=\rho-\lambda^2$, where $\rho=0,1,2,\ldots$.

In the line of this example we now turn to the more general case $\mu\neq 0$ but keep the $a_{rs}^{(k)}$ matrix finite. As a first example we assume that the expansion (12) of the transformation matrix terminates, and $a_{rs}^{(1)}$ are the only nonzero coefficients. In other words, $a_{rs}^{(2)}=a_{rs}^{(3)}=\cdots=0$. In this case the system (17) is also finite because starting from $l=3$ all the higher-order equations are equivalent to equations corresponding to $l=2$. Taking into account symmetry properties (22) of the matrix, the system reduces to four equations

$$\begin{aligned} &\overline{a_{11}}+2\mu\overline{a_{12}}+2\lambda\overline{a_{12}^2}-\lambda(E+\lambda^2)=0, \qquad 2\mu\overline{a_{11}}+\overline{a_{12}}+2\lambda\overline{a_{11}}\,\overline{a_{12}}+\lambda\mu=0, \\ &(E+\lambda^2)\overline{a_{11}}+\mu\overline{a_{12}}-\lambda(E+\lambda^2)=0, \qquad \mu\overline{a_{11}}+(E+\lambda^2)\overline{a_{12}}+\lambda\mu=0, \end{aligned} \tag{29}$$

where we denote $\overline{a_{kl}}=a_{kl}^{(1)}$ for convenience. Let μ be nontrivial and $0<\mu\leqslant(E+\lambda^2)$. Then, after some algebra, one can show that the system (29) is equivalent to the transformation matrix

$$\{a_{rs}(z)\}=\begin{pmatrix} 1+\dfrac{1+\mu^2}{4\lambda z} & -\dfrac{\mu}{2\lambda z} \\ \dfrac{\mu}{2\lambda z} & 1-\dfrac{1+\mu^2}{4\lambda z} \end{pmatrix} \tag{30}$$

and two other conditions: $E+\lambda^2=1$ and $4\lambda^2+\mu^2=1$. From the $a_{12}(z)$ element in (30) it also follows that $A=\mu+2\lambda a_{12}^{(1)}=0$.

Thus the very assumption that the transformation matrix terminates gave us the form of the matrix, the values of $E+\lambda^2$ and A, showing that they correspond to a degenerate solution of (25). In addition the system has energy $E=1-\lambda^2$ only if the atomic level separation 2μ and the atom–boson field coupling λ obey condition $4\lambda^2+\mu^2=1$. The corresponding eigenfunction $\binom{F_1(z)}{F_2(z)}$ is given by (28) and $\binom{f_1(z)}{f_2(z)}$ can be found by applying (11). One can easily show that $f_1(z)$ and $f_2(z)$ belong to the Bargmann–Fock space. This solution agrees with the first root of the Kuś series.[3]

In an analogous way one can show that if the transformation matrix terminates from the third-order coefficients onwards, $a_{rs}^{(3)}=a_{rs}^{(4)}=\cdots=0$, and $0<\mu\leqslant(E+\lambda^2)$, then the transformation matrix functions are

$$\begin{aligned} a_{11}(z)=a_{22}(-z)&=1+\frac{2\lambda+\dfrac{\mu^2}{2\lambda}}{z}+\frac{\lambda^2+\mu^2+\dfrac{\mu^4-\mu^2}{8\lambda^2}}{z^2}, \\ a_{12}(z)=a_{21}(-z)&=-\frac{\mu}{2\lambda z}+\frac{\mu(6\lambda^2+\mu^2-1)}{4\lambda^2 z^2}, \end{aligned} \tag{31}$$

i.e., again $A=0$ and the remaining conditions are $E+\lambda^2=2$ and $32\lambda^4-32\lambda^2+12\lambda^2\mu^2-5\mu^2+\mu^4+4=0$, which corresponds to the second root of the Kuś series. In this way all solutions of the Rabi Hamiltonian characterized by a terminating $\{a_{rs}(z)\}$ can be generated. They are found to coincide with all known exact solutions.

V. DISCUSSION

The Rabi Hamiltonian describes the coupling between a two-level system and a single mode through a linear interaction term $\lambda\sigma_1(a^+ + a)$. This problem is relevant in quantum optics but also appears in molecular physics as the simplest example of vibronic coupling.[11,12]

In Bargmann–Fock space it can be represented by a system of two first-order differential equations, as shown in (20). For $\mu=0$ this system separates into two independent equations:

$$\begin{aligned} (z+\lambda)\frac{d}{dz}f_1(z)&=(E-\lambda z)f_1(z), \\ (z-\lambda)\frac{d}{dz}f_2(z)&=(E+\lambda z)f_2(z). \end{aligned} \tag{32}$$

This situation corresponds to a highly symmetric case with two uncoupled harmonic oscillators that are displaced to the left and to the right in coordinate space,[9] and cross at the coordinate origin. From this perspective the introduction of the level separation 2μ may be viewed as a symmetry-lowering perturbation, which couples the two oscillators.

If we now compare the original system (20) to the canonical one (21), we still have essentially a set of two displaced oscillators—but now the coupling term no longer corresponds to μ but to $\mu+2\lambda a_{12}^{(1)}$! Hence the canonical transformation provides a degree of freedom that allows us to

perform a displacement in the space of the coupling parameter itself. We can thus adjust $a_{12}^{(1)}$ in such a way that it compensates for the energy gap, by requiring $a_{12}^{(1)}=-\mu/2\lambda$, or $A=0$. System (21) then becomes

$$z\frac{d}{dz}F_1(z)=(E-\lambda z+\lambda^2)F_1(z), \qquad z\frac{d}{dz}F_2(z)=(E+\lambda z+\lambda^2)F_2(z). \tag{33}$$

This system again describes two degenerate harmonic oscillators that are displaced in coordinate space and also underwent a translation in z space over $+$ or $-\lambda$.

We thus have shown that the exact solutions that are found for $A=0$ can be mapped onto the energy spectrum of a degenerate harmonic oscillator. A similar result can also be obtained for the Juddian exact solutions of the $E\otimes e$ Jahn–Teller Hamiltonian.[13]

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Boson–fermion model with two-body interactions: Exact results

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A one-dimensional boson–fermion model with two-body interactions between the two types of chiral fermions is considered. It is shown that the model is exactly soluble and the general Bethe eigenstates are constructed. On the basis of the Bethe ansatz equations, the ground state, the low lying elementary excitations, and the thermodynamics are also given in some closed integral equations. © *1996 American Institute of Physics.* [S0022-2488(96)03305-2]

I. INTRODUCTION

A many-body problem plays a very important role in modern physics, especially in statistical physics and condensed matter physics. After the establishment of quantum mechanics, very many methods had been developed to approach this problem. However, most of the theories are approximate and exact results are still rare. Although many efforts have been done in this aspect, the exact results were only obtained in a few special two-dimensional classical models and one-dimensional quantum models. At present, perhaps the most powerful method to approach one-dimensional quantum soluble models is the Bethe ansatz method. After the elegant work of Bethe,[1] a dozen of models have been solved with his brilliant ansatz. Great achievements have been reached in $1+1$-dimensional quantum field theory[2–4] and condensed matter physics.[5,6] Among the exactly soluble models, there is a special type, i.e., the N wave interaction model[7] in which there are interactions breaking the conservation of the particle numbers. Such interactions put the eigenstates of the Hamiltonian into the coherentlike states. The first Bethe ansatz result of the quantum three wave interaction model was given by Wadati and co-workers after some lengthy calculations.[8] Very recently, a systematic method to approach such interacting systems has been developed by one of the present authors and co-workers.[9]

In this article, we study the boson–fermion model with two-body interactions in one dimension. It is shown that this model is also Bethe ansatz soluble.

The Hamiltonian we shall consider reads

$$H=\int\left\{-i\left[Q_1^\dagger\frac{\partial}{\partial x}Q_1-Q_3^\dagger\frac{\partial}{\partial x}Q_3\right]+\nu Q_2^\dagger Q_2+cQ_1^\dagger Q_3^\dagger Q_3Q_1+g[Q_1^\dagger Q_3^\dagger Q_2+Q_2^\dagger Q_3Q_1]\right\}dx, \tag{1}$$

where the $Q_j^\dagger$s(Q_j's) are particle creation (annihilation) operators. $Q_1^\dagger$ and $Q_3^\dagger$ create spinless chiral fermions with different chiral indices ±1 and $Q_2^\dagger$ creates localized bosons; g is the ''contraction-decay'' coupling constant; c describes the coupling constant between Q_1 and Q_3 particles. Note such an interaction in the Tomonaga model[10] is irrelevant but indeed relevant in the present model as in the Luttinger model;[11] ν is a positive number which denotes the virtual level of the bosons. In our model, we define the bosons being localized. Thus the bosons may describe the bi-polaron

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states or the dimer states.[13] Although the bosons are static initially, the spontaneous decay into itinerant fermions does allow them to behave itinerantly. The outline of this article is the following. In Sec. II we construct the eigenstates of the model Hamiltonian. Through the consideration of a two-body state, the general eigenstates can be constructed with a theorem. In Sec. III, the ground state or the physical vacuum (Fermi sea) is discussed in a cut-off scheme because the energy spectrum is not bounded from below. Some elementary excitations are given in Sec. IV. It is found that all the four types of elementary excitations fall into the particle-hole scheme with the ''back flow'' of the Fermi sea compensated. The thermodynamics is given in Sec. V by a closed set of integral equations. As checks, some special cases are studied on the basis of the integral equations.

II. CONSTRUCTION OF THE EIGENSTATES

We shall follow the method developed in Ref. 9 to construct the eigenstates of the Hamiltonian (1). Traditionally, the Bethe ansatz method is used to construct the common eigenstates of the Hamiltonian, the total momentum, and the particle number(s). However, the total particle number is not conserved in the present model. Fortunately, the quantities

$$N_1=\int [Q_1^\dagger Q_1+Q_2^\dagger Q_2]dx, \quad N_2=\int [Q_3^\dagger Q_3+Q_2^\dagger Q_2]dx, \tag{2}$$

which we call ''pseudoparticle numbers'' and the total momentum

$$P=-i\int \sum_{j=1}^{3} Q_j^\dagger \frac{\partial}{\partial x} Q_j \, dx \tag{3}$$

are conserved. Therefore, we can specify the eigenstates by $|N_1,N_2\rangle$. To show the procedure clearly, it is convenient to consider first the $N_1=N_2=1$ state. Such a state is the simplest nontrivial state which gives the main information about the general eigenstates. The $|1,1\rangle$ state can be written as

$$|1,1\rangle=\int dx_1\, dx_2\, \Psi(x_1|x_2)Q_1^\dagger(x_1)Q_3^\dagger(x_2)|0\rangle+\int dy\, \Psi_1(y)Q_2^\dagger(y)|0\rangle, \tag{4}$$

where $|0\rangle$ is the vacuum state defined by $Q_j|0\rangle=0$. The Schrödinger equation $H|1,1\rangle=E|1,1\rangle$ leads to

$$\begin{gathered}-i\left[\frac{\partial}{\partial x_1}-\frac{\partial}{\partial x_2}\right]\Psi(x_1|x_2)+[g\Psi_1(x_1)+c\Psi(x_1|x_2)]\delta(x_1-x_2)=E\Psi(x_1|x_2),\\ \nu\Psi_1(y)+g\Psi(y|y)=E\Psi_1(y),\end{gathered} \tag{5}$$

where E is the eigenvalue. To solve the above equations, we make the following ansatz:

$$\begin{gathered}\Psi(x_1|x_2)=\exp[ikx_1+iqx_2][\theta(x_1-x_2)+\theta(x_2-x_1)S(k,q)],\\ \Psi_1(y)=S^+(k,q)\Psi(y|y),\end{gathered} \tag{6}$$

where $\theta(x)$ is the step function with $\theta(0)=\frac{1}{2}$. Other choices of $\theta(0)$ value induce nothing but the renormalization of the coupling constants c and g. The discontinuity of $\Psi(x_1|x_2)$ at $x_1=x_2$ is due to the linear kinetic energy term in the Hamiltonian. Substituting Eq. (6) into Eq. (5) we deduce the two-body S matrix and the contraction matrix S^+ as

$$S(k,q)=S^{-1}(q,k)=e^{i\phi}\,\frac{k-q-\nu+i\mu}{k-q-\nu-i\mu^*},$$
$$S^{+}(k,q)=\frac{g}{k-q-\nu}, \tag{7}$$

with $\mu=g^2/(4+ic)$ and $e^{i\phi}=(4-ic)/(4+ic)$. Then the state $|1,1\rangle$ defined in Eq. (4) is an eigenstate with the eigenenergy $E=k-q$.

Now we turn to construct the general eigenstate with arbitrary N_1 and N_2. Such an eigenstate can be written as

$$\begin{aligned}|N_1,N_2\rangle=&\int\sum_{M=0}^{\min[N_1,N_2]}\Psi_M(x_1,\ldots,x_{N_1-M}|y_1,\ldots,y_{N_2-M}|z_1,\ldots,z_M)\\&\times[M!(N_1-M)!(N_2-M)!]^{-1}\\&\times\prod_{i=1}^{N_1-M}Q_1^{\dagger}(x_i)dx_i\prod_{j=1}^{N_2-M}Q_3^{\dagger}(y_j)dy_j\prod_{l=1}^{M}Q_2^{\dagger}(z_l)dz_l|0\rangle.\end{aligned} \tag{8}$$

Notice that the $Q_1^{\dagger}(x_i)$s and $Q_3^{\dagger}(y_j)$s in the products have a well defined order. That means that if $i<i'$, $Q_1^{\dagger}(x_i)$ must be on the left-hand side of $Q_1^{\dagger}(x_{i'})$. From the Schrödinger equation $H|N_1,N_2\rangle=E|N_1,N_2\rangle$ we get

$$\begin{aligned}&\left\{-i\sum_i\frac{\partial}{\partial x_i}+i\sum_j\frac{\partial}{\partial y_j}+M\nu\right\}\Psi_M+g\sum_{l=1}^{M}\Psi_{M-1}(\ldots,z_l,z_i,\ldots|\ldots,z_{l-1},z_{l+1},\ldots)\\&+g\sum_{i,j}(-1)^{N_1-M-i+j-1}\Psi_{M+1}(\ldots,x_{i-1},x_{i+1},\ldots|\ldots,y_{j-1},y_{j+1},\ldots|x_i,\ldots)\\&\times\delta(x_i-y_j)+c\sum_{i,j}\delta(x_i-y_j)\Psi_M=E\Psi_M.\end{aligned} \tag{9}$$

To give the explicit form of Ψ_M, it is convenient to construct first Ψ_0. We define the color indices of the coordinates x_i and y_j as $\alpha_i=1$ and $\alpha_{N_1+j}=-1$, respectively. Also, we introduce the color indices of the momenta as $\gamma_i=1$ for $\{k_1,\ldots,k_{N_1}\}$ and $\gamma_{N_1+j}=-1$ for $\{q_1,\ldots,q_{N_2}\}$, where k_is and q_js are the momenta carried by the Q_1 and Q_3 particles, respectively. A Q_2 particle may carry a momentum k_i+q_j as shown in Eq. (6). Introduce the notations

$$\{s_1,\ldots,s_N\}=\{k_1,\ldots,k_{N_1};q_1,\ldots,q_{N_2}\},$$
$$\{t_1,\ldots,t_N\}=\{x_1,\ldots,x_{N_1};y_1,\ldots,y_{N_2}\},$$

and then make the following ansatz:

$$\Psi_0(x_1,\ldots,x_{N_1}|y_1,\ldots,y_{N_2})=\sum_{P,Q} A_P(Q)\exp\left[i\sum_{j=1}^{N} s_{P_j}t_{Q_j}\right]$$
$$\times\prod_{j=1}^{N}\delta_{\alpha_{Q_j}}^{\gamma_{P_j}}\theta(t_{Q_1}<\cdots<t_{Q_N})=\sum_{Q,P}\Psi_0[Q,P]. \tag{10}$$

Above we have put $N=N_1+N_2$. P,Q are permutations of (1,..., N) and $A_P(Q)$s are constants which satisfy

$$A_{\ldots,P_i,P_{i+1},\ldots,}(Q)=-A_{\ldots,P_{i+1},P_{i\ldots,}}(Q), \tag{11}$$

due to the antisymmetry of fermion wave functions. The general eigenstates can be constructed by the following theorem.

Theorem: The constants $A_P(Q)$s in Eq. (10) satisfy

$$A_{\ldots,P_i,P_{i+1},\ldots,}(\ldots,Q_i,Q_{i+1},\ldots,)=S(P_i,P_{i+1})A_{\ldots,P_{i+1},P_i,\ldots,}(\ldots,Q_{i+1},Q_i,\ldots), \tag{12}$$

with the S matrix

$$S(P_i,P_j)=e^{i\phi}\frac{s_{P_i}-s_{P_j}-\nu+i\mu}{s_{P_i}-s_{P_j}-\nu-i\mu^*}\quad\text{for}\ \ \gamma_{P_i}=1,\gamma_{P_j}=-1,$$

$$S(P_i,P_j)=e^{-i\phi}\frac{s_{P_i}-s_{P_j}+\nu+i\mu^*}{s_{P_i}-s_{P_j}+\nu-i\mu}\quad\text{for}\ \ \gamma_{P_i}=-1,\gamma_{P_j}=1, \tag{13}$$

$$S(P_i,P_j)=1\quad\text{for}\ \ \gamma_{P_i}=\gamma_{P_j}.$$

Then the wave function (10) is uniquely defined. Ψ_M in Eq. (8) is the M order contraction of Ψ_0. A z_l coordinate corresponds to the contraction of a pair

$$\{x_i=z_l,y_j=z_l|i>N_1-M,\quad j>N_2-M\}.$$

In a given range $[Q,P]$, put

$$x_i=z_l=t_{Q_m},\quad y_j=z_l=t_{Q_{m+1}};\ \ k^{(l)}=s_{P_m},\quad q^{(l)}=s_{P_{m+1}},$$

and

$$\Psi_M[Q,P]=\sum_{Q,P}\prod_{l=1}^{M}S^+(k^{(l)},q^{(l)})(-1)^{N_1-M-i+j-1}\Psi_0[Q,P].$$

Then the state defined in Eq. (8) is an eigenstate with the eigenenergy

$$E=\sum_{i=1}^{N_1}k_i-\sum_{j=1}^{N_2}q_j.$$

Proof: The above theorem can be demonstrated directly from Eq. (9). In a given coordinate and momentum arrangement $[Q,P]$, the corresponding term $\Psi_M[Q,P]$ of Ψ_M can be expressed as

$$\Psi_M[Q,P]=A_M[Q,P]\prod_{i=1}^{N_1-M}\exp(ik_i'x_i)\prod_{j=1}^{N_2-M}\exp(iq_j'y_j)\prod_{l=1}^{M}\exp[i(k^{(l)}+q^{(l)})z_l],$$

k_i' and $k^{(l)}$ belong to $\{k_1,\ldots,k_{N_1}\}$ and q_j' and $q^{(l)}$ belong to $\{q_1,\ldots,q_{N_2}\}$. $A_M[Q,P]$ is a constant. The theorem defines

$$\Psi_{M-1}[Q,P](\ldots,z_l|z_l,\ldots|\ldots,z_{l-1},z_{l+1},\ldots)=\frac{1}{S^+(k^{(l)},q^{(l)})}\Psi_M[Q,P],$$

$$\begin{aligned}&\Psi_{M+1}[Q,P](\ldots,x_{i-1},x_{i+1},\ldots|\ldots,y_{j-1},y_{j+1},\ldots|x_i,\ldots)\\&\quad=(-1)^{N_1-M-i+j-1}S^+(k_i',q_j')\Psi_M[Q,P].\end{aligned}$$

Thus we have

$$\begin{aligned}&M_\nu\Psi_M[Q,P]+g\sum_{l=1}^{M}\Psi_{M-1}[Q,P](\ldots,z_l|z_l,\ldots|\ldots,z_{l-1},z_{l+1},\ldots)\\&\quad=\sum_{l=1}^{M}(k^{(l)}-q^{(l)})\Psi_M[Q,P]\end{aligned}\tag{14}$$

and

$$\begin{aligned}&-i\left\{\sum_{i=1}^{N_1-M}\frac{\partial}{\partial x_i}-\sum_{j=1}^{N_2-M}\frac{\partial}{\partial y_j}\right\}\Psi_M[Q,P]+\sum_{i,j}[c+gS^+(k_i',q_j')]\Psi_M[Q,P]\delta(x_i-y_j)\\&\quad=\left\{\sum_{i=1}^{N_1-M}k_i'-\sum_{j=1}^{N_2-M}q_j'\right\}\Psi_M[Q,P].\end{aligned}\tag{15}$$

Substituting Eqs. (14) and (15) into Eq. (9) we find that Eq. (9) is an identity if $E=\Sigma_{i=1}^{N_1}k_i-\Sigma_{j=1}^{N_2}q_j$. Then the state (8) with the functions Ψ_Ms defined in the theorem is really an eigenstate. (QED)

From the periodic conditions

$$\Psi_M(\ldots,x_i|\ldots,y_j,\ldots)=\Psi_M(\ldots,x_i+L,\ldots)=\Psi_M(\ldots,y_j+L,\ldots)$$

we get the following Bethe ansatz equations:

$$e^{ik_iL}=e^{iN_2\phi}\prod_{j=1}^{N_2}\frac{k_i-q_j-\nu+i\mu}{k_i-q_j-\nu-i\mu^*},\quad e^{iq_jL}=e^{-iN_1\phi}\prod_{i=1}^{N_1}\frac{q_j-k_i+\nu+i\mu^*}{q_j-k_i+\nu-i\mu},\tag{16}$$

where L is the length of the system.

III. PHYSICAL VACUUM

Take the logarithm of Eq. (16),

$$k_i L = 2\pi I_i + \sum_j \Theta(k_i, q_j) + N_2 \phi, \quad q_j L = 2\pi J_j - \sum_i \Theta(k_i, q_j) - N_1 \phi, \tag{17}$$

where I_i and J_j are integers or half-odd integers and

$$\Theta(k,q) = -2 \tan^{-1} \frac{k - q - \nu - \mu_I}{\mu_R}$$

with

$$\mu_R = \mathrm{Re}\ \mu, \mu_I = \mathrm{Im}\ \mu.$$

There are no two I_is or two J_js and then two k_is or two q_js being equal. It can be deduced from Eq. (16) that the present model has no bound state. That means the spectrum of the Hamiltonian must be given in real $\{k,q\}$ sets. A set of $\{I_i, J_j\}$ defines a unique eigenstate of the Hamiltonian and Eq. (17) gives a complete set of the solutions.[12]

Because the energy spectrum is not bounded from below, a cutoff K should be introduced. The cutoffs are defined as $k_i > -K$ and $q_j < K$. In the ground state, all I_is and J_js must be consecutive numbers. Now we consider the thermodynamic limit of the system with $N \to \infty$, $L \to \infty$, and $N/L = D$ keeping finite. Introducing the density functions

$$\rho_0(k) = \frac{1}{L(k_{i+1} - k_i)}, \quad \sigma_0(q) = \frac{1}{L(q_{j+1} - q_j)}, \tag{18}$$

and taking the infinite limit we get

$$\begin{aligned} 1 &= 2\pi\rho_0(k) - \int_0^K \frac{2\mu_R \sigma_0(q)\, dq}{[k - q - \nu - \mu_I]^2 + \mu_{R^2}}, \\ 1 &= 2\pi\sigma_0(q) - \int_{-K}^0 \frac{2\mu_R \rho_0(k)\, dk}{[q - k + \nu + \mu_I]^2 + \mu_{R^2}}. \end{aligned} \tag{19}$$

Here we have put the Fermi level at zero.

The Fermi sea consists thus of all negative k-states and all positive q-states are filled with cutoffs. The density of ground state energy is

$$E_g/L = \int_{-K}^0 k\rho_0(k)\, dk - \int_0^K q\sigma_0(q)\, dq, \tag{20}$$

and the momentum density is

$$P_g/L = \int_{-K}^0 k\rho_0(k)\, dk + \int_0^K q\sigma_0(q)\, dq, \tag{21}$$

with the cutoff K determined by

$$D = \int_{-K}^0 \rho_0(k)\, dk + \int_0^K \sigma_0(q)\, dq. \tag{22}$$

IV. ELEMENTARY EXCITATIONS

The excitations are described by the ''quasiholes'' in the Fermi sea and the ''quasiparticles'' above the Fermi level. There are four types of such excitations. In an isolated system, the number of quasiholes is exactly the same of that of quasiparticles. For an excited state, Eq. (17) shows that the quantum numbers I_is and J_js are also in the same two lattices, but not occupied consecutively. We shall call the empty lattice sites of I_i and J_j holes. Now let

$$\begin{aligned} Lh_1(k) &= kL - N_2\phi - \sum_j \Theta(k,q_j), \\ Lh_2(q) &= qL + N_1\phi + \sum_i \Theta(k_i,q). \end{aligned} \tag{23}$$

Those values of k and q where $Lh_1(k)=2\pi I$ and $Lh_2(q)=2\pi J$ are ks and qs. Those values of k and q where $Lh_1(k)=2\pi I^h$ and $Lh_2(q)=2\pi J^h$ are k^hs and q^hs. Thus

$$\frac{dh_1(k)}{dk}=2\pi[\rho(k)+\rho^h(k)], \quad \frac{dh_2(q)}{dq}=2\pi[\sigma(q)+\sigma^h(q)], \tag{24}$$

where $\rho(k),\sigma(q)$ and $\rho^h(k),\sigma^h(q)$ are the particle and hole densities, respectively, in an excited state. For low lying excitations, there are only few quasiholes in the Fermi sea and few quasiparticles above the Fermi level. We may define the densities of quasihole states in the Fermi sea as

$$\rho^h(k)=\frac{1}{L}\sum \delta(k-k^h), \quad \sigma^h(q)=\frac{1}{L}\sum \delta(q-q^h), \tag{25}$$

and the densities of quasiparticle states above the Fermi level as

$$\frac{1}{L}\sum \delta(k-k^2), \quad \frac{1}{L}\sum \delta(q-q^p), \tag{26}$$

where the symbol Σ denotes the summation of h or p. From Eq. (23) we obtain

$$\begin{aligned} 1 &= 2\pi\rho(k) + \frac{2\pi}{L}\sum \delta(k-k^h) - \int_0^K a(k,q)\sigma(q)dq - \frac{1}{L}a(k,q^p), \\ 1 &= 2\pi\sigma(q) + \frac{2\pi}{L}\sum \delta(q-q^h) - \int_{-K}^0 a(k,q)\rho(k)dk - \frac{1}{L}a(k^p,q). \end{aligned} \tag{27}$$

Above we have put

$$-K<k<0, \quad 0<q<K, \quad a(k,q)=\frac{2\mu_R}{[k-q-\nu-\mu_i]^2+\mu_{R^2}}.$$

Defining

$$F(k)=L[\rho(k)-\rho_0(k)]+\sum \delta(k-k^h),$$
$$H(q)=L[\sigma(q)-\sigma_0(q)]+\sum \delta(q-q^h), \tag{28}$$

then we have

$$2\pi F(k)-\int_0^K a(k,q)H(q)dq=\sum a(k,q^p)-\sum a(k,q^h),$$
$$2\pi H(q)-\int_{-K}^0 a(k,q)F(k)dk=\sum a(k^p,q)-\sum a(k^h,q). \tag{29}$$

The excitation energy is then given by

$$\epsilon=\sum |k^p|+\sum |k^h|+\sum |q^p|+\sum |q^h|+\int_{-K}^0 kF(k)dk-\int_0^K qH(q)dq, \tag{30}$$

where the last two terms are usually called back flow of the Fermi sea. Notice that here $k^p,q^h>0$ and $k^h,q^p<0$. When $\mu\to\infty$, the fermions are too hard to close each other and the system will behave as two noninteracting subsystems. In this case, $a(k,q)\to 0$ and $F(k),H(q)\to 0$. The excitations are exactly described by the quasiparticles and quasiholes. It is just the anticipated result.

V. THERMODYNAMICS

We construct the thermodynamics following the standard method developed by Yang and Yang.[12] At finite temperature, the method used to describe the low lying excitations is inappropriate because the number of quasiparticles and quasiholes becomes a large quantity. Taking the infinite limit of Eq. (17) with Eq. (24) we obtain

$$1=2\pi[\rho(k)+\rho^h(k)]-\int_{-\infty}^K a(k,q)\sigma(q)dq,$$
$$1=2\pi[\sigma(q)+\sigma^h(q)]-\int_{-K}^{\infty} a(k,q)\rho(k)dk. \tag{31}$$

The energy density is

$$E/L=\int_{-K}^{\infty} k\rho(k)dk-\int_{-\infty}^K q\sigma(q)dq \tag{32}$$

and

$$D=\int_{-K}^{\infty}\rho(k)dk+\int_{-\infty}^K \sigma(q)dq. \tag{33}$$

The entropy of the state described by $\rho(k)$ and $\sigma(q)$ is not zero because of the empty sites in the I_i and J_j lattices which allow many wave functions of approximately the same energy to be described by $\rho(k),\rho^h(k)$ and $\sigma(q),\sigma^h(q)$. In an interval dk, the total number of ks and holes is $L(\rho+\rho^h)dk$. Thus the choices of states in dk with given $\rho(k)$ and $\rho^h(k)$ is

$$\frac{[L(\rho+\rho^h)dk]!}{[L\rho dk]![L\rho^h dk]!}.$$

For $\sigma(q)$ and $\sigma^h(q)$ we have the same discussion. Then the density of the total entropy is given by

$$S/L=\int_{-K}^{\infty}[(\rho+\rho^h)\ln(\rho+\rho^h)-\rho\ \ln\ \rho-\rho^h\ \ln\ \rho^h]dk$$
$$+\int_{-\infty}^{K}[(\sigma+\sigma^h)\ln(\sigma+\sigma^h)-\sigma\ \ln\ \sigma-\sigma^h\ \ln\ \sigma^h]dq. \tag{34}$$

The partition function can be written as

$$Z=\int D\sigma\ D\sigma^h\ D\rho\ D\rho^h\ \exp(S-E/T+AN/T), \tag{35}$$

where A is the Lagrange multiplier. At the thermal equilibrium, we should maximize the contribution to the partition function from the states described by ρ,ρ^h and σ,σ^h. The equilibrium values of ρ and σ are then obtained from variation. The above described procedure leads to the following equations for the equilibrium ρ and σ:

$$\begin{aligned} k+T\ \ln\frac{\rho}{\rho^h}-\frac{T}{2\pi}\int_{-\infty}^{K}a(k,q)\ln\left(1+\frac{\sigma}{\sigma^h}\right)dq=A,\\ -q+T\ \ln\frac{\sigma}{\sigma^h}-\frac{T}{2\pi}\int_{-K}^{\infty}a(k,q)\ln\left(1+\frac{\rho}{\rho^h}\right)dk=A. \end{aligned} \tag{36}$$

Introducing the notations $\exp[\epsilon_1(k)/T]=\rho^h(k)/\rho(k)$ and $\exp[\epsilon_2(q)/T]=\sigma^h(q)/\sigma(q)$, we may rewrite Eq. (36) as

$$\begin{aligned} A=k-\epsilon_1(k)-\frac{T}{2\pi}\int_{-\infty}^{K}a(k,q)\ln[1+\exp(-\epsilon_2/T)]dq,\\ A=-q-\epsilon_2(q)-\frac{T}{2\pi}\int_{-K}^{\infty}a(k,q)\ln[1+\exp(-\epsilon_1/T)]dk. \end{aligned} \tag{37}$$

Multiply Eq. (37) by $\rho(k)$ and $\sigma(q)$, respectively, with integral and then sum them to obtain

$$AD=\int_{-K}^{\infty}\rho(k-\epsilon_1)dk+\int_{-\infty}^{K}\sigma(-q-\epsilon_2)dq+T\int_{-\infty}^{K}\left\{\frac{1}{2\pi}-\sigma[1+\exp(\epsilon_2/T)]\right\}$$
$$\times\ln[1+\exp(-\epsilon_2/T)]dq+T\int_{-K}^{\infty}\left\{\frac{1}{2\pi}-\rho[1+\exp(\epsilon_1/T)]\right\}\ln[1+\exp(-\epsilon_1/T)]dk. \tag{38}$$

Now rewriting S/L as

$$S/L=\int_{-K}^{\infty}(\rho+\rho^h)\ln[1+\exp(-\epsilon_1/T)]dk+\frac{1}{T}\int_{-K}^{\infty}\rho\epsilon_1\,dk$$
$$+\int_{-\infty}^{K}(\sigma+\sigma^h)\ln[1+\exp(-\epsilon_2/T)]dq+\frac{1}{T}\int_{-\infty}^{K}\sigma\epsilon_2 dq, \tag{39}$$

we obtain the density of free energy

$$F/L=AD-\frac{T}{2\pi}\left\{\int_{-K}^{\infty}\ln[1+\exp(-\epsilon_1/T)]dk+\int_{-\infty}^{K}\ln[1+\exp(-\epsilon_2/T)]dq\right\}. \tag{40}$$

Below we shall check some special cases.

A. A=Chemical potential

By thermodynamics we have

$$F=-PL+NB, \tag{41}$$

where P and B are the pressure and chemical potential, respectively. The pressure is thus given by

$$P=-N\frac{\partial A}{\partial L}-\frac{N}{2\pi D}\left[\int_{-K}^{\infty}\frac{dk}{1+\exp(\epsilon_1/T)}\frac{\partial\epsilon_1}{\partial A}+\int_{-\infty}^{K}\frac{dq}{1+\exp(\epsilon_2/T)}\frac{\partial\epsilon_2}{\partial A}\right]\frac{\partial A}{\partial L}$$
$$+\frac{T}{2\pi}\left\{\int_{-K}^{\infty}\ln[1+\exp(-\epsilon_1/T)]dk+\int_{-\infty}^{K}\ln[1+\exp(-\epsilon_2/T)]dq\right\}. \tag{42}$$

Differentiating Eq. (37) with respect to A, we obtain

$$1=-\frac{\partial\epsilon_1}{\partial A}+\frac{1}{2\pi}\int_{-\infty}^{K}a(k,q)\frac{\partial\epsilon_2/\partial A}{1+\exp(\epsilon_2/T)}dq,$$
$$1=-\frac{\partial\epsilon_2}{\partial A}+\frac{1}{2\pi}\int_{-K}^{\infty}a(k,q)\frac{\partial\epsilon_1/\partial A}{1+\exp(\epsilon_1/T)}dk. \tag{43}$$

Comparing the above equations with Eq. (31) we get

$$-\frac{\partial\epsilon_1}{\partial A}=2\pi\rho(k)[1+\exp(\epsilon_1/T)],\quad -\frac{\partial\epsilon_2}{\partial A}=2\pi\sigma(q)[1+\exp(\epsilon_2/T)]. \tag{44}$$

Substituting Eq. (44) into Eq. (42) we find

$$P=\frac{T}{2\pi}\left\{\int_{-K}^{\infty}\ln[1+\exp(-\epsilon_1/T)]dk+\int_{-\infty}^{K}\ln[1+\exp(-\epsilon_2/T)]dq\right\}. \tag{45}$$

From Eqs. (40) and (41) with Eq. (45) we conclude that A is the chemical potential.

B. $\mu\to\infty$

In this case, the integrals in Eq. (37) contribute nothing. Thus

$$\epsilon_1(k)=k-A,\quad \epsilon_2(q)=-q-A. \tag{46}$$

From Eq. (31) we deduce

$$\rho(k)=\frac{1}{2\pi\left[1+\exp\left(\frac{k-A}{T}\right)\right]}\,\theta(k+K),$$
$$\sigma(q)=\frac{1}{2\pi\left[1+\exp\left(\frac{-q-A}{T}\right)\right]}\,\theta(K-q). \tag{47}$$

The Lagrange multiplier can be obtained from Eq. (33) as

$$A=T\,\ln[\exp(\pi D/T)-1]-K. \tag{48}$$

Notice that the cutoff K does not depend on temperature. When $T\to 0$, $A\to -K+\pi D$ and from Eq. (22) we obtain

$$K=\pi D,\quad \zeta=e^{A/T}=1-\exp(-K/T). \tag{49}$$

The free energy is given by

$$F/L=TD\,\ln\left[1-\exp\left(-\frac{K}{T}\right)\right]-\frac{T^2}{\pi}\int_{-K/T}^{\infty}\ln[1+\zeta e^{-x}]dx. \tag{50}$$

C. $\mu\to 0$, $\nu\to 0$

As $\mu\to 0$, $\nu\to 0$, $a(k,q)\to 2\pi\delta(k-q)$, so Eq. (37) becomes

$$A=k-\epsilon_1(k)-T\,\ln[1+\exp\{-\epsilon_2(k)/T\}]\,\theta(K-k),$$
$$A=-q-\epsilon_2(q)-T\,\ln[1+\exp\{-\epsilon_1(q)/T\}]\,\theta(q+K). \tag{51}$$

Thus we have

$$\epsilon_1(k)=[k-A]\,\theta(k-K)+\left[\frac{1}{2}\,(k-A)+T\,\ln\sinh\left(-\frac{A}{T}\right)-T\,\ln\cosh\frac{k+A}{2T}\right]\theta(K-|k|) \tag{52}$$

and

$$\epsilon_2(q)=[-q-A]\,\theta(-K-q)+\left[-\frac{1}{2}\,(q+A)+T\,\ln\sinh\left(-\frac{A}{T}\right)-T\,\ln\cosh\frac{A-q}{2T}\right]\theta(K-|q|). \tag{53}$$

From Eq. (31) we have

$$1=2\pi\rho(k)[1+\exp(\epsilon_1/T)]+2\pi\sigma(k)\,\theta(K-k),$$
$$1=2\pi\sigma(q)[1+\exp(\epsilon_2/T)]+2\pi\rho(q)\,\theta(q+K). \tag{54}$$

Thus the thermodynamics can be constructed from Eqs. (33) and (40) with Eqs. (52), (53), and (54).

VI. CONCLUSION

In conclusion, we have established the exact eigenstates of a boson–fermion model with two-body interactions. The physical properties including the ground state, the low lying elementary excitations, and the thermodynamics have been studied in a cut-off scheme. In the present model, the cutoff K is only a parameter which is relevant to the physical data in a concrete system. In fact, we can take the scaling limit $K\to\infty$. In this case, the quantity $F-E_g$ (free energy minus the ground state energy) is indeed convergent. It should be pointed out that the model Hamiltonian is not analytic at $\mu_R=0$ due to the special form of the ''contraction–decay'' interaction which breaks the particle hole symmetry. That means that this type of interactions cannot be turned on adiabatically. This is why the $\mu\to 0$ limit does not give the results of a free fermion system as discussed in the above section.

We would like to point out that even for the particles with arbitrary moving velocities $(v_1\neq v_2\neq v_3)$, the model is also solvable with the same algebra. At first glance, it seems that the linear spectrum of the bosons with a finite moving velocity is ill-defined. However, we notice that the bosons are nothing but the ''fusion'' of two fermions in our model. Thus they behave as hard core bosons. That means the bosons obey Fermi-like statistics rather than Bose statistics. The system has a well defined ground state (Fermi sea) even the velocity of the bosons takes a finite value. Such a result can also be deduced from the Bethe ansatz equations. The energy for a given eigenstate determined uniquely by the two set of real numbers $\{k\}$ and $\{q\}$ which obey the Fermi statistics.

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Exact results on a Dirac-like Lee model

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A one-dimensional massive Lee model is studied via the Bethe ansatz method. The exact engenstates and the energy spectrum are obtained. The general picture of the excitations is discussed. © *1996 American Institute of Physics.*
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I. INTRODUCTION

In the past few decades, a dozen models have been solved via the Bethe ansatz[1] and the Bethe–Yang ansatz.[2] In this paper, we consider a new Bethe ansatz soluble model, e.g., the Dirac-like Lee model. The Lee model[3] plays an important role in the quantum field theory. Recently, similar models have been proposed to describe the high Tc superconductivity.[4,5]

The Hamiltonian we shall consider reads as

$$\mathbf{H}=\int dx\Big\{-i\sum_{r=\pm} r\Psi_r^\dagger(x)\,\frac{\partial}{\partial x}\,\Psi_r(x)+m[\Psi_+^\dagger(x)\Psi_-(x)+\Psi_-^\dagger(x)\Psi_+(x)]$$
$$+g[\Psi_+^\dagger(x)\Psi_-^\dagger(x)b(x)+b^\dagger(x)\Psi_-(x)\Psi_+(x)]\Big\}, \tag{1}$$

where $\Psi_r^\dagger(x)(\Psi_r(x))$ are the creation (annihilation) operators of the fermions and $b^\dagger(x)(b(x))$ is the creation (annihilation) operator of the bosons. m and g are real constants. The massive term in (1) may be induced by either the electron–phonon $(2k_F)$ interaction or the backward scattering among the electrons. The bosons, however, may represent a variety of physical situations phenomenologically, such as the Cooper-pair-like bound state or the dimer state. We would like to point out that the Hamiltonian (1) is similar to that of the massive Thirring model.[6]

A special feature of the Lee model is that the particle numbers are no longer conserved. It can be easily read off from (1). However, the quantity

$$\mathbf{N}=\int\Big[\sum_{r=\pm}\Psi_r^\dagger(x)\Psi_r(x)+2b^\dagger(x)b(x)\Big]dx, \tag{2}$$

is conserved. Therefore, we can establish the common eigenstates of **H** and **N**.

II. BETHE STATES

To show the procedure clearly, it is convenient to consider the $N=2$ case first. Such a state is the simplest nontrivial state, which gives the main information about the general engenstates. As done in the massive Thirring model,[6] we introduce the operator

$$\Psi_\alpha^\dagger(x)=e^{\alpha/2}\Psi_+^\dagger(x)+e^{-\alpha/2}\Psi_-^\dagger(x), \tag{3}$$

where α takes values in the lines Im $\alpha=0$ and Im $\alpha=\pi$. An $N=2$ eigenstate can be written as

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$$|\alpha_1,\alpha_2\rangle=\int dx_1\ dx_2\ f(x_1,x_2)\Psi^{\dagger}_{\alpha_1}(x_1)\Psi^{\dagger}_{\alpha_2}(x_2)|0\rangle+\int dy\ h(y)b^{\dagger}(y)|0\rangle, \tag{4}$$

where $|0\rangle$ is the pseudovacuum state defined by $\Psi_r(x)|0\rangle=b(x)|0\rangle=0$. The Schrödinger equation $H|\alpha_1,\alpha_2\rangle=E(\alpha_1,\alpha_2)|\alpha_1,\alpha_2\rangle$ gives

$$\begin{aligned}\int\ dx_1\ dx_2\Bigg\{&\sum_{r=\pm}\left[-ire^{r\alpha_1/2}\frac{\partial}{\partial x_1}+me^{-r\alpha_1/2}\right]f(x_1,x_2)\Psi^{\dagger}_r(x_1)\Psi^{\dagger}_{\alpha_2}(x_2)|0\rangle\\&+\Psi^{\dagger}_{\alpha_1}(x_1)\sum_{r=\pm}\left[-ire^{r\alpha_2/2}\frac{\partial}{\partial x_2}+me^{-r\alpha_2/2}\right]f(x_1,x_2)\Psi^{\dagger}_r(x_2)|0\rangle\Bigg\}+g\int dy\ h(y)\\&\times\Psi^{\dagger}_+(y)\Psi^{\dagger}_-(y)|0\rangle+2g\int dx\ f(x,x)\sinh\frac{\alpha_1-\alpha_2}{2}\,b^{\dagger}(x)|0\rangle=E(\alpha_1,\alpha_2)|\alpha_1,\alpha_2\rangle.\end{aligned} \tag{5}$$

Make the following ansatz:

$$\begin{aligned}f(x_1,x_2)&=\exp\{ix_1m\ \sinh\ \alpha_1+ix_2m\ \sinh\ \alpha_2\}[1+i\lambda(\alpha_1,\alpha_2)\epsilon(x_1-x_2)],\\h(x)&=S^{+}(\alpha_1,\alpha_2)f(x,x),\end{aligned} \tag{6}$$

where $\epsilon(x)=\theta(x)-\theta(-x)$ and $\theta(x)$ is the step function. Substituting (6) into (5), we readily obtain

$$E(\alpha_1,\alpha_2)=m\ \cosh\ \alpha_1+m\ \cosh\ \alpha_2, \tag{7}$$

$$S^{+}(\alpha_1,\alpha_2)=\frac{2g\ \sinh[(\alpha_1-\alpha_2)/2]}{m\ \cosh\ \alpha_1+m\ \cosh\ \alpha_2}, \tag{8}$$

$$\lambda(\alpha_1,\alpha_2)=-\frac{g^2}{4m}\frac{\tanh[(\alpha_1-\alpha_2)/2]}{\cosh\ \alpha_1+\cosh\ \alpha_2}. \tag{9}$$

Through the same procedure, we can establish the general eigenstates with arbitrary N by introducing the ladder wave functions f_M,[7]

$$\begin{aligned}|\alpha_1,\ldots,\alpha_N\rangle=\int&\sum_{M=0}^{[N/2]}\sum_{\{i_k<j_k\}}f_M(x_1,\ldots,x_{i_k-1},x_{i_k+1},\ldots,x_N|x_{i_1}=x_{j_1},\ldots,x_{i_M}=x_{j_M})\\&\times\prod_{\substack{l=1\\l\neq\{i_k,j_k\}}}^{N}\Psi^{\dagger}_{\alpha_l}(x_l)dx_l\prod_{k=1}^{M}b^{\dagger}(x_{i_k})dx_{i_k}|0\rangle,\end{aligned} \tag{10}$$

where $\{i_k<j_k\}$ denotes the choices of i_k's and j_k's with the restrictions $i_k<j_k$ and $i_k\neq i_{k'}$, $j_{k'}$ for $k\neq k'$. After some manipulations we deduce the ladder wave function f_M as

$$\begin{aligned}&f_M(x_1,\ldots,x_{i_k-1},x_{i_k+1},\ldots,x_N|x_{i_1}=x_{j_1},\ldots,x_{i_M}=x_{j_M})\\&=\prod_{l=1}^{N}e^{imx_l\ \sinh\ \alpha_l}\prod_{1\leqslant m<n\leqslant N}[1+i\lambda(\alpha_m,\alpha_n)\epsilon(x_m\end{aligned} \tag{11}$$

$$-x_n)]\prod_{k=1}^{M}\zeta_k\frac{2g\ \sinh[(\alpha_{i_k}-\alpha_{j_k})/2]}{m\ \cosh\ \alpha_{i_k}+m\ \cosh\ \alpha_{j_k}},$$

where $\zeta_k=(-1)^{i_k-j_k+1}$ is induced by the contraction process of two fermions to a boson. It is easy to verify that with f_M defined in (11), the state (10) is really an eigenstate of the Hamiltonian (1) with the eigenenergy and the momentum,

$$E(\alpha_1,\ldots,\alpha_N)=\sum_{l=1}^{N}m\ \cosh\ \alpha_l,\quad P(\alpha_1,\ldots,\alpha_N)=\sum_{l=1}^{N}m\ \sinh\ \alpha_l. \tag{12}$$

Imposing the periodic conditions in f_M's we obtain the following Bethe ansatz equation:

$$e^{iLm\ \sinh\ \alpha_j}=\prod_{i=1}^{N}\frac{\cosh\ \alpha_j+\cosh\ \alpha_i+ic\ \tanh[(\alpha_j-\alpha_i)/2]}{\cosh\ \alpha_j+\cosh\ \alpha_i-ic\ \tanh[(\alpha_j-\alpha_i)/2]}, \tag{13}$$

where L is the length of the system and $c=g^2/4m$. The physical properties of the present model (1) are uniquely determined by the Bethe ansatz equation (13). The physical vacuum or the ground state is the state in which all the α modes in the line Im $\alpha=\pi$ are filled. Suppose $\beta=$Re α. By taking the limit $L\to\infty$ in (13), we deduce that the density of β in the ground state satisfies the following integral equation:

$$m\ \cosh\ \beta=2\pi\rho(\beta)+\int_{-\Lambda}^{\Lambda}\frac{2c}{\cosh[(\beta-\beta')/2]}\frac{\cosh[(\beta+\beta')/2]-\sinh\ \beta\ \sinh[(\beta-\beta')/2]}{(\cosh\ \beta+\cosh\ \beta')^2+c^2\ \tanh^2[(\beta-\beta')/2]}\rho(\beta')d\beta', \tag{14}$$

where $\Lambda\to\infty$ is a cutoff for the modes β that renormalizes the mass m and the velocities of the modes.[6]

III. ELEMENTARY EXCITATIONS

Based on the Bethe ansatz equation (13), we can discuss the excitations of the system. The simplest excitation possible is obtained by moving a mode from $\alpha=\beta+i\pi$ and placing it at $\alpha=\beta'$, where β and β' are real. In free field theory, this particle–hole pair is a state with a fermion and an antifermion. The antifermion (hole) has energy $-m\cosh(\beta+i\pi)=m\cosh\beta$, and the fermion has energy $m\cosh\beta'$. In the interacting system, the energy has the same form to that of the free system. Given a β, we can choose β' arbitrarily to satisfy the Bethe ansatz equation (13) because c is a positive number. This is not the case of the massive Thirring model as described in Ref. 6, where there may be some restriction for the choice of β'.

There are also other possible excitations in the interacting theory. The modes can be put in the complex plane. Generally, we must be careful to place modes symmetrically about the lines Im $\alpha=\pi$ and or Im $\alpha=0$ (mod 2π) to ensure the energy and the momentum to be real. An imaging α ($\alpha\neq n\pi$) introduces the possibility of an exponentially growing wave function in some direction. However, the coefficient of the exponentially growing term vanishes if we choose the complex modes properly. The excitations for the present model have special features because the two-body scattering matrix is not a function of $\alpha_i-\alpha_j$: (i) Only the two strings with position-dependent lengths may exist apart from the origin. The failure of Lorentz invariance in Lee-type models like this one leads to the position dependence of the length of strings; (ii) the n-body bound state corresponds to a bent n string. Here a bent string means that the real parts of the roots are not equal, hence the string is not a straight line parallel to the imaginary axis and may be bent

in the complex plane. A bent $2n$ string is composed by n conjugate pairs and a bent $2n+1$ string is composed by n conjugate pairs plus a mode in the lines Im $\alpha=0,\ \pi$. Below we discuss some special cases.

A. Two-string solutions

The two-string excitation is obtained by moving two modes in the line Im $\alpha=\pi$ to the strip $|\text{Im }\alpha|<\pi$ conjugately. Suppose the two string has the form

$$\alpha_{\pm}=\beta\pm i\Delta(\beta), \tag{15}$$

where β, $\Delta(\beta)$ are real. The complex roots are determined either from the zeros or poles from the right side of the Bethe ansatz equation (13) because of the $L\to\infty$ behavior of the left side. We deduce that

$$\sin\ \Delta(\beta)=\frac{(c^2+16\cosh^2\ \beta)^{1/2}-c}{4\cosh\ \beta}. \tag{16}$$

Obviously, there are two solutions for a given β. One is $\Delta_1=\arcsin\{[(c^2+16\cosh^2\beta)^{1/2}-c]/4\cosh\beta\}$ and the other is $\Delta_2=\pi-\Delta_1$. The length of the string depends on both its position and the constant c. The position of the string is completely determined by the positions of the holes.[6,8]

B. Bent three-strings

One type of the bent three-string is composed by a conjugate pair $\alpha_{\pm}=\beta\pm i\Delta(\beta)$ and a real mode β_0. To meet the Bethe ansatz equation, $\alpha_{\pm}$ and β_0 must satisfy

$$\cosh\ \alpha_{+}+\cosh\ \beta_0+ic\ \tanh\frac{\alpha_{+}-\beta_0}{2}=0,\quad \sin\ \Delta(\beta)>0. \tag{17}$$

For a given β, β_0 and $\Delta(\beta)$ are determined by the following equations:

$$\begin{aligned}\cosh\ \beta\ \cos\ \Delta+\cosh\ \beta_0&=\frac{c\ \sin\ \Delta}{\cosh(\beta-\beta_0)+\cos\ \Delta},\\ \sinh\ \beta\ \sin\ \Delta+\frac{\sinh(\beta-\beta_0)}{\cosh(\beta-\beta_0)+\cos\ \Delta}&=0.\end{aligned} \tag{18}$$

For $\beta=0$, we have $\beta_0=0$. This solution is a normal three-string. The other type of the bent three-string is composed by a conjugate pair $\alpha_{\pm}=\beta\pm i\Delta$ and a mode $\beta_0+i\pi$. β, β_0, and Δ satisfy the equations

$$\begin{aligned}\cosh\ \beta\ \cos\ \Delta-\cosh\ \beta_0&=\frac{c\ \sin\ \Delta}{-\cosh(\beta-\beta_0)+\cos\ \Delta},\\ \sinh\ \beta\ \sin\ \Delta+\frac{\sinh(\beta-\beta_0)}{\cosh(\beta-\beta_0)-\cos\ \Delta}&=0.\end{aligned} \tag{19}$$

C. *n* string on the imaginary axis

Higher strings can be constructed by the same procedures. Any string, consisting of $2s+1$ modes, where s is either an integer or a half-integer, has its modes at α_s, $\alpha_{s-1},\ldots,\alpha_{-s}$, where

$$\cosh\ \alpha_j+\cosh\ \alpha_{j-1}+ic\ \tanh\ \tfrac{1}{2}(\alpha_j-\alpha_{j-1})=0.$$

In the special case where all the modes lie on the imaginary axis, the equation can be simplified. For a $2n$ string,

$$\alpha_{j\pm}=\pm i\Delta_j,\quad j=\frac{1}{2},\ldots,\frac{n}{2}-1, \tag{20}$$

we have the solutions

$$\begin{aligned}&\sin\ \Delta_{1/2}=\frac{(c^2+16)^{1/2}-c}{4},\\ &\cos\ \Delta_{j+1}+\cos\ \Delta_j=c\ \tan\frac{\Delta_{j+1}-\Delta_j}{2},\quad \text{for } j\geqslant\frac{1}{2}.\end{aligned} \tag{21}$$

For a $2n+1$ string,

$$\alpha_0=0,\quad \alpha_{j\pm}=\pm i\Delta_j,\quad j=1,2,\ldots,n, \tag{22}$$

we have the solution

$$\begin{aligned}&1+\cos\ \Delta_1=c\ \tan\frac{\Delta_1}{2},\\ &\cos\ \Delta_{j+1}+\cos\ \Delta_j=c\ \tan\frac{\Delta_{j+1}-\Delta_j}{2},\quad \text{for } j\geqslant 1.\end{aligned} \tag{23}$$

Note by moving the modes by $i\pi$ we can obtain a string symmetric to the line Im $\alpha=\pi$.

IV. CONCLUDING REMARKS

In conclusion, we have established the exact eigenstates of a massive Lee model. The elementary excitations are discussed. It is found that the general complex excitations are bent strings. Some special cases are discussed.

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Microcanonical ensemble and algebra of conserved generators for generalized quantum dynamics

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It has recently been shown, by application of statistical mechanical methods to determine the canonical ensemble governing the equilibrium distribution of operator initial values, that complex quantum field theory can emerge as a statistical approximation to an underlying generalized quantum dynamics. This result was obtained by an argument based on a Ward identity analogous to the equipartition theorem of classical statistical mechanics. We construct here a microcanonical ensemble which forms the basis of this canonical ensemble. This construction enables us to define the microcanonical entropy and free energy of the field configuration of the equilibrium distribution and to study the stability of the canonical ensemble. We also study the algebraic structure of the conserved generators from which the microcanonical and canonical ensembles are constructed, and the flows they induce on the phase space. © *1996 American Institute of Physics.* [S0022-2488(96)00511-7]

I. INTRODUCTION

Generalized quantum dynamics[1,2] is an analytic mechanics on a symplectic set of operator-valued variables, forming an operator-valued phase space $\mathscr{S}$. These variables are defined as the set of linear transformations, in general, local (noncommuting) quantum fields, on an underlying real, complex, or quaternionic Hilbert space (Hilbert module), for which the postulates of a real, complex, or quaternionic quantum mechanics are satisfied.[2–6] The dynamical (generalized Heisenberg) evolution, or flow, of this phase space is generated by the total trace Hamiltonian $\mathbf{H}=\mathbf{Tr}\,H$, where for any operator O we have

$$\mathbf{O}\equiv\mathbf{Tr}\;O\equiv\mathrm{Re}\;\mathrm{Tr}(-1)^F O=\mathrm{Re}\sum_n\;\langle n|(-1)^F O|n\rangle, \tag{1.1}$$

H is a function of the operators $\{q_r(t)\},\{p_r(t)\}$, $r=1,2,\ldots,N$ (realized as a sum of monomials, or a limit of a sequence of such sums; in the general case of local noncommuting fields, the index r contains continuous variables), and $(-1)^F$ is a grading operator with eigenvalue $1(-1)$ for states in the boson (fermion) sector of the Hilbert space. Operators are called bosonic or fermionic in type if they commute or anticommute, respectively, with $(-1)^F$; for each r, p_r and q_r are of the same type.

The derivative of a total trace functional with respect to some operator variation is defined with the help of the cyclic property of the **Tr** operation. The variation of any monomial O consists of terms of the form $\mathrm{O}_L\,\delta x_r\mathrm{O}_R$, for x_r one of the $\{q_r\},\{p_r\}$, which, under the **Tr** operation, can be brought to the form

$$\delta\mathbf{O}=\delta\mathbf{Tr}\;O=\pm\,\mathbf{Tr}\;O_R O_L\,\delta x_r\,,$$

so that sums and limits of sums of such monomials permit the construction of

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$$\delta\mathbf{O}=\mathbf{Tr}\sum_r \frac{\delta\mathbf{O}}{\delta x_r}\,\delta x_r, \tag{1.2}$$

uniquely defining $\delta\mathbf{O}/\delta x_r$.

Assuming the existence of a total trace Lagrangian[1,2] $\mathbf{L}=\mathbf{L}(\{q_r\},\{\dot{q}_r\})$, the variation of the total trace action

$$\mathbf{S}=\int_{-\infty}^{\infty}\mathbf{L}(\{q_r\},\{\dot{q}_r\})dt \tag{1.3}$$

results in the operator Euler–Lagrange equations

$$\frac{\delta\mathbf{L}}{\delta q_r}-\frac{d}{dt}\frac{\delta\mathbf{L}}{\delta\dot{q}_r}=0. \tag{1.4}$$

As in classical mechanics, the total trace Hamiltonian is defined as a Legendre transform,

$$\mathbf{H}=\mathbf{Tr}\sum_r p_r\dot{q}_r-\mathbf{L}, \tag{1.5}$$

where

$$p_r=\frac{\delta\mathbf{L}}{\delta\dot{q}_r}. \tag{1.6}$$

It then follows from (1.4) that

$$\frac{\delta\mathbf{H}}{\delta q_r}=-\dot{p}_r, \quad \frac{\delta\mathbf{H}}{\delta p_r}=\epsilon_r\dot{q}_r, \tag{1.7}$$

where $\epsilon_r=1(-1)$ according to whether p_r,q_r are of bosonic (fermionic) type.

Defining the generalized Poisson bracket

$$\{\mathbf{A},\mathbf{B}\}=\mathbf{Tr}\sum_r \epsilon_r\left(\frac{\delta\mathbf{A}}{\delta q_r}\frac{\delta\mathbf{B}}{\delta p_r}-\frac{\delta\mathbf{B}}{\delta q_r}\frac{\delta\mathbf{A}}{\delta p_r}\right), \tag{1.8a}$$

one sees that

$$\frac{d\mathbf{A}}{dt}=\frac{\partial\mathbf{A}}{\partial t}+\{\mathbf{A},\mathbf{H}\}. \tag{1.8b}$$

Conversely, if we define

$$\mathbf{x}_s(\eta)=\mathbf{Tr}(\eta x_s), \tag{1.9a}$$

for η an arbitrary, constant operator (of the same type as x_s, which denotes here q_s or p_s), then

$$\frac{d\mathbf{x}_s(\eta)}{dt}=\mathbf{Tr}\sum_r \epsilon_r\left(\frac{\delta\mathbf{x}_s(\eta)}{\delta q_r}\frac{\delta\mathbf{H}}{\delta p_r}-\frac{\delta\mathbf{H}}{\delta q_r}\frac{\delta\mathbf{x}_s(\eta)}{\delta p_r}\right), \tag{1.9b}$$

and comparing the coefficients of η on both sides, one obtains the Hamiltonian equations (1.7) as a consequence of the Poisson bracket relation (1.8b).

The Jacobi identity is satisfied by the Poisson bracket of (1.8a),[7] and hence the total trace functionals have many of the properties of the corresponding quantities in classical mechanics.[8] In particular, canonical transformations take the form

$$\delta \mathbf{x}_s(\eta) = \{\mathbf{x}_s(\eta), \mathbf{G}\}, \tag{1.10a}$$

which implies that

$$\delta p_r = -\frac{\delta \mathbf{G}}{\delta q_r}, \quad \delta q_r = \epsilon_r \frac{\delta \mathbf{G}}{\delta p_r}, \tag{1.10b}$$

with the generator $\mathbf{G}$ any total trace functional constructed from the operator phase space variables. Time evolution then corresponds to the special case $\mathbf{G} = \mathbf{H}\, dt$.

It has recently been shown by Adler and Millard[9] that a canonical ensemble can be constructed on the phase space $\mathscr{S}$, reflecting the equilibrium properties of a system of many degrees of freedom. Since the operator

$$\tilde{C} = \sum_r (\epsilon_r q_r p_r - p_r q_r) = \sum_{r,B} [q_r, p_r] - \sum_{r,F} \{q_r, p_r\}, \tag{1.11}$$

where the sums are over bosonic and fermionic pairs, respectively, is conserved under the evolution (1.7) induced by the total trace Hamiltonian, the canonical ensemble must be constructed taking this constraint into account. This is done by constructing the conserved quantity $\mathbf{Tr}\, \tilde{\lambda}\tilde{C}$, for some given constant anti-Hermitian operator $\tilde{\lambda}$.

In the general case, in the presence of the fermionic sector, the graded trace of the Hamiltonian is not bounded from below, and the partition function may be divergent. When the equations of motion induced by the Lagrangian $\mathbf{L}$ coincide with those induced by the ungraded total trace of the same Lagrangian,

$$\hat{\mathbf{L}} = \mathrm{Re\ Tr}\ L$$

without the factor $(-1)^F$, the corresponding ungraded total trace Hamiltonian $\hat{\mathbf{H}}$ is conserved. It may therefore be included as a constraint functional in the canonical ensemble, along with the new conserved quantity $\hat{\mathbf{Tr}}\, \hat{\tilde{\lambda}}\hat{\tilde{C}}$ (see Appendices 0 and C of Ref. 9), where

$$\hat{\tilde{C}} = \sum_r [q_r, p_r] = \sum_{r,B} [q_r, p_r] + \sum_{r,F} [q_r, p_r]. \tag{1.12}$$

It was argued that the Ward identities derived from the canonical ensemble imply that $\hat{\tilde{\lambda}}$ and $\tilde{\lambda}$ are functionally related, so that they may be diagonalized in the same basis (Appendix F of Ref. 9). It was then shown that, since the ensemble averages depend only on $\tilde{\lambda}$ and $(-1)^F$, the ensemble average of any operator must commute with these operators. Since the ensemble-averaged operator $\langle \tilde{C} \rangle_{AV}$ is anti-self-adjoint, if one furthermore assumes it is completely degenerate (with eigenvalue $i_{\mathrm{eff}}\hbar$), the ensemble average of the theory then reduces to the usual complex quantum field theory. In this paper, we construct a microcanonical ensemble from which the canonical ensemble of Ref. 9 can be obtained following the usual methods of statistical mechanics. This construction gives some insight into the interpretation of the parameters, relates the canonical and microcanonical entropies, and identifies the generalized free energy. It also permits estimates of the statistical fluctuations admitted by the canonical ensemble, and error bounds on the Ward identity which we shall treat elsewhere. We give, in this framework, a self-consistency proof of the

stability of the canonical ensemble. We then go on to discuss the algebraic structure of the canonical generators related to the conserved operators $\tilde{C}$ and $\hat{\tilde{C}}$, and the flows on phase space induced by these generators.

II. THE MICROCANONICAL AND CANONICAL ENSEMBLES

Introducing a complete set of states $\{|n\rangle\}$ in the underlying Hilbert space, the phase space operators are completely characterized by their matrix elements $\langle m|x_r|n\rangle \equiv (x_r)_{mn}$, which have the form

$$(x_r)_{mn} = \sum_A (x_r)^A_{mn} e_A , \tag{2.1}$$

where A takes the values 0,1 for complex Hilbert space, 0,1,2,3 for quaternion Hilbert space (technically, a Hilbert module), and just the one value 0 for real Hilbert space, and the e_A are the associated hypercomplex units (unity, complex, or quaternionic units[2]). The mathematical procedures we establish here are applicable to more general Hilbert modules; arguments are given in Ref. 2, however, for restricting our attention to these three cases, and we shall therefore concentrate on the real, complex, and quaternionic structures in the examination of specific properties. The phase space measure is then defined as

$$d\mu = \prod_A d\mu^A, \quad d\mu^A \equiv \prod_{r,m,n} d(x_r)^A_{mn} , \tag{2.2}$$

where redundant factors are omitted according to adjointness conditions. The measure defined in this way is invariant under canonical transformations induced by the generalized Poisson bracket.[9]

We then define the microcanonical ensemble in terms of the set of states in the underlying Hilbert space which satisfy δ-function constraints on the values of the two total trace functionals $\mathbf{H}$ and $\hat{\mathbf{H}}$ and the matrix elements of the two conserved operator quantities $\tilde{C}$ and $\hat{\tilde{C}}$ discussed in the previous section. The volume of the corresponding submanifold in phase space is given by

$$\Gamma(E,\hat{E},\tilde{\nu},\hat{\tilde{\nu}}) = \int d\mu\, \delta(E-\mathbf{H})\, \delta(\hat{E}-\hat{\mathbf{H}}) \prod_{n\leqslant m,A} \delta(\nu^A_{nm} - \langle n|(-1)^F \tilde{C}|m\rangle^A)\, \delta(\hat{\nu}^A_{nm} - \langle n|\hat{\tilde{C}}|m\rangle^A), \tag{2.3}$$

where we have used the abbreviations $\tilde{\nu} \equiv \{\nu^A_{nm}\}$ and $\hat{\tilde{\nu}} \equiv \{\hat{\nu}^{\ A}_{nm}\}$ for the parameters in the arguments on the left-hand side. The factor $(-1)^F$ in the term with $\tilde{C}$ is not essential, but convenient in obtaining the precise form given in Ref. 9 for the canonical distribution. The entropy associated with this ensemble is given by

$$S_{\mathrm{mic}}(E,\hat{E},\tilde{\nu},\hat{\tilde{\nu}}) = \log\, \Gamma(E,\hat{E},\tilde{\nu},\hat{\tilde{\nu}}). \tag{2.4}$$

As we shall see, it is not possible to associate a temperature to this structure in the usual simple way.

The operators $\tilde{C}$ and $\hat{\tilde{C}}$ are defined in terms of sums over degrees of freedom. In the context of the application to quantum field theory, the enumeration of degrees of freedom includes continuous parameters, corresponding to the measure space of the fields. These operators may therefore be decomposed into parts within a certain (large) region of the measure space, which we denote as b, corresponding to what we shall consider as a *bath*, in the sense of statistical mechanics, and within another (small) part of the measure space, which we denote as s, corresponding to what we shall consider as a *subsystem*. We shall assume that the functionals $\mathbf{H}$ and $\hat{\mathbf{H}}$ may also be

decomposed additively into parts associated with b and s; this assumption is equivalent to the presence of interactions in the Hamiltonian or Lagrangian operators which are reasonably localized in the measure space of the fields (the difference in structure between the Lagrangian and Hamiltonian consists of operators that are explicitly additive), so that the errors in assuming additivity are of the nature of ''surface terms.'' The constraint parameters may then be considered to be approximately additive as well, and we may rewrite the microcanonical ensemble as

$$\begin{aligned}\Gamma(E,\hat{E},\tilde{\nu},\hat{\tilde{\nu}}) = \int & d\mu_b d\mu_s dE_s d\hat{E}_s (d\nu^s)(d\hat{\nu}^s)\,\delta(E-E_s-\mathbf{H}_b) \\ & \times \delta(E_s-\mathbf{H}_s)\,\delta(\hat{E}-\hat{E}_s-\hat{\mathbf{H}}_b)\,\delta(\hat{E}_s-\hat{\mathbf{H}}_s) \\ & \times \prod_{n\leqslant m,A} \delta(\nu^A_{nm}-\nu^{A,s}_{nm}-\langle n|(-1)^F\tilde{C}_b|m\rangle^A)\,\delta(\nu^{A,s}_{nm}-\langle n|(-1)^F\tilde{C}_s|m\rangle^A) \\ & \times \delta(\hat{\nu}^A_{nm}-\hat{\nu}^{A,s}_{nm}-\langle n|\hat{\tilde{C}}_b|m\rangle^A)\,\delta(\hat{\nu}^{A,s}_{nm}-\langle n|\hat{\tilde{C}}_s|m\rangle^A). \end{aligned} \tag{2.5}$$

We recognize the integrations over $d\mu_s$ and $d\mu_b$ in (2.5) in terms of the corresponding microcanonical subensembles, for the bath b and subsystem s, respectively, i.e., we may write (2.5) as

$$\Gamma(E,\hat{E},\tilde{\nu},\hat{\tilde{\nu}}) = \int dE_s\; d\hat{E}_s (d\nu^s)(d\hat{\nu}^s)\Gamma_b(E-E_s,\hat{E}-\hat{E}_s,\tilde{\nu}-\tilde{\nu}_s,\hat{\tilde{\nu}}-\hat{\tilde{\nu}}_s)\Gamma_s(E_s,\hat{E}_s,\tilde{\nu}_s,\hat{\tilde{\nu}}_s). \tag{2.6}$$

We now assume that the integrand in (2.6) has a maximum for a large number of degrees of freedom that dominates the integral. In the treatment of the statistical mechanics of classical particles, the number of degrees of freedom generally vastly exceeds the number of variables controlling the constraint hypersurfaces in the phase space; in our case, due to the presence of the constraints imposed by the operators $\tilde{C}$ and $\hat{\tilde{C}}$, there are an infinite number of variables, and the question of the development of a significant maximum may be more delicate. We will demonstrate, however, that due to the semidefinite form of the autocorrelation matrix of the fluctuations, the canonical distribution that we obtain with this assumption is at least locally stable.

Let us, for brevity, define

$$\xi=\{\xi_i\}\equiv\{E,\hat{E},\tilde{\nu},\hat{\tilde{\nu}}\}, \tag{2.7}$$

where the index i refers to the elements of the set of variables, so that (2.6) takes the form

$$\Gamma(\Xi)=\int d\xi_s \Gamma_b(\Xi-\xi_s)\Gamma_s(\xi_s), \tag{2.8a}$$

where Ξ corresponds to the set of total properties for the whole ensemble. A necessary condition for an extremum in all of the variables at $\xi_s=\xi$ is then

$$\frac{\partial}{\partial\xi}[\Gamma_b(\Xi-\xi)\Gamma_s(\xi)]\big|_{\bar{\xi}}=0, \tag{2.8b}$$

which implies that

$$\frac{1}{\Gamma_s(\xi)}\frac{\partial\Gamma_s}{\partial\xi_i}(\xi)\big|_{\bar{\xi}}=\frac{1}{\Gamma_b(\Xi-\xi)}\frac{\partial\Gamma_b}{\partial\Xi_i}(\Xi-\xi)\big|_{\bar{\xi}}. \tag{2.8c}$$

The logarithmic derivatives in (2.8c) define a set of quantities analogous to the (reciprocal) temperature of the usual statistical mechanics, i.e., equilibrium-fixing Lagrange parameters common to the bath and the subsystem. We write these separately as

$$\tau = \frac{\partial}{\partial E} \log \Gamma_s(\xi)|_{\bar{\xi}}, \quad \hat{\tau} = \frac{\partial}{\partial \hat{E}} \log \Gamma_s(\xi)|_{\bar{\xi}},$$
$$\lambda^A_{nm} = -\frac{\partial}{\partial \nu^A_{nm}} \log \Gamma_s(\xi)|_{\bar{\xi}}, \quad \hat{\lambda}^A_{nm} = -\frac{\partial}{\partial \hat{\nu}^A_{nm}} \log \Gamma_s(\xi)|_{\bar{\xi}}. \tag{2.9}$$

According to the definition of entropy (2.4), the bath phase space volume is given by

$$\Gamma_b(\Xi - \xi_s) = e^{S_b(\Xi - \xi_s)} \cong e^{S_b(\Xi)} \exp\left\{ -\sum_i \xi_{i,s} \frac{\partial S_b}{\partial \Xi_i}(\Xi) \right\}. \tag{2.10}$$

Neglecting the small shift in argument $\Xi \to \Xi - \xi_s$, it follows from (2.8a)–(2.8c), (2.9), and (2.10) that

$$\Gamma_b(\Xi - \xi_s) \cong e^{S_b(\Xi)} \exp\left\{ -\tau E_s - \hat{\tau}\hat{E}_s + \sum_{n \leqslant m, A} (\nu^{A,s}_{nm} \lambda^A_{nm} + \hat{\nu}^{A,s}_{nm} \hat{\lambda}^A_{nm}) \right\}. \tag{2.11}$$

We now return to (2.6), replacing the phase space volume of the bath, Γ_b, by the approximate form (2.11), and the subsystem phase space volume Γ_s by the phase space integral over the constraint δ-functions, i.e. (we use the equality henceforth, although it should be understood that we have included just the dominant contribution),

$$\begin{aligned} \Gamma(\Xi) = \int & d\mu_s \, dE_s \, d\hat{E}_s (d\nu^s)(d\hat{\nu}^s) \delta(E_s - \mathbf{H}_s) \delta(\hat{E}_s - \hat{\mathbf{H}}_s) \\ & \times \prod_{n \leqslant m, A} \delta(\nu^{A,s}_{nm} - \langle n | (-1)^F \widetilde{C}_s | m \rangle^A) \delta(\hat{\nu}^{A,s}_{nm} - \langle n | \hat{\widetilde{C}}_s | m \rangle^A) \\ & \times e^{S_b(\Xi)} \exp\left\{ -\tau E_s - \hat{\tau}\hat{E}_s + \sum_{n \leqslant m, A} (\nu^{A,s}_{nm} \lambda^A_{nm} + \hat{\nu}^{A,s}_{nm} \hat{\lambda}^A_{nm}) \right\}. \end{aligned} \tag{2.12}$$

Carrying out the integrals over the parameters, the δ-functions imply the replacement of the parameters E_s, $\hat{E}_s$, $\nu^{A,s}_{nm}$, and $\hat{\nu}^{A,s}_{nm}$ in the exponent by the corresponding phase space quantities. For the product

$$\lambda^A_{nm} \langle n | (-1)^F \widetilde{C}_s | m \rangle^A, \tag{2.13}$$

we note that the anti-self-adjoint property of $\widetilde{C}_s$ implies that

$$\langle n | (-1)^F \widetilde{C}_s | m \rangle = -\langle m | (-1)^F \widetilde{C}_s | n \rangle^*, \tag{2.14}$$

with * denoting conjugation of the hypercomplex units, so that

$$\begin{aligned} \langle n | (-1)^F \widetilde{C}_s | m \rangle^0 &= -\langle m | (-1)^F \widetilde{C}_s | n \rangle^0, \\ \langle n | (-1)^F \widetilde{C}_s | m \rangle^A &= \langle m | (-1)^F \widetilde{C}_s | n \rangle^A, \quad A \neq 0, \end{aligned} \tag{2.15}$$

for all three cases of real, complex, or quaternionic Hilbert spaces. Thus we have

$$\mathrm{Re}\ \lambda_{nm}\langle m|(-1)^F\tilde{C}_s|n\rangle=-\sum_A \lambda^A_{nm}\langle n|(-1)^F\tilde{C}_s|m\rangle^A. \tag{2.16a}$$

Defining the operator $\tilde{\lambda}$ for which the matrix elements are

$$\langle n|\tilde{\lambda}|n\rangle^A=\lambda^A_{nn},\quad \langle n|\hat{\lambda}|m\rangle^A=\tfrac{1}{2}\lambda^A_{nm},\quad n<m, \tag{2.16b}$$

we see that the sum over $n\leqslant m$ of the expression (2.16a) is $\mathbf{Tr}\ \tilde{\lambda}\tilde{C}_s$. A similar result holds for the last term of (2.12) [in this case, since we did not insert the factor $(-1)^F$, we obtain the $\hat{\mathbf{Tr}}$ functional]. The volume in phase space is then

$$\Gamma(\Xi)=e^{S_b(\Xi)}\int d\mu_s\ \exp-\{\tau\mathbf{H}_s+\hat{\tau}\hat{\mathbf{H}}_s+\mathbf{Tr}\ \tilde{\lambda}\tilde{C}_s+\hat{\mathbf{Tr}}\ \hat{\tilde{\lambda}}\hat{\tilde{C}}_s\}, \tag{2.17}$$

so that the normalized canonical distribution function (with the subscripts s removed) is given by

$$\rho=Z^{-1}\ \exp-\{\tau\mathbf{H}+\hat{\tau}\hat{\mathbf{H}}+\mathbf{Tr}\ \tilde{\lambda}\tilde{C}+\hat{\mathbf{Tr}}\ \hat{\tilde{\lambda}}\hat{\tilde{C}}\}, \tag{2.18}$$

where

$$Z=\int d\mu\ \exp-\{\tau\mathbf{H}+\hat{\tau}\hat{\mathbf{H}}+\mathbf{Tr}\ \tilde{\lambda}\tilde{C}+\hat{\mathbf{Tr}}\ \hat{\tilde{\lambda}}\hat{\tilde{C}}\}. \tag{2.19}$$

This formula coincides with that obtained by Adler and Millard.[9] Note that the operators $\tilde{\lambda}$ and $\hat{\tilde{\lambda}}$ appear as an infinite set of inverse ''temperatures,'' i.e., equilibrium Lagrange parameters associated both with the bath and the subsystem, corresponding to the conserved matrix elements of $(-1)^F\tilde{C}$ and $\hat{\tilde{C}}$.

We finally remark that the microcanonical entropy defined in (2.4) provides the Jacobian of the transformation from the integration over the measure of $\mathscr{S}$ in (2.19) to an integral over the parameters defining the microcanonical shells. To see this, we rewrite (2.19) as

$$\begin{aligned}Z=\int d\mu\ dE\ d\hat{E}(d\nu)(d\hat{\nu})\,\delta(E-\mathbf{H})\,\delta(\hat{E}-\hat{\mathbf{H}})\prod_{n\leqslant m,A}\delta(\nu^A_{nm}-\langle n|(-1)^F\tilde{C}|m\rangle^A)\\ \times\delta(\hat{\nu}^A_{nm}-\langle n|\hat{\tilde{C}}|m\rangle^A)\exp-\{\tau E+\hat{\tau}\hat{E}+\mathbf{Tr}\ \tilde{\lambda}\tilde{\nu}+\hat{\mathbf{Tr}}\ \hat{\tilde{\lambda}}\hat{\tilde{\nu}}\},\end{aligned} \tag{2.20a}$$

where we have defined the anti-self-adjoint parametric operators $\tilde{\nu}$ and $\hat{\tilde{\nu}}$ by

$$\nu^A_{nm}=\langle n|(-1)^F\tilde{\nu}|m\rangle^A,\quad \hat{\nu}^A_{nm}=\langle n|\hat{\tilde{\nu}}|m\rangle^A. \tag{2.20b}$$

The phase space integration over the δ-function factors reproduces the volume of the microcanonical shell associated with these parameters, i.e., the exponential of the microcanonical entropy, so that the partition function can be written as

$$Z=\int dE\ d\hat{E}(d\nu)(d\hat{\nu})e^{S_{\mathrm{mic}}(E,\hat{E},\tilde{\nu},\hat{\tilde{\nu}})}\ \exp-\{\tau E+\hat{\tau}\hat{E}+\mathbf{Tr}\ \tilde{\lambda}\tilde{\nu}+\hat{\mathbf{Tr}}\ \hat{\tilde{\lambda}}\hat{\tilde{\nu}}\}. \tag{2.21}$$

III. STABILITY AND THERMODYNAMIC RELATIONS

In this section, we study the stability of the canonical ensemble as associated with the dominant contribution to the microcanonical phase space volume. To this end, we formally define the free energy A as the negative of the logarithm of the partition function,

$$Z \equiv e^{-A(\tau,\hat{\tau},\tilde{\lambda},\hat{\tilde{\lambda}})}, \tag{3.1}$$

so that (2.19) can be written as

$$1 = \int d\mu\ e^{A(\tau,\hat{\tau},\tilde{\lambda},\hat{\tilde{\lambda}})} \exp -\{\tau \mathbf{H} + \hat{\tau}\hat{\mathbf{H}} + \mathbf{Tr}\ \tilde{\lambda}\tilde{C} + \hat{\mathbf{Tr}}\ \hat{\tilde{\lambda}}\hat{\tilde{C}}\}. \tag{3.2}$$

Differentiating with respect to (the hypercomplex index A should not be confused with the conventional symbol for the free energy) τ, $\hat{\tau}$, and the matrix elements λ^A_{nm}, $\hat{\lambda}^A_{nm}$, we obtain [as in Eqs. (49) of Ref. 9]

$$\frac{\partial A}{\partial \tau} = \langle \mathbf{H} \rangle_{AV}, \tag{3.3}$$

$$\frac{\partial A}{\partial \hat{\tau}} = \langle \hat{\mathbf{H}} \rangle_{AV}, \tag{3.4}$$

and using

$$\begin{aligned} \mathbf{Tr}\ \tilde{\lambda}\tilde{C} &= -\sum_{n \leqslant m, A} \lambda^A_{nm} \langle n|(-1)^F \tilde{C}|m\rangle^A, \\ \hat{\mathbf{Tr}}\ \hat{\tilde{\lambda}}\hat{\tilde{C}} &= -\sum_{n \leqslant m, A} \hat{\lambda}^A_{nm} \langle n|\hat{\tilde{C}}|m\rangle^A, \end{aligned} \tag{3.5}$$

we find

$$\frac{\partial A}{\partial \lambda^A_{nm}} = -\langle\langle n|(-1)^F \tilde{C}|m\rangle^A\rangle_{AV} \equiv -\langle C^A_{nm}\rangle_{AV}, \tag{3.6}$$

$$\frac{\partial A}{\partial \hat{\lambda}^A_{nm}} = -\langle\langle n|\hat{C}|m\rangle^A\rangle_{AV} \equiv -\langle \hat{C}^A_{nm}\rangle_{AV}. \tag{3.7}$$

We now consider the identity

$$0 = \int d\mu (\mathbf{H} - \langle \mathbf{H} \rangle_{AV}) e^{A(\tau,\hat{\tau},\tilde{\lambda},\hat{\tilde{\lambda}})} \exp -\{\tau \mathbf{H} + \hat{\tau}\hat{\mathbf{H}} + \mathbf{Tr}\ \tilde{\lambda}\tilde{C} + \hat{\mathbf{Tr}}\ \hat{\tilde{\lambda}}\hat{\tilde{C}}\}. \tag{3.8}$$

Differentiating with respect to τ, one finds

$$0 = \int d\mu \left(\frac{\partial A}{\partial \tau} - \mathbf{H} \right) (\mathbf{H} - \langle \mathbf{H} \rangle_{AV}) e^{A(\tau,\hat{\tau},\tilde{\lambda},\hat{\tilde{\lambda}})} \exp -\{\tau \mathbf{H} + \hat{\tau}\hat{\mathbf{H}} + \mathbf{Tr}\ \tilde{\lambda}\tilde{C} + \hat{\mathbf{Tr}}\ \hat{\tilde{\lambda}}\hat{\tilde{C}}\} - \frac{\partial \langle \mathbf{H} \rangle_{AV}}{\partial \tau}, \tag{3.9}$$

so that, from (3.3), we find that (as in Ref. 9)

$$\langle (\mathbf{H} - \langle \mathbf{H} \rangle_{AV})^2 \rangle_{AV} = -\frac{\partial \langle \mathbf{H} \rangle_{AV}}{\partial \tau} = -\frac{\partial^2 A}{\partial \tau^2} \geqslant 0. \tag{3.10}$$

In fact, applying this argument to all of the parameters, we now show that A is a locally convex function. With this result, we will prove the stability of the canonical ensemble.

The derivative of (3.8) with respect to $\hat{\tau}$ yields, using the second of (3.3),

$$\langle(\mathbf{H}-\langle\mathbf{H}\rangle_{AV})(\hat{\mathbf{H}}-\langle\hat{\mathbf{H}}\rangle_{AV})\rangle=-\frac{\partial\langle\mathbf{H}\rangle_{AV}}{\partial\hat{\tau}}=-\frac{\partial^2 A}{\partial\tau\partial\hat{\tau}}. \tag{3.11}$$

In the same way that we obtained (3.10), we also find (using $\hat{\mathbf{H}}-\langle\hat{\mathbf{H}}\rangle_{AV}$ as a factor in the integrand)

$$\langle(\hat{\mathbf{H}}-\langle\hat{\mathbf{H}}\rangle_{AV})^2\rangle_{AV}=-\frac{\partial\langle\hat{\mathbf{H}}\rangle_{AV}}{\partial\hat{\tau}}=-\frac{\partial^2 A}{\partial\hat{\tau}^2}\geqslant 0. \tag{3.12}$$

We consider next the identity

$$0=\int d\mu(C^A_{nm}-\langle C^A_{nm}\rangle_{AV})e^{A(\tau,\hat{\tau},\tilde{\lambda},\hat{\lambda})}\exp-\{\tau\mathbf{H}+\hat{\tau}\hat{\mathbf{H}}+\mathbf{Tr}\,\tilde{\lambda}\tilde{C}+\hat{\mathbf{Tr}}\,\hat{\tilde{\lambda}}\hat{\tilde{C}}\}. \tag{3.13}$$

Differentiating with respect to $\lambda^B_{n'm'}$ and $\hat{\lambda}^B_{n'm'}$, we find

$$\frac{\partial^2 A}{\partial\lambda^A_{nm}\partial\lambda^B_{n'm'}}=-\langle(C^A_{nm}-\langle C^A_{nm}\rangle_{AV})(C^B_{n'm'}-\langle C^B_{n'm'}\rangle_{AV})\rangle_{AV},$$

$$\frac{\partial^2 A}{\partial\hat{\lambda}^A_{nm}\partial\lambda^B_{n'm'}}=-\langle(\hat{C}^A_{nm}-\langle\hat{C}^A_{nm}\rangle_{AV})(C^B_{n'm'}-\langle C^B_{n'm'}\rangle_{AV})\rangle_{AV},$$

$$\frac{\partial^2 A}{\partial\hat{\lambda}^A_{nm}\partial\hat{\lambda}^B_{n'm'}}=-\langle(\hat{C}^A_{nm}-\langle\hat{C}^A_{nm}\rangle_{AV})(\hat{C}^B_{n'm'}-\langle\hat{C}^B_{n'm'}\rangle_{AV})\rangle_{AV}. \tag{3.14}$$

Finally, we differentiate (3.8) with respect to λ^A_{nm} and $\hat{\lambda}^A_{nm}$ to obtain

$$\frac{\partial^2 A}{\partial\tau\partial\lambda^A_{nm}}=\langle(\mathbf{H}-\langle\mathbf{H}\rangle_{AV})(C^A_{nm}-\langle C^A_{nm}\rangle_{AV})\rangle_{AV} \tag{3.15}$$

and

$$\frac{\partial^2 A}{\partial\tau\partial\hat{\lambda}^A_{nm}}=\langle(\mathbf{H}-\langle\mathbf{H}\rangle_{AV})(\hat{C}^A_{nm}-\langle\hat{C}^A_{nm}\rangle_{AV})\rangle_{AV}, \tag{3.16}$$

as well as the corresponding identity with coefficient $\hat{\mathbf{H}}-\langle\hat{\mathbf{H}}\rangle_{AV}$ to obtain

$$\frac{\partial^2 A}{\partial\hat{\tau}\partial\lambda^A_{nm}}=\langle(\hat{\mathbf{H}}-\langle\hat{\mathbf{H}}\rangle_{AV})(C^A_{nm}-\langle C^A_{nm}\rangle_{AV})\rangle_{AV} \tag{3.17}$$

and

$$\frac{\partial^2 A}{\partial\hat{\tau}\partial\hat{\lambda}^A_{nm}}=\langle(\hat{\mathbf{H}}-\langle\hat{\mathbf{H}}\rangle_{AV})(\hat{C}^A_{nm}-\langle\hat{C}^A_{nm}\rangle_{AV})\rangle_{AV}. \tag{3.18}$$

Combining (3.3)–(3.18), we find that the Taylor expansion of A through second derivatives is given by

$$
\begin{aligned}
&A(\tau+\delta\tau,\hat{\tau}+\delta\hat{\tau},\tilde{\lambda}+\delta\tilde{\lambda},\hat{\tilde{\lambda}}+\delta\hat{\tilde{\lambda}}) \\
&\quad = A(\tau,\hat{\tau},\tilde{\lambda},\hat{\tilde{\lambda}}) + \delta\tau\langle\mathbf{H}\rangle_{AV} + \delta\hat{\tau}\langle\hat{\mathbf{H}}\rangle_{AV} - \sum_{n\leqslant m,A} (\delta\lambda^A_{nm}\langle C^A_{nm}\rangle_{AV} + \delta\hat{\lambda}^A_{nm}\langle\hat{C}^A_{nm}\rangle_{AV}) \\
&\qquad - \frac{1}{2}\left\langle \left[\delta\tau(\mathbf{H}-\langle\mathbf{H}\rangle_{AV}) + \delta\hat{\tau}(\hat{\mathbf{H}}-\langle\hat{\mathbf{H}}\rangle_{AV}) \right.\right. \\
&\qquad \left.\left. - \sum_{m\leqslant n,A} \delta\lambda^A_{nm}(C^A_{nm}-\langle C^A_{nm}\rangle_{AV}) + \delta\hat{\lambda}^A_{nm}(\hat{C}^A_{nm}-\langle\hat{C}^A_{nm}\rangle_{AV}) \right]^2 \right\rangle_{AV} ;
\end{aligned}
\tag{3.19}
$$

the uniform negative sign of the quadratic term in the expansion indicates that A is a locally convex function, and shows that the matrix of second derivatives of A is negative semidefinite.

We now turn to the alternative expression of (2.21) for the partition function, defined in terms of an integral over the parameters of a sequence of microcanonical ensembles. The existence of a maximum in the integrand which dominates the integration assures the stability of the canonical ensemble; we now show that (3.19) implies the self-consistency of our assumption of a maximum.

Returning to (2.21), we see that the conditions for a maximum of the integrand at $\xi=\underline{\xi}$ are that there be a stationary point, i.e., that

$$
\begin{aligned}
&\tau = \frac{\partial}{\partial E} S_{\mathrm{mic}}(\xi)\Big|_{\underline{\xi}}, \quad \hat{\tau} = \frac{\partial}{\partial \hat{E}} S_{\mathrm{mic}}(\xi)\Big|_{\underline{\xi}}, \\
&\lambda^A_{nm} = -\frac{\partial}{\partial \nu^A_{nm}} S_{\mathrm{mic}}(\xi)\Big|_{\underline{\xi}}, \quad \hat{\lambda}^A_{nm} = -\frac{\partial}{\partial \hat{\nu}^A_{nm}} S_{\mathrm{mic}}(\xi)\Big|_{\underline{\xi}},
\end{aligned}
\tag{3.20}
$$

together with the requirement that the integrand should decrease in all directions, so that this point corresponds to a maximum. To make our demonstration of stability more transparent, let us define

$$
\chi = \{\chi_i\} = \{\tau, \hat{\tau}, -\lambda^A_{nm}, -\hat{\lambda}^A_{nm}\}, \tag{3.21}
$$

so that (3.20) takes the form

$$
\chi_i = \frac{\partial S_{\mathrm{mic}}}{\partial \xi_i}\Big|_{\underline{\xi}}, \tag{3.22}
$$

where the indices i are in the correspondence implied by (3.20), together with the requirement that the second derivative matrix

$$
\frac{\partial^2 S_{\mathrm{mic}}}{\partial \xi_i \partial \xi_j} = \frac{\partial \chi_i}{\partial \xi_j} \tag{3.23}
$$

should be positive definite. However, the values of E, $\hat{E}$, ν^A_{nm}, and $\hat{\nu}^A_{nm}$ are equal to $\mathbf{H}$, $\hat{\mathbf{H}}$, C^A_{nm}, and $\hat{C}^A_{nm}$ in the microcanonical ensemble, as seen from (2.3). If the stationary values are those given by (3.3), (3.4), (3.6) and (3.7), then we must have

$$
\xi_i = \frac{\partial A}{\partial \chi_i}, \tag{3.24}
$$

which implies that the matrix inverse to the right-hand side of (3.23) is given by

$$\frac{\partial \xi_j}{\partial \chi_i} = \frac{\partial^2 A}{\partial \chi_i \partial \chi_j}, \tag{3.25}$$

which we have shown to be a negative semidefinite matrix. This in turn implies that the matrix on the right-hand side of (3.23) is negative definite, giving the condition needed to assure that the stationary point in (3.20) is indeed a maximum.

Assuming this maximum dominates the integration, then the logarithm of the integral in (2.21) (up to an additive term which is relatively small for a large number of degrees of freedom) may be approximated by

$$A \cong \tau E + \hat{\tau}\hat{E} + \mathbf{Tr}\ \tilde{\lambda}\tilde{C} + \hat{\mathbf{Tr}}\ \hat{\tilde{\lambda}}\hat{\tilde{C}} - S_{\mathrm{mic}}(E, \hat{E}, \tilde{C}, \hat{\tilde{C}}), \tag{3.26}$$

where the arguments are at the extremal values, giving the analog of the standard thermodynamical result $A = E - TS$ for the free energy.

IV. THE OPERATORS $\tilde{C}$ and $\hat{\tilde{C}}$ AS GENERATORS

The microcanonical ensemble is constructed as a set of elements of $\mathscr{S}$, which satisfy a constraint described by the value of **H**. This subset of $\mathscr{S}$ is invariant to the flow generated by **H**, where we define the flow induced by a functional according to the canonical transformation formulas of (1.10a) and (1.10b). As we have remarked above, the space is further restricted by values of $\hat{\mathbf{H}}$ and, in the canonical ensemble, the values of $\mathbf{Tr}\ \tilde{\lambda}\tilde{C}$ and $\hat{\mathbf{Tr}}\ \hat{\tilde{\lambda}}\hat{\tilde{C}}$. Since these four quantities have vanishing Poisson brackets with each other under our present assumptions, the flow generated by all of these functionals lies in the constrained subset of $\mathscr{S}$. In constructing the microcanonical ensemble, we constrain the values of the conserved operators $\tilde{C}$ and $\hat{\tilde{C}}$, i.e., we constrain the values of all total trace functionals constructed by projection from these operators. It is therefore instructive to study the action of general total trace functionals projected from $\tilde{C}$ and $\hat{\tilde{C}}$ as generators of canonical transformations on the phase space.

We first remark that it was pointed out in Ref. 9 that a canonical generator of unitary transformations on the basis of the underlying Hilbert space has the form

$$\mathbf{G}_{\tilde{f}} = -\mathbf{Tr} \sum_r\ [\tilde{f},\ p_r] q_r, \tag{4.1}$$

where $\tilde{f}$ is bosonic. Using (1.11) and the cyclic properties of **Tr**, one sees that

$$\mathbf{G}_{\tilde{f}} = -\mathbf{Tr}\ \tilde{f} \sum_r\ (p_r q_r - \epsilon_r q_r p_r) = \mathbf{Tr}\ \tilde{f}\tilde{C}. \tag{4.2}$$

We thus see that the conserved operator $\tilde{C}$ has the additional role of inducing the action of unitary transformations on the underlying Hilbert space.

That this action preserves the algebraic properties of functionals of the type $\mathbf{G}_{\tilde{f}}$ can be seen by computing the Poisson bracket,

$$\{\mathbf{G}_{\tilde{f}}, \mathbf{G}_{\tilde{g}}\} = \mathbf{Tr} \sum_r\ \epsilon_r \left(\frac{\delta \mathbf{G}_{\tilde{f}}}{\delta q_r} \frac{\delta \mathbf{G}_{\tilde{g}}}{\delta p_r} - \frac{\delta \mathbf{G}_{\tilde{g}}}{\delta q_r} \frac{\delta \mathbf{G}_{\tilde{f}}}{\delta p_r} \right). \tag{4.3a}$$

We use the result that

$$\delta \mathbf{G}_{\tilde{f}} = \mathbf{Tr}\ \tilde{f}\delta\tilde{C} = \mathbf{Tr}\sum_r \{\epsilon_r(\tilde{f}q_r - q_r\tilde{f})\delta p_r - (\tilde{f}p_r - p_r\tilde{f})\delta q_r\} \tag{4.3b}$$

to obtain

$$\frac{\delta \mathbf{G}_{\tilde{f}}}{\delta q_r} = -[\tilde{f},\ p_r], \quad \frac{\delta \mathbf{G}_{\tilde{f}}}{\delta p_r} = \epsilon_r[\tilde{f},\ q_r], \tag{4.4}$$

and hence, expanding out the commutators,

$$\{\mathbf{G}_{\tilde{f}}, \mathbf{G}_{\tilde{g}}\} = -\mathbf{Tr}\sum_r \{p_r\tilde{f}q_r\tilde{g} - p_r\tilde{f}\tilde{g}q_r - \tilde{f}p_rq_r\tilde{g} + \tilde{f}p_r\tilde{g}q_r - p_r\tilde{g}q_r\tilde{f} + p_r\tilde{g}\tilde{f}q_r + \tilde{g}p_rq_r\tilde{f} - \tilde{g}p_r\tilde{f}q_r\}. \tag{4.5}$$

The first and last terms on the right cancel under the **Tr**, as do the fourth and fifth. These cancellations do not depend on the grading under the trace, since they involve only cycling of the bosonic operators $\tilde{f},\tilde{g}$. The remaining terms can be rearranged to the form

$$\{\mathbf{G}_{\tilde{f}}, \mathbf{G}_{\tilde{g}}\} = -\mathbf{Tr}\sum_r [\tilde{f},\ \tilde{g}](p_rq_r - \epsilon_r q_r p_r) = \mathbf{Tr}[\tilde{f},\ \tilde{g}]\tilde{C} = \mathbf{G}_{[\tilde{f},\ \tilde{g}]}. \tag{4.6}$$

These relations, corresponding to the group properties of integrated charges in quantum field theory, can be generalized to a ''local'' algebra. Defining

$$\mathbf{G}_{\tilde{f}r} = \mathbf{Tr}\ \tilde{f}\tilde{C}_r, \tag{4.7a}$$

where

$$\tilde{C}_r = \epsilon_r q_r p_r - p_r q_r, \tag{4.7b}$$

one obtains in the same way that

$$\{\mathbf{G}_{\tilde{f}r}, \mathbf{G}_{\tilde{g}s}\} = \delta_{rs}\mathbf{G}_{[\tilde{f},\ \tilde{g}]r}. \tag{4.8}$$

In studying the flows induced by conserved operators, we shall also need the properties of generators projected from $\hat{\tilde{C}}$. We therefore define

$$\hat{\mathbf{G}}_{\tilde{f}} = \mathbf{Tr}\ \tilde{f}\hat{\tilde{C}}. \tag{4.9}$$

Note that, in terms of this definition,

$$\hat{\mathbf{Tr}}\ \hat{\tilde{\lambda}}\hat{\tilde{C}} = \mathbf{Tr}(-1)^F\hat{\tilde{\lambda}}\hat{\tilde{C}} = \hat{\mathbf{G}}_{(-1)^F\tilde{\lambda}}$$

Substituting (1.12), we find that the operator derivatives of $\hat{\mathbf{G}}_{\tilde{f}}$ with respect to the phase space variables are

$$\begin{aligned} \frac{\delta}{\delta q_r}\hat{\mathbf{G}}_{\tilde{f}} &= -(-1)^F[(-1)^F\tilde{f},\ p_r] = -(\tilde{f}p_r - \epsilon_r p_r\tilde{f}), \\ \frac{\delta}{\delta p_r}\hat{\mathbf{G}}_{\tilde{f}} &= (-1)^F[(-1)^F\tilde{f},\ q_r] = \tilde{f}q_r - \epsilon_r q_r\tilde{f}. \end{aligned} \tag{4.10}$$

Computing Poisson brackets in the same way as above, we find that the algebra of the generators $\mathbf{G}_{\tilde{f}}$ and $\hat{\mathbf{G}}_{\tilde{f}}$ closes,

$$\{\hat{\mathbf{G}}_{\tilde{f}},\hat{\mathbf{G}}_{\tilde{g}}\}=\mathbf{G}_{[\tilde{f},\,\tilde{g}]},\quad \{\hat{\mathbf{G}}_{\tilde{f}},\mathbf{G}_{\tilde{g}}\}=\{\mathbf{G}_{\tilde{f}},\hat{\mathbf{G}}_{\tilde{g}}\}=\hat{\mathbf{G}}_{[\tilde{f},\,\tilde{g}]}, \tag{4.11}$$

giving a structure reminiscent of the vector and axial-vector charge algebra in quantum field theory. Just as the vector and axial-vector charge algebra can be diagonalized into two independent chiral charge algebras, so the algebra of (4.6) and (4.11) can be diagonalized into two independent algebras

$$\mathbf{G}_{\pm\,\tilde{f}}=\tfrac{1}{2}(\mathbf{G}_{\tilde{f}}\pm\hat{\mathbf{G}}_{\tilde{f}}), \tag{4.12}$$

which obey the algebra

$$\{\mathbf{G}_{\pm\,\tilde{f}},\mathbf{G}_{\pm\,\tilde{g}}\}=\mathbf{G}_{\pm[\tilde{f},\,\tilde{g}]},\quad \{\mathbf{G}_{+\,\tilde{f}},\mathbf{G}_{-\,\tilde{g}}\}=0. \tag{4.13}$$

Defining a ''local'' version of $\hat{\mathbf{G}}_{\tilde{f}}$ by

$$\hat{\mathbf{G}}_{\tilde{f}r}=\mathbf{Tr}\;\tilde{\tilde{f}}\hat{\tilde{C}}_r, \tag{4.14}$$

where

$$\hat{\tilde{C}}_r=q_rp_r-p_rq_r, \tag{4.15}$$

the algebras of (4.11) and (4.13) can be converted to local versions analogous to (4.8).

We now turn to the flows associated with $\mathbf{G}_{\tilde{f}}$ and $\hat{\mathbf{G}}_{\tilde{f}}$ when used as canonical generators. Beginning with $\mathbf{G}_{\tilde{f}}$, we consider its action on the function $\mathbf{x}_s(\eta)$ defined in (1.9a), for which $\delta\mathbf{x}_s(\eta)=\mathbf{Tr}\;\eta\delta x_s$. Defining a parameter γ along the motion generated by $\mathbf{G}_{\tilde{f}}$, we choose δx_s as $dx_s/d\gamma$, so that by (1.10a) we have

$$d\mathbf{x}_s(\eta)=\{\mathbf{x}_s(\eta),\mathbf{G}_{\tilde{f}}\}d\gamma. \tag{4.16}$$

Comparing (1.10b) with (4.4) and (4.16) gives

$$\frac{dq_s}{d\gamma}=[\tilde{f},\,q_s],\quad \frac{dp_s}{d\gamma}=[\tilde{f},\,p_s]. \tag{4.17}$$

In both the boson and fermion sectors we see that, as a solution of the differential equations (4.17), $\mathbf{G}_{\hat{f}}$ induces the action of a unitary group generated by $\tilde{f}$,

$$x_s(\gamma)=e^{\tilde{f}\gamma}x_s(0)e^{-\tilde{f}\gamma}. \tag{4.18}$$

The unitary transformation (4.18) preserves the supremum operator norm

$$\|x_s\|=\sup_{\{|n\rangle\}}\frac{|\langle n|x_s|n\rangle|}{|\langle n|n\rangle|}, \tag{4.19}$$

where the supremum is taken over all states $|n\rangle$ in Hilbert space. {The spectrum of x_s may be unbounded; the argument we have given above then applies to all bounded functions of the x_s, for which the operator norm exists. There is, moreover, a possibility that in the unbounded case, a phase space operator may be an eigenfunction of $\tilde{f}$, in the sense that $[\tilde{f},\,x_s]=\sigma_s x_s$ for some real

σ_s. The transformation (4.17) would then correspond to dilation, therefore admitting conformal transformations on some subset of the phase space $\mathscr{S}$ (for which preservation of the operator norm does not form an obstacle).}

We next consider the canonical transformation induced on $\mathbf{x}_s(\eta)$ by the functional $\hat{\mathbf{G}}_{\tilde{f}}$ defined in (4.9). Introducing a parameter $\hat{\gamma}$ along the motion generated by $\hat{\mathbf{G}}_{\tilde{f}}$, we have in this case by (1.10a)

$$d\mathbf{x}_s(\eta)=\{\mathbf{x}_s(\eta),\hat{\mathbf{G}}_{\tilde{f}}\}d\hat{\gamma}. \tag{4.20}$$

Comparing (1.10b) with (4.10) and (4.20) gives

$$\begin{aligned}\frac{dq_s}{d\hat{\gamma}}&=\epsilon_s(-1)^F[(-1)^F\tilde{f},\ q_s]=\epsilon_s\tilde{f}q_s-q_s\tilde{f},\\ \frac{dp_s}{d\hat{\gamma}}&=(-1)^F[(-1)^F\tilde{f},\ p_s]=\tilde{f}p_s-\epsilon_s p_s\tilde{f}.\end{aligned} \tag{4.21}$$

For the bosonic sector, (4.21) can be rewritten as

$$\frac{dq_s}{d\hat{\gamma}}=[\tilde{f},\ q_s],\quad \frac{dp_s}{d\hat{\gamma}}=[\tilde{f},\ p_s], \tag{4.22}$$

and can be integrated as a unitary transformation for both q_s and p_s,

$$x_s(\hat{\gamma})=e^{\tilde{f}\hat{\gamma}}x_s(0)e^{-\tilde{f}\hat{\gamma}}. \tag{4.23}$$

For the fermionic sector, however, the grading index $(-1)^F$ anticommutes with q_s and p_s and $\epsilon_s=-1$; consequently, the differential equations (4.21) in this case take the form

$$\frac{dq_s}{d\hat{\gamma}}=-\{\tilde{f},q_s\},\quad \frac{dp_s}{d\hat{\gamma}}=\{\tilde{f},p_s\}, \tag{4.24}$$

and involve *anticommutators* with the operator $\tilde{f}$, i.e., a graded action. We note, however, that the total trace Lagrangians for which $\tilde{\tilde{C}}$ is conserved are ones in which the fermion fields appear as bosonic bilinears of the form p_rq_s; for these bilinears, and for the reverse ordered bosonic bilinears q_sp_r, we find from (4.24) that

$$\frac{d(p_rq_s)}{d\hat{\gamma}}=[\tilde{f},\ p_rq_s],\quad \frac{d(q_sp_r)}{d\hat{\gamma}}=-[\tilde{f},\ q_sp_r]. \tag{4.25}$$

The solution of these differential equations is the unitary group action

$$(p_rq_s)(\hat{\gamma})=e^{\tilde{f}\hat{\gamma}}(p_rq_s)(0)e^{-\tilde{f}\hat{\gamma}},\quad (q_sp_r)(\hat{\gamma})=e^{-\tilde{f}\hat{\gamma}}(q_sp_r)(0)e^{\tilde{f}\hat{\gamma}}, \tag{4.26}$$

which preserves the supremum operator norm of the bilinears p_rq_s and q_sp_r. However, it is easy to see that for fermionic operators, the supremum operator norm of (4.19) is not preserved by the evolution of (4.24). For example, to lowest order in $\delta\hat{\gamma}$, for the fermionic coordinate variable q_s we have

$$(n,q_s(\delta\hat{\gamma})n)=(n,q_sn)-[(n,\tilde{f}q_sn)+(n,q_s\tilde{f}n)]\delta\hat{\gamma}+O((\delta\hat{\gamma})^2).$$

Now, letting $n=g+h\,\delta\hat{\gamma}$, we obtain

$$(n,q_s(\delta\hat{\gamma})n)=(g,q_sg)+[(h,q_sg)+(g,q_sh)]\delta\hat{\gamma}-[(g,\tilde{f}q_sg)+(g,q_s\tilde{f}g)]\delta\hat{\gamma}+O((\delta\hat{\gamma})^2).$$

Taking $h=\tilde{f}g$, we see that $(g,q_sh)=(g,q_s\tilde{f}g)$ cancels the fifth term on the right, but $(h,q_sg)=(\tilde{f}g,q_sg)=-(g,\tilde{f}q_sg)$ does not cancel the fourth. The action of the diagonalized generators defined in (4.12) is therefore norm preserving on bosonic, but not on fermionic operators.

Finally, it is also useful to define parameters $\gamma_\pm$ along the flows generated by $\mathbf{G}_{\pm\tilde{f}}$ according to

$$d\mathbf{x}_s(\eta)=\{\mathbf{x}_s(\eta),\mathbf{G}_{\pm\tilde{f}}\}d\gamma_\pm, \tag{4.27a}$$

so that

$$\frac{dx_s}{d\gamma_\pm}=\frac{1}{2}\left(\frac{dx_s}{d\gamma}\pm\frac{dx_s}{d\hat{\gamma}}\right). \tag{4.27b}$$

Then taking sums and differences of (4.17), (4.22), and (4.24), we find that for bosons (with x_s either q_s or p_s)

$$\frac{dx_s}{d\gamma_+}=[\tilde{f},\,x_s],\quad \frac{dx_s}{d\gamma_-}=0, \tag{4.28a}$$

which integrate to

$$x_s(\gamma_+)=e^{\tilde{f}\gamma}x_s(0)e^{-\tilde{f}\gamma},\quad x_s(\gamma_-)=x_s(0). \tag{4.28b}$$

Similarly, for fermions we find that

$$\begin{aligned}&\frac{dq_s}{d\gamma_+}=-q_s\tilde{f},\quad \frac{dp_s}{d\gamma_+}=\tilde{f}p_s,\\ &\frac{dq_s}{d\gamma_-}=\tilde{f}q_s,\quad \frac{dp_s}{d\gamma_-}=-p_s\tilde{f},\end{aligned} \tag{4.29a}$$

which integrate to

$$\begin{aligned}&q_s(\gamma_+)=q_s(0)e^{-\tilde{f}\gamma_+},\quad p_s(\gamma_+)=e^{\tilde{f}\gamma_+}p_s(0),\\ &q_s(\gamma_-)=e^{\tilde{f}\gamma_-}q_s(0),\quad p_s(\gamma_-)=p_s(0)e^{-\tilde{f}\gamma_-}.\end{aligned} \tag{4.29b}$$

This identifies $\mathbf{G}_{\pm\tilde{f}}$ as the generators of the one-sided unitary transformations acting on the fermions which are discussed in Refs. 1 and 2.

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Decay of correlations and uniqueness of Gibbs lattice systems with nonquadratic interaction

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The aim of this paper is to develop the classical lattice models with unbounded spin to the case of nonquadratic polynomial interaction. We demonstrate that the distinct relation between the growths of potentials leads to the uniqueness and the fast decay of correlations for Gibbs measure. © *1996 American Institute of Physics.* [S0022-2488(96)00611-1]

There is an approach initiated in Refs. 1–3 to describe the probability measures on infinite-dimensional spaces in the terms of conditional distributions. This approach has already found its nontrivial applications to the natural construction of the different models in the quantum field theory, mathematical and statistical physics.[4–7]

The effective criteria on the existence and uniqueness of such systems were obtained (see Dobrushin's criterion[1,2,8] and Dobrushin–Shlosman mixing condition[9,10]). In the essence of the Dobrushin-type criteria lie the keen variational estimates on the one-point conditional measures, which admit iteration and application of the fixed point arguments. Moreover, such estimates were used in the applications to the lattice spin systems of the statistical physics to the study of decay of correlations, differentiability of pressure, and the connected questions.[11–17]

In the noncompact spin case the check of Dobrushin's conditions is rather complicated because of the principle unboundedness of interaction potentials. The results in this direction were mainly centered around the regular interactions,[11,18–23] i.e., when the many-point potentials in the Hamiltonian admit the quadratic domination, for example with the quadratic two-point potentials

$$H(x)=\sum_{k\in\mathbb{Z}^d} F(x_k)+\lambda\sum_{k,j\in\mathbb{Z}^d} b_{k-j}(x_k-x_j)^2.$$

On the other hand, a wide class of models with nonregular interaction, associated with massless free lattice field, perturbed by $(\nabla\varphi)^4$,

$$H(x)=\sum_{|k-j|=1}(x_k-x_j)^2+\lambda\sum_{|k-j|=1}(x_k-x_j)^4,$$

has already obtained a detail investigation through various techniques.[24–28] In particular, it was shown that the exponential decay of correlations for such systems does not occur for all $\lambda>0$,[24] i.e., the Dobrushin uniqueness technique does not work for such Hamiltonians.

In this paper we demonstrate that there is a wide class of the Gibbs lattice systems which *do not fulfill* the regularity assumption but have the fast decay of correlations. The aim of this paper is to show that the application of Dobrushin's uniqueness technique for the Hamiltonian

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$$H(x)=\sum_{k\in\mathbb{Z}^d} F(x_k)+\lambda\sum_{k,j\in\mathbb{Z}^d} G_{k-j}(x_k-x_j)$$

with polynomials $\{G_j\}$ requires the distinct correlations between the growths of the interaction potentials $\{G_j\}$ and self-action $\{F\}$. This gives us the possibility of treating the problem of the existence, uniqueness, and the *exponentially* fast decay of correlations in the case of *nonquadratic* polynomial interaction. We base our investigation on the scheme of Refs. 1, 2, 8, 12, 13, and 16 and apply the Brascamp–Lieb inequality[29] to obtain estimates on the distance in variations.

Consider $\mathbb{Z}^d$ to be a d-dimensional integer lattice, to each point of which corresponds the linear spin space $\mathbb{R}^1$. Let $\mathcal{G}\{\mu_\Lambda\}$ denote the set of Gibbs measures[1–3] on the product σ-algebra on $\mathbb{R}^{\mathbb{Z}^d}$. It means that the corresponding conditional measures $\{\mu_\Lambda\}$ in the finite volumes of the lattice $\Lambda\subset\mathbb{Z}^d$ are defined by

$$d\mu_\Lambda=\frac{1}{Z_\Lambda}\exp\left\{-\lambda\sum_{\{k,j\}\cup\Lambda\neq\varnothing} G_{k-j}(x_k-x_j)\right\}\times\prod_{k\in\Lambda} e^{-F(x_k)}dx_k, \tag{1}$$

i.e., for all cylinder bounded functions $f\in C_{b,\mathrm{cyl}}(\mathbb{R}^{\mathbb{Z}^d})$ we have $\mu(\mu_\Lambda(f))=\mu(f)$, where $\mu(f)$ denotes the expectation and Z_Λ is a normalization factor.

We put the following conditions on the interactive potentials $\{F,G_j\}$ in the Gibbs measure (1).

(A) Self-action potentials $F\in C^2(\mathbb{R}^1)$, fulfill $F(0)=0$, $\exists\varepsilon>0$ $\inf_{x\in\mathbb{R}}F''(x)\geqslant\varepsilon$ and have no more than the exponential growth on the infinity $\exists c,a\colon\forall x|F(x)|\leqslant ce^{a|x|}$.

(B) Interaction potentials $\{G_j\in C^2(\mathbb{R}^1)\}_{j\in\mathbb{Z}^d\setminus\{0\}}$, fulfill $G_j(0)=0$, $\forall j\in\mathbb{Z}^d\setminus\{0\}\forall x\in\mathbb{R}^1\colon G_j''(x)\geqslant 0$ and $\exists r_0\forall j\colon|j|>r_0\Rightarrow G_j\equiv 0$.

(C) Growth condition $\forall k\in\mathbb{Z}^d|k|\leqslant r_0$

$$\sup_{x_k,x_0\in\mathbb{R}^1}\frac{|G_k''(x_k-x_0)|}{\sqrt{F''(x_k)}\sqrt{F''(x_0)}}<\infty.$$

Immediately remark that condition C states the domination of the one-point potentials over the interaction. It always holds for the quadratic and less than quadratic interaction due to $\sup|G''|\leqslant$const. Actually condition C permits the consideration of the interaction $\{G_j\}$ to be of polynomial type.

The following theorem states the uniqueness and the exponentially fast decay of correlations for the Gibbs measure (1). The existence of such a measure and finiteness of its moments is shown in Theorem 2.

Theorem 1. *Suppose conditions A–C hold and the set of measures $\mu\in\mathcal{G}\{\mu_\Lambda\}$, which satisfy*

$$m_\mu=\sup_{k\in\mathbb{Z}^d}\int_{\mathbb{R}^{\mathbb{Z}^d}}\rho^2(x_k,0)d\mu<\infty,\quad \rho(x,y)=\left|\int_y^x\sqrt{F''(s)}ds\right|, \tag{2}$$

is nonempty. Denote

$$\gamma_d=\sum_{k\in\mathbb{Z}^d} e^{d(k,0)}\sup_{x_k,x_0\in\mathbb{R}^1}\frac{|G''(x_k-x_0)|}{\sqrt{F''(x_k)}\sqrt{F''(x_0)}}$$

for some transitional invariant semimetric $d(k,j)$ on the lattice $\mathbb{Z}^d$.

Then $\forall\lambda\in[0,1/\gamma_d)$ measure $\tilde{\mu}\in\mathcal{G}\{\mu_\Lambda\}$, $m_{\tilde{\mu}}<\infty$, is unique and has exponentially fast decay of correlations, i.e.,

$$\sum_{k\in\mathbb{Z}^d} e^{d(k,0)}|\mathrm{cov}_{\tilde{\mu}}(f,\tau_k g)| \leqslant \frac{1}{1-\lambda\gamma_d}\left(\sum_{k\in\mathbb{Z}^d} e^{d(k,0)}\delta_k(f)\right)\left(\sum_{j\in\mathbb{Z}^d} e^{d(j,0)}\delta_j(g)\right). \tag{3}$$

Above τ_κ is a shift operator on vector $k\in\mathbb{Z}^d$,

$$\delta_k(f)=\sup_{x\in\mathbb{R}^{\mathbb{Z}^d}}\left|\frac{\partial_k f(x)}{\sqrt{F''(x_k)}}\right|, \quad \partial_k f(x)=\frac{\partial f(x)}{\partial x_k}, \quad x=\{x_k\}_{k\in\mathbb{Z}^d}. \tag{4}$$

Inequality (3) is understood on the cylinder bounded differentiable functions $f,g \in C^1_{b,\mathrm{cyl}}(\mathbb{R}^{\mathbb{Z}^d})$ such that $\Sigma_{j\in\mathbb{Z}^d} e^{d(j,0)}\delta_j(f)<\infty$.

Proof: We discuss the main tool, which enables us to deal with the polynomial interaction in the Gibbs measure. First note that the usual estimate on the covariance[30,31]

$$\mathrm{cov}_\mu(f,f)\equiv\int_{\mathbb{R}^1}\left(f-\int_{\mathbb{R}^1} f d\mu\right)^2 d\mu \leqslant \frac{1}{\varepsilon}\int_{\mathbb{R}^1}\left|\frac{\partial f}{\partial x}\right|^2 d\mu, \tag{5}$$

for the probability measure $\mu, d\mu=e^{-F(x)}dx$ on the line $\mathbb{R}^1$, holds for *arbitrary* function $F\in C^2(\mathbb{R})$ such that $F''(x)\geqslant\varepsilon>0$ for all $x\in\mathbb{R}^1$. Actually the above inequality (5) is not optimal and in Ref. 29 (Th.4.1) it was found that the next weighted generalization is true:

$$\mathrm{cov}_\mu(f,f)\leqslant\int_{\mathbb{R}^1}\frac{1}{F''(x)}\left|\frac{\partial f}{\partial x}\right|^2 d\mu, \tag{6}$$

with the weight $1/F''$, which in the cases when F'' grows on the infinity improves inequality (5).

Introduce the family of one-point conditional measures $\{\mu_k\}_{k\in\mathbb{Z}^d}$

$$d\mu_k=\frac{1}{Z_k}\exp\left\{-\lambda\sum_{j:j\neq k} G_{k-j}(x_k-x_j)\right\}e^{-F(x_k)}\,dx_k, \tag{7}$$

where Z_k is a normalization factor. Below we also understand the measure μ_k as the operator of conditional expectation

$$\mu_k: C^1_{b,\mathrm{cyl}}(\mathbb{R}^{\mathbb{Z}^d})\ni f\to\mu_k(f)\overset{\mathrm{def}}{\equiv}\int_{\mathbb{R}^1_k} f d\mu_k\in C^1_{b,\mathrm{cyl}}(\mathbb{R}^{\mathbb{Z}^d}).$$

The next identity for $j,k\in\mathbb{Z}^d$, $j\neq k$,

$$\partial_j\mu_k(f)=\mu(\partial_j f)-\lambda\,\mathrm{cov}_{\mu_k}(f,\partial_j G_{k-j}(x_k-x_j))$$

leads to

$$\begin{aligned}\delta_j(\mu_k(f))=\sup\left|\frac{\partial_j(\mu_k(f))}{\sqrt{F''}}\right|&=\sup\left|\mu_k\left(\frac{\partial_j f}{\sqrt{F''(x_j)}}\right)-\lambda\,\mathrm{cov}_{\mu_k}\left(f,\frac{\partial_j G_{k-j}(x_k-x_j)}{\sqrt{F''(x_j)}}\right)\right|\\ &\leqslant\delta_j(f)+\lambda\,\sup\left|\mathrm{cov}_{\mu_k}\left(f,\frac{\partial_j G_{k-j}(x_k-x_j)}{\sqrt{F''(x_j)}}\right)\right|.\end{aligned} \tag{8}$$

Using the convexness of G_j we obtain the following consequence of the weighted inequality (6):

$$\mathrm{cov}_{\mu_k}(f,f)\leqslant\int_{\mathbb{R}^1}\frac{|\partial_k f|^2}{F''(x_k)+\Sigma_{j\neq k}G''_{k-j}(x_k-x_j)}\,d\mu_k\leqslant\int_{\mathbb{R}^1}\frac{|\partial_k f|^2}{F''(x_k)}\,d\mu_k\leqslant[\delta_k(f)]^2. \tag{9}$$

Inequality (9) enables us to estimate the second term in (8):

$$\begin{aligned}\sup\left|\mathrm{cov}_{\mu_k}\left(f,\frac{\partial_j G_{k-j}(x_k-x_j)}{\sqrt{F''(x_j)}}\right)\right|&\leqslant\sup\,\mathrm{cov}^{1/2}_{\mu_k}(f,f)\,\mathrm{cov}^{1/2}_{\mu_k}\left(\frac{\partial_j G_{k-j}(x_k-x_j)}{\sqrt{F''(x_j)}},\frac{\partial_j G_{k-j}(x_k-x_j)}{\sqrt{F''(x_j)}}\right)\\&\leqslant\delta_k(f)\left(\int_{\mathbb{R}^1}\frac{|\partial_k\partial_j G(x_k-x_j)|^2}{F''(x_k)F''(x_j)}\,d\mu_k\right)^{1/2}\\&\leqslant\delta_k(f)\sup\frac{|G''_{k-j}(x_k-x_j)|}{\sqrt{F''(x_k)}\sqrt{F''(x_j)}}.\end{aligned}$$

Finally from (8) we obtain that

$$\delta_j(\mu_k(f))\leqslant\delta_j(f)+\lambda C_{kj}\delta_k(f) \tag{10}$$

with

$$C_{kj}=\sup_{x_k,x_j\in\mathbb{R}^1}\frac{|G''_{k-j}(x_k-x_j)|}{\sqrt{F''(x_k)}\sqrt{F''(x_j)}}.$$

The estimate (10) is a key point of the Dobrushin's uniqueness technique and the special structure of the *covariance* matrix C_{kj} permits the polynomiality of $\{G_j\}$ in the interaction.

Below we follow the scheme of Refs. 12, 13, and 16. The principal modification lies in the use of weighted inequality (6) and weighted estimate on covariances (10).

1. Uniqueness of the Gibbs measure. As in Ref. 12 we say that the vector $\{a_j\}_{j\in\mathbb{Z}^d}$ is an estimate for probability measures μ,ν if $\forall f\in C^\infty_{b,\mathrm{cyl}}(\mathbb{R}^{\mathbb{Z}^d})$: $\Sigma_{k\in\mathbb{Z}^d}\delta_k(f)<\infty$ we have

$$\left|\int_{\mathbb{R}^{\mathbb{Z}^d}} f\,d\mu-\int_{\mathbb{R}^{\mathbb{Z}^d}} f\,d\nu\right|\leqslant\sum_{j\in\mathbb{Z}^d}a_j\delta_j(f). \tag{11}$$

For any two measures $\mu_1,\mu_2\in\mathcal{G}\{\mu_\Lambda\}$ with property (2) there is an estimate $\tilde{a}=\{\tilde{a}_j\equiv m_0\equiv\mathrm{const}\}_{j\in\mathbb{Z}^d}$ with $m_0=m^{1/2}_{\mu_1}+m^{1/2}_{\mu_2}$. To show this, note first that for $f\in C^1_{b,\mathrm{cyl}}(\mathbb{R}^{\mathbb{Z}^d})$ with $\Sigma_{k\in\mathbb{Z}^d}\delta_k(f)<\infty$ we have

$$|f(x)-f(y)|\leqslant\sum_{i\in\mathbb{Z}^d}\delta_i(f)\rho(x_i,y_i)$$

and therefore

$$\begin{aligned}\left|\int_{\mathbb{R}^{\mathbb{Z}^d}} f\,d\mu_1-\int_{\mathbb{R}^{\mathbb{Z}^d}} f\,d\mu_2\right|&=\left|\int_{\mathbb{R}^{\mathbb{Z}^d}}(f(x)-f(0))d\mu_1-\int_{\mathbb{R}^{\mathbb{Z}^d}}(f(x)-f(0))d\mu_2\right|\\&\leqslant\sum_{k\in\mathbb{Z}^d}\delta_k(f)\int_{\mathbb{R}^{\mathbb{Z}^d}}\rho(x_k,0)\{d\mu_1(x)+d\mu_2(x)\}\leqslant m_0\sum_{k\in\mathbb{Z}^d}\delta_k(f).\end{aligned} \tag{12}$$

By (10) the operator $f \to \mu_k(f)$ preserves the class of functions $\{f \in C^1_{b,\mathrm{cyl}}(\mathbb{R}^{\mathbb{Z}^d}): \Sigma_{k\in\mathbb{Z}^d}\delta_k(f) < \infty\}$. From (10) and (12) we have

$$\begin{aligned}|\mu_1(f)-\mu_2(f)| &= |(\mu_1-\mu_2)(\mu_k(f))| \\ &\leqslant \sum_{j\in\mathbb{Z}^d} \tilde{a}_j \delta_j(\mu_k(f)) \\ &\leqslant \sum_{j:j\neq k} \tilde{a}_j \delta_j(f) + \lambda\,\delta_k(f) \sum_{i:i\neq k} \tilde{a}_i C_{ki}. \end{aligned} \tag{13}$$

Iterating the above estimate by choosing some enumeration $k_1,\ldots,k_n$, of the points of lattice $\mathbb{Z}^d$ one can in a purely algebraic way achieve the following estimate (see Ref. 12, Lemma 2.3):

$$|\mu_1(f)-\mu_2(f)| \leqslant \lambda \sum_{k\in\mathbb{Z}^d} \delta_k(f)\left(\sum_{j\in\mathbb{Z}^d} \tilde{a}_j C_{kj}\right),$$

which gives

$$|\mu_1(f)-\mu_2(f)| \leqslant \sum_{k\in\mathbb{Z}^d} (\tilde{a}(\lambda C)^n)_k \delta_k(f)$$

for all $n \geqslant 0$.

Due to

$$\begin{aligned}\|\tilde{a}(\lambda C)^n\|_{l_\infty(\mathbb{Z}^d)} &= m_0 \sup_{k\in\mathbb{Z}^d} \sum_{j\in\mathbb{Z}^d} \{(\lambda C)^n\}_{kj} \\ &= m_0 \sup_{k\in\mathbb{Z}^d} \lambda^n \sum_{j(1)\in\mathbb{Z}^d} \cdots \sum_{j(n-1)\in\mathbb{Z}^d} \sum_{j\in\mathbb{Z}^d} C_{kj(1)}\cdots C_{j(n-1)j} \\ &\leqslant m_0 \left(\sup_{k\in\mathbb{Z}^d} \lambda \sum_{j\in\mathbb{Z}^d} C_{kj}\right)^n \\ &\leqslant m_0(\lambda\gamma_d)^n \to 0, \quad n\to\infty, \end{aligned} \tag{14}$$

we obtain the uniqueness of the Gibbs measure.

2. Decay of correlations. Fix function $g \in C^1_{b,\mathrm{cyl}}(\mathbb{R}^{\mathbb{Z}^d})$ such that $\int_{\mathbb{R}^{\mathbb{Z}^d}} g\, d\mu = 1$, $g>0$ and $\Sigma_{k\in\mathbb{Z}^d} e^{d(k,0)}\delta_k(g) < \infty$. Then measure $d\nu = g\, d\mu$ for the unique measure $\mu \in \mathcal{G}\{\mu_\Lambda\}$ with property (2) has the same property

$$\sup_{k\in\mathbb{Z}^d} \int_{\mathbb{R}^{\mathbb{Z}^d}} \rho(x_k,0)\, d\nu(x) \leqslant \|g\|_{C_b} m_\mu^{1/2} < \infty.$$

In analog to (12) this gives the estimate $\tilde{a} = \{\tilde{a}_j \equiv m_\mu^{1/2}(\|g\|_{C_b} + 1)\}_{j\in\mathbb{Z}^d}$ on measures μ and ν

$$|\mu(f)-\nu(f)| \leqslant \sum_{k\in\mathbb{Z}^d} \tilde{a}_k \delta_k(f) = m_\mu^{1/2}(\|g\|_{C_b}+1) \sum_{k\in\mathbb{Z}^d} \delta_k(f).$$

Now we prove that if $\{a_j\}_{j\in\mathbb{Z}^d}$ is an estimate, then $\{\Sigma_{j\in\mathbb{Z}^d} a_j C_{jk} + b_k\}_{k\in\mathbb{Z}^d}$ for $b_k = \delta_k(g)$ is an estimate too. Indeed

$$|\mu(f)-\nu(f)|\leqslant\left|(\mu-\nu)_y\left\{\int_{\mathbb{R}_k} f(\cdot|y)d\mu_k(\cdot|y)\right\}\right|$$
$$+\left|\nu_y\left\{\int_{\mathbb{R}_k} f(\cdot|y)d\mu_k(\cdot|y)-\int_{\mathbb{R}_k} f(\cdot|y)d\nu_k(\cdot|y)\right\}\right|$$
$$=\sum_{j\in\mathbb{Z}^d}\tilde{a}_j\delta_j(\mu_k(f))+\left|\nu_y\left\{\int_{\mathbb{R}_k} f(\cdot|y)d\mu_k(\cdot|y)-\int_{\mathbb{R}_k} f(\cdot|y)d\nu_k(\cdot|y)\right\}\right|. \quad (15)$$

Using (10) the first term in (15) can be estimated by

$$\sum_{j\neq k}\tilde{a}_j\delta_j(f)+\lambda\,\delta_k(f)\left\{\sum_{i\neq k}\tilde{a}_i C_{ik}\right\}.$$

We apply inequality (6) to the second term. We use that $d\nu=g\,d\mu$, so $d\nu_k=[g/\mu_k(g)]d\mu_k$ and obtain

$$\left|\nu_y\left\{\int f\,d\mu_k(\cdot|y)-\int f\,d\nu_k(\cdot|y)\right\}\right|=\left|\nu_y\left\{\int[f-\mu_k(f)]\left(d\mu_k-\frac{g}{\mu_k(g)}\,d\mu_k\right)\right\}\right|$$
$$=\left|\mu_y\left\{\frac{g}{\mu_k(g)}\int(f-\mu_k(f))(g-\mu_k(g))d\mu_k\right\}\right|.$$

The result of integration on $\mathbb{R}_k$ does not depend on variable $x_k\in\mathbb{R}_k$, therefore we continue:

$$\left|\mu_y\left\{\frac{g}{\mu_k(g)}\int(f-\mu_k(f))(g-\mu_k(g))d\mu_k\right\}\right|=\left|\mu\left\{\int_{\mathbb{R}_k}(f-\mu_k(f))(g-\mu_k(g))d\mu_k\right\}\right|$$
$$\leqslant\sup\,\mathrm{cov}^{1/2}_{\mu_k}(f,f)\mathrm{cov}^{1/2}_{\mu_k}(g,g)\leqslant\delta_k(f)\,\delta_k(g)$$
$$=b_k\delta_k(f).$$

Finally we have obtained the estimate on (15):

$$|\mu(f)-\nu(f)|\leqslant\sum_{j\neq k}\tilde{a}_j\delta_j(f)+\delta_k(f)\left\{\sum_{i\neq k}\tilde{a}_i\lambda C_{ik}+b_k\right\}. \quad (16)$$

By iteration of (16) as in Refs. 12, 13, and 16, one achieves that $(\tilde{a}\lambda C+b)$ is an estimate, too:

$$|\mu(f)-\nu(f)|\leqslant\sum_{k\in\mathbb{Z}^d}\{\tilde{a}_i\lambda C_{ik}+b_k\}\,\delta_k(f). \quad (17)$$

The vector $b\Sigma_{n=0}^{\infty}(\lambda C)^n$ is also an estimate because of the following convergence in $l_\infty(\mathbb{Z}^d)$:

$$b\sum_{n=0}^{N}(\lambda C)^n+\tilde{a}(\lambda C)^{N+1}\to b\sum_{n=0}^{\infty}(\lambda C)^n,\quad N\to\infty.$$

Thus we achieve estimate[12,13,16]

$$|\mathrm{cov}_\mu(f,g)|=\left|\int_{\mathbb{R}^{\mathbb{Z}^d}} f\,d\nu-\int_{\mathbb{R}^{\mathbb{Z}^d}} f\,d\mu\right|\leqslant\sum_{k,j\in\mathbb{Z}^d}D_{kj}\delta_k(f)\,\delta_j(g) \quad (18)$$

for $D=\Sigma_{n=0}^{\infty}(\lambda C)^n$. Therefore

$$|\mathrm{cov}_\mu(f,\tau_i g)|e^{d(i,0)} \leqslant \sum_{k,j\in\mathbb{Z}^d} e^{d(j,k)} D_{jk} e^{d(k,0)} \delta_k(f\,) e^{d(i,j)} \delta_{j-i}(g).$$

Summing up on $i\in\mathbb{Z}^d$ we have the required decay of correlations for $g>0$.

The case of arbitrary $g \in C^1_{b,\mathrm{cyl}}(\mathbb{R}^{\mathbb{Z}^d})$ with $\Sigma_{k\in\mathbb{Z}^d} e^{d(k,0)}\delta_k(g) < \infty$ is obviously due to the identity $\mathrm{cov}_\mu(f,c_1 g + c_2) = c_1\,\mathrm{cov}_\mu(f,g)$ ■

Theorem 2: *Under conditions A–C the set of Gibbs measures $\mathcal{G}\{\mu_\Lambda\}$ with condition*

$$m_\mu = \sup_{k\in\mathbb{Z}^d} \int_{\mathbb{R}^{\mathbb{Z}^d}} \rho^2(x_k,0)\, d\mu(x) < \infty \tag{19}$$

is nonempty.

Moreover, at the coupling interaction constant $\lambda\in[0,1/\gamma_d)$, the Gibbs measure $\tilde{\mu}$ of Theorem 1 fulfills the estimate

$$\sup_{k\in\mathbb{Z}^d} \int_{\mathbb{R}^{\mathbb{Z}^d}} \exp\{a x_k^2\}\, d\tilde{\mu} \leqslant \exp\left(\frac{a}{\epsilon - 2a}\right) \tag{20}$$

for all $a\in[0,\epsilon/2)$.

Proof: Let

$$\mathcal{U}_\Lambda = \sum_{k\in\Lambda} F(x_k) + \lambda \sum_{\{k,j\}\subset\Lambda} G_{k-j}(x_k - x_j)$$

and consider the family of Gibbs measures $\{\mu_\Lambda\}$ with the free boundary conditions in the finite volumes $\Lambda\subset\mathbb{Z}^d$

$$d\mu^0_\Lambda = \frac{1}{Z}\, e^{-\mathcal{U}_\Lambda}\, dx_\Lambda\,.$$

The potentials $(\mathcal{U}_\Lambda)'' \geqslant \epsilon I$ are convex, so the measures μ^0_Λ satisfy inequality (24) in form[30,31]

$$\mathrm{cov}_{\mu^0_\Lambda}(f,f\,) \leqslant \frac{1}{\epsilon} \int_{\mathbb{R}^\Lambda} \sum_{k\in\Lambda} |\partial_k f|^2\, d\mu^0_\Lambda.$$

Substituting $f = x_k$ and using that $\int_{\mathbb{R}^\Lambda} x_k d\mu^0_\Lambda \equiv 0$ by the symmetry of μ^0_Λ, we have that uniformly on Λ and $k\in\Lambda$

$$\sup_{\Lambda\subset\mathbb{Z}^d,\ k\in\Lambda} \int_{\mathbb{R}^\Lambda} x_k^2\, d\mu^0_\Lambda \leqslant 1/\epsilon. \tag{21}$$

The convexness of the potentials $\mathcal{U}_\Lambda$ also implies the Log–Sobolev inequality for the measures $\{\mu^0_\Lambda\}$:[30]

$$\int_{\mathbb{R}^\Lambda} f^2 \ln f^2\, d\mu^0_\Lambda - \int_{\mathbb{R}^\Lambda} f^2\, d\mu^0_\Lambda \ln \int_{\mathbb{R}^\Lambda} f^2\, d\mu^0_\Lambda \leqslant \frac{2}{\epsilon} \int_{\mathbb{R}^\Lambda} \sum_{k\in\Lambda} |\partial_k f(x_\Lambda)|^2\, d\mu^0_\Lambda(x_\Lambda). \tag{22}$$

Fix $\Lambda\subset\mathbb{Z}^d$ and $k\in\Lambda$. Consider increasing on $n\geqslant 1$ sequence of functions:

$$f_n=\begin{cases} -n, & x_k<-n,\\ x_k, & |x_k|\leqslant n,\\ n, & x_k>n. \end{cases}$$

As in Ref. 31 introduce the sequence of functions $h_n(a)=\int_{\mathbb{R}^\Lambda}\exp(af_n^2)d\mu_\Lambda^0\geqslant 1$ on half-line $a\in[0,\infty)$, increasing on both a and n with all derivatives $h_n^{(k)}(a)>0$, $a>0$. Then for $g_n=\exp(af_n^2/2)$ we apply the Log–Sobolev inequality (22):

$$\begin{aligned} ah_n'(a)&=\int_{\mathbb{R}^\Lambda} af_n^2\,\exp(af_n^2)d\mu_\Lambda^0=\int_{\mathbb{R}^\Lambda} g_n^2\,\ln\, g_n^2 d\mu_\Lambda^0\\ &\leqslant\frac{2}{\varepsilon}\int_{\mathbb{R}^\Lambda}\sum_{j\in\Lambda}|\partial_j g_n|^2\,d\mu_\Lambda^0+h_n(a)\ln\, h_n(a)\\ &\leqslant\frac{2}{\varepsilon}\,a^2\int_{\mathbb{R}^\Lambda} f_n^2\,\exp(af_n^2)d\mu_\Lambda^0+h_n(a)\ln\, h_n(a). \end{aligned}$$

Therefore the family $h_n(a)$, increasing on both n and $a\geqslant 0$, $h_n(0)=1$, satisfy the inequality $a(1-2a/\varepsilon)h_n'(a)\leqslant h_n(a)\ln h_n(a)$. To find the major function we must set $h(0)=1$ and take the highest growth of its derivative, so $a(1-2a/\varepsilon)h'(a)=h(a)\ln h(a)$ and

$$h(a)=\exp[aD/(1-2a/\varepsilon)]$$

for some D. The restriction on D we obtain from the highest growth of h_n at zero,

$$h_n'(0)=\int_{\mathbb{R}^\Lambda} f_n^2\,d\mu_\Lambda^0\leqslant\int_{\mathbb{R}^\Lambda} x_k^2\,d\mu_\Lambda^0(x)=D<\infty,$$

and achieve estimate

$$h_n(a)\leqslant\exp\left\{\frac{a}{1-2a/\varepsilon}\int_{\mathbb{R}^\Lambda} x_k^2\,d\mu_\Lambda^0(x)\right\}.$$

Tending $n\to\infty$ we obtain the estimate of the next form at $a\in[0,\varepsilon/2)$,

$$\int_{\mathbb{R}^\Lambda}\exp(ax_k^2)d\mu_\Lambda^0\leqslant\exp\left(\frac{a}{1-2a/\varepsilon}\int_{\mathbb{R}^\Lambda} x_k^2\,d\mu_\Lambda^0\right),$$

which by (21) gives

$$\forall\, a\in[0,\varepsilon/2)\qquad\sup_{\Lambda\subset\mathbb{Z}^d,k\in\Lambda}\int_{\mathbb{R}^\Lambda}\exp(ax_k^2)d\mu_\Lambda^0<\exp\left(\frac{a}{\varepsilon-2a}\right).\tag{23}$$

Compactness of the function $\exp(ax_k^2)$ leads by the Prochorov's theorem[7] to the existence of the weak local limit $\tilde{\mu}$,

$$\lim_{\Lambda\nearrow\mathbb{Z}^d}\int_{\mathbb{R}^\Lambda} f(x_\Lambda)d\mu_\Lambda^0=\int_{\mathbb{R}^{\mathbb{Z}^d}} f(x)d\tilde{\mu},$$

on any cylinder function $f\in C_{b,\mathrm{cyl}}(\mathbb{R}^{\mathbb{Z}^d})$.

Due to the finiteness of the interaction radius (condition B), the limit measure $\tilde{\mu}$ has the conditional measures $\{\mu_\Lambda\}$ in the finite volumes, i.e., $\tilde{\mu}\in\mathcal{G}\{\mu_\Lambda\}$ and the set of the Gibbs measures is nonempty. From (23) we also have that the measure $\tilde{\mu}$ is tempered, i.e.,

$$\sup_{k\in\mathbb{Z}^d}\int_{\mathbb{R}^{\mathbb{Z}^d}}\exp(ax_k^2)d\tilde{\mu}<\exp\left(\frac{a}{\varepsilon-2a}\right),\quad a\in[0,\varepsilon/2),$$

which obviously gives the statement (20). ■

Model 1: Let the potentials be defined by

$$F(x_k)=(1+x_k^2)^{2n+1}\quad\text{and}\quad G_{k-j}(x_k-x_j)=b_{k-j}(x_k-x_j)^{2n+2}$$

and assume that the coefficients $\{b_j\}_{j\in\mathbb{Z}^d}$ satisfy

$$\forall j\in\mathbb{Z}^d\ \ b_j\geqslant 0\ \text{ and }\ \exists r_0\forall|j|>r_0: b_j=0.$$

Then for

$$0\leqslant\lambda<\frac{1}{(n+1)2^{2n+1}\|b\|_d},\quad \|b\|_d=\sum_{j\in\mathbb{Z}^d}b_j e^{d(j,0)}<\infty$$

the statements of Theorems 1 and 2 are valid.

Model 2. Lattice spin system on Riemannian manifold. Denote $M=M_k$, $k\in\mathbb{Z}^d$, a noncompact Riemannian manifold with covariant derivative ∂_k and Ricci curvature tensor Ric_k.

Let potentials $F_k(x_k)$, $G_{kj}(x_k,x_j)$ satisfy

(1) $F_k\in C^2(M)$, $\exists\varepsilon>0\forall x_k\in M_k\ \mathrm{Ric}_k+\partial_k\partial_k F(x_k)\geqslant\varepsilon$;

(2) $G_{kj}\in C^2(M\times M)$, $\exists\alpha\in\mathbb{R}^1\partial_k\partial_k G_{kj}(x_k,x_j)\geqslant-\alpha$, $k,j\in\mathbb{Z}^d$ and $G_{kj}\equiv 0$, for $|k-j|\geqslant r_0$;

(3) $\alpha_{k,j}=\sup_{x\in M^{\mathbb{Z}^d}}\|B^{-1/2}(x_k)B^{-1/2}(x_j)\partial_k\partial_j G_{kj}(x_k,x_j)\|_{TM_k\times TM_j}<\infty$,

where $B(x_k)=\mathrm{Ric}_k(x_k)+\partial_k\partial_k F_k(x_k)$ and $\|\cdot\|_{TM_k\times TM_j}$ is a standard Hilbert norm on tangent space to $M_k\times M_j$.

Then for $\lambda\in[0,\min(\varepsilon/\alpha(2r_0+1)^d,1/\gamma_d))$ the lattice system, described by Hamiltonian

$$H=\sum_{k\in\mathbb{Z}^d}F_k(x_k)+\lambda\sum_{|k-j|\leqslant r_0}G_{kj}(x_k,x_j),$$

has exponentially fast decay of correlations and the Gibbs measure is unique.[32] Above $\gamma_d=\sup_{k\in\mathbb{Z}^d}\Sigma_{j\in\mathbb{Z}^d}e^{d(k,j)}\alpha_{kj}$.

This result is achieved by the scheme of this paper. One needs to consider

$$\delta_k(f)=\sup_{x\in M^{\mathbb{Z}^d}}\|(\mathrm{Ric}_k+\partial_k\partial_k F(x_k))^{-1/2}\partial_k f(x)\|_{TM_k}$$

and apply in corresponding places the following generalization of the Brascamp–Lieb inequality (6) to the case of arbitrary Riemannian manifold:[32] under condition $\exists\varepsilon>0$ $\mathrm{Ric}+\partial\partial F\geqslant\varepsilon$ we have

$$\mathrm{cov}_\mu(f,f)\leqslant\int_M\langle(\mathrm{Ric}+\partial\partial F)^{-1}\partial f,\partial f\rangle d\mu,\quad f\in C_b^1(M),\tag{24}$$

with probability measure $d\mu=e^{-F}\,d\sigma$ (σ denotes Riemannian volume on manifold M) and Riemannian pairing $\langle\cdot,\cdot\rangle$ on tangent space to manifold.

Developing idea of Helffer[28,33] we can shortly explain inequality (24) in the following way. Take $u=\partial H_\mu^{-1}(g-\int g\ d\mu)$ for $H_\mu=\partial_\mu^*\partial$ with dual gradient $\partial_\mu^* v=-\operatorname{div} v+\langle \partial F, v\rangle$. Then $\partial_\mu^* u=H_\mu H_\mu^{-1}(g-\int g\ d\mu)=g-\int g\ d\mu$ and we have

$$\operatorname{cov}_\mu(g,g)=\int g\left(g-\int g\ d\mu\right)d\mu=\int \langle u,\partial g\rangle d\mu$$

$$=\int \langle (H_\mu+\mathrm{Ric}+\partial\partial F)^{-1}\partial g,\partial g\rangle d\mu$$

$$\leqslant \int_M \langle (\mathrm{Ric}+\partial\partial F)^{-1}\partial g,\partial g\rangle d\mu,$$

where we used the positivity of H_μ and $u=(H_\mu+\mathrm{Ric}+\partial\partial F)^{-1}\partial g$ by a simple commutation $\partial g=\partial\partial_\mu^* u=(\partial_\mu^*\partial+\mathrm{Ric}+\partial\partial F)u$.

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Integration of thermodynamic identities for a relativistic general equation of state

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In a recent paper Mason and Kgathi have integrated some well-known thermodynamic identities for an equation of state $p=nkT$ and thereby have obtained some explicit expressions for the thermodynamic variables concerned. In the present paper we integrate the same identities for a more general equation of state $p=p(n,T)$ and thereby obtain more general expressions for the same thermodynamic variables. © *1996 American Institute of Physics.*
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I. INTRODUCTION

In a recent paper Mason and Kgathi[1] have shown that the well-known thermodynamic identities,

$$d\mu = T\,dS + K\,dn \tag{1a}$$

and

$$\mu = TS + Kn - p, \tag{1b}$$

together can be integrated for an equation of state,

$$p = nkT. \tag{2}$$

Here μ is the total energy density, T is the temperature in Kelvin, S is the entropy per unit volume, n is the particle number density, K is the chemical potential per particle, k is Boltzmann's constant, and p is the pressure. The purpose of the present paper is to integrate equations (1) for a more general equation of state,

$$p = p(n,T). \tag{3}$$

II. SOLUTIONS

Equations (1) and (3) can be combined to give

$$\mu(s,n) = S\,\frac{\partial\mu(S,n)}{\partial S} + n\,\frac{\partial\mu(S,n)}{\partial n} - p(n,T), \tag{4}$$

where

$$T = \frac{\partial\mu(S,n)}{\partial S}, \tag{5a}$$

$$K = \frac{\partial\mu(S,n)}{\partial n}. \tag{5b}$$

Also, by virtue of Eq. (5a), one can rewrite Eq. (4) as

$$\mu(S,n)=S\,\frac{\partial\mu(S,n)}{\partial S}+n\,\frac{\partial\mu(S,n)}{\partial n}-p\left(n,\frac{\partial\mu}{\partial S}\right). \tag{6}$$

Equation (6) is a nonlinear partial differential equation for $\mu(S,n)$ that can be solved as follows.

Differentiating Eq. (6) wrt S while treating n as constant one gets

$$S\,\frac{\partial^2\mu(S,n)}{\partial S^2}+n\,\frac{\partial^2\mu(S,n)}{\partial S\;\partial n}-\frac{p(n,(\partial\mu/\partial S))}{\partial(\partial\mu/\partial S)}\,\frac{\partial^2\mu}{\partial S^2}=0, \tag{7}$$

which by virtue of Eq. (5a) can be rewritten as

$$S\,\frac{\partial T(S,n)}{\partial S}+n\,\frac{\partial T(S,n)}{\partial n}-\frac{\partial p(n,T)}{\partial T}\cdot\frac{\partial T(S,n)}{\partial S}=0. \tag{8}$$

Treating S as a function of n and T, one can rewrite Eq. (8) as

$$S(n,T)-n\,\frac{\partial S(n,T)}{\partial n}=\frac{\partial p(n,T)}{\partial T},$$

which can be easily integrated as

$$S=n\,\frac{\partial}{\partial T}\left(f(T)-\int\frac{1}{n^2}\,p(n,T)dn\right), \tag{9}$$

where $f(T)$ is an arbitrary function of T.

Equation (5a) can now be integrated wrt S by treating n as constant to give

$$\mu=\int T\,dS+\alpha(n)=TS-\int S\,dT+\alpha(n), \tag{10}$$

where $\alpha(n)$ is an arbitrary function of n while $\int S\,dT$ represents an integration of S wrt T, treating n as constant.

From Eqs. (9) and (10) one gets

$$\mu=nT\left[f'(T)-\int\frac{1}{n^2}\,\frac{\partial p(n,T)}{\partial T}\,dn-n\left[f(T)-\int\frac{1}{n^2}\,p(n,T)dn\right]+\alpha(n)\right]. \tag{11}$$

Equations (9) and (11) together give a form for μ as a function of S and n where T is a parameter. Obviously any solution $\mu(S,n)$ of Eq. (6) must be of this form. But any μ of the form given by Eqs. (9) and (11) together may not satisfy Eq. (6), because the equations (9) and (11) are essentially obtained from Eq. (7), which was obtained by differentiation of Eq. (6) wrt S. So putting Eqs. (9) and (11) back into Eq. (6) and using relations like

$$\left(\left.\frac{\partial\mu}{\partial n}\right|_{\substack{S\text{ as}\\ \text{constant}}}\right)=\left(\left.\frac{\partial\mu}{\partial n}\right|_{\substack{T\text{ as}\\ \text{constant}}}\right)-\left(\left.\frac{\partial\mu}{\partial T}\right|_{\substack{n\text{ as}\\ \text{constant}}}\right)\left(\frac{\partial S(n,T)/\partial n}{\partial S(n,T)/\partial T}\right),$$

one gets after a little calculation,

$$n\,\frac{d\alpha(n)}{dn}=\alpha(n),$$

which gives $\alpha(n)=nL$, where L is a constant of integration. Putting this form of $\alpha(n)$ back into Eq. (11), it is easy to see that the constant of integration L can be easily absorbed into $f(T)$. Hence one gets finally

$$\mu=n\left[T\left\{f'(T)-\int \frac{1}{n^2}\frac{\partial p(n,T)}{\partial T}\,dn\right\}-\left\{f(T)-\int \frac{1}{n^2}\,p(n,T)dn\right\}\right]. \tag{12}$$

III. CONCLUSION

In summary, we have integrated the thermodynamic identities given by (1a) and (1b) for any equation of state of the form (3). On integration the total energy density function μ is expressed as a function of other thermodynamic variables n and T, as is given by Eq. (12), the entropy per unit volume S is obtained as a function of n and T, and is given by Eq. (9).

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The low activity phase of some Dirichlet series

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We show that a rigorous statistical mechanics description of some Dirichlet series is possible. Using the abstract polymer model language of statistical mechanics and the polymer expansion theory we characterize the *low activity* phase by the suitable exponential decay of the truncated correlation functions. © *1996 American Institute of Physics.* [S0022-2488(96)01511-3]

I. INTRODUCTION

The idea to relate number theory and equilibrium statistical mechanics or, more precisely, zeta functions and partition functions, is now already quite old. One motivation for pursuing this idea lies in the probabilistic aspects of the prime number distribution. Statistical mechanics as an intrinsically probabilistic theory is hoped to be an appropriate language for these phenomena. The book[1] by Kac nicely presents this kind of probabilistic reasoning.

More concretely, the formulation of the famous Lee–Yang theorem was influenced by a paper[2] by Pólya on the Riemann zeta function. In that paper Pólya took the asymptotics of the Fourier transformed zeta function and proved for its inverse Fourier transform the ''Riemann hypothesis,'' saying that the nonreal zeroes have real part $\frac{1}{2}$.

As described by Kac in Ref. 2, the method of Pólya's proof inspired the first version of the Lee–Yang theorem (which says that the partition function of ferromagnetic Ising models has only zeroes on the unit circle of the activity plane).

This led to the natural question whether inversely the Riemann hypothesis or simpler number-theoretical questions could be proven by some statistical mechanics method.

In recent years two approaches have been followed. In one of them the Riemann zeta function $\zeta(s)$ itself was interpreted as partition function of a system of *interacting primes* at inverse temperature s (see Refs. 3–6). In the last-mentioned paper the system was shown to exhibit a phase transition at $s=1$ with type I states (resp. type III) at low (resp. high) temperature.

In the second approach mentioned the quotient $\zeta(s-1)/\zeta(s)$ is interpreted as a partition function at the inverse temperature s (see Refs. 7–13).

It was shown that the partition function described a spin chain with asymptotically translation-invariant long-range ferromagnetic interaction (the *number-theoretical spin chain*). The point $s=2$ corresponds to a phase transition where magnetization jumps from 0 to 1.

Although there exist versions of the Lee–Yang theorem predicting zero-free half-planes in the inverse temperature plane, unfortunately these theorems cannot be applied to the above spin chain, since its interaction includes multi-body terms.

In this paper, using the general polymer model approach of statistical mechanics, we propose a criterium to interpret a large class of Dirichlet series as grand canonical partition functions of hard-core interacting systems.

The criterium involves a finite-volume approximation and a precise notion of activity. We

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present two possible polymerizations: the first is based on the notion of Euler product and works for multiplicative arithmetical functions, the second covers a wider class of cases.

We show that the natural thermodynamical quantities of the polymer model, like correlation functions, carry a deep number-theoretical meaning being the probability of suitable divisibility properties.

In order to control the behavior of the correlation functions we apply the polymer expansion technique by means of the Kirkwood–Salsburg iterative equations: the low activity expansion theory enables us to prove the exponential decay of all the truncated correlation functions and provides, in general, a full analytical control of the low temperature phase.

This shows that the language of polymer models is not only formally but also analytically adequate to describe the considered class of Dirichlet series.

Our approach clarifies the statistical mechanics meaning of the absolute convergence theory for the Dirichlet series and introduces new perspectives on it; moreover, it has the merit to point out the natural limits of each polymerization. The polymerizations treated in this work, like similar techniques in number theory, provide an approximation of the Dirichlet function which works well for the large real part of the complex plane but its results are too nonuniform elsewhere, especially on the critical strip.

We believe that, in order to obtain new analytical results from the number-theoretical point of view, one has to search for different polymerizations, for instance the high temperature ones, or better to explore more subtle strategies like the *rearrangement* procedure for polymer models (see Refs. 14 and 15) which, in some cases, provide a good control of the asymptotic behavior of the correlation functions in the interesting regions of the phase space.

All these ideas can be improved and tested with the study of the number theoretical spin chain: the interacting objects there are not directly related to primes and could suggest different types of polymerization based on groups of spins (see Ref. 13). Moreover the approximant family φ_k (Refs. 7 and 8) of the Euler totient function could really be seen as a systematic way to rearrange the Euler totient function φ thought as a *bare* interaction. We will return to these questions elsewhere.

Notation: Sums (resp. products) over empty sets equal zero (resp. one). We write $\mathbb{N}:=\{1,2,3,...\}$ for the integers, $\mathbb{N}_0:=\mathbb{N}\cup\{0\}$ and $\mathbb{P}\equiv\{2,3,5,...\}$ for the primes. If n divides m, we write $n|m$ and the symbol $\Sigma_{n|m}$ denotes a sum over all the divisors of m; (n,m) is the greatest common divisor of m and n.

II. THE POLYMER EXPANSION

Statistical mechanics seeks to describe the collective behavior of a large number of similar particles. One assumes that these particles are enclosed in a finite region $\Lambda\subset S$ of space S (typically $S=\mathbb{R}^d$ or $S=\mathbb{Z}^d$) and then considers the thermodynamic limit $\Lambda\nearrow S$.

The mutual interaction between the particles in a configuration σ is encoded by their total energy $H_\Lambda(\sigma)$. At inverse temperature s the probability of that configuration is given by $\exp(-sH_\Lambda(\sigma))/Z_\Lambda(s)$,

$$Z_\Lambda(s):=\sum_\sigma \exp(-sH_\Lambda(\sigma)) \tag{1}$$

being the partition function for volume Λ.

So the basic objects of statistical mechanics are the Boltzmann factors $\exp(-sH_\Lambda(\sigma))$ of the configurations.

Whereas the above Gibbs probability measures for the finite volume Λ are real-analytic in the parameter s, in the thermodynamic limit $\Lambda\nearrow S$ nonanalyticities arise which are called phase transitions. Different asymptotic Gibbs measures may then be compatible with a given interaction and inverse temperature.

This phenomenon is typical for random fields, i.e., random functions in several variables, and is of central interest in today's theory of probability.

Thus one basic problem of statistical mechanics consists of determining regions in parameter space (e.g., in the s plane) where intensive quantities like the free energy $|\Lambda|^{-1}\ln(Z_\Lambda(s))$ stay analytic in the thermodynamic limit.

Many of the techniques employed in that context recently turned out to be related, the common ground being the abstract *polymer model* formulation (see Refs. 16–18).

In the abstract setting one starts with a denumerable set $P\equiv\{\gamma_1,\gamma_2,...\}$ whose elements are called *polymers* and with an assigned reflexive symmetric relation of *incompatibility* between each of the two of them.

In the concrete application of a two-dimensional Ising model, the polymers may be the contours enclosing a region of constant spin direction, or the subgraphs of the nearest-neighbor graph, depending on whether one is interested in small or large temperatures; the incompatibility between two of them is simply the mutual overlapping.

Thus one may associate to a *k-polymer* $X:=\{\gamma_1,\ldots,\gamma_k\}\in P^k$ an undirected graph $G(X)=(V(X),E(X))$ with vertex set $V(X):=\{1,\ldots,k\}$, vertices $i\neq j$ being connected by the edge $\{\gamma_i,\gamma_j\}\in E(X)$ if γ_i and γ_j are incompatible. Accordingly the k-polymer X is called connected if $G(X)$ is path connected and (completely) disconnected if it has no edges $[E(X)=\varnothing]$.

The corresponding subsets of P^k are called C^k resp. D^k, with $D^0:=P^0:=\{\varnothing\}$ consisting of a single element. Moreover $P^\infty:=\cup_{k=0}^\infty P^k$ with the subsets $D^\infty:=\cup_{k=0}^\infty D^k$ and $C^\infty:=\cup_{k=1}^\infty C^k$. We write $|X|:=k$ if $X\in P^k$; indicating with $X(\gamma)$ the multiplicity of γ in X it results in $k=\Sigma_i X(\gamma_i)$. It is useful to define the function $c(X):=\Pi_i X(\gamma_i)!$. We will indicate with a hat the Abelianized set: for instance $\hat{P}^\infty$ is the set of Abelian words (which we also call polymer configurations) which arises if one identifies k-polymers $X=\{\gamma_1,\ldots,\gamma_k\}$, $Y=\{\delta_1,\ldots,\delta_k\}\in P^\infty$ if $\delta_{\pi(i)}=\gamma_i$ for some permutation π.

Statistical weights or activities $z:P\to\mathbb{C}$ of the polymers are multiplied to give the activities $z^X:=\Pi_{i=1}^k z(\gamma_i)$ of k-polymers.

The thermodynamical properties of the model are defined through the partition function

$$Z=\sum_{X\in\hat{D}^\infty} z^X. \tag{2}$$

We observe that no multiple occurrence of a polymer is allowed since the incompatibility relation is reflexive; for this reason the sum is finite when P has finite cardinality which corresponds to a finite volume in the concrete cases.

It has to be stressed that the polymer models are not statistical mechanics models in the usual form (1). They are useful devices to study the true models in the *low activity* regime of the phase diagram: for this reason a given model is often mapped into different polymer models according to each different phase regime.

One is mainly interested in the $|P|\to\infty$ limit (thermodynamic limit) for the mean values of the configuration functions h:

$$\langle h\rangle_z=\frac{\Sigma_{X\in\hat{D}^\infty}h(X)z^X}{\Sigma_{X\in\hat{D}^\infty}z^X}, \tag{3}$$

and especially for the correlation functions

$$\rho_z(Y)=\langle\chi_Y\rangle_z, \tag{4}$$

where χ_Y is the characteristic function of Y. Often the dependence of the correlation functions on the activity is studied in terms of parameters such as, for instance in statistical mechanics, the inverse temperature or a magnetic field.

An important quantity to be studied in the thermodynamic limit is the free energy density, or pressure, which turns out to be (see, for instance, Refs. 16 and 19) up to a suitable normalization factor

$$\ln(Z)=\sum_{X\in\hat{P}^{\infty}}\frac{n^{T}(X)}{c(X)}z^{X}, \tag{5}$$

with $n^T(X):=n_+(X)-n_-(X)$, $n_\pm(X)$ being the number of subgraphs of $G(X)$ connecting all the vertices of $G(X)$ with an even (resp. odd) number of edges. The structure of the factors n^T implies that the previous sum is actually supported only on $\hat{C}^{\infty}$.

We notice that, although in the partition sum only compatible configurations of polymer may appear, the free energy contains contribution from all the configuration and also coincident polymers (multiplicities) are allowed.

Formula (5) is important from the conceptional as well as from the analytical point of view. It is complemented by the so-called tree estimate $|n^T(X)|\leqslant|\tau(G(X))|$, where $\tau(G)$ denotes the set of maximal subtrees of the connected graph G. This inequality is useful, since there exist techniques to estimate the number of subtrees. As an example, a theorem by Cayley says that the complete (all edges present) graph $K(k)$ with k vertices contains $|\tau(K(k))|=k^{k-2}$ maximal trees.

It is easy to check that the simplest example $P=\{p\}$, i.e., $Z=1+z$, of a polymer model reduces the formula (5) to the Taylor expansion for the logarithm $\ln(Z)=\Sigma_{k=1}^{\infty}[(-1)^{k-1}/k]z^k$, since $n^T(K(k))=(-1)^{k-1}(k-1)!$ (the last formula showing, by the way, that the tree estimate is nonoptimal).

So even for a finite cardinality of P one needs bounds on the activities to ensure convergence of the free energy. In the statistical mechanics applications such bounds are given in terms of energy (or activity) and entropy bounds.

III. DIRICHLET SERIES

A basic object of analytic number theory is the Dirichlet series consisting of terms of the form $e^{-s\lambda_n}$ whose exponents $\{\lambda_n\}_{n\in\mathbb{N}}$ are a real-valued sequence strictly increasing to $\lim_{n\to\infty}\lambda_n=\infty$.

A formal series of the form

$$\sum_{n=1}^{\infty}a(n)e^{-s\lambda_n} \tag{6}$$

with complex coefficients $a(n)$ and argument s is called a general Dirichlet series. In this context functions $A:\mathbb{N}\to\mathbb{C}$ are called *arithmetical functions*.

Dirichlet series have abscissae $\sigma_a(\sigma_c)$ of *absolute* (resp. *conditional*) convergence. For $\lambda_n:=n$ Eq. (6) is a power series in $x:=e^{-s}$ so that σ_a and σ_c coincide.

For $\lambda_n:=\ln(n)$ Eq. (6) is called an ordinary Dirichlet series, and we write it in the form

$$Z_a(s):=\sum_{n=1}^{\infty}a(n)n^{-s}. \tag{7}$$

In that case $0\leqslant\sigma_a-\sigma_c\leqslant1$.

The simplest choice $a(n):=1$ of coefficients leads to the Riemann zeta function $\zeta(s)=\Sigma_{n=1}^{\infty}n^{-s}$ with inverse $1/\zeta(s)=\Sigma_{n=1}^{\infty}\mu(n)n^{-s}$, with the Möbius function μ (see Appendix A). In that case $\sigma_a=1$ and $\frac{1}{2}\leqslant\sigma_c\leqslant1$, the Riemann hypothesis being $\sigma_c=\frac{1}{2}$.

Many Dirichlet series arising in number theory can be written as a Euler product (see Ref. 20):

$$\sum_{n=1}^{\infty} a(n)n^{-s} = \prod_{p\in\mathbb{P}} f_p(p^{-s}). \tag{8}$$

By the fundamental theorem of arithmetic this is the case exactly if the arithmetical function $n\mapsto a(n)$ is *multiplicative*, that is, it is not identically zero, and

$$a(mn) = a(m)a(n) \quad \text{if gcd } (m,n) = 1.$$

Then $f_p(x) = \Sigma_{k=0}^{\infty}\, a(p^k)x^{-k}$. For example, $\zeta(s) = \Pi_{p\in\mathbb{P}}(1 - p^{-s})^{-1}$.

The product

$$Z_f(s)Z_g(s) = Z_{f*g}(s) \tag{9}$$

of Dirichlet series has coefficients

$$f*g(n) = \sum_{d|n} f(d)g\left(\frac{n}{d}\right), \tag{10}$$

which are given by the Dirichlet convolution product $f*g$ of the arithmetical functions of the factors.

With pointwise addition and Dirichlet multiplication the set of arithmetical functions becomes an associative algebra with unit I, $I(n) = \delta_{1,n}$ (a so-called monoid). It is easy to prove that when $f(1)\neq 0$ a Dirichlet inverse $f^{(-1)}$ exists.

Dirichlet series are used in number theory in order to make use of analytic tools in the theory of prime numbers. As an example, the prime number theorem states that the number $\pi(x) = |\{p\in\mathbb{P}|p\leqslant x\}|$ of primes smaller than x is asymptotic to $x/\ln x$. This can be shown by analyzing $\zeta'(s)/\zeta(s)$ for $\mathrm{Re}(s) = 1$, which is on the line containing the pole.

In order to give a statistical mechanics interpretation of (some) Dirichlet series as polymer partition functions we have to identify the sums (7) and (2). This can be done, of course, in many ways: the main point is that in the partition sum each polymer can only have simple multiplicity.

We propose two types of polymerization: the first works for multiplicative arithmetical functions and is based on the notion of Euler product, the second is more general. We introduce both of them because the first admits a special treatment in the convergence theorems leading to better convergence estimates (see Appendix B).

A. Multiplicative polymerization

(i) If we now interpret $\zeta(s) = \Sigma_{n=1}^{\infty}\, e^{-s\,\ln(n)}$ as a partition function for an infinite system with state space $n\in\mathbb{N}$ and energies $\ln(n)$, then $\zeta'(s)/\zeta(s)$ is minus the expectation of the internal energy. Moreover, in the notation of the previous section,

$$\zeta(s) = \prod_{p\in\mathbb{P}} (1-p^{-s})^{-1} = \sum_{X\in\hat{D}^{\infty}} z_s^X,$$

taking the primes as the polymers ($P := \mathbb{P}$), assuming different primes to be compatible and setting the activities $z_s(p) := 1/(p^s - 1)$; moreover

$$\zeta'(s)/\zeta(s) = \frac{d}{ds}\ln(\zeta(s)) = -\sum_{p\in\mathbb{P}} \ln(p)\cdot z_s(p).$$

(ii) Alternatively one may consider the set $P:=\{p^n | p\in\mathbb{P}, n\in\mathbb{N}\}$ of prime powers as polymers with the activities $z_s(x):=x^{-s}$ for $x\in P$ and call $p_1^{n_1}, p_2^{n_2} \in P$ incompatible iff $p_1=p_2$. Then, again, $\zeta(s)$ can be written as a polymer model (2) and thus its logarithm may be written using formula (5).

Clearly this kind of game can be played with any Dirichlet series having a Euler product (8). Then for the first choice $P=\mathbb{P}$ of polymers the activities are $z_s(p):=f_p(p^{-s})-1$, whereas $z_s(p^k):=a(p^k)p^{-sk}$ in the second case.

It is clear that when the multiplicative arithmetical function $a:\mathrm{N}\to\mathbb{C}$ is a square-free function (that is, it vanishes on integers containing squares), then both polymer model interpretations lead to the same activity $z_s(p) = a(p)e^{-s\ln p}$, $z_s(p^k)=0$ for $k>1$. The function a plays the role of an interaction.

B. General polymerization

1. Square-free case

A large class of *square-free* Dirichlet series admit the interpretation of polymer models where each prime number is considered a polymer. For instance we can consider the family of arithmetical functions $\phi=\omega f$ where f is multiplicative (and possibly positive to have a genuine probabilistic framework) and the function ω is defined as

$$\omega(n)=\begin{cases} 1, & \text{if } n=1,p, \\ \displaystyle\prod_{pp'|n} g(p,p'), & \text{otherwise,} \end{cases} \tag{11}$$

where $g(p,p')$ takes values 0,1 and is a symmetric function vanishing on the diagonal. We stress that the previous conditions define a *class* of matrices [of entries $g(p,p')$] and correspondingly a class of square-free arithmetical functions ϕ not necessarily multiplicative. Two primes with $g(p,p')=0$ are called incompatible; two integers are incompatible if there are two incompatible primes in the respective decomposition.

Some examples of incompatibility are the following: p,p' are compatible polymers when

$-p\neq p'$;

$-|p-p'|>\text{const}$;

$-|p-p'|>\log\sqrt{pp'}$.

The first case corresponds to the square-free function $|\mu|$ (see Appendix A) in which the only interaction is the Fermi statistic; the relative zeta function is $Z_{|\mu|}(s)=\zeta(s)/\zeta(2s)$. The interest of the third case will be clear in the section on convergence.

The fundamental theorem of arithmetic on the unique decomposition of an integer into primes permits the formal identification of the function

$$Z_\phi(s)=\sum_{n\neq\mathbb{N}}\phi(n)n^{-s}, \tag{12}$$

with a partition function of a polymer system in which each prime has activity $z_s(p) = f(p)e^{-s\log p}$ and the function ω play the role of the hard-core interaction.

2. Non-square-free case

An important observation is that to treat the case of non-square-free Dirichlet series we have simply to change the polymer identification: the polymers are now the prime powers

$P:=\{p^n | p\in\mathbb{P}, n\in\mathbb{N}\}\equiv\{2,3,4,5,7,8,9,...\}$ with the activities $z_s(x):=f(x)x^{-s}$ for $x\in P$. The class of arithmetical function treated in this way is defined by $\phi=f\omega$ where f is multiplicative and

$$\omega(n)=\begin{cases}1, & \text{if } n=1,p^k,\\ \displaystyle\prod_{x,x'\in P, xx'|n} g(x,x'), & \text{otherwise,}\end{cases} \tag{13}$$

where $g(x,x')$ takes values 0 and 1 and is a symmetric function vanishing on all the couples $(x,x')=(p^k,p^{k'})$. The previous conditions define a *class* of matrices and correspondingly a class of arithmetical functions ϕ in general not square-free nor multiplicative.

Also in this case there are plenty of examples; for instance, the second and third example of the previous polymerization can be rephrased exactly in this one. The simplest example is just the Riemann zeta function: it corresponds to the element of the previous class in which $f(n)=1$ and $g(x,x')=1$ if $(x,x')\neq(p^k,p^{k'})$ which says that two polymers are incompatible when they are power of the same prime and they are compatible otherwise.

This means that the Riemann zeta function admits the interpretation of the partition function of a hard-core interacting polymer system.

IV. THE HARD-CORE MODELS

Let us consider, for simplicity, the square-free case with $\phi=\omega$. We introduce now a family of approximating functions ω_k depending on an integer k; the meaning of this approximation is just the finite volume approximation in statistical mechanics which manifests itself with a finite number of polymers. The corresponding partition function becomes a finite series for each k and the problem to control the thermodynamical limit for the correlation functions concerns the possibility of obtaining bounds which are uniform in k.

We first define the kth set of square-free integers $\mathbb{N}_k$ as the integers of the form

$$n=p_1^{\alpha_1}p_2^{\alpha_2}\cdots p_k^{\alpha_k}, \quad \text{where } \alpha_i=0 \text{ or } 1, \tag{14}$$

and $p_1,\ldots,p_k$ are the first k prime numbers. Then, for instance, $\mathbb{N}_0=\{1\}$, $\mathbb{N}_1=\{1,2\}$, $\mathbb{N}_2=\{1,2,3,6\}$, $\mathbb{N}_3=\{1,2,3,5,6,10,15,30\}$, etc., and $|\mathbb{N}_k|=2_k$. Now we define

$$\omega_k(n)=\begin{cases}\omega(n), & \text{if } n\in\mathbb{N}_k,\\ 0, & \text{otherwise.}\end{cases} \tag{15}$$

It is easy to prove that

$$\omega_k(n)=\omega(n) \quad \text{for } n\leqslant p_k, \tag{16}$$

and

$$\omega_k(n)=0 \quad \text{for } n>p_1\cdots p_k. \tag{17}$$

The origin of this approximation is quite simple: we consider the natural numbers progressively generated by prime numbers; the nature of the function ω implies that for each generation only a finite quantity of integers gives a contribution.

Remark: The above mechanism induces in general a one-to-one correspondence between the functions of the variable $(\alpha_1,\ldots,\alpha_k)$ and the kth approximation of a square-free arithmetical functions.

It clearly turns out that the approximating zeta function admits the interpretation of a grand canonical partition function for a system of k particles interacting via a hard-core two-body potential:

$$Z_{\omega_k}(s)=\sum_{n\in\mathbb{N}}\omega_k(n)n^{-s}=\sum_{\alpha}\prod_i p_i^{-s\alpha_i}\prod_{i<j}[1+\alpha_i\alpha_j(g(p_i,p_j)-1)], \tag{18}$$

where $\alpha=(\alpha_1,\ldots,\alpha_k)$. A mean values are

$$\langle f\rangle_k(s)=\frac{\Sigma_\alpha f(\alpha)\Pi_i p_i^{-s\alpha_i}\Pi_{i<j}[1+\alpha_i\alpha_j(g(p_i,p_j)-1)]}{Z_{\omega_k}(s)}. \tag{19}$$

The basic objects of our model are the r-points ($r\leqslant k$) correlation functions:

$$\langle\alpha_{i_1}\cdots\alpha_{i_r}\rangle_k(s), \tag{20}$$

with $i_1<i_2<\cdots<i_r$; it is interesting to notice that, by comparing with (20), they represent the probability of divisibility by the integer $p_{i_1}\cdots p_{i_r}$. Without loss we assume $i_1,\ldots,i_r\leqslant k$ because otherwise (20) vanishes.

One of our main problems is to study the limit $k\to\infty$ of the correlation functions, and to prove that they describe, indeed, the equilibrium state of a system of interacting polymers defined by the partition function (18).

There are various approaches in the study of the properties of the polymer models. One of them, the one we consider here, is based on the use of the Kirkwood–Salsburg-type iterative equations to control the analytical behavior of the correlation functions and related quantities. We will follow the ideas of Ref. 19 (see also Refs. 21 and 22) with a different proof of the convergence theorems according to the number theoretical framework which requires a slightly different identification of interaction and activity function.

V. THE ITERATIVE EQUATION FOR THE CORRELATIONS

The analytic control of a polymer model is based on two interrelated axioms carrying a deep statistical mechanics meaning.

Activity Bound: There exists a constant $a<1$ and a positive function $v(\gamma)$ (the volume) such that

$$|z(\gamma)|\leqslant a^{v(\gamma)}. \tag{21}$$

Defining $N(\gamma,x)$ as the number of γ-incompatible polymers for which the function v stay inside the interval $[x,x+1)$, we impose the following.

Entropy Bound: There exists a constant c such that

$$N(\gamma,x)\leqslant v(\gamma)c^x. \tag{22}$$

From an analytic point of view the two requirements are simply saying that the terms we sum have to be not too large and not too many. In our context the activity bound can be naturally fulfilled with the choice $a=e^{-s}$ and $v(p)=\log(p)$ and the entropy bound defines the class of function we are treating. It is easy to see that the three concrete examples of the general polymerization fulfill the entropy axiom for any $c>1$; for each of them one could actually improve the general convergence strategy we are going to present.

Our first goal is to express the correlation function at the temperature s as a zeta function:

$$\langle\alpha_{i_1}\cdots\alpha_{i_r}\rangle_k(s)=\sum_l\langle n\rangle(l)l^{-s}, \tag{23}$$

where $n = p_{i_1}\cdots p_{i_r}$. The algebraic properties of the Dirichlet convolution imply that Eq. (23) can be solved in the arithmetical function $\langle n\rangle$ and the solution is

$$\langle n\rangle = n^{-s}(\omega_k^{(-1)} * D_n\omega_k), \tag{24}$$

where we have introduced the operation D_n as

$$D_n f(k) = f(nk). \tag{25}$$

One immediately realizes that the arithmetic function corresponding to the correlations of a square-free model *is not* square-free. This is because the Dirichlet inverse operation does not conserve the square-free property and it is the main motivation to introduce a formalism able to handle generic polymer configurations with the suitable convolution. Moreover, it also implies that, even for finite k, the correlation's zeta function is no more a finite series; we want to show how it is possible to control its properties in the limit $k\to\infty$ using the statistical mechanics method of the iterative equations. This will provide a statistical mechanics meaning to the limiting correlations and a new point of view in the study of some number theoretical quantities.

The idea, which is a central one in statistical mechanics, is to study the ''interaction'' between one particle and the remaining ones or, in number theoretical terms, to have some control on the nonmultiplicativity of the ω.

Defining the function

$$\Gamma_n := \omega_k^{(-1)} * D_n\omega_k, \tag{26}$$

we consider an integer of the form pn, where p is a prime compatible with n (otherwise $\Gamma_{pn}=0$). By definition we have

$$\Gamma_{pn}(l) = \sum_{d|l} \omega_k^{(-1)}(d)\,\omega_k\left(pn\,\frac{l}{d}\right); \tag{27}$$

indicating $\Sigma_{k\subset n}$ a sum over all the divisors of n counted with multiplicity (see Appendix A), we first observe that

$$\omega_k\left(pn\,\frac{l}{d}\right) = \omega_k\left(n\,\frac{l}{d}\right)\sum_{r\subset l/d}^{p} \lambda(r), \tag{28}$$

where the Σ^p means a sum over all square-free integers build on p-incompatible primes and the function λ is the Liouville function defined by $\lambda(n)=(-1)^{\Omega(n)}$ where Ω is the number of prime factors counted with multiplicity. Since $\omega(p)=1$, the previous formula gives an evaluation of how much the interaction ω deviates from a completely multiplicative function; it can be proved, for instance, observing that the factor $G(p,h)$ defined by

$$\omega(ph) = \omega(h)G(p,h) \tag{29}$$

is

$$G(p,h) = \prod_{p'\subset h} g(p,p') = \prod_{p'\subset h} ((g(p,p')-1)+1) = \sum_{r\subset h}{}^{p}(-1)^{\Omega(r)}, \tag{30}$$

which is the (28) since the integer pn is supposed to be compatible. Substituting the (28) inside the (27) we have

$$\Gamma_{pn}(l)=\sum_{d|l}\ \omega_k^{(-1)}(d)\,\omega_k(p)\,\omega_k\left(n\,\frac{l}{d}\right)\sum_{r\subset l/d}^{p}\ \lambda(r), \tag{31}$$

and interchanging the summation order

$$\Gamma_{pn}(l)=\sum_{r\subset l}^{p}\ \lambda(r)\sum_{d|l/r}\ \omega_k^{(-1)}(d)\,\omega_k\left(\frac{nl}{d}\right), \tag{32}$$

which is, up to renaming the sets,

$$\Gamma_{pn}(l)=\sum_{r\subset l}^{p}\ \lambda(r)\Gamma_{nr}\left(\frac{l}{r}\right). \tag{33}$$

This is the iterative equation we want to consider. In order to control its solutions we observe that, by inspection, it lives naturally as an equation for the *two-variable* arithmetical function Γ; moreover, defining the ''index'' of the quantity $\Gamma_n(l)$ as $\Omega(nl)$, Eqs. (33) can be solved iteratively observing that they allow us to compute the family of index $\Omega(nl)+1$ in terms of that whose index is $\Omega(nl)$. This fact not only makes it possible to study the iterative solutions with the initial condition $\Gamma_1(1)=1$ but it also gives hints on the suitable Banach space structure to be introduced in order to make use of the contraction principle.

VI. THE CONTRACTION REGIME FOR THE ITERATION

In our number-theoretical context we can introduce the seminorms for the family of the $\langle n\rangle(l)$ with $\Omega(nl)=m$, depending on a parameter δ to be optimized at the end,

$$N_m(\delta)=\sup_{n,1\leqslant\Omega(n)\leqslant m}\ \sum_{l,\Omega(nl)=m}\ |\langle n\rangle(l)|l^{-s}n^{(s-\delta)}. \tag{34}$$

We claim that, for suitable values of δ, this norm is contractive for the iterative equations. The proof is along the following lines. Using the (33) we observe that it holds the bound

$$\sum_{l,\Omega(nl)=m}\ |\langle pn\rangle(l)|l^{-s}(pn)^{(s-\delta)}\leqslant\sum_{l,\Omega(nl)=m}\ p^{-s}\sum_{r\subset l}^{p}\ r^{s}|\langle rn\rangle\left(\frac{l}{r}\right)|l^{-s}(pn)^{(s-\delta)}, \tag{35}$$

since the Liouville function is bounded in modulus by one. It follows that

$$\sum_{l,\Omega(nl)=m}\ |\langle pn\rangle(l)|l^{-s}(pn)^{(s-\delta)}\leqslant N_m(\delta)p^{-\delta}\sum_{r}^{p}\ r^{-(s-\delta)}, \tag{36}$$

where the last sum runs over the square-free r build on p-incompatible primes. We also observe that, since r runs over square-free integers,

$$\sum_{r}^{p}\ e^{-(s-\delta)\,\log r}\leqslant\sum_{n=0}^{\infty}\ \frac{1}{n!}\left(\sum_{p'}\ {}^{p}e^{-(s-\delta)\,\log p'}\right)^{n}. \tag{37}$$

Making use of the entropy bound it is possible to control the sum on p-incompatible primes, observing that it can be written as

$$\sum_{v=1}^{\infty} \sum_{p',v\leqslant \log p'<v+1} e^{-(s-\delta)\log p'} = \tag{38}$$

$$\leqslant \log p \sum_{v=1}^{\infty} (ce^{-(s-\delta)})^{v} = \log p \, \frac{ce^{-(s-\delta)}}{1-ce^{-(s-\delta)}}, \tag{39}$$

provided $ce^{-s}<e^{-\delta}$; we notice that the extension of the previous sum up to infinity makes the resulting bound uniform in k. Taking the supremum norm of (35) we obtain

$$N_{m+1}(\delta)\leqslant N_m(\delta)\exp\left(\log 2\left(-\delta+\frac{ce^{-(s-\delta)}}{1-ce^{-(s-\delta)}}\right)\right), \tag{40}$$

which means that we are in the contraction regime when $ce^{-s}<\delta e^{-\delta}/(1+\delta)$. The right-hand side can easily be optimized, observing that it is, on the positive real line, a function with the only maximum reached at the *golden ratio* $\delta=(\sqrt{5}-1)/2$ (see Ref. 23 for a discussion). The previous convergence theorem means that the limit $k\to\infty$ of the correlation functions exists in the range defined by

$$ce^{-s}<\frac{\overline{\delta}e^{-\overline{\delta}}}{1+\delta}\approx e^{-1.58} \tag{41}$$

and describes the equilibrium state of a hard-core interacting polymer system.

An easy corollary to be used in the control of connected correlations functions is that, for all the s defined by the (41), one has the bound

$$N_{m+1}\leqslant N_m e^{-\rho}, \tag{42}$$

where, defining the positive number $\epsilon := \overline{\delta e^{-\overline{\delta}}}/(1+\delta)-ce^{-s}$, one has $\rho=\epsilon e^{\overline{\delta}}\log 2(2+\overline{\delta})$. In particular, it is possible to check that, since $N_1\leqslant 1$, it results that $N_m\leqslant e^{-m\rho}$.

The reader should compare this general result with the one for the multiplicative case (Appendix B), where one has optimal convergence estimates.

VII. THE EXPONENTIAL DECAY OF THE CORRELATIONS

The statistical mechanics theory of the low activity expansion gives a systematic way to obtain bounds for the free energy and for all its derivatives with respect to external parameters. It is well known that those bound are equivalent to the bounds for the truncated correlation function and are usually given in terms of the distance between the polymers.

In our context the convolutory algebra permits a natural rephrasing of all these properties: the bounds we present are given in terms of the volume of each polymer, i.e., $\log p$.

The quantities we are mainly interested in are the generalization of the two-point truncated correlation function

$$\langle \alpha_{i_1},\alpha_{i_2}\rangle^{T}(s) := \langle \alpha_{i_1}\alpha_{i_2}\rangle(s)-\langle \alpha_{i_1}\rangle(s)\langle \alpha_{i_2}\rangle(s). \tag{43}$$

This function represents the deviation from the independence of the two events ''p_{i_1} divides an integer'' and ''p_{i_2} divides an integer.'' As for the simple correlations, an easy computation shows that it is possible to express them as Dirichlet series of a suitable arithmetical function:

$$\langle \alpha_{i_1},\alpha_{i_2}\rangle^{T}(s)=\sum_{l} (p_{i_1}p_{i_2})^{-s}(\Gamma_{p_{i_1}p_{i_2}}-\Gamma_{p_{i_1}}*\Gamma_{p_{i_2}})l^{-s}. \tag{44}$$

We recognize that the two-point truncated expectation is the Dirichlet series of the arithmetical function given by the second order of the formal logarithm of the functions Γ with respect to the *lower variable*:

$$\Gamma^T := \log \Gamma. \tag{45}$$

Let us clarify the geometrical meaning of the operations which naturally appear considering the simple and the truncated correlation functions. First we notice that for the operation D_n it holds (see Ref. 24) the Leibnitz rule with respect to the circle product (see Appendix A):

$$D_n(f \circ g) = D_n f \circ g + f \circ D_n g. \tag{46}$$

From it one can easily prove that the operation ∂_n, defined by

$$\partial_n f(k) = f(nk)\, \frac{c(nk)}{c(k)}, \tag{47}$$

plays the role of a *multiple* derivative with respect to the Dirichlet product since it fulfills the composition rule $\partial_{n_1}\partial_{n_2} = \partial_{n_1 n_2}$ and, when n is a prime number, the Leibnitz rule with respect to the Dirichlet multiplication. This can be seen observing that defining the operation $\mathscr{D}$ from the set of the one-variable to that of the two-variable arithmetical functions by

$$(\mathscr{D} f\ )(n,k) = f(nk)\, \frac{c(nk)}{c(n)c(k)}; \tag{48}$$

it holds for it the important property:

$$\mathscr{D}(f * g) = \mathscr{D} f * \mathscr{D} g, \tag{49}$$

where the convolution on the right-hand side is the two-variable Dirichlet convolution.

In particular it holds the

$$\partial_p \ \mathrm{Exp}\ f = \partial_p f * \mathrm{Exp}\ f, \tag{50}$$

and

$$\partial_p \ \mathrm{Log}\ g = g^{(-1)} * \partial_p g. \tag{51}$$

Since ω is a square-free function $D_n\omega = \partial_n\omega$, we have, with $\omega^T := \mathrm{Log}\ \omega$,

$$\partial_n \omega^T = \Gamma_n^T. \tag{52}$$

Choosing $n = p$ it holds $\partial_p \omega^T = \Gamma_p$, which is

$$\omega^T(pn) = \frac{c(n)}{c(pn)}\, \Gamma_p(n). \tag{53}$$

This relation enables us to obtain a bound, inside our contraction regime, on a quantity which represents the free energy density centered around the prime p:

$$\sum_{l=1, p|l}^{\infty} \omega^T(l) l^{-s}. \tag{54}$$

In fact applying Eq. (53) and the contraction scheme for the norm one has

$$\sum_{l=1,p|l}^{\infty} \omega^T(l) l^{-s} \leqslant \sum_{k=1}^{\infty} \sum_{l,\Omega(pl)=k} |\Gamma_p(l)| p^{-s} l^{-s} \tag{55}$$

$$\leqslant p^{-(s-\overline{\delta})} \sum_{k=1}^{\infty} e^{-\rho k} = e^{-(s-\overline{\delta})\log p} \frac{e^{-\rho}}{1-e^{-\rho}}, \tag{56}$$

which is the claimed exponential decay in terms of the polymer volume (notice that $s > \overline{\delta}$ in the contraction regime). In the same way it is possible to obtain the decay for the multiple truncated correlations functions; let us show it for the two-point case.

From (44) we have

$$|\langle \alpha_{i_1}, \alpha_{i_2} \rangle^T(s)| \leqslant (p_{i_1} p_{i_2})^{-s} \sum_{l=1}^{\infty} (|\Gamma_{p_{i_1} p_{i_2}}(l)| + |\Gamma_{p_{i_1}} * \Gamma_{p_{i+2}}(l)|) l^{-s}. \tag{57}$$

The term with the convolution product on the right-hand side is bounded using the (56) and the multiplicative property of the relative Dirichlet series. For the first terms one has

$$\sum_{l=1}^{\infty} |\Gamma_{p_{i_1} p_{i_2}}(l)| l^{-s} = (p_{i_1} p_{i_2})^{\overline{\delta}} \sum_{k=2}^{\infty} \sum_{l,\Omega(p_{i_1} p_{i_2})=k} \langle p_{i_1} p_{i_2} \rangle(l) l^{-s} (p_{i_1} p_{i_2})^{(s-\overline{\delta})} \tag{58}$$

$$\leqslant (p_{i_1} p_{i_2})^{\overline{\delta}-s} \sum_{k=2}^{\infty} e^{-k\rho} = e^{-(s-\delta)\log(p_{i_1} p_{i_2})} \frac{e^{-2\rho}}{1-e^{-\rho}}. \tag{59}$$

Summing the two contributions we obtain

$$|\langle \alpha_{i_1}, \alpha_{i_2} \rangle^T(s)| \leqslant e^{-(s-\overline{\delta})\log(p_{i_1} p_{i_2})} \left(\frac{e^{-2\rho}}{1-e^{-\rho}} + \frac{e^{-2\rho}}{(1-e^{-\rho})^2} \right), \tag{60}$$

which is the desired result. In the same way one can obtain the same exponential decay for all the other truncated correlation functions.

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APPENDIX A: SOME ARITHMETICAL FUNCTIONS

Some arithmetical functions considered on this work are the identity for the pointwise multiplication:

$$u(n) = 1 \quad \forall n, \tag{A1}$$

the identity for the Dirichlet product:

$$I(n) = \begin{cases} 1, & \text{if } n = 1, \\ 0, & \text{otherwise,} \end{cases} \tag{A2}$$

the identity map from $\mathbb{N}$ to $\mathbb{N}$:

$$N(n)=n \tag{A3}$$

and the ''square'' function:

$$Q(n)=\begin{cases}1, & \text{if } n \text{ is a square,}\\ 0, & \text{otherwise}\end{cases} \tag{A4}$$

In terms of them it is easy to express other important functions: the Möbius function

$$\mu=u^{-1}, \tag{A5}$$

its absolute value

$$|\mu|=u*Q^{(-1)}. \tag{A6}$$

and the Liouville function

$$\lambda=\mu*Q=|\mu|^{(-1)}. \tag{A7}$$

It can be useful to introduce another convolution product: considering an integer as an unordered sequence of primes $n \equiv \{p_{i_1},\ldots,p_{i_1},p_{i_2},\ldots,p_{i_2},\ldots,p_{i_n}\}$, the natural definition of convolution is the sum over all the subsequences

$$f\circ g(n)=\sum_{d\subset n} f(d)g\left(\frac{n}{d}\right), \tag{A8}$$

where, for instance, the set of subsequences of 4 is {1,2,2,4}. It is easy to see that it is related to the Dirichlet one by

$$f\circ g(n)=\sum_{d|n} f(d)g\left(\frac{n}{d}\right)c\left(d,\frac{n}{d}\right), \tag{A9}$$

where $c(l,m)=c(lm)/c(l)c(m)$ with $c(p_{i_1}^{\alpha_{i_1}}\cdots p_{i_k}^{\alpha_{i_k}}) = \Pi_{j=1}^{k}\alpha_{i_k}!$. This property is equivalent to the fact that the $\circ$-product plays the role of the convolution for the deformed zeta functions with the noncharacter activity $\tilde{z}(n)=n^{-s}/c(n)$;

$$\tilde{Z}_f(s)=\sum_n f(n)\tilde{z}(n), \tag{A10}$$

i.e., it holds

$$\tilde{Z}_f(s)\tilde{Z}_g(s)=\tilde{Z}_{f\circ g}(s). \tag{A11}$$

For both the convolution products it is possible to define the powers of a function and, in some cases, power series like exponential and logarithm: Defining the sets of arithmetical functions $\mathscr{A}_0$ and $\mathscr{A}_1$, respectively, by the conditions $f(1)=0$ and $f(1)=1$ it is possible to construct well-defined power series in the convolution products; in particular, the arithmetical function corresponding to the exponential for $f\in\mathscr{A}_0$ is

$$\text{Exp } f=\sum_{k=0}^{\infty}\frac{f^{(k)}}{k!} \tag{A12}$$

and the logarithm, for $h\in\mathscr{A}_1$ which is, defining $h=I+\tilde{h}$,

TABLE I. Values of some arithmetical functions on the first 10 integers.

Function	1	2	3	4	5	6	7	8	9	10
Q	1	0	0	1	0	0	0	0	1	0
$Q^{(-1)}$	1	0	0	−1	0	0	0	0	−1	0
λ	1	−1	−1	1	−1	1	−1	−1	1	1
μ	1	−1	−1	0	−1	1	−1	0	0	1
ω_3	1	1	1	0	1	1	0	0	0	1
$\omega_3^{(-1)}$	1	−1	−1	1	−1	1	0	−1	1	1
$D_2\omega_3$	1	0	1	0	1	0	0	0	0	0
$\omega_3^{(-1)} * D_2\omega_3$	1	−1	0	1	0	0	0	−1	0	0

$$\mathrm{Log}\, h = \sum_{k=0}^{\infty} (-1)^k \frac{\tilde{h}^{(k)}}{k}. \tag{A13}$$

It is easy to see that the operation Exp: $\mathscr{A}_0 \to \mathscr{A}_1$ and Log: $\mathscr{A}_1 \to \mathscr{A}_0$ are mutually inverse.

From a combinatorial point of view, the main advantage to considering the circle product is that it permits the definition of the exponential of a function as the sum over the *partitions*. Example: the $\circ$-exponential of f in $12 = 2^2 \cdot 3$ is in fact

$$\mathrm{Exp}(f\ )(12) = f(12) + 2\, f(2) f(6) + f(3) f(4) + f(2) f(2) f(3). \tag{A14}$$

On the other hand, the Dirichlet exponential implies the important *formal* property:

$$Z_f(s) = \exp(Z_{\mathrm{Log}\, f}(s)), \tag{A15}$$

which permits us to obtain the *free energy* series expansion starting from the partition function series expansion on a Dirichlet series.

APPENDIX B: CONVERGENCE IN THE MULTIPLICATIVE CASE

First keeping within the context of general polymer models, we set $\psi(X) := \phi(X) z^X$ so that the partition function equals $Z = \Sigma_{X \in \hat{P}^\infty} \psi(X)$. Then the probability that the k-polymer X is present is defined by

$$\rho(X) := \frac{\Sigma_{Y \in \hat{P}^\infty} \psi(Y \cdot X)}{\Sigma_{Y \in \hat{P}^\infty} \psi(Y)} = \sum_{Y \in \hat{P}^\infty} \Delta_X(Y) \tag{B1}$$

with $\Delta_X(Y) = (\psi^{-1} * D_X \psi)(Y)$.

The terms $\Delta_X(Y)$ meet the following recursive equation wrt addition of a polymer $\gamma \in P$ to X:

$$\Delta_{\gamma \cdot X}(Y) = z(\gamma) \sum_{S \subset Y}{}^{\gamma} (-1)^{|S|} \Delta_{X \cdot S}(Y/S). \tag{B2}$$

Here the superscript γ means that summation is restricted to multi-polymers S of Y which are incompatible with γ.

We now express the correlation function

$$\rho_k(X) = \langle \alpha_{i_1} \cdots \alpha_{i_r} \rangle_k(s) = \sum_{Y \in \mathbb{N}} \Delta_X^k(Y)$$

at the inverse temperature s as a series in the activities. By definition $\Delta_X^k(Y) = (\omega_k^{-1} * D_X \omega_k)(Y) \cdot z^X z^Y$, with D_n defined in (25).

Now by (B2) for a prime $p \in \mathbb{P}_k$

$$\Delta_{p\cdot X}^k(Y) = z_s(p) \sum_{S|Y} {}^p(-1)^{|S|} \Delta_{S\cdot X}^k(Y/S) = z_s(p) \sum_{S:p|S|Y} \lambda(S) \Delta_{S\cdot X}^k(Y/S), \tag{B3}$$

since $S \in \mathbb{N}$ is incompatible with $p \in \mathbb{N}$ iff $p|S$. Furthermore, for an integer S of the form $S = \Pi_i p_i^{\alpha_i}$, by definition $|S| = \Sigma_i \alpha_i = \Omega(S)$. Moreover, the Liouville function λ is defined by $\lambda(S) = (-1)^{\Omega(S)}$, showing (B3).

Equations (B3) are the iterative equations we want to consider. Defining the ''index'' of the quantity $\Delta_X^k(Y)$ as $\Omega(XY)$, the equations (B3) can be solved iteratively observing that give the family of index $\Omega(XY)+1$ in terms of that whose index is $\Omega(XY)$. This fact not only makes it possible to study the iterative solutions with the initial condition $\Delta_1^k(1)=1$, but it also gives hints on the suitable Banach space structure to be introduced in order to make use of the contraction principle.

In our number-theoretical context the seminorms N_m^δ have the form

$$N_m^\delta(\rho_k) = \sup_{X \in \mathbb{N}} \sum_{Y \in \mathbb{N}, \Omega(XY)=m} |\Delta_X^k(Y)| e^{-(\ln(a)+\delta)v(X)} = \sup_{X \in \mathbb{N}} \sum_{Y \in \mathbb{N}, \Omega(XY)=m} |\Delta_X^k(Y)| X^{(A'-\delta')} \tag{B4}$$

with $A' - \ln(a)/\ln 2$, $\delta' = \delta/\ln 2$, and $v(X) = \ln(X)/\ln(2)$.

In the multiplicative case $\omega = |\mu|$ we can improve the convergence estimate to the optimal value:

$$\begin{aligned} N_m^\delta(\rho_k) &= \sup_{X \in \mathbb{N}} \sum_{Y \in \mathbb{N}, \Omega(XY)=m} |\omega_k^{-1} * D_X \omega_k(Y)| |z^X z^Y| e^{-(\ln(a)+\delta)v(X)} \\ &= \sup_{X \in \hat{P}_k^\infty} \sum_{Y \in \hat{P}_k^\infty, \Omega(XY)=m} |\omega^{-1} * D_X \omega(Y)| |z^X z^Y| e^{-(\ln(a)+\delta)v(X)}. \end{aligned} \tag{B5}$$

Remember that $\mathbb{P}_k$ consists of the first k primes. So

$$\hat{P}_k^\infty = \{n \in \mathbb{N} | p \in \mathbb{P} \quad \text{and} \quad p|n \Rightarrow p \in \mathbb{P}_k\}.$$

Since we have assumed $\omega = |\mu|$, $\omega^{-1} = \lambda$. So

$$\omega^{-1} * D_X \omega(Y) = \sum_{d|Y} \lambda(Y/d) |\mu|(Xd) = \sum_{d|Y,(d,X)=1} \lambda(Y/d) = \begin{cases} \lambda(Y), & p|Y \Rightarrow p|X (p \in \mathbb{P}) \\ 0, & \text{otherwise} \end{cases}.$$

Now if there is an m-independent bound b on the minimal number of prime factors of an X which attains the supremum in (B4), then $m \mapsto N_m^\delta(\rho_k)$ converges exponentially fast to zero, since then there are only $\mathcal{O}(b^m)$ terms in the sum (B4). Then we are done.

So we can assume wlog that the maximal number of prime factors of the X grows with m. Now since $m+1 \geqslant 2$, the $\widetilde{X} \in \mathbb{N}$ which attain the supremum in $N_{m+1}^\delta(\rho_k)$ are unequal to 1 so that we can write them in the form $\widetilde{X}_0 = pX$ and assume that $p \in \mathbb{P}$ is the largest prime factor. Then we use the recursion relation (B2):

$$N_{m+1}^\delta(\rho_k) = \sup_{\widetilde{X} \in \mathbb{N}} \sum_{Y \in \mathbb{N}, \Omega(\widetilde{X}Y)=m+1} |\Delta_{\widetilde{X}}^k(Y)| \widetilde{X}^{(A'-\delta')}$$

$$
\begin{aligned}
&= \sum_{Y\in\mathbb{N},\ \Omega(XY)=m} |\Delta^k_{pX}(Y)|(pX)^{(A'-\delta')} \\
&= \sum_{Y\in\mathbb{N},\ \Omega(XY)=m} |z_s(p) \sum_{S:p|S|Y} \lambda(S)\Delta^k_{XS}(Y/S)|(pX)^{(A'-\delta')} \\
&\leqslant p^{-\delta'} \sum_{Y\in\mathbb{N},\ \Omega(XY)=m} \ \sum_{S:p|S|Y} |\Delta^k_{XS}(Y/S)|(SX)^{(A'-\delta')} S^{(\delta'-A')} \\
&= p^{-\delta'} \sum_{S:p|S} S^{(\delta'-A')} \sum_{Y:S|Y,\Omega(XY)=m} |\Delta^k_{XS}(Y/S)|(SX)^{(A'-\delta')} \\
&\leqslant p^{-\delta'} \sum_{S:p|S} S^{(\delta'-A')} N^{\delta}_m(\rho_k) \\
&= p^{-A'}\zeta(A'-\delta')N^{\delta}_m(\rho_k). \qquad \text{(B6)}
\end{aligned}
$$

Now we assume that $A'>1$ and $\delta'=\frac{1}{2}(A'-1)$. Then as m and thus p become large, the constant $c:=p^{-A'}\zeta(A'-\delta')$ in

$$N^{\delta}_{m+1}(\rho)\leqslant cN^{\delta}_m(\rho)$$

coming from (B6) is getting strictly smaller than one, implying convergence. In other words, we have absolute convergence if $|z(p)|\leqslant p^{-1-\varepsilon}$ for some $\varepsilon>0$. This is clearly optimal.

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Criteria for inverted temperatures in evaporation–condensation processes

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A recent criterion for shock waves which predicts the behaviors of the internal energy across the shock is extended to a vapor between two interfaces. We look at the predictions of monotonic or not behavior and at the possible inversion of the internal energy inside the gas. We consider different discrete Boltzmann models, construct new classes of exact solutions (models with a rest particle and models leading to 3×3 Riccati systems), and verify the criteria predictions. © *1996 American Institute of Physics.* [S0022-2488(96)03111-8]

I. INTRODUCTION

Twenty-five years[1] ago a remarkable and paradoxal result was found in the kinetic treatment of slow evaporation/condensation between two parallel liquid surfaces: The temperature of the vapor at the warm interface can be below the one of the cold wall, the so-called ''inverted temperature gradient paradox.'' Experiments and many numerical, analytical, and ''controversial'' studies using the continuous Boltzmann kinetic theory have been performed[2] and, very recently, the discrete kinetic theory.[3]

In the context of the shock waves, a criterion[4] was established to predict, from the knowledge of the two equilibrium states, whether or not the temperature across the shock could present nonmonotonic behavior.

Could the two phenomena be linked in the sense that the criterion for shock waves could be applied to predict the temperature inversion in the vapor between two interfaces? This conjecture is the motivation of the present work. Our tool is discrete kinetic theory with a finite number of velocities and we deal only with internal energy.[5] In fact, the same criterion with a slight modification could be applied to the two phenomena but with an important difference. We try to see whether the change of sign of the derivative of the internal energy which, for shock waves, can be predicted by the macroscopic quantities at the upstream and downstream states, could similarly be predicted from the knowledge of the vapor near the two interfaces. However, for shock waves we cannot have equal masses or pressures in the two equilibrium states. No such restriction applies to the vapor. For the vapor our result is that, in general, the inversion arises after a transition where the masses are equal near the two interfaces. Moreover, before and after this transition the internal energy is monotonic, either increasing or decreasing. We call this effect ''strict inversion.'' On the other hand, for shock waves, we obtain an overshoot with the internal energy increasing and decreasing. In some cases we still find this effect for the gas between two interfaces and we call this ''partial inversion.''

We find two new classes for the exact solutions[6] of the discrete Boltzmann models[7] (DBMs). First, for stationary solutions, the linear differential term of the rest particle density being zero, the sum of the collision terms of the rest particle is also zero. Thus, when a rest particle is present, in addition to the usual nonlinear differential system for the other densities, we must add these identically zero nonlinear terms. For instance, instead of the usual quadratic, cubic, quartic,..., nonlinearities, here we find a ratio of a cubic polynomial by a linear one. Second, we obtain also exact solutions for a 6×6 nonlinear differential system of DBMs. Taking into account the three

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linear differential conservation laws (that we integrate with three integration constants), we are reduced to a 3×3 Riccati differential system. We seek Riccati scalar-type solutions for the 3×3 system. From the number of parameters and the number of constraints, the surprising result is that we obtain a scaling parameter and exact solutions without any restriction on the coefficients of the nonlinear 3×3 Riccati system.

We recall the criterion for shock waves[4] in one dimension with the variable $\eta=x-\zeta t$. Let us assume for the mass $M(\eta)$, the momentum $J(\eta)$, and the energy $E(\eta)$ the existence of η-dependent ''shock profiles:'' $c_1+c_2/D(\eta)$ with $D(\eta)$ monotonic. Call $M_\pm$, $J_\pm$, and $E_\pm$ the values at the upstream and downstream states and define

$$\begin{aligned}&\lambda_\pm := M_\pm\mu + J_\pm(J_+M_- - J_-M_+),\\ &\mu := M_+E_- - M_-E_+, \quad P_\lambda=\lambda_-\lambda_+ .\end{aligned} \tag{1.1}$$

Depending whether $P_\lambda\geqslant0$ or <0, the internal energy is monotonic or not. In Sec. II we derive the same criterion for a gas between two interfaces, the $M_\pm$,..., being now the states of the gas near the two interfaces, the only change being that the momentum is a constant $J_\pm=j$. The two interfaces being parallel we call z a perpendicular axis. For the connection with classical discrete models and, due to the boundary conditions, for their modification we refer to the thesis of d'Almeida and to Ref. 3. For instance, we recall the Cabannes[3] results for two cubic $10v_i$ models with velocity v_i coordinates (x,y,z):

$$v_i:(\pm\alpha_x,\pm\alpha_y,\pm\alpha_z),\quad (0,0,\pm a),\quad \alpha_x=\alpha_y=\alpha_z=1,\quad a=1,2. \tag{1.2}$$

For the second model with $a=2$ (and for the first one with $a=1$) Cabannes has found inversion effects (and nothing). Here we will study models in $d=2,3$ dimensions (in the paper we write $d^*:=d-1$) which are generalizations and extensions of (1.2). In Sec. II B we construct a class of DBMs such that the velocities have only one projection on the $z>0$ axis and another opposite on $z<0$. Applying the criterion we prove that the internal energy is monotonic and, for exact solutions of two collision terms, without inversion. On the contrary, in Secs. III and IV we study other DBMs (with and without a rest particle) with different projections on the $z>0$ axis (opposite for $z<0$). We verify the predictions given by the criterion and observe partial and strict inversions but in general strict inversion alone.

We explain the determination[2,3] of the macroscopic quantities at the two interfaces or walls: $M_{w,\pm}$ for the masses and $E_{wI,\pm}$ for the internal energies which are associated to isotropic Maxwellians. We apply the following boundary conditions:[2,3] At a given wall we retain only the densities associated to the emitted molecules. More explicitly for any density N_i, associated to a velocity with α_z for z-component, depending whether $\alpha_z>0$ or <0, we retain N_i at the interface with z-component negative or positive.

From the boundary conditions and the geometry of the flow we require that the densities with velocities symmetrical to the z-axis are equal. More explicitly, to any velocity with coordinates $(\alpha_x,\alpha_y,\alpha_z)$ exist other velocities with coordinates $(\pm\alpha_x,\pm\alpha_y,\alpha_z)$. For stationary solutions with a variable η, we assume that the associated densities are equal. The important point is that these associated velocities have both the same speed and the same projection on the z axis. In the standard discrete velocity models we eliminate the velocities parallel to the two interfaces. For the two-dimensional (three) models, with $(x,z)[(x,y,z)]$ coordinates and the interfaces parallel to the x axis [(x,y) plane], we do not consider velocities along the x axis [in the (x,y) plane]. The distinctions between the models become the number of projections of the velocities along the z axis and the fact that the velocities are along the z axis or not.

For the gas near the two interfaces $\eta=\pm\frac{1}{2}$ we define $N_{i,\pm}$, $M_{\pm}$, $E_{\pm}$, and $E_{I\pm}$ for the density N_i, the mass M, the energy E, and the internal energy E_I. We will construct mainly two classes of exact stationary solutions for nonlinear differential systems with quadratic and quartic nonlinearities:

$$D(\eta):=1+\lambda e^{\nu\eta}>0, \quad \eta\in[-\tfrac{1}{2},\tfrac{1}{2}], \tag{1.3a}$$

$$N_i(\eta)=n_{0i}+n_i/D(\eta), \tag{1.3b}$$

$$N_i(\eta)=n_{0i}+n_i/D^{1/3}(\eta). \tag{1.3c}$$

If we find $N_{i,+}=N_{i,-}$, for instance for a transition value, for the monotonic (1.3a)–(1.3c) solutions this means $N_i(\eta)=$const. We can find either $\lambda=0$ or ∞ while before and after the transition, λ changes sign.

II. CRITERIA FOR THE INVERSIONS OF THE INTERNAL ENERGY

Let us call N_i the densities associated to the projection $e_i\neq 0$ of the velocities along the z axis. *We consider stationary solutions with N_i depending only on z*. To N_i we associate the linear differential terms $l_i=e_i\partial_z N_i$, we write the differential mass conservation law, we integrate, and we find that the momentum along the z axis, $J(z)$, is a constant:

$$\Sigma l_i=0\rightarrow J(z)=\Sigma e_i N_i(z)=j=\text{const.}$$

Taking into account the Knudsen number we write η instead of z for the variable.

We study both partial and strict inversions for the internal energy $\tau(\eta)$ defined from the mass, the energy, and the momentum j which is a constant:

$$\tau(\eta)=2E(\eta)/M(\eta)-[j/M(\eta)]^2, \quad \eta\in[-\tfrac{1}{2},\tfrac{1}{2}]. \tag{2.1a}$$

We associate two parameters $\lambda_{\pm}$, which depend on the macroscopic quantities:

$$\lambda_{\pm}:=M_{\pm}\mu+j^2(M_{-}-M_{+}), \quad P_{\lambda}=\lambda_{+}\lambda_{-}, \tag{2.1b}$$

their product with μ written down in (1.1). As we shall see, the derivative $\partial_\eta\tau$ does not change sign if $P_\lambda\geqslant 0$, contrary to the case where $P_\lambda<0$. For this last case, called partial inversion, there exists an extremum for $\tau(\eta)$ and in our examples we find a maximum leading to an overshoot. For the second effect, called strict inversion, at the warm interface with internal energy T_w^+ which can be either at $\eta=\frac{1}{2}$ or $-\frac{1}{2}$, we associate τ^+ for the gas and similarly τ^- at the cold interface $T_w^-<T_w^+$. The strict inversion exists when $\tau^->\tau^+$. We consider a family of $\tau(\eta)$ functions, depending on one arbitrary parameter a. It can happen that for a particular transition value $a=a_0$ both $\lambda_{\pm}=0$ whereas, before and after that value, both $\lambda_{\pm}$ have the same sign which is changing across the transition value while $P_\lambda>0$. As we shall see, the sign of $\tau^--\tau^+$ changes across that value and a strict inversion exists for either $a>a_0$ or $a<a_0$. Of course in the whole interval around a_0, the inequality $T_w^-<T_w^+$ must remain valid.

A. Criterion for partial inversion

We assume (i) *j is a constant*, (ii) *both $M(\eta)$ and $E(\eta)$ are of the type $c_1+c_2/D(\eta)$ with c_i=constants and D is a monotonic η function, without roots for $\eta\in[-\frac{1}{2},\frac{1}{2}]$. We define $D_{\pm}=D(\eta=\pm 1/2)$ and write the energy*:

$$E(\eta)(D_{-}-D_{+})=E_{-}D_{-}-E_{+}D_{+}+D_{+}D_{-}(E_{+}-E_{-})/D(\eta), \tag{2.2}$$

while $M(\eta)$ is obtained with the substitution $E_{\pm}\rightarrow M_{\pm}$. We define α, β, and γ and get the derivative of the internal energy written down in (2.1a):

$$\alpha:=(M_-D_- - M_+D_+)\mu - j^2(M_+ - M_-)(D_-D_+),$$

$$\beta:=\mu(M_+ - M_-)D_+D_-, \quad \gamma:=(DM)^3(D_- - D_+)^2/2D_+D_-, \tag{2.3a}$$

$$\gamma\partial_\eta\tau(\eta)/\partial_\eta D(\eta)=\alpha D(\eta)+\beta.$$

For the sign of the derivative we use

$$D_\pm\alpha+\beta=D_\pm(D_- - D_+)\lambda_\pm,$$

$$(D_+\alpha+\beta)(D_-\alpha+\beta)=D_-D_+(D_+ - D_-)^2\lambda_+\lambda_-, \tag{2.3b}$$

and deduce, for $\eta\in[-\frac{1}{2},\frac{1}{2}]$, that τ is monotonic or not depending on whether $\lambda_+\lambda_-\geqslant 0$ or <0. In the following we study different classes of models differing by their positive projections along the z axis, perpendicular to the interfaces: either the same or different.

B. A class of models without partial inversion

We notice that, for models with $M_\pm=M=$const., Eq. (2.1b) yields

$$\lambda_\pm=M^2(E_- - E_+),$$

$$P_\lambda=\lambda_-\lambda_+=M^4(E_- - E_+)^2\geqslant 0. \tag{2.4}$$

This leads to a monotonic internal energy and partial inversion cannot exist. We construct a simple class of models with v_i in two and three ($d=2,3$) dimensions satisfying $M_+=M_-$. They have two speeds, $4(d-1)+2$ v_i, and generalize the first Cabannes model:

$$v_i:(\pm\alpha_x,\pm\alpha_y,\alpha_z=\pm 1), \quad (0,0,\pm 1), \quad \alpha_y=0 \quad \text{for } d=2. \tag{2.5a}$$

To v_i we associate densities N_i and, from the boundary conditions, all N_i, with associated v_i symmetrical with respect to the z axis, are equal. There remain four independent densities:

$$N_1:(\alpha_x>0,\alpha_y\geqslant 0,1), \quad N_5:(0,0,1),$$

$$N_3:(-\alpha_x,-\alpha_y,-1), \quad N_6:(0,0,-1). \tag{2.5b}$$

We consider stationary z-dependent solutions. In Appendix A 1 we write the three conservation laws, linear combinations of the differential terms $l_i=\alpha_z\partial_\eta N_i$. We integrate the momentum conservation law along the z axis and obtain that the mass is a constant:

$$d^*:=d-1, \quad 2d^*(l_1-l_3)+l_5-l_6=0,$$

$$M(\eta)=2d^*(N_1+N_3)+N_5+N_6=\text{const}=M_\pm. \tag{2.5c}$$

There exist generalizations of these models in $d=2,3$ with $\alpha_z=\pm 1$ and leading to $M_-=M_+$. We must check that the models do not share spurious conservation laws. We present a model with $8(d-1)+2$, velocities, three speeds,

$$1, \quad \sqrt{1+\alpha_x^2+\alpha_y^2}, \quad \sqrt{1+4\alpha_x^2+4\alpha_y^2}, \tag{2.6a}$$

$\alpha_z=\pm 1$ and from the z-axis symmetry, there are only six independent densities:

$$N_1:(\alpha_x>0,\alpha_y>0,1),\quad N_2:(2\alpha_x,2\alpha_y,1),\quad N_3(0,0,1), \tag{2.6b}$$

while N_{i+3}, $i=1,2,3$, are associated to velocities opposite to those of N_i. Collisions not conserving the number of particles with a given speed exist and the models are acceptable:

$$\begin{gathered}4[1+\alpha_x^2+\alpha_y^2]=3[1]+[1+4\alpha_x^2+4\alpha_y^2],\\ N_1^3N_4-N_3^2N_2N_6,\quad N_4^3N_1-N_5N_6^2N_3.\end{gathered} \tag{2.6c}$$

The linear differential momentum conservation law still leads to $M_+=M_-$:

$$2d^*\Sigma(l_i-l_{i+3})=0,\quad i=1,2,3\rightarrow M(\eta)=\text{const.} \tag{2.6d}$$

C. Criterion for strict inversion

Let $E_{wI\pm}$ be the internal energy at the walls. Depending whether

$$Q=(E_{I-}-E_{I+})(E_{wI-}-E_{wI+})<0\quad\text{or}\quad\geqslant 0, \tag{2.7}$$

we have a strict inversion or not. For a strict inversion alone we assume (i) *both* $\lambda_\pm=0$ *for some particular value* a_0 *of one arbitrary parameter* a *building up the solutions of the densities*, (ii) $\lambda_+\lambda_->0$ *for* $a\neq a_0$ *and both* $\lambda_\pm$ *change of sign when* a *crosses the* a_0 *value*. From (2.1b) we deduce for a_0 that both $M_+=M_-$, $E_+=E_-$, and $\tau^+=\tau^-$, whereas for $a\neq a_0$ they are different. From (2.3b) we get that for $a>a_0$ and $a<a_0$ both $D_\pm\alpha+\beta$ have the same sign which are opposite when a crosses the a_0 value. The same property holds for $D\alpha+\beta$ and the derivative $\partial_\eta\tau$ and τ is monotonic but increasing and decreasing when a crosses the a_0 value. Consequently, either for $a>a_0$ or $a<a_0$, necessarily $\tau^->\tau^+$ and the transition value leads to a strict inversion effect. We must verify that the hot and cold interfaces remain at the same interface during the transition where a strict inversion occurs. Later we will illustrate this strict inversion with different examples.

D. Partial proof for a class of models without strict inversion

For the class of models (2.5a)–(2.5c) with ± 1 for the projections of the velocities along the z axis, for different collision terms, we have *numerically not found any strict inversion. We have not a general proof, independent of the choice of the collision terms*, as done in Sec. II B for the partial inversion. For the study, done in Appendix A 1, we first give, for $E_{I\pm}$ and Q defined in (2.7),

$$\begin{gathered}E_{I-}-E_{I+}=c_1(N_{1,-}-N_{1,+}),\\ Q=c_2(N_{1,-}N_{6,+}-N_{3,+}N_{5,-})(N_{1,-}-N_{1,+}),\quad c_i>0\end{gathered} \tag{2.8}$$

without strict inversion if $Q\geqslant 0$. *Second, assuming a binary collision term, we prove* $Q\geqslant 0$ *for the solutions. Third, we add a quaternary collision term and solve the nonlinear equation for a class of exact solutions, proving there is no strict inversion*. More explicitly we show that for $\lambda\leqslant 0$ [defined in (1.3a)] the positivity is violated whereas $Q\geqslant 0$ for $\lambda>0$.

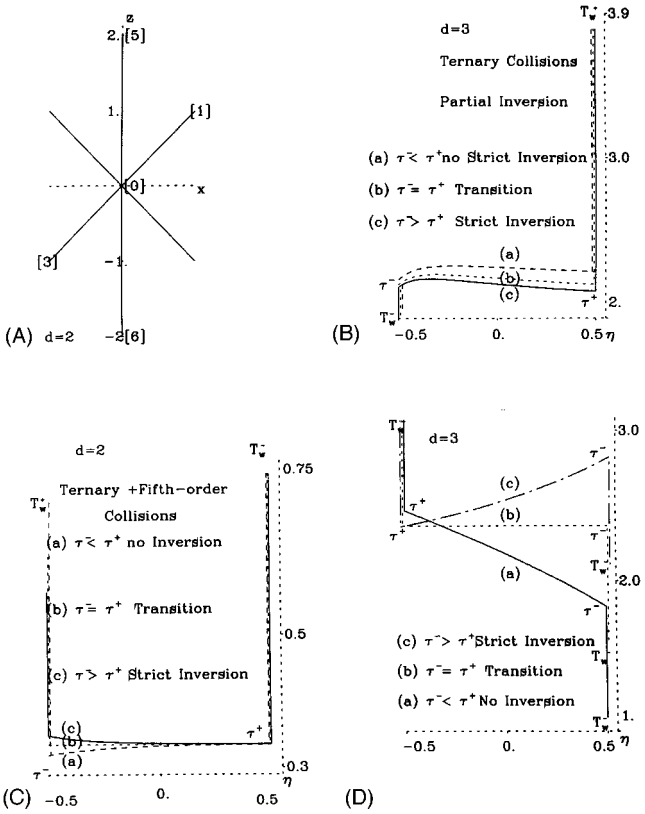

FIG. 1. (A) Models with four and five independent densities. (B) Model with four independent densities: partial and strict Inversions, ternary Collisions. (C) Model with four independent densities: strict inversion, ternary plus fifth-order collisions. (D) Model with five independent densities and a rest particle: strict inversion.

III. MODELS WITH FOUR AND FIVE INDEPENDENT DENSITIES AND TWO $z>0$ VELOCITY PROJECTIONS

We study two classes of models in two dimensions, $d=2$ [cf. Fig. 1(A)], and three dimensions, $d=3$, symmetrical with respect to the z axis. From the boundary conditions there are only four and five (rest particle present) independent densities. In $d=2,3$ we consider models with six and ten velocities (or seven and eleven when a rest particle is present):

$$v_i:(\pm\alpha_x,\pm\alpha_y,\alpha_z=\pm 1),\quad (0,0\pm 2),\quad v_0:(0,0,0)$$
$$\alpha_y=0 \text{ for } d=2,\quad \alpha_x^2+\alpha_y^2=1 \text{ if } v_0 \text{ is present,} \tag{3.1a}$$

generalizing (v_0 absent) the second Cabannes model. To v_i we associate stationary densities $N_i(z)$ and, from the boundary conditions, we write the remaining independent N_i:

$$N_1:(\alpha_x>0,\alpha_y\geqslant 0,1),\quad N_5:(0,0,2),$$
$$N_3:(-\alpha_x,-\alpha_y,-1),\quad N_6:(0,0,-2),\quad N_0:(0,0,0). \tag{3.1b}$$

The difference, with the previous models in Sec. II B, is that the $\alpha_z=\pm 2$ values for N_5 and N_6 are different from ± 1 for N_1 and N_3. It follows that the differential momentum conservation law does not lead to a constant mass. In Appendix A 2 a we write down the three linear differential con-

servation laws (N_0-independent), deduce three differential relations for N_3, N_5, N_6 in terms of N_1, we integrate, and we obtain relations (N_0-independent) for the densities and the momentum j along the z axis, with integration constants a_i:

$$N_3 = N_1 + a_3, \quad N_5 + d^* N_1/2 = a_5 > 0, \quad N_6 + d^* N_1/2 = a_6 > 0, \tag{3.2a}$$

$$j = 2d^*(N_1 - N_3) + 2(N_5 - N_6) = 2(a_5 - a_6 - d^* a_3). \tag{3.2b}$$

All collision terms can be written in terms of $N_1(\eta)$ (with the Knudsen number).

At this stage we discuss models without N_0 and for the connection with the boundary near the interfaces, we write for the gas both the masses and internal energies:

$$\begin{aligned} N_{i,\pm} &:= N_i(\eta = \pm 1/2), \quad M_\pm = 2d^*(N_{1,\pm} + N_{3,\pm}) + N_{5,\pm} + N_{6,\pm}, \\ E_{I\pm} &= [2d^*(1 + \alpha_x^2 + \alpha_y^2)(N_{1,\pm} + N_{3,\pm}) + 4(N_{5,\pm} + N_{6,\pm})]/M_\pm - (j/M_\pm)^2, \end{aligned} \tag{3.3}$$

which can be rewritten with only the $N_{1,\pm}$ values and the constants a_k. For the transition towards a strict inversion we easily write the difference:

$$E_{I+} - E_{I-} = [N_{1,+} - N_{1,-}] F(N_{1,-}, N_{1,+}, a_3, a_5, a_6) \tag{3.4}$$

with $F \neq 0$ for $N_{1,-} = N_{1,+}$. For a transition we have two possibilities:

(i) $N_{1,-} = N_{1,+}$. For monotonic solutions, of the (1.3a)–(1.3c) type, this means that $N_1(\eta)$ is a constant as well as the other densities, the mass, and the internal energy. The transition is characterized by constant microscopic and macroscopic quantities.

(ii) $N_{1,-} \neq N_{1,+}$ and necessarily $F = 0$ in (3.4). In this case the microscopic and macroscopic quantities are not constant at the transition. Adding N_0 (in M), written in terms of N_i or N_1, does not change the discussion of the two (i) and (ii) cases.

At the interfaces or at the walls we associate macroscopic quantities (respectively N_1, N_5 and N_3, N_6 to the interfaces at $\eta = \mp\frac{1}{2}$). At $\eta = -\frac{1}{2}$ we get

$$\begin{aligned} M_{w,-} &= 4d^* N_{1,-} + 2N_{5,-}, \\ E_{wI-} &= [4d^*(1 + \alpha_x^2 + \alpha_y^2) N_{1,-} + 8N_{5,-}]/M_{w,-}, \end{aligned} \tag{3.5}$$

while at $\eta = \frac{1}{2}$ we get $M_{w,+}$ and E_{wI+} with the substitution of $N_{3,+}, N_{6,+}$ to $N_{1,-}, N_{5,-}$.

Finally we define as kinetic temperature (internal energy) T_w^+ at the warm interface and T_w^- at the cold interface satisfying the inequality

$$T_w^+ = \sup(E_{wI+}, E_{wI-}), \quad T_w^- = \inf(E_{wI+}, E_{wI-}). \tag{3.6}$$

This fixes the $\eta = \pm\frac{1}{2}$ value for warmness and coldness. For the gas at the warm and cold interfaces we deduce the masses $M^\pm$ (from $M_\pm$) and we call $\tau^\pm$ the associated limit values of the internal energies ($E_{I\pm}$). If we find solutions with $\tau^- > \tau^+$ we have a strict inversion. We write the internal energy τ and the mass M inside the gas:

$$\begin{aligned} M(\eta) &= 2d^*(N_1 + N_3) + 2(N_5 + N_6) + N_0, \\ \tau(\eta) &= [2d^*(1 + \alpha_x^2 + \alpha_y^2)(N_1 + N_3) + 8(N_5 + N_6)]/M - (j/M)^2. \end{aligned} \tag{3.7}$$

We have a partial inversion if $\tau(\eta)$ is nonmonotonic for $\eta \in [-\frac{1}{2}, \frac{1}{2}]$. In Secs. III A (without rest particle) and III B (with rest particle) we first, with the conservation laws (3.2a), eliminate N_3, N_5

and N_6 and second, solve the nonlinear equation for N_1. We give examples where either both effects exist or only one. At the transition we give examples where either microscopic and macroscopic quantities are constant or not.

A. Models, without rest particle, with four independent densities

We consider ternary and fifth-order collisions with associated parameters θ_3 and θ_5:

$$X:=3(N_3^2N_5-N_1^2N_6), \quad \partial_\eta N_1=(\theta_3+N_1N_3\theta_5)X,$$
$$f_1:=3a_3(2a_5-d^*a_3/2), \quad f_0:=3a_5a_3^2, \tag{3.8}$$
$$\partial_\eta N_1=[3jN_1^2/2+f_1N_1+f_0][\theta_3+\theta_5N_1(N_1+a_3)],$$

and j written down in (3.2b). We get either a quadratic Riccati scalar equation ($\theta_5=0$) or a quartic nonlinear equation. With solutions of the type (1.3a)–(1.3c) in Appendices A 2 b and c, we determine n_{01}, n_1, and γ. Once N_1 is known we deduce, with (3.2a), all n_{0i}, n_i, and N_i.

In all figures of the paper we present three solutions: (a) without strict inversion $\tau^-<\tau^+$, (b) transition $\tau^-=\tau^+$, and (c) with a strict inversion $\tau^->\tau^+$. In Fig. 1(B) ($d=2$, only ternary collisions) we observe both partial and strict inversions with parameter values: Fig. 1(B): $N_{1,-}=0.673$, $N_{3,-}=0.679$, $N_{6,-}=3.107$, $N_{5,-}$ varying in (a)–(c).

Fig. 1(B)	$N_{5,-}$	T_w^-	T_w^+	τ^-	τ^+	M^-	M^+	λ_-	λ_+	λ
(a)	0.081	2.06	<3.8	2.24	<2.29	8.6	>5.13	+	−	−
(b)	0.0315	2.02	<3.8	2.21	$=2.21$	8.54	>5.07	+	−	−
(c)	0.005	2.0	<3.8	2.2	>2.174	8.52	>5.04	+	−	−

(3.9a)

We note that $\lambda_\pm\neq 0$ have opposite signs so that the criterion $\lambda_-\lambda_+<0$ for nonmonotonic $\tau(\eta)$ is always satisfied. The only equality at (b) is $\tau^-=\tau^+$, nevertheless λ, defined in (1.3a) is $\neq 0$, $\neq\infty$, $N_{1,-}\neq N_{1,+}$. *Consequently the transition is of the type (ii) with densities and macroscopic quantities which are η-dependent functions.*

In Fig. 1(C) ($d=3$ and fifth-order collision included) with only a strict inversion, the momentum $j=-4.091$ and two other constants are fixed while λ is varying:

Fig. 1(C)	T_w^-	T_w^+	τ^-	τ^+	M^-	M^+	λ_-	λ_+	λ
(a)	0.7	<0.74	0.318	<0.334	6.24	<6.47	−	−	$+0.075$
(b)	0.62	<0.74	0.33	$=0.33$	6.48	$=6.48$	0	0	0
(c)	0.56	<0.74	0.348	>0.334	6.72	>6.48	+	+	-0.092

(3.9b)

For the transition curve (b) we verify both $\lambda_\pm=0$ and $\lambda=0$ and the changes of signs between (a) and (c). From the criterion $\lambda_-\lambda_+\geqslant 0$ we verify that $\tau(\eta)$ is monotonic. Due to $\lambda_\pm<0$ in (a), >0 in (c), and$=0$ at the transition (b) we see that the curves (a) and (c) are monotonic but either increasing or decreasing. *Due to $\lambda=0$ or $N_{1,-}=N_{1,+}$, the transition is of the (i) type, with constants for all densities and macroscopic quantities.*

B. Models with a rest particle and five independent densities

We add the rest particle density N_0 to the previous models and for N_1 and N_3 the speed of the associated velocities is $\sqrt{2}$. Binary collisions including N_0 of the type [4]+[0]=[2]+[2] are pos-

sible, while for the collisions without N_0, we keep in (3.8) only the ternary X collision term. For the stationary solution there is no differential term associated to the rest particle density N_0. From the sum of the two collision terms including N_0 we get

$$N_0=[N_1^2+N_3^2]/(N_5+N_6)=[2N_1^2+2a_3N_1+a_3^2]/[-d^*N_1+a_5+a_6], \tag{3.10a}$$

leading to an analytic expression of N_0 in terms of N_1, because the relations (3.2a) for N_3, N_5, and N_6 are still valid. In order to distinguish the collisions with and without N_0, we add a cross section θ_2 and substitute (3.10a) for N_0 in the collision term:

$$\begin{aligned}&\partial_\eta N_1=X+\theta_2(N_0N_5-N_1^2),\\ &[-d^*N_1+a_5+a_6]\partial_\eta N_1(\eta)=[3jN_1^2+f_1N_1+f_0][-d^*N_1+a_5+a_6+\theta_2/3].\end{aligned} \tag{3.10b}$$

We finally have a nonlinear differential equation for N_1 alone which is an unusual DBM equation. The study is done in Appendix A 2 d and, except for N_0, we still find solutions of the (1.3a) and (1.3b) type. We start with a_3, a_5, and a_6 as arbitrary parameters and from the coefficients of D^{-q} in (3.10b) we deduce successively n_{01} as a solution of a quadratic equation and θ_2, n_1, and γ. For the masses $M_{w,\pm}$ at the interfaces we can add N_0 or

$$N_{1,-}^2/N_{5,-} \quad \text{at} \quad \eta=-\tfrac{1}{2}, \quad N_{3,+}^2/N_{6,+} \quad \text{at} \quad \eta=\tfrac{1}{2},$$

but we have not found any significant difference concerning the existence of a strict inversion. In Fig. 1(D) we present the three solutions (a), (b), and (c) for $d=3$ (warm interface at $\eta=-\frac{1}{2}$). We give the values of the fixed parameters and λ which is varying:

Fig. 1(D): $N_{1,-}=0.1021$, $N_{3,-}=0.3019$, $N_{5,-}=0.5015$

Fig. 1(D)	T_w^-	T_w^+	τ^-	τ^+	M^-	M^+	λ_-	λ_+	λ
(a)	1.05	<3.07	2.12	<2.36	2.87	>2.38	+	+	$+83.10^{-5}$
(b)	1.6	<3.07	2.36	$=2.36$	2.38	$=2.38$	0	0	0
(c)	2.11	<3.07	2.81	>2.36	1.76	<2.38	−	−	-97.10^{-5}

(3.11)

For the transition curve (b) we find both $\lambda_\pm=0$ and $\lambda=0$, $N_{1,-}=N_{1,+}$, and the changes of signs between (a) and (c). We still have a transition of the (i) type with densities and macroscopic quantities which are constant. Concerning the masses we always notice $M^->M^+$ in Fig. 1(B) while in Fig. 1(C) [contrary to Fig. 1(D)], when there exists a strict inversion the inequality $M^->M^+$ is reversed when there is no inversion. In Figs. 1(B)–1(D) [contrary to Fig. 1(C)] we observe, near and at the two interfaces, the normal pattern: $\tau^->T_w^-$ and $\tau^+<T_w^+$. This was also observed previously.[2,3]

IV. MODELS WITH SIX INDEPENDENT DENSITIES

A. Riccati scalar solutions to a 3×3 Riccati system

We start with a 6×6 differential Riccati system, with only quadratic nonlinear terms, satisfied by six densities X_i, $i=1,..,6$. In DBMs these densities satisfy three linear differential equations for the conservation laws of mass, momentum, and energy:

$$\sum_{j=1}^{6} c_{ij}\partial_\eta X_j=0, \quad i=1,2,3.$$

We rewrite the linear system such that three $\partial_\eta X_k$, $k=4,5,6$, are linear combinations of three other $\partial_\eta X_i$, $i=1,2,3$. We integrate, introducing three constants a_k, $k=4,5,6$, and the three densities X_k are linear combinations of the X_i with the three constants a_k. The three remaining X_i satisfy a 3×3 Riccati system:

$$\partial_\eta X_i=\sum_{j=1}^{3} X_j(a_{ij}X_i+b_{ij})+\sum_{j\neq i,k\neq i,j\leqslant k} a_{ijk}X_jX_k+c_i, \quad i=1,2,3, \tag{4.1}$$

with quadratic and linear terms, a_{ij} and a_{ijk} independent on the integration parameters a_j while the b_{ij} and c_i are respectively linear and quadratic in these parameters. We look at solutions of the scalar Riccati type (1.3a) and (1.3b):

$$X_i(\eta)=x_{0i}+x_i/D(\eta), \quad D(\eta)=1+\lambda e^{\gamma\eta}. \tag{4.2a}$$

We show that such solutions, with ten parameters x_i, x_{0i}, a_i, and γ, satisfying nine relations [coefficients of D^{-k}, $k=0,1,2$ in (4.1)] exist. We define scaled parameters

$$\beta_{ij}=x_j/x_1, \quad \alpha_{1j}=x_{0j}/x_{01}, \quad \lambda_k=a_k/x_{01}, \quad \overline{b_{ij}}=b_{ij}/x_{01}, \quad \overline{c_i}=c_i/x_{01}^2, \tag{4.2b}$$

the $\overline{b_{ij}}$, $\overline{c_i}$ being, respectively, linear and quadratic in λ_k. We will see that x_{01} is finally an arbitrary scaling parameter. First, from the three D^{-2} relations, we get

$$\gamma/x_1=\sum_{j,k} [a_{ij}\beta_{1j}+a_{ijk}\beta_{1k}\beta_{1j}/\beta_{1i}], \quad i=1,2,3. \tag{4.3a}$$

On the rhs we have two independent relations for β_{12}, β_{13}:

$$\sum_j \beta_{1j}\beta_{1l}(a_{1j}-a_{lj})+\sum_{j,k} \beta_{1j}\beta_{1k}(a_{1jk}\beta_{1l}-a_{ljk})=0, \quad l=2,3. \tag{4.3b}$$

We deduce β_{12} and β_{13} as solutions of two coupled polynomials with coefficients a_{ij} and a_{ijk} independent on the a_k. Second, we get from the three D^{-1} relations with $i=1,2,3$

$$\frac{-\gamma}{x_{01}}=\left[\sum_j a_{ij}(\beta_{1j}\alpha_{1i}+\beta_{1i}\alpha_{1j})+\sum_{jk} a_{ijk}(\alpha_{1j}\beta_{1k}+\alpha_{1k}\beta_{1j})+\sum_j \overline{b_{ij}}\beta_{1j}\right] \Big/ \beta_{1i}, \tag{4.4a}$$

On the rhs we have two independent relations, for α_{12} and α_{13} with coefficients $\overline{b_{ij}}$, which are linear in λ_k. We substract the two relations for $i=1,2$ and $i=1,3$:

$$\sum \beta_{1j}(a_{1j}\beta_{1l}-a_{lj}\alpha_{1l})+\beta_{1l}\alpha_{1j}(a_{1j}-a_{lj})+\sum (\beta_{1k}\alpha_{1j}+\beta_{1j}\alpha_{1k})(a_{1jk}\beta_{1l}-a_{ljk})$$

$$=\sum \beta_{1j}(\overline{b_{lj}}-\overline{b_{1j}}\beta_{1l}), \quad l=2,3. \tag{4.4b}$$

The β_{12} and β_{13} are known from (4.3b) and *the two (4.4b) relations* lead to α_{12} and α_{13}, which are linear combinations of b_{ij} or equivalently of λ_k, $k=4,5,6$. Third, we get from the three constant relations D^0 of (4.1)

$$\sum_j a_{ij}\alpha_{1i}\alpha_{1j}+\sum_{jk} a_{ijk}\alpha_{1j}\alpha_{1k}+\sum_j \overline{b_{ij}}\alpha_{1j}+\overline{c_i}=0, \quad i=1,2,3. \tag{4.5}$$

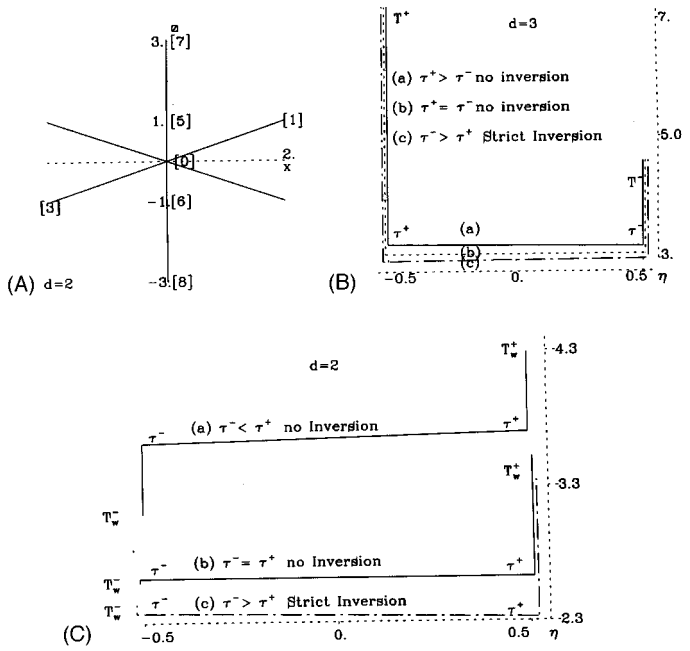

FIG. 2. (A) Models with six independent densities and three speeds. (B) Model with six independent densities, $d=3$, and strict inversion. (C) Model with six independent densities, $d=2$, and strict inversion

We substitute α_{12} and α_{13} given by (4.4b), and which are linear in λ_k, into (4.5). We get three quadratic polynomials in λ_k that we solve and the λ_k and α_{1l} are known. With β_{ij}, α_{1j}, and λ_k known, from (4.3a–4.4a) we deduce γ/x_1, γ/x_{01}, and x_1/x_{01}. Finally we consider x_{01} as a scaling parameter and all ratios of x_i, x_{0i}, γ, and a_k by x_{01} are known.

B. Models with six densities and four velocities along the *z*-axis

We consider models with $8v_i$ in $d=2$ [Fig. 2(A)], coordinates $(x,y=0,z)$ for the velocities, and $12v_i$ in $d=3$ with four velocities along the z axis:

$$v_i:(\pm\alpha_x,\pm\alpha_y,\alpha_z=\pm 1),\quad \alpha_x^2+\alpha_y^2=4,\quad \alpha_y=0\ \ d=2,\quad \alpha_y\neq 0\ \ d=3,$$
$$(0,0,\alpha_z=\pm 1),\quad (0,0,\alpha_z=\pm 3). \tag{4.6a}$$

To the v_i we associate the densities N_i. From the boundary conditions all N_i with associated v_i symmetrical with the z axis are equal. There remain six independent densities:

$$N_1:(\alpha_x>0,\alpha_y\geqslant 0,1),\quad N_5:(0,0,1),\quad N_7:(0,0,3),$$
$$N_3:(-\alpha_x,-\alpha_y,-1),\quad N_6:(0,0,-1),\quad N_8:(0,0,-3). \tag{4.6b}$$

The speeds being 1, 3, and $\sqrt{5}$ it follows that collisions of the type $2[5]=[1]+[9]$ are possible. In Appendix B 1 we write down the differential conservation laws, deduce N_3, N_6, and N_8 as linear combination of N_1, N_5, and N_7 with constants a_k, $k=3,6,8$, write the collision terms leading to an heavy 3×3 Riccati system of the (4.1) type for N_1, N_5, and N_7:

$$\partial_\eta N_5 = N_5^2((d-7)/3+1/d^*)+N_5(6(2-d)+2d^{*2}/3)(N_1+3N_7/d^*)+d^*[(13-4d)N_1^2$$
$$+2(a_6+3a_3)N_1+a_3^2-a_8N_5]+81N_7^2/d^*+18N_1N_7(4-d)+N_5 2a_3(2-d)+18N_7a_3,$$

$$\partial_\eta N_1 = N_1^2(2d-3)-9N_7^2+N_1[3N_5+(11-2d)N_7]+N_5(9N_7+N_5)/d^*+a_6(N_7-N_1)+a_3N_5, \tag{4.6c}$$

$$\partial_\eta 3N_7/d^* = N_1^2+N_7(9N_7+2d^*N_1+a_6).$$

We obtain, for (1.3a) and (1.3b) type of solutions, the ratios of the parameters n_i, n_{0i}, a_k, and γ by n_{01}. Furthermore, we write down $M_{w,\pm}$ and $E_{wI\pm}$ at the two interfaces and for the gas, both the mass and the energy. A sufficient condition that these last quantities, and consequently the internal energy, be equal at the two interfaces is that the three densities N_1, N_5, and N_7 be also equal. For our solution of the (1.3a) and (1.3b) type, we can thus find a transition towards a strict inversion with constant densities and macroscopic quantities for the gas. On the contrary, at the wall, $E_{wI\pm}$ will be different.

In Fig. 2(B) for $d=3$ (warm interface at $\eta=-\frac{1}{2}$) and in Fig. 2(C) for $d=2$ (warm interface at $\eta=\frac{1}{2}$) we still present the three solutions (a), (b), and (c) with a strict inversion. We present the values of the fixed parameters $\beta_{1,l}$ and $\alpha_{1,l}$ and of λ defined in (4.2b) and (1.3a):

Figs.	β_{17}	β_{15}	α_{17}	α_{15}	$N_{1,-}$
2(B)	−0.462	1.387	7.45	0.748	0.215
2(C)	0.0579	1.122	0.0886	3.333	0.015

Figs.	T_w^-	T_w^+	τ^-	τ^+	M^-	M^+	λ_-	λ_+	λ
2(B)(a)	4.593	<7.189	3.17	<3.2	<2.61	<2.63	+	+	−10.0
2(B)(b)	4.592	<7.197	3.04	=3.04	2.81	=2.81	0	0	∞
2(B)(c)	4.59	<7.202	2.95	>2.92	2.97	>2.96	−	−	+13.0
2(C)(a)	3.10	<4.29	3.63	<3.7	2.38	<2.48	−	−	−1.8
2(C)(b)	2.6	<3.52	2.63	=2.63	0.40	=0.40	0	0	∞
2(C)(c)	2.44	<3.34	2.37	>2.33	0.48	>0.475	+	+	+5.0

(4.7)

For the two transition (b) curves we find $\lambda_\pm=0$ and $\lambda=\infty$ or $N_{i,-}=N_{i,+}$ and changes of signs between (a) and (c). *For the gas we still have a transition with constants for the densities and the macroscopic quantities* (contrary to $T_w^\pm$ at the walls which are different). The difference between the two pictures is the fact that $\tau^-<T_w^-$ in Figs. 2(B) and 2(C), curve (c), while the pattern is normal in Fig. 2(c), curves (a) and (b).

C. Models with six densities and two velocities along the *z* axis

For these models with $10v_i$ [$d=2$, Fig. 3(A)] and $18v_i$ ($d=3$), speeds 3 and $\sqrt{3}$, only two velocities are along the z axis with z coordinates ± 3:

$$v_i:(\pm\alpha_x,\pm\alpha_y,\alpha_z=\pm 1),\quad (\pm 2\alpha_x,\pm 2\alpha_y,\alpha_z=\pm 1),\quad (0,0,\alpha_z=\pm 3),$$
$$\alpha_x^2+\alpha_y^2=2,\quad \alpha_y=0 d=2,\quad \alpha_y[\neq]d=3. \tag{4.8a}$$

From the boundary conditions all N_i with v_i symmetrical with respect the z axis are equal. There still remain six independent densities:

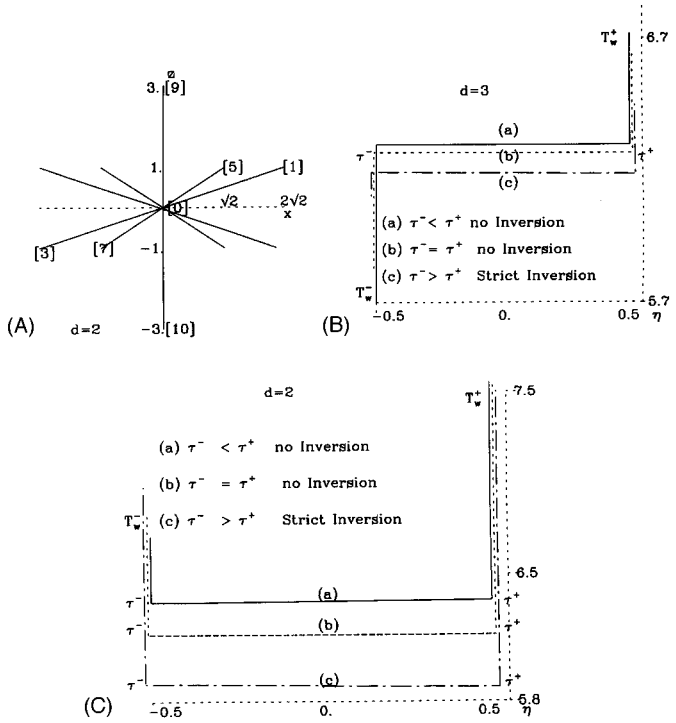

FIG. 3. (A) Models with six independent densities and two speeds. (B) Model with six independent densities, $d=3$, and strict inversion. (C) Model with six independent densities, $d=2$, and strict inversion.

$$N_1:(2\alpha_x>0,2\alpha_y\geqslant 0,1),\quad N_5:(\alpha_x,\alpha_y,1),\quad N_9:(0,0,3),$$
$$N_3:(-2\alpha_x,-2\alpha_y,-1),\quad N_7:(-\alpha_x,-\alpha_y,-1),\quad N_{10}:(0,0,-3). \tag{4.8b}$$

In Appendix B 2 we write the collision terms, the differential conservation laws, deduce N_7, N_3, and N_{10} as a linear combination of N_1, N_5, and N_9 with constants a_k, $k=3,7,10$, leading to a 3×3 Riccati system of the (4.1) type for N_1, N_5, and N_9:

$$\partial_\eta N_1=-2N_1^2-2N_9^2+N_5^2+N_5N_9(1+(27-4d^{*2})/6d^*)-N_1(N_5+N_9(27+4d^{*2})/6d^*+a_3+a_7)$$
$$+N_9(a_7+a_{10})+N_5a_3,$$
$$3\partial_\eta N_9/2d^*=2(N_1^2+N_9^2+N_1N_5)+N_9[(27+4d^{*2})N_1/6d^*+N_5(2d-5)/3-a_7-a_{10}]+N_1a_3, \tag{4.8c}$$
$$\partial_\eta N_5=N_5[2d^*(N_5+N_1)/3+3N_9+a_7-a_{10}]+a_7[3N_1+N_9(2d+7)/2d^*+a_3]$$

with $d^*=d-1$. For solutions of the (1.3a) and (1.3b) type, we find the ratios of the parameters n_i, n_{0i}, a_k, and γ by n_{01}, like for the previous model. We write also $M_{w,\pm}$ and $E_{wI\pm}$ at the two interfaces and both the mass and the energy for the gas. A sufficient condition for the equality of the internal energy at $\eta=\pm\frac{1}{2}$ is the equality of N_1, N_5, and N_7 at $\eta=\pm\frac{1}{2}$. For (1.3a) and (1.3b) type solutions we can find a transition with, for the gas, densities and macroscopic quantities constant (at the walls $E_{wI\pm}$ are different).

In Fig. 3(B) for $d=3$ (warm interface at $\eta=-\frac{1}{2}$) and in Fig. 3(C) for $d=2$ (warm interface at $\eta=1/2$) we still present three solutions with curves (a)–(c), the fixed parameters values, and the three values for λ:

Figs.	β_{19}	β_{15}	α_{19}	α_{15}	$N_{1,-}$
3(B)	5.040	6.374	−0.3684	−0.1489	0.011
3(C)	1.847	2.514	−0.3169	−0.2827	0.025

$$\left|\begin{array}{cccccccccc} \text{Figs.} & T_w^- & T_w^+ & \tau^- & \tau^+ & M^- & M^+ & \lambda_- & \lambda_+ & \lambda \\ 3(B)(a) & 5.7< & 6.72 & 6.294< & 6.296 & 3.52< & 3.54 & - & - & -0.13 \\ 3(B)(b) & 5.83< & 6.25 & 6.26= & 6.26 & 3.17= & 3.17 & 0 & 0 & 0 \\ 3(B)(c) & 6.1< & 6.48 & 6.188> & 6.184 & 2.61> & 2.58 & + & + & +0.28 \end{array}\right|, \quad (4.9)$$

$$\left|\begin{array}{ccccccccc} 3(C)(a) & 6.71< & 7.55 & 6.34< & 6.35 & 0.426< & 0.429 & - & - & -0.11 \\ 3(C)(b) & 6.82< & 7.53 & 6.16= & 6.16 & 0.41= & 0.41 & 0 & 0 & 0 \\ 3(C)(c) & 6.98< & 7.50 & 5.89> & 5.87 & 0.385> & 0.383 & + & + & +0.17 \end{array}\right|.$$

The transition cases (b) still correspond to $\lambda_{\pm}=0$ and $\lambda=0$, their changes of signs between (a) and (c) and, due to $\lambda=0$, to *constant densities* $N_i(\eta)$. *At the transition (b) both the masses and the internal energies are constant while these quantities are different at the two walls*. The difference between the two pictures is still $\tau^- < T_w^-$ in Fig. 3(C) and the opposite in Fig. 3(B). For the masses near the interfaces, in Figs. 2(B), 2(C), 3(B), and 3(C) we notice $M^- > M^+$ when there exists a strict inversion and the reversed inequality when there is no inversion.

V. CONCLUSION

In this paper we have applied and modified, to a vapor between two interfaces, a criterion previously established for shock waves. However, we look at stationary solutions (not shock waves) and we have eliminated the velocities parallel to the two interfaces. Our results confirm, generalize, and extend those of Ref. 3. The two different effects (either partial inversion, where the internal energy between the two interfaces is not monotonic, or strict inversion, where the internal energy of the gas is larger at the cold interface) have been illustrated with different possibilities: either both effects exist or only one or none. Summarizing the results for the nonexistence or existence of at least one effect: (i) no effect when only one $z>0$ projection of the velocities exists and (ii) at least one effect when more than one positive $z>0$ projection exists. With different models we have verified that the distinctions (i) and (ii) hold whatever the number and location of the velocities are, parallel to the z axis or oblique. For models of the type (i) we can prove, without explicit construction of the solutions, that no partial inversion can occur. This is an immediate consequence of the fact that the mass inside the gas remains constant. On the contrary for the nonexistence of a strict inversion, we must construct explicitly the solutions. We have given the proof for two collision terms, verified numerically for some other collisions; however, we have not a general proof independent of the collision terms.

Summarizing the results for the existence of both effects or only one (strict inversion), we find a distinction at the transition where the values of the internal energy at the two interfaces are the same: (i) both the masses and the densities are the same at the two interfaces and only the strict inversion occurs and (ii) they are different and we find both effects. In the first case, due to the fact that our particular solutions (1.3a)–(1.3c) for the densities are monotonic, the densities and all macroscopic quantities of the gas are necessarily constant at the transition. On the contrary, in the second case the microscopic and macroscopic quantities are not constant.

If we want to enlarge the present exact results, we can either introduce rest particles in the models with six independent densities or we can consider more general models with eight, ten,..., densities. However, in these cases, taking into account the fact that the number of linear conservation laws remains three, we are reduced to $5\times5,7\times7,...$, nonlinear systems and the determination of exact solutions becomes more and more difficult. Another possible extension is the deter-

mination of density solutions which are not monotonic. We know that this is possible for Riccati systems.[8] At the transition, the equality at the two interfaces will not necessarily lead to constant solutions. However, these solutions are more difficult to handle. It will be useful to establish the connection between these results of the discrete theory with those of the continuous one. We notice also a recent study[9] of evaporation/condensation in the scope of the Navier–Stokes equations.

ACKNOWLEDGMENT

We thank G. Ripka for the improvement in the presentation.

APPENDIX A: EXACT SOLUTIONS FOR MODELS WITH FOUR AND FIVE DENSITIES

1. No strict inversion for a model with ±1 for the *z*-axis velocities projections

We study the models (2.5a)–(2.5c), like Fig. 1(A) but $\alpha_z=\pm 1$ for N_5 and N_6, with four independent velocities N_1, N_3, N_5, and N_6. We have the three linear differential conservation laws:

$$\begin{gathered} 2d^*(l_1\pm l_3)+l_5\pm l_6=0, \\ d^*:=d-1, \quad 2d^*(1+\alpha_x^2+\alpha_y^2)(l_1+l_3)+(l_5+l_6)=0. \end{gathered} \tag{A1a}$$

We deduce l_3, l_5, and l_6 from l_1, integrate and get N_3, N_5, and N_6 from N_1:

$$N_3-N_1=a_3, \quad N_5+2d^*N_1=a_5>0, \quad N_6+2d^*N_1=a_6>0. \tag{A1b}$$

Taking into account $M_-=M_+$, we get for the gas at $\eta=\pm\frac{1}{2}$ the difference

$$E_{I-}+E_{I+}=2(E_--E_+)/M=c_1(N_{1-}-N_{1+}), \quad c_1>0, \tag{A2a}$$

and for the internal energy at the two interfaces,

$$\begin{gathered} E_{wI-}-E_{wI+}=c_2(N_{1,-}N_{6,+}-N_{1,+}N_{5,-}), \quad c_2>0, \\ j=a_5-a_6-2d^*a_3, \quad E_{wI-}-E_{wI+}=c_2((N_{1,-}-N_{1,+})a_5-jN_{1,-}-a_3a_5). \end{gathered} \tag{A2b}$$

If the product Q of the two differences (2.7) is positive, there is no strict inversion

$$\begin{gathered} Q/c_1c_2:=a_5(N_{1,-}-N_{1,+})^2+\overline{Q}>0 \quad \text{if } \overline{Q}>0, \\ \overline{Q}=-(jN_{1,-}+a_3a_5)(N_{1,-}-N_{1,+}), \end{gathered} \tag{A2c}$$

and $\overline{Q}>0$ *is a sufficient condition for the nonexistence of a strict inversion.*

(i) First, we can prove $Q>0$ for a simple example of a binary collision:

$$\begin{gathered} \partial_\eta N_1(\eta)=N_3N_5-N_1N_6=jN_1(\eta)+a_3a_5, \quad N_1(\eta)=-a_3a_5/j+ce^{j\eta}, \\ c=\text{const}, \quad \overline{Q}=jc^2(1-e^{-j})\geqslant 0. \end{gathered} \tag{A3}$$

(ii) Second, we add a quaternary collision term $\theta_4(N_5^2N_3^2-N_1^2N_6^2)$, $\theta_4>0$,

$$\partial_\eta N_1(\eta)=(jN_1(\eta)+a_3a_5)[1+\theta_4(-4d^*N_1^2(\eta)+(j+2a_6)N_1(\eta)+a_3a_5)]. \tag{A4a}$$

For cubic $j\neq 0$ nonlinearity, we have found two exact solutions with the same $j\gamma<0$:

$$D=1+\lambda e^{\gamma\eta}>0, \quad j\neq 0, \quad N_1=n_{01}+N_1/D^{1/2}. \tag{A4b}$$

Solution 1: $a_3, a_5, \theta_4, N_{1,-}$, arbitrary: $a_6=2d^*a_3+a_5$, $n_{01}=a_5/4d^*$, $n_1^2 4d^*=1/\theta_4+a_6a_5/2d^*$:

$$j=-4d^*a_3, \quad j\gamma=-8d^*(jn_1)^2<0 \tag{A4c}$$

Solution 2: a_3, a_5, a_6 arbitrary: $n_{01}=(j+2a_6)/12d^*-a_3a_5/3j$, $n_1=n_{01}+a_3a_5/j$, $1/\theta_4=4d^*n_{01}^2-n_{01}(j+2a_6)-a_3a_5$.

With $\lambda>0$ we get both sign of $\overline{Q}=j\lambda(e^{-\gamma}-1)>0$ and positivity for θ_4, solutions 1 and 2. We give the proof for solution 1 and notice

$$a_6>0\rightarrow y:=2d^*a_3/a_5>-1, \quad 2\sqrt{2}d^*|n_1|/a_5>\sqrt{1+y}. \tag{A5a}$$

First we assume $\lambda=0$ or $N_{1,-}=N_{1,+}$, find four cases, and with (A1b) for N_3, N_5, and N_6,

$$\begin{gathered}
n_1<0, \quad a_3>0\rightarrow N_1=a_5/4d^*-|n_1|<a_5(1-\sqrt{2})/4d^*<0,\\
n_1<0, \quad a_3<0\rightarrow 4d^*Ns_3/a_5<y+\sqrt{1+y}[\sqrt{1+y}-\sqrt{2}]<0,\\
n_1>0, \quad a_3>0\rightarrow N_5<a_5(1-\sqrt{2})/2<0,\\
n_1>0, \quad a_3<0\rightarrow N_6/a_5<1/2+y-\sqrt{1+y}/\sqrt{2}<0.
\end{gathered} \tag{A5b}$$

Second, for $\lambda<0$, $D(\lambda<0)<D(\lambda=0)=1$, we define $\tilde{N}_i=N_i(\lambda=0)$ with four cases:

$$\begin{gathered}
n_1<0, \quad a_3>0\rightarrow N_1(\lambda)=n_{01}-n_1|\sqrt{D(\lambda)}<\tilde{N}_1<0,\\
n_1<0, \quad a_3<0\rightarrow N_3(\lambda)=\tilde{N}_3+|n_1|(1-1\sqrt{D(\lambda)})<0,\\
n_1>0\rightarrow N_1(\lambda)=n_{01}+|n_1|\sqrt{D(\lambda)}>\tilde{N}_1,\\
n_1>0, \quad a_3>0\rightarrow N_5(\lambda)<-2d^*\tilde{N}_1+a_5=\tilde{N}_5<0,\\
n_1>0, \quad a_3<0\rightarrow N_6(\lambda)<2d^*\tilde{N}_1+a_6=\tilde{N}_6<0.
\end{gathered} \tag{A5c}$$

For $j=0$ *we have found one exact solution* $N_1=n_{01}+n_1/D$:
Solution 3: a_3, a_5, θ_4, $N_{1,-}$ arbitrary: $a_6=a_5-2d^*a_3$, $\gamma=-4d^*\theta_4 n_1 a_3 a_5$,

$$n_{01}^2-n_{01}a_6/2d^*=-n_{01}(n_1+n_{01})=(a_3a_5+1/\theta_4)/4d^* \tag{A5d}$$

$N_i>0$, sign $\overline{Q}=a_3n_1\lambda(e^{-\gamma}-1)>0$ for $\lambda>0$ and positivity violated for $\lambda\leqslant 0$.

2. Models with ±1, ±2 for the *z*-axis velocity projections (Sec. III)

a. Conservation laws for stationary solutions

We call $l_i=e_i\partial_\eta N_i$ with $e_i=\pm 1$ for N_1 and N_3,$=\pm 2$ for N_5 and N_6, and$=0$ for N_0. We have $l_0=0$ and for the three linear differential conservation laws

$$\begin{gathered}
2d^*(1+\alpha_x^2+\alpha_y^2)(l_1+l_3)+4(l_5+l_6)=0,\\
2d^*(l_1\pm l_3)+(3\mp 1)(l_5\pm l_6)/2=0, \quad l_1=-l_3=-l_5/d^*=l_6/d^*.
\end{gathered} \tag{A6}$$

We integrate and, from N_1, find (3.2a) for N_3, N_5, and N_6. *We note that the masses associated to the densities with the same speed satisfy* $N_1+N_3\neq$const. and $N_5+N_6\neq$const.

b. Only ternary collisions for the Sec. III A models with $N_0=0$, $\theta_5=0$

In (3.8) for N_1 solutions (1.3a) and (1.3b), from the coefficients of D^{-q}, $q=0,1,2$ we get

$$3jn_{01}^2/2+f_1n_{01}+f_0=0\rightarrow n_{01}\rightarrow n_1=-2n_{01}-f_1/3j\rightarrow\gamma=n_1 3j/2. \tag{A7}$$

c. Ternary and fifth-order collisions for the Sec. III A models with $N_0=0$

In (3.8), $\theta_5\neq0$, we get a quartic nonlinearity with a_3, a_5, a_6, θ_3, and θ_5 dependent coefficients:

$$\overline{f_1}:=f_1/a_3,\quad \overline{\theta_{35}}=(\theta_3/\theta_5)(j/a_3)^2,\quad A_4=1,\quad A_3=2\,\overline{f_1}/3+j,$$
$$A_2=2j(a_5+\overline{f_1}/3)+\overline{\theta_{35}},\quad A_1=3j^2a_5+\overline{f_1\theta_{35}},\quad A_0=3ja_5\overline{\theta_{35}}, \tag{A8}$$
$$\frac{\partial_\eta N_1(\eta)}{(1.5j\theta_5)}=\sum_{k=0}^{4}A_k\left(\frac{a_3}{j}\right)^{4-k}N_1^k(\eta),$$

For (1.3a)–(1.3c) solutions, with $D^{-q/3}$ coefficients, we get from const, $D^{-2/3}$, and D^{-1}

$$n_{01}=-(a_3/4j)A_3,\quad A_2=3A_3^2/8\rightarrow\overline{\theta_{35}}=-2j(a_5+\overline{f_1}/3)+3A_3^2/8, \tag{A9a}$$
$$3A_3^4/32-2A_1A_3+8A_0=0\rightarrow\overline{\theta_{35}}=\frac{A_3[3A_3^3/32-6a_5j^2]}{[2A_3\overline{f_1}-24ja_5]}.$$

Here $\overline{f_1}$ and j are arbitrary. From (A8) and (A9a) we get, A_3, a_5 (quadratic equation), and $\overline{\theta_{35}}$ and deduce successively a_j, θ_3/θ_5, A_k, and n_{01}. From $D^{-4/3}$ and $D^{-1/3}$ we get γ and n_1:

$$2\gamma/9j=(a_3/j)^3(A_3^3/16-A_1)=n_1^3. \tag{A9b}$$

We know the $N_1(\eta)$ solution (1.3)–(1.3c) and the other N_i with (3.2a).

d. Binary and ternary collisions for the Sec. III B models with $N_0\neq0$

We write the rhs of (3.10b) as a cubic $Z(N_1)$ polynomial with j, f_0, and f_1 defined in (3.2b)–(3.8):

$$b_0:=-d^*f_1+3(a_5+a_6)j/2,\quad c_0:=-d^*f_0+f_1(a_5+a_6),\quad d_0=f_0(a_5+a_6),$$
$$Z(N_1)=-3jd^*N_1^3/2+N_1^2(b_0+\theta_2j/2)+N_1(c_0+\theta_2+f_1/3)+d_0+\theta_2f_0/3, \tag{A10}$$

while the (3.10b) lhs is the product of the derivative by a first-order polynomial. For N_1 solutions of the (1.3a) and (1.3b) type, from D^{-q}, $q=0,1,2,3$, we successively get n_{01}, θ_2, n_1, and γ:

$$\sum_{q=0}^{2}A_qn_{01}^1=0,\quad e_0:=j(a_5+a_6)/2d^*+f_1/3,\quad A_0:=d_0e_0+d^*f_0^2/3,$$

$$A_1 := c_0 e_0 + 2 f_1 f_0 d^*/3 + j d_0/2, \quad A_2 := b_0 e_0 + d^*(j f_0 + f_1^2/3) + c_0 j/2,$$
$$\theta_2 = d^*[3 j n_{01}^2/2 + f_1 n_{01} + f_0]/[j n_{01}/2 + e_0], \tag{A11}$$
$$n_1 = \omega_2/3d^* - 2n_{01} - 2 f_1/3j, \quad \gamma = 3 j n_1/2.$$

With $N_1(\eta)$, from (3.2a) we get all other $N_i(\eta)$ densities and, from (3.10a), $N_0(\eta)$.

APPENDIX B: EXACT SOLUTIONS FOR MODELS WITH SIX INDEPENDENT DENSITIES

1. Scalar Riccati-type solutions for the Sec. IV B models

For stationary solutions we define the differential terms $l_i = e_i \partial_\eta N_i$, $e_i = \pm 1$ for $i = 1, 3, 5$, and $6, = \pm 3$ for N_7 and N_8, write the linear differential conservation laws

$$2d^*(l_1 \pm l_3) + l_5 \pm l_6 + (2 \mp 1)(l_7 \pm l_8) = 0,$$
$$10 d^*(l_1 + l_3) + l_5 + l_6 + 9(l_7 + l_8) = 0, \tag{B1a}$$

deduce l_3, l_6, and l_8 from l_1, l_5, and l_7, integrate, and get N_3, N_6, and N_8 from N_1, N_5, and N_7:

$$N_3 = 3N_1 + (N_5 + 9N_7)/d^* + a_3, \quad N_6 = -2d^* N_1 - 9N_7 + a_6,$$
$$N_8 = -[6N_7 + 2d^* N_1 + N_5]/3 + a_8. \tag{B1b}$$

We write the collision terms and the nonlinear equations for three densities N_1, N_5, and N_7:

$$X_1 = N_3 N_5 - N_1 N_6, \quad X_0 = N_7 N_6 - N_1^2, \quad X_{00} = N_8 N_5 - N_3^2,$$
$$\partial_\eta N_1 = X_0 + X_1, \quad \partial_\eta N_5 = -d^*(2X_1 + X_{00}), \quad 3\partial_\eta N_7 = -d^* X_0. \tag{B2}$$

We substitute (B1b) and get the 3×3 (4.6c) system for N_1, N_5, and N_7. For N_i of the (1.3a) and (1.3b) type, we define $\beta_{1j} = n_j/n_{1,j} = 5,7$, and from the coefficients of D^{-2} we obtain two polynomials of the (4.3b) type and we deduce a polynomial for β_{17}:

$$\beta_{15}\beta_{17}[3 + (\beta_{15} + 9\beta_{17})/d^*] - \beta_{17}^2[5d - 14 + 9\beta_{17}] - (2d^{*2}/3 - 3 + 2d)\beta_{17} - d^*/3 = 0,$$
$$d = 2{:}6075\beta_{17}^4 + 1140\beta_{17}^3 + 116\beta_{17}^2 + 40\beta_{17} - 3 = 0. \tag{B3}$$

As explained in Sec. IV A, n_{01} is a scaling parameter. We define $\lambda_k = a_k/n_{01}$, $\alpha_{1j} = n_{0j}/n_{01}, j = 5,7$, and get from the two constant relations of the N_1 and N_7 collision terms in (4.6c)

$$\lambda_6 = 9\alpha_{17} + 2d^* + 1/\alpha_{17}, \quad \lambda_3 = -3 - 9\alpha_{17} - \alpha_{15}/d^* + 1/\alpha_{17}\alpha_{15}. \tag{B4}$$

From the two D^{-1} relations for the N_1 and N_7 collision terms, substituting λ_6 and λ_3 given by (B4) we obtain a polynomial relation for α_{17}, α_{15}:

$$A\alpha_{15}^2 + B\alpha_{15} + C = 0, \quad A := -(\beta_{15} + 9\beta_{17})/d^* - 3, \quad C := -\beta_{15}/\alpha_{17},$$
$$B := \alpha_{17}[5d^* + 9\beta_{17} + 2d^{*2}/3\beta_{17}] + (4 - d - 3\beta_{17})/3\alpha_{17} + 2(2 - d) - 9\beta_{17} + 2d^*/\beta_{17}. \tag{B5}$$

We start with α_{17} as an arbitrary parameter, we deduce α_{17}, λ_6, and λ_8 from (B5) and (B4), and we see from (4.6c) that a_8 or λ_8 enters only in the collision term for N_5 and linearly in the coefficient of D^{-1}. From the two D^{-1} relations for N_1 and N_5 we deduce λ_8 as a function of α_{17}.

Substituting all parameters deduced from α_{17} into the constant term of the (4.6c) N_5 equation fixes α_{17} and all other values except the scaling parameter n_{01} and λ in $D(\eta)$ of (1.3a). Finally we write the mass and the internal energy at the wall $\eta=-\frac{1}{2}$:

$$M_{w,-}=4d^*N_{1,-}+2N_{5,-}+2N_{7,-},$$
$$E_{wI-}=(20d^*N_{1,-}+2N_{5,-}+18N_{7,-})/M_{w,-}, \tag{B6}$$

while at $\eta=\frac{1}{2}$ we get $M_{w,+}$, E_{wI+} with the substitution of $N_{3,+}$, $N_{6,+}$, $N_{8,+}$ to $N_{1,-}$, $N_{5,-}$, $N_{7,-}$. The hot and cold interfaces are still defined by (3.6). With (B1b) we write the mass M and the energy E in terms of N_1, N_5, N_7:

$$M(\eta)=8(2d^*N_1+N_5+3N_7)/3+2d^*a_3+a_6+a_8,$$
$$2E(\eta)=8(4d^*N_1+N_5+9N_7)+10d^*a_3+a_6+9a_8, \tag{B7}$$
$$N_{i,-}=N_{i,+}, \quad i=1,5,7\rightarrow M^-=M^+, \quad E^-=E^+\rightarrow\tau^-=\tau^+.$$

2. Scalar Riccati-type solutions for the Sec. IV C models

For stationary solutions we define the linear differential terms $l_i=e_i\partial_\eta N_i$, $e_i=\pm1$ for $i=1,5,3,7$, $e_i=\pm3$ for N_9, N_{10}. We write the linear differential conservation laws:

$$2d^*(l_1\pm l_3+l_5\pm l_7)+(2\mp1)(l_9\pm l_{10})=0,$$
$$6d^*(3(l_1+l_3)+l_5+l_7)+9(l_9+l_{10})=0, \tag{B8a}$$

We deduce l_3, l_7, and l_{10} from l_1, l_5, and l_9, we integrate, and we get N_3, N_7, and N_{10} from N_1, N_5, and N_9:

$$N_7=N_5+a_7, \quad N_3=2N_1+N_5+9N_9/2d^*+a_3,$$
$$N_{10}=-2d^*(N_1+N_5)/3-2N_9+a_{10}. \tag{B8b}$$

We write the collision terms and the equations for three densities N_1, N_5, and N_9:

$$X_1=N_9N_{10}-N_1N_3, \quad X_2=N_3N_5-N_1N_7,$$
$$X_3=N_3N_7-N_5N_{10}, \quad X_4=N_1N_5-N_9N_7, \tag{B9}$$
$$\partial_\eta N_1=X_1+X_2-X_3, \quad \partial_\eta N_5=-X_2+X_3-X_4, \quad 3\partial_\eta N_9=2d^*(-X_1+X_3).$$

We substitute (B8b) and get the 3×3 (4.8c) equation for N_1, N_5, and N_9. For N_i of the (1.2a) and (1.2b) type with $D=1+\lambda e^{\gamma\eta}$. We define $\beta_{1j}=n_j/n_{1,j}=5,9$, and, from the coefficients of D^{-2}, we obtain two polynomials of the (4.3) type:

$$d=2,3:3(12d-47)\beta_{19}^2+19(2d+1)\beta_{19}+12(9d-13)=0,$$
$$\beta_{15}(8\beta_{19}/3-4d^*)=(4d-13)\beta_{19}^2+(6d+13)\beta_{19}/3+4d^*; \tag{B10}$$

n_{01} is still a scaling parameter. We define $\lambda_k=a_k/n_{01}$, $\alpha_{1j}=n_{0j}/n_{01}$, $j=5,9$, and from the two constant relations of the N_1 and N_9 collision terms in (4.8c) we get

$$\lambda_3=-\alpha_{15}-1-9\alpha_{19}/2d^*+\lambda_7/\alpha_{15}, \tag{B11}$$

$$\lambda_{10}=(1+\alpha_{15})/\alpha_{19}+2\alpha_{19}+\alpha_{15}(2d-5)/3+\lambda_7(1/\alpha_{15}\alpha_{19}-1).$$

From the three D^{-1} relations for the N_1, N_5, and N_9 collision terms, substituting λ_3 and λ_{10} we obtain two rational fractions of polynomials P_j, Q_j, with α_{19}-dependent coefficients,

$$\lambda_7/\alpha_{19}=P_1(\alpha_{15})/Q_1(\alpha_{15})=S_1(\alpha_{15})/T_1(\alpha_{15}), \tag{B12}$$

linear in α_{15}. *We start with* α_{19} *arbitrary*, we deduce α_{15}, λ_7, λ_3, λ_{10} from (B12) and (B11), all parameters substituted into the constant term of (4.8c) for N_5 fixed α_{19} and all parameters except n_{01}, and λ in $D(\eta)$. Finally we write $M_{w,-}$, E_{wI-} and $M(\eta), E(\eta)$ with (B8b):

$$M_{w,-}=4d^*(N_{1,-}+N_{5,-})+2N_{9,-},$$

$$E_{wI-}=(4d^*(9N_{1,-}+3N_{5,-})+18N_{9,-})/M_{w,-},$$

$$M(\eta)=16d^*(N_1+N_5)/3+8N_9+2d^*(a_3+a_7)+a_{10}, \tag{B13}$$

$$E(\eta)=12d^*(2N_1+N_5)+36N_9+3d^*(3a_3+a_7)+9a_{10}/2,$$

$$N_{i,-}=N_{i,+}, \quad i=1,5,9\rightarrow M^-=M^+, \quad E^-=E^+\rightarrow\tau^-=\tau^+,$$

while we get $M_{w,+}, E_{wI+}$ with the substitution of $N_{3,+}$, $N_{6,+}$, $N_{10,+}$ to $N_{1,-}$, $N_{5,-}$, $N_{9,-}$.

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Extension of Giacomini's results concerning invariants for one-dimensional time-dependent potentials

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One-dimensional time-dependent potentials are considered for which an invariant can be expressed in terms of the potential and the momentum according to the formulation of Giacomini. New solutions of Giacomini's equations are derived. In addition, possibilities are discussed for extending Giacomini's approach to more general systems. © *1996 American Institute of Physics.*
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I. INTRODUCTION

Giacomini[1] has presented a formalism for examining Hamiltonian systems in which a one-dimensional potential admits an invariant that can be expressed solely as a function of the potential and the momentum, and he derived some solutions of the associated equations. In Sec. II, we summarize Giacomini's formalism and derive some additional solutions of his equations. In Sec. III, we explore the possibility of extending Giacomini's approach to cases where the invariant cannot be expressed solely as a function of a potential and the momentum. The starting point for that discussion is the work of Lewis *et al.*,[2] who deduced all one-degree-of-freedom Hamiltonians $H(q,p,t)$ for which a specified function of (q,p,t) is an invariant. Certain differential identities that are used in Sec. III are given in the Appendix.

The one-degree-of-freedom Hamiltonian $H(q,p,t)$ under consideration is that associated with a one-dimensional potential $V(q,t)$,

$$H(q,p,t)=\tfrac{1}{2}p^2+V(q,t). \tag{1.1}$$

An invariant for this system is any function $I(q,p,t)$ whose total time derivative vanishes:

$$0=\frac{dI}{dt}=I_t(q,p,t)+[I,\,H]=I_t(q,p,t)+I_q p-I_p V_q\,, \tag{1.2}$$

where $[I,\,H]$ is the Poisson bracket of I with H. Potentials for which (1.2) can be solved analytically to give an invariant are usually identified by invoking some symmetry of the system, or by using a direct method, in which some functional restriction of the potential or the invariant is postulated. For example, it may be possible to apply Noether's theorem,[3–5] or to apply the theory of extended Lie groups.[6] Examples of the use of direct methods can be found in Refs. 7–11.

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II. NEW SOLUTIONS OF GIACOMINI'S FORMALISM

Giacomini[1] has developed a theoretical framework that defines exact invariants for a certain class of one-dimensional time-dependent potentials and he used the relevant equations to determine examples of such potentials. Giacomini's result begins with the ansatz that the invariant is expressible as a function of two arguments, $V(q,t)$ and p:

$$I(q,p,t)\rightarrow I[V(q,t),p]=I(v,p) \quad \{v=V(q,t)\}. \tag{2.1}$$

Then (1.2) can be written as

$$\left[\frac{V_t(q,t)}{V_q(q,t)}+p\right]I_v[V(q,t),p]-I_p[V(q,t),p]=0. \tag{2.2}$$

In order for (2.2) to have a solution, $V(q,t)$ must satisfy

$$V_t(q,t)=f[V]V_q(q,t), \tag{2.3}$$

where f is an arbitrary function. The implicit solution of (2.3) is

$$\Phi[V]-t-\frac{q}{f[V]}=0, \tag{2.4}$$

where also Φ is an arbitrary function. As a result, the equation for $I(v,p)$ is

$$[f(v)+p]I_v(v,p)-I_p(v,p)=0, \tag{2.5}$$

whose characteristic equation is

$$\frac{dv}{dp}+f(v)+p=0. \tag{2.6}$$

Giacomini treated the case

$$f(v)=a_1v^2+a_2v+a_3, \tag{2.7}$$

where (a_1,a_2,a_3) are arbitrary constants, analytically in terms of Airy functions.

New solutions of Giacomini's relations (2.5) and (2.6) can be obtained by defining a function $X(v)$ as

$$X(v)=\frac{1}{p+f(v)}, \tag{2.8}$$

where p is to be interpreted as a function of v along a characteristic of (2.5) that is determined by solving (2.6). By differentiating (2.8) with respect to v and using (2.6) we find that $X(v)$ satisfies the Abel equation of the first kind[12]

$$\frac{dX}{dv}=X^3-\frac{df}{dv}X^2. \tag{2.9}$$

By means of the transformation from $X(v)$ to $U(v)$ defined by[12]

$$U(v)=\frac{[X(v)-X_2(v)]}{[X_1(v)]^{1/3}}, \tag{2.10}$$

where

$$X_1(v)=-\frac{1}{3}\frac{d^2f}{dv^2}-\frac{2}{27}\left(\frac{df}{dv}\right)^3, \quad X_2(v)=\frac{1}{3}\frac{df}{dv}, \tag{2.11}$$

(2.9) is transformed to

$$\frac{dU}{dv}=X_1{}^{2/3}\left[1-\left(3X_1{}^{-2/3}X_2^2+\frac{1}{3}X_1{}^{-5/3}\frac{dX_1}{dv}\right)U+U^3\right]. \tag{2.12}$$

We shall use (2.12) for finding solutions to the characteristic equation (2.6).

Equation (2.12) can be solved analytically if it is separable. In order for it to be separable, the coefficient of U must be a constant, which we denote by K. This gives the following condition on $f(v)$:

$$\left[9\frac{d^3f}{dv^3}+15\frac{d^2f}{dv^2}\left(\frac{df}{dv}\right)^2+2\left(\frac{df}{dv}\right)^5\right]^3=\left(\frac{K}{3}\right)^3\left[9\frac{d^2f}{dv^2}+2\left(\frac{df}{dv}\right)^3\right]^5. \tag{2.13}$$

We have found three values of K for which (2.13) can be solved in terms of implicit relations that do not involve integrals; these values are $K=3/2^{2/3}$, $K=3(A^2-6)/[2A(A^2-9)]^{2/3}$ ($A=$const $\neq\pm3$, $\neq0$, $\neq\sqrt{6}$), and $K=0$. In addition, a general partial treatment of (2.13) can be given in terms of implicit relations that involve an indefinite integral. [It has been pointed out by the referee of this paper that (2.13) is formally integrable for all values of K because (2.13) has three Lie point symmetries.]

A. $K=3/2^{2/3}$

This choice of K leads to

$$f(v)=a_2v+a_3, \tag{2.14}$$

where a_2 and a_3 are arbitrary constants. This is a case analyzed by Giacomini (Giacomini's form with $a_1=0$).[1] For $f(v)=a_1v^2+a_2v+a_3$, which is the most general form for which Giacomini solved his equations, (2.13) cannot be satisfied if $a_1\neq0$. This is associated with the fact that (2.6) can only be solved with Airy functions in this case, but Airy functions do not solve $dU/dV=[X_1(V)]^{2/3}(1-KU+U^3)$.

B. $K=3(A^2-6)/[2A(A^2-9)]^{2/3}$, $A=$const$\neq\pm3$

In this case, we find

$$f(v)=A\sqrt{v}. \tag{2.15}$$

It is interesting to note that one is also led to (2.15) by considering the Lie invariance properties of (2.6).[13] The invariant associated with (2.15) is given by

$$I[V(q,t),\,p]=\ln(2V+p^2+A\sqrt{V}p)-A\int^{\sqrt{V}/p}\frac{dy}{(2y^2+Ay+1)} \tag{2.16}$$

and, from (2.4), the potential is determined from

$$\Phi[V]-t-\frac{q}{A\sqrt{V}}=0. \tag{2.17}$$

It is instructive to examine the special case $A=0$. Then $f(v)=0$, (2.3) implies $V(q,t)$ is a function of q only, and (2.16) reduces to $I[V(q,t),\ p]=\ln(2V+p^2)$. Thus, the energy is conserved, as expected.

C. $K=0$

With this choice, (2.13) reduces to

$$9\frac{d^3f}{dv^3}+15\frac{d^2f}{dv^2}\left(\frac{df}{dv}\right)^2+2\left(\frac{df}{dv}\right)^5=0. \tag{2.18}$$

This equation can be integrated completely in terms of three arbitrary constants as follows. Because (2.18) is autonomous and depends only on the derivatives of f, we introduce

$$W=\frac{d^2f}{dv^2} \tag{2.19}$$

and

$$F=\frac{df}{dv}, \tag{2.20}$$

in which case (2.18) is transformed into the first-order differential equation

$$9W\frac{dW}{dF}+15WF^2+2F^5=0. \tag{2.21}$$

This equation can be integrated by changing variable to

$$Z=W/F^3. \tag{2.22}$$

The result is

$$|Z+\tfrac{2}{9}|^{-2}|Z+\tfrac{1}{3}|^3|F|^3=C_1, \tag{2.23}$$

where C_1 is an arbitrary positive constant. Moreover, since by construction we have $W=dF/dv$, we also have $Z=(dF/dv)/F^3$, which can be written in the form

$$dv=\frac{1}{F^3}\frac{dF}{dZ}\frac{dZ}{Z}. \tag{2.24}$$

Using $dF/dZ=-FZ/[3(Z+2/9)(Z+1/3)]$, which is obtained from (2.21) and (2.22), and $|F|=C_1^{1/3}|Z+2/9|^{2/3}/|Z+1/3|$, which is obtained from (2.23), (2.24) becomes

$$dv=-\frac{\varepsilon_1}{3C_1^{2/3}}\frac{(Z+\frac{1}{3})}{|Z+\frac{2}{9}|^{7/3}}\,dZ, \tag{2.25}$$

where ε_1 is the sign of $(Z+\frac{2}{9})$. This relation, which is valid for $C_1\neq 0$, can be integrated to yield

$$v+C_2=C_1^{-2/3}[\varepsilon_1|Z+\tfrac{2}{9}|^{-1/3}+\tfrac{1}{36}|Z+\tfrac{2}{9}|^{-4/3}], \tag{2.26}$$

where C_2 is a constant of integration. Using (2.20), (2.25), and the expression for F in terms of Z, we can obtain

$$df = -\frac{\epsilon_1\epsilon_2\epsilon_3}{3C_1^{1/3}}\frac{dZ}{|Z+\frac{2}{9}|^{5/3}}, \tag{2.27}$$

where ϵ_2 and ϵ_3 are, respectively, the signs of $Z+\frac{1}{3}$ and F. This can be integrated to give f as a function of Z:

$$f + C_3 = \frac{\epsilon_2\epsilon_3}{2C_1^{1/3}}|Z+\tfrac{2}{9}|^{-2/3}, \tag{2.28}$$

where C_3 is a constant of integration.

It is now possible to derive the relation between the function f and the potential V for $K=0$. Combining (2.26) and (2.28), and substituting $v=V(q,t)$ from (2.1), an easy calculation yields

$$V(q,t)+C_2=\epsilon_1\sqrt{2/C_1}\sqrt{\epsilon_2\epsilon_3(f(V)+C_3)}+(f(V)+C_3)^2/9, \quad C_1\neq 0. \tag{2.29}$$

$C_1=0$ and $C_1=\infty$ are interesting special cases. For $C_1=0$, we use (2.23) to get $-\frac{1}{3}=Z=(dF/dv)/F^3$, which can be integrated to give $f(v)=[6(v+k_1)]^{1/2}+k_2$, where k_1 and k_2 are arbitrary constants. If $k_1=k_2=0$, this corresponds to (2.15) of Case B with $A=\sqrt{6}$. For $C_1=\infty$, we may use (2.29) to obtain $f(v)=[3(v+C_2)]^{1/2}-C_3$. If $C_2=C_3=0$, this corresponds to (2.15) with $A=3$, which was excluded in our discussion of Case B.

For $K\equiv 3X_1^{-2/3}X_2^2+(1/3)X_1^{-5/3}(dX_1/dv)=0$, (2.12) can be integrated and the constant of integration equals the invariant that we seek:

$$I[v,p]=\int^U \frac{dU'}{1+U'^3}-\int^v [X_1(v')]^{2/3}\,dv'. \tag{2.30}$$

Here U as defined by (2.10) depends on v; it also depends parametrically on the constant that labels the characteristic. The constant can be expressed as a function of v and p, so that U can in fact be expressed directly in terms of v and p. The result, which can be found by combining (2.8) and (2.10), we denote by $U(v,p)$:

$$U(v,p)=\frac{1-[p+f(v)]X_2(v)}{[p+f(v)][X_1(v)]^{1/3}}. \tag{2.31}$$

Thus, the formula for the invariant in terms of (q,p,t) is

$$I[V(q,t),p]=\int^{U[V(q,t)p]}\frac{dU'}{1+U'^3}-\int^{V(q,t)}[X_1(v')]^{2/3}\,dv'. \tag{2.32}$$

Carrying out the integrations in (2.32) is a lengthy calculation. The result is

$$\begin{aligned} I[V(q,t),p]=\frac{1}{6}&\left\{\ln\left[\frac{(1+U[V(q,t),p])^3}{1+U[V(q,t),p]^3}\right]+\epsilon_2\ln\left[\frac{(1+|f[V(q,t)]+C_3|)^3}{1+|f[V(q,t)]+C_3|^3}\right]\right\}\\ &+\frac{1}{\sqrt{3}}\left[\arctan\left(\frac{2U[V(q,t),p]-1}{\sqrt{3}}\right)+\epsilon_2\arctan\left(\frac{2|f[V(q,t)]+C_3|-1}{\sqrt{3}}\right)\right]. \end{aligned} \tag{2.33}$$

The constants ϵ_1 and ϵ_3 do not appear in this formula because, in the derivation, certain quantities occur raised to fractional powers. In order for those quantities to be positive, ϵ_1 and ϵ_3 are required to have the values $\epsilon_1=1$ and $\epsilon_3=-1$.

D. General treatment of Eq. (2.13)

Introduce functions W and F as in (2.19) and (2.20) so that (2.13) becomes

$$\left(9W\frac{dW}{dF}+15WF^2+2F^5\right)^3=\left(\frac{K}{3}\right)^3(9W+2F^3)^5. \tag{2.34}$$

Then, with Z as defined by (2.22), this can be transformed to

$$9FZ\frac{dZ}{dF}+27Z^2+15Z+2=\frac{K}{3}(9Z+2)^{5/3}, \tag{2.35}$$

$$\frac{9ZdZ}{27Z^2+15Z+2-\frac{K}{3}(9Z+2)^{5/3}}=-\frac{dF}{F}. \tag{2.36}$$

Defining Y by

$$Y=(9Z+2)^{1/3}\Rightarrow dY=3Y^{-2}dZ, \tag{2.37}$$

we can write (2.36) as

$$\frac{(Y^3-2)dY}{Y(Y^3-KY^2+1)}=-\frac{dF}{F}, \tag{2.38}$$

which can be integrated to give

$$\ln(F^4|Y^4-KY^3+Y|)+\int\frac{3KY^2+1}{Y^4-KY^3+Y}\,dY=0. \tag{2.39}$$

From this relation F can be obtained as a function of Y and then of Z. Equation (2.22) gives the relation between F and W, which leads to an equation relating d^2f/dv^2 and df/dv. This equation can be solved in principle to give $f(v)$.

III. AN APPROACH FOR EXTENDING GIACOMINI'S ANSATZ

Attempts to generalize ansatz (2.1), which is the basis of Giacomini's formalism, have not led to equations from which new invariant/potential pairs have been derived. In this section we generalize Giacomini's formalism within the context of the theoretical framework of Lewis *et al.*[2] Although this generalization has not led to new invariant/potential pairs, it is sufficiently general to hold the promise of new results.

A. The result of Lewis *et al.*

Lewis *et al.*[2] showed that all Hamiltonians $H(q,p,t)$ for which a specified function $\tilde{P}(q,p,t)$ is an invariant are given by

$$H(q,p,t)=K(t)-F_t[\tilde{P}(q,p,t),t]-\int^q G_t[q',\tilde{P}(q,p,t),t]dq', \tag{3.1}$$

where $G(q,P,t)$ is the inverse of $\tilde{P}(q,p,t)$,

$$p=G(q,P,t)\leftrightarrow P=\tilde{P}(q,p,t), \tag{3.2}$$

and where $F(P,t)$ and $K(t)$ are arbitrary functions. For a given $H(q,p,t)$, the function $F(P,t)$ can be determined and a canonically conjugate second invariant can be constructed.[14] We note in passing that (3.1) is related to the Hamilton–Jacobi equation through a Type-Two generating function $S(q,P,t)$ for a canonical transformation that is defined by

$$S(q,P,t)=\int^{q} G(q',P,t)dq'+F(P,t)-\int^{t} K(t')dt', \tag{3.3}$$

with $p=S_q(q,P,t)$ and $Q=S_P(q,P,t)$. From (3.3), $G(q,P,t)$ and $S(q,P,t)$ are related by

$$G(q,P,t)=S_q(q,P,t). \tag{3.4}$$

As a result, (3.1) can be written in terms of (q,P,t) as

$$H[q,S_q(q,P,t),t]+S_t(q,P,t)=0, \tag{3.5}$$

which is the Hamilton–Jacobi equation. In the remainder of this paper we shall not use the generating function $S(q,P,t)$.

Equation (3.1) written in terms of the variables (q,P,t) and the function $G(q,P,t)$ is

$$H[q,G(q,P,t),t]=K(t)-F_t(P,t)-\int^{q} G_t(q',P,t)dq'. \tag{3.6}$$

Differentiating (3.6) with respect to q gives

$$H_q[q,G(q,P,t),t]+H_p[q,G(q,P,t),t]G_q(q,P,t)=-G_t(q,P,t), \tag{3.7}$$

where $H_q(q,p,t)$ and $H_p(q,p,t)$ are the derivatives with respect to q and p of $H(q,p,t)$. We now specialize to the case of motion in a time-dependent potential $V(q,t)$,

$$H(q,p,t)=\tfrac{1}{2}p^2+V(q,t). \tag{3.8}$$

Then (3.7) becomes

$$G_t(q,P,t)+G(q,P,t)G_q(q,P,t)=-V_q(q,t), \tag{3.9}$$

which determines the functions $G(q,P,t)$ that are allowable for a given potential $V(q,t)$. If we associate $G(q,P,t)$ with the momentum density as a function of (q,t) of a fluid of particles acted upon by a force density $-V_q(q,t)$, then (3.9) is the equation of motion of that fluid.

Giacomini's ansatz (2.1) is equivalent to demanding that $G(q,P,t)$ be expressible in terms of a function G of two arguments, where the two arguments are $V(q,t)$ and P:

$$G(q,P,t)=\overline{G}[V(q,t),P]. \tag{3.10}$$

Our objective is to explore the consequences of generalizing (3.10) to allow the two arguments to be arbitrary functions of (q,P,t). That is, we assume that $G(q,P,t)$ can be written as

$$G(q,P,t)=\overline{G}(x,y)=\overline{G}[f(q,P,t),h(q,P,t)], \tag{3.11}$$

where the variables x and y are defined in terms of arbitrary functions $f(q,P,t)$ and $h(q,P,t)$ by

$$x=f(q,P,t), \quad y=h(q,P,t). \tag{3.12}$$

The idea is to restrict $f(q,P,t)$ and $h(q,P,t)$ in such a way as to facilitate finding functions $G(q,P,t)$ that solve (3.9) for some new potentials $V(q,t)$. In Sec. III C we shall demonstrate that

Giacomini's equations can be derived easily by choosing $h(q,P,t)=P$ and taking $f(q,P,t)$ to be an arbitrary function of (q,t). With the ansatz (3.11),(3.9) can be written as

$$\overline{G_x}(x,y)f_t(q,P,t)+\overline{G_y}(x,y)h_t(q,P,t)+\overline{G}(x,y)[\overline{G_x}(x,y)f_q(q,P,t)+\overline{G_y}(x,y)h_q(q,P,t)] = -V_q(q,t). \tag{3.13}$$

Equation (3.13) is a very general equation that can be arbitrarily nonlinear. If we were to specify $G(x,y)$, which is a function of only two arguments, then there generally would be solutions, because $f(q,P,t)$ and $h(q,P,t)$ are unspecified functions of three arguments. However, viewed in that way, the equations are too complicated and general to be amenable to analysis. The approach that we adopt is to view (3.13) as an equation for $G(x,y)$. Because $G(x,y)$ is a function of only two arguments, this imposes consistency conditions on $V_q(q,t)$ and on the coefficients of $G(x,y)$ and its derivatives. In the remainder of this paper we examine (3.13) as an equation for $G(x,y)$.

B. Consistency conditions

The derivatives of (3.13) with respect to q, P, and t involve $\overline{G}(x,y)$ and the derivatives of $\overline{G}(x,y)$ with respect to x and y. Thus, (3.13) and the derivatives of (3.13) up to some order with respect to q, P, and t may be viewed as a system of algebraic equations for $G(x,y)$ and those derivatives of $G(x,y)$ that appear up to that order. Equation (3.13) involves three functions of (x,y) [i.e., $G(x,y)$ and its first derivatives]. The four equations comprising (3.13) and its three first derivatives involve six functions of (x,y) [i.e., $G(x,y)$ and its first and second derivatives]. The ten equations comprising (3.13) and its first and second derivatives involve ten functions of (x,y) [i.e., $G(x,y)$ and its first, second, and third derivatives]. The twenty equations comprising (3.13) and its first, second and third derivatives involve 15 functions of (x,y) [i.e., $G(x,y)$ and its first, second, third, and fourth derivatives]. The ten equations comprising (3.13) and its first and second derivatives are unique in that there are exactly the same number of functions of (x,y) as there are equations. Thus, one might consider solving that algebraic system of ten equations for $G(x,y)$ and its first, second, and third derivatives. One would then have the consistency conditions that the algebraically obtained solutions for $G(x,y)$ and its first, second, and third derivatives [in terms of $f(q,P,t),h(q,P,t),V(q,t)$ and their derivatives] would need to satisfy in order to be consistent with one another. For example, if the algebraic solutions for $G(x,y)$ and its first derivatives were given by

$$\overline{G}[f(q,P,t),h(q,P,t)]=\Lambda^{(0)}(q,P,t), \tag{3.14}$$

$$\overline{G_x}[f(q,P,t),h(q,P,t)]=\Lambda^{(1)}(q,P,t), \tag{3.15}$$

$$\overline{G_y}[f(q,P,t),h(q,P,t)]=\Lambda^{(2)}(q,P,t), \tag{3.16}$$

where $\Lambda^{(0)}(q,P,t)$, $\Lambda^{(1)}(q,P,t)$, and $\Lambda^{(2)}(q,P,t)$ were defined as explicit functions of $f(q,P,t),h(q,P,t),V(q,t)$, and their derivatives, then the relation

$$\Lambda^{(0)}_q(q,P,t)=\Lambda^{(1)}(q,P,t)f_q(q,P,t)+\Lambda^{(2)}(q,P,t)h_q(q,P,t) \tag{3.17}$$

would need to hold. Similarly for the P and t derivatives.

Two salient facts are encountered in an attempt to solve the ten equations for $\overline{G}(x,y)$ and its first, second, and third derivatives. First, there is a subsidiary consistency condition that must be satisfied by the three first derivatives of (3.13) in order that they be soluble for the second derivatives of $\overline{G}(x,y)$. Second, proceeding beyond that condition leads to extremely complex equations. We shall not proceed beyond that condition here.

The derivatives of (3.13) with respect to q, P, and t can be viewed as a system of three linear equations for the three second derivatives of $G(x,y)$. In matrix form they are

$$A\begin{pmatrix} \overline{G_{xx}} \\ \overline{G_{xy}} \\ \overline{G_{yy}} \end{pmatrix} = \beta, \tag{3.18}$$

where

$$A = \begin{pmatrix} f_q(f_t+\overline{Gf}_q) & [h_q(f_t+\overline{Gf}_q)+f_q(h_t+\overline{Gh}_q)] & h_q(h_t+\overline{Gh}_q) \\ f_P(f_t+\overline{Gf}_q) & [h_P(f_t+\overline{Gf}_q)+f_P(h_t+\overline{Gh}_q)] & h_P(h_t+\overline{Gh}_q) \\ f_t(f_t+\overline{Gf}_q) & [h_t(f_t+\overline{Gf}_q)+f_t(h_t+\overline{Gh}_q)] & h_t(h_t+\overline{Gh}_q) \end{pmatrix}, \tag{3.19}$$

$$\beta = \begin{pmatrix} -\overline{G_x(f_t+\overline{Gf}_q)_q}-\overline{G_y(h_t+\overline{Gh}_q)_q}-V_{qq} \\ -\overline{G_x(f_t+\overline{Gf}_q)_P}-\overline{G_y(h_t+\overline{Gh}_q)_P} \\ -\overline{G_x(f_t+\overline{Gf}_q)_t}-\overline{G_y(h_t+\overline{Gh}_q)_t}-V_{qt} \end{pmatrix}. \tag{3.20}$$

The matrix A is singular, corresponding to a null vector n of its transpose:

$$\tilde{A}n=0, \quad n=\begin{pmatrix} f_th_P-f_Ph_t \\ -f_th_q+f_qh_t \\ -f_qh_P+f_Ph_q \end{pmatrix}. \tag{3.21}$$

The subsidiary consistency condition for (3.18) is

$$\tilde{n}\beta=0. \tag{3.22}$$

The meaning of this condition can be understood clearly by transforming variables from (q,P,t) to (x,y,t), where x and y are defined by (3.12). Denote the inverse transformation by

$$q=r(x,y,t), \quad P=s(x,y,t). \tag{3.23}$$

Derivatives of $f(q,P,t)$ and $h(q,P,t)$ are related to derivatives of $r(x,y,t)$ and $s(x,y,t)$ by the derivatives of the identities

$$x\equiv f[r(x,y,t),s(x,y,t),t], \quad y\equiv h[r(x,y,t),s(x,y,t),t]. \tag{3.24}$$

Those relations are presented in the Appendix.

Completely in terms of (x,y,t), we can express (3.13) as

$$\overline{G_x}[(r_ys_t-r_ts_y)+s_y\overline{G}]-\overline{G_y}[(r_xs_t-r_ts_x)+s_x\overline{G}]=(r_ys_x-r_xs_y)V_q[r(x,y,t),t]. \tag{3.25}$$

Since $\overline{G}(x,y)$ is not a function of t, the derivative of (3.25) with respect to t is

$$\overline{G_x}[(r_ys_t-r_ts_y)_t+s_{yt}\overline{G}]-\overline{G_y}[(r_xs_t-r_ts_x)_t+s_{xt}\overline{G}]=\{(r_ys_x-r_xs_y)V_q[r(x,y,t),t]\}_t. \tag{3.26}$$

The consistency condition (3.22) is the same as the condition obtained by subtracting the product of $(r_ys_x-r_xs_y)_t$ with (3.25) from the product of $(r_ys_x-r_xs_y)$ with (3.26).

If we view (3.25) and (3.26) as equations for $\overline{G}(x,y)$ given $r(x,y,t)$, $s(x,y,t)$, and $V[r(x,y,t),t]$, three approaches come to mind for performing an analysis. None of them has proven fruitful. The first approach is to eliminate $G(x,y)$ algebraically from (3.25) and (3.26).

Note that the case $(s_y\overline{G_x}-s_x\overline{G_y})=0$ is not of interest. This is because that case would imply $s(x,y,t)=$[function of $G(x,y)$ and t], so that $G(x,y)$ could be expressed as a function of $s(x,y,t)$ and t; in that event, the invariant $\widetilde{P}(q,p,t)$ would have to be a function of p and t alone. The result for $(s_yG_x-s_xG_y)\neq 0$ can be written as

$$\frac{\partial}{\partial t}\left\{\frac{[(r_ys_t-r_ts_y)\overline{G_x}-(r_xs_t-r_ts_x)\overline{G_y}]}{(s_y\overline{G_x}-s_x\overline{G_y})}\right\}=\frac{\partial}{\partial t}\left\{\frac{[(r_ys_x-r_xs_y)V_q]}{(s_y\overline{G_x}-s_x\overline{G_y})}\right\}, \tag{3.27}$$

which can be immediately integrated to give

$$A(x,y)(s_y\overline{G_x}-s_x\overline{G_y})+[(r_ys_t-r_ts_y)\overline{G_x}-(r_xs_t-r_ts_x)\overline{G_y}]=[(r_ys_x-r_xs_y)V_q], \tag{3.28}$$

where $A(x,y)$ is arbitrary. However, comparison with (3.25) shows that

$$A(x,y)=\overline{G}(x,y), \tag{3.29}$$

so that (3.28) is really the same as (3.25).

The second approach is to solve (3.25) and (3.26) algebraically for $\overline{G_x}(x,y)$ and $\overline{G_y}(x,y)$ and then impose the compatibility condition that the cross derivatives must be equal:

$$\overline{G_{xy}}(x,y)=\overline{G_{yx}}(x,y). \tag{3.30}$$

This condition is very complicated and will not be pursued further.

The third approach is to construct a linear combination of (3.25) and (3.26) which does not contain the nonlinear products $G(x,y)G_x(x,y)$ and $G(x,y)G_y(x,y)$. This requires

$$0=s_xs_{yt}-s_ys_{xt}\Rightarrow\frac{\partial}{\partial t}\left(\frac{s_x}{s_y}\right)=0\Rightarrow s(x,y,t)=s_0[u(x,y),t], \tag{3.31}$$

where $s_0[z,t]$ and $u(x,y)$ are arbitrary functions. The linear combination of (3.25) and (3.26) is a linear differential equation that can be solved formally. With that solution, (3.25) can be reduced to another formally soluble linear differential equation. Unfortunately, the formal solutions of the linear differential equations involve arbitrary functions whose occurrence prevents practical use of the formal solutions.

C. A different approach in (x,y,t) space

Let us view (3.25) as an equation for $s(x,y,t)$ given $r(x,y,t)$, $\overline{G}(x,y)$, and $V_q(q,t)$. In that case, it is appropriate to write (3.25) in the form

$$(r_y\overline{G_x}-r_x\overline{G_y})s_t-\{r_yV_q[r(x,y,t),t]-r_t\overline{G_y}+\overline{GG_y}\}s_x+\{r_xV_q[r(x,y,t),t]-r_t\overline{G_x}+\overline{GG_x}\}s_y=0. \tag{3.32}$$

We can recover Giacomini's equations from (3.32) as follows. Assume

$$f(q,P,t)=A(q,t),\quad h(q,P,t)=P, \tag{3.33}$$

which implies that the inverse functions can be written as

$$r(x,y,t)=B(x,t),\quad s(x,y,t)=y. \tag{3.34}$$

Then (3.32) reduces to

$$B_xV_q[B(x,t),t]-B_t\overline{G_x}+\overline{GG_x}=0. \tag{3.35}$$

Differentiation with respect to x gives

$$B_t\overline{G_{xy}}=(\overline{GG_x})_y, \tag{3.36}$$

which implies that $B_t(x,t)$ is a function of x alone:

$$B_t(x,t)=-f(x)\Rightarrow\frac{A_t(q,t)}{A_q(q,t)}=f[A]. \tag{3.37}$$

Applying (3.37) to (3.35) shows that $B_xV_q[B(x,t),t]$ is a function of x alone:

$$\frac{V_q}{A_q}=S'[A(q,t)]\Rightarrow V(q,t)=S[A(q,t)]+\alpha(t), \tag{3.38}$$

where S and α are arbitrary. Without loss of generality, we can take $S(A)=A$ and $\alpha=0$. Then, (3.37) becomes

$$V_t=f(V)V_q, \tag{3.39}$$

which is identical to (2.3). Finally, (3.5) can now be written as

$$1+f(x)\overline{G_x}+\overline{GG_x}=0. \tag{3.40}$$

Equations (3.39) and (3.40) constitute Giacomini's result expressed in terms of (x,y,t). Giacomini expressed (3.40) in terms of an invariant function $I[V(q,t),p]$. Here $I(x,p)$ is the inverse of $G(x,y)$:

$$p=\overline{G}(x,y)\leftrightarrow y=I(x,p). \tag{3.41}$$

Differentiation of the identity

$$y\equiv I[x,\overline{G}(x,y)] \tag{3.42}$$

with respect to x yields

$$\overline{G_x}=-\frac{I_x}{I_p}. \tag{3.43}$$

Combining this with (3.11) gives

$$[f(x)+p]I_x-I_p=0, \tag{3.44}$$

which is the actual equation derived by Giacomini.

In order to obtain a generalization of Giacomini's equations in terms of the variables (x,y,t), we would need to generalize (2.4) and (3.40). Perhaps this could be achieved with the following approach. Assume

$$f_q(q,P,t)=a[f,P]V_q, \quad f_t(q,P,t)=b[f,P]V_q, \tag{3.45}$$

$$h(q,P,t)=P, \quad s(x,y,t)=y. \tag{3.46}$$

From (3.45), $f(q,P,t)$ must satisfy

$$f_t - \frac{b}{a} f_q = 0, \tag{3.47}$$

whose solution is

$$\Omega[f,P] = \frac{b}{a} t + q, \tag{3.48}$$

where Ω is arbitrary. Equation (3.48) is a generalization of (2.4). If we express $a[f,P]$ as

$$a[f,P] = \frac{1}{A_f[f,P]}, \tag{3.49}$$

then (3.45) implies

$$A[f(q,P,t),P] = V(q,t) + \gamma(P,t), \tag{3.50}$$

where γ is arbitrary. As a result of (3.46), (3.32) now reduces to

$$A_f[f,P] + A_f[f,P] b[f,P] \overline{G_x}(x,y) + \overline{G}(x,y) \overline{G_x}(x,y) = 0, \tag{3.51}$$

which is a generalization of (3.40). For (3.48) and (3.51) to be legitimate generalizations of (2.4) and (3.40), it is imperative that (3.47) and (3.49) be satisfied in a way that does not make $V(q,t)$ depend upon P when it is calculated from (3.50).

APPENDIX: RELATIONS AMONG THE DERIVATIVES OF *f*, *h*, *r*, AND *s*

Define the transformation from variables (q,P,t) to variables (x,y,t) by

$$x = f(q,P,t), \quad y = h(q,P,t), \tag{3.12}$$

and define the inverse transformation by

$$q = r(x,y,t), \quad P = s(x,y,t). \tag{3.23}$$

The formulas relating the first derivatives of $f(q,P,t)$ and $h(q,P,t)$ to the first derivatives of $r(x,y,t)$ and $s(x,y,t)$ can be obtained from the first derivatives of the identities

$$x \equiv f[r(x,y,t),s(x,y,t),t], \quad y \equiv h[r(x,y,t),s(x,y,t),t]; \tag{A1}$$

the identities are linear in the derivatives. The relations are

$$f_q = \frac{s_y}{r_x s_y - r_y s_x}, \quad f_p = -\frac{r_y}{r_x s_y - r_y s_x}, \quad f_t = \frac{r_y s_t - r_t s_y}{r_x s_y - r_y s_x}, \tag{A2}$$

$$h_q = -\frac{s_x}{r_x s_y - r_y s_x}, \quad h_p = \frac{r_x}{r_x s_y - r_y s_x}, \quad h_t = \frac{r_t s_x - r_x s_t}{r_x s_y - r_y s_x}, \tag{A3}$$

$$r_x = \frac{h_p}{f_q h_p - f_p h_q}, \quad r_y = -\frac{f_p}{f_q h_p - f_p h_q}, \quad r_t = \frac{f_p h_t - f_t h_p}{f_q h_p - f_p h_q}, \tag{A4}$$

$$s_x = -\frac{h_q}{f_q h_p - f_p h_q}, \quad s_y = \frac{f_q}{f_q h_p - f_p h_q}, \quad s_t = \frac{f_t h_q - f_q h_t}{f_q h_p - f_p h_q}. \tag{A5}$$

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A second invariant for one-degree-of-freedom, time-dependent Hamiltonians given a first invariant

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An explicit formula for a second invariant of a one-degree-of-freedom time-dependent Hamiltonian is derived in terms of the Hamiltonian and an assumed first invariant. If the first invariant is expressed as a function of two canonical functions, a transformation to an autonomous Hamiltonian system is possible. © *1996 American Institute of Physics.* [S0022-2488(96)02411-5]

I. INTRODUCTION

Considerable attention has been paid in recent years to the question of finding invariants for one-degree-of-freedom, time-dependent Hamiltonian systems. In this paper we assume that one invariant is known as an explicit function of two canonically conjugate variables and time, and we derive an explicit formula for a second invariant in terms of the Hamiltonian and the assumed first invariant. The two invariants are canonically conjugate to one another. Then we consider the special case in which the assumed first invariant is expressed as a function of *two* arguments, which are canonically conjugate functions of the canonical variables and time. This is always possible in principle, but such an expression for the invariant may not be known for a particular problem. If it is known, then a related *autonomous* Hamiltonian system can be derived that leads to a simplification of the formula for the second invariant. The related autonomous system is in terms of a new time variable that is defined separately for each value of the assumed first invariant.

By an invariant we mean any function $\tilde{I}(q,p,t)$ whose total time derivative vanishes:

$$0=\frac{d\tilde{I}}{dt}=\tilde{I}_t(q,p,t)+[\tilde{I},H]=\tilde{I}_t(q,p,t)+\tilde{I}_q(q,p,t)H_p(q,p,t)-\tilde{I}_p(q,p,t)H_q(q,p,t), \quad (1.1)$$

where $[\tilde{I},H]$ is the Poisson bracket of $\tilde{I}$ with H, and Hamilton's equations of motion have been taken into account in the evaluation of the total time derivative.

Our starting point is the formulation of Lewis *et al.*,[1] who gave an expression for all Hamiltonians $H(q,p,t)$ for which a specified function $\tilde{I}(q,p,t)$ is an invariant. In addition to the general case in which $\tilde{I}(q,p,t)$ is given explicitly as a function of the *three* arguments (q,p,t), they also treat the special case in which $\tilde{I}(q,p,t)$ is expressed as an explicit function of *two* arguments which are canonically conjugate to one another. The results of Lewis *et al.*[1] allow a simple, elegant derivation of a canonically conjugate second invariant within the framework of canonical transformation theory. A derivation of an equivalent canonically conjugate second invariant from a different point of view was given earlier by Dewisme and Bouquet.[2]

In Sec. II, we derive the general formula for a second invariant in terms of the Hamiltonian and the assumed first invariant. In Sec. III, we consider the special case in which the assumed first invariant is expressed as a function of two canonically conjugate functions and we present an

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example. In Appendix A we verify a required mathematical property of a function that is introduced in the derivation of the second invariant. In Appendix B we demonstrate directly that the general expression for a second invariant derived in this paper and the general expression derived by Dewisme and Bouquet[2] both satisfy the equation that defines an invariant and that they both are canonically conjugate to the assumed first invariant.

II. THE GENERAL CASE

Lewis *et al.*[1] showed that all Hamiltonians $H(q,p,t)$ for which a specified function $\tilde{I}(q,p,t)$ is an invariant are given by

$$H(q,p,t)=K(t)-F_t[\tilde{I}(q,p,t),t]-\int_{q_0}^{q}G_t[q',\tilde{I}(q,p,t),t]dq', \tag{2.1}$$

where $G(q,I,t)$ is the inverse of $\tilde{I}(q,p,t)$,

$$p=G(q,I,t)\leftrightarrow I=\tilde{I}(q,p,t), \tag{2.2}$$

and where $F(I,t)$ and $K(t)$ are arbitrary functions and q_0 is a constant. Consider a canonical transformation from variables (q,p,t) to variables (J,I,t),

$$J=\tilde{J}(q,p,t), \quad I=\tilde{I}(q,p,t), \tag{2.3}$$

such that the new Hamiltonian is $K(t)$. Then the functions $\tilde{J}(q,p,t)$ and $\tilde{I}(q,p,t)$ are canonically conjugate invariants of $H(q,p,t)$. A result of Lewis *et al.*[1] is that a Type Two generating function $S(q,I,t)$ for the canonical transformation from variables (q,p,t) to variables (J,I,t) is given by

$$S(q,I,t)=F(I,t)+\int_{q_0}^{q}G(q',I,t)dq'. \tag{2.4}$$

The transformation equations are

$$p=S_q(q,I,t), \quad \tilde{J}(q,p,t)=S_I[q,\tilde{I}(q,p,t),t], \tag{2.5}$$

and

$$K(t)=H(q,p,t)+S_t[q,\tilde{I}(q,p,t),t], \tag{2.6}$$

which is equivalent to (2.1). If we arbitrarily choose $K(t)=0$ and use (2.5) to write (2.6) in terms of (q,I,t), the result is the Hamilton–Jacobi equation for $S(q,I,t)$. There is an analogous result if one of the other generating functions is used mutatis mutandis, but the equation analogous to (2.6) would not normally be called the Hamilton–Jacobi equation.

We assume that both the Hamiltonian $H(q,p,t)$ and a first invariant $\tilde{I}(q,p,t)$ are given. In order to determine the second invariant $\tilde{J}(q,p,t)$, we shall determine a suitable function $F(I,t)$ that occurs in (2.1). Equation (2.1) written in terms of the variables (q,I,t) is

$$H[q,G(q,I,t),t]=K(t)-F_t(I,t)-\int_{q_0}^{q}G_t(q',I,t)dq'. \tag{2.7}$$

Integration of (2.7) with respect to t gives

$$F(I,t)-F(I,t_0)=\int_{t_0}^{t}K(t')dt'-\int_{t_0}^{t}H[q,G(q,I,t'),t']dt'-\int_{q_0}^{q}G(q',I,t)dq'+\int_{q_0}^{q}G(q',I,t_0)dq', \tag{2.8}$$

where t_0 is a constant. That this formula for $F(I,t)$ is indeed independent of q is verified in Appendix A. For that verification and for the remainder of the derivation of the second invariant, we use the following identities that relate the derivatives of $G(q,I,t)$ and $\tilde{I}(q,p,t)$:

$$G_q(q,I,t)=-\frac{\tilde{I}_q[q,G(q,I,t),t]}{\tilde{I}_p[q,G(q,I,t),t]}, \tag{2.9}$$

$$G_I(q,I,t)=\frac{1}{\tilde{I}_p[q,G(q,I,t),t]}, \tag{2.10}$$

$$G_t(q,I,t)=-\frac{\tilde{I}_t[q,G(q,I,t),t]}{\tilde{I}_p[q,G(q,I,t),t]}. \tag{2.11}$$

They can be derived by differentiating the identity

$$I=\tilde{I}[q,G(q,I,t),t] \tag{2.12}$$

with respect to q, I, and t and solving the resulting three equations for the derivatives of $G(q,I,t)$.

Now that we have $F(I,t)$ we can use (2.4) and (2.5) to calculate the second invariant $\tilde{J}(q,p,t)$. Taking $F(I,t_0)=0$, the generating function $S(q,I,t)$ is given by

$$S(q,I,t)=\int_{t_0}^{t}K(t')dt'+\int_{q_0}^{q}G(q',I,t_0)dq'-\int_{t_0}^{t}H[q,G(q,I,t'),t']dt', \tag{2.13}$$

and its derivative with respect to I is

$$S_I(q,I,t)=\int_{q_0}^{q}G_I(q',I,t_0)dq'-\int_{t_0}^{t}H_p[q,G(q,I,t'),t']G_I(q,I,t')dt'$$
$$=\int_{q_0}^{q}\frac{1}{\tilde{I}_p[q',G(q',I,t_0),t_0]}dq'-\int_{t_0}^{t}\frac{H_p[q,G(q,I,t'),t']}{\tilde{I}_p[q,G(q,I,t'),t']}dt'. \tag{2.14}$$

In order to obtain (2.14) we have used the identity (2.10). The second invariant $\tilde{J}(q,p,t)$ is obtained directly from (2.14) by replacing the variable I by the function $\tilde{I}(q,p,t)$.

The expression for the second invariant specified by (2.14) is very similar to, but different than, the expression given by Dewisme and Bouquet in Eq. (2.7) of Ref. 2. That both expressions are indeed invariants canonically conjugate to $\tilde{I}(q,p,t)$ is verified directly in Appendix B.

III. THE FIRST INVARIANT GIVEN AS A FUNCTION OF TWO CANONICALLY CONJUGATE FUNCTIONS

We now suppose that the first invariant, $\tilde{I}(q,p,t)$, is given as a function of two canonically conjugate functions:

$$\tilde{I}(q,p,t)\rightarrow\tilde{I}(x,y), \tag{3.1}$$

where

$$x=\tilde{x}(q,p,t), \quad y=\tilde{y}(q,p,t), \tag{3.2}$$

$$[\tilde{x}(q,p,t),\tilde{y}(q,p,t)]=1. \tag{3.3}$$

As is demonstrated by Lewis *et al.*,[1] a representation in the form (3.1) with canonically conjugate functions $\tilde{x}$ and $\tilde{y}$ is always possible in principle for any invariant. Although a realization of (3.1) may not be available in a particular case, such a representation is a natural generalization of the form of invariants that are quadratic in the momentum for the case of a particle moving in a potential.[3] The treatment leading to a second invariant is analogous to that for the general case, the canonical variables (x,y) replacing (q,p). However, because $\tilde{I}(x,y)$ does not depend on t, the treatment is simpler.

Define $G(x,I)$ as the inverse of $\tilde{I}(x,y)$,

$$y=G(x,I)\leftrightarrow I=\tilde{I}(x,y). \tag{3.4}$$

All Hamiltonians $H(x,y,t)$ for which a specified function $\tilde{I}(x,y)$ is an invariant are given by

$$H(x,y,t)=K(t)-F_t[\tilde{I}(x,y),t], \tag{3.5}$$

where $F(I,t)$ and $K(t)$ are arbitrary functions. Consider a canonical transformation from variables (x,y,t) to variables (J,I,t),

$$J=\tilde{J}(x,y,t), \quad I=\tilde{I}(x,y), \tag{3.6}$$

such that the new Hamiltonian is $K(t)$. Then the functions $\tilde{J}(x,y,t)$ and $\tilde{I}(x,y)$ are canonically conjugate invariants of $H(q,p,t)$. A Type Two generating function $S(x,I,t)$ for the canonical transformation from variables (x,y,t) to variables (J,I,t) is given by

$$S(x,I,t)=F(I,t)+\int_{x_0}^{x} G(x',I)dx', \tag{3.7}$$

where x_0 is a constant. The transformation equations are

$$y=S_x(x,I,t), \quad \tilde{J}(x,y,t)=S_I[x,\tilde{I}(x,y),t], \tag{3.8}$$

and

$$K(t)=H(x,y,t)+S_t[x,\tilde{I}(x,y),t], \tag{3.9}$$

which is equivalent to (3.5).

Equation (2.1) written in terms of the variables (x,I,t) is

$$H[q,G(x,I),t]=K(t)-F_t(I,t). \tag{3.10}$$

Integration of (3.10) with respect to t gives

$$F(I,t)-F(I,t_0)=\int_{t_0}^{t} K(t')dt'-\int_{t_0}^{t} H[x,G(x,I),t']dt', \tag{3.11}$$

where t_0 is a constant. That this formula for $F(I,t)$ is indeed independent of x is verified in Appendix A.

Now that we have $F(I,t)$ we can use (3.7) and (3.8) to calculate the second invariant $\tilde{J}(x,y,t)$. Taking $F(I,t_0)=0$, the generating function $S(x,I,t)$ is given by

$$S(x,I,t)=\int_{t_0}^{t}K(t')dt'+\int_{x_0}^{x}G(x',I)dx'-\int_{t_0}^{t}H[x,G(x,I,t'),t']dt', \tag{3.12}$$

and its derivative with respect to I is

$$\begin{aligned}S_I(x,I,t)&=\int_{x_0}^{x}G_I(x',I)dx'-\int_{t_0}^{t}H_y[x,G(x,I),t']G_I(x,I)dt'\\&=\int_{x_0}^{x}\frac{1}{\tilde{I}_y[x',G(x',I)]}\,dx'-\int_{t_0}^{t}\frac{H_y[x,G(x,I),t']}{\tilde{I}_y[x,G(x,I)]}\,dt'.\end{aligned} \tag{3.13}$$

In order to obtain (3.13) we have used the identity analogous to (2.10). The second invariant $\tilde{J}(x,y,t)$ is obtained directly from (3.13) by replacing the variable I by the function $\tilde{I}(x,y)$.

It is possible to convert the Hamiltonian system in terms of (x,y,t) to an autonomous system by introducing a new time variable T that is defined separately on each level curve of $\tilde{I}(x,y)$. This leads to an elegant expression for $\tilde{J}(x,y,t)$. Hamilton's equations for the Hamiltonian given by (3.5) are

$$\dot{x}(t)=-F_{tI}[\tilde{I}(x,y),t]\tilde{I}_y(x,y),\quad \dot{y}(t)=F_{tI}[\tilde{I}(x,y),t]\tilde{I}_x(x,y). \tag{3.14}$$

Define the new time variable T by

$$T=-F_I(I,t), \tag{3.15}$$

and define $X(T)=x(t)$ and $Y(T)=y(t)$. Then Hamilton's Eqs. (3.14) can be written as an autonomous Hamiltonian system in (X,Y,T),

$$\frac{dX}{dT}=\tilde{I}_y(X,Y)=h_Y(X,Y),\quad \frac{dY}{dT}=-\tilde{I}_x(X,Y)=-h_X(X,Y), \tag{3.16}$$

whose Hamiltonian is

$$h(X,Y)=\tilde{I}(X,Y). \tag{3.17}$$

Thus, a canonically conjugate second invariant written in terms of (X,Y,T) is immediately given by

$$\tilde{\tilde{J}}(X,Y,T)=-T+\int_{X_0}^{X}\frac{1}{h_Y\{X',G[X',h(X,Y)]\}}\,dX', \tag{3.18}$$

and in terms of (x,y,t) by

$$\tilde{J}(x,y,t)=F_I[\tilde{I}(x,y),t]+\int_{x_0}^{x}\frac{1}{\tilde{I}_y\{x',G[x',\tilde{I}(x,y)]\}}\,dx'. \tag{3.19}$$

As an example, we consider the system discussed in Sec. IV C of Ref. 1. The Hamiltonian in terms of (q,p,t) is

$$H(q,p,t)=\tfrac{1}{2}p^2+V(q,t), \tag{3.20}$$

where the potential is

$$V(q,t)=-\frac{1}{2}\left(\frac{\dot{\alpha}_1 q+\dot{\beta}_1}{\alpha_1}\right)^2-\frac{\dot{\alpha}_1}{\alpha_1^2}\left(\frac{1}{2}\,\dot{\alpha}_1 q+\dot{\beta}_1\right)q+\frac{1}{\alpha_1}\left(\frac{1}{2}\,\ddot{\alpha}_1 q+\ddot{\beta}_1\right)q$$
$$-\alpha_1^2\,\ln(\alpha_1 q+\beta_1)-\frac{\alpha_1^2}{2(\alpha_1 q+\beta_1)^2}\int^t \alpha_1^2(t')dt' \tag{3.21}$$

and $\alpha_1(t)$ and $\beta_1(t)$ are two arbitrary functions of time. An invariant for this system is

$$\tilde{I}(x,y)=xy^2+\ln y, \tag{3.22}$$

where x and y are defined by

$$x=\tilde{x}(q,p,t)=\frac{1}{2}\,(\alpha_1 q+\beta_1)^2+\frac{\alpha_1(\alpha_1 q+\beta_1)\int^t\alpha_1^2(t')dt'}{p-\dfrac{\alpha_1}{(\alpha_1 q+\beta_1)}\int^t\alpha_1^2(t')dt'+\dfrac{(\dot{\alpha}_1 q+\dot{\beta}_1)}{\alpha_1}}, \tag{3.23}$$

$$y=\tilde{y}(q,p,t)=\frac{p}{\alpha_1(\alpha_1 q+\beta_1)}+\frac{(\dot{\alpha}_1 q+\dot{\beta}_1)}{\alpha_1^2(\alpha_1 q+\beta_1)}-\frac{1}{(\alpha_1 q+\beta_1)^2}\int^t\alpha_1^2(t')dt'. \tag{3.24}$$

The function $F(I,t)$ is

$$F(I,t)=-\alpha_1^2(t)I, \tag{3.25}$$

and the new time is

$$T=\int^t\alpha_1^2(t')dt'. \tag{3.26}$$

For this example, the new time is independent of I. The autonomous Hamiltonian is

$$h(X,Y)=XY^2+\ln Y \tag{3.27}$$

and Hamilton's equations are

$$\frac{dX}{dT}=2XY+\frac{1}{Y},\quad \frac{dY}{dT}=-Y^2. \tag{3.28}$$

A second invariant canonically conjugate to I is

$$J=-T+\frac{1}{Y}=-\int^t\alpha_1^2(t')dt'+\frac{1}{\tilde{y}(q,p,t)}. \tag{3.29}$$

Direct integration of (3.28) yields

$$X(T)=(T+c_1)^2[c_2+\ln(T+c_1)],\quad Y(T)=(T+c_1)^{-1}, \tag{3.30}$$

where c_1 and c_2 are constants of integration equal to J and I, respectively.

APPENDIX A: VERIFICATION OF THE FUNCTIONAL DEPENDENCE OF $F(I,t)$

In order to verify that the rhs of (2.8) is independent of q, we evaluate its derivative with respect to q:

$$\frac{\partial}{\partial q}\,\mathrm{rhs}(2.8) = -\frac{\partial}{\partial q}\int_{t_0}^{t} H[q,G(q,I,t'),t']dt' - G(q,I,t) + G(q,I,t_0). \tag{A1}$$

The first term can be transformed as follows:

$$\begin{aligned} &-\frac{\partial}{\partial q}\int_{t_0}^{t} H[q,G(q,I,t'),t']dt' \\ &\quad = -\int_{t_0}^{t} \frac{1}{\widetilde{I}_p[q,G(q,I,t'),t']}\{H_q[q,G(q,I,t'),t']\widetilde{I}_p[q,G(q,I,t'),t'] \\ &\qquad - H_p[q,G(q,I,t'),t']\widetilde{I}_q[q,G(q,I,t'),t']\}dt' \end{aligned} \tag{A2}$$

In order to obtain (A2) we have used the identity (2.9). The expression in the curly brackets in (2.10) is minus the Poisson bracket of $\widetilde{I}$ with H. Therefore we may use (1.1) to obtain

$$-\frac{\partial}{\partial q}\int_{t_0}^{t} H[q,G(q,I,t'),t']dt' = -\int_{t_0}^{t} \frac{\widetilde{I}_t[q,G(q,I,t'),t']}{\widetilde{I}_p[q,G(q,I,t'),t']}\,dt' = \int_{t_0}^{t} G_t(q,I,t')dt'. \tag{A3}$$

In order to obtain (A3) we have used the identity (2.11). Finally, by substituting (A3) into (A1), we obtain

$$\frac{\partial}{\partial q}\,\mathrm{rhs}(2.8) = 0, \tag{A4}$$

as is required in order that (2.8) be a valid formula for $F(I,t)$.

The derivative of the rhs of (3.11) with respect to x can be evaluated as follows:

$$\begin{aligned} \frac{\partial}{\partial x}\,\mathrm{rhs}(3.11) &= -\frac{\partial}{\partial x}\int_{t_0}^{t} H[x,G(x,I),t']dt' \\ &= -\int_{t_0}^{t} \frac{1}{\widetilde{I}_y[x,G(x,I),t']}\{H_x[x,G(x,I),t']\widetilde{I}_y[x,G(x,I)] \\ &\quad - H_y[x,G(x,I),t']\widetilde{I}_x[x,G(x,I)]\}dt'. \end{aligned} \tag{A5}$$

In order to obtain (A5) we have used the identity analogous to (2.9). The expression in the curly brackets in (A5) is minus the Poisson bracket of $\widetilde{I}$ with H. Therefore, since $\widetilde{I}(x,y)$ is not an explicit function of t, we obtain

$$\frac{\partial}{\partial x}\,\mathrm{rhs}(3.11) = 0, \tag{A6}$$

as is required in order that (3.11) be a valid formula for $F(I,t)$.

APPENDIX B: DIRECT VERIFICATION OF EQ. (2.14) AND OF THE CORRESPONDING RESULT OF DEWISME AND BOUQUET

The expression for $\widetilde{J}(q,p,t)$ specified by (2.5) and (2.14) is very similar to, but different than, the expression given by Dewisme and Bouquet in Eq. (2.7) of Ref. 2. The two expressions may

differ by a function of the invariant $\tilde{I}(q,p,t)$. Here we verify directly that both expressions are indeed invariants canonically conjugate to $\tilde{I}(q,p,t)$. For that purpose we substitute the expressions into (1.1) and evaluate their Poisson brackets with $\tilde{I}(q,p,t)$.

1. $\tilde{J}(q,p,t)$ specified by Eq. (2.14)

The total time derivative of $\tilde{J}(q,p,t)$ is

$$\frac{d}{dt}\tilde{J}(q,p,t)=\tilde{J}_t(q,p,t)+[J,H]=S_{It}+S_{II}\tilde{I}_t+S_{Iq}H_p+S_{II}[I,H]=S_{It}+S_{Iq}H_p=-\frac{H_p(q,p,t)}{\tilde{I}_p(q,p,t)}$$
$$+\left\{\frac{1}{\tilde{I}_p(q,p,t_0)}-\int_{t_0}^{t}\frac{\partial}{\partial q}\frac{H_p[q,G(q,I,t'),t']}{\tilde{I}_p[q,G(q,I,t'),t']}\,dt'\right\}H_p(q,p,t). \tag{B1}$$

The integral in (B1) can be evaluated by transforming the integrand to a derivative with respect to t holding (q,I) fixed. In order to do that, we use the derivative with respect to p of (1.1),

$$0=\tilde{I}_{tp}+\tilde{I}_{qp}H_p+\tilde{I}_qH_{pp}-\tilde{I}_{pp}H_q-\tilde{I}_pH_{qp}, \tag{B2}$$

along with (2.10), (1.1), and (2.12):

$$\frac{\partial}{\partial q}\frac{H_p[q,G(q,I,t),t]}{\tilde{I}_p[q,G(q,I,t),t]}=\frac{1}{\tilde{I}_p^2}\{[H_{pq}+H_{pp}G_q]\tilde{I}_p-H_p[\tilde{I}_{pq}+\tilde{I}_{pp}G_q]\}$$
$$=\frac{1}{\tilde{I}_p^2}\{\tilde{I}_{tp}+\tilde{I}_{pp}G_t\}=-\frac{\partial}{\partial t}\frac{1}{\tilde{I}_p[q,G(q,I,t),t]}. \tag{B3}$$

Substitution of (B3) into (B1) immediately shows satisfaction of (1.1).

The following evaluation demonstrates that $\tilde{J}(q,p,t)$ and $\tilde{I}(q,p,t)$ are canonically conjugate:

$$[J,I]=\frac{1}{\tilde{I}_p(q,p,t_0)}\tilde{I}_p(q,p,t)-\left\{\int_{t_0}^{t}\frac{\partial}{\partial q}\frac{H_p[q,G(q,I,t'),t']}{\tilde{I}_p[q,G(q,I,t'),t']}\,dt'\right\}\tilde{I}_p(q,p,t)$$
$$=\left\{\frac{1}{\tilde{I}_p(q,p,t_0)}+\int_{t_0}^{t}\frac{\partial}{\partial t'}\frac{1}{\tilde{I}_p[q,G(q,I,t'),t']}\,dt'\right\}\tilde{I}_p(q,p,t)=1. \tag{B4}$$

2. $\tilde{J}(q,p,t)$ as given by Dewisme and Bouquet

The expression for $\tilde{J}(q,p,t)$ given by Dewisme and Bouquet in Eq. (2.7) of Ref. 2, written in the notation of the present paper, is

$$\tilde{J}(q,p,t)=S_I[q,\tilde{I}(q,p,t),t],$$

as in (2.5), but where $S_I(q,I,t)$ is given by

$$S_I(q,I,t)=\int_{q_0}^{q}\frac{1}{\tilde{I}_p[q',G(q',I,t),t]}\,dq'-\int_{t_0}^{t}\frac{H_p[q_0,G(q_0,I,t'),t']}{\tilde{I}_p[q_0,G(q_0,I,t'),t']}\,dt', \tag{B5}$$

instead of by (2.14). The total time derivative of this $\tilde{J}(q,p,t)$ is

$$\frac{d}{dt}\,\widetilde{J}(q,p,t)=-\frac{H_p(q_0,p,t)}{\widetilde{I}_p(q_0,p,t)}+\int_{q_0}^{q}\frac{\partial}{\partial t}\,\frac{1}{\widetilde{I}_p[q',G(q',I,t),t]}\,dq'+\frac{H_p(q,p,t)}{\widetilde{I}_p(q,p,t)}. \tag{B6}$$

The integral in (B6) can be evaluated by using (B3). It follows immediately that (1.1) is satisfied.

Verification of the Poisson bracket relation $[J,I]=1$ is very simple when $S_I(q,I,t)$ is given by (B5).

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Inhibition of chaotic escape from a potential well using small parametric modulations

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It is shown theoretically for the first time that, depending on its period, amplitude, and initial phase, a periodic parametric modulation can suppress a chaotic escape from a potential well. The instance of the Helmholtz oscillator is used to demonstrate, by means of Melnikov's method, that parametric modulations of the linear or quadratic potential terms inhibit chaotic escape when certain resonance conditions are met. © *1996 American Institute of Physics.* [S0022-2488(96)03709-7]

I. INTRODUCTION

Escape from a potential well is a general problem in the physical sciences. One finds it in very different contexts: the escape of stars from a stellar system,[1] the orbits of a photon near a Schwarzschild black hole,[2] the photodissociation of molecules as described by the driven Morse oscillator,[3] the capsizing of a boat subjected to trains of regular waves,[4] and the stochastic escape of a trapped ion induced by a resonant laser field,[5] to quote a few. All of these systems (except the integrable one of Ref. 2) present a common characteristic: before escape, chaotic transients of unpredictable duration are usually observed for orbits starting from chaotic generic phase space regions (such as those surrounding separatrices), in both Hamiltonian[1,3,5] and dissipative[4] systems. As the application of weak parametric modulations (PMs) is an effective technique for taming chaos arising from such a wide class of dynamical systems,[6] one might conjecture that there would be a similar efficacy for suppressing chaotic escape. The approach is of the nonfeedback type, and is easily implemented in practical systems, where the performance of a specific nonlinear system with a potential well subjected to a periodic excitation would generally be considered optimal if it operates in a periodic mode (i.e., inside the well).

For the sake of clarity, we shall concentrate in this paper on the simplest model for a universal chaotic escape situation—the Helmholtz oscillator.[7] We first added a weak PM of the quadratic term,

$$\ddot{x}=x-\beta[1+\eta\,\sin(\Omega t+\phi)]x^2-\delta\dot{x}+\gamma\,\sin(\omega t), \tag{1}$$

where x is the displacement, Ω, η and ϕ are the normalized frequency, amplitude, and initial phase, respectively, of the PM ($\eta\ll 1$), which will have an inhibitory effect on the chaotic escape of the remaining system ($\delta,\gamma\ll 1$),[8] and ω, δ, and γ are the normalized parameters of frequency, damping coefficient, and driving term amplitude, respectively. We shall then apply instead a PM of the linear term

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$$\ddot{x}=x[1+\eta' \sin(\Omega' t+\phi')]-\beta x^2-\delta\dot{x}+\gamma \sin(\omega t), \tag{2}$$

where Ω', η', and ϕ' are the normalized frequency, amplitude, and initial phase, respectively, of the PM ($\eta' \ll 1$), and compare the results.

II. MELNIKOV ANALYSIS

Melnikov's method (MM) is the main analytical technique currently available to provide a criterion for the occurrence of homoclinic (and heteroclicic) chaos in a dynamical system, and is today considered standard. As is well known, MM predictions are both approximate (the MM is a first-order perturbative method) and limited (only valid for orbits starting at points sufficiently near the separatrix). However, they are highly valued because of the quite general scarcity of analytical results in the theory of chaos. Since it has been described many times by different authors, we shall not discuss it in detail here, but refer the interested reader to that literature.[9–13]

A. Melnikov function

The application of MM to Eq. (1) involves calculating the Melnikov function,

$$M(t_0)=-\delta\int_{-\infty}^{\infty}\dot{x}_0^2(t)dt+\gamma\int_{-\infty}^{\infty}\dot{x}_0(t)\sin[\omega(t+t_0)]dt-\beta\eta\int_{-\infty}^{\infty}\dot{x}_0(t)x_0^2(t)\sin[\Omega(t+t_0)+\phi]dt, \tag{3}$$

where

$$x_0(t)=\frac{3}{2\beta}\operatorname{sech}^2\left(\frac{t}{2}\right),$$
$$\dot{x}_0(t)=-\frac{3}{2\beta}\operatorname{sech}^2\left(\frac{t}{2}\right)\tanh\left(\frac{t}{2}\right), \tag{4}$$

is the parametric representation of the separatrix of the underlying conservative system ($\delta=\gamma=\eta=0$). After substituting Eq. (4) into Eq. (3) and computing the resulting integrals with the aid of standard integral tables,[14] Eq. (3) can be written as

$$M(t_0)=-C-A\cos(\omega t_0)+B\cos(\Omega t_0+\phi), \tag{5}$$

with

$$C=\frac{6\delta}{5\beta^2},$$
$$A=\frac{6\pi\gamma}{\beta}\omega^2\operatorname{cosech}(\pi\omega), \tag{6}$$
$$B=\frac{3\pi\eta}{5\beta^2}\Omega^2(\Omega^2+1)(\Omega^2+4)\operatorname{cosech}(\Omega\pi).$$

As is well known,[11–13] the Melnikov function $M(t_0)$ measures the distance between the perturbed stable and unstable manifolds in the Poincaré section at t_0. If $M(t_0)$ has a simple zero, then a homoclinic bifurcation occurs, signifying the possibility of chaotic behavior, i.e., only *necessary* conditions for steady chaos are obtained from MM, and therefore one always has the

possibility of finding *sufficient* conditions for the elimination of even transient chaos. Indeed, we shall show in the following that the MM provides, for the system under consideration, sufficient conditions for the inhibition of chaotic escape.

B. Escape Inhibition Theorem (EIT)

Suppose that for $\eta=0$ the system (1) undergoes a chaotic escape for which the associated Melnikov function $M_0(t_0)\equiv -C+A\cos(\omega t_0)$ has simple zeros, i.e., $A-C\equiv d\geqslant 0$, where the equal sign corresponds to the case of tangency between the stable and unstable manifolds. If we now let the PM act on the system ($\eta\neq 0$) in such a way that $B>d$, i.e., $A-B-C<0$, this relationship provides a necessary condition for $M(t_0)$ to always have the same sign, specifically $M(t_0)<0$, which is

$$\eta>\left(1-\frac{C}{A}\right)R, \tag{7}$$

with

$$R=\frac{10\gamma\beta\omega^2}{\Omega^2(\Omega^2+1)(\Omega^2+4)}\left[\frac{\sinh(\pi\Omega)}{\sinh(\pi\omega)}\right]. \tag{8}$$

For general Ω and ϕ ($0\leqslant\phi\leqslant 2\pi$), we shall see that this condition is not sufficient to assure the negativity of $M(t_0)$. In order to achieve such a sufficient condition, we shall first need three lemmas.

Lemma I: Let Ω/ω be irrational. Then there exists an $\overline{t_0}$ such that $B\cos(\Omega\overline{t_0}+\phi)-A\cos(\omega\overline{t_0})>A-B$.

Lemma II: Let $p\omega=q\Omega$ for some positive integers p and q. Then a t_0^* exits such that $\cos(\omega t_0^*)=\cos(\Omega t_0^*+\phi)=-1$ if and only if

$$\frac{p}{q}=\frac{2m-1-\phi/\pi}{2n-1}, \tag{9}$$

for some integers m and n.

Remark: Observe that a requirement for Eq. (9) to be fulfilled for some integers m and n is $\phi=m_1\pi/m_2$, $m_{1,2}$ integers.

Lemma III: Let $g(t;p,q)=[1-\cos(pt/q)]/(1-\cos t)$, t real, p and q integers. Then g is finite if and only if $q=1$. One also has that $0\leqslant g(t;p,1)\leqslant p^2$.

It is obvious that for Eq. (7) to also be a sufficient condition for $M(t_0)$ to be negative for all t_0, one must have

$$A-B\geqslant B\cos(\Omega t_0+\phi)-A\cos(\omega t_0). \tag{10}$$

We now look for the values of ω, Ω, and ϕ, permitting Eq. (10) to be fulfilled for all t_0. From Lemma I, a resonance condition is required: $p\omega=q\Omega$. In such a situation, Lemma II provides a condition for Eq. (10) to be satisfied for an infinity of t_0 values. Thus, let us assume that p, q, and ϕ verify Eq. (9). We can then rewrite Eq. (10) in the form

$$\frac{A}{B}\geqslant\frac{1-\cos(p\tau/q)}{1-\cos\tau}, \tag{11}$$

with $\tau\equiv\omega t_0-(2n-1/2)\pi$. Finally, if $q=1$, Lemma III provides a condition for Eq. (11) to be fulfilled for all τ:

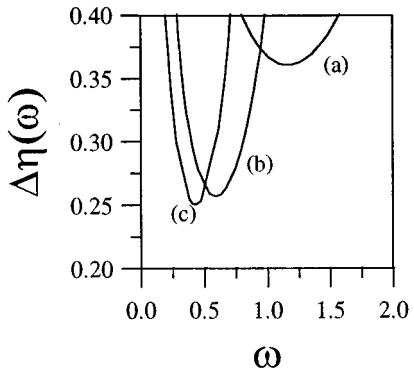

FIG. 1. Function $\Delta\eta(\omega)=\eta_{\max}-\eta_{\min}$ vs ω for δ=const, β=const, γ=const, and $\Omega=p\omega$: (a) $p=1$; (b) $p=2$; (c) $p=3$.

$$\eta \leqslant \frac{R}{p^2}, \tag{12}$$

with R given by (8). The proofs of the lemmas are quite straightforward, so they will not be included here. In brief we have the following.

Escape Inhibition Theorem (EIT): Let $\Omega=p\omega$, p an integer, such that $p=(2m-1-\phi/\pi)/(2n-1)$ is satisfied for some integers m and n. Then $M(t_0)$ always has the same sign, i.e., $M(t_0)<0$, if and only if the following condition is fulfilled:

$$\eta_{\min} < \eta \leqslant \eta_{\max},$$

$$\eta_{\min}=\left(1-\frac{C}{A}\right)R, \tag{13}$$

$$\eta_{\max}=\frac{R}{p^2}.$$

Remarks: First, note that, for a given set of parameters satisfying the theorem's hypothesis, as the resonance order p is increased, the allowed interval $]\eta_{\min},\eta_{\max}]$ for escape inhibition shrinks rapidly. One may therefore expect only the first few resonances to be suitable for suppressing chaotic escape (as, in fact, we observed in numerical experiments). Figure 1 shows the width $\Delta\eta(\omega)=\eta_{\max}-\eta_{\min}$ vs ω for δ,γ=const. There exist a minimum-range frequency for each resonance. Observe that the minimum $\omega_{\min}$ is lower as the resonance order is increased. The asymptotic behavior $\Delta\eta(\omega\to 0,\infty)=\infty$ means that chaotic escape is impossible in these limits. Second, we can test the EIT theoretically by considering the limiting case $\delta=0$. From Eqs. (9) and (13), one has $\phi=0$, $\Omega=\omega$, and $\eta=R$ as a necessary and sufficient condition for eliminating stochastic escape. But this is the obvious result arising from a direct analysis of Eq. (5). Third, the EIT imposes having $\phi=0$ ($\phi=\pi$) for odd (even) values of p. Note that since distinct ϕ values imply different initial conditions for the complete system (1), the above results provide information about the *extension* and *structure* of the basin of attraction of the regularized (periodic) orbits inside the well.

C. Case of a PM of the linear term

We now compare the above results with those corresponding to the application of a PM of the linear term as in Eq. (2). Proceeding similarly to the quadratic case, the Melnikov function corresponding to Eq. (2) is

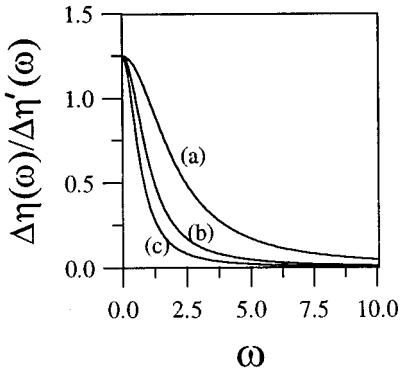

FIG. 2. Function $\Delta\eta(\omega)/\Delta\eta'(\omega)$ [Eq. (17)] vs ω for several values of p: (a) $p=1$; (b) $p=2$; (c) $p=3$.

$$M'(t_0) = -C - A\cos(\omega t_0) + B\cos(\Omega' t_0 + \phi'), \tag{14}$$

with

$$B' = \frac{3\pi\eta'}{\beta^2}\,\Omega'^2(\Omega'^2+1)\,\mathrm{cosech}(\pi\Omega'), \tag{15}$$

and C, A given by Eq. (6). Note that Eqs. (5) and (14) become identical with the substitutions: $B\to B'$, $\Omega\to\Omega'$, $\phi\to\phi'$. Therefore (cf. Sec. II B), one obtains a similar escape inhibition theorem (that we shall denote EIT′): Let $\Omega'=p\omega$, p an integer, such that $p=(2m-1-\phi'/\pi)/(2n-1)$ is satisfied for some integers m and n. Then $M'(t_0)$ always has the same sign, i.e., $M'(t_0)<0$, if and only if

$$\begin{aligned} &\eta'_{\min} < \eta' \leqslant \eta'_{\max}, \\ &\eta'_{\min} = \left(1 - \frac{C}{A}\right) R', \\ &\eta'_{\max} = \frac{R'}{p^2}, \\ &R' = \frac{2\gamma\beta\omega^2}{\Omega'^2(\Omega'^2+1)}\left[\frac{\sinh(\pi\Omega')}{\sinh(\pi\omega)}\right]. \end{aligned} \tag{16}$$

The same remarks hold as for EIT. In order to compare the quadratic and linear cases we set $\Omega=\Omega'$, $\phi=\phi'$ and define $\Delta\eta'(\omega) = \eta'_{\max} - \eta'_{\min}$. We then obtain [cf. Eqs. (13) and (16)]

$$\frac{\Delta\eta(\omega)}{\Delta\eta'(\omega)} = \frac{5}{p^2\omega^2+4}. \tag{17}$$

Figure 2 shows the relative width $\Delta\eta(\omega)/\Delta\eta'(\omega)$ vs ω for several values of p. First, observe that for $\omega=1/p$, $\Delta\eta(\omega)=\Delta\eta'(\omega)$, whereas for $\omega>1/p$ ($\omega<1/p$) one has $\Delta\eta(\omega)<\Delta\eta'(\omega)$ [$\Delta\eta(\omega)>\Delta\eta'(\omega)$], i.e., the effectiveness of the quadratic PM (in the frequency domain) relative to the linear PM rises with decreasing resonance order, and *vice versa*. Second, with fixed p, the asymptotic behavior $[\Delta\eta/\Delta\eta'](\omega\to\infty)=0$ means that a linear PM inhibits chaotic escape much more easily (i.e., for a larger interval of amplitudes) than a quadratic PM for small driving periods

of the primary chaos-inducing modulation. From the other limit $(\Delta\eta/\Delta\eta')(\omega\to 0)=5/4$, we deduce the opposite result for large driving periods, i.e., for resonances with orbits (of the conservative Helmholtz oscillator) very close to the separatrix (for which $T=\infty$).

III. CONCLUSIONS

We have shown here for the first time that the application of periodic PM is an efficient procedure for suppressing chaotic escape from a potential well. Analytical estimates of the ranges of parameters for inhibition were found by means of the Melnikov analysis of the example of the Helmholtz oscillator. The cases of PMs of the linear and quadratic potential terms were studied and compared. It was demonstrated that a PM of the linear (quadratic) term suppress chaotic escape more efficiently than that of the quadratic (linear) term for small (large) driving periods of the primary chaos-inducing modulation.

ACKNOWLEDGMENTS

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Lie algebraic structures of (1+1)-dimensional Lax integrable systems

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An approach of constructing isospectral flows K_l, nonisospectral flows σ_k and their implicit representations of a general Lax integrable system is proposed. By introducing product function matrices, it is shown that the two sets of flows and of related symmetries both constitute infinite-dimensional Lie algebras with respect to the commutator $[\![\cdot,\cdot]\!]$ given in this paper. Algebraic properties for some well-known integrable systems such as the AKNS system, the generalized Harry Dym system, and the n-wave interaction system are obtained as particular examples. © *1996 American Institute of Physics.* [S0022-2488(96)00311-8]

I. INTRODUCTION

Many (1+1)-dimensional Lax integrable systems, such as the AKNS system, the generalized Harry Dym (HD) system, and the n-wave interaction system, possess a couple of isospectral flows K_l and nonisospectral flows σ_k. For an integrable system with a recursion operator, by using the hereditariness of this operator, an infinite-dimensional Lie algebra constituted by the flows K_l and σ_k can be derived. In recent years, there are some new methods that do not use the concept of hereditary symmetry in the study of the algebraic structure of the flows. On the basis of Fokas–Fuchssteiner's idea of the master symmetry, Cheng *et al.*[1,2] have introduced the notion of semi-product Lie algebra of Lax operator. From here, they have suggested a direct approach to derive the commutator relations of flows for some integrable systems. Following this line and assuming that there exists a recursion operator for flows and some other restrictive conditions, Ma[3] has further given the algebraic structure of Lax operator and corresponding flows for the spectral problem $L\phi=\lambda\phi$. However, the applied scope of Ma's results is very limited. In Refs. 4–6, we have introduced the implicit representations of the flows of some soliton systems by using the zero-curvature equation and have also obtained the algebraic properties of these flows by simple computation.

In this paper, we would like to consider the algebraic properties of an integrable system associated with the general linear problem

$$\phi_x=M(\eta,u)\phi, \tag{1.1a}$$

$$\phi_t=N(t,x,\eta,u)\phi. \tag{1.1b}$$

We first put forward a simple method to derive respectively its isospectral flows K_l, nonisospectral flows σ_k (may be no recursion operator), and their implicit representations. Then we introduce the notion and some Lie commutator equalities of product function matrices which play crucial roles in our theory. As a result, the infinite-dimensional Lie algebraic structures of the flows and related symmetries of the general Lax integrable system can be derived naturally. Finally we shall apply our results to several known integrable systems such as the AKNS system, the generalized HD system, and the n-wave interaction system.

The method used in this paper is universal and can be extended to some high-dimensional Lax integrable systems. Thus it is revealed that there exists a close relationship between infinite-dimensional Lie algebra of flows and Lax integrability of corresponding evolution equations.

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This paper is organized as follows. Section II gives the notion of the Gateaux derivative and some required derivation formulas. In Sec. III we derive the isospectral flows K_l and nonisospectral flows σ_k of a general integrable system associated with the linear problem (1.1) and their implicit representations. In Sec. IV we introduce product function matrices and related Lie commutator equalities. In Sec. V, we derive Lie algebraic structure of flows K_l and σ_k of the general Lax integrable system. Finally, we apply the results obtained to some classical integrable systems in Sec. VI.

II. GATEAUX DERIVATIVE

Let $x \in R^n$, $u=u(t,x)=(u_1,u_2,\ldots,u_s)^T$, where $u_i=u_i(t,x) \in S(R^n)$ (the space of rapidly decreasing functions). Suppose $f=f(t,x,u)=(f_1,f_2,\ldots,f_m)^T$ with $f_i=f_i(t,x,u,Du,D^2u,\ldots,D^ru)$, in which $D^ru = D_1^{r_1}D_2^{r_2}\cdots D_n^{r_n}u$, $D_iu=\partial u/\partial x_i$, and r is a set of non-negative integers $\{r_1,r_2,\ldots,r_n\}$, is a C^∞ differentiable vector filed with respect to x, u, Du, D^2u,..., and D^ru. By $V^{(m)}$ denote a complex linear space constructed by these vector fields. By $Q^{(m)}$ denote a set composed of all the linear operators [in the form of $T=T(t,x,u)$] acting on the vector field space $V^{(m)}$ and being C^∞ differentiable for x and u as well. Obviously, $Q^{(m)}$ is also a linear space. In addition, by $Q_0^{(m)}$ denote a subspace described by all the $m\times m$ function matrices in $Q^{(m)}$.

Definition 1: Let $f \in V^{(m)}$, $h \in V^{(s)}$, and $T \in Q^{(m)}$. Then

$$f'[h]=f'(u)[h]=\frac{d}{d\varepsilon}\,f(u+\varepsilon h)\big|_{\varepsilon=0} \tag{2.1a}$$

and

$$T'[h]=T'(u)[h]=\frac{d}{d\varepsilon}\,T(u+\varepsilon h)\big|_{\varepsilon=0} \tag{2.1b}$$

are called, respectively, the Gateaux derivatives of the vector field f and linear operator T in the direction h with respect to u, or called the G-derivative for short.

From the definition, we obtain the following.

Lemma 1: Let $f \in V^{(m)}$, $h \in V^{(s)}$, and T, $S \in Q^{(m)}$. Then the Leibniz formulas

$$(Tf\,)'[h]=T'[h]f+Tf'[h] \tag{2.2a}$$

and

$$(TS)'[h]=T'[h]S+TS'[h] \tag{2.2b}$$

are valid.

Clearly, $T' \in Q^{(m)}$, and the G-derivative can also be defined. So we have the following lemma.

Lemma 2: Let $f,g \in V^{(s)}$ and $T \in Q^{(m)}$. Then

$$(T')'[f]g=(T')'[g]f. \tag{2.3}$$

Definition 2: Let $f,g \in V^{(s)}$. Then

$$[\![f,\,g]\!]=f'[g]-g'[f] \tag{2.4}$$

is named the commutator of vector fields f and g.

Lemma 3: Linear space $V^{(s)}$ constitutes a Lie algebra with respect to the commutator operation (2.4).[7]

Lemma 1 together with Lemma 2 immediately implies the following.

Lemma 4: Let $f,g\in V^{(s)}$ and $T\in Q^{(m)}$. Then

$$(T'[f])'[g]-(T'[g])'[f]=T'[[\![f,\ g]\!]]. \tag{2.5}$$

III. ISOSPECTRAL AND NONISOSPECTRAL FLOWS

Let η be a spectral parameter and $\mathscr{S}(Q_0^{(m))}$ be a linear space containing all the polynomials of η on $Q_0^{(m)}$.

Suppose that the couple of function matrices $M=M(\eta,u)$ and $N=N(t,x,\eta,u)$ in the linear problem (1.1) belong to $\mathscr{S}(Q_0^{(m)})$. The compatible condition of (1.1) is

$$M_t-N_x+[M,\ N]=0, \tag{3.1}$$

where $[M,N]=MN-NM$ and $x\in R'$. Usually, (3.1) is called the zero-curvature equation.

From Eq. (3.1), if one can derive a hierarchy of isospectral evolution equations

$$u_t=K_l,\quad K_l\in V^{(s)},\quad l=0,1,2,\ldots, \tag{3.2}$$

or of nonisospectral evolution equations

$$u_t=\sigma_k,\quad \sigma_k\in V^{(s)},\quad k=0,1,2,\ldots\ . \tag{3.3}$$

Then (3.2) or (3.3) are called to be Lax integrable.

In the isospectral case, $M_t=M'[u_t]=M'[K_l]$. It follows that Eq. (3.1) can be written as

$$M'[K_l]=N_{l,x}+[N_l,\ M], \tag{3.4}$$

where $N_l=N_l(t,x,\eta,u)\in\mathscr{S}(Q_0^{(m)})$. While for nonisospectrum, $M_t=M'[\sigma_k]+M_\eta\eta_t$; then Eq. (3.1) implies

$$M'[\sigma_k]=P_{k,x}+[P_k,\ M]-M_\eta\eta^{\alpha k+\beta}, \tag{3.5}$$

where $P_k=P_k(t,x,\eta,u)\in\mathscr{S}(Q_0^{(m)})$, $\eta_t=\eta^{\alpha k+\beta}$, and α, β, and k are all integers. Equations (3.4) and (3.5) are named respectively the implicit representations of the hierarchies of evolution equations (3.2) and (3.3) (or of the flows K_l and σ_k).

In what follows, we shall discuss a sufficient condition under which the above implicit representations are existential and unique. Suppose that for the given function matrix $M=M(\eta,u)\in\mathscr{S}(Q_0^{(m)})$ and vector field $Y=Y(t,x,u)\in V^{(s)}(Y|_{u=0}=0)$, the matrix equation

$$M'[X-\eta^\alpha Y]=N_x+[N,\ M] \tag{3.6}$$

possesses unique solutions $X=X(t,x,u)\in V^{(s)}$ and $N=N(t,x,\eta,u)\in\mathscr{S}(Q_0^{(m)})$ which meet the condition

$$N|_{u=0}=\delta_0 M|_{u=0}\eta^\mu, \tag{3.7a}$$

where $\alpha(\alpha\neq 0)$ and μ are integers and δ_0 is given by

$$\delta_0=\begin{cases}1, & \text{if } Y=0,\\ 0, & \text{if } Y\neq 0.\end{cases} \tag{3.7b}$$

Then for each j there exists a unique vector field $K_j\in V^{(s)}$ with $K_j|_{u=0}=0$ [see (3.16) and (3.17)] and a unique function matrix $U_j\in\mathscr{S}(Q_0^{(m)})$ $(j=0,1,\ldots,l)$, which satisfy in turn the following:

$$M'[K_0]=U_{0,x}+[U_0,\ M],\quad U_0=M|_{u=0}\eta^\mu, \tag{3.8a}$$

$$M'[K_j-\eta^{\alpha}K_{j-1}]=U_{j,x}+[U_j,\ M],\quad U_j|_{u=0}=0\quad (j=1,2,...,l). \tag{3.8b}$$

Equation (3.8) suggests

$$\begin{aligned} M'[K_l]&=M'[K_0]\eta^{\alpha l}+\sum_{j=1}^{l} M'[K_j-\eta^{\alpha}K_{j-1}]\eta^{\alpha(l-j)}\\ &=\sum_{j=0}^{l} U_{j,x}\eta^{\alpha(l-j)}+\left[\sum_{j=0}^{l} U_j\eta^{\alpha(l-j)},\ M\right], \end{aligned} \tag{3.9}$$

that is to say, the vector field K_l possesses a unique implicit representation (3.4) where

$$N_l=\sum_{j=0}^{l} U_j\eta^{\alpha(l-j)}\in Q_0^{(m)},\quad N_l|_{u=0}=M|_{u=0}\eta^{\alpha l+\mu}. \tag{3.10}$$

In the same way, if we suppose that there exist a vector field $\sigma_0\in V^{(s)}$ $(\sigma_0|_{u=0}=0)$ and a function matrix $W_0\in\mathscr{S}(Q^{(m)})$ which satisfy

$$M'[\sigma_0]=W_{0,x}+[W_0,\ M]-M_{\eta}\eta^{\beta} \tag{3.11a}$$

and

$$W_0|_{u=0}=(p_0xM|_{u=0}+A_0)\eta^{\beta-1}, \tag{3.11b}$$

here $p_0=p_0(t)\in Q_0^{(1)}$, $A_0=A_0(t)\in Q_0^{(m)}$, both depend on given spectral problem. Then for each j there also must exist uniquely a vector field σ_j with $\sigma_j|_{u=0}=0$ [see (3.18)] and a function matrix $W_j\in\mathscr{S}(Q_0^{(m)})(j=1,2,\ldots,k)$ which satisfy in turn

$$M'[\sigma_j-\eta^{\alpha}\sigma_{j-1}]=W_{j,x}+[W_j,\ M],\quad W_j|_{u=0}=0\quad (j=1,2,...,k). \tag{3.12}$$

Equation (3.11) coupled with (3.12) yields

$$\begin{aligned} M'[\sigma_k]&=M'[\sigma_0]\eta^{\alpha k}+\sum_{j=1}^{k} M'[\sigma_j-\eta^{\alpha}\sigma_{j-1}]\eta^{\alpha(k-j)}\\ &=\sum_{j=0}^{k} W_{j,x}\eta^{\alpha(k-j)}+\left[\sum_{j=0}^{k} W_j\eta^{\alpha(k-j)},\ M\right]-M_{\eta}\eta^{\alpha k+\beta}. \end{aligned} \tag{3.13}$$

That means the vector field σ_k possesses the implicit representation (3.5) where

$$P_k=\sum_{j=0}^{k} W_j\eta^{\alpha(k-j)}\in\mathscr{S}(Q_0^{(m)}),\quad P_k|_{u=0}=(p_0xM|_{u=0}+A_0)\eta^{\alpha k+\beta-1}. \tag{3.14}$$

It should be noted that if Eq. (3.6) has unique solutions meeting Condition (3.7), then the matrix equation

$$M'[X]=N_x+[N,\ M],\quad N|_{u=0}=0, \tag{3.15}$$

only admits zero solutions $X=0$ and $N=0$. As a result, the solutions σ_0 and W_0 of (3.11) are unique, and so is the implicit representation of σ_k.

From the above note, it is easy to know that if Eq. (3.6) possesses solutions $X\in V^{(s)}$ and $N\in\mathscr{S}(Q_0^{(m)})$ meeting Condition (3.7), the two following propositions are equivalent:

(1) The solutions satisfying Eq. (3.6) and Condition (3.7) are unique.
(2) In (3.15), operator M' is an injective homomorphism and from $N|_{u=0}=0$ it can be deduced that $N=0$.

Furthermore, from (3.8), we have

$$M'[K_0]|_{u=0}=0, \quad M'[K_j-\eta^{\alpha}K_{j-1}]|_{u=0}=0 \quad (j=1,2,...,l). \tag{3.16}$$

Because M' is an injective homomorphism (so is $M'|_{u=0}$), (3.16) suggests

$$K_j|_{u=0}=0 \quad (j=0,1,...,l). \tag{3.17}$$

Similarly, (3.12) associated with the assumption $\sigma_0|_{u=0}=0$ yields also

$$\sigma_j|_{u=0}=0 \quad (j=1,2,...,k). \tag{3.18}$$

The above results can be generalized to the following theorem:

Theorem 1: Suppose that for any given vector field $Y=Y(t,x,u)\in V^{(s)}(Y|_{u=0}=0)$ the function matrix equation (3.6) possesses unique solutions vector field $X=X(t,x,u)\in V^{(s)}$ and function matrix $N=N(t,x,\eta,u)\in\mathscr{L}(Q_0^{(m)})$ which satisfy the condition (3.7). Then the vector field $K_l\in V^{(s)}$ constructed in turn by (3.8) meets the condition (3.17) and has a unique implicit representation (3.4), in which the function matrix $N_l=N_l(t,x,\eta,u)\in\mathscr{L}(Q_0^{(m)})$ is described by (3.10). While if there exist solutions $\sigma_0\in V^{(s)}$ $(\sigma_0|_{u=0}=0)$ and $W_0\in\mathscr{L}(Q_0^{(m)})$ satisfying (3.11), then the vector field $\sigma_k\in V^{(s)}$ constructed in turn by (3.11) and (3.12) satisfies Condition (3.18) and has also a unique implicit representation (3.5) where $P_k=P_k(t,x,\eta,u)\in\mathscr{L}(Q_0^{(m)})$ is expressed by (3.14) and p_0 and A_0 in (3.14) satisfy

$$[A_0,\ M|_{u=0}]=-p_0M|_{u=0}+M_{\eta}|_{u=0}\eta. \tag{3.19}$$

Here it suffices to deduce (3.19). In fact, substituting the condition (3.14) into Eq. (3.5) and noticing $M'[\sigma_k]|_{u=0}=0$ yield (3.19) easily.

IV. PRODUCT FUNCTION MATRICES AND RELATED ALGEBRAIC STRUCTURES

In this section, we first introduce the notion of product function matrices.

Definition 4: Suppose, respectively K_l and $\sigma_k\in V^{(s)}$ are the isospectral and nonisospectral flows of the Lax integrable system associated with the linear problem (1.1) and have the unique implicit representations (3.4) and (3.5). Then

$$\langle N_l,\ N_k\rangle=N_l'[K_k]-N_k'[K_l]+[N_l,\ N_k], \tag{4.1a}$$

$$\langle N_l,P_k\rangle=N_l'[\sigma_k]-P_k'[K_l]+[N_l,P_k]+N_{l,\eta}\eta^{\alpha k+\beta}, \tag{4.1b}$$

$$\langle P_l,P_k\rangle=P_l'[\sigma_k]-P_k'[\sigma_l]+[P_l,\ P_k]+P_{l,\eta}\eta^{\alpha k+\beta}-P_{k,\eta}\eta^{\alpha l+\beta} \tag{4.1c}$$

are named three kinds of product function matrices.

Concerning the product function matrices, we give the following theorems:

Theorem 2: Suppose that $\langle N_l,\ N_k\rangle$, $\langle N_l,\ P_k\rangle$, and $\langle P_l,\ P_k\rangle$ are defined by (4.1) and $\beta-1=\alpha i_0$ (i_0 integer). Then we have

$$M'[[K_l,\ K_k]]=\langle N_l,\ N_k\rangle_x+[\langle N_l,\ N_k\rangle,\ M], \tag{4.2a}$$

$$M'[[K_l,\ \sigma_k]]=\langle N_l,\ P_k\rangle_x+[\langle N_l,\ P_k\rangle,\ M], \tag{4.2b}$$

$$M'[[\sigma_l,\ \sigma_k]]=\langle P_l,\ P_k\rangle_x+[\langle P_l,\ P_k\rangle,\ M]-\alpha(l-k)M_\eta\eta^{\alpha(l+k+i_0)+\beta}. \tag{4.2c}$$

Proof: We only prove the equality (4.2b); the other equalities (4.2a) and (4.2c) can be obtained similarly. Respectively, from the representations (3.4) and (3.5), we have

$$(M'[K_l])'[\sigma_k]=N'_{l,x}[\sigma_k]+[N'_l[\sigma_k],\ M]+[N_l,\ P_{k,x}]+[N_l,\ [P_k,\ M]]-[N_l,\ M_\eta]\eta^{\alpha k+\beta} \tag{4.3a}$$

and

$$\begin{aligned}(M'[\sigma_k])'[K_l]=&P'_{k,x}[K_l]+[P'_k[K_l],\ M]+[P_k,\ N_{l,x}]\\&+[P_k,\ [N_l,\ M]]-N_{l,x\eta}\eta^{\alpha k+\beta}-[N_l,\ M]_\eta\eta^{\alpha k+\beta}.\end{aligned} \tag{4.3b}$$

Because of

$$[N_l,\ [P_k,\ M]]-[P_k,\ [N_l,\ M]]=[[N_l,\ P_k],\ M],$$

(4.3) suggests

$$\begin{aligned}(M'[K_l])'[\sigma_k]-(M'[\sigma_k])'[K_l]=&(N'_l[\sigma_k]-P'_k[K_l]+[N_l,\ P_k]+N_{l,\eta}\eta^{\alpha k+\beta})_x\\&+[N'_l[\sigma_k]-P'_k[K_l]+[N_l,\ P_k]+N_{l,\eta}\eta^{\alpha k+\beta},\ M].\end{aligned} \tag{4.4}$$

From (4.4) and using Lemma 4 and Definition 4, we obtain (4.2b) immediately.

Theorem 3: Suppose that the matrices N_l and P_k are respectively described by (3.10) and (3.14). Then

$$\langle N_l,\ N_k\rangle|_{u=0}=0, \tag{4.5a}$$

$$\langle N_l,\ P_k\rangle|_{u=0}=(\alpha l+\mu+p_0)N_{l+k+i_0}|_{u=0}, \tag{4.5b}$$

$$\langle P_l,\ P_k\rangle|_{u=0}=\alpha(l-k)P_{l+k+i_0}|_{u=0}. \tag{4.5c}$$

Proof: By Theorem 1, we know $K_i|_{u=0}=0$ and $\sigma_j|_{u=0}=0$. Thus

$$N'_l[K_k]|_{u=0}=N'_k[K_l]|_{u=0}=N'_l[\sigma_k]|_{u=0}=0, \tag{4.6a}$$

$$P'_l[\sigma_k]|_{u=0}=P'_k[\sigma_l]|_{u=0}=P'_k[K_l]|_{u=0}=0. \tag{4.6b}$$

Recalling the condition (3.10) we obtain

$$\langle N_l,\ N_k\rangle|_{u=0}=[N_l,\ N_k]|_{u=0}=[M|_{u=0},\ M|_{u=0}]\eta^{\alpha(l+k)+2\mu}=0. \tag{4.7}$$

Next, using (3.14), we have

$$\begin{aligned}\langle N_l,\ P_k\rangle|_{u=0}=&[N_l,\ P_k]|_{u=0}+N_{l,\eta}\eta^{\alpha k+\beta}|_{u=0}\\=&[M,\ A_0]|_{u=0}\eta^{\alpha(l+k+i_0)+\mu}+M_\eta|_{u=0}\eta^{\alpha(l+k+i_0)+\mu+1}\\&+(\alpha l+\mu)M|_{u=0}\eta^{\alpha(l+k+i_0)+\mu}.\end{aligned} \tag{4.8}$$

Substitution of (3.19) into (4.8) yields (4.5b). At last, it follows from a similar argument that

$$\begin{aligned}\langle P_l,\ P_k\rangle|_{u=0}&=[P_l,\ P_k]|_{u=0}+P_{l,\eta}\eta^{\alpha k+\beta}|_{u=0}-P_{k,\eta}\eta^{\alpha l+\beta}|_{u=0}\\&=\alpha(l-k)(p_0xM|_{u=0}+A_0)\,\eta^{\alpha(l+k+i_0)+\beta-1}\\&=\alpha(l-k)P_{l+k+i_0}|_{u=0}.\end{aligned}\tag{4.9}$$

V. LIE ALGEBRAIC STRUCTURE OF THE FLOWS K_l AND σ_k

In this section, we use the equalities (4.2) and (4.5) which the product function matrices satisfy to derive the Lie algebraic structure of the flows K_l and σ_k.

Theorem 4: Suppose respectively that the isospectral flows K_l and nonisospectral flows σ_k have the unique implicit representations (3.4) and (3.5), and that N_l and P_k are described by (3.10) and (3.14). Then

$$[\![K_l,\ K_k]\!]=0,\tag{5.1a}$$

$$[\![K_l,\ \sigma_k]\!]=(\alpha l+\mu+p_0)K_{l+k+i_0},\tag{5.1b}$$

$$[\![\sigma_l,\ \sigma_k]\!]=\alpha(l-k)\sigma_{l+k+i_0}.\tag{5.1c}$$

Proof: Since the implicit representation of K_0 is unique, i.e., (3.8a) has solitary solutions, it follows that (3.15) only admits zero solutions and so does Eq. (4.2a) [under the condition (4.5a)]. That is to say, (5.1a) is valid. Next, set

$$\theta=[\![K_l,\ \sigma_k]\!]-(\alpha l+\mu+p_0)K_{l+k+i_0},\tag{5.2a}$$

$$\widetilde{N}=\langle N_l,\ P_k\rangle-(\alpha l+\mu+p_0)N_{l+k+i_0}.\tag{5.2b}$$

Obviously, $\theta\in V^{(s)}$ and $\widetilde{N}\in\mathscr{L}(Q_0^{(m)})$. By Theorem 1 we have

$$M'[K_{l+k+i_0}]=N_{l+k+i_0,x}+[N_{l+k+i_0},\ M].\tag{5.3}$$

Then it follows from (4.2b), (5.3), and (4.5b) that

$$M'[\theta]=\widetilde{N}_x+[\widetilde{N},\ M],\quad \widetilde{N}|_{u=0}=0,\tag{5.4}$$

has only zero solutions $\theta=0$ and $\widetilde{N}=0$; that means (5.1b) is true. At last, set

$$\omega=[\![\sigma_l,\ \sigma_k]\!]-\alpha(l-k)\sigma_{l+k+i_0},\tag{5.5a}$$

$$\widetilde{P}=\langle P_l,\ P_k\rangle-\alpha(l-k)P_{l+k+i_0};\tag{5.5b}$$

clearly, $\omega\in V^{(s)}$ and $\widetilde{P}\in\mathscr{L}(Q_0^{(m)})$. By Theorem 1 we also know

$$M'[\sigma_{l+k+i_0}]=P_{l+k+i_0,x}+[P_{l+k+i_0},\ M]-M_\eta\eta^{\alpha(l+k+i_0)+\beta}.\tag{5.6}$$

Similarly, (5.6) together with (4.2c) and (4.5c) yields

$$M'[\omega]=\widetilde{P}_x+[\widetilde{P},\ M],\quad \widetilde{P}|_{u=0}=0.\tag{5.7}$$

Hence we have $\omega=0$ and $\widetilde{P}=0$, which means (5.1c) is also right.

If by $\mathscr{A}$ we denote an infinite-dimensional linear space which is generated by all the isospectral flows K_l and nonisospectral flows σ_k, and by $\mathscr{A}_1$ and $\mathscr{A}_2$ denote two subspaces of $\mathscr{A}$ which

are generated respectively by all the isospectral flows K_l and nonisospectral flows σ_k, then Theorem 4 shows that $\mathscr{A}$ constitutes an infinite-dimensional Lie algebra with respect to the binary operation (2.4), and $\mathscr{A}_1$ and $\mathscr{A}_2$ are, respectively, a commutative subalgebra and a Virasoro subalgebra of $\mathscr{A}$.

Furthermore, in the above proof, we have already obtained $\langle N_l, N_k\rangle=0$, $\widetilde{N}=0$, and $\widetilde{P}=0$. Therefore, the following result holds.

Corollary 1: The function matrices N_l and P_k in the implicit representations of K_l and σ_k satisfy the following algebraic relations:

$$\langle N_l, N_k\rangle=0, \tag{5.8a}$$

$$\langle N_l, P_k\rangle=(\alpha l+\mu+p_0)N_{l+k+i_0}, \tag{5.8b}$$

$$\langle P_l, P_k\rangle=\alpha(l-k)P_{l+k+i_0}, \tag{5.8c}$$

which are similar to those of K_l and σ_k for $[\![\cdot,\cdot]\!]$.

From Theorem 4, we can still deduce K symmetry, τ symmetry, and their infinite-dimensional Lie algebra structure of a general isospectral evolution equation.

Corollary 2: The two sets of symmetries of Eq. (3.2) are K_j and $\tau_k^l=(\alpha l+\mu+p_0)tK_{l+k+i_0}+\sigma_k$, and satisfy the following Lie algebraic relations:

$$[\![K_j, K_k]\!]=0, \tag{5.9a}$$

$$[\![K_j, \tau_k^l]\!]=(\alpha j+\mu+p_0)K_{j+k+i_0}, \tag{5.9b}$$

$$[\![\tau_j^l, \tau_k^l]\!]=\alpha(j-k)\tau_{j+k+i_0}^l. \tag{5.9c}$$

VI. APPLICATION

1. To AKNS system

It is well-known that the hierarchies of isospectral and nonisospectral evolution equations of the AKNS system are

$$u_t=K_l, \quad K_l=L^l(2\gamma u) \quad (l=0,1,2,\ldots) \tag{6.1.1a}$$

and

$$u_t=\sigma_k, \quad \sigma_k=L^k(x\gamma u) \quad (k=0,1,2,\ldots), \tag{6.1.1b}$$

where K_l, and $\sigma_k\in V^{(2)}$ and L is a recursion operator given by

$$L=\tfrac{1}{2}(\gamma \mathrm{D}-2\gamma u \mathrm{I} u^T\delta), \tag{6.1.2a}$$

$$\gamma=\begin{pmatrix}-1 & 0\\ 0 & 1\end{pmatrix}, \quad \delta=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \quad u=\begin{pmatrix}q\\ r\end{pmatrix}, \tag{6.1.2b}$$

$$\mathrm{D}=\frac{\partial}{\partial x}, \quad \mathrm{I}=\int_{-\infty}^{x}\cdot\, dx, \quad \mathrm{DI}=\mathrm{ID}=1. \tag{6.1.2c}$$

Set

$$M=\begin{pmatrix} -\eta & q \\ r & \eta \end{pmatrix}. \tag{6.1.3}$$

Then the hierarchies (6.1.1) are associated with the linear problem (1.1).

Now, we explain that the flows K_l and σ_k have respectively the unique implicit representations (3.4) and (3.5) with $\alpha=1$, $\mu=-1$, $\beta=0$, $p_0=1$, and $A_0=0$.

By Theorem 1, first, we have to prove that for any given vector field $Y=(Y_1,Y_2)^T\in V^{(2)}(Y|_{u=0}=0)$, Eq. (3.6) has only a couple of solutions $X=(X_1,X_2)^T\in V^{(2)}$ and $N\in Q_0^{(2)}$ satisfying Condition (3.7). Here, $\alpha=1$ and $\mu=-1$. For this sake, write (3.6) in the following form:

$$\begin{pmatrix} 0 & X_1-\eta Y_1 \\ X_2-\eta Y_2 & 0 \end{pmatrix}=N_x+[N,\ M]. \tag{6.1.4}$$

Setting

$$N=N(t,x,u)=\begin{pmatrix} A & B \\ C & -A \end{pmatrix}, \tag{6.1.5}$$

we have

$$A_x=qC-rB, \tag{6.1.6a}$$

$$X_1-\eta Y_1=B_x+2\eta B+2qA, \tag{6.1.6b}$$

$$X_2-\eta Y_2=C_x-2\eta C-2rA. \tag{6.1.6c}$$

Comparing the coefficients of the same powers of η and noticing N independent of η yield

$$A=\mathrm{I}u^T\delta\gamma F-\delta_0,\quad Y=2\gamma F, \tag{6.1.7a}$$

$$X=2L\gamma F+2\delta_0\gamma u, \tag{6.1.7b}$$

where $F=(B,C)^T$, and δ_0 is given by (3.7b). Further, we have

$$A=\tfrac{1}{2}\,\mathrm{I}u^T\delta Y-\delta_0,\quad F=\tfrac{1}{2}\,\gamma Y, \tag{6.1.8a}$$

$$X=LY+2\delta_0\gamma u. \tag{6.1.8b}$$

It is obvious that for any given $Y\in V^{(2)}(Y|_{u=0}=0)$, the unique vector field X and unique function matrix N respectively defined by (6.1.8b) and (6.1.8a) satisfy (3.6) and (3.7). Especially, when $Y=0$ (6.1.8) gives

$$X=K_0=2\gamma u,\quad N=U_0=\gamma. \tag{6.1.9}$$

Second, by a similar discussion, it is easy to get the solutions of (3.11) with $\beta=0$, $p_0=1$, and $A_0=0$:

$$\sigma_0=x\gamma u\quad(\sigma_0|_{u=0}=0),\quad W_0=x\gamma. \tag{6.1.10}$$

From the above statements, it is shown that if we choose $\alpha=1$, $\beta=0$, $\mu=-1$, $p_0=1$, and $A_0=0$, then Theorem 4 holds for the AKNS system. That means the following:

Theorem 5: The isospectral flows K_l and nonisospectral flows σ_k of the AKNS system constitute an infinite-dimensional Lie algebra, and possess the following commutator relations (also see Ref. 4):

$$[\![K_l,\ K_k]\!]=0, \tag{6.1.11a}$$

$$[\![K_l,\ \sigma_k]\!]=lK_{l+k-1}, \tag{6.1.11b}$$

$$[\![\sigma_l,\ \sigma_k]\!]=(l-k)\sigma_{l+k-1}. \tag{6.1.11c}$$

Recalling Corollary 2 (or directly using Theorem 5) we have the following.

Corollary 3: The two sets of symmetries of the Eq. (6.1.1a) are K_j and $\tau_k^{\,l}=ltK_{l+k-1}+\sigma_k$ which constitute a Lie algebra with the following commutator relations:

$$[\![K_j,\ K_k]\!]=0, \tag{6.1.12a}$$

$$[\![K_j,\ \tau_k^{\,l}]\!]=jK_{j+k-1}, \tag{6.1.12b}$$

$$[\![\tau_j^{\,l},\ \tau_k^{\,l}]\!]=(j-k)\tau_{j+k-1}^{\,l}. \tag{6.1.12c}$$

2. To generalized HD system

In this subsection, we will consider the second-order linear spectral problem:

$$\psi_{xx}+\left(\sum_{i=0}^{h} u_i\eta^i\right)\psi=0, \quad u_h=-1. \tag{6.2.1}$$

If we set $\phi_1=\psi$, $\phi_2=\psi_x$, and $\phi=(\phi_1,\phi_2)^T$, (6.2.1) can be written in the form of (1.1a) where

$$M=\sum_{i=0}^{h} M_i\eta^i=\begin{pmatrix} 0 & 1 \\ -\sum_{i=0}^{h} u_i\eta^i & 0 \end{pmatrix}, \tag{6.2.2a}$$

$$M_i=\begin{pmatrix} 0 & \delta_{0,i} \\ -u_i & 0 \end{pmatrix} \quad (i=0,1,...,h). \tag{6.2.2b}$$

From Eq. (3.1), one can obtain the hierarchies of isospectral and nonisospectral evolution equations,[6,8,9] i.e.,

$$u_t=K_l, \quad K_l=\mathrm{D}L^l u \quad (l=0,1,2,\ldots) \tag{6.2.3a}$$

and

$$u_t=\sigma_k, \quad \sigma_k=\tfrac{1}{2}\mathrm{D}L^k(hxu+\theta \mathrm{I}u) \quad (k=0,1,2,\ldots), \tag{6.2.3b}$$

where

$$u=u(t,x)=(u_0,u_1,u_2,\ldots,u_{h-1})^T, \tag{6.2.4a}$$

$$L=\sum_{i=0}^{h-2} E_{i+1,i}+\sum_{i=0}^{h-1} J_i E_{i,h-1}, \tag{6.2.4b}$$

$$\theta=\sum_{i=0}^{h-1}(h-2i)E_{ii}, \tag{6.2.4c}$$

D and I are described by (6.1.2c). The operators J_i and the $h\times h$ matrices E_{ij} are respectively given by

$$J_i=\tfrac{1}{4}\delta_{0i}\mathrm{D}^2+u_i-\tfrac{1}{2}\mathrm{I}u_{i,x}\quad(i=0,1,...,h-1) \tag{6.2.4d}$$

and

$$(E_{ij})_{kl}=\delta_{ik}\delta_{jl}. \tag{6.2.4e}$$

For convenience, we appoint that if a vector field $Z\in V^{(h)}$, then Z has the following form:

$$Z=(Z_0,Z_1,Z_2,..,Z_{h-1})^T. \tag{6.2.5}$$

In Eq. (3.6) and Condition (3.7), we take $\alpha=1$, $\mu=0$, X and $Y\in V^{(h)}$, $N\in\mathscr{L}(Q_0^{(2)})$, and

$$N=\overline{N}+q(M-M_0),\quad \overline{N}=\begin{pmatrix}\overline{A} & \overline{B}\\ \overline{C} & -\overline{A}\end{pmatrix}, \tag{6.2.6}$$

where $\overline{A}$, $\overline{B}$, $\overline{C}$, and q are all undetermined functions independent of η. It follows that (3.6) can be written as

$$M'[X-\eta Y]=(\overline{N}+q(M-M_0))_x+[\overline{N},\,M]-q[M_0,\,M]. \tag{6.2.7}$$

Substituting (6.2.2a) into (6.2.7) and comparing the coefficients of the same powers of η yield

$$M_0'[X]=\overline{N}_x+[\overline{N},\,M_0], \tag{6.2.8a}$$

$$M_i'[X]-M_{i-1}'[Y]=(qM_i)_x+[\overline{N},\,M_i]-q[M_0,\,M_i]\quad(i=1,2,...,h-1), \tag{6.2.8b}$$

$$-M_{h-1}'[Y]=(qM_h)_x+[\overline{N},\,M_h]-q[M_0,\,M_h]. \tag{6.2.8c}$$

From (6.2.8a), (6.2.8b), and (6.2.8c), respectively, we have

$$\overline{A}_x=u_0\overline{B}+\overline{C},\quad \overline{B}_x+2\overline{A}=0,\quad X_0=-\overline{C}_x-2u_0\overline{A}, \tag{6.2.9a}$$

$$q=\overline{B},\quad X_i=2\mathrm{D}J_i\overline{B}+Y_{i-1} \tag{6.2.9b}$$

and

$$\overline{B}=\tfrac{1}{2}\mathrm{I}Y_{h-1}+\delta_0, \tag{6.2.9c}$$

where (6.2.9a) implies

$$X_0=2\mathrm{D}J_0\overline{B}. \tag{6.2.10}$$

Substituting (6.2.9c) into (6.2.9a), (6.2.9b), and (6.2.10), we obtain easily

$$\overline{A}=-\tfrac{1}{4}Y_{h-1}, \tag{6.2.11a}$$

$$q=\overline{B}=\tfrac{1}{2}\mathrm{I}Y_{h-1}+\delta_0, \tag{6.2.11b}$$

$$\overline{C}=-\tfrac{1}{4}\big(D+2u_0\mathrm{I}\big)Y_{h-1}-\delta_0 u_0, \tag{6.2.11c}$$

and

$$X=\mathrm{D}LIY+\delta_0 u_x, \tag{6.2.11d}$$

where δ_0 is given by (3.7b). By now, we have proved that for any given $Y\in V^{(h)}(Y|_{u=0}=0)$, the unique vector field $X\in V^{(h)}$ and unique function matrix $N\in\mathscr{G}(Q_0^{(2)})$ respectively defined by (6.2.11d) and (6.2.11a)–(6.2.11c) satisfy (3.6) and (3.7). In particular, when $Y=0$, we obtain

$$X=K_0=u_x, \quad N=U_0=M. \tag{6.2.12}$$

Next, in order to find the solutions of (3.11), we take

$$W_0=\widetilde{W}_0+\widetilde{q}(M-M_0), \quad \widetilde{W}_0=\begin{pmatrix}\widetilde{A}_0 & \widetilde{B}_0\\ \widetilde{C}_0 & -\widetilde{A}_0\end{pmatrix} \tag{6.2.13}$$

and $\widetilde{W}_0$ is independent of η. Substituting (6.2.13) into (3.11a) (with $\beta=1$) and comparing the coefficients of the same powers of η lead to

$$M_0'[\sigma_0]=\widetilde{W}_{0,x}+[\widetilde{W}_0,\ M_0], \tag{6.2.14a}$$

$$M_i'[\sigma_0]=(\widetilde{q}M_i)_x+[\widetilde{W}_0,\ M_i]-\widetilde{q}[M_0,\ M_i]-iM_i \quad (i=1,2,...,h-1), \tag{6.2.14b}$$

$$0=(\widetilde{q}M_h)_x+[\widetilde{W}_0,\ M_h]-\widetilde{q}[M_0,\ M_h]-hM_h. \tag{6.2.14c}$$

From these equalities, an argument similar to above yields

$$\sigma_0=\tfrac{1}{2}\mathrm{D}(hxu+\theta\mathrm{I}u) \quad (\sigma_0|_{u=0}=0), \quad W_0=\frac{h}{4}(\gamma+2xM), \tag{6.2.15}$$

which meet (3.11) with $p_0=h/2$ and $A_0=h\gamma/4$, where θ and γ are given by (6.2.4c) and (6.1.2b), respectively.

So it follows from Theorem 1 that the flows K_l and σ_k possess respectively the unique implicit representations (3.4) and (3.5).

In light of the results described in Sec. V, we obtain immediately the following.

Theorem 6: The isospectral flows K_l and nonisospectral flows σ_k of the generalized HD system associated with the linear problem (1.1) [in which M is given by (6.2.2)] constitute an infinite-dimensional Lie algebra, and possess the following commutator relations (also see Ref. 6):

$$[\![K_l,\ K_k]\!]=0, \tag{6.2.16a}$$

$$[\![K_l,\ \sigma_k]\!]=\Big(l+\frac{h}{2}\Big)K_{l+k}, \tag{6.2.16b}$$

$$[\![\sigma_l,\ \sigma_k]\!]=(l-k)\sigma_{l+k}. \tag{6.2.16c}$$

Corollary 4: The two sets of symmetries of Eq. (6.2.3a) are K_j and $\tau_k^{\,l}=(l+h/2)tK_{l+k}+\sigma_k$ which constitute a Lie algebra with the following relations:

$$[\![K_j,\ K_k]\!]=0, \tag{6.2.17a}$$

$$[\![K_j,\ \tau^{\ l}_k]\!]=\left(j+\frac{h}{2}\right)K_{j+k}, \tag{6.2.17b}$$

$$[\![\tau^{\ l}_j,\ \tau^{\ l}_k]\!]=(j-k)\tau^{\ l}_{j+k}. \tag{6.2.17c}$$

3. To *n*-wave interaction system

In the linear problem (1.1), set

$$M=\eta H+S \tag{6.3.1}$$

and $H,\ S\ \in Q_0^{(n)}$ and $N\in\mathscr{S}(Q_0^{(n)})$ where H is a constant diagonal matrix:

$$H=\mathrm{diag}(h_1,h_2,h_3,\ldots,h_n)\quad (h_i\neq h_j, i\neq j), \tag{6.3.2a}$$

$$S=S(t,x,u)=\sum_{i,j=1\ i\neq j}^{n} u_{ij}E_{ij}, \tag{6.3.2b}$$

in which the vector field $u\ \in\ V^{(n(n-1))}$ is described by

$$u=(u_{12},u_{13},\ldots,u_{1n},u_{21},u_{23},\ldots,u_{ij},\ldots,u_{n,n-1})^T\quad (i\neq j). \tag{6.3.2c}$$

The $n(n-1)$ u_{ij}'s are nonzero functionally independent potentials and the $n\times n$ matrices E_{ij}'s are given by (6.2.4e).

Then, from the compatible condition (3.1) of (1.1), we can obtain isospectral and nonisospectral flows K_l and σ_k of the n-wave interaction system. In a general way, it is very difficult to write these flows in the form $K_l=\Phi^l K_0$ and $\sigma_k=\Phi^k\sigma_0$, where $\Phi\ \in\ Q^{(n(n-1))}$ is some operator. Therefore, Ma's method (see Ref. 3) cannot be applied to construct the flows' Lie algebra for this kind of Lax integrable system. However, our method has such advantage indeed, because we derive the isospectral and nonisospectral flows and their Lie algebraic properties without using the recursion operator Φ of the integrable system.

In fact, by Theorem 4, we only need to prove that there exist respectively the unique implicit representations (3.4) and (3.5) for flows K_l and σ_k of the n-wave interaction system.

For simplicity, in what follows, we make the appointment that

$$Z=(Z_{12},Z_{13},\ldots,Z_{1n},Z_{21},Z_{23},\ldots,Z_{ij},\ldots,Z_{n,n-1})^T\quad (i\neq j), \tag{6.3.3}$$

if vector field $Z\ \in\ V^{(n(n-1))}$.

Now, in Eq. (3.6) and the condition (3.7), for any given $Y\ =\ Y(t,x,u)\ \in\ V^{(n(n-1))}(Y|_{u=0}\ =\ 0)$, we take $X\ =\ X(t,x,u)\ \in\ V^{(n(n-1))}$ $N=N(t,x,u)\in Q_0^{(n)}$ and $\alpha=1$, $\mu=-1$. Then (3.6) can be written in the form

$$S'[X]-\eta S'[Y]=N_x+\eta[N,\ H]+[N,\ S]. \tag{6.3.4}$$

Comparison of the coefficients of the same powers of η in the above equality yields

$$\sum_{i,j=1 i\neq j}^{n} X_{ij}E_{ij}=N_x+[N,\ S],\qquad \sum_{i,j=1 i\neq j}^{n} Y_{ij}E_{ij}=[H,\ N]. \tag{6.3.5}$$

Further, let I and δ_0 be described respectively by (6.1.2c) and (3.7b). We have

$$N_{ij}=\frac{Y_{ij}}{h_i-h_j}\quad (i\neq j), \tag{6.3.6a}$$

$$N_{ii}=\mathrm{I}\sum_{k=1,k\neq i}^{n}\frac{u_{ki}Y_{ik}+u_{ik}Y_{ki}}{h_k-h_i}+\delta_0 h_i, \tag{6.3.6b}$$

and

$$\begin{aligned}X_{ij}=&\frac{Y_{ij,x}}{h_i-h_j}+\sum_{k=1,k\neq i,j}^{n}\left(\frac{u_{kj}Y_{ik}}{h_i-h_k}-\frac{u_{ik}Y_{kj}}{h_k-h_j}\right)\\&+u_{ij}\mathrm{I}\left(\sum_{k=1,k\neq i}^{n}\frac{u_{ki}Y_{ik}+u_{ik}Y_{ki}}{h_k-h_i}-\sum_{k=1,k\neq j}^{n}\frac{u_{kj}Y_{jk}+u_{jk}Y_{kj}}{h_k-h_j}\right)\\&+u_{ij}\delta_0(h_i-h_j)\quad(i\neq j),\end{aligned} \tag{6.3.6c}$$

which immediately shows that for any given vector field $Y\in V^{(n(n-1))}(Y|_{u=0}=0)$. Equation (3.6) has unique solutions X and N satisfying the condition (3.7), and in particular, if $Y=0$, the solutions X and N are given respectively by

$$X=K_0,\quad K_{0ij}=(h_i-h_j)u_{ij}\quad(i\neq j), \tag{6.3.7a}$$

and

$$N=U_0=H. \tag{6.3.7b}$$

Second, taking $\beta=0$, $p_0=1$, and $A_0=0$ in (3.11), we have

$$S'[\sigma_0]=W_{0,x}+\eta[W_0,\,H]+[W_0,\,S]-H. \tag{6.3.8}$$

Here, $\sigma_0\in V^{(n(n-1))}$ and $W_0\in Q_0^{(n)}$ are all independent of η. Equation (6.3.8) implies

$$\sum_{i,j=1i\neq j}^{n}\sigma_{0ij}E_{ij}=W_{0,x}+[W_0,\,S]-H,\quad[W_0,\,H]=0, \tag{6.3.9}$$

which suggests a couple of solutions σ_0 and W_0 described respectively by

$$\sigma_{0ij}=(h_i-h_j)xu_{ij}\quad(i\neq j,\sigma_0|_{u=0}=0) \tag{6.3.10a}$$

and

$$W_0=xH. \tag{6.3.10b}$$

So we have shown that the conditions of Theorem 1 are satisfied for the n-wave interaction system. That is to say, the flows K_l and σ_k of this system can be generated by (3.8), and (3.11), and (3.12), respectively and have their unique implicit representations.

Further, according to the results of Sec. V, we have the following.

Theorem 7: The isospectral flows $K_l\in V^{(n(n-1))}$ and nonisospectral flows $\sigma_k\in V^{(n(n-1))}$ of the n-wave interaction system associated with the linear problem (1.1) [in which M is described by (6.3.1)] constitute an infinite-dimensional Lie algebra, and possess the following commutator relations:

$$[K_l,\,K_k]=0, \tag{6.3.11a}$$

$$[K_l,\,\sigma_k]=lK_{l+k-1}, \tag{6.3.11b}$$

$$[\sigma_l,\ \sigma_k]=(l-k)\sigma_{l+k-1}. \tag{6.3.11c}$$

Theorem 7 shows that the flows' commutator relations of the n-wave interaction system are independent of wave number n. Therefore, if set $n=2$ and $h_1=-h_2=1$, then (6.3.11a)–(6.3.11c) becomes (6.1.11a)–(6.1.11c). That is to say, isospectral flows K_l and nonisospectral flows σ_k of the n-wave interaction system constitute the same infinite-dimensional Lie algebraic structure as the AKNS system. The similar conclusion for symmetries of the two systems is also valid. So we have the following.

Corollary 5: The two sets of symmetries of the isospectral equation $u_t=K_l$ are K_j and $\tau_k^{\,l}=ltK_{l+k-1}+\sigma_k$, which constitute a Lie algebra with the following relations:

$$[K_j,\ K_k]=0, \tag{6.3.12a}$$

$$[K_j,\ \tau_k^{\,l}]=jK_{j+k-1}, \tag{6.3.12b}$$

$$[\tau_j^{\,l},\ \tau_k^{\,l}]=(j-k)\tau_{j+k-1}^{\,l}. \tag{6.3.12c}$$

As mentioned earlier, it is not easy to derive the general explicit expressions of the flows K_l and σ_k of the n-wave interaction system, which leads to the algebraic properties of these flows and related symmetries have not been reported in any literature up to now. So we have enough reason to believe that Theorem 7 and *Corollary 5* obtained by means of the so-called ''implicit representations'' are new results.

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On the polynomial first integrals of the (a,b,c) Lotka–Volterra system

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Using elementary differential algebraic techniques, we prove that the 3D Lotka–Volterra dynamical system has no other nontrivial polynomial first integrals than the previously known ones. © *1996 American Institute of Physics.*
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I. INTRODUCTION

The (a,b,c) or 3D Lotka–Volterra dynamical system[1,2]

$$\dot{x}=x(cy+z), \quad \dot{y}=y(az+x), \quad \dot{z}=z(bx+y), \tag{1}$$

where (a,b,c) are three real (or complex) parameters, appears in various areas of science such as ecology (in which it models a three-species competition), plasma physics (in which it approximates the Vlasov–Poisson equation), and so on.

It can be generalized by adding an isotropic linear damping term. Indeed, the dynamical system

$$\dot{x}=x(\lambda+cy+z), \quad \dot{y}=y(\mu+az+x), \quad \dot{z}=z(\nu+bx+y), \tag{2}$$

reduces to Eq. (1), if $\lambda=\mu=\nu$, by setting

$$x'=xe^{-\lambda t}, \quad y'=ye^{-\lambda t}, \quad z'=ze^{-\lambda t}, \quad t'=e^{\lambda t},$$

and then dropping the primes. It may be worth noticing that the linear term isotropy is a necessary condition for Eq. (2) to have the Painlevé property.[3]

Up to now, using various techniques (extension of the Lie symmetry method,[4] Painlevé analysis[3]), the following cases of polynomial integrability of the system (1) have been found (see Refs. 4 and 5 for further matter):

1. $abc=-1\Rightarrow I=x-cy-b^{-1}z$;

2. $abc=-1\Rightarrow I=x^{ab}y^{-b}z$; one sees that this integral can be made a polynomial iff $(a,b,c)\in(\mathbf{Q}^{-})^3$;

3. $abc=1$ and $a=-(c+1)^{-1}$ and $b=-(c+1)/c\Rightarrow I=x^2+c^2y^2+c^2(c+1)^{-2}z^2-2cxy+2c^2(c+1)^{-1}xz+2c(c+1)^{-1}yz$.

The aim of this paper is to show that there are no other cases of polynomial integrability and no other polynomial first integrals than these ones and their combinations when the parameters are real, which is the case in the biological and physical applications. We will prove this result in the following way. In Sec. II, we recall the definition and the general properties of the Darboux polynomials of a polynomial dynamical system. Then we establish some useful features of the Darboux polynomials of the Lotka–Volterra system. Section III is devoted to the proof of the result itself; and Sec. IV summarizes our results.

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II. ON THE DARBOUX POLYNOMIALS OF THE LOTKA–VOLTERRA SYSTEM

Consider an autonomous polynomial dynamical system

$$\dot{x}_i = V_i(x_1,\ldots,x_n), \quad i = 1\cdots n. \tag{3}$$

It induces a derivation D—i.e., a linear endomorphism such that $D(fg)=D(f)g+fD(g)$—on the space of real (or complex) polynomials in n variables, called *derivation associated to (or with respect to) the system* (3), which reads

$$Df = \sum_{i=1}^{n} f_{x_i} V_i .$$

Then a Darboux polynomial[6] of Eq. (3) is a polynomial $f(x_1,\ldots,x_n)$ such that there is another polynomial $p(x_1,\ldots,x_n)$ satisfying $Df=pf$. The couple (p,f) may also be called a *Darboux element*. The following properties of Darboux elements can be shown easily:

(1) If m is the greatest of deg V_i, $i=1\cdots n$, then deg $p \leqslant m-1$.
(2) The product of two Darboux polynomials is still Darboux, namely ($Df_1=p_1f_1$ and $Df_2=p_2f_2$)$\Rightarrow D(f_1f_2)=(p_1+p_2)(f_1f_2)$. This can be generalized to any number of factors.
(3) All the irreducible factors of a Darboux polynomial are Darboux. Thus the search for Darboux polynomials can be restricted to irreducible f.
(4) If the dynamical system (3) is homogeneous of degree m, i.e., all V_i are homogeneous of degree m, then p is homogeneous of degree m—1 and all homogeneous components of f are Darboux. Thus the search can be restricted to homogeneous f.

Darboux polynomials give rise to numerous (polynomial or not) first integral search techniques for polynomial dynamical systems, such as the Prelle–Singer procedure.[7] Indeed a polynomial first integral f is a Darboux polynomial with $p=0$. Up to now, only semidecisive procedures are known; however it is possible to find a reciprocal for some dynamical systems. This shall we undertake with the (a,b,c) system, using its homogeneity and symmetry properties.

These properties yield first that for any Darboux element (p,f), p is homogeneous of first degree and f can be taken homogeneous; so the definition equation for the Darboux polynomials of (1) is

$$x(cy+z)f_x + y(az+x)f_y + z(bx+y)f_z = (\alpha x+\beta y+\gamma z)f, \tag{4}$$

where α, β, γ as well as the coefficients of f are *a priori* complex. For a Darboux polynomial f, the coefficients α, β, γ in Eq. (4) may be denoted $\alpha(f),\beta(f),\gamma(f)$.

The following statements are evident:

• The Lotka–Volterra system (1) is invariant by simultaneous cyclical permutations of (x,y,z) and (a,b,c); and identically Eq. (4) is invariant by simultaneous cyclical permutations of (x,y,z), (a,b,c), and (α,β,γ).

• x, y, and z—and thus all monomials—are Darboux polynomials of the system (1).

The following notations will be of constant use. For any polynomial $g(x,y,z)$ we shall write $\hat{g}(y,z)=g(0,y,z)$, $\widetilde{g}(x,z)=g(x,0,z)$, $\overline{g}(x,y)=g(x,y,0)$. These restriction operators commute with derivation with respect to the *other* variables.

Proposition 2.1: Let f be a (homogeneous) solution of degree m to Eq. (4). Then if $\gamma\neq 0$, f has no z^m term and thus reads $f(x,y,z)=x\varphi(x,y,z)+y\psi(x,y,z)$.

Since the polynomial f is homogeneous, we use Euler's theorem:

$$xf_x + yf_y + zf_z = mf.$$

Eliminating, e.g., f_x between this equality and Eq. (4), we find that

$$yf_y(az+x-cy-z)+zf_z(bx+y-cy-z)=[\alpha x+(\beta-mc)y+(\gamma-m)z]f.$$

Setting $x=0$ and $y=0$ [and $F(z)=f(0,0,z)$] yields

$$-z^2F'(z)=(\gamma-m)zF(z),$$

thus $F=\lambda z^{m-\gamma}$. But, as f is homogeneous of degree m, the only term containing only z is necessarily z^m. Hence, if $\gamma\neq 0$, we have $F=0$, which means that $f(x,y,z)$ is in the ideal generated by x and y.

Proposition 2.2: Let f be a solution of Eq. (4). Then $(\gamma\notin\mathbf{N}\Rightarrow y|f)$ *and* $(\gamma\notin a\mathbf{N}\Rightarrow x|f)$, *and, cyclically*:

- $(\beta\notin\mathbf{N}\Rightarrow x|f)$ and $(\beta\notin c\mathbf{N}\Rightarrow z|f)$;
- $(\alpha\notin\mathbf{N}\Rightarrow z|f)$ and $(\alpha\notin b\mathbf{N}\Rightarrow y|f)$.

If $\gamma\notin\mathbf{N}$ or $\gamma\notin a\mathbf{N}$, then $\gamma\neq 0$, and thus $f(x,y,z)=x\varphi(x,y,z)+y\psi(x,y,z)$. Setting this in Eq. (4) yields

$$xD\varphi+yD\psi=(\alpha x+\beta y+\gamma z-cy-z)x\varphi+(\alpha x+\beta y+\gamma z-az-x)y\psi. \tag{5}$$

Suppose $\gamma\notin\mathbf{N}$. Set $y=0$ in Eq. (5):

$$x\widetilde{D\varphi}=(\alpha x+(\gamma-1)z)x\widetilde{\varphi}.$$

The operator $\varphi\mapsto\widetilde{\varphi}$ commutes with the derivations with respect to x and z, hence

$$xz\left(\frac{\partial\widetilde{\varphi}}{\partial x}+b\,\frac{\partial\widetilde{\varphi}}{\partial z}\right)=(\alpha x+(\gamma-1)z)\widetilde{\varphi}. \tag{6}$$

So x divides the right-hand side; since $\gamma\notin\mathbf{N}$, $\gamma-1\neq 0$, and x does not divide $[ax+(\gamma-1)z]$. Thus $x|\widetilde{\varphi}$.

Setting $\widetilde{\varphi}=x\varphi_1$ we get

$$\frac{\partial\widetilde{\varphi}}{\partial x}=x\,\frac{\partial\varphi_1}{\partial x}+\varphi_1,\quad \frac{\partial\widetilde{\varphi}}{\partial z}=x\,\frac{\partial\varphi_1}{\partial z},$$

and Eq. (6), after some calculations, may be rewritten as

$$xz\left(\frac{\partial\varphi_1}{\partial x}+b\,\frac{\partial\varphi_1}{\partial z}\right)=[\alpha x+(\gamma-2)z]\varphi_1.$$

Since $\gamma\neq 2$, one has $x|\varphi_1$, so $x^2|\widetilde{\varphi}$; and if $\gamma\notin\mathbf{N}$ the same argument can be repeated indefinitely. The polynomial $\widetilde{\varphi}$ is divisible by any power of x, hence is zero. As $\widetilde{\varphi}(x,z)=\varphi(x,0,z)$, this means that φ is divisible by y; hence $f=x\varphi+y\psi$ is divisible by y. QED.

If we now assume $\gamma\notin a\mathbf{N}$, setting $x=0$ in Eq. (5) yields

$$yz\left(a\,\frac{\partial\hat{\psi}}{\partial y}+\frac{\partial\hat{\psi}}{\partial z}\right)=[\beta y+(\gamma-a)z]\widetilde{\varphi}.$$

By recurrence it can be shown as above that $\hat{\psi}$ is divisible by any power of y, hence is zero, hence that $x|\psi$ and f is divisible by x.

This leads to the following statement, a characterization of the ''eigenvalues'' of the Darboux polynomials of the system (1), which will be a fundamental tool for proving our main result.

Proposition 2.3: Let f be a nonzero Darboux polynomial. Then there exist two positive integers γ_1 and γ_2 such that $\gamma=\gamma_1+\gamma_2 a$.

Suppose $\gamma \notin \mathbf{N}+\mathbf{N}a$. So $\gamma \notin \mathbf{N}$ and $\gamma \notin Na$. Hence by Proposition 2.2 f is divisible by x:

$$f = xf_1 \quad \text{and} \quad Df_1 = [\alpha x + \beta y + (\gamma - 1)z]f_1.$$

But $\gamma - 1$ cannot be in $\mathbf{N}+\mathbf{N}a$ unless γ be in it. As this procedure can be repeated indefinitely, f may be divided by an infinity of powers of x, hence is zero. Contradiction.

This result allows to classify all the Darboux polynomials of Eq. (1) when $(a,b,c) \in (\mathbf{R}\backslash\mathbf{Q}^+)^3$, as is shown in the two following propositions.

Proposition 2.4: Let f be a solution of Eq. (4). If a is neither zero nor a positive rational number, then f reads

$$f = x^{\gamma_1} y^{\gamma_2} f_1, \tag{7}$$

where the positive integers γ_1 and γ_2 satisfy $\gamma(f) = \gamma_1 + a\gamma_2$ and f_1 is a solution to Eq. (4) such that $\gamma(f_1) = 0$.

If $a \notin \mathbf{Q}^+$, $\mathbf{N} \cap \mathbf{N}a = \{0\}$. If γ is zero, setting $\gamma_1 = \gamma_2 = 0$ yields the result. If not, then either $\gamma \notin \mathbf{N}$ or $\gamma \notin \mathbf{N}a$. Assume $\gamma \notin \mathbf{N}$; f can be divided by y. Let this procedure be repeated as many times as it can, and let γ_2 be the number of times it can. We have $f = y^{\gamma_2} f_0$, and f_0 is solution to Eq. (4) with $\gamma(f_0) = \gamma(f) - a\gamma_2$. This $\gamma_1 = \gamma(f_0)$ must be integer since we had to stop the division procedure of f by y.

Thus either $\gamma_1 = 0$ or $\gamma_1 \notin \mathbf{N}a$. In the first case, Eq. (7) is satisfied with $f_1 = f_0$. In the second case, f_0 can be divided γ_1 times by x, and Eq. (7) is satisfied with $f_1 = f_0 / x^{\gamma_1}$.

Assume now $\gamma \in \mathbf{N}^*$; applying only the second step of the above procedure yields the same conclusion. In both cases, it follows from the basic properties of Darboux polynomials that f_0 is solution to Eq. (4) with $\gamma(f_0) = 0$ and that $\gamma(f) = \gamma_1 + a\gamma_2$.

Theorem 2.5: *Let f be a solution of Eq. (4). If none of the three system parameters is zero or a positive rational number, then there exist three positive integers p,q,r and a polynomial first integral I of Eq. (1)—which may be trivial—such that*

$$f = x^p y^q z^r I \tag{8}$$

and

$$\alpha = q + br, \quad \beta = r + cp, \quad \gamma = p + aq. \tag{9}$$

By cyclical permutations Proposition 2.4 can be rewritten as statements on α and β. These three results will be successively used in the following algorithm:

(1) Set $n = 0$ and $f_n = f$.
(2) Applying Proposition 2.4 for α yields
$$f_n = y^{\alpha_1} z^{\alpha_2} f_{n+1}, \quad \alpha(f_{n+1}) = 0.$$
(3) If f_{n+1} is a first integral, go to the final step, else increment n by one.
(4) Applying Proposition 2.4 for β yields
$$f_n = z^{\beta_1} x^{\beta_2} f_{n+1}, \quad \beta(f_{n+1}) = 0.$$
(5) If f_{n+1} is a first integral, go to the final step, else increment n by one.
(6) Applying Proposition 2.4 for γ yields
$$f_n = x^{\gamma_1} y^{\gamma_2} f_{n+1}, \quad \gamma(f_{n+1}) = 0.$$
(7) If f_{n+1} is a first integral, go to the final step, else increment n by one and return to step 2.
(8) (Final step) Set $I = f_{n+1}$ and, using the sequence of equations linking f_i to f_{i+1}, $i = 1 \cdots n$ given by the algorithm, determine the exponents (p,q,r) in Eq. (8).

At every step, one has $\deg f_{i+1} \leqslant \deg f_i$; and when three consecutive terms of the sequence are of same degree, they are equal and $\alpha(f_i)=\beta(f_i)=\gamma(f_i)=0$, so f_i is a first integral. Thus the algorithm converges in a finite number of steps. Once the existence of (p,q,r) is proven, Eq. (9) follow by the basic properties of Darboux polynomials.

III. POLYNOMIAL FIRST INTEGRALS

Proposition 3.1 Let f be a polynomial first integral of degree m with a nonzero z^m term. Then a must be nonzero and there exists a polynomial $k(x,y,z)$ such that

$$f=\lambda\left[(z-bx)^m+\left(z-\frac{y}{a}\right)^m-z^m\right]+xyk(x,y,z).$$

The homogeneity of f yields $f(x,y,z)=x\varphi(x,y,z)+y\psi(x,y,z)+\lambda z^m$. Thus, $Df=0$ reads

$$xD\varphi+yD\psi=-(cy+z)x\varphi-(az+x)y\psi-\lambda(mbx+my)z^m. \tag{10}$$

Set $y=0$ in Eq. (10)

$$\widetilde{xD\varphi}=-zx\widetilde{\varphi}-\lambda mbxz^m.$$

Simplifying by x we get after some calculations:

$$xz\left(\frac{\partial\widetilde{\varphi}}{\partial x}+b\,\frac{\partial\widetilde{\varphi}}{\partial z}\right)=-z\widetilde{\varphi}-\lambda mbz^m. \tag{11}$$

This shows that

$$x\,|-\widetilde{\varphi}-\lambda mbz^{m-1}.$$

Hence we set

$$\varphi_0=\widetilde{\varphi}=x\varphi_1-\lambda mbz^{m-1},$$

then the derivatives of $\widetilde{\varphi}$ are

$$\frac{\partial\widetilde{\varphi}}{\partial x}=x\,\frac{\partial\varphi_1}{\partial x}+\varphi_1,\quad \frac{\partial\widetilde{\varphi}}{\partial z}=x\,\frac{\partial\varphi_1}{\partial z}-\lambda(m-1)mbz^{m-2}.$$

Putting these expressions in Eq. (11) gives

$$xz\left(x\,\frac{\partial\varphi_1}{\partial x}+\varphi_1+b\,\frac{\partial\varphi_1}{\partial z}\right)=-zx\varphi_1-z\lambda(-mb)z^{m-1}-\lambda mbz^m.$$

The last two terms compensate; in all other terms x is in factor and we simplify:

$$xz\left(\frac{\partial\varphi_1}{\partial x}+b\,\frac{\partial\varphi_1}{\partial z}\right)=-2z\varphi_1+\lambda mb(m-1)bz^{m-1}.$$

By recurrence, we get a sequence of PDE,

$$xz\left(\frac{\partial\varphi_k}{\partial x}+b\,\frac{\partial\varphi_k}{\partial z}\right)=-(k+1)z\varphi_k+\lambda(k+1)(-b)^{k+1}C_m^{k+1}z^{m-k}, \tag{12}$$

linked by the recurrence formula

$$\varphi_{k-1}=x\varphi_k+\lambda(-b)^k C_m^k z^{m-k}. \tag{13}$$

As $\deg\varphi_0=\deg\varphi=m-1$, this formula shows that $\deg\varphi_k=m-1-k$; thus $\deg\varphi_{m-1}=0$ and $\varphi_{m-1}=C=\text{cst}$. Then Eq. (12) reads

$$xz0=-mzC+\lambda m(-b)^m z^1$$

or $C=\lambda(-b)^m$. Hence the sequence of Eq. (13) yields finally

$$\tilde{\varphi}=\lambda\sum_{k=0}^{m-1} x^k(-b)^{k+1}C_m^{k+1}z^{m-1-k}$$

or, since $\tilde{\varphi}=\varphi(.,0,.)$:

$$\varphi=\frac{\lambda}{x}\left[(z-bx)^m-z^m\right]+yK_1(x,y,z). \tag{14}$$

We now determine ψ similarly. Setting $x=0$ in Eq. (10) yields

$$yz\left(a\,\frac{\partial\hat{\psi}}{\partial y}+\frac{\partial\hat{\psi}}{\partial z}\right)=-az\hat{\psi}+\lambda(-m)z^m. \tag{15}$$

Thus,

$$y|-a\hat{\psi}+\lambda(-m)z^{m-1}.$$

This shows $a\neq 0$, otherwise we get the contradiction $y|\lambda z^{m-1}$ with $\lambda\neq 0$. Now, Eq. (15) is integrated by a method similar to that used for Eq. (11). So we find that

$$\psi=\frac{\lambda}{y}\left[\left(z-\frac{y}{a}\right)^m-z^m\right]+xK_2(x,y,z).$$

Since $f=x\varphi+y\psi+\lambda z^m$ we have

$$f=\lambda_1[(z-bx)^m+(z-y/a)^m-z^m]+xyk_1(x,y,z), \tag{16}$$

which we had to prove.

Using the variable and coefficient symmetry, we get the following results:

• if f is a polynomial first integral with nonzero y^m term then $c\neq 0$ and

$$f=\lambda_2[(y-az)^m+(y-x/c)^m-y^m]+xzk_2(x,y,z), \tag{17}$$

• if f is a polynomial first integral with nonzero x^m term then $b\neq 0$ and

$$f=\lambda_3[(x-cy)^m+(x-z/b)^m-x^m]+zyk_3(x,y,z). \tag{18}$$

These facts yield a first distinction between polynomial first integrals.

Proposition 3.2: Let f be a polynomial first integral of degree m of (1). Then the coefficients of x^m, y^m, z^m—which we will call the extremal terms*—are either all zero or all nonzero.*

Assume that the z^m term is zero, i.e., $f=x\varphi+y\psi$. The equivalent of Eq. (11) in that case is

$$xz\left(\frac{\partial\tilde{\varphi}}{\partial x}+b\,\frac{\partial\tilde{\varphi}}{\partial z}\right)=-z\tilde{\varphi}.$$

Thus, $x|\widetilde{\varphi}$, then repeating the proof of Proposition 2.2 yields $\widetilde{\varphi}=0$; or $y|\varphi$ and thus $y|f$. In particular the x^m term in f is zero.

Suppose the coefficient of y^m is nonzero. Then $c\neq 0$ and Eq. (17) shows that the coefficient of x^m is nonzero. Contradiction.

The variable symmetry allows to complete the proof: if any of the extremal terms is zero, so are the other two. QED.

The first integrals with no extremal terms are characterized by the following statement.

Proposition 3.3: Let f be a polynomial first integral of degree m, with no x^m, y^m, z^m terms. Then:

• *the system parameters (a,b,c) are negative rational numbers whose product is -1;*

• *we have $f=x^p y^q z^r I$, where I is another polynomial first integral—which may be trivial—and (p,q,r) satisfy Eq. (9) with $\alpha=\beta=\gamma=0$, i.e.,*

$$q+br=0, \quad r+cp=0, \quad p+aq=0. \tag{19}$$

If f has no extremal terms, it reads

$$f(x,y,z)=xy\varphi(x,y,z)+xz\chi(x,z)+yz\psi(y,z),$$

i.e., all terms divisible by xyz have been put in φ. Then $Df=0$ yields

$$\begin{aligned}&(bx+y)z(x\chi+y\psi+xz\chi_z+yz\psi_z+xy\varphi_z)+y(x+az)(x\varphi+z\psi+yz\psi_y+xy\varphi_y)\\&+x(cy+z)(z\chi+y\varphi+xz\chi_x+xy\varphi_x)=0,\end{aligned} \tag{20}$$

thus, setting $x=0$,

$$(y+az)\psi+yz(a\psi_y+\psi_z)=0.$$

Hence we have $z|\psi$; by recurrence we can show that ψ is divisible by any power of z. Thus $\psi=0$.

If similarly we set $y=0$ in Eq. (20), we get

$$(bx+z)\chi+xz(\chi_x+g\chi_z)=0.$$

Hence $x|\chi$; by recurrence we show that χ is divisible by any power of x. Thus $\chi=0$.

Finally, replacing z with 0 in Eq. (20) yields

$$(x+cy)\overline{\varphi}+xy(c\overline{\varphi_x}+\overline{\varphi_y})=0.$$

Hence $\overline{\varphi}=0$, which means $\varphi=zQ$. Thus we have $f=xyzQ$. Then $Df=0$ reads

$$xyzDQ+[(1+b)x+(1+c)y+(1+a)z]xyzQ=0.$$

By definition, Q is thus a Darboux polynomial with $\alpha(Q)=-(1+b)$, $\beta(Q)=-(1+c)$, $\gamma(Q)=-(1+a)$. Proposition 2.3 shows that the parameters (a,b,c) are strictly negative. Indeed, if, e.g., $a\geqslant 0$, it yields $\gamma\geqslant 0$, but $\gamma=-1-a<0$. Hence Theorem 2.5 holds for Q and $Q=x^{p_1}y^{q_1}z^{r_1}I$. Hence $f=x^p y^q z^r I$ with $p=p_1+1$, etc.

We check that (a,b,c) satisfy Eq. (19). Those imply $a,b,c\in\mathbf{Q}^-$, since p,q,r are positive integer numbers. Moreover, in order for this linear system to admit a nonzero solution (p,q,r), it is necessary that its determinant be zero; but this determinant is precisely $abc+1$. QED.

As for the first integrals with extremal terms, we shall prove that when (a,b,c) are real the condition $abc=\pm 1$ is a necessary one for their existence.

Proposition 3.4: Let f be a polynomial first integral of degree m with extremal terms. Then the system parameters satisfy $(-abc)^m=1$. Thus, if they are real the condition $abc=\pm 1$ holds, the plus sign being excluded if m is odd. Moreover, f satisfies in all cases:

$$f=\lambda((-a)^m((z-bx)^m-z^m-(-bx)^m)+(y-az)^m+(y-x/c)^m-y^m)+xyzQ(x,y,z). \tag{21}$$

First, the presence of all extremal terms implies that the three system parameters are nonzero. Hence the three expressions (16), (17), and (18) for f hold. We can identify the terms without the variable x in Eqs. (16) and (17):

$$\lambda_2(y-az)^m=\lambda_1(z-y/a)^m.$$

Hence $\lambda_1=\lambda_2(-a)^m$. Then we identify the terms containing x in factor:

$$\lambda_2[(y-x/c)^m-y^m]+xzk_2=\lambda_2(-a)^m[(z-bx)^m-z^m]+xyk_1. \tag{22}$$

The identification of the coefficients of x^m yields $(-1/c)^m=(ab)^m$; in other words, $-abc$ must be an mth root of unity. Since the parameters are real, we must have $abc=-1$ if m is odd and $abc=\pm 1$ if m is even.

Setting $y=0$ in Eq. (22) and recalling the compensation of the x^m terms, we get

$$xz\tilde{k}_2=\lambda_2(-a)^m[(z-bx)^m-z^m-(-bx)^m],$$

hence the equality

$$xzk_2=\lambda_2(-a)^m[(z-bx)^m-z^m-(-bx)^m]+xyzQ,$$

which combined to Eq. (17) yields Eq. (21).

Up to now, all computations could have been carried with real or complex parameters and/or Darboux elements. However, the assumption of reality for (a,b,c) will play a crucial role for completing the proof of the result announced in the Introduction.

Indeed, there are only two real roots of unity: 1 (''first'' root) and -1 (square or ''second'' root). The above Proposition suggests that when $abc=\pm 1$ a polynomial first integral of first or second degree *may* exist; but we know it *does*. Then the most natural idea is to compare these known first integrals to Eq. (21). But the latter contains a polynomial Q which seems hard to determine: we have exhausted all the arithmetic arguments. Now we have got it: if $\deg f=1$ or 2, then the $xyzQ$ term in Eq. (21) must be zero. *This allows us to guess what the least-degree first integral should be and at what condition it is a first integral*. We are now able to prove that in both cases the polynomial first integrals reduce to the known ones.

Now, in the case where the parameters can be complex, Proposition 3.4 suggests that other cases can exist, and indeed they do.[5] But they cannot be found out by the above theory. When $-abc$ is a *primitive* mth root of unity, a polynomial first integral needs to be of degree at least m. Thus, it cannot be derived from Eq. (21) because of the $xyzQ$ term. In other words, we can check that this formula holds in the integrability cases with complex parameters, *but it does not allow to guess new cases nor to discard their existence*. We intend to reserve the problem of integrability with complex parameters for a future publication.

Theorem 3.5: *If $abc=-1$, the generators of the algebra of polynomial first integrals are*:

• *in all cases, the first integral $f_1=abx+y-az$*;

• *when, moreover, $(a,b,c)\in(\mathbf{Q}^-)^3$, $x^py^qz^r$, where (p,q,r) is the least positive integer solution to the system (19).*

We shall use the following algorithm:

1. If f has no extremal terms, apply Proposition 3.3 as many times as f can be factored by $x^p y^q z^r$. Finally, we get either a constant, or a first integral of strictly lower degree, with extremal terms. In the first case we have $f=\lambda(x^p y^q z^r)^i$ for some i, which is in the algebra defined by our statement. In the second case, go to the following step.

2. If f possesses extremal terms, it satisfies Eq. (21). Indeed, setting $c=-1/ab$ and $m=1$, this formula does read $f=\lambda f_1=\lambda(abx+y-az)$, and for $m=2$, $f=\lambda(f_1)^2$—we recall that if deg $f<3$, the term $xyzQ$ must be zero. Suppose $m=\deg f\geqslant 3$. The terms in the expansion of $(f_1)^m$ which do not contain xyz in factor are the ones in factor of λ in Eq. (21). Consequently

$$f=\lambda(f_1)^m+xyzQ_1.$$

On the other hand, we check that $Df_1=(1+abc)xy=0$, hence $xyzQ_1$ is a polynomial first integral with no extremal terms. If it is zero, then $f=(f_1)^m$, else return to the first step.
As the first step produces an integral of strictly lower degree, this algorithm must terminate in a finite number of steps. So we shall obtain an expression of f in function of f_1 and $x^p y^q z^r$.

Theorem 3.6: *If* $abc=1$, *polynomial first integrals exist on the extra condition that* $1+b+ab=0$, *and in this case the algebra they span is generated by* $f_2=a^2b^2x^2-2abxy+y^2-2ayz-2a^2bxz+a^2z^2$.
We know that for $abc=1$ the degree of the integral is necessarily even: $m=2k$. When $k=1$ and $c=1/ab$, Eq. (21) reads $f=\lambda f_2$—since the term $xyzQ$ must then be zero. If we calculate the derivative of this function with respect to the system (1), we find

$$Df_2=-4axyz(1+b+ab),$$

thus, as $a\neq 0$, f_2 cannot be a first integral unless $1+b+ab=0$.

For $k>1$, Eq. (21) shows $f-(f_2)^k=xyzQ_1$, or, since f is assumed to be a first integral,

$$D[f-(f_2)^k]=0-D[(f_2)^k]=D(xyzQ_1),$$

which yields

$$4akxyz(1+b+ab)(f_2)^{k-1}=xyz\{DQ_1+[(1+b)x+(1+c)y+(1+a)z]Q_1\}.$$

The linear differential operator in Q_1 which appears in the right-hand side has been studied in the proof of Proposition 3.3. In particular, a necessary condition for its kernel to be nontrivial is $abc=-1$, which is clearly not true. Hence, this operator is injective, and, if $1+b+ab=0$, we have $Q_1=0$ and $f=\lambda(f_2)^k$.

The rest of the proof will be devoted to show that the case $1+b+ab\neq 0$ is in fact impossible. Suppose *ab absurdo* that $1+b+ab\neq 0$; then the previous equation reads

$$\mu(f_2)^{k-1}=\{DQ_1+[(1+b)x+(1+c)y+(1+a)z]Q_1\}, \tag{23}$$

with $\mu\neq 0$. Setting then $z=0$ in this equality yields

$$xy\left(c\,\frac{\partial\overline{Q_1}}{\partial x}+\frac{\partial\overline{Q_1}}{\partial y}\right)+[(1+b)x+(1+c)y]\overline{Q_1}=\mu(abx-y)^{2k-2}. \tag{24}$$

Clearly if Eq. (23) admits a polynomial solution—which must be of degree $2k-3$—then Eq. (24) does. We shall integrate this equation by the method of characteristics.

Equation (24) is equivalent to the following system:

$$\dot{x}=cxy,\quad \dot{y}=xy,$$

$$\dot{u}=-[(1+b)x+(1+c)y]u+\mu(abx-y)^{2k-2}, \tag{25}$$

by the correspondence $u(t)=\overline{Q_1}[x(t),y(t)]$.

The first two equations can be uncoupled from the third one. Their quotient yields $\dot{x}/\dot{y}=c$, thus, $\dot{x}=c\dot{y}$ or $x=c(y-y_0)$, where y_0 is an integration constant. Then the second becomes $\dot{y}=cy(y-y_0)$, a separable variable equation which easily integrates as

$$y=\frac{y_0}{1-e^{cy_0t}},$$

and, since $x=c(y-y_0)$,

$$x=\frac{cy_0e^{cy_0t}}{1-e^{cy_0t}}.$$

Setting $X=e^{cy_0t}$ and $Y=y_0$, we get

$$x=\frac{cXY}{1-X},\quad y=\frac{Y}{1-X}.$$

Before we integrate the third equation in Eq. (25), we remark that $\overline{Q_1}$ is a homogeneous polynomial of degree $2k-3$ in (x,y) iff $u(t)$ can be written as $u=Y^{2k-3}A(X)/(1-X)^{2k-3}$ where $A(X)$ is a polynomial of degree $2k-3$. Then we get

$$\dot{u}=\frac{\partial}{\partial X}\left(\frac{Y^{2k-3}A(X)}{(1-X)^{2k-3}}\right)\frac{dX}{dt},$$

with $dX/dt=cy_0e^{cy_0t}=cXY$ and $dY/dt=0$.

Then the third equation in Eq. (25) reads

$$cXY\left[\frac{A'(X)(1-X)^{2k-3}+(2k-3)(1-X)^{2k-4}A(X)}{(1-X)^{4k-6}}\right]Y^{2k-3}$$
$$=\frac{Y^{2k-3}A(X)}{(1-X)^{2k-3}}\left(\frac{-c(1+b)XY-(1+c)Y}{1-X}\right)+\mu\left(\frac{abcXY-Y}{1-X}\right)^{2k-2}.$$

Since $abc=1$, the last term simplifies as Y^{2k-2}. Multiplying then this equation by $(1-X)^{2k-2}$ and dividing it by Y^{2k-2} yields

$$cX[A'(X)(1-X)+(b+2k-2)A(X)]+(1+c)A(X)=\mu(1-X)^{2k-2}. \tag{26}$$

The latter is a linear differential equation. Notice, that $c\neq-1$ for otherwise we would have $X|\mu(1-X)^{2k-2}$ which is impossible since $\mu\neq0$. The general solution to the homogeneous equation is

$$A(X)=K(1-X)^{b+2k-1+1/c}X^{-(1+1/c)}. \tag{27}$$

Let the constant vary: $K=K(X)$. Then Eq. (26) becomes

$$K'(X)=\frac{\mu}{c}X^{1/c}(1-X)^{-(2+b+1/c)}.$$

For any $\alpha\in\mathbf{R}$, we denote $(\alpha)_n=\alpha(\alpha+1)\cdots(\alpha+n-1)$; i.e., the generating function of the $(\alpha)_n$ being $(1-X)^{-\alpha}$, we have

$$K'(X)=\frac{\mu}{c}\sum_{n=0}^{\infty}(2+b+1/c)_n\frac{X^{n+1/c}}{n!}.$$

We see that if there exists $n\in\mathbf{N}$ such that $n+1/c=-1$, the function K has a logarithmic singularity at 0; and so does A.

Hence, if A is a polynomial, then necessarily $c\notin-\mathbf{N}^*$ and the indefinite integral is calculated as

$$K(X)=\frac{\mu}{c}\sum_{n=0}^{\infty}(2+b+1/c)_n\frac{X^{n+1+1/c}}{(n+1+1/c)n!}+k$$

($k=$cst), and so

$$A(X)=(1-X)^{b+2k-1+1/c}\left(\frac{\mu}{c}\sum_{n=0}^{\infty}(2+b+1/c)_n\frac{X^n}{(n+1+1/c)n!}+kX^{-(1+1/c)}\right).$$

Clearly, the integral series in this formula is not equal to a power of $1-X$. Thus A being a polynomial implies that $(2+b+1/c)_n$ is zero for n sufficiently large, i.e., $2+b+1/c=-n_1\in-\mathbf{N}$ and that $b+2k-1+1/c\in\mathbf{N}$; since the value of this integer must be at most $\deg A=2k-3$, we get once more the condition $2+b+1/c\in-\mathbf{N}$.

This is the only possibility of existence of a polynomial solution to Eq. (26)—hence to Eq. (24). If it holds, we check that $\deg A=2k-3$. But the analysis carried out by suppressing the variable z can be achieved by setting $x=0$ or $y=0$ and hence we get the three equalities

$$2+b+1/c=-n_1,\quad 2+a+1/b=-n_2,\quad 2+c+1/a=-n_3, \tag{28}$$

where n_1, n_2, $n_3\in\mathbf{N}$. Since $abc=1$, there are two possibilities: either the three parameters are positive, or one is positive, e.g., a and the other two are negative. The first possibility is excluded by Eq. (28).

Thus, if $a>0$ and $b,c<0$, the second equation yields $0<a=-n_2-2-1/b$ or $-1/b>n_2+2\geqslant 2$ and hence $|b|<1/2$. In the same way we get $|1/c|<1/2$. Then the first equation in Eq. (28) yields $-n_1=2+b+1/c>2-1/2-1/2=1$, a contradiction.

Consequently, it is absurd to assume the existence of a polynomial solution to Eq. (23). Hence, in the case $abc=1, 1+b+ab\neq 0$, there cannot be a polynomial first integral to the dynamical system (1).

IV. CONCLUSION

We have proved the following characterization of all existence cases and values of polynomial first integrals for the Lotka–Volterra dynamical system with real parameters.

(1) The (a,b,c) Lotka–Volterra system cannot have a nontrivial polynomial first integral unless $abc=\pm 1$.
(2) If $abc=1$, the algebra of polynomial first integrals is generated by the integral $I_2=a^2b^2x^2-2abxy+y^2-2ayz-2a^2bxz+a^2z^2$ if $1+b+ab=0$, and trivial if not.
(3) If $abc=-1$ and $(a,b,c)\notin(\mathbf{Q}^-)^3$, this algebra is generated by $I_1=abx+y-az$.
(4) If $abc=-1$ and $(a,b,c)\in(\mathbf{Q}^-)^3$, the generators are $I_1=abx+y-az$ and $x^py^qz^r$, where (p,q,r) is the least strictly positive solution to the linear system (19).

Our method yields no characterization of the integrability cases for complex parameters. It gives however a necessary, but clearly not sufficient, condition for their existence, which is effectively satisfied by all known cases.[5]

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Symmetries of discrete dynamical systems

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Differential–difference equations of the form $\ddot{u}_n = F_n(t, u_{n-1}, u_n, u_{n+1})$ are classified according to their continuous Lie point symmetry groups. It is shown that for nonlinear equations, the symmetry group can be at most seven-dimensional. The integrable Toda lattice is a member of this class and has a four-dimensional symmetry group. © *1996 American Institute of Physics.* [S0022-2488(96)03906-0]

I. INTRODUCTION

The purpose of this article is to classify differential–difference equations ($D\Delta E$) of the form

$$\Delta_n \equiv \ddot{u}_n(t) - F_n(t, u_{n-1}(t), u_n(t), u_{n+1}(t)) = 0, \tag{1.1}$$

into conjugacy classes and to determine the Lie point symmetries for each conjugacy class. Conjugacy is considered under a group of ''allowed transformations,'' preserving the form of Eq. (1.1), while possibly changing the function F_n. We restrict the allowed transformations to be fiber preserving, i.e., to have the form

$$u_n(t) = \Omega_n(\tilde{u}_n(\tilde{t}), t, g), \quad \tilde{t} = \tilde{t}(t, g), \quad \tilde{n} = n, \tag{1.2}$$

where Ω_n and $\tilde{t}$ are some locally smooth and monotonous (invertible) functions, and g represents the group parameters. These functions are such that $\tilde{u}_n(\tilde{t})$ satisfies an equation of the form (1.1) with F_n replaced by some function $\tilde{F}_n(\tilde{t}, \tilde{u}_k(\tilde{t}))$ $k = n-1, n, n+1$.

With this formulation, Lie symmetries of Eq. (1.1) are special cases of allowed transformations, namely, those for which we have

$$\tilde{F}_n(\tilde{t}, \tilde{u}_k(\tilde{t})) = F_n(\tilde{t}, \tilde{u}_k(\tilde{t})). \tag{1.3}$$

In this article we restrict to Lie point symmetries only. The algorithm for calculating them for a given equation was presented in our earlier articles[1,2] and was called ''the intrinsic method'' in Ref. 2. Thus we assume that the Lie algebra of the symmetry group is realized by vector fields of the form

$$\hat{X} = \tau(t, u_n)\partial_t + \phi_n(t, u_n)\partial_{u_n}, \tag{1.4}$$

and request that the prolongation $\mathrm{pr}\,\hat{X}$ of $\hat{X}$ should annihilate the equation on its solution set

$$\mathrm{pr}\,\hat{X}\Delta_n|_{\Delta_n = 0} = 0. \tag{1.5}$$

The prolongation formula for $D\Delta E$ was given earlier.[1] This definition of Lie point symmetries [as in Eqs. (1.2),...,(1.5)] is closely related to that of Maeda[3] for difference equations, and also to that of Quispel *et al.*[4] We note that the restriction $\tilde{n} = n$ is an important one and significantly cuts down

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on the number of symmetries of a difference equation, as opposed to a differential one. Symmetries transforming the discrete variables, can also be incorporated systematically, but that is a topic for a different article.[5]

Our motivation is the same as for classifying differential equations according to their symmetries. Dynamical systems of the form (1.1) occur in many applications, ranging from classical mechanics to molecular physics, or mathematical biology.[6–8] If the function $F_n(t,u_k)$ is such that Eq. (1.1) allows a nontrivial symmetry group, then it is usually possible to obtain exact analytical solutions satisfying certain symmetry requirements.

A different aspect is the possible connection between symmetries and integrability. Indeed, integrable equations, be they differential, or differential–difference ones, tend to have large Lie point symmetry groups. For instance, the Korteweg–de Vries equation with variable coefficients was shown to have at most a four-dimensional Lie point symmetry group.[9] More important, it has a four-dimensional symmetry algebra precisely if it is equivalent, under point transformations, to the KdV equation itself.

In the same context, we mention that integrable equations involving three independent variables (like the Kadomtsev–Petviashvili, Davey–Stewartson, 3-wave equations, and others) have infinite dimensional Lie point symmetry algebras with a specific Kac–Moody–Virasoro structure.[10–13] Interestingly enough, this is also true when one of the three variables is discrete, as in the two-dimensional Toda lattice.[1,2]

In short, nonlinear differential and differential–difference equations with large Lie point symmetry groups are prime candidates for being integrable, or having some of the attributes of integrability.[14]

Throughout this article we impose some restrictions.

(1) Only point symmetries are considered, i.e., all elements of the symmetry algebra have the form (1.4).

(2) The interaction F_n and the vector field $\hat{X}$ depend continuously on n. This rules out terms of the type $[A\pm(-1)^nB]$ in F_n, or ϕ_n. Such terms will be considered elsewhere, once we treat systems of $D\Delta E$. Indeed, they correspond to treating even and odd values of n separately.

(3) In the bulk of the article the interaction F_n is assumed to be nonlinear and coupled, i.e.,

$$\frac{\partial^2 F_n}{\partial u_i \partial u_k} \neq 0, \quad \left(\frac{\partial F_n}{\partial u_{n-1}}, \frac{\partial F_n}{\partial u_{n+1}}\right) \neq (0,0) \tag{1.6}$$

(on some open set of values of the variables). The linear case is considered in Sec. VIII.

(4) The interaction F_n involves only nearest neighbors on the lattice, i.e., depends on u_n, u_{n+1}, u_{n-1}, but not say on u_{n+2}.

(5) We only list the ''maximal'' symmetry algebras for a given interaction F_n. Thus if F_n allows say a five-dimensional symmetry algebra, we will not include it among those with symmetry algebras of dimension $\dim L \leqslant 4$.

In Sec. II we present the determining equations for the symmetries and introduce the classification group, i.e., the allowed transformations. We also find all interactions F_n with one-dimensional symmetry algebras. Section III is devoted to interactions with abelian symmetry algebras. We denote them $\mathrm{A}_{i,k}$, where the first index shows the dimension of the algebra. This turns out to satisfy $1 \leqslant \dim L \leqslant 4$. All nilpotent nonabelian symmetry algebras are found in Sec. IV. We call them $\mathrm{N}_{i,k}$ with i indicating the dimension. In this case we have $3 \leqslant \dim L \leqslant 5$. Solvable symmetry algebras $\mathrm{SN}_{i,k}$ with nonabelian nilradicals are treated in Sec. V. There exist eight classes of such algebras. Their dimensions are four, or six. Section VI is devoted to solvable symmetry algebras with abelian nilradicals $\mathrm{SA}_{i,k}$. Their dimensions satisfy $3 \leqslant \dim L \leqslant 5$ and there are altogether 30 inequivalent symmetry algebras of this type. In Sec. VII we treat nonsolvable symmetry algebras. They all contain $\mathrm{sl}(2,\mathbb{R})$ as a subalgebra. Their dimensions are $\dim L = 3$, 4, 5, and 7 and there exist five inequivalent ones. Linear equations were so far excluded from consid-

eration and are investigated in Sec. VIII. Their symmetry algebras are infinite-dimensional, but this just reflects the linear superposition principle. A summary of results and some conclusions are presented in the final Sec. IX.

II. FORMULATION OF THE PROBLEM AND EQUATIONS WITH ONE-DIMENSIONAL SYMMETRY ALGEBRAS

In order to implement the symmetry algorithm (1.5) for Eq. (1.1), we need the second prolongation of the vector field (1.4). We use the general formulas presented earlier,[1,2] i.e., in our case

$$\mathrm{pr}^{(2)}\, X=\tau(t,u_n)\partial_t+\sum_{k=n-1}^{n+1}\phi_k(t,u_k)\partial_{u_k}+\phi_n^{tt}\partial_{\ddot{u}_n}, \tag{2.1}$$

$$\phi_n^{tt}=D_t^2\phi_n-(D_t^2\tau)_{\dot{u}_n}-2(D_t\tau)_{\ddot{u}_n}, \tag{2.2}$$

where D_t is the total derivative.

We apply $\mathrm{pr}^{(2)}\, X$ to Eq. (1.1), eliminate the $\ddot{u}_n$ terms using Eq. (1.1) and then request that the coefficients of $(\dot{u}_n)^k$, $k=0,1,2,3$ should vanish. We find that, for any F_n that depends nontrivially on at least one u_k, $k\neq n$, the coefficients in the vector field (1.4) satisfy

$$\phi_n(t,u_n)=(\tfrac{1}{2}\dot{\tau}(t)+a_n)u_n+\beta_n(t),\quad \tau(t,u_n)=\tau(t),\quad \dot{a}_n=0. \tag{2.3}$$

Moreover, the constants a_n and functions $\tau(t)$, $\beta_n(t)$ satisfy the remaining determining equation (the coefficient of the term independent of $\dot{u}_n$)

$$\tfrac{1}{2}\dddot{\tau}u_n+\ddot{\beta}_n+(a_n-\tfrac{3}{2}\dot{\tau})F_n-\tau F_{n,t}-\sum_{\alpha=n-1}^{n+1}[(\tfrac{1}{2}\dot{\tau}+a_\alpha)u_\alpha+\beta_\alpha]F_{n,u_\alpha}=0. \tag{2.4}$$

Let us now determine the allowed transformation (1.2). Substituting Eq. (1.2) into Eq. (1.1) and requiring that the terms $(\dot{\tilde{u}}_n)^2$ and $\ddot{\tilde{u}}_n$ be absent, we find that the allowed transformation (1.2) must be linear and satisfy

$$u_n(t)=\frac{A_n}{\sqrt{\dot{\tilde{t}}_t}}\,\tilde{u}_n(\tilde{t})+B_n(t),\quad \tilde{t}=\tilde{t}(t),\quad A_{n,t}=0,\quad \dot{\tilde{t}}\neq 0,\quad A_n\neq 0,\quad \tilde{n}=n. \tag{2.5}$$

Equation (1.1) is transformed into

$$\ddot{\tilde{u}}_n=\frac{1}{A_n}\,(\dot{\tilde{t}})^{-3/2}\left\{F_n(t,u_k)+\left[-\tfrac{3}{4}A_n(\dot{\tilde{t}})^{-5/2}(\ddot{\tilde{t}})^2+\frac{A_n}{2}\,(\dot{\tilde{t}})^{-3/2}\dddot{\tilde{t}}\right]\tilde{u}_n(\tilde{t})-\ddot{B}_n\right\}, \tag{2.6}$$

where t, u_{n-1}, u_n, and u_{n+1} must be expressed in terms of $\tilde{t}$, $\tilde{u}_k$, using Eq. (1.2).

The vector field

$$\hat{X}=\tau(t)\partial_t+[(\tfrac{1}{2}\dot{\tau}(t)+a_n)u_n+\beta_n(t)]\partial_{u_n}, \tag{2.7}$$

is transformed into

$$\hat{X}=\tau(t)\dot{\tilde{t}}\partial_{\tilde{t}}+\left\{\left[\frac{\tau}{2}\,\ddot{\tilde{t}}(\dot{\tilde{t}})^{-1}+\frac{1}{2}\,\dot{\tau}+a_n\right]\tilde{u}_n+(\dot{\tilde{t}})^{1/2}A_n^{-1}\left[\left(\frac{1}{2}\,\dot{\tau}+a_n\right)B_n+\beta_n-\tau\dot{B}_n\right]\right\}\partial_{\tilde{u}_n}. \tag{2.8}$$

Let us now assume that the interaction F_n is given and that it is invariant under a one parameter symmetry group, generated by the vector field (2.7), with coefficients satisfying Eq. (2.4). Let us now use the allowed transformation (2.6) to simplify the vector field $\hat{X}$, i.e., transform it into a convenient ''canonical'' form. Once this is done, we insert the coefficients of the canonical vector field into the determining equation (2.4) and solve this equation for $F_n(t,u_k)$. This is easy to do, since we have a first order linear partial differential equation and we simply apply the method of characteristics.

We see from Eq. (2.8) that three different possibilities occur.

A. $\tau(t)\neq 0$

If we have $\tau(t)\neq 0$ (in some open neighborhood), we choose $\tilde{t}(t)$ and $B_n(t)$ to satisfy

$$\frac{d\tilde{t}}{dt}=[\tau(t)]^{-1}, \quad \tau\frac{dB_n}{dt}-\left(\frac{1}{2}\dot{\tau}+a_n\right)B_n-\beta_n=0.$$

We obtain

$$A_{1,1}: \quad \hat{X}=\partial_t+a_n u_n\partial_{u_n}, \tag{2.9}$$

and using Eq. (2.4) with $\tau=1$, $\beta_n=0$ we find

$$F_n(t,u_k)=f_n(\xi_k)e^{a_n t}, \quad \xi_k=u_k e^{-a_k t}, \quad k=n-1,n,n+1. \tag{2.10}$$

In particular, for $a_n=0$ we have invariance with respect to time translations: F_n does not depend on t.

B. $\tau(t)=0$, $a_n\neq 0$

We choose $B_n=-\beta_n(t)/a_n$ and obtain

$$A_{1,2}: \quad \hat{X}=a_n u_n\partial_n, \tag{2.11}$$

$$F_n(t,u_k)=u_n f_n(t,\xi_k), \quad \xi_k=u_k^{a_n}u_n^{-a_k}, \quad k=n\pm 1. \tag{2.12}$$

The vector field (2.11) can be interpreted as generating site dependent (n dependent) dilations of the function u_n.

C. $\tau(t)=0$, $a_n=0$, $\beta_n(t)\neq 0$

In this case we already have

$$A_{1,3}: \quad \hat{X}=\beta_n(t)\partial_{u_n}, \tag{2.13}$$

and obtain

$$F_n(t,u_k)=\frac{\ddot{\beta}_n}{\beta_n}u_n+f_n(t,\xi_k), \quad \xi_k=\beta_n(t)u_k-\beta_k(t)u_n, \quad k=n\pm 1. \tag{2.14}$$

In this case allowed transformations provide the equivalence

$$\beta_n(t)\sim\beta_n(t)(\tilde{t}_t)^{-1/2}A_n^{-1}. \tag{2.15}$$

In particular, if $\beta_n(t)$ factorizes as a function of n and t, i.e., $\beta_n(t)=\mu_n h(t)$, $\dot{\mu}_n=0$, we can transform $\beta_n(t)$ into $\beta_n(t)=1$. In this case the vector field (2.13) corresponds to a translation of the dependent variable: $u_n \to u_n + c$.

We see that the existence of a one-dimensional symmetry algebra imposes a certain restriction on the form of F_n. Instead of being an arbitrary function of four variables, it will involve a function of only three ''symmetry'' variables. By allowed transformations it can be taken into one of three ''standard'' form Eq. (2.10), (2.12), or (2.14).

Below we shall always assume that F_n and one of the symmetry generators is already in standard form and will show how F_n is further restricted by the existence of a higher dimensional symmetry algebra.

The strategy that we shall follow is to proceed ''structurally.'' Thus we shall first find all interactions that allow abelian symmetry algebras (of any dimension N, but it turns out that in this case we have $N \leqslant 4$). We then proceed to classify nilpotent (nonabelian) symmetry algebras. For these we find that their dimensions satisfy $3 \leqslant N \leqslant 5$. The classification of abelian and nilpotent symmetry algebras is then used to find all solvable (nonabelian) Lie algebras. To do this we use a known result, namely, that a solvable Lie algebra L of dimension $\dim L = d$, has a (unique) nilradical $\mathrm{NR}(L)$ of dimension $\dim \mathrm{NR}(L) \geqslant d/2$. The nilradical is defined as the maximal nilpotent ideal of a Lie algebra.[15] Finally, we shall construct all nonsolvable Lie algebras. These are either simple, or they have a nontrivial Levi decomposition[15,16] into a semidirect sum of a simple Lie algebra and a solvable one (the radical, i.e., the maximal solvable ideal, unique up to equivalence).

III. ABELIAN SYMMETRY ALGEBRAS

The procedure that we adopt for finding all interactions F_n allowing abelian symmetry algebras is an inductive one. We start from each of the $\dim L = 1$ cases found in Sec. II, and then add further generators X_i of the form (2.7), commuting with those that have already been standardized. Thus X_1 is chosen in the form (2.9), (2.11), or (2.13), respectively. We then add X_2, satisfying $[X_1, X_2]=0$ and take F_n in the form (2.10), (2.12), or (2.14), as the case may be. The generator X_2 is first simplified, using allowed transformations that leave the space $\{X_1\}$ invariant. The standardized X_2 and F_n are then inserted into the determining equation (2.4) and this is solved for the arbitrary function f_n in Eq. (2.10), (2.12), or (2.14), respectively. Thus we obtain two-dimensional abelian symmetry algebras and the corresponding interactions, again in ''canonical forms.'' To obtain higher dimensional symmetry algebras, we successively add further linearly independent vector fields to the already established ''canonical'' algebras and impose further restrictions on F_n. The results for $\dim L = 2$ can be summed up in theorem that we state without proof. The interaction F_n throughout satisfies condition (1.6).

Theorem 1: *There exist precisely 5 classes of interactions F_n for which Eq. (1.1) allows a two-dimensional abelian symmetry algebra. The algebras and interaction functions can be represented as follows:*

$$A_{2,1}: \quad X_1 = \partial_t + a_{1n} u_n \partial_{u_n}, \quad X_2 = a_{2n} u_n \partial_{u_n}, \tag{3.1}$$

$$F_n = u_n f_n(\xi_k), \quad \xi_k = u_k^{a_{2n}} u_n^{-a_{2k}} e^{(a_{1n}a_{2k} - a_{1k}a_{2n})t}, \quad a_{2n} \not\equiv 0, \quad k = n-1, n+1. \tag{3.2}$$

$$A_{2,2}: \quad X_1 = \partial_t + a_n u_n \partial_{u_n}, \quad X_2 = e^{a_n t} \partial_{u_n}, \tag{3.3}$$

$$F_n = a_n^2 u_n + e^{a_n t} f_n(\xi_k), \quad \xi_k = u_k e^{-a_k t} - u_n e^{-a_n t}, \quad k = n-1, n+1. \tag{3.4}$$

$$A_{2,3}: \quad X_1 = a_{1n} u_n \partial_{u_n}, \quad X_2 = a_{2n} u_n \partial_{u_n}, \tag{3.5}$$

$$F_n = u_n f_n(t,\xi), \quad \xi = u_{n-1}^{\alpha_{n+1n}} u_n^{\alpha_{n-1n+1}} u_{n+1}^{\alpha_{nn-1}}, \quad \alpha_{kl} = a_{1k}a_{2l} - a_{1l}a_{2k} \neq 0. \tag{3.6}$$

$$A_{2,4}: \quad X_1 = \beta_{1n}(t)\partial_{u_n}, \quad X_2 = \beta_{2n}(t)\partial_{u_n}, \quad \begin{vmatrix} \beta_{1n} & \beta_{2n} \\ \beta_{1n+1} & \beta_{2n+1} \end{vmatrix} \neq 0, \tag{3.7}$$

$$F_n = \frac{(\beta_{1n}\ddot{\beta}_{2n} - \ddot{\beta}_{1n}\beta_{2n})u_{n+1} - (\beta_{1n+1}\ddot{\beta}_{2n} - \ddot{\beta}_{1n}\beta_{2n+1})u_n}{\beta_{1n}\beta_{2n+1} - \beta_{1n+1}\beta_{2n}} + f_n(t,\xi), \tag{3.8}$$

$$\xi = (\beta_{1n}\beta_{2n+1} - \beta_{1n+1}\beta_{2n})u_{n-1} + (\beta_{1n+1}\beta_{2n-1} - \beta_{1n-1}\beta_{2n+1})u_n + (\beta_{1n-1}\beta_{2n} - \beta_{1n}\beta_{2n-1})u_{n+1}.$$

$$A_{2,5}: \quad X_1 = \partial_{u_n}, \quad X_2 = t\partial_{u_n}, \tag{3.9}$$

$$F_n = f_n(t,\xi_k), \quad \xi_k = u_k - u_n, \quad k = n-1, n+1. \tag{3.10}$$

Comments: (1) Notice that for $A_{2,1},\ldots,A_{2,4}$ the interaction involves an arbitrary function f_n of two variables. For $A_{2,5}$ f_n depends on three variables. In all cases we require $f_n \neq 0$. (2) It is easy to verify that no algebra in the representative list is conjugate to any other one in the list (under allowed transformations) and that any two-dimensional abelian symmetry algebra is conjugate to precisely one in the list.

For $\dim L = 3$ we proceed in the same manner. We start from the algebras $A_{2,1},\ldots A_{2,5}$ and add a further linearly independent element X_3, commuting with X_1 and X_2. Again, without proof, we present the following result.

Theorem 2: *Precisely four classes of three-dimensional abelian symmetry algebras exist. They are represented by the following ones.*

$$A_{3,1}: \quad X_1 = \partial_t + a_n u_n \partial_{u_n}, \quad X_2 = b_n u_n \partial_{u_n}, \quad X_3 = c_n u_n \partial_{u_n}. \tag{3.11}$$

$$F_n = u_n f_n(\xi),$$

$$\xi = u_{n-1}^{\alpha_{n+1n}} u_n^{\alpha_{n-1n+1}} u_{n+1}^{\alpha_{nn-1}} \exp(a_{n-1}\alpha_{nn+1} + a_{n+1}\alpha_{n-1n} + a_n\alpha_{n+1n-1})t, \tag{3.12}$$

$$\alpha_{km} = b_k c_m - b_m c_k.$$

$$A_{3,2}: \quad X_1 = \partial_t + a_n u_n \partial_{u_n}, \quad X_2 = e^{a_n t}\partial_{u_n}, \quad X_3 = \gamma_n e^{a_n t}\partial_{u_n}, \quad \gamma_{n+1} \neq \gamma_n, \quad \dot{\gamma}_n = 0. \tag{3.13}$$

$$F_n = a_n^2 u_n + e^{a_n t} f_n(\xi),$$

$$\xi = (\gamma_n - \gamma_{n+1})u_{n-1}e^{-a_{n-1}t} + (\gamma_{n+1} - \gamma_{n-1})u_n e^{-a_n t} + (\gamma_{n-1} - \gamma_n)u_{n+1}e^{-a_n t}, \tag{3.14}$$

$$A_{3,3}: \quad X_1 = \beta_{1n}(t)\partial_{u_n}, \quad X_2 = \beta_{2n}(t)\partial_{u_n}, \quad X_3 = [\lambda_1(t)\beta_{1n}(t) + \lambda_2(t)\beta_{2n}(t)]\partial_{u_n}, \tag{3.15}$$

$$\ddot{\lambda}_1\beta_{1n} + 2\dot{\lambda}_1\dot{\beta}_{1n} + \ddot{\lambda}_2\beta_{2n} + 2\dot{\lambda}_2\dot{\beta}_{2n} = 0, \quad \begin{vmatrix} \beta_{1n} & \beta_{1n+1} \\ \beta_{2n} & \beta_{2n+1} \end{vmatrix} \neq 0, \quad \dot{\lambda}_1\dot{\lambda}_2 \neq 0. \tag{3.16}$$

F_n as in Eq. (3.8)

$$A_{3,4}: \quad X_1 = \partial_{u_n}, \quad X_2 = t\partial_{u_n}, \quad X_3 = \beta_n(t)\partial_{u_n}, \quad \beta_{n+1} \neq \beta_n, \quad \ddot{\beta}_n \neq 0. \tag{3.17}$$

$$F_n=\frac{\ddot{\beta}_n}{\beta_{n+1}-\beta_n}\,(u_{n+1}-u_n)+f_n(t,\xi),$$

$$\xi=(\beta_n-\beta_{n+1})u_{n-1}+(\beta_{n+1}-\beta_{n-1})u_n+(\beta_{n-1}-\beta_n)u_{n+1}. \tag{3.18}$$

Comments: (1) Equation (3.16) can be solved in all generality to yield

$$\beta_{1n}=\frac{1}{\sqrt{\dot{\lambda}_1}}\,\phi(t),\quad \beta_{2n}=\frac{1}{\sqrt{\dot{\lambda}_2}}\left[\gamma_n-\int_0^t\sqrt{\frac{\dot{\lambda}_1(s)}{\dot{\lambda}_2(s)}}\,\dot{\phi}_n(s)ds\right],\quad \dot{\gamma}_n=0. \tag{3.19}$$

We see that interaction (3.8) always allows the two-dimensional symmetry algebra $A_{2,4}$. If the functions β_{1n} and β_{2n} satisfy Eq. (3.16), i.e., can be expressed in terms of one function $\phi_n(t)$ of n and t, two functions $\lambda_1(t)$ and $\lambda_2(t)$ of t alone, and one function γ_n of n, then the symmetry algebra is three-dimensional.

(2) For $\ddot{\beta}_n=0$ in Eq. (3.17) the interaction $F_n=f_n(t,\xi)$ allows a four-dimensional symmetry algebra, a special case of Eq. (3.34) below.

(3) The algebra $\{X_i=\beta_{in}(t)\partial_{u_n},\ i=1,2,3\}$ with β_{in} satisfying

$$\begin{vmatrix}\beta_{1n-1} & \beta_{2n-1} & \beta_{3n-1}\\ \beta_{1n} & \beta_{2n} & \beta_{3n}\\ \beta_{1n+1} & \beta_{2n+1} & \beta_{3n+1}\end{vmatrix}\neq 0, \tag{3.20}$$

is not listed above. The reason is that the corresponding invariant equation has the form

$$\ddot{u}_n=A_n(t)u_n+B_n(t)u_{n-1}+C_n(t)u_{n+1}+D_n(t).$$

Thus the equation is linear (inhomogeneous) and the invariance algebra is a reflection of the linear superposition principle (see Sec. VIII below).

(4)The algebra $\{X_i=a_{in}u_n\partial_{u_n},\ i=1,2,3\}$ also corresponds only to a system of decoupled linear equations.

The algebras $A_{3,1}$ and $A_{3,2}$ cannot be extended to four-dimensional ones, or rather, the corresponding invariant equations would be linear. Hence, for $\dim L\geqslant 4$ the symmetry algebra must have the form $X_i=\beta_{in}(t)\partial_{u_n}$, $i=1,2,\cdots$. At most two of the functions $\beta_{in}(t)$ can be linearly independent as functions of n, otherwise the equation would be linear. If all β_{in} are proportional to $\beta_{1n}(t)$, then L is at most two-dimensional. Hence, we need only consider

$$X_1=\beta_{1n}(t)\partial_{u_n},\quad X_2=\beta_{2n}(t)\partial_{u_n},\quad \beta_{1n}\beta_{2n+1}-\beta_{1n+1}\beta_{2n}\neq 0,$$

$$X_3=[\lambda_1(t)\beta_{1n}(t)+\lambda_2(t)\beta_{2n}(t)]\partial_{u_n},\quad X_4=[\mu_1(t)\beta_{1n}(t)+\mu_2(t)\beta_{2n}(t)]\partial_{u_n}. \tag{3.21}$$

We consider separately the cases $\lambda_1\lambda_2=0$ (or $\mu_1\mu_2=0$) and $\lambda_1\lambda_2\mu_1\mu_2\neq 0$.

In both cases we find that the existence of an abelian symmetry algebra of the type (3.21) ($\dim L=4$) implies that the interaction has the form

$$F_n=P_n(t)u_{n+1}+Q_n(t)u_n+f_n(t,\xi), \tag{3.22}$$

$$\xi=(\gamma_n-\gamma_{n+1})u_{n-1}+(\gamma_{n+1}-\gamma_{n-1})u_n+(\gamma_{n-1}-\gamma_n)u_{n+1}, \tag{3.23}$$

$$\gamma_{n+1}\neq\gamma_n,\quad \dot{\gamma}_n=0,\quad f_{n,\xi\xi}\neq 0.$$

Let us now find the abelian symmetries for interaction (3.22). We already know that they have the form $X_i = \beta_{in}(t)\partial_{u_n}$. Substituting Eq. (3.22) into Eq. (2.4) and solving the corresponding determining equations, we find

$$\beta_{in}(t)=\phi_i(t)+\gamma_n\psi_i(t), \quad i=1,2, \tag{3.24}$$

where the functions $\phi_i(t)$ and $\psi_i(t)$ satisfy

$$\ddot{\phi}_i+\ddot{\psi}_i\gamma_n-(\phi_i+\psi_i\gamma_{n+1})P_n-(\phi_i+\psi_i\gamma_n)Q_n=0, \quad i=1,2. \tag{3.25}$$

The two equations (3.25) determine the dependence of P_n and Q_n on n. The condition $\beta_{2n}(t)\neq\lambda(t)\beta_{1n}(t)$ implies $\phi_1\psi_2-\phi_2\psi_1\neq 0$, and we obtain

$$\begin{aligned} P_n&=-\frac{1}{\gamma_n-\gamma_{n+1}}[A+(B+C)\gamma_n+D\gamma_n^2], \\ Q_n&=\frac{1}{\gamma_n-\gamma_{n-1}}[A+B\gamma_n+C\gamma_{n+1}+D\gamma_n\gamma_{n+1}], \end{aligned} \tag{3.26}$$

where A, B, C, and D are arbitrary functions of time t. The determining equations for the symmetries X_i with β_{in} as in Eq. (3.24) reduce to

$$\ddot{\psi}-B\psi+D\phi=0, \quad \ddot{\phi}+C\phi-A\psi=0. \tag{3.27}$$

The general solution of Eq. (3.27) involves four arbitrary constants, hence the abelian symmetry algebra L will be precisely four-dimensional and never larger.

Allowed transformations make it possible to exchange the roles of ϕ_i and ψ_i, hence of (B,D) and (C,A). Two cases can be distinguished.

(1) $A\neq 0$ (or equivalently, $D\neq 0$). We reduce Eq. (3.27) to

$$\psi=\frac{1}{A}(\ddot{\phi}+C(t)\phi), \tag{3.28}$$

$$\dddot{\phi}^{\cdot}+2A\left(\frac{1}{A}\right)^{\cdot}\dddot{\phi}+A\left[\left(\frac{1}{A}\right)^{\cdot\cdot}+\frac{C-B}{A}\right]\ddot{\phi}+2A\left(\frac{C}{A}\right)^{\cdot}\dot{\phi}+A\left[\left(\frac{C}{A}\right)^{\cdot\cdot}+\frac{DA-BC}{A}\right]\phi=0. \tag{3.29}$$

A basis for the symmetry algebra is obtained in the form

$$X_i=\left[\phi_i+\frac{1}{A}(\ddot{\phi}_i+C\phi_i)\gamma_n\right]\partial_{u_n}, \quad i=1,\ldots,4, \tag{3.30}$$

where $\phi_1,\ldots\phi_4$ are four linearly independent solutions of Eq. (3.29). Using allowed transformations we can set $\phi_1=1$ and hence

$$\left(\frac{C}{A}\right)^{\cdot\cdot}+\frac{DA-BC}{A}=0. \tag{3.31}$$

(2) $A=D=0$. Using allowed transformations we set $\phi_1=1$ and thus $C=0$, and $\phi_2=t$.

Then ψ_1 and ψ_2 are two linearly independent solutions of the equation

$$\ddot{\psi}-B(t)\psi=0. \tag{3.32}$$

We arrive at the following result.

Theorem 3: *An abelian symmetry algebra of Eq. (1.1) satisfying conditions (1.6) can be at most four-dimensional. A four-dimensional symmetry algebra occurs in the following two cases.*

$$A_{4,1}: \quad X_1=\partial_{u_n}, \quad X_2=t\partial_{u_n}, \quad X_3=\psi_1(t)\gamma_n\partial_{u_n}, \quad X_4=\psi_2(t)\gamma_n\partial_{u_n}, \tag{3.33}$$

$$\gamma_{n+1}\neq\gamma_n, \quad \dot{\gamma}_n=0.$$

$$F_n=\frac{B_n(t)\gamma_n}{\gamma_n-\gamma_{n+1}}(u_n-u_{n+1})+f_n(t,\xi), \quad f_{n,\xi\xi}\neq 0, \tag{3.34}$$

with ξ as in Eq. (3.23) and ψ_1, ψ_2 satisfying Eq. (3.32) and hence also

$$\psi_1\dot{\psi}_2-\dot{\psi}_1\psi_2=\text{const.} \tag{3.35}$$

$$A_{4,2}: \quad X_i=[\phi_i(t)+\psi_i(t)\gamma_n]\partial_{u_n}, \quad i=1,\ldots,4, \tag{3.36}$$

$$F_n=\frac{1}{\gamma_n-\gamma_{n+1}}[A(t)+(B(t)+C(t))\gamma_n+D(t)\gamma_n\gamma_{n+1}]u_{n+1}$$
$$+\frac{1}{\gamma_n-\gamma_{n+1}}[A(t)+B(t)\gamma_n+C(t)\gamma_{n+1}+D(t)\gamma_n\gamma_{n+1}]u_n+f_n(t,\xi), \tag{3.37}$$

where $(A,D)\neq(0,0)$, ϕ_i and ψ_i are solutions of Eq. (3.27), ξ is as in Eq. (3.23), and $f_{n,\xi\xi}\neq 0$.

IV. NILPOTENT NONABELIAN SYMMETRY ALGEBRAS

Nilpotent nonabelian Lie algebras L exist for dim $L\geqslant 3$. For dim $L=3$ the only such algebra is the Heisenberg algebra with commutation relations

$$[X_2,X_3]=X_1, \quad [X_1,X_2]=[X_1,X_3]=0. \tag{4.1}$$

To construct all such algebras, we let X_1 run through the three possible standard forms (2.9), (2.11), and (2.13). The generators X_2 and X_3 are taken in generic form, and further simplified by allowed transformations, after the commutation relations (4.1) are imposed. We thus obtain two mutually nonconjugate representative Heisenberg algebras, namely,

$$N_{3,1}: \quad X_1=\partial_{u_n}, \quad X_2=\partial_t, \quad X_3=t\partial_{u_n}, \tag{4.2}$$

$$F_n=f_n(\xi_k), \quad \xi_k=u_k-u_n, \quad k=n+1,n-1. \tag{4.3}$$

$$N_{3,2}: \quad X_2=\partial_t+a_nu_n\partial_{u_n}, \quad X_3=(t+\gamma_n)e^{a_nt}\partial_{u_n}, \quad X_1=e^{a_nt}\partial_{u_n}, \tag{4.4}$$

$$\dot{a}_n=0, \quad \dot{\gamma}_n=0, \quad \gamma_n\neq\gamma_{n+1},$$

$$F_n=\frac{a_n^2(\gamma_{n+1}-\gamma_n)-2a_n}{\gamma_{n+1}-\gamma_n}u_n+\frac{2a_n}{\gamma_{n+1}-\gamma_n}u_{n+1}e^{(a_n-a_{n+1})t}+e^{a_nt}f_n(\xi),$$

$$\xi=(\gamma_n-\gamma_{n+1})u_{n-1}e^{-a_{n-1}t}+(\gamma_{n+1}-\gamma_{n-1})u_ne^{-a_nt}+(\gamma_{n-1}-\gamma_n)u_{n+1}+e^{-a_{n+1}t}. \tag{4.5}$$

Notice that the algebra (4.2) is obtained from Eq. (4.4) by setting $a_n=0$, $\gamma_n=0$, however, interaction (4.3) is more general than the one obtained from Eq. (4.5) by setting $a_n=\gamma_a=0$. Hence $N_{3,1}$ is *not* a special case of $N_{3,2}$.

Every nonabelian nilpotent Lie algebra contains a Heisenberg subalgebra, so we can proceed to higher dimensions, by adding further operators to $N_{3,1}$, or $N_{3,2}$.

The algebra $N_{3,1}$ thus yields a five-dimensional Lie algebra, namely,

$$N_{5,1}: \quad X_1=\partial_{u_n}, \quad X_2=t\partial_{u_n}, \quad X_3=\left(\frac{kt^2}{2}+\gamma_n\right)\partial_{u_n}, \quad X_4=\left(\frac{kt^3}{6}+\gamma_n t\right)\partial_{u_n}, \tag{4.6}$$

$$X_5=\partial_t, \quad k=0,1,$$

$$F_n=\frac{2k}{\gamma_{n+1}-\gamma_n}(u_{n+1}-u_n)+f_n(\xi), \tag{4.7}$$

ξ as in Eq. (3.23). The commutation relations are

$$\begin{pmatrix}[X_5,X_1]\\ [X_5,X_2]\\ [X_5,X_3]\\ [X_5,X_4]\end{pmatrix}=\begin{pmatrix}0 & & & \\ 1 & 0 & & \\ & k & 0 & \\ & & 1 & 0\end{pmatrix}\begin{pmatrix}X_1\\ X_2\\ X_3\\ X_4\end{pmatrix}, \quad [X_i,X_k]=0, \quad i,k=1,2,3,4. \tag{4.8}$$

If we leave out the generator X_4, we obtain a four-dimensional nilpotent subalgebra. However, the corresponding invariant interaction is again Eq. (4.7), so this subalgebra need not be listed separately. We mention that $\{X_1,\ldots,X_4\}$ is an abelian subalgebra of $N_{5,1}$. It corresponds to $A_{4,2}$ of Sec. III, with $A=2k$, $B=C=D=0$.

Finally, the Lie algebra $N_{3,2}$ can be extended to a four-dimensional nilpotent symmetry algebra of a nonlinear interaction precisely if we have

$$a_n\neq a_{n+1}, \quad \gamma_n=-\frac{1}{2a_n}. \tag{4.9}$$

The result is

$$N_{4,1}: \quad X_1=a_n e^{a_n t}\partial_{u_n}, \quad X_2=(-a_n t+\tfrac{1}{2})e^{a_n t}\partial_{u_n},$$

$$X_3=(\tfrac{1}{2}a_n t^2-\tfrac{t}{2})e^{a_n t}\partial_{u_n}, \quad X_4=\partial_t+a_n u_n\partial_{u_n}, \tag{4.10}$$

$$F_n=\frac{(a_n)^2}{a_{n+1}-a_n}[4a_n e^{(a_n-a_{n+1})t}u_{n+1}-(3a_{n+1}+a_n)u_n]+e^{a_n t}f_n(\xi),$$

$$\xi=(a_n-a_{n+1})u_{n-1}e^{-a_{n-1}t}+(a_{n+1}-a_{n-1})u_n e^{-a_n t}+(a_{n-1}-a_n)u_{n+1}e^{-a_{n+1}t}. \tag{4.11}$$

The commutation relations are

$$\begin{pmatrix}[X_4,X_1]\\ [X_4,X_2]\\ [X_4,X_3]\end{pmatrix}=\begin{pmatrix}0 & 0 & 0\\ 1 & 0 & 0\\ 0 & 1 & 0\end{pmatrix}\begin{pmatrix}X_1\\ X_2\\ X_3\end{pmatrix}, \quad [X_i,X_k]=0, \quad i,k=1,2,3. \tag{4.12}$$

We can sum up the results as follows:

Theorem 4: *Four classes of nonlinear interactions with nilpotent symmetry algebras exist. They are represented by $N_{3,1}$, $N_{3,2}$, $N_{4,1}$, and $N_{5,1}$, respectively.*

V. SOLVABLE SYMMETRY ALGEBRAS WITH NONABELIAN NILRADICALS

All nilpotent symmetry algebras were classified in Sec. IV. Let us now embed them into solvable Lie algebras as nilradicals and find the corresponding invariant interactions. In all cases it is possible to add at most one element Y outside the nilradical. The commutation relations are hence those of the nilradical plus the relation

$$[X_i, Y] = A_{ik} X_k, \tag{5.1}$$

where A is some fixed matrix.

A. Nilradical $N_{3,1}$

To the basis elements $\{X_1, X_2, X_3\}$ of Eq. (4.2) we add a general element Y of the form (2.7). Imposing the commutation relations (5.1) we find that $\tau(t)$ in Y must satisfy either $\tau = t$ or $\tau = 0$. We consider the two cases separately. Simplifying by allowed transformations and solving the determining equations, we find that the symmetry algebras can be at most four-dimensional. We obtain four classes of such symmetry algebras and they can be represented as follows. The nilradical is as in Eq. (4.2) with commutation relations (4.1).

Below we list Y, the matrix A, the elements of which figure in Eq. (5.1), and the invariant interactions.

$$\mathrm{SN}_{4,1}: \quad Y = t\partial_t + (\tfrac{1}{2} + a) u_n \partial_{u_n}$$

$$A = \begin{pmatrix} \frac{1}{2}+a & & \\ & 1 & \\ & & -\frac{1}{2}+a \end{pmatrix}, \quad a \neq -\frac{1}{2}, \tag{5.2}$$

$$F_n = (u_{n+1} - u_n)^{(a-3/2)/(a+1/2)} f_n(\xi), \quad \xi = \frac{u_{n-1} - u_n}{u_{n+1} - u_n}.$$

$$\mathrm{SN}_{4,2}: \quad Y = t\partial_t + (2u_n + t^2)\partial_{u_n}$$

$$A = \begin{pmatrix} 2 & & \\ & 1 & 2 \\ & 0 & 1 \end{pmatrix}, \tag{5.3}$$

$$F_n = \ln(u_{n+1} - u_n) + f_n(\xi), \quad \xi = \frac{u_{n-1} - u_n}{u_{n+1} - u_n},$$

$$\mathrm{SN}_{4,3}: \quad Y = t\partial_t + \gamma_n \partial_{u_n}, \quad \gamma_{n-1} \neq \gamma_n,$$

$$A = \begin{pmatrix} 0 & & \\ & 1 & \\ & & -1 \end{pmatrix}, \tag{5.4}$$

$$F_n = \exp\left(-2 \frac{u_{n+1} - u_n}{\gamma_{n+1} - \gamma_n} \right) f_n(\xi),$$

with ξ as in Eq. (3.23)

$$\mathrm{SN}_{4,4}: \quad Y=u_n\partial_{u_n},$$

$$A=\begin{pmatrix} 1 & & \\ & 0 & \\ & & 1 \end{pmatrix}, \tag{5.5}$$

$$F_n=(u_{n+1}-u_n)f_n(\xi), \quad \xi=\frac{u_{n-1}-u_n}{u_{n+1}-u_n}.$$

B. Nilradical $N_{3,2}$ and $N_{4,1}$

Proceeding as for $N_{3,1}$, we find that no solvable symmetry algebras with nilradicals $N_{3,2}$ or $N_{4,1}$ exist for nonlinear equations.

C. Nilradical $N_{5,1}$

We start from the algebra $N_{5,1}$ with basis as in Eq. (4.6) and commutation relations as in Eq. (4.8). We add a further operator Y and find that this is possible only for $k=0$ in Eq. (4.6). For γ_n generic we find that the corresponding solvable algebras are six-dimensional. The case $\gamma_n=A+(-1)^nB$ would lead to a seven-dimensional Lie algebra, but by caveat we do not consider such algebras in this article.

For generic γ_n with $\gamma_{n+1}\neq\gamma_n$ we have the nilradical (4.6) and commutation relations (4.8) with $k=0$. The interaction will in all cases be

$$F_n=f_n(\xi), \tag{5.6}$$

with ξ as in Eq. (3.23). Four nonequivalent cases occur:

$$\mathrm{SN}_{6,1}: \quad Y=t\partial_t+(\tfrac{1}{2}+a)u_n\partial_{u_n},$$

$$F_n=c_n\xi^{(a-3/2)/(a+1/2)}, \quad a\neq-\tfrac{1}{2}, a\neq\tfrac{3}{2},$$

$$A=\mathrm{diag}\{\tfrac{1}{2}+a,-\tfrac{1}{2}+a,\tfrac{1}{2}+a,-\tfrac{1}{2}+a,1\} \tag{5.7}$$

$$\mathrm{SN}_{6,2}: \quad Y=t\partial_t+[2u_n+(a+b\gamma_n)t^2]\partial_{u_n}, \quad (a,b)\neq(0,0)$$

$$F_n=c_n+(a+b\gamma_n)\ln\xi,$$

$$A=\begin{pmatrix} 2 & & & & \\ & 1 & & & \\ & 0 & 2 & & \\ & 0 & 0 & 1 & \\ & 2a & 0 & 2b & 1 \end{pmatrix} \tag{5.8}$$

$$\mathrm{SN}_{6,3}: \quad Y=t\partial_t+\rho_n\partial_{u_n}, \quad \rho_n\neq A+B\gamma_n, \quad \dot{\rho}_n=0, \tag{5.9}$$

$$F_n=c_n\exp\left(-\frac{2\xi}{(\gamma_n-\gamma_{n+1})\rho_{n-1}+(\gamma_{n+1}-\gamma_{n-1})\rho_n+(\gamma_{n-1}-\gamma_n)\rho_{n+1}}\right), \tag{5.10}$$

$$A=\mathrm{diag}\{0,-1,0,-1,1\}.$$

Theorem 5: *Seven classes of solvable symmetry algebras with nonabelian nilradicals exist for equations of type (1.1). Their dimension can be 4, or 6 and the algebras and invariant interactions are represented above as* $SN_{4,1},\ldots,SN_{4,4}$, *with nilradical* $N_{3,1}$ *and* $SN_{6,1},\ldots,SN_{6,3}$ *with nilradical* $N_{5,1}$.

VI. SOLVABLE LIE ALGEBRAS WITH ABELIAN NILRADICALS

A. General strategy

We shall run through all abelian Lie algebras of Sec. IV and denote their basis elements X_i. We extend them by a nonnilpotent element Y in the general form (2.7). We then find the invariant interaction $F_n(t,u_{n-1},u_n,u_{n+1})$, keeping it only if F_n is nonlinear and coupled. We then check whether the considered algebra is maximal among those that leave the obtained equation (1.1) invariant. We shall only list maximal symmetry algebras. Once a maximal symmetry algebra is found, we check whether we can add further non-nilpotent elements Y_i, to the Lie algebra. If that is the case, we then obtain the further restricted interaction F_n.

We use several results on the structure of solvable Lie algebras.[15–22]

(1) The nilradical $\mathrm{NR}(L)$ of a solvable Lie algebra is uniquely defined (up to conjugacy) and its dimension satisfies

$$\dim \mathrm{NR}(L) \geqslant \tfrac{1}{2}\dim L. \tag{6.1}$$

(2) The derived algebra is contained in the nilradical $D(L)\subseteq NR(L)$.

(3) If the nilradical $\{X_1,\ldots,X_n\}$ is abelian, then the commutation relations for the solvable Lie algebra L can be written as

$$[X_i,Y_k]=(A_k)_{ij}X_j, \quad [A_k,A_l]=0, \quad [Y_i,Y_k]=c_{ik}^l,X_l, \quad [X_i,X_k]=0. \tag{6.2}$$

The matrices A_k commute and are linearly nilindependent (i.e., no nontrivial linear combination of them is a nilpotent matrix).

If only one element Y outside the nilradical exists, we have

$$[X_i,Y]=A_{ik}X_k, \tag{6.3}$$

and the non-nilpotent matrix A can be taken in Jordan canonical form.

(4) A partial classification of solvable Lie algebras exists.[17–22]

B. dim NR(L)=1

The commutation relation is Eq. (6.3) with $A=1$; X_1 runs through the standard forms (2.9), (2.11), and (2.13). The algebra (2.11) cannot be extended, nor can Eq. (2.9) for $a_n\neq 0$. The remaining cases provide four solvable Lie algebras and the corresponding interactions. They are

$$\mathrm{SA}_{2,1}: \quad X=\partial_t, \quad Y=t\partial_t+(\tfrac{1}{2}+a_n)u_n\partial_{u_n}, \quad a_n\neq -\tfrac{1}{2}, \tag{6.4}$$

$$F_n=u_n^{\alpha_n}f_n(\xi_{n-1},\xi_{n+1}),$$

$$\xi_k=u_k^{a_n+1/2}u_n^{-a_k-1/2}, \quad k=n-1,n+1, \quad \alpha_n=\frac{a_n-3/2}{a_n+1/2}, \tag{6.5}$$

$$\mathrm{SA}_{2,2}: \quad X=\partial_t, \quad Y=t\partial_t+\partial_{u_n} \tag{6.6}$$

$$F_n=e^{-2u_n}f_n(\xi_{n-1},\xi_{n+1}),$$

$$\xi_k = u_k - u_n, \quad k = n-1, n+1,$$

$$\mathrm{SA}_{2,3}: \quad X = e^{(a_n-1)t}\partial_{u_n}, \quad Y = \partial_t + a_n u_n \partial_{u_n}, \tag{6.7}$$

$$F_n = (a_n-1)^2 u_n + e^{a_n t} f_n(\xi_{n-1}, \xi_{n+1}),$$

$$\xi_k = u_k e^{-a_k t} - u_n e^{-a_n t}, \quad k = n-1, n+1,$$

$$\mathrm{SA}_{2,4}: \quad X = \beta_n(t)\partial_{u_n}, \quad Y = u_n \partial_{u_n},$$

$$F_n = \frac{\ddot{\beta}_n}{\beta_n} u_n + (\beta_n u_{n+1} - \beta_{n+1} u_n) f_n(t, \xi), \quad \xi = \frac{\beta_n u_{n-1} - \beta_{n-1} u_n}{\beta_n u_{n+1} - \beta_{n+1} u_n}. \tag{6.8}$$

We see that in all cases the interaction involves an arbitrary function f_n of two variables. For algebra $\mathrm{SA}_{2,1}$, $\mathrm{SA}_{2,2}$, and $\mathrm{SA}_{2,3}$ the transformations act nontrivially on time and induce a gauge transformation of u_n. For $\mathrm{SA}_{2,4}$ we have pure gauge transformations.

C. dim NR(L)=2

Five classes of two-dimensional abelian symmetry algebras exist, namely, $A_{2,1},\ldots,A_{2,5}$ of Sec. III. We have dim $L=3$, or 4. The algebra $A_{2,3}$ does not allow any solvable extensions; the others do, at least in special cases. We shall present the Lie algebras, interactions F_n and matrices A of Eq. (6.3).

1. NR(L)=$A_{2,1}$

We must take $a_n=0$ and we obtain a decomposable Lie algebra, namely,

$$\mathrm{SA}_{3,1}: \quad X_1 = \partial_t, \quad X_2 = b_n u_n \partial_{u_n}, \quad Y = t\partial_t + (\tfrac{1}{2} + c_n) u_n \partial_{u_n}, \quad c_n \neq -\tfrac{1}{2}.$$

$$A = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}. \tag{6.9}$$

The invariant interaction is

$$F_n = u_n [u_{n+1}^{b_n} u_n^{-b_{n+1}}]^{4/(\alpha_{nn+1})} f_n(\xi), \quad \xi = u_{n-1}^{\alpha_{nn+1}} u_n^{\alpha_{n+1n-1}} u_{n+1}^{\alpha_{n-1n}},$$

$$\alpha_{km} = b_m - b_k - 2(b_k c_m - b_m c_k). \tag{6.10}$$

2. NR(L)=$A_{2,2}$

For $a_n \neq 0$ we get just one extension, namely,

$$\mathrm{SA}_{3,2}: \quad X_1 = e^{a_n t}\partial_{u_n}, \quad X_2 = \partial_t + a_n u_n \partial_{u_n}, \quad Y = u_n \partial_{u_n},$$

$$F_n = a_n^2 u_n + (u_{n+1} e^{(a_n - a_{n+1})t} - u_n) f_n(\xi), \tag{6.11}$$

$$\xi = \frac{u_{n-1} e^{-a_{n-1}t} - u_n e^{-a_n t}}{u_{n+1} e^{-a_{n+1}t} - u_n e^{-a_n t}}.$$

The commutation relations are as in the case (6.9).

For $a_n=0$, further possibilities arise, namely,

$$\mathrm{SA}_{3,3}: \quad X_1=\partial_t, \quad X_2=\partial_{u_n}, \quad Y=t\partial_t+\gamma_n\partial_{u_n},$$

$$F_n=\exp\left(-2\frac{u_n-u_{n+1}}{\gamma_n-\gamma_{n+1}}\right)f_n(\xi), \quad \gamma_n\neq\gamma_{n+1}, \tag{6.12}$$

$$\xi=(\gamma_n-\gamma_{n+1})u_{n-1}+(\gamma_{n+1}-\gamma_{n-1})u_n+(\gamma_{n-1}-\gamma_n)u_{n+1}.$$

The commutation relations are as in the case (6.9).

$$\mathrm{SA}_{3,4}: \quad X_1=\partial_t, \quad X_2=\partial_{u_n}, \quad Y=t\partial_t+(\tfrac{1}{2}+a)u_n\partial_{u_n}, \quad a\neq-\tfrac{1}{2}$$

$$F_n=(u_{n+1}-u_n)^{(a-3/2)/(a+1/2)}f_n(\xi), \quad \xi=\frac{u_{n-1}-u_n}{u_{n+1}-u_n}. \tag{6.13}$$

$$A=\begin{pmatrix}1 & 0\\ 0 & a+\frac{1}{2}\end{pmatrix}, \tag{6.14}$$

$$\mathrm{SA}_{3,5}: \quad X_1=\partial_{u_n}, \quad X_2=\partial_t, \quad Y=t\partial_t+(u_n+t)\partial_{u_n}, \quad F_n=(u_{n+1}-u_n)^{-1}f_n(\xi),$$

$$\xi=\frac{u_{n-1}-u_n}{u_{n+1}-u_n}, \quad A=\begin{pmatrix}1 & 0\\ 1 & 1\end{pmatrix}. \tag{6.15}$$

3. $NR(L)=A_{2,4}$

When the nilradical is $A_{2,4}$ the additional operator Y can be further simplified so as to have $\tau=1$, or $\tau=0$, $a_n\neq0$. Moreover, the case with $\tau=0$ leads to F_n linear. We obtain the following three-dimensional Lie algebras

$$\mathrm{SA}_{3,6}: \quad X_1=e^{(a_n-1)t}\partial_{u_n}, \quad X_2=\gamma_n e^{(a_n-p)t}\partial_{u_n}, \quad Y=\partial_t+a_nu_n\partial_{u_n},$$

$$F_n=(a_n-1)^2u_n-\frac{\gamma_n}{\gamma_n-\gamma_{n+1}}(p-1)(2a_n-p-1)[u_n-u_{n+1}e^{(a_n-a_{n+1})t}]+e^{a_nt}f_n(\xi),$$

$$\xi=(\gamma_n-\gamma_{n+1})u_{n-1}e^{-a_{n-1}t}+(\gamma_{n+1}-\gamma_{n-1})u_ne^{-a_nt}+(\gamma_{n-1}-\gamma_n)u_{n+1}e^{-a_{n+1}t}, \quad \gamma_{n+1}\neq\gamma_n, \tag{6.16}$$

with

$$A=\begin{pmatrix}1 & 0\\ 0 & p\end{pmatrix} \tag{6.17}$$

$$\mathrm{SA}_{3,7}: \quad X_1=e^{(a_n-p)t}\cos(t-\alpha_n)\partial_{u_n}, \quad X_2=e^{(a_n-p)t}\sin(t-\alpha_n)\partial_{u_n}, \quad Y=\partial_t+a_nu_n\partial_{u_n},$$

$$F_n=[(a_n-p)^2-1-2(a_n-p)\cot(\alpha_n-\alpha_{n+1})]u_n+\frac{2(a_n-p)}{\sin(\alpha_n-\alpha_{n+1})}u_{n+1}e^{(a_n-a_{n+1})t}+e^{a_nt}f_n(\xi),$$

$$\xi=u_{n-1}e^{-a_{n-1}t}\sin(\alpha_n-\alpha_{n+1})+u_ne^{-a_nt}\sin(\alpha_{n+1}-\alpha_{n-1})$$
$$+u_{n+1}e^{-a_{n+1}t}\sin(\alpha_{n-1}-\alpha_n), \quad \alpha_n\neq\alpha_{n+1}, \tag{6.18}$$

with

$$A=\begin{pmatrix} p & 1 \\ -1 & p \end{pmatrix}, \tag{6.19}$$

$$\begin{gathered} \mathrm{SA}_{3,8}: \quad X_1=e^{(a_n-1)t}\partial_{u_n}, \quad X_2=(-t+\gamma_n)e^{(a_n-1)t}\partial_{u_n}, \quad Y=\partial_t+a_n u_n\partial_{u_n}, \\ F_n=(a_n-1)^2u_n-\frac{2(a_n-1)}{\gamma_n-\gamma_{n+1}}(u_n-u_{n+1})e^{(a_n-a_{n+1})t}+e^{a_n t}f_n(\xi), \end{gathered} \tag{6.20}$$

with ξ as in Eq. (6.16) and

$$A=\begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}. \tag{6.21}$$

4. $NR(L)=A_{2,5}$

We add Y in the general form (2.7) to X_1 and X_2. The commutation relations imply $\tau=\tau_0+\tau_1 t+\tau_2 t^2$, $a_n=a$. Using allowed transformations we set $\beta_n(t)=0$. Four inequivalent three-dimensional symmetry algebras are obtained.

$$\begin{gathered} \mathrm{SA}_{3,9}: \quad X_1=\partial_{u_n}, \quad X_2=t\partial_{u_n}, \quad Y=u_n\partial_{u_n}, \\ F_n=(u_{n+1}-u_n)f_n(t,\xi), \quad \xi=\frac{u_{n-1}-u_n}{u_{n+1}-u_n}, \end{gathered} \tag{6.22}$$

with

$$A=\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{6.23}$$

$$\mathrm{SA}_{3,10}: \quad X_1=\partial_{u_n}, \quad X_2=-t\partial_{u_n}, \quad Y=\partial_t+u_n\partial_{u_n}, \tag{6.24}$$

$$F_n=(u_{n+1}-u_n)f_n(\xi_{n-1},\xi_{n+1}), \quad \xi_k=e^{-t}(u_k-u_n), \quad k=n\pm 1,$$

with

$$A=\begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}, \tag{6.25}$$

$$\begin{gathered} \mathrm{SA}_{3,11}: \quad X_1=\partial_{u_n}, \quad X_2=t\partial_{u_n}, \quad Y=t\partial_t+(\tfrac{1}{2}+a)u_n\partial_{u_n}, \\ F_n=(u_{n+1}-u_n)^{(a-3/2)/(a+1/2)}f_n(\xi_{n-1},\xi_{n+1}), \\ \xi_k=(u_k-u_n)t^{-a-1/2}, \quad a\neq-\tfrac{1}{2}, k=n\pm 1, \end{gathered} \tag{6.26}$$

with

$$A=\begin{pmatrix} a+\frac{1}{2} & 0 \\ 0 & a-\frac{1}{2} \end{pmatrix}, \tag{6.27}$$

$$\mathrm{SA}_{3,12}: \quad X_1=\partial_{u_n}, \quad X_2=t\partial_{u_n}, \quad Y=(t^2+1)\partial_t+(t+a)u_n\partial_{u_n},$$

$$F_n=(u_{n+1}-u_n)(t^2+1)^{-2}f_n(\xi_{n-1},\xi_{n+1}), \tag{6.28}$$

$$\xi_k=(t^2+1)^{-1/2}(u_k-u_n)e^{-a\ \arctan t}, \quad k=n\pm 1,$$

with

$$A=\begin{pmatrix} a & 1 \\ -1 & a \end{pmatrix}. \tag{6.29}$$

We see that for algebras $\mathrm{SA}_{3,1},\ldots,\mathrm{SA}_{3,8}$ the interaction F_n involves an arbitrary function f_n of one variable ξ. None of these algebras can be further extended by another symmetry operator $\widetilde{Y}$, outside the nilradical. Indeed, the existence of such an operator would force the interaction to be linear.

The situation is different for algebras $\mathrm{SA}_{3,9},\ldots,\mathrm{SA}_{3,12}$, where F_n involves an arbitrary function of two variables. Extensions of these algebras lead to two inequivalent four-dimensional solvable Lie algebras with two-dimensional nilradicals, namely, the following:

$$\mathrm{SA}_{4,1}: \quad X_1=\partial_{u_n}, \quad X_2=t\partial_{u_n}, \quad Y_1=u_n\partial_{u_n}, \quad Y_2=(t^2+1)\partial_t+tu_n\partial_{u_n},$$

$$F_n=(u_{n+1}-u_n)(t^2+1)^{-2}f_n(\xi), \quad \xi=\frac{u_{n-1}-u_n}{u_{n+1}-u_n}. \tag{6.30}$$

$$\mathrm{SA}_{4,2}: \quad X_1=\partial_{u_n}, \quad X_2=t\partial_{u_n}, \quad Y_1=u_n\partial_{u_n}, \quad Y_2=t\partial_t+\tfrac{1}{2}u_n\partial_{u_n},$$

$$F_n=(u_{n+1}-u_n)t^{-2}f_n(\xi), \quad \xi=\frac{u_{n+1}-u_n}{u_{n-1}-u_n}. \tag{6.31}$$

D. dim NR(L)=3

1. $NR(L)=A_{3,1}$

This algebra can figure as a nilradical only for $a_n=0$. We then obtain

$$\mathrm{SA}_{4,3}: \quad X_1=\partial_t, \quad X_2=b_nu_n\partial_{u_n}, \quad X_3=c_nu_n\partial_{u_n}, \quad Y=t\partial_t+(\tfrac{1}{2}+a_n)u_n\partial_{u_n},$$

$$F_n=p_nu_n\xi^{-2/\alpha}, \quad \begin{vmatrix} b_n & b_{n+1} \\ c_n & c_{n+1} \end{vmatrix}\neq 0,$$

$$\xi=u_{n-1}^{\alpha_{nn+1}}u_n^{\alpha_{n+1n-1}}u_{n+1}^{\alpha_{n-1n}}, \quad \alpha_{km}=b_mc_k-b_kc_m, \tag{6.32}$$

$$\alpha=(\tfrac{1}{2}+a_{n-1})\alpha_{n,n+1}+(\tfrac{1}{2}+a_n)\alpha_{n+1,n-1}+(\tfrac{1}{2}+a_{n+1})\alpha_{n-1n},$$

$$A=\begin{pmatrix} 1 & & \\ & 0 & \\ & & 0 \end{pmatrix}. \tag{6.33}$$

2. $NR(L)=A_{3,2}$

The algebra $A_{3,2}$ can serve as a nilradical only for $a_n=0$. We add Y as usual and it turns out that we must have τ of the form $\tau=\tau_1 t+\tau_0$. However, the invariant interactions obtained are either linear, or such that they allow a symmetry algebra with a larger (four-dimensional) nilradical. Hence, no algebras L with $\mathrm{NR}(L)=A_{3,2}$ are obtained.

3. $NR(L)=A_{3,3}$

Using allowed transformations we can simplify $\tau(t)$ in the additional operator Y to be $\tau=1$, or $\tau=0$. We can always set $\beta_n(t)\to 0$ in Y. For a four-dimensional symmetry algebra the nonzero commutation relations will be as in Eq. (6.3) (with $1\leqslant i,\ k\leqslant 3$). We list the matrices A below. Inequivalent symmetry algebras are distinguished by the Jordan canonical forms of A.

The algebras we obtain are

$$\mathrm{SA}_{4,4}:\quad X_1=(2a_n-p_2-p_3)e^{(a_n-p_1)t}\partial_{u_n},$$

$$X_2=(2a_n-p_1-p_3)e^{(a_n-p_2)t}\partial_{u_n},$$

$$X_3=(2a_n-p_1-p_2)e^{(a_n-p_3)t}\partial_{u_n},\quad p_1<p_2<p_3, \tag{6.34}$$

$$Y=\partial_t+a_n u_n\partial_{u_n},\quad a_{n+1}\neq a_n,$$

$$F_n=A_n u_n+B_n e^{(a_n-a_{n+1})t}u_{n+1}+e^{a_n t}f_n(\xi),$$

$$\xi=(a_n-a_{n+1})u_{n-1}e^{-a_{n-1}t}+(a_{n+1}-a_{n-1})u_n e^{-a_n t}+(a_{n-1}-a_n)u_{n+1}e^{-a_{n+1}t},$$

$$A_n=\frac{1}{2(a_{n+1}-a_n)}\{2a_{n+1}[-3a_n^2+2a_n(p_1+p_2+p_3)-p_1p_2-p_2p_3-p_3p_1]$$
$$-2a_n(a_n-p_1-p_2-p_3)^2+(p_1+p_2)(p_2+p_3)(p_3+p_1)\},$$

$$B_n=\frac{1}{2(a_{n+1}-a_n)}(2a_n-p_1-p_2)(2a_n-p_2-p_3)(2a_n-p_3-p_1),$$

$$A=\mathrm{diag}(p_1,p_2,p_3). \tag{6.35}$$

$$\mathrm{SA}_{4,5}:\quad X_1=e^{(a_n-p)t}\cos(t-\gamma_n)\partial_{u_n},$$

$$X_2=e^{(a_n-p)t}\sin(t-\gamma_n)\partial_{u_n},\quad X_3=e^{(a_n-q)t}\cos\gamma_n\partial_{u_n},\quad Y=\partial_t+a_n u_n\partial_{u_n}, \tag{6.36}$$

$$\tan\gamma_n=\frac{(2a_n-p-q)(p-q)+1}{2(a_n-p)},\quad a_{n+1}\neq a_n,$$

$$F_n=[(a_n-p)^2-1-2(a_n-p)\cot(\gamma_n-\gamma_{n+1})]u_n+2\frac{a_n-p}{\sin(\gamma_n-\gamma_{n+1})}u_{n+1}e^{(a_n-a_{n+1})t}+e^{a_n t}f_n(\xi),$$

$$\xi=u_{n-1}e^{-a_{n-1}t}\sin(\gamma_n-\gamma_{n+1})+u_n e^{-a_n t}\sin(\gamma_{n+1}-\gamma_{n-1})+u_{n+1}e^{-a_{n+1}t}\sin(\gamma_{n-1}-\gamma_n)$$

$$A=\mathrm{diag}\left[\begin{pmatrix} p & 1\\ -1 & p\end{pmatrix},q\right]. \tag{6.37}$$

$$\mathrm{SA}_{4,6}: \quad X_1=\tfrac{1}{2}[(a_n-1)^2-(a_n-p)^2]e^{(a_n-1)t}\partial_{u_n},$$

$$X_2=\{-\tfrac{1}{2}[(a_n-1)^2-(a_n-p)^2]t+(a_n-1)\}e^{(a_n-1)t}\partial_{u_n},$$

$$X_3=(a_n-1)e^{(a_n-p)t}\partial_{u_n}, \quad p\neq 1,$$

$$Y=\partial_t+a_nu_n\partial_{u_n}, \quad a_{n+1}\neq a_n, \tag{6.38}$$

$$F_n=\frac{a_n-1}{a_{n+1}-a_n}[(a_{n+1}-1)(2p-3a_n+1)-(a_n-p)^2]u_n$$
$$+\frac{(a_n-1)(2a_n-1-p)^2}{a_{n+1}-a_n}u_{n+1}e^{(a_n-a_{n+1})t}+e^{a_nt}f_n(\xi),$$

with ξ as for algebra $\mathrm{SA}_{4,4}$.

$$A=\mathrm{diag}\left[\begin{pmatrix}1&0\\1&1\end{pmatrix},p\right]. \tag{6.39}$$

$$\mathrm{SA}_{4,7}: \quad X_1=(2a_n-1)e^{a_nt}\partial_{u_n}, \quad X_2=[(2a_n-1)t+1]e^{a_nt}\partial_{u_n},$$

$$X_3=2a_ne^{(a_n-1)t}\partial_{u_n}, \quad Y=\partial_t+a_nu_n\partial_{u_n}, \tag{6.40}$$

$$F_n=\frac{[a_n(a_n-a_{n+1})-(2a_{n+1}-1)(2a_n-1)]a_n}{a_n-a_{n+1}}u_n+\frac{(2a_n-1)^2a_n}{a_n-a_{n+1}}u_{n+1}e^{(a_n-a_{n+1})t}+e^{a_nt}f_n(\xi),$$

with ξ as for algebra $\mathrm{SA}_{4,4}$.

$$A=\mathrm{diag}\left[\begin{pmatrix}0&0\\1&0\end{pmatrix},1\right]. \tag{6.41}$$

$$\mathrm{SA}_{4,8}: \quad X_1=(a_n-1)e^{(a_n-1)t}\partial_{u_n}, \quad X_2=(-(a_n-1)t+\tfrac{1}{2})e^{(a_n-1)t}\partial_{u_n},$$

$$X_3=\tfrac{1}{2}[(a_n-1)t^2-t]e^{(a_n-1)t}\partial_{u_n}, \quad Y=\partial_t+a_nu_n\partial_{u_n},$$

$$F_n=\frac{(a_n-1)^2}{a_{n+1}-a_n}\{[(a_{n+1}-a_n)-4(a_{n+1}-1)]u_n+4(a_n-1)u_{n+1}e^{(a_n-a_{n+1})t}\}+e^{a_nt}f_n(\xi), \tag{6.42}$$

with ξ as for algebra $\mathrm{SA}_{4,4}$.

$$A=\begin{pmatrix}1&0&0\\1&1&0\\0&1&1\end{pmatrix}. \tag{6.43}$$

We see that the matrix A in Eq. (6.43) is indecomposable. The case (6.35) corresponds to the decomposition $1+1+1$, while Eqs. (6.37), (6.39), and (6.41) correspond to the decomposition $2+1$, with different structures of the 2×2 block.

4. NR(L)=$A_{3,4}$

We take $\{X_1, X_2, X_3\}$ as in Eq. (3.17) and add Y in the form (2.7). The commutation relations (6.3) imply that the coefficients in Y must satisfy $a_{n+1}=a_n$ and $\tau=\tau_0+\tau_1 t+\tau_2 t^2$. By allowed transformations we take τ into one of the following: $\tau=0,1,t,1+t^2$. Moreover, $\beta_n(t)$ of Y can be set equal to zero. We find that $\tau=0$ leads to a linear equation. The values $\tau=1$, t and t^2+1 lead to five different four-dimensional symmetry algebras. However, none of them is maximal among those existing for the given interaction F_n. In each case the abelian nilradical can be extended to a four-dimensional one and the corresponding maximal symmetry algebras will appear below.

E. dim NR(L)=4

1. NR(L)=$A_{4,1}$

We take $X_1,\ldots X_4$ as in Eq. (3.33). The additional element Y must again satisfy $a_{n+1}=a_n$, $\tau=1$, t or t^2+1, $\beta_n(t)=0$.

Up to allowed transformations the following five-dimensional symmetry algebras represent all possibilities. In each case we list the algebra, the interaction and the matrix A of Eq. (6.3).

$$\mathrm{SA}_{5,1}: \quad X_1=-\partial_{u_n}, \quad X_2=t\partial_{u_n}, \quad X_3=e^t\gamma_n\partial_{u_n},$$

$$X_4=e^{-t}\gamma_n\partial_{u_n}, \quad Y=\partial_t+au_n\partial_{u_n}, \quad a\neq 0$$

$$F_n=\frac{\gamma_n(u_{n+1}-u_n)}{\gamma_{n+1}-\gamma_n}+e^{at}f_n(\xi), \tag{6.44}$$

$$\xi=[(\gamma_n-\gamma_{n+1})u_{n-1}+(\gamma_{n+1}-\gamma_{n-1})u_n+(\gamma_{n-1}-\gamma_n)u_{n+1}]e^{-at},$$

$$A=\mathrm{diag}\left\{\begin{pmatrix} a & 0\\ 1 & a\end{pmatrix}, a-1, a+1\right\}.$$

$$\mathrm{SA}_{5,2}: \quad X_1=-\partial_{u_n}, \quad X_2=t\partial_{u_n}, \quad X_3=-\gamma_n\partial_{u_n},$$

$$X_4=t\gamma_n\partial_{u_n}, \quad Y=\partial_t+u_n\partial_{u_n}, \quad F_n=e^t f_n(\xi), \tag{6.45}$$

$$A=\mathrm{diag}\left\{\begin{pmatrix} 1 & 0\\ 1 & 1\end{pmatrix}, \begin{pmatrix} 1 & 0\\ 1 & 1\end{pmatrix}\right\}.$$

Here, ξ is as in case $\mathrm{SA}_{5,1}$ with $a=1$

$$\mathrm{SA}_{5,3}: \quad X_1=-\partial_{u_n}, \quad X_2=t\partial_{u_n}, \quad X_3=\gamma_n \sin t\partial_{u_n},$$

$$X_4=\gamma_n \cos t\partial_{u_n}, \quad Y=\partial_t+au_n\partial_{u_n}, \tag{6.46}$$

$$F_n=-\frac{\gamma_n(u_{n+1}-u_n)}{\gamma_{n+1}-\gamma_n}+e^{at}f_n(\xi), \quad A=\mathrm{diag}\left\{\begin{pmatrix} a & 0\\ 1 & a\end{pmatrix}, \begin{pmatrix} a & -1\\ 1 & a\end{pmatrix}\right\}.$$

Again, ξ as in case $\mathrm{SA}_{5,1}$.

$$\mathrm{SA}_{5,4}: \quad X_1=\partial_{u_n}, \quad X_2=t\partial_{u_n}, \quad X_3=t^{1/2+a-p}\gamma_n\partial_{u_n},$$

$$X_4=t^{1/2-a+p}\gamma_n\partial_{u_n}, \quad Y=t\partial_t+(\tfrac{1}{2}+a)u_n\partial_{u_n},$$

$$F_n=\frac{[(a-p)^2-\frac{1}{4}]\gamma_n(u_{n+1}-u_n)}{(\gamma_{n+1}-\gamma_n)t^2}+t^{a-3/2}f_n(\xi), \tag{6.47}$$

$$\xi=[(\gamma_n-\gamma_{n+1})u_{n-1}+(\gamma_{n+1}-\gamma_{n-1})u_n+(\gamma_{n-1}-\gamma_n)u_{n+1}]t^{-a-1/2},$$

$$A=\mathrm{diag}(\tfrac{1}{2}+a,-\tfrac{1}{2}+a,p,a-p),\quad p\neq a.$$

$$\mathrm{SA}_{5,5}:\quad X_1=\partial_{u_n},\quad X_2=t\partial_{u_n},\quad X_3=\gamma_n\sqrt{t}\,\cos(\ln t)\partial_{u_n},$$

$$X_4=\gamma_n\sqrt{t}\,\sin(\ln t)\partial_{u_n},\quad Y=t\partial_t+(\tfrac{1}{2}+a)u_n\partial_{u_n},$$

$$F_n=-\frac{5}{4}\frac{\gamma_n(u_{n+1}-u_n)}{(\gamma_{n+1}-\gamma_n)t^2}+e^{at}f_n(\xi),\quad A=\mathrm{diag}\left\{a+\frac{1}{2},a-\frac{1}{2},\begin{pmatrix}a & 1\\ -1 & a\end{pmatrix}\right\}, \tag{6.48}$$

with ξ as in case $\mathrm{SA}_{5,1}$

$$\mathrm{SA}_{5,6}:\quad X_1=\partial_{u_n},\quad X_2=t\partial_{u_n},\quad X_3=\gamma_n\sqrt{t^2+1}\,\cos(q\ \arctan\ t)\partial_{u_n},$$

$$X_4=\gamma_n\sqrt{t^2+1}\,\sin(q\ \arctan\ t)\partial_{u_n},\quad Y=(t^2+1)\partial_t+(t+a)u_n\partial_{u_n},$$

$$F_n=\frac{(1-q^2)\gamma_n(u_{n+1}-u_n)}{(\gamma_{n+1}-\gamma_n)(t^2+1)^2}+\frac{e^{a\ \arctan\ t}}{(t^2+1)^{3/2}}f_n(\xi),$$

$$\xi=\{(\gamma_n-\gamma_{n+1})u_{n-1}+(\gamma_{n+1}-\gamma_{n-1})u_n+(\gamma_{n-1}-\gamma_n)u_{n+1}\}\frac{e^{-a\ \arctan\ t}}{(t^2+1)^{1/2}},$$

$$A=\mathrm{diag}\left\{\begin{pmatrix}a & 1\\ -1 & a\end{pmatrix},\begin{pmatrix}a & q\\ -q & a\end{pmatrix}\right\},\quad q>0. \tag{6.49}$$

$$\mathrm{SA}_{5,7}:\quad X_1=\partial_{u_n},\quad X_2=-t\partial_{u_n},\quad X_3=(-\ln t+\gamma_n)\partial_{u_n},$$

$$X_4=(t\ \ln\ t+\gamma_n t)\partial_{u_n},\quad Y=t\partial_t+(\tfrac{1}{2}+a)u_n\partial_{u_n}, \tag{6.50}$$

$$F_n=\frac{u_{n+1}-u_n}{t^2(\gamma_{n+1}-\gamma_n)}+t^{a-3/2}f_n(\xi),$$

$$A=\begin{pmatrix}\frac{1}{2}+a & & & \\ 0 & -\frac{1}{2}+a & & \\ 1 & 0 & \frac{1}{2}+a & \\ 0 & 1 & 0 & -\frac{1}{2}+a\end{pmatrix} \tag{6.51}$$

with ξ as in the case $\mathrm{SA}_{5,4}$.

None of the algebras $\mathrm{SA}_{4,3},\ldots,\mathrm{SA}_{4,8}$ nor $\mathrm{SA}_{5,1},\ldots,\mathrm{SA}_{5,7}$ can be extended by a further element Y_2, outside the nilradical.

Let us sum things up as theorem.

Theorem 6: *Altogether 31 classes of solvable symmetry algebras with abelian nilradicals exist for Eq. (1.1). Their dimensions are 2, 3, 4, and 5. Each class is represented by one algebra in this Section, namely, $SA_{2,1},\ldots,SA_{2,4}$; $SA_{3,1},\ldots,SA_{3,12}$; $SA_{4,1},\ldots,SA_{4,8}$, and $SA_{5,1},\ldots,SA_{5,7}$.*

VII. NONSOLVABLE SYMMETRY ALGEBRAS

A nonsolvable Lie algebra must contain a simple subalgebra. The only simple Lie algebra that can be realized in terms of vector fields of the form (2.7) is $\mathrm{sl}(2,\mathbb{R})$. Upto allowed transformations it can only be realized, together with the corresponding invariant interaction, as

$$\mathrm{NS}_{3,1}: \quad X_1=\partial_t, \quad X_2=t\partial_t+\tfrac{1}{2}u_n\partial_{u_n}, \quad X_3=t^2\partial_t+tu_n\partial_{u_n}, \tag{7.1}$$

$$F_n=\frac{1}{u_n^3}\,f_n(\xi_{n-1},\xi_{n+1}), \quad \xi_k=\frac{u_k}{u_n}. \tag{7.2}$$

We now write the determining equation (2.4) for F_n in the form (7.2) and look for additional symmetries. As a result we obtain algebras containing (7.1), plus further vector fields, forming the radical of the final symmetry algebra. They are

$$\mathrm{NS}_{4,1}: \quad X_4=a_nu_n\partial_{u_n}, \quad a_{n+1}\neq a_n,$$

$$F_n=u_n^{-3}\left(\frac{u_{n+1}}{u_n}\right)^{(4a_n)/(a_{n+1}-a_n)} f_n(\xi), \tag{7.3}$$

$$\xi=u_{n+1}^{a_{n-1}-a_n}u_n^{a_{n+1}-a_{n-1}}u_{n-1}^{a_n-a_{n+1}}.$$

$$\mathrm{NS}_{5,1}: \quad X_4=a_nu_n\partial_{u_n}, \quad X_5=b_nu_n\partial_{u_n},$$

$$a_{n+1}\neq a_n, \quad b_{n+1}\neq b_n, \quad b_n\neq\lambda a_n,$$

$$F_n=c_nu_n[u_{n-1}^{(b_{n+1}a_n-b_na_{n+1})}u_n^{(b_{n-1}a_{n+1}-b_{n+1}a_{n+1})}u_{n+1}^{(b_na_{n-1}-b_{n-1}a_n)}]^{4/\alpha_n}, \tag{7.4}$$

$$\alpha_n=b_{n-1}(a_n-a_{n+1})+b_n(a_{n+1}-a_{n-1})+b_{n+1}(a_{n-1}-a_n).$$

$$\mathrm{NS}_{5,2}: \quad X_4=\partial_{u_n}, \quad X_5=t\partial_{u_n}, \tag{7.5}$$

$$F_n=(u_{n+1}-u_n)^{-3}f_n(\xi), \quad \xi=\frac{u_{n+1}-u_n}{u_{n-1}-u_n}.$$

$$\mathrm{NS}_{7,1}: \quad X_4=\partial_{u_n}, \quad X_5=t\partial_{u_n}, \quad X_6=\gamma_n\partial_{u_n}, \quad X_7=t\gamma_n\partial_{u_n}, \tag{7.6}$$

$$F_n=[(\gamma_n-\gamma_{n+1})u_{n-1}+(\gamma_{n+1}-\gamma_{n-1})u_n+(\gamma_{n-1}-\gamma_n)u_{n+1}]^{-3}.$$

To sum up:

Theorem 7: *Nonsolvable symmetry algebras of Eq. (1.1) can have dimensions 3, 4, 5, or 7. There are 5 classes of them, $NS_{3,1}$, $NS_{4,1}$, $NS_{5,1}$, $NS_{5,2}$, and $NS_{7,1}$.*

VIII. SYMMETRIES OF LINEAR DIFFERENTIAL–DIFFERENCE EQUATIONS

Let us now consider the case excluded in the rest of this article, namely when Eq. (1.1) has the form

$$\ddot{u}_n = A_n(t)u_{n-1} + B_n(t)u_n + C_n(t)u_{n+1} + D_n(t), \tag{8.1}$$

i.e., is a linear inhomogeneous $D\Delta E$. Substituting into the determining equation (2.4) and reading off the coefficients of u_{n-1}, u_{n+1}, u_n, and 1 we obtain four equations.

$$[(a_n - a_{n-1}) - 2\dot{\tau}]A_n - \tau\dot{A}_n = 0, \tag{8.2}$$

$$[(a_n - a_{n+1}) - 2\dot{\tau}]C_n - \tau\dot{C}_n = 0, \tag{8.3}$$

$$\tfrac{1}{2}\dddot{\tau} - 2\dot{\tau}B_n - \tau\dot{B}_n = 0, \tag{8.4}$$

$$\ddot{\beta}_n + (a_n - \tfrac{3}{2}\dot{\tau})D_n - \tau\dot{D}_n - \beta_{n-1}A_n - \beta_n B_n - \beta_{n+1}C_n = 0. \tag{8.5}$$

For A_n and C_n generic, Eqs. (8.2) and (8.3) imply

$$\tau = 0, \quad a_{n+1} = a_n \equiv a. \tag{8.6}$$

Equation (8.4) is satisfied identically and Eq. (8.5) has the following solutions:

(1) For $a = 0$ we have

$$X(\beta) = \beta_n(t)\partial_{u_n}, \tag{8.7}$$

where $\beta_n(t)$ is a solution of the homogeneous equation, i.e., Eq. (8.1) with $D_n(t) = 0$.

(2) For $a \neq 0$ choose $a = -1$. We then have

$$X_I = [u_n - \beta^{(t)}_{n,I}]\partial_{u_n}, \tag{8.8}$$

where $\beta_{n,I}$ is any solution of the inhomogeneous equation (8.1).

Thus the symmetry algebra is infinite dimensional, but this simply reflects the linear superposition principle. This is still a useful property. Indeed the existence of an infinite-dimensional symmetry algebra can serve as a criterion of linearizability by point transformations for equations of the form (1.1), just as in the case of partial differential equations.[23] The linearizing transformations would of course not be amongst the allowed transformations (2.5).

Now let us find additional symmetries existing for special forms of Eq. (8.1). Allowed transformation preserve linearity, so we can use them to simplify the vector field X.

Let one additional symmetry generator exist.

A. $\tau = 0$

For $A_n \neq 0$, or $C_n \neq 0$ we find $a_{n+1} = a_n$ and we reobtain the generator (8.8) and hence nothing new.

For $A_n = C_n = 0$ Eq. (8.1) decouples into

$$\ddot{u}_n = B_n(t)u_n + D_n(t). \tag{8.9}$$

For each n separately we obtain an $sl(3,\mathbb{R})$ symmetry algebra, as in the case for any linear, or linearizable ODE.[24]

B. $\tau \neq 0$

We transform τ into $\tau = 1$ and consider X in the form (2.9). Solving the determining equations (8.2),...,(8.4) for the coefficients A_n, B_n, C_n, D_n, we find that such an additional symmetry exists only for

TABLE I. The results of the symmetry classification of the nonlinear $D\Delta E$ (1.1).

dim L	A	N	SN	SA	NS	T
7	0	0	0	0	1	1
6	0	0	3	0	0	3
5	0	1	0	7	2	10
4	2	1	4	8	1	16
3	4	2	0	12	1	19
2	5	0	0	4	0	9
1	3	0	0	0	0	3

$$\ddot{u}_n = R_n e^{(a_n - a_{n-1})t} u_{n-1} + B_n u_n + S_n e^{(a_n - a_{n+1})t} u_n + W_n e^{a_n t},$$
$$\dot{R}_n = \dot{B}_n = \dot{W}_n = \dot{S}_n = 0, \quad X = \partial_t + a_n u_n \partial_{u_n}. \tag{8.10}$$

A two-dimensional additional symmetry algebra for coupled equations (R_n and S_n not both vanishing) can exist only if we have $A_n = 0$, or $C_n = 0$ and also $a_n = 0$ in Eq. (8.10). For instance, for $C_n = 0$, $A_n \neq 0$, we have

$$F_n = A_n u_{n-1} + D_n, \quad X_1 = \partial_t, \quad X_2 = t\partial_t + [(\tfrac{1}{2} + 2n + \rho)u_n + \beta_n]\partial_{u_n}, \tag{8.11}$$

where ρ and β_n satisfy

$$\ddot{\beta}_n + (2n + \rho - \tfrac{3}{2})D_n - \beta_{n-1} A_n = 0.$$

If, in particular, we also have $D_n = 0$, then the entire symmetry algebra is as follows:

$$\ddot{u}_n = A_n u_{n-1}, \tag{8.12}$$

$$X_1 = \partial_t, \quad X_2 = t\partial_t + (\tfrac{1}{2} + 2n) u_n \partial_{u_n},$$

$$X_3 = \partial_{u_n}, \quad X(\beta) = \beta_n(t) \partial_{u_n},$$

where $\beta_n(t)$ is a solution of Eq. (8.12).

IX. CONCLUSIONS

(1) The results of the symmetry classification of the nonlinear $D\Delta E$ (1.1) are summed up in Table I.

In the first row A, N, SN, SA, NS, and T mean abelian, nilpotent, solvable with nonabelian nilradical, solvable with abelian nilradical, nonsolvable, and total, respectively. In the second to fifth column we give the number of each type of symmetry algebra for each dimension dim L. The total number for each dimension is given in the last column.

The A, N, SN, SA, and NS type symmetry algebras are reviewed in Secs. III–VII, respectively.

We see that we have dim $L \leqslant 7$. For dim $L = 6$, or 7 the interactions F_n are completely specified (up to 1 or more functions of n). Several types of ''symmetry variables'' occur for the higher dimensional symmetry algebras. Let us denote them as follows:

$$\xi=(\gamma_n-\gamma_{n+1})u_{n-1}+(\gamma_{n+1}-\gamma_{n-1})u_n+(\gamma_{n-1}-\gamma_n)u_{n+1},$$
$$\eta=\xi h(t),\quad \zeta=p_{n-1}(t)u_{n-1}+p_n(t)u_n+p_{n+1}u_{n+1},$$
$$\rho=\frac{u_{n+1}-u_n}{u_{n-1}-u_n},\quad \sigma=u_{n-1}^{a_{n-1}}u_n^{a_n}u_{n+1}^{a_{n+1}}, \tag{9.1}$$

where γ_n and q_n depend only on n, $h(t)$ is some (specific in each case) function of t and $p_n(t)$ is a (specific) function of n and t.

We can write the interactions having symmetry algebras of dimension $5\leqslant\dim L\leqslant 7$ as follows:

$$\mathrm{NS}_{7,1}:\quad F_n=c_n\xi^{-3}, \tag{9.2}$$

$$\mathrm{SN}_{6,1}:\quad F_n=c_n\xi^{p}, \tag{9.3a}$$

$$\mathrm{SN}_{6,2}:\quad F_n=c_n+(a+b\gamma_n)\ln\,\xi, \tag{9.3b}$$

$$\mathrm{SN}_{6,3}:\quad F_n=c_n+e^{b_n\xi}, \tag{9.4a}$$

$$\mathrm{SN}_{6,4}:\quad F_n=c_n\xi^{-1}, \tag{9.4b}$$

$$\mathrm{SN}_{6,5}:\quad F_n=\frac{2k}{\gamma_{n+1}-\gamma_n}+f_n(\xi), \tag{9.4c}$$

$$\mathrm{SA}_{5,1},\ldots,\mathrm{SA}_{5,7}:\quad F_n=\frac{\alpha(t)+\beta(t)\gamma_n}{\gamma_{n+1}-\gamma_n}(u_{n+1}-u_n)+g(t)f_n(\eta), \tag{9.5a}$$

where the functions of α, β, g, and h are different in each case

$$\mathrm{NS}_{5,1}:\quad F_n=c_n\sigma, \tag{9.5b}$$

$$\mathrm{SN}_{5,2}:\quad F_n=(u_{n+1}-u_n)^{-3}f_n(\rho). \tag{9.5c}$$

For $1\leqslant\dim L\leqslant 4$, see Secs. II, III, and VI.

(2) Among the interactions with four-dimensional symmetry algebras a case of particular interest is $\mathrm{SN}_{4,3}$ of Eq. (5.4). This case contains the well-known and integrable Toda lattice.[25] Indeed, if we choose

$$\gamma_n=2n,\quad f_n(\xi)=-1+e^{1/2\xi}, \tag{9.6}$$

we obtain the equation

$$u_{n,tt}=e^{u_{n-1}-u_n}-e^{u_n-u_{n+1}}. \tag{9.7}$$

Thus the Toda lattice is not singled out by its Lie point symmetry group, at least not by symmetries generated by vector fields of the type (1.4). Instead, it comes in a family involving two arbitrary functions, γ_n and $f_n(\xi)$. Nor is the Toda lattice the one with the largest symmetry group of the considered type. This distinction goes to the interaction (9.2).

(3) The connection between Lie point symmetries of $D\Delta E$ and their integrability remains open. We plan to investigate other types of symmetries of Eq. (1.1), or at least special cases thereof in the near future.

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The behavior of nearby trajectories in magnetic billiards

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In chaos theory the separation of infinitesimally close trajectories has great importance. In present paper this behavior is investigated for classical magnetic billiard systems on Riemannian manifolds. The separation of the trajectories during the bounceless segments as well as at the reflections is studied generally, with a method similar to that of Jacobi fields for geodesic flows. For two-dimensional manifolds the results are also given in a natural coordinate frame, and they are illustrated in special (homogeneous) cases. We relate our issues to the known properties of the curvature of the horocycles, too. © *1996 American Institute of Physics.* [S0022-2488(96)00609-3]

I. INTRODUCTION

The geodesic motion on Riemannian manifolds became a very important model in ergodic theory, since due to the theorem of Lobatchewski and Hadamard[1] the geodesic flow on the unitary tangent bundle of any compact Riemannian manifold with negative curvature shows strongly stochastic properties, it is a *C*-system, ergodic, mixing and has positive entropy.[2,3] With the method of Jacobi fields[4] it has been shown that on Riemannian manifolds with negative curvature the separation of nearby geodesic trajectories is exponential and the long-time evolution depends very sensitively on the initial conditions, i.e., the system is chaotic.

Slightly more difficult systems are the billiards, which were also traditionally investigated in chaos theory[5–9] and later from the point of view of quantum chaos, too.[10–12] In these systems a particle moves freely (along geodesic segments) in a bounded region of a Riemannian manifold, and changes its velocity according to the law of elastic reflection at the boundaries of the billiard. The long-time behavior of nearby trajectories is controlled by two effects; by the separation of the geodesic segments between subsequent bounces, and by the reflections themselves, which can focus or defocus the bunch of trajectories. The first effect is essentially equivalent with that mentioned in the previous paragraph, and depends on the curvature of the Riemannian manifold, while the second one is an instantaneous, local effect, which does not depend on the properties of the manifold, but only on the curvature of the billiard boundary at the reflection point and on the angle of reflection. A conventional way, motivated by geometric optical analogies, for keeping track of these separating effects is to follow the evolution of the curvature of the horocycle (wavefront in geometric optics) along the investigated bunch of trajectories.[5,6,8,11,13,14] The curvature κ of the horocycle satisfies a first-order ordinary differential equation along the geodesic segments, and it has jumps depending on the angle of reflection and on the curvature of the wall at the bounces. Having known the time (or parameter) dependence of κ, one can get the transverse separation of nearby trajectories by integration.

A bit more complicated family of systems are billiards with force field, which results in that the particle no longer follows geodesic segments between the subsequent bounces. Special types of these systems are the magnetic billiards, in which a charged particle moves in the billiard under the action of magnetic Lorentz force, that changes only the direction of its velocity, but does not change its kinetic energy. These systems also have a great importance in chaos theory because of their (relative) simplicity and richness.[14–17] The presence of the magnetic field breaks the time-

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reversal symmetry of the system, and strongly influences the behavior of nearby trajectories during the bounceless segments as well as at the reflections. Changing the value of the magnetic field one can study the transition from completely integrable systems to soft or hard chaos.[14,17] Since the Schrödinger equation can be relatively easily treated in magnetic billiards with numerical methods, these systems also provide a good framework for studying the quantum mechanical aspects of classical chaos.[18]

In this paper we study magnetic billiard systems from a classical point of view, and derive some formulas describing the separation of nearby trajectories during the bounceless periods and at the reflections. With the help of these formulas one can calculate the Lyapunov exponent for special trajectories. We summarize the main results of the paper along with its organization.

In Sec. II the bounceless motion of a charged particle is studied on a Riemannian manifold with magnetic field, and, using a method similar to that of Jacobi fields for geodesics,[4] a generalization of the Jacobi equation[4] is also derived for this case. This latter equation describes the infinitesimal separation of nearby trajectories in magnetic systems. In Appendix A a mathematical addendum is given about the properties of vector fields along mappings needed in Sec. II.

From Sec. III our attention is restricted to two-dimensional systems. In the third section we rewrite the Jacobi equation obtained in Sec. II in a more expressing form using a naturally chosen coordinate frame along the investigated trajectory, and discuss the behavior of its solutions. It is shown that the positive (Gaussian) curvature and the presence of the magnetic field locally stabilize the given bunch of trajectories, the behavior of which is also influenced by the transverse inhomogeneity of the magnetic field. The results are illustrated in simple, homogeneous cases, with special emphasis on the Bolyai–Lobatchewski plane with constant magnetic field.[18] Appendix B contains a brief survey of the cycles and isometries of the hyperbolic plane using its pseudosphere model.[10]

In Sec. IV the bouncing effects are investigated, and a formula is derived, which gives the jump of the Jacobi field at the reflections. In contrast with geodesic billiards, at the presence of magnetic field this jump depends on the value of the field, too; moreover, the field can also change the focusing or defocusing character of the bounce. We illustrate this in a simple case using purely classical geometrical tools in Appendix C.

In Sec. V we relate our method, using generalized Jacobi fields along the trajectories for calculating the behavior of nearby trajectories, to the method which uses the curvature κ of horocycles. We express κ with the help of the Jacobi field, rewrite our results as equations for κ, and show that they agree with the known results when the magnetic field is zero,[5,6,8,11,13] or when the magnetic field is homogeneous and the curvature of the billiard plane is zero.[14]

Our main results are summarized again in Sec. VI.

II. INFINITESIMAL VARIATIONS AND GENERALIZED JACOBI EQUATION

From this section, in differential geometrical calculations we generally adopt the notations of Ref. 4. For a smooth manifold $M, T_x(M)$ denotes its tangent space at the point $x \in M$, $T(M)$ and $\pi_M: T(M) \to M$ denotes the tangent bundle and its canonical projection to M. $\mathscr{F}(M)$ is the algebra of smooth functions on M and $\mathscr{V}(M)$ is the Lie algebra of smooth vector fields on M. For a differentiable mapping $f: N \to M$ we denote its differential (resp. its differential at a point $p \in N$) with f_* [resp. with $(f_*)_p$]. The tensor field $f^*\Omega$ is the pull back of the covariant tensor field Ω given on M to the manifold N. The set of smooth vector fields along f is denoted by $\mathscr{V}_f$. If $\mathbf{\nabla}: \mathscr{V}(M) \times \mathscr{V}(M) \to \mathscr{V}(M)$ is a connection of M, then the induced connection $\tilde{\mathbf{\nabla}}: \mathscr{V}(N) \times \mathscr{V}_f \to \mathscr{V}_f$ is distinguished by a tilde. Since our derivations are strongly based on the concept of vector fields along mappings,[19] we give the definition and summarize the basic properties of this notion in Appendix A.

Let $(M, \langle \cdot, \cdot \rangle)$ be an m-dimensional Riemannian manifold with scalar product $\langle \cdot, \cdot \rangle$, and let us denote its Levi-Civita connection, torsion, and curvature tensor with $\mathbf{\nabla}$, $T(=0)$ and R, respectively.

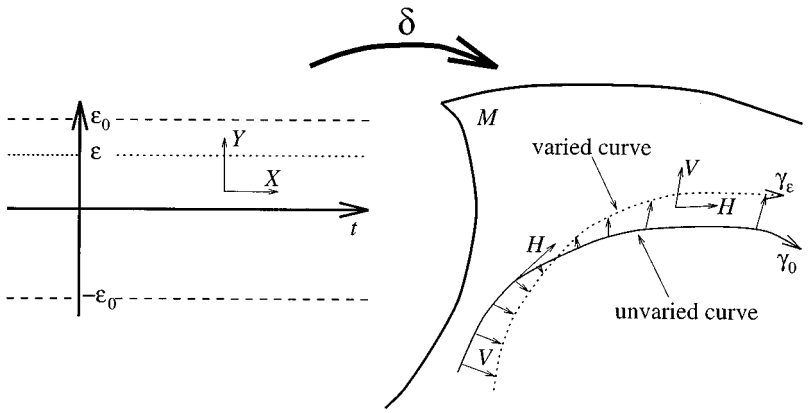

FIG. 1. The variation of a trajectory.

Let B be a given antisymmetric tensor field of type (1,1) [i.e., $\langle X,B(X)\rangle=0$ for all $X\in\mathscr{V}(M)$]. This plays the role of the magnetic field in our system. The equation of motion of a particle of unit charge and mass is

$$\nabla_{\dot\gamma}\dot\gamma=B(\dot\gamma), \tag{1}$$

where $\gamma:\mathfrak{R}\to M$ gives the trajectory of the particle parametrized with time. For physical reasons we assume furthermore that in the investigated system every solution of Eq. (1) is complete, so the motion of the particle can always be followed infinitely both backwards and forwards in time. Multiplying the equation with $\dot\gamma$ we get that $(d/dt)\langle\dot\gamma,\dot\gamma\rangle = 2\langle\dot\gamma,\nabla_{\dot\gamma}\dot\gamma\rangle = 2\langle\dot\gamma,B(\dot\gamma)\rangle = 0$, so the speed (kinetic energy) of the particle is constant. We can assume, without loss of generality, that

$$|\dot\gamma|^2=1. \tag{2}$$

(Otherwise one should change the scale of time and magnetic field by $|\dot\gamma|$.)

The following two concepts help us to handle the behavior of nearby trajectories (Fig. 1).

Definition 1: Let $\gamma_0:\mathfrak{R}\to M$ be a solution of the equation of motion (1). A differentiable mapping $\delta:\mathfrak{R}\times(-\varepsilon_0,\varepsilon_0)\to M$ $(\varepsilon_0>0)$ is said to be a *variation of the curve* γ_0, if $\delta(t,0)=\gamma_0(t)$ $(t\in\mathfrak{R})$, and the curves $\gamma_\varepsilon:\mathfrak{R}\to M$ defined by $\gamma_\varepsilon(t):=\delta(t,\varepsilon)$ also satisfy Eq. (1). The curves γ_ε are the *varied curves*. If the varied curves satisfy also the additional condition (2), δ is called a *special variation.*

Definition 2: Let γ_0 be a solution of Eq. (1), and let δ be a variation of it. The *infinitesimal variation* of γ_0 corresponding to the variation δ is a smooth vector field $V_0\in\mathscr{V}_{\gamma_0}$ along γ_0, for which $V_0(t)=(\partial/\partial\varepsilon)|_{(t,0)}\delta(t,\varepsilon)$. In accordance with the previous definition, V_0 is called a *special infinitesimal variation* if it is induced by a special variation. We denote the set of infinitesimal variations (resp. special infinitesimal variations) along γ_0 with $\mathscr{J}_{\gamma_0}$ (resp. with $\mathscr{SJ}_{\gamma_0}$).

It is intuitively clear that a (special) infinitesimal variation of a trajectory describes the relative motion of another particle moving (at the same speed) along an infinitesimally close path. Since the possible initial conditions of a trajectory constitute a finite-dimensional manifold, it is also expectable that the set $\mathscr{J}_\gamma$ (or $\mathscr{SJ}_\gamma$) of (special) infinitesimal variations along γ form a finite-dimensional subspace of the infinite-dimensional vector space $\mathscr{V}_\gamma$. In the following we define a finite-dimensional subspace of $\mathscr{V}_\gamma$, whose elements are called (special) generalized Jacobi fields, and show that these vector fields are exactly the (special) infinitesimal variations of γ.

Definition 3: Let $\gamma:\mathfrak{R}\to M$ be a solution of the equation of motion (1). A vector field $V\in\mathscr{V}_\gamma$ along γ is a *generalized Jacobi field along* γ, if it satisfies the following second-order ordinary differential equation called *generalized Jacobi equation*:

$$V''=(\nabla_V B)(\dot\gamma)+B(V')-R(V,\dot\gamma)\dot\gamma, \tag{3}$$

where R is the curvature tensor of M, and $V'\in\mathscr{V}_\gamma$ is the derivative $\tilde\nabla_{\partial/\partial t}V$ of $V\in\mathscr{V}_\gamma$ with respect to the parameter $t\in\mathfrak{R}$ of γ. If V beside the equation (3) also satisfies the condition

$$\langle V',\dot\gamma\rangle=0, \tag{4}$$

then V is said to be a *special* (generalized) *Jacobi field*. The set of (generalized) Jacobi fields and special (generalized) Jacobi fields along γ are denoted by $\mathscr{J}_\gamma$ and $\mathscr{SJ}_\gamma$, respectively.

We note that, if the magnetic field is zero, the first two terms on the right side of Eq. (3) vanish, and the generalized Jacobi equation simplifies to the usual Jacobi equation for geodesic variations.[4] In this paper variations of geodesics are not treated, so for the sake of brevity the attribute (generalized) of Jacobi fields and Jacobi equation is omitted.

Since Eq. (3) and condition (4) are linear in V, $\mathscr{J}_\gamma$ and $\mathscr{SJ}_\gamma$ are vector spaces over $\mathfrak{R}$. To give a particular solution $V\in\mathscr{J}_\gamma$ of (3), $V(t_0)$, $V'(t_0)\in T_{\gamma(t_0)}(M)$ must be prescribed (arbitrarily) at a given instant of time t_0. This means, that $\dim\mathscr{J}_\gamma=2m$ $[m=\dim(M)]$.

A straightforward calculation shows that for a Jacobi field $V\in\mathscr{J}_\gamma$ the scalar product $p:=\langle V',\dot\gamma\rangle$ is independent of time. Indeed, $dp/dt = d/dt\langle V',\dot\gamma\rangle = \langle V'',\dot\gamma\rangle + \langle V',\nabla_{\dot\gamma}\dot\gamma\rangle$, and inserting V'' from (3) and $\nabla_{\dot\gamma}\dot\gamma$ from (1) we obtain

$$\frac{dp}{dt}=\frac{d}{dt}\langle V',\dot\gamma\rangle=-\langle R(V,\dot\gamma)\dot\gamma,\dot\gamma\rangle+\langle(\nabla_V B)(\dot\gamma),\dot\gamma\rangle+\langle B(V'),\dot\gamma\rangle+\langle B(\dot\gamma),V'\rangle=0, \tag{5}$$

which is zero due to the properties of the curvature tensor and the antisymmetry of B. So if the condition (4) is satisfied at an arbitrary instant of time, then it holds for all parameter values $t\in\mathfrak{R}$. It means that $\mathscr{SJ}_\gamma$ is a hyperplane ($2m-1$-dimensional subspace) of $\mathscr{J}_\gamma$. It is also easy to show that for every $a\in\mathfrak{R}$, $a\dot\gamma\in\mathscr{V}_\gamma$ is a special Jacobi field.

The following theorem gives the connection between the (special) Jacobi fields and the (special) infinitesimal variations along a trajectory γ.

Theorem 4: For every solution $\gamma_0:\mathfrak{R}\to M$ of the equation of motion (1), the set $\mathscr{T}_{\gamma_0}$ of infinitesimal variations of γ_0 is identical with the set $\mathscr{J}_{\gamma_0}$ of Jacobi fields along γ_0. Moreover, for a solution η_0 of the equation (1), which also satisfies the condition (2), the set $\mathscr{ST}_{\eta_0}$ of special infinitesimal variations of η_0 is identical with the set $\mathscr{SJ}_{\eta_0}$ of special Jacobi fields along η_0.

Proof: First we prove that every infinitesimal variation of γ_0 satisfies the Jacobi equation. Let $\delta:\mathfrak{R}\times(-\varepsilon_0,\varepsilon_0)\to M(\varepsilon_0>0)$ be a variation of γ_0, and let us denote the canonical base vector fields on the parameter plane $\mathfrak{R}\times(-\varepsilon_0,\varepsilon_0)$ with $X:=\partial/\partial t$ and $Y:=\partial/\partial\varepsilon$, where t is the first and ε is the second coordinate of the parameter plane (Fig. 1). The *longitudinal vector field* $H\in\mathscr{V}_\delta$ and the *transverse vector field* $V\in\mathscr{V}_\delta$ are constructed from these base fields with the help of δ_*:

$$H:=\delta_* X,\quad V:=\delta_* Y. \tag{6}$$

[If the mapping δ were injective, the vector fields X and Y could be simply pushed forward to the manifold M. But generally δ is not injective; moreover, it usually has critical points along γ_0 (conjugate points). This is the reason why H and V have to be defined as vector fields along δ.]

It is clear that $V(t,0)$ is just the infinitesimal variation corresponding to δ at the point $\gamma_0(t)$, and that the longitudinal vector field H consists of the tangent vectors of the varied curves, i.e., $H(t,\varepsilon)=\dot\gamma_\varepsilon(t)$. Since the varied curves also obey Eq. (1), we have

$$\tilde{\nabla}_X H = B(H) \tag{7}$$

for H ($\tilde{\nabla}$ denotes the covariant derivation on $\mathscr{T}_\delta$ induced by ∇). Differentiating Eq. (7) with respect to Y, we obtain

$$\tilde{\nabla}_Y \tilde{\nabla}_X H = \tilde{\nabla}_Y (B(H)). \tag{8}$$

Now we transform this equation into a form which does not contain derivations of H or V with respect to Y, so in which it is enough to know H and V along γ_0. Using (A2) and the facts that $T=0$ and $[X,Y]=0$, we have

$$\tilde{\nabla}_X V = \tilde{\nabla}_Y H. \tag{9}$$

Using (A3) and (9), the left side of Eq. (8) can be rewritten in the following form:

$$\tilde{\nabla}_Y \tilde{\nabla}_X H = R(V,H)H + \tilde{\nabla}_X \tilde{\nabla}_Y H + \tilde{\nabla}_{[Y,X]} H = R(V,H)H + \tilde{\nabla}_X \tilde{\nabla}_X V. \tag{10}$$

The right side of (8) can be written as follows:

$$\tilde{\nabla}_Y (B(H)) = (\tilde{\nabla}_Y B)(H) + B(\tilde{\nabla}_Y H) = (\tilde{\nabla}_Y B)(H) + B(\tilde{\nabla}_X V). \tag{11}$$

Putting together the two sides (10) and (11), considering the equation obtained at $\varepsilon=0$, and writing $\dot{\gamma}_0(t)$ in place of $H(t,0)$, we obtain

$$R(V,\dot{\gamma}_0)\dot{\gamma}_0 + V'' = (\nabla_V B)(\dot{\gamma}_0) + B(V'), \tag{12}$$

which agrees with the Jacobi equation (3).

For a special variation δ of the curve η_0, the property (4) of the corresponding infinitesimal variation V can be proved using a similar trick. Let X, Y, H, and V be the same vector fields as before. Since δ is a special variation, we have

$$\langle H,H\rangle = 1 \tag{13}$$

for H. Differentiating it with respect to Y and using (9), we find that

$$\tilde{\nabla}_Y \langle H,H\rangle = 2\langle \tilde{\nabla}_Y H, H\rangle = 2\langle \tilde{\nabla}_X V, H\rangle = 0. \tag{14}$$

Considering it at $\varepsilon=0$, we find that $\langle V', \dot{\eta}_0\rangle = 0$, so V is indeed a special Jacobi field.

Now we sketch the proof of the theorem in the opposite direction. Let $\tilde{V}$ be a given Jacobi field along the trajectory γ_0. From $\tilde{V}$ we construct a variation δ, for which the transverse vector field $V \in \mathscr{T}_\delta$ is identical with $\tilde{V}$ along γ_0. Since both $\tilde{V}$ and $V|_{\varepsilon=0}$ are Jacobi fields, to prove their equality it is enough to show that they and their first derivatives with respect to $\dot{\gamma}_0$ agree at a single point of γ_0. However, using (9) the derivations with respect to tangent vectors of γ_0 can be rewritten as derivations with respect to transverse vectors. The construction of δ can be followed in Fig. 2.

Let $\nu:(-\varepsilon_0,\varepsilon_0)\to M(\varepsilon_0>0)$ be a smooth injective curve, for which $\nu(0)=\gamma_0(0)$ and $\dot{\nu}(0) = \tilde{V}(0)$. Let G and $K \in \mathscr{T}_\nu$ be the vector fields along ν, obtained by autoparallel translation of $\dot{\gamma}_0(0)$ and $\tilde{V}'(0)$ along ν, respectively. Let us define the ''longitudinal'' vector field $\tilde{H}$ along ν by

$$\tilde{H}(\varepsilon) := G(\varepsilon) + \varepsilon K(\varepsilon) \tag{15}$$

[$\varepsilon \in (-\varepsilon_0,\varepsilon_0)$]. It comes immediately from this construction that

$$\nabla_{\tilde{V}(0)} \tilde{H} = K(0) = \tilde{V}'(0). \tag{16}$$

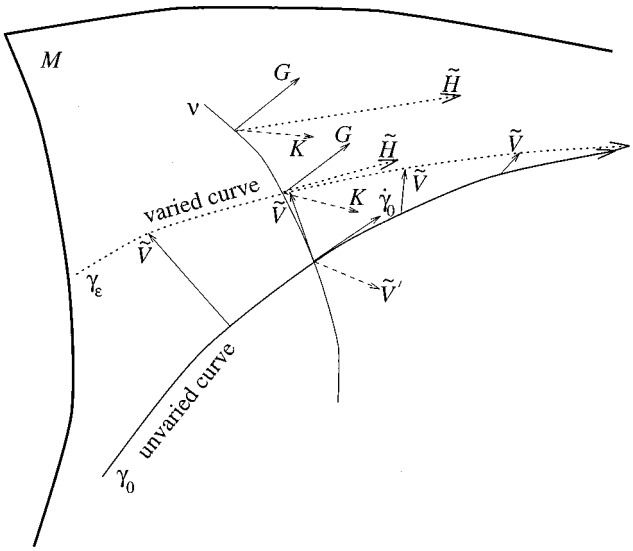

FIG. 2. The construction of the variation from the Jacobi field.

Now let us define the varied curves γ_ε $[\varepsilon\in(-\varepsilon_0,\varepsilon_0)]$ as the solutions of Eq. (1) with initial conditions $\gamma_\varepsilon(0)=\nu(\varepsilon)$ and $\dot{\gamma}_\varepsilon(0)=\widetilde{H}(\varepsilon)$, and define the variation with $\delta(t,\varepsilon):=\gamma_\varepsilon(t)$. (It is a simple consequence of the construction that δ is indeed a smooth variation of γ_0.)

Let X, Y and H, $V\in\mathscr{V}_\delta$ denote the canonical vector fields on the parameter plane and the longitudinal, transverse vector field along δ, respectively, as before. Due to the construction of δ, H coincides with $\widetilde{H}$ and V coincides with $\dot{v}$ along ν, so especially V agrees with $\widetilde{V}$ and $\dot{\nu}$ at $\gamma_0(0)$ and $\nabla_{V(0,0)}H=\nabla_{\widetilde{V}(0)}\widetilde{H}$. Using (16) and (9), this means, that V' agrees with $\widetilde{V}'$ at $\gamma_0(0)$. Since the values and the first derivatives of the Jacobi fields V and $\widetilde{V}\in\mathscr{J}_{\gamma_0}$ coincide at $\gamma_0(0)$, V agrees with $\widetilde{V}$ along the whole trajectory.

If η_0 is a trajectory satisfying condition (2) and $\widetilde{V}$ is a special Jacobi field, we must construct a special variation inducing $\widetilde{V}$. For this reason the equation (15) defining $\widetilde{H}$ has to be slightly changed:

$$\widetilde{H}(\varepsilon):=\frac{G(\varepsilon)+\varepsilon K(\varepsilon)}{|G(\varepsilon)+\varepsilon K(\varepsilon)|}. \tag{17}$$

Since in this case $|\dot{\eta}_0|=1$ and $\langle V',\dot{\eta}_0\rangle=0$, the denominator in (17) is of order $1+\varepsilon^2$, and (16) remains valid. With this modification $|\widetilde{H}|=1$, so the corresponding δ is a special variation. The proof can be finished in the same way as in the previous case.

This completes the proof of Theorem 4.

Q.E.D.

We note, that the Jacobi field $V(t)=a\dot{\gamma}(t)$ $(a\in\mathfrak{R})$ along γ corresponds to the variation $\delta(t,\varepsilon)=\gamma(t+a\varepsilon)$, which is a translation of γ in its parameter line $\mathfrak{R}$.

For a Jacobi field $V\in\mathscr{J}_\gamma$ let $p:=\langle V',\dot{\gamma}\rangle\in\mathfrak{R}$. [As we have seen in (5), p is independent of time.] A simple calculation shows that p is the rate of change of the speed of the varied trajectories γ_ε as a function of ε:

$$\left.\frac{\partial}{\partial\varepsilon}\right|_{(t,0)}|\dot{\gamma}_\varepsilon(t)|=\left.\frac{\partial}{\partial\varepsilon}\right|_{(t,0)}|H(t,\varepsilon)|=\frac{\langle\widetilde{\nabla}_Y H(t,0),H(t,0)\rangle}{|H(t,0)|}=\frac{\langle V',\dot{\gamma}_0\rangle}{|\dot{\gamma}_0|}=p. \tag{18}$$

[Here the notations were introduced before, and Eqs. (2) and (9) were used.] It is also clear that for a special infinitesimal variation p is zero; namely, this is the condition (4) in Definition 3 of special Jacobi fields.

III. SPECIAL FORMULAS FOR TWO-DIMENSIONAL MANIFOLDS

From here our study is restricted to two-dimensional manifolds. The low dimensionality enables us to introduce a natural coordinate system along the trajectories, in which the Jacobi equation (3) and condition (4) can be written in a more adequate form.

Let $(M,\langle\cdot,\cdot\rangle)$ be a two-dimensional Riemannian manifold with magnetic field B, and let Ω denote the antisymmetric tensor field of type (1,1) corresponding to the volume form ω [i.e., $\langle\Omega(Y),X\rangle=\omega(X,Y)$ for all $X,Y\in\mathscr{X}(M)$]. Due to the properties of the metric tensor and the volume form, Ω satisfies the following two conditions:

$$\Omega^2=-1, \quad \nabla\Omega=0. \tag{19}$$

(The effect of Ω on a tangent vector is just a rotation of 90° in the tangent plane.)

Since $\dim(M)=2$, the magnetic field B can be uniquely written in the form

$$B=\beta\Omega, \tag{20}$$

where $\beta\in\mathscr{F}(M)$ is a smooth function.

Let $V\in\mathscr{J}_\gamma$ be a Jacobi field along the trajectory γ of unit speed ($|\dot\gamma|=1$), and let us denote the (strength of the) magnetic field along γ by $\beta_\gamma:=\beta\circ\gamma:\mathfrak{R}\to\mathfrak{R}$. Inserting (20) into the Jacobi equation (3), we obtain

$$V''=V(\beta)\dot\gamma^\perp+\beta_\gamma\Omega(V')-R(V,\dot\gamma)\dot\gamma, \tag{21}$$

where $V(\beta)$ is the derivative of β in the direction of V, and $\dot\gamma^\perp:=\Omega(\dot\gamma)$ denotes the vector field of unit vectors perpendicular to $\dot\gamma$ along the trajectory.

Since $\dim(M)=2$, $V\in\mathscr{J}_\gamma$ can be uniquely written in the form

$$V=a\dot\gamma+b\dot\gamma^\perp, \tag{22}$$

where a and b are functions on $\mathfrak{R}$. The coordinate function a describes the *longitudinal* separation of nearby trajectories, while function b shows the relative motion of two infinitesimally closed trajectories in the *transverse* direction.

In the following theorem the Jacobi equation (21) is expressed with the help of these coordinate functions.

Theorem 5: A vector field $V=a\dot\gamma+b\dot\gamma^\perp\in\mathscr{X}_\gamma$ along the trajectory γ of unit speed on a two-dimensional manifold M is a Jacobi field if and only if the coordinate functions a and b of V satisfy for some $p\in\mathfrak{R}$ the following system of differential equations:

$$a'=p+\beta_\gamma b, \quad b''=-b(r+\beta_\gamma^2-\beta_\gamma^\perp)-\beta_\gamma p, \tag{23}$$

where $\beta_\gamma^\perp:=\dot\gamma^\perp(\beta)$ denotes the derivative of β with respect to $\dot\gamma^\perp$, $\beta_\gamma=\beta\circ\gamma$, and $r:=\langle R(\dot\gamma^\perp,\dot\gamma)\dot\gamma,\dot\gamma^\perp\rangle:\mathfrak{R}\to\mathfrak{R}$ is the sectional (Gaussian) curvature of M along γ. Here V is a special Jacobi field, if $p=0$.

If $V\in\mathscr{J}_\gamma$ is a Jacobi field, then the constant p is

$$p=\langle V',\dot\gamma\rangle=a'-\beta b\in\mathfrak{R}. \tag{24}$$

(It is in accordance with our previous notation.)

It is worth mentioning that (23) is not a real coupled system of differential equations; the second equation of (23) is an ordinary differential equation only for b. Having known the initial conditions $a(t_0),b(t_0),a'(t_0),b'(t_0)\in\Re$, expression (24) gives the value of p, the time dependence of b can be obtained by solving the second equation of (23), and inserting it into the first equation of (23), an integration gives the function $a(t)$.

Proof: First we prove the ''only if'' part of the theorem. Let $V=a\dot{\gamma}+b\dot{\gamma}^{\perp}\in\mathcal{J}_{\gamma}$ be a Jacobi field. Using the expressions (19) and (20) and the equation of motion (1), the derivatives of V can be written as follows:

$$V'=(a'-\beta_{\gamma}b)\dot{\gamma}+(b'+\beta_{\gamma}a)\dot{\gamma}^{\perp}, \tag{25}$$

$$V''=(a''-\beta_{\gamma}'\,b-2\beta_{\gamma}\,b'-b^2a)\dot{\gamma}+(b''+\beta_{\gamma}'a+2\beta_{\gamma}\,a'-\beta_{\gamma}^2\,b)\gamma^{\perp}. \tag{26}$$

Substituting these equations as well as expression (22) into the Jacobi equation (21), using again the properties (19) of Ω and the symmetry properties of R, we obtain the following system of ordinary differential equations for the coordinate functions a and b:

$$a''=\beta_{\gamma}'b+\beta_{\gamma}b'=(\beta_{\gamma}\,b)', \quad b''=-b(r-\beta_{\gamma}^{\perp})-\beta_{\gamma}a'. \tag{27}$$

With the help of the expression (24) for p, it is easy to transform this system of equations into the desired form (23), and it is also obvious that, if V is a special Jacobi field, then $p=0$. This proves the ''only if'' part of the theorem, and following the calculations backwards, one can easily check, that the ''if'' part is also true.

Q.E.D.

If the factor $r+\beta_{\gamma}^2-\beta_{\gamma}^{\perp}$ were constant on the right side of the second equation of (23) then the solution $b(t)$ would be an exponential or a harmonic (sine or cosine) function depending on the sign of $r+\beta_{\gamma}^2-\beta_{\gamma}^{\perp}$. According to this fact, a trajectory γ is said to be *locally stable* at a point $\gamma(t_0)$, if $r+\beta_{\gamma}^2-\beta_{\gamma}^{\perp}>0$ at that point, and *locally instable*, if $r+\beta_{\gamma}^2-\beta_{\gamma}^{\perp}<0$. The negative curvature causes instability, the presence of the magnetic field works against it, and the inhomogeneity of the magnetic field also influences the stability of the trajectories. (The fact that the magnetic field suppresses chaos has been also observed in Ref. 17.)

In the remaining part of this section the results obtained are illustrated by presenting particular cases, where the Gaussian curvature r and the magnetic field β is constant. In this case $\beta^{\perp}=0$, so the stability of the trajectories depends (globally) on the sign of $r+\beta^2$. If the scalar curvature is positive, the trajectories are stable for every value β of the magnetic field. It is more interesting that in the case of negative curvature the trajectories can be either stable or instable, depending on the strength of the magnetic field.

First we study in detail the motion of a charged particle on the hyperbolic (Bolyai–Lobatchewski) plane, denoted by S, for which $r=-1$. This means, that for magnetic fields $|\beta|<1$ the trajectories are instable, and for fields $|\beta|>1$ the trajectories are stable.[18] In Appendix B we summarize some basic facts connected with the cycles and isometries of the hyperbolic plane using the pseudosphere model.[10]

For a trajectory $\gamma:\Re\to S$ let the image of the mapping γ (as a subset of S) be called the *path* of the particle (or the *path* belonging to the trajectory γ). The following theorem relates the cycles of the hyperbolic plane to the paths of charged particles.

Theorem 6: The possible paths of charged particles moving on the hyperbolic plane in constant nonzero magnetic field are the cycles. If the charge, mass, and speed of the particle is unit, then for magnetic fields $|\beta|<1$ the paths are hypercycles, for $|\beta|>1$ the paths are circles, and at the magnetic fields $|\beta|=1$ the particles move along paracycles.

The possible directed paths (i.e., the directed cycles) constitute in a natural way a three-dimensional differentiable manifold P. The points of P can be identified with the paths belonging

to trajectories of unit speed, and the tangent plane $T_\gamma(P)$ at the point $\gamma \in P$ can be brought into one-to-one correspondence with the factor space $\mathscr{J}_\gamma/\Re\dot{\gamma}$, where $\Re\dot{\gamma} \subset \mathscr{S}\mathscr{J}_\gamma$ is a one-dimensional subspace of the (special) Jacobi fields.

Proof: It is a direct consequence of the rich symmetry (homogeneity and isotropy) of the hyperbolic plane S, and the autonomity of the equation of motion (1), that the trajectories can be translated along themselves. Indeed, for every two tangent vectors $\dot{\gamma}(t_0)$ and $\dot{\gamma}(t_1)$ $(t_0, t_1 \in \Re)$ of a solution γ of (1), there is an isometry of S, which transforms the first vector into the second one. (See Lemma 14.) Since the equation of the motion is independent of time, this isometry transforms the path of the trajectory γ onto itself.

It is also obvious that the trajectories are curves of constant curvature. The equation of motion (1) just tells us that the curvature of a solution γ of speed $v = |\dot{\gamma}|$ in magnetic field β is $|\nabla_{\dot{\gamma}/|\dot{\gamma}|}\dot{\gamma}/|\dot{\gamma}|| = (\beta/v^2)|\dot{\gamma}^\perp| = \beta/v$. So, using Lemma 17, the trajectories of unit speed are hypercycles of altitude $\operatorname{artanh}|\beta|$, if $|\beta|<1$; paracycles, if $|\beta|=1$, and circles of radius $\operatorname{arcoth}|\beta|$, if $|\beta|>1$. This proves the first part of the theorem.

For defining a differentiable structure on the set of directed cycles we use the pseudosphere model of the hyperbolic plane. Let $(\mathbf{V}, \langle\cdot,\cdot\rangle)$ be the three-dimensional Minkowskian vector space into which the pseudosphere S is embedded. (See Lemma 12 and Definition 13 in Appendix B.) First we prove that the set of all oriented affine hyperplanes (i.e., two-dimensional affine subspaces) of $\mathbf{V}$ possesses a natural differentiable structure. For this reason, let us introduce (beside the Minkowskian structure $\langle\cdot,\cdot\rangle$) a Riemannian (positive definite) scalar product $g: \mathbf{V}\times\mathbf{V} \to \Re$ on $\mathbf{V}$. With the help of this multiplication every directed hyperplane of $\mathbf{V}$ can be unambiguously characterized by its (g-orthogonal) normal (unit) vector and its distance from the origin of $\mathbf{V}$ measured in the direction of the normal vector. (The normal vector gives also the orientation of the hyperplane.) So the hyperplanes are in one-to-one correspondence with the points of the product manifold $N\times\Re$, where N is the g-unit sphere of $\mathbf{V}$, and the differentiable structure of $N\times\Re$ can be carried over to the set of affine hyperplanes of $\mathbf{V}$. It is also easy to show that this is a canonical differentiable structure, i.e., independent of the special choice of the scalar product g.

According to Lemma 17, the cycles are the plane sections of the pseudosphere S in $\mathbf{V}$. Since the affine hyperplanes intersecting the pseudosphere in more than one point correspond to the elements of an open subset of $N\times\Re$, the cycles indeed form in a natural way a differentiable submanifold P of the manifold of all affine hyperplanes of $\mathbf{V}$.

As we have seen, the curvature of a trajectory of speed v in magnetic field β is β/v. This means that at an appropriate value of the magnetic field β every cycle (of arbitrary curvature) can be realized as the path belonging to a trajectory of unit speed, so the points of P can be regarded as the paths belonging to the trajectories of unit speed.

To establish the correspondence between the tangent plane $T_\gamma(P)$ and the factor space $\mathscr{J}_\gamma/\Re\dot{\gamma}$ is also easy, but a bit more cumbersome. In Definition 1 the magnetic field is fixed during the variation of a trajectory, and the speed of the varied trajectories can be changed, while the points of P are regarded as paths of trajectories of unit speed, corresponding to different values of the magnetic field. So, first the varied trajectories have to be brought into correspondence with the trajectories of unit speed. This can be easily done by relating a trajectory of speed v at magnetic field β to the trajectory of unit speed belonging to the same path at magnetic field β/v. Using this connection, the variation of a trajectory $\gamma \in P$ is just a curve in the manifold P, and an infinitesimal variation, or Jacobi field along γ corresponds to a tangent vector in $T_\gamma(P)$. It is also evident that $\mathscr{J}_\gamma$ has to be factorized with $\Re\dot{\gamma}$, since the infinitesimal variations $\Re\dot{\gamma}$ move γ along itself, so they present the null vector in $T_\gamma(P)$.

This completes the proof of Theorem 6.

Q.E.D.

Figure 3 shows the variation of a hypercycle and a circle on the pseudosphere model. The behavior of the transverse coordinates b can be clearly seen in both cases. This figure also illustrates that in the manifold of the cycles P there is a preferred path between every pair of different points $\Sigma, \Pi \in P$ consisting of the plane sections of S with planes having a common line

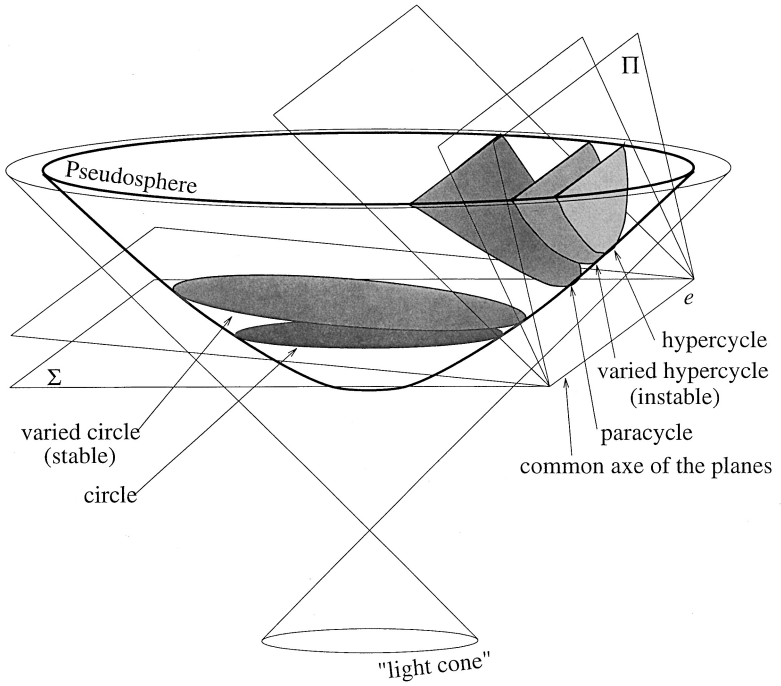

FIG. 3. The variation of a hypercycle and a circle.

e with Σ and Π. (If Σ and Π are parallel, then all the other planes are parallel with them, and e is the ideal line.)

Similar considerations can be followed for constant positive curvature. In the case of $r=1$, the two-dimensional manifold is the unit sphere embedded into a three-dimensional Euclidean vector space. The trajectories of curvature β/v are just the circles of radius $\operatorname{arcctg}(\beta/v)$ (measured on the sphere), and these curves are also the plane sections of the unit sphere.

For $r=0$ the trajectories are the usual circles on the two-dimensional Euclidean plane.

IV. THE EFFECT OF THE BOUNCES

Till now the behavior of nearby trajectories of charged particles in magnetic systems has been studied during the bounceless segments. However, in billiards the reflections also strongly influence the separation of close trajectories. At the bouncing point(s) neither the *variation* nor the *infinitesimal variation of a bouncing trajectory* is smooth, the variation is continuous there, and the Jacobi field and its first derivative have certain jump at the reflection point. In the ongoing section this effect is investigated in detail for two-dimensional systems, and a formula is derived which gives the jump of the Jacobi field and its derivative in terms of the magnetic field, the angle of reflection, and the curvature of the billiard wall at the reflection point.

For this purpose the definition of the variation and infinitesimal variation (Definitions 1 and 2) should be slightly modified for bouncing trajectories. [The bouncing trajectories are continuous curves, which are everywhere smooth, except at the bouncing point, they satisfy the equation of motion (1) for parameter values before and after the reflection, and obey the law of elastic reflection at the bouncing point.]

Definition 7: The mapping δ: $\mathfrak{R}\times(-\varepsilon_0,\varepsilon_0)\to M$ $(\varepsilon_0>0)$ is a *variation of the bouncing trajectory* γ_0, if the varied trajectories $\gamma_\varepsilon(t)=\delta(t,\varepsilon)$ $(|\varepsilon|<\varepsilon_0)$ are also trajectories of charged particles bouncing on the billiard wall according to the law of elastic reflection, and δ is smooth on its domain before and after the reflection. The *infinitesimal variation* V_0 *of the bouncing trajectory*

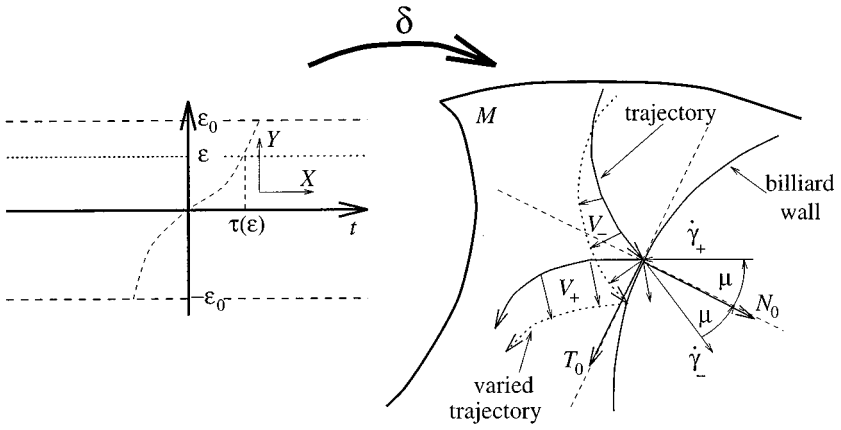

FIG. 4. The variation of a bouncing trajectory.

γ_0 corresponding to the variation δ is defined similarly as in Definition 2, $V_0(t)=\partial/\partial\varepsilon|_{(t,0)}\delta(t,\varepsilon)$, but in this case V_0 has a jump at the reflection point, since the variation δ is not smooth there.

The letters ω, Ω, and $B=\beta\Omega$ $[\beta\in\mathscr{F}(M)]$ denote the same tensor fields on the two-dimensional Riemannian manifold $(M,\langle\cdot,\cdot\rangle)$ as in the previous section. Let $\nu\colon \mathfrak{R}\to M$ be the billiard wall parametrized in such a way that $T:=\dot{\nu}$ is its unit tangent vector and the unit normal vector $N:=\Omega(\dot{\nu})$ points outwards of the billiard (Fig. 4). Let $\gamma\colon \mathfrak{R}\to M$ be the trajectory of a particle of unit speed bouncing on ν at the point $\nu(0)=\gamma(0)$, and let V be an infinitesimal variation of it. The values of the vector fields T, $N\in\mathscr{V}_\nu$ at the bouncing point are denoted by $T_0,N_0\in T_{\nu(0)}(M)$. Since γ obeys the law of elastic reflection,

$$\dot{\gamma}_+=\dot{\gamma}_- -2\langle\dot{\gamma}_-,N_0\rangle N_0, \tag{28}$$

where (and in the remaining sections further on) the subscripts ''$-$'' and ''$+$'' distinguish the vectors (and coordinates) just before and just after the reflection, respectively. The coordinates $a_\pm,b_\pm\in\mathfrak{R}$ of $V_\pm\in T_{\gamma(0)}(M)$ are defined by the following two formulas:

$$V_-=a_-\dot{\gamma}_-+b_-\dot{\gamma}_-^{\perp}, \tag{29}$$

$$V_+=a_+\dot{\gamma}_++b_+\gamma_+^{\perp}, \tag{30}$$

where $\dot{\gamma}_\pm^{\perp}=\Omega(\dot{\gamma}_\pm)\in T_{\gamma(0)}(M)$, like before. Let the angle of reflection, directed from the velocity vector $\dot{\gamma}_-$ (just before the reflection) to the normal vector N_0, be denoted by μ, as it is shown in Fig. 4. This means that

$$N_0=\dot{\gamma}_-\cos(\mu)+\dot{\gamma}_-^{\perp}\sin(\mu), \tag{31}$$

$$T_0=\dot{\gamma}_-\sin(\mu)-\dot{\gamma}_-^{\perp}\cos(\mu). \tag{32}$$

Let β and q be the value of the magnetic field and the curvature of the billiard wall at the bouncing point, respectively, where the curvature q is defined by the equation

$$\nabla_{T_0}T=-qN_0. \tag{33}$$

Since N points outwards of the billiard, q is positive if the billiard wall is focusing at the reflection point and negative if it is defocusing.

The following theorem gives the jump of the Jacobi field and its first derivative.

Theorem 8: Using the notations introduced above, the infinitesimal variation V_+ of a bouncing trajectory γ of unit speed and its first derivative V'_+ just after the reflection can be calculated by the following formulas:

$$V_+ = V_- - 2\langle V_-, N_0\rangle N_0, \tag{34}$$

$$V'_+ = V'_- - 2\langle V'_-, N_0\rangle N_0 + 2\frac{\langle \beta N_0 + q\dot{\gamma}_-^{\perp}, V_-\rangle}{\cos(\mu)}\,(\dot{\gamma}_-\,\sin(2\mu) - \dot{\gamma}_-^{\perp}\,\cos(2\mu)), \tag{35}$$

where V_- and V'_- are the infinitesimal variation and its first derivative just before the reflection.

These equations result in the following connections between the coordinates and their derivatives at the reflection point:

$$a_+ = a_-, \quad b_+ = -b_-; \tag{36}$$

$$a'_+ = a'_- - 2\beta b_-, \quad b'_+ = -b'_- + 2b_-\frac{q+\beta\,\sin(\mu)}{\cos(\mu)}. \tag{37}$$

We remark that Eq. (34) or (36) means that V_+ is simply the reflection of V_- in the line of T_0.

Proof: First we prove the assumptions (34) and (35). Let δ be a variation of γ corresponding to the infinitesimal variation V, and let X,Y and $H_{\leftarrow}, V_{\leftarrow}$ (or $H_{\rightarrow}, V_{\rightarrow}$) be the canonical vector fields on the parameter plane and the longitudinal, transverse vector field before (or after) the bounce, respectively. [This means that $H_{\leftarrow}(0,0)=\dot{\gamma}_-$, $H_{\rightarrow}(0,0)=\dot{\gamma}_+$, $V_{\leftarrow}(0,0)=V_-$ and $V_{\rightarrow}(0,0)=V_+$.] To avoid unnecessary technical difficulties, let us suppose that δ is regular at the point $t=\varepsilon=0$, and let $Z=\xi X+\eta Y$ be the vector on the parameter plane, for which $\delta_* Z = T_0$ holds. This means that

$$T_0 = \xi\dot{\gamma}_- + \eta V_- = \xi\dot{\gamma}_+ + \eta V_+. \tag{38}$$

Since the velocity vector $\dot{\gamma}_+$ is the reflection of the vector $\dot{\gamma}_-$ in the line of T_0, it follows from the previous equation that the infinitesimal variation vector V_+ is also the reflection of the vector V_- in this axis; this proves assumptions (34) and (36) of the theorem. [In the second equation of (36) the negative sign appears because the reflection of $\dot{\gamma}_-^{\perp}$ in T_0 is $-\dot{\gamma}_+^{\perp}$.]

With the help of the formulas (31), (32), and (29) the factors ξ,η can be easily expressed in terms of the angle of reflection and the (coordinates of the) infinitesimal variation vector before the bounce:

$$\xi = \frac{\langle N_0, V_-\rangle}{\langle \dot{\gamma}_-^{\perp}, V_-\rangle} = \sin(\mu) + \frac{a_-}{b_-}\cos(\mu),$$
$$\eta = -\frac{\cos(\mu)}{\langle \dot{\gamma}_-^{\perp}, V_-\rangle} = -\frac{\cos(\mu)}{b_-}. \tag{39}$$

Since the varied trajectories satisfy the law of elastic reflection,

$$H_{\rightarrow}(\tau(\varepsilon),\varepsilon) = H_{\leftarrow}(\tau(\varepsilon),\varepsilon) - 2\langle H_{\leftarrow}(\tau(\varepsilon),\varepsilon), N\rangle N, \tag{40}$$

where the function $\tau(\varepsilon)$ gives the parameter value corresponding to the bounce of the varied trajectory γ_ε. Differentiating this equation with respect to the vector $Z=\xi X+\eta Y$ at the point $t=\varepsilon=0$, and using Eq. (28) as well as the expressions

$$\widetilde{\nabla}_Z H_{\leftrightarrow} = \xi \widetilde{\nabla}_X H_{\leftrightarrow} + \eta \widetilde{\nabla}_Y H_{\leftrightarrow} = \beta \xi \dot{\gamma}_{\pm}^{\perp} + \eta V'_{\pm}, \tag{41}$$

$$\widetilde{\nabla}_Z N = \Omega(\widetilde{\nabla}_Z T) = -q\Omega(N_0) = qT_0, \tag{42}$$

we obtain

$$V'_+ = V'_- - 2\langle V'_-, N_0\rangle N_0 + \frac{-2(\xi\beta+q)}{\eta}(\langle \dot{\gamma}_-, N_0\rangle T_0 + \langle \dot{\gamma}_-, T_0\rangle N_0). \tag{43}$$

[For deriving the expressions (41) and (42) and Eq. (43), the connection (9), the equation of motion (1), and the properties (19) of the tensor Ω are to be used.]

With the help of Eqs. (31) and (32), it is easy to show that

$$\langle \dot{\gamma}_-, N_0\rangle T_0 + \langle \dot{\gamma}_-, T_0\rangle N_0 = \dot{\gamma}_- \sin(2\mu) - \dot{\gamma}_-^{\perp} \cos(2\mu). \tag{44}$$

Using this, and substituting ξ, η from (the coordinate free expression of) (39) into Eq. (43), Eq. (35) of the theorem can be obtained.

Differentiating the expressions (29) and (30) at $t=0$ with respect to $\dot{\gamma}_-$ and $\dot{\gamma}_+$, respectively, and in the second equation replacing the vectors $\dot{\gamma}_+, \dot{\gamma}_+^{\perp}$ in terms of the vectors $\dot{\gamma}_-, \dot{\gamma}_-^{\perp}$ using the low of elastic reflection (28), one can express the vectors V'_- and V'_+ in the basis $\{\dot{\gamma}_-, \dot{\gamma}_-^{\perp}\} \subset T_{\gamma(0)}(M)$:

$$V'_- = (a'_- - \beta b_-)\dot{\gamma}_- + (b'_- + \beta a_-)\dot{\gamma}_-^{\perp}, \tag{45}$$

$$\begin{aligned} V'_+ = {} & (-(a'_+ + \beta b_-)\cos(2\mu) + (b'_+ + \beta a_-)\sin(2\mu))\dot{\gamma}_- \\ & + (-(a'_+ + \beta b_-)\sin(2\mu) - (b'_+ + \beta a_-)\cos(2\mu))\dot{\gamma}_-^{\perp}. \end{aligned} \tag{46}$$

Substituting these expressions, as well as expression (29), into Eq. (35) and using the conditions (31) and (32), after straightforward calculations one can derive Eqs. (37).

This completes the proof of Theorem 8.

Q.E.D.

It can be seen from Eqs. (37) [or (35)] that the presence of the magnetic field really influences the behavior of nearby trajectories at the instant of the bounce. A reflection at an angle μ on a wall of curvature q in magnetic field β causes the same jump in the transverse part of the infinitesimal variation and its first derivative, as a reflection on a wall of curvature $q' = q + \beta\sin(\mu)$, without magnetic field. If $|\beta| > |q|$, at appropriate value of μ the magnetic field can even change the focusing or defocusing character of the wall.

In Appendix C we give an elementary proof of Eqs. (36) and (37) in a special case, where b'_- and the curvature q of the billiard wall are zero.

V. RELATION WITH THE CURVATURE OF THE HOROCYCLES

In this section we relate our method for calculating the separation of nearby trajectories in billiard systems to the earlier method of Bunimovich and Sinai[5,6,8] according to which the transverse separation of the trajectories can be obtained by integrating the curvature of the *horocycles* along the trajectory investigated.

Let $\gamma: \mathfrak{R} \to M$ be a trajectory of unit speed in the two-dimensional manifold $(M, \langle\cdot,\cdot\rangle)$ with magnetic field $B = \beta\Omega$, let δ be a variation of γ corresponding to the infinitesimal variation $V_0 = a\dot{\gamma} + b\dot{\gamma}^{\perp} \in \mathscr{V}_{\gamma}$, and let X, Y and $H, V \in \mathscr{V}_{\delta}$ be the canonical base fields on the parameter plane and the longitudinal, transverse vector fields, respectively. The vector field $\Omega(H) \in \mathscr{V}_{\delta}$ perpendicular to H is denoted by $H^{\perp}$.

Definition 9: The *horocycles* corresponding to the variation δ of the trajectory γ (of unit speed) are the integral curves of the vector field $H^{\perp}$ perpendicular to the varied trajectories. Assuming that δ is regular at the point $(t,0)$, the *curvature* $\kappa(t)$ *of the horocycle* at the point $\gamma(t)$ is defined by the following equation:

$$\widetilde{\nabla}_{P(t)} \frac{H^{\perp}}{|H^{\perp}|} = -\kappa(t)\dot{\gamma}(t), \tag{47}$$

where $P(t)$ is the vector of the parameter plane, for which $\delta_* P(t) = \Omega(\dot{\gamma}(t)) = \dot{\gamma}^{\perp}(t)$ holds. [Due to the negative sign in Eq. (47), the curvature κ is positive, if the varied trajectories diverge.]

In the following theorem we calculate the curvature κ of the horocycles as a function of the infinitesimal variation, and give expressions describing the evolution of κ along the trajectory as well as at the bouncings.

Theorem 10: Using the notations introduced above, the curvature κ is given by the following equation:

$$\kappa = \frac{\langle V_0', \dot{\gamma}^{\perp}\rangle - \beta_{\gamma}\langle V_0, \dot{\gamma}\rangle}{\langle V_0, \dot{\gamma}^{\perp}\rangle} = \frac{b'}{b} = (\ln|b|)', \tag{48}$$

where $\beta_{\gamma} = \beta \circ \gamma$.

The curvature κ_+ just after a reflection at an angle μ on a wall of curvature q is

$$\kappa_+ = \kappa_- - 2\frac{q + \beta\,\sin(\mu)}{\cos(\mu)}, \tag{49}$$

where κ_- is the curvature of the horocycle just before the bounce and β is the value of the magnetic field at the reflection point.

Assuming that the horocycles correspond to a special variation, their curvature obey the following differential equation:

$$\kappa' = -r - \beta_{\gamma}^2 + \beta_{\gamma}^{\perp} - \kappa^2, \tag{50}$$

where $r:\mathfrak{R}\to\mathfrak{R}$ is the scalar curvature of M along γ, and $\beta_{\gamma}^{\perp}(t) = \dot{\gamma}^{\perp}(t)(\beta)$ is the derivative of β in the direction perpendicular to $\dot{\gamma}(t)$.

[We emphasize that the statements (48) and (49) are valid for any variation, while the last formula is valid only for special variations.]

Proof: Let $P(t) = \chi(t)X + \psi(t)Y$ be the vector of the parameter plane for which $\delta_* P(t) = \dot{\gamma}^{\perp}(t)$ holds. This means, that $\dot{\gamma}^{\perp} = \chi\dot{\gamma} + \psi V_0$, and a simple calculation shows that

$$\chi = -\frac{\langle V_0, \dot{\gamma}\rangle}{\langle V_0, \dot{\gamma}^{\perp}\rangle}, \quad \psi = \frac{1}{\langle V_0, \dot{\gamma}^{\perp}\rangle}. \tag{51}$$

The curvature κ of the horocycles is calculated directly, according to its definition:

$$\widetilde{\nabla}_P \frac{H^{\perp}}{|H^{\perp}|} = -P(|H^{\perp}|)\dot{\gamma}^{\perp} + \widetilde{\nabla}_P H^{\perp}, \tag{52}$$

where the differentiations $P(|H^{\perp}|)$ and $\widetilde{\nabla}_P H^{\perp}$ can be further simplified:

$$P(|H^{\perp}|) = (\chi X + \psi Y)(|H|) = \psi \left.\frac{\partial}{\partial\varepsilon}\right|_{\varepsilon=0} |H| = \psi\langle V_0', \dot{\gamma}\rangle = \psi p, \tag{53}$$

$$\tilde{\nabla}_P H^{\perp} = \Omega(\tilde{\nabla}_P H) = \chi\Omega(\tilde{\nabla}_X \dot{\gamma}) + \psi\Omega(\tilde{\nabla}_Y H) = -\chi\beta_\gamma \dot{\gamma} + \psi\Omega(V_0'). \tag{54}$$

[We have used Eqs. (1), (9), (18), and (19).] Substituting $\Omega(V_0')$ with $\langle V_0', \dot{\gamma}\rangle \dot{\gamma}^{\perp} - \langle V_0', \dot{\gamma}^{\perp}\rangle \dot{\gamma}$ in Eq. (54) and putting the expressions (53) and (54) into Eq. (52), we obtain

$$\tilde{\nabla}_P \frac{H^{\perp}}{|H^{\perp}|} = -(\chi\beta_\gamma + \psi\langle V_0', \dot{\gamma}^{\perp}\rangle)\dot{\gamma}. \tag{55}$$

With the help of this equation, using expressions (51) and Eqs. (22) and (25) for χ,ψ and V_0, V_0', respectively, it is easy to prove assumption (48) of the theorem.

The conjecture (49) describing the jump of the curvature κ at the reflection can be proved by dividing the second equation of (37) with $b_+ = -b_-$.

Differentiating Eq. (48) we get $\kappa' = (b''b - b'^2)/b^2$, from which $b'' = b(\kappa' + \kappa^2)$ follows. Substituting it into the second equation of (23), and using that $p = 0$ for special variations, assumption (50) of the theorem can be also proved.

Q.E.D.

The results of Theorem 10 are in accordance with the earlier results of Bunimovich and Sinai[5,6,8] in the case of $\beta = 0$.

Following a given bunch of trajectories in a billiard system, with the help of the equations (49) and (50) the evolution of the curvature κ of the horocycles can be determined as a function of time, and, according to the connection (48), the integral $\int_0^t \kappa(t)dt = \ln(|b(t)|/|b(0)|)$ gives the logarithm of the transverse stretching. [Due to the second equation of (36), the absolute value of the transverse coordinate is continuous at the bounces.]

VI. CONCLUSIONS

In the present article the behavior of nearby trajectories has been investigated in classical magnetic billiard systems on Riemannian manifolds with a method which is similar to that of Jacobi fields for geodesic flows. The relative motion of two particles moving infinitesimally close to each other is described by the *infinitesimal variation* vector field along one of the trajectories (Definitions 2 and 7). In the bounceless segments the infinitesimal variations of the trajectories satisfy a second-order ordinary differential equation, which is the usual Jacobi equation in the lack of magnetic field (Theorem 4). Restricting our studies to two-dimensional systems, differential equations describing the transverse as well as the longitudinal behavior of nearby trajectories have been derived (Theorem 5). The transverse behavior depends on the (Gaussian) curvature of the manifold, on the value of the magnetic field, and its derivative in transverse direction. The positive curvature and the presence of the magnetic field suppress chaos.

The bouncing effects have been also investigated in two-dimensional billiards, and a formula describing the jump of the infinitesimal variation and its derivative at the reflections has been given (Theorem 8). These jumps depend not only on the curvature of the wall and on the angle of incidence, but also on the value of the magnetic field at the bouncing point. The magnetic field can even change the focusing or defocusing character of the wall.

We have expressed the curvature κ of the curves perpendicular to a bunch of trajectories (*horocycles*, Definition 9) in terms of the infinitesimal variation. It has been shown that in the bounceless segments κ obeys a first-order differential equation containing the (Gaussian) curvature of the manifold, the magnetic field, and its derivative in transverse direction, and at the reflections κ has a definite jump depending on the curvature of the wall, the angle of incidence, and the value of the magnetic field (Theorem 10). In the lack of magnetic field our results are in accordance with the known properties of κ.

After finishing this work the author was informed that another paper[14] is being published on partially similar topics on two-dimensional Euclidean surface. The author of Ref. 14 has also obtained Eq. (49) of theorem 10 describing the jump of the curvature κ of the horocycles at reflections in presence of magnetic field, and he has given the bounceless evolution of κ in

homogeneous magnetic field. [It is the solution of Eq. (50) in the special case of $r=\beta_\gamma^\perp=0$.] Furthermore, Ref. 14 contains nice applications for the evaluation of the Lyapunov exponent in different magnetic billiard systems.

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APPENDIX A: VECTOR FIELDS ALONG DIFFERENTIABLE MAPPINGS

In this Appendix the basic properties of the *vector fields along differentiable mappings* are summarized.

Definition 11: Let $f:N\to M$ be a smooth mapping. A differentiable mapping $X:N\to T(M)$ is a (differentiable) *vector field along* f, if $\pi_M\circ X=f$ holds. The set of vector fields along f is denoted by $\mathscr{T}_f$.

The most common examples for this concept are $f_*U\in\mathscr{T}_f$ and $V\circ f\in\mathscr{T}_f$, where $U\in\mathscr{T}(N)$, $V\in\mathscr{T}(M)$. For vector fields along f essentially the same calculus can be developed as for those on M. A covariant derivation $\nabla:\mathscr{T}(M)\times\mathscr{T}(M)\to\mathscr{T}(M)$ of M can be naturally extended to one $\tilde{\nabla}:\mathscr{T}(N)\times\mathscr{T}_f\to\mathscr{T}_f$ on $\mathscr{T}_f$, so it is reasonable to derivate an element of $\mathscr{T}_f$ with respect to a vector field on N. If δ is regular at the point $n\in N$, then for every $P\in T_n(N)$ and $U\in\mathscr{T}(N)$

$$\tilde{\nabla}_P\delta_*U=\nabla_{(\delta_*)_nP}V, \tag{A1}$$

where $V\in\mathscr{T}(M)$ is an arbitrary vector field on M, for which $V\circ\delta=\delta_*U$ holds in an open neighborhood of $n\in N$. The derivation $\tilde{\nabla}$ satisfies the usual algebraic axioms [$\mathscr{F}(N)$-linearity in its first and Leibnitz rule in its second argument], and for the torsion tensor T and curvature tensor R of M it is also valid that

$$(f^*T)(X,Y)=T(f_*X,f_*Y)=\tilde{\nabla}_Xf_*Y-\tilde{\nabla}_Yf_*X-f_*[X,Y], \tag{A2}$$

$$R(f_*X,f_*Y)Z=\tilde{\nabla}_X\tilde{\nabla}_YZ-\tilde{\nabla}_Y\tilde{\nabla}_XZ-\tilde{\nabla}_{[X,Y]}Z, \tag{A3}$$

where $X,Y\in\mathscr{T}(N)$ and $Z\in\mathscr{T}_f$. The detailed proofs of these properties can be found in Ref. 19.

APPENDIX B: THE PSEUDOSPHERE MODEL AND SOME PROPERTIES OF THE HYPERBOLIC PLANE

In this Appendix the pseudosphere model of the hyperbolic plane is introduced, and using it in a series of lemmas with short proofs or references the basic properties of the isometries and the cycles of the Bolyai–Lobatchewski plane are summarized.

Let $(\mathbf{V},\langle\cdot,\cdot\rangle)$ be an oriented, arrow-oriented three-dimensional vector space with an indefinite scalar product $\langle\cdot,\cdot\rangle$ of signature $(-,+,+)$ on it. For the sake of simplicity we use the attributes introduced in the theory of special relativity (spacelike, lightlike, timelike, future/past oriented) for characterizing the vectors and hyperplanes of $\mathbf{V}$. Let $S\subset\mathbf{V}$ be the set of future-oriented timelike unit vectors.

Lemma 12: S is a two-dimensional, oriented, noncompact, simply connected embedded submanifold of $\mathbf{V}$, which inherits a (positive definite) Riemannian metrics from $\mathbf{V}$. Equipped with this Riemannian structure (denoted also by $\langle\cdot,\cdot\rangle$), S is diffeomorphic with the hyperbolic plane.

The inherited metrics is positive definite because of the fact that the tangent plane $T_x(S)$ at any point $x\in S$ is just the spacelike affine hyperplane through x orthogonal to the vector $x\in\mathbf{V}$. It is also easy to show that S is homogeneous and isotropic (see Lemma 14), so it has constant curvature. The detailed proof of Lemma 12 can be found in Ref. 10.

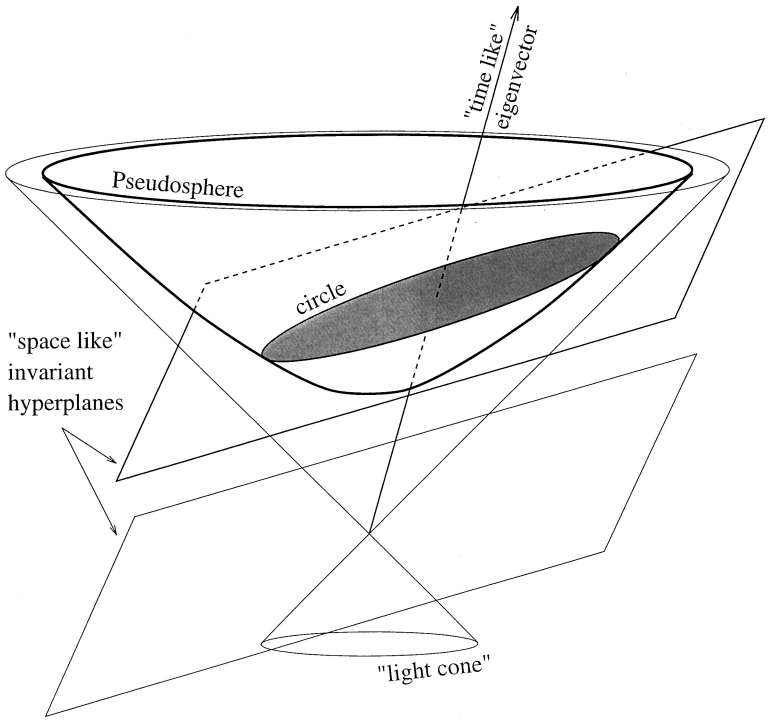

FIG. 5. The elliptic isometries.

Definition 13: The set S equipped with its inherited Riemannian structure is called the *pseudosphere*.

The following lemma gives a survey of the isometries of the hyperbolic plane using the pseudosphere model.

Lemma 14: Every arrow-orientation-preserving $\langle\cdot,\cdot\rangle$-orthogonal transformation of $\mathbf{V}$ leaves S fixed, and induces and isometry on the pseudosphere S. Conversely, every isometry of S can be uniquely extended to an arrow-orientation-preserving orthogonal transformation of $\mathbf{V}$. An isometry of S is orientation-preserving if and only if it is induced by an orientation-preserving orthogonal transformation of $\mathbf{V}$.

Every orientation and arrow-orientation-preserving transformation $\mathbf{O}$ of $\mathbf{V}$ which is not the identity can be put into one of the following three classes:

(i) The characteristic equation of $\mathbf{O}$ has three different roots; one of them is 1, which belongs to a timelike eigenvector, and the other two eigenvalues are complex numbers of unit absolute values conjugate to each other. The (spacelike) affine hyperplanes perpendicular to the timelike eigenspace are invariant under the effect of $\mathbf{O}$. (The effect of $\mathbf{O}$ is simply a rotation in the invariant planes around the timelike eigenvector.) The isometries of the hyperbolic plane induced by this kind of orthogonal transformations are called *elliptic isometries (rotations)*. The elliptic isometries have one fixed point (the center of the rotation), which is the intersection of S and the timelike eigenspace of $\mathbf{O}$. The rotations having the same center form a one-parameter subgroup of the isometry group of S. (See Fig. 5.)

(ii) The characteristic equation of $\mathbf{O}$ has three different real roots; one of them is 1, which belongs to a spacelike eigenvector, the other two real eigenvalues are reciprocal to each other, and the corresponding eigenvectors are lightlike vectors perpendicular to the spacelike eigenspace. The (timelike) affine hyperplanes perpendicular to the spacelike eigenvec-

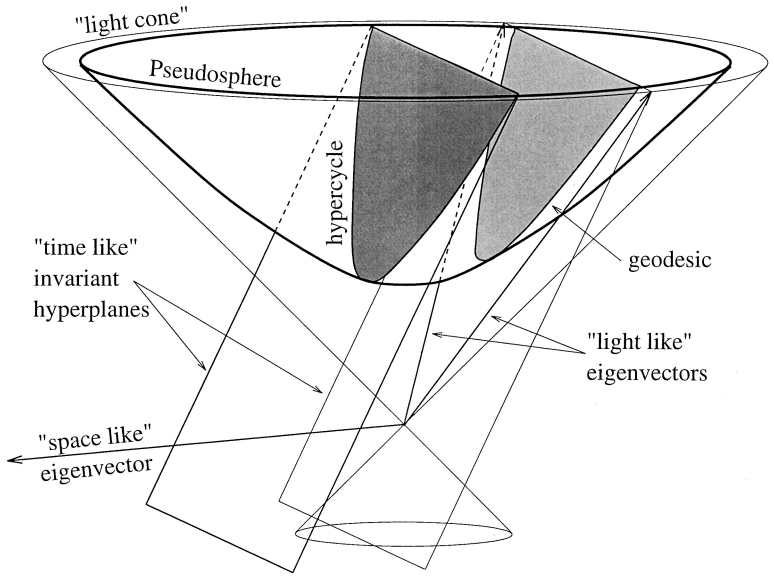

FIG. 6. The hyperbolic isometries.

tor are invariant under the transformation **O**. (This transformation is similar to the Lorentz boosts in the theory of special relativity.) The isometries of the hyperbolic plane induced by this kind of orthogonal transformations are called *hyperbolic isometries (translations)*. The hyperbolic isometries do not have fixed points, but they have a (not pointwise) fixed line, which is the intersection of S and the hyperplane spanned by the two lightlike eigenspaces. The translations having the same invariant line form a one-parameter subgroup of the isometry group of S. (See Fig. 6.)

(iii) The 1 is a three times degenerate root of the characteristic equation of **O**. **O** has only one lightlike eigenspace, and the (lightlike) hyperplanes orthogonal to it are invariant under the transformation. (In the invariant plane the effect of **O** is a shearing along the lightlike eigenvector.) The isometries of the hyperbolic plane induced by this kind of orthogonal transformations are called *parabolic isometries*. The parabolic isometries have neither fixed points nor invariant lines, but they have a fixed ideal point lying ''infinitely far'' in the direction of the lightlike eigenvector of the transformation. (This means that for every line directed towards this ideal point, the transformed image of the line also tends to this point.) The parabolic transformations having the same ideal point (or the same lightlike eigenvector) form a one-parameter subgroup of the isometry group of S. (See Fig. 7.)

The statements of this lemma can be proved step by step using standard linear algebraic methods.

It follows from Lemma 14 that for every pair of unit tangent vectors of the pseudosphere S there exists exactly one isometry of S, which transforms the first vector into the second vector. This means that the hyperbolic plane is homogeneous and isotropic, and its isometry group is a three-dimensional Lie group.

Now let us overview the properties of the most important curves (called the *cycles*) of the hyperbolic plane on the pseudosphere model.

Definition 15: The set of points lying at a distance $r>0$ from a fixed point o of the hyperbolic plane is called the *circle* of center o and radius r. The set of points lying at a distance $d\geqslant 0$ from a fixed geodesic line γ; on one side of γ is called the hypercycle of base line γ and altitude d. (Specially the geodesic lines are hypercycles of altitude zero.) A curve perpendicular to a bunch of

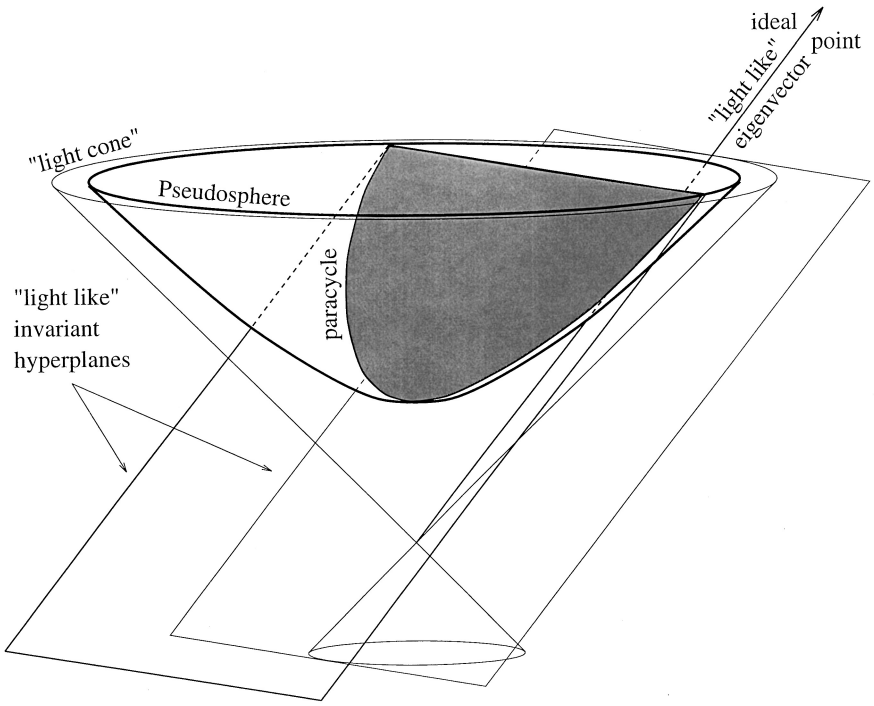

FIG. 7. The parabolic isometries.

geodesic lines tending towards the same ideal point in one direction is called *paracycle* (or sometimes *horocycle*). The circles, hypercycles, and paracycles together are named *cycles*.

Definition 16: A curve γ on a Riemannian manifold M is said to be *translatable along itself*, if there exists a one parameter subgroup of the isometry group of M, every element of which transforms the curve onto itself.

Lemma 17: Every cycle of the hyperbolic plane can be translated along itself. For circles, this translation is realized by a one-parameter subgroup of elliptic isometries, for hypercycles by hyperbolic isometries, and the subgroups of parabolic isometries translate the paracycles along themselves. [In other words, the circles (resp. the hypercycles, paracycles) are the orbits of the action of one-parameter subgroups of elliptic (resp. hyperbolic, parabolic) isometries.] Every cycle is a curve of constant curvature, a circle of radius r has curvature $\coth(r)$, a horocycle of altitude d has curvature $\tanh(d)$, and the curvature of the paracycles is 1. On the contrary, every (unextendable) curve of the hyperbolic plane, which has constant curvature, or which is translatable along itself, is a cycle.

On the pseudosphere model of the hyperbolic plane the cycles are exactly the sections of S with affine hyperplanes of $\mathbf{V}$. The intersections of hyperplanes containing the origin of $\mathbf{V}$ give the geodesic lines, the timelike affine hyperplanes intersect the pseudosphere in hypercycles, the lightlike affine hyperplanes in paracycles, and the intersections of S with spacelike affine hyperplanes are the circles. (See Figs. 5–7.)

It follows immediately from Definition 15 and lemma 14 that the cycles are translatable curves along themselves, and for the three different types of cycles the translations are realized by different types of isometries as stated in the lemma. It also means that the curvature of the cycles is constant, and a direct calculation using elementary techniques gives its value. It is also easy to show the converse of the first two statements. The assertion in the second paragraph of the lemma can be proved with the help of Lemma 14. For every cycle there is a one-parameter isometry

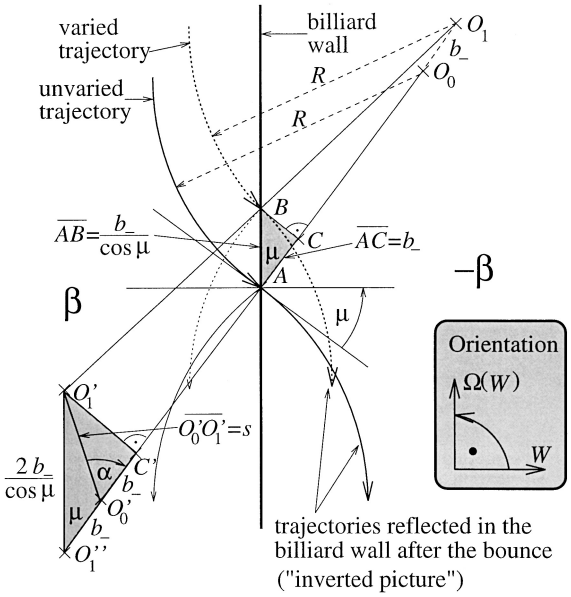

FIG. 8. The ''inverted picture'' of the bouncing trajectories for straight billiard wall.

subgroup of S, which transforms the cycle along itself. According to Lemma 14, there is a family of affine hyperplanes parallel to each other in $\mathbf{V}$, which are invariant under the one-parameter isometry subgroup. The investigated cycle is the intersection of S and one of these invariant affine planes.

APPENDIX C: ELEMENTARY ILLUSTRATION OF THE BOUNCING EFFECT

In this Appendix we give an elementary demonstration of the equations (36) and (37) describing the jump of the infinitesimal variation and its first derivative at the bounce in a special case, where the derivative of the transverse infinitesimal variation b' and the curvature q of the billiard wall are zero at the reflection point. Since the curvature of the manifold M does not play any role in the bouncing effects, it is assumed furthermore that $(M,\langle\cdot,\cdot\rangle)$ is the Euclidean plane. For the sake of simplicity, we deal only with special variations.

It is better to work in an ''*inverted picture,*'' i.e., reflect the trajectories after the bounce in the wall of the billiard. In this case the billiard wall can be considered as the boundary between two domains of opposite magnetic field, which the particles cross without changing their velocities (Fig. 8). It can be also seen that the infinitesimal variation is everywhere continuous in the inverted picture.

Let us use the usual notations $a_-, b_- \in \mathfrak{R}$ and $a'_-, b'_- \in \mathfrak{R}$ (introduced in Sec. IV) for describing the coordinates of the (special) infinitesimal variation and their derivatives just before the bounce, respectively. For distinguishing the coordinates (and their derivatives) in the inverted picture from the ordinary ones after the bounce, we use a tilde above the letters. Since the reflection in the billiard wall changes the orientation of the plane, the transverse coordinate changes sign in the inverted picture, but the longitudinal one remains unaltered, i.e.,

$$a_+ = \tilde{a}_+, \quad a'_+ = \tilde{a}'_+, \quad b_+ = -\tilde{b}_+, \quad b'_+ = -\tilde{b}'_+. \tag{C1}$$

As the infinitesimal variation is continuous in the inverted picture, $a_- = \tilde{a}_+$, $b_- = \tilde{b}_+$, and this together with (C1) proves Eqs. (36).

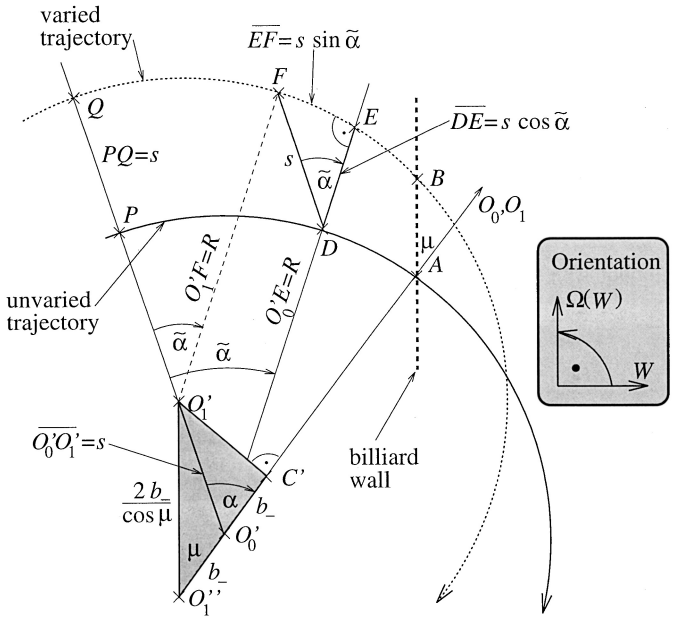

FIG. 9. The trajectories after the bounce in the ''inverted picture.''

To prove the equations (37) in the special case of $b'_- = q = 0$, let us consider the two infinitesimally close trajectories of unit speed in Fig. 8, where $0<\mu<\pi/2$ is the angle of reflection, $\beta>0$ is the magnetic field, and $R=1/\beta$ is the radius of the trajectories. Since $b'_- = 0$, the centers O_0, O_1 of the incident trajectories and the reflection point A of the unvaried trajectory are collinear, and $\overline{O_0O_1} = b_- > 0$. The centers O_0', O_1' of the trajectories after the bounce (in the inverted picture) are obtained by reflecting the centers O_0, O_1 of the incident trajectories in the bouncing points A,B, respectively. Let O_1'' be the central inverse image of O_1 in the point A, and let C, resp. C' be the foot of the perpendicular dropped from the points B, resp. O_1', to meet the line O_0O_0'. The triangles ABC and $O_1''O_1'C'$ are similar in the ratio of 2. Further on we assume that the variation is small, i.e., the angle $\angle BO_1A \ll 1$ or equivalently $b_- \ll R\cot(\mu)$. This means that the angle of incidence of the varied trajectory is also (approximately) μ, and $\overline{AC} \approx \overline{C'O_0'} \approx b_- = \overline{O_0O_1} = \overline{O_0'O_1''}$.

It can be seen in Fig. 8 that $\overline{AB} \approx b_-/\cos(\mu)$, so $\overline{O_1'O_1''} \approx 2b_-/\cos(\mu)$, and the angle $\angle O_0'O_1''O_1' = \mu$. Let us denote the angle $\angle O_1'O_0'O_0$ with α (directed in the way shown in Figs. 8 and 9), and let $s := \overline{O_0'O_1'}$ (Fig. 9). Applying the sine rule to the triangle $O_0'O_1'O_1''$,

$$s\,\sin(\alpha) = \sin(\mu)\,\frac{2b_-}{\cos(\mu)}. \tag{C2}$$

In order to determine the derivatives $\tilde{a}'_+, \tilde{b}'_+$ of the coordinates of the (special) infinitesimal variation just after the bounce (in the inverted picture), let us consider two particles starting from the points P,Q and moving along the trajectories shown in Fig. 9 at unit speed. (The points P, Q, O_0', and O_1' are collinear.) After the time $R\tilde{\alpha}$, where $\tilde{\alpha} = \angle QO_1'F = \angle PO_0'D$ is the angle of the arcs covered, the particles are at the points D, F, and the longitudinal, resp. transverse, distance between them are $\tilde{a}_+(\tilde{\alpha}) = -\overline{EF} = -s\,\sin(\tilde{\alpha})$, resp. $\tilde{b}_+(\tilde{\alpha}) = \overline{DE} = s\,\cos(\tilde{\alpha})$. (Since the variation is small, DEF is a right triangle.) Differentiating these expressions with respect to time (i.e., with respect to $R\tilde{\alpha}$) at $\tilde{\alpha}=\alpha$,

$$\tilde{a}'_+ = \frac{d}{d(R\tilde{\alpha})}\bigg|_\alpha (-s\,\sin(\tilde{\alpha})) = -s\beta\,\cos(\alpha) = -\beta\overline{O'_0C'} = -\beta b_-\,, \tag{C3}$$

$$\tilde{b}'_+ = \frac{d}{d(R\tilde{\alpha})}\bigg|_\alpha (s\,\cos(\tilde{\alpha})) = -s\beta\,\sin(\alpha) = -\beta\,\sin(\mu)\,\frac{2b_-}{\cos(\mu)}. \tag{C4}$$

[The right triangle $O'_0C'O'_1$ shows that $s\,\cos(\alpha)=b_-$, and we used expression (C2) in Eq. (C4).]

Inserting the connections (C1) into Eqs. (C3) and (C4), and using the fact that for special variations $a'_\pm = \beta b_\pm$ [see the first equation of (23) in Theorem 5, with $p=0$], it is easy to obtain Eqs. (37) in the special case of $b'_- = q = 0$.

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Integration of the Einstein–Dirac equations

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The problem of exact integration of the Einstein–Dirac equation is studied. To solve this set of equations metrics admitting complete separation of variables in the Dirac equation are considered. At the first stage Stäckel spaces of types (3.1) and (3.0) are studied. For the first case obtained solutions contain arbitrary functions depending on one variable only (five real functions for the Einstein–Weyl equations and four real functions for the Einstein–Dirac ones). For the second one all solutions belonging to the diagonal metrics of Bianchi type 1 are found. © *1996 American Institute of Physics.* [S0022-2488(96)02909-X]

I. INTRODUCTION

Exact integration of the Einstein–Dirac equations is one of the complicated problems in the modern mathematical physics. As far as we know at this writing only few exact solutions of these equations have been found (see, for example Refs. 1, 2 and references therein). Our approach is based on using metrics of the space-times for which the Dirac equation can be integrated by complete separation of variables method. Many authors studied these metrics (see Refs. 3–9). In the papers, metrics admitting Yano–Killing tensors or Yano vectors were studied. Using these geometrical objects one can construct symmetry operators of the Dirac equation. These spaces have been found in Ref. 10. Other trend was investigate in Ref. 11 where all spaces for which the Dirac equations can be integrated by diagonalization and separation of variables have been found. In the paper[12] it was proved that if the Dirac equation admits complete separation of variables the Hamilton–Jacobi equation can be integrated by complete separation of variables in the same coordinate set too. In other words, spaces for which Dirac equation can be separated belong to the class of Stäckel spaces (Riemannian space is called the Stäckel one if in this space the Hamilton–Jacobi equation can be integrated by the complete separation of variables[13,14]). Recall the main states of the theory of Stäckel spaces (see Refs. 14–16). Let g_{ij} be a metric tensor of the Riemannian space V_n. The Hamilton–Jacobi equation

$$g^{ij}S_{,i}S_{,j}=m^2 \tag{1.1}$$

admits complete separation of variables if coordinate set $\{u^i\}$ exists for which the complete integral can be presented in the form:

$$S=\sum_{i=1}^{n} S_i(u^i,\lambda_1,\ldots,\lambda_n). \tag{1.2}$$

It was proved that the separation takes place if and only if the metric tensor g_{ij} can be put in the form

$$g_{ij}=\sum_{\nu=N}^{n} (\Phi^{-1})^{\nu}_{n} h^{ij}_{\nu}(u^{\nu}), \tag{1.3}$$

$$\Phi^{\mu}_{\nu}=\Phi^{\mu}_{\nu}(u^{\nu}), \quad h^{ij}_{\nu}=\delta^i_{\nu}\delta^j_{\nu}h^{\nu\nu}_{\nu}+(\delta^i_{\nu}\delta^j_{p}+\delta^i_{p}\delta^j_{\nu})h^{ij}_{\nu}+\delta^i_{p}\delta^j_{q}h^{pq}_{\nu},$$

$$p,q=1,\ldots N, \quad \nu,\mu=N+1,\ldots,n.$$

One can verify, that V_n admits mutually commuting Killing vectors and tensors:

$$Y^i_p=\delta^i_p, \quad Y^{ij}_\nu=\sum_{\nu=N}^{n}(\Phi^{-1})^\mu_\nu h^{ij}_\mu. \tag{1.4}$$

These geometrical objects form a so called compete set. Next designations are adopted in the theory. Riemannian space is called the Stäckel one of type (N,N_0) if the metric tensor can be presented in the form (1.3). N is the number of the Killing vectors entering into the complete set,

$$N_0=N-\mathrm{rank}|g_{ij}Y^i_pY^j_q|. \tag{1.5}$$

If V_n has the Lorentz signature $(+,-,-,-)$, number N_0 may take a value of 0 or 1. Hence there are seven types of Stäckel spaces with signature $(+,-,-,-)$: four non-null types (N,0) and three null types (N,1).

According to the definition the Dirac equation

$$(\gamma^i(x)\hat{D}_i-m)\Psi=0 \tag{1.6}$$

can be integrated by complete separation of variables if any Ψ may be present in the separated form:

$$\Psi=\hat{S}(u)\hat{\varphi}_0(u^0,\lambda),\hat{\varphi}_1(u^1,\lambda),\hat{\varphi}_2(u^2,\lambda),\hat{\varphi}_3(u^3,\lambda). \tag{1.7}$$

Here

$$\det\hat{S}(u)\neq 0, \quad [\hat{\varphi}_i,\hat{\varphi}_j]=0.$$

(The analogous definition takes place for the squared Dirac equation.[11,12] Another approach to the problem of separation of variables for the Dirac equation has been studied in Ref. 17.) In Ref. 3 it was proved that the existence of Yano vectors or Yano–Killing tensors is the necessary condition of the separation. Moreover, g_{ij} must have the form (1.3). (The space belongs to the Stäckel one.) In Ref. 10 it was found that only spaces $(2,N_0)$ can admit Yano vectors or Yano–Killing tensors. Hence only six types of spaces for which Ψ can be present in the form (1.7) exist. There are two types $(3,N_0)$ and four types $(2,N_0)$ (two types with Yano vector and two types with Yano–Killing tensor) satisfying these conditions. Thus all appropriate metrics are known now and it is possible to consider the problem of integration of the Einstein–Dirac equations for the case when the Dirac equation can be integrated by complete separation of variables. We try to solve the problem of the complete classification of the Einstein–Dirac spaces for which the Dirac equation admits complete separation of variables. Note that a similar problem has been solved for the case when gravitational field interacts with a vector one (Einstein–Maxwell equation[18–20]). Therefore the problem of classification for the interacting spinor and gravitational fields can be regarded as a part of the general classification problem. We begin our investigation from the spaces of types (3,1) and (3,0). (For the last type we restrict ourselves to the case when the metric has Bianchi type I form.) Other types will be considered in the next papers. Moreover, at the first stage it is possible to suppose that solutions of the Dirac equation have separate forms.

II. FIELD EQUATIONS

In the present section we restrict our attention to the case when the space-time has a form of Stäckel space of type (3.1). The Metric tensor for this case has a form:

$$g^{\mu\nu}=g^{\nu\mu}(x^0), \quad g^{00}=0, \quad \nu,\mu=0,1,2,3.$$

Obviously the space admits three Killing vectors $Y_p{}^i$. To write Einstein–Dirac equations one has to use Newman–Penrose formalism.[21,22] Let us introduce the complex tetrad in the form

$$\begin{gathered} l^i=(1,0,0,0), \ \ n^i=(0,1,\beta_2,\beta_3), \quad m^i=(0,0,v,u) \\ l_i=(0,1,0,0), \quad n_i=(1,0,0,0), \\ m_i=(0,i(\beta_3 u-\beta_2 v)/G,-iu/G,iv/G)), \\ G\equiv i(u\overline{v}-\overline{u}v), \quad \overline{\beta_2}=\beta_2, \quad \overline{\beta_3}=\beta_3. \end{gathered} \tag{2.1}$$

All functions depend on x^0 only, bar means complex conjugation. From (2.1) it follows

$$D=\partial_0, \quad \Delta=\partial_1+\beta_2\partial_2+\beta_3\partial_3, \quad \delta=v\partial_2+u\partial_3 (\partial_i\equiv\partial/\partial x^i), \tag{2.2}$$

$$\begin{gathered} \kappa=\lambda=\nu=\mu=0, \quad \alpha=i(\dot{\beta}_3\overline{v}-\dot{\beta}_2\overline{u})/4G, \quad 2\overline{\beta}=\overline{\tau}=\overline{\lambda}=2\alpha, \\ \sigma=i(\dot{v}u-\dot{u}v)/G, \quad \rho=i(\mathring{v}u-\mathring{u}v+\dot{u}\overline{v}-\dot{v}\overline{u})/2G=\dot{G}/2G, \\ \varepsilon=i(\mathring{u}v-\mathring{v}u+\dot{u}\overline{v}-\dot{v}\overline{u})/4G. \end{gathered} \tag{2.3}$$

Dots mean derivatives with respect to the variable x^0. Using (2.2) and (2.3) one can find spinor components of the Weyl tensor

$$\begin{gathered} \psi_0=\dot{\sigma}-\sigma(2\rho+4\varepsilon), \quad \psi_1=\mathring{\alpha}-(\rho+2\varepsilon)\overline{\alpha}-3\sigma\alpha, \\ 3\psi_2=-16\alpha\overline{\alpha}, \quad \psi_3=\psi_4=0, \end{gathered} \tag{2.4}$$

and spinor components of the Ricci tensor

$$\begin{gathered} \Phi_{00}=\dot{\rho}-\rho^2-\sigma\overline{\sigma}, \quad \Phi_{01}=\dot{\overline{\alpha}}-(3\rho+2\varepsilon)\overline{\alpha}-\sigma\alpha, \\ \Phi_{11}=-6\alpha\overline{\alpha}, \quad \Phi_{02}=-4\alpha^2, \quad 3\Lambda=2\alpha\overline{\alpha}, \quad \Phi_{12}=\Phi_{22}=0. \end{gathered} \tag{2.5}$$

In this formalism the Einstein–Dirac equations have the form

$$\Phi_{\alpha\beta'\gamma\delta'}+\varepsilon_{\alpha\gamma}\varepsilon_{\beta'\delta'}H=aT_{\alpha\beta'\gamma\delta'}, \tag{2.6}$$

$$\nabla_{\alpha\beta'}\xi^{\alpha}=m_0\eta_{\beta'}, \quad \nabla_{\alpha'\beta}\eta^{\alpha'}=m_0\xi_{\beta}. \tag{2.7}$$

Here $m_0=m/\sqrt{2}$, m is the mass of a spinor particle, $\Phi_{00'00'}=\Phi_{00}$, $\Phi_{00'01'}=\Phi_{01}$, $\Phi_{01'01'}=\Phi_{02}$, $\Phi_{01'11'}=\Phi_{12}$, $\Phi_{11'11'}=\Phi_{22}$, $\Phi_{00'11'}=2(\Phi_{11}-3\Lambda)$, $\Phi_{01'10'}=-2(\Phi_{11}+3\Lambda)$, $\xi_{\alpha'}=\overline{\xi_{\alpha}}$, $\alpha,\beta,\gamma,\delta=0,1$, H is the cosmological constant, $a=$const, and $T_{\alpha\beta'\gamma\delta'}$ is the stress-energy tensor of the particle with spin 1/2. It has the form

$$T_{\alpha\beta'\gamma\delta'}=ik[T(\xi)_{\alpha\beta'\gamma\delta'}-T(\eta)_{\alpha\beta'\gamma\delta'}], \tag{2.8}$$

$$T(\varphi)_{\alpha\beta'\gamma\delta'}=\varphi_{\delta'}\nabla_{\alpha\beta'}\varphi_{\gamma}+\varphi_{\beta}\nabla_{\gamma\delta'}\varphi_{\alpha}-\varphi_{\alpha}\nabla_{\alpha\beta'}\varphi_{\delta'}-\varphi_{\alpha}\nabla_{\gamma\delta'}\varphi_{\beta'}. \tag{2.9}$$

Here

$$\nabla_{00'}\varphi_0=D\varphi_0-\varepsilon\varphi_0+\kappa\varphi_1, \quad \nabla_{00'}\varphi_1=D\varphi_1-\pi\varphi_0+\varepsilon\varphi_1,$$

$$\nabla_{01'}\varphi_0=\delta\varphi_0-\beta\varphi_0+\sigma\varphi_1,\quad \nabla_{01'}\varphi_1=\delta\varphi_1-\mu\varphi_0+\beta\varphi_1,$$
$$\nabla_{10'}\varphi_0=\overline{\delta}\varphi_0-\alpha\varphi_0+\rho\varphi_1,\quad \nabla_{10'}\varphi_1=\overline{\delta}\varphi_1-\lambda\varphi_0+\alpha\varphi_1, \tag{2.10}$$
$$\nabla_{11'}\varphi_0=\Delta\varphi_0-\gamma\varphi_0+\tau\varphi_1,\quad \nabla_{11'}\varphi_1=\Delta\varphi_1-\nu\varphi_0+\gamma\varphi_1,$$
$$\nabla_{\alpha\beta'}\varphi_{\gamma'}=\overline{(\nabla_{\beta\alpha'}\varphi_{\gamma})}.$$

For the Einstein–Weyl case $m=\eta_\alpha=0$. Using (2.10) one can find function $T(\varphi)_{\alpha\beta'\gamma\delta'}$:

$$T(\varphi)_{00'00'}=\varphi_{0'}D\varphi_0-\varphi_0D\varphi_{0'}-(\varepsilon-\overline{\varepsilon})\varphi_0\varphi_{0'}+\kappa\varphi_{0'}\varphi_1-\overline{\kappa}\varphi_0\varphi_{1'},$$
$$2T(\varphi)_{00'01'}=\varphi_{1'}D\varphi_0-\varphi_0D\varphi_{1'}+\varphi_{0'}\delta\varphi_0-\varphi_0\delta\varphi_{0'}+\varphi_0\varphi_{0'}(\overline{\alpha}-\beta+\overline{\pi})$$
$$+\kappa\varphi_1\varphi_{1'}-(\varepsilon+\overline{\varepsilon}+\overline{\rho})\varphi_0\varphi_{1'}+\sigma\varphi_{0'}\varphi_1,$$
$$T(\varphi)_{01'01'}=\varphi_{1'}\delta\varphi_0-\varphi_0\delta\varphi_{1'}+\sigma\varphi_1\varphi_{1'}+\overline{\lambda}\varphi_0\varphi_{0'}-(\beta+\overline{\alpha})\varphi_0\varphi_{1'},$$
$$2T(\varphi)_{01'11'}=\varphi_{1'}\delta\varphi_1-\varphi_1\delta\varphi_{1'}+\varphi_{1'}\Delta\varphi_0-\varphi_0\Delta\varphi_{1'}+\overline{\nu}\varphi_0\varphi_{0'}$$
$$+(\beta-\overline{\alpha}+\tau)\varphi_1\varphi_{1'}-(\overline{\gamma}+\gamma+\mu)\varphi_0\varphi_{1'}+\overline{\lambda}\varphi_1\varphi_{0'},$$
$$T(\varphi)_{11'11'}=\varphi_{1'}\Delta\varphi_1-\varphi_1\Delta\varphi_{1'}+(\gamma-\overline{\gamma})\varphi_1\varphi_{1'}-\nu\varphi_0\varphi_{1'}+\overline{\nu}\varphi_1\varphi_{0'},$$
$$2T(\varphi)_{00'11'}=\varphi_{1'}D\varphi_1-\varphi_1D\varphi_{1'}+\varphi_{0'}\Delta\varphi_0-\varphi_0\Delta\varphi_{0'}+(\varepsilon-\overline{\varepsilon})\varphi_1\varphi_{1'}$$
$$+(\overline{\gamma}-\gamma)\varphi_0\varphi_{0'}-(\overline{\tau}+\pi)\varphi_0\varphi_{1'}+(\tau+\overline{\pi})\varphi_1\varphi_{0'},$$
$$2T(\varphi)_{01'10'}=\varphi_{0'}\delta\varphi_1-\varphi_0\overline{\delta}\varphi_{1'}+\varphi_{1'}\overline{\delta}\varphi_0-\varphi_1\delta\varphi_{0'}+(\overline{\mu}-\mu)\varphi_0\varphi_{0'}$$
$$+(\rho-\overline{\rho})\varphi_1\varphi_{1'}+(\beta+\overline{\alpha})\varphi_{0'}\varphi_1-(\alpha+\overline{\beta})\varphi_0\varphi_{1'}.$$

Let us transform tetrad (2.1) in the following manner:

$$\widetilde{l}\to l,\quad \widetilde{n}\to n,\quad \widetilde{m}\to m\ \exp i\theta(x^0). \tag{2.11}$$

Then

$$\widetilde{\alpha}\to\alpha\ \exp-i\theta,\quad \widetilde{\beta}\to\beta\ \exp i\theta,\quad \widetilde{\tau}\to\tau\ \exp i\theta,\quad \widetilde{\pi}\to\pi\ \exp-i\theta. \tag{2.12}$$

Other spin coefficients do not transform. If function θ will be chosen in the form

$$2\theta=-i\ \ln(\alpha/\overline{\alpha})$$

coefficients α,β,τ,π become real functions

$$\overline{\alpha}=\alpha=\beta=\tau/2=\pi/2. \tag{2.13}$$

Then Einstein–Dirac equations can be present in the form

$$(D+\varepsilon-\rho)\xi_1-(\overline{\delta}+\alpha)\xi_0=m_0\eta_{0'},\quad (\delta-\alpha)\xi_1-\Delta\xi_0=m_0\eta_{1'},$$
$$(D-\varepsilon-\rho)\eta_{1'}-(\delta+\alpha)\eta_{0'}=m_0\xi_0,\quad (\overline{\delta}-\alpha)\eta_{1'}-\Delta\eta_{0'}=m_0\xi_1; \tag{2.14}$$

$$\xi_{1'}\Delta\xi_1-\xi_1\Delta\xi_{1'}-\eta_{1'}\Delta\eta_1+\eta_1\Delta\eta_{1'}=0; \tag{2.15}$$

$$\xi_{1'}\delta\xi_1-\xi_1\delta\xi_{1'}+\xi_{1'}\Delta\xi_0-\xi_0\Delta\xi_{1'}+2\alpha\xi_1\xi_{1'}$$
$$-[\eta_{1'}\delta\eta_1-\eta_1\delta\eta_{1'}+\eta_{1'}\Delta\eta_0-\eta_0\Delta\eta_{1'}+2\alpha\eta_1\eta_{1'}]=0; \tag{2.16}$$

$$iak[\xi_{1'}D\xi_0-\xi_0D\xi_{1'}+\xi_{0'}\delta\xi_0-\xi_0\delta\xi_{0'}+2\alpha\xi_0\xi_{0'}-\rho\xi_0\xi_{1'}+\sigma\xi_{0'}\xi_1-\eta_{1'}D\eta_0+\eta_0D\eta_{1'}$$
$$-\eta_{0'}\delta\eta_0+\eta_0\delta\eta_{0'}-2\alpha\eta_0\eta_{0'}+\rho\eta_0\eta_{1'}-\sigma\eta_{0'}\eta_1]=4[\alpha(3\rho+2\varepsilon+\sigma)-\dot{\alpha}]; \tag{2.17}$$

$$ika\{\xi_1[(D+\varepsilon-\rho)\xi_1-(\overline{\delta}+\alpha)\xi_0]-\xi_1[(D-\varepsilon-\rho)\xi_{1'}-(\delta+\alpha)\xi_{0'}]+\xi_{0'}[\Delta\xi_0-(\delta-\alpha)\xi_1]$$
$$-\xi_0[\Delta\xi_{0'}-(\overline{\delta}-\alpha)\xi_{1'}]-\eta_{1'}[(D-\varepsilon-\rho)\eta_1-(\overline{\delta}+\alpha)\eta_0]+\eta_1[(D-\varepsilon-\rho)\eta_{1'}$$
$$-(\delta+\alpha)\eta_{0'}]-\eta_{0'}[\Delta\eta_0-(\delta-\alpha)\eta_1]+\eta_0[\Delta\eta_{0'}-(\overline{\delta}-\alpha)\eta_{1'}]\}=16\alpha^2-4H; \tag{2.18}$$

$$ika[\xi_{0'}\delta\xi_1-\xi_0\overline{\delta\xi}_{1'}-\xi_{1'}\overline{\delta\xi}_0-\xi_1\delta\xi_{0'}+2\alpha(\xi_{0'}\xi_1-\xi_0\xi_{1'})-\eta_{0'}\delta\eta_1+\eta_0\overline{\delta\eta}_{1'}$$
$$-\eta_{1'}\overline{\delta\eta}_0+\eta_1\delta\eta_{0'}-2\alpha(\eta_{0'}\eta_1-\eta_0\eta_{1'})]=-32\alpha^2+2H. \tag{2.19}$$

Separated solutions of Eqs. (2.13) have the form

$$\xi_a=\varphi_a\ \exp\ i(\lambda_1x^1+\lambda_2x^2+\lambda_3x^3),\quad \eta_a=\psi_a\ \exp-i(\lambda_1x^1+\lambda_2x^2+\lambda_3x^3),$$
$$\varphi_a=\varphi_a(x^0),\quad \psi_a=\psi_a(x^0),\quad \lambda_1,\lambda_2,\lambda_3=\text{const}. \tag{2.20}$$

One can show that Eqs. (2.6) are compatible if and only if $\lambda_p=0$. That is why we shall suppose that

$$\xi_\alpha=\xi_\alpha(x^0),\quad \eta_\alpha=\eta_\alpha(x^0). \tag{2.21}$$

III. EINSTEIN–WEYL EQUATIONS

First we consider the case when $m=\eta_a=0$. Then Eqs. (2.6) and (2.7) have the form

$$ika[\xi_{0'}\dot{\xi}_0-\xi_0\dot{\xi}_{0'}-2\varepsilon\xi_0\xi_{0'}]=-2(\dot{\rho}-\rho^2-\sigma\overline{\sigma}); \tag{3.1}$$

$$\xi_{1'}\dot{\xi}_0-\xi_0\dot{\xi}_{1'}-\rho\xi_0\xi_{1'}+\sigma\xi_{0'}\xi_1=0; \tag{3.2}$$

$$\sigma\xi_1\xi_{1'}=0; \tag{3.3}$$

$$H=0; \tag{3.4}$$

$$\dot{\xi}_1=(\rho-\varepsilon)\xi_1+\alpha\xi_0; \tag{3.5}$$

$$\alpha\xi_1=0. \tag{3.6}$$

From Eqs. (3.5) and (3.6) it follows that $\alpha=0$. If function $\xi_1\neq 0$ from Eq. (3.4) it follows $\sigma=0$. Using Eqs. (3.2) and (3.5) one can show that

$$\xi_{0'}\dot{\xi}_0-\xi_0\dot{\xi}_{0'}-2\varepsilon\xi_0\xi_{0'}=0. \tag{3.7}$$

By this is meant that $T_{\alpha\beta'\gamma\delta'}\equiv 0$. That is why from Eq. (3.4) it follows that $\xi_1=0$. To find ξ_0 one has to solve Eq. (3.1). Let us present ξ_0 in the form

$$\xi_0=X\ \exp\ iY\quad (\overline{X}=X,\ \ \overline{Y}=Y). \tag{3.8}$$

Then Eq. (3.1) can be written in the form

$$akX^2[\dot{Y}+i\varepsilon]=\dot{\rho}-\rho^2-\sigma\overline{\sigma}. \tag{3.9}$$

Obviously $\dot{Y}+i\varepsilon \neq 0$ (otherwise $T_{\alpha\beta'\gamma\delta'}\equiv 0$). Then

$$X=[(\dot{\rho}-\rho^2-\sigma\overline{\sigma})/ak(\dot{Y}+i\varepsilon)]^{1/2}. \tag{3.10}$$

Let us consider condition

$$\alpha=0.$$

From Eq. (2.3) it follows

$$\dot{\beta}_3\overline{v}-\dot{\beta}_2\overline{u}=0\Rightarrow\dot{\beta}_2=\dot{\beta}_3=0\Rightarrow\beta_2,\beta_3=\text{const}.$$

These conditions are equivalent to $\beta_2=\beta_3=0$. Thus obtained solution can be written in the form

$$l^i=(1,0,0,0),\quad n^i=(0,1,0,0),\quad m^i=(0,0,v,u),$$

$$\xi_\alpha=\delta_{\alpha 0}[(\dot{\rho}-\rho^2-\sigma\overline{\sigma})/ak(\dot{Y}+i\varepsilon)]^{1/2}\exp iY,\quad H=0.$$

Here Y,v,u are arbitrary functions depending on X^0 only, $\overline{Y}=Y$. Functions ρ,σ,ε can be found from Eq. (2.3). Note that the obtained metric belongs to Petrov type N.

IV. EINSTEIN–DIRAC EQUATIONS

Using (2.21) one can present Dirac equations in the following form:

$$\begin{aligned}(D+\varepsilon-\rho)\xi_1-\alpha\xi_0&=m_0\eta_{0'},\\ (D-\varepsilon-\rho)\eta_{1'}-\alpha\eta_{0'}&=m_0\xi_0;\end{aligned} \tag{4.1}$$

$$\left.\begin{aligned}\alpha\xi_1+m_0\eta_{1'}&=0,\\ m_0\xi_1+\alpha\eta_{1'}&=0;\end{aligned}\right\}\Rightarrow\alpha=m_0,\quad \eta_{1'}=-\xi_1. \tag{4.2}$$

Let us put (4.2) into (4.1). In result we shall obtain

$$\begin{aligned}(D-\rho)\eta_1=0\Rightarrow\eta_1&=c|G|^{1/2},\quad c=\text{const},\\ \xi_0&=-(\eta_{0'}+\varepsilon\eta_{1'}/m_0).\end{aligned} \tag{4.3}$$

From Eqs. (2.18), (2.19) and (4.3) it follows

$$H=8m_0^2, \tag{4.4}$$

$$ika(\eta_0\eta_{1'}-\eta_1\eta_{0'}-\varepsilon\eta_1\eta_{1'}/m_0)=4m_0. \tag{4.5}$$

Thus cosmological constant H is determined by the mass of a spinor. Other equations have the form

$$\begin{aligned}ika[\eta_1\dot{\eta}_{0'}-\eta_{1'}\dot{\eta}_0+\varepsilon\eta_1\dot{\eta}_{1'}/m_0+\rho(\eta_0\dot{\eta}_{1'}-\eta_1\dot{\eta}_{0'}+(\eta_0\eta_{1'}-\eta_{0'}\eta_1-\varepsilon\eta_1\eta_{1'}/m_0)\\ \times(2\varepsilon+\sigma+\rho)]=4m_0(3\rho+2\varepsilon+\sigma);\end{aligned} \tag{4.6}$$

$$ika[2(\eta_0\dot{\eta}_{0'}-\eta_{0'}\dot{\eta}_0)+(\dot{\varepsilon}+\varepsilon\rho)(\eta_1\eta_{0'}+\eta_0\eta_{1'})/m_0-2\varepsilon^2(\eta_0\eta_{1'}-\eta_{0'}\eta_1-\varepsilon\eta_1\eta_{1'}/m_0)$$
$$-\varepsilon(\eta_1\dot{\eta}_{0'}+\dot{\eta}_0\eta_{1'})/m_0]=-2(\dot{\rho}-\rho^2-\sigma\overline{\sigma}). \tag{4.7}$$

Equation (4.6) is consequent from Eqs. (4.3) and (4.7). Indeed from Eqs. (4.3) and (4.7) it follows

$$\dot{\varepsilon}\eta_1\dot{\eta}_{1'}=m_0[\dot{\eta}_0\eta_{1'}-\dot{\eta}_{0'}\eta_1+\rho(\eta_0\eta_{1'}-\eta_1\eta_{0'})]-2\varepsilon\rho\eta_1\eta_{1'}. \tag{4.8}$$

Using Eq. (4.8) one can present Eq. (4.6) in the form

$$\rho[iak(\eta_0\eta_{1'}-\eta_{0'}\eta_1-\varepsilon\eta_1\eta_{1'}/m_0)-4m_0]=0.$$

The left-hand side of Eq. (4.7) can be transformed in the following way:

$$ik[2(\eta_0\dot{\eta}_{0'}-\eta_{0'}\dot{\eta}_0)+(\dot{\varepsilon}+\varepsilon\rho)(\eta_1\eta_{0'}+\eta_0\eta_{1'})/m_0-\varepsilon(\eta_1\dot{\eta}_{0'}+\dot{\eta}_0\eta_{1'})/m_0]-8\varepsilon^2$$
$$=ika[2(\eta_0\dot{\eta}_{0'}-\eta_{0'}\dot{\eta}_0)+(\eta_1\eta_{0'}+\eta_0\eta_{1'})(\dot{\eta}_0\eta_{1'}-\dot{\eta}_{0'}\eta_1+\rho(\eta_0\eta_{1'}-\eta_1\eta_{0'}))/\eta_1\eta_{1'}$$
$$-2\varepsilon\rho/m_0-\varepsilon(\eta_1\dot{\eta}_{0'}+\dot{\eta}_0\eta_{1'})/m_0+\varepsilon\rho(\eta_1\eta_{0'}+\eta_{1'}\eta_0)/m_0]-8\varepsilon^2$$
$$=4m_0(\eta_1\eta_{0'}+\eta_0\eta_{1'})^{\cdot}/\eta_1\eta_{1'}-8\varepsilon^2.$$

Thus Eq. (4.7) is equivalent to

$$(\eta_0\eta_{1'}+\eta_{0'}\eta_1)^{\cdot}=\eta_1\eta_{1'}(\rho^2-\dot{\rho}+\sigma\overline{\sigma}+4\varepsilon^2)/2m_0. \tag{4.9}$$

Let us present function η_0 in the form

$$\eta_0=\eta_1 X=cXG^{1/2}.$$

Then from Eqs. (4.5) and (4.8) it follows

$$X=\frac{1}{2}\left\{\frac{1}{\eta_1\eta_{1'}}\left[\int(\rho^2+\sigma\overline{\sigma}+4\varepsilon^2-\dot{\rho})\ \frac{\eta_1\eta_{1'}}{2m_0}\ dx^0-\frac{4im_0}{ka}\right]+\frac{\varepsilon}{m_0}\right\}.$$

Here $\eta_1=c|G|^{1/2}$ functions ρ, σ, and ε have the form (2.3). To determine tetrad one has to solve Eq. (4.2):

$$\alpha=(\dot{\beta}_3\overline{v}-\dot{\beta}_2\overline{u})/(u\overline{v}-\overline{u}v)=4m_0. \tag{4.10}$$

From Eq. (4.9) it follows

$$\dot{\beta}_2=4m_0(v+\overline{v}),\quad \dot{\beta}_3=4m_0(u+\overline{u}).$$

Thus

$$v=(\dot{\beta}_2+iq_2)/8m_0,\quad u=(\dot{\beta}_3+iq_3)/8m_0, \tag{4.11}$$

q_2 and q_3 are arbitrary functions depending on x^0.

Let us present obtained solutions in the final form

$$l^i=(1,0,0,0),\quad n^i=(0,1,\beta_2,\beta_3),$$

$$m^i=(1,0,(\dot{\beta}_3+iq_3)/8m_0,(\dot{\beta}_3+iq_3)/8m_0),$$

$$\xi_1=-4m_0\overline{p}(\dot{\beta}_3q_2-\dot{\beta}_2q_3),\quad \eta_1=4m_0p(\dot{\beta}_3q_2-\dot{\beta}_2q_3);$$

$$\xi_0=\frac{-\overline{p}(\dot\beta_3q_2-\dot\beta_2q_3)^{-1/2}}{2}\left\{-(\dot\beta_3q_2-\dot\beta_2q_3)^{\cdot}+2\int\left(\frac{[(\dot\beta_3q_2-\dot\beta_2q_3)^{\cdot}]^2}{\dot\beta_3q_2-\dot\beta_2q_3}+\ddot\beta_2\dot q_3-\ddot\beta_3\dot q_2\right)dx^0\right.$$
$$\left.+i\left[\ddot\beta_3\dot\beta_2-\ddot\beta_2\dot\beta_3+\dot q_3q_2-\dot q_2q_3+\frac{1}{kap\overline{p}}\right]\right\};$$

$$\eta_0=\frac{p(\dot\beta_3q_2-\dot\beta_2q_3)^{-1/2}}{2}\left\{-(\dot\beta_3q_2-\dot\beta_2q_3)^{\cdot}+2\int\left(\frac{[(\dot\beta_3q_2-\dot\beta_2q_3)^{\cdot}]^2}{\dot\beta_3q_2-\dot\beta_2q_3}+\ddot\beta_2\dot q_3-\ddot\beta_3\dot q_2\right)dx^0\right.$$
$$\left.+i\left[\ddot\beta_3\dot\beta_2-\ddot\beta_2\dot\beta_3+\dot q_3q_2-\dot q_2q_3-\frac{1}{kap\overline{p}}\right]\right\}.$$

Here $p=\text{const}$, β_2, β_3, q_2, q_3 are arbitrary functions depending on x^0 only, and $H=8m_0^2=(2m)^3$.

V. BIANCHI TYPE I METRIC

We intend to consider others types of the Stäckel spaces in the next paper. In this paper we consider in addition to the spaces of type (3,1) the special case of the spaces of type (3.0) for which the Killing vectors entering into the complete set are spacelike and non-null. These metrics are known as Bianchi type I. The diagonal metrics of this type has a form:

$$dS^2=dx^{0^2}-\sum_{i=1}^{3}(dx^i\exp\alpha_i)^2,\quad \alpha_i=\alpha_i(x^0).$$

Let us introduce the complex tetrad:

$$l^\alpha=\frac{1}{\sqrt2}(\delta_0^\alpha-\delta_1^\alpha\exp-\alpha_1),\quad l_\alpha=\frac{1}{\sqrt2}(\delta_\alpha^0+\delta_\alpha^1\exp\alpha_1),$$

$$n^\alpha=\frac{1}{\sqrt2}(\delta_0^\alpha+\delta_1^\alpha\exp-\alpha_1),\quad n_\alpha=\frac{1}{\sqrt2}(\delta_\alpha^0-\delta_\alpha^1\exp\alpha_1),\tag{5.1}$$

$$m^\alpha=\frac{1}{\sqrt2}(\delta_2^\alpha\exp-\alpha_2-i\delta_3^\alpha\exp-\alpha_3),\quad m_\alpha=-\frac{1}{\sqrt2}(\delta_\alpha^2\exp\alpha_2-i\delta_\alpha^3\exp\alpha_3).$$

Using (5.1) let us find the spin coefficients the spinor components of the Ricci tensor and the Weyl one,

$$\kappa=\alpha=\beta=\tau=\pi=\nu=0,$$

$$\mu=-\rho=\frac{1}{2\sqrt2}(\dot\alpha_2+\dot\alpha_3),\quad \sigma=-\lambda=\frac{1}{2\sqrt2}(-\dot\alpha_2+\dot\alpha_3),\tag{5.2}$$

$$\varepsilon=-\gamma=\frac{\dot\alpha_1}{2\sqrt2},$$

$$\Phi_{00}=\Phi_{22}=\frac{1}{4}\,(-\ddot{\alpha}_2-\ddot{\alpha}_3-\dot{\alpha}_2^2-\dot{\alpha}_3^2-\dot{\alpha}_1(\dot{\alpha}_2+\dot{\alpha}_3)),$$

$$\Phi_{01}=\Phi_{21}=0,\quad \Phi_{11}=\frac{1}{4}\,(\dot{\alpha}_2\dot{\alpha}_3-\dot{\alpha}_1^2-\ddot{\alpha}_1), \tag{5.3}$$

$$12\Lambda=\ddot{\alpha}_1+\ddot{\alpha}_2+\ddot{\alpha}_3+\dot{\alpha}_1^2+\dot{\alpha}_2^2+\dot{\alpha}_3^2+\dot{\alpha}_1\dot{\alpha}_2+\dot{\alpha}_1\dot{\alpha}_3+\dot{\alpha}_2\dot{\alpha}_3,$$

$$4\Phi_{02}=\ddot{\alpha}_2-\ddot{\alpha}_3+(\dot{\alpha}_2-\dot{\alpha}_3)(\dot{\alpha}_2+\dot{\alpha}_3+\dot{\alpha}_1),$$

$$\Psi_0=\Psi_4=\frac{1}{4}\,(-\ddot{\alpha}_2+\ddot{\alpha}_3-\dot{\alpha}_2^2+\dot{\alpha}_3^2+\dot{\alpha}_1(\dot{\alpha}_2-\dot{\alpha}_3)),\quad \Psi_1=\Psi_3=0, \tag{5.4}$$

$$6\Psi_2=-\ddot{\alpha}_1-\dot{\alpha}_1^2-\dot{\alpha}_2\dot{\alpha}_3+\frac{1}{2}\,(\ddot{\alpha}_2+\ddot{\alpha}_3+\dot{\alpha}_2^2+\dot{\alpha}_3^2+\dot{\alpha}_1\dot{\alpha}_2+\dot{\alpha}_1\dot{\alpha}_3).$$

One can show that Einstein equations (2.6)–(2.7) are simultaneous only if $\xi_a=\xi_a(x^0)$, $\eta_a=\eta_a(x^0)$. In this case Dirac equation (2.7) will take the form:

$$\dot{\xi}_0=-\frac{(\dot{\alpha}_1+\dot{\alpha}_2+\dot{\alpha}_3)}{2}\,\xi_0-m\eta_{1'},\quad \dot{\eta}_{0'}=-\frac{(\dot{\alpha}_1+\dot{\alpha}_2+\dot{\alpha}_3)}{2}\,\eta_{0'}-m\xi_1$$

$$\dot{\xi}_1=-\frac{(\dot{\alpha}_1-\dot{\alpha}_2+\dot{\alpha}_3)}{2}\,\xi_1+m\eta_{0'},\quad \dot{\eta}_{1'}=-\frac{(\dot{\alpha}_1+\dot{\alpha}_2+\dot{\alpha}_3)}{2}\,\eta_{1'}+m\xi_0. \tag{5.5}$$

Let us denote

$$\xi_a=\varphi_\alpha\,\exp-\frac{\Omega}{2},\quad \eta_{a'}=i\varepsilon_{a'b'}\chi^{b'}\,\exp-\frac{\Omega}{2}.$$

Using (5.5) one can find that φ_a,χ_a have the form

$$\varphi_a=p_a\,\exp imx^0+q_a\,\exp-imx^0,\quad \chi^{a'}=p_a\,\exp imx^0+q_a\,\exp-imx^0,$$

$$p_a,q_a=\text{const},\quad p_{a'}=\overline{p_a},\quad \overline{q_{a'}}=q_a. \tag{5.6}$$

Let us enumerate all components of the tensor $T_{ab'cd'}$:

$$T_{00'11'}=T_{11'11'}=T_{00'00'}, \tag{5.7}$$

$$T_{00'00'}=\frac{ikm_0}{\sqrt{2}}\,(\xi_0\eta_1-\xi_{0'}\eta_{1'}+\eta_{0'}\xi_{1'}-\eta_0\xi_1),$$

$$T_{01'01'}=\frac{ik}{2\sqrt{2}}\,(-\dot{\alpha}_2+\dot{\alpha}_3)(\xi_1\xi_{1'}-\xi_0\xi_{0'}-\eta_1\eta_{1'}+\eta_0\eta_{0'}), \tag{5.8}$$

$$T_{00'01'}=T_{01'11'}=T_{01'10'}=0.$$

Now Einstein equations can be present in the equivalent form

$$\ddot{\alpha}_p+\dot{\alpha}_p^2-\dot{\alpha}_s\dot{\alpha}_q=c\,\exp-\Omega,\quad (p,q,s\neq),$$

$$\dot{\alpha}_1\dot{\alpha}_2+\dot{\alpha}_1\dot{\alpha}_3+\dot{\alpha}_2\dot{\alpha}_3=-H-c\ \exp-\Omega, \tag{5.9}$$

$$p,q,s\neq 1,2,3 c=\sqrt{2}m_0 a k(q_0 q_{0'}+q_1 q_{1'}-p_0 p_{0'}-p_1 p_{1'}),$$

$$\begin{aligned}(\dot{\alpha}_1-\dot{\alpha}_2)(p_0p_{1'}+q_0q_{1'}+p_{0'}p_1+q_{0'}q_1)&=(\dot{\alpha}_1-\dot{\alpha}_3)(p_0p_{1'}+q_0q_{1'}+p_{0'}p_1+q_{0'}q_1)\\&=(\dot{\alpha}_2-\dot{\alpha}_3)(p_0p_{0'}+q_0q_{0'}+p_{1'}p_1+q_{1'}q_1)=0.\end{aligned} \tag{5.10}$$

Equations (5.9) can be integrated:

$$\begin{aligned}\alpha_p&=-\frac{1}{3}\left[\varepsilon b_p\int\ \frac{\exp\ \Omega d\Omega}{\sqrt{l^2\ \exp 2\Omega-3H-3c\ \exp\ \Omega}}+\Omega\right],\\ \varepsilon x^0&=\int\ \frac{d\Omega}{\sqrt{l^2\ \exp 2\Omega-3H-3c\ \exp\ \Omega}}.\\ b_1&=l_1+l_2, b_2=l_3-2l_2,\quad b_3=l_2-2l_3,\\ l_q&=\text{const},\quad \varepsilon=\pm 1,\quad l^2=l_2^2+l_3^2-l_2l_3.\end{aligned} \tag{5.11}$$

One can show that the conditions (5.10) lead to the next variants

$$\text{I.}\ \ \alpha_1=\alpha_2=\alpha_3\Rightarrow l_p=0,\quad \text{II.}\ \ \alpha_2=\alpha_3\Rightarrow l_2=l_3=l.$$

Let us enumerate all obtained solutions:

$$\xi_a=\varphi_a Q^{1/3},\quad \eta_{a'}=i\varepsilon_{a'b'}\chi^{b'}Q^{1/3}$$

$[\phi_a,\chi^b$ have the form (5.6)]

$$\text{I.}\ \ dS^2=dx^{0^2}-Q^{2/3}[dx^{1^2}+dx^{2^2}+dx^{3^2}],$$

$$(1)\ \ H=0,\quad c<0,\quad Q=\frac{3|c|}{4}\ x^{0^2}, \tag{5.12}$$

$$(2)\ \ H<0,\quad c>0,\quad Q=|\frac{c}{H}|\mathrm{ch}^2\left(\frac{\sqrt{3|H|}}{2}\ x^{0^2}\right), \tag{5.13}$$

$$(3)\ \ H>0,\quad c<0,\quad Q=|\frac{c}{H}|\sin^2\left(\frac{\sqrt{3|H|}}{2}\ x^{0^2}\right), \tag{5.14}$$

$$(4)\ \ H<0,\quad c<0,\quad Q=|\frac{c}{H}|\mathrm{sh}^2\left(\frac{\sqrt{3|H|}}{2}\ x^{0^2}\right); \tag{5.15}$$

$$\text{II.}\ \ dS^2=dx^{0^2}-Q^{2/3}[W^{-4/3}dx^{1^2}+W^{2/3}(dx^{2^2}+dx^{3^2})],\quad c=\xi|c|,\quad \xi^2=1,$$

$$(1)\quad H=0\quad Q=\frac{3c}{4}\left(\frac{4l^2}{9c^2}-x^{0^2}\right),\quad W=\frac{2l/3c+x^0}{2l/3c-x^0}, \tag{5.16}$$

$$(2)\quad H<0,\quad y^2=-1-\frac{4Hl^2}{3c^2},\quad Q=\frac{\xi|c|}{2H}\ (\xi-y\ \mathrm{sh}\ \sqrt{3|H|}x^0), \tag{5.17}$$

$$W=\frac{\xi y+\mathrm{sh}(\sqrt{3|H|}x^0)+(2l\sqrt{3|H|}/3c)\ \mathrm{ch}\ \sqrt{3|H|}x^0}{\xi-y\ \mathrm{sh}\ \sqrt{3|H|}x^0},$$

$$(3)\quad H<0,\quad y^2=1+\frac{4Hl^2}{3c^2},\quad Q=-\frac{\xi c}{2H}\ (y\ \mathrm{ch}(\sqrt{3|H|}x^0)-\xi), \tag{5.18}$$

$$W=\frac{-\xi y+\mathrm{ch}(\sqrt{3|H|}x^0)+(2l\sqrt{3|H|}/3c)\ \mathrm{sh}\ \sqrt{3|H|}x^0}{\xi-y\ \mathrm{ch}\ \sqrt{3|H|}x^0},$$

$$(4)\quad H>0,\quad y^2=1+\frac{4Hl^2}{3c^2},\quad Q=\frac{\xi c}{2H}\ (y\ \cos(\sqrt{3|H|}x^0)-\xi), \tag{5.19}$$

$$W=\frac{\xi y-\cos(\sqrt{3/|H|}x^0)+(2l\sqrt{3|H|}/3c)\ \sin\ \sqrt{3|H|}x^0}{\xi-y\ \cos\sqrt{3|H|}x^0}.$$

VI. CONCLUSION

(1) One can show that if for solutions obtained in Sec. III and IV spinor fields will be directed to zero $\xi_a, \eta_a \to 0$ the metrics take the form

$$dS^2=2dx^0x^1-g_{pq}(x^0)dx^pdx^q,\quad p,q=2,3. \tag{6.1}$$

Moreover $R_{\alpha\beta}=0$. It is known that such metrics describe a gravitational plain wave. Thus the obtained solution can be interpreted as plain gravitational wave interacting with a spinor field. As functions determining metric tensor are arbitrary one can find solutions with or without singularity. Solutions with neutrinos belong to Petrov type N. They can be regarded as a model of interacting plain gravitational and plain neutrino waves.

Solutions with massive spinor belong to Petrov type II (or D). Nevertheless they can be regarded as a plain wave too. All functions in this case depend on x^0 only. Let us transform the coordinate set in the following manner

$$x^0=u^0-u^1,\quad x^1=u^0+u^1,\quad x^2=u^2,\quad x^3=u^3.$$

Then all functions will depend on (u^0-u^1) only. In these coordinates $T_{00}>0$ and (u^0-u^1) have the same sense as for the electromagnetic wave in the flat space-time.

(2) Bianchi type I case. The spaces of this type for the general case describe the heterogeneous cosmological model. (Note that case when cosmological constant equals to zero was considered in).[23] They can be regarded as a generalization of the Kasner solutions. All of them have the

singular points. Apparently pulsating solution (5.19) is the same. It has infinitely large number of the repeating singular points. Let us calculate components $T_{\alpha\beta}$ for all obtained solutions

$$T_{00}=\frac{ikm}{\sqrt{2}}\,\frac{(q_0q_{0'}+q_1q_{1'}-p_0p_{0'}-p_1p_{1'})}{\exp(\alpha_1+\alpha_2+\alpha_3)}=\frac{c}{2G}\,\exp 2\Omega,$$

$$T_{0i}=T_{ij}=0,\quad i,j=1,2,3.$$

If $c>0$ T_{00} and energy are positive. Note in conclusion that (5.12)–(5.15) belong to the class of the conformally flat spaces, solutions (5.16)–(5.19) to Petrov type D ones.

ACKNOWLEDGMENTS

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Four dimensional quantum topology changes of space–times

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Topology changing processes in the WKB approximation of four dimensional quantum cosmology with a negative cosmological constant are investigated. As Riemannian manifolds, which describe quantum tunnelings of space–time, constant negative curvature solutions of the Einstein equation, i.e., hyperbolic geometries are considered. Using four dimensional polytopes, one can explicitly construct hyperbolic manifolds with topologically nontrivial boundaries which describe topology changes. These instantonlike solutions are constructed out of 8-cells, 16-cells, or 24-cells and have several points at infinity called cusps. The hyperbolic manifolds are noncompact because of the cusps but have finite volumes. Topology change amplitudes in the WKB approximation in terms of the volumes of these manifolds are evaluated and it was found that the more complicated the topology changes, the more likely are suppressed. © *1996 American Institute of Physics.* [S0022-2488(96)04409-X]

I. INTRODUCTION

In classical gravity the topology change of the universe can be considered only in the case where a normally assumed principle like causality is violated.[1] In quantum gravity, on the other hand, topology changing processes are rather ubiquitous. For example, topology changes can happen in the birth of the universe, in the evaporation of a black hole, and so on. Moreover, the topology changes, if possible by any mechanism either in classical or quantum gravity, may induce important physical effects.

Recently there have been new progress in the investigation of topology changes. In $(2+1)$-dimensional simplified models, the topology changes have been demonstrated to happen indeed by some explicit examples. In three dimensional space–times with a negative cosmological constant, two kinds of topology changes have been investigated. The first one was associated with the existence of a compactified three dimensional black hole solution (or a higher genus universe with a negative cosmological constant). One of present authors (M.S.) showed that its analytical continuation around the coordinate singularity of the space–time may provide a process of topology change.[2] The second one was in the context of quantum cosmology. Siino *et al.*[3] constructed topology changing solutions by quantum tunneling. To discuss more physical topology changes these works should be generalized to four dimensional space–times. The former will be generalized to the $(3+1)$-dimensional compact hyperbolic cosmology.[4] The purpose of the present article is the generalization of the latter. That is to say, we investigate quantum topology changes in a cosmological model through tunneling processes in four dimensions.

According to Gibbons and Hartle,[5] a quantum tunneling space–time is semiclassically ap-

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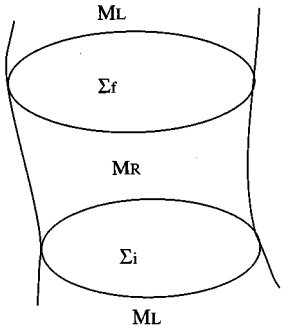

FIG. 1. A manifold with a Euclidean signature M_R interpolates the two manifolds with a Lorentz signature M_L through $\Sigma_{i,f}$.

proximated by a Riemannian manifold with totally geodesic boundaries. In Ref. 3, the authors found some constantly curved Riemannian manifolds with topologically nontrivial, totally geodesic boundaries. If such a manifold has two connected pieces of boundary components with different topologies, it describes a process of topology change between the two Lorentzian space–times connected on the boundaries. Such 3-manifolds were constructed out of regular truncated polyhedra embedded in a hyperbolic 3-space. In the present article, we discuss the topology change of the universe along the same line but in four dimensions. The four dimensional analog of polyhedra is called polytope and we shall construct four dimensional Riemannian manifolds by four dimensional regular truncated polytopes embedded in a hyperbolic 4-space.[6] The resultant manifolds describe topology change of a vacuum universe with a negative cosmological constant.

In Sec. II we briefly review quantum tunnelings of space–times in general, and give a mathematical preliminary for hyperbolic space and quotient manifolds. Section III gives topology changing solutions in four dimensional space–times of a constant negative curvature. We investigate their amplitudes and discuss the strong rigidity of the tunneling manifolds in Sec. IV. Section V is devoted to summary and discussions.

II. QUANTUM TUNNELING OF SPACE–TIMES AND HYPERBOLIC MANIFOLDS

A. Quantum tunneling of space–times: Formalism

In the context of quantum cosmology, a quantum tunneling should be described by Riemannian path integral formalism proposed by Hartle and Hawking.[7] We would like to appeal to the WKB approximation to compute tunneling amplitudes, since exact computations are almost hopeless in four dimensions. In this case, a quantum tunneling means a transition (classically forbidden) from a spatial hypersurface Σ_i to another spatial hypersurface Σ_f. By topology change of space–time it is meant that Σ_f is topologically different from Σ_i. These hypersurfaces may consist of some disconnected components.

Gibbons and Hartle[5] showed that, in the WKB approximation, the tunneling process is described by a Riemannian manifold which has the boundary components Σ_i and Σ_f. In the ADM formalism, a spatial hypersurface Σ is characterized by a spatial metric h_{ij} and an extrinsic curvature K_{ij} on it. In a semiclassical picture, an ordinary space–time manifold M_L with a Lorentzian signature (Lorentzian manifold) and a quantum tunneling manifold M_R with a Euclidean signature (Riemannian manifold) are connected on the hypersurface Σ (see Fig. 1). The spatial metric h_{ij} can be uniquely defined from the viewpoints of both regions, because it is independent of the time coordinates. However, the hypersurfaces connecting M_L and M_R cannot be arbitrarily chosen. Now we work out the condition the connecting hypersurfaces should satisfy. By a lapse function N and a shift vector N^i, the extrinsic curvature of Σ is defined as

$$K_{ij}=-\frac{1}{2N}\left(\frac{\partial h_{ij}}{\partial \tau}-D_{(i}N_{j)}\right), \tag{1}$$

in the Riemannian manifold, where τ is the time coordinate in this region, and it is defined as

$$K_{ij}=-\frac{1}{2N}\left(\frac{\partial h_{ij}}{\partial t}-D_{(i}N_{j)}\right), \tag{2}$$

in the Lorentzian manifold, where t is the time coordinate in this region. In these definitions, D_i is the covariant derivative with respect to h_{ij}. Since the time τ in M_R is analytically continued to the time t in M_L as $\tau=it$ at Σ, the analytical continuation of geometrical variables, h_{ij} and K_{ij}, requires vanishing K_{ij} and N_i at Σ. Hereafter the boundary hypersurfaces with vanishing extrinsic curvature will be called totally geodesic boundaries. Then on the connecting hypersurface, it must be totally geodesic.

For the sake of cosmological interest and simplicity, in the present article, we consider a vacuum space–time with a cosmological constant. If we further assume vanishing Weyl curvature, the space–time has a geometry with constant curvature. Thus the Riemannian tunneling manifold M_R becomes locally isometric to one of the following cases, S^4 (4-sphere), R^4 (4-plane), or H^4 (4-hyperboloid). In Ref. 5, however, it was proved that if a 4-manifold has two pieces of disconnected boundaries Σ_i and Σ_f, the space–time should violate the energy condition at some points. The energy condition states

$$R_{\mu\nu}V^{\mu}V^{\nu}>0 \tag{3}$$

for all vector V^{μ}. Therefore, we can exclude S^4 from our considerations of topology changing manifolds because the curvature of it is positive definite.

From the Gauss–Codazzi equation, the vanishing extrinsic curvature makes Σ_i and Σ_f also have constant curvatures (locally isometric to S^3, R^3, or H^3) if the 4-manifold has a constant curvature. To consider topology changes we need a variety of topologies. The Riemannian manifold locally isometric to R^4 does not satisfy this requirement because the topology of Σ is too restricted (see Ref. 8). On the other hand, since the variety of hyperbolic 3-manifolds (Riemannian manifolds locally isometric to H^3) is very rich, we will consider the Riemannian manifolds which are locally isometric to H^4. A vacuum space–time with a negative cosmological constant can serve our purpose. Then the main question we want to answer is: Can we construct a hyperbolic 4-manifold with totally geodesic boundaries Σ_i and Σ_f which have different topologies?

Mathematically, hyperbolic 4-manifolds are quotient manifolds of a 4-hyperboloid H^4 by discrete subgroups of its isometry group SO(4,1). The fundamental region of this quotient 4-manifold is a 4-polytope (four dimensional objects bounded by a collection of polyhedra) embedded into H^4. Intuitively, a quotient manifold means taking some copies of the fundamental regions with their faces identified pairwisely. If we need a 4-manifold with boundaries, some of the 3-faces of the fundamental regions should remain unidentified which form the 3-boundaries of the 4-manifold. Previously, some $(2+1)$-dimensional analog of this have been discussed.[3] Although it is more complicated in four dimensions, by similar procedures, we can determine the fundamental region and then the identifications of its 3-faces in hyperbolic geometry.[6]

B. Hyperbolic geometry and the Klein model

To give a hyperbolic, structure of four dimensional polytopes we embed them into H^4. In our constructions, we use an n-dimensional Klein model (projective model)[6] as the model of hyperbolic geometry. The n-Klein model is a model on an open n-disk

$$D^n=\{x^i\in R^n | x^i x_i<1\}, \tag{4}$$

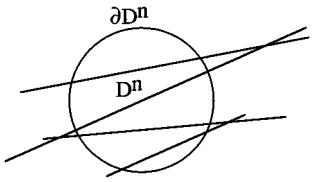

FIG. 2. A two dimensional example. There are some lines not intersecting each other inside the Klein model D^n. They are parallel lines and intersect outside the sphere at infinity ∂D^n.

in which a metric is

$$ds^2=\frac{1}{1-r^2}\left(\frac{dr^2}{1-r^2}+r^2d\Omega_{n-1}^2\right). \tag{5}$$

As r goes to 1, one approaches a sphere at infinity ∂D^n. This metric gives a constant sectional curvature -1 and has a hyperbolic structure. Then this Klein model is isometric to the spatial hypersurface of the well-known n-dimensional open-universe ($k=-1$).

Here, we briefly review the important properties of this model. First, it is easy to find that all totally geodesic (extrinsic curvature vanishing) $m(<n)$-hypersurfaces are m-planes in this model. Then we can construct totally geodesic boundaries by connecting such m-planes. For example, if $m=n-1$, the m-planes bound a polytope. We know that each m-plane can be identified with another by the isometry SO(n,1) of H^n. By these identifications we shall construct quotient manifolds. A more important property arises when we consider ideal points outside the sphere at infinity ∂D^n. As depicted in Fig. 2, most of ''parallel'' $(n-1)$-planes, which do not intersect each other inside the Klein model D^n but intersect outside the sphere at infinity ∂D^n. For our purpose we consider situations in which some $(n-1)$-planes share only one point ''a'' outside the sphere at infinity. The $(n-1)$-planes form a pyramid with the vertex a. There ought to exist a special cone which is tangent to the sphere at infinity. There exists an (n-1)-plane which intersects the cone at the tangent points (exemplified in Fig. 3). The virtue of the Klein model is that this $(n-1)$-plane is orthogonal to all of the planes forming the pyramid.

These facts facilitate our procedure of construction of tunneling manifolds. As an example, we show a simple case of a 2-Klein model of H^2. In Fig. 4, two regular triangles are drawn in the 2-Klein model so that each vertex protrudes from D^2. As mentioned above, we can draw dotted lines which are orthogonal to the edges of the triangle and truncate off the vertices along these dotted lines. We call such a truncation a regular truncation. Gluing the triangles so that the labeled

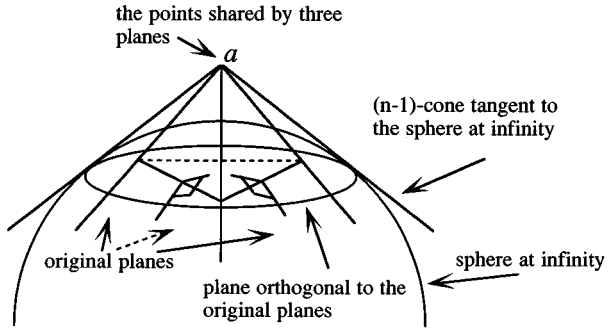

FIG. 3. Three planes share the point a outside the sphere. The cone with the vertex a, is tangent to the sphere at infinity. Then the plane through the tangent points is perpendicular to the three planes.

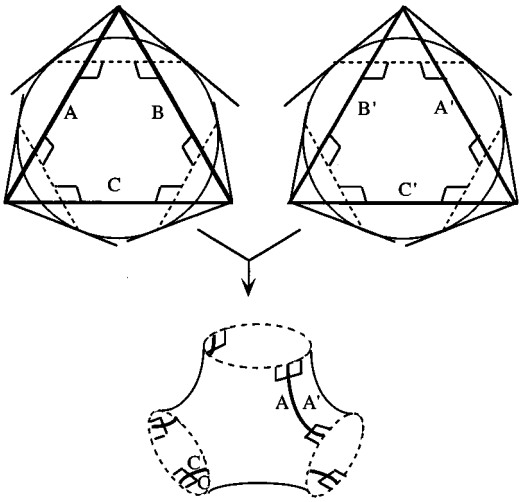

FIG. 4. Two hexagons made by regular truncations of triangles are glued. The resultant space is one of the simplest topology changing manifolds.

edges match each other, we get a hyperbolic manifold with three S^1 boundaries. Since the lines composing the boundaries are geodesic and orthogonal to the edges of the regular triangle, the boundaries become smooth totally geodesic S^1.[9]

Finally, we should remark upon the relation between the size of an object bounded by planes and the angles between these planes. In the hyperbolic geometry, if we enlarge the size of the object, the angles decrease. When the size approaches zero, the angles become the same values in Euclidean geometry. An angle on the sphere at infinity ∂D^n vanishes. We have no well-defined angle outside the sphere at infinity ∂D^n.

C. Four dimensional polytopes

First we prepare regular truncated 4-polytopes in the 4-Klein model of hyperbolic 4-space H^4. Regular 4-polytopes are 5-cell, 8-cell, 16-cell, 24-cell, 120-cell, and 600-cell.[10] For example, ''5-cell'' means that there are five congruent polyhedra which bound the 4-polytope. We shall consider large polytopes in the 4-Klein model in the following sense:

(1) All the vertices are outside of the sphere at infinity.
(2) Each edge of polytopes has intersection with the sphere at infinity.

The above conditions guarantee that a single ideal vertex shared by 3-planes which are cells (polyhedra) bounding the polytope can be regularly truncated off. As a generalization of the discussion in the last subsection, to a vertex, there is a unique 3-plane which is perpendicular to the polyhedra bounding the polytope. Also as mentioned in the previous subsection, the dicellular angle (the angle between two adjacent polyhedra in a 4 dimensional space) decreases as the size of the polytope increases in the hyperbolic geometry. To produce a regular and smooth structure after gluing of polytopes, we choose the size of the polytope to make dicellular angles become $2\pi/n$ (n is an integer). Then the size of the polytopes are restricted further to some discrete values. From a geometrical calculation we can find the allowed dicellular angles of the polytopes. The allowed polytopes are shown in Table I.

The first column gives the names of polytopes and the second column the polyhedra which bound the polytope. Allowed dicellular angles are shown in the third column. The fourth column shows polyhedra produced by regular truncations. The solid angles of these polyhedra at their

TABLE I. The first column is the name of polytopes, which are bounded by the polyhedra on the second column. The third column gives possible dicellular angles. After regular truncation, there appear new polyhedra shown in the fourth column whose vertices have a solid angle on the fifth column.

Polytope	Bounding polyhedra	Dicellular angle	Polyhedra made by truncation	Solid angle around the vertices
5-cell	5 tetrahedra	$\pi/3$	5 tetrahedra	0
8-cell	8 hexahedra	$\pi/3$	16 tetrahedra	0
16-cell	16 tetrahedra	$\pi/2$	8 octahedra	0
24-cell	24 octahedra	$2\pi/5$	24 hexahedra	$4\pi/20$
	24 octahedra	$\pi/3$	24 hexahedra	0
120-cell	120 dodecahedra	$\pi/3$	600 tetrahedra	0
600-cell	600 tetrahedra	$2\pi/3$	120 icosahedra	$4\pi/12$

vertices are in the fifth column. Here, it should be noted that the edges of the polytope are tangent to the sphere at infinity except for the cases of a 24-cell with a dicellular angle $2\pi/5$ and a 600-cell with a dicellular angle $2\pi/3$. Therefore, in most situations, vertices made by the truncation are on the sphere at infinity. (This aspect is reflected in the fifth column since the vertices at infinity have vanishing solid angles.) In these cases, the truncated polytopes are of course noncompact (exemplified for the case of 8-cell in the next section). Calculating the volume, however, in the next section, we find that their volumes are finite. In the present article, we only consider these noncompact cases. By allowing the points at infinity, the construction of the tunneling manifold becomes much easier. Because a constructed object is required to be a manifold, we should consider completeness of the construction which gives a restriction at every vertex generally. However, in the special cases with vertices on the sphere at infinity, these restrictions do not exist.

In the next section we shall demonstrate some examples of constructions of Riemannian manifolds which describe topology changing processes. One of such Riemannian manifolds is constructed from 12 8-cells which are 4-polytopes bounded by eight congruent hexahedra. The development of such an 8-cell on 3-space is shown in Fig. 5. Gluing faces in four dimensions according to the arrows in Fig. 5, we get a 4-dimensional polytope bounded by these eight hexahedra, which has 16 vertices.

III. RIEMANNIAN MANIFOLDS WITH TOTALLY GEODESIC BOUNDARIES

A. Construction from an 8-cell

We can adjust the size of the embedded 8-cell so that all the dicellular angles are $\pi/3$. Then we can show that all vertices are located outside the sphere at infinity ∂D^4. This 8-cell satisfies the two conditions given in the previous section. The edges of the 8-cell are coincidentally tangent to

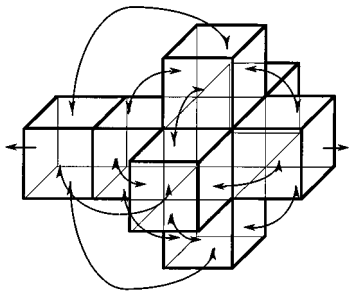

FIG. 5. The development of an 8-cell. Gluing the faces of the hexahedra along the arrows in four dimensions, we get the 8-cell of a 4-dimensional polytope.

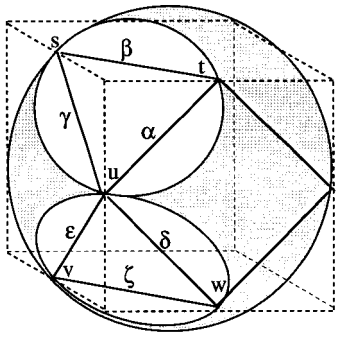

FIG. 6. The shaded sphere is a sphere at infinity in the 3-Klein model. Each edge of the hexahedra is tangent to the sphere at $s,t,u\cdots$. The sphere is cut by planes through $s,t,u\cdots$. Along these planes we truncate the vertices of the hexahedron.

the sphere at infinity. Each hexahedron of the 8-cell is embedded into an induced 3-Klein model (sub-model of the 4-Klein model) as shown in Fig. 6. In this three dimensional figure, all vertices are also outside the sphere at infinity ∂D^3 and all edges are tangent to the sphere.

To get smooth totally geodesic boundary hypersurfaces, we truncate every vertex of the 8-cell in an analogous way as we did in the 2-dimensional example in Sec. II B. Let us pay attention to the four hexahedra having a vertex in common in Fig. 5. The property of the Klein model guarantees the existence of a unique 3-hyperplane which is perpendicular to all of the four hexahedra as mentioned in the previous section. In this way we cut out the regions near the 16 vertices of the 8-cell by these perpendicular 3-hyperplanes to get a regular truncated 8-cell embedded completely in the 4-Klein model. The truncation of 8-cell induces truncation on every hexahedron bounding the 8-cell. The resultant hexahedron is shown in Fig. 6. On each hexahedron the truncation of the vertex of the 8-cell makes a triangle with its vertices on the sphere at infinity ∂D^3. It is noticed that the triangles share vertices with adjacent triangles [for example, the vertex (u) is shared by the two adjacent triangles Δstu and Δuvw in Fig. 6]. In this case, any edge of the original hexahedron can be completely truncated off by the two truncations of the two adjacent vertices connected by the edge (see Fig. 6).

Because four hexahedra share one vertex in an 8-cell (see Fig. 7), each 3-boundary of the

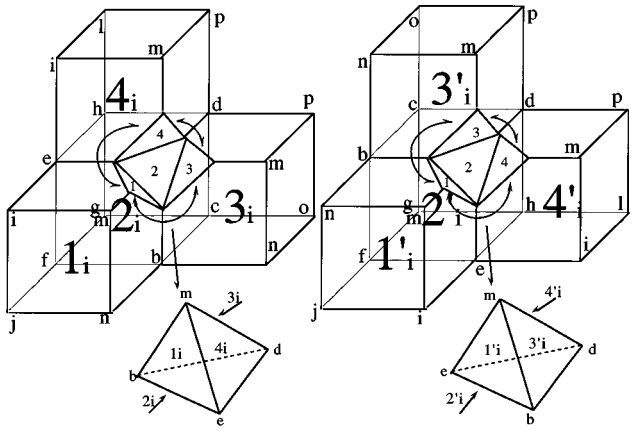

FIG. 7. A part of the 8-cell in Fig. 5. Four hexahedra meet at a vertex. When we truncate the vertex, a tetrahedron appears. We label the faces and the vertices of the tetrahedra at the vertices (a) by the index number of the cell which the face belongs to and the vertices of the 8-cells on the opposite side of (a), respectively.

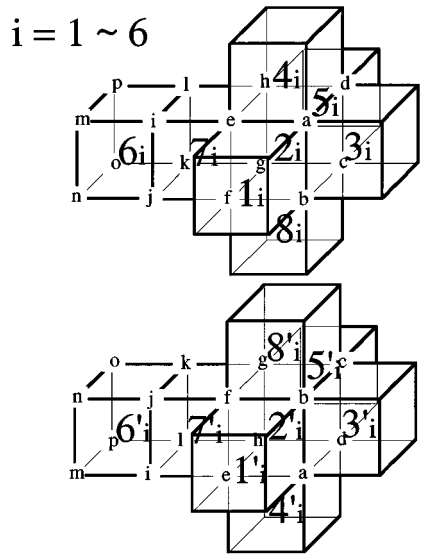

FIG. 8. Two types of 8-cells. Upper ones are left-handed while lower ones (with primes) are right-handed. The corresponding cells with the same number which are primed and unprimed are identified (for example, 1_1 and $1_1'$, 4_1 and $4_3'\cdots$).

8-cell made by the truncation of a vertex is bounded by four triangles. From Fig. 7 we see that the 3-boundary is a tetrahedron whose vertices are on the sphere at infinity. (To the cases of other 4-polytopes, see the fourth column of the Table I). Since each tetrahedron is orthogonal to the hexahedra in the hyperbolic 4-space, the dihedral angle of the tetrahedron, which equals the dicellular angle of the 8-cell, is $\pi/3$. The volume integration tells us that such tetrahedra have finite volumes[6] though they are noncompact. A single 8-cell includes 16 vertices and therefore has 16 tetrahedra as the boundary after regular truncations.

The next step is to find a certain gluing of appropriate number of regular truncated hyperbolic 8-cells by identifying the hexahedra, so that the resultant space becomes a smooth manifold and the collection of the tetrahedra produced by regular truncations form smooth 3-boundaries of the manifold. In mathematical language, we want to find a discrete subgroup of the isometry group SO(4,1) so that the quotient space of H^4 by the discrete subgroup is a manifold. First, we would like to try a generalization to four dimensions of what was illustrated in the simple two dimensional example and see whether a manifold can be formed or not. Below is an example of the trial.

We prepare two regular truncated 8-cells and put them in the position so that they have a reflection symmetry as depicted in Fig. 8. Gluing the hexahedra $X(=1\text{–}8)$ and $X'(=1'\text{–}8')$ so that all vertices $(a)\text{–}(p)$ match, we get a 4-space with 16 boundary components. To make sure smoothness of this 4-space in terms of hyperbolic geometry, it is sufficient to check the smoothness on the boundaries since the dicellular angles of the 8-cell equal the dihedral angles of the tetrahedra on the boundaries. The inside of a truncated hyperbolic 8-cell is smooth and regular. We can nicely glue the two hexahedra in four dimensions because the hexahedra are totally geodesic. Therefore, singular structures possibly appear only on the faces, edges and/or vertices of each hexahedron. From Fig. 6 we see that the singularity should appear on the boundary tetrahedra if any. The gluing of the hexahedra induces the gluing on the boundary tetrahedra. Fig. 7, for example, shows that the gluing of two tetrahedra corresponding to the vertex (a) both in the unprimed and primed 8-cells is determined by the identifications of the truncated hexahedra around the vertex (a). Since each unprimed hexahedron is identified with its primed partner, every face of unprimed tetrahedron is glued with its primed partner so that all vertices match. In this

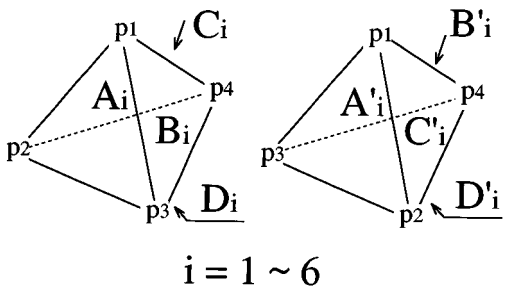

FIG. 9. Six unprimed tetrahedra and six primed tetrahedra. Twelve tetrahedra constitute $M_B 8$.

configuration, the topology of this space composed of the two tetrahedra is S^3. Nevertheless, we have only $2\pi/3$ turning around each edge of the tetrahedra after gluing, since only two edges of the tetrahedra with the dihedral angle $\pi/3$ are identified into one edge. This means a singularity by the deficit angle $2\pi-2\times\pi/3=4\pi/3$. Therefore, we fail to get a smooth manifold by a simple minded generalization of the 2-dimensional example in the previous section.

However, there is a way to improve the construction so that we can get a neat manifold, i.e., without a deficit angle. We consider a branched covering space of this singular space. The appropriate branched covering space can be given by a sixfold cover (12 tetrahedra) of the original singular space. The faces and vertices of the twelve tetrahedra are labeled as Fig. 9 ($i=1$–6). The following pairs of the faces of unprimed and primed tetrahedra are glued so that all labeled vertices match:

$$
\begin{aligned}
&A_1-A_1'B_1-B_3'C_1-C_2'D_1-D_4', \quad A_2-A_2'B_2-B_1'C_2-C_4'D_2-D_3',\\
&A_3-A_3'B_3-B_2'C_3-C_5'D_3-D_6', \quad A_4-A_4'B_4-B_6'C_4-C_1'D_4-D_5',\\
&A_5-A_5'B_5-B_4'C_5-C_6'D_5-D_1', \quad A_6-A_6'B_6-B_5'C_6-C_3'D_6-D_2'.
\end{aligned}
\tag{6}
$$

For instance, A_1 is matched with A_1'. All the vertices p_1,p_2,p_3 of A_1 are identified to the vertices p_1,p_2,p_3 of A_1', respectively.

Figure 10 shows consistency of the gluing around every edge. There are twelve edges in the sixfold covering space after the gluing. There are six dihedral angles which meet at one edge so that there is no deficit angle since each dihedral angle is $\pi/3$.

On the other hand, the vertices of the tetrahedra are on the sphere at infinity ∂D^3. By the gluing, these vertices are identified into four points at infinity, p_1,p_2,p_3,p_4. Such points at infinity are called cusps in the hyperbolic geometry. They are not singularities of the manifold but open boundaries at infinity.[6] Topologically a cusp looks like a torus crossing a half-open interval (see Fig. 11). The boundary space composed of twelve tetrahedra is a noncompact smooth manifold, which is called M_{B8} in the present paper.

The cusp will not cause any serious physical problem because one cannot observe the infinity of the universe. On the contrary, the existence of such structures at infinity renders the manifold of primary importance. It is a known fact in mathematics that there is a family of almost isometric compact manifolds limiting a cusped manifold.[11] It is expected that the limiting cusped manifold shares common characters of the family. Furthermore, the cusped manifold is the simplest one among the family in some sense. Hence, admitting the cusp to our manifold, we get the following simplest example of topology changing of space–time by quantum tunneling.

Now we expect that the branched covering proceeded above can be straightforwardly extended to the whole of 8-cells. Since the sixfold cover of the boundary 3-space produced by the simple minded identification is the smooth 3-manifold M_{B8}, the sixfold cover of the 4-space

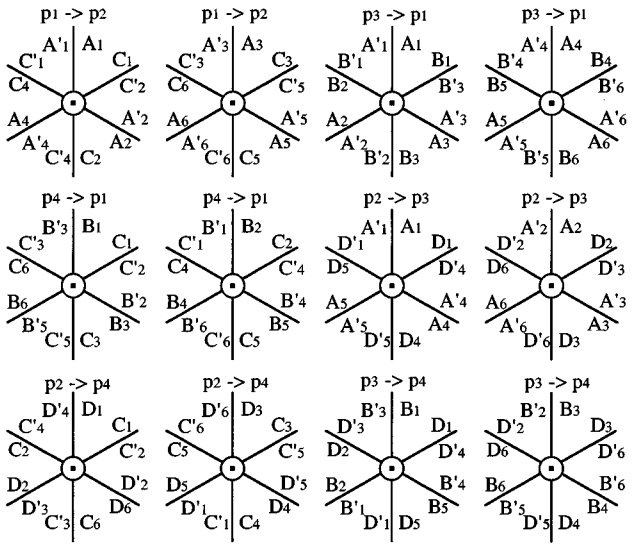

FIG. 10. The consistency check of the manifold which is composed of the tetrahedra in Fig. 9 with the rule of Eq. (6). Six dihedral angles meet at the edges in Fig. 9. Since each dihedral angle is $\pi/3$, there is no deficit angle.

produced by the simple minded identification will have smooth boundary manifolds, M_{B8}s. We prepare six pairs of unprimed and primed 8-cells as Fig. 8 (the pairs are labeled by $i=1$–6). Every vertex and cell (hexahedron) of the 8-cells are also labeled in Fig. 8. All subsequent gluings will be done so that these labeled vertices are matched. We determine the gluing of hexahedra around each vertex (a) of 8-cells (cell 1_i–cell 4_i, so that they induce gluing (6) on a tetrahedron made by the truncation of the vertex (a) to form M_{B8}. Figure 7 shows the tetrahedron by the truncation of each vertex (a). In this figure, each face of a tetrahedron is labeled by an index of the cell which the face belongs to, and each vertex of the tetrahedron is labeled by the same character as that of the nearest vertex of the hexahedron.

From Figs. 7 and 9 we find a correspondence, $1_i \equiv A_i$, $4_i \equiv B_i$, $3_i \equiv C_i$, $2_i \equiv D_i$. By Eq. (6), the gluing of the hexahedra, which constructs M_{B8} from the tetrahedra produced by the truncation of the vertex (a) are the following:

$$1_1-1_1'4_1-4_3'3_1-3_2'2_1-2_4', \quad 1_2-1_2'4_2-4_1'3_2-3_4'2_2-2_3',$$
$$1_3-1_3'4_3-4_2'3_3-3_5'2_3-2_6', \quad 1_4-1_4'4_4-4_6'3_4-3_1'2_4-2_5', \tag{7}$$

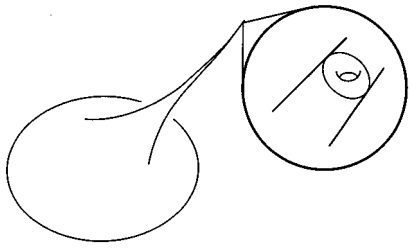

FIG. 11. An intuitive picture of a cusped hyperbolic manifold. The cusp topologically looks like a torus cross a half-open interval.

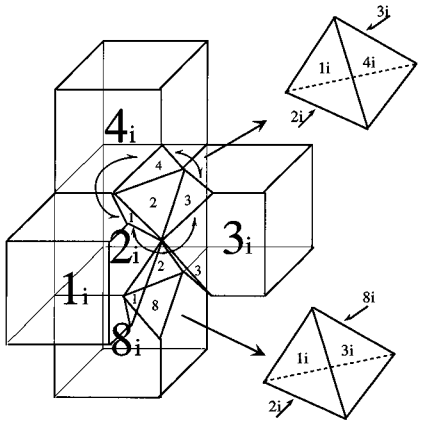

FIG. 12. If we treat 8_i as if it were 4_i, a tetrahedron from vertex (a) and a tetrahedron from vertex (b) would be symmetric under the inversion.

$$1_5-1_5'4_5-4_4'3_5-3_6'2_5-2_1', \quad 1_6-1_6'4_6-4_5'3_6-3_3'2_6-2_2'.$$

It is a nontrivial problem to determine whether it is possible or not for the tetrahedra produced by the truncations of the other vertices $(b)-(p)$ to form M_{B8}s by appropriate choices of gluing of the other cells (cell 5–cell 8). Determining the other gluings as shown below, we can see that two adjacent tetrahedra, e.g., formed by the truncations of vertices (a) and (b) (see Fig. 12), are symmetric under the inversion because of the symmetry of the 8-cell

$$\begin{aligned}
&5_1-5_1'8_1-8_3'7_1-7_2'6_1-6_4', \quad 5_2-5_2'8_2-8_1'7_2-7_4'6_2-6_3',\\
&5_3-5_3'8_3-8_2'7_3-7_5'6_3-6_6', \quad 5_4-5_4'8_4-8_6'7_4-7_1'6_4-6_5',\\
&5_5-5_5'8_5-8_4'7_5-7_6'6_5-6_1', \quad 5_6-5_6'8_6-8_5'7_6-7_3'6_6-6_2'.
\end{aligned} \tag{8}$$

Since the inversion of one M_{B8} gives another M_{B8}, each group of 12 tetrahedra forms one M_{B8} at each vertex $(b)-(p)$. Therefore, the glued twelve 8-cells have 16 M_{B8}s on their boundary. Here, a fact should be noticed that the tetrahedra are orthogonal to the cells (hexahedra) of the 8-cell, which guarantees that the M_{B8} is smooth at the points at which the tetrahedra join. Then M_{B8} on the boundary is a totally geodesic smooth manifold in H^4.

Of course, these identifications are orientation preserving isometry transformation because of the reflection symmetry between the unprimed and primed 8-cells. The resultant space is orientable.

To check that this 4-space is a complete smooth 4-manifold, we consider the neighborhood of the faces, edges and vertices. In four dimensions, when we turn around each face completely, the total angle should be 2π for consistency. We shall check this consistency on the boundary of it. On the boundary 3-hypersurface, we should check whether it is 2π or not around the edges (α,β,γ... in Fig. 6) of the tetrahedra. This consistency is guaranteed by our previous analysis where we have shown that the boundary consists of several pieces of the manifolds M_{B8} (see Fig. 10). The remaining vertices after the regular truncation (s,t,u... in Fig. 6) cause no problem since they form 4-cusps at infinity. Hence this space is a complete smooth non-compact hyperbolic 4-manifold with totally geodesic 3-boundaries. The boundaries are sixteen M_{B8}s.

B. Other solutions

As shown in Table I, there are seven kinds of 4-polytopes admitting regular truncations. Geometrical calculations reveal that two of them, 24-cell with a dicellular angle $2\pi/5$ and 600-cell with a dicellular angle $2\pi/3$, are compact and the others are noncompact after regular truncations. We can apply our method for the 12 noncompact 8-cells to these noncompact cases. By a similar method, we can successfully get complete smooth hyperbolic 4-manifolds with totally geodesic 3-boundaries in the two cases. One of them is the case of a 16-cell (bounded by 16 tetrahedra) with a dicellular angle $\pi/2$ and the other is the case of a 24-cell (bounded by 24 octahedra) with a dicellular angle $\pi/3$. Four 16-cells form a manifold whose 3-boundaries are eight M_{B16}s (we consider a twofold cover of a simple minded identifications), where an M_{B16} with six cusps is composed of four octahedra. Similarly, 6 24-cells also constitute a manifold whose 3-boundaries are 24 M_{B24}s (we consider a threefold cover of a simple minded identifications), where an M_{B24} with eight cusps is composed of six hexahedra.

Here, we would like to point out a peculiarity of the hyperbolic manifold by referring to a mathematical fact. For three or four dimensional hyperbolic manifold $M_{3,4}$, the fundamental group $\pi_1(M_{3,4})$ determines $M_{3,4}$ uniquely up to an isometry and a choice of normalizing constants.[12] This has been known as the Mostow rigidity. Then it is sometimes sufficient to determine the homology group H_1 of the hyperbolic manifold in order to distinguish the manifolds, where H_1 is an Abelian group such that $H_1=\pi_1/[\pi_1,\pi_1]$. To characterize the boundaries topologically we calculate the corresponding homology groups,[13]

$$H_1(M_{B8})=Z+Z+Z+Z; \tag{9}$$

$$H_1(M_{B16})=Z+Z+Z+Z+Z+Z; \tag{10}$$

$$H_1(M_{B24})=Z+Z+Z+Z+Z+Z+Z+Z. \tag{11}$$

Clearly they are topologically inequivalent. Since the rank of the free finite Abelian group part of H_1 counts the number of two dimensional holes,[13] M_{Bn} has a more complicated topological structure than M_{Bm} has if $n>m$. On the other hand, the torsion-free property may be considered as a pleasant feature of the universe because otherwise the universe might be non-orientable. If we had a method which can produce a solution whose boundaries have torsion part, much more solutions could be found.

Incidentally, it is impossible to construct a solution from 5-cells or 120-cells in our way. The remaining regular truncated polytopes are compact. In the compact case, we should check consistency also around the vertices of the regular truncated polytopes. However, it is too complicated for us to work out this consistency check and we need more advanced techniques. This is our project in future.[14]

IV. TOPOLOGY CHANGING AMPLITUDE AND STRONG RIGIDITY

We have constructed three hyperbolic 4-manifolds with totally geodesic boundaries. From Gibbons and Hartle[5] and Siino *et al.*,[3] these manifolds can be regarded as instantons causing topology changes by quantum tunneling. For example, the manifold of 12 8-cells can describe the topology changes: ''from nothing to sixteen M_{B8}s,'' ''from one M_{B8} to fifteen M_{B8}s'' or ''from two M_{B8}s to fourteen M_{B8}s,'' and so on (see Fig. 13). It is also worthy of notice that by plumbing them we can get infinite series of topology changing solutions as exemplified in Fig. 13. Since each boundary is totally geodesic, the gluing is perfect to make a neat manifold when we identify two boundary components of the same shape and size.

We have demonstrated topology changing processes between nontrivial spatial topologies in four dimensions by quantum tunneling, which cannot be reduced to a lower dimensional subspace. Brill constructed a 4-dimensional topology changing solution which, in fact, is effectively a direct

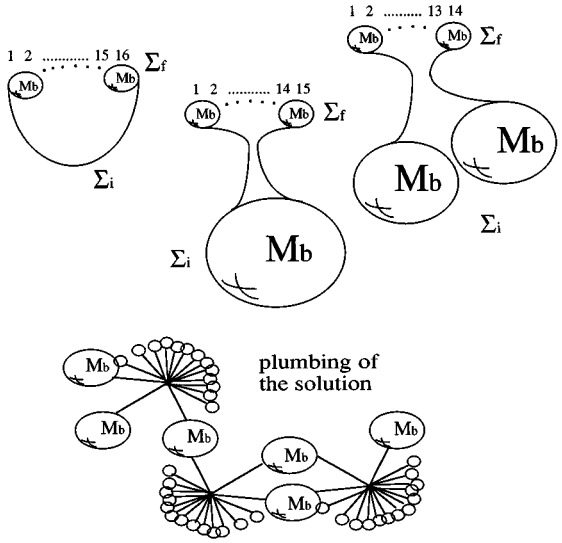

FIG. 13. A Riemannian manifold with 16 boundaries is regarded as a topology change solution ''from nothing to sixteen M_{B8}s'' ''from one M_{B8} to fifteen M_{B8}s,'' or ''from two M_{B8}'s to fourteen M_{B8}s,'' and so on. Furthermore, by plumbing of the solution we can obtain various types of topology change solutions.

product of a topology changing two dimensional space–time and the other two dimensional space.[9] Of course, the pair creation of charged black holes,[15] in an extended sense, is also a process of topology change. The Riemannian manifold for that process has a single totally geodesic 3-boundary which can be interpreted as a topology change from ''nothing'' to the space containing a pair of black holes. However, the present paper gives descriptions of processes which include not only the creation of the universe from ''nothing'' but also the change from n M_B to m $M_B (n \neq m)$. Both of initial and final spatial hypersurfaces (Σ_i and Σ_f) have nontrivial topologies.

Now let us evaluate the tunneling amplitude for these topology changes. In the context of the Hawking's Riemannian path integral, the amplitude can be formally described as

$$T(h_i, h_f) = \sum_{M_R} \int \mathscr{D}g \, \exp(-S_E[g]), \tag{12}$$

where h_i and h_f are the 3-dimensional metrics on the initial and final spatial hypersurfaces Σ_i and Σ_f, respectively. S_E is the Euclidean action,

$$S_E = -\frac{1}{16\pi G} \int_{M_R} (R - 2\Lambda) \sqrt{g} d^4x + \frac{1}{8\pi G} \int_{\partial M_R} K \sqrt{h} d^3x. \tag{13}$$

The path integral is over smooth 4-metric g on the Riemannian manifold M_R which has appropriate boundaries Σ_i and Σ_f by assumption. In our cases, M_R is one of the 4-manifolds which have been constructed in the previous section. Then we can evaluate the path integral (12) in the WKB approximation for the topology changing processes. The second term comes from the contribution of the boundaries other than $\Sigma_{i,f}$, namely, that of the open boundaries at the cusps. It is easy to see by explicit calculation that K vanishes at the cusps. Since our solution has a constant negative curvature $R = 4\Lambda < 0$, the classical action S_E is proportional to the 4-volume of the space–time and is given by

TABLE II. The topology changing manifolds that we have constructed. The first column is the polytope we have used. The resultant manifolds have the boundaries on the second column whose homology group H_1 are shown in the third column. The volume of solutions are displayed on the fourth column.

Building block	Boundary $\Sigma_{i,f}$	$H_1(\Sigma)$	The volume of solutions
8-cell×12	$16\times M_{B8}$	$Z+Z+Z+Z$	$\frac{4\pi^2}{3}\times 12$
16-cell×4	$8\times M_{B16}$	$Z+Z+Z+Z+Z+Z$	$\frac{4\pi^2}{3}\times 4$
24-cell×6	$24\times M_{B24}$	$Z+Z+Z+Z+Z+Z+Z+Z$	$\frac{4\pi^2}{3}\times 30$

$$\overline{S_E}=\frac{1}{8\pi G}\frac{V}{|\Lambda|}, \tag{14}$$

where V is a numerical value of the volume of M_R in the case of $\Lambda=-3$. It follows from Eq. (14) that the WKB approximation of the tunneling amplitude is exponentially suppressed for a tunneling manifold of a large volume. Then we intuitively expect that the topology change between more complicated topologies requires a larger volume of tunneling manifold and is more suppressed provided that the WKB prefactors are of the same order.

Though our manifolds have cusps, their volumes are finite. Following Kellerhals,[16] the hyperbolic volumes of the 4-polytopes that we have used are calculated as

$$\text{Volume(truncated 8-cells)}=\frac{4\pi^2}{3}, \tag{15}$$

$$\text{Volume(truncated 16-cells)}=\frac{4\pi^2}{3}, \tag{16}$$

$$\text{Volume(truncated 24-cells)}=\frac{20\pi^2}{3}, \tag{17}$$

and the volume of the manifolds are summarized in Table II.

The volume of a constant curvature space is given by the Gauss–Bonnet theorem,[17]

$$\chi(M)=\frac{1}{32\pi^2}\int_M \epsilon_{abcd}\mathscr{R}^{ab}\wedge\mathscr{R}^{cd}-\frac{1}{32\pi^2}\int_{\partial M}\epsilon_{abcd}\left(2\theta^{ab}\wedge\mathscr{R}^{cd}-\tfrac{4}{3}\theta^{ab}\wedge\theta^c_e\wedge\theta^c_e\wedge\theta^{ed}\right), \tag{18}$$

where $\mathscr{R}^{ab}$ and θ^{ab} are the curvature 2-form and the second fundamental form. Since the boundary ∂M is totally geodesic, θ^{ab} vanishes there. The Euler numbers $\chi(M)$ are combinatorially determined as

$$\chi(\text{tunneling manifold consisting of 12 8-cells})=12, \tag{19}$$

$$\chi(\text{tunneling manifold consisting of 4 16-cells})=4, \tag{20}$$

$$\chi(\text{tunneling manifold consisting of 6 24-cells})=30, \tag{21}$$

and agree with Eq. (18) and the volumes given in Table II.

Roughly speaking, more polytopes are needed to get a manifold with a more complicated topological structure. Then we expect that the volumes are largely related to the topological structure (just the Euler number in a constant curvature space). The larger volume will imply a

more complicated topological structure. Now let us recall one of the peculiarities of the hyperbolic manifold, Mostow rigidity. For three or four dimensional hyperbolic manifold $M_{3,4}$, the fundamental group $\pi_1(M_{3,4})$ determines $M_{3,4}$ uniquely up to an isometry and a choice of normalizing constant.[12] Therefore, our tunneling manifolds include no degrees of freedom of deformation[8] as long as the manifold is hyperbolic. If we include nonzero Weyl curvature, the manifold can become inhomogeneous and the degrees of freedom of deformation becomes dynamical. In such a situation, the quantum theory of the dynamical degrees of freedom have to be developed for a quantum topology change theory.

V. SUMMARY AND DISCUSSIONS

In the present paper, we have found instantons which describe topology changing processes by quantum tunneling of spatial hypersurfaces of space–times which are locally anti-de Sitter. Here we summarize our results in the Table II.

It may be intuitively expected that the more complicated is the topology of the universe which topologically changes, the larger is the volume of the tunneling manifold. Let us investigate whether this is the case in our examples. From Table II, however, we cannot easily draw a conclusion directly since the number of boundary manifolds are different. Quantitatively, we can compare a set of three topology changing manifolds with $16\times M_{B8}$, a set of six topology changing manifolds with $8\times M_{B16}$ and a set of two topology changing manifolds with $24\times M_{B24}$. All the sets have 48 boundaries though they are not arcwise connected. Then the corresponding manifolds have volumes $48\pi^2$, $32\pi^2$, and $80\pi^2$, respectively. The result is just not what we expected. Although the third one is much larger than the other two, which means that M_{B24} is more unlikely to appear comparing to the other two, the first one and the second one are comparable. What is more, the probability for the first one to appear is smaller than that for the second one. Since $H_1(\Sigma)$ characterizes the topological structure of Σ by Eqs. (9), (10), and (11), the boundary of the first one is simpler than that of the second one. However, their volumes imply that the topology of the first one is more complicated than the topology of the second one. Nevertheless, we cannot conclude that the tunneling of M_{B16} has the maximum of probability. There might be a smaller manifold describing the topology change of M_{B8}s. If we could find the relation between the volume of the solution (the Euler number) and the boundary of it, the relation would explain this.

One might think that our constructions are too restricted. First, the identification is determined so as to preserve the symmetry of the polytope. Second, the resultant polytopes are identical with each other. From these restrictions, for example, one cannot consistently identify the polyhedra which bound a single polytope. Our restrictions made the construction simple. However, it may well be the case that there are much more solutions which have been ruled out by the restrictions. To complete the discussion about the topology change by quantum tunneling, we should relax these restrictions. Then the structure of the tunneling manifold becomes more involved. Constructing such complicated cases will need the aid of computer.

When we evaluate the topology changing amplitude, the formalism of Hartle and Hawking has been used. However, the exact no-boundary condition in the original formalism of Hartle and Hawking does not allow the existence of boundary at infinity. In our solutions, the tunneling manifolds have cusped boundaries at infinity. Since the cusped boundaries are infinitely small and the manifolds have finite volumes, we may generalize the formalism of Hartle and Hawking to such a case. If we stick to impose the no-boundary condition in a strict sense, we need compact tunneling manifolds. An investigation in this direction is also in progress.[14]

People might be disturbed by the existence of the cusps. If we study the effect of ''matter fields'' or fluctuations of the metric (''one-loop corrections''), the boundary conditions at the cusps are needed. The conditions and the effects will be studied in appropriately simplified situation.[18] Furthermore, some people might insist that the cusps do not allow one to use Einstein–Hilbert action and the idea of a smooth manifold in this arbitrary small scale. A calculation in the $(2+1)$-dimensional gravity will reveal something about this as a simplified case. On the other

hand, it observationally causes no problem since the cusps are at infinity and we cannot ''see'' them. We see only the pattern of spatial periodicity.[19] If we observe the pattern of the spatial periodicity as the super large scale structure of the universe, we may be able to determine the topology of our universe and to know whether the universe has the cusps or not.

In the case of the topology change in $(2+1)$-dimensional quantum tunneling, the rigidity of the hyperbolic manifold is easier to understand. While hyperbolic 2-boundaries have moduli parameters as the dynamical degrees of freedom, the tunneling manifolds do not allow any deformation corresponding to them, which is consistent with the rigidity. In four dimensional case, however, the situation is different because the 3-boundary is also rigid as well as the tunneling manifold itself. The dynamical degrees of freedom will appear only when we allow nonzero Weyl curvature. In such a case the gravitational degrees of freedom should be considered. As a first step we can consider the linear perturbation of them. If we quantize these degrees of freedom, we expect particles be created. This might cause a quantum instability of topology changing solutions if the backreaction to the space–time is too large.

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Einstein's equations in the presence of signature change

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We discuss Einstein's field equations in the presence of signature change using variational methods, obtaining a generalization of the Lanczos equation relating the distributional term in the stress tensor to the discontinuity of the extrinsic curvature. In particular, there is no distributional term in the stress tensor, and hence no surface layer, precisely when the extrinsic curvature is continuous, in agreement with the standard result for constant signature. © *1996 American Institute of Physics.* [S0022-2488(96)02611-4]

I. INTRODUCTION

Classical cosmological models containing an initial region of Euclidean signature joined to a final region with the usual Lorentzian signature were introduced by Ellis *et al.*[1,2] A basic feature of this work is the use of the Darmois junction conditions at the surface where the signature changes. This assumption has been questioned by Hayward,[3] who prefers to assume the stronger conditions appropriate for quantum cosmology. We argue here in favor of the Darmois approach by *deriving* these junction conditions from the Einstein-Hilbert action.

What are Einstein's equations in the presence of signature change? Formal computation quickly goes astray: A signature-changing metric is necessarily degenerate at the hypersurface of signature change. The Geroch-Traschen conditions[4] for the existence of a distributional curvature tensor thus fail to be satisfied, and it is not clear whether a preferred connection exists. Supposing that a suitable distributional connection is available, the distributional curvature tensor could be readily constructed, but it would still be unclear at best how to reverse its trace with the degenerate metric to obtain a distributional Einstein tensor.

We adopt instead a variational approach, and begin with the natural generalization of the Einstein-Hilbert action to signature change, subtracting the standard surface term used in the nondegenerate case in the presence of boundaries. We choose to work with a discontinuous metric, as this permits the introduction of a frame which is orthonormal almost everywhere. Having made these choices, we find that the variations proceed unchanged from the degenerate case, and we recover the identical result: The Darmois conditions (continuity of the extrinsic curvature) ensure the absence of a surface layer, and the Lanczos equation relates the discontinuity of the extrinsic curvature to the surface stress tensor. The former result agrees with one of Embacher's variational principles;[5] the latter result is new.

The paper is organized as follows. In Section II we introduce the necessary notation for dealing with signature change, and introduce the concept of an ''almost'' orthonormal frame. In Section III we review the standard Einstein-Hilbert variational principle for Einstein's equations, showing that the usual derivation applies without change. Finally, in Section IV we discuss our results.

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II. NOTATION

Let Σ be a (smooth) hypersurface in a smooth n-dimensional manifold M which divides M into disjoint open regions $M^\pm$ with smooth, nondegenerate metric tensors $g^\pm$. We will assume that the limits $g^\pm|_\Sigma$ exist, and that the pullbacks of $g^\pm|_\Sigma$ to Σ agree. The common pullback is the induced metric on Σ, which will be further assumed to be nondegenerate and which will be denoted by h. In particular, we are assuming that Σ is not null.

A tensor field F is said to be *regularly discontinuous*[6,7] if F is continuous on $M^\pm$ and if the one-sided limits,

$$F^\pm|_\Sigma = \lim_{\to\Sigma^\pm} F, \tag{1}$$

exist. The *discontinuity* of F is the tensor on Σ defined by

$$[F]_\Sigma = F^+|_\Sigma - F^-|_\Sigma . \tag{2}$$

Note that F itself need only be defined on $M^\pm$. In the *continuous metric* approach, one assumes that $[g]_\Sigma = 0$; this is the standard assumption for constant signature. If the signatures of $g^\pm$ differ, $g^\pm|_\Sigma$ will necessarily be degenerate ($\det g^\pm|_\Sigma = 0$) in this approach, whereas for constant signature one can also assume that $g^\pm|_\Sigma$ is nondegenerate. In the *nondegenerate metric* approach, one instead assumes that $g^\pm|_\Sigma$ are not degenerate. If the signatures of $g^\pm$ differ, this necessarily implies that $[g]_\Sigma \neq 0$; in this case, we will refer to this approach as the *discontinuous metric* approach. The two approaches are mutually exclusive in the presence of signature change, whereas for constant signature one normally makes both sets of assumptions.

Introduce an orthonormal (with respect to h) frame on Σ, i.e. a basis $\{\hat{e}^i, i = 1 \ldots n-1\}$ of 1-forms on Σ. In each of $M^\pm$ separately, we can extend this to a smooth orthonormal frame $\{e^a_\pm\} = \{e^0_\pm, e^i_\pm\}$ with $e^i|_\Sigma = \hat{e}^i$. We have $[e^i]_\Sigma = 0$ by construction, and we will further *assume* that $[e^0]_\Sigma = 0$. This can always be done in the continuous metric approach, although if the signature changes we have $e^0_\pm|_\Sigma = 0$. For discontinuous metrics, this is a further restriction on $g^\pm$, which amounts to assuming that both 1-sided notions of the unit normal vector to Σ are the same—which would imply continuity of the metric if the signature were constant—or equivalently that proper time/distance from Σ is a C^1 coordinate. Let $\{X^\pm_a\}$ denote the basis of vector fields on $M^\pm$ which is dual to $\{e^a_\pm\}$. Note that in the presence of signature change, $X^\pm_0$ will admit limits to Σ only in the discontinuous case.

Consider the separate Hodge dual operators defined by $g^\pm$ on $M^\pm$, both written as $*$, and the Hodge dual operator defined by h on Σ, written as $\hat{*}$. The metric volume element on Σ is

$$\hat{*}1 = e^1_\pm \wedge \cdots \wedge e^{n-1}_\pm, \tag{3}$$

and the metric volume elements on $M^\pm$ are

$$*1 = e^0_\pm \wedge e^1_\pm \wedge \cdots \wedge e^{n-1}_\pm, \tag{4}$$

which admit continuous limits to Σ by assumption. For discontinuous metrics, this provides the usual Leray decomposition,

$$*1 = e^0 \wedge \hat{*}1, \tag{5}$$

where e^0 here denotes the common limit of $e^0_\pm$ to Σ. However, in the continuous metric approach for a signature-changing metric, these limits are identically zero!

We therefore take the nondegenerate metric approach in the remainder of the paper, resulting in discontinuous metrics if the signature changes. We emphasize that this choice means that both

$$[e^0]_\Sigma = 0 = [X_0]_\Sigma\,, \tag{6}$$

so that there is a continuous ''orthonormal'' frame on all of M, which in turn defines a continuous, nondegenerate, volume element on all of M.

Metric-compatible connection 1-forms $\omega^a_{\pm b}$ on $M^\pm$ satisfy

$$dg_{ab} = \omega^m{}_a g_{mb} + \omega^m{}_b g_{ma}\,, \tag{7}$$

and have torsion

$$T^a = de^a + \omega^a{}_b \wedge e^b, \tag{8}$$

where we have dropped the $\pm$ index. For an orthonormal frame $\{e^a\}$,

$$dg_{ab} = 0, \tag{9}$$

and the unique metric-compatible, torsion-free connection is given by[8]

$$2g_{am}\omega^m{}_b = g_{mn}e^m i_{X_a}(i_{X_b}(de^n)) + g_{an}i_{X_b}(de^n) - g_{mb}i_{X_a}(de^m), \tag{10}$$

where

$$g_{ab} = g(X_a, X_b). \tag{11}$$

By assumption, g_{ab} is regularly discontinuous. We will further assume that the connection 1-forms $\omega^a{}_b$ are regularly discontinuous. Physically, this means that not only $g^\pm$ but also their derivatives admit 1-sided limits to Σ, so that $M^\pm \cup \Sigma$ are (pseudo) Riemannian manifolds-with-boundary.

III. VARIATIONAL APPROACH

We first review the Palatini formalism for obtaining Einstein's equations in vacuum for nondegenerate metrics. We then show by example how to include matter fields, and finally consider degenerate metrics.

A. Nondegenerate metrics

The Einstein-Hilbert action on a manifold with nondegenerate metric but without boundary can be written in terms of the Lagrangian density

$$\mathscr{L}_{EH} = g_{ac}R^c{}_b \wedge *(e^a \wedge e^b), \tag{12}$$

where the curvature 2-forms $R^a{}_b$ are defined by

$$R^a{}_b = d\omega^a{}_b + \omega^a{}_c \wedge \omega^c{}_b\,, \tag{13}$$

We adopt the Palatini approach and vary the action separately with respect to e^a and $\omega^a{}_b$, noting that g_{ac} is constant, $R^c{}_b$ is independent of e^a, and the remaining factor is independent of $\omega^a{}_b$.

Taking the ω variation first, if $\omega \mapsto \omega + \delta\omega$ then

$$\begin{aligned}\delta_\omega R^a{}_b &= \delta(d\omega^a{}_b + \omega^a{}_c \wedge \omega^c{}_b) \\ &= d(\delta\omega^a{}_b) + \delta\omega^a{}_c \wedge \omega^c{}_b + \omega^a{}_c \wedge \delta\omega^c{}_b\,.\end{aligned} \tag{14}$$

Thus,

$$\delta_\omega \mathscr{L}_{EH} = g_{ac}\delta_\omega R^c{}_b \wedge *(e^a \wedge e^b)$$

$$= g_{ac} d(\delta\omega^c{}_b \wedge *(e^a \wedge e^b)) + g_{ac}\delta\omega^c{}_b \wedge d*(e^a \wedge e^b)$$
$$+ g_{ac}\delta\omega^c{}_d \wedge \omega^d{}_b \wedge *(e^a \wedge e^b) - g_{ac}\delta\omega^d{}_b \wedge \omega^c{}_d \wedge *(e^a \wedge e^b). \quad (15)$$

Since there is no boundary, the surface term does not contribute. Furthermore, using (7) in the last term yields

$$-g_{ac}\delta\omega^d{}_b \wedge \omega^c{}_d = g_{cd}\delta\omega^d{}_b \wedge \omega^c{}_a, \quad (16)$$

so that requiring that $\delta_\omega R^a{}_b$ vanish for arbitrary variations in ω results in

$$D*(e^a \wedge e^b) := g_{ac}\delta\omega^c{}_b (d*(e^a \wedge e^b) + \omega^b{}_m \wedge *(e^a \wedge e^m) + \omega^a{}_m \wedge *(e^m \wedge e^b)) = 0. \quad (17)$$

Working in 4 dimensions for convenience and introducing the totally antisymmetric tensor η_{abcd} with $\eta_{0123} = 1$, whose indices are raised and lowered with g_{ab} we have

$$*(e^a \wedge e^b) = \frac{1}{2!}\eta^{ab}{}_{cd}(e^c \wedge e^d), \quad (18)$$

which leads directly to

$$D*(e^a \wedge e^b) = *(T^a \wedge e^b + e^a \wedge T^b) = 2*(T^a \wedge e^b). \quad (19)$$

The result of the ω variation is thus that the connection must be torsion-free

$$T^a = 0. \quad (20)$$

(We have assumed that the connection is metric-compatible. A similar computation starting instead from the assumption that the connection is torsion-free leads to the requirement that the connection be metric-compatible. A general computation, making no *a priori* restriction on the connection, results in an equation relating the nonmetricity of the connection to its torsion.[9])

Moving on to the e variation, we obtain

$$\delta_e *(e^a \wedge e^b) = \delta_e\left(\frac{1}{2!}\eta^{ab}{}_{cd}e^c \wedge e^d\right)$$

$$= \eta^{ab}{}_{cd}e^c \wedge \delta e^d$$

$$= -*(e^a \wedge e^b \wedge e^m g_{md}) \wedge \delta e^d$$

$$= -i_{X_d} *(e^a \wedge e^b) \wedge \delta e^d, \quad (21)$$

where we have used[8]

$$*(\phi \wedge X^\flat) = i_X * \phi, \quad (22)$$

where $X^\flat$ denotes the 1-form which is the metric dual of the vector field X. Thus

$$\delta_e \mathscr{L}_{EH} = 2g_{ac}R^c{}_b \wedge i_{X_d} *(e^a \wedge e^b) \wedge \delta e^d$$

$$= 2G_d \wedge \delta e^d, \quad (23)$$

where the right-hand-side defines[8] the Einstein 1-form G_d, which is related to the Einstein tensor G by

$$G_a = G(X_a, X_b)e^b. \tag{24}$$

Thus, in the absence of a matter Lagrangian, we obtain the vacuum Einstein equations

$$G_a = 0. \tag{25}$$

B. Matter terms

Before considering boundaries, we show by example what changes need to be made in the presence of matter. Consider for simplicity a massless scalar field Φ, with Lagrangian density

$$2\,\mathscr{L}_\Phi = d\Phi \wedge *d\Phi. \tag{26}$$

The field equations

$$d*d\Phi = 0 \tag{27}$$

are derived by varying $\mathscr{L}_\Phi$ with respect to Φ.[10] The stress 1-forms are obtained by varying $\mathscr{L}_\Phi$ with respect to e^a. We first note that

$$\begin{aligned} 0 = \delta_e d\Phi &= \delta_e(X_a(\Phi)e^a) \\ &= \delta X_a(\Phi)e^a + X_a(\Phi)\,\delta e^a. \end{aligned} \tag{28}$$

The variation is thus essentially a variation of $*$, and we obtain

$$\begin{aligned} \delta_e *d\Phi &= \delta_e(X_a(\Phi)*e^a) \\ &= \delta_e\left(X_a(\Phi)\frac{1}{3!}\,\eta^a_{bcd}e^b \wedge e^c \wedge e^d \right) \\ &= \delta X_a(\Phi)*e^a + X_a(\Phi)\frac{1}{2}\,\eta^a_{bcd}e^b \wedge e^c \wedge \delta e^d \\ &= -X_a(\Phi)*\delta e^a + X_a(\Phi)*(e^a \wedge e^m g_{md}) \wedge \delta e^d \\ &= -i_{X_a}(d\Phi)*\delta e^a + X_a(\Phi)i_{X_d}(*e^a) \wedge \delta e^d, \end{aligned} \tag{29}$$

where we have again used (22). Thus,

$$\begin{aligned} 2\,\delta_e\mathscr{L}_\Phi &= d\Phi \wedge \delta_e *d\Phi \\ &= -i_{X_a}(d\Phi)d\Phi \wedge *\delta e^a + d\Phi \wedge i_{X_d}(*d\Phi) \wedge \delta e^d \\ &= -i_{X_a}(d\Phi)\,\delta e^a \wedge *d\Phi + d\Phi \wedge i_{X_a}(*d\Phi) \wedge \delta e^a \\ &= i_{X_a}(d\Phi)*d\Phi \wedge \delta e^a + d\Phi \wedge i_{X_a}(*d\Phi) \wedge \delta e^a, \end{aligned} \tag{30}$$

so that the stress 1-forms are

$$2*\tau_a = 2\frac{\delta \mathscr{L}}{\delta e^a} = i_{X_a}(d\Phi)*d\Phi + d\Phi \wedge i_{X_a}(*d\Phi). \tag{31}$$

The stress 1-forms are related to the stress tensor T by

$$\tau_a = T(X_a, X_b)e^b \tag{32}$$

[compare (24)]. If we now take as our total Lagrangian

$$\mathscr{L} = \mathscr{L}_{EH} - 16\pi G \mathscr{L}_\Phi, \tag{33}$$

then the variation with respect to ω is unchanged, and the variation with respect to e yields Einstein's equations in the form

$$G_a = 8\pi G \tau_a. \tag{34}$$

C. Signature change

We now consider a manifold M divided as before into disjoint open regions $M^\pm$ by a hypersurface Σ. We will take as our Lagrangian the piecewise sum of the Einstein-Hilbert Lagrangians. For variations with support away from Σ, everything is as before, and we obtain Einstein's equations separately in the two regions. But for variations of ω in a neighborhood of Σ, the surface term which we previously discarded would now contribute, and we do not wish to impose any *a priori* conditions on the smoothness of the variations of ω, and thus implicitly on ω itself. We thus modify the Einstein-Hilbert action by adding a surface term,

$$\mathscr{L}_g = \mathscr{L}_{EH} - d(g_{ac}\omega^c{}_b \wedge *(e^a \wedge e^b)), \tag{35}$$

and note that this will precisely cancel the surface term in the variation of ω. We emphasize that this change in the action has nothing to do with signature change, and is required for the standard, constant signature case.[5,11]

We thus consider the theory with action,

$$\mathscr{S} = \int_{M^+} \mathscr{L}_g^+ + \int_{M^-} \mathscr{L}_g^-, \tag{36}$$

and reiterate that variations with support away from Σ lead as expected to Einstein's equations and the torsion-free condition separately in the two regions. If we now assume that

$$[e^a]_\Sigma = 0, \tag{37}$$

and consider continuous variations of e^a across the boundary, we obtain on each side a surface term of the form

$$-\int_\Sigma \delta_e(g_{ac}\omega^c{}_b \wedge *(e^a \wedge e^b)) = \int_\Sigma g_{ac}\omega^c{}_b \wedge i_{X_d} *(e^a \wedge e^b) \wedge \delta e^d, \tag{38}$$

where we have used (21). Consider the term

$$\rho_d := g_{ac}\omega^c{}_b \wedge i_{X_d} *(e^a \wedge e^b), \tag{39}$$

and note that only the pullback $\hat{\rho}_d$ of ρ_d occurs in (38). A tedious but straightforward computation making repeated use of identities like

$$g_{am}g_{bn}*(e^m\wedge e^n)=g_{bn}i_{X_a}*e^n=i_{X_a}i_{X_b}*1, \tag{40}$$

$$\omega^a{}_b\wedge i_{X_c}\alpha=-i_{X_c}(\omega^a{}_b\wedge\alpha)+i_{X_c}\omega^a{}_b\wedge\alpha, \tag{41}$$

$$g_{00}*(e^0\wedge e^i)=\hat{*}e^i, \tag{42}$$

shows that

$$\hat{\rho}_0=-2\omega^i{}_j(X_i)\hat{*}e^j, \tag{43}$$

$$\hat{\rho}_i=(2\omega^0{}_j(X_i)-2\delta_{ij}\delta^{kl}\omega^0{}_k(X_l))\hat{*}e^j, \tag{44}$$

and we see at once that $\hat{\rho}_0$ is continuous, as it only depends on the frame at Σ. Requiring that (38) vanish for arbitrary variations, we thus obtain the boundary condition

$$[\hat{\rho}_i]_\Sigma=0. \tag{45}$$

The extrinsic curvature of Σ is defined by (the 1-sided limits to Σ of)

$$K(X,Y)=-\nabla_X e^0(Y). \tag{46}$$

(One usually assumes X_0 is geodesic to ensure that K only has components tangent to Σ; it is in any case only these components which matter. One can therefore without loss of generality restrict X and Y to the tangent space to Σ, which is spanned by $\{X_i:i=1,\ldots,n-1\}$.) We have

$$K(X_i,X_j)=-(\nabla_{X_i}e^0)(X_j)=\omega^0{}_c(X_i)e^c(X_j)=\omega^0{}_j(X_i). \tag{47}$$

We define the trace of K by

$$\text{tr } K:=h^{ij}K(X_i,X_j)=\delta^{ij}K(X_i,X_j). \tag{48}$$

Inserting (47) and (48) into (45) and (44), we see that the e variation yields

$$0=[\hat{\rho}_i]_\Sigma=(2[K(X_i,X_j)]_\Sigma-2\delta_{ij}[\text{tr}]_\Sigma K)\hat{*}e^j, \tag{49}$$

which is equivalent to

$$[K(X_i,X_j)]_\Sigma=0, \tag{50}$$

so that the extrinsic curvature must be continuous.

D. Lanczos equation

If the matter Lagrangian contains a surface term of the form

$$\mathscr{S}_\Sigma=\int_\Sigma \mathscr{L}_\Sigma, \tag{51}$$

then there will be a surface stress tensor of the form

$$\hat{*}\tau_i^\Sigma=\frac{\delta\mathscr{L}_\Sigma}{\delta e^i}. \tag{52}$$

Relating this to the variation of the (surface term of the) Einstein-Hilbert action yields the Lanczos equation[12,13] in the form

$$[\hat{\rho}_i]_\Sigma = 16\pi G \tau_i^\Sigma , \tag{53}$$

or equivalently

$$([K(X_i,X_j)]_\Sigma - \delta_{ij}[\mathrm{tr}]_\Sigma K)e^j = 8\pi G \tau_i^\Sigma , \tag{54}$$

relating the discontinuity in the extrinsic curvature to the surface stress tensor. This equation is identical in form to that obtained when the metric is nondegenerate.

IV. DISCUSSION

We reiterate that there are no canonical ''Einstein's equations'' in the presence of signature change. One can try to construct a theory by formal substitution of a signature-changing metric into equations derived for constant signature, but it is not at all obvious that the resulting theory could be derived from an appropriate starting principle. For instance, for continuous, signature-changing metrics there is no (metric) volume element at the surface of signature change, so in this approach it is not clear what one should mean by a surface layer. And for discontinuous metrics, it is not even clear whether a (distributional) metric-compatible connection exists, since the standard computational techniques involve contracting the distributional derivatives of the metric with the discontinuous metric. One intriguing possibility involves a connection which is merely discontinuous but not metric-compatible.[14] Even with a discontinuous (as opposed to distributional) connection, however, the formal computation of Einstein's equations fails in general: While a distributional curvature tensor (or 2-form) can be constructed, with a signature-changing metric there is no way to take the trace to obtain the Einstein tensor.

Our results agree with Embacher[5] that the boundary condition obtained from the action (35) is precisely that the extrinsic curvature be continuous, which is the well-known Darmois junction condition for the absence of a surface layer.[15] Our derivation thus supports the work of several authors[1,2,16,17] who postulate the Darmois conditions for Einstein's equations in the presence of signature change. Hellaby and Dray[16–18] have pointed out, however, that in the presence of signature change the Darmois junction conditions are not sufficient to obtain the usual conservation laws, in contrast to the usual situation.[4,19–22] We note in particular that the Kossowski and Kriele claim[23] that the Darmois conditions lead to a surface layer which was missed by Ellis is incorrect,[24] as it is based on a smoothness assumption which does not hold in the Darmois approach.

We emphasize that not only does our work support our previous claims that the Darmois junction conditions are precisely the conditions for there to be no surface layer in the presence of signature change, but it also derives the precise relationship between the discontinuity in the extrinsic curvature and the stress tensor of the surface layer, namely the Lanczos equation.

Our theory is constructed using standard variational techniques from a straightforward generalization of the standard Einstein-Hilbert Lagrangian. A surface term is added to avoid having to specify continuity conditions on the connection variations without knowing anything in advance about the continuity of the connection itself. It is remarkable that even though our metric is discontinuous, there is still a continuous frame which is orthonormal almost everywhere, and we work with this frame to avoid having to vary the metric.

One might question whether our variations of the frame e^a are indeed arbitrary. There are two separate issues here, the first being that we have restricted our variations so that away from Σ the frame remains orthonormal. This is merely a reflection of the gauge freedom in Einstein's theory to work with a preferred category of frames, such as coordinate bases, null tetrads, or orthonormal frames. The second issue is at first sight more worrisome: Our class of nearly orthonormal frames for signature-changing metrics uniquely determines e^0 at Σ, so that

$$\delta e^0|_\Sigma = 0 \tag{55}$$

(which also restricts the variations $\delta e^i|_\Sigma$ to be tangent to Σ). The careful reader will have noticed that we have not tried to *derive* the condition $[\hat{\rho}_0]=0$ from the variational principle; we now see that this can not in fact be done. Fortunately, this condition is identically satisfied. This is just a reflection of the fact that we have fixed the hypersurface Σ, so that $X_0|_\Sigma$ is a geometric object, the normal vector field to the given surface. So long as Σ is fixed, there is no physical or geometric content to varying X_0, or equivalently varying its dual e^0. This point of view is supported by the fact that, if one permits such variations in the nondegenerate case, one obtains no new information. In any case, we expect our results to generalize directly to permit continuous variations of an arbitrary (non-orthonormal) frame e^a, yielding the same results. Strong evidence for this claim is provided by the fact that Embacher[5] obtains the same results as we do by varying (35) with respect to the metric and connection in a coordinate basis.

Similar results to those obtained here were derived earlier for the scalar field[10,25] from several different approaches, including a variational principle. These results agree with those obtained by Ellis *et al.*[1,2] for the coupled Einstein-Klein/Gordon system. Carfora and Ellis[26] have recently given a an elegant approach to signature changing spacetimes, in which the Darmois conditions are generalized to allow a diffeomorphism of the surface Σ of signature change.

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Kinks and geodesic incompleteness

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The problem of geodesic incompleteness is examined for space–times with Finkelstein–Misner kinks. A discussion of spherically symmetric kink space–times is followed by specific examples in which geodesics, initially incomplete in the original space–time, are shown to be extendible by the Kruskal technique. The structure of the two Kruskal patches and their matching at the patch boundaries are worked out in detail for one such example. Comments are made concerning a possible link between extendibility and energy conditions. It is shown that the kinds of spherically symmetric kink space–times examined in the present paper do not satisfy the strong energy condition. © *1996 American Institute of Physics.* [S0022-2488(96)01711-2]

I. INTRODUCTION

Kink space–times were originally discovered by Finkelstein and Misner[1] and were further studied by Finkelstein and McCollum[2] who showed how kink space–times which were geodesically incomplete when presented in terms of so-called ''rotational'' coordinates could sometimes be extended by performing a Kruskal transformation[3] to obtain new coordinates which range over a larger geodesically complete manifold. Finkelstein and McCollum also raised the question of whether a geodesically complete kink space–time could arise from a physically reasonable source, and they formulated a set of conditions that (a certain class of) spherically symmetric kink space–times would need to satisfy if the source were to be physically reasonable.

More recently, Chamblin (Ref. 4, pp. 376–377) has raised questions concerning the relationship between kinking and geodesic incompleteness. In further work, Chamblin[5] studies chronological asymptotically flat kink space–times that satisfy the strong and generic energy conditions (and are already maximally extended). He argues that such a space–time will be timelike and null (i.e., nonspacelike) geodesically incomplete *in an absolute sense*. That is to say, the space–time cannot be further extended to a geodesically complete space–time. The de Sitter kink space–time, which does not satisfy the energy conditions, was previously extended by Dunn, Harriott, and Williams.[6] The purpose of the present paper is to pursue this tie between incompleteness and energy conditions by examining other examples of spherically symmetric kink space–times. Such space–times are characterized by a tipping over of the light cones as r varies from 0 to ∞. The angle of tilt of the light cones will be denoted by α, which will be assumed to be a function of r, but not of t. Although it is always possible to find a *local* coordinate system in which $\alpha(r)$ is zero, it is not possible to do this *globally* when there are kinks. Throughout the present paper, we shall

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impose the boundary conditions $\alpha(0)=0$ and $\alpha(\infty)=\pi$, which correspond to a kink number of one.

II. SIMPLEST SPHERICALLY SYMMETRIC KINKS

The simplest spherically symmetric space–time with a kink present is given by[2,6–11]

$$ds^2=-\cos 2\alpha\ dt^2-2\sin 2\alpha\ dt\ dr+\cos 2\alpha\ dr^2+r^2\ d\Omega^2.$$

This is a special case of the space–time discussed by Letelier and Wang.[12,13] The Christoffel symbols and the Ricci and Einstein tensors are listed in Appendix A. Examples of such space–times include the de Sitter kink space–time[9,10] and the Tolman–Hawking and Schwarzschild kink space–times discussed by González-Díaz.[11] (See also Ref. 14.)

Since α varies from 0 to π, there will be two horizons: one at $\alpha=\pi/4$ and the other at $\alpha=3\pi/4$. For the example of the de Sitter kink space–time, the horizons are of the cosmological kind and the geodesics can be straightened by transforming to Kruskal coordinates.[6] For other examples, it may not be possible to extend the geodesics at $\alpha=\pi/4$ and $\alpha=3\pi/4$, but if it is possible, since one cannot expect to find a coordinate system that will straighten the geodesics at both $\alpha=\pi/4$ and $\alpha=3\pi/4$ simultaneously, two coordinate patches will be needed to describe the resulting geodesically complete space–time with Kruskal coordinates.[2] In terms of the original α, the coordinate patches correspond to the ranges $0\leqslant\alpha\leqslant\pi/2$ (first patch) and $\pi/2\leqslant\alpha\leqslant\pi$ (second patch). There is a further difficulty concerning the joining together of the two patches. The smooth joining of such patches requires the metric and its first derivatives to be continuous at the boundary (the Lichnerowicz junction conditions[15]) or alternatively, and more covariantly, that the first and second fundamental forms of the boundary three-manifold be the same for both patches (the Darmois junction conditions[16–18]). This is not the case for the de Sitter kink space–time.[19]

The two patches are most easily described in terms of a new time coordinate[2,6]

$$\overline{t}=t+h(r),$$

with $h(r)$ chosen to satisfy

$$\frac{dh}{dr}=\frac{\sin 2\alpha-\kappa}{\cos 2\alpha},$$

where $\kappa=+1$ for the first patch and $\kappa=-1$ for the second patch. The apparent singularities at $\alpha=\pi/4$ for $\kappa=+1$ and at $\alpha=3\pi/4$ for $\kappa=-1$ (i.e., for $\sin\alpha=\kappa\cos\alpha$) can be removed by using the identities

$$\sin 2\alpha\mp 1\equiv(\cos\alpha\mp\sin\alpha)^2,$$

$$\cos 2\alpha\equiv(\cos\alpha-\sin\alpha)(\cos\alpha+\sin\alpha)$$

to rewrite the derivative dh/dr as

$$\frac{dh}{dr}=\frac{\kappa\sin\alpha-\cos\alpha}{\sin\alpha+\kappa\cos\alpha}.$$

This is clearly well defined and hence $h(r)$ is also well defined, thus ensuring that the kink number will not be affected by the transformation to the new time coordinate $\overline{t}$. The metric is transformed to

$$ds^2=-\cos 2\alpha\ d\overline{t}^2-2\kappa\ d\overline{t}\ dr+r^2\ d\Omega^2,$$

and will be geodesically incomplete at $\alpha=\pi/4$ for $\kappa=+1$ and at $\alpha=3\pi/4$ for $\kappa=-1$, angles which correspond to the same $\sin\alpha=\kappa\cos\alpha$ condition under which trouble originally arose for dh/dt.

Kruskal coordinates,[3] U, V, are given by[2,6]

$$U=\mp e^{\gamma t}\exp\left(2\gamma\kappa\int_{0/A}^{r}\frac{dr}{\cos 2\alpha}\right),$$

$$V=\mp\frac{1}{\gamma a_\kappa}e^{-\gamma t},$$

where the lower limit of integration $0/A$ refers to the choices $r=0$ or $r=A$ at the start of the first or second patches, respectively, where a_κ denotes the values of r at the horizons which occur at a_{+1} in the first patch and at a_{-1} in the second patch, and where γ is a constant. The metric becomes

$$ds^2=-2F(U,V)dU\,dV+r^2\,d\Omega^2,$$

with F given by

$$F=\frac{-a_\kappa\cos 2\alpha}{2\gamma}\exp\left(-2\gamma\kappa\int_{0/A}^{r}\frac{dr}{\cos 2\alpha}\right).$$

(The factor of $-a_\kappa$ in this expression for F was omitted by error in our earlier paper.)[6] The constant γ, which has so far been undetermined, must be chosen so that the function F is finite and nonzero when $\sin\alpha=\kappa\cos\alpha$ (i.e., as $r\to a_\kappa$). When γ is chosen in this way, the extension process is complete. If no such γ can be found, then the Kruskal extension fails.

If the possibility of extending a nonspacelike geodesically incomplete kink space–time to one that is geodesically complete hinges, in part, on the energy conditions being satisfied,[5] then it is appropriate to review these energy conditions and also the physical conditions that were put forward by Finkelstein and McCollum.[2] Following the procedure of Hawking and Ellis (Ref. 20, p. 89), consider the eigenvalue equation

$$(G_{\mu\nu}-\lambda g_{\mu\nu})\xi^\nu=0.$$

The components G_μ^ν of the Einstein tensor are listed in Appendix A. In terms of the function

$$\mu(r):=\tfrac{1}{2}(r-r\cos 2\alpha)=r\sin^2\alpha,$$

introduced by Finkelstein and McCollum,[2] the eigenvalues are given by

$$\lambda_0=\lambda_1=2r^{-2}\,\partial_r\mu,\quad \lambda_2=\lambda_3=-r^{-1}\,\partial_r^2\mu.$$

Corresponding eigenvectors are

$$E_0=(\cos\alpha,\sin\alpha,0,0),\quad E_1=(\sin\alpha,-\cos\alpha,0,0),$$

$$E_2=(0,0,r^{-1},0),\quad E_3=(0,0,0,(r\sin\theta)^{-1}).$$

The eigenvector E_0 is timelike (with the remaining eigenvectors being spacelike) and so, of the four canonical forms listed by Hawking and Ellis (Ref. 20, p. 89), this situation is *Type I*. The $\{E_\alpha\}$ form an orthonormal basis and the tetrad components of the metric tensor are computed according to

$$\overline{g}_{\alpha\beta}=g(E_\alpha,E_\beta)=g_{\mu\nu}E^\mu_\alpha E^\nu_\beta=\mathrm{diag}(-1,1,1,1).$$

Note that $\overline{g^{\alpha\beta}}=\overline{g}_{\alpha\beta}$. It is straightforward to calculate the tetrad components $\overline{G}^{\alpha\beta}$ of the Einstein tensor and hence, using the Einstein equations $G^{\alpha\beta}=T^{\alpha\beta}$, the tetrad components $T^{\alpha\beta}$ of the energy-momentum tensor are found to be $\|T^{\alpha\beta}\|=\mathrm{diag}(\rho,p_1,p_2,p_3)$, where

$$\rho=2r^{-2}\,\partial_r\mu,\quad p_1=-2r^{-2}\,\partial_r\mu,\quad p_2=p_3=-r^{-1}\,\partial_r^2\mu.$$

The weak energy condition states that the energy density as measured by any observer is non-negative, and this is equivalent to requiring $\rho\geqslant 0$ and $\rho+p_\alpha\geqslant 0$, for $\alpha=1, 2, 3$ (Ref. 20, p. 90). These inequalities imply $\partial_r\mu\geqslant 0$ and $\partial_r(r^{-2}\,\partial_r\mu)\leqslant 0$. The strong energy condition holds for a *Type I* energy-momentum tensor provided that, for $\alpha=1, 2, 3$, $\rho+p_\alpha\geqslant 0$ and $\rho+\Sigma p_\alpha\geqslant 0$ (Ref. 20, p. 95). The latter condition is equivalent to $\partial_r^2\mu\leqslant 0$. Note that the strong energy condition does *not* imply the weak energy condition (Ref. 21, p. 219). We now list some physical conditions for $\mu(r)$:

(a) $\partial_r\mu\geqslant 0$ for all r,
(b) $\partial_r(r^{-2}\partial_r\mu)\leqslant 0$ for all r,
(c) $\mu=O(r^3)$ as $r\to 0$ (i.e., $|G^\nu_\mu|<\infty$ at $r=0$),
(d) $0\leqslant\mu/r\leqslant 1$ (i.e., $0\leqslant\sin^2\alpha\leqslant 1$),
(e) $\partial_r^2\mu\leqslant 0$ for all r.

Taken together, conditions (a) and (b) have been shown to be equivalent to the weak energy condition. From Appendix A,

$$G^t_t=G^r_r=-2r^{-2}\partial_r\mu,$$

$$G^\theta_\theta=G^\varphi_\varphi=-r^{-1}\partial_r^2\mu,$$

and so requiring $\mu=O(r^3)$ as $r\to 0$ will ensure that G^ν_μ, and hence T^ν_μ, is finite at the origin. This is condition (c). Condition (d) follows from the definition $\mu:=r\sin^2\alpha$. For present purposes, one needs a somewhat stronger condition than (d) since, to ensure the presence of a kink, we are imposing the boundary conditions $\alpha(0)=0$ and $\alpha(\infty)=\pi$. Thus we require μ to satisfy

(f) $\lim_{r\to 0}(\mu/r)=\lim_{r\to\infty}(\mu/r)=0$,

with μ/r attaining its maximum value of 1 at the value of r corresponding to $\alpha=\pi/2$. Our conditions (a), (c), and (d) agree with the corresponding conditions given by Finkelstein and McCollum (Ref. 2, p. 2253). However, our condition (b) differs from Finkelstein and McCollum's condition (b).

Taken together, conditions (b) and (e) have been shown to be equivalent to the strong energy condition. However, for the kind of spherically symmetric one-kink metrics being discussed, conditions (d) and (f) *must* be satisfied. From condition (f), $\lim_{r\to 0}(\mu/r)=0$ implies that, for small r, $\mu=O(r^{1+c})$ with $c>0$. Hence, for small $r>0$, $\partial_r\mu=O(r^c)>0$ and $\partial_r^2\mu=O(r^{c-1})>0$. The latter inequality violates condition (e), thus showing that the strong energy condition cannot be satisfied by kink metrics of this kind.

In the present paper, the space–times considered are spherically symmetric and have one kink on each hypersurface of constant t. Note that Alty[22] has given a formula for counting the number of kinks on a closed three-manifold or hypersurface within any nonsingular (3+1)-dimensional space–time. An alternative formula has been given by Torre.[23] (See also Ref. 24 for an earlier approach and Ref. 25 for a formula that is valid in 1+1 dimensions.) This concludes the analysis for general α. In Secs. III–V, specific functional forms for α will be chosen.

III. STEREOGRAPHIC KINK

Let the functional form of $\alpha(r)$ be given by

$$\tan(\alpha/2)=r/a,$$

where a is a positive constant and $0\leqslant r<\infty$. Since α varies continuously from $\alpha(0)=0$ to $\alpha(\infty)=\pi$, the resulting metric describes a one-kink space–time. The function $\mu(r)$ is given by

$$\mu=\frac{4a^2r^3}{(a^2+r^2)^2}.$$

Of conditions (a)–(f), only conditions (c), (d), and (f) hold. Thus not even the *weak* energy condition is satisfied. This space–time can be aptly called the ''stereographic kink space–time,'' since the angle α is mapped into a radial distance r in accordance with the usual stereographic projection from a sphere onto a plane with radial coordinate r. The first patch corresponds to the range $0\leqslant r\leqslant a$, and the second patch corresponds to the range $a\leqslant r<\infty$. The $r=a_\kappa$ (i.e., $\sin\alpha=\kappa\cos\alpha$) horizons are located at $r=a_\pm=a(2^{1/2}\mp1)$, where we are abbreviating a_{+1} to a_+ and a_{-1} to a_-. The derivative dh/dr is given by

$$\frac{dh}{dr}=\frac{\kappa 2ar-(a^2-r^2)}{2ar+\kappa(a^2-r^2)},$$

and it is straightforward to show (Ref. 26, §2.103, p. 57) that, to within an arbitrary constant,

$$h(r)=-\kappa r-2^{1/2}\{a_+\ \ln(r+\kappa a_+)+a_-\ \ln(-\kappa r+a_-)\}.$$

Both dh/dr and $h(r)$ are well defined everywhere.

The constants a_+ and a_- satisfy the equations

$$a_+a_-=a^2,$$

$$a_+^2=[3-2(2^{1/2})]a^2,$$

$$a_-^2=[3+2(2^{1/2})]a^2,$$

$$a_-^{-2}-a_+^{-2}=-4(2^{1/2})a^{-2},$$

which lead to

$$\begin{aligned}\frac{1}{\cos 2\alpha}&=\frac{(a^2+r^2)^2}{(a^2-r^2)^2-(2ar)^2}\\&=1+\frac{8a^2r^2}{(a^2-r^2)^2-(2ar)^2}\\&=1+\frac{8a^2r^2}{(r^2-a_+^2)(r^2-a_-^2)}\\&=1-2^{1/2}a^4\left\{\frac{a_-^{-2}}{r^2-a_+^2}-\frac{a_+^{-2}}{r^2-a_-^2}\right\}\\&=1-2^{-1/2}a^2\left\{a_-^{-1}\left(\frac{1}{r-a_+}-\frac{1}{r+a_+}\right)-a_+^{-1}\left(\frac{1}{r-a_-}-\frac{1}{r+a_-}\right)\right\},\end{aligned}$$

and hence, ignoring the constant factor coming from the lower integration limit, to

$$\int^r \frac{dr}{\cos 2\alpha} = r - 2^{-1/2}a^2\{a_-^{-1}(\ln|r-a_+| - \ln|r+a_+|) - a_+^{-1}(\ln|r-a_-| - \ln|r+a_-|)\}.$$

This expression is undefined at $r=a_+$ which occurs in the first patch, and at $r=a_-$ which occurs in the second patch. The constant γ must now be chosen (if possible) so that F is nowhere zero and nowhere infinite. Since

$$\cos 2\alpha = (r^2+a^2)^{-2}(r-a_+)(r+a_+)(r-a_-)(r+a_-),$$

it follows from the equation for F given in Sec. II that the appropriate choices for γ are $\gamma=-2^{-1/2}a^{-2}a_-$ in the first patch, and $\gamma=-2^{-1/2}a^{-2}a_+$ in the second patch. More concisely, $\gamma=-2^{-1/2}a^{-2}a_{-\kappa}$. Since the resulting F is a complicated function of r, it will not be easy to express F as an explicit function of U and V (as was done in the de Sitter case[6]).

IV. NEWTONIAN KINK

The example

$$\mu = \frac{2ar^2}{a^2+r^2}$$

was considered some years ago[7] and was shown to reproduce the Newtonian potential for large r. We shall call it the ''Newtonian kink.'' Conditions (a), (b), (d), and (f) are satisfied, but not conditions (c) or (e). Thus the weak energy condition is satisfied. The angle α is related to r by

$$\sin\alpha = \left(\frac{2ar}{a^2+r^2}\right)^{1/2}, \quad \cos\alpha = \frac{a-r}{(a^2+r^2)^{1/2}},$$

so that the boundary between patches is located at $r=a$. The roots of $\cos 2\alpha$ are $a_\pm = a(2\mp 3^{1/2})$. From

$$a_+a_- = a^2, \quad a_+ + a_- = 4a, \quad a_-^{-1} - a_+^{-1} = -2a^{-1}3^{1/2},$$

it follows that

$$\cos 2\alpha = 1 - \frac{4ar}{r^2+a^2} = \frac{(r-a_+)(r-a_-)}{r^2+a^2},$$

and

$$\frac{1}{\cos 2\alpha} = 1 + \frac{4ar}{(r-a_+)(r-a_-)} = 1 - 2a^2 3^{1/2}\left\{\frac{1}{a_-(r-a_+)} - \frac{1}{a_+(r-a_-)}\right\}.$$

Hence, neglecting the constant factor coming from the lower integration limit,

$$\int^r \frac{dr}{\cos 2\alpha} = r - 2a^2 3^{-1/2}(a_-^{-1}\ln|r-a_+| - a_+^{-1}\ln|r-a_-|).$$

It follows from the equation for F given in Sec. II that F will be nowhere zero and nowhere infinite if we choose $\gamma=-(3^{1/2}/4)a^2a_-$ in the first patch and $\gamma=-(3^{1/2}/4)a^2a_+$ in the second patch.

V. FINKELSTEIN–McCOLLUM KINK

Finkelstein and McCollum[2] proposed

$$\mu=\left(\frac{3}{2+1/r}\right)^3=\frac{27r^3}{8r^3+12r^2+6r+1},$$

which violates condition (e) but satisfies the remaining conditions. Hence μ satisfies the weak but not the strong energy condition. It is interesting to note that Finkelstein and McCollum's condition (b) is also satisfied. The above μ implies

$$\cos 2\alpha=\frac{8r^3-42r^2+6r+1}{8r^3+12r^2+6r+1}.$$

The numerator factorizes as

$$8r^3-42r^2+6r+1=8(r+b)(r-a_+)(r-a_-),$$

where

$$b=\tfrac{1}{2}(3^{3/2}-5)\approx 0.0981,\quad a_+=\tfrac{1}{4},\quad a_-=\tfrac{1}{2}(3^{3/2}+5)\approx 5.0981,$$

so that problems with geodesic incompleteness arise at a_+ in the first patch and at a_- in the second patch. The boundary between patches occurs at $r=1$.

$$\begin{aligned}\frac{1}{\cos 2\alpha}&=1+\frac{27r^2}{4(r+b)(r-a_+)(r-a_-)}\\&=1+\frac{27}{4}\left[\frac{1}{r+b}+\frac{(a_++a_-)r-a_+a_-}{(r+b)(r-a_+)(r-a_-)}\right]\\&=1+\frac{27}{4}\left[\frac{b^2}{(a_++b)(a_-+b)(r+b)}-\frac{a_+^2}{(b+a_+)(a_--a_+)(r-a_+)}\right.\\&\quad\left.+\frac{a_-^2}{(b+a_-)(a_--a_+)(r-a_-)}\right].\end{aligned}$$

Requiring F to be nowhere zero and nowhere infinite in the two patches implies

$$\gamma=-\frac{2(b+a_\kappa)(a_--a_+)}{27a_\kappa^2}.$$

This gives $\gamma=-2$ in the first patch ($\kappa=+1$), and $\gamma\approx-0.0718$ in the second patch ($\kappa=-1$). The above values of a_+ and a_- agree with those of Finkelstein and McCollum but the above values of γ do not [Ref. 2, Eqs. (37) and (38), p. 2256].

VI. SPHERICALLY SYMMETRIC KINKS WITH $\chi\neq 0$

A slightly more general form of metric than that of Sec. II is given by

$$ds^2=-e^{\chi}\cos 2\alpha\ dt^2-2\sin 2\alpha\ dt\ dr+e^{-\chi}\cos 2\alpha\ dr^2+r^2\ d\Omega^2.$$

Again, this is a special case of the metric discussed by Letelier and Wang.[12,13] The Christoffel symbols and the Ricci and Einstein tensors are listed in Appendix B. After a change of time coordinate,

$$\overline{t}=t+h(r), \quad \frac{dh}{dr}=\frac{\sin 2\alpha-\kappa}{e^{\chi}\cos 2\alpha},$$

the method of extension proceeds as in Sec. II, with

$$U=\mp e^{\gamma \overline{t}}\exp\left(2\gamma\kappa\int_{0/A}^{r}\frac{dr}{e^{\chi}\cos 2\alpha}\right),$$

$$V=\mp\frac{1}{\gamma a_{\kappa}}e^{-\gamma \overline{t}},$$

$$F=\frac{-a_{\kappa}e^{\chi}\cos 2\alpha}{2\gamma}\exp\left(-2\gamma\kappa\int_{0/A}^{r}\frac{dr}{e^{\chi}\cos 2\alpha}\right).$$

The function μ defined in Sec. II will now be generalized by defining

$$\mu(r):=\tfrac{1}{2}(r-re^{\chi}\cos 2\alpha).$$

The eigenvalue analysis is similar to before and the energy-momentum tensor can be shown to be of *Type I*, with the elements of $\|T^{\alpha\beta}\|=\mathrm{diag}(\rho,p_1,p_2,p_3)$ being related to $\partial_r\mu$ and $\partial_r^2\mu$ exactly as before, except that the generalized μ is now being used. The form of conditions (a), (b), and (e) is unchanged, as is the relationship between these conditions and the weak and strong energy conditions. However, for the generalized μ, the other conditions listed in Sec. II must be modified:

(c′) $|G^{\nu}_{\mu}|<\infty$ at $r=0$,
(d′) $0\leqslant\sin^2\alpha\leqslant 1$,
(f′) $\alpha(0)=\lim_{r\to 0}(\sin\alpha)=\lim_{r\to\infty}(\sin\alpha)=0$,

with, as before, the understanding that the presence of the kink will force α to pass through $\pi/2$ so that $\sin\alpha$ will attain its maximum value of 1. The discussion of the strong energy condition that was presented at the end of Sec. II can be adapted to the present situation by noting that a space–time with a well-defined kink number requires the metric to be continuous, and so e^{χ} must be a regular function of r in the neighborhood of $r=0$. The fact that e^{χ} is regular at $r=0$ implies that, for small r, the (generalized) μ satisfies $\mu=O(r^{1+c})$ with $c>0$. One can now deduce, following the argument of Sec. II, that the strong energy condition cannot be satisfied by the more general spherically symmetric kink metrics discussed in this section.

VII. EXAMPLE

As an example, let α be the same as for the ''Newtonian'' kink of Sec. IV and let e^{χ} be given by

$$e^{\chi}=\frac{2(r^2+a^2)}{a(a_{-}-a_{+})}.$$

The (r^2+a^2) in the numerator is chosen so that it will cancel with the similar term in the denominator of $\cos 2\alpha$. The constant factors are chosen for later convenience, remembering also that e^{χ} must be dimensionless. Conditions (a), (c′), and (e) are violated. Conditions (b), (d′), and (f′) are satisfied.

It follows from Sec. IV that

$$e^{\chi}\cos 2\alpha=\frac{2(r-a_+)(r-a_-)}{a(a_--a_+)},$$

where $a_\pm=a(2\mp 3^{1/2})$ and $a_+<a<a_-$. Horizons occur at $r=a_+$ in the first patch and at $r=a_-$ in the second patch. The boundary between the two patches occurs at $r=a$.

$$\int_{0/a}^{r}\frac{dr}{e^{\chi}\cos 2\alpha}=\frac{1}{2}\,a\int_{0/a}^{r}\left(\frac{1}{r-a_-}-\frac{1}{r-a_+}\right)dr=\frac{1}{2}\,a\left[\ln\left|\frac{r-a_-}{r-a_+}\right|\right]_{0/a}^{r}.$$

Consider the first patch, $0\leqslant r\leqslant a$;

$$\int_0^r\frac{dr}{e^{\chi}\cos 2\alpha}=\frac{1}{2}\,a\left[\ln\left(\frac{a_--r}{a_+-r}\right)\right]_0^r=\frac{1}{2}\,a\,\ln\left(\frac{a_+(a_--r)}{a_-(a_+-r)}\right).$$

From the equation for F given in Sec. VI, it follows that F will be finite and nonzero if $\gamma=-a^{-1}$. This leads to

$$F=\frac{a_+^2(r-a_-)^2}{a_-(a_--a_+)}.$$

Recall that $a=(a_+a_-)^{1/2}$ and define

$$\lambda:=\left(\frac{a_-}{a_+}\right)^{1/2}=\frac{a_--a}{a-a_+}\approx 3.732.$$

It follows that

$$U=\mp\lambda^2 e^{-\overline{t}/a}\left(\frac{a_+-r}{a_--r}\right),\quad V=\pm\lambda e^{\overline{t}/a},\quad UV=-\lambda^3\left(\frac{a_+-r}{a_--r}\right).$$

These formulas for F, U, V, and UV are valid for $0\leqslant r\leqslant a$. It follows that, for the first patch,

$$r=a_+\lambda^2\left(\frac{\lambda+UV}{\lambda^3+UV}\right)$$

and

$$F=\frac{a_+\lambda^4(a_--a_+)}{(\lambda^3+UV)^2}.$$

The first patch is illustrated in Fig. 1. Regions I_+ and II_+ are *original* regions. (Following González-Díaz,[14] a $\pm$ subscript indicates that the region is in the first/second patch.) Within $I_+\cup II_+$, $r=0$ corresponds to the hyperbola $UV=-\lambda$; $r=a_+$ corresponds to the line $U=0$ (for $V>0$), and $r=a$ corresponds to the hyperbola $UV=\lambda^2$. The extension is performed by allowing V to be negative in the formulas above. This creates the *new* regions III_+ and IV_+ of Fig. 1. The line $r=a_+$, $t=-\infty$ (i.e., $V=0$) forms the boundary between the original and the new regions.

Now consider the second patch, $a\leqslant r<\infty$:

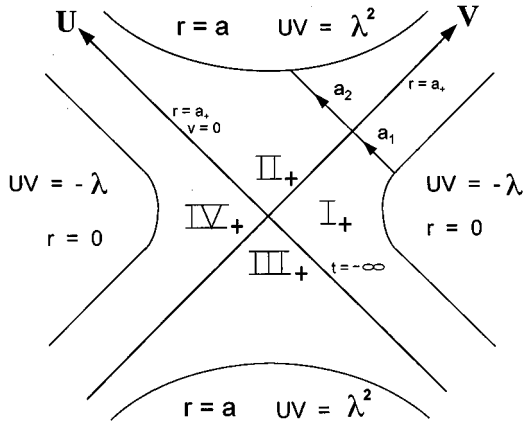

FIG. 1. First patch.

$$\int_a^r \frac{dr}{e^{\chi}\cos 2\alpha} = \frac{1}{2}\,a\left[\ln\left(\frac{a_- - r}{r - a_+}\right)\right]_a^r = \frac{1}{2}\,a\,\ln\left(\frac{a_- - r}{\lambda(r-a_+)}\right).$$

From the equation for F given in Sec. VI, it follows that F will be finite and nonzero if $\gamma = -a^{-1}$. This leads to

$$F = \frac{-\lambda a_-(r-a_+)^2}{a_- - a_+},$$

$$U = \mp\lambda^{-1}e^{-\overline{t/a}}\left(\frac{a_- - r}{r-a_+}\right), \quad V = \pm\lambda^{-1}e^{\overline{t/a}}, \quad UV = -\lambda^{-2}\left(\frac{a_- - r}{r-a_+}\right),$$

and

$$r = \frac{a_-(1-UV)}{1-\lambda^2 UV}, \quad F = \frac{-a_-\lambda(a_- - a_+)}{(1-\lambda^2 UV)^2}.$$

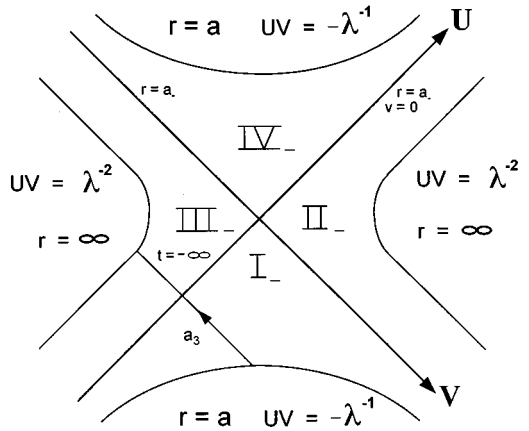

FIG. 2. Second patch.

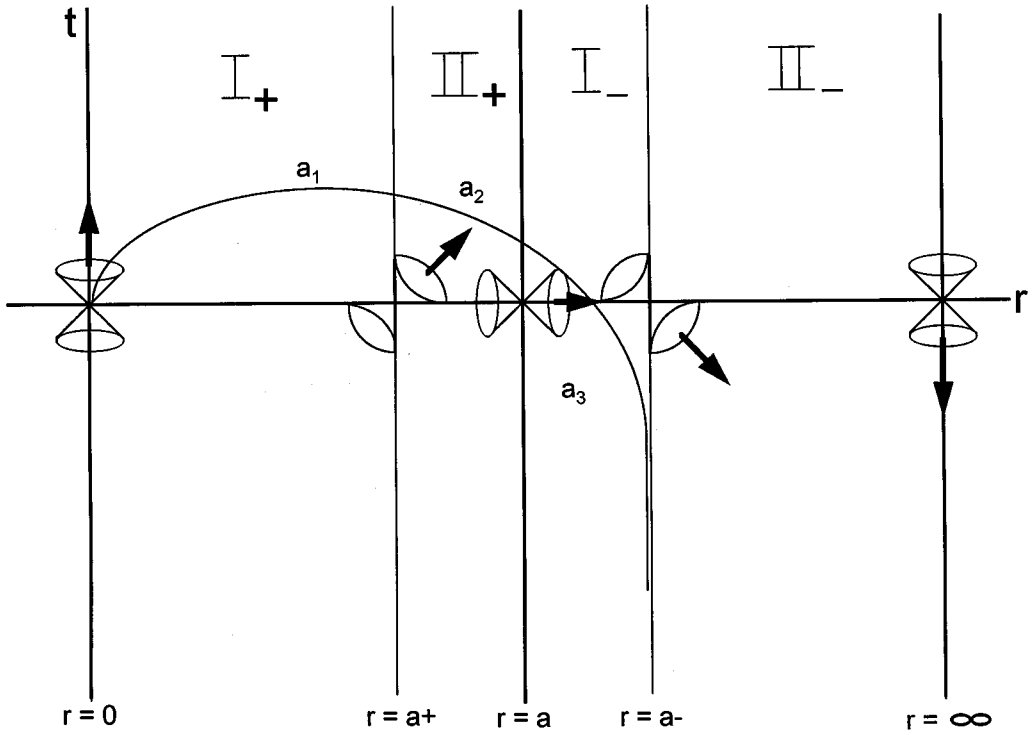

FIG. 3. Kink in rotational coordinates.

The second patch is illustrated in Fig. 2. Regions I_- and II_- are *original* regions. The line $r=a_-$, $t=-\infty$ (i.e., $V=0$) forms the boundary between $I_-\cup II_-$ and the union $III_-\cup IV_-$ of the two *new* regions, III_- and IV_-. The two $UV=\lambda^{-2}$ hyperbolas correspond to $r=\infty$ and the two $UV=-\lambda^{-1}$ hyperbolas correspond to $r=a$. The lower of the two latter hyperbolas (i.e., the $UV=-\lambda^{-1}$ hyperbola of region I_-) is to be joined with the corresponding $r=a$, $UV=\lambda^2$ hyperbola of region II_+ in the upper part of Fig. 1. Physical time is measured upwards in Figs. 1 and 2, and an example of a null geodesic $a_1a_2a_3$ is pictured starting from $r=0$, crossing from I_+ into II_+ and then into I_-, and finally into the new region III_-. The part of this geodesic that is within the original region $I_+\cup II_+\cup I_-$ is illustrated in rotational coordinates in Fig. 3.

Let Σ^+ denote the upper $UV=\lambda^2$ hyperbola in region II_+ of the first patch and let Σ^- denote the lower $UV=-\lambda^{-1}$ hyperbola in region I_- of the second patch. In constructing the kink space–time, one needs to show that Σ^+ and Σ^- can be smoothly joined. The rotational coordinates t,r,θ,φ span $II_+\cup I_-$ and it is easily shown that, in these coordinates, $g_{\mu\nu}$ and $\partial_\lambda g_{\mu\nu}$ are continuous across $\Sigma^\pm$. Thus the Lichnerowicz junction conditions[15] are satisfied and so smooth joining is possible. Although this implies that the Darmois junction conditions[16–18] are also satisfied, it is instructive to check these conditions in the UV-coordinate systems of the two patches. Following Lake,[18] let Σ denote a three-space within the (3+1)-dimensional space–time manifold and let the coordinates intrinsic to Σ be denoted by ξ^i, $i=1,2,3$. Let the equation for Σ be given in terms of the space–time coordinates by $x^\mu=x^\mu(\xi^i)$. Now define the intrinsic metric of Σ (Gauss' first fundamental form) by

$$\gamma_{ij} := \frac{\partial x^\mu}{\partial \xi^i}\frac{\partial x^\nu}{\partial \xi^j} g_{\mu\nu},$$

and the extrinsic curvature of Σ (Gauss' second fundamental form) by

$$K_{ij} := \frac{\partial x^\mu}{\partial \xi^i} \frac{\partial x^\nu}{\partial \xi^j} \nabla_\mu n_\nu,$$

where the unit vector n^λ is normal to Σ and can be found by writing the equation for Σ in the form $f(x^\mu(\xi^i))=0$ and putting

$$n_\lambda = \pm \left| g^{\mu\nu} \frac{\partial f}{\partial x^\mu} \frac{\partial f}{\partial x^\nu} \right|^{-1/2} \frac{\partial f}{\partial x^\lambda}.$$

An alternative and more convenient formula for K_{ij} is given by[17,18]

$$K_{ij} = -n_\lambda \left(\frac{\partial^2 x^\lambda}{\partial \xi^i \partial \xi^j} + \frac{\partial x^\mu}{\partial \xi^i} \frac{\partial x^\nu}{\partial \xi^j} \Gamma^\lambda_{\mu\nu} \right).$$

For the first patch, choose the intrinsic coordinates on Σ^+ to be $(\xi^1,\xi^2,\xi^3)=(V,\theta,\varphi)$ and note that, on Σ^+, $\partial U/\partial V = -\lambda^2 V^{-2}$. The first and second fundamental forms on Σ^+ will be denoted by γ^+_{ij} and K^+_{ij}, respectively. For the second patch, choose the intrinsic coordinates on Σ^- to be $(\xi^1,\xi^2,\xi^3)=(V,\theta,\varphi)$ and note that, on Σ^-, $\partial U/\partial V = \lambda^{-1} V^{-2}$. The first and second fundamental forms on Σ^- will be denoted by γ^-_{ij} and K^-_{ij}, respectively. The two Darmois conditions are $\gamma^+_{ij}=\gamma^-_{ij}$ and $K^+_{ij}=K^-_{ij}$, for $i,j=1,2,3$. It is straightforward to show that

$$\gamma^+_{VV} = \gamma^-_{VV} = \tfrac{1}{3} a (a_- - a_+) V^{-2},$$

$$\gamma^+_{\theta\theta} = \gamma^-_{\theta\theta} = a^2, \quad \gamma^+_{\varphi\varphi} = \gamma^-_{\varphi\varphi} = a^2 \sin^2\theta,$$

with the remaining components of $\gamma^\pm_{ij}$ being zero. Thus the first Darmois condition is satisfied.

The components of the unit normal vector on Σ^+ and Σ^- are, respectively,

$$n^+_U = (\lambda^2 C)^{-1} V, \quad n^+_V = (CV)^{-1} \quad n^+_\theta = n^+_\varphi = 0,$$

$$n^-_U = \lambda C^{-1} V, \quad n^-_V = -(CV)^{-1}, \quad n^-_\theta = n^-_\varphi = 0,$$

where

$$C = 2^{1/2} a^{-1} (a_-^{1/2} + a_+^{1/2})(a_- - a_+)^{-1/2}.$$

Care has been taken to choose the signs of $n^\pm_\mu$ so that n^+_μ is directed outwards from II_+ and n^-_μ is directed into I_-. It can now be shown that

$$K^+_{VV} = K^-_{VV} = -2C^{-1}(\lambda-1)(\lambda+1)^{-1} V^{-2},$$

$$K^+_{\theta\theta} = K^-_{\theta\theta} = -2C^{-1},$$

with $K^\pm_{\varphi\varphi} = \sin^2\theta K^\pm_{\theta\theta}$ and the remaining components of $K^\pm_{ij}$ being zero. Thus the second Darmois condition is satisfied.

VIII. SUMMARY

The problem of geodesic incompleteness was considered for two kinds of spherically symmetric kink space–times. Conditions that these space–times might satisfy were discussed in relation to the weak and strong energy conditions, and it was shown that the strong energy condition could not be satisfied. Examples were introduced and, in each case, the constant γ necessary to

perform the Kruskal extension was computed. In the most complicated of these examples, a judicious choice of the function e^{χ} enabled the transformation between tr-coordinates and UV-coordinates to be calculated explicitly and the Kruskal patches to be constructed. The junction conditions were shown to hold across the hypersurface located at the join of the two patches.

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APPENDIX A: EINSTEIN TENSOR FOR SIMPLEST SPHERICALLY SYMMETRIC KINK

For the metric

$$ds^2 = -\cos 2\alpha\ dt^2 - 2\sin 2\alpha\ dt\ dr + \cos 2\alpha\ dr^2 + r^2\ d\Omega^2,$$

with $\alpha = \alpha(r)$, the nonzero Christoffel symbols are as follows:

$$\Gamma^t_{tt} = \sin^2 2\alpha\ \partial_r\alpha, \quad \Gamma^t_{tr} = \Gamma^r_{tt} = -\sin 2\alpha\ \cos 2\alpha\ \partial_r\alpha,$$

$$\Gamma^t_{rr} = (1 + \cos^2 2\alpha)\partial_r\alpha, \quad \Gamma^r_{tr} = -\sin^2 2\alpha\ \partial_r\alpha,$$

$$\Gamma^t_{\theta\theta} = r\ \sin 2\alpha, \quad \Gamma^t_{\varphi\varphi} = r\ \sin^2\ \theta\ \sin 2\alpha,$$

$$\Gamma^r_{rr} = \sin 2\alpha\ \cos 2\alpha\ \partial_r\alpha, \quad \Gamma^r_{\theta\theta} = -r\ \cos 2\alpha,$$

$$\Gamma^\theta_{r\theta} = \Gamma^\varphi_{r\varphi} = r^{-1}, \quad \Gamma^r_{\varphi\varphi} = -r\ \sin^2\ \theta\ \cos 2\alpha,$$

$$\Gamma^\theta_{\varphi\varphi} = -\sin\ \theta\ \cos\ \theta, \quad \Gamma^\varphi_{\theta\varphi} = \cot\ \theta.$$

With Δ defined as

$$\Delta := 2r^{-2}\partial_r(r\ \sin^2\ \alpha),$$

the nonzero components of the Ricci tensor are

$$R_{tt} = -R_{rr} = -(2r)^{-1}\ \cos 2\alpha\ \partial_r(r^2\Delta),$$

$$R_{tr} = -(2r)^{-1}\ \sin 2\alpha\ \partial_r(r^2\Delta),$$

$$R_{\theta\theta} = r^2\Delta, \quad R_{\varphi\varphi} = r^2\ \sin^2\ \theta\Delta,$$

with the curvature scalar being given by

$$R = 2r^{-2}\partial_r^2(r^2\ \sin^2\ \alpha) = 2\Delta + r^{-1}\partial_r(r^2\Delta).$$

The nonzero mixed components of the Einstein tensor are

$$G^t_t = G^r_r = -\Delta, \quad G^\theta_\theta = G^\varphi_\varphi = -(2r)^{-1}\partial_r(r^2\triangle).$$

The $\mu(r)$ of Finkelstein and McCollum[2] is related to $\triangle$ by

$$\Delta := 2r^{-2}\partial_r\mu,$$

whence

$$G^t_t = G^r_r = -2r^{-2}\partial_r \mu, \quad G^\theta_\theta = G^\varphi_\varphi = -r^{-1}\partial_r^2 \mu.$$

APPENDIX B: EINSTEIN TENSOR FOR SPHERICALLY SYMMETRIC KINK WITH $\chi=0$

For the metric

$$ds^2 = -e^\chi \cos 2\alpha \; dt^2 - 2 \sin 2\alpha \; dt \; dr + e^{-\chi} \cos 2\alpha \; dr^2 + r^2 \; d\Omega^2,$$

with $\alpha=\alpha(r)$ and $\chi=\chi(r)$, the nonzero Christoffel symbols are as follows:

$$\Gamma^t_{tt} = e^\chi \sin 2\alpha (\sin 2\alpha \; \partial_r \alpha - \tfrac{1}{2} \cos 2\alpha \; \partial_r \chi),$$

$$\Gamma^t_{tr} = \cos 2\alpha (-\sin 2\alpha \partial_r \alpha + \tfrac{1}{2} \cos 2\alpha \; \partial_r \chi),$$

$$\Gamma^r_{tt} = e^{2\chi} \cos 2\alpha (-\sin 2\alpha \; \partial_r \alpha + \tfrac{1}{2} \cos 2\alpha \; \partial_r \chi),$$

$$\Gamma^t_{rr} = e^{-\chi}[(1+\cos^2 2\alpha)\partial_r \alpha + \tfrac{1}{2} \sin 2\alpha \; \cos 2\alpha \partial_r \chi],$$

$$\Gamma^r_{tr} = e^\chi \sin 2\alpha (-\sin 2\alpha \partial_r \alpha + \tfrac{1}{2} \cos 2\alpha \; \partial_r \chi),$$

$$\Gamma^t_{\theta\theta} = r \; \sin 2\alpha, \quad \Gamma^t_{\varphi\varphi} = r \; \sin^2 \; \theta \sin 2\alpha,$$

$$\Gamma^r_{rr} = \cos 2\alpha (\sin 2\alpha \; \partial_r \alpha - \tfrac{1}{2} \cos 2\alpha \; \partial_r \chi),$$

$$\Gamma^r_{\theta\theta} = -re^\chi \cos 2\alpha, \quad \Gamma^\theta_{r\theta} = \Gamma^\varphi_{r\varphi} = r^{-1},$$

$$\Gamma^r_{\varphi\varphi} = -re^\chi \sin^2 \; \theta \cos 2\alpha, \quad \Gamma^\theta_{\varphi\varphi} = -\sin \; \theta \cos \; \theta,$$

$$\Gamma^\varphi_{\theta\varphi} = \cot \; \theta.$$

Define Φ by

$$\Phi = r^{-2}\partial_r (r - re^\chi \cos 2\alpha)$$

(noting that $\Phi=\Delta$ whenever $\chi=0$). The nonzero Ricci tensor components and the Ricci scalar are

$$R_{tt} = -(2r)^{-1} e^\chi \cos 2\alpha \; \partial_r (r^2 \Phi),$$

$$R_{tr} = -(2r)^{-1} \sin 2\alpha \; \partial_r (r^2 \Phi),$$

$$R_{rr} = (2r)^{-1} e^{-\chi} \cos 2\alpha \; \partial_r (r^2 \Phi),$$

$$R_{\theta\theta} = r^2 \Phi, \quad R_{\varphi\varphi} = r^2 \sin^2 \; \theta \Phi, \quad R = 2\Phi + r^{-1} \; \partial_r (r^2 \Phi).$$

The nonzero mixed components of the Einstein tensor are

$$G^t_t = G^r_r = -\Phi, \quad G^\theta_\theta = G^\varphi_\varphi = -(2r)^{-1} \partial_r (r^2 \Phi).$$

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Topological properties of single gravisolitons

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The possibility of assigning topological properties to gravisolitons has been recently discussed by Belinsky, who considered perturbations of certain diagonal metrics with two commuting Killing vectors. The discussion given by Belinsky relies on the properties of the solitonic part of the projection of the four-dimensional space–time metric onto the two-dimensional space spanned by the Killing vectors. In that context, for single soliton perturbations, he finds two types of, in principle, disjoint solutions, characterized respectively by the functions $\mu_{\rm in}$ and $\mu_{\rm out}$, such that one can assign a ''topological charge'' to the corresponding space–time. In this article we analyze this problem, studying in detail the single soliton perturbation of a Bianchi-type VI_0 background, and prove that when we consider the full four-dimensional metric, it is possible to construct locally smooth extensions that connect sectors associated to $\mu_{\rm in}$ to sectors associated to $\mu_{\rm out}$. Therefore, the concept of ''topological charge'' for this type of gravisolitons needs to be revised. Some ideas in this direction are discussed in this paper. We also show that this behavior is not restricted to the particular case of a Bianchi-type VI_0 background, but holds in general for the whole set of diagonal background metrics considered by Belinsky. An interesting side result is that the soliton perturbation ''erases'' the ''cosmological'' singularity that appears naturally in the background metrics, and that they can be extended to regions not covered in the original charts. In the particular case of a Bianchi-type VI_0 background, the resulting extended metric is regular everywhere. Finally we present an extension of the soliton metric to the background by matching these metrics through a null hypersurface. This extension requires the presence of a ''null dust'' on the matching hypersurface, and therefore the resulting space–time is not a vacuum everywhere. © *1996 American Institute of Physics.* [S0022-2488(96)01911-1]

I. INTRODUCTION

The possibility of assigning topological properties to gravisolitons has been recently discussed by Belinsky,[1] who considered perturbations of certain diagonal metrics with two commuting Killing vectors. These are of the form

$$ds^2=f_0(-dt^2+dz^2)+\alpha e^{u_0}(dx^1)^2+\alpha e^{-u_0}(dx^2)^2, \tag{1}$$

where f_0, α, and u_0 are functions of t and z. If we set $t=\xi-\eta$ and $z=\xi+\eta$, α and u_0 satisfy the equations

$$\alpha_{,\xi\eta}=0, \tag{2}$$

$$(\alpha u_{o,\xi})_{,\eta}+(\alpha u_{o,\eta})_{,\xi}=0. \tag{3}$$

We may then write

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$$\alpha = a(\xi) + b(\eta), \tag{4}$$

where a and b are arbitrary functions, and define

$$\beta = a(\xi) - b(\eta) \tag{5}$$

so that α and β are linearly independent solutions of the wave equation (2).

According to Ref. 1, the one-soliton metric on this background can be written in the form

$$ds^2 = f(t,z)(dz^2 - dt^2) + g_{ab}dx^a dx^b, \tag{6}$$

where $a,b = 1,2$ ($x^1 = x$, $x^2 = y$), and we have

$$g = \begin{pmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{pmatrix} = \frac{1}{2|\mu|\cosh(\rho)} \begin{pmatrix} (\mu^2 e^{\rho} + \alpha^2 e^{-\rho}) e^{u_0} & \alpha^2 - \mu^2 \\ \alpha^2 - \mu^2 & (\alpha^2 e^{\rho} + \mu^2 e^{-\rho}) e^{-u_0} \end{pmatrix} \tag{7}$$

and

$$f = c_0 f_0 \alpha^{1/2} |\mu| \cosh(\rho) (\alpha^2 - \mu^2)^{-1}. \tag{8}$$

We notice that any solution of the vacuum Einstein equations that can be written in the form (6) is defined up to an arbitrary constant multiplying the coefficient f. On this account, and for further convenience, we have explicitly included the real parameter c_0 in (8). The sign of this constant will determine the timelike or spacelike nature of the vectors $\partial/\partial t$ and $\partial/\partial z$.

The function $\mu(t,z)$ is a solution of the quadratic equation

$$\mu^2 + 2(\beta - w)\mu + \alpha^2 = 0 \tag{9}$$

in which w is an arbitrary real constant and the function $\rho(t,z)$ can be found by quadratures from the differential equations

$$\begin{aligned} \rho_{,\xi} &= (\alpha + \mu)(\alpha - \mu)^{-1} u_{0,\xi}, \\ \rho_{,\eta} &= (\alpha - \mu)(\alpha + \mu)^{-1} u_{0,\eta}. \end{aligned} \tag{10}$$

Following the notation of Ref. 1, the solutions of (9) can be written as

$$\begin{aligned} \mu_{\text{in}} &= (w - \beta)\{1 - [1 - \alpha^2 (w - \beta)^{-2}]^{1/2}\}, \\ \mu_{\text{out}} &= (w - \beta)\{1 + [1 - \alpha^2 (w - \beta)^{-2}]^{1/2}\}. \end{aligned} \tag{11}$$

These definitions are motivated by the fact that if $\mu = \mu_{\text{in}}$, then the values of μ are inside the interval $[-\alpha, \alpha]$, while for $\mu = \mu_{\text{out}}$ the corresponding values are outside that interval. It is clear from the previous expressions that the property, e.g., $\mu = \mu_{\text{in}}$ (or $\mu = \mu_{\text{out}}$), is maintained in any neighborhood where (7) and (8) are well defined and regular, since the functions f and ρ are singular when $\mu = \pm\alpha$.

The discussion given by Belinsky in Ref. 1 relies on the properties of the solitonic part of the projection of the four-dimensional space–time metric onto the two-dimensional space spanned by the Killing vectors. In that context, for single soliton perturbations, and in accordance with the previous discussion, he finds two types of, in principle, disjoint solutions, characterized respectively by having either $\mu = \mu_{\text{in}}$ or $\mu = \mu_{\text{out}}$, in such a way that one can assign a ''topological charge'' to the corresponding space–time.

There are, however, some difficulties in this interpretation when we look at the complete set of metric coefficients characterizing the solitonic solutions. As indicated in Ref. 1, we have

$$\mu_{\text{in}}\mu_{\text{out}}=\alpha^2. \tag{12}$$

Then, if we call ρ_{in} and ρ_{out} the functions ρ, defined by (10), associated respectively with μ_{in} and μ_{out}, it is easy to check that for any ρ_{in} we may choose ρ_{out} such that $\rho_{\text{in}}=-\rho_{\text{out}}$. However, as can be seen by making the appropriate replacements in (7) and (8), this means that if we call f_{in} and g^{in}_{ab} the metric coefficients in (7) and (8) corresponding to a solution with μ_{in} and ρ_{in}, and f_{out} and g^{out}_{ab} those corresponding to a solution with μ_{out} and ρ_{out}, and the same c_0, we have

$$g^{\text{in}}_{11}=g^{\text{out}}_{11}, \quad g^{\text{in}}_{12}=-g^{\text{out}}_{12},$$

$$g^{\text{in}}_{22}=g^{\text{out}}_{22}, \quad f^{\text{in}}=-f^{\text{out}}.$$

Since a change in sign in g_{12} corresponds to an isometry where we change the sign of either x^1 or x^2, we conclude that a solution with μ_{in} and ρ_{in}, and a certain choice of c_0, is indistinguishable from that corresponding to μ_{out} and ρ_{out} and the opposite sign of c_0. This discrete symmetry bears a certain formal resemblance to that present for the kink and anti-kink solitons in the Sine–Gordon equation, in the sense that one is formally indistinguishable from the other if we include the change $x\rightarrow -x$ as a symmetry operation. We also remark that a change in sign in c_0 corresponds to a change in the choice of which of $\partial/\partial t$ or $\partial/\partial z$ is timelike.

In this article we analyze these properties in detail, studying the particular example of the single soliton perturbation of a Bianchi-type VI_0 background. We show that when we consider the full four-dimensional metric, it is possible to construct locally smooth extensions that connect sectors associated to μ_{in} to sectors associated to μ_{out}. Furthermore, by some rather natural restrictions on the coordinate ranges, it is possible to give a simple and interesting geometrical interpretation to the soliton metric, where we find sectors with $\mu=\mu_{\text{in}}$ and sectors with $\mu=\mu_{\text{out}}$. Therefore, our results seem to indicate that the concept of ''topological charge'' for this type of gravisolitons needs to be revised. Some ideas in this direction are discussed in this paper in Sec. V, where the present case is compared to that of the Sine–Gordon equation.[2]

We also show that this behavior is not restricted to the particular case of a Bianchi-type VI_0 background, but holds likewise for the whole set of diagonal background metrics considered by Belinsky. An interesting general property, obtained as a side result in our derivation, is that the soliton perturbation ''erases'' the ''cosmological'' singularity that appears naturally in the background metrics. The proofs are given in two Appendices.

Finally we present an extension of the soliton metric to the background, by matching these metrics through the null hypersurfaces $\mu^2=\alpha^2$. These extensions require the presence of a ''null dust'' on the matching hypersurface, and therefore the resulting space–time is not a vacuum everywhere.

II. THE METRIC

We consider a single real pole soliton perturbation of a seed metric that is a particular case of the metrics of the form (1), and corresponds to a vacuum Bianchi-type VI_0 metric.[3] This seed metric can be written in the form

$$ds^2=f_0(dz^2-dt^2)+te^{2kz}dx^2+te^{-2kz}dy^2, \tag{13}$$

where $f_0=\exp(k^2t^2)/\sqrt{t}$ *and* $k>0$.

In the case of (13), $\alpha=t$, we may take $\beta=z$, and the functions μ and ρ can be written as

$$\mu_\epsilon = \omega - z + \epsilon[(\omega - z)^2 - t^2]^{1/2}, \tag{14}$$

$$\rho = 2k\epsilon[(\omega - z)^2 - t^2]^{1/2}, \tag{15}$$

where ω is an arbitrary constant and $\epsilon = \pm 1$. Comparing with Ref. 1, we have $\mu_{+1} = \mu_{\text{in}}$ and $\mu_{-1} = \mu_{\text{out}}$. Without loss of generality, we may set $\omega = 0$ in what follows, on account of the homogeneity of the background.

It is clear from these definitions that the coefficients g_{ij} depend only on t^2. Replacing the definitions of μ and ρ in (8), we have

$$f = c_0 \exp(k^2 t^2)|\mu|\cosh(\rho)/(\alpha^2 - \mu^2). \tag{16}$$

Therefore, the metric depends only on t^2, and any region with t restricted to $t<0$ is isometric to an appropriate region where $t>0$. Since there is, in principle, a singularity for $t=0$, on account of the vanishing of $\alpha = \det(g)^{1/2}$, we only need to consider $t>0$ in our analysis of the geometrical properties of the metric.

The single soliton metric resulting from (13) is a well-defined vacuum solution of Einstein's equations, only if we restrict to $z^2 > t^2$, because μ is complex when $z^2 < t^2$, and the metric is no longer real. Therefore, the regions $z>0$ and $z<0$ correspond to separate charts in the (t,z) plane. It is not difficult to show, however, that a single soliton metric defined for certain fixed c_0 and ϵ, in the region $z<0$, is isometric to a single soliton metric with the same c_0, but the opposite sign for ϵ, defined in the region $z>0$.[4] Since we are considering both signs for ϵ, we may, without loss of generality, restrict our discussion to the sector $z>0$, $t>0$, with $z>t$.

We now notice that, besides those already mentioned, there is also a singularity in f for $z^2 = t^2$, since in that case we have $\alpha^2 = \mu^2$, and the denominator vanishes. The consequences of the presence of this type of singularity in solitonic solutions have been analyzed in detail in Ref. 5. In the present case, the procedures developed in Ref. 5 to handle this problem may be applied as follows: if we consider the general form of the metric (6), together with the restriction $z>0$, $t>0$, which defines a sector whose boundaries are at $t=0$ corresponding to the vanishing of $\det(g)$, and $t=z$, where the square root in μ vanishes, we notice that we still have two possible choices for ϵ, and two signs for c_0. With the given restrictions, the coefficient f may be written as

$$f = c_0 \epsilon \frac{\exp(k^2 t^2)\cosh(\rho)}{2(z^2 - t^2)^{1/2}}. \tag{17}$$

This implies that $\partial/\partial t$ is timelike if $c_0\epsilon > 0$, corresponding to the choice made in Ref. 1, but $\partial/\partial t$ is spacelike when $c_0\epsilon > 0$, which is also a solution, not considered in Ref. 1.

We take first the case $c_0\epsilon > 0$, and notice that μ can be written in the form

$$\mu_\epsilon = -[(z-t)^{1/2} - \epsilon(z+t)^{1/2}]^2/2. \tag{18}$$

This suggests[5] the introduction of new coordinates u and v, given by

$$u = +(z+t)^{1/2}, \quad v = -(z-t)^{1/2}. \tag{19}$$

The region $z>t>0$ in the t,z plane is then mapped one-to-one to the region $u>-v>0$ in the u,v plane, and using (19) we find

$$\mu_\epsilon = -(u + \epsilon v)^2/2, \tag{20}$$

$$\rho = -2k\epsilon uv, \tag{21}$$

$$\alpha = t = (u^2 - v^2)2, \tag{22}$$

$$z=(u^2+v^2)/2. \tag{23}$$

The metric coefficients g_{ab} in the coordinate system $\{u,v,x,y\}$ are simply obtained by replacing, in the corresponding functions, the appropriate functional dependencies in u and v [Eqs. (20)–(23)]. Taking into account that $\epsilon=\pm 1$, this gives the following expressions for g_{ab}:

$$g_{11}=\frac{(u+v)^2\ \exp(k(u-v)^2)+(u-v)^2\ \exp(k(u+v)^2)}{4\cosh(2kuv)},$$

$$g_{12}=-\frac{\epsilon uv}{\cosh(2kuv)}, \tag{24}$$

$$g_{22}=\frac{(u+v)^2\exp(-k(u-v)^2)+(u-v)^2\ \exp(-k(u+v)^2)}{4\cosh(2kuv)}.$$

Then, using the relation $-dt^2+dz^2=4uv\,du\,dv$, after the coordinate transformation (19), we find

$$ds^2=-2\tilde{f}(u,v)\,du\,dv+\tilde{g}_{ab}(u,v)\,dx^a dx^b, \tag{25}$$

with $\tilde{g}_{ab}(u,v)=g_{ab}(t(u,v),z(u,v))$ and

$$\tilde{f}=\mathscr{C}_0\ \cosh(2kuv)\exp(k^2(u^2-v^2)^2/4), \tag{26}$$

where $\mathscr{C}_0=c_0\epsilon$ is a positive constant, on account of our choice $c_0\epsilon>0$.

The results summarized in (24) and (26), though rather surprising, because it is apparent that almost all information on ϵ (and, therefore, on μ_{in} and μ_{out}) has been lost, except for the sign of the coefficient g_{12}, are in agreement with the discussion in Sec. I. Moreover, as indicated, even this sign has no *a priori* (local) geometrical meaning, because it can be changed to the opposite by a linear isometry in x^1 and x^2. The situation may be different, however, if we consider global properties of the solitonic solutions.

We remark again that (25) is isometric to (6) in the region $u>-v>0$. However, it is clear from (24) and (26) that the solitonic metric (25) is well defined and regular for $v=0$ (that is, $z=t$) and for $u>v>0$. The region $u>v>0$ in (25) corresponds, therefore, to a locally smooth extension of (6) through the hypersurface $z=t$, where the coordinate system of (6) is singular.

To clarify the nature of this extension to $v>0$, we consider again the metric in (t,z) coordinates, but now in the case $c_0\epsilon<0$, where $\partial/\partial t$ is spacelike. We define new coordinates u and v by

$$u=+(z+t)^{1/2},\quad v=(z-t)^{1/2}, \tag{27}$$

which now map one-to-one the region $z>t>0$ in the t,z plane to the region $u>v>0$ in the u,v plane. If we carry out the same procedures as in the previous case, we find exactly the same forms (24) and (26) for the transformed metric coefficients (up to an isometry of the form $x\to -x$), provided we define, in this case, the positive constant $\mathscr{C}_0$ by $\mathscr{C}_0=-c_0\epsilon$. This metric is, in this case, defined for $v>0$, but, on account of the previous discussion, it is trivially smoothly extended to the region $v<0$. Thus, if we consider the metric defined by (24) and (26) in the whole region $u>0$, $-u<v<u$, we find that all the single soliton metrics derived from (13), with a given value of $|c_0|$, and any ϵ, can be isometrically mapped to either the region $v>0$, or the region $v<0$, of a single (u,v) chart, where the metric takes the form (24) and (26), with $\mathscr{C}_0=|c_0|$. In other words, all forms of the single soliton metrics derived from (13) are contained in the extended (u,v) chart.

Going back to the question of the distinction between μ_{in} and μ_{out}, we notice that going from $v<0$ to $v>0$ corresponds formally to the change $v\to -v$. However, a change in sign in the

coordinate v is equivalent to the change $\epsilon \to -\epsilon$ along with a change of sign in f. Therefore, the original sector $z>t>0$ of an ϵ-type single soliton metric is smoothly extended to a similar sector, $z>t>0$, of a $-\epsilon$-type single soliton metric, but with the opposite sign for the c_0 parameter, that is, to a sector where $\partial/\partial t$ is spacelike and $\partial/\partial z$ is timelike. Thus, the metric (25) smoothly matches a region of space–time where $\mu=\mu_{\text{in}}$ with a region where $\mu=\mu_{\text{out}}$, a result that does not agree, in principle, with that described in Ref. 1. We shall comment more on this below, but first we will consider further extensions of (25), and show the interesting fact that in these the solitonic perturbation ''erases'' the ''cosmological singularity'' present in (13) for $t=0$.

As a final comment on this section, we remark that the possibility of smoothly extending the soliton metric through the hypersurfaces $\mu^2=\alpha^2$ is not restricted to the Bianchi-type VI_0 metrics, but, as shown in Appendix B, holds for general single soliton transformations of background metrics of the form (1).

III. GEOMETRICAL INTERPRETATION

The metric (25) is regular everywhere in the region $u>|v|$, but, since we have $\det(g)^{1/2}=(u^2-v^2)/2$, it is singular for $u=\pm v$. In this section we analyze the nature of these singularities of the soliton solution and show that with appropriate choices and restrictions on the coordinate systems, the metric can be made regular both for $u=v$ and $u=-v$.

The analysis is simplified if we introduce new coordinates, τ and R, related to u and v by

$$\tau=u+v, \quad R=u-v. \tag{28}$$

In terms of these coordinates, the metric coefficients take the form

$$2\tilde{f}(u,v)du\,dv=F(\tau,R)(-d\tau^2+dR^2)=\tfrac{1}{2}\mathscr{C}_0\cosh[k(R^2-\tau^2)/2]\exp(k^2R^2\tau^2/4)(-d\tau^2+dR^2) \tag{29}$$

and

$$g=\frac{1}{4\cosh[k(R^2-\tau^2)/2]}\begin{pmatrix}\tau^2\exp(kR^2)+R^2\exp(k\tau^2) & \epsilon(R^2-\tau^2)\\ \epsilon(R^2-\tau^2) & \tau^2\exp(-kR^2)+R^2\exp(-k\tau^2)\end{pmatrix}. \tag{30}$$

We notice that $\det(g_{ab})=R^2\tau^2/4$. That is, the singularities for $u=v$ and $u=-v$ appear in this coordinate system as singularities for $R=0$ and $\tau=0$. To analyze their structure, we consider the behavior of the metric coefficients in the limits $R\to 0$ and $\tau\to=0$.

We first notice that near $R=0$ we have

$$g\simeq\frac{1}{4\cosh[k\tau^2/2]}\begin{pmatrix}\tau^2+R^2\exp(k\tau^2) & -\epsilon\tau^2\\ -\epsilon\tau^2 & \tau+R^2\exp(-k\tau^2)\end{pmatrix} \tag{31}$$

while

$$2F(\tau,R)\simeq\mathscr{C}_0\cosh[k\tau^2/2], \tag{32}$$

These results suggest that we may ''diagonalize'' the metric (near $R=0$ and to order R^2) by introducing a ''rotation'' in the x,y plane, defining new coordinates η and Φ by the relations

$$x=\Phi-\epsilon\eta, \quad y=\Phi+\epsilon\eta. \tag{33}$$

With this change of coordinates the Killing part of the metric becomes

$$g_{\Phi\Phi}=\frac{R^2\ \cosh(k\tau^2)+\tau^2\cosh(kR^2)+(R^2-\tau^2)}{2\ \cosh(k(R^2-\tau^2)/2)}, \tag{34}$$

$$g_{\eta\Phi}=\frac{R^2\ \sinh(k\tau^2)+\tau^2\ \sinh(kR^2)}{2\ \cosh(k(R^2-\tau^2)/2)}, \tag{35}$$

$$g_{\eta\eta}=\frac{R^2\ \cosh(k\tau^2)+\tau^2\ \cosh(kR^2)-(R^2-\tau^2)}{2\ \cosh(k(R^2-\tau^2)/2)}, \tag{36}$$

and in the limit $R\to 0$, the leading orders of the metric coefficients are of the form

$$F=\tfrac{1}{2}\mathscr{C}_0\ \cosh(k\tau^2/2)+\mathscr{O}(R^2), \tag{37}$$

$$g_{\Phi\Phi}=\cosh(k\tau^2/2)R^2+\mathscr{O}(R^4), \tag{38}$$

$$g_{\Phi\eta}=\mathscr{O}(R^2), \tag{39}$$

$$g_{\eta\eta}=\frac{\tau^2}{\cosh(k\tau^2/2)}+\mathscr{O}(R^2). \tag{40}$$

However, then the singularity for $R=0$ is removed if we choose $C_0=2$, restrict Φ and R to the ranges $0\leqslant R<\infty$, $0\leqslant\Phi\leqslant 2\pi$, and identify $\Phi=0$ and $\Phi=2\pi$, because in this case, for $\tau\neq 0$, the singularity along $R=0$ can be interpreted as the coordinate singularity along a regular symmetry axis in cylindrical spatial coordinates.[6]

Similarly, taking as before $\mathscr{C}_0=2$, near $\tau=0$, the leading orders of the metric coefficients are of the form

$$\begin{aligned} F&=\cosh(kR^2/2)+O(\tau^2),\\ g_{\Phi\Phi}&=\frac{R^2}{\cosh(kR^2/2)}+O(\tau^2),\\ g_{\Phi\eta}&=O(\tau^2),\\ g_{\eta\eta}&=\cosh(kR^2/2)\,\tau^2+O(\tau^4). \end{aligned} \tag{41}$$

This form of the metric coefficients implies that the singularity for $\tau=0$ is of the Rindler type. It can be removed by the following coordinate transformation:[7]

$$T=\tau\ \cosh(\eta),\quad Z=\tau\ \sinh(\eta). \tag{42}$$

This transformation maps the region $\tau>0$, $-\infty<\eta<+\infty$, of the (τ,η) plane to the region $T\geqslant|Z|$ of the (T,Z) plane. However, after replacing the new coordinates in the metric coefficients, it is easy to check that the new metric is defined for *all* values of T and Z, and the already defined ranges for Φ and R, and can be, therefore, naturally extended to the regions $|T|<|Z|$.

We notice, however, that the extended regions $|T|<|Z|$ do not correspond to any of the regions defined by the ''canonical'' chart (t,z,x^1,x^2). This is easily seen if we transform the metric to new coordinates $\tilde{\tau}$ and $\tilde{\eta}$ defined by

$$T=\tilde{\tau}\ \sinh(\tilde{\eta}), \tag{43}$$

$$Z=\tilde{\tau}\ \cosh(\tilde{\eta}). \tag{44}$$

In this case the new metric coefficients corresponding to the regions $|T|<|Z|$ have the same formal expressions as (29) and (30) but with the (formal) replacement $\tau\to i\tilde{\tau}$. Since the metric depends on τ only through τ^2, the net effect is that $\partial/\partial\tilde{\tau}$ is now *spacelike*. Moreover, the determinant of g_{ab}, namely α^2, is now given by $-\tilde{\tau}^2R^2$, and becomes negative. Therefore, one of the Killing vectors changes from spacelike to timelike when we cross the boundary $\tau^2=0$, and the metric is actually *stationary* in the regions $|T|<|Z|$.

This dependence of the metric on τ^2 implies also that the solitonic metric is symmetric also with respect to T, where the metric is regular for $T=0$. Therefore $T=0$ corresponds to a moment of time symmetry for the whole space–time.

One may shed more light on the nature of the symmetries of this space–time by considering the Killing vector $\partial/\partial\eta$. In the chart (τ,η,R,Φ), its norm is given by $g_{\eta\eta}$. In the coordinate chart (T,R,Φ,Z), in the overlap region $T^2>Z^2$, we have

$$\frac{\partial}{\partial\eta}=T\,\frac{\partial}{\partial Z}+Z\,\frac{\partial}{\partial T}, \tag{45}$$

but it is clear that the right-hand side of (45) provides a smooth, well-defined extension for $\partial/\partial\eta$ to the whole (T,R,Φ,Z) chart, which is also a Killing vector field. We shall retain the name $\partial/\partial\eta$ for this extended field. Its norm is given by

$$\frac{\partial}{\partial\eta}\cdot\frac{\partial}{\partial\eta}=\frac{R^2\,\sinh[k(T^2-Z^2)]+(T^2-Z^2)\sinh(kR^2)}{2\,\cosh[k(R^2+Z^2-T^2)/2]} \tag{46}$$

and, therefore, $\partial/\partial\eta$ is spacelike for $T^2>Z^2$, timelike when $T^2<Z^2$, and null on the hypersurface $T^2=Z^2$.

In particular, in the region $T^2>Z^2$, for fixed τ, the trajectories of $\partial/\partial\eta$ generate a spacelike hypersurface that nowhere touches the null hypersurfaces $T^2=Z^2$. This latter hypersurface, which corresponds to $\tau=0$ is, in turn, smoothly generated by the trajectories of the *extended* $\partial/\partial\eta$, but has no image on the (τ,η,R,Φ) chart, since $\tau=0$ is outside that chart.

It is interesting to look at the form of the fronts corresponding to either $u=0$ or $v=0$. From the equalities

$$-4\epsilon uv=\tau^2-R^2=T^2-Z^2-R^2, \tag{47}$$

we find that these null hypersurfaces correspond to (topological) spheres which are contracting for $T<0$ and expanding for $T>0$. The constant T two-dimensional sections of these hypersurfaces approach a spherical shape for small $|T|$, but their form is distorted in general, on account of the nonflat nature of the background where they propagate. However, suppose now that we look at the functions $\mu_{\rm in}$ and $\mu_{\rm out}$ in the region $u>-v>0$, with u and v considered as functions of T, R, and Z. We have

$$\mu_{\rm in}=-\tfrac{1}{2}(T^2-Z^2), \tag{48}$$

$$\mu_{\rm out}=-\tfrac{1}{2}R^2, \tag{49}$$

$$\alpha^2=\tfrac{1}{4}(T^2-Z^2)R^2. \tag{50}$$

As we approach and cross the boundary $v=0$ from $v<0$ to $v>0$, we move from the region $T^2-Z^2>R^2$, where $|\mu_{\rm in}|<\alpha$ to the region $T^2-Z^2>R^2$, where $|\mu_{\rm in}|>\alpha$, while the opposite is true for $|\mu_{\rm out}|$. This confirms our assertion that the extension through $v=0$ connects a region associated to $\mu_{\rm in}$ to one associated to $\mu_{\rm out}$. However, as we have already indicated, there seems to be no natural isometrically invariant way of assigning either μ to the extended soliton metric. We shall comment more on this below.

Summarizing results, we have found that the solitonic metrics can be extended to define a space–time where the metric is regular everywhere. These space–times contain, in general, two stationary regions separated by a nonstationary region, isometric to the original soliton metric. The hypersurface where we have the transition from stationary to nonstationary corresponds to the original ''cosmological singularity,'' which is, therefore, eliminated by the soliton transformation. This behavior is not restricted to the Bianchi-type VI_0 background. In Appendix A we show that this ''cosmological singularity'' appears, in general, for background metrics of the form (1), and that it is ''cancelled'' in the soliton transformation.

IV. MATCHING THE SOLITON SOLUTION TO THE BACKGROUND

We have already indicated that in the original chart $\{t,z,x,y\}$ there is a singularity in the coefficient f when $\mu\to\pm\alpha$. However, since we also have in this case $\rho\to 0$, the remaining coefficients g_{ab} $(a,b=x,y)$ have a finite limit which coincides with that of the corresponding coefficients in the background metric. It is then tempting to try to find an extension of the soliton metric that matches it to the background through the hypersurfaces $z=\pm t$, where we have $\mu^2=\alpha^2$.

Let us consider again the soliton metric in the sector $z>t>0$. The coordinate singularity in f can be eliminated if we apply the coordinate transformation (19). The matching hypersurface $z=t$ is then approached by taking the limit $v=0$ from the region $v<0$, and we have the following expansions for the solitonic metric coefficients near $v=0$:

$$\tilde{f}=c_0\epsilon\,\exp(k^2u^4/4)+\mathcal{O}(v^2), \tag{51}$$

$$g_{11}=\frac{u^2}{2}\exp(ku^2)+\mathcal{O}(v^2), \tag{52}$$

$$g_{12}=\epsilon uv+\mathcal{O}(v^2), \tag{53}$$

$$g_{22}=\frac{u^2}{2}\exp(-ku^2)+\mathcal{O}(v^2). \tag{54}$$

We may, on the other hand, introduce the coordinate change

$$u=+(z+t)^{1/2},\quad v=-(z-t) \tag{55}$$

in the region $t>z>0$ of the background metric. The matching surface is then approached by taking the limit $v=0$ from positive values of v. In this case, the expansions for the seed metric coefficients for $v>0$, near $v=0$, are

$$\tilde{f}=\sqrt{2}\,\exp(k^2u^4/4)+\sqrt{2}\,\exp(k^2u^4/4)\,\frac{1-k^2u^4}{2u^2}\,v+\mathcal{O}(v^2), \tag{56}$$

$$g_{11}=\frac{u^2-v}{2}\exp(ku^2)+\mathcal{O}(v^2), \tag{57}$$

$$g_{12}=0, \tag{58}$$

$$g_{22}=\frac{u^2-v}{2}\exp(-ku^2)+\mathcal{O}(v^2). \tag{59}$$

Therefore, we conclude that, if we take $c_0\epsilon=\sqrt{2}$ in (51), the solitonic metric and the background metric can be matched continuously through the null hypersurface $v=0$. We notice, how-

ever, that although the metric coefficients are continuous in $v=0$, their first derivatives have finite jumps on this hypersurface. Since this is a null hypersurface, this type of behavior of the metric can be interpreted in terms of the presence of a matter shell (null dust) or of an impulsive gravitational wave, depending on the detailed structure of the singularity. This interpretation can be inferred from the fact that the Ricci tensor may, in this case, contain terms of the form[8] $\delta(v)$ or $\theta(v)$. On the other hand, because of the continuity of the metric coefficients, there will be terms containing a $\delta(v)$ function only in those components of the Ricci tensor that contain a second derivative of a metric coefficient with respect of the v coordinate. The only component of the Ricci tensor satisfying this requirement is R_{vv}, which, for a general metric of the form (7) and (8), can be written as

$$R_{vv}=\frac{\alpha_{,vv}}{\alpha}+\text{terms with lower derivatives in } v, \tag{60}$$

where the ''terms with lower derivatives in v'' give actually a vanishing contribution, on account of the fact that the metric is a vacuum solution for $v\neq 0$.

To compute R_{vv}, near the hypersurface $v=0$, we write α in the form

$$\alpha=\frac{u^2}{2}-\frac{v^2}{2}\,(1-\theta(v))-\frac{v}{2}\,\theta(v), \tag{61}$$

which leads to

$$R_{vv}=\frac{\delta(v)}{u^2}, \tag{62}$$

while the other components of the Ricci tensor vanish. The corresponding energy-momentum tensor can be interpreted as representing surface distribution of null dust located on $v=0$ with a positive energy density ρ proportional to u^{-2}.

In order to have a more symmetric space–time, we may consider the solitonic solution (6) in the region $-z>t>0$ and match it again to the background metric on the hypersurface $z=-t$. This is easily achieved by a simple modification of the previous procedure. The result is that, for any $t\neq 0$, we have two solitonic regions, one for $z>t$ and the other for $-z>t$, matched to the background metric through the hypersurfaces $|z|=t$. The matching requires the presence of surface distributions of null dust, with nonvanishing positive energy density, confined to the hypersurfaces $|z|=t$.

We notice that again the matching does not impose any condition on the functions μ, and it is possible to have solitons of the same or opposite sign for ϵ in the solitonic regions.

V. FINAL COMMENTS

The analysis carried out in this paper shows that the solitonic metrics considered by Belinsky in Ref. 1 can be locally (smoothly) extended in such a way that in a single chart the function μ satisfies, e.g., $|\mu|<|\alpha|$ in one region, and $|\mu|>|\alpha|$ in another. The distinction between μ_{in} and μ_{out} as indicating a topological characteristic of the solution does not appear then to be as clear as inferred from the considerations given in Ref. 1.

This situation is somewhat worsened if we consider also the equivalence of the metrics under isometric mappings, for, in this case, we have shown that a metric obtained using, say, μ_{in}, is isometric to a metric obtained starting with μ_{out}.

There is here, however, an important point that makes again contact with the topological character of some classical solitons. Consider, for instance, the Sine–Gordon equation,

$$\frac{\partial^2\phi(x,t)}{\partial t^2}-\frac{\partial^2\phi(x,t)}{\partial x^2}+\sin\ \phi(x,t)=0. \tag{63}$$

As is well known, it is possible to construct soliton solutions of this equation, known as *kinks* and *antikinks*, which are different solutions as long as we do not consider as equivalent situations related by the transformation $x\rightarrow -x$, which leaves the equation invariant, but changes a *kink* into an *antikink*. In other words, even though (63) is invariant under $x\rightarrow -x$, to be able to distinguish between the two types of topological solitons, we must exclude this *discrete* transformation[9] for there is no *intrinsic* property that we can use to distinguish between a kink and an antikink. Therefore, if we consider that solutions of (63) related by coordinate transformations (discrete or not) are equivalent, then the only apparent way of deducing the existence of two different solutions is by introducing some additional structure that defines a preferential orientation on the x axis. This structure could be the result of the presence of fields in the physical situation considered, or we could consider a solution of (63) with a kink and an antikink. In the latter case, we could easily recognize the difference between the kink and antikink solutions in the asymptotic regions of the multi-kink solution.

Similarly, the isometry that makes the solutions related to $\mu_{\rm in}$ and to $\mu_{\rm out}$ equivalent is a *discrete* transformation that corresponds to change in the orientation of the space axis. If we exclude these changes, we still have *two* types of soliton, and, although the reference to $\mu_{\rm in}$ and to $\mu_{\rm out}$ is essentially lost, they in some sense resemble even more the *kink* and *antikink* solutions of (63) because they are indistinguishable under certain discrete symmetry of their governing equation, but correspond to different solutions for a given *fixed* orientation of the space axis. Again, just as in the case of (63), where, assuming that $\phi(x,t)$ represents some physical quantity, we would not know if the situation corresponds to a kink or an antikink until we fix an orientation for the x axis, we have in the gravisoliton case a sort of ''rotation'' or ''twist'' that allows us to distinguish between a ''gravisoliton'' and an ''antigravisoliton,'' only after we have somehow fixed the orientation of the space axis of our reference system, but there is no intrinsic feature that we can use to distinguish one from the other.

Finally, it is also possible that, as in the case of the solutions of (63), in the gravitational case we could note the differences between the two types of gravisolitons analyzing multisoliton solutions, along lines similar to those given in Ref. 1. This possibility will be considered elsewhere.

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APPENDIX A: BEHAVIOR NEAR $\alpha=0$

In this Appendix we consider the behavior of a general metric of the form (1) near $\alpha=0$. We assume that $g^{\mu\nu}\alpha_{,\nu}$ is timelike. It is clear from (1) and (4) that in any neighborhood here both $a(\xi)$ and $b(\eta)$ and their first derivatives are nonvanishing we may choose coordinates t and z that preserve the form (1) and where $\alpha=t$. We impose the (mild) restriction that there is such a coordinate system in a neighborhood of $\alpha=0$. Then, the vacuum Einstein equations for (1) can be put in the form

$$\frac{\partial^2 u_0(t,z)}{\partial z^2}-\frac{\partial^2 u_0(t,z)}{\partial t^2}-\frac{1}{t}\frac{\partial u_0(t,z)}{\partial t}=0 \tag{A1}$$

and

$$\frac{1}{f_0}\frac{\partial f_0}{\partial z}=t\,\frac{\partial u_0}{\partial t}\frac{\partial u_0}{\partial z}, \tag{A2}$$

$$\frac{1}{f_0}\frac{\partial f_0}{\partial t}=-\frac{1}{2t}+\frac{t}{2}\left(\frac{\partial u_0}{\partial t}\right)^2+\frac{t}{2}\left(\frac{\partial u_0}{\partial z}\right)^2. \tag{A3}$$

It is easily checked that (A1) is precisely the integrability condition for the system (A2) and (A3). We therefore assume that $u_0(t,z)$ is regular near $t=0$. Then we may write

$$u_0(t,z)=u_{00}(z)+u_{01}(z)t+u_{02}(z)t^2+u_{03}(z)t^3+u_{04}(z)t^4+\cdots . \tag{A4}$$

Replacing in (A1) we find that the coefficients of odd powers of t should be zero. The function $u_{00}(z)$ is arbitrary, and the other coefficients are determined once u_{00} is given. In particular we have

$$u_{02}(z)=\frac{1}{4}\frac{d^2u_{00}}{dz^2};\quad u_{04}(z)=\frac{1}{64}\frac{d^4u_{00}}{dz^4};\quad \cdots . \tag{A5}$$

We notice that the simplest choice for u_{00}, namely $u_{00}=2kz$, corresponds to the Bianchi-type VI_0 background.

Using this result in (A2) and (A3), we find the behavior of f_0 near $t=0$. This is given by

$$\ln f_0=\ln C_0-\frac{1}{2}\ln t+\frac{1}{4}t^2\left(\frac{du_{00}}{dz}\right)^2+\mathcal{O}(t^4). \tag{A6}$$

Therefore, for a general $u_0(t,z)$, regular near $t=0$, the function f_0 is the product $t^{-1/2}$ times a regular part. In other words, in all these metrics f_0 contains a factor $\alpha^{-1/2}$, which can be associated to a ''cosmological'' singularity. This factor is precisely cancelled in the single soliton transformation, which, therefore, has the effect of ''erasing'' the singularity.

APPENDIX B: BEHAVIOR NEAR $|\mu|=|\alpha|$

In this Appendix we consider the behavior of a general metric of the form (1) near $|\mu|=|\alpha|$. We assume that $g^{\mu\nu}\alpha_{,\nu}$ is timelike. In particular, we assume that $da/d\xi$ and $db/d\eta$ are nonvanishing in a neighborhood of the region where $|\mu|=|\alpha|$. We may then define new coordinates u and v, given by

$$u=[2a(\xi)-w]^{1/2},\quad v=-[-2b(\eta)-w]^{1/2}. \tag{B1}$$

In these new coordinates we have

$$\alpha=\tfrac{1}{2}(u^2-v^2),\quad \mu=-\tfrac{1}{2}(u+\epsilon v)^2,\quad \beta=\tfrac{1}{2}(u^2-v^2)+w, \tag{B2}$$

and the condition $|\mu|=|\alpha|$ is satisfied for either $u=0$ or $v=0$.

It is easy to check that the equations for ρ can be written in the form

$$\rho_{,u}=-\epsilon\frac{v}{u}u_{0,u},\quad \rho_{,v}=-\epsilon\frac{u}{v}u_{0,v}. \tag{B3}$$

The integrability condition for ρ is

$$2\alpha u_{0,}uv+\alpha_{,u}u_{0,v}+\alpha_{,v}u_{0,u}=0, \tag{B4}$$

which is equivalent to (3), in u,v coordinates.

We shall analyze the behavior of the metric coefficients near $v=0$. We assume regularity of u_0 in the sense that it admits an expansion of the form

$$u_0(u,v)=u_{o0}(u)+u_{o1}(u)v+u_{o2}(u)v^2+u_{o3}(u)v^3+\cdots . \tag{B5}$$

Then, (B4) puts no restriction on $u_{o0}(u)$, but u_{o1} must be of the form $u_{o1}=C/u$, where C is a constant, while the other terms should satisfy equations such as

$$2u^2\frac{du_{o2}}{du}+2uu_{o2}=\frac{du_{o0}}{du}, \tag{B6}$$

which do not mix coefficients of even and odd powers of v. If we replace (B5) in (B3), we find that ρ should be of the form

$$\rho(u,v)=-\epsilon uu_{o1}\ln v-2\epsilon uu_{o2}v+\cdots . \tag{B7}$$

If we further require regularity of u_0 near $u=0$, we should have $u_{o1}=0$, and all coefficients of odd powers of v should also vanish. The coefficients of even powers of v can, on the other hand, be chosen such that the expansion (B5) is regular and nontrivial near $u=0$. With this restriction we have that ρ vanishes at least as v for $v=0$. A simple example is, of course, the Bianchi-type VI_0 case analyzed in this paper, where $\rho=-2k\epsilon uv$.

Going back to the general form of the metric, if, as required by the regularity conditions on u_0, $\rho=0$ when $v=0$, that is, when $\mu^2=\alpha^2$, then g_{ab} is regular in a neighborhood of $v=0$, and coincides with the background metric for $v=0$. However, the full metric is not regular because there is a vanishing denominator and, therefore, a singularity in f. It is easy to show that singularity is related to coordinate choice and can be eliminated by an adequate change of coordinates. Namely, if we consider u and v as new coordinates, it is easy to verify that

$$\begin{aligned} f(t,z)(dz^2-dt^2)&=c_0f_0\alpha^{1/2}|\mu|\,\frac{\cosh(\rho)}{(\alpha^2-\mu^2)}\,d\xi d\eta \\ &=\sqrt{2}\epsilon c_0f_0(u^2-v^2)^{1/2}\cosh(\rho)\left(\frac{db}{d\eta}\frac{da}{d\xi}\right)^{-1}dudv, \end{aligned}$$

and, clearly, the last expression is regular for $v=0$, and the singularity has been cancelled.

[1] V. A. Belinsky, Phys. Rev. D **44**, 3109 (1991).
[2] The fact that there is no fundamental difference between ''in'' and ''out'' solitons, and the possibility of extending the single soliton metric to the background, are contained in one of authors (AG) doctoral thesis, (Universidad Nacional de Córdoba, December, 1994). After submission of this paper we learned that similar results are indicated by P. Kordas in his thesis (University of London, 1995). We are grateful to the referee for this latter reference.
[3] M. A. H. MacCallum, Ph.D. thesis, University of Cambridge, 1970.
[4] The isometry requires also that x and y be exchanged.
[5] M. C. Diaz and R. J. Gleiser, Gen. Rel. Gravit. **20**, 517 (1988).
[6] The choice $\mathscr{C}_0=2$, once we impose the restriction $0\leqslant\Phi\leqslant 2\pi$, with $\Phi=0$ identified with $\Phi=2\pi$, is the natural one, if we want to avoid a ''conical singularity'' for $R=0$. These ''conical singularities'' have been used to represent ''thin cosmic strings,'' but, for simplicity, we are not including this possibility in our discussion. Similarly, we do not consider more complex ''cut and paste'' type of singularities that would result from different identifications in the range of Φ.
[7] A similar transformation, but with a rescaling in T and Z, may be used to remove the singularity in the case $\mathscr{C}_0\neq 2$.
[8] See, e.g., R. Geroch and J. Traschen, Phys. Rev. **36**, 1017 (1987), for a formal treatment the sense of the theory of distributions.
[9] Incidentally, from a three-dimensional point of view, this would correspond to a reflection on the $x=0$ plane.

Noncommutative structure of singularities in general relativity

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Initial and final singularities in the closed Friedman world model are typical examples of *malicious* singularities. They form the single point of Schmidt's *b*-boundary of this model and are not Hausdorff separated from the rest of space–time. The method of noncommutative geometry, developed by A. Connes and his co-workers, is applied to this case. We rephrase Schmidt's construction in terms of the groupoid G of orthonormal frames over space–time and carry out the ''desingularization'' process. We define the line bundle $\tau:\Omega^{1/2}\rightarrow G$ over G and change the space of its cross sections into an involutive algebra. This algebra is represented in the space of operators on a Hilbert space and, with the norm inherited from these operators, it becomes a C^*-algebra. The initial and final singularities of the closed Friedman model are given by two distinct representations of this C^*-algebra in the space of operators acting on the Hilbert space $L^2(O(3,1))$. © *1996 American Institute of Physics.* [S0022-2488(96)01009-2]

I. INTRODUCTION

The problem of correctly defining singularities which appear in relativistic cosmology and relativistic astrophysics has been recently less investigated than it deserves. This is probably so because of the prevailing opinion that in the quantum gravity theory singularities will be irrevocably eliminated. However, this is not at all certain,[1] and—as we shall argue in the present paper—it may turn out that the study of classical singularities could suggest some indications concerning the looked for quantum gravity theory. Besides, the nature of classical singularities is interesting from the mathematical point of view and certainly deserves further study.

In the famous theorems of Hawking and Penrose on the existence of singularities, the latter were effectively identified with the geodesic incompleteness of space–time.[2] It was Schmidt[3] who proposed a very elegant construction of a singular boundary of space–time. Singularities were understood by him as points of this boundary, called *b-boundary* of space–time, and identified not only with the endpoints of (timelike and null) incomplete geodesics but also with the endpoints (in the generalized affine parameter) of timelike curves of bounded acceleration. This definition of singularities was soon accepted as the best available one within the framework of relativistic theories of gravitation. However, its popularity suddenly ended when Bosshard[4] and Johnson[5] demonstrated that in the closed Friedman world model the initial and final singularities formed the single point of the *b*-boundary, and that *b*-boundaries of the closed Friedman model and of the Schwarzschild solution are not Hausdorff separated from the rest of space–time. Some attempts to modify Schmidt's construction were lacking either the required generality or the original elegance.[6] In practice, Schmidt's construction was soon eliminated from current research.

We have returned to Schmidt's definition of singularities by looking at it from a slightly

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different perspective. In our previous works[7] we have demonstrated that all troubles connected with the b-boundary construction have their origin in the fact that it is carried out in the bad category, namely in the category of smooth manifolds, whereas space–times with their singularities, from their very nature, go beyond this category. We have also shown that one can effectively work with the b-completed closed Friedman model (i.e., with its space–time together with its b-boundary) within the category of structured spaces. The structured space concept is based on the idea of ''algebraization'' of geometry, and it was Koszul who, in his classical paper,[8] gave a dictionary for translating geometry into algebra. By a *structured space* we mean the pair (M,C), where M is a topological space and C the sheaf of algebras of real functions on M such that, for any open set $U \in M$ and any functions $f_1,\ldots,f_n \in C(U)$, $\omega \in C^\infty(\mathbf{R})$, one has $\omega \circ (f_1,\ldots,f_n) \in C(U)$. The sheaf C is called the *differential structure* on M. The theory of structured spaces, developed in Ref. 9, is a strong generalization of the theory of smooth manifolds (any function belonging to the differential structure is *ex definitione* assumed to be smooth). By using the theory of structured spaces one can safely work with the b-completed closed Friedman M space–time as long as one deals with local cross sections of $C(U)$ and local vector fields on $U \subset M$. However, one must be cautious since there exists the unique differential structure which can be prolonged to the b-completed space–time, namely the one consisting only of constant functions. If one ''touches'' either of the two singularities (i.e., if one prolongs the differential structure to the singularity), pathologies immediately occur: the differential structure consists only of constant functions, there exist only zero derivations of such functions, i.e., zero vector fields, and consequently the ''bundle length'' of a curve joining the singularity with any point in space–time is zero, and everything shrinks to the single point.

To deal with similar ''pathological situations,'' Alain Connes[10] developed his noncommutative approach to geometry. This approach is a further generalization as compared with our structured space theory. Functional algebras appearing in the differential structure of structured spaces, being functional, are always commutative. In Connes' approach, the entire information about a given geometry is encoded in a non-necessarily commutative algebra. If this algebra happens to be commutative, it is essentially equivalent to the complex counterpart of our differential structure. Noncommutative algebras are indispensable in dealing with strongly singular situations. The aim of the present paper is to analyze space–times with b-boundaries, and in particular b-completed space–time of the closed Friedman model, within the framework of Connes' noncommutative geometry. We strictly follow Connes method; our only modification consists in replacing the ordinary concept of smoothness (in the manifold category) by its generalized counterpart in the theory of differential spaces.

In Sec. II we give a short account of Schmidt's construction and rephrase it in terms of the groupoid theory. In Sec. III we discuss the groupoid counterpart of singular fibers. By constructing the suitable line bundle on this groupoid we perform what could be called the *desingularization* process. Cross sections of this line bundle with suitably defined convolution (as ''multiplication'' of cross sections) and involution form a (noncommutative) involutive algebra. This algebra can be represented in the space of operators on a Hilbert space and, with the norm inherited from these operators, it becomes a C^*-algebra. With the help of this algebra we gain the insight into the structure of the initial and final singularities in the Friedman model. All this is presented in Sec. IV. Section V contains a discussion of the obtained results. Both initial and final singularities are given in terms of the algebra of operators acting on the Hilbert space $L^2(O(3,1))$ of square integrable functions defined on the Lorentz group [let us notice that by replacing $O(3,1)$ by its double covering we are led to the spinorial formalism]. It might well be that classical singularities are not entirely classical; they somehow seem to know that in the extreme conditions of shrinking quantum structures must be used to model physical processes.

II. FRAME BUNDLE OVER SPACE–TIME AS A GROUPOID

Schmidt's construction of the b-boundary of space–time can be summarized in the following way (details can be found in Ref. 3). Let M be a space–time carrying the Lorentz metric, and OM

(the connected component of) the orthonormal frame bundle over M, $\pi:OM\to M$. The Levi–Civita connection in M determines the family of uniformly equivalent Riemannian (positive definite) metrics on OM. We select one of them and notice that further construction does not depend of the particular choice. With the help of this metric we determine the distance function on OM and construct, in the usual way, the Cauchy completion $\overline{OM}$ of OM. The Lorentz group acts on OM to the right, $OM\times O(3,1)\to OM$, and since this action maps Cauchy sequences into Cauchy sequences, we can naturally extend the action of $O(3,1)$ into $\overline{OM}$, i.e., $\overline{OM}\times O(3,1)\to\overline{OM}$. The quotient space $\overline{M}:=\overline{OM}/O(3,1)$ is called the b-*completion* of space–time M. Here M turns out to be open and dense in $\overline{M}$, and $\partial_b M=\overline{M}\backslash M$ is said to be the b-*boundary* of M. (The above construction in the category of structured spaces is presented in Refs. 7 and 9.)

To treat M as a noncommutative space we shall apply Connes' method to our case and regard the fiber bundle of orthonormal frames over M as a groupoid. This could look like a slight change of perspective, but it has important consequences. Our construction applies to any space–time with its b-boundary, but in what follows we can think about the b-completed space–time of the closed Friedman world model, and regard it as a typical case to which noncommutative methods have to be applied.

For the groupoid definition, see Ref. 10 or 11; here we shall describe the groupoid $\overline{G}=\overline{OM}\lhd O(3,1)$ called the groupoid of orthonormal frames over $\overline{M}$. Elements of G are pairs of orthonormal frames. Therefore, an element $\gamma=(p,pg)$ of G (one can also write $\gamma=(p,g)$) can be interpreted as an arrow beginning at the orthonormal frame $p\in\overline{OM}$ and ending at the frame $pg\in\overline{OM}$, or equivalently as the element g of the group $O(3,1)$ transforming p into pg. Two arrows (p,g_1) and (q,g_2) can be composed if $pg_1=q$. The set of all composable arrows is denoted by $G^{(2)}$. Elements of the form (p,pe), where e is the unit of $O(3,1)$, should be regarded as loops beginning and ending at p. The set of all such loops is denoted by $G^{(0)}$. This interpretation is obvious for $p\in OM$. It can also be extended to ''singular fibers'' $\overline{OM}\backslash OM$ with a suitable understanding of ''singular frames,'' as it is discussed below.

It should be noticed that the groupoid G of orthonormal frames over $\overline{M}$ is smooth as a structured space. Indeed, the differential structure on $\overline{OM}$ can be pulled back from the Euclidean space in which it is embedded, and $O(3,1)$ itself carries the smooth manifold structure. In fact $\overline{G}$ is a D_0 structured space of constant dimension (for details concerning smooth structured spaces see Ref. 9). We thus have the following.

Proposition 2.1: The semidirect product $\overline{G}=\overline{OM}\lhd O(3,1)$, where $\overline{OM}$ is the Cauchy completed total space of the fiber bundle of orthonormal frames over the b-completion $\overline{M}$ of space–time M, is a groupoid. □

The above construction can locally be presented in the following way. Let φ be a map of an atlas on the manifold M (for the time being we consider space–time M without its b-boundary). To every point $p\in OM$, i.e., to every frame at $x\in M$, there corresponds its matrix representation $A_{p,\varphi}$ in the local map φ. The matrix representation of the point $pg\in\pi^{-1}(x)$ is the matrix $A_{pg,\varphi}$, and consequently the arrow $\gamma=(p,pg)$ can be represented by the matrix $A_{\gamma,\varphi}=A_{p,\varphi}+iA_{pg,\varphi}$.

Our strategy in the following will be to extend this representation to singular frames and then to define a suitable (complex) C^*-algebra which would encode the geometric information about space–time with its b-boundary.

III. THE STRUCTURE OF SINGULAR FIBERS

Let us consider a singular fiber $\overline{G}^{(2)}_{x_0}\subset\overline{G^{(2)}}$ where $x_0\in\partial_b M:=\overline{M}\backslash M$. The pairs belonging to $\overline{G}^{(2)}_{x_0}$ are no longer the pairs of orthonormal frames, but rather the pairs of limits of Cauchy sequences of orthonormal frames. Let $\overline{p}=\lim_{n\to\infty}p_n$ and $\overline{pg}=\lim_{n\to\infty}p_ng$, $g\in O(3,1)$, where p_n and p_ng are Cauchy sequences in OM. From Schmidt's construction[3] it follows that these limits always exist.

To see how singularities of this kind can be analyzed, let us consider the most pathological situation that can arise. Let us suppose that the singular fiber $\pi^{-1}(x_0)$, where $x_0 \in \partial_b M$, degenerates to a single point. In Refs. 7 and 9 such singularities were called *malicious singularities*. They appear in the closed Friedman model and in the Schwarzschild solution (Refs. 4 and 5). We immediately have the following.

Lemma 3.1: The following conditions are equivalent:

(i) $x_0 \in \partial_b M$ is a malicious singularity,
(ii) $G^{(2)}_{x_0} = \{(p,e)\} = \overline{G^{(0)}_{x_0}}$,
(iii) the isotropy group Γ_p of the point $p \in \pi^{-1}(x_0)$ coincides with the group $O(3,1)$. ■

Proof: To see the equivalence of (i) and (ii) it is enough to notice that if $p = \pi^{-1}(x_0)$, then, for every $g \in O(3,1)$, one has $pg = p$, and the equivalence of (i) and (iii) follows from the fact that p is a fixed point of the action of $O(3,1)$. □

The following sets will be useful in the sequel

$$G^p = \{\gamma \in \overline{G} : r(\gamma) = p\} = \{(p,g) : g \in O(3,1)\},$$

$$G_q = \{\gamma \in \overline{G} : s(\gamma) = q\} = \{(qg^{-1}, q) : g \in O(3,1)\}.$$

The first of these sets consists of all arrows that begin at $p \in \overline{OM}$, the second of all arrows that end at $q \in \overline{OM}$.

Lemma 3.2: The sets G^p and G_q can be given the structure of the group manifold $O(3,1)$. ■

Proof: The sets G^p and G_p can be written in the form $G^p = \{p\} \times O(3,1)$, $G_q = \{qg^{-1}\} \times O(3,1)$ from which the bijection between these sets and the set $O(3,1)$ is evident. With the help of this bijection the manifold structure can be carried out from $O(3,1)$ to G^p and G_q. □

It should be noticed that this structure of the sets G^p and G_q is preserved also in the malicious singularity.

Let $\varphi : M \to \mathbf{R}^n$ be a map belonging to an atlas on M and D_φ its domain. The map $\tilde{\varphi}$ on OM is said to be *associated* to the map φ if it is of the form $\tilde{\varphi} : \pi^{-1}(D_\varphi) \to \mathbf{R}^n \times \mathbf{R}^d$, where $d = \dim O(3,1)$. The map φ is said to be *accessible* (*to the singularity*) if $\mathrm{cl}\, D_{\tilde{\varphi}} \cap \partial_c OM \neq \varnothing$, where $\partial_c OM$ is the Cauchy boundary of OM. From Schmidt's construction[3] it follows that for every $x_0 \in \partial_b M$ there exists an accessible map (i.e., a map from the domain of which x_0 can be reached). It should be noticed that the set $\mathrm{cl}\, D_{\tilde{\varphi}}$ is $O(3,1)$-saturated, i.e., $\mathrm{cl}\, D_{\tilde{\varphi}} \cap \pi^{-1}(x_0) \supset \pi^{-1}(x_0)$, $x_0 \in \partial_b M$.

If p is an element of a singular fiber (not necessarily over the malicious singularity), from the Schmidt's construction one has $p = \lim_{n\to\infty} p_n$, where $p_n \in \pi^{-1}(D_\varphi)$, φ being an accessible map, and correspondingly $\gamma_n = (p_n, g)$. This gives us the local matrix representation of the singular fiber

$$A_{\gamma,\varphi} = \lim_{n\to\infty} A_{\gamma_n, p},$$

where

$$A_{\gamma_n,\varphi} = A_{p_n,\varphi} + iA_{p_n g,\varphi}.$$

The convergence of matrices should be understood in the following way. The obvious bijection $A_{p,\varphi} \mapsto p$ can be treated as a homeomorphism with the help of which we can pull back the Riemannian metric from OM to the space of matrices. The ''limit matrices'' $A_{\gamma,\varphi}$ should be understood as equivalence classes of the corresponding matrix sequences. Let us notice that if $x_0 \in \partial_b M$ is a malicious singularity, the singular fiber $\pi^{-1}(x_0)$ has the local matrix representation

$A_{p,\varphi} + iA_{p,\varphi}$, where φ is an accessible map on M. This trivially follows from the fact that the singular fiber consists of the one ''limit frame'' p which is represented by a loop.

IV. DESINGULARIZATION OF SPACE–TIME

Now—strictly following Connes's method—we construct the line bundle $\tau:\Omega^{1/2}\to\overline{G}$ over the groupoid G where $\Omega^{1/2} = \cup_{\gamma\in\overline{G}}\Omega^{1/2}_{\gamma}$ and $\Omega^{1/2}_{\gamma}$ is of the form

$$\Omega^{1/2}_{\gamma}=\{\rho:\wedge^k T_{\gamma}(G^p)\otimes\wedge^k T_{\gamma}(G_q)\to\mathbf{C}:$$

$$\rho(\lambda\nu)=|\lambda|^{1/2}\rho(\nu),\quad \lambda\in\mathbf{R},\quad \nu\in\wedge^k T_{\gamma}(G^p)\otimes\wedge^k T_{\gamma}(G_q)\}$$

for $\gamma=(p,q)=(p,pg)$. Here $k=\dim(G^p)=\dim(G_q)$ and, for $G^p = G_q=O(3,1)$, $k=6$. For $\gamma=(p,pg)$, one has $T_{\gamma}(O(3,1))\simeq o(3,1)$, where $o(3,1)$ is the Lie algebra of the Lorentz group $O(3,1)$. It can be easily seen that the line bundle τ: $\Omega^{1/2}\to G$ is trivial. It should be emphasized that the trivial structure of this line bundle is preserved at singularities (even malicious ones). This is the first important step in the process of ''desingularization of space–time.''

Let $C^{\infty}_c(G,\Omega^{1/2})$ denote the space of smooth sections with compact support of the bundle τ: $\Omega^{1/2}\to G$. In the space of sections $C^{\infty}_c(G,\Omega^{1/2})$ we define the *convolution* in the following way:

$$(s*t)(\gamma)=\int_{G_p} s(\gamma_1)t(\gamma_2),$$

where $s,t\in C^{\infty}_c(\overline{G},\Omega^{1/2})$, and $\gamma=(p,pg)$, $\gamma=\gamma_1\circ\gamma_2$. The integral is well defined since $s(\gamma_1)t(\gamma_2)$ is a one-density and it does not depend on the particular composition $\gamma=\gamma_1\circ\gamma_2$.

For each $s\in C^{\infty}_c(G,\Omega^{1/2})$ we also define the *involution* $s\mapsto s^*$ by $s^*(\gamma)=\overline{s(\gamma^{-1})}$.

Now we can formulate our final result:

Theorem 4.1: Let $G=\overline{OM}\triangleleft O(3,1)$ be the groupoid of orthonormal frames over space–time M with its b-boundary.

(1) With convolution and involution defined above $C^{\infty}_c(\overline{G},\Omega^{1/2})$ is an involutive algebra.

(2) For each $q\in G^{(0)}$ the expression

$$(\pi_q(s)\xi)\gamma=\int_{G_q} s(\gamma_1)\xi(\gamma_1^{-1}\gamma),$$

$\gamma\in G_q$, $\xi\in L^2(G_q)$, $s\in C^{\infty}_c(\overline{G},\Omega^{1/2})$, defines an involutive (nongenerate) representation

$$\pi_q: C^{\infty}_c(\overline{G},\Omega^{1/2})\to \mathrm{End}\, L^2(G_q)$$

of $C^{\infty}_c(\overline{G},\Omega^{1/2})$ in the Hilbert space $L^2(G_q)$ of the square integrable functions on the manifold G_q.

(3) The completion of $C^{\infty}_c(\overline{G},\Omega^{1/2})$ with respect to the norm

$$\|s\|=\sup_{q\in G^{(0)}}\|\pi_q(s)\|$$

is a C^*-algebra; it will be denoted by $C^*(\overline{OM})$. ■

Proof is the repetition of the proof given by Connes[12] with minor changes following from the fact that G is smooth in the sense of structured spaces. □

Every representation π_q, $q \in \overline{OM}$, can be prolonged to the representation of $C^*(\overline{OM})$, and part (2) of theorem 4.1 remains valid also for $C^*(\overline{OM})$. The C^*-algebra $C^*(\overline{OM})$ is a noncommutative counterpart of the algebra of functions on a given space, and it conveys all relevant information about space–time with singularities.

V. INTERPRETATION

How is the noncommutative C^*-algebra $C^*(\overline{OM})$ related to the geometry of space–time $\overline{M} = M \cup \partial_b M$ with its b-boundary? In noncommutative geometry there is no concept of point, but in some respects it could be replaced by the concept of state. If $\mathscr{A}$ is a C^*-algebra, π a representation of $\mathscr{A}$ in the Hilbert space $\mathscr{H}$, and $\xi \in \mathscr{H}$, then $a \mapsto (\pi(a)\xi,\xi)$ is a positive form on $\mathscr{A}$. If additionally this positive form is suitably normed, it is called a *state*. We have, therefore, a correspondence between (equivalence classes of) representations of $\mathscr{A}$ in a Hilbert space and states of $\mathscr{A}$ (the state is pure if and only if the corresponding representation is nonzero and irreducible).[13] In the present work we have shown that the initial and final singularities of the closed Friedman world model, understood as the b-boundary points, are distinct structures given by two representations

$$\pi_{p_i}: C^*(\overline{OM}) \to \text{End } L^2(G_{p_i}),$$

$i=1,2$, where p_1 is the single ''limit frame'' in the singular fiber over the initial singularity, and p_2 is the single ''limit frame'' in the singular fiber over the final singularity. Therefore, although the initial and final singularities, in the sense of Schmidt, cannot be regarded as points (or regions) in space–time (even if space–time is modelled by a structured space), they can be treated as the states of the universe.

Of course, we can apply the above-presented method to space–time M with no singularities. In such a case, we obtain a noncommutative C^*-algebra $C^*(OM)$; being noncummutative this algebra loses information about individual points and their neighborhoods, but instead it informs us about the states of the closed Friedman universe. As should be expected, such states coincide with space sections $t=$const of the Friedman model [indeed, because of the maximal symmetry of such space sections, it is easy to show that all corresponding representations of the algebra $C^*(OM)$ are equivalent]. Consequently, if we look at the history of the closed Friedman universe as a sequence of states, the initial and final singularities are full rights elements of this history.

The C^*-algebra $C^*(OM)$ must be strongly related to the (commutative) algebra $\mathscr{F}(M)$ of complex functions on the manifold M. Mathematically speaking $C^*(OM)$ and $\mathscr{F}(M)$ are strongly Morita equivalent. The concept of strong Morita equivalence plays the role of the isomorphism in the theory of C^*-algebras. In particular, two strongly Morita equivalent C^*-algebras have the same space of equivalence classes of irreducible representations.

Since the closed Friedman space–time M is a solution to Einstein field equations, the algebra $C^*(OM)$ contains full information about this solution. Using our former terminology[14] we can say that $C^*(OM)$ is a *noncommutative Einstein algebra of the closed Friedman world model*. Consequently, $C^*(\overline{OM})$ is the extension of this Einstein algebra to the b-completed closed Friedman space–time, and as such it can be regarded as a generalization of Einstein equations to the space–time with singularities. In this sense, the noncommutative approach to general relativity leads to its essential generalization.

Let us notice that the pathological behavior of the closed Friedman space–time with b-boundary is produced by forming the quotient $M = \overline{OM}/O(3,1)$. In the desingularization process, described in the preceding sections, this quotient has nowhere been used. Moreover, based on the C^*-algebra $C^*(\overline{OM})$ one can develop the measure theory, the K-theory, differential and integral calculi, as it has been done by Connes himself[10,15] and his co-workers.[16] In this sense, singularities, even the malicious ones, are no longer geometrically nontractable entities.

The method of dealing with singularities presented in this paper can be applied to any singularities understood as b-boundary points but, of course, it would be rather meaningless to apply this method to milder types of singularities which could be analyzed with the help of simpler and more standard strategies. On the other hand, the present method seems to be the only possible one as far as the malicious singularities are concerned. Singularities of this type, as proved in Refs. 7 and 9, always lead to typically nonlocal (non-Hausdorff) situations.

It is a striking fact that classical singularities are represented by typically quantum object $\mathrm{End}\, L^2(G_p)$, the algebra of operators on the Hilbert space of square integrable functions. Moreover, if we replace the Lorentz group $O(3,1)$ by its double covering $SL(2,\mathbf{C})$ we are automatically led to the spinor formalism. We should also notice that in the construction of the object $\mathrm{End}\, L^2(G_p)$ typically relativistic concepts (Lorentz frame bundle, Lorentz metric, connection, etc.) are involved and they nicely interact with typically quantum concepts (Hilbert space with its scalar product, bounded operators, etc.). We would like to emphasize that this interaction of relativistic and quantum structures was not put into our model by hand (it was not even intended), but it came to surface quite unexpectedly. It seems as if classical singularities knew something about quantum phenomena acting in the beginning and in the end of the closed Friedman universe.

It is tempting to speculate that beneath the Planck threshold smooth (commutative) geometry breaks down and essentially global, perhaps strongly singular, noncommutative geometry (with no points and no time instances) takes over. The space of states of such a quantum noncommutative universe (the counterpart of superspace in quantum canonical theory) would be the space of states of the corresponding C^*-algebra $\mathscr{A}$, and (Hermitian) elements of $\mathscr{A}$ could be regarded as the quantum gravity counterpart of observables in the usual quantum theory. Then one could try to proceed in analogy with the standard quantization methods.

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The equivalence of Darmois-Israel and distributional method for thin shells in general relativity

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A distributional method to solve the Einstein's field equations for thin shells is formulated. The familiar field equations and jump conditions of Darmois-Israel formalism are derived. A careful analysis of the Bianchi identities shows that, for cases under consideration, they make sense as distributions and lead to jump conditions of Darmois-Israel formalism. © *1996 American Institute of Physics.* [S0022-2488(96)03711-5]

I. INTRODUCTION

The study of hypersurfaces of discontinuity in general relativity began in the early twenties.[1–3] But it has been revived through new questions raised in cosmology and black-hole physics. Domain walls separating two coexisting different phases in inflationary scenarios,[4] bubble dynamics,[5] wormholes,[6] signature changes,[7] and interior structures of black-holes[8] are just some of the recent applications of the thin shell formalism of general relativity.

The traditional and most widely used method of handling such problems is that of Darmois-Israel (DI), based on the Gauss-Kodazzi decomposition of space-time.[9,10] It expresses the surface properties in terms of the jump of extrinsic curvature across the layer directly as functions of the layer's intrinsic coordinates. Thus the four-dimensional coordinates may be chosen freely and independently, adapted to the symmetry requirements, on the two sides of the layer. This is the very practical advantage of that method which has found its final formulation in the outstanding paper of Israel.[9] The geometric conditions for the layer to be considered as a boundary of two different manifolds glued together at this boundary were first formulated by Darmois.[3] Those are the minimum conditions which had been assumed by Israel. There are other conditions formulated by Lichnerowicz,[11,12] which means basically continuous coordinates across the layer, and seems to be necessary for using distributional tensor calculus. It is interesting to note that Sen,[2] in this relatively unknown paper, used the same conditions, without any further discussion, derived the reduced Einstein's equations for the general case, and solved it for the spheric symmetric $2+1$ dimensional mass distribution. The O'Brien-Synge conditions[13,14] are in most cases equivalent to the Lichnerowicz ones, so we are not going to consider them here.[15] Because of the restrictive choice of coordinates the Lichnerowicz conditions are not usually used. But there are cases where the distributional method, and therefore the Lichnerowicz conditions, are more suitable for calculation. The case of a cylindrically symmetric thin layer, for example, has been solved by the distributional method using these conditions.[16]

There have been attempts to formulate the problem of a thin layer in general relativity using distributional methods, familiar in other part of physics. In fact many physical systems, classical and relativistic, undergo very rapid transitions of their state of motion. Think of shock waves in hydrodynamics. Although the state of the system need not be described by discontinuous functions

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of space and time, or by functions having discontinuity in their first or second derivatives, a mathematical description of the system which is based on the distribution valued states of the system gives an accurate picture of some important aspects of the physical problem. Usually such a description is more amenable to treatment than the treatment which contains a smooth description of the physical state. This has not only been used in classical hydrodynamics, but also has been applied in the relativistic case. Lichnerowicz[11,12] has given a discussion of hydrodynamic and gravitational shock wave problems by using curvature tensors for space-time which contain a Dirac δ function with support on a submanifold. Y. Choquet-Bruhat has used similar methods to treat high-frequency gravitational waves.[17]

Rapid changes of physical quantities occur also in electromagnetism. One might have, for example, some charge distribution which is confined to a one- or two-dimensional region of space that is small compared with characteristic distances of the problem. This distribution of charge can be replaced by a concentrated source, and the problem can be formulated in the sense of distributions, but not of smooth functions. There is a natural mathematical framework in electromagnetism. Recall that linear operations, including differentiations, make sense when applied to distributions. Hence, Maxwell's equations, by virtue of their linearity in both fields and sources, make sense as equations on these distributions. This means that the machinery of distribution theory is available in electromagnetism, and guarantees that distributional Maxwell fields with distributional charge-currents make physical sense, and at the same time gives a well defined and detailed sense in which a distributional charge density must approximate our real smooth charge density distribution.

In general relativity, where the field equations are non-linear, the use of distributional objects seem not to be trivial. Although Raju[18] claims to give an analytical formalism to deal with the occurrence of jump discontinuities in the metric across a hypersurface, using a non-linear theory of distributions,[18,19] his method does not seem to be conclusive. The application he mentions is for a continuous metric where no non-linear distributional operations are needed. Anyhow, here the mathematical framework cannot be as simple as for electromagnetism. Efforts to implement distributional methods in general relativity go back to works of Papapetrou and Treder.[20] Nariai,[21] aiming to understand the O'Brien-Synge junction conditions, and demanding the Einstein's tensor to be free of δ functions, uses continuous metrics and so brings in distributions in the formalism, which is consequently used by Kumar.[22] Papapetrou and Hamoui[23,24] then try to formulate a general method with application to a spherical symmetric thin layer. Their method has then been reformulated and corrected by Evans.[25] Lichnerowicz[12] gives a detailed mathematical analysis of distributions in curved space-time and comes to the conclusion that the classical properties of the covariant derivatives and all of the corresponding formulas are valid for tensor distributions. Barrabes[26] uses tensor distributions specially to include null hyper-surfaces in the shell dynamics.

Taub[27] is interested in relativistic hydrodynamics and shock waves but also discusses the previous accounts on the concentrated 2- and 3-dimensional sources. Israel[28] and Taub[27] give a formulation for a 2-dimensional concentrated mass distribution. These attempts have been criticized by Geroch and Traschen[29] who gave an extensive and thorough analysis of concentrated mass distributions in general relativity. This work is a milestone in all the discussions about the validity of distributional Einstein's field equations and its applications to concentrated sources. There the authors define some regularity conditions for metrics, for which the distributional tensor calculations are allowed. Hence, for example, the line source case should be handled with care, although some authors have criticized it.[30] The $(2+1)$-dimensional case, as a result of this work, should not cause any problem, as far as the continuity of the metric is assured. We have thereafter used distributional tensors to solve Einstein's equations directly, without any use of Gauss-Kodazzi decompositions. The coordinates have to be prepared to make them continuous at the hypersurface of discontinuity, but the method has been applied easily for several cases.[16,31,32] Naturally, there should be no difference in the results using either the distributional- or Gauss-Kodazzi-method. But the complete equivalence has never been demonstrated explicitly, and the

role of jump conditions by using the distributional method has never been clearly stated.

With the results of Geroch and Traschen in mind, we show here that all the dynamical- and constraint-equations derived by the DI-formalism results very naturally in the distributional method, without any need to define a new covariant derivative. For the sake of transparency, we limit ourselves to the non-null shells. The null case can be treated along the same line as this paper.[33]

In section II we review shortly the DI formalism and give the necessary formulae. Section III begins with the formulation of the distributional method. Covariant derivative of distributions and some useful formulae are given in section III A, and the Einstein's equations for a thin shell in section III B. Section III C deals with the conservation laws and the Bianchi identities. In this section we will see the full equivalence of the two methods. We end with a conclusion in section IV.

Conventions and definitions: We use the signature $(-+++)$, and follow the curvature conventions of Misner, Thorn, and Wheeler (MTW).[10] However, our sign convention for extrinsic curvature is that of Israel,[9] which is the opposite of MTW. The Greek indices run from 0 to 3 and Latin indices from 1 to 3. A semicolon indicates covariant derivatives with respect to either the four-metric of the whole space-time or the three-metric of the layer. There will, however, be no confusion because the kind of indices and objects used makes the difference transparent. The symbol $\nabla^{\pm}$ denotes the covariant derivative with respect to either of the metrics of partial manifolds $M^{\pm}$ which are to be glued together.

The square brackets $[F]$ are used to indicate the jump of any quantity F at the layer, and bars $\overline{F}$ the arithmetic mean of it. As we are going to work with distributional valued tensors, there may be terms in a tensor quantity F proportional to some δ-function. These terms are indicated by $\underline{F}$.

II. DARMOIS-ISRAEL FORMALISM

Assume two space-times M^+ and M^- with boundaries Σ^+ and Σ^-. M^+ and M^- may have been cut from space-times M_1 and M_2, respectively, but this is irrelevant for our task of glueing these together. Coordinates on the two space-time manifolds are defined independently as x_+^μ and x_-^μ, and the metrics denoted by $g^+_{\alpha\beta}(x_+^\mu)$ and $g^-_{\alpha\beta}(x_-^\mu)$. The induced metrics on the boundaries are called $g^+_{ij}(\xi_+^k)$ and $g^-_{ij}(\xi_-^k)$, where $\xi_\pm^k$ are intrinsic coordinates on $\Sigma_\pm$, respectively. Bringing these 3- and 4-dimensional quantities in connection is trivially done with the help of tetrads defining on Σ.[34]

Now, to paste the manifolds together we demand that the boundaries be isometric having the same coordinates

$$\xi_+^k = \xi_-^k = \xi^k.$$

The identification

$$\Sigma_+ = \Sigma_- =: \Sigma$$

gives us the single glued manifold $M = M_+ \cup M_-$.

This is the minimum requirement for glueing two manifolds together. Formulated as

$$[g_{ij}] = 0 \tag{1}$$

gives together with the continuity of the second fundamental form on Σ

$$[K_{ij}] = 0 \tag{2}$$

the Darmois conditions. Both conditions should be satisfied if Σ is just a boundary surface. But in the case of a thin shell we do not expect the second condition to be satisfied. In fact, the matter content of the shell should lead to a jump in the extrinsic curvature K_{ij}.

The condition (1) leaves the coordinates in $M^{\pm}$ free. If we assume the continuity of the coordinates $x_{\pm}^{\mu}$ at Σ we then have to require

$$[g_{\mu\nu}]=0, \tag{3}$$

which together with the corresponding equation for derivatives of the metric

$$\left[\frac{\partial g_{\mu\nu}}{\partial x^{\alpha}}\right]=0 \tag{4}$$

gives the Lichnerowicz conditions. In the following we just assume condition (1) or (3), respectively.

On Σ we define a three-bein

$$e_i=\frac{\partial}{\partial \xi^i}$$

having the components

$$e_i^{\mu}=\frac{\partial x^{\mu}}{\partial \xi^i}\ . \tag{5}$$

The induced metric on Σ is given by the scalar product

$$g_{ij}=e_i\cdot e_j=g_{\mu\nu}e_i^{\mu}e_j^{\nu}\ . \tag{6}$$

Note that, because of the assumed isometry, this metric is the same on both faces Σ_+ and Σ_-. We note that the subscripts of the three-beins on Σ are not the component indices, but as this distinction is trivial we prefer for the sake of simplicity not to use parentheses to distinguish them, as is usually done.

We choose the parametric equation for Σ in the form

$$\Phi(x^{\mu}(\xi^i))=0, \tag{7}$$

having the unit normal four-vector n^{μ} given by

$$n_{\mu}=\alpha^{-1}\partial_{\mu}\Phi, \tag{8}$$

where

$$\alpha=\pm\sqrt{\left(\left|g^{\nu\gamma}\frac{\partial f}{\partial x^{\nu}}\frac{\partial f}{\partial x^{\gamma}}\right|\right)}. \tag{9}$$

Therefore

$$n_{\mu}e_i^{\mu}=0, \tag{10}$$

and

$$n_{\mu}n^{\mu}=\epsilon, \tag{11}$$

where $\epsilon=+1$ or -1 for Σ to be time- or space-like, respectively. We suppose n^μ to be directed from M^- to M^+, i.e., in the direction of increasing a space- or time-like coordinate corresponding to time- or space-like Σ. Therefore we have to take the positive (negative) sign in (9) for time-(space-)like Σ. This choice gives us the useful relation

$$\text{sign } \alpha=\frac{|\alpha|}{\alpha}=\epsilon.$$

The choice of the Lichnerowicz condition (3) makes it possible to have a unique normal vector for each case. As we want to concentrate on the formulation of the distributional method and avoid any undue complications, we leave aside the case of null hypersurfaces.

Now, in general the metrics in M^+ and M^- need not to be continuous at Σ, but they could be. However, the normal extrinsic curvature (second fundamental form) is not continuous for a thin shell. It is defined by

$$K^\pm_{ij}=e^\mu_i e^\nu_j \nabla^\pm_\mu n_\nu=-n_\mu e^\nu_j \nabla^\pm_\nu e^\mu_i=-n_\mu e^\nu_i \nabla^\pm_\nu e^\mu_j=K^\pm_{ji}. \tag{12}$$

Now, we have all the prerequisites to write the Einstein's equation for the hypersurface. These are 10 equations which will be written in components normal and tangent to the hypersurface. The first and second contracted Gauss-Kodazzi equations are[9,10]

$$G_{\mu\nu}n^\mu n^\nu=\tfrac{1}{2}\,(K^2-K_{ij}K^{ij}-\epsilon^3 R), \tag{13}$$

$$G_{\mu\nu}e^\mu_i n^\nu=K^j_{i;j}-K_{,i}, \tag{14}$$

where ${}^3R$ and ${}^3G$ are the Ricci scalar and Einstein tensor of the three metric g_{ij}, respectively. Now, to discover the effect the energy-momentum tensor S_{ij} of Σ on the space-time geometry, we perform a ''pill-box'' integration of Einstein's equations across Σ:

$$S_{\mu\nu}=\lim_{\Sigma\to 0}\int_{-\Sigma}^{\Sigma}\left(T_{\mu\nu}-g_{\mu\nu}\frac{\Lambda}{\kappa}\right)dn=\frac{1}{\kappa}\lim_{\Sigma\to 0}\int_{-\Sigma}^{\Sigma}G_{\mu\nu}dn, \tag{15}$$

where n is the proper distance through Σ in the direction of the normal n_μ. $S_{\mu\nu}$ is the associated 4-tensor of energy momentum of the shell. The equations (13), (14) have the physical meaning that no moment associated with the surface layer flows out of Σ. Therefore $S_{\mu\nu}$ vanishes off the hypersurface Σ, which is expressed as

$$S_{\mu\nu}n^\nu=0. \tag{16}$$

The energy momentum 4- and 3-tensors are related as

$$S^{\mu\nu}=e^\mu_i e^\nu_j S^{ij}. \tag{17}$$

The covariant derivative of such a tensor relative to the corresponding connections is given by[9]

$$\nabla^\pm_\nu S^{\mu\nu}=e^\mu_i S^{ij}_{;j}-\epsilon S^{ij}K^\pm_{ij}n^\mu, \tag{18}$$

which leads to the following useful relation

$$e^\mu_i \nabla_\nu S^\nu_\mu=S^j_{i:j}. \tag{19}$$

Similarly we can associate to the 3-tensor K_{ij} defined on Σ, the corresponding 4-dimensional tensor:

$$K^{\mu\nu}=K^{ij}e_i^\mu e_j^\nu, \tag{20}$$

satisfying

$$K^{\mu\nu}n_\nu=0. \tag{21}$$

The remaining components of the Einstein's equations lead to the following non-vanishing result

$$\lim_{\Sigma\to 0}\int_{-\Sigma}^{\Sigma} G_{\mu\nu}e_i^\mu e_j^\nu dn=\epsilon([K_{ij}]-g_{ij}[K])=\kappa S_{ij}. \tag{22}$$

This distributional equivalent of Einstein's equations is called *Lanczos* equation, which partly determines the dynamic of the thin shell. The other dynamical equations come from the defining equation of the matter contents of the shell. Now, the two Gauss-Kodazzi equations act as constraints. The first one (13) is the so-called ''Hamiltonian''- and the second one (14) the ''ADM''-constraint. Note however that these equations are valid in M^+ and M^- on taking the limits as one approaches the layer Σ. Therefore we are actually faced with 8 equations, the sum and difference of which give us the junction conditions. The Hamiltonian constraint along with the Einstein's or Lanczos equations then give the *evolution identity*:

$$S^{ij}\overline{K_{ij}}=-[T_{\mu\nu}n^\mu n^\nu-\Lambda/\kappa] \tag{23}$$

and

$${}^3R+(\overline{K_{ij}}\,\overline{K^{ij}}-K^2)=2\epsilon\kappa\overline{(T_{\mu\nu}n^\mu n^\nu-\Lambda/\kappa)}+\frac{\epsilon\kappa^2}{4}\left(S^{ij}S_{ij}-\frac{S^2}{2}\right). \tag{24}$$

The ADM constraint gives the *conservation identity*

$$S^i_{j;i}=-\epsilon[T_{\mu\nu}n^\mu e_j^\nu] \tag{25}$$

and

$$\overline{K^i_{j;i}}-\overline{K_{,j}}=\kappa\overline{(T_{\mu\nu}n^\mu e_i^\nu)}. \tag{26}$$

Not all of these jump conditions are independent. Usually one takes the evolution identity (23) and the conservation identity (25) as the proper junction conditions, which in addition to the Lanczos equation should be satisfied.[35]

III. DISTRIBUTIONAL METHOD

Here we intend to give a formulation of the Einstein's equations for the case where there exists a hypersurface of concentrated source immersed in an otherwise arbitrary space-time, not necessarily vacuum. We assume the metric to be continuous at the hypersurface:

$$[g_{\mu\nu}]=0. \tag{27}$$

Otherwise we would have to consider non-linear operations of distributions such as $\delta\theta$ or $\delta\delta$. The disadvantage of having a continuous metric across the shell pays off by the simplicity of the method to calculate specific solutions.[16,31,32]

Write the metric in the following form

$$g_{\mu\nu}=g^+_{\mu\nu}\theta(\Phi(x))+g^-_{\mu\nu}\theta(-\Phi(x)), \tag{28}$$

where θ is the step function and

$$g^{+}_{\mu\nu}|_{\Phi(x)=0}=g^{-}_{\mu\nu}|_{\Phi(x)=0}. \tag{29}$$

This condition guarantees the smoothness of the metric on the hypersurface. Should this not be the case we try a coordinate transformation $x=x(x')$ having a jump in the first derivative:

$$\frac{\partial x^{\mu}}{\partial x'^{\rho}}=\alpha^{+\mu}_{\rho}\theta(\Phi(x))+\alpha^{-\mu}_{\rho}\theta(-\Phi(x)). \tag{30}$$

The condition for the new metric to be continuous comes out to be

$$\alpha^{+\mu}_{\rho}\alpha^{+\nu}_{\sigma}g^{+}_{\mu\nu}|_{\Phi(x)=0}=\alpha^{-\mu}_{\rho}\alpha^{-\nu}_{\sigma}g^{-}_{\mu\nu}|_{\Phi(x)=0}. \tag{31}$$

We assume from now on that the metric is smooth everywhere, C^1 at the hypersurface and C^{∞} on both sides of it.

Although the metric is continuous on Σ, its derivatives, and so the corresponding connections, are discontinuous. Nevertheless the connection corresponding to the metric $g_{\mu\nu}$ can be written in the following compact form:

$$\Gamma^{\rho}_{\mu\nu}=\tfrac{1}{2}\ g^{\rho\sigma}(g_{\mu\sigma,\nu}+g_{\nu\sigma,\mu}-g_{\mu\nu,\sigma})=\theta(\Phi(x))\Gamma^{+\rho}{}_{\mu\nu}+\theta(-\Phi(x))\Gamma^{-\rho}{}_{\mu\nu}, \tag{32}$$

where $\Gamma^{\pm\rho}{}_{\mu\nu}$ are the ordinary connections on $M^{\pm}$. The above connection has jump discontinuities on Σ.

To write the field equations for the hypersurface we need the formulation of the energy-momentum tensor of the shell. Generally it can be written in the form

$$\breve{T}_{\mu\nu}=CS_{\mu\nu}\delta(\Phi(x)), \tag{33}$$

where C is a constant to be calculated. We integrate the above equation in the direction of the normal to the hypersurface

$$\int \breve{T}_{\mu\nu}dn=CS_{\mu\nu}\int \delta(\Phi(x))dn=CS_{\mu\nu}\left|\frac{dn}{d\Phi}\right|. \tag{34}$$

Therefore, using the definition (15), we obtain

$$C=\left|\frac{d\Phi}{dn}\right| \tag{35}$$

and

$$\breve{T}_{\mu\nu}=S_{\mu\nu}\left|\frac{d\Phi}{dn}\right|\delta(\Phi(x)). \tag{36}$$

Note that in the literature one usually takes $C=1$, which is correct just for special cases. But in general the factor C is necessary (see also Ref. 33). Now, the derivative of Φ in the normal direction can be written in terms of unit normal vector n^{μ}:

$$C=\left|\frac{d\Phi}{dn}\right|=|n^{\mu}\partial_{\mu}\Phi|=|\epsilon\alpha|=|\alpha|, \tag{37}$$

where we have used (8)–(11). Therefore (33) will be written in the form

$$\check{T}_{\mu\nu}=S_{\mu\nu}|n^{\sigma}\partial_{\sigma}\Phi|\,\delta(\Phi(x))=CS_{\mu\nu}\delta(\Phi(x))=|\alpha|S_{\mu\nu}\delta(\Phi(x)). \tag{38}$$

A. Covariant derivative of distributional valued tensors

There is no need to change the ordinary concept of covariant derivative, as it has been carefully shown by Lichnerowicz.[12] In fact, all the known properties of covariant derivative and the corresponding formulae in a pseudo-Riemannian manifold are valid for tensor distributions. But for the sake of convenience of calculation we refer to some useful formulae. Consider first an arbitrary vector A^{μ} defined as

$$A^{\mu}=\theta(\Phi)A^{+}+\theta(-\Phi)A^{-}, \tag{39}$$

where $A^{\pm}$ has the support on $M^{\pm}$. It is therefore useful to define the operator

$$\nabla=\theta(\Phi)\nabla^{+}+\theta(-\Phi)\nabla^{-}. \tag{40}$$

We can now write the covariant derivative of a distributional valued vector A^{μ} in terms of the covariant derivatives of its defining parts in $M^{\pm}$. The following relation is easily obtained:

$$A^{\mu}_{;\nu}=\nabla_{\nu}A^{\mu}+[A^{\mu}]\partial_{\nu}\Phi\,\delta(\Phi). \tag{41}$$

This relation can be generalized easily for a distributional tensor of any rank. The covariant derivative of the tensor

$$T^{(\rho)}=\theta(\Phi)T^{+(\rho)}+\theta(-\Phi)T^{-(\rho)}, \tag{42}$$

where (ρ) stands for any number of indices, is calculated to be

$$T^{(\rho)}{}_{;\nu}=\nabla_{\nu}T^{(\rho)}+[T^{(\rho)}]\partial_{\nu}\Phi\,\delta(\Phi). \tag{43}$$

In case a tensor has the support on Σ its covariant derivative is in the usual form. Take the tensor $\check{T}^{\mu\nu}$ from (33). Its covariant derivative can be written

$$(\check{T}^{\mu\nu})_{;\rho}=(CS^{\mu\nu})_{;\rho}\delta(\Phi)+CS^{\mu\nu}(\delta(\Phi))_{,\rho}=(CS^{\mu\nu})_{;\rho}\delta(\Phi)+CS^{\mu\nu}\partial_{\rho}\Phi\,\delta'(\Phi). \tag{44}$$

We will need this relation later to discuss the conservation laws.

B. The field equations

Einstein's field equations are valid on both sides of the hypersurface as usual. So we concentrate our procedure on Σ, where we expect the curvature and Einstein tensor to be proportional to δ. That means that in calculating the connection coefficients and the components of the Ricci tensor we can ignore terms not proportional to δ. Hence, e.g., the terms in the Ricci tensor

$$R_{\mu\nu}=\Gamma^{\rho}_{\mu\rho,\nu}-\Gamma^{\rho}_{\mu\nu,\rho}+\Gamma^{\sigma}_{\mu\rho}\Gamma^{\rho}_{\sigma\nu}-\Gamma^{\sigma}_{\mu\nu}\Gamma^{\rho}_{\rho\sigma} \tag{45}$$

proportional to Γ's can be ignored. The only relevant terms are

$$\check{R}_{\mu\nu}=\check{\Gamma}^{\rho}_{\mu\rho,\nu}-\check{\Gamma}^{\rho}_{\mu\nu,\rho}. \tag{46}$$

Now,

$$\Gamma^{\rho}_{\mu\rho}=\frac{1}{2g}\,g_{,\mu}, \tag{47}$$

where g is the determinant of the metric. The δ distribution can only occur in the second derivatives of the metric. Therefore

$$\breve{\Gamma}^{\rho}_{\mu\rho,\nu}=\frac{1}{2g}\,\breve{g}_{,\mu\nu}. \tag{48}$$

Similarly, for the second term in the Ricci tensor we have

$$\breve{\Gamma}^{\rho}_{\mu\nu,\rho}=\tfrac{1}{2}\,g^{\rho\sigma}(\breve{g}_{\sigma\mu,\nu\rho}+\breve{g}_{\sigma\nu,\mu\rho}-\breve{g}_{\mu\nu,\sigma\rho}). \tag{49}$$

Having the metric in the form (28) we obtain

$$\breve{g}_{\alpha\beta,\mu\nu}=[g_{\alpha\beta,\mu}](\partial_\nu\Phi)\,\delta(\Phi(x)) \tag{50}$$

and

$$\breve{g}_{,\mu\nu}=[g_{,\mu}]\partial_\nu\Phi\,\delta(\Phi(x)). \tag{51}$$

As a result we obtain for terms in the Ricci tensor proportional to δ

$$\begin{aligned}\breve{R}_{\mu\nu}&=\left(\frac{1}{2g}\,[g_{,\mu}]\partial_\nu\Phi-g^{\rho\sigma}([g_{\sigma\mu,\nu}]+[g_{\sigma\nu,\mu}]-[g_{\mu\nu,\sigma}])\partial_\rho f\right)\delta(f(x))\\&=\left(\frac{1}{2g}\,[g_{,\mu}]\partial_\nu\Phi-[\Gamma^{\rho}_{\mu\nu}]\partial_\rho\Phi\right)\delta(\Phi(x)).\end{aligned} \tag{52}$$

This enables us to write the Einstein's equations for the layer:

$$\breve{G}_{\mu\nu}=\kappa\breve{T}_{\mu\nu}. \tag{53}$$

Defining

$$Q_{\mu\nu}=(\alpha)^{-1}\left(\frac{1}{2g}\,[g_{,\mu}]\delta^{\rho}_{\nu}-[\Gamma^{\rho}_{\mu\nu}]\right)\partial_\rho\Phi=\left(\frac{1}{2g}\,[g_{,\mu}]\delta^{\rho}_{\nu}-[\Gamma^{\rho}_{\mu\nu}]\right)n_\rho \tag{54}$$

we obtain, using (38) and (52) for the energy momentum tensor, the field equations in the 4-dimensional form

$$Q_{\mu\nu}-\tfrac{1}{2}\,g_{\mu\nu}Q=\epsilon\kappa S_{\mu\nu}, \tag{55}$$

where $Q=Q_{\mu\nu}g^{\mu\nu}$, and we have used the relation $\epsilon=|\alpha|/\alpha$. Note that $Q_{\mu\nu}$ is a tensor with support on Σ. This equation, for the time-like case, has been first derived, without using the hitherto unknown distributional calculus, by Sen.[2] We would like, therefore, to coin it by *Sen equation*. The three dimensional form of the Sen equation is readily obtained by decomposing it to tangential- and normal-components to Σ. Multiplying (54) with n^μ we obtain

$$S_{\mu\nu}n^\nu=0, \tag{56}$$

which is the same relation as (16). This tells us immediately that the components corresponding to $S_{\mu\nu}n^\mu n^\nu$ and $S_{\mu\nu}n^\mu e^\nu_i$ identically vanishes. To obtain the proper 3-dimensional components we notice first that

$$Q_{ij}=Q_{\mu\nu}e^\mu_i e^\nu_j=-[\Gamma^{\rho}_{\mu\nu}]n_\rho e^\mu_i e^\nu_j=[K_{ij}]. \tag{57}$$

Therefore, we obtain from the Sen equation

$$Q_{ij}=\epsilon\kappa(S_{ij}-\tfrac{1}{2}\,g_{ij}S), \tag{58}$$

which is equivalent to the Lanczos equation (22).

We have therefore seen that the explicit method of writing the Einstein's field equations for a regular metric which is continuous without having continuous derivatives leads to the equation (55) and is equivalent to the DI-formalism based on the Gauss-Codazzi formalism. In practice, one begins with known solutions of the Einstein's equations in $M^{\pm}$, and after making sure the continuity of the metric on Σ, tries to solve equations (55). In the following we will show that the jump conditions of DI-formalism follows from the Bianchi identities corresponding to the metric (28), and are therefore implicit in the equations we have used.

C. Conservation laws

We have now all the prerequisites to evaluate the Bianchi identities and the conservation of energy momentum tensor of our pasted space-time. The energy momentum of the whole space-time, including the cosmological terms $\Lambda^{\pm}$ is

$$T^{\mu\nu}=\breve{T}^{\mu\nu}+(T^{+\mu\nu}-\Lambda^{+}/\kappa g^{+\mu\nu})\,\theta(\Phi)+(T^{-\mu\nu}-\Lambda^{-}/\kappa g^{-\mu\nu})\,\theta(-\Phi), \tag{59}$$

where $\breve{T}^{\mu\nu}$ is defined in (38). Having in mind that the covariant divergences of $T^{\pm\mu\nu}$ and $g^{\pm\mu\nu}$ with respect to the corresponding connections vanishes, we obtain

$$T^{\mu\nu}{}_{;\nu}=(\breve{T}^{\mu\nu})_{;\nu}+[T^{\mu\nu}-\Lambda/\kappa]\partial_{\nu}\Phi\,\delta(\Phi), \tag{60}$$

where we have used the relation (43). Now inserting for $\breve{T}^{\mu\nu}$ from (38) and using (44) we obtain an equation having terms proportional to $\delta(\Phi)$ and $\delta'(\Phi)$. Each term vanishes independently. The term proportional to $\delta'(\Phi)$ gives

$$(S^{\mu\nu}\partial_{\nu}\Phi)(n^{\sigma}\partial_{\sigma}\Phi)=0, \tag{61}$$

which leads to the (56) and ensures the orthogonality of the energy-momentum tensor of Σ to the hypersurface normal n^{μ}. We use in the following this relation to simplify the remaining calculations. The term proportional to δ is

$$(CS^{\mu\nu})_{,\nu}+CS^{\mu\rho}\Gamma^{\nu}_{\nu\rho}+CS^{\rho\nu}\Gamma^{\mu}_{\rho\nu}+[T^{\mu\nu}-\Lambda/\kappa g^{\mu\nu}]\partial_{\nu}\Phi)\,\delta(\Phi)=0. \tag{62}$$

We have left $\delta(\Phi)$ as proportionality factor to stress its influence especially on terms containing Γ's and $g^{\mu\nu}$'s. Note that the third term containing Γ's contains terms like $\theta\cdot\delta$, i.e., product of distributions. This is in analogy to the elementary problem of evaluating the electrostatic force on a sheet of charge.[5] There the linearity of electrostatic equation resolve the ambiguity. But how about our case where the Einstein equations are non-linear? We have already shown that in the case of thin shells the only terms contributing to the Einstein tensor are the derivatives of the connection, or the second derivative of the metric, which appear linearly. It is then easily seen that in the case of a layer the Einstein's equations leads to a Poisson-like equation corresponding to the Sen equation (55) for concentrated distribution, where the second derivative can be replaced by (50) and (51). Therefore, in analogy to the electromagnetic case, we can use the linearity of (55) to show that

$$\Gamma^{\mu}_{\rho\nu}\delta(\Phi)=\tfrac{1}{2}\,(\Gamma^{+\mu}{}_{\rho\nu}+\Gamma^{-\mu}{}_{\rho\nu})\,\delta(\Phi). \tag{63}$$

Using this result and multiplying equation (62) by n_μ, we obtain the component in the normal direction.

$$(CS^{\mu\nu})_{,\nu}n_\mu + CS^{\rho\nu}\overline{\Gamma^{\mu}_{\rho\nu}}n_\mu = \epsilon[T^{\mu\nu} - \Lambda/\kappa g^{\mu\nu}]n_\mu \partial_\nu \Phi. \tag{64}$$

Using the relations (63) and the definition of the extrinsic curvature (12), we obtain the final result

$$S^{ij}\overline{K_{ij}} = \epsilon[T^{\mu\nu}n_\mu n_\nu - \Lambda/\kappa]. \tag{65}$$

This is the evolution identity (23) derived as one of the jump conditions in the Darmois-Israel method. Here it is just a consequence of the Bianchi identities. To obtain the remaining three equations we multiply (64) by e^i_μ. Using (19) we obtain

$$S^i_{j;i} = -\epsilon[T_{\mu\nu}n^\mu e^\nu_i], \tag{66}$$

which is the conservation identity (25). It gives the conservation law for the energy momentum tensor of the layer. We therefore see that our explicit distributional method of solving the Einstein's equations gives all the dynamical and constraint equations of the Darmois-Israel method, and is therefore equivalent to it.

IV. CONCLUSION

We have seen that, based on the Lichnerowicz condition (3), a distributional method can be formulated to solve Einstein's field equations for a thin shell, which is equivalent to the Darmois-Israel formalism, and gives all the necessary equations and jump conditions formulated there. In fact, it has been shown that the jump conditions are a consequence of the Bianchi identities, and therefore implicit in the formalism, once the Lichnerowicz condition is satisfied. This makes the distributional formalism easy to apply, especially when explicit solutions are to be found, and it pays off the disadvantage of the continuity of the coordinates across the shell.

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Gravitational and electromagnetic perturbations of the Schwarzschild solution

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It is shown that the complete metric and vector potential perturbations of the Schwarzschild solution can be expressed in terms of radial functions that share several differential properties. The energy flux of the incident, reflected, and absorbed gravitational and electromagnetic waves is given and the polarization changes are also analyzed. © *1996 American Institute of Physics.* [S0022-2488(96)03609-2]

I. INTRODUCTION

The perturbations of space–times describing black holes have been the subject of numerous investigations, making use of diverse methods (see, e.g., Ref. 1). The simplest of these space–times corresponds to the Schwarzschild solution, which describes a static, uncharged black hole, and the study of its perturbations was initiated some time ago, originally in connection with the stability of the Schwarzschild black hole[2–4] (see also Refs. 5–7 and the references cited therein). Although it is generally believed that the perturbations of the Schwarzschild solution are fairly well understood, as we shall show below, some existing results are wrong or incomplete.

The aim of this paper is twofold; we show that the gravitational and the electromagnetic perturbations of the Schwarzschild solution can be expressed in terms of radial functions that obey sets of equations of the same form. This allows us to show that the Teukolsky–Starobinsky identities, which in the case of the gravitational and the electromagnetic perturbations involve differential operators of order four and two, respectively, follow from a single basic identity [Eq. (30) below]. We also give expressions for all the components of the perturbed conformal curvature and of the electromagnetic perturbations. The energy fluxes at spatial infinity and at the horizon are then calculated and it is *explicitly* shown that the energy carried by the gravitational or electromagnetic waves is conserved. We show that an ingoing circularly polarized gravitational wave produces an elliptically polarized scattered wave, even though the black hole does not rotate. Throughout this paper we make use of the Newman–Penrose notation.

II. DEBYE POTENTIALS

As shown in Refs. 8–11, the metric perturbations of an algebraically special solution of the Einstein vacuum field equations, in a frame such that $\Psi_0=\Psi_1=0$ (or, equivalently, $\kappa=\sigma=0$), are given by

$$\begin{aligned} h_{\mu\nu}=2\{&l_\mu l_\nu[(\delta+3\beta+\overline{\alpha}-\tau)(\delta+4\beta+3\tau)-\overline{\lambda}(D+4\epsilon+3\rho)]\\ &+m_\mu m_\nu(D+3\epsilon-\overline{\epsilon}-\rho)(D+4\epsilon+3\rho)-l_{(\mu}m_{\nu)}[(D+3\epsilon+\overline{\epsilon}-\rho+\overline{\rho})(\delta+4\beta+3\tau)\\ &+(\delta+3\beta-\overline{\alpha}-\tau-\overline{\pi})(D+4\epsilon+3\rho)]\}\psi_{\mathrm{G}}+\text{c.c.}, \end{aligned} \tag{1}$$

up to the gauge transformations $h_{\mu\nu}\mapsto h_{\mu\nu}-2\nabla_{(\mu}\xi_{\nu)}$, where ξ_μ is an arbitrary vector field, with the complex scalar potential ψ_{G} governed by the equation

$$[(\Delta+3\gamma-\overline{\gamma}+\overline{\mu})(D+4\epsilon+3\rho)-(\overline{\delta}+3\alpha+\overline{\beta}-\overline{\tau})(\delta+4\beta+3\tau)-3\Psi_2]\psi_{\mathrm{G}}=0. \tag{2}$$

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The Schwarzschild solution can be specified by the null tetrad,

$$l^\mu\partial_\mu=\partial_r+\frac{r^2}{\chi}\,\partial_t,\quad n^\mu\partial_\mu=-\frac{1}{2}\,\frac{\chi}{r^2}\left(\partial_r-\frac{r^2}{\chi}\,\partial_t\right),$$
$$m^\mu\partial_\mu=\frac{1}{\sqrt{2}r}\,(\partial_\theta+i\,\mathrm{cosec}\;\theta\partial_\varphi),\quad \overline{m^\mu}\partial_\mu=\frac{1}{\sqrt{2}r}\,(\partial_\theta-i\,\mathrm{cosec}\;\theta\partial_\varphi), \tag{3a}$$

with

$$\chi\equiv r^2-2Mr. \tag{3b}$$

The nonvanishing spin coefficients can be conveniently expressed as

$$\rho=-D\,\ln r,\quad \mu=\Delta\,\ln r,\quad \gamma=\Delta\,\ln r\chi^{-1/2},$$
$$\beta=\delta\,\ln\sin^{1/2}\theta,\quad \alpha=-\overline{\delta}\,\ln\sin^{1/2}\theta, \tag{4}$$

and the only nonvanishing component of the Weyl spinor is

$$\Psi_2=-\frac{M}{r^3}. \tag{5}$$

Since ψ_{G} has spin weight -2, we seek solutions of Eq. (2) of the form

$$\psi_{\mathrm{G}}=r^3Y_{-2}(r)e^{-i\omega t}{}_{-2}Y_{jm}(\theta,\varphi), \tag{6}$$

where the ${}_sY_{jm}$ are spin-weighted spherical harmonics.[12] Substituting Eqs. (3)–(6) into Eq. (2) one obtains the ordinary differential equation,

$$\mathscr{D}^*\,\frac{r^6}{\chi}\,\mathscr{D}Y_{-2}=\eta^2\,\frac{r^6}{\chi^2}\left(1+\frac{6M}{\eta^2r}\right)Y_{-2}, \tag{7}$$

where

$$\mathscr{D}^*\equiv\partial_r+\frac{i\omega r^2}{\chi},\quad \mathscr{D}\equiv\partial_r-\frac{i\omega r^2}{\chi} \tag{8}$$

and

$$\eta\equiv[(j-1)(j+2)]^{1/2}. \tag{9}$$

If one introduces the function[13]

$$X_{-1}\equiv\frac{r^6}{\eta^2\chi}\,\mathscr{D}\,Y_{-2}, \tag{10}$$

then Eq. (7) is equivalent to the system of first-order equations,

$$\mathscr{D}\,Y_{-2}=\eta^2\,\frac{\chi}{r^6}\,X_{-1},\quad \mathscr{D}^*X_{-1}=\frac{r^6}{\chi^2}\left(1+\frac{6M}{\eta^2r}\right)Y_{-2}. \tag{11}$$

On the other hand, the vector potential perturbations of an algebraically special solution of the Einstein vacuum field equations, in a frame such that $\Psi_0=\Psi_1=0$ are given by[14,9,10]

$$b_\mu = l_\mu(\delta+2\beta+\tau)\psi_{\mathrm{E}} - m_\mu(D+2\epsilon+\rho)\psi_{\mathrm{E}} + \text{c.c.}, \tag{12}$$

where the complex scalar potential ψ_{E} satisfies

$$[(\Delta+\gamma-\overline{\gamma}+\overline{\mu})(D+2\epsilon+\rho) - (\overline{\delta}+\alpha+\overline{\beta}-\overline{\tau})(\delta+2\beta+\tau)]\psi_{\mathrm{E}} = 0. \tag{13}$$

Commuting the derivatives acting on ψ_{E}, making use of the fact that $\kappa=\sigma=\Psi_1=0$, one obtains

$$[(D+3\epsilon+\overline{\epsilon}+2\rho-\overline{\rho})(\Delta+2\gamma+\mu) - (\delta+3\beta-\overline{\alpha}+2\tau+\overline{\pi})(\overline{\delta}+2\alpha+\pi) - 6\Psi_2]\psi_{\mathrm{E}} = 0. \tag{14}$$

Using the fact that ψ_{E} has spin weight -1, we look for solutions of Eq. (14) of the form

$$\psi_{\mathrm{E}} = \frac{\chi}{r^3} X_{-2}(r) e^{-i\omega t}\, {}_{-1}Y_{jm}(\theta,\varphi). \tag{15}$$

Then, substituting Eqs. (3a), (4), and (15) into Eq. (14), one finds that

$$\mathscr{D}\frac{\chi^2}{r^6}\mathscr{D}^* X_{-2} = \eta^2 \frac{\chi}{r^6}\left(1+\frac{12M}{\eta^2 r}\right) X_{-2}. \tag{16}$$

Therefore, introducing the function

$$Y_{-1} \equiv \frac{\chi^2}{r^6}\mathscr{D}^* X_{-2}, \tag{17}$$

Eq. (16) is equivalent to

$$\mathscr{D} Y_{-1} = \eta^2 \frac{\chi}{r^6}\left(1+\frac{12M}{\eta^2 r}\right) X_{-2}, \quad \mathscr{D}^* X_{-2} = \frac{r^6}{\chi^2} Y_{-1} \tag{18}$$

[cf. Eqs. (11)].

Equations (11) and (18) can be written in the common form

$$\mathscr{D} Y_{-k} = \eta^2 \frac{\chi}{r^6}\left(1+\frac{2q_k}{\eta^2 r}\right) X_{-l}, \quad \mathscr{D}^* X_{-l} = \frac{r^6}{\chi^2}\left(1+\frac{q_l}{\eta^2 r}\right) Y_{-k} \quad (k,l=1,2;\ k\neq l), \tag{19}$$

where

$$q_1 \equiv 6M, \quad q_2 \equiv 0. \tag{20}$$

In the study of the perturbations of the Reissner–Nordström solution, Chandrasekhar[15,5] obtained a set of equations identical to Eqs. (19). It must be noticed, however, that in the present case there is no need to make infinitesimal tetrad rotations as in Refs. 15 and 5. The solution of Eqs. (19) can be expressed in terms of a single function $Z_k^{(+)}$ or $Z_k^{(-)}$, which obeys the Schrödinger-type equation,[15,5]

$$\left(-\frac{d^2}{dr_*^2} + V_k^{(\pm)}\right) Z_k^{(\pm)} = \omega^2 Z_k^{(\pm)}, \tag{21}$$

where r_* is defined by $dr_*/dr=r^2/\chi$ and

$$V_k^{(\pm)}\equiv \pm q_l \frac{df_k}{dr_*}+q_l^2 f_k^2+\eta^2(\eta^2+2)f_k,$$
$$f_k\equiv \frac{\chi}{r^3(\eta^2 r+q_l)} \quad (k,l=1,2;\ \ k\neq l). \tag{22}$$

The solution of Eqs. (19) is given by

$$Y_{-k}=V_k^{(\pm)}Z_k^{(\pm)}+(W_k^{(\pm)}+2i\omega)\left(\frac{d}{dr_*}+i\omega\right)Z_k^{(\pm)},$$
$$\eta^2 X_{-l}=\mp q_l Z_k^{(\pm)}+f_k^{-1}\left(\frac{d}{dr_*}+i\omega\right)Z_k^{(\pm)} \quad (k\neq l), \tag{23}$$

with

$$W_k^{(\pm)}\equiv -\frac{d}{dr_*}\ln f_k\mp q_l f_k \quad (k\neq l). \tag{24}$$

It may be noticed that, since q_2 vanishes, the potentials $V_1^{(+)}$ and $V_1^{(-)}$, which correspond to the electromagnetic perturbations, coincide and, similarly, that $W_1^{(+)}=W_1^{(-)}$; therefore, Eqs. (21)–(24) yield only one expression for Y_{-1} and X_{-2}. On the other hand, Eqs. (3b), (20), and (22) give two distinct potentials,

$$V_2^{(+)}=\frac{\chi}{r^5}\frac{\eta^4(\eta^2+2)r^3+6\eta^4 Mr^2+36\eta^2M^2r+72M^3}{(\eta^2 r+6M)^2} \tag{25}$$

and

$$V_2^{(-)}=\frac{\chi}{r^5}[(\eta^2+2)r-6M]. \tag{26}$$

The potentials $V_2^{(+)}$ and $V_2^{(-)}$ were originally obtained by Zerilli[3] and by Regge and Wheeler,[2] respectively, in the study of the polar and axial metric perturbations of the Schwarzschild metric. Chandrasekhar and Detweiler[16] proved that the reflection and transmission coefficients corresponding to the potential barriers $V_2^{(+)}$ and $V_2^{(-)}$ are the same (also see Refs. 5 and 15 and Sec. IV).

In the present treatment, the functions $Z_2^{(+)}$ and $Z_2^{(-)}$ lead to the same set of solutions of Eqs. (11) and, as we shall show in Sec. IV, the reflection and transmission coefficients for the gravitational waves impinging on a Schwarzschild black hole coincide with those of the potential barrier employed to express the solution of Eqs. (11) [Eqs. (23)]; therefore, without any further calculation or without having to relate the functions $Z_2^{(+)}$ and $Z_2^{(-)}$ that produce a given perturbation, it follows that the reflection and transmission coefficients for $V_2^{(+)}$ and $V_2^{(-)}$ must coincide. (It may be remarked that in Ref. 5 it is shown that the perturbed value of Ψ_4, with respect to the tetrad (3), can be expressed in terms of the radial functions Y_{-2}, which are given in terms of either $Z_2^{(+)}$ or $Z_2^{(-)}$ by Eq. (23); this fact alone does not imply the equality of the reflection and transmission coefficients for $V_2^{(+)}$ and $V_2^{(-)}$ since the computation of the reflection and transmission coefficients of the black hole requires the knowledge of the corresponding perturbed value of Ψ_0 [see Eqs. (51), (53) and (56) below].) Note also that the meaning of the functions Y_{-k} and X_{-l} appearing in the present treatment differs from that of analogous functions introduced by Chandrasekhar.[15,5]

III. THE DIFFERENTIAL IDENTITIES

Since the complete perturbations (gravitational or electromagnetic) are given in terms of derivatives of a single scalar potential, there must exist differential identities relating the perturbed quantities. In fact, some differential relations of this type (called Teukolsky–Starobinsky identities) were obtained in the study of the Kerr metric perturbations. In terms of the notation used here, the Teukolsky–Starobinsky identities can be expressed as[17–19,5]

$$\chi^2\mathscr{D}^*\mathscr{D}^*\mathscr{D}^*\mathscr{D}^*r^3Y_{+2}\propto r^3Y_{-2}, \quad \chi^2\mathscr{D}\mathscr{D}\mathscr{D}\mathscr{D}r^3Y_{-2}\propto r^3Y_{+2}, \tag{27}$$

for the gravitational perturbations, and

$$\chi\mathscr{D}^*\mathscr{D}^*\frac{\chi}{r^3}X_{+2}\propto\frac{\chi}{r^3}X_{-2}, \quad \chi\mathscr{D}\mathscr{D}\frac{\chi}{r^3}X_{-2}\propto\frac{\chi}{r^3}X_{+2}, \tag{28}$$

in the case of the electromagnetic perturbations, where Y_{+k} and X_{+l} are radial functions satisfying the differential equations

$$\mathscr{D}^*Y_{+k}=\eta^2\frac{\chi}{r^6}\left(1+\frac{2q_k}{\eta^2 r}\right)X_{+l}, \quad \mathscr{D}X_{+l}=\frac{r^6}{\chi^2}\left(1+\frac{q_l}{\eta^2 r}\right)Y_{+k} \quad (k\neq l), \tag{29}$$

[cf. Eqs. (19)].

Since the radial dependence of the scalar potentials ψ_{G} and ψ_{E} is determined by similar equations [Eqs. (19)], it is not surprising that the identities (27)–(28) can be derived from a single relation. Indeed, the functions $X_{\pm k}$ can be normalized in such a way that[20]

$$\eta^2r^3\mathscr{D}^*\mathscr{D}^*\frac{\chi}{r^3}X_{+k}+q_kr^2\mathscr{D}^*\frac{1}{r}\mathscr{D}^*\frac{\chi}{r^2}X_{+k}=C_kX_{-k} \tag{30}$$

and

$$\eta^2r^3\mathscr{D}\mathscr{D}\frac{\chi}{r^3}X_{-k}+q_kr^2\mathscr{D}\frac{1}{r}\mathscr{D}\frac{\chi}{r^2}X_{-k}=\widetilde{C}_kX_{+k}, \tag{31}$$

where C_k and $\widetilde{C}_k$ are constants such that

$$\widetilde{C}_k=\overline{C_k}, \quad \text{for } \omega \text{ real.} \tag{32}$$

When $k=2$, owing to the fact that $q_2=0$, Eqs. (30) and (31) reduce to

$$\chi\mathscr{D}^*\mathscr{D}^*\frac{\chi}{r^3}X_{+2}=\frac{C_2}{\eta^2}\frac{\chi}{r^3}X_{-2}, \quad \chi\mathscr{D}\mathscr{D}\frac{\chi}{r^3}X_{-2}=\frac{\widetilde{C}_2}{\eta^2}\frac{\chi}{r^3}X_{+2}, \tag{33}$$

which correspond to Eqs. (28).

On the other hand, applying the operator $\mathscr{D}^*$ to both sides of Eq. (30) and making use of Eq. (19), one readily finds that

$$\eta^2\frac{\chi^2}{r^4}\mathscr{D}^*\mathscr{D}^*\mathscr{D}^*\frac{\chi}{r^2}X_{+k}=C_kY_{-l} \quad (k\neq l). \tag{34}$$

In an analogous manner, one obtains the identity

$$\eta^2 \frac{\chi^2}{r^4} \mathscr{D}\mathscr{D}\mathscr{D} \frac{\chi}{r^2} X_{-k} = \widetilde{C}_k Y_{+l} \quad (k \neq l). \tag{35}$$

Setting $k=1$ in Eqs. (34) and (35), and eliminating $X_{\pm 1}$ in favor of $Y_{\pm 2}$, making use of Eqs. (19) and (29), one obtains

$$\chi^2 \mathscr{D}^* \mathscr{D}^* \mathscr{D}^* \mathscr{D}^* r^3 Y_{+2} = C_1 r^3 Y_{-2}, \quad \chi^2 \mathscr{D}\mathscr{D}\mathscr{D}\mathscr{D} r^3 Y_{-2} = \widetilde{C}_1 r^3 Y_{+2}, \tag{36}$$

which correspond to Eqs. (27).

From Eqs. (19) and (29) one can derive two additional useful identities,

$$r^2 \mathscr{D}^* \mathscr{D}^* \mathscr{D}^* r^2 Y_{+k} = \eta^2 r \mathscr{D}^* \mathscr{D}^* \frac{\chi}{r^3} X_{+l} + 2q_k \mathscr{D}^* \mathscr{D}^* \frac{\chi}{r^3} X_{+l} - 4q_k \mathscr{D}^* \frac{\chi}{r^4} X_{+l} \quad (k \neq l) \tag{37}$$

and

$$r^2 \mathscr{D}\mathscr{D}\mathscr{D} r^2 Y_{-k} = \eta^2 r \mathscr{D}\mathscr{D} \frac{\chi}{r^3} X_{-l} + 2q_k \mathscr{D}\mathscr{D} \frac{\chi}{r^3} X_{-l} - 4q_k \mathscr{D} \frac{\chi}{r^4} X_{-l} \quad (k \neq l). \tag{38}$$

The value of $C_k \widetilde{C}_k$ can be obtained by eliminating X_{+k} from Eqs. (30) and (31) and making use repeatedly of Eqs. (19), this gives

$$C_k \widetilde{C}_k = \eta^4 (\eta^2 + 2)^2 + 4\omega^2 q_k^2. \tag{39}$$

The phase of C_k depends on the relative normalization of the functions X_{-k} and X_{+k}.

IV. REFLECTION, TRANSMISSION, AND ABSORPTION OF GRAVITATIONAL AND ELECTROMAGNETIC WAVES

All the components of the perturbed Weyl spinor, distinguished with a superscript B, can be calculated making use of Eq. (1) and the relation[21]

$$\Psi^{\mathrm{B}}_{ACDE} = \tfrac{1}{2} \nabla_{(A}{}^{R'} \nabla_C{}^{S'} h_{DE)R'S'} + \tfrac{1}{4} h^{\mu}{}_{\mu} \Psi_{ACDE}. \tag{40}$$

Then, by means of a straightforward but lengthy computation, using Eqs. (1), (3), (4), and (6) one obtains

$$\begin{aligned}
\overline{\Psi^{\mathrm{B}}_0} &= (\mathscr{D}\mathscr{D}\mathscr{D}\mathscr{D} r^3 Y_{-2}) e^{-i\omega t} {}_{-2}Y_{jm}(\theta,\varphi), \\
\overline{\Psi^{\mathrm{B}}_1} &= -\frac{\eta}{\sqrt{2}} (\mathscr{D}\mathscr{D}\mathscr{D} r^2 Y_{-2}) e^{-i\omega t} {}_{-1}Y_{jm}(\theta,\varphi), \\
\overline{\Psi^{\mathrm{B}}_2} &= \frac{\eta\sqrt{\eta^2+2}}{2r} (\mathscr{D} r^2 \mathscr{D}\, Y_{-2}) e^{-i\omega t} Y_{jm}(\theta,\varphi), \\
\overline{\Psi^{\mathrm{B}}_3} &= -\frac{\eta(\eta^2+2)}{2\sqrt{2}} \mathscr{D}\, Y_{-2} e^{-i\omega t} {}_1Y_{jm}(\theta,\varphi), \\
\overline{\Psi^{\mathrm{B}}_4} &= \frac{\eta^2(\eta^2+2)}{4r} Y_{-2} e^{-i\omega t} {}_2Y_{jm}(\theta,\varphi) - \frac{3iM\omega}{r} \overline{Y_{-2}} e^{i\omega t}\ \overline{{}_{-2}Y_{jm}(\theta,\varphi)}.
\end{aligned} \tag{41}$$

[In order to obtain the reduced expression for $\overline{\Psi_4^{\mathrm{B}}}$ given by Eq. (41) one has to employ repeatedly Eq. (2) or (11).[22,23]] Similarly, from Eqs. (3), (4), (12), (13), and (15) it follows that the components of the electromagnetic field perturbations are given by

$$\overline{\varphi_0}=\left(\mathscr{D}\mathscr{D}\frac{\chi}{r^3}X_{-2}\right)e^{-i\omega t}{}_{-1}Y_{jm}(\theta,\varphi),$$

$$\overline{\varphi_1}=-\frac{\sqrt{\eta^2+2}}{\sqrt{2}}\left(\frac{1}{r}\mathscr{D}\frac{\chi}{r^3}X_{-2}\right)e^{-i\omega t}Y_{jm}(\theta,\varphi), \tag{42}$$

$$\overline{\varphi_2}=\frac{(\eta^2+2)}{2}\frac{\chi}{r^5}X_{-2}e^{-i\omega t}{}_1Y_{jm}(\theta,\varphi).$$

Alternative expressions for the perturbations (41) and (42) can be obtained, making use of the differential relations (11), (33), (36), and (38). In particular, Ψ_0^{B} and Ψ_4^{B}, which are invariant under the gauge transformations $h_{\mu\nu}\mapsto h_{\mu\nu}-2\nabla_{(\mu}\xi_{\nu)}$ and represent the ingoing and outgoing gravitational radiation, respectively (see below), are given by

$$\overline{\Psi_0^{\mathrm{B}}}=\widetilde{C}_1\frac{r^3}{\chi^2}Y_{+2}e^{-i\omega t}{}_{-2}Y_{jm}(\theta,\varphi), \tag{43a}$$

$$\overline{\Psi_4^{\mathrm{B}}}=\frac{1}{4r}\{\eta^2(\eta^2+2)Y_{-2}e^{-i\omega t}{}_2Y_{jm}(\theta,\varphi)-12iM\omega\overline{Y_{-2}}e^{i\omega t}\ \overline{{}_{-2}Y_{jm}(\theta,\varphi)}\}. \tag{43b}$$

Equations (43) correspond to Eqs. (362) and (363) of Sec. 32 of Ref. 5; however, Eq. (43b) is not equivalent to the corresponding expression given in Ref. 5.

Since the potentials $V_k^{(\pm)}$ are of short range, $Z_k^{(\pm)}$ have the asymptotic behaviors $e^{\pm i\omega r_*}$ both for $r_*\to\infty$ and $r_*\to-\infty$ (the horizon of the black hole) and from Eqs. (23) one can find the asymptotic forms of Y_{-k} and X_{-l}.[5] If the functions $Z_k^{(\pm)}$ have the asymptotic behavior $e^{-i\omega r_*}$ for $r\to\infty$, then Eqs. (41) and (42) show that

$$\Psi_i^{\mathrm{B}}=O\left(\frac{1}{r^{1+i}}\right),\quad \varphi_i=O\left(\frac{1}{r^{1+i}}\right),$$

which means that, for ingoing waves, Ψ_0^{B} and φ_0 represent the ingoing fields and that these perturbations satisfy the ''peeling property'' (see Ref. 24). Similarly, if $Z_k^{(\pm)}$ have the asymptotic behavior $e^{i\omega r*}$ for $r_*\to\infty$,

$$\Psi_i^{\mathrm{B}}=O\left(\frac{1}{r^{5-i}}\right),\quad \varphi_i=O\left(\frac{1}{r^{3-i}}\right);$$

hence, at spatial infinity, Ψ_4^{B} and φ_2 represent the outgoing fields.

By definition, under a rotation through an angle ϕ determined by $m^\mu\mapsto e^{i\phi}m^\mu$, a quantity ξ with spin weight s transforms as $\xi\mapsto e^{is\phi}\xi$; therefore, since $\overline{\Psi_0^{\mathrm{B}}}$, $\overline{\Psi_4^{\mathrm{B}}}$, $\overline{\varphi_0}$, and $\overline{\varphi_2}$ have spin weight -2, 2, -1, and 1, respectively, if any of these quantities is proportional to $e^{i\omega t}$ or to $e^{-i\omega t}$, the corresponding field has circular polarization, while the presence of both factors, $e^{i\omega t}$ and $e^{-i\omega t}$, means that the field has elliptic polarization. Thus, at spatial infinity, the ingoing gravitational waves and the (ingoing and outgoing) electromagnetic waves given by Eqs. (41) and (42) have right (left) circular polarization if $\omega>0$ ($\omega<0$). (Note that φ_0 and φ_2 have opposite spin weights, but they represent waves propagating in opposite directions.) On the other hand, the outgoing gravitational waves given by Eqs. (41) will be elliptically polarized (unless $M\omega Y_{-2}$ vanishes).

Equation (43b) deserves some comments. First, the presence of a term proportional to $e^{i\omega t}$ is a consequence of considering *real* metric perturbations [Eq. (1)]. Second, unless $M\omega Y_{-2}$, or $M\omega Y_{+2}$, vanishes, there are no real gravitational perturbations such that all the components of the perturbed Weyl spinor have a time dependence of the form $e^{i\omega t}$ (or $e^{-i\omega t}$). Third, the presence of both factors $e^{i\omega t}$ and $e^{-i\omega t}$ in Ψ_4^{B} has an objective physical meaning: it signifies that the outgoing gravitational waves are elliptically polarized if the ingoing gravitational waves are circularly polarized. In most previous investigations on black hole perturbations (see, e.g., Ref. 5) it is assumed that all the perturbed quantities have a time dependence of the form $e^{-i\omega t}$, which, as remarked above, is not consistent if the metric perturbations are real [see also Ref. 7, Eqs. (3.97) and (3.98)] and, furthermore, it amounts to assuming that the helicity of the gravitational waves is left unchanged by the scattering from the black hole. Note that in the case of the scattering of electromagnetic waves, a circularly polarized ingoing wave gives rise to a circularly polarized outgoing wave (a result that is not obvious).

Assuming that there are no waves emerging from the horizon, the functions $Z_k^{(\pm)}$ have the asymptotic forms

$$\begin{aligned} Z_k^{(\pm)} &\to A_k^{(\pm)} e^{-i\omega r_*} + B_k^{(\pm)} e^{i\omega r_*} \quad (r_* \to +\infty), \\ &\to D_k^{(\pm)} e^{-i\omega r_*} \qquad\qquad\quad (r_* \to -\infty). \end{aligned} \tag{44}$$

Since the potentials $V_k^{(\pm)}$ are real, from Eq. (21) it follows that the amplitudes

$$R_k^{(\pm)} \equiv \frac{B_k^{(\pm)}}{A_k^{(\pm)}}, \quad T_k^{(\pm)} \equiv \frac{D_k^{(\pm)}}{A_k^{(\pm)}}, \tag{45}$$

satisfy

$$|R_k^{(\pm)}|^2 + |T_k^{(\pm)}|^2 = 1. \tag{46}$$

Expressing the radial functions Y_{-k}, X_{-l} in terms of $Z_k^{(\pm)}$, by means of Eqs. (23), and assuming that $Z_k^{(\pm)}$ have the asymptotic forms (44), from Eqs. (41) and (42) one finds that when $r_* \to \infty$,

$$\begin{gathered} \frac{1}{4} r\overline{\Psi_0^{\mathrm{B}}} \to -\omega^2[\eta^2(\eta^2+2) \pm 12iM\omega] A_2^{(\pm)} e^{-i\omega(t+r_*)}\, {}_{-2}Y_{jm}, \\ r\overline{\Psi_4^{\mathrm{B}}} \to -\omega^2[\eta^2(\eta^2+2) B_2^{(\pm)} e^{-i\omega(t-r_*)}\, {}_2Y_{jm} - 12iM\omega \overline{B_2^{(\pm)}} e^{i\omega(t-r_*)}\ \overline{{}_{-2}Y_{jm}}], \\ \frac{1}{2} r\overline{\varphi_0} \to -i\omega\eta(\eta^2+2) A_1 e^{-i\omega(t+r_*)}\, {}_{-1}Y_{jm}, \\ r\overline{\varphi_2} \to i\omega\eta(\eta^2+2) B_1 e^{-i\omega(t-r_*)}\, {}_1Y_{jm}. \end{gathered} \tag{47}$$

Similarly, when $r_* \to -\infty$ (the horizon of the black hole),

$$\begin{gathered} \chi^2 \overline{\Psi_0^{\mathrm{B}}} \to 4i\omega\left(i\omega + \frac{1}{4M}\right)(2M)^3[\eta^2(\eta^2+2) \pm 12iM\omega] D_2^{(\pm)} e^{-i\omega(t+r_*)}\, {}_{-2}Y_{jm}, \\ \chi\overline{\varphi_0} \to -4iM\omega\eta(\eta^2+2) D_1 e^{-i\omega(t+r_*)}\, {}_{-1}Y_{jm}. \end{gathered} \tag{48}$$

(We have supressed the superscript $(\pm)$ in the coefficients A_1, B_1, and D_1, since there is no difference between $Z_1^{(+)}$ and $Z_1^{(-)}$ [see Eqs. (21)–(24)].)

From Eqs. (47) and (48) it follows that the functions $Z_2^{(+)}$ and $Z_2^{(-)}$, satisfying the boundary conditions (44), give rise to the same gravitational perturbations, provided that the coefficients $A_2^{(\pm)}$, $B_2^{(\pm)}$, and $D_2^{(\pm)}$ are related by

$$\begin{gathered}[\eta^2(\eta^2+2)+12iM\omega]A_2^{(+)}=[\eta^2(\eta^2+2)-12iM\omega]A_2^{(-)},\\ B_2^{(+)}=B_2^{(-)},\\ [\eta^2(\eta^2+2)+12iM\omega]D_2^{(+)}=[\eta^2(\eta^2+2)-12iM\omega]D_2^{(-)},\end{gathered} \tag{49}$$

which, among other things, implies that [see Eqs. (45)]

$$R_2^{(+)}=\frac{\eta^2(\eta^2+2)+12iM\omega}{\eta^2(\eta^2+2)-12iM\omega}\,R_2^{(-)},\quad T_2^{(+)}=T_2^{(-)}. \tag{50}$$

(An alternative proof of these relations was given by Chandrasekhar.[15,5])

Using Eqs. (47) one finds that the flux of energy per unit time of the gravitational or electromagnetic radiation coming from infinity is given by

$$\frac{dE_{\text{in}}^{\text{grav}}}{dt}=\frac{1}{4\pi\omega^2}\lim_{r\to\infty}\int\left|\frac{1}{4}\,r\Psi_0^{\text{B}}\right|^2 d\Omega=\frac{\omega^2}{4\pi}\,[\eta^4(\eta^2+2)^2+144M^2\omega^2]|A_2^{(\pm)}|^2 \tag{51}$$

and

$$\frac{dE_{\text{in}}^{\text{em}}}{dt}=\frac{1}{2\pi}\lim_{r\to\infty}\int\left|\frac{1}{2}\,r\varphi_0\right|^2 d\Omega=\frac{\omega^2}{2\pi}\,\eta^2(\eta^2+2)^2|A_1|^2, \tag{52}$$

respectively. Similarly, since the power flux per unit solid angle of the outgoing gravitational and electromagnetic waves is

$$\frac{d^2E_{\text{out}}^{\text{grav}}}{dt\,d\Omega}=\frac{1}{4\pi\omega^2}\lim_{r\to\infty}|r\Psi_4^{\text{B}}|^2,\quad \frac{d^2E_{\text{out}}^{\text{em}}}{dt\,d\Omega}=\frac{1}{2\pi}\lim_{r\to\infty}|r\varphi_2|^2, \tag{53}$$

respectively, the *time-averaged* flux of energy per unit time of the outgoing gravitational waves is

$$\left\langle\frac{dE_{\text{out}}^{\text{grav}}}{dt}\right\rangle=\frac{\omega^2}{4\pi}\,[\eta^4(\eta^2+2)^2+144M^2\omega^2]|B_2^{(\pm)}|^2, \tag{54}$$

and the flux of energy per unit time of the outgoing electromagnetic waves is

$$\frac{dE_{\text{out}}^{\text{em}}}{dt}=\frac{\omega^2}{2\pi}\,\eta^2(\eta^2+2)^2|B_1|^2. \tag{55}$$

Finally, using the fact that the flux of energy across the event horizon is given by

$$\begin{gathered}\frac{d^2E_{\text{hole}}^{\text{grav}}}{dt\,d\Omega}=\frac{1}{64\pi}\lim_{r\to 2M}\frac{|\chi^2\Psi_0^{\text{B}}|^2}{(2M)^6[\omega^2+1/(4M)^2]},\\ \frac{d^2E_{\text{hole}}^{\text{em}}}{dt\,d\Omega}=\frac{1}{8\pi}\lim_{r\to 2M}\frac{|\chi\varphi_0|^2}{(2M)^2}\end{gathered} \tag{56}$$

[see Ref. 17 and Ref. 5, Eq. (258) of Chap. 8 and Eq. (516) of Chap. 9], from Eqs. (48) one obtains

$$\frac{dE^{\text{grav}}_{\text{hole}}}{dt}=\frac{\omega^2}{4\pi}\,[\,\eta^4(\,\eta^2+2)^2+144M^2\omega^2]|D_2^{(\pm)}|^2, \tag{57}$$

$$\frac{dE^{\text{em}}_{\text{hole}}}{dt}=\frac{\omega^2}{2\pi}\,\eta^2(\,\eta^2+2)^2|D_1|^2. \tag{58}$$

Thus, Eqs. (45), (46), (51), (52), (54), (55), (57), and (58) explicitly show that the energy carried by the gravitational or the electromagnetic perturbations is conserved. (Note that in order for these conservation relations to hold, it may be necessary to consider the time-averaged flux of energy [see Eq. (54)].) Furthermore, one has

$$\frac{\langle dE^{\text{grav}}_{\text{out}}/dt\rangle}{dE^{\text{grav}}_{\text{in}}/dt}=|R_2^{(\pm)}|^2,\quad \frac{dE^{\text{grav}}_{\text{hole}}/dt}{dE^{\text{grav}}_{\text{in}}/dt}=|T_2^{(\pm)}|^2 \tag{59}$$

and

$$\frac{dE^{\text{em}}_{\text{out}}/dt}{dE^{\text{em}}_{\text{in}}/dt}=|R_1|^2,\quad \frac{dE^{\text{em}}_{\text{hole}}/dt}{dE^{\text{em}}_{\text{in}}/dt}=|T_1|^2, \tag{60}$$

which means that the energy reflection and transmission coefficients for the gravitational and electromagnetic waves do coincide with the reflection and transmission coefficients for the potential barriers $V_2^{(\pm)}$ and V_1, respectively, in the Schrödinger-type equations (21). Note that the ''conservation relations'' (46) can be properly interpreted as expressions of the conservation of energy only after the energy fluxes (51), (52), (54), (55), (57), and (58) are derived, which requires, in particular, the knowledge of Ψ_0^{B} and Ψ_4^{B} with the correct relative normalization.

V. CONCLUDING REMARKS

As pointed out in Sec. II, Eqs. (19), which we take as the basic equations for the (uncoupled) gravitational and electromagnetic perturbations of the Schwarzschild solution, possess the form of a set of equations found in the study of the coupled gravitational and electromagnetic perturbations of the Reissner–Nordström solution,[15,5] although with a different meaning for the functions Y_{-k} and X_{-l}. This fact suggests that, going in the opposite direction, the equations for the gravitational and electromagnetic perturbations of some solutions of the Einstein vacuum field equations can be written in a form useful in the study of the coupled perturbations of the charged version of the background solution.

The derivations presented here illustrate the many simplifications that follow from the use of the Debye potentials in the study of perturbations.

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A null-tetrad approach to Kerr–Schild gravitational fields in matter

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The null tetrad formalism is used to investigate the structure of the Einstein field equations for Kerr–Schild gravitational fields in the presence of an elastic solid source. It is shown that such equations may be reduced to five nonlinear partial differential equations for five variables. It turns out that, when the interior solutions admit the same preferred null congruence of the vacuum ones and some compatibility conditions hold, it is possible to reduce them to a linear system and to develop a method of solution which closely resembles the ''variation of the arbitrary constants'' for ordinary differential equations. In the present paper, the above technical framework is developed in general and applied to two simple examples, deferring to future work the approach to the Kerr–interior problem. © *1996 American Institute of Physics.* [S0022-2488(96)02509-1]

I. INTRODUCTION

In a recent paper[1] a new approach to the problem of finding the sources of the Kerr metric was presented. The key idea of such a paper was to search for elastic-solid sources within the same algebraic class to which the Kerr metric itself belongs, namely the Kerr–Schild[2] one (KS in what follows). In that paper it was shown that any stationary KS field in elastic matter may be obtained by solving three *linear* partial differential equations for the gravitational field and a set of six nonlinear, but algebraic, relations for the stresses. Such results lead to a new class of exact solutions which may be interpreted as describing elastic sources of the Kerr metric, the matching surface being an oblate spheroid. However, some open problems remain. First, the matching of the interior solution with the Kerr vacuum is not smooth, so that it is necessary to interpret the corresponding jump of the exterior curvature as a surface distribution; this fact strongly depends on the specific choice of the matching surface, but if one tries to change this choice one has to face a very difficult potential problem in Newtonian theory. Moreover, it is difficult to study the physical behavior of the stresses when the rotation rate becomes high.

The above results were obtained by means of a coordinate-dependent method. However, it is well known that the use of the Newman–Penrose (NP) formalism[3] proves very useful in dealing with KS gravitational fields. Recent developments in this area regard the ''generalized'' Kerr–Schild problem both in vacuum[4] and in presence of matter[5] and the generalization of the Kerr theorem to the nonstationary case.[6] The suitability of the NP formalism arises essentially because the preferred null direction of the KS geometry is a natural candidate for one of the null vectors of the NP tetrad. In fact, this observation was the starting point of the work by Debney, Kerr, and Schild (DKS)[7] who characterized the KS solutions of the Einstein and Einstein–Maxwell equations having a nonvanishing complex expansion. Here arises also the idea of the present paper, in which the search for exact KS solutions for the gravitational equations in elastic matter is conducted by making use of the tetrad formalism. Our main result is that, assuming as a source a non-prestressed elastic material, the gravitational field equations in the tetrad formalism can be reduced to five partial differential equations for five variables which have interesting properties. Such equations may in fact be written in a form which makes them directly comparable to that of vacuum, and this comparison suggests the possibility of constructing some nonvacuum solutions starting from the DKS vacuum ones. This may be done with a method which closely recalls the

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''variation of the arbitrary constants'' for ordinary differential equations. It consists of choosing a vacuum solution and imposing that the corresponding nonvacuum one have the same preferred null congruence. This fixes two of the three quantities that characterize the gravitational field and, whenever the appropriate compatibility conditions hold, the determination of the field variables can be reduced to the integration of two suitable, linear differential forms. This quite unexpected result shows the way in which linearity comes into play using the null-tetrad formalism.

The present paper presents the framework of this null-tetrad approach to KS gravitational fields in elastic matter; the method described above is thus developed in general but only applied to two simple examples, deferring to a future work the application to the problem of the sources of the Kerr and the Kerr–Newman metric. To construct our examples we start from a Newman–Unti–Tamburino (NUT)[8] vacuum solution having a null Killing vector and from the Schwarzschild solution, respectively. The first choice gives rise to an independent derivation of a class of solutions originally due to Kowalczyński and Plebański,[9] while the second one produces a new class of (generally singular) nonstationary solutions, which, for certain choices of the integration parameters, reduces to an already known regular, static and spherically symmetric subclass.[10]

The paper is structured as follows. The null-tetrad formalism for KS fields is briefly recalled in Sec. II. The energy-momentum tensor and the Einstein field equations in the tetrad form are obtained in Secs. III and IV. Section V contains an overview on the vacuum DKS solutions, while the method of reduction of the nonvacuum field equations is presented in Sec. VI. The two examples are finally treated in Secs. VII and VIII, respectively. The paper ends with some concluding remarks and an outline about future work on this subject.

II. NULL-TETRAD FORMALISM FOR KERR–SCHILD FIELDS

Let $\mathscr{M}$ be the general-relativistic space–time equipped with the pseudo-Riemannian metric tensor $g_{\mu\nu}$ [$\mu,\nu=0,1,2,3$, signature $(-,+,+,+)$].[11]

Introduce at each point of $\mathscr{M}$ a tetrad of independent vectors $e_a{}^\mu$ ($a,b=1,2,3,4$) such that $e_a{}^\mu e^b{}_\mu=\delta_a^b$, where $e^b{}_\mu$ is the dual tetrad. We denote by e^a the linear differential forms $e^a{}_\mu dx^\mu$. The tetrad components of a tensor $T_{\mu\nu}$ are given by $T_{ab}=T_{\mu\nu}e_a{}^\mu e_b{}^\nu$. The directional derivatives along tetrad vectors will always be denoted by a comma preceding the index a, so that, for example,

$$f_{,a}:=e_a{}^\mu\partial_\mu f$$

for any scalar function f. The tetrad components of the covariant derivatives $e_a{}^\mu\boldsymbol{\nabla}_\mu$ will instead be denoted by a semicolon, while the symbol ''∂'' with a subscript will be always reserved for the partial derivative.

In the tetrad formalism the role of the Christoffel symbols is played by the Ricci rotation coefficients, defined by

$$\Gamma^a{}_{bc}:=-e^a{}_{\mu;\nu}e_b{}^\mu e_c{}^\nu.$$

For instance, the covariant derivative of a tensor reads

$$T^a{}_{b;c}=T^a{}_{b,c}-\Gamma^d{}_{bc}T^a{}_d+\Gamma^a{}_{dc}T^d{}_b\,.$$

The Ricci coefficients also determine the commutator between directional derivatives along tetrad vectors:

$$T^{\cdot\cdot}_{\cdot\cdot,[ab]}:=\tfrac{1}{2}\,(T^{\cdot\cdot}_{\cdot\cdot,ab}-T^{\cdot\cdot}_{\cdot\cdot,ba})=T^{\cdot\cdot}_{\cdot\cdot,c}\Gamma^c{}_{[ab]}\,.$$

We adopt the Newman–Penrose choice for the tetrad, which consists of using four null vectors such that $\underline{e}_1$ and $\underline{e}_2$ are complex conjugates while $\underline{e}_3$ and $\underline{e}_4$ are real. However, we will not

use the Newman–Penrose notations and conventions but rather that used by Debney, Kerr, and Schild. The scalar products between the tetrad vectors are therefore given by

$$g_{ab}=g_{\mu\nu}e_a{}^{\mu}e_b{}^{\nu}=\begin{pmatrix}0&1&0&0\\1&0&0&0\\0&0&0&1\\0&0&1&0\end{pmatrix} \tag{2.1}$$

whereas in the standard convention g_{34} equals *minus* one.

The numerical values 1,2,3,4 will always refer to tetrad indexes. These are raised and lowered by performing the permutation 1,2,3,4↦2,1,4,3. The complex conjugate of a real geometrical object may be obtained by applying the permutation 1,2,3,4↦2,1,3,4.

We are going to consider here only space–times which are of the Kerr–Schild type, namely we assume that the metric tensor may be put into the form

$$g_{\mu\nu}=\eta_{\mu\nu}+2hl_{\mu}l_{\nu},$$

where $\eta_{\mu\nu}$ is the metric tensor of Minkowski space, h is a scalar function, and l^{μ} is a null vector with respect to both the flat and the curved metric. It is therefore natural to pick l^{μ} as one of the null real vectors of the tetrad, say $\underset{\sim}{e}_4$. Starting with a system of pseudo-Cartesian coordinates $x^{\mu}=(x,y,z,t)$ such that the Minkowski metric assumes its canonical form, and introducing the null coordinates

$$\xi=\frac{x+iy}{\sqrt{2}},\quad \overline{\xi}=\frac{x-iy}{\sqrt{2}},$$

$$u=\frac{z+t}{\sqrt{2}},\quad v=\frac{z-t}{\sqrt{2}},$$

the line element reads

$$ds^2=2\ d\xi\ d\overline{\xi}+2\ du\ dv+2h(e^3)^2. \tag{2.2}$$

It is well known that a general field of null directions in Minkowski space may be parametrized in the form

$$e^3=du+\overline{Y}d\xi+Yd\overline{\xi}-\overline{Y}Ydv,$$

where Y is a complex function, so far arbitrary. The null tetrad may be completed as follows:

$$e^1=d\xi-Ydv,\qquad e^2=d\overline{\xi}-\overline{Y}dv,\qquad e^4=dv+he^3.$$

The directional derivatives of a scalar function f therefore read

$$\begin{aligned}f_{,1}&=\partial_{\xi}f-\overline{Y}\partial_u f,\\ f_{,2}&=\partial_{\overline{\xi}}f-Y\partial_u f,\qquad f_{,3}=\partial_u f-hf_{,4},\\ f_{,4}&=\partial_v f+Y\partial_{\xi}f+\overline{Y}\partial_{\overline{\xi}}f-Y\overline{Y}\partial_u f.\end{aligned} \tag{2.3}$$

The tetrad components R_{ab} of the Ricci tensor can now be calculated in terms of the three unknowns $h, Y, \overline{Y}$ and their derivatives in the following way. Starting from the first Cartan equation

$$de^a = \Gamma^a{}_{bc} e^b \wedge e^c,$$

one can calculate the quantities $\Gamma_{a[bc]}$ (listed in Appendix A). The Ricci rotation coefficients $\Gamma^a{}_{bc}$ are then obtained by

$$\Gamma_{abc} = -\Gamma_{bac} = \Gamma_{a[bc]} + \Gamma_{b[ca]} - \Gamma_{c[ab]},$$

and, finally, the tetrad components of the Riemann and the Ricci tensor can be deduced from the second Cartan equation

$$\tfrac{1}{2} R^a{}_{bcd} e^c \wedge e^d = d\Gamma^a_b + \Gamma^a_c \wedge \Gamma^c_b,$$

where $\Gamma^a_b = \Gamma^a{}_{bc} e^c$.

We shall consider KS fields characterized by the following properties of the congruence of null curves having $\underline{e}_4$ as the tangent vector:

(1) the curves are geodesic, so that

$$\Gamma_{424} = -Y_{,4} = 0; \tag{2.4}$$

(2) the complex expansion (expansion $+i$ rotation),

$$Z := -\Gamma_{421} = Y_{,1}, \tag{2.5}$$

is nonzero.

For such gravitational fields, the tetrad components R_{ab} of the Ricci tensor may be easily calculated. Any real, symmetric tensor in the null tetrad formalism is completely identified by four real components (with the values 12,33,34,44 of the indexes) and three complex components, the remaining three being obtainable by complex conjugation. In particular, for the Ricci tensor we have the following seven independent components:

$$R_{24} = 0, \qquad R_{44} = 0, \qquad R_{22} = -2Y_{,2}[h_{,4} + h(\overline{Z} - Z)],$$

$$R_{34} = -[h_{,4} + h(\overline{Z} - Z)],4 - 2Z[h_{,4} + h(\overline{Z} - Z)],$$

$$R_{12} = -(Z + \overline{Z})[h_{,4} + h(\overline{Z} - Z)] - 2hZ^2 + 2hY_{,2}\overline{Y}_{,1}, \tag{2.6}$$

$$R_{23} = -[h_{,4} + h(\overline{Z} - Z)]_{,2} + [h_{,4} + h(\overline{Z} - Z)]Y_{,3} - 2Y_{,3}hZ + 2Y_{,2}(h_{,1} - h\overline{Y}_{,3}),$$

$$R_{33} = -2(hZ)_{,3} + 2Z\overline{Z}h^2 - 2(h_{,1} - h\overline{Y}_{,3})Y_{,3} - 2hZ[h_{,4} + h(\overline{Z} - Z)] + 2(h_{,1} - h\overline{Y}_{,3})_{,2} + 2h^2\overline{Y}_{,1}Y_{,2}.$$

III. THE "CONSTITUTIVE CONSTRAINT" EQUATION AND THE STRUCTURE OF THE ENERGY-MOMENTUM TENSOR

In this section we obtain the structure of the energy-momentum tensor, which is obviously needed to write the Einstein field equations, in the case of an elastic material acting as a source of a KS geometry. This problem has been extensively treated in a recent paper,[1] so here we simply

express the main results in the tetrad formalism. For a detailed discussion and a brief introduction on the basic structures of relativistic elasticity we refer the reader to that paper.

The energy tensor of an elastic body may be written as

$$T_{\mu\nu}=\epsilon u_\mu u_\nu+\Pi_{\mu\nu}, \tag{3.1}$$

where ϵ is the energy density, u^μ is the velocity field of the material, and $\Pi_{\mu\nu}$ is the stress tensor (sometimes called the ''pressures tensor''). It is symmetric and orthogonal to the velocity ($\Pi_{\mu\nu}u^\nu=0$). The state of strain of the material is characterized by another symmetric, orthogonal tensor $H_{\mu\nu}$ and, in order to describe the physical state of the material, the relation connecting the strain and the stress must be given. For a generic, isotropic material such a relation may be obtained observing that the energy density is a function of three independent strain invariants, for which we choose the following definition:

$$I_1:=\tfrac{1}{2}(\mathrm{Tr}\ K-4),$$

$$I_2:=\tfrac{1}{4}[\mathrm{Tr}\ K^2-(\mathrm{Tr}\ K)^2]+3,$$

$$I_3:=\tfrac{1}{2}(\det K-1),$$

where the symbols $\det K$ and $\mathrm{Tr}\,K$ denote the determinant and the trace, respectively, of the auxiliary tensor

$$K^\mu_\nu:=H^\mu_\nu-u^\mu u_\nu.$$

The resulting stress–strain relation is the following:

$$\Pi_{\mu\nu}=\left(\frac{\partial\epsilon}{\partial I_3}\det K-\epsilon\right)(g_{\mu\nu}+u_\mu u_\nu)+\left(\frac{\partial\epsilon}{\partial I_1}-\mathrm{Tr}\ K\,\frac{\partial\epsilon}{\partial I_2}\right)H_{\mu\nu}+\frac{\partial\epsilon}{\partial I_2}H_{\mu\rho}H^\rho_\nu. \tag{3.2}$$

In order to calculate the tetrad expression of the above quantities, it is convenient to start with the pseudo-Cartesian coordinates x,y,z,t. Greek indexes will always refer to such coordinates; no confusion between their numerical values and that of tetrad indexes may occur since we shall only need the ''temporal'' components (i.e., zero-components) of the tetrad vectors.

It may be shown that relativistic elasticity has a ''gauge invariance'' which allows the choice of the ''comoving gauge'' or, in other words, the kinematical description of the material such that the velocity field has the simple form

$$u^\mu=(1/\sqrt{-g_{00}})\,\delta^\mu_0.$$

In what follows, we consider only the case of non-prestressed materials, deferring a more general treatment to a future paper in which the problem of the sources of the Kerr field will be analyzed in details. For non-prestressed bodies, it may be shown that the expression of the strain in the comoving frame is simply given by

$$H_{\mu\nu}=\delta_{ij}\delta^{\ i}_\mu\delta^{\ j}_\nu.$$

We can now calculate the required tetrad expression of the energy tensor. First of all, we observe that

$$u^a=\Gamma e^a{}_0, \qquad u_a=\Gamma(-e_a{}^0+2hk\delta^3_a),$$

where we have defined

$$\Gamma := \frac{1}{\sqrt{-g_{00}}} = \sqrt{\frac{1}{1-2hk^2}},$$

$$k := l_0 = \frac{1}{\sqrt{2}}\,(1+Y\overline{Y}).$$

The tetrad version of the strain reads

$$H_{ab} = g_{ab} + e_a{}^0 e_b{}^0 - 2h\,\delta_a^3\delta_b^3.$$

The square of such a tensor is then

$$H_{ac}H_b^c = H_{ab} - 2hQ_{ab},$$

where

$$Q_{ab} := \delta_a^3\delta_b^3 - k(e_a{}^0\delta_b^3 + e_b{}^0\delta_a^3) + k^2 e_a{}^0 e_b{}^0.$$

From $K_{ab} = H_{ab} - u_a u_b$ it follows

$$\det K = 1/\Gamma^2, \qquad \mathrm{Tr}\, K = 4 - 2hk^2.$$

Inserting the above results in (3.1) and (3.2), one readily obtains the tetrad version of the energy-momentum tensor:

$$T_{ab} = \epsilon u_a u_b + \left(\frac{1}{\Gamma^2}\frac{\partial\epsilon}{\partial I_3} - \epsilon\right)(g_{ab} + u_a u_b) + \left[\frac{\partial\epsilon}{\partial I_1} - (3-2hk^2)\,\frac{\partial\epsilon}{\partial I_2}\right]H_{ab} - 2h\,\frac{\partial\epsilon}{\partial I_2}\,Q_{ab}.$$

It may be shown that, if the null vector l^μ of a KS metric is geodesic, then it is an eigenvector of the Einstein tensor.[12] All the KS space–times considered here have a geodesic null vector [Eq. (2.4)], so that the energy tensor of the material has to satisfy $T^\mu_\nu l^\nu = -\epsilon l^\mu$. This equation may be interpreted as a condition on the state equation of the body, and therefore has been called ''constitutive constraint.'' [1] The tetrad version of such a constraint reads

$$T_{a4} = -\epsilon g_{a4}, \tag{3.3}$$

that is,

$$-(\delta_a^3 + k e_a{}^0)\left(\frac{\partial\epsilon}{\partial I_3} + \frac{\partial\epsilon}{\partial I_1} - 3\,\frac{\partial\epsilon}{\partial I_2}\right) = 0.$$

Therefore, the constraint implies

$$\frac{\partial\epsilon}{\partial I_3} + \frac{\partial\epsilon}{\partial I_1} = 3\,\frac{\partial\epsilon}{\partial I_2}. \tag{3.4}$$

This result obviously agrees with that previously obtained[1] using a coordinate-dependent method.

From now on, we assume that the energy density, regarded as a function of the strain invariants, satisfies (3.4). Using such an equation to eliminate $\partial\epsilon/\partial I_1$ in the expression of the energy tensor, we obtain

$$T_{ab} = -(\epsilon + k^2\mathscr{P})g_{ab} - k\mathscr{P}\,(e_a{}^0\delta_b^3 + e_b{}^0\delta_a^3) + \mathscr{P}\,(1+2hk^2)\,\delta_a^3\delta_b^3, \tag{3.5}$$

where

$$\mathscr{P} := 2h\left(\frac{\partial \epsilon}{\partial I_3} - \frac{\partial \epsilon}{\partial I_2}\right).$$

We stress that the material described by Eq. (3.5) is *not* a perfect fluid. In fact, although such a material is described by the energy density and only one principal stress $\mathscr{P}$, it may be easily verified that the corresponding energy tensor (3.5) is anisotropic. It becomes isotropic only if $\mathscr{P}$ vanishes. In this case, however, the energy tensor turns out to be proportional to the metric ($T_{ab} = -\epsilon g_{ab}$) and it follows from $T^b_{a;b} = 0$ that ϵ has to be a constant. Thus the resulting ''perfect fluid'' is formally equivalent to a cosmological constant term in the vacuum Einstein field equations.

IV. THE EINSTEIN FIELD EQUATIONS

We consider here the Einstein field equations in the form $G_{ab} = -T_{ab}$ owing to our choice of units and to the useful convention $T_{ab} = 8\pi T^{\text{true}}_{ab}$ (in other words, we adsorb the factor 8π into the definition of ϵ and $\mathscr{P}$). Due to $R^a_a = 2(R_{12} + R_{34})$, one has $G_{12} = -R_{34}$, $G_{34} = -R_{12}$, while $G_{ab} = R_{ab}$ for the other components. From the constitutive constraint (3.3) we have $T_{24} = T_{44} = 0$. But, from (2.6), one has $R_{24} = R_{44} = 0$ and therefore the corresponding field equations hold identically. Using (3.5) and (2.6) the field equations to be satisfied turn out to be the following:

$$\begin{gathered} R_{22} = 0, \qquad R_{12} = -\epsilon, \qquad R_{34} = -(\epsilon + k^2\mathscr{P}), \\ R_{13} = -(k\overline{Y}/\sqrt{2})\mathscr{P}, \qquad R_{23} = -(kY/\sqrt{2})\mathscr{P}, \qquad R_{33} = Y\overline{Y}\mathscr{P}. \end{gathered} \tag{4.1}$$

We start considering equation $R_{22} = 0$. From (2.6) we obtain either $Y_{,2} = 0$ or $h_{,4} + h(\overline{Z} - Z) = 0$. We remind the reader that, in the vacuum case, the Goldberg–Sachs theorem assures that $Y_{,2}$ vanishes and therefore the e^3 congruence is shear-free. In the nonvacuum case, the vanishing of $h_{,4} + h(Z - Z)$ gives $R_{34} = 0$, which is consistent with the sources only if $\epsilon + k^2\mathscr{P}$ vanishes too. It may be verified that this situation corresponds to a very particular case in which the energy-momentum tensor has limiting (stringlike or monopolelike) properties.[13] We shall not further investigate this case in the present paper, and therefore, from now on, we proceed assuming $\epsilon + k^2\mathscr{P}$ to be nonvanishing. This implies that the e^3 congruence is shear-free:

$$Y_{,2} = 0, \tag{4.2}$$

so that

$$dY = Y_{,a}e^a = Ze^1 + Y_{,3}e^3. \tag{4.3}$$

The field equation $R_{22} = 0$ is now satisfied. Due to (4.2), the remaining equations reduce to the following:

$$\begin{gathered} [R_{12}] \mapsto (Z + \overline{Z})[h_{,4} + h(\overline{Z} - Z)] + 2hZ^2 = \epsilon, \\ [R_{34}] \mapsto [h_{,4} + h(\overline{Z} - Z)]_{,4} + 2Z[h_{,4} + h(\overline{Z} - Z)] = \epsilon + k^2\mathscr{P}, \\ [R_{13}] \mapsto [h_{,4} + h(Z - \overline{Z})]_{,1} - [h_{,4} + h(Z - \overline{Z})]\overline{Y}_{,3} + 2\overline{Y}_{,3}h\overline{Z} = k\overline{Y}\mathscr{P}/\sqrt{2}, \\ [R_{23}] \mapsto [h_{,4} + h(\overline{Z} - Z)]_{,2} - [h_{,4} + h(\overline{Z} - Z)]Y_{,3} + 2Y_{,3}hZ = kY\mathscr{P}/\sqrt{2}, \\ [R_{33}] \mapsto 2(hZ)_{,3} - 2Z\overline{Z}h^2 + 2(h_{,1} - h\overline{Y}_{,3})Y_{,3} + 2hZ[h_{,4} + h(\overline{Z} - Z)] - 2(h_{,1} - h\overline{Y}_{,3})_{,2} = -Y\overline{Y}\mathscr{P}. \end{gathered} \tag{4.4}$$

The equations above are a system of five partial differential equations for the five unknowns (three real and two complex conjugate) $\epsilon,\mathscr{P},h,Y,\overline{Y}$. Therefore, we expect them to allow the determination of such fields.

We shall now elaborate the field equations ending up with a form which makes them directly comparable with the DKS vacuum ones.

Rewrite the equation $[R_{12}]$ in the form

$$h_{,4}+h\,\frac{Z^2+\overline{Z^2}}{Z+\overline{Z}}=\frac{\epsilon}{Z+\overline{Z}}.$$

If $\epsilon=0$, this is obviously a vacuum equation and, from the DKS work, we know that its general solution is proportional to $Z+\overline{Z}$, the factor of proportionality having zero fourth tetrad derivative (this is a consequence of the commutation relation $Z_{,4}=-Z^2$, see Appendix B). Then, we can write

$$h=\tfrac{1}{2}M(Z+\overline{Z}), \tag{4.5}$$

where

$$M_{,4}=\frac{2\epsilon}{(Z+\overline{Z})^2}. \tag{4.6}$$

The field equation $[R_{12}]$ is thus equivalent to the above equation. It is easy to check that, using (4.5) and (4.6) in the equation $[R_{34}]$, one obtains

$$\epsilon_{,4}=k^2\mathscr{P}(Z+\overline{Z}). \tag{4.7}$$

This equation, as we shall see, coincides with the ''conservation'' equation $T^b_{4;b}=0$.

Consider now the equation $[R_{23}]$ and its complex conjugate. Using Eqs. (4.5) and (4.6), it reduces to

$$M_{,2}-3\,\frac{\overline{Z}}{Z}\,Y_{,3}M=\Lambda,$$

where we have defined

$$\Lambda:=\frac{1}{Z^2}\left[\left(\frac{\epsilon}{Z+\overline{Z}}\right)_{,2}-\frac{\epsilon}{Z+\overline{Z}}Y_{,3}-\frac{Yk\mathscr{P}}{\sqrt{2}}\right]. \tag{4.8}$$

The real equation $[R_{33}]$ may finally be simplified using all the previous results. A rather cumbersome but straightforward calculation (in which the commutation relations listed in Appendix B play a key role) leads to

$$M_{,3}-\frac{Y_{,3}}{Z}\,M_{,1}-\frac{\overline{Y_{,3}}}{\overline{Z}}M_{,2}=-\frac{\epsilon}{Z+\overline{Z}}M+\mathscr{K}$$

with

$$\mathscr{K}:=\frac{1}{2Z\overline{Z}}[-Y\overline{Y}\mathscr{P}+(Z\Lambda)_{,1}+(\overline{Z\Lambda})_{,2}-Z\Lambda\overline{Y}_{,3}-\overline{Z\Lambda}Y_{,3}]. \tag{4.9}$$

Summarizing, the field equations (4.4) may be rewritten as follows:

$$M_{,1}=3\frac{Z}{\overline{Z}}\overline{Y}_{,3}M+\overline{\Lambda},\qquad M_{,2}=3\frac{\overline{Z}}{Z}Y_{,3}M+\Lambda,$$

$$M_{,3}=\frac{Y_{,3}}{Z}M_{,1}+\frac{\overline{Y}_{,3}}{\overline{Z}}M_{,2}-\frac{\epsilon}{Z+\overline{Z}}M+\mathscr{K},\tag{4.10}$$

$$M_{,4}=\frac{2\epsilon}{(Z+\overline{Z})^2},\qquad \epsilon_{,4}=k^2\mathscr{P}(Z+\overline{Z}).$$

Together with the Einstein field equations, obviously we have to take into account their compatibility conditions (due to Bianchi identities), which in the presence of matter fields are equivalent to the ''conservation'' equations $T^b_{a;b}=0$ for the energy tensor.

In our case, these equations may be written as follows:

$$(\epsilon+k^2\mathscr{P})_{,1}=k^2\overline{Y}_{,3}\mathscr{P}+\frac{k\mathscr{P}\overline{Y}}{\sqrt{2}}(Z+2\overline{Z})+\frac{k\overline{Y}}{\sqrt{2}}\mathscr{P}_{,4},$$

$$(\epsilon+k^2\mathscr{P})_{,2}=k^2Y_{,3}\mathscr{P}+\frac{k\mathscr{P}Y}{\sqrt{2}}(\overline{Z}+2Z)+\frac{kY}{\sqrt{2}}\mathscr{P}_{,4},\tag{4.11}$$

$$\hat{D}\epsilon=0,\qquad \epsilon_{,4}=k^2\mathscr{P}(Z+\overline{Z}),$$

where we have introduced the differential operator $\hat{D}$ whose action on a scalar function f is given by

$$\hat{D}f:=(1/\sqrt{2})[Yf_{,1}+\overline{Y}f_{,2}+k\sqrt{2}f_{,3}+(hk\sqrt{2}-1)f_{,4}].\tag{4.12}$$

It is easy to check that this expression is the tetrad version of the partial derivative with respect to the pseudo-Cartesian t-coordinate. Therefore, owing to the Bianchi identity $\hat{D}\epsilon=0$, the energy of the source must be a stationary function.

V. THE VACUUM CASE: AN OVERVIEW ON THE DEBNEY–KERR–SCHILD SOLUTIONS

In the present section, we briefly overview the integration of the vacuum equations originally due to Debney, Kerr, and Schild.[14] This account is essential for our purposes, and, moreover, we hope that it may be useful for the readers.

When no matter is present, $\epsilon=\mathscr{P}=0$ and therefore Λ and $\mathscr{K}$ vanish. As a consequence, Eqs. (4.10) reduce to

$$M_{,1}=3\frac{Z}{\overline{Z}}\overline{Y}_{,3}M,\qquad M_{,2}=3\frac{\overline{Z}}{Z}Y_{,3}M,$$

$$M_{,3}=\frac{Y_{,3}}{Z}M_{,1}+\frac{\overline{Y}_{,3}}{\overline{Z}}M_{,2},\qquad M_{,4}=0.\tag{5.1}$$

Observe now that, as a consequence of (2.4) and (4.3), the three functions Y, $\overline{Y}$, and M each satisfy the same pair of partial differential equations

$$X_{,4}=0, \quad X_{,3}-\frac{Y_{,3}}{Z}X_{,1}-\frac{\overline{Y}_{,3}}{\overline{Z}}X_{,2}=0. \tag{5.2}$$

However, the base space on which such functions are defined is four dimensional, and Y and $\overline{Y}$ are functionally independent according to the hypothesis of a nonvanishing Z. Therefore, any other function satisfying (5.2) must be functionally dependent on Y and $\overline{Y}$. Thus, we can put

$$M=\frac{m}{P^3}, \tag{5.3}$$

where m is a constant and $P=P(Y,\overline{Y})$ is a real function. The equations for $M_{,3}$ and $M_{,4}$ are now satisfied while the equation for $M_{,2}$ may be rewritten as

$$Y_{,3}=-\frac{ZP_{\overline{Y}}}{P}, \tag{5.4}$$

where $P_{\overline{Y}}=\partial P/\partial\overline{Y}$. It follows that also $Y_{,3}/Z=-P_{\overline{Y}}/P$ depends only on Y and $\overline{Y}$, so that

$$\left(\frac{Y_{,3}}{Z}\right)_{,2}=\overline{Z}\left(\frac{Y_{,3}}{Z}\right)_{\overline{Y}},$$

and, using the commutation relations of Appendix B,

$$\left(\frac{Y_{,3}}{Z}\right)_{\overline{Y}}=\frac{1}{\overline{Z}}\left(\frac{Y_{,3}}{Z}\right)_{,2}=\frac{1}{\overline{Z}}\left(\frac{Y_{,32}}{Z}-\frac{Y_{,3}}{Z^2}Z_{,2}\right)=\left(\frac{Y_{,3}}{Z}\right)^2.$$

Thus, (5.4) implies

$$P_{\overline{Y}Y}=-\left(P\,\frac{Y_{,3}}{Z}\right)_{\overline{Y}}=0.$$

Since P is real. P_{YY} vanishes, too, and therefore P must be a bilinear function in Y and $\overline{Y}$:

$$P=pY\overline{Y}+qY+\overline{q}\overline{Y}+c \tag{5.5}$$

with p and c real constants and q complex constant. Finally, one reaches the following formula for dY:

$$dY=\frac{Z}{P}\,(Pe^1-P_{\overline{Y}}e^3), \tag{5.6}$$

that is, using the explicit expression of the tetrad vectors,

$$dY=\frac{Z}{P}\,[(qY+c)(d\xi-Ydv)-(pY+\overline{q})(du+Yd\overline{\xi})]. \tag{5.7}$$

This differential equation may now be integrated and the general solution is given in implicit form by

$$F=0,$$
$$F:=\phi(Y)+(qY+c)(\xi-Yv)-(pY+\overline{q})(u+Y\overline{\xi}), \tag{5.8}$$

where $\phi(Y)$ is an arbitrary analytic function. This result, not completely straightforward in our opinion, is given without an explicit proof in the original DKS paper; we sketch then a proof in what follows.

The function Y defined by (5.7) identifies a particular class of geodesic, shear-free congruences characterized by (4.3). However, Kerr's theorem[15] states that all such congruences are given implicitly by an equation of the form

$$\mathscr{F}(Y,\lambda_1,\lambda_2)=0, \tag{5.9}$$

where $\mathscr{F}$ is a *completely arbitrary* analytic function of the quantities

$$\lambda_1=\xi-Yv, \quad \lambda_2=u+Y\overline{\xi}.$$

Therefore, all we have to do is to identify which further restrictions are imposed on $\mathscr{F}$ by the Einstein field equations. Comparing (4.3) with (5.6), we see that Y satisfies *one* more equation besides $Y_{,2}=Y_{,4}=0$ (which are the hypotheses of Kerr's theorem), namely (5.4). Using $Z=\partial_\xi Y-Y\partial_u Y$ and (5.5), such equation gives

$$(pY+\overline{q})\partial_\xi Y=-(qY+c)\partial_u Y.$$

However, if Y is defined implicitly by (5.9), one has

$$\partial_\xi Y=-\frac{1}{\mathscr{F}_Y}\frac{\partial\mathscr{F}}{\partial\lambda_1}, \quad \partial_u Y=-\frac{1}{\mathscr{F}_Y}\frac{\partial\mathscr{F}}{\partial\lambda_2},$$

and therefore $\mathscr{F}$ must be a solution of

$$(pY+\overline{q})\frac{\partial\mathscr{F}}{\partial\lambda_1}+(qY+c)\frac{\partial\mathscr{F}}{\partial\lambda_2}=0.$$

This linear partial differential equation in three independent variables fixes only the dependence of $\mathscr{F}$ on λ_1 and λ_2. Thus, it is easy to check that its general solution is given by

$$\mathscr{F}(Y,\lambda_1,\lambda_2)=\tilde{\mathscr{F}}(Y,\tau),$$

where $\tilde{\mathscr{F}}$ is a new arbitrary analytic function, and

$$\tau:=(qY+c)\lambda_1-(pY+\overline{q})\lambda_2.$$

It follows that the general solution of (5.7) is given by

$$\tilde{\mathscr{F}}(Y,(qY+c)(\xi-Yv)-(pY+\overline{q})(u+Y\overline{\xi}))=0.$$

This equation defines Y as a function of τ, but also τ as a function of Y, and therefore one can substitute it (without loss or gain in generality) with the DKS formula (5.8).

Returning to the solution of the field equations, and differentiating (5.8), we readily obtain

$$Z=-\frac{P}{F_Y}. \tag{5.10}$$

Summarizing, the vacuum DKS solutions are given by the following line element:

$$ds^2=2\ d\xi\ d\overline{\xi}+2\ du\ dv+m\ \frac{Z+\overline{Z}}{P^3}\ (du+\overline{Y}d\xi+Yd\overline{\xi}-Y\overline{Y}dv)^2, \tag{5.11}$$

where P, Y, and Z are defined by (5.5), (5.8), and (5.10), respectively. It may be shown[12] that all such solutions are algebraically special, the null vector $\underline{e}_4$ being a multiple principal null direction of the Weyl tensor.

The solutions (5.11) may be simplified by coordinate transformations because all of them admit at least one group of motions. In fact, introducing the real, linear differential operator

$$\hat{K}:=K^\mu\partial_\mu=c\,\partial_u+\overline{q\partial}_\xi+q\partial_{\overline{\xi}}-p\,\partial_v\,,$$

it is easy to check that $\hat{K}Y=0$. Moreover, $\hat{K}$ commutes with the directional derivatives along $\underline{e}_1$ and $\underline{e}_2$, so that $\hat{K}Z$ also vanishes. It follows that K^μ is a Killing vector of the DKS metrics. Since K^μ has constant components, it is also a translational Killing vector of flat space–time. In the three cases in which $\eta_{\mu\nu}K^\mu K^\nu$ is (a) negative, (b) positive, or (c) zero, one can, without loss of generality, make the following choice for the coefficients in P:

$$\text{(a)}p=c=1/\sqrt{2},q=0;\quad \text{(b)}p=-c=-1/\sqrt{2},q=0;\quad \text{(c)}p=q=0,c=1. \tag{5.12}$$

Correspondingly, one has

$$\text{(a)}P=k,\quad K^\mu\partial_\mu=(1/\sqrt{2})(\partial_u-\partial_v),$$

$$\text{(b)}P=(1/\sqrt{2})(1-Y\overline{Y}),\quad K^\mu\partial_\mu=(1/\sqrt{2})(\partial_u+\partial_v),$$

$$\text{(c)}P=1,\quad K^\mu\partial_\mu=\partial_u\,.$$

The case (a) evidently corresponds to stationary space–times ($K^\mu\partial_\mu=\hat{D}$).

One may now ask whether the DKS solutions admit additional Killing vectors. In particular, a physically interesting case is obviously that of axially symmetric space–times. The generator of rotations along the z axis written in the x,y,z,t coordinates is obviously given by

$$\hat{\Phi}:=\Phi^\mu\partial_\mu=\mathrm{x}\partial_\mathrm{y}-y\,\partial_\mathrm{x}=i(\overline{\xi\partial}_{\overline{\xi}}-\xi\partial_\xi).$$

It is not difficult to verify that Φ^μ is a Killing vector for the metric (2.2) if and only if

$$\hat{\Phi}Y=-iY,\quad \hat{\Phi}h=0.$$

In each of the three cases listed in (5.12), the first of such equations implies

$$\phi=Y\phi_Y\,.$$

Once this condition is satisfied, one has $\hat{\Phi}P=\hat{\Phi}Z=\hat{\Phi}\overline{Z}=0$ so that $\hat{\Phi}h=0$ holds identically due to the relation

$$h=\frac{1}{2}\ (Z+\overline{Z})\ \frac{m}{P^3}.$$

It follows that axisymmetric DKS solutions exist only if ϕ is a linear homogeneous function of Y. If the Killing vector K^μ is timelike, one obtains stationary, axially symmetric KS fields. In particular, the choice $\phi=-iaY$ with a real a leads to the Kerr solution of mass m and angular momentum ma, and therefore $\phi=0$ leads to the Schwarzschild solution.

VI. THE NONVACUUM CASE: A METHOD OF REDUCTION OF THE FIELD EQUATIONS

We turn now to the Einstein field equations in matter [Eqs. (4.10)]. Such equations are five highly nonlinear partial differential equations for the five unknowns $\epsilon, \mathscr{P}, M, Y, \overline{Y}$. We know a *particular* solution of them, namely the DKS vacuum field $\epsilon = \mathscr{P} = 0$ and $Y, \overline{Y}, M$ given by the equations (5.3), (5.5), and (5.8) above. In general, of course, knowledge of vacuum solutions is of little help in solving the coupled Einstein–matter problem. However, there are interesting cases in which generating techniques may be applied to vacuum solutions to obtain nonvacuum ones. We shall now try to construct one such technique to obtain some solutions of our equations. It will turn out that it is, in fact, possible to obtain solutions using an approach similar to the method of variation of the arbitrary constants familiar from the theory of ordinary differential equations.

The idea is the following. The first four equations in (4.10) look like the vacuum ones [Eqs. (5.1)] with the addition of a source term on the right-hand side. This suggests the ansatz

$$M = \frac{N}{\overline{P^3}},$$

where P is defined in (5.5) and N is a new unknown. Such a function is a ''variation of the constant'' m which appears in the vacuum case. The equation for $M_{,2}$ now gives

$$N_{,2} - 3\overline{Z}N\left(\frac{P\overline{_Y}}{P} + \frac{Y_{,3}}{Z}\right) = P^3\Lambda. \tag{6.1}$$

The above formula would effectively correspond to the result of a ''variation of the arbitrary constants'' with respect to the vacuum solution if the term in brackets vanishes. Evidently, this is possible whenever the equation (5.4) (which is a field equation for vacuum fields) holds in the nonvacuum case too. Therefore, in order to proceed with our construction, we have to *assume* the validity of such an equation as a condition on Y.[16] From now on, we introduce such a condition as an explicit assumption. It must, however, be remarked that (5.4) and its complex conjugate have now to be considered as additional partial differential equations ''superimposed'' on a system of five equations for five variables and must be compatible with such equations. Therefore, it is not guaranteed *a priori* that the resulting system does admit, in general, solutions different from the ''trivial'' vacuum ones.

Recall now that the field equations in vacuum give only one differential equation for Y, namely (5.4). Therefore, if (5.4) is satisfied also in the matter case, the function Y turns out to be the same as in vacuum. In such a case, in order to obtain a solution in matter, one can choose an explicit DKS solution for Y (choice of ϕ, p, q, c) as a ''seed.'' Then, the gravitational field turns out to be described by the *vacuum* fields Y and $\overline{Y}$ and by the function h, which is given in terms of N by the relation

$$h = \frac{1}{2}(Z + \overline{Z})\frac{N}{\overline{P^3}}. \tag{6.2}$$

The physical properties of the elastic material are described by the functions ϵ and $\mathscr{P}$, and the three unknowns $N, \epsilon, \mathscr{P}$ are governed by the following eight equations (Einstein+Bianchi):

$$\begin{gathered} N_{,1} = P^3\overline{\Lambda}, \qquad N_{,2} = P^3\Lambda, \\ N_{,3} = -P\overline{_Y}P^2\overline{\Lambda} - P_Y P^2\Lambda - \frac{\epsilon}{Z+\overline{Z}}N + P^3\mathscr{K}, \quad N_{,4} = P^3\frac{2\epsilon}{(Z+\overline{Z})^2}, \end{gathered} \tag{6.3}$$

$$(\epsilon+k^2\mathscr{P})_{,1}=-\frac{k^2P_Y\overline{Z}}{P}\mathscr{P}+\frac{k\mathscr{P}\overline{Y}}{\sqrt{2}}(Z+2\overline{Z})+\frac{k\overline{Y}}{\sqrt{2}}\mathscr{P}_{,4},$$

$$(\epsilon+k^2\mathscr{P})_{,2}=-\frac{k^2P_{\overline{Y}}Z}{P}\mathscr{P}+\frac{k\mathscr{P}Y}{\sqrt{2}}(\overline{Z}+2Z)+\frac{kY}{\sqrt{2}}\mathscr{P}_{,4}, \tag{6.4}$$

$$\hat{D}\epsilon=0, \qquad \epsilon_{,4}=k^2\mathscr{P}(Z+\overline{Z}).$$

As we have already stressed, once a seed solution has been explicitly chosen, one has to check whether this ''seed'' is such as to generate a nonvacuum solution. This requirement may be expressed in terms of the integrability conditions on the above equations, conditions which may be obtained using the commutation relations between tetrad derivatives (Appendix B). It turns out to be very complicated to identify *all* the compatible DKS seeds. Fortunately, however, the set of such ''seeds'' turns out to be not empty. In the present paper we shall concentrate only on two simple but interesting cases which are generated by two Petrov type D vacuum solutions and will be discussed in the next two sections.

VII. A SIMPLE EXAMPLE: THE KOWALCZYŃSKI–PLEBAŃSKI SOLUTIONS

As a first example of the procedure outlined above, we are going to deduce within our formalism a simple class of solutions originally due to Kowalczyński and Plebański.[9]

We start from vacuum solutions having a null Killing vector K^μ and restrict ourselves to the ''Kerr choice'' for ϕ, namely $\phi(Y)=-iaY$. These assumptions imply that $P=1$ and that the ''seed'' vacuum solution is

$$Y=Y(\xi,v)=\frac{\xi}{v+ia}. \tag{7.1}$$

It may be verified[17] that this seed corresponds to one of the NUT[8] solutions, the constant a being related to the NUT parameter.

As far as the material source is concerned, we consider only the case $\epsilon=\text{const}=\lambda$ and $\mathscr{P}=0$, so that the energy tensor ($T_{ab}=\lambda g_{ab}$) is formally equivalent to a cosmological constant term in the vacuum Einstein field equations. It follows that the ''conservation'' equations (6.4) hold identically.

From (7.1) one obtains that $Y_{,3}$ vanishes and that

$$Z=Z(v)=\frac{1}{v+ia};$$

thus $Z_{,1}$ and $Z_{,2}$ both vanish together with their complex conjugates due to Eqs. (2.3). In turn, this implies that Λ and $\mathscr{K}$ vanish [Eqs. (4.8) and (4.9)] and Eqs. (6.3) reduce to

$$N_{,1}=N_{,2}=0, \qquad N_{,3}=-\frac{\lambda}{Z+\overline{Z}}N, \qquad N_{,4}=\frac{2\lambda}{(Z+\overline{Z})^2}.$$

This system of equations is compatible, as one may readily check observing that

$$dN = N_{,3}e^3 + N_{,4}e^4 = \frac{1}{2}\lambda\left(\frac{v^2+a^2}{v}\right)^2 dv, \tag{7.2}$$

and thus N is a function of v only. Straightforward integration now yields

$$N(v) = \frac{\lambda}{2}\left(\frac{v^3}{3} + 2a^2 v - \frac{a^4}{v}\right) + m_0,$$

where m_0 is an arbitrary constant. Finally, due to (6.2), we end up with the Kowalczyński–Plebański result

$$h(v) = \frac{1}{2}(Z+\overline{Z})N(v) = \frac{1}{2}m_0(Z+\overline{Z}) + \frac{\lambda}{2}Z\overline{Z}\left(\frac{v^4}{3} + 2a^2v^2 - a^4\right).$$

VIII. GENERATION OF SOLUTIONS STARTING FROM THE SCHWARZSCHILD "SEED"

As we have seen, among the DKS solutions, the stationary ones contain the Kerr field and therefore the Schwarzschild one. It is of obvious physical interest to investigate whether the seeds corresponding to such solutions generate interior solutions. In the present paper we shall focus our attention only on the most simple case, namely the Schwarzschild one.

Letting $\phi=0$ and assuming stationariety ($P=k$), Eq. (5.8) reads

$$\overline{\xi}Y^2 + \mathrm{z}\sqrt{2}Y - \xi = 0,$$

[where $\mathrm{z}=(u+v)/\sqrt{2}$] so that Y is given by a quadratic equation. We choose the positive root and therefore set

$$Y = \frac{r-\mathrm{z}}{\overline{\xi}\sqrt{2}},$$

where $r = \sqrt{\mathrm{x}^2+\mathrm{y}^2+\mathrm{z}^2}$ is the radial coordinate of a spherical system in the flat base space.

It turns out that the complex expansion actually is real,

$$Z = \frac{r-\mathrm{z}}{\xi\overline{\xi}\sqrt{2}} = \overline{Z},$$

and the commutation relations then imply $Z_{,2} = \overline{Z}_{,2} = 0$ together with their complex conjugates. Moreover, one has

$$k = \frac{1}{\sqrt{2}}(1 + Y\overline{Y}) = rZ. \tag{8.1}$$

Applying the "$\hat{D}$" operator (4.12) to the last equation in (6.4), and observing that $\hat{D}$ commutes with the directional derivative along e_4 when DY vanishes, we see that $\mathscr{P}$ is stationary if ϵ and Y are. Therefore, the Bianchi identities (6.4) may be rearranged in terms of the tetrad derivatives of the auxiliary function

$$\eta := \epsilon + k^2\mathscr{P},$$

and read

$$\eta_{,1}=\frac{k\overline{Y}}{\sqrt{2}}\,[\mathscr{P}_{,4}+2Z\mathscr{P}], \qquad \eta_{,2}=\frac{kY}{\sqrt{2}}\,[\mathscr{P}_{,4}+2Z\mathscr{P}],$$
$$\hat{D}\,\eta=0, \qquad \eta_{,4}=k^2[\mathscr{P}_{,4}+2Z\mathscr{P}]. \tag{8.2}$$

The above equations may be rewritten (formally, at the present stage) as

$$d\,\eta=(\mathscr{P}_{,4}+2Z\mathscr{P})\left[\overline{Y}d\xi+Yd\overline{\xi}+\frac{1}{\sqrt{2}}\,(1-Y\overline{Y})dz\right]. \tag{8.3}$$

We remind the reader that, in the above formula, both Y and $\overline{Y}$ are *known* functions coming from the chosen seed solution. Using the seed explicitly, one obtains

$$d\,\eta=(\mathscr{P}_{,4}+2Z\mathscr{P})\,\frac{r-\mathrm{z}}{\xi\overline{\xi}\sqrt{2}}\,(\overline{\xi}\,d\xi+\xi\,d\overline{\xi}+\mathrm{z}\,dz)=(\mathscr{P}_{,4}+2Z\mathscr{P})Zr\,dr. \tag{8.4}$$

Therefore, in order to assure the compatibility of the above equation, η must be a function of r only and the relation

$$\mathscr{P}_{,4}+2Z\mathscr{P}=\frac{1}{rZ}\,\frac{d\,\eta}{dr} \tag{8.5}$$

must hold. Using (8.1) and $\mathscr{P}=(\eta-\epsilon)/k^2$, this gives

$$\eta_{,4}-\epsilon_{,4}+2Z(\,\eta-\epsilon)=Zr\,\frac{d\,\eta}{dr}. \tag{8.6}$$

It is now convenient to introduce the angles $\vartheta=\arctan(\sqrt{x^2+y^2}/z)$ and $\varphi=\arctan(y/x)$ of the spherical system of coordinates in the base space. It is easy to check that

$$r_{,4}=Zr, \quad \vartheta_{,4}=\varphi_{,4}=0.$$

and then

$$\epsilon_{,4}=\frac{\partial\epsilon}{\partial r}\,r_{,4}+\frac{\partial\epsilon}{\partial\vartheta}\,\vartheta_{,4}+\frac{\partial\epsilon}{\partial\varphi}\,\varphi_{,4}=Zr\,\frac{\partial\epsilon}{\partial r},$$

while

$$\eta_{,4}=Zr\,\frac{d\,\eta}{dr}.$$

It follows that (8.6) reads

$$\frac{\partial\epsilon}{\partial r}=\frac{2}{r}\,(\,\eta-\epsilon),$$

for every arbitrary choice of η. The general solution, denoting

$$\eta=f(r),$$

is then given by

$$\epsilon = \frac{E(\vartheta,\varphi)}{r^2} + \frac{2}{r^2}\int_{r_0}^{r} s f(s)\,ds,$$

$$\mathscr{P} = \frac{1}{(Zr)^2}\,(f(r) - \epsilon(r,\vartheta,\varphi)),$$

where $f(r)$ and $E(\vartheta,\varphi)$ are arbitrary functions.

The above procedure allowed us to calculate the material variables ϵ and $\mathscr{P}$ independently from N. Therefore, (6.3) now become linear differential equations in N only. Denoting by C the action of $\hat{D}$ on N, a simple calculation shows that such equations can be written as follows:

$$N_{,1} = \left(\frac{r^3\epsilon}{2}\right)_{,1} - \frac{\overline{Y}r^2 f(r)}{\sqrt{2}}, \qquad N_{,2} = \left(\frac{r^3\epsilon}{2}\right)_{,2} - \frac{Y r^2 f(r)}{\sqrt{2}},$$

$$N_{,3} = \left(\frac{r^3\epsilon}{2}\right)_{,3} + \frac{C}{rZ} - \frac{r f(r)}{2Z}\left(1 - Y\overline{Y} - 2\frac{N}{r}\right), \qquad N_{,4} = \left(\frac{r^3\epsilon}{2}\right)_{,4} - Z f(r) r^3.$$

Defining the auxiliary function

$$L := N - \frac{r^3\epsilon}{2},$$

we can write the following formula for the differential of L:

$$dL = \frac{1}{Zr}\,[C - r^2 f(r)]\left[\overline{Y}d\xi + Y d\overline{\xi} + \frac{1}{\sqrt{2}}\,(1 - Y\overline{Y})dz\right] + C\,dt = [C - r^2 f(r)]\,dr + C\,dt. \quad (8.7)$$

In order to assure the compatibility of the above equation we must calculate C explicitly. A quite long but straightforward calculation gives

$$C = \hat{D}N = \tfrac{1}{2}r^2(E_{,12} + E_{,21}) = \tfrac{1}{2}r^2\Delta E,$$

where Δ denotes the flat Laplace operator. Therefore $C = r^2\Delta E/2$ is a function of θ and φ only, and the necessary and sufficient condition for the compatibility of (8.7) is $C = \text{const}$. It follows that the function E must be a solution of the equation

$$\frac{\partial^2 E}{\partial\vartheta^2} + \frac{\cos\vartheta}{\sin\vartheta}\frac{\partial E}{\partial\vartheta} + \frac{1}{\sin^2\vartheta}\frac{\partial^2 E}{\partial\varphi^2} = 2C.$$

It is easy to check that such an equation admits a regular solution only if C vanishes, and in such a case the solution is constant. Therefore, nonsingular solutions of our problem exist only if C is zero and E is a constant or, in other words, if L depends on r only. In any case, we have

$$L(r,t) = C(r - r_0) - \int_{r_0}^{r} s^2 f(s)\,ds + Ct,$$

and finally

$$N(r,\vartheta,\varphi,t) = C(r - r_0) + \int_{r_0}^{r} s(r - s) f(s)\,ds + \frac{1}{2}\,rE(\vartheta,\varphi) + Ct. \quad (8.8)$$

The line element we have obtained reads, therefore, as follows:

$$ds^2 = -dt^2 + dr^2 + r^2(d\vartheta^2 + \sin^2\vartheta d\varphi^2) + \frac{2N(r,\vartheta,\varphi,t)}{r}(dt+dr)^2. \tag{8.9}$$

For $N=m=$const, this is the Schwarzschild line element (in the so-called Eddington form), as it must be. For $C=0$ and $E=$const, this is a static, spherically symmetric interior solution.[10] It satisfies the familiar mass-density relation for spherically symmetric static fields, namely

$$\frac{\partial N}{\partial r} = \frac{1}{2} r^2 \epsilon.$$

In the general case in which C is nonvanishing, the line element (8.9) describes an interior Kerr–Schild geometry which has no easily recognizable symmetries. As far as we are aware such metrics are new, but their physical meaning is doubtful because they are necessarily singular in $\theta=0$ or $\theta=\pi$.

IX. CONCLUDING REMARKS

The main problems in solving the Einstein field equations are obviously due to their intrinsic nonlinearity. However, since the work by Gürses and Gürsey,[18] it is known that an underlying linear structure exists in the case of Kerr–Schild space–times both in the vacuum and in the electrovacuum case. As was recently shown,[1] this linear structure comes into play also in the case of elastic matter, and allows the decoupling of the equations governing the gravitational field (which are linear partial differential equations) from those governing the material quantities (which turn out to be algebraic).

In the present paper we have shown that, if the same problem is approached using the null-tetrad formalism, linearity appears under the quite unexpected form of the possibility of ''variation of the arbitrary constants.'' This result appears to be promising in the perspective of solving some of the open problems left unsolved in Ref. 1. In fact, approaching the field equations using the coordinate-dependent method, one has to solve a boundary value problem for an elliptic, although linear, equation. Therefore, one is immediately faced with the absence of explicit sets of eigenfunctions if the boundary is not trivial. Here instead, although the null-tetrad machinery is somewhat intricate, the ''variation of arbitrary constants'' should allow us to study, for example, the matching problem with the Kerr metric, starting with a seed metric whose principal null direction satisfies the boundary conditions however complicated they can be. We think, in addition, that the possibility of expressing the stresses in terms of invariant tetrad components should result in facilitating the analysis of the physical properties of the sources even in the general case of prestressed bodies. It might be necessary to consider such bodies in order to satisfy the compatibility conditions in the Kerr case. Work in this direction is now in progress.

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APPENDIX A: $\Gamma_{a[bc]}$ COEFFICIENTS

The nonvanishing skew-symmetric part of the Ricci rotation coefficients in the case of a geodesic ($Y_{,4}=0$) Kerr–Schild geometry are given by

$$
\begin{array}{llll}
2\Gamma_{1[14]}=-\overline{Y}_{,1}, & 2\Gamma_{1[34]}=-\overline{Y}_{,3}, & 2\Gamma_{2[24]}=-Y_{,2}, & 2\Gamma_{3[32]}=hY_{,3}-h_{,2},\\
2\Gamma_{1[13]}=h\overline{Y}_{,1}, & 2\Gamma_{2[14]}=-Z, & 2\Gamma_{2[34]}=-Y_{,3}, & 2\Gamma_{3[43]}=h_{,4},\\
2\Gamma_{1[23]}=h\overline{Z}, & 2\Gamma_{2[13]}=hZ, & 2\Gamma_{3[12]}=h(\overline{Z}-Z), & 2\Gamma_{4[12]}=\overline{Z}-Z,\\
2\Gamma_{1[24]}=-\overline{Z}, & 2\Gamma_{2[23]}=hY_{,2}, & 2\Gamma_{3[31]}=hY_{,3}-h_{,1}, & 2\Gamma_{4[31]}=\overline{Y}_{,3}.
\end{array}
$$

APPENDIX B: COMMUTATION RULES IN THE SHEAR-FREE CASE

For $Y_{,2}=0$, the commutation rules coming from the above Ricci coefficients read

$$2f_{[12]}=(Z-\overline{Z})(f_{,3}+hf_{,4}),$$

$$2f_{[13]}=hZf_{,1}-\overline{Y}_{,3}(f_{,3}+hf_{,4})+f_{,4}h_{,1},$$

$$2f_{[14]}=-Zf_{,1},$$

$$2f_{[34]}=-(Y_{,3}f_{,1}+\overline{Y}_{,3}f_{,2}+h_{,4}f_{,4}),$$

$$2f_{[23]}=h\overline{Z}f_{,2}-Y_{,3}(f_{,3}+hf_{,4})+f_{,4}h_{,2}.$$

Applying such formulas to Y, it follows

$$Z_{,2}=(Z-\overline{Z})Y_{,3}, \qquad Z_{,3}=Y_{,31}+hZ^2-Y_{,3}\overline{Y}_{,3},$$

$$Z_{,4}=-Z^2, \qquad Y_{,34}=-ZY_{,3}, \qquad Y_{,32}=(Y_{,3})^2.$$

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Heat kernel for nonminimal operators on a Kähler manifold

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The heat kernel expansion for a general nonminimal operator on the spaces $C^\infty(\Lambda^k)$ and $C^\infty(\Lambda^{p,q})$ is studied. The coefficients of the heat kernel asymptotics for this operator are expressed in terms of the Seeley coefficients for the Hodge–de Rham Laplacian. © *1996 American Institute of Physics.* [S0022-2488(96)01509-5]

Let M be a compact Reimannian manifold of dimension m without boundary. If M is equipped with integrable complex structure, one can split tagential indices into holomorphic and antiholomorphic ones and define space of differential forms $C^\infty(\Lambda^{p,q})$. The exterior differential d can be also split into a sum $d=\partial+\bar\partial$ of anticommuting nilpotent operators: $\partial^2=\bar\partial^2=\partial\bar\partial+\bar\partial\partial=0$. If M is a Kähler manifold, the corresponding ''Laplacians'' can be reduced to the Hodge–de Rham Laplacian:

$$\partial\partial^*+\partial^*\partial=\overline{\partial\,\partial^*}+\overline{\partial^*\partial}=\tfrac{1}{2}\Delta=\tfrac{1}{2}(\delta d+d\delta). \tag{1}$$

Using these first order differential operators one can construct a (nonminimal) second order differential operator:

$$\mathscr{D}=g_1\partial\partial^*+g_2\partial^*\partial+g_3\overline{\partial\,\partial^*}+g_4\overline{\partial^*\partial}+g_5\partial\bar\partial^*+g_5^*\bar\partial\partial^*, \tag{2}$$

with real constants $g_1,\ldots,g_4$ and a complex constant g_5. For some values of the constants this operator reduces to that considered previously in the paper,[1] where one can find some motivations for studying nonminimal operators. Such operators appear naturally in quantum gauge theories after imposing gauge conditions.[2–5]

For a self-adjoint second order operator L with non-negative eigenvalues $\{\lambda_\nu\}$ one can define the integrated heat kernel

$$\mathrm{Tr}(e^{-tL})=\sum_\nu e^{-t\lambda_\nu}. \tag{3}$$

As $t\to 0_+$, there is an asymptotic expansion of the form

$$\mathrm{Tr}(e^{-tL})=\frac{1}{(4\pi)^{m/2}}\sum_{n=0}^{\infty}a_n(L)t^{(2n-m)/2}. \tag{4}$$

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In this paper, we study the heat kernel expansion for the nonminimal operator $\mathscr{D}$ (2) and relate the Seeley coefficients $a_n(\mathscr{D})$ to that for the Laplace operator $a_n(\Delta)$. General expressions for $a_n(\Delta)$, $n=0,1,2,3$ suitable for the spaces of differential forms can be found in the paper.[6] In particular cases, this problem was solved in Refs. 1, 3–5. In a sense, we suggest an extension of the Theorem 1.2 of Ref. 1 for the case of complex geometry.

First we study the heat kernel for $\mathscr{D}$ acting on the space of k forms, $C^\infty(\Lambda^k)$. Next the case $\mathscr{D}$: $C^\infty(\Lambda^{p,q})\to C^\infty(\Lambda^{p,q})$ is considered. This assumes some restrictions on the constants in Eq. (2), but a more detailed information can be obtained.

Consider the heat kernel for nonminimal operators acting on the space $C^\infty(\Lambda^k)$ of k forms. Let us discuss some properties of first order operators D_1 and D_2, which will be used later to build up a general nonminimal second order operator $\mathscr{D}$.

Lemma 1: Let D_1 and D_2 be operators on $C^\infty(\Lambda)$ having the following properties: (a) D_1, D_2: $C^\infty(\Lambda^k)\to C^\infty(\Lambda^{k+1})$, (b) $D_1^2=D_2^2=0$, (c) $D_1D_2 + D_2D_1 = D_1D_2^* + D_2^*D_1 = 0$, (d) $D_1D_1^* + D_1^*D_1=\alpha\Delta,\ D_2D_2^*+D_2^*D_2=\beta\Delta,\ \alpha,\beta\neq 0$. Then

(1) $C^\infty(\Lambda^k)=\mathrm{Ker}(\Delta)\oplus\mathrm{im}(D_1)\oplus\mathrm{im}(D_1^*)=\mathrm{Ker}(\Delta)\oplus\mathrm{im}(D_2)\oplus\mathrm{im}(D_2^*)$,
(2) $C^\infty(\Lambda^k)=\mathrm{Ker}(\Delta)\oplus(D_1D_2)_k\oplus(D_1D_2^*)_k\oplus(D_1^*D_2)_k\oplus(D_1^*D_2^*)_k$.
(3) The following mappings are isomorphisms:

$$(D_1D_2)_k \overset{D_1D_1^*}{\leftrightarrow} (D_1^*D_2)_{k-1},\quad (D_1^*D_2)_k \overset{D_2D_2^*}{\leftrightarrow} (D_1^*D_2^*)_{k-1},$$

$$(D_1D_2^*)_k \overset{D_1D_1^*}{\leftrightarrow} (D_1^*D_2^*)_{k-1},\quad (D_1D_2)_k \overset{D_2D_2^*}{\leftrightarrow} (D_1D_2^*)_{k-1},$$

where operators D act from right to left, and D^* act from left to right. We introduced the notation $(AB)_k=\mathrm{im}(A)\cap\mathrm{im}(B)\cap C^\infty(\Lambda^k)$.

(4) Let $\Delta_k=\Delta\big|_{C^\infty(\Lambda^k)}$, $f(t,D)=\mathrm{Tr}\,\exp(-tD)f(t,A,B,k)=\mathrm{Tr}\,\exp[-t\Delta|_{(AB)_k}]$. Then in these notations

$$f(t,D_1^*,D_2^*,k)=\sum_{l=0}^{k}(-1)^l(l+1)(f(t,\Delta_{k-l})-\beta_{k-l}), \tag{5}$$

where β_k denote Betti numbers.

Proof: The proof of the first statement repeats standard proof[7] of the same property for operator d. The decomposition 2. can be obtained by repeating twice the decompositions 1. The third statement follows from the anticommutativity properties (b) and (c). To prove the last statement observe that all spaces appearing in the second statement of Lemma 1 are eigenspaces of the Laplace operator. Hence,

$$f(t,\Delta_k)=\beta_k+f(t,D_1,D_2,k)+f(t,D_1^*,D_2,k)+f(t,D_1,D_2^*,k)+f(t,D_1^*,D_2^*,k), \tag{6}$$

$$f(t,D_1,D_2,k)=f(t,D_1^*,D_2,k-1)=f(t,D_1,D_2^*,k-1)=f(t,D_1^*,D_2^*,k-2). \tag{7}$$

Now we can express $f(t,D_1^*,D_2^*)$ from Eq. (6) and by repeated use of Eq. (7) obtain

$$f(t,D_1^*,D_2^*,k)=-f(t,D_1^*,D_2^*,k-1)+\sum_{l=0}^{k}(-1)^l(f(t,\Delta_{k-l})-\beta_{k-l}). \tag{8}$$

Now the statement of the Lemma follows by induction. □

It is easy to see that the operators

$$D_1 = x_1\partial + y_1\overline{\partial}, \quad D_2 = x_2\partial + y_2\overline{\partial}, \tag{9}$$

satisfy conditions of Lemma 1 provided the equation $x_1x_2^* + y_1y_2^* = 0$ holds for complex parameters x_1, x_2, y_1, and y_2. The constants α and β are real and positive: $\alpha = \frac{1}{2}(|x_1|^2 + |y_1|^2)$, $\beta = \frac{1}{2}(|x_2|^2 + |y_2|^2)$. The nonminimal operator

$$\begin{aligned}\mathscr{D} &= aD_1D_1^* + bD_1^*D_1 + cD_2D_2^* + dD_2^*D_2 \\ &= (a|x_1|^2 + c|x_2|^2)\partial\partial^* + (b|x_1|^2 + d|x_2|^2)\partial^*\partial + (a|y_1|^2 + c|y_2|^2)\overline{\partial\,\partial^*} \\ &\quad + (b|y_1|^2 + c|y_2|^2)\overline{\partial^*}\,\overline{\partial} + [(a-b)x_1y_1^* + (c-d)x_2y_2^*]\partial\overline{\partial^*} + [(a-b)y_1x_1^* + (c-d)y_2x_1^*]\overline{\partial}\partial^*\end{aligned} \tag{10}$$

with real constants a, b, c, d is the most general hermitian operator on $C^\infty(\Lambda^k)$ which can be constructed using ∂, ∂, ∂^*, and ∂^*. This operator has the form (2).

The following Theorem gives the heat kernel asymptotics for $\mathscr{D}$.

Theorem 1. Let D_1 and D_2 satisfy conditions of Lemma 1. Then the coefficients a_n of the heat kernel expansion for the operator $\mathscr{D}$ (10) have the form

$$\begin{aligned}a_n[\mathscr{D}|_{C^\infty(\Lambda^k)}] &= (\alpha a + \beta c)^{n-(m/2)}\sum_{l=0}^{k-2}(-1)^{k-l}(k-l-1)a_n(\Delta_l) - [(\alpha a + \beta d)^{n-(m/2)} \\ &\quad + (\alpha b + \beta c)^{n-(m/2)}]\sum_{l=0}^{k-1}(-1)^{k-l}(k-l)a_n(\Delta_l) + (\alpha b + \beta d)^{n-(m/2)}\sum_{l=0}^{k}(-1)^{k-l} \\ &\quad \times (k-l+1)a_n(\Delta_l).\end{aligned}$$

Proof consists in repeated use of Lemma 1. Note, that to ensure existence of all traces of exponentials for positive t one should take non-negative a, b, c, d.

Consider nonminimal operators on $C^\infty(\Lambda^{p,q})$. To ensure that $\mathscr{D}$ maps $C^\infty(\Lambda^{p,q})$ on itself we should choose $D_1 = \partial$, $D_2 = \partial$. The following notations will be useful:

$$(AB)_{p,q} = \mathrm{im}(A) \cap \mathrm{im}(B) \cap C^\infty(\Lambda^{p,q}), \quad \Delta_{p,q} = \Delta|_{C^\infty(\Lambda^{p,q})}. \tag{11}$$

Other notations are modified by replacing k by p,q in Lemma 1. $\beta_{p,q}$ will denote Hodge numbers.

Next Lemma replaces the Lemma 1.

Lemma 2. 1: $C^\infty(\Lambda^{p,q}) = \mathrm{Ker}(\Delta_{p,q}) \oplus (\partial\overline{\partial})_{p,q} \oplus (\partial\overline{\partial^*})_{p,q} \oplus (\partial^*\overline{\partial})_{p,q} \oplus (\partial^*\overline{\partial^*})_{p,q}$.

2. The following maps are isomorphisms:

$$(\partial\overline{\partial})_{p,q} \overset{\partial,\partial^*}{\leftrightarrow} (\partial^*\overline{\partial})_{p-1,q}, \quad (\partial^*\overline{\partial})_{p,q} \overset{\overline{\partial\,\partial^*}}{\leftrightarrow} (\partial^*\overline{\partial^*})_{p,q-1},$$

$$(\partial\overline{\partial^*})_{p,q} \overset{\partial,\partial^*}{\leftrightarrow} (\partial^*\overline{\partial^*})_{p-1,q}, \quad (\partial\overline{\partial})_{p,q} \overset{\overline{\partial\,\partial^*}}{\leftrightarrow} (\partial\overline{\partial^*})_{p,q-1},$$

where the operators ∂ and $\overline{\partial}$ act from right to left, and the operators ∂^* and $\overline{\partial^*}$ act from left to right.

4. $f(t,\partial^*,\overline{\partial^*},p,q) = \Sigma_{k,l=0}^{p,q}(-1)^{k+l}(f(t,\Delta_{p-k,q-l}) - \beta_{p-k,q-l})$.

The proof repeats that of Lemma 1 with minor modifications Now we can prove the following theorem.

Theorem 2: Let $\mathscr{D} = a\,\partial\partial^* + b\,\partial^*\partial + c\,\overline{\partial\,\partial^*} + d\,\overline{\partial^*}\,\overline{\partial}$ on $C^\infty(\Lambda^{p,q})$. Then

$$a_n(\mathscr{D}) = \left(\frac{b+d}{2}\right)^{n-(m/2)} a_n(\Delta_{p,q}) + \left[\left(\frac{b+c}{2}\right)^{n-(m/2)} - \left(\frac{b+d}{2}\right)^{n-(m/2)}\right] a_n(\Delta_{p,q-1}) + \left[\left(\frac{a+d}{2}\right)^{n-(m/2)} - \left(\frac{b+d}{2}\right)^{n-(m/2)}\right] a_n(\Delta_{p-1,q}) + \left[\left(\frac{a+c}{2}\right)^{n-(m/2)} + \left(\frac{b+d}{2}\right)^{n-(m/2)} - \left(\frac{a+d}{2}\right)^{n-(m/2)} - \left(\frac{b+c}{2}\right)^{n-(m/2)}\right] \sum_{k,l=0}^{p-1,q-1} (-1)^{p+q-k-l} a_n(\Delta_{k,l}).$$

In this paper, we expressed the heat kernel coefficients for nonminimal operators on $C^\infty(\Lambda^k)$ and $C^\infty(\Lambda^{p,q})$ in terms of the Seeley coefficients for the Laplace operators on the same spaces. Expressions for the heat kernel asymptotics applicable for Laplacian on differential forms can be found in the literature.[6]

The fact that underlying manifold is Kählerian was used only to relate $\partial\partial^* + \partial^*\partial$ and $\partial\partial^* + \partial^*\partial$ to $\Delta = \delta d + d\delta$. With some modifications our results can be extended to a general complex manifold. Another generalization could consist in adding an endomorphism E to the operator $\mathscr{D}$.

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Towards the canonical tensor operators of $u_q(3)$. I. The maximal null space case

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Generalizing the SU(3) canonical tensor operator concept (Biedenharn and Louck) to the quantum algebra $u_q(3)$, the Wigner–Clebsch–Gordan coefficients of $u_q(3)$ with repeating irreducible representations are considered. Extremal projectors of the quantum algebra $u_q(3)$ in terms of the ordered generator polynomials are used for evaluation of the bilinear combinations of the $u_q(3)$ canonical isoscalar factors. Explicit expressions of the $u_q(3)$ isofactors, corresponding to the maximal null space case of the $u_q(3)$ unit canonical tensor operators, and their normalization factors (denominator functions) are presented. The transposition and conjugation phase factors for the SU(3) and $u_q(3)$ canonical isofactors are correlated with phases and zeros of boundary isofactors. Invariance of the canonical isofactors (or absence of such invariance) under interchange of the tensor operator and the initial or final state parameters is correlated with the existence and invariance (or numerical degeneracy) of the usual splitting (distinctive) conditions. Some oversights of previous publications are disclosed. © *1996 American Institute of Physics.* [S0022-2488(96)00509-9]

I. INTRODUCTION

The matrix elements of the canonical unit SU(3) tensor operators[1–4] provide the most universal complete algebraic system of the orthonormal coupling (Wigner–Clebsch–Gordan) coefficients of SU(3) group with the repeating irreducible representations (irreps) in the direct product decomposition. The canonical SU(3) tensor operators are determined by the null space inclusion property,[4–6] together with their Hermitian and conjugation properties and vanishing conditions[2,3,6] of certain SU(3):U(2) projective operators and corresponding maximal shift isoscalar factors (isofactors). Biedenharn, Louck, and collaborators solved explicitly[5–7] the normalization problem of the canonical SU(3) isofactors. The definite advance for the evaluation of the explicit canonical SU(3) isofactors is presented by the recursive construction of the SU(3) tensor operators,[8] although an additional orthogonalization procedure is necessary in the general case.

With the growing interest in the Wigner–Racah irreducible tensor calculus of the quantum groups, some elementary coupling coefficients for the quantum algebra $u_q(3)$ were considered by Smirnov *et al.*[9,10] and Lienert and Butler.[11] Some multiplicity-free isoscalar factors (isofactors) for the unitary quantum algebra $u_q(n)$ of an arbitrary rank were considered by Gould and Biedenharn[12] (with presented pattern calculus rules) and by Ališauskas and Smirnov[13] (for the coupling of arbitrary and one-parametric irreps, and for the semistretched and stretched coupling). Ališauskas[14] proposed alternative recursive constructions for the biorthogonal systems of $u_q(n)$ isofactors with the repeating irreps in the coproduct decomposition.

Biedenharn and Tarlini[15] presented a definition of the q-tensor operators transforming under representations of q-deformed universal enveloping algebras and compatible with the coproduct expansion rules and Klimyk[16] reconsidered the Wigner–Eckart theorem for the quantum group as dual to $u_q(n)$ Hopf algebra. In both cases their matrix elements are proportional to the coupling (Wigner–Clebsch–Gordan) coefficients of the quantum algebra. The explicit symmetric (multiplicity-free) tensor operators of $u_q(k)$ were expressed[13] in terms of the $u_q(k+1)$ generators. However, contrary to the $u_q(2)$ case[17,18] and the SU(3) case, even for the rank (1 1) the separate

components of the self-conjugate minimal null space canonical tensor operator of $u_q(3)$ are rather complicated (and, as a rule, nonlinear) functions[19] of $u_q(3)$ generators. Hence, the matrix elements of the simplest non-multiplicity-free $u_q(3)$ unit canonical tensor operator of the rank (1 1), presented by Smirnov and Kharitonov,[19] cannot be written straightforwardly from the matrix elements of the $u_q(3)$ generators, as it was done in the SU(3) case.[20,21]

In general, the external multiplicity labels of the all orthonormal analytical systems of the SU(3)⊃U(2) isofactors (including the matrix elements of the unit canonical tensor operators, the paracanonical[22,23] and pseudocanonical[22] isofactors) may be associated with solution of the internal SU(3)⊃U(2)⊃U(1)⊗U(1) weight multiplicity problem and represented by the operator (Gelfand–Weyl–Biedenharn) patterns[2–7] (or by the external isospin type parameters[22]) with the different distribution of the null spaces [which inclusion property[5,6] is not exceptional[24] just for the canonical tensor operators and defining condition (1.26b) of Ref. 6 is insufficient]. In all these cases isofactors [matrix elements of the SU(3):U(2) projective operators] with the fixed multiplicity label may be expressed[6] in terms of the definite numerator polynomials (or the multiple terminated series) in the free irrep parameters of SU(3) and U(2), with the linear numerator pattern calculus factors and the corresponding SU(3) and U(2)-invariant denominator polynomials under the square root sign. For all three analytical systems,[22] the guessed denominator functions[5,7,23,24] and the boundary[23,24] SU(3)⊃U(2) isofactors are determined completely by their polynomial, reduction, and symmetry properties and zeros [associated with the null spaces and the additional selection rules in frames of SU(2)]. Since the overlaps of the biorthogonal systems of $u_q(3)$ isofactors[14] are expressed in terms of the multiple balanced terminated basic hypergeometric series [and are invariant with respect to the substitution $q \to q^{-1}$, similarly as the $u_q(2)$ Racah coefficients], the analogical unambiguous extrapolation is possible for the paracanonical and pseudocanonical isofactors of $u_q(3) \supset u_q(2)$, although the proof is rather problematic.

For the fixed rank, shifts, and multiplicity label of the $u_q(3)$ canonical tensor operators, we may also deduce the analogical structure of their matrix elements, with rational numerator functions and the corresponding q-pattern calculus factors and $u_q(3)$ denominator functions under the square root sign, such that the expressions are valid for the entire values of parameters of initial state and give zeros in the null space region. However, appearing q-phases provide serious difficulties for the extrapolation of the SU(3) denominator G-function[7,25] for the $u_q(3)$ canonical tensor operators. {Note, that the role of Milne's[26] q-analog $[G]_m^{(3)}$ or, respectively, the well-poised multiple series $W_m^{(3)}$, cf. introduced by Holman *et al.*[27] SU(3) invariant G-function, for the $u_q(3)$ irreducible tensor operators[15] is not clear.}

In this paper, some important constructive elements of the explicit matrix elements of the $u_q(3)$ canonical tensor operators are presented and some distinction and symmetry problems of the $u_q(3)$ canonical isofactors are considered [together with some questionable aspects of the SU(3) case]. Unambiguous orthonormal systems of the $u_q(3) \supset u_q(2)$ isofactors may be derived from special bilinear combinations of isofactors, including, respectively, single, two, or other restricted number of values of the multiplicity labels, i.e., by means of the Gram-Schmidt process. Such bilinear combinations (presented for the paracanonical and pseudocanonical cases in Ref. 14) could be expressed by means of the integration of three qD-matrices, if the q-integration technique[28] could be extended to the quantum group space of $u_q(3)$, or using the q-boson realizations of the $u_q(3) \supset u_q(2)$ basis states. In Sec. II of this paper, we apply an easier approach—the generalized projection operator technique[8,9] and $u_q(2)$-irreducible properties[13] of the $u_q(3)$ generator powers and their ordered products for the explicit construction of the restricted bilinear combinations of the $u_q(3)$ canonical isofactors, equivalent to the SU(3) canonical isofactors for $q=1$.

The different $u_q(3)$ tensor operators may be constructed in analogy with (2.10) of Ref. 8 by means of the stretched coupling [see Eq. (4.10) of Ref. 13] of the maximal null space canonical tensor operator and the (q-self-adjoint) minimal null space canonical tensor operator, varying each rank. Since both the auxiliary q-tensor operators are still available[19] only in the case of rank (1 1),

it may be suitable to use construction (2.10) of Ref. 8 step by step, taking $k=1$, and to postpone the final (correct) construction of the orthogonal SU(3) and $u_q(3)$ canonical isofactors to a later publication, reconsidering below only some questionable aspects of orthogonality. Therefore, in Sec. III, the expressions for the product of isofactors with a single (extreme) value of the canonical multiplicity label are considered. Some of our results are different in formal structure from those[8] of SU(3) only by the appearance of rather complicated q-phases, but the explicit expressions for the square of the extreme maximal null space isofactor and the corresponding normalization factors, presented in Sec. III [as well as the expression for the most general bilinear combinations of the $u_q(3)$ canonical isofactors in Sec. II], were never published before, even in the SU(3) version. After unsuccessful efforts to rearrange this normalization factor in the generic $q\neq 1$ case into form, related to the G-function,[7,25] we observed that the first presented solution does not cover all the cases of the matrix elements of the maximal null space $u_q(3)$ canonical tensor operators, unless the normalization factor is expressed in a more convenient form, which was eliminated from the product of two different extreme canonical isofactors. The second version of the projection operator and the symmetries of the $u_q(3)$ canonical isofactors were indispensable for this purpose.

The essential advantage of the canonical tensor operators consists of their elementary behavior under conjugation and transposition. The symmetry properties of their matrix elements in the $u_q(3)$ case should be consistent with their depending on the multiplicity label phase relations of the SU(3) canonical isofactors[1,8] and include the corresponding q-factors,[29] but unquestionable (cf. Refs. 8 and 30) complete phase factors are correlated with the conjugation and transposition ($1\leftrightarrow 3$) invariant extreme isofactors, derived in Sec. III. In Sec. IV, we (re)consider the symmetry phase factors of the SU(3) and $u_q(3)$ canonical isofactors, correlating them also with the definite zeros of the SU(3) isofactors [similar to zeros of $C_{000}^{l_1 l_2 l}$ for l_1+l_2+l odd in the SU(2) case[31]]. Besides, we anticipate conditions for the existence or absence of the $1\leftrightarrow 2$ and $2\leftrightarrow 3$ S_2-irreducible transposition symmetry[32] of the $u_q(3)$ and SU(3) canonical isofactors, associated with the observed invariance or the degeneracy of the distinctive conditions. We also discuss the contradictions between the Derome[32] and Biedenharn *et al.*[30] approaches to this problem, when some parameters before and after transposition coincide.

We use here the same notations for irreps and basis states of $u_q(3)$ as were used in Ref. 8 for SU(3), with $(a\ \ b)$ for the mixed tensor irreps (more convenient to catch symmetries in the presented below results),

$$a=m_{13}-m_{23},\quad b=m_{23}-m_{33}\ \text{ where }\ [m_{13},m_{23},m_{33}] \tag{1.1a}$$

is a Young frame (partition). The basis states are labeled by the hypercharge y, the isospin i and its projection i_z:

$$y=m_{12}+m_{22}-\tfrac{2}{3}\,(m_{13}+m_{23}+m_{33}),\quad i=\tfrac{1}{2}\,(m_{12}-m_{22}),\quad i_z=m_{11}-\tfrac{1}{2}\,(m_{12}+m_{22}), \tag{1.1b}$$

where m_{ij} are the Gelfand–Tsetlin parameters. Sometimes the parameter

$$z=\tfrac{1}{3}\,(b-a)-\tfrac{1}{2}\,y=m_{23}-\tfrac{1}{2}\,(m_{12}+m_{22}) \tag{1.1c}$$

is more convenient than y, because

$$i\pm z\geqslant 0,\quad a+z-i\geqslant 0,\quad b-z-i\geqslant 0 \tag{1.1d}$$

are integers. For the state of irrep $(a\ \ b)$ in the coproduct $(a'b')\otimes(a''b'')$ decomposition,

$$z=z'+z''+v\ \ \text{where}\ \ v=\tfrac{1}{3}\,(a'-b'+a''-b''-a+b). \tag{1.2}$$

The multiplicity r of irrep $(a\ \ b)$ in the coproduct $(a'b')\otimes(a''b'')$ decomposition (intertwining number) is equal to[8,22]

$$r=\min r_{\alpha\beta\gamma}+1 \quad (\alpha=1,2,3;\beta=1,2,3;\gamma=1,2) \tag{1.3a}$$

where integers $r_{\alpha\beta\gamma}$ form the following $3\times3\times2$ array (the third dimension of which is represented by a skew shift in plane):

$$|r_{\alpha\beta\gamma}|=\begin{vmatrix} b'-a''+a+v & & b-v & & b' & \\ & a'-b''+b-v & & b & & b'+v \\ a & & a-a'+b''+v & & a''-v & \\ & a+v & & a''-b'+b-v & & a'' \\ a'-v & & b'' & & b'+b''-b+v & \\ & a' & & b''+v & & a'+a''-a-v \end{vmatrix} \tag{1.3b}$$

with equidistant parameters in the layers, rows, and columns:

$$r_{\alpha\beta2}-r_{\alpha\beta1}=r_{\alpha'\beta'2}-r_{\alpha'\beta'1}=v, \quad r_{\alpha\beta\gamma}-r_{\alpha\beta'\gamma}=r_{\alpha'\beta\gamma}-r_{\alpha'\beta'\gamma}. \tag{1.3c}$$

Similar to the SU(3) canonical tensor operators,[1–6] the matrix elements of $u_q(3)$ canonical unit tensor operators coincide with the coupling coefficients of $u_q(3)$,

$$\left\langle \begin{matrix} ab \\ yii_z \end{matrix} \middle| T^{(a''b'')t,q}_{y''i''i''_z} \middle| \begin{matrix} a'b' \\ y'i'i'_z \end{matrix} \right\rangle_q = \begin{bmatrix} (a'b') & \overset{t}{(a''b'')} & (a\ \ b) \\ y'i' & y''i'' & y\ \ i \end{bmatrix}^{(3)}_q \begin{bmatrix} i' & i'' & i \\ i'_z & i''_z & i_z \end{bmatrix}^{(2)}_q, \tag{1.4}$$

which are expressed on the rhs in terms of the $u_q(3)\downarrow u_q(3)$ isofactors (with the external canonical multiplicity label t written over the irrep which corresponds to the irreducible tensor operator) and Clebsch–Gordan coefficients of $u_q(2)$. In order to escape some ambiguities and complications in the analytical expressions and, especially, in the phases,[30] we prefer to use the linear external multiplicity label $t=\min(m''_{13}-\gamma_{12},\gamma_{22}-m''_{33})+1$ instead of the operator Gelfand–Weyl–Biedenharn pattern[3–7] $\Gamma_t=\left(\begin{smallmatrix}\gamma_{11}\\ \gamma_{12}\ \ \gamma_{22}\end{smallmatrix}\right)$, usual in the case of the partition type notations. In accordance with (2.7) of Ref. 8 [cf. (1.11) of Ref. 6], the multiplicity label t of the canonical tensor operator $T^{(a''b'')t,q}_{y''i''i''_z}$ accepts values 1,2,...,$\mathscr{M}$, where $\mathscr{M}$ is the number of independent tensor operators,

$$\mathscr{M}=\min r_{\alpha'\beta'\gamma}+1 (\alpha'=2,3;\beta'=2,3;\gamma=1,2), \tag{1.5a}$$

with the tensor operator characterizing parameters, presented as $2\times2\times2$ subarray

$$|r_{\alpha'\beta'\gamma}|=\begin{vmatrix} \Delta_1 & & p-\Delta_2 & \\ & p-\Delta_3 & & a'' \\ b'' & & \Delta_3 & \\ & \Delta_2 & & p-\Delta_1 \end{vmatrix}, \tag{1.5b}$$

expressed in terms of the shift parameters $\Delta_1,\Delta_2,\Delta_3(p=a''+b'')$ used in Refs. 5–7.

The null space property of the $u_q(3)$ canonical tensor operator $T^{(a''b'')t,q}_{y''i''i''_z}$ with the definite shifts of $u_q(3)$ irrep parameters means the complete vanishing of its matrix elements (and canonical isofactors) for[4,6,8]

$$t \leqslant \mathscr{M} - r, \tag{1.6}$$

when acting on the subspace $\mathscr{N}_t$ of an infinite dimensional Hilbert space $\mathscr{H}$ of all irreps $(a'b')$. Vanishing of the $u_q(3)$ canonical isofactors for

$$i'' + |i - i'| > a'' + b'' - t + 1 \tag{1.7a}$$

is another important generalization of the distinctive property[6] of the SU(3) canonical tensor labeling scheme. Particularly, in analogy with the SU(3) case,[2,3,8,33] it may be supposed that the complete system of the independent $u_q(3)$ isofactors is ensured by their vanishing condition for the sufficient shifts of the q-isospin,

$$|i - i'| > i''_{\mathrm{m}} - t + 1 \tag{1.7b}$$

[i.e., the $u_q(3){:}u_q(2)$ projective operators with the definite shifts of the $u_q(2)$ irrep parameters are zero operators[6]]. To some extension, a sufficient distinction may be ensured even by vanishing (i.e., equal to zero values) of isofactors for

$$i_{\mathrm{m}} - i' > i''_{\mathrm{m}} - t + 1, \tag{1.7c}$$

where isospin accepts the maximal values

$$i = i_{\mathrm{m}} \equiv \tfrac{1}{2}(a+b), \quad i'' = i''_{\mathrm{m}} \equiv \tfrac{1}{2}(a''+b'').$$

We are using also the notations

$$y_{\mathrm{m}} = \tfrac{1}{3}(a-b), \quad z_{\mathrm{m}} = \tfrac{1}{2}(b-a).$$

At first, conditions (1.7a)–(1.7c) may be proved by induction for the $u_q(3)$ self-adjoint tensor operator of the rank $(k\ \ k)$ in the minimal null space case with $t = k+1$. In order to prove that vanishing condition (1.7c) yields the vanishing conditions (1.7b) and (1.7a) for the general $u_q(3)$ canonical isofactors, we use the recursive construction (cf. Ref. 8) of the independent tensor operators

$$\widetilde{T}^{(a''b'')t,q}_{y''i''i''_z} = \left[T^{(t-1,t-1)t,q} T^{(a''-t+1,b''-t+1)1,q} \right]^{(a''b'')t,q}_{y''i''i''_z}, \tag{1.8}$$

derived by means of the stretched coupling of the self-adjoint minimal null space tensor operator $T^{(t-1,t-1)t,q}_{y_3 j_3 m_3}$ [with trivial shift of $u_q(3)$ irreps and restricted shift of $u_q(2)$ irreps for special $j_3 = t-1$] and maximal null space tensor operator $T^{(a''-t+1,b''-t+1)1,q}_{y_1 j_1 m_1}$ [which ensure the null space properties of the full operator (1.8)]. However, contrary to conjecture presented in Ref. 8, the orthogonalization process begun from the maximal value of t is as a rule necessary. Otherwise, the null space condition (1.6) is mainly (but incompletely) ensured by construction (1.8). Therefore, the superfluous tensor operators that appeared should be eliminated and the canonical tensor operators can be obtained only by the Gram–Schmidt process begun from the maximal value of t, although the tensor operators (1.8) with $t=1$ and $\mathscr{M}$ (after normalization) are always canonical.

Of course, conditions (1.7a)–(1.7c) are trivially satisfied (and, therefore, they seemed meaningless[6]) for the maximal null space tensor operators. Nevertheless, for the complete proof of the canonical distinctiveness, we need to find such triplet of parameters $i', i'' = i''_{\mathrm{m}}$, and i with

$$|i-i'|=i''_{\rm m}-t+1 \quad (\text{at least } i_{\rm m}-i'=i''_{\rm m}-t+1 \text{ and/or } i'_{\rm m}-i=i''_{\rm m}-t+1), \tag{1.9}$$

for which isofactor does not vanish and a Gram–Schmidt process from the bilinear combinations of isofactors may be ensured. However, in Secs. III and IV, some ambiguous situations (associated to the absence of the transposition $1\leftrightarrow 2$ or $2\leftrightarrow 3$ symmetry of the canonical isofactors) will be demonstrated, for which condition (1.9) (and beginning of any numerical Gram–Schmidt procedure) is impossible, because the corresponding values of parameters in triplet are not allowed (e.g., they are nonlexical[4,6]) for any value of t. Hence, the distinction properties (1.7a)–(1.7c) for special values of the irrep parameters may be degenerated, since the null space of the SU(3):U(2) and $u_q(3):u_q(2)$ projective operators may exceed the corresponding null space of the SU(3) and $u_q(3)$ canonical operators, contrary to Lemma 1.1, postulated in Ref. 6. Theorems 1.1 and 1.2 of Ref. 6 also turned out to be questionable. Nevertheless, Theorem 1.2 may be correct under the additional restrictions, when isofactors or matrix elements are conjugation invariant and expressed as ratios of the most simple non-singular functions. In such degenerated cases the analytical continuation procedure from the generic (non-degenerated) region may be helpful, as well as the remaining universal properties[1–7] of the canonical tensor operators.

II. EXTREMAL PROJECTORS AND BILINEAR COMBINATIONS OF $U_q(3)$ ISOFACTORS

As in Refs. 9 and 13, we use the Cartan–Weyl generators $E_{ik}(i,j,k=1,2,3)$ of the unitary quantum algebra $u_q(3)=U_q(u(3))$, which satisfy the commutation relations

$$[E_{ii},E_{kk}]=0, \quad [E_{ii},E_{jk}]=\delta_{ij}E_{ik}-\delta_{ik}E_{ji}, \tag{2.1a}$$

$$[E_{ik},E_{ki}]=[E_{ii}-E_{kk}], \tag{2.1b}$$

where $[x]$ and $[x]!$ are q-numbers and q-factorials, respectively:

$$[x]=\frac{(q^x-q^{-x})}{(q-q^{-1})}, \quad [x]!=[x][x-1]\ldots[2][1], \quad [1]!=[0]!=1. \tag{2.2}$$

The composite generators may be expressed in terms of the q-deformed commutators

$$E_{13}=[E_{12},E_{23}]_q\equiv E_{12}E_{23}-qE_{23}E_{12}, \tag{2.3a}$$

$$E_{31}=[E_{32},E_{21}]_{q^{-1}}\equiv E_{32}E_{21}-q^{-1}E_{21}E_{32}, \tag{2.3b}$$

and satisfy the Serre identities

$$[E_{ik},[E_{ik},E_{kl}]_q]_{q^{-1}}=0 \quad (i,k,l=1,2,3, \text{ or } 3,2,1), \tag{2.4a}$$

$$[E_{12},E_{32}]=[E_{21},E_{23}]=0. \tag{2.4b}$$

Generators E_{12} and E_{21} are chosen for the canonical $u_q(2)$ subalgebra, used for labeling of the basis states.

We use the coproduct expansion rules[9]

$$\Delta(E_{ii})=E_{ii}\otimes 1+1\otimes E_{ii}, \tag{2.5a}$$

$$\Delta(E_{ii+1})=E_{ii+1}\otimes q^{1/2(E_{ii}-E_{i+1,i+1})}+q^{-1/2(E_{ii}-E_{i+1,i+1})}\otimes E_{ii+1}, \tag{2.5b}$$

$$\Delta(E_{i+1i})=E_{i+1i}\otimes q^{1/2(E_{ii}-E_{i+1,i+1})}+q^{-1/2(E_{ii}-E_{i+1,i+1})}\otimes E_{i+1i}, \tag{2.5c}$$

as well as special coproduct formulas

$$\Delta(E_{13})=[\Delta(E_{12}),\Delta(E_{23})]_q=E_{13}\otimes q^{1/2(E_{11}-E_{33})}-(q-q^{-1})q^{-1/2(E_{22}-E_{33})}E_{12}\otimes E_{23}q^{1/2(E_{11}-E_{22})}+q^{-1/2(E_{11}-E_{33})}\otimes E_{13}, \tag{2.6a}$$

$$\Delta(E_{31})=[\Delta(E_{32}),\Delta(E_{21})]_{q^{-1}}=E_{31}\otimes q^{1/2(E_{11}-E_{33})}+(q-q^{-1})q^{-1/2(E_{11}-E_{22})}E_{32}\otimes E_{21}q^{1/2(E_{22}-E_{33})}+q^{-1/2(E_{11}-E_{33})}\otimes E_{31} \tag{2.6b}$$

for the composite generators E_{13} and E_{31} [see Eqs. (7.5) and (7.6) of Ref. 9] and the corresponding q-binomial and q-trinomial expansions[9] of the generator powers.

For the maximal isospin state $|aby_{\rm m}i_{\rm m}i_{\rm m}\rangle_q$ with $y_{\rm m}=1/3(a-b)$, $i_{\rm m}=1/2(a+b)$, $z_{\rm m}=1/2(b-a)$, the maximal projector of the quantum algebra $u_q(3)$ accepts the following form:

$$\mathscr{P}^{(ab)q}_{y_{\rm m}i_{\rm m}i_{\rm m},y_{\rm m}i_{\rm m}i_{\rm m}}=\sum_{n_1n_2n_3}\frac{(-1)^{n_1+n_2+n_3}q^{n_3}[a+1]![b+1]![a+b+2]!}{[n_1]![a+n_1+1]![n_2]![b+n_2+1]![n_3]![a+b+n_3+2]!}\times E_{31}^{n_1}E_{13}^{n_1}E_{21}^{n_3}E_{12}^{n_3}E_{23}^{n_2}E_{32}^{n_2}. \tag{2.7}$$

Contrary to the SU(3) case, we cannot go immediately from the highest weight projector[9] to (2.7) by a simple relabeling of subscripts in generators, but we need to check the identities

$$E_{13}\mathscr{P}^{(ab)q}_{i_{\max},i_{\max}}=E_{32}\mathscr{P}^{(ab)q}_{i_{\max},i_{\max}}=\mathscr{P}^{(ab)q}_{i_{\max},i_{\max}}E_{31}=\mathscr{P}^{(ab)q}_{i_{\max},i_{\max}}E_{23}=0, \tag{2.8}$$

using the generator transposition formulas, similarly as it was done in Ref. 9.

We may write a more universal projection operator as

$$\mathscr{P}^{(ab)q}_{y_{\rm m}i_{\rm m}i_{\rm m};yii}=\langle aby_{\rm m}i_{\rm m}i_{\rm m}|E_{13}^{a+z-i}E_{32}^{b-z-i}|abyii\rangle_q^{-1}\mathscr{P}^{(ab)q}_{y_{\rm m}i_{\rm m}i_{\rm m},y_{\rm m}i_{\rm m}i_{\rm m}}E_{13}^{a+z-i}E_{32}^{b-z-i}\mathscr{P}^{i,q}_{ii} \tag{2.9a}$$

$$=d_3[ab]\left(\frac{[a]![b]![a+b+1]![i+z]![i-z]![a+z+i+1]![b-z+i+1]!}{[2i+1]![a+z-i]![b-z-i]!}\right)^{1/2}\times\sum_{n_1n_2n_3}\frac{(-1)^{n_1+n_2}q^{(n_1+1)n_3}[a+b+n_1+n_2+n_3+2]!}{[n_1]![a+n_1+1]![n_2]![b+n_2+n_3+1]![n_3]![a+b+n_1+n_3+2]!}\times\frac{1}{[a+b+n_2+n_3+2]!}E_{21}^{n_3}E_{31}^{n_1}E_{23}^{n_2}E_{13}^{a+z-i+n_1+n_3}E_{32}^{b-z-i+n_2+n_3}\mathscr{P}^{i,q}_{ii} \tag{2.9b}$$

where $d_3[ab]=[a+1][b+1][a+b+2]$ and

$$\mathscr{P}^{i,q}_{ii}=\sum_{n'}\frac{(-1)^{n'}[2i+1]!}{[n']![2i+n'+1]!}E_{21}^{n'}E_{12}^{n'} \tag{2.10}$$

is the maximal projector of $u_q(2)$. For the rearrangement of (2.9a) [as well as (2.7)] to (2.9b), we use the transposition formulas presented in Appendix of Ref. 9, condition $E_{12}\mathscr{P}^{i,q}_{i}=0$, and summation formula (cf. Ref. 34)

$$\sum_s\frac{q^{s(a+b+c)}}{[s]![b-s]![c-s]![a+s]!}=\frac{q^{bc}[a+b+c]!}{[b]![c]![a+b]![a+c]!}. \tag{2.11}$$

By the way, we may also write the weight lowering operator for acting into the maximal isospin state:

$$\widetilde{F}\begin{pmatrix} ab \\ yii \end{pmatrix}|aby_{\rm m}i_{\rm m}i_{\rm m}\rangle_q=|abyii\rangle_q \tag{2.12a}$$

where

$$\widetilde{F}\begin{pmatrix} ab \\ yii \end{pmatrix}=\left(\frac{[2i+1]![a+z-i]![a+z+i+1]![b-z-i]![b-z+i+1]![i-z]!}{[a]![b]![a+b+1]![i+z]!}\right)^{1/2}$$
$$\times\sum_s \frac{q^{-s(2i+s+1)}[i+z+s]!}{[s]![a+z-i-s]![b-z-i-s]![2i+s+1]!}E_{21}^{s}E_{31}^{a+z-i-s}E_{23}^{b-z-i-s}. \tag{2.12b}$$

In accordance with condition (1.7c), we may express the bilinear combinations of isofactors as follows:

$$\sum_{t=1}^{\hat{I}'-i_{\rm m}+i''_{\rm m}+1}\begin{bmatrix} (a'b') & \overset{t}{(a''b'')} & (a\ \ b) \\ y'i' & y''i'' & y\ \ i \end{bmatrix}_q^{(3)}\begin{bmatrix} (a'b') & \overset{t}{(a''b'')} & (a\ \ b) \\ \hat{y}'\hat{I}' & y''_{\rm m}i''_{\rm m} & y_{\rm m}i_{\rm m} \end{bmatrix}_q^{(3)}$$
$$=\left(\begin{bmatrix} \hat{I}' & i''_{\rm m} & i_{\rm m} \\ i_{\rm m}-i''_{\rm m} & i''_{\rm m} & i_{\rm m} \end{bmatrix}_q^{(2)}\right)^{-1}\sum_{m'}\begin{bmatrix} i' & i'' & i \\ m' & i-m' & i \end{bmatrix}_q^{(2)}$$
$$\times\left\langle \begin{matrix}(a'b')\\ \hat{y}'\hat{I}'i_{\rm m}-i''_{\rm m}\end{matrix}\right|_q\left\langle \begin{matrix}(a''b'')\\ y''_{\rm m}i''_{\rm m}i''_{\rm m}\end{matrix}\right|_q\mathscr{P}^{(ab)q}_{y_{\rm m}i_{\rm m}i_{\rm m};y\ i\ i}\left|\begin{matrix}(a'b')\\ y'i'm'\end{matrix}\right\rangle_q\left|\begin{matrix}(a''b'')\\ y''i''i-m'\end{matrix}\right\rangle_q. \tag{2.13}$$

Although (2.13) provides an overcomplete system of non-orthogonal $u_q(3)$ isofactors, the direct canonical resolution of the multiplicity problem from the triangular system of equations (2.13) (i.e., by means of the Gram–Schmidt process) is not always possible (see Sec. IV).

We expand the powers of generators in (2.9b) when substituted into (2.13) in accordance with coproduct rules.[9] Operators $E_{21}^{n_3}$, $E_{31}^{n_1}$ and $E_{23}^{n_2}$ give only a single term in the coproduct expansion of (2.13) in accordance with formulas (7.9), (7.11) and (7.8) of Ref. 9, respectively, with the operators

$$q^{n_3(E_{11}-E_{22})/2+n_1(E_{11}-E_{33})/2+n_2(E_{22}-E_{33})/2},$$

acting in the space of the second irrep $(a''b'')$. Expansion of E_{13}^{k} $(k=a+z-i+n_1+n_3)$ in accordance with (7.10) of Ref. 9 gives a sum with a single summation parameter, as well as expansion of E_{32}^{l} $(l=b-z-i+n_2+n_3)$ in accordance with (7.9). Moreover, the powers of operators E_{13} and E_{32} acting in the second space are fixed by the shift conditions for the isospin projection and the hypercharge. Thus, the total number of sums (seven) does not exceed the SU(3) case[8] and we may write

$$\sum_t \begin{bmatrix} (a'b') & \overset{t}{(a''b'')} & (a\ \ b) \\ y'i' & y''i'' & y\ \ i \end{bmatrix}_q^{(3)} \begin{bmatrix} (a'b') & \overset{t}{(a''b'')} & (a\ \ b) \\ \hat{y}'\hat{I}' & y''_{\rm m} i''_{\rm m} & y_{\rm m} i_{\rm m} \end{bmatrix}_q^{(3)}$$

$$= (-1)^{\hat{I}'+i''_{\rm m}-i_{\rm m}} q^{(\hat{I}'-i_{\rm m}+i''_{\rm m})(\hat{I}'-i''_{\rm m}+i_{\rm m}+1)/2} ([i_{\rm m}+i''_{\rm m}-\hat{I}']![i_{\rm m}+i''_{\rm m}+\hat{I}'+1]!)^{1/2} d_3[a\ \ b]$$

$$\times \left(\frac{[a]![b]![i+z]![i-z]![a+z+i+1]![b-z+i+1]!}{[2i+1]![a+z-i]![b-z-i]![a''+b'']!} \right)^{1/2}$$

$$\times \sum_{n_1,n_2,n_3,m'} \frac{(-1)^{n_1+n_2} q^{Q_1} [a+b+n_1+n_2+n_3+2]!}{[n_1]![n_2]![n_3]![a+n_1+1]![b+n_2+n_3+1]!}$$

$$\times \frac{[a+z-i+n_1+n_3]![b-z-i+n_2+n_3]!}{[a+b+n_1+n_3+2]![a+b+n_2+n_3+2]![a''+z''-i+m']!} \begin{bmatrix} i' & i'' & i \\ m' & i-m' & i \end{bmatrix}_q^{(2)}$$

$$\times \frac{1}{[a-a''+v+z'-m'+n_1+n_3]![b''-z''-i+m']![b-b''-z'-v-m'+n_2+n_3]!}$$

$$\times \left\langle \begin{matrix} (a'b') \\ \hat{y}'\hat{I}' i_{\rm m} - i''_{\rm m} \end{matrix} \middle| E_{21}^{n_3} E_{31}^{n_1} E_{23}^{n_2} E_{13}^{a-a''+v+z'-m'+n_1+n_3} E_{32}^{b-b''-z'-v-m'+n_2+n_3} \middle| \begin{matrix} (a'b') \\ y'i'm' \end{matrix} \right\rangle_q$$

$$\times \left\langle \begin{matrix} (a''b'') \\ y''_{\rm m} i''_{\rm m} i''_{\rm m} \end{matrix} \middle| E_{13}^{a''+z''-i+m'} E_{32}^{b''-z''-i+m'} \middle| \begin{matrix} (a''b'') \\ y''i''i-m' \end{matrix} \right\rangle_q , \tag{2.14}$$

where

$$\hat{y}' = y_{\rm m} - y''_{\rm m} = \tfrac{1}{3}(a-b-a''+b'') = \tfrac{1}{3}(a'-b') - v$$

and q-phase

$$\begin{aligned} Q_1 = {} & (n_1+1)n_3 - \tfrac{1}{2}(a''+z''-i+m')(a-a''+2n_1-n_2+n_3) \\ & + \tfrac{1}{2} a''(a-a''+v+z'-m'+n_1+n_3) \\ & + \tfrac{1}{2}(b-b''-z'-v-m'+n_2+n_3)(b''-a''-3z''+m'-i) \\ & - \tfrac{1}{2}(b'-a'-3z'-m')(b''-z''-i+m') \\ & + \tfrac{1}{2}(a''+b'')n_3 + \tfrac{1}{2} a''n_1 - \tfrac{1}{2} b''n_2; \end{aligned} \tag{2.15}$$

$$(b'-a'-3z' = \tfrac{3}{2} y',\ \ b''-a''-3z'' = \tfrac{3}{2} y'')$$

appeared from the above mentioned coproduct expansion of the generator powers, after substituting the proper values of E_{ii}.

We express the matrix elements of the generator powers as follows:[13]

$$\left\langle \begin{matrix} (ab) \\ yim \end{matrix} \middle| E_{21}^n \middle| \begin{matrix} (ab) \\ yim+n \end{matrix} \right\rangle_q = \left(\frac{[i+m+n]![i-m]!}{[i+m]![i-m-n]!} \right)^{1/2}, \tag{2.16}$$

$$\left\langle \begin{matrix}(ab)\\ y'i'm'\end{matrix}\middle| E_{23}^{r}E_{13}^{p-r}\middle|\begin{matrix}(ab)\\ yim\end{matrix}\right\rangle_q = \delta_{z-p/2,z'}\delta_{m+p/2-r,m'}q^{(i+p/2-i')(i+p/2+i'+1)/2-p(i-m)/2-rm} \times\frac{\Gamma[abiz]([p-r]![r]![2i+1])^{1/2}}{\nabla[\frac{1}{2}p,i,i']\Gamma[abi'z']}\begin{bmatrix} i & \frac{1}{2}p & i' \\ m & \frac{1}{2}p-r & m'\end{bmatrix}^{(2)}_{q^{-1}}, \tag{2.17a}$$

$$\left\langle \begin{matrix}(ab)\\ y'i'm'\end{matrix}\middle| E_{31}^{r}E_{32}^{p-r}\middle|\begin{matrix}(ab)\\ yim\end{matrix}\right\rangle_q = \delta_{z+p/2,z'}\delta_{m+p/2-r,m'}(-1)^{i+p/2-i'+r} \times q^{(i+p/2-i')(i-p/2+i'+1)/2-p(i'-m')/2-r(m'+1)} \times\frac{\Gamma[abi'z'](p-r]![r]![2i+1])^{1/2}}{\nabla[\frac{1}{2}p,i,i']\Gamma[abiz]}\begin{bmatrix} i & \frac{1}{2}p & i' \\ m & \frac{1}{2}p-r & m'\end{bmatrix}^{(2)}_{q}, \tag{2.17b}$$

where the Clebsch–Gordan coefficients of $u_q(2)$ are presented in Refs. 13, 35, 36, and

$$\nabla[abc]=\left(\frac{[a+b-c]![a-b+c]![a+b+c+1]!}{[b+c-a]!}\right)^{1/2}, \tag{2.18}$$

$$\Gamma[abiz]=\left(\frac{[i+z]![a+z-i]![a+z+i+1]!}{[i-z]![b-z-i]![b-z+i+1]!}\right)^{1/2}. \tag{2.19}$$

The last matrix element on the rhs of Eq. (2.14) may be expressed without sum as follows:

$$\begin{aligned}&\left\langle \begin{matrix}(a''b'')\\ y''_{\rm m}i''_{\rm m}i''_{\rm m}\end{matrix}\middle| E_{13}^{a''+z''-i+m'}E_{32}^{b''-z''-i+m'}\middle|\begin{matrix}(a''b'')\\ y''i''i-m'\end{matrix}\right\rangle_q \\ &\quad=\frac{[a''+z''-i+m']![b''-z''-i+m']!}{[i-z''-m']!} \\ &\quad\times\left(\frac{[i''-z'']![a'']![b'']!}{[i''+z'']![a''+z''-i'']![b''-z''-i'']!}\right. \\ &\quad\left.\times\frac{[a''+b''+1]![2i''+1][i''+i-m']!}{[a''+z''+i''+1]![b''-z''+i''+1]![i''-i+m']!}\right)^{1/2}.\end{aligned} \tag{2.20}$$

Finally, the total number of sums in (2.14) is seven, including two isospin-type parameters of the intermediate states (which appear after acting with a power of E_{32} into $|a'b'\rangle_q$, but before acting with $E_{31}^{n_1}$) and a single sum of the $u_q(2)$ Clebsch–Gordan coefficient, appearing in accordance with Eq. (2.17a).

III. ISOFACTORS CHARACTERIZED BY THE MAXIMAL NULL SPACE

The three sums vanish in Eq. (2.14) for the canonical tensor operators, characterized by the maximal null space, when $\hat{I}' = i_{\rm m} - i''_{\rm m} \geqslant |\hat{z}'|$ [here $\hat{z}' \equiv 1/2(b'-a'+v)$] and label t accepts the single value $t=1$. Hence, we obtain

$$\begin{aligned}
&\left[\begin{matrix}\overset{t=1}{(a'b')} & (a''b'') & (ab)\\ y'i' & y''i'' & yi\end{matrix}\right]^{(3)}_{q}\left[\begin{matrix}\overset{t=1}{(a'b')} & (a''b'') & (ab)\\ \hat{y}'\hat{I}' & y''_{\mathrm{m}}i''_{\mathrm{m}} & y_{\mathrm{m}}i_{\mathrm{m}}\end{matrix}\right]^{(3)}_{q}\\
&\quad=\mathscr{N}_{(a''b'')}[a'b';ab]\,\frac{([a+1][b+1][a+b+2])^{1/2}}{\nabla[ii'i'']\Gamma[a'b'i'z']R[a''b''i''z'']}\\
&\quad\times\left(\frac{[2i'+1][i''-z'']![a+z+i+1]![b-z+i+1]![i+z]![i-z]!}{[i''+z'']![a+z-i]![b-z-i]!}\right)^{1/2}\\
&\quad\times\sum_{n_1,n_2,m',j'}\frac{(-1)^{(b''+v-b+z'+m'+n_2)/2-i'+j'+n_1}q^{Q_2}[2j'+1]}{[n_1]![n_2]![a+n_1+1]![b+n_2+1]![a+b+n_1+2]![a+b+n_2+2]!}\\
&\quad\times\frac{[a+b+n_1+n_2+2]![a+z-i+n_1]![b-z-i+n_2]!}{[i-m'-z'']![i''-i+m']![a'+a''-a-v-n_1]!}\\
&\quad\times\frac{[i''+i-m']![a-a''+v+n_1]![b'-a''+a+v+n_1+1]!}{\nabla^2[\frac{1}{2}(a-a''+v+z'-m'+n_1),i_{\mathrm{m}}-i''_{\mathrm{m}}+\frac{1}{2}(n_1+n_2),j']}\\
&\quad\times\frac{\Gamma^2[a',b',j',\frac{1}{2}(b-b''-v+z'-m'+n_2)]}{\nabla^2[\frac{1}{2}(b-b''-v-z'-m'+n_2),j',i']}
\end{aligned}\tag{3.1}$$

where the summation parameters satisfy the conditions[8]

$$\max(0,a''-a-v)\leqslant n_1\leqslant a'+a''-a-v,\quad 0\leqslant n_2\leqslant b'+b''-b+v,$$

$$i-i''\leqslant m'\leqslant\min(i',i-z''),$$

$$\max\{\tfrac{1}{2}(b-b''-v-z'+m'+n_2),\tfrac{1}{2}|b-b''-v+z'-m'+n_2|\}\leqslant j',$$

$$j'\leqslant\min\{b'-\tfrac{1}{2}(b-b''-v+z'-m'+n_2),\tfrac{1}{2}(b-b''-v-z'-m'+n_2)+i'\}$$

and are restricted by the non-negative integer values of the denominator q-factorial arguments. Besides, in (3.1) notations (2.18) and (2.19), together with those presented below, are used:

$$\begin{aligned}
&\mathscr{N}_{(a''b'')}[a'b';ab]\\
&\quad=\left(\frac{[a+1]![b+1]![a+b+2]![2i_{\mathrm{m}}-2i''_{\mathrm{m}}+1]![a'+\hat{z}'-\hat{I}']![b'-\hat{z}'-\hat{I}']!}{[\hat{I}'+\hat{z}']![\hat{I}'-\hat{z}']![a'+\hat{z}'+\hat{I}'+1]![b'-\hat{z}'+\hat{I}'+1]!}\right)^{1/2}
\end{aligned}\tag{3.2a}$$

$$=\left(\frac{[a+1]![b+1]![a+b+2]![a'+a''-a-v]![b'+b''-b+v]![a+b-a''-b''+1]!}{[a-a''+v]![b-b''-v]![a'-b''+b-v+1]![b'-a''+a+v+1]!}\right)^{1/2},\tag{3.2b}$$

$$R[abiz]=\left(\frac{[a+z-i]![a+z+i+1]![b-z-i]![b-z+i+1]!}{[2i+1][a]![b]![a+b+1]!}\right)^{1/2}, \tag{3.3}$$

$$\begin{aligned}Q_2=&(n_1-n_2)(i+z''-m')-\tfrac{1}{2}(a''+z''-i+m')(a-a'')-\tfrac{1}{2}(b''-z''-i+m')(\tfrac{3}{2}y'-m')\\&+\tfrac{1}{2}(\tfrac{3}{2}y''-i+m')(b-b''-v-z'-m')+\tfrac{1}{2}a''(a-a''+v+z'-m')+\tfrac{1}{2}(i'+i''-i)\\&\times(i-i'+i''+1)-(i+1)(i'-m')+j'(j'+1)-\tfrac{1}{4}(b-b''-v-z'+m'+n_2)\\&\times(b-b''-v-z'+m'+n_2+2)-2n_1z''.\end{aligned} \tag{3.4}$$

Notation (3.3) is also used in the expression[13] for the stretched $u_q(3)$ isofactors:

$$\begin{aligned}\begin{bmatrix}(a'b') & (a''b'') & (a'+a'',b'+b'')\\ (z')i' & (z'')i'' & (z'+z'')i\end{bmatrix}^{(3)}_q&=q^{(a'b''-a''b')/2+z'(a''+b'')-z''(a'+b')}\\&\times\frac{R[a'+a'',b'+b'',i,z'+z'']}{R[a'b'i'z']R[a''b''i''z'']}\begin{bmatrix}i' & i'' & i\\ z' & z'' & z\end{bmatrix}^{(2)}_q,\end{aligned} \tag{3.5}$$

which, of course, corresponds to a multiplicity-free case of (3.1).

The following particular case of (3.1) with $i'=i-i''_{\mathrm{m}}$ is especially important for the solution of its normalization problem:

$$\begin{aligned}&\begin{bmatrix}(a'b') & \overset{t=1}{(a''b'')} & (ab)\\ y'i-i''_{\mathrm{m}} & y''_{\mathrm{m}}i''_{\mathrm{m}} & yi\end{bmatrix}^{(3)}_q\begin{bmatrix}(a'b') & \overset{t=1}{(a''b'')} & (ab)\\ \hat{y}'i_{\mathrm{m}}-i''_{\mathrm{m}} & y''_{\mathrm{m}}i''_{\mathrm{m}} & y_{\mathrm{m}}i_{\mathrm{m}}\end{bmatrix}^{(3)}_q\\&=\left(\frac{[2i'+1]![i+z]![i-z]![a'+z'+i']![b'-z'-i']![a+z+i+1]![b-z+i+1]!}{[2i+1]![i'+z']![i'-z']![a+z-i]![b-z-i]![a'+z'+i'+1]![b'-z'+i'+1]!}\right)^{1/2}\\&\times q^{a''(a+z-i)/2-b''(b-z-i)/2}(d_3[ab])^{1/2}\mathscr{N}_{(a''b'')}[a'b';ab]\mathscr{D}^2\begin{pmatrix}q,t=1\\ a''b''\end{pmatrix}[a'b';ab],\end{aligned} \tag{3.6}$$

where

$$\begin{aligned}&\mathscr{D}^2\begin{pmatrix}q,t=1\\ a''b''\end{pmatrix}[a'b';ab]\\&=\mathscr{D}^2\begin{pmatrix}q^{-1},t=1\\ b''a''\end{pmatrix}[b'a';ba]\end{aligned} \tag{3.7a}$$

$$=\sum_{n_1,n_2}\frac{(-1)^{n_1+n_2}q^{a''n_1-b''n_2}[a+b+n_1+n_2+2]!}{[n_1]![n_2]![a+n_1+1]![b+n_2+1]![a+b+n_1+2]![a+b+n_2+2]!}$$

$$\times\frac{[a-a''+v+n_1]![b'-a''+a+v+n_1+1]![b-b''-v+n_2]![a'-b''+b-v+n_2+1]!}{[a'+a''-a-v-n_1]![b'+b''-b+v-n_2]![a+b-a''-b''+n_1+n_2+1]!}. \tag{3.7b}$$

Taking $i=i_{\mathrm{m}}, y=y_{\mathrm{m}}$, we obtain square of isofactor

$$\begin{bmatrix} (a'b') & \overset{t=1}{(a''b'')} & (ab) \\ \hat{y}'i_{\mathrm{m}}-i''_{\mathrm{m}} & y''_{\mathrm{m}}i''_{\mathrm{m}} & y_{\mathrm{m}}i_{\mathrm{m}} \end{bmatrix}^{(3)}_{q} = \mathscr{N}_{(a''b'')}[a'b';ab]\mathscr{D}\begin{pmatrix} q,t=1 \\ a''b'' \end{pmatrix}[a'b';ab]. \tag{3.8}$$

Now (3.8) may be inserted into the lhs of (3.1) to express the normalized isofactor of the maximal null space case, but some reasoning was necessary for choice of the sign of the boundary canonical isofactor. Acceptance of the separate isofactors (3.8) being positive requires use of the supplementary phase factors $(-1)^{b'-b}$ or $(-1)^{v}$ for the multiplicity-free[13] isofactors of $u_q(3)$ (with parameter $b''=0$, or in the semistretched case, respectively). We see that the denominator q-factorials $[a-a''+v]!$ and $[b-b''-v]!$, restricting the regions of non-vanishing for (3.1) and (3.6)–(3.8), cancel and the matrix elements of the $u_q(3)$ canonical tensor operator with $t=1$ may be obtained by an analytical continuation procedure and may exist also for $a-a''+v$ or $b-b''-v$ negative. Really, the sum over n_1,n_2,m',j' on the rhs of (3.1) is restricted only by the triangular and betweenness conditions (1.1d), but the rhs of (3.7b) is indefinite for negative $a-a''+v$ or $b-b''-v$. The latter problem was escaped in Ref. 8 for the SU(3) isofactors, after the corresponding double sum (at first rearranged into the $G^1_{b'+b''-b+v}$-function) has been transformed by means of its reduction formulas[6,7] into the $G^1_{b''}$-function.[5,7,25]

We tried to replace some ratios of q-factorials in the first and the last rows of Eq. (3.7b) separately by the q-analogs of the Vandermonde formulas,[34] in analogy with (3.17) of Ref. 8, but we failed to transform the double sum (3.7b) into another form, related to the denominator polynomials[5–7] of the SU(3) maximal null space tensor operators.[25] Unfortunately, after summation over n_1 (or n_2), it was impossible to take the sum over the second original summation parameter n_2 (or n_1) because of the non-balanced (i.e., non-correlated with the difference of the factorial argument sums in numerator and denominator) q-power, unless $b''=0$ (or $a''=0$).

In order to obtain more convenient expressions for the denominator function $\mathscr{D}^2\left(\begin{smallmatrix} q,t=1 \\ a''b'' \end{smallmatrix}\right)$, let us consider another product (trivial bilinear combination) of isofactors, corresponding to the maximal null space tensor operator:

$$\begin{bmatrix} (a'b') & \overset{t=1}{(a''b'')} & (ab) \\ y'_{\mathrm{m}}i'_{\mathrm{m}} & y''_{\mathrm{m}}i''_{\mathrm{m}} & \hat{y}i'_{\mathrm{m}}-i''_{\mathrm{m}} \end{bmatrix}^{(3)}_{q}\begin{bmatrix} (a'b') & \overset{t=1}{(a''b'')} & (ab) \\ \hat{y}'i_{\mathrm{m}}-i''_{\mathrm{m}} & y''_{\mathrm{m}}i''_{\mathrm{m}} & y_{\mathrm{m}}i_{\mathrm{m}} \end{bmatrix}^{(3)}_{q}. \tag{3.9}$$

Formula (3.1) gives a triple sum for (3.9), which is not preferable to (3.7b). Otherwise, an alternative expression (3.15) of Ref. 8, together with the Vandermonde formula, gives a double sum in the corresponding denominator function of the SU(3) maximal null space tensor operator. Hence, it is expedient to derive a q-analog of the projection operator (3.3b) of Ref. 8:

$$\mathscr{P}^{(ab)q}_{yii;y_{\rm m}i_{\rm m}i_{\rm m}}$$

$$=\widetilde{F}\begin{pmatrix} ab \\ yii \end{pmatrix}\mathscr{P}^{(ab)q}_{y_{\rm m}i_{\rm m}i_{\rm m};y_{\rm m}i_{\rm m}i_{\rm m}} \tag{3.10a}$$

$$=d_3[ab]([a]![b]![a+b+1]![2i+1]![i-z]![a+z-i]!$$

$$\times[a+z+i+1]![b-z-i]![b-z+i+1]!/[i+z]!)^{1/2}$$

$$\times\sum_{n_1n_2ur}\frac{(-1)^{n_1+n_2}q^{u(i+z+1)+r(a-2i+n_1-r)}[a+b+n_1+n_2-u+2]!}{[u]![a+n_1-u+1]![n_2-u]![b+n_2+1]![a+b+n_1+2]![a+b+n_2+2]!}$$

$$\times\frac{1}{[b-z-i-r+u]!}\sum_s\frac{q^{-s(a+n_1-u+1)}[i+z+s]!}{[s]![a+z-i-s]![r-s-u]![n_1-r+s]![2i+s+1]!}$$

$$\times E_{21}^rE_{31}^{a+z-i-r+n_1}E_{23}^{b-z-i-r+n_2}E_{13}^{n_1}E_{32}^{n_2}\mathscr{P}^{i_{\rm m},q}_{i_{\rm m}i_{\rm m}}. \tag{3.10b}$$

Formula (3.10b) is obtained, using in (3.10a) our formulas (2.9b), (2.12b), and the generator transposition formulas.[9] The sum over s is more convenient if transformed (cf. Refs. 8 and 34) into

$$\sum_s\ldots=\frac{[i+z]!q^{-(r-u)(a+z-i)}}{[i-z]![n_1-u]![a+z-i-r+n_1]!}$$

$$\times\sum_s(-1)^s\frac{q^{s(i+z-n_1+r)}[i-z+s]![a+z-i+n_1-s-u]!}{[s]![a+z-i-s]![r-s-u]![2i+s+1]!}. \tag{3.11}$$

However, the coproduct expansions (2.6a) and (2.6b) of the E_{31} and E_{13} powers in the matrix elements of projector (3.10b) give some additional sums in the expression of (3.9) to compare with the SU(3) case [see Eq. (3.3b) of Ref. 8]. An expression without additional sums may be obtained for the following bilinear combination of isofactors:

$$\sum_t\begin{bmatrix}(a'b') & \overset{t}{(a''b'')} & (ab)\\ y'_{\rm m}i'_{\rm m} & y''_{\rm m}i''_{\rm m} & \hat{y}i''_{\rm m}-i'_{\rm m}\end{bmatrix}^{(3)}_q\begin{bmatrix}(a'b') & \overset{t}{(a''b'')} & (ab)\\ y'_{\rm m}i'_{\rm m} & \hat{y}''i_{\rm m}-i''_{\rm m} & y_{\rm m}i_{\rm m}\end{bmatrix}^{(3)}_q. \tag{3.12}$$

After permutation of the both states to be coupled in (3.12), relabeling of the parameters $a',b',y',i'\leftrightarrow a'',b'',y'',i''$, and q-inversion: $q\rightarrow q^{-1}$ (together with an elementary phase factor), product (3.9) may be presented as

$$\begin{bmatrix}(a'b') & \overset{t=1}{(a''b'')} & (ab)\\ y'_{\rm m}i'_{\rm m} & y''_{\rm m}i''_{\rm m} & \hat{y}i'_{\rm m}-i''_{\rm m}\end{bmatrix}^{(3)}_q\begin{bmatrix}(a'b') & \overset{t=1}{(a''b'')} & (ab)\\ \hat{y}'i_{\rm m}-i''_{\rm m} & y''_{\rm m}i''_{\rm m} & y_{\rm m}i_{\rm m}\end{bmatrix}^{(3)}_q$$

$$=(-1)^{b''+v}q^{-Q_3}\left(\frac{d_3[ab][a'+b'+1]}{d_3[a'b'][2i'_{\rm m}-2i''_{\rm m}+1]}\right)^{1/2}\mathscr{N}_{(a''b'')}[a'b';ab]$$

$$\times\mathscr{N}_{(a''b'')}[ba;b'a']\mathbf{D}^2\begin{pmatrix}q,t=1\\ a''b''\end{pmatrix}[a'b';ab] \tag{3.13}$$

with

$$\mathbf{D}^2\begin{pmatrix} q,t=1 \\ a''b'' \end{pmatrix}[a'b';ab]$$

$$= q^{b''(a'-b''+b-v+2)-a''(b'-a''+a+v+2)}\mathbf{D}^2\begin{pmatrix} q^{-1},t=1 \\ a''b'' \end{pmatrix}[ba;b'a'] \tag{3.14a}$$

$$= (-1)^{b'-b+v}q^{a''(a''-a-v-1)-b''(b''-b+v-1)+b'-b+v}$$
$$\times\frac{[a'']![b'']![a'-b''+b-v+1]![b'-a''+a+v+1]![b'-a''+v]!}{[b'+b''+v+1]![a'+a''+b-v+2]![b'+b''+a+v+2)]!}$$
$$\times\sum_{s,u}\ \frac{(-1)^{s+u}q^{s(b''-b+v)-u(a''+b-v+2)}[a''+b''-s-u]![s+u]!}{[s]![a-a'+b''+v-s]![b-b'+a''-v-s]![b'-b+v+s]!}$$
$$\times\frac{[a'-b''-v+s]!}{[a'+b'-a''-b''+s+1]![u]![a'+a''-a-v-u]![b'+b''-b+v-u]!}$$
$$\times\frac{[a'+b'+a''+b''-u+2]!}{[b-b'-v+u]![a'+a''-v-u+1]!} \tag{3.14b}$$

and

$$Q_3=\tfrac{1}{2}\,b''(a'-b''+b-v+1)-\tfrac{1}{2}\,a''(b'-a''+a+v+1). \tag{3.15}$$

The factors in the first row of the rhs of Eq. (3.13) are mainly motivated by the symmetry properties of the $u_q(3)$ canonical isofactors, presented in the last section of this paper, but the equivalence question for the denominator functions (3.7b) and (3.14b), including the above presented distribution of q-powers between (3.13) and (3.14b), should be considered separately, unless $q=1$.

Taking into account the generic structure of the $t=1$ isofactors with the extreme shift of $u_q(2)$ irreps, grounded on the pattern calculus[12] principles, the ratio of such isofactors may be expressed as follows:

$$\begin{bmatrix} & \overset{t=1}{} & \\ (a'b') & (a''b'') & (ab) \\ \hat{y}'i_{\mathrm{m}}-i''_{\mathrm{m}} & y''_{\mathrm{m}}i''_{\mathrm{m}} & y_{\mathrm{m}}i_{\mathrm{m}} \end{bmatrix}^{(3)}_{q}\left(\begin{bmatrix} & \overset{t=1}{} & \\ (a'b') & (a''b'') & (ab) \\ y'_{\mathrm{m}}i'_{\mathrm{m}} & y''_{\mathrm{m}}i''_{\mathrm{m}} & \hat{y}i'_{\mathrm{m}}-i''_{\mathrm{m}} \end{bmatrix}^{(3)}_{q}\right)^{-1}$$
$$= (-1)^{b''+v}q^{Q_3}\left(\frac{d_3[a'b'][2i'_{\mathrm{m}}-2i''_{\mathrm{m}}+1]}{d_3[ab][a'+b'+1]}\right)^{1/2}\frac{\mathscr{N}_{(a''b'')}[a'b';ab]}{\mathscr{N}_{(a''b'')}[ba;b'a']}. \tag{3.16}$$

Particularly, the q-power in formula (3.16) is extrapolated from the multiplicity-free isofactors,[13] respectively, with $a=a'+a''-v$, or $b=b'+b''+v$, or $b''=0$, or $a''=0$. The single sums remaining in the corresponding formulas (4.5), (3.4), or (3.16) of Ref. 13 were taken, respectively, by means of the basic generalizations[34] of the Vandermonde, balanced, and Carlson formulas [see, for example, (3.11) and (3.15) of Ref. 13].

However, (3.14b) is also indefinite for $b'-a''+v<0$, or $a'-b''-v<0$ and $a-a''+v<0$. It is evident that the infinities (poles) of the denominator function, appearing together with the negative arguments of the numerator q-factorials, determine the null space for

$$a'-b''-v<0 \quad \text{and} \quad a-a''+v<0 \quad \text{both together} \tag{3.17a}$$

(i.e., $r_{\alpha 1\gamma}<r_{\alpha 2\gamma}$ and $r_{\alpha 1\gamma}<r_{\alpha 3\gamma}$), or

$$b-b''-v<0 \quad \text{and} \quad b'-a''+v<0 \quad \text{both together} \tag{3.17b}$$

(i.e., $r_{1\beta\gamma}<r_{3\beta\gamma}$ and $r_{1\beta\gamma}<r_{2\beta\gamma}$). Otherwise, if the null space situation is excluded, we should use the symmetry relations (3.7a) or (3.14a) of the denominator functions for $b'-a''+v<0$ in order to get expressions without indefinities, unless both $b'-a''+v<0$ and $a-a''+v<0$, when Eq. (3.14b) can be used only together with relation (3.14a). In general, for the fixed rank $(a''b'')$ and shifts $\Delta_1,\Delta_2,\Delta_3$ [see array (1.5b)] of the q-tensor operator $T^{(a''b'')1,q}$, we may choose such a version of the denominator function, where indefinities appear only together with singularities (poles). Hence, the left (generic) isofactor with $t=1$ on the lhs of (3.1) may accept non-zero values, although $i_{\mathrm{m}}-i''_{\mathrm{m}}<0$ and the right isofactor is equal to 0. In this case we get the null space of the $u_q(3):u_q(2)$ extreme projective operator, exceeding the null space of the corresponding canonical tensor operator.

For final fixation of the phases in the symmetry relations (4.2a) and (4.2b), it is expedient to write the following expression of special isofactors:

$$\begin{bmatrix} & {\scriptstyle t=1} & \\ (a'b') & (a''b'') & (ab) \\ y'_{\mathrm{m}}i'_{\mathrm{m}} & \hat{y}''i'' & y_{\mathrm{m}}i_{\mathrm{m}} \end{bmatrix}^{(3)}_{q}$$

$$=\frac{(-1)^{v+i''+\hat{z}''}q^{Q_4}}{\mathscr{D}\begin{pmatrix} q,t=1 \\ a''b'' \end{pmatrix}[a'b';ab]R[a''b''i''\hat{z}'']}$$

$$\times\left(\frac{[a'+b'+1][a+b+2][a+1]![b+1]![a']![b']![i_{\mathrm{m}}+i'_{\mathrm{m}}-i'']![i_{\mathrm{m}}+i'_{\mathrm{m}}+i''+1]!}{[2i'_{\mathrm{m}}+2i''_{\mathrm{m}}+3][a'+a''-v+1]![b'+b''+v+1]![b+a''-v+1]![a+b''+v+1]!}\right)^{1/2}$$

$$\times\frac{([2i''_{\mathrm{m}}+i_{\mathrm{m}}+i'_{\mathrm{m}}-i''+2]![2i''_{\mathrm{m}}+i_{\mathrm{m}}+i'_{\mathrm{m}}+i''+3]!)^{1/2}}{[a'+a''+b-v+2]![b'+b''+a+v+2]!}\begin{bmatrix} i''_{\mathrm{m}}+i_{\mathrm{m}}+1 & i'' & i'_{\mathrm{m}}+i''_{\mathrm{m}}+1 \\ \hat{z}' & \hat{z}'' & \hat{z} \end{bmatrix}^{(2)}_{q}, \tag{3.18}$$

where

$$Q_4=\tfrac{1}{2}\{\hat{z}''(a+b+4)+b''(b-b'-v)-a''(a-a'+v)+i''_{\mathrm{m}}(b'-a'+a''-b'')+v(i''_{\mathrm{m}}-i'_{\mathrm{m}})\},$$

$$\hat{z}'=\tfrac{1}{2}(b'-a'+v), \quad \hat{z}''=\tfrac{1}{2}(b''-a''+v), \quad \hat{z}=\tfrac{1}{2}(b-a-v). \tag{3.19}$$

Formula (3.18) may be derived directly from Eq. (3.15) of Ref. 8 in the $q=1$ case, but for arbitrary q we use projector (3.10b), together with transformations, applied between (3.12) and (3.13), explicit expressions[36] and symmetry properties[35] of the $u_q(2)$ Clebsch–Gordan coefficients.

Let us consider the simplest non-trivial example—special cases of the denominator function (3.7b) and (3.14b) for $a''=b''=1$, $a'=a$, $b'=b$, $v=0$. It may be written as

$$\mathscr{D}^2\begin{pmatrix} q,t=1 \\ 11 \end{pmatrix}[ab;ab]=\frac{f_2[ab]}{[a+b+1][a+b+2][a+b+3][a][a+1][a+2][b][b+1][b+2]} \tag{3.20}$$

in terms of function

$$f_2[ab]=[a+b+3][b+2]([a+b][a+2]-q[a][a+b+1])+[a+b+1][b]([a][a+b+4] -q^{-1}[a+2][a+b+3]) \tag{3.21a}$$

$$=q^{b-a}\{[2][a+b+4][a+b]-q^{-b+1}[a][a+b+4] -q^{-b-3}[a+b][a+2]+[2][a][a+2]\} \tag{3.21b}$$

$$=[2]([a+1][a+b+2]q^{-a-1}+[b+1]^2q^{a+b+2}-q^{a+b+2}-q^{b-a}-q^{-a-b-2}) \tag{3.21c}$$

$$=[2]([a-b][a+b+2]q^{-a-b-2}+[b+1][a+2b+3]-q^{a+b+2}-q^{b-a}-q^{-a-b-2}), \tag{3.21d}$$

where (3.21a) (where 4 is the initial formal total degree of a,b in the $q=1$ case polynomial) is obtained, respectively, from (3.7b) and reduced with considerable efforts to (3.21c) and (3.21d); the corresponding version (3.21b) of Eq. (3.14b) is more simple *ab initio*. Perhaps, function $f_2[ab]$ accepts the simplest form after the multiplication by q^{b+1} and substitution $q\to q^{-1}$ into the normalization factor[19] $g_{\lambda\mu}(q)$ of the canonical tensor operators of rank (1 1):

$$f_2[ab]=[2]\{q^{-a-1}([a+b+3][a]+[b])+q^{a+b+2}[b][b+2]\}. \tag{3.22}$$

It is invariant with respect to interchange $a\leftrightarrow b$, together with substitution $q\to q^{-1}$. For $q=1$, function $f_2[ab]$ turns into the usual quantity, related to the eigenvalue of the SU(3) Casimir operator

$$f_2(ab)=2(a^2+ab+b^2+3a+3b). \tag{3.23}$$

Some blocks of (3.14b) may be associated with the rhs of (2.11), but the rearrangement of the denominator function $\mathbf{D}^2\binom{q,t=1}{a''b''}$ into an analogue of G-function[7,25] is possible only in the $q=1$ case.[37] The requirement of the $q\to q^{-1}$ antisymmetry for the normalization factors makes any straightforward extrapolation of the denominator functions[5,7] of the SU(3) canonical tensor operators rather problematic. The necessity to fix two parameters from subarray (1.5b) in Eqs. (3.7b) and (3.14b) also restricts the possibility of introducing q-analog of G-function (for which fixation of a single parameter is sufficient).

We considered also the properties of Milne's[26] q-analog $[G]^{(3)}_m$ of the introduced by Holman *et al.*[27] invariant G-function (in terms of the well-poised series $W^{(3)}_m$), using Ref. 38 for agreement of notations. [Note that the G-functions, as introduced in Ref. 27, satisfy the complete explicit symmetry under permutations of array (1.5b), but present problems when reducing the total degree of polynomial, i.e., rearranging sums of fractions into polynomials of minimal degree]. However, we didn't find any coincidence of the generic q case even with our Eq. (3.21) or (3.22). Non-balanced and quadratic in the summation parameters q-powers of the well-poised series $[W]^{(3)}_m$, when presented in terms of the symmetrical q-factorials (2.2), appear in contradiction with the requirement of the $q\to q^{-1}$ antisymmetry under conjugation.

IV. SOME SYMMETRIES AND DISTINCTION PROBLEM OF THE SU(3) AND $u_q(3)$ CANONICAL ISOFACTORS

The symmetry properties of the matrix elements of the $u_q(3)$ canonical tensor operators should be consistent with the symmetry properties of the SU(3) canonical isofactors[1,8] (cf. also Ref. 30) and include the corresponding q-factors.[29] We prefer to use the SU(3) conjugation relation

$$|abyii_z\rangle_q^* = (-1)^{a+b+z+i_z}|b,a,-y,i,-i_z\rangle_{q^{-1}} \tag{4.1}$$

[with the phase factor $(-1)^{\rho(3)}$, $\rho(n)=\Sigma_{j=1}^{n}\Sigma_{i=1}^{j}m_{ij}$, in the Gelfand–Tsetlin parameters, cf. Ref. 1] instead of (2.20) of Ref. 30 [which gives the phase factor $(-1)^{a+b}$ if applied twice]. The $u_q(3)$ unit tensor operator conjugation and transposition (Hermitian) properties give the following $S_2\times S_2$ symmetry of isofactors:

$$\begin{bmatrix} (a'b') & \overset{t}{(a''b'')} & (ab) \\ y'i' & y''i'' & yi \end{bmatrix}_q^{(3)} = (-1)^{t-1+i'+i''-i}\begin{bmatrix} (b'a') & \overset{t}{(b''a'')} & (ba) \\ -y'i' & -y''i'' & -yi \end{bmatrix}_{q^{-1}}^{(3)} \tag{4.2a}$$

$$= (-1)^{a''+b''+v+t-1+i''-z''}q^{-3y''/2} \times \left(\frac{[2i'+1]d_3[ab]}{[2i+1]d_3[a'b']}\right)^{1/2}\begin{bmatrix} (ba) & \overset{t}{(a''b'')} & (b'a') \\ -yi & y''i'' & -y'i' \end{bmatrix}_{q^{-1}}^{(3)} \tag{4.2b}$$

together with q-inversion. Dependencies of the phase factors on the basis labels are the same as for other external labeling schemes of SU(3) isofactors[22,23,39] [e.g., labeled by means of SU(3) invariant operators[22,39] in the SU(3)⊗SU(3) enveloping algebra] and for the multiplicity-free isofactors[13] of $u_q(3)$. Dependence of the phase factors on the multiplicity label t is completely determined by the number $t-1$ of the self-adjoined minimal null space operators in the canonical tensor operator[1,8,30,33] under consideration, but the total phase factors in (4.2a) and (4.2b) are consistent with (3.18), as well as with (4.1). In accordance with (4.2a) or (4.2b), the SU(3) canonical isofactors with the sign change and coinciding after permutation parameters should be equal to 0.

However, the phase factors, obtained by extrapolation from the matrix elements of the elementary self-adjoined tensor operators and presented in Eq. (2.16b) of Ref. 8, should be corrected, as well as the phase factors of the SU(3) 3-j coefficients.[30] Of course, some alternatives in the phase choice are possible for different phase systems, but the conjugation properties of the evidently non-vanishing SU(3) isofactors

$$\begin{bmatrix} \overset{t=1}{(a'a')} & (a''a'') & (aa) \\ 0i_{\mathrm{m}}-i''_{\mathrm{m}} & 0i''_{\mathrm{m}} & 0i_{\mathrm{m}} \end{bmatrix}^{(3)} \quad (a\geqslant a'') \tag{4.3a}$$

[see Eq. (3.8)] should not contradict with phase factor in Eq. (4.2a). Especially, the phase factor asymmetry with respect to the permutation $a'\leftrightarrow b'$, $a''\leftrightarrow b''$, $a\leftrightarrow b$ [contrary to proposition (4.11) of Ref. 30] cannot be allowed, because it sometimes induces improper sign changes of the conjugation invariant canonical isofactors or 3-j coefficients, e.g., for the triplet of irreps (5 5), (3 3), and (4 4) with the shifts $\Delta_1=2$, $\Delta_2=3$, $\Delta_3=4$ and the operator pattern $\Gamma_1=(_5{}^2{}_0)$ of the rank [6 3 0] tensor operator in the partition-type notations. Besides, for this triplet (and in the all cases with $\Delta_1\neq\Delta_3$) the use of $\Gamma_1=(_0{}^{-2}{}_{-5})$ as multiplicity label in the coproduct $[0,-5,-10]\otimes[0,-3,-6]\rightarrow$

$[-4,-8,-12]$ decomposition is incompatible with condition (2.11) of Ref. 30 between the weights and shifts. The conjugation of irreps (in the partition-type notations) interchanges the order and signs of shifts, but formal conjugation of the operator pattern changes only the signs of shifts. Of course, the equivalence relation $\Gamma_1 \cong (_6{}^4{}_1) \neq (_5{}^2{}_0)$ (used together with $[0,-3,-6] \cong [6,3,0]$) does not improve the situation, but the operator pattern $(_6{}^4{}_1)$ is consistent with the transposed triplet of irreps (4 4), (3 3), and (5 5), as well as the general Γ_1 is consistent with the triplet $(ba)\otimes(a''b'') \rightarrow (b'a')$.

Otherwise, the phase factor $(-1)^{a''+b''+v} = (-1)^{a'-b'-a+b}$ in (4.2b) is determined by explicit isofactors (3.18) and does not contradict with the explicit multiplicity-free isofactors[13] after correlation of the fixed signs of the corresponding boundary cases. It is also consistent with the vanishing properties of special SU(3) isofactors

$$\begin{bmatrix} & \overset{t=1}{} & \\ (ba) & (a''b'') & (ab) \\ -y_{\mathrm{m}} i_{\mathrm{m}} & \hat{y}'' i'' & y_{\mathrm{m}} i_{\mathrm{m}} \end{bmatrix}^{(3)}, \tag{4.3b}$$

[with $\hat{y}'' = 2y_{\mathrm{m}}$, $i'' \geqslant |\frac{1}{2}(b''-a''+v)| = |b-a-v)|$], corresponding to zeros of the Clebsch–Gordan coefficients of SU(2) on the rhs of Eq. (3.18), related in frames of the Regge symmetry to the SU(2) Wigner coefficients with equal to 0 projections of angular momentum. In its turn, the q-power in (3.14a) may be found using the general version of (4.2b), together with (3.18).

Using elementary $u_q(3)$ Wigner–Clebsch–Gordan coefficients for the coupling $(b'''a''')\otimes(a'''b''') \rightarrow (0\ 0)$ [which are consistent with (4.2b) in the $a=b=0$ case], together with the phase factor $(-1)^{a'+a''+a'''}$, we may introduce the $u_q(3)$ 3-j coefficients (cf. Refs. 30 and 40)

$$\begin{pmatrix} & \overset{t}{} & \\ (a'b') & (a''b'') & (a'''b''') \\ y'i'i'_z & y''i''i''_z & y'''i'''i'''_z \end{pmatrix}^{(3)}_{q} = (-1)^{\psi+a'+a''+b'''+z'''+i'''_z} q^{-(3y'''+i'''_z)/2} \left(\frac{[2]}{d_3[a'''b''']} \right)^{1/2} \times \begin{bmatrix} & \overset{t}{} & \\ (a'b') & (a''b'') & (b'''a''') \\ y'i' & y''i'' & -y'''i''' \end{bmatrix}^{(3)}_{q} \begin{bmatrix} i' & i'' & i''' \\ i'_z & i''_z & -i'''_z \end{bmatrix}^{(2)}_{q} \tag{4.4}$$

for coupling of three irreps $(a'b')\otimes(a''b'')\otimes(a'''b''') \rightarrow (0\ 0)$. In accordance with Pluhař *et al.*[39] and Biedenharn *et al.*[30] (see Sec. V) for $\psi=0$ or v we obtain coinciding (but not equivalent with that presented in Ref. 30) conjugation and transposition $1 \leftrightarrow 3$ phase factors $(-1)^{v+t-1}$ [here $v = \frac{1}{3}(a'+a''+a'''-b'-b''-b''')$] of the $u_q(3)$ 3-j coefficients (together with the q-inversion $q \rightarrow q^{-1}$ in the both cases). However, these phase factors are different, if $\psi = a'+a''+a'''$ or $b'+b''+b'''$. Note, that our self-consistent conjugation phase factor (4.1) is sufficient for motivation (but, of course, not for the proof) of the phase factors in (4.2a) and (4.2b) in the $t=1$ case.

There are two different possible approaches to the permutations $1 \leftrightarrow 2$ or $1 \leftrightarrow 3$ in the canonical isofactors and 3-j coefficients of $u_q(3)$ or SU(3). Extending results discussed in Sec. VI and the conclusion of Ref. 22 about three versions of the canonical labeling, we may write explicitly also the relations between the isofactors with the permuted first and second irreps or the permuted and conjugated third and second irreps:

$$\begin{bmatrix} (a'b') & \overset{t}{(a''b'')} & (ab) \\ y'i' & y''i'' & yi \end{bmatrix}^{(3)}_{q} = (-1)^{\varphi_{12}+t-1+i'+i''-i} \begin{bmatrix} \overset{t}{(a''b'')} & (a'b') & (ab) \\ y''i'' & y'i' & yi \end{bmatrix}^{(3)}_{q^{-1}} \tag{4.5a}$$

$$= (-1)^{\varphi_{32}+t-1+i'+z'} q^{3y'/2} \left(\frac{[2i''+1]d_3[ab]}{[2i+1]d_3[a''b'']} \right)^{1/2} \times \begin{bmatrix} (a'b') & (ba) & \overset{t}{(b''a'')} \\ y'i' & -yi & -y''i'' \end{bmatrix}^{(3)}_{q^{-1}}, \tag{4.5b}$$

but in this case we are also transposing the multiplicity label t of the tensor operator of rank $(a''b'')$, together with selection rules (1.7). Hence, this operation means transition to a labeling scheme[22] different from the canonical one, similar to transition between two versions of the paracanonical[22,23] labeling or between six versions of the pseudocanonical[22] labeling. We are not able to specify phases φ_{12} and φ_{32} until we have concrete applications of (4.5a) and (4.5b) with fixed phase systems of these new labeling schemes.

Invariance in the absolute value of SU(3) 3-j coefficients under transposition of the irrep parameters, without special attachment to any definite labeling scheme, was usual according to de Swart,[40] although Derome[32] warned care should be taken when some transposed irreps are equivalent. Transposition of the isofactor parameters and multiplicity label, together with the change of its labeling scheme, was also used for the different labeling schemes[22,23] of the SU(3) isofactors and may be used without restriction (but with some distrust if irreps before and after transposition coincide) for isofactors of arbitrary non-multiplicity-free group, derived by means of the definite Gram–Schmidt process. Similar to any transformation of an arbitrary vector together with its coordinate system, these two dual operations both together give an identity (up to a possible sign change) and always may be associated[30] with the one-dimensional irrep of S_3, although the proof presented in Ref. 30 is unquestionable only when the below-discussed distinctive (splitting) conditions (factually always associated with a definite Gram–Schmidt process) are not spoiled. Nevertheless, it is not evident how the operations of different nature (4.2a), (4.2b), (4.5a), and (4.5b) (which leave invariant or change the labeling scheme) may be joined into a single representation of S_3, since unambiguous Derome's[32] character analysis of the S_3 or S_2 irreducible structure cannot be applied to relations (4.5a) or (4.5b) [unlike as to Eqs. (4.2a) or (4.2b)] (neither zeros of isofactors may be predicted).

Otherwise, instead of Eq. (4.5a) or (4.5b), we may write the numerical symmetry relations[29,30]

$$\begin{bmatrix} (a'b') & \overset{t}{(a''b'')} & (ab) \\ y'i' & y''i'' & yi \end{bmatrix}^{(3)}_{q} = \sum_{t'} B_{t,t'} (-1)^{i'+i''-i} \begin{bmatrix} (a''b'') & \overset{t'}{(a'b')} & (ab) \\ y''i'' & y'i' & yi \end{bmatrix}^{(3)}_{q^{-1}}, \tag{4.6a}$$

$$= \sum_{t''} \widetilde{B}_{t,t''} (-1)^{i'+z'} q^{3y'/2} \left(\frac{[2i''+1]d_3[ab]}{[2i+1]d_3[a''b'']} \right)^{1/2} \times \begin{bmatrix} (a'b') & \overset{t''}{(ba)} & (b''a'') \\ y'i' & -yi & -y''i'' \end{bmatrix}^{(3)}_{q^{-1}}, \tag{4.6b}$$

preserving the canonical (or other fixed) labeling scheme. When irreps before and after transposition coincide, the orthogonal (unitary) expansion matrices $B_{t,t'}$ and/or $\widetilde{B}_{t,t''}$ are representation matrices[32,41] with definite S_2 or S_3 irreducible (or reducible) structure, similar to the antidiagonal transition matrices in the case of the odd permutations for the external labeling scheme of Ref. 39. (Note that for isofactors of some groups[32] the two-dimensional irreducible representation of S_3 may also appear.)

As the simplest situation with non-trivial transition matrices $B_{t,t'}$ and $\widetilde{B}_{t,t''}$, the following example may be considered: In agreement with the presented-above and transposed conditions (1.7b) and (1.7c) and tabulated[19] expressions of the $u_q(3)$ canonical tensor operators, we may write the following evident relations:

$$\begin{bmatrix} & \overset{t=2}{} & \\ (2\ \ 1) & (1\ \ 1) & (2\ \ 1) \\ \frac{1}{3}\ \frac{3}{2} & 00 & \frac{1}{3}\ \frac{3}{2} \end{bmatrix}^{(3)}_{q} \neq 0, \quad \begin{bmatrix} & \overset{t=2}{} & \\ (2\ \ 1) & (1\ \ 1) & (2\ \ 1) \\ \frac{1}{3}\ \frac{3}{2} & 01 & \frac{1}{3}\ \frac{1}{2} \end{bmatrix}^{(3)}_{q} = 0, \tag{4.7a}$$

$$\begin{bmatrix} & \overset{t=2}{} & \\ (1\ \ 1) & (2\ \ 1) & (2\ \ 1) \\ 00 & \frac{1}{3}\ \frac{3}{2} & \frac{1}{3}\ \frac{3}{2} \end{bmatrix}^{(3)}_{q} = 0, \quad \begin{bmatrix} & \overset{t=2}{} & \\ (1\ \ 1) & (2\ \ 1) & (2\ \ 1) \\ 01 & \frac{1}{3}\ \frac{3}{2} & \frac{1}{3}\ \frac{3}{2} \end{bmatrix}^{(3)}_{q} \neq 0, \tag{4.7b}$$

when for a ''transposed'' canonical labeling scheme we obtain

$$\begin{bmatrix} \overset{t=2}{} & & \\ (2\ \ 1) & (1\ \ 1) & (2\ \ 1) \\ \frac{1}{3}\ \frac{3}{2} & 00 & \frac{1}{3}\ \frac{3}{2} \end{bmatrix}^{(3)}_{q} = 0, \quad \begin{bmatrix} \overset{t=2}{} & & \\ (2\ \ 1) & (1\ \ 1) & (2\ \ 1) \\ \frac{1}{3}\ \frac{3}{2} & 01 & \frac{1}{3}\ \frac{3}{2} \end{bmatrix}^{(3)}_{q} \neq 0, \tag{4.7c}$$

$$\begin{bmatrix} \overset{t=2}{} & & \\ (1\ \ 1) & (2\ \ 1) & (2\ \ 1) \\ 00 & \frac{1}{3}\ \frac{3}{2} & \frac{1}{3}\ \frac{3}{2} \end{bmatrix}^{(3)}_{q} \neq 0, \quad \begin{bmatrix} \overset{t=2}{} & & \\ (1\ \ 1) & (2\ \ 1) & (2\ \ 1) \\ 01 & \frac{1}{3}\ \frac{3}{2} & \frac{1}{3}\ \frac{3}{2} \end{bmatrix}^{(3)}_{q} = 0. \tag{4.7d}$$

Hence, we verify that even 2×2 matrix $B_{t,t'}$ is non-diagonal. A similar situation [and non-diagonal matrix $B_{t,t'}$ in (4.6a)] occurs for the $u_q(3)$ canonical isofactors with $(a''b'')=(1\ 1)$, $(a'b')=(a\ \ b)$, $a>1$, $b\geqslant 1$ or $a\geqslant 1$, $b>1$, with exception of the $a=b$ case for SU(3).

Favorably for the SU(3) and $u_q(3)$ canonical labeling scheme (but never for the non-trivial cases of the paracanonical[22,23] and some other labeling schemes), these expansion matrices $B_{t,t'}$ are usually diagonal for an elementary transposition (odd permutation) of the coinciding irreps in the canonical isofactors and always diagonal (what will be proved below) when the all three irreps in the canonical 3-j coefficient of SU(3) or $u_q(3)$ are equivalent. Otherwise, the antidiagonal form of the expansion matrices for the odd permutations of the SU(3) isofactors in the labeling scheme of Ref. 25 ensures the appearance of the two-dimensional reducible representations and solely one-dimensional irreps of S_3 for the all values of representation parameters of the SU(3) isofactors, in addition to the special cases, considered by Derome.[32]

Moreover, the sufficient conditions of the one-to-one correspondence between the isofactors on the lhs and the rhs of (4.6a) and (4.6b), labeled by t and t' [associated, respectively, with irreps $(a''b'')$ and $(a'b')$ and taking values, as a rule, in the different intervals], may be strictly formulated for the SU(3) and $u_q(3)$ canonical tensor operators. For this purpose, let us reconsider

conditions (1.7b) and (1.7c). Following Hecht[20] and Refs. 8, 22, and 30, it may be supposed that for a given triplet $(a'b')(a''b'')(a\ \ b)$ of SU(3) or $u_q(3)$ irreps at least one triplet of the basis state labels (the initiation point) exists, for which only a single value of the external multiplicity label with non-vanishing isofactor is possible. (Usually, from such point a Gram–Schmidt process is begun). For example, exactly three initiation points exist for the (non-trivial) paracanonical[22,23] external labeling scheme. For the SU(3) and $u_q(3)$ canonical isofactors, sometimes many such initiation points may be chosen, with the parameters $i',i''_{\mathrm{m}},i,y',y''_{\mathrm{m}},y$, satisfying the following conditions:

$$|i-i'|=i''_{\mathrm{m}}-\mathscr{M}+r, \quad y=y'+y''_{\mathrm{m}} \tag{4.8}$$

and, possibly, forming two isolated sets (for $i-i'>0$ and $i-i'<0$, respectively), when the multiplicities $\mathscr{M}=r$. For example, represented by (4.7) isofactors have more than two initiation points for tensor of rank (1 1) and a mutually shared initiation point for the both tensor operators of rank (2 1).

Specifying the parameters $i=i_{\mathrm{m}}$, $y=y_{\mathrm{m}}$ as in (2.13), (2.14), and (3.1) and taking into account possible additional restrictions in the null space case, we may write condition (4.8) for the first main initiation point as

$$i'_{\mathrm{init.}}=i_{\mathrm{m}}-i''_{\mathrm{m}}+\mathscr{M}-r\geqslant|\hat{z}'|, \quad \hat{z}'=\tfrac{1}{2}(b'-a'+v), \quad \text{and } i'_{\mathrm{init.}}\geqslant i''_{\mathrm{m}}-i_{\mathrm{m}}$$
$$\text{if } i_{\mathrm{m}}-i''_{\mathrm{m}}<0 \quad \text{in addition.} \tag{4.9a}$$

Otherwise, condition (4.8) with special parameters $i'=i'_{\mathrm{m}}$, $y'=y'_{\mathrm{m}}$ gives the second main initiation point

$$i_{\mathrm{init.}}=i'_{\mathrm{m}}-i''_{\mathrm{m}}+\mathscr{M}-r\geqslant|\hat{z}|, \quad \hat{z}=\tfrac{1}{2}(b-a-v), \quad \text{and } i_{\mathrm{init}}\geqslant i''_{\mathrm{m}}-i'_{\mathrm{m}} \quad \text{if } i'_{\mathrm{m}}-i''_{\mathrm{m}}<0 \quad \text{in addition.} \tag{4.9b}$$

However, the above discussed problems with the normalization factor (3.7b) or (3.14b) are caused by the absence of some initiation points. We see that such triplets $(a'b'),(a''b''),(a\ \ b)$ of SU(3) or $u_q(3)$ irreps are also possible, for which the initiation points of the canonical splitting scheme are missing, since neither (4.8), nor at least (4.9a) or (4.9b) may be satisfied. [Of course, the initiation points presented as (3.1)–(3.3) of Ref. 30, perhaps with intention to escape the ambiguities of attaching the operator pattern to the first or third irrep, may also be non-existent, when $a''+b''>a+b$ and $a''+b''>a'+b'$ without the null space situation.] Contrary to the paracanonical and pseudocanonical isofactors[22,23] (for which the numerical transitions from the biorthogonal to orthogonal sets are always possible), the canonical isofactors cannot always be obtained immediately from the bilinear combinations of isofactors (solving the triangular systems of equations in numerical or analytical forms, i.e., by a Gram–Schmidt process) but only by an analytical continuation procedure (extrapolation) from the region with infinite (but countable) number of points, in which initiation points are existing. (Note that the numerical approach of Draayer and Akiyama[42] and its analytical generalization[8] are independent of our initiation problem.)

Using array (1.3b), together with its equidistantness properties (1.3c) and relations

$$i_{\mathrm{m}}-i''_{\mathrm{m}}=\tfrac{1}{2}(r_{111}-r_{331}), \quad \hat{z}'=\tfrac{1}{2}(r_{131}-r_{311}),$$

$$i'_{\mathrm{m}}-i''_{\mathrm{m}}=\tfrac{1}{2}(r_{111}-r_{221}), \quad \hat{z}=\tfrac{1}{2}(r_{121}-r_{211}),$$

it may be shown that the initiation points of each [either (4.9a) or (4.9b)] type may disappear and the nearest allowed value of $\hat{i}'_{\mathrm{min}}>i'_{\mathrm{init.}}$ or $\hat{i}_{\mathrm{min}}>i_{\mathrm{init.}}$ (with the remaining parameters chosen as above) is not distinctive (i.e., not sufficient) for the canonical labeling of the external multiplicity

with fixed position of the tensor operator labels. For example, only one initiation point from two sets exists when non-diagonal parameter $r_{13\gamma}$ (respectively, $r_{12\gamma}$, or $r_{31\gamma}$, or $r_{21\gamma}$) from array (1.3b) strictly exceeds eight remaining parameters $r_{\alpha\beta\gamma}$ in the same layer of (1.3b). Separately for concrete versions of $\mathscr{M}-r$ we also prove that both inequalities (4.9a) and (4.9b) have no solutions when non-diagonal parameter $r_{32\gamma}$, i.e., b'' or $b''+v$ (or, respectively, $r_{23\gamma}$, i.e., a'' or $a''-v$), strictly exceeds eight remaining parameters $r_{\alpha\beta\gamma}$ in the same layer of (1.3b), i.e.,

$$r_{32\gamma}>r_{\alpha\beta\gamma}>0 \quad \text{unless} \quad \alpha=3,\ \beta=2 \quad \text{both together}, \tag{4.10a}$$

or

$$r_{23\gamma}>r_{22\gamma}, \quad r_{23\gamma}>r_{33\gamma}, \quad r_{23\gamma}>r_{21\gamma}, \quad r_{23\gamma}>r_{13\gamma}. \tag{4.10b}$$

(The both conditions, for maximal $r_{32\gamma}$ and for maximal $r_{23\gamma}$, are written above in the different, but equivalent forms).

Hence, we found the regions of the irrep parameters $(a'b')(a''b'')(a\ \ b)$, for which conditions (1.7a)–(1.7c) are not sufficient for the canonical splitting. We see that initiation points may be absent without the null space situation for parameters $r_{1\beta\gamma}$ or $r_{\alpha1\gamma}$ accepting intermediate values, respectively, between $r_{2\beta\gamma}$ and $r_{3\beta\gamma}$, or between $r_{\alpha2\gamma}$ and $r_{\alpha3\gamma}$, for example, in the case of the coproduct decomposition $(12)\otimes(31)\to(21)$ or $(24)\otimes(51)\to(42)$. Using recursive construction (2.13) of Ref. 8 [which is equivalent for $t=\mathscr{M}$ with algorithm of Draayer and Akiyama[42] in the SU(3) case], we see that isofactor

$$\begin{bmatrix} & \overset{t}{} & \\ (1\ \ 2) & (3\ \ 1) & (2\ \ 1) \\ -\frac{1}{3}\,\frac{1}{2} & \frac{2}{3}\,2 & \frac{1}{3}\,\frac{3}{2} \end{bmatrix}^{(3)}_{q} \tag{4.11a}$$

does not vanish for the both values of the multiplicity label $t=1,2$. Of course, their parameters with the maximal shift $|i'-i|=2$ are impossible and system of equations (2.13) is unsolvable in terms of the canonical isofactors, without using results of Sec. III. Otherwise, labels of (4.11a) corresponds to an initiation point, associated with the last tensor of rank $(2\ \ 1)$ or, respectively, with the isofactor

$$\begin{bmatrix} & \overset{t=1}{} & \\ (1\ \ 2) & (1\ \ 2) & (1\ \ 3) \\ -\frac{1}{3}\,\frac{1}{2} & -\frac{1}{3}\,\frac{3}{2} & -\frac{2}{3}\,2 \end{bmatrix}^{(3)}_{q}. \tag{4.11b}$$

Since (4.11a) has a definite symmetry, described by (4.2b), the transposition matrix $B_{t,t'}$ of (4.6a) for (4.11b) [and in the all cases, described by the conditions (4.10a) or (4.10b)] is non-diagonal, in spite of the coinciding first and second irreps, and corresponds to a reducible representation of S_2 according Derome.[32]

Therefore, dependency (4.10a) or (4.10b) between the isofactor parameters forbids any symmetries associated with the interchange of the SU(3) tensor operator and initial or final labels, even if the corresponding irreducible representations coincide. For example, recursive construction (2.13) of Ref. 8 (equivalent with the approach of Ref. 42) never gives 0 for isofactors

$$\begin{bmatrix} & \overset{t=2}{} & \\ (3\ \ 2) & (3\ \ 2) & (5\ \ 3) \\ \frac{1}{3}\,\frac{5}{2} & \frac{1}{3}\,\frac{5}{2} & \frac{2}{3}\,i \end{bmatrix}^{(3)} \quad (1\leqslant i\leqslant 4), \tag{4.11c}$$

which should appear at least for two values of i in the case of diagonal matrix $B_{t,t'}$ in (4.3c). Thus, the canonical resolution of the SU(3) external multiplicity problem sometimes is not optimal with respect to Derome's[32] approach.

Let us consider another concrete example of the irrep parameters with absent initiation points of the canonical isofactors. We take the canonical tensor operator of rank (6 4) for the coproduct decomposition $(2\ 4)\otimes(6\ 4)\rightarrow(3\ 3)$, with non-vanishing isofactors for $t=4$ and 5. The initiation points for the tensor operators of the rank (3 3) and (2 4) exist (but are not common for the both operators) and correspond to the isofactors of the alternative labeling schemes

$$\begin{bmatrix} & \overset{1}{} & \\ (2\ 4) & (6\ 4) & (3\ 3) \\ -\frac{1}{3}2 & \frac{1}{3}5 & 0\ 3 \end{bmatrix}_q^{(3)} \quad \text{and} \quad \begin{bmatrix} \overset{1}{} & & \\ (2\ 4) & (6\ 4) & (3\ 3) \\ -\frac{1}{3}3 & \frac{1}{3}5 & 0\ 2 \end{bmatrix}_q^{(3)}. \tag{4.12a}$$

The corresponding canonical isofactors cannot be extracted immediately from the bilinear combinations of the type (2.14) by any Gram–Schmidt process, but generalized to $u_q(3)$ recursive construction (2.13) of Ref. 8 (see also Ref. 42) may be useful, when applying our Eq. (2.14) for normalization (unless the q-analog for the denominator function[5,7] will be derived). This construction, together with non-vanishing values of the multiplicity-free isofactors[13]

$$\begin{bmatrix} (2\ 4) & (2\ 0) & (3\ 3) \\ -\frac{1}{3}2 & \frac{1}{3}1 & 0\ 3 \end{bmatrix}_q^{(3)} \quad \text{and} \quad \begin{bmatrix} (2\ 4) & (2\ 0) & (3\ 3) \\ -\frac{1}{3}3 & \frac{1}{3}1 & 0\ 2 \end{bmatrix}_q^{(3)}, \tag{4.12b}$$

allows us to prove that

$$\begin{bmatrix} & \overset{t=5}{} & \\ (2\ 4) & (6\ 4) & (3\ 3) \\ -\frac{1}{3}2 & \frac{1}{3}5 & 0\ 3 \end{bmatrix}_q^{(3)} \neq 0, \quad \begin{bmatrix} & \overset{t=5}{} & \\ (2\ 4) & (6\ 4) & (3\ 3) \\ -\frac{1}{3}3 & \frac{1}{3}5 & 0\ 2 \end{bmatrix}_q^{(3)} \neq 0. \tag{4.12c}$$

Finally, the absence of the initiation points for this case of the canonical coupling is also proved, taking into account that triplets satisfying (4.8) (1, 5, 3 or 3, 5, 1) are not allowed.

Similar to formula (3.6) with inserted Eq. (3.8) and the non-singular version of the denominator function (3.14b), expression (4.7) of Ref. 43 for the SU(3) isofactors with extreme shifts of the SU(2) irreps [or Eq. (5.8) of Ref. 8 which, nevertheless, is correct] may give zero for parameters satisfying conditions (4.10a) or (4.10b) [e.g., for triplet $(2\ 4)\otimes(6\ 2)\rightarrow(4\ 2)$], without the null space situation of the canonical tensor operator. Hence, we conclude that the null space of SU(3):U(2) and $u_q(3):u_q(2)$ projective operators may exceed the null space of the SU(3) and $u_q(3)$ canonical tensor operators, contrary to Lemma 1.1 and Theorem 1.1 of Ref. 6. Since the tertium non datur principle now is questionable in the proof of Theorem 1.2 of Ref. 6, the defining conditions (1.26b) of the canonical tensor operators[6] should be replenished. Particularly, now it is not evident that the isofactor vanishing condition (1.7a) is completely determined by the null space inclusion property $\mathcal{N}_1 \supset \mathcal{N}_2 \supset \cdots \supset \mathcal{N}_{\mathcal{M}}$, just together with the conjugation invariance, without any supplementary condition. Paradoxically, we see that construction (2.13) of Ref. 8 is conjugation invariant (up to sign) independently on its orthogonality, as well as the isofactors on the left-hand and right-hand sides of Eqs. (4.6a) and (4.6b), although matrices $B_{t,t'}$ and $\widetilde{B}_{t,t''}$ may be non-diagonal. The author did not find any reason why some unitary transformation with the non-diagonal matrix elements, vanishing on the disjunctive complement of $\mathcal{N}_{t'}$ in $\mathcal{N}_t$, for $t'>t$ cannot be invented, similar to the transformation between the canonical and pseudocanonical isofactors.

Hence, together with the arguments versus the null space inclusion property being sufficient for the canonical splitting, the author understood that the SU(3) isofactors with $t\neq 1$ or $\mathcal{M}$,

constructed by means of (2.13) of Ref. 8, may be non-orthogonal. Besides, the Gram–Schmidt process begun from $t=1$ (actually from $t=2$) spoils for $\mathscr{M}>2$ (when the set of isofactors is overcomplete), the null space inclusion property [perhaps, with exception of the rank (2 2) case]. [In this last case, (2.13) of Ref. 8 does not contradict with the results, tabulated in Ref. 44, but the null spaces also coincide.] The overlaps of the SU(3) isofactors from Ref. 8 were considered for the tensor operators of the multiplicity 4 and rank (3 3) and were expanded in terms of the overlaps (3.6) of the dual (biorthogonal) SU(3) coupled states[22] by means of the expansion coefficients (5.1) from Ref. 8 and expressed in terms of polynomials and linear functions in a,b by means of the computer algebra. Since the non-diagonal overlaps with unequal $t=2,3,4$ were expressed purely in terms of the linear functions in a,b, without any non-trivial polynomials, our approach of Ref. 8 does not seem hopeless for the final explicit construction of the SU(3) and $u_q(3)$ canonical tensor operators.

We see that some oversights of Ref. 8 and Refs. 6 and 30 are ''dual'' in a similar sense as the biorthogonal coupled bases:[22] the bases with subscripts are overcomplete and the bases with superscripts present additional definition problems. Hence, our Eq. (2.13) and the corresponding algorithm from Ref. 30, or used in Sec. VI of Ref. 22 distinctive conditions (6.1a,b), do not ensure sometimes the null space inclusion properties, when the corresponding initiation points are not correlated as above with the canonical splitting. Nevertheless, our Eq. (2.13) is overcomplete for the algorithm, consistent with the Braunschweig conjecture.[45,46] Particularly, the Williams[46] construction of the orthogonal SU(3) coupling coefficients is also equivalent to the numerical Gram-Schmidt procedure, whose initiation points may be either associated with some ''transposed'' version of the canonical labeling scheme [in analogy with (1.9), or (4.9a,b)], or may not be correlated with any considered analytical solution of the external multiplicity problem (although isofactors with the coinciding irreps should be equivalent up to sign with the canonical ones for the multiplicity 2). The above presented arguments may show some transposition symmetry of the coupling coefficients[46] being not universal, although the alternative symmetry relations[46] under definite restrictions may be equivalent to our results.

It is evident that matrix $B_{t,t'}$ accepts in (4.6a) a shift-diagonal form, if the initiation points for the tensor operators of rank $(a''b'')$ and $(a'b')$ are mutually related by the same transposition $(a'b')\leftrightarrow(a''b'')$. This is possible when $i'_{\mathrm{m}}-i''_{\mathrm{m}}-\mathscr{M}+r=i''_{\mathrm{m}}-i'_{\mathrm{m}}$, or in the inverse situation (appearing after the transposition), also when the null space appears before and/or after transposition (and Lemma 1.1 of Ref. 6 is valid). Thus, relation (4.6a) may be reduced to the phase factor when diagonal parameter $r_{33\gamma}$ of array (1.3b) exceeds all the remaining parameters of the same layer:

$$r_{33\gamma}\geqslant r_{\alpha\beta\gamma} \tag{4.13a}$$

with the corresponding shift $r_{11\gamma}-r_{22\gamma}$ or $r_{22\gamma}-r_{11\gamma}$ between t and t'. Similarly, the transposition $(b\ \ a)\leftrightarrow(a''b'')$ [with the antidiagonal transposition of the both layers of array (1.3b)] gives only phase factor in (4.6b) when

$$r_{22\gamma}\geqslant r_{\alpha\beta\gamma} \tag{4.13b}$$

with the corresponding shift $\pm\,2(i_{\mathrm{m}}-i''_{\mathrm{m}})$ of t. Supremacy of the parameter $r_{11\gamma}$ determines the possibility of transposition $(b'a')\leftrightarrow(a\ \ b)$ for the external multiplicity label, associated with tensor operator of rank $(a'b')$ or $(a\ \ b)$. Relations (4.13a) and (4.13b) turn into equalities and determine the S_3 transposition invariance (up to sign) of the SU(3) or $u_q(3)$ canonical 3-j coefficients, when the all three irreps are equivalent. Of course, conditions (4.13a) and (4.13b) are satisfied and Lemma 1.1 of Ref. 6 is not violated for the self-conjugated tensor operators with $v=0$ and in some their vicinity.

The vanishing (non-vanishing) properties of the canonical SU(3) isofactors with coinciding parameters allows us to fix some phases also in (4.6a) and (4.6b), when $B_{t,t'}$ or $\widetilde{B}_{t,t''}$ are diagonal. For example, non-vanishing of isofactors

$$\begin{bmatrix} & \overset{t=1}{} & \\ (a'b') & (a'b') & (a\ \ b) \\ y'_{\mathrm{m}}i'_{\mathrm{m}} & y'_{\mathrm{m}}i'_{\mathrm{m}} & \frac{2}{3}(b-a)0 \end{bmatrix}^{(3)} \quad \text{for } v=a'-b'=b-a \tag{4.14a}$$

or, in general,

$$\begin{bmatrix} & \overset{t_0}{} & \\ (a'b') & (a'b') & (a\ \ b) \\ y'_{\mathrm{m}}i'_{\mathrm{m}} & y'_{\mathrm{m}}i'_{\mathrm{m}} & 2y'_{\mathrm{m}}\ \ t_0-1 \end{bmatrix}^{(3)} \quad \text{with } t_0=|b'-a'+v|+1 \tag{4.14b}$$

do not contradict with (4.6a), if we include into $B_{t,t'}$ the phase factor $(-1)^{v+t-t_0}$, together with the corresponding shifts of t, determined by (4.13a) and $t_0=\mathscr{M}-r+1$ in the general $[(a'b')\neq(a''b'')]$ case. The same phase factor $(-1)^v$ appears for transposition $1\leftrightarrow 2$ in the multiplicity-free cases, without dependence on condition (4.13a).

We see that alternatives in the symmetry properties of the canonical isofactors and possibilities in abbreviating tables depend on what—diagonal or non-diagonal—position is accepted by the maximal entry of array (1.3b), when the external multiplicity of the SU(3) or $u_q(3)$ tensor operator or in the isofactors is determined by the minimal entry [in the opposite row, column, and layer of subarray (1.5b)]. Note that only diagonal entries belong to two different subarrays $2\times2\times2$ of the type (1.5b), or related with (1.5b) by the corresponding transposition. Remember that the denominator functions[5–7] and the boundary SU(3) isofactors (orthogonalization of which leads in a shortest way to the canonical ones—see Sec. V of Ref. 8) are dermined only for a fixed integer value of at least single entry of subarray (1.5b) and the multiplicity label t. Thus, the interchange of the tensor operator and initial (or, respectively, final) basis labels in the canonical SU(3) or $u_q(3)$ isofactors may give the coinciding (when the Gram–Schmidt processes are allowed before and after transposition) or alternative (transposed) numerical versions of the canonical splitting (with changed position of the tensor operator in its matrix element). The differences of the t shifts after such interchange and the different alternatives between the Gram–Schmidt and analytical continuation processes forbid speaking about the uniqueness of the canonical resolution of the external multiplicity problem analytical in all 12 isofactor parameters, unless (before) the position of the tensor operator in isofactor is fixed. The definition ambiguity of the canonical tensor operators may be excluded, if the null space inclusion property is used together with the linear independence condition of the all non-zero $u_q(3):u_q(2)$ [or SU(3):U(2)] projective operators.

Nevertheless, in addition to the symmetries, induced by conditions (4.13a), and (4.13b), some simple symmetries of the canonical isofactors may be caused by accidental initiation points. For example, vanishing of special SU(3) isofactors

$$\begin{bmatrix} & \overset{t=2}{} & \\ (1\ \ 1) & (a\ \ a) & (a\ \ a) \\ 0\ \ 0 & 0\ \ a & 0\ \ a \end{bmatrix}^{(3)}=0, \quad \begin{bmatrix} & \overset{t=2}{} & \\ (a\ \ a) & (1\ \ 1) & (a\ \ a) \\ 0\ \ a & 0\ \ 0 & 0\ \ a \end{bmatrix}^{(3)}=0 \tag{4.15a}$$

[in accordance with condition (1.7c) in the first case, and in accordance with the conjugation symmetry (4.2a), or with the tabulated isofactor expressions in the second case] induces the complete $S_3\times S_2$ symmetry of the canonical SU(3) isofactors for coupling $(a\ \ a)\otimes(1\ \ 1)\rightarrow(a\ \ a)$. In accordance with (3.18) and (4.2b), accidental initiation points exist also for SU(3) isofactors

$$\left[\begin{array}{ccc} & \overset{t}{} & \\ (1\ \ 2) & (3\ \ 1) & (2\ \ 1) \\ -\frac{1}{3}\frac{3}{2} & \frac{2}{3}\,i'' & \frac{1}{3}\frac{3}{2} \end{array}\right]^{(3)} \tag{4.15b}$$

with $t=1$ and 2 for $i''=0$ (or 2) and 1, respectively [cf. isofactors (4.11a) and (4.11b)].

In general, when all three irreps are self-adjoint, i.e., for coupling $(a'a')\otimes(a''a'')\to(a\ \ a)$, one or two independent versions of the canonical labeling may exist in accordance with satisfied condition (4.13a) or (4.13b). Anyway, the elements of matrices $B_{t,t'}$ and $\widetilde{B}_{t,t''}$ with the positions of different parity in rows and columns are 0, since the transpositions do not mix states with the different irreducible behavior under conjugation. Returning to the triplet of irreps (5 5), (3 3), and (4 4), we may predict that the canonical labeling scheme is completely invariant under transposition for $t=2$, but $t=1$ and $t=3$ states of the rank (3 3) tensor mix after transposition. [There is one-to-one correspondence between the all matrix elements of the rank (4 4) and (5 5) tensors]. However, the symmetries of this type are not satisfied by the corresponding $u_q(3)$ isofactors.

In spite of absent initiation point on the lhs or rhs of Eq. (4.6a) or (4.6b), zeros may be found in unitary matrices $B_{t,t'}$ and $\widetilde{B}_{t,t''}$ from the analysis of the original and transposed conditions (1.7). Distribution and number of zeros depend on the degree to which (4.9a) or (4.9b) are spoiled and determine some restrictions for the remaining non-vanishing matrix elements. For example, isofactor without any initiation point

$$\left[\begin{array}{ccc} & \overset{t}{} & \\ (2\ \ 3) & (4\ \ 2) & (3\ \ 2) \\ -\frac{1}{3}\frac{5}{2} & \frac{2}{3}3 & \frac{1}{3}\,\hat{i} \end{array}\right]^{(3)}_{q} \qquad \left(\hat{i}=\frac{1}{2},\frac{3}{2},\frac{5}{2}\right) \tag{4.16}$$

may be expanded according (4.6a) by means of the matrix $B_{t,t'}$ with $B_{31}=0$ and some dependencies (e.g., $B_{12}B_{23}=B_{13}B_{22}$) between the remaining matrix elements.

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Quantum Clifford algebras from spinor representations

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A general theory of quantum Clifford algebras is presented, based on a quantum generalization of the Cartan theory of spinors. We concentrate on the case when it is possible to apply the quantum-group formalism of bicovariant bimodules. The general theory is then singularized to the quantum SL(n,$\mathbb{C}$) group case, to generate explicit forms for the whole class of braidings required. The corresponding spinor representations are introduced and investigated. Starting from our Clifford algebras we introduce the quantum-Euclidean underlying spaces compatible with different choices of *-structures from where the analogues of Dirac and Laplace operators are built. Using the formalism developed, quantum Spin(n) groups are defined. © *1996 American Institute of Physics.* [S0022-2488(96)01709-4]

I. INTRODUCTION

In this paper we present a general theory of quantum Clifford algebras and spinors based on the incorporation, into the quantum context, of Cartan's theory of spinors.[1,2] Our approach depends essentially on constructing the ''spinor representation'' that would lead us to the proper way of defining the abstract algebra.

In Cartan's classical theory, spinors are considered as elements of the graded exterior algebra over one of the two isotropic subspaces into which the underlying $2n$ or $2n+1$-dimensional Euclidean or pseudo-Euclidean space W decomposes. These two isotropic subspaces are mutually dual and hence we can write $W=V\oplus V'$ for even-dimensional spaces and $W=M\oplus V\oplus V'$ for odd-dimensional spaces, where dim $V=$dim $V'=n$, and dim $M=1$. Spinors are based on V, and if any vector $\mathbf{w}$ in W is written as the unique decomposition $\mathbf{w}=x^0\hat{e}_0+x+f$, where $\hat{e}_0$ is a unit vector in M and $x\in V$, $f\in V'$, then the generators of the Clifford algebra acting on a spinor ξ are determined by the relations

$$H(\mathbf{w})\xi=x\wedge\xi+\iota_f\xi+x^0S\xi, \tag{1}$$

where S is the parity operator which acts on homogeneous spinors $\xi^{(p)}\in V^{\wedge p}$ according to

$$S\xi^{(p)}=(-1)^p\xi^{(p)}. \tag{2}$$

In our quantum construction we shall start from a vector space V endowed with a braiding $\sigma:V^{\otimes 2}\to V^{\otimes 2}$ satisfying the Hecke condition $\sigma^2=(1-q)\sigma+q1$ for some $q\in\mathbb{R}$, such that V and σ

(together with the dual V' and $\mathbb{C}$) with the usual tensor products (and appropriate subspaces and factor-spaces) generate a braided monoidal category. Moreover, we ask that the contraction map between V' and V is functorial [see diagrams (32) and (33)].

We can define $V^{\wedge}$, the exterior braided algebra of V, as $T(V)/J$ where $T(V)$ is the tensor algebra of V and J is the ideal of $T(V)$ generated by $\ker(A)$. Here $A=\Sigma_{k\geqslant 0}^{\oplus}A_k$, and A_k is defined on $V^{\otimes k}$ by $A_k=\Sigma_{\pi\in S_k}(-1)^{l(\pi)}\sigma_\pi$, where σ_π are operators obtained by replacing transpositions in the minimal decomposition of π by the corresponding σ-twists, and $l(\pi)$ is the length of π. We then have $A_k^2=c_kA_k$ with $c_k\neq 0$. Under our assumptions $T(V)=\ker(A)\oplus\mathrm{Im}(A)$, therefore $T(V)/J\simeq\mathrm{Im}(A)$, so we can identify $V^{\wedge}$ with $\mathrm{Im}(A)$, a subspace of $T(V)$. Explicitly, we will assume the following identifications:

$$[\varphi+\ker(A)]\leftrightarrow A(\varphi),$$

where $\varphi\in T(V)$.

This identification allows us to define a transformation $\iota_f:V^{\wedge}\to V^{\wedge}$ for any $f\in V'$ given by $\iota_f(\eta)=\Sigma f(\eta_{i_1})\eta_{i_2}\otimes\cdots\otimes\eta_{i_k}$ for $\eta=\Sigma\eta_{i_1}\otimes\eta_{i_2}\otimes\cdots\otimes\eta_{i_k}$. Having this operation we can define, for any $\mathbf{w}\in W$, an action on $V^{\wedge}$ by means of the relation (1), so we have a map $H:W\to L(V^{\wedge})$. We then find that $Cl(W)$, the algebra generated by $H(W)$, is isomorphic to $T(W)/J$ where J is the ideal generated by the elements $x\otimes y+(1/q)\sigma(x\otimes y)$; $x\otimes f+\sigma(x\otimes f)-\langle\sigma(x\otimes f)\rangle$; $f\otimes x+\sigma^{-1}(f\otimes x)-f(x)$; $f\otimes g+(1/q)\sigma(f\otimes g)$. Here $x,y\in V$; $f,g\in V'$, while $\langle,\rangle:V'\otimes_{\mathbb{C}}V\to\mathbb{C}$ denotes the contraction map and the symbol σ is used for all the braidings in the above-mentioned braided monoidal category.

We recall that $T(W)$ is a *filtered algebra* with filtration

$$T^d(W)=\sum_{i\leqslant d}W^{\otimes i}.$$

This filtration induces a filtration in $Cl(W)$. The corresponding graded algebra

$$\mathrm{gr}[Cl(W)]=\sum{}^{\oplus}Cl(W)^{i+1}/Cl(W)^i,$$

is naturally isomorphic, as a vector space, to $V^{\wedge}\otimes V'^{\wedge}$, while the product is appropriately ''deformed'' with the help of σ.

Moreover, it is possible to introduce a braiding τ in W, which depends exclusively on the initial braiding σ, such that the mentioned graded algebra is isomorphic, in a natural manner, to the corresponding τ-exterior algebra $W^{\wedge}$. From this point of view, our Clifford algebra can be interpreted as a *Chevalley–Kähler-type deformation* of the exterior algebra. It is worth noticing that this fact can be used as a starting point[3] for constructing quantum Clifford algebras, as in the classical theory. Such a generalization of the Chevalley–Kähler construction works for arbitrary braids.

The paper is organized in the following way. In Sec. II we shall review some basic facts about Hecke algebras and quantum groups, which are then applied to the cases of (general) quantum $\mathrm{SL}(n)$ groups. We shall also explain why it is possible to apply the theory of compact quantum groups in the noncompact context. In Sec. III a general theory of quantum Clifford algebras is given, together with some concrete examples and computations. Section IV is devoted to a more detailed study of the spinor representation. We shall prove that this representation is faithful and irreducible, as in the classical theory. Questions related to the spinor scalar product and the associated *-structure on the Clifford algebras will be discussed also. In Sec. V we construct the flip-over operators starting from the fundamental representation of $\mathrm{SL}_q(n,\mathbb{C})$. In Sec. VI we intro-

duce and investigate quantum Euclidean underlying spaces induced by our Clifford algebras. We also discuss different choices of *-structures. Finally, in Sec. VII we use our formalism to describe briefly the general procedure for defining quantum Spin(n) groups.

As a concrete example of constructing the braided monoidal category generated by V, V', $\mathbb{C}$, and $\sigma: V\otimes V\to V\otimes V$, we shall consider the case when a quantum group formalism of bicovariant bimodules can be applied. More specifically, we let G be a quantum group and $\mathscr{A}$ be the associated Hopf algebra of ''polynomial functions'' on G. We then take V as a right $\mathscr{A}$-module and right $\mathscr{A}$-comodule. Under some necessary and sufficient conditions we have that $V\simeq\Gamma_{\text{inv}}$=left invariant elements of a bicovariant bimodule Γ. Then, if in the category of bicovariant bimodules $\mathscr{T}_G$ we take the braided monoidal category generated by Γ, Γ' (dual to Γ), $\mathscr{A}$, (including the appropriate submodules and factor-modules) and consider the left invariant part of the objects of this last category we obtain the required braided monoidal category.

Our approach differs from others appearing in the literature (Refs. 4–6) in that the procedure followed in these papers consists essentially in deforming $Cl(W)$ by stressing its presentation in terms of generators and relations rather than its representation in $V^{\wedge}$. In this case if we consider an appropriate (Hecke) braiding $\sigma: W\otimes W\to W\otimes W$, it is natural to define the corresponding Clifford algebra $\widetilde{Cl}(W)$ as the factor algebra $T(W)/K$ where K is the ideal generated by elements $x\otimes y+(1/q)\sigma(x\otimes y)-(x,y)1$, where $x,y\in W$ and $(,)$ is an appropriate (σ-symmetric) bilinear form. Thus the corresponding graded algebra is simply $W^{\wedge}$. A problem with this approach is that if $W=V\oplus V'$, then it is not possible to have a representation of $\widetilde{Cl}(W)$ a la Cartan, because it is not possible to have that $\sigma(V\otimes V')=V'\otimes V$ and $\sigma(V'\otimes V)=V\otimes V'$ at the same time (the Hecke relation is incompatible with that, if the braid is not symmetric).

Another approach for deforming Clifford algebras is due to Hayashi,[7] where an analogy is made between the usual presentation of $Cl(W)$ by generators and relations with the Chevalley generators of the enveloping algebra $\mathscr{U}(X)$ of a symmetrizable generalized Cartan matrix X. The corresponding quantum Clifford algebra is then obtained in analogy with the quantized enveloping algebra. In this case a representation of the quantum Clifford algebra is given on a usual exterior algebra. The resulting quantum Clifford algebra turns out to be a direct product of classical Clifford algebras. It is worth noticing that our Clifford algebra is also isomorphic to the full endomorphism algebra $L(V^{\wedge})$, via the representation H (if $V^{\wedge}$ is finite dimensional).

It is interesting to consider possible physical applications of the formalism of quantum Clifford algebras from the point of view of introducing ''quantized'' space–time models. Logically, several possibilities are open. Perhaps the most natural approach is to define the corresponding space–time algebra starting from relations defining the quantum Clifford algebra. The space–time algebra is then generated by W, and quadratic relations obtained by requiring that the square of the generic vector from W is the space–time ''distance.'' In this picture the deviation from classical of the generating relations for quantum Clifford algebras is responsible for the noncommutativity of the space–time algebra. However, given a compatible *-structure, the space–time algebra is uniquely fixed. Essentially, it will be a variant of a ''quantum plane.''

On the other hand, it is possible to relax such a relation between the Clifford algebra and the ''space–time,'' and to introduce axiomatically the analogues of spin bundles. The advantage of such approach is in its flexibility, since the ''horizontal'' and the ''vertical'' parts of the formalism become relatively independent. In particular, it is possible to introduce a concept of a classical spinor structure on a quantum space.[8] The material presented here constitutes a base for further studies related to these matters.

II. HECKE ALGEBRAS, BICOVARIANT BIMODULES, AND INTERTWINERS FOR QUANTUM GROUPS

A. On Hecke algebras

Let $q\in\mathbb{C}\setminus\{0\}$ be a complex number and $n\geqslant 2$ an integer. By definition in Ref. 9, the corresponding Hecke algebra $H_{n,q}$ is described by generators $\sigma_1,\ldots,\sigma_{n-1}$ and relations

$$\sigma_i^2=(1-q)\sigma_i+q1, \tag{3}$$

$$\sigma_i\sigma_j=\sigma_j\sigma_i, \quad \text{if } |i-j|\geqslant 2, \tag{4}$$

$$\sigma_i\sigma_{i+1}\sigma_i=\sigma_{i+1}\sigma_i\sigma_{i+1}. \tag{5}$$

In what follows, it will be assumed that $q>0$. The algebra $H_{n,q}$ is finite dimensional, moreover $\dim H_{n,q}=n!$. It can be understood as a deformation of the functional algebra of the symmetric group S_n. A natural basis in $H_{n,q}$ is given by elements $([\pi]_q)_{\pi\in S_n}$, where $[\pi]_q$ denotes the element obtained by replacing transpositions in a *minimal* decomposition of the permutation π with the corresponding generators σ_i.

In this article Hecke algebras will appear via their representations, which will be of the following particular kind: Let V be a vector space and $\sigma: V\otimes V\to V\otimes V$ be an arbitrary braid operator satisfying the Hecke relation of the form (3). Then there exists the unique representation D_σ of the algebra $H_{n,q}$ in the space $V^{\otimes n}$ satisfying $D_\sigma(\sigma_i)=id^{i-1}\otimes\sigma\otimes id^{n-i-1}$. For our purposes, we shall further assume that the space V is a carrier of an irreducible representation υ of an appropriate quantum group G, such that σ intertwines the square of this representation. This condition will ensure that all entities constructed intrinsically from V and σ are G-covariant, in a natural manner. In fact, we shall go beyond this and assume that V, υ, and σ are interpretable in the framework of the theory of bicovariant bimodules[10] over G. More precisely, it will be assumed that V consists of left-invariant elements of some bicovariant bimodule Γ over G such that the representation υ can be viewed as the restriction of the right action of G on Γ, and such that σ becomes (the ''left-invariant part'' of) the canonical flip-over operator.

In our considerations, the main object associated to σ and V will be the corresponding *braided exterior algebra* $V^\wedge$. This algebra can be described as the factor algebra of the tensor algebra $V^\otimes$ through the ideal J generated by $\ker(I-\sigma)$. This ideal coincides with the kernel of the corresponding ''total antisymmetrizer'' $A: V^\otimes\to V^\otimes$, which is explicitly given by

$$A=\sum_{n\geqslant 0}^{\oplus} A_n,$$

where $A_n: V^{\otimes n}\to V^{\otimes n}$ are operators given by

$$A_n=\sum_{\pi\in S_n}(-1)^{l(\pi)}\sigma_\pi,$$

and σ_π are operators obtained by replacing transpositions in the minimal decomposition of π by the corresponding σ-twists. In other words,

$$\sigma_\pi=D_\sigma([\pi]_q).$$

In consequence, the following decomposition holds:

$$V^\otimes=\ker(A)\oplus\mathrm{Im}(A).$$

In fact, due to the Hecke relation, it follows that A is a projection operator, up to a multiplication constant in each $V^{\otimes k}$. Explicitly, we have

$$A_k^2=c_kA_k, \tag{6}$$

where

$$c_k=\left(\sum_{\pi\in S_k} q^{l(\pi)}\right). \tag{7}$$

The algebra $V^{\wedge}$ can be naturally identified, with the help of A, with the space $\mathrm{Im}(A)$. In what follows it will be assumed that the identification

$$V^{\wedge}\ni(\varphi+J)\leftrightarrow A(\varphi)\in V^{\otimes}$$

is made.

It is very important to observe that all our considerations apply for general Hecke braidings (with $q>0$), and in particular it is not necessary to assume that dimensions of braided exterior algebra spaces $V^{\wedge k}$ are classical (for example, classical *symmetric* algebras are included trivially in the procedure).

B. On bicovariant bimodules

In this subsection we shall summarize the most important elements of the theory of bicovariant bimodules over (compact matrix) quantum groups. We shall basically follow Ref. 10, in a slightly different notation.

1. Structure of bicovariant bimodules

Let Γ be a bicovariant bimodule over G, and let ${}_\Gamma\phi:\Gamma\to\Gamma\otimes\mathscr{A}$ and $\phi_\Gamma:\Gamma\to\mathscr{A}\otimes\Gamma$ be the right and the left action of G on Γ, respectively. These maps satisfy the following identities

$$(id\otimes\epsilon)_\Gamma\phi=id, \tag{8}$$

$$(\epsilon\otimes id)\phi_\Gamma=id, \tag{9}$$

$${}_\Gamma\phi(a\theta)=\phi(a)_\Gamma\phi(\theta), \tag{10}$$

$${}_\Gamma\phi(\theta a)={}_\Gamma\phi(\theta)\phi(a), \tag{11}$$

$$\phi_\Gamma(a\theta)=\phi(a)\phi_\Gamma(\theta), \tag{12}$$

$$\Phi_\Gamma(\theta a)=\phi_\Gamma(\theta)\phi(a), \tag{13}$$

$$(id\otimes\phi)_\Gamma\phi=({}_\Gamma\phi\otimes id)_\Gamma\phi, \tag{14}$$

$$(\phi\otimes id)\phi_\Gamma=(id\otimes\phi_\Gamma)\phi_\Gamma, \tag{15}$$

$$(\phi_\Gamma\otimes id)_\Gamma\phi=(id\otimes_\Gamma\phi)\phi_\Gamma. \tag{16}$$

Let $V=\Gamma_{\mathrm{inv}}$ be the space of left-invariant elements of Γ. The space V possesses a natural right $\mathscr{A}$-module structure. This structure is given by

$$\theta\circ a=\kappa(a^{(1)})\theta a^{(2)}, \tag{17}$$

where $\kappa:\mathscr{A}\to\mathscr{A}$ is the antipode map. Equivalently, we have

$$\theta\circ a=P(\theta a), \tag{18}$$

where $P:\Gamma\to V$ is the canonical projection onto left-invariant elements. This map is given by

$$P(\varphi)=\sum_i \kappa(a_i)\varphi_i,$$

where $\Sigma_i a_i\otimes\varphi_i=\phi_\Gamma(\varphi)$.

The space V is right-invariant in the sense that

$$_\Gamma\phi(V)\subseteq V\otimes\mathscr{A}. \tag{19}$$

Let $v:V\to V\otimes\mathscr{A}$ be the restriction of $_\Gamma\phi$ on V. This map is a representation of G (in other words V is a right $\mathscr{A}$-comodule).

The module and comodule structures on V are mutually related in the following way:

$$v(\theta\circ a)=\sum_k (\theta_k\circ a^{(2)})\otimes\kappa(a^{(1)})c_k a^{(3)}, \tag{20}$$

where

$$v(\theta)=\sum_k \theta_k\otimes c_k. \tag{21}$$

The map $I:\mathscr{A}\otimes V\to\Gamma$ given by

$$I(a\otimes\theta)=a\theta \tag{22}$$

is a left $\mathscr{A}$-module isomorphism. If we identify the two spaces (with the help of I), then the right $\mathscr{A}$-module structure on Γ is given by

$$(a\otimes\theta)b=ab^{(1)}\otimes(\theta\circ b^{(2)}). \tag{23}$$

Further, left and right actions of G on Γ are given by

$$\phi_\Gamma(a\otimes\theta)=a^{(1)}\otimes a^{(2)}\theta, \tag{24}$$

$$_\Gamma\phi(a\otimes\theta)=\sum_k a^{(1)}\otimes\theta_k\otimes a^{(2)}c_k. \tag{25}$$

Consequently, Γ is completely determined by $(V,v,\circ)$.

Let $\sigma:V\otimes V\to V\otimes V$ be (the left-invariant part of) the canonical flip-over operator.[10] The following identities hold:

$$\sigma(\eta\otimes\theta)=\sum_k \theta_k\otimes(\eta\circ c_k), \tag{26}$$

$$\sigma^{-1}(\theta\otimes\eta)=\sum_k [\eta\circ\kappa^{-1}(c_k)]\otimes\theta_k. \tag{27}$$

The map σ intertwines the square $v^2:V\otimes V\to V\otimes V\otimes\mathscr{A}$ with itself.

2. Reconstruction problematics

Let V be a vector space, $v:V\to V\otimes\mathscr{A}$ be a representation of G on V, and $\circ$ be a right $\mathscr{A}$-module structure on V. Let us assume that (20) holds, and let us define a left $\mathscr{A}$-module Γ as the free structure $\Gamma=\mathscr{A}\otimes V$.

It then follows that formula (23) defines a right module structure on Γ, while formulas (24) and (25) define the left and the right action of G on Γ. Endowed with all these structures, Γ becomes a bicovariant bimodule. Moreover, $V=\Gamma_{\text{inv}}$ and the initial $\circ$ and v are understood as associated right $\mathscr{A}$-module and comodule structures on V, respectively. In such a way, the circle is closed.

3. Some technical criteria for compatibility between the module and the comodule structure on V

Let us assume that a (finite-dimensional) vector space V is endowed with a right $\mathscr{A}$-comodule structure $v:V\to V\otimes\mathscr{A}$ as well as with a right $\mathscr{A}$-module structure $\circ$. Let $\sigma:V\otimes V\to V\otimes V$ be a linear map given by (26). This map is always bijective (independently of mutual compatibility between $\circ$ and v) and its inverse is given by (27).

Let us assume that the matrix elements of the representation v together with the matrix elements of the contragradient representation $\kappa(v)^{\mathrm{T}}$ generate the algebra $\mathscr{A}$.

Lemma II.1: The following conditions are equivalent:

(i) Equality (20) holds for each $\theta\in V$ and $a\in\mathscr{A}$.

(ii) The map σ intertwines v^2.

Proof: If equality (20) holds, then $\Gamma=\mathscr{A}\otimes V$ becomes in a natural manner a bicovariant bimodule over G and σ becomes its canonical flip-over operator. Therefore (ii) holds.

Conversely, let us assume that (ii) holds.

Let us fix a basis $e_1,\ldots e_n\in V$. Matrix elements v_{ij} of v are given by

$$v(e_i)=\sum_j e_j\otimes v_{ji}. \tag{28}$$

The intertwining property of σ can be expressed as

$$v^{\otimes 2}\sigma(e_i\otimes e_j)=\sum_k v^{\otimes 2}[e_k\otimes(e_i\circ v_{kj})]=\sum_{k,n}(e_n\otimes v_{nk})v[e_i\circ v_{kj}]=(\sigma\otimes id)v^{\otimes 2}(e_i\otimes e_j)$$

$$=\sum_{k,l}\sigma(e_k\otimes e_l)\otimes v_{ki}v_{lj}=\sum_{k,l,n}e_n\otimes(e_k\circ v_{nl})\otimes v_{ki}v_{lj}.$$

In other words,

$$\sum_{k,l}(e_k\circ v_{nl})\otimes v_{ki}v_{lj}=\sum_k(1\otimes v_{nk})v[e_i\circ v_{kj}].$$

Now multiplying by $1\otimes\kappa(v_{mn})$ both sides, and summing over the n we obtain

$$\sum_{k,l,n}(e_k\circ v_{nl})\otimes\kappa(v_{mn})v_{ki}v_{lj}=v[e_i\circ v_{mj}].$$

Hence, (20) holds for all a of the form v_{ij}.

Similarly, using (26) and the intertwining property of σ^{-1} we conclude that (20) holds for all a of the form $\kappa^{-1}(v_{ij})$. To complete the proof it is sufficient to observe that v_{ij} and $\kappa^{-1}(v_{ij})$ generate $\mathscr{A}$, and that if (20) holds for $a,b\in\mathscr{A}$, then it holds also for $a+\alpha b$ and ab.

Let us now assume that the matrix elements v_{ij} are mutually linearly independent.

Lemma II.2: If (20) holds for each $a\in\mathscr{A}$ and for one nonzero vector $\theta\in V$, then it holds for all vectors θ (and for all $a\in\mathscr{A}$).

Proof: Without a lack of generality we can assume that $\theta=e_i$, for some fixed i. Equation (20) (for this choice of θ) implies

$$(1\otimes a^{(1)})v(e_i\circ a^{(2)})(1\otimes\kappa(a^{(3)}))=\sum_j (e_j\circ a)\otimes v_{ji}.$$

Acting by $v\otimes id$ on both sides of the above equality, and using the comodule property and (20) we obtain

$$\sum_{kn} (e_k\circ a^{(4)})\otimes\kappa(a^{(3)})v_{kn}a^{(5)}\otimes a^{(1)}\kappa(a^{(2)})v_{ni}a^{(6)}\kappa(a^{(7)})$$

$$=\sum_{kn} (e_k\circ a^{(2)})\otimes\kappa(a^{(1)})v_{kn}a^{(3)}\otimes v_{ni}=\sum_j v(e_j\circ a)\otimes v_{ji}.$$

Hence

$$v(e_j\circ a)=\sum_k (e_k\circ a^{(2)})\otimes\kappa(a^{(1)})v_{kj}a^{(3)},$$

for an arbitrary j (because of linear independence of the v_{ij}). □

4. The dual bimodule

Assume now that a bicovariant bimodule Γ over G is specified by $(V,v,\circ)$. Then the corresponding *dual bimodule* Γ' can be specified by the triple $(V',v^c,\circ)$ where $v^c:V'\to V'\otimes A$ is the conjugate representation, while $\circ$ is the right $\mathscr{A}$-module structure on V defined by

$$\langle f\circ a,\theta\rangle=\langle f,\theta\circ\kappa^{-1}(a)\rangle. \tag{29}$$

Here, $f\in V'$, $\theta\in V$, and $\langle,\rangle$ is the contraction map. By a straightforward generalization of Woronowicz's considerations, we conclude that for any two bicovariant bimodules Γ_1 and Γ_2 there exists the canonical bimodule isomorphism $\sigma:\Gamma_1\otimes_{\mathscr{A}}\Gamma_2\to\Gamma_2\otimes_{\mathscr{A}}\Gamma_1$. Let V_i be the space of left-invariant elements of Γ_i. The left invariant part of this flip-over operator is an operator σ: $V_1\otimes V_2\to V_2\otimes V_1$, explicitly given by (26), where now $\eta\in V_1$ and $\theta\in V_2$ [with the inverse given by (27)]. Under these conditions all possible braid-type equations are satisfied.

We shall denote by $\mathscr{T}_G$ the *category* of bicovariant bimodules over G. Morphisms in this category are bimodule homomorphisms intertwining the corresponding right and left actions of G. Endowed with canonical braidings, $\mathscr{T}_G$ becomes a *braided monoidal category*.[11] Every *bicovariant algebra* is automatically an algebra in the category $\mathscr{T}_G$ (the product map is functorial with respect to all braidings). In what follows we shall use, without risk of confusion, the same symbol σ for all possible braidings appearing in the category $\mathscr{T}_G$.

If Γ_1 and Γ_2 are bicovariant bimodules determined by $(V_1, v_1, \circ)$ and $(V_2, v_2, \circ)$, respectively, then the product bimodule $\Gamma=\Gamma_1\otimes_{\mathscr{A}}\Gamma_2$ is determined by $(V,v,\circ)$ where $V=V_1\otimes V_2$, while v is the product of v_1 and v_2 and $\circ$ is given by

$$(\theta\otimes\eta)\circ a=(\theta\circ a^{(1)})\otimes(\eta\circ a^{(2)}). \tag{30}$$

If Γ is a bicovariant algebra, then Γ_{inv} is its subalgebra and we have

$$(\theta\eta)\circ a=(\theta\circ a^{(1)})(\eta\circ a^{(2)}), \tag{31}$$

for each θ, $\eta\in\Gamma_{\text{inv}}$.

It is also worth noticing that the contraction map between V and V' is functorial, in a natural manner. In other words,

Lemma II.3. The diagrams

$$\begin{array}{ccccc} V'\otimes & V & \otimes\Psi & \xrightarrow{(\sigma\otimes id)(id\otimes\sigma)} & \Psi\otimes & V' & \otimes V \\ \langle,\rangle\otimes id & \downarrow & & & & \downarrow & id\otimes\langle,\rangle, \\ \mathbb{C} & \otimes & \Psi & \xrightarrow[\cong]{} & \Psi & \otimes & \mathbb{C} \end{array} \tag{32}$$

$$\begin{array}{ccccc} \Psi\otimes & V' & \otimes V & \xrightarrow{(id\otimes\sigma)(\sigma\otimes id)} & V'\otimes & V & \otimes\Psi \\ id\otimes\langle,\rangle & \downarrow & & & & \downarrow & \langle,\rangle\otimes id \\ \Psi & \otimes & \mathbb{C} & \xrightarrow[\cong]{} & \mathbb{C} & \otimes & \Psi \end{array} \tag{33}$$

are commutative. Here $\Psi\in\{V,V'\}$.

Proof: Let us check diagrams (32). Diagrams (33) can be checked similarly. By direct computation we have

$$\begin{aligned} (id\otimes\langle,\rangle)(\sigma\otimes id)(id\otimes\sigma)(f\otimes\theta\otimes\eta) &= (id\otimes\langle,\rangle)(\sigma\otimes id)\Big(f\otimes\sum_l \eta_l\otimes(\theta\circ d_l)\Big) \\ &= (id\otimes\langle,\rangle)\Big(\sum_l \eta_l\otimes(f\circ d_l^{(1)})\otimes(\theta\circ d_l^{(2)})\Big) \\ &= \sum_l \eta_l\otimes\langle f\circ d_l^{(1)},\theta\circ d_l^{(2)}\rangle \\ &= \sum_l \eta_l\otimes\langle f,(\theta\circ d_l^{(2)})\circ\kappa^{-1}(d_l^{(1)})\rangle \\ &= \sum_l \eta_l\otimes\langle f,\theta\circ(d_l^{(2)}\kappa^{-1}(d_l^{(1)}))\rangle \\ &= \sum_l \eta\otimes\langle f,\theta e(d_l)\rangle = \eta\otimes\langle f,\theta\rangle, \end{aligned}$$

where $\Sigma_l \eta_l\otimes d_l = v(\eta)$ or $v^c(\eta)$ depending on the choice of Ψ. □

In fact, the above diagrams hold for an arbitrary $\Psi\in\mathscr{T}_G$.

C. Quantum SL(n,$\mathbb{C}$) groups

For application of the above general theory to the construction of the quantum Clifford algebras, which we present in Sec. III, we shall require the consideration of the specific case of the special linear groups. Following Ref. 12, let us consider a vector space $V=\mathbb{C}^n$, and a linear operator $\sigma: V\otimes V\to V\otimes V$ given by

$$\sigma(e_i\otimes e_j)=\mu(e_j\otimes e_i),\quad i<j,$$

$$\sigma(e_i\otimes e_i)=e_i\otimes e_i,$$

$$\sigma(e_i\otimes e_j)=\mu(e_j\otimes e_i)+(1-\mu^2)(e_i\otimes e_j),\quad i>j,$$

where $\mu\in(-1,1)\backslash\{0\}$. This operator is a Hecke braiding with $q=\mu^2$. A quantum deformation of the SL(n) group can be described as follows (it is obviously equivalent to the R-matrix definition[13]). Let $\mathscr{H}$ be the algebra generated by the elements $u_{ij}(i,j\in\{1,\ldots,n\})$ and the following relations

$$\sum_{kl}\sigma_{kl}^{ij}u_{km}u_{ln}=\sum_{kl}u_{ik}u_{jl}\sigma_{mn}^{kl}, \tag{34}$$

$$\sum_{\pi\in S_n}(-\mu)^{l(\pi)}u_{\pi_1\zeta_1}\cdots u_{\pi_n\zeta_n}=(-\mu)^{l(\zeta)}. \tag{35}$$

The meaning of relation (34) is that σ intertwines the square of the ''fundamental representation'' $v:V\to V\otimes\mathscr{A}$ [$v(e_i)=\Sigma_j e_j\otimes u_{ji}$, where e_i are the absolute basis vectors]. Relation (35) corresponds to the classical determinant requirement. Geometrically, it means that the reduction of the nth power of v on the one-dimensional subspace $V^{\wedge n}\subseteq V^{\otimes n}$ gives a trivial representation. Condition (35) can be also rewritten in the form

$$\sum_{\pi\in S_n}(-\mu)^{l(\pi)}u_{\zeta_1\pi_1}\cdots u_{\zeta_n\pi_n}=(-\mu)^{l(\zeta)}. \tag{36}$$

The Hopf algebra structure, the coproduct ϕ: $\mathscr{H}\to\mathscr{H}\otimes\mathscr{H}$, the counit ϵ: $\mathscr{H}\to\mathbb{C}$, and the antipode κ: $\mathscr{H}\to\mathscr{H}$ are specified by

$$\phi(u_{ij})=\sum_k u_{ik}\otimes u_{kj},\quad \epsilon(u_{ij})=\delta_{ij},$$

$$\kappa(u_{ij})=(-\mu)^{i-j}\sum_{\pi\in S_{n-1}}u_{\pi_1 1}\cdots u_{\pi_{i-1}i-1}u_{\pi_{i+1}i+1}\cdots u_{\pi_n n}.$$

In the formula for the antipode, permutations $\pi\in S_{n-1}$ are represented by sequences $(\pi_1,\ldots,\pi_{i-1},\pi_{i+1},\pi_n)$ of numbers $(1,\ldots,j-1,j+1,\ldots,n)$.

All operators of the form $D_\sigma(\varphi)$ (where $\varphi\in H_{n,q}$) intertwine the nth power of the fundamental representation u. Let us observe that the flip-over operator σ is borrowed from the theory of quantum SU(n) groups,[14] which are *compact quantum objects* (σ is a canonical intertwiner of the square of the fundamental representation of this group). In particular,[14] operators belonging to the image of the corresponding Hecke algebra representations are the only intertwiners of u^n.

Moreover, in all algebraic considerations with the above-described quantum SL(n,$\mathbb{C}$) group it is possible to deal with its *compact form* $S_\mu U(n)$. This is based on the fact that the Hopf algebras representing these two groups are isomorphic, the only difference being that the algebra $\mathscr{A}$ representing $S_\mu U(n)$ possesses the *-structure. Speaking in classical terms, the elements of the algebra $\mathscr{H}$ correspond to *holomorphic* polynomial functions on the quantum space SL(n) (and in the framework of this picture it is not possible to introduce the *-conjugation). On the other hand the elements of $\mathscr{A}$ correspond to all polynomial functions on $S_\mu U(n)$.

It is important to stress that the above argumentation only applies for the ''holomorphic part'' of the theory of the quantum SL(n) group. For example, if the full theory is considered (as for

example in Ref. 15), then the corresponding ''functional algebra'' $\mathscr{B}$ on the quantum SL(n) group is much larger (because then $\mathscr{B}$ represents all polynomial functions), and there exists the canonical Hopf algebra epimorphism $j:\mathscr{B}\to\mathscr{A}$ (the dualized inclusion map).

III. ON QUANTUM CLIFFORD ALGEBRAS

In this section we shall present a general construction of quantum Clifford algebras (for even-dimensional vector spaces), together with the corresponding spinor representation. The main geometrical classical idea that will be incorporated into the quantum context is that the spinor space is interpretable as the exterior algebra built over one of two isotropic (with respect to a given quadratic form) subspaces, into which the initial vector space decomposes. These subspaces are mutually dual, in a natural manner. The duality between them is realized via the scalar product. Therefore we can *start* from a vector space V (endowed with the appropriate structures) and *define* the ''total'' vector space as the direct sum $W=V\oplus V'$.

In the next subsection general considerations will be given. After that, the theory will be illustrated for the concrete example of four-dimensional spinors built from the quantum SL(2,$\mathbb{C}$) group, and its fundamental representation.

A. General considerations

Let G be a compact matrix quantum group. The algebra of polynomial functions on G will be denoted by $\mathscr{A}$. The quantum group structure is specified by the coproduct $\phi:\mathscr{A}\to\mathscr{A}\otimes\mathscr{A}$, the counit $\epsilon:\mathscr{A}\to\mathbb{C}$, and the antipode $\kappa:\mathscr{A}\to\mathscr{A}$. The result of an $(n-1)$-fold coproduct of $a\in\mathscr{A}$ will be denoted by $a^{(1)}\otimes\cdots\otimes a^{(n)}$.

Let $v:V\to V\otimes\mathscr{A}$ be an irreducible representation of G in a (finite dimensional) unitary vector space V. Let us assume that the space V possesses a unital right $\mathscr{A}$-module structure $\circ$, such that the compatibility condition (20) holds. In other words, V is understood as the left-invariant part of a bicovariant bimodule Γ over G, and v is the restriction on V of the corresponding right action of G on Γ. Let us assume that the corresponding canonical flip-over operator σ (eventually modified by an inessential multiplication constant) satisfies the Hecke condition

$$\sigma^2=(1-q)\sigma+qI,$$

for some $q>0$ (however, this assumption is not essential for our constructions).

Let $V^\wedge$ be the corresponding exterior algebra. This algebra is also naturally isomorphic to the subalgebra of left-invariant elements of the bicovariant[10] exterior algebra $\Gamma^\wedge$.

The following identities hold:

$$\sigma(m^\wedge\otimes id)=(id\otimes m^\wedge)(\sigma\otimes id)(id\otimes\sigma), \tag{37}$$

$$\sigma(id\otimes m^\wedge)=(m^\wedge\otimes id)(id\otimes\sigma)(\sigma\otimes id), \tag{38}$$

where $m^\wedge:V^\wedge\otimes V^\wedge\to V^\wedge$ is the multiplication map in $V^\wedge$. These identities express ''functoriality'' of $m^\wedge$, with respect to the natural braiding in $V^\wedge$, and follow directly from the fact that $V^\wedge\cong\Gamma^\wedge_{\mathrm{inv}}$. Indeed, using (31) we find

$$\begin{aligned}\sigma(m^\wedge\otimes id)(\theta\otimes\eta\otimes\zeta)&=\sum_k\ \zeta_k\otimes(\theta\eta)\circ c_k=\sum_k\ \zeta_k\otimes(\theta\circ c_k^{(1)})(\eta\circ c_k^{(2)})\\&=\sum_k\ (id\otimes m^\wedge)(\sigma\otimes id)(\theta\otimes\zeta_k\otimes(\eta\circ c_k))\\&=(id\otimes m^\wedge)(\sigma\otimes id)(id\otimes\sigma)(\theta\otimes\eta\otimes\zeta),\end{aligned}$$

for each $\zeta,\theta,\eta\in V^\wedge$, where $\Sigma_k\zeta_k\otimes c_k=v^\wedge(\zeta)$ and $v^\wedge:V^\wedge\to V^\wedge\otimes\mathscr{A}$ is the natural multiplicative extension of v (the restriction of the right action of G on $V^\wedge$). Property (37) follows similarly.

Let us now define the action $H: W \to L(V^{\wedge})$ of vectors from $V \oplus V' = W$ on $V^{\wedge}$ by the following formulas:

$$H(x)\xi = x \wedge \xi, \tag{39}$$

$$H(f\ )\xi = (f \otimes id)\xi = \iota_f \xi, \tag{40}$$

where $x \in V$, $f \in V'$ and in (40) the space $V^{\wedge}$ is realized as a subspace in $V^{\otimes}$ (with the help of the antisymmetrizer A).

For each $f \in V'$ the map $\iota_f : V^{\wedge} \to V^{\wedge}$ satisfies the following ''braided'' Leibniz rule:

$$\iota_f(\theta\eta) = \iota_f(\theta)\eta + (-1)^{\partial\theta} m\sigma^{-1}(\iota_f \otimes id)\sigma(\theta \otimes \eta). \tag{41}$$

This follows easily from the definition of ι_f as a contraction, as well as from the definition of the embedding $V^{\wedge} \hookrightarrow V^{\otimes}$.

Proposition III.1: The following identities hold:

$$H(x)H(y) + \frac{1}{q}\sum_k H(y_k)H(x_k) = 0, \tag{42}$$

$$H(f\ )H(g) + \frac{1}{q}\sum_l H(g_l)H(f_l) = 0, \tag{43}$$

$$H(f\ )H(x) + \sum_i H(x_i')H(f_i') = f(x), \tag{44}$$

$$H(y)H(g) + \sum_j H(g_j')H(y_j') = \sum_j g_j'(y_j'). \tag{45}$$

Here, $x, y \in V$ and $f, g \in V'$, while

$$\sum_k y_k \otimes x_k = \sigma(x \otimes y), \quad \sum_l g_l \otimes f_l = \sigma(f \otimes g),$$

$$\sum_i x_i' \otimes f_i' = \sigma^{-1}(f \otimes x), \quad \sum_j g_j' \otimes y_j' = \sigma(y \otimes g).$$

Proof: Identities (42) and (43) follow directly from the definition of exterior algebras over V and V', as well as from the fact that $I + \sigma/q$ is the projector on the space of σ-symmetric elements of $V \otimes V$ and $V' \otimes V'$. Identities (44) and (45) are mutually equivalent. Let us check (44). First, observe that the introduced ''contraction'' between V' and $V^{\wedge}$ can be naturally extended to a map $\iota: V'^{\wedge} \otimes V^{\wedge} \to V^{\wedge}$ such that

$$\iota_{uw} = \iota_u \iota_w \tag{46}$$

for each $u, w \in V'^{\wedge}$, where $\iota_{uw}(x) = \iota(u, w \otimes x)$.

Now, by the use of the braided Leibniz rule (41) and the identities

$$\sigma(\iota \otimes id) = (id \otimes \iota)(\sigma \otimes id)(id \otimes \sigma), \tag{47}$$

$$\sigma(id \otimes \iota) = (\iota \otimes id)(id \otimes \sigma)(\sigma \otimes id), \tag{48}$$

we obtain, by a direct computation,

$$\begin{aligned} H(f\ )H(x)\xi &= f(x)\xi - m^{\wedge}\sigma^{-1}(\iota_f \otimes id)\sigma(x\otimes\xi) \\ &= f(x)\xi - m^{\wedge}\sigma^{-1}(\iota\otimes id)(id\otimes\sigma)(f\otimes x\otimes\xi) \\ &= f(x)\xi - m^{\wedge}(id\otimes\iota)(\sigma^{-1}\otimes id)(f\otimes x\otimes\xi) = f(x)\xi - \sum_i H(x_i')H(f_i')\xi. \end{aligned}$$

□

Motivated by the above proposition we can *define* abstract quantum Clifford algebras. In fact, let $Cl(W)$ be a unital associative algebra generated by the vector space $W=V\oplus V'$ and the following relations

$$xy + \frac{1}{q}\sum_k y_k x_k = 0, \tag{49}$$

$$fg + \frac{1}{q}\sum_l g_l f_l = 0, \tag{50}$$

$$fx + \sum_i x_i' f_i' = f(x). \tag{51}$$

Definition III.1: The constructed algebra is called the quantum Clifford algebra associated to (V,σ).

The relations defining the algebra $Cl(W)$ can be written in a compact form as

$$\vartheta\eta + \sum_k \eta_k\vartheta_k = f(\vartheta,\eta).$$

Here, $\Sigma_k \eta_k\otimes\vartheta_k = \tau(\vartheta\otimes\eta)$ and $\tau: W^{\otimes 2}\to W^{\otimes 2}$ is a braiding given by the block matrix

$$\tau = \begin{pmatrix} \sigma/q & 0 & 0 & 0 \\ 0 & 0 & \sigma^{-1} & 0 \\ 0 & \sigma & 0 & 0 \\ 0 & 0 & 0 & \sigma/q \end{pmatrix},$$

and f is the corresponding bilinear form on W, extending the contraction map [uniquely determined by relations (49)–(51)].

To end this section, we observe that a quantum analogue of the Clifford algebra for the odd-dimensional case can be introduced as follows. We put

$$W = V\oplus V'\oplus M,$$

where M is a one-dimensional space, and define $Cl(W,\sigma)$ to be the abstract algebra generated by the spaces V and V', the corresponding relations (42)–(45), as well as by an element S satisfying $S^2=1$, $Sx+xS=0$, and $Sf+fS=0$, for each $x\in V$ and $f\in V'$.

IV. SPINOR REPRESENTATIONS

In this section we shall introduce the spinor representation. The braided exterior algebra $V^{\wedge}$ will play the role of the space of algebraic spinors.

A. Algebraic spinors

From the relations defining $Cl(W)$ and the braided Leibniz rule (41) for ι, it follows that the map $H:W\to L(V^{\wedge})$ can be uniquely extended to a unital homomorphism $H:Cl(W)\to L(V^{\wedge})$.

Definition IV.1: The introduced homomorphism H is called the spinor representation.

Proposition IV.1: The algebra $Cl(W)$ acts on $V^{\wedge}$ faithfully and irreducibly.

Proof: We shall prove that each nonzero vector $\xi\in V^{\wedge}$ is cyclic for H, which immediately implies that H is irreducible.

Without a lack of generality we can assume that ξ is homogeneous ($\xi\in V^{\wedge k}$).

Let us first observe that the spaces $V'^{\wedge}$ and $V^{\wedge}$ are mutually dual, in a natural manner. The corresponding pairing $\langle,\rangle:V'^{\wedge}\otimes V^{\wedge}\to\mathbb{C}$ can be explicitly constructed by taking the restriction of the natural pairing $\langle,\rangle:V'^{\otimes}\otimes V^{\otimes}\to\mathbb{C}$. Second, we have

$$\langle\varphi,\xi\rangle=c_k\iota(\varphi\otimes\xi), \tag{52}$$

for each $\varphi\in V'^{\wedge k}$. In particular, there exists $f\in V'^{\wedge}$ such that $\iota(f\otimes\xi)=1$. In other words, 1 can be obtained by acting with the operators $H(f)$ (where $f\in V'$) on ξ, and taking appropriate linear combinations. Consequently, ξ is cyclic for H, because 1 is cyclic for the left regular representation of $V^{\wedge}$ on itself.

Let us prove that H is faithful. From the relations defining $Cl(W)$ it follows that the inclusions $V\hookrightarrow W$ and $V'\hookrightarrow W$ can be extended to inclusions of algebras $V^{\wedge}\hookrightarrow Cl(W)$ and $V'^{\wedge}\hookrightarrow Cl(W)$. Moreover, from the same relations we conclude that the map $\mu:V^{\wedge}\otimes V'^{\wedge}\to Cl(W)$, given by

$$\mu(\xi\otimes\varphi)=\xi\varphi,$$

is bijective. Using this, Eq. (52), and the fact that $V^{\wedge}$ and $V'^{\wedge}$ are mutually dual, it is easy to see that the vectors ξ distinguish elements of $V^{\wedge}\otimes V'^{\wedge}$. More precisely, let us consider the maps of the form $\delta_{\xi}:V^{\wedge}\otimes V'^{\wedge}\to V^{\wedge}$ given by

$$\delta_{\xi}(\Theta)=H[\mu(\Theta)]\xi.$$

If $\Theta\in\ker(\delta_{\xi})$ for each $\xi\in V^{\wedge}$, then we have $\Theta=0$. In other words, the representation H is faithful. □

In the odd-dimensional case, the corresponding spinor representation can be constructed essentially in the same way as in the even-dimensional case. The additional generator S acts as the parity operator. According to Proposition IV.1 (applied to the Clifford algebra generated by V and V'), the operator $H(S)$ can be expressed algebraically through the operators $H(x)$, where $x\in V,V'$, if $V^{\wedge}$ is finite dimensional.

To end this section we shall briefly consider other possible approaches for introducing spinors, following Ref. 3. First, we give a more concise general definition.

Let $\varpi:V'^{\wedge}\to\mathbb{C}$ be a linear multiplicative functional, specified by $\varpi(1)=1$ and $\varpi(V')=\{0\}$. This gives a left $V'^{\wedge}$-module structure on the number field $\mathbb{C}$. On the other hand, $Cl(W)$ is naturally a right $V'^{\wedge}$-module (the multiplication on the right). Let $\mathscr{S}$ be a left $Cl(W)$-module, given by

$$\mathscr{S}=Cl(W)\otimes_{*}\mathbb{C},$$

where the tensor product is taken over $V'^{\wedge}$.

Proposition IV.2: The modules $(V^{\wedge},H)$ and $\mathscr{S}$ are naturally isomorphic. The isomorphism is explicitly given by

$$V^{\wedge} \ni \xi \leftrightarrow \xi \otimes_* 1 \in \mathscr{S}.$$

Proof: The statement follows from the relations defining the quantum Clifford algebra. □

Let us now assume for a moment that we are dealing with classical Clifford algebras. Then spinors can be viewed in another (but equivalent) way as elements of the left $Cl(W)$-ideal, generated by a volume element of V'.

An analogous description of spinors works in the quantum context if there exists a ''volume element'' in the braided exterior algebra $V'^{\wedge}$. More precisely, let us assume that there exists (a volume element) $\omega \in V'^{\wedge} \setminus \{0\}$ satisfying $x\omega = 0$, for each $x \in V'$.

Proposition IV.3: Let $\mathscr{I}_\omega$ be a left ideal in $Cl(W)$ generated by ω. Then there exists the unique $Cl(w)$-module map $i_\omega : V^{\wedge} \to \mathscr{I}_\omega$ satisfying $i_\omega(1) = \omega$.

Proof: The statement easily follows from the definition of the spinor module $\mathscr{I} = (\mathrm{V}^{\wedge}, \mathrm{H})$, and its simplicity. □

B. Scalar products and *-structures

In this subsection we shall introduce a natural scalar product in the spinor space, and investigate its properties. With the help of this scalar product, a *-structure on the corresponding quantum Clifford algebra will be introduced. The construction generalizes classical considerations in the case when the underlying space is endowed with an Euclidean (strictly positive) scalar product. Pseudo-Euclidean spaces are dealt with in a forthcoming paper.

Let us assume that the space V is endowed with a unitary structure, such that the braiding σ: $V^{\otimes 2} \to V^{\otimes 2}$ is Hermitian with respect to the corresponding scalar product. Let $j : V \to V'$ be the canonical antilinear map (induced by the scalar product). In what follows it will be assumed that V' is endowed with the corresponding j-induced scalar product (so that j is antiunitary).

We can now introduce a *-involution in the main vector space $W = V \oplus V'$, by means of the block matrix.

$$* = \begin{pmatrix} 0 & j^{-1} \\ j & 0 \end{pmatrix}.$$

We shall prove that this involution can be extended to a *-structure on the Clifford algebra $Cl(W)$.

Assume that $V^{\wedge}$ is realized as a subspace of completely σ antisymmetric elements of the tensor algebra $V^{\otimes}$. Furthermore, let us assume that $V^{\wedge}$ is endowed with the scalar product $\langle , \rangle$ given by

$$\langle \varphi, \psi \rangle = c_n(\varphi, \psi),$$

where $(,)$ is the scalar product in $V^{\otimes}$, and $\varphi, \psi \in V^{\wedge n}$, while

$$c_n = (n_q)!, \quad n_q = \frac{1 - q^n}{1 - q}, \quad \text{for } q \neq -1.$$

By definition, the elements of different degrees are orthogonal.

Lemma IV.1: We have

$$\langle H(x)\varphi, \psi \rangle = \langle \varphi, H(x^*)\psi \rangle, \tag{53}$$

for each $x \in W$ and $\varphi, \psi \in V^{\wedge}$.

Proof: Clearly, it is sufficient to check the above equation for elements $x \in V$, $\varphi \in V^{\wedge n-1}$, and $\psi \in V^{\wedge n}$. A direct calculation gives

$$\langle H(x)\varphi,\psi\rangle = c_n(A_{1n-1}(x\otimes\varphi),\psi) = c_n(x\otimes\varphi,A^{\dagger}_{1n-1}\psi) = c_n\left(\sum_{i=0}^{n-1} q^i\right)(x\otimes\varphi,\psi)$$
$$= c_{n-1}(\varphi,H(x^*)\psi) = \langle\varphi,H(x^*)\psi\rangle.$$

□

Therefore, the *-involution is compatible with the spinor representation H. Having in mind that the H is an isomorphism between $Cl(W)$ and $L(V^{\wedge})$, we can define a *-structure on the whole $Cl(W)$ by requiring that

$$\langle H(a)\varphi,\psi\rangle = \langle\varphi,H(a^*)\psi\rangle,$$

for each $a\in Cl(W)$. Evidently, this gives an antimultiplicative and involutive extension of the previously introduced map.

V. FLIP-OVER OPERATOR AND *q*-CLIFFORD ALGEBRA

In order to obtain concrete relations that will enable a comparison of our results with those of other authors, we focus our attention on the q-Clifford algebra for a $2n$-dimensional total vector space W, with basis $\{e_i,e_i'\}_{i=1}^n$, and quantum group $\mathrm{SL}_q(n,\mathbb{C})$ with metric representation on V given by $v(e_i)=\Sigma_j e_j\otimes u_{ji}$.

Following the methodology developed in the general theory contained in Sec. II, one arrives at the following results:

$$H(e_i')H(e_j)+\sum_{k,l}(\sigma^{-1})_{ij}{}^{kl}H(e_k)H(e_l') = \delta_{ij}E, \tag{54}$$

where

$$\sigma^{-1}(e_i'\otimes e_j) = \sum_{k,l}(\sigma^{-1})_{ij}{}^{kl}e_k\otimes e_l', \tag{55}$$

and E is the identity operator. The inverse relation is given by

$$H(e_i)H(e_j')+\sum_{k,l}(\sigma)_{ij}{}^{kl}H(e_k')H(e_l) = \eta_{ij}E, \tag{56}$$

with

$$\sigma(e_i\otimes e_j') = \sum_{k,l}(\sigma)_{ij}{}^{kl}e_k'\otimes e_l \quad\text{and}\quad \eta_{ij}\equiv\sum_{l}(\sigma)_{ij}{}^{ll}. \tag{57}$$

We also have

$$H(e_i)H(e_j)+\frac{1}{\mu^2}\sum_{k,l}(\sigma)_{ij}{}^{kl}H(e_k)H(e_l) = 0, \tag{58}$$

where

$$\sigma(e_i\otimes e_j) = \sum_{k,l}(\sigma)_{ij}{}^{kl}e_k\otimes e_l, \tag{59}$$

and

$$H(e_i')H(e_j')+\frac{1}{\mu^2}\sum_{k,l}(\sigma)_{ij}{}^{kl}H(e_k')H(e_l')=0, \tag{60}$$

where

$$\sigma(e_i'\otimes e_j')=\sum_{k,l}(\sigma)_{ij}{}^{kl}e_k'\otimes e_l'. \tag{61}$$

To compute the flip-over operators, we use the formalism of bicovariant bimodules. Here, we shall denote by $\tilde{\sigma}$ the canonical intertwiners given by formula (26). Up to a multiplication constant, $\tilde{\sigma}:V\otimes V\to V\otimes V$ coincides with the flip-over operator $\sigma:V\otimes V\to V\otimes V$. In fact, the condition $\tilde{\sigma}=\beta\sigma$ with $\beta\in\mathbb{R}^+$ uniquely fixes the corresponding right $\mathscr{A}$-module structure $\circ$ on V. Applying (26) and (27) and making use of the fact that

$$\kappa^{-1}(u)=F^{-1}\kappa(u)F, \tag{62}$$

where $\kappa(u)=u^\dagger$, and $F:V\to V$ is the canonical intertwiner[16] between u and its double contragradient u^{cc}, which in our case is explicitly given by $Fe_k=\mu^{2k-n-1}e_k$, we obtain expressions for $e_i\circ u_{kj}$ and $e_i\circ u_{kj}^*$. Using the definition (29) of $\circ$ in the dual space we obtain the expressions for $e_i'\circ u_{kj}$ and $e_i'\circ u_{kj}^*$.

The right $\mathscr{A}$-module structures on V and V' (cf. equations given in the Appendix) enable us to compute the remaining three flip-over operators. A direct calculation based on (26) and (27) gives

$$\tilde{\sigma}(e_i\otimes e_i')=\frac{1}{\beta}e_i'\otimes e_i+\frac{1-\mu^{-2}}{\beta}\sum_{k<i}\mu^{2(i-k)}e_k'\otimes e_k,$$

$$\tilde{\sigma}(e_i\otimes e_j')=\frac{1}{\beta\mu}e_j'\otimes e_i,\quad i\neq j,$$

$$\tilde{\sigma}^{-1}(e_i'\otimes e_i)=\beta e_i\otimes e_i'+\beta(1-\mu^2)\sum_{k<i}e_k\otimes e_k',$$

$$\tilde{\sigma}^{-1}(e_i'\otimes e_j)=\beta\mu e_j\otimes e_i',\quad i\neq j,$$

$$\tilde{\sigma}(e_i'\otimes e_i)=\frac{1}{\beta}e_i\otimes e_i'+\frac{1-\mu^{-2}}{\beta}\sum_{k>i}e_k\otimes e_k', \tag{63}$$

$$\tilde{\sigma}(e_i'\otimes e_j)=\frac{1}{\beta\mu}e_j\otimes e_i',\quad i\neq j,$$

$$\tilde{\sigma}(e_i'\otimes e_i')=\beta e_i'\otimes e_i',$$

$$\tilde{\sigma}(e_i'\otimes e_j')=\beta(1-\mu^2)e_i'\otimes e_j'+\mu\beta e_j'\otimes e_i',\quad i<j,$$

$$\tilde{\sigma}(e_i'\otimes e_j')=\beta\mu e_j'\otimes e_i',\quad i>j.$$

We can renormalize these flip-over operators $\tilde{\sigma}$ in such a way that they become extensions of the initial Hecke braiding $\sigma:V\otimes V\to V\otimes V$. This involves multiplying by β the ''mixing operators'' acting on $V\otimes V'$ and $V'\otimes V$ and, dividing by β the braid operator in $V'\otimes V'$. We denote by

σ all these new operators. From the quantum determinant condition (35) it is straightforward to determine that $\beta=\mu^{(1-n)/n}$. For the four-dimensional case, the q-Clifford algebra generated by $H(W)$ becomes

$$H(e_i)H(e'_j)+L_{ij}{}^{kl}H(e'_k)H(e_l)=\eta_{ij}E, \tag{64}$$

with

$$L=\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & \mu^{-1} & 0 \\ 0 & \mu^{-1} & 0 & 0 \\ (\mu^2-1) & 0 & 0 & 1 \end{pmatrix}$$

and

$$\eta=\begin{pmatrix} 1 & 0 \\ 0 & \mu^2 \end{pmatrix};$$

$$H(e_i)H(e_j)+M_{ij}{}^{kl}H(e_k)H(e_l)=0,$$

with

$$M=\mu^{-2}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & \mu & 0 \\ 0 & \mu & (1-\mu^2) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix};$$

$$H(e'_i)H(e'_j)+M'_{ij}{}^{kl}H(e'_k)H(e'_l)=0, \tag{65}$$

with

$$M'=\mu^{-2}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & (1-\mu^2) & \mu & 0 \\ 0 & \mu & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

For the four-dimensional case, it is also possible to arrive at the above q-Clifford algebra by a stepwise procedure, which consists of making use of the definition of the action of the operator H on each element of the basis, applied twice on a spinor $\xi=\xi^0+\xi^1e_1+\xi^2e_2+\xi^3e_1\wedge e_2$. For example, the double action of $H(e_1)H(e'_1)$ on ξ results in

$$H(e_1)H(e'_1)\xi=e_1\wedge(\iota_{e'_1}\xi)=\xi^1e_1+\xi^3e_1\wedge e_2, \tag{66}$$

and, similarly,

$$H(e'_1)H(e_1)\xi=\iota_{e'_1}(e_1\wedge\xi)=\xi^0+\xi^2e_2. \tag{67}$$

Adding these two expressions yields

$$(H(e_1)H(e_1')+H(e_1')H(e_1))\xi=E\xi, \tag{68}$$

which coincides with our previous result.

Finally we consider the matrix $\hat{R}=PR$ [corresponding to the quantum group $\mathrm{SL}_q(2,\mathbb{C})$[13]] that satisfies both the Hecke condition and the braid equation. In matrix form we have

$$\hat{R}=\begin{pmatrix} \mu^{-1} & 0 & 0 & 0 \\ 0 & \mu^{-1}-\mu & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & \mu^{-1} \end{pmatrix}.$$

Furthermore, since for this case

$$\mu^{-1}\sigma=\begin{pmatrix} \mu^{-1} & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & \mu^{-1}-\mu & 0 \\ 0 & 0 & 0 & \mu^{-1} \end{pmatrix},$$

with σ corresponding to the flip-over operator on $V\otimes V$, which also satisfies the Hecke condition, both matrices are related by the similarity transformation

$$S\hat{R}S^{-1}=\mu^{-1}\sigma, \tag{69}$$

with

$$S=\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

This enables us to obtain a relation between the R matrix, which determines the quantum group $\mathrm{SL}_q(2,\mathbb{C})$, and the operator σ, which establishes the anticommutation relations of the Clifford algebra.

VI. *q*-CLIFFORD ALGEBRAS AND *q*-DIRAC OPERATOR

In this section we use the q-Clifford algebra to construct a real q-space and a differential calculus associated to this space. We also build up the q-Dirac and the q-Klein–Gordon scalar operators from the dual q-Clifford algebra.

We shall introduce a formal background for the coordinates and the derivation operators, based on our q-Clifford algebras, and define a consistent *-structure which will allow us to describe real q-Euclidean spaces and the corresponding differential calculi. We also describe an interesting and purely quantum phenomenon which appears in the presented theory, which is related to a certain nonuniqueness of our q-Clifford algebras, as well as of the algebras of coordinates and derivations.

A. Differential calculus in isotropic basis

Consider a bilinear map $\langle,\rangle: W\times W\to\mathbb{C}$, given by the matrix elements figuring in the q-Clifford algebra relations

$$2\langle e_\alpha, e_\beta\rangle=f_{\alpha\beta}=(e_\alpha e_\beta+m\tau(e_\alpha\otimes e_\beta)), \tag{70}$$

with $e_\alpha = \{e_i, e_i'\}_{i=1}^n$. The introduced ''scalar product'' is τ-symmetric $\langle \mathbf{w}\otimes\mathbf{z}\rangle = \langle \tau(\mathbf{w}\otimes\mathbf{z})\rangle$, and nondegenerate, because the only contributions of the braid τ to (70) come from the part which mixes elements in V with elements in V', which is involutive due to relations (63).

Following the classical Cartan theory, we would like to satisfy the fundamental property of spinor transformations $H(\mathbf{w})$ associated with a vector $\mathbf{w}$, that is,

$$H(\mathbf{w})H(\mathbf{w}) = \langle \mathbf{w},\mathbf{w}\rangle E. \tag{71}$$

Maintaining the above relation for the quantum case will make it also possible to preserve the geometric interpretation of the spinor transformations $H(\mathbf{u})$ as ''plane inversions'' in a subspace perpendicular to the unit vector $\mathbf{u}$. This in turn will be important for the construction of a spinor algebra, a natural q-spinor bilinear inner product, and its relations to the Hermitian product introduced in the previous section.

Relation (71) implies

$$\sum_{\alpha\beta} w^\alpha w^\beta \otimes e_\alpha \otimes e_\beta \in \mathscr{B}\otimes \mathrm{Im}(1+\tau), \tag{72}$$

where $\mathscr{B}$ is the algebra generated by the coordinates $w^\alpha = \{w^1,\ldots,w^n,w'^1,\ldots,w'^n\}$ in the isotropic basis.

The above relation is equivalent to

$$0 = [id\otimes(1-\tau_1)](w^\alpha w^\beta \otimes e_\alpha \otimes e_\beta), \tag{73}$$

where τ_1 is an operator on W satisfying

$$\ker(1-\tau_1) = \mathrm{Im}(1+\tau).$$

An explicit solution for this is given by a braiding

$$\tau_1 = \begin{pmatrix} \sigma & 0 & 0 & 0 \\ 0 & 0 & \sigma^{-1} & 0 \\ 0 & \sigma & 0 & 0 \\ 0 & 0 & 0 & \sigma \end{pmatrix}, \tag{74}$$

where, as already mentioned, σ denotes all functorial extensions of the original σ (the domain is clear from the context).

From (73) we immediately obtain the following algebra for the coordinates w^α:

$$w^\alpha w^\beta = m\,\tau_1^\tau(w^\alpha\otimes w^\beta). \tag{75}$$

In explicit form,

$$\begin{aligned} w^i w^j &= \mu w^j w^i, \quad i<j, \\ w'^i w'^j &= \mu^{-1} w'^j w'^i, \quad i<j, \\ w^i w'^j &= \mu w'^j w^i, \quad i\neq j, \\ w^i w'^i &= w'^i w^i + \sum_{l>i} (1-\mu^2) w'^l w^l. \end{aligned} \tag{76}$$

Note that essentially the same algebra is obtained in Ref. 17 for the four-dimensional case. The basic difference being that in our approach the commutation relations (76) on the underlying base space are imposed by the ansatz (71) on the q-Clifford algebra.

To complete the algebra, we also need an algebra Σ of q-symbolic derivations $\{\partial_i,\partial_i'\}_{i=1}^n$. Relations for the algebra Σ follow by dualizing relations (75) and noting that for an arbitrary braiding η there corresponds a braiding $\psi\eta^{\tau}\psi$ acting in the dual space. Here ψ denotes the standard transposition operator (if we include the dual spaces in the braided monoidal category generated by η and require the functoriality of the contraction map). Thus we get the following symmetric algebra for the Σ space of q-derivations

$$\begin{aligned}
&\partial_i\partial_j=\mu^{-1}\partial_j\partial_i, \quad i<j,\\
&\partial_i'\partial_j'=\mu\partial_j'\partial_i', \quad i<j,\\
&\partial_i\partial_j'=\mu\partial_j'\partial_i, \quad i\neq j,\\
&\partial_i\partial_i'=\partial_i'\partial_i+\sum_{l<i}(1-\mu^2)\partial_l'\partial_l.
\end{aligned} \tag{77}$$

We shall be needing in addition the braided Leibniz rule with actions of q-derivations both from the left and from the right. The braided Leibniz rule with derivations from the left is given by

$$\partial_\alpha w^\beta=\delta_\alpha^\beta+(\mathscr{T}^{-1})_{\alpha\epsilon}^{\beta\gamma}w^\epsilon\partial_\gamma. \tag{78}$$

To determine the coefficients in (78) we use the functoriality relation

$$(id\otimes c)(\mathscr{T}^{-1}\otimes id)(\partial_\alpha\otimes w^\beta\otimes w^\gamma)=(c\otimes id)(id\otimes\eta)(\partial_\alpha\otimes w^\beta\otimes w^\gamma), \tag{79}$$

where c denotes contraction. This enables us to find the relation between $\mathscr{T}^{-1}$ and the braiding η in the space of coordinates. We obtain

$$(\mathscr{T}^{-1})_{\alpha\epsilon}^{\beta\gamma}=\eta^{\beta\gamma}{}_{\alpha\epsilon}, \tag{80}$$

with

$$\eta\equiv\begin{cases}
\mu^{-2}\sigma^{\tau} \;:\; (\alpha,\beta)=(i,j),\\
\mu^{-2}(\sigma)^{\tau} \;:\; (\alpha,\beta)=(i',j'),\\
(\tilde{\sigma}^{-1})^{\tau} \;:\; (\alpha,\beta)=(i',j),\\
(\sigma)^{\tau} \;:\; (\alpha,\beta)=(i,j').
\end{cases}$$

In explicit form, using (78)–(80), the Leibniz rule with action from the left is

$$\partial_i w^j=\mu^{-1}w^j\partial_i, \quad i\neq j$$

$$\partial_i w^i=1+\mu^{-2}w^i\partial_i+(\mu^{-2}-1)\sum_{k<i}w^k\partial_k,$$

$$\partial_i' w'^j=\mu^{-1}w'^j\partial_i', \quad i'\neq j',$$

$$\partial_i' w'^i=1+\mu^{-2}w'^i\partial_i'+(\mu^{-2}-1)\sum_{k>i}w'^k\partial_k',$$

$$\begin{aligned}
\partial_i' w^j &= \mu w^j \partial_i', \quad i<j,\\
\partial_i' w^j &= \mu w^j \partial_i' + (1-\mu^2) w^i \partial_j', \quad i>j,\\
\partial_i' w^i &= w^i \partial_i',\\
\partial_i w'^j &= \mu^{-1} w'^j \partial_i,\\
\partial_i w'^j &= \mu^{-1} w'^j \partial_i + (1-\mu^{-2}) \mu^{2(i-j)} w'^i \partial_j, \quad i>j,\\
\partial_i w'^i &= w'^i \partial_i.
\end{aligned} \tag{81}$$

In a similar manner, we obtain the Leibniz rule with q-derivation action from the right. Thus

$$w^\beta \overleftarrow{\partial}_\alpha = \delta_\alpha^\beta + \eta_{\epsilon\alpha}^{\gamma\beta} \overleftarrow{\partial}_\gamma w^\epsilon, \tag{82}$$

where

$$\eta \equiv \begin{cases} \mu^{-2}\sigma^\tau \ : \ (\beta,\alpha)=(j,k),\\ \mu^{-2}(\sigma)^\tau \ : \ (\beta,\alpha)=(j',k'),\\ (\sigma^{-1})^\tau \ : \ (\beta,\alpha)=(j',k),\\ (\sigma)^\tau \ : \ (\beta,\alpha)=(j,k'). \end{cases}$$

Explicitly, we have

$$w^j \overleftarrow{\partial}_k = \mu^{-1} \overleftarrow{\partial}_k w^j, \quad j \neq k, \tag{83}$$

$$w^j \overleftarrow{\partial}_j = 1 + \mu^{-2} \overleftarrow{\partial}_j w^j + (\mu^{-2}-1) \sum_{i>j} \overleftarrow{\partial}_i w^i, \tag{84}$$

$$w'^j \overleftarrow{\partial}_k' = \mu^{-1} \overleftarrow{\partial}_k' w'^j, \quad j \neq k, \tag{85}$$

$$w'^j \overleftarrow{\partial}_j' = 1 + \mu^{-2} \overleftarrow{\partial}_j' w'^j + (\mu^{-2}-1) \sum_{i<j} \overleftarrow{\partial}_i' w'^i, \tag{86}$$

$$w'^j \overleftarrow{\partial}_k = \mu \overleftarrow{\partial}_k w'^j + (1-\mu^2) \overleftarrow{\partial}_j w'^k, \quad j<k \tag{87}$$

$$w'^j \overleftarrow{\partial}_k = \mu \overleftarrow{\partial}_k w'^j, \quad j>k, \tag{88}$$

$$w'^j \overleftarrow{\partial}_j = \overleftarrow{\partial}_j w'^j, \tag{89}$$

$$w^j \overleftarrow{\partial}_k' = \mu^{-1} \overleftarrow{\partial}_k' w^j + (1-\mu^{-2}) \mu^{2(k-j)} \overleftarrow{\partial}_j w^k, \quad j<k \tag{90}$$

$$w^j \overleftarrow{\partial}_k' = \mu^{-1} \overleftarrow{\partial}_k' w^j, \quad j>k, \tag{91}$$

$$w^j \overleftarrow{\partial}_j' = \overleftarrow{\partial}_j' w^j. \tag{92}$$

The left and right partial derivatives used above are related to the differential by the following symbolic expression

$$d=\sum_{\alpha} dw^{\alpha}\,\partial_{\alpha}=\sum_{\alpha}\overleftarrow{\partial}_{\alpha}\,dw^{\alpha}. \tag{93}$$

Note that all the expressions derived in this section are automatically consistent, because all constructions are intrinsic, and are performed in a braided monoidal category. An alternative and explicit way to check consistency could be based on an approach similar to that followed by Pusz and Woronowicz[12] and Wess and Zumino.[18] Essentially such a procedure consists of introducing a flip operator C between differentials and coordinates which is required to satisfy the relations

$$E+C=\tau_1^{\tau}+C\tau_1^{\tau}, \tag{94}$$

$$(id\otimes\tau_1^{\tau})(C\otimes id)(id\otimes C)=(C\otimes id)(id\otimes C)(\tau_1^{\tau}\otimes id). \tag{95}$$

B. On two natural Clifford algebras

As we have seen, starting from $Cl(W)$ it is possible to construct a q-analogue of the polynomial algebra over W. This algebra is generated by W and relations resulting from the requirement that the expression

$$\left(\sum_i e_i' x_i' + e_i x_i\right)^2=\langle \mathbf{x},\mathbf{x}\rangle$$

be scalar. This leads to the braided-symmetric algebra $\mathscr{B}$ over W, based on the operator τ_1^{τ}. However, using the induced commutation relations for the partial derivatives, it is easy to show that the square of the symbolic ''Dirac operator''

$$\boldsymbol{\nabla}=\sum_i e_i'\,\partial_i' + e_i\partial_i$$

is not a scalar operator.

On the other hand, it is possible to adopt a different point of view, which consists of introducing a new Clifford algebra, starting from the explicit requirement that ∇^2 be a scalar operator and that relations between partial derivatives are assumed the same as in (77).

In other words we should look for such a braiding $\widetilde{\tau}: W^{\otimes 2}\to W^{\otimes 2}$ which is related to $\psi\tau_1\psi$ in the same way as τ is to τ_1^{τ} [see Eqs. (73) and (74)]. Explicitly

$$\widetilde{\tau}=\psi\tau^{\tau}\psi.$$

This leads to the following expression for the Laplacian:

$$\Delta=\nabla^2=\sum_i \partial_i'\partial_i\,. \tag{96}$$

Note, however, that this new Clifford algebra would exchange the role of coordinates and derivatives figuring in their commutation relations and when applying twice the procedure we would return to the starting point.

In the classical case both Clifford algebras coincide. However, from the point of view of introducing quantum space models, there is *a priori* no reason to favor one q-Clifford algebra over the other. Furthermore, from the perspective of developing an analogue of the Hamiltonian for-

malism, it may be desirable to work simultaneously with the two Clifford algebras, since one of them is intrinsically connected with coordinates, and the other is connected with derivation operators.

C. Real *q*-space and corresponding differential calculus

Let $\mathscr{W}$ be the algebra generated by the coordinates w^α, the left and right partial derivatives, and all the above-mentioned relations. We can now extend the antimultiplicative $*$-involution introduced in Sec. IV to the whole algebra $\mathscr{W}$.

For simplicity in what follows we shall restrict ourselves to the four-dimensional case. Clearly the results can be readily generalized to arbitrary dimensions.

In the isotropic basis $\{e_i, e_i'\}_{i=1}^2$ of the vector space W, the $*$-operation is given by

$$e_1^* = e_1', \quad e_1'^* = e_1, \tag{97}$$

$$e_2^* = e_2', \quad e_2'^* = e_2. \tag{98}$$

This *-operation induces the following *-operation for partial derivatives:

$$(\partial_1)^* = \overleftarrow{\partial}_1', \quad (\partial_2)^* = \overleftarrow{\partial}_2', \tag{99}$$

$$(\partial_1')^* = \overleftarrow{\partial}_1, \quad (\partial_2')^* = \overleftarrow{\partial}_2. \tag{100}$$

The $*$ is extended to the whole algebra $\mathscr{W}$ by making use of the properties

$$*^2 = id, \quad (w^\alpha w^\beta)^* = w^{\beta *} w^{\alpha *},$$

$$(\partial_\alpha w^\beta)^* = w^{\beta *} (\partial_\alpha)^*, \quad (w^\alpha \overleftarrow{\partial}_\beta)^* = (\overleftarrow{\partial}_\beta)^* w^{\alpha *}.$$

It is easy to verify that, with these relations, the algebra is consistent. Furthermore, defining reality by means of the condition $\mathbf{w}^* = \mathbf{w}$, we can apply the above formalism to construct the Dirac and Klein–Gordon operators for the case of q-deformed Euclidean spaces.

Clearly, to the generator level, the resulting expressions will reproduce the ones in the classical case. However, for computations with these operators involving higher-order terms in the generators, the quantum nature of the algebra will appear.

It is important to mention that the above *-structure is not unique. Another natural choice is to adopt a ''quantum plane'' viewpoint, and to consider the $*$ invariant under the natural action of a certain quantum group. In the considered case, the group is $S_\mu U(2)$. Explicitly, the *-structure is then given by

$$w^{1*} = w'^1, \quad w'^{1*} = w^1, \quad w^{2*} = \mu^2 w'^2, \quad w'^{2*} = \mu^{-2} w^2, \tag{101}$$

and

$$(\partial_1)^* = \mu^2 \overleftarrow{\partial}'_1, \quad (\partial_2)^* = \overleftarrow{\partial}'_2, \quad (\partial_1')^* = \mu^{-2} \overleftarrow{\partial}_1, \quad (\partial_2')^* = \overleftarrow{\partial}_2. \tag{102}$$

From this we construct the ''real'' basis of vectors $\{a_i\}_{i=1}^4$:

$$a_1 = e_1 + e_1', \tag{103}$$

$$a_2 = e_2 + \mu^2 e_2', \tag{104}$$

$$a_3 = i(e_1 - e_1'), \tag{105}$$

$$a_4 = i(\mu^2 e_2 - e_2'). \tag{106}$$

Making use of (106) it immediately follows that

$$\langle a_i, a_j \rangle \equiv g_{ij} \equiv \begin{cases} 1 \ : \ i=j=1 \ \text{ or } \ i=j=3, \\ \frac{1}{2}(1+\mu^{-2}) \ : \ i=j=2, \\ \dfrac{\mu^2}{2}(1+\mu^2) \ : \ i=j=4, \\ \dfrac{i}{2}(1-\mu^2) \ : \ i=2, \ j=4, \\ \dfrac{-i}{2}(1-\mu^2) \ : \ i=4, \ j=2, \\ 0 \ : \ \text{otherwise.} \end{cases}$$

Note that the g_{ij} can be seen as the coefficients of a ''q-metric,'' appearing in the corresponding q-Clifford algebra

$$a_i a_j + m\tau(a_i \otimes a_j) = 2g_{ij}. \tag{107}$$

In the basis (106), the coordinates of any ''real'' vector $\mathbf{A} \in W$ are given in terms of the former isotropic coordinates by

$$A^1 = \tfrac{1}{2}(w^1 + w'^1), \tag{108}$$

$$A^2 = \tfrac{1}{2}(w^2 + \mu^2 w'^2), \tag{109}$$

$$A^3 = \frac{i}{2}(w'^1 - w^1), \tag{110}$$

$$A^4 = \frac{i}{2}(-\mu^{-2} w^2 + w'^2). \tag{111}$$

Substituting (108)–(111) in the algebra (76), we obtain the following commutation relations for the A^i:

$$A^2 A^4 = A^4 A^2, \tag{112}$$

$$A^2 A^1 - iA^2 A^3 = \mu(A^1 A^2 - iA^3 A^2), \tag{113}$$

$$A^3 A^4 + iA^1 A^4 = \mu^{-1}(A^4 A^3 + iA^4 A^1), \tag{114}$$

$$A^1 A^3 - A^3 A^1 = \frac{i}{2}(\mu^{-2} - 1)(A^2 A^2 + \mu^4 A^4 A^4). \tag{115}$$

Note that from the relations (76) and (101), it follows that the ''q-distance'' defined as the fundamental bilinear form is ''real,'' i.e.,

$$\langle w, w \rangle = w'^1 w^1 + w'^2 w^2 = \langle w, w \rangle^*, \tag{116}$$

and it is also central to the algebra $\mathscr{B}$.

If we now write the q-distance in terms of the ''real'' coordinates, we have

$$\langle w,w\rangle = A^i A^j g_{ij} = A^1 A^1 + A^3 A^3 + \tfrac{1}{2}(1+\mu^{-2})(A^2 A^2 + \mu^4 A^4 A^4). \tag{117}$$

Observe that (117) has the Euclidean metric as the classical limit. The q-derivations $\{\partial/\partial A^i\}$, corresponding to the real coordinates A^i, follow directly from the chain rule

$$\frac{\partial}{\partial A^i} = \frac{\partial w^j}{\partial A^i}\frac{\partial}{\partial w^j} \equiv \frac{\partial w^j}{\partial A^i}\,\partial_j\,. \tag{118}$$

We thus obtain

$$\frac{\partial}{\partial A^1} = \partial_1 + \partial_1'\,, \tag{119}$$

$$\frac{\partial}{\partial A^2} = \partial_2 + \mu^{-2}\partial_2'\,, \tag{120}$$

$$\frac{\partial}{\partial A^3} = i(\partial_1 - \partial_1'), \tag{121}$$

$$\frac{\partial}{\partial A^4} = i(\mu^2\partial_2 - \partial_2'), \tag{122}$$

and $\partial A^i/\partial A^j = \delta_{ij}$, $(\partial/\partial A^i)^* = \overleftarrow{\partial}/\partial A^i$.

Note also that, in contrast to the solution suggested in Ref. 19, where conjugation of partial derivatives involves nonlinear terms of arbitrary order, our *-operation preserves the space of partial derivatives, intertwining the left and right differential structures.

Another approach in constructing a differential calculus is given in Ref. 20, where analogues of the Laplacian (see Sec. VI B) and the metric observable are similar to the entities considered here. On the other hand, our approach is fully based on the general theory of Clifford algebras, and does not presume a unique *-structure, since quantum groups are used mainly as auxiliary entities for the construction of the corresponding braidings (via the formalism of bicovariant bimodules). Thus we believe that our formalism would be less restrictive because one could exploit the nonuniqueness of the *-operator to investigate several possible q-Euclidean spaces with the same classical limit, as we commented before.

VII. QUANTUM GROUPS FROM CLIFFORD ALGEBRAS

Our above described general theory of quantum Clifford algebras based on a deformation of Cartan's theory of spinors can be readily applied to the construction of the different q-groups associated with the underlying Euclidean and pseudo-Euclidean spaces, as well as to the construction of their corresponding double covering quantum spin groups.

Indeed, by requiring that the fundamental property of spinor transformations [Eq. (71)] be preserved in the quantum case, and using the linearity of $H(\mathbf{w})$, a noncommutative algebra $\mathscr{B}$ with a consistent *-structure can be imposed for which the generators are the ''coordinates'' of the underlying (pseudo)-Euclidean space.

The fundamental representation of the corresponding quantum group comes from providing the algebra $\mathscr{B}$ with the structure of a comodule on which this quantum group coacts. By further requiring that the resulting quantum group leaves invariant the fundamental quadric $\langle \mathbf{x},\mathbf{x}\rangle$ results in the $O_q(n-h,h)$ groups associated to the possible signatures $(n-h,h)$ of the q-spaces.

To derive the corresponding double-covering q-spin groups, we use our Clifford algebra to define a q-spinor representation by

$$\xi=\sum_{p=0}^{\nu}\sum_{k_1<\cdots<k_p}\xi^{k_1\cdots k_p}\otimes H_{k_1}\cdots H_{k_p}\cdot 1. \tag{123}$$

The spinor components $\xi^{k_1\cdots k_p}$ generate a noncommutative algebra.

We also introduce the involutive and antimultiplicative τ-transpose operation, $\xi\in S\to\xi^{\tau}\in S'$, which maps linearly spinors in S to spinors in the dual space S'. This operation is uniquely defined by its action on the generators of the Clifford algebra:

$$1^{\tau}=1',H_i^{\tau}=H_i',(H_i')^{\tau}=H_i,(H_iH_j\cdots H_l\cdots H_p)^{\tau}=H_p'\cdots H_l'\cdots H_j'H_i', \tag{124}$$

which defines a right action of the initial Clifford algebra in the dual space.

Hence

$$\xi^{\tau}=\sum_{p=0}^{\nu}\sum_{k_1<\cdots<k_p}\xi^{k_1\cdots k_p}\otimes 1'\cdot H_{k_p}'\cdots H_{k_1}'. \tag{125}$$

Note that by virtue of (39)–(40) and (124) the elements $\{(H_{k_1}\cdots H_{k_p}\cdot 1)^{\tau}=1'\cdot H_{k_p}'\cdots H_{k_1}'\}$ form a basis reciprocal to $\{H_{k_1}\cdots H_{k_p}\cdot 1\}$, $k_1<\cdots<k_p$, which allows us to define a scalar product for homogeneous spinors of p-degree, given by

$$\begin{aligned}[(\xi^{(p)})^{\tau},\ \eta^{(p)}]:&=\sum_{k_1<\cdots<k_p}\xi^{k_1\cdots k_p}\eta^{k_1\cdots k_p}[1'\cdot H_{k_p}'\cdots H_{k_1}',H_{k_1}\cdots H_{k_p}\cdot 1]\\&=\sum_{k_1<\cdots<k_p}\xi^{k_1\cdots k_p}\eta^{k_1\cdots k_p}1'\cdot H_{k_p}'\cdots H_{k_1}'\cdot H_{k_1}\cdots H_{k_p}\cdot 1\\&=\sum_{k_1<\cdots<k_p}\xi^{k_1\cdots k_p}\eta^{k_1\cdots k_p}.\end{aligned} \tag{126}$$

Requiring that the scalar product of any two spinors respects gradation, we thus have

$$[\xi^{\tau},\ \eta]=\sum_{p=0}^{\nu}\sum_{k_1<\cdots<k_p}\xi^{k_1\cdots k_p}\eta^{k_1\cdots k_p}. \tag{127}$$

(Note that the above formula for the scalar product reduces to the definition used in Sec. IV when the spinor components become $\mathbb{C}$-numbers). Now, in analogy to the classical Cartan spinor theory, we introduce a spinor metric operator C, acting on spinors via the q-Clifford product, by

$$C=\sum_{p=0}^{\nu}(-1)^{p(p+1)/2}\sum_{\substack{\pi\in S_{\nu}\\ \pi(1)<\cdots<\pi(p)\\ \pi(p+1)<\cdots<\pi(\nu)}}(-1)^{l(\pi)}a^{p}_{\pi(1)\cdots\pi(p)}(\mu)H_{\pi(1)}\cdots H_{\pi(p)}(H_{\pi(p+1)}\cdots H_{\pi(\nu)})^{\tau}, \tag{128}$$

where $a^{p}_{\pi(1)\cdots\pi(p)}(\mu)$ are μ-parameter-valued commuting quantities such that in the classical limit they are equal to one.

This allows us to define a fundamental spinor bilinear by means of

$$(\xi,\xi)=[\xi^{\tau},C\cdot\xi]. \tag{129}$$

The quantum Spin (n) groups can then be constructed by introducing a matrix with block-diagonal entries, giving these entries the structure of a Hopf algebra and requiring that:

(1) each block sub-matrix should be unimodular,
(2) the fundamental spinor bilinear be central in the spinor components algebra,
(3) the fundamental spinor bilinear be invariant under the coaction map,
(4) we have

$$\delta:(\xi,H_\alpha\xi)\mapsto\sum_\beta t_{\alpha\beta}\otimes(\xi,H_\beta\xi),$$

where $t_{\alpha\beta}$ are the elements of the corresponding q-orthogonal groups.

Conditions (2) and (3) fix uniquely and consistently the parameters in (128), while (4) establishes the covering character of the q-spin groups.

The details of this procedure, which applies to arbitrary dimensions, are beyond the scope of this work, and will be presented in a forthcoming separate paper.

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APPENDIX: RIGHT $\mathscr{A}$-MODULE STRUCTURES ON V AND V' FOR SL(n,$\mathbb{C}$)

From (26)–(29) we get the following right $\mathscr{A}$-module structure on V:
for $i<j$,

$$e_i\circ u_{kj}=\delta_{kj}\beta\mu e_i,\quad e_j\circ u^*_{ii}=\frac{1}{\mu\beta}\,e_j,$$

$$e_j\circ u^*_{ij}=\frac{\mu^2-1}{\beta\mu^{2(1+i-j)}}\,e_i,\quad e_j\circ u^*_{ik}=0,\quad k\neq\{i,j\};$$

for $i>j$,

$$e_i\circ u_{ij}=\beta(1-\mu^2)e_j,\quad e_i\circ u_{jj}=\beta\mu e_i,$$

$$e_i\circ u_{kj}=0,\quad k\neq\{i,j\},\quad e_j\circ u^*_{ik}=\frac{\delta_{ki}}{\beta\mu}\,e_j;$$

and finally, for $i=j$,

$$e_i\circ u^*_{ik}=\frac{1}{\beta}\,\delta_{ik}e_i,\quad e_i\circ u_{ki}=\delta_{ki}\beta e_i,$$

where $\beta=\mu^{1-n/n}$ (as follows from the quantum determinant condition).

Now using the definition (29) of $\circ$ in the dual space V' we obtain for $i\neq j$,

$$e'_i\circ u^*_{ji}=0,\quad e'_i\circ u^*_{ij}=\begin{cases}\beta(1-\mu^2)e'_j & \text{if } i<j,\\ 0 & \text{if } i>j,\end{cases}$$

$$e'_i\circ u^*_{jj}=\beta\mu e'_i,\quad e'_i\circ u^*_{kj}=0,\quad k\neq\{i,j\},\quad e'_i\circ u_{kj}=0,\quad k\neq\{i,j\},$$

$$e_i' \circ u_{ij} = 0, \quad e_i' \circ u_{jj} = \frac{1}{\beta\mu}\, e_i', \quad e_i' \circ u_{ji} = \begin{cases} \dfrac{\mu^2 - 1}{\beta\mu^2}\, e_j' & \text{if } j > i, \\ 0 \quad \text{if } j < i, \end{cases}$$

and the relations

$$e_i' \circ u_{ii} = \frac{1}{\beta}\, e_i', \quad e_i' \circ u_{ii}^* = \beta e_i',$$

when $i = j$.

The right $\mathscr{A}$-module structures on V and V' enable us to compute in an analogous way the remaining three flip-over operators. We shall omit listing them.

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An ill-posed problem of the continuation of transient data for a hyperbolic equation in a three-dimensional inhomogeneous half-space

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A time-domain data continuation problem for a second order hyperbolic equation in a three-dimensional inhomogeneous half-space, which is a common problem in time-domain layer-stripping, is considered. Two different approaches, namely the local continuation approach and the wave-splitting approach, are used to propagate the surface data (the Dirichlet and Neumann data) to the data at deeper planes. The local continuation approach requires a regularization in order to obtain a stable numerical result. The wave-splitting approach uses larger transverse spatial domain of dependence, and gives reasonably stable results even without any additional smoothing process. © *1996 American Institute of Physics.*
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I. INTRODUCTION AND STATEMENT OF THE PROBLEM

For any time-domain layer-stripping approach to an inverse problem, one has to propagate the transient wave field (the Dirichlet data) and its normal derivative (the Neumann data) to the next layer below (layer by layer) starting from the surface data which can be obtained from experimental measurements. In the present paper we treat such a data continuation problem for the following second order hyperbolic equation:

$$(\partial_t^2-\partial_z^2)u=F(x,y,z,t;u), \tag{1}$$

where

$$F(x,y,z,t;u)=a_1\partial_x^2u+a_2\partial_y^2u+A_1\partial_xu+A_2\partial_yu+A_3\partial_zu-b\partial_tu, \tag{2}$$

and where the coefficients a_1, a_2, A_j $(j=1,2,3)$, b are functions of spatial variables (x,y,z). The data continuation problem is to determine the internal field u and its normal derivative $\partial_z u$ from the surface data, i.e., $u|_{z=0}$ and $(\partial_z u)|_{z=0}$. Such a data continuation problem is in general ill-posed in the high-dimensional case. The ill-posedness can be illustrated by a simple example in homogeneous space with $a_1=a_2=1$ and $A_1=A_2=A_3=b=0$. Assume that the exact surface data are $u|_{z=0}=v_0(x,y,t),(\partial_z u)|_{z=0}=0$ and the corresponding solution to the internal field is $u=w(x,y,z,t)$. Now if there is a small perturbation (error) to the field at the surface such that $u|_{z=0}=v_0(x,y,t)+\epsilon\sin(k_1x)\sin(k_2y)\sin(kt)$ (ϵ is a small constant, and $k_1^2+k_2^2>k^2$), then the solution to the internal field becomes $u = w + \epsilon \sin(k_1x)\sin(k_2y)\sin(kt)\cosh(\sqrt{k_1^2+k_2^2-k^2}z)$, which has an exponentially growing error as the depth z increases. Some mathematical aspects of the propagation problem in a homogeneous space have been considered in Refs. 1 and 2. In the present paper, we give two alternative approaches to the ill-posed problem of the continuation of the transient data in an three-dimensional inhomogeneous half-space. The first approach is to use the local continuation formulas for which a regularization process is necessary. The second ap-

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proach is to use the dynamic integro-differential equations for the split fields (see, e.g., Refs. 3–8 for wave-splittings and their applications to inverse problems). In the wave-splitting approach, a larger transverse spatial domain of dependence is used, and the continuation results are reasonably stable even without any additional smoothing process. Once a successful continuation approach has been established, one can use the wave front condition, which relates the split fields at the wave front to the material parameters, to reconstruct these parameters.[7]

II. APPROACH ONE: LOCAL CONTINUATION FORMULAS

A. Local continuation theorem

In order to obtain a local continuation formula that can be employed in the next subsection, we prove a continuation theorem for the hyperbolic equation (1).

The continuation problem involves determining the values of u in some region of the half-space $z>0$ for a range of value of t, given the Dirichlet and Neumann values of u on the plane $z=0$,

$$u=v_0(x,y,t), \quad \frac{\partial u}{\partial z}=v_1(x,y,t); \quad z=0, \quad |t-t_0|<T. \tag{3}$$

To specify the conditions on the data and the coefficients of Eq. (1), we need to introduce the local Banach space A_s of analytic functions $w(x,y)$ in the transverse variables (x,y), whose norm is defined as follows:

$$\|w\|_s=\sum_{l=0}^{\infty}\sum_{p=0}^{\infty}\frac{s^{l+p}}{l!p!}\left|\frac{\partial^{l+p}w(0,0)}{\partial^p x\partial^l y}\right|, \tag{4}$$

where s is real and $s>0$. We will assume that v_0, v_1 belong to A_{s_0}, and v_0 is a C^1, v_1 a C^0 function of time. For $|t-t_0|\leqslant\tau$, $v_0\in C^1(A_{s_0},[t_0-\tau,t_0+\tau])$, $v_1\in C^0(A_{s_0},[t_0-\tau,t_0+\tau])$.

We will also assume that the coefficients a_1, a_2, A_j $(j=1,2,3)$ and b belong to A_{s_0} and are continuous functions of z for $0\leqslant z\leqslant T$, and so the solution of Eq. (1) will be in the following (z,t) domain:

$$D_T=\{(z,t)|0\leqslant z\leqslant T, \ z-T<t-t_0<T-z\}. \tag{5}$$

We use the following norm:

$$\|u\|_{s,D_T}=\max_{(z,t)\in D_T}\|u\|_s(z,t), \tag{6}$$

for functions $u(x,y,z,t)$, which are analytic in (x,y) and continuous in (z,t) in the domain D_T.

Equation (1) can be transformed in the following integral differential form:

$$u(x,y,z,t)=u_0(x,y,z,t)-\frac{1}{2}\int_0^z\int_{t-z+z'}^{t+z-z'}F(x,y,z',t';u)dt'dz', \tag{7}$$

where

$$u_0=\frac{1}{2}[v_0(x,y,t+z)+v_0(x,y,t-z)]+\frac{1}{2}\int_{t-z}^{t+z}v_1(x,y,t')dt'. \tag{8}$$

Differentiating Eq. (7) with respect to z and t, we obtain the additional equations

$$\frac{\partial u}{\partial z}=\frac{\partial u_0}{\partial z}-\frac{1}{2}\int_0^z [F(x,y,z',t+z-z';u)+F(x,y,z',t-z+z';u)]dz', \tag{9}$$

and

$$\frac{\partial u}{\partial t}=\frac{\partial u_0}{\partial t}-\frac{1}{2}\int_0^z [F(x,y,z',t+z-z';u)-F(x,y,z',t-z+z';u)]dz'. \tag{10}$$

By setting

$$U=\begin{bmatrix} u \\ \partial_z u \\ \partial_t u \end{bmatrix}, \quad U^0=\begin{bmatrix} u_0 \\ \partial_z u_0 \\ \partial_t u_0 \end{bmatrix}, \tag{11}$$

the systems of Eqs. (7)–(10) can be expressed in the following operator form:

$$U=U^0+T[U]. \tag{12}$$

As will be shown in a subsequent theorem, the above system of equations can be solved by successive approximation,

$$U^{n+1}=U^0+T[U^n], \quad n=0,1,2,\ldots, \tag{13}$$

starting from U^0 [given by Eq. (11)]. To show convergence of the iteration process, we need to introduce the sequence V^n,

$$V^n=U^{n+1}-U^n, \quad n=0,1,2,\ldots . \tag{14}$$

Obviously, we have

$$V^0=T[U^0], \tag{15}$$

$$V^n=T[V^{n-1}], \quad n=1,2,3,\ldots . \tag{16}$$

From the definitions (4)–(6), and Eq. (8), it follows that there exists a positive real constant α such that for $0<s\leqslant s_0$,

$$\max\left\{\|u_0\|_{s,D_T}, \left\|\frac{\partial u_0}{\partial z}\right\|_{s,D_T}, \left\|\frac{\partial u_0}{\partial t}\right\|_{s,D_T}\right\}\leqslant\alpha. \tag{17}$$

Thus, the components of U^0 satisfy the inequality

$$\|U_j^0\|_{s,D_T}\leqslant\alpha, \quad 0<s\leqslant s_0, \quad j=1,2,3. \tag{18}$$

To obtain estimates for $V^{(n)}$ we need to introduce the constant β such that

$$\max\{\|a_1\|_{s_0,D_T},\|a_2\|_{s_0,D_T},\|A_j\|_{s_0,D_T}(j=1,2,3),\|b\|_{s_0,D_T}\}\leqslant\beta. \tag{19}$$

Set

$$\rho_0=\beta(32+6s_0), \tag{20}$$

and choose the positive real constant a_0 such that

$$a_0\rho_0<1,\ \ a_0^2\rho_0<1,\ \ a_0s_0<T,\ \ a_0<T. \tag{21}$$

Let

$$\rho=\max[a_0\rho_0,a_0^2\rho_0], \tag{22}$$

it then follows that $\rho<1$. In the following lemma we will need the following decreasing sequence

$$a_n=a_{n-1}/[1+1/n^2],\quad n=1,2,3,\ldots\ . \tag{23}$$

Note that the sequence $\{a_n\}$ is bounded away from zero.

Lemma: For $0\leqslant z<a_n(s_0-s)$, $|t-t_0|\leqslant z$, the following inequalities hold:

$$\|V_1^n\|_s(z,t)<\lambda_0\rho^n z/[a_n(s_0-s)-z], \tag{24}$$

$$\|V_j^n\|_s(z,t)<\lambda_0\rho^n a_n z/[a_n(s_0-s)-z]^2,\quad j=2,3, \tag{25}$$

where

$$\lambda_0=4\beta\alpha[8+s_0+s_0^2/2]\max[a_0,a_0^2]. \tag{26}$$

See the Appendix for the proof of the above lemma.

It can now be shown that the method of successive approximation (13) converges.

Restricting (z,t) to the region $0\leqslant z<a_{n+1}(s_0-s)$, $|t-t_0|\leqslant z$, it follows from the lemma that

$$\sum_{k=0}^{n}\|V_1^k\|_s\leqslant\lambda_0\sum_{k=0}^{n}\frac{\rho^k z}{[a_k(s_0-s)-z]},$$

$$\sum_{k=0}^{n}\|V_j^k\|_s\leqslant\lambda_0\sum_{k=0}^{n}\frac{\rho^k a_k z}{[a_k(s_0-s)-z]^2},\quad j=2,3.$$

Using the result that $z<a_{n+1}(s_0-s)\leqslant a_0(s_0-s)$, and relation (23), it follows that

$$\sum_{k=0}^{n}\|V_1^k\|_s\leqslant\lambda_0\sum_{k=0}^{n}\frac{\rho^k a_{k+1}}{[a_k-a_{k+1}]}\leqslant\lambda_0\sum_{k=0}^{n}\rho^k(k+1)^2, \tag{27}$$

$$\sum_{k=0}^{n}\|V_j^k\|_s\leqslant\frac{\lambda_0}{(s_0-s)}\sum_{k=0}^{n}\frac{\rho^k a_{k+1}a_k}{(a_k-a_{k+1})^2}\leqslant\frac{\lambda_0}{(s_0-s)}\sum_{k=0}^{n}\rho^k[(k+1)^4+(k+1)^2],\quad j=2,3. \tag{28}$$

Since the constant a_0 has been chosen so that $\rho<1$, the series on the right-hand sides of the above two inequalities converge. Thus, it follows from the above two inequalities that the left-hand sides converge. From Eq. (14) it follows that

$$U^{n+1}=U^0+\sum_{k=0}^{n}V^k. \tag{29}$$

Thus for $n>m$,

$$\|U_j^n - U_j^m\|_s = \left\| \sum_{k=m+1}^{n} V_j^k \right\| \leqslant \sum_{k=m+1}^{n} \|V_j^k\|, \quad j=1,2,3, \tag{30}$$

which implies that U_j^n, $j=1,2,3$, converge. We can now state the theorem.

Local Continuation Theorem: For $0 \leqslant z < a_\infty(s_0 - s)$, $|t - t_0| \leqslant z$, where $a_\infty = \lim_{n\to\infty} a_n$, the sequence $\{U^n\}$ converges, and the solution $u(x,y,z,t)$ to the system of Eqs. (1)–(3) exists such that $u(x,y,z,t)$ is an analytic function in A_s and a C^1 function in z and t.

B. Finite-difference formulas

Here we give the finite-difference formulas of the local continuation theorem for the following acoustic wave equation:

$$\partial_t^2 u - \rho \nabla \cdot \left(\frac{1}{\rho} \nabla u \right) + b \partial_t u = 0, \tag{31}$$

where $\rho(x,y,z)$ is the density, and $b(x,y,z)$ is the dissipation coefficient (the velocity has a value of unity). Consider the problem of determining the value of u and $\partial u/\partial z$ on $z=h$ (h is small for use in a finite-difference formula) for Eq. (31), given the data $u = v_0$, $\partial u/\partial z = v_1$ on the plane $z=0$. We will assume that the data v_0, v_1, are piecewise analytic in the transverse variables (x,y), with v_0, v_1 being C^1 and C^0 functions of t, respectively, over certain intervals, with the discontinuities in x, y and t being of a wave front type (on the intersection of a characteristic surface and the plane $z=0$). In this paper we will treat the case where the discontinuity is a wave front moving in the positive z-direction. For the wave front moving in the opposite direction or combined directions, the theorem in the previous subsection has to be properly modified.

To apply the theorem in the previous subsection, we take $a_1 = a_2 = 1$, $(A_1, A_2, A_3) = -\nabla(\ln \rho)$. For small values of $z=h$, we take the approximate solution of system (12), given by the iterate $U^1 = U^0 + T(U^0)$, where U^0 is given by Eq. (11). Thus, it follows from Eqs. (2), (7), (8), and (9) that the solution to the above order is

$$u(x,y,h,t) = u_0(x,y,h,t) - \frac{1}{2} \int_0^h \int_{t-h+z'}^{t+h-z'} F(x,y,z',t';u_0)\, dt'\, dz', \tag{32}$$

$$\partial_z u(x,y,h,t) = \partial_z u_0(x,y,h,t) - \frac{1}{2} \int_0^h [F(x,y,z',t+h-z';u_0) + F(x,y,z',t-h+z';u_0)]\, dz', \tag{33}$$

where

$$\begin{aligned} u_0(x,y,z,t) &= \frac{1}{2}[v_0(x,y,t+z) + v_0(x,y,t-z)] + \frac{1}{2} \int_{t-z}^{t+z} v_1(x,y,t')\, dt', \\ F(x,y,z,t;u_0) &= (\partial_x^2 + \partial_y^2) u_0 - \nabla(\ln \rho) \cdot \nabla u_0 - b \partial_t u_0. \end{aligned} \tag{34}$$

Therefore, the sought-for expressions for u and $\partial u/\partial z$ at $z=h$ are

$$\begin{aligned} u(x,y,h,t) = {} & \frac{1}{2}[v_0(x,y,t+h) + v_0(x,y,t-h)] + \frac{1}{2} \int_{t-h}^{t+h} v_1(x,y,t')\, dt' - \frac{h^2}{2} [(\partial_x^2 + \partial_y^2) v_0 \\ & - (\partial_x v_0) \partial_x (\ln \rho)|_{z=0} - (\partial_y v_0) \partial_y (\ln \rho)|_{z=0} - v_1 \partial_z (\ln \rho)|_{z=0} - b \partial_t v_0] + O(h^3), \end{aligned} \tag{35}$$

$$[\partial_z u](x,y,h,t)=\tfrac{1}{2}[\partial_t v_0(x,y,t+h)-\partial_t v_0(x,y,t-h)]+\tfrac{1}{2}[v_1(x,y,t+h)+v_1(x,y,t-h)]$$
$$-h[(\partial_x^2+\partial_y^2)v_0-(\partial_x v_0)\partial_x(\ln\rho)|_{z=0}-(\partial_y v_0)\partial_y(\ln\rho)|_{z=0}$$
$$-v_1\partial_z(\ln\rho)|_{z=0}-b\partial_t v_0]+O(h^2). \tag{36}$$

Repeatedly applying the above two formulas, one can propagate the data $(u,\partial_z u)$ layer by layer (from the surface data) to the data at the planes $z=nh$, $n=1,2,3,\ldots$. Note that in the repeated application of the formulas, the smoothness parameter s_0 has to be replaced by s_n, $n=1,2,3,\ldots$, which is related to h through the constant $h<a_\infty(s_n-s_{n+1})$, $n=1,2,3,\ldots$. This limits the range of continuation with respect to z.

In order to obtain some reliable reference data to compare with our continuation results, we generate the data with either an explicit solution (in the case of a homogeneous medium) or a finite-difference time-domain method. In all the numerical examples, we assume that the medium above the surface $z=0$ is homogeneous and non-dissipative, and a point source is located at the point $\mathbf{r}_0=(0,0,z_0)(z_0<0)$ in the homogeneous upper half-space $z<0$ (the inhomogeneity is confined in the lower half-space $z>0$). The incident field in an entirely homogeneous space satisfies the following equation:

$$\partial_t^2 p^i-\nabla^2 p^i=\delta(\mathbf{r}-\mathbf{r}_0)f(t), \tag{37}$$

which has the solution

$$p^i=\frac{f(t-|\mathbf{r}-\mathbf{r}_0|)}{4\pi|\mathbf{r}-\mathbf{r}_0|}. \tag{38}$$

In all the numerical examples in the present paper, we choose the position of the point source to be $z_0=-0.5$, and $f(t)$ to be

$$f(t)=\begin{cases}\sin^2(\pi t/t_0), & \text{when } 0\leqslant t\leqslant t_0,\\ 0, & \text{otherwise,}\end{cases}$$

where $t_0=0.4$.

Numerical example 1 (case of a homogeneous medium): Consider the simplest case when the whole space is homogeneous and non-dissipative. The surface fields and their normal derivatives can be obtained from the explicit solution (38). We choose $\Delta x=\Delta y=\Delta z=2\Delta t=0.005$, and calculate the field and its normal derivative at the point (0,0,0.1), which is on the 20th layer, using the local continuation formulas (35) and (36). The continuation results are given by the dotted lines in Figs. 1(a) and 1(b), where the corresponding exact values [obtained from (38)] are given by the solid lines. Numerical results in Figs. 1(a) and 1(b) show that the continuation scheme is not stable, which is mainly due to the second order transverse spatial derivatives of the fields in the formulas (35) and (36). Thus, one needs to regularize[9] (smooth) the data before using the finite-difference formulas (35) and (36). In the next subsection, we describe a way to regularize the data.

C. Regularization

To obtain reliable second order transverse spatial derivatives of the field u, we need to smooth u to at least twice differentiable in respect with the transverse spatial variables $\mathbf{x}=(x,y)$. Define a function

$$S(\mathbf{x})=\frac{e^{-2\gamma\sqrt{|\mathbf{x}|+4}}}{2\pi\sqrt{|\mathbf{x}|+4}}. \tag{39}$$

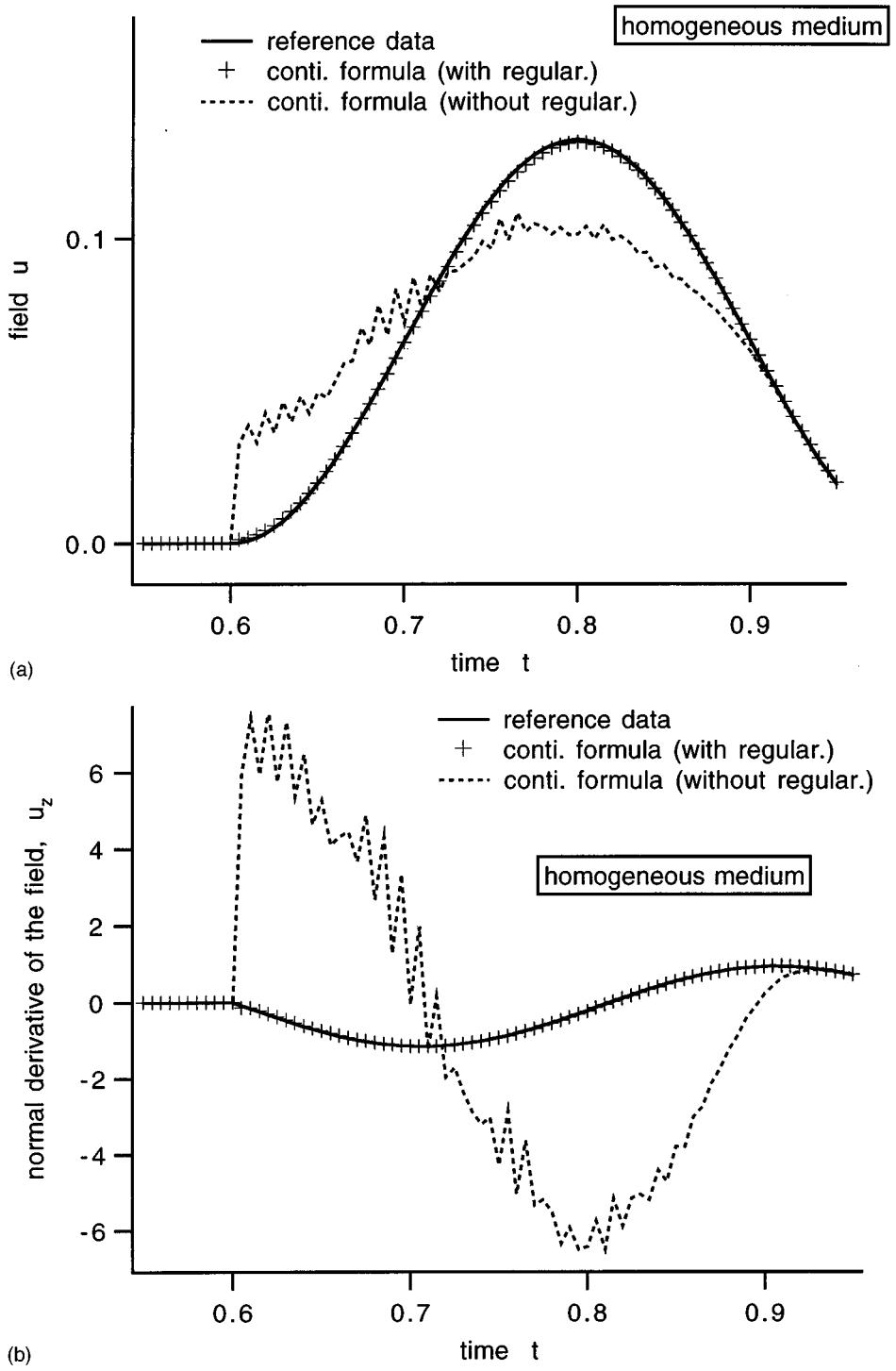

FIG. 1. (a) and (b) The local continuation formulas for data continuation in a homogeneous space. The solid lines are the exact reference data at a point (0,0,0.1) obtained from Eq. (38). The dotted lines are the corresponding continuation results using the local continuation formulas (35) and (36) without regularization. Here we choose $\Delta x=\Delta y=\Delta z=2\Delta t=0.005$, and the point (0,0,0.1) is at the 20th layer. The crosses are the corresponding continuation results using the regularization formula (43) with $d=0.005$.

Its Fourier transformation is

$$\widetilde{S}(\overline{\mathbf{x}})\equiv(\mathbf{F}^{-1}S)(\overline{\mathbf{x}})=\int S(\mathbf{x})e^{i\mathbf{x}\overline{\mathbf{x}}}d\mathbf{x}=2\pi\int_0^\infty S(\mathbf{x})J_0(|\mathbf{x}||\overline{\mathbf{x}}|)|\mathbf{x}|d|\mathbf{x}|=\frac{\exp(-2\sqrt{|\overline{\mathbf{x}}|^2+(2\gamma)^2})}{\sqrt{|\overline{\mathbf{x}}|^2+(2\gamma)^2}}. \tag{40}$$

If we choose γ such that it satisfies $\gamma=1/2e^{-4\gamma}$, i.e.,

$$\gamma=0.21315138, \tag{41}$$

then $S(\mathbf{x})$ and $\widetilde{S}(\overline{\mathbf{x}})$ are a pair of Fejer kernels (cf. e.g., Ref. 10), since $\widetilde{S}(0)=1$, $S(-\mathbf{x})=S(\mathbf{x})$, and $S,\ \widetilde{S}\in L_1$.

Define

$$S_d(\mathbf{x})\equiv\frac{1}{d^2}\,S\left(\frac{\mathbf{x}}{d}\right)=\frac{1}{2\pi}\cdot\frac{\exp[(-2\gamma/d)(\sqrt{|\mathbf{x}|^2+(2d)^2})]}{d\sqrt{|\mathbf{x}|^2+(2d)^2}}, \tag{42}$$

then we have the following theorem.

Regularization Theorem: If $u\in L_1$ and is bounded, then the following formula holds:

$$\lim_{d\to+0}\int_{R^2}S_d(\mathbf{x}-\overline{\mathbf{x}})u(\overline{\mathbf{x}})d\overline{\mathbf{x}}=u(\mathbf{x}). \tag{43}$$

Proof: Introduce the Fejer mean of u defined as

$$u_d(\mathbf{u})=\int_{R^2}e^{-i\mathbf{x}\overline{\mathbf{x}}}\widetilde{S}_d(d\overline{\mathbf{x}})\widetilde{u}(\overline{\mathbf{x}})d\overline{\mathbf{x}}, \tag{44}$$

where $\widetilde{S}_d$ and $\widetilde{u}$ are the inverse Fourier transform of S_d and u, respectively. Since $u\in L_1$, according to Theorem 1.13 in Ref. 10, we have

$$u_d(\mathbf{u})\equiv\int_{R^2}S_d(\mathbf{x}-\overline{\mathbf{x}})u(\overline{\mathbf{x}})d\overline{\mathbf{x}}. \tag{45}$$

Also since $u\in L_1$ and is bounded, we have (cf. Theorem 1.15 in Ref. 10),

$$\lim_{d\to+0}u_d(\mathbf{x})=u(\mathbf{x}). \tag{46}$$

Equation (43) follows immediately from the above two equations. The regularization theorem is thus proved.

Note that if the sources have spatial compact support (e.g., in a point source case), the field $u(x,y,z,t)$ is non-zero only within a finite region $\sqrt{x^2+y^2}<D_0$ on a plane $z=z_0$ at any finite time $t=t_0$, and thus obviously $u\in L_1(R^2)$. Using the regularization formula (43), we first test the homogeneous case as described in the numerical example 1. The crosses in Figs. 1(a) and 1(b) are the continuation results using the local continuation formulas (35) and (36) with u being smoothed [using the formula (43) with $d=0.005$] for each time at each layer. These numerical results indicate that the local continuation formulas give quite good continuation results in a homogeneous space if the regularization formula (43) is also used. In the next example we test the local continuation formulas (with the regularization) for a case of an inhomogeneous medium.

Numerical example 2 (the case of an inhomogeneous medium): In this numerical example, we consider an inhomogeneous half-space with the following synthetic density profile:

$$\rho(x,y,z)=1+2\sin^2(\pi z)\exp[-(x^2+y^2/4+z^2/9)], \quad z\geqslant 0. \tag{47}$$

The dissipation coefficient is chosen to be $b=0$ in the whole space. The reference data for the fields and their normal derivatives are calculated with a finite-difference time-domain method, in which one computes the fields step by step in time starting from the trivial initial condition for the fields (see Refs. 11 and 12) for a detailed description; our Connection machine with a memory of 2 GByte in RAM has enough memory to set all the boundary surfaces in x-, y-, and z- directions of the computation domain to be far enough away so that putting the fields to zero at the boundary surfaces will have no effect on the fields at the receiving points and during the time periods of interest). We then use the local continuation formulas (35) and (36) to migrate the surface data (obtained from the finite-difference time-domain method) to the data at the plane $z=0.1$ inside the inhomogeneous medium with $\Delta x=\Delta y=\Delta z=2\Delta t=0.005$. The formula (43) is used to regularize the data at each time and at each layer with $d=0.005$. The crosses in Figs. 2(a) and 2(b) are the continuation results at the point $(x,y)=(0,0)$ on the plane $z=0.1$ (the solid lines are the corresponding reference data). The continuation results appear to be quite good.

Note that in the local continuation formulas, one has to do the regularization (spatial convolution) at each time and at each layer (the spatial convolution is done only after computing u and $\partial_z u$ for all time steps and locations). As shown in Ref. 13, the analyticity of the data can guarantee the stability of the solution to the inverse problem. By such a spatial convolution, the analyticity of the data can be restored after the data continuation in deeper layers. In the next section, we give another approach for the data continuation, which does not require such a regularization.

III. APPROACH TWO: WAVE-SPLITTING FORMULAS

The acoustic wave equation (31) can be written in matrix form as

$$\partial_z\begin{bmatrix} u \\ \partial_z u\end{bmatrix}=\begin{bmatrix} 0 & 1 \\ \Box+(\nabla^T \ln\rho)\cdot\nabla^T+b\partial_t & (\partial_z \ln\rho)\end{bmatrix}\begin{bmatrix} u \\ \partial_z u\end{bmatrix}\equiv D\begin{bmatrix} u \\ \partial_z u\end{bmatrix}, \tag{48}$$

where $\Box=\partial_t^2-\partial_x^2-\partial_y^2$, and $\partial^T=(\partial_x,\partial_y)$. The total field can be decomposed into a down-going component u^+ and an up-going component u^- as follows:

$$\begin{bmatrix} u^+ \\ u^-\end{bmatrix}=\frac{1}{2}\begin{bmatrix} 1 & -K \\ 1 & K\end{bmatrix}\begin{bmatrix} u \\ \partial_z u\end{bmatrix}\equiv T\begin{bmatrix} u \\ \partial_z u\end{bmatrix}, \tag{49}$$

where K is the wave-splitting operator, which has the following explicit expression (see Ref. 4 for a detailed mathematical description of the wave-splitting operator):

$$\mathbf{K}u=\frac{1}{2\pi}\int_0^t\int_0^{2\pi} u(x+(t-s)\cos\theta, y+(t-s)\sin\theta, z, s)\,d\theta\,ds. \tag{50}$$

Differentiating Eq. (49) with respect to z and using Eq. (48), yields

$$\partial_z\begin{bmatrix} u^+ \\ u^-\end{bmatrix}=TDT^{-1}\begin{bmatrix} u^+ \\ u^-\end{bmatrix}. \tag{51}$$

After a formal matrix calculation, one obtains[7]

$$(\partial_z+K^{-1})u^+=f, \tag{52}$$

$$(\partial_z-K^{-1})u^-=-f, \tag{53}$$

where K^{-1} is the inverse of K, and

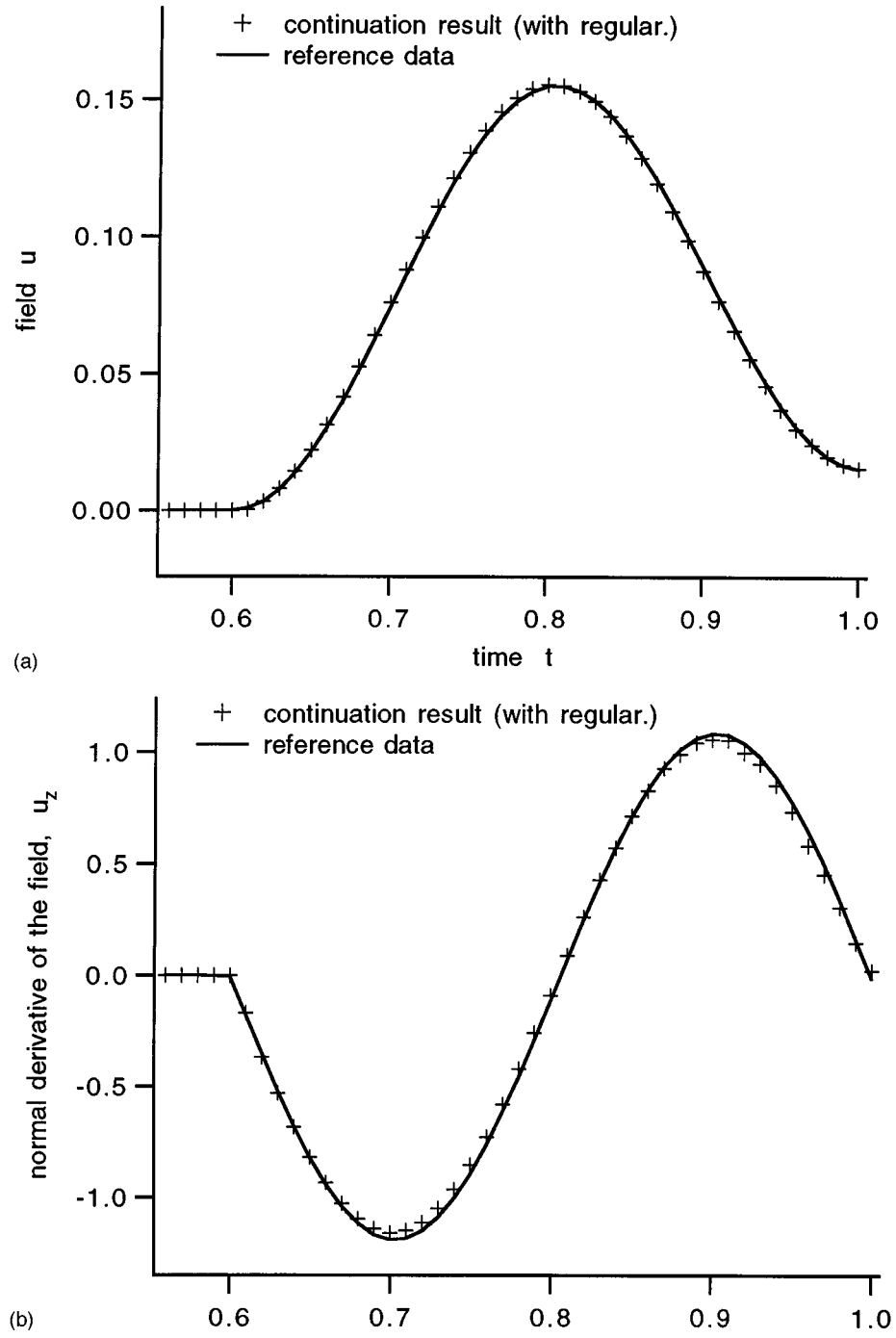

FIG. 2. (a) and (b) Data continuation using the local continuation formulas (with the regularization) in an inhomogeneous half-space with a synthetic density profile $\rho(x,y,z)=1+2\sin^2(\pi z)\exp[-(x^2+y^2/4+z^2/9)]$, for $z\geqslant 0$ (the dissipation coefficient $b\equiv 0$). The solid lines are the reference data at a point $(x,y)=(0,0)$ on the plane $z=0.1$, calculated with a finite-difference time-domain method. The crosses are the corresponding continuation results using the local continuation formulas with $\Delta x=\Delta y=\Delta z=2\Delta t=0.005$. The regularization parameter is chosen to be $d=0.005$.

$$f=-\tfrac{1}{2}K[(\nabla^T \ln \rho)\cdot\nabla^T+b\partial_t](u^+ +u^-)+\tfrac{1}{2}K[(\partial_z \ln \rho)K^{-1}](u^+ -u^-). \tag{54}$$

The operator K^{-1} can be expressed in the following form:[12]

$$\mathbf{K}^{-1}=\partial_t-\mathbf{L}, \tag{55}$$

where

$$\mathbf{L}u=\frac{1}{2\pi}[\partial_x^2(\mathbf{L}_1u)+\partial_y^2(\mathbf{L}_2u)-2\partial_{xy}^2(\mathbf{L}_3u)], \tag{56}$$

with

$$\mathbf{L}_1u=\int_0^t\int_0^{2\pi}\sin^2\theta\, u(x+(t-s)\cos\theta, y+(t-s)\sin\theta, z, s)\,d\theta ds, \tag{57}$$

$$\mathbf{L}_2u=\int_0^t\int_0^{2\pi}\cos^2\theta\, u(x+(t-s)\cos\theta, y+(t-s)\sin\theta, z, s)\,d\theta ds, \tag{58}$$

$$\mathbf{L}_3u=\int_0^t\int_0^{2\pi}\sin\theta\cos\theta\, u(x+(t-s)\cos\theta, y+(t-s)\sin\theta, s)\,d\theta ds. \tag{59}$$

Note that the integrations in the expressions (57)–(59) have a smoothing effect to the data u, and thus the spatial second order derivatives in the expression (56) is not a serious problem in the numerical evaluation of the operator $\mathbf{L}$.

From the dynamic integro-differential equations (52) and (53) for the split fields, we obtain the following approximations:

$$u^+(x,y,z+h,t)=\frac{1}{2\pi}\int\int_{D(x,y,t)}\frac{h}{R^3}[u^+(x',y',z,t-R)+R\partial_t u^+(x',y',z,t-R)]dx'dy' + hf(x,y,z,t)+O(h^2), \tag{60}$$

$$u^-(x,y,z+h,t)=u^-(x',y',z,t+h)-h[\mathbf{L}u^- +f](x,y,z,t)+O(h^2), \tag{61}$$

where $R=\sqrt{(x-x')^2+(y-y')^2+h^2}$, and $D(x,y,t)$ is a disk with center (x,y) and radius t at the z plane. Note that if $f=0$, then Eq. (60) gives the free-space integral formula.[6]

When both u^+ and u^- are calculated at a plane, the internal field u and its normal derivative $\partial_z u$ at that plane can be immediately obtained by

$$u=u^+ +u^-, \tag{62}$$

$$\partial_z u=K^{-1}[u^- -u^+]. \tag{63}$$

Numerical example 3 (using wave-splitting approach). In this numerical example, we consider an inhomogeneous half-space with the following synthetic profile for the dissipation coefficient:

$$b(x,y,z)=100\sin^2(\pi z)\exp[-(x^2+y^2/4+z^2/9)], \quad z\geq 0 \tag{64}$$

(the density ρ is a constant everywhere). The solid and dashed lines are the reference data for the fields at points (0,0,0.1) and (0.2,0,0.1), respectively, calculated with the finite-difference time-domain method. The dotted line is the free-space (i.e., when $b\equiv 0$) solution for the field u at the point (0,0,0.1), and the difference between the solid line and the dotted line indicates the magni-

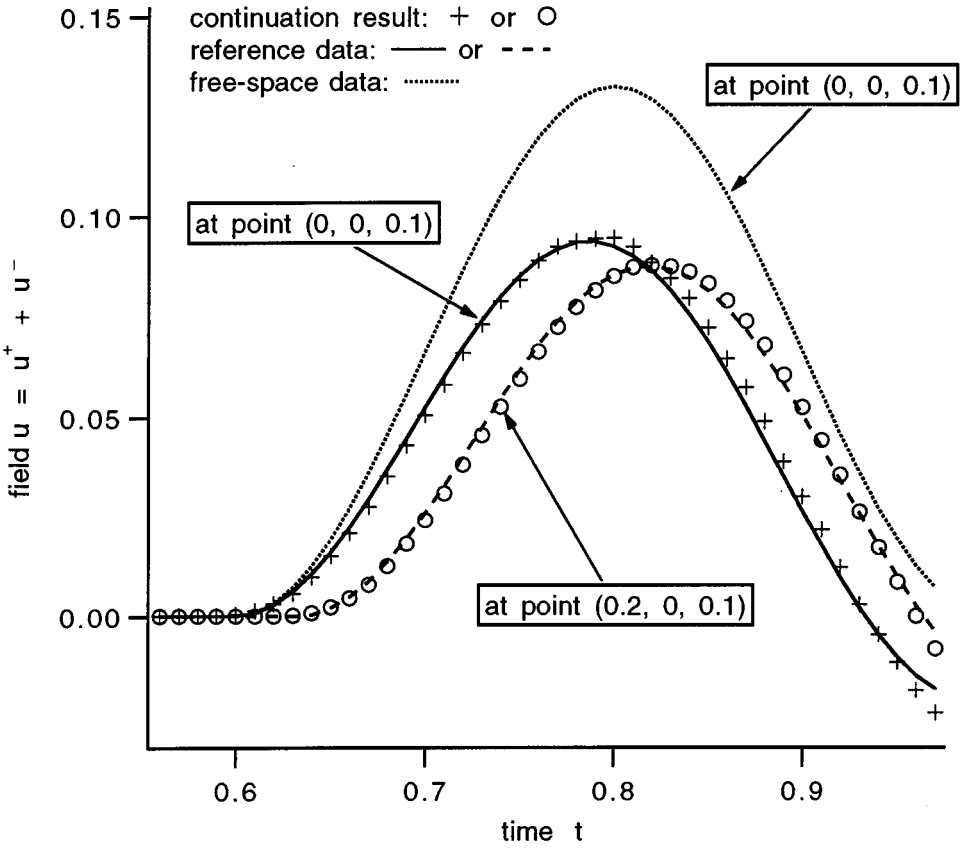

FIG. 3. Data continuation using the wave-splitting formulas (60) and (61) in an inhomogeneous half-space with a synthetic dissipation coefficient profile $b(x,y,z)=100\sin^2(\pi z)\exp[-(x^2+y^2/4+z^2/9)]$, $z\geqslant 0$ (the density ρ is constant everywhere). The solid and dashed lines are the reference data at points (0,0,0.1) and (0.2,0,0.1), respectively, calculated with a finite-difference time-domain method. The crosses and circles are the corresponding continuation data using the wave-splitting formulas with $\Delta x=\Delta y=\Delta z=2\Delta t=0.02$.

tude of scattering due to the dissipation. We use the wave-splitting formulas (60) and (61) to propagate the split fields at the surface (i.e., the incident field, and the reflected field obtained from the finite-difference time-domain method) to the split fields at the plane $z=0.1$ inside the inhomogeneous medium, with $\Delta x=\Delta y=\Delta z=2\Delta t=0.02$. The continuation results are output at two points (0,0,0.1) and (0.2,0,0.1) by the crosses and circles, respectively, in Fig. 3. One sees from Fig. 3 that the continuation data using the wave-splitting approach is smooth, even without any additional smoothing process. To compare with the local continuation approach described in the previous section, we plot the fields at a plane $z=0.1$ with a fixed time $t=0.8$ in Figs. 4(a)–4(c). Figure 4(a) is the reference data calculated by the finite-difference time-domain method. Figure 4(b) is the continuation result obtained by the wave-splitting formulas. Figure 4(c) is the continuation result obtained by the local continuation formulas (with regularization). Both the local continuation approach (with regularization) and the wave-splitting approach give quite good continuation results.

The reason why the wave-splitting approach gives stable results even without any additional smoothing process, is that it takes a larger transverse spatial domain of dependence. Notice that the transverse spatial domain of dependence of the operator K or L is a disk area with radius t. Therefore, if one wants to calculate the field at a point x on the plane $z=h$ up to the time $t=T$, the

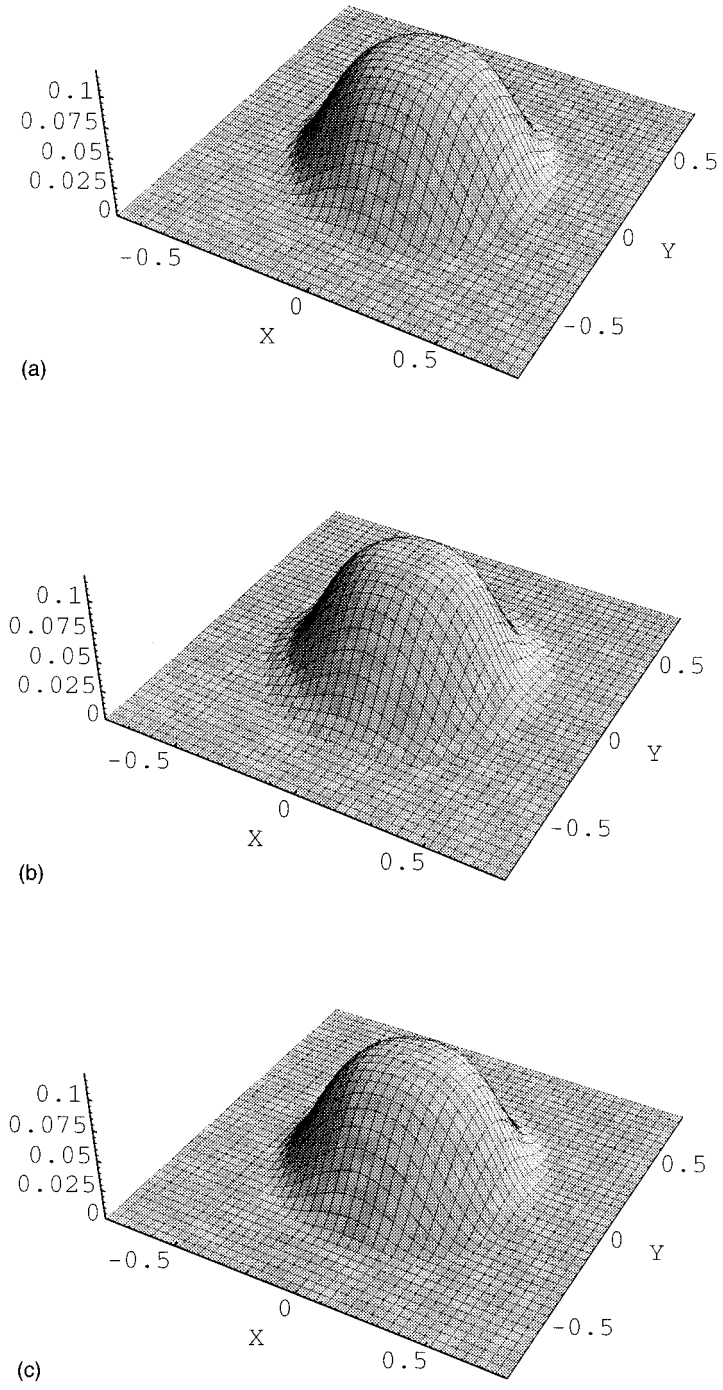

FIG. 4. (a)–(c) Data continuation results at a plane $z=0.1$ with a fixed time $t=0.8$ in an inhomogeneous half-space with a synthetic dissipation coefficient profile $b(x,y,z)=100\sin^2(\pi z)\exp[-(x^2+y^2/4+z^2/9)]$, $z\geqslant 0$ (then density ρ is constant everywhere). (a) is the reference data calculated by the finite-difference time-domain method. (b) and (c) are the corresponding continuation results obtained from the wave-splitting formulas and the local continuation formulas (with the regularization), respectively.

transverse spatial domain of dependence on the surface data is a disk area centered at x with radius T for the wave-splitting formulas (60) and (61), while for the local continuation formulas (35) and (36) the transverse spatial domain of dependence on the surface data is merely a disk centered at x with radius h. Thus, in a sense, the wave-splitting approach stabilizes the ill-posedness by using a larger transverse spatial domain of dependence.

IV. CONCLUSION

In the present paper we have considered the ill-posed problem of the time-domain data continuation for a second order hyperbolic equation in a three-dimensional inhomogeneous half-space. Two different approaches, namely the local continuation approach and the wave-splitting approach, have been used to propagate the surface data (the fields and their normal derivatives) to the data at deeper planes. A local continuation theorem has been given, and its finite-difference form has been used for the data continuation. To obtain a stable continuation result, a regularization process at each time at each plane is necessary in the local continuation approach. The wave-splitting approach uses a larger transverse spatial domain of dependence, and gives reasonably stable results even without any additional smoothing process. Numerical implementations for both the local continuation and the wave-splitting approaches are very suitable for parallel computing (without a parallel machine, the computation time for obtaining the results in Numerical examples 2 and 3 will be several years).

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APPENDIX: PROOF OF THE LEMMA IN SECTION II A

Since

$$F(x,y,z,t;V)=(a_1\partial_x^2+a_2\partial_y^2+A_1\partial_x+A_2\partial_y)V_1+A_3V_2-bV_3, \tag{A1}$$

it follows for $0<s\leqslant s_0,(z,t)\in D_T$, on using the following properties of analytic functions in A_{s_0} (see, e.g., Ref. 13):

$$\|\partial_x^2 u\|_s,\|\partial_y^2 u\|_s\leqslant \frac{4}{(s'-s)^2}\,\|u\|_{s'},\quad 0<s<s'<s_0,$$

$$\|\partial_x u\|_s,\|\partial_y u\|_s\leqslant \frac{1}{s'-s}\,\|u\|_{s'},\quad 0<s<s'<s_0,$$

$$\|u\|_s\leqslant\|u\|_{s'},\quad 0<s<s'<s_0,$$

that

$$\|F(x,y,z,t;V)\|_s(z,t)\leqslant\beta\left[\frac{8}{(s'-s)^2}+\frac{2}{(s'-s)}\right]\|V_1\|_{s'}+\beta\|V_2\|_{s'}+\beta\|V_3\|_{s'}. \tag{A2}$$

Thus, from the relation [the first component of Eq. (16)],

$$V_1^n(x,y,z,t) = -\frac{1}{2}\int_0^z \int_{t-z+z'}^{t+z-z'} F(x,y,z',t';V^{n-1})\,dz'\,dt', \tag{A3}$$

where $n=1,2,...$, it follows that for $(z,t)\in D_T$,

$$\|V_1^n\|_s(z,t) \leqslant \frac{1}{2}\,\beta\int_0^z \int_{t-z+z'}^{t+z-z'} \left\{ \left[\frac{8}{(s'-s)^2} + \frac{2}{(s'-s)} \right] \|V_1^{n-1}\|_{s'} + \|V_2^{n-1}\|_{s'} + \|V_3{}^{n-1}\|_{s'} \right\} dt'\,dz'. \tag{A4}$$

When $n=0$, V_j^{n-1}, $j=1,2,3$, on the right-hand side of Eq. (A4) should be replaced by U_j^0.

In a similar manner, it can be shown using the second and third components of Eq. (16) that of $j=2,3$,

$$\|V_j^n\|_s(z,t) \leqslant \max_{|t'-t|\leqslant z-z'} \beta\int_0^z \left\{ \left[\frac{8}{(s'-s)^2} + \frac{2}{(s'-s)} \right] \|V_1^{n-1}\|_{s'} + \|V_2^{n-1}\|_{s'} + \|V_3^{n-1}\|_{s'} \right\} dz', \tag{A5}$$

for $n=1,2,...$, and when $n=0$, V_j^{n-1} on the right-hand side of Eq. (A5) should be replaced by U_j^0.

Define the following sequence:

$$s_n'(z) = (s_0 + s - z/a_n)/2, \quad n=0,1,2,3,\ldots\ . \tag{A6}$$

The lemma can now be proved by induction. For $n=0$, take $s' = s_0'(z') = (s + s_0 - z'/a_0)/2$ in expressions (A4), (A5), and restrict z so that $0\leqslant z < a_0(s_0-s)$, $|t-t_0|\leqslant z$. Using Eq. (18) and the inequality $s_0(z')-s \leqslant s_0/2$, it can be shown that

$$\|V_1^0\|_s(z,t) \leqslant 4a_0^2\beta\alpha\left(8 + s_0 + \frac{s_0^2}{2}\right)\int_0^z \frac{(z-z')\,dz'}{[a_0(s_0-s)-z']^2} \leqslant \lambda_0 \cdot \frac{z}{[a_0(s_0-s)-z]}. \tag{A7}$$

In a similar manner, it can be shown that

$$\|V_j^0\|_s(z,t) \leqslant \lambda_0 a_0 \int_0^z \frac{dz'}{[a_0(s_0-s)-z']^2} \leqslant \frac{\lambda_0 z a_0}{[a_0(s_0-s)-z]^2}, \tag{A8}$$

for $0\leqslant z < a_0(s_0-s)$.

Hence, inequalities (24) and (25) hold for $n=0$.

Assume that inequalities (24) and (25) hold for $n-1$. Then set $s' = s_n'(z') = (s + s_0 - z'/a_n)/2$ in Eq. (A4), restrict z so that $0\leqslant z < a_n(s_0-s)$, use the inequalities $a_n \leqslant a_{n-1} \leqslant \cdots \leqslant a_0$, and $[a_{n-1}(s_0-s)-z'] \geqslant [a_n(s_0-s)-z']$ valid for $0\leqslant z' < a_n(s_0-s)$ to obtain

$$\|V_1^n\|_s(z,t) \leqslant a_n a_0 \beta\lambda_0\rho^{n-1}(32+6s_0)\int_0^z \frac{(z-z')z'\,dz'}{[a_0(s_0-s)-z']^3} \leqslant \lambda_0\rho^n \cdot \frac{z}{[a_0(s_0-s)-z]}. \tag{A9}$$

The last inequality is obtained by straightforward integration.

In a similar manner, it can be shown from Eq. (A5) for $0\leqslant z < a_n(s_0-s)$, $|t-t_0 \leqslant z|$, that

$$\|V_j^n\|_s(z,t) \leqslant a_0 a_n \lambda_0 \rho^{n-1}\rho_0 \int_0^z \frac{z'\,dz'}{[a_0(s_0-s)-z']^3} \leqslant \lambda_0\rho^n \cdot \frac{z a_n}{[a_0(s_0-s)-z]^2}. \tag{A10}$$

The lemma is thus proved.

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On the Lie algebras generated by two two-forms in Minkowski space–time

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In relativity, planes and two-forms play important roles in the description of physical configurations or objects. When these configurations or objects interact, or are superposed, the corresponding planes or two-forms appear associated by pairs, and the *relative position* of the pair allows the classification of the particular form of the interaction. Here it is shown that in Minkowski space a pair of planes may adopt 35 relative positions. This result allows the almost complete characterization of the dimension of the Lie (sub)algebras (of the Lorentz group) generated by a pair of two-forms in terms of the relative position of their invariant planes. Furthermore, it is shown that, apart from Patera *et al.* algebras F_2 and F_5 (for which the eigenvalues' ratios have to be computed as well), the position of their invariant planes is also sufficient to determine the algebra itself generated by two two-forms. © *1996 American Institute of Physics.* [S0022-2488(96)03811-X]

I. INTRODUCTION

A smooth surface, the evolution of a rod, a string, a point mass with spin, a polarized photon; any of these objects define, in relativistic macroscopic physics, a (two-dimensional) *plane* at every point of its space–time support.[1]

Consequently, the study of shocks, diffusion, or interaction of any two of these elements involves the analysis of the different *relative positions* that the associated planes may have in Minkowski space–time.

Planes appear also naturally in relativity in many other domains, such as perfect fluids with heat flow,[2] anisotropic fluids,[3] tilted cosmologies,[4] magnetohydrodynamics,[5] two perfect fluid sources,[6] or regular or pure radiative electromagnetic fields.[7]

Thus, their junctions, shocks, phase changes, or chemical reactions across a hypersurface, their interactions,[8] or superpositions in a domain are processes that involves the study of the relative position of the pair of planes that they define. And so is also the description of the evolution of any of the above objects in these media.

The study of the variety of these relative positions not only induces a classification of the corresponding physical situations, allowing an easier analysis of them, but may help, in some cases, in the search of first integrals of the motion.[9]

Here we show that there exist 35 different relative positions for a pair of planes in Minkowski space–time (Theorem 1).

Relativistic Helmholtz vorticity of fluid currents,[10] Minkowski description of electromagnetic fields,[11] or infinitesimal generators (algebra) of Lorentz transformations[12] are perhaps the best-known examples of space–time two-forms. However, many other important two-forms have been considered in relativity, such as principal Riemann,[13] Killing–Yano,[14] Hertz potential,[15] or Frenkel intrinsic angular momentum[16] two-forms.

As two-forms in space–time univocally determine nonspacelike planes, our Theorem 1 di-

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rectly applies to the characterization of the *relative position of two two-forms*, and may help to find conserved quantities for the corresponding field equations.[17]

At any point of the space–time, a two-form amounts to an infinitesimal generator (element of its algebra) of a local Lorentz transformation; this interpretation of *any* two-form may be of interest in some problems related to adapted observers or frames.[12] Moreover, the determination of a Lorentz transformation by the corresponding Lorentz algebra two-form reduces the parametrization to its intrinsic elements.[18] In Ref. 19 it was shown a striking property of the commutator of two two-forms, namely that it defines an internal binary operation on the space of planes: the invariant planes of the commutator depend exclusively on the invariant planes of the two-forms (and not on their eigenvalues).

This last property strongly suggests that the Lie (sub)algebra (of the Lorentz group) generated by two two-forms depends essentially on the relative position of its invariants planes, and very little on their eigenvalues. In the second part of the article we examine this question. Our main result (Theorem 3) is that, apart from a special case of regular two-forms for which the ratio of eigenvalues are needed, the algebra generated by two two-forms *depends exclusively* on the relative position of the principal planes of the two-forms.

In the above-mentioned interpretation of any two-form as generator of a Lorentz transformation, but also in other situations,[20] one is naturally lead to consider the Baker–Campbell–Hausdorff formula[21] for the two-form associated to a product of two Lorentz transformations. Our Theorem 3 directly applies to simplify its general expression; this will be seen in a later work.

II. PRELIMINARIES

Let (V_4,g) be Minkowski space and P and Q be two planes (two-dimensional linear subspaces of V_4). In order to render easier the study of their relative position, it is convenient to range the intersections of them and their (biunivocally determinated) orthogonal planes $P^\perp$ and $Q^\perp$ as a 2×2 matrix:

$$\mathscr{D}(P,Q)\equiv\begin{pmatrix} P\cap Q & P\cap Q^\perp \\ P^\perp\cap Q & P^\perp\cap Q^\perp \end{pmatrix}.$$

The set of these matrices $\mathscr{D}(P,Q)$ will be denoted by $\mathscr{D}$. These matrices have the following properties $\forall P,Q$ (Proposition 2 of Ref. 19):

$$\begin{gathered}(\mathscr{D}(P,Q))_{ij}\ \perp(\mathscr{D}(P,Q))_{mn}\quad\forall(i,j)\neq(m,n),\\ \dim(\mathscr{D}(P,Q))_{11}=\dim((P,Q))_{22},\\ \dim(\mathscr{D}(P,Q))_{22}=\dim(\mathscr{D}(P,Q))_{21}.\end{gathered}\tag{1}$$

By reasons explained in Ref. 19 we are interested by the following transformations of $\mathscr{D}$ (bijections of $\mathscr{D}$):

$$\begin{aligned}&\mathrm{t}:\mathscr{D}(P,Q)\mapsto\mathscr{D}^{\mathrm{t}}(P,Q)\equiv\mathscr{D}(Q,P),\\ &\mathrm{c}:\mathscr{D}(P,Q)\mapsto\mathscr{D}^{\mathrm{c}}(P,Q)\equiv\mathscr{D}(P,Q^\perp),\\ &\mathrm{r}:\mathscr{D}(P,Q)\mapsto\mathscr{D}^{\mathrm{r}}(P,Q)\equiv\mathscr{D}(P^\perp,Q),\\ &\mathrm{l}:\mathscr{D}(P,Q)\mapsto\mathscr{D}^{\mathrm{l}}(P,Q)\equiv\mathscr{D}(l(P),l(Q)),\end{aligned}\tag{2}$$

where $\mathrm{l}\in\mathscr{L}$, $\mathscr{L}$ being the Lorent group.

TABLE I. Planes determined by $\mathscr{D}(P,Q)$.

m_0	m_{10}^0	m_{10}^2	m_1^0	m_1^3	m_1^1	m_{20}	m_{21}
$\begin{pmatrix}0&0\\0&0\end{pmatrix}$	$\begin{pmatrix}a&0\\0&b\end{pmatrix}$	$\begin{pmatrix}i&0\\0&p\end{pmatrix}$	$\begin{pmatrix}a&b\\c&d\end{pmatrix}$	$\begin{pmatrix}i&i\\p&q\end{pmatrix}$	$\begin{pmatrix}i&i\\i&i\end{pmatrix}$	$\begin{pmatrix}R&0\\0&R^\perp\end{pmatrix}$	$\begin{pmatrix}I&i\\i&I^\perp\end{pmatrix}$
Undetermined	$P=a+c'$ $Q=a+c''$	$P=i+i'$ $Q=i+i''$	$P=a+b$ $Q=a+c$	$P=i+i'$ $Q=i+p$	$P=i+p$ $Q=i+p'$	$P=R$ $Q=R$	$P=I$ $Q=I$

Let us consider the subgroups of transformations of $\mathscr{D}$ generated by the elements {t}, {t,cr}, {t,c,r}, and {l}, respectively. Apart from those given by (2), the images of the matrix $\mathscr{D}(P,Q)$ by the transformations of the subgroup generated by {t,c,r} are

$$\begin{aligned}&\mathscr{D}^{\mathrm{tr}}(P,Q)=\mathscr{D}(Q^\perp,P),\quad \mathscr{D}^{\mathrm{cr}}(P,Q)=\mathscr{D}(P^\perp,Q^\perp),\\&\mathscr{D}^{\mathrm{tcr}}(P,Q)=\mathscr{D}(Q^\perp,P^\perp),\quad \mathscr{D}^{\mathrm{tc}}(P,Q)=\mathscr{D}(Q^\perp,P).\end{aligned}\tag{3}$$

This subgroup, which is the same as the one generated by {tr,t}, is the dihedral group D_4. The subgroups generated by {t,cr} and {t} are, respectively, the dihedral group D_2 and the permutation group S_2.

Two results are needed. The first result says (Proposition 3 of Ref. 19) that *in Minkowski space the elements of* $\mathscr{D}/(D_4\times\mathscr{S})$ *are*

$$\begin{gathered}\left[\begin{pmatrix}0&0\\0&0\end{pmatrix}\right]\equiv m_0,\quad \left[\begin{pmatrix}a&0\\0&b\end{pmatrix}\right]\equiv m_{10}^0,\quad \left[\begin{pmatrix}i&0\\0&p\end{pmatrix}\right]\equiv m_{10}^2,\\ \left[\begin{pmatrix}a&b\\c&d\end{pmatrix}\right]\equiv m_1^0,\quad \left[\begin{pmatrix}i&i\\p&q\end{pmatrix}\right]\equiv m_1^3,\quad \left[\begin{pmatrix}i&i\\i&i\end{pmatrix}\right]\equiv m_1^1,\\ \left[\begin{pmatrix}R&0\\0&R^\perp\end{pmatrix}\right]\equiv m_{20},\quad \left[\begin{pmatrix}I&i\\i&I^\perp\end{pmatrix}\right]\equiv m_{21},\end{gathered}\tag{4}$$

where a, b, c, d, p, and q *are non-null directions,* i *is a null one, and* R *and* I *are respectively a non-null and a null plane.*

The second result says (Proposition 4 of Ref. 19) that *the components of the matrix* $\mathscr{D}(P,Q)$ *determine the planes* P *and* Q *as indicated in Table I, where* $\{a,b,c,d,\}$ *is a tetrad of orthogonal directions,* $\{a,b,c'\}$ *and* $\{a,b,c''\}$ *are different orthogonal triads,* $\{i,i',i''\}$ *is a triad of null directions, and* p *and* p' *are different and nonorthogonal directions which are orthogonal to the null directions of each case.*

III. RELATIVE POSITION

In a linear space, the relative position of two planes (P,Q) is determined by the dimension of their common elements, $\dim(P\cap Q)$; thus *in* V_4 *there are three relative positions for a pair of planes.*

If the linear space is endowed with a Euclidean metric, which associates to every plane its orthogonal, the (qualitative) relative positions of two planes are determined by the dimensions of relevant intersections of pairs of planes taken from the set $\{P,Q,P^\perp,Q^\perp\}$; i.e., by the dimension matrix $\mathrm{D}(P,Q)$ such that $(\mathrm{D}(P,Q))_{ij}=\dim(\mathscr{D}(P,Q))_{ij}$. Thus, from (1) it is easy to see that *in four-dimensional Euclidean space* (V_4,g_e), *there are six relative positions for a pair of planes,* corresponding to the dimension matrices

$$\begin{pmatrix}0&0\\0&0\end{pmatrix}\begin{pmatrix}1&0\\0&1\end{pmatrix}\begin{pmatrix}0&1\\1&0\end{pmatrix}\begin{pmatrix}1&1\\1&1\end{pmatrix}\begin{pmatrix}2&0\\0&2\end{pmatrix}\begin{pmatrix}0&2\\2&0\end{pmatrix}.$$

If the linear space is endowed with a Lorentzian metric, which associates to every plane also a causal character, the (qualitative) relative position of a pair of planes will be determined by the corresponding matrix $\mathrm{D}(P,Q)$ but also by the causal character of P and Q and the elements of $\mathscr{D}(P,Q)$. The object of this section is to characterize all of them.

Let us be slightly more precise. The six above-mentioned relative positions of the Euclidean case correspond to elements of $\mathscr{D}/(D_2\times O)$, bijectively related to the set D of dimension matrices $\mathrm{D}(P,Q)$. Here D_2 appears because the pairs (P,Q), (Q,P), $(P^\perp,Q^\perp)$, and $(Q^\perp,P^\perp)$ have the same relative position. However, in Minkowski space because of the causal character, we have to distinguish between (P,Q) and $(P^\perp,Q^\perp)$. Thus, in addition to the causal character of P and Q, we have to consider the group S_2 in place of D_2 (and, of course, $\mathscr{L}$ in place of O).

Denoting by c_P the causal character of the plane P ($c_P=-,0,+$, resp. if P is timelike, null, spacelike), by $c(P,Q)$ the couple of causal characters of P and Q, $c(P,Q)\equiv(c_P,c_Q)$, and by $\mathscr{C}$ the set $\{c(P,Q)\}\forall P,Q$, we are led to give the following definition:

Definition 1. The relative position of two planes P *and* Q *is the element of* $\mathscr{C}/S_2\times\mathscr{D}/(S_2\times\mathscr{L})$ *that contains* $(c(P,Q),\mathscr{D}(P,Q))$.

From (2)–(4) it is easy to compute the elements of $\mathscr{D}/(S_2\times\mathscr{L})$; one has[22]

$$\begin{gathered}
\left[\begin{pmatrix}0&0\\0&0\end{pmatrix}\right]\equiv m_0,\\
\left[\begin{pmatrix}0&t\\e&0\end{pmatrix}\right]\equiv m_{01}^{-+},\quad \left[\begin{pmatrix}0&e\\e'&0\end{pmatrix}\right]\equiv m_{01}^{++},\quad \left[\begin{pmatrix}0&i\\e&0\end{pmatrix}\right]\equiv m_{01}^{0+},\\
\left[\begin{pmatrix}t&0\\0&e\end{pmatrix}\right]\equiv m_{10}^{-+},\quad \left[\begin{pmatrix}e&0\\0&e'\end{pmatrix}\right]\equiv m_{10}^{++},\quad \left[\begin{pmatrix}e&0\\0&t\end{pmatrix}\right]\equiv m_{10}^{-+},\\
\left[\begin{pmatrix}i&0\\0&e\end{pmatrix}\right]\equiv m_{10}^{0+},\quad \left[\begin{pmatrix}e&0\\0&i\end{pmatrix}\right]\equiv m_{10}^{+0},\\
\left[\begin{pmatrix}t&e\\e'&e''\end{pmatrix}\right]\equiv m_1^{-+},\quad \left[\begin{pmatrix}e&e'\\e''&t\end{pmatrix}\right]\equiv m_1^{+-},\quad \left[\begin{pmatrix}e&t\\e'&e''\end{pmatrix}\right]\equiv m_1^{++},\\
\left[\begin{pmatrix}i&i\\e&e'\end{pmatrix}\right]\equiv m_1^{0+},\quad \left[\begin{pmatrix}e&i\\e'&i\end{pmatrix}\right]\equiv m_1^{+0},\quad \left[\begin{pmatrix}i&i\\i&i\end{pmatrix}\right]\equiv m_1^{00},\\
\left[\begin{pmatrix}T&0\\0&E\end{pmatrix}\right]\equiv m_{20}^{-+},\quad \left[\begin{pmatrix}E&0\\0&T\end{pmatrix}\right]\equiv m_{20}^{+-},\quad \left[\begin{pmatrix}0&T\\E&0\end{pmatrix}\right]\equiv m_{02},\\
\left[\begin{pmatrix}I&i\\i&I^\perp\end{pmatrix}\right]\equiv m_{21},\quad \left[\begin{pmatrix}i&I\\I^\perp&i\end{pmatrix}\right]\equiv m_{12},
\end{gathered}\tag{5}$$

where t and i are, respectively, a timelike and a null direction; e, e', and e'' are spacelike directions, and T, I, and E are, respectively, a timelike plane, a null plane, and a spacelike plane. We are thus able to prove the following result:

Theorem 1: *In Minkowski space there are 35 relative positions for a pair of planes. They are characterized in Table II.*

TABLE II. Relative positions of a pair of planes.

$\mathscr{C}/S_2$	$\mathscr{D}/(S_2\times\mathscr{S})$	Symbol
$[(-,-)]$	m_0	$\Pi_{6,1}$
	m_{01}^{++}	$\Pi_{6,2}$
	m_{10}^{++}	$\Pi_{3,1}$
	m_{10}^{+-}	$\Pi_{3,2}$
	m_{1}^{-+}	$\Pi_{3,3}$
	m_{10}^{0+}	$\Pi_{2,1}$
	m_{20}	$\Pi_{1,1}$
$[(-,0)]$	m_0	$\Pi_{6,3}$
	m_{01}^{++}	$\Pi_{6,4}$
	m_{10}^{++}	$\Pi_{3,4}$
	m_{1}^{0+}	$\Pi_{2,2}$
$[(-,+)]$	m_0	$\Pi_{6,5}$
	m_{01}^{++}	$\Pi_{6,6}$
	m_{01}^{-+}	$\Pi_{6,7}$
	m_{01}^{0+}	Π_{4}
	m_{10}^{++}	$\Pi_{3,5}$
	m_{1}^{++}	$\Pi_{3,6}$
	m_{02}	$\Pi_{2,1}$
$[(0,0)]$	m_0	$\Pi_{6,8}$
	m_{01}^{++}	$\Pi_{6,9}$
	m_{10}^{++}	$\Pi_{3,7}$
	m_{1}^{00}	$\Pi_{2,2}$
	m_{12}	$\Pi_{2,3}$
	m_{21}	$\Pi_{1,2}$
$[(0,+)]$	m_0	$\Pi_{6,10}$
	m_{01}^{++}	$\Pi_{6,11}$
	m_{10}^{++}	$\Pi_{3,8}$
	m_{1}^{+0}	$\Pi_{3,9}$
$[(+,+)]$	m_0	$\Pi_{6,12}$
	m_{01}^{++}	$\Pi_{6,13}$
	m_{10}^{++}	$\Pi_{3,10}$
	m_{10}^{+0}	$\Pi_{3,11}$
	m_{10}^{+-}	$\Pi_{3,12}$
	m_{1}^{+-}	$\Pi_{3,13}$
	m_{20}^{+-}	$\Pi_{1,3}$

Proof: Suppose $[\mathscr{D}(P,Q)]=m_0$; let $\{a,b,a',b'\}$ be its characteristic tetrad (Definition 1 of Ref. 19) and $\{K,K^{\perp}\}$ its characteristic planes (Definition 2 of Ref. 19); then $a+a'=K$, $b+b'=K^{\perp}$, $P=a+b$, and $Q=a'+b'$. Taking into account that the characteristic planes are not null and that $a\not\perp a'$ and $b\not\perp b'$ one has that $[c(P,Q)]$ can be any element of $\mathscr{C}/S_2$.

Suppose $[\mathscr{D}(P,Q)]=m_{10}^{++}$; from the Table I one has $P=e+c'$ and $Q=e+c''$, verifying $c'\perp e\perp c''$ and $c'\not\perp c''$. Then P has the causal character of c' and Q has the character of c''. As c' and c'' can have any causal character, $[c(P,Q)]$ can be any element of $\mathscr{C}/S_2$.

Suppose $[\mathscr{D}(P,Q)]=m_{01}^{++}$. Then, one has $[\mathscr{D}(P^{\perp},Q)]=m_{10}^{++}$; by the preceding argument $[c(P^{\perp},Q)]$ is any element of $\mathscr{C}/S_2$, so that $[c(P,Q)]$ do as well.

Finally, let us take any other element m of $\mathscr{D}/(S_2\times\mathscr{S})$. It is easily deduced from (2), (3), (5), and Table I that $\mathscr{D}(P,Q)\in m$ implies that $[c(P,Q)]$ is univocally determined.

Then, Table II follows. □

IV. BASIC NOTIONS ABOUT TWO-FORMS

Every two-form F has two independent *invariant scalars*, namely $\phi_F \equiv (F,*F)$ and $\psi_F \equiv (F,F)$, where $*$ is the Hodge dual operator and $(.,.)$ stands for the scalar product induced by g: $(F,G) \equiv -(1/2)\mathrm{tr}(FG)$, tr being the trace operator and FG the (cross-)product of two-forms.[23]

A nonvanishing two-form F is called *null* if $\phi_F^2 + \psi_F^2 = 0$, *regular* otherwise, *simple* if $\phi_F = 0$, and *unitary* if it is simple and $\psi_F = -1$.

The *principal directions* of F are the common eigendirections of F and $*F$, which are necessarily null. Let $\pm\alpha$ and $\pm i\tilde{\alpha}$ be the eigenvalues of a regular two-form verifying $\alpha > 0$, $\phi_F = -2\alpha\tilde{\alpha}$, and $\psi = -\alpha^2 + \tilde{\alpha}^2$. Then F admits a unique decomposition of the form $F = \alpha U - \tilde{\alpha} * U$, where U is unitary. The pair $\{U, *U\}$ is called the *geometry* of F. For a null F, it is the pair $\{F, *F\}$ itself which is called the *geometry* of F.

It is *always* possible to write univocally any two-form F in terms of its geometry $\{U, *U\}$ as $F = \alpha U - \tilde{\alpha} * U$, where the *weights* α and $\tilde{\alpha}$ take the values $\alpha = 1$ and $\tilde{\alpha} = 0$ when U is null. This decomposition is useful when (as in the present case) only algebraic calculations are involved.

An *inner direction* x of a simple two-form F is a direction such that any of its elements $\hat{x}$ verifies $\hat{x} \wedge F = 0$, where $\wedge$ stands for the exterior product. The plane of inner directions will be noted $\pi(F)$. The *invariant planes* of a two-form F are the planes of inner directions of its geometry: $\{\pi(U), \pi(*U)\}$. It is clear that $\pi(*U) = \pi(U)^{\perp}$.

There are six invariant scalars for a pair of two-forms, F and G, namely ϕ_F, ψ_F, ϕ_G, ψ_G, and the two *mixed invariant scalars* $\rho_{FG} \equiv (F,*G)$ and $\sigma_{FG} \equiv (F,G)$. The geometrical meaning of the mixed invariant scalars is as follows (see Lemma 2 in Ref. 19 for a proof):

Lemma 1: The planes $\pi(F)$ and $\pi(G)$ of simple two-forms F and G have common directions if, and only if, the mixed invariant ρ_{FG} vanishes.

It is to be noted that, because of the identity $\sigma_{FG} = -\rho_{F*G}$, this lemma also asserts that $\pi(F)$ and $\pi(*G)$ have common directions if, and only if, $\sigma_{FG} = 0$.

Let us recall that two-forms build the Lie algebra of Lorentz group with the commutator as the Lie bracket

$$[F,G] = FG - GF;$$

the properties of its geometry have been studied in Ref. 19. Now we are concerned with the subalgebras $\mathscr{A}(F,G)$ of the Lie algebra of Lorentz group generated by two-forms F and G.

V. A BASIS FOR THE SUBALGEBRAS GENERATED BY TWO TWO-FORMS

Let us consider the set

$$\mathscr{G}(F,G) \equiv \{F, G, *F, *G, [F,G], *[F,G]\}$$

associated to two-forms F and G and let $\mathscr{L}(\mathscr{G}(F,G))$ denote the linear space generated by $\mathscr{G}(F,G)$.

Taking into account the identities $FG - *G*F = -\sigma_{FG} g$ and $[F,*G] = *[F,G]$, one has

$$\begin{aligned} [[F,G],F] &= -\sigma_{FG} F + \psi_F G + \rho_{FG} *F - \phi_F *G, \\ [[F,G],G] &= -\psi_G F + \sigma_{FG} G + \phi_G *F - \rho_{FG} *G, \end{aligned} \tag{6}$$

and it is clear that all the elements of $\mathscr{A}(F,G)$ may be expressed as a linear combination of the elements of $\mathscr{G}(F,G)$. Therefore, the following holds:

Lemma 2: For any two-forms F and G, one has $\mathscr{A}(F,G) \subset \mathscr{L}(\mathscr{G}(F,G))$.

Thus we can always select a basis of $\mathscr{A}(F,G)$ from $\mathscr{G}(F,G)$. Concerning the dimension of $\mathscr{L}(\mathscr{G}(F,G))$, we have the following.

Proposition 1: For nonproportional two-forms F and G, one has

$$\dim \mathscr{L}(\mathscr{G}(F,G)) \in \{2,4,6\}.$$

This dimension is 2 if, and only if, they have the same principal directions, it is 4 if, and only if, they have one common principal direction and at least one that is not common, and it is 6 if, and only if, they have no common principal directions.

Proof: Let $\{U,*U\}$ and $\{V,*V\}$ be the geometries of F and G, respectively. As the elements of $\mathscr{G}(F,G)$ may be expressed as linear combinations of the elements of $\mathscr{G}(U,V)$ and vice versa, it is clear that $\dim \mathscr{L}(\mathscr{G}(F,G))=\dim \mathscr{L}(\mathscr{G}(U,V))$. Hence, we only have to prove the proposition for the two-forms U and V.

Let us remember that U and V have same principal directions iff $U=\lambda V+\mu *V$ ($\lambda=1$ and $\mu=0$ if they are regular). Hence, if they have the same principal directions $\dim \mathscr{L}\{U,V,*U,*V\}=2$; and as $[U,\ V]=0$ (Proposition 8 from Ref. 19), $\dim \mathscr{L}(\mathscr{G}(U,V))=2$.

If U and V have one common principal direction and at least one noncommon, $\dim \mathscr{L}\{U,V,*U,*V\}=4$. Then there exist some vectors x, y, and z verifying $U=x\wedge y$, $V=x\wedge z$, and $(x,x)=0$. Since

$$[U,\ V]=-(x,x)y\wedge z-(x,z)U+(x,y)V=-(x,z)U+(x,y)V, \tag{7}$$

it follows that $\dim \mathscr{L}(\mathscr{G}(U,V))=4$.

If U and V have no common principal directions, $\dim \mathscr{L}\{U,V,*U,*V\}=4$ and $\dim \mathscr{L}(\mathscr{G}(U,V))\geqslant 4$. Suppose $\dim \mathscr{L}(\mathscr{G}(U,V))=4$ so that

$$[U,\ V]=\lambda U+\mu V+\nu *U+\xi *V,$$

and then

$$[[U,\ V],\ U]=-(\lambda\mu-\xi\nu)U-(\mu^2-\xi^2)V-(\lambda\xi+\mu\nu)*U-2\mu\xi *V,$$

$$[[U,\ V],\ V]=(\lambda^2-\nu^2)U+(\lambda\mu-\xi\nu)V-2\lambda\nu *U+(\lambda\xi+\mu\nu)*V.$$

However, from (6), $\phi_U=2\mu\xi=0$ and $\phi_V=-2\lambda\nu=0$, so that all the solutions for λ, μ, ν, and ξ lead to expressions of the form (7) implying the existence of common principal directions. Thus $\dim \mathscr{L}(\mathscr{G}(U,V))>4$. Suppose $\dim \mathscr{L}(\mathscr{G}(U,V))=5$, and then either $\dim \mathscr{L}\{U,V,*U,*V,[U,V]\}=5$ or $\dim \mathscr{L}\{U,V,*U,*V,*[U,V]\}=5$ or both. Assume the first condition verified so that

$$*[U,\ V]=\lambda U+\mu V+\nu *U+\xi *V+\chi[U,\ V]$$

and call $A\equiv\lambda U+\mu V+\nu *U+\xi *V$. It follows

$$[U,\ V]=-*A-\chi *[U,\ V]=-\chi A-*A-\chi^2[U,\ V],$$

and we obtain

$$(\chi\lambda-\nu)U+(\chi\mu-\xi)V+(\chi\nu+\lambda)*U+(\chi\xi+\mu)*V+(1+\chi^2)[U,\ V]=0.$$

Following our assumption this expression leads to the incompatibility $1+\chi^2=0$. The same conclusion is obtained assuming the other conditions, so that $\dim \mathscr{L}(\mathscr{G}(U,V))=6$ for U and V having no common principal directions. □

VI. DIMENSION OF THE ALGEBRAS GENERATED BY TWO SIMPLE TWO-FORMS

Let U and V be simple noncommuting two-forms (they do not have the same principal directions; see Proposition 8 in Ref. 19), and let ψ, ψ', ρ, and σ be their nonzero invariant scalars. From (6) we obtain

$$[[U,\ V],\ U]=-\sigma U+\psi V+\rho *U,\quad [[U,\ V],\ V]=-\psi' U+\sigma V-\rho *V. \tag{8}$$

Therefore, $\rho=0$ implies $\dim \mathscr{A}(U,V)\leqslant 3$. Conversely, when $\dim \mathscr{A}(U,V)\leqslant 3$, from (8) we have either $\rho=0$ or

$$*U=\lambda U+\mu V+\nu[U,\ V],\quad *V=\lambda' U+\mu' V+\nu'[U,\ V]. \tag{9}$$

However, if (9) is verified, then $\nu\nu'\neq 0$; hence we can obtain $[U,\ V]$ in two different ways from (9) and, equating them, we have

$$(\lambda'\nu-\lambda\nu')U+\nu' *U=(\mu\nu'-\mu'\nu)V+\nu *V,$$

and so U and V would have same geometry. Thus $\dim \mathscr{A}(U,V)\leqslant 3\Leftrightarrow\rho=0$. Then, from Lemma 1 and (7), we have the following:

Lemma 3: For noncommuting simple two-forms U and V, one has

(i) $\dim \mathscr{A}(U,V)=2$ *if, and only if, they have one common inner principal direction, and*
(ii) $\dim \mathscr{A}(U,V)=3$ *if, and only if, they have one common non-null inner direction.*

Let us suppose now $\dim \mathscr{A}(U,V)=4$. The last lemma implies $\rho\neq 0$, and, from (8), we get

$$[[[U,\ V],\ U],\ V]=-\sigma[U,\ V]+\rho *[U,\ V]; \tag{10}$$

hence, $\dim \mathscr{A}(U,V)=4\ \Rightarrow\ \dim \mathscr{L}(\mathscr{G}(U,V))=4$. Therefore, from Proposition 1 and Lemma 3, U and V must have one common principal direction and no common inner directions for both two-forms. Conversely, when U and V have a common principal direction and no common inner directions, $\dim \mathscr{L}(\mathscr{G}(U,V))=4$ (Proposition 1) and $\dim \mathscr{A}(U,V)\leqslant 4$ (Lemma 2). As $\rho\neq 0$, $\dim \mathscr{A}(U,V)=4$ (Lemma 3). Thus, the following lemma has been proved:

Lemma 4: The necessary and sufficient condition for $\dim \mathscr{A}(U,V)=4$ *is that the simple two-forms U and V have one common principal direction and no common inner directions.*

Finally, suppose $\dim \mathscr{A}(U,V)=6$.[24] By Lemmas 3 and 4, the two-forms U and V have neither common principal directions nor common inner directions. Conversely, by Proposition 1 when U and V have neither common principal directions nor common inner directions, $\dim \mathscr{L}(\mathscr{G}(U,V))=6$. As $\rho\neq 0$, from (8) and (10), the two-forms U, V, $[U,\ V]$, $[[U,\ V],U]$, $[[U,\ V],V]$ and $[[[U,V],U],V]$ are linearly independent; hence[24] $\dim \mathscr{A}(U,V)=6$. We have shown the following result:

Lemma 5: The necessary and sufficient condition for $\dim \mathscr{A}(U,V)=6$ *is that the simple two-forms U and V have neither common principal directions nor common inner directions.*

As a corollary of the last results and Proposition 8 of Ref. 19 we have the next proposition:

Proposition 2: Let U and V be nonproportional simple two-forms. It holds that

(i) $\dim \mathscr{A}(U,V)=2$ *and* $[U,\ V]=0$ *if, and only if, all principal directions are common;*
(ii) $\dim \mathscr{A}(U,V)=2$ *and* $[U,\ V]\neq 0$ *if, and only if, there is one common principal direction and at least one noncommon principal direction;*
(iii) $\dim \mathscr{A}(U,V)=3$ *if, and only if, there is only one common non-null inner direction;*
(iv) $\dim \mathscr{A}(U,V)=4$ *if, and only if, there is only one common principal direction and no common inner directions; and*
(v) $\dim \mathscr{A}(U,V)=6$ *if, and only if, there are neither common principal directions nor common inner directions.*

Hence, the following is now evident.

Corollary 1: The dimension of the algebra $\mathscr{A}(U,V)$ *generated by the simple two-forms U and V is d when the relative position of the planes of inner directions is* Π_d, *as given in Table II.*

VII. DIMENSION OF THE ALGEBRA GENERATED BY ANY TWO TWO-FORMS

Here we shall consider pairs of noncommuting two-forms such that at least one is not simple, say $F=\alpha U-\tilde{\alpha}*U$ and $G=\beta V-\tilde{\beta}*V$ such that $\psi_U=-1$ and $\psi_V\in\{-1,0\}$.

Suppose that F and G have only one common principal direction; then lemma 2 and proposition 1 imply $\dim \mathscr{A}(F,G)\leqslant 4$. Since U is unitary but V is unitary or null, (7) gives

$$[U,\ V]=\gamma U+\delta V \tag{11}$$

(note that $\gamma^2\in\{1,0\}$, $\delta^2=1$, and that $\gamma=0$ iff V is null). Hence,

$$[F,\ G]=\gamma\beta F+\delta\alpha G-\gamma\tilde{\beta}*F-\delta\tilde{\alpha}*G. \tag{12}$$

For F not simple and $\dim \mathscr{L}\{F,G,*F,*G\}=4$, $\dim \mathscr{A}(F,G)\geqslant 3$. Then, $\dim \mathscr{A}(F,G)\in\{3,4\}$. In order to have $\dim \mathscr{A}(F,G)=3$ we must impose $[[F,\ G],\ F]$, $[[F,\ G],\ G]\in\mathscr{L}\{F,G,[F,\ G]\}$. Taking into account (11) and (12) we get

$$[[f,\ G],\ G]=\gamma\delta(\alpha\beta-\tilde{\alpha}\tilde{\beta})F-(\alpha^2-\tilde{\alpha}^2)G+\gamma\delta(\alpha\tilde{\beta}+\tilde{\alpha}\beta)*F+2\alpha\tilde{\alpha}*G,$$

$$[[F,\ G],\ F]=(\beta^2-\tilde{\beta}^2)F+\gamma\delta(\alpha\beta-\tilde{\alpha}\tilde{\beta})G-2\beta\tilde{\beta}*F-\gamma\delta(\alpha\tilde{\beta}+\tilde{\alpha}\beta)*G,$$

so, $\dim \mathscr{A}(F,G)=3$ iff $\gamma(\alpha\tilde{\beta}-\tilde{\alpha}\beta)=0$; equivalently, G is null or the ratio of the weights of F equals the ratio of the weights of G.

Lemma 6: Let F and G be two-forms such that at least one is not simple. Then

(i) $\dim \mathscr{A}(F,G)=3$ *if, and only if, there is only one common principal direction and either one of the two-forms is null or, being regular, their weights' ratios coincide, and*

(ii) $\dim \mathscr{A}(F,G)=4$ *if, and only if, they are regular, have only one common principal direction and their weights' ratios are different.*

Finally, assume that they have no common principal direction. By Proposition 1 $\dim \mathscr{L}(\mathscr{I}(F,G))=6$ and by Lemma 6 $\dim \mathscr{A}(F,G)>4$, hence[24] it is 6. Conversely, when $\dim \mathscr{A}(F,G)=6$, from Lemma 2 and Proposition 1 they do not have any common principal direction. We have shown the following result:

Lemma 7: Let F and G be two-forms such that at least one is not simple. Then, the necessary and sufficient condition for $\dim \mathscr{A}(F,G)=6$ *is that they do not have common principal directions.*

As a corollary of proposition 8 of Ref. 19, and due to Lemmas 3–7 we have the following theorem:

Theorem 2: *Let F and G be nonproportional two-forms. Then*

(i) $\dim \mathscr{A}(F,G)=2$ *and* $[F,\ G]=0$ *if, and only if, they have the same principal directions;*

(ii) $\dim \mathscr{A}(F,G)=2$ *and* $[F,\ G]\neq 0$ *if, and only if, they are simple, have only one common principal direction, and at least one noncommon principal one;*

(iii) $\dim \mathscr{A}(F,G)=3$ *if, and only if, either they are simple and have only one non-null common direction or they are not simple, have one common principal direction and their weights' ratios coincide, or one is null, the other is not simple and have one common principal direction;*

(iv) $\dim \mathscr{A}(F,G)=4$ *if, and only if, they are both regular, have one common principal direction and their weights' ratios do not coincide; and*

(v) $\dim \mathscr{A}(F,G)=6$ *if, and only if, there are not common principal directions and, when they are simple, neither common inner directions.*

This theorem shows that the relative position of the geometries of a pair of two-forms determines the dimension of the algebra that they generate except in the case of regular two-forms

TABLE III. Subalgebras of the Lie algebra of Lorentz group.

Dimension	Type		Basis
0	R_1	F_{15}	
1	R_2	F_{13}	A_1
1	R_3	F_{14}	A_3
1	R_4	F_{12}	A_2
1	R_5	F_{11}	$A_1+\lambda A_2$ $(\lambda\neq 0)$
2	R_6	F_8	$A_1,\ A_3$
2	R_7	F_9	$A_1,\ A_2$
2	R_8	F_{10}	$A_3,\ A_4$
3	R_9	F_7	$A_1,\ A_3,\ A_4$
3	R_{10}	F_4	$A_1,\ A_3,\ A_5$
3	R_{11}	F_6	$A_2,\ A_3,\ A_4$
3	R_{12}	F_5	$A_1+\lambda A_2,\ A_3,\ A_4$ $(\lambda\neq 0)$
3	R_{13}	F_3	$A_2,\ A_3-A_5,\ A_4-A_6$
5	R_{14}	F_2	$A_1,\ A_2,\ A_3,\ A_4$
6	R_{15}	F_1	$A_1,\ A_2,\ A_3,\ A_4,\ A_5,\ A_6$

verifying the conditions that only one is simple and have one common principal direction. In this case we have to compute the weights' ratio of each one to discriminate between dimensions 3 and 4.

VIII. ALGEBRAS GENERATED BY TWO TWO-FORMS

Table III gives the subalgebras of the Lie algebra of Lorentz group. Each type corresponds to a class of conjugation by the orthochronous proper Lorentz group (connected component of the identity), except for the types where it the real number λ appears; each λ defines a different conjugation class. In the type column the Rs and the Fs correspond, respectively, to notations by Schell (see Ref. 25) and by Patera *et al.* (see Ref. 26); the last column includes a basis of each type in terms of the two-forms associated to a real null tetrad $\{l,m,p,q\}$.[27] We have made use of the notation:

$$\begin{aligned} &A_1=l\wedge m, \quad A_3=l\wedge p, \quad A_5=m\wedge p,\\ &A_2=p\wedge q, \quad A_4=l\wedge q, \quad A_6=m\wedge q. \end{aligned} \tag{13}$$

In this section we will see which types of these algebras can be generated by a pair of two-forms and which are the necessary and sufficient conditions for a pair of two-forms to generate a given type. These conditions will be expressed in terms of the geometric ingredients of the two-forms.

There are four types of subalgebras of dimension 1. Three of them (R_2,R_3,R_4) correspond to each causal character (resp., timelike, null, spacelike) of the plane of inner directions of a simple two-form. Type R_5 corresponds to classes of algebras generated by a nonsimple two-form, where λ is related to the weights' ratio of the two-form. It is clear that these types can be generated by two proportional two-forms with the characteristics listed above.

There are three types of subalgebras of dimension 2: R_6 is nonconmutative and R_7 and R_8 are conmutative; the former corresponds to regular geometry, and the latter to null geometry. From Theorem 2 we obtain the following result:

Lemma 8: For nonproportional two-forms F and G,

TABLE IV. The three-dimensional algebras of the Lorentz group.

Schell type	R_9	R_{10}	R_{11}	R_{12}	R_{13}
Bianchi type	V	VIII	VII_0	VII_h $(h\neq 0)$	IX

(i) *$\mathscr{A}(F,G)$ is an R_6-algebra if, and only if, they are simple, have only one common principal direction and at least one noncommon principal one,*

(ii) *$\mathscr{A}(F,G)$ is an R_7-algebra if, and only if, they are regular and have the same geometry, and*

(iii) *$\mathscr{A}(F,G)$ is an R_8-algebra if, and only if, they are null and have the same principal direction.*

Table IV shows the three-dimensional subalgebras of the Lorentz group and the correspondence between the Schell types and the Kramer *et al.*[29] notation of Bianchi[28] types.

The three planes of inner directions of the elements of the basis of R_{10}, R_{11}, and R_{13} (see Table III) generate a timelike, null, and spacelike hyperplane, respectively; for R_9 they generate all Minkowski space. Moreover, for types R_9, R_{10}, R_{11}, and R_{13}, any linear combination of the elements of the basis is simple, but this does not hold for R_{12}. We deduce that R_9, R_{10}, R_{11}, and R_{13} can only be generated by a pair of simple two-forms and that R_{12} can only be generated by a pair where at least one is not simple. By Proposition 2, the two-forms generating R_9, R_{10}, R_{11}, and R_{13} have a non-null common inner direction; taking into account (7), these two-forms and their commutator belong to a hyperplane; consequently R_9 cannot be generated by a pair of two-forms.

For algebras R_{10}, R_{11}, and R_{13} it is verified that

$$\pi([F,G])=(\mathrm{tr}\ \mathscr{D}(\pi(F),\pi(G)))^{\perp}.$$

This follows directly from the theorem of Ref. 19 and 7. Then, with the aid of Table II and relations (5), the relative position of the plane of inner directions of F and G that generate algebras R_{10}, R_{11}, and R_{13} may be obtained without difficulty. The result is given by the following lemma:

Lemma 9: The algebra $\mathscr{A}(F,G)$ generated by the two-forms F and G is never R_9 and it is R_{10}, R_{11} or *R_{13} if, and only if, F and G are simple and the relative position of the planes of inner directions is $\Pi_{3,r}$ with $r\in\{1,2,3,4,5,6,7,8,10\}$, $r\in\{9,11\}$, or $r\in\{12,13\}$, respectively.*

For R_{12} we have the result of part (i) of Lemma 6:

Lemma 10: Let F and G be two-forms with geometries $\{U,*U\}$ and $\{V,*V\}$, respectively. Then, $\mathscr{A}(F,G)$ is a R_{12} if, and only if, F and G are such that at least one is not simple and the relative position of $(\pi(U),\pi(V))$ is $\Pi_{2,2}$ or is $\Pi_{2,1}$ and their weights' ratio coincide.

Here R_{14} and R_{15} are the only algebras of dimension 4 and 6, respectively, so we only have to use Table II and (5) to express the conditions of Theorem 2 in terms of the relative position of the geometry. Then, taking into account Lemmas 8–10, we have the following theorem:

Theorem 3: *Let F and G be nonproportional two-forms and $\pi(U)$ and $\pi(V)$ the nonspacelike planes of its geometries. The algebra $\mathscr{A}(F,G)$ generated by F and G is*

(i) *never R_9,*

(ii) *R_7 or R_8 if the relative position of $(\pi(U),\pi(V))$ is $\Pi_{1,1}$ or $\Pi_{2,r}$ with $r\in\{1,2\}$,*

(iii) *R_6, R_{10}, R_{11}, R_{13}, R_{14},* or *R_{15}, if F and G are simple and the relative position of $(\pi(F),\pi(G))$ is $\Pi_{2,\cdot}$ for R_6, $\Pi_{3,r}$ with $r\in\{1,2,3,4,5,6,7,8,10\}$ for R_{10}, $\Pi_{3,r}$ with $r\in\{9,11\}$ for R_{11}, $\Pi_{3,r}$ with $r\in\{12,13\}$ for R_{13}, Π_4 for R_{14}, or $\Pi_{6,\cdot}$ for R_{15}, and*

(iv) *R_{12} or R_{15} if F and G are not both simple and the relative position of the planes $(\pi(U),\pi(V))$ is $\Pi_{2,2}$ for R_{12} or $\Pi_{3,r}$, $r\in\{1,2,3,4,7\}$, or $\Pi_{6,r'}$, $r'\in\{1,2,3,4,8,9\}$ for R_{15}. R_{12}, or R_{14} if they are not both simple, the relative position of the planes $(\pi(U),\pi(V))$ is $\Pi_{2,1}$ and their weights' ratios, respectively, coincide or differ.*

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[1] For a surface, this plane is the tangent one at the point, which, depending on its physical materialization, may have any causal orientation. For the rod or the string, the plane at every point is the one determined by the orientation of the object and its space–time velocity. For the point mass with spin, the appropriate plane is that defined by the spin two-form [see Ref. 16 or, for example, J. Ibañez, J. Martin, and E. Ruiz, Gen. Rel. Grav. **16**(3), 225 (1984) and references therein]. For the photon, it is the lightlike plane determined by the polarization and its null direction of propagation.

[2] In Landau and Lifchitz's as well as in Eckart's schemes; in both cases the plane is that defined by the velocity and the heat flow vectors. Such fluids may be of interest in the study of inhomogeneous universes; see, for example, J. Triginer and D. Pavón, Class. Quant. Grav. **12**, 689 (1995).

[3] The anisotropic fluids concerned here are those that, like in spherical symmetry, admit an isotropic two-surface, the plane in question being then that containing the fluid velocity and the anisotropic direction.

[4] That is, cosmologies in which the velocity of the cosmological (usually perfect) fluid does not coincide with that of the observers at rest with respect to the *instants* (spacelike hypersurfaces) of symmetry.

[5] In (perfect) relativistic magnetohydrodynamics, the plane is that determined by the velocity of the fluid and the magnetic field. For the subject, see, for example, B. Coll, Ann. Inst. Henri Poincaré **25**(4), 363 (1976) and references therein.

[6] Some astrophysical and cosmological situations seem to correspond to the sum of two perfect fluids. See G. S. Hall and D. A. Negm, Int. J. Theo. Phys. 25(4), 405 (1986); J. J. Ferrando, J. A. Morales, and M. Portilla, Gen. Rel. Grav. **22**(9), 1021 (1990) and references therein. In this case the plane is necessarily the spacelike eigenplane of the energy tensor.

[7] An electromagnetic field is described by a two-form (see Ref. 11), and it is well known [G. Y. Rainich, Trans. Am. Math. Soc. **27**, 106 (1925)] that a regular (resp. null) two-form in space–time is strictly equivalent to a $2+2$ weighted (resp. degenerated) local almost product structure, which may always be determined by its nonspacelike field of planes.

[8] Of particular importance is that of fluids (or magnetofluids) in the presence of pure radiative electromagnetic fields (relativistic cosmology), that of regular fields with radiation or that of two beam pure radiative interferences (relativistic optics) or that of the interaction of two spinning particles (relativistic mechanics and astronomy).

[9] Consider a system of two interacting point particles in Newtonian gravity, and let us associate to every one of them the plane containing its velocity and the relative position vector. In this case there are only two relative positions for the planes: they coincide or they cut each other. The statement that every one of these relative positions is *permanent* is equivalent to that of the *conservation* of the direction of the angular momentum. In some other more complicated relativistic systems for which we do not know first integrals, the analysis of the evolution of each of the possible relative positions of associate planes, easier to do in general, may help us to find some of these integrals.

[10] The classical Helmholtz vorticity [H. Helmholtz, Crelle's J. **55**, 25 (1858)], was extended to relativity by Synge [J. L. Synge, Proc. Lond. Math. Soc. **43**, 376 (1937)], and appears at present in all the studies involving relativistic fluids.

[11] Minkowski was the first to show that the electric and magnetic fields are in fact the components of a second-order skew-symmetric form (Nach. der K. Gessellschaft der Wissenschaften zu Göttingen Math. Phys. Klas. 53–111 (1908).

[12] Lorentz transformations in the exponential domain may be expressed in terms of the corresponding Lie algebra element, which is represented in Minkowski space by a constant antisymmetric form. In many problems in relativity, mainly those related to adapt *observers* (timelike directions) or *reference systems* (tetrads) to particular data, *local* Lorentz transformations (point dependent) are needed; they are then defined by an (exterior) two-form.

[13] These forms (antidual eigenforms of the Riemann tensor, or their real part), omnipresent in complex formalisms of general relativity, seem to have been first considered by Pirani in his analysis of the three Petrov types [F. A. E. Pirani, Phys. Rev. **105** (3), 1089 (1957)] and by Bel in his completion to five of those three types [Ll. Bel, Cahiers Phys. **138**, 59 (1962)].

[14] The Killing–Yano two-forms are potentiallike generators of some second-order Killing tensors (see for instance, Ref. 29). They are of importance in questions related to the symmetries of the space–time and in the problem of separation of variables of the Laplacian or the geodesic equations [see, for instance, S. Benenti, ''L'intégration de l'équation d'Hamilton-Jacobi par séparation des variables: histoire et résultats récents,'' in *La ''Mécanique analytique'' de Lagrange et son héritage* (Acta Acad. Scient. Taurinensis, Torino, 1990), pp. 119–144, and references therein].

[15] That Hertz potentials for electromagnetic field [H. Hertz, Ann. Phys. Lpz. **36**, 1 (1889)] can be defined in any space–time (Debye particular Hertz potentials cannot) was shown in J. M. Cohen and L. S. Kegeles, Phys. Rev. D **10**(4), 1070 (1974).

[16] The introduction in relativity of the spin two-form was due to J. Frenkel [Zeit. Phys. **37**, 243 (1926)], the equations of motions for spinning particles in a gravitational field were due to A. Papapetrou, [Proc. R. Soc. Lond., A **209**, 248 (1951)], and the interaction of two such particles was studied by Ibañez, Martin, and Ruiz (see reference in Ref. 1).

[17] By the same method indicated in Ref. 9.

[18] See comments on this subject in Ref. 19.

[19] B. Coll and F. San José, J. Math. Phys. **38**, 4350 (1995).

[20] For example, those given rise to effects of the *Thomas precession* type [cf. L. M. Thomas, Nature **117** (2945), 514 (April, 1926)].

[21] Let $L \equiv \exp F$ and $M \equiv \exp G$ be two (field of) Lorentz transformations generated by the two-forms F and G, respec-

tively. The product transformation $N \equiv LM$ is of the form $N \equiv \exp H$ where $H \equiv F \bullet G$ is given by the so-called BCH formula. See Ref. 19 for references.

[22] Subscripts denote dimension of a component of each diagonal and superscripts the causal character of the elements of the principal diagonal if they are not zero and of the second one otherwise.

[23] In local coordinates one has $(*F)_{\alpha\beta} \equiv (1/2)\,\eta_{\alpha\beta\gamma\delta} F^{\gamma\delta}$ and $(FG)_{\alpha\beta} \equiv F_{\alpha\rho} G^{\rho}_{\beta}$, where $\eta_{\alpha\beta\gamma\delta}$ is the volume element induced by the Minkowski metric g.

[24] It is well known that the Lorentz group has no subgroup of dimension 5; see, for instance, Ref. 25.

[25] J. F. Schell, J. Math. Phys. **2**, 202 (1961).

[26] J. Patera, P. Winternitz, and H. Zassenhaus, J. Math. Phys. **16**, 1597 (1975).

[27] That means: $(l,l)=(m,m)=(l,p)=(l,q)=(m,p)=(m,q)=(p,q)=0$ and $(l,m)=-(p,p)=-(q,q)=1$.

[28] L. Bianchi, Soc. Ital. Mem. di Mat. **11**, 267 (1897).

[29] D. Kramer, H. Stephani, M. MacCallum, and E. Herlt, *Exact Solutions of the Einstein's Field Equations* (VEB Deutscher Verlag der Wissenschaften, Berlin, 1980).

Determinants of Dirac operators with local boundary conditions

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We study functional determinants for Dirac operators on manifolds with boundary. We give, for local boundary conditions, an explicit formula relating these determinants to the corresponding Green's functions. We finally apply this result to the case of a bidimensional disk under baglike conditions. © *1996 American Institute of Physics.* [S0022-2488(96)00306-4]

I. INTRODUCTION

It is well known that functional determinants have wide application in quantum and statistical physics. Typically, one faces the necessity of defining a regularized determinant for elliptic differential operators. In this context, the Dirac first-order differential operator plays a central role.

Seeley's construction of complex powers of elliptic differential operators provides a powerful tool to regularize such determinants: the so-called ζ-function method.[1]

In the case of boundaryless manifolds, this construction has been largely studied and applied (see, for instance, Ref. 2 and references therein).

For manifolds with boundary, the study of complex powers was performed in Refs. 3 and 4 for the case of local boundary conditions, while for the case of nonlocal conditions, this task is still in progress (see, for example, Ref. 5).

In general, the regularized determinant turns out to be nonlocal and, so, it cannot be expressed in terms of just a finite number of Seeley's coefficients. However, such determinant can always be obtained from the Green's function in a finite number of steps involving these coefficients. For boundaryless manifolds this was proved in Ref. 6, while for a particular type of local boundary condition the procedure was introduced in Ref. 7.

The aim of this paper is to give the explicit relationship between determinants and the corresponding Green's functions of Dirac operators under general local elliptic boundary conditions.

Dirac operators defined on manifolds with boundaries have been the subject of a vast literature (see, for instance, Refs. 8 and 9 and references therein), mainly concerning anomalies and index theorems. However, in these papers, the emphasis was put on nonlocal boundary conditions of the type introduced in Ref. 10. We leave for a forthcoming publication the treatment of such conditions.

The outline of this paper is as follows:

In Sec. II we introduce some general definitions and conventions concerning elliptic boundary problems for Dirac operators.

In Sec. III we present a formula relating the determinant of the Dirac operator with its Green's function for the case of local boundary conditions.

In Sec. IV, an explicit computation of the determinant of a Dirac operator in a bidimensional disk with baglike boundary conditions is performed, making use of the results in Sec. III.

II. ELLIPTIC BOUNDARY PROBLEMS, COMPLEX POWERS, AND REGULARIZED DETERMINANTS

Throughout this paper we will be concerned with boundary value problems associated to first-order elliptic operators

$$D: C^{\infty}(M,E) \to C^{\infty}(M,F), \tag{1}$$

where M is a bounded closed domain in $\mathbf{R}^{\nu}$ with smooth boundary ∂M, and E and F are k-dimensional complex vector bundles over M.

In a collar neighborhood of ∂M in M, we will take coordinates $\underline{\underline{x}}=(x,t)$, with t the inward normal coordinate and x local coordinates for ∂M (that is, $t>0$ for points in $M\backslash\partial M$ and $t=0$ on ∂M), and conjugated variables $\underline{\underline{\xi}}=(\xi,\tau)$.

As stated in the Introduction, we will mainly consider the Euclidean Dirac operator. Let us recall that the free Euclidean Dirac operator $i\not{\partial}$ is defined as

$$i\not{\partial} = \sum_{\mu=0}^{\nu-1} i\gamma_{\mu} \frac{\partial}{\partial x_{\mu}}, \tag{2}$$

where the matrices γ_{μ} satisfy

$$\gamma_{\mu}\gamma_{\alpha} + \gamma_{\alpha}\gamma_{\mu} = 2\delta_{\mu\alpha}, \tag{3}$$

and that, given a gauge potential $A=\{A_{\mu},\ \mu=0,...,\nu-1\}$ on M, the coupled Dirac operator is defined as

$$D(A) = i\not{\partial} + \not{A}, \tag{4}$$

with $\not{A}=\Sigma_{\mu=0}^{\nu-1}\gamma_{\mu}A_{\mu}$.

One of the most suitable tools for studying boundary problems is the Calderón projector Q.[11,12] For the case we are interested in, D of order 1 as in (1), Q is a (not necessarily orthogonal) projection from $[L^2(\partial M, E_{/\partial M})]$ onto the subspace $\{(T\varphi/\varphi)\in\ker(D)\}$, being T: $C^{\infty}(M,E)\to C^{\infty}(\partial M, E_{/\partial M})$ the trace map.

As shown in Ref. 11, Q is a zeroth-order pseudodifferential operator and its principal symbol $q(x;\xi)$, which depends only on the principal symbol of D, $\sigma_1(D)=a_1(x,t;\xi,\tau)$, turns out to be the $k\times k$ matrix

$$q(x;\xi) = \frac{1}{2\pi i} \int_{\Gamma} (a_1^{-1}(x,0;0,1)a_1(x,0;\xi,0) - z)^{-1}\, dz, \tag{5}$$

where Γ is any simple closed contour oriented clockwise and enclosing all poles of the integrand in $\mathrm{Im}(z)<0$.

Here Q is not unique, since it can be constructed from any fundamental solution of D, but its principal symbol $q(x;\xi)$ is uniquely determined.[11]

According to Calderón[11] and Seeley,[12] elliptic boundary conditions can be defined in terms of $q(x;\xi)$.

Definition 1: Let us assume that the *rank* of $q(x;\xi)$ is a constant r (as is always the case for $\nu\geqslant 3$).[11]

A zeroth-order pseudodifferential operator B: $[L^2(\partial M,E_{/\partial M})]\to[L^2(\partial M,G)]$, with G an r-dimensional complex vector bundle over ∂M, gives rise to an *elliptic boundary condition* for a first-order operator D as in (1) if, $\forall\xi{:}|\xi|\geqslant 1$,

$$\operatorname{rank}(b(x;\xi)q(x;\xi))=\operatorname{rank}(q(x;\xi))=r, \tag{6}$$

where $b(x;\xi)$ coincides with the principal symbol of B for $|\xi|\geqslant 1$.

In this case we say that

$$D\varphi=\chi \ \text{ in } \ M, \quad BT\varphi=f \ \text{ on } \ \partial M, \tag{7}$$

is an *elliptic boundary problem*, and denote by D_B the closure of D acting on the sections $\varphi\in C^\infty(M,E)$ satisfying $B(T\varphi)=0$.

An elliptic boundary problem such as (7) has a solution $\varphi\in H^1(M,E)$ for any (χ,f) in a subspace of $L^2(M,E)\times H^{1/2}(\partial M,G)$ of finite codimension. Moreover, this solution is unique up to a finite-dimensional kernel.[11] In other words, the operator

$$(D,BT){:}H^1(M,E)\to L^2(M,E)\times H^{1/2}(\partial M,G) \tag{8}$$

is Fredholm.

When B is a local operator, Definition 1 yields the classical local elliptic boundary conditions, also called Lopatinsky–Shapiro conditions (see, for instance, Ref. 13).

For Euclidean Dirac operators on $\mathbf{R}^\nu$, $E_{/\partial M}=\partial M\times\mathbf{C}^k$, local boundary conditions arise when the action of B is given by the multiplication by a $k/2\times k$ matrix of functions defined on ∂M.

Owing to *topological obstructions*, chiral Dirac operators in even dimensions, $\mathscr{D}$, do not admit local elliptic boundary conditions (see, for example, Ref. 14). Nevertheless, it is easy to see from Definition 1 that local boundary conditions can be defined for the full, either free or coupled, Euclidean Dirac operator

$$D(A)=\begin{pmatrix} 0 & \mathscr{D}^\dagger \\ \mathscr{D} & 0 \end{pmatrix}$$

on M.

We now sketch Seeley's construction of the complex powers of the operator D under a local elliptic boundary condition B.[3,4,15]

Definition 2: The elliptic boundary problem (7) admits a cone of Agmon's directions if there is a cone Λ in the λ-complex plane such that

(1) $\forall\overline{x}\in M$, $\forall\overline{\xi}\neq 0$, Λ contains no eigenvalues of the matrix $\sigma_1(D)(\overline{x,\xi})$,
(2) $\forall\xi{:}|\xi|\geqslant 1$, $\operatorname{rank}(b(x;\xi)q(\lambda)(x;\xi))=\operatorname{rank}(q(\lambda)(x;\xi))$, $\forall\lambda\in\Lambda$,

where $q(\lambda)$ denotes the principal symbol of the Calderón projector $Q(\lambda)$ associated to $D-\lambda I$, with λ included in $\sigma_1(D-\lambda I)$ [i.e., considering λ of degree one in the expansion of $\sigma(D-\lambda I)$ in homogeneous functions].[3,15]

An expression for $q(\lambda)(x;\xi)$ is obtained from (5):

$$q(\lambda)(x;\xi)=\frac{1}{2\pi i}\int_\Gamma (a_1^{-1}(x,0;0,1;0)a_1(x,0;\xi,0;\lambda)-z)^{-1}\,dz, \tag{9}$$

where $a_1(x;t;\xi,\tau;\lambda)=\sigma_1(D-\lambda I)$, with λ considered of degree one as stated above.

Henceforth, we assume the existence of an Agmon's cone Λ. Moreover, we will consider only boundary conditions B giving rise to a discrete spectrum $\operatorname{sp}(D_B)$. Note that this is always the case

for elliptic boundary problems unless $\mathrm{sp}(D_B)$ is the whole complex plane (see, for instance, Ref. 13). Now, for $|\lambda|$ large enough, $\mathrm{sp}(D_B)\cap\Lambda$ is empty, since there is no λ in $\mathrm{sp}(\sigma_1(D_B))\cap\Lambda$. Then, $\mathrm{sp}(D_B)\cap\Lambda$ is a finite set.

The usual definition of elliptic boundary conditions through ordinary differential equations in the normal variable can be recovered from Defn. 1 by introducing the ''partial symbol'' at the boundary:[3] Let us write

$$\sigma(D-\lambda I)=a_0(x,t;\xi,\tau;\lambda)+a_1(x,t;\xi,\tau;\lambda), \tag{10}$$

with a_l homogeneous of degree l in $(\overline{\xi,\lambda})$. We replace the coefficients of D by their Taylor expansions in powers of t, and group the resulting terms according to their degree of homogeneity in $(1/t,\xi,-i\partial_t,\lambda)$. More precisely, we set

$$a^{(j)}=a^{(j)}(x,t,\xi,-i\partial_t,\lambda)=\sum_{l-k=j}\frac{t^k}{k!}\,a_l^k(x,0,\xi,-i\partial_t,\lambda), \tag{11}$$

with $a_l^k=\partial_t^k a_l$.

Let us denote $\sigma'(D-\lambda I)=\Sigma_j a^{(j)}$ the partial symbol of $D-\lambda I$ at the boundary.

Now, condition (2) is equivalent to the following:

(2′) $\forall\lambda\in\Lambda$, $\forall x\in\partial M$, $\forall g\in\mathbf{C}^r$, the initial value problem

$$\sigma_1'(D)(x;\xi)u(t)=\lambda u(t),$$

$$b(x;\xi)u(t)\big|_{t=0}=g,$$

has, for each $\xi\neq 0$, a unique solution satisfying $\lim_{t\to\infty}u(t)=0$. This is the form under which this condition is stated in Ref. 3.

For $\lambda\in\Lambda$ not in $\mathrm{sp}(D_B)$, an asymptotic expansion of the symbol of $R(\lambda)=(D_B-\lambda I)^{-1}$ can be explicitly given:[3]

$$\sigma(R(\lambda))\sim\sum_{j=0}^{\infty}c_{-1-j}-\sum_{j=0}^{\infty}d_{-1-j}, \tag{12}$$

where the *Seeley coefficients* c_{-1-j} and d_{-1-j} satisfy

$$\sum_{j=0}^{1}a_{1-j}\circ\sum_{j=0}^{\infty}c_{-1-j}=I \tag{13}$$

with a_{1-j} as in (10), $\circ$ denoting the usual composition of homogeneous symbols, and

$$\sigma'(D-\lambda)\circ\sum_{j=0}^{\infty}d_{-1-j}=0,$$

$$\sigma'(B)\circ\sum_{j=0}^{\infty}d_{-1-j}=\sigma(B)\circ\sum_{j=0}^{\infty}c_{-1-j}\quad\text{at}\quad t=0, \tag{14}$$

$$\lim_{t\to\infty}d_{-1-j}=0.$$

Note that condition (2′) implies the existence and unicity of the solution of (14).

The coefficients $c_{-1-j}(x,t;\xi,\tau;\lambda)$ and $d_{-1-j}(x,t;\xi,\tau;\lambda)$ are meromorphic functions of λ with poles at those points where $\det[\sigma_1(D-\lambda)(x,t;\xi,\tau)]$ vanishes. The c_{-1-j}s are homogeneous of degree $-1-j$ in (ξ,τ,λ); the d_{-1-j}s are also homogeneous of degree $-1-j$, but in $(1/t,\xi,\tau,\lambda)$.[3]

This gives an approximation to $(D_B-\lambda)^{-1}$, a parametrix constructed as[3]

$$P_K(\lambda)=\sum_{\varphi}\ \psi\left[\sum_{j=0}^{K} Op(\theta_2 c_{-1-j})-\sum_{j=0}^{K} Op'(\theta_1 d_{-1-j})\right]\varphi, \tag{15}$$

where φ is a partition of the unity, $\psi\equiv 1$ in $\mathrm{Supp}(\varphi)$,

$$\begin{aligned}\theta_2(\xi,\tau,\lambda)&=\chi(|\xi|^2+|\tau|^2+|\lambda|^2),\\ \theta_1(\xi,\lambda)&=\chi(|\xi|^2+|\lambda|^2),\end{aligned} \tag{16}$$

with

$$\chi(t)=\begin{cases}0, & t\leqslant\frac{1}{2},\\ 1, & t\geqslant 1,\end{cases} \tag{17}$$

and

$$\begin{aligned}Op(\sigma)h(x,t)&=\int \sigma(x,t;\xi,\tau)\hat{h}(\xi,\tau)e^{i(x\xi+t\tau)}\,\frac{d\xi}{(2\pi)^{\nu-1}}\,\frac{d\tau}{2\pi},\\ Op'(\sigma)h(x,t)&=\int\int \tilde{\sigma}(x,t;\xi,s)\tilde{h}(\xi,s)e^{ix\xi}\,\frac{d\xi}{(2\pi)^{\nu-1}}\,\frac{ds}{2\pi},\end{aligned} \tag{18}$$

where $\hat{h}(\xi,\tau)$ is defined in (30) and

$$\tilde{h}(\xi,s)=\int h(x,s)e^{-ix\xi}\,dx. \tag{19}$$

Moreover, it can be proved from (12) that, for $\lambda\in\Lambda$,

$$\|R(\lambda)\|_{L^2}\leqslant C|\lambda|^{-1}, \tag{20}$$

with C a constant.[3,15]

The estimate (20) allows for expressing the complex powers of D_B as

$$D_B^z=\frac{i}{2\pi}\int_\Gamma \lambda^z R(\lambda)\,d\lambda \tag{21}$$

for $\mathrm{Re}\,z<0$, where Γ is a closed path lying in Λ, enclosing the spectrum of D_B.[4] Note that such a curve Γ always exists for $\mathrm{sp}(D_B)\cap\Lambda$ finite.

For $\mathrm{Re}\,z\geqslant 0$, one defines

$$D_B^z=D^l\circ D_B^{z-l}, \tag{22}$$

for l a positive integer such that $\mathrm{Re}(z-l)<0$.

If $\mathrm{Re}(z)<-\nu$, the power D_B^z is an integral operator with continuous kernel $J_z(x,t;y,s)$ and, consequently, it is trace class. As a function of z, $\mathrm{Tr}(D_B^z)$ can be extended to a meromorphic

function in the whole complex plane **C**, with only simple poles at $z=j-\nu$, $j=0,1,2,...$, and vanishing residues when $z=0,1,2,...$.[4] Throughout this paper, analytic functions and their meromorphic extensions will be given the same name.

The function $\mathrm{Tr}(D_B^z)$ is usually called $\zeta_{(D_B)}(-z)$ because of its similarity with the classical Riemann ζ-function: if $\{\lambda_j\}$ are the eigenvalues of D_B, $\{\lambda_j^z\}$ are the eigenvalues of D_B^z; so $\mathrm{Tr}(D_B^z)=\Sigma\lambda_j^z$ when D_B^z is a trace class operator.

A regularized determinant of D_B can then be defined as

$$\mathrm{Det}(D_B)=\exp\left[-\frac{d}{dz}\,\mathrm{Tr}(D_B^z)\right]\Bigg|_{z=0}. \tag{23}$$

Now, let $D(\alpha)$ be a family of elliptic differential operators on M sharing their principal symbol and analytically depending on α. Let B give rise to an elliptic boundary condition for all of them, in such a way that $D(\alpha)_B$ is invertible and the boundary problems they define have a common Agmon's cone. Then, the variation of $\mathrm{Det}\,D(\alpha)_B$ with respect to α is given by (see, for example, Refs. 10 and 16)

$$\frac{d}{d\alpha}\ln\mathrm{Det}\,D(\alpha)_B=\frac{d}{dz}\left[z\mathrm{Tr}\left\{\frac{d}{d\alpha}\,(D(\alpha)_B)D(\alpha)_B^{z-1}\right\}\right]\Bigg|_{z=0}. \tag{24}$$

Note that, under the assumptions made, $(d/d\alpha)(D(\alpha)_B)$ is a multiplication operator.

Given α_0 and α_1, the quotient $\mathrm{Det}(D(\alpha_1))_B/\mathrm{Det}(D(\alpha_0))_B$ can be obtained by integrating the variation in (24) along a path from α_0 to α_1.

Although $J_z(x,t;x,t;\alpha)$, the kernel of $D(\alpha)_B^z$ evaluated at the diagonal, can be extended to the whole z-complex plane as a meromorphic function, the rhs in (24) cannot be simply written as the integral over M of the finite part of

$$\mathrm{tr}\left\{\frac{d}{d\alpha}\,(D(\alpha)_B)J_{z-1}(x,t;x,t;\alpha)\right\} \tag{25}$$

at $z=0$ (where tr means matrix trace). In fact, $J_{z-1}(x,t;x,t;\alpha)$ is in general nonintegrable in the variable t near ∂M for $z\approx 0$.

Nevertheless, an integral expression for the rhs in (24) will be constructed in Sec. (III), from the integral expression for $\mathrm{Tr}(D(\alpha)_B^{z-1})$ holding in a neighborhood of $z=0$ and obtained in the following way:[4]

if $T>0$ is small enough, the function $j_z(x;\alpha)$, defined as

$$j_z(x;\alpha)=\int_0^T J_z(x,t;x,t;\alpha)\,dt \tag{26}$$

for $\mathrm{Re}\,z<1-\nu$, admits a meromorphic extension to **C** as a function of z. So, if V is a neighborhood of ∂M defined by $t<\epsilon$, with ϵ small enough, $\mathrm{Tr}(D(\alpha)_B^{z-1})$ can be written as the finite part of

$$\int_{M/V}\mathrm{tr}\;J_{z-1}(x,t;x,t;\alpha)dx\;dt+\int_{\partial M}\mathrm{tr}\;j_{z-1}(x;\alpha)dx, \tag{27}$$

where a suitable partition of the unity is understood.

III. GREEN'S FUNCTIONS AND DETERMINANTS

In this section, we will give an expression for $(d/d\alpha)\ln\mathrm{Det}[D(\alpha)_B]$ in terms of $G_B(x,t;y,s;\alpha)$, the Green's function of $D(\alpha)_B$ [i.e., the kernel of the operator $D(\alpha)_B^{-1}$].

With the notation of Sec. II, (24) can be rewritten as

$$\frac{d}{d\alpha}\ln \operatorname{Det} D(\alpha)_B = \operatorname*{F.P.}_{z=0}\int_M \operatorname{tr}\left[\frac{d}{d\alpha}(D(\alpha)_B)J_{-z-1}(x,t;x,t;\alpha)\right]d\overline{x}, \tag{28}$$

where the rhs must be understood as the finite part of the meromorphic extension of the integral at $z=0$.

The finite part of $J_{-z-1}(x,t;x,t;\alpha)$ at $z=0$ does not coincide with the regular part of $G_B(x,t;y,s;\alpha)$ at the diagonal, since the former is defined through an analytic extension.

However, it can be shown that there exists a relation between them, involving a finite number of Seeley's coefficients. In fact, for boundaryless manifolds this problem has been studied in Ref. 6, by comparing the iterated limits F.P. $\lim_{z\to -1}\{\lim_{\overline{y}\to\overline{x}} J_z(x,t;y,s;\alpha)\}$ and R.P. $\lim_{\overline{y}\to\overline{x}}\{\lim_{z\to -1} J_x(x,t;y,s;\alpha)\}=$R.P. $\lim_{\overline{y}\to\overline{x}} G_B(x,t;y,s;\alpha)$.

In the case of manifolds with boundary, the situation is more involved owing to the fact that the finite part of the extension of $J_z(x,t;x,t;\alpha)$ at $z=-1$ is not integrable near ∂M. (A first approach to this problem appears in Ref. 7). Nevertheless, as mentioned in Sec. II, a meromorphic extension of $\int_0^T J_z(x,t;x,t;\alpha)dt$, with T small enough, can be performed and its finite part at $z=-1$ turns to be integrable in the tangential variables. A similar result holds, *a fortiori*, for $\int_0^T t^n J_z(x,t;x,t;\alpha)dt$, with $n=1,2,3...$. Then, near the boundary, the Taylor expansion of the function $A_\alpha=(d/d\alpha)D(\alpha)_B$ will naturally appear, and the limits to be compared are F.P. $\lim_{z\to -1}\{\lim_{\overline{y}\to\overline{x}}\int_0^T t^n J_z(x,t;y,s;\alpha)dt\}$ and R.P. $\lim_{\overline{y}\to\overline{x}}\{\lim_{z\to -1}\int_0^T t^n J_z(x,t;y,s;\alpha)dt\}$ $=$R.P. $\lim_{\overline{y}\to\overline{x}}\int_0^T t^n G_B(x,t;y,s;\alpha)dt$.

The starting point for this comparison is to carry out asymptotic expansions and to analyze the terms for which the iterated limits do not coincide (or do not even exist).

An expansion of $G_B(x,t,y,s)$ in $M\backslash\partial M$ in homogeneous and logarithmic functions of $(\overline{x}-\overline{y})$ can be obtained from (12) for $\lambda=0$:

$$G_B(x,t,y,s)=\sum_{j=1-\nu}^{0} h_j(x,t,x-y,t-s)+M(x,t)\log|(x,t)-(y,s)|+R(x,t,y,s), \tag{29}$$

with h_j the Fourier transform $\mathscr{F}^{-1}(c_{-\nu-j})$ of $c_{-\nu-j}$ for $j>0$ and $h_0=\mathscr{F}^{-1}(c_{-\nu})-M(x,t)\log|(x,t)-(y,s)|$. The function $M(x,t)$ will be explicitly defined below [see (35)]. Our convention for the Fourier transform is

$$\begin{aligned}\mathscr{F}(f\,)(\overline{\xi})&=\hat{f}(\overline{\xi})=\int f(\overline{x})e^{-i\overline{x}\cdot\overline{\xi}}\,d\overline{x},\\ \mathscr{F}^{-1}(\hat{f}\,)(\overline{x})&=f(\overline{x})=\frac{1}{(2\pi)^\nu}\int \hat{f}(\overline{\xi})e^{i\overline{x}\cdot\overline{\xi}}\,d\overline{\xi}.\end{aligned} \tag{30}$$

For $t>0$, $R(x,t,y,s)$ is continuous even at the diagonal $(y,s)=(x,t)$. Nevertheless, $R(x,t,y,s)|_{(y,s)=(x,t)}$ is not integrable because of its singularities at $t=0$. On the other hand, the functions $t^n R(x,t,y,t)$ are integrable with respect to the variable t for $y\neq x$ and $n=0,1,2,...$. An expansion of $\int_0^\infty t^n R(x,t,y,t)dt$ in homogeneous and logarithmic functions of $(x-y)$ can also be obtained from (12):

$$\int_0^\infty t^n R(x,t,y,t)dt=\sum_{j=n+2-\nu}^{0} g_{j,j+n+2-\nu}(x,x-y)+M_n(x)\log(|x-y|)+R_n(x,y), \tag{31}$$

where $R_n(x,y)$ is continuous even at $y=x$, and $g_{j,j+n+2-\nu}$ is the Fourier transform of the (homogeneous extension of) $\int_0^\infty t^n \widetilde{d}_{-1-j}(x,t,\xi,t,0)dt$, with

$$\tilde{d}_{-1-j}(x,t,\xi,s,\lambda)=-\int_{\Gamma^-} e^{-is\tau}\, d_{-1-j}(x,t,\xi,\tau,\lambda)\,d\tau \tag{32}$$

for Γ^- a closed path enclosing the poles of $d_{-1-j}(x,t,\xi,\tau,\lambda)$ lying in $\{\mathrm{Im}\,\tau>0\}$.

Since $\tilde{d}_{-1-j}$ is homogeneous of degree $-j$ in $(1/t,\xi,1/s,\lambda)$, $g_{j,j+n+2-\nu}$ turns out to be homogeneous of degree $j+n+2-\nu$ in $x-y$.

From the forementioned comparison, the following Theorem can be shown to hold (the proof will be given in Ref. 17):

Theorem 1: *Let M be a bounded closed domain in $\mathbf{R}^\nu$ with smooth boundary ∂M and E a k-dimensional complex vector bundle over M.*

Let $(D_\alpha)_B$ *be a family of elliptic differential operators of first order, acting on the sections of E, with a fixed local boundary condition B on ∂M, and denote by $J_z(x,t;x,t;\alpha)$ the meromorphic extension of the evaluation at the diagonal of the kernel of $(D_\alpha)_B^z$.*

Let us assume that, for each α, $(D_\alpha)_B$ is invertible, the family is differentiable with respect to α, and $\partial/\partial\alpha(D_\alpha)_B f = A_\alpha f$, with A_α a differentiable function.

If V is a neighborhood of ∂M defined by $t<\epsilon$ and $T>0$ small enough, then

(a)

$$\frac{\partial}{\partial\alpha}\ln\mathrm{Det}(D_\alpha)_B=\operatorname*{F.P.}_{z=-1}\left[\int_{\partial M}\int_0^T \mathrm{tr}\{A_\alpha(x,t)J_z(x,t;x,t;\alpha)\}dt\,dx\right]$$
$$+\operatorname*{F.P.}_{z=-1}\left[\int_{M/V}\mathrm{tr}\{A_\alpha(\overline{x})J_z(\overline{x;x;\alpha})\}d\overline{x}\right], \tag{33}$$

where a suitable partition of the unity is understood. (This expression must be understood as the finite part at $z=-1$ of the meromorphic extension.)

(b) For every α, the integral $\int_0^T A_\alpha(x,t)J_z(x,t;x,t;\alpha)dt$ is a meromorphic function of z, for each $x\in\partial M$, with a simple pole at $z=-1$. Its finite part (dropping, from now on, the index α for the sake of simplicity) is given by

$$\operatorname*{F.P.}_{z=-1}\int_0^T A(x,t)J_z(x,t;x,t)dt=-\int_0^T A(x,t)\int_{|(\xi,\tau)|=1}\frac{i}{2\pi}\int_\Gamma\frac{\ln\lambda}{\lambda}\,c_{-\nu}(x,t;\xi,\tau;\lambda)d\lambda\,\frac{d\sigma_{\xi,\tau}}{(2\pi)^\nu}\,dt$$
$$+\sum_{l=0}^{\nu-2}\frac{\partial_t^l A(x,0)}{l!}\int_{|\xi|=1}\int_0^\infty t^l\,\frac{i}{2\pi}$$
$$\times\int_\Gamma\frac{\ln\lambda}{\lambda}\,\tilde{d}_{-(\nu-1)+l}(x,t;\xi,t;\lambda)d\lambda\,dt\,\frac{d\sigma_\xi}{(2\pi)^{\nu-1}}+\lim_{y\to x}\left\{\int_0^T A(x,t)\right.$$
$$\times\left[G_B(x,t;y,t)-\sum_{l=1-\nu}^{0}h_l(x,t;x-y,0)-M(x,t)\,\frac{\Omega_\nu}{(2\pi)^\nu}\,(\ln|x\right.$$
$$\left.-y|^{-1}+\mathscr{K}_\nu)\right]dt+\sum_{j=0}^{\nu-2}\sum_{l=0}^{\nu-2-j}\frac{\partial_t^l A(x,0)}{l!}\,g_{j,l-(\nu-2-j)}(x,x-y)$$
$$\left.+\sum_{l=0}^{\nu-2}\frac{\partial_t^l A(x,0)}{l!}\,M_{\nu-2-l}(x)\,\frac{\Omega_{\nu-1}}{(2\pi)^{\nu-1}}\,(\ln|x-y|^{-1}+\mathscr{K}_{\nu-1})\right\}, \tag{34}$$

with

$$M(x,t)=\frac{1}{\Omega_\nu}\int_{|(\xi,\tau)|=1} c_{-\nu}(x,t;\xi,\tau;0)\,d\sigma_{\xi,\tau},$$
$$M_j(x)=\frac{1}{\Omega_{\nu-1}}\int_{|\xi|=1}\int_0^\infty t^{\nu-2-j}\tilde{d}_{-1-j}(x,t;\xi,t;0)\,dt\;d\sigma_\xi, \tag{35}$$

where $\Omega_n=\mathrm{Area}(S^{n-1})$, $\mathscr{K}_\nu=\ln 2-\frac{1}{2}\gamma+\frac{1}{2}\Gamma'(\nu/2)/\Gamma(\nu/2)$ *with* γ *the Euler's constant and where* h_l *and* g_l *are related to the Green's function* G_B *as in (29) and (31),*

$$h_{1-\nu+j}(x,t;w,u)=\mathscr{F}^{-1}_{(\xi,\tau)}[c_{-1-j}(x,t;(\xi,\tau)/|(\xi,\tau)|;0)|(\xi,\tau)|^{-1-j}](w,u),$$
$$h_0(x,t;w,u)=\mathscr{F}^{-1}_{(\xi,\tau)}[\mathrm{P.V.}\{(c_{-\nu}(x,t;(\xi,\tau)/|(\xi,\tau)|;0)-M(x,t))|(\xi,\tau)|^{-\nu}\}](w,u),$$
$$g_{j,l}(x,w)=\mathscr{F}^{-1}_{\xi}\left[\int_0^\infty t^n\tilde{d}_{-1-j}(x,t;\xi/|\xi|,t;0)\,dt\,|\xi|^{-1-j-n}\right](w),$$

with

$$l=j+n-\nu+2,$$

and

$$g_{j,0}(x,w)=\mathscr{F}^{-1}_{\xi}\left[\mathrm{P.V.}\left[\int_0^\infty t^{\nu-j-2}\tilde{d}_{-1-j}(x,t;\xi/|\xi|,t;0)\,dt-M_j(x)\right]|\xi|^{-(\nu-1)}\right](w). \tag{36}$$

(c) The integral $\int_{M\setminus V}\mathrm{tr}[A(\overline{x})J_z(\overline{x;x})]d\overline{x}$ in the second term on the rhs of (33) is a meromorphic function of z with a simple pole at $z=-1$. Its finite part is given by

$$\begin{aligned}\underset{z=-1}{\mathrm{F.P.}}\int_{M\setminus V}\mathrm{tr}[A(\overline{x})J_z(\overline{x;x})]d\overline{x}=&\int_{M\setminus V}A(\overline{x})\int_{|\overline{\xi}|=1}\frac{i}{2\pi}\int\frac{\ln\lambda}{\lambda}\,c_{-\nu}(\overline{x,\xi};\lambda)d\lambda\,\frac{d\overline{\xi}}{(2\pi)^\nu}\\&+\int_{M\setminus V}\lim_{y\to\overline{x}}A(\overline{x})\Bigg[G_B(\overline{x,y})-\sum_{l=1-\nu}^{0}h_l(\overline{x,x-y})\\&-M(\overline{x})\frac{\Omega_\nu}{(2\pi)^\nu}(\ln|\overline{x-y}|^{-1}+\mathscr{K}_\nu)\Bigg]d\overline{x}.\end{aligned} \tag{37}$$

This Theorem gives a closed expression for the evaluation of the determinant when the associated Green's function is known.

Awful as it looks, (34) is not so complicated: In the first place, all terms can be systematically evaluated. Moreover, the terms containing h_l subtract the singular part of the Green's function in the interior of the manifold [see (29)] and can thus be easily identified from the knowledge of G_B. $R(x,t,y,t)$, the regular part so obtained, is still nonintegrable near the boundary. Those terms containing $g_{j,l}$ subtract the singular part of the integrals $\int_0^T t^n R(x,t,y,t)\,dt$ [see (31)]. Finally, the terms containing $c_{-\nu}$ and $d_{-\nu+1}$ arise as a consequence of having replaced an analytic regularization by a *point splitting* one.

Even though Seeley's coefficients c and $\tilde{d}$ are to be obtained through an iterative procedure, which can make their evaluation a tedious task, in the cases of physical interest only the few first of them are needed. In fact, for the two-dimensional example in Sec. IV we will only need two such coefficients.

IV. TWO-DIMENSIONAL DIRAC OPERATOR ON A DISK

In this section, we will use the method previously discussed to evaluate the determinant of the operator $D=i\not{\partial}+\not{A}$ acting on functions defined on a two-dimensional disk of radius R. A family of local baglike[18] elliptic boundary conditions will be assumed.

We take A_μ to be an Abelian field in the Lorentz gauge; as it is well known, it can be written as $A_\mu=\epsilon_{\mu\nu}\partial_\nu\phi$ ($\epsilon_{01}=-\epsilon_{10}=1$). For ϕ we choose a smooth bounded function $\phi=\phi(r)$. Notice that, with these assumptions, $A_r=0$ and $A_\theta(r)=-\partial_r\phi(r)$. We call

$$\Phi=\oint_{r=R} A_\theta R\, d\theta=-2\pi R\partial_r\phi(r)\big|_{r=R}. \tag{38}$$

The free Dirac operator in polar coordinates is

$$i\not{\partial}=i\left(\gamma_r\partial_r+\frac{1}{r}\,\gamma_\theta\partial_\theta\right), \tag{39}$$

with

$$\gamma_r=\begin{pmatrix}0 & e^{-i\theta}\\ e^{i\theta} & 0\end{pmatrix},\quad \gamma_\theta=\begin{pmatrix}0 & -ie^{-i\theta}\\ ie^{i\theta} & 0\end{pmatrix}. \tag{40}$$

With these conventions, the full Dirac operator can be written as

$$D=e^{-\gamma_5\phi(r)}i\not{\partial}e^{-\gamma_5\phi(r)}. \tag{41}$$

Now, in order to perform our calculations, we consider the family of operators

$$D_\alpha=i\not{\partial}+\alpha\not{A}=e^{-\alpha\gamma_5\phi(r)}i\not{\partial}e^{-\alpha\gamma_5\phi(r)},\quad \text{with } 0\leqslant\alpha\leqslant 1, \tag{42}$$

which will allow us to go smoothly from the free to the full Dirac operator. If we call

$$W(\alpha)=\ln\,\mathrm{Det}(D_\alpha)_B, \tag{43}$$

where B represents the elliptic boundary condition, we have

$$\frac{\partial}{\partial\alpha}\,W(\alpha)=\mathrm{F.P.}_{z=0}[\mathrm{Tr}(\not{A}(D_\alpha)_B^{-z-1})]. \tag{44}$$

From the Theorem in Sec. III we obtain

$$\frac{\partial}{\partial\alpha}W(\alpha)=\frac{1}{(2\pi)^2}\,\mathrm{tr}\Bigg\{\int\lim_{y\to x}\Bigg[\int\Bigg[\not{A}(t)\Bigg(4\pi^2G_B(x,t,y,t)-\frac{1}{|x-y|}\int e^{i\xi(x-y)/|x-y|}c_{-1}$$
$$\times\Bigg(x,t;\frac{(\xi,\tau)}{|(\xi,\tau)|};0\Bigg)d\xi\,d\tau-\int_{|(\xi,\tau)|\geqslant 1}e^{i\xi(x-y)}c_{-2}(x,t;\xi,\tau;0)d\xi\,d\tau$$
$$-\int\frac{i}{2\pi}\int_\Gamma\frac{\ln\lambda}{\lambda}\,c_{-2}$$
$$\times\Bigg(x,t;\frac{(\xi,\tau)}{|(\xi,\tau)|};\lambda\Bigg)d\lambda\,d\sigma_{\xi,\tau}\Bigg)+\not{A}(0)\Bigg(\int_{|\xi|\geqslant 1}e^{i\xi(x-y)}\tilde{d}_{-1}(x,t;\xi,t;0)d\xi$$
$$+\int\frac{i}{2\pi}\int_\Gamma\frac{\ln\lambda}{\lambda}\,\tilde{d}_{-1}$$
$$\times\Bigg(x,t;\frac{\xi}{|\xi|},t;\lambda\Bigg)d\lambda\,d\sigma_\xi\Bigg)\Bigg]dt\Bigg]dx\Bigg\},\tag{45}$$

where the Fourier transforms of c_{-2} and $\tilde{d}_{-1}$ have been left explicitly indicated.

Now, the coefficients c and $\tilde{d}$ in the previous equation are those appearing in the asymptotic expansion of the resolvent $(D_\alpha-\lambda I)^{-1}$.

From (41), the symbol of $(D_\alpha-\lambda I)$ is

$$\sigma(D_\alpha-\lambda I)=(-\not{\xi}-\lambda I)+\alpha\not{A}=a_1(\theta,t,\xi,\tau,\lambda)+a_0(\theta,t,\xi,\tau,\lambda),\tag{46}$$

where

$$a_1=-\not{\xi}-\lambda I,\quad a_0=\alpha\not{A}.\tag{47}$$

The required Seeley's c-coefficients are given by[2]

$$c_{-1}=\frac{1}{(\lambda^2-\xi^2-\tau^2)}\,(\not{\xi}-\lambda I),$$
$$c_{-2}=\frac{\alpha}{(\lambda^2-\xi^2)^2}\,(2\lambda\xi_\mu A_\mu I-(\lambda^2-\xi^2)\not{A}-2\xi_\mu A_\mu\not{\xi}),\tag{48}$$

where $\not{\xi}=\xi\gamma_\theta+\tau\gamma_t$.

As regards the boundary contributors to the parametrix, i.e., the coefficients d_{-1-j}, they are the solutions of (14). In our case, the equation to be solved is

$$(-\lambda I-\xi\gamma_\theta+i\gamma_t\partial_t)d_{-1}=0,\tag{49}$$

with boundary conditions

$$b_0d_{-1}=b_0c_{-1}\quad\text{at } t=0,\tag{50}$$

plus the vanishing of d_{-1} as $t\to+\infty$. Equation (49) can be recast in the form

$$\partial_td_{-1}=-Md_{-1},\tag{51}$$

where $M=\xi\gamma_5+i\lambda\gamma_t$. It can be easily verified that

$$\mathrm{tr}(M)=0, \quad M^2=(\xi^2-\lambda^2)I. \tag{52}$$

So, M has eigenvalues $\pm\sqrt{\xi^2-\lambda^2}$, corresponding to the eigenvectors

$$u_{\pm}=\begin{pmatrix} ie^{-i\theta}(\xi\pm\sqrt{\xi^2-\lambda^2}) \\ \lambda \end{pmatrix}. \tag{53}$$

Since $d_{-1}\to 0$ for $t\to\infty$, we obtain

$$d_{-1}(x,t;\xi,\tau;\lambda)=e^{-t\sqrt{\xi^2-\lambda^2}}u_{+}\otimes\begin{pmatrix} f \\ g \end{pmatrix}^{\dagger}, \tag{54}$$

where the vector $\binom{f}{g}$ must be determined from the boundary condition at $t=0$ ($r=R$), given by (50).

We now consider a parametric family of baglike local boundary conditions leading to an elliptic boundary problem,

$$b_0=(1,we^{-i\theta}), \tag{55}$$

with w a nonzero complex constant. (Notice that these boundary conditions reduce to those of an MIT bag[18] when $w=\pm 1$.)

We define the operator $(D_\alpha)_B$ as the differential operator in (41), acting on the dense subspace of functions satisfying

$$B\psi\equiv b_0\psi|_{t=0}=0. \tag{56}$$

It is easy to verify that this operator has no normalizable zero modes. (Notice that these are not the most general local elliptic boundary conditions. In fact, zero modes would in general arise if one allowed w to depend on θ.)

Now, from (50) and the expression for c_{-1} given in (48), it turns out that

$$\begin{pmatrix} f \\ g \end{pmatrix}^{\dagger}=\frac{e^{i\theta}}{(\xi^2+\tau^2-\lambda^2)(\lambda w+i\xi+i\sqrt{\xi^2-\lambda^2})}\,(\lambda+w(-i\xi+\tau) \quad e^{-i\theta}(i\xi+\tau+\lambda w)). \tag{57}$$

Placing this expression into (54), and taking into account (32), we finally obtain

$$\begin{aligned}\tilde{d}_{-1}=&\pi i\,\frac{e^{-(u+t)\sqrt{\xi^2-\lambda^2}}}{\sqrt{\xi^2-\lambda^2}(iw\lambda-\xi-\sqrt{\xi^2-\lambda^2})}\\ &\times\begin{pmatrix} (\xi+\sqrt{\xi^2-\lambda^2})(i\lambda+w(\xi+\sqrt{\xi^2-\lambda^2})) & e^{-i\theta}(\xi+\sqrt{\xi^2-\lambda^2})(iw\lambda-\xi+\sqrt{\xi^2-\lambda^2}) \\ -i\lambda e^{i\theta}(i\lambda-w(\xi+\sqrt{\xi^2-\lambda^2})) & -i\lambda(iw\lambda-\xi+\sqrt{\xi^2-\lambda^2}) \end{pmatrix}.\end{aligned} \tag{58}$$

In order to apply (45), we look for the function $G_B(x,y)$ satisfying

$$D_\alpha G_B(x,y)=\delta(x,y), \quad BG_B(x,y)|_{x\in\partial\Omega}=0, \tag{59}$$

where D_α and B are given by Eqs. (41) and (56), respectively. Now, with the notation

$$\begin{aligned} x=(x_0,x_1)=(r\ \cos\ \theta, r\ \sin\ \theta), \quad X=x_0+ix_1=re^{i\theta}, \\ y=(y_0,y_1)=(\rho\ \cos\ \varphi,\rho\ \sin\ \varphi), \quad Y=y_0+iy_1=\rho e^{i\varphi}, \end{aligned} \tag{60}$$

it is easy to see that $G_B(x,y)$ is given by

$$G_B(x,y)=\frac{1}{2\pi i}\begin{pmatrix} \dfrac{Rwe^{\alpha(\phi(x)+\phi(y)-2\phi(R))}}{XY^*-R^2} & \dfrac{e^{\alpha(\phi(x)-\phi(y))}}{X-Y} \\ \dfrac{e^{-\alpha(\phi(x)-\phi(y))}}{(X-Y)^*} & \dfrac{Re^{-\alpha(\phi(x)+\phi(y)-2\phi(R))}}{w(XY^*-R^2)^*} \end{pmatrix}. \tag{61}$$

With these elements at hand, we now perform the calculation of the determinant.

From (61), one can see that

$$G_B(\theta,r,\varphi,r)\underset{\varphi\to\theta}{\sim}\ \text{diagonal matrix}+\frac{1}{2\pi ir(\theta-\varphi)}\,\gamma_\theta. \tag{62}$$

When placed into (45), we obtain for the first term on the rhs

$$\mathrm{tr}\{A_\theta\gamma_\theta G_B(\theta,r,\varphi,r)\}\underset{\varphi\to\theta}{\sim}\frac{A_\theta}{\pi ir(\theta-\varphi)}. \tag{63}$$

For the second term in (45)

$$-\frac{1}{4\pi^2|x-y|}\int d\xi\,d\tau\,e^{i\xi(x-y)/|x-y|}c_{-1}\left(x,t;\frac{(\xi,\tau)}{|(\xi,\tau)|};\lambda=0\right)\underset{\varphi\to\theta}{\sim}\frac{-1}{2\pi ir(\theta-\varphi)}\,\gamma_\theta, \tag{64}$$

which exactly cancels the singularity of the Green's function. Therefore, the contribution of the first two terms in (45) vanishes.

As regards the third term,

$$\begin{aligned}
&\frac{-1}{(2\pi)^2}\,\mathrm{tr}\int \lim_{y\to x}\mathcal{A}(t)\int_{|(\xi,\tau)|\geqslant 1}e^{i\xi(x-y)}c_{-2}(x,t;\xi,\tau;0)\,d\xi\,d\tau\,dx\,dt\\
&\quad=\frac{-\alpha}{2\pi^2}\lim_{y\to x}\int A_\theta^2 d^2x\int_{|(\xi,\tau)|\geqslant 1}e^{i\xi(x-y)}\,\frac{(\tau^2-\xi^2)}{(\xi^2+\tau^2)^2}\,d\xi\,d\tau\\
&\quad=-\frac{\alpha}{\pi}\int A_\theta^2 d^2x\,\lim_{y\to x}\int_{|x-y|}^{\infty}J_2(u)\,\frac{du}{u}\\
&\quad=\frac{-\alpha}{2\pi}\int A_\nu A_\nu\,d^2x.
\end{aligned} \tag{65}$$

where $J_2(u)$ is the Bessel function of order two.

Now, the fourth term in (45) is

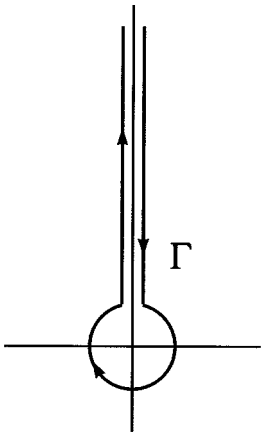

FIG. 1. The Contour Γ.

$$\frac{-1}{(2\pi)^2}\,\mathrm{tr}\int \mathcal{A}(t)\int\ \frac{i}{2\pi}\int_\Gamma \ln\lambda\, c_{-2}\left(x,t;\frac{(\xi,\tau)}{|(\xi,\tau)|};\lambda\right)\frac{d\lambda}{\lambda}\,d\sigma_{\xi,\tau}\,dx\,dt$$
$$=\frac{-i\alpha}{4\pi^3}\int A_\theta^2\,d^2x\int_\Gamma\frac{\ln\lambda}{(\lambda^2-1)^2}\int(1-\lambda^2-2\xi^2)d\sigma_{\xi,\tau}\,\frac{d\lambda}{\lambda}$$
$$=\frac{i\alpha}{2\pi^2}\int A_\theta^2\,d^2x\,2\pi i\int_0^\infty\frac{\mu\,d\mu}{(\mu^2+1)^2}$$
$$=\frac{-\alpha}{2\pi}\int A_\nu A_\nu\,d^2x. \tag{66}$$

This term gives rise to a contribution identical to that of (65).

The last term in (45) is

$$\frac{i}{(2\pi)^3}\,\mathrm{tr}\int\mathcal{A}(0)\sum_{\xi=\pm1}\int_\Gamma\ln\lambda\,\tilde{d}_{-1}\left(x,t;\frac{\xi}{|\xi|},t;\lambda\right)\frac{d\lambda}{\lambda}\,dx\,dt$$
$$=\frac{i\Phi}{(2\pi)^2}\int_\Gamma\frac{u\,\ln\lambda}{(1+u^2\lambda^2)}\left[\lambda\sqrt{1+u^2}-i\sqrt{1-\lambda^2}\right]\frac{d\lambda}{\sqrt{1-\lambda^2}}, \tag{67}$$

where $u=(1-w^2)/2w$. We choose the curve Γ as in Fig. 1.

Therefore, (67) reads

$$-\frac{\Phi}{2\pi}\,u\int_0^\infty\frac{1}{(1-u^2\mu^2)}\left[\mu\,\frac{\sqrt{1+u^2}}{\sqrt{1+\mu^2}}-1\right]d\mu=\frac{-\Phi}{4\pi}\ln w^2. \tag{68}$$

Putting all pieces together [(65), (66), and (68)], we finally find

$$\ln \mathrm{Det}(D)_B - \ln \mathrm{Det}(i\partial\!\!\!/)_B = -\frac{1}{2\pi}\int_\Omega A_\nu A_\nu \, d^2x - \frac{\Phi}{4\pi}\ln w^2$$

$$= -\frac{1}{2\pi}\int_\Omega A_\nu A_\nu \, d^2x$$

$$-\frac{1}{4\pi}\ln w^2 \int_{\partial\Omega} A_\nu \, dx_\nu . \tag{69}$$

The first term is the integral, restricted to the region Ω, of the same density appearing in the well-known case of the whole plane.[19] The second term is well defined for every $w \neq 0$, and vanishes for a null total flux, $\Phi = 0$. For $w = 0$, b_0 in (55) does not define an elliptic boundary problem. It is also interesting to notice that this term vanishes in the case of MIT bag boundary conditions, i.e., $w = \pm 1$.

This calculation is to be compared with the case of the compactified plane,[2] where the determinant can be expressed in terms of just the kernel of the z-power of the operator analytically extended to $z = 0$, which is a local quantity. The presence of boundaries makes the evaluation more involved, since even in simple cases as the present (or the half-plane treated in Ref. 7), the knowledge of the Green's function of the problem is needed.

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Differential calculi on quantum Minkowski space

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The differential calculus on n-dimensional ($n\geqslant 3$) quantum Minkowski space covariant with respect to left action of κ-Poincaré group is constructed and its uniqueness is shown. © *1996 American Institute of Physics.* [S0022-2488(96)03909-6]

I. INTRODUCTION

The κ-Poincaré algebra, introduced in Ref. 1, provides a Hopf algebra deformation of standard Poincaré algebra which depends on dimensionful parameter κ. Its global counterpart, κ-Poincaré group P_κ has been constructed by Zakrzewski.[2] It is a free *-algebra generated by the hermitean elements $\Lambda^\mu{}_\nu$, a^μ, subject to the following conditions:

$$
\begin{gathered}
(g^{\mu\nu}=\mathrm{diag}(+---)):\quad [a^\mu,a^\nu]=\frac{i}{\kappa}\,(\delta^\mu_0 a^\nu-\delta^\nu_0 a^\mu),\\
[\Lambda^\mu{}_\nu,\Lambda^\alpha{}_\beta]=0,\quad [\Lambda^\mu{}_\nu,a^\alpha]=-\frac{i}{\kappa}\,((\Lambda^\mu{}_0-\delta^\mu_0)\Lambda^\alpha{}_\nu+(\Lambda^0{}_\nu-\delta^0_\nu)g^{\mu\alpha}),\\
\Delta(\Lambda^\mu{}_\nu)=\Lambda^\mu{}_\alpha\otimes\Lambda^\alpha{}_\nu,\quad \Delta(\alpha^\mu)=\Lambda^\mu{}_\nu\otimes a^\nu+a^\mu\otimes I,\quad S(\Lambda^\mu{}_\nu)=\Lambda_\nu{}^\mu,\\
S(a^\mu)=-\Lambda_\nu{}^\mu a^\nu.\quad \epsilon(\Lambda^\mu{}_\nu)=\delta^\mu_\nu,\quad \epsilon(a^\mu)=0.
\end{gathered}
\tag{1}
$$

It appears[2,3] that one can also define a noncommutative generalization of Minkowski spacetime—the κ-Minkowski space $\mathcal{M}_\kappa$. The κ-Poincaré group acts on $\mathcal{M}_\kappa$ covariantly from the left. Once one accepts the idea that the κ-deformed Poincaré symmetry can have something to do with reality, the next step is to find the natural generalizations of standard geometric notions related to Minkowski space. The first step toward this directions was made by Sitarz[4] who showed that one cannot construct four-dimensional differential calculus on $\mathcal{M}_\kappa$ which is covariant with respect to infinitesimal left action of $\mathcal{P}_\kappa$. He sketched also the construction of five-dimensional covariant calculus.

In the present paper we consider the problem of the classification of differential calculi on $\mathcal{M}_\kappa$ which are covariant with respect to the left *global* action of κ-Poincaré group on $\mathcal{M}_\kappa$. No restriction is made concerning the dimensionality of spacetime (i.e., the indices μ, ν, etc., in Eq. (1) run from 0 to $n-1$) except $n\geqslant 3$. We show that the lowest dimensional nontrivial left-covariant calculus is $n+1$-dimensional and is unique. Its construction is given explicitly and the result coincides with the suggestion of Sitarz.

As a main tool we use the beautiful Woronowicz theory of differential calculi.[5] In Sec. II we show that the Woronowicz theory can be immediately extended to deal with the problem of covariant differential calculi on quantum spaces. This natural extension provides a nice framework to discuss our problem. In Sec. III we use the scheme developed in Sec. II to show that there is a

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unique $n+1$-dimensional calculus on $\mathcal{M}_\kappa$ which is left-covariant with respect to the action of $\mathcal{P}_\kappa$. This calculus is explicitly constructed and shown to be lowest-dimensional nontrivial calculus on $\mathcal{M}_\kappa$.

The results obtained here were briefly reported in Ref. 6. Let us also mention that the differential calculi on quantum spacetimes covariant with respect to other deformations of Poincaré group were considered by Podleś.[7]

II. COVARIANT DIFFERENTIAL CALCULI

Let us first indicate how one can extend the Woronowicz theory of differential calculi[5] to the following situation: Assume that the quantum group $\mathcal{B}$ acts on quantum space $\mathcal{A}$; one looks for differential calculi on $\mathcal{A}$ on which the covariant action of $\mathcal{B}$ can be defined as ''induced'' by the action of $\mathcal{B}$ on $\mathcal{A}$. All proofs are omitted as being a straightforward extension of those given by Woronowicz.

Let $\mathcal{A}$ be an algebra with unity (quantum space). The starting point in Woronowicz construction is the universal bimodule $\mathcal{A}^2 \subset \mathcal{A}\otimes\mathcal{A}$ defined by

$$\mathcal{A}^2 = \left\{ \sum_k a_k \otimes b_k \in \mathcal{A}\otimes\mathcal{A} \Big| \sum_k a_k b_k = 0 \right\},$$

$$c\left(\sum_k a_k \otimes b_k\right) = \sum_k c a_k \otimes b_k, \quad \left(\sum_k a_k \otimes b_k\right) c = \sum_k a_k \otimes b_k c. \tag{2}$$

The universal differential $D: \mathcal{A} \to \mathcal{A}^2$ is given by $da = I\otimes a - a\otimes I$.

It can be easily shown that any other calculus is obtained from the universal one by dividing by an appropriately chosen sub-bimodule $\mathcal{N} \subset \mathcal{A}^2$.

Let now ρ_L be a left action of a quantum group $\mathcal{B}$ on $\mathcal{A}$, i.e., a homomorphism $\rho_L : \mathcal{A} \to \mathcal{B}\otimes\mathcal{A}$ obeying

$$(\mathrm{id}\otimes\rho_L)\circ\rho_L = (\Delta\otimes\mathrm{id})\circ\rho_L, \quad (\epsilon\otimes\mathrm{id})\circ\rho_L = \mathrm{id}. \tag{3}$$

Let us define the action $\tilde{\rho}_L$ of $\mathcal{B}$ on $\mathcal{A}^2$ as follows: Let

$$q = \sum_i x_i \otimes y_i \in \mathcal{A}\otimes\mathcal{A}, \quad \rho_L(x_i) = \sum_k a_i{}^k \otimes x_i{}^k \in \mathcal{B}\otimes\mathcal{A},$$

$$\rho_L(y_i) = \sum_l b_i{}^l \otimes y_i{}^l \in \mathcal{B}\otimes\mathcal{A}; \tag{4a}$$

then

$$\tilde{\rho}_L(q) = \sum_{i,k,l} a_i{}^k b_i{}^l \otimes x_i{}^k \otimes y_i{}^l. \tag{4b}$$

Obviously, $\tilde{\rho}_L : \mathcal{A}\otimes\mathcal{A} \to \mathcal{B}\otimes\mathcal{A}\otimes\mathcal{A}$; however, it is straightforward to show that $\tilde{\rho}_L : \mathcal{A}^2 \to \mathcal{B}\otimes\mathcal{A}^2$. Following the same lines as in Ref. 5, one easily proves the following properties of $\tilde{\rho}_L$

(i_L) for $x \in \mathcal{A}$, $y \in \mathcal{A}^2$

$$\tilde{\rho}_L(xy) = \rho_L(x)\tilde{\rho}_L(y), \quad \tilde{\rho}_L(yx) = \tilde{\rho}_L(y)\rho_L(x)$$

(ii_L)

$$\tilde{\rho}_L \circ D = (\mathrm{id} \otimes D) \circ \rho_L \tag{5}$$

(iii_L)

$$(\mathrm{id} \otimes \tilde{\rho}_L) \circ \tilde{\rho}_L = (\Delta \otimes \mathrm{id}) \circ \tilde{\rho}_L, \quad (\epsilon \otimes \mathrm{id}) \circ \tilde{\rho}_L = \mathrm{id}.$$

Property (iii_L) means that $\tilde{\rho}_L$ is the left action of $\mathscr{B}$ on $\mathscr{A}^2$ while (i), (ii) can be summarized by saying that $\tilde{\rho}_L$ is the lift of ρ_L to $\mathscr{A}^2$ ($\tilde{\rho}_L$ is the left action of $\mathscr{B}$ on universal differential calculus on $\mathscr{A}$ induced from the left action ρ_L). Moreover, let us note that the following formula holds:

$$\tilde{\rho}_L \left(\sum_i x_i D y_i \right) = \sum_i \rho_L(x_i)(\mathrm{id} \otimes D) \rho_L(y_i) \tag{6}$$

which is a counterpart of Eq. (1.15) of Ref. 5.

Now, assume that $\mathscr{N} \subset \mathscr{A}^2$ is a subbimodule such that

$$\tilde{\rho}_L(\mathscr{N}) \subset \mathscr{B} \otimes \mathscr{N}. \tag{7}$$

Then the differential calculus (Γ, d) determined by $\mathscr{N}$ has the following property:

$$\sum_i x_i \, dy_i = 0 \Rightarrow \sum_i \rho_L(x_i)(\mathrm{id} \otimes d) \rho_L(y_i) = 0. \tag{8}$$

Therefore,

$$\tilde{\rho}_L \left(\sum_i x_i \, dy_i \right) = \sum_i \rho_L(x_i)(\mathrm{id} \otimes d) \rho_L(y_i) \tag{9}$$

is well defined linear mapping from Γ into $\mathscr{B} \otimes \Gamma$. Formulate (i_L)–(iii_L) and Eq. (6) hold upon replacing $\mathscr{A}^2$ by Γ and D by d.

We shall say that (Γ, d) is left-covariant with respect to the action of $\mathscr{B}$.

All the above results can be extended mutatis mutandis to right actions. Let $\rho_R : \mathscr{A} \to \mathscr{A} \otimes \mathscr{B}$ be right action of $\mathscr{B}$ on $\mathscr{A}$

$$(\rho_R \otimes \mathrm{id}) \circ \rho_R = (\mathrm{id} \otimes \Delta) \circ \rho_R, \quad (\mathrm{id} \otimes \epsilon) \circ \rho_R = \mathrm{id}. \tag{10}$$

For

$$q = \sum_i x_i \otimes y_i \in \mathscr{A} \otimes \mathscr{A}, \quad \rho_R(x_i) = \sum_k x_i{}^k \otimes a_i{}^k \in \mathscr{A} \otimes \mathscr{B},$$

$$\rho_R(y_i) = \sum_l y_i{}^l \otimes b_i{}^l \in \mathscr{A} \otimes \mathscr{B}, \tag{11a}$$

we put

$$\tilde{\rho}_R(q) = \sum_{i,k,l} x_i{}^k \otimes y_i{}^l \otimes a_i{}^k b_i{}^k, \tag{11b}$$

Again $\tilde{\rho}_R : \mathscr{A}^2 \to \mathscr{A}^2 \otimes \mathscr{B}$ obeys

(i_R) for $x \in \mathscr{A}$, $y \in \mathscr{A}^2$

$$\tilde{\rho}_R(xy)=\rho_R(x)\tilde{\rho}_R(y), \quad \tilde{\rho}_R(yx)=\tilde{\rho}_R(y)\rho_R(x),$$

(ii_R)

$$\tilde{\rho}_R\circ D=(D\otimes \mathrm{id})\circ\rho_R \tag{12}$$

(iii_R)

$$(\tilde{\rho}_R\otimes \mathrm{id})\circ\tilde{\rho}_R=(\mathrm{id}\otimes\Delta)\circ\tilde{\rho}_R, \quad (id\otimes\epsilon)\circ\tilde{\rho}_R=\mathrm{id}$$

as well as

$$\tilde{\rho}_R\left(\sum_i x_i D y_i\right)=\sum_i \rho_R(x_i)(D\otimes \mathrm{id})\rho_R(y_i). \tag{13}$$

Now assume $\mathcal{N}\in\mathcal{A}^2$ to be a sub-bimodule such that $\tilde{\rho}_R(\mathcal{N})\subset\mathcal{N}\otimes\mathcal{B}$. Then, for the calculus (Γ,d) determined by $\mathcal{N}$, (i_R)–(iii_R) and Eq. (13) hold with appropriate replacements $\mathcal{A}^2\to\Gamma$, $D\to d$.

Finally, let the pair (ρ_L,ρ_R) of actions of $\mathcal{B}$ on $\mathcal{A}$ be given. We assume that ρ_L,ρ_R commute

$$(\mathrm{id}\otimes\rho_R)\circ\rho_L=(\rho_L\otimes \mathrm{id})\circ\rho_R. \tag{14}$$

We say that (Γ,d) is bicovariant with respect to the action of $\mathcal{B}$ on $\mathcal{A}$ if it is left- and right-covariant. Then, it has all properties of left- and right-covariant calculi together with the following one [cf. Eq. (1.20) of Ref. 5];

$$(\mathrm{id}\otimes\tilde{\rho}_R)\circ\tilde{\rho}_L=(\tilde{\rho}_L\otimes \mathrm{id})\circ\tilde{\rho}_R. \tag{15}$$

Let us now discuss the problem of infinitesimal action of $\mathcal{B}$ on $\mathcal{A}$. Let χ be any element of the Hopf algebra dual to $\mathcal{B}$. We put

$$\chi_{\rho_L}=(\chi\otimes \mathrm{id})\circ\rho_L, \quad \chi_{\tilde{\rho}_L}=(\chi\otimes \mathrm{id})\circ\tilde{\rho}_L. \tag{16}$$

The first definition, introduced by Woronowicz,[8] coincides with the one used by Majid and Ruegg.[3] The second one is equivalent to the proposal of Sitarz[4]

$$\begin{aligned}\chi_{\tilde{\rho}_L}(x\ dy)&=(\chi\otimes \mathrm{id})(\rho_L(x)(\mathrm{id}\otimes d)\rho_L(y))\\&=[(\chi_{(1)}\otimes \mathrm{id})\rho_L(x)](\mathrm{id}\otimes d)[(\chi_{(2)}\otimes \mathrm{id})\rho_L(y)]\\&=\chi_{(1)\rho_L}(x)(\mathrm{id}\otimes d)\chi_{(2)\rho_L}(y),\end{aligned} \tag{17}$$

where $\Delta\chi=\chi_{(1)}\otimes\chi_{(2)}$. Analogous definitions can be given for ρ_R and $\tilde{\rho}_R$.

From the above discussion it follows then that in order to check whether a calculus on $\mathcal{A}$ is consistent with the action of $\mathcal{B}$ on $\mathcal{A}$ it is sufficient to check the property $\tilde{\rho}_L(\mathcal{N})\subset\mathcal{B}\otimes\mathcal{N}$ $(\tilde{\rho}_R(\mathcal{N})\subset\mathcal{N}\otimes\mathcal{B})$.

This simplifies considerably if $\mathcal{A}$ itself is a quantum group and $\mathcal{N}$ defines (say) left-covariant calculus on it. Then $\mathcal{N}=r^{-1}(\mathcal{A}\otimes\mathcal{R})$ where $\mathcal{R}$ is a right ideal in $\ker\epsilon$; any element of $\mathcal{A}\otimes\mathcal{R}$ can be written as

$$t=\sum_i a_i\otimes x_i b_i, \tag{18}$$

where $a_i, b_i \in \mathscr{A}$ and x_i are generators of $\mathscr{R}$. From the very definition of the operation r^{-1} the following formula follows immediately:[5]

$$r^{-1}(t) = \sum_{i,l} a_i S(b^{l'}{}_i) r^{-1}(I \otimes x_i) b^{l''}{}_i, \tag{19a}$$

where

$$\Delta(b_i) = \sum_{l} b^{l'}{}_i \otimes b^{l''}{}_i. \tag{19b}$$

The properties (5) applied to the universal calculus imply

$$\widetilde{\rho}_L(r^{-1}(t)) = \sum_{i,l} \rho_L(a_i S(b^{l'}{}_i) \widetilde{\rho}_L(r^{-1}(I \otimes x_i)) \rho_L(b^{l''}{}_i). \tag{20}$$

Therefore it is sufficient to check that

$$\widetilde{\rho}_L(r^{-1}(I \otimes x_i)) \subset \mathscr{B} \otimes \mathscr{N} \tag{21}$$

for all generators x_i of $\mathscr{R}$.

Let us now pass to the external algebra. Given $\widetilde{\rho}_L : \Gamma \to \mathscr{B} \otimes \Gamma$ we define $\widetilde{\rho}_L^{\otimes 2} : \Gamma^{\otimes 2} \to \mathscr{B} \otimes \Gamma^{\otimes 2}$ by

$$\widetilde{\rho}_L^{\otimes 2}(\omega_1 \otimes \omega_2) = \sum_{k,l} a_{1k} a_{2l} \otimes \omega_{1k} \otimes \omega_{2l} \tag{22}$$

extended by linearity; here $\omega_i \in \Gamma$ and

$$\widetilde{\rho}_L(\omega_i) = \sum_{k} a_{ik} \otimes \omega_{ik}, \quad i = 1,2. \tag{23}$$

Let us assume that $\mathscr{A}$ is a quantum group, (Γ, d)—a bicovariant calculus on it and let σ be the module homomorphism defined in Proposition 3.1 of Ref. 5. Then $\Gamma^{\wedge 2}$ is defined as

$$\Gamma^{\wedge 2} = \Gamma^{\otimes 2} / \ker(I - \sigma) \tag{24}$$

and, in order to have a consistent action of $\mathscr{B}$ on $\Gamma^{\wedge 2}$ we must only check that

$$(\mathrm{id} \otimes \sigma) \circ \widetilde{\rho}_L^{\otimes 2} = \widetilde{\rho}_L^{\otimes 2} \circ \sigma. \tag{25}$$

Due to the property

$$\widetilde{\rho}_L^{\otimes 2}(xy) = \rho_L(x) \widetilde{\rho}_L^{\otimes 2}(y), \quad x \in \mathscr{A}, \quad y \in \Gamma^{\otimes 2} \tag{26}$$

it is sufficient to verify Eq. (25) for the basic elements only.

III. LEFT-COVARIANT CALCULI ON κ-MINKOWSKI SPACE

The n-dimensional κ-Minkowski space $\mathscr{M}_\kappa$ is an $*$-algebra with unity generated by n hermitian elements x^μ subject to the following conditions:[2,3]

$$[x^\mu, x^\nu] = \frac{i}{\kappa} (\delta_0^\mu x^\nu - \delta_0^\nu x^\mu). \tag{27}$$

$\mathcal{M}_\kappa$ can be equipped with the structure of the quantum group by putting

$$\Delta x^\mu = I\otimes x^\mu + x^\mu \otimes I, \quad S(x^\mu) = -x^\mu, \quad \epsilon(x^\mu) = 0. \tag{28}$$

The left action of n-dimensional κ-Poincaré group $\mathcal{P}_\kappa$ on $\mathcal{M}_\kappa$ can be defined as follows:

$$\rho_L(I) = I\otimes I, \quad \rho_L(x^\mu) = \Lambda^\mu{}_\nu \otimes x^\nu + a^\mu \otimes I \tag{29}$$

extended by linearity and multiplicativity.

We want to find a left-covariant (with respect to action of $\mathcal{P}_\kappa$) calculi on $\mathcal{M}_\kappa$. The proof will be given for $n=4$. However, for general $n\geqslant 3$ the proof goes along the same way. As the first step let us note that $\mathcal{M}_\kappa$ is a subgroup of $\mathcal{P}_\kappa$. Indeed, $\Pi:\mathcal{P}_\kappa \to \mathcal{M}_\kappa$ given

$$\Pi(a^\mu) = x^\mu, \quad \Pi(\Lambda^\mu{}_\nu) = \delta^\mu_\nu I \tag{30}$$

is an epimorphism obeying

$$\Delta_{\mathcal{M}} \circ \Pi = (\Pi\otimes\Pi)\circ\Delta_{\mathcal{P}}. \tag{31a}$$

Moreover, it is immediate to check that

$$(\Pi\otimes \mathrm{id})\circ\rho_L = \Delta_{\mathcal{M}}. \tag{31b}$$

Let $\tilde{\rho}_L$ be the extension of ρ_L to $\mathcal{M}^2_\kappa$. Equations (8), (31), and the results contained in Ref. 5 imply that any calculus on $\mathcal{M}_\kappa$ left-covariant with respect to action of $\mathcal{P}_\kappa$ is also left-covariant with respect to action of $\mathcal{M}_\kappa$ on itself. Therefore the relevant sub-bimodule $\mathcal{N}$ is of the form $r^{-1}(\mathcal{M}_\kappa\otimes\mathcal{R})$ where $\mathcal{R}$ is a right ideal in $\ker\epsilon_{\mathcal{M}}$.

Let $\mathcal{R}$ be any ideal in $\ker\epsilon_{\mathcal{M}}$. Any $a\in\mathcal{R}$ can be written as ($\boldsymbol{\mu}\equiv(\mu_0,\mu_k)$)

$$a = \sum_{\mu_0,\mu_k} c_{\boldsymbol{\mu}} (x^0)^{\mu_0} \prod_{k=1}^{n-1} (x^k)^{\mu_k}. \tag{32}$$

Let us call $|\mu| = \mu_0 + \Sigma_{k=1}^{n-1}\mu_k$; obviously, $c_{\boldsymbol{\mu}}=0$ for $|\mu|=0$; further, let

$$\mu(a) = \max_{c_{\boldsymbol{\mu}}\neq 0} |\mu|, \quad \mu(\mathcal{R}) = \min_{a\in\mathcal{R}} \mu(a). \tag{33}$$

Obviously, $\mu(\mathcal{R})\geqslant 1$; let us first assume that $\mu(\mathcal{R})=1$. This means that $c_0 x^0 + c_k x^k \in \mathcal{R}$ for some (not all zero) constants c_0, c_k. But

$$\tilde{\rho}_L(r^{-1}(I\otimes c_\mu x^\mu)) = c_\mu \Lambda^\mu{}_\nu \otimes r^{-1}(I\otimes x^\nu). \tag{34}$$

Therefore, $x^\mu\in\mathcal{R}$ for all μ, i.e., $\mathcal{R}=\ker\epsilon_{\mathcal{M}}$ and the corresponding calculus is trivial.

As the next step let us take $\mu(\mathcal{R})=2$. It is straightforward to check that

$$\tilde{\rho}_L(r^{-1}(I\otimes x^{\mu\nu})) = \Lambda^\mu{}_\alpha \Lambda^\nu{}_\beta \otimes r^{-1}(I\otimes x^{\alpha\beta}), \tag{35}$$

where

$$x^{\mu\nu} \equiv x^\mu x^\nu + \frac{i}{\kappa}(g^{\mu\nu}x^0 - g^{0\mu}x^\nu). \tag{36}$$

Due to the fact that Λ's commute among themselves we can write a standard representation theory of Lorentz group. First of all, we note that $r^{-1}(I\otimes x^{\mu\nu})$ transform as a second order symmetric [$x^{\mu\nu}=x^{\nu\mu}$ due to Eqs. (27) and (36)] tensor. It carries $D^{(1,1)}\oplus D^{(0,0)}$ representation of

Lorentz group. Let us first take all $x^{\mu\nu}$ as generators of $\mathscr{R}$. Then $(x^0)^2=x^{00}\in\mathscr{R}$ and $x^ix^0=x^{i0}\in\mathscr{R}$, i.e., $[(x^0)^2,x^i]\in\mathscr{R}$; therefore $x^ix^0+x^0x^i\in\mathscr{R}$ and $x^0x^i\in\mathscr{R}$. However, $x^{0i}=x^0x^i-(i/\kappa)x^i\in\mathscr{R}$ which implies $x^i\in\mathscr{R}$. Then Poincaré invariance implies $x^0\in\mathscr{R}$ and our calculus is trivial.

To improve the situation we can only, due to condition (21), subtract $D^{(0,0)}$ or $D^{(1,1)}$. Obviously, subtracting $D^{(1,1)}$ gives larger calculus, so we will subtract $D^{(0,0)}$.

It is not difficult to check that for general $n\geqslant 3$ the following lemma holds.

Lemma: Let $\mathscr{R}\subset\ker\epsilon_{\mathscr{M}}$ be right ideal generated by the elements

$$x^\mu x^\nu+\frac{i}{\kappa}(g^{\mu\nu}x^0-g^{0\mu}x^\nu)-\frac{1}{n}g^{\mu\nu}\left(x^2+\frac{i(n-1)}{\kappa}x^0\right). \tag{37}$$

Then

(a) $\mathscr{R}$ defines a left-$\mathscr{P}_\kappa$-covariant calculus on $\mathscr{M}_\kappa$,

(b) $a\in\mathscr{R}$ implies $S(a)^*\in\mathscr{R}$,

(c) $\ker\epsilon_{\mathscr{M}}/\mathscr{R}$ is spanned by x^μ and by

$$\varphi\equiv x^2+\frac{i}{\kappa}(n-1)x^0. \tag{38}$$

Now, we can construct the relevant calculus. The left-invariant forms are

$$\tau^\mu=\pi r^{-1}(I\otimes x^\mu)=dx^\mu,\quad \tau=\pi r^{-1}(I\otimes\varphi)=d\varphi-2x_\mu dx^\mu \tag{39}$$

and they appear to be also right-invariant. The commutation rules are easily derived according to the standard procedure of Ref. 5

$$[\tau^\mu,x^\nu]=\frac{i}{\kappa}g^{0\mu}\tau^\nu-\frac{i}{\kappa}g^{\mu\nu}\tau^0+\frac{1}{n}g^{\mu\nu}\tau,\quad [\tau,x^\mu]=-\frac{n}{\kappa^2}\tau^\mu \tag{40}$$

while the hermicity properties read

$$(\tau^\mu)^*=\tau^\mu,\quad \tau^*=-\tau. \tag{41}$$

The left action of $\mathscr{P}_\kappa$ on $\mathscr{M}_\kappa$ is easily calculated to be

$$\tilde{\rho}_L(\tau^\mu)=\Lambda^\mu{}_\nu\otimes\tau^\nu,\quad \tilde{\rho}_L(\tau)=I\otimes\tau. \tag{42}$$

In order to construct the external algebra we first verify property (25) for the bimodule homomorphism σ: $\sigma(\tau^\mu\otimes\tau^\nu)=\tau^\nu\otimes\tau^\mu$, $\sigma(\tau\otimes\tau^\mu)=\tau^\mu\otimes\tau$, $\sigma(\tau^\mu\otimes\tau)=\tau\otimes\tau^\mu$. The external algebra implied by σ takes the standard form

$$\tau^\mu\wedge\tau^\nu=-\tau^\nu\wedge\tau^\mu,\quad \tau\wedge\tau^\mu=-\tau^\mu\wedge\tau. \tag{43}$$

Moreover,

$$d\tau^\mu=0,\quad d\tau=-2\,d\tau^\mu\wedge d\tau_\mu. \tag{44}$$

From the discussion carried out above it follows that the $n+1$-dimensional calculus described by Eqs. (39)–(43) is the lowest dimensional nontrivial calculus on $\mathscr{M}_\kappa$ covariant with respect to the left action of $\mathscr{P}_\kappa$. This is due to the fact that all differential calculi with $\mu(\mathscr{R})\geqslant 3$ have higher dimensions.

Finally, let us compare our calculus with that proposed by Sitarz.[4] Our Eqs. (40) agree with Eqs. (60) of Ref. 4 under the identification: $x^\mu \to ix^\mu$, $\tau \to (4/\kappa^2)\varphi$. In the two-dimensional case there is also an agreement provided the replacement $\tau \to (2/\kappa^2)\varphi$ is made; also the multiplication rules for one-forms [Eqs. (58) of Ref. 4] coincide in this case.

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Solving nonlinear recursions

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A general method to map a polynomial recursion on a matrix linear one is suggested. The solution of the recursion is represented as a product of a matrix multiplied by the vector of initial values. This matrix is product of *transfer* matrices whose elements depend only on the polynomial and not on the initial conditions. The method is valid for systems of polynomial recursions and for polynomial recursions of arbitrary order. The only restriction on these recurrent relations is that the highest-order term can be written in explicit form as a function of the lower-order terms (existence of a normal form). A continuous analog of this method is described as well. © *1996 American Institute of Physics.*
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I. INTRODUCTION

Recurrent relations take a central place in various fields of science. For example, numerical solution of differential equations and models of evolution of a system involve, in general, recursions.

By now, only linear recursions could be solved[1–3] while even the simplest nonlinearity usually made an analytic solution impossible. A good example for this is a rather simple recursion, the logistic map, $y_{n+1}=\lambda y_n(1-y_n)$. The analysis of its behavior, while based on roundabout approaches, has revealed many unusual features.

In this paper we propose a new approach to the solution of polynomial recursions. It turns out that the coefficients of the i-th iteration of the polynomial depend linearly on the coefficients of the $(i-1)$-th iteration. Using this fact we succeed in writing down the general solution of the recursion.

To make this paper more readable we include some auxiliary material on linear recursions as well as an introductory example.

II. INTRODUCTORY EXAMPLE: LOGISTIC MAPPING

To demonstrate our approach we begin with the recursion equation known as the logistic mapping:

$$y_{n+1}=\lambda y_n(1-y_n) \quad \text{with} \quad y_0\equiv y. \tag{1}$$

Very recently it was shown by Rabinovich *et al.*[4] that the solution of this recursion is given by

$$y_n=\langle \mathbf{e}|\mathbf{T}^n|\mathbf{y}\rangle, \tag{2}$$

where $\mathbf{T}$ is a transfer matrix with elements

$$T_{jk}=(-1)^{k-j}\binom{j}{k-j}\lambda^j. \tag{3}$$

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The vectors $|\mathbf{y}\rangle$ and $\langle\mathbf{e}|$ are correspondingly a set of y's powers and the first ort defined as

$$|\mathbf{y}\rangle=\{y^j\}_{j=1}^{2^n} \quad \text{and} \quad \langle\mathbf{e}|=[\delta_{j1}]_{j=1}^{2^n}, \tag{4}$$

where δ_{jk} is the Kronecker symbol.

Equations (2) and (3) were derived in Ref. 4 by consideration of a branching process. However, knowing the representation of the solution (2) one can obtain the matrix elements (3) in a ''one-line'' way. Namely, we have to find a matrix $\mathbf{T}$ that transforms a column $\{y^j\}$ to a column $\{[\lambda y(1-y)]^j\}$. Expanding this last expression

$$[\lambda y(1-y)]^j=\sum_{i=0}^{j}(-1)^i\binom{j}{i}\lambda^j y^{j+i}=\sum_{k=j}^{2j}(-1)^{k-j}\binom{j}{k-j}\lambda^j y^k=\sum_{k=j}^{2j}T_{jk}y^k$$

and extending the last summation over all natural numbers {due to the vanishing of the binomials $\binom{j}{k-j}$ for k outside the interval $[j,2j]$} we immediately recover Eq. (3) for the elements of the matrix $\mathbf{T}$.

III. GENERAL CASE OF FIRST-ORDER POLYNOMIAL RECURSION

Here we consider a first-order recursion equation in its normal form

$$y_{n+1}=P(y_n), \tag{5}$$

where $P(x)$ is a polynomial of degree m:

$$P(x)=\sum_{k=0}^{m}a_k x^k, \quad a_m\neq 0. \tag{6}$$

Let $y_0\equiv y$ be an initial value for the recursion (5). We denote by $|\mathbf{y}\rangle$ the column vector of powers of y

$$|\mathbf{y}\rangle=\{y^j\}_{j=0}^{\infty}$$

and the vector $\langle\mathbf{e}|$ is a row vector

$$\langle\mathbf{e}|=[\delta_{j1}]_{j=0}^{\infty}.$$

It should be emphasized that j runs from 0, since in the general case $a_0\neq 0$. In this notation $\langle\mathbf{e}|\mathbf{y}\rangle$ is a scalar product that yields

$$\langle\mathbf{e}|\mathbf{y}\rangle=y. \tag{7}$$

Theorem: For any recursion of the type of Eq. (5) there exists a matrix $\mathbf{T}=\{T_{jk}\}_{j,k=0}^{\infty}$ such that

$$y_n=\langle\mathbf{e}|\mathbf{T}^n|\mathbf{y}\rangle. \tag{8}$$

Proof: For $n=0$ the statement of the theorem is valid [see Eq. (7)]. We introduce the column vector $|\mathbf{y}_1\overset{\text{def}}{=}\{y_1^j\}_{j=0}^{\infty}$, where $y_1=P(y)$. Let $\mathbf{T}$ be a matrix such that

$$|\mathbf{y}_1\rangle=\mathbf{T}|\mathbf{y}\rangle. \tag{9}$$

The existence of this matrix will be proven later on. If such a matrix exists, then, analogically to Eq. (7), we have

$$y_1 = \langle \mathbf{e}|\mathbf{y}_1\rangle = \langle \mathbf{e}|\mathbf{T}|\mathbf{y}\rangle.$$

Therefore, the statement of the theorem is true for $n=1$ as well.

Assume that Eq. (8) is valid for $n=l$ and any initial value y. Then y_{l+1} can be represented as $y_{l+1}=\langle \mathbf{e}|\mathbf{T}^l|\mathbf{y}_1\rangle$, where $y_1=P(y)$ is considered as a new initial value of the recursion. Then, using Eq. (9) one gets

$$y_{l+1} = \langle \mathbf{e}|\mathbf{T}^l|\mathbf{y}_1\rangle = \langle \mathbf{e}|\mathbf{T}^l\mathbf{T}|\mathbf{y}\rangle = \langle \mathbf{e}|\mathbf{T}^{l+1}|\mathbf{y}\rangle.$$

To prove the existence of the matrix $\mathbf{T}$ we use $|\mathbf{y}_1\rangle \overset{\text{def}}{=} \{P^j(y)\}_{j=0}^{\infty}$. In turn, $P^j(y)$ is the jm-th degree polynomial

$$P^j(y) = \left(\sum_{i=0}^{m} a_i y^i\right)^j = \sum_{k=0}^{jm} T_{jk} y^k, \tag{10}$$

and we infer that $\mathbf{T}=\{T_{jk}\}_{j,k=0}^{\infty}$ obeys Eq. (9).

Note that for j and k satisfying $k \geqslant jm$ we have $T_{jk}\equiv 0$. Therefore, each row is finite (i.e., there is only a finite number of nonzero matrix elements in each row). This proves the existence of powers of $\mathbf{T}$ and completes the proof.

The method of this section can be generalized to an arbitrary analytic function in the right-hand side of Eq. (5).[5]

IV. SPECIAL CASES

A. The binomial case, $P(x)=a_p x^p + a_q x^q$

As one can see, in the general case elements of the matrix $\mathbf{T}$ have a form of rather complicated sums. However, they are degenerated to a fairly simple expression, when the polynomial (6) has only two terms. In this case one gets

$$P^j(y) = (a_p y^p + a_q y^q)^j = \sum_{i=0}^{j} \binom{j}{i} a_p^{j-i} a_q^i y^{p(j-i)+qi}.$$

Denoting

$$k = p(j-i)+qi, \quad i = l(k) = (q-p)^{-1}(k-pj),$$

we have

$$P^j(y) = \sum_{k=jp}^{jq} y^k \binom{j}{l(k)} a_p^{j-l(k)} a_q^{l(k)}.$$

Thus, the matrix elements T_{jk} are

$$T_{jk} = \binom{j}{l(k)} a_p^{j-l(k)} a_q^{l(k)}.$$

By substituting here $p=1$, $q=2$, $a_p=-a_q=\lambda$, we immediately recover the solution for the logistic map, Eq. (3).

B. The trinomial case, $P(x)=a_0+a_px^p+a_qx^q$, $a_0\neq 0$

Here, the transfer matrix $\mathbf{T}$ admits the following decomposition:

$$\mathbf{T}=\mathbf{A}\mathbf{T}_0,$$

where $\mathbf{T}_0$ is the matrix corresponding to the polynomial $P_0(x)=a_px^p+a_qx^q$ and $\mathbf{A}$ is an upper-triangular matrix. Indeed, let us consider $P_0(x)=a_px^p+a_qx^q$ and the corresponding matrix $\mathbf{T}_0$. It yields

$$\mathbf{T}_0|\mathbf{y}\rangle=|\mathbf{y}_1'\rangle\overset{\text{def}}{=}\{P_0^j(y)\}_{j=0}^{\infty}.$$

For the matrix $\mathbf{T}$ one gets

$$\mathbf{T}|\mathbf{y}\rangle=|\mathbf{y}_1\rangle\overset{\text{def}}{=}\{P(y)^j\}_{j=0}^{\infty},$$

$$P^j(y)=\sum_{i=0}^{j}\binom{j}{i}a_0^{j-i}(a_py^p+a_qy^q)^i.$$

Denoting in the last line $A_{ji}\equiv\binom{j}{i}a_0^{j-i}$ one obtains $|\mathbf{y}_1\rangle=\mathbf{A}|\mathbf{y}_1'\rangle=\mathbf{A}\mathbf{T}_0|\mathbf{y}\rangle=\mathbf{T}|\mathbf{y}\rangle$, and $\mathbf{T}=\mathbf{A}\mathbf{T}_0$.

V. NONCONSTANT COEFFICIENTS

As shown in Ref. 4 a generalization of Eq. (1),

$$y_{n+1}=\lambda_n y_n(1-y_n)\quad\text{with}\quad y_0\equiv y,\tag{11}$$

can be solved using a similar approach. The solution is

$$y_n=\langle\mathbf{e}|\mathbf{T}_n\cdots\mathbf{T}_2\mathbf{T}_1|\mathbf{y}\rangle,\tag{12}$$

where the matrix elements of $\mathbf{T}_i$ are now i-dependent:

$$(T_i)_{jk}=(-1)^{k-j}\binom{j}{k-j}(\lambda_i)^j.\tag{13}$$

The same argument is valid for an arbitrary recursion $y_{n+1}=P_n(n,y_n)$ and therefore solution Eq. (8) takes the form of Eq. (12) with the obvious changes ($a_0,\ldots,a_m$ become i-dependent functions) in the corresponding matrix elements.

VI. THE RICCATI RECURSION

This name is commonly used for the equation

$$y_{n+1}y_n+a_n'y_{n+1}+b_n'y_n+c_n'=0.$$

However, by a proper change of variable[1,2] this equation can be reduced to a linear one and then treated by conventional techniques. Here we shall be dealing with the following recursion:

$$y_{n+1}=a_n+b_ny_n+c_ny_n^2\quad\text{with}\quad y_0\equiv y.$$

This is a possible (asymmetric) discrete analog of the Riccati differential equation.[6] It is well known that the latter cannot be solved in quadratures.

The general results of the two previous sections can be employed to write down the solution of this recursion. Namely, the solution reads

$$y_n = \langle \mathbf{e} | \mathbf{T}_n \cdots \mathbf{T}_2 \mathbf{T}_1 | \mathbf{y} \rangle,$$

where the matrix $\mathbf{T}_i$ is a product of two matrices

$$\mathbf{T}_i = \mathbf{A}_i \mathbf{S}_i$$

with matrix elements

$$(\mathbf{A}_i)_{jk} = \binom{j}{k} a_i^{j-k} \quad \text{and} \quad (\mathbf{S}_i)_{jk} = \binom{j}{k-j} b_i^{2j-k} c_i^{k-j}.$$

VII. SYSTEM OF LINEAR FIRST-ORDER RECURSIONS

The next three sections deal with linear recursions. They are well known,[1,2] but we include those sections to help the understanding of subsequent sections, devoted to systems of nonlinear recursions.

The solution of a system of linear first-order recursions in the most general case is rather trivial, but for the sake of clarity we shall demonstrate it on a 2×2 homogeneous system

$$\begin{aligned} u_{n+1} &= (\lambda_{11})_n u_n + (\lambda_{12})_n v_n \quad \text{with} \quad u_0 \equiv u, \\ v_{n+1} &= (\lambda_{21})_n u_n + (\lambda_{22})_n v_n \quad \text{with} \quad v_0 \equiv v. \end{aligned} \tag{14}$$

Introducing the vector $\langle \mathbf{x}_n | = (u_n, v_n)$ and the matrix

$$\mathbf{\Lambda}_n = \begin{pmatrix} (\lambda_{11})_n & (\lambda_{12})_n \\ (\lambda_{21})_n & (\lambda_{22})_n \end{pmatrix},$$

one rewrites Eq. (14) as follows:

$$|\mathbf{x}_{n+1}\rangle = \mathbf{\Lambda}_n |\mathbf{x}_n\rangle$$

and, thus,

$$|\mathbf{x}_{n+1}\rangle = \mathbf{\Lambda}_n \ldots \mathbf{\Lambda}_0 |\mathbf{x}_0\rangle,$$

where $\langle \mathbf{x}_0 | = (u, v)$ is an initial vector.

Further generalization to a homogeneous system of N linear equations of first order is straightforward.

VIII. LINEAR EQUATION WITH NONCONSTANT COEFFICIENTS

The result of the previous section allows one to solve linear recursions of an arbitrary order with nonconstant coefficients. As usual, we start with the simplest case—a second-order equation

$$x_{n+1} + \lambda_n x_n + \mu_{n-1} x_{n-1} = 0. \tag{15}$$

Denoting $y_n \equiv \mu_{n-1} x_{n-1}$ we obtain the system

$$x_{n+1} = -\lambda_n x_n - y_n, \quad y_{n+1} = \mu_n x_n. \tag{16}$$

The solution of this equation is written as in the previous section but now

$$\mathbf{\Lambda}_n=\begin{pmatrix} -\lambda_n & -1 \\ \mu_n & 0 \end{pmatrix}$$

and the initial vector is $(x_1,\mu_0 x_0)$, where x_0 and x_1 are initial values of the recursion (15).

The method we used to transform Eq. (15) to Eq. (16) is well known in the theory of differential equations,[7] but it is useful for the simplest case of constant coefficients only.

Again, the generalization of (16) for a linear equation of arbitrary order is quite simple.

IX. SYSTEM OF LINEAR HIGHER-ORDER RECURSIONS

The generalization to higher orders is rather obvious. The simplest example is

$$\begin{aligned} &x_{n+1}+(\lambda_{11})_n x_n+(\lambda_{12})_n x_{n-1}+(\mu_{11})_n y_n+(\mu_{12})_n y_{n-1}=0, \\ &y_{n+1}+(\mu_{21})_n y_n+(\mu_{22})_n y_{n-1}+(\lambda_{21})_n x_n+(\lambda_{22})_n x_{n-1}=0. \end{aligned} \tag{17}$$

One proceeds as in the previous section with new variables $u_n=x_{n-1}$ and $v_n=y_{n-1}$. Then, the system (17) takes the form

$$\begin{gathered} x_{n+1}+(\lambda_{11})_n x_n+(\lambda_{12})_n u_n+(\mu_{11})_n y_n+(\mu_{12})_n v_n=0, \\ y_{n+1}+(\mu_{21})_n y_n+(\mu_{22})_n v_n+(\lambda_{21})_n x_n+(\lambda_{22})_n u_n=0, \\ u_{n+1}-x_n=0, \quad v_{n+1}-y_n=0, \end{gathered}$$

i.e., the vector (x_n,y_n,u_n,v_n) is transformed by the transfer matrix

$$\mathbf{\Lambda}_n=\begin{pmatrix} -(\lambda_{11})_n & -(\mu_{11})_n & -(\lambda_{12})_n & -(\mu_{12})_n \\ -(\lambda_{21})_n & -(\mu_{21})_n & -(\lambda_{22})_n & -(\mu_{22})_n \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

and subject to appropriate initial conditions.

X. SYSTEM OF NONLINEAR FIRST-ORDER RECURSIONS

Actually, very little is known about systems of nonlinear recursions.[8] We now extend our method of Sec. III to deal with systems of nonlinear equations. Let us demonstrate it on the following example:

$$\begin{aligned} &u_{n+1}=\lambda u_n(1-v_n) \quad \text{with } u_0\equiv u, \\ &v_{n+1}=\mu v_n(1-u_n) \quad \text{with } v_0\equiv v. \end{aligned} \tag{18}$$

Proceeding here as in Sec. III, we are checking the transformation of a product $u^j v^k$:

$$\begin{aligned} [\lambda u(1-v)]^j[\mu v(1-u)]^k &= \sum_{r,s} \lambda^j u^j (-1)^r \binom{j}{r} v^r \mu^k v^k (-1)^s \binom{k}{s} u^s \\ &= \sum_{p,q} u^p v^q (-1)^{(p-j)+(q-k)} \binom{j}{q-k} \binom{k}{p-j} \lambda^j \mu^k. \end{aligned} \tag{19}$$

We prefer to proceed with the aid of multidimensional matrices[9] as being the most natural way. However, a possibility of using traditional two-dimensional matrices also exists.[5]

Indeed, introducing here a four-dimensional matrix $\mathbf{T}$ with the elements

$$T_{jkpq}=(-1)^{(p-j)+(q-k)}\binom{j}{q-k}\binom{k}{p-j}\lambda^j\mu^k$$

(it can also be viewed as an ordinary matrix on the space of index pairs) we basically return to the familiar transfer-matrix construction but for more complex objects. Namely, we shall operate with a two-dimensional matrix $\mathbf{X}$, defined as a direct product of vectors $|\mathbf{u}\rangle$ and $|\mathbf{v}\rangle$:

$$X_{jk}=u^j v^k.$$

Here the matrix $\mathbf{X}$ plays the same role as the vector $|\mathbf{y}\rangle$ in Sec. III. The four-dimensional matrix $\mathbf{T}$ is analogous to its two-dimensional relative $\mathbf{T}$. The multiplication of such matrices is defined rather naturally:

$$\mathbf{X}_1\mathbf{X}_2=\sum_{p,q}(X_1)_{pq}(X_2)_{pq},\quad (\mathbf{TX})_{jk}=\sum_{p,q}T_{jkpq}X_{pq},\quad (\mathbf{T}_1\mathbf{T}_2)_{jkpq}=\sum_{rs}(T_1)_{jkrs}(T_2)_{rspq}.$$

Note that the matrix analog of the scalar product of vectors is just a contraction, $\mathbf{X}_1\mathbf{X}_2$, in the tensor algebra nomenclature.

As in Sec. X, one can obtain the solution of the system in the form

$$u_n=\mathbf{E}_1\mathbf{T}^n\mathbf{X},\quad v_n=\mathbf{E}_2\mathbf{T}^n\mathbf{X},$$

where, as usual,

$$(\mathbf{E}_1)_{jk}=\delta_{1j}\delta_{0k},\quad (\mathbf{E}_2)_{jk}=\delta_{0j}\delta_{1k}.$$

Further generalization of this approach is also rather simple. In the general case of m first-order nonlinear equations

$$x_{n+1}^{(i)}=P_i(x_n^{(1)},\ldots,x_n^{(m)}),\quad i=1,\ldots,m, \tag{20}$$

one has to consider the $2m$-dimensional transfer matrix $\mathbf{T}$. To construct it we are checking as before the product

$$P_{j_1,\ldots,j_m}\equiv P_1^{j_1}\cdots P_m^{j_m},$$

and the m-dimensional matrix $\mathbf{X}$, defined as a direct product of m vectors of initial values $|\mathbf{x}^{(1)}\rangle,\ldots,|\mathbf{x}^{(m)}\rangle$.

The polynomial $P_{j_1,\ldots,j_m}$ depends on m variables $x^{(1)},\ldots,x^{(m)}$ and therefore can be represented as

$$P_{(j_1,\ldots,j_m)}(x^{(1)},\ldots,x^{(m)})=\mathbf{T}_{(j_1,\ldots,j_m)}\mathbf{X},$$

where $\mathbf{T}_{j_1,\ldots,j_m}$ is a constant multidimensional matrix of coefficients of the polynomial $P_{j_1\ldots,j_m}$. This matrix $\mathbf{T}_{j_1,\ldots,j_m}$ is the $(j_1,\ldots,j_m)$-th m-section of the transfer matrix $\mathbf{T}$.

Then defining the matrix $\mathbf{E}_i$ by

$$(\mathbf{E}_i)_{j_1,\ldots,j_i,\ldots,j_m}=\delta_{0j_1}\ldots\delta_{1j_i}\ldots\delta_{0j_m}$$

one can write down the solution of the system in the form

$$x_n^{(i)} = \mathbf{E}_i \mathbf{T}^n \mathbf{X}.$$

XI. SYSTEM OF NONLINEAR HIGHER-ORDER RECURSIONS

We are not going to write down even the simplest example, but the scheme is quite obvious: introduction of new variables to bring each equation to the first-order structure and, then, construction of a transfer matrix (as in the two previous sections).

XII. CONTINUOUS ANALOG OF THE TRANSFER MATRIX

In this section we present a continuous generalization of our transfer matrix technique. We consider the general case, the multivariable function, $f:\mathbf{R}^n \to \mathbf{R}^n$. We do not try to establish the exact conditions for existence of all the functions involved, but merely describe the algorithm.

Let

$$F_{x\to s}[\varphi(\mathbf{x},\mathbf{t})] = (2\pi)^{-n} \int_{\mathbf{R}^n} \exp(-i\langle \mathbf{x},\mathbf{s}\rangle)\varphi(\mathbf{x},\mathbf{t})d\mathbf{x},$$

where $\langle \mathbf{x},\mathbf{s}\rangle$ is the scalar product of two real vectors $\mathbf{x}$ and $\mathbf{s}$, be the Fourier transform of the function $\varphi:\mathbf{R}^{2n}\to\mathbf{C}$, $\mathbf{s},\mathbf{x},\mathbf{t}\in\mathbf{R}^n$ and $F_{s\to x}^{-1}$ be the corresponding inverse Fourier transform.[10] Then, we define the transfer kernel of the function $f:\mathbf{R}^n\to\mathbf{R}^n$ as Fourier transform $T(\mathbf{t},\mathbf{s}) = F_{x\to s}\exp[i\langle f(\mathbf{x}),\mathbf{t}\rangle]$.

For example, let us consider the logistic map, $f(x)=\lambda x(1-x)$. Then the transfer kernel is the function[11]

$$T(t,s) = \int_{-\infty}^{\infty} \exp[-ixs + it\lambda x(1-x)]dx = \sqrt{\frac{\pi}{t\lambda}} \exp\left[-\frac{i\pi}{4} + \frac{i(t\lambda - s)^2}{4t\lambda}\right].$$

We define the product of the transfer kernels $S(\mathbf{t},\mathbf{s})$ and $T(\mathbf{t},\mathbf{s})$ of the functions $g(\mathbf{x})$ and $f(\mathbf{x})$ by

$$S\odot T(\mathbf{t},\mathbf{s}) \overset{\text{def}}{=} \int_{\mathbf{R}^n} S(\mathbf{t},\tau)T(\tau,\mathbf{s})d\tau.$$

Theorem: The product, $S\odot T(\mathbf{t},\mathbf{s})$, of the transfer kernels $S(\mathbf{t},\mathbf{s})$ and $T(\mathbf{t},\mathbf{s})$ is the transfer kernel of the composition $g\circ f(\mathbf{x})$, where $g\circ f(\mathbf{x})\equiv g(f(\mathbf{x}))$.

Indeed, performing the inverse Fourier transform for the function $S\odot T(\mathbf{t},\mathbf{s})$ one gets

$$F_{s\to x}^{-1}[S\odot T(\mathbf{t},\mathbf{s})] = \int_{\mathbf{R}^n} S(\mathbf{t},\tau)F_{s\to x}^{-1}[T(\tau,\mathbf{s})]d\tau = \int_{\mathbf{R}^n} S(\mathbf{t},\tau)\exp[i\langle f(\mathbf{x}),\tau\rangle]d\tau$$
$$= F_{\tau\to f(\mathbf{x})}^{-1}[S(\mathbf{t},\tau)] = \exp[i\langle g\circ f(\mathbf{x}),t\rangle].$$

One can see that the product of the transfer kernels is defined in analogy to the matrix product and we can obtain the solution of the recursion (see Sec. III) in the form

$$y_n^{(j)} = -\ln\{F_{s\to y}^{-1}[\mathbf{T}^n(\mathbf{t},\mathbf{s})]\big|_{\mathbf{t}=i\mathbf{e}_j}\}$$

where $\mathbf{e}_j = \{\delta_{jk}\}_{k=1}^n$.

XIII. SUMMARY

In this paper we have presented a new method to obtain the solution of arbitrary polynomial recursions. The method has been generalized to systems of multivariable recursions and recursions of arbitrary order, in analogy to the solution of linear recursions, also presented in this paper.

Generally, the solution is obtained in the form of a matrix power, applied to the vectors of initial values. We have presented a way to construct such a matrix.

Famous and important examples, such as the logistic map and the Riccati recursion, have been considered and the corresponding matrices have been written down explicitly.

We also generalized the method in another direction. It is shown that instead of transfer matrix one can use transfer kernel which can be considered as a continuous matrix.[12]

While the investigation of the solutions found is beyond the scope of the paper this challenging task deserves a few words. For example, the logistic map solution (2) can be used to construct a generating function.[4] Unfortunately, this latter may have an essential singularity. Therefore, it is more natural to construct an exponential generating function $\phi(z) \equiv \Sigma_n^{\infty}(1/n!) y_n z^n = \langle \mathbf{e} | \exp(z\mathbf{T}) | \mathbf{y} \rangle$. Then, one can try to understand the parametric dependence of the logistic map asymptotics from a steepest descent of the Cauchy integral

$$y_n = \frac{1}{2\pi i} \oint_{C_0} \frac{\phi(z)}{z^{n+1}}\, dz,$$

where the contour C_0 includes the origin of coordinates.

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Rigged Hilbert spaces for chaotic dynamical systems

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We consider the problem of rigging for the Koopman operators of the Renyi and the baker maps. We show that the rigged Hilbert space for the Renyi maps has some of the properties of a strict inductive limit and give a detailed description of the rigged Hilbert space for the baker maps. © *1996 American Institute of Physics.* [S0022-2488(96)01809-9]

I. INTRODUCTION

The notion of a generalized spectral decomposition of self-adjoint operators on a Hilbert space goes back to Dirac,[1] who assumed that a given self-adjoint operator A must be of the form

$$A=\int_{\sigma(A)} d\lambda\ \lambda|\lambda)(\lambda|, \tag{1}$$

where $\sigma(A)$ is the spectrum of the operator A. This formula is a straightforward generalization of the familiar decomposition of a self-adjoint operator on a finite-dimensional Hilbert space

$$A=\sum_i \lambda_i|e_i)(e_i|, \tag{2}$$

where λ_i and e_i are the eigenvalues and eigenvectors of A, respectively. In infinite-dimensional Hilbert spaces, however, the situation is not so simple. The notion of an eigenvalue is replaced by the spectrum, but eigenvectors can be associated only with the discrete part of the spectrum. Nevertheless, a precise meaning can be given to the decomposition (1), if we replace eigenvectors by ''generalized eigenvectors,'' which will, in general, lie outside the given Hilbert space. This is achieved by replacing the initial Hilbert space $\mathscr{H}$ by a dual pair $(\Phi,\Phi^\times)$, where Φ is a locally convex space, which is a dense subspace of $\mathscr{H}$ endowed with a topology, stronger than the Hilbert space topology. This procedure is referred to as rigging and the triple

$$\Phi\subset\mathscr{H}\subset\Phi^\times \tag{3}$$

is called a *rigged Hilbert space* (see Refs. 2–5 for details). Gelfand[3,4] was the first to give a precise meaning to the generalized eigenvectors, which was later elaborated by Maurin.[5] Although generalized eigenvectors have a very natural physical interpretation, generalized spectral decompositions have not been used in physics for a long time. Only a few papers had appeared by the end of the 1960s (see, for example, Refs. 6–8), followed by a series of papers by Bohm and Gadella (see Ref. 2 and references therein). The latter publications are particularly significant, because they provide the basis for a rigorous and systematic approach to the problems of irreversibility and resonances in unstable quantum systems like the Friedrichs model.[9] The same ideas can be extended to chaotic dynamical systems, like Kolmogorov systems or exact systems.[10,11] The observable phase functions of dynamical systems evolve according to the Koopman operator[10]

$$Vf(x)=f(Sx),$$

where S is an endomorphism or an automorphism of a measure space, and f is a square-integrable phase function.

The spectrum of the Koopman operator determines the time scales of the approach to equilibrium very much in analogy with quantum unstable systems, where the spectra of the Hamiltonians determine the decay rates. More precisely, the eigenvalues of the Koopman operator or that of its adjoint, known as the Frobenius–Perron operator, are the resonances of the power spectrum.[12–15] Eigenvalues and eigenvectors of simple chaotic systems have recently been constructed by several authors.[16–24]

The question of the existence of a generalized spectral decomposition of extensions of the Koopman operator was raised and resolved by Antoniou and Tasaki.[17–19] This issue is delicate, because the original Gelfand–Maurin theory was constructed for operators which admit a spectral theorem,[25] like normal operators, giving a generalized spectrum identical with the Hilbert space spectrum. The Koopman operator of unstable systems, however, either does not admit a spectral theorem, as in the case of exact systems,[18] or the generalized spectrum is very different from the Hilbert space spectrum, as in the case of Kolmogorov systems.[19] The original Gelfand–Maurin theory had to be extended[17–19] to arbitrary dual pairs $(\Phi,\Phi^{\times})$ of linear topological spaces.

Summarizing for the reader's convenience, a dual pair $(\Phi,\Phi^{\times})$ of linear topological spaces constitutes a rigged Hilbert space for the linear endomorphism V of the Hilbert space $\mathscr{H}$ if the following conditions are satisfied:

(1) Φ is a dense subspace of $\mathscr{H}$.
(2) Φ is complete and its topology is stronger than the one induced by $\mathscr{H}$.
(3) Φ is stable with respect to the adjoint $V^{\dagger}$ of V, i.e., $V^{\dagger}\Phi\subset\Phi$.
(4) The adjoint $V^{\dagger}$ is continuous on Φ

The extension V_{ext} of V to the dual $\Phi^{\times}$ of Φ is then defined in the standard way as follows:

$$(\phi|V_{\text{ext}}f)=(V^{\dagger}\phi|f),$$

for every $\phi\in\Phi$.

In the sequel we shall not distinguish between V and V_{ext} if confusion is unlikely to arise.

The choice of the test function space Φ depends on the specific operator V and on the physically relevant questions to be asked about the system. For self-adjoint operators V, for example, the generalized spectral theorem can be justified for nuclear test function spaces; for normal operators this condition may be relaxed.[26,27]

Here, we shall discuss the problem of rigging for the generalized spectral decompositions of the Koopman operators for two specific but typical models of chaotic systems, namely, the Renyi maps and the baker maps.

In the case of the Renyi map various riggings exist[28] and our task will be to choose a tight rigging within spaces of analytic test functions. We call a rigging ''tight'' if the test function space

is the (set theoretically) largest possible within a chosen family of test function spaces, such that the physically relevant spectral decomposition is meaningful. This notion of tightness is more general than that of Fredricks.[7] It turns out that the topology of this rigged Hilbert space enjoys some of the properties of a strict inductive limit of Banach spaces, which greatly simplifies convergence arguments.

The construction of the rigged Hilbert space for the baker map, on the other hand, reveals a different aspect of the problem of rigging. In fact, here the problem is to understand the very nature of the rigging, since the test function space is the tensor product of the space of polynomials with the space of square-integrable functions corresponding to the expanding and contracting fibers. Our task will be to investigate the properties of this rigged Hilbert space.

II. RIGGED HILBERT SPACES FOR THE RENYI MAPS

In this section we discuss the rigged Hilbert spaces for the Koopman operator of the general β-adic Renyi map.

The β-adic Renyi map S on the interval $[0,1)$ is the multiplication, modulo 1, by the integer $\beta \geqslant 2$

$$S:[0,1)\to[0,1): \quad x\mapsto Sx=\beta x(\mathrm{mod}\ 1).$$

The probability densities $\rho(x)$ evolve according to the Frobenius–Perron operator U (Ref. 11):

$$U\rho(x)\equiv \sum_{y,S(y)=x} \frac{1}{|S'(y)|}\,\rho(y)=\frac{1}{\beta}\sum_{r=0}^{\beta-1}\rho\left(\frac{x+r}{\beta}\right).$$

The Frobenius–Perron operator is a partial isometry on the Hilbert space L^2 of all square integrable functions over the unit interval; it is, moreover, the dual of the isometric Koopman operator V:

$$V\rho(x)=U^{\dagger}\rho(x)=\rho(Sx).$$

In Ref. 18 two of us (I.A. and S.T.) constructed a spectral decomposition of the Koopman operator using a general algorithm based on the subdynamics decompositions. The Koopman operator can be expressed as follows:

$$V=\sum_{n=0}^{\infty} \frac{1}{\beta^n}\,|\widetilde{B}_n)(B_n|, \tag{4}$$

where $B_n(x)$ is the nth-degree Bernoulli polynomial defined by the generating function (Ref. 29, §9)

$$\frac{ze^{zx}}{e^z-1}=\sum_{n=0}^{\infty}\frac{B_n(x)}{n!}\,z^n$$

and

$$|\widetilde{B}_n)=\begin{cases} |1), & n=0,\\ \dfrac{(-1)^{(n-1)}}{n!}\{\delta^{(n-1)}(x-1)-\delta^{(n-1)}(x)\}), & n=1,2,\ldots . \end{cases}$$

The bras $(\cdot|$ and kets $|\cdot)$ denote linear and antilinear functionals, respectively. Formula (4) defines a spectral decomposition for the Koopman and Frobenius–Perron operators in the following sense:

$$(\rho|Vf)=(U\rho|f)=\sum_{n=0}^{\infty}\frac{1}{\beta^n}(\rho|\widetilde{B}_n)(B_n|f),$$

for any density function ρ and observable f in the appropriate pair (Φ,Φ^x). Consequently, the Frobenius–Perron operator acts on density functions as

$$U\rho(x)=\int_0^1 dx'\ \rho(x')+\sum_{n=1}^{\infty}\frac{\rho^{(n-1)}(1)-\rho^{(n-1)}(0)}{n!\beta^n}B_n(x).$$

The orthonormality of the system $|\widetilde{B}_n)$ and $(B_n|$ follows immediately, while the completeness relation is just the Euler–MacLaurin summation formula for the Bernoulli polynomials (Ref. 29, §9)

$$\rho(x)=\int_0^1 dx'\ \rho(x')+\sum_{n=1}^{\infty}\frac{\rho^{(n-1)}(1)-\rho^{(n-1)}(0)}{n!}B_n(x). \tag{5}$$

The Bernoulli polynomials are the only polynomial eigenfunctions as any polynomial can be uniquely expressed as a linear combination of the Bernoulli polynomials.

The spectral decomposition (4) has no meaning in the Hilbert space L^2, as the derivatives $\delta^{(n)}(x)$ of Dirac's delta function appear as right eigenvectors of V. A natural way to give meaning to formal eigenvectors of operators which do not admit eigenvectors in Hilbert space is to extend the operator to a suitable rigged Hilbert space. A suitable test function space is the space $\mathscr{P}$ of polynomials. The space $\mathscr{P}$ fulfills the following conditions:

(i) $\mathscr{P}$ is dense in L^2 (see Ref. 30, ch. 15),
(ii) $\mathscr{P}$ is a nuclear LF-space (Ref. 30, ch. 51) and thus, complete and barreled,
(iii) $\mathscr{P}$ is stable with respect to the Frobenius–Perron operator U, and
(iv) U is continuous with respect to the topology of $\mathscr{P}$, because U preserves the degree of polynomials.

It is, therefore, an appropriate rigged Hilbert space, which gives meaning to the spectral decomposition of V.

We shall, however, look for a tight rigging. The test functions should at least provide a domain for the Euler–MacLaurin summation formula (5). The requirement of absolute convergence of the series (5) means that

$$\sum_{n=1}^{\infty}\left|\frac{\phi^{(n-1)}(y)}{n!}B_n(x)\right|<\infty\quad(y=0,1).$$

This implies[18] that the appropriate test functions are restrictions on $[0,1)$ of entire functions of exponential type c with $0<c<2\pi$. For simplicity we identify the test functions space with the space $\mathscr{E}_c$ of entire functions $\phi(z)$ of exponential type $c>0$ such that

$$|\phi(z)|\leqslant Ke^{c|z|},\quad \forall z\in\mathbb{C},\quad \text{for some } K>0.$$

Each member of the whole family $\mathscr{E}_c$, $0<c<2\pi$, is a suitable test function space, since properties (1)–(4) are fulfilled. Indeed, each space $\mathscr{E}_c$ is a Banach space with norm (Ref. 30, ch. 22):

$$\|\phi\|_c\equiv\sup_{z\in\mathbb{C}}|\phi(z)|e^{-c|z|},$$

which is dense in the Hilbert space L^2, as $\mathscr{E}_c$ includes the polynomial space $\mathscr{P}$. Each $\mathscr{E}_c$ is stable under the Frobenius–Perron operator U, and it is easily verified that U is continuous on $\mathscr{E}_c$. Now, observe that the spaces are ordered

$$\mathscr{E}_c \subset \mathscr{E}_{c'}, \quad c<c',$$

and consider the space

$$\tilde{\mathscr{E}}_{2\pi} \equiv \bigcup_{c<2\pi} \mathscr{E}_c.$$

The space $\tilde{\mathscr{E}}_{2\pi}$, also preserved by U, is the (set theoretically) largest test function space in our case. Since $\tilde{\mathscr{E}}_{2\pi}$ is a natural generalization of the space $\mathscr{P}$ of polynomials, we want to equip it with a topology which is a generalization of the topology of $\mathscr{P}$.

Recall that $\mathscr{P}$ was given the strict inductive limit topology of the spaces $\mathscr{P}^n$ of all polynomials of degree $\leqslant n$. A very important property of this topology is that the strict inductive limit of complete spaces is complete. Moreover, it is exceptionally simple to describe convergence in this topology. For example, a sequence $\{w_n\}$ of polynomials converges in $\mathscr{P}$ if and only if the degrees of all w_n are uniformly bounded by some n_0 and $\{w_n\}$ converges in $\mathscr{P}^{n_0}$.

We cannot, however, define the strict inductive topology on $\tilde{\mathscr{E}}_{2\pi}$ because for $c<c'$ the topology on $\mathscr{E}_c$ induced by $\mathscr{E}_{c'}$ is essentially stronger than the initial one. Nevertheless, as we shall see in the theorem below, it is possible to define a topology on $\tilde{\mathscr{E}}_{2\pi}$, which is a natural extension of the topology on $\mathscr{P}$ in the following sense.

Theorem 1: There is a locally convex topology $\mathscr{T}$ on $\tilde{\mathscr{E}}_{2\pi}$ for which it is a nuclear, complete Montel space. Moreover, a sequence $\{f_n\} \subset \tilde{\mathscr{E}}_{2\pi}$ is convergent in the $\mathscr{T}$ topology if and only if there is $c_0 \in (0,2\pi)$ such that 1° f_n, $n=1,2,...$, are of exponential type c_0 and 2° $\{f_n\}$ converges in $\|\cdot\|_{c_0}$-norm.

Proof: Denote by $\hat{f}$ the Fourier transform of a function f and by $\check{f}$ its converse. By Schwartz's extension of the Paley–Wiener theorem (Ref. 31, vol. II, p. 106) a function f belongs to $\mathscr{E}_c$ if and only if $\hat{f}$ is a distribution with compact support contained in the interval $[-c, c]$.

Note that, if the function $f \in \tilde{\mathscr{E}}_{2\pi}$ is integrable or square integrable, then $\hat{f}$ is a function. However, for an arbitrary function its Fourier transform is correctly defined only as a distribution with compact support, i.e., as a continuous linear functional on the space $C^\infty(\Omega)$ of all infinitely differentiable functions on the interval $\Omega=(-2\pi, 2\pi)$, endowed with the topology of uniform convergence on compact subsets of Ω of functions together with all their derivatives.

The Fourier transform, therefore, establishes an isomorphism between $\tilde{\mathscr{E}}_{2\pi}$ and the topological dual $C^\infty(\Omega)^x$ of the space $C^\infty(\Omega)$. Consequently, the strong dual topology of $C^\infty(\Omega)^x$ can be transported through the inverse Fourier transform to the space $\tilde{\mathscr{E}}_{2\pi}$. The strong dual topology is the topology of uniform convergence on bounded subsets of $C^\infty(\Omega)$. Then $C^\infty(\Omega)^x$ is nuclear (Ref. 30, p. 530), complete (Ref. 31, vol I, p. 89), and a Montel space (Ref. 30, prop. 34.4 and 36.10). In this way we obtain on $\tilde{\mathscr{E}}_{2\pi}$ a topology with the same properties.

We shall now prove the second part of the theorem. Let $\{f_n\}$ be convergent to zero in $\tilde{\mathscr{E}}_{2\pi}$. This means that $\{\check{f}_n\}$ converges in $C^\infty(\Omega)^x$. Therefore $\{\check{f}_n\}$ is a bounded subset of $C^\infty(\Omega)^x$, which implies (Ref. 30, th. 34.4, p. 359) that the supports of all f_n are contained in a compact set $K \subset \Omega$.

Take c with $c<2\pi$ and $K \subset (-c,c)$. Therefore [see Ref. 31, vol. I, th. XXVI and the remark afterwards which remains true if we replace $\mathbb{R}^1$ by the open set $\Omega=(-2\pi,2\pi)$], there is a number $p \geqslant 0$ and a family of continuous functions $g_{j,n}$ such that the supports of $g_{j,n}$ are contained in the interval $(-c,c)$,

$$\check{f}_n = \sum_{j \leqslant p} D^j g_{j,n}$$

(D^j denotes the jth derivative, classical or in the sense of distributions) and $g_{j,n}(x)$ converges uniformly to zero as $n\to\infty$.

Using the above representation of $\check{f}_n$ we obtain that $\check{f}_n$ converges to zero uniformly on each set U_A:

$$U_A\equiv\left\{ f\in C^\infty(\Omega):\ \sup_{x\in[-c,c]}\left|\frac{d^j}{dx_j}f(x)\right|\leqslant A,\quad j=0,1,\ldots,p\right\},$$

where $A>0$. Indeed, for each j

$$|\langle D^j g_{j,n},f\rangle|=\left|(-1)^j\int_{-c}^{c}g_{j,n}(x)\,\frac{d^j}{dx_j}f(x)dx\right|$$

$$\leqslant A\int_{-c}^{c}|g_{j,n}(x)|dx\to 0,$$

as $n\to\infty$.

Let us take any $c_0\in(c,2\pi)$. Then for each $z\in\mathbb{C}$ the function

$$x\mapsto e^{izx}e^{-c_0|z|},\quad |x|\leqslant c, \tag{6}$$

belongs to U_A. Indeed

$$\left|\frac{d^j}{dx_j}\left(e^{izx}e^{-c_0|z|}\right)\right|\leqslant|z|^j e^{|z|(|x|-c_0)}=|z|^j e^{|z|(|x|-c)}e^{-(c_0-c)|z|}$$

$$\leqslant|z|^j e^{-(c_0-c)|z|}.$$

The right-hand side is bounded, for each $j=0,1,\ldots,p$, by some constant A_j. Thus taking $A=\max_{0\leqslant j\leqslant p}A_j$ we see that the functions (6) belong to U_A, for each $z\in\mathbb{C}$.

From

$$f_n(z)=(\check{f}_n)\hat{}\,(z)$$

and uniform convergence of $\check{f}_n$ on U_A we have

$$\sup_{z\in\mathbb{C}}|f_n(z)|e^{-c_0|z|}=\sup_{z\in\mathbb{C}}|\langle\,\check{f}_n,e^{iz}e^{-c_0|z|}\rangle|\to 0,$$

as $n\to\infty$, which means that $\|f_n\|_{c_0}\to 0$. This proves 2°. Condition 1° is also satisfied because we have chosen $c_0>c$. Thus, the supports of the $\check{f}_n$s are also contained in $(-c_0,c_0)$ and by the Paley–Wiener–Schwartz theorem the f_ns are of exponential type c_0.

The converse of the second part of the theorem is now trivial. If $\{f_n\}$ satisfies 1° and 2°, then by applying the Paley–Wiener–Schwartz theorem again we obtain convergence of $\{\check{f}_n\}$ in $C^\infty(\Omega)^x$.

Remark 1: Using the above method one can show an analogous criterion of convergence for bounded nets in $\tilde{\mathscr{E}}_{2\pi}$ but not for an arbitrary net.

Remark 2: Note that it is not always possible to obtain convergence of the type given in the above theorem. Actually, to prove the second part of the theorem we needed the following property:

Let F be a Frechet space and let $\{x_n'\}$ be a sequence in its dual F' which converges to zero in the strong dual topology. Then there exists an open subset U of F such that

$$|\langle x_n', x\rangle| \to 0, \quad \text{uniformly for } x \in U. \tag{7}$$

As mentioned in Ref. 32, some concrete F-spaces have this property although it is not true in general. It was stated there as an open problem to describe those F-spaces for which (7) is true. This situation motivated us to include the full proof.

Remark 3: An alternative but less constructive proof of the theorem can be found in Ref. 28. It is based on a theorem by Raikov[33] and the nuclearity of the imbedding

$$\mathscr{E}_c \hookrightarrow \mathscr{E}_{c'}, \quad c < c'.$$

III. THE RIGGED HILBERT SPACE FOR THE BAKER TRANSFORMATIONS

The β-adic, $\beta = 2,3,...$, baker's transformation B on the unit square $[0, 1)\times[0, 1)$ is a two-step operation: (1) squeeze the 1×1 square to a $\beta\times 1/\beta$ rectangle and (2) cut the rectangle into β $(1\times 1/\beta)$ rectangles and pile them up to form another 1×1 square:

$$(x,y) \mapsto B(x,y) = \left(\beta x - r, \frac{y+r}{\beta}\right), \quad \text{for } \frac{r}{\beta} \leqslant x < \frac{r+1}{\beta}, \quad r = 0,\ldots,\beta-1.$$

The invariant measure of the β-adic baker transformation is the Lebesgue measure on the unit square. The probability densities $\rho(x,y)$ evolve according to the Frobenius–Perron operator U (Ref. 11):

$$U\rho(x,y) \equiv \rho(B^{-1}(x,y)) = \rho\left(\frac{x+r}{\beta}, \beta y - r\right), \quad \text{for } \frac{r}{\beta} \leqslant y < \frac{r+1}{\beta}, \quad r = 0,\ldots,\beta-1.$$

The Frobenius–Perron and Koopman operators are unitary on the Hilbert space $L^2_{x,y}$ of square integrable functions over the unit square and has a countably degenerate Lebesgue spectrum on the unit circle plus the simple eigenvalue 1 associated with the equilibrium (as is the case for all Kolmogorov automorphisms).

The β-adic baker automorphism B is the natural extension[34] of the β-adic Renyi map on the unit interval $[0, 1)$, described in the previous section.

It was shown in Ref. 19 that the Koopman operator V has a spectral decomposition involving Jordan blocks

$$V = |\tilde{f}_{00})(f_{00}| + \sum_{\nu=1}^{\infty} \left\{ \sum_{r=0}^{\nu} \frac{1}{\beta^\nu} |\tilde{f}_{\nu,r})(f_{\nu,r}| + \sum_{r=0}^{\nu-1} |\tilde{f}_{\nu,r+1})(f_{\nu,r}| \right\}. \tag{8}$$

The vectors $f_{\nu,j}$ and $\tilde{f}_{\nu,j}$ are linear functionals over the spaces $L^2_x \otimes \mathscr{P}_y$ and $\mathscr{P}_x \otimes L^2_y$, respectively, with well-defined inner product $(f_{\nu,r}|\tilde{f}_{\nu',r'}) = \delta_{\nu\nu'}\delta_{rr'}$, and $\Sigma_{\nu=0}^{\infty}\Sigma_{r=0}^{\nu}|\tilde{f}_{\nu,r})(f_{\nu,r}| = I$. Moreover,

$$(f_{\nu,r}|V = \begin{cases} \frac{1}{\beta^\nu}((f_{\nu,r}| + (f_{\nu,r+1}|), & r = 0,\ldots,\nu-1, \\ \frac{1}{\beta^\nu} f_{\nu,r}, & r = \nu, \end{cases}$$

$$V|\tilde{f})_{\nu,r} = \left\{ \frac{1}{\beta^\nu}(|\tilde{f}_{\nu,r}) + |\tilde{f}_{\nu,r-1})), \quad r = 1,\ldots,\nu, \right.$$

$$\left. \frac{1}{\beta^\nu} \tilde{f}_{\nu,r}, \quad r = 0. \right.$$

While the Koopman operator V is unitary in the Hilbert space $L^2_{x,y}$ and thus has spectrum on the unit circle $|z|=1$ in the complex plane, the spectral decomposition (8) includes the numbers $1/\beta^{\nu}<1$ which are not in the Hilbert space spectrum. The spectral decomposition (8) also shows that the Frobenius–Perron operator has Jordan-block parts despite the fact that it is diagonalizable in the Hilbert space. As both $f_{\nu,j}$ and $\tilde{f}_{\nu,j}$ contain distributions, the spectral decomposition (8) has no meaning in the Hilbert space $L^2_{x,y}$ but only on the subspaces $L^2_x \otimes \mathscr{P}_y$ and $\mathscr{P}_x \otimes L^2_y$. Therefore, our purpose is to define an appropriate topology on these spaces. We shall give the construction for $\mathscr{P}_x \otimes L^2_y$ only; a similar argument applies to $L^2_x \otimes \mathscr{P}_y$.

We will start from the most natural, i.e., the strict inductive limit topology, which coincides with other, apparently stronger, tensor product topologies.

Let us consider the space $\mathscr{P}\otimes L^2$ (for simplicity we omit the subscripts x and y), where $\mathscr{P}$ is the space of all polynomials w of finite degree:

$$w=\sum_{k=0}^{n} a_k x^k, \tag{9}$$

L^2_y is the space of all square integrable functions on the space $Y=[0, 1]$.

Let $\mathscr{P}^n$ be the space of all polynomials of degree $\leqslant n$. For a w of the form (9),

$$\|w\|_n = \max_{0\leqslant k\leqslant n} |a_k|$$

defines a norm on $\mathscr{P}^n$. Then $\mathscr{P}$ is defined as the union $\cup_n \mathscr{P}^n$ with the strict inductive limit topology (Ref. 30, sec. 13).

Similarly $\mathscr{P}\otimes L^2$ was defined in Ref. 19 as the strict inductive limit of the spaces $\mathscr{P}^n \otimes L^2$ endowed with the topology τ, generated by the norms

$$\left\| \sum_{k=1}^{n} x^k \otimes \phi_k \right\|_n = \max_{0\leqslant k\leqslant n} \|\phi\|_{L^2}. \tag{10}$$

It is very easy to see that $(\cup_n \mathscr{P}^n)\otimes L^2 = \cup_n (\mathscr{P}^n \otimes L^2)$. Thus, we have, *algebraically*,

$$\mathscr{P}\otimes L^2 = (\varinjlim \mathscr{P}^n)\otimes L^2 = \varinjlim (\mathscr{P}^n \otimes L^2),$$

and, as we will see below, also topologically.

In fact, it will be shown that the τ-topology defined by the seminorms (10) is also, roughly speaking, the only natural locally convex tensor product topology on the space $\mathscr{P}\otimes L^2$.

This will be done in three steps:

(1) τ is a cross-seminorm topology, i.e., the tensor product seminorm (10) is a cross-norm[35] when restricted to the Banach spaces $\mathscr{P}^n$ and L^2. Indeed, for $w\in\mathscr{P}^n$, $f\in L^2$,

$$\begin{aligned}\|w\otimes f\|_n &= \left\| \sum_{k=1}^{n} a_k x^k \otimes f \right\|_n = \left\| \sum_{k=1}^{n} x^k \otimes (a_k f) \right\|_n \\ &= \max_{0\leqslant k\leqslant n} \|a_k f\|_{L^2} = \max_{0\leqslant k\leqslant n} |a_k| \|f\|_{L^2} \\ &= \|w\|_n \|f\|_{L^2}.\end{aligned}$$

(2) The τ-topology is weaker than the projective topology (shortly π-topology) on the tensor product $\mathscr{P}\otimes L^2$ (see Ref. 30, sec. 43, for the definition). Indeed, consider an element $\tilde{f}=\Sigma_{i=1}^{N} w_i\otimes f_i$ of the space $\mathscr{P}\otimes L^2$ and let n be the maximal degree of $w_i, i=1,\ldots,N$. Then we can write $w_i=\Sigma_{k=0}^{N} a_k^{(i)}x^k$, $i=1,\ldots,N$ (some $a_k^{(i)}$ can be zero). Therefore

$$\begin{aligned}\tilde{f}&=\left\|\sum_{i=1}^{N} w_i\otimes f_i\right\|_n=\left\|\sum_{i=1}^{N}\left(\sum_{k=0}^{n} a_k^{(i)}x^k\right)\otimes f_i\right\|_n\\&=\left\|\sum_{k=0}^{n}\left(\sum_{i=1}^{N} a_k^{(i)}f_i\right)\otimes x^k\right\|_n\\&=\max_{0\leq k\leq n}\left\|\sum_{i=1}^{N} a_k^{(i)}f_i\right\|_{L^2}\leq\max_{0\leq k\leq n}\sum_{i=1}^{N}|a_k^{(i)}|\|f_i\|_{L^2}.\end{aligned}$$

Denote by R the right-hand side in the above inequalities and let k_0 be the index which realizes the maximum of R. Then

$$\begin{aligned}R&=\sum_{i=1}^{N}|a_{k_0}^{(i)}|\|f_i\|_{L^2}\leq\sum_{i=1}^{N}\max_{0\leq k\leq n}|a_k^{(i)}|\|f_i\|_{L^2}\\&=\sum_{i=1}^{N}\|w_i\|_n\|f_i\|_{L^2}.\end{aligned}$$

Therefore, we obtain the inequality

$$\|\tilde{f}\|_n\leq\sum_{i=1}^{N}\|w_i\|_n\|f_i\|_{L^2},$$

which does not depend on the particular representation of $\tilde{f}$. Thus $\|\tilde{f}\|_n\leq\|\tilde{f}\|_{\pi,n}$, where $\|\cdot\|_{\pi,n}$ denotes the π-seminorm corresponding to the seminorm $\|\cdot\|_n$ on $\mathscr{P}$ and $\|\cdot\|_{L^2}$.

(3) The τ-topology is stronger than the ε-topology (see Ref. 30, sec. 43 for the definition) on $\mathscr{P}\otimes L^2$. To see this let us first note that the space $\mathscr{P}$ with its topology can be identified with the space $C_c^0(X)$ of continuous functions on X with compact support (Ref. 30, p. 132), provided we take as the locally compact space the set $\mathbb{N}\cup\{0\}$ with the discrete topology. In such a case, functions with compact support are just sequences with at most finitely many nonzero elements and the family of seminorms is here precisely the same as that for $\mathscr{P}$ described above. Similarly, $\mathscr{P}\otimes L^2$ with the τ-topology can be identified with $C_c^0(X;L^2)$ which is a subspace of the space $C^0(X;L^2)$ of all continuous functions on X with values in L^2 (see Ref. 30, p. 412 for the definition of the topology).

On the other hand, $C_c^0(X;L^2)$ is topologically isomorphic with $C_c^o(X)\,\hat{\otimes}_\epsilon L^2$ ($\hat{}$ denotes completion). Since the topology induced by $C^0(X;L^2)$ on $C_c^0(X;L^2)$ is weaker than the τ-topology we obtain that *the ε-topology on $\mathscr{P}\otimes L^2$ is weaker than τ-topology.*

Therefore after completion we obtain

$$\mathscr{P}\hat{\otimes}_\pi L^2\subset\mathscr{P}\hat{\otimes}_\tau L^2\subset\mathscr{P}\hat{\otimes}_\epsilon L^2.$$

However, since $\mathscr{P}$ is a nuclear space we have (Ref. 30, th. 50.1)

$$\mathscr{P}\hat{\otimes}_e L^2\cong\mathscr{P}\hat{\otimes}_\pi L^2$$

($\cong$ denotes topological isomorphism). Because $\mathscr{P}\otimes L^2$ is already complete in the τ-topology[19] we obtain the following.

Theorem 2: The τ-topology on $\mathscr{P}\otimes L^2$ coincides with the ε and the π topology.

IV. CONCLUDING REMARKS

(1) We have characterized the natural rigged Hilbert spaces of analytic functions associated with the prototype of dynamical systems, namely the Renyi and the baker transformations. In the case of the Renyi map, we constructed a tight rigged Hilbert space $\tilde{\mathscr{E}}_{2\pi}$ within the spaces of analytic functions, which gives meaning to the simple resonance spectrum. We have shown that $\tilde{\mathscr{E}}_{2\pi}$ inherits the crucial properties of strict inductive limits of Banach spaces without being a strict inductive limit itself. For the baker maps we characterized the topology of the tensor product which gives meaning to the multiple resonance spectrum.

(2) We expect that these rigged Hilbert space topologies are typical for chaotic maps, if the evolution of analytic densities is considered. In the case of nonanalytic densities we may have test function spaces satisfying properties (1)–(4) with different extension properties.

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On the structure of projective group representations in quaternionic Hilbert space

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A structure theorem concerning projective quaternionic representations is stated and proved. A corollary to the structure theorem is then proved, answering a question recently posed by Adler. © *1996 American Institute of Physics.* [S0022-2488(96)01309-6]

I. INTRODUCTION

In a recent paper,[1] Adler builds on some of the material in his book,[2] specifically that which concerns general, multicentral and central quaternionic projective representations. He asks if a multicentral representation can be constructed that is not central or if it can be proved that a multicentral representation must always be central. For a given Lie group G, the answers to these questions depend on the connectedness of the group. If G is not connected, it is possible to construct a multicentral representation that is not central and we provide an example of such in this paper. Our main result, however, is to prove that if G is connected, then a multicentral representation must also be central. This is actually a corollary to a structure theorem that divides irreducible representations into three types according to the reality and commutativity of the projective phases.

II. USEFUL TERMS AND COMMON THEMES

For a general introduction to quaternions and their application to quantum mechanics, we refer the reader to Adler's book.[2]

The quaternions include both real and complex numbers, and by a suitable categorization the commutativity properties of the different types of quaternion can be concisely summarized. In this paper, we use the following categories in the proof of the structure theorem and of its corollary.

Definition 1: A real number has vanishing i, j, and k coefficients.

Definition 2: A complex number has vanishing j and k coefficients. It is the most general α-symplectic quaternion.

Definition 3: A strictly complex number has vanishing j and k coefficients but nonvanishing i coefficient.

Definition 4: A skew-complex number has vanishing 1 and i coefficients. It is a purely β-symplectic quaternion.

Definition 5: A strictly quaternionic number has nonvanishing β-symplectic part.

It should be noted that these definitions are dependent on the choice of i, j, and k, so the quaternionic basis must be specified before the above terms can be used.

Other useful quaternionic quantities are phases. A phase is a real, complex or quaternionic number that has unit norm, in other words it is an element of, respectively, $U(1,\mathbb{R})$, $U(1,\mathbb{C})$ or $U(1,\mathbb{H})$. A real phase must then be ± 1 while a complex phase can be parametrised as the familiar $\exp(i\theta)$.

The connectedness of G is crucial to the structure theorem and is used several times in the proof. Typically, we will deduce that, for each a in G, a certain quantity dependent on a must

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have one of two mutually exclusive ''disconnected'' properties, P or Q. We use disconnected to mean that it is impossible to have a smooth transition from P to Q. Since G is connected, either property P holds for all a or property Q holds for all a; there cannot be one region of G where P is satisfied and one where Q is since the regions' boundary would be a discontinuity. To determine which property holds for all a, it then suffices to test which property holds for some particular a, such as the multiplicative identity 1.

As a tool for applying the consequences of connectedness, it is useful to be able to perturb group elements by a small amount. If we perturb a group element a by a small amount, we write the new group element as $a\delta a$ where δa is a group element in some neighborhood of the identity; letting δa tend to 1 then defines a limiting process that generates elements tending to a.

III. THE STRUCTURE THEOREM AND ITS COROLLARY

Let G be a connected Lie group with identity element 1, and suppose that V is a quaternionic Hilbert space with a privileged set of (quaternionic) orthonormal basis elements $\{|f\rangle\}$. Let

$$U: G \to U(V, \mathscr{H})$$

be a smooth assignment from a group element a to a unitary right-linear operator U_a on V. We say that U is a projective quaternionic representation if $U_1 = 1$ and

$$\Omega(b,a) = U_{ba}^{-1} U_b U_a$$

is diagonal on the basis $\{|f\rangle\}$ for all group elements b and a, that is

$$\Omega(b,a) = \sum_f |f\rangle \omega(f,b,a) \langle f|$$

for some quaternionic phase $\omega(f,b,a)$ called the projective phase. The above definition of a representation is partially dependent on the choice of basis; a representation which is projective with respect to one basis need not be projective with respect to another. However, one can safely reray a basis

$$|f\rangle \mapsto |f\rangle \phi_f$$

$$\omega(f,b,a) \mapsto \overline{\phi_f} \omega(f,b,a) \phi_f,$$

where the ϕ_f are quaternionic phases, without changing the projective nature of the map U—this reraying affects the ω but not the Ω. Let us also make the technical assumption that U is irreducible, in the sense that there does not exist a partition of the basis elements into two sub-bases with respect to which the operators U_a are block-diagonal for all group elements a. A reducible representation can easily be expressed as the direct sum of irreducible ones, so this is not a severe restriction. There are three obvious ways to make such a representation. The first way is to start with a genuine representation (so that

$$U_{ba} = U_b U_a$$

for all b and a); this is, of course, automatically a quaternionic projective representation in any basis. We can modestly generalize this by requiring only that the representation be real-projective, that is, so that

$$U_{ba} = \pm U_b U_a.$$

A second way is to start with a complex projective representation on a complex space $V_{\mathbb{C}}$, so that one has complex operators $U_a^{\mathbb{C}}$ such that

$$U_{ba}^{\mathbb{C}}\omega(b,a)=U_b^{\mathbb{C}}U_a^{\mathbb{C}}$$

for some complex phase $\omega(b,a)$, and extend it to a projective quaternionic representation on $V_{\mathbb{C}} \oplus V_{\mathbb{C}}j$ in the canonical manner. The third way is to start with a real projective representation, $U_a^{\mathbb{R}}$ on a real space $V_{\mathbb{R}}$ and tensor product it with an otherwise arbitrary phase map

$$\sigma: G \to U(1,\mathbb{H})$$

to obtain a quaternionic projective representation on the quaternionic space $V_{\mathbb{R}} \otimes \mathbb{H}$. The following theorem states that these three methods are, up to a reraying, the only ways to create irreducible projective quaternionic representations.

Structure Theorem: *Let U be an irreducible projective representation of a connected Lie group G. There then exists a reraying of the basis $|f\rangle$ under which one of the following three possibilities must hold.*

(1) U is a real projective representation (type I). That is, $\omega(f,b,a)=\omega(b,a)$ is independent of $|f\rangle$ and is equal to ± 1 for each b and a.
(2) U is the extension of a complex projective representation (type II). That is, the matrix elements $\langle f|U_a|f'\rangle$ are complex and $\omega(f,b,a)=\omega(b,a)$ is independent of $|f\rangle$ and is a complex phase.
(3) U is the tensor product of a real projective representation and a quaternionic phase (type III). That is, there exists a decomposition

$$U_a = U_a^{\mathbb{R}} \sum_f |f\rangle \sigma_a \langle f|,$$

where the unitary operator $U_a^{\mathbb{R}}$ has real matrix elements, σ_a is a quaternionic phase and

$$U_{ba}^{\mathbb{R}} = \pm U_b^{\mathbb{R}} U_a^{\mathbb{R}}$$

for all b and a.

It should be noted that the three cases are not mutually exclusive; for example, a one-dimensional type I representation is a type III representation with real σ_a and a one-dimensional type II representation is a type III representation with complex σ_a.

We use this structure theorem to answer Adler's question. Let a multicentral projective representation be one in which $\Omega(b,a)$ commutes with U_b and U_a for all b and a, and let a central projective representation be one in which $\Omega(b,a)$ commutes with U_c for all a, b, and c. Our answer is then as follows.

Corollary 1: Any multicentral quaternionic projective representation of a connected Lie group is central.

The requirement that G is connected is not redundant, as shown in the following example. Set G to be the union of two copies of the quaternionic phase group $U(1,\mathbb{H})$ labeled by $+$ and $-$, respectively, with these labels combining under Z_2. Let U be the one-dimensional representation defined by $U_{a_+} = a$ and $U_{a_-} = 1$ for all $a \in U(1,\mathbb{H})$. The whole system is now a quaternionic projective representation of $Z_2 \times U(1,\mathbb{H})$, which is not connected, the operators multiplying according to Table I. By inspection, for each row $\Omega(b,a)$ commutes with U_a and with U_b, so the representation is multicentral, but $\Omega(b,a)$ does not generally commute with all U_c, so the representation is not central.

TABLE I. Representation for $Z_2 \times U(i,\mathscr{H})$.

a	b	ba	U_a	U_b	U_{ba}	$\Omega(b,a)$
a_+	b_+	ba_+	a	b	ba	1
a_+	b_-	ba_-	a	1	1	a
a_-	b_+	ba_-	1	b	1	b
a_-	b_-	ba_+	1	1	ba	ba

IV. PROOF OF THE STRUCTURE THEOREM

Following Adler's analysis,[1] we begin with the crucial observation that

Statement 1:

$$U_a^{-1}\Omega(b,c)U_a=\Omega(bc,a)^{-1}\Omega(b,ca)\Omega(c,a),$$

is unitary and diagonal for all a, b, and c.
We may therefore, write this unitary diagonal operator as

$$U_a^{-1}\Omega(b,c)U_a=\sum_f |f\rangle \nu(f,a,b,c)\langle f|, \tag{1}$$

where the ν are quaternionic phases that are formed from the ω,

$$\nu(f,a,b,c)=\omega(f,bc,a)^{-1}\omega(f,b,ca)\omega(f,c,a).$$

We multiply Eq. (1) on the left by U_a and take matrix elements to give

$$\omega(f,b,c)\langle f|U_a|f'\rangle=\langle f|U_a|f'\rangle \nu(f',a,b,c). \tag{2}$$

If the underlying algebra was commutative and the matrix elements of U_a were invertible, we could cancel the matrix elements and conclude that the ω were independent of f. Since the quaternions are not commutative, we can only expect to show that the conjugacy class of the ω is independent of f.

We shall use Eq. (2) for various values of f and f' to derive a relationship that involves the ω but not the ν. However, it is necessary to first ensure that the matrix elements of U_a are invertible for suitable a, $|f\rangle$ and $|f'\rangle$. This motivates the following.

Definition 6: We say that two basis states $|f_1\rangle$ and $|f_2\rangle$ are directly connected if there exists a basis state $|f_3\rangle$ (which may be equal to $|f_1\rangle$ or $|f_2\rangle$ or both) and a group element a such that $\langle f_1|U_a|f_3\rangle$ and $\langle f_2|U_a|f_3\rangle$ are both nonzero (and hence invertible).

The relationship of direct connectivity is symmetric but is not necessarily an equivalence relation. In order to form equivalence classes, we shall also define a completion of direct connectivity.

Definition 7: We say that two basis states $|f\rangle$ and $|f'\rangle$ are indirectly connected if there exists a non-negative integer n and a sequence of basis states $|f_0\rangle,\ldots,|f_n\rangle$ with $|f_0\rangle=|f\rangle$ and $|f_n\rangle=|f'\rangle$ such that $|f_i\rangle$ and $|f_{i+1}\rangle$ are directly connected for all $0\leqslant i<n$.

It can easily be verified that indirect connectivity is an equivalence relation. Note, that two states which are directly connected are automatically indirectly connected. This allows us to propose the following.

Proposition 1: All basis states are indirectly connected to each other.

Suppose this were not true. Then one can partition the basis states into two nonempty classes A and A' such that no state in A is directly connected to any state in A'. To do this, pick any basis state $|f_0\rangle$ and let A be the set of all states indirectly connected to $|f_0\rangle$; by the hypothesis that not

all states are indirectly connected, A and its complement A' are nonempty. Let V_A and $V_{A'}$ be the subspaces of V spanned by the states of A and those of A' respectively, so that $V = V_A \oplus V_{A'}$. Choose a basis state $|f\rangle$ from A and a group element a. Then the Hilbert space state $U_a|f\rangle$ can have components from states in A or components from states in A' but not both, since that would contradict the fact that A and A' are not directly connected. Since $|f\rangle$ is normalized and since U_a is unitary, $U_a|f\rangle$ is also normalized and hence lies either in the unit sphere of V_A or in the unit sphere of $V_{A'}$ for each a. When a is the multiplicative group identity 1, $U_a|f\rangle$ lies in (the unit sphere of) V_A; by the connectivity argument, $U_a|f\rangle$ lies in V_A for all a, and since $|f\rangle$ was an arbitrary basis state of A, this means that U maps V_A to V_A. Similarly it must map $V_{A'}$ to $V_{A'}$. Hence U is reducible, contradicting the assumptions of the theorem, and the proposition is proved.

Corollary 2: For any basis states $|f_1\rangle$ and $|f_2\rangle$ there exists a quaternionic phase $\phi(f_1, f_2)$ such that

$$\omega(f_2, b, c) = \phi(f_1, f_2)\omega(f_1, b, c)\overline{\phi(f_1, f_2)}, \tag{3}$$

for all b and c.

Since $|f_1\rangle$ and $|f_2\rangle$ are indirectly connected by the previous proposition, it is sufficient to prove this corollary for the case when the states are directly connected and then to use induction. (The claim is trivial when the states are the same.) We may thus assume the existence of a group element a and a state $|f_3\rangle$ such that $\langle f_1|U_a|f_3\rangle$ and $\langle f_2|U_a|f_3\rangle$ are invertible. Substituting f_1 for f and f_3 for f' and then f_2 for f and f_3 for f' in Eq. (2) and eliminating the ν dependence yields Eq. (3) with

$$\phi(f_1, f_2) = \frac{\langle f_2|U_a|f_3\rangle[\langle f_1|U_a|f_3\rangle]^{-1}}{|\langle f_2|U_a|f_3\rangle[\langle f_1|U_a|f_3\rangle]^{-1}|} = \overline{\phi(f_2, f_1)}.$$

Corollary 2 can now be used to simplify the problem as follows. Choose a fixed basis state $|f_0\rangle$; all other basis states may now be rerayed,

$$|f\rangle \mapsto |f\rangle\phi(f, f_0),$$

without changing the projective nature of the representation U. Under this reraying, Eq. (3) implies that

$$\omega(f, b, c) \mapsto \omega(f_0, b, c);$$

in other words, $\omega(f, b, c) = \omega(b, c)$ is independent of the basis state $|f\rangle$.

There are then three cases depending on the range of the ω. We list them here and then consider each in turn.

(1) The $\omega(b, c)$ are real for all b and c.
(2) The ω are not always real, but they commute with each other.
(3) There exist $\omega(b, c)$ and $\omega(b', c')$ which do not commute with each other.

For the first case, since the ω must have unit magnitude, each is therefore, ± 1—this is the first case of the structure theorem so the representation is of type I.

Another way to state the second case is to say that there exists a single reraying under which the ω are all complex. In this case, we must re-examine Eq. (2), which is an identity of the form $pr = rq$. Now the ν are each the product of three of the ω; in particular, the ν are also complex. We can then use the following fact.

Quaternionic Identity 1: If the p is strictly complex, q are complex and r is quaternionic such that

$$pr = rq,$$

then either $p=q$, in which case r is also complex, or $p=q^*$, in which case r is skew-complex. (This is easily proved by decomposing all quantities into complex and skew-complex components.) Since it is assumed that $\omega(b,c)$ is not real for at least one pair b and c, this means that, for each a, U_a either has all complex matrix elements or all skew-complex matrix elements. However, since U_a never completely vanishes and is complex when $a=1$, we can use the connectedness of G as before to show that U_a must be complex for all a—this is the second case of the structure theorem so the representation is of type II.

For the third case, we must again re-examine Eq. (2). Since the ω are independent of $|f\rangle$ and the ν are formed from the ω, the ν are also independent of $|f\rangle$. Thus, whenever x is any matrix element of U_a, we have

$$\omega(b,c)x=x\nu(a,b,c). \tag{4}$$

When x and y are two nonzero matrix elements of U_a, a double application of Eq. (4) gives, after some manipulation, that

$$\omega(b,c)xy^{-1}=x\nu(a,b,c)y^{-1}=xy^{-1}\omega(b,c),$$

in other words, xy^{-1} commutes with $\omega(b,c)$. Similarly, xy^{-1} commutes with $\omega(b',c')$. Now we use the following fact.

Quaternionic Identity 2: If p, q, and r are quaternions such that r commutes with both p and q, but p and q do not themselves commute, then r must be real.

Hence, xy^{-1} is real for all pairs of nonzero matrix elements x and y of U_a. This is equivalent to saying that the nonzero matrix elements of U_a all have the same quaternionic phase, so we can separate U_a into the product of a real matrix $U_a^{\mathbb{R}}$ and a quaternionic phase matrix Σ_a,

$$\Sigma_a=\sum_f |f\rangle\sigma_a\langle f|,$$

so that

$$U_a=U_a^{\mathbb{R}}\Sigma_a=\Sigma_a U_a^{\mathbb{R}}.$$

Since U_a and Σ_a are unitary, $U_a^{\mathbb{R}}$ must also be unitary. Repeatedly using the fact that real matrices commute with constant diagonal ones (we recall that the Ω are constant diagonal), we find that

$$(U_{ba}^{\mathbb{R}})^{-1}U_b^{\mathbb{R}}U_a^{\mathbb{R}}$$

is simultaneously real unitary and constant diagonal and must, therefore, be plus or minus the identity. Thus, we have achieved the third case of the structure theorem and the representation is of type III.

Since these are the only three possibilities for the ω, the structure theorem is proved.

V. PROOF OF THE STRUCTURE THEOREM'S COROLLARY

We may again assume without loss of generality that the representation is irreducible, in which case the structure theorem applies. Representations of type I and type II are automatically central, so we immediately pass to consideration of type III representations. Here, we effectively have a one-dimensional projective quaternionic representation

$$a\mapsto\sigma_a.$$

Since the real part $U_a^{\mathbb{R}}$ of the representation is real-projective and commutes with constant diagonal operators, the multicentrality condition reduces to the quaternion-valued constraint

$$[\sigma_{ba}^{-1}\sigma_b\sigma_a,\sigma_a]=[\sigma_{ba}^{-1}\sigma_b\sigma_a,\sigma_b]=0. \tag{5}$$

One immediate consequence of multicentrality is

Statement 2: If any two of σ_a, σ_b, and σ_{ba} commute, then all three commute.

Our task is to show that in fact $\sigma_{ba}^{-1}\sigma_b\sigma_a$ commutes with all σ_c, meaning that the representation is also central. We may assume that the σ_a do not all commute with one another as if they did, the representation would be of type II which is always central. This lack of total commutativity may be stated as follows.

Statement 3: For any choice of i, there is an a such that σ_a is strictly quaternionic and so does not commute with any strictly complex number.

In particular, this means that we can always find an a such that σ_a is not real.

Given that there are some noncommuting phases, centrality is equivalent to the statement that

$$\sigma_{ba}=\pm\sigma_b\sigma_a \tag{6}$$

for all a and b, in other words the representation must, after all, be of type I. We begin by observing that from Eq. (5) and from quaternionic identity 2, we have that

Statement 4: $\sigma_{ba}=\pm\sigma_b\sigma_a$ is true whenever σ_a and σ_b do not commute.

This is actually a special case of a more general statement.

Proposition 2: Unless exactly two of σ_a, σ_b, and σ_{ba} are real, it is true that $\sigma_{ba}=\pm\sigma_b\sigma_a$.

In other words, if none of, one of, or all three of σ_a, σ_b, and σ_{ba} are real, then Eq. (6) holds. By statement 4, we may begin by assuming that σ_a and σ_b commute and hence by statement 2, they also commute with σ_{ba}. We can then reray them to be complex, in which case, statement 3 allows us to find a c such that σ_c does not commute with any of σ_a, σ_b, or σ_{ba}.

If all three of σ_a, σ_b, and σ_{ba} are real, then the proposition is trivially true, so we can assume that at most one of them is real. This gives four cases as follows.

(1) σ_b, σ_a, and σ_{ba} are all strictly complex.
(2) σ_b is real but σ_a and σ_{ba} are strictly complex.
(3) σ_a is real but σ_b and σ_{ba} are strictly complex.
(4) σ_{ba} is real but σ_b and σ_a are strictly complex.

In the first case, we have from statement 4 that

$$\sigma_{cb}=\pm\sigma_c\sigma_b;$$

since this is the product of something strictly complex and something strictly quaternionic, it is also strictly quaternionic. Hence, by statement 4 again,

$$\sigma_{cba}=\pm\sigma_{cb}\sigma_a=\pm\sigma_c\sigma_b\sigma_a,$$

On the other hand, another application of statement 4 gives that

$$\sigma_{cba}=\pm\sigma_c\sigma_{ba},$$

which on canceling σ_c means that Eq. (6) holds and the proposition is true.

In the second case, we again have from statement 4 that

$$\sigma_{cba}=\pm\sigma_c\sigma_{ba},$$

so σ_{cba} is strictly quaternionic and does not commute with σ_a. Hence, by statement 2, none of σ_{cba}, σ_{cb}, or σ_a can commute with each other and hence by statement 4,

$$\sigma_{cba}=\pm\sigma_{cb}\sigma_a;$$

therefore,

$$\sigma_c \sigma_{ba} = \pm \sigma_{cb} \sigma_a$$

or, after rearrangement,

$$\sigma_a \sigma_{ba}^{-1} = \pm \sigma_{cb}^{-1} \sigma_c .$$

However, the left-hand side of this equation is the product of two strictly complex quantities and hence is complex while the right-hand side commutes with σ_c by statement 2; thus, both sides must be equal to ± 1 or, since σ_b is real, to $\pm \sigma_b$. Hence Eq. (6) holds and the proposition is again true.

The third and fourth cases are handled in a similar manner to the above treatment of the second case, although σ_{bac} is considered instead of σ_{cba} in the third case.

We now develop an important corollary to this proposition by introducing the following definitions.

Definition 8: σ is locally constant at x if there is a neighborhood V_x around x such that $\sigma_x = \sigma_y$ for all y in V_x.

Definition 9: If σ_x is real and σ is locally constant at x, then σ_x is strongly real.

The corollary to proposition 2 is then as follows.

Corollary 3: Unless exactly two of σ_a, σ_b, and σ_{ba} are strongly real, it is true that $\sigma_{ba} = \pm \sigma_b \sigma_a$.

This is trivially true if σ_a, σ_b, and σ_{ba} are all strongly real, since they are then real and Eq. (6) holds. Suppose, then, that neither σ_a nor σ_b are strongly real: then we can find (multiplicative) perturbations $a\,\delta a$ and $b\,\delta b$ of a and b for which $\sigma_{a\,\delta a}$ and $\sigma_{b\,\delta b}$ are not real so that proposition 2 applies. Letting δa and δb tend to 1 and using the continuity of σ, Eq. (6) continues to hold and hence the proposition is true. The other two cases are handled similarly.

We wish to prove that Eq. (6) always holds, and we shall do this by showing that there is no a such that σ_a is strongly real, allowing us to apply corollary 3. A convenient origin for our argument is the multiplicative identity of G.

Proposition 3: σ_1 is real but is not strongly real.

Since σ_a commutes with itself, statement 2 implies that σ_1 commutes with all σ_a. Since not all σ commute, quaternionic identity 2 means that σ_1 is real. We will now prove that σ_1 is not strongly real.

Suppose that σ_1 is strongly real, so that

$$\sigma_{\delta a} = \pm 1 \tag{7}$$

for all δa in the neighborhood V_1. Let a be any group element such that σ_a is not real; by continuity, we can then find a neighborhood V_1^a of 1 such that $\sigma_{a\,\delta a}$ is also not real and is not equal to $-\sigma_a$ for all δa in V_1^a. Then, by proposition 2, we may conclude that

$$\sigma_{a\,\delta a} = \sigma_a$$

for all δa in $V_1 \cap V_1^a$—in other words, σ is locally constant at a whenever σ_a is not real. We will now generate a contradiction to the supposition that σ_1 is strongly real.

We use the connectedness of G to construct a trajectory from a, where σ_a is not real, to the identity,

$$\{a(t) : t \in [0,1]\}; \quad a(0) = a, \quad a(1) = 1.$$

At $t=0$, $\sigma_{a(t)} = \sigma_a$ but at $t=1$, $\sigma_{a(t)} \neq \sigma_a$. Let t_0 be the first time that $\sigma_{a(t)}$ departs from σ_a; more precisely,

$$t_0 = \sup\{s : \sigma_{a(t)} = \sigma_a \forall 0 \leqslant t < s\}.$$

By continuity, we then have that $\sigma_{a(t_0)} = \sigma_a$ so that $\sigma_{a(t_0)}$ is not real. Now, by the argument in the previous paragraph, which we recall follows from the supposition that σ_1 is strongly real, σ is locally constant at a. However, this means that

$$\sigma_{a(t_0+\delta t)} = \sigma_{a(t_0)}$$

for all sufficiently small δt. However, this contradicts the definition of t_0, which means that σ_1 cannot be strongly real, proving the proposition.

Since σ_1 is not strongly real, we ought to be able to prove the converse result of the conclusion of the second paragraph of the above proof, and this is in fact the case.

Corollary 4: If σ_a is not real, then σ is not locally constant at a.

If σ is locally constant at a, then for all $a\,\delta a$ in the neighborhood V_a of a,

$$\sigma_{a\,\delta a} = \sigma_a;$$

now, σ_a is not real and so by proposition 2,

$$\sigma_{a\,\delta a} = \pm \sigma_a \delta_{\delta a},$$

which, with the previous equation, means that Eq. (7) is again true. However, that implies that σ_1 is strongly real, which contradicts the proposition.

Corollary 5: If at least two of σ_a, σ_b, and σ_{ba} are not strongly real, then all three phases are not strongly real.

Suppose that σ_a and σ_b are not strongly real but that σ_{ba} is. Since σ_a is not strongly real, corollary 4 implies that σ is not locally constant at a. Thus, we can find a δa close to 1 such that $\sigma_{a\,\delta a}$ is not equal to $\pm\sigma_a$ or ± 1; in particular $\sigma_{a\,\delta a}$ is not strongly real, so by corollary 3,

$$\sigma_b \sigma_{a\,\delta a} = \pm \sigma_{ba\,\delta a}.$$

However, since σ_{ba} is strongly real,

$$\sigma_{ba\,\delta a} = \pm \sigma_{ba} = \pm \sigma_b \sigma_a,$$

contradicting the fact that $\sigma_{a\,\delta a} \neq \pm \sigma_a$. The other two cases are handled similarly.

Corollary 6: For δa sufficiently close to 1, $\sigma_{\delta a}$ is not strongly real.

Choose a such that σ_a is not real. By continuity, $\sigma_{a\,\delta a}$ is also not real for δa sufficiently close to 1. Since σ_a and $\sigma_{a\,\delta a}$ are not real, they are not strongly real, so by corollary 5, $\sigma_{\delta a}$ is also not strongly real.

With one main step remaining, we are now very close to our goal.

Proposition 4: There is no a such that σ_a is strongly real.

Suppose there exists an a such that σ_a is strongly real. We use the connectedness of G to construct a trajectory from a to the identity,

$$\{a(t) : t \in [0,1]\}; \quad a(0) = a, \quad a(1) = 1.$$

At $t=0$, $\sigma_{a(t)} = \sigma_a$ and hence is strongly real, but at $t=1$, $\sigma_{a(t)} = \sigma_1$ which is not strongly real. Let t_0 be the first time that $\sigma_{a(t)}$ is not strongly real; more precisely,

$$t_0 = \sup\{s : \sigma_{a(t)} \text{ is strongly real } \forall 0 \leqslant t < s\}.$$

The definition of t_0 means that $\sigma_{a(t)}$ is strongly real for all $t < t_0$ and that, for all $\epsilon > 0$, we can find $\delta t \in [0, \epsilon]$ such that $\sigma_{a(t_0+\delta t)}$ is not strongly real.

Suppose $\sigma_{a(t_0)}$ was itself strongly real. There is then a neighborhood $V_{a(t_0)}$ such that σ is real and constant in that neighborhood. However, this lets us choose an $\epsilon>0$ such that $a(t_0 + \delta t) \in V_{a(t_0)}$ for all $\delta t \in [0,\epsilon]$; since σ is real and constant in this neighborhood, this means that $\sigma_{a(t_0+\delta t)}$ is also strongly real, contradicting the definition of t_0.

Suppose, then, that $\sigma_{a(t_0)}$ is not strongly real. Choose δa near 1 such that

$$a(t_0)\,\delta a = a(t_0 - \delta t),$$

where δt is, as usual, small and positive. Since $\sigma_{a(t_0)}$ and, by corollary 6, $\sigma_{\delta a}$ are not strongly real, by corollary 5, $\sigma_{a(t_0-\delta t)}$ is not strongly real, again contradicting the definition of t_0.

Since $\sigma_{a(t_0)}$ must be either strongly real or not strongly real, the supposition that σ_a was strongly real is false and we have proved the proposition. By corollary 3, therefore, Eq. (6) is always true, so that the representation is central, in the case that the σ_a do not all commute. All cases now having been covered, we have also proved the main corollary.

An alternative to the last couple of steps is to form H, the set of all $a \in G$ such that σ_a is not strongly real. H is then a subgroup of G by corollary 5. We then prove that H is an open subset of G, and that $G\backslash H$, the set of all $a \in G$ such that σ_a is strongly real, is also an open subset of G. However, by the definition of connectedness, there is no way to partition G as the union of two disjoint nonempty open sets, and since 1 is in H by proposition 3, it must be $G\backslash H$ that is empty, proving proposition 4.

The above proof of the corollary to the structure theorem shows that for a multicentral (and hence central) type III representation, either all the σ_a commute and can thus be rerayed to be complex—so the representation is type II—or the σ satisfy Eq. (6)—so the representation is type I. The only irreducible multicentral projective quaternionic representations are, therefore, either real projective representations or extensions of complex projective representations.

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The absolute rigidity of the Neveu–Schwarz and Ramond superalgebras

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We prove that the second cohomology group with coefficients in the adjoint module of both the infinite-dimensional Lie superalgebras $k(1)$ and $k^+(1)$, as well as their unique central extensions, which are known as the Neveu–Schwarz and the Ramond superalgebras, respectively, is equal to zero. This particularly implies that all these Lie superalgebras are rigid, i.e. they can only be deformed in a trivial manner. © *1996 American Institute of Physics.* [S0022-2488(96)03809-1]

I. INTRODUCTION

From the general theory on deformations of algebraic structures (see, e.g., Ref. 1), we learn that constructions of deformations involve cohomology computations. The infinitesimal part of an algebra deformation can be represented as an element of the second cohomology group with coefficients in the adjoint representation. An algebra is called rigid if all its deformations are trivial, i.e. any algebra that is obtained from it by deformation is isomorphic to the original algebra by means of an isomorphism that depends on the deformation parameter, which reduces to the identity mapping when this deformation parameter is set equal to zero. A sufficient condition for the rigidity of an algebra is that its second cohomology group is equal to zero. Therefore, algebras that satisfy this condition are usually called absolutely rigid.

In recent years quite a number of papers have been written on the topic of deformations of nilpotent subalgebras of graded infinite-dimensional Lie algebras (see, e.g., Refs. 2–6). These works show that the nilpotent subalgebras have several nontrivial deformations that have a fairly simple algebraic description. In Refs. 7 and 8 the author shows that the situation is similar in the case of graded infinite-dimensional Lie superalgebras. With respect to the corresponding graded Lie (super)algebras, one could say there is common consent that these Lie (super)algebras are rigid. In this paper we show that the results of the cohomology computations for the positive nilpotent part of the Neveu–Schwarz and the Ramond Lie superalgebras presented in Ref. 7, can be fruitfully used to prove that these Lie superalgebras are absolutely rigid. In fact, the presented method of rigidity proving is another illustration of the usefulness of studying these nilpotent subalgebras.

The Neveu–Schwarz and Ramond superalgebras are usually called super-Virasoro algebras since they can be viewed as superanalogs of the Virasoro algebra. As the Virasoro algebra arises as the unique (up to equivalence) central extension of the Witt algebra, they are the unique central extensions of the simple Lie superalgebras $k(1)$ and $k^+(1)$, respectively (see, e.g., Ref. 9). Both superalgebras appear in mathematical physics (see, e.g., Refs. 10 and 11). For instance, in superstring theory (see, e.g., Ref. 12) the Neveu–Schwarz algebra describes the super-Virasoro algebra in the bosonic sector, whereas the Ramond algebra describes the super-Virasoro algebra in the fermionic sector.

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The Neveu–Schwarz algebra can be presented as the $\mathbb{Z}_2$-graded vector space with $\{L_p, D\}_{p\in\mathbb{Z}}$ as a basis of the even homogeneous part and $\{G_q\}_{q+1/2\in\mathbb{Z}}$ as a basis of the odd homogeneous part. Its commutator is defined by

$$\begin{aligned}
[L_p, L_q] &= (p-q)L_{p+q} + \tfrac{1}{8}(p^3-p)\,\delta_{p+q,0}D,\\
[L_p, G_q] &= (\tfrac{1}{2}p-q)G_{p+q},\\
[G_p, G_q] &= 2L_{p+q} + \tfrac{1}{2}(p^2-\tfrac{1}{4})\,\delta_{p+q,0}D,
\end{aligned} \tag{1}$$

and the property that D is a central element. The Ramond algebra has $\{L_p, D\}_{p\in\mathbb{Z}}$ as a basis of the even homogeneous part and $\{F_q\}_{q\in\mathbb{Z}}$ as a basis of the odd homogeneous part. It is equipped with the commutator

$$\begin{aligned}
[L_p, L_q] &= (p-q)L_{p+q} + \tfrac{1}{8}p^3\,\delta_{p+q,0}D,\\
[L_p, F_q] &= (\tfrac{1}{2}p-q)F_{p+q},\\
[F_p, F_q] &= 2L_{p+q} + \tfrac{1}{2}p^2\,\delta_{p+q,0}D,
\end{aligned} \tag{2}$$

where D is defined to be central.

II. THE RIGIDITY OF $k(1)$ AND NS

The Lie superalgebra $k(1)$ (see Ref. 9) is defined as the $\mathbb{Z}_2$-graded vector space $\mathbb{C}[t,t^{-1},\theta]$ equipped with the commutator

$$[f,g] = \left(2f - \theta\frac{\partial f}{\partial\theta}\right)\frac{\partial g}{\partial t} - \frac{\partial f}{\partial t}\left(2g - \theta\frac{\partial g}{\partial\theta}\right) - (-1)^{|f|}\frac{\partial f}{\partial\theta}\frac{\partial g}{\partial\theta}, \quad f,g\in\mathbb{C}[t,t^{-1},\theta]. \tag{3}$$

The parameter t is even and the parameter θ is odd. The symbol $|f|$ denotes the parity of the element f in $\mathbb{C}[t,t^{-1},\theta]$. As basis of $k(1)$ we choose $\{e_p\}_{p\in\mathbb{Z}}$ where

$$e_{2p} = t^{p+1}, \quad e_{2p-1} = \theta t^p \quad (p\in\mathbb{Z}). \tag{4}$$

Note that the elements in this basis are homogeneous, in particular, the parity of e_p equals p modulo 2. The unique central extension of $k(1)$, which we denote by NS, is determined by the 2-cocycle $c\in Z^2(k(1))$, defined as

$$c(f\wedge g) = \mathrm{Res}\left\{\left(\frac{\partial f}{\partial\theta} - \theta\frac{\partial f}{\partial t}\right)\frac{\partial^2 g}{\partial t^2} - (-1)^{|f|}\frac{\partial^2 f}{\partial t^2}\left(\frac{\partial g}{\partial\theta} - \theta\frac{\partial g}{\partial t}\right)\right\}. \tag{5}$$

In this formula the symbol Res denotes the residue, i.e., $\mathrm{Res}(h)$ is the coefficient of the term θt^{-1} in $h\in\mathbb{C}[t,t^{-1},\theta]$. The wedge ($\wedge$) in formula (5) denotes the $\mathbb{Z}_2$-graded antisymmetric tensor product, so for homogeneous elements f and g in $k(1)$ we have

$$f\wedge g = f\otimes g - (-1)^{|f||g|}g\otimes f = -(-1)^{|f||g|}g\wedge f.$$

Naturally a basis for NS is found by adding the central element γ to the given basis of $k(1)$. The linear map φ defined by

$$\varphi(t^{p+1}) = 2L_{-p}, \quad \varphi(\theta t^q) = G_{1/2-q}, \quad \varphi(\gamma) = \tfrac{1}{4}D \quad (p,q\in\mathbb{Z}) \tag{6}$$

is an isomorphism that explicitly describes the connection between the description of the Neveu–Schwarz algebra given in (1) and the one presented above. Besides the $\mathbb{Z}_2$ grading of NS,

$$NS=\bigoplus_{j\in\mathbb{Z}_2} NS_j, \quad NS_0=(\bigoplus_{j\in\mathbb{Z}}\langle e_{2j}\rangle)\oplus\langle\gamma\rangle, \quad NS_1=\bigoplus_{j\in\mathbb{Z}}\langle e_{2j-1}\rangle,$$

which describes NS as a superspace, the element e_0 defines an inner grading on $k(1)$ and NS by means of its adjoint action. The basis elements are homogeneous with respect to this inner $\mathbb{Z}$ grading. We denote the eigenspace of $ad(e_0)$ corresponding to the eigenvalue λ by $NS_{(\lambda)}$; then we have

$$NS=\bigoplus_{\lambda\in\mathbb{Z}} NS_{(\lambda)}, \quad NS_{(0)}=\langle e_0,\gamma\rangle, \quad NS_{(\lambda)}=\langle e_\lambda\rangle \quad (\lambda\in\mathbb{Z}\backslash\{0\}). \tag{7}$$

We remark that the inner grading is compatible with the $\mathbb{Z}_2$ grading in the sense that a homogeneous element of degree λ has parity λ modulo 2. For later use we write out explicitly the commutators of the basis elements:

$$\begin{aligned}
[e_{2j},e_{2k}]&=2(k-j)e_{2j+2k}+2k(k^2-1)\delta_{j+k,0}\gamma,\\
[e_{2j-1}e_{2k}]&=(k-2j+1)e_{2j+2k-1},\\
[e_{2j-1},e_{2k-1}]&=e_{2j+2k-2}+2k(k-1)\delta_{j+k,1}\gamma,\\
[e_j,\gamma]&=0.
\end{aligned} \tag{8}$$

The commutators in $k(1)$ are the same with the omission of all terms involving the central element γ.

Theorem 1: *The second cohomology group of $k(1)$ with coefficients in the adjoint representation is equal to zero:*

$$H^2(k(1);k(1))=0.$$

Proof: The $\mathbb{Z}$ grading of $k(1)$ induces a $\mathbb{Z}$ grading on the cochain complex $(C^\bullet(k(1);k(1)),d)$, so we can write

$$C^q(k(1);k(1))=\prod_{\lambda\in\mathbb{Z}} C^q(k(1);k(1))_{(\lambda)} \quad (q\in\mathbb{Z}),$$

and similarly for the corresponding cohomology groups. For details on the coboundary operator on this cochain complex and the corresponding cohomology groups we simply refer to Refs. 8, 13, and 14. Since nonzero cohomology classes can only exist at degree zero (see, e.g., Ref. 8 or 15), we know that

$$H^q(k(1);k(1))_{(\lambda)}=0 \quad (q\in\mathbb{Z}),$$

for all degrees λ not equal to zero. This observation reduces the work to be done considerably; we can confine ourselves to studying homogeneous 2-cocycles of degree zero.

An arbitrary 2-cocycle of degree zero can be written as

$$c(e_j\wedge e_k)=\alpha_{j,k}e_{j+k} \quad (j,k\in\mathbb{Z}), \tag{9}$$

with coefficients $\alpha_{j,k}\in\mathbb{C}$ satisfying $\alpha_{j,k}=-(-1)^{jk}\alpha_{k,j}$. A cocycle represents a cohomology class, in general; it is, however, not unique since there exist other cohomologically equivalent cocycles.

By application of coboundary corrections, we will determine a set of conditions for the coefficients $\alpha_{j,k}$ such that each cohomology class has a unique representative with coefficients that satisfy these specific conditions.

Lemma 1: An arbitrary cohomology class of $H^2(k(1);k(1))_0$ *can be represented by a 2-cocycle as described by formula (9), with coefficients* $\alpha_{j,k}$ *satisfying*

$$\alpha_{-1,1}=\alpha_{0,1}=0, \quad \alpha_{j,k}=0 \quad (jk>0).$$

Proof: We perform coboundary corrections in several steps. We refer to each step by the condition it imposes on the coefficients $\alpha_{j,k}$.

Step 1: $\alpha_{j,k}=0 \quad (j,k\in\mathbb{Z}_{>0})$

We define the Lie supersubalgebra of $k(1)$ spanned by the homogeneous elements of positive degree and denote it by

$$k(1)_+ = \bigoplus_{\lambda\in\mathbb{Z}_{>0}} k(1)_{(\lambda)}.$$

In Ref. 7 we proved (by application of the Feigin–Fuchs spectral sequence; for its definition see Ref. 16) that $H^2(\mathrm{k}(1)_+;\mathrm{k}(1)_+)_{(0)}=0$; hence the restriction of c to $\wedge^2(k(1)_+)$ is a coboundary. So there exists an element b_1 in $C^1(\mathrm{k}(1)_+;\mathrm{k}(1)_+)_{(0)}$ such that $d(b_1)(e_j\wedge e_k)=c(e_j\wedge e_k)$ for all $j,k\in\mathbb{Z}_{>0}$. We expand b_1 trivially from $k(1)_+$ to $k(1)$ by defining $b_1(e_j)=0$ for all $j\in\mathbb{Z}_{\leqslant 0}$ and we replace c by $c'=c-d(b_1)$. The 2-cocycle c' has coefficients $\alpha'_{j,k}$ satisfying $\alpha'_{j,k}=0$ for all $j,k\in\mathbb{Z}_{>0}$. From here on we will denote c' again by c.

Step 2: $\alpha_{j,k}=0 \quad (j,k\in\mathbb{Z}_{<0})$

Similar to the previous step, we define

$$k(1)_- = \bigoplus_{\lambda\in\mathbb{Z}_{<0}} k(1)_{(\lambda)};$$

this is the Lie supersubalgebra of $k(1)$ spanned by the homogeneous elements of negative degree. It is isomorphic to $k(1)_+$ by the isomorphism φ: $k(1)_+\to k(1)_-$, satisfying

$$\begin{cases} \varphi(e_{2j})=-e_{-2j} \\ \varphi(e_{2j-1})=ie_{1-2j} \end{cases} \quad (j\in\mathbb{Z}_{>0}).$$

Hence, $H^2(k(1)_-;k(1)_-)_{(0)}=0$ and there exists an element b_2 in $C^1(k(1);k(1))_{(0)}$ such that $(d(b_2)-c)(e_j\wedge e_k)=0$, $(j,k\in\mathbb{Z}_{<0})$, and $b_2(e_j)=0$, $(j\in\mathbb{N})$. In particular, we have $d(b_2)(e_j\wedge e_k)=0$ for all $j,k\in\mathbb{Z}_{>0}$, so $d(b_2)$ respects the previous conditions for the coefficients $\alpha_{j,k}$. We adjust c to $c-d(b_2)$ and obtain $\alpha_{j,k}=0$ for all $j,k\in\mathbb{Z}_{<0}$.

Step 3: $\alpha_{0,1}=0$

We define the element b_3 in $C^1(k(1);k(1))_{(0)}$ by $b_3(e_j)=\delta_{j,0}e_0 \quad (j\in\mathbb{Z})$. The coboundary $d(b_3)$ satisfies $d(b_3)(e_j\wedge e_k)=0 \quad (jk>0)$, so it respects the preceding conditions for the coefficients $\alpha_{j,k}$. Since $d(b_3)(e_0\wedge e_1)=e_1$ we can adjust c such that $\alpha_{0,1}$ becomes zero.

Step 4: $\alpha_{-1,1}=0$

Define $b_4\in C^1(k(1);k(1))_{(0)}$ by $b_4(e_j)=je_j \quad (j\in\mathbb{Z}_{>0})$ and $b_4(e_j)=0 \quad (j\in\mathbb{Z}_{\leqslant 0})$. One easily verifies that $d(b_4)(e_j\wedge e_k)=0$ for $jk\geqslant 0$, hence the coboundary $d(b_4)$ respects the preceding conditions for $\alpha_{j,k}$. On account of $d(b_4)(e_{-1}\wedge e_1)=e_0$ it is possible to adjust c such that $\alpha_{-1,1,}=0$. □

It is not yet clear that a representative of the form described in the previous lemma is unique. We will prove that any 2-cocycle that satisfies these conditions is equal to zero. The cocycle condition $d(c)=0$ gives rise to four types of equations for the coefficients $\alpha_{j,k}$. Since we will need them frequently we write down these equations explicitly: $d(c)(e_{2j}\wedge e_{2k}\wedge e_{2l})=0$ gives

$$(k-j)\alpha_{2j+2k,2l}-(l-j)\alpha_{2j+2l,2k}+(l-k)\alpha_{2l+2k,2j}$$
$$-(l+k-j)\alpha_{2k,2l}+(j+l-k)\alpha_{2j,2l}-(j+k-l)\alpha_{2j,2k}=0; \tag{10}$$

$d(c)(e_{2j-1}\wedge e_{2k}\wedge e_{2l})=0$ gives

$$(k-2j+1)\alpha_{2j+2k-1,2l}-(l-2j+1)\alpha_{2j+2l-1,2k}+2(l-k)\alpha_{2k+2l,2j-1}$$
$$-(l+k-2j+1)\alpha_{2k,2l}+(2l+2j-k-1)\alpha_{2j-1,2l}-(2j+2k-l-1)\alpha_{2j-1,2k}=0; \tag{11}$$

$d(c)(e_{2j-1}\wedge e_{2k-1}\wedge e_{2l})=0$ gives

$$\alpha_{2j+2k-2,2l}-(l-2j+1)\alpha_{2j+2l-1,2k-1}-(l-2k+1)\alpha_{2k+2l-1,2j-1}$$
$$-\alpha_{2k-1,2l}-\alpha_{2j-1,2l}-2(j+k-l-1)\alpha_{2j-1,2k-1}=0; \tag{12}$$

and $d(c)(e_{2j-1}\wedge e_{2k-1}\wedge e_{2l-1})=0$ gives

$$\alpha_{2j+2k-2,2l-1}+\alpha_{2j+2l-2,2k-1}+\alpha_{2k+2l-2,2j-1}-(k+l-2j)\alpha_{2k-1,2l-1}$$
$$-(j+l-2k)\alpha_{2j-1,2l-1}-(j+k-2l)\alpha_{2j-1,2k-1}=0. \tag{13}$$

By substituting specific values for j, k, and l in these equations we prove in several steps that all coefficients $\alpha_{j,k}$ are equal to zero. Again we refer to each step by the condition it imposes on the coefficients.

Step 1: $\alpha_{0,p}=0$ $(p\in\mathbb{Z})$

We substitute $(j,l)=(k,0)$ in (12) and find $\alpha_{4k-2,0}=2\alpha_{2k-1,0}$. In particular $k=1$ yields $\alpha_{0,2}=0$, then by substituting $(j,k,l)=(0,\mathbb{Z}_{>0},\mathbb{Z}_{>0})$ in (10) we find $(l-k)(\alpha_{2l+2k,0}-\alpha_{2l,0}-\alpha_{2k,0})=0$ and $\alpha_{0,2l}=l\alpha_{0,2}=0$ for all $l\in\mathbb{Z}_{>0}$. A similar proof can be given for $l\in\mathbb{Z}_{<0}$ since putting $(j,k,l)=(0,1,0)$ in (12) yields $\alpha_{-1,0}=0$.

Step 2: $\alpha_{-1,p}=\alpha_{1,p}=0$ $(p\in\mathbb{Z})$

We already have $\alpha_{-1,p}=0$ for $p\leqslant 1$; in order to show that $\alpha_{-1,p}=0$ for $p\geqslant 2$ we take $(j,k,l)=(0,1,\mathbb{Z}_{>0})$ and $(j,k,l)=(0,\mathbb{Z}_{>0},1)$ in (12), yielding $-(l-1)\alpha_{-1,2l+1}-\alpha_{-1,2l}=0$ and $-2(1-k)\alpha_{-1,2k+1}-\alpha_{-1,2}-2(k-2)\alpha_{-1,2k-1}=0$. The choice $l=1$ in the first equation gives $\alpha_{-1,2}=0$, and by that the second one yields $\alpha_{-1,2k+1}=(k-2)\alpha_{-1,2k-1}/(k-1)$. The choice $k=2$ gives $\alpha_{-1,5}=0$ and by induction we find $\alpha_{-1,2p+1}=0$ for $p\geqslant 2$. Then again, the first implies $\alpha_{-1,p}=0$ for all $p\geqslant 4$. The last case $\alpha_{-1,3}=0$ follows from substituting $(j,k,l)=(10,0,2)$ in (13). The case $\alpha_{1,p}=0$ for all $p\in\mathbb{Z}$ can be handled similarly.

Step 3: $\alpha_{2,2p}=\alpha_{-2,2p}=0$ $(p\in\mathbb{Z})$

We consider $\alpha_{2,2p}$ with $p\in\mathbb{Z}_{<0}$. Putting $(j,k,l)=(1,1,-1)$ in (12) yields $\alpha_{-2,2}=0$ and $(j,k,l)=(-1,\mathbb{Z}_{<0},1)$ in (10) gives $(k+1)\alpha_{2k-2,2}-(k+2)\alpha_{2k,2}=0$. So by taking $k=-2$ we obtain $\alpha_{2,-6}=0$ and inductively $\alpha_{2,2p}=0$ for all $p\leqslant -3$. The condition $\alpha_{2,-4}=0$ follows from $(j,k,l)=(-3,-2,1)$ in (10). The case $\alpha_{-2,2p}$ can be handled similarly.

Step 4: $\alpha_{4,2p}=0$ $(p\in\mathbb{Z})$

We only need to consider $p<-1$. We substitute $(j,k,l)=(-1,\mathbb{Z}_{<0},2)$ in (10) and obtain $(k+1)\alpha_{2k-2,4}-(k+3)\alpha_{2k,4}=0$. The choice $k=-3$ yields $\alpha_{4,2p}=0$ for $p\leqslant -4$. By combining $k=-2$ with $(j,k,l)=(-3,-2,2)$ in (10), we obtain $\alpha_{4,-6}=\alpha_{4,-4}=0$ and hence $\alpha_{4,2p}=0$ for all p in $\mathbb{Z}$.

Step 5: $\alpha_{2n,2p}=0$ $(n,p\in\mathbb{Z})$

We only need to consider $\alpha_{2n,2p}$ with $n\in\mathbb{N}$ and $p\in\mathbb{Z}$. The cases $n=0,1,2$ are already evident. We proceed by induction, assuming that $\alpha_{2j,2p}=0$ for all $j\leqslant n$. Substituting $(j,k,l)=(p,1,n)$ in (10) gives $(n-1)\alpha_{2n+2,2p}=0$.

Step 6: $\alpha_{2,p}=0$, $(p\in\mathbb{Z})$

We only need to consider odd p. Put $(k,l)=(1,1)$ in (13), then $\alpha_{2,2j-1}=0$.

Step 7: $\alpha_{3,p}=0$ $(p\in\mathbb{Z})$

We put $(j,k)=(2,0)$ in (12) and (13) and find $\alpha_{2l,3}-(l+1)\alpha_{3,2l-1}=0$ and $\alpha_{2l-2,3}-(l+2)\alpha_{3,2l-1}=0$. Setting $l=-2$ yields by induction $\alpha_{3,p}=0$ for $p\leqslant -6$. The case $p=-4$ follows from, e.g., $(j,k,l)=(2,-10,-12)$ in (11) and putting $l=-1$ and $l=-2$ in the equations above yield $\alpha_{3,-3}=\alpha_{3,-5}=0$. By this and previous steps all coefficients $\alpha_{3,p}$ are equal to zero.

Step 8: $\alpha_{n,p}=0$ $(n,p\in\mathbb{Z})$

We only need to prove this for $n\in\mathbb{N}$ and $p\in\mathbb{Z}$. We use induction on n. The cases $n=0,1,2,3$ are evident on account of previous steps. It is completed by the substitutions

$$(j,k,l)=(1,p,n) \text{ in } (11), \quad (1-n)\alpha_{2n+1,2p}=0 \quad (n\geqslant 2),$$

$$(j,k,l)=(p+1,1,n) \text{ in } (12), \quad (1-n)\alpha_{2n+1,2p+1}=0 \quad (n\geqslant 2),$$

$$(j,k,l)=(p+1,1,n) \text{ in } (13), \quad \alpha_{2n,2p+1}=0.$$

This completes the proof that any 2-cocycle of degree zero is a coboundary. So by the previous remarks on the inner grading we have $H^2(k(1);k(1))=0$.

We will use the same technique to prove that the central extension NS is rigid.

Theorem 2: *The second cohomology group of NS with coefficients in the adjoint representation is equal to zero*:

$$H^2(NS;NS)=0.$$

Proof: Due to the inner grading of NS it suffices to prove that $H^2(NS;NS)_0=0$. An arbitrary 2-cocycle of degree zero can be written as

$$\begin{aligned} c(e_j\wedge e_k)&=\alpha_{j,k}e_{j+k}+\delta_{j+k,0}\beta_k\gamma \quad (j,k\in\mathbb{Z}),\\ c(\gamma\wedge e_j)&=\lambda_j e_j+\delta_{j,0}\mu\gamma \quad (j\in\mathbb{Z}), \end{aligned} \tag{14}$$

where $\alpha_{j,k}$, β_k, λ_j, and μ are complex numbers satisfying

$$\alpha_{j,k}=-(-1)^{jk}\alpha_{k,j} \quad (j,k\in\mathbb{Z}), \quad \beta_{-k}=-(-1)^k\beta_k \quad (k\in\mathbb{Z}).$$

Again we use coboundary corrections to choose representatives of a specific form. The notation will be similar to the one in Theorem 1.

Lemma 2: An arbitrary cohomology class of $H^2(NS;NS)_0$ *can be represented by a 2-cocycle as described by formula (14), with coefficients satisfying*

$$\alpha_{-1,1}=\alpha_{0,1}=\beta_1=\beta_3=\lambda_1=0, \quad \alpha_{j,k}=0 \quad (jk>0).$$

Proof:

Step 1: $\alpha_{-1,1}=\alpha_{0,1}=0$ $\alpha_{j,k}=0$ $(jk>0)$

Use the coboundaries $d(b_l)$ $(1\leqslant l\leqslant 4)$, where b_l is the extension of the element b_l given in Theorem 1, defined by $b_l(\gamma)=0$.

Step 2: $\lambda_1=0$

We define b_5 in $C^1(NS;NS)_{(0)}$ by $b_5(\gamma)=e_0$, $b_5(e_j)=0$, $(j\in\mathbb{Z})$; then $d(b_5)(\gamma\wedge e_1)=e_1$ so we obtain $\lambda_1=0$.

Step 3: $\beta_1=0$

We define b_6 in $C^1(NS;NS)_{(0)}$ by $b_6(\gamma)=0$, $b_6(e_l)=\delta_{l,0}\gamma$, $(l\in\mathbb{Z})$, and we see that $d(b_6)(e_{-1}\wedge e_1)=-\gamma$. By this β_1 becomes zero.

Step 4: $\beta_3=0$

Define b_7 in $C^1(NS;NS)_{(0)}$ by $b_7(\gamma)=\gamma$, $b_7(e_l)=0$, $(l\in\mathbb{Z})$; then $d(b_7)(e_{-3}\wedge e_3)=-4\gamma$; hence β_3 becomes zero.

It can easily be verified that all these corrections respect the preceding ones. □

We will prove that any representative c of this form is equal to zero. For that purpose we write out some consequences of the cocycle condition $d(c)=0$:

$$d(c)(\gamma\wedge e_{2j-1}\wedge e_{2k-1})=(\lambda_{2j+2k-2}-\lambda_{2k-1}-\lambda_{2j-1})e_{2j+2k-2}+\delta_{j+k,1}(\mu-\lambda_{2j-1}2j(j-1)-\lambda_{2k-1}2k(k-1))\gamma=0, \tag{15}$$

$$d(c)(\gamma\wedge e_{2j-1}\wedge e_{2k})=(k-2j+1)(\lambda_{2j+2k-1}-\lambda_{2k}-\lambda_{2j-1})e_{2j+2k-1}=0, \tag{16}$$

$$d(c)(\gamma\wedge e_{2j}\wedge e_{2k})=2(k-j)(\lambda_{2j+2k}-\lambda_{2j}-\lambda_{2k})e_{2j+2k}+2k\delta_{j+k,0}(2\mu-(k^2-1)(\lambda_{2j}+\lambda_{2k}))\gamma=0. \tag{17}$$

We take $(j,k)=(1,0)$ in (15) and $k=0$ in (16) and obtain $\mu=\lambda_0=0$. By substituting $j=1$ in (15) and (16), we find $\lambda_k=\lambda_1=0$ for all $k\in\mathbb{Z}$. Since the equations (10)–(13) still hold, we conclude that $\alpha_{j,k}=0$ for all j and k in $\mathbb{Z}$. Finally, we prove that the coefficients β_j are equal to zero,

$$d(c)(e_{2j-1}\wedge e_{2k-1}\wedge e_{2-2j-2k})=-\{\beta_{2-2j-2k}+(3j+k-2)\beta_{2k-1}+(3k+j-2)\beta_{2j-1}\}\gamma=0, \tag{18}$$

$$d(c)(e_{2j}\wedge e_{2k}\wedge e_{-2j-2k})=2\{(k-j)\beta_{2j+2k}-(2j+k)\beta_{2k}+(2k+j)\beta_{2j}\}\gamma=0. \tag{19}$$

We substitute $(j,k)=(1,1)$ and $(j,k)=(1,2)$ in (18) and obtain $\beta_2=\beta_4=0$. The choice $j=1$ in (19) yields $\beta_{2k+2}=[(k+2)/(k-1)]\beta_{2k}$ $(k\neq 1)$, and by induction all β_{2k} are equal to zero. Then $j=k$ in (18) implies $\beta_{2k-1}=0$ for all k in $\mathbb{Z}$ and the proof is complete. □

III. THE RIGIDITY OF $k^+(1)$ AND R

The Lie superalgebra $k^+(1)$ (see Ref. 9) looks quite similar to $k(1)$; it consists of the $\mathbb{Z}_2$-graded vector space $\mathbb{C}[t,t^{-1},\theta\sqrt{t}]$ equipped with the commutator of formula (3). We define a basis of $k^+(1)$ by $\{e_p\}_{p\in\mathbb{Z}}$, where

$$e_{2p}=t^{p+1},\quad e_{2p-1}=\theta t^p\sqrt{t}\quad (p\in\mathbb{Z}).$$

The elements in this basis are homogeneous; the parity of e_p is p modulo 2. The Ramond algebra is the unique central extension of $k^+(1)$. It is described by the 2-cocycle of formula (5) and we shall denote it by R. Let γ denote the central element of R. An isomorphism that relates this description with the one presented by formula (2) in the Introduction can be given by

$$\varphi(t^{p+1})=2L_{-p}+\tfrac{1}{16}\delta_{p,0}D,\quad \varphi(\theta t^q\sqrt{t})=F_{-q},\quad \varphi(\gamma)=\tfrac{1}{4}D\quad (p,q\in\mathbb{Z}). \tag{20}$$

We will use the inner grading of R corresponding to the special element $\frac{1}{2}e_0$. This boils down to

$$R=\bigoplus_{\lambda\in\mathbb{Z}}R_{(\lambda)},\quad R_{(\lambda)}=\langle e_{2l-1},e_{2\lambda}\rangle\quad (\lambda\in\mathbb{Z}\backslash\{0\}),\quad R_{(0)}=\langle e_{-1},e_0,\gamma\rangle.$$

The basis elements are homogeneous with respect to this $\mathbb{Z}$ grading, however, the $\mathbb{Z}_2$ grading of R is not compatible with this $\mathbb{Z}$ grading. To be more precise, we have

$$R_{(\lambda)}=R_{(\lambda),0}\oplus R_{(\lambda),1}=\langle e_{2\lambda}\rangle\oplus\langle e_{2\lambda-1}\rangle\quad (\lambda\neq 0)$$

and

$$R_{(0)}=R_{(0),0}\oplus R_{(0),1}=\langle e_0,\gamma\rangle\oplus\langle e_{-1}\rangle.$$

This makes the rigidity proof in this case slightly more technical than the one presented in the previous section. For later use we write out the commutators of the basis elements:

$$\begin{aligned}
[e_{2j},e_{2k}]&=2(k-j)e_{2j+2k}+2k(k^2-1)\,\delta_{j+k,0}\gamma,\\
[e_{2j-1},e_{2k}]&=(k-2j)e_{2j+2k-1},\\
[e_{2j-1},e_{2k-1}]&=e_{2j+2k}+2(k^2-\tfrac{1}{4})\,\delta_{j+k,0}\gamma,\\
[e_j,\gamma]&=0.
\end{aligned}\tag{21}$$

The commutators in $k^+(1)$ are as described above with the omission of all the terms involving the central element γ.

Theorem 3: *The even part of the second cohomology group of $k^+(1)$ with coefficients in the adjoint representation is equal to zero:*

$$H^2(k^+(1);k^+(1))=0.$$

Proof: Due to the inner grading of $k^+(1)$, we only need to prove $H^2(k^+(1);k^+(1))_{(0),0}=0$, i.e. we can restrict ourselves to studying even 2-cocycles of degree zero. We will use the same technique as described in the two proofs of the previous section, therefore we will confine ourselves to shortly indicating the various steps without discussing them in detail.

An even 2-cocycle c of degree zero is of the following form:

$$\begin{aligned}
c(e_{2j}\wedge e_{2k})&=\alpha_{2j,2k}e_{2j+2k},\\
c(e_{2j-1}\wedge e_{2k})&=\alpha_{2j-1,2k}e_{2j+2k-1},\\
c(e_{2j-1}\wedge e_{2k-1})&=\alpha_{2j-1,2k-1}e_{2j+2k},
\end{aligned}\tag{22}$$

with $\alpha_{j,k}\in\mathbb{C}$ and $\alpha_{j,k}=-(-1)^{jk}\alpha_{k,j}$ $(j,k\in\mathbb{Z})$.

Lemma 3: An arbitrary cohomology class of $H^2(k^+(1);k^+(1))_{(0),0}$ can be represented by a 2-cocycle as described by formula (22), with coefficients $\alpha_{j,k}$ satisfying

$$\alpha_{-2,-1}=\alpha_{-2,1}=\alpha_{0,1}=0,\quad \alpha_{j,k}=0\quad (j,k>0;j,k<-1).$$

Proof:

Step 1: $\alpha_{j,k}=0$ $(j,k>0)$

Define

$$k^+(1)_+=\bigoplus_{\lambda\in\mathbb{Z}_{>0}}k^+(1)_{(\lambda)};$$

this is the Lie supersubalgebra of $k^+(1)$ spanned by the homogeneous elements of positive degree. From Ref. 7 we know that $H^2(k^+(1)_+;k^+(1)_+)_{(0)}=0$; hence the restriction of c to $\wedge^2(k^+(1)_+)$ is a coboundary. By subtracting $d(b_1)$ from c, where b_1 denotes the trivial expansion of the element that yields the coboundary mentioned above, we obtain a 2-cocycle with coefficients $\alpha_{j,k}$ satisfying the described property.

Step 2: $\alpha_{j,k}=0$ $(j,k<-1)$

Define

$$k^+(1)_- = \bigoplus_{\lambda \in \mathbb{Z}_{<0}} k^+(1)_{(\lambda)}$$

and note that $k^+(1)_-$ is isomorphic to $k^+(1)_+$ by the isomorphism $\varphi: k^+(1)_+ \to k^+(1)_-$, given by

$$\begin{cases} \varphi(e_{2j}) = -e_{-2j} \\ \varphi(e_{2j-1}) = ie_{-2j-1} \end{cases} \quad (j \in \mathbb{Z}_{>0}).$$

By a similar argument as given in Step 1, we obtain $\alpha_{j,k}=0$ for $j,k<-1$.

Step 3: $\alpha_{0,1}=0$

Use $d(b_2)$ with $b_2(e_j)=\delta_{j,0}e_0$ $(j \in \mathbb{Z})$; then $d(b_2)(e_0 \wedge e_1)=2e_1$.

Step 4: $\alpha_{-2,-1}=0$

Use $d(b_3)$ with $b_3(e_j)=\delta_{j+1,0}e_{-1}$ $(j \in \mathbb{Z})$; then $d(b_3)(e_{-2} \wedge e_{-1})=e_{-3}$.

Step 5: $\alpha_{-2,1}=0$

Define b_4 by $b_4(e_{2j})=je_{2j}, b_4(e_{2j-1})=je_{2j-1}$ $(j \in \mathbb{Z}_{\leqslant 0})$, and $b_4(e_j)=0$ $(j \in \mathbb{Z}_{>0})$; then $d(b_4)(e_{-2} \wedge e_1)=-3e_{-1}$.

One can easily verify that each coboundary respects the conditions that have been imposed on the coefficients $\alpha_{j,k}$ in preceding steps. □

By similar inductive arguments, as demonstrated in the preceding theorems, one can prove that any 2-cocycle of the form described in the lemma is equal to zero. By that the proof is complete. □

Theorem 4: *The even part of the second cohomology group of R with coefficients in the adjoint representation is equal to zero*:

$$H^2(R;R)_0=0.$$

Proof: Due to the inner grading of R, it is sufficient to prove that $H^2(R;R)_{(0),0}=0$. An arbitrary even 2-cocycle of degree zero can be written as

$$\begin{gathered} c(e_{2j} \wedge e_{2k}) = \alpha_{2j,2k}e_{2j+2k} + \delta_{j+k,0}\beta_{2k}\gamma, \\ c(e_{2j-1} \wedge e_{2k}) = \alpha_{2j-1,2k}e_{2j+2k-1}, \\ c(e_{2j-1} \wedge e_{2k-1}) = \alpha_{2j-1,2k-1}e_{2j+2k} + \delta_{j+k,0}\beta_{2k-1}\gamma, \\ c(c\gamma \wedge e_j) = \lambda_j e_j + \delta_{j,0}\mu\gamma, \end{gathered} \tag{23}$$

where $\alpha_{j,k}, \beta_k, \lambda_j$, and μ are complex numbers such that

$$\alpha_{j,k} = -(-1)^{jk}\alpha_{k,j} \quad (j,k \in \mathbb{Z}), \quad \beta_{-2k} = -\beta_{2k}, \quad \beta_{2k-1} = \beta_{-2k-1} \quad (k \in \mathbb{Z}).$$

Lemma 4: An arbitrary cohomology class of $H^2(R;R)_{(0),0}$ can be represented by a 2-cocycle as described by formula (23), with coefficients $\alpha_{j,k}$ satisfying

$$\alpha_{-2,-1}=\alpha_{-2,1}=\alpha_{0,1}=0, \quad \alpha_{j,k}=0 \quad (j,k>0; j,k<-1),$$

and coefficients β_k and λ_j that satisfy

$$\beta_1=\beta_2=\lambda_2=0.$$

Proof: It is evident that the restrictions from Step 1–5 from Theorem 3 can also be obtained for $\alpha_{j,k}$ in this case. Furthermore, we perform the following steps.

Step 1: $\beta_2=0$

Use $d(b_1)$ with $b_1(e_j)=\delta_{j,0}\gamma$ $(j \in \mathbb{Z})$, and $b_1(\gamma)=0$; then $d(b_1)(e_{-2} \wedge e_2)=-4\gamma$.

Step 2: $\beta_1=0$

Use $d(b_2)$ with $b_2(\gamma)=\gamma$ and $b_2(e_j)=0$ $(j\in\mathbb{Z})$; then $d(b_2)(e_{-3}\wedge e_1)=-\frac{3}{2}\gamma$.

Step 3: $\lambda_2=0$

Use $d(b_3)$ with $b_3(\gamma)=e_0$ and $b_3(e_j)=0$ $(j\in\mathbb{Z})$; then $d(b_3)(\gamma\wedge e_2)=2e_2$. □

We will prove that any 2-cocycle c given by (23), with coefficients satisfying the conditions of the preceding lemma, is equal to zero,

$$d(c)(\gamma\wedge e_{2j}\wedge e_{2k})=2(k-j)(\lambda_{2j+2k}-\lambda_{2j}-\lambda_{2k})e_{2j+2k}+\delta_{j+k,0}2k(2\mu-(k^2-1)(\lambda_{2j}+\lambda_{2k}))\gamma=0, \tag{24}$$

$$d(c)(\gamma\wedge e_{2j-1}\wedge e_{2k})=(k-2j)(\lambda_{2j+2k-1}-\lambda_{2j-1}-\lambda_{2k})e_{2j+2k-1}=0, \tag{25}$$

$$d(c)(\gamma\wedge e_{2j-1}\wedge e_{2j-1})=(\lambda_{4j}-2\lambda_{2j-1})e_{4j}+\delta_{j,0}(\mu+\lambda_{-1})\gamma=0. \tag{26}$$

From the substitution $(j,k)=(-1,1)$ in (24), we obtain $\mu=0$. Then $j=0$ in (26) yields $\lambda_{-1}=0$. From $k=1$ in (25) we conclude $\lambda_{2j-1}=\lambda_{-1}=0$ for all $j\in\mathbb{Z}$. Finally, Eq. (25) implies $\lambda_{2k}=0$ for all $k\in\mathbb{Z}$.

Since the conditions for the coefficients $\alpha_{j,k}$ from Lemma 4 coincide with the conditions in Lemma 3, the proof of the preceding theorem implies that all coefficients $\alpha_{j,k}$ are equal to zero. In order to show that β_k equals zero for all $k\in\mathbb{Z}$, we write out the following two expressions:

$$d(c)(e_{2j}\wedge e_{2k}\wedge e_{-2j-2k})=2\{(k-j)\beta_{2j+2k}-(k+2j)\beta_{2k}+(2k+j)\beta_{2j}\}\gamma=0, \tag{27}$$

$$d(c)(e_{2j-1}\wedge e_{2k-1}\wedge e_{-2j-2k})=\{\beta_{2j+2k}-(k+3j)\beta_{2k-1}-(j+3k)\beta_{2j-1}\}\gamma=0. \tag{28}$$

We take $(j,k)=(1,1)$ in (28) and obtain $\beta_4=0$. Then by inductive use of Eq. (27) we conclude that $\beta_{2k}=0$ for all $k\in\mathbb{Z}$. Finally, $j=1$ in (28) gives $\beta_{2k-1}=0$ for all $k\in\mathbb{Z}$. This completes the proof that any even 2-cocycle of degree zero is a coboundary. □

IV. SOME FINAL REMARKS

The even parts of the Lie superalgebras NS and R are isomorphic to the Virasoro algebra. Therefore one could consider the rigidity proofs of these superalgebras, as extensions of a rigidity proof for the Virasoro algebra. In fact, this is how the presented technique has arisen. This technique can also be used with respect to W algebras, work on this is in progress.

In the introductory part of this paper we mentioned the possibility of deforming Lie superalgebras. A deformation of a Lie superalgebra L is defined by a new commutator on L, which is a power series in a formal parameter, with the zeroth-order term equal to the bracket of L. Since the parameter involved is usually even, it is only the even part of the cohomology group of L that is of interest with respect to the rigidity of L. Nevertheless, one can formally carry out the construction of a deformation of L by using an odd parameter, such deformations are therefore called odd deformations. For details on this we refer to Ref. 8. On account of $\mathbb{Z}$ homogeneity; the cocycle that describes an odd deformation needs to be odd. By consequence, a sufficient condition for the rigidity of a Lie superalgebra with respect to these kinds of odd deformations is that the odd component of its second cohomology group with coefficients in the adjoint module is equal to zero. From Theorems 1 and 2 we learn that $k(1)$ and NS satisfy this condition. We can give proofs similar to the ones given in Theorems 3 and 4, to show that $H^2(k^+(1);k^+(1))_1=0$ and $H^2(R;R)_1=0$. Hence, we can conclude that the Lie superalgebras $k(1)$, $k^+(1)$, NS, and R are also rigid with respect to odd deformations.

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Asymptotics of oscillatory Riemann–Hilbert problems

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A classical method of stationary phase for oscillatory integrals is generalized to oscillatory Riemann–Hilbert problems of the kind arising in the theory of integrable nonlinear equations. The proposed approach is developed for the phase with N first-order stationary points, and the final formulas can immediately be applied to the problem of long-time behavior of the solutions of equations such as the NLS, KdV, mKdV sine-Gordon, and others. © *1996 American Institute of Physics.* [S0022-2488(96)01111-5]

I. INTRODUCTION

It is well known that the Riemann–Hilbert problem (RHP) plays an important role in the study of a certain class of nonlinear evolution equations.[1] In particular, the long-time behavior of the solution of the initial value problem for the evolution equation can be found by finding a viable method of asymptotic analysis of the RHP. A great progress has already been made when that is the 2×2 matrix RHP on the real axis with oscillations in its conjugation matrix: this will also be treated here. However, the results obtained in this paper are more general, and the approach used allows us to formulate these results in the spirit of the method of stationary phase.

The mentioned oscillatory Riemann–Hilbert problem is a search for a matrix $M(\lambda)$ analytic in λ for $\operatorname{Im}\lambda\neq0$, satisfying a conjugation condition on the real axis, and normalized at infinity:

$$M_+(\lambda)=M_-(\lambda)G(\lambda,t),\quad \lambda\in R,$$

$$M(\infty)=I, \tag{1.1}$$

where the jump (conjugation) matrix, $G(\lambda,t)$ is given by

$$G(\lambda,t)=\begin{pmatrix} 1+p(\lambda)q(\lambda) & p(\lambda)e^{-it\theta(\lambda)} \\ q(\lambda)e^{it\theta(\lambda)} & 1 \end{pmatrix}. \tag{1.2}$$

Solving a nonlinear wave equation by the inverse scattering method, one looks for potentials

$$u(t)=\lim_{\lambda\to\infty}\lambda M_{12}(\lambda),\quad v(t)=\lim_{\lambda\to\infty}\lambda M_{21}(\lambda). \tag{1.3}$$

In this paper, we study (1.1) with general phase, assuming that it has N first-order stationary phase points. More precisely, it is supposed that

(A) $p(\lambda)$, $q(\lambda)$ belong to the Schwartz space.

(B) $\theta\in C^\infty(R)$, $\operatorname{Im}\theta(\lambda)=0$, $\theta(\lambda)\sim\lambda^d$ as $\lambda\to\pm\infty$, where d is some integer. The asymptotics are differentiable.

(C) The first derivative of θ vanishes only in points $\lambda_1,\ldots,\lambda_N$, where $\theta''(\lambda_n)\neq0$.

(D) $1+p(\lambda)q(\lambda)>0$ for all $\lambda\in R$.

Conditions A and B can be chosen weaker but we use them in order to simplify formulations of some results. On the contrary, assumptions C and D are strict.

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Theorem: Let conditions A, B, C, and D be satisfied. Then, there is a number t_0 such that the solution of the RHP exists at least for $t \geqslant t_0$. The leading asymptotics of the potentials are given as the sum of contributions from the distinct stationary phase points:

$$u(t)=\sum_{n=1}^{N} u_0^n(t)+O(t^{-3/4}\ln t), \quad v(t)=\sum_{n=1}^{N} v_0^n(t)+O(t^{-3/4}\ln t). \tag{1.4}$$

The functions u_0^n and v_0^n are determined by

$$u_0^n=\frac{i\nu_n}{\varepsilon_n\sqrt{|\nu_n\theta''(\lambda_n)t|}}\frac{p(\lambda_n)}{\sqrt{|p(\lambda_n)q(\lambda_n)|}}\exp\{-it\theta(\lambda_n)-i\nu_n\ln|\theta''(\lambda_n)t|+i\alpha_n(\lambda_1,\ldots,\lambda_N)\}, \tag{1.5a}$$

$$v_0^n=\frac{i\nu_n}{\varepsilon_n\sqrt{|\nu_n\theta''(\lambda_n)t|}}\frac{q(\lambda_n)}{\sqrt{|p(\lambda_n)q(\lambda_n)|}}\exp\{it\theta(\lambda_n)+i\nu_n\ln|\theta''(\lambda_n)t|-i\alpha_n(\lambda_1,\ldots,\lambda_N)\}, \tag{1.5b}$$

where

$$\varepsilon_n=\operatorname{sgn}\theta''(\lambda_n), \quad \nu_n=-\frac{1}{2\pi}\varepsilon_n\ln(1+p(\lambda_n)q(\lambda_n)),$$

and

$$\alpha_n(\lambda_1\cdots\lambda_N)=\varepsilon_n\frac{\pi}{4}+\arg\Gamma(i\nu_n)+\sum_{k=1,k\neq n}^{N}2\nu_k\ln|\lambda_n-\lambda_k| + \frac{1}{\pi}\int_{\theta'(z)<0}\ln|z-\lambda_n|d\ln(1+p(z)q(z))$$

(here Γ is the standard gamma function). Moreover, for $|\operatorname{Im}\lambda|\geqslant a>0$, one has

$$M(\lambda)=\begin{pmatrix} \delta(\lambda) & \delta^{-1}(\lambda)\sum_{n=1}^{N} u_0^n/(\lambda-\lambda_n) \\ \delta(\lambda)\sum_{n=1}^{N} v_0^n/(\lambda-\lambda_n) & \delta^{-1}(\lambda) \end{pmatrix}+O(t^{-3/4}\ln t), \tag{1.6}$$

where

$$\delta(\lambda)=\exp\left\{\frac{1}{2\pi i}\int_{\theta'(z)<0}\frac{\ln(1+p(z)q(z))}{z-\lambda}\,dz\right\}.$$

The order of decay of the corrections in formulas (1.4) and (1.6) is not the best possible one: the estimates for these corrections in (1.4) and (1.6) for the nondiagonal elements of $M(\lambda)$ can be improved to order $t^{-3/2}\ln t$. The error term for the diagonal part of $M(\lambda)$ in (1.6) must be $O(t^{-1}\ln t)$.

The first *direct* method for analyzing the asymptotics of the factorization problem (1.1) was proposed by Its.[2] Its considered the nonlinear Schrödinger equation (NLS) [the phase, $\theta(\lambda)=(\lambda-\lambda_0)^2$, has one stationary point in this case] and showed that problem (1.1) could be reduced, up to small errors which decay as $t\to\infty$, to a model RHP, which in turn was explicitly

solvable. The extension of those ideas to the phase with more then one stationary point led to the necessity of involving the technique (which is quite difficult itself) from the theory of isomonodromic deformations.[3]

The second was presented by Deift and Zhou[4] who investigated the modified Korteweg–de Vries equation (mKdV). The phase, $\theta(\lambda)=4(\lambda^3-3\lambda_0^2\lambda)$, has two stationary points in this case. They separated the contribution from the distinct stationary phase points and derived the model RH problem by deforming contours in the spirit of the classical method of steepest descent. In other words, they reduced the situation with two stationary phase points to the situation with one stationary phase point. The Deift–Zhou procedure is a general and rigorous approach to analyzing oscillatory RHPs of the form (1.1).

We emphasize that only the direct approaches to (1.1) have been described, i.e., those not involving *a priori* ansatz for the asymptotic form of the solution of an integrable nonlinear equation (the further references can be found in Refs. 3 and 4). We mention also that formulas (1.4) and (1.5) have already appeared in the literature[5] but as a hypothesis.

Before describing the background of this paper and its relationship with earlier works, let us recall the classical theory of oscillatory integrals. Note that if $p(\lambda)=0$, we derive that

$$v(t)=\frac{i}{2\pi}\int_{-\infty}^{\infty} q(\lambda)e^{it\theta(\lambda)}\,d\lambda, \quad u(t)=0. \tag{1.7}$$

For studying (1.7) there exist two commonly known approaches: the method of steepest descent and the method of stationary phase. The main idea of the first is an appropriate deformation of the contour of integretion. This method can be applied only if q and θ are analytic, but it may give more detailed information about the asymptotic behavior of (1.7) and can be used when the contour is not the real axis. The method of stationary phase is based on integration by parts and is applicable when q and θ are smooth functions. In this paper, we advocate the point of view that all results obtained for oscillatory integrals can be generalized to oscillatory RHPs (1.1). Indeed, it has been shown by the authors of Ref. 4 that one can investigate (1.1) by deforming the conjugation contour of (1.1). It is worth mentioning that in Ref. 4 a special technique of rational approximations of q was developed to include not only analytic q. The theorem posed in this Introduction establishes a result which, in the classical theory, is stated by the method of stationary phase. It is interesting to note that formulas (1.4) and (1.5) become classical if one passes to the limit $p\to 0$ and takes into account that the potentials in this case are given by (1.7).

The present paper is closely related to Refs. 2 and 4. We proceed by conjugating the original RHP (1.1) to

$$\begin{gathered} M_+^{\Phi}(\lambda)=M_-^{\Phi}(\lambda)\Phi_-^{-1}(\lambda)G(\lambda,t)\Phi_+(\lambda), \quad \lambda\in R, \\ M^{\Phi}(\infty)=I, \end{gathered} \tag{1.1}$$

where piecewise analytical matrix function Φ is constructed explicitly: this is a way of Ref. 2 as well. The transformation (1.8) is employed both to localize the problem and to derive the model RHP. The latter was introduced in Ref. 2. The scheme of proof in the method of Ref. 2 was not developed rigorously. As it was demonstrated in Ref. 4, the most successful way for justification of asymptotics is to use the operator approach to the RHP of Beals and Coifman.[6] This is also applied here in a manner similar to Ref. 4, however, on the basis of completely different estimates.

As a final remark, we say a few words on the relationship between the steepest descent method and the method of stationary phase. Suppose it is desired to evaluate an integral

$$I(t)=\int_a^b q(\lambda)e^{it\theta(\lambda)}\,d\lambda$$

as $t\to\infty$, where $q(\lambda)$ and $\theta(\lambda)$ are smooth, and $\theta(\lambda)$ is real. If $q(\lambda)$ is analytic, and $\theta(\lambda)$ is real analytic, and if, in addition, for some (small) $\varepsilon>0$,

$$\text{Im } \theta(\lambda)>0 \quad \text{for } a<\text{Re } \lambda<b, \quad 0<\text{Im } \lambda<\varepsilon, \tag{1.8}$$

then the above integral can be deformed to an integral on a contour lying in $a<\text{Re}\,\lambda<b$, $0<\text{Im}\,\lambda<\varepsilon$. But then $\text{Re}\, i\theta(\lambda)<0$, and as $t\to\infty$, the leading contributions to $I(t)$ clearly arises from small neighborhoods of a and b. These observations, in particular, are taken for the ground of the method in Ref. 4.

Now as $\theta(\lambda)$ is real analytic, it follows from (1.8) and the Cauchy–Riemann equations that

$$\theta'(\lambda)=\frac{\partial \text{ Re } \theta}{\partial(\text{Re } \lambda)}(\lambda)=\frac{\partial \text{ Im } \theta}{\partial(\text{Im } \lambda)}(\lambda)>0,$$

and hence as $\theta'(\lambda)\neq 0$ in (a,b) one can evaluate $I(t)$ asymptotically simply integrating by parts on the real axis. In other words analyticity is not needed to evaluate $I(t)$ as $t\to\infty$: all that is needed are familiar to (1.8) conditions on the signature of $\theta'(\lambda)$ on appropriate subintervals of R. This is the basis of the method in the present paper.

II. THE SCALAR RIEMANN–HILBERT PROBLEM

In this section, we discuss the properties of the solution of the scalar factorization problem:

$$\begin{gathered}\delta_+(\lambda)=\delta_-(\lambda)(1+p(\lambda)q(\lambda)), \quad \lambda\in D_-,\\ \delta_+(\lambda)=\delta_-(\lambda), \quad \lambda\in D_+,\\ \delta(\infty)=1,\end{gathered} \tag{2.1}$$

where

$$D_+=\{\lambda:\lambda\in R,\theta'(\lambda)>0\}, \quad D_-=\{\lambda:\lambda\in R,\theta'(\lambda)<0\}. \tag{2.2}$$

The role of $\delta(\lambda)$ will be made clear in the sequel.

The problem (2.1) has a unique solution in the class of bounded functions. It is given by the following formula:

$$\ln\,\delta(\lambda)=\frac{1}{2\pi i}\int_{D_-}\frac{\ln(1+p(\lambda)q(\lambda))}{z-\lambda}\,dz. \tag{2.3}$$

Standard theorems concerning singular integrals reveal that $\delta_\pm$ are smooth functions in the domain $D_+\cup D_-$. The preceding as well as following statements are a consequence of conditions A and D.

Assume for the moment that

$$\nu(\lambda)=-\frac{1}{2\pi}\ln(1+p(\lambda)q(\lambda)) \tag{2.4}$$

is analytic in some small neighborhood of the stationary phase point λ_n. Then, one can verify calculating the jump on the left-hand side of

$$\ln\,\delta(\lambda)-i\varepsilon_n\nu(\lambda)\ln(\varepsilon_n(\lambda-\lambda_n))=\Lambda(\lambda) \tag{2.5}$$

that Λ is analytic in a neighborhood of λ_n. We choose the principle branch of the logarithm, and ε_n denotes sgn $\theta''(\lambda_n)$.

Now, consider the general case. Let $\varphi(\lambda)$ be a finite function whose support contains only one stationary phase point λ_n and $\varphi(\lambda)=1$ if $|\lambda-\lambda_n|\leqslant r, r>0$. Furthermore, split $\nu(\lambda)$ as follows:

$$\begin{gathered}\nu(\lambda)=\nu^1(\lambda)\varphi(\lambda)+(\nu(\lambda)-\nu^1(\lambda))\varphi(\lambda)+\nu(\lambda)(1-\varphi(\lambda)),\\ \nu^1(\lambda)=\sum_{k=0}^{m+1}\frac{\nu^{(k)}(\lambda_n)}{k!}(\lambda-\lambda_n)^k.\end{gathered}\tag{2.6}$$

Divide (2.3) into three Cauchy integrals in accordance with (2.6). The density of the third Cauchy integral is zero when $z\in I_n$ (I_n denotes the interval $|z-\lambda_n|<r$), hence analytic in the circle $|\lambda-\lambda_n|<r$. The density of the second Cauchy integral can be extended by zero from $D_-\cap I_n$ to I_n: the extension belongs to $C^{m+1}(I_n)$. Therefore, this integral produces the piecewise analytic function whose boundary values are in $C^m(I_n)$. The first term in (2.6) is analytic in the circle $|\lambda-\lambda_n|<r$. Thus (2.5) and (2.6) give rise to the proceeding representation for $\delta(\lambda)$ in a small neighborhood of λ_n:

$$\ln\,\delta(\lambda)=i\varepsilon_n\nu^1(\lambda)\ln\,\varepsilon_n(\lambda-\lambda_n)+\Lambda^1(\lambda).\tag{2.7}$$

In (2.7), Λ^1 is analytic for $\operatorname{Im}\lambda\neq 0$, $|\lambda-\lambda_n|<r$, and its boundary values, $\Lambda^1_\pm$, belong to $C^m(I_n)$. Note also that

$$\Lambda^1_+(\lambda_n)=\Lambda^1_-(\lambda_n)\equiv i\gamma(\lambda_n).\tag{2.8}$$

From (2.7) it is easy to see that the local behavior of $\delta(\lambda)$ at λ_n is described by

$$\begin{gathered}\delta^{\,n}(\lambda)=(\lambda-\lambda_n)^{i\nu_n}\varepsilon_n^{i\nu_n}e^{i\gamma(\lambda_n)},\quad -\pi<\arg\,\varepsilon_n(\lambda-\lambda_n)<\pi,\\ \nu_n=\varepsilon_n\nu(\lambda_n)\equiv\operatorname{sgn}\,\theta''(\lambda_n)\nu(\lambda_n).\end{gathered}\tag{2.9}$$

We summarize the results as follows:

Proposition 2.1: Let $\delta(\lambda)$ be a solution of (2.1) in the class of bounded functions. Then,

(1) it is unique, and $\delta_\pm$ are smooth functions in $D_+\cup D_-$, and

(2) in a sufficiently small neighborhood of the stationary phase point λ_n, the following estimates are valid:

$$\left|\frac{d^k}{d\lambda^k}\,\delta_\pm(\lambda)\right|\leqslant\frac{C}{|\lambda-\lambda_n|^k},\tag{2.10}$$

$$|\delta(\lambda)-\delta^n(\lambda)|\leqslant C|\lambda-\lambda_n|\ln|\lambda-\lambda_n|.\tag{2.11}$$

A simple way to derive an explicit expression for $\gamma(\lambda_n)$ is to obtain it through

$$e^{2i\gamma(\lambda_n)}=\lim_{\lambda\to\lambda_n}|\lambda-\lambda_n|^{-2i\nu_n}\delta_+(\lambda)\delta_-(\lambda).\tag{2.12}$$

Direct calculations lead to

$$\gamma(\lambda_n)=\sum_{k=1,k\neq n}^{N}\nu_k\,\ln|\lambda_n-\lambda_k|+\frac{1}{2\pi}\int_{D_-}\ln|z-\lambda_n|d\,\ln(1+p(z)q(z)).\tag{2.13}$$

Here we have used the fact that

$$\ln\ \delta_+(\lambda)\delta_-(\lambda)=\sum_{k=1}^{N} 2i\nu_k \ln|\lambda-\lambda_k|-2i\int_{D_-} \ln|z-\lambda|\,d\nu(z). \tag{2.14}$$

Identity (2.14) is found by integration by parts.

In later sections, we shall thoroughly investigate the piecewise analytic matrix

$$m(\lambda)=M(\lambda)e^{-\sigma_3 \ln \delta(\lambda)}. \tag{2.15}$$

It satisfies the following factorization problem:

$$m_+(\lambda)=m_-(\lambda)(b^-)^{-1}b^+, \quad m(\infty)=I, \tag{2.16}$$

where $b^{\pm}$ are triangular matrices,

$$b^+(\lambda)=\begin{pmatrix} 1 & 0 \\ \overline{\rho(\lambda,t)} & 1 \end{pmatrix}, \quad b^-(\lambda)=\begin{pmatrix} 1 & -\rho(\lambda,t) \\ 0 & 1 \end{pmatrix} \tag{2.17a}$$

if $\lambda\in D_+$,

$$b^+(\lambda)=\begin{pmatrix} 1 & \rho(\lambda,t) \\ 0 & 1 \end{pmatrix}, \quad b^-(\lambda)=\begin{pmatrix} 1 & 0 \\ -\overline{\rho(\lambda,t)} & 1 \end{pmatrix} \tag{2.17b}$$

if $\lambda\in D_-$. Here, we have introduced the notations:

$$\rho(\lambda,t)=p(\lambda)\delta_+(\lambda)\delta_-(\lambda)e^{-it\theta(\lambda)}, \quad \overline{\rho(\lambda,t)}=q(\lambda)\delta_+^{-1}(\lambda)\delta_-^{-1}(\lambda)e^{it\theta(\lambda)}. \tag{2.18}$$

It is clear that one may find the potentials, u and v, through the solutions of (2.16) by the same formulas (1.3) with $m(\lambda)$ in place of $M(\lambda)$.

III. OPERATOR FORMULATION OF THE RHP

As in Ref. 4 we shall employ the method of Beals and Coifman[6] in order to construct the singular integral equation associated with (2.16). It will be the basis for later proofs. All the results in this section can be found in Ref. 6. They are given here merely for convenience of subsequent use.

We begin with classical properties of Cauchy operators,

$$(C_\pm f\ )(\lambda)=\frac{1}{2\pi i}\lim_{\varepsilon\to 0}\int_{-\infty}^{\infty}\frac{f(z)}{z-(\lambda\pm i\varepsilon)}\,dz, \quad \varepsilon>0. \tag{3.1}$$

A natural way of treating $C_\pm$ is to regard them as operators in $L_2(R)$. The Fourier transform gives

$$(C_\pm f\ )(\lambda)=\pm\int_{-\infty}^{\infty}\hat{f}(s)H(\mp s)e^{-is\lambda}\,ds, \tag{3.2}$$

where $H(s)$ is the Heavyside unit symbol. It follows trivially from (3.2) that $\pm C_\pm$ are bounded operators from $L_2(R)$ to $L_2(R)$; moreover, they are mutually complementary orthogonal projection operators.

Introduce

$$C_w f=C_+(fw^-)+C_-(fw^+), \tag{3.3}$$

where

$$w^{\pm}=\pm(b^{\pm}-I) \tag{3.4}$$

and

$$w=w^{+}+w^{-}. \tag{3.5}$$

The operator C_w in (3.3) acts on the space of 2×2 matrix-valued functions. It is understood throughout the article that the L_2 and L_∞-norms, respectively, in this space are conventionally given by

$$\|f\|^2_{L_2(R)}=\int_{-\infty}^{\infty}\text{trace } ff^{*}\, d\lambda, \quad \|f\|_{L_\infty(R)}=\sup_{\lambda}|f(\lambda)|,$$

and $|f|$ denotes $\max_{ij}|f_{ij}|$. The matrices $w^{\pm}$ are ambiguously determined by the jump matrix of the RHP. However, we shall call them the data of the RHP, pointing out explicitly the chosen factorization of the jump matrix.

Let μ be a solution of the basic integral equation

$$\mu=I+C_w\mu. \tag{3.6}$$

If the solution of Eq. (3.6) exists, then one defines the solution of RHP (2.16) as

$$m(\lambda)=I+\frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{\mu(z)w(z)}{z-\lambda}\,dz. \tag{3.7}$$

Indeed, simple calculations show that

$$m_{\pm}(\lambda)=I+C_{\pm}(\mu w^{+})+C_{\pm}(\mu w^{-})=\pm\mu w^{\pm}+I+C_w\mu=\mu(I\pm w^{\pm})=\mu b^{\pm}(\lambda), \tag{3.8}$$

which implies (2.16). It is not necessary, but sufficient, to suppose that $w^{\pm}\in L_2(R)\cap L_\infty(R)$. Then, C_w is a bounded map from $L_\infty(R)$ to $L_2(R)$; hence, $C_w(I)\in L_2(R)$,

$$\|C_w(I)\|_{L_2(R)}\leqslant\|w^{-}\|_{L_2(R)}+\|w^{+}\|_{L_2(R)}. \tag{3.9}$$

This fact, along with the uniqueness of the solution of the RHP, reveals that Eq. (3.6) has a unique solution if $id-C_w$ is invertible as an operator from $L_2(R)$ to $L_2(R)$. As an operator in $L_2(R)$, C_w has norm dominated by

$$\|C_w\|\leqslant\|w^{-}\|_{L_\infty}\|C_{+}\|+\|w^{+}\|_{L_\infty}\|C_{-}\|\leqslant\|w^{-}\|_{L_\infty}+\|w^{+}\|_{L_\infty}. \tag{3.10}$$

In particular, the solution of the RHP exists when $\|w^{-}\|_{L_\infty}+\|w^{+}\|_{L_\infty}<1$. In addition, note that if Eq. (3.6) has a solution μ, then $\mu-I\in L_2(R)$.

Examine the question of what happens if the factorization data of the jump matrix $(b^{\pm})$ are changed. Set $b^{\pm}=Ub'^{\pm}$, where the matrix U is invertable. Then one has the following relation:[7]

$$(id-C_w)=(id-C_{w'})\hat{U}, \tag{3.11}$$

here $\hat{U}$ is an operator of right multiplication by U $(\hat{U}f=fU)$. In fact,

$$\begin{aligned}(id-C_{w'})\hat{U}f&=fU-C_{+}(fU(I-b'^{-}))+C_{-}(fU(I-b'^{+}))\\&=fU-C_{+}(f(U-b^{-}))-C_{-}(f(b^{+}-U))\\&=f-C_{+}(fw^{-})-C_{-}(fw^{+})=(id-C_w)f.\end{aligned}$$

IV. LOCALIZATION PRINCIPLE

In this section, we shall show that only small neighborhoods of the stationary phase points give an essential contribution to the potentials. This fact will help us to reduce the original Riemann–Hilbert problem to some RHPs with one stationary phase point. First, we shall discuss some asymptotic properties of singular integrals. The method of stationary phase based on integration by parts[8] is the most useful for this purpose.

Lemma 1: Let $f\in C^{2k-1}(R)$, $k>1$, and

(1) supp $f\subset D_+$ or supp $f\subset D_-$.

Suppose also that for any set of non-negative integers β, α_i such that $\Sigma_{m=0}^{n}\ \alpha_m=\Sigma_{m=0}^{n}\ m\alpha_m=n-\beta$,

(2) $f^n_{\beta,\alpha_0,\ldots,\alpha_n}\to 0$ as $\lambda\to\pm\infty$, $n<k$.

(3) $f^k_{\beta,\alpha_0,\ldots,\alpha_k}|\theta'|^d\in L_1$ at $\pm\infty$, $d=1,\ \frac{1}{2}$, where $f^n_{\beta,\alpha_0,\ldots,\alpha_n}=|f^{(\beta)}||\theta'|^{\beta+d-2n}|\theta'|^{\alpha_0}\cdots|\theta^{(n+1)}|^{\alpha_n}$. Then,

$$\lim_{\varepsilon\to 0}\frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{f(z)e^{it\theta(z)}}{z-(\lambda+i\varepsilon)}\,dz=\operatorname{sgn}\varepsilon H(\operatorname{sgn}\varepsilon\theta'(\lambda))f(\lambda)e^{it\theta(\lambda)}+I_0(\lambda),\tag{4.1}$$

where $H(\lambda)$ is the Heavyside unit symbol, and for $I_0(\lambda)$, one has the estimates

$$\|I_0\|_{L_\infty(R)}\leqslant\frac{C}{t^{k-1}},\quad \|I_0\|_{L_2(R)}\leqslant\frac{C}{t^{k-1/2}}.\tag{4.2}$$

Proof: It is sufficient to prove the lemma for supp $f\subset D_+$, since the proof when supp $f\subset D_-$ is similar. It is enough to prove the result for $\varepsilon<0$, since for $\varepsilon>0$ it follows immediately from the fact that $\pm C_\pm$ are complementary orthogonal projection operators.

Represent the left-hand side of (4.1) in the form (3.2):

$$I_0(\lambda)=\frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{f(z)e^{it\theta(z)}}{z-(\lambda-i0)}\,dz=-\int_0^{\infty}\hat f_t(s)e^{-is\lambda}\,ds.$$

Applying integration by parts, we get

$$\hat f_t(s)=\frac{1}{2\pi}\int_{-\infty}^{\infty}f(\lambda)e^{it\theta(\lambda)+is\lambda}\,d\lambda=\frac{(-1)^k}{2\pi i^k}\int_{-\infty}^{\infty}f_k(\lambda,s,t)e^{it\theta(\lambda)+is\lambda}\,d\lambda,$$

where

$$f_k(\lambda,s,t)=\frac{d}{d\lambda}\left(\frac{1}{\omega(\lambda)}\,f_{k-1}(\lambda,s,t)\right),\quad f_0(\lambda)=f(\lambda),$$

$$\omega(\lambda)=t\theta'(\lambda)+s>0\quad\text{for}\quad\lambda\in\operatorname{supp}f,\quad s>0.$$

Note that

$$f_k(\lambda,s,t)=\sum_{\beta=0}^{k}f^{(\beta)}(\lambda)\omega^{\beta-2k}C^k_\beta(\omega,\omega',\ldots,\omega^{(k)}),$$

where C^k_β are homogeneous polynomials of order $k-\beta$ whose coefficients, $C^k_{\beta\alpha_0\cdots\alpha_k}\omega^{\alpha_0}\cdots(\omega^{(k)})^{\alpha_k}$, are nonzero only if $\Sigma^k_{m=0}m\alpha_m=k-\beta$. We now use the Minkowski integral inequality,

$$\left(\int_0^\infty |\hat{f}_t(s)|^p \, ds \right)^{1/p} \leqslant \frac{1}{2\pi} \int_{-\infty}^{\infty} d\lambda \left(\int_0^\infty ds |f_k(\lambda,s,t)|^p \right)^{1/p}. \tag{4.3}$$

Since $\omega^{(m)}$ does not depend on s for $m>0$, the first integral on the right-hand side of (4.3) can be easily calculated; one derives

$$\|I_0\|_{L_\infty} \leqslant \int_0^\infty |\hat{f}_t(s)| ds \leqslant \frac{1}{t^{k-1}} \frac{1}{2\pi} \frac{1}{k-1} \sum_{\beta=0}^{k} \int_{-\infty}^{\infty} |f^{(\beta)}(\lambda)| |\theta'(\lambda)|^{\beta+1-2k} |C_\beta^k(\lambda)| d\lambda,$$

$$\|I_0\|_{L_2} = \sqrt{2\pi} \left(\int_0^\infty |\hat{f}_t(s)|^2 ds \right)^{1/2} \leqslant \frac{1}{t^{k-1/2}} \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{2k-1}} \sum_{\beta=0}^{k} \int_{-\infty}^{\infty} |f^{(\beta)} \times (\lambda)| |\theta'(\lambda)|^{\beta+1/2-2k} |C_\beta^k(\lambda)| d\lambda.$$

In the above inequalities, $|C_\beta^k(\lambda)|$ denote $\Sigma_{\alpha_0 \cdots \alpha_k} |C^k_{\beta\alpha_0\cdots\alpha_k}| |\theta'(\lambda)|^{\alpha_0} |\theta''(\lambda)|^{\alpha_1} \cdots |\theta^{(k+1)}(\lambda)|^{\alpha_k}$. The lemma is evident.

To separate the contributions from the distinct stationary phase points, we shall employ a partition of unity:

$$\sum_{n=1}^{N} \varphi_n(\lambda) + \varphi(\lambda) + \psi(\lambda) = 1,$$

where φ, ψ, $\varphi_n \in C^\infty(R)$, $\varphi_n(\lambda)=1$ if $|\lambda-\lambda_n| \leqslant 3\epsilon/4$, $\varphi_n(\lambda)=0$ if $|\lambda-\lambda_n|>\epsilon$, supp $\varphi \subset D_+$, supp $\varphi \subset D_-$, and ϵ is some positive number such that there is only one stationary phase point λ_n in supp φ_n.

Set

$$\begin{aligned} \rho_\pm^\varphi &= C_\pm(\varphi\rho), \quad \rho_\pm^\psi = C_\pm(\psi\rho), \\ \overline{\rho}_\pm^{\,\varphi} &= C_\pm(\varphi\overline{\rho}), \quad \overline{\rho}_\pm^{\,\psi} = C_\pm(\psi\overline{\rho}). \end{aligned} \tag{4.4}$$

One can apply Lemma 1 to (4.4). Indeed, Proposition 2.1 shows that $\varphi\rho$, $\psi\rho$, $\varphi\overline{\rho}$, and $\psi\overline{\rho}$ are smooth functions whose supports are in D_+ or D_-. Conditions A and B imposed on θ, p, and q make premises (2) and (3) of the lemma fulfilled as well. It is convenient to summarize the properties of (4.4) as follows:

Proposition 4.1: For any given k, there are constants $C(k)$ independent on t such that

$$\rho_-^\varphi = -\rho\varphi + \rho_+^\varphi, \quad \|\rho_+^\varphi\| \leqslant \frac{C(k)}{t^k}, \quad \rho_+^\psi = \rho\psi + \rho_-^\psi, \quad \|\rho_-^\psi\| \leqslant \frac{C(k)}{t^k},$$

$$\overline{\rho}_+^{\,\varphi} = \overline{\rho\varphi} + \overline{\rho}_-^{\,\varphi}, \quad \|\overline{\rho}_-^{\,\varphi}\| \leqslant \frac{C(k)}{t^k}, \quad \overline{\rho}_-^{\,\psi} = -\overline{\rho\psi} + \overline{\rho}_+^{\,\psi}, \quad \|\overline{\rho}_+^{\,\psi}\| \leqslant \frac{C(k)}{t^k}.$$

Here, $\|\rho\|$ denotes the L_∞- or L_2-norms.

Suppose that $m^L(\lambda)$ is a solution of the RHP

$$m_+^L(\lambda) = m_-^L(\lambda)(b_L^-)^{-1} b_L^+, \quad m^L(\infty) = I, \tag{4.5}$$

where $b_L^{\pm}$ are related to the data $w_L^{\pm}$ given by $w_L^{\pm}=\Sigma_{n=1}^{N}\varphi_n w^{\pm}$ [see (3.4)]. It is clear that these data are not zero only in neighborhoods of the stationary phase points. In the following sections, we shall prove that the operator $id - C_{w_L}$ associated with (4.5) is invertible as an operator in L_2 if t is large enough, and the norm of its inverse is bounded when $t\to\infty$.

Proposition 4.2: There is a number t_0 such that the solution of the RHP (2.16) exists at least for $t\geqslant t_0$. Moreover, for any given k, one has

$$|m(\lambda)-m^L(\lambda)|\leqslant\frac{C(k)}{t^k}\quad\text{if } |\mathrm{Im}\,\lambda|\geqslant a>0, \tag{4.6}$$

and

$$u(t)=u^L(t)+O\left(\frac{1}{t^k}\right),\quad v(t)=v^L(t)+O\left(\frac{1}{t^k}\right). \tag{4.7}$$

Proof: Introduce the piecewise analytical matrix function

$$\Phi(\lambda)=\begin{pmatrix}1 & 0\\ -\overline{\rho}^{\varphi}_{+}(\lambda) & 1\end{pmatrix}\begin{pmatrix}1 & -\rho^{\psi}_{+}(\lambda)\\ 0 & 1\end{pmatrix},\quad \mathrm{Im}\,\lambda>0,$$

$$\Phi(\lambda)=\begin{pmatrix}1 & -\rho^{\varphi}_{-}(\lambda)\\ 0 & 1\end{pmatrix}\begin{pmatrix}1 & 0\\ -\overline{\rho}^{\psi}_{-}(\lambda) & 1\end{pmatrix},\quad \mathrm{Im}\,\lambda<0.$$

Because $|\Phi(\lambda)-I|\leqslant Ct^{-k}$ when $|\mathrm{Im}\,\lambda|\geqslant a>0$, it is sufficient to prove the results for matrix

$$m^{\Phi}(\lambda)=m(\lambda)\Phi(\lambda), \tag{4.8}$$

which satisfies the factorization problem

$$\begin{gathered}m^{\Phi}_{+}(\lambda)=m^{\Phi}_{-}(\lambda)(b^{-}_{\Phi})^{-1}b^{+}_{\Phi},\quad b^{\pm}_{\Phi}=b^{\pm}\Phi_{\pm},\\ m^{\Phi}(\infty)=I.\end{gathered} \tag{4.9}$$

It follows from Proposition 4.1 that the data of the RHP (4.9) can be decomposed in the form

$$w^{\pm}_{\Phi}=w^{\pm}_{L}+w^{\pm}_{R}, \tag{4.10}$$

where $w_R^{\pm}$ are small in the sense of the L_2- or L_∞-norms, viz.,

$$\|w^{\pm}_{R}\|_{L_\infty(R)},\|w^{\pm}_{R}\|_{L_2(R)}\leqslant\frac{C}{t^k}. \tag{4.11}$$

The basic integral equation,

$$\mu^{\Phi}=I+C_{w_\Phi}\mu^{\Phi}, \tag{4.12}$$

can be equivalently rewritten as

$$\begin{gathered}A(\mu^{\Phi}-\mu^{L})=(id-C_{w_L})^{-1}C_{w_R}\mu^{L},\\ A=id-(id-C_{w_L})^{-1}C_{w_R},\end{gathered} \tag{4.13}$$

provided that $id - C_{w_L}$ is invertible. The norm of C_{w_R} converges to zero as $t\to\infty$. Therefore, the operator A has an inverse if t is large enough. This leads to the desired existence of the solution of (4.12) and hence of (4.9).

From (3.7) and (4.10), one has

$$m^{\Phi}(\lambda)-m^{L}(\lambda)=\frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{w_R(z)}{z-\lambda}\,dz+\frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{(\mu^{\Phi}-\mu^{L})w_{\Phi}}{z-\lambda}\,dz+\frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{(\mu^{L}-I)w_R}{z-\lambda}\,dz, \tag{4.14}$$

and for $|\mathrm{Im}\,\lambda|\geqslant a>0$

$$|m^{\Phi}(\lambda)-m^{L}(\lambda)|\leqslant C\{\|w_R\|_{L_2}+\|\mu^{\Phi}-\mu^{L}\|_{L_2}\|w_{\Phi}\|_{L_2}+\|\mu^{L}-I\|_{L_2}\|w_R\|_{L_2}\}. \tag{4.15}$$

Inserting (4.11) and the estimate

$$\|\mu^{\Phi}-\mu^{L}\|_{L_2}\leqslant C(\|w_R^{+}\|_{L_2}+\|w_R^{-}\|_{L_2}+(\|w_R^{+}\|_{L_\infty}+\|w_R^{-}\|_{L_\infty})\|\mu^{L}-I\|_{L_2}), \tag{4.16}$$

which is a consequence of (4.13), in (4.15), one derives (4.6).

To complete the proof, observe that

$$w_R=\begin{pmatrix}0 & \rho_{+}^{\varphi}-\rho_{-}^{\psi}\\ \overline{\rho_{+}^{\psi}}-\overline{\rho_{-}^{\varphi}} & 0\end{pmatrix}+w_I. \tag{4.17}$$

In the splitting of (4.17), each element of w_I belongs to $L_1(R)$ as a sum of the functions like $\rho\varphi\overline{\rho_{+}^{\psi}},\rho_{+}^{\varphi}\overline{\rho_{+}^{\psi}}\cdots$; its L_1-norm is dominated by $\|\rho_{+}^{\varphi}\|_{L_2}+\|\rho_{-}^{\psi}\|_{L_2}+\|\overline{\rho_{+}^{\varphi}}\|_{L_2}+\|\overline{\rho_{-}^{\psi}}\|_{L_2}\leqslant C(k)t^{-k}$. Multiply (4.14) by λ and pass to the limit $\lambda\to\infty$. In the process of estimating this limit, only the first term of (4.14) is troublesome. However, note that

$$\frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{w^{R}-w^{I}}{z-\lambda}\,dz=\begin{pmatrix}0 & \rho_{+}^{\varphi}(\lambda)\\ \overline{\rho_{+}^{\psi}}(\lambda) & 0\end{pmatrix},$$

if $\mathrm{Im}\,\lambda\geqslant 0$. The above formula and analogous one for $\mathrm{Im}\,\lambda\leqslant 0$, together with (4.17), say that

$$\left|\lim_{\lambda\to\infty}\frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{\lambda w^{R}(z)}{z-\lambda}\,dz\right|\leqslant\frac{C}{t^{k}},\quad \mathrm{Im}\,\lambda\neq 0.$$

Now, the asymptotics of (4.7) are evident.

The proof of Proposition 4.2 illuminates the reason why the original RHP (1.1) was conjugated to the RHP (2.16) in which the jump matrix had factorization (2.17). To have a better grasp of that, it is useful to review the proof for the phase with no stationary points. Let $\theta'(\lambda)>0$ for definiteness. Then, one must choose the factorization (2.17a). Split $\rho(\overline{\rho})$ in the form $\rho=\rho_{+}-\rho_{-}$ $(\overline{\rho}=\overline{\rho_{+}}-\overline{\rho_{-}})$. Since ρ_{+}, $\overline{\rho_{-}}$ are small while $\rho_{-}(\overline{\rho_{+}})$ can be incorporated into m_{-} (m_{+}), we conclude that $\Phi(\psi=0)$ is an approximating solution of (2.16), and the potentials decrease to higher order in t.

In the rest of this section, we pursue the study of oscillatory singular integrals. Before formulating our results, let us introduce some notations. Set

$$\begin{aligned}\rho_n&=p(\lambda_n)e^{-it\theta(\lambda_n)}\delta_{+}^{n}(\lambda)\delta_{-}^{n}(\lambda)e^{-it\varepsilon_n\kappa_n(\lambda-\lambda_n)^2},\\ \overline{\rho_n}&=q(\lambda_n)e^{it\theta(\lambda_n)}(\delta_{+}^{n}(\lambda))^{-1}(\delta_{-}^{n}(\lambda))^{-1}e^{it\varepsilon_n\kappa_n(\lambda-\lambda_n)^2},\end{aligned} \tag{4.18}$$

and

$$h(\lambda)=H(\varepsilon_n(\lambda-\lambda_n)),\quad e(\lambda)=H(-\varepsilon_n(\lambda-\lambda_n)), \tag{4.19}$$

where $\kappa_n=\frac{1}{2}|\theta''(\lambda_n)|$ and $\epsilon_n=\operatorname{sgn}\theta''(\lambda_n)$. Then, define

$$\begin{aligned}&\rho_{\pm}^{h}=C_{\pm}((\rho\varphi_n-\rho_n)h),\quad \rho_{\pm}^{e}=C_{\pm}((\rho\varphi_n-\rho_n)e),\\ &\overrightarrow{\rho}_{\pm}^{h}=C_{\pm}((\overrightarrow{\rho\varphi}_n-\overrightarrow{\rho_n})h),\quad \overrightarrow{\rho}_{\pm}^{e}=C_{\pm}((\overrightarrow{\rho\varphi}_n-\overrightarrow{\rho_n})e).\end{aligned} \tag{4.20}$$

Proposition 4.3:

$$\rho_{-}^{h}=-(\rho\varphi_n-\rho_n)h+\rho_{+}^{h},\quad \|\rho_{+}^{h}\|_{L_\infty}\leqslant Ct^{-1/2}\ln t,\quad \|\rho_{+}^{h}\|_{L_2}\leqslant Ct^{-3/4}\ln t,$$

$$\rho_{+}^{e}=(\rho\varphi_n-\rho_n)e+\rho_{-}^{e},\quad \|\rho_{-}^{e}\|_{L_\infty}\leqslant Ct^{-1/2}\ln t,\quad \|\rho_{-}^{e}\|_{L_2}\leqslant Ct^{-3/4}\ln t,$$

$$\overrightarrow{\rho}_{+}^{h}=(\overrightarrow{\rho\varphi}_n-\overrightarrow{\rho_n})h+\overrightarrow{\rho}_{-}^{h},\quad \|\overrightarrow{\rho}_{-}^{h}\|_{L_\infty}\leqslant Ct^{-1/2}\ln t,\quad \|\overrightarrow{\rho}_{-}^{h}\|_{L_2}\leqslant Ct^{-3/4}\ln t,$$

$$\overrightarrow{\rho}_{-}^{e}=-(\overrightarrow{\rho\varphi}_n-\overrightarrow{\rho_n})e+\overrightarrow{\rho}_{+}^{e},\quad \|\overrightarrow{\rho}_{+}^{e}\|_{L_\infty}\leqslant Ct^{-1/2}\ln t,\quad \|\overrightarrow{\rho}_{+}^{e}\|_{L_2}\leqslant Ct^{-3/4}\ln t.$$

Proof: We prove the estimates for ρ_{-}^{e} in the case when $\varepsilon_n=-1$, because the proofs for the other estimates are similar. Notice that $\rho\varphi_n$ can be rewritten for $\lambda-\lambda_n\geqslant 0$ in the form

$$\rho\varphi_n=\varphi_n e^{-it\theta}\delta_{+}^{2}r,\quad r(\lambda)=\frac{p(\lambda)}{1+p(\lambda)q(\lambda)}.$$

Set

$$\rho^{1}\varphi_n=\varphi_n e^{-it\theta}\delta_{+}^{2}r^{1},\quad r^{1}(\lambda)=\sum_{m=0}^{3}\frac{r^{(m)}(\lambda_n)}{m!}(\lambda-\lambda_n)^m.$$

Since

$$\rho\varphi_n-\rho^{1}\varphi_n=\operatorname{Re}^{-it\theta},\quad R(\lambda)=\varphi_n(\lambda)\,\delta_{+}^{2}(\lambda)(r(\lambda)-r^{1}(\lambda)),$$

$e(\lambda)R(\lambda)$ belongs to $C^{3}(R)$ [because of (2.10)], and $\operatorname{supp} eR\subset D_{-}$, Lemma 1 yields

$$\|C_{-}((\rho-\rho^{1})\varphi_n e)\|_{L_\infty}\leqslant Ct^{-1},\quad \|C_{-}((\rho-\rho^{1})\varphi_n e)\|_{L_2}\leqslant Ct^{-3/2}. \tag{4.21}$$

Now we replace the phase by its Taylor's series:

$$\theta^{1}(\lambda)=\sum_{m=0}^{5}\frac{\theta^{(m)}(\lambda_n)}{m!}(\lambda-\lambda_n)^m.$$

Let

$$\rho^{\tau}=e^{-it\theta^{\tau}}\delta_{+}^{2}r^{1},\quad \theta^{\tau}(\lambda)=\theta^{1}(\lambda)+\tau(\theta(\lambda)-\theta^{1}(\lambda)).$$

Then

$$C_{-}((\rho^{1}-\rho^{0})\varphi_n e)=-it\int_{0}^{1}d\tau C_{-}((\theta-\theta^{1})\rho^{\tau}\varphi_n e). \tag{4.22}$$

Recall that $\varphi_n(\lambda)=0$ for $|\lambda-\lambda_n|\geqslant\varepsilon$. Until now, ε was arbitrary; at this point, however, choose ε such that

$$\frac{\theta^{1\prime}(\lambda)}{\theta'(\lambda)}\geqslant a>0 \quad \text{for } |\lambda-\lambda_n|\leqslant\varepsilon.$$

This condition guarantees that $\theta^{\tau}(\lambda)$ has only one stationary point λ_n in supp φ_n. Application of Lemma 1, taken together with the Minkowski integral inequality, to (4.22) results in

$$\|C_-((\rho^1-\rho^0)\varphi_n e)\|_{L_\infty}\leqslant Ct^{-1}, \quad \|C_-((\rho^1-\rho^0)\varphi_n e)\|_{L_2}\leqslant Ct^{-3/2}. \tag{4.23}$$

By virtue of Lemma 1, it is also easy to show that the L_2- and L_∞-norms of $C_-(\rho_n(1-\varphi_n)e)$ decay to higher order as $t\to\infty$.

To conclude the proof, it remains to evaluate $C_-((\rho^0-\rho_n)\varphi_n e)$. Note that $(\rho^0-\rho_n)\varphi_n$ has an analytic continuation in the quadrant $|\lambda-\lambda_n|<\frac{3}{4}\varepsilon$, $\mathrm{Re}(\lambda-\lambda_n)>0$, $\mathrm{Im}\,\lambda>0$ [indeed, $\varphi_n(\lambda)=1$ if $|\lambda-\lambda_n|\leqslant\frac{3}{4}\varepsilon$, $\delta_+^n\delta_-^n=(\delta_+^n)^2/(1+p(\lambda_n)q(\lambda_n))$ if $\lambda-\lambda_n>0$]. Let $\Gamma=\Gamma_1\cup\Gamma_2\cup\Gamma_3$ be the contour which consists of an interval joining λ_n with $\lambda_n+\varepsilon' e^{i\pi/4}$ (Γ_1), an arc joining $\lambda_n+\varepsilon' e^{i\pi/4}$ with $\lambda_n+\varepsilon'$ (Γ_2), and a ray joining $\lambda_n+\varepsilon'$ with $+\infty$ (Γ_3). Here, ε' is a positive number less than $\frac{3}{4}\varepsilon$. Write

$$C_-((\rho^0-\rho_n)\varphi_n e)=\frac{1}{2\pi i}\int_{\lambda_n}^{\infty}\frac{(\rho^0(z)-\rho_n(z))\varphi_n(z)}{z-(\lambda-i0)}\,dz=\frac{1}{2\pi i}\int_{\Gamma_1}\frac{\rho^0(z)-\rho_n(z)}{z-\lambda}\,dz$$
$$+\frac{1}{2\pi i}\int_{\Gamma_2\cup\Gamma_3}\frac{(\rho^0(z)-\rho_n(z))\varphi_n(z)}{z-(\lambda-i0)}\,dz. \tag{4.24}$$

It is possible to choose ε' such that $\mathrm{Im}\,\theta^1(\lambda)\leqslant 0$ as $\lambda\in\Gamma_1\cup\Gamma_2$, $\mathrm{Im}\,\theta^1(\varepsilon' e^{i\pi/4})<0$, and $\theta^{1\prime}(\lambda)\neq 0$ as $\lambda\in\Gamma_2$. Therefore, the second integral on the right-hand side of (4.24) can be estimated by integration by parts for $\lambda\notin[\varepsilon',\varepsilon]$. However, notice that the variation of ε leads to the appearance in (4.24) of a small correction described by Lemma 1. Eventually, one derives appropriate L_2 and L_∞ evaluations for this integral.

Consider the first integral on the right-hand side of (4.24). Since

$$|\delta_+^2(\lambda)r^1(\lambda)-(\delta_+^n(\lambda))^2 r^1(\lambda_n)|\leqslant C|\lambda-\lambda_n|\ln|\lambda-\lambda_n|,$$

which is true because of (2.11), and since

$$|e^{-it\theta^1(\lambda)}-e^{it\theta^0(\lambda)}|\leqslant t|\theta^1(\lambda)-\theta^0(\lambda)|,$$

which is true if $\mathrm{Im}\,\theta^1(\lambda)$ and $\mathrm{Im}\,\theta^0(\lambda)\leqslant 0$, one obtains

$$\left|\frac{1}{2\pi i}\int_{\Gamma_1}\frac{\rho^0(z)-\rho_n(z)}{z-\lambda}\,dz\right|\leqslant C_1\int_0^{\varepsilon' e^{i\pi/4}}\frac{|z|\ln|z|e^{it\kappa_n\,\mathrm{Im}\,z^2}}{|z-(\lambda-\lambda_n)|}\,dz+C_2 t\int_0^{\varepsilon' e^{i\pi/4}}\frac{|z|^3 e^{it\kappa_n\,\mathrm{Im}\,z^2}}{|z-(\lambda-\lambda_n)|}\,dz$$
$$\leqslant C\,\frac{\ln t}{\sqrt{t}}\int_0^{\infty e^{i\pi/4}}\frac{(|z|\ln|z|+|z|^3)e^{i\kappa_n\,\mathrm{Im}\,z^2}}{|z-\xi|}\,dz=\frac{\ln t}{\sqrt{t}}f(\xi), \tag{4.25}$$

where $\xi=\sqrt{t}(\lambda-\lambda_n)$. The function f, determined through (4.25), is a function of ξ only obviously belonging to $L_2\cap L_\infty$. This completes the proof.

It should be pointed out that the above proof is a combination of ideas from Refs. 8 and 9.

V. MODEL RIEMANN–HILBERT PROBLEM

It has been explained that the asymptotic investigation of the RHP (2.16) is equivalent to the RHP (4.5). That the jump matrix in (4.5) is unity everywhere except small neighborhoods of the stationary phase points allows us to divide the factorization problem (4.5) into N simpler problems. As it turns out, the solution of (4.5) can be expressed, up to small errors, in terms of the solutions of the following RH problems:

$$\begin{gathered}\phi_+^n(\lambda)=\phi_-^n(\lambda)(b_n^-)^{-1}b_n^+, \quad n=1,\ldots,N,\\ \phi(\infty)=I,\end{gathered} \tag{5.1}$$

where $b_n^\pm$ are associated with the data $w_n^\pm=\varphi_n w^\pm$ ($b_n^\pm=I\pm\varphi_n w^\pm$). More precisely, it is a product of ϕ^n, while the potentials, u^L and v^L are a sum of potentials of (5.1). Before proving these statements rigorously, we shall conduct a comprehensive asymptotic analysis of (5.1).

On the other hand, problems (5.1) can be reduced, again up to small errors, to explicitly solvable ones. It is suitable to begin with these problems. To produce them, ρ and $\overline{\rho}$ in (2.16) should be replaced by ρ_n and $\overline{\rho_n}$ of (4.18), respectively. In new notations, after this substitution, one gets

$$\begin{aligned}\psi_+^M(\lambda)&=\psi_-^M(\lambda)(b_M^-)^{-1}b_M^+\\ &=\psi_-^M(\lambda)\begin{pmatrix}1 & \rho_n(\lambda)\\ 0 & 1\end{pmatrix}\begin{pmatrix}1 & 0\\ \overline{\rho_n}(\lambda) & 1\end{pmatrix}, \quad \varepsilon_n(\lambda-\lambda_n)>0\\ &=\psi_-^M(\lambda)\begin{pmatrix}1 & 0\\ \overline{\rho_n}(\lambda) & 1\end{pmatrix}\begin{pmatrix}1 & \rho_n(\lambda)\\ 0 & 1\end{pmatrix}, \quad \varepsilon_n(\lambda-\lambda_n)<0,\\ \psi^M(\infty)&=I.\end{aligned} \tag{5.2}$$

A more clear form of (5.2) is obtained with the following change of variables. Set

$$\xi=\varepsilon_n\sqrt{2\kappa_n t}(\lambda-\lambda_n), \quad -\pi<\arg\,\xi<\pi. \tag{5.3}$$

Then

$$\rho_n=p^0\xi_+^{i\nu_n}\xi_-^{i\nu_n}e^{-i\varepsilon_n\xi^2/2}, \quad \overline{\rho_n}=q^0\xi_+^{-i\nu_n}\xi_-^{-i\nu_n}e^{i\varepsilon_n\xi^2/2}, \tag{5.4}$$

where

$$p^0=p(\lambda_n)e^{-i\beta(\lambda_n)}, \quad q^0=q(\lambda_n)e^{i\beta(\lambda_n)}, \quad \beta=t\theta(\lambda_n)-2\gamma(\lambda_n)+\nu_n\ln 2\kappa_n t. \tag{5.5}$$

Inserting (5.3)–(5.5) into (5.2), we learn that

$$\psi_+^0(\xi)=\psi_-^0(\xi)\xi_-^{i\nu_n\sigma_3}\exp\left\{-i\sigma_3\varepsilon_n\frac{\xi^2}{2}\right\}v^{\varepsilon_n}\exp\left\{i\sigma_3\varepsilon_n\frac{\xi^2}{2}\right\}\xi_+^{-i\nu_n\sigma_3}. \tag{5.6}$$

Here, $\psi^0(\xi)$ is determined by the identity $\psi^M(\lambda)=\psi^0(\xi)$, and

$$v^1=\begin{pmatrix}1+p^0q^0 & p^0\\ q^0 & 1\end{pmatrix}, \quad v^{-1}=\begin{pmatrix}1 & -p^0\\ -q^0 & 1+p^0q^0\end{pmatrix}.$$

One thing which is worth mentioning is that, in the case when $\varepsilon_n=-1$, the substitution (5.3) maps the upper half-plane onto the lower half-plane and vice versa. This means that it is necessary to invert the jump matrix of (5.2) in deriving (5.6), whereas $\psi^M(\lambda\pm i0)=\psi^0(\xi\mp i0)$.

A natural method for solving (5.6) is to consider the piecewise analytic function $\Psi(\xi) = \psi_0(\xi)\xi^{i\nu_n\sigma_3}\exp(-i\sigma_3\varepsilon_n\xi^2/2)$. It happens that the jump matrix of Ψ is independent on ξ; hence, $(d\Psi/d\xi)\Psi^{-1}$ is an analytic function easily calculated through its known behavior at infinity. This results in a linear equation for Ψ which can be solved explicitly in terms of parabolic-cylinder functions. However, we shall find the solution of (5.6) directly, without calling on the linear equation.

Let

$$D_{i\nu}(z), \quad D_{i\nu}(-z), \quad D_{-i\nu-1}(iz), \quad D_{-i\nu-1}(-iz) \tag{5.7}$$

be the standard notations for the parabolic-cylinder functions. Recall that they are entire for any ν. Introduce

$$\Psi_1(\xi)=\begin{pmatrix} e^{\pi\nu/2}D_{i\nu}(i\alpha\xi) & ye^{-\pi\nu}D_{-i\nu-1}(-\alpha\xi) \\ -\overline{y}e^{\pi\nu/2}D_{i\nu-1}(i\alpha\xi) & e^{-\pi\nu}D_{-i\nu}(-\alpha\xi)\end{pmatrix}\alpha^{-i\nu\sigma_3},$$

$$\Psi_2(\xi)=\begin{pmatrix} e^{\pi\nu/2}D_{i\nu}(i\alpha\xi) & -yD_{-i\nu-1}(\alpha\xi) \\ -\overline{y}e^{\pi\nu/2}D_{i\nu-1}(i\alpha\xi) & D_{-i\nu}(\alpha\xi)\end{pmatrix}\alpha^{-i\nu\sigma_3},$$

$$\Psi_3(\xi)=\begin{pmatrix} e^{-\pi\nu/2}D_{i\nu}(-i\alpha\xi) & -yD_{-i\nu-1}(\alpha\xi) \\ \overline{y}e^{-\pi\nu/2}D_{i\nu-1}(-i\alpha\xi) & D_{-i\nu}(\alpha\xi)\end{pmatrix}\alpha^{-i\nu\sigma_3},$$

$$\Psi_4(\xi)=\begin{pmatrix} e^{-\pi\nu/2}D_{i\nu}(-i\alpha\xi) & ye^{\pi\nu}D_{-i\nu-1}(-\alpha\xi) \\ \overline{y}e^{-\pi\nu/2}D_{i\nu-1}(-i\alpha\xi) & e^{\pi\nu}D_{-i\nu}(-\alpha\xi)\end{pmatrix}\alpha^{-i\nu\sigma_3},$$

where y, $\overline{y}$, and ν satisfy the constraint $\nu=y\overline{y}$. Any three of the functions from the set (5.7) are linearly dependent as solutions of the same second-order linear differential equation. The exact connection formulas can be found in Ref. 10. Using them, one easily checks

$$\Psi_2(\xi)=\Psi_1(\xi)S_1, \quad \Psi_3(\xi)=\Psi_2(\xi)S_2, \quad \Psi_4(\xi)=\Psi_3(\xi)S_3, \tag{5.8}$$

where S_k are triangular matrices given by

$$S_1=\alpha^{i\nu\sigma_3}\begin{pmatrix} 1 & \dfrac{i\sqrt{2\pi}e^{-\pi\nu}}{\overline{y\Gamma}(i\nu)} \\ 0 & 1\end{pmatrix}\alpha^{-i\nu\sigma_3}, \quad S_2=\alpha^{i\nu\sigma_3}\begin{pmatrix} 1 & 0 \\ \dfrac{i\sqrt{2\pi}}{y\Gamma(-i\nu)} & 1\end{pmatrix}\alpha^{-i\nu\sigma_3},$$

$$S_3=\alpha^{i\nu\sigma_3}\begin{pmatrix} 1 & -\dfrac{i\sqrt{2\pi}e^{\pi\nu}}{\overline{y\Gamma}(i\nu)} \\ 0 & 1\end{pmatrix}\alpha^{-i\nu\sigma_3}, \quad \sigma_3=\begin{pmatrix} 1 & 0 \\ 0 & -1\end{pmatrix}.$$

Taking the asymptotic expansion of $D_{i\nu}(z)$ as $z\to\infty$,

$$D_{i\nu}(z)=z^{i\nu}e^{-z^2/4}\left(1+O\left(\frac{1}{z^2}\right)\right), \quad |\arg z|<\frac{3\pi}{4}, \tag{5.9}$$

and setting $\alpha = e^{-i\varepsilon_n\pi/4}$, one observes

$$\Psi_k(\xi)=\left(\begin{pmatrix} 1 & -ye^{i\varepsilon_n\pi/4}/\xi \\ -\varepsilon_n\overline{y}e^{-i\varepsilon_n\pi/4}/\xi & 1\end{pmatrix}+O\left(\frac{1}{|\xi|^2}\right)\right)e^{-i\varepsilon_n(\xi^2/4)\sigma_3+i\nu\sigma_3\ln\xi} \tag{5.10}$$

if $\xi\in\Omega_k(\varepsilon_n)$, $\xi\to\infty$,

$$\Omega_k(1)=\left\{\xi:-\frac{3\pi}{2}+\frac{k\pi}{2}<\arg\,\xi<-\frac{\pi}{2}+\frac{k\pi}{2}\right\},$$

$$\Omega_k(-1)=\left\{\xi:-2\pi+\frac{k\pi}{2}<\arg\,\xi<-\pi+\frac{k\pi}{2}\right\},\quad k=1,2,3,4.$$

Ending our construction, we demand that y, $\overline{y}$, and ν be chosen so that

$$\nu=\nu_n,\quad p^0=\frac{i\sqrt{2\pi}e^{-\varepsilon_n\pi\nu_n/2}}{\overline{y\Gamma}(i\nu_n)},\quad q^0=\frac{\varepsilon_n i\sqrt{2\pi}e^{-\varepsilon_n\pi\nu_n/2}}{y\Gamma(-i\nu_n)}. \tag{5.11}$$

Identities (5.11) are consistent with the constraint $\nu=y\overline{y}$. Indeed,

$$p^0q^0=-\varepsilon_n\frac{2\pi e^{-\varepsilon_n\pi\nu_n}}{\nu_n\Gamma(i\nu_n)\Gamma(-i\nu_n)}=-\varepsilon_n 2i\,\sin(i\pi\nu_n)e^{-\varepsilon_n\pi\nu_n}=-1+e^{-\varepsilon_n 2\pi\nu_n}.$$

Now, there are no obstacles to achieve the desired goal of solving (5.6). In fact, from (5.8), (5.10), and (5.11) it is seen that

$$\psi^0(\xi)=\begin{cases}\Psi_3(\xi)\xi^{-i\nu_n\sigma_3}e^{i(\xi^2/4)\sigma_3}, & \text{Im }\xi>0,\\ \Psi_1(\xi)\xi^{-i\nu_n\sigma_3}e^{i(\xi^2/4)\sigma_3}, & \text{Im }\xi<0,\end{cases}$$

is a solution of (5.6) when $\varepsilon_n=1$, while

$$\psi^0(\xi)=\begin{cases}\Psi_4(\xi)\xi^{-i\nu_n\sigma_3}e^{-i(\xi^2/4)\sigma_3}, & \text{Im }\xi>0,\\ \Psi_2(\xi)\xi^{-i\nu_n\sigma_3}e^{-i(\xi^2/4)\sigma_3}, & \text{Im }\xi<0,\end{cases}$$

is a solution of (5.6) when $\varepsilon_n=-1$.

The solution of (5.2) has been found explicitly. At this point, consider the operator $id-C_{w_M}$ related to (5.2) $[w_M^{\pm}=\pm(b_M^{\pm}-I), w_M=w_M^{+}+w_M^{-}]$. Dealing with the operator form of the RHP which was discussed in Sec. III, the following result from Refs. 4 and 7 is very useful:

Lemma 2: Let $\phi(\lambda)$ be a piecewise analytic invertible matrix, with $\phi(\infty)=I$. Define

$$w_\phi=w_\phi^{+}+w_\phi^{-},\quad w_\phi^{\pm}=\pm(b_\phi^{\pm}-I),$$

$$b^{\pm}=b_\phi^{\pm}\phi_{\pm},\quad w^{\pm}=\pm(b^{\pm}-I).$$

Then

$$(id-C_w)=(id-C_\phi)(id-C_{w_\phi}),$$

$$(id-C_{\phi^{-1}})(id-C_\phi)=(id-C_\phi)(id-C_{\phi^{-1}})=id,$$

where

$$C_\phi f=C_+(f(I-\phi_-))+C_-(f(\phi_+-I)),$$

$$C_{\phi^{-1}}f=C_+(f(I-\phi_-^{-1}))+C_-(f(\phi_+^{-1}-I)).$$

Proof: In fact,

$$
\begin{aligned}
C_\phi C_{w_\phi} &= C_\phi(C_+(\cdot w_\phi^-)+C_-(\cdot w_\phi^+)) \\
&= C_+[(C_+(\cdot w_\phi^-)+C_-(\cdot w_\phi^+))(I-\phi_-)]+C_-[(C_+(\cdot w_\phi^-)+C_-(\cdot w_\phi^+))(\phi_+-I)] \\
&= C_+(C_+(\cdot w_\phi^-)(I-\phi_-))+C_-(C_-(\cdot w_\phi^+)(\phi_+-I)) \\
&= C_+(\cdot w_\phi^-(I-\phi_-))-C_-(\cdot w_\phi^+(\phi_+-I))=C_{w_\phi}-C_w+C_\phi,
\end{aligned}
$$

whereas

$$
w_\phi^-(I-\phi_-)=w_\phi^- - w^- + (I-\phi_-), \quad w_\phi^+(\phi_+-I)=w^+ - w_\phi^+ + (I-\phi_+).
$$

The rest of the lemma is proved with similar calculations.

Return to the operator $(id - C_{w_M})$. Application of Lemma 2 in the case when $\phi(\lambda)=\psi^M(\lambda)$ and $b^\pm = b_M^\pm$ leads to

$$
(id-C_{w_M})^{-1}=\hat{\mu}^M(id-C_{\phi^{-1}}). \tag{5.12}
$$

In the above formula, $\hat{\mu}^M$ denotes right multiplication by μ^M ($\hat{\mu}^M f = f\mu^M$),

$$
(\mu^M)^{-1}=b_M^+(\psi_+^M)^{-1}=b_M^-(\psi_-^M)^{-1}=b_\phi^\pm. \tag{5.13}
$$

We have also used the identity

$$
(id-C_{w_\phi})f=f(\mu^M)^{-1}.
$$

From (5.12) one concludes that $(id - C_{w_M})^{-1}$ exists and is bounded as $t\to\infty$. In addition, since $C_{\phi^{-1}}I = 0$, μ^M is a solution of the basic integral equation.

Formula (5.13) gives a useful representation for μ^M which, after simplification by (5.8) and (5.11), takes the form

$$
\mu^M(\lambda;\varepsilon_n=1)=\begin{cases}\Psi_2(\xi)\xi^{-i\nu_n\sigma_3}e^{i(\xi^2/4)\sigma_3}, & \xi>0,\\ \Psi_4(\xi)\xi_+^{-i\nu_n\sigma_3}e^{i(\xi^2/4)\sigma_3}, & \xi<0,\end{cases} \tag{5.14a}
$$

$$
\mu^M(\lambda;\varepsilon_n=-1)=\begin{cases}\Psi_3(\xi)\xi^{-i\nu_n\sigma_3}e^{-i(\xi^2/4)\sigma_3}, & \xi>0,\\ \Psi_1(\xi)\xi_-^{-i\nu_n\sigma_3}e^{-i(\xi^2/4)\sigma_3}, & \xi<0.\end{cases} \tag{5.14b}
$$

From (5.10) and (5.14) we learn that

$$
\mu^M(\lambda)=\tilde{\mu}^M(\xi)=I+O(1/\xi) \quad \text{as} \quad \xi\to\pm\infty,
$$

whence

$$
\|\mu^M-I\|_{L_2}\leqslant Ct^{-1/4}. \tag{5.15}
$$

Let u^n, v^n and u_0^n, v_0^n be potentials of the RHPs (5.1) and (5.2), respectively. Note that u_0^n and v_0^n can be obtained from (5.5), (5.10), and (5.11). The result of these calculations is given by (1.5).

Proposition 5.1. There is a number t_0 such that the solution of RHP (5.1) exists at least for $t\geqslant t_0$. Moreover,

$$
|\phi^n(\lambda)-\psi^M(\lambda)|\leqslant Ct^{-3/4}\ln t \quad \text{if } |\operatorname{Im}\lambda|\geqslant a>0 \tag{5.16}
$$

and

$$u^n(t)=u_0^n(t)+O(t^{-3/4}\ln t),\quad v^n(t)=v_0^n(t)+O(t^{-3/4}\ln t). \tag{5.17}$$

Proof: The proof is virtually the same as the proof of Proposition (4.2). Here we use the piecewise analytical matrix $\Phi(\lambda)$ determined by

$$\Phi(\lambda)=\begin{pmatrix} 1 & 0 \\ -\overline{\rho^h_+}(\lambda) & 1 \end{pmatrix}\begin{pmatrix} 1 & -\rho^e_+(\lambda) \\ 0 & 1 \end{pmatrix},\quad \operatorname{Im}\lambda>0,$$

$$\Phi(\lambda)=\begin{pmatrix} 1 & -\rho^h_-(\lambda) \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ -\overline{\rho^e_-}(\lambda) & 1 \end{pmatrix},\quad \operatorname{Im}\lambda<0.$$

Passing to the new RHP (4.9) with $b\pm$ replaced by $b_n^{\pm}$ and with

$$m^{\Phi}(\lambda)=\phi^n(\lambda)\Phi(\lambda),$$

one deduces from Proposition 4.3 that the data of (4.9) can be decomposed in the form

$$w_{\Phi}^{\pm}=w_M^{\pm}+w_R^{\pm},$$

where $w_M^{\pm}$ are the data of (5.2) while $w_R^{\pm}$ have small L_2- and L_∞-norms which are dominated by

$$\|w_R^{\pm}\|_{L_2}\leqslant Ct^{-3/4}\ln t,\quad \|w_R^{\pm}\|_{L_\infty}\leqslant Ct^{-1/2}\ln t. \tag{5.18}$$

Due to the estimates (4.15) and (4.16) with ψ^M,μ^M in place of m^L,μ^L and due to inequalities (5.15) and (5.18), one gets

$$|m^{\Phi}(\lambda)-\psi^M(\lambda)|\leqslant Ct^{-3/4}\ln t \quad \text{if } |\operatorname{Im}\lambda|\geqslant a>0,$$

$$\|\mu^{\Phi}-\mu^M\|_{L_2}\leqslant Ct^{-3/4}\ln t. \tag{5.19}$$

To derive (5.16), it is sufficient to note that

$$|\Phi(\lambda)-I|\leqslant Ct^{-1}\ln t \quad \text{if } |\operatorname{Im}\lambda|\geqslant a>0.$$

Instead of the splitting (4.17), we now have

$$w_R=\begin{pmatrix} -\overline{\rho^e_+}\rho_n h-\rho^h_+\overline{\rho_n}e & \rho^h_+-\rho^e_- \\ \overline{\rho^e_+}-\overline{\rho^h_-} & -\overline{\rho^h_-}\rho_n e-\rho^e_-\overline{\rho_n}h \end{pmatrix}+w_I,$$

where again each element of w_I belongs to $L_1(R)$ but with L_1-norm decaying as $t^{-3/4}\ln t$. Since the diagonal elements of w_R-w_I do not play any role in the evaluation of the potentials u^n and v^n, the end of the proof is similar to that of Proposition 4.2.

Proposition 5.2: The operator $id-C_{w_n}$ related to (5.1) has an inverse at least for large t, and this is bounded as $t\to\infty$.

Proof: Let $(id-C_{w_\Phi})$ be the operator associated with the new RHP (4.9). Because of the identity

$$id-C_{w_\Phi}=(id-C_{w_M})(id-(id-C_{w_M})^{-1}C_{w_R})$$

and estimates (5.18), $(id-C_{w_\Phi})$ is invertible at least for large t. Using Lemma 2, the proof is complete.

Proposition 5.3: Let μ^n be the solution of the basic integral equation related to (5.1). Then

$$\|\mu^n-\mu^M\|_{L_2}\leqslant Ct^{-3/4}\ln t. \tag{5.20}$$

Proof: From (3.8) it is easily seen that $\mu^\Phi=\mu^n$, where Φ was determined in the proof of Proposition 5.1. Therefore, inequality (5.19) implies (5.20).

Proposition 5.4: For any real λ which is not in the support of φ_n, the following estimate is valid:

$$\begin{aligned}\mu^n(\lambda)=\phi_+^n(\lambda)=\phi_-^n(\lambda)&=\mu^M(\lambda)+O(t^{-3/4}\ln t)\\&=I+\begin{pmatrix}0 & u_0^n/(\lambda-\lambda_n)\\ v_0^n/(\lambda-\lambda_n) & 0\end{pmatrix}\\&\quad+O(t^{-3/4}\ln t).\end{aligned} \tag{5.21}$$

Proof: Take the representation (3.7) for the solution of the RHP:

$$\phi_+^n(\lambda)=\phi_-^n(\lambda)=I+\frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{\mu^M(z)w_n(z)}{z-\lambda}\,dz+\frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{(\mu^n(z)-\mu^M(z))w_n(z)}{z-\lambda}\,dz. \tag{5.22}$$

The second integral in the above formula is evaluated by

$$\frac{1}{2\pi}\frac{1}{|\lambda-\lambda_n|-\varepsilon}\|\mu^n-\mu^M\|_{L_2}\|w_n\|_{L_2}\leqslant Ct^{-3/4}\ln t.$$

The first is equal to $C_{w_n}(\mu^M)(\lambda)$, whereas $w_n^{\pm}(\lambda)=0$. Hence, one may show that

$$\phi_+^n(\lambda)=\phi_-^n(\lambda)=\mu^M(\lambda)+C_{w_n-w_M}(\mu^M)(\lambda)+O(t^{-3/4}\ln t). \tag{5.23}$$

Define

$$R^n(\lambda)=C_{w_n-w_M}(\mu^M)(\lambda)=C_+(\mu^M(w_n^--w_M^-))(\lambda)+C_-(\mu^M(w_n^+-w_M^+))(\lambda).$$

It turns out that

$$|R^n(\lambda)|\leqslant C\frac{\ln t}{t}; \tag{5.24}$$

thus (5.21) follows from (5.23). To obtain (5.24), one should consider each element of the matrix $R^n(\lambda)$ distinguishing two cases: $\varepsilon_n=1$, and $\varepsilon_n=-1$; for instance, we illustrate the proof of (5.24) for $R_{12}^n(\lambda)$, assuming that $\varepsilon_n=1$.

A straightforward calculation yields

$$\mu^M(w_n^--w_M^-)=\begin{pmatrix}\mu_{12}^M(\overline{\rho\varphi}_n-\overline{\rho}_n)e & \mu_{11}^M(\rho\varphi_n-\rho_n)h\\ \mu_{22}^M(\overline{\rho\varphi}_n-\overline{\rho}_n)e & \mu_{21}^M(\rho\varphi_n-\rho_n)h\end{pmatrix},$$

$$\mu^M(w_n^+-w_M^+)=\begin{pmatrix}\mu_{12}^M(\overline{\rho\varphi}_n-\overline{\rho}_n)h & \mu_{11}^M(\rho\varphi_n-\rho_n)e\\ \mu_{22}^M(\overline{\rho\varphi}_n-\overline{\rho}_n)h & \mu_{21}^M(\rho\varphi_n-\rho_n)e\end{pmatrix}.$$

Therefore,

$$R_{12}^n(\lambda)=C_+(\mu_{11}^M(\rho\varphi_n-\rho_n)h)(\lambda)+C_-(\mu_{11}^M(\rho\varphi_n-\rho_n)e)(\lambda)$$
$$=C_+(d^h(\rho_+^h-\rho_-^h))(\lambda)+C_-(d^e(\rho_+^e-\rho_-^e))(\lambda),$$

where we have used (5.14a) and replaced μ_{11}^M by

$$d^h=(\Psi_2)_{11}\xi^{-i\nu_n}e^{i\xi^2/4}=e^{\pi\nu_n/4}D_{i\nu_n}(i\alpha\xi)\xi^{-i\nu_n}e^{i\xi^2/4}$$

or

$$d^e=(\Psi_4)_{11}\xi_+^{-i\nu_n}e^{i\xi^2/4}=e^{-3\pi\nu_n/4}D_{i\nu_n}(-i\alpha\xi)\xi^{-i\nu_n}e^{i\xi^2/4}.$$

Notice that $d^h(d^e)$ is an analytic bounded function in the sector $-\pi<\arg(\lambda-\lambda_n)<\pi/2$ $[0<\arg(\lambda-\lambda_n)<3\pi/2]$ with unit behavior at infinity [see (5.9)],

$$d^h(\lambda)=1+O\left(\frac{1}{|\xi|^2}\right),\quad d^e(\lambda)=1+O\left(\frac{1}{|\xi|^2}\right).$$

Hence, $d^h\rho_-^h(d^e\rho_+^e)$ belongs to the null space of $C_+(C_-)$. This means that

$$R_{12}^n=C_+(d^h\rho_+^h)(\lambda)-C_-(d^e\rho_-^e)(\lambda)$$
$$=\rho_+^h(\lambda)+\rho_-^e(\lambda)+C_+((d^h-1)\rho_+^h)(\lambda)-C_-((d^e-1)\rho_-^e)(\lambda).$$

Let

$$\Gamma_{\lambda_n}^+=\{\lambda:\lambda=\lambda_n+ze^{i\pi/4},z\in R\},\quad \Gamma_{\lambda_n}^-=\{\lambda:\lambda=\lambda_n+ze^{-i\pi/4},z\in R\}.$$

Recall that $\rho_+^h(\rho_-^e)$ is the boundary value of the analytic, in the complex plane with the cut $\lambda-\lambda_n\geqslant 0(\lambda-\lambda_n\leqslant 0)$, function $\rho^h(\rho^e)$. Deforming the contour of integration, we deduce

$$R_{12}^n(\lambda)=\rho_+^h(\lambda)+\rho_-^e(\lambda)+(d^h(\lambda)-1)\rho_+^h(\lambda)h(\lambda)+(d^e(\lambda)-1)\rho_-^e(\lambda)e(\lambda)$$
$$+\frac{1}{2\pi i}\int_{\Gamma_{\lambda_n}^+}\frac{(d^h(z)-1)\rho^h(z)}{z-\lambda}\,dz+\frac{1}{2\pi i}\int_{\Gamma_{\lambda_n}^+}\frac{(d^e(z)-1)\rho^e(z)}{z-\lambda}\,dz.$$

The last identity reveals that

$$|R_{12}^n(\lambda)|\leqslant C_1(|\rho_+^h(\lambda)|+|\rho_-^e(\lambda)|)+C_2\frac{t^{-1/4}}{|\lambda-\lambda_n|}(\|\rho^h\|_{L_2(\Gamma_{\lambda_n}^+)}+\|\rho^e\|_{L_2(\Gamma_{\lambda_n}^+)}).\qquad(5.25)$$

Reviewing the proof of Proposition 4.3, one sees that

$$|\rho_+^h(\lambda)|,|\rho_-^e(\lambda)|\leqslant C\frac{\ln t}{t},\quad \|\rho^h\|_{L_2(\Gamma_{\lambda_n}^+)},\|\rho^e\|_{L_2(\Gamma_{\lambda_n}^+)}\leqslant Ct^{-3/4}\ln t.$$

Thus, estimate (5.25) implies

$$|R_{12}^n(\lambda)|\leqslant C\frac{\ln t}{t}.$$

The contour $\Gamma_{\lambda_n}^-$ is needed when the case $\varepsilon_n=-1$ is considered.

VI. THE PROOF OF THE THEOREM

We take up the investigation of the RHP (2.16), which is equivalent to the original one (1.1). In Sec. IV, (2.16) was reduced, without loss of asymptotic information, to the factorization problem (4.5), provided the operator associated with (4.5) was invertible at least for large t. The data of the RHP (4.5) had support localized in neighborhoods (which could be chosen arbitrarily small) of the stationary phase points. This result, namely, Proposition (4.2), is in complete correspondence with analogous ones from the asymptotic theory of oscillatory integrals, known as the localization principle. The next problem is to separate the contributions from the distinct stationary phase points. The present section is dedicated to it.

Consider the piesewise analytic matrix $m^{L\phi}$ defined through

$$m^L(\lambda)=m^{L\phi}(\lambda)\phi^1(\lambda), \tag{6.1}$$

where ϕ^1 is the solution of (5.1) with $n=1$. It evidently satisfies the following factorization problem:

$$m_+^{L\phi}(\lambda)=m_-^{L\phi}(\lambda)(b_{L\phi}^-)^{-1}b_{L\phi}^+, \quad m^{L\phi}(\infty)=I. \tag{6.2}$$

We choose the decomposition of the jump matrix in the form

$$b_{L\phi}^-=\mu^1 b_L^-(\phi_-^1)^{-1}, \quad b_{L\phi}^+=\mu^1 b_L^+(\phi_+^1)^{-1}. \tag{6.3}$$

Since $(\mu^1)^{-1}=b_1^-(\phi_-^1)^{-1}=b_1^+(\phi_+^1)^{-1}$, it occurs that

$$w_{L\phi}^{\pm}=\sum_{n=2}^{N}\varphi_n\mu^1 w^{\pm}(\mu^1)^{-1}. \tag{6.4}$$

Furthermore, estimate (5.21) gives rise to the splittings

$$w_{L\phi}^{\pm}=\sum_{n=2}^{N}\varphi_n w^{\pm}+w_R^{\pm}\equiv w_{L'}^{\pm}+w_R^{\pm}, \tag{6.5}$$

in which the corrections $w_R^{\pm}$ are small, viz.,

$$\|w_R^{\pm}\|_{L_2},\|w_R^{\pm}\|_{L_\infty}\leqslant Ct^{-1/2}. \tag{6.6}$$

Moreover,

$$w_R^{\pm}=\sum_{n=2}^{N}\varphi_n(V_1w^{\pm}-w^{\pm}V_1)+w_I^{\pm}\equiv w_V^{\pm}+w_I^{\pm}, \tag{6.7}$$

where

$$V_1=\begin{pmatrix}0 & u_0^1/(\lambda-\lambda_1)\\ v_0^1/(\lambda-\lambda_1) & 0\end{pmatrix}, \quad \|w_I^{\pm}\|_{L_1},\|w_I^{\pm}\|_{L_2},\|w_I^{\pm}\|_{L_\infty}\leqslant Ct^{-3/4}\ln t. \tag{6.8}$$

Let $m^{L'}(\lambda)$ be the solution of the RHP with data $w_{L'}^{\pm}$,

$$\begin{gathered}m_+^{L'}(\lambda)=m_-^{L}(\lambda)(b_{L'}^-)^{-1}b_{L'}^+, \quad b_{L'}^{\pm}=I\pm w_{L'}^{\pm},\\ m^{L'}(\infty)=I,\end{gathered} \tag{6.9}$$

and let $id - C_{w_{L'}}$ have an inverse which is bounded as $t\to\infty$. Then, rewriting the basic integral equation related to (6.2) in the form (4.13), one gets

$$\|\mu^{L\phi}-\mu^{L'}\|_{L_2}\leqslant C(\|C_{w_R}I\|_{L_2}+(\|w_R^+\|_{L_\infty}+\|w_R^-\|_{L_\infty})\|\mu^{L'}-I\|_{L_2}). \tag{6.10}$$

Inequalities (6.6) and (6.10) imply that

$$\|\mu^{L\phi}-\mu^{L'}\|_{L_2}\leqslant Ct^{-1/2}. \tag{6.11}$$

To proceed, we must suppose that $\|\mu^k\|_{L_\infty}\leqslant C$. Then, Lemma 2 and relation (3.11) reveal

$$(id-C_{w_L})^{-1}=\hat{\mu}^1(id-C_{w_{L\phi}})^{-1}(id-C_{\phi^{-1}}), \tag{6.12}$$

where $\phi=\phi^1$, $\hat{\mu}^1 f=f\mu^1$. Thus $id - C_{w_L}$ is invertible at least for large t [see (6.5) and (6.6)], and $(id - C_{w_L})^{-1}$ is bounded as $t\to\infty$. In addition, $\mu^L=\mu^{L\phi}\mu^1$ because $C_{\phi^{-1}}I = 0$. The last identity and (6.11) show

$$\|\mu^L-\mu^{L'}\mu^1\|_{L_2}\leqslant Ct^{-1/2};$$

hence

$$\|\mu^L-I\|_{L_2}\leqslant\|\mu^1-I\|_{L_2}+\|\mu^1\|_{L_\infty}\|\mu^{L'}-I\|_{L_2}+Ct^{-1/2}.$$

It is clear that the same arguments work with respect to $id - C_{w_{L'}}$. Continuing the induction, which consist of a finite number of steps, we find

$$\|\mu^L-I\|_{L_2}\leqslant\sum_{k=1}^{N} C_k\|\mu^k-I\|_{L_2}+C_0t^{-1/2}\leqslant Ct^{-1/4},\quad \|\mu^{L'}-I\|_{L_2}\leqslant Ct^{-1/4}. \tag{6.13}$$

We now want to improve estimate (6.11). Note that the leading terms of $w_R^{\pm}$ have been found explicitly. These are of order $t^{-1/2}$ but contain oscillations as well. Taking this into account, one observes

$$\|C_{w_V}I\|_{L_2}\leqslant Ct^{-3/4},\quad \|C_{w_R}I\|_{L_2}\leqslant Ct^{-3/4}\ln t. \tag{6.14}$$

Hence

$$\|\mu^{L\phi}-\mu^{L'}\|_{L_2}\leqslant Ct^{-3/4}\ln t. \tag{6.15}$$

Return to the RHP (4.5). Using the analogous of formula (4.14), we derive

$$m^{L\phi}(\lambda)-m^{L'}(\lambda)=\frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{w_V(z)}{z-\lambda}\,dz+O(t^{-3/4}\ln t)=O(t^{-3/4}\ln t), \tag{6.16}$$

provided $|\mathrm{Im}\,\lambda|\geqslant a>0$. Here, the oscillations in $w_V^{\pm}$ have been taken into account again. Then

$$m^L(\lambda)=m^{L'}(\lambda)\phi^1(\lambda)+O(t^{-3/4}\ln t),\quad |\mathrm{Im}\,\lambda|\geqslant a>0, \tag{6.17}$$

and

$$u^L=u^{L'}+u^1+O(t^{-3/4}\ln t),\quad v^L=v^{L'}+v^1+O(t^{-3/4}\ln t), \tag{6.18}$$

where $u^{L'}$ and $v^{L'}$ are the potentials of (6.9). It is obvious from (6.17) that, applying induction on the number of stationary phase points, we eventually obtain

$$m^L(\lambda)=\phi^N(\lambda)\cdots\phi^1(\lambda)+O(t^{-3/4}\ln t),\quad |\mathrm{Im}\,\lambda|\geqslant a>0, \tag{6.19}$$

and

$$u^L=\sum_{n=1}^{N} u^n+O(t^{-3/4}\ln t),\quad v^L=\sum_{n=1}^{N} v^n+O(t^{-3/4}\ln t). \tag{6.20}$$

The evaluations from Propositions (4.2) and (5.1) and the above ones complete the proof of the theorem.

Since there is one hole in the above proof, we describe briefly another approach in the end of this section. First, note that the assumption $\|\mu^k\|_{L_\infty}\leqslant C$ has been used in two places. One is the existence proof of $(id-C_{w_L})^{-1}$. Second, it has been needed in the proof of estimates (6.13). However, it is possible to state these results independently of whether $\mu^k\in L_\infty$ or not. Indeed, we know that the operators associated with the RHP (5.1), $id-C_{w_n}$, are invertible. Further, inspection reveals the following identities:

$$\begin{aligned}
&(id-C_{w_L})\left(id+\sum_{k=1}^{N} C_{w_k}(id-C_{w_k})^{-1}\right)=id-\sum_{k,n,k\neq n}^{N} C_{w_k}C_{w_n}(id-C_{w_n})^{-1},\\
&\left(id+\sum_{k=1}^{N} C_{w_k}(id-C_{w_k})^{-1}\right)(id-C_{w_L})=id-\sum_{k,n,k\neq n}^{N} (id-C_{w_k})^{-1}C_{w_k}C_{w_n}.
\end{aligned} \tag{6.21}$$

Recall that $C_{w_L}=\Sigma_{k=1}^{N}C_{w_k}$. Evidently, if the operators on the right-hand side of (6.21) are invertible, then $(id-C_{w_L})^{-1}$ exists. The former is true for large t because of the inequalities

$$\|C_{w_k}C_{w_n}\|_{L_2\to L_2}\leqslant Ct^{-1/4},\quad k\neq n.$$

The latter can be found by the method of stationary phase since $C_{w_n}f$ is an analytic function whose derivatives are bounded in t for any $f\in L_2$ in some neighborhood of $\mathrm{supp}\,w_k$ ($\mathrm{supp}\,w_k\cap\mathrm{supp}\,w_n=\varnothing$, $n\neq k$). The desired evaluations (6.13) are now consequence of

$$\|C_{w_L}I\|_{L_2}\leqslant Ct^{-1/4}.$$

We have developed our approach, assuming that the phase of the RHP (1.1) is a smooth function on the real axis; however, the RHPs which arise in the theory of integrable nonlinear equations (e.g., sine–Gordon) may have a phase with poles on the real axis. These cases can easily be incorporated into the method presented here if we assume that $p(\lambda)$ and $q(\lambda)$ have zeros of appropriate order at the poles of the phase. Therefore, the theorem is still valid for such p, q, and θ.

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Factorization of scattering matrices due to partitioning of potentials in one-dimensional Schrödinger-type equations

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The one-dimensional Schrödinger equation and two of its generalizations are considered, as they arise in quantum mechanics, wave propagation in a nonhomogeneous medium, and wave propagation in a nonconservative medium where energy may be absorbed or generated. Generically, the zero-energy transmission coefficient vanishes when the potential is nontrivial, but in the exceptional case this coefficient is nonzero, resulting in tunneling through the potential. It is shown that any nontrivial exceptional potential can always be fragmented into two generic pieces. Furthermore, any nontrivial potential, generic or exceptional, can be fragmented into generic pieces in infinitely many ways. The results remain valid when Dirac delta functions are included in the potential and other coefficients are added to the Schrödinger equation. For such Schrödinger equations, factorization formulas are obtained that relate the scattering matrices of the fragments to the scattering matrix of the full problem. © *1996 American Institute of Physics.*
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I. INTRODUCTION

In this paper we consider the one-dimensional Schrödinger equation and two of its generalizations. The Schrödinger equation (2.1) describes the quantum mechanical behavior of a particle interacting with the potential $V(x)$. From the corresponding transmission coefficient $T(k)$ we obtain the probability $|T(k)|^2$ that a particle of energy k^2 can tunnel through this potential. Generically, the zero-energy transmission coefficient is zero and hence a zero-energy particle cannot tunnel through a nontrivial potential. However, in the exceptional case, the transmission coefficient does not vanish at zero energy. In this paper, we analyze certain aspects of this exceptional case. With the help of a factorization formula, we show that a nontrivial exceptional potential can always be fragmented into generic pieces; i.e., a nontrivial potential allowing tunneling at zero energy can always be decomposed into pieces none of which allow such tunneling. The factorization formula (2.17) used to obtain this result allows us to express the scattering coefficients corresponding to a potential in terms of the scattering coefficients corresponding to its fragments. We show that similar factorization formulas hold for certain generalized Schrödinger equations describing the wave propagation in one-dimensional nonhomogeneous or nonconservative media. For such generalized Schrödinger equations, the generic and exceptional cases are again determined by the zero-energy behavior of the transmission coefficients.

The generalized Schrödinger equation (3.3) can be analyzed by locally transforming it into a finite number of Schrödinger equations; the results obtained in Sec. II show that each of these Schrödinger equations can be chosen to have generic potentials. In Sec. III we obtain the corresponding factorization formula for Eq. (3.3). This formula, Eq. (3.15), brings insight to the analy-

sis of wave scattering in a one-dimensional nonhomogeneous medium and allows us to see how the scattering process can be viewed as resulting both from ''soft scatterers''[1] (responsible for continuous changes in the medium parameters) and from ''hard scatterers''[1] (responsible for discontinuous changes in the medium parameters). This formula also explains how the total scattering matrix can be obtained in terms of the scattering matrices of the individual fragments localized in space.

In Sec. IV, we generalize the factorization formula (2.17) in a different way to analyze how the scattering process takes place in a one-dimensional nonconservative medium governed by the generalized Schrödinger equation (4.1), where energy absorption or generation may occur. Although the scattering matrix is no longer unitary when energy absorption or generation is present, we still have a factorization formula, namely Eq. (4.5), showing how the scattering resulting from the fragments is superposed to give the total scattering.

The small-energy analysis of the exceptional case for these three equations usually requires elaborate calculations. In addition to giving insight into the scattering process, the factorization formulas associated with these equations are expected to simplify the small-energy analysis of the wavefunctions and scattering coefficients.

II. SCHRÖDINGER EQUATION

Consider the one-dimensional Schrödinger equation

$$\frac{d^2\psi(k,x)}{dx^2}+k^2\psi(k,x)=V(x)\psi(k,x), \tag{2.1}$$

where k^2 is energy, x is the space coordinate, and $V(x)$ is a real-valued potential belonging to $L_1^1(\mathbf{R})$, i.e., $\int_{-\infty}^{\infty} dx\ (1+|x|)|V(x)|$ is finite. The scattering solutions of Eq. (2.1) are those that behave like $e^{\pm ikx}$ as $x\to+\infty$ and $x\to-\infty$. There are two linearly independent scattering solutions $f_l(k,x)$ and $f_r(k,x)$ of Eq. (2.1), known as the Jost solutions from the left and from the right, respectively, satisfying the boundary conditions

$$f_l(k,x)=\begin{cases} e^{ikx}+o(1), & x\to+\infty, \\ \dfrac{1}{T(k)}\,e^{ikx}+\dfrac{L(k)}{T(k)}\,e^{-ikx}+o(1), & x\to-\infty, \end{cases} \tag{2.2}$$

$$f_r(k,x)=\begin{cases} \dfrac{1}{T(k)}\,e^{-ikx}+\dfrac{R(k)}{T(k)}\,e^{ikx}+o(1), & x\to+\infty, \\ e^{-ikx}+o(1), & x\to-\infty, \end{cases} \tag{2.3}$$

where $T(k)$ is the transmission coefficient and $R(k)$ and $L(k)$ are the reflection coefficients from the right and from the left, respectively. The scattering matrix associated with Eq. (2.1) is defined as

$$\mathbf{S}(k)=\begin{bmatrix} T(k) & R(k) \\ L(k) & T(k) \end{bmatrix}, \tag{2.4}$$

and it satisfies

$$\mathbf{S}(-k)=\overline{\mathbf{S}(k)}, \quad k\in\mathbf{R}, \tag{2.5}$$

where the overline denotes complex conjugation. The scattering matrix is unitary; thus,

$$|T(k)|^2+|R(k)|^2=|T(k)|^2+|L(k)|^2=1, \quad k\in\mathbf{R}, \tag{2.6}$$

and from Eq. (2.5) we see that

$$R(k)T(-k)+L(-k)T(k)=0, \quad k\in\mathbf{R}. \tag{2.7}$$

It is also known that the determinant of $\mathbf{S}(k)$ is given by

$$T(k)^2-R(k)L(k)=\frac{T(k)}{T(-k)}, \quad k\in\mathbf{R}. \tag{2.8}$$

For a potential in $L^1_1(\mathbf{R})$, the corresponding scattering matrix is well understood. Generically, the transmission coefficient vanishes linearly as $k\to 0$ and $R(0)=L(0)=-1$. In the exceptional case, we have $T(0)\neq 0$ and hence $|R(0)|=|L(0)|<1$. There are other characterizations of these two cases. For example, the potential $V(x)$ is exceptional if and only if $f_l(0, x)$ and $f_r(0, x)$ are linearly dependent. Equivalently, $V(x)$ is exceptional if and only if at least one of $f_l(0, x)$ and $f_r(0, x)$ is bounded; in that case both of these functions are bounded for $x\in\mathbf{R}$. Furthermore, the potential $V(x)$ is exceptional if and only if

$$\int_{-\infty}^{\infty} dx\ V(x)f_l(0, x)=0, \tag{2.9}$$

which is equivalent to $\int_{-\infty}^{\infty} dx\ V(x)f_r(0, x)=0$ because $f_l(0, x)$ and $f_r(0, x)$ are linearly dependent in the exceptional case. Moreover, the exceptional case occurs if and only if $f_l'(0, -\infty)=0$ or $f_r'(0, +\infty)=0$. Here and throughout the paper the prime denotes the spatial derivative and we interpret $f_l'(0, -\infty)$ as $\lim_{x\to-\infty} f_l'(0, x)$ and interpret $f_r'(0, +\infty)$ as $\lim_{x\to+\infty} f_r'(0, x)$.

If the potential has support on a half-line, i.e., if $V(x)=0$ for $x>b$ or $x<a$ for some constants a and b, we have the exceptional case if and only if $f_r'(0, x)=0$ for all $x\geqslant b$ or $f_l'(0, x)=0$ for all $x\leqslant a$, respectively. For example, when $V(x)=0$ for $x>b$, the linear dependence of $f_l(0, x)$ and $f_r(0, x)$ in the exceptional case requires that $f_r(0, x)$ is a constant for $x\geqslant b$ and hence $f_r'(0, b)=0$; in the generic case, since $f_r(0, x)$ is linear for $x\geqslant b$ and linearly independent of $f_l(0, x)$, it follows that $f_r'(0, b)\neq 0$. Note that $f_l(0, x)$ and $f_l'(0, x)$ cannot simultaneously vanish at the same x value; otherwise, we would have $f_l(0, x)=0$ for $x\in\mathbf{R}$ contradicting $f_l(0,+\infty)=1$. Similarly, $f_r(0, x)$ and $f_r'(0, x)$ cannot simultaneously vanish at the same x value. Thus, if $V(x)=0$ for $x<a$ and if $f_l(0, a)=0$, then $V(x)$ must be generic. Similarly, if $V(x)=0$ for $x>b$ and $f_r(0, b)=0$, then $V(x)$ must be generic.

In the exceptional case, let γ denote the constant

$$\gamma=\frac{f_l(0, x)}{f_r(0, x)}. \tag{2.10}$$

We have[2]

$$\begin{bmatrix} f_l(-k,x) \\ f_r(-k,x) \end{bmatrix}=\begin{bmatrix} T(k) & -R(k) \\ -L(k) & T(k) \end{bmatrix}\begin{bmatrix} f_r(k,x) \\ f_l(k,x) \end{bmatrix}, \quad k\in\mathbf{R}, \tag{2.11}$$

and hence from Eqs. (2.10) and (2.11) at $k=0$ we get

$$\gamma=\frac{T(0)}{1+R(0)}=\frac{1+L(0)}{T(0)}. \tag{2.12}$$

Using Eqs. (2.7), (2.8), and (2.12), we obtain

$$T(0)=\frac{2\gamma}{\gamma^2+1}, \quad L(0)=-R(0)=\frac{\gamma^2-1}{\gamma^2+1}. \tag{2.13}$$

Further information on the generic and exceptional cases can be found in Refs. 2–6. For later reference, we summarize some of the necessary and sufficient conditions for the exceptional case.

Proposition 2.1: A potential $V\in L_1^1(\mathbf{R})$ is exceptional if and only if $f_l'(0,-\infty)=0$ or equivalently if and only if $f_r'(0,+\infty)=0$. If $V(x)$ vanishes for $x>b$, it is exceptional if and only if $f_r'(0,b)=0$. Similarly, if $V(x)$ vanishes for $x<a$, it is exceptional if and only if $f_l'(0,a)=0$.

The trivial potential $V(x)=0$ is exceptional. If $V(x)$ is nontrivial and $V(x)\geqslant 0$, then $V(x)$ is generic. The exceptional case is unstable in the sense that a small change in the potential usually makes the case generic. As an example, consider the square-well potential: the exceptional case occurs at the exact depths when a bound state is added to the potential; at any other depth the square-well potential is generic.

The distinction between the generic and exceptional cases becomes relevant when the small-energy behavior of the scattering coefficients and of the wavefunctions is considered. In many instances one has to deal with quantities involving the factor $T(k)/k$. In the generic case this factor remains bounded and continuous as $k\to 0$, but in the exceptional case it behaves as $T(0)/k$ with $T(0)\neq 0$. In some applications the factor $T(k)/k$ is multiplied by a continuous function $g(k)$ and one has to prove, for example, the integrability of the product $g(k)T(k)/k$ as $k\to 0$. In the generic case this integrability holds automatically, but in the exceptional case one has to prove, for instance, that $g(k)$ is of order $|k|^{\gamma}$ for some $\gamma\in(0,1]$ as $k\to 0$. This is one of the reasons why proofs tend to be more elaborate in the exceptional case than in the generic case. In this Section we show among other things that an exceptional potential can always be ''fragmented'' into two generic pieces and that a matrix closely related to the scattering matrix can be written as a product of factors, where each factor carries the information pertaining to one fragment. The term ''fragment'' will be made precise below. We expect our results to offer simplifications in dealing with exceptional potentials.

We now consider Eq. (2.1) and first explain the term fragment used in this paper. Choose a partition $-\infty<x_1<x_2<\cdots<x_n<+\infty$ of the real line $\mathbf{R}$ and define

$$V_{j,j+1}(x)=\begin{cases} V(x), & x\in(x_j,x_{j+1}),\\ 0, & x\notin(x_j,x_{j+1}),\end{cases}$$

so that

$$V(x)=\sum_{j=0}^{N} V_{j,j+1}(x), \tag{2.14}$$

where in Eq. (2.14) and below we use the convention that $x_0=-\infty$ and $x_{N+1}=+\infty$. We call $V_{j,j+1}(x)$ a fragment of $V(x)$. In analogy to Eq. (2.4) we let

$$\mathbf{S}_{j,j+1}(k)=\begin{bmatrix} T_{j,j+1}(k) & R_{j,j+1}(k)\\ L_{j,j+1}(k) & T_{j,j+1}(k)\end{bmatrix}$$

denote the scattering matrix associated with the potential $V_{j,j+1}(x)$, where each matrix $\mathbf{S}_{j,j+1}(k)$ only carries the information pertaining to the fragment $V_{j,j+1}(x)$. Using the scattering coefficients, we introduce the matrices

$$\Lambda(k)=\begin{bmatrix} \dfrac{1}{T(k)} & -\dfrac{R(k)}{T(k)} \\ \dfrac{L(k)}{T(k)} & \dfrac{1}{T(-k)} \end{bmatrix}, \quad \Lambda_{j,j+1}(k)=\begin{bmatrix} \dfrac{1}{T_{j,j+1}(k)} & -\dfrac{R_{j,j+1}(k)}{T_{j,j+1}(k)} \\ \dfrac{L_{j,j+1}(k)}{T_{j,j+1}(k)} & \dfrac{1}{T_{j,j+1}(-k)} \end{bmatrix}. \tag{2.15}$$

Note that each matrix in Eq. (2.15) can be written as the product of two matrices in the following way:

$$\Lambda(k)=\begin{bmatrix} \dfrac{1}{T(k)} & -\dfrac{R(k)}{T(k)} \\ \dfrac{L(k)}{T(k)} & \dfrac{1}{T(-k)} \end{bmatrix}=\begin{bmatrix} 1 & 0 \\ L(k) & T(k) \end{bmatrix}\begin{bmatrix} \dfrac{1}{T(k)} & -\dfrac{R(k)}{T(k)} \\ 0 & 1 \end{bmatrix}. \tag{2.16}$$

Note also that using Eq. (2.7) it is possible to express the entries of each matrix in Eq. (2.15) in terms of the transmission coefficient and only one of the reflection coefficients; for example, we have

$$\Lambda(k)=\begin{bmatrix} \dfrac{1}{T(k)} & -\dfrac{R(k)}{T(k)} \\ -\dfrac{R(-k)}{T(-k)} & \dfrac{1}{T(-k)} \end{bmatrix}=\begin{bmatrix} \dfrac{1}{T(k)} & \dfrac{L(-k)}{T(-k)} \\ \dfrac{L(k)}{T(k)} & \dfrac{1}{T(-k)} \end{bmatrix}.$$

It is known[7] that $\Lambda(k)$ can be written as the product

$$\Lambda(k)=\Lambda_{0,1}(k)\Lambda_{1,2}(k)\cdots\Lambda_{N,N+1}(k). \tag{2.17}$$

It can be proved that Eq. (2.17) remains valid if we allow the potential $V(x)$ to contain a finite number of Dirac delta functions. When delta functions are included, the proof of Eq. (2.17) can be obtained from Eqs. (3.15) and (3.16) in the special case $H(x)\equiv 1$. If all the fragments in Eq. (2.14) are delta-function potentials, Eq. (2.17) reduces to Eq. (3.17). In Sec. III we will elaborate on the inclusion of delta functions.

The matrices $\Lambda(k)$ and $\Lambda_{j,j+1}(k)$ are usually called transition matrices. The reason for this terminology is as follows, which at the same time proves Eq. (2.17). Any scattering solution $\psi(k,x)$ of (2.1) obeys $\psi(k,x)=c_1e^{ikx}+c_2e^{-ikx}+o(1)$ as $x\to+\infty$ and $\psi(k,x)=d_1e^{ikx}+d_2e^{-ikx}+o(1)$ as $x\to-\infty$, where c_1,c_2,d_1,d_2 are function of k alone. By using Eqs. (2.2), (2.3), and (2.8), we can relate the vectors $[c_1\ c_2]$ and $[d_1\ d_2]$ corresponding to each of the Jost solutions $f_l(k,x)$ and $f_r(k,x)$, and hence we obtain $[d_1\ d_2]^t=\Lambda(k)[c_1\ c_2]^t$. We use the superscript t to denote the transpose. Hence $\Lambda(k)$ provides the link between the asymptotics of the solutions of Eq. (2.1) at $+\infty$ and those at $-\infty$ when the functions $e^{\pm ikx}$ are chosen as an (asymptotic) basis. Now let $N=1$, i.e., the partition is simply $-\infty<x_1<+\infty$. Let $\psi_{1,2}(k,x)$ be the solution of Eq. (2.1) with the potential $V_{1,2}(x)$ that satisfies $\psi_{1,2}(k,x)=\psi(k,x)$ for $x\geqslant x_1$, and let $\psi_{0,1}(k,x)$ be the solution of Eq. (2.1) with the potential $V_{0,1}(x)$ such that $\psi_{0,1}(k,x)=\psi(k,x)$ for $x\leqslant x_1$. Then $\psi_{1,2}(k,x)=\tilde{d}_1e^{ikx}+\tilde{d}_2e^{-ikx}$ for $x\leqslant x_1$, where $[\tilde{d}_1\ \tilde{d}_2]^t=\Lambda_{1,2}(k)[c_1\ c_2]^t$. Since $\psi(k,x_1)=\psi_{0,1}(k,x_1)=\psi_{1,2}(k,x_1)$ and $\psi'(k,x_1)=\psi'_{0,1}(k,x_1)=\psi'_{1,2}(k,x_1)$, it follows that $\psi_{0,1}(k,x)=\tilde{d}_1e^{ikx}+\tilde{d}_2e^{-ikx}$ for $x\geqslant x_1$. So $\Lambda_{0,1}(k)[\tilde{d}_1\ \tilde{d}_2]^t=[d_1\ d_2]^t$, and hence $[d_1\ d_2]^t=\Lambda_{0,1}(k)\Lambda_{1,2}(k)[c_1\ c_2]^t$. Thus, $\Lambda(k)=\Lambda_{0,1}(k)\Lambda_{1,2}(k)$, proving Eq. (2.17) when $N=1$. For $N\geqslant 2$ the result follows by induction.

For later use we note that when $N=1$, from Eqs. (2.15) and (2.17) we obtain

$$\frac{1}{T(k)}=\frac{1-R_{0,1}(k)L_{1,2}(k)}{T_{0,1}(k)T_{1,2}(k)}. \tag{2.18}$$

Now we return to Eq. (2.1) and discuss some consequences of Eqs. (2.17) and (2.18). The first result concerns resonant energies. These are energies at which the potential is perfectly transparent; in other words, energies $k_i^2 \geq 0$ where $|T(k_i)|=1$. Because of Eq. (2.5), $T(-k) = \overline{T(k)}$ for real k, and hence it is sufficient to consider the resonant frequencies only for $k_i \geq 0$. Typically, if $V(x)$ is a square-well potential, the existence of such resonant energies is well known (p. 94 of Ref. 8). There are also some general existence results[9] concerning resonances for potentials that are symmetric with respect to the midpoint of the potential barrier. The resonant energies play an important role in tunneling spectroscopy.[10] Here we consider a related but somewhat different problem. We consider the one-parameter family of potentials

$$V_\xi(x)=V_{0,1}(x+\xi)+V_{1,2}(x-\xi), \tag{2.19}$$

where $\xi>0$ is a real parameter. In other words, we take a potential $V(x)$ consisting of two fragments $V_{0,1}(x)$ and $V_{1,2}(x)$ and vary the distance between them by changing ξ. The goal is to adjust the distance between the fragments so that the transmission coefficient has magnitude 1. Let $T_\xi(k)$ denote the transmission coefficient for $V_\xi(x)$, and fix any $k=k_0 \geq 0$. Then we ask: are there any values of ξ for which $|T_\xi(k_0)|=1$? The answer when $k_0>0$ is contained in the next theorem. The analysis for $k_0=0$ will be given at the end of this section.

Theorem 2.2: Consider the potential $V_\xi(x)$ defined in Eq. (2.19) with the corresponding transmission coefficient $T_\xi(k)$. For any fixed $k_0>0$, there are three possibilities: (i) $|T_\xi(k_0)|=1$ for all $\xi>0$, (ii) there is no $\xi>0$ for which $|T_\xi(k_0)|=1$, (iii) the values $\xi>0$ for which $|T_\xi(k_0)|=1$ form an infinite sequence tending to $+\infty$.

Proof: Before starting the proof we remark that case (i) occurs when both of the fragments have a common resonant energy, that is when $|T_{0,1}(k_0)|=|T_{1,2}(k_0)|=1$; case (ii) occurs when $|T_{0,1}(k_0)|\neq|T_{1,2}(k_0)|$; case (iii) occurs when $|T_{0,1}(k_0)|=|T_{1,2}(k_0)|\neq 1$. For example, if $V(x)$ is symmetric about $x=x_1$ and hence $V_{0,1}(x_1-x)=V_{1,2}(x_1+x)$, then we are either in case (i) or case (iii); the same is true if $V_{1,2}(x)$ is a translate of $V_{0,1}(x)$.

The reflection coefficients from the right and left associated with the potentials $V_{0,1}(x+\xi)$ and $V_{1,2}(x-\xi)$ are given by $R_{0,1}(k)e^{2ik\xi}$ and $L_{1,2}(k)e^{2ik\xi}$, respectively. The transmission coefficients of the individual fragments are not affected by the shifts $\pm\xi$. Thus, by Eq. (2.18), $|T_\xi(k_0)|=1$ if and only if

$$|T_{0,1}(k_0)||T_{1,2}(k_0)|=|1-R_{0,1}(k_0)L_{1,2}(k_0)e^{4ik_0\xi}|. \tag{2.20}$$

Clearly, if $R_{0,1}(k_0)=L_{1,2}(k_0)=0$, then, by Eq. (2.6), $|T_{0,1}(k_0)|=|T_{1,2}(k_0)|=1$, and Eq. (2.20) holds independently of ξ, which is case (i). If $R_{0,1}(k_0)=0$ but $L_{1,2}(k_0)\neq 0$ (or vice versa), then $|T_{0,1}(k_0)|=1$ and $|T_{1,2}(k_0)|<1$ (or vice versa). Then Eq. (2.20) does not hold for any ξ. This is a special case of case (ii). Now suppose that $R_{0,1}(k_0)$ and $L_{1,2}(k_0)$ are both nonzero. Note the inequality

$$1-ab \geq (1-a^2)^{1/2}(1-b^2)^{1/2}, \quad a,b\in[0,1],$$

with the equality holding if and only if $a=b$. Using this inequality with $a=|R_{0,1}(k_0)|$ and $b=|L_{1,2}(k_0)|$, we see that Eq. (2.20) holds if and only if $|R_{0,1}(k_0)|=|L_{1,2}(k_0)|$ and

$$R_{0,1}(k_0)L_{1,2}(k_0)e^{4ik_0\xi}=|R_{0,1}(k_0)||L_{1,2}(k_0)|.$$

Hence, if $|R_{0,1}(k_0)|\neq|L_{1,2}(k_0)|$, then we are in case (ii). If $|R_{0,1}(k_0)|=|L_{1,2}(k_0)|$, then we set

$$R_{0,1}(k_0)L_{1,2}(k_0)=|R_{0,1}(k_0)||L_{1,2}(k_0)|e^{i\varphi(k_0)},$$

and we see that the values ξ are given by $4k_0\xi+\varphi(k_0)=2\pi n$, where n is any integer large enough to ensure $\xi>0$. Hence $\xi_n=\pi n/(2k_0)-\varphi(k_0)/(4k_0)$ is the desired sequence in case (iii). ■

Next we give some results concerning the nature of the point $k=0$. Let $f_{l;j,j+1}(k,x)$ and $f_{r;j,j+1}(k,x)$ denote the Jost solutions from the left and from the right, respectively, for the potentials $V_{j,j+1}(x)$. Since the potentials $V_{j,j+1}(x)$ have compact support for $j=1,\ldots,N-1$, using Proposition 2.1 we can conclude that $V_{j,j+1}(x)$ is generic if and only if $f'_{l;j,j+1}(k,x_j)\neq 0$ or if and only if $f'_{r;j,j+1}(k,x_{j+1})\neq 0$. Equivalently, $V_{j,j+1}(x)$ is exceptional if and only if $f'_{l;j,j+1}(k,x_j)=0$ or if and only if $f'_{r;j,j+1}(k,x_{j+1})=0$. This characterization also applies to the fragments $V_{0,1}(x)$ and $V_{N,N+1}(x)$ if we use $f'_{l;0,1}(k,x_0)$ and $f'_{r;N,N+1}(k,x_{N+1})$, respectively.

Theorem 2.3: Consider a potential $V(x)$ given in Eq. (2.14) with $N\geqslant 1$. Then:

(i) $\Rightarrow$ If all $N+1$ of the fragments are exceptional, then $V(x)$ is exceptional.

(ii) $\Rightarrow$ If exactly one fragment is generic, then $V(x)$ is generic.

Proof: (i) We give two proofs of (i) illustrating different aspects of the problem. First let $N=1$. Then, from Eq. (2.18) we see that if both $T_{0,1}(0)$ and $T_{1,2}(0)$ are nonzero, then the transmission coefficient $T(k)$ corresponding to $V(x)$ cannot vanish at $k=0$. Using induction, it then follows from Eq. (2.18) that if none of the transmission coefficients $T_{j,j+1}(k)$ vanish at $k=0$, then $T(k)$ cannot vanish at $k=0$. Hence (i) is proved. Alternatively, one can argue by using the zero-energy Jost solutions. Let $M_{j,j+1}$ denote the transfer matrix such that

$$\begin{bmatrix} \psi(0,x_j) \\ \psi'(0,x_j)\end{bmatrix}=M_{j,j+1}\begin{bmatrix} \psi(0,x_{j+1}) \\ \psi'(0,x_{j+1})\end{bmatrix},\quad j=1,\ldots,N-1,$$

for any zero-energy solution of Eq. (2.1). Notice that

$$f_{l;j,j+1}(0,x_{j+1})=1,\quad f'_{l;j,j+1}(0,x_{j+1})=0.$$

Hence, if $V_{j,j+1}(x)$ is exceptional, then $[1\ 0]^t$ is an eigenvector of $M_{j,j+1}$ corresponding to the eigenvalue $f_{l;j,j+1}(0,x_j)$; if $V_{j,j+1}(x)$ is generic, then $[1\ 0]^t$ is not an eigenvector of $M_{j,j+1}$, since in that case $f'_{l;j,j+1}(0,x_j)\neq 0$ and $f'_{l;j,j+1}(0,x_{j+1})=0$. Furthermore, we have $f_l(0,x_N)=f_{l;N,N+1}(0,x_N)$ for $x\in[x_N,+\infty)$ and hence $f'_l(0,x_N)=0$ whenever $V_{N,N+1}(x)$ is exceptional. Since all fragments are assumed exceptional, and hence $[1\ 0]^t$ is a common eigenvector of all matrices $M_{j,j+1}$, it follows that

$$\begin{bmatrix} f_l(0,x_1) \\ f'_l(0,x_1)\end{bmatrix}=M_{1,2}\cdots M_{N-1,N}\begin{bmatrix} f_l(0,x_N) \\ 0\end{bmatrix}=c\begin{bmatrix} 1 \\ 0\end{bmatrix},$$

where $c=\Pi_{n=1}^{N} f_{l;n,n+1}(0,x_n)$. Now notice that $f_l(0,x)$ satisfies $f''_l(0,x)=V_{0,1}(x)f_l(0,x)$ with the boundary conditions $f_l(0,x_1)=c$ and $f'_l(0,x_1)=0$; since $V_{0,1}(x)$ is exceptional, $f_l(0,x)$ must be a constant multiple of $f_r(0,x)$ in the interval $(-\infty,x_1]$. Hence $V(x)$ is exceptional.

(ii) When $N=1$ and exactly one of the two fragments is generic, then the assertion immediately follows from Eq. (2.18). Indeed, from Eqs. (2.15) and (2.17) we have

$$\frac{1}{T_{1,2}(k)}=\frac{1-L_{0,1}(-k)L(k)}{T_{0,1}(-k)T(k)},$$

and hence if $T(0)\neq 0$ and $T_{0,1}(0)\neq 0$, we must have $T_{1,2}(0)\neq 0$. Consequently, if both $V(x)$ and $V_{0,1}(x)$ are exceptional, $V_{1,2}(x)$ has to be exceptional. A similar argument shows that if $T(0)\neq 0$ and $T_{1,2}(0)\neq 0$, we must have $T_{0,1}(0)\neq 0$. When $N\geqslant 2$, assume that the generic fragment is $V_{j_0,j_0+1}(x)$. Multiply Eq. (2.17) by $T_{j_0,j_0+1}(k)$ so that

$$T_{j_0,j_0+1}(k)\Lambda(k)=\Lambda_{0,1}(k)\cdots[T_{j_0,j_0+1}(k)\Lambda_{j_0,j_0+1}(k)]\cdots\Lambda_{N,N+1}(k). \tag{2.21}$$

Now let $k\to 0$ in Eq. (2.21). Since in the generic case, $\lim_{k\to 0} T(k)/k = ic_0$ for some real, nonzero constant c_0 (p. 303 of Ref. 5), we have $T_{j_0,j_0+1}(0)/\overline{T_{j_0,j_0+1}(0)} = -1$. Also, $R(0)=L(0)=-1$ in the generic case. Thus on the right-hand side of Eq. (2.21) we get

$$\lim_{k\to 0}\,[T_{j_0,j_0+1}(k)\Lambda(k)] = \Lambda_{0,1}(0)\Lambda_{1,2}(0)\cdots\begin{bmatrix} 1 & 1 \\ -1 & -1 \end{bmatrix}\cdots\Lambda_{N,N+1}(0).$$

Since $\det \Lambda_{j,j+1}(k)=1$, the matrices $\Lambda_{j,j+1}(0)$ are invertible and hence it follows that the matrix product in Eq. (2.21) is nonzero as $k\to 0$. This implies that $\lim_{k\to 0}[k\Lambda(k)]\neq 0$ and hence $V(x)$ must be generic. As in (i), one could also use the transfer matrices to give an alternate proof of part (ii). ■

Theorem 2.4: Any nontrivial potential, generic or exceptional, can be fragmented into at least two generic pieces. There are infinitely many different ways of fragmenting a nontrivial potential into generic pieces.

Proof: If suffices to show that if a given portion contains an exceptional piece that is not identically zero, then that piece can further be partitioned into infinitely many generic pieces. Suppose that $V_{j,j+1}(x)$ is exceptional and not identically zero. Then there is a subinterval of (x_j, x_{j+1}) on which $f_l'(0, x) \neq 0$. Choosing any point in this subinterval to partition $V_{j,J+1}(x)$ yields two fragments that are both generic.

An alternate proof can be given as follows. Let $f_{l;j,j+1}(k,x)$ be the corresponding Jost solution from the left for the potential $V_{j,j+1}(x)$. From Eq. (2.9) we have

$$\int_{x_j}^{x_{j+1}} dx\; V_{j,j+1}(x) f_{l;j,j+1}(0, x) = 0. \tag{2.22}$$

Then for any $z\in\mathbf{R}$, consider the fragmentation of $V_{j,j+1}(x)$ given by

$$V_{j,j+1}(x) = \theta(z-x)V_{j,j+1}(x) + \theta(x-z)V_{j,j+1}(x), \tag{2.23}$$

where $\theta(x)$ is the Heaviside function, i.e., $\theta(x)=1$ if $x>0$ and $\theta(x)=0$ if $x<0$. The fragments given in Eq. (2.23) have to be generic for an infinite number of values $z\in(x_j,x_{j+1})$, because $V_{j,j+1}(x)$ is nontrivial and so the integral obtained by replacing the lower limit in (2.22) by z has to be nonzero for some z, and hence, by continuity, for infinitely many z. ■

One can also consider fragmentations that contain exceptional pieces. From Theorem 2.3 we already know that a generic potential cannot be divided into two exceptional fragments. A generic potential can be divided into one generic and one exceptional piece if and only if there is a point x_1 where either $f_l'(0, x_1) = 0$ or $f_r'(0, x_1) = 0$. In the first case, the piece to the right of x_1 is exceptional while the piece to the left of x_1 is generic. In the second case, the types of the pieces are reversed. We may or may not be able to fragment a nontrivial exceptional potential into two nontrivial exceptional pieces. For example, the square-well potential supported on $0<x<a$ becomes exceptional at the depths $-j^2\pi^2/a^2$ with $j=1, 2, 3,...$, and hence the square-well potential given by

$$V(x) = \begin{cases} -\pi^2, & x\in(0,1), \\ 0, & \text{elsewhere}, \end{cases}$$

cannot be fragmented into two nontrivial exceptional pieces. A nontrivial exceptional potential can be cut into two nontrivial exceptional pieces if and only if there is a point x_1 where $f_l'(0, x_1) = 0$. If we have an exceptional potential we can choose each zero of $f_l'(0, x)$ as a separation point.

This will give the partition into the largest possible number of exceptional pieces, and that number may be finite or infinite. Example 3.1 demonstrates that an exceptional potential can be fragmented into an infinite number of exceptional pieces. If $V(x)$ is generic, then choosing the zeros of $f_l'(0,x)$ [respectively, $f_r'(0,x)$] as separation points, we obtain a partition where all pieces are exceptional except one, namely $V_{0,1}(x)$ [respectively, $V_{N,N+1}(x)$].

We note that if more than one fragment of $V(x)$ is generic, then $V(x)$ may be generic or exceptional. The following example illustrates this point.

Example 2.5: Assume

$$V_{0,1}(x)=\frac{-4e^{\sqrt{2}x}}{(1+e^{\sqrt{2}x})^2}\,\theta(-x),\quad V_{1,2}(x)=\frac{-4e^{-\sqrt{2}x}}{(1+e^{-\sqrt{2}x})^2}\,\theta(x).$$

Both $V_{0,1}(x)$ and $V_{1,2}(x)$ are generic, and in fact we have

$$T_{0,1}(k)=T_{1,2}(k)=\frac{k(k+i/\sqrt{2})}{k^2+1/4},\quad R_{0,1}(k)=L_{1,2}(k)=\frac{-1}{4k^2+1}.$$

Note that corresponding to $V(x)=V_{0,1}(x)+V_{1,2}(x)$ we have

$$T(k)=\frac{k+i/\sqrt{2}}{k-i/\sqrt{2}},\quad R(k)=0,$$

which is the exceptional case.

On the other hand, in terms of $u(x)$ and $v(x)$ given by

$$u(x)=8[4(3+2\sqrt{2})e^{\sqrt{2}x}-64e^{2x}+8e^{(2+\sqrt{2})x}-e^{(2+2\sqrt{2})x}+4(3-2\sqrt{2})e^{(4+\sqrt{2})x}],$$

$$v(x)=8+8e^{2x}-(3+2\sqrt{2})e^{\sqrt{2}x}-(3-2\sqrt{2})e^{(2+2\sqrt{2})x},$$

let us define

$$V_{0,1}(x)=\frac{u(x)}{v(x)^2}\,\theta(-x),\quad V_{1,2}(x)=\frac{-e^{-\sqrt{2}x}}{(1+e^{-\sqrt{2}x}/4)^2}\,\theta(x),$$

both of which are generic with the corresponding transmission coefficients

$$T_{0,1}(k)=\frac{50k(k+i)(\sqrt{2}k+i)}{50\sqrt{2}k^3+70ik^2+13\sqrt{2}k+31i},\quad T_{1,2}(k)=\frac{25k(\sqrt{2}k+i)}{25\sqrt{2}k^2+15ik+4\sqrt{2}}.$$

The sum $V(x)=V_{0,1}(x)+V_{1,2}(x)$ is a generic potential with the scattering coefficients given by

$$T(k)=\frac{2k(k+i)}{2k^2+1},\quad R(k)=\frac{-1}{2k^2+1}.$$

Finally, we analyze $T_\xi(0)$ corresponding to the potential $V_\xi(x)$ given in Eq. (2.19), as the analysis of $T_\xi(k)$ for $k=0$ was omitted from Theorem 2.2. In order to have $|T_\xi(0)|=1$, it is necessary that $V_\xi(x)$ is exceptional, and hence we first analyze the conditions for which $V_\xi(x)$ is exceptional. Let $F_l(k,x)$ and $F_r(k,x)$ denote the Jost solutions from the left and from the right, respectively, for the potential $V_\xi(x)$. Let us also use $f_l(k,x)$ and $f_r(k,x)$ to denote the Jost solutions from the left and from the right, respectively, for the potential $V(x)$. Note that $V_\xi(x)=0$ for $x\in(x_1-\xi,x_1+\xi)$, and hence we have

$$F_l(0,x)=\begin{cases} f_l(0,x+\xi)\left[1-2\xi\dfrac{f_l'(0,x_1)}{f_l(0,x_1)}-2\xi f_l'(0,x_1)^2\displaystyle\int_{x+\xi}^{x_1}\frac{dt}{f_l(0,t)^2}\right], & x\leqslant x_1-\xi,\\ (x-x_1-\xi)f_l'(0,x_1)+f_l(0,x_1), & x\in[x_1-\xi,\,x_1+\xi],\\ f_l(0,x-\xi), & x\geqslant x_1+\xi, \end{cases} \tag{2.24}$$

$$F_r(0,x)=\begin{cases} f_r(0,x+\xi), & x\leqslant x_1-\xi,\\ (x-x_1+\xi)f_r'(0,x_1)+f_r(0,x_1), & x\in[x_1-\xi,\,x_1+\xi],\\ f_r(0,x-\xi)\left[1+2\xi\dfrac{f_r'(0,x_1)}{f_r(0,x_1)}-2\xi f_r'(0,x_1)^2\displaystyle\int_{x_1}^{x-\xi}\frac{dt}{f_r(0,t)^2}\right], & x\geqslant x_1+\xi. \end{cases} \tag{2.25}$$

From Eqs. (2.24) and (2.25) we see that $V_\xi(x)$ is exceptional if and only if the ratio $F_r(0,x)/F_l(0,x)$ is independent of x; since $F_l(0,x)$ and $F_r(0,x)$ are linear functions in the interval $x\in[x_1-\xi,x_1+\xi]$, we can conclude that $V_\xi(x)$ is exceptional if and only if

$$\frac{F_r(0,x_1+\xi)}{F_l(0,x_1+\xi)}=\frac{F_r(0,x_1-\xi)}{F_l(0,x_1-\xi)},$$

from which we obtain

$$\xi=\frac{[f_l(0,x_1);f_r(0,x_1)]}{2f_l'(0,x_1)f_r'(0,x_1)}=\frac{d_r-d_l}{2d_rd_l}, \tag{2.26}$$

where $[f;g]=fg'-f'g$ denotes the Wronskian and we have defined

$$d_l=\frac{f_l'(0,\ x_1)}{f_l(0,\ x_1)},\quad d_r=\frac{f_r'(0,\ x_1)}{f_r(0,\ x_1)}.$$

The cases in which $f_l(0,x_1)=0$ and $f_r(0,x_1)=0$ are included by setting $d_l=\infty$ and $d_r=\infty$, respectively.

(a) If $d_l\neq0$ and $d_r\neq0$, then there is exactly one value of ξ given by Eq. (2.26) for which $V_\xi(x)$ is exceptional provided the right-hand side of Eq. (2.26) is positive. Otherwise, $V_\xi(x)$ is generic.

(b) If $d_l=d_r=0$, i.e., if $f_l'(0,x_1)=f_r'(0,x_1)=0$, then both fragments and hence also $V(x)$ are exceptional. Thus, $V_\xi(x)$ is exceptional for all $\xi\geqslant0$.

(c) If $d_l\neq0$ and $d_r=0$, then $V_{0,1}(x)$ is exceptional and $V_{1,2}(x)$ is generic. Thus, $T_{0,1}(0)\neq0$, $T_{1,2}(0)=0$, $R_{1,2}(0)=-1$, and $|L_{0,1}(0)|<1$, and Eq. (2.18) shows that $T_\xi(0)=0$ and hence we are in the generic case for all $\xi\geqslant0$. This is also in agreement with Theorem 2.3 (ii).

(d) If $d_l=0$ and $d_r\neq0$, then the analysis is similar to case (c); thus $V_\xi(x)$ is generic for all $\xi\geqslant0$.

(e) If $d_l\neq0$ and $d_r=\infty$, then $f_l'(0,x_1)\neq0$ and $f_r(0,x_1)=0$; both fragments are generic. From Eq. (2.26) we see that $V_\xi(x)$ is exceptional only when $\xi=1/(2d_l)$ provided that $d_l>0$. Otherwise $V_\xi(x)$ is generic, and in particular $V(x)$ is generic.

(f) If $d_l=\infty$ and $d_r\neq0$, the analysis is similar to case (e). Then, from Eq. (2.26) we see that $V_\xi(x)$ is exceptional only when $\xi=-1/(2d_r)$ provided that $d_r<0$. Otherwise $V_\xi(x)$ is generic, and in particular $V(x)$ is generic.

(g) If $d_l=0$ and $d_r=\infty$, from (2.26) in the limiting case it is seen that no ξ exists for which $V_\xi(x)$ is exceptional. Similarly, if $d_l=\infty$ and $d_r=0$, $V_\xi(x)$ is always generic.

(h) If $d_l=d_r=\infty$, we have $f_l(0,x_1)=f_r(0,x_1)=0$ and hence $f_l(0,x)$ and $f_r(0,x)$ are linearly dependent. Thus, $V(x)$ is exceptional. However, as seen from Eq. (2.26), $V_\xi(x)$ is generic for every $\xi>0$. In other words, $T_\xi(0)\neq0$ for $\xi=0$ but $T_\xi(0)=0$ for all $\xi>0$.

Once all the ξ values are obtained in cases (a), (b), (e), and (f) for which V_ξ is exceptional, one needs to determine which of these ξ values correspond to $|T_\xi(0)|=1$. For example, in case (b), we can proceed as follows. From Eq. (2.18) we have

$$\frac{1}{T_\xi(0)}=\frac{1-R_{0,1}(0)L_{1,2}(0)}{T_{0,1}(0)T_{1,2}(0)}, \tag{2.27}$$

and hence $T_\xi(0)$ is independent of ξ. Let $\gamma_{0,1}$ be the constant defined as in Eq. (2.10) giving the ratio of the zero-energy Jost solutions for the potential $V_{0,1}(x)$, and let $\gamma_{1,2}$ be defined similarly for the potential $V_{1,2}(x)$. As in Eq. (2.13), we have

$$R_{0,1}(0)=\frac{1-\gamma_{0,1}^2}{1+\gamma_{0,1}^2}, \quad L_{1,2}(0)=\frac{\gamma_{1,2}^2-1}{1+\gamma_{1,2}^2}. \tag{2.28}$$

Using Eq. (2.28) in Eq. (2.27) we obtain

$$T_\xi(0)=\frac{2\gamma_{0,1}\gamma_{1,2}}{1+\gamma_{0,1}^2\gamma_{1,2}^2},$$

from which we see that $|T_\xi(0)|=1$ if and only if $\gamma_{0,1}\gamma_{1,2}=\pm 1$.

III. WAVE PROPAGATION IN A NONHOMOGENEOUS MEDIUM

The fragmentation of an exceptional potential into two generic pieces has important consequences in direct and inverse scattering problems associated with wave propagation, where the governing equations are related to the Schrödinger equation or its variants. One such differential equation is given by

$$\frac{d^2\psi(k,x)}{dx^2}+\frac{k^2}{c(x)^2}\,\psi(k,x)=Q(x)\psi(k,x), \tag{3.1}$$

or by its time domain equivalent

$$\frac{\partial^2\phi(t,x)}{\partial x^2}-\frac{1}{c(x)^2}\,\frac{\partial^2\phi(t,x)}{\partial t^2}=Q(x)\phi(t,x). \tag{3.2}$$

Equation (3.1) describes the quantum mechanical behavior of a particle when the potential also depends on its energy. Equations (3.1) and (3.2) describe the propagation of waves in a one-dimensional nonhomogeneous, nonabsorptive medium where the wavespeed is $c(x)$ and the restoring force density is $Q(x)$. These equations can be analyzed by transforming them into Schrödinger equations by using local Liouville transformations.[11] In the special (but still significant) case $Q(x)=0$, the potential in the transformed Schrödinger equation is always exceptional. One important outcome of Theorem 2.4 is that it is possible to choose the local Liouville transformations in such a way that all the resulting fragments of the transformed Schrödinger equations are either generic or pertain to a potential vanishing identically. This leads to considerable simplifications in the small-k analysis of Eqs. (3.1) and (3.2). For example, consider Eq. (3.25) of Ref. 11 where the Jost solutions and their space derivatives are expressed as a product of matrices, each of which is expressed in terms of the quantities related to one fragment only. The matrices in Eq. (3.25) of Ref. 11 contain the factor $t_{j-1,j}(k)/k$, where $t_{j-1,j}(k)$ is the transmission coefficient corresponding to the jth fragment; that factor remains continuous as $k\to 0$ if the jth piece is generic and it is singular if the jth piece is exceptional. Hence, by fragmenting the exceptional pieces into generic ones, it becomes obvious that the Jost solutions and their space derivatives are continuous at $k=0$.

Let us write Eq. (3.1) as

$$\psi''(k,x)+k^2H(x)^2\psi(k,x)=Q(x)\psi(k,x), \quad x\in\mathbf{R}. \tag{3.3}$$

Our assumptions on $Q(x)$ and $H(x)$ are as follows:

(H1) $H(x)$ is strictly positive, piecewise continuous with possible discontinuities in $H(x)$ or $H'(x)$ occurring at the N points $x_1<\cdots<x_N$.

(H2) $H(x)\to H_\pm$ as $x\to\pm\infty$, where $H_\pm$ are positive constants.

(H3) $H-H_\pm\in L^1(\mathbf{R}^\pm)$, where $\mathbf{R}^-=(-\infty,0)$ and $\mathbf{R}^+=(0,+\infty)$.

(H4) H' is absolutely continuous on (x_n,x_{n+1}) and $2H''H-3(H')^2\in L^1_1(x_n,x_{n+1})$ for $n=0,\ldots,N$, where $x_0=-\infty$ and $x_{N+1}=+\infty$.

(H5) $Q(x)$ is real valued and of the form $Q(x)=W(x)+\Sigma_{j=1}^N c_j\delta(x-x_j)$, where $W\in L^1_1(\mathbf{R})$ and $\delta(x)$ is the Dirac delta function.

Conditions (H1)–(H5), without the delta-function terms in (H5), were introduced in Ref. 11, where the inverse scattering problem for Eq. (3.3), namely the recovery of the coefficient $H(x)$ from an appropriate set of scattering data, was studied. Hypothesis (H1) allows for abrupt changes in the material properties of the medium in which the wave propagates. In (H5) we have now included delta functions because they are often useful in working out explicitly solvable examples. Moreover, it is of interest to see how some of the results are affected by delta functions superimposed on discontinuities in $H(x)$ and $H'(x)$. The delta-function potential $V(x)=\alpha\delta(x-a)$ corresponds to

$$T(k)=\frac{k}{k+i\alpha/2}, \quad R(k)=\frac{-i\alpha/2}{k+i\alpha/2}\,e^{2ika}, \quad L(k)=\frac{-i\alpha/2}{k+i\alpha/2}\,e^{-2ika}, \tag{3.4}$$

from which we see that it is a generic potential.

As for Eq. (2.1), Eq. (3.3) also has two linearly independent scattering solutions, namely the Jost solutions $f_l(k,x)$ and $f_r(k,x)$ satisfying the boundary conditions

$$f_l(k,x)=\begin{cases} e^{ikH_+x}+o(1), & x\to+\infty,\\ \dfrac{1}{T_l(k)}\,e^{ikH_-x}+\dfrac{L(k)}{T_l(k)}\,e^{-ikH_-x}+o(1), & x\to-\infty,\end{cases}$$

$$f_r(k,x)=\begin{cases} \dfrac{1}{T_r(k)}\,e^{-ikH_+x}+\dfrac{R(k)}{T_r(k)}\,e^{ikH_+x}+o(1), & x\to+\infty,\\ e^{-ikH_-x}+o(1), & x\to-\infty.\end{cases}$$

Here, $T_l(k)$ and $T_r(k)$ are the transmission coefficients from the left and from the right, respectively, and $L(k)$ and $R(k)$ are the reflection coefficients from the left and from the right, respectively. Associated with Eq. (3.3) is the scattering matrix

$$\mathbf{S}(k)=\begin{bmatrix} T_l(k) & R(k)\\ L(k) & T_r(k)\end{bmatrix}. \tag{3.5}$$

The matrix $\mathbf{S}(k)$ is not unitary unless $H_+=H_-$; we have $\mathbf{S}(-k)=\overline{\mathbf{S}(k)}$ for real k, and

$$H_+T_l(k)=H_-T_r(k), \quad \text{Im } k\geqslant 0,$$

$$T_r(-k)T_l(k)+|R(k)|^2=T_r(k)T_l(-k)+|L(k)|^2=1, \quad k\in\mathbf{R},$$

$$R(k)T_r(-k)+L(-k)T_r(k)=0, \quad k\in\mathbf{R}.$$

In the study of the scattering matrix $\mathbf{S}(k)$ given in Eq. (3.5), one again has to distinguish between the generic case and the exceptional case. As in Sec. II, in the generic case the transmission coefficients vanish linearly as $k\to 0$, whereas in the exceptional case we have $T_l(0)\neq 0$ and $T_r(0)\neq 0$. Furthermore, in the generic case $R(0)=L(0)=-1$, while in the exceptional case $|R(0)|=|L(0)|<1$. The coefficient $H(x)$ in Eq. (3.3) has no influence on the leading behavior of the transmission coefficients as $k\to 0$, and hence the generic and exceptional cases are determined by the potential $Q(x)$ only. All the characterizations of the two cases for the Schrödinger equation hold verbatim also for Eq. (3.3). If $Q(x)=0$ in Eq. (3.3), we have the exceptional case. If $Q(x)$ is nontrivial and $Q(x)\geqslant 0$ in Eq. (3.3), then we have the generic case. All the differences between the two cases as $k\to 0$ outlined in Sec. II also exist[11–13] in the wave propagation problem associated with Eq. (3.3).

Let us generalize the factorization formula (2.17) to the scattering problem for Eq. (3.3). Under the Liouville transformation

$$y=y(x)=\int_0^x ds\ H(s), \quad \psi(k,x)=\frac{1}{\sqrt{H(x)}}\ \phi(k,y), \tag{3.6}$$

Eq. (3.3) is transformed into

$$\frac{d^2\phi(k,y)}{dy^2}+k^2\phi(k,y)=V(y)\,\phi(k,y), \tag{3.7}$$

where

$$V(y)=V(y(x))=\frac{H''(x)}{2H(x)^3}-\frac{3}{4}\frac{H'(x)^2}{H(x)^4}+\frac{Q(x)}{H(x)^2}. \tag{3.8}$$

Since, by (H1), $H(x)$ and $H'(x)$ are allowed to have jump discontinuities at x_j for $j=1,\ldots,N$, the function $V(y)$ is undefined at $y_j=y(x_j)$ for $j=1,\ldots,N$. In agreement with Eq. (3.6), we set $y_0=y(x_0)=-\infty$ and $y_{N+1}=y(x_{N+1})=+\infty$. Then $V(y)$ is well defined in each of the intervals (y_j,y_{j+1}) for $j=0,\ldots,N$, and (H4) ensures that $V\in L_1^1$ on these intervals. In view of (H5), the solutions of Eq. (3.3) satisfy the conditions

$$\psi(k,x_n-0)=\psi(k,x_n+0), \quad \psi'(k,x_n+0)-\psi'(k,x_n-0)=c_n\psi(k,x_n). \tag{3.9}$$

As a result, by using Eqs. (3.6) and (3.9), we deduce that the solutions of Eq. (3.7) satisfy the self-adjoint boundary conditions

$$\phi(k,y_n-0)=\sqrt{q_n}\ \phi(k,y_n+0), \tag{3.10}$$

$$\frac{d\phi(k,y_n-0)}{dy}=\nu_n\phi(k,y_n+0)+\frac{1}{\sqrt{q_n}}\frac{d\phi(k,y_n+0)}{dy}, \tag{3.11}$$

where

$$q_n=\frac{H(x_n-0)}{H(x_n+0)},$$

$$\nu_n=\frac{1}{2\sqrt{H(x_n-0)H(x_n+0)}}\left[\frac{H'(x_n-0)}{H(x_n-0)}-\frac{H'(x_n+0)}{H(x_n+0)}-2c_n\right]. \tag{3.12}$$

The scattering matrix corresponding to Eq. (3.7) equipped with these boundary conditions is known as the ''reduced scattering matrix''[11] and is given by

$$\sigma(k)=\begin{bmatrix}\tau(k) & \rho(k)\\ \ell(k) & \tau(k)\end{bmatrix},$$

where $\tau(k)$ is the reduced transmission coefficient and $\rho(k)$ and $\ell(k)$ are the reduced reflection coefficients from the right and from the left, respectively. The reduced scattering matrix is unitary and its entries are related to the scattering matrix $\mathbf{S}(k)$ given in Eq. (3.5) as follows:[11]

$$\tau(k)=\sqrt{\frac{H_+}{H_-}}\,T_l(k)e^{ikA}=\sqrt{\frac{H_-}{H_+}}\,T_r(k)e^{ikA}, \tag{3.13}$$

$$\rho(k)=R(k)e^{2ikA_+}, \quad \ell(k)=L(k)e^{2ikA_-},$$

where

$$A_\pm=\pm\int_0^{\pm\infty} ds\,[H_\pm-H(s)], \quad A=A_++A_-.$$

The points y_j generate a partition of the real line, and so we define

$$V_{j,j+1}(y)=\begin{cases}V(y), & y\in(y_j,y_{j+1}),\\ 0, & \text{elsewhere.}\end{cases}$$

We let $\tau_{j,j+1}(k)$, $\rho_{j,j+1}(k)$, and $\ell_{j,j+1}(k)$ denote the transmission coefficient and the reflection coefficients from the right and from the left, respectively, for the potential $V_{j,j+1}(y)$, and, as in Eq. (2.15), we define

$$\Lambda(k)=\begin{bmatrix}\dfrac{1}{\tau(k)} & -\dfrac{\rho(k)}{\tau(k)}\\ \dfrac{\ell(k)}{\tau(k)} & \dfrac{1}{\tau(-k)}\end{bmatrix}, \quad \Lambda_{j,j+1}(k)=\begin{bmatrix}\dfrac{1}{\tau_{j,j+1}(k)} & -\dfrac{\rho_{j,j+1}(k)}{\tau_{j,j+1}(k)}\\ \dfrac{\ell_{j,j+1}(k)}{\tau_{j,j+1}(k)} & \dfrac{1}{\tau_{j,j+1}(-k)}\end{bmatrix}. \tag{3.14}$$

By suppressing the k-dependence of the transition matrices in Eq. (3.14), we have the generalization of Eq. (2.17) in the case of Eq. (3.3) given by[13]

$$\Lambda=\Lambda_{0,1}F_1\Lambda_{1,2}F_2\Lambda_{2,3}\cdots F_N\Lambda_{N,N+1}, \tag{3.15}$$

where F_j for $j=1,\ldots,N$ are the matrices defined by

$$F_j(k)=\begin{bmatrix}\alpha_n+\dfrac{\nu_n}{2ik} & \left(\beta_n+\dfrac{\nu_n}{2ik}\right)e^{-2iky}\\ \left(\beta_n-\dfrac{\nu_n}{2ik}\right)e^{2iky_n} & \alpha_n-\dfrac{\nu_n}{2ik}\end{bmatrix},$$

with

$$\alpha_n=\frac{1}{2}\left[\sqrt{\frac{H(x_n-0)}{H(x_n+0)}}+\sqrt{\frac{H(x+0)}{H(x_n-0)}}\right], \quad \beta_n=\frac{1}{2}\left[\sqrt{\frac{H(x_n-0)}{H(x_n+0)}}-\sqrt{\frac{H(x_n+0)}{H(x_n-0)}}\right],$$

and where the constants ν_n are given in Eq. (3.12).

The matrices F_j account for the internal boundary conditions (3.10) and (3.11). In order to justify Eq. (3.15), again consider the case $N=1$ first. Using notations similar to those used below Eq. (2.17), we let $\phi(k,y)$ be a solution of Eq. (3.7) such that $\phi(k,y)=c_1e^{iky}+c_2e^{-iky}$ as $y\to+\infty$, and we define $\phi_{1,2}(k,y)$ and $\phi_{0,1}(k,y)$ as solutions of Eq. (3.7) for the fragments $V_{0,1}(y)$ and $V_{1,2}(y)$ such that $\phi_{1,2}(k,y)=\phi(k,y)$ for $y>y_1$ and $\phi_{0,1}(k,y)=\phi(k,y)$ for $y<y_1$. Then, $\phi_{1,2}(k,y)=\tilde{d}_1e^{iky}+\tilde{d}_2e^{-iky}$ for $y<y_1$ and $\phi_{0,1}(k,y)=\tilde{c}_1e^{iky}+\tilde{c}_2e^{-iky}$ for $y>y_1$, with suitable constants $\tilde{d}_1$, $\tilde{d}_2$, $\tilde{c}_1$, and $\tilde{c}_2$. Now the coefficients $\tilde{d}_1$ and $\tilde{d}_2$ are related to the coefficients $\tilde{c}_1$ and $\tilde{c}_2$ through the boundary conditions (3.10) and (3.11) by setting $\phi(k,y_1-0)=\phi_{0,1}(k,y_1)$, $\phi'(k,y_1-0)=\phi'_{0,1}(k,y_1)$, and $\phi(k,y_1+0)=\phi_{1,2}(k,y_1)$, $\phi'(k,y_1+0)=\phi'_{1,2}(k,y_1)$. This yields

$$\begin{bmatrix} e^{iky_1} & e^{-iky_1} \\ ike^{iky_1} & -ike^{-iky_1} \end{bmatrix}\begin{bmatrix} \tilde{c}_1 \\ \tilde{c}_2 \end{bmatrix}=\begin{bmatrix} \sqrt{q_1} & 0 \\ \nu_1 & \dfrac{1}{\sqrt{q_1}} \end{bmatrix}\begin{bmatrix} e^{iky_1} & e^{-iky_1} \\ ike^{iky_1} & -ike^{-iky_1} \end{bmatrix}\begin{bmatrix} \tilde{d}_1 \\ \tilde{d}_2 \end{bmatrix},$$

from which we obtain $[\tilde{c}_1\ \tilde{c}_2]^t=F_1[\tilde{d}_1\ \tilde{d}_2]^t$. This proves Eq. (3.15) when $N=1$, and the general case follows by induction. Note that F_n can be written as a product of three matrices, namely

$$F_n=\Lambda(x_n-0,\,x_n)\Lambda[x_n,x_n]\Lambda(x_n,x_n+0), \tag{3.16}$$

where

$$\Lambda(x_n-0,\,x_n)=\begin{bmatrix} \alpha_n^-+\dfrac{\nu_n^-}{2ik} & \left(\beta_n^-+\dfrac{\nu_n^-}{2ik}\right)e^{-2iky_n} \\ \left(\beta_n^--\dfrac{\nu_n^-}{2ik}\right)e^{2iky_n} & \alpha_n^--\dfrac{\nu_n^-}{2ik} \end{bmatrix},$$

$$\Lambda[x_n,x_n]=\begin{bmatrix} 1-\dfrac{c_n}{2ik} & \dfrac{c_n}{2ik}\,e^{-2iky_n} \\ -\dfrac{c_n}{2ik}\,e^{2iky_n} & 1+\dfrac{c_n}{2ik} \end{bmatrix},$$

$$\Lambda(x_n,x_n+0)=\begin{bmatrix} \alpha_n^++\dfrac{\nu_n^+}{2ik} & \left(\beta_n^++\dfrac{\nu_n^+}{2ik}\right)e^{-2iky_n} \\ \left(\beta_n^+-\dfrac{\nu_n^+}{2ik}\right)e^{2iky_n} & \alpha_n^+-\dfrac{\nu_n^+}{2ik} \end{bmatrix},$$

with

$$\alpha_n^{\mp}=\frac{1}{2}\left[\sqrt{H(x_n\mp0)}+\frac{1}{\sqrt{H(x_n\mp0)}}\right],\quad \beta_n^{\mp}=\pm\frac{1}{2}\left[\sqrt{H(x_n\mp0)}-\frac{1}{\sqrt{H(x_n\mp0)}}\right],$$

$$\nu_n^{\mp}=\frac{\pm1}{2\sqrt{H(x_n\mp0)}}\,\frac{H'(x_n\mp0)}{H(x_n\mp0)}.$$

We remark that the transition matrix $\Lambda(x_n-0,x_n)$ is due to the hard scatterer caused by a jump in $H(x)$ from $H(x_n-0)$ to 1 and a jump in $H'(x)$ from $H'(x_n-0)$ to 0. The transition matrix $\Lambda[x_n,x_n]$ is due to the hard scatterer $c_n\delta(x-x_n)$, as seen from Eq. (3.4). The transition matrix $\Lambda(x_n,x_n+0)$ is due to the hard scatterer caused by a jump in $H(x)$ from 1 to $H(x_n+0)$ and a

jump in $H'(x)$ from 0 to $H'(x_n+0)$. The transition matrices $\Lambda_{n,n+1}(k)$ in Eq. (3.15) are due to the soft scatterers $V_{n,n+1}(y)$. In the special case when $H(x)=1$ and $W(x)=0$ in (H5), Eq. (3.15) takes the form

$$\Lambda=\Lambda[x_1,x_1]\cdots\Lambda[x_N,x_N], \tag{3.17}$$

which describes scattering by a superposition of delta functions located at $x_1,\ldots,x_N$.

We mention one application of the factorization formula (3.15) in the inverse scattering problem for Eq. (3.3) concerning the large-k asymptotics of $\tau(k)$, $\rho(k)$, and $\ell(k)$; we refer the reader to Refs. 11–13 for details: it is known that from the large-k asymptotics of a reduced reflection coefficient one can recover the ratios q_n and ν_n (cf. Ref. 13, where the case $c_n=0$ was studied). It is seen from Eq. (3.12) that the coefficients c_n affect the large-k asymptotics through the constants ν_n and thus contribute in the same manner as the jumps in the derivative of $H(x)$. We also see that c_n can be chosen suitably to cancel the contribution from a jump in $H'(x)$.

In the recovery of $H(x)$ in Eq. (3.3), the distinction between the exceptional and generic cases is important. For example, in the absence of bound states, given the scattering data consisting of a reduced reflection coefficient and $Q(x)$, one obtains a one-parameter family of $H(x)$ in the exceptional case and a unique $H(x)$ in the generic case.[11–13] Therefore, in the exceptional case one must include either H_+ or H_- in the scattering data for the unique recovery of $H(x)$; however, in the generic case, H_+ or H_- cannot be specified in the scattering data and instead these constants are themselves recovered during the inversion procedure.

Finally in this section we give an example of an exceptional potential that can be fragmented into an infinite number of only exceptional pieces.

Example 3.1: In Eq. (3.3) choose $Q(x)=0$ and

$$H(x)=\begin{cases}1+\left(\dfrac{\sin x}{x}\right)^3, & x\neq 0,\\ 2, & x=0.\end{cases} \tag{3.18}$$

Note that $H(x)$ is strictly positive and bounded, $H_\pm=1$, and

$$H'(x)=\begin{cases}\dfrac{3\sin^2 x}{x^4}\,[x\cos x-\sin x], & x\neq 0,\\ 0, & x=0,\end{cases}$$

$$H''(x)=\begin{cases}\dfrac{3\sin x}{x^5}\,[x^2(3\cos^2 x-1)-6x\cos x\sin x+4\sin^2 x], & x\neq 0,\\ 0, & x=0,\end{cases}$$

and hence H, H', and H'' are all continuous on $\mathbf{R}$. Since $Q(x)=0$, we are in the exceptional case, and hence the transmission coefficients $T_l(k)$ and $T_r(k)$ cannot vanish at $k=0$. Note that $H(n\pi)=1$, $H'(n\pi)=0$, and $H''(n\pi)=0$ for any integer n. Using Eq. (3.6) let us define $y_n=y(n\pi)$. Now consider the potential $V(y)$ obtained by using Eq. (3.18) and $Q(x)=0$ in Eq. (3.8). That potential must be exceptional, and in fact from Eq. (3.13) it can be seen that the transmission coefficient $\tau(k)$ corresponding to the potential $V(y)$ cannot vanish at $k=0$. Now let us fragment $V(y)$ as $V(y)=\sum_{n=-\infty}^{\infty}V_{n,n+1}(y)$, where we have defined

$$V_{n,n+1}(y)=\begin{cases}V(y), & y\in(y_n,y_{n+1}),\\ 0, & \text{elsewhere.}\end{cases} \tag{3.19}$$

The following argument shows that each $V_{n,n+1}(y)$ is exceptional. Since $Q(x)=0$ in Eq. (3.3), the corresponding zero-energy Jost solution is given by $f_l(0,x)=1$ for $x\in\mathbf{R}$. Using Eq. (5.1) of Ref. 11, we see that the zero-energy Jost solution from the left of Eq. (3.7) is given by

$$g_l(0,y)=g_l(0,y(x))=\sqrt{H(x)}.$$

Hence, we obtain

$$g_l'(0,y)=\frac{dg_l(0,y)}{dy}=\frac{dx}{dy}\,\frac{d\sqrt{H(x)}}{dx}=\frac{H'(x)}{2H(x)^{3/2}}. \tag{3.20}$$

Since $H'(n\pi)=0$, from Eq. (3.20) we see that $g_l'(0,y_n)=0$, and hence we can choose y_n as the separation points to fragment $V(y)$ into only exceptional pieces, which are given by Eq. (3.19).

IV. WAVE PROPAGATION IN A NONCONSERVATIVE MEDIUM

The wave propagation in a one-dimensional nonconservative medium is described, in the frequency domain, by the generalized Schrödinger equation

$$\psi''(k,x)+k^2\psi(k,x)=[ikP(x)+Q(x)]\psi(k,x),\quad x\in\mathbf{R}, \tag{4.1}$$

where k is the wave number, $P(x)$ represents the joint effect of energy absorption and generation, and $Q(x)$ stands for the restoring force density. In the time domain Eq. (4.1) corresponds to

$$\frac{\partial^2 u}{\partial x^2}-\frac{\partial^2 u}{\partial t^2}-P(x)\,\frac{\partial u}{\partial t}=Q(x)u,\quad t,x\in\mathbf{R},$$

where the wavespeed is equal to one. We will assume that $Q(x)$ is real valued and belongs to $L_1^1(\mathbf{R})$, and that $P(x)$ is real valued and belongs to $L^1(\mathbf{R})$. We have energy absorption when $P(x)\leqslant 0$ and energy generation when $P(x)\geqslant 0$; however, our results in this section are valid without assuming that $P(x)$ is positive or negative.

The scattering solutions of Eq. (4.1) are those behaving like e^{ikx} or e^{-ikx} as $x\to\pm\infty$, and such solutions occur when $k^2>0$. Among the scattering solutions are the Jost solution from the left $f_l(k,x)$ and the Jost solution from the right $f_r(k,x)$ satisfying the boundary conditions (2.2) and (2.3), respectively. The scattering matrix $\mathbf{S}(k)$ associated with Eq. (4.1) has the form (2.4). When $P(x)$ is purely imaginary, the inverse scattering problem for Eq. (4.1) was analyzed by Jaulent and Jean;[14–17] in this case the scattering matrix $\mathbf{S}(k)$ is unitary and hence the reflection coefficients cannot exceed one in absolute value. An incomplete study of the same problem when $P(x)$ is real was outlined in Ref. 18. In that case the differential equation (4.1) is no longer self-adjoint and the scattering matrix $\mathbf{S}(k)$ is no longer unitary. Consequently, the analysis of the direct and inverse scattering problems for real $P(x)$ is much more complicated than for imaginary $P(x)$.

We are interested in the analog of the factorization formula (2.17). As in Sec. II, let us partition the real axis $\mathbf{R}$ into $x_0<x_1<x_2<\cdots<x_N<x_{N+1}$ with $x_0=-\infty$ and $x_{N+1}=+\infty$. Consider the analog of Eq. (4.1) given by

$$\psi''(k,x)+k^2\psi(k,x)=[ikP_{j,j+1}(x)+Q_{j,j+1}(x)]\psi(k,x), \tag{4.2}$$

where we have defined the fragments

$$P_{j,j+1}(x)=\begin{cases}P(x), & x\in(x_j,x_{j+1}),\\ 0, & \text{elsewhere},\end{cases} \tag{4.3}$$

$$Q_{j,j+1}(x)=\begin{cases} Q(x), & x\in(x_j,x_{j+1}),\\ 0, & \text{elsewhere.}\end{cases} \tag{4.4}$$

Let the scattering matrix associated with Eq. (4.2) be given by

$$\mathbf{s}_{j,j+1}(k)=\begin{bmatrix} t_{j,j+1}(k) & r_{j,j+1}(k)\\ l_{j,j+1}(k) & t_{j,j+1}(k)\end{bmatrix}.$$

Proceeding as in the previous sections or as in Ref. 7 or Ref. 13 we obtain

$$\Lambda(k)=\Lambda_{0,1}(k)\Lambda_{1,2}(k)\cdots\Lambda_{N,N+1}(k), \tag{4.5}$$

where we have defined the transition matrices

$$\Lambda(k)=\begin{bmatrix} \dfrac{1}{T(k)} & -\dfrac{R(k)}{T(k)}\\ \dfrac{L(k)}{T(k)} & \dfrac{T(k)^2-L(k)R(k)}{T(k)}\end{bmatrix}, \tag{4.6}$$

$$\Lambda_{j,j+1}(k)=\begin{bmatrix} \dfrac{1}{t_{j,j+1}(k)} & -\dfrac{r_{j,j+1}(k)}{t_{j,j+1}(k)}\\ \dfrac{l_{j,j+1}(k)}{t_{j,j+1}(k)} & \dfrac{t_{j,j+1}(k)^2-l_{j,j+1}(k)r_{j,j+1}(k)}{t_{j,j+1}(k)}\end{bmatrix}. \tag{4.7}$$

As in the previous sections, the transition matrix given in Eq. (4.6) provides the link between the asymptotics of the scattering solutions of Eq. (4.1) at $+\infty$ and those at $-\infty$ when $e^{\pm ikx}$ are chosen as an asymptotic basis; the transition matrices in Eq. (4.7) have similar interpretations. Again, each of the matrices in Eqs. (4.6) and (4.7) can be decomposed as in Eq. (2.16). Note that the (2,2) entry in Eq. (4.6) is analytic in the lower-half complex plane $\mathbf{C}^-$ and in general cannot be replaced by $1/T(-k)$; however, it is known that[14] this entry is equal to $1/\mathscr{T}(-k)$, where $\mathscr{T}(k)$ is the transmission coefficient associated with the differential equation obtained from Eq. (4.1) by changing the sign of $P(x)$.

Again one has to distinguish between the generic and exceptional cases in studying the scattering and inverse scattering problems for Eq. (4.1). As for Eq. (3.3), the potential $Q(x)$ alone determines whether we have the generic case or the exceptional case. The difficulties arising in proofs in the exceptional case outlined in the previous sections remain true also for Eq. (4.1), and by choosing each fragment in the partitioning (4.3) and (4.4) to be either generic or identically zero we expect simplifications in the small k-analysis of the direct and inverse scattering problems for Eq. (4.1).

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ℓ^P interpolation and optimized bounds on pairwise interacting fermion systems

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We derive a set of inequalities which relate the translation invariant problem of N identical particles with pairwise interactions to an independent particle problem. These inequalities apply to attractive power law potentials $V(r)=r^q$, $1\leqslant q\leqslant\infty$, and superpositions of such potentials; they become identities in the harmonic oscillator case $q=2$. We use the inequalities to derive new upper and lower bounds for the ground state energies of fermion systems, which interact through these potentials. These bounds improve all previous results in the range $1\leqslant q\leqslant\infty$; they reduce to the exact answer in the harmonic oscillator case. © *1996 American Institute of Physics.* [S0022-2488(96)01109-7]

I. INTRODUCTION

Since the pioneering works of Fischer and Ruelle on the thermodynamic limit,[1] of Dyson and Lenard on the stability of matter,[2] and of Lévy-Leblond on the nonsaturation of gravitational forces,[3] a great deal of interest has been devoted to the derivation of lower bounds for the ground state energies of many particle systems in terms of two particle spectra.

In Ref. 4 we have shown that for boson systems, or particles of different masses, previous bounds could be considerably improved by a simple technique. The improved bounds coincide with the exact answer for harmonic interactions. This has a number of applications, for instance in relating baryon to meson masses in the quark model.

Pairwise interacting N fermion systems present a variety of interesting applications. In that case, however, the methods introduced in Ref. 4 are not able to produce any improvements to the bounds obtained by the Fischer–Ruelle–Dyson–Lenard–Lévy-Leblond (FRDL3)[1–3] technique. This is quite frustrating in the harmonic oscillator case which can be solved exactly, and where the FRDL3 bound differs from the exact result by a factor of $\sqrt{2}$. Similarly, the attractive Coulomb case can be calculated for large N with the Thomas–Fermi method. In that case, the FRDL3 result is off by a factor of ~ 3.

One reason for this difficulty in improving the FRDL3 bounds can be traced back to the known difficulty of constructing an orthogonal set of N particle wavefunctions which satisfies the three conditions of being completely antisymmetric, translationally invariant, and of being eigenfunctions of an independent particle Hamiltonian. This can only be done in the harmonic case.

In this paper, we present a new approach to the N fermion problem with pairwise interactions which deals with the particular class of potentials

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$$V(r)=\int_1^\infty r^q \mu(q)\,dq, \quad \mu \geqslant 0.$$

Although, this class does not include some cases of practical interest such as the Coulomb and Yukawa potentials, or the quark–quark confining potentials, the results are nevertheless very interesting insofar as (1) they systematically improve the FRDL3 results; (2) they produce *both* upper *and* lower bounds; and (3) they reduce to the exact answer in the harmonic case.

The derivation of these new bounds relies on the existence of a set of inequalities which is interesting as such. The proof of these inequalities is nontrivial, it requires the techniques of $\mathcal{L}^P$ interpolation, and the Riesz–Thorin interpolation theorem. For the class of potentials under consideration, these inequalities allow us to relate an N-body problem with pairwise interactions and translation invariance to an independent particle problem whose solution is known.

In Sec. I, we state the problems under consideration and recall previous bounds. In Sec. II, we use the inequalities to derive the upper and lower bounds on fermion systems, and we draw our first conclusions. Finally, in Sec. III, we give the derivation of the inequalities themselves.

II. POSITION OF THE PROBLEM

Consider a system of N identical particles with pairwise interactions $V_{ij} \equiv V(r_i - r_j)$, of Hamiltonian

$$H^N = \sum_{i=1}^N p_i^2 + \sum_{i=1}^N \sum_{j=i+1}^N V_{ij} \tag{1}$$

(for simplicity we have set the mass equal to $\frac{1}{2}$).

We denote by $\epsilon_n(\mu)$ the energy levels of a particle of mass $\mu/2$ placed in the potential $V(r)$ centered at the origin, of Hamiltonian $h = p^2/\mu + V(r)$, by g_n their degeneracies, and by $f_N(\mu)$ the ground state energy of N independent fermions, of spin s and mass $\mu/2$, each placed in this potential, of Hamiltonian

$$\tilde{H}^N = \sum_{i=1}^N h_i = \sum_{i=1}^N \left(\frac{p_i^2}{\mu} + V(r_i) \right). \tag{2}$$

We have

$$f_N(\mu) = (2s+1) \sum_{n=1}^k g_n \epsilon_n(\mu) + r\,\epsilon_{k+1}(\mu), \tag{3}$$

where the integer k is defined in terms of N by

$$(2s+1) \sum_{n=1}^k g_n + r = N < (2s+1) \sum_{n=1}^{k+1} g_n, \quad r \geqslant 0. \tag{4}$$

In the Coulomb case, $V = -1/r$, we have $\epsilon_n(\mu) = -\mu/4n^2$, $g_n = n^2$, and, for large N, $f_N(\mu) \approx -(\mu/4)(2s+1)^{2/3}(3N)^{1/3}$.

In the three-dimensional harmonic oscillator $V = r^2$, $\epsilon_n(\mu) = (2n+1)/\sqrt{\mu}$, $g_n = n(n+1)/2$, and, for large N, $f_N(\mu) \approx (6N)^{4/3}/((2s+1)^{1/3} 4\sqrt{\mu})$.

Following an argument due originally to Fischer and Ruelle,[1] one can obtain a lower bound on the N-particle ground state energy E^N, in terms of the two-particle spectrum, by rewriting the Hamiltonian (1) as a sum of N terms

$$H^N=\frac{1}{2}\sum_{i=1}^{N} H_i, \tag{5}$$

$$H_i=\sum_{j=1,j\neq i}^{N}\left(\frac{2p_j^2}{(N-1)}+V_{ij}\right). \tag{6}$$

If $|\Omega\rangle$ is the N particle ground state, $E^N=\langle\Omega|H^N|\Omega\rangle$, and therefore

$$E^N=\frac{N}{2}\langle\Omega|H_i|\Omega\rangle. \tag{7}$$

In Eq. (6), H_i appears as the Hamiltonian of $N-1$ independent particles of mass $\mu/2=(N-1)/4$, placed in the field of particle i considered as infinitely massive. Since $\langle H_i\rangle$ is larger than the ground state energy of this system, one obtains the desired lower bounds.

For bosons, we have

$$E_B^N\geqslant\frac{N(N-1)}{2}\,\epsilon_1(\mu=(N-1)/2), \tag{8}$$

which yields in the Coulomb and harmonic cases

$$E_B^N\geqslant 3N\sqrt{(N-1)/2}\quad(V=r^2), \tag{9a}$$

$$E_B^N\geqslant -N(N-1)^2/16\quad(V=1/r). \tag{9b}$$

In the case of fermions, the antisymmetry of $|\Omega\rangle$ imposes retention of only those levels of H_i which correspond to antisymmetric states in the $N-1$ particles $j=1,\ldots,N,j\neq i$. The minimal requirement is therefore to distribute evenly the $N-1$ particles over the $N-1$ lowest eigenstates of the one-particle Hamiltonian. One thus obtains

$$E_F^N\geqslant\frac{N}{2}\,f_{N-1}(\mu=(N-1)/2). \tag{10}$$

For large N, in the harmonic and Coulomb cases, respectively, one obtains

$$E_F^N\geqslant\frac{6^{4/3}}{2^{1/2}4(2s+1)^{1/3}}\,N^{11/6}\quad(V=r^2), \tag{11a}$$

$$E_F^N\geqslant-\frac{(2s+1)^{2/3}3^{1/3}}{16}\,N^{7/3}\quad(V=-1/r). \tag{11b}$$

These bounds are off by factors of $\sqrt{2}$ (harmonic case, which is exactly soluble) and ≈ 3 (Coulomb case, which can be treated by the Thomas–Fermi method for large N).

In the case of bosons (more generally, nonidentical particles), we have improved the above bounds[4] in what we believe is an optimal way.

We use the identity

$$N\sum_{i=1}^{N} p_i^2=\sum_{1\leqslant i<j\leqslant N}\sum(p_i-p_j)^2+\left(\sum_{i=1}^{N} p_i\right)^2, \tag{12}$$

valid for any set of N vectors p_i, $i=1,\ldots,N$ of R^k, to separate out the center-of-mass motion in (1) as

$$H^N = H^N_{\rm rel} + P^2/N, \tag{13}$$

where the relative Hamiltonian is

$$H^N_{\rm rel} = \sum_{1\leqslant i<j\leqslant N}\sum \left(\frac{1}{N}(p_i-p_j)^2 + V_{ij}\right) \tag{14}$$

and $P=\Sigma p_i$ is the total momentum.

In the N body center-of-mass frame $\langle P\rangle = 0$ [this can be made rigorous by adding, e.g., a term $\alpha^2(\Sigma r_i/N)^2$ which commutes with $H^N_{\rm rel}$ and letting α^2 tend to zero], and therefore

$$E^N = \frac{N(N-1)}{2}\langle\Omega|\left(\frac{4}{N}\left(\frac{p_i-p_j}{2}\right)^2 + V_{ij}\right)|\Omega\rangle. \tag{15}$$

Since $(p_i-p_j)/2$ and (r_i-r_j) satisfy canonical commutation relations, one obtains, for bosons

$$E^N_B \geqslant \frac{N(N-1)}{2}\,\epsilon_1(\mu = N/4), \tag{16}$$

which improves (8) since $\epsilon_n(\mu)$ increases with $1/\mu$.

This new lower bound becomes the exact answer for a harmonic interaction: $E^N = 3(N-1)\sqrt{N}$, and we have shown[4] that it is very close to the exact answer for the power-law potentials $V=r^q$, $-1\leqslant q\leqslant 5$, including the Coulomb case (we thank J. M. Richard for making new tests for $q>3$, $N=3$).

In fermion systems, however, this procedure does not help. We can, of course, perform a decomposition of H^N similar to (5) and (6):

$$H^N = \frac{1}{2}\sum_{i=1}^{N} H_i, \tag{17}$$

$$H_i = \sum_{j=1, j\neq i}^{N}\left(\frac{4}{N}\left(\frac{p_j-p_i}{2}\right)^2 + V_{ij}\right), \tag{18}$$

but H_i is no longer an independent particle Hamiltonian, and it cannot be diagonalized in general. In fact, although $(p_j-p_i)/2$ and (r_j-r_i) have canonical commutation relations, (p_j-p_i) and (r_k-r_i) do not commute.

Here H_i can be viewed as describing the motion of $N-1$ independent particles of mass $N/2$, placed in the field of a much lighter particle i of mass $N/(2(N+1))$. This problem has no simple solution in general. The difficulty we meet here is also related to the known difficulty of constructing fully antisymmetric N-particle wavefunctions which are both eigenstates of an $N-1$ independent particle Hamiltonian and translationally invariant.

No recasting of the kinetic term, such as (12) or the many analogous formulas one can write, can do the job, and it seems impossible to improve the fermionic bound (10) in a simple way without further specifying the potential.

This situation is rather frustating with regards to the harmonic interaction, where we know the exact answer and the bound (10) is off by a factor of $\sqrt{2}$.

A naïve conjecture, following from the inspection of Eq. (14), and assuming the first $N-1$ levels of the Hamiltonian $(4/N)p^2+V(r)$ are equally populated, such as what would occur in a Slater determinant, would lead to

$$E_F^N \geqslant \frac{N}{2} f_{N-1}(\mu = N/4), \tag{19}$$

which, in the harmonic case, reduces to $\sqrt{N} f_{N-1}(1)$, giving the right answer asymptotically in N. However, it does not seem possible to prove such a conjecture in a simple way.

III. DERIVATION OF NEW FERMIONIC BOUNDS

Improved bounds on fermion systems may be obtained by further specifying the potential. In what follows, we restrict ourselves to power-law potentials,

$$V(r) = r^q, \quad 1 \leqslant q \leqslant \infty, \tag{20}$$

which include the harmonic case $q=2$ and the infinite square well $q=\infty$, and superpositions of such potentials.

It is instructive to recall the solution of the harmonic case. Consider the independent particle Hamiltonian

$$\widetilde{H}^N = \sum_{i=1}^N p_i^2 + N \sum_{i=1}^N r_i^2; \tag{21}$$

the ground-state energy of the totally antisymmetric solution is

$$\widetilde{E}^N = \sqrt{N} f_N \tag{22}$$

[from now on we write f_N instead of $f_N(1)$ since we know that the eigenvalues of $ap^2 + br^q$ scale as $a^{q/(q+2)} b^{2/(q+2)}$, and therefore $f_N(\mu)$ can be expressed in terms of $f_N(1)$].

Using the identity (12) both for the kinetic and potential terms, we obtain

$$\widetilde{H}^N = H_{\mathrm{rel}}^N + \left(\frac{P^2}{N} + N^2 X^2 \right), \tag{23}$$

where $X = \Sigma r_i / N$ is the center of gravity of the system. The second term on the right-hand side of (23) is a one-particle Hamiltonian which commutes with H_{rel}^N. Therefore the ground state energy of $\widetilde{H}^N$ is the sum of ground state energies $\widetilde{E}^N = E^N + \sqrt{N} \epsilon_1$, that is to say,

$$E^N = \sqrt{N}(f_N - \epsilon_1). \tag{24}$$

In order to derive upper and lower bounds for fermion systems with $V(r) = r^q$ potentials, we will follow a similar procedure, and we will make use of the following inequalities.

Consider N vectors r_i, $i = 1, \ldots, N$, of R^3, and $1 \leqslant q \leqslant \infty$. Then

$$4 \sum_{1 \leqslant i < j \leqslant N} \sum \left| \frac{r_i - r_j}{2} \right|^q + N^2 \left| \frac{\Sigma_{i=1}^N r_i}{N} \right|^q \geqslant N \sum_{i=1}^N |r_i|^q, \tag{25}$$

$$\sum_{1 \leqslant i < j \leqslant N} \sum |r_i - r_j|^q + \left| \sum_{i=1}^N r_i \right|^q \leqslant N \sum_{i=1}^N |r_i|^q, \tag{26}$$

where the upper inequality holds for $1 \leqslant q \leqslant 2$, and the lower one for $2 \leqslant q \leqslant \infty$; $|r|$ is the Euclidean norm of $r \in R^3$.

The proof of these inequalities is given in the next section. Notice that both of them become identities for $q=2$ since they reduce to (12).

The physical interest of such inequalities lies in the fact that they allow us to relate a problem of translationally invariant pairwise interaction to an independent particle problem.

Indeed, both inequalities are of the form

$$\sum_{1\leqslant i<j\leqslant N}\sum |r_i-r_j|^q+a|X|^q\geqslant b\sum_{i=1}^{N}|r_i|^q, \tag{27}$$

where $X=\Sigma r_i/N$ is the position of the center of gravity. We therefore have the *operator* inequalities

$$\sum_{i=1}^{N} p_i^2+\sum\sum |r_i-r_j|^q+a|X|^q\geqslant\sum_{i=1}^{N}(p_i^2+b|r_i|^q). \tag{28}$$

The right-hand side of (28) is an independent-particle Hamiltonian whose (antisymmetric) ground state energy is

$$\widetilde{E}_f^N=b^{2/(q+2)}f_N. \tag{29}$$

Using (12) the left-hand side can be rewritten as the sum of two commuting Hamiltonians, the Hamiltonian we are interested in $H_{\rm rel}^N$, and a one-particle Hamiltonian

$$h=\frac{P^2}{N}+a|X|^q \tag{30}$$

whose ground state energy is $a^{2/(q+2)}N^{-q(q+2)}\epsilon_1$. $H_{\rm rel}^N$ and h commute, their eigenstates factorize, and their eigenvalues add.

Since (28) is an operator inequality, we therefore have the bounds

$$E_f^N+a^{2/(q+2)}N^{-q/(q+2)}\epsilon_1\geqslant b^{2/(q+2)}f_N. \tag{31}$$

Inserting the actual values of the coefficients a and b, as can be read from Eqs. (25) and (26), we obtain the following upper and lower bounds for the ground state energy E_1^N of a N fermion system with pairwise interactions $|r_i-r_j|^q$. For $1\leqslant q\leqslant 2$,

$$2^{[2(q-2)]/(q+2)}[N^{2/(q+2)}f_N-N^{(4-q)/(q+2)}\epsilon_1]\leqslant E_F^N\leqslant N^{2/(q+2)}f_N-N^{q/(q+2)}\epsilon_1 \tag{32}$$

and, for $2\leqslant q\leqslant\infty$, the inequalities are reversed. At $q=2$, we recover the exact harmonic oscillator results.

Since, for $V=r^q, f_N\sim N^{(5q+6)/(3q+6)}$ as $N\to\infty$ in three dimensions, as it can be shown from semi-classical estimates valid in the large N limit for power potentials, the f_N terms dominate over the ϵ_1 terms at large N, and, for simplicity, we concentrate on this limit for the discussion:

$$2^{[2(q-2)]/(q+2)}\leqslant\lim_{N\to\infty}[E_F^N/N^{2/(q+2)}f_N]\leqslant 1, \tag{33}$$

the upper and lower inequalities corresponding respectively to $1\leqslant q\leqslant 2$ and to $2\leqslant q\leqslant\infty$.

For $q=1$, the upper and lower bounds differ by a factor $2^{2/3}=1.59$; the lower bound is the same as the previous result (10). For $q=\infty$ (infinite square well) the upper and lower bounds differ by a factor of 4 and again the lower bound coincides with (10).

In all the range $1<q<\infty$, the previous result (10) is improved. The maximal improvement occurs for the harmonic case $q=2$, where these bounds reduce to the exact answer.

This approach provides *both* upper and lower bounds.

We shall exploit this fact in turning to the more general class of potentials which are linear superpositions of power law potentials (20):

$$V(r)=\int_1^\infty r^q \mu(q)\ dq. \tag{34}$$

In principle, since we have both upper and lower inequalities in the two ranges $1\leqslant q\leqslant 2$ and $2\leqslant q\leqslant\infty$, we should be able to write upper and lower bounds for this class of potentials.

Consider first the simplest case which corresponds to linear superpositions (34) with positive weights and $q\geqslant 2$,

$$V(r)=\int_2^\infty r^q \mu(q)\ dq, \quad \mu(q)\geqslant 0, \tag{35}$$

a particular case of which is entire functions with positive expansion coefficients and no linear term (a constant can always be subtracted out).

From the inequalities (25) and (26), we readily obtain, writing down (35) on both sides,

$$\sum_{1\leqslant i<j\leqslant N}\sum V(r_i-r_j)+V\left(\sum\ r_i\right)\geqslant N\sum_{i=1}^N\ V(r_i), \tag{36}$$

$$\sum\sum\ V(r_i-r_j)+\frac{N^2}{4}\ V\left(\frac{2\Sigma r_i}{N}\right)\leqslant\frac{N}{4}\sum_{i=1}^N\ V(2r_i). \tag{37}$$

Adding the kinetic terms and taking into account that the eigenvalues of $ap^2+bV=b(a/bp^2+V)$ are directly expressed in terms of those of V: $\epsilon_n(\mu=b/a)$, and that multiplying r by a constant is equivalent to rescaling the mass by the inverse squared of this constant, one obtains the bounds

$$E_F^N\geqslant N f_N(\mu=N)-\epsilon_1(\mu=1/N), \tag{38}$$

$$E_F^N\leqslant\frac{N}{4}\ f_N\left(\mu=\frac{N}{16}\right)-\frac{N^2}{4}\ \epsilon_1\left(\mu=\frac{N^3}{16}\right). \tag{39}$$

For potentials of the class

$$V(r)=\int_1^2 r^q\mu(q)dq, \quad \mu\geqslant 0, \tag{40}$$

the signs of these two bounds are simply reversed.

The bounds (38) and (39) are quite remarkable in that they hold for any potential of the classes (35) and (40), and are expressed in terms of the two-particle spectrum. They reduce to the particular cases (32) for power law potentials, and become exact for a harmonic potential.

We notice that, although (38) reproduces the harmonic result, it is different from the naïve conjecture (19). It is only for potentials of the class (35) that (38) is an improvement over the result (10).

For the more general superposition (34) with positive weights, one can obtain similar formulas but these are more complicated to write. The N-body results are expressed in terms of two-body spectra corresponding not to the original potential but to a modified one:

$$\tilde{V}(r)=\int_1^2 \frac{(2r)^q}{4}\,\mu(q)dq+\int_2^\infty r^q\mu(q)dq=V(r)-\int_1^2\left(1-\frac{2^q}{4}\right)r^q\mu(q)dq. \tag{41}$$

For weights of alternating signs, sticking to the class (35) for simplicity, one can write the potential $V(r)$ as

$$V(r)=V_+(r)-V_-(r) \tag{42}$$

with

$$V_\pm(r)=\int_2^\infty r^q\mu_\pm(q)\,dq, \quad \mu_\pm(q)\geqslant 0. \tag{43}$$

In order to write lower bounds, for instance, one uses inequality (36) for V_+ and inequality (37) for V_- in order to obtain

$$H^N+\frac{P^2}{N}+V_+(NX)-\frac{N^2}{4}\,V_-(2X)\geqslant\sum_{i=1}^N\left[p_i^2+NV_+(r_i)-\frac{N}{4}\,V_-(2r_i)\right]. \tag{44}$$

Leaving aside the one-particle Hamiltonian for the center-of-mass variable X in the left-hand side, this inequality allows us to relate H^N to an independent-particle Hamiltonian where the potential is no longer $V(r)$ but the effective potential

$$\tilde{V}(r)=V_+(r)-\tfrac{1}{4}V_-(2r). \tag{45}$$

In general, however, this is of no use in deriving lower bounds because in many cases of interest $\tilde{V}(r)$ is unbounded from below. Consider, for instance

$$V=-\lambda r^2\,\exp(-r), \tag{46}$$

which possesses two-body bound states for λ large enough, and pertains to the class under consideration. For this potential, one has

$$V_+(r)=r^2\,\sinh r, \quad V_-(r)=r^2\,\cosh r, \tag{47}$$

therefore the effective potential $\tilde{V}(r)$ entering on the right-hand side of (44) is

$$\tilde{V}(r)=r^2\,\sinh r-r^2\,\cosh 2r, \tag{48}$$

which is unbounded from below.

Upper bounds can nevertheless be obtained in such cases.

Lower bounds can only be obtained if $\mu(q)$ oscillates in a bounded region in q (for instance, if V is a polynomial in r).

IV. PROOF OF THE INEQUALITIES

We now give the proof of the inequalities (25) and (26). The keypoint in this proof is due to Jean-Michel Bony.

Consider N_1 vectors x_i, $i=1,\ldots,N_1$, of R^3 (or R^k in general) and let $|x_i|$ denote the usual Euclidean norm of x_i.

The set $X=\{x_1,x_2,\ldots,x_{N_1}\}$ can be considered as a point in $(R^3)^{N_1}$. In this latter space one defines the $\mathcal{L}^P$ norm of X, noted $\|x\|_p$, $p\geqslant 1$, associated with the positive coefficients $\gamma_1,\gamma_2,\ldots,\gamma_{N_1}$ as

$$\|X\|_p=(\gamma_1|x_1|^p+\gamma_2|x_2|^p+\cdots+\gamma_{N_1}|x_{N_1}|^p)^{1/p}. \tag{49}$$

Consider a point $Y=\{y_1,y_2,\ldots,y_{N_2}\}$ of $(R^3)^{N_2}$ with the ℓ^p norm $\|Y\|_p=(\Sigma_{i=1}^{N_2}\delta_i|y_i|^p)^{1/p}$, δ_i positive, and an injective linear transformation L from $X\in(R^3)^{N_1}$ to $Y\in(R^3)^{N_2}$ noted $Y=LX$, such that, for $1\leqslant p_2\leqslant p_1\leqslant+\infty$,

$$\|LX\|_{p_1}\leqslant c_1\|X\|_{p_1}, \tag{50a}$$

$$\|LX\|_{p_2}\leqslant c_2\|X\|_{p_2}. \tag{50b}$$

The Riesz–Thorin interpolation theorem[5] states that for all p between p_2 and p_1

$$p_1\geqslant p\geqslant p_2,\quad \|LX\|_p\leqslant C_p\|X\|_p, \tag{51}$$

with

$$C_p=C_2^{1-\theta}C_1^{\theta}, \tag{52}$$

θ being given in terms of p, p_2, and p_1 by

$$\frac{1}{p}=\frac{\theta}{p_1}+\frac{1-\theta}{p_2}. \tag{53}$$

Returning to our problem, we first consider $X=\{x_1,x_2,\ldots,x_N\}\in(R^3)^N$ with the ℓ^P norm

$$\|X\|_p=\left(N\sum_{i=1}^{N}|x_i|^p\right)^{1/p} \tag{54}$$

and $Y=\{\{v_{ij}\},w\}\in(R^3)^{N'}$, $N'=N(N-1)+1$, where

$$v_{ij}=\frac{x_i-x_j}{2},\quad w=\sum_{i=1}^{N}\frac{x_i}{N}, \tag{55a}$$

the inverse transformation being

$$x_i=\frac{(w+2\Sigma_{j=1}^{N}v_{ij})}{N}. \tag{55b}$$

Equations (55a) and (55b) provide a bijection of $(R^3)^N$ and its image $\mathcal{J}$ in $(R^3)^{N'}$ which is such that

$$v_{ij}+v_{ji}=0,\quad v_{ij}+v_{jk}+v_{ki}=0.$$

The ℓ^p norm of Y is defined by

$$\|Y\|_p+\left(2\sum_{i=1}^{N}\sum_{\substack{j=1\\ i\neq j}}^{N}|v_{ij}|^p+N^2|w|^p\right)^{1/p}. \tag{56}$$

For $p=2$, these norms are equal since they reduce to the identity (12): $\|X\|_2=\|Y\|_2$.

For $p=1$, using the identity

$$x_i=\frac{1}{N}\left(\sum_{j=1}^{N}(x_i-x_j)+\sum_{j=1}^{N}x_j\right),$$

one has

$$|x_i|\leqslant\frac{1}{N}\left(\sum_{j=1}^{N}|x_i-x_j|+\left|\sum_{j=1}^{N}x_j\right|\right).$$

Therefore, by summing over i,

$$N\sum|x_i|\leqslant 2\sum_{\substack{i=1\\ i\neq j}}^{N}\sum_{j=1}^{N}\left|\frac{x_i-x_j}{2}\right|+N^2\left|\frac{\Sigma x_i}{N}\right|. \tag{57}$$

In other words, $\|X\|_1\leqslant\|Y\|_1$, and by the Riesz–Thorin interpolation theorem

$$\|X\|_p\leqslant\|Y\|_p, \quad 1\leqslant p\leqslant 2,$$

which proves the inequality (25) in this case.

For $p>2$, the inequality is reversed. Indeed

$$\|X\|_\infty\geqslant\|Y\|_\infty, \tag{58}$$

which can be seen as follows. Let $|x_i|=\sup_j|x_j|$. It is obvious that $|x_i|\geqslant|x_j-x_k|/2\ \forall j,k$ and $|x_i|\geqslant|\Sigma x_i|/N$.

So, $\sup_j|x_j|\geqslant\sup(|v_{ij}|,|w|)$.

The only case we need to consider is when all vectors are collinear and of equal moduli. If all vectors are equal, both sides of (58) are equal. If p vectors are equal to x and $(N-p)$ to $-x$, one easily checks that $N\Sigma|x_i|\geqslant 2\Sigma\Sigma|v_{ij}|$, this becoming an inequality for $p=N/2$.

Therefore, (58) holds and, since $\|X\|_2=\|Y\|_2$,

$$\|X\|_p\geqslant\|Y\|_p \quad \text{for } p\geqslant 2,$$

which completes the proof of inequality (25). This inequality is *saturated*, i.e., it becomes an equality, when either all x_i are equal, or $N/2$ of the x_i are equal to x and the other $N/2$ are equal to $-x$ (N even).

Turning to inequality (26), we now replace (55) by

$$v_{ij}=(x_i-x_j), \quad w=\sum_{i=1}^{N}x_i, \tag{59}$$

and we define the ℓ^p norm of Y by

$$\|Y\|_p=\left(\frac{1}{2}\sum_{\substack{i=1\\ i\neq j}}^{N}\sum_{j=1}^{N}|x_i-x_j|^p+\left|\sum_{i=1}^{N}x_i\right|^p\right)^{1/p}, \tag{60}$$

$\|X\|_p$ being defined as previously.

For $p=2$ we still have $\|X\|_2=\|Y\|_2$, of course.

The proof that $\|Y\|_1\geqslant\|X\|_1$ is straightforward. We have

$$|x_i-x_j|\leqslant|x_i|+|x_j|, \quad \left|\sum\ x_i\right|\leqslant\sum\ |x_i|.$$

Therefore

$$\frac{1}{2}\sum_{\substack{i=1\\ i\neq j}}^{N}\sum_{j=1}^{N}|x_i-x_j|+\left|\sum_{i=1}^{N}x_i\right|\leqslant N\sum_{i=1}^{N}|x_i|.$$

and

$$\|Y\|_p\leqslant\|X\|_p \tag{61}$$

for $1\leqslant p\leqslant 2$, which proves (26) in that range of values of p.

Notice that we also have for any $\lambda\geqslant 0$

$$\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}|x_i-x_j|+\lambda^2\left|\frac{\Sigma x_i}{\lambda}\right|\leqslant(N-1+\lambda)\sum_{i=1}^{N}|x_i|,$$

$$\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}|x_i-x_j|^2+\lambda^2\left|\frac{\Sigma x_i}{\lambda}\right|^2\leqslant N\sum_{i=1}^{N}|x_i|^2,$$

which lead to a set of λ-dependent inequalities valid for $1\leqslant p\leqslant 2$ where one makes full use of the Riesz–Thorin interpolation theorem, in particular Eq. (52).

In practice, we have found out that, by optimizing in λ, one does improve the upper bound in the range $1\leqslant p\leqslant 2$, but not asymptotically in N. One can readily check that, for $p=1$, the upper bound can be brought down to $E_F^N\leqslant(N-1)^{2/3}\,(f_N^3-N\epsilon_1^3)^{1/3}$ instead of $E_F^N\leqslant N^{2/3}\,f_N-N^{1/3}\epsilon_1$. The improvement is only felt for small values of N.

Finally, for $p\to+\infty$ we want to prove that

$$\left(\frac{1}{2}\sum\sum\ |x_i-x_j|^p+\left|\sum\ x_i\right|^p\right)^{1/p}\geqslant N^{1/p}\left(\sum\ |x_i|^p\right)^{1/p}. \tag{62}$$

Let x_1 be one of the vectors of largest norm $|x_1|\geqslant|x_i|$, $i=2,\ldots,N$. If one other vector, x_2, of nonvanishing norm points in the backward hemisphere of x_1, that is to say $x_1\cdot x_2/|x_1||x_2|<0$, then $|x_1-x_2|\geqslant|x_1|$ and the inequality holds.

If all vectors x_i, $i\neq 1$, point in the forward hemisphere of x_1 and at least one is of nonzero norm, then $|\Sigma x_i|>|x_1|$ and the inequality holds.

If all vectors vanish except x_1, both sides of (62) are equal.

Therefore, $\|X\|_\infty\leqslant\|Y\|_\infty$, and $\|X\|_p\leqslant\|Y\|_p$ for $p\geqslant 2$, which completes the proof of inequality (26). This inequality is saturated when all x_i vanish except one of them.

One can derive, in a similar manner, a variety of other inequalities, for instance by using Jacobi variables.

The Riesz–Thorin interpolation theorem actually applies to a much larger class of problems since it applies to measure spaces, with positive measure, in general. Notice, for instance, by dividing Eq. (25) by N^2, one can rewrite it in integral form as

$$2\int\int\left|\frac{x(u)-x(v)}{2}\right|^p d\mu(u)d\mu(v)+\left|\int x(u)d\mu(u)\right|^p\geqslant\int|x(u)|^p\,d\mu(u),$$

where we have introduced a positive measure such that $\int d\mu(u)=1$. In order to recover (25) we set

$$d\mu(u)=\frac{1}{N}\sum_{i=1}^{N}\delta(u-x_i)du.$$

In this more general formulation, these inequalities may turn out to be useful in dealing with systems with an infinite number of degrees of freedom.

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Interchannel resonances at a threshold

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Fermi's Golden Rule, the perturbation theoretic formula for calculating the half-width of a resonance, is not applicable to the case of a transition from a bound state into an open channel, when the energy of the bound state is exactly at the threshold of the continuum. We study solvable models of this phenomenon. The exact results coincide in leading order with the formulas found by modifying Fermi's Golden Rule. © *1996 American Institute of Physics.* [S0022-2488(96)03011-3]

I. INTRODUCTION

An interchannel resonance in quantum mechanical scattering is considered as arising by a perturbation of a bound state in a closed channel, with the bound state energy lying in a region where other channels are open.[1] In the case of a small perturbation, the half-width of the resonance is in general calculated with **Fermi's Golden Rule** (FGR).[2–4] If the unperturbed Hamiltonian H_0 (which is the kinetic energy plus interchannel potentials) with a bound state $|\varphi\rangle$ in the closed channel and continuum wavefunctions ψ_k in the open channel (we will consider only one open channel) is perturbed by αV, then FGR gives the imaginary part of the resonance energy as a product of

(1) α^2,
(2) the absolute square of the transition matrix element $\langle\varphi|V\psi_k\rangle$,
(3) the spectral density in the open channel, and
(4) the constant π.

A mathematical treatment, using complex scaling,[5] confirms Fermi's Golden Rule as the contribution to perturbation theory in second order, with the exception of *the case where the energy of the bound state does coincide with the threshold of the continuous spectrum in the open channel*. When trying to apply FGR to such a case, one observes the following facts:

(a) The transition matrix element is zero in general; only in the case of an open s-channel with a zero-energy inner-channel resonance may it be nonvanishing at the threshold.
(b) The spectral density at the threshold is infinite.

So FGR gives either infinity or an undecided value of zero times infinity; up to now we don't know for sure whether the bound state turns into a resonance, and, in case it should do so, we don't have a perturbation-theoretic formula for its lifetime.

Such cases actually do occur with atoms.[6] In principle they could also appear with nuclei or in solid state physics, where the channels are the bands of electron states, and where a bound state is located at an impurity. For semiconductors just the resonances near a band edge (=threshold) are of particular importance.[7]

In this paper we study simple solvable models: first, a one-dimensional lattice model with two bands. Then we make a comparison with a simplified model, which keeps only the barest essentials. This serves as an argument for the validity of the solvable continuum models with a separable potential for coupling of the channels. The continuum models are one-dimensional or the radial parts of a rotation-invariant three-dimensional system.

The leading term in an expansion of the lifetime turns out to be proportional to a half-integer-

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exponentiated coupling constant. We end up with a conjecture how to modify FGR to get a generally valid formula for the imaginary part of the resonance energy.

II. A ONE-DIMENSIONAL LATTICE MODEL

We consider a one-dimensional lattice $\mathbf{Z}$, carrying two channels, which would be translation invariant, if there were not an impurity at the point denoted by $n=0$. We consider only a local action of the impurity, so we can restrict the Hilbert space for each channel to the space of even functions. (The odd functions are zero at $n=0$ and are not affected by the impurity.) So it is enough to consider the half-space with points $n\geqslant 0$, and the even wavefunctions can be represented by elements of the Hilbert space $\ell^2(\mathbf{N})$ with the norm for $\psi=(\psi_n)\in\ell^2(\mathbf{N})$ given by

$$\|\psi\|^2=|\psi_0|^2=2\sum_{n=1}^{\infty}|\psi_n|^2. \tag{1}$$

In each channel there is a kinetic energy K:

$$(K\psi)_n=\begin{cases}2\psi_n-\psi_{n-1}-\psi_{n+1}, & n\geqslant 1\\ 2\psi_0-2\psi_1, & n=0.\end{cases}$$

The complete system with two bands is modelled in the Hilbert space $\ell^2(\mathbf{N})\oplus\ell^2(\mathbf{N})$. One channel gives a band shifted by a positive energy b, so, without impurity, the Hamiltonian would be $(K+b\mathbf{1})\oplus K$. The impurity is represented by a negative local inner-channel potential $(-w\delta_{n,0})\oplus(-v\delta_{n,0})$, where w is positive.

We are interested in the bound state in the upper band. It has the wavefunction

$$\varphi_n=ce^{-n\gamma_0},\quad c=(\coth\ \gamma_0)^{-1/2}, \tag{2}$$

where

$$2\sinh\ \gamma_0=w \tag{3}$$

and a binding energy which we consider as exactly equal to the relative shift of the bands:

$$b=2\cosh\ \gamma_0-2. \tag{4}$$

Now we collect all these contributions as the unperturbed Hamiltonian H_0. In matrix notation

$$H_0=\begin{pmatrix}b\mathbf{1}+K-w\delta_{n,0} & 0\\ 0 & K-v\delta_{n,0}\end{pmatrix} \tag{5}$$

it has the bound state $\binom{\varphi_n}{0}$ with energy zero, which equals the lower band edge of the lower channel.

Next we add a perturbation αV by an impurity at the point $n=0$, which introduces a coupling of the channels. For explanations see the discussion in Sec. III. We define

$$H_\alpha=H_0+\alpha V,\quad V=\delta_{n,0}\begin{pmatrix}\mathbf{1} & t^*\\ t & u\end{pmatrix},\quad t\in\mathbf{C},\quad u\in\mathbf{R}. \tag{6}$$

In the open channel the resonance state should behave like a Gamow function,[8] so, to solve the equation, we make the ansatz

$$\psi_n = \begin{pmatrix} e^{-n\gamma} \\ a \cdot e^{ikn} \end{pmatrix}, \tag{7}$$

$$(H_\alpha - E)\psi = 0, \tag{8}$$

and search for solutions with $\mathrm{Im}(k) < 0$, $E \to 0$, $a \to 0$, and $\gamma \to \gamma_0$ as $\alpha \to 0$.

Inserting (7) into (8) gives for the components $((H_\alpha - E)\psi)_n$ for $n \geqslant 1$ the equations

$$E = 2 - 2\cosh\,\gamma + b = 2 - 2\cos\,k, \tag{9}$$

$$\begin{aligned} b + 2 - 2e^{-\gamma} - w - E + \alpha(1 + t^* a) &= 0, \\ (2 - 2e^{ik} - v - E)a + \alpha(ua + t) &= 0. \end{aligned} \tag{10}$$

Expressing E by the appropriate parts of (9) we transform (10) to

$$a = \frac{-\alpha t}{\alpha u - v - 2i\,\sin\,k} = \frac{\alpha - w + 2\sinh\,\gamma}{-t^* \alpha} \tag{11}$$

and

$$\alpha^2(t^* t - u) + \alpha(f + ug) - fg = 0, \tag{12}$$

where we have introduced

$$\begin{aligned} f &:= v + 2i\,\sin\,k, \\ g &:= w - 2\sinh\,\gamma. \end{aligned} \tag{13}$$

Considering, by way of Eq. (9), E, γ, f, and g as analytic functions of the uniformizing complex variable k,

$$\gamma = \gamma(k) = \mathrm{arcosh}(b/2 + \cos\,k) \tag{14}$$

with

$$\lim_{k \to 0} \gamma(k) = \gamma_0 > 0,$$

we will be mainly interested in the behavior of these functions of k near zero. The expansions are

$$\begin{aligned} E &= k^2 - \frac{k^4}{12} + O(k^6), \\ f &= v + 2ik - \frac{i}{3}\,k^3 + O(k^5), \\ g &= k^2\,\coth\,\gamma_0 + \left(\frac{1}{w} + \frac{2}{w^3} - \frac{\sqrt{w^2+4}}{12w}\right)k^4 + O(k^6) =: c^{-2}k^2 + dk^4 + O(k^6). \end{aligned} \tag{15}$$

The goal is to get E as a function of real α by way of k. Using Eq. (12) it seems easier first to consider α as a complex-valued function of k, and then to invert this to a function $k(\alpha)$. Four different cases have to be treated separately:

(a) If $t^* t - u = 0$,

$$\alpha=\frac{f\cdot g}{f+ug}\begin{cases}(c^{-2}k^2+dk^4)\left(1-\dfrac{t^*t}{c^2v}\,k^2+i\,\dfrac{2t^*t}{c^2v}\,k^3\right)+O(k^6), & \text{if } v\neq 0,\\ (c^{-2}k^2+dk^4)\left(1+i\,\dfrac{t^*t}{2c^2}\right)k+O(k^5), & \text{if } v=0.\end{cases}\tag{16a}$$

(b) If $t^*t-u\neq 0$, the solution of the quadratic equation with $\alpha\to 0$ as $k\to 0$ has to be chosen:

$$\begin{aligned}\alpha&=\frac{f+ug}{2(t^*t-u)}\left(\sqrt{1+\frac{4fg(t^*t-u)}{(f+ug)^2}}-1\right)\\&=\begin{cases}(c^{-2}k^2+dk^4)\left(1-\dfrac{t^*t}{c^2v}\,k^2+2it^*t\,\dfrac{c^{-2}}{v^2}\,k^3\right)+O(k^6), & \text{if } v\neq 0,\\ (c^{-2}k^2+dk^4)\left(1+i\,\dfrac{t^*t}{2c^2}\,k\right)+O(k^4), & \text{if } v=0.\end{cases}\end{aligned}\tag{16b}$$

The leading contributions to the power series for the case b are independent of u and identical to the power series in case a, where we may replace u by t^*t. However, the distinction between absence and presence of an impurity well, $v=0$ and $v\neq 0$, is important.
For $v\neq 0$,

$$\alpha=c^{-2}k^2-\left(\frac{t^*t}{vc^4}-d\right)+i\,\frac{2t^*t}{vc^4}\,k^5+O(k^6).$$

For $v=0$,

$$\alpha=c^{-2}k^2+i\,\frac{t^*t}{2c^4}\,k^3+O(k^4).\tag{17}$$

In all the cases $\alpha(k)$ is an analytic function of k in some neighborhood of $k=0$, which is a zero point of second order, so the function can be inverted to give k as an analytic function of the square root of α.[9,10] Its expansion is
for $v\neq 0$,

$$\begin{aligned}k&=c\alpha^{1/2}+\frac{1}{2}\left(t^*t\,\frac{c}{v}-c^5d\right)\alpha^{3/2}-it^*t\,\frac{c^2}{v^2}\,\alpha^2+O(\alpha^{5/2}),\\E&=c^2\alpha+\left(t^*t\,\frac{c^2}{v}-c^6d-\frac{c^4}{12}\right)\alpha^2-it^*t\,\frac{2c^3}{v^2}\,\alpha^{5/2}+O(\alpha^3);\end{aligned}\tag{18}$$

for $v=0$,

$$\begin{aligned}k&=c\alpha^{1/2}-i\,\frac{t^*t}{4}\,\alpha+O(\alpha^{3/2}),\\E&=c^2\alpha-it^*t\,\frac{c}{2}\,\alpha^{3/2}+O(\alpha^2).\end{aligned}\tag{19}$$

III. DISCUSSION

The model has been chosen to investigate the basic mathematical structure, with best possible ease in computation. The impurity's potential and the perturbation are therefore assumed to act locally at one point only. From there on everything is as general as possible. For the closed

channel the inner-channel part of the perturbing potential has been set equal to one in Eq. (6). The reason is the following: If it were zero, the bound state would under perturbation not turn into a resonance, but would remain a bound state. [This can be checked with the ansatz of a wavefunction $\Phi_n = \binom{e^{-\gamma n}}{a \cdot e^{-\kappa n}}$, and proceeding in a similar way as for the resonance.] So we are only interested in the case where this inner-channel perturbation is strictly positive, and we may use the freedom of shifting the normalization between the coupling constant and the potential V to set this matrix element equal to one.

The threshold behavior of the open channel, connected with the absence or presence of an impurity well, determines the leading term for the imaginary part: If $v \neq 0$, there is a nonvanishing effective range of the impurity and the continuum wavefunctions at low energy tend to stay away from it. The transition probability from the bound state to the continuum increases with the coupling constant α more slowly than in other cases. If $v=0$, there is no effective range, the transitions are not hindered, and the high spectral density of the continuum effects an increase of Im $(E(\alpha))$ faster than α^2. These effects will be discussed in closer detail for the continuum models.

IV. THE SIMPLIFIED LATTICE MODEL

To pave the way for simple continuum models, we simplify this two-band model by ignoring any inner-channel effects in the closed channel, except for the change in energy. So, we replace H_α by $PH_\alpha P$, with the projection operator

$$P = \begin{pmatrix} |\varphi\rangle\langle\varphi| & 0 \\ 0 & 1 \end{pmatrix}, \tag{20}$$

where $|\varphi\rangle$ is the unperturbed bound state (2).

So we work in the restricted Hilbert space $P[\ell^2(\mathbf{N}) \oplus \ell^2(\mathbf{N})] \cong \mathbf{C} \oplus \ell^2(\mathbf{N})$, where the closed channel is represented by only one state. Moreover, we feel free to replace the inner-channel part u of the perturbation V by t^*t, because the leading terms in the expansion of (16b) are identical to those of (16a).

The Hilbert space is $\mathscr{H} = \mathbf{C} \oplus \ell^2(\mathbf{N})$, the Hamiltonian $H_\alpha = H_0 + \alpha V$,

$$H_0 = \begin{pmatrix} 0 & 0 \\ 0 & K - v\,\delta_{n0} \end{pmatrix}, \quad V = \begin{pmatrix} c^2 & ct^*\delta_{n0} \\ ct\,\delta_{n0} & t^*t\,\delta_{n0} \end{pmatrix}. \tag{21}$$

With the ansatz for the unnormalized resonance wavefunction

$$\Psi = \begin{pmatrix} 1 \\ a \cdot e^{ikn} \end{pmatrix} \tag{22}$$

inserted into $(H_\alpha - E)\Psi = 0$, we get

$$\begin{aligned} E &= 2(1 - \cos k), \\ a &= (E/\alpha c - c)/t^*, \\ \alpha &= \frac{c^{-2}(1 - \cos k)(v + 2i \sin k)}{v/2 + i \sin k + t^*tc^{-2}(1 - \cos k)}. \end{aligned} \tag{23}$$

This α is an analytic function of k, with the power series in a neighborhood of the origin

$$\alpha=\begin{cases} c^{-2}k^2+\left(\dfrac{t^*t}{vc^4}-\dfrac{1}{12c^2}\right)k^4-ik^5+O(k^6) & \text{for } v\neq 0,\\ c^{-2}k^2+i\,\dfrac{t^*t}{2c^4}\,k^3+O(k^4) & \text{for } v=0. \end{cases} \tag{24}$$

These functions can be inverted to a function of $\sqrt{\alpha}$, analytic in a neighborhood of the origin: For $v\neq 0$,

$$\begin{aligned} k&=c\alpha^{1/2}+\left(\frac{t^*t}{2vc^2}-\frac{1}{24}\right)c^3\alpha^{3/2}-i\,\frac{t^*tc^2}{v^2}\,\alpha^2+O(\alpha^{5/2}),\\ E&=c^2\alpha+\frac{t^*tc^2}{v}\,\alpha^2-i\,\frac{2t^*tc^3}{v^2}\,\alpha^{5/2}+O(\alpha^3). \end{aligned} \tag{25}$$

For $v=0$,

$$\begin{aligned} k&=c\alpha^{1/2}-i\left(\frac{t^*t}{4}\right)\alpha+O(\alpha^{3/2}),\\ E&=c^2\alpha-i\,\frac{t^*tc}{2}\,\alpha^{3/2}+O(\alpha^2). \end{aligned} \tag{26}$$

The leading contributions both to the real part and to the imaginary part of the energy in (25) and (26) are identical to those in the formulas (18) and (19).

V. A SIMPLE CONTINUUM MODEL

The studies of the lattice model encourage us to use two simple building blocks: To keep only a single bound state, representing the closed channel, and to consider a rank one operator as the perturbation V, coupling the bound state to the open channel. In the open channel we consider the particle to be free. Everything is reflection or rotation invariant in one or three dimensions.

The Hilbert space is now

$$\mathscr{H}=\mathbf{C}\oplus\mathscr{L}^2(\mathbf{R}_+)=\left\{\begin{pmatrix} p\\ |\psi\rangle\end{pmatrix}, p\in\mathbf{C}, |\psi\rangle=\psi(x)\in\mathscr{L}^2(\mathbf{R}_+)\right\}.$$

As Hamiltonian we consider

$$H_\alpha=H_0+\alpha V,\quad H_0=\begin{pmatrix}0&0\\0&K_\nu\end{pmatrix},\quad V=\begin{pmatrix}c^2 & c\langle v|\\ c|v\rangle & |v\rangle\langle v|\end{pmatrix}, \tag{27}$$

with $c>0$, $v(x)=O(e^{-\kappa x})$ for some $\kappa>0$, as $x\to\infty$. The kinetic energy, plus the angular momentum barrier, is either

$$K_\nu=-\frac{d^2}{dx^2}+\frac{\ell(\ell+1)}{x^2},\quad \ell=\nu-\frac{1}{2}\in\mathbf{N} \tag{28}$$

with Dirichlet-boundary conditions (b.c.) at $x=0$, or $K_\nu=-d^2/dx^2$ with Neumann (b.c.) at $x=0$ and $\nu=-\frac{1}{2}$. The models in one dimension are either of parity -1 or $+1$, concerning the reflection at $x=0$ in $\mathscr{L}^2(\mathbf{R})$. They can thus be reduced to models on the half line $\mathbf{R}_+$, with $\nu=\pm\frac{1}{2}$, the sign of ν corresponding to the sign of the parity.

The index ν is chosen in such a way that it coincides with the standard indication of the Bessel functions, which, multiplied by $\sqrt{\pi kx/2}$, give the eigenfunctions of K_ν.

The **formal** ansatz for the resonance wavefunction at positive α is

$$\Psi_\alpha = \begin{pmatrix} 1 \\ \psi_\alpha(x) \end{pmatrix}, \tag{29}$$

supposed to be a solution of the differential equation

$$(H_\alpha - E(\alpha))\Psi_\alpha = 0, \tag{30}$$

with the asymptotic behavior

$$\psi_\alpha(x) \sim e^{ikx} \quad \text{at } x \to \infty, \text{ with } \mathrm{Im}(k) < 0, \quad \mathrm{Re}(k) > 0. \tag{31}$$

A discussion of this asymptotic behavior would involve mathematical subtleties, especially if $v(x)$ is not of compact support. So we will instead analyze these formulas first for negative coupling constants α. There we get unnormalized bound states Ψ_α with negative energies $E(\alpha)$, the asymptotic behavior as in (31), but with $k = k(\alpha) = i\sqrt{-E(\alpha)}$. Then we may consider the analytic continuation of $E(\alpha)$ and $\psi_\alpha(x)$ to positive α. This is again achieved by inverting the function $\alpha(k)$.

Inserting (27) and (29) into (30) gives the pair of equations

$$\begin{aligned} \alpha c^2 + \alpha c \langle v | \psi_\alpha \rangle - E = 0, \\ (K_\nu - E)|\psi_\alpha\rangle + \alpha(c + \langle v|\psi_\alpha\rangle)|v\rangle = 0. \end{aligned} \tag{32}$$

The second equation is transformed to

$$|\psi_\alpha\rangle = -\alpha(c + \langle v|\psi_\alpha\rangle)(K_\nu - E)^{-1}|v\rangle = -\frac{E}{c}(K_\nu - E)^{-1}|v\rangle. \tag{33}$$

Multiplying (33) by $\langle v|$, and eliminating $\langle v|\psi_\alpha\rangle$ from the pair of equations, we get

$$\alpha = \frac{E}{c^2 - E\langle v|(K_\nu - E)^{-1}|v\rangle}. \tag{34}$$

For negative real energies E, (34) gives negative real α. In the uniformizing variable k, this function $\alpha(k)$ can be analytically continued into the region $\mathrm{Im}(k) > -\kappa$ (Appendix A). In Appendix B we prove that the energies $E = k^2$ in the unphysical sheet, giving positive real $\alpha(k)$, are actually poles of the resolvent of H_α. In Appendix A it is shown that

$$\langle v|(K_\nu - k^2)^{-1}|v\rangle = F(k) - ik^{2\nu}G(k), \tag{35}$$

with $F(k)$ and $G(k)$ analytic functions of k, real and even for $k \in \mathbf{R}$. $G(0)$ is the absolute square of a scaled transition matrix element from $|v\rangle$ into the continuum of K_ν at energy zero: $|t|^2 = G(0)$. The analytic function $\alpha(k)$ can be split into a real and an imaginary part, for $k \in \mathbf{R}$, and expanded in powers of k:

$$\alpha(k) = \frac{k^2}{c^2 - k^2F(k) - ik^{2\nu+2}G(k)} = \frac{k^2}{c^2} + O(k^4) + i\left[\frac{|t|^2}{c^4}k^{2\nu+4} + O(k^{2\nu+6})\right]. \tag{36}$$

To invert it, we have to form the square root:

$$\alpha^{1/2}(k)=\frac{k}{c}+O(k^3)+i\left[\frac{|t|^2}{2c^3}\,k^{2\nu+3}+O(k^{2\nu+5})\right]. \tag{37}$$

In both equations the remaining contributions, which we indicate by the order of their leading terms, have real-valued expansion coefficients. The inversion of this function near $k=0$ gives the searched for expansions of k and of E in the square root of the coupling constant:

$$k(\alpha^{1/2})=c\,\alpha^{1/2}+O(\alpha^{3/2})-i\left[\frac{c^{2\nu+1}}{2}\,|t|^2\alpha^{\nu+3/2}+O(\alpha^{\nu+5/2})\right], \tag{38}$$

$$E(\alpha^{1/2})=c^2\alpha+O(\alpha^2)-i[c^{2\nu+2}|t|^2\alpha^{\nu+2}+O(\alpha^{\nu+3})]. \tag{39}$$

VI. DISCUSSION

The leading term in the expansion of the real part of the resonance energy is precisely as in ordinary first-order perturbation theory. The leading term in the expansion of the negative imaginary part increases as $\alpha^{3/2}$ for $\nu=-\frac{1}{2}$, where standard FGR would give infinity times α^2. In the other cases, for $\nu\geqslant\frac{1}{2}$, the increase is slower than α^2. Now it turns out that the leading term in the expansion can be calculated with a **modified FGR**:

As a *first step* one has to take into account the shift in energy of the bound state to $E_\alpha=c^2\alpha$.

Then as a *second step* one has to proceed with standard FGR, applied to the bound state with the shifted energy.

In the present case this procedure gives the transition matrix element to the wavefunction $b_\nu(kx)$ in the open channel (see Appendix A)

$$t_k:=\sqrt{\frac{2}{\pi}}\,c\int_0^\infty v^*(x)b_\nu(kx)dx\overset{k\to0}{\sim}ck^{\nu+1/2}\sqrt{\frac{2}{\pi}}\,t. \tag{40}$$

The spectral density is $1/2k$. Evaluating all the contributions at $k=\sqrt{E_\alpha}$, one gets

$$\frac{\Gamma}{2}=|\mathrm{Im}\;E(\alpha)|=\frac{\pi}{2k}\,|t_k|^2\alpha^2=c^{2\nu+2}|t|^2\alpha^{\nu+2}, \tag{41}$$

precisely the leading term in (39).

Concerning the relevance of the model for physics, one has to observe that the wavefunctions in the continuum of an open channel with a short range potential behave as in the open channel without a potential and with Dirichlet b.c., *unless there is a zero energy bound state or inner-channel resonance*. In an open channel with $l=0$ and a zero-energy resonance, the wavefunctions behave as in the open channel with Neumann b.c. and the transition matrix element into the continuum stays finite at $E=0$.

The exponential falloff of the perturbing potential in the model corresponds to the exponential decrease of the bound state wavefunction to be incorporated in the model: Consider the case of two particles with the bound state Φ in the closed channel,

$$\Phi(\mathbf{x},\mathbf{y})=\varphi_1(\mathbf{x})\varphi_2(\mathbf{y})$$

perturbed by an interaction $\alpha W(\mathbf{x}-\mathbf{y})$. It enables transitions into an open channel, where the second particle with y-coordinate is still bounded with the wavefunction $\varphi_3(\mathbf{y})$, but the first particle is free. In this open channel the general wavefunction is

$$\Psi(x,y)=\psi(\mathbf{x})\varphi_3(\mathbf{y}),$$

the transition matrix element is

$$\langle \Psi | \alpha W | \Phi \rangle = \langle \psi | \alpha v \rangle$$

with

$$v(\mathbf{x}) = \varphi_1(\mathbf{x}) \int d^3y\, W(\mathbf{x}-\mathbf{y}) \varphi_3^*(\mathbf{y}) \varphi_2(\mathbf{y}).$$

The decay of $v(\mathbf{x})$ is thus determined by the decay of the bound state wavefunction $\varphi_1(\mathbf{x})$.

There remains the problem of the behavior of continuum wavefunction in the open channel in the presence of a long range potential.

APPENDIX A: ANALYTIC CONTINUATION

The solutions to the differential equation

$$((K_\nu - k^2) f\ )(x) = 0$$

are given by the transformed Bessel and Hankel functions b_ν and e_ν:

$$\begin{aligned} b_\nu(kx) &:= (\pi kx/2)^{1/2} J_\nu(kx), \\ e_\nu(kx) &:= (\pi kx/2)^{1/2} H_\nu^{(1)}(kx). \end{aligned} \tag{A1}$$

The asymptotic behavior is[11]

$$b_\nu(kx) \overset{kx\to 0}{\sim} \frac{\sqrt{\pi}}{\Gamma(\nu+1)} \left(\frac{kx}{2}\right)^{\nu+1/2}, \tag{A2}$$

$$e_\nu(kx) \overset{kx\to\infty}{\sim} e^{i(kx - \pi(\nu+1/2)/2)}. \tag{A3}$$

The Wronskian

$$b_\nu \frac{d}{dx} e_\nu - e_\nu \frac{d}{dx} b_\nu = ik. \tag{A4}$$

The Green's function $G_{\nu,k}(x,y)$, the kernel of the resolvent $(K_\nu - k^2)^{-1}$ for $\mathrm{Im}\, k > 0$, is thus

$$G_{\nu,k}(x,y) = \frac{i}{k} [\Theta(y-x) b_\nu(kx) e_\nu(ky) + \Theta(x-y) b_\nu(ky) e_\nu(kx)]. \tag{A5}$$

For half-integer-valued ν, it is an entire function of k.

Since in the limit $x\to\infty$ $v(x) = O(e^{-\kappa x})$, the integration

$$\int_0^\infty dx \int_0^\infty dy\, v^*(x) G_{\nu,k}(x,y) v(y)$$

converges for $\mathrm{Im}\, k > -\kappa$. So does the integration with $G_{\nu,k}$ replaced by the kernel $(d/dk)(kG_{\nu,k})$, and the existence of a continuation of the analytic function

$$kQ(x) := k\langle v | (K_\nu - k^2)^{-1} | v \rangle$$

is established for Im $k>-\kappa$. In order to distinguish between real and imaginary coefficients of the expansions, we use the transformed Neumann functions

$$n_\nu(kx):=(\pi kx/2)^{1/2}N_\nu(kx)$$

and split

$$e_\nu=b_\nu+in_\nu. \tag{A6}$$

The Green's function is now written as

$$G_{\nu,k}(x)=\frac{i}{k}\,b_\nu(ky)b_\nu(kx)+\frac{1}{k}\,[\Theta(y-x)n_\nu(ky)b_\nu(kx)+\Theta(x-y)b_\nu(ky)n_\nu(kx)]. \tag{A7}$$

The Bessel and Neumann functions take real values at positive real arguments. So, *for positive real* k, we may split $Q(k)$ into real and imaginary parts:

$$Q(k)=F(k)+ik^{2\nu}G(k), \tag{A8}$$

$$F(k)=-\frac{1}{k}\int_0^\infty dx\int_0^\infty dy\,\Theta(y-x)n_\nu(ky)b_\nu(kx)[v^*(y)v(x)+v(y)v^*(x)]. \tag{A9}$$

The product $n_\nu(ky)b_\nu(kx)$ lifts the singularity of $1/k$. For half-integer-valued ν, $F(k)$ has an analytic expansion in powers of k^2:

$$G(k)=k^{-(2\nu+1)}\left|\int_0^\infty dx v^*(x)b_\nu(kx)\right|^2 \overset{k\to0}{\to}|t|^2, \tag{A10}$$

with the ''scaled transition matrix element''

$$t:=\lim_{k\to0}k^{-(\nu+1/2)}\int_0^\infty dx v^*(x)b_\nu(kx)=\frac{\sqrt{\pi}}{2^{\nu+1/2}\Gamma(\nu+1)}\int_0^\infty dx v^*(x)x^{\nu+1/2}. \tag{A11}$$

At $k\sim0$, $G(k)$ has an analytic expansion in powers of k^2.

APPENDIX B: POLES OF THE RESOLVENT

We split the Hamiltonian H_α as

$$H_\alpha=L+W,\quad L:=\begin{pmatrix}\alpha c^2 & 0\\ 0 & K+\alpha|v\rangle\langle v|\end{pmatrix},\quad W:=\begin{pmatrix}0 & \alpha c\langle v|\\ \alpha c|v\rangle & 0\end{pmatrix} \tag{B1}$$

(we simply write K instead of K_ν) and use the iterated resolvent equation in the Hilbert space $\mathbf{C}\oplus\mathscr{L}^2(\mathbf{R})$,

$$(H_\alpha-E)^{-1}=(L-E+W)^{-1}=\frac{1}{L-E}-\frac{1}{L-E}\,W\,\frac{1}{L-E+W}=\frac{1}{L-E}-\frac{1}{L-E}\,W\,\frac{1}{L-E}$$
$$+\frac{1}{L-E}\,W\,\frac{1}{L-E}\,W\,\frac{1}{L-E+W} \tag{B2}$$

to calculate the matrix element with $(\,{}^1_{|0\rangle})$:

$$r:=(1,\langle 0|)\,\frac{1}{L+W-E}\begin{pmatrix}1\\|0\rangle\end{pmatrix}. \tag{B3}$$

We get

$$r=\frac{1}{\alpha c^2-E}+\frac{\alpha^2 c^2}{\alpha c^2-E}\,\langle v|\frac{1}{K+\alpha|v\rangle\langle v|-E}\,|v\rangle r. \tag{B4}$$

Again we use the resolvent equation, now in the smaller Hilbert space $\mathscr{L}^2(\mathbf{R}_+)$:

$$\frac{1}{K-E+\alpha|v\rangle\langle v|}=\frac{1}{K-E}-\frac{\alpha}{K-E}\,|v\rangle\langle v|\,\frac{1}{K-E+\alpha|v\rangle\langle v|}. \tag{B5}$$

Taking the expectation value of (B5) with $|v\rangle$, we get an equation, to be transformed to

$$\langle v|\,\frac{1}{K-E+\alpha|v\rangle\langle v|}\,|v\rangle=\frac{\langle v|\,\frac{1}{K-E}\,|v\rangle}{1+\alpha\langle v|\,\frac{1}{K-E}\,|v\rangle}. \tag{B6}$$

Inserting (B6) in (B4) and solving for r results in

$$r=\frac{1+\alpha\langle v|(K-E)|v\rangle}{\alpha c^2-E-\alpha E\langle v|(K-E)^{-1}|v\rangle}. \tag{B7}$$

Due to the asymptotic bound at large x

$$v(x)=O(e^{-\kappa x}), \tag{B8}$$

the matrix element $\langle v|(K-k^2)^{-1}|v\rangle$ can be continued to an analytic function of k, for $\mathrm{Im}\,k>-\kappa$. The poles of the matrix element $r=r(k)$ in this region are the zeroes of the denominator of (B7). Finding these zeroes amounts to solving Eq. (34).

Other matrix elements of the resolvent involve the same denominator.

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Transmission of conduction electrons through a symmetric pair of delta-barriers or delta-wells embedded in a semiconductor or a metal

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The transmission coefficient $T(k_0)$ is calculated for conduction electrons incident with a wave vector k_0 upon a double barrier (double well) formed of two equal delta-barriers (of two equal delta-wells) embedded in a one-dimensional (1-D) semiconductor or in a 1-D metal. The stationary Schrödinger–Wannier equation $E(-i\partial/\partial x)\psi+V(x)\psi=\mathscr{E}\psi$ is solved for $V(x)=\gamma[\delta(x+a/2)+\delta(x-a/2)]$ (with real and time-independent parameters γ, a) and $\mathscr{E}=E(k_0)>0$. (The interband transitions are neglected.) The operator $E(-i\partial/\partial x)$ corresponds to a given (possibly nonquadratic) dispersion function $E(k)$ of the conduction electrons $[E(0)=0]$. It is shown that $T(k_0)$ is an oscillating function reaching the maximum value $[T(k_0)\to 1]$ on an infinite set $\{K^{(j)}\}$ of values of k_0. The shape of $T(k_0)$ depends on the shape of the dispersion function $E(k)$ in a simple way: $T(k_0)=T_{\rm par}(mv(k_0)/\hbar))$ where $T_{\rm par}(k_0)$ means the transmission coefficient in the special case when the dispersion function is quadratic, $E_{\rm par}(k)=\hbar^2k^2/2m$, and $v(k)=(1/\hbar)\partial E(k)/\partial k$ is the group velocity due to $E(k)$. [Here $E(k)$ is taken as an increasing function.]
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I. INTRODUCTION

A. Physical motivation

The use of delta-function pseudopotentials is an old and frequent approach in the solid state physics. For instance, in general discussions of the behavior of conduction electrons in metallic polycrystals, interfaces between crystalline grains were often interpreted as very thin potential energy barriers (cf. e.g., Refs. 1 and 2) and afterwards, from mathematical grounds, simplified as delta-barriers.[3] Similarly, a narrow quantum well (e.g., a sandwich structure with a very thin inner layer) can be approximated as a delta-well. In the literature, we could find examples that even the potential energy of point defects was sometimes modelled as a delta-potential, or (more correctly) as $\sim-(2\pi\sigma^2)^{-3/2}\exp[-(\mathbf{r}-\mathbf{r}_i)^2/2\sigma^2]$, where σ is a small real parameter. Such a point-defect potential may correspond to a deep level in a 3-D semiconductor and we can put it into conformity with the spirit of the well-known Koster–Slater theory.[4,5] (For brief information about this theory cf. e.g., Ref. 6.) If these point defects are densely packed along a plane (and at present there are modern techniques of the so-called delta-doping enabling to implant atomically thin layers of dopants in a crystalline structure), we may approximately replace the sum $\sim-\Sigma_i(2\pi\sigma^2)^{-1/2}\exp[-(\mathbf{r}-\mathbf{r}_i)^2/2\sigma^2]$ by an averaged function approximated as $\gamma\delta(x)$ (with $\gamma<0$).

Generally, if we can verify that a quantum mechanical method is adequate for solving a problem in which the potential energy is taken as a delta-function, we may believe that the same method is also applicable for solving more realistic (and potentially more difficult) problems.

Thus, there is good motivation to study Bloch electrons near a delta-barrier or a delta-well embedded in a crystalline lattice.

In this paper, we will consider the delta-barrier or the delta-well as an abstraction in a context of the mesoscopic quantum physics. Therefore, we will not focus attention on the Bloch wavefunctions themselves. Instead, we will pay heed to envelope wavefunctions. The only fact which

we will explicitly take into account from the Bloch theory is the existence of dispersion functions $E_n(\mathbf{k})$ defining the electron energy bands. For the sake of simplicity, we will consider one energy band only, the conduction band; therefore, we omit the band index n and write the dispersion function as $E(\mathbf{k})$. We assume that $E(\mathbf{k})$ is an analytical function of the variable $\mathbf{k}$.

Obviously, the equation $E(-i\boldsymbol{\nabla})\psi_0(\mathbf{r})=\mathscr{E}\psi_0(\mathbf{r})$ is satisfied by the plane waves $\psi_0(\mathbf{r})\sim\exp(i\mathbf{k}\cdot\mathbf{r})$ if $\mathscr{E}=E(\mathbf{k})$. In spite of this fact, it is not trivial to solve the delta-barrier or delta-well problem if $E(\mathbf{k})$ is a general function. That is why papers which dealt with delta-potentials $\gamma\delta(x)$ in crystals specified, as a rule, the dispersion law, i.e., the dependence $E=E(\mathbf{k})$, in the parabolic form,

$$E_{\mathrm{par}}(\mathbf{k})=\hbar^2k^2/2m.$$

However, there are only a few cases where the parabolic dispersion law of the conduction electrons is actually a good approximation. First of all, we can mention two such cases:

(1) the $A^{\mathrm{III}}B^{\mathrm{V}}$ semiconductors (if energies of the conduction electrons are close to the lower boundary of the conduction band) and
(2) the alkaline metals (then the electron energies may be as high as the Fermi energy).

In the majority of other cases, we have to assume that the dispersion function $E(\mathbf{k})$ of the conduction electrons is not quadratic.

In our recent papers[7,8] where we have already gone beyond the quadratic approximation of the function $E(\mathbf{k})$, we have derived, having employed the one-band Schrödinger–Wannier equation[9] (the same equation which has been used in the Koster–Slater theory[4,5] for the envelope wave-functions of the conduction electrons), general formulas for the reflection (transmission) coefficient from (through) a *single* delta-barrier or a *single* delta-well. The one-band Schrödinger–Wannier equation differs from the usual Schrödinger equation solely in the kinetic energy term: in the **r**-representation, we have to use the operator $E(-i\boldsymbol{\nabla})$ instead of the usual kinetic energy operator $-\hbar^2\nabla^2/2m$. In general, the McLaurin development of the function $E(\mathbf{k})$ may involve an infinite number of terms; in other words, $E(-i\boldsymbol{\nabla})$ may mean a functional differential operator. Therefore, if the potential energy is of the form $\gamma\delta(x)$, it is uneasy to formulate correct boundary conditions at $x=0$. Fortunately, these conditions can be avoided (as we have shown right in Refs. 7 and 8) if one uses the **k**-representation.

The purpose of the present paper is to show that our former analysis[7,8] can readily be extended. Now we will consider *two* equal delta-barriers ($\gamma>0$) or *two* equal delta-wells ($\gamma<0$) instead of one. To avoid formal complications, we will solve the problem in the one-dimensional version.

Before formulating our problem mathematically, let us mention some relevant configurations on which it may have a special bearing. First, there are planar faults of the crystalline periodicity consisting of two closely positioned parallel defect planes. Such faults were really observed. Here we can discuss, e.g., pairs of stacking faults or pairs of twin planes. For example, recently Rosová *et al.*[10–12] presented thorough electron microscopic observations of pairs of twin planes (the so-called twin lamellae in the electron micrographs) in YBaCuO—in the material most reputed as one of the high-temperature superconductors. We believe that the idea of modelling an effective potential energy of conduction electrons by pairs of delta-functions in such a case can be supported by arguments of the theory of pseudopotentials[13] well known to solid state theorists.

Second, in view of interesting applications in the semiconductor electronics, there is one specifically good reason why a detailed analysis of the situation with the potential energy defined as a sum of two delta-functions may be worth doing: if a conduction electron is to travel across a double barrier or a double well, its transmission coefficient $T(k_0)$ has to manifest the phenomenon of the ideal transparency at ''resonances.'' Indeed, microelectronic structures in which the potential energy of electrons is modelled as a symmetric double barrier are nowadays a matter to which

great attention is being paid in connection with the *resonant tunnelling transistors*.[14–17] Until now, any theoretical analysis of the resonant tunnelling through pairs of equal barriers was always confined to the case when the dispersion dependence $E=E(k)$ was taken parabolic. Moreover, if the shape of these barriers was not taken as rectangular, the tunnelling probability through them was almost always calculated approximately, mainly within the framework of the WKB approximation. Notwithstanding, if these barriers are taken as delta-barriers, the calculations can be done without resorting to such an approximation. That is why we may consider even solutions concerning the simplified situation where the symmetric double barrier is composed of delta-functions as truly archetypal for the theory of the resonant tunnelling transistors.

Admittedly, we must say that if $E(k)\equiv E_{\mathrm{par}}(k)$, the problem of deriving the transmission probability [then we write it as $T_{\mathrm{par}}(k_0)$] with the potential energy in the form of two equal delta-functions is not new: for instance, Galindo and Pascual devote much attention to this problem in their monograph.[18] Nevertheless, without repeating their way of derivations, we intend to generalize their results. Our intent is to show a general way of deriving the oscillating transmission coefficient $T(k_0)$ under the assumption that $E=E(k)$ may be a nonparabolic dependence.

B. Mathematical preliminaries

In accordance to what has just been said, the majority of calculations in the present paper concern the Hamiltonian

$$H(x)=E\left(-\mathrm{i}\,\frac{\partial}{\partial x}\right)+\gamma\left[\delta\left(x+\frac{a}{2}\right)+\delta\left(x-\frac{a}{2}\right)\right]. \tag{1}$$

(Only at the end of this paper, the Hamiltonian will be written in a more general form.)

We assume that the function $E(k)$ (a real function if k is real) is known in advance. We take $E(0)=0$ and

$$E(-k)\equiv E(k). \tag{2}$$

For the sake of simplicity, we take $E(k)$ as a growing function if $k>0$.

Condition (2) implies that

$$E(k)=\sum_{n=1}^{\infty} a_n k^{2n}. \tag{3}$$

As in Ref. 7, we do not confine the definition region of $E(k)$ to the (first) Brillouin zone and stipulate formally that

$$E(k)/|k|\to\infty \tag{4}$$

if $|k|\to\infty$. Of course, we assume that the function $E(k)$ is realistic enough if values of $|k|$ are not too high, namely if the energies $E(k)$ lie still well below the upper boundary of the band under consideration. Therefore, condition (4) corresponds to nothing more than to a mathematical extrapolation.

In particular, if $E(k)$ defines the conduction band in a narrow-gap semiconductor, we may exemplify our derivations by taking $E(k)$ in the form of the well-known Kane function[19–23]

$$E_{\mathrm{Kane}}(k)=\frac{E_g}{2}\left[\left(1+\frac{2\hbar^2k^2}{mE_g}\right)^{1/2}-1\right], \tag{5}$$

where E_g is the width of the forbidden gap. [In the case of metals for which our calculations are also applicable, $E(k)$ should be exemplified by another function.]

Before ending this Section, let us make two remarks.

First, even if the Kane function does not respect condition (4), we can easily make a mathematical amendment: to secure the fulfillment of condition (4), it is sufficient to multiply $E_{\mathrm{Kane}}(k)$ by a convenient formal factor $\Phi(u)$, fulfilling the conditions $\Phi(0)=1$, $\Phi(u)\to\infty$, with $u=\varepsilon k^2$, where $\varepsilon>0$ is a very small constant. Essentially, as we have shown in Refs. 7 and 8, condition (4) is only to guarantee that there is a finite lower bound for all eigenenergies of $H(x)$ even in the case when $\gamma<0$ and that the transmission coefficient $T(k_0)$ does not tend (on the average) to a value different from unity if $|k_0|\to\infty$.

Second, $E(k)$ need not be an entire function (i.e., a function analytical on the whole complex k-plane $\mathscr{D}_\infty$) and the function $E_{\mathrm{Kane}}(k)$ is really not. We stipulate, however, the existence of a domain $\mathscr{D}$ involving both the real k-semiaxes (the point zero may be excluded) and the infinite point and assume that the function $E(k)$ is analytical in $\mathscr{D}$. In the case of the Kane function, we define $\mathscr{D}=\mathscr{D}_\infty-\mathscr{I}$, where $\mathscr{I}$ is an interval on the imaginary k-axis with boundaries defined by the values $\mathrm{Im}\,k_d=-(1/\hbar)\sqrt{mE_g/2}-\varepsilon$ and $\mathrm{Im}\,k_u=+(1/\hbar)\sqrt{mE_g/2}+\varepsilon$. If k is complex in formula (5), we might formally discuss two separated analytical branches of the function $E_{\mathrm{Kane}}(k)$ in $\mathscr{D}$. From physical reasons, however, we do only accept the branch for which $E_{\mathrm{Kane}}(k)>0$ if $k\neq 0$ is real.

II. THE TRANSMISSION COEFFICIENT

A. Some relations formulated via the *x*-representation

In the x-representation, the stationary one-band Schrödinger–Wannier equation reads

$$\left\{E\left(-\mathrm{i}\frac{\partial}{\partial x}\right)+\gamma\left[\delta\left(x+\frac{a}{2}\right)+\delta\left(x-\frac{a}{2}\right)\right]\right\}\psi_{k_0}(x)=E(k_0)\psi_{k_0}(x). \tag{6}$$

Without loss of generality, we may confine ourselves to considering a conduction electron incident upon the pair of the delta-barriers or of the delta-wells from the left (i.e., we may take $k_0>0$). Then we take the (envelope) wavefunction in the form

$$\psi_{k_0}(x)=[1-\Theta(x+a/2)][\exp(\mathrm{i}k_0x)+B\ \exp(-\mathrm{i}k_0x)]+[\Theta(x+a/2)-\Theta(x-a/2)]$$
$$\times[F\ \cos(k_0x)+G\ \sin(k_0x)]+\Theta(x-a/2)C\ \exp(\mathrm{i}k_0x) \tag{7}$$

or

$$\psi_{k_0}(x)=\exp(\mathrm{i}k_0x)+B\ \exp(-\mathrm{i}k_0x)+\Theta(x+a/2)[F\ \cos(k_0x)+G\ \sin(k_0x)-\exp(\mathrm{i}k_0x)$$
$$-B\ \exp(-\mathrm{i}k_0x)]+\Theta(x-a/2)[C\ \exp(\mathrm{i}k_0x)-F\ \cos(k_0x)-G\ \sin(k_0x)]. \tag{8}$$

Here, $\Theta(x)$ is the Heaviside step function: $\Theta(x)=0$ if $x<0$ and $\Theta(x)=1$ if $x>0$. Since the function $\psi_{k_0}(x)$ is continuous at $x=\pm a/2$, we obtain the equations

$$\psi_{k_0}(-a/2)=\exp(-\mathrm{i}k_0a/2)+B\ \exp(\mathrm{i}k_0a/2)=F\ \cos(k_0a/2)-G\ \sin(k_0a/2), \tag{9}$$

$$\psi_{k_0}(a/2)=C\ \exp(\mathrm{i}k_0a/2)=F\ \cos(k_0a/2)+G\ \sin(k_0a/2). \tag{10}$$

From them, we obtain the expressions

$$F=\frac{\exp(-\mathrm{i}k_0a/2)+(C+B)\exp(\mathrm{i}k_0a/2)}{2\cos(k_0a/2)}, \tag{11}$$

$$G=\frac{-\exp(-\mathrm{i}k_0a/2)+(C-B)\exp(\mathrm{i}k_0a/2)}{2\sin(k_0a/2)}. \tag{12}$$

When inserting (11) and (12) into (8), we obtain $\psi_{k_0}(x)$ as a function of two complex coefficients: $B \equiv B(k_0)$ and $C \equiv C(k_0)$.

The transmission coefficient is

$$T = \frac{|C|^2}{|B|^2 + |C|^2}. \tag{13}$$

However, since

$$|B|^2 + |C|^2 = 1 \tag{14}$$

(we will verify this explicitly), then

$$T(k_0) = |C(k_0)|^2. \tag{15}$$

The complementary probability, i.e.,

$$R(k_0) = 1 - T(k_0) = |B(k_0)|^2, \tag{16}$$

is the reflection coefficient.

Thus, the basic problem is to calculate the coefficients B and C.

B. Form of the wavefunction in the *k*-representation

Let $M_K(k)$, $N_K(k)$, $P_K(k)$, etc., be the Fourier originals to $m_K(x)$, $n_K(x)$, $p_K(x)$:

$$m_K(x) = \int_{-\infty}^{\infty} \mathrm{d}k M_K(k) \exp(\mathrm{i}kx), \tag{17}$$

etc.

We assume that K is a real parameter. The Fourier original to the exponential

$$m_K(x) = \exp(\mathrm{i}Kx) \tag{18}$$

is the delta function

$$M_K(k) = \delta(k - K). \tag{19}$$

The Fourier original to the generalized analytical function

$$n_K(x) = \Theta(x) \exp(\mathrm{i}Kx) \tag{20}$$

is

$$N_K(k) = \frac{1}{2}\,\delta(k-K) - \frac{\mathrm{i}}{2\pi}\,\mathrm{v.p.}\,\frac{1}{k-K} = \frac{1}{2}\,\delta(k-K) - \frac{\mathrm{i}}{4\pi}\left(\frac{1}{k-K-\mathrm{i}\epsilon} + \frac{1}{k-K+\mathrm{i}\epsilon}\right). \tag{21}$$

(In the last relation, ϵ is a positive infinitesimal quantity. The symbol v.p. means the Cauchy principal value.[24])

In the wavefunction (8), we have also got the terms of the type

$$p_K(x) = \Theta(x-b) \exp(\mathrm{i}Kx), \tag{22}$$

$$q_{k_0}(x) = \Theta(x-b) \cos(k_0 x), \tag{23}$$

$$r_{k_0}(x)=\Theta(x-b)\sin(k_0x). \tag{24}$$

Respectively, they correspond to the Fourier originals

$$P_K(k)=\exp[-\mathrm{i}(k-K)b]N_K(k), \tag{26}$$

$$\begin{aligned}Q_{k_0}(k)&=\tfrac{1}{2}(\exp[-\mathrm{i}(k-k_0)b]N_{k_0}(k)+\exp[-\mathrm{i}(k+k_0)b]N_{-k_0}(k))\\&=\tfrac{1}{2}\exp(-\mathrm{i}k_0b)(\exp(\mathrm{i}k_0b)N_{k_0}(k)+\exp(-\mathrm{i}k_0b)N_{-k_0}(k)),\end{aligned} \tag{27}$$

$$\begin{aligned}R_{k_0}(k)&=\frac{1}{2\mathrm{i}}\,(\exp[-\mathrm{i}(k-k_0)b]N_{k_0}(k)-\exp[-\mathrm{i}(k+k_0)b]N_{-k_0}(k))\\&=\frac{1}{2\mathrm{i}}\exp(-\mathrm{i}k_0b)(\exp(\mathrm{i}k_0b)N_{k_0}(k)-\exp(-\mathrm{i}k_0b)N_{-k_0}(k)),\end{aligned} \tag{28}$$

where $N_K(k)$ is given by expression (21). (In our case, b is equal either to $-a/2$ or to $a/2$.)

We define the Fourier original $\phi_{k_0}(k)$ to $\psi_{k_0}(x)$ as well:

$$\psi_{k_0}(x)=\int_{-\infty}^{\infty}\mathrm{d}k\,\phi_{k_0}(k)\exp(\mathrm{i}kx). \tag{29}$$

When employing the wavefunction (8) on the lhs of (29) and utilizing correspondingly, term by term, the Fourier originals (19), (21), (26), (27), and (28), we obtain the decomposition

$$\phi_{k_0}(k)=\phi^{\delta}_{k_0}(k)+\phi^{\mathrm{vp}}_{k_0}(k) \tag{30}$$

where

$$\phi^{\delta}_{k_0}(k)=\tfrac{1}{2}[(1+C)\,\delta(k-k_0)+B\,\delta(k+k_0)] \tag{31}$$

is the ''delta function part.'' The ''valeur principale part'' $\phi^{\mathrm{vp}}_{k_0}(k)$ will be calculated in the next section.

C. Solution of the Schrödinger–Wannier equation in the *k*-representation

The function $\phi_{k_0}(k)$ has to obey the Schrödinger–Wannier equation

$$[E(k)-E(k_0)]\phi_{k_0}(k)=-\frac{\gamma}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}k'\,\phi_{k_0}(k')\left\{\exp\left[-\mathrm{i}(k'-k)\,\frac{a}{2}\right]+\exp\left[\mathrm{i}(k'-k)\,\frac{a}{2}\right]\right\}. \tag{32}$$

Equation (32) results directly from Eq. (6) if the convolution theorem is applied. [Note that the Fourier original to $\delta(x-b)$ is $\exp(-\mathrm{i}kb)/2\pi$.] However, according to (29), we have

$$\psi_{k_0}\left(-\frac{a}{2}\right)=\int_{-\infty}^{\infty}\mathrm{d}k'\,\phi_{k_0}(k')\exp\left(-\mathrm{i}k'\,\frac{a}{2}\right), \tag{33a}$$

$$\psi_{k_0}\left(\frac{a}{2}\right)=\int_{-\infty}^{\infty}\mathrm{d}k'\,\phi_{k_0}(k')\exp\left(\mathrm{i}k'\,\frac{a}{2}\right), \tag{33b}$$

and thus we may write the Schrödinger–Wannier equation in the form

$$[E(k)-E(k_0)]\phi_{k_0}(k)=-\frac{\gamma}{2\pi}\left[\psi_{k_0}\left(-\frac{a}{2}\right)\exp\left(\mathrm{i}k\,\frac{a}{2}\right)+\psi_{k_0}\left(\frac{a}{2}\right)\exp\left(-\mathrm{i}k\,\frac{a}{2}\right)\right]. \tag{34}$$

Obviously,

$$[E(k)-E(k_0)]\phi^{\delta}_{k_0}(k)=0. \tag{35}$$

Therefore, instead of (34), we may write the equation

$$[E(k)-E(k_0)]\phi^{\mathrm{vp}}_{k_0}(k)=-\frac{\gamma}{2\pi}\left[\psi_{k_0}\left(-\frac{a}{2}\right)\exp\left(\mathrm{i}k\,\frac{a}{2}\right)+\psi_{k_0}(a)\exp\left(-\mathrm{i}k\,\frac{a}{2}\right)\right]. \tag{36}$$

According to the very definition of the function $\phi^{\mathrm{vp}}_{k_0}(k)$, if any product of this function with an analytical function is to be integrated with respect to the variable k, the integration has to be done in the Cauchy sense. So we have to exempt two infinitesimally short intervals centered in the points $\pm k_0$, i.e., $(-k_0-\epsilon,-k_0+\epsilon)$ and $(k_0-\epsilon,k_0+\epsilon)$, from the real k-axis. Then, as $E(k)\neq E(k_0)$ for all values of k outside these intervals, we may divide Eq. (36) by $E(k)-E(k_0)$. Thus we obtain the expression

$$\phi^{\mathrm{vp}}_{k_0}(k)=-\frac{\gamma}{2\pi}\,\mathrm{v.p.}\left[\psi_{k_0}\left(-\frac{a}{2}\right)\,\frac{\exp(\mathrm{i}ka/2)}{E(k)-E(k_0)}+\psi_{k_0}\left(\frac{a}{2}\right)\,\frac{\exp(-\mathrm{i}ka/2)}{E(k)-E(k_0)}\right]. \tag{37}$$

Its Fourier image is

$$\psi^{\mathrm{vp}}_{k_0}(x)=\int_{-\infty}^{\infty}\mathrm{d}k\,\phi^{\mathrm{vp}}_{k_0}(k)\exp(\mathrm{i}\,kx). \tag{38}$$

Formulas (37) and (38) imply that we have to cope with the calculation of the integral

$$\mathrm{v.p.}\int_{-\infty}^{\infty}\mathrm{d}k\,\frac{\exp[\mathrm{i}k(x-b)]}{E(k)-E(k_0)}=\frac{1}{2}\int_{-\infty}^{\infty}\mathrm{d}\,k\,\frac{\exp[\mathrm{i}k(x-b)]}{E(k-\mathrm{i}\,\epsilon)-E(k_0)}+\frac{1}{2}\int_{-\infty}^{\infty}\mathrm{d}\,k\,\frac{\exp[\mathrm{i}k(x-b)]}{E(k+\mathrm{i}\,\epsilon)-E(k_0)}. \tag{39}$$

In Sec. IB, we have defined (for k taken as a complex variable) the domain $\mathscr{D}$ and the interval $\mathscr{I}$. Now we add the definition of the subdomain $\mathscr{D}^{+}\subset\mathscr{D}$ and of the subinterval $\mathscr{I}^{+}\subset\mathscr{I}$ by the condition $\mathrm{Im}\,k>0$. (Analogically, we say that $k\in\mathscr{D}^{-}\subset\mathscr{D}$ or $k\in\mathscr{I}^{-}\subset\mathscr{I}$ if $\mathrm{Im}\,k<0$.) The function $1/[E(k-\mathrm{i}\epsilon)-E(k_0)]$ has two single poles, $k^{+}_{1,2}=\pm k_0+\mathrm{i}\epsilon$, lying in $\mathscr{D}^{+}$, while $1/[E(k+\mathrm{i}\epsilon)-E(k_0)]$ has two single poles, $k^{-}_{1,2}=\pm k_0-\mathrm{i}\epsilon$, lying in $\mathscr{D}^{-}$. If $x>b$, we define a closed contour Γ^{+} consisting of five parts as follows. The first part is the negative half of the real k-axis. The second and third parts of Γ^{+} are the left-hand and right-hand boundaries of $\mathscr{I}^{+}$. The fourth part is the positive half of the real k-axis. The final (fifth) part is an infinitely large semicircle (centered at $k=0$) lying in $\mathscr{D}^{+}$. Similarly, if $x<b$, we define the closed contour Γ^{-} as the mirror image (with respect to the real k-axis) of Γ^{+}. Then, using the theorem of residua, we obtain the results

$$\frac{1}{2}\int_{-\infty}^{\infty}\mathrm{d}k\,\frac{\exp[\mathrm{i}k(x-b)]}{E(k-\mathrm{i}\epsilon)-E(k_0)}$$
$$=\frac{1}{2}\oint_{\Gamma^+}\mathrm{d}k\,\frac{\exp[\mathrm{i}k(x-b)]}{E(k-\mathrm{i}\epsilon)-E(k_0)}$$
$$=\mathrm{i}\pi\Theta(x-b)(\mathrm{res}_{k=k_0+\mathrm{i}\epsilon}+\mathrm{res}_{k=-k_0+\mathrm{i}\epsilon})\,\frac{\exp[\mathrm{i}k(x-b)]}{E(k-\mathrm{i}\epsilon)-E(k_0)}$$
$$=i\pi\Theta(x-b)\,\frac{\exp[\mathrm{i}k_0(x-b)]-\exp[-\mathrm{i}k_0(x-b)}{E'(k_0)},\tag{40+}$$

$$\frac{1}{2}\int_{-\infty}^{\infty}\mathrm{d}k\,\frac{\exp[\mathrm{i}k(x-b)]}{E(k+\mathrm{i}\epsilon)-E(k_0)}=-\frac{1}{2}\oint_{\Gamma^-}\mathrm{d}k\,\frac{\exp[\mathrm{i}k(x-b)]}{E(k+\mathrm{i}\epsilon)-E(k_0)}$$
$$=-\mathrm{i}\pi[1-\Theta(x-b)](\mathrm{res}_{k=k_0-\mathrm{i}\epsilon}+\mathrm{res}_{k=-k_0-\mathrm{i}\epsilon})\,\frac{\exp[\mathrm{i}k(x-b)]}{E(k+\mathrm{i}\epsilon)-E(k_0)}$$
$$=-\mathrm{i}\pi[1-\Theta(x-b)]\,\frac{\exp[\mathrm{i}k_0(x-b)]-\exp[-\mathrm{i}k_0(x-b)]}{E'(k_0)}.\tag{40-}$$

Here we have introduced the symbol $\oint$ in the usual sense, i.e., we have reserved it for the anticlockwise integration. When integrating along Γ^+ (Γ^-), we observe that the contributions due to the left-hand and right-hand sides of $\mathscr{T}^+$ ($\mathscr{T}^-$) exactly cancel out.

For brevity, we have introduced the symbol

$$E'(k)=\frac{\mathrm{d}E(k)}{\mathrm{d}k}.\tag{41}$$

[Note that $E'(k)>0$ and $E'(-k)=-E'(k)$.]

In this way we have derived the formula

$$\mathrm{v.p.}\int_{-\infty}^{\infty}\mathrm{d}k\,\frac{\exp(\mathrm{i}kX)}{E(k)-E(k_0)}=-2\pi[2\Theta(X)-1]\,\frac{\sin(k_0X)}{E'(k_0)}.\tag{42}$$

With its aid, formulas (37) and (38) yield us the function

$$\psi_{k_0}^{\mathrm{vp}}(x)=-\frac{\gamma}{E'(k_0)}\left\{\psi_{k_0}\left(-\frac{a}{2}\right)\left[2\Theta\left(x+\frac{a}{2}\right)-1\right]\sin\left[k_0\left(x+\frac{a}{2}\right)\right]\right.$$
$$\left.+\psi_{k_0}\left(\frac{a}{2}\right)\left[2\Theta\left(x-\frac{a}{2}\right)-1\right]\sin\left[k_0\left(x-\frac{a}{2}\right)\right]\right\}.\tag{43}$$

Hence

$$\psi_{k_0}^{\mathrm{vp}}\left(-\frac{a}{2}-0\right)=\frac{\gamma}{E'(k_0)}\,\psi_{k_0}\left(\frac{a}{2}\right)\sin(k_0a)=\frac{\gamma}{E'(k_0)}\,C\,\exp\left(\mathrm{i}k_0\,\frac{a}{2}\right)\sin(k_0a),\tag{44}$$

$$\psi_{k_0}^{\mathrm{vp}}\left(\frac{a}{2}+0\right)=\frac{\gamma}{E'(k_0)}\,\psi_{k_0}\left(-\frac{a}{2}\right)\sin(k_0a)=\frac{\gamma}{E'(k_0)}\left[\exp\left(-\mathrm{i}k_0\,\frac{a}{2}\right)+B\,\exp\left(\mathrm{i}k_0\,\frac{a}{2}\right)\right]\sin(k_0a).\tag{45}$$

[Here we have employed formulas (9) and (10).]

However, the respective Fourier images to functions (30) and (31) are

$$\psi_{k_0}(x)=\psi^{\delta}_{k_0}(x)+\psi^{\mathrm{vp}}_{k_0}(x), \tag{46}$$

$$\psi^{\delta}_{k_0}(x)=\tfrac{1}{2}[(C+1)\exp(\mathrm{i}k_0x)+B\ \exp(-\mathrm{i}k_0x)]. \tag{47}$$

The function (46) is continous. When taking x equal to $-a/2-0$ and to $a/2+0$, and bearing in mind expressions (44) and (45), we obtain the following two linear algebraic equations for the coefficients B and C:

$$\exp\left(-\mathrm{i}k_0\frac{a}{2}\right)+B\ \exp\left(\mathrm{i}k_0\frac{a}{2}\right)=\frac{1}{2}\left[(C+1)\exp\left(-\mathrm{i}k_0\frac{a}{2}\right)+B\ \exp\left(\mathrm{i}k_0\frac{a}{2}\right)\right]$$
$$+\frac{\gamma}{E'(k_0)}\ C\ \exp\left(\mathrm{i}k_0\frac{a}{2}\right)\sin(k_0a), \tag{48}$$

$$C\ \exp\left(\mathrm{i}k_0\frac{a}{2}\right)=\frac{1}{2}\left[(C+1)\exp\left(\mathrm{i}k_0\frac{a}{2}\right)+B\ \exp\left(-\mathrm{i}k_0\frac{a}{2}\right)\right]$$
$$+\frac{\gamma}{E'(k_0)}\left[\exp\left(-\mathrm{i}k_0\frac{a}{2}\right)+B\ \exp\left(\mathrm{i}k_0\frac{a}{2}\right)\right] \tag{49}$$

[cf. again (9) and (10)].
Their solution is

$$B(k_0)=\exp(-\mathrm{i}k_0a)\ \frac{2\gamma[E'(k_0)\cos(k_0a)+\gamma\ \sin(k_0a)]}{D(k_0)}, \tag{50}$$

$$C(k_0)=\mathrm{i}\ \exp(-\mathrm{i}k_0a)\ \frac{[E'(k_0)]^2}{D(k_0)}, \tag{51}$$

where

$$D(k_0)=-2\gamma E'(k_0)\cos(k_0a)+[[E'(k_0)]^2-2\gamma^2]\sin(k_0a)$$
$$+\mathrm{i}E'(k_0)[E'(k_0)\cos(k_0a)+2\gamma\ \sin(k_0a)]. \tag{52}$$

D. General result for the transmission coefficient $T(k_0)$

The square of the absolute value of (52) is

$$|D(k_0)|^2=[E'(k_0)]^4+4\gamma^2[E'(k_0)\cos(k_0a)+\gamma\ \sin(k_0a)]^2. \tag{53}$$

When calculating $|C(k_0)|^2$, we obtain the formula

$$T(k_0)=\frac{[E'(k_0)]^4}{[E'(k_0)]^4+4\gamma^2[E'(k_0)\cos(k_0a)+\gamma\ \sin(k_0a)]^2} \tag{54}$$

giving the probability with which a conduction electron with the wavevector k_0 can travel across the system of two equal delta-barriers or delta-wells that are the distance a apart. The complementary probability, i.e., the reflection coefficient which is equal to $|B(k_0)|^2$, then is

$$R(k_0)=\frac{4\gamma^2[E'(k_0)\cos(k_0a)+\gamma\,\sin(k_0a)]^2}{[E'(k_0)]^4+4\gamma^2[E'(k_0)\cos(k_0a)+\gamma\,\sin(k_0a)]^2}. \tag{55}$$

The identity $T+R=1$ proves exactly the validity of identity (14).

III. DISCUSSION AND CONCLUDING REMARKS

A. The oscillations of the transmission coefficient $T(k_0)$

When introducing the group velocity

$$v(k)=\frac{1}{\hbar}\,E'(k), \tag{56}$$

we may rewrite formula (54) in the form

$$T(k_0)=\frac{[\hbar v(k_0)]^4}{[\hbar v(k_0)]^4+4\gamma^2[\hbar v(k_0)\cos(k_0a)+\gamma\,\sin(k_0a)]^2}. \tag{57}$$

According to this formula, there are values of k_0 at which $T(k_0)$ is equal to unity. This ideal transparency of the symmetric delta-function double barrier or double well takes place at all values of k_0 that are equal to the roots $K^{(j)}$ of the equation

$$\hbar v(K^{(j)})=-\gamma\,\tan(K^{(j)}a). \tag{58}$$

Notice that

$$v_{\rm par}(k)=\frac{\hbar k}{m}, \tag{59}$$

while

$$v_{\rm Kane}(k)=\frac{\hbar k}{m}\left[1+\frac{2\hbar^2k^2}{mE_g}\right]^{-1/2}. \tag{60}$$

Let us introduce the dimensionless parameters

$$\kappa=k_0a, \tag{61}$$

$$\beta=\frac{m\gamma a}{\hbar^2}. \tag{62}$$

Then we define the dimensionless function $\eta(\kappa)$,

$$E(k_0)=\frac{\hbar^2}{ma^2}\,\eta(\kappa). \tag{63}$$

In particular,

$$\eta_{\rm par}(\kappa)=\tfrac{1}{2}\kappa^2, \tag{64}$$

$$\eta_{\rm Kane}(\kappa)=\frac{\eta_g}{2}\left[\left(1+\frac{2\kappa^2}{\eta_g}\right)^{1/2}-1\right]. \tag{65}$$

In the latter formula, we have used η_g instead of E_g:

$$E_g=\frac{\hbar^2}{ma^2}\,\eta_g\,. \tag{66}$$

Clearly, $\hbar^2/ma^2$ and a are, respectively, the units for energies and distances. After defining the dimensionless group velocity

$$v(\kappa)=\frac{\mathrm{d}\eta(\kappa)}{\mathrm{d}\kappa}, \tag{67}$$

we obtain the functions

$$v_{\mathrm{par}}(\kappa)=\kappa, \tag{68}$$

$$v_{\mathrm{Kane}}(\kappa)=\frac{\kappa}{(1+2\kappa^2/\eta_g)^{1/2}}. \tag{69}$$

Thus, according to formula (57), we obtain the function

$$\mathscr{T}(\kappa)=\frac{[v(\kappa)]^4}{[v(\kappa)]^4+4\beta^2[v(\kappa)\cos(\kappa)+\beta\,\sin(\kappa)]^2} \tag{70}$$

so that

$$\mathscr{T}_{\mathrm{par}}(\kappa)=\frac{\kappa^4}{\kappa^4+4\beta^2[\kappa\,\cos(\kappa)+\beta\,\sin(\kappa)]^2} \tag{71}$$

[cf. formula (A12) in the Appendix] and

$$\mathscr{T}_{\mathrm{Kane}}(\kappa)=\frac{\kappa^4}{\kappa^4+4\beta^2(1+2\kappa^2/\eta_g)[\kappa\,\cos(\kappa)+\beta(1+2\kappa^2/\eta_g)^{1/2}\,\sin(\kappa)]^2}. \tag{72}$$

In Fig. 1, we compare $\mathscr{T}_{\mathrm{par}}(\kappa)$ (the upper frame) with $\mathscr{T}_{\mathrm{Kane}}(\kappa)$ (the lower frame). Both the frames are equally scaled. The vertical dashed lines correspond to $\kappa=j\pi$, while the dotted lines correspond to $\kappa=(j-1/2)\pi$, $j=1,2,\ldots$. The full curved lines correspond to the double delta-function barrier with $\beta=5$ and the dashed curved lines correspond to the double delta-function well with $\beta=-5$. The curves showing $\mathscr{T}_{\mathrm{Kane}}(\kappa)$ concern the value $\eta_g=120$.

As it is seen from formula (70), the values $\mathscr{T}(j\pi/2)$ (with an arbitrary integer j) are always for β and for $-\beta$ equal to one another. (In both the frames of Fig. 1, the full curved line and the dashed curved line intersect one another just at $\kappa=j\pi/2$.)

In the dimensionless variables that we are now using formula (58) reads

$$v(\kappa^{(j)})=-\beta\,\tan(\kappa^{(j)}), \tag{73}$$

so that

$$v_{\mathrm{par}}(\kappa^{(j)})=\kappa^{(j)}, \tag{74}$$

$$v_{\mathrm{Kane}}(\kappa^{(j)})=\kappa^{(j)}[1+2\kappa^{(j)^2}/\eta_g]^{-1/2}. \tag{75}$$

If $\beta>0$ and $j\to\infty$, the position $\kappa_{\mathrm{par}}^{(j)}$ of the jth maximum of the function $\mathscr{T}_{\mathrm{par}}(\kappa)$ $(=1)$ tends to the value $(j-1/2)\pi$ from the right. In the double-well case, however, for $j\to\infty$, we find that

$\kappa_{\rm par}^{(j)} \to (j + 1/2)\pi$ from the left for $-1<\beta<0$ if $-1<\beta<0$ and $\kappa_{\rm par}^{(j)} \to (j - 1/2)\pi$ from the left if $\beta<-1$. On the other hand, the asymptotic behavior of the position $\kappa_{\rm Kane}^{(j)}$ of the jth maximum of the function $\mathscr{T}_{\rm Kane}(\kappa)$ $(=1)$ is different. Formula (75) implies that $\upsilon_{\rm Kane}(\kappa) \to \kappa(\eta_g/2)^{1/2}$ if $\kappa \to \infty$. Therefore, if $\beta>0$ and $j \to \infty$, the position $\kappa_{\rm Kane}^{(j)}$ of the jth maximum of the function $\mathscr{T}_{\rm par}(\kappa)$ $(=1)$ tends to the value $j\pi - \arctan[(\eta_g/2)^{1/2}/\beta)]$ from the right. In the double-well case, we find for $j \to \infty$ that $\kappa_{\rm Kane}^{(j)} \to j\pi + \arctan[(\eta_g/2)^{1/2}/|\beta|]$ from the left if $-1<\beta<0$ and $\kappa_{\rm Kane}^{(j)} \to j\pi - \arctan[(\eta_g/2)^{1/2}/|\beta|]$ from the left if $\beta<-1$.

B. The transmission coefficient as a function of energy

If we depict the transmission coefficient T as a function of the energy $E(k_0)$, and not as function of k_0 (in contrast to the Sec. III A), the difference between $T_{\rm par}$ and $T_{\rm Kane}$ becomes even more visible.

Since $E(k)$ has been taken as a growing function of $|k|$, we may equally say that $|k|$ is a growing function of E. In particular, after inverting formulas (64) and (65), we obtain the functions

$$\kappa_{\rm par}(\eta) = (2\eta)^{1/2}, \tag{76}$$

$$\kappa_{\rm Kane}(\eta) = (2\eta)^{1/2}[1 + \eta/\eta_g]^{1/2}. \tag{77}$$

Correspondingly, we define the functions

$$\tilde{\mathscr{T}}_{\rm par}(\eta) \equiv \mathscr{T}(\kappa_{\rm par}(\eta)), \tag{78}$$

$$\tilde{\mathscr{T}}_{\rm Kane}(\eta) \equiv \mathscr{T}(\kappa_{\rm Kane}(\eta)). \tag{79}$$

These functions are shown in Fig. 2. The vertical dashed lines are erected at $\eta = \eta_{\rm par}(j\pi)$ (in the upper frame) and at $\eta = \eta_{\rm Kane}(j\pi)$ (in lower frame). Respectively, the vertical dotted lines are erected at $\eta = \eta_{\rm par}((j-1/2)\pi)$ and at $\eta = \eta_{\rm Kane}((j-1/2)\pi)$. The shifts of the vertical dashed (dotted) lines of the lower frame against the corresponding vertical dashed (dotted) lines of the upper frame demonstrate the extent of the deviation from the parabolicity if $E_{\rm par}(k)$ is replaced by $E_{\rm Kane}(k)$ with preserving the same effective mass m at $k=0$:

$$\frac{1}{m} = \frac{1}{\hbar^2}\left.\frac{\partial^2 E_{\rm par}(k)}{\partial k^2}\right|_{k=0} = \frac{1}{\hbar^2}\left.\frac{\partial^2 E_{\rm Kane}(k)}{\partial k^2}\right|_{k=0}. \tag{80}$$

Evidently, the number of the maxima in the lower frame is higher than in the upper frame, in correspondence with the fact that the curve $E = E_{\rm Kane}(k)$ lies below the curve $E = E_{\rm par}(k)$.

C. The limiting case when $a \to 0$

In our previous paper,[7] we have calculated the transmission coefficient $T_\gamma^{\rm single}(k_0)$ for conduction electrons incident upon a single delta-function potential of the strength γ:

$$T_\gamma^{\rm single}(k_0) = \frac{[\hbar\upsilon(k_0)]^2}{[\hbar\upsilon(k_0)]^2 + \gamma^2}. \tag{81}$$

According to formula (57), if $a \to +0$, i.e., if two delta-potentials of the strength γ join together, the pair of these delta-potentials gives the same transmission probability $T(k_0)$ as one single delta-potential but with the strength 2γ :

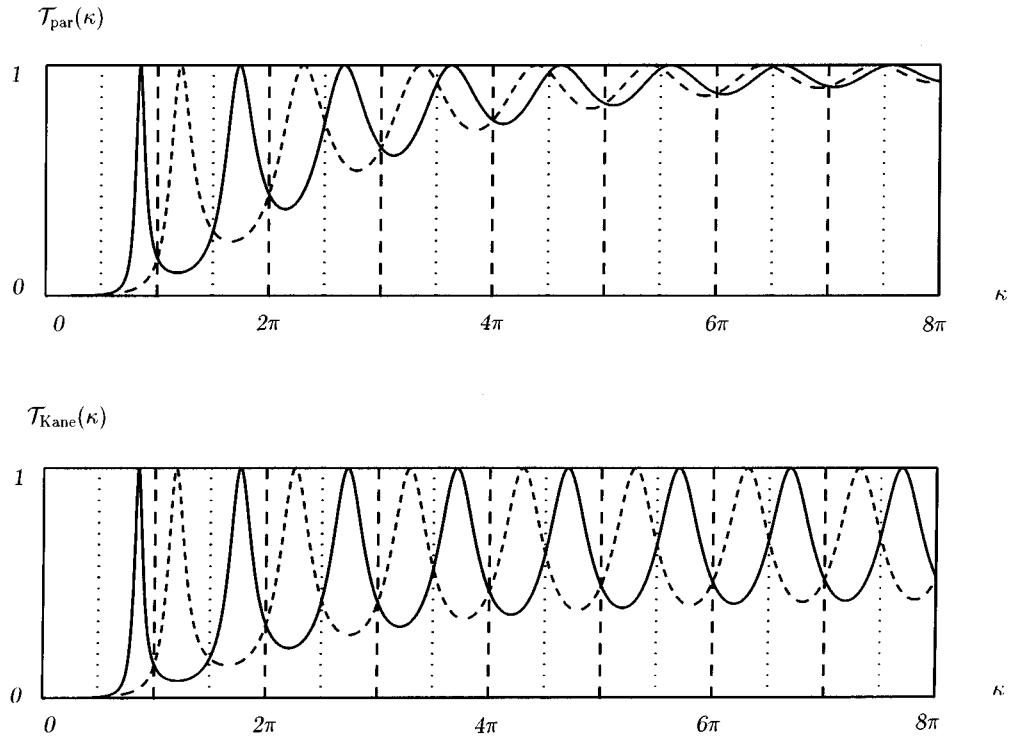

FIG. 1. The upper frame: the transmission coefficient $\mathcal{T}=\mathcal{T}_{\mathrm{par}}(\kappa)$ [i.e., if $E(k)=E_{\mathrm{par}}(k)$] for $\beta=5$ (full curved line) and for $\beta=-5$ (dashed curved line). The lower frame: the transmission coefficient $\mathcal{T}=\mathcal{T}_{\mathrm{Kane}}(\kappa)$ [i.e., if $E(k)=E_{\mathrm{Kane}}(k)$] for $\beta=5$ (full curved line) and for $\beta=-5$ (dashed curved line) ($\eta_g=120$).

$$\lim_{a\to+0} T(k_0)=T_{2\gamma}^{\mathrm{single}}(k_0). \tag{82}$$

D. Difficulties with boundary conditions in the *x*-representation

Our main intent in the present paper was to demonstrate explicitly that it is really advantageous to solve the Schrödinger–Wannier equation in the k-representation since then we are free of difficulties which otherwise arise with boundary conditions in the x-representation whenever the potential energy term of the Hamiltonian involves at least one delta-function, provided that $E(k)$ is a nonquadratic function. (Of course, there are no difficulties with boundary conditions followed from the overall continuity of any envelope wavefunction; actually, problems arise only with boundary conditions formulated for derivatives—and not only for the first-order derivative but also for higher-order derivatives—of the envelope wavefunction.)

Fortunately, if we focus attention on eigenfunction $\psi(x)\equiv\psi_{k_0}(x)$ due to positive eigenenergies $\mathscr{E}=E(k_0)$, then for any position x_s of the delta-function potential $\sim\delta(x-x_s)$, we *may* write a relation which looks like a boundary condition involving derivatives of $\psi_{k_0}(x)$.

We will now briefly elucidate this statement with a more general Hamiltonian than (1). We define the Hamiltonian

$$H_S(x)=E\left(-\mathrm{i}\frac{\partial}{\partial x}\right)+\sum_{s=1}^{\infty}\gamma_s\delta(x-x_s), \tag{83}$$

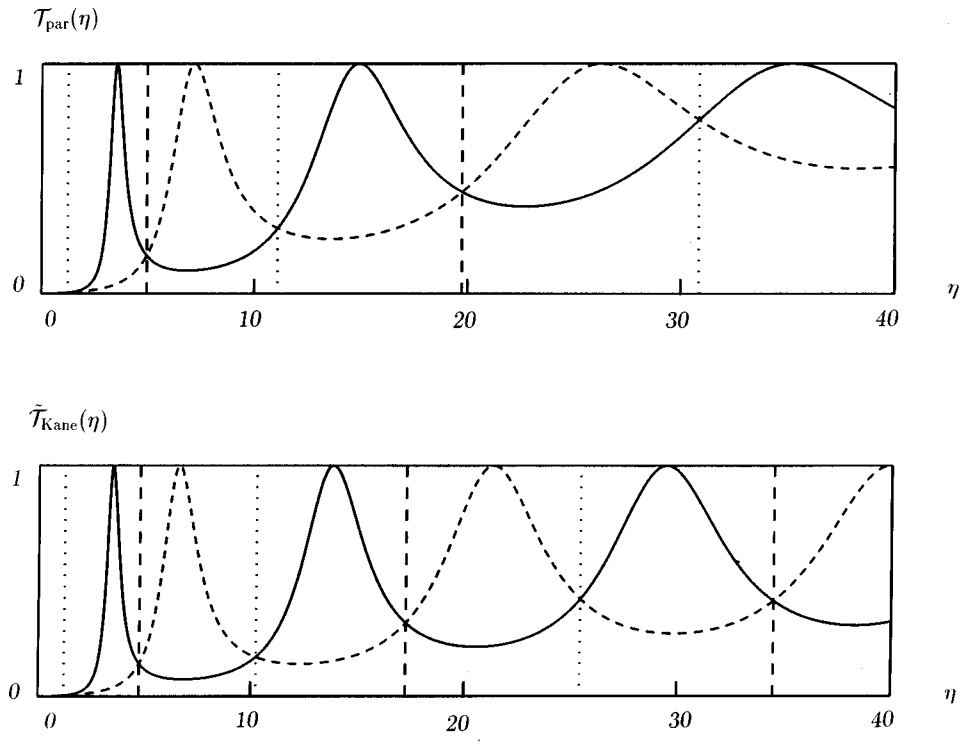

FIG. 2. The same as in Fig. 1 ($\beta=\pm 5$) but the corresponding transmission coefficients are taken as functions of the energy parameter η: $\tilde{\mathcal{T}}_{\rm par}(\eta)=\mathcal{T}_{\rm par}(\kappa)$, $\tilde{\mathcal{T}}_{\rm Kane}(\eta)=\mathcal{T}_{\rm Kane}(\kappa)$ ($\eta_g=120$).

assuming that the (real) values γ_s and x_s are arbitrary but $x_1<x_2<\ldots<x_S$. In (83), we assume that the operator $E(-\mathrm{i}\partial/\partial x)$ corresponds to an arbitrary dispersion function $E(k)$. [Regard only condition (4).] In particular, we define also

$$H_{S,\rm par}(x)=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+\sum_{s=1}^{\infty}\gamma_s\delta(x-x_s). \tag{84}$$

Let $\Psi_{\rm par}(x,t)$ be an arbitrary wavefunction satisfying the Schrödinger–Wannier equation

$$\mathrm{i}\hbar\,\frac{\partial\Psi_{\rm par}(x,t)}{\partial t}=H_{S,\rm par}(x)\Psi_{\rm par}(x,t). \tag{85}$$

Since $H_{S,\rm par}(x)$ is a second-order differential operator, we may write down the boundary conditions

$$-\frac{\hbar^2}{2m}\left[\left.\frac{\partial\Psi_{\rm par}(x,t)}{\partial x}\right|_{x=x_s+0}-\left.\frac{\partial\Psi_{\rm par}(x,t)}{\partial x}\right|_{x=x_s-0}\right]+\gamma_s\Psi_{\rm par}(x_s)=0. \tag{86}$$

If we prefer to use the group velocity $v_{\rm par}(k)$ [cf. formula (59)], we can rewrite equation (86) into the form

$$-\mathrm{i}\left(\frac{\hbar}{2}\right)\left[v_{\mathrm{par}}\left(-\mathrm{i}\,\frac{\partial}{\partial x}\right)\Psi_{\mathrm{par}}(x,t)\Big|_{x=x_s+0}-v_{\mathrm{par}}\left(-\mathrm{i}\,\frac{\partial}{\partial x}\right)\Psi_{\mathrm{par}}(x,t)\Big|_{x=x_s-0}\right]+\gamma_s\Psi_{\mathrm{par}}(x_s,t)=0. \tag{87}$$

[The envelope wavefunction $\Psi_{\mathrm{par}}(x,t)$ itself is continuous but its first derivative $\partial\Psi_{\mathrm{par}}(x,t)/\partial x$ is discontinuous at $x=x_s$.]

Let us now discuss stationary wavefunctions

$$\Psi_{\mathscr{E}}(x,t)=\exp(-\mathrm{i}\,\mathscr{E}t/\hbar)\,\tilde{\psi}_{\mathscr{E}}(x) \tag{88}$$

in the case when $E(k)$ [satisfying condition (4)] is not a quadratic function.

In accordance with the way of derivations which we have decided to follow in Sec. II, we may make the following general statement:

if $\mathscr{E}=E(k_0)>0$, then for $\tilde{\psi}_{\mathscr{E}}(x)=\psi_{k_0}(x)$ we may write the identities

$$-\mathrm{i}\left(\frac{\hbar}{2}\right)\left[v\left(-\mathrm{i}\frac{\partial}{\partial x}\right)\psi_{k_0}(x)\Big|_{x=x_s+0}-v\left(-\mathrm{i}\frac{\partial}{\partial x}\right)\psi_{k_0}(x)\Big|_{x=x_s-0}\right]+\gamma_s\psi_{k_0}(x_s)=0 \tag{89}$$

where the operator $v(-\mathrm{i}\partial/\partial\mathrm{x})$ derives from the group velocity $v(k)$ [cf. formula (54)] by replacing the argument k by $-\mathrm{i}\partial/\partial\mathrm{x}$.

We do not call equalities (89) boundary conditions since generally, if $E(k)$ is not quadratic, equalities (89) cannot be employed in the case when $\mathscr{E}<0$ [if $\psi_{k_0}(x)$ is replaced by $\tilde{\psi}_{\mathscr{E}}(x)$]. [In general, the localized wavefunctions $\tilde{\psi}_{\mathscr{E}}(x)$ for $\mathscr{E}<0$ cannot be constructed as finite sums of exponentials. Therefore, if $\mathscr{E}<0$, not only that is it dubious whether equalities (89) are valid but it is also questionable for which functions these equalities are usable at all.]

To conclude this discussion, we state that in the case of the equation

$$\mathrm{i}\hbar\,\frac{\partial\Psi(x,t)}{\partial t}=H_S(x)\Psi(x,t) \tag{90}$$

concerning a nonquadratic dispersion function $E(k)$, we may surely rely upon the equalities

$$-\mathrm{i}\left(\frac{\hbar}{2}\right)\left[v\left(-\mathrm{i}\,\frac{\partial}{\partial x}\right)\Psi(x,t)\Big|_{x=x_s+0}-v\left(-\mathrm{i}\frac{\partial}{\partial x}\right)\Psi(x,t)\Big|_{x=x_s-0}\right]+\gamma_s\Psi(x_s,t)=0,\quad s=1,\ldots,S \tag{91}$$

provided that none of the constants γ_s is negative.

E. The possibility of a direct translation of results from the case when the dispersion law $E=E(k)$ is parabolic to the case when it is nonparabolic

In this section hand in hand with equalities (89), we will state the validity of the following corollary:

Corollary: Let $\mathscr{A}_{\mathrm{par}}$ be a quantum mechanical coefficient determining the nonlocalized wavefunction $\psi_{k_0}(x)$ derived from the equation

$$H_{S,\mathrm{par}}(x)\,\psi_{k_0,\mathrm{par}}(x)=E(k_0)\,\psi_{k_0,\mathrm{par}}(x) \tag{92}$$

[$E(k_0)>0$ and k_0 is an arbitrary real fixed value]. After introducing the variables $\kappa_s=k_0x_s$ ($s=1,2,\ldots,S$), we consider $\mathscr{A}_{\mathrm{par}}$ as a function of $S+1$ *independent* variables $k_0,\kappa_1,\ldots,\kappa_S$: $\mathscr{A}_{\mathrm{par}}\equiv\mathscr{A}_{\mathrm{par}}(k_0,\kappa_1,\ldots,\kappa_S)$.

If $H_{S,\mathrm{par}}(x)$ is replaced by $H_S(x)$ [respecting condition (4)], the function $\mathscr{A}_{\mathrm{par}}(k_0,\kappa_1,\ldots,\kappa_S)$ is transformed into another function, $\mathscr{A}(k_0,\kappa_1,\ldots,\kappa_S)$, in correspondence with the equation

$$H_S(x)\psi_{k_0}(x)=E(k_0)\psi_{k_0}(x). \tag{93}$$

Then

$$\mathscr{A}(k_0,\kappa_1,\ldots,\kappa_S)\equiv\mathscr{A}_{\mathrm{par}}(mv(k_0)/\hbar,\kappa_1,\ldots,\kappa_S). \tag{94}$$

(Recall that $k_0=mv_{\mathrm{par}}(k_0)/\hbar$.)

Undoubtedly, identity (94) is of appreciable practical value since to solve the Wannier–Schrödinger equation in the case when $E(-\mathrm{i}\partial/\partial x)$ is a second-order differential operator is evidently an easier task [because of the possibility to use the x-representation and the boundary conditions (87)] than to solve this equation in any other case where $E(-\mathrm{i}\partial/\partial x)$ corresponds to a nonquadratic function $E(k)$. A general way of how to obtain the exact solution of the Schrödinger equation [for $E(k)\equiv E_{\mathrm{par}}(k)$ and $\mathscr{E}>0$] with δ-function potentials of arbitrary position and strength has been presented by Reading and Sigel.[25] (For a simplified alternative to their derivations cf. Ref. 26.)

To suggest the proof of formula (94), let us dissect the real x-axis on $S+1$ intervals $\equiv(x_{j-1},x_j)$ $(j=1,2,\ldots,S+1)$ with $x_0=-\infty$ and $x_{S+1}=\infty$. Taking $k_0>0$, we write

$$\psi_{k_0}(x)=[1-\Theta(x-x_1)][\exp(\mathrm{i}k_0x)+B\ \exp(-\mathrm{i}k_0x)]+\sum_{s=1}^{S-1}[\Theta(x-x_s)-\Theta(x-x_{s+1})]$$
$$\times[F_s\ \cos(k_0x)+G_s\ \sin(k_0x)]+\Theta(x-x_S)C\ \exp(\mathrm{i}k_0x). \tag{95}$$

As it is seen, here we have $2S$ coefficients: B, $\{F_s,G_s\}$ and C; $s=1,\ldots,S-1$. For these coefficients, we obtain S linear algebraic equations simply from the continuity of function (95). Subsequently we can carry out analogical calculations as in Sec. II C. This means that we are to solve the Schrödinger–Wannier equation in the k-representation at first and afterwards return to the x-representation. If we choose $x=x_s-0$ (or $x=x_s+0$) in the wavefunction $\psi_{k_0}(x)$ obtained in this way, we arrive at S new linear equations (independent of the former ones) for B, $\{F_s,G_s\}$ and C. These equations involve the derivative $E'(k_0)$ as a parameter. Thus, we can indeed derive $2S$ independent linear algebraic equations for $2S$ coefficients of the wavefunction $\psi_{k_0}(x)$. Each coefficient is derived uniquely and whichever dispersion function $E(k)$ is used, the formal expression for each coefficient is the same: it a function of the variables $\kappa_s=k_0x_s$ (which occur as arguments in sines and cosines; $s=1,\ldots,S$) and of $E'(k_0)=\hbar v(k_0)$. However, this function can also be obtained in a different way if we use the function $E_{\mathrm{par}}(k)$ in the role of $E(k)$. If we prefer to express any coefficient—let us call it $\mathscr{A}$—as a function of k_0 and κ_s instead of $v(k)$ and κ_s $(s=1,,\ldots,S)$, we obtain right equality (94).

Simultaneously, we can clarify the validity of identities (89). If we take into consideration any interval x_{j-1},x_j [cf. the definition of $\psi_{k_0}(x)$ by expression (95)], we may state that

$$v\left(-\mathrm{i}\frac{\partial}{\partial x}\right)\exp(\pm ik_0x)=\pm v(k_0)\exp(\pm ik_0x). \tag{96}$$

In the special case when $E(k)\equiv E_{\mathrm{par}}(k)$, these equalities, when respected in relations (89), have yielded correct values for each coefficient $\mathscr{A}_{\mathrm{par}}(k_0,\kappa_1,\ldots,\kappa_S)$. Then, if the dependence of the corresponding coefficient $\mathscr{A}(k_0,\kappa_1,\ldots,\kappa_S)$ on $v(k)$ is to be [according to formula (94)] the same for nonquadratic functions $E(k)$ as for the quadratic one, it is only then possible if relations (89) are valid generally, i.e., not only in the case when $E(k)\equiv E_{\mathrm{par}}(k)$.

Finally, it is instructive to exemplify identity (94) with the transmission coefficient $T(k_0)$ which we have calculated so carefully in this paper for the double delta-function potential. In the

Appendix, we present the calculation of $T_{\rm par}(k_0)$ within the framework of the x-representation as well. Now we have $S=2$, $\gamma_1=\gamma_2=\gamma$, $\kappa_1=-k_0a/2$, $\kappa_2=k_0a/2$. According to (A12), we have the function

$$T_{\rm par}(k_0)=\frac{k_0^4}{k_0^4+4(m\gamma/\hbar^2)^2[k_0\ \cos(\kappa_2-\kappa_1)+(m\gamma/\hbar^2)\sin(\kappa_2-\kappa_1)]^2}. \tag{97}$$

If we substitute $mv(k_0)/\hbar$ for k_0 in the rhs (retaining the variables κ_1 and κ_2 intact), we obtain the expression

$$T_{\rm par}\left(\frac{mv(k_0)}{\hbar}\right)=\frac{[\hbar v(k_0)]^4}{[\hbar v(k_0)]^4+4\gamma^2[\hbar v(k_0)\cos(\kappa_2-\kappa_1)+\gamma\ \sin(\kappa_2-\kappa_1)]^2}. \tag{98}$$

However, the rhs of (98) is nothing but the expression for $T(k_0)$ according to formula (57). Thus, we have indeed verified that

$$T(k_0)\equiv T_{\rm par}(mv(k_0)/\hbar), \tag{99}$$

in full concordance with the general equality (94).

We close this paper by expressing our hope that the line of thought as it has been presented here may have rewarding potentialities especially in view of some interesting problems occurring in the theory of mesoscopic phenomena.

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APPENDIX: COEFFICIENT $T_{\rm par}(k_0)$ FOR THE PARABOLIC DISPERSION LAW $E=E_{\rm par}(k)$

Within the framework of the x-representation, the traditional way of calculating $T_{\rm par}(k_0)$ for a symmetric delta-function double barrier (double well), if $E=\hbar^2k^2/(2m)$, is as follows.

We solve the Schrödinger equation

$$-\frac{{\rm d}^2}{{\rm d}\xi^2}\psi+2\beta[\,\delta(\xi+1/2)+\delta(\xi-1/2)\,]\psi=\kappa^2\psi. \tag{A1}$$

Here we have introduced the dimensionless parameters (59) and (60) and the dimensionless variable

$$\xi=x/a. \tag{A2}$$

We assume that the solution is of the form

$$\psi(\xi)=\Theta(\xi+\tfrac{1}{2})[\exp({\rm i}\kappa\xi)+B\ \exp(-{\rm i}\kappa\xi)]+[\Theta(\xi+\tfrac{1}{2})-\Theta(\xi-\tfrac{1}{2})]$$
$$\times[F\ \cos(\kappa\xi)+G\ \sin(\kappa\xi)]+\Theta(\xi-\tfrac{1}{2})C\ \exp({\rm i}\kappa\xi). \tag{A3}$$

From the continuity of the wavefunction $\psi(\xi)$, we obtain the equations

$$\exp\left(-\frac{{\rm i}\kappa}{2}\right)+B\ \exp\left(\frac{{\rm i}\kappa}{2}\right)=F\ \cos\left(\frac{\kappa}{2}\right)-G\ \sin\left(\frac{\kappa}{2}\right), \tag{A4}$$

$$C\ \exp\left(\mathrm{i}\frac{\kappa}{2}\right)=F\ \cos\left(\frac{\kappa}{2}\right)+G\ \sin\left(\frac{\kappa}{2}\right). \tag{A5}$$

Equations (A4) and (A5) are, of course, equally correct whichever dispersion function $E(k)$ is taken into consideration.

However, the usability of the following step which we are now intending to do is strictly limited to the parabolicity of the dependence $E=E(k)$ [or $\eta=\eta(\kappa)$].

When integrating (A1) with respect to ξ from $-a/2-\varepsilon$ to $-a/2+\varepsilon$ and from $a/2-\varepsilon$ to $a/2+\varepsilon$ (where $\varepsilon>0$ is an infinitesimal quantity), we obtain, respectively, the equations

$$\frac{2\beta+\mathrm{i}\kappa}{\kappa}\exp\left(\frac{-\mathrm{i}\kappa}{2}\right)+\frac{2\beta-\mathrm{i}\kappa}{\kappa}\exp\left(\frac{\mathrm{i}\kappa}{2}\right)B=F\ \sin\left(\frac{\kappa}{2}\right)+G\ \cos\left(\frac{k}{2}\right), \tag{A6}$$

$$\frac{2\beta-\mathrm{i}\kappa}{\kappa}\exp\left(\frac{\mathrm{i}\kappa}{2}\right)C=F\ \sin\left(\frac{\kappa}{2}\right)-G\ \cos\left(\frac{\kappa}{2}\right). \tag{A7}$$

Equation (A6) represents a linear relation between the left-hand and right-hand first derivatives of $\psi(\xi)$ at $\xi=-\frac{1}{2}$. Similarly, Eq. (A7) is a linear relation between the left-hand and right-hand first derivatives of $\psi(\xi)$ at $\xi=\frac{1}{2}$. If $E(k)$ is quadratic, then it is needless to try to find relations between higher-order derivatives of $\psi(\xi)$ at $\xi=\pm\frac{1}{2}$. Only if $E(k)$ were a nonquadratic function, then higher-order derivatives of $\psi(\xi)$ would have indispensably to be reckoned with. Nevertheless, the method of the k-representation, as we have employed it in Sec. II, has enabled us fully to miss any complications with the higher-order derivatives in boundary conditions at all.

Equations (A5) and (A7) imply the relations

$$F=C\ \exp\left(\frac{\mathrm{i}\kappa}{2}\right)\left[\cos\left(\frac{\kappa}{2}\right)+\frac{2\beta-\mathrm{i}\kappa}{\kappa}\sin\left(\frac{\kappa}{2}\right)\right], \tag{A8}$$

$$G=C\ \exp\left(\frac{\mathrm{i}\kappa}{2}\right)\left[\sin\left(\frac{\kappa}{2}\right)-\frac{2\beta-\mathrm{i}\kappa}{\kappa}\cos\left(\frac{\kappa}{2}\right)\right]. \tag{A9}$$

After inserting (A8) and (A9) into (A4) and (A6), we obtain two linear equations for C and B. Their solutions are

$$C=\mathrm{i}\,\frac{\kappa^2\ \exp(-\mathrm{i}\kappa)}{-2\beta\kappa\ \cos\ \kappa+(\kappa^2-2\beta^2)\sin\ \kappa+\mathrm{i}\kappa(\kappa\ \cos\ \kappa+2\beta\ \sin\ \kappa)}. \tag{A10}$$

$$B=\frac{2\beta\ \exp(-\mathrm{i}\kappa)(\kappa\ \cos\ \kappa+\beta\ \sin\ \kappa)}{-2\beta\kappa\ \cos\ \kappa+(\kappa^2-2\beta^2)\sin\ \kappa+\mathrm{i}\kappa(\kappa\ \cos\ \kappa+2\beta\ \sin\ \kappa)}. \tag{A11}$$

Correspondingly, denoting $\mathscr{T}_{\mathrm{par}}(\kappa)\equiv|C|^2$ and $\mathscr{R}_{\mathrm{par}}(\kappa)\equiv|B|^2$, we obtain the functions

$$\mathscr{T}_{\mathrm{par}}(\kappa)=\frac{\kappa^4}{\kappa^4+4\beta^2(\kappa\ \cos\ \kappa+\beta\ \sin\ \kappa)^2}, \tag{A12}$$

$$\mathscr{R}_{\mathrm{par}}(\kappa)=\frac{4\beta^2(\kappa\ \cos\ \kappa+\beta\ \sin\ \kappa)^2}{\kappa^4+4\beta^2(\kappa\ \cos\ \kappa+\beta\ \sin\ \kappa)^2}. \tag{A13}$$

When returning to the variables k_0 and γ and using the denotation

$$E'_{\mathrm{par}}(k_0)=\frac{\mathrm{d}E_{\mathrm{par}}(k_0)}{\mathrm{d}k_0}=\frac{\hbar^2 k_0}{m}, \tag{A14}$$

we may state that formulas (A12) and (A13) are in full agreement with formulas (54) and (55) if $E(k)\equiv E_{\mathrm{par}}(k)$.

Finally, let us point out that Galindo and Pascual[18] have derived expression (A12) for the transmission coefficient [cf. their formula (4.133)] by means of another method. Their calculation has relied on Jost functions.

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Localization of the photon on phase space

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We obtain phase space representations of the Poincaré group for zero mass particles of all helicities, including photons. A natural quantization scheme for massless particles arises, and a covariant phase space localization operator is found.
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I. INTRODUCTION

In this paper we investigate the particle-like nature of the photon and other massless relativistic objects.

An elementary particle in relativistic theory is, according to Newton and Wigner,[1] described mathematically by a unitary, irreducible representation of the Poincaré group together with a collection of localization operators transforming covariantly. The conventional view adheres to two specific tenets: (i) the localization operators are described through the use of a Borel structure on the space or the space–time of the theory, and covariance is with respect to the Euclidean subgroup; (ii) the localization operators are to be projection operators.

While maintaining the assumption regarding the representation, we advance an extension of the conventional view concerning the localization operators, proposing that (i) the localization operators be described through the use of a Borel structure in the phase space of the theory, and covariance be with respect to the full Poincaré group; (ii) the localization operators are not *a priori* restricted to be projection operators.

It appears that a completely satisfactory description is not to be found in either of the conventional formulations of classical relativistic particle mechanics in space–time or of relativistic quantum mechanics. Employing a framework reflecting but extending and unifying these two formulations, we take as fundamental a phase space formulation of relativistic particle mechanics. We also allow a measurement theory in quantum mechanics based upon unsharp measurement (positive operator-valued measures, systems of covariance) rather than one based solely on sharp measurement (projection-valued measures, systems of imprimitivity). Our position is founded upon recent developments in classical relativistic particle mechanics and quantum mechanics as outlined in the following.

In the realm of classical mechanics we adopt the apparatus of symplectic geometry to describe Hamiltonian systems.[2–5] We follow generally the treatment of relativistic particle mechanics as advanced by Künzle,[6] Souriau,[7] and exposited further by Woodhouse.[8]

In the domain of quantum mechanics, we recall that elementary relativistic systems are associated with irreducible representations of the Poincaré group,[9] and that elementary particles require, in addition, a covariant notion of localizability.[1] For localization describable by projection operators[10] these two characteristics of elementary particles merge to form a system of imprimitivity[11] with respect to a Euclidean subgroup of the Poincaré group.[12] Within this scheme the photon fails to be localizable. Hegerfeldt[13] proved more generally that covariant localization of elementary relativistic systems by projection operators is inconsistent even for massive systems. In order to treat localizability of the photon it was suggested[14,15] that positive operator-valued measures be employed. Positive operator-valued measures are now an essential ingredient in quantum measurement theory.[16–20] Independent of these developments, phase space representations of the

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Poincaré group with a concept of unsharp localizability for massive particles were discovered by Prugovečki[21] and further elaborated by Ali and Prugovečki.[22]

The following is our strategy:

(i) identify symplectic homogeneous spaces (phase spaces) of the Poincaré group relevant to massless particles;
(ii) construct unitary representations of the Poincaré group on Hilbert spaces of functions on these phase spaces;
(iii) define the phase space localization operators on such Hilbert spaces;
(iv) carry out harmonic decompositions of these representations into irreducible components on which the projected localization operators define covariant positive operator-valued measures.

Summary of the results:

(i) We construct informationally complete covariant localization operators for elementary massless particles of arbitrary *helicity/spin* in explicit form.
(ii) The operator for localization within a region of phase space is realized as an integral with respect to a density; consequently, to a measurable function on classical phase space there corresponds an operator obtained by averaging the function with respect to this density, itself an operator. This correspondence defines a natural quantization scheme bearing some similarity to suggestions of Berezin,[23] Prugovečki,[24] Ali and Prugovečki,[25] Schroeck,[26,27] Ali and Emch,[28] and Ali and Doebner.[29]

In quantum mechanics over phase space, a quantization scheme may also be defined as follows: to each measurable function f, associate the operator of multiplication by f, and restrict this operator to the irreducible subspace which is the Hilbert space of the physical system. Choosing f to be the characteristic function for a measurable set, one obtains a localization operator. The localization operator so obtained may be used to produce a quantization scheme in the manner outlined in the previous paragraph. The result is the same quantization scheme with which we began. In this sense, there is a natural equivalence between quantization and localization. This equivalence is both conceptual and practical.

This formalism also yields a dequantization scheme whereby a classical probability density on phase space is naturally associated with a density operator in conventional quantum mechanics so that classical and quantum expectations agree. In this respect these two correspondences are dual.

II. GROUP STRUCTURE, GEOMETRIC STRUCTURE, DEFINITIONS, AND NOTATION

Minkowski space–time and energy-momentum space are both identified with $\mathbb{R}^4$ equipped with the Minkowski metric $g \equiv \mathrm{diag}(1,-1,-1,-1)$. We identify $\mathbb{R}^4$ with the set of 2×2 Hermitian matrices according to the correspondence:

$$(p^0,p^1,p^2,p^3) \leftrightarrow \begin{pmatrix} p^0+p^3 & p^1-ip^2 \\ p^1+ip^2 & p^0-p^3 \end{pmatrix} \tag{1}$$

using the boldface notation $\mathbf{p}$ in either situation. The Minkowski inner product $g(\mathbf{p},\mathbf{p})$ is expressed

$$g(\mathbf{p},\mathbf{p}) = \det\begin{pmatrix} p^0+p^3 & p^1-ip^2 \\ p^1+ip^2 & p^0-p^3 \end{pmatrix}. \tag{2}$$

The Minkowski inner product is abbreviated

$$\mathbf{p}\cdot\mathbf{q} \equiv g(\mathbf{p},\mathbf{q}). \tag{3}$$

The identification in (1) permits a flexible expression of the natural action of elements A of $SL(2,\mathbb{C})$, the double cover of the Lorentz group on $\mathbb{R}^4$, as follows:

$$\mathbf{p} \mapsto A \cdot \mathbf{p} \equiv A\mathbf{p}A^{\dagger}. \tag{4}$$

The Poincaré group, $\mathscr{P}$, is taken to be the semi-direct product:

$$\mathscr{P} = \mathbb{R}^4 \oslash \mathscr{L}, \quad \mathscr{L} \equiv SL(2,\mathbb{C}). \tag{5}$$

Two closed subgroups of $\mathscr{P}$ of particular relevance in the representation theory of massless spinning particles are

(a) $H_1 \equiv \mathbb{R}^4 \oslash SL(2,\mathbb{C})_{\mathbf{p}}$,
(b) $H_2 \equiv \mathbb{R}\mathbf{p} \oslash SL(2,\mathbb{C})_{\mathbf{p}}$,

where $SL(2,\mathbb{C})_{\mathbf{p}}$, the stability subgroup of the future-pointing null vector $\mathbf{p}$ in $\mathbb{R}^4$ viewed as energy-momentum space, consists of those $A \in SL(2,\mathbb{C})$ satisfying the condition $A \cdot \mathbf{p} = \mathbf{p}$. Case (a) occurs in the theory of induced irreducible representations where the homogeneous space $\mathscr{P}/H_1$ is the conventional momentum space (future null cone). Topologically, $\mathscr{P}/H_1$ is homeomorphic to $\mathbb{R}^1 \times S^2$. In case (b), $\mathscr{P}/H_2$ is the symplectic homogeneous space identified by Souriau[3] (see also Ref. 8) as the phase space of the photon. Topologically, $\mathscr{P}/H_2$ is homeomorphic to $\mathbb{R}^3 \times \mathbb{R}^1 \times S^2$.

The orbit $\mathscr{O}_{\mathbf{p}}$ of $\mathbf{p}$ under $SL(2,\mathbb{C})$ consists of all points $A \cdot \mathbf{p}$, $A \in SL(2,\mathbb{C})$. When $\mathbf{p}$ is a future-pointing null vector ($p^0 > 0$), then $\mathscr{O}_{\mathbf{p}}$ is the future null cone V_0^+:

$$V_0^+ = \{\mathbf{p} | g(\mathbf{p},\mathbf{p}) = 0,\ p^0 > 0\}. \tag{6}$$

Henceforth, $\mathbf{p}_o$ denotes the point $(1,0,0,1) \in V_0^+$.

If $\mathbf{q}$ belongs to $\mathscr{O}_{\mathbf{p}}$ with $\mathbf{q} = A \cdot \mathbf{p}$, then the stabilizers of $\mathbf{q}$ and $\mathbf{p}$ are related:

$$SL(2,\mathbb{C})_{\mathbf{q}} = A SL(2,\mathbb{C})_{\mathbf{p}} A^{-1}.$$

A computation shows that $SL(2,\mathbb{C})_{\mathbf{p}_o}$ is the subgroup of matrices A of the form $A = \left(\begin{smallmatrix} 1 & z \\ 0 & 1 \end{smallmatrix}\right) \times \left(\begin{smallmatrix} \tau & 0 \\ 0 & \tau^{-1} \end{smallmatrix}\right)$, $|\tau| = 1$, $z \in \mathbb{C}$. If θ is the angle of right-hand rotation about the (0,0,1)-axis in $\mathbb{R}^3$ when A acts on $\mathbb{R}^4$ by (4), then $\tau = e^{-i\theta/2}$; the matrices of the type $\left(\begin{smallmatrix} \tau & 0 \\ 0 & \tau^{-1} \end{smallmatrix}\right)$ form a group isomorphic to $O(2)^{\sim}$, a double cover of $O(2)$. The matrices of the type $\left(\begin{smallmatrix} 1 & z \\ 0 & 1 \end{smallmatrix}\right)$ form a group isomorphic to $\mathbb{R}^2$. Therefore, the group $SL(2,\mathbb{C})_{\mathbf{p}_o}$ is isomorphic to $E(2)^{\sim} = \mathbb{R}^2 \oslash O(2)^{\sim}$, a double cover of the Euclidean group of $\mathbb{R}^2$.[9] For any $\mathbf{p} = (p^0, \vec{p}) \in V_0^+$, an element of $SL(2,\mathbb{C})_{\mathbf{p}} \cong E(2)^{\sim}$ factorizes similarly into a product of a translation preceded by a rotation in $\mathbb{R}^3$ about the axis $\vec{p}$.

We now describe the homogeneous spaces $\mathscr{P}/H_1$ and $\mathscr{P}/H_2$ and their left-invariant measures in coordinates. For this, we use the general fact that $G/G_{\mathbf{x}}$ is diffeomorphic to $\mathscr{O}_{\mathbf{x}}$ the G-orbit of $\mathbf{x}$ under the action of the group G through the diffeomorphism $AG_{\mathbf{x}} \mapsto A \cdot \mathbf{x}$, $A \in G$. Let $H_0 \equiv SL(2,\mathbb{C})_{\mathbf{p}_o}$ so that $\mathscr{L}/H_0 = SL(2,\mathbb{C})/SL(2,\mathbb{C})_{\mathbf{p}_o}$. In the present case, $SL(2,\mathbb{C})/SL(2,\mathbb{C})_{\mathbf{p}_o}$ is diffeomorphic to V_0^+ by the mapping

$$A\ SL(2,\mathbb{C})_{\mathbf{p}_o} \mapsto A \cdot \mathbf{p}_o. \tag{7}$$

Since $SL(2,\mathbb{C})$ and $E(2)^{\sim} = \mathbb{R}^2 \oslash O(2)^{\sim}$ are unimodular Lie groups, the homogeneous space $SL(2,\mathbb{C})/SL(2,\mathbb{C})_{\mathbf{p}_o}$ has an $SL(2,\mathbb{C})$-invariant measure unique up to scalar multiples. On the other hand, V_0^+ also has the $SL(2,\mathbb{C})$-invariant measure ν, which when V_0^+ is identified with $\mathbb{R}^3$ by $\mathbf{p} = (p^0, \vec{p}) = (p^0, p^1, p^2, p^3) \mapsto \vec{p}$, is given by

$$d\nu(\mathbf{p}) = (p^0)^{-1} dp^1 \wedge dp^2 \wedge dp^3, \tag{8}$$

where $p^0=|\vec{p}|$, and which, when V_0^+ is identified with $\mathbb{R}^+\times\mathbb{R}^2$ by $\mathbf{p}\mapsto(p^0+p^3,p^1,p^2)$, is given by

$$d\nu(\mathbf{p})=(p^0+p^3)^{-1}d(p^0+p^3)\wedge dp^1\wedge dp^2. \tag{9}$$

The diffeomorphism (7) identifies these three invariant measures. From this, we obtain the following:

(a) The homogeneous space $\mathscr{L}/H_0 = \mathrm{SL}(2,\mathbb{C})/\mathrm{SL}(2,\mathbb{C})_{\mathbf{p}_o}$ is diffeomorphic to V_0^+ and possesses the $\mathrm{SL}(2,\mathbb{C})$-invariant measure ν.

(b) The homogeneous space $\mathscr{P}/H_1 = \mathbb{R}^4\circledcirc\mathrm{SL}(2,\mathbb{C})/\mathbb{R}^4\circledcirc\mathrm{SL}(2,\mathbb{C})_{\mathbf{p}_o}$ is diffeomorphic to $\mathrm{SL}(2,\mathbb{C})/\mathrm{SL}(2,\mathbb{C})_{\mathbf{p}_o}$ and hence $\mathscr{P}/H_1$ is also diffeomorphic to V_0^+. From (7) and (8) $\mathscr{P}/H_1$ possesses the $\mathscr{P}$-invariant measure ν.

(c) The homogeneous space $\mathscr{P}/H_2 = \mathbb{R}^4\circledcirc\mathrm{SL}(2,\mathbb{C})/\mathbb{R}\mathbf{p}_o\circledcirc\mathrm{SL}(2,\mathbb{C})_{\mathbf{p}_o}$ may be described as the space of cosets $(\mathbf{a},A)(\mathbb{R}\mathbf{p}_o\circledcirc\mathrm{SL}(2,\mathbb{C})_{\mathbf{p}_o}) = (\mathbf{a}+\mathbb{R}A\cdot\mathbf{p}_o, A\mathrm{SL}(2,\mathbb{C})_{\mathbf{p}_o})$ which corresponds by (7) to $(\mathbf{a}+\mathbb{R}\mathbf{p},\mathbf{p})$ where $\mathbf{p}=A\cdot\mathbf{p}_o$. Thus, $\mathscr{P}/H_2$ is seen to be diffeomorphic to the bundle $\cup_{\mathbf{p}\in V_0^+}\mathbb{R}^4/\mathbb{R}\mathbf{p}$. Consequently, a $\mathscr{P}$-invariant measure on $\mathscr{P}/H_2$ is seen to be

$$d\mu(\mathbf{a}+\mathbb{R}\mathbf{p},\mathbf{p})=d\lambda_{\mathbf{p}}(\mathbf{a})d\nu(\mathbf{p}), \tag{10}$$

where $d\lambda_{\mathbf{p}}(\mathbf{a})$ is the Lebesgue measure on the three-dimensional quotient space $\mathbb{R}^4/\mathbb{R}\mathbf{p}$ of $\mathbb{R}^4$. We stress that in using this measure, one must necessarily integrate over the $\mathbb{R}^4/\mathbb{R}\mathbf{p}$ coordinates first.

We turn now to a brief description of the symplectic structure of the homogeneous space $\mathscr{P}/H_2$ by paralleling results obtained for the case of relativistic massive spinning particles (Refs. 30–32). For $\lambda\in\mathbb{R}$, let $\mathscr{E}_\lambda$ denote the evolution space of triples (Ref. 7): $(\mathbf{q},\ \mathbf{p},\ \mathbf{s})\in\mathbb{R}^4\times\mathbb{R}^4\times\mathbb{R}^4$, satisfying the conditions: $\mathbf{p}\in V_0^+$, $\mathbf{s}=\lambda\mathbf{p}$. The origin of the latter condition is the classical mechanical requirement that $g(\mathbf{p},\mathbf{s})=0$ and the additional requirement that $\mathbf{s}$ be a null vector (Ref. 33). Spacelike $\mathbf{s}$ leads to continuous spin representations which are not treated here. If $\lambda\neq0$, then λ is the classical counterpart of *helicity/spin*; the sign of λ labels the two circular polarizations (Ref. 3). If $\lambda=0$, $\mathscr{E}_0$ will be understood to be the set of pairs: $(\mathbf{q},\mathbf{p})\in\mathbb{R}^4\times\mathbb{R}^4$, $\mathbf{p}\in V_0^+$. For $\lambda\neq0$, $\mathscr{E}_\lambda$ is topologically $\mathbb{R}^4\times\mathbb{R}\times S^2$.

For the Minkowski space–time $M=(\mathbb{R}^4,g)$ and any point $\mathbf{q}\in M$, define $V_0^+(\mathbf{q})\equiv\{\mathbf{p}\in T_{\mathbf{q}}^*M:\mathbf{p}$ is future pointing and null$\}$. This is essentially the V_0^+ introduced earlier. If $(\mathbf{e}_0,\ \mathbf{e}_1,\ \mathbf{e}_2,\ \mathbf{e}_3)$ is a Lorentz frame at $\mathbf{q}$ [i.e., $g(\mathbf{e}_a,\mathbf{e}_b)=g_{ab}$] and $(\boldsymbol{\theta}^0,\ \boldsymbol{\theta}^1,\ \boldsymbol{\theta}^2,\ \boldsymbol{\theta}^3)$ is the dual frame at $\mathbf{q}$, any $\mathbf{p}\in V_0^+(\mathbf{q})$ may be expressed $\mathbf{p}=p_a\boldsymbol{\theta}^a$. We may always choose a Lorentz frame so that $\mathbf{p}=\boldsymbol{\theta}^0-\boldsymbol{\theta}^3$. In arbitrary coordinates, this may be written $p_\mu=\theta^0_\mu-\theta^3_\mu$, or $p^\mu=e^\mu_0+e^\mu_3$. Define

$$\mathbf{S}\equiv\lambda\,\boldsymbol{\theta}^1\wedge\boldsymbol{\theta}^2;\quad \text{i.e.,}\ \ S_{\rho\sigma}=\lambda(\theta^1_\rho\theta^2_\sigma-\theta^1_\sigma\theta^2_\rho). \tag{11}$$

With this choice, regarding $\mathbf{S}$ as the angular momentum tensor relative to the origin $\mathbf{q}$ of the frame $(\mathbf{e}_a)$, one computes the corresponding Pauli-Lubanski spin vector

$$s^\mu=\tfrac{1}{2}\epsilon^{\mu\rho\sigma\tau}S_{\rho\sigma}p_\tau. \tag{12}$$

In coordinate free terms,

$$\mathbf{s}=*(\mathbf{p}\wedge\mathbf{S}), \tag{13}$$

where $*$ denotes the Hodge dual mapping for M. From the definition of $\mathbf{S}$ we find that $\mathbf{s}=\lambda\mathbf{p}$.

On the bundle $\mathrm{Lor}(M)$ of Lorentz frames over M, with coordinates (q^α,e^α_a), define the two-form

$$\Omega = dp_\mu \wedge dq^\mu + (2\lambda^2)^{-1}(dS^\alpha_\beta \wedge S^\beta_\gamma dS^\gamma_\alpha), \tag{14}$$

where, as before, $S^{\alpha\beta}=\lambda(e_1^\alpha e_2^\beta - e_1^\beta e_2^\alpha)$ and $p_\mu = \theta^0_\mu - \theta^3_\mu$. (See Ref. 3, p. 190, equation ♣, with "η"$=+1$ and Ref. 6.) Regard the evolution space $\mathscr{E}_\lambda$ as a subset of the Lorentz bundle by the injection

$$\begin{gathered} \iota: \mathscr{E}_\lambda \to \mathrm{Lor}(M), \\ \iota: (\mathbf{q},\mathbf{p},\mathbf{s}) \mapsto (q^\alpha, e^\alpha_a), \end{gathered} \tag{15}$$

where

$$\mathbf{p} = \boldsymbol{\theta}^0 - \boldsymbol{\theta}^3 \quad \text{and} \quad \lambda \mathbf{p} = *(\mathbf{p} \wedge \mathbf{S}). \tag{16}$$

Then we pull back Ω to obtain the two-form $\iota^*\Omega$ on $\mathscr{E}_\lambda$. On $\mathscr{E}_\lambda$, $\iota^*\Omega$ is degenerate, with a one-dimensional kernel. Thus, Ω induces a symplectic structure on the six-dimensional phase space $\mathscr{E}_\lambda/\ker(\iota^*\Omega)$. The action of $\mathscr{P}$ on $\mathscr{E}_\lambda$ is given by

$$(a,A)(\mathbf{q},\mathbf{p},\mathbf{s}) = (A^{-1}\cdot(\mathbf{q}-\mathbf{a}),\ A^{-1}\cdot\mathbf{p},\ A^{-1}\cdot\mathbf{s}). \tag{17}$$

This induces an action on $\mathscr{E}_\lambda/\ker(\iota^*\Omega)$, and shows (see Ref. 3, pp. 189–192 and Ref. 5, pp. 341–343) that $\mathscr{E}_\lambda/\ker(\iota^*\Omega)$ may be identified with the bundle $\cup_{\mathbf{p}\in V_0^+}\mathbb{R}^4/\mathbb{R}\mathbf{p}$ and hence with $\mathscr{P}/H_2$. Alternatively, the phase space $\mathscr{E}_\lambda/\ker(\iota^*\Omega)$ and its symplectic structure may be identified with the coadjoint orbit of the Poincaré group corresponding to the point $(\mathbf{p}, S)$ as in (16) and its canonical symplectic structure (Ref. 34).

The following notation will be used for the canonical projections π_i and (local) Borel cross sections σ_i:

(0)

$$\begin{gathered} \pi_0: \mathrm{SL}(2,\mathbb{C}) \to \mathrm{SL}(2,\mathbb{C})/\mathrm{SL}(2,\mathbb{C})_{\mathbf{p}_o} \cong V_0^+ \ \text{ by } \ \pi_0(A) = A\cdot\mathbf{p}_o; \\ \sigma_0: \mathrm{SL}(2,\mathbb{C})/\mathrm{SL}(2,\mathbb{C})_{\mathbf{p}_o} \to \mathrm{SL}(2,\mathbb{C}) \ \text{ with } \ \pi_0\circ\sigma_0(\mathbf{p}) = \mathbf{p}. \end{gathered} \tag{18}$$

(1)

$$\begin{gathered} \pi_1: \mathbb{R}^4 \oslash \mathrm{SL}(2,\mathbb{C}) \to \mathbb{R}^4 \oslash \mathrm{SL}(2;\mathbb{C})/\mathbb{R}^4 \oslash \mathrm{SL}(2,\mathbb{C})_{\mathbf{p}_o} \cong V_0^+ \ \text{ by } \ \pi_1(\mathbf{a},A) = A\cdot\mathbf{p}_o; \\ \sigma_1: \mathbb{R}^4 \oslash \mathrm{SL}(2,\mathbb{C})/\mathbb{R}^4 \oslash \mathrm{SL}(2,\mathbb{C})_{\mathbf{p}_o} \to \mathbb{R}^4 \oslash \mathrm{SL}(2,\mathbb{C}) \ \text{ with } \ \pi_1\circ\sigma_1(\mathbf{p}) = \mathbf{p}. \end{gathered} \tag{19}$$

(2)

$$\begin{gathered} \pi_2: \mathbb{R}^4 \oslash \mathrm{SL}(2,\mathbb{C}) \to \mathbb{R}^4 \oslash \mathrm{SL}(2,\mathbb{C})/\mathbb{R}\mathbf{p}_o \oslash \mathrm{SL}(2,\mathbb{C})_{\mathbf{p}_o} \ \text{ by } \ \pi_2(\mathbf{a},A) = (\mathbf{a}+\mathbb{R}A\cdot\mathbf{p}_o, A\cdot\mathbf{p}_o); \\ \sigma_2: \mathbb{R}^4 \oslash \mathrm{SL}(2,\mathbb{C})/\mathbb{R}\mathbf{p}_o \oslash \mathrm{SL}(2,\mathbb{C})_{\mathbf{p}_o} \to \mathbb{R}^4 \oslash \mathrm{SL}(2,\mathbb{C}) \ \text{ with } \ \pi_2\circ\sigma_2(\mathbf{a}+\mathbb{R}\mathbf{p},\mathbf{p}) = (\mathbf{a}+\mathbb{R}\mathbf{p},\mathbf{p}). \end{gathered} \tag{20}$$

III. INDUCED MASSLESS REPRESENTATIONS OF THE POINCARÉ GROUP

In this section we develop the representations of the Poincaré group induced from irreducible representations of the two subgroups H_1 and H_2. These are respectively the standard irreducible representation on the null cone, and the phase space representation.

A. Induced massless representations of the Poincaré group on the null cone

The Mackey[11] procedure of induced representations will be employed to obtain massless unitary irreducible representations of $\mathscr{P}$. In this way we will recover not only the ''standard'' irreducible representations for massless spinning particles, but also unitarily equivalent representations that are analogous to the phase space representations.

The unitary irreducible representations M_λ of $O(2)^\sim$ are parametrized by $\lambda \in \frac{1}{2}\mathbb{Z}$ and act on $\mathscr{H}_0 = \mathbb{C}$. If $R(\psi)$ denotes rotation by ψ, then $M_\lambda(R(\psi)) = \exp(i\lambda\psi)$.

The unitary irreducible representation Λ_λ of $E(2)^\sim = \mathbb{R}^2 \circledcirc O(2)^\sim$ induced from M_λ is given by

$$\Lambda_\lambda(z,\tau) \equiv \Lambda(\chi_0, M_\lambda; (z,\tau)) = \chi_0(z) M_\lambda(\tau) = \tau^\lambda, \tag{21}$$

where, using the notation from Sec. II, (z,τ) denotes an element of $E(2)^\sim$. The representation space of Λ_λ is $\mathscr{H}_0 = \mathbb{C}$.

We are now ready to describe the unitary irreducible representations of the subgroup H_1 of the Poincaré group corresponding to massless particles with quantized spin (helicity). Continuous spin representations will not be considered.

Massless discrete spin unitary irreducible representations of $H_1 = \mathbb{R}^4 \circledcirc [\mathrm{SL}(2,\mathbb{C})]_{\mathbf{p}_o} = \mathbb{R}^4 \circledcirc E(2)^\sim$ arise from the choice of a character $\chi_{\boldsymbol{\xi}}$ where $\boldsymbol{\xi}$ is any vector in the $\mathrm{SL}(2,\mathbb{C})$-orbit of $\mathbf{p}_o$, and one of the representations Λ_λ, $\lambda \in \frac{1}{2}\mathbb{Z}$, of $E(2)^\sim$. Denoting this representation by $\Lambda_{\boldsymbol{\xi}\lambda}$ and using the notation of Sec. II, we have

$$\Lambda_{\boldsymbol{\xi}\lambda}(\mathbf{k},(z,\tau)) \equiv \Lambda(\chi_{\boldsymbol{\xi}}, \Lambda_\lambda; (\mathbf{k},(z,\tau))) = \chi_{\boldsymbol{\xi}}(\mathbf{k}) \Lambda_\lambda(z,\tau) = \exp\{i\boldsymbol{\xi}\cdot\mathbf{k}\}\tau^\lambda. \tag{22}$$

We induce a representation of $\mathscr{P}$ from this representation of H_1.

Theorem 3.1: *Let $\boldsymbol{\xi} \in V_0^+$, and $\lambda \in \frac{1}{2}\mathbb{Z}$. The Hilbert space of the representation is*

$$\mathscr{H}_{\mathrm{mom}}^{\boldsymbol{\xi}\lambda} = L^2_\nu(\mathscr{P}/H_1). \tag{23}$$

The induced unitary irreducible representation $U^{\boldsymbol{\xi}\lambda}$ of $\mathscr{P}$ is given by

$$[U^{\boldsymbol{\xi}\lambda}(\mathbf{a},A)F](\mathbf{p}) = \exp\{i[\sigma_0(\mathbf{p})\cdot\boldsymbol{\xi}]\cdot\mathbf{a}\} M_\lambda(\sigma_0(\mathbf{p})^{-1} A \sigma_0(A^{-1}\cdot\mathbf{p})) F(A^{-1}\cdot\mathbf{p}). \tag{24}$$

To obtain the familiar representation,[9] one identifies $\mathscr{P}/H_1 = V_0^+$ with $\mathbb{R}^3$ by $\mathbf{p} = (p^0, \vec{p}) \mapsto \vec{p}$ and $\mathscr{H}_{\mathrm{mom}}^{\boldsymbol{\xi}\lambda}$ with $L^2_\nu(\mathbb{R}^3)$, $d\nu(\vec{p}) = \|\vec{p}\|^{-1} d\vec{p}$, and one chooses $\boldsymbol{\xi} = \mathbf{p}_o$ to obtain

$$[U^{\mathbf{p}_o\lambda}(\mathbf{a},A)F](\mathbf{p}) = \exp\{i\mathbf{p}\cdot\mathbf{a}\} M_\lambda(\sigma_0(\mathbf{p})^{-1} A \sigma_0(A^{-1}\cdot\mathbf{p})) F(A^{-1}\cdot\mathbf{p}). \tag{25}$$

A unitarily equivalent representation is obtained by choosing $\boldsymbol{\xi} = \mathbf{q}_o \equiv (\frac{1}{2}, 0, 0, -\frac{1}{2})$ (that is, $\mathbf{q}_o$ is a future null vector $\mathbf{k}$ such that $\mathbf{k}\cdot\mathbf{p}_o = 1$), and $\mathbf{q} = \sigma_0(\mathbf{p})\cdot\mathbf{q}_o$, to obtain

$$[U^{\mathbf{q}_o\lambda}(\mathbf{a},A)F](\mathbf{p}) = \exp\{i\mathbf{q}\cdot\mathbf{a}\} M_\lambda(\sigma_0(\mathbf{p})^{-1} A \sigma_0(A^{-1}\cdot\mathbf{p})) F(A^{-1}\cdot\mathbf{p}). \tag{26}$$

The choices $\lambda = \pm\frac{1}{2}$ have been identified as the neutrino representations, and the cases $\lambda = \pm 1$ as the photon representations (Refs. 9 and 35–37). The graviton has been associated with $\lambda = \pm 2$. The choices ''$\pm$'' reflect the two-valued nature of helicity.

B. Induced massless representations of the Poincaré group on phase space

Because the phase space representations will be induced from representations of $H_2 \equiv \mathbb{R}\mathbf{p}_o \circledcirc [\mathrm{SL}(2,\mathbb{C})]_{\mathbf{p}_o} \cong \mathbb{R} \circledcirc E(2)^\sim$, $\mathbf{p}_o = (1,0,0,1)$, it is useful to describe the unitary irreducible representations of H_2.

In the notation of Sec. II, let $(\kappa\mathbf{p}_o,(z,\tau))\in\mathbb{R}\mathbf{p}_o\oslash E(2)^{\sim}=\mathbb{R}\mathbf{p}_o\oslash[\mathrm{SL}(2,\mathbb{C})]_{\mathbf{p}_o}\equiv H_2$. Let χ_β be a character for $\mathbb{R}$: $\chi_\beta(\kappa)=\exp\{i\beta\kappa\}$, $\beta\in\mathbb{R}$. Again, we denote irreducible unitary representations of $E(2)^{\sim}$ by M_λ, as in (21). We obtain then the irreducible unitary representation $\Lambda_{\beta\lambda}$ of H_2:

$$\Lambda_{\beta\lambda}(\kappa,(z,\tau))=\Lambda(\chi_\beta,M_\lambda;(\kappa\mathbf{p}_o,(z,\tau)))=\chi_\beta(\kappa)M_\lambda(z,\tau)=\exp\{i\beta\kappa\}\tau^\lambda, \tag{27}$$

where β is any real number, $\lambda\in\frac{1}{2}\mathbb{Z}$.

From these representations of H_2, we now obtain phase space representations of $\mathscr{P}$.

Theorem 3.2: *Let $\beta\in\mathbb{R}$, and $\lambda\in\frac{1}{2}\mathbb{Z}$. The Hilbert space of the representation is*

$$\mathscr{H}_{\mathrm{phase}}^{\beta\lambda}=L^2_\mu(\mathscr{P}/H_2), \tag{28}$$

where μ is the $\mathscr{P}$-invariant measure on $\mathscr{P}/H_2$ defined in (10). Recalling from Sec. II the identification of $\mathscr{P}/H_2$ with $\mathbb{R}^3\times V_0^+$ by $(\mathbf{k}+\mathbb{R}\mathbf{p},\mathbf{p})\mapsto(\mathbf{k},\mathbf{p})$, we identify elements of $\mathscr{H}_{\mathrm{phase}}^{\beta\lambda}$ as functions F: $\mathbb{R}^3\times V_0^+\to\mathbb{C}$ satisfying $F(\mathbf{k}+\alpha\mathbf{p},\mathbf{p})=F(\mathbf{k},\mathbf{p})$, for all $\alpha\in\mathbb{R}$. The induced unitary irreducible representation $U^{\beta\lambda}$ of $\mathscr{P}$ is given by

$$[U^{\beta\lambda}(\mathbf{a},A)F](\mathbf{k},\mathbf{p})=\Lambda_{\beta\lambda}(h_2(\mathbf{b},B)[h_2((\mathbf{a},A)^{-1}(\mathbf{b},B))]^{-1})F((\mathbf{a},A)^{-1}(\mathbf{k},\mathbf{p})), \tag{29}$$

where, for $(\mathbf{k},\mathbf{p})$, $(\mathbf{b},B)$ is any element of $\mathscr{P}$ such that $\pi_2(\mathbf{b},B)=(\mathbf{k}+\mathbb{R}\mathbf{p},\mathbf{p})$ and where h_2: $\mathscr{P}\to H_2$ by $g\mapsto[\sigma_2\circ\pi_2(g)]^{-1}g$.

Proof: The induced representation space $\mathscr{H}_{\mathrm{phase}}^{\beta\lambda}\equiv L^2_\mu(\mathscr{P}/H_2)$ consists of functions f: $\mathscr{P}\to\mathbb{C}$ such that $f\circ\sigma_2$ is square integrable on $\mathscr{P}/H_2$ and

$$f(gh)=\Lambda_{\beta\lambda}(h^{-1})f(g) \tag{30}$$

for all $h\in H_2$, $g\in\mathscr{P}$. On such functions we define the left quasi-regular representation $U^{\Lambda_{\beta\lambda}}\equiv U^{\beta\lambda}$ by

$$[U^{\beta\lambda}(g)f](g')=f(g^{-1}g') \tag{31}$$

for all $g,g'\in\mathscr{P}$. Since $h_2(g)=[\sigma_2\circ\pi_2(g)]^{-1}g$ is an element in H_2, (30) becomes

$$f(g)=\Lambda_{\beta\lambda}(h_2(g)^{-1})f(\sigma_2\circ\pi_2(g)). \tag{32}$$

It follows that

$$[U^{\beta\lambda}(g)f](g')=f(g^{-1}g')=\Lambda_{\beta\lambda}([h_2(g^{-1}g')]^{-1})f(\sigma_2\circ\pi_2(g^{-1}g')).$$

Then, by replacing f with $U^{\beta\lambda}(g)f$ in (32), we obtain

$$\begin{aligned}[U^{\beta\lambda}(g)f](\sigma_2\circ\pi_2(g'))&=\Lambda_{\beta\lambda}(h_2(g'))[U^{\beta\lambda}(g)f](g')\\&=\Lambda_{\beta\lambda}(h_2(g'))\Lambda_{\beta\lambda}([h_2(g^{-1}g')]^{-1})f(\sigma_2\circ\pi_2(g^{-1}g'))\\&=\Lambda_{\beta\lambda}(h_2(g')[h_2(g^{-1}g')]^{-1})f(\sigma_2(g^{-1}\pi_2(g'))).\end{aligned} \tag{33}$$

Note that, in (33), $\Lambda_{\beta\lambda}(h_2(g')[h_2(g^{-1}g')]^{-1})$ depends on g' only through $\pi_2(g')$. In order to simplify (33), define

$$F(\mathbf{k},\mathbf{p})\equiv f(\sigma_2(\mathbf{k}+\mathbb{R}\mathbf{p},\mathbf{p})). \tag{34}$$

It follows that $F(\mathbf{k}+\alpha\mathbf{p},\mathbf{p})=F(\mathbf{k},\mathbf{p})$ for all $\alpha\in\mathbb{R}$, and also, from (33), that such functions F are form invariant under the action of $\mathscr{P}$ defined by

$$[U^{\beta\lambda}(g)F](\mathbf{k},\mathbf{p})\equiv[U^{\beta\lambda}(g)f](\sigma_2(\mathbf{k}+\mathbb{R}\mathbf{p},\mathbf{p})). \tag{35}$$

Equation (33) becomes

$$[U^{\beta\lambda}(\mathbf{a},A)F](\mathbf{k},\mathbf{p})=\Lambda_{\beta\lambda}(h_2(\mathbf{b},B)[h_2((\mathbf{a},A)^{-1}(\mathbf{b},B))]^{-1})F(A^{-1}\cdot(\mathbf{k}-\mathbf{a}),A^{-1}\mathbf{p}), \quad (36)$$

for any $(\mathbf{b},B)$ such that $\pi_2(\mathbf{b},B)=(\mathbf{k}+\mathbf{R}\mathbf{p},\mathbf{p})$. Since $f\circ\sigma_2\in L^2_\mu(\mathscr{P}/H_2)\equiv\mathscr{H}^{\beta\lambda}_{\text{phase}}$, by an abuse of notation, we write $F\in\mathscr{H}^{\beta\lambda}_{\text{phase}}$.

Equation (36) may, in turn, be simplified by lifting the action of $\mathscr{P}$ on $\mathscr{P}/H_2$ to an action of $\mathscr{P}$ on $\mathbb{R}^4\times V_0^+$ defined by

$$(\mathbf{a},A)^{-1}(\mathbf{k},\mathbf{p})\equiv(A^{-1}\cdot(\mathbf{k}-\mathbf{a}),A^{-1}\mathbf{p}). \quad (37)$$

This results in

$$[U^{\beta\lambda}(\mathbf{a},A)F](\mathbf{k},\mathbf{p})=\Lambda_{\beta\lambda}(h_2(\mathbf{b},B)[h_2((\mathbf{a},A)^{-1}(\mathbf{b},B))]^{-1})F((\mathbf{a},A)^{-1}(\mathbf{k},\mathbf{p})), \quad (38)$$

for any $(\mathbf{b},B)$ such that $\pi_2(\mathbf{b},B)=(\mathbf{k}+\mathbb{R}\mathbf{p},\mathbf{p})$ with $F\in\mathscr{H}^{\beta\lambda}_{\text{phase}}$.□

The expression (38) is a general phase space representation of $\mathscr{P}$ depending on the arbitrary choice of section σ_2. Any section σ_2 may be expressed in the form

$$\sigma_2(\mathbf{k}+\mathbb{R}\mathbf{p},\mathbf{p})=(\mathbf{k},-\kappa(\mathbf{k},\mathbf{p})\mathbf{p},A(\mathbf{k},\mathbf{p})) \quad (39)$$

where

$$\mathbf{p}=A(\mathbf{k},\mathbf{p})\cdot\mathbf{p}_o,\quad \kappa(\mathbf{k}+\alpha\mathbf{p},\mathbf{p})=\kappa(\mathbf{k},\mathbf{p})+\alpha,\quad A(\mathbf{k}+\alpha\mathbf{p},\mathbf{p})=A(\mathbf{k},\mathbf{p}) \quad (40)$$

for all $\alpha\in\mathbb{R}$. From this one computes

$$h_2(\mathbf{b},B)\equiv(\kappa(\mathbf{b},\mathbf{p})\mathbf{p}_o,A(\mathbf{b},\mathbf{p}))^{-1}B),\quad \mathbf{p}=B\cdot\mathbf{p}_o,$$

and

$$\begin{aligned}&h_2(\mathbf{b},B)[h_2((\mathbf{a},A)^{-1}(\mathbf{b},B))]^{-1}\\&\quad=([\kappa(\mathbf{b},\mathbf{p})-\kappa((\mathbf{a},A)^{-1}(\mathbf{b},\mathbf{p}))]\mathbf{p}_o,[A(\mathbf{b},\mathbf{p})]^{-1}A[A((\mathbf{a},A)^{-1}(\mathbf{b},\mathbf{p}))]).\end{aligned} \quad (41)$$

Equation (38) now reads

$$\begin{aligned}[U^{\beta\lambda}(\mathbf{a},A)F](\mathbf{k},\mathbf{p})&=\exp\{i\beta(\kappa(\mathbf{k},\mathbf{p})-\kappa[(\mathbf{a},A)^{-1}(\mathbf{k},\mathbf{p})])\}\\&\quad\times M_\lambda\{[A(\mathbf{k},\mathbf{p})]^{-1}A[A((\mathbf{a},A)^{-1}(\mathbf{k},\mathbf{p}))]\}F((\mathbf{a},A)^{-1}(\mathbf{k},\mathbf{p})).\end{aligned} \quad (42)$$

In order to compare (42) with (26), we choose

$$A(\mathbf{k},\mathbf{p})=\sigma_0(\mathbf{p}),\quad \kappa(\mathbf{k},\mathbf{p})=\mathbf{k}\cdot\mathbf{q}, \quad (43)$$

where $\mathbf{q}$ is a null vector such that $\mathbf{p}\cdot\mathbf{q}=1$. This special choice of section yields

$$[U^{\beta\lambda}(\mathbf{a},A)F](\mathbf{k},\mathbf{p})=\exp\{i\beta\mathbf{a}\cdot\mathbf{q}\}M_\lambda(\sigma_0(\mathbf{p})^{-1}A\sigma_0(A^{-1}\mathbf{p}))F((\mathbf{a},A)^{-1}(\mathbf{k},\mathbf{p})) \quad (44)$$

with $F\in\mathscr{H}^{\beta\lambda}_{\text{phase}}$ and $M_\lambda(\tau)$ given by (21). By setting $\beta=1$, the representation (44) is strikingly similar to the representation (26). Note also that (40) precludes the choice $\kappa(\mathbf{k},\mathbf{p})=\mathbf{k}\cdot\mathbf{p}$; so, we may not obtain such a similarity between (42) and (26), the standard irreducible representation.

The choice (43) for the section is special, leading directly to the orthogonality relations which follow. Other choices give more complicated relations. The variety of results so obtainable have been worked out for the 1+1-dimensional Poincaré group but only in representations with trivial multiplier (Ref. 38).

IV. ORTHOGONALITY RELATIONS

We now introduce an isometry from $L^2_\nu(\mathscr{P}/H_1)$ to a closed subspace of $L^2_\mu(\mathscr{P}/H_2)$ by first deriving an appropriate orthogonality relation. The orthogonality relation will play many additional roles subsequently.

For this, it is convenient to establish a coordinate system, so that some of the computations are easier to follow. As always, we choose $\mathbf{p}_o=(1,0,0,1)$; then $\mathbf{p}_o\cdot\mathbf{p}_o=0$. We also choose $\mathbf{q}_o$, $\mathbf{u}_o$, $\mathbf{v}_o\in\mathbb{R}^4$ such that $\mathbf{q}_o\cdot\mathbf{q}_o=0$, $\mathbf{u}_o\cdot\mathbf{u}_o=\mathbf{v}_o\cdot\mathbf{v}_o=-1$, $\mathbf{p}_o\cdot\mathbf{q}_o=1$, $\mathbf{p}_o\cdot\mathbf{u}_o=\mathbf{p}_o\cdot\mathbf{v}_o=\mathbf{q}_o\cdot\mathbf{u}_o=\mathbf{q}_o\cdot\mathbf{v}_o=\mathbf{u}_o\cdot\mathbf{v}_o=0$. Define, for $\mathbf{p}\in V_0^+$, $\mathbf{q}_\mathbf{p}\equiv\sigma_0(\mathbf{p})\cdot\mathbf{q}_o$, $\mathbf{u}_\mathbf{p}\equiv\sigma_0(\mathbf{p})\cdot\mathbf{u}_o$, $\mathbf{v}_\mathbf{p}\equiv\sigma_0(\mathbf{p})\cdot\mathbf{v}_o$. Then any vector $\mathbf{a}\in\mathbb{R}^4$ may be written in coordinates as

$$\mathbf{b}=(\mathbf{b}\cdot\mathbf{q}_\mathbf{p})\mathbf{p}+(\mathbf{b}\cdot\mathbf{p})\mathbf{q}_\mathbf{p}-(\mathbf{b}\cdot\mathbf{u}_\mathbf{p})\mathbf{u}_\mathbf{p}-(\mathbf{b}\cdot\mathbf{v}_\mathbf{p})\mathbf{v}_\mathbf{p}; \tag{45}$$

i.e., by (43),

$$\mathbf{b}-\kappa(\mathbf{b},\mathbf{p})\mathbf{p}=(\mathbf{b}\cdot\mathbf{p})\mathbf{q}_\mathbf{p}-(\mathbf{b}\cdot\mathbf{u}_\mathbf{p})\mathbf{u}_\mathbf{p}-(\mathbf{b}\cdot\mathbf{v}_\mathbf{p})\mathbf{v}_\mathbf{p}. \tag{46}$$

In this coordinate system, the invariant measure (10) on $\mathbb{R}^3\times\mathbb{R}^1\times S^2$ becomes

$$d\mu(\mathbf{b}+\mathbb{R}\mathbf{p},\mathbf{p})=d\lambda_\mathbf{p}(\mathbf{b})\,d\nu(\mathbf{p})=d(\mathbf{b}\cdot\mathbf{p})d(\mathbf{b}\cdot\mathbf{u}_\mathbf{p})d(\mathbf{b}\cdot\mathbf{v}_\mathbf{p})(p^0)^{-1}dp^1\wedge dp^2\wedge dp^3. \tag{47}$$

Theorem 4.1: *(Orthogonality) Let $U^{\mathbf{p}_o\lambda}$ be the irreducible zero mass representation of the Poincaré group on $L^2_\nu(\mathscr{P}/H_1)$ as in Theorem 3.1, (25). Let $\mathscr{E}$ be the multiplication operator on $L^2_\nu(\mathscr{P}/H_1)$ given by*

$$(\mathscr{E}\psi)(\mathbf{k})=\mathscr{E}(\mathbf{k})\,\psi(\mathbf{k}). \tag{48}$$

Let η_1, η_2, φ_1, $\varphi_2\in L^2_\nu(\mathscr{P}/H_1)$. Let W_η be defined by

$$W_\eta: L^2_\nu(\mathscr{P}/H_1)\to\mathbb{C}^\mathscr{P}, \tag{49}$$

$$[W_\eta(\varphi)](\mathbf{b},B)=\langle\mathscr{E}U^{\mathbf{p}_o\lambda}(\mathbf{b},B)\,\eta,\varphi\rangle. \tag{50}$$

For any section σ_2 given by (39) with $\kappa(\mathbf{k},\mathbf{p})=\mathbf{k}\cdot\mathbf{q}$, $W_\eta(\varphi)$ as a function on $\mathscr{P}/H_2$ is defined by

$$[W_\eta(\varphi)](\mathbf{a}+\mathbb{R}\mathbf{p},\mathbf{p})\equiv[W_\eta(\varphi)](\sigma_2(\mathbf{a}+\mathbb{R}\mathbf{p},\mathbf{p})). \tag{51}$$

Define positive operator C on $L^2_\nu(\mathscr{P}/H_2)$ by

$$(C^2\eta)(\mathbf{p})\equiv 4(2\pi)^3(p^0+p^3)^{-2}\eta(\mathbf{p}). \tag{52}$$

If

$$\mathscr{E}(\mathbf{k})=\sqrt{k^0}=((k^1)^2+(k^2)^2+(k^3)^2)^{1/4}, \tag{53}$$

then

$$\langle W_{\eta_2}(\varphi_2),W_{\eta_1}(\varphi_1)\rangle_{L^2_\mu(\mathscr{P}/H_2)}=\langle\eta_1,C^2\eta_2\rangle_{L^2_\nu(\mathscr{P}/H_1)}\langle\varphi_2,\varphi_1\rangle_{L^2_\nu(\mathscr{P}/H_1)}; \tag{54}$$

conversely (54) holds for all η_1, $\eta_2\in D(C)$, φ_1, $\varphi_2\in L^2_\nu(\mathscr{P}/H_1)$ iff $|\mathscr{E}(\mathbf{p})|=\sqrt{p^0}$.

Proof: In the computation below, we shall use a delta function property; we begin with a derivation of this property: From (46) we compute,

$$(\mathbf{p}-\mathbf{t})\cdot(\mathbf{b}-\kappa(\mathbf{b},\mathbf{k})\mathbf{k})=(\mathbf{b}\cdot\mathbf{k})((\mathbf{p}-\not{\ell})\cdot\mathbf{q}_\mathbf{k})-(\mathbf{b}\cdot\mathbf{u}_\mathbf{k})((\mathbf{p}-\not{\ell})\cdot\mathbf{u}_\mathbf{k})-(\mathbf{b}\cdot\mathbf{v}_\mathbf{k})((\mathbf{p}-\not{\ell})\cdot\mathbf{v}_\mathbf{k}). \tag{55}$$

Hence

$$\int d\lambda_{\mathbf{k}}(\mathbf{b})\exp\{i(\mathbf{p}-\mathbf{t})\cdot(\mathbf{b}-\kappa(\mathbf{b},\mathbf{k})\mathbf{k})\} = \int d(\mathbf{b}\cdot\mathbf{k})d(\mathbf{b}\cdot\mathbf{u}_{\mathbf{k}})d(\mathbf{b}\cdot\mathbf{v}_{\mathbf{k}})\exp\{i[(\mathbf{b}\cdot\mathbf{k})((\mathbf{p}-\mathbf{t})\cdot\mathbf{q}_{\mathbf{k}}) - (\mathbf{b}\cdot\mathbf{u}_{\mathbf{k}})((\mathbf{p}-\mathbf{t})\cdot\mathbf{u}_{\mathbf{k}})]\}\exp\{-i(\mathbf{b}\cdot\mathbf{v}_{\mathbf{k}})((\mathbf{p}-\mathbf{t})\cdot\mathbf{v}_{\mathbf{k}})]\}$$
$$= (2\pi)^3\delta((\mathbf{p}-\mathbf{t})\cdot\mathbf{q}_{\mathbf{k}})\delta((\mathbf{p}-\mathbf{t})\cdot\mathbf{u}_{\mathbf{k}})\delta((\mathbf{p}-\mathbf{t})\cdot\mathbf{v}_{\mathbf{k}}). \quad (56)$$

Now if $\mathbf{p}$ is any null vector, from (45) we may write

$$\mathbf{p} = (\mathbf{p}\cdot\mathbf{k})\mathbf{q}_{\mathbf{k}} + (\mathbf{p}\cdot\mathbf{q}_{\mathbf{k}})\mathbf{k} - (\mathbf{p}\cdot\mathbf{u}_{\mathbf{k}})\mathbf{u}_{\mathbf{k}} - (\mathbf{p}\cdot\mathbf{v}_{\mathbf{k}})\mathbf{v}_{\mathbf{k}}.$$

Then, for purposes of integration after applying the δ-functions in (56), one obtains

$$0 = \mathbf{p}\cdot\mathbf{p} = 2(\mathbf{p}\cdot\mathbf{k})(\mathbf{p}\cdot\mathbf{q}_{\mathbf{k}}) - (\mathbf{p}\cdot\mathbf{u}_{\mathbf{k}})^2 - (\mathbf{p}\cdot\mathbf{v}_{\mathbf{k}})^2 = 2(\mathbf{p}\cdot\mathbf{k})(\mathbf{t}\cdot\mathbf{q}_{\mathbf{k}}) - (\mathbf{t}\cdot\mathbf{u}_{\mathbf{k}})^2 - (\mathbf{t}\cdot\mathbf{v}_{\mathbf{k}})^2.$$

If also $\mathbf{t}\cdot\mathbf{t}=0$, then

$$0 = 2(\mathbf{t}\cdot\mathbf{k})(\mathbf{t}\cdot\mathbf{q}_{\mathbf{k}}) - (\mathbf{t}\cdot\mathbf{u}_{\mathbf{k}})^2 - (\mathbf{t}\cdot\mathbf{v}_{\mathbf{k}})^2;$$

consequently,

$$\mathbf{p}\cdot\mathbf{k} = \mathbf{t}\cdot\mathbf{k}.$$

We may therefore restate (56) in the symbolic form

$$\int d\lambda_{\mathbf{k}}(\mathbf{b})\exp\{-i(\mathbf{p}-\mathbf{t})\cdot(\mathbf{b}-\kappa(\mathbf{b},\mathbf{k})\mathbf{k})\} = (2\pi)^3\delta(\mathbf{p}-\mathbf{t}). \quad (57)$$

We see from this form that the result is independent of the choice made for the basis elements $\mathbf{q}_o$, $\mathbf{u}_o$, $\mathbf{v}_o$.

We now use (57) to prove the theorem. Initially assume either that η_1,η_2 are such that $U^{\mathbf{p}_o\lambda}(\sigma_2\circ\pi_2(\mathbf{b},B))\eta_i$ is in the domain of $\mathscr{E}$ for all $(\mathbf{b},B)\in\mathscr{P}$, or that φ_1,φ_2 are in the domain of $\mathscr{E}$. We have, for $\mathbf{k}\equiv B\cdot\mathbf{p}_o$,

$$\langle\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2\circ\pi_2(\mathbf{b},B))\eta_i,\varphi_i\rangle = \langle\mathscr{E}U^{\mathbf{p}_o\lambda}(\mathbf{b}-\kappa(\mathbf{b},\mathbf{k})\mathbf{k},\sigma_0(\mathbf{k}))\eta_i,\varphi_i\rangle$$
$$= \int d\nu(\mathbf{p})\mathscr{E}(\mathbf{p})\exp\{-i\mathbf{p}\cdot(\mathbf{b}-\kappa(\mathbf{b},\mathbf{k})\mathbf{k})\}$$
$$\times\overline{M_\lambda(\sigma_0(\mathbf{p})^{-1}B\sigma_0(B^{-1}\cdot\mathbf{p})\eta_i(\sigma_0(\mathbf{k})^{-1}\mathbf{p}))}\varphi_i(\mathbf{p}). \quad (58)$$

However,

$$\langle W_{\eta_2}(\varphi_2),W_{\eta_1}(\varphi_1)\rangle_{L^2_\mu(\mathscr{P}/H_2)} = \int_{\mathscr{P}/H_2} d\mu((\pi^2(\mathbf{b},B))\overline{[W_{\eta_1}(\varphi_1)](\sigma_2(\pi_2(\mathbf{b},B)))}$$
$$\times[W_{\eta_2}(\varphi_2)](\sigma_2(\pi_2(\mathbf{b},B)))$$
$$= \int_{\mathscr{P}/H_2} d\mu(\pi_2(\mathbf{b},B))\langle\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\pi_2(\mathbf{b},B)))\eta_1,\varphi_1\rangle$$
$$\times\langle\varphi_2,\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\pi_2(\mathbf{b},B)))\eta_2\rangle$$
$$= \int_{\mathscr{P}/H_2} d\mu(\mathbf{b}-\kappa(\mathbf{b},\mathbf{k})\mathbf{k},\mathbf{k})\int d\nu(\mathbf{p})d\nu(\mathbf{t})$$

$$
\begin{aligned}
&\times \exp\{-i(\mathbf{p}-\mathbf{t})\cdot(\mathbf{b}-\kappa(\mathbf{b},\mathbf{k})\mathbf{k})\}\overline{M_\lambda(\sigma_0(\mathbf{p})^{-1}B\sigma_0(B^{-1}\cdot\mathbf{p}))}\\
&\times M_\lambda(\sigma_0(\mathbf{t})^{-1}B\sigma_0(B^{-1}\cdot\mathbf{t}))\overline{\mathscr{E}(\mathbf{p})}\mathscr{E}(\mathbf{t})\\
&\times\overline{\eta_1(\sigma_0(\mathbf{k})^{-1}\mathbf{p})}\,\eta_2(\sigma_0(\mathbf{k})^{-1}\mathbf{t})\varphi_1(\mathbf{p})\overline{\varphi_2(\mathbf{t})}\\
=&\int d\nu(\mathbf{p})d\nu(\mathbf{t})\overline{\mathscr{E}(\mathbf{p})}\mathscr{E}(\mathbf{t})\varphi_1(\mathbf{p})\overline{\varphi_2(\mathbf{t})M_\lambda(\sigma_0(\mathbf{p})^{-1}B\sigma_0(B^{-1}\cdot\mathbf{p}))}\\
&\times M_\lambda(\sigma_0(\mathbf{t})^{-1}B\sigma_0(B^{-1}\cdot\mathbf{t}))\delta(\mathbf{p}-\mathbf{t})(2\pi)^3\\
&\times\int d\nu(\mathbf{k})\overline{\eta_1(\sigma_0(\mathbf{k})^{-1}\mathbf{p})}\,\eta_2(\sigma_0(\mathbf{k})^{-1}\mathbf{t})\\
=&\int d\nu(\mathbf{p})\varphi_1(\mathbf{p})\overline{\varphi_2(\mathbf{p})}|\mathscr{E}(\mathbf{p})|^2(p^0)^{-1}\\
&\times\left[(2\pi)^3\int d\nu(\mathbf{k})\overline{\eta_1(\sigma_0(\mathbf{k})^{-1}\mathbf{p})}\,\eta_2(\sigma_0(\mathbf{k})^{-1}\mathbf{p})\right]\\
=&\int d\nu(\mathbf{p})\varphi_1(\mathbf{p})\overline{\varphi_2(\mathbf{p})}|\mathscr{E}(\mathbf{p})|^2(p^0)^{-1}N_{12}(\mathbf{p})\\
=&\langle\varphi_2,EN_{12}\varphi_1\rangle_{L^2_\nu(P/H_1)},
\end{aligned}
\tag{59}
$$

where

$$
N_{12}(\mathbf{p})\equiv(2\pi)^3\int d\nu(\mathbf{k})\overline{\eta_1(\sigma_0(\mathbf{k})^{-1}\mathbf{p})}\,\eta_2(\sigma_0(\mathbf{k})^{-1}\mathbf{p})
\tag{60}
$$

and

$$
E(\mathbf{p})=|\mathscr{E}(\mathbf{p})|^2(p^0)^{-1}.
$$

We shall show that N_{12} is independent of $\mathbf{p}$. Recall $\eta(\mathbf{k})=f(0,\sigma_0(\mathbf{k}))$ for some f transforming under $U^{\mathbf{p}_o\lambda}$ as in (25). Then

$$
N_{12}=(2\pi)^3\int d\nu(\mathbf{k})\overline{f_1(0,\sigma_0(\mathbf{k})^{-1}\sigma_0(\mathbf{p}))}f_2(0,\sigma_0(\mathbf{k})^{-1}\sigma_0(\mathbf{p})).
\tag{61}
$$

Define F by $F(0,\sigma_0(\mathbf{p}))=f(0,\sigma_0(\mathbf{p})^{-1})$. Then, by the SL(2,$\mathbb{C}$) invariance of ν,

$$
\begin{aligned}
N_{12}&=(2\pi)^3\int d\nu(\mathbf{k})\overline{F_1(0,\sigma_0(\mathbf{p})^{-1}\sigma_0(\mathbf{k}))}F_2(0,\sigma_0(\mathbf{p})^{-1}\sigma_0(\mathbf{k}))\\
&=(2\pi)^3\int d\nu(\mathbf{k})\overline{F_1(0,\sigma_0(\mathbf{k}))}F_2(0,\sigma_0(\mathbf{k}))=(2\pi)^3\int d\nu(\mathbf{k})\overline{f_1(0,\sigma_0(\mathbf{k})^{-1})}f_2(0,\sigma_0(\mathbf{k})^{-1}).
\end{aligned}
$$

Also, we have from (7) and (18), $\sigma_0(\mathbf{k})^{-1}=\sigma_0(\tilde{\mathbf{k}})h(\mathbf{k})$ for some null vector $\tilde{\mathbf{k}}$, and some element $h(\mathbf{k})$ of $E(2)^{\sim}$. Using (22) and the analog of (30) common to any induction procedure, we obtain

$$
N_{12}=(2\pi)^3\int d\nu(\mathbf{k})\overline{f_1(\sigma_0(\tilde{\mathbf{k}})h(\mathbf{k}))}f_2(0,\sigma_0(\tilde{\mathbf{k}})h(\mathbf{k}))=(2\pi)^3\int d\nu(\mathbf{k})\overline{f_1(0,\sigma_0(\tilde{\mathbf{k}}))}f_2(0,\sigma_0(\tilde{\mathbf{k}})).
$$

With a similar computation, one also shows that the last expression is independent of any particular choice for σ_0, any other choice again differing by an $E(2)\tilde{}$-valued function acting on the right. To proceed, it then suffices to compute $\tilde{\mathbf{k}}$ using any convenient choice of section σ_0. We do this in the Appendix in order to extract the Jacobian $d\tilde{\mathbf{k}}/d\mathbf{k}$, which is all we need for what follows. We obtain

$$[(\tilde{k})^0]^{-1} d\tilde{\mathbf{k}}/d\mathbf{k} = -4[k^0]^{-1}[k^0+k^3]^{-2}. \tag{62}$$

Using this, and substituting $\tilde{\mathbf{k}}=\mathbf{r}$, we compute

$$\begin{aligned} N_{12} &= (2\pi)^3 \int d\nu(\mathbf{k}) \overline{f_1(0,\sigma_0(\tilde{\mathbf{k}}))} f_2(0,\sigma_0(\tilde{\mathbf{k}})) = (2\pi)^3 \int d\nu(\mathbf{k}) \overline{\eta_1(\tilde{\mathbf{k}})}\, \eta_2(\tilde{\mathbf{k}}) \\ &= (2\pi)^3 \int \frac{d\mathbf{k}}{k^0} \overline{\eta_1(\tilde{\mathbf{k}})}\, \eta_2(\tilde{\mathbf{k}}) = (2\pi)^3 \int d\mathbf{k}\, \frac{d\mathbf{k}}{d\tilde{\mathbf{k}}} \frac{1}{k^0} \overline{\eta_1(\tilde{\mathbf{k}})}\, \eta_2(\tilde{\mathbf{k}}) \\ &= (2\pi)^3 \int d\mathbf{r}\, \frac{d\tilde{\mathbf{r}}}{d\mathbf{r}} \frac{1}{\tilde{r}^0} \overline{\eta_1(\mathbf{r})}\, \eta_2(\mathbf{r}) = 4(2\pi)^3 \int \frac{d\mathbf{r}}{r^0} (r^0+r^3)^{-2} \overline{\eta_1(\mathbf{r})}\, \eta_2(\mathbf{r}) \\ &= \langle \eta_1, C^2 \eta_2 \rangle_{L^2_\nu(P/H_1)}. \end{aligned} \tag{63}$$

Then (59) becomes

$$\langle W_{\eta_2}(\varphi_2), W_{\eta_1}(\varphi_1) \rangle_{L^2_\mu(\mathscr{P}/H_2)} = \langle \varphi_2, E\varphi_1 \rangle_{L^2_\nu(P/H_1)} \langle \eta_1, C^2 \eta_2 \rangle_{L^2_\nu(P/H_1)}$$

which equals

$$\langle \varphi_2, \varphi_1 \rangle_{L^2_\nu(P/H_1)} \langle \eta_1, C^2 \eta_2 \rangle_{L^2_\nu(P/H_1)}$$

iff $E(\mathbf{p})=1$, i.e., $|\mathscr{E}(\mathbf{p})| = \sqrt{p^0}$.

This proves (54) under the initial assumptions on η_1,η_2 or φ_1,φ_2. However, C^2 acting on $L^2_\nu(\mathscr{P}/H_1)$, being an operator of pointwise multiplication by a function that is nonzero, has dense range. Thus (54) and (52) have unique bounded linear extensions. □

The integral (63) is geometrically more transparent if one uses the coordinates $\{p^0+p^3, p^1, p^2\}$ rather than $\{p^1,p^2,p^3\}$. Here as in (10), there is the constraint $p^0+p^3 \geqslant 0$. The Jacobian for this transformation is $p^0/(p^0+p^3)$ and (63) becomes

$$\begin{aligned} N_{12} &= 4(2\pi)^3 \int \frac{dp^1 dp^2 dp^3}{p^0} (p^0+p^3)^{-2} \overline{\eta_1(\mathbf{p})}\, \eta_2(\mathbf{p}) \\ &= 4(2\pi)^3 \int d(p^0+p^3) dp^1 dp^2 (p^0+p^3)^{-3} \overline{\eta_1(\mathbf{p})}\, \eta_2(\mathbf{p}) \end{aligned} \tag{64}$$

where the integral is over the half-space $p^0+p^3 \geqslant 0$.

Corollary 4.2: With the notation above and choosing $\eta_1=\eta_2=\eta$ so that $N_{11} \equiv \|C\eta\|^2 = 1$, then W_η is an isometry: $W_\eta : L^2_\nu(\mathscr{P}/H_1) \to L^2_\mu(\mathscr{P}/H_2)$. Defining the representation $U^{\eta,\lambda}$ of $\mathscr{P}$ on the range of W_η in $L^2_\mu(\mathscr{P}/H_2)$ by intertwining,

$$U^{\eta,\lambda} \equiv W_\eta U^{\mathbf{p}_o \lambda} W_\eta^{-1}, \tag{65}$$

then $U^{\eta,\lambda}$ is an irreducible representation of $\mathscr{P}$.

Proof: One need only show that W_η is a closed operator, the proof of which is straightforward. Then the range of W_η is closed subspace $\mathscr{H}_\eta$ of $L^2_\mu(\mathscr{P}/H_2)$. □

In a similar fashion, one could begin with the representation $U^{\beta\lambda}$ on $L^2_\mu(\mathscr{P}/H_2)$ as in (29), and form the pull-back representation $W_\eta^{-1}U^{\beta\lambda}W_\eta$ on $L^2_\nu(\mathscr{P}/H_1)$. Since $U^{\beta\lambda}$ is not irreducible, as we show below, this is not as useful.

Notation: Henceforth, we shall say that η is admissible if $N\equiv\|C\eta\|^2<\infty$. Furthermore, the symbol η will henceforth be reserved to denote an admissible vector.

The projection: $L^2_\mu(\mathscr{P}/H_2)\to$the range of W_η will be denoted P^η.

V. PHASE SPACE LOCALIZATION AND INTERTWINING WITH PHASE SPACE REPRESENTATIONS

We recall the familiar result that, for massive irreducible representations of the Poincaré group, there are Euclidean covariant Euclidean space localization operators[1,12] allowing one to define ''massive elementary particles.'' This result has been generalized to show the existence of phase space localization operators covariant under the action of the entire Poincaré group.[31] On the other hand, it was also shown[1,12] that no Euclidean covariant Euclidean space localization operator existed for the photon or for other massless particles of helicity greater than 1. We shall next show that this precludes intertwining the standard irreducible massless representations with any left-quasiregular representation on phase space such as is given in (44). Nevertheless, we shall exhibit explicitly the phase space representation intertwined via the W_η given above.

Definition: Define the family $A\equiv\{A(\Delta)|\Delta$ a Borel set in $\mathscr{P}/H_2\}$ on $L^2_\mu(\mathscr{P}/H_2)$ through multiplication by characteristic functions χ_Δ for Borel sets Δ:

$$\begin{aligned}&\Delta\mapsto A(\Delta)=M_{\chi_\Delta};\\ &[A(\Delta)f](\mathbf{y})=\chi_\Delta(\mathbf{y})f(\mathbf{y})a.e.\mathbf{y},\quad f\in L^2_\mu(\mathscr{P}/H_2).\end{aligned}\tag{66}$$

On $L^2_\nu(\mathscr{P}/H_1)$ define the family A_η by

$$A_\eta\equiv\{A_\eta(\Delta)|\Delta=\text{Borel set of } \mathscr{P}/H_2\},\tag{67}$$

where

$$A_\eta(\Delta)\equiv W_\eta^{-1}P^\eta A(\Delta)W_\eta\equiv W_\eta^{-1}P^\eta A(\Delta)P^\eta W_\eta.\tag{68}$$

Since A is the phase space localization operator on $L^2_\mu(\mathscr{P}/H_2)$, and A_η is its pullback to the irreducible representation space $L^2_\nu(\mathscr{P}/H_1)$, A_η is the natural choice for a phase space localization operator for massless particles.

Definition: Let G be a group on $\mathscr{P}/H_2$ and let U be a representation of G on $L^2_\mu(\mathscr{P}/H_2)$. The phase space localization operator A is said to be G-covariant with respect to U if and only if

$$U(g)A(\Delta)U(g)^{-1}=A(g\cdot\Delta)\ \text{ for all }\ \Delta\in\text{Borel}(\mathscr{P}/H_2),\quad g\in G.$$

Theorem 5.1: *The family $A=\{A(\Delta)|\Delta=$Borel set in $\mathscr{P}/H_2\}$ is a $\mathscr{P}$-covariant projection-valued measure (PVM) on $L^2_\mu(\mathscr{P}/H_2)$ with respect to $U^{\beta\lambda}$ of (44) [and not with respect to $U^{\eta,\lambda}$ of (65)]. A_η is a positive operator-valued measure (POVM) on $L^2_\nu(\mathscr{P}/H_1)$.*

Proof: That A is a PVM is trivial. To see the covariance, choose $f\in L^2_\mu(\mathscr{P}/H_2)$. Now, from (44) we have, for $\varphi\equiv\kappa(\mathbf{k},\mathbf{p})-\kappa((\mathbf{b},B)^{-1}(\mathbf{k},\mathbf{p}))$,

$$\begin{aligned}&[U^{\beta\lambda}(\mathbf{b},B)A(\Delta)U^{\beta\lambda}(\mathbf{b},B)^{-1}F](\mathbf{k},\mathbf{p})\\ &\quad=\exp\{i\beta\varphi\}M_\lambda(\sigma_0(\mathbf{p})^{-1}B\sigma_0(B^{-1}\mathbf{p}))[A(\Delta)U^{\beta\lambda}(\mathbf{b},B)^{-1}F](B^{-1}\cdot(\mathbf{k}-\mathbf{b}),B^{-1}\cdot\mathbf{p})\end{aligned}$$

$$= \begin{cases} 0 & \text{if } (B^{-1}\cdot(\mathbf{k}-\mathbf{b}), B^{-1}\cdot\mathbf{p}) \notin \Delta \\ F(\mathbf{k},\mathbf{p}) & \text{if } (B^{-1}\cdot(\mathbf{k}-\mathbf{b}), B^{-1}\cdot\mathbf{p}) \in \Delta \end{cases}$$

$$= [A((\mathbf{b},B)\circ\Delta)F](\mathbf{k},\mathbf{p}) \tag{69}$$

where

$$(\mathbf{k},\mathbf{p}) \in (\mathbf{b},B)\circ\Delta \quad \text{iff} \quad (\mathbf{b},B)^{-1}(\mathbf{k},\mathbf{p}) = (B^{-1}\cdot(\mathbf{k}-\mathbf{b}), B^{-1}\cdot\mathbf{p}) \in \Delta.$$

Hence, A is $\mathscr{P}$-covariant with respect to $U^{\beta\lambda}$. Since A_η is the projection of a PVM, it is a POVM. □

As a consequence of Theorem 5.1, we have the following:

Result: Let U be an irreducible representation of $\mathscr{P}$ on a Hilbert space $\mathscr{H}$. Let W intertwine U with the left-regular representation V of $\mathscr{P}$ on $L^2_\mu(\mathscr{P}/H_2)$. Let P denote the projection of $L^2_\mu(\mathscr{P}/H_2)$ onto the range of W. Let B be defined by

$$B(\Delta) = W^\dagger P A(\Delta) W, \quad \Delta \in \text{Borel}(\mathscr{P}/H_2),$$

where A is the phase space localization operator defined above. Then B is a $\mathscr{P}$-covariant localization operator on $\mathscr{H}$.

Proof: Since $WU(g) = V(g)W$ for all $g \in \mathscr{P}$, one has $U(g)W^\dagger W = W^\dagger W U(g)$ for all $g \in \mathscr{P}$. Since U is irreducible, $W^\dagger W = \gamma \mathbf{1}$ for some $\gamma > 0$. Then

$$(\gamma^{-1} W W^\dagger) W\phi = \gamma^{-1} W(W^\dagger W)\phi = W\phi$$

for all $\phi \in \mathscr{H}$. Therefore, if $f \in L^2_\mu(\mathscr{P}/H_2)$ is orthogonal to the range of W, then

$$\langle \gamma^{-1} W W^\dagger f, W\phi\rangle = \gamma^{-1}\langle W^\dagger f, W^\dagger W\phi\rangle = \langle W^\dagger f, \phi\rangle = \langle f, W\phi\rangle = 0.$$

Thus, $\gamma^{-1} W W^\dagger = P$. It follows by intertwining that $V(g)P = PV(g)$ for all $g \in \mathscr{P}$. Hence, for all $g \in \mathscr{P}$,

$$U(g^{-1})B(\Delta)U(g) = U(g^{-1})W^\dagger P A(\Delta) W U(g) = W^\dagger V(g^{-1}) P A(\Delta) V(g) W$$
$$= W^\dagger P V(g^{-1}) A(\Delta) V(g) W = W^\dagger P A(g\cdot\Delta) W = B(g\cdot\Delta).$$

□

In particular, if we take W to be W_η defined through (51) and $B = A_\eta$, then if W_η intertwined the irreducible representation $U^{\xi\lambda}$ in (24) with $U^{\beta\lambda}$ in (29) or (44), it follows that A_η would define a $\mathscr{P}$-covariant configuration space localization operator, and hence a Euclidean space localization operator covariant under the Euclidean subgroup of $\mathscr{P}$. This would contradict the result of Wightman (Ref. 12, pp. 850, 862). One concludes that W_η cannot intertwine $U^{\xi\lambda}$ with any phase space representation of $\mathscr{P}$ such as $U^{\beta\lambda}$.

To obtain the same result without relying on Wightman's result, we may do the following: Define a Euclidean subgroup of $\mathscr{P}$, by first picking a preferred time axis. In the basis defining the notation of (45), the time direction corresponds to $\mathbf{p}+2\mathbf{q}_\mathbf{p}$. Then, $(\mathbf{u}_\mathbf{p}, \mathbf{v}_\mathbf{p}, \mathbf{p}-2\mathbf{q}_\mathbf{p})$ forms a basis of spacelike vectors in what may viewed as ordinary momentum space. This identification of ''ordinary space'' is not Poincaré invariant, but is invariant under the subgroup $\text{SL}(2,\mathbb{C})_{\mathbf{p}+2\mathbf{q}_\mathbf{p}} \cong O(3)$ of $\text{SL}(2,\mathbb{C})$. Then $\mathbb{R}^4 \circledcirc \text{SL}(2,\mathbb{C})_{\mathbf{p}+2\mathbf{q}_\mathbf{p}} \cong \mathbb{R}^4 \circledcirc O(3)$ includes the Euclidean group $E(3) = [\mathbb{R}^4/(\mathbf{p}+2\mathbf{q}_\mathbf{p})] \circledcirc \text{SL}(2,\mathbb{C})_{\mathbf{p}+2\mathbf{q}_\mathbf{p}}$.

The next theorem isolates the desired intertwining condition.

Theorem 5.2: *For $U^{p_o\lambda}$ as in (25), $U^{\beta\lambda}$ as in (29), and W_η as in (49) and (50), then*

$$W_\eta U^{\mathbf{p}_o\lambda}(g) = U^{\beta\lambda}(g) W_\eta \tag{70}$$

iff $g \in \mathscr{P}$ *satisfies*

$$\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(g^{-1}\cdot\mathbf{x}))\eta = U^{\mathbf{p}_o\lambda}(g^{-1})\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta, \quad a.e. \quad \mathbf{x}. \tag{71}$$

Proof: We have

$$\begin{aligned}[W_\eta U^{\mathbf{p}_o\lambda}(g)\varphi](\mathbf{x}) &\equiv [W_\eta U^{\mathbf{p}_o\lambda}(g)\varphi](\sigma_2(\mathbf{x})). = \langle \mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta, U^{\mathbf{p}_o\lambda}(g)\varphi\rangle \\ &= \langle U^{\mathbf{p}_o\lambda}(g^{-1})\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta, \varphi\rangle. \end{aligned} \tag{72}$$

On the other hand,

$$\langle \mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(g^{-1}\cdot\mathbf{x}))\eta, \varphi\rangle = [W_\eta\phi](\sigma_2(g^{-1}\cdot\mathbf{x})) \equiv [W_\eta\phi](g^{-1}\cdot\mathbf{x}) = U^{\beta\lambda}(g)[W_\eta\varphi](\mathbf{x}). \tag{73}$$

Since both (72) and (73) hold for all φ, then (70) is equivalent to (71). □

The condition (71) is the source of the general failure of achieving Euclidean covariance in the massless representations of the Poincaré group. To see this, suppose $g \in \mathbb{R}^4 \circledcirc \mathrm{SL}(2,\mathbb{C})_{\mathbf{p}+2\mathbf{q}_\mathbf{p}}$. It follows that $\mathscr{E}U^{\mathbf{p}_o\lambda}(g) = U^{\mathbf{p}_o\lambda}(g)\mathscr{E}$. Then (71) reduces to showing that

$$U^{\mathbf{p}_o\lambda}(\sigma_2(g^{-1}\cdot\mathbf{x}))\eta = U^{\mathbf{p}_o\lambda}(g^{-1}\sigma_2(\mathbf{x}))\eta, \quad a.e. \quad \mathbf{x}.$$

By using σ_2 as defined in (39) and (43) and setting $\mathbf{x}=(\mathbf{k},\mathbf{p})$ and $g=(\mathbf{b},B)$, one shows that this is equivalent to

$$U^{\mathbf{p}_o\lambda}((-\mathbf{b}\cdot\mathbf{q})\mathbf{p}, A(\mathbf{k},\mathbf{p})^{-1}BA(B^{-1}(\mathbf{k}-\mathbf{b}), B^{-1}\mathbf{p}))\eta = \eta \quad \text{for all } (\mathbf{k},\mathbf{p}).$$

For $U^{\mathbf{p}_o\lambda}$ as in (25), this requires $\eta=0$.

For comparison, we note that a similar analysis in the massive case has a nontrivial solution, namely that η be rotation invariant (Ref. 31).

We exhibit precisely the form of the irreducible unitary phase space representation intertwined from $U^{\mathbf{p}_o\lambda}$ by (65).

Theorem 5.3: *The irreducible representation* $U^{\eta,\lambda}$ *intertwined from* $U^{\mathbf{p}_o\lambda}$ *by (65) is given, for* $N=\|C\eta\|^2$*, by the integral representation*

$$[U^{\eta,\lambda}(g)(P^\eta f)](\mathbf{x}) = N^{-1}\int d\mu(\mathbf{y})\langle \mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\pi, U^{\mathbf{p}_o\lambda}(g)\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{y}))\eta\rangle(P^\eta f)(\mathbf{y}). \tag{74}$$

Proof: From (72) we have

$$[W_\eta U^{\mathbf{p}_o\lambda}(g)\varphi](\mathbf{x}) = \langle U^{\mathbf{p}_o\lambda}(g^{-1})\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta, \varphi\rangle.$$

Using the orthogonality relation (54), this reads

$$\begin{aligned}[W_\eta U^{\mathbf{p}_o\lambda}(g)\varphi](\mathbf{x}) &= N^{-1}\langle W_\eta U^{\mathbf{p}_o\lambda}(g^{-1})\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta, W_\eta\varphi\rangle \\ &= N^{-1}\int d\mu(\mathbf{y})\overline{[W_\eta U^{\mathbf{p}_o\lambda}(g^{-1})\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta](\mathbf{y})}[W_\eta\varphi](\mathbf{y}).\end{aligned}$$

From the definition (50) of W_η, this may be written

$$\begin{aligned}&[W_\eta U^{\mathbf{p}_o\lambda}(g)W_\eta^{-1}W_\eta\varphi](\mathbf{x}) \\ &\quad = [W_\eta U^{\mathbf{p}_o\lambda}(g)\varphi](\mathbf{x})\end{aligned}$$

$$= N^{-1} \int d\mu(\mathbf{y}) \langle \mathscr{E} U^{\mathbf{p}_o \lambda}(\sigma_2(\mathbf{x}))\eta, U^{\mathbf{p}_o \lambda}(g)\mathscr{E} U^{\mathbf{p}_o \lambda}(\sigma_2(\mathbf{y}))\eta \rangle [W_\eta \varphi](\mathbf{y}).$$

By (65), (74) follows. □

Again we see that (74) does not correspond to the left-quasiregular representation for the action of g unless (72) is satisfied.

VI. QUANTIZATION AND DEQUANTIZATION

With the results above, we may define a natural quantization scheme. On $L^2_\mu(\mathscr{P}/H_2)$, and for f a measurable function on $\mathscr{P}/H_2$, define the operator M_r by

$$[M_r f](\mathbf{y}) \equiv r(\mathbf{y}) f(\mathbf{y}). \tag{75}$$

For $\psi \in L^2_\nu(\mathscr{P}/H_1)$, define $A_\eta(r)\psi$ by

$$A_\eta(r)\psi \equiv W_\eta^{-1} P^\eta M_r W_\eta \psi. \tag{76}$$

Theorem 6.1: (Quantization):

$$A_\eta(r) = \int_{\mathscr{P}/H_2} r(\mathbf{x}) |\mathscr{E} U^{\mathbf{p}_o \lambda}(\sigma_2(\mathbf{x}))\eta\rangle\langle \mathscr{E} U^{\mathbf{p}_o \lambda}(\sigma_2(\mathbf{x}))\eta| d\mu(\mathbf{x}). \tag{77}$$

Proof: Let ψ, $\varphi \in L^2_\nu(\mathscr{P}/H_1)$. We have,

$$\begin{aligned}\langle \varphi, A_\eta(r)\psi\rangle &= \langle \varphi, W_\eta^{-1} P^\eta M_r W_\eta \psi\rangle = \langle W_\eta \varphi, P^\eta M_r W_\eta \psi\rangle = \langle W_\eta \varphi, M_r W_\eta \psi\rangle \\ &= \int \overline{[W_\eta \phi](\mathbf{x})} [M_r W_\eta \psi](\mathbf{x}) d\mu(\mathbf{x}) \\ &= \int \langle \varphi, \mathscr{E} U^{\mathbf{p}_o \lambda}(\sigma_2(\mathbf{x}))\eta\rangle r(\mathbf{x}) \langle \mathscr{E} U^{\mathbf{p}_o \lambda}(\sigma_2(\mathbf{x}))\eta, \psi\rangle d\mu(\mathbf{x}).\end{aligned}$$

□

Remark: If $r(\mathbf{x}) \equiv 1$, a.e. $\mathbf{x}$, then (77) shows that $A_\eta(r) = 1$. Alternatively,

$$\int_{\mathscr{P}/H_2} |U^{\mathbf{p}_o \lambda}(\sigma_2(\mathbf{x}))\eta\rangle\langle U^{\mathbf{p}_o \lambda}(\sigma_2(\mathbf{x}))\eta| d\mu(\mathbf{x}) = \mathscr{E}^{-2}. \tag{78}$$

We introduce the notation

$$T^\eta(\mathbf{x}) \equiv |\mathscr{E} U^{\mathbf{p}_o \lambda}(\sigma_2(\mathbf{x}))\eta\rangle\langle \mathscr{E} U^{\mathbf{p}_o \lambda}(\sigma_2(\mathbf{x}))\eta|. \tag{79}$$

Then Theorem 6.1 may be reexpressed

$$A_\eta(r) = \int_{\mathscr{P}/H_2} r(\mathbf{x}) T^\eta(\mathbf{x}) d\mu(\mathbf{x}). \tag{80}$$

There is also a natural dequantization scheme:

Theorem 6.2. *(Dequantization): Let ρ be a density operator in $L^2_\nu(\mathscr{P}/H_1)$, and define*

$$R_\rho(\mathbf{x}) \equiv \mathrm{Tr}(\rho T^\eta(\mathbf{x})). \tag{81}$$

Then R_ρ is a classical probability density over the phase space $\mathscr{P}/H_2$ and, moreover,

$$\mathrm{Tr}(\rho A_\eta(r)) = \int_{\mathscr{P}/H_2} R_\rho(\mathbf{x}) r(\mathbf{x}) d\mu(\mathbf{x}); \tag{82}$$

i.e., the quantum and classical expectations agree, making the quantization map and the dequantization map dual in the sense of (82).

Proof: The theorem follows from (80), (81), and the interchangeability of trace with the integral. □

Two questions which we now ask are:

(1) Which operators in $L^2_\nu(\mathscr{P}/H_1)$ may be written in the form (76) and (80) for some measurable function r?
(2) Does the set of expressions in (81), $\{R_\rho(\mathbf{x}) \equiv \mathrm{Tr}(\rho T^\eta(\mathbf{x})) | \mathbf{x} \in \mathscr{P}/H_2\}$, uniquely determine ρ?

To analyze this, we introduce the concept of ''informational completeness:''

Definition: A collection $\{A_\alpha | \alpha \in I\}$ of operators acting on Hilbert space $\mathscr{H}$ is said to be informationally complete iff, for ρ_1 and ρ_2 any positive trace class operators of trace one on $\mathscr{H}$, the equality $\mathrm{Tr}(\rho_1 A_\alpha) = \mathrm{Tr}(\rho_2 A_\alpha)$ for all $\alpha \in I$, implies $\rho_1 = \rho_2$.

A result of P. Busch[39] shows that, if $\{A_\alpha | \alpha \in I\}$ is informationally complete, then the closure of the span of $\{A_\alpha | \alpha \in I\} \cup \{\mathbf{1}\}$ [in the sense of a topology related to the form $A \mapsto \mathrm{Tr}(\rho A)$] includes all of $\mathscr{B}(\mathscr{H})$. In this sense, possessing the informational completeness property implies a positive response to both questions. This has a physical interpretation if the A_α are all quantum observables (that is, they are self-adjoint, or at least symmetric operators), since the positive traceclass operators of trace one on $\mathscr{H}$ are the quantum statistical density operators and $\mathrm{Tr}(\rho A)$ is just quantum expectation. The question of informational completeness is addressed as we introduce families of localization operators below.

VII. INFORMATIONAL COMPLETENESS OF THE LOCALIZATION OPERATOR

To demonstrate the informational completeness property, we will use the mathematical trick of introducing an action of the Heisenberg group on an extension of the phase space representation of zero mass particles. Then we will employ the known informational completeness property of the Wigner coefficients of the Heisenberg group:

Consider $\phi \in L^2(V_0^+, d\nu)$, $d\nu(\mathbf{k}) = d(\mathbf{k}\cdot\mathbf{q}_0) d(\mathbf{k}\cdot\mathbf{u}_0) d(\mathbf{k}\cdot\mathbf{v}_0)/\mathbf{k}\cdot\mathbf{q}_0$. Since, for $\mathbf{k} \in V_0^+$, $\mathbf{k}\cdot\mathbf{p}_0 = [(\mathbf{k}\cdot\mathbf{u}_0)^2 + (\mathbf{k}\cdot\mathbf{v}_0)^2]/2\mathbf{k}\cdot\mathbf{q}_0$, we may consider $V_0^+ \cong \mathbb{R}^+ \times \mathbb{R}^2$, and functions ϕ in V_0^+ to be functions ϕ of $(\mathbf{k}\cdot\mathbf{q}_0, \mathbf{k}\cdot\mathbf{u}_0, \mathbf{k}\cdot\mathbf{v}_0)$ in $\mathbb{R}^+ \times \mathbb{R}^2$ which are extended to all of $\mathbb{R}^3$ with support on the closure of V_0^+. We set

$$j: V_0^+ \to \mathbb{R}^3, \quad j(\mathbf{k}) = (\mathbf{k}\cdot\mathbf{q}_0, \mathbf{k}\cdot\mathbf{u}_0, \mathbf{k}\cdot\mathbf{v}_0). \tag{83}$$

Similarly, j^{-1}: $\mathbb{R}^3 \to V_0^+ \cup V_0^- \cup \{\mathbf{0}\}$, and j^{-1} maps $\mathbf{x} \in \mathbb{R}^3$ into V_0^+ iff $\mathbf{x} = (x_0, x_1, x_2)$ with $x_0 > 0$.

We may now define the bijective isometry

$$J: L^2(V_0^+, d\nu) \to L^2(\mathbb{R}^3), \quad J: \phi(\mathbf{k}) \to |\mathbf{k}\cdot\mathbf{q}_0|^{-1/2} \widetilde{\phi}(j(\mathbf{k})). \tag{84}$$

By (64), η is admissible iff

$$\int_{\mathbb{R}^2} d(\mathbf{k}\cdot\mathbf{u}_0) d(\mathbf{k}\cdot\mathbf{v}_0) \int_{\mathbb{R}^+} d(\mathbf{k}\cdot\mathbf{q}_0) (\mathbf{k}\cdot\mathbf{q}_0)^{-3} |\eta(\mathbf{k})|^2 < \infty.$$

Thus, as a function of $\mathbf{k}\cdot\mathbf{q}_0$, if η is smooth, it may be extended smoothly to a function on $\mathbb{R}^3$.

Now, for $t \in \mathbb{R}$, $\mathbf{r}' \in V_0^+$, $\mathbf{r}'\cdot\mathbf{q}_0 = 0$ (the ''prime'' $'$ will henceforth signal this condition), define

$$l(\mathbf{r}') = (\mathbf{r}'\cdot\mathbf{p}_0, -\mathbf{r}'\cdot\mathbf{u}_0, -\mathbf{r}'\cdot\mathbf{v}_0) \in \mathbb{R}^3. \tag{85}$$

These are the coordinates of $\mathbf{r}\prime=(\mathbf{r}\prime\cdot\mathbf{p}_0)\mathbf{q}_0-(\mathbf{r}\prime\cdot\mathbf{u}_0)\mathbf{u}_0-(\mathbf{r}\prime\cdot\mathbf{v}_0)\mathbf{v}_0$ *relative to the basis* $\{\mathbf{q}_0,\mathbf{u}_0,\mathbf{v}_0\}$; *with respect to the Minkowski metric, this basis is dual to the basis* $\{\mathbf{p}_0, -\mathbf{u}_0, -\mathbf{v}_0\}$ *for which the coordinates are given by the map* j.

Next, for such $\mathbf{r}\prime$ *and for* $\mathbf{s}\in\mathbb{R}^4$, *define a representation* W *of the Heisenberg group by*

$$W(t,l(\mathbf{r}'),j(\mathbf{s})):L^2(\mathbb{R}^3)\to L^2(\mathbb{R}^3),$$

$$[W(t,l(\mathbf{r}'),j(\mathbf{s}))J\phi](\mathbf{x})=e^{-i\pi l(\mathbf{r}')\cdot j(\mathbf{s})}e^{i2\pi(t+l(\mathbf{r}')\cdot(\mathbf{x}+j(\mathbf{s})))}[J\phi](\mathbf{x}+j(\mathbf{s})),\quad \mathbf{x}\in\mathbb{R}^3, \tag{86}$$

where $l(\mathbf{r}')\cdot j(\mathbf{s})$ and $l(\mathbf{r}')\cdot(\mathbf{x}+j(\mathbf{s}))$ employs the usual inner product in $\mathbb{R}^3$. Because $\mathbf{r}'\cdot\mathbf{q}_0=0$, these two inner products agree with the Minkowski inner products $\mathbf{r}'\cdot\mathbf{s}$ and $\mathbf{r}'\cdot(j^{-1}(\mathbf{x})+\mathbf{s})$, and we may write

$$[W(t,l(\mathbf{r}'),j(\mathbf{s}))J\phi](\mathbf{x})=e^{-i\pi\mathbf{r}'\cdot\mathbf{s}}e^{i2\pi(t+\mathbf{r}'\cdot(j^{-1}(\mathbf{x})+\mathbf{s}))}[J\phi](\mathbf{x}+j(\mathbf{s})). \tag{87}$$

One verifies the Heisenberg relation

$$W(t,l(\mathbf{r}'),j(\mathbf{s}))W(u,l(\mathbf{q}'),j(\mathbf{p}))=W(t+u+(\mathbf{q}'\cdot\mathbf{s}+\mathbf{r}'\cdot\mathbf{p})/2,l(\mathbf{r}')+l(\mathbf{q}'),j(\mathbf{s})+j(\mathbf{p})),$$

$$\mathbf{q}'\cdot\mathbf{q}_0=0. \tag{88}$$

The Heisenberg orthogonality relations are computed and expressed as

$$\int_{\mathbb{R}^6}d(\mathbf{r}'\cdot\mathbf{p}_0)d(\mathbf{r}'\cdot\mathbf{u}_0)d(\mathbf{r}'\cdot\mathbf{v}_0)d(\mathbf{s}\cdot\mathbf{q}_0)d(\mathbf{s}\cdot\mathbf{u}_0)d(\mathbf{s}\cdot\mathbf{v}_0)\langle J\phi_1,W(0,l(\mathbf{r}'),j(\mathbf{p}))J\phi_2\rangle_{L^2(\mathbb{R}^3)}$$
$$\times\langle W(0,l(\mathbf{r}'),j(\mathbf{s}))J\phi_3,J\phi_4\rangle_{L^2(\mathbb{R}^3)}=\langle J\phi_3,J\phi_2\rangle_{L^2(\mathbb{R}^3)}\langle J\phi_1,J\phi_4\rangle_{L^2(\mathbb{R}^3)}. \tag{89}$$

If we denote by U the action of the Poincaré group on $L^2(V_0^-)$ with invariant measure $d\nu(\mathbf{k})=d(\mathbf{k}\cdot\mathbf{q}_0)d(\mathbf{k}\cdot\mathbf{u}_0)d(\mathbf{k}\cdot\mathbf{v}_0)/|\mathbf{k}\cdot\mathbf{q}_0|$ corresponding to the same helicity as the representation U on $L^2(V_0^+)$, then the Heisenberg operators are computed to have the following covariance with respect to our section of the Poincaré group:

Theorem 7.1: For $\mathbf{x}=(\mathbf{a}+\mathbb{R}\mathbf{p},\mathbf{p})$, $\sigma(\mathbf{x})=(\mathbf{a}',A_{\mathbf{p}})$, $\mathbf{a}'=\mathbf{a}-(\mathbf{a}\cdot\mathbf{q}_{\mathbf{p}})\mathbf{p}$ (*hence* $\mathbf{a}'\cdot\mathbf{q}_0=0$), *then*

$$U(\sigma(\mathbf{x}))^{-1}J^{-1}W(0,l(\mathbf{r}'),j(\mathbf{s}))JU(\sigma(\mathbf{x}))=e^{i\mathbf{a}'\cdot\mathbf{s}}J^{-1}W(0,l(A_{\mathbf{p}}^{-1}\mathbf{r}'),j(A_{\mathbf{p}}^{-1}\mathbf{s}))J. \tag{90}$$

We may now reexpress the expected values of the phase space localization operators as follows:

$$\begin{aligned}
&\langle\phi_2,T_\eta(\mathbf{x})\phi_1\rangle_{L^2(V_0^+)}\\
&\quad=\langle U(\sigma(\mathbf{x}))\eta,\phi_1\rangle_{L^2(V_0^+)}\langle\phi_1,U(\sigma(\mathbf{x}))\eta\rangle_{L^2(V_0^+)}\\
&\quad=\langle JU(\sigma(\mathbf{x}))\eta,J\phi_1\rangle_{L^2(\mathbb{R}^3)}\langle J\phi_1,JU(\sigma(\mathbf{x}))\eta\rangle_{L^2(\mathbb{R}^3)}\\
&\quad=\int_{\mathbb{R}^6}d(\mathbf{r}'\cdot\mathbf{p}_0)d(\mathbf{r}'\cdot\mathbf{u}_0)d(\mathbf{r}'\cdot\mathbf{v}_0)d(\mathbf{s}\cdot\mathbf{q}_0)d(\mathbf{s}\cdot\mathbf{u}_0)d(\mathbf{s}\cdot\mathbf{v}_0)\\
&\qquad\times\langle J\phi_2,W(0,l(\mathbf{r}'),j(\mathbf{s}))J\phi_1\rangle_{L^2(\mathbb{R}^3)}\langle W(0,l(\mathbf{r}'),j(\mathbf{s}))JU(\sigma(\mathbf{x}))\eta,JU(\sigma(\mathbf{x}))\eta\rangle_{L^2(\mathbb{R}^3)}\\
&\quad=\int_{\mathbb{R}^6}d(\mathbf{r}'\cdot\mathbf{p}_0)d(\mathbf{r}'\cdot\mathbf{u}_0)d(\mathbf{r}'\cdot\mathbf{v}_0)d(\mathbf{s}\cdot\mathbf{q}_0)d(\mathbf{s}\cdot\mathbf{u}_0)d(\mathbf{s}\cdot\mathbf{v}_0)\\
&\qquad\times\langle J\phi_2,W(0,l(\mathbf{r}'),j(\mathbf{s}))J\phi_1\rangle_{L^2(\mathbb{R}^3)}e^{-i\mathbf{a}'\cdot\mathbf{s}}\langle W(0,l(A_{\mathbf{p}}^{-1}\mathbf{r}'),j(A_{\mathbf{p}}^{-1}\mathbf{s}))J\eta,J\eta\rangle_{L^2(\mathbb{R}^3)}
\end{aligned}$$

$$
\begin{aligned}
&= \int_{\mathbb{R}^6} d(\mathbf{r}'\cdot\mathbf{p}_0)d(\mathbf{r}'\cdot\mathbf{u}_0)d(\mathbf{r}'\cdot\mathbf{v}_0)d(\mathbf{s}\cdot\mathbf{q}_0)d(\mathbf{s}\cdot\mathbf{u}_0)d(\mathbf{s}\cdot\mathbf{v}_0)e^{-il(\mathbf{a}')\cdot j(\mathbf{s})} \\
&\quad\times\langle J\phi_2, W(0,l(\mathbf{r}'-\mathbf{q}_\mathbf{p}),j(\mathbf{s}))J\phi_1\rangle_{L^2(\mathbb{R}^3)} \\
&\quad\times\langle W(0,l(A_\mathbf{p}^{-1}(\mathbf{r}'-\mathbf{q}_\mathbf{p})),j(A_\mathbf{p}^{-1}\mathbf{s}))J\eta, J\eta\rangle_{L^2(\mathbb{R}^3)},
\end{aligned}
\tag{91}
$$

where we have introduced the shift $\mathbf{r}'\to\mathbf{r}'-\mathbf{q}_\mathbf{p}$, $\mathbf{q}_\mathbf{p}=A_\mathbf{p}\mathbf{q}_0$, in order to ''center'' the last factor in $j(V_0^+)$.

Next, as in the informational completeness proof for the affine group,[40] we introduce a ''chirp,'' c. Define

$$
c(\mathbf{t}) = e^{i\pi\mathbf{t}\cdot\mathbf{t}}, \quad \mathbf{t}\in\mathbb{R}^3. \tag{92}
$$

Take

$$
J\eta = cg, \quad \text{some } g\in L^2(\mathbb{R}^3). \tag{93}
$$

Then

$$
\begin{aligned}
&\langle W(0,l(A_\mathbf{p}^{-1}(\mathbf{r}'-\mathbf{q}_\mathbf{p}),j(A_\mathbf{p}^{-1}\mathbf{s})))J\eta, J\eta\rangle_{L^2(\mathbb{R}^3)} \\
&\quad=\langle W(0,l(A_\mathbf{p}^{-1}(\mathbf{r}'-\mathbf{q}_\mathbf{p}),j(A_\mathbf{p}^{-1}\mathbf{s})))cg, cg\rangle_{L^2(\mathbb{R}^3)} \\
&\quad=\int_{\mathbb{R}^3} d^3\mathbf{t}\overline{c(\mathbf{t})g(\mathbf{t})}e^{-i\pi(A_\mathbf{p}^{-1}(\mathbf{r}'-\mathbf{q}_\mathbf{p}))\cdot A_\mathbf{p}^{-1}\mathbf{s}}e^{i2\pi(A_\mathbf{p}^{-1}(\mathbf{r}'-\mathbf{q}_\mathbf{p}))\cdot(j^{-1}\mathbf{t}+A_\mathbf{p}^{-1}\mathbf{s})}c(\mathbf{t}+j(\mathbf{s}))g(\mathbf{t}+j(\mathbf{s})) \\
&\quad=\langle W(0,l(A_\mathbf{p}^{-1}(\mathbf{r}'-\mathbf{q}_\mathbf{p})+j(A_\mathbf{p}^{-1}\mathbf{s}),j(A_\mathbf{p}^{-1}\mathbf{s})))g, g\rangle_{L^2(\mathbb{R}^3)} \\
&\quad=\langle W(0,l(A_\mathbf{p}^{-1}\mathbf{r}'-\mathbf{q}_0)+j(A_\mathbf{p}^{-1}\mathbf{s}),j(A_\mathbf{p}^{-1}\mathbf{s}))g, g\rangle_{L^2(\mathbb{R}^3)}.
\end{aligned}
\tag{94}
$$

Finally, also as in the informational completeness proof for the affine group, we show that by replacing η with a delta sequence $\{\eta_\lambda\}$, we may isolate the Fourier transform of all Wigner coefficients $\langle W(0,l(A_\mathbf{p}^{-1}\mathbf{r}' - \mathbf{q}_0) + j(A_\mathbf{p}^{-1}\mathbf{s}),j(A_\mathbf{p}^{-1}))g, g\rangle_{L^2(\mathbb{R}^3)}$. As an example, if one takes $g=g_\lambda\in L^2(\mathbb{R}^3)$,

$$
g_\lambda(\mathbf{t}) = Ne^{-\pi\mathbf{t}\cdot\mathbf{t}/\lambda^2}, \tag{95}
$$

N a normalization constant, then one obtains

$$
\begin{aligned}
&\langle W(0,l(A_\mathbf{p}^{-1}\mathbf{r}'-\mathbf{q}_0)+j(A_\mathbf{p}^{-1}\mathbf{s}),j(A_\mathbf{p}^{-1}\mathbf{s}))g_\lambda, g_\lambda\rangle_{L^2(\mathbb{R}^3)} \\
&\quad=e^{-i\pi j(A_\mathbf{p}^{-1}\mathbf{s})\cdot j(A_\mathbf{p}^{-1}\mathbf{s})/(2\lambda^2)}e^{-\pi\lambda^2\{l[A_\mathbf{p}^{-1}\mathbf{r}'-\mathbf{q}_0]+j(A_\mathbf{p}^{-1}\mathbf{s})\}\cdot\{l[A_\mathbf{p}^{-1}\mathbf{r}'-\mathbf{q}_0]+j(A_\mathbf{p}^{-1}\mathbf{s})\}/2} \\
&\quad=e^{-\pi j(A_\mathbf{p}^{-1}\mathbf{s})\cdot j(A_\mathbf{p}^{-1}\mathbf{s})/(2\lambda^2)}\lambda^{-3}2^{-5/2}K_\lambda(l[A_\mathbf{p}^{-1}\mathbf{r}'-\mathbf{q}_0]+j[A_\mathbf{p}^{-1}\mathbf{s}])
\end{aligned}
\tag{96}
$$

where $\{K_\lambda|\lambda>0,\lambda^{-1}\to0^+\}$ is a delta sequence (Ref. 27, pp. 309–310). Also, in the limit $\lambda^{-1}\to0^+$, the first exponential converges to 1. We therefore have

$$
\begin{aligned}
&\lambda^3 2^{5/2}\langle\phi_2, T_{\eta_\lambda}(\mathbf{x})\phi_1\rangle_{L^2(V_0^+)} \\
&=\lambda^3 2^{5/2}\int_{\mathbb{R}^6} d(\mathbf{r}'\cdot\mathbf{p}_0)d(\mathbf{r}'\cdot\mathbf{u}_0)d(\mathbf{r}'\cdot\mathbf{v}_0)d(\mathbf{s}\cdot\mathbf{q}_0)d(\mathbf{s}\cdot\mathbf{u}_0)d(\mathbf{s}\cdot\mathbf{v}_0)e^{-il(\mathbf{a}')\cdot j(\mathbf{s})} \\
&\quad\times\langle J\phi_2, W(0,l(\mathbf{r}'-\mathbf{q}_\mathbf{p}),j(\mathbf{s}))J\phi_1\rangle_{L^2(\mathbb{R}^3)}\langle W(0,l(A_\mathbf{p}^{-1}(\mathbf{r}'-\mathbf{q}_\mathbf{p}),j(A_\mathbf{p}^{-1}\mathbf{s}))cg_\lambda, cg_\lambda\rangle_{L^2(\mathbb{R}^3)}
\end{aligned}
$$

$$= \int_{\mathbb{R}^6} d(\mathbf{r}'\cdot\mathbf{p_0})d(\mathbf{r}'\cdot\mathbf{u_0})d(\mathbf{r}'\cdot\mathbf{v_0})d(\mathbf{s}\cdot\mathbf{q_0})d(\mathbf{s}\cdot\mathbf{u_0})d(\mathbf{s}\cdot\mathbf{v_0})e^{-il(\mathbf{a}')\cdot j(\mathbf{s})}$$
$$\times\langle J\phi_2, W(0,l(\mathbf{r}'-\mathbf{q_p}),j(\mathbf{s}))J\phi_1\rangle_{L^2(\mathbb{R}^3)} e^{-\pi j(A_{\mathbf{p}}^{-1}\mathbf{s})\cdot j(A_{\mathbf{p}}^{-1}\mathbf{s})/(2\lambda^2)}$$
$$\times K_\lambda(l[A_{\mathbf{p}}^{-1}\mathbf{r}'-\mathbf{q}_0]+j[A_{\mathbf{p}}^{-1}\mathbf{s}])$$
$$\to_{\lambda^{-1}\to 0^+} \int_{\mathbb{R}^3} d(\mathbf{s}\cdot\mathbf{q_0})d(\mathbf{s}\cdot\mathbf{u_0})d(\mathbf{s}\cdot\mathbf{v_0})e^{-il(\mathbf{a}')\cdot j(\mathbf{s})}\langle J\phi_2, W(0,l(\mathbf{r}'\cdot\mathbf{q_p}),j(\mathbf{s}))J\phi_1\rangle_{L^2(\mathbb{R}^3)}. \quad (97)$$

Similarly, for

$$\rho = \sum_k \gamma_k P_{\phi_k}$$

any density operator in $L^2_\nu(V_0^+)$,

$$\lambda^3 2^{5/2}\mathrm{Tr}_{L^2_\nu(V_0^+)}(\rho T_{\eta_\lambda}(\mathbf{x})) \to_{\lambda^{-1}\to 0^+} \int_{\mathbb{R}^3} d(\mathbf{s}\cdot\mathbf{q_0})d(\mathbf{s}\cdot\mathbf{u_0})d(\mathbf{s}\cdot\mathbf{v_0})e^{-il(\mathbf{a}')\cdot j(\mathbf{s})}$$
$$\times \mathrm{Tr}_{L^2(\mathbb{R}^3)}[J\rho J^{-1}W(0,l(\mathbf{r}'-\mathbf{q_p}),j(\mathbf{s}))]. \quad (98)$$

Here $\mathbf{r}'$ is given by

$$l[A_{\mathbf{p}}^{-1}\mathbf{r}'-\mathbf{q}_0]+j[A_{\mathbf{p}}^{-1}\mathbf{s}]=0; \quad (99)$$

i.e.,

$$(A_{\mathbf{p}}^{-1}\mathbf{r}'\cdot\mathbf{p_0}+1, -A_{\mathbf{p}}^{-1}\mathbf{r}'\cdot\mathbf{u_0}, -A_{\mathbf{p}}^{-1}\mathbf{r}'\cdot\mathbf{v_0})+(A_{\mathbf{p}}^{-1}\mathbf{s}\cdot\mathbf{q_0}, A_{\mathbf{p}}^{-1}\mathbf{s}\cdot\mathbf{u_0}, A_{\mathbf{p}}^{-1}\mathbf{s}\cdot\mathbf{v_0})=0; \quad (100)$$

so,

$$\mathbf{r}'\cdot\mathbf{p_0} = (\mathbf{p}\cdot\mathbf{q_0})^{-1}[1+(\mathbf{r}'\cdot\mathbf{u_0})(\mathbf{p}\cdot\mathbf{u_0})+(\mathbf{r}'\cdot\mathbf{v_0})(\mathbf{p}\cdot\mathbf{v_0})]-\mathbf{s}\cdot\mathbf{q_0},$$
$$\mathbf{r}'\cdot\mathbf{u_0} = \mathbf{s}\cdot\mathbf{u_0}-(\mathbf{p}\cdot\mathbf{u_0})(\mathbf{s}\cdot\mathbf{q_0})(\mathbf{p}\cdot\mathbf{q_0})^{-1}, \quad (101)$$
$$\mathbf{r}'\cdot\mathbf{v_0} = \mathbf{s}\cdot\mathbf{v_0}-(\mathbf{p}\cdot\mathbf{v_0})(\mathbf{s}\cdot\mathbf{q_0})(\mathbf{p}\cdot\mathbf{q_0})^{-1}.$$

Hence

$$l(\mathbf{r}'-\mathbf{q_0}) = (-\mathbf{p}\cdot\mathbf{q_0}+(\mathbf{p}\cdot\mathbf{q_0})^{-1}+(\mathbf{p}\cdot\mathbf{q_0})^{-1}[(\mathbf{s}'\cdot\mathbf{u_0})(\mathbf{p}\cdot\mathbf{u_0})+(\mathbf{s}'\cdot\mathbf{v_0})(\mathbf{p}\cdot\mathbf{v_0})]-(\mathbf{s}\cdot\mathbf{q_0})$$
$$\times(\mathbf{p}\cdot\mathbf{q_0})^{-2}[(\mathbf{p}\cdot\mathbf{u_0})^2+(\mathbf{p}\cdot\mathbf{v_0})^2]-\mathbf{s}\cdot\mathbf{q_0},\ \mathbf{s}\cdot\mathbf{u_0}-(\mathbf{p}\cdot\mathbf{u_0})(\mathbf{s}\cdot\mathbf{q_0})(\mathbf{p}\cdot\mathbf{q_0})^{-1},$$
$$\mathbf{s}\cdot\mathbf{v_0}-(\mathbf{p}\cdot\mathbf{v_0})(\mathbf{s}\cdot\mathbf{q_0})(\mathbf{p}\cdot\mathbf{q_0})^{-1}). \quad (102)$$

Therefore, the map $(\mathbf{p},\mathbf{s})\mapsto(l(A_{\mathbf{p}}^{-1}\mathbf{r}'-\mathbf{q}_0), j(\mathbf{s}))$, $V_0^+\times\mathbb{R}^4\to\mathbb{R}^6$ is surjective, and all Wigner coefficients $\mathrm{Tr}_{L^2(\mathbb{R}^3)}[J\rho J^{-1}W(0,l(\mathbf{r}'-\mathbf{q_p}),j(\mathbf{s}))]$ may be obtained by Fourier transform. By the informational completeness of these coefficients[40] $J\rho J^{-1}$, and hence ρ, is determined uniquely.

For consistency with the original problem in $L^2_\nu(V_0^+)$, one needs to work with a slightly different delta sequence than this Gaussian net $\{\eta_\lambda\}$ for the informational completeness since none of these η_λ are supported on V_0^+; however, as the example shows, it is enough for the distribution to be centered at $\mathbf{q_p}\in V_0^+$, and this may be accomplished with suitably supported delta sequences.

VIII. EXPLICIT FORMULAS FOR P^η AND W_η^{-1}

To simplify subsequent analysis, we present explicit expressions for P^η and W_η^{-1}.

Theorem 8.1: *Let $f\in L^2_\mu(\mathscr{P}/H_2)$. Define P by*

$$(Pf)(\mathbf{z})\equiv\|C\eta\|^{-2}\int_{\mathscr{P}/H_2} d\mu(\mathbf{x})\langle\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{z}))\eta,\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta\rangle f(\mathbf{x}). \tag{103}$$

Then P is the projection P^η from $L^2_\mu(\mathscr{P}/H_2)$ to the range of W_η.

Proof: (1) $Pf\in$Range of W_η since we may rewrite the integral in (103) in the form

$$\int d\mu(\mathbf{x})f(\mathbf{x})[W_\eta(\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta)](\mathbf{z}).$$

$$(2)\quad (PW_\eta\varphi)(\mathbf{z})=\|C\eta\|^{-2}\int d\mu(\mathbf{x})\langle\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{z}))\eta,\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta\rangle\langle\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta,\varphi\rangle$$
$$=\langle\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{z}))\eta,\varphi\rangle=(W_\eta\varphi)(\mathbf{z}).$$

Therefore P is the identity on the range of W_η.

$$(3)\quad (PPf)(\mathbf{z})=\|C\eta\|^{-2}\int d\mu(\mathbf{x})\langle\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{z}))\eta,\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta\rangle(Pf)(\mathbf{x})$$
$$=\|C\eta\|^{-4}\int d\mu(\mathbf{x})d\mu(\mathbf{y})\langle\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{z}))\eta,\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta\rangle$$
$$\times\langle\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta,\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{y}))\eta\rangle f(\mathbf{y})$$
$$=\|C\eta\|^{-2}\int d\mu(\mathbf{y})\langle\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{z}))\eta,\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{y}))\eta\rangle f(\mathbf{y})$$
$$=(Pf)(\mathbf{z}).$$

Therefore

$$P^2=P.$$

(4) P is an integral operator with kernel K such that $\overline{K(\mathbf{x},\mathbf{y})}=K(\mathbf{y},\mathbf{x})$. Thus

$$P=P^\dagger. \qquad \square$$

Theorem 8.2: *$W_\eta^{-1}:P^\eta L^2_\mu(\mathscr{P}/H_2)\to L^2_\nu(\mathscr{P}/H_1)$ is given by*

$$W_\eta^{-1}(P^\eta f)=N^{-1}\int (P^\eta f)(\mathbf{x})\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta\, d\mu(\mathbf{x}), \tag{104}$$

where $N=\|C\eta\|^2$.

Proof: Recall, $(W_\eta\varphi)(\mathbf{x})=\langle\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta,\varphi\rangle$. Also, since for $f\in L^2_\mu(\mathscr{P}/H_2)$, there exists a unique $\varphi\in L^2_\nu(\mathscr{P}/H_1)$ such that $P^\eta f=W_\eta\varphi$, then for any $\psi\in L^2_\nu(\mathscr{P}/H_1)$ we compute

$$\left\langle\psi,N^{-1}\int (P^\eta f)(\mathbf{x})\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta\, d\mu(\mathbf{x})\right\rangle=\left\langle\psi,N^{-1}\int (W_\eta\varphi)(\mathbf{x})\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta\, d\mu(\mathbf{x})\right\rangle$$
$$=N^{-1}\int (W_\eta\varphi)(\mathbf{x})\overline{(W_\eta\psi)(\mathbf{x})}d\mu(\mathbf{x})=\langle\psi,\varphi\rangle$$
$$=\langle\psi,W_\eta^{-1}P^\eta f\rangle. \qquad \square$$

Theorem 8.3: *For P^{η} and W_{η} as above,*

$$P^{\eta}=\|C\eta\|^{-2}W_{\eta}W_{\eta}^{\dagger}. \tag{105}$$

Proof: From the orthogonality theorem we have

$$[W_{\eta}W_{\eta}^{\dagger}W_{\eta}\varphi](\mathbf{x})=\langle \mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta, W_{\eta}^{\dagger}W_{\eta}\varphi\rangle=\langle W_{\eta}\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta, W_{\eta}\varphi\rangle$$
$$=\|C\eta\|^2\langle \mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta,\varphi\rangle=\|C\eta\|^2[W_{\eta}\varphi](\mathbf{x}).$$

Thus $\|C\eta\|^{-2}W_{\eta}W_{\eta}^{\dagger}$ is the identity on the range of W_{η}. If f is orthogonal to the range of W_{η}, then

$$W_{\eta}W_{\eta}^{\dagger}f(\mathbf{x})=\langle \mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta, W_{\eta}^{\dagger}f\rangle=\langle W_{\eta}\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta, f\rangle=0. \qquad \square$$

With these results, we may present an alternate proof of the integral representation for $U^{\eta,\lambda}$ as intertwined from $U^{\mathbf{p}_o\lambda}$ and given in Theorem 5.3, (74).

Alternative Proof of Theorem 5.3:

$$[U^{\eta,\lambda}(g)(P^{\eta}f\ )](\mathbf{x})=(W_{\eta}U^{\mathbf{p}_o\lambda}(g)W_{\eta}^{-1}P^{\eta}f\ )(\mathbf{x})=\langle \mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta, U^{\mathbf{p}_o\lambda}(g)W_{\eta}^{-1}P^{\eta}f\rangle$$
$$=N^{-1}\left\langle \mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta, U^{\mathbf{p}_o\lambda}(g)\int (P^{\eta}f\ )(\mathbf{y})\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{y}))\eta\, d\mu(\mathbf{y})\right\rangle$$
$$=N^{-1}\int d\mu(\mathbf{y})\langle \mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta, U^{\mathbf{p}_o\lambda}(g)\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{y}))\eta\rangle(P^{\eta}f\ )(\mathbf{y}). \qquad \square$$

Corollary 8.4: Theorem 5.3 (74) may also be written, using Theorem 8.1, to read

$$[U^{\eta,\lambda}(g)(P^{\eta}f\ )](\mathbf{x})=N^{-1}\int d\mu(\mathbf{y})\langle \mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta, U^{\mathbf{p}_o\lambda}(g)\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{y}))\eta\rangle\|C\eta\|^{-2}$$
$$\times\int d\mu(\mathbf{z})\langle \mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{y}))\eta, \mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{z}))\eta\rangle f(\mathbf{z})$$
$$=N^{-1}\int d\mu(\mathbf{z})\langle \mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta, U^{\mathbf{p}_o\lambda}(g)\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{z}))\eta\rangle f(\mathbf{z}). \tag{106}$$

This provides a explicit integral representation.

IX. COVARIANCE ASPECTS OF THE LOCALIZATION OPERATOR

We next determine the covariance properties of the phase space localization operators for the photon and other zero mass particles. For notation, see Sec. V.

Theorem 9.1: $A_{\eta}(\Delta)\varphi = N^{-1}\int_{\Delta}d\mu(\mathbf{y})\langle \mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{y}))\eta,\varphi\rangle \mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{y}))\eta$; *i.e.,*

$$A_{\eta}(\Delta)=N^{-1}\int_{\Delta}d\mu(\mathbf{y})|\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{y}))\eta\rangle\langle \mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{y}))\eta|=N^{-1}\int_{\Delta}d\mu(\mathbf{y})T^{\eta}(\mathbf{y}). \tag{107}$$

Proof: In fact, (107) follows immediately from (80); but for reasons given below, we offer an independent proof here:

$$A_{\eta}(\Delta)\varphi=W_{\eta}^{-1}P^{\eta}A(\Delta)W_{\eta}\varphi=N^{-1}\int_{\mathscr{P}/H_2}d\mu(\mathbf{x})(P^{\eta}A(\Delta)W_{\eta}\varphi)(\mathbf{x})\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta$$

$$
\begin{aligned}
&= N^{-2}\int_{\mathscr{P}/H_2} d\mu(\mathbf{x})\int_{\mathscr{P}/H_2} d\mu(\mathbf{y})\\
&\quad\times\langle \mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta, \mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{y}))\eta\rangle (A(\Delta)W_\eta\varphi)(\mathbf{y})\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta\\
&= N^{-2}\int_{\mathscr{P}/H_2} d\mu(\mathbf{x})\int_{\Delta} d\mu(\mathbf{y})\langle \mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta, \mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{y}))\eta\rangle\\
&\quad\times(W_\eta\varphi)(\mathbf{y})\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta\\
&= N^{-2}\int_{\mathscr{P}/H_2} d\mu(\mathbf{x})\int_{\Delta} d\mu(\mathbf{y})\langle \mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta, \mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{y}))\eta\rangle\\
&\quad\times\langle \mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{y}))\eta,\varphi\rangle\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta\\
&= N^{-2}\int_{\Delta} d\mu(\mathbf{y})\int_{\mathscr{P}/H_2} d\mu(\mathbf{x})\langle \mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{y}))\eta,\varphi\rangle\\
&\quad\times\langle \mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta, \mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{y}))\eta\rangle\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta\\
&= N^{-1}\int_{\Delta} d\mu(\mathbf{y})\langle \mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{y}))\eta,\varphi\rangle\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{y}))\eta. \qquad \square
\end{aligned}
$$

Equation (107) proves that $\Delta\to A_\eta(\Delta)$ is an absolutely continuous POVM with respect to the invariant measure, and A_η has operator density T^η. Then using the theory of integration with respect to a POVM one may establish a quantization scheme.[41] The specific quantization scheme from that theory gives precisely (80). Hence, one could have defined A and A_η by (66) and (68), and then derived the quantization scheme. In contrast, in Sec. V the localization is derived from the quantization scheme (75) and (76). *Theorem* 6.1 shows the equivalence of these two approaches.

Theorem 9.2: *As an operator on* $L^2_\nu(\mathscr{P}/H_1)$, A_η *satisfies*

$$\mathscr{E}U^{\mathbf{p}_o\lambda}(g)\mathscr{E}^{-1}A_\eta(\Delta)\mathscr{E}^{-1}U^{\mathbf{p}_o\lambda}(g)^{-1}\mathscr{E}=A_\eta(g[\Delta]). \tag{108}$$

Proof:

$$
\begin{aligned}
\mathscr{E}U^{\mathbf{p}_o\lambda}(g)\mathscr{E}^{-1}A_\eta(\Delta)\varphi &= \mathscr{E}N^{-1}\int_{\Delta} d\mu(\mathbf{y})\langle \mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{y}))\eta,\varphi\rangle U^{\mathbf{p}_o\lambda}(g\sigma_2(\mathbf{y}))\eta\\
&= \mathscr{E}N^{-1}\int_{y\in\Delta} d\mu(g\cdot\mathbf{y})\langle \mathscr{E}U^{\mathbf{p}_o\lambda}(g^{-1}\sigma_2(g\cdot\mathbf{y}))\eta,\varphi\rangle U^{\mathbf{p}_o\lambda}(\sigma_2(g\cdot\mathbf{y}))\eta\\
&= N^{-1}\int_{g[\Delta]} d\mu(\mathbf{z})\langle \mathscr{E}U^{\mathbf{p}_o\lambda}(g^{-1}\sigma_2(\mathbf{z}))\eta,\varphi\rangle\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{z}))\eta\\
&= N^{-1}\int_{g[\Delta]} d\mu(\mathbf{z})\langle \mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{z}))\eta,\mathscr{E}^{-1}U^{\mathbf{p}_o\lambda}(g)\mathscr{E}\varphi\rangle\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{z}))\eta\\
&= A_\eta(g[\Delta])\mathscr{E}^{-1}U^{\mathbf{p}_o\lambda}(g)\mathscr{E}\varphi.
\end{aligned}
$$

Thus

$$\mathscr{E}U^{\mathbf{p}_o\lambda}(g)\mathscr{E}^{-1}A_\eta(\Delta)=A_\eta(g[\Delta])\mathscr{E}^{-1}U^{\mathbf{p}_o\lambda}(g)\mathscr{E}. \qquad \square$$

Corollary 9.3: $\Delta\to\mathscr{E}^{-1}A_\eta(\Delta)\mathscr{E}^{-1}$ *defines a non-normalized POVM transforming covariantly under* $U^{\mathbf{p}_o\lambda}$:

$$U^{\mathbf{p}_o\lambda}(g)(\mathscr{E}^{-1}A_\eta(\Delta)\mathscr{E}^{-1})U^{\mathbf{p}_o\lambda}(g^{-1})=\mathscr{E}^{-1}A_\eta(g[\Delta])\mathscr{E}^{-1}. \tag{109}$$

Proof: From (108), the covariance follows. For the normalization

$$\mathscr{E}^{-1}A_\eta(\mathscr{P}/H_2)\mathscr{E}^{-1}=\mathscr{E}^{-2}, \quad \text{not } \mathbf{1}. \qquad \square$$

Remark: Equation (109) may be reexpressed

$$\mathscr{E}^{-1}A_\eta(\Delta)\mathscr{E}^{-1}\varphi=N^{-1}\int_\Delta d\mu(\mathbf{y})\langle U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{y}))\eta,\varphi\rangle U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{y}))\eta, \tag{110}$$

or

$$\mathscr{E}^{-1}A_\eta(\Delta)\mathscr{E}^{-1}=N^{-1}\int_\Delta d\mu(\mathbf{y})|U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{y}))\eta\rangle\langle U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{y}))\eta|. \tag{111}$$

It is not known at this time if this family of phase space localization operators reduces, by marginality, to the family of configuration space localization operators of Kraus[42] in the photon case.

X. THE ANALOG OF THE WIGNER TRANSFORM

We define a transform in analogy to the Wigner transform of nonrelativistic massive quantum theory:

Definition: The Wigner transform will be defined in the massless Poincaré case by

$$\rho\mapsto\{\mathrm{Tr}(\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))C^{-2}\rho)|\mathbf{x}\in\mathscr{P}/H_2\}, \tag{112}$$

and the Weyl dequantization by

$$B\mapsto\{\mathrm{Tr}(\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))B)|\mathbf{x}\in\mathscr{P}/H_2\} \tag{113}$$

where B is any operator such that almost every $\mathrm{Tr}(\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))B)$ exists.

Remark: As in the massive, nonrelativistic case, the right-hand side of (112) does not generally define a probability density, and (112) does not define a proper dequantization scheme.

Theorem 10.1: *Let $\eta\in D(C^2)$ and let η be admissible. Then the one-dimensional projection $P_{C^2\eta}$ is given by*

$$P_{C^2\eta}=\|C^2\eta\|^{-2}\int_{\mathscr{P}/H_2}\langle\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x})),C^2\eta\rangle\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))d\mu(\mathbf{x}). \tag{114}$$

Proof: Let $\psi,\ \varphi\in D(\mathscr{E})$. Then

$$\begin{aligned}&\langle\psi,\|C^2\eta\|^{-2}\int_{\mathscr{P}/H_2}\langle\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta,C^2\eta\rangle\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))d\mu(\mathbf{x})\varphi\rangle\\&=\|C^2\eta\|^{-2}\int_{\mathscr{P}/H_2}d\mu(\mathbf{x})\langle\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta,C^2\eta\rangle\langle\psi,\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\varphi\rangle\\&=\|C^2\eta\|^{-2}\langle C^2\eta,\varphi\rangle\langle\psi,C^2\eta\rangle=\langle\psi,P_{C^2\eta}\varphi\rangle\end{aligned}$$

for a dense set of φ,ψ. Hence, it holds for all $\varphi,\ \psi\in L^2_\nu(\mathscr{P}/H_1)$. $\square$

Theorem 10.2: *Let ρ be a density operator in $L^2_\nu(\mathscr{P}/H_1)$. Then*

$$\rho=\int_{\mathscr{P}/H_2}\mathrm{Tr}(\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))C^{-2}\rho)\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))d\mu(\mathbf{x}); \tag{115}$$

i.e., $\{\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))C^{-2}|\mathbf{x}\in\mathscr{P}/H_2\}$ *is informationally complete in* $L^2_\nu(\mathscr{P}/H_1)$.

Proof: Begin with $\rho=\Sigma\rho_i P_{\psi_i}$, ψ_i in the range of C^2. Then, write $\psi_i=C^2\varphi_i$:

$$\begin{aligned}\rho&=\sum_i \rho_i\|C^2\varphi_i\|^{-2}\int_{\mathscr{P}/H_2}\langle\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\varphi_i,C^2\varphi_i\rangle\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))d\mu(\mathbf{x})\\&=\sum_i \rho_i\|\psi_i\|^{-2}\int_{\mathscr{P}/H_2}\langle\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))C^{-2}\psi_i,\psi_i\rangle\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))d\mu(\mathbf{x})\\&=\int_{\mathscr{P}/H_2}\mathrm{Tr}(\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))C^{-2}\sum_i \rho_i\|\psi_i\|^{-2}|\psi_i\rangle\langle\psi_i|)\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))d\mu(\mathbf{x})\\&=\int_{\mathscr{P}/H_2}\mathrm{Tr}(\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))C^{-2}\rho)\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))d\mu(\mathbf{x}).\end{aligned}$$ □

This theorem does not carry direct physical meaning since physical observables are self-adjoint or symmetric operators, while the operators $\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))C^{-2}$ are not even symmetric.

Theorem 10.3:

$$\mathrm{Tr}(\rho B)=\int_{P/H_2}\mathrm{Tr}(\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))C^{-2}\rho)\mathrm{Tr}(\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))B)d\mu(\mathbf{x}); \tag{116}$$

that is, the quantum expectation and the analog of the classical expectation coincide.

Theorem 10.4: *For section* σ_2 *as in (39) and (40), operators* $U^{\mathbf{p}_o\lambda}$ *as in (25), and* $\mathscr{E}$ *as in (48) and (53), the set*

$$\{\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))|\mathbf{x}\in\mathscr{P}/H_2\} \tag{117}$$

is informationally complete in $L^2_\nu(\mathscr{P}/H_1)$. *Furthermore, the reconstruction of vector states* P_ψ *from the set* $\{\mathrm{Tr}(P_\psi\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x})))|\mathbf{x}\in\mathscr{P}/H_2\}$ *is particularly simple.*

Proof: Informational completeness follows from Theorem 10.2 and the invertibility of C^{-2}.

For the reconstruction of vector states, let $\{e_j|j=1,2,3,...\}$ be an orthonormal basis for $L^2_\nu(\mathscr{P}/H_1)$. Then

$$\begin{aligned}&\int_{\mathscr{P}/H_2}d\mu(\mathbf{x})\langle e_j,\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta\rangle\mathrm{Tr}(P_\psi\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x})))\\&\quad=\int_{\mathscr{P}/H_2}d\mu(\mathbf{x})\langle e_j,\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta\rangle\langle\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\psi,\psi\rangle\\&\quad=\langle\psi,C^2\eta\rangle\langle e_j,\psi\rangle.\end{aligned}$$

Since

$$\langle\psi,C^2\eta\rangle\psi=\sum_j\langle\psi,C^2\eta\rangle\langle e_j,\psi\rangle e_j,$$

one can construct normalized vector ψ up to a constant phase from the set

$$\{\mathrm{Tr}(P_\psi\mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x})))|\mathbf{x}\in\mathscr{P}/H_2\}.$$ □

This approach also gives a formula for reconstructing P_ψ from its Wigner transform (112). In particular,

$$\int_{\mathscr{P}/H_2} d\mu(\mathbf{x})\langle e_j, \mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta\rangle \mathrm{Tr}(P_\psi \mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x})))$$

$$= \int_{\mathscr{P}/H_2} d\mu(\mathbf{x})\langle e_j, \mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))\eta\rangle\langle \mathscr{E}U^{\mathbf{p}_o\lambda}(\sigma_2(\mathbf{x}))C^{-2}\psi, \psi\rangle = \langle \psi, \eta\rangle\langle e_j, \psi\rangle, \tag{118}$$

from which we can determine normalized ψ up to a constant phase, and hence P_ψ.

XI. COMPARISON WITH OTHER RESULTS

The methods used here are closest to those of Ali and Antoine[38,43] and Ali, Antoine, and Gazeau[44] in their treatment of the Poincaré group in two dimensions, but differ in several essential ways. First of all, in our treatment we intertwine irreducible representations with representations in $L^2_\mu(\mathscr{P}/H_2)$, but not with the left-quasiregular representation on $L^2_\mu(\mathscr{P}/H_2)$. Second, our orthogonality result (54) exhibits a factoring into a factor involving only the resolution generators and a second term that is independent of the resolution generators; this factorization plays a role in the proof of informational completeness. Furthermore, their treatment of the Poincaré group in two dimensions deals only with the massive case with a recent extension to the massless case,[45] while the present work deals with the massless case in the full four dimensions. In a sequel paper, we shall treat the massive case as well, but even there our two approaches will differ, this latter difference occurring since we use methods parallel to the general scheme employed to discuss informational completeness of Wigner coefficients and localization operators in the Heisenberg, affine, and Galilei groups;[40] in that setting, the presence of nontrivial cocycles requires a modification of the standard process. In the four-dimensional Poincaré group there are no nontrivial cocycles; however, for the two-dimensional Poincaré group, there is a one-dimensional manifold of inequivalent multiplier representations based on distinct cocycles (Ref. 46, pp. 478–484). For this reason, two-dimensional Galilean theory is closer to the two-dimensional Poincaré theory than the corresponding four-dimensional cases (and may be related by group contraction). Ali *et al.* discuss only the representation based on the trivial multiplier representation. The difference is in the nature of the approaches, ours beginning with the identification of the physically relevant and classically motivated homogeneous spaces, after which all related induced representations play a role. Fourth, the inclusion of all three spatial dimensions allows for spin and helicity. The nontrivial restrictions on the resolution generators under rotations that derive from the intertwining property are inherently connected with the identification of the value of *spin/helicity*. This simply cannot be discussed in the two-dimensional setting.

Points of similarity of their approach and ours are also manifold and include: the operator $\mathscr{E}$ appearing in (48) and (50), as well as the choice between the localization operator A_η transforming under a nonunitary representation of the group $\mathscr{P}$ [Eq. (108)] versus $\mathscr{E}^{-1}A_\eta\mathscr{E}^{-1}$ transforming covariantly under the ''proper'' unitary representation but being normalized to $\mathscr{E}^{-2}$ [Eq. (109)] are both consistent with the results of Ali *et al.* and would not be anticipated from results of others known to us.

Our approach here is different in spirit from all prior treatments based on deforming results in the massive case to massless ones by taking ''suitable'' limits. The treatment of the massive case, in particular, will be seen in the sequel to have no terms corresponding to the $\mathscr{E}$ factors here; therefore, the essential introduction of this $\mathscr{E}$ will not be obtained by any such limiting process, nor will the travelling coordinate system introduced in (64) arise in such a limit. In fact, essential

structural differences should occur between the massive and massless cases, since the geometry of the corresponding homogeneous spaces is different because the little groups for the two cases are different.

APPENDIX: CHOICE OF CROSS SECTION FOR $SL(2,\mathbb{C})/[SL(2,\mathbb{C})]_{(1,0,0,1)}$

If $a\neq 0$, then the element $\left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right)$ of $SL(2,\mathbb{C})$ may be factored uniquely in the form

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} |a| & 0 \\ |a|ca^{-1} & |a|^{-1} \end{pmatrix} \begin{pmatrix} a|a|^{-1} & b|a|^{-1} \\ 0 & a^{-1}|a| \end{pmatrix}. \tag{A1}$$

The last factor is in $H_1=[SL(2,\mathbb{C})]_{(1,0,0,1)}$.

The set of elements for which this decomposition fails ($a=0$) is of Haar measure zero; consequently, we may impose the condition $a\neq 0$ when integrating over the group.

Henceforth, for $A=\left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right)$, we define

$$\theta_A \equiv a|a|^{-1} \tag{A2}$$

and almost everywhere choose the canonical projection π_0 and Borel section σ_0 by

$$\pi_0 : SL(2,\mathbb{C}) \to SL(2,\mathbb{C})/[SL(2,\mathbb{C})]_{(1,0,0,1)}, \tag{A3}$$

$$\pi_0(A) = \pi_0\left(\begin{pmatrix} a & b \\ c & d \end{pmatrix}\right) = \begin{pmatrix} a & b \\ c & d \end{pmatrix} H_1 = \begin{pmatrix} |a| & 0 \\ |a|ca^{-1} & |a|^{-1} \end{pmatrix} H_1$$

$$\equiv \left\{ \begin{pmatrix} |a| & 0 \\ |a|ca^{-1} & |a|^{-1} \end{pmatrix} \begin{pmatrix} \theta & z \\ 0 & \theta^{-1} \end{pmatrix}, \ |\theta|=1, z\in\mathbb{C} \right\};$$

$$\sigma_0 : SL(2,\mathbb{C})/[SL(2,\mathbb{C})]_{(1,0,0,1)} \to SL(2,\mathbb{C}),$$

$$\sigma_0 = \pi_0\left(\begin{pmatrix} a & b \\ c & d \end{pmatrix}\right) \mapsto \sigma_0 \circ \pi_0\left(\begin{pmatrix} a & b \\ c & d \end{pmatrix}\right) \equiv \begin{pmatrix} |a| & 0 \\ |a|ca^{-1} & |a|^{-1} \end{pmatrix}. \tag{A4}$$

We may parametrize the cosets with the parameters $ca^{-1}\in\mathbb{C}$, $|a|\in\mathbb{R}^+$ up to a set of measure zero. Next, set

$$\mathbf{p}_0 = \begin{pmatrix} 2 & 0 \\ 0 & 0 \end{pmatrix} \tag{A5}$$

and

$$\mathbf{p} \equiv A\cdot\mathbf{p}_0. \tag{A6}$$

Then

$$\begin{pmatrix} p^0+p^3 & p^1-ip^2 \\ p^1+ip^2 & p^0-p^3 \end{pmatrix} = A\begin{pmatrix} 2 & 0 \\ 0 & 0 \end{pmatrix}A^\dagger = 2\begin{pmatrix} |a|^2 & a\overline{c} \\ \overline{ac} & |c|^2 \end{pmatrix}; \tag{A7}$$

so;

$$\begin{gathered} p^0>0, \quad \mathbf{p}\cdot\mathbf{p}=0, \\ p^0+p^3=2|a|^2, \quad p^1+ip^2=2\overline{ac}. \end{gathered} \tag{A8}$$

Conversely, every future-pointing null vector $\mathbf{p}\in\mathbb{R}^4$ uniquely determines a class in $\mathrm{SL}(2,\mathbb{C})/\mathrm{SL}(2,\mathbb{C})_{(1,0,0,1)}$ and a unique $\sigma_0\circ\pi_0(A)$. For such $\mathbf{p}$ we define $A_{\mathbf{p}}$ by

$$A_{\mathbf{p}}\equiv\begin{pmatrix}((p^0+p^3)/2)^{1/2} & 0\\ (p^1+ip^2)/(2(p^0+p^3))^{1/2} & (2/(p^0+p^3))^{1/2}\end{pmatrix}=\sigma_0\circ\pi_0(A). \tag{A9}$$

In this way, we may identify $\mathrm{SL}(2,\mathbb{C})/\mathrm{SL}(2,\mathbb{C})_{(1,0,0,1)}$ with V_0^+. From (A9),

$$A_{\mathbf{p}}^{-1}\equiv\begin{pmatrix}(2/(p^0+p^3))^{1/2} & 0\\ (-p^1-ip^2)/(2(p^0+p^2))^{1/2} & ((p^0+p^3)/2)^{1/2}\end{pmatrix}\equiv A_{\tilde{\mathbf{p}}}, \tag{A10}$$

where

$$\begin{aligned}\tilde{p}^{\,0}+\tilde{p}^{\,3}&=4(p^0+p^3)^{-1},\\ \tilde{p}^{\,1}&=-2p^1(p^0+p^3)^{-1},\\ \tilde{p}^{\,2}&=-2p^2(p^0+p^3)^{-1},\\ \tilde{p}^{\,0}-\tilde{p}^{\,3}&=p^0-p^3.\end{aligned} \tag{A11}$$

From (A11), the Jacobian (62) follows.

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Multi-periodic coherent states and the WKB exactness

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We construct the path integral formula in terms of a ''multi-periodic'' coherent state as an extension of the Nielsen–Rohrlich formula for spin. We make an exact calculation of the formula and show that, when a parameter corresponding to the magnitude of spin becomes large, the leading order term of the expansion coincides with the exact result. We also give an explicit correspondence between the trace formula in the multi-periodic coherent state and the one in the ''generalized'' coherent state. © *1996 American Institute of Physics.* [S0022-2488(96)03911-4]

I. INTRODUCTION

Spin, a system being subject to the SU(2) group, is a simple and pedagogical model so that many useful results and discussions have been made. In the framework of the path integral, it is applied to, for example, the explanation of the Fermi–Bose transmutation.[1–3]

In quantum mechanics there exist few systems which are solved exactly, so various approximations such as the perturbation or the variational method have been invented to give useful results. The most suitable one in the path integral formalism is the WKB approximation, which can be stated as the stationary phase method in quantum mechanics. Although the WKB approximation is useful, the result differs from the exact one in general. However, it is known that there exist some systems in which they coincide with each other, for example, the harmonic oscillator: this is a kind of trivial example since the approximation gives the same form with the original action which is the Gaussian to be integrated exactly.

In the stationary phase approximation in finite dimensions, the conditions that an approximation gives the exact result of the integral has been discovered by Duistermaat and Heckman,[4,5] so that the fact is called as the DH theorem.

Recently there have been some discussions[6–9] that the WKB approximation gives the exact result (we call this fact the **WKB exactness**) in the trace formula of spin in connection with the DH theorem. However, there are some unsatisfactory points in the preceding discussions, for example, the manner of construction of the trace formula and the use of the continuum path integral. By paying attention to the above points, we have shown the WKB exactness in terms of the spin coherent state[10] with the form

$$Z=\lim_{N\to\infty}\int\prod_{i=1}^{N}d\mu(\xi_i,\xi_i^*)\exp\left[iJ\sum_{k=1}^{N}\left\{2i\,\log\left(\frac{1+\xi_k^*\xi_k}{1+\xi_k^*\xi_{k-1}}\right)+\Delta th\,\frac{1-\xi_k^*\xi_{k-1}}{1+\xi_k^*\xi_{k-1}}\right\}\right]\Bigg|_{\xi_N=\xi_0},\tag{1.1}$$

where J is the magnitude of spin and h is the external magnetic field. We have also extended the WKB exactness in terms of the ''generalized'' coherent state.[11]

As for path integrals for spin, there exists another expression, the Nielsen–Rohrlich formula,[12,13] which is constructed in terms of the periodic coherent state. Its trace formula is

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$$Z=\sum_{n=-\infty}^{\infty}\lim_{N\to\infty}\int_{2n\pi}^{2(n+1)\pi}\frac{d\varphi_N}{2\pi}\int_{-\infty}^{\infty}\prod_{i=1}^{N-1}\frac{d\varphi_i}{2\pi}\int_{-J-1/2+\varepsilon}^{J+1/2-\varepsilon}\prod_{j=1}^{N}\frac{dp_j}{2\pi}$$
$$\times\exp\left[i\sum_{k=1}^{N}(p_k+J)(\varphi_k-\varphi_{k-1})-\Delta t\sum_{k=1}^{N}h(k)p_k\right]\Bigg|_{\varphi_N=\varphi_0+2n\pi}, \tag{1.2}$$

where ε is positive infinitesimal. On the other hand, the trace formula of the spin coherent state is (1.1). The two representations look quite different despite starting from the same Hamiltonian. The integration domain of ps and the existence of infinite sum lead to the observation that the phase space is considered to be the ''punctured sphere'', while the phase space of the spin coherent state is $CP^1\simeq S^2$, the ''sphere.'' In the latter case, the WKB exactness holds. However, in the former case, from (1.2), the equations of motion are

$$\begin{aligned}\varphi_k-\varphi_{k-1}&=h(k)\Delta t,\\ p_k-p_{k-1}&=0,\end{aligned} \tag{1.3}$$

which does not meet the boundary condition $\varphi_N=\varphi_0+2n\pi$ in a general $h(k)$. Thus there seems to be no classical solutions. We have clarified this puzzle in Ref. 14. The phase space of the Nielsen–Rohrlich formula is not ''punctured'' and the appearance of the infinite sum is superficial. The trace formula is equivalent to that of the spin coherent state. By rewriting (1.2) to

$$Z=\sum_{n=-\infty}^{\infty}e^{i2n\pi J}\lim_{N\to\infty}\int_{2n\pi}^{2(n+1)\pi}\frac{d\varphi_N}{2\pi}\int_{-\infty}^{\infty}\prod_{i=1}^{N-1}\frac{d\varphi_i}{2\pi}\int_{0}^{\pi}\prod_{j=1}^{N}\lambda\sin\theta_j d\theta_j$$
$$\times\exp\left\{i\lambda\sum_{k=1}^{N}\cos\theta_k(\varphi_k-\varphi_{k-1}-h\Delta t)\right\}\Bigg|_{\varphi_N=\varphi_0+2n\pi}, \tag{1.4}$$

the WKB exactness also holds in this case.

Although the extension of the Nielsen–Rohrlich formula has been attempted,[15] the explicit form has not yet been obtained. In this paper we construct the path integral formula and clarify the WKB exactness.

The contents of this paper are as follows. In Sec. II, we define the ''multi-periodic'' coherent state to construct the path integral formula. In Sec. III, we make an exact calculation of the trace formula. We establish a relationship with the trace formula to that of the generalized coherent state in Sec. IV. Then we perform the WKB approximation to confirm the WKB exactness in Sec. V. The last section is devoted to the discussion.

II. CONSTRUCTION OF THE TRACE FORMULA

First we make up the $u(N+1)$ algebra and the representation space by means of $N+1$ harmonic oscillators. The method is called the Schwinger boson method.[16] The commutation relations of oscillators are

$$[a_\alpha,\ a_\beta^\dagger]=\delta_{\alpha\beta},\quad [a_\alpha,\ a_\beta]=[a_\alpha^\dagger,\ a_\beta^\dagger]=0,\quad \alpha,\beta=1,\ldots,N+1, \tag{2.1}$$

and the Fock space is

$$\{|m^1,\ldots,m^{N+1}\rangle\},\quad m^\alpha=0,1,2,\ldots,\ \text{with}\ \alpha=1,\ldots,N+1,$$

$$|m^1,\ldots,m^{N+1}\rangle\equiv\frac{1}{\sqrt{m^1!\cdots m^{N+1}!}}(a_1^\dagger)^{m^1}\cdots(a_{N+1}^\dagger)^{m^{N+1}}|0\rangle,\tag{2.2}$$

$$a_\alpha|0\rangle=0.$$

By putting

$$E_{\alpha\beta}=a_\alpha^\dagger a_\beta,\quad \alpha,\beta=1,\ldots,N+1,\tag{2.3}$$

the $u(N+1)$ algebra

$$[E_{\alpha\beta},\,E_{\gamma\delta}]=\delta_{\beta\gamma}E_{\alpha\delta}-\delta_{\delta\alpha}E_{\gamma\beta}\tag{2.4}$$

is realized.

The Fock space (2.2) is too large to be the representation space of $U(N+1)$. We restrict the representation space with the identity operator

$$\mathbf{1}_Q\equiv\sum_{\|m\|=Q}|m^1,\ldots,m^{N+1}\rangle\langle m^1,\ldots,m^{N+1}|,\tag{2.5}$$

where we have used the abbreviation

$$\|m\|\equiv\sum_{\alpha=1}^{N+1}m^\alpha.\tag{2.6}$$

Now we introduce the highest weight vector defined by

$$\begin{aligned}&E_{N+1,N+1}|Q;N+1\rangle\rangle=Q|Q;N+1\rangle\rangle,\\&E_{N+1,\alpha}|Q;N+1\rangle\rangle=0,\quad \alpha=1,\ldots,N,\end{aligned}\tag{2.7}$$

where $E_{\alpha,N+1}(E_{N+1,\alpha})$ is the lowering (raising) operator of $u(N+1)$. We can identify

$$|Q;N+1\rangle\rangle\equiv|\overset{1}{0},\ldots,\overset{N}{0},\ \overset{N+1}{Q}\ \rangle.\tag{2.8}$$

The ''multi-periodic'' coherent state is defined by

$$\begin{aligned}|\boldsymbol{\varphi}\rangle\equiv|\varphi^1,\varphi^2,\ldots,\varphi^N\rangle&\equiv\frac{1}{(2\pi)^{N/2}}\sum_{\|m\|=Q}\sqrt{\frac{m^{N+1}!}{m^1!\cdots m^N!Q!}}\prod_{\alpha=1}^{N}(e^{-im^\alpha\varphi^\alpha}(E_{\alpha,N+1})^{m^\alpha})|Q;N+1\rangle\rangle\\&=\frac{1}{(2\pi)^{N/2}}\sum_{\|m\|=Q}e^{-i\Sigma_{\alpha=1}^N m^\alpha\varphi^\alpha}|m^1,m^2,\ldots,m^{N+1}\rangle,\end{aligned}\tag{2.9}$$

which satisfies periodicity

$$|\varphi^1,\ldots,\varphi^\alpha+2n\pi,\ldots,\varphi^N\rangle=|\varphi^1,\ldots,\varphi^\alpha,\ldots,\varphi^N\rangle,\quad n:\text{integer}.\tag{2.10}$$

The inner product is

$$\langle \boldsymbol{\varphi}|\boldsymbol{\varphi}'\rangle = \frac{1}{(2\pi)^N} \sum_{\|m\|=Q} e^{i\Sigma_{\alpha=1}^N m^\alpha(\varphi^\alpha - \varphi^{\alpha'})}, \tag{2.11}$$

and the resolution of unity is

$$\int_0^{2\pi} d\boldsymbol{\varphi}|\boldsymbol{\varphi}\rangle\langle\boldsymbol{\varphi}| = \mathbf{1}_Q, \tag{2.12}$$

where

$$\int_0^{2\pi} d\boldsymbol{\varphi} \equiv \int_0^{2\pi} \prod_{\alpha=1}^N d\varphi^\alpha. \tag{2.13}$$

To construct the path integral formula, we utilize the next relation: For $m_0, m_1 \in \mathbf{Z}$,

$$\sum_{m=m_0}^{m_1} e^{im\varphi} f(m) = \sum_{n=-\infty}^{\infty} \int_{m_0-\varepsilon}^{m_1+\varepsilon} dp e^{ip(\varphi+2n\pi)} f(p), \quad 0<\varepsilon<1. \tag{2.14}$$

We rewrite (2.11) with the aid of (2.14) to

$$\begin{aligned}
\langle \varphi|\varphi'\rangle &= \frac{1}{(2\pi)^N} \sum_{m^1=0}^{Q} \sum_{m^2=0}^{Q-m^1} \cdots \sum_{m^N=0}^{Q-\Sigma_{\alpha=1}^{N-1} m^\alpha} e^{i\Sigma_{\alpha=1}^N m^\alpha(\varphi^\alpha-\varphi^{\alpha'})} \\
&= \frac{1}{(2\pi)^N} \sum_{m^1=0}^{Q} \sum_{m^2=0}^{Q-m^1} \cdots \sum_{m^{N-1}=0}^{Q-\Sigma_{\alpha=1}^{N-2} m^\alpha} e^{i\Sigma_{\alpha=1}^N m^\alpha(\varphi^\alpha-\varphi^{\alpha'})} \\
&\quad \times \sum_{n^N=-\infty}^{\infty} \int_{-\varepsilon_N}^{Q-\Sigma_{\alpha=1}^{N-1} m^\alpha+\varepsilon_N} dp^N e^{ip^N(\varphi^N-\varphi^{N\prime}+2n^N\pi)} \\
&= \cdots = \frac{1}{(2\pi)^N} \sum_{n^1=-\infty}^{\infty} \cdots \sum_{n^N=-\infty}^{\infty} \int_{-\varepsilon_1}^{Q+\varepsilon_1} dp^1 \int_{-\varepsilon_2}^{Q-p^1+\varepsilon_2} dp^2 \cdots \int_{-\varepsilon_{N-1}}^{Q-\Sigma_{\alpha=1}^{N-2} p^\alpha+\varepsilon_{N-1}} dp^{N-1} \\
&\quad \times \int_{-\varepsilon_N}^{Q-\Sigma_{\alpha=1}^{N-1} p^\alpha+\varepsilon_N} dp^N e^{i\Sigma_{\alpha=1}^N p^\alpha(\varphi^\alpha-\varphi^{\alpha'}+2n^\alpha\pi)},
\end{aligned} \tag{2.15}$$

where we restrict $0<\varepsilon_\alpha \leqslant 1/(2^{\alpha-1}(N+1))$ for later convenience. We make a change of variables such that

$$\tilde{p}^\alpha = p^\alpha + \frac{1}{2^{\alpha-1}(N+1)}, \tag{2.16}$$

with

$$\lambda \equiv \frac{Q}{2} + \frac{1}{N+1},$$

$$\tilde{\varepsilon}_\alpha \equiv -\varepsilon_\alpha + \frac{1}{2^{\alpha-1}(N+1)}, \quad 0 \leqslant \tilde{\varepsilon}_\alpha < \frac{1}{2^{\alpha-1}(N+1)}, \tag{2.17}$$

which leads to

$$\int_{-\varepsilon_\alpha}^{Q-\Sigma_{\beta=1}^{\alpha-1}p^\beta+\varepsilon_\alpha} dp^\alpha \to \int_{\tilde{\varepsilon}_\alpha}^{2\lambda-\Sigma_{\beta=1}^{\alpha-1}\tilde{p}^\beta-\tilde{\varepsilon}_\alpha} d\tilde{p}^\alpha. \tag{2.18}$$

Equation (2.15) then becomes

$$\begin{aligned}\langle\boldsymbol{\varphi}|\boldsymbol{\varphi}'\rangle = \frac{1}{(2\pi)^N}\sum_{n^1=-\infty}^{\infty}\cdots\sum_{n^N=-\infty}^{\infty}\int_{\varepsilon_1}^{2\lambda-\varepsilon_1}dp^1\int_{\varepsilon_2}^{2\lambda-p^1-\varepsilon_2}dp^2\cdots\int_{\varepsilon_{N-1}}^{2\lambda-\Sigma_{\alpha=1}^{N-2}p^\alpha-\varepsilon_{N-1}}dp^{N-1}\\ \times\int_{\varepsilon_N}^{2\lambda-\Sigma_{\alpha=1}^{N-1}p^\alpha-\varepsilon_N}dp^N e^{i\Sigma_{\alpha=1}^{N}[p^\alpha-1/(2^{\alpha-1}(N+1))](\varphi^\alpha-\varphi^{\alpha\prime}+2n^\alpha\pi)},\end{aligned} \tag{2.19}$$

where the tildes have been omitted.

We adopt a Hamiltonian as

$$\hat{H}\equiv\sum_{\alpha=1}^{N+1}c_\alpha a_\alpha^\dagger a_\alpha, \tag{2.20}$$

where we have assumed that all cs are different from each other and independent of time. The matrix element of the Hamiltonian is

$$\begin{aligned}\langle\boldsymbol{\varphi}|\hat{H}|\boldsymbol{\varphi}'\rangle &= \left\{\sum_{\alpha=1}^{N}(c_\alpha-c_{N+1})\frac{1}{i}\frac{\partial}{\partial\varphi^\alpha}+c_{N+1}Q\right\}\langle\boldsymbol{\varphi}|\boldsymbol{\varphi}'\rangle\\ &= \frac{1}{(2\pi)^N}\sum_{n^1=-\infty}^{\infty}\cdots\sum_{n^N=-\infty}^{\infty}\int_{\varepsilon_1}^{2\lambda-\varepsilon_1}dp^1\cdots\int_{\varepsilon_N}^{2\lambda-\Sigma_{\alpha=1}^{N-1}p^\alpha-\varepsilon_N}\\ &\quad\times dp^N e^{i\Sigma_{\alpha=1}^{N}[p^\alpha-1/(2^{\alpha-1}(N+1))](\varphi^\alpha-\varphi^{\alpha\prime}+2n^\alpha\pi)}\left[\sum_{\alpha=1}^{N}\mu_\alpha\left(p^\alpha-\frac{1}{2^{\alpha-1}(N+1)}\right)+c_{N+1}Q\right],\end{aligned} \tag{2.21}$$

where $\mu_\alpha\equiv c_\alpha-c_{N+1}$.

From now on we put $\tilde{\varepsilon}_\alpha=0$ for simplicity. [See (2.17) for the range of $\tilde{\varepsilon}_\alpha$.]

The Feynman kernel is defined by

$$K(\boldsymbol{\varphi}_F,\boldsymbol{\varphi}_I;T)\equiv\langle\boldsymbol{\varphi}_F|e^{-i\hat{H}T}|\boldsymbol{\varphi}_I\rangle=\lim_{M\to\infty}\langle\boldsymbol{\varphi}_F|(1-i\Delta t\hat{H})^M|\boldsymbol{\varphi}_I\rangle,\quad \Delta t\equiv T/M, \tag{2.22}$$

or explicitly

$$
\begin{aligned}
K(\boldsymbol{\varphi}_F,\boldsymbol{\varphi}_I;T) &= \lim_{M\to\infty}\int_0^{2\pi}\prod_{i=1}^{M-1} d\boldsymbol{\varphi}_i \prod_{j=1}^{M}\langle\boldsymbol{\varphi}_j|(1-i\Delta t\hat{H})|\boldsymbol{\varphi}_{j-1}\rangle\Bigg|_{\boldsymbol{\varphi}_0=\boldsymbol{\varphi}_I}^{\boldsymbol{\varphi}_M=\boldsymbol{\varphi}_F} \\
&= \lim_{M\to\infty}\int_0^{2\pi}\prod_{i=1}^{M-1} d\boldsymbol{\varphi}_i \prod_{j=1}^{M}\Bigg[\frac{1}{(2\pi)^N}\sum_{n_j^1=-\infty}^{\infty}\cdots\sum_{n_j^N=-\infty}^{\infty}\int_0^{2\lambda} dp_j^1\cdots \\
&\quad\times\int_0^{2\lambda-\Sigma_{\alpha=1}^{N-1}p_j^\alpha} dp_j^N e^{i\Sigma_{\alpha=1}^{N}[p^\alpha-1/(2^{\alpha-1}(N+1))](\Delta\varphi_j^\alpha+2n_j^\alpha\pi)}\Bigg[1-i\Delta t \\
&\quad\times\Bigg\{\sum_{\alpha=1}^{N}\mu_\alpha\Bigg(p_j^\alpha-\frac{1}{2^{\alpha-1}(N+1)}\Bigg)+c_{N+1}Q\Bigg\}\Bigg]\Bigg]\Bigg|_{\varphi_0=\varphi_I}^{\varphi_M=\varphi_F} \\
&= \lim_{M\to\infty}\int_0^{2\pi}\prod_{i=1}^{M-1} d\boldsymbol{\varphi}_i \prod_{j=1}^{M}\Bigg\{\frac{1}{(2\pi)^N}\sum_{n_j^1=-\infty}^{\infty}\cdots\sum_{n_j^N=-\infty}^{\infty}\int_0^{2\lambda} dp_j^1\cdots\int_0^{2\lambda-\Sigma_{\alpha=1}^{N-1}p_j^\alpha} dp_j^N\Bigg\} \\
&\quad\times\exp\Bigg[i\sum_{k=1}^{M}\Bigg\{\sum_{\alpha=1}^{N}\Bigg(p_k^\alpha-\frac{1}{2^{\alpha-1}(N+1)}\Bigg)(\Delta\varphi_k^\alpha+2n_k^\alpha\pi) \\
&\quad-\Delta t\Bigg\{\sum_{\alpha=1}^{N}\mu_\alpha\Bigg(p_k^\alpha-\frac{1}{2^{\alpha-1}(N+1)}\Bigg)+c_{N+1}Q\Bigg\}\Bigg\}\Bigg]\Bigg|_{\varphi_0=\varphi_I}^{\varphi_M=\varphi_F},
\end{aligned}
\tag{2.23}
$$

where the resolution of unity (2.12) has been inserted in the first equality and $\Delta\varphi_k^\alpha\equiv\varphi_k^\alpha-\varphi_{k-1}^\alpha$ has been put and $O((\Delta t)^2)$ terms, which finally vanish in $M\to\infty$ limit, have been omitted in the last equality. We introduce new variables such that

$$
\begin{aligned}
n_k^{\alpha'} &= \sum_{l=1}^{k} n_l^\alpha, \\
\varphi_k^{\alpha'} &= \varphi_k^\alpha+2n_k^{\alpha'}\pi,
\end{aligned}
\tag{2.24}
$$

to give

$$
\begin{aligned}
\Delta\varphi_k^\alpha+2n_k^\alpha\pi &= \Delta\varphi_k^{\alpha'}, \\
\sum_{n_i^{\alpha'}=-\infty}^{\infty}\int_{2n_i^{\alpha'}\pi}^{2(n_i^{\alpha'}+1)\pi} d\varphi_i^{\alpha'} &= \int_{-\infty}^{\infty} d\varphi_i^{\alpha'}.
\end{aligned}
\tag{2.25}
$$

The kernel is then rewritten

$$
\begin{aligned}
K(\boldsymbol{\varphi}_F,\boldsymbol{\varphi}_I;T)=&\lim_{M\to\infty}\int_{-\infty}^{\infty}\prod_{i=1}^{M-1}d\boldsymbol{\varphi}_i\sum_{n_M^1=-\infty}^{\infty}\cdots\sum_{n_M^N=-\infty}^{\infty}\prod_{j=1}^{M}\\
&\times\left\{\int_0^{2\lambda}\frac{dp_j^1}{2\pi}\cdots\int_0^{2\lambda-\Sigma_{\alpha=1}^{N-1}p_j^\alpha}\frac{dp_j^N}{2\pi}\right\}\exp\left[i\sum_{k=1}^{M}\left\{\sum_{\alpha=1}^{N}\left(p_k^\alpha-\frac{1}{2^{\alpha-1}(N+1)}\right)\Delta\varphi_k^\alpha\right.\right.\\
&\left.\left.-\Delta t\left\{\sum_{\alpha=1}^{N}\mu_\alpha\left(p_k^\alpha-\frac{1}{2^{\alpha-1}(N+1)}\right)+c_{N+1}Q\right\}\right\}\right]\Bigg|_{\varphi_0^\alpha=\varphi_I^\alpha}^{\varphi_M^\alpha=\varphi_F^\alpha+2n_M^\alpha\pi}\\
=&e^{-iQc_{N+1}T+i\Sigma_{\alpha=1}^{N}[1/(2^{\alpha-1}(N+1))]\mu_\alpha T}\sum_{n^1=-\infty}^{\infty}\cdots\sum_{n^N=-\infty}^{\infty}\\
&\times e^{-i\Sigma_{\alpha=1}^{N}[1/(2^{\alpha-1}(N+1))](\varphi_F^\alpha-\varphi_I^\alpha+2n^\alpha\pi)}\lim_{M\to\infty}\int_{-\infty}^{\infty}\prod_{i=1}^{M-1}d\boldsymbol{\varphi}_i\prod_{j=1}^{M}\\
&\times\left\{\int_0^{2\lambda}\frac{dp_j^1}{2\pi}\cdots\int_0^{2\lambda-\Sigma_{\alpha=1}^{N-1}p_j^\alpha}\frac{dp_j^N}{2\pi}\right\}\exp\left[i\sum_{k=1}^{M}\sum_{\alpha=1}^{N}p_k^\alpha\Phi_k^\alpha\right]\Bigg|_{\varphi_0^\alpha=\varphi_I^\alpha}^{\varphi_M^\alpha=\varphi_F^\alpha+2n^\alpha\pi},
\end{aligned}
\tag{2.26}
$$

where primes have been omitted and n_M^α has been written as n^α and $\Phi_k^\alpha\equiv\Delta\varphi_k^\alpha-\Delta t\mu_\alpha$ in the last equality.

Further, we make a change of variables such that

$$
\begin{aligned}
p^{1\prime}&=p^1-\lambda,\\
p^{2\prime}&=p^2-\frac{\lambda-p^{1\prime}}{2},\\
&\vdots\\
p^{\alpha\prime}&=p^\alpha-\frac{\lambda-\Sigma_{\beta=1}^{\alpha-1}2^{\beta-1}p^{\beta\prime}}{2^{\alpha-1}},\\
&\vdots\\
p^{N\prime}&=p^N-\frac{\lambda-\Sigma_{\beta=1}^{N-1}2^{\beta-1}p^{\beta\prime}}{2^{N-1}},
\end{aligned}
\tag{2.27}
$$

which leads to

$$
\int_0^{2\lambda-\Sigma_{\beta=1}^{\alpha-1}p^\beta}dp^\alpha\to\int_{-(\lambda-\Sigma_{\beta=1}^{\alpha-1}2^{\beta-1}p^{\beta\prime})/2}^{(\lambda-\Sigma_{\beta=1}^{\alpha-1}2^{\beta-1}p^{\beta\prime})/2}dp^{\alpha\prime},
\tag{2.28}
$$

where we use the notations

$$\left.\begin{array}{l}\displaystyle\sum_{\beta=a}^{b} f(\beta)=0\\ \displaystyle\prod_{\beta=a}^{b} f(\beta)=1\end{array}\right\} \quad \text{for } b<a \tag{2.29}$$

for simplicity. We then obtain the kernel

$$\begin{aligned}K(\boldsymbol{\varphi}_F,\boldsymbol{\varphi}_I;T)=&e^{-iQc_{N+1}T+i\Sigma_{\alpha=1}^{N}1/(2^{\alpha-1}(N+1))\mu_\alpha T}\sum_{n^1=-\infty}^{\infty}\cdots\sum_{n^N=-\infty}^{\infty}\\ &\times e^{-i\Sigma_{\alpha=1}^{N}1/(2^{\alpha-1}(N+1))(\varphi_F^\alpha-\varphi_I^\alpha+2n^\alpha\pi)}\\ &\times\lim_{M\to\infty}\int_{-\infty}^{\infty}\prod_{i=1}^{M-1}d\boldsymbol{\varphi}_i\prod_{j=1}^{M}\left\{\int_{-\lambda}^{\lambda}\frac{dp_j^1}{2\pi}\int_{-(\lambda-p_j^1)/2}^{(\lambda-p_j^1)/2}\frac{dp_j^2}{2\pi}\cdots\right.\\ &\left.\times\int_{-(\lambda-\Sigma_{\beta=1}^{N-1}2^{\beta-1}p_j^\beta)/2^{N-1}}^{(\lambda-\Sigma_{\beta=1}^{N-1}2^{\beta-1}p_j^\beta)/2^{N-1}}\frac{dp_j^N}{2\pi}\right\}\\ &\times\exp\left[i\sum_{k=1}^{M}\sum_{\alpha=1}^{N}\left(p_k^\alpha+\frac{\lambda-\Sigma_{\beta=1}^{\alpha-1}2^{\beta-1}p_k^\beta}{2^{\alpha-1}}\right)\Phi_k^\alpha\right]\Bigg|_{\varphi_0^\alpha=\varphi_I^\alpha}^{\varphi_M^\alpha=\varphi_F^\alpha+2n^\alpha\pi},\end{aligned} \tag{2.30}$$

where we have again omitted primes.

To compare with the θ-expression of the Nielsen–Rohrlich formula (1.4), we make a change of variables such that

$$p_k^\alpha=\lambda\left(\prod_{\beta=1}^{\alpha-1}\sin^2\frac{\theta_k^\beta}{2}\right)\cos\theta_k^\alpha,\quad \alpha=1,\ldots,N, \tag{2.31}$$

with the Jacobian

$$\frac{\partial(p)}{\partial(\theta)}=(-1)^N\lambda^N\prod_{\alpha=1}^{N}\left\{\left(\sin^2\frac{\theta_k^\alpha}{2}\right)^{N-\alpha}\sin\theta_k^\alpha\right\}, \tag{2.32}$$

to obtain

$$\begin{aligned}K(\boldsymbol{\varphi}_F,\boldsymbol{\varphi}_I;T)=&e^{-iQc_{N+1}T+i\Sigma_{\alpha=1}^{N}[1/(2^{\alpha-1}(N+1))]\mu_\alpha T}\sum_{n^1=-\infty}^{\infty}\cdots\sum_{n^N=-\infty}^{\infty}\\ &\times e^{-i\Sigma_{\alpha=1}^{N}[1/(2^{\alpha-1}(N=1))](\varphi_F^\alpha-\varphi_I^\alpha+2n^\alpha\pi)}\\ &\times\lim_{M\to\infty}\int_{-\infty}^{\infty}\prod_{i=1}^{M-1}d\boldsymbol{\varphi}_i\prod_{j=1}^{M}\left\{\lambda^N\int_0^\pi\left(\sin^2\frac{\theta_j^1}{2}\right)^{N-1}\right.\\ &\left.\times\sin\theta_j^1\frac{d\theta_j^1}{2\pi}\cdots\int_0^\pi\sin^2\frac{\theta_j^{N-1}}{2}\sin\theta_j^{N-1}\frac{d\theta_j^{N-1}}{2\pi}\int_0^\pi\sin\theta_j^N\frac{d\theta_j^N}{2\pi}\right\}\\ &\times\exp\left[i\sum_{k=1}^{M}\sum_{\alpha=1}^{N}2\lambda\left(\prod_{\beta=1}^{\alpha-1}\sin^2\frac{\theta_k^\beta}{2}\right)\cos^2\frac{\theta_k^\alpha}{2}\Phi_k^\alpha\right]\Bigg|_{\varphi_0^\alpha=\varphi_I^\alpha}^{\varphi_M^\alpha=\varphi_F^\alpha+2n^\alpha\pi}.\end{aligned} \tag{2.33}$$

The trace formula is defined by

$$Z \equiv \int_0^{2\pi} d\boldsymbol{\varphi} \langle \boldsymbol{\varphi} | e^{-i\hat{H}T} | \boldsymbol{\varphi} \rangle = \int_0^{2\pi} d\boldsymbol{\varphi} K(\boldsymbol{\varphi}, \boldsymbol{\varphi}; T), \tag{2.34}$$

whose explicit form is

$$\begin{aligned} Z = & e^{-iQc_{N+1}T + i[1/(N+1)]\Sigma_{\alpha=1}^{N} 2^{-\alpha+1}\mu_\alpha T} \sum_{n^1=-\infty}^{\infty} \cdots \sum_{n^N=-\infty}^{\infty} e^{-i[1/(N+1)]\Sigma_{\alpha=1}^{N} 2^{-\alpha+2} n^\alpha \pi} \\ & \times \lim_{M\to\infty} \prod_{\alpha=1}^{N} \left\{ \int_{2n^\alpha\pi}^{2(n^\alpha+1)\pi} d\varphi_M^\alpha \right\} \int_{-\infty}^{\infty} \prod_{i=1}^{M-1} d\boldsymbol{\varphi}_i \prod_{j=1}^{M} \left\{ \lambda^N \int_0^\pi \left(\sin^2 \frac{\theta_j^1}{2} \right)^{N-1} \right. \\ & \left. \times \sin\, \theta_j^1 \frac{d\theta_j^1}{2\pi} \cdots \int_0^\pi \sin^2 \frac{\theta_j^{N-1}}{2} \sin\, \theta_j^{N-1} \frac{d\theta_j^{N-1}}{2\pi} \int_0^\pi \sin\, \theta_j^N \frac{d\theta_j^N}{2\pi} \right\} \\ & \times \exp\left[2i\lambda \sum_{k=1}^{M} \sum_{\alpha=1}^{N} \left(\prod_{\beta=1}^{\alpha-1} \sin^2 \frac{\theta_k^\beta}{2} \right) \cos^2 \frac{\theta_k^\alpha}{2}\, \Phi_k^\alpha \right] \Bigg|_{\varphi_0^\alpha = \varphi_M^\alpha - 2n^\alpha\pi} . \end{aligned} \tag{2.35}$$

This is the counterpart of the θ-expression of the Nielsen–Rohrlich formula. Actually, in the $N=1$ case, by putting $Q=2J$ and $c_1=-c_2=h/2$, (2.35) becomes

$$\begin{aligned} Z = & \sum_{n=-\infty}^{\infty} e^{i2n\pi J} \lim_{M\to\infty} \int_{2n\pi}^{2(n+1)\pi} \frac{d\varphi_M}{2\pi} \int_{-\infty}^{\infty} \prod_{i=1}^{M-1} \frac{d\varphi_i}{2\pi} \prod_{j=1}^{M} \\ & \times \left\{ \lambda \int_0^\pi \sin\, \theta_j d\theta_j \right\} \exp\left[i\lambda \sum_{k=1}^{M} \cos\, \theta_k (\Delta\varphi_k - h\Delta t) \right], \end{aligned} \tag{2.36}$$

which is just the Nielsen–Rohrlich formula (1.4).

III. EXACT CALCULATION

To claim the WKB exactness, we need the exact calculation to be compared with the result of the WKB approximation. We have already obtained the exact result in another expression (the generalized coherent state).[11] However, we make an exact calculation in this expression to be self-contained.

By changing variables such that

$$p_k^\alpha = \left(\prod_{\beta=1}^{\alpha-1} \sin^2 \frac{\theta_k^\beta}{2} \right) \cos^2 \frac{\theta_k^\alpha}{2}, \tag{3.1}$$

with the Jacobian

$$\frac{\partial(p)}{\partial(\theta)} = (-1)^N 2^{-N} \prod_{\alpha=1}^{N} \left\{ \left(\sin^2 \frac{\theta_k^\alpha}{2} \right)^{N-\alpha} \sin\, \theta_k^\alpha \right\}, \tag{3.2}$$

the trace formula (2.35) becomes

$$Z=e^{-iQc_{N+1}T+i[1/(N+1)]\Sigma_{\alpha=1}^{N}2^{-\alpha+1}\mu_\alpha T}\sum_{n^1=-\infty}^{\infty}\cdots\sum_{n^N=-\infty}^{\infty}e^{-i[1/(N+1)]\Sigma_{\alpha=1}^{N}2^{-\alpha+1}\mu_\alpha T}$$
$$\times\lim_{M\to\infty}\prod_{i=1}^{M}\left\{(2\lambda)^N\int_0^1 dp_i^1\cdots\int_0^{1-\Sigma_{\alpha=1}^{N-1}p_i^\alpha}dp_i^N\right\}$$
$$\times\prod_{\alpha=1}^{N}\left\{\int_{2n^\alpha\pi}^{2(n^\alpha+1)\pi}\frac{d\varphi_M^\alpha}{2\pi}\int_{-\infty}^{\infty}\prod_{j=1}^{M-1}\frac{d\varphi_j^\alpha}{2\pi}\right\}\prod_{\alpha=1}^{N}e^{2i\lambda\Sigma_{k=1}^{M}p_k^\alpha\Phi_k^\alpha}. \tag{3.3}$$

Rewriting the exponent to

$$\sum_{k=1}^{M}p_k^\alpha\Phi_k^\alpha=\sum_{k=1}^{M-1}(p_k^\alpha-p_{k-1}^\alpha)\varphi_k^\alpha+(p_M^\alpha-p_1^\alpha)\varphi_M^\alpha+p_1^\alpha 2n^\alpha\pi-\Delta t\mu_\alpha\sum_{k=1}^{M}p_k^\alpha, \tag{3.4}$$

and performing the φ_i-integrals ($i=1,\ldots,N-1$) as the δ-functions, we obtain

$$Z=e^{-iQc_{N+1}T+i[1/(N+1)]\Sigma_{\alpha=1}^{N}2^{-\alpha+1}\mu_\alpha T}\sum_{n^1=-\infty}^{\infty}\cdots\sum_{n^N=-\infty}^{\infty}e^{-i[1/(N+1)]\Sigma_{\alpha=1}^{N}2^{-\alpha+1}2n^\alpha\pi}$$
$$\times\lim_{M\to\infty}\prod_{i=1}^{M}\left\{(2\lambda)^N\int_0^1 dp_i^1\cdots\int_0^{1-\Sigma_{\alpha=1}^{N-1}p_i^\alpha}dp_i^N\right\}$$
$$\times\prod_{\alpha=1}^{N}\left[\int_{2n^\alpha\pi}^{2(n^\alpha+1)\pi}\frac{d\varphi_M^\alpha}{2\pi}e^{2i\lambda\{(p_M^\alpha-p_1^\alpha)\varphi_M^\alpha+p_1^\alpha 2n^\alpha\pi-\Delta t\mu_\alpha\Sigma_{k=1}^{M}p_k^\alpha\}}\prod_{j=1}^{M-1}\left\{\frac{1}{2\lambda}\,\delta(p_j^\alpha-p_{j+1}^\alpha)\right\}\right]$$
$$\times e^{-iQc_{N+1}T+i[1/(N+1)]\Sigma_{\alpha=1}^{N}2^{-\alpha+1}\mu_\alpha T}\sum_{n^1=-\infty}^{\infty}\cdots\sum_{n^N=-\infty}^{\infty}e^{-i[1/(N+1)]\Sigma_{\alpha=1}^{N}2^{-\alpha+1}2n^\alpha\pi}(2\lambda)^N$$
$$\times\int_0^1 dp_M^1\cdots\int_0^{1-\Sigma_{\alpha=1}^{N-1}p_M^\alpha}dp_M^N e^{2i\lambda\Sigma_{\alpha=1}^{N}(2n^\alpha\pi-\mu_\alpha T)p_M^\alpha}. \tag{3.5}$$

By applying the integral relation (1.7) with $I=0$, $L=1$, $u=2\lambda$, and $\Phi^\alpha=2n^\alpha\pi-\mu_\alpha T$, (3.5) becomes

$$Z=e^{-iQc_{N+1}T+i[1/(N+1)]\Sigma_{\alpha=1}^{N}2^{-\alpha+1}\mu_\alpha T}\sum_{n^1=-\infty}^{\infty}\cdots\sum_{n^N=-\infty}^{\infty}e^{-i[1/(N+1)]\Sigma_{\alpha=1}^{N}2^{-\alpha+1}2n^\alpha\pi}$$
$$\times\left[\sum_{\alpha=1}^{N}\frac{e^{i2\lambda(2n^\alpha\pi-\mu_\alpha T)}}{i(2n^\alpha\pi-\mu_\alpha T)\Pi_{\substack{\beta=1\\\beta\neq\alpha}}^{N}i\{2(n^\alpha-n^\beta)\pi-(\mu_\alpha-\mu_\beta)T\}}+\frac{(-1)^N}{\Pi_{\alpha=1}^{N}i(2n^\alpha\pi-\mu_\alpha T)}\right]. \tag{3.6}$$

First we calculate each term of the α-sum. We set

$$
\begin{aligned}
Z_\alpha &= e^{-iQc_{N+1}T+i[1/(N+1)]\Sigma_{\beta=1}^{N}2^{-\beta+1}\mu_\beta T}\sum_{n^1=-\infty}^{\infty}\cdots\sum_{n^N=-\infty}^{\infty}e^{-i[1/(N+1)]\Sigma_{\beta=1}^{N}2^{-\beta+1}2n^\beta\pi}\\
&\quad\times\frac{e^{2i\lambda(2n^\alpha\pi-\mu_\alpha T)}}{i(2n^\alpha\pi-\mu_\alpha T)}\prod_{\substack{\beta=1\\ \beta\neq\alpha}}^{N}\frac{1}{i\{2(n^\alpha-n^\beta)\pi-(\mu_\alpha-\mu_\beta)T\}}\\
&= e^{-iQc_\alpha T}e^{-i[1/(N+1)]2^{-N+1}\mu_\alpha T}\sum_{n^\alpha=-\infty}^{\infty}\frac{e^{i[1/(N+1)]2^{-N+1}2n^\alpha\pi}}{i(2n^\alpha\pi-\mu_\alpha T)}\\
&\quad\times\prod_{\substack{\beta=1\\ \beta\neq\alpha}}^{N}\left[e^{i[1/(N+1)]2^{-\beta+1}\tilde{\mu}_\beta T}\sum_{\tilde{n}^\beta=-\infty}^{\infty}\frac{e^{i[1/(N+1)]2^{-\beta+1}2\tilde{n}^\beta\pi}}{i(2\tilde{n}^\beta\pi+\tilde{\mu}_\beta T)}\right],
\end{aligned}
\tag{3.7}
$$

where $\tilde{n}^\beta=n^\alpha-n^\beta$ and $\tilde{\mu}_\beta\equiv c_\beta-c_\alpha=\mu_\beta-\mu_\alpha$ $(\beta\neq\alpha)$. We apply the formula

$$
\sum_{n=-\infty}^{\infty}\frac{e^{2n\pi i\varepsilon}}{2n\pi+\varphi}=\frac{e^{i(1/2-\varepsilon)\varphi}}{2\sin\varphi/2},\quad 0<\varepsilon<1,
\tag{3.8}
$$

with

$$
\begin{aligned}
&\varepsilon=\frac{1}{N+1}2^{-N+1},\quad \varphi=-\mu_\alpha T\quad\text{for }\alpha,\\
&\varepsilon=\frac{1}{N+1}2^{-\beta+1},\quad \varphi=\tilde{\mu}_\beta T\quad\text{for }\beta\neq\alpha,
\end{aligned}
\tag{3.9}
$$

to find

$$
Z_\alpha=e^{-iQc_\alpha T}\frac{1}{1-e^{i\mu_\alpha T}}\prod_{\substack{\beta=1\\ \beta\neq\alpha}}^{N}\frac{1}{1-e^{-i\tilde{\mu}_\beta T}}=\frac{e^{-iQc_\alpha T}}{\Pi_{\substack{\beta=1\\ \beta\neq\alpha}}^{N+1}(1-e^{-i\tilde{\mu}_\beta T})},
\tag{3.10}
$$

where $\tilde{\mu}_{N+1}\equiv c_{N+1}-c_\alpha=-\mu_\alpha$. Next the calculation of the last term in (3.6) is

$$
\begin{aligned}
Z_{N+1}&\equiv e^{-iQc_{N+1}T+i[1/(N+1)]\Sigma_{\alpha=1}^{N}2^{-\alpha+1}\mu_\alpha T}\\
&\quad\times\sum_{n^1=-\infty}^{\infty}\cdots\sum_{n^N=-\infty}^{\infty}e^{-i[1/(N+1)]\Sigma_{\alpha=1}^{N}2^{-\alpha+1}2n^\alpha\pi}\frac{(-1)^N}{\Pi_{\alpha=1}^{N}i(2n^\alpha\pi-\mu_\alpha T)}\\
&= e^{-iQc_{N+1}T}\prod_{\alpha=1}^{N}\left[e^{i[1/(N+1)]2^{-\alpha+1}\mu_\alpha T}\sum_{\tilde{n}^\alpha=-\infty}^{\infty}\frac{e^{i[1/(N+1)]2^{-\alpha+1}2\tilde{n}^\alpha\pi}}{i(2\tilde{n}^\alpha\pi+\mu_\alpha T)}\right]=\frac{e^{-iQc_{N+1}T}}{\Pi_{\alpha=1}^{N}(1-e^{-i\mu_\alpha T})},
\end{aligned}
\tag{3.11}
$$

where we have put $\tilde{n}^\alpha=-n^\alpha$ in the second equality and applied (3.8) in the last equality. Thus

$$
Z=\sum_{\alpha=1}^{N+1}Z_\alpha=\sum_{\alpha=1}^{N+1}\frac{e^{-iQc_\alpha T}}{\Pi_{\substack{\beta=1\\ \beta\neq\alpha}}^{N+1}\{1-e^{-i(c_\beta-c_\alpha)T}\}}.
\tag{3.12}
$$

This is the exact result of the trace formula and just the same as that of the generalized coherent state. We here note that (3.12) can be written in the determinant form:

$$Z=\left|\begin{array}{cccc} 1 & 1 & \cdots & 1 \\ e^{-ic_1T} & e^{-ic_2T} & \cdots & e^{-ic_{N+1}T} \\ \vdots & \vdots & \ddots & \vdots \\ e^{-i(N-1)c_1T} & e^{-i(N-1)c_2T} & \cdots & e^{-i(N-1)c_{N+1}T} \\ e^{-i(Q+N)c_1T} & e^{-i(Q+N)c_2T} & \cdots & e^{-i(Q+N)c_{N+1}T} \end{array}\right| \Bigg/ \left|\begin{array}{cccc} 1 & 1 & \cdots & 1 \\ e^{-ic_1T} & e^{-ic_2T} & \cdots & e^{-ic_{N+1}T} \\ \vdots & \vdots & \ddots & \vdots \\ e^{-i(N-1)c_1T} & e^{-i(N-1)c_2T} & \cdots & e^{-i(N-1)c_{N+1}T} \\ e^{-iNc_1T} & e^{-iNc_2T} & \cdots & e^{-iNc_{N+1}T} \end{array}\right|.$$

For detailed calculation, see Appendix B.

IV. RELATIONSHIP TO THE GENERALIZED COHERENT STATE

In this section we establish a relationship with (2.35) to the trace formula in terms of the generalized coherent state by an explicit calculation.

By definition, the trace formula in terms of the multi-periodic coherent state is

$$Z=\lim_{M\to\infty}\int_0^{2\pi}\prod_{i=1}^{M} d\boldsymbol{\varphi}_i \prod_{k=1}^{M}\langle\boldsymbol{\varphi}_k|(1-i\Delta t\hat{H})|\boldsymbol{\varphi}_{k-1}\rangle\Big|_{\boldsymbol{\varphi}_M=\boldsymbol{\varphi}_0}. \tag{4.1}$$

Inserting the completeness

$$\mathbf{1}_Q=\sum_{\|m\|=Q}|m^1,\ldots,m^{N+1}\rangle\langle m^1,\ldots,m^{N+1}|, \tag{4.2}$$

and noting

$$\begin{aligned}\langle\boldsymbol{\varphi}|m^1,\ldots,m^{N+1}\rangle&=\frac{1}{(2\pi)^{N/2}}\,e^{i\Sigma_{\alpha=1}^{N}m^\alpha\varphi^\alpha},\\ \hat{H}|m^1,\ldots,m^{N+1}\rangle&=\left(\sum_{\alpha=1}^{N}\mu_\alpha m^\alpha+c_{N+1}Q\right)|m^1,\ldots,m^{N+1}\rangle,\end{aligned} \tag{4.3}$$

and putting

$$\theta_i^\alpha=-\varphi_i^\alpha+2\pi, \tag{4.4}$$

we rewrite (4.1) as

$$Z=\lim_{M\to\infty}\prod_{i=1}^{M}\left[\sum_{\|m_i\|=Q}\int_0^{2\pi}\frac{d\boldsymbol{\theta}_i}{(2\pi)^N}\,e^{-i\Sigma_{\alpha=1}^{N}m_i^\alpha\Delta\theta_i^\alpha}\left\{1-i\Delta t\left(\sum_{\alpha=1}^{N}\mu_\alpha m_i^\alpha+c_{N+1}Q\right)\right\}\right]\Bigg|_{\varphi_M=\varphi_0}, \tag{4.5}$$

where

$$\int_0^{2\pi} d\boldsymbol{\theta}_i \equiv \int_0^{2\pi} \prod_{\alpha=1}^{N} d\theta_i^\alpha ,$$
$$\Delta\theta_i^\alpha \equiv \theta_i^\alpha - \theta_{i-1}^\alpha . \tag{4.6}$$

If we write (4.5) as

$$Z = \lim_{M\to\infty} \prod_{i=1}^{M} \left[\sum_{\|m_i\|=Q} \int_0^{2\pi} \frac{d\boldsymbol{\theta}_i}{(2\pi)^N} e^{-i\Sigma_{\alpha=1}^{N}(m_i^\alpha - m_{i+1}^\alpha)\theta_i^\alpha} \left\{ 1 - i\Delta t \left(\sum_{\alpha=1}^{N} \mu_\alpha m_i^\alpha + c_{N+1}Q \right) \right\} \right] \Bigg|_{\varphi_M=\varphi_0} , \tag{4.7}$$

we find $m_i^\alpha = m_{i+1}^\alpha$ from the $\boldsymbol{\theta}$-integrals (δ-functions). By inserting the identity[11]

$$\frac{(N+Q)!}{\mathbf{l}!} \int_0^{\infty} \prod_{\alpha=1}^{N} du^\alpha \frac{(u^1)^{l^1}\cdots(u^N)^{l^N}}{(1+u^1+\cdots u^N)^{N+Q+1}} = 1,$$
$$l! \equiv l^1!\ldots l^{N+1}!, \tag{4.8}$$

into (4.5), the trace formula becomes

$$\begin{aligned} Z = \lim_{M\to\infty} \prod_{i=1}^{M} \Bigg[\sum_{\|m_i\|=Q} & \frac{(N+Q)!}{Q!} \int_0^{2\pi} \frac{d\boldsymbol{\theta}_i}{(2\pi)^N} \int_0^{\infty} \frac{\Pi_{\alpha=1}^{N} du_i^\alpha}{(1+u_i^1+\cdots+u_i^N)^{N+1}} \\ & \times \frac{((u_i^1)^{1/2}e^{-i\theta_i^1})^{m_i^1}\cdots((u_i^N)^{1/2}e^{-i\theta_i^N})^{m_i^N}}{(1+u_i^1+\cdots+u_i^N)^{Q/2}} \\ & \times \frac{((u_{i-1}^1)^{1/2}e^{i\theta_{i-1}^1})^{m_i^1}\cdots((u_{i-1}^N)^{1/2}e^{i\theta_{i-1}^N})^{m_i^N}}{(1+u_{i-1}^1+\cdots+u_{i-1}^N)^{Q/2}} \frac{Q!}{\mathbf{m}!} \left\{ 1 - i\Delta t \left(\sum_{\alpha=1}^{N} \mu_\alpha m_i^\alpha + c_{N+1}Q \right) \right\} \Bigg] \Bigg|_{\boldsymbol{\theta}_M=\boldsymbol{\theta}_0} , \end{aligned} \tag{4.9}$$

where $m_i^\alpha = m_{i+1}^\alpha$ and $u_0^\alpha = u_M^\alpha$ have been used. Then putting

$$(u_i^\alpha, \theta_i^\alpha) \to \xi_i^\alpha ; \quad \xi_i^\alpha = \sqrt{u_i^\alpha} e^{i\theta_i^\alpha}, \tag{4.10}$$

we obtain

$$
\begin{aligned}
Z=&\lim_{M\to\infty}\prod_{i=1}^{M}\left[\sum_{\|m_i\|=Q}\int d\mu(\boldsymbol{\xi}_i,\boldsymbol{\xi}_i^{\dagger})\right.\\
&\times\sqrt{\frac{Q!}{\mathbf{m}!}}\frac{(\xi_i^{1*})^{m_i^1}\cdots(\xi_i^{N*})^{m_i^N}}{(1+\boldsymbol{\xi}_i^{\dagger}\boldsymbol{\xi}_i)^{Q/2}}\sqrt{\frac{Q!}{\mathbf{m}!}}\frac{(\xi_{i-1}^{1})^{m_i^1}\cdots(\xi_{i-1}^{N})^{m_i^N}}{(1+\boldsymbol{\xi}_{i-1}^{\dagger}\xi_{i-1})^{Q/2}}\\
&\left.\times\left\{1-i\Delta t\left(\sum_{\alpha=1}^{N}\mu_\alpha m_i^\alpha+c_{N+1}Q\right)\right\}\right]\Bigg|_{\boldsymbol{\xi}_M=\boldsymbol{\xi}_0}\\
=&\lim_{M\to\infty}\prod_{i=1}^{M}\left[\sum_{\|m_i\|=Q}\int d\mu(\boldsymbol{\xi}_i,\boldsymbol{\xi}_i^{\dagger})\langle\boldsymbol{\xi}_i|(1-i\Delta t\hat{H})|m^1,\ldots,m^{N+1}\rangle\langle m^1,\ldots,m^{N+1}|\boldsymbol{\xi}_{i-1}\rangle\right]\Bigg|_{\boldsymbol{\xi}_M=\boldsymbol{\xi}_0}\\
=&\lim_{M\to\infty}\prod_{i=1}^{M}d\mu(\boldsymbol{\xi}_i,\boldsymbol{\xi}_i^{\dagger})\prod_{j=1}^{M}\langle\boldsymbol{\xi}_j|(1-i\Delta t\hat{H})|\boldsymbol{\xi}_{j-1}\rangle\Bigg|_{\boldsymbol{\xi}_M=\boldsymbol{\xi}_0},
\end{aligned}
\tag{4.11}
$$

which is nothing but the trace formula in terms of the generalized coherent state.[11]

V. THE WKB APPROXIMATION

In the Nielsen–Rohrlich formula, the WKB approximation is applicable to the θ-expression instead of the p-expression. In this section we perform the WKB approximation to the θ-expression of the trace formula in terms of the multi-periodic coherent state. The WKB approximation in this case is the large $Q(\lambda)$ expansion.

Writing (2.35) as

$$
\begin{aligned}
Z=&\sum_{n^1=-\infty}^{\infty}\cdots\sum_{n^N=-\infty}^{\infty}\lim_{M\to\infty}\prod_{\alpha=1}^{N}\left\{\int_{2n^\alpha\pi}^{2(n^\alpha+1)\pi}d\varphi_M^\alpha\right\}\int_{-\infty}^{\infty}\prod_{i=1}^{M-1}d\boldsymbol{\varphi}_i\prod_{j=1}^{M}\\
&\times\left\{\lambda^N\int_0^\pi\left(\sin^2\frac{\theta_j^1}{2}\right)^{N-1}\sin\theta_j^1\frac{d\theta_j^1}{2\pi}\cdots\int_0^\pi\left(\sin^2\frac{\theta_j^{N-1}}{2}\right)\right.\\
&\left.\times\sin\theta_j^{N-1}\frac{d\theta_j^{N-1}}{2\pi}\int_0^\pi\sin\theta_j^N\frac{d\theta_j^N}{2\pi}\right\}e^{iS^{(n^\alpha)}}
\end{aligned}
\tag{5.1}
$$

with the action

$$
\begin{aligned}
S^{(n^\alpha)}\equiv&-Qc_{N+1}T+\frac{1}{N+1}\sum_{\alpha=1}^{N}2^{-\alpha+1}\mu_\alpha T-\frac{1}{N+1}\sum_{\alpha=1}^{N}2^{-\alpha+2}n^\alpha\pi\\
&+2\lambda\sum_{k=1}^{M}\sum_{\alpha=1}^{N}\left(\prod_{\beta=1}^{\alpha-1}\sin^2\frac{\theta_k^\beta}{2}\right)\cos^2\frac{\theta_k^\alpha}{2}\Phi_k^\alpha,
\end{aligned}
\tag{5.2}
$$

we find the equations of motion;

$$
\left(\prod_{\beta=1}^{\alpha-1}\sin^2\frac{\theta_k^\beta}{2}\right)\cos^2\frac{\theta_k^\alpha}{2}-\left(\prod_{\beta=1}^{\alpha-1}\sin^2\frac{\theta_{k+1}^\beta}{2}\right)\cos^2\frac{\theta_{k+1}^\alpha}{2}=0,
\tag{5.3a}
$$

$$\left(\prod_{\beta=1}^{\alpha-1}\sin^2\frac{\theta_k^\beta}{2}\right)\sin\theta_k^\alpha\left[-\Phi_k^\alpha+\sum_{\gamma=\alpha+1}^{N}\left(\prod_{\delta=\alpha+1}^{\gamma-1}\sin^2\frac{\theta_k^\delta}{2}\right)\cos^2\frac{\theta_k^\gamma}{2}\,\Phi_k^\gamma\right]=0. \tag{5.3b}$$

Now we solve the first equation(s), (5.3a). In the $\alpha=1$ case the equation is

$$\cos^2\frac{\theta_k^1}{2}=\cos^2\frac{\theta_{k+1}^1}{2}, \tag{5.4}$$

and its solution is

$$\theta_k^1=\theta_{k+1}^1=\theta^1=\text{const.} \tag{5.5}$$

In the $\alpha=2$ case the equation is

$$\sin^2\frac{\theta^1}{2}\left(\cos^2\frac{\theta_k^2}{2}-\cos^2\frac{\theta_{k+1}^2}{2}\right)=0, \tag{5.6}$$

and its solutions are

(i) $\theta^1=0$ [in this case the remaining equations of (5.3a) hold with arbitrary θ^α for $\alpha\geqslant 2$],
(ii) $\theta^1=C_1\neq 0,\ \theta_k^2=\theta_{k+1}^2=\theta^2=\text{const.}$

By a similar consideration, we obtain the solutions

$$\begin{aligned}(\theta^1,\theta^2,\ldots,\theta^N)&=(0,*,*,\ldots,*,*),\\&=(C_1,0,*,\ldots,*,*),\\&=(C_1,C_2,0,\ldots,*,*),\\&\ \ \vdots\\&=(C_1,C_2,C_3,\ldots,C_{N-1},0),\end{aligned} \tag{5.7}$$

where $C_\alpha=\text{const}\neq 0$ $(1\leqslant\alpha\leqslant N-1)$, and $*$ denotes an arbitrary number. Next we solve (5.3b). The solution $(C_1,C_2,\ldots,C_{I-1},0,*,\ldots,*)$ of (5.7) satisfies the equations for $\alpha\geqslant I$ because $\theta_k^I=0$. In the $\alpha=I-1$ case the equation is

$$\sin C_{I-1}(-\Phi_k^{I-1}+\Phi_k^I)=0. \tag{5.8}$$

Because $-\Phi_k^{I-1}+\Phi_k^I=-(\Delta\varphi_k^{I-1}-\mu_{I-1}\Delta t)+(\Delta\varphi_k^I-\mu_I\Delta t)=0$ is not compatible with the boundary condition for any given T, the solution is

$$C_{I-1}=\pi. \tag{5.9}$$

Therefore we obtain

$$C_1=C_2=\cdots=C_{I-1}=\pi. \tag{5.10}$$

Considering about all Is, finally we obtain the solutions of (5.3):

$$
\begin{aligned}
(\theta_k^1,\theta_k^2,\ldots,\theta_k^N) &= (0,*,*,\ldots,*,*),\\
&= (\pi,0,*,\ldots,*,*),\\
&= (\pi,\pi,0,\ldots,*,*),\\
&\ \ \vdots\\
&= (\pi,\pi,\pi,\ldots,\pi,0),\\
&= (\pi,\pi,\pi,\ldots,\pi,\pi),
\end{aligned}
\tag{5.11}
$$

with φs being arbitrary for all α and κ.

First we consider the WKB approximation around $(\theta_k^1,\ldots,\theta_k^N)=(\pi,\pi,...,\pi)$. Putting

$$
\theta_k^\alpha = \pi - \frac{x_k^\alpha}{\sqrt{\lambda}}, \quad \alpha = 1,\ldots,N, \tag{5.12}
$$

we write the trace formula as

$$
\begin{aligned}
Z = e^{-iQc_{N+1}T + i[1/(N+1)]\Sigma_{\alpha=1}^N 2^{-\alpha+1}\mu_\alpha T} & \sum_{n^1=-\infty}^{\infty} \cdots \sum_{n^N=-\infty}^{\infty} e^{-i[1/(N+1)]\Sigma_{\alpha=1}^N 2^{-\alpha+2} n^\alpha \pi}\\
\times \lim_{M\to\infty} \prod_{\alpha=1}^N & \left\{ \int_{2n^\alpha\pi}^{2(n^\alpha+1)\pi} d\varphi_M^\alpha \right\} \int_{-\infty}^{\infty} \prod_{i=1}^{M-1} d\boldsymbol{\varphi}_i \prod_{j=1}^{M} \left\{ \lambda^N \int_0^\infty \left(\cos^2 \frac{x_j^1}{2\sqrt{\lambda}} \right)^{N-1} \right.\\
\times \sin \frac{x_j^1}{\sqrt{\lambda}} & \left. \frac{dx_j^1}{2\pi\sqrt{\lambda}} \cdots \int_0^\infty \cos^2 \frac{x_j^{N-1}}{2\sqrt{\lambda}} \sin \frac{x_j^{N-1}}{\sqrt{\lambda}} \frac{dx_j^{N-1}}{2\pi\sqrt{\lambda}} \int_0^\infty \sin \frac{x_j^N}{\sqrt{\lambda}} \frac{dx_j^N}{2\pi\sqrt{\lambda}} \right\}\\
\times \exp & \left[2i\lambda \sum_{k=1}^M \sum_{\alpha=1}^N \left(\prod_{\beta=1}^{\alpha-1} \cos^2 \frac{x_k^\beta}{2\sqrt{\lambda}} \right) \left(\sin^2 \frac{x_k^\alpha}{2\sqrt{\lambda}} \right) \Phi_k^\alpha \right].
\end{aligned}
\tag{5.13}
$$

The leading order term ($O((1/\lambda)^0)$) becomes

$$
\begin{aligned}
Z_{N+1} \equiv e^{-iQc_{N+1}T + i[1/(N+1)]\Sigma_{\alpha=1}^N 2^{-\alpha+1}\mu_\alpha T} & \sum_{n^1=-\infty}^{\infty} \cdots \sum_{n^N=-\infty}^{\infty} e^{-i[1/(N+1)]\Sigma_{\alpha=1}^N 2^{-\alpha+2} n^\alpha \pi}\\
\times \lim_{M\to\infty} \prod_{\alpha=1}^N & \left[\int_{2n^\alpha\pi}^{2(n^\alpha+1)\pi} \frac{d\varphi_M^\alpha}{2\pi} \int_{-\infty}^{\infty} \prod_{i=1}^{M-1} \frac{d\varphi_i^\alpha}{2\pi} \int_0^\infty \prod_{j=1}^{M} x_j^\alpha dx_j^\alpha \right.\\
\times \exp & \left. \left\{ \frac{i}{2} \sum_{k=1}^M (x_k^\alpha)^2 (\Phi_k^\alpha + i\delta_M) \right\} \right],
\end{aligned}
\tag{5.14}
$$

where δ_M has been introduced, which is given for each M and finally put as zero, to ensure the convergence of the x-integrals. By the form of (5.14), each x_j^α-integral can be performed independently to give

$$Z_{N+1}=e^{-iQc_{N+1}T+i[1/(N+1)]\Sigma_{\alpha=1}^{N}2^{-\alpha+1}\mu_\alpha T}\sum_{n^1=-\infty}^{\infty}\cdots\sum_{n^N=-\infty}^{\infty}e^{-i[1/(N+1)]\Sigma_{\alpha=1}^{N}2^{-\alpha+2}n^\alpha\pi}$$
$$\times\lim_{M\to\infty}\prod_{\alpha=1}^{N}\left[\int_{2n^\alpha\pi}^{2(n^\alpha+1)\pi}\frac{d\varphi_M^\alpha}{2\pi}\int_{-\infty}^{\infty}\prod_{i=1}^{M-1}\frac{d\varphi_i^\alpha}{2\pi}\prod_{j=1}^{M}\frac{1}{i(\mu_\alpha\Delta t-\Delta\varphi_j^\alpha-i\delta_M)}\right]. \quad (5.15)$$

Noting that

$$\int_{-\infty}^{\infty}\frac{d\varphi_i^\alpha}{2\pi i}\frac{1}{\mu_\alpha\Delta t-\varphi_{j+1}^\alpha+\varphi_j^\alpha-i\delta_M}\frac{1}{\mu_\alpha\Delta t-\varphi_j^\alpha+\varphi_{j-1}^\alpha-i\delta_M}=\frac{1}{\mu_\alpha 2\Delta t-\varphi_{j+1}^\alpha+\varphi_{j-1}^\alpha-2i\delta_M}, \quad (5.16)$$

we perform the φ-integrals to obtain

$$Z_{N+1}=e^{-iQc_{N+1}T+i[1/(N+1)]\Sigma_{\alpha=1}^{N}2^{-\alpha+1}\mu_\alpha T}\prod_{\alpha=1}^{N}\left[i\sum_{n^\alpha=-\infty}^{\infty}\frac{e^{i[1/(N+1)]2^{-\alpha+2}n^\alpha\pi}}{2n^\alpha\pi-\mu_\alpha T}\right]$$
$$=e^{-iQc_{N+1}T}\prod_{\alpha=1}^{N}\left[e^{i[1/(N+1)]2^{-\alpha+1}\mu_\alpha T}\sum_{\tilde{n}^\alpha=-\infty}^{\infty}\frac{e^{i2\tilde{n}^\alpha\pi[1/(N+1)]2^{-\alpha+1}}}{i(2\tilde{n}^\alpha\pi+\mu_\alpha T)}\right], \quad (5.17)$$

where we have put $\delta_M=0$ and $\tilde{n}^\alpha=-n^\alpha$ in the second equality. Application of the formula (3.8), noting

$$0<\frac{1}{N+1}2^{-\alpha+1}<1, \quad (5.18)$$

gives the final form

$$Z_{N+1}=e^{-iQc_{N+1}T}\prod_{\alpha=1}^{N}\left[e^{i[1/(N+1)]2^{-\alpha+1}\mu_\alpha T}\frac{e^{i(1/2-2^{-\alpha+1}/(N+1))\mu_\alpha T}}{2i\sin\frac{\mu_\alpha T}{2}}\right]$$
$$=\frac{e^{-iQc_{N+1}T}}{\Pi_{\alpha=1}^{N}(1-e^{-i\mu_\alpha T})}=\frac{e^{-iQc_{N+1}T}}{\Pi_{\alpha=1}^{N}\{1-e^{-i(c_\alpha-c_{N+1})T}\}}. \quad (5.19)$$

Next we perform the WKB approximation around

$$(\theta_k^1,\ldots,\theta_k^N)=(\overset{1}{\pi},\overset{2}{\pi},\ldots,\overset{I-1}{\pi},\overset{I}{0},\overset{I+1}{*},\ldots,\overset{N}{*}), \quad (5.20)$$

for $I=1,\ldots,N$ [$(\theta_k^1,\ldots,\theta_k^N)=(\pi,\pi,...,\pi,0)$ is a special case of (5.20)]. We put

$$\theta_k^\alpha=\pi-\frac{x_k^\alpha}{\sqrt{\lambda}},\quad \alpha=1,\ldots,I-1,\quad \theta_k^I=\frac{x_k^I}{\sqrt{\lambda}}, \quad (5.21)$$

and leave $\theta_\kappa^\alpha(\alpha=I+1,\ldots,N)$ unchanged because they are arbitrary numbers which have no expansion points. The leading order term of the trace formula then becomes

$$
\begin{aligned}
Z_I = & e^{-iQc_{N+1}T+i[1/(N+1)]\Sigma_{\alpha=1}^{N}2^{-\alpha+1}\mu_\alpha T}\sum_{n^1=-\infty}^{\infty}\cdots\sum_{n^N=-\infty}^{\infty}e^{-i[1/(N+1)]\Sigma_{\alpha=1}^{N}2^{-\alpha+1}2n^\alpha\pi} \\
& \times\lim_{M\to\infty}\prod_{\alpha=1}^{N}\left\{\int_{2n^\alpha\pi}^{2(n^\alpha+1)\pi}d\varphi_M^\alpha\right\}\int_{-\infty}^{\infty}\prod_{i=1}^{M-1}d\varphi_i \\
& \times\prod_{j=1}^{M}\left\{\int_0^\infty x_j^1\frac{dx_j^1}{2\pi}\cdots\int_0^\infty x_j^{I-1}\frac{dx_j^{I-1}}{2\pi}\int_0^\infty 2^{-2(N-I)}\right. \\
& \left.\times(x_j^I)^{2(N-I)+1}\frac{dx_j^I}{2\pi}\int_0^\pi\left(\sin^2\frac{\theta_j^{I+1}}{2}\right)^{N-I-1}\sin\theta_j^{I+1}\frac{d\theta_j^{I+1}}{2\pi}\cdots\int_0^\pi\sin\theta_j^N\frac{d\theta_j^N}{2\pi}\right\} \\
& \times e^{2i\lambda(2n^I\pi-\mu_I T)}\exp\left[\frac{i}{2}\sum_{k=1}^{M}\sum_{\alpha=1}^{I-1}(x_k^\alpha)^2(\Phi_k^\alpha-\Phi_k^I)-\frac{i}{2}\sum_{k=1}^{M}(x_k^I)^2\Phi_k^I\right. \\
& \left.+\frac{i}{2}\sum_{k=1}^{M}(x_k^I)^2\sum_{\alpha=I+1}^{N}\left(\prod_{\beta=I+1}^{\alpha-1}\sin^2\frac{\theta_k^\beta}{2}\right)\cos^2\frac{\theta_k^\alpha}{2}\Phi_k^\alpha\right] \\
= & e^{-iQc_IT}\hat{Z}_I e^{-i[1/(N+1)]2^{-I+1}\mu_I T+i[1/(N+1)]\Sigma_{\alpha=I+1}^{N}2^{-\alpha+1}\mu_\alpha T} \\
& \times\sum_{n^I=-\infty}^{\infty}\cdots\sum_{n^N=-\infty}^{\infty}e^{i[1/(N+1)]2^{-I+1}2n^I\pi-[1/(N+1)]\Sigma_{\alpha=I+1}^{N}2^{-\alpha+1}2n^\alpha\pi} \\
& \times\lim_{M\to\infty}\prod_{\alpha=I}^{N}\left\{\int_{2n^\alpha\pi}^{2(n^\alpha+1)\pi}\frac{d\varphi_M^\alpha}{2\pi}\int\prod_{i=1}^{M-1}\frac{d\varphi_i^\alpha}{2\pi}\right\} \\
& \times\prod_{j=1}^{M}\left\{2^{-(N-I)}\int_0^\infty(x_j^I)^{2(N-I)+1}dx_j^I e^{-(i/2)(x_j^I)^2\Phi_j^I}\int_0^\pi\left(\sin^2\frac{\theta_j^{I+1}}{2}\right)^{N-I-1}\right. \\
& \left.\times\sin\theta_j^{I+1}d\theta_j^{I+1}\cdots\int_0^\pi\sin\theta_j^N d\theta_j^N\exp\left[\frac{i}{2}(x_j^I)^2\sum_{\alpha=I+1}^{N}\left(\prod_{\beta=I+1}^{\alpha-1}\sin^2\frac{\theta_j^\beta}{2}\right)\cos^2\frac{\theta_j^\alpha}{2}\Phi_j^\alpha\right]\right\},
\end{aligned}
\tag{5.22}
$$

where

$$
\begin{aligned}
\hat{Z}_I \equiv & e^{i[1/(N+1)]\Sigma_{\alpha=1}^{I-1}2^{-\alpha+1}\tilde{\mu}_\alpha T}\sum_{n^1=-\infty}^{\infty}\cdots\sum_{n^{I-1}=-\infty}^{\infty}e^{i[1/(N+1)]\Sigma_{\alpha=1}^{I-1}2^{-\alpha+1}2(n^I-n^\alpha)\pi} \\
& \times\lim_{M\to\infty}\prod_{\alpha=1}^{I-1}\left\{\int_{2n^\alpha\pi}^{2(n^\alpha+1)\pi}\frac{d\varphi_M^\alpha}{2\pi}\int_{-\infty}^{\infty}\prod_{i=1}^{M-1}\frac{d\varphi^\alpha}{2\pi}\int_0^\infty\prod_{j=1}^{M}x_j^\alpha dx_j^\alpha\right. \\
& \left.\times\exp\left[\frac{i}{2}\sum_{k=1}^{M}(x_k^\alpha)^2(\Phi_k^\alpha-\Phi_k^I)\right]\right\},
\end{aligned}
\tag{5.23}
$$

with $\tilde{\mu}_\alpha\equiv\mu_\alpha-\mu_I$. We can calculate $\hat{Z}_I$ by the way similar to the $(\theta_k^1,\ldots,\theta_k^N)=(\pi,\ldots,\pi)$ case by substituting $N\to I-1$ and $\Phi_k^\alpha\to\Phi_k^\alpha-\Phi_k^I$ to obtain

$$\hat{Z}_I = e^{i[1/(N+1)]\Sigma_{\alpha=1}^{N-1} 2^{-\alpha+1}\tilde{\mu}_\alpha T} \sum_{n^1=-\infty}^{\infty} \cdots \sum_{n^{I-1}=-\infty}^{\infty} e^{i[1/(N+1)]\Sigma_{\alpha=1}^{I-1} 2^{-\alpha+1} 2(n^I - n^\alpha)\pi}$$
$$\times \prod_{\alpha=1}^{I-1} \left[\frac{1}{-i\{2(n^\alpha - n^I)\pi - (\mu_\alpha - \mu_I)T\}} \right]$$
$$= \prod_{\alpha=1}^{I-1} \left[e^{i[1/(N+1)]2^{-\alpha+1}\tilde{\mu}_\alpha T} \sum_{\tilde{n}^\alpha=-\infty}^{\infty} \frac{e^{i[1/(N+1)]2^{-\alpha+1} 2\tilde{n}^\alpha \pi}}{i(2\tilde{n}^\alpha + \tilde{\mu}_\alpha T)} \right] = \prod_{\alpha=1}^{I-1} \frac{1}{1 - e^{-i\tilde{\mu}_\alpha T}}, \tag{5.24}$$

where $\tilde{n}^\alpha = n^I - n^\alpha$. For the remaining part of (5.22), changing variables such that

$$p_k^\alpha = \left(\prod_{\beta=I+1}^{\alpha-1} \sin^2 \frac{\theta_k^\beta}{2} \right) \cos^2 \frac{\theta_k^\alpha}{2}, \quad \alpha = I+1, \ldots, N, \tag{5.25}$$

with the Jacobian

$$\frac{\partial(\pi)}{\partial(\theta)} = (-1)^{N-I} 2^{-N+I} \prod_{\alpha=I+1}^{N} \left\{ \left(\sin^2 \frac{\theta_k^\alpha}{2} \right)^{N-\alpha} \sin \theta_k^\alpha \right\}, \tag{5.26}$$

gives the form of the leading order term

$$Z_I = e^{-iQc_I T} \hat{Z}_I e^{-i[1/(N+1)]2^{-I+1}\mu_I T + i[1/(N+1)]\Sigma_{\alpha=I+1}^{N} 2^{-\alpha+1}\mu_\alpha T}$$
$$\times \sum_{n^I=-\infty}^{\infty} \cdots \sum_{n^N=-\infty}^{\infty} e^{i[1/(N+1)]2^{-I+1} 2n^I \pi - i[1/(N+1)]\Sigma_{\alpha=I+1}^{N} 2^{-\alpha+1} 2n^\alpha \pi}$$
$$\times \lim_{M\to\infty} \prod_{\alpha=1}^{N} \left\{ \int_{2n^\alpha \pi}^{2(n^\alpha+1)\pi} \frac{d\varphi_M^\alpha}{2\pi} \int_{-\infty}^{\infty} \prod_{i=1}^{M-1} \frac{d\varphi_i^\alpha}{2\pi} \right\}$$
$$\times \prod_{j=1}^{M} \left\{ \int_0^\infty (x_j^I)^{2(N-I)+1} dx_j^I e^{-(i/2)(x_j^I)^2 \Phi_j^I} \int_0^1 dp_j^{I+1} \int_0^{1-p_j^{I+1}} dp_j^{I+2} \cdots \right.$$
$$\left. \times \int_0^{1-\Sigma_{\alpha=I+1}^{N-1} p_j^\alpha} dp_j^N \exp\left[\frac{i}{2} (x_j^I)^2 \sum_{\alpha=I+1}^{N} p_j^\alpha \Phi_j^\alpha \right] \right\}. \tag{5.27}$$

By putting $u_j = \frac{1}{2}(x_j^I)^2$ and applying the integral relation (1.7) with $L = I+1$, $u = u_j$, $\Phi^\alpha = \Phi_j^\alpha$, u-integrals becomes

$$\int_0^\infty (u_j)^{N-I} du_j e^{-iu_j\Phi_j^I} \int_0^1 dp_j^{I+1} \cdots \int_0^{1-\Sigma_{\alpha=I+1}^{N-1} p_j^\alpha} dp_j^N e^{iu_j \Sigma_{\alpha=I+1}^N p_j^\alpha \Phi_j^\alpha}$$

$$= \int_0^\infty (u_j)^{N-I} du_j e^{-iu_j\Phi_j^I} (iu_j)^{-N+(I+1)-1} \left[\sum_{\alpha=I+1}^N \frac{1}{\Phi_j^\alpha \Pi_{\substack{\beta=I+1 \\ \beta\neq\alpha}}^N (\Phi_j^\alpha - \Phi_j^\beta)} e^{iu_j\Phi_j^\alpha} \right.$$

$$\left. + \frac{(-1)^{N-(I-1)+1}}{\Pi_{\beta=I+1}^N \Phi_j^\beta} \right] = \lim_{\delta\to 0} i^{-N+I} \left[\sum_{\alpha=I+1}^N \frac{1}{\Phi_j^\alpha \Pi_{\substack{\beta=I+1 \\ \beta\neq\alpha}}^N (\Phi_j^\alpha - \Phi_j^\beta)} \int_0^\infty du_j e^{iu_j(\Phi_j^\alpha - \Phi_j^I + i\delta)} \right.$$

$$\left. + \frac{(-1)^{N-I}}{\Pi_{\beta=I+1}^N \Phi_j^\beta} \int_0^\infty du_j e^{-iu_j(\Phi_j^I - i\delta)} \right] = i^{-N+I-1} \left\{ -\sum_{\alpha=I+1}^N \frac{1}{\Phi_j^\alpha \Pi_{\substack{\beta=I \\ \beta\neq\alpha}}^N (\Phi_j^\alpha - \Phi_j^\beta)} \right.$$

$$\left. + \frac{(-1)^{N-I}}{\Pi_{\beta=I}^N \Phi_j^\beta} \right\} = \frac{1}{i\Phi_j^I \Pi_{\beta=I+1}^N i(\Phi_j^I - \Phi_j^\beta)}, \tag{5.28}$$

where the regularization parameter δ has been introduced for the u_j-integrals to converge in the third equality and the relation (1.6) has been applied in the last equality. Thus (5.27) becomes

$$Z_I = e^{-iQc_I T} \hat{Z}_I e^{-i[1/(N+1)]2^{-I+1}\mu_I T + i[1/(N+1)]\Sigma_{\alpha=I+1}^N 2^{-\alpha+1}\mu_\alpha T}$$

$$\times \sum_{n^I=-\infty}^\infty \cdots \sum_{n^N=-\infty}^\infty e^{i[1/(N+1)]2^{-I+1}2n^I\pi - i[1/(N+1)]\Sigma_{\alpha=I+1}^N 2^{-\alpha+1}2n^\alpha\pi}$$

$$\times \lim_{M\to\infty} \int_{2n^I\pi}^{2(n^I+1)\pi} \frac{d\varphi_M^I}{2\pi} \int_{-\infty}^\infty \prod_{i=1}^{M-1} \frac{d\varphi_i^I}{2\pi} \prod_{j=1}^M \frac{1}{i\Phi_j^I} \prod_{\alpha=I+1}^N$$

$$\times \left\{ \int_{2n^\alpha\pi}^{2(n^\alpha+1)\pi} \frac{d\varphi_M^\alpha}{2\pi} \int_{-\infty}^\infty \prod_{i=1}^{M-1} \frac{d\varphi_i^\alpha}{2\pi} \prod_{j=1}^M \frac{1}{(\Phi_j^I - \Phi_j^\alpha)} \right\}$$

$$= e^{-iQc_I T} \hat{Z}_I e^{-i[1/(N+1)]2^{-I+1}\mu_I T + i[1/(N+1)]\Sigma_{\alpha=I+1}^N 2^{-\alpha+1}\mu_\alpha T}$$

$$\times \sum_{n^I=-\infty}^\infty \cdots \sum_{n^N=-\infty}^\infty e^{i1/(N+1)2^{-I+1}2n^I\pi - i[1/(N+1)]\Sigma_{\alpha=I+1}^N 2^{-\alpha+1}2n^\alpha\pi}$$

$$\times \frac{1}{i(2n^I\pi - \mu_I T)} \prod_{\alpha=I+1}^N \frac{1}{i\{2(n^I - n^\alpha)\pi - (\mu_I - \mu_\alpha)T\}}, \tag{5.29}$$

where the φ-integrals have been performed by noting (5.16). Putting

$$\tilde{n}^\alpha = n^I - n^\alpha, \quad \tilde{\mu}_\alpha \equiv c_\alpha - c_I = \mu_\alpha - \mu_I, \quad \alpha = I+1,\ldots,N,$$

$$\tilde{\mu}_{N+1} \equiv c_{N+1} - c_I = -\mu_I, \tag{5.30}$$

we obtain

$$
\begin{aligned}
Z_I &= e^{-iQc_I T}\hat{Z}_I e^{i[1/(N+1)]2^{-N+1}\tilde{\mu}_{N+1}T} \sum_{n^I=-\infty}^{\infty} \frac{e^{i[1/(N+1)]2^{-N+1}2n^I\pi}}{i(2n^I\pi+\tilde{\mu}_{N+1}T)} \\
&\quad \times \prod_{\alpha=I+1}^{N} \left[e^{i[1/(N+1)]2^{-\alpha+1}\tilde{\mu}_\alpha T} \sum_{\tilde{n}^\alpha=-\infty}^{\infty} \frac{e^{i[1/(N+1)]2^{-\alpha+1}2\tilde{n}^\alpha\pi}}{i(2\tilde{n}^\alpha\pi+\tilde{\mu}_\alpha T)} \right] \\
&= e^{-iQc_I T}\hat{Z}_I e^{i[1/(N+1)]2^{-N+1}\tilde{\mu}_{N+1}T} \frac{e^{i(1/2-[1/(N+1)]2^{-N+1})\tilde{\mu}_{N+1}T}}{2i\,\sin\dfrac{\tilde{\mu}_{N+1}T}{2}} \\
&\quad \times \prod_{\alpha=I+1}^{N} \left[e^{i1/(N+1)2^{-\alpha+1}\tilde{\mu}_\alpha T} \frac{e^{i(1/2-[1/(N+1)]2^{-\alpha+1})\tilde{\mu}_\alpha T}}{2i\,\sin\dfrac{\tilde{\mu}_\alpha T}{2}} \right] \\
&= e^{-iQc_I T}\hat{Z}_I \frac{1}{1-e^{-i\tilde{\mu}_{N+1}T}} \prod_{\alpha=I+1}^{N} \frac{1}{1-e^{-i\tilde{\mu}_\alpha T}} = \frac{e^{-iQc_I T}}{\prod_{\substack{\alpha=1 \\ \alpha\neq I}}^{N+1}(1-e^{-i\tilde{\mu}_\alpha T})},
\end{aligned}
\tag{5.31}
$$

where we have applied the formula (3.8) in the second equality and put the explicit form of $\hat{Z}_I$, (5.24), in the last equality. Thus the total contribution of the WKB approximation becomes

$$
Z_{\mathrm{WKB}} = \sum_{\alpha=1}^{N+1} Z_\alpha = \sum_{\alpha=1}^{N+1} \frac{e^{-iQc_\alpha T}}{\prod_{\substack{\beta=1 \\ \beta\neq\alpha}}^{N+1}\{1-e^{-i(c_\beta-c_\alpha)T}\}},
\tag{5.32}
$$

which is the same with the exact calculation (3.12). Therefore we can conclude that *the WKB exactness holds in the multi-periodic coherent state*.

VI. DISCUSSION

In this paper we have constructed the trace formula in terms of the multi-periodic coherent state as an extension of the Nielsen–Rohrlich formula for spin. We have made an exact calculation of the trace formula and performed the WKB approximation to show the WKB exactness. We have also clarified a connection between the trace formula and that of the generalized coherent state.

The result obtained in this paper is perfectly parallel with the generalized coherent state.[11] Similar argument in terms of another coherent state may be possible. However, the WKB exactness will not hold in arbitrary coherent states. Now we have the problem that *what kind of coherent states make the system WKB exact.*

The extension to the Grassmann manifold from CP^N have been made.[17] The corresponding extension from the multi-periodic coherent state will be also possible.

The extension to supersymmetric $CP^1(CP^N)$ model is also attractive. There is an expectation that by the fermion contribution the result of the continuum path integral coincides with the discrete one.

The extension to field theories is more important. There are some attempts in this field.[18–20] However, they still seem to be insufficient in the mathematical point of view.

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APPENDIX A: SOME USEFUL RELATIONS

1. The Vandermonde's determinant

We define

$$\Delta_k \equiv \prod_{\alpha=k}^{n} \prod_{\beta=k}^{\alpha-1} (a_\alpha - a_\beta) = \begin{vmatrix} 1 & 1 & \cdots & 1 \\ a_k & a_{k+1} & \cdots & a_n \\ a_k^2 & a_{k+1}^2 & \cdots & a_n^2 \\ \vdots & \vdots & \ddots & \vdots \\ a_k^{n-k} & a_{k+1}^{n-k} & \cdots & a_n^{n-k} \end{vmatrix},$$

$$\Delta_k(\alpha) \equiv \begin{vmatrix} a_k & a_{k+1} & \cdots & a_{\alpha-1} & a_{\alpha+1} & \cdots & a_n \\ a_k^2 & a_{k+1}^2 & \cdots & a_{\alpha-1}^2 & a_{\alpha+1}^2 & \cdots & a_n^2 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ a_k^{n-k} & a_{k+1}^{n-k} & \cdots & a_{\alpha-1}^{n-k} & a_{\alpha+1}^{n-k} & \cdots & a_n^{n-k} \end{vmatrix}, \tag{A1}$$

$$\tilde{\Delta}_k(\alpha) \equiv \begin{vmatrix} 1 & \cdots & 1 & 1 & \cdots & 1 \\ a_k & \cdots & a_{\alpha-1} & a_{\alpha+1} & \cdots & a_n \\ a_k^2 & \cdots & a_{\alpha-1}^2 & a_{\alpha+1}^2 & \cdots & a_n^2 \\ \vdots & & \vdots & \vdots & & \vdots \\ a_k^{n-k-1} & \cdots & a_{\alpha-1}^{n-k-1} & a_{\alpha+1}^{n-k-1} & \cdots & a_n^{n-k-1} \end{vmatrix} = \prod_{\substack{\beta=k \\ \beta\neq\alpha}}^{n} \prod_{\substack{\gamma=k \\ \gamma\neq\alpha}}^{\beta-1} (a_\beta - a_\gamma),$$

$$P_k \equiv \prod_{\alpha=k}^{n} a_\alpha = a_k a_{k+1} \cdots a_n .$$

Here Δ_k is known as the Vandermonde's determinant and $\Delta_k(\alpha)$ is its cofactor apart from sign factor $(-1)^{\alpha-k}$. We then find the relations (Laplace expansion)

$$\Delta_k = \sum_{\alpha=k}^{n} (-1)^{\alpha-k} \Delta_k(\alpha),$$

$$\Delta_k(\alpha) = \frac{P_k}{a_\alpha} \tilde{\Delta}_k(\alpha). \tag{A2}$$

We rewrite $\Delta_k(\alpha)$ by another expression. Since

$$\prod_{\substack{\beta=k \\ \beta\neq\alpha}}^{n} (a_\alpha - a_\beta) = (-1)^{n-\alpha} \Delta_k \frac{1}{\tilde{\Delta}_k(\alpha)} = (-1)^{n-\alpha} \frac{P_k}{a_\alpha} \frac{\Delta_k}{\Delta_k(\alpha)}, \tag{A3}$$

we have

$$\Delta_k(\alpha) = (-1)^{n-\alpha} \frac{P_k}{a_\alpha \prod_{\substack{\beta=k \\ \beta\neq\alpha}}^{n} (a_\alpha - a_\beta)} \Delta_k . \tag{A4}$$

Substituting (A4) into the first relation in (A2), we then find

$$\sum_{\alpha=k}^{n} \frac{P_k}{a_\alpha \Pi_{\substack{\beta=k \\ \beta\neq\alpha}}^{n}(a_\alpha - a_\beta)} = (-1)^{n-k}, \tag{A5}$$

and, picking out the $\alpha=k$ term,

$$\frac{1}{a_k \Pi_{\beta=k+1}^{n}(a_k - a_\beta)} = -\sum_{\alpha=k+1}^{n} \frac{1}{a_\alpha \Pi_{\substack{\beta=k \\ \beta\neq\alpha}}^{n}(a_\alpha - a_\beta)} + \frac{(-1)^{n-k}}{P_k}. \tag{A6}$$

2. Some integral

We claim

$$\begin{aligned} A(L) &\equiv \int_0^{1-\Sigma_{\gamma=I+1}^{L-1} p^\gamma} dp^L e^{iu\Phi^L p^L} \cdots \int_0^{1-\Sigma_{\gamma=I+1}^{N-1} p^\gamma} dp^N e^{iu\Phi^N p^N} \\ &= (iu)^{-N+L-1} \left[\sum_{\alpha=L}^{N} \frac{1}{\Phi^\alpha \Pi_{\substack{\beta=L \\ \beta\neq\alpha}}^{N}(\Phi^\alpha - \Phi^\beta)} e^{iu(1-\Sigma_{\gamma=I+1}^{L-1} p^\gamma)\Phi^\alpha} + \frac{(-1)^{N-L+1}}{\Pi_{\beta=L}^{N}\Phi^\beta} \right], \\ &\quad \text{for } L = N, N-1, \ldots, I+1. \end{aligned} \tag{A7}$$

We prove this relation by mathematical induction. In the $L=N$ case we can examine (A7) by an explicit calculation. Now we assume that (A7) holds in L. We then calculate in the $L-1$ case:

$$\begin{aligned} A(L-1) &\equiv \int_0^{1-\Sigma_{\gamma=I+1}^{L-2} p^\gamma} dp^{L-1} e^{iu\Phi^{L-1} p^{L-1}} \cdots \int_0^{1-\Sigma_{\gamma=I+1}^{N-1} p^\gamma} dp^N e^{iu\Phi^N p^N} \\ &= \int_0^{1-\Sigma_{\gamma=I+1}^{L-2} p^\gamma} dp^{L-1} A(L) \\ &= (-1)^{-N+L-1} \left[\sum_{\alpha=L}^{N} \frac{1}{\Phi^\alpha \Pi_{\substack{\beta=L \\ \beta\neq\alpha}}^{N}(\Phi^\alpha - \Phi^\beta)} e^{iu(1-\Sigma_{\gamma=I+1}^{L-2} p^\gamma)\Phi^\alpha} \right. \\ &\quad \times \int_0^{1-\Sigma_{\gamma=I+1}^{L-1} p^\gamma} dp^{L-1} e^{iu(\Phi^{L-1}-\Phi^\alpha)p^{L-1}} \\ &\quad \left. + \frac{(-1)^{N-L+1}}{\Pi_{\beta=L}^{N}\Phi^\beta} \int_0^{1-\Sigma_{\gamma=I+1}^{L-2} p^\gamma} dp^{L-1} e^{iu\Phi^{L-1} p^{L-1}} \right] \\ &= (iu)^{-N+(L-1)-1} \left[\sum_{\alpha=L}^{N} \frac{1}{\Phi^\alpha \Pi_{\substack{\beta=L-1 \\ \beta\neq\alpha}}^{N}(\Phi^\alpha - \Phi^\beta)} e^{iu\Phi^\alpha(1-\Sigma_{\gamma=I+1}^{L-2})p^\gamma} \right. \\ &\quad \left. + \left\{ -\sum_{\alpha=L}^{N} \frac{1}{\Phi^\alpha \Pi_{\substack{\beta=L-1 \\ \beta\neq\alpha}}^{N}(\Phi^\alpha - \Phi^\beta)} + \frac{(-1)^{N-L+1}}{\Pi_{\beta=L-1}^{N}\Phi^\beta} \right\} \right. \end{aligned}$$

$$\times e^{iu\Phi^{L-1}(1-\Sigma_{\gamma=I+1}^{L-2}p^{\gamma})}+\frac{(-1)^{N-(L-1)+1}}{\Pi_{\beta=L-1}^{N}\Phi^{\beta}}\Bigg]$$

$$=(iu)^{-N+(L-1)-1}\Bigg[\sum_{\alpha=L}^{N}\frac{1}{\Phi^{\alpha}\Pi_{\substack{\beta=L-1\\ \beta\neq\alpha}}^{N}(\Phi^{\alpha}-\Phi^{\beta})}$$

$$\times e^{iu\Phi^{\alpha}(1-\Sigma_{\gamma=I+1}^{L-2})p^{\gamma}}+\frac{1}{\Phi^{L-1}\Pi_{\beta=L}^{N}(\Phi^{L-1}-\Phi^{\beta})}$$

$$\times e^{iu\Phi^{L-1}(1-\Sigma_{\gamma=I+1}^{L-2}p^{\gamma})}+\frac{(-1)^{N-(L-1)+1}}{\Pi_{\beta=L-1}^{N}\Phi^{\beta}}\Bigg]$$

$$=(-1)^{-N+(L-1)-1}\Bigg[\sum_{\alpha=L-1}^{N}\frac{1}{\Phi^{\alpha}\Pi_{\substack{\beta=L-1\\ \beta\neq\alpha}}^{N}(\Phi^{\alpha}-\Phi^{\beta})}$$

$$\times e^{-u\Phi^{\alpha}(1-\Sigma_{\gamma=I+1}^{L-2}p^{\gamma})}+\frac{(-1)^{N-(L-1)+1}}{\Pi_{\beta=L-1}^{N}\Phi^{\beta}}\Bigg]. \tag{A8}$$

Equation (A8) indicates that (A7) in the $L-1$ case holds if it holds in the L case. Thus we conclude that (A7) holds for $L=N,N-1,\ldots,I+1$.

APPENDIX B: THE DETERMINANT FORM OF THE EXACT RESULT

Utilizing the relation in Appendix A, we rewrite the exact result of the trace formula in the determinant form.

By assigning

$$k=1,\quad n=N+1,\quad a_{\alpha}=e^{-ic_{\alpha}T}, \tag{B1}$$

(A3) becomes

$$\prod_{\substack{\beta=1\\ \beta\neq\alpha}}^{N+1}(e^{-ic_{\alpha}T}-e^{-ic_{\beta}T})=(-1)^{N+1-\alpha}\frac{\Delta_1}{\tilde{\Delta}_1(\alpha)}. \tag{B2}$$

By means of (B2), we rewrite (3.12) to

$$Z=\sum_{\alpha=1}^{N+1}\frac{e^{-iQc_\alpha T}}{\prod_{\substack{\beta=1\\ \beta\neq\alpha}}^{N+1}\{1-e^{-i(c_\beta-c_\alpha)T}\}}=\sum_{\alpha=1}^{N+1}\frac{e^{-iQc_\alpha T}}{e^{iNc_\alpha T}\prod_{\substack{\beta=1\\ \beta\neq\alpha}}^{N+1}(e^{-ic_\alpha T}-e^{-ic_\beta T})}$$

$$=\sum_{\alpha=1}^{N+1}\frac{e^{-i(Q+N)c_\alpha T}}{(-1)^{N+1-\alpha}\dfrac{\Delta_1}{\tilde{\Delta}_1(\alpha)}}=\frac{1}{\Delta_1}\sum_{\alpha=1}^{N+1}$$

$$\times(-1)^{N+1+\alpha}e^{-i(Q+N)c_\alpha T}\begin{vmatrix} 1 & \cdots & 1 & 1 & \cdots & 1 \\ e^{-ic_1T} & \cdots & e^{-ic_{\alpha-1}T} & e^{-ic_{\alpha+1}T} & \cdots & e^{-ic_{N+1}T} \\ e^{-i2c_1T} & \cdots & e^{-i2c_{\alpha-1}T} & e^{-i2c_{\alpha+1}T} & \cdots & e^{-i2c_{N+1}T} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ e^{-i(N-1)c_1T} & \cdots & e^{-i(N-1)c_{\alpha-1}T} & e^{-i(N-1)c_{N+1}T} & \cdots & e^{-i(N-1)c_{N+1}T} \end{vmatrix}$$

$$=\frac{1}{\Delta_1}\begin{vmatrix} 1 & 1 & \cdots & 1 \\ e^{-ic_1T} & e^{-ic_2T} & \cdots & e^{-ic_{N+1}T} \\ \vdots & \vdots & \ddots & \vdots \\ e^{-i(N-1)c_1T} & e^{-i(N-1)c_2T} & \cdots & e^{-i(N-1)c_{N+1}T} \\ e^{-i(Q+N)c_1T} & e^{-i(Q+N)c_2T} & \cdots & e^{-i(Q+N)c_{N+1}T} \end{vmatrix}. \tag{B3}$$

This is the determinant form (3.13).

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Hamiltonian structure of Dubrovin's equation of associativity in 2-d topological field theory

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A third order Monge-Ampère type equation of associativity that Dubrovin has obtained in 2-d topological field theory is formulated in terms of a variational principle subject to second class constraints. Using Dirac's theory of constraints this degenerate Lagrangian system is cast into Hamiltonian form and the Hamiltonian operator is obtained from the Dirac bracket. There is a new type of Kac-Moody algebra that corresponds to this Hamiltonian operator. In particular, it is not a W-algebra. © *1996 American Institute of Physics.* [S0022-2488(96)01811-7]

I. INTRODUCTION

Witten has introduced model-independent recursion relations which can be regarded as the qualitative definition of the topological phase of two dimensional gravity.[1] The validity of these relations is based on purely geometrical considerations such as intersection theory and makes no reference to the details of the physical model. The equations of associativity for the Frobenius algebra satisfied by the n-point function are third order Monge-Ampère equations. In this paper we shall consider the Hamiltonian structure of

$$u_{ttt}=u_{xtt}u_{xxx}-u_{txx}{}^2 \tag{1}$$

that Dubrovin[2] has obtained as an equation of associativity in 2-d topological field theory. Our approach will closely follow the discussion of the multi-Hamiltonian structure of the Monge-Ampère equation,[3] starting with a field theory formulation of Dubrovin's equation (1) itself.

We shall show that Eq. (1) can be derived from a variational principle with a degenerate Lagrangian and using Dirac's theory of constraints[4] cast it into Hamiltonian form. The resulting Dirac bracket yields the Hamiltonian operator. The Kac-Moody algebra associated with this Hamiltonian operator is not a W-algebra.

The Hamiltonian structure of Eq. (1) has also been discussed by Mokhov and Ferapontov[5] who based their considerations on a system of equations of hydrodynamic type.[6] They found that Eq. (1) is equivalent to a non-diagonizable 3-component Hamiltonian system of hydrodynamic type and obtained a first order Hamiltonian operator of Dubrovin-Novikov type. The Hamiltonian operator that results from our approach is different from that of Mokhov and Ferapontov.

II. SYSTEM OF EVOLUTION EQUATIONS

Dubrovin's equation (1) is third order in time and in order to cast it into Hamiltonian form we need to express it as a triplet of first order nonlinear evolution equations. For this purpose we introduce auxiliary variables

$$p=u_x, \quad q=u_t, \quad r=u_{tt}, \tag{2}$$

which results in

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$$\begin{aligned} p_t &= q_x, \\ q_t &= r, \\ r_t &= p_{xx} r_x - {q_{xx}}^2 \end{aligned} \tag{3}$$

and it is worth noting that this split of Eq. (1) into the system (3) is not unique. Now the vector field

$$\mathbf{X} = q_x \frac{\partial}{\partial p} + r \frac{\partial}{\partial q} + (p_{xx} r_x - {q_{xx}}^2) \frac{\partial}{\partial r} \tag{4}$$

defines the flow. In the discussion of the Hamiltonian structure of this system we shall use $u^i, i = 1,2,3$, for the variables p, q, r, respectively.

III. DIRAC BRACKET

It can be verified directly that the Lagrangian density which yields the first order equations of motion (3) is given by

$$\mathscr{L} = p r_t - \tfrac{1}{2} q_x q_t - p_x p_{xx} q_t - p_x q_{xx} p_t - q r_x - \tfrac{1}{2} q_x^2 p_{xx} \tag{5}$$

and we note that it is linear in the velocities. Thus the canonical momenta

$$\begin{aligned} \pi_p &= -p_x q_{xx}, \\ \pi_q &= -p_x p_{xx} - \tfrac{1}{2} q_x, \\ \pi_r &= p \end{aligned} \tag{6}$$

cannot be inverted for the velocities and we have a degenerate Lagrangian system. They satisfy the canonical Poisson bracket relations

$$\{\pi_k(x), u^i(y)\} = \delta_k^i \delta(x-y) \tag{7}$$

with all others vanishing. The passage to a Hamiltonian formulation of this system requires the use of Dirac's theory of constraints[4] since the Lagrangian (5) is degenerate.

Following Dirac we introduce the primary constraints from Eqs. (6)

$$\begin{aligned} \phi_1 &= \pi_p + p_x q_{xx}, \\ \phi_2 &= \pi_q + p_x p_{xx} + \tfrac{1}{2} q_x, \\ \phi_3 &= \pi_r - p \end{aligned} \tag{8}$$

and calculating the Poisson brackets of the constraints

$$\begin{aligned} \{\phi_1(x), \phi_1(y)\} &= q_{xx} \delta_x(x-y) - q_{yy} \delta_y(y-x), \\ \{\phi_1(x), \phi_2(y)\} &= p_y \delta_{xx}(y-x) + p_x \delta_{yy}(x-y) - p_{xx} \delta_y(x-y) \\ \{\phi_1(x), \phi_3(y)\} &= \delta(x-y), \\ \{\phi_2(x), \phi_2(y)\} &= \tfrac{1}{2} \delta_x(x-y) - \tfrac{1}{2} \delta_y(y-x), \\ \{\phi_2(x), \phi_3(y)\} &= 0, \\ \{\phi_3(x), \phi_3(y)\} &= 0 \end{aligned} \tag{9}$$

we find that the constraints (8) are second class as they do not vanish modulo the constraints.

The total Hamiltonian of Dirac is given by

$$H_T=\int\left(\frac{1}{2}q_x^2p_{xx}+qr_x+c^i\phi_i\right)dx, \tag{10}$$

where summation over $i=1,2,3$ is implied and c^i are Lagrange multipliers. The condition that the constraints are maintained in time

$$\{\phi_i(x),H_T\}=0 \tag{11}$$

gives rise to no further constraints. Instead, using Eqs. (9), we find that the Lagrange multipliers are determined from Eq. (11)

$$c^1=q_x,\quad c^2=r,\quad c^3=p_{xx}r_x-q_{xx}{}^2$$

and finally from Eq. (10) we have

$$H_T=\int\left\{q_x\pi_p+r\pi_q+(p_{xx}r_x-q_{xx}{}^2)\pi_r-\frac{1}{2}rq_x-pq_{xx}{}^2+pr_xp_{xx}\right\}dx \tag{12}$$

for the total Hamiltonian. Given any smooth function of the canonical variables $\mathscr{A}$, all the equations of motion are satisfied in the form of Hamilton's equations

$$\mathscr{A}_t=\{\mathscr{A}(x),H_T\} \tag{13}$$

with this total Hamiltonian.

In order to construct the Dirac bracket we need the inverse J^{ik} of the matrix of Poisson brackets of the constraints. The definition of the inverse is simply

$$\int\{\phi_i(x),\phi_k(z)\}J^{kj}(z,y)dz=\delta_i^j\delta(x-y), \tag{14}$$

which results in a set of differential equations for J^{ik}. Starting with the Poisson bracket relations (9) we find that Eq. (14) can be solved readily to yield

$$\begin{aligned}
J^{11}(x,y)&=0,\\
J^{12}(x,y)&=0,\\
J^{13}(x,y)&=\delta(x-y),\\
J^{22}(x,y)&=-\theta(x-y),\\
J^{23}(x,y)&=p_{xx}\delta(x-y),\\
J^{33}(x,y)&=(p_{xx}^2-2q_{xx})\delta_x(x-y)+(p_{xx}p_{xxx}-q_{xxx})\delta(x-y)
\end{aligned} \tag{15}$$

for the inverse of (9). From this result the Dirac bracket can be constructed readily.

IV. HAMILTONIAN OPERATOR

The transition from the Dirac bracket to the Hamiltonian operator is given by

$$\{u^i(x),u^k(y)\}_D=J^{ik}(x,y)\equiv J^{ik}(x)\,\delta(x-y) \tag{16}$$

and from Eqs. (16) and (15) it follows that the Hamiltonian operator corresponding to the degenerate Lagrangian (5) is

$$J=\begin{pmatrix} 0 & 0 & -1 \\ 0 & D_x^{-1} & -p_{xx} \\ 1 & p_{xx} & D_x q_{xx}+q_{xx}D_x-p_{xx}D_x p_{xx} \end{pmatrix}, \tag{17}$$

where D_x^{-1} the inverse of D_x. We refer to Ref. 7 for the definition and properties of D_x^{-1} in particular,

$$D_x^{-1}f=\frac{1}{2}\left(\int_{-\infty}^{x}-\int_{x}^{\infty}\right)f(\xi)d\xi \tag{18}$$

and the integrals are taken in the principal value sense. We should note that the Hamiltonian operator (17) is not a truly nonlocal operator. In the variables p,q,r for which there is a local expression for the Lagrangian (5) there is a nonlocal piece in the Hamiltonian operator, but this operator will become a local operator if in place of p,q,r we use variables that contain higher x-derivatives of u.

Finally, in Dirac's theory second class constraints hold as strong equations and therefore one can eliminate the momenta from Eqs. (6) to obtain the total Hamiltonian density

$$\mathscr{H}_D=\tfrac{1}{2}q_x^2 p_{xx}+rq_x \tag{19}$$

of Dirac. It can be directly verified that this quantity is conserved for the flow (4) and this is the Hamiltonian function appropriate to the operator (17). That is, the equations of motion (3) are cast into the form

$$u_t^i=\mathbf{X}(u^i)=J^{ik}\delta_k H_D \tag{20}$$

of Hamilton's equations, where δ_k denotes the variational derivative with respect to u^k and H_D is the integral of the density $\mathscr{H}_D$.

The proof of the Jacobi identities for (17) follows from the fact that it is simply the Hamiltonian operator corresponding to the Dirac bracket according to Eq. (16) and there is a general proof of the Jacobi identities for Dirac brackets.[4]

There are two additional conserved densities for Eqs. (3),

$$\begin{aligned} \mathscr{C} &= r-q_x p_{xx}, \\ \mathscr{P} &= \tfrac{1}{2}q_x^2+rp_x+\tfrac{1}{2}p_x^2 q_{xx}, \end{aligned} \tag{21}$$

which consist of the Casimir and momentum, respectively. Inserting P in place of H_D in Eq. (20) we end up with the trivial flow.

V. SYMPLECTIC STRUCTURE

The symplectic structure of the equations of motion (3) is obtained by integrating the 2-form density[8]

$$\omega=\tfrac{1}{2}du^i\wedge K_{ij}du^j \tag{22}$$

over the spatial variable, where K is the ''inverse'' of J. This is just the Poisson bracket of the constraints (9), or we may invert (17) to obtain

$$K=\begin{pmatrix} q_{xx}D_x+D_x q_{xx} & -p_{xx}D_x & 1 \\ -D_x p_{xx} & D_x & 0 \\ -1 & 0 & 0 \end{pmatrix} \tag{23}$$

and we find the symplectic 2-form

$$\omega = dp \wedge dr + q_{xx} dp \wedge dp_x - p_{xx} dp \wedge dq_x + \frac{1}{2} dq \wedge dq_x , \tag{24}$$

which can be directly verified to be a closed 2-form. By invoking the Poincaré lemma, in a local neighborhood we can write

$$\omega = d\alpha, \quad \alpha = (q_x p_{xx} - r) dp - \tfrac{1}{2} q_x dq, \tag{25}$$

where the coefficient of dp is essentially the Casimir of (17). The closure of the symplectic 2-form (24) is equivalent to the satisfaction of the Jacobi identities by the Hamiltonian operator (17).

VI. KAC-MOODY ALGEBRA

Hamiltonian operators associated with integrable nonlinear evolution equations give rise to Kac-Moody (KM) algebras.[9] There is an explicit algorithm for the construction of the KM algebra from the Hamiltonian operator which is essentially based on Fourier analysis. Thus using

$$p(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{i}{n^2} \mathscr{P}_n e^{inx} dn, \quad q(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{1}{n^2} \mathscr{Q}_n e^{inx} dn,$$

$$r(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathscr{R}_n e^{inx} dn,$$

we find

$$\begin{aligned}
&[\mathscr{P}_m, \mathscr{P}_n] = 0, \\
&[\mathscr{P}_m, \mathscr{Q}_n] = 0, \\
&[\mathscr{P}_m, \mathscr{R}_n] = m^2 \delta_{n,-m}, \\
&[\mathscr{Q}_m, \mathscr{Q}_n] = m^3 \delta_{n,-m}, \\
&[\mathscr{Q}_m, \mathscr{R}_n] = -m^2 \mathscr{P}_{m+n}, \\
&[\mathscr{R}_m, \mathscr{R}_n] = (m-n) \mathscr{Q}_{m+n} + \Sigma_{k=-\infty}^{\infty} k \mathscr{P}_{m-k} \mathscr{P}_{k+n} ,
\end{aligned} \tag{26}$$

which is not a W-algebra, but rather of a new type. We note that no normal ordering is needed in the last one of Eqs. (26) because all the $\mathscr{P}_n$ commute.

VII. CONCLUSION

We have presented a Hamiltonian formulation of Dubrovin's equation of associativity in 2-d topological field theory. A different Hamiltonian structure for this equation was obtained by Mokhov and Ferapontov earlier. In a subsequent paper[11] we shall show that these two Hamiltonian structures can be combined to yield the bi-Hamiltonian structure of Dubrovin's equation, which by the theorem of Magri[10] will provide a proof of its complete integrability.

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Classical and quantum implications of the causality structure of two-dimensional space–times with degenerate metrics

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The causality structure of two-dimensional manifolds with degenerate metrics is analyzed in terms of global solutions of the massless wave equation. Certain novel features emerge. Despite the absence of a traditional Lorentzian Cauchy surface on manifolds with a Euclidean domain, it is possible to uniquely determine a global solution (if it exists), satisfying well-defined matching conditions at the degeneracy curve, from Cauchy data on certain spacelike curves in the Lorentzian region. In general, however, no global solution satisfying such matching conditions will be consistent with this data. Attention is drawn to a number of obstructions that arise prohibiting the construction of a bounded operator connecting asymptotic single particle states. The implications of these results for the existence of a unitary quantum field theory are discussed. © *1996 American Institute of Physics.* [S0022-2488(96)01311-4]

I. INTRODUCTION

If S is a spacelike (acausal) domain in a space–time M, then one defines its domain of dependence $D(S)$ as the set of points p such that all nonterminating timelike curves from p intersect S.[1] Furthermore, one says that an acausal hypersurface S is a Cauchy hypersurface if $D(S)=M$. The existence of a Cauchy hypersurface is equivalent to M being globally hyperbolic.

Kundt first[2] discussed the nonexistence of certain topologically nontrivial space–times assuming that every geodesic is complete. Geroch[1] exploited the notion of global hyperbolicity to reach a similar conclusion. There has been recent interest in the behavior of both classical and quantum fields on background manifolds that admit metrics with both Euclidean[3] and variable signatures[1,2,4–16] as well as in space–times that are not globally hyperbolic.[17]

For information that propagates according to the wave equation for a scalar field, a specification of the field and its normal derivative on any spacelike surface S is sufficient to determine a unique solution to the equation on the domain of dependence of S. A manifold with a degenerate metric is not globally hyperbolic and it is therefore of interest to investigate the influence of this degeneracy on the propagation of massless scalar fields satisfying

$$d\star d\psi=0, \tag{1}$$

where $\star$ is the Hodge map associated with an ambient metric tensor field g.

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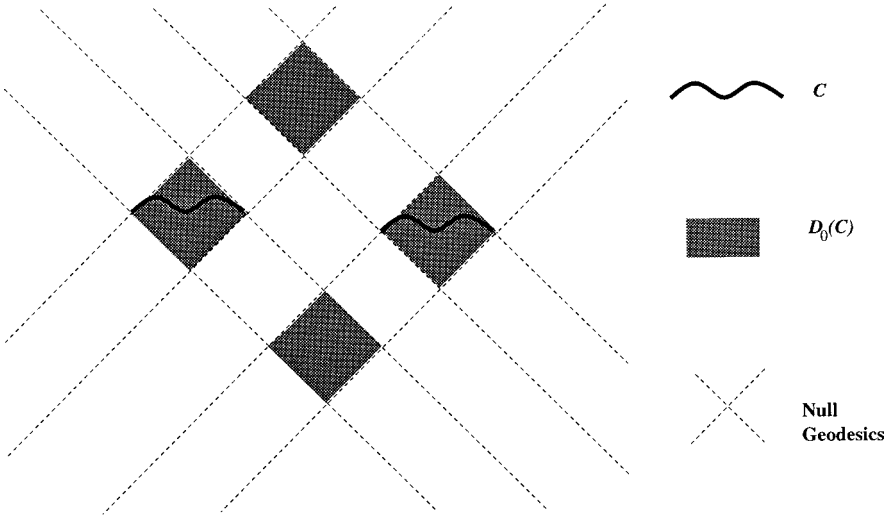

FIG. 1. Domain of null dependence of C, $D_0(C)\subset L\cup\Sigma$.

In this article we address this question in the context of a metric that partitions a two-dimensional manifold into three disjoint sets: a Lorentzian region L, a Euclidean region E, and a one-dimensional subset Σ where the metric is degenerate.

In a region where g has Euclidean signature (1) is the (elliptic) Laplace equation. The traditional data for this equation is the specification of ψ on the boundary of any Euclidean domain since this will fix a solution uniquely in such a region. However, we show below that a specification of ψ and its normal derivative on any arc of the boundary is also sufficient to uniquely determine the interior solution should it exist. This result proves of relevance when we discuss the propagation of hyperbolic data from a Lorentzian to a Euclidean domain.

In a region where g has Lorentzian signature (1) is the (hyperbolic) *massless* wave equation, and it is possible to contemplate data on disjoint spacelike curves (Fig. 1).

Since information travels along null geodesics we redefine the domain of dependence. Thus if C is a spacelike (acausal) domain in a Lorentzian region $L\subset M$, then its *domain of null dependence* $D_0(C)$ is the set of points p such that all nonterminating null curves from p intersect C. For $C\subset L$ and $\Sigma'\subset\Sigma$ we define $D_0(C\cup\Sigma')$ to be all the points $p\in L$ where both null geodesics that intersect at p either intersect C or terminate on Σ', where they are not tangent.

From Fig. 1 we see that if C is not connected, then $D_0(C)$ may contain regions disjoint from C.

Consider now a spacelike arc $C\subset L$ on which standard Cauchy data for (1) is prescribed (Fig. 2). Furthermore, suppose that the domain of null dependence of C intersects Σ nontrivially, i.e., the intersection is one-dimensional. Then we show below that if a global solution exists and agrees with the data on C, then it is unique in E. Such a solution provides Cauchy data on Σ which together with that on C enables one to construct the solution on the domain of null dependence $D_0(C\cup\Sigma)$. In general no such global solution exists, as will be illustrated in example 1 below.

If the intersection $D_0(C)\cap\Sigma$ is trivial, then the theorem below is not applicable. In this case more than one global solution may exist compatible with the Cauchy data on C. Example 2 will illustrate this situation.

In Sec. V we review the standard prescription that is adopted to construct a quantum field theory on a fixed globally hyperbolic manifold. With the aid of explicit examples, we draw attention to the obstructions that arise when one attempts to implement this prescription on a two-dimensional manifold with a degenerate metric. We offer reasons why we believe that a

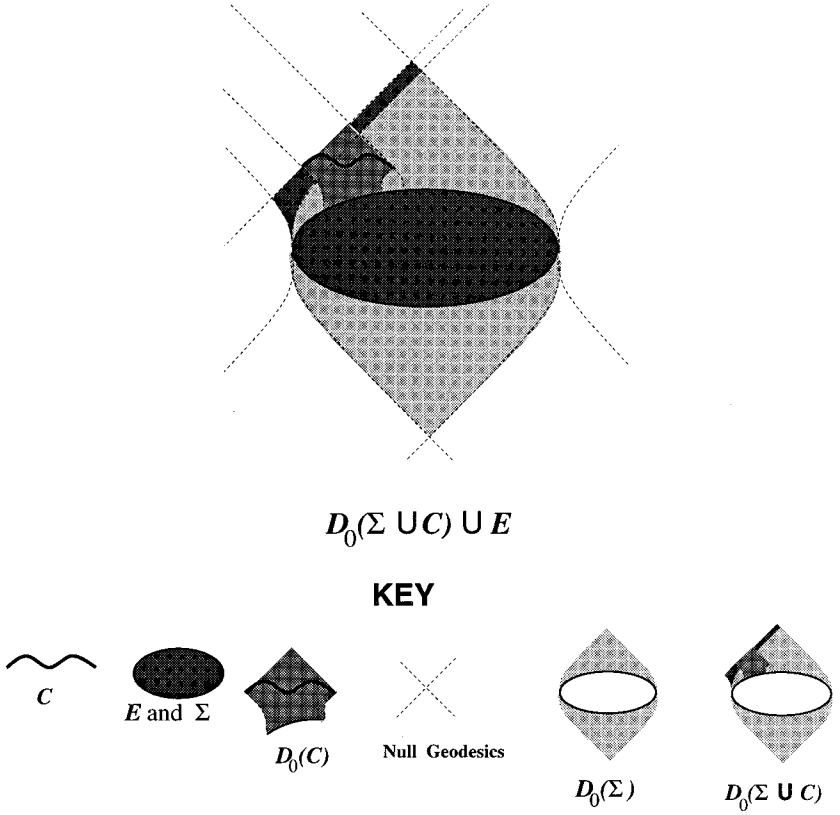

FIG. 2. $D_0(C\cup\Sigma)\cup E$.

bounded unitary scattering matrix in the presence of nondynamical signature change may not exist.

II. CONSTRUCTION OF COORDINATE SYSTEMS

Given a two-dimensional manifold (L,g^L) with a (nondegenerate) Lorentzian metric g^L, a *null coordinate system* (η_+,η_-) is one in which the metric may be written

$$g^L=\Omega^L(\eta_+,\eta_-)(d\eta_+\otimes d\eta_- + d\eta_-\otimes d\eta_+), \tag{2}$$

where Ω^L is a real function. Similarly for a two-dimensional manifold (E,g^E) with a (nondegenerate) Euclidean metric g^E, a *complex isothermal coordinate system* $(z,\overline{z})$ is one in which the metric may be written

$$g^E=\Omega^E(z,\overline{z})(dz\otimes d\overline{z}+dz\otimes d\overline{z}), \tag{3}$$

where Ω^E is a real positive function. It is known that one can construct a null coordinate system about any point in $p\in L$ and that one can construct a complex isothermal coordinate system about any point $p\in E$.

In this section we give conditions for the construction of null and complex isothermal coordinate systems for a two-dimensional manifold $M=L\cup\Sigma\cup E$ with a signature changing metric g.

We assume that Σ is (locally) parametrized by a C^ω monotonic function $\Sigma:I\mapsto\Sigma$, with $\sigma\in I\subset\mathbb{R}$. (The symbol Σ will be used for both the map and its image.) Given $p\in\Sigma$, we say Σ is *null at* p if

$$g\left(\Sigma_\star \frac{\partial}{\partial\sigma},\ \Sigma_\star \frac{\partial}{\partial\sigma}\right)\Big|_p = 0. \tag{4}$$

If Σ is null at p, then null geodesics in $L\cup\Sigma$ are tangent to Σ at p.

For $p\in\Sigma$ such that Σ is not null at p, Lemma 1 below shows that there exists a coordinate system about p in L which can be extended to Σ, and Lemma 2 below shows that there exists a complex isothermal coordinate system about p that extends to Σ.

Lemma 2 is a modification of the standard proof for the existence of isothermal coordinates (Ref. 18, Vol. IV, pp. 455–460). However, to simplify matters we restrict our attention to the case where g is analytic and can be written in *absolute time* form[9] about a point $p\in\Sigma$; that is there exist coordinates (t,x) about p such that the metric can be written

$$g = tdt\otimes dt + h(t,x)^2 dx\otimes dx, \tag{5}$$

where h is a real positive C^ω function. In this coordinate system the curve Σ is given by $t=0$. Then g^E is given by the restriction

$$g^E = g|_{t>0}. \tag{6}$$

From Ref. 9 (theorem 1) we know that sufficient conditions for writing g in absolute time form about $p\in\Sigma$ are

(i) Σ is not null at p,
(ii) with respect to any coordinate system, $\det(g_{ab})$ has a nonzero differential at p, and
(iii) $\{g_{ab}\}$ is C^ω in a neighborhood of p.

With respect to both the null and complex isothermal coordinate system we then derive the general solution of (1), specifying both its value and *normal derivative* on Σ. This data is used to match the solutions across Σ.

Lemma 1: Extension of Null Coordinate System: Given $p\in\Sigma$ such that Σ is not null at p, there exists a neighborhood of p, $U^L\subset L\cup\Sigma$ and a C^0 function

$$\Phi^L: U^L \mapsto \{(\eta_+,\eta_-)\in\mathbb{R}^2 |\, \eta_- \leqslant \eta_+\} \tag{7}$$

such that the restriction

$$\Phi^L|_L : U^L\cap L \mapsto \{(\eta_+,\eta_-)\in\mathbb{R}^2 |\, \eta_- < \eta_+\} \tag{8}$$

is a C^∞ diffeomorphism and a null coordinate system. Also

$$\Phi^L|_\Sigma : U^L\cap\Sigma \mapsto \{(\eta_+,\eta_-)\in\mathbb{R}^2 |\, \eta_- = \eta_+\}, \tag{9}$$

where

$$\eta_+\circ\Sigma(\sigma) = \eta_-\circ\Sigma(\sigma) = \sigma. \tag{10}$$

Proof: Every point $x\in L$ near p lies on the intersection of two null geodesics. We can choose U^L such that for all $x\in U^L\cap L$, both the null geodesics that intersect x also intersect Σ near p where they are not tangent. Thus for each x this gives two points, $q_1,q_2\in\Sigma$ (See Fig. 3). Let $\eta_+(x)$ be the larger of $\{\Sigma^{-1}(q_1),\Sigma^{-1}(q_2)\}$ and $\eta_-(x)$ the smaller. This construction gives a well-defined C^∞ map Φ^L, which is a diffeomorphism in the set described. Furthermore, since $\eta_\pm$=constant are null geodesics, $\partial/\partial\eta_\pm$ are null, so the metric is given by (2). ■

With respect to a null coordinate system the Lorentzian Hodge maps are given by

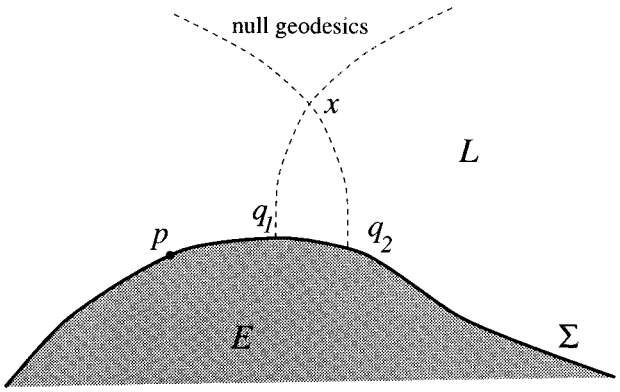

FIG. 3. Intersection of the null geodesics from x with Σ at q_1 and q_2.

$$\star 1 = \Omega^L d\eta_+ \wedge d\eta_- , \tag{11}$$

$$\star d\eta_+ = -d\eta_+ , \tag{12}$$

$$\star d\eta_- = d\eta_- , \tag{13}$$

so the wave equation (1) for $\psi^L : U^L \to \mathbb{C}$ is

$$\frac{\partial^2 \psi^L}{\partial \eta_+ \partial \eta_-} d\eta_+ \wedge d\eta_- = 0, \tag{14}$$

and its solution in this region is

$$\psi^L = \psi^L_+(\eta_+) + \psi^L_-(\eta_-), \tag{15}$$

where $\psi^L_\pm : U^L \to \mathbb{C}$. We define the value of the ψ^L on Σ and the normal derivative $\mathcal{N}\psi^L_\Sigma$ of ψ^L on Σ by

$$\psi^L_\Sigma : \Sigma \mapsto \mathbb{C}, \quad \psi^L_\Sigma(x) = \lim_{y \to x, y \in L} \psi^L(y), \tag{16}$$

$$\mathcal{N}\psi^L_\Sigma : \Sigma \mapsto \mathbb{C}, \quad \mathcal{N}\psi^L_\Sigma(x) = i_{\partial/\partial\sigma}\left(\Sigma^\star \left(\lim_{y \to x, y \in L} \star d\psi^L|_y \right) \right). \tag{17}$$

With respect to the coordinate systems (η_+, η_-) given in Lemma 1, these are given by

$$\psi^L_\Sigma(x) = \psi^L_+(\eta_+(x)) + \psi^L_-(\eta_-(x)), \tag{18}$$

$$\begin{aligned}
\mathcal{N}\psi^L_\Sigma(x) &= i_{\partial/\partial\sigma}\left(\Sigma^\star \lim_{y \to x, y \in L} \star d(\psi^L_+(\eta_+) + \psi^L_-(\eta_-))|_y \right) \\
&= i_{\partial/\partial\sigma}\left(\Sigma^\star \lim_{y \to x, y \in L} (\psi^{L\prime}_+ \star d\eta_+ + \psi^{L\prime}_- \star d\eta_-)|_y \right) \\
&= i_{\partial/\partial\sigma}\left(\Sigma^\star \lim_{y \to x, y \in L} (-\psi^{L\prime}_+ d\eta_+ + \psi^{L\prime}_- d\eta_-)|_y \right) \\
&= i_{\partial/\partial\sigma}(\Sigma^\star(-\psi^{L\prime}_+ d\eta_+ + \psi^{L\prime}_- d\eta_-)|_x) \\
&= -\psi^{L\prime}_+ \frac{\partial \eta_+ \circ \Sigma}{\partial \sigma} + \psi^{L\prime}_- \frac{\partial \eta_- \circ \Sigma}{\partial \sigma} \\
&= -\psi^{L\prime}_+(\eta_+(x)) + \psi^{L\prime}_-(\eta_-(x)),
\end{aligned} \tag{19}$$

since $\partial\eta_{\pm}\circ\Sigma/\partial\sigma=1$. Thus the normal derivative exists so long as Σ is not null.

Lemma 2: Extension of Complex Isothermal Coordinate System: Given $p\in\Sigma$ such that g is analytic and can be written in absolute time form (5) about a point $p\in\Sigma$, then there exists a neighborhood of p, $U^E\subset E\cup\Sigma$ and a C^0 function

$$\Phi^E: U^E\mapsto\{z\in\mathbb{C}|\mathrm{Im}(z)\geqslant 0\} \tag{20}$$

such that the restriction

$$\Phi^E|_E: U^E\cap E\mapsto\{z\in\mathbb{C}|\mathrm{Im}(z)>0\} \tag{21}$$

is a C^ω diffeomorphism, and a complex isothermal coordinate. Also

$$\Phi^E|_\Sigma: U^E\cap\Sigma\mapsto\mathbb{R}. \tag{22}$$

Proof: Let g be written as in (5), so that p is given by $t=0$, $x=x_0$, and g^E is given by (6). Let

$$\omega=h dx+i\sqrt{t}dt \tag{23}$$

so that

$$g^E=\omega\otimes\overline{\omega}+\overline{\omega}\otimes\omega. \tag{24}$$

We seek a nonvanishing integrating factor $\lambda(t,x)$, and a complex coordinate $z(t,x)$ such that

$$\omega\lambda=dz. \tag{25}$$

Consider the extension of ω to $\mathbb{R}^+\times\mathbb{C}$ given by

$$\omega=h(t,\xi)d\xi+i\sqrt{t}dt, \tag{26}$$

where $t\in\mathbb{R}$, $t>0$, and $\xi\in\mathbb{C}$, and where $h(t,\xi)$ is the analytic extension of $h(t,x)$ with respect to its second argument. Let

$$X=\frac{-i\sqrt{t}}{h}\frac{\partial}{\partial\xi}+\frac{\partial}{\partial t}, \tag{27}$$

a vector field on $\mathbb{R}^+\times\mathbb{C}$, which is an annihilator of ω, i.e., $\omega(X)=0$. The solution curves of X are the set of curves $t\mapsto(t,\xi(t))$, where $\xi(t)$ are solutions to the differential equation

$$\frac{dx}{dt}=-i\frac{\sqrt{t}}{h(x,t)}. \tag{28}$$

We note that the component of X in the t direction is 1, and the component of X in the imaginary ξ direction is

$$-\frac{\sqrt{t}\ \mathrm{Re}(h)}{|h|^2}, \tag{29}$$

which, near $t=0$, $\xi=x_0$, is bounded above by $\sqrt{t}$ times some factor. Therefore, near $p=(0,x_0)$, all solution curves of (28) that intersect the half-plane $\{t=0,\ \mathrm{Im}(\xi)>0\}$ also intersect the plane $\{\mathrm{Im}(\xi)=0,\ t>0\}$ and visa versa (see Fig. 4). Thus we have the map

$$\Phi^E: U^E\mapsto\{z\in\mathbb{C}|\mathrm{Im}(z)\geqslant 0\},\quad \Phi^E:(t,x)\mapsto z, \tag{30}$$

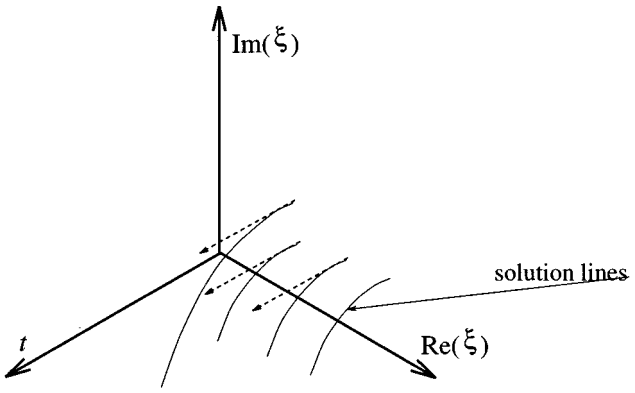

FIG. 4. The solution lines of X intersecting with the half-plane $\{\mathrm{Im}(\xi)=0,\ t>0\}$ and the half-plane $\{t=0,\ \mathrm{Im}(\xi)>0\}$ where they are parallel to the field $\partial/\partial t$.

where the solution curve connects the point $(t=t,\mathrm{Re}(\xi)=x,\mathrm{Im}(\xi)=0)\in\{\mathrm{Im}(\xi)=0,t>0\}$ to the point $(t=0,\xi=z)\in\{t=0,\mathrm{Im}(\xi)>0\}$. This map satisfies (21), and (22). Since z now labels each solution curve, and is thus a constant along it, $X(z)\equiv dz(X)=0$. In general

$$dz=\lambda\,\omega+\mu_1\overline{\omega}+\mu_2 dt, \tag{31}$$

but contracting with $\partial/\partial\overline{\xi}$ implies that $\mu_1=0$ since z and ω are analytic. Contracting with X gives $\mu_2=0$ so (25) holds.

Substituting dz into (24) gives (3) with $\Omega^E=1/\lambda\overline{\lambda}$. ■

The Euclidean Hodge maps are given with respect to the $(z,\overline{z})$ coordinate system by

$$\star 1=\Omega^2 dz\wedge d\overline{z}, \tag{32}$$

$$\star dz=-i dz, \tag{33}$$

$$\star d\overline{z}=i d\overline{z}, \tag{34}$$

so Laplace's equation for $\psi^E:U\to\mathbb{C}$ is

$$\frac{\partial^2\psi^E}{\partial z\,\partial\overline{z}}dz\wedge d\overline{z}=0 \tag{35}$$

and its solution in this region is

$$\psi^E=\psi^E_+(z)+\overline{\psi^E_-(z)}, \tag{36}$$

where $\psi^E_\pm:U\to\mathbb{C}$. Since $\partial\psi^E_\pm/\partial\overline{z}=0$ these are analytic functions. We define ψ^E_Σ and $\mathscr{N}\psi^E_\Sigma$ by replacing the symbol L with E in (16) and (17). These are given by

$$\psi^E_\Sigma(p)=\psi^E_+(p)+\overline{\psi^E_-(p)}, \tag{37}$$

$$\mathscr{N}\psi^E_\Sigma(p)=-i\psi^{E\prime}_+\frac{\partial z}{\partial\sigma}+\overline{i\psi^{E\prime}_-}\,\frac{\partial\overline{z}}{\partial\sigma}. \tag{38}$$

We have

$$\frac{\partial z}{\partial \sigma} = \frac{dx}{d\sigma} \in \mathbb{R} - \{0\}, \tag{39}$$

hence

$$\mathcal{N}\psi^E_\Sigma(p) = i\,\frac{dx}{d\sigma}\,(-\psi^{E\prime}_+ + \overline{\psi^{E\prime}_-}). \tag{40}$$

So the normal derivative exists about the point $p \in \Sigma$ so long as Σ is not null.

III. UNIQUENESS LEMMA

Lemma 3: Let $(E \cup \Sigma, g)$ be a closed pathwise connected manifold with boundary $\Sigma = \partial E$, with a Riemannian metric g which is degenerate on Σ and analytic in a neighborhood of Σ. Let there be only isolated points on Σ about which g cannot be written in absolute time form. Given a nontrivial curve $C: I \mapsto \Sigma$ where I is some interval in $\mathbb{R}$ parametrized by s and two functions $u^E, v^E: E \mapsto \mathbb{C}$ that satisfy Laplace's equation $d \star d\psi = 0$ on the interior of E, then $u^E_\Sigma|_C = v^E_\Sigma|_C$ and $\mathcal{N}u^E_\Sigma|_C = \mathcal{N}v^E_\Sigma|_C$ if and only if $u^E = v^E$.

In these equations $u^E_\Sigma(x), \mathcal{N}u^E_\Sigma(x)$ are defined by replacing ψ by the symbol u in the Euclidean version of (16) and (17).

Proof: Let (U^E, Ψ^E) be a complex isothermal chart of E about a point $p \in C(I)$ given by Lemma 2 above. For the solution $w^E = u^E - v^E$, it follows that $w^E_\Sigma|_C = 0$ and $\mathcal{N}w^E_\Sigma|_C = 0$. Thus from (37) and (40) we have

$$w^E_\pm(z) = 0 \quad \forall z \in \Psi^E \circ C(I). \tag{41}$$

Hence $w^E_\pm$ are analytic functions on the domain $\Psi^E(U^E \cap E) \subset \mathbb{C}$ where $\mathrm{Im}(\Psi^E(U^E \cap E)) > 0$. They are continuous functions on the domain $\Psi^E(U^E) \subset \mathbb{C}$ where $\mathrm{Im}(\Psi^E(U^E \cap \Sigma)) = 0$. One can perform a Schwartz reflection[19] about $\mathrm{Im}(z) = 0$ to produce an analytic function on a domain with a nontrivial subset of $\Psi^E(\Sigma)$ in its interior. Since $\Psi^E(C)$ is not a distinct collection of points

$$w^E_\pm(z) = 0 \quad \forall z \in \Psi^E(U^E). \tag{42}$$

For any other chart $(\widetilde{U}, \widetilde{\Psi})$ where $U \cap \widetilde{U} \neq \varnothing$, since

$$w^E_\pm(z) = 0 \quad \forall z \in \widetilde{\Psi}(\widetilde{U} \cap U), \tag{43}$$

then

$$w^E_\pm(z) = 0 \quad \forall z \in \widetilde{\Psi}(\widetilde{U}). \tag{44}$$

Thus $w^E_\pm = 0$, or $u^E = v^E$ on E. ■

This is a uniqueness proof, not an existence proof. Given two functions $f_1, f_2: C(I) \mapsto \mathbb{C}$ there will in general be no solution $u: E \mapsto \mathbb{C}$ to Laplace's equation such that $u|_C = f_1$ and $i_{C\star}\partial/\partial s \star u = f_2$ for any neighborhood of $C(I)$.

Example 1: Let $\Psi^E(U^E) = \{z \in \mathbb{C} | \mathrm{Im}(z) < 0\}$ and $\Psi^E(C) = \{z \in \mathbb{C} | \mathrm{Im}(z) = 0\}$. Let

$$\psi^E_\Sigma(x) = \begin{cases} e^{(-1/x^2)}, & x > 0, \\ 0, & x \leqslant 0, \end{cases}$$
$$\mathcal{N}\psi^E_\Sigma(x) = 0 \quad \forall x \in \mathbb{R}, \tag{45}$$

where $x \in \Psi^E(C)$. According to Lemma 3, the data on $x<0$ implies that $\psi(z)=0\ \forall z \in \Psi^E(U^E)$, while the data on $x>0$ implies that $\psi(z)=\exp(-1/x^2)\ \forall z \in \Psi^E(U^E)$. Thus there is no solution to Laplace's equation on $\Psi^E(U^E)$ consistent with this boundary data.

This does not contradict the Cauchy–Kowalewski theorem[20,21] on the existence of solutions to PDE's with analytic Cauchy data since the data (45) is not analytic.

IV. UNIQUENESS THEOREM

In order to match Euclidean solutions to Lorentzian solutions, we must adopt some boundary conditions along the degeneracy curve Σ.

The class of boundary conditions adopted here relate boundary data in a **linear** and **pointwise invertible** manner. Thus for $J:\Sigma \mapsto GL_2(\mathbb{C})$

$$\begin{pmatrix} \psi^L_\Sigma(x) \\ \mathcal{N}\psi^L_\Sigma(x) \end{pmatrix} = J(x) \begin{pmatrix} \psi^E_\Sigma(x) \\ \mathcal{N}\psi^E_\Sigma(x) \end{pmatrix}. \tag{46}$$

The ''natural'' boundary conditions given by continuity of ψ and its normal derivative across Σ correspond to

$$J(x)=\mathbf{1}. \tag{47}$$

We note in passing that the theorem below is applicable even when ψ is restricted such that $\mathcal{N}\psi^E_\Sigma(x)=\mathcal{N}\psi^L_\Sigma(x)=0$.

Theorem: *Let (M,g) be a two-dimensional manifold M with a metric g that is degenerate along a curve Σ, partitioning M into a Lorentzian domain L and a connected Euclidean domain E. Let g be analytic in a neighborhood of Σ, and let there only be isolated points on Σ where g cannot be written in absolute time form. Let $C \subset L$ be an acausal curve, parametrized by s, such that $D_0(C)\cap\Sigma$ contains an arc. Given two solutions of (1) $u,v:M\mapsto\mathbb{C}$ satisfying any boundary condition in the class above, then $u|_C=v|_C$ and $(C^\star \star du)(\partial/\partial s)=(C^\star \star dv)(\partial/\partial s)$ if and only if $u|_{D_0(C\cup\Sigma)\cup E} = v|_{D_0(C\cup\Sigma)\cup E}$, i.e., u and v agree on the entire shaded area indicated in Fig. 2.*

Proof: Since u and v have the same Cauchy data on C, then if $w=u-v$ it follows that $w|_{D_0(C)} = 0$. Hence w has zero Cauchy data on the Lorentzian side of $D_0(C)\cap\Sigma$, i.e.,

$$w^L_\Sigma(x)=0 \quad \text{and} \quad \mathcal{N}w^L_\Sigma(x)=0 \quad \forall x \in D_0(C)\cap\Sigma. \tag{48}$$

In these equations $w^L_\Sigma(x)$, $\mathcal{N}w^L_\Sigma(x)$, $w^E_\Sigma(x)$, and $\mathcal{N}w^E_\Sigma(x)$ are defined by replacing ψ by w in (16) and (17). Since the boundary conditions are linear and pointwise invertible, we have zero Cauchy data for w on the Euclidean side of $D_0(C)\cap\Sigma$, i.e.,

$$w^E_\Sigma(x)=0 \quad \text{and} \quad \mathcal{N}w^E_\Sigma(x)=0 \quad \forall x \in D_0(C)\cap\Sigma. \tag{49}$$

Hence $w|_E=0$ from Lemma 3. This now implies zero Cauchy data for w on the Euclidean side of the whole of Σ, i.e.,

$$w^E_\Sigma(x)=0 \quad \text{and} \quad \mathcal{N}w^E_\Sigma(x)=0 \quad \forall x \in \Sigma. \tag{50}$$

Thus these boundary conditions give zero Cauchy data for w on the Lorentzian side of the *whole* of Σ. Since the Cauchy data for w on C is zero as well, it follows that $w|_{D_0(C\cup\Sigma)\cup E} = 0$. ■

Again we note that this is a uniqueness theorem. In general no solution to (1) on M will exist satisfying (46) with Cauchy data on some C satisfying the conditions of this theorem. The requirement that $D_0(C)\cap\Sigma$ is nontrivial is necessary. If the domain of null dependence of C contains a single point in common with the Euclidean domain E, it is not difficult to construct a situation in which there exists more than one solution on E compatible with the Cauchy data.

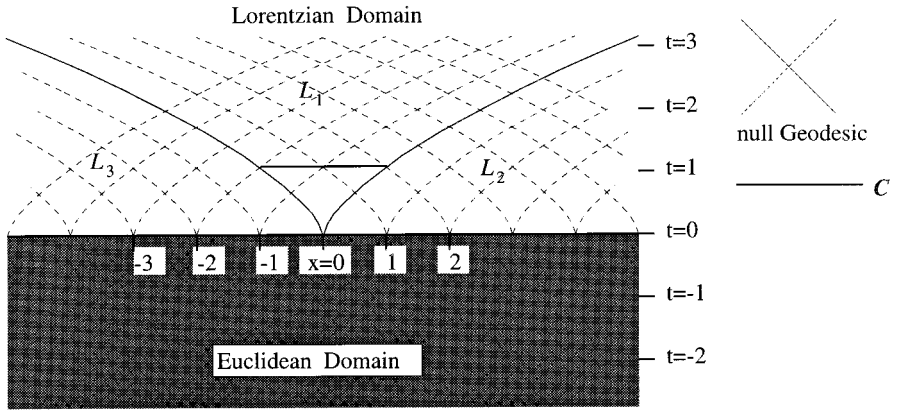

FIG. 5. Example where $D_0(C)\cap\Sigma$ is trivial.

Example 2: Let $M=\mathbb{R}^2$ and $g=-\frac{9}{4}tdt\otimes dt+dx\otimes dx$. We wish to find solutions that have zero Cauchy data on $C=\{(-1,x),-1\leqslant x\leqslant 1\}$. The null geodesics (denoted by dotted lines in Fig. 5) are given by $x\pm t^{(3/2)}=$const. Clearly one solution that also satisfies the natural boundary conditions (47) is $\psi=0$ on M. However, one readily verifies that another solution is

$$\psi|_L(x,t)=\begin{cases}0, & x+t^{3/2}>0, x-t^{3/2}<0 \quad (L_1 \text{ in Fig. 5}),\\ (1-i)\sqrt{x-t^{3/2}}, & x-t^{3/2}>0, t>0 \quad (L_2 \text{ in Fig. 5}),\\ (1-i)\sqrt{-x-t^{3/2}}, & x+t^{3/2}>0, t>0 \quad (L_3 \text{ in Fig. 5}),\end{cases} \tag{51}$$

$$\psi|_E(x,t)=(\sqrt{x+it^{3/2}})+i\overline{(\sqrt{x+it^{3/2}})}, \tag{52}$$

where $\sqrt{\ }:\{z\in\mathbb{C}:\mathrm{Im}(z)\leqslant 0\}\mapsto\{z\in\mathbb{C}:\mathrm{Re}(z)\geqslant 0,\mathrm{Im}(z)\leqslant 0\}$.

In a two-dimensional universe with a known degenerate metric one might imagine one could use the theorem above to predict the behavior of the scalar field beyond causally connected regions. However, realistic Cauchy data that is obtained from physical measurements will contain errors. Since it is possible to find global solutions that lie arbitrarily close to such data in the domain of the Cauchy curve but are arbitrarily disparate elsewhere, one must conclude that the propagation of such errors cannot be controlled.

Example 3: Referring to Fig. 5, enlarge C to $\hat{C}=\{(t=1,x):|x|<2\}$. Assume the ''experimental'' data given on $\hat{C}$ prescribes that a function and its normal derivative are zero to an accuracy ϵ. If ϵ is zero, then the theorem above implies that the only global solution is identically zero. For $\epsilon>0$, given any continuous function $f:\mathbb{R}\mapsto\mathbb{C}$ such that $f(x)=0$, $\forall|x|\leqslant 3$, then from the Boltzano–Wiesstrass theorem there exists a polynomial $\mathscr{P}:\mathbb{R}\mapsto\mathbb{C}$ such that $|\mathscr{P}(x)-f(x)|<\epsilon/2$, $\forall x\leqslant 5$. The function $\mathscr{P}(x+it^{3/2})$ solves Laplace's equation (1) in the Euclidean domain and $|\mathscr{P}(x)|<\epsilon/2$ on the interval $\{(t=0,x):|x|<3\}$. However, this function extends to a global solution of (1) on $\mathbb{R}^2$ and is consistent with the ''experimental'' Cauchy data on $\hat{C}$ within the prescribed error. This is similar to Hadamard's example[22] demonstrating that certain initial value problems are not *well posed* for Laplace's equation.

V. IMPLICATIONS FOR QUANTIZATION

The standard method[23–25] for constructing a quantum field theory in a curved space–time is to consider a globally hyperbolic manifold M possessing Cauchy surfaces C^{in} and C^{out} in (asymptotically) flat regions upon which one sets up Hilbert spaces $\mathscr{H}(C^{\text{in}})\oplus\overline{\mathscr{H}(C^{\text{in}})}$ and $\mathscr{H}(C^{\text{out}})\oplus\overline{\mathscr{H}(C^{\text{out}})}$ of solutions to local field equations.

The Klein–Gordon Hermitian bilinear form is defined as

$$\langle u,v\rangle_C=\frac{1}{2\pi i}\int_C \overline{u}\star dv - v\star d\overline{u}, \tag{53}$$

where u,v are Cauchy data on a Cauchy surface C for solutions to the scalar wave (Klein–Gordon) equation. For C in a flat region of space–time, the (maximal) subspace of positive frequencies, $\mathscr{H}(C)$, is defined by some timelike vector field which is Killing in this region, such that the restriction of $\langle,\rangle_C$ to $\mathscr{H}(C)$ is positive definite. The restriction of $\langle,\rangle_C$ to its conjugate $\overline{\mathscr{H}(C)}=\{\overline{u}|u\in\mathscr{H}(C)\}$ is negative definite. We have

$$\langle u,v\rangle_C=\langle u_+,v_+\rangle_C+\langle\overline{u_-},\overline{v_-}\rangle_C \tag{54}$$

where $u=u_+ +\overline{u_-}$, $v=v_+ +\overline{v_-}$, and $u_\pm,v_\pm\in\mathscr{H}(C)$. The Hilbert space $\mathscr{H}(C)\oplus\overline{\mathscr{H}(C)}$ is defined with respect to the ''true'' inner product

$$\langle\langle u,v\rangle\rangle_C=\langle u_+,v_+\rangle_C-\langle\overline{u_-},\overline{v_-}\rangle_C. \tag{55}$$

For any solution $u:M\mapsto\mathbb{C}$ there is Cauchy data associated with $u^{\text{in}}\in\mathscr{H}(C^{\text{in}})\oplus\overline{\mathscr{H}(C^{\text{in}})}$ for u, and Cauchy data associated with $u^{\text{out}}\in\mathscr{H}(C^{\text{out}})\oplus\overline{\mathscr{H}(C^{\text{out}})}$. The corresponding quantum system is said to be *unitary* if $\langle u^{\text{in}},v^{\text{in}}\rangle_{C^{\text{in}}}=\langle u^{\text{out}},v^{\text{out}}\rangle_{C^{\text{out}}}$. This is guaranteed for a globally hyperbolic manifold since the current $\overline{u}\star du-u\star d\overline{u}$ is conserved. The linear map $\mathscr{A}:\mathscr{H}(\mathscr{C}^{\text{in}})\oplus\overline{\mathscr{H}(\mathscr{C}^{\text{in}})}\mapsto\mathscr{H}(\mathscr{C}^{\text{out}})\oplus\overline{\mathscr{H}(\mathscr{C}^{\text{out}})}$ defined by $u^{\text{in}}\mapsto u^{\text{out}}=\mathscr{A}u^{\text{in}}$ may be represented as

$$\mathscr{A}=\begin{pmatrix}\alpha & \beta\\ \overline{\beta} & \overline{\alpha}\end{pmatrix} \tag{56}$$

and defines the Bogolubov transformations:

$$\alpha:\mathscr{H}(C^{\text{in}})\mapsto\mathscr{H}(C^{\text{out}}), \tag{57}$$

$$\beta:\mathscr{H}(C^{\text{in}})\mapsto\overline{\mathscr{H}(C^{\text{out}})}. \tag{58}$$

From these one may construct the Scattering matrix in a Fock space basis of many particle states in the quantum theory. The expectation value of the particle number density with respect to the image of a Fock space vacuum state under this Scattering matrix can be shown to be $\Sigma_{ij}|\beta_{ij}|^2$. For a finite theory β must be Hilbert–Schmidt, i.e., $\Sigma_{ij}|\beta_{ij}|^2<\infty$ (Ref. 23, p. 140). This implies that $\mathscr{A}$ must be bounded.

It is of interest to see to what extent the formalism above breaks down in the context of a quantum field theory of massless scalar particles in a background two-dimensional space–time with a degenerate metric. We approach this by considering a simple example in which we can readily calculate the Bogolubov coefficients. Let M be a cylinder with coordinates $\{(\tau,\theta)|-\infty<\tau<\infty,0\leqslant\theta<2\pi\}$, together with the axially symmetric metric

$$g=g_{\tau\tau}(\tau)d\tau\otimes d\tau+g_{\theta\theta}(\tau)d\theta\otimes d\theta, \tag{59}$$

where $g_{\theta\theta}(\tau)>0$ for all τ. Here M has a Euclidean region E (where $g_{\tau\tau}>0$) sandwiched between two Lorentzian regions labelled L^{in} and L^{out} (where $g_{\tau\tau}<0$). Let there be a flat region $L^{\text{in}}_{\text{flat}}\subset L^{\text{in}}$, i.e., where $g_{\tau\tau}=-1$, $g_{\theta\theta}=1$, containing the Cauchy surface $C^{\text{in}}\subset L^{\text{in}}_{\text{flat}}$. Similarly let $C^{\text{out}}\subset L^{\text{out}}_{\text{flat}}\subset L^{\text{out}}$. Let Σ^{in} be the degeneracy ring $\tau=\tau^{\text{in}}$ that partitions E from L^{in}. Similarly suppose Σ^{out} is the degeneracy ring $\tau=\tau^{\text{out}}>\tau^{\text{in}}$ that partitions E from L^{out}. See Ref. 15 for explicit details of such a construction.

A transformation to complex coordinates, such that the metric may be written as (3), is given by

$$z=\Psi(\tau,\theta)=e^{i\theta}\exp\left(\int_{\tau^{\rm in}}^{\tau}\left(\frac{g_{\tau\tau}(\tau')}{g_{\theta\theta}(\tau')}\right)^{1/2}d\tau'\right)\quad\text{where}\quad \tau^{\rm in}\leqslant\tau\leqslant\tau^{\rm out},\quad 0\leqslant\theta<2\pi. \tag{60}$$

Thus $\Psi(E)$ is an annulus about the origin with radii 1 and e^{ξ} where

$$\xi=\int_{\tau^{\rm in}}^{\tau^{\rm out}}\left(\frac{g_{\tau\tau}(\tau')}{g_{\theta\theta}(\tau')}\right)^{1/2}d\tau'. \tag{61}$$

A convenient basis of nonzero mode solutions to (1) in the Lorentzian flat domain $L^{\rm in}_{\rm flat}$ is

$$\{e^{\rm in}_k=|2\pi k|^{-1/2}e^{-i(|k|\tau+k\theta)},\overline{e^{\rm in}_k}=|2\pi k|^{-1/2}e^{i(|k|\tau+k\theta)}\}_{k\in\mathbb{Z},k\neq 0}, \tag{62}$$

where (τ,θ) lie in $L^{\rm in}_{\rm flat}$. This basis is in 1-to-1 correspondence with the set of Cauchy data on $C^{\rm in}$ and hence provides a basis of one-particle in-states for $\mathscr{H}(C^{\rm in})\oplus\overline{\mathscr{H}(C^{\rm in})}$, with $\{e^{\rm in}_k\}$ giving a basis for $\mathscr{H}(C^{\rm in})$. A basis of one-particle out-states is likewise defined from $\{e^{\rm out}_k,\overline{e^{\rm out}_k}\}$ where (τ,θ) lie in $L^{\rm out}_{\rm flat}$.

The Bogolubov coefficients can easily be calculated from the matching conditions (47):

$$\alpha_{kk}=\cosh(k\xi)\quad \alpha_{kj}=0,\quad j\neq k, \tag{63}$$

$$\beta_{kk}=i\,\sinh(k\xi),\quad \beta_{kj}=0,\quad j\neq k. \tag{64}$$

It is obvious that β is not Hilbert–Schmidt. Furthermore, it is easy to verify that the linear map $\mathscr{A}:\mathscr{H}(C^{\rm in})\oplus\overline{\mathscr{H}(C^{\rm in})}\mapsto\mathscr{H}(C^{\rm out})\oplus\overline{\mathscr{H}(C^{\rm out})}$ is not even bounded. This follows since one can construct a solution u on M which has a pole on $\Sigma^{\rm out}$, e.g.,

$$u(\tau,\theta)=\frac{1}{\Psi(\tau,\theta)-\Psi(\tau^{\rm out},0)}. \tag{65}$$

Now $\|u^{\rm in}\|_{C^{\rm in}}<\infty$ but $\|u^{\rm out}\|_{C^{\rm out}}=\infty$, which could not happen if $\mathscr{A}$ were bounded. ($\|\mathscr{A}(u^{\rm in})\|_{C^{\rm out}}=\|u^{\rm out}\|\leqslant\|\mathscr{A}\|\|u^{\rm in}\|_{C^{\rm in}}$.) However on the subspace consisting of finite sums of basis elements above, the mapping $\mathscr{A}$ has a unitary restriction. Furthermore, it can be shown that if $u:M\mapsto\mathbb{C}$ is bounded, and $u^{\rm in}\in\mathscr{H}(C^{\rm in})\oplus\overline{\mathscr{H}(C^{\rm in})}$ is associated Cauchy data, then $\langle u^{\rm in},u^{\rm in}\rangle_{C^{\rm in}}=\langle\mathscr{A}u^{\rm in},\mathscr{A}u^{\rm in}\rangle_{C^{\rm out}}$.

In order to construct $\mathscr{A}$ from initial Cauchy data $u^{\rm in}\in\mathscr{H}(C^{\rm in})\oplus\overline{\mathscr{H}(C^{\rm in})}$, one or more of the following obstructions may arise when attempting to calculate the corresponding element $u^{\rm out}\in\mathscr{H}(C^{\rm out})\oplus\overline{\mathscr{H}(C^{\rm out})}$:

(1) There is no compatible solution in any Euclidean neighborhood of $\Sigma^{\rm in}$. An illustration of this has been given in example 1.

(2) Although a solution in a neighborhood of $\Sigma^{\rm in}$ exists, this solution has a ''natural boundary'' which prevents it propagating to $\Sigma^{\rm out}$. For example, consider the analytic function $f:\mathbb{D}\mapsto\mathbb{C}$,

$$f(z)=\sum_{n=0}^{\infty}\left(\frac{z}{R}\right)^{(n!)}, \tag{66}$$

where $\mathbb{D}\subset\mathbb{C}$ is the open disk of radius R. This function is infinite for all $z=Re^{p/q}$, $p,q\in\mathbb{Z}$, and is therefore said to have a natural boundary on $\partial\mathbb{D}$. It cannot be analytically continued beyond $\partial\mathbb{D}$. If $1<R<e^{\xi}$, then $\Psi(\Sigma^{\rm in})\subset\mathbb{D}$ and $\Psi(\Sigma^{\rm out})\not\subset\mathbb{D}$, hence the state in $\mathscr{H}(C^{\rm in})\oplus\overline{\mathscr{H}(C^{\rm in})}$ corresponding to f cannot be propagated to $\Sigma^{\rm out}$.

(3) The state propagates to Σ^{out} but contains a singularity on Σ^{out}. This may give an infinite norm for the state at C^{out}.

(4) An analytic continuation of the state on Σ^{in} to Σ^{out} exists with singularities in E. Such singularities can give rise to nontrivial de Rham periods and contribute to the breakdown of unitarity. In Ref. 15 it is suggested that a resolution to this problem is to excise those domains where such solutions are singular by attaching extra tubes to the manifold. This correlates the space of allowable Cauchy data to the global topology of the manifold. One can then restore unitarity for this particular initial state by labelling some of the tubes as ''in'' and the others as ''out.'' This resolution works for any particular state but cannot be applied to the entire space of states without removing the entire Euclidean domain.

VI. CONCLUSIONS

One of the most striking results of the theorem above is that a space–time with a Euclidean domain does not necessarily require a traditional Cauchy surface in order for one to be able to predict a global solution of the (scalar) wave equation. Cauchy data on any acausal curve may be sufficient. To effect such a prediction it is only necessary that (i) the domain of null dependence of the acausal curve has a nontrivial intersection with the Euclidean domain, (ii) the solution in the two domains is connected by ''linear pointwise-invertible'' junction conditions, and (iii) the boundary of the Euclidean domain is a Cauchy curve for the whole Lorentzian domain. If the degenerate metric possesses a spacelike Killing isometry in the Lorentzian domain, then (iii) is automatic.

For example, a two-dimensional cosmology may be modelled with a metric that is induced by appropriately immersing a paraboloid in Minkowski three-space. If the Euclidean domain corresponds to a parabolic cap, then the ring of signature change is a Cauchy curve for the prediction of solutions to the wave equation for the whole paraboloid. However, every acausal segment in the Lorentzian region provides a family of (disconnected) domains of null determination. If one such domain has a nontrivial intersection with the ring of signature change, then any global solution satisfying the junction conditions above can be calculated from just the Cauchy data on the original segment. However, in general, given arbitrary Cauchy data on such a segment, there may be no such global solution.

Although our results have relied fundamentally on the conformal structure of the scalar wave equation and the dimensionality of the background manifold, we speculate that many of these features will persist in theories that lack conformal symmetry, such as the massive Klein–Gordon equation in three or more dimensions. The extension of our methods would exploit the general theory of elliptic partial differential equations.[20–22,27]

The traditional construction of a local quantum field theory on a space–time relies on a number of features that are conspicuously absent on manifolds with a degenerate metric. Most notably it proves difficult to construct a space of asymptotic quantum states that can be connected by a unitary Scattering matrix.

Although it is not difficult to find subspaces of bounded Lorentzian solutions, such solutions may become singular when continued to a Euclidean region via a broad class of matching conditions. Thus a well-behaved Lorentzian solution can propagate into the future without attenuation and pass smoothly into a Euclidean domain where it may rapidly explode. For example, for any $0<r<1$ consider the sum of two packets

$$u(\tau,\theta)=\frac{1}{1-re^{i(\theta+\hat{\tau})}}+\frac{1}{1-re^{i(\theta-\hat{\tau})}}, \tag{67}$$

where

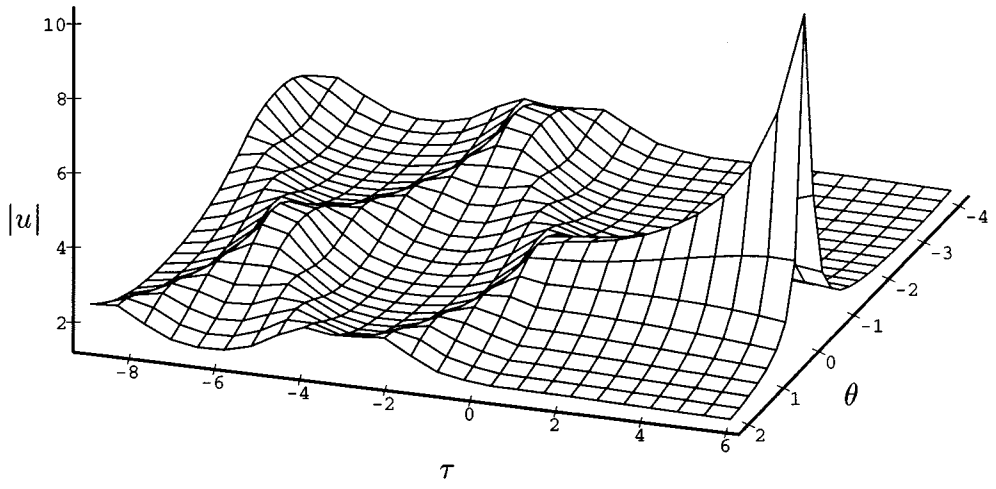

FIG. 6. Evolution with τ of the modulus of a pair of counterrotating Lorentzian wavepackets u across a metric degeneracy at $\tau=0$. The angular coordinate for the cylindrical manifold is denoted by $0\leqslant\theta<2\pi$.

$$\hat{\tau}=\int_{\tau}^{\tau^{\mathrm{in}}}\left(\frac{-g_{\tau\tau}(\tau')}{g_{\theta\theta}(\tau')}\right)^{1/2}d\tau' \tag{68}$$

for $(\tau,\theta)\in L^{\mathrm{in}}$, and

$$u(\tau,\theta)=\frac{1}{1-z}+\frac{\overline{z}}{\overline{z}-r^2} \tag{69}$$

for $(\tau,\theta)\in E$ where $z=\Psi(\tau,\theta)$ is given by (60). This is illustrated in Fig. 6, with $r=0.4$, for the cylindrical manifold M above. For $\tau<\tau^{\mathrm{in}}$, the bounded Lorentzian wave packets counterrotate around the cylinder unattenuated, until they reach the signature ring at $\tau^{\mathrm{in}}=0$. This Lorentzian solution is then matched to the Euclidean one using the junction condition (47), but with the additional constraint that the normal derivatives on either side of the degeneracy curve vanish. The solution clearly becomes an exploding peak as it diffuses into the Euclidean region, becoming singular before escaping to the Lorentzian domain.

We have also explicitly demonstrated several other obstructions than can arise when trying to construct unitary operators in a basis of asymptotic states. Although we cannot prove that no such construction is possible, the results above lead us to strongly suspect that without a radical departure from traditional methods a local unitary quantum field theory on a background with a fixed topology and degenerate metric does not exist. This conclusion does not necessarily rule out classical geometries with signature change. A more comprehensive analysis would consider a coupled field and geometry system with dynamic topology. Such a quantum geometry would then allow classical histories describing a manifold with a topology consistent with the corresponding bounded global field configuration. In the weak-field semi-classical limit such coupled states might select a self-consistent classical background geometry with a degenerate metric upon which one could construct an approximate quantum matter field description.

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Scattering in one dimension: The coupled Schrödinger equation, threshold behaviour and Levinson's theorem

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We formulate scattering in one dimension due to the coupled Schrödinger equation in terms of the S matrix, the unitarity of which leads to constraints on the scattering amplitudes. Levinson's theorem is seen to have the form $\eta(0)=\pi(n_b+\frac{1}{2}n-\frac{1}{2}N)$, where $\eta(0)$ is the phase of the S matrix at zero energy, n_b the number of bound states with nonzero binding energy, n the number of half-bound states, and N the number of coupled equations. In view of the effects due to the half-bound states, the threshold behaviour of the scattering amplitudes is investigated in general, and is also illustrated by means of particular potential models. © *1996 American Institute of Physics.* [S0022-2488(96)03112-X]

I. INTRODUCTION

The quantum mechanics of one-dimensional scattering describes many actual physical phenomena to a good approximation. (For example, see Ref. 1 for a review of tunneling times.) One-dimensional models are furthermore often employed to gain deeper insight into the approximations used in order to make the more complex three-dimensional systems tractable. It is therefore not surprising that there have been many articles, also in this journal, dealing with various aspects of such scattering. In particular a number of papers have appeared in recent years on the threshold behaviour of one-dimensional scattering and Levinson's theorem.[2–7] These studies have been limited to systems without coupling.

In this paper we wish to investigate scattering described by a system of coupled differential equations with a particular interest in developing a formulation for Levinson's theorem and in gaining insight into the threshold properties of the scattering amplitudes. This work can be seen as a special case of multichannel scattering for which the threshold energies are equal. In subsequent work, we intend to generalize to the case of differing threshold energies. Although in previous work on one-dimensional scattering one has at times employed a ''partial wave'' analysis[7,8] or a parity-eigenstate representation,[2,6] we have chosen to use the traditional, more ''physical,'' approach involving states with incident waves coming from a single direction.

In Sec. II we express the scattering properties in terms of the S matrix, the unitarity of which leads to specifiable constraints on the scattering amplitudes. For the proof of the generalized Levinson's theorem we make use of the complete set of orthonormal states of the Hamiltonian; this is an alternative to the approach involving the analyticity of the scattering amplitudes. The proof of Levinson's theorem depends on the threshold properties of the scattering amplitudes. These properties are of interest in their own right, especially in connection with scattering time delay and advance,[6] and therefore we discuss the zero-energy behaviour of the amplitudes at some length.

The factorization of the S matrix is generalized to the coupled system in Sec. III. We also

indicate that there is a class of finitely periodic matrix potentials for which the scattering amplitudes can be found in a way analogous to the case with no coupling.

In Sec. IV we discuss a number of specific potential models to elucidate and amplify general results. We conclude with a brief discussion of our results in Sec. V.

II. *S*-MATRIX FORMULATION

The one-dimensional scattering problem has been studied in terms of the S matrix by a number of authors. (See, for example, Refs. 7, 9–12.) We extend the formalism to include a matrix potential function. The Schrödinger equation for a stationary state of such a system is

$$-\frac{d^2\Psi}{dx^2}+V(x)\Psi=k^2\Psi, \tag{2.1}$$

where $V(x)$ is a real, symmetric $N\times N$ matrix, k^2 the energy of the system, and $\Psi(k,x)$ the wave function, which is an N-dimensional column vector. For large values of $|x|$ the potential matrix $V(x)$ approaches zero sufficiently fast, so that in the asymptotic region $\Psi(k,x)$ represents a free-particle wave function. To ensure this we will take $V(x)=\mathbf{0}$ for $|x|>R$, R being the range of the potential. (The boldface $\mathbf{0}$ and $\mathbf{1}$ refer to the zero and identity $N\times N$ matrices, respectively.) Furthermore, we assume that $|V_{ij}(x)|$ is integrable for $i,j=1,\ldots,N$.

The physical scattering solutions of Eq. (2.1) at a given energy k^2 can be written as the columns of $N\times N$ matrices $\psi(k,x)$ and $\tilde{\psi}(k,x)$ which are uniquely determined by the boundary conditions,

$$\psi(k,x)\sim\begin{cases}\mathbf{1}e^{ikx}+\rho(k)e^{-ikx}, & x\to-\infty\\ \tau(k)e^{ikx}, & x\to\infty\end{cases} \tag{2.2}$$

and

$$\tilde{\psi}(k,x)\sim\begin{cases}\tilde{\tau}(k)e^{-ikx}, & x\to-\infty\\ \mathbf{1}e^{-ikx}+\tilde{\rho}(k)e^{ikx}, & x\to\infty.\end{cases} \tag{2.3}$$

We will refer to ψ and $\tilde{\psi}$ as the solution matrices. Note that the columns of ψ contain the wave functions with an incident wave from the left, whereas the columns of $\tilde{\psi}$ include those with an incident wave from the right. The $N\times N$ matrices $\rho,\tilde{\rho},\tau,\tilde{\psi}$ are generalizations of the usual reflection and transmission amplitudes.[13,14] The set of N-dimensional column vectors of matrices ψ and $\tilde{\psi}$ represent solutions of Eq. (2.1). The linear independency of these solutions can be shown by considering the $2N\times 2N$ matrix,

$$W(\psi,\tilde{\psi})=\begin{pmatrix}\psi & \tilde{\psi}\\ \psi' & \tilde{\psi}'\end{pmatrix}, \tag{2.4}$$

in which the prime indicates the derivative with respect to x. In Appendix A we show that the $\det W(\psi,\tilde{\psi})$ is a constant, which is nonzero if and only if the solutions are linearly independent. Its value, determined from the asymptotic forms of ψ and $\tilde{\psi}$, is

$$\det W(\psi,\tilde{\psi})=\det(\tau(k))(-2ik)^N. \tag{2.5}$$

Thus when both k and $\det\tau(k)$ are nonzero, the columns of ψ and $\tilde{\psi}$ give $2N$ linearly independent solutions.

In order to define the S matrix, we consider the general solution matrix in the asymptotic region,

$$\Phi(k,x)\sim\begin{cases}Ae^{ikx}+B'e^{-ikx}, & x\to-\infty\\ A'e^{ikx}+Be^{-ikx}, & x\to\infty,\end{cases} \tag{2.6}$$

where A,A',B,B' are $N\times N$ matrices. Since the unprimed matrices are associated with incoming waves and the primed matrices with outgoing waves, the S matrix can be defined as the matrix that transforms the coefficients of the incoming waves into those of the outgoing waves,[7,15] so that

$$\begin{pmatrix}A'\\ B'\end{pmatrix}=S\begin{pmatrix}A\\ B\end{pmatrix}=\begin{pmatrix}S_{aa} & S_{ab}\\ S_{ba} & S_{bb}\end{pmatrix}\begin{pmatrix}A\\ B\end{pmatrix}. \tag{2.7}$$

Clearly, S is a $2N\times 2N$ matrix. We can write it in terms of the transmission and reflection amplitudes by making use of the special cases for which $(A,B)=(\mathbf{1},\mathbf{0})$ and $(A,B)=(\mathbf{0},\mathbf{1})$. The result is

$$S=\begin{pmatrix}S_{aa} & S_{ab}\\ S_{ba} & S_{bb}\end{pmatrix}=\begin{pmatrix}\tau & \tilde{\rho}\\ \rho & \tilde{\tau}\end{pmatrix}. \tag{2.8}$$

The S matrix contains $4N^2$ complex elements or $8N^2$ real parameters. As we will see below there are a number of relations between the transmission and reflection amplitudes, which will reduce the number of independent real parameters.

A. Relation between reflection and transmission amplitudes

Constraints on the transmission and reflection amplitudes follow from the Schrödinger equation (2.1). Consider two solution matrices $\psi_1(k,x)$ and $\psi_2(k,x)$, then

$$\psi_2''=(k^2-V)\psi_2 \quad \text{and} \quad \psi_2^{\dagger\prime\prime}=\psi_2^\dagger(k^2-V), \tag{2.9}$$

so that

$$\psi_2^{\dagger\prime\prime}\psi_1=\psi_2^\dagger(k^2-V)\psi_1. \tag{2.10}$$

The Schrödinger equation, Eq. (2.1), for ψ_1 premultiplied by $\psi_2^\dagger$ yields

$$\psi_2^\dagger\psi_1''=\psi_2^\dagger(k^2-V)\psi_1. \tag{2.11}$$

Subtracting Eqs. (2.10) and (2.11), we obtain

$$\psi_2^{\dagger\prime\prime}\psi_1-\psi_2^\dagger\psi_1''=\frac{d}{dx}[\psi_2^{\dagger\prime}\psi_1-\psi_2^\dagger\psi_1']=0, \tag{2.12}$$

which leads to

$$\psi_2^{\dagger\prime}\psi_1-\psi_2^\dagger\psi_1'=\text{ constant matrix}. \tag{2.13}$$

If we now insert the asymptotic forms of ψ or $\tilde{\psi}$ for ψ_1 or ψ_2 into Eq. (2.13) and equate the expression at $-\infty$ to that at $+\infty$, we obtain the following relations:

$$\tau^\dagger\tau+\rho^\dagger\rho=\tilde{\tau}^\dagger\tilde{\tau}+\tilde{\rho}^\dagger\tilde{\rho}=\mathbf{1}, \tag{2.14}$$

$$\rho^\dagger\tilde{\tau}+\tau^\dagger\tilde{\rho}=\tilde{\tau}^\dagger\rho+\tilde{\rho}^\dagger\tau=\mathbf{0}. \tag{2.15}$$

Equations (2.14) and (2.15) are equivalent to the statement that $S^\dagger S = I$, where I is the $2N \times 2N$ identity matrix.

Further relations are found by using the time-reversal symmetry of the system. Since $V(x)$ is real, the complex conjugate solution matrices ψ^* and $\tilde{\psi}^*$ are also solutions of the Schrödinger equation. By complex conjugating Eq. (2.6), we see that the roles of the incoming and outgoing asymptotic waves are reversed, and indeed Eq. (2.7) is valid when $A \to B'^*$, $B \to A'^*$, $A' \to B^*$, and $B' \to A^*$. Thus Eq. (2.7) may be written as

$$\begin{pmatrix} B^* \\ A^* \end{pmatrix} = S \begin{pmatrix} B'^* \\ A'^* \end{pmatrix}. \tag{2.16}$$

Multiplying on the left by $S^\dagger$ and using $S^\dagger S = I$, we find that

$$\begin{pmatrix} B'^* \\ A'^* \end{pmatrix} = S^\dagger \begin{pmatrix} B^* \\ A^* \end{pmatrix}, \tag{2.17}$$

which leads to

$$\begin{pmatrix} A' \\ B' \end{pmatrix} = \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ \mathbf{1} & \mathbf{0} \end{pmatrix} S^T \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ \mathbf{1} & \mathbf{0} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix}, \tag{2.18}$$

where S^T is the transpose of S. Thus

$$S = \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ \mathbf{1} & \mathbf{0} \end{pmatrix} S^T \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ \mathbf{1} & \mathbf{0} \end{pmatrix}, \tag{2.19}$$

from which it follows that

$$\tilde{\tau} = \tau^T, \quad \rho = \rho^T, \quad \text{and} \quad \tilde{\rho} = \tilde{\rho}^T. \tag{2.20}$$

Inserting these expressions into Eqs. (2.14) and (2.15), we obtain

$$\tilde{\tau}\tilde{\tau}^\dagger + \rho\rho^\dagger = \tau\tau^\dagger + \tilde{\rho}\tilde{\rho}^\dagger = \mathbf{1}, \tag{2.21}$$

$$\tau\rho^\dagger + \tilde{\rho}\tilde{\tau}^\dagger = \rho\tau^\dagger + \tilde{\tau}\tilde{\rho}^\dagger = \mathbf{0}. \tag{2.22}$$

These equations yield the other half of the unitarity condition of the S matrix, so that

$$S^\dagger S = S S^\dagger = I. \tag{2.23}$$

For a parity-invariant potential function, i.e., $V(-x) = V(x)$, there are further constraints on the transmission and reflection amplitudes. In that case the amplitudes are symmetric matrices and the two types of amplitudes are the same, i.e.,

$$\rho = \tilde{\rho} = \rho^T = \tilde{\rho}^T, \quad \text{and} \quad \tau = \tilde{\tau} = \tilde{\tau}^T = \tau^T. \tag{2.24}$$

There is also a useful relation between the scattering amplitudes at k and at $-k$, which is easily obtained by generalizing the result for uncoupled potentials.[7] Since $\psi^*(-k,x)$ and $\tilde{\psi}^*(-k,x)$ are solution matrices of the Schrödinger equation with the same boundary conditions as $\psi(k,x)$ and $\tilde{\psi}(k,x)$ respectively, we find that

$$\tau^*(-k) = \tau(k), \quad \rho^*(-k) = \rho(k), \quad \tilde{\tau}^*(-k) = \tilde{\tau}(k), \quad \tilde{\rho}^*(-k) = \tilde{\rho}(k). \tag{2.25}$$

From these relations it follows immediately that the reflection and transmission amplitudes at threshold (i.e., $k=0$) are real.

B. Levinson's theorem

Levinson's theorem in its most common formulation for a spherically symmetric potential gives a relationship of the scattering phase shifts at zero and infinite energy. The theorem has also been studied for one-dimensional systems without coupling.[2,5] We generalize the theorem to the matrix-potential case. Levinson's theorem is a consequence of the orthogonality and completeness relation of the eigenstates of the total Hamiltonian.

The scattering states of the Schrödinger equation (2.1) defined by Eqs. (2.2) and (2.3) along with the bound states can be used to form a complete orthonormal set of eigenstates. Suppose that there are n_b bound states whose orthonormal wave functions are denoted by the column vectors $\psi_{E_j}(x)$ with $E_j(<0)$ referring to the bound state energy. In case of degenerate bound states, we label the state vectors with subscript E_j, but allow the possibility of different subscripts j for the same energy in order to include all independent bound-state vectors. For example, one could have $E_j=E_i$ where $i \neq j$ when E_i is a degenerate energy eigenvalue. The orthonormality relations are

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} dx\,\psi_j^{\dagger}(k,x)\,\psi_i(k',x)=\frac{1}{2\pi}\int_{-\infty}^{\infty} dx\,\tilde{\psi}_j^{\dagger}(k,x)\,\tilde{\psi}_i(k',x)=\delta_{ij}\delta(k'-k), \tag{2.26}$$

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx\,\psi_j^{\dagger}(k,x)\,\psi_{E_i}(x)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx\,\tilde{\psi}_j^{\dagger}(k,x)\,\psi_{E_i}(x)=0, \tag{2.27}$$

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} dx\,\tilde{\psi}_j^{\dagger}(k,x)\,\psi_i(k',x)=0 \quad \text{and} \quad \int_{-\infty}^{\infty} dx\,\psi_{E_j}^{\dagger}(x)\,\psi_{E_i}(x)=\delta_{ij}\,, \tag{2.28}$$

where ψ_i and $\tilde{\psi}_i$ are the ith columns of the ψ and $\tilde{\psi}$ matrices, respectively. Thus the completeness relation is

$$\sum_{j=1}^{n_b}\psi_{E_j}(x)\,\psi_{E_j}^{\dagger}(x')+\sum_{i=1}^{N}\frac{1}{2\pi}\int_0^{\infty} dk\,\psi_i(k,x)\,\psi_i^{\dagger}(k,x')$$

$$+\sum_{i=1}^{N}\frac{1}{2\pi}\int_0^{\infty} dk\,\tilde{\psi}_i(k,x)\,\tilde{\psi}_i^{\dagger}(k,x')=\mathbf{1}\delta(x-x'). \tag{2.29}$$

The completeness relation may be written in a more compact form in terms of the matrices themselves rather than the column vectors, i.e.,

$$\sum_{j=1}^{n_b}\psi_{E_j}(x)\,\psi_{E_j}^{\dagger}(x')+\frac{1}{2\pi}\int_0^{\infty} dk[\,\psi(k,x)\,\psi^{\dagger}(k,x')+\tilde{\psi}(k,x)\,\tilde{\psi}^{\dagger}(k,x')\,]=\mathbf{1}\delta(x-x'). \tag{2.30}$$

For the free-particle case when $V(x)=\mathbf{0}$, there are no bound states and the completeness relation is

$$\frac{1}{2\pi}\int_0^{\infty} dk[\,\psi^0(k,x)\,\psi^{0\dagger}(k,x')+\tilde{\psi}^0(k,x)\,\tilde{\psi}^{0\dagger}(k,x')\,]=\mathbf{1}\delta(x-x'). \tag{2.31}$$

We now subtract Eq. (2.31) from Eq. (2.30), set $x'=x$, and integrate over x from $-\mathscr{R}$ to $\mathscr{R}$. The resulting equation may be written as

$$\int_0^\infty dk \int_{-\mathscr{R}}^{\mathscr{R}} dx [\psi(k,x)\psi^\dagger(k,x) + \widetilde{\psi}(k,x)\widetilde{\psi}^\dagger(k,x) - \psi^0(k,x)\psi^{0\dagger}(k,x) - \widetilde{\psi}^0(k,x)\widetilde{\psi}^{0\dagger}(k,x)]$$

$$= -2\pi \int_{-\mathscr{R}}^{\mathscr{R}} dx \sum_{j=1}^{n_b} \psi_{E_j}(x)\psi_{E_j}^\dagger(x). \tag{2.32}$$

The trace of Eq. (2.32) in the limit as $\mathscr{R}$ approaches infinity gives

$$-2\pi n_b = \lim_{\mathscr{R}\to\infty} \int_0^\infty dk \int_{-\mathscr{R}}^{\mathscr{R}} dx \, \mathrm{Tr}[\psi(k,x)\psi^\dagger(k,x) + \widetilde{\psi}(k,x)\widetilde{\psi}^\dagger(k,x)$$

$$- \psi^0(k,x)\psi^{0\dagger}(k,x) - \widetilde{\psi}^0(k,x)\widetilde{\psi}^{0\dagger}(k,x)]. \tag{2.33}$$

To perform the integration over x in the right side of Eq. (2.33), we use the identity

$$\mathrm{Tr}[\psi\psi^\dagger] = \frac{1}{2k}\frac{\partial}{\partial x}\left\{ \mathrm{Tr}\left[\frac{\partial\psi}{\partial k}\frac{\partial\psi^\dagger}{\partial x} - \frac{\partial^2\psi}{\partial x \partial k}\psi^\dagger \right] \right\}, \tag{2.34}$$

which may be obtained by taking the derivative with respect to k of the Schrödinger equation (2.1). Since in the limit $\mathscr{R}$ exceeds the range of the potential, we can insert the asymptotic forms of the wave functions in Eq. (2.33) to obtain

$$-2\pi n_b = \lim_{\mathscr{R}\to\infty} \int_0^\infty \frac{dk}{2k} \mathrm{Tr}\Bigg[-2ik\left(\frac{\partial\tau}{\partial k}\tau^\dagger + \frac{\partial\rho}{\partial k}\rho^\dagger + \frac{\partial\widetilde{\tau}}{\partial k}\widetilde{\tau}^\dagger + \frac{\partial\widetilde{\rho}}{\partial k}\widetilde{\rho}^\dagger \right)$$

$$- i(\rho + \widetilde{\rho})e^{2ik\mathscr{R}} + i(\rho^\dagger + \widetilde{\rho}^\dagger)e^{-2ik\mathscr{R}} \Bigg]. \tag{2.35}$$

Following Newton and Jost[16] we define the phase as

$$\eta(k) = \frac{1}{2i} \ln \det S(k), \tag{2.36}$$

where we require $\eta(k)$ to be continuous for $k \in (0,\infty)$. Since the S matrix is unitary, we may write $S = U^\dagger S_D U$, where U is a real orthogonal matrix and S_D is the diagonal matrix $S_D = \mathrm{diag}(e^{i\delta_1}, \ldots, e^{i\delta_{2N}})$ where the δ_j's are real phases.[17] Let us write therefore $S = e^{i\Delta}$ where $\Delta = U^\dagger \Delta_D U$ for $\Delta_D = \mathrm{diag}(\delta_1, \ldots, \delta_{2N})$. Then

$$2i\,\eta(k) = \ln \det S(k) = \ln \det S_D(k) = \sum_{j=1}^{2N} i\,\delta_j(k) = \mathrm{Tr}[i\Delta_D(k)] \tag{2.37}$$

and

$$2i\frac{\partial\eta}{\partial k} = \mathrm{Tr}\left[\frac{\partial i\Delta_D}{\partial k}\right] = \mathrm{Tr}\left[S_D^\dagger \frac{\partial S_D}{\partial k}\right] = \mathrm{Tr}\left[S^\dagger \frac{\partial S}{\partial k}\right] = \mathrm{Tr}\left[\frac{\partial\tau}{\partial k}\tau^\dagger + \frac{\partial\rho}{\partial k}\rho^\dagger + \frac{\partial\widetilde{\tau}}{\partial k}\widetilde{\tau}^\dagger + \frac{\partial\widetilde{\rho}}{\partial k}\widetilde{\rho}^\dagger\right]. \tag{2.38}$$

Thus Eq. (2.35) may be written as

$$\eta(0) - \eta(\infty) = \pi n_b - \lim_{\mathscr{R}\to\infty} X(\mathscr{R}), \tag{2.39}$$

where

$$X(\mathscr{R})=\frac{1}{2}\int_0^\infty \frac{dk}{2k}\,\mathrm{Tr}[\,i(\rho(k)+\tilde{\rho}(k))e^{2ik\mathscr{R}}-i(\rho^\dagger(k)+\tilde{\rho}^\dagger(k))e^{-2ik\mathscr{R}}] \tag{2.40}$$

$$=\frac{i}{4}\int_{-\infty}^{\infty}\frac{dk}{k}\,\mathrm{Tr}[\rho(k)+\tilde{\rho}(k)]e^{2ik\mathscr{R}}. \tag{2.41}$$

In the next section we show that $\rho(k)\sim O(1/k)$ for large $|k|$, so that the integration in Eq. (2.41) converges for large $|k|$. We now take the limit as $\mathscr{R}$ approaches ∞, using the relation

$$\lim_{\mathscr{R}\to\infty}\frac{e^{2ik\mathscr{R}}}{k}=i\pi\delta(k), \tag{2.42}$$

where $\delta(k)$ is the Dirac delta function. In that limit $X(\mathscr{R})$ goes to $-(\pi/4)\,\mathrm{Tr}[\rho(0)+\tilde{\rho}(0)]$, so that the statement of Levinson's theorem now is

$$\eta(0)=\pi n_b+\frac{\pi}{4}\,\mathrm{Tr}[\rho(0)+\tilde{\rho}(0)], \tag{2.43}$$

where we have set $\eta(\infty)$ equal to zero. In the next section we also show that

$$\mathrm{Tr}[\rho(0)+\tilde{\rho}(0)]=-2(N-n), \tag{2.44}$$

where n is the number of ''half-bound states.''[10,11,18] Thus in its final form Levinson's theorem states,

$$\eta(0)=\pi(n_b+\tfrac{1}{2}n-\tfrac{1}{2}N). \tag{2.45}$$

This expression of the theorem is consistent with that for the uncoupled case given in Ref. 11.

C. Threshold behaviour of ρ and τ

The threshold behaviour of reflection and transmission amplitudes and coefficients has been discussed recently in several articles.[2,4,6,7] In order to study the behaviour of the ρ and τ matrices at $k=0$, we introduce a different set of solutions of the Schrödinger equation, since according to Eq. (2.5) the columns of ψ and $\tilde{\psi}$ fail to be linearly independent at $k=0$. Let $\phi(k,x)$ and $\chi(k,x)$ be solution matrices of Eq. (2.1) which satisfy the boundary conditions,

$$\begin{aligned}\phi(k,-R)&=\chi'(k,-R)=\mathbf{1}\\ \phi'(k,-R)&=\chi(k,-R)=\mathbf{0},\end{aligned} \tag{2.46}$$

where R is the range of the potential as defined at the beginning of Sec. II. By evaluating $\det W(\phi,\chi)$ at $x=-R$ and using the results of Appendix A, we readily show that for all x and k the $\det W(\phi,\chi)=1$, where the matrix W is defined as in Eq. (2.4). Thus unlike the column vectors of ψ and $\tilde{\psi}$, the column vectors of ϕ and χ are linearly independent at zero energy.

In order to obtain the scattering amplitudes, we expand ψ in terms of ϕ and χ so that

$$\psi(k,x)=\phi(k,x)B(k)+\chi(k,x)C(k), \tag{2.47}$$

where $B(k)$ and $C(k)$ are matrices of expansion coefficients. Evaluating ψ and ψ' at $\pm R$ using Eqs. (2.2) and (2.47), we obtain four equations involving $B(k),C(k),\rho(k)$ and $\tau(k)$. By eliminating three of these we find that ρ can expressed in terms of ϕ and χ and their derivatives evaluated at R. Thus

$$\rho(k)=\{k^2\chi(k,R)+ik[\chi'(k,R)+\phi(k,R)]-\phi'(k,R)\}^{-1}$$
$$\times\{k^2\chi(k,R)+ik[\chi'(k,R)-\phi(k,R)]+\phi'(k,R)\}e^{-2ikR}. \tag{2.48}$$

Similarly by expanding $\tilde{\psi}$ in terms of ϕ and χ we obtain

$$\tilde{\rho}(k)=\{k^2\chi(k,R)-ik[\chi'(k,R)-\phi(k,R)]+\phi'(k,R)\}$$
$$\times\{k^2\chi(k,R)+ik[\chi'(k,R)+\phi(k,R)]-\phi'(k,R)\}^{-1}e^{-2ikR}, \tag{2.49}$$

$$\tilde{\tau}(k)=2ik\{k^2\chi(k,R)+ik[\chi'(k,R)+\phi(k,R)]-\phi'(k,R)\}^{-1}e^{-2ikR}, \tag{2.50}$$

and, since $\tau(k)=\tilde{\tau}^T(k)$,

$$\tau(k)=2ik\{k^2\chi^T(k,R)+ik[\chi'^T(k,R)+\phi^T(k,R)]-\phi'^T(k,R)\}^{-1}e^{-2ikR}. \tag{2.51}$$

Thus all four scattering amplitudes, and consequently the S matrix, are determined by ϕ and χ and their derivatives evaluated at R. In Appendix B it is shown that $\phi(k,x)$ and $\chi(k,x)$ are entire functions of complex k for all $x\in[-R,R]$ so that the analytic properties of the scattering amplitudes can be determined using these wave functions. By inserting the expressions for the large real k behaviour of the wave functions, Eqs. (B16) and (B17), into the expressions for the scattering amplitudes, we obtain

$$\tau(k)\sim\mathbf{1}+O(1/k) \quad \text{and} \quad \rho(k)\sim\mathbf{0}+O(1/k) \quad \text{for } k\to\infty, \tag{2.52}$$

and similar expressions for $\tilde{\tau}$ and $\tilde{\rho}$.

If $\det[\phi'(0,R)]\neq 0$, the reflection and transmission amplitudes at zero energy are

$$\rho(0)=\tilde{\rho}(0)=-\mathbf{1} \quad \text{and} \quad \tau(0)=\tilde{\tau}(0)=\mathbf{0}. \tag{2.53}$$

The case for which $\det[\phi'(0,R)]=0$ needs special attention. In order to understand the significance of this condition, we look at the bound states of the system. In the Schrödinger equation (2.1) for bound states, we denote the bound-state energy as $\alpha^2=-k^2$ with $\alpha>0$. The bound-state wave functions can be expressed as column vectors of a matrix $\psi_b(\alpha,x)$ with the asymptotic boundary conditions,

$$\psi_b(\alpha,x)\sim\begin{cases}e^{\alpha x}Q, & x\leqslant -R\\ e^{-\alpha x}T, & x\geqslant R\end{cases} \tag{2.54}$$

where Q and T are matrices of constants. The number of independent bound states at a given energy will depend on the rank of the matrix ψ_b, and consequently cannot exceed N. Proceeding as we did for the scattering states, we expand the bound-state wave functions in terms of the functions $\phi_b(\alpha,x)$ and $\chi_b(\alpha,x)$ which are solution matrices of the Schrödinger equation with energy $-\alpha^2$ and satisfy the boundary conditions

$$\phi_b(\alpha,-R)=\chi_b'(\alpha,-R)=\mathbf{1}, \quad \chi_b(\alpha,-R)=\phi_b'(\alpha,-R)=\mathbf{0}. \tag{2.55}$$

Thus

$$\psi_b(\alpha,x)=\phi_b(\alpha,x)\beta(\alpha)+\chi_b(\alpha,x)\gamma(\alpha), \tag{2.56}$$

where β and γ are matrices of expansion coefficients. At R and $-R$ we match the asymptotic form of the wave function, Eq. (2.54), and its derivative to the expanded form, Eq. (2.56), and its derivative. Eliminating T,Q and γ from the four equations so obtained, we are left with the equation

$$\{\alpha^2\chi_b(\alpha,R)+\alpha[\chi_b'(\alpha,R)+\phi_b(\alpha,R)]+\phi_b'(\alpha,R)\}\beta(\alpha)=0. \tag{2.57}$$

Since one of the four matching equations is $Q=\beta(\alpha)e^{\alpha R}$, there will be bound states only if the matrix $\beta(\alpha)$ contains nonzero entries. Such a nontrivial matrix exists only when

$$\det\{\alpha^2\chi_b(\alpha,R)+\alpha[\chi_b'(\alpha,R)+\phi_b(\alpha,R)]+\phi_b'(\alpha,R)\}=0. \tag{2.58}$$

This is the bound-state eigenvalue equation for energy $-\alpha^2$. In contrast to the case with no coupling, the bound-state eigenenergies can be degenerate.

Let us consider the eigenstates when $\alpha=0$. These will occur only if $\det[\phi_b'(0,R)]=0$. In general the solutions represented by the columns vectors of $\psi_b(0,x)$ are bounded but not square integrable; hence they are referred to as half-bound states.[19] The restriction on the potential function that it vanishes for $|x|\geqslant R$, precludes the possibility of having normalizable state functions at zero energy. For this to be the case a linear combination of the columns of ψ_b would yield $\Psi(0,x)=0$ for $|x|\geqslant R$. Such a boundary condition would lead to the trivial solution of Eq. (2.1). Normalizable zero-energy bound states can exist for potentials which are less restrictive than those of this paper.[18]

Since $\phi(0,x)$ and $\phi_b(0,x)$ are solutions of the same system of differential equations and both have the same boundary conditions, $\phi_b(0,x)=\phi(0,x)$. Thus the condition that

$$\det[\phi'(0,R)]=0 \tag{2.59}$$

is equivalent to the condition for the existence of half-bound states.

Consider the matrix eigenvalue equation,

$$\phi'(0,R)\tilde{\beta}=\lambda\tilde{\beta}, \tag{2.60}$$

where $\tilde{\beta}$ is a column vector and λ is its eigenvalue. There will be a nontrivial solution only if

$$\det[\phi'(0,R)-\lambda\mathbf{1}]=0. \tag{2.61}$$

Suppose the eigenvalues obtained are $\lambda_1,\cdots,\lambda_N$. At least one of these must be zero if there is a half-bound state. Actually there may be $n(\leqslant N)$ zero eigenvalues. We can order these in the following way: $0,\ldots,0,\lambda_{n+1},\ldots,\lambda_N$. These n zero eigenvalues will have n linearly independent eigenvectors associated with them, which represent n distinct half-bound states.

We now return to the discussion of reflection and transmission amplitudes. The inverse of $\tilde{\tau}$ of Eq. (2.50) can be written as

$$2ik\,\tilde{\tau}^{-1}(k)=\{k^2\chi(k,R)+ik[\chi'(k,R)+\phi(k,R)]-\phi'(k,R)\}e^{2ikR}. \tag{2.62}$$

If this equation is combined with Eq. (2.49), we obtain

$$2ik\tilde{\rho}(k)\tilde{\tau}^{-1}(k)=\{k^2\chi(k,R)-ik[\chi'(k,R)-\phi(k,R)]+\phi'(k,R)\}. \tag{2.63}$$

The factor in the curly brackets of Eq. (2.62) is precisely that in the determinant of Eq. (2.58) (with $k=i\alpha$), i.e., it is the factor which determines the bound states of the system. In Appendix B we show that matrices ϕ and χ are elementwise entire functions of k. From Eq. (2.62) and the fact that $\tilde{\tau}^T=\tau$ we see that $2ik\tau^{-1}(k)$ and $(2ik)^N$ det $\tau^{-1}(k)$ are also entire functions of k. According to Eqs. (2.58) and (2.62) det $\tau^{-1}(k)$ has a zero at $k=i\alpha$ when $-\alpha^2$ is the energy of a bound state. Thus det $\tau(k)$ has poles (possibly multiple) on the positive imaginary axis of the complex k plane. In the absence of a half-bound state, det $\tau^{-1}(k)$ has an Nth order pole at $k=0$ and det τ has an Nth order zero at $k=0$. Since there can be no more than N half-bound states det $\tau(k)$ and $\tau(k)$ are analytic in a neighborhood of $k=0$.

In the following we consider real k. Taking the limits as k goes to zero of Eqs. (2.62) and (2.63) we obtain

$$\lim_{k\to 0} 2ik\tilde{\tau}^{-1}(k) = -\phi'(0,R) \quad \text{and} \quad \lim_{k\to 0} 2ik\tilde{\rho}(k)\tilde{\tau}^{-1}(k) = \phi'(0,R). \tag{2.64}$$

Similarly using Eq. (2.51) and the transpose of Eq. (2.48), we get

$$\lim_{k\to 0} 2ik\tau^{-1}(k) = -\phi'^{T}(0,R) \quad \text{and} \quad \lim_{k\to 0} 2ik\rho(k)\tau^{-1}(k) = \phi'^{T}(0,R). \tag{2.65}$$

We introduce unitary matrices $U(k)$ and $V(k)$ which diagonalize τ (Ref. 20), so that

$$\tau_D(k) = U^{\dagger}(k)\tau(k)V(k) \quad \text{and} \quad 2ik\tau_D^{-1} = V^{\dagger}(k)2ik\tau^{-1}(k)U(k). \tag{2.66}$$

In the limit as k approaches zero $U(0)$ and $V(0)$ also diagonalize $\phi'^{T}(0,R)$, i.e., $\phi_D'^{T}(0,R) = V^{\dagger}(0)\phi'^{T}(0,R)U(0)$, so that

$$\lim_{k\to 0} 2ik\tau_D^{-1}(k) = -\phi_D'^{T}(0,R). \tag{2.67}$$

We define the matrix

$$r(k) \equiv V^{\dagger}(k)\rho(k)V(k), \tag{2.68}$$

so that

$$\lim_{k\to 0} 2ikr(k)\tau_D{}^{-1}(k) = \phi_D'^{T}(0,R). \tag{2.69}$$

Combining Eqs. (2.67) and (2.69) gives

$$r(0)\phi_D'^{T}(0,R) = -\phi_D'^{T}(0,R). \tag{2.70}$$

The matrices $\phi'^{T}(0,R)$ and $\phi_D'^{T}(0,R)$ have the same rank (Ref. 20). Thus $\phi_D'^{T}(0,R)$ will have the same number of nonzero diagonal elements as there are nonzero eigenvalues of $\phi'^{T}(0,R)$ or $\phi'(0,R)$. Writing $\phi_D'^{T}(0,R) = \mathrm{diag}(0,\cdots,0,s_{n+1},\cdots,s_N)$ and using Eq. (2.70) we see that the matrix $r(0)$ must have the form

$$r(0) = \begin{pmatrix} R_{11} & \mathbf{0} \\ R_{21} & -\mathbf{1} \end{pmatrix}, \tag{2.71}$$

where the matrices R_{11}, R_{21}, $\mathbf{0}$ and $\mathbf{1}$ have dimensions $n\times n$, $(N-n)\times n$, $n\times(N-n)$ and $(N-n)\times(N-n)$, respectively.

To study the behaviour of $\tau_D(k)$ near $k=0$, we consider the Hermitian positive semi-definite matrix $T(k) = \tau^{\dagger}(k)\tau(k)$, whose real nonnegative eigenvalues we denote by $t_1^2(k),\ldots,t_N^2(k)$. The singular values of $\tau(k)$ are defined as the nonnegative square root of these, i.e., $t_1(k),\ldots,t_N(k)$, and they form the diagonal elements of $\tau_D(k)$ in Eq. (2.66), so that $\tau_D(k) = \mathrm{diag}(t_1(k),\ldots,t_N(k))$. (Ref. 20) Since $\tau(k)$ is analytic in the neighborhood of $k=0$, so is $T(k)$. For small real $k>0$, we invoke a theorem of Rellich[21] which states that the eigenvalues of $T(k)$ are convergent power series of k. Furthermore, using Eq. (2.25), we note that $T(k) = T^{T}(-k)$ and the eigenvalues of $T(k)$ and $T(-k)$ are the same. Thus taking the eigenvalues in the same order, we find that $t_i^2(-k) = t_i^2(k)$. Hence the $t_i^2(k)$'s are power series of k^2 and the

$t_i(k)$'s are power series of k. Thus we may write $\tau_D(k) = \mathrm{diag}(t_1 + t_{11}k + \cdots, \ldots, t_N + t_{N1}k + \cdots)$ and $\tau_D^{-1}(k) = \mathrm{diag}((t_1 + t_{11}k + \cdots)^{-1}, \ldots, (t_N + t_{N1}k + \cdots)^{-1})$, where the t_i's and t_{ij}'s are constants. In order that

$$\lim_{k\to 0} 2ik\tau_D^{-1}(k) = \lim_{k\to 0} \mathrm{diag}(2ik(t_1 + t_{11}k + \cdots)^{-1}, \ldots, 2ik(t_N + t_{N1}k + \cdots)^{-1}) \tag{2.72}$$

$$= \mathrm{diag}(0, \ldots, 0, -s_{n+1}, \ldots, -s_N), \tag{2.73}$$

the quantities $t_1, \ldots, t_n \neq 0$ and $t_{n+1} = \cdots = t_N = 0$. The matrix $\tau_D(0)$ therefore has the form $\tau_D(0) = \mathrm{diag}(t_1, \ldots, t_n, 0, \ldots, 0)$ where the first n diagonal elements are nonzero.

Recall that $\tau^T = \tilde{\tau}$ and therefore $(\tau^T)^{-1} = \tilde{\tau}^{-1}$, and that $\tilde{\rho} = \tilde{\rho}^T$. The second part of Eq. (2.64) becomes

$$\lim_{k\to 0} 2ik\tau^{-1}(k)\tilde{\rho}(k) = \phi'^T(0,R). \tag{2.74}$$

The same U and V can be used to obtain

$$\lim_{k\to 0} 2ik\tau_D{}^{-1}(k)\tilde{r}(k) = \phi_D'^T(0,R), \tag{2.75}$$

where

$$\tilde{r}(k) = U^\dagger(k)\tilde{\rho}(k)U(k). \tag{2.76}$$

As before the structure of $\tilde{r}(0)$ may be determined, and it is

$$\tilde{r}(0) = \begin{pmatrix} \tilde{R}_{11} & \tilde{R}_{12} \\ \mathbf{0} & -\mathbf{1} \end{pmatrix}. \tag{2.77}$$

In order to simplify Eq. (2.43) we write

$$\begin{aligned} \mathrm{Tr}[\rho(0) + \tilde{\rho}(0)] &= \mathrm{Tr}[r(0) + \tilde{r}(0)] \\ &= -2(N-n) + \mathrm{Tr}[R_{11}^{n\times n} + \tilde{R}_{11}^{n\times n}], \end{aligned} \tag{2.78}$$

where the superscripts refer to the dimensions of the matrices. All that remains is to evaluate the last term of the right side of this equation. At zero energy the scattering amplitudes are real. Using this fact along with the relations that $\tilde{\tau} = \tau^T$ and $\rho = \rho^T$ in Eq. (2.15), we obtain

$$\tau(0)\rho(0) + \tilde{\rho}(0)\tau(0) = \mathbf{0}. \tag{2.79}$$

By applying the diagonalization transformation of τ, we find that

$$\tau_D(0)r(0) + \tilde{r}(0)\tau_D(0) = \mathbf{0}. \tag{2.80}$$

In matrix form this equation may be written

$$\begin{pmatrix} A_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}\begin{pmatrix} R_{11} & \mathbf{0} \\ R_{21} & -\mathbf{1} \end{pmatrix} + \begin{pmatrix} \tilde{R}_{11} & \tilde{R}_{12} \\ \mathbf{0} & -\mathbf{1} \end{pmatrix}\begin{pmatrix} A_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix} = \mathbf{0}, \tag{2.81}$$

where $A_1 = \mathrm{diag}(t_1, \cdots, t_n)$ and the block matrices have the appropriate dimensions. From Eq. (2.81) it follows that

$$A_1 R_{11} + \tilde{R}_{11} A_1 = \mathbf{0}^{n\times n}. \tag{2.82}$$

Consequently, the second term in the right side of Eq. (2.78) is zero, and we have the simple relation

$$\mathrm{Tr}[\rho(0) + \tilde{\rho}(0)] = -2(N-n) \tag{2.83}$$

In light of the discussion of the $N=1$ normal and anomalous threshold behaviour,[4,7] our result seems surprising since the right side of Eq. (2.83) is an integer, whereas the anomalous threshold effect for parity-noninvariant potentials gives values for $\rho(0)$ which lie between 0 and 1. However, if one considers the sum of $\rho(0)$ and $\tilde{\rho}(0)$ in the uncoupled case, one obtains an even integer. For a parity-invariant potential, i.e., $V(-x)=V(x)$, ρ and $\tilde{\rho}$ are equal and the zero-energy value of ρ will always be an integer.

III. SEGMENTED POTENTIALS AND FACTORIZATION OF THE *S* MATRIX

For the Schrödinger equation without coupling it is well known that the reflection and transmission amplitudes satisfy a factorization formula. That is, if the potential is subdivided into a number of sections, then the total transmission and reflection amplitudes for the system can be expressed in terms of the amplitudes for each of the truncated pieces of the potential. The recent proof of Aktosun[22] may be generalized immediately to the case of N coupled equations.

Following Aktosun, then, we subdivide the real line into J pieces. The boundaries of the segments are denoted by x_i, $i=0,\ldots,J$, with $-R=x_0<x_1<\ldots<x_{J-1}<x_J=R$. The potential may then be written as a sum of truncated potentials as follows:

$$V(x) = \sum_{j=0}^{J-1} V_j(x), \tag{3.1}$$

where

$$V_j(x) = \begin{cases} V(x), & x_j<x<x_{j+1} \\ 0, & \text{otherwise.} \end{cases} \tag{3.2}$$

The single indices on the truncated potentials should not be confused with the implicit double indices which label the various elements of the potential matrix.

For a given j, then, let us define the matrix

$$\Lambda_j(k) = \begin{pmatrix} \tau_j^{-1}(k) & -\tau_j^{-1}(k)\tilde{\rho}_j(k) \\ \rho_j(k)\tau_j^{-1}(k) & (\tilde{\tau}_j^{\dagger}(k))^{-1} \end{pmatrix}, \tag{3.3}$$

where $\tau_j(k)$, $\tilde{\tau}_j(k)$, $\rho_j(k)$, $\tilde{\rho}_j(k)$ represent the various amplitude matrices for the truncated potentials with the usual boundary conditions. The amplitudes for the original potential are similarly arranged into a matrix,

$$\Lambda(k) = \begin{pmatrix} \tau^{-1}(k) & -\tau^{-1}(k)\tilde{\rho}(k) \\ \rho(k)\tau^{-1}(k) & (\tilde{\tau}^{\dagger}(k))^{-1} \end{pmatrix}, \tag{3.4}$$

and the factorization formula is then simply given by

$$\Lambda(k) = \prod_{j=0}^{J-1} \Lambda_j(k), \tag{3.5}$$

where the factors on the right side of the equation are ordered so that factors with lower subscripts occur to the left of the ones with higher subscripts. The proof of Eq. (3.5) is completely analogous to that advanced by Aktosun in the $N=1$ case and so we shall not review it here. The only added complication is the fact that the various amplitude matrices do not generally commute, but this has been properly accounted for in the definitions of the Λ matrices. The utility of Eq. (3.5) will become apparent below when we use it to derive the amplitudes for scattering from two different delta-function matrix potentials in terms of the amplitudes for scattering from each of them separately.

This approach effectively factorizes the S matrix in the sense that if the S matrix of the jth potential segment, i.e.,

$$S_j(k)=\begin{pmatrix} \tau_j(k) & \tilde{\rho}_j(k) \\ \rho_j(k) & \tilde{\tau}_j(k) \end{pmatrix}, \tag{3.6}$$

is known, then the scattering amplitudes of the potential segment are determined, and from them $\Lambda_j(k)$. Using Eq. (3.5) we can obtain $\Lambda(k)$ for the whole potential, and this allows us to solve for the scattering amplitudes and the S matrix of the whole potential.

Another generalization of the uncoupled to the coupled problem involves the finitely periodic potentials, recently discussed by a number of authors.[3,23–25] In the derivation of the factorization formula, Eq. (3.5), we have to be careful in the ordering of the products such as $\rho\tau^{-1}$. This non-commutativity of the amplitude matrices would typically prevent us from generalizing the closed-form solutions of the finitely periodic potentials. There are however classes of potentials for which the various amplitude matrices do commute with each other and for which the results for no coupling *can* be generalized.

An example of such a class of potentials consists of those potentials which can be expressed as

$$V(x)=U\ \mathrm{diag}[v_1(x),v_2(x),\ldots,v_N(x)]U^T, \tag{3.7}$$

where U is a constant (real) orthogonal matrix. Note that the potentials of Eq. (3.7) include as a subclass those of the form $V(x)=v(x)M$, where $v(x)$ is a real-valued function of x and M is a constant symmetric matrix. Such potentials have been used previously in various applications (see, for example, Ref. 26). It is easy to prove that when the potential is diagonalizable by a constant orthogonal matrix, then all of the amplitude matrices (as well as their inverses and hermitian conjugates) commute with each other.

If we use potentials of this type to construct finitely periodic potentials with nonoverlapping subpotentials, the analysis of Rozman *et al.*[23,24] follows in the same way for the matrix potential problem and the expressions for the amplitude matrices are straight forward generalizations of their results.

IV. POTENTIAL MODELS

Below we consider some potential models which lend themselves to solutions in closed form. These models help to elucidate some of the results obtained in the previous sections.

A. Constant potential matrix

An example of a potential for which solutions can be obtained in closed form is the square-well or square-barrier potential matrix for which

$$V(x)=\begin{cases} V_0 & \text{for } a\leqslant x\leqslant b \text{ where } a\geqslant -R \text{ and } b\leqslant R \\ 0 & \text{otherwise,} \end{cases} \tag{4.1}$$

where V_0 is a real symmetric $N\times N$ matrix. The Schrödinger equation (2.1) is equivalent to a first-order differential equation of the matrix function $W(x)=W(\phi,\chi)$ of Eq. (A2), i.e.,

$$W'(x)=F(x)W(x), \tag{4.2}$$

where

$$F(x)=\begin{pmatrix} \mathbf{0} & \mathbf{1} \\ V(x)-k^2 & \mathbf{0} \end{pmatrix}, \tag{4.3}$$

with the boundary condition $W(-R)=I$. As we saw earlier the function $W(x)$ provides the advantage of giving solutions that are linearly independent at $k=0$. In addition, Eq. (4.2) gives us an initial value problem, rather than the two-point boundary condition problem of the original Schrödinger equation. Solving for the scattering amplitudes numerically is simpler for the initial value problem. An alternative to this approach is the variable amplitude formulation which also casts the problem into a system of first order differential equations with an initial value condition.[13,14] In principle, Eq. (4.2) can be used to solve the Schrödinger equation for any arbitrary potential matrix.

For the constant potential matrix the differential equation Eq. (4.2) can be integrated starting at $x=-R$ over the three regions $(-R,a),(a,b)$ and (b,R) in turn.[27] The result is

$$\begin{aligned} W(R)=&\begin{pmatrix} \cos\, k(R-b) & k^{-1}\sin k(R-b) \\ -k\sin k(R-b) & \cos\, k(R-b) \end{pmatrix}\begin{pmatrix} \cosh\, K(b-a) & K^{-1}\sinh K(b-a) \\ K\sinh K(b-a) & \cosh\, K(b-a) \end{pmatrix} \\ &\times\begin{pmatrix} \cos\, k(a+R) & k^{-1}\sin k(a+R) \\ -k\sin k(a+R) & \cos\, k(a+R) \end{pmatrix}, \end{aligned} \tag{4.4}$$

where $K^2=V_0-k^2$. To simplify matters, but still to allow us to study a model with a potential function without definite parity, we set $a=-R$, so that we obtain explicit forms for the wave functions at $x=R$.

$$\begin{aligned} \phi(k,R)&=\cos\, k(R-b)\cosh\, K(R+b)+k^{-1}\sin k(R-b)K\sinh K(R+b), \\ \phi'(k,R)&=-k\sin k(R-b)\cosh\, K(R+b)+\cos\, k(R-b)K\sinh K(R+b), \\ \chi(k,R)&=\cos\, k(R-b)K^{-1}\sinh K(R+b)+k^{-1}\sin k(R-b)\cosh\, K(R+b), \\ \chi'(k,R)&=-k\sin k(R-b)K^{-1}\sinh K(R+b)+\cos\, k(R-b)\cosh\, K(R+b). \end{aligned} \tag{4.5}$$

These expressions can be inserted in the equations for ρ, $\tilde{\rho}$, τ, $\tilde{\tau}$, Eqs. (2.48) to (2.51), to obtain the scattering amplitudes.

Note that $K^2=V_0-k^2$ is a real symmetric matrix and may therefore be diagonalized by an orthogonal transformation U, giving $K_D^2=UK^2U^T$. The diagonal matrix K_D has the square root of the diagonal elements of K_D^2 along its diagonal. Thus $K=U^TK_DU$, which is a symmetric matrix. Consequently, ϕ,ϕ',χ,χ' are symmetric matrices, which leads to $\tau=\tilde{\tau}$. Furthermore, since each of the wave-function matrices or their derivatives at R is a power series (or polynomial) of the matrix K, the wave-function matrices commute. It is not difficult to show that in the case of $b=R$, i.e., when the potential function has even parity, $\rho(k)=\tilde{\rho}(k)$.

The threshold behaviour of the transition amplitudes for a potential lacking specific parity can be studied explicitly with this model. Since Levinson's theorem involves the trace of the ampli-

tudes at zero energy, we need to consider the diagonalized forms of the amplitudes only. We diagonalize each of the wave-function matrices of Eq. (4.5) using the same orthogonal matrix U for each, and we denote the diagonal matrices at zero energy as

$$\begin{aligned}\phi_D(0,R) &= \mathrm{diag}(p_1,\ldots,p_N), \phi_D'(0,R) = \mathrm{diag}(\lambda_1,\ldots,\lambda_N),\\ \chi_D(0,R) &= \mathrm{diag}(x_1,\ldots,x_N), \chi_D'(0,R) = \mathrm{diag}(x_1',\ldots,x_N').\end{aligned} \tag{4.6}$$

When there is no half-bound state, we obtain, by inserting these expressions into Eqs. (2.48) and (2.51),

$$\rho(0)=\rho_D(0)=-\mathbf{1} \quad \text{and} \quad \tau(0)=\tau_D(0)=\mathbf{0}. \tag{4.7}$$

When there are n half-bound states and $\det \phi'(0,R)=0$, we write $\phi_D'(0,R) = \mathrm{diag}(0,\ldots,0,\lambda_{n+1},\ldots,\lambda_N)$. Using Eq. (2.13) we find that

$$\phi^{\dagger\prime}(k,x)\chi(k,x)-\phi^{\dagger}(k,x)\chi'(k,x)=-\mathbf{1}. \tag{4.8}$$

In general the matrices ϕ and χ are real and for the constant potential matrix they are symmetric as well. Thus

$$\phi'(0,R)\chi(0,R)-\phi(0,R)\chi'(0,R)=\phi_D\prime(0,R)\chi_D(0,R)-\phi_D(0,R)\chi_D\prime(0,R)=-\mathbf{1}. \tag{4.9}$$

From this relation it follows that $x_i'=1/p_i$ for $i=1,\ldots,n$, and furthermore,

$$\rho_D(0)=\mathrm{diag}\left(\frac{1-p_1^2}{1+p_1^2},\ldots,\frac{1-p_n^2}{1+p_n^2},-1,\ldots,-1\right), \tag{4.10}$$

$$\tilde{\rho}_D(0)=\mathrm{diag}\left(-\frac{1-p_1^2}{1+p_1^2},\ldots,-\frac{1-p_n^2}{1+p_n^2},-1,\ldots,-1\right), \tag{4.11}$$

$$\tau_D(0)=\tilde{\tau}_D(0)=\mathrm{diag}\left(\frac{2p_1}{1+p_1^2},\ldots,\frac{2p_n}{1+p_n^2},0,\ldots,0\right). \tag{4.12}$$

Clearly the relation (2.83) is satisfied by Eqs. (4.10) and (4.11). For the parity-invariant potential obtained by setting $b=R$ in Eq. (4.5) , $\phi(0,R)=\chi'(0,R)$. Hence $p_i=x_i'$ for $i=1,\ldots,N$, and it follows that $p_i^2=1$. Such a potential therefore yields transition amplitudes of the form

$$\rho_D(0)=\tilde{\rho}_D(0)=\mathrm{diag}(0,\ldots,0,-1,\ldots,-1) \quad \text{and} \quad \tau_D(0)=\mathrm{diag}(\pm 1,\ldots,\pm 1,0,\ldots,0). \tag{4.13}$$

When the ith diagonal element of $\phi_D(0,x)$ is an even (odd) function, then the ith diagonal element of $\tau_D(0)$ will have a plus (minus) sign with the one. The converse is not necessarily true.

Consider the special case of $N=1$. For the parity-invariant potential with a half-bound state, one has $\rho(0)=0$ and $\tau(0)=\pm 1$. The plus sign corresponds to $\phi(0,x)$ being an even solution and the negative sign to it being an odd solution. When there is no half-bound state, then $\rho(0)=-1$ and $\tau(0)=0$. In the case of a potential without definite parity, $\rho(0)=\tilde{\rho}(0)=-1$ and $\tau(0)=\tilde{\tau}(0)=0$ when the potential does not support a half-bound state. When there is a half-bound state, $\tau(0)$ and $\tilde{\tau}(0)$ are not equal to zero, nor are the ρ's equal to -1. However, the sum of the ρ's is an integer, i.e., $\rho(0)+\tilde{\rho}(0)=0$. These results, which are clearly valid for the square-well potential, are actually valid for any $N=1$ potential function.

B. Models involving delta-function potentials

We now consider two examples involving delta functions for which results can be obtained in closed form. The results exhibit qualitative features which are also found in much more complicated examples. First we examine the case of a single delta-function matrix potential positioned at the origin. Then we will use the factorization formula derived earlier to look at the case for which there are two delta-function matrices symmetrically positioned on both sides of the origin.

1. Delta function at the origin

We write the Schrödinger equation for this case as

$$\left(-\frac{d^2}{dx^2}+\delta(x)\lambda\right)\psi=k^2\psi, \tag{4.14}$$

where λ is an $N\times N$ symmetric matrix, and ψ can be taken to be either a column vector solution or a solution matrix. The former approach will be used when we consider bound states and the latter when we examine scattering solutions.

First consider the scattering solutions. Since the potential has even parity, we immediately have the result that $\tilde{\rho}=\rho$ and $\tilde{\tau}=\tau$. Thus we need only consider the solution with the incident wave from the left,

$$\psi(k,x)=\begin{cases}\mathbf{1}e^{ikx}+\rho e^{-ikx}, & x\leqslant 0\\ \tau e^{ikx}, & x\geqslant 0.\end{cases} \tag{4.15}$$

Here we see the utility of working directly with a matrix of column eigenvectors (as opposed to working with individual column vectors); ρ and τ may be solved for directly in terms of matrix operations. The scattering amplitudes are

$$\rho(k)=(2ik-\lambda)^{-1}\lambda, \tag{4.16}$$

$$\tau(k)=\mathbf{1}+\rho(k)=2ik(2ik-\lambda)^{-1}. \tag{4.17}$$

Of particular interest to us, due to its connection with the version of Levinson's theorem given in Eq. (2.43), is the quantity $\mathrm{Tr}[\rho(0)+\tilde{\rho}(0)]$. If λ^{-1} exists, then $\rho(0)=-\mathbf{1}$ and $\mathrm{Tr}[\rho(0)+\tilde{\rho}(0)]=2\,\mathrm{Tr}[\rho(0)]=-2N$, as expected. If λ is not invertible, however, we must be a bit more careful.

In order to determine the significance of the noninvertibility of λ, consider the bound-state solutions of Eq. (4.14). Setting $\alpha^2=-k^2$ and insisting that $\alpha\geqslant 0$, we find that the column eigenvector for the bound state is

$$\Psi_b(\alpha,x)=\begin{cases}Ae^{\alpha x}, & x\leqslant 0\\ Ae^{-\alpha x}, & x\geqslant 0,\end{cases} \tag{4.18}$$

where A is a normalized column matrix. By integrating Eq. (4.14) over an infinitesimal interval including the origin, we obtain an expression between the derivatives of $\Psi_b(\alpha,x)$ on both sides of the origin, which leads to the relation

$$(2\alpha+\lambda)A=0. \tag{4.19}$$

In order to avoid the trivial solution, we demand that

$$\det(2\alpha+\lambda)=0. \tag{4.20}$$

The nonnegative values of α which solve the above equation define the bound-state energies. Clearly there is at least one half-bound state if $\det \lambda = 0$.

Returning to the scattering problem, we find that the easiest way to proceed is to first diagonalize the matrix λ. Since λ is real and symmetric, the diagonalization can be accomplished by using an orthogonal matrix U, so that

$$\lambda_D = U \lambda U^{-1}, \tag{4.21}$$

where λ_D is diagonal and $U^{\mathrm{T}} = U^{-1}$. If we now define

$$\psi_D \equiv U \psi U^{-1}, \tag{4.22}$$

we see that Eq. (4.14) may be rewritten as

$$\left(-\frac{d^2}{dx^2} + \delta(x) \lambda_D \right) \psi_D = k^2 \psi_D . \tag{4.23}$$

The orthogonal transformation similarly transforms the boundary conditions, Eq. (4.15), to

$$\psi_D(k,x) = \begin{cases} \mathbf{1} e^{ikx} + \rho_D(k) e^{-ikx}, & x \leqslant 0 \\ \tau_D(k) e^{ikx}, & x \geqslant 0. \end{cases} \tag{4.24}$$

We see here another advantage of working directly with square matrices. If we had been working with column-vector wave functions, the transformed wave functions would have been given by $U\Psi$, so that the normalization of the incoming wave would in general have been changed. Working with $N \times N$ wave-function matrices gives the above result that the form of the boundary conditions is unchanged under the transformation. In fact the transformed wave function is itself a diagonal matrix, and we essentially have N decoupled copies of the problem with no coupling, with (possibly) different potential strengths. [Note that this same trick can be employed any time the potential is of the form $V(x) = v(x) M$, where M is a real symmetric matrix. Diagonalizing M gives N decoupled systems with potentials $V_i(x) = m_i v(x)$, $i = 1,\ldots,N$, where the m_i are the eigenvalues of the matrix M.]

Suppose now that $\det \lambda = 0$. Then it follows that λ has at least one zero eigenvalue. Let us again suppose that there are in fact n zero eigenvalues, so that

$$\lambda_D = \mathrm{diag}(0,\ldots,0,\lambda_{n+1},\ldots,\lambda_N), \tag{4.25}$$

where the λ_i, $i = n+1,\ldots,N$, are the remaining (nonzero) eigenvalues. Then the diagonalized reflection and transmission amplitude matrices are given by

$$\rho_D(k) = \mathrm{diag}\left(0,\ldots,0, \frac{\lambda_{n+1}}{2ik - \lambda_{n+1}}, \ldots, \frac{\lambda_N}{2ik - \lambda_N} \right) \tag{4.26}$$

and

$$\tau_D(k) = \mathrm{diag}\left(1,\ldots,1, \frac{2ik}{2ik - \lambda_{n+1}}, \ldots, \frac{2ik}{2ik - \lambda_N} \right), \tag{4.27}$$

so that

$$\mathrm{Tr}[\rho(0) + \tilde{\rho}(0)] = 2\,\mathrm{Tr}[\rho_D(0)] = -2(N-n). \tag{4.28}$$

Thus we see in this example how the trace of $\rho(0)+\tilde{\rho}(0)$ keeps track of the number of half-bound states in the system. In fact it is easy to verify that Levinson's theorem holds for the coupled system, since it holds separately for each decoupled equation of the diagonalized problem. (The proof follows on noting that the determinant of the S matrix is unchanged under the transformation which diagonalizes ρ and τ.)

It is instructive to consider the relation

$$2ik\tau_D^{-1}(k)=\ \mathrm{diag}(2ik,\ldots,2ik,2ik-\lambda_{n+1},\ldots,2ik-\lambda_N), \tag{4.29}$$

which follows from Eq. (4.27). It demonstrates for this model that in the limit as $k\to 0$ the expression Eq. (2.65) is real, as expected.

2. Potential with two delta functions

We now turn to a slightly more complicated example, in which there are two delta-function matrix potentials, one at $x=a$ and the other at $x=-a$. The $N=1$ version of this model was studied by Senn.[4] The Schrödinger equation for this case is given by

$$\left(-\frac{d^2}{dx^2}+\delta(x+a)\lambda+\delta(x-a)\tilde{\lambda}\right)\psi=k^2\psi, \tag{4.30}$$

with boundary conditions

$$\psi(k,x)=\begin{cases}\mathbf{1}e^{ikx}+\rho(k)e^{-ikx}, & x\leqslant -a\\ \tau(k)e^{ikx}, & x\geqslant a,\end{cases} \tag{4.31}$$

for the wave incident from the left and

$$\tilde{\psi}(k,x)=\begin{cases}\tilde{\tau}(k)e^{-ikx}, & x\leqslant -a\\ \mathbf{1}e^{-ikx}+\tilde{\rho}(k)e^{ikx}, & x\geqslant a,\end{cases} \tag{4.32}$$

for the wave incident from the right. Rather than solve the Schrödinger equation again, we may now simply substitute the results of the previous section into the factorization formula, Eq. (3.5). (Some care must be taken with the reflection amplitude matrices, for they acquire a phase when the potential is translated. The transmission amplitude matrices are, however, unchanged.) An evaluation of the resulting expressions yields

$$\rho(k)=(\lambda e^{-4ika}+(2ik+\lambda)(2ik-\tilde{\lambda})^{-1}\tilde{\lambda})\Gamma^{-1}(k,a;\lambda,\tilde{\lambda})\lambda^{-1}, \tag{4.33}$$

$$\tau(k)=-4k^2e^{-2ika}(2ik-\tilde{\lambda})^{-1}\Gamma^{-1}(k,a;\lambda,\tilde{\lambda})\lambda^{-1}, \tag{4.34}$$

$$\tilde{\rho}(k)=(2ik-\tilde{\lambda})^{-1}\Gamma^{-1}(k,a;\lambda,\tilde{\lambda})((2ik-\lambda)\lambda^{-1}\tilde{\lambda}e^{-4ika}+2ik+\tilde{\lambda}), \tag{4.35}$$

$$\tilde{\tau}(k)=\tau^T(k), \tag{4.36}$$

where

$$\Gamma(k,a;\lambda,\tilde{\lambda})=(2ik-\lambda)\lambda^{-1}e^{-2ika}-(2ik-\tilde{\lambda})^{-1}\tilde{\lambda}e^{2ika}. \tag{4.37}$$

Let us assume for the moment that both λ^{-1} and $\tilde{\lambda}^{-1}$ exist so that the above expressions are well defined. (For $k>0$, it is actually sufficient that only one or the other exists—it is possible to rewrite the expressions so that they contain only $\tilde{\lambda}^{-1}$ and not λ^{-1}.) Performing a Taylor expansion of ρ and $\tilde{\rho}$ for small k, we find that in the typical case $\rho(0)=\tilde{\rho}(0)=-\mathbf{1}$, so that

$\mathrm{Tr}[\rho(0)+\tilde{\rho}(0)]=-2N$, as expected. The atypical case is defined by the condition $\det(\lambda^{-1}+\tilde{\lambda}^{-1}+2a)=0$, which, as we shall see, is also the condition for a half-bound state.

Let us then work out the bound-state condition. This may be done in a manner similar to that for the single delta-function case to obtain

$$\det \Gamma(i\alpha,a;\lambda,\tilde{\lambda})=0. \tag{4.38}$$

Solutions of Eq. (4.38) with $\alpha>0$ correspond to bound states. As $\alpha\to 0$, Eq. (4.38) yields the half-bound-state condition,

$$\det(\lambda^{-1}+\tilde{\lambda}^{-1}+2a)=0. \tag{4.39}$$

Alternatively, if we employ the wave functions ϕ and χ of Sec. II C. for the model potential and use Eq. (2.58) as the condition for the bound state, we obtain the equation

$$\det([(\lambda+2\alpha)(\tilde{\lambda}+2\alpha)-\lambda\tilde{\lambda}e^{-4\alpha a}]/2\alpha)=0, \tag{4.40}$$

which in the limit as α approaches zero reduces to

$$\det(\lambda+\tilde{\lambda}+2a\lambda\tilde{\lambda})=0. \tag{4.41}$$

This equation is preferred over Eq. (4.39) since it is not artificially singular when one of the inverse matrices does not exist.

Let us now consider an explicit example with $N=2$. Since one of the two matrices λ or $\tilde{\lambda}$ may always be diagonalized by an orthogonal transformation, we will let λ be diagonal right from the start. An example which gives a half-bound state for $a=1$ is one for which

$$\lambda=\begin{pmatrix} -\frac{1}{2} & 0 \\ 0 & -1 \end{pmatrix}, \quad \tilde{\lambda}=\begin{pmatrix} -6 & -2 \\ -2 & -1 \end{pmatrix}. \tag{4.42}$$

Figure 1 shows a parametric plot of $\rho_{11}(k)$ as a function of k in the complex plane for the cases $a=0.95$, $a=1.00$, and $a=1.05$. In the two typical cases ($a=0.95,1.05$), $\rho_{11}(0)=-1$, while for the atypical case ($a=1$), $\rho_{11}(0)=0.777\cdots$. This is then the analog of Senn's ''threshold anomaly'' for the generalized matrix version of his model.[4] Examination of the other diagonal reflection amplitudes yields the expected result that $\mathrm{Tr}[\rho(0)+\tilde{\rho}(0)]$ is equal to -4 in the typical case and -2 in the case where one half-bound state exists.

The behaviour of $\rho_{11}(k)$ as a function of k may strike the reader as being somewhat peculiar: for sufficiently large k as k increases, $\rho_{11}(k)$ traces out a never-ending counter-clockwise spiral towards the origin. A plot of the argument of $\rho_{11}(0)$ for the three cases would show that the phase shifts are not bounded—they keep on increasing to infinity. This peculiar feature does not exist when there is no coupling (the phase shifts are bounded due to Levinson's theorem), but is a rather generic feature of $N>1$ models. The important thing to bear in mind when $N>1$ is that the phase shift which obeys Levinson's theorem is defined as being proportional to the logarithm of the determinant of the S matrix. This phase shift can in general be a nontrivial function of the ''physical'' phase shifts associated with the scattering amplitudes.

Figure 2 shows a plot of

$$f(\alpha,a;\lambda,\tilde{\lambda})=\det([(\lambda+2\alpha)(\tilde{\lambda}+2\alpha)-\lambda\tilde{\lambda}e^{-4\alpha a}]/2\alpha), \tag{4.43}$$

as a function of α for $a\approx 1$. The inset in this figure shows an expanded view of the function near the origin for the three cases $a=0.95,1.00$, and 1.05. In addition to the two regular bound states

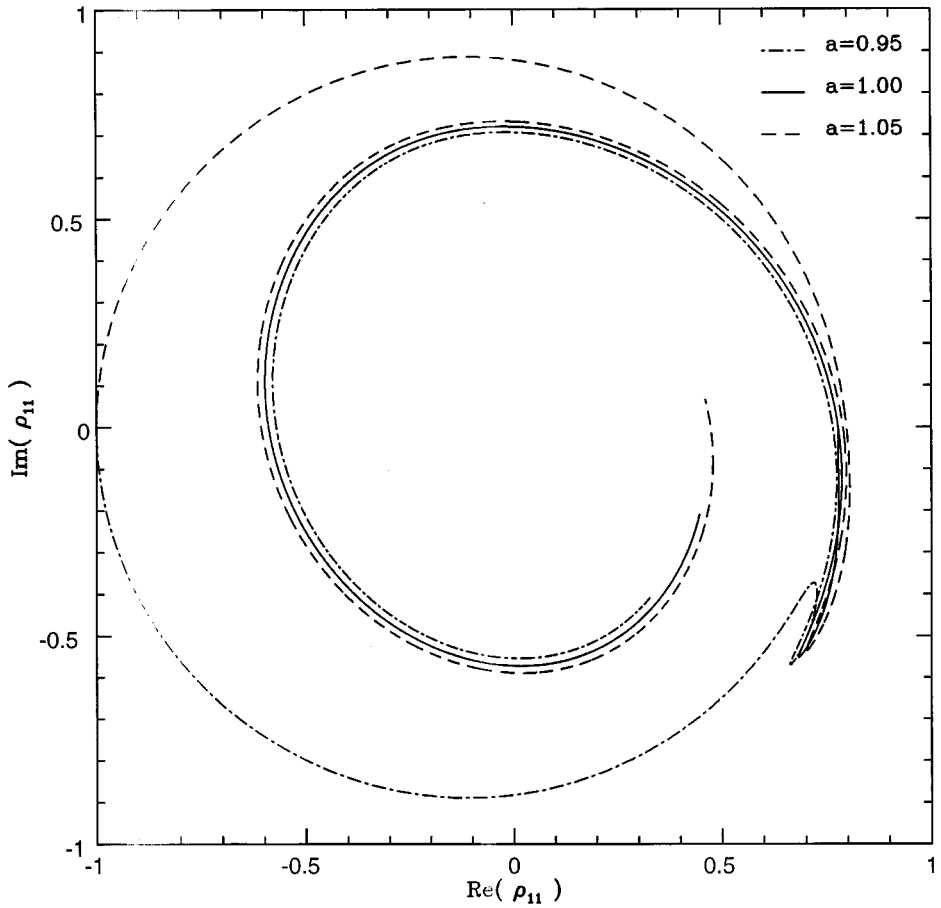

FIG. 1. Plot of the $\mathrm{Im}(\rho_{11}(k))$ vs the $\mathrm{Re}(\rho_{11}(k))$ for $k=0$ to $k=5$ for double delta-function matrix potential. For the $a=1.05$ case the curve reverses the direction of travel around the origin when $k\simeq 1.1$.

that all three cases possess (near $\alpha=0.5164$ and $\alpha=3.3508$), the $a=1.05$ case has an extra bound state near $\alpha=0.0259$, and the $a=1.00$ case has a new bound state just emerging at $\alpha=0$.

Finally, Fig. 3 shows a plot of the ''Levinson's theorem'' phase shift as a function of k for the three cases. Clearly this phase shift is well-behaved and is bounded. As the potential ''strength'' is adjusted so that the system goes through a half-bound state the phase shift at $k=0$ jumps by π in two increments of $\pi/2$.

V. DISCUSSION

In this section we make a few observations. The problem of one-dimensional coupled-equation scattering using a representation of wave functions which have incoming waves from the left or the right is readily solvable. Despite the advantages of a ''partial wave'' representation[7,8] or a parity-eigenstate representation[2,6] for parity-invariant potential functions, our analysis (which is valid for any potential) is quite manageable.

The use of wave function matrices (see Refs. 16 and 28 for three-dimensional scattering and also Refs. 13 and 14 for one-dimensional scattering) rather than column-vector wave functions, leads to simplified notation for a number of relations, e.g., the closure relation, Eq. (2.30). One also finds that performing a unitary transformation on the scattering wave function matrix does not

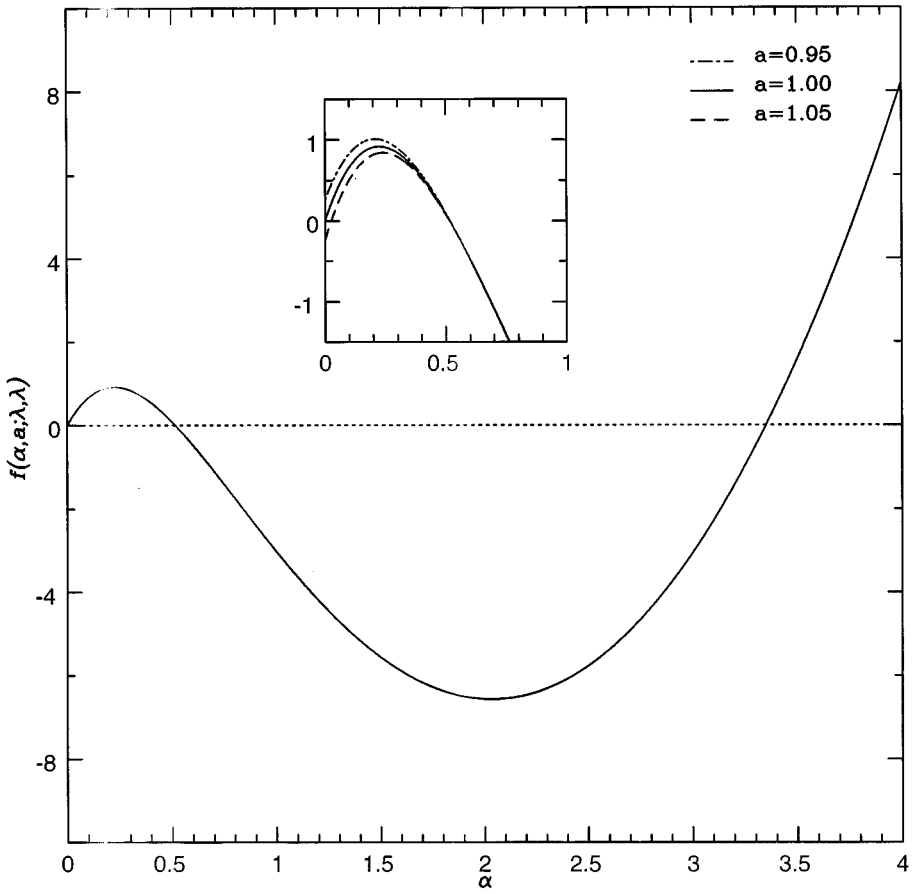

FIG. 2. The determinant function for the double delta-function potential graphed as a function of α.

alter the normalization of the incoming waves, whereas it does for column wave functions. The introduction of the real matrix wave function solutions ϕ and χ has two distinct advantages. In the first place the Schrödinger equation for the scattering problem can be reduced to a system of first-order differential equations with one-point boundary conditions, Eq. (4.2). The scattering amplitudes (and the S matrix) are algebraic expressions of these functions evaluated at R. Furthermore, unlike the solution matrices ψ and $\tilde{\psi}$, matrices ϕ and χ have linearly independent columns at threshold and consequently are convenient for investigating threshold behaviour.

Our starting point with the wave functions ψ and $\tilde{\psi}$, which gives the definition of the reflection amplitudes ρ and $\tilde{\rho}$, yields a generalized and simplified understanding of threshold behaviour. Whereas previous work[4,7] indicates that for parity-noninvariant potentials the reflection amplitude at threshold can have noninteger values, unlike that for parity-invariant potentials, we find that $\mathrm{Tr}[\rho(k)+\tilde{\rho}(k)]$ at threshold is always an integer [see Eq. (2.83)]. The results of de Bianchi,[2] however, already imply such a relation, as well as noninteger reflection amplitudes at threshold, for some parity-noninvariant potentials with no coupling.

Finally, the phases of the reflection and transmission amplitudes of the coupled system are not simple functions of k, as is the case for uncoupled scattering, for which these phases satisfy the appropriate form of Levinson's theorem. The phase η of the S matrix, which appears in Levinson's theorem, is in general a nontrivial function of the phases of the scattering amplitudes.

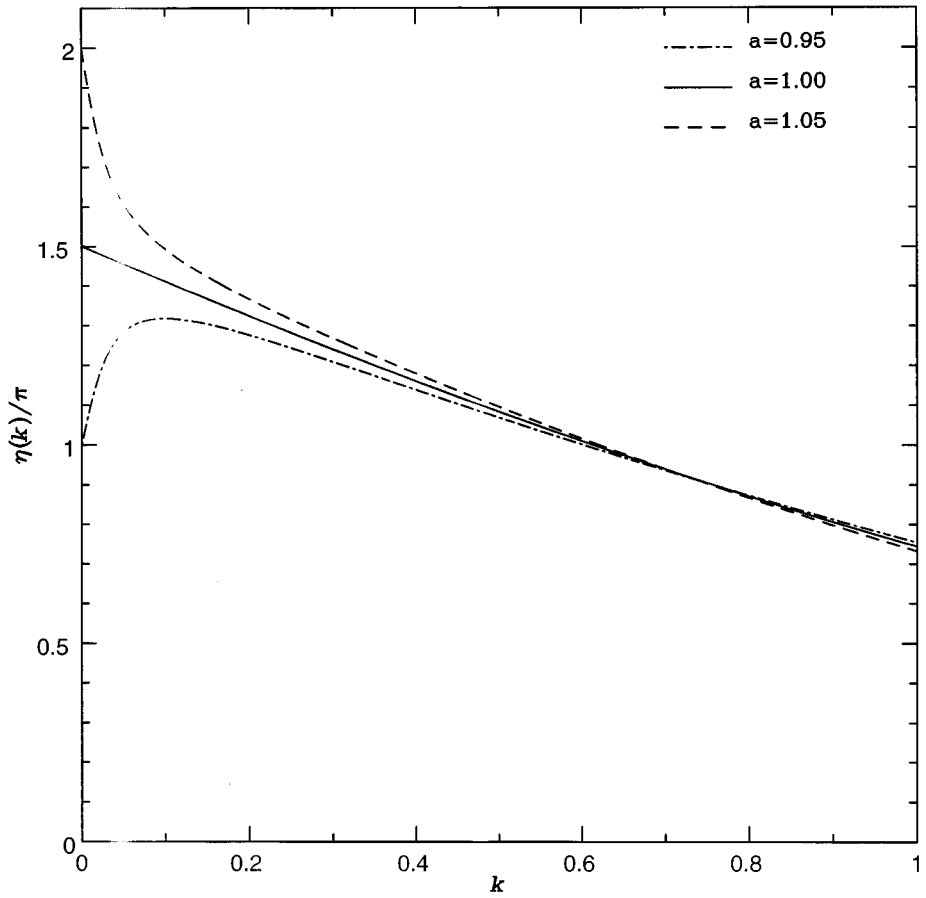

FIG. 3. The phase of the S matrix (divided by π) of the double delta-function potential as a function of k. For k larger than shown on the graph the three curves remain close to one another and approach zero as $k\to\infty$.

Furthermore, the function $\eta(k)$ is bounded, unlike the phases of the scattering amplitudes which are not necessarily bounded.

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APPENDIX A: SOME PROPERTIES OF SOLUTIONS OF THE SCHRÖDINGER EQUATION

In this Appendix we determine the condition for linear independence of the solutions of the Schrödinger equation. Consider the matrix Schrödinger equation

$$-\frac{d^2\psi}{dx^2}+V(x)\psi=k^2\psi, \tag{A1}$$

where ψ is the $N\times N$ solution matrix whose columns are solutions to Eq. (2.1). Suppose we have two such solution matrices, f and $\tilde{f}$. We define a $2N\times 2N$ matrix functional

$$W(f,\tilde{f})=\begin{pmatrix} f & \tilde{f} \\ f' & \tilde{f}' \end{pmatrix}, \tag{A2}$$

in which the prime indicates the derivative with respect to x. Since f and $\tilde{f}$ satisfy Eq. (A1) the matrix W is a solution of the matrix equation,

$$W'=FW, \tag{A3}$$

where

$$F=\begin{pmatrix} \mathbf{0} & \mathbf{1} \\ V-k^2 & \mathbf{0} \end{pmatrix}. \tag{A4}$$

Lemma 1: $(\det\ W)'=0$ for all $x\in(-\infty,\infty)$.

Proof: Let us write f and $\tilde{f}$ in terms of their N-component row vectors:

$$f=\begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ f_N \end{pmatrix} \quad \text{and} \quad \tilde{f}=\begin{pmatrix} \tilde{f}_1 \\ \tilde{f}_2 \\ \vdots \\ \tilde{f}_N \end{pmatrix}. \tag{A5}$$

We then obtain (Ref. 27)

$$(\det\ W)'=\det\begin{pmatrix} f_1' & \tilde{f}_1' \\ f_2 & \tilde{f}_2 \\ \vdots & \vdots \\ f_N & \tilde{f}_N \\ f_1' & \tilde{f}_1' \\ f_2' & \tilde{f}_2' \\ \vdots & \vdots \\ f_N' & \tilde{f}_N' \end{pmatrix}+\cdots+\det\begin{pmatrix} f_1 & \tilde{f}_1 \\ f_2 & \tilde{f}_2 \\ \vdots & \vdots \\ f_N' & \tilde{f}_N' \\ f_1' & \tilde{f}_1' \\ f_2' & \tilde{f}_2' \\ \vdots & \vdots \\ f_N' & \tilde{f}_N' \end{pmatrix}+\det\begin{pmatrix} f_1 & \tilde{f}_1 \\ f_2 & \tilde{f}_2 \\ \vdots & \vdots \\ f_N & \tilde{f}_N \\ f_1'' & \tilde{f}_1'' \\ f_2' & \tilde{f}_2' \\ \vdots & \vdots \\ f_N' & \tilde{f}_N' \end{pmatrix}+\cdots+\det\begin{pmatrix} f_1 & \tilde{f}_1 \\ f_2 & \tilde{f}_2 \\ \vdots & \vdots \\ f_N & \tilde{f}_N \\ f_1' & \tilde{f}_1' \\ f_2' & \tilde{f}_2' \\ \vdots & \vdots \\ f_N'' & \tilde{f}_N'' \end{pmatrix}. \tag{A6}$$

The first N determinants in the sum on the right are zero because they have two equivalent rows. In order to show that the remaining terms are also zero, we write the Schrödinger equation, Eq. (A1), as

$$\psi''(x)=M(x)\psi(x), \tag{A7}$$

where $M(x)$ is an $N\times N$ matrix. Furthermore we write $M(x)$ in terms of row vectors

$$M(x)=\begin{pmatrix} m_1(x) \\ m_2(x) \\ \vdots \\ m_N(x) \end{pmatrix}. \tag{A8}$$

Then the matrix in the ith second-derivative term of Eq. (A6) may be written as

$$\begin{pmatrix} f_1 & \tilde{f}_1 \\ \vdots & \vdots \\ f_N & \tilde{f}_N \\ f_1' & \tilde{f}_1' \\ \vdots & \vdots \\ f_i'' & \tilde{f}_i'' \\ \vdots & \vdots \\ f_N' & \tilde{f}_N' \end{pmatrix} = \begin{pmatrix} \mathbf{1} & & & & \mathbf{0} & & \\ & 1 & & & & & \\ & & \ddots & & & & \\ & & & 1 & & & \\ m_i(x) & & & & 0 & & \\ & & & & & 1 & \\ & & & & & & \ddots \\ & & & & & & & 1 \end{pmatrix} (W). \tag{A9}$$

The determinant of the matrix on the right side of Eq. (A9) is zero, and consequently the $(\det W)' = 0$. The $\det W$ is a constant function of x.

Lemma 2: The solutions contained in the columns of f and $\tilde{f}$ are linearly independent if and only if $\det W \neq 0$ for all $x \in (-\infty, \infty)$.

Proof: First suppose that $\det W \neq 0$. We consider a linear combination of solutions which is equal to the trivial solution,

$$f\mathbf{h} + \tilde{f}\tilde{\mathbf{h}} = \mathbf{o} \quad \text{for all } x, \tag{A10}$$

where $\mathbf{h}$ and $\tilde{\mathbf{h}}$ are N-component column vectors of constants and $\mathbf{o}$ is the N-component zero column vector. A similar relation holds for the derivatives of f and $\tilde{f}$, so that

$$W\mathbf{c} = \mathbf{o}, \tag{A11}$$

where

$$\mathbf{c} = \begin{pmatrix} \mathbf{h} \\ \tilde{\mathbf{h}} \end{pmatrix}, \tag{A12}$$

and $\mathbf{c}$ and $\mathbf{o}$ are now $2N$-component column vectors. If $\det W \neq 0$ for some x, which according to the previous result means it is nonzero for all x, $\mathbf{c} = \mathbf{o}$ and the column solutions contained in f and $\tilde{f}$ are linearly independent.

Suppose now that $\det W = 0$. If $\det W = 0$ for some $x = x_0$, then the system of linear equations $W(x_0)\mathbf{c} = \mathbf{o}$ has a nontrivial solution $\mathbf{c}$. We form a column solution of the system of differential equations, Eq. (A3), $\mathbf{w}(x) = W(x)\mathbf{c}$ which vanishes at x_0. This is the trivial solution of Eq. (A3); $\mathbf{w}(\mathrm{x}) = \mathbf{o}$ for all x. It follows that the column solutions contained in f and $\tilde{f}$ are linearly dependent.

APPENDIX B: ANALYTIC PROPERTIES OF THE SOLUTION MATRICES ϕ AND χ

We consider solution matrices $\phi(k,x)$ and $\chi(k,x)$ of Eq. (A1) with boundary conditions $\phi(k,-R) = \chi'(k,-R) = \mathbf{1}$ and $\phi'(k,-R) = \chi(k,-R) = \mathbf{0}$, where R is the range of the potential. According to a theorem of Poincaré an ordinary differential equation containing an entire function of some parameter has solutions which are entire functions of the parameter provided these solutions have boundary conditions which are independent of the parameter. We will show that ϕ and χ are entire functions of k, following a similar derivation for partial-wave solutions in three-dimensional scattering.[28,29]

It is straightforward to verify that the matrix functions ϕ and χ with the given boundary conditions are solutions of integral equations of the Volterra type,

$$\phi(k,x)=\mathbf{1}\cos k(x+R)+\int_{-R}^{x}dx'\,\frac{\sin k(x-x')}{k}V(x')\phi(k,x') \tag{B1}$$

$$\chi(k,x)=\mathbf{1}\frac{\sin k(x+R)}{k}+\int_{-R}^{x}dx'\,\frac{\sin k(x-x')}{k}V(x')\chi(k,x'). \tag{B2}$$

In order to show that each element of the solution matrices is an entire function of k, we rewrite Eq. (B1) in the form

$$\phi(k,x)=\mathbf{1}\cos k(x+R)+\int_{-R}^{x}dx'\int_{0}^{x-x'}dt\,\cos ktV(x')\phi(k,x'). \tag{B3}$$

We solve Eq. (B3) by successive approximations of the form

$$\phi(k,x)=\sum_{s=0}^{\infty}\phi^{(s)}(k,x), \tag{B4}$$

where

$$\phi^{(s)}(k,x)=\int_{-R}^{x}dx'\int_{0}^{x-x'}dt\,\cos ktV(x')\phi^{(s-1)}(k,x'),\quad s\geqslant 1$$

and

$$\phi^{(0)}(k,x)=\mathbf{1}\cos k(x+R). \tag{B5}$$

Thus

$$|\phi_{ij}^{(s)}(k,x)|\leqslant\int_{-R}^{x}dx'\int_{0}^{x-x'}dt|\cos kt|\sum_{l}|V_{il}(x')||\phi_{lj}^{(s-1)}(k,x')|,\quad s\geqslant 1 \tag{B6}$$

and

$$|\phi_{ij}^{(0)}(k,x)|=\delta_{ij}|\cos k(x+R)|. \tag{B7}$$

Denoting $\Im k$ for the imaginary part of k and using the relation $|\cos kt|\leqslant\cosh \Im kt$ for t real, we obtain upon iteration

$$\begin{aligned}|\phi_{ij}^{(s)}(k,x)|&\leqslant\sum_{i'j'}|\phi_{i'j'}^{(s)}(k,x)|\\&\leqslant\left(\frac{\sinh(2\Im kR)}{\Im k}\right)^{s}\cosh(2\Im kR)\int_{-R}^{x}dx_1\int_{-R}^{x_1}dx_2\cdots\int_{-R}^{x_{s-1}}dx_s\\&\quad\times\sum_{i',j',l_1,\ldots,l_s}|V_{i'l_1}(x_1)||V_{l_1l_2}(x_2)|\cdots|V_{l_sj'}(x_s)|.\end{aligned} \tag{B8}$$

Since the integrand is a symmetric function under the interchange of any pair (x_i,x_j),

$$|\phi_{ij}^{(s)}(k,x)| \leqslant \left(\frac{\sinh(2\Im kR)}{\Im k}\right)^s \cosh(2\Im kR)\frac{1}{s!} \times \sum_{i',j',l_1,\ldots,l_s} \int_{-R}^{x} dx_1 |V_{i'l_1}(x_1)| \cdots \int_{-R}^{x} dx_s |V_{l_s j'}(x_s)|. \tag{B9}$$

Let

$$M_0 = \max_{i,j} \int_{-R}^{R} dx' |V_{ij}(x')| < \infty. \tag{B10}$$

Then

$$|\phi_{ij}^{(s)}(k,x)| \leqslant \left(\frac{\sinh(2\Im kR)}{\Im k}\right)^s \cosh(2\Im kR)\frac{N^{s+2}}{s!} M_0^s. \tag{B11}$$

Thus the series $\Sigma_s \phi_{ij}^{(s)}$ converges absolutely and uniformly for $x \in [-R,R]$ and for every region in the complex k plane. To determine the existence of $(\partial\phi/\partial k)(k,x)$, we differentiate Eq. (B3) with respect to k,

$$\frac{\partial \phi}{\partial k}(k,x) = -(x+R)\mathbf{1}\sin k(x+R) - \int_R^x dx' \int_0^{x-x'} dt\, t \sin kt V(x')\phi(k,x') + \int_R^x dx' \int_0^{x-x'} dt \cos kt\, V(x')\frac{\partial \phi}{\partial k}(k,x'). \tag{B12}$$

When Eq. (B4) is differentiated with respect to k it yields

$$\frac{\partial \phi}{\partial k}(k,x) = \sum_{s=0}^{\infty} \frac{\partial \phi^{(s)}}{\partial k}(k,x), \tag{B13}$$

where now we have

$$\frac{\partial \phi^{(s)}}{\partial k}(k,x) = \int_R^x dx' \int_0^{x-x'} dt \cos kt\, V(x')\frac{\partial \phi^{(s-1)}}{\partial k}(k,x') \tag{B14}$$

with

$$\frac{\partial \phi^{(0)}}{\partial k}(k,x) = -(x+R)\mathbf{1}\sin k(x+R) - \int_R^x dx' \int_0^{x-x'} dt\, t \sin kt\, V(x')\phi(k,x'). \tag{B15}$$

It is not difficult to show that

$$\left|\frac{\partial \phi_{ij}^{(0)}}{\partial k}(k,x)\right|$$

is bounded, and the convergence of series (B13) follows in the same manner as that of $\phi(k,x)$. Since $\phi(k,x)$ and its derivative with respect to k exist for all k, $\phi(k,x)$ is an entire function of k. Similarly $\chi(k,x)$ can be shown to be an entire function of k.

For real k the behaviour of $\phi(k,x)$ and $\chi(k,x)$ as k becomes very large can be determined by iterating Eqs. (B1) and (B2). Thus

$$\phi(k,x)\underset{k\to\infty}{\sim}\mathbf{1}\cos k(x+R)+\frac{1}{k}\int_{-R}^{x}dx'\sin k(x-x')V(x')\cos k(x'+R)+O(1/k^2) \tag{B16}$$

and

$$\chi(k,x)\underset{k\to\infty}{\sim}\mathbf{1}\frac{\sin k(x+R)}{k}+\frac{1}{k^2}\int_{-R}^{x}dx'\sin k(x-x')V(x')\sin k(x'+R)+O(1/k^3). \tag{B17}$$

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Special-relativistic harmonic oscillator modeled by Klein–Gordon theory in anti-de Sitter space

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It is shown that the one-particle sector of the Klein–Gordon theory in the universal covering space of the anti-de Sitter space (CAdS) can be interpreted, in a natural way, as a special-relativistic oscillator in Minkowski space. The quantum wave functions have a significantly different behavior with respect to the nonrelativistic ones. The energy spectrum coincides, up to the ground state energy, with that of the nonrelativistic oscillator. The requirement of having the adequate nonrelativistic limit for the special-relativistic oscillator theory turns out to be equivalent to the imposition of the Dirichlet-type boundary condition at spatial infinity on CAdS Klein–Gordon functions. © *1996 American Institute of Physics.*
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I. INTRODUCTION

The nonrelativistic oscillator is one of the simplest and most useful system in physics. However, despite its simplicity, there is not a well-established relativistic generalization in the literature. The first proposal for a special-relativistic harmonic oscillator was given by Yukawa,[1] followed by the work of Feynman *et al.*[2] and further developed in Ref. 3. These works are all based on the naive covariant generalization $x^\mu x_\mu$ of the nonrelativistic potential thus leading to quantum timelike excitations, the interpretation of which presents some difficulties. On the other hand, Itô *et al.*[4] (see also Refs. 5 and 6) introduced a Dirac equation which is linear in both coordinates and momenta. In the nonrelativistic limit, the equation satisfied by the large components is that of ordinary oscillator with a spin-orbit coupling term.

Recently a new proposal for the special-relativistic harmonic oscillator was outlined in Ref. 7 (see also Ref. 8). It is based in the natural generalization of the symmetry algebra of quantum operators of a relativistic free system (i.e., the Poincaré algebra)

$$[\hat{E},\,\hat{x}]=-i\,\frac{\hbar}{m}\,\hat{p},\quad [\hat{E},\,\hat{p}]=0,\quad [\hat{x},\,\hat{p}]=i\hbar\left(1+\frac{1}{mc^2}\,\hat{E}\right),\tag{1}$$

and that of a nonrelativistic harmonic oscillator (i.e., the Lie algebra of the Newton group)

$$[\hat{E},\,\hat{x}]=-i\,\frac{\hbar}{m}\,\hat{p},\quad [\hat{E},\,\hat{p}]=im\omega^2\hbar\hat{x},\quad [\hat{x},\,\hat{p}]=i\hbar.\tag{2}$$

Here $\hat{E}$, $\hat{p}$, and $\hat{x}$ are the energy (with the rest-mass energy subtracted), momentum, and boost operators in the center of momentum frame. The proposed symmetry for the $(1+1)$ special-relativistic oscillator was defined in terms of the unique Lie algebra which allows it to be contracted to the above algebras

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$$[\hat{E},\,\hat{x}]=-i\,\frac{\hbar}{m}\,\hat{p},\quad [\hat{E},\,\hat{p}]=im\omega^2\hbar\hat{x},\quad [\hat{x},\,\hat{p}]=i\hbar\left(1+\frac{1}{mc^2}\,\hat{E}\right). \tag{3}$$

This Lie algebra corresponds to that of the SO(1,2) group. Related approaches can be seen in Ref. 9.

The aim of this paper is to further elaborate on this proposal. In Sec. II we shall interpret it geometrically showing that a static (1+1) anti-de Sitter metric can be used to simulate a one-dimensional special-relativistic oscillator. More precisely, we shall show that the one-particle sector of the Klein–Gordon field theory on the universal covering space of the anti-de Sitter space (CAdS), with the positive frequencies defined with respect to the global timelike Killing vector, can be interpreted in terms of a special-relativistic oscillator in Minkowski space. The results obtained in this way can be seen as complementary to those found by group theoretical methods[10–12] for the one-dimensional oscillator.[7,13] The main goal of this paper is to extend to three spatial dimensions the proposal (3) for a (1+1) special-relativistic oscillator. This will be done in Sec. III by making use of the geometrical interpretation developed in Sec. II. Obviously, the proper space–time of the special-relativistic oscillator theory is Minkowski space (CAdS is just an auxiliary concept) and this should be taken into account in the interpretation of the corresponding wavefunctions. We will show that a specific boundary condition, usually required as a way to recover a well-defined Cauchy problem[14] in AdS, is now needed to recover the quantum mechanics of the nonrelativistic harmonic oscillator. Moreover, the adequate physical interpretation of the special-relativistic oscillator wave functions involves some sort of Newton–Wigner type transformation of the associated Klein–Gordon functions. In Sec. IV we shall state our conclusions.

II. ANTI-DE SITTER SPACE AND THE ONE-DIMENSIONAL SPECIAL-RELATIVISTIC OSCILLATOR

The basic ingredient in the proposal of Ref. 7 for a special-relativistic oscillator is the SO(1,2) group symmetry. The Lie algebra commutators of this group can be thought of as the natural generalization of those of the relativistic free particle and the nonrelativistic oscillator. Due to anti-de Sitter (AdS) space is a homogeneous space of the SO(1,2) group. It is therefore natural to regard the harmonic oscillator interaction in (1+1) Minkowski space as equivalent to a free system in AdS space (more precisely, in its universal covering space, which has the topology of $\mathbb{R}^2$).[15] However, this definition for a special-relativistic oscillator is incomplete. Owing to general covariance we must specify which particular CAdS metric properly simulates the relativistic oscillator interaction in Minkowski space. To solve this ambiguity we can resort to the nonrelativistic limit. To adjust the nonrelativistic limit we have to choose g_{00} as

$$g_{00}=1+\frac{\omega^2}{c^2}\,x^2. \tag{4}$$

Assuming now a static form for the metric, the requirement of having a CAdS geometry determines the remaining component of the metric:

$$ds^2=\left(1+\frac{\omega^2}{c^2}\,x^2\right)c^2dt^2-\frac{1}{1+(\omega^2/c^2)x^2}\,dx^2. \tag{5}$$

The timelike geodesic trajectories of motion can be obtained from the Lagrangian

$$\mathscr{L}=-mc\,\sqrt{1-\frac{1}{1+(\omega^2/c^2)x^2}\,\frac{v^2}{c^2}+\frac{\omega^2}{c^2}\,x^2}, \tag{6}$$

where m is the (reduced) mass of the system. Moreover, it is easy to see that the timelike geodesics in the metric (5) are periodic and with a period $2\pi/\omega$ independent of the amplitude. The underlying SO(1,2) symmetry is realized by Poisson brackets between the three constants of motion

$$C_{(a)}=mg_{\mu\nu}f^{\mu}_{(a)}\frac{dx^{\nu}}{d\tau}, \tag{7}$$

where $f^{\mu}_{(a)}$, $a=1,2,3$, are the Killing vectors of (5).

$$f^{\mu}_{1}=(1,0), \tag{8}$$

$$f^{\mu}_{2}=\left(\frac{(\omega/c)\,x}{\sqrt{1+(\omega^2/c^2)\,x^2}}\cos\,\omega t,\sqrt{1+\frac{\omega^2}{c^2}\,x^2}\,\sin\,\omega t\right), \tag{9}$$

$$f^{\mu}_{3}=\left(-\frac{(\omega/c)x}{\sqrt{1+(\omega^2/c^2)x^2}}\sin\,\omega t,\sqrt{1+\frac{\omega^2}{c^2}\,x^2}\cos\,\omega t\right). \tag{10}$$

The Killing vectors realize the algebra (3). Here f^{μ}_{1}, f^{μ}_{2}, and f^{μ}_{3} lead to the energy, boost, and momentum generators, respectively. It is also interesting to note that the periodic character of the trajectories of motion of the oscillator can be traced back to the existence of closed timelike lines in AdS space.

From (6) it is straightforward to compute the Hamiltonian of the model

$$H^2=m^2c^4+p^2c^2+m^2\omega^2c^2x^2+2\omega^2x^2p^2+\frac{\omega^4}{c^2}\,x^4p^2. \tag{11}$$

Physically we can think of this Hamiltonian as the one describing the dynamics of a (special-relativistic) harmonic oscillator system in the center of the momentum frame. The AdS symmetry is the responsiblility of the nonlinear terms in (11). We must remark that (11) differs essentially from the naive definition[16]

$$(H-\tfrac{1}{2}m\omega^2x^2)^2=m^2c^4+p^2c^2. \tag{12}$$

In contrast with (12), our model (11) will lead to square-integrable quantum wavefunctions. With the standard substitutions $H\to i\hbar\partial/\partial t$, $p\to -i\hbar\partial/\partial x$, $x\to x$ [we have used the same notation for the ''position'' operator and the ''boost'' operator $\hat{x}$ of (3)] and introducing the parameters α and β to account for the normal ordering ambiguities of the classical function (11):

$$x^4p^2\to -\hbar^2\left(x^4\frac{d^2}{dx^2}+4x^3\frac{d}{dx}+\alpha x^2\right), \tag{13}$$

$$x^2p^2\to -\hbar^2\left(x^2\frac{d^2}{dx^2}+2x\frac{d}{dx}+\beta\right). \tag{14}$$

The quantum counterpart of (11) yields to

$$\left\{ \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \left(1+\frac{\omega^2}{c^2}x^2\right)^2 \frac{\partial^2}{\partial x^2} - 4\frac{\omega^2}{c^2}x\left(1+\frac{\omega^2}{c^2}x^2\right)\frac{\partial}{\partial x} + \left[\left(\frac{mc}{\hbar}\right)^2 - 2\beta\frac{\omega^2}{c^2}\right]\left(1+\frac{\omega^2}{c^2}x^2\right) - (\alpha-2\beta)\frac{\omega^4}{c^4}x^2\right\}\Psi(x,t)=0. \tag{15}$$

This equation turns out be the Klein–Gordon equation in AdS space[17]

$$\left(\Box + \frac{m^2c^2}{\hbar^2} + \xi R\right)\phi = 0, \tag{16}$$

where $\Box$ is the D'Alembertian operator for the AdS metric (5), $R=-2\omega^2/c^2$ is the scalar curvature, and ξ is a numerical factor. The equivalence is obtained through the transformation

$$\Psi = \frac{1}{\sqrt{1+(\omega^2/c^2)x^2}}\,\phi, \tag{17}$$

and requires a restriction on the parameters α and β: $\alpha=\xi+\frac{1}{2}$ and $\beta=2\xi+2$.

It is worthwhile to remark that the transformation (17) can be understood in terms of the Klein–Gordon scalar product in curved space (see, for instance Ref. 17)

$$\langle \phi_1 | \phi_2 \rangle = i\int_\Sigma d\sigma_\mu \sqrt{g} g^{\mu\nu}(\phi_1 \overleftrightarrow{\partial}_\nu \phi_2^*), \tag{18}$$

where Σ is the initial value hypersurface. For the line element (5) and choosing Σ as $t=0$, (18) becomes

$$\langle \phi_1 | \phi_2 \rangle = -i\int \frac{dx}{1+(\omega^2/c^2)x^2}(\phi_1 \overleftrightarrow{\partial}_0 \phi_2^*). \tag{19}$$

For stationary states the scalar product (19) is proportional to the standard $L^2(\mathbb{R},dx)$ scalar product of Schrödinger-type wavefunctions

$$\langle \Psi_1 | \Psi_2 \rangle = \int dx \Psi_1^* \Psi_2. \tag{20}$$

In general a sort of Newton–Wigner-type transformation is required to convert (19) into (20). From now on we shall be mainly concerned with the Klein–Gordon equation although the physical wavefunctions are the Schrödinger-type wavefunctions verifying the equation (15).

The D'Alembertian operator for the AdS metric (5) is

$$\Box = \frac{1}{1+(\omega^2/c^2)x^2}\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - 2\frac{\omega^2}{c^2}x\frac{\partial}{\partial x} - \left(1+\frac{\omega^2}{c^2}x^2\right)\frac{\partial^2}{\partial x^2}. \tag{21}$$

To solve the Klein–Gordon equation we shall first look for positive frequency states. To find the spatial dependence of the wavefunctions we shall further propose the ansatz

$$\phi(x,t) = e^{-i\lambda\omega t}\left(1+\frac{\omega^2}{c^2}x^2\right)^{-\lambda/2}\phi^\lambda(x), \tag{22}$$

where λ is an arbitrary positive parameter. The wavefunction (22) verifies the Klein–Gordon equation (16) if the function $\phi^\lambda(x)$ satisfies the following differential equation;

$$\left\{\left(1+\frac{\omega^2}{c^2}x^2\right)\frac{d^2}{dx^2}-2\frac{\omega^2}{c^2}(\lambda-1)x\frac{d}{dx}+\frac{\omega^2}{c^2}(\lambda(\lambda-1)-N^2+2\xi)\right\}\phi^{\lambda}(x)=0, \tag{23}$$

where $N=mc^2/\hbar\omega$. In terms of the variable $w=-(\omega^2/c^2)x^2$, (23) is a standard hypergeometric equation

$$\left\{(1-w)w\frac{d^2}{dw^2}+\left(\frac{1}{2}-\left(\frac{3}{2}-\lambda\right)w\right)\frac{d}{dw}-\frac{1}{4}(\lambda(\lambda-1)-N^2+2\xi)\right\}\phi^{\lambda}(w)=0. \tag{24}$$

The vanishing of the Klein–Gordon functions at infinity restricts the allowed values of the λ parameter. We obtain

$$\lambda=\tfrac{1}{2}+n+\gamma, \tag{25}$$

where $n=0,1,2,...$, and

$$\gamma=\pm\tfrac{1}{2}\sqrt{1+4N^2-8\xi}. \tag{26}$$

So mathematically we obtain two distinct set of states according to the positive and negative sign of γ. However, in order to obtain the nonrelativistic limit of the eigenenergies we must choose the positive sign. Therefore the energy spectrum of the (1+1) relativistic oscillator is given by

$$E_n=\left(\frac{1}{2}+n+\frac{1}{2}\sqrt{1+4\frac{m^2c^4}{\hbar^2\omega^2}-8\xi}\right)\hbar\omega. \tag{27}$$

In the limit $c\to\infty$ the spectrum behaves as

$$E_n\to E_n^{NR}+mc^2, \tag{28}$$

where $E_n^{NR}=(\frac{1}{2}+n)\hbar\omega$ are the standard eigenenergies of the (1+1) nonrelativistic oscillator. The equation (27) makes clear the physical meaning of the ξ parameter. It is related with the zero-point energy of the relativistic oscillator. The consistence of theory is related to the unitarity of the representation of the AdS algebra (3) which only requires the positivity of the energy (27) (see later on in this section). Therefore the range of ξ is naturally restricted as $1+4(m^2c^4/\hbar^2\omega^2)-8\xi>0$.

Introducing the variable $z=-i\frac{\omega}{c}x$ and for the discrete values (25), the equation (23) turns out to be the equation of Gegenbauer polynomials[18]

$$\left\{(1-z^2)\frac{d^2}{dz^2}-(1-2(n+\gamma))z\frac{d}{dz}-n(n+2\gamma)\right\}\phi_n^{\lambda}(z)=0. \tag{29}$$

Therefore the Klein–Gordon energy-eigenstates are

$$\phi_n^{\gamma}(x,t)=N_n^{\gamma}e^{-i(E/\hbar)t}\left(1+\frac{\omega^2}{c^2}x^2\right)^{-\lambda/2}C_n^{-(n+\gamma)}\left(-i\frac{\omega}{c}x\right), \tag{30}$$

where N_n^{γ} are appropriate normalization constants

$$(N_n^{\gamma})^{-2}=\sqrt{\pi}\frac{c}{\omega}\frac{4^n}{n!}\frac{(2\gamma)!}{(2\gamma+n)!}\left[\frac{(\gamma+n)!}{(\gamma)!}\right]^2\frac{1}{\gamma+n+\frac{1}{2}}\frac{\Gamma(\gamma+1)}{\Gamma(\gamma+\frac{1}{2})}. \tag{31}$$

Let us now consider the interpretation of the solutions of the wave equations (15) and/or (16). It is well known that the Klein–Gordon wavefunctions—with the scalar product (18)—cannot be interpreted as probability density amplitudes. The definition of ''position'' observable is problem-

atical, even for the free relativistic particle.[19] One has to introduce a new field—representing the same abstract state—with respect to which the scalar product takes the L^2-form (see, for instance, Refs. 20 and 21).

A positive-frequency solution of the Klein–Gordon equation [with the energy spectrum (27)] is given by

$$\phi(x,t)=\sum_{n=0}^{\infty} \frac{1}{\sqrt{2E_n/\hbar}}\,\tilde{c}_n\phi_n^{\gamma}(x)e^{-iE_nt/\hbar}, \tag{32}$$

where $\tilde{c}_n$ are complex numbers. The inner product on these states is

$$\|\phi\|^2=\sum_{n=0}^{\infty}|\tilde{c}_n|^2. \tag{33}$$

Given the state $\{\tilde{c}_n\}\in l^2$, one can define the Newton–Wigner field[20]

$$\phi_{\mathrm{NW}}(x,t)=\sum_{n=0}^{\infty}\tilde{c}_n\phi_n^{\gamma}(x)e^{-iE_nt/\hbar}, \tag{34}$$

with respect to which the scalar product turns out to be

$$\|\phi_{\mathrm{NW}}\|^2=\int_{-\infty}^{+\infty}|\phi_{\mathrm{NW}}(x,t)|^2\rho(x)dx, \tag{35}$$

where $\rho(x)=(1+(\omega^2/c^2)x^2)^{-1}$. Since our special-relativistic oscillator lies in flat Minkowski space, $|\phi_{\mathrm{NW}}|^2$ cannot be properly interpreted as a probability density in position space and a further transformation is required. Defining now the ''Schrödinger''-type wavefunction

$$\Psi(x,t)=\sum_{n=0}^{\infty}\frac{\tilde{c}_n}{\sqrt{1+(\omega^2/c^2)x^2}}\,\phi_n^{\gamma}(x)e^{-iE_nt/\hbar}=\frac{1}{\sqrt{1+(\omega^2/c^2)x^2}}\,\phi_{\mathrm{NW}}(x,t), \tag{36}$$

the inner product takes now the adequate form (20)

$$\|\Psi\|^2=\int_{-\infty}^{+\infty}|\Psi(x,t)|^2dx \tag{37}$$

to properly interpret $|\Psi(x,t)|^2$ as the probability density for observations of x at time t. Therefore, both the Newton–Wigner and Schrödinger-type states are (generalized) eigenfunctions of the position operator $\hat{x}$ ($\hat{x}\phi_{\mathrm{NW}}=x\phi_{\mathrm{NW}}$). In analogy with the analysis of Ref. 19 we can push down this action on the solution space. In our case this leads to a complicated expression in terms of the enveloping algebra of the AdS Lie algebra.

The normalized energy-eigenstates represented by Schrödinger wave functions are

$$\Psi_n^{\gamma}(x,t)=N_n^{\gamma}e^{-i(E/\hbar)t}\left(1+\frac{\omega^2}{c^2}\,x^2\right)^{-(\lambda+1)/2}C_n^{-(n+\gamma)}\left(-i\,\frac{\omega}{c}\,x\right), \tag{38}$$

with the orthonormality relations

$$\langle \Psi_n^\gamma | \Psi_m^\gamma \rangle = N_n^\gamma N_m^\gamma \int_{-\infty}^{\infty} \frac{dx}{1+(\omega^2/c^2)x^2} \left(1+\frac{\omega^2}{c^2}\,x^2\right)^{-(1+2\gamma+n+m)/2}$$
$$\cdot\, C_n^{-(n+\gamma)}\left(-i\,\frac{\omega}{c}\,x\right) C_m^{-(m+\gamma)}\left(-i\,\frac{\omega}{c}\,x\right) = \delta_{nm}\,. \tag{39}$$

We must stress that the Hermite polynomials $H_n(\zeta)$, where $\zeta = \sqrt{m\omega/\hbar}\;x$, are naturally recovered in the nonrelativistic limit

$$\lim_{c\to\infty} \frac{i^n n!}{N^{n/2}}\, C_n^{-(n+\gamma)}\left(-i\,\frac{\zeta}{\sqrt{N}}\right) = H_n(\zeta). \tag{40}$$

We also have

$$\lim_{c\to\infty} \frac{N^n}{(n!)^2}\,(N_n^\gamma)^2 = \sqrt{\frac{m\omega}{\hbar\pi}}\,\frac{1}{n!\,2^n}, \tag{41}$$

where the rhs of (41) has the normalization constants of the Hermite polynomials. Therefore, the lhs of (40), without the limit, can be seen as a relativistic generalization of the Hermite polynomials. In fact, it is not difficult to check that they are proportional to the so-called relativistic Hermite polynomials of Refs. 7, 13, and 22.

We would like to remark at this point that, although the expression (38) allows us to show the proper nonrelativistic limit of the relativistic wave functions, the formula (39) is not the standard orthogonality relation for the Gegenbauer polynomials. However, introducing a new variable $y = [(\omega/c)x]/\sqrt{1+(\omega^2/c^2)x^2} \in [-1,1]$, and using the following relation between Gegenbauer polynomials,

$$C_n^{-(n+\gamma)}\left(-i\,\frac{\omega}{c}\,x\right) = i^n 2^n\,\frac{(2\gamma)!(\gamma+n)!}{(\gamma)!(2\gamma+n)!}\left(1+\frac{\omega^2}{c^2}\,x^2\right)^{n/2} C_n^{\gamma+1/2}\left(\frac{(\omega/c)x}{\sqrt{1+(\omega^2/c^2)x^2}}\right), \tag{42}$$

the expression (39) can be converted into the standard orthogonality relation[18]

$$\langle \Psi_n^\gamma | \Psi_m^\gamma \rangle = N_n^\gamma N_m^\gamma\,\frac{c}{\omega}\,2^{(n+m)}\left(\frac{(2\gamma)!}{(\gamma)!}\right)^2 \frac{(\gamma+n)!(\gamma+m)!}{(2\gamma+n)!(2\gamma+m)!}$$
$$\cdot \int_{-1}^{1} dy\,(1-y^2)^\gamma C_n^{\gamma+1/2}(y) C_m^{\gamma+1/2}(y) = \delta_{nm}\,. \tag{43}$$

This result can be used to characterize immediately the Hilbert $\mathscr{H}$ space of the theory. The completeness theorem (see, for instance Ref. 23) for the orthogonal polynomials of compact support in the space of square-integrable functions implies that the set of wavefunctions Ψ_n^γ provides an orthonormal basis for the Hilbert space $\mathscr{H} \equiv L^2([-1,1],(c/\omega)[1/(1-y^2)^{3/2}]dy) \approx L^2(\mathbb{R},dx)$.

To finish this section we shall consider the construction of the quantum physical operators. One is tempted to propose the Killing vectors

$$\hat{C}_{(a)} = i\hbar f^\mu_{(a)}\,\frac{\partial}{\partial x^\mu}, \tag{44}$$

acting on Newton–Wigner functions ϕ_{NW} (they are solutions of the invariant Klein–Gordon equation), as the quantum operators associated to the classical observables (7). The operators $\hat{C}_{(a)}$ do not leave invariant the measure $d\mu = dx/[1+(\omega^2/c^2)x^2] = \rho(x)dx$ of the scalar product (35)

$$\langle \phi_{1_{\mathrm{NW}}} | \phi_{2_{\mathrm{NW}}} \rangle = \int d\mu \phi^*_{1_{\mathrm{NW}}} \phi_{2_{\mathrm{NW}}}. \tag{45}$$

Therefore, the representation $g \to U(g)$ defined by

$$U(g)\phi_{\mathrm{NW}}(x,t) = \phi_{\mathrm{NW}}(g^{-1}(x,t)), \tag{46}$$

where $g(x,t)$ is the finite group action in the space–time, is not unitary. Nevertheless, the representation defined by

$$U(g)\phi_{\mathrm{NW}}(x,t) = \left(\frac{d\mu_g}{d\mu}\right)^{1/2} \phi_{\mathrm{NW}}(g^{-1}(x,t)), \tag{47}$$

where $d\mu_g/d\mu$ is the Radon–Nikodim derivative of μ_g with respect to μ, is unitary. A straightforward calculation leads to the following expression;

$$U(g)\phi_{\mathrm{NW}}(x,t) = \sqrt{\frac{1+x'^2}{1+x^2}}\, \phi_{\mathrm{NW}}(g^{-1}(x,t)), \tag{48}$$

where $(x',t') \equiv g(x,t)$. This corrects the expression of the operators (44) and then the proper quantum operators acting on $\phi_{\mathrm{NW}}(x,t)$ read as

$$\hat{C}_1 = i\hbar \frac{\partial}{\partial x^0}, \tag{49}$$

$$\begin{aligned}\hat{C}_2 = {} & i\hbar \frac{(\omega/c)x}{\sqrt{1+(\omega^2/c^2)x^2}} \cos \omega t \frac{\partial}{\partial x^0} + i\hbar \sqrt{1+\frac{\omega^2}{c^2}x^2} \sin \omega t \frac{\partial}{\partial x} \\ & + i\hbar \frac{(\omega/c)\, x}{\sqrt{1+(\omega^2/c^2)x^2}} \sin \omega t \frac{\partial}{\partial \phi_{\mathrm{NW}}},\end{aligned} \tag{50}$$

$$\begin{aligned}\hat{C}_3 = {} & i\hbar \frac{-(\omega/c)x}{\sqrt{1+(\omega^2/c^2)x^2}} \sin \omega t \frac{\partial}{\partial x^0} + i\hbar \sqrt{1+\frac{\omega^2}{c^2}x^2} \cos \omega t \frac{\partial}{\partial x} \\ & + i\hbar \frac{(\omega/c)x}{\sqrt{1+(\omega^2/c^2)x^2}} \cos \omega t \frac{\partial}{\partial \phi_{\mathrm{NW}}}.\end{aligned} \tag{51}$$

Finally, the transformation (36) allows us to obtain the action of the quantum operators on the physical (relativistic oscillator) wavefunctions Ψ.

In conclusion, the Schrödinger wavefunctions (38) provide an orthonormal basis of the carrier space for unitary, lowest-weight representations of the symmetry algebra so(1,2). Moreover, the lowest-weight representation of the so(1,2) algebra are characterized by a unique parameter,[24] $E_0/\hbar\omega = \frac{1}{2} + \gamma$ in our case, and, therefore, our Hilbert space construction is unique, up to unitary equivalence, if we assume the existence of a ground state (i.e., a lowest weight state). Finally we want to comment on the issue of the zero-point energy. For the (1+1) relativistic oscillator we

have $E_0/\hbar\omega > \frac{1}{2}$. This means that not all the lowest-weight representations ($E_0/\hbar\omega \in [0, +\infty]$) can be realized physically. The natural barrier $E_0/\hbar\omega = \frac{1}{2}$ corresponds to the so-called Mock representation.[24]

III. THE THREE-DIMENSIONAL SPECIAL-RELATIVISTIC OSCILLATOR

In this section we shall extend our study of the one-dimensional special-relativistic oscillator to the three-dimensional case. To this end we shall first find out the appropriate form of the (1+3) metric. Imposing the nonrelativistic limit and assuming the static form for the metric and the spherical symmetry of the (1+3) AdS space we can write

$$ds^2 = \left(1 + \frac{\omega^2}{c^2} r^2\right) c^2 dt^2 - F(r) dr^2 - G(r)(d\theta^2 + \sin^2 \theta d\varphi^2), \tag{52}$$

where $0 \leqslant \theta \leqslant \pi$ and $0 \leqslant \varphi \leqslant 2\pi$ are the usual spherical coordinates. Moreover, to recover the one-dimensional oscillator when the angular coordinates are frozen we have to choose the function $F(r)$ as follows:

$$F(r) = \frac{1}{1 + (\omega^2/c^2) r^2}. \tag{53}$$

Imposing now the anti-de Sitter geometry we find that the appropriate line element should read as

$$ds^2 = \left(1 + \frac{\omega^2}{c^2} r^2\right) c^2 dt^2 - \frac{dr^2}{1 + (\omega^2/c^2) r^2} - r^2(d\theta^2 + \sin^2 \theta d\varphi^2). \tag{54}$$

The geodesics of (54) can be derived from the Lagrangian

$$\mathscr{L} = -mc \sqrt{1 + \frac{\omega^2}{c^2} r^2 - \frac{v^2}{c^2} + \frac{\omega^2}{c^4} \frac{(\mathbf{x}\cdot\mathbf{v})^2}{1 + (\omega^2/c^2) r^2}}, \tag{55}$$

and, according with our scheme, we can view the above Lagrangian as defining a three-dimensional special-relativistic oscillator in Minkowski space. The SO(3,2) symmetry (i.e., the generalisation of the three-dimensional Poincaré and Newton algebras),

$$[\hat{E}, \hat{x}^i] = -i \frac{\hbar}{m} \hat{p}^i, \quad [\hat{E}, \hat{p}^i] = im\omega^2 \hbar \hat{x}^i, \quad [\hat{x}^i, \hat{p}^j] = i\hbar \left(1 + \frac{1}{mc^2} \hat{E}\right) \delta^{ij} \tag{56}$$

(we have omitted the rotation generators), can be realized now by the Killing vectors of (54).

The next step now is to compute the Hamiltonian. We obtain

$$H^2 = \left(1 + \frac{\omega^2}{c^2} r^2\right) (m^2 c^4 + p^2 c^2 + \omega^2 (\mathbf{x}\cdot\mathbf{p})^2). \tag{57}$$

As in the one-dimensional oscillator it is not difficult to test that the wave equation associated with the Hamiltonian (57) can be transformed, with a particular normal-ordering prescription, into a Klein–Gordon equation. Introducing the parameters α, β, η, and ϱ for the operator ordering ambiguities of the classical function (57),

$$x_i^4 p_i^2 \to -\hbar^2 \left(x_i^4 \frac{\partial^2}{\partial x_i^2} + 4x_i^3 \frac{\partial}{\partial x_i} + \alpha x_i^2\right), \tag{58}$$

$$x_i^2 p_i^2 \to -\hbar^2 \left(x_i^2 \frac{\partial^2}{\partial x_i^2} + 2x_i \frac{\partial}{\partial x_i} + B \right), \tag{59}$$

$$x_i^3 p_i \to -i\hbar \left(x_i^3 \frac{\partial}{\partial x_i} + \eta x_i^2 \right), \tag{60}$$

$$x_i p_i \to -i\hbar \left(x_i \frac{\partial}{\partial x_i} + \varrho \right), \tag{61}$$

the Schrödinger equation leads to the Klein–Gordon equation in AdS space with metric (54) ($R=-12\omega^2/c^2$). The Schrödinger and Newton–Wigner-type wavefunctions are related by

$$\Psi = \frac{1}{\sqrt{1+(\omega^2/c^2)r^2}}\, \phi_{\mathrm{NW}}. \tag{62}$$

The normal ordering parameters are then fixed as

$$\alpha = \frac{11}{2} + 8\xi, \quad \beta = \frac{1}{2} + 2\xi, \quad \eta = \frac{3}{2}, \quad \varrho = \frac{1}{2}. \tag{63}$$

So, there is only one free parameter left, which is essentially the curvature factor ξ.

Now we want to solve the corresponding Klein–Gordon equation. The D'Alembertian operator is given by

$$\Box = \frac{1}{1+(\omega^2/c^2)r^2} \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - 2\frac{\omega^2}{c^2} r \frac{\partial}{\partial r} - \left(1 + \frac{\omega^2}{c^2} r^2 \right) \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{\mathbf{L}^2}{r^2}, \tag{64}$$

where $\mathbf{L}^2$ is the orbital angular momentum operator

$$\mathbf{L}^2 = -\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) - \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\varphi^2}. \tag{65}$$

Separation of variables and an ansatz analogous to that of (22) leads to the following set of positive frequency modes:

$$\phi(\mathbf{x},t) = e^{-i\lambda\omega t} Y_m^l(\theta,\varphi) \left(1 + \frac{\omega^2}{c^2} r^2 \right)^{-\lambda/2} r^l \phi_l^\lambda(r), \tag{66}$$

where $Y_m^l(\theta,\varphi)$ are the spherical harmonics and the functions $\phi_l^\lambda(r)$ are required to verify the equation

$$\left\{ \left(1 + \frac{\omega^2}{c^2} r^2 \right) \frac{d^2}{dr^2} - 2\frac{\omega^2}{c^2} r(\lambda - l - 2) \frac{d}{dr} + 2\frac{l+1}{r} \frac{d}{dr} + \frac{\omega^2}{c^2} \left(\lambda(\lambda - 2l - 3) + l(l+3) - N^2 + 12\xi \right) \right\} \phi_l^\lambda(r) = 0. \tag{67}$$

In terms of the variable $\rho = -(\omega^2/c^2)r^2$, the above equation turns out to be a hypergeometric differential equation

$$\left\{(1-\rho)\rho\,\frac{d^2}{d\rho^2}+\left(l+\frac{3}{2}-\left(l+\frac{5}{2}-\lambda\right)\rho\right)\frac{d}{d\rho}-\frac{1}{4}\,(\lambda(\lambda-2l-3)+l(l+3)-N^2+12\xi)\right\}\phi_l^{\lambda}(\rho)=0. \tag{68}$$

The ordinary regularity condition at the origin and the square integrability of the functions yield to the following energy spectrum ($\lambda=E/\hbar\omega$):

$$E_n=\left(\frac{3}{2}+2n+l+\frac{1}{2}\,\sqrt{9+4\,\frac{m^2c^4}{\hbar^2\omega^2}-48\xi}\right)\hbar\omega, \tag{69}$$

where $n,l=0,1,2,3,\ldots$. We have chosen the positive sign of the square root of (69) ($\gamma = +\frac{1}{2}\times\sqrt{9+4N^2-48\xi}$) to fit the nonrelativistic approximation

$$E_n \xrightarrow{c\to\infty} E_n^{NR}+mc^2, \tag{70}$$

where $E_n^{NR}=(\frac{3}{2}+2n+l)\hbar\omega$ is the ordinary energy spectrum of three-dimensional nonrelativistic oscillator. The range of ξ is now restricted as $9+4N^2-48\xi>0$.

We must mention at this point that the choice of the positive sign of the square root of (69) parallels the Dirichlet-type boundary conditions imposed on the solution of the Klein–Gordon equation on the Einstein static universe in $1+3$ dimensions associated with AdS space[14] (see also Ref. 25 for the $1+2$ case). The negative sign corresponds to the Newmann boundary condition. Both boundary conditions allow us to solve the problem of the lack of global hyperbolicity in the standard AdS theory. However, in our relativistic oscillator interpretation the Dirichlet-type boundary condition emerges as the natural one to properly recover the quantum nonrelativistic oscillator.

For the values (69) the regular hypergeometric functions solving (68) are

$$\phi_{nl}^{\lambda(r)}={}_2F_1\left(-n,n+l+\frac{3}{2}-\lambda,l+\frac{3}{2};-\frac{\omega^2}{c^2}\,r^2\right). \tag{71}$$

Rewriting the dimensionless parameter $(\omega^2/c^2)r^2$ as $(m\omega/\hbar N)r^2$, it is easy to check that, in the limit $c\to\infty$, the functions (71) become the confluent hypergeometric ones appearing in the nonrelativistic wavefunctions

$$\lim_{c\to\infty}{}_2F_1\left(-n,n+l+\frac{3}{2}-\lambda,l+\frac{3}{2};-\frac{m\omega}{\hbar}\,\frac{r^2}{N}\right)={}_1F_1\left(-n,l+\frac{3}{2};\,\frac{m\omega}{\hbar}\,r^2\right). \tag{72}$$

Taking into account the relation of Jacobi polynomials with the hypergeometric functions[18]

$${}_2F_1(-n,n+\alpha+\beta+1,\alpha+1;z)=\frac{n!}{(\alpha+1)_n}\,P_n^{(\alpha,\beta)}(1-2z), \tag{73}$$

we obtain the following set of wavefunctions

$$\Psi_{nlm}^{\gamma}(\mathbf{x},t)=C_{nl}^{\gamma}e^{-t(E/\hbar)t}Y_m^l(\theta,\varphi)\left(1+\frac{\omega^2}{c^2}\,r^2\right)^{-(\lambda+1)/2}r^lP_n^{[l+1/2,-\lambda]}\left(1+2\,\frac{\omega^2}{c^2}\,r^2\right). \tag{74}$$

where C_{nl}^{γ} are appropriate normalization constants

$$(C_{nl}^{\gamma})^{-2}=\frac{1}{2(\omega/c)^{2l+3}(2l+3)}\,\frac{\Gamma(\gamma+n+1)\Gamma(n+l+\frac{3}{2})}{n!\Gamma(2n+l+\frac{3}{2}+\gamma)\;\Gamma(n+l+\frac{3}{2}+\gamma)}, \tag{75}$$

with respect to the scalar product

$$\langle \Psi^{\gamma}_{nls} | \Psi^{\gamma}_{ml's'} \rangle = C^{\gamma}_{nl} C^{\gamma}_{ml'} \int_{-1}^{1} \int_{0}^{2\pi} \int_{0}^{\infty} d(\cos\,\theta) d\varphi \, \frac{r^2 dr}{1+(\omega^2/c^2) r^2}$$
$$\cdot \left(1+\frac{\omega^2}{c^2}\, r^2 \right)^{-(3+2\gamma+n+(m)+2l+2l')/2} r^{(l+l')} Y^{l}_{s}(\theta,\varphi) Y^{l'}_{s'}(\theta,\varphi)$$
$$\cdot P^{[l+1/2,-\lambda]}_{n}\left(1+2\frac{\omega^2}{c^2} r^2 \right) P^{[l'+1/2,-\lambda]}_{m}\left(1+2\,\frac{\omega^2}{c^2}\, r^2 \right). \tag{76}$$

Observe that the polynomials $P^{[l+1/2,-\lambda]}_{n}$ have the appropriate $c\to\infty$ limit

$$\lim_{c\to\infty} P^{[l+1/2,-\lambda]}_{n}\left(1+2\,\frac{m\omega}{\hbar}\,\frac{r^2}{N} \right) = L^{(l+1/2)}_{n}\left(\frac{m\omega}{\hbar}\, r^2 \right), \tag{77}$$

where $L^{(l+1/2)}_{n}$ are the generalized Laguerre polynomials. To illustrate our special-relativistic generalization of them we give the first few polynomials

$$P^{[l+1/2,-(l+3/2+\gamma)]}_{0}\left(1+2\,\frac{\zeta^2}{N} \right) = 1, \tag{78}$$

$$P^{[l+1/2,-(l+5/2+\gamma)]}_{1}\left(1+2\,\frac{\zeta^2}{N} \right) = \left(l+\frac{3}{2} \right) - 2\,\frac{\gamma}{N}\,\zeta^2, \tag{79}$$

$$P^{[l+1/2,-(l+7/2+\gamma)]}_{2}\left(1+2\,\frac{\zeta^2}{N} \right) = \frac{1}{2}\left(l+\frac{3}{2} \right)\left(l+\frac{5}{2} \right) - \frac{1}{2}\,\frac{\gamma(l+\frac{5}{2})}{N}\,\zeta^2 + \frac{1}{8}\,\frac{\gamma(\gamma+1)}{N^2}\,\zeta^4. \tag{80}$$

Although the relation (73) leads to a set of polynomials with the appropriate nonrelativistic limit, the scalar product (76) is not the standard orthogonality relation of the Jacobi polynomials. However, introducing an alternative relation between the hypergeometric functions and the Jacobi polynomials

$${}_2F_1\left(-n,-n-\alpha,\beta+1;\,\frac{x+1}{x-1} \right) = \frac{n!}{(\beta+1)n}\left(\frac{2}{x-1} \right)^{n} P^{(\alpha,\beta)}_{n}(x), \tag{81}$$

we can rewrite the wavefunctions as

$$\Psi^{\gamma}_{nlm}(\mathbf{x},t) = C^{\gamma}_{nl} e^{-i(E/\hbar)t} Y^{l}_{m}(\theta,\varphi) \cdot \left(1+\frac{\omega^2}{c^2}\, r^2 \right)^{-(\lambda+1)/2+n} r^{l} P^{[\gamma,l+1/2]}_{n}\left(\frac{-1+(\omega^2/c^2) r^2}{1+(\omega^2/c^2) r^2} \right). \tag{82}$$

In terms of the new variable $x=[-1+(\omega^2/c^2)r^2]/[1+(\omega^2/c^2)r^2]\in[-1,1]$, the scalar product (76) turns out to be

$$\langle \Psi^{\gamma}_{nls} | \Psi^{\gamma}_{ml's'} \rangle = C^{\gamma}_{nl} C^{\gamma}_{ml'} 2^{-(\gamma+l+5/2)} \left(\frac{\omega}{c} \right)^{-(2l+3)} \delta_{ll'}\,\delta_{ss'}$$
$$\cdot \int_{-1}^{1} dx (1-x)^{\gamma} (1+x)^{l+1/2} P^{[\gamma,l+1/2]}_{n}(x) P^{[\gamma,l+1/2]}_{m}(x). \tag{83}$$

As in the (1+1) case, we observe again that the inner product (83) reproduces the standard orthogonality relation for Jacobi polynomials. The completeness theorem for orthogonal polynomials implies that states Ψ^{γ}_{nlm} constitutes an orthonormal basis for the Hilbert space $L^2(\mathbb{R}^3, r^2 dr d\varphi d(\cos\theta))$. Finally we would like to remark that the irreducible representations of the (1+3) AdS algebra are determined up to equivalence by two parameters:[26] the lowest eigenvalue of the Hamiltonian and the spin of the particle. Since we are dealing with a spinless particle our construction is uniquely characterized by the ground state energy.

IV. CONCLUSIONS AND FINAL COMMENTS

In this paper we have provided a physical interpretation of the one-particle sector of the Klein–Gordon theory in terms of a special-relativistic oscillator in Minkowski space. The system is exactly solvable and leads to radial energy eigenfunctions composed of a weight-function

$$\left(1+\frac{\omega^2}{c^2}\,r^2\right)^{-(3/2+2n+1+(1/2)\sqrt{9+4(m^2c^4/\hbar^2\omega^2)-48\xi}+1)/2}, \tag{84}$$

reducing to the Gaussian one $e^{-(1/2)(m\omega/\hbar)r^2}$ in the limit $c\to\infty$, and a polynomial

$$r^l P_n^{[l+1/2,-\lambda]}\left(1+2\,\frac{\omega^2}{c^2}\,r^2\right), \tag{85}$$

going to its nonrelativistic counterpart.

We observe from the expression (84) that the probability density for the relativistic oscillator is less confined in the classical region than the corresponding one of the nonrelativistic oscillator. It penetrates more appreciably in the classically forbidden region. This can be understood in terms of the behavior of the null geodesics in AdS. They go to infinity in a finite lapse of the coordinate time t used in the metrics (5) and (54). So, that, in the limit $N=0$, the geodesics are not confined in a finite region of space and this fact is partially reflected by the asymptotic behavior of the wave functions. Despite this, the spacing of the energy levels is identical to the nonrelativistic one. However, for the ground state energy we have

$$E_0=\hbar\omega\left(\tfrac{3}{2}+\tfrac{1}{2}\sqrt{9+4N^2-48\xi}\right), \tag{86}$$

representing some sort of mixing between the nonrelativistic zero-point energy $\frac{3}{2}\hbar\omega$ and the relativistic rest mass energy. The mixing is just parametrized by the curvature factor ξ.

It is remarkable that the lack of global hyperbolicity of AdS space is physically incorporated by choosing those solutions with the adequate nonrelativistic limit. This way of truncating the space of solutions, which is natural in our special-relativistic oscillator theory, turns out to be equivalent to the imposition of the Dirichlet-type boundary condition at infinity.

Another point which merits some comment is the question of how to extend our approach to spinning particles. When dealing with spin $\frac{1}{2}$ particles one could construct the corresponding wave equation by means of Dirac equation in the AdS background, i.e.,

$$(i\gamma^{\mu}(\partial_{\mu}-\Gamma_{\mu})-mc/\hbar)\Psi=0, \tag{87}$$

where $\gamma^{\mu}=e^{\mu}_{\alpha}\gamma^{\alpha}$ are the Dirac matrices in AdS space (e^{μ}_{α} are the vierbeins) and Γ_{μ} is the spin connection. Using the identity

$$R_{\mu\nu\sigma\rho}\gamma^{\mu}\gamma^{\nu}\gamma^{\sigma}\gamma^{\rho}=-2R, \tag{88}$$

where $R_{\mu\nu\sigma\rho}$ is the Riemann curvature tensor, it is not difficult to see that the Dirac equation (87) implies a Klein–Gordon equation with $\xi=\frac{1}{4}$:

$$\left(\Box+\left(\frac{mc}{\hbar}\right)^2+\frac{1}{4}R\right)\Psi=0. \tag{89}$$

The term $\frac{1}{4}R$ plays the role of the standard spin-dependent term $(q/2)F_{\mu\nu}\sigma^{\mu\nu}$ which appears when coupling the Dirac field with an electromagnetic potential. Note that this term is now diagonal in the spin components and then the energy spectrum should be similar to that of the spinless oscillator.

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Prepotential of $N=2$ SU(2) Yang–Mills gauge theory coupled with a massive matter multiplet

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We discuss the $N=2$ SU(2) Yang–Mills theory coupled with a massive matter in the weak coupling. In particular, we obtain the instanton expansion of its prepotential. Instanton contributions in the mass-less limit are completely reproduced. We study also the double scaling limit of this massive theory and find that the prepotential with instanton corrections in the double scaling limit coincides with that of $N=2$ SU(2) Yang–Mills theory without matter. © *1996 American Institute of Physics.* [S0022-2488(96)04511-2]

I. INTRODUCTION

As is well-known, low energy properties of $N=2$ supersymmetric Yang–Mills gauge theory are dominated by a holomorphic function (prepotential) and were recently studied by Seiberg and Witten.[1,2] In particular, they showed that the quantum moduli space was described by a kind of special geometry[3] and identified the quantum moduli space of $N=2$ SU(2) Yang–Mills theory without matter with the moduli space of a certain elliptic curve. Though they did not explicitly calculate the prepotential with instanton corrections, they qualitatively discussed the monopole and dyon masses, the metric on the quantum moduli space and a version of Olive–Montonen electric-magnetic duality and found that the strongly coupled vacuum turned out to be a weakly coupled theory of monopoles.

After the discovery of Seiberg and Witten,[1,2] generalizations for other gauge group theories coupled with or without several matters[4–9] have been discussed. The instanton expansion of the prepotential for pure SU(2) and SU(3) theories[6] and SU(2) theory with mass-less matters[10] have been found, but prepotentials of the massive SU(2) thories have not been established quantitatively so far. For this reason, we can not say that the non-perturbative aspects of quantum moduli space have been understood in detail even for the case of $N=2$ SU(2) Yang–Mills theory when massive N_f matters[11] are introduced. In fact, instanton calculations for massive theory do not seem to be discussed in the literature. Thus we will study the quantum moduli spaces of $N=2$ SU(2) Yang–Mills gauge theories coupled with massive matters in this and subsequent papers.[12] In particular, we will study the quantum moduli space of $N=2$ SU(2) Yang–Mills theory coupled with a massive matter at weak coupling in this paper.

The paper organizes as follows. In the next section, we derive the Picard–Fuchs equation for massive $N_f=1$ $N=2$ SU(2) Yang–Mills theory and discuss the property of its solutions. It is noteworthy that the order of the differential equation is three in contrast with that of the mass-less theory whose order of the Picard–Fuchs equation is two. We also obtain the monodromy matrix near the weak coupling limit. In Sec. III, we derive the prepotential and its instanton expansion. The result coincides with the previous result[10] if the matter is mass-less. Considerations on double scaling limit of the $N_f=1$ massive theory are done in Sec. IV. We will see that we can reproduce the instanton expansion of the $N_f=0$ theory. Section V is a summary.

II. THE PICARD–FUCHS EQUATION

Quantum moduli space of $N_f=1$, $N=2$ SU(2) Yang–Mills theory can be described by a kind of hyperelliptic curve

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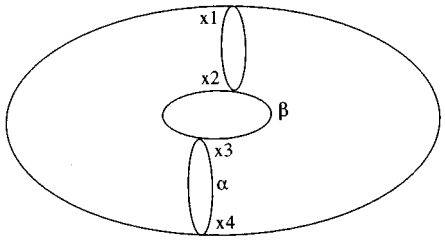

FIG. 1. The hyperelliptic curve as a genus 1 Riemann surface.

$$y^2=(x^2-u)^2-\Lambda_1^3(x+m), \tag{2.1}$$

and the meromorphic 1-form[13] which is given by

$$\lambda_1=\frac{\sqrt{2}xdx}{4\pi iy}\left[\frac{x^2-u}{2(x+m)}-2x\right], \tag{2.2}$$

where $x, y\in\mathbf{C}$, u is the gauge invariant parameter, Λ_1 is the dynamical mass scale of this theory and m is the bare mass of the hypermultiplet.[9] Formulation by an elliptic curve can also be found.[2]

This curve has four branching points. In particular, near the weak coupling limit ($u=\infty$), they will be

$$\begin{aligned}
x_1&=-\sqrt{u}-\frac{i\Lambda_1^{3/2}}{2u^{1/4}}+\frac{i\Lambda_1^{3/2}m}{4u^{3/4}}+\ldots,\\
x_2&=-\sqrt{u}+\frac{i\Lambda_1^{3/2}}{2u^{1/4}}-\frac{i\Lambda_1^{3/2}m}{4u^{3/4}}+\ldots,\\
x_3&=\sqrt{u}-\frac{\Lambda_1^{3/2}}{2u^{1/4}}-\frac{\Lambda_1^{3/2}m}{4u^{3/4}}+\ldots,\\
x_4&=\sqrt{u}+\frac{\Lambda_1^{3/2}}{2u^{1/4}}+\frac{\Lambda_1^{3/2}m}{4u^{3/4}}+\ldots\ .
\end{aligned} \tag{2.3}$$

Since we can take the cuts to run from x_1 to x_2 and x_3 to x_4, we may identify this curve as a genus one Riemann surface, as shown in Fig. 1. We then identify α-cycle as a loop going around the cut from x_4 to x_3 counterclockwise and β-cycle from x_3 to x_2. As is obvious from the figure, the intersection of these cycles is $\alpha\cap\beta=1$.

Now we can define periods $a(u), a_D(u)$ of λ_1 by

$$a(u)=\oint_\alpha \lambda_1, \tag{2.4}$$

$$a_D(u)=\oint_\beta \lambda_1. \tag{2.5}$$

$a(u)$ is identified with the scalar component of the $N=1$ chiral multiplet and $a_D(u)$ is its dual. We are interested in their evaluation, but it is not so easy to accomplish it exactly. So we take a method of the Picard–Fuchs equation. It is given by

$$\frac{d^3\Pi_1}{du^3}+\frac{3\Delta_1(m)+\Delta_1'(m)(4m^2-3u)}{\Delta_1(m)(4m^2-3u)}\frac{d^2\Pi_1}{du^2} - \frac{8[4(2m^2-3u)(4m^2-3u)+3(3\Lambda_1^3m-4u^2)]}{\Delta_1(m)(4m^2-3u)}\frac{d\Pi_1}{du}=0, \tag{2.6}$$

where

$$\Delta_1(m)=27\Lambda_1^6+256\Lambda_1^3m^3-288\Lambda_1^3mu-256m^2u^2+256u^3, \tag{2.7}$$

and $\Pi_1=\int_\gamma \lambda_1$, γ is a suitable 1-cycle and $\Delta_1' = d\Delta_1/du$. Note that $\Delta_1(m)$ is the discriminant of the curve (2.1). It is easy to find that (2.6) has no symmetry over the u-plane and the mass plays a role to break the symmetry. Equation (2.6) has obviously regular singular points which are solutions to $\Delta_1(m)=0$ and $4m^2-3u=0$. These singular points correspond to mass-less states. Since we are going to treat only weak coupling limit in this paper, we do not discuss the behaviour of the moduli space near these singular points, but they should be discussed elsewhere. We have checked that (2.6) can also be obtained as a result of the double scaling limit of the Picard–Fuchs equation of the massive $N_f=2$ theory.[12]

In the case of mass-less limit ($m\to 0$), this third order differential equation reduces to the second one,

$$\frac{d^3\Pi_1}{du^3}-\frac{\Delta_1(0)-\Delta_1'(0)u}{\Delta_1(0)u}\frac{d^2\Pi_1}{du^2}+\frac{64u}{\Delta_1(0)}\frac{d\Pi_1}{du}=0, \tag{2.8}$$

i.e.,

$$(27\Lambda_1^6+256u^3)\frac{d^2\Pi_1}{du^2}+64u\Pi_1=0, \tag{2.9}$$

where we set the integration constant as 0 because it can be shown directly. This equation has already been obtained and solved.[10]

The mechanism of this reduction is explained as follows. When the matter is massive, λ_1 will acquire an extra simple pole corresponding to $x=-m$ in contrast with the mass-less case. At first sight, even if $m=0$, λ_1 seems to have a pole at $x=0$, but the locus of the pole can be canceled out between denominator and numerator of λ_1. Accordingly, in general, the number of poles of massive meromorphic 1-form is equal to that of the mass-less meromorphic 1-form plus 1. Since the differentiation reduces the order[14] by 1, the reduction will require one step more when λ_1 is massive. Therefore the order of the differential equation which the periods of λ_1 should satisfy will increase one more than that of mass-less λ_1, i.e., the order will be three and this observation is consistent with (2.6) and (2.9).

In order to get the solutions to (2.6) near $u=\infty$, we take $z=1/u$. After this change of variable, we use Frobenius's method. Then we find that its indicial equation has three roots, i.e., 0, $-1/2$, $-1/2$ (double roots). The solution $\rho_0(z)$ corresponding to the index 0 is in fact trivial, i.e., it is a constant,

$$\rho_0(z)=\epsilon. \tag{2.10}$$

However, this constant ϵ may depend on Λ_1 or m and will be determined below. Geometrically, ϵ corresponds to the residue contribution of the pole of the meromorphic 1-form. Of course, ϵ must

vanish in the mass-less limit because the mass-less theory does not have such a pole. Thus ϵ is a function of the mass. On the other hand, there are two independent solutions corresponding to the index $-1/2$. One of them is

$$\rho_1(z)=z^{-1/2}\sum_{i=0}^{\infty} a_i z^i, \tag{2.11}$$

where the first several expansion coefficients a_i are given in appendix A. We find that a_n can be represented by a polynomial of $\Lambda_1^{3i}m^j$ with $2n=3i+j$, where i and j are some non-negative integers. The other solution behaves logarithmically. It is

$$\rho_2(z)=\rho_1(z)\ln z+z^{-1/2}\sum_{i=1}^{\infty} b_i z^i, \tag{2.12}$$

where the first several coefficients b_i are given in appendix B. Note that b_n can also be represented by a polynomial of $\Lambda_1^{3i}m^j$ with $2n=3i+j$. But this time, non-negative integers i and j must move over all combinations.

Since we would like to get $a(u)$ and $a_D(u)$, let us consider whether we can express them as linear combinations of ρ_0, ρ_1 and ρ_2. First, in order to see an asymptotic behaviour of $a(u)$ near $u=\infty$, we must calculate the lower order expansion of the integral (2.4). This is done in appendix C. Making a comparison ρ_1 and ρ_0 with (C4), we can see that

$$a(u)=n\rho_0(z)+\frac{\rho_1(z)}{\sqrt{2}}, \tag{2.13}$$

where we identified

$$\rho_0(z)=-\frac{\sqrt{2}}{4}\,m. \tag{2.14}$$

It is easy to find that $a(u)$ can be expressed by a hypergeometric function in the mass-less limit.[10] $a_D(u)$ can be written as a linear combination of ρ_0, ρ_1 and ρ_2 by comparison it with (C7),

$$a_D(u)=A\rho_2(z)+B\rho_1(z)+n'\rho_0(z), \tag{2.15}$$

where

$$A=-\frac{i3\sqrt{2}}{4\pi}, \quad B=\frac{i\sqrt{2}}{4\pi}\,c, \tag{2.16}$$

and $c=-6+8\ln 2-i\pi-6\ln\Lambda_1$.

From these explicit expressions for the periods, we can easily find that the monodromy matrix near $u=\infty$ acts to the three objects ${}^t(a_D,a,\epsilon)$ as

$$\begin{pmatrix} a_D \\ a \\ \epsilon \end{pmatrix} \to \begin{pmatrix} -1 & 3 & 2n'-3n \\ 0 & -1 & 2n \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} a_D \\ a \\ \epsilon \end{pmatrix}. \tag{2.17}$$

Note that the monodromy matrix is now quantized by the winding number n and n'. Since these winding numbers are arbitrary, we may say that there are ''many'' monodromy matrices near $u=\infty$. This observation will be valid even near the regular singular points.

III. PREPOTENTIAL

Let us try to construct the prepotential $\mathscr{F}_1$ which is a solution to the following differential equation

$$a_D(u)=\frac{d\mathscr{F}_1}{da}, \tag{3.1}$$

but we use a new variable $\tilde{a}=a-n\epsilon$ for convenience. For that purpose, first, we must express u as a series of $\tilde{a}$. We can easily get it from (2.13), i.e.,

$$\begin{aligned} u=&2\tilde{a}^{\,2}+\frac{\Lambda_1^3 m}{16\tilde{a}^{\,2}}-\frac{3\Lambda_1^6}{2048\tilde{a}^{\,4}}+\frac{5\Lambda_1^6 m^2}{4096\tilde{a}^{\,6}}-\frac{7\Lambda_1^9 m}{65536\tilde{a}^{\,8}}+\frac{1}{\tilde{a}^{\,10}}\left(\frac{153\Lambda_1^{12}}{67108864}+\frac{9\Lambda_1^9 m^3}{131072}\right)\\ &-\frac{715\Lambda_1^{12}m^2}{67108864\tilde{a}^{\,12}}+\frac{1}{\tilde{a}^{\,14}}\left(\frac{1131\Lambda_1^{15}m}{2147483648}+\frac{1469\Lambda_1^{12}m^4}{268435456}\right)-\frac{1}{\tilde{a}^{\,16}}\left(\frac{1155\Lambda_1^{18}}{137438953472}\right.\\ &\left.+\frac{2625\Lambda_1^{15}m^3}{2147483648}\right)-\frac{1}{\tilde{a}^{\,18}}\left(\frac{667879\Lambda_1^{18}m^2}{1099511627776}+\frac{148819\Lambda_1^{15}m^5}{17179869184}\right)+\cdots . \end{aligned} \tag{3.2}$$

Inserting (3.2) into (2.15) and integrating it over $\tilde{a}$, we can obtain the prepotential

$$\mathscr{F}_1=\frac{i\tilde{a}^{\,2}}{\pi}\left[\frac{3}{4}\ln\left(\frac{\tilde{a}}{\Lambda_1}\right)^2+\frac{3}{4}\left(-1+\frac{c}{3}+\ln 2\right)-\frac{\sqrt{2}\pi}{4i\tilde{a}}n'm-\frac{m^2}{4\tilde{a}^{\,2}}\ln\tilde{a}+\sum_{i=2}^{\infty}\mathscr{F}_i^{\,1}\tilde{a}^{\,-2i}\right], \tag{3.3}$$

where the first several coefficients $\mathscr{F}_i^{\,1}$ are recorded in appendix D. Note that $\mathscr{F}_n^{\,1}$ is expressed again by a polynomial of $\Lambda_1^{3i}m^j$ with $2n=3i+j$. We can find that our result (3.3) is consistent with the mass-less $N_f=1$ theory[10] when $m=0$. It is interesting to note that (3.3) has a curious term proportional to $(\ln\tilde{a})/\tilde{a}^{\,2}$ in the brackets. However, we can find that[15]

$$\begin{aligned} \mathscr{F}_s^{\,1}=&\left(\tilde{a}-\frac{m}{\sqrt{2}}\right)^2\ln\left(\tilde{a}-\frac{m}{\sqrt{2}}\right)+\left(\tilde{a}+\frac{m}{\sqrt{2}}\right)^2\ln\left(\tilde{a}+\frac{m}{\sqrt{2}}\right)\\ =&2\tilde{a}^{\,2}\ln\tilde{a}+m^2\ln\tilde{a}+\frac{3}{2}m^2-\frac{m^4}{24\tilde{a}^{\,2}}-\frac{m^4}{240\tilde{a}^{\,4}}-\cdots . \end{aligned} \tag{3.4}$$

Thus we may rewrite (3.3) as

$$\begin{aligned} \mathscr{F}_1=&\frac{i\tilde{a}^{\,2}}{\pi}\left[\frac{3}{4}\ln\left(\frac{\tilde{a}}{\Lambda_1}\right)^2+\frac{3}{4}\left(-1+\frac{c}{3}+\ln 2\right)-\frac{\sqrt{2}\pi}{4i\tilde{a}}n'm-\frac{1}{4\tilde{a}^{\,2}}\mathscr{F}_s^{\,1}+\frac{1}{2}\ln\tilde{a}+\frac{3m^2}{8\tilde{a}^{\,2}}\right.\\ &\left.+\sum_{i=2}^{\infty}\tilde{\mathscr{F}}_i^{\,1}\tilde{a}^{\,-2i}\right], \end{aligned} \tag{3.5}$$

where $\tilde{\mathscr{F}}_i^{\,1}$ is the Λ_1 dependent part of $\mathscr{F}_i^{\,1}$.

IV. DOUBLE SCALING LIMIT

In this section, we examine the double scaling limit of the massive $N_f=1$ theory discussed in previous sections.

To begin with, let us discuss the Picard–Fuchs equation. Since the $N_f=1$ curve turns to the $N_f=0$ curve in the double scaling limit ($m\to\infty$, $\Lambda_1\to 0$, $m\Lambda_1^3=\Lambda_0^4$ fixed, where Λ_0 is a dynamical parameter of the $N_f=0$ theory), in other words, $N=2$ SU(2) Yang–Mills theory is considered as a low energy theory of the massive $N_f=1$ theory,[2] we may expect that (2.6) reduces to the Picard–Fuchs equation of the $N_f=0$ theory. In fact, we find that (2.6) in the double scaling limit is given by

$$\frac{d^3\Pi_1}{du^3}+\frac{3\cdot 256m^2(\Lambda_0^4-u^2)-2\cdot 256m^2u\cdot 4m^2}{256m^2(\Lambda_0^4-u^2)\cdot 4m^2}\frac{d^2\Pi_1}{du^2}-\frac{32\cdot 8m^4}{256m^2(\Lambda_0^4-u^2)\cdot 4m^2}\frac{d\Pi_1}{du}=0, \tag{4.1}$$

i.e.,

$$\frac{d^2\Pi_1}{du^2}-\frac{1}{4(\Lambda_0^4-u^2)}\Pi_1=\text{constant}. \tag{4.2}$$

Equation (4.2) shows the global $\mathbf{Z}_2$ symmetry over the u-plane. At first sight, this can be seen as the Picard–Fuchs equation of $N=2$ SU(2) Yang–Mills theory without matter.[6,16] However, we can not say that Π_1 also reduces to that of $N_f=0$ Picard–Fuchs equation because there is no reason why the relation

$$\Pi_1(u,m,\Lambda_1)\quad\overset{\text{double scaling limit}}{\longrightarrow}\quad\Pi_0(u,\Lambda_0) \tag{4.3}$$

should hold, where Π_0 is a representative of the $N_f=0$ period integral. So we can not insist that the integration constant on the right hand side of (4.2) must be 0.

More precisely speaking, the meromorphic 1-form λ_1 in the double scaling limit will behave as

$$\begin{aligned}\lambda_1&\to\frac{\sqrt{2}xdx}{4\pi i\tilde{y}}\left[\frac{x^2-u}{2m}\left(1-\frac{x}{m}+\frac{x^2}{m^2}-\cdots\right)-2x\right]\\&=\frac{\sqrt{2}x(x^2-u)dx}{8\pi im\tilde{y}}\left(1-\frac{x}{m}+\frac{x^2}{m^2}-\cdots\right)-\frac{\sqrt{2}x^2dx}{2\pi i\tilde{y}},\end{aligned} \tag{4.4}$$

where $\tilde{y}^2=(x^2-u)^2-\Lambda_0^4$ is the curve for the $N_f=0$ theory. The first term in the last expression is an ''extra'' 1-form which depends on the mass m while the second is nothing other than the meromorphic 1-form of the $N_f=0$ theory. Therefore, naively speaking, the solutions to (2.6) consist of the contributions originating from this extra 1-form and λ_0, in the double scaling limit. In fact, (2.10) and (2.12) diverge to infinity in the double scaling limit as is easy to find. Accordingly, when we discuss the low energy version of $N_f=1$ theory, we must carefully treat (4.3). Though ρ_0, ρ_1 and ρ_2 are indeed solutions to (2.6) for finite Λ_1 and m, nothing gives an assurance that they constitute fundamental solutions even for infinitely large Λ_1 or m. Recall that we have obtained the solutions to (2.6), assuming that Λ_1 and m are finite. Consequently, there must be a gap between Π_1 in the double scaling limit and Π_0. This gap will appear as divergence due to the large mass.

Next, let us directly examine the above observations, focusing on the periods $a(u)$ and $a_D(u)$. As for the residue part of the periods, i.e., ρ_0, it moves to infinity due to $m\to\infty$. However, the heavy quark with large mass can be integrated out,[2] so we can eliminate the residue dependence of the periods. We can see that among the expansion coefficients $a_n(n>1)$ of $a(u)$, only the coefficients of even degree survive in the double scaling limit and those of the odd degrees vanish.

Accordingly, we may then say that $a(u)$ converges to a solution to (4.2). In other words, $a(u)$ is not affected by the contributions from the extra 1-form. This fact suggests that $a(u)$ has a nice property which is valid under the double scaling. It is easy to check that the period $a(u)$ in the double scaling limit can be again expressed as a hypergeometric function. In order to see the behaviour of $a_D(u)$, on the other hand, we must rewrite it as a series of $a(u)$ and then take the double scaling limit. We can easily see that the expansion coefficients b_n's diverge to infinity in the double scaling limit. This means that the contributions for $a_D(u)$ from the extra 1-form are non-trivial. Since it is hard to see the difference with the period over β-cycle of the $N_f=0$ theory in this situation, we should first arrange $a_D(u)$ with some ''good'' variable. For that purpose, we take $a(u)$ as the good variable. From (3.2), $a_D(u)$ will be expanded as

$$a_D(u)=n'\epsilon+\sqrt{2}a[B-A\ \ln 2-2A\ \ln a]+\frac{A}{\sqrt{2}}\left[\frac{m^2}{3a}+\frac{m}{72a^3}\,(-3\Lambda_1^3+2m^3)\right.$$
$$\left.+\frac{1}{46080a^5}\,(45\Lambda_1^6+256m^6)+\frac{m^2}{86016a^7}\,(-105\Lambda_1^6+128m^6)+\cdots\right], \tag{4.5}$$

where ϵ, A and B are given in (2.14) and (2.16). Note that each coefficient of $a^{-2i+1}(i>0)$ consists of a finite part and a ''divergent'' part and the latter is always proportional to m^{2l}, $l\in\mathbf{N}$. However, since the heavy quark with large mass must be integrated out[2] as has been mentioned above, it would be enough to consider the finite parts. The divergence due to the large mass can be eliminated in that sense. Accordingly, if we extract only finite contributions we can arrive at a correct answer to get the periods $a_D(u)$ of the $N_f=0$ theory. The reader may ask how to deal with the constants A and B in (4.5) under the double scaling. These constants should be replaced with those of the $N_f=0$ theory. This is because the initial conditions for the Picard–Fuchs equation of the $N_f=1$ theory are different from those of the $N_f=0$ theory. In this way, Π_1 reduces to Π_0 and under this situation the integration constant in (4.2) will be 0. Then (4.2) is nothing other than the Picard–Fuchs equation of the $N_f=0$ theory. Of course, this time we must change Π_1 to Π_0 in (4.2).

Let us examine the double scaling limit of the prepotential. From the above discussions, we can drop the large mass dependence of the prepotential. Then, the procedure to do it consists of two steps. The first one is to take the double scaling limit of the first six terms in the brackets in (3.5). The second one is to consider the double scaling limit of the instanton expansion coefficients.

In order to accomplish the first step, we use a trick. Recall that we can add or subtract infinity related to the mass because of the reason described before. Thus,

$$\frac{3}{4}\ln\left(\frac{a}{\Lambda_1}\right)^2+\frac{3}{4}\,C=\frac{3}{4}\ln\left(\frac{a}{\Lambda_1}\right)^2+\frac{3}{4}\,C+\ln\left[\left(\frac{a}{m}\right)^{1/2}\cdot e^{D/2-3C/4}\right]$$
$$=\ln\left(\frac{a}{\Lambda_0}\right)^2+\frac{D}{2}, \tag{4.6}$$

where[17] $C=-1+\ln 2+c/3$, $D=-6+6\ln 2$ and $\tilde{a}$ is now replaced with a. Note that this trick essentially corresponds to the replacement of the ''initial'' conditions described above. Since the remaining two terms can be integrated out, we have dropped them here.

For the expansion coefficients $\tilde{\mathcal{F}}_i^1$, we can easily find that they will then be

$$\tilde{\mathcal{F}}_2^1\to-\frac{\Lambda_0^4}{64},\quad \tilde{\mathcal{F}}_3^1\to 0,\quad \tilde{\mathcal{F}}_4^1\to-\frac{5\Lambda_0^8}{32768},\quad \tilde{\mathcal{F}}_5^1\to 0,$$
$$\tilde{\mathcal{F}}_6^1\to-\frac{3\Lambda_0^{12}}{524288},\quad \tilde{\mathcal{F}}_7^1\to 0,\quad \tilde{\mathcal{F}}_8^1\to-\frac{1469\Lambda_0^{16}}{4294967296},\quad \tilde{\mathcal{F}}_9^1\to 0. \tag{4.7}$$

Then we can get the following ''renormalized'' prepotential $\hat{\mathcal{F}}_1$ in the double scaling limit:

$$\hat{\mathscr{F}}_1=\frac{ia^2}{\pi}\left[\ln\left(\frac{a}{\Lambda_0}\right)^2+\frac{D}{2}-\frac{\Lambda_0^4}{2^6\cdot a^4}-\frac{5\Lambda_0^8}{2^9\cdot a^6}-\frac{3\Lambda_0^{12}}{2^{19}\cdot a^8}-\frac{1469\Lambda_0^{16}}{2^{32}\cdot a^{10}}-\cdots\right]. \tag{4.8}$$

This agrees with the result of $N_f=0$ pure Yang–Mills theory.[6]

V. SUMMARY

We have studied the moduli space of $N=2$ SU(2) Yang–Mills theory coupled with a matter multiplet at weak coupling. In particular, we have determined its prepotential and monodromy matrix. For general values of Λ_1 and m, we have established that the two periods of the meromorphic 1-form can be written as

$$\begin{aligned} a(u)&=-\frac{\sqrt{2}}{4}nm+\frac{1}{2}\sqrt{2u}\left[1+\sum_{i=2}^{\infty}a_i(\Lambda_1^3,m)u^{-i}\right],\\ a_D(u)&=-\frac{\sqrt{2}}{4}n'm+\frac{3i}{2\pi}\tilde{a}(u)\ln\left(\frac{u}{\Lambda_1^2}\right)+\sqrt{u}\sum_{i=0}^{\infty}a_{D_i}(\Lambda_1^3,m)u^{-i}, \end{aligned} \tag{5.1}$$

where $a_i(\Lambda_1^3,m)$ and $a_{D_i}(\Lambda_1^3,m)$ are homogeneous polynomials of order $2i$, instead of the formulas noted before.[2,10] And we have proposed the exact expression for the prepotential as in (3.5). The coefficients of instanton expansion in the mass-less limit completely recovered. On the other hand, we have succeeded in constructing the $N_f=0$ theory as a low energy theory of the massive $N_f=1$ and have found that we can recover the instanton expansion of the prepotential of the $N_f=0$ theory.

Finally, we give some comments. Since the massive $N_f=1$ theory can be considered as a low energy theory of the massive $N_f=2$ theory,[2] all our results will be expected to be reproduced from it. In addition to this, it will be interesting to reconstruct our results in the languages of integrable systems such as Whitham hierarchy and so on.[16,18] The discussions in this paper should be compared with those approaches, but such considerations unfortunately are not proceeded at present.

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APPENDIX A: EXPANSION COEFFICIENTS (1)

The first several coefficients of ρ_1 are

$$\begin{aligned} &a_0=1,\quad a_1=0,\quad a_2=-\frac{\Lambda_1^3 m}{16},\\ &a_3=\frac{3\Lambda_1^6}{1024},\quad a_4=-\frac{15\Lambda_1^6 m^2}{1024},\quad a_5=\frac{35\Lambda_1^9 m}{16384},\\ &a_6=-\frac{105\Lambda_1^9}{4194304}(3\Lambda_1^3+256m^3),\quad a_7=\frac{3465\Lambda_1^{12}m^2}{2097152},\\ &a_8=-\frac{3003\Lambda_1^{12}m}{67108864}(3\Lambda_1^3+80m^3),\quad a_9=\frac{15015\Lambda_1^{15}}{4294967296}(\Lambda_1^3+384m^3). \end{aligned} \tag{A1}$$

APPENDIX B: EXPANSION COEFFICIENTS (2)

The first several coefficients of ρ_2 are

$$b_1=\frac{1}{3}\,m^2,\quad b_2=\frac{m}{72}\,(3\Lambda_1^3+4m^3),$$

$$b_3=\frac{1}{23040}\,(-45\Lambda_1^6+480\Lambda_1^3m^3+512m^6),$$

$$b_4=\frac{m^2}{21504}\,(-21\Lambda_1^6+224\Lambda_1^3m^3+256m^6),$$

$$b_5=\frac{m}{276480}\,(-120\Lambda_1^9+1575\Lambda_1^6m^3+1920\Lambda_1^3m^6+2048m^9), \tag{B1}$$

$$b_6=\frac{1}{415236096}\,(9801\Lambda_1^{12}-937728\Lambda_1^9m^3+1419264\Lambda_1^6m^6+2162688\Lambda_1^3m^9+2097152m^{12}),$$

$$b_7=\frac{m^2}{5725224960}\,(323505\Lambda_1^{12}+13453440\Lambda_1^9m^3+15375360\Lambda_1^6m^6 +23855104\Lambda_1^3m^9+20971520m^{12}),$$

$$b_8=\frac{m}{3019898880}\,(45837\Lambda_1^{15}-5636520\Lambda_1^{12}m^3+4392960\Lambda_1^9m^6 +7028736\Lambda_1^6m^9+10485760\Lambda_1^3m^{12}+8388608m^{15}),$$

$$b_9=\frac{1}{13799729922048}\,(-9689337\Lambda_1^{18}+3483611712\Lambda_1^{15}m^3+16467010560\Lambda_1^{12}m^6 +16728391680\Lambda_1^9m^9+29198647296\Lambda_1^6m^{12}+41070624768\Lambda_1^3m^{15}+30064771072m^{18}).$$

APPENDIX C: LOWER ORDER EXPANSION OF THE PERIODS

In this appendix, we show that the lower order expansion of the period integral (2.4) in detail as an example. However, we must treat (2.4) carefully because this α-cycle is defined to be a usual homology basis. Recall that the meromorphic 1-form was constructed under the assumption such that the asymptotic behaviour of $a(u)$ at $u=\infty$ was to be $a(u)\sim\sqrt{u/2}$ even if the theory was massive.[9] Therefore even if we evaluate the period (2.4) by direct calculation, we can not obtain the correct contribution from the pole.[2] When the cycle may cross the pole, then the integration must pick up the residue of the pole. However, since the α-cycle in (2.4), as we have stated above, avoids the pole, we must study the case such that the cycle deforms from α to α', which encloses the pole and the two branching points x_3 and x_4 as shown in Fig. 2. As is easily seen from this figure, the direction of α' is the same as that of δ, which encloses only the pole. However, taking into account an effect for topological deformation, we can find that the α-cycle can be identified with the loop α'' in the figure. Namely, if the α-cycle should move on another covering of this x-plane and back onto the original one, it will enclose x_1 and x_2, i.e., another cut. But this time, the directions of α and α'' will be different. Therefore when α'' crosses the pole, the direction of α''' which is a deformation of α'' and that of δ will be different. This fact causes the sign of the residue to change. The reader may ask that the sign of the integral over the α'' should be reflected.

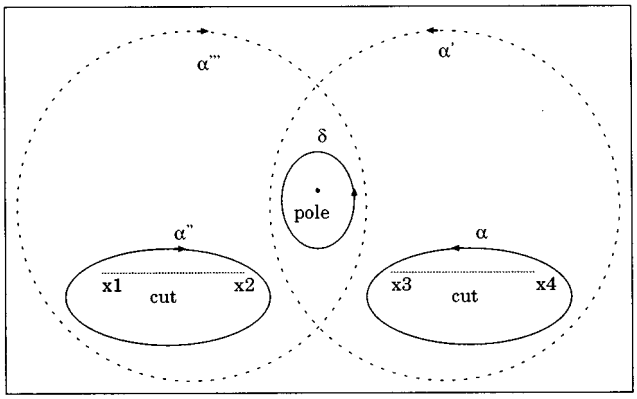

FIG. 2. Deformations of α-cycle on the x-plane.

Of course it is right. But since we usually use the convention such that the overall sign of $a(u)$ without the residue contribution, for example, to be $+$, e.g., $a(u) \sim +\sqrt{u/2}$ in $N=2$ $SU(2)$ Yang-Mills theory, we should change the sign of the residue instead of that of the integral in order to preserve the convention.

From these discussions, the true expression for the massive period $a(u)$ should be defined by

$$a(u):\ \oint_{\tilde{\alpha}} \lambda_1 = \oint_{\alpha} \lambda_1 + \oint_{\delta} \lambda_1$$

$$= \oint_{\alpha} \lambda_1 + 2\pi i n \cdot \mathrm{Res}(\lambda_1)|_{\text{at } x=-m}, \tag{C1}$$

where $\tilde{\alpha}$ is a certain member of the family of α-cycle which may include the pole and the cut inside the loop, δ is a small loop around the pole and $n=0,\pm 1$. If $\tilde{\alpha}$ avoids the pole, then $\tilde{\alpha}=\alpha$ and $n=0$. If $\tilde{\alpha}$ encloses the pole and the directions of $\tilde{\alpha}$ and δ coincide, $n=+1$. If the directions are different while $\tilde{\alpha}$ encloses the pole, then $n=-1$. To clarify, we should further comment on the number n. We have treated only the case such that $\tilde{\alpha}$ winds once around the pole, but we may also allow the case such that it winds several times around the pole. In this time, n can be interpreted as winding number and will be $n \in \mathbf{Z}$.

Now, let us evaluate (C1). First, note that

$$\oint_{\alpha} \lambda_1 = 2\int_{x_4}^{x_3} \lambda_1. \tag{C2}$$

On the right hand side, the factor 2 is required because the integral over α-cycle contains an integral from x_4 to x_3 and from x_3 to x_4 on the other side of the cut. In order to calculate (C2), we introduce a new variable t such as$x = \sqrt{u}t$. Then (C2) will be

$$\oint_{\alpha} \lambda_1 = \frac{2\sqrt{2}}{4\pi i} \int_{x_4/\sqrt{u}}^{x_3/\sqrt{u}} \frac{utdt}{\sqrt{u^2(t^2-1)^2 - \Lambda_1^3(\sqrt{u}t+m)}} \left[\frac{u(t^2-1)}{2(\sqrt{u}t+m)} - 2\sqrt{ut} \right]$$

$$= \frac{i}{4\pi} \sqrt{2u} \int_{x_4/\sqrt{u}}^{x_3/\sqrt{u}} \frac{(3\sqrt{u}t^3 + 4mt^2 + \sqrt{u}t)}{\sqrt{u}t+m} \left[\frac{1}{t^2-1} + \frac{\Lambda_1^3 m}{2u^2(t^2-1)^3} + \frac{3\Lambda_1^6 t^2}{8u^3(t^2-1)^5} + \cdots \right] dt$$

$$= \frac{1}{2} \sqrt{2u} \left(1 - \frac{\Lambda_1^3 m}{16u^2} + \cdots \right). \tag{C3}$$

Taking the contribution from the pole into account, we can arrive at

$$a(u)=-\frac{\sqrt{2}}{4}nm+\frac{1}{2}\sqrt{2u}\left(1-\frac{\Lambda_1^3 m}{16u^2}+\cdots\right). \tag{C4}$$

On the other hand, the integration over β-cycle is not well-defined, as well. This can be seen by evaluating its lower order expansion. (2.5) will be

$$\oint_\beta \lambda_1=\frac{i}{4\pi}\sqrt{2u}\left(3\ln u+8\ln 2-i\pi-6-6\ln\Lambda_1+\frac{im\pi}{\sqrt{u}}+\cdots\right). \tag{C5}$$

At first sight, this integration seems to be $a_D(u)$ with the contribution from the pole. In fact, this observation is not wrong. However, (C5) does not contain the possibilities such that the β-cycle does not enclose the pole, for example. In other words, the topological deformation of β-cycle as in the case of α-cycle is (partially) ignored. Since the pole merely contributes as only a constant term, (C5) will be well-defined as the period over the β-cycle avoiding the pole, if the constant term is extracted. Therefore the true definition of $a_D(u)$ will be

$$\begin{aligned} a_D(u):&=\oint_{\tilde\beta}\lambda_1 \\ &=\oint_\beta\lambda_1+\oint_\delta\lambda_1 \\ &=\oint_\beta\lambda_1+2\pi i n'\cdot\mathrm{Res}(\lambda_1)\big|_{\text{at } x=-m}, \end{aligned} \tag{C6}$$

where $\tilde\beta$ is a certain member of β-cycle which may enclose the pole and the cut, β in (C6) means now a loop avoiding the pole and $n'=0,\pm1$. If the loop $\tilde\beta$ winds around the pole several times, then $n'\in\mathbf{Z}$. In this way we can arrive at

$$a_D(u)=-\frac{\sqrt{2}}{4}n'm+\frac{i}{4\pi}\sqrt{2u}(3\ln u+8\ln 2-i\pi-6-6\ln\Lambda_1+\cdots). \tag{C7}$$

APPENDIX D: EXPANSION COEFFICIENTS (3)

The first several coefficients of the prepotential (3.3) are listed below:

$$\begin{gathered} \mathscr{F}_2^1=-\frac{1}{64}\Lambda_1^3 m+\frac{m^4}{96},\quad \mathscr{F}_3^1=\frac{3\Lambda_1^6}{16384}+\frac{m^6}{960}, \\ \mathscr{F}_4^1=-\frac{5\Lambda_1^6 m^2}{32768}+\frac{m^8}{5376},\quad \mathscr{F}_5^1=\frac{7\Lambda_1^9 m}{786432}+\frac{m^{10}}{23040}, \\ \mathscr{F}_6^1=-\frac{153\Lambda_1^{12}}{1073741824}-\frac{3\Lambda_1^9 m^3}{524288}+\frac{m^{12}}{84480}, \\ \mathscr{F}_7^1=\frac{715\Lambda_1^{12}m^2}{1073741824}+\frac{m^{14}}{279552}, \\ \mathscr{F}_8^1=-\frac{1131\Lambda_1^{15}m}{42949672960}-\frac{1469\Lambda_1^{12}m^4}{4294967296}+\frac{m^{16}}{860160}, \\ \mathscr{F}_9^1=\frac{385\Lambda_1^{18}}{1099511627776}+\frac{525\Lambda_1^{15}m^3}{8589934592}+\frac{m^{18}}{2506752}. \end{gathered} \tag{D1}$$

The relation between $\mathscr{F}_i^1$ and $\tilde{\mathscr{F}}_i^1$ is

$$\tilde{\mathscr{F}}_i^1:=\mathscr{F}_i^1-(\text{term proportional to } m^{2i}). \tag{D2}$$

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Symmetry and history quantum theory: An analog of Wigner's theorem

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The basic ingredients of the ''consistent histories'' approach to quantum theory are a space $\mathcal{UP}$ of ''history propositions'' and a space $\mathcal{D}$ of ''decoherence functionals.'' In this article we consider such history quantum theories in the case where $\mathcal{UP}$ is given by the set of projectors $\mathcal{P}(\mathcal{V})$ on some Hilbert space $\mathcal{V}$. We define the notion of a ''physical symmetry of a history quantum theory'' (PSHQT) and specify such objects exhaustively with the aid of an analog of Wigner's theorem. In order to prove this theorem we investigate the structure of $\mathcal{D}$, define the notion of an ''elementary decoherence functional,'' and show that each decoherence functional can be expanded as a certain combination of these functionals. We call two history quantum theories that are related by a PSHQT ''physically equivalent'' and show explicitly, in the case of history quantum mechanics, how this notion is compatible with one that has appeared previously. © *1996 American Institute of Physics.* [S0022-2488(96)00212-5]

I. INTRODUCTION

In this paper we discuss the mathematical aspects of a notion of ''symmetry'' in a history quantum theory, such as the decoherent histories approach to quantum theory initiated by Griffiths,[1] Omnès,[2] and Gell-Mann and Hartle.[3] Given the major importance symmetries play in almost every physical theory, one would like to know what the counterpart of this concept is in theories who place the emphasis on ''histories'' and ''decoherence functionals'' rather than propositions and states at a fixed time point (as is done in standard quantum theory). This involves the problem of giving a meaning to the notion of two history theories being equivalent, when consistent sets can be called equivalent, etc.[4]

These matters are not settled yet, but I will show that, in case we adopt a particular notion of ''symmetry,'' it is possible to assign a well-defined meaning to such concepts. In order to understand where these ideas fit into the structure of such history quantum theories, we have to rewrite the decoherent histories approach in a way that describes the ingredients of such a theory in a more transparent way.

The clarification of the structural content of history quantum theories (HQT) is due to C. J. Isham,[5] who extracted the basic features of these theories in the form of a set of axioms which determine the mathematical content of the framework of such theories. The aim is to place history quantum theories—as an entirely new approach to the problem of defining and constructing quantum theories—on an equally firm mathematical base as other, already existing approaches to quantum theories. The explanation of why the axioms take the particular form chosen is a very deep one and is partly motivated by problems arising in the area of quantum gravity, in particular the so-called ''problem of time;'' it uses ideas of ''quasi-temporal'' logic and much more. These matters have been discussed at some length by Isham,[5] Isham and Linden,[6] and Schreckenberg,[7] and the reader is referred to those sources for a deeper appreciation of ''history quantum theories.''

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In this paper I will adopt a working, practical approach. I will mainly restrict myself to the case of the history version of finite-dimensional quantum mechanics. This will prove to be an ideal model to illustrate the concept of ''symmetry'' introduced in this article.

Our discussion will be based on an investigation of how the mathematical structure of history quantum theories suggests a notion of ''physical symmetries of history quantum theories.'' It is striking—and indeed very satisfying—that the concept developed here is compatible with a definition and a result presented by Gell-Mann and Hartle in Ref. 4, even though this was not the original goal of the enterprise. This speaks on the one hand for the physical insight and arguments which led Gell-Mann and Hartle to the notion of 'physical equivalence', and, on the other hand, it shows the strength of the mathematical formalism developed by Isham[5] in order to capture the main ideas of the decoherent histories program in a precise manner. Because of this relation among the results, the physical arguments presented in Ref. 4 can, to some extent, be regarded as *physical* arguments in favor of the notion developed here and, vice versa, the arguments presented here as a precise *mathematical* statement about such objects, which possess a *very* transparent description.

We will begin with an introduction to the formalism introduced in Ref. 5, recall the classification theorem for decoherence functionals proven in Ref. 8, and remind the reader of the content of Wigner's theorem, which will be central to our investigation. In Sec. II we reformulate the standard requirements for ''physical symmetries'' given by Wigner in a way that is more suited to our problem in that it avoids some of the interpretative difficulties that arise when one is trying to induce a notion of symmetry in history quantum theories from symmetries defined at a single time point. We proceed by defining ''physical symmetries of a history quantum theory'' (PSHQT) and show that a particular subset of PSHQT can be induced by unitary or antiunitary operators $\hat{U}$ on $\mathscr{V}$, which I call ''homogeneous symmetries.'' We show that these symmetries possess a characterization *à la* Wigner. We investigate the structure of the space $\mathscr{D}$ in some detail to show in Sec. III that, in fact, PSHQT are in one-to-one correspondence with homogeneous symmetries and can thus be characterized by an analog of Wigner's theorem. We call two history quantum theories which are related by a physical symmetry of a history quantum theory *physically equivalent*. This expression first appeared in Ref. 4 and we show explicitly, for history quantum mechanics, how the notion of ''physical equivalence''—as introduced in Ref. 4—is naturally induced by a subset of the set of PSHQT. In the closing section IV we mention some ways one could try to proceed in order to find a satisfactory *physical* interpretation of the symmetries considered in this article.

A. Decoherent histories and history quantum theory

1. The algebraic structure for HQT

In the decoherent histories approach the two main ingredients are the so-called ''histories,'' namely sequences of Schrödinger picture projection operators $\alpha := (\alpha_{t_1}, \alpha_{t_2}, \ldots, \alpha_{t_n})$, with $t_1 < t_2 < \cdots < t_n$, defined on the single time Hilbert space $\mathscr{H}$, and ''decoherence functionals,'' namely a complex-valued functional d of pairs of histories. For normal quantum mechanics the latter is given by

$$d_{(H,\rho)}(\alpha,\beta) := \mathrm{tr}_{\mathscr{H}}(\widetilde{C}_\alpha^\dagger \rho_{t_0} \widetilde{C}_\beta), \tag{I.1}$$

where the ''class'' operator $\widetilde{C}_\alpha$ (Ref. 3) is defined to be

$$\widetilde{C}_\alpha := \alpha_{t_1}(t_1)\alpha_{t_2}(t_2)\cdots\alpha_{t_n}(t_n) \tag{I.2}$$

with $\{\alpha_{t_i}(t_i) := e^{(i/\hbar)H(t_i-t_0)}\alpha_{t_i}e^{-(i/\hbar)H(t_i-t_0)}\}$ being the associated Heisenberg picture operators. For the ease of exposition, all histories α will be defined on n arbitrary, but fixed, time points.

This functional $d(\alpha,\beta)$ is an extension of the formula $d(\alpha,\alpha)$ in standard quantum mechanics for the joint probability of finding all the properties $\alpha := (\alpha_{t_1},\alpha_{t_2},\ldots,\alpha_{t_n})$ with $t_1<t_2<\cdots<t_n$ in a time-ordered sequence of measurements. The aim is to determine with the aid of certain ''consistency conditions'' on $d(\alpha,\beta)$ such histories, on which $d(\alpha,\alpha)$ defines a probability distribution.

The expression for the decoherence functional is rather messy: it is difficult to isolate the contribution of the histories α and β to the evaluation. Whereas before they were defined as sequences of Schrödinger operators, they enter now as a product of Heisenberg operators. Hence the evolution operator should belong intrinsically to the decoherence functional as does the density matric ρ.

The separation that I have in mind of the contribution to $d_{(H,\rho)}(\alpha,\beta)$ of (i) the histories, and (ii) a part which encodes all the properties of the decoherence functional, is best illustrated by an analogous expression in standard quantum mechanics. Namely, the probability $p(x\in[a,\,b])$ of finding that the eigenvalue x of an observable X lies in the interval $[a,b],a,b\in\mathbb{R}$, given the state ρ of the system, is evaluated as

$$p(x\in[a,b],\rho)=\mathrm{tr}_{\mathscr{H}}(P^X_{[a,b]}\rho). \tag{I.3}$$

One can immediately refer to the density operator to describe the contribution of the state and to the projection operator $P^X_{[a,b]}$—as the mathematical representation of the question asked—to describe the contribution of the corresponding observable to the value $p(x\in[a,b],\rho)$. This is, of course, due to Gleason's theorem which establishes a one-to-one correspondence between states and density operators.

The appropriate rewriting of the expression for $d_{(H,\rho)}(\alpha,\beta)$, which is described in detail in Ref. 8, relies on the mathematical identity

$$\mathrm{tr}_{\mathscr{H}}(A_1A_2\ldots A_m)=\mathrm{tr}_{\otimes\mathscr{H}^m}(A_1\otimes\cdots\otimes A_mS), \tag{I.4}$$

which allows us to express the trace of a product of m operators $\{A_m\}$ by means of the trace of a single operator $A_1\otimes\cdots\otimes A_m$ on the m-fold tensor product space $\mathscr{V}_m:=\otimes\mathscr{H}^m$ and a universal operator S.

Forgetting for a moment the ρ in (I,1), $d_{(H,\rho)}(\alpha,\beta)$ is given by the product of $2n$ Heisenberg operators. Using formula (I.4) we deduce that histories enter the decoherence functional in the following way:

$$\tilde{\alpha}=\alpha_{t_1}(t_1)\otimes\alpha_{t_2}(t_2)\otimes\cdots\otimes\alpha_{t_n}(t_n). \tag{I.5}$$

Heisenberg operators are just Schrödinger operators multiplied on the left and right by the evolution operators $U(t_i,t_0)$ and its inverse. Expression (I.4) shows that this dependence can be thrown onto the universal operator S, allowing us to represent histories by Schrödinger-picture operators

$$\alpha=\alpha_{t_1}\otimes\alpha_{t_2}\otimes\cdots\otimes\alpha_{t_n}\in P(\mathscr{V}_n), \tag{I.6}$$

which contribute to the value for $d_{(H,\rho)}(\alpha,\beta)$ through

$$d_{(H,\rho)}(\alpha,\beta)=\mathrm{tr}_{\mathscr{V}_n\otimes\mathscr{V}_n}(\alpha\otimes\beta X_{(H,\rho)}), \tag{I.7}$$

for some operator $X_{(H,\rho)}$ defined on $\mathscr{V}_n\otimes\mathscr{V}_n$. The time-ordered strings of projection operators $(\alpha_{t_1},\alpha_{t_2},\ldots,\alpha_{t_n})$ are now represented by a homogeneous projection operator $\alpha_{t_1}\otimes\alpha_{t_2}\otimes\cdots\otimes\alpha_{t_n}$ on the n-fold tensor product space $\mathscr{V}_n=\otimes_{i=1}^n\mathscr{H}_{t_i}$ and one can easily see that this association is

one-to-one. This motivates the definition of a space $\mathcal{UP}$ of ''history propositions'' (also called ''universal propositions'' or ''propositions about the universe''), which is given by the set of *all* projection operators $\alpha \in \mathcal{P}(\mathcal{V}_n)$ on the n-fold tensor product space.

By these means we have achieved the aim of separating the contribution of the histories to the value $d_{(H,\rho)}(\alpha,\beta)$ in that the operator $X_{(H,\rho)}$ encodes now all of the dynamical information and the initial conditions of the system under investigation.

One can also convince oneself that the decoherence functional (I.7) satisfies the following properties:

$$\begin{aligned} &\circ \text{Hermiticity: } d(\alpha,\beta) = d(\beta,\alpha)^* \quad \forall\, \alpha,\beta \in \mathcal{P}(\mathcal{V}_n), \\ &\circ \text{Positivity: } d(\alpha,\alpha) \geqslant 0 \quad \forall\, \alpha \in \mathcal{P}(\mathcal{V}_n), \\ &\circ \text{Additivity: } d(\alpha \oplus \beta,\gamma) = d(\alpha,\gamma) + d(\beta,\gamma), \\ &\circ \text{Normalization: } d(1,1) = 1, \end{aligned} \tag{I.8}$$

which are the usual requirements for decoherence functionals in the consistent histories approach when expressed in this formalism. The operation ''$\oplus$'' is given by the addition of two orthogonal projectors, i.e., history propositions, in $\mathcal{P}(\mathcal{V}_n)$.

This example seems to suggest that it might be worth trying to define a *history quantum theory* as a theory which has two main ingredients: A space of history propositions $\mathcal{UP}$ which, in this paper, will be the space of propositions $\mathcal{P}(\mathcal{V})$ onto a Hilbert space $\mathcal{V}$; and a decoherence functional $d \in \mathcal{D}$, where $\mathcal{D}$ denotes the space of all decoherence functionals, that is, all those functionals defined on $\mathcal{P}(\mathcal{V}) \times \mathcal{P}(\mathcal{V})$ which possess the properties (I.8) mentioned above. Thus $\mathcal{V}$ does not necessarily have to be of the tensor-product form $\mathcal{V}_n$, and $d \in \mathcal{D}$ will in general not be of the form $d_{(H,\rho)}$. In this formalism, *consistent sets of history propositions with respect to a* $d \in \mathcal{D}$ correspond to certain partitions of the unit operator on $\mathcal{V}$ into mutually orthogonal projectors $\{\alpha_i\}_{i=1}^{m \leqslant \dim \mathcal{V}}$ such that

$$d(\alpha_i,\alpha_j) = \delta_{ij} d(\alpha_i,\alpha_i) \quad \forall\, i,j \in \{1,2,\ldots,m\}. \tag{I.9}$$

The properties (I.8) of $d \in \mathcal{D}$ ensure that the values $d(\alpha_i,\alpha_i)$ determine a probability distribution on the Boolean algebra generated by the $\{\alpha_i\}_{i=1}^{m \leqslant \dim \mathcal{V}}$.

2. The classification theorem

We want to base our investigations of symmetries on the expression (I.7) of the decoherence functional. However, in order to do so, we must first be sure that it is not only a lucky coincidence that we are able to cast this *particular* decoherence functional for the history version of quantum mechanics in the above form. The formalism for decoherent histories is not simply restricted to models with unitary evolution, inclusions of final density matrices, and the like. Therefore, in order to formulate a notion of symmetry that is valid for all these cases, we have to find out whether every decoherence functional, i.e., every functional satisfying the properties (I.8) listed above, can be written in the form (I.7). The clear cut answer to this is given by the following theorem (see Ref. 8), which is valid for any theory in which the history propositions are given by projectors on a finite-dimensional Hilbert space $\mathcal{V}$.

Theorem:[8] If $\dim \mathcal{V} > 2$, decoherence functionals d are in one-to-one correspondence with operators $X = X_1 + iX_2$ on $\mathcal{V} \otimes \mathcal{V}$ according to the rule

$$d(\alpha,\beta) = \mathrm{tr}_{\mathcal{V}\otimes\mathcal{V}}(\alpha \otimes \beta X) \tag{I.10}$$

with the restriction that

$$(a) X^\dagger = MXM \quad \text{with} \quad M(|v\rangle \otimes |w\rangle) := |w\rangle \otimes |v\rangle, \quad \forall |v\rangle, |w\rangle \in \mathscr{V}, \tag{I.11}$$

$$(b) \mathrm{tr}_{\mathscr{V}\otimes\mathscr{V}}(\alpha \otimes \alpha X_1) \geq 0, \tag{I.12}$$

$$(c) \mathrm{tr}_{\mathscr{V}\otimes\mathscr{V}}(X_1) = 1. \tag{I.13}$$

The restrictions on the operator X on $\mathscr{V}\otimes\mathscr{V}$ reflect the requirements (I.8). We denote by $\mathscr{X}_{\mathscr{D}}$ the set of all such operators X. This theorem which has been extended to arbitrary von Neumann algebras without factor of type II in Ref. 9, is the cornerstone of the forthcoming investigation. It allows us to shift the investigation of the properties of decoherence functionals $d \in \mathscr{D}$, where $\mathscr{D}$ denotes the space of all decoherence functionals, to an analysis of the properties of the associated operator $X_d \in \mathscr{X}_{\mathscr{D}}$, which, as we emphasize once again, carries all of the ''dynamical'' content as well as the ''initial conditions'' of the model under investigation.

It is important to understand the origin of these requirements. Condition (I.11) reflects the Hermiticity requirement. The action of M on $\alpha\otimes\beta$ is given by $M(\alpha\otimes\beta)M = (\beta\otimes\alpha)$. Equation (I.11) follows then from the condition

$$d(\alpha,\beta) = \mathrm{tr}_{\mathscr{V}\otimes\mathscr{V}}(\alpha\otimes\beta X) = \mathrm{tr}_{\mathscr{V}\otimes\mathscr{V}}(\beta\otimes\alpha X^\dagger) = d(\beta,\alpha)^*.$$

Condition (I.12) stems from the fact that, since $X^\dagger = MXM$ is equivalent to the pair of conditions

$$X_1 = MX_1M, \quad X_2 = -MX_2M, \tag{I.14}$$

it follows that

$$\mathrm{tr}_{\mathscr{V}\otimes\mathscr{V}}(\alpha\otimes\alpha X_2) = -\mathrm{tr}_{\mathscr{V}\otimes\mathscr{V}}(\alpha\otimes\alpha MX_2M) = -\mathrm{tr}_{\mathscr{V}\otimes\mathscr{V}}(M(\alpha\otimes\alpha)MX_2) = -\mathrm{tr}_{\mathscr{V}\otimes\mathscr{V}}(\alpha\otimes\alpha X_2), \tag{I.15}$$

and so $\mathrm{tr}_{\mathscr{V}\otimes\mathscr{V}}(\alpha\otimes\alpha X_2) = 0$ is implied already by the Hermiticity requirement (I.11).

It will be advantageous later to think of $d(\alpha,\beta)$ as the value of the complex-valued functional

$$\begin{aligned} &\mathrm{tr}: \mathscr{P}(\mathscr{V})\otimes\mathscr{P}(\mathscr{V}) \times \mathscr{X}_{\mathscr{D}} \to \mathbb{C} \\ &(\alpha\otimes\beta; X_d) \mapsto \mathrm{tr}_{\mathscr{V}\otimes\mathscr{V}}(\alpha\otimes\beta X_d). \end{aligned} \tag{I.16}$$

B. Wigner's theorem

In order to understand fully the importance of Wigner's result it is crucial to distinguish between the notion of a *symmetry* and that of a *physical symmetry*.

Definition: On a complex Hilbert space $\mathscr{H}$ a *symmetry* is a unitary or antiunitary operator U. Thus it leaves invariant the modulus of the inner product of any pair of two vectors $|v\rangle, |w\rangle \in \mathscr{H}$, that is

$$|\langle v,w\rangle|^2 = |\langle Uv, Uw\rangle|^2, \quad \forall |v\rangle, |w\rangle \in \mathscr{H}. \tag{I.17}$$

This definition is only a mathematical one; it has, *a priori*, no motivation by physical arguments. Note also that it does *not* impose any further defining properties on U, such as commutativity with the Hamiltonian operator. Such requirements only enter at a much later stage, motivated by analogs of the assumption in classical mechanics, that a particular physical system evolves along the flowlines of a specific, Hamiltonian, vector field.

On the other hand, a physical system at a *fixed moment of time* is described in quantum mechanics by a state $\sigma \in \mathscr{S}: \mathscr{P}(\mathscr{H}) \to \mathbb{R}$, that is, a normalized $[\sigma(1)=1]$, positive-valued functional which is additive on disjoint projectors. The states are, via Gleason's theorem, in one-to-one correspondence with density operators ρ on $\mathscr{H}$ according to the rule

$$\sigma(\alpha,\rho)=\mathrm{tr}_{\mathscr{H}}(\alpha\rho),\quad \forall\,\alpha\in\mathscr{P}(\mathscr{H}), \tag{I.18}$$

where ρ is defined by the properties

$$\rho=\rho^{\dagger},\quad \rho\geqslant 0,\quad \mathrm{tr}_{\mathrm{H}}(\rho)=1. \tag{I.19}$$

The set of all density operators is often denoted by $\mathscr{W}_{\mathscr{S}}$.

The *physical* assumption is now that all that matters are the relations among the states, which can be entirely described by means of their overlaps, that is the transition amplitudes $\mathrm{tr}_{\mathscr{H}}(\rho_1\rho_2)$.

In the finite-dimensional case the self-adjointness of ρ implies that for every density operator there exists an orthonormal basis $\{|\psi_i\rangle\}$ such that

$$\rho=\sum\, r_i P_{|\Psi_i\rangle},\quad \sum\, r_i=1,\quad r_i\geqslant 0. \tag{I.20}$$

Density operators of the form $P_{|\Psi_i\rangle}:=|\,\Psi_i\rangle\langle\Psi_i|\in\mathscr{W}_{\mathscr{SP}}$ are called *pure*. Every density operator possesses an expansion in terms of pure density operators, also representing ''rays'' of $\mathscr{H}$; instead of $\mathscr{W}_{\mathscr{SP}}$ we also use sometimes the notation $\mathscr{R}(\mathscr{H})$. Therefore, the invariance requirement on the transition amplitude between two arbitrary states ρ_1 and ρ_2 can be reduced to the requirement that

$$\mathrm{tr}_{\mathscr{H}}(P_{|\Psi^1\rangle}P_{|\Psi^2\rangle})=\mathrm{tr}_{\mathscr{H}}(P^{\xi}_{|\Psi^1\rangle}P^{\xi}_{|\Psi^2\rangle}), \tag{I.21}$$

for arbitrary one-dimensional pure density operators $P_{|\Psi^1\rangle}$ and $P_{|\Psi^2\rangle}$ and an affine map ξ: $\mathscr{W}_{\mathscr{SP}}\to\mathscr{W}_{\mathscr{SP}}$, that is a map satisfying $\xi(\Sigma_i c_i P_{|\Psi^i\rangle})=\Sigma_i c_i\xi(P_{|\Psi^i\rangle})\equiv\Sigma_i c_i P^{\xi}_{|\Psi^i\rangle}, c_i\in\mathbb{C}$.

Definition: A *physical symmetry* is an affine bijection $\xi:\mathscr{W}_{\mathscr{SP}}\to\mathscr{W}_{\mathscr{SP}}$; $P_{|\Psi\rangle}\mapsto P^{\xi}_{|\Psi\rangle}$, such that the transition amplitude between pure density operators remains invariant, i.e., that

$$\mathrm{tr}_{\mathscr{H}}(P_{|\Psi_1\rangle}P_{|\Psi_2\rangle})=\mathrm{tr}_{\mathscr{H}}(P^{\xi}_{|\Psi_1\rangle}P^{\xi}_{|\Psi_2\rangle}),\quad \forall|\Psi_1\rangle,|\Psi_2\rangle\in\mathscr{H}. \tag{I.22}$$

Theorem:[10] (*Wigner*) Every symmetry induces a physical symmetry and, conversely, every one-to-one map $\xi:\mathscr{W}_{\mathscr{SP}}\to\mathscr{W}_{\mathscr{SP}}$ preserving orthogonality between rays is a physical symmetry and can be implemented by a unitary or antiunitary operator U on $\mathscr{H}$.

II. SYMMETRY AND HISTORY QUANTUM THEORY

The notion of symmetry discussed in the last section arose from discussing quantum mechanics at a single, fixed time point $t\in\mathbb{R}$ with a corresponding Hilbert space $\mathscr{H}$. At a single time point physics is described in terms of the pair $(\mathscr{S},\mathscr{L})$, where $\mathscr{S}$ is the set of states and $\mathscr{L}$ is the lattice of projection operators on $\mathscr{H}$. In order to define physical symmetries in quantum mechanics—in the sense specified by Wigner—only the knowledge of one part of this pair was required, namely the knowledge of the properties of the set of states $\mathscr{S}$, via the map

$$\mathrm{tr}:\mathscr{W}_{\mathscr{SP}}\times\mathscr{W}_{\mathscr{SP}}\to\mathbb{R}$$

$$(P_{|\Psi_1\rangle}:P_{|\Psi_2\rangle})\mapsto\mathrm{tr}_{\mathscr{H}}(P_{|\Psi_1\rangle}P_{|\Psi_2\rangle}). \tag{II.1}$$

The properties of the lattice of propositions $\mathscr{L}=\mathscr{P}(\mathscr{H})$ did not enter in full.

In order to arrive at a notion of symmetry for HQTs, recall that in a history quantum theory the pair $(\mathscr{UP},\mathscr{D})$ can be seen as a formal analogue of the pair $(\mathscr{L},\mathscr{S})$. Comparing the two expressions

$$\mathrm{tr}_{\mathscr{H}}(\rho_1\rho_2)\quad and\quad \mathrm{tr}_{\mathscr{T}\otimes\mathscr{T}}(\alpha\otimes\beta X_d) \tag{II.2}$$

reveals immediately the mathematical difference between them. In contrast to the quantum mechanical case at a single time point, in HQTs the map

$$\mathrm{tr}:\mathscr{P}(\mathscr{V})\otimes\mathscr{P}(\mathscr{V})\times\mathscr{X}_{\mathscr{D}}\to\mathbb{C}$$

$$(\alpha\otimes\beta)\times X_d\mapsto\mathrm{tr}_{\mathscr{V}\otimes\mathscr{V}}(\alpha\otimes\beta X_d) \tag{II.3}$$

intertwines the properties of $\mathscr{UP}=\mathscr{P}(\mathscr{V})$ and $\mathscr{X}_{\mathscr{D}}$. This is not surprising, since the classification theorem is more to be regarded as an analog of Gleason's theorem, which in a similar manner intertwines properties of $\mathscr{L}$ and $\mathscr{S}$.

The invariance requirement for the expression $\mathrm{tr}_{\mathscr{H}}(\rho_1\rho_2)$ has a direct physical meaning. In HQTs the formal analog of a density operator ρ is an operator $X_d\in\mathscr{X}_{\mathscr{D}}$ so that the first guess for symmetries might be to look for transformations which leave ''transition amplitudes between different X_d'' invariant. However, such a requirement would be hard to interpret since HQTs deal with ''history propositions'' as entities in their own right. The theory is completely specified by choosing *a particular* decoherence functional, which is kept fixed throughout. Since the notion of ''time'' in a specific history quantum theory is determined by the choice of the structure of the space of history propositions—for example, the nature of ''time'' as a parameter $t\in\mathbb{R}$ in quantum mechanics is mirrored in the definition of $\mathscr{P}(\mathscr{V}_n)=\mathscr{P}(\otimes_{i=1}^{n}\mathscr{H}_{t_i})$—and decoherence functionals associate numbers with these pairs of history propositions *as an entity*, a change of the decoherence functional must not occur.

How can we nonetheless use, at least at the mathematical level, the existing notion of a physical symmetry and later on Wigner's theorem, to define a corresponding notion for HQTs that does not suffer from the difficulty mentioned above? The main idea is to characterize the notion of a *physical symmetry* in a form which exploits the pairing (I.18) between density operators $\rho\in\mathscr{W}_{\mathscr{S}}$ and propositions $\alpha\in\mathscr{P}(\mathscr{H})$ given by Gleason's theorem.

A. Alternative specification of physical symmetries

We start by neglecting entirely the considerations from which the expression

$$\mathrm{tr}_{\mathscr{H}}(P_{|\Psi\rangle}P_{|\Phi\rangle}) \tag{II.4}$$

originally arose. Pure density operators belong trivially to the space of projection operators $\mathscr{P}(\mathscr{H})$ and therefore, instead of thinking of the map (II.1) as a pairing between states, one can think of it as a map

$$\mathrm{tr}:\{\mathscr{R}(\mathscr{H})\subset\mathscr{P}(\mathscr{H})\}\times\mathscr{W}_{\mathscr{S}^p}\to\mathbb{R}$$

$$P_{|\Psi\rangle}\times P_{|\Phi\rangle}\mapsto\mathrm{tr}_{\mathscr{H}}(P_{|\Psi\rangle}P_{|\Phi\rangle}) \tag{II.5}$$

that establishes a pairing between a subset of the space of propositions and the set of pure states. Therefore, we see immediately that Wigner's result can be read as follows: Wigner's theorem determines all bijections

$$\xi:\mathscr{R}(\mathscr{H})\times\mathscr{W}_{\mathscr{S}^p}\to\mathscr{R}(\mathscr{H})\times\mathscr{W}_{\mathscr{S}^p}$$

$$(P_{|\Phi\rangle},P_{|\Psi\rangle})\mapsto(P^{\xi}_{|\Phi\rangle},P^{\xi}_{|\Psi\rangle}) \tag{II.6}$$

that leave invariant the pairing

$$\mathrm{tr}_{\mathscr{H}}(P_{|\Psi\rangle}P_{|\Phi\rangle})=\mathrm{tr}_{\mathscr{H}}(P^{\xi}_{|\Psi\rangle}P^{\xi}_{|\Phi\rangle}). \tag{II.7}$$

Now, when seen from this perspective, it is natural to ask whether or not Wigner's theorem specifies completely all affine one-to-one maps

$$V:\mathscr{P}(\mathscr{H})\times\mathscr{W}_{\mathscr{S}}\rightarrow\mathscr{P}(\mathscr{H})\times\mathscr{W}_{\mathscr{S}}$$

$$(\alpha,\rho)\mapsto(\alpha^V,\rho^V) \tag{II.8}$$

such that the pairing between propositions and density operators is left invariant for all $\alpha\in\mathscr{P}(\mathscr{H})$ and all $\rho\in\mathscr{W}_{\mathscr{S}}$, i.e.,

$$\mathrm{tr}_{\mathscr{H}}(\alpha\rho)=\mathrm{tr}_{\mathscr{H}}(\alpha^V\rho^V). \tag{II.9}$$

The map is required to be affine since the space $\mathscr{W}_{\mathscr{S}}$ is a convex space. Convex combinations of elements of $\mathscr{W}_{\mathscr{S}}$ are again density operators.

Note that the question posed is not trivial: The space of projectors $\mathscr{P}(\mathscr{H})$ is a disjoint union of compact Grassmann manifolds and therefore allows for a much wider class of transformation than just unitary or antiunitary operators U on $\mathscr{H}$. The three conditions these maps have to satisfy are

$$^*V:\mathscr{P}(\mathscr{H})\rightarrow\mathscr{P}(\mathscr{H}), \tag{II.10}$$

$$^*V:\mathscr{W}_{\mathscr{S}}\rightarrow\mathscr{W}_{\mathscr{S}}, \tag{II.11}$$

$$^*\mathrm{tr}_{\mathscr{H}}(\alpha\rho)=\mathrm{tr}_{\mathscr{H}}(\alpha^V\rho^V). \tag{II.12}$$

If we consider transformations on $\mathscr{P}(\mathscr{H})$, the interesting transformations are given by transforming projectors of different dimensions to each other. So consider, for example, the transformation

$$G:\mathscr{P}(\mathscr{H})\rightarrow\mathscr{P}(\mathscr{H})$$

$$\alpha\mapsto G[\alpha], \tag{II.13}$$

whereby a particular one-dimensional projector $P_{|\Phi\rangle}$ is mapped into an m-dimensional one, $G[P_{|\Phi\rangle}]$, $m>1$. Such a transformation might be bijective on $P(\mathscr{H})$ and even obey requirement (II.12).

Now, regarding $P_{|\Phi\rangle}$ as a pure *density operator*, we see immediately that the trace of its image under G is $\mathrm{tr}_{\mathscr{H}}(G[P_{|\Phi\rangle}])=m$. Therefore, such a map does not comply with the requirement (II.11). Thus, only maps which map rays into rays are allowed and, therefore, all maps obeying the conditions (II.8) and (II.9) are determined by Wigner's theorem.

This reformulation of ''physical symmetries'' in terms of the intersection of different sets of transformations fulfilling (II.10), (II.11), or (II.12), respectively, possesses the advantage of never having to consider ''transition amplitudes between states at a fixed moment of time.'' Physical symmetries just preserve the intertwining between $(\mathscr{L},\mathscr{S})$ via Gleason's theorem by transforming $\mathscr{L}$ *and* $\mathscr{S}$ by the same transformation *into itself*.

This fact justifies trying to define symmetries of a history quantum theory by exact analogs of the requirements (II.10)–(II.12), i.e., by replacing

$$\{\mathscr{P}(\mathscr{H});\mathscr{W}_{\mathscr{S}};\mathrm{tr}_{\mathscr{H}}(\alpha\rho)\}\leftrightarrow\{\mathscr{P}(\mathscr{V})\otimes\mathscr{P}(\mathscr{V});\mathscr{X}_{\mathscr{D}};\mathrm{tr}_{\mathscr{V}\otimes\mathscr{V}}(\alpha\otimes\beta X_d)\}. \tag{II.14}$$

This notion of a ''symmetry of a history quantum theory'' does not suffer from the interpretative difficulty mentioned above.

Through this choice, we will build in an invariance requirement for the values $d(\alpha,\beta)$ of the decoherence functional from the very start. Some physical arguments for such a choice can be found in Refs. 4, 11, and 12. I will discuss its relevance at various stages in this paper.

B. Definition and proposition

Definition: A *physical symmetry of a history quantum theory* (PSHQT) is any affine one-to-one map

$$\mathcal{Q}:\mathcal{P}(\mathcal{V})\otimes\mathcal{P}(\mathcal{V})\times\mathcal{X}_{\mathcal{G}}\to\mathcal{P}(\mathcal{V})\otimes\mathcal{P}(\mathcal{V})\times\mathcal{X}_{\mathcal{G}}$$

$$([\alpha\otimes\beta],X_d)\mapsto([\alpha\otimes\beta]^{\mathcal{Q}},X_d^{\mathcal{Q}}) \tag{II.15}$$

that preserves the value of the pairing between history propositions and operators associated with decoherence functionals, i.e.,

$$\mathrm{tr}_{\mathcal{V}\otimes\mathcal{V}}(\alpha\otimes\beta X_d)=\mathrm{tr}_{\mathcal{V}\otimes\mathcal{V}}([\alpha\otimes\beta]^{\mathcal{Q}}X_d^{\mathcal{Q}}). \tag{II.16}$$

We state once again the three requirements such a map has to fulfill:

$$*\mathcal{Q}:\mathcal{P}(\mathcal{V})\otimes\mathcal{P}(\mathcal{V})\to\mathcal{P}(\mathcal{V})\otimes\mathcal{P}(\mathcal{V}), \tag{II.17}$$

$$*\mathcal{Q}:\mathcal{X}_{\mathcal{G}}\to\mathcal{X}_{\mathcal{G}}, \tag{II.18}$$

$$*\mathrm{tr}_{\mathcal{V}\otimes\mathcal{V}}(\alpha\otimes\beta X_d)=\mathrm{tr}_{\mathcal{V}\otimes\mathcal{V}}([\alpha\otimes\beta]^{\mathcal{Q}}X_d^{\mathcal{Q}}). \tag{II.19}$$

Each condition separately determines a set of transformations, but only the intersection of these sets may be called a PSHQT. The word *physical* is chosen since this definition parallels the one for physical symmetries given by Wigner. Again, the history propositions $\alpha\in\mathcal{P}(\mathcal{V})$ *and* the decoherence functionals, represented by $X_d\in\mathcal{X}_{\mathcal{G}}$, are transformed *together* by the same transformation. We call two history quantum theories that are related by a physical symmetry of a history quantum theory *physically equivalent*. Furthermore, as will be shown later, this definition encompasses the notion of ''physical equivalence,'' first introduced and justified through physical arguments by Gell-Mann and Hartle in Ref. 4. It is easy to see that the following Lemma holds.

Lemma: The relation among two history quantum theories (hqt_1,hqt_2) of being *physically equivalent*, denoted by $hqt_1\sim hqt_2$, is an equivalence relation. Thus it is (i) reflexive: $hqt_1\sim hqt_1$, (ii) symmetric: $hqt_1\sim hqt_2\Rightarrow hqt_2\sim hqt_1$, and (iii) transitive: $(hqt_1\sim hqt_2)$ and $(hqt_2\sim hqt_3)\Rightarrow(hqt_1\sim hqt_3)$.

There is an obvious class of transformations on $\mathcal{V}\otimes\mathcal{V}$ that fulfills all three conditions (II.17)–(II.18) stated above:

Definition: A *homogeneous symmetry* on $\mathcal{V}\otimes\mathcal{V}$ is a unitary operator $\hat{U}\otimes\hat{U}$ where $\hat{U}$ may be a unitary or antiunitary operator on $\mathcal{V}$.

Lemma: Every homogeneous symmetry induces a PSHQT, i.e., {HS}⊂{PSHQT}.

Proof: A homogeneous symmetry induces the maps

$$\begin{aligned}\alpha\otimes\beta&\mapsto\hat{U}\otimes\hat{U}[\alpha\otimes\beta]\hat{U}^{\dagger}\otimes\hat{U}^{\dagger},\\ X_d&\mapsto\hat{U}\otimes\hat{U}X_d\hat{U}^{\dagger}\otimes\hat{U}^{\dagger},\end{aligned} \tag{II.20}$$

so that for all $\alpha\otimes\beta\in\mathcal{P}(\mathcal{V})\otimes\mathcal{P}(\mathcal{V})$ and all $X_d\in\mathcal{X}_{\mathcal{G}}$ it holds that

$$d(\alpha,\beta)=\mathrm{tr}_{\mathcal{V}\otimes\mathcal{V}}[(\hat{U}\alpha\hat{U}^{\dagger}\otimes\hat{U}\beta\hat{U}^{\dagger})(\hat{U}\otimes\hat{U}X_d\hat{U}^{\dagger}\otimes\hat{U}^{\dagger})]. \tag{II.21}$$

One can easily check that $\hat{U}\otimes\hat{U}X_d\hat{U}^{\dagger}\otimes\hat{U}^{\dagger}$ fulfills the defining properties for an operator $X_{d'}\in\mathcal{X}_{\mathcal{G}}$ given by the classification theorem. □

Homogeneous symmetries possess a different characterization, which can easily be derived from Wigner's theorem for quantum mechanics. Recall the definition of the map M used in the classification theorem for decoherence functionals:

$$M:\mathscr{V}\otimes\mathscr{V}\to\mathscr{V}\otimes\mathscr{V}$$

$$|u\rangle\otimes|v\rangle\mapsto|v\rangle\otimes|u\rangle, \tag{II.22}$$

for all $|u\rangle,|v\rangle\in\mathscr{V}\otimes\mathscr{V}$. As a result, its action on projection operators of the form $\alpha\otimes\beta$ is given by

$$M(\alpha\otimes\beta)M=(\beta\otimes\alpha),\quad \forall\,\alpha\otimes\beta\in P(\mathscr{V})\otimes P(\mathscr{V}). \tag{II.23}$$

In particular, this holds true for $\alpha,\beta\in\mathscr{R}(\mathscr{V})$, i.e., projection operators belonging to the space $\mathscr{R}(\mathscr{V})$ of rays of $\mathscr{V}$.

Let $\tau=\tau_1\otimes\tau_2$ denote a map

$$\tau:\mathscr{R}(\mathscr{V})\otimes\mathscr{R}(\mathscr{V})\to\mathscr{R}(\mathscr{V})\otimes\mathscr{R}(\mathscr{V})$$

$$P_{|\Psi\rangle}\otimes P_{|\Phi\rangle}\mapsto[P_{|\Psi\rangle}\otimes P_{|\Phi\rangle}]^{\tau}:=P_{|\Psi\rangle}^{\tau_1}\otimes P_{|\Phi\rangle}^{\tau_2}, \tag{II.24}$$

where τ_1 and τ_2 denote transformations on the space of pure density operators. A map τ is said to *commute* with M if $(M\circ\tau)[P_{|\Psi\rangle}\otimes P_{|\Phi\rangle}]=(\tau\circ M)[P_{|\Psi\rangle}\otimes P_{|\Phi\rangle}]$ for all elements $P_{|\Psi\rangle}\otimes P_{|\Phi\rangle}\in\mathscr{R}(\mathscr{V})\otimes\mathscr{R}(\mathscr{V})$, written symbolically as $[\tau, M]=0$.

Definition: A homogeneous symmetry of a history quantum theory (HSHQT) is a one-to-one map $\tau:\mathscr{R}(\mathscr{V})\otimes\mathscr{R}(\mathscr{V})\to\mathscr{R}(\mathscr{V})\otimes\mathscr{R}(\mathscr{V})$ that preserves the transition amplitude between two elements, i.e.,

$$\mathrm{tr}_{\mathscr{V}\otimes\mathscr{V}}([P_{|\Psi_1\rangle}\otimes P_{|\Phi_1\rangle}][P_{|\Psi_2\rangle}\otimes P_{|\Phi_2\rangle}])=\mathrm{tr}_{\mathscr{V}\otimes\mathscr{V}}([P_{|\Psi_1\rangle}\otimes P_{|\Phi_1\rangle}]^{\tau}[P_{|\Psi_2\rangle}\otimes P_{|\Phi_2\rangle}]^{\tau}),$$

and commutes with the map M, that is $[\tau, M]=0$.

Proposition: Every homogeneous symmetry induces a HSHQT and, conversely, every one-to-one map $\tau:\mathscr{R}(\mathscr{V})\otimes\mathscr{R}(\mathscr{V})\to\mathscr{R}(\mathscr{V})\otimes\mathscr{R}(\mathscr{V})$ that preserves orthogonality between the rays and commutes with M is a HSHQT and can be implemented by a unitary or antiunitary operator $\hat{U}\otimes\hat{U}$ on $\mathscr{V}\otimes\mathscr{V}$. Symbolically,

$$\{\mathrm{HSHQT}\}\cong\{\mathrm{HS}\}.$$

Proof: The transition amplitude between two elements $[P_{|\Psi_1\rangle}\otimes P_{|\Phi_1\rangle}],[P_{|\Psi_2\rangle}\otimes P_{|\Phi_2\rangle}]\in\mathscr{R}(\mathscr{V})\otimes\mathscr{R}(\mathscr{V})$ is given by

$$\mathrm{tr}_{\mathscr{V}\otimes\mathscr{V}}([P_{|\Psi_1\rangle}\otimes P_{|\Phi_1\rangle}][P_{|\Psi_2\rangle}\otimes P_{|\Phi_2\rangle}])=\mathrm{tr}_{\mathscr{V}}(P_{|\Psi_1\rangle}P_{|\Psi_2\rangle})\mathrm{tr}_{\mathscr{V}}(P_{|\Phi_1\rangle}P_{|\Phi_2\rangle}). \tag{II.25}$$

Therefore, by Wigner's theorem, all transformations preserving orthogonality and the transition amplitude can be implemented by operators $\hat{U}\otimes\hat{V}$, where $\hat{U}$ and $\hat{V}$ are either unitary or antiunitary operators on $\mathscr{V}$. Requiring these transformations to commute with M concludes the proof. □

Remark: It is important to understand why only transformations of the form $\hat{U}\otimes\hat{U}$ are admitted, and not, for example, operators of the form

$$\sum_i c_i\hat{U}_i\otimes\hat{U}_i,\quad \sum_i c_i=1,\quad c_i\in\mathbb{R}. \tag{II.26}$$

The reason is that, starting from $d(\alpha,\beta)$, only those transformations $\tilde{T}:\alpha\otimes\beta\mapsto\tilde{T}(\alpha\otimes\beta)\tilde{T}^{\dagger}$ on $\mathscr{V}\otimes\mathscr{V}$ are allowed for which

$$\tilde{T}(\alpha\otimes\beta)\tilde{T}^{\dagger}=\alpha'\otimes\beta'. \tag{II.27}$$

It is possible for these transformations only to write them as $d(\alpha,\beta)\mapsto d'(\alpha',\beta')$.

We have therefore established the following relation among the three sets of transformations:

$$\{\text{HSHQT}\}\cong\{\text{HS}\}\subset\{\text{PSHQT}\}. \tag{II.28}$$

We argued that PSHQTs determined by conditions (II.17)–(II.19) is an appropriate notion for symmetries of history quantum theories. What we want to show now is that all PSHQTs are given by homogeneous symmetries of the form $\hat{U}\otimes\hat{U}$. In view of (II.28) it remains to be shown that $\{\text{HS}\}\supset\{\text{PSHQT}\}$.

C. The structure of $\mathscr{D}$

In order to show that all PSHQTs can be characterized by means of rays in $\mathscr{R}(\mathscr{V})\otimes\mathscr{R}(\mathscr{V})$, we have to discuss in more detail the structure of the space of decoherence functionals. Comparison with the case in standard quantum mechanics shows that what we now have to look for is a notion of ''elementary decoherence functionals,'' out of which all other decoherence functionals can be built by a certain superposition. The requirement (II.19) for PSHQT,

$$\mathrm{tr}_{\mathscr{V}\otimes\mathscr{V}}(\alpha\otimes\beta X_d)=\mathrm{tr}_{\mathscr{V}\otimes\mathscr{V}}([\alpha\otimes\beta]^{\mathbb{C}}X_d^{\mathbb{C}}),$$

can then be reduced to a requirement that has to hold only for all elementary decoherence functionals. We start our investigation with the following observation:

Lemma: For any finite set $\{d^{(i)}\}_{i=1}^{n}$, $d^{(i)}\in\mathscr{D}$, it holds that $d:=\Sigma_i r_i d^{(i)}\in\mathscr{D}, r_i\in\mathbb{R}$, provided that

$$r_i\in\mathbb{R}\quad\forall i\in\{1,2,\ldots,n\},$$

$$\sum_i r_i d^{(i)}(\alpha,\alpha)\geqslant 0\quad\forall\alpha\in\mathscr{UP}, \tag{II.29}$$

$$\sum_i r_i=1.$$

These conditions reflect the requirements for d of Hermiticity, positivity, and normalization. We call such superpositions of decoherence functionals a *weak convex combination* of decoherence functionals. All convex combinations are weak convex combinations, but the converse is not true. For a convex combination it is required that $r_i\geqslant 0$; the second condition in (II.29) does not imply $r_i\geqslant 0$. It seems natural to look for so-called ''pure decoherence functionals'' which can not be written as weak convex combination of other decoherence functionals. An argument first given by N. Linden[13] shows that *any* decoherence functional can be written as the sum of two other decoherence functionals. Thus there can be no pure decoherence functionals. Nonetheless, in this context we are only interested in a convenient expansion of an arbitrary decoherence functional by what I will call *elementary decoherence functionals*. This will suffice to prove an analog of Wigner's theorem in the next section. I will show explicitly how these elementary decoherence functionals reflect Linden's argument. The same notions apply *mutatis mutandis* for the associated operators $X_d\in\mathscr{X}_{\mathscr{D}}$.

By the classification theorem[8] we know that for every decoherence functional $d\in\mathscr{D}$ its associated operator X_d can be written as a sum of two self-adjoint operators $X_d=X_1+iX_2$ subject to the conditions

$$X_1=MX_1M;\quad X_2=-MX_2M;\quad \mathrm{tr}_{\mathscr{V}\otimes\mathscr{V}}(\alpha\otimes\alpha X_1)\geqslant 0;\quad \mathrm{tr}_{\mathscr{V}\otimes\mathscr{V}}(X_1)=1. \tag{II.30}$$

We seek an expansion for the real part X_1 and the imaginary part X_2 of X_d as a weak convex combination of decoherence functionals d^e that can not be written as a weak convex combination.

Proposition: For each $X=X_1+iX_2\in\mathscr{X}_{\mathscr{D}}$ there exist two orthonormal bases (ONB) $\{|e_i\rangle\}$ and $\{|b_i\rangle\}$ on $\mathscr{V}$ such that X can be written as

$$X=\sum_{i,j}\lambda_{ij}X_1^{(ij)}+i\sum_{l,m}\kappa_{lm}X_2^{[lm]}, \tag{II.31}$$

where

$$X_1^{(ij)}=\tfrac{1}{2}(P_{|e_i\rangle}\otimes P_{|e_j\rangle}+P_{|e_j\rangle}\otimes P_{|e_i\rangle});$$
$$\lambda_{ij}=\lambda_{ji},\quad \sum_{i,j}\lambda_{ij}=1,\quad \sum_{i,j}a_{ii}\lambda_{ij}a_{jj}\geqslant 0,\quad \lambda_{ij}\in\mathbb{R}, \tag{II.32}$$

and

$$X_2^{[lm]}=\tfrac{1}{2}(P_{|b_l\rangle}\otimes P_{|b_m\rangle}-P_{|b_m\rangle}\otimes P_{|b_l\rangle});$$
$$\kappa_{lm}=-\kappa_{ml},\quad \kappa_{lm}\in\mathbb{R}. \tag{II.33}$$

Remark: The positivity requirement $\mathrm{tr}_{\mathscr{V}\otimes\mathscr{V}}(\alpha\otimes\alpha X_1)\geqslant 0$ gives rise to the condition $\Sigma_{i,j}a_{ii}\lambda_{ij}a_{jj}\geqslant 0$ for an arbitrary projector $\alpha=\Sigma_{ij}a_{ij}|e_i\rangle\langle e_j|$ on $\mathscr{V}$ when expanded in the basis $\{|e_i\rangle\langle e_j|\}$.

Proof: The proof is a constructive one; it follows the proof of the classification theorem in Ref. 8.

For each $\alpha\in\mathscr{P}(\mathscr{V})$ define a function $d_\alpha(\beta)\colon\mathscr{P}(\mathscr{V})\to\mathbb{C}$ where $d_\alpha(\beta):=d(\alpha,\beta)$. Let $\mathfrak{R}d_\alpha$ and $\mathfrak{T}d_\alpha$ denote the real and imaginary parts of d_α, so that

$$d_\alpha(\beta)=\mathfrak{R}d_\alpha(\beta)+i\mathfrak{T}d_\alpha(\beta) \tag{II.34}$$

with $\mathfrak{R}d_\alpha(\beta)\in\mathbb{R}$ and $\mathfrak{T}d_\alpha(\beta)\in\mathbb{R}$. We will develop the argument only for the real part $\mathfrak{R}d_\alpha(\beta)$. The biadditivity condition on the $d\in\mathscr{D}$ requires that $\mathfrak{R}d_\alpha(\beta_1\oplus\beta_2)=\mathfrak{R}d_\alpha(\beta_1)+\mathfrak{R}d_\alpha(\beta_2)$ for any orthogonal pair of projectors β_1 and β_2. Since d is assumed to be bounded, the same holds true for its real part $\mathfrak{R}d_\alpha$. For any $r\in\mathbb{R}$, the quantity

$$\kappa_r(\beta):=r\ \dim(\beta)=r\ \mathrm{tr}(\beta) \tag{II.35}$$

is a real additive function of β, and hence so are $\mathfrak{R}d_\alpha+\kappa_r$ for any $r\in\mathbb{R}$.

In Ref. 8 it was shown that there exists for each $\alpha\in\mathscr{P}(\mathscr{V})$ two real numbers $r_\alpha,\mu_a\in\mathbb{R}$ such that there exists a density operator $\rho_\alpha^{\mathfrak{R}}$ on $\mathscr{V}$ for which it holds that

$$\mathfrak{R}d_\alpha(\beta)=\mathrm{tr}_{\mathscr{V}}\left(\left(\frac{1}{\mu_\alpha}\rho_\alpha^{\mathfrak{R}}-r_\alpha\right)\beta\right)=\mathrm{tr}_{\mathscr{V}}(Y_\alpha^{\mathfrak{R}}\beta), \tag{II.36}$$

where $Y_\alpha^{\mathfrak{R}}:=(1/\mu_\alpha)\rho_\alpha^{\mathfrak{R}}-r_\alpha$. Since $\rho_\alpha^{\mathfrak{R}}$ is a density operator, there exists an orthonormal basis $\{|e_i\rangle\}_{i=1}^{\dim\mathscr{V}}$ and positive numbers $w_\alpha^i\in\mathbb{R}$ such that $\rho_\alpha^{\mathfrak{R}}=\Sigma_i w_\alpha^i P_{|e_i\rangle}$ and therefore

$$Y_\alpha^{\mathfrak{R}}=\sum_i\left(\frac{w_\alpha^i}{\mu_a}-r_\alpha\right)P_{|e_i\rangle}. \tag{II.37}$$

The additivity condition $d(\alpha_1\oplus\alpha_2,\beta)=d(\alpha_1,\beta)+d(\alpha_2,\beta)$ implies that

$$\mathrm{tr}_{\mathscr{V}}(Y_{\alpha_1\oplus\alpha_2}^{\mathfrak{R}}\beta)=\mathrm{tr}_{\mathscr{V}}(Y_{\alpha_1}^{\mathfrak{R}}\beta)+\mathrm{tr}_{\mathscr{V}}(Y_{\alpha_2}^{\mathfrak{R}}\beta), \tag{II.38}$$

which, since it is true for all $\beta \in \mathscr{P}(\mathscr{V})$ (and hence for all operators on $\mathscr{V}$), implies that the operator-valued map $\alpha \mapsto Y_\alpha^{\mathfrak{R}}$ is itself additive in the sense that

$$Y_{\alpha_1 \oplus \alpha_2}^{\mathfrak{R}} = Y_{\alpha_1}^{\mathfrak{R}} + Y_{\alpha_2}^{\mathfrak{R}} \tag{II.39}$$

for all disjoint pairs of projectors α_1 and α_2 on the Hilbert space $\mathscr{V}$.

Let $\{|c_i\rangle\}_{i=1}^{\dim \mathscr{V}}$ be an orthonormal basis of $\mathscr{V}$; let $\{\langle c_i|\}_{i=1}^{\dim \mathscr{V}}$ denote its dual basis. Let $\{B_{ij} := |c_i\rangle\langle c_j|;\ i,j=1,2,\ldots,N\}$ be a vector-space basis for the operators on $\mathscr{V}$, so that the operators $Y_\alpha^{\mathfrak{R}}$ can be expanded as $Y_\alpha^{\mathfrak{R}} = \Sigma_{i,j=1} y_{ij}^{\mathfrak{R}}(\alpha) B_{ij}$. Then relation (II.39) shows that the complex expansion coefficients $y_{ij}^{\mathfrak{R}}(\alpha)$, $i,j=1,2,\ldots,\dim \mathscr{V}$, must satisfy the additivity condition:

$$y_{ij}^{\mathfrak{R}}(\alpha_1 \oplus \alpha_2) = y_{ij}^{\mathfrak{R}}(\alpha_1) + y_{ij}^{\mathfrak{R}}(\alpha_2). \tag{II.40}$$

Since $Y_\alpha^{\mathfrak{R}}$ is a bounded operator, its expansion coefficient functions $\alpha \mapsto y_{ij}^{\mathfrak{R}}(\alpha) \forall\, \alpha \in \mathscr{P}(\mathscr{V})$ are bounded as well. It was shown[8] that there exists an operators $\Lambda_{ij}^{\mathfrak{R}}$ on $\mathscr{V}$ such that

$$y_{ij}(\alpha) = \mathrm{tr}_{\mathscr{V}}(\alpha \Lambda_{ij}^{\mathfrak{R}}), \tag{II.41}$$

and therefore

$$Y_\alpha = \sum_{i,j=1}^{N} \mathrm{tr}_{\mathscr{V}}(\alpha \Lambda_{ij}^{\mathfrak{R}}) B_{ij}. \tag{II.42}$$

In particular,

$$\mathfrak{R}d(\alpha,\beta) = \mathrm{tr}_{\mathscr{V}}\left\{ \sum_{i,j} (\mathrm{tr}_{\mathscr{V}}(\alpha \Lambda_{ij}^{\mathfrak{R}})) B_{ij} \beta \right\} = \sum_{i,j} \mathrm{tr}_{\mathscr{V}}(\alpha \Lambda_{ij}^{\mathfrak{R}}) \mathrm{tr}_{\mathscr{V}}(B_{ij}\beta). \tag{II.43}$$

We define an operator $X^{\mathfrak{R}}$ on $\mathscr{V} \otimes \mathscr{V}$ by

$$X^{\mathfrak{R}} := \sum_{ij} \Lambda_{ij}^{\mathfrak{R}} \otimes B_{ij}, \tag{II.44}$$

for which it holds that $\mathfrak{R}d(\alpha,\beta) = \mathrm{tr}_{\mathscr{V}\otimes\mathscr{V}}(\alpha \otimes \beta X^{\mathfrak{R}})$.

From now on we choose the particular set of $\{|e_i\rangle\}$ of eigenvectors of the operator $\rho_\alpha^{\mathfrak{R}}$ as an orthonormal basis for $\mathscr{V}$, i.e., $B_{ij} = |e_i\rangle\langle e_j|$. As an operator on $\mathscr{V}$, $\Lambda_{ij}^{\mathfrak{R}}$ possesses an expansion

$$\Lambda_{ij}^{\mathfrak{R}} = \sum_{k,l} \lambda_{kl}^{ij} B_{kl}, \tag{II.45}$$

so that

$$X^{\mathfrak{R}} = \sum_{i,j,k,l} \lambda_{kl}^{ij} B_{kl} \otimes B_{ij}. \tag{II.46}$$

However, from Eq. (II.37) we see that, by using the basis $\{|e_i\rangle\}$, this sum reduces to

$$X^{\mathfrak{R}} = \sum_{i,k,l} \lambda_{kl}^{ii} B_{kl} \otimes b_{ii}, \tag{II.47}$$

since only the $B_{ii} = P_{|e_i\rangle}$ appear in the expansion of $Y_\alpha^{\mathfrak{R}}$.

Remember now that $X^{\mathfrak{R}}$ stands for the real part X_1 of X_d, the operator associated with a decoherence functional $d \in \mathscr{D}$. As such it has to fulfill that

$$X^{\mathfrak{R}} = M X^{\mathfrak{R}} M, \tag{II.48}$$

where M was defined through the action $M(A \otimes B)M = (B \otimes A)$ for arbitrary operators A and B on $\mathscr{V}$. This requirement is strong enough to reduce (II.47) to

$$X^{\mathfrak{R}} = \sum_{i,k} \lambda^{ii}_{kk} B_{kk} \otimes B_{ii}\,. \tag{II.49}$$

Since $B_{ii} = |e_i\rangle\langle e_i| = P_{|e_i\rangle}$, we see that the real part $X^{\mathfrak{R}} \equiv X_1$ of the operator X_d associated with a decoherence functional $d \in \mathscr{D}$ can be written as

$$X_1 \equiv X^{\mathfrak{R}} = \sum_{i,j} \lambda_{ij} P_{|e_1\rangle} \otimes P_{|e_j\rangle}\,, \tag{II.50}$$

where $\lambda_{ij} := \lambda^{ii}_{jj}$. It is easy to see that these coefficients must obey

$$\lambda_{ij} = \lambda_{ji}\,, \quad \sum_{i,j} \lambda_{ij} = 1, \quad \sum_{i,j} a_{ii} \lambda_{ij} a_{jj} \geqslant 0, \tag{II.51}$$

which follow from the requirements of Hermiticity, normalization, and positivity. The $a_{ii} \in \mathbb{R}$ are expansion coefficients of an arbitrary projector $\alpha = \Sigma_{ij} a_{ij} |e_i\rangle\langle e_j|$ on $\mathscr{V}$ when expanded in the basis $\{|e_i\rangle\langle e_j|\}$.

Note that the operators $P_{|e_i\rangle} \otimes P_{|e_j\rangle}$ are not themselves operators associated with decoherence functionals. They do not obey the $X^{\dagger} = MXM$ requirement. By defining

$$X_1^{(ij)} := \tfrac{1}{2}(P_{|e_i\rangle} \otimes P_{|e_j\rangle} + P_{|e_j\rangle} \otimes P_{|e_i\rangle}), \tag{II.52}$$

we see that $X_1^{(ij)}$ is an operator that can be associated with a decoherence functional. This concludes the proof of the proposition for the real part.

By the same procedure we obtain the expansion (II.33) for the imaginary part X_2 of X_d in terms of projectors $P_{|b_i\rangle}$ for a different orthonormal basis $\{|b_i\rangle\}$. This concludes the proof. □

Note that the imaginary part X_2 in itself is not an operator that can be associated with a $d \in \mathscr{D}$. Thus, we have shown the following Corollary.

Corollary: There exists a one-to-one correspondence between elementary decoherence functionals $d^e \in \mathscr{D}$ and operators $X_{d^e} \in \mathscr{X}_{\mathscr{D}}$ which are given by the following expression:

$$X^{(ij)[lm]}_{d^e} = X_1^{(ij)} + i \kappa_{lm} X_2^{[lm]}, \quad \kappa_{lm} \in \mathbb{R}, \tag{II.53}$$

where the operators $X_1^{(ij)}$ and $X_2^{[lm]}$ are defined as above. Note that there is no sum over repeated indices.

We have thus shown that every decoherence functional can be written as a weak convex combination of elementary decoherence functionals. I now want to show why these X_{d^e} must not be called ''pure decoherence functionals.''

We show that every elementary decoherence functional can be written as the sum of two decoherence functionals as follows. Due to the fact that the imaginary part X_2' of an operator $X' \in \mathscr{X}_{\mathscr{D}}$ associated with arbitrary decoherence functional $d' \in \mathscr{D}$ can be added to the operator X_{d^e} associated with an elementary decoherence functional $d^e \in \mathscr{X}_{\mathscr{D}}$ to produce a new decoherence functional, one can calculate that

$$X_{d^e} = \tfrac{1}{2}(X_{d^e} + iX_2') + \tfrac{1}{2}(X_{d^e} - iX_2'). \tag{II.54}$$

Both terms $(X_{d^e} + iX_2')$ and $(X_{d^e} - iX_2')$ in this expression are proper decoherence functionals, even though iX_2' in itself is *not* a decoherence functional. Thus, elementary decoherence functionals are not pure, but they still account for the simplest expansion of an arbitrary decoherence functional and this is all that is needed for the proof of the analog of Wigner's theorem.

We have now all the tools at hand to prove the following theorem.

III. AN ANALOG OF WIGNER'S THEOREM

Recall that, up to this point, we know about the following relation between the sets of ''homogeneous symmetries of a history quantum theory, ''homogeneous symmetries,'' and ''physical symmetries of a history quantum theory:''

$$\{\text{HSHQT}\} \cong \{\text{HS}\} \subset \{\text{PSHQT}\}. \tag{III.1}$$

We are now going to show that the sets {HS} and {PSHQT} are identical.

A. The theorem

Theorem: There exists a one-to-one correspondence between homogeneous symmetries and physical symmetries of history quantum theories. Thus each PSHQT is given by an operator $\hat{U} \otimes \hat{U}$ and induces a HSHQT; conversely, every one-to-one map τ: $\mathscr{R}(\mathscr{V}) \otimes \mathscr{R}(\mathscr{V}) \to \mathscr{R}(\mathscr{V}) \otimes \mathscr{R}(\mathscr{V})$ that preserves orthogonality between the rays and commutes with M can be implemented by a unitary operator $\hat{U} \otimes \hat{U}$ on $\mathscr{V} \otimes \mathscr{V}$, where $\hat{U}$ may be unitary or antiunitary.

Proof: We will first look for one-to-one maps which leave invariant the pairing between history propositions and decoherence functionals and map the set of rays into itself, *and then* restrict those transformations to homogeneous symmetries via the condition that they must map $\mathscr{X}_{\mathscr{D}}$ into itself.

We first consider the invariance requirement for the values of $d(\alpha,\beta)$. This has to hold true for *all* decoherence functionals. In particular, for the functionals $X_1^{(ij)}$ the relevant number is

$$2\,\mathrm{tr}_{\mathscr{V}\otimes\mathscr{V}}(\alpha \otimes \beta X_1^{(ij)}) = \mathrm{tr}_{\mathscr{V}}(\alpha P_{|e_i\rangle})\mathrm{tr}_{\mathscr{V}}(\alpha P_{|e_j\rangle}) + \mathrm{tr}_{\mathscr{V}}(\alpha P_{|e_j\rangle})\mathrm{tr}_{\mathscr{V}}(\beta P_{|e_i\rangle}), \tag{III.2}$$

for some ONB $\{|e_i\rangle\}$ of $\mathscr{V}$.

Recall that the requirement of the invariance of the imaginary part of a decoherence functional leads us to consider

$$2\,\mathrm{tr}_{\mathscr{V}\otimes\mathscr{V}}(\alpha \otimes \beta X_2^{[ij]}) = \mathrm{tr}_{\mathscr{V}}(\alpha P_{|b_i\rangle})\mathrm{tr}_{\mathscr{V}}(\beta P_{|b_j\rangle}) - \mathrm{tr}_{\mathscr{V}}(\alpha P_{|b_j\rangle})\mathrm{tr}_{\mathscr{V}}(\beta P_{|b_i\rangle}), \tag{III.3}$$

for some ONB $\{|b_i\rangle\}$ of $\mathscr{V}$.

Therefore, considering those decoherence functionals X_d for which $|b_i\rangle = |e_i\rangle$ for all $i \in \{1,2,\ldots,\dim \mathscr{V}\}$, and $\lambda_{ij} = \kappa_{ij}$ for all $i,j \in \{1,2,\ldots,\dim \mathscr{V}\}$, we see that the invariance requirement amounts to requiring that

$$\mathrm{tr}_{\mathscr{V}}(\alpha P_{|e_i\rangle})\mathrm{tr}_{\mathscr{V}}(\beta P_{|e_j\rangle}) \tag{III.4}$$

should remain invariant under the appropriate transformations. At first we take the case when $\alpha \otimes \beta \in \mathscr{R}(\mathscr{V}) \otimes \mathscr{R}(\mathscr{V})$. By Wigner's theorem, the transformations leaving (III.4) invariant are given by operators $\hat{U} \otimes \hat{V}$ whereby $\hat{U}$ and $\hat{V}$ are unitary or antiunitary operators on $\mathscr{V}$. Even though these transformations leave the value of $d(\alpha,\beta)$ invariant, they do not comply with the condition of mapping the set $\mathscr{X}_{\mathscr{D}}$ into itself.

To see this, recall that an element $X_d \in \mathscr{X}_{\mathscr{D}}$ is required to satisfy the condition $X_d^\dagger = MX_dM$, which is equivalent to $X_1^{(ij)} = MX_1^{(ij)}M$ and $X_2^{[ij]} = -MX_2^{[ij]}M$. Consider the following particular decoherence functional $X_1^{(ii)}$ under such a mapping:

$$\mathscr{X}_{\mathscr{D}} \ni P_{|e_i\rangle} \otimes P_{|e_i\rangle} \mapsto P^{\hat{U}}_{|e_i\rangle} \otimes P^{\hat{V}}_{|e_i\rangle}. \tag{III.5}$$

Since

$$M[P^{\hat{U}}_{|e_i\rangle} \otimes P^{\hat{V}}_{|e_i\rangle}]M \neq P^{\hat{U}}_{|e_i\rangle} \otimes P^{\hat{V}}_{|e_i\rangle}, \tag{III.6}$$

we see that its image under the map $\hat{U} \otimes \hat{V}$ does not belong to $\mathscr{X}_{\mathscr{D}}$. To comply with this requirement we need to require that $[\hat{U} \otimes \hat{V}, M] = 0$, i.e., consider only those operators of the form $\hat{U} \otimes \hat{U}$.

What is now left to show is that there can be no other transformations obeying conditions (II.17)–(II.19), even if we allow for arbitrary transformations $G = (G_0, G_0)$:

$$G: \mathscr{P}(\mathscr{V}) \otimes \mathscr{P}(\mathscr{V}) \to \mathscr{P}(\mathscr{V}) \otimes \mathscr{P}(\mathscr{V})$$

$$\alpha \otimes \beta \mapsto \alpha^{G_0} \otimes \beta^{G_0}. \tag{III.7}$$

The argument is much the same as in the standard quantum mechanical case: consider a transformation $G = (G_0, G_0)$ that maps a one-dimensional projector $\alpha \in \mathscr{P}(\mathscr{V})$ into $\alpha^{G_0} \in \mathscr{P}(\mathscr{V})$, an m-dimensional one, $m > 1$. Therefore,

$$\alpha \otimes \alpha \mapsto \alpha^{G_0} \otimes \alpha^{G_0}.$$

It is easy to see that there exists a $d \in \mathscr{D}$ such that $X_d = \alpha \otimes \alpha$ (see also Ref. 14). However, since $\mathrm{tr}_{\mathscr{V} \otimes \mathscr{V}}(\alpha^{G_0} \otimes \alpha^{G_0}) = m^2$, there exists no decoherence functional $d^{G_0} \in \mathscr{D}$ for which $\alpha^{G_0} \otimes \alpha^{G_0}$ is the associated operator $X_{d^{G_0}}$. This concludes the proof. □

B. Discussion

The result of the theorem shows that every PSHQT can be induced by a unitary or antiunitary operator $\hat{U}$ on $\mathscr{V}$ as follows:

$$\begin{aligned} \mathscr{UP}: \quad & \alpha \mapsto \tilde{\alpha} := \hat{U} \alpha \hat{U}^\dagger, \\ \mathscr{D}: \quad & X_d \mapsto X_{\tilde{d}} := \tilde{X}_d \equiv \hat{U} \otimes \hat{U} X_d \hat{U}^\dagger \otimes \hat{U}^\dagger. \end{aligned} \tag{III.8}$$

As a consequence of this transformation, the invariance

$$d(\alpha, \beta) = \tilde{d}(\tilde{\alpha}, \tilde{\beta}) \tag{III.9}$$

for all $d \in \mathscr{D}$ and all $\alpha, \beta \in P(\mathscr{V})$ follows by the property of the trace.

By looking at the definition for a PSHQT from which this theorem arose, it seems rather unnecessary to proceed via the use of elementary decoherence functionals. We could have started immediately by looking for all transformations obeying condition (II.17); then, restrict to those which map $\mathscr{X}_{\mathscr{D}}$ into itself. However, since it was not known to which extent $\mathscr{X}_{\mathscr{D}}$ can accommodate more general transformations G on $\mathscr{P}(\mathscr{V})$, it seems a sensible way to follow this hybrid path. In particular, we circumvented the problem of specifying all transformations that map $\mathscr{X}_{\mathscr{D}}$ into itself.

A central requirement in the proof of the theorem was the invariance of the value $d(\alpha, \beta) \in \mathbb{C}$ for all pairs $\alpha, \beta \in \mathscr{P}(\mathscr{V})$. A closer inspection reveals that the existence of *complex*-valued functionals makes it possible to reduce the invariance requirement to the form (III.4). However, it is

neither necessary to consider *complex*-valued functionals nor to require invariance for *all* pairs (α,β). We can investigate the possibility of softening the invariance requirement to hold only for the ''diagonal'' values of $d\in\mathscr{D}$, i.e., $d(\alpha,\alpha)$. Then we are led to the condition that

$$\mathrm{tr}_{\mathscr{T}\otimes\mathscr{T}}(\alpha\otimes\alpha X_1^{(ij)})=\mathrm{tr}_{\mathscr{T}}(\alpha P_{|e_i\rangle})\mathrm{tr}_{\mathscr{T}}(\alpha P_{|e_j\rangle}) \tag{III.10}$$

has to remain invariant. In this case we see that we will end up with the same transformations $\hat{U}\otimes\hat{U}$ on $\mathscr{T}\otimes\mathscr{T}$ as requiring $d(\alpha,\beta)$ to remain invariant for *all* pairs (α,β). This is due to the fact that restricting to projectors of the form $\alpha\otimes\alpha$ can be formulated with the aid of the same operator M which is used to formulate the defining property $X^\dagger=MXM$ for decoherence functionals. Therefore, the requirement on the diagonal part only is strong enough to enforce it onto the value of d on any pair (α,β).

The particular feature of physical symmetries of history quantum theories is their property of being implemented by a unitary or antiunitary operator $\hat{U}$ on $\mathscr{T}$. As a consequence, each partition of the unit operator in $\mathscr{T}$ into mutually orthogonal projectors, that is a set of projectors $\{\alpha_i\}$, such that

$$\{\alpha_i\}_{i=1}^{m\leqslant\dim\mathscr{T}},\quad \oplus_{i=1}^m\alpha_i=1, \tag{III.11}$$

is mapped into another partition of unity. In particular, the cardinality of this set is preserved. Now, much emphasis in the decoherent histories approach is placed on finding consistent sets of history propositions with respect to a particular decoherence functional $d\in\mathscr{D}$. In the formalism used here, consistent sets are naturally associated with particular partitions of unity,[14] namely those for which it holds that

$$d(\alpha_i,\alpha_j)=\delta_{ij}d(\alpha_i,\alpha_i)\quad\forall i,j\in\{1,2,\ldots,m\}. \tag{III.12}$$

We see therefore that a PSHQT will always map consistent sets into sets of the *same* cardinality. There has been some discussion[11,12] whether or not one should allow for transformations between consistent sets of different cardinality. We see that, at least in this context, this possibility is excluded if one agrees on the definition of PSHQT presented in this article.

C. Physical symmetries of history quantum mechanics

The main aim of this section is to show that the notion of ''physical equivalence,'' introduced in Ref. 4, is—when expressed in this formalism—a particular example of a physical symmetry of history quantum mechanics. It also serves the purpose of providing the explicit form of the decoherence functional for this theory.

Remember that, for standard quantum mechanics when looked at from the perspective of the history program, the space of history propositions $\alpha\in\mathscr{UP}$ is given by projectors $\alpha\in\mathscr{P}(\mathscr{V}_n)=\mathscr{P}(\otimes_{i=1}^n\mathscr{H}_{t_i})$. The particular decoherence functional is associated with an operator

$$X_{(H,\rho_{t_0},\rho_{t_f})}=\frac{1}{\mathrm{tr}_{\mathscr{H}}(\rho_{t_0}\rho_{t_f}(t_f))}\,\tilde{X}_{(H,\rho_{t_0},\rho_{t_f})} \tag{III.13}$$

on $\mathscr{V}_n\otimes\mathscr{V}_n$, where I also have inserted a final density operator at time t_f. When evaluated on homogeneous projectors $\alpha_h=\alpha_{t_1}\otimes\alpha_{t_2}\otimes\cdots\otimes\alpha_{t_n}$, the value of $d_{(H,\rho_{t_0},\rho_{t_f})}(\alpha_h,\beta_h)$ is given by

$$d_{(H,\rho_{t_0},\rho_{t_f})}(\alpha_h,\beta_h)=\frac{1}{\mathrm{tr}_{\mathscr{H}}(\rho_{t_0}\rho_{t_f}(t_f))}\,\mathrm{tr}_{\mathscr{V}\otimes\mathscr{V}}(\alpha_h\otimes\beta_h\widetilde{X}_{(H,\rho_{t_0},\rho_{t_f})})$$

$$=\frac{1}{\mathrm{tr}_{\mathscr{H}}(\rho_{t_0}\rho_{t_f}(t_f))}\,\mathrm{tr}_{\mathscr{H}}(\widetilde{C}^{\dagger}_{\alpha_h}\rho_{t_0}\widetilde{C}_{\beta_h}\rho_{t_f}(t_f)),\tag{III.14}$$

which coincides with the form of the decoherence functional usually employed in the histories approach. However, note once again that $d_{(H,\rho_{t_0},\rho_{t_f})}(\alpha,\beta)$ is defined *for all* $\alpha,\beta\in\mathscr{P}(\mathscr{V})$. By following the procedure outlined in Ref. 8, one shows that the operator $\widetilde{X}_{(H,\rho_{t_0},\rho_{t_f})}$ is given by

$$\begin{aligned}\widetilde{X}_{(H,\rho_{t_0},\rho_{t_f})}=&[U(t_1,t_0)^{\dagger}\rho_{t_0}U(t_1,t_0)\otimes U(t_2,t_1)^{\dagger}\otimes\cdots\otimes U(t_n,t_{n-1})^{\dagger}]\\&\otimes[U(t_2,t_1)\otimes U(t_3,t_2)\otimes\cdots\otimes U(t_n,t_{n-1})\otimes U(t_f,t_n)\rho_{t_f}U(t_f,t_n)^{\dagger}]\\&\times(R_{(n)}\otimes 1_{t_1}\otimes 1_{t_2}\otimes\cdots\otimes 1_{t_n})S_{(2n)}(R_{(n)}\otimes 1_{t_1}\otimes 1_{t_2}\otimes\cdots\otimes 1_{t_n}).\end{aligned}\tag{III.15}$$

The last three lines involve universal operators $R_{(n)}$ and $S_{(2n)}$ that arise by rewriting products of operators in terms of tensor-products.[8] Thus they are system independent. This operator is defined on $\mathscr{V}_n\otimes\mathscr{V}_n$ and encodes the initial and final density operators as well as the dynamical evolution in the form of the evolution operator $U(t_i,t_{i-1})$. This is the purest description of the content of the decoherence functional one can write down. It has a very transparent form.

Recall[4] that ''two triples $(\{C_\alpha\},H,\rho)$ and $(\{\widetilde{C}_\alpha\},\widetilde{H},\widetilde{\rho})$ are called 'physically equivalent' if there are fields and conjugate momenta $(\Phi(x),\pi(x))$ and $(\Phi(x),\widetilde{\pi}(x))$, respectively, in which the triples' histories, Hamiltonian, and initial condition take the same form.'' As an example, the explicit transformation $(\alpha_{t_i}(t_i)\mapsto V\alpha_{t_i}(t_i)V^{\dagger},H\mapsto VHV^{\dagger},\rho\mapsto V\rho V^{\dagger})$ for a fixed unitary operator V on $\mathscr{H}$ was shown to lead to physically equivalent triples.

Remark: In order not to use the same symbol twice, I used the notation V instead of U as in Ref. 4 for the unitary operator; in the context of history quantum mechanics $U(t_i,t_{i-1})$ already denotes the evolution operator.

First, notice that a transformation of the Heisenberg projection operators

$$\alpha_{t_i}(t_i)\mapsto V\alpha_{t_i}(t_i)V^{\dagger}\quad\forall i\in\{1,2,\ldots,n\}\tag{III.16}$$

is identical to the transformation

$$\alpha_{t_i}(t_i)\mapsto VU(t_i,t_0)V^{\dagger}[V\alpha_{t_i}V^{\dagger}]VU(t_i,t_0)V^{\dagger},\quad\forall i\in\{1,2,\ldots,n\}\tag{III.17}$$

that is a pair of transformations

$$\alpha_{t_i}\mapsto V\alpha_{t_i}V^{\dagger}\quad\forall i\in\{1,2,\ldots,n\};\quad H\mapsto VHV^{\dagger},\tag{III.18}$$

where the α_{t_i} denote the Schrödinger projection operators. This is important since in the formalism used here only a string $\alpha_h=\alpha_{t_1}\otimes\alpha_{t_2}\otimes\cdots\otimes\alpha_{t_n}$ of *Schrödinger projection operators* corresponds to a homogeneous history proposition $\alpha_h\in\mathscr{UP}=\mathscr{P}(\mathscr{V}_n)$. Now, defining the unitary operator $\hat{U}_V:=V\otimes V\otimes\cdots\otimes V$, n times, remembering that $\rho\mapsto V\rho V^{\dagger}$ and that the decoherence functional is given by Eq. (III.15), we see that the effect of this transformations on $\widetilde{X}_{(H,\rho_{t_0},\rho_{t_f})}$ is given by $\widetilde{X}_{(H,\rho_{t_0},\rho_{t_f})}\mapsto(\hat{U}_V\otimes\hat{U}_V)\widetilde{X}_{(H,\rho_{t_0},\rho_{t_f})}(\hat{U}_V^{\dagger}\otimes\hat{U}_V^{\dagger})$. Thus, this transformation between physically equivalent triples can be described as follows:

The transformation of the history propositions $\alpha_h \in \mathscr{P}(\mathscr{V}_n)$ as well as the operator $X_{(H,\rho_{t_0},\rho_{t_f})}$ by a unitary $\hat{U}_V \in B(\mathscr{V}_n)$ clearly leaves invariant the values of $d(\alpha_h,\beta_h)$ since

$$d(\alpha_h,\beta_h)=\mathrm{tr}_{\mathscr{V}\otimes\mathscr{V}}[(\hat{U}_V\alpha_h\hat{U}_V^\dagger\otimes\hat{U}_V\beta_h\hat{U}_V^\dagger)(\hat{U}_V\otimes\hat{U}_V X_{(H,\rho_{t_0},\rho_{t_f})}\hat{U}_V^\dagger\otimes\hat{U}_V^\dagger)], \qquad \text{(III.19)}$$

which is the definition of physical symmetry of a history quantum theory for which $\mathscr{UP}=P(\mathscr{V}_n)$. Note that, in general, not all unitary operators $\hat{U}$ on $\mathscr{V}_n$ need to be of the form $\hat{U}_V$ for a unitary operator V on the single-time Hilbert space $\mathscr{H}$.

IV. SUMMARY AND OUTLOOK

In this article we proposed a notion of a ''homogeneous symmetry'' (HS) and of a ''physical symmetry of a history quantum theory'' (PSHQT). We proved an analog of Wigner's theorem which states that there exists a one-to-one correspondence between both HS and PSHQT. It has been shown that each PSHQT can be induced by a unitary or antiunitary operator $\hat{U}$ on $\mathscr{V}$. History quantum theories that are related by a PSHQT are called ''physically equivalent'' and we showed explicitly in the case of history quantum mechanics how this notion encompasses the notion of physical equivalence introduced by Gell-Mann and Hartle in Ref. 4 in case one is dealing with a finite-dimensional, single-time Hilbert space $\mathscr{H}_t$ at a finite number of time points $(t_1,t_2,\ldots,t_n)$. An extension to infinite-dimensional $\mathscr{H}_t$ as well as to a continuous range of time points is clearly desirable since such spaces occur naturally in the context of *continuous histories*.[15,16]

In this article we also investigated the structure of the space of decoherence functionals; in particular, we defined the notion of an ''elementary decoherence functional'' in terms of which every decoherence functional can be expanded. We showed that these decoherence functionals are not pure, an observation that agrees with a result by Linden[13] that there exist no pure decoherence functionals. These elementary decoherence functionals were employed in order to perform some proofs but have *never* been assigned any status other than a technical one. In particular, we never calculated ''transition amplitudes between decoherence functionals,'' something that entirely contradicts the spirit of history quantum theories. Do these elementary decoherence functionals possess any physical interpretation?

While the definition of symmetry presented here has very convenient properties, it does not treat consistent sets of history propositions in any way preferred to other elements $\alpha \in \mathscr{P}(\mathscr{V})$. However, since these are the sets one ultimately wants to determine, it is reasonable to ask for a notion of symmetry which mirrors their importance. Reflecting a moment about the structure of consistent sets, one notices that this amounts to asking for an approach which places its emphasis on Boolean subalgebras of the space $\mathscr{P}(\mathscr{V})$. Via the use of the consistency conditions on the values of the decoherence functional, some of these Boolean algebras, namely the ones associated with consistent sets, are selected. Within each of these algebras classical reasoning without running into logical paradoxes is possible, whereas reasoning about elements belonging to different consistent sets leads, in general, to inconsistencies in the use of the values $d(\alpha,\alpha)$ of the decoherence functional as probabilities. The theory of ''Boolean manifolds,'' [17] which seem to be the most appropriate objects to describe history quantum theories,[7,18] allows one to describe the structure of $\mathscr{P}(\mathscr{V})$ in these terms and therefore, one is led to the problem of defining a transformation theory on Boolean manifolds. This is a task for future research.

By proving a classification theorem for decoherence functionals—an analog of Gleason's theorem in the context of history quantum theories—and the analog of Wigner's theorem presented here, we have laid the mathematical foundations for an approach to quantum theory from the point of view of the history program.

In history quantum theories the decoherence functional can be thought of as providing the ''dynamical'' content of the theory. In standard quantum mechanics, when investigated from the point of view of the history program, this is manifest in that the space of history propositions $\mathscr{UP}$

is given by Schrödinger picture projection operators and thus represents the ''kinematical''—as opposed to ''dynamical''—ingredient of the theory. In contrast, the decoherence functional (III.15) contains the evolution operator and the initial and final density operators and thus provides the ''dynamical'' specification of the model under investigation. In a companion paper[19] we will use the analog of Wigner's theorem presented in this article to define and to investigate the properties of ''symmetries of decoherence functionals.''

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Lie algebra cohomology and group structure of gauge theories

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We explicitly construct the adjoint operator of coboundary operator and obtain the Hodge decomposition theorem and the Poincaré duality for the Lie algebra cohomology of the infinite-dimensional gauge transformation group. We show that the adjoint of the coboundary operator can be identified with the BRST adjoint generator $Q^\dagger$ for the Lie algebra cohomology induced by BRST generator Q. We also point out an interesting duality relation—Poincaré duality—with respect to gauge anomalies and Wess–Zumino–Witten topological terms. We consider the consistent embedding of the BRST adjoint generator $Q^\dagger$ into the relativistic phase space and identify the noncovariant symmetry recently discovered in QED with the BRST adjoint Nöther charge $Q^\dagger$. © *1996 American Institute of Physics.*
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I. INTRODUCTION

The theory of gauge fields is based on symmetry principles and the hypothesis of locality of fields. The principle of local gauge invariance determines all the forms of the interactions and allows the geometrical description of the interactions.[1] However the quantization of gauge fields leads to difficulties due to the constraints arising from the gauge symmetry. These difficulties of the quantization of constrained systems can be circumvented by the extension of phase space including the anticommuting ghost variables.[2] In this approach, the original gauge symmetry is transformed into the so-called BRST symmetry in the extended phase space.[3,4] The BRST symmetry will determine all the forms of the interactions and the algebraic and topological properties of the fields in the quantum theory.[5]

The question that comes naturally to mind is how we recover the original gauge invariant space consisting of only physical degrees of freedom from the extended phase space with ghosts[4–6] and what is the physical spectrum with the group invariant structure. In order to study the algebraic and topological structures of gauge theories, we follow the point of view of Ref. 7 about the ghost fields and the BRST transformation. That is, we identify the ghost field with the Cartan–Maurer form on an infinite-dimensional Lie group G_∞—the group of gauge transformation—and the BRST generator Q with the coboundary operator s on its Lie algebra $\mathcal{G}$. Through these identifications, we have the natural framework to construct the Lie algebra cohomology induced by the BRST generator Q. This Lie algebra cohomology will be related to the group invariants of the configuration space of gauge fields and matter fields.

The organization of this paper is as follows. In Sec. II, we construct the cochain complex on $\mathcal{G}$ with values in a $\mathcal{G}$-module.[8–10] With the pairing between Lie algebra $\mathcal{G}$ and its dual space $\mathcal{G}^*$, we define a chain as an element of the dual space to the cochain and a dual operation s_* of s. We define a positive-definite inner product and construct an adjoint operator $s^\dagger$ of s using the Hodge duality operation. We obtain the Hodge decomposition theorem, Poincaré duality, and Künneth formula analogous to the de Rham cohomology.[11]

In Sec. III, we show that the adjoint of the coboundary operator can be identified with the BRST adjoint generator $Q^\dagger$ for the Lie algebra cohomology induced by BRST generator Q and

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each cohomology class on a polynomial space is characterized by the gauge invariant polynomials with a particular group invariant structure imposed on the cochain (or chain) space. We discuss the physical implications of the Lie algebra cohomology in the contexts of gauge anomaly and the effective action with the symmetry group G spontaneously broken to a subgroup H. The Lie algebra cohomology allows us algebraic and topological characterization of them and provides an interesting duality relation—Poincaré duality—between them. In Sec. IV, we apply this cohomology to QED and QCD. In order to consider the consistent embedding of the BRST adjoint generator $Q^\dagger$ into the relativistic phase space, we introduce the nonminimal sector of BRST generator.[4] Through this procedure, we find the BRST-like Nöther charge $Q^\dagger$ corresponding to the adjoint of the BRST generator Q, which generates a new kind of noncovariant symmetry in QED in Refs. 12 and 13. Section V contains discussion and some comments.

II. LIE ALGEBRA COHOMOLOGY

Let P be a principal bundle with a structure group G (a compact Lie group with the invariant inner product defined on its Lie algebra g) over a differentiable manifold M (flat Minkowski space or Euclidean space $\mathbf{R}^n$). The gauge transformation group G_∞—an automorphism of P—and its Lie algebra $\mathcal{G}$ can be identified with the set of C^∞-functions on M taking values in the structure group G and its Lie algebra g, respectively. One defines the dual spaces g^* of g and $\mathcal{G}^*$ of $\mathcal{G}$ as follows:[10]

$$\langle x,X\rangle=\sum_{a=1}^{dimG} X^a x_a, \quad \text{for } X\in g(\mathcal{G}),\ x\in g^*(\mathcal{G}^*). \tag{2.1}$$

The space–time dependence of the elements of G_∞, $\mathcal{G}$, and $\mathcal{G}^*$ will be suppressed unless otherwise explicitly indicated and an L^2-norm will be assumed in the inner product (2.1) between $\mathcal{G}$ and $\mathcal{G}^*$.[14] Using the pairing between Lie algebra g ($\mathcal{G}$) and its dual space g^* ($\mathcal{G}^*$), the coadjoint action of G (G_∞) on g^* ($\mathcal{G}^*$) is defined by

$$\langle X,Ad_g^* x\rangle=\langle Ad_{g^{-1}}X,x\rangle \quad \text{for } g\in G(G_\infty),\ x\in g^*(\mathcal{G}^*). \tag{2.2}$$

Consider a p-cochain w^p, an element of $C^p(\mathcal{G};R)$, where C^p is an antisymmetric p-linear map on $\mathcal{G}$ with values in a left $\mathcal{G}$-module R with the ring structure.[8–11] The space of cochains on $\mathcal{G}$ is the direct sum of the spaces of p-cochains:

$$C^*=\oplus_{p=0}^{dimG} C^p. \tag{2.3}$$

We introduce on C^* the operators $i(\vartheta)(x)$ and $\epsilon(\vartheta^*)(x)$ on a point $x\in M$ defined as follows:

$$i(\vartheta): C^p\to C^{p-1}, \quad \forall\,\vartheta\in\mathcal{G}$$

by

$$(i(\vartheta)(x)w^p)(\vartheta_1,\ldots,\vartheta_{p-1})(y)=w^p(\vartheta,\vartheta_1,\ldots,\vartheta_{p-1})(y)\,\delta(x-y), \quad w^p\in C^p; \tag{2.4}$$

and

$$\epsilon(\vartheta^*): C^p\to C^{p+1}, \quad \forall\,\vartheta^*\in\mathcal{G}^*$$

by

$$(\epsilon(\vartheta^*)(x)w^p)(\vartheta_1,\ldots,\vartheta_{p+1})(y)=\sum_{l=1}^{p+1}(-1)^{l+1}\langle\vartheta^*(x),\vartheta_l(y)\rangle w^p(\vartheta_1,\ldots,\hat{\vartheta}_l,\ldots,\vartheta_{p+1})(y), \tag{2.5}$$

where $\hat{}$ indicates omission. Denote by $\{\theta_a\}$, $a=1,\ldots,N\equiv dim G$, a basis of $\mathscr{G}$ and by $\{\theta^{*a}\}$ the basis of $\mathscr{G}^*$ such that

$$\langle\theta^{*a}(x),\theta_b(y)\rangle=\delta^a_b\delta(x-y). \tag{2.6}$$

Then straightforward calculations using the definitions (2.4) and (2.5) lead to the following relations:[10]

$$\{i(\theta_a),i(\theta_b)\}\equiv i(\theta_a)\circ i(\theta_b)+i(\theta_b)\circ i(\theta_a)=0,$$

$$\{\epsilon(\theta^{*a}),\epsilon(\theta^{*b})\}=0,$$

$$\{\epsilon(\theta^{*a}),i(\theta_b)\}=\langle\theta^{*a},\theta_b\rangle\mathbf{1}=\delta^a_b\mathbf{1}, \tag{2.7}$$

where $\circ$ denotes the map composition. Then, for example, the p-cochain $w^p\in C^p$ can be constructed using the operator $\epsilon(\theta^*)$ as follows:

$$w^p=\sum\ \frac{1}{p!}\underbrace{\epsilon(\theta^{*a})\circ\epsilon(\theta^{*b})\circ\cdots\circ\epsilon(\theta^{*c})}_{p\ \text{elements}}\phi^{(p)}_{ab\ldots c},\quad\text{where}\quad\phi^{(p)}_{ab\ldots c}\in R. \tag{2.8}$$

It must be kept in mind that the operations in Eqs. (2.4)–(2.8) must be understood as defined on a point $x\in M$ and we have omitted delta-function on M in Eq. (2.7). This shorthand notation will be used throughout this paper if it raises no confusion.

Let $s:C^p\to C^{p+1}$ be the coboundary operator, i.e., $s^2=0$ (Refs. 7–10) defined on $C^*(\mathscr{G};R)$ by

$$(sw^p)(\theta_1,\ldots,\theta_{p+1})(x)=\sum_{l=1}^{p+1}(-1)^{l+1}\theta_l\cdot w^p(\theta_1,\ldots,\hat{\theta}_l,\ldots,\theta_{p+1})(x)$$

$$+\sum_{l<n}(-1)^{l+n}w^p([\theta_l,\theta_n],\theta_1,\ldots,\hat{\theta}_l,\ldots,\hat{\theta}_n,\ldots,\theta_{p+1})(x), \tag{2.9}$$

where a dot means the linear transformation of R defined by an element of $\mathscr{G}$. The coboundary operator s can then be expressed in terms of $\epsilon(\theta^*)$ and $i(\theta)$ as follows:

$$s=\sum_{a=1}^{N}\int_M\theta_a\cdot\epsilon(\theta^{*a})-\sum_{a<b}^{N}\int\int_M i([\theta_a,\theta_b])\circ\epsilon(\theta^{*a})\circ\epsilon(\theta^{*b}), \tag{2.10}$$

where the integrations are defined over M.

Now we define a chain complex C as the dual space of the cochain complex C^* using the duality (2.1),[9,11] namely,

$$\langle,\rangle:C^p\times C_p\to R$$

by

$$(w^p,v_p)\mapsto\langle w^p,v_p\rangle=\int_{v_p} w^p,\quad w^p\in C^p \text{ and } v_p\in C_p, \tag{2.11}$$

where we set $\langle w^p,v_q\rangle=0$ if $p\neq q$, and C^* and C are augmented compleces, that is, $C^p=C_p=0$ for $p<0$.[8,11] The duality (2.11) allows us to define an operator $s_*:C_p(\mathcal{G}^*;R)\to C_{p-1}(\mathcal{G}^*;R)$ dual to s:

$$\langle sw^{p-1},v_p\rangle=\langle w^{p-1},s_*v_p\rangle,\quad w^{p-1}\in C^{p-1} \text{ and } v_p\in C_p. \tag{2.12}$$

Obviously, Eq. (2.12) shows us $s^2=0$ implies $s_*^2=0$. Thus we will identify s_* with the boundary operator acting on the chains $\{v_p\}$. Of course, the above procedures defining the chain complex is completely analogous to the ordinary homology theory.[8,9,11]

Let us introduce the Hodge star duality operation whose action on the cochain space is defined as follows:

$$*:C^p\to C^{N-p} \tag{2.13}$$

by

$$(*w^p)(\theta_{a_{p+1}},\ldots,\theta_{a_N})=\sum\frac{1}{p!}w^p(\theta_{b_1},\ldots,\theta_{b_p})\epsilon^{b_1\ldots b_p}{}_{a_{p+1}\ldots a_N}. \tag{2.14}$$

As the de Rham cohomology, we want to define the adjoint operator $s^\dagger$ of s (Refs. 9 and 15) under the new nondegenerate inner product defined by

$$(w_1,w_2)=\int_{u_N} w_1\wedge *w_2 \tag{2.15}$$

with the N-chain u_N satisfying $s_*u_N=0$. Then

$$(sw_1,w_2)=(w_1,s^\dagger w_2), \tag{2.16}$$

and $s^\dagger:C^p\to C^{p-1}$ is given by

$$s^\dagger=(-1)^{N\cdot p+N+1}*\circ s\circ *. \tag{2.17}$$

For convenience, we have taken the Cartan–Killing metric g_{ab} of the semi-simple Lie subalgebra as positive definite:

$$g_{ab}=-\tfrac{1}{2}c^l_{ad}c^d_{bl}=\delta_{ab},$$

where $[\theta_a(x),\theta_b(y)]=c^l_{ab}\theta_l(x)\delta(x-y)$. The operator $s^\dagger$ is nilpotent since $s^{\dagger 2}\propto *s^2*=0$. Using the definitions in Eqs. (2.17), (2.9), and (2.14), one can determine the action of $s^\dagger$ on a p-cochain w^p:

$$\begin{aligned}(s^\dagger w^p)(\theta_1,\ldots,\theta_{p-1})(x)=&-\sum_{l=p}^{N}\theta_l\cdot w^p(\theta_l,\theta_1,\ldots,\theta_{p-1})(x)\\&-\sum_{l=1}^{p-1}\sum_{a<b}(-1)^{l+1}c^l_{ab}w^p(\theta_a,\theta_b,\theta_1,\ldots,\hat{\theta}_l,\ldots,\theta_{p-1})(x).\end{aligned} \tag{2.18}$$

Similarly, the adjoint operator $s^\dagger$ can be expressed in terms of $\epsilon(\theta^*)$ and $i(\theta)$ as follows

$$s^{\dagger}=-\sum_{a=1}^{N}\int_{M}\theta_a\cdot i(\theta_a)+\sum_{a<b,c}^{N}\int_{M}c_{ab}^{c}\epsilon(\theta^{*c})\circ i(\theta_a)\circ i(\theta_b). \tag{2.19}$$

Let us define an operator $\delta\equiv s\circ s^{\dagger}+s^{\dagger}\circ s$ corresponding to the Laplacian, which clearly takes p-cochains back into p-cochains as

$$\delta: C^p\rightarrow C^p.$$

The straightforward calculation using Eq. (2.7) and the Jacobi identity for c_{ab}^{c} leads to the following expression for the Laplacian δ:

$$\delta=-\int_{M}\left(\sum\ \theta_a\cdot\theta_a+\sum\ c_{ab}^{c}\theta_a\cdot\epsilon(\theta^{*c})\circ i(\theta_b)+\frac{1}{2}\sum\ c_{ab}^{c}c_{ae}^{d}\epsilon(\theta^{*c})\circ i(\theta_b)\cdot\epsilon(\theta^{*d})\circ i(\theta_e)\right). \tag{2.20}$$

Considering the formal resemblance to the de Rham cohomology, it will be sufficient to state, without proof, only the important results which are necessary for later applications. For mathematical details of homology and cohomology theory, see Refs. 8, 9, and 11.

We define the p-th cohomology group of the Lie algebra $\mathcal{G}$ by the equivalence class of the p-cochains $C^p(\mathcal{G};R)$, that is, the kernel of s modulo its image:

$$H^p(\mathcal{G};R)\equiv Ker^p s/\mathrm{Im}^p s,\quad p=0,\ldots,N. \tag{2.21}$$

Then the nondegenerating inner product (2.11) provides a natural pairing between p-th cohomology group $H^p(\mathcal{G};R)$ and p-th homology group $H_p(\mathcal{G}^*;R)$,

$$H^p(\mathcal{G};R)\otimes H_p(\mathcal{G}^*;R)\rightarrow R,$$

so that *the inner product (2.11) establishes the duality of the vector spaces* $H^p(\mathcal{G};R)$ *and* $H_p(\mathcal{G}^*;R)$, the de Rham theorem.[11]

The following result is the direct consequence of the positive definiteness of the inner product (2.15):

The ''harmonic'' p-cochain $w^p\in Harm(\mathcal{G};R)$, *i.e.,* $\delta w^p=0$ *is satisfied if and only if it is exact, i.e.,* $sw^p=0$ *and co-exact, i.e.,* $s^{\dagger}w^p=0$.

The adjointness of the operator s and $s^{\dagger}$ under the nondegenerate inner product (2.15) and their nilpotency leads to the so-called Hodge decomposition theorem in the cochain space in a unique way:[9,15]

Any p-cochain w^p *can be uniquely decomposed as a sum of exact, co-exact, and harmonic forms, i.e.,*

$$w^p=\delta_H^p\oplus sw^{p-1}\oplus s^{\dagger}w^{p+1},\quad p=0,\ldots,N, \tag{2.22}$$

where δ_H^p is a harmonic p-cochain. The Hodge decomposition theorem (2.22) implies *the isomorphism between the p-th cohomology space* $H^p(\mathcal{G};R)$ *and the p-th harmonic space* $Harm^p(\mathcal{G};R)$.

The Hodge star operator $*$ maps $C^p\rightarrow C^{N-p}$ and commute with the Laplacian δ. Thus $*$ induces an isomorphism

$$Harm^p(\mathcal{G};R)\approx Harm^{N-p}(\mathcal{G};R).$$

Consequently, $H^{N-p}(\mathcal{G};R)$ *and* $H^p(\mathcal{G};R)$ *are isomorphic as vector spaces,*

$$H^{N-p}(\mathcal{G};R)\approx H^p(\mathcal{G};R). \tag{2.23}$$

This is just the Poincaré duality.[11]

If the Lie algebra $\mathcal{G}$ is a direct sum of semi-simple Lie algebras and/or Abelian $u(1)$ algebras, that is, $\mathcal{G}=\mathcal{G}_1\oplus\mathcal{G}_2$ and thus each of these algebras $\mathcal{G}_\alpha$ is an ideal of $\mathcal{G}$, then a total p-cochain C^p will be a sum of a tensor product of cochains corresponding to each Lie algebra $\mathcal{G}_\alpha$,

$$C^p=\oplus_{q+r=p}C_1^q\otimes C_2^r,$$

and $w^p\in C^p$ will be given by

$$w^p=\sum_{q=0}^{p} w_1^q\times w_2^{p-q},\quad w_1^q\in C_1^q,\quad w_2^{p-q}\in C_2^{p-q}.$$

The map $w^p\in C^p$ on $\mathcal{G}$ is defined by

$$w^p(\theta_1,\ldots,\theta_q;\xi_1,\ldots,\xi_{p-q})=w_1^q(\theta_1,\ldots,\theta_q)w_2^{p-q}(\xi_1,\ldots,\xi_{p-q}),\quad \theta_i\in\mathcal{G}_1,\quad \xi_i\in\mathcal{G}_2.$$

Then $H^p(\mathcal{G};R)$ can be decomposed into a sum of a product of each $H^q(\mathcal{G}_1;R)$ and $H^{p-q}(\mathcal{G}_2;R)$:

$$H^p(\mathcal{G};R)=\oplus_{q=0}^{p}[H^q(\mathcal{G}_1;R)\otimes H^{p-q}(\mathcal{G}_2;R)]. \tag{2.24}$$

This is known as the Künneth formula for a product space (in our case, a product group $G_1\otimes G_2$).[11,15]

III. GROUP STRUCTURE OF GAUGE THEORIES

In this section we will show that the group invariant structures of the gauge theory can be described by the Lie algebra cohomology induced by the BRST generator Q in the algebra of invariant polynomials on $\mathcal{G}$ with the generalized Poisson bracket,[4] taking the complete correspondence with the results of Sec. II. It will provide the algebraic and the topological characterization with respect to group invariant structures in the gauge theory and exhibit a very remarkable connection between the BRST symmetry and the differential and algebraic geometry.

Consider any physical system with gauge transformation group G_∞ and its compact Lie algebra $\mathcal{G}$ with N generators G_a, $a=1,\ldots,N$, satisfying the following Lie algebra:

$$[G_a(x),G_b(y)]=gf_{ab}^cG_c(x)\delta(x-y),\quad a,b,c=1,\ldots,N. \tag{3.1}$$

Corresponding to each generator, we introduce a ghost $\eta^a(x)$ and an antighost $\rho_a(x)$ which satisfy the following Poisson bracket relations:

$$\{\eta^a,\eta^b\}=\{\rho_a,\rho_b\}=0,\quad \{\eta^a,\rho_b\}=\delta_b^a. \tag{3.2}$$

Then we can construct the nilpotent BRST generator[4]

$$Q=\int_M G_a\eta^a-\frac{1}{2}g\int_M f_{ab}^c\rho_c\eta^a\eta^b, \tag{3.3}$$

and its nilpotency

$$Q^2=0 \tag{3.4}$$

follows from the Lie algebra (3.1) together with the Jacobi identity.

If one identifies the operators $\epsilon(\theta^{*a})(x)$ and $i(\theta_a)(x)$ in Sec. II with the ghost $\eta^a(x)$ and the antighost $\rho_a(x)$, respectively,[10] the expression (2.10) about the coboundary operator s exactly agrees with the BRST generator Q, where structure constants $c^l_{ab}=gf^l_{ab}$ and G_a is any representation for θ_a. Rewrite the BRST generator as

$$Q=\int_M\left(J_a\eta^a-\frac{1}{2}\,\tau_a\eta^a\right), \tag{3.5}$$

where $J_a=G_a+\tau_a$. $\tau_a=g\rho_m f^m_{al}\eta^l$ satisfies the same algebra as G_a and commutes with it. Then BRST s-transformation law with respect to a field $\mathscr{F}(x)$ is defined as follows,

$$s.\mathscr{F}(x)=[Q,.\mathscr{F}(x)\}, \tag{3.6}$$

where the symbol $[,\}$ is the generalized Poisson bracket. Thus the s-transformations with respect to the ghost field η and ρ by Q are

$$s\,\eta^a=-\tfrac{1}{2}\,gf^a_{bc}\eta^b\eta^c,\quad s\rho_a=J_a. \tag{3.7}$$

According to Ref. 7, we identify the ghost field $\eta(x)$ with a left-invariant Cartan–Maurer form on the group G_∞. With this interpretation of the ghost field $\eta(x)$, the first equation in Eq. (3.7) is just the Cartan–Maurer equation with respect to ''exterior derivative'' s for forms $\eta(x)$ on G_∞. It is also obvious that the adjoint operator $s^\dagger$ of s introduced in Sec. II can be constructed in terms of η and ρ. We define the corresponding generator by $Q^\dagger$ and it is given by

$$Q^\dagger=-\int_M\left(G^a\rho_a-\frac{1}{2}\,gf^{ab}_c\eta^c\rho_a\rho_b\right)=-\int_M\left(J^a\rho_a-\frac{1}{2}\,\tau^a\rho_a\right). \tag{3.8}$$

One can easily check this generator is also nilpotent, i.e., $Q^{\dagger 2}=0$ as stated in Sec. II.

The generator $Q^\dagger$ first appeared in Ref. 16 to find the gauge invariant interactions in string theory and then in Ref. 17 to construct the BRST complex and the cohomology of compact Lie algebra. The Lie algebra cohomology in this paper is quite different from the BRST cohomology constructed in Ref. 18, so we use the nomenclature, Lie algebra cohomology, in order to avoid confusion with the BRST cohomology since these two cohomologies have been often confused in the literature. In fact, the cohomology of Ref. 17 corresponds to the Lie algebra cohomology in this paper as long as the space–time dependences of the Lie group G_∞ and the Lie algebra $\mathscr{G}$ are fixed. However, it is necessary to consider the infinite-dimensional Lie group and Lie algebra in order that the BRST generator may be viewed as the coboundary operator for the Lie algebra cohomology.[7]

The $s^\dagger$-transformation with respect to a field $\mathscr{F}(x)$ is defined by

$$s^\dagger.\mathscr{F}(x)=[Q^\dagger,.\mathscr{F}(x)\}. \tag{3.9}$$

Then the $s^\dagger$-transformations with respect to the ghost fields η and ρ are

$$s^\dagger\eta^a=-J^a,\quad s^\dagger\rho_a=\tfrac{1}{2}\,gf^{bc}_a\rho_b\rho_c. \tag{3.10}$$

The above equations show that one can identify the antighost ρ_a with the Cartan–Maurer form with respect to the ''exterior derivative'' $s^\dagger$ as well.

Since Q and $Q^\dagger$ are nilpotent, it follows that Q and $Q^\dagger$ invariant by G_∞, i.e.,

$$[Q,J_a]=0,\quad [Q^\dagger,J_a]=0. \tag{3.11}$$

One finds that Q and $Q^\dagger$ satisfy the supersymmetrylike algebra that closes into a Laplacian generator Δ,

$$\{Q,Q^\dagger\}=-\Delta, \quad [\Delta,Q]=0, \quad [\Delta,Q^\dagger]=0, \tag{3.12}$$

where the Laplacian Δ can be computed in terms of the Casimir generators[16]

$$\Delta=\frac{1}{2}\int_M (J^a J_a+G^a G_a). \tag{3.13}$$

The operator δ: $C^p\to C^p$ in Sec. II corresponds to this generator and it has exactly the same expression as Δ if it is rewritten in terms of Casimir operators.

Following the same scheme as those in Refs. 19 and 20, we construct the cochains on $\mathcal{G}$ spanned by the polynomial $\omega_{(p)}=Tr\,\eta^p$, where $\eta=\eta^a T_a$ and T_a is a generator of g. That is, a p-dimensional cochain $C^p(\mathcal{G};R)$ corresponding to Eq. (2.8) is spanned by elements of the space of $w^p=\wedge^r\omega_{(p_r)}\cdot\phi(\Sigma p_r=p)$, where ϕ is an element of R, i.e., $\mathcal{G}$-module of symmetric polynomials on $\mathcal{G}$ without (anti-)ghosts. Then $\omega_{(p)}=0$ if p is even and $\omega_{(p)}$ is a ''closed'' p-form - a p-cocycle, i.e., $s\omega_{(p)}=0$ by Eq. (3.7). Notice, for semi-simple groups G, $\omega_{(1)}=0$.[15] Let us reexpress the p-cochain w^p as the following form:

$$w^p=\sum \frac{1}{p!}\,\eta^{a_1}\eta^{a_2}\cdots\eta^{a_p}\cdot\phi^{(p)}_{a_1a_2\cdots a_p}. \tag{3.14}$$

Note that the results such as Hodge decomposition theorem, Poincaré duality, and Künneth formula in Sec. II will be reproduced here in the same manner as well. In Sec. II, we stated the isomorphism between the p-th cohomology space $H^p(\mathcal{G};R)$ and the p-th harmonic polynomial space $Harm^p(\mathcal{G};R)$. Therefore, the BRST invariant polynomial space can be summarized as the *harmonic* polynomial space $\delta w^p=0$, whose solutions are represented by

$$[G_a,w^p]=0, \tag{3.15}$$

and

$$[\tau_a,w^p]=[g\rho_m f^{\ m}_{al}\eta^l,w^p]=0. \tag{3.16}$$

The second condition reads, in components,

$$f^{\ m}_{a[a_1}\phi^{(p)}_{a_2\cdots a_p]m}=0, \tag{3.17}$$

where the square bracket denotes complete antisymmetrization over the enclosed indices.[17] The first condition (3.15) imposes the G-invariance—G-singlet—on the polynomial ($\mathcal{G}$-module) and the second one imposes very important constraints about the group invariant structures. For the $p=0$ and $p=N$, the conditions (3.15) and (3.16) are always satisfied trivially as long as they are associated with the G-invariant polynomials, which leads to the conclusion that the zeroth and the N-th cohomology spaces require only the space of G-singlet. For semi-simple groups G, there are no solutions satisfying the condition (3.16) for $p=1,2,4$ since there is no cohomology basis $\wedge^r\omega_{(p_r)}$ to be closed and for $p=N-1$, $N-2$, $N-4$ by Poincaré duality (2.23), so that their cohomologies $H^p(\mathcal{G};R)$ vanish. Note that the gauge group SU(2) is cohomologically trivial so that the group invariant structure in the SU(2) gauge theory is similar to electrodynamics. In this respect, we would like to refer to the interesting analysis[21] which arrives at the same conclusion under the different approach. If one $U(1)$ factor is present (for example, $SU(2)\times U(1)$, $U(2)$, etc.),

then $H^1(\mathcal{G};R)$ is non-trivial since $\omega_{(1)}$ is nonzero.[15,19] For $G=\mathrm{SU}(N)$, $N\geqslant 3$, there exist nontrivial cohomologies $H^3(\mathcal{G};R)$ and $H^5(\mathcal{G};R)$ whenever the symmetric polynomials $\phi^{(3)}$ and $\phi^{(5)}$ are proportional to the structure constants as follows, respectively:

$$\phi^{(3)}_{abc}=f_{abc}\cdot\phi, \quad \phi^{(5)}_{abcde}=d_{amn}f_{mbc}f_{nde}\cdot\phi, \tag{3.18}$$

where $d_{abc}=1/2TrT_a\{T_b,T_c\}$ and ϕ is any G-singlet. These follow directly from the expansion (3.14)[7,22] or Eq. (3.17) with the Jacobi identity.

It is worth mentioning, for $G=\mathrm{SU}(3)$, the nontrivial cohomologies $H^3(\mathcal{G};R)$ and $H^5(\mathcal{G};R)$ are related with each other by Poincaré duality (2.23). The solution of the descent equations corresponding to the Wess–Zumino consistency conditions in gauge theories[23] shows that the polynomials $\omega_{(3)}$ and $\omega_{(5)}$ corresponding to the third and the fifth cohomologies (3.18) respectively generate the two dimensional and the four dimensional gauge anomaly[7,19] (see also recent analysis[24] by Sorella, where the cohomology basis $\omega_{(3)}$ and $\omega_{(5)}$ have a fundamental importance on solving the descent equations). Thus, from the results of these literatures, we can conclude that two and four dimensional $SU(3)$ anomalies are related to each other by the Poincaré duality; in other words, the gauge anomaly in two dimensional QCD implies the existence of the anomaly in four dimensional QCD as long as d-cohomology is trivial.[7,19,20] This observation is also applied to the problem yielding the general G-invariant effective action[25] with the symmetry group G spontaneously broken to the subgroup H since the G-invariant effective actions for homogeneous spaces G/H can be understood as the Lie algebra cohomology problem of the manifold G/H. For example, in the case for $\mathrm{SU}(3)\times\mathrm{SU}(3)$ spontaneously broken to the subgroup SU(3), the two dimensional Poincaré-dual of the Wess–Zumino–Witten term in four dimensional theory is the Goldstone–Wilczek topological current.[26]

IV. COHOMOLOGY IN QED AND QCD

In this section, we want to see whether it is possible to find a corresponding adjoint generator $Q^\dagger$ of the nilpotent Nöther charge Q in relativistic theories and what the role of the adjoint $Q^\dagger$ in the Lagrangian formulation is. That is, the solution we want to find out is how to embed the adjoint $Q^\dagger$ of Q into the relativistic phase space. In order to construct the relativistic phase space, it is then necessary to incorporate the Lagrange multipliers and their conjugate momenta and the associated ghost pairs into the phase space.[4,27] In that case we will have the two kinds of first-class constraints composed of Gauss constraints and gauge-fixing constraints in the extended phase space. Thus the consistent embedding of the BRST adjoint generator $Q^\dagger$ into the relativistic phase space means that the $Q^\dagger$ is the adjoint generator with respect to the total Lie algebra $\mathcal{G}$ composed of a direct sum of two ideals $\mathcal{G}_1$ and $\mathcal{G}_2$ corresponding to the Gauss and the gauge-fixing constraint algebras, respectively, and it can be realized as a Nöther charge in configuration space.

First, consider the BRST (and anti-BRST) invariant effective QED Lagrangian. (Our BRST treatments are parallel with those of Baulieu's paper.[5])

$$\begin{aligned}\mathcal{L}_{\mathrm{eff}}&=-\tfrac{1}{4}F_{\mu\nu}F^{\mu\nu}+\overline{\psi}(i\gamma^\mu D_\mu-m)\psi-\tfrac{1}{2}\,\overline{ss}(A_\mu^2+\alpha\overline{cc})\\&=-\frac{1}{4}F_{\mu\nu}F^{\mu\nu}+\overline{\psi}(i\gamma^\mu D_\mu-m)\psi+A_\mu\partial^\mu b+\frac{\alpha}{2}\,b^2-\partial_\mu\overline{c}\partial^\mu c,\end{aligned} \tag{4.1}$$

where $D_\mu=\partial_\mu+ieA_\mu$ is the covariant derivative with the metric $g_{\mu\nu}=(1,-1,-1,-1)$. The explicit BRST transformations are

$$sA_\mu=\partial_\mu c, \quad sc=0,$$

$$s\overline{c}=b, \quad sb=0,$$

$$s\psi = -iec\psi. \tag{4.2}$$

We introduced an auxiliary field b to achieve off-shell nilpotency of the BRST (and the anti-BRST) transformation. Then the nilpotent Nöther charge generated by the BRST symmetry reads as

$$Q = \int d^3x\{(\partial_i F^{io} - J_0)c + b\dot{c}\}, \tag{4.3}$$

where J_0 is a charge density defined by

$$J_0 = e\overline{\psi}\gamma_0\psi. \tag{4.4}$$

The constraint functions G^i consist of two commuting groups, $G^i = (\Phi, b)$, $i = 1,2$, where $\Phi = \partial_i F^{io} - J_0$ is a Gauss law constraint in the theory and b is the momentum canonically conjugate to the Lagrange multiplier A_0 so that it generates a gauge transformation, δA_0. Thus adding the nonminimal sector in the BRST generator, the Lie algebra $\mathcal{G}$ is composed of a direct sum of two Abelian ideals $\mathcal{G}_1$ and $\mathcal{G}_2$ corresponding to the $u(1)$ generators Φ and b, respectively. In a similar fashion, let the ghost fields split as follows:

$$\eta^i = (c, \pi_{\bar{c}} = \dot{c}), \quad \rho^i = (\pi_c = -\dot{\bar{c}}, c). \tag{4.5}$$

Then the BRST charge Q with respect to the total Lie algebra $\mathcal{G}$ can be written as a linear combination of each $u(1)$ subalgebra sectors

$$Q = \int d^3x G^i \alpha_{ij} \eta^j, \tag{4.6}$$

where

$$\alpha_{ij} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

Since the constraints in the relativistic phase space for Abelian gauge theories impartially generate $u(1)$ Lie algebras and the Künneth formula (2.24) shows $H(\mathcal{G};R)$ is the product of each $H(\mathcal{G}_1;R)$ and $H(\mathcal{G}_2;R)$, we expect that the adjoint $Q^\dagger$ corresponding to the total Lie algebra $\mathcal{G}$ similarly should be a linear combination of each subalgebra sector. Therefore, according to Eq. (3.8), one can guess the form of the generator $Q^\dagger$ must be the following: $Q^\dagger = -\int d^3x G^i \beta_{ij} \rho^j$. Note that we have a degree of freedom to the extent of multiplicative factor in defining the BRST generator Q or its adjoint generator $Q^\dagger$ for a given Lie algebra $\mathcal{G}$ as long as it does not affect the nilpotency of Q or $Q^\dagger$. Using this degree of freedom either in the Lie algebra $\mathcal{G}_2$ or in the $\mathcal{G}_1$ sector in defining the adjoint generator $Q^\dagger$, we take the following choices for the matrix β_{ij} which will allow the well-defined canonical mass dimension for $Q^\dagger$:

$$\beta_{ij} = \begin{pmatrix} 1 & 0 \\ 0 & -\nabla^2 \end{pmatrix} \text{or} \begin{pmatrix} -\nabla^{-2} & 0 \\ 0 & 1 \end{pmatrix}. \tag{4.7}$$

These choices make the BRST adjoint $Q^\dagger$ the symmetry generator of the Lagrangian (4.1) and so complete the consistent embedding of $Q^\dagger$ into the relativistic phase space.

Alternatively, in the case of the Abelian gauge theory, we can also obtain the BRST adjoint generator $Q^\dagger$ through an appropriate redefinition about the constraint functions G^i and the ghost fields (4.5) as follows:

$$G^i=(\Phi,\sqrt{-\nabla^2}b),\quad \eta^i=\left(c,\frac{1}{\sqrt{-\nabla^2}}\dot{c}\right),\quad \rho^i=(-\overrightarrow{\dot{c}},\sqrt{-\nabla^2}\overline{c}),$$

$$G^i=\left(\frac{1}{\sqrt{-\nabla^2}}\Phi,b\right),\quad \eta^i=(\sqrt{-\nabla^2}c,\dot{c}),\quad \rho^i=\left(-\frac{1}{\sqrt{-\nabla^2}}\overrightarrow{\dot{c}},c\right), \tag{4.8}$$

and $\beta_{ij}=\alpha_{ij}$ since the redefinition does not affect their algebra.

Then the adjoint generator $Q^\dagger$ can take the local expression in Ref. 13 or the nonlocal one in Ref. 12. The explicit form of the BRST adjoint generator $Q^\dagger$ for the local type is

$$Q^\dagger=\int d^3x\{(\partial_i F^{io}-J_0)\overrightarrow{\dot{c}}+b\nabla^2\overline{c}\}. \tag{4.9}$$

Thus the explicit transformations defined by (3.9) are that

$$s^\dagger A_0=-\nabla^2\overline{c},\quad s^\dagger A_1=-\partial_0\partial_i\overline{c},$$

$$s^\dagger c=(\partial_i F^{io}-J_0),\quad s^\dagger\overline{c}=0,$$

$$s^\dagger\psi=ie\overrightarrow{c}\psi,\quad s^\dagger b=0. \tag{4.10}$$

In Ref. 13, it has been shown that this noncovariant transformation is a symmetry of the Lagrangian (4.1) and there also exists the same kind of symmetry in the Landau–Ginzburg and the Chern–Simons theories and the Nöther charge $Q^\dagger$ imposes strong constraint on state space. As discussed in Ref. 13, the symmetry generated by $Q^\dagger$ is realized in quite a different way compared to the BRST symmetry: while the gauge-fixing term in the effective QED Lagrangian (4.1), i.e., $A_\mu\partial^\mu b+(\alpha/2)b^2\rightarrow-(1/2\alpha)(\partial_\mu A^\mu)^2$, remains invariant under the transformation (4.10), the variation from the ghost term is canceled up to the total derivative by the variation from the original gauge-invariant classical Lagrangian which remains invariant under the BRST transformation (4.2). These differences in the way of realizing the symmetries imply that the BRST adjoint symmetry can give the different superselection sector from the BRST symmetry[28] (as it is also seen from the Hodge decomposition theorem (2.22) which is a canonical decomposition into a direct sum of linearly independent subspaces) unlike the recent comment.[29]

If we use, instead, the matrix

$$\beta_{ij}=\begin{pmatrix}\frac{1}{-\nabla^2} & 0\\ 0 & 1\end{pmatrix}$$

in Eq. (4.9), we will obtain the nonlocal symmetry in Ref. 12. Of course, in this case, we must impose the good boundary conditions on fields. But there is no reason to introduce the nonlocality and it seems unnatural since the generator $Q^\dagger$ must be the adjoint of the generator Q of the local gauge transformation.

In non-Abelian gauge theory, the BRST charge Q incorporated with a compactifiable gauge fixing (e.g., the covariant or the Coulomb gauge) can generate a well-defined gauge transformation only on the interior of a bounded region, whose boundary is so-called the Gribov horizon, because of the existence of the Gribov copies.[30] The adjoint generator in the configuration space can be understood as the generator of transformation consistent with the gauge fixing condition.[12,13] Thus, in the configuration space, there may not exist the globally well-defined expression of the adjoint generator $Q^\dagger$ of non-Abelian gauge theory compatible with the gauge fixing condition unlike QED

on account of the topological obstructions such as the Gribov ambiguity. But it does not imply that there can not exist the local expression of $Q^{\dagger}$, because the difficulty posed by the Gribov ambiguity can be avoided[31] by finding a local cross section on a finite local covering and using the Faddeev–Popov trick locally. Nevertheless, it seems a nontrivial problem to find the solution for the consistent embedding into the relativistic phase space for the non-Abelian gauge theory such as QCD. This problem remains for a future work. We want to focus our attention on the construction of su(3) Lie algebra cohomology in QCD.

Consider the BRST (and anti-BRST) invariant effective QCD Lagrangian:

$$\begin{aligned}\mathscr{L}_{\text{eff}} &= -\tfrac{1}{4} F^a_{\mu\nu} F^{a\mu\nu} + \overline{\Psi}(i\gamma^\mu D_\mu - M)\Psi - \tfrac{1}{2}\,\overline{ss}(A^a_\mu A^{a\mu} + \alpha \overline{C^a} C^a) \\ &= -\frac{1}{4} F^2_{\mu\nu} + \overline{\Psi}(i\gamma^\mu D_\mu - M)\Psi + A_\mu \partial^\mu B + \frac{\alpha}{2} B^2 + \frac{\alpha}{2} gB[C,\overline{C}] \\ &\quad - \partial_\mu \overline{C} D^\mu C + \frac{\alpha}{2} g^2 [\overline{C}, C]^2, \end{aligned} \tag{4.11}$$

where quark fields Ψ are taken to transform according to the fundamental $SU(3)$ representation, the Yang–Mills vector potential A_μ, a pair of anticommuting ghosts C,C and the auxiliary field B take values in the adjoint representation of a SU(3) Lie group. The QCD Lagrangian (4.11) is invariant with respect to the following BRST transformations:[5]

$$\begin{aligned} &sA_\mu = D_\mu C, \quad sC = -\frac{g}{2}[C,C], \\ &s\overline{C} = B, \quad sB = 0, \\ &s\Psi = -gC\Psi. \end{aligned} \tag{4.12}$$

D_μ defines the covariant derivatives of $SU(3)$ Yang–Mills symmetry group. The corresponding conserved nilpotent BRST generator is given by

$$Q = \int d^3x \left\{ (D_i F^{io} - J_0 + g[\overleftarrow{\overline{C}}, C])^a C^a + B^a (D_0 C)^a - \frac{1}{2} g[\overleftarrow{\overline{C}}, C]^a C^a \right\}, \tag{4.13}$$

where J^a_0 is a matter color charge density defind by

$$J^a_0 = -ig\overline{\Psi}\gamma_0 T^a \Psi. \tag{4.14}$$

The constraint functions G^A are composed of two commuting groups, $G^A = (\Phi^a, B^a)$, where $\Phi^a = (D_i F^{io} - J_0)^a$ is the original Gauss-law constraints in the theory generating $su(3)$ Lie algebra:

$$[\Phi_a, \Phi_b] = g f^c_{ab} \Phi_c, \tag{4.15}$$

and B^a is the momenta canonically conjugate to the Lagrange multiplier A^a_0 and generates $u(1)$ Lie algebras. In the similar fashion as QED, one can split the ghosts as follows:

$$\eta^A = (C^a, \Pi^a_C = (D_0 C)^a), \quad \rho^A = (\Pi^a_C = -\overleftarrow{\overline{C^a}}, \overline{C^a}). \tag{4.16}$$

Note that $s\Pi^a_{\bar{C}} = 0$, so that we can identify the ghost $\Pi^a_{\bar{C}}$ with the Cartan–Maurer form on $U(1)$ group. Of course, the BRST generator Q in Eq. (4.13) is exactly the same form of Eq. (3.3). Let us rewrite the BRST generator Q as the form of Eq. (3.5),

$$Q = \int d^3x \left\{ J_a C^a + B_a \Pi^a_{\bar{C}} - \frac{1}{2}\, \tau_a C^a \right\}, \tag{4.17}$$

where the generator J^a and the generator of the ghost representation τ_a (Ref. 16) are given by

$$J^a = (D_i F^{io} - J_0 + g[\overleftarrow{\bar{C}}, C])^a = \Phi^a + \tau^a, \quad \tau^a = g[\overleftarrow{\bar{C}}, C]^a. \tag{4.18}$$

The generators J_a and τ_a satisfy the same $su(3)$ algebra:

$$[J_a, J_b] = g f^{\ c}_{ab} J_c, \quad [\tau_a, \tau_b] = g f^c_{ab} \tau_c. \tag{4.19}$$

The nontriviality of the principal fiber bundle does not admit a global section which would provide a global gauge fixing. The nonexistence of a global section of the bundle entails that it is not possible to continuously fix the gauge globally. Then the Gribov ambiguity is a consequence of the fact that there exists a topological obstruction to the existence of a global gauge fixing condition.[31] This means that a global gauge fixing must contain discontinuities coming from the global geometry of the gauge theory. Thus the BRST charge (4.13) or (4.17) will also contain these discontinuities as long as it is not restricted to a fundamental modular region because it is involved with the global gauge fixing.

Since the two groups of the constraint functions $G^A = (\Phi^a, B^a)$ commute with each other, the total Lie algebra $\mathcal{G}$ including the nonminimal sectors B^a is composed of the $su(3)$ non-Abelian ideal and the eight $u(1)$ Abelian ideals:

$$\mathcal{G} = \oplus su(3) \oplus \oplus_{\alpha=1}^{8} u(1)_\alpha. \tag{4.20}$$

In order to construct only the cohomology of the color $su(3)$ Lie algebra for the reasons explained above, we drop the Abelian sectors from the BRST generator Q through the direct restriction on the cochain space (3.14), in other words, considering only $su(3)$ subcochain complex. Note that this restriction to a subalgebra sector of the cochain space is always possible in terms of the Künneth formula (2.24). The BRST adjoint $Q^\dagger$ defined on the cochain $C^*(su(3);R)$ is equal to

$$Q^\dagger = -\int d^3x \left\{ J^a \Pi^a_C - \frac{1}{2}\, \tau^a \Pi^a_C \right\}. \tag{4.21}$$

Then the Laplacian Δ of the $su(3)$ subalgebra sector can be represented in terms of the generators J_a and the original constraints Φ_a,

$$\Delta = \tfrac{1}{2} \int d^3x \{ J^a J_a + \Phi^a \Phi_a \}, \tag{4.22}$$

which is equal to the expression given by Eq. (3.13) for $su(3)$ cohomology. Thus the harmonic polynomials of the $su(3)$ algebra sector must satisfy the following conditions,

$$[\Phi^a, w^p] = [(D_i F^{io} - J_0)^a, w^p] = 0, \quad a = 1, \ldots, 8, \tag{4.23}$$

and

$$[\tau^a, w^p] = [g f^a_{bc} \overleftarrow{\bar{C}^b} C^c, w^p] = 0, \quad a = 1, \ldots, 8. \tag{4.24}$$

From the arguments in Sec. III, we see that the solutions of Eqs. (4.23) and (4.24) exist trivially for $p=0$ and $p=8$ as long as they are given by the gauge invariant polynomials because they are singlets under the adjoint representation of the su(3) Lie algebra. But the cohomologies $H^p(\mathrm{su}(3);R)$ for $p=1$, 2, 4, 6, and 7 vanish. For $p=3$ and 5, there always exist non-trivial cohomologies $H^3(\mathrm{su}(3);R)$ and $H^5(\mathrm{su}(3);R)$ whose structures are given by Eq. (3.18) and they are related to each other by the Poincaré duality (2.23). Since the Lie algebra cohomology proves the nontrivial property of group invariant structures, the nonvanishing Lie algebra cohomologies $H^p(\mathrm{su}(3);R)$ can be related to the gauge invariants in $SU(3)$ gauge theory. It remains to investigate the deep relation between the gauge invariant configuration of gauge and matter fields in the space–time and the Lie algebra cohomology.

V. DISCUSSION

We have constructed the Lie algebra cohomology of the group of gauge transformation and obtained the Hodge decomposition theorem and the Poincaré duality. As long as a Lie algebra has a nondegenerate Cartan–Killing metric so that the underlying manifold is orientable, we can always define a unique (up to a multiplicative factor) adjoint of the coboundary operator under a nondegenerate inner product using a Hodge duality. However, for Lie algebras such as the Virasoro algebra for which no Cartan–Killing metric exists, the adjoint can not be unique. Indeed, for the Virasoro algebra, the adjoint of BRST generator defined by Niemi[32] is different from ours and that in Ref. 16.

We also considered the consistent extension of the Lie algebra cohomology into the relativistic phase space in order to obtain the Lagrangian formulation. In order to do that, we extended the Lie algebra by including the nonminimal sector of BRST generator and defined the adjoint generator with respect to the total Lie algebras corresponding to the constraint algebras in the extended phase space. We have pointed out that the generator $Q^\dagger$ constructed through this procedure corresponds to the adjoint of the BRST generator Q generating local gauge transformation and generates the noncovariant local or nonlocal symmetry in QED in Refs. 12 and 13 and there is no reason to introduce the nonlocality necessarily.

We have remarked that, in non-Abelian gauge theory, there may not exist the globally well-defined expression of the adjoint generator compatible with the gauge fixing condition due to the Gribov ambiguity being a topological obstruction coming from the global geometry of the gauge theory. But, as explained in Sec. IV, the adjoint $Q^\dagger$ in the non-Abelian gauge theory can exist locally (or perturbatively), so that it can generate new symmetry at least locally (or perturbatively). Then it will be interesting to study the role of the symmetry generated by the generator $Q^\dagger$ and the Ward identity of this symmetry in the local (or perturbative) sense and we think they are the important topics to need further study, including the relation between the Lie algebra cohomology and the global geometry of the gauge theory.

Note that the Lie algebra cohomology constructed here is quite different from the BRST cohomology in Refs. 6, 18, and 33. In the two cohomologies, the role of ghost fields is quite different and each inner product to obtain Hodge theory is defined by the definitely different schemes. It can be shown[34] that there is no paired singlet in the BRST cohomology so that higher cohomologies with nonzero ghost number vanish as long as the asymptotic completeness is assumed. Therefore the ghost number characterizing cohomology classes in this paper has different meaning from the ghost number of state space. The distinction between the BRST cohomology and the Lie algebra cohomology will be further clarified.[34]

In QCD, there are nontrivial cohomologies $H^p(\mathrm{su}(3);R)$ for $p=0$, 8 and $p=3$, 5 and they are, respectively, related to each other by the Poincaré duality. Since the Lie algebra cohomology proves the nontrivial property of group invariant structures, the nonvanishing Lie algebra cohomologies $H^p(\mathrm{su}(3);R)$ may be deeply related to the colorless combination of $SU(3)$ color charges which satisfy the su(3) Lie algebra. Then it will be very interesting to investigate the relation between the color confinement and the su(3) cohomology.

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On q-deformed supersymmetric classical mechanical models

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Based on the idea of quantum groups and para-Grassmannian variables, we present a generalization of supersymmetric classical mechanics with a deformation parameter $q=\exp(2\pi i/k)$ dealing with the $k=3$ case. The coordinates of the q-superspace are a commuting parameter t and a para-Grassmannian variable θ, where $\theta^3=0$. The generator and covariant derivative are obtained, as well as the action for some possible superfields. © *1996 American Institute of Physics.* [S0022-2488(96)00812-2]

I. INTRODUCTION

In the last few years, quasi triangular Hopf algebras or quantum groups[1–3] have attracted alot of attention from physicists. One of the most interesting features is that such structures can be related to underlying symmetries on spaces where the coordinates are noncommutative.[4]

It has been shown that the creation and annihilation operators of the q-deformed harmonic oscillator,[5]

$$aa^{\dagger}-qa^{\dagger}a=q^{-N}, \tag{1}$$

possess a classical limit where these operators can be understood as coordinates obeying[6]

$$\theta^k=0, \tag{2}$$

where k is an integer, and the q-factor of the deformation is a prime root of unity, $q^k=1$. In general, the properties of these coordinates are generalizations of the associated with Grassmannian variables. Promoting these coordinates to functions of a (nondeformed) parameter t, it was shown that it is possible to write down an action for such fields that, when added to the action of a commuting field, has a symmetry resembling supersymmetry,[7] and it has also been how to functional integrate on a heterotic quantum field theory.[8] The aim of this article is to show a way to understand the transformations on such fields and the action invariances, as resulting from a superspace formulation of a classical mechanical model where its coordinates are the para-Grassmann variables (a q-superspace) and noncommuting fields.

In the next section we briefly review para-Grassmann variables and also how we construct coordinates and actions from them. Section III is devoted to the construction of the q-superspace, transformations between its coordinates, and the induced transformations on the q-superfields defined on it. Invariant quadratic actions are constructed in Sec IV, in particular for a free particle and the harmonic oscillator. We leave some final comments to the last section.

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II. PARA-GRASSMANNIAN VARIABLES AND THEIR RELATION TO QUERMIONIC COORDINATES

We start this section by introducing a para-Grassmannian variable θ and its derivative, $\partial/\partial\theta \equiv \partial_\theta$ obeying[9]

$$\theta^k = 0, \quad \partial_\theta{}^k = 0, \tag{3}$$

for a positive integer k.

If we demand that the action of ∂_θ on θ^n is proportional to θ^{n-1}, it turns out that it becomes necessary to deform the Leibnitz rule to be

$$\partial_\theta(ab) = (\partial_\theta a)b + g(a)(\partial_\theta b), \tag{4}$$

where a and b are arbitrary polynomials in θ, and $g(a)$ is an automorphism of the algebra satisfying

$$g(\alpha a + \beta b) = \alpha g(a) + \beta g(b), \quad g(ab) = g(a)g(b), \tag{5}$$

where α and β are c-numbers.

Choosing $a = \theta$ in (4), we see that ∂_θ and θ must obey a q-deformed commutation (q-commutation) relation

$$[\partial_\theta, \theta]_q \equiv \partial_\theta\theta - q\,\theta\partial_\theta = 1, \tag{6}$$

implying for θ the automorphism

$$g(\theta) = q\,\theta. \tag{7}$$

This derivative, however, is not unique. Indeed, we could change the power 1 in Eq. (6) by any other integer, thus for each value of k one can define $k-1$ different derivatives. For the specific case $k=3$, one may also define another derivative δ_θ (Ref. 10) that q-commutes with θ as

$$[\delta_\theta, \theta]_{q^2} \equiv \delta_\theta\theta - q^2\,\theta\delta_\theta = 1, \tag{8}$$

and its Leibnitz rule differs from Eq. (4) by changing $g(a)$ to $g(g(a))$. These two derivatives have the following q-commutation relation

$$\partial_\theta\delta_\theta - q\,\delta_\theta\partial_\theta = 1.$$

As in the Grassmannian case, it is not possible to define the integral over θ as the inverse of the derivative. However, if we impose translation invariance and homogenity for the integral, it must be of the form

$$\int d\theta\ \theta^n \alpha\,\delta_{n,k-1}. \tag{9}$$

It is interesting to notice that, for $k=2$ and $q=-1$, Eq. (1) becomes the usual anticommutator, consistent with Eqs. (3) and (6), which are the conditions for Grassmannian variables. Taking $k\to\infty$, Eq. (1) becomes the usual commutator. The meaning of this limit in Eq. (3) is that, if we Taylor expand a function of these variables, it will become a series [obviously, if $\theta^k=0$, k finite, a Taylor expansion will be a polynomial of degree $(k-1)$] being

$$f = a_0 + \theta a_1 + \theta^2 a_2 + \cdots + \theta^{k-1} a_{k-1}, \tag{10}$$

where we can promote the functions of a (commuting) parameter t.

Let us recall that in the Grassmannian case we have two different coordinates: one that behaves like θ (a fermionic coordinate), and another that behaves like θ^0, a bosonic (commuting) coordinate. In the para-Grassmannian case, we will have k different types of coordinates, each one corresponding to a power of θ, and again θ^0 being a commuting one. We call $\psi^{(i)}(t)$ the q-fermionic generalization of the coordinates or, simply, the quermionic coordinates, and its label (i) indicates the sector to which it belongs.

In a recent work,[7] it was emphasized that two quermions of different sectors obey the q-commutation relation

$$\psi^{(i)}\psi^{(j)}=q_{(i,j)}\psi^{(j)}\psi^{(i)}, \tag{11}$$

where the parameters $q_{(i,j)}$ are simply powers of q, $q^k=1$.

The particular case $k=3$ was taken, and an action which extends the supersymmetric point particle through the use of these generalized fields was constructed. This generalized particle was described by the coordinates $(x(t),\psi^{(1)}(t),\psi^{(2)}(t))$, in the same way as a supersymmetric point particle is described by the coordinates $(x(t),\psi(t))$. The shown action involving the quermions was given by

$$S=\int dt\left(\frac{1}{2}\dot{x}^2-qC^{(s)^2}\dot{\psi}^{(2)}\psi^{(1)}\right), \tag{12}$$

with the mass equal to one. The second term in (12) resembles the classical fermionic equation of motion. The cocycle-type factor $C^{(s)^2}$ was required because the product of two objects of different sectors, $A^{(r)}B^{(s)}$, must behave like an object of the sector $(r+s)$ mod 3. In that work, it emphasized the necessity of the factor Cq-superfield, paying the price of writing a suitable ''algebra'' of this factors. For instance, the cocycle-type factor $C^{(s)}$ that could be seen as a sector-counter had a relation

$$C^{(s)}A^{(i)}=q^iA^{(i)}C^{(s)}, \tag{13}$$

and adding the choice $[\psi^{(1)},\psi^{(2)}]_q=0$, which takes all the fields as real, the second term in the action equation (12) was left real and a zeroth sector representative.

Another interesting feature to recall was the transformation (the variations of a field, from now on, will be written as Δ to one not to be confused with the derivative δ)

$$\Delta x=qC^{(s)}\epsilon^{(1)}\psi^{(2)},\quad \Delta\psi^{(1)}=q^2C^{(s)^2}\epsilon^{(1)}\dot{x},\quad \Delta\psi^{(2)}=\pm q\epsilon^{(1)}\psi^{(1)}, \tag{14}$$

on the action (12) reaching

$$\Delta S=\pm\int dt\,\frac{d}{dt}\,(\epsilon^{(1)}\psi^{(1)^2}), \tag{15}$$

where $[\epsilon^{(1)},\psi^{(1)}]_q=[\psi^{(2)},\epsilon^{(1)}]_q=0$ was used. Such a transformation is similar to a supersymmetric one: the parameter $\epsilon^{(1)}$ is a noncommuting one, the action transforms as a total derivative, and one of the fields, $\psi^{(1)}$, transforms as a total derivative, which can be taken as indicating that $\psi^{(1)}$ is the highest term in a θ-expansion of some superfield. One could also write transformations among the fields with a parameter belonging to the sector two. However, it can be shown that this transformation is not a symmetry of the action (12).[7]

III. THE q-SUPERSPACE AND q-SUPERFIELDS

We begin to construct a q-superspace formulation that will recover the structure concerning the quermionic coordinates presented in the last section. As previously stated, we will consider in detail only the $k=3$ case, which represents the nilpotency and produces an interesting expression $1+q+q^2=0$. It emphasizes that the q and q^2 cases have no crucial difference. Some of the ideas discussed here and in the next section have been discussed also in Refs. 11 and 12 and more recently in Ref. 13 (this interesting work appeared when we had just finished this paper).

The q-superspace coordinates are $(t;\theta)$, where t is a c-number to be identified with time and θ is a para-Grassmannian variable obeying $\theta^3=0$, and both are taken as real parameters.

Let us now introduce transformations between these coordinates that are translations on the q-superspace. We write them as

$$\theta' = \theta + \varepsilon, \quad t' = t + q^C \theta^2 \varepsilon, \tag{16}$$

where ε is an infinitesimal constant in the same sector as θ and C can assume the values 1,2,3. Clearly, the exponent 3 will give us a trivial factor restricting then our set of possible choices. The translation in q-superspace fixes the mass dimensions of θ and ε to be $-\frac{1}{3}$. Although the translation term in t does not commute with the infinitesimal parameter ε, it still belongs to the same sector as t. [Remember that we met this issue when we wrote down the action for the quermionic components, Eq. (12), and we introduced the cocycle-like factor $C^{(s)}$ to correct the statistics.] We will say that two terms are homogeneous if both belong to the same sector. Defining the q-commutator to be

$$[A,B]_q \equiv AB - qBA, \tag{17}$$

we choose

$$[\theta,\varepsilon]_{q^{2C}} = 0. \tag{18}$$

It is after determining these q-commutation relations that we set the q factors in (16) to preserve the reality condition for the coordinates. We could choose q^C instead of q^{2C} in (18) (i.e., take $[\varepsilon,\theta]_{q^{2C}} = 0$). With this choice we necessarily have to change $q \leftrightarrow q^2$ in Eq. (16).

After introducing the q-superspace (t,θ), our next step is to write down a function of these variables. As in the supersymmetric case, let us expand this function in a Taylor series on θ. This expansion is a polynomial of degree 2 [for the generic case $\theta^k=0$, the polynomial goes up to the order $(k-1)$],

$$X(t;\theta) = x(t) + q^{B_2}\theta\psi^{(2)}(t) + q^{2B_1}\theta^2\psi^{(1)}(t). \tag{19}$$

The coordinate $x(t)$ is a commuting function, the $\psi^{(i)}(t)$ are the q-supersymmetric partners of the coordinate $x(t)$, and their dimensions are $[\psi^{(j)}] = -j/3$. We take their quommutators to be

$$[\psi^{(1)},\psi^{(2)}]_{q^A}=0, \quad [\varepsilon,\psi^{(j)}]_{q^{D_j}}=0, \quad [\theta,\psi^{(j)}]_{q^{B_j}}=0, \tag{20}$$

where the last expression guarantees that X is real and the others complete a deformed algebra.

The infinitesimal coordinate transformations (16) induce a variation on the q-superfield $X(t,\theta)$ of the form

$$X(t',\theta') - X(t,\theta) = \Delta X = \varepsilon Q X. \tag{21}$$

We can get the realization of the q-supersymmetric generator transformation, Q, by Taylor expanding the lhs of this equation. Choosing the factors to keep the reality condition we have

$$X(\theta',t')-X(\theta,t)=\varepsilon\frac{\partial X}{\partial\theta}+q^{2C}\varepsilon\theta^2\frac{\partial X}{\partial t}. \tag{22}$$

With this expansion, and using Eq. (16), Q becomes

$$Q=q^{2C}\theta^2\frac{\partial}{\partial t}+\frac{\partial}{\partial\theta}. \tag{23}$$

We notice that the generator is in the θ^2 sector, and its canonical dimension is $[Q]=\frac{1}{3}$. A straightforward calculation shows that $Q^3=-\partial_t$. This means that the q-supersymmetric transformations are the cubic roots of time translations.

Explicitly computing the rhs of (21), we obtain the X variation as

$$\Delta X=q^{B_2}\varepsilon\psi^{(2)}-q^{2B_1+2+C}\theta\varepsilon\psi^{(1)}+q^{2C}\theta^2\varepsilon\hat{x}. \tag{24}$$

Bearing in mind the reality condition we find from ΔX and X itself some relations among the q exponents. Finally we reach

$$2C=2B_2=B_1,\quad D_2=D_1+1. \tag{25}$$

The above relations do not fix completely the q-commutators among the variables [see (20)] we are considering, since we still have at our disposal three free coefficients. We may choose the variables $2C=D_2=1$ and $A=2$, thus fixing all the other ones (remember that for the $k=3$ nilpotency we have only two relevant choices for the exponents). With such a choice, the q-superspace translation becomes

$$\theta'=\theta+\varepsilon,\quad t'=t+q^2\theta^2\varepsilon, \tag{26}$$

while the q-su becomes

$$X(t)=x+q^2\theta\psi^{(2)}+q^2\theta^2\psi^{(1)}. \tag{27}$$

The q-SUSY generator,

$$Q=q\theta^2\partial_t+\partial_\theta, \tag{28}$$

yields the transformation

$$\Delta X=q\varepsilon\theta^2\dot{x}+q^2\varepsilon\psi^{(2)}-q\varepsilon\theta\psi^{(1)}, \tag{29}$$

or in components

$$\Delta x=q^2\varepsilon\psi^{(2)},\quad \Delta\psi^{(1)}=\varepsilon\dot{x},\quad \Delta\psi^{(2)}=q\varepsilon\psi^{(1)}. \tag{30}$$

Moreover, they have the q-commutators

$$\varepsilon\theta=q^2\theta\varepsilon,\quad \theta\psi^{(j)}=q^j\psi^{(j)}\theta,\quad \varepsilon\psi^{(j)}=q^j\psi^{(j)}\varepsilon, \tag{31}$$

which let on the same structure as the one present in Sec. II. This structure allows us to take the q-commutation relation between the two quermionic coordinates, which read

$$\psi^{(1)}\psi^{(2)}=q^2\psi^{(2)}\psi^{(1)}. \tag{32}$$

Having written down the q-superspace transformations and the variations on the q-superfield, let us now construct a q-covariant derivative, D, that is, a differential operator that obeys

$$[D,Q]_q=0, \tag{33}$$

$$D(\Delta X)=\Delta(DX). \tag{34}$$

We could try for D the same structure that appears in the q-SUSY generator, i.e., to take $D=q^{\alpha}\theta^2\partial_t+aq^{\beta}\partial_\theta$, $(\alpha,\beta=1,2,3;\ a\in C)$. However, it turns out not to be possible to find an operator with this structure and q-commuting with Q. The only operator that obeys (34) is Q itself, but it obviously does not obey (33).

To construct the coordinates of level 3 permit us to introduce two differential operators, ∂_θ and δ_θ. Using the second one it is possible to show that the operator

$$D=\theta^2\partial_t+q\,\delta_\theta \tag{35}$$

satisfies the conditions (33) and (34).

As in the supersymmetric case, the component fields can be defined by projecting the superfield on different sectors, using the covariant derivatives on $\theta=0$:

$$X|_{\theta=0}=x, \quad DX|_{\theta=0}=\psi^{(2)}, \quad D^2X|_{\theta=0}=-\psi^{(1)}. \tag{36}$$

From now on, we will neglect the subscript $\theta=0$.

We also notice some relations between different powers of D and Q that will become useful later:

$$D.|=q^2Q.|, \quad D^2.|=qQ^2.|, \quad D^3.|=-\partial_t.|. \tag{37}$$

Besides the above-defined bosonic superfield, we can also construct sectors one and two superfields. Their θ expansion can be taken to be

$$\Lambda^{(1)}=\lambda^{(1)}+\theta A+q\,\theta^2\lambda^{(2)} \tag{38}$$

and

$$\Xi^{(2)}(t)=\xi^{(2)}+q\,\theta\xi^{(1)}+\theta^2F, \tag{39}$$

where the superscripts indicate the sectors to which the fields belongs, and A and F are bosonic fields.

The dimension of the q-superfield $\Xi^{(2)}$ is taken to be $\frac{2}{3}$, its bosonic component F being dimensionless and, as we will see later, behaving as an auxiliary field. We cannot, however, take the dimension of the q-superfield $\Lambda^{(1)}$ to be $\frac{1}{3}$, since this would imply a negative dimension for the component field $\lambda^{(2)}$. Thus take its dimension to be $\frac{4}{3}$. This, however, will produce different equations of motion for its quermionic components, as we will see in the next section.

We assume that the fields $\xi^{(j)}$ have the same behavior as $\psi^{(j)}$ with respect to the q-commutations relations with each other, with θ and with ϵ.

IV. EXAMPLES OF SUPERACTIONS

In this section, we are going to make a general discussion about simply quadratic actions that are functions of the q-superfields introduced in the previous section and give some examples of them.

The action for a generic superfield Φ must be of the form

$$S=\int dtd\theta\mathscr{L}(\Phi,\dot{\Phi},D\Phi,D^2\Phi), \tag{40}$$

where $\mathscr{P}$ is a polynomial in Φ and its derivatives. $\mathscr{P}$ must behave like θ^2, belonging to the sector two (since $\int d\theta = \partial_\theta^2$, and S is scalar), and since the measure has mass dimension $-\frac{1}{3}$ and S is dimensionless, its dimension must be $\frac{1}{3}$.

By comparing the expression for the covariant derivative and the θ-integration, we notice the rule

$$\int d\theta = q^2 D^2|. \tag{41}$$

Let us now perform a transformation on the action

$$\Delta S = \int dt\ d\theta\ \Delta\mathscr{P}(\Phi, \dot{\Phi}, D\Phi, D^2\Phi), \tag{42}$$

since the Jacobian is one, which can be seen by the t independence of the θ translation. Since $\mathscr{P}$ is a superfield, its variation is of the form of Eq. (21). Using this and Eq. (41), we arrive at the conclusion

$$\Delta S = -q\varepsilon \int dt\ \alpha_t \mathscr{P}. \tag{43}$$

and the transformations Eq. (16) generates symmetries of the action.

Let us now write an action of the q-superfields X, $\Lambda^{(1)}$, and $\Xi^{(2)}$ defined in Sec. III, and compute their equations of motion. We begin with the bosonic superfield X. Its quadratic action is

$$S_X = -\frac{m}{2} \int dt\ d\theta\ q^2 (D^2 X)(D^2 X), \tag{44}$$

where m is a commuting mass parameter. By explicit computation of its θ integral, or by use of Eq. (41), this action can be written down in components as

$$S_X = m \int dt \left(\frac{1}{2} \dot{x}^2 - 2q \dot{\psi}^{(2)} \psi^{(1)} \right), \tag{45}$$

where the difference with the Sec. I action is due to the different initial superactions in these cases.

Although the variational calculus of the quermionic coordinates presents several difficulties to overcome (for instance, how to do the variation with respect to a quermion), it is clear that the equation of motion arising from the above Lagrangian is, up to multiplicative factors $D\dot{X} = 0$, giving in components $\ddot{x} = \psi^{(j)} = 0$ $(j = 1,2)$. Computing its q-supersymmetric variation, we obtain

$$\Delta S^X = q\varepsilon \int dt\ \frac{\partial \psi^{(1)^2}}{\partial t}. \tag{46}$$

We notice that the action given by Eq. (44), its variation Eq. (46), and the variation of the component fields Eq. (30) are, up to factors, equal to Eqs. (12), (15), and (14), respectively, recalling that the presence of such cocycle-type factors was because the q-commutation homogeneity assumption had been used. Thus we see that the q-superfield X describes the dynamics of a free particle partners.

The quadratic action for the q-superfield $\Lambda^{(1)}$ is

$$S_\Lambda = -\frac{m}{2} \int dt d\theta (\dot{\Lambda}^{(1)})^2. \tag{47}$$

By convenience the mass parameter was taken to be the same as in the X action. In components, the action turns out to be

$$S_\Lambda = \frac{m}{2} \int dt(\dot{A}^2 + 2q\dot{\lambda}^{(2)}\dot{\lambda}^{(1)}) \tag{48}$$

It is interesting to notice that the equation of motion for $\Lambda^{(1)}$, obtained from its action, $\ddot{\Lambda}^{(1)}=0$, gives in component $\ddot{A}=\ddot{\lambda}^{(i)}=0$. Thus this q-superfield also represents a free particle, but its quermionic partners obey an equation of motion that is of second order in the time derivative, whereas in the case of q-superfield X it is of first order. The q-supersymmetric variation of the S_Λ is

$$\Delta S_\Lambda = \varepsilon \int dt \frac{\partial(\dot{\Lambda}^{(1)})^2}{\partial t}. \tag{49}$$

We now consider the quadratic action for the q-superfield $\Xi^{(2)}$. It is

$$S_\Xi = m \int dt\ d\theta (D\Xi^{(2)})^2. \tag{50}$$

In component fields, the action reads

$$S_\Xi = m \int dt[2q\dot{\xi}^{(2)}\xi^{(1)} + F^2]. \tag{51}$$

The equation of motion for $\Xi^{(2)}$ is $D^2\Xi^{(2)}=0$, giving $F=\dot{\xi}^{(j)}=0$, meaning, as it was anticipated, that the bosonic coordinate F is an auxiliary one. The variation of S_Ξ is

$$\Delta S_\Xi = -\varepsilon \int dt\ \frac{\alpha \xi^{(1)^2}}{\partial t}. \tag{52}$$

The superfields X and $\Xi^{(2)}$ can have a quadratic action with a mixed term

$$S_{X\Xi} = m\omega \int dt d\theta q^2 X \Xi^{(2)}, l \tag{53}$$

where ω has a mass^{-1} dimension. In components we write this action as

$$S_{X\Xi} = m\omega \int dt(Fx + q^2\psi^{(1)}\xi^{(2)} + q\psi^{(2)}\xi^{(1)}). \tag{54}$$

Summing up the actions (44), (50), and (54), $S_{HO}=S_X+S_\Xi+S_{X\Xi}$, and its bosonic part is

$$S_{HO} = \int dtm\left(\frac{1}{2}\dot{x}^2 + \frac{1}{2}F^2 + \omega F x\right). \tag{55}$$

Computing the equation of motion of the auxiliary field F and reintroducing it in the action, it becomes

$$S_x = \int dt\left[\frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega x\right], \tag{56}$$

which is the action for the harmonic oscillator.

V. CONCLUSIONS

In this article, we presented a generalization of some supersymmetric classical mechanical models where the superspace has a noncommuting coordinate nilpotent of order 3, and the commutation relations among the several objects of the model are deformed by powers of a parameter q. Translations on the q-superspace induce transformations on the fields, and the operational realization of the supersymmetric generator is obtained by a suitable Taylor expansion. The covariant derivative was also introduced, in which we used a second kind of partial para-Grassmannian derivative. In spite of the supersymmetric structure similarity, we are facing a slightly different situation. In fact, because of the presence of two derivatives, such as the forward and the backward one, it resembles a lattice approach. In a recent work,[13] the authors showed the roles played by the covariant derivative D and the symmetry generator Q, present in this work, are the left and right action of G_3 group.

After introducing superfields belonging to different sectors, we were able to construct quadratic actions for each one. These actions are, up to total derivatives, invariant under the q-supersymmetric transformations. Using a naive approach, it is possible to extract from these actions the equations of motion since there is no, up to now, well-defined differential calculus on these quermionic coordinates. We intend to discuss this subject in a forthcoming publication. We also showed that imposing the ''on-shell'' constraint to the auxiliary fields, it is possible to get the harmonic oscillator as a bosonic sector of a simple suitable linear combination of the actions.

It should also be interesting to study this formulation from a field theoretical point of view, in particular in the $(2+1)$-dimensional case. We might also try to understand if such fields are representations of some q-deformed algebra, either a q-Poincaré or a q-Clifford one.

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Inverse problem in nonstationary multidimensional medium

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The problem of a scalar wave propagation from the point impulsive source in the layer of a nonstationary multidimensional medium is considered. The boundary problem for the wave equation is reformulated in the problem with the initial condition using the invariant imbedding method. The integral-differential inverse procedures of the various orders were obtained from the imbedding equations using the singularities method. The order of inverse procedure is defined by the degree of a polynomial in the analytical representation of the medium characteristic near the layer boundary. It was shown that the coefficients of the polynomial are calculated with the help of the differential characteristics of the point impulsive source in the inhomogeneous medium. The cause and character of the multidimensional inverse problem overdefiniteness are considered. The application of the proposed procedure for a statistical problem is discussed. © *1996 American Institute of Physics.* [S0022-2488(96)04311-3]

I. INTRODUCTION

For the study of direct and inverse wave problems in the regular and random media, the imbedding method[1,2] has been developed which allows simultaneously the creation of the strict inverse procedures[3–5] and the employment of the effective statistical approaches using the Markov process approximation.[1,2,6] This is different from the integral equation method[7,8] and the deferential method,[9,10] both of which have some difficulties pertaining to the application in statistical theory.[1,2]

The nature of most of the media examined in optics, acoustics, plasma physics, and radio science is described by mathematical models with spatial and time inhomogeneous refractive index. The inverse procedure obtained by the imbedding method was considered for multidimensional stationary[11,12] and one-dimensional nonstationary[13] media. The subject of the present paper is to extend the previous results on common case for the promotion of the inverse problem research in remote sensing based on the statistical approach,[14] which is a strict alternative to the line radiation transfer theory, which uses the usual transfer equation[15] and does not account for the statistical effects.[16,17]

In the present paper, the mathematical model accepted in statistical theory[1,2] is employed. The boundary-value wave problem for this model is reformulated in the problem with the initial condition and the imbedding equation is written. The inverse procedure is obtained from the imbedding equation by a singularities method.[5,18]

The main step of the inverse procedure is the ''layer stripping'' process,[11,12] which can be realized in the different versions. In conclusion, the extension of the obtained procedure on statistical problems and the derivation way of the evolution equations for the statistical characteristics of backscattering are discussed.

II. THE STATEMENT OF THE PROBLEM

The scalar wave propagation in the layer of inhomogeneous nonstationary medium that occupies the part of the space $L_0 \leqslant x \leqslant L$ will be considered. The wave is created by the point impulsive source on the boundary of the layer $x = L$ and is described by the equation[15]

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$$\left[\frac{\partial^2(1+\varepsilon(x,\boldsymbol{\rho},t))}{\partial t^2}-c^2\Delta\right]G(x,\boldsymbol{\rho},t;L,\boldsymbol{\rho}_0,t_0)=\delta(x-L)\,\delta(\boldsymbol{\rho}-\boldsymbol{\rho}_0)\,\delta(t-t_0), \tag{1}$$

where $\varepsilon(x,\boldsymbol{\rho},t)$ is the continuous and smooth characteristic of the scattering medium in the layer $L_0\leqslant x\leqslant L$, $\boldsymbol{\rho}$ and $\boldsymbol{\rho}_0$ are the vectors in the plane of constant x, c is the signal velocity in the homogeneous medium outside of the layer, where $\varepsilon=0$, Δ is Laplacian, and the Dirac δ-functions are in the right part of this equation.

It will be assumed that $-1<\varepsilon(x,\boldsymbol{\rho},t)<\mu$ and all first partial derivatives of $\varepsilon(x,\boldsymbol{\rho},t)$ are bounded. However, when some variants of the inverse procedure will be discussed in Sec. VII, the existence and bound of higher derivatives will be supposed.

Equation (1) is used in the different areas of physics, for example, in optics, acoustics, radio science, etc., where the wave propagation is considered in the medium with a transient impedance or refractive index. The wave equation is taken here in a simpler form to show an approach, which may be extended to the waves of a more complex nature.

The solution of the mixed (initial and boundary values) problem for Eq. (1) will be analyzed. There are the discontinuities of $\varepsilon(x,\boldsymbol{\rho},t)$ on two planes $x=L_0$ and $x=L$, which divide the space into three areas. It will be supposed that G and $\partial G/\partial x$ are continuous on the boundaries of the layer and there are only the going away waves outside of the layer. These six boundary values for three space areas are enough to solve the above-mentioned problem, if they are completed by the initial conditions: $G=0$ for $t<t_0$. In Sec. IV, this mixed problem will be represented in the convenient form for obtaining the imbedding equations in Sec. V. First, the wave operator in (1) will be written through the Neumann operator[12] in Sec. III.

We shall proceed from the existence of a solution of the above-formulated problem for the Eq. (1),[15] which is a Green's function describing the field of the point impulsive source. This solution is the generalized function,[19] which will be considered on the plane $x=L$. The evolution equations of the solution, when L is a variable parameter, will be found in Sec. V. The behavior of singularities and the regular part of the solution will be considered in Sec. VI with the intention of creating the inverse procedure in Sec. VII.

III. THE CASE OF THE HOMOGENEOUS SPACE

The factorization of the wave operator (1) in the free space will be needed below. In the homogeneous space, (see for example Ref. 15) the solution of (1) is

$$g(x-L,\boldsymbol{\rho}-\boldsymbol{\rho}_0,t-t_0)=\frac{\theta(t-t_0)}{4\pi c^2(t-t_0)}\,\delta[c(t-t_0)-\sqrt{(x-L)^2+(\boldsymbol{\rho}-\boldsymbol{\rho}_0)^2}]$$

$$\equiv\frac{\theta(t-t_0)}{2\pi c}\,\delta[c^2(t-t_0)^2-(x-L)^2-(\boldsymbol{\rho}-\boldsymbol{\rho}_0)^2], \tag{2a}$$

where $\theta(t-t_0)$ is the Heaviside function. Let us write the equation for (2). If $\epsilon=0$ everywhere, Eq. (1) may be presented in the form

$$\left[\frac{\partial}{\partial x}+\hat{M}(\boldsymbol{\rho},t)\right]\left[\frac{\partial}{\partial x}-\hat{M}(\boldsymbol{\rho},t)\right]g(x-L,\boldsymbol{\rho}-\boldsymbol{\rho}_0,t-t_0)=-\delta(x-L)\,\delta(\boldsymbol{\rho}-\boldsymbol{\rho}_0)\,\delta(t-t_0)/c^2, \tag{2b}$$

where the introduced operator is defined as[2]

$$\hat{M}^2(\boldsymbol{\rho},t)=\frac{\partial^2}{c^2\partial t^2}-\Delta_{\boldsymbol{\rho}},\quad \Delta_{\boldsymbol{\rho}}=\partial^2/\partial y^2+\partial^2/\partial z^2.$$

In the regions $x>L$ and $x<L$ the function g satisfies the first-order equations $[\partial/\partial x \pm \hat{M}(\boldsymbol{\rho},t)]g=0$, which describe the free going away waves. The signs correspond to the directions of the waves. The solutions of these equations we can write as[2]

$$g(x-L,\boldsymbol{\rho}-\boldsymbol{\rho}_0,t-t_0)=\exp[-|x-L|\hat{M}(\boldsymbol{\rho},t)]g_0(\boldsymbol{\rho}-\boldsymbol{\rho}_0,t-t_0), \tag{3}$$

where $g_0(\boldsymbol{\rho}-\boldsymbol{\rho}_0,t-t_0)=g(0,\boldsymbol{\rho}-\boldsymbol{\rho}_0,t-t_0)$. Differentiating (3) twice with respect to x we shall find

$$[\partial^2/\partial x^2-\hat{M}^2(\boldsymbol{\rho},t)]g(x-L,\boldsymbol{\rho}-\boldsymbol{\rho}_0,t-t_0)=-2\,\delta(x-L)\hat{M}(\boldsymbol{\rho},t)g_0(\boldsymbol{\rho}-\boldsymbol{\rho}_0,t-t_0). \tag{4}$$

Then we see that it follows from the comparison of (2b) with (4)

$$\hat{M}(\boldsymbol{\rho},t)g_0(\boldsymbol{\rho}-\boldsymbol{\rho}_0,t-t_0)=(1/2c^2)\,\delta(\boldsymbol{\rho}-\boldsymbol{\rho}_0)\,\delta(t-t_0). \tag{5}$$

We shall present the operator $\hat{M}(\boldsymbol{\rho},t)$ in the integral form by the identity

$$\hat{M}(\boldsymbol{\rho},t)f(\boldsymbol{\rho},t)=\int d\boldsymbol{\rho}_1 dt_1 \hat{M}(\boldsymbol{\rho},t)\,\delta(\boldsymbol{\rho}-\boldsymbol{\rho}_1)\,\delta(t-t_1)f(\boldsymbol{\rho}_1,t_1). \tag{6}$$

Hence we defined the kernel of the operator as

$$M(\boldsymbol{\rho}-\boldsymbol{\rho}_1,t-t_1)=\hat{M}(\boldsymbol{\rho},t)\,\delta(\boldsymbol{\rho}-\boldsymbol{\rho}_1)\,\delta(t-t_1). \tag{7}$$

Acting by $\hat{M}(\boldsymbol{\rho},t)$ on (5) we can obtain also for the kernel of the operator

$$M(\boldsymbol{\rho}-\boldsymbol{\rho}_1,t-t_1)=2c^2\hat{M}^2(\boldsymbol{\rho},t)g_0(\boldsymbol{\rho}-\boldsymbol{\rho}_1,t-t_1). \tag{8}$$

Differentiating in the right part of (8), we yield the explicit form of the kernel[2]

$$M(\boldsymbol{\rho}-\boldsymbol{\rho}_1,t-t_1)=-\frac{2}{(t-t_1)}\frac{\partial}{\partial t}\,g_0(\boldsymbol{\rho}-\boldsymbol{\rho}_1,t-t_1). \tag{9a}$$

Substituting second expression (2a) in (9a) and differentiating it here, using the formulas,

$$\delta'(t-t_1)=-\delta(t-t_1)/(t-t_1) \quad \text{and} \quad \int d\boldsymbol{\rho}_1\delta[c^2(t-t_1)^2-(\boldsymbol{\rho}-\boldsymbol{\rho}_1)^2]|_{t\to t_1}=\pi,$$

which may be derived by the standard technique of the generalized functions,[15,19] it can be shown that

$$\hat{M}(\boldsymbol{\rho},t)f(\boldsymbol{\rho},t)=\frac{1}{c}\frac{\partial}{\partial t}\,f(\boldsymbol{\rho},t)-\frac{2c}{\pi}\int d\boldsymbol{\rho}_1 dt_1\,\theta(t-t_1)\,\delta'[c^2(t-t_1)^2-(\boldsymbol{\rho}-\boldsymbol{\rho}_1)^2]f(\boldsymbol{\rho}_1,t_1), \tag{9b}$$

where δ' is the derivative of the δ-function and, in the agreement with its definition,[15] is the spatial derivative of $f(\boldsymbol{\rho}_1,t_1)$ normal to the nonstationary circle $c^2(t-t_0)^2-(\boldsymbol{\rho}-\boldsymbol{\rho}_0)^2=0$. The example (9b) of two members decomposition of the kernel (9a) will be used in Sec. VI.

By the action of inverse operator $\hat{M}^{-1}(\boldsymbol{\rho},t)$ on (5), the kernel of the inverse operator is obtained:

$$M^{-1}(\boldsymbol{\rho}-\boldsymbol{\rho}_1,t-t_1)=\hat{M}^{-1}(\boldsymbol{\rho},t)\,\delta(\boldsymbol{\rho}-\boldsymbol{\rho}_1)\,\delta(t-t_1)=2c^2g_0(\boldsymbol{\rho}-\boldsymbol{\rho}_1,t-t_1). \tag{9c}$$

Substituting the first expression of (2a) in (9c), we come exactly to the result (2.3) of Ref. 12. It is clear that the $\hat{M}^{-1}(\boldsymbol{\rho},t)$ is the Neumann operator in free space, hence the $\hat{M}(\boldsymbol{\rho},t)$ is its inversion.

IV. THE BOUNDARY CONDITIONS

Following the method[1,2] we shall write the noted above (in Sec. II) boundary conditions in the convenient form for obtaining the imbedding equations. The solution of (1) is $G(x,\boldsymbol{\rho},t;L,\boldsymbol{\rho}_0,t_0)=\exp[-(x-L)\hat{M}(\boldsymbol{\rho},t)]G(L,\boldsymbol{\rho},t;L,\boldsymbol{\rho}_0,t_0)$ for $x>L$ and $G(x,\boldsymbol{\rho},t;L,\boldsymbol{\rho}_0,t_0)=\exp[(x-L)M(\boldsymbol{\rho},t)]G(L_0,\boldsymbol{\rho},t;L,\boldsymbol{\rho}_0,t_0)$ for $x<L_0$. Differentiating these expressions with respect to x and accounting for the jump $\partial/\partial x G(x,\boldsymbol{\rho},t;L,\boldsymbol{\rho}_0,t_0)|_{x=L-0}^{x=L+0}=-(1/c^2)\,\delta(\boldsymbol{\rho}-\boldsymbol{\rho}_0)\delta(t-t_0)$ and the continuity of G and $\partial/\partial x G$, we obtain the relations in the layer on the inside of the boundaries. After this evolution, we have the problem in the layer instead of (1).

$$\left[\frac{\partial^2}{\partial x^2}-\hat{M}^2(\boldsymbol{\rho},t)\right]G(x,\boldsymbol{\rho},t;L,\boldsymbol{\rho}_0,t_0)=\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\,\varepsilon(x,\boldsymbol{\rho},t)G(x,\boldsymbol{\rho},t;L,\boldsymbol{\rho}_0,t_0),$$

$$\left[\frac{\partial}{\partial x}+\hat{M}(\boldsymbol{\rho},t)\right]G(x,\boldsymbol{\rho},t;L,\boldsymbol{\rho}_0,t_0)|_{x=L-0}=(1/c^2)\,\delta(\boldsymbol{\rho}-\boldsymbol{\rho}_0)\,\delta(t-t_0), \tag{10}$$

$$\left[\frac{\partial}{\partial x}-\hat{M}(\boldsymbol{\rho},t)\right]G(x,\boldsymbol{\rho},t;L,\boldsymbol{\rho}_0,t_0)|_{x=L_0+0}=0.$$

The imbedding method allows us to reformulate this boundary problem to the problem with the initial conditions. Following Refs. 1 and 2, we shall obtain the imbedding equations, which will be used for the investigation of the inverse problem below.

V. IMBEDDING EQUATIONS

Having in mind that L is a variable parameter in a correspondence with the essence of the imbedding method,[1,2] we differentiate (10) with respect to L. The equation and the second boundary condition give directly the necessary result. The first boundary condition yields

$$\left[\frac{\partial}{\partial x}+\hat{M}(\boldsymbol{\rho},t)\right]\left[\frac{\partial}{\partial x}+\frac{\partial}{\partial L}\right]G(x,\boldsymbol{\rho},t;L,\boldsymbol{\rho}_0,t_0)|_{x=L}=0. \tag{11}$$

Two components in (11) $[\partial/\partial x+\hat{M}(\boldsymbol{\rho},t)]G(x,\boldsymbol{\rho},t;L,\boldsymbol{\rho}_0,t_0)|_{x=L}$ are found by using Eq. (10) and the operation of $\hat{M}(\boldsymbol{\rho},t)$ on the first boundary condition (10). Its obtained instead of (10).

$$\left[\frac{\partial^2}{\partial x^2}-\hat{M}^2(\boldsymbol{\rho},t)\right]\frac{\partial}{\partial L}\,G(x,\boldsymbol{\rho},t;L,\boldsymbol{\rho}_0,t_0)=\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\,\varepsilon(x,\boldsymbol{\rho},t)\,\frac{\partial}{\partial L}\,G(x,\boldsymbol{\rho},t;L,\boldsymbol{\rho}_0,t_0),$$

$$\left[\frac{\partial}{\partial x}+\hat{M}(\boldsymbol{\rho},t)\right]\frac{\partial}{\partial L}\,G(x,\boldsymbol{\rho},t;L,\boldsymbol{\rho}_0,t_0)|_{x=L}=-\frac{1}{c^2}\,\hat{M}(\boldsymbol{\rho},t)\,\delta(\boldsymbol{\rho}-\boldsymbol{\rho}_0)\,\delta(t-t_0)$$

$$-\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\,\varepsilon(L,\boldsymbol{\rho},t)G_L(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0), \tag{12}$$

$$\left[\frac{\partial}{\partial x}-\hat{M}(\boldsymbol{\rho},t)\right]\frac{\partial}{\partial L}\,G(x,\boldsymbol{\rho},t;L,\boldsymbol{\rho}_0,t_0)|_{x=L_0}=0,$$

where $G_L(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0)=G(L,\boldsymbol{\rho},t;L,\boldsymbol{\rho}_0,t_0)$.

We see from the comparison of (10) with (12) that the solution of (10) is a Green's function for the problem (12). It means that $\partial G/\partial L$ is expressed through G by the integral relationship, which yields with respect to (6) and (7) the expression

$$\left[\frac{\partial}{\partial L}+\hat{M}(\boldsymbol{\rho}_0,t_0)\right]G(x,\boldsymbol{\rho},t;L,\boldsymbol{\rho}_0,t_0)$$

$$=-\int d\boldsymbol{\rho}_1 dt_1 G(x,\boldsymbol{\rho},t;L,\boldsymbol{\rho}_1,t_1)\,\frac{\partial^2}{\partial t_1^2}\,\varepsilon(L,\boldsymbol{\rho}_1,t_1)G_L(\boldsymbol{\rho}_1,t_1;\boldsymbol{\rho}_0,t_0). \tag{13}$$

$\hat{M}(\boldsymbol{\rho}_0,t_0)$ is defined above in (7)–(9); it operates on $\boldsymbol{\rho}_0,t_0$. We have to exchange in (7) $\boldsymbol{\rho}\to\boldsymbol{\rho}_1$, $\boldsymbol{\rho}_1\to\boldsymbol{\rho}_0$ (and the same for t). The expression (13) may be considered as the equation for $G(x,\boldsymbol{\rho},t;L,\boldsymbol{\rho}_0,t_0)$, if it be completed by the initial condition

$$G(x,\boldsymbol{\rho},t;L,\boldsymbol{\rho}_0,t_0)|_{L=x}=G_x(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0). \tag{14}$$

We need the equation for $G_L(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0)$ and write

$$\frac{\partial G_L(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0)}{\partial L}=\left(\frac{\partial}{\partial x}+\frac{\partial}{\partial L}\right)G(x,\boldsymbol{\rho},t;L,\boldsymbol{\rho}_0,t_0)|_{x=L}\,.$$

Here the first component is found using the first boundary condition (10); the second is calculated by the using of (13). A result is obtained as

$$\left[\frac{\partial}{\partial L}+\hat{M}(\boldsymbol{\rho},t)+\hat{M}(\boldsymbol{\rho}_0,t_0)\right]G_L(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0)$$

$$=\frac{1}{c^2}\,\delta(\boldsymbol{\rho}-\boldsymbol{\rho}_0)\,\delta(t-t_0)-\int d\boldsymbol{\rho}_1 dt_1 G_L(\boldsymbol{\rho},t;\boldsymbol{\rho}_1,t_1)\,\frac{\partial^2}{\partial t_1^2}\,\varepsilon(L,\boldsymbol{\rho}_1,t_1)G_L(\boldsymbol{\rho}_1,t_1;\boldsymbol{\rho}_0,t_0) \tag{15}$$

with the obvious initial condition $G_L(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0)|_{L=L_0}=g_0(\boldsymbol{\rho}-\boldsymbol{\rho}_0,t-t_0)$.

How it will be shown that the value $G_L(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0)$ plays the main role in the inverse problem. This is a field on the plane $x=L$ from the point impulsive source on same plane, which may be measured in the remote sensing. The difference $G_L(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0)-g_0(\boldsymbol{\rho}-\boldsymbol{\rho}_0,t-t_0)$ is a backscattering field from the layer of the inhomogeneous medium. Below we shall consider the solution of Eq. (1) only on the plane $x=L$ and Eq. (15) will be used only.

VI. THE METHOD OF THE SINGULARITIES

The important element of the differential approach for inverse problems is the method of the singularities.[5,18,20] In order to make its generalization for the multidimensional problem, we shall perform the solution of (15) as

$$G_L(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0)=\theta(t-t_0)H_L(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0), \tag{16}$$

where $\theta(t-t_0)$ is the Heaviside function.

The substitution of (16) in (15) and the application of (9b) give the expression with two kinds of singularities $\theta(t-t_0)$ and $\delta(t-t_0)$. Comparing the coefficients before these singularities to zero, we obtain two equations:

$$\frac{\partial}{\partial L}\,H_L(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0)+\frac{1}{c}\,\frac{\partial}{\partial t}\,H_L(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0)-\frac{1}{c}\,\frac{\partial}{\partial t_0}\,H_L(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0)$$

$$-\frac{2c}{\pi}\int_{t_0}^{t}dt_1\int \boldsymbol{\rho}_1 H_L(\boldsymbol{\rho},t;\boldsymbol{\rho}_1,t_1)\,\delta'[c^2(t_1-t_0)^2-(\boldsymbol{\rho}_1-\boldsymbol{\rho}_0)^2]$$

$$-\frac{2c}{\pi}\int_{t_0}^{t}dt_1\int \boldsymbol{\rho}_1 \delta'[c^2(t-t_1)^2-(\boldsymbol{\rho}-\boldsymbol{\rho}_1)^2]H_L(\boldsymbol{\rho}_1,t_1;\boldsymbol{\rho}_0,t_0)$$

$$=h_L(\boldsymbol{\rho}_0,t_0)\varepsilon(L,\boldsymbol{\rho}_0,t_0)\frac{\partial}{\partial t_0}H_L(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0)$$

$$-h_L(\boldsymbol{\rho},t)\frac{\partial}{\partial t}[\varepsilon(L,\boldsymbol{\rho},t)H_L(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0)]$$

$$+\int_{t_0}^{t}dt_1\int d\boldsymbol{\rho}_1\frac{\partial}{\partial t_1}[H_L(\boldsymbol{\rho},t;\boldsymbol{\rho}_1,t_1)]\frac{\partial}{\partial t_1}\varepsilon(L,\boldsymbol{\rho}_1,t_1)H_L(\boldsymbol{\rho}_1,t_1;\boldsymbol{\rho}_0,t_0), \quad (17a)$$

$$c^2\varepsilon(L,\boldsymbol{\rho}_0,t_0)h_L^2(\boldsymbol{\rho}_0,t_0)+2c\cdot h_L(\boldsymbol{\rho}_0,t_0)-1=0. \quad (17b)$$

The value $h_L(\boldsymbol{\rho}_0, t_0)$ in (17b) is determined by the relationship

$$H_L(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0)|_{t\to t_0}=h_L(\boldsymbol{\rho}_0,t_0)\,\delta(\boldsymbol{\rho}-\boldsymbol{\rho}_0), \quad (18)$$

which is the distribution of the source field in the initial moment t_0. The amplitude $h_L(\boldsymbol{\rho}_0,t_0)$ of this distribution is defined, in the agreement with (17b), by the characteristic of the medium $\varepsilon(L,\boldsymbol{\rho}_0,t_0)$ in the point of the source,

$$h_L(\boldsymbol{\rho}_0,t_0)=\frac{(\sqrt{1+\varepsilon(L,\boldsymbol{\rho}_0,t_0)}-1)}{c\varepsilon(L,\boldsymbol{\rho}_0,t_0)}. \quad (19)$$

Note, a sign before the square root in (19) is chosen so that for the homogeneous medium

$$H_L(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0)|_{t\to t_0}=g_0(\boldsymbol{\rho}-\boldsymbol{\rho}_0,t-t_0)|_{t\to t_0}=(1/2c)\,\delta(\boldsymbol{\rho}-\boldsymbol{\rho}_0).$$

The δ' in (17a) is the derivative of the δ-function. In the agreement with its definition,[15] the expressions under the integrals in the left part of (17a) are the spatial derivative of $H_L(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0)$ normal to the nonstationary circles $c^2(t_1-t_0)^2-(\boldsymbol{\rho}_1-\boldsymbol{\rho}_0)^2=0$ or $c^2(t-t_1)^2-(\boldsymbol{\rho}-\boldsymbol{\rho}_1)^2=0$ in the plane $x=L$. These terms describe the transverse propagation of the wave and are written in (17a) formally as the longitudinal terms, which simplifies the analysis of the multidimensional problem.

Equation (17a) allows us to obtain the relation between the partial derivative of $\varepsilon(L,\boldsymbol{\rho}_0,t_0)$ with respect to L and the partial derivatives of $H_L(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0)$ with respect to t and t_0 for $t=t_0$. Putting in (17a) $t=t_0$, we have

$$\frac{\partial h_L(\boldsymbol{\rho}_0,t_0)}{\partial L}+\frac{A_L(\boldsymbol{\rho}_0,t_0)}{c}-\frac{B_L(\boldsymbol{\rho}_0,t_0)}{c}=h_L(\boldsymbol{\rho}_0,t_0)\varepsilon(L,\boldsymbol{\rho}_0,t_0)[B_L(\boldsymbol{\rho}_0,t_0)-A_L(\boldsymbol{\rho}_0,t_0)]$$
$$-\frac{[h_L(\boldsymbol{\rho}_0,t_0)]^2\partial\varepsilon(L,\boldsymbol{\rho}_0,t_0)}{\partial t_0}. \quad (20)$$

The values A and B introduced here are the characteristics of the point source on the boundary of the inhomogeneuos medium in initial moment. They are defined by the expressions

$$\left.\frac{\partial H_L(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0)}{\partial t}\right|_{t\to t_0}=A_L(\boldsymbol{\rho}_0,t_0)\,\delta(\boldsymbol{\rho}-\boldsymbol{\rho}_0), \quad (21)$$

$$\left.\frac{\partial H_L(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0)}{\partial t_0}\right|_{t\to t_0} = B_L(\boldsymbol{\rho}_0,t_0)\,\delta(\boldsymbol{\rho}-\boldsymbol{\rho}_0).$$

Using (17b), (19), and (20), we can obtain

$$\frac{\partial \varepsilon(L,\boldsymbol{\rho}_0,t_0)}{\partial L} = \frac{2(1-ch_L(\boldsymbol{\rho}_0,t_0))^2[A_L(\boldsymbol{\rho}_0,t_0) - 2\partial h_L(\boldsymbol{\rho}_0,t_0)/\partial t_0 - B_L(\boldsymbol{\rho}_0,t_0)]}{[ch_L(\boldsymbol{\rho}_0,t_0)]^4}. \tag{22}$$

Hence the derivative of $\varepsilon(L,\boldsymbol{\rho}_0,t_0)$ with respect to L is defined by the time derivatives of the field on the boundary of the medium in initial moment.

Differentiating (17a) with respect to t and t_0, putting $t=t_0$, and combining the obtained expressions, we can find $\partial^2\varepsilon(L,\boldsymbol{\rho}_0,t_0)/\partial L^2$, which will be defined by second time derivatives of the field on the boundary in initial moment.

The procedure of the differentiation may be repeated over and over again and the higher derivatives of ε with respect to L can be found. In principle, from the time behavior of the field on the plane $x=L$ in initial moment, all L derivatives of ε can be calculated and the Taylor series of ε can be completed, which allows us to reconstruct the behavior of ε to the left from the plane $x=L$. It can be considered like the inverse procedure, but the nonlinearity of Eq. (17a) creates the difficulties in calculation of very high derivatives. The more effective way will be discussed in next section.

Note the some features of the wave propagation. On the plane $x=L$, the value of $H_L(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0)$ is singular on the front of the wave. Behind the front, the wave can have also the singularities, when the reflection of the wavefront from the medium or from the plane $x=L_0$ comes to the surface $x=L$. This moment and greater time were not considered above. To do it, the solution of (15), instead of (16), would have to be presented in the form

$$G_L(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0) = \theta(t-t_0)H_L(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0) + \theta(t-t_0')\widetilde{H}_L(\boldsymbol{\rho},t;\boldsymbol{\rho}_0',t_0'), \tag{23}$$

where $\boldsymbol{\rho}_0'$ and t_0' are the point on the plane $x=L$ and the moment of the reflection appearance. Substituting (23) in (15) and separating the singularities as above, we can obtain the equation for $\widetilde{H}_L(\boldsymbol{\rho},t;\boldsymbol{\rho}_0',t_0')$, which is not closed, because the value H presents there. (We have to define H and $\widetilde{H}$ jointly.) The separation of the singularities was considered in detail for the one-dimensional case in Ref. 20.

When the second wavefront reflection appears on the plane $x=L$, the third term has to be included in (23) and the third equation has to be obtained, etc. This approach allows us to separate and to observe individually the moves of all singularities, which will promote the development of the algorithms and numerical methods.

With the purpose of simplifying the examination of an inverse procedure, the case when the reflections of the wavefront are absent will be considered below.

VII. INVERSE PROBLEM

The inverse procedure for the multidimensional nonstationary medium may be obtained by the use of the evolution equations (17a) and (17b). These equations allow us to apply the ''layer stripping'' process for the value $H_L(\boldsymbol{\rho},t;\ \boldsymbol{\rho}_0,t_0)$, which is used so successfully in other simpler cases.[11–13] The main step in the ''layer stripping'' process is to employ Eq. (17a) to obtain a value of $H_{L-\delta L}(\boldsymbol{\rho},\ t;\boldsymbol{\rho}_0,t_0)$ on a surface $x=L-\delta L(\,\delta L>0)$ for a finite time interval, from knowledge of this value $H_L(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0)$ on an adjacent surface $x=L$, where two surface are an infinitesimal distance apart.

The field $H_L(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0)$ on the plane $x=L$ of the point source on the same plane for finite time interval may be measured. The $H_L(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0)$ is observed on the bounded region in R^6, which is

chosen in an agreement with the condition where $\varepsilon(x,\boldsymbol{\rho},t)$ have to be reconstructed. The feature of the inverse problem with the nonstationary medium is a necessity to repeat the experiments with the medium many times and to make the measurements in every case for the different t_0, which is the initial moment of the source action. For example, the time periodical media are comfortable to examine. The $\boldsymbol{\rho}_0$ is another free variable parameter in an experiment. When the scattering data $H_L(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0)$ are obtained, the step of inverse procedure is carried out.

Putting $t\to t_0$ in $H_L(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0)$ and using (17b), we find $\varepsilon(L,\boldsymbol{\rho}_0,t_0)$ on the plane $x=L$. Substituting $H_L(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0)$ and $\varepsilon(L,\boldsymbol{\rho}_0,t_0)$ in Eq. (17a) and determining $\partial H_L/\partial L$, the value of $H_{L-\delta L}(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0)$ is obtained so $H_{L-\delta L}=H_L-(\partial H_L/\partial L)\cdot\delta L$. The operation $t\to t_0$ in $H_{L-\delta L}(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0)$ takes $\varepsilon(L-\delta L,\boldsymbol{\rho}_0,t_0)$ on the surface $x=L-\delta L$.

This step may be repeated many times and $\varepsilon(x,\boldsymbol{\rho},t)$ can be reconstructed to the left from $x=L$. The procedure stops in two cases. We arrive at the plane $x=L_0$ or the definition region of $H_{L-n\times\delta L}(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0)$ is tightened to the point in R^6 where n is the number of a procedure step and $n\times\delta L$ is the transference distance of the right layer boundary. The structure of Eq. (17a) is such that a definition region of $H_{L-n\times\delta L}(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0)$ is decreased on every procedure step. If the distance $n\times\delta L$ of an inversion is not enough, we have to make the observation region of $H_L(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0)$ in the measurements more broad.

Above we had in view the line ''layer stripping'' process for the value $H_L(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0)$ so that $H_{L-\delta L}=H_L-(\partial H_L/\partial L)\cdot\delta L$ and the value $\varepsilon(L,\boldsymbol{\rho},t)$ was constant in δL infinitesimal layer. We discussed the scheme of first order. There is an opportunity to create the higher order procedure. The value $\varepsilon(L,\boldsymbol{\rho},t)$ may be presented in the δL-layer by a k-polynomial in L, whose coefficient calculations are considered in the previous section. Substituting this polynomial in Eq. (17a), solving it in the δL-layer, and getting $H_{L-\delta L}(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0)$ from $H_L(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0)$, we realize the k-order ''layer stripping'' process and accordingly the same inverse procedure. The address to a high-order procedure will promote the improvement of the stability and convergence of inversion. In principle, the questions of stability and convergence of the procedure may be considered as in the well-researched one-dimensional case,[3,4] and the complete analysis of the procedure features will be carried out in the future, when an algorithm will be created and the numerical experiments will be realized.

The $H_L(\boldsymbol{\rho},t;\boldsymbol{\rho}_0,t_0)$ in R^6 is used for the reconstruction of the $\varepsilon(x,\boldsymbol{\rho},t)$ in R^4. We see a over-definiteness that is the attribute and characteristic property of the multidimensional inverse problem,[21] which comes from the structure of Eq. (17a) and is explained physically by the transverse propagation, in the direction across to the x-axis.

VIII. CONCLUSION

The same application of the obtained results will be discussed here. Equation (17a) is a differential equation of a first order with respect to L. This allows us to apply the approximation of the Markov process[1,2] for the analysis of the statistical inverse problem.[6] Hence, the proposed above inverse procedure may be used directly in the statistical transfer theory[1,2] for a determination of a multidimensional random medium characteristics. The apparatus of a Markov process approximation developed in Refs. 16 and 17 for a derivation of an evolution equation for the backscattering statistical characteristics may be applied to (17a) and the generalization of the present procedure for statistical inverse problem may be obtained.

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A temperature and mass dependence of the linear Boltzmann collision operator from group theory point of view

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The Lie group of the transformations affecting the parameters of the linear Boltzmann collision operator such as temperature of background gas and ratio of masses of colliding particles and molecules is discovered. The group also describes the conservation laws for collisions and main symmetries of the collision operator. New algebraic properties of the collision operator are derived. Transformations acting on the variables and parameters and leaving the linear Boltzmann kinetic equation invariant are found. For the constant collision frequency the integral representation of solutions for nonuniform case in terms of the distribution function of particles drifting in a gas with zero temperature is deduced. The new exact relaxation solutions are obtained too. © *1996 American Institute of Physics.*
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I. INTRODUCTION

Last year's steady interest remains in studying groups of symmetry of the mathematical physics equations. It is so especially in the case where the transformations taken into consideration affect the parameters of an equation as well as its variables, that is, the basis of the renormgroup ideology.[1] Here, we will study the linear kinetic equation that in particular describes nonuniform spatial drift of charged particles through a gas in the electromagnetic field. It is useful, first, to consider (from the group theory point of view) the character of dependence on parameters of the collision integral as the most complicated term of this equation. Also, such a consideration is interesting, because it results in quite remarkable mathematical constructions, and permits us to understand deeper properties of the collision operator. The evolution due to collisions of the distribution function of particles having mass m_1 (for example, ions) with particles of mass m_2 (molecules), distributed on speed according to the distribution function $\Psi(\boldsymbol{u})$, is defined by the operator of collisions[2] $\hat{I}$:

$$\left(\frac{\partial f}{\partial t}\right)_C = \hat{I}(\Psi) f, \tag{1}$$

where

$$[\hat{I}f](\boldsymbol{v}) = \int \nu(\mathrm{v})\chi(\mu,\mathrm{v})[f(\boldsymbol{v}')\Psi(\boldsymbol{u}') - f(\boldsymbol{v})\Psi(\boldsymbol{u})]d\Omega_{\boldsymbol{v}'}d\boldsymbol{u}, \tag{2}$$

$\mathbf{v}=\boldsymbol{v}-\boldsymbol{u}$ is relative velocity, $\mu=(\mathbf{v}\cdot\mathbf{v}')/\mathrm{v}^2$ is the cosine of scattering angle: $d\Omega_{\mathbf{v}'}$ is the element of solid angle near $\mathbf{v}'$, $\nu=N\mathrm{v}\sigma$ and $\chi=(1/\sigma)d\sigma/d\Omega$ are the frequency of collisions and probability of scattering into solid angle; $\boldsymbol{v},\boldsymbol{v}'$; $\boldsymbol{u},\boldsymbol{u}'$ are velocities of ions and molecules before and after a collision; $\boldsymbol{v}$, $\boldsymbol{u}$, $\mathbf{v}'$ and $\boldsymbol{v}'$, $\boldsymbol{u}'$, $\boldsymbol{v}$ are connected with the idempotent transformation:

$$\boldsymbol{v}' = \frac{m\boldsymbol{v} + \boldsymbol{u} + \mathbf{v}'}{1+m}, \quad \boldsymbol{v} = \frac{m\boldsymbol{v}' + \boldsymbol{u}' + \mathbf{v}}{1+m},$$

$$\boldsymbol{u}' = \frac{m\boldsymbol{v} + \boldsymbol{u} - m\mathbf{v}'}{1+m}, \quad \boldsymbol{u} = \frac{m\boldsymbol{v}' + \boldsymbol{u}' - m\boldsymbol{v}}{1+m}, \tag{3}$$

$$\mathbf{v} = \boldsymbol{v} - \boldsymbol{u}, \quad \mathbf{v}' = \boldsymbol{v}' - \boldsymbol{u}',$$

where $m = m_1/m_2$.

We will consider only elastic collisions. Because of this we will have

$$\mathrm{v} = \mathrm{v}'. \tag{4}$$

Many properties of the collision operator can be found more easily for the conjugate operator and then they can be transferred on the collision operator. If the scalar product is defined as

$$(\varphi, f) = \int \varphi(\boldsymbol{v}) f(\boldsymbol{v}) d\boldsymbol{v}, \tag{5}$$

then the conjugate operator determined by the condition

$$(\varphi, \hat{I} f) = (\tilde{\hat{I}} \varphi, f), \tag{6}$$

obviously ($d\mathbf{v} d\mathbf{u} d\Omega_{\mathbf{v}'} = d\mathbf{v}' d\mathbf{u}' d\Omega_{\mathbf{v}}$), will have the form

$$[\tilde{\hat{I}} \varphi](\boldsymbol{v}) = \int \nu(\mathrm{v}) \chi(\mathrm{v}, \mu) [\varphi(\boldsymbol{v}') - \varphi(\boldsymbol{v})] \Psi(\boldsymbol{u}) d\Omega_{\mathbf{v}'} d\boldsymbol{u}. \tag{7}$$

II. TEMPERATURE DEPENDENCE OF THE COLLISION OPERATOR

Let us introduce special notation $\hat{J}$ for the collision operator for collisions with scattering centers that are at rest before a collision, i.e., when $\Psi(\boldsymbol{u}) = \delta(\boldsymbol{u})$:

$$\hat{J} = \hat{I}(\delta(\boldsymbol{u})). \tag{8}$$

The collision operator $\hat{I}$ can be expressed through the operator $\hat{J}$ with the help of a simple transformation[3,4] $F: \hat{J} \to \hat{I}$. This transformation has a clear physical meaning consisting in that the process of scattering on moving center can be considered in the system of reference where this center is at rest. Indeed, the action of the collision operator can be reduced to the next operations. The scattering centers should be separated on groups according to the velocity, and one should get over to the system where scattering centers of a chosen group are at rest, act by the collision operator $\hat{J}$, return to the initial system, and integrate over all groups, i.e.,

$$\hat{I} = F(\hat{J}) = \int d\boldsymbol{u} \Psi(\boldsymbol{u}) e^{-\boldsymbol{u}\nabla} \hat{J} e^{\boldsymbol{u}\nabla}, \tag{9}$$

where $e^{\boldsymbol{u}\nabla}$ is the operator of translation on the vector $\boldsymbol{u}$ in the velocity space,

$$e^{\boldsymbol{u}\nabla} f(\boldsymbol{v}) = f(\boldsymbol{v} + \boldsymbol{u}), \quad \text{where } \nabla = \frac{\partial}{\partial \boldsymbol{v}}. \tag{10}$$

The transformation F has an interesting algebraic property. The successive action of the transformations F_{Ψ_1} and F_{Ψ_2}, induced by the distribution functions $\Psi_1(\boldsymbol{u})$ and $\Psi_2(\boldsymbol{u})$, is the transformation induced by convolution of the input distribution functions:

$$F_{\Psi_1}\otimes F_{\Psi_2}=F_{\Psi_2}\otimes F_{\Psi_1}=F_{\Psi_{12}},$$
$$\Psi_{12}=\Psi_1\circ\Psi_2=\Psi_2\circ\Psi_1=\int \Psi_1(\boldsymbol{u}-\boldsymbol{u}')\Psi_2(\boldsymbol{u}')d\boldsymbol{u}'. \tag{11}$$

In practicality, in the important case when a distribution of scattering centers (molecules) is the Maxwellian distribution with temperature T,

$$\Psi(\boldsymbol{u})=\Psi_T(u)=\left(\frac{m_2}{2\pi kT}\right)^{3/2} e^{-m_2u^2/2kT}, \tag{12}$$

the family of the transformations F_T, $0\leqslant T<\infty$, is an Abelian semigroup:

$$F_{T=0}=1, \quad F_{T_1}\otimes F_{T_2}=F_{T_2}\otimes F_{T_1}=F_{T_1+T_2}. \tag{13}$$

Property (13) follows from a closure of the family of the Maxwellian distributions, $\Psi_T(\boldsymbol{u})$, $0\leqslant T<\infty$, relatively to the convolution:

$$\int d\boldsymbol{u}'\Psi_{T_1}(\boldsymbol{u}-\boldsymbol{u}')\Psi_{T_2}(\boldsymbol{u}')=\Psi_{T_1+T_2}(\boldsymbol{u}). \tag{14}$$

Differentiating transformation F_T (9) with respect to temperature T at zero, bearing in mind the property of Maxwellians,

$$\frac{\partial}{\partial T}\Psi_T(\boldsymbol{v})=\frac{k}{2m_2}\nabla^2\Psi_T(\boldsymbol{v}), \tag{15}$$

we will have an expression for the generator q of the temperature transformations' semigroup. An action of the generator q on the operator $\hat{I}$ is expressed through the double commutator $(\hat{a}*\hat{b}\equiv[\hat{a},\hat{b}]\equiv\hat{a}\hat{b}-\hat{b}\hat{a})$:

$$q(\hat{I})=\frac{k}{2m_2}\boldsymbol{\nabla}*\boldsymbol{\nabla}*\hat{I}\equiv\frac{k}{2m_2}[\boldsymbol{\nabla},[\boldsymbol{\nabla},\hat{I}]]=\frac{k}{2m_2}(\nabla^2\hat{I}-2\boldsymbol{\nabla}\hat{I}\boldsymbol{\nabla}+\hat{I}\nabla^2). \tag{16}$$

According to expression (16), the collision operator satisfies the differential equation:

$$\frac{\partial}{\partial T}\hat{I}=\frac{k}{2m_2}\boldsymbol{\nabla}*\boldsymbol{\nabla}*\hat{I}\equiv\frac{k}{2m_2}[\boldsymbol{\nabla},[\boldsymbol{\nabla},\hat{I}]]. \tag{17}$$

We will denote by the operator belonging to some algebra K marked from the right side with the sign $*$ (i.d. $\hat{a}*$, $\hat{a}\subseteq K$) the linear map $\hat{a}*$: $K\rightarrow\hat{a}*K$ of the algebra K into itself:

$$\hat{a}*\hat{b}\equiv\hat{a}\hat{b}-\hat{b}\hat{a}, \quad \hat{a},\hat{b}\subseteq K. \tag{18}$$

Later we will need the next simple properties of such maps:

$$[\hat{a}*,\hat{b}*]=[\hat{a},\hat{b}]*, \quad [\hat{a}*,\hat{b}]=[\hat{a},\hat{b}*]=[\hat{a},\hat{b}],$$
$$\hat{a}\hat{b}*+\hat{b}\hat{a}*=\hat{a}*\hat{b}*+(\hat{b}\hat{a})*. \tag{19}$$

Taking into account definitions (18), we can express the collision operator in terms of the collision operator of the scattering on molecules at rest before the collision with the help of the transformation F_T:

$$\hat{I}=e^{(kT/2m_2)\nabla*\nabla*}\hat{J}. \tag{20}$$

III. MASS DEPENDENCE OF THE COLLISION OPERATOR

It can be seen from Eq. (3) that the derivative of the velocity after collision with respect to the variable $\ln(1+m)$ is equal to a difference of the velocities before and after the collision:

$$\xi=\ln(1+m), \quad \frac{\partial \boldsymbol{v}'}{\partial \xi}=\boldsymbol{v}-\boldsymbol{v}'. \tag{21}$$

So,

$$\frac{\partial}{\partial \xi}\tilde{\hat{I}}=(\boldsymbol{v}\tilde{\hat{I}}-\tilde{\hat{I}}\boldsymbol{v})\boldsymbol{\nabla}=(\boldsymbol{v}*\tilde{\hat{I}})\boldsymbol{\nabla}=(\boldsymbol{\nabla}\boldsymbol{v}*-\boldsymbol{\nabla}*\boldsymbol{v}*)\tilde{\hat{I}}. \tag{22}$$

Conjugating expression (22) and using the usual properties of conjugation,

$$(\hat{a}\hat{b})\tilde{}=\tilde{\hat{b}}\tilde{\hat{a}} \quad \text{and} \quad \tilde{\boldsymbol{\nabla}}=-\boldsymbol{\nabla}, \quad \tilde{\boldsymbol{v}}=\boldsymbol{v}, \tag{23}$$

one gets a formula for differentiation of the collision operator $\hat{I}$ on ξ:

$$\frac{\partial}{\partial \xi}\hat{I}=\boldsymbol{\nabla}\boldsymbol{v}*\hat{I}. \tag{24}$$

Thus, the semigroup of the transformations, $e^{\xi\boldsymbol{\nabla}\boldsymbol{v}*}$, $\infty>\xi\geqslant 0$, describes the mass dependence of the collision operator and together with the transformation F_T allows the expression of the operator $\hat{I}$ in terms of the operator $\hat{\chi}$ that describes a process of scattering on the infinitely heavy ($m=0$) centers being at rest. The operator $\hat{\chi}$ is the simplest collision operator. So, we have

$$\hat{I}=e^{(kT/2m_2)\boldsymbol{\nabla}*\boldsymbol{\nabla}*+\ln(1+m)\boldsymbol{\nabla}\boldsymbol{v}*}\hat{\chi}, \tag{25}$$

$$[\hat{\chi}f](\boldsymbol{v})=\int \nu(\mathrm{v})\chi(\mu,\mathrm{v})[f(\mathbf{v}')-f(\boldsymbol{v})]d\Omega_{\mathbf{v}'}, \quad \text{here } \mathbf{v}'^2=\mathbf{v}^2=\boldsymbol{v}^2, \quad \tilde{\hat{\chi}}=\hat{\chi}. \tag{26}$$

One can notice that the generators of the temperature and mass transformations commutate:

$$[\boldsymbol{\nabla}*\boldsymbol{\nabla}*,\boldsymbol{\nabla}\boldsymbol{v}*]=0. \tag{27}$$

Due to (17), (23), and (22), the conjugate collision operator can be represented in the form

$$\tilde{\hat{I}}=e^{(kT/m_2)\boldsymbol{\nabla}*\boldsymbol{\nabla}*+\ln(1+m)(\boldsymbol{\nabla}\boldsymbol{v}*-\boldsymbol{\nabla}*\boldsymbol{v}*)}\hat{\chi}. \tag{28}$$

IV. ENERGY CONSERVATION LAW

The energy conservation law for scattering on an infinitely heavy center being at rest is reduced to the fact that the squares of velocities before and after collision remain equal, or in other words,

$$\boldsymbol{v}^2 * \hat{\chi} = 0, \tag{29}$$

and the operator $\hat{\chi}$ is a stationary object with respect to the group of transformations defined by generator $\boldsymbol{v}^2 *$:

$$e^{\alpha \boldsymbol{v}^2 *} \hat{\chi} = \hat{\chi}. \tag{30}$$

One more property of symmetry is added in the case of the constant collision frequency ($\nu = \text{const}$, the so-called Maxwell's particles) frequently used in the kinetic theory:

$$\nabla^2 * \hat{\chi} = 0, \quad \text{when} \quad \nu = \text{const}, \quad \chi(\mu, \mathrm{v}) = \chi(\mu). \tag{31}$$

V. LIE ALGEBRA AND GROUP

To create from the set of generators $\boldsymbol{\nabla} * \boldsymbol{\nabla} *$, $\boldsymbol{\nabla} \boldsymbol{v} *$, $v^2 *$, $\boldsymbol{\nabla}^2 *$ the basis of Lie algebra, one needs to add to it three more elements: $\boldsymbol{\nabla} * \boldsymbol{v} *$, $\boldsymbol{v} * \boldsymbol{v} *$ $(\boldsymbol{v} \boldsymbol{\nabla}) *$. This seven-dimensional Lie algebra is determined by commutative relations that look most simple in the bases:

$$P_1 = \frac{1}{\sqrt{8}} \nabla * \nabla *, \quad P_2 = \frac{1}{2} \nabla * \boldsymbol{v} *, \quad P_3 = \frac{1}{\sqrt{8}} \boldsymbol{v} * \boldsymbol{v} *,$$

$$Q_1 = \frac{1}{\sqrt{8}} \nabla^2 *, \quad Q_2 = \frac{1}{2} (\boldsymbol{v} \nabla) *, \quad Q_3 = \frac{1}{\sqrt{8}} v^2 *, \tag{32}$$

$$S = M - Q_2 - P_2,$$

where

$$M = \nabla \boldsymbol{v} *,$$

and can be represented in the form

$$[P_i, P_k] = 0,$$

$$[Q_i, P_k] = e_{ikl} b_{lm} P_m, \quad [Q_i, Q_k] = e_{ikl} b_{lm} Q_m, \tag{33}$$

$$[S, P_k] = P_k, \quad [S, Q_k] = 0,$$

where e_{ikl} is the antisymmetric Levi-Civita tensor and b_{lm} is an antidyogonal matrix

$$b = \begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad \tilde{b} = b, \quad b^2 = 1. \tag{34}$$

Explicit values of commutators (32) are given in Table I. For convenience we give commutative relations for the generator of mass transformations M separately:

TABLE I. Values of the commutators $[A_\alpha, A_\beta]$.

$A_\alpha \backslash A_\beta$	P_1	P_2	P_3	Q_1	Q_2	Q_3	S
$P_1=\frac{1}{\sqrt{8}}\nabla*\nabla*$	0	0	0	0	P_1	P_2	$-P_1$
$P_2=\frac{1}{2}\nabla*\boldsymbol{v}*$	0	0	0	$-P_1$	0	P_3	$-P_2$
$P_3=\frac{1}{\sqrt{8}}\boldsymbol{v}*\boldsymbol{v}*$	0	0	0	$-P_2$	$-P_3$	0	$-P_3$
$Q_1=\frac{1}{\sqrt{8}}\nabla^2*$	0	P_1	P_2	0	Q_1	Q_2	0
$Q_2=\frac{1}{2}(\boldsymbol{v}\nabla)*$	$-P_1$	0	P_3	$-Q_1$	0	Q_3	0
$Q_3=\frac{1}{\sqrt{8}}v^2*$	$-P_2$	$-P_3$	0	$-Q_2$	$-Q_3$	0	0
$S=\nabla\boldsymbol{v}*-\frac{1}{2}(\boldsymbol{v}\nabla)*-\frac{1}{2}\nabla*\boldsymbol{v}*$	P_1	P_2	P_3	0	0	0	0

$$[M,P_1]=0,\quad [M,P_2]=P_2,\quad [M,P_3]=2P_3,$$
$$[M,Q_1]=-Q_1-P_1,\quad [M,Q_2]=0,\quad [M,Q_3]=Q_3+P_3. \tag{35}$$

As it follows from Table I, AP, AQ, APQ, and APS (where AP is the Lie algebra with bases elements P_i, APS is the Lie algebra with bases elements P_i, S, and so on) are subalgebras of Lie algebra $APQS$ (32). Moreover APQ and APS are ideals, and AP is commutative ideal. Matrices T_{ik} of adjoint representation[5] of the subgroup GQ, defined by the expression

$$G^{-1}(q)Q_iG(q)=T_{ik}(q)Q_k,\quad G(q)=e^{q_1Q_1}e^{q_2Q_2}e^{q_3Q_3}, \tag{36}$$

can be obtained with the help of the formula

$$e^ABe^{-A}=B+\frac{1}{1!}[A,B]+\frac{1}{2!}[A,[A,B]]+\cdots. \tag{37}$$

These matrixes have the form

$$T(q)=\begin{vmatrix} e^{q_2} & q_3e^{q_2} & \frac{q_3^2}{2}e^{q_2} \\ -q_1e^{q_2} & 1-q_1q_3e^{q_2} & q_3\left(1-\frac{q_1q_3}{2}e^{q_2}\right) \\ \frac{q_1^2}{2}e^{q_2} & -q_1\left(1-\frac{q_1q_3}{2}e^{q_2}\right) & \left(1-\frac{q_1q_3}{2}e^{q_2}\right)^2e^{-q_2} \end{vmatrix}. \tag{38}$$

One can see from (33) that the generators P_i are being transformed according to the same representation:

$$G^{-1}(q)P_iG(q)=T_{ik}(q)P_k. \tag{39}$$

Matrices of the conjugated representation $\overline{T_{ik}}(q)$,

$$G(q)Q_kG^{-1}(q)=Q_i\overline{T_{ik}}(q),\quad G(q)P_kG^{-1}(q)=P_i\overline{T_{ik}}(q), \tag{40}$$

accordingly have the form

$$\overline{T(q)}=\widetilde{T}^{-1}(q)=\begin{vmatrix} \left(1-\frac{q_1q_3}{2}\,e^{q_2}\right)^2 e^{-q_2} & q_1\left(1-\frac{q_1q_3}{2}\,e^{q_2}\right) & \frac{q_1^2}{2}\,e^{q_2} \\ -q_3\left(1-\frac{q_1q_3}{2}\,e^{q_2}\right) & 1-q_1q_3e^{q_2} & q_1e^{q_2} \\ \frac{q_3^2}{2}\,e^{q_2} & -q_3e^{q_2} & e^{q_2} \end{vmatrix}. \tag{41}$$

Parameters of the product of two elements from subgroup GQ,

$$G(q)G(q')=G(q''),\quad G(q'),G(q''),G(q)=e^{q_1Q_1}e^{q_2Q_2}e^{q_3Q_3}\in GQ, \tag{42}$$

are defined by formulas

$$q_1''=q_1+\frac{q_1'}{1-q_3q_1'/2}\,e^{-q_2},\quad q_2''=(q_2+q_2')\ln\left(1-\frac{q_3q_1'}{2}\right)^2,\quad q_3''=q_3'+\frac{q_3}{1-q_3q_1'/2}\,e^{-q_2'}; \tag{43}$$

parameters of the inverse element have the form

$$G^{-1}(q)=G(q'),$$
$$q_1'=\frac{q_1e^{q_2}}{(q_1q_2/2)e^{q_2}-1},\quad q_2'=-q_2\,\ln\left(\frac{q_1q_2}{2}\,e^{q_2}-1\right)^2,\quad q_3'=\frac{q_3e^{q_2}}{(q_1q_2/2)e^{q_2}-1}. \tag{44}$$

The connection with parameters of the exponential parametrization for a group element from GQ is given by formula

$$e^{q_1Q_1}e^{q_2Q_2}e^{q_3Q_3}=e^{q_1'Q_1+q_2'Q_2+q_3'Q_3},$$
$$q_1'=\frac{q_1q_2}{1-e^{-q_2}},\quad q_2'=\frac{q_1q_2q_3}{2(1-e^{-q_2})}+q_2,\quad q_3'=\frac{q_2q_3}{1-e^{-q_2}}. \tag{45}$$

The summands of the element S are a basis of the subalgebra:

$$[Q_2,M]=[Q_2,P_2]=0,\quad [M,P_2]=P_2. \tag{46}$$

The multiplication formula,

$$e^{q_2Q_2}e^{\xi M}e^{p_2P_2}e^{q_2'Q_2}e^{\xi' M}e^{p_2'P_2}=e^{q_2''Q_2}e^{\xi'' M}e^{p_2''P_2},$$
$$p_2''=p_2'+p_2e^{-\xi'},\quad \xi''=\xi+\xi',\quad q_2''=q_2+q_2', \tag{47}$$

and the correspondence formula,

$$e^{p_2P_2}e^{\xi M}=e^{p_2'P_2+\xi' M},$$
$$\xi'=\xi,\quad p_2'=\frac{\xi p_2}{\exp(\xi)-1},\quad p_2=\frac{\exp(\xi')-1}{\xi'}\,p_2', \tag{48}$$

follow from (46). That yields useful relations:

$$e^{sS}=e^{-sQ_2}e^{(1-\exp(s))P_2}e^{sM}=e^{(1-\exp(s))P_2}e^{sM}e^{-sQ_2},$$
$$e^{\ln(1+m)(M-2P_2)}=e^{-2mP_2}e^{\ln(1+m)M}. \tag{49}$$

For the entire group $GPQS$, the formula of two elements' product reads

$$G(p,q,s)=e^{p_iP_i}e^{q_1Q_1}e^{q_2Q_2}e^{q_3Q_3}e^{sS}=e^{p_iP_i}e^{sS}e^{q_1Q_1}e^{q_2Q_2}e^{q_3Q_3}\in GPQS,$$
$$G(p,q,s)G(p',q',s')=G(p'',q'',s''),$$
$$p_i''=p_i+e^s\overline{T_{ik}}(q)p_k', \tag{50}$$
$$q_1''=q_1+\frac{q_1'e^{-q_2}}{1-q_3q_1'/2},\quad q_2''=q_2+q_2'+\ln\left(1-\frac{q_3q_1'}{2}\right)^2,\quad q_3''=q_3'+\frac{q_3e^{-q_2'}}{1-q_3q_1'/2},$$
$$s''=s+s'.$$

The representation conjugated with adjoint one of the group is given by the formulas

$$G(p,q,s)P_kG^{-1}(p,q,s)=P_ie^s\overline{T_{ik}}(q),$$
$$GQ_kG^{-1}=Q_i\overline{T_{ik}}+P_1(p_1\overline{T_{2k}}-p_2\overline{T_{1k}})+P_2(p_1\overline{T_{3k}}-p_3\overline{T_{1k}})+P_3(p_2\overline{T_{3k}}-p_3\overline{T_{2k}}), \tag{51}$$
$$GSG^{-1}=-P_ip_i+S.$$

VI. SOME CONSEQUENCES

We will call as extended collision operator the following operator:

$$\hat{I}_g(p,q,s)=e^{p_iP_i}e^{sS}e^{q_1Q_1}e^{q_2Q_2}e^{q_3Q_3}\hat{\chi}, \tag{52}$$

which one can obtain acting by a transformation from the group $GPQS$ (50) on the simplest collision operator $\hat{\chi}$ for collisions with infinitely heavy centers being at rest.

As follows from (28) and (49) and also from property (30) and formulas (54), (55), and (37), the conjugated operator is connected with the collision operator by the relation

$$\tilde{\hat{I}}=e^{-2mP_2}\hat{I}=e^{\sqrt{2}(m_1/kT)Q_3}\hat{I}. \tag{53}$$

Taking into account (25), (49), and the first part of (53), one can express the collision operator $\hat{I}$ and the conjugated collision operator $\tilde{\hat{I}}$ in terms of the extended operator $\hat{I}_g$ with accordingly chosen parameters:

$$\hat{I}=\hat{I}_g(p,q,s),$$
$$p_1=\sqrt{2}\,\frac{kT}{m_2},\quad p_2=m,\quad p_3=0;\quad q_1=0,\quad q_2=\ln(1+m),\quad q_3=0;\quad s=\ln(1+m); \tag{54}$$

$$\tilde{\hat{I}}=\hat{I}_g(p,q,s), \tag{55}$$

$$p_1=\sqrt{2}\,\frac{kT}{m_2},\quad p_2=-m,\quad p_3=0;\quad q_1=0,\quad q_2=\ln(1+m),\quad q_3=0;\quad s=\ln(1+m).$$

Energy conservation law (29) yields the identity for the extended collision operator:

$$G(p,q,s)Q_3G^{-1}(p,q,s)\hat{I}_g(p,q,s)=0. \tag{56}$$

An explicit form of (56) can be obtained with the help of (51) and (41):

$$\left\{\frac{q_1^2}{2}\,Q_1+q_1Q_2+Q_3+q_1\left(p_1-p_2\,\frac{q_1}{2}\right)P_1+\left(p_1-p_3\,\frac{q_1^2}{2}\right)P_2+(p_2-p_3q_1)P_3\right\}\hat{I}_g(p,q,s)=0. \tag{57}$$

In the case of the constant collision frequency, we add two more identities due to (31), (29), and (33):

$$G(p,q,s)Q_1G^{-1}(p,q,s)\hat{I}_g(p,q,s)=0,\quad G(p,q,s)Q_2G^{-1}(p,q,s)\hat{I}_g(p,q,s)=0,$$
$$\text{when}\quad \nu=\text{const},\quad \chi(\mu,v)=\chi(\mu). \tag{58}$$

We can get the explicit form of them using (51) and (41) accordingly:

$$\left\{\left(1-\frac{q_1q_3}{2}\,e^{q_2}\right)^2e^{-q_2}Q_1-q_3\left(1-\frac{q_1q_3}{2}\,e^{q_2}\right)Q_2+\frac{q_3^2}{2}\,e^{q_2}Q_3+\left[-p_1q_3\left(1-\frac{q_1q_3}{2}\,e^{q_2}\right)\right.\right.$$
$$\left.-p_2\left(1-\frac{q_1q_3}{2}\,e^{q_2}\right)^2e^{-q_2}\right]P_1+\left[p_1\,\frac{q_3^2}{2}\,e^{q_2}-p_3\left(1-\frac{q_1q_3}{2}\,e^{q_2}\right)^2e^{-q_2}\right]P_2$$
$$\left.+\left[p_2\,\frac{q_3^2}{2}\,e^{q_2}+p_3q_3\left(1-\frac{q_1q_3}{2}\,e^{q_2}\right)\right]P_3\right\}\hat{I}_g(p,q,s)=0,$$
$$\text{when}\quad \nu=\text{const},\quad \chi(\mu,v)=\chi(\mu); \tag{59}$$

$$\left\{q_1\left(1-\frac{q_1q_3}{2}\,e^{q_2}\right)Q_1+(1-q_1q_3e^{q_2})Q_2-q_3e^{q_2}Q_3+\left[p_1(1-q_1q_3e^{q_2})\right.\right.$$
$$\left.-p_2q_1\left(1-\frac{q_1q_3}{2}\,e^{q_2}\right)\right]P_1-\left[p_1q_3e^{q_2}+p_3q_1\left(1-\frac{q_1q_3}{2}\,e^{q_2}\right)\right]P_2$$
$$\left.-[p_2q_3e^{q_2}+p_3(1-q_1q_3e^{q_2})]P_3\right\}\hat{I}_g(p,q,s)=0;$$
$$\text{when}\quad \nu=\text{const},\quad \chi(\mu,v)=\chi(\mu). \tag{60}$$

Identities (57), (59), and (60) with the parameters given by (54) for the operator $\hat{I}$ are reduced to the form

$$\left(v^{2}*+\frac{2kT}{m_2}\,\nabla*\boldsymbol{v}*+m\boldsymbol{v}*\boldsymbol{v}*\right)\hat{I}=0; \tag{61}$$

$$(\nabla^{2}*-m\nabla*\nabla*)\hat{I}=0,\quad \text{when}\quad \nu=\text{const},\quad \chi(\mu,\text{v})=\chi(\mu); \tag{62}$$

$$\left((\boldsymbol{v}\boldsymbol{\nabla})*+\frac{kT}{m_2}\boldsymbol{\nabla}*\boldsymbol{\nabla}*\right)\hat{I}=0,\quad \text{when}\quad \nu=\text{const},\quad \chi(\mu,\text{v})=\chi(\mu). \tag{63}$$

The temperature transformation that gets the collision operator $\hat{I}$ can be represented by the similitude

$$\begin{aligned}\hat{I}&=Ge^{[(1+m)/m](\sqrt{2}kT/m_2)Q_1}G^{-1}Ge^{[-(1+m)/m](\sqrt{2}kT/m_2)Q_1}\hat{\chi}=e^{(kT/2m_1)\nabla^2}*\hat{J}'\\&=e^{(kT/2m_1)\nabla^2}\hat{J}'e^{-(kT/2m_1)\nabla^2},\end{aligned} \tag{64}$$

where

$$\hat{J}'=e^{\ln(1+m)M}\hat{\chi}',$$

$$\hat{\chi}'=e^{-(1+m)(kT/2m_1)\nabla^2}\hat{\chi}e^{(1+m)(kT/2m_1)\nabla^2}.$$

In the case the collision frequency does not depend on the velocity, we have $\hat{\chi}'=\hat{\chi}$ due to property (31) and consequently $\hat{J}'=\hat{J}$. Therefore, for that case the collision operator $\hat{I}$ is expressed in terms of the collision operator $\hat{J}$ for collisions with molecules at rest with the help of the simple similitude:

$$\hat{I}=e^{(kT/2m_1)\nabla^2}*\hat{J}=e^{(kT/2m_1)\nabla^2}\hat{J}e^{-(kT/2m_1)\nabla^2},\quad \text{when}\quad \nu=\text{const},\quad \chi(v,\mu)=\chi(\mu), \tag{65}$$

which is based on the Gauss transformation:[6]

$$e^{(kT/2m_1)\nabla^2}f(\boldsymbol{v})=\left(\frac{m_1}{2\pi kT}\right)^{3/2}\int d\boldsymbol{v}'e^{-m_1(\boldsymbol{v}-\boldsymbol{v}')^2/2kT}f(\boldsymbol{v}'). \tag{66}$$

VII. TRANSFORMATIONS FROM THE RENORMGROUP OF THE BOLTZMANN LINEAR KINETIC EQUATION

We use the term *renormgroup* here to underline that the group transformations affect not only the variables $\boldsymbol{v}$, $\boldsymbol{r}'$, t, but the problem's parameters T, m, $\mathbf{w}$, too. Thus, we use the renormgroup ideology.[1]

Let us consider nonuniform drift of charged particles through the gas of heated molecules in the electric and magnetic fields.[7] The distribution function of charged particles $f(\boldsymbol{v},\boldsymbol{r},t)$ satisfies the Boltzmann kinetic equation with the extended operator parameters p, q, s taken from (54):

$$\frac{\partial f}{\partial t}+\boldsymbol{v}\boldsymbol{\nabla}_{\boldsymbol{r}}f+(\boldsymbol{w}+\boldsymbol{v}\times\Omega)\boldsymbol{\nabla}f=\hat{I}_g(p,q,s)f, \tag{67}$$

where $\mathbf{w}=e\boldsymbol{E}/m$, $\Omega=e\boldsymbol{B}/mc$, $\boldsymbol{\nabla}_{\boldsymbol{r}}=\partial/\partial\boldsymbol{r}$, $\boldsymbol{\nabla}=\partial/\partial\boldsymbol{v}$.

The operator of the left part of Eq. (67),

$$\hat{L}=\frac{\partial}{\partial t}+\boldsymbol{v}\nabla_{\boldsymbol{r}}+(\boldsymbol{w}+\boldsymbol{v}\times\Omega)\boldsymbol{\nabla},$$

is transformed by generators from the AQ algebra as follows:

$$Q_1\hat{L}=\frac{1}{\sqrt{8}}\,[\nabla^2,\hat{L}]=\frac{1}{\sqrt{2}}\,\boldsymbol{\nabla}\boldsymbol{\nabla}_{\boldsymbol{r}},$$

$$Q_2\hat{L}=\tfrac{1}{2}\,[\boldsymbol{v}\boldsymbol{\nabla},\hat{L}]=\tfrac{1}{2}\,(\boldsymbol{v}\boldsymbol{\nabla}_{\mathbf{r}}-\boldsymbol{w}\boldsymbol{\nabla}), \tag{68}$$

$$Q_3\hat{L}=\frac{1}{\sqrt{8}}\,[v^2,\hat{L}]=-\frac{1}{\sqrt{2}}\,\boldsymbol{w}\boldsymbol{v}.$$

It is easy to see that the action of the operators affecting the problem's parameter $\boldsymbol{w}$ and spatial variable $\boldsymbol{r}$ leads to the same results:

$$\frac{1}{\sqrt{2}}\,(\boldsymbol{\nabla}_{\boldsymbol{r}}\nabla_{\boldsymbol{w}})*\hat{L}=\frac{1}{\sqrt{2}}\,[\boldsymbol{\nabla}_{\boldsymbol{r}}\boldsymbol{\nabla}_{\boldsymbol{w}},\hat{L}]=\frac{1}{\sqrt{2}}\,\boldsymbol{\nabla}\boldsymbol{\nabla}_{\boldsymbol{r}},$$

$$-\tfrac{1}{2}\,(\boldsymbol{r}\boldsymbol{\nabla}_{\boldsymbol{r}}+\boldsymbol{w}\boldsymbol{\nabla}_{\boldsymbol{w}})*\hat{L}=-\tfrac{1}{2}\,[(\boldsymbol{r}\boldsymbol{\nabla}_{\boldsymbol{r}}+\boldsymbol{w}\boldsymbol{\nabla}_{\boldsymbol{w}}),\hat{L}]=\tfrac{1}{2}\,(\boldsymbol{v}\boldsymbol{\nabla}_{\boldsymbol{r}}-\boldsymbol{w}\boldsymbol{\nabla}), \tag{69}$$

$$\frac{1}{\sqrt{2}}\,(\boldsymbol{w}\boldsymbol{r})*\hat{L}=\frac{1}{\sqrt{2}}\,[\boldsymbol{w}\boldsymbol{r},\hat{L}]=-\frac{1}{\sqrt{2}}\,\boldsymbol{w}\boldsymbol{v}.$$

Therefore, the difference of the operators from (68) and (69) gives us the set of generators commutating with operator $\hat{L}$. The group constructed on their base keeps the operator $\hat{L}$ invariant,

$$e^{(\overline{q_1}/\sqrt{8})\,(\nabla^2-2\boldsymbol{\nabla}_{\boldsymbol{r}}\boldsymbol{\nabla}_{\boldsymbol{w}})*}\hat{L}=e^{(\overline{q_1}/\sqrt{8})(\nabla^2-2\boldsymbol{\nabla}_{\boldsymbol{r}}\boldsymbol{\nabla}_{\boldsymbol{w}})}\hat{L}\,e^{-(\overline{q_1}/\sqrt{8})(\nabla^2-2\boldsymbol{\nabla}_{\boldsymbol{r}}\boldsymbol{\nabla}_{\boldsymbol{w}})}=\hat{L},$$

$$e^{(\overline{q_2}/2)\,(\boldsymbol{v}\boldsymbol{\nabla}+\boldsymbol{r}\boldsymbol{\nabla}_{\boldsymbol{r}}+\boldsymbol{w}\boldsymbol{\nabla}_{\boldsymbol{w}})*}\hat{L}=e^{(\overline{q_2}/2)\,(\boldsymbol{v}\boldsymbol{\nabla}+\boldsymbol{r}\boldsymbol{\nabla}_{\boldsymbol{r}}+\boldsymbol{w}\boldsymbol{\nabla}_{\boldsymbol{w}})}\hat{L}\,e^{-(\overline{q_2}/2)(\boldsymbol{v}\boldsymbol{\nabla}+\boldsymbol{r}\boldsymbol{\nabla}_{\boldsymbol{r}}+\boldsymbol{w}\boldsymbol{\nabla}_{\boldsymbol{w}})}=\hat{L}, \tag{70}$$

$$e^{(\overline{q_3}/\sqrt{8})(v^2-2\boldsymbol{w}\boldsymbol{r})*}\hat{L}=e^{(\overline{q_3}/\sqrt{8})(v^2-2\boldsymbol{w}\boldsymbol{r})}\hat{L}\,e^{-(\overline{q_3}/\sqrt{8})(v^2-2\boldsymbol{w}\boldsymbol{r})}=\hat{L}.$$

The extended collision operator $\hat{I}_g(p,q,s)$ is transformed under the GQ group, because operators (69) do not affect the velocity and commutate with $\hat{I}_g(p,q,s)$:

$$e^{(\overline{q_1}/\sqrt{8})(\nabla^2-2\boldsymbol{\nabla}_{\boldsymbol{r}}\boldsymbol{\nabla}_{\boldsymbol{w}})*}\hat{I}_g(p,q,s)=e^{\overline{q_1}Q_1}\hat{I}_g(p,q,s)=\hat{I}_g(p',q',s'),$$

$$e^{(\overline{q_2}/2)(\boldsymbol{v}\boldsymbol{\nabla}+\boldsymbol{r}\boldsymbol{\nabla}_{\boldsymbol{r}}+\boldsymbol{w}\boldsymbol{\nabla}_{\boldsymbol{w}})*}\hat{I}_g(p,q,s)=e^{\overline{q_2}Q_2}\hat{I}_g(p,q,s)=\hat{I}_g(p',q',s'), \tag{71}$$

$$e^{(\overline{q_3}/\sqrt{8})(v^2-2\boldsymbol{w}\boldsymbol{r})*}\hat{I}_g(p,q,s)=e^{\overline{q_3}Q_3}\hat{I}_g(p,q,s)=\hat{I}_g(p',q',s').$$

Therefore, the kinetic equation (67) is invariant regarding the transformations with parameters $\overline{q_1}$, $\overline{q_2}$, and $\overline{q_3}$ due to properties (70), (71), (42), and (43). The transformations have the form

$$p_i'=\overline{T_{ik}}(\overline{q})p_k,\quad s'=s,$$

$$q_1'=\overline{q_1}+\frac{q_1e^{-\overline{q_2}}}{1-\overline{q_3}q_1/2},\quad q_2'=\overline{q_2}+q_2+\ln\left(1-\frac{\overline{q_3}q_1}{2}\right)^2,\quad q_3'=q_3+\frac{\overline{q_3}e^{-q_2}}{1-\overline{q_3}q_1/2},$$

$$f'(\boldsymbol{v},\boldsymbol{r},t;\boldsymbol{w},p',q',s')=e^{(\overline{q_1}/\sqrt{8})(\nabla^2-2\boldsymbol{\nabla}_{\boldsymbol{r}}\boldsymbol{\nabla}_{\boldsymbol{w}})}e^{(\overline{q_2}/2)(\boldsymbol{v}\boldsymbol{\nabla}+\boldsymbol{r}\boldsymbol{\nabla}_{\boldsymbol{r}}+\boldsymbol{w}\boldsymbol{\nabla}_{\boldsymbol{w}})}e^{(\overline{q_3}/\sqrt{8})(v^2-2\boldsymbol{w}\boldsymbol{r})}f(\boldsymbol{v},\boldsymbol{r},t;\boldsymbol{w},p,q,s,). \tag{72}$$

We will give three simple examples of using the transformation (72).

Example 1: If we change the parameters p, q, and s in problem (67) and take them from (55), we will have $\hat{I}_g(p,q,s)=\tilde{\hat{I}}$. For these parameters a constant N_0 becomes the solution of Eq. (67)

due to the property of the conjugated collision operator, $\tilde{\hat{I}}N_0 = 0$. Transformation (72) with parameters $\overline{q_3} = -\sqrt{2}m_1/kT$ and $\overline{q_1} = \overline{q_2} = 0$ transforms [see (53)] $\tilde{\hat{I}}$ into $\hat{I}$ so that, with the help of this transformation, we can get the classic Maxwell–Boltzmann solution for problem (67):

$$f = N_0 e^{-(m_1/2kT)(v^2 - 2\mathbf{wr})}. \tag{73}$$

Example 2: The extended collision operator with parameters p, q, and s given by formula (54) at $T=0$ is the collision operator $\hat{J}$ for collisions with molecules being at rest before collision. In the case of the constant collision frequency, transformation (72) with parameters $\overline{q_1} = \sqrt{2}kT/m_1$ and $\overline{q_2} = \overline{q_3} = 0$ transforms the operator $\hat{J}$ into $\hat{I}$ due to property (65). Therefore, transformation (72) with those parameters makes it possible to express the distribution function of charged particles drifting in a heated gas ($T \neq 0$) in terms of the distribution function of charged particles drifting in a cold gas ($T=0$):

$$f(\mathbf{v},\mathbf{r},t;\mathbf{w},T) = e^{(kT/2m_1)(\nabla^2 - 2\nabla_r \nabla_w)} f(\mathbf{v},\mathbf{r},t;\mathbf{w},\ T=0), \quad \text{when} \quad \nu = \text{const}, \quad \chi(\mu,\text{v}) = \chi(\mu). \tag{74}$$

Using the property of the Fourier transformation,

$$\hat{F}\nabla_r \hat{F}^{-1} = i\mathbf{k}, \quad [\hat{F}f](\mathbf{k}) = \frac{1}{(2\pi)^{3/2}} \int d\mathbf{r} e^{-i\mathbf{kr}} f(\mathbf{r}), \tag{75}$$

and formulas (66), (10), we get the integral representation of transformation (74):

$$f(\mathbf{v},\mathbf{r},t;\mathbf{w},T) = \left(\frac{m_1}{2\pi kT}\right)^{3/2} \int \frac{d\mathbf{v}'\, d\mathbf{r}'\, d\mathbf{k}}{(2\pi)^3} e^{-m_1(\mathbf{v}-\mathbf{v}')^2/2kT + i\mathbf{k}(\mathbf{r}-\mathbf{r}')} \times f\left(\mathbf{v}',\mathbf{r}',t;\mathbf{w} - i\frac{kT}{m_1}\mathbf{k},\ T=0\right) \quad \text{when} \quad \nu = \text{const}, \quad \chi(\mu,\text{v}) = \chi(\mu). \tag{76}$$

Formula (76) gives a generalization of the Wannier[8] theorem of convolution on the spatial not uniform case with presence of the magnetic field.

Example 3: When $\nu = \text{const}$, and $\chi(\mu,\text{v}) = \chi(\mu)$, a class of the exact solutions of the equation

$$\frac{\partial f}{\partial t} + \mathbf{v}\nabla_r f + (\mathbf{w} + \mathbf{v} \times \Omega)\nabla f = \hat{I} f, \tag{77}$$

describing spatial and velocity relaxation of the plasma charged component in the electric and magnetic fields has the form

$$f(\mathbf{v},\mathbf{r},t) = e^{-(m_1/2kT)(v^2 - 2\mathbf{wr})} e^{-(kT/2m_1)(\nabla^2 - 2\nabla_r\nabla_w)} e^{t[\tilde{\hat{J}} - \mathbf{v}\nabla_r - (\mathbf{w}+\mathbf{v}\times\Omega)\nabla]} p_n(\mathbf{v},\mathbf{r}), \tag{78}$$

where $p_n(\mathbf{v},\mathbf{r})$ is an arbitrary polynomial of the order n of the velocity and radius vector components, and the function

$$\varphi(\mathbf{v},\mathbf{r},t) = e^{t[\tilde{\hat{J}} - \mathbf{v}\nabla_r - (\mathbf{w}+\mathbf{v}\times\Omega)\nabla]} p_n(\mathbf{v},\mathbf{r}) \tag{79}$$

is a solution of the equation

$$\frac{\partial \varphi}{\partial t} + \mathbf{v}\nabla_r \varphi + (\mathbf{w} + \mathbf{v} \times \Omega)\nabla\varphi = \tilde{J}\varphi. \tag{80}$$

In fact, the linear vector space of polynomials of the order not greater than n is invariant with respect to the operator

$$\hat{H}=\tilde{\tilde{J}}-\boldsymbol{v}\boldsymbol{\nabla}_{\boldsymbol{r}}-(\boldsymbol{w}+\boldsymbol{v}\times\Omega)\boldsymbol{\nabla},$$

and therefore the operator is represented by the matrix in that space. Thus the exponential in (78) and (79) is a function in terms of the matrix and its action on a polynomial is defined by the usual rules.[9] A simple example of a solution (nonpositive) from class (78) is the solution ($n=1$)

$$f=e^{-(m_1/2kT)(v^2-2\boldsymbol{w}\boldsymbol{r})}\left\{c_0+\boldsymbol{c}_1[(\lambda+\Omega\times)\boldsymbol{r}+\boldsymbol{v}-\boldsymbol{w}t]+\boldsymbol{c}_{2+}\left(\boldsymbol{v}-\frac{\boldsymbol{w}}{\lambda-i\Omega}\right)e^{(\lambda-i\Omega)t}\right.$$
$$\left.+\boldsymbol{c}_{2-}\left(\boldsymbol{v}-\frac{\boldsymbol{w}}{\lambda+i\Omega}\right)e^{(\lambda+i\Omega)t}+\boldsymbol{c}_{2\mathrm{II}}\left(\boldsymbol{v}-\frac{\boldsymbol{w}}{\lambda}\right)e^{\lambda t}\right\}, \tag{81}$$

where c_0 is an arbitrary constant, $\boldsymbol{c}_1$ is an arbitrary vector constant, $\boldsymbol{c}_{2+}$, $\boldsymbol{c}_{2-}$, $\boldsymbol{c}_{2\mathrm{II}}$ are the cyclic components of an arbitrary vector constant those can be effectively used[10] for description the ionospheric magnetoactive plasma dynamic,

$$\boldsymbol{c}_{2\pm}=-\frac{\Omega\times(\Omega\times\pm i\Omega)}{2\Omega^2}\boldsymbol{c}_2,\quad \boldsymbol{c}_{2\mathrm{II}}=\frac{\Omega\times\Omega\times+\Omega^2}{\Omega^2}\boldsymbol{c}_2,$$

where $\lambda=\lambda_1^0$ is the eigenvalue[4,11] of the conjugated collision operator, $\tilde{\tilde{J}}\boldsymbol{v}=\lambda_1^0\boldsymbol{v}$.

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Rigorous estimates of small scales in turbulent flows

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We derive rigorous bounds on the length scale of determining local averages (volume elements) for the 3-D Navier-Stokes Equations. These length scale estimates are related to Kolmogorov's notion of a dissipation length scale in turbulent flows.
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I. INTRODUCTION

We consider the Navier-Stokes Equations (NSE)

$$\begin{cases} \dfrac{\partial}{\partial t}u-\nu\Delta u+(u\cdot\nabla)u+\nabla p=f \\ \nabla\cdot u=0 \end{cases},$$

in the cube $\Omega=[0,L]^3$. The above equations are subject to either periodic or Dirichlet boundary conditions. Let us divide Ω into N^3 small sub-cubes, $\{Q_j\}_{j=1}^{N^3}$, each with side of length $\ell=LN^{-1}$. Let us denote by

$$\overline{w_j}=\frac{1}{|Q_j|}\int_{Q_j} w(x)dx, \quad \text{for } j=1,2,\ldots,N^3,$$

the average of the function w in the small cube Q_j, and we set

$$\overline{\eta(w)}=\left(\sum_{j=1}^{N^3}|\overline{w_j}|^2\right)^{1/2}.$$

Following Ref. 1 (see also Ref. 2) we say that the set of sub-cubes $\{Q_j\}_{j=1}^{N^3}$ is a set of determining volume elements if for any two solutions $u(t),v(t)$ of the NSE, $\overline{\eta((u(t)-v(t)))}\to 0$, $t\to\infty$, implies $\|u(t)-v(t)\|\to 0$ as $t\to\infty$, in some reasonable norm $\|\cdot\|$. This concept was inspired by the notions of determining modes and determining nodes which were introduced by Foias and Prodi in Ref. 3 and by Foias and Temam in Ref. 4, respectively. These ideas were developed in an attempt to identify and study the finite number of degrees of freedom in turbulent flows. Rigorous *global* estimates on the number of determining modes, determining nodes and determining volume elements were established in Refs. 5, 6, and 2, respectively. An

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improvement of these global estimates was recently reported in Ref. 7. Moreover, a unified treatment of these concepts and more general ones, such as determining finite elements, has been recently developed in Refs. 8 and 9.

The above mentioned estimates are global in the sense that they are independent of the individual solution. In this paper, however, we give an upper bound on the minimal number of determining volume elements, N^3, or equivalently a lower bound on the size of determining finite volume elements (cubes), ℓ, in terms of the viscosity, and a modified mean rate of dissipation. The latter is a function of the individual solution. It is noteworthy that estimates for the number of determining volume elements that we provide here are the same as those established in Ref. 10 for the number of determining modes. This study is complementary to other rigorous work identifying small length scales in solutions of the NSE.[10–14]

II. PRELIMINARIES

We denote by $L^p(D)$ the usual Lebesgue spaces in the domain D, and by $H^k(D)$ the usual L^2 Sobolev spaces of index k in the domain D. Hereafter c_i, for $i=1,2,\ldots$, will denote positive dimensionless universal constants.

First let us prove the following version of the Poincaré inequality.

Lemma 2.1: *For every* $w \in H^1(Q_j)$ *we have*

$$\|w\|^2_{L^2(Q_j)} \leq 2|\overline{w_j}|^2 \ell^3 + c_1 \ell^2 \|\nabla w\|^2_{L^2(Q_j)}, \tag{1}$$

$$\|w\|^2_{L^2(\Omega)} \leq 2(\overline{\eta(w)})^2 \ell^3 + c_1 \ell^2 \|\nabla w\|^2_{L^2(\Omega)}. \tag{2}$$

Proof: By the Poincaré inequality we have

$$\|w - \overline{w_j}\|_{L^2(Q_j)} \leq c_1 \ell \|\nabla w\|_{L^2(Q_j)},$$

where c_1 is a universal constant independent of w and Q_j. From the above we get

$$\|w\|_{L^2(Q_j)} \leq |Q_j|^{1/2} |\overline{w_j}| + c_1 \ell \|\nabla w\|_{L^2(Qj)},$$

which establishes (1). To prove (2) we sum the (1) over $j=1,\ldots,N^3$.

Let us recall the following Lemma from Ref. 5 (see also Ref. 2).

Lemma 2.2: *Let* α *be a locally integrable real valued function on* $(0,\infty)$ *satisfying, for some* $0<T<\infty$, *the following conditions:*

$$\liminf_{t\nearrow\infty} \frac{1}{T}\int_t^{t+T} \alpha(\tau)\,d\tau = \gamma > 0,$$

$$\limsup_{t\to\infty} \frac{1}{T}\int_t^{t+T} \alpha^-(\tau)\,d\tau = \Gamma < \infty,$$

where $\alpha^- = \max\{-\alpha,0\}$. *Further, let* β *be a real valued locally integrable function defined on* $(0,\infty)$ *such that*

$$\lim_{t\to\infty} \frac{1}{T}\int_t^{t+T} \beta^+(\tau)\,d\tau = 0,$$

where $\beta^+ = \max\{\beta,0\}$. *Suppose that* ξ *is an absolutely continuous non-negative function on* $(0,\infty)$ *such that*

$$\frac{d}{dt}\xi+\alpha\xi\leqslant\beta, \qquad \text{a.e. on } (0,\infty).$$

Then $\xi(t)\to 0$ *as* $t\to\infty$.

III. MAIN RESULTS

We now state our main result:

Theorem 3.1: *Let* u *be any solution of the NSE. Suppose that the length of the side of* Q_j, *for* $j=1,\ldots,N^3$, *is small enough so that*

$$\ell^{-2}\geqslant\frac{4c_1}{\nu}\inf_{T>0}\left(\limsup_{t\to\infty}\frac{1}{T}\int_t^{t+T}\|\nabla u(s)\|_{L^\infty(\Omega)}ds\right). \tag{3}$$

Then for any solution v *of the NSE for which* $\overline{\eta}((u(t)-v(t)))\to 0$, *as* $t\to\infty$, *we have* $\|u(t)-v(t)\|_{L^2(\Omega)}\to 0$, *as* $t\to\infty$.

Proof: Let us set $w=u-v$. Then, w satisfies

$$\frac{\partial w}{\partial t}-\nu\Delta w+(u\cdot\nabla)w+(w\cdot\nabla)u-(w\cdot\nabla)w+\nabla(p_u-p_v)=0,$$

where p_u and p_v are the pressure fields corresponding to the solutions u and v respectively. Multiply the above equation by w and integrate over Ω to obtain

$$\frac{1}{2}\frac{d}{dt}\|w\|^2_{L^2(\Omega)}-\nu\int_\Omega\Delta w(x)\cdot w(x)dx+\int_\Omega((w(x)\cdot\nabla)u(x))\cdot w(x)dx+\int_\Omega((u(x)\cdot\nabla)w(x))\cdot w(x)dx-\int_\Omega((w(x)\cdot\nabla)w(x))\cdot w(x)dx=0.$$

Notice that $\int_\Omega\nabla(p_u(x)-p_v(x))\cdot w(x)dx=0$ because $\nabla\cdot w=0$ and $w|_{\partial\Omega}=0$ (or periodic). Integrate by parts the above equations and use again the facts that $\nabla\cdot u=\nabla\cdot w=0$ and that $w|_{\partial\Omega}=0$ (or periodic) to get

$$\frac{1}{2}\frac{d}{dt}\|w\|^2_{L^2(\Omega)}+\nu\|\nabla w\|^2_{L^2(\Omega)}=-\int_\Omega[(w(x)\cdot\nabla)u(x)]\cdot w(x)dx. \tag{4}$$

Now, we estimate the right hand side

$$\left|\int_\Omega((w(x)\cdot\nabla)u(x))\cdot w(x)dx\right|\leqslant\|\nabla u\|_{L^\infty(\Omega)}\|w\|^2_{L^2(\Omega)}.$$

Hence equation (4) becomes:

$$\frac{1}{2}\frac{d}{dt}\|w\|^2_{L^2(\Omega)}+\nu\|\nabla w\|^2_{L^2(\Omega)}\leqslant\|w\|^2_{L^2(\Omega)}\|\nabla u\|_{L^\infty(\Omega)},$$

and from (2) we have

$$\frac{1}{2}\frac{d}{dt}\|w\|^2_{L^2(\Omega)}+\left(\frac{\nu}{c_1\ell^2}-\|\nabla u\|_{L^\infty(\Omega)}\right)\|w\|^2_{L^2(\Omega)}\leqslant\frac{2\nu\ell}{c_1}(\overline{\eta}(w))^2.$$

Let $T_*>0$ be chosen such that

$$\inf_{T>0}\left(\limsup_{t\to\infty}\frac{1}{T}\int_t^{t+T}\left\|\nabla u(s)\right\|_{L^\infty(\Omega)}ds\right)\leqslant\limsup_{t\to\infty}\frac{1}{T_*}\int_t^{t+T_*}\|\nabla u(s)\|_{L^\infty(\Omega)}ds\leqslant\frac{\nu}{2c_1\ell^2}.$$

Now, we apply Lemma 2.2 with $\alpha(t)=\nu/c_1\ell^2-\|\nabla u(t)\|_{L^\infty(\Omega)}$, $\beta(t)=(2\nu\ell/c_1)(\overline{\eta}(w))^2$ and $T=T_*$ to conclude the Theorem.

Let u be any solution of the NSE. Following the conventional theory of turbulence we set

$$\epsilon=\frac{\nu}{L^3}\langle\|\nabla u\|^2_{L^2(\Omega)}\rangle,$$

the mean rate of energy dissipation, where $\langle\cdot\rangle$ denotes some kind of ensemble average (usually taken to be time average). Following Kolmogorov[15] we identify a small length scale in the flow to be

$$\ell_K\sim\left(\frac{\nu^3}{\epsilon}\right)^{1/4}.$$

By analogy let us define a modified mean rate of energy dissipation,

$$\epsilon_\infty=\nu\inf_{T>0}\left(\limsup_{t\to\infty}\frac{1}{T}\int_t^{t+T}\|\nabla u(s)\|^2_{L^\infty(\Omega)}ds\right),$$

and a modified small length scale:

$$\ell_{K,\infty}=\frac{1}{\sqrt{4c_1}}\left(\frac{\nu^3}{\epsilon_\infty}\right)^{1/4}.$$

As a corollary of the above Theorem we have:

Corollary 3.2: *If the side of each of the cubes Q_j, for $j=1,\ldots,N^3$, is small enough, in particular if $\ell\leqslant\ell_{K,\infty}$, then the cubes are determining volume elements.*

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Explicit solutions of supersymmetric KP hierarchies: Supersolitons and solitinos

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Wide classes of explicit solutions of the Manin-Radul and Jacobian supersymmetric KP hierarchies are constructed by using line bundles over complex supercurves based on the Riemann sphere. Their construction extends several ideas of the standard KP theory, such as wave functions, ∂-equations and τ-functions. Thus, supersymmetric generalizations of N-soliton solutions, including a new purely odd ''solitino'' solution, as well as rational solutions, are found and characterized. © *1996 American Institute of Physics.* [S0022-2488(96)02112-3]

I. INTRODUCTION

The most appealing aspects of the theory of the KP hierarchy have a rich geometrical content and it is likely that this fact is at the heart of the relevance of integrable systems in modern theoretical physics.[1,2] For example, a common feature of the explicit methods of solutions is that they frequently involve geometric objects such as Grassmannians, algebraic curves, Abelian functions, and holomorphic line bundles.[3–9] This also happens to be true in the context of supersymmetric KP (SKP) hierarchies[10,11] and it is expected that some of these integrable systems are to find applications in string theory and quantum gravity.[12–14] The aim of this article is to show how line bundles over complex supercurves can be used to provide efficient methods of solution for the SKP hierarchies formulated by Manin and Radul (MRKP)[15] and Mulase and Rabin (JKP).[10,11] Both hierarchies have attracted much attention because of their important mathematical content. Apart from sharing many of the standard integrability properties, among their reductions they have a supersymmetric generalization of the KdV hierarchy with a rich Hamiltonian structure[15–17] and they are relevant from the point of view of superconformal algebra.[18–20] A basic goal of our study is to generalize some of the standard methods of solution arising in the KP theory and to characterize the classes of solutions they determine. In particular we want to investigate solutions of soliton type and their relationship with the standard KP solitons. To this end we extend some strategies of the Grassmannian approach for constructing several types of solutions and apply them to the SKP hierarchies.

This work is based on the concept of super-wave function for a system of Sato equations of supersymmetric type. As it is known from our experience with the KP hierarchy, the notion of wave function is what allows us to derive methods of solution based on the resolution of analytic problems. Despite the seemingly great diversity of these methods, they exhibit a common ingredient: the presence of holomorphic line bundles[6–8] whose sections turn to be the wave functions. Actually, the wave functions are special types of sections satisfying certain conditions as functions of the spectral parameter. These conditions are formulated in several forms depending on the particular approach which is being adopted. For example, they may be expressed by means of a ∂-equation[21,22] or by selecting a subspace of an infinite-dimensional Grassmanian.[7] In this article we characterize the super-wave functions as certain sections of deformations of holomorphic line bundles over complex supercurves based on the Riemann sphere together with the corresponding points in the super-Grassmannian. Finally we also offer a ∂-equation description of them. Then we compute several families of solutions including supersymmetric N-soliton solutions possessing an interesting composite odd structure, and a genuine supersymmetric family of solutions without a bosonic counterpart, unrelated to any class of solution of the standard KP theory, that we call *solitino* solutions. They exhibit a remarkable nonlinear superposition principle and a Fourier-like

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dependence on the bosonic variables. It is worth mentioning that the solutions found in the present work can also be determined, although in a less straigthforward way, through the bilinear formalism proposed in Ref. 23.

The first part of Section II is concerned with a brief review of SKP hierarchies in terms of pseudodifferential operators, including the formulation of Sato equations. The notion of super-wave function is analyzed in the second part of this section. In particular, we describe in detail the derivation of the corresponding expressions for the vacuum super-wave functions. The characterization of super-wave functions as sections of (super) holomorphic line bundles over complex supermanifolds is described in the first part of Section III, and finally in Section IV we relate the above constructions to the supergroup and bilinear formalism.

II. SUPER KP HIERARCHIES

A. Sato equations for super KP hierarchies

The MRKP and JKP hierarchies can be described in a unified way with the help of an algebra $\mathscr{E}$ of super-pseudodifferential operators:[24]

$$X=\sum_{n\leqslant N} a_n(x,\theta,\mathbf{t},\boldsymbol{\tau})D^n, \quad N\in\mathbb{N}, \tag{1}$$

where the coefficients a_n are elements of a supercommutative algebra

$$\mathscr{S}=\mathbb{C}[[x,\mathbf{t}]]\otimes\Lambda(\theta,\boldsymbol{\tau})\otimes\mathscr{A}.$$

Here, x is an even variable, θ is an odd variable, $\mathbf{t}=\{t_n\}_{n=1}^{\infty}$ and $\boldsymbol{\tau}=\{\tau_n\}_{n=1}^{\infty}$ are infinite sets of even and odd variables, respectively, and $\mathscr{A}$ denotes a given complex Grassmann algebra of finite or infinite dimension. The superdifferential operator D is defined as the derivation on $\mathscr{S}$ given by

$$D=\frac{\partial}{\partial\theta}+\theta\frac{\partial}{\partial x},$$

satisfying the identity

$$D^2=\partial\equiv\frac{\partial}{\partial x}.$$

We will denote by $X=X_+ + X_-$ the decomposition of elements $X\in\mathscr{E}$ into positive ($n\geqslant 0$) and negative ($n<0$) powers D^n of D.

Both algebras $\mathscr{S}$ and $\mathscr{E}$ have natural $\mathbb{Z}_2$-graduations

$$\mathscr{S}=\mathscr{S}_{\bar{0}}\oplus\mathscr{S}_{\bar{1}}, \quad \mathscr{E}=\mathscr{E}_{\bar{0}}\oplus\mathscr{E}_{\bar{1}}.$$

An operator (1) is said to have parity p if and only if ($\forall n\leqslant N$) the coefficients a_n have parity $n+p$ mod 2. We may also introduce body maps ϵ on $\mathscr{S}$ and $\mathscr{E}$ (Ref. 24) and, in particular, the body of an operator (1) is given by

$$\epsilon(X)=\sum_{n\ \text{even}}\epsilon(a_n)D^n.$$

Notice that $\epsilon(X)$ is not the even part of X.

The Sato equations for the SKP hierarchies can be written as

$$\frac{\partial K}{\partial t_n} = -(K\partial^n K^{-1})_- K,$$
$$\frac{DK}{D\tau_n} = -(KA_n K^{-1})_- K, \quad n \geqslant 1, \tag{2}$$

for an even $K \in \mathscr{E}$ of the form

$$K = 1 + \sum_{n=1}^{\infty} w_n(x, \theta, \mathbf{t}, \boldsymbol{\tau}) D^{-n}. \tag{3}$$

Notice that $p(w_{2n}) = 0$ and $p(w_{2n+1}) = 1$ so that $p(K) = 0$.

For the MRKP hierarchy the superderivations $D/D\tau_n$ and the operators A_n in (2) are

$$\frac{D}{D\tau_n} = \frac{\partial}{\partial \tau_n} - \sum_{m \geqslant 1} \tau_m \frac{\partial}{\partial t_{n+m-1}}, \quad A_n = D^{2n-1}.$$

while for the JKP version

$$\frac{D}{D\tau_n} = \frac{\partial}{\partial \tau_n}, \quad A_n = (D - \theta D^2) D^{2n-2} = \frac{\partial}{\partial \theta} D^{2n-2}.$$

These hierarchies generalize the standard KP hierarchy in the sense that, as one easily shows, the body $\epsilon(K)$ of a solution K of (2) satisfies the Sato equations for the KP hierarchy in the variables t_n.

By identifying the coefficients of the powers of D in the system (2) one finds infinite systems of superdifferential equations involving the superfunctions $\{w_n\}$. Simpler equations can be obtained by imposing a reduction condition of the type[15]

$$\frac{\partial K}{\partial t_r} = 0, \tag{4}$$

for some $r \geqslant 2$. Indeed, if one introduces the operator

$$L = KDK^{-1} = D + \sum_{n=1}^{\infty} u_n D^{-n+1}, \tag{5}$$

the constraint (4) is equivalent to

$$(L^{2r})_- = (KD^{2r}K^{-1})_- = 0,$$

and it turns out that the operator

$$\mathscr{L} = L^{2r}$$

satisfies the Lax equations

$$\frac{\partial \mathscr{L}}{\partial t_n} = [(\mathscr{L}^{n/r})_+, \mathscr{L}]. \tag{6}$$

The coefficients of the expansion of $(\mathscr{L}^{n/r})_+$ in powers of D are differential polynomials in the coefficients of $\mathscr{L}$ (Ref. 15), so that (6) leads to a system of superdifferential equations for the coefficients of $\mathscr{L}$ which constitutes a supersymmetric generalization of the rth KdV hierarchy.

For example if we asssume (4) for $r=2$, then the operator $\mathscr{L}=L^4$ is of the form

$$\mathscr{L}=D^4+v_1D+v_0,$$

where v_0 and v_1 can be expressed in terms of the coefficients of K as

$$v_0=-2[\partial w_2+(\partial w_1)w_1], \quad v_1=-2\partial w_1. \tag{7}$$

Furthermore, it is easy to find

$$(\mathscr{L}^{3/2})_+=D^6+\frac{3}{2}v_1D^3+\frac{3}{2}v_0D^2+\frac{3}{4}\partial v_1D+\frac{3}{4}\partial v_0,$$

so that the equation corresponding to (6) for $n=3$ reads ($t=t_3$)

$$\begin{aligned}\frac{\partial v_0}{\partial t}&=\frac{1}{4}[\partial(\partial^2v_0+3v_1Dv_0+3v_0^2)],\\ \frac{\partial v_1}{\partial t}&=\frac{1}{4}[\partial(\partial^2v_1+3v_1Dv_1+6v_0v_1)],\end{aligned} \tag{8}$$

which is the supersymmetric Korteweg-de Vries (SKdV) equation of Manin-Radul.[15]

B. Super-wave functions for super KP hierarchies

The notion of super-wave function for a SKP hierarchy requires the introduction of a spectral parameter (z,α), where z denotes a complex variable and α is a new Grassmann variable. The superparameter (z,α) represents local supercoordinates on a complex supercurve $\mathscr{C}$ (see for instance, Ref. 25, and references therein for the notions of supergeometry used in the following) with structure sheaf $\mathscr{O}$ and not being necessarily a super-Riemann surface (SRS). Let p be a point in the body of $\mathscr{C}$ and D a disk containing p. We shall denote by $\mathscr{O}^*$ the restriction of sheaf of superfunctions $\mathscr{O}$ to $D-\{p\}$.

Definition 1:[11–20,24] *A vacuum super-wave function is a superfunction* $f_0\in\mathscr{O}^*\otimes\mathscr{S}$ *that satisfies*

$$\begin{aligned}\frac{\partial f_0}{\partial t_n}&=\partial^n f_0,\\ \frac{Df_0}{D\tau_n}&=A_nf_0, \quad n\geqslant 1.\end{aligned} \tag{9}$$

Hence, a super-wave function f_0 depends on the variables $(z,\alpha;x,\theta,\mathbf{t},\boldsymbol{\tau})$, and is a solution of the linear system (9). We can find solutions of (9) using the ansazt,

$$f_0=Ve^{zx+\alpha\theta}, \tag{10}$$

with V a super-pseudodifferential operator in $\mathscr{E}$ and satisfying the initial condition $V|_{\mathbf{t}=\mathbf{0},\boldsymbol{\tau}=\mathbf{0}}=1$. Then, V must verify

$$\frac{\partial V}{\partial t_n}=\partial^n\cdot V,$$

$$\frac{DV}{D\tau_n}=A_n\cdot V,\quad n\geqslant 1.$$

It is easy to see that for the MRKP hierarchy

$$V=\exp\left[\sum_{n=1}^{\infty} t_n\partial^n\right]\cdot\left[1+\sum_{n=1}^{\infty}\tau_n D^{2n-1}\right]$$

and

$$f_0=\exp\left[zx+\alpha\theta+\sum_{n=1}^{\infty} z^n t_n+(\alpha-z\theta)\sum_{n=1}^{\infty} z^{n-1}\tau_n\right].$$

Respectively for the JKP hierarchy

$$V=\exp\left[\sum_{n=1}^{\infty} t_n\partial^n+\sum_{n=1}^{\infty}\tau_n\frac{\partial}{\partial\theta}D^{2n-2}\right]$$

and

$$f_0=\exp\left[zx+\alpha\theta+\sum_{n=1}^{\infty} z^n t_n+\alpha\sum_{n=1}^{\infty} z^{n-1}\tau_n\right].$$

Henceforth we will write both expressions of the vacuum super-wave function f_0 as

$$f_0=\exp\left[zx+\sum_{n=1}^{\infty} z^n(t_n+\theta\tau_n)+(\alpha-\lambda)\left(\theta+\sum_{n=1}^{\infty} z^{n-1}\tau_n\right)\right],\tag{11}$$

where $\lambda=\lambda(z,\theta,\boldsymbol{\tau})$ denotes a function which for the MRKP hierarchy is

$$\lambda(z,\theta,\boldsymbol{\tau})=z\theta-\sum_{n=1}^{\infty} z^n\tau_n,\tag{12}$$

and for the JKP hierarchy is given by

$$\lambda(z,\theta,\boldsymbol{\tau})=z\theta.\tag{13}$$

For brevity's sake, we will often omit the arguments of the superfunctions which are irrelevant or clear from the context.

It should be noticed that

$$Df_0=(\lambda-\alpha)f_0,\quad D^2f_0=zf_0,\tag{14}$$

so that the action of inverse powers of D on f_0 may be defined as

$$D^{-1}f_0=D\cdot D^{-2}f_0=(\lambda-\alpha)z^{-1}f_0.\tag{15}$$

It is now evident that we can ''dress'' the vacuum super-wave function to obtain solutions of Sato's equations (2) introducing the notion of a super-wave function.

Let $H(\Omega)$ denote the set of complex valued holomorphic functions of z on a certain region Ω of the complex plane, and $\mathcal{O}_\Omega=H(\Omega)\otimes\Lambda(\alpha)$ the superalgebra of superfunctions of the trivial $(1|1)$-superspace over Ω.

Definition 2: Let Ω *and* $\mathscr{O}_\Omega$ *as before. A super-wave function for a SKP hierarchy is an even element* $f=f(z,\alpha;x,\theta;\mathbf{t},\boldsymbol{\tau})$ *of the algebra*

$$\mathscr{O}_\Omega\otimes\mathbb{C}[[x,\mathbf{t}]]\otimes\Lambda(\theta,\boldsymbol{\tau})\otimes\mathscr{A},$$

which satisfies the properties:
(P1) f *is a solution of an infinite system of equations:*

$$\begin{aligned}\frac{\partial f}{\partial t_n}&=P_n f,\\ \frac{Df}{D\tau_n}&=Q_n f,\quad n\geqslant 1,\end{aligned}\tag{16}$$

with $P_n,Q_n\in\mathscr{E}$ *being superdifferential operators*

$$(P_n)_-=(Q_n)_-=0.$$

(P2) f *can be decomposed as a product:*

$$f=f'\cdot f_0,\tag{17}$$

where f' *admits a Laurent expansion on* $r<|z|<r'$ *of the form:*

$$f'=1+\sum_{n=1}^{\infty}w_{2n}z^{-n}+(\alpha-\lambda)\sum_{n=1}^{\infty}w_{2n-1}z^{-n},\tag{18}$$

with $w_n\in\mathscr{S}$ *for all* $n\geqslant 1$.

Then a super-wave function f is obtained by dressing the vacuum super-wave function f_0 using an operator K satisfying Sato's equations.

Theorem 1: *Let* f *be a super-wave function for an SKP hierarchy and* f_0 *the vacuum super-wave function (11), then there is an operator* K *such that*

$$f=Kf_0.\tag{19}$$

and K *verifies Sato's equations (2). Conversely, any solution of Sato's equations (2) provides a super-wave function* f *for a SKP hierarchy by means of Eq. (19).*

Proof: To prove this fact, we observe that as a consequence of properties (14) and (15) of f_0, the operator K in (19) has the required form (3) with the coefficients w_n being the same as those of the expansion (18) of f'. On the other hand (16), (19) and (9) imply

$$\frac{\partial K}{\partial t_n}f_0+K\partial^n f_0=P_nKf_0,$$

so that we deduce

$$\frac{\partial K}{\partial t_n}K^{-1}=P_n-K\partial^nK^{-1}.$$

But this equation obviously leads to

$$P_n=(K\partial^nK^{-1})_+$$

and

$$\frac{\partial K}{\partial t_n} = -(K\partial^n K^{-1})_- K.$$

In the same way one shows that K satisfies the Sato equations for the flows associated with the variables τ_n. Thus, we have obtained in this way a one-to-one correspondence between solutions K of Sato's equation and super-wave functions f_0.

Conversely, if $f=Kf_0$, then because of (2), and (9), f verifies (16) with $P_n=(K\partial^n K^{-1})_+$ and $Q_n=(KA_nK^{-1})_+$. Moreover, because of the expansion (3) of the operator K follows the expansion (18) of the transition superfunction f'.

It is worth noticing that, as it should be expected, the body of a super-wave function for a SKP hierarchy constitutes a wave function for the standard KP hierarchy.

III. LINE BUNDLES AND EXPLICIT SOLUTIONS OF THE SKP HIERARCHIES

A. Super-wave functions as sections of line bundles

Contrary to the situation in the bosonic case, the description of the SKP flows must be done not on line bundles over a supercurve but on line bundles over a family of supercurves parametrized by θ, $\boldsymbol{\tau}$. To be precise, we are going to consider a family $\mathscr{M}(\theta, \tau)$ of compact complex supermanifolds of dimension (1,1) *parametrized* by the set of global Grassmann variables $(\theta,\boldsymbol{\tau})$. We will describe this structure in detail. Let $\mathscr{U}=(U;z,\alpha)$ and $\mathscr{U}'=(U';z',\alpha')$ be two charts, where the pair $\{U,U'\}$ is a covering of the Riemann sphere, for instance,

$$U=\{z\in\mathbb{C}\,|\,|z|<r\},\quad U'^0=\{z\in\mathbb{C}\,|\,|z|>r'\},\quad 0<r'<r,$$

with the two systems of coordinates being related through the equations

$$z'=\frac{1}{z},\quad \alpha'=\alpha-\lambda(z,\theta,\boldsymbol{\tau}). \tag{20}$$

Here $\lambda(z,\theta,\boldsymbol{\tau})$ is the function defined in (12) and (13) and the transformation $\alpha\mapsto\alpha'$ will be called a super-Schiffer transformation. Notice that these supermanifolds are of extended type in the sense of Rogers[26] because superfunctions on $\mathscr{M}(\theta,\boldsymbol{\tau})$ depend not only on the local coordinates (z,α) of the supermanifold but also on the global variables $(\theta,\boldsymbol{\tau})$. In general, the equation (20) for the super-Schiffer transformation $\alpha\mapsto\alpha'$ does not extend holomorphically throughout U', generically it has a pole of order 1 at ∞, and the supermanifold structures defined by the transition superfunctions (20) are not equivalent to the trivial super-Riemann sphere.

Thus we can think on the supermanifold structures defined by the $(\theta,\boldsymbol{\tau})$-dependent transition functions (20) as tracing a path on the moduli space of complex supercurves. See Ref. 27 for the description of universal deformations on the supermoduli space of supercurves. We could consider further deformations of our complex supercurves but we will simplify the description of super-wave functions by considering only the supercurves parametrized by θ and $\boldsymbol{\tau}$ by means of (20).

We shall consider then the family $\mathscr{L}(x,\mathbf{t})$ of holomorphic line bundles over $\mathscr{M}(\theta,\boldsymbol{\tau})$ with transition function given by the vacuum super-wave function f_0 of a SKP hierarchy. Our purpose now will be to characterize holomorphic sections of these bundles. Such sections will be determined by pairs

$$(\mathscr{U},\phi),\quad (\mathscr{U}',\phi'),$$

defined on the patches U and U', and where ϕ and ϕ' are even superfunctions

$$\phi\in M(U)\otimes\Lambda(\alpha)\otimes\mathbb{C}[[x,\mathbf{t}]]\otimes\Lambda(\theta,\boldsymbol{\tau})\otimes\mathscr{A},$$

$$\phi'\in M(U')\otimes\Lambda(\alpha')\otimes\mathbb{C}[[x,\mathbf{t}]]\otimes\Lambda(\theta,\boldsymbol{\tau})\otimes\mathscr{A},$$

verifying the overlapping condition,

$$\phi=\phi'\cdot f_0,\quad \forall z\in U\cap U'. \tag{21}$$

Here, $M(U)$ and $M(U')$ denote the sets of complex valued meromorphic functions of z on U and U', respectively.

Comparing our last equation (21) with the factorization property for a super-wave function (17), we immediately see that wide classes of super-wave functions for the SKP hierarchies can be obtained from special sections of $\mathscr{L}(x,\mathbf{t})$. We will search for the conditions defining subsets

$$\mathscr{W}\subset M(U)\otimes\Lambda(\alpha)\otimes\mathbb{C}[[x,\mathbf{t}]]\otimes\Lambda(\theta,\boldsymbol{\tau})\otimes\mathscr{A}, \tag{22}$$

whose elements will be super-wave functions.

Definition 3: A subspace $\mathscr{W}$ of the the superalgebra $M(U)\otimes\Lambda(\alpha)\otimes\mathbb{C}[[x,\mathbf{t}]]\otimes\Lambda(\theta,\boldsymbol{\tau})\otimes\mathscr{A}$ will be called an asympotic super-module if it verifies:

(C1) *$\mathscr{W}$ is a left-module over the algebra of superdifferential operators generated by D and $\{(\partial/\partial t_n),(\partial/\partial\tau_n)\}_{n\geqslant 1}$ with coefficients in $\mathscr{S}$.*

(C2) *There is only one even section of the line superbundle $\mathscr{L}(x,\mathbf{t})$ given by the local expressions,*

$$(\mathscr{U},f),\quad (\mathscr{U}',f'), \tag{23}$$

such that $f\in\mathscr{W}$ and f' is holomorphic on U' with $f'|_{\{z=\infty\}}=1$.

In Section III we will construct explicitly several examples of asymptotic super-modules for complex supercurves with body manifold the Riemann sphere. For more general complex supercurves $\mathscr{M}$ with body manifold an arbitrary compact Riemann surface Σ, the previous characterization works similarly. To construct the subspaces $\mathscr{W}$ we should choose first a line bundle $\mathscr{L}$ over $\mathscr{M}$ such that $\dim H^0(\mathscr{M},\mathscr{L})=\dim H^1(\mathscr{M},\mathscr{L})=0$. Then, fixing a point $p\in\Sigma$ and a local trivialization in a neighborhood of it, we define the new bundle $\mathscr{L}\otimes\mathscr{L}_p$ possessing the required properties. Notice that the cohomological requirements on $\mathscr{L}$ implies that $\deg E=0$ where E is the underlying complex line bundle over the Riemann surface. For the Riemann sphere case, this implies that $\deg\mathscr{L}=-1$ and the complex supercurve is not a SRS.

We can prove now the following theorem characterizing super-wave functions using asymptotic super-modules.

Theorem 2: *Given an asymptotic super-module $\mathscr{W}$, the superfunction*

$$f=f'\cdot f_0,\quad z\in U\cap U',$$

defined by the unique section associated to it is a super-wave function for the associated SKP hierarchy.

Proof: To see this, observe that from (C2) in Def. 3 we deduce

$$f'=1+\sum_{n=1}^{\infty}w_{2n}(z')^n+\alpha'\cdot\sum_{n=1}^{\infty}w_{2n-1}(z')^n=1+\sum_{n=1}^{\infty}w_{2n}z^{-n}+(\alpha-\lambda)\sum_{n=1}^{\infty}w_{2n-1}z^{-n}.$$

Therefore f satisfies the condition (P2) for super-wave functions. On the other hand, by using (14) we get that for $z\in U\cap U'$

$$\begin{aligned} D^{2n}f-w_1D^{2n-1}f&=[z^n+O(z^{n-1})]f_0,\\ D^{2n+1}f+w_1D^{2n}f&=[-(\alpha-\lambda)z^n+O(z^{n-1})]f_0. \end{aligned} \tag{24}$$

As a consequence, we may determine superdifferential operators $P_n, Q_n \in \mathscr{E}$ such that

$$\frac{\partial f}{\partial t_n} - P_n f = O\left(\frac{1}{z}\right) \cdot f_0,$$
$$\frac{Df}{D\tau_n} - Q_n f = O\left(\frac{1}{z}\right) \cdot f_0, \quad n \geqslant 1. \tag{25}$$

Then, it is easy to see that (C2) implies that both $\partial f/\partial t_n - P_n f$ and $Df/D\tau_n - Q_n f, n \geqslant 1$, vanish, and therefore f satisfies the condition (P1) for super-wave functions.

Solutions to a reduced hierarchy (4) can be obtained by imposing on $\mathscr{W}$ the additional condition

$$z^r \cdot \mathscr{W} \subset \mathscr{W}. \tag{26}$$

Indeed, in that case the super-wave function f associated with $\mathscr{W}$ satisfies

$$\frac{\partial f}{\partial t_r} = z^r \cdot f,$$

so that f' and K are independent on t_r.

B. Solitons and solitinos

We will now construct several examples of asymptotic super-modules and the corresponding super-wave functions.

Let us consider the subset of superfunctions ϕ which are analytic for all $z \in U$, with the possible exception of simple poles contained in a fixed subset $\{q_i\}_{i=1}^N$, and such that the corresponding residues satisfy

$$\mathrm{Res}(\phi, q_i) = (c_i + \alpha\omega_i) \cdot \phi(p_i, \alpha), \quad i = 1, \ldots, N, \tag{27}$$

where $\{c_i\}_{i=1}^N \in \mathscr{A}_0$ and $\{\omega_i\}_{i=1}^N \in \mathscr{A}_1$ are given, and $\{p_i\}_{i=1}^N$ is a fixed subset of points of U different from $\{q_i\}_{i=1}^N$. This subspace will be denoted by $\mathscr{W}(\mathbf{q}, \mathbf{p}; \mathbf{c}, \boldsymbol{\omega})$, where $\mathbf{q} = (q_1, \ldots, q_N)$, etc.

Theorem 3: *The subspace $\mathscr{W}(\mathbf{q}, \mathbf{p}; \mathbf{c}, \boldsymbol{\omega})$ is an asymptotic super-module and its elements are super-wave functions for a SKP hierarchy.*

Proof: In order to prove that $\mathscr{W}(\mathbf{q}, \mathbf{p}; \mathbf{c}, \boldsymbol{\omega})$ verifies the required conditions (C1) and (C2) of Def. 3, let us note that the corresponding superfunction f must be of the form

$$f = \left[1 + \sum_{i=1}^{N} \frac{a_i + (\alpha - \lambda)\beta_i}{z - q_i}\right] \cdot f_0, \tag{28}$$

where the unknown coefficients a_i and β_i are even and odd elements of $\mathscr{S}$, respectively. Thus computing the residues, (27) implies

$$a_i + (\alpha - \lambda(q_i))\beta_i = (b_i + \alpha\gamma_i)\left[1 + \sum_{j=1}^{N} \frac{a_j + (\alpha - \lambda(p_i))\beta_j}{p_i - q_j}\right], \tag{29}$$

for all $i = 1, \ldots, N$, where $b_i, \gamma_i \in \mathscr{S}$ are given by

$$b_i = e(p_i) c_i e(q_i)^{-1}, \quad \gamma_i = e(p_i)\left[\omega_i + c_i \sum_{n \geqslant 1} (p_i^{n-1} - q_i^{n-1})\tau_n\right] e(q_i)^{-1},$$

and with $e(z)$ denoting the superfunction

$$e(z)=\exp\left[zx+\sum_{n\geqslant 1} z^n(t_n+\theta\tau_n)-\lambda(z)\left(\theta+\sum_{n\geqslant 1} z^{n-1}\tau_n\right)\right].$$

From (29) the following linear system for the coefficients a_i and β_i follows

$$\begin{aligned}&\sum_j\left[\delta_{ij}-\frac{b_i}{p_i-q_j}\right]\cdot a_j-\sum_j\left[\delta_{ij}\lambda(q_i)-\frac{b_i\lambda(p_i)}{p_i-q_j}\right]\cdot\beta_j=b_i,\\ &-\sum_j\frac{\gamma_i}{p_i-q_j}\cdot a_j+\sum_j\left[\delta_{ij}+\frac{\gamma_i\lambda(p_i)-b_i}{p_i-q_j}\right]\cdot\beta_j=\gamma_i.\end{aligned}\tag{30}$$

This is a uniquely solvable system since the body of the matrix of coefficients is the invertible numerical matrix,

$$\begin{pmatrix}\delta_{ij}-\dfrac{\epsilon(b_i)}{p_i-q_j} & 0\\ 0 & \delta_{ij}-\dfrac{\epsilon(b_i)}{p_i-q_j}\end{pmatrix}.\tag{31}$$

Therefore we conclude that (28) is a super-wave function.

Theorem 1 allows the identification of the coefficients of the expansion of the super-wave function with the coefficients of the expansion of the operator K solving Sato's equations (2). Observe then for f given by eq. (28), the first two coefficients of the expansion of the associated solution K of Sato equations are

$$w_1=\sum_{i=1}^{N}\beta_i,\quad w_2=\sum_{i=1}^{N}a_i.\tag{32}$$

We consider the following two different cases for the system (30).

1. Supersoliton solutions: $\epsilon(c_i)=0,\forall i\neq 1,\ldots,N$

From (30) it is easy to see that the body of f is the wave function associated with the N-soliton solution of the KP hierarchy. Therefore the solution of the SKP hierarchy provided by f is a supersymmetric generalization of the standard multisoliton solutions. For example, it is rather simple to derive the explicit solution for $N=1$. In this case, the constraints (27) reduce to

$$\mathrm{Res}(\phi,q)=(c+\alpha\omega)\phi(p,\alpha).$$

Then one finds

$$f=\left[1+\frac{a+(\alpha-\lambda)\beta}{z-q}\right]\cdot f_0,$$

with

$$\begin{aligned}a&=\frac{(q-p)b}{q-p+b}+\frac{\lambda(p)b+(q-p)\lambda(q)}{(q-p+b)^3}(q-p)^2\gamma,\\ \beta&=\frac{(p-q)^2}{(q-p+b)^2}\gamma.\end{aligned}\tag{33}$$

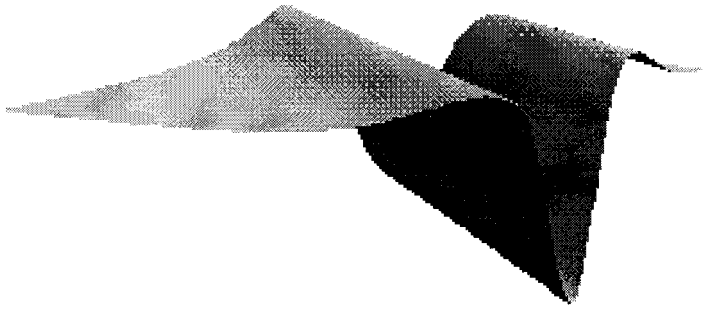

FIG. 1. Composite structure of a single supersoliton, $(h_1(x,t), q=1, x_0=1)$.

If we take $p=-q$, then it follows that $z^2\cdot\mathscr{W}\subset\mathscr{W}$, so that f becomes a super-wave function for the supersymmetric KdV hierarchy. In particular, it provides a solution of the SKdV equation (8). To simplify the expression of this solution we set $t_n=0$, $\forall n\neq 3$, and $\tau_n=0$, $\forall n\geqslant 1$. Thus, from (7), (32) and (33), we find

$$\begin{aligned} v_0&=2\left(q^2+\theta\omega\frac{q^3}{c}\right)\operatorname{sech}^2[q(x-x_0+q^2t)]-3\,\theta\omega\frac{q^3}{c}\operatorname{sech}^4[q(x-x_0+q^2t)],\\ v_1&=\omega\frac{2q^2}{c}\sinh[q(x-x_0+q^2t)]\operatorname{sech}^3[q(x-x_0+q^2t)], \end{aligned} \tag{34}$$

where

$$x_0=\frac{1}{q}\log\left(\frac{c}{2q}\right).$$

The expression of v_0 may be described as a supersymmetric dressing of the standard soliton of the KdV equation. Writing $v_0=h_0(x,t)+h_1(x,t)\,\theta\omega$ and $v_1=h_2(x,t)\,\omega$, in Fig. 1 we show the composite structure of h_1, the $\theta\omega$ component of the superfunction v_0.

On the other hand, it is worth noticing that the odd superfunction v_1 is proportional to a function h_2 of (x,t) which represents also a composite structure (see Fig. 2) which propagates without deformation along the x axis.

2. Solitino solutions: $c_i=0, \forall i=1,\ldots,N$

In this case (29) and (30) reduces to

$$\begin{aligned} a_i&=\lambda(q_i)\cdot\beta_i,\\ \gamma_i&=\sum_{j=1}^{N}\left[\delta_{ij}+\gamma_i\frac{\lambda(p_i)-\lambda(q_j)}{p_i-q_j}\right]\beta_j. \end{aligned} \tag{35}$$

This system can be solved in terms of the nilpotent matrix

$$\Delta_{ij}=\frac{\lambda(p_i)-\lambda(q_j)}{p_i-q_j}\gamma_i. \tag{36}$$

Indeed, as $\Delta^N\boldsymbol{\gamma}=0$ the solution of (35) is

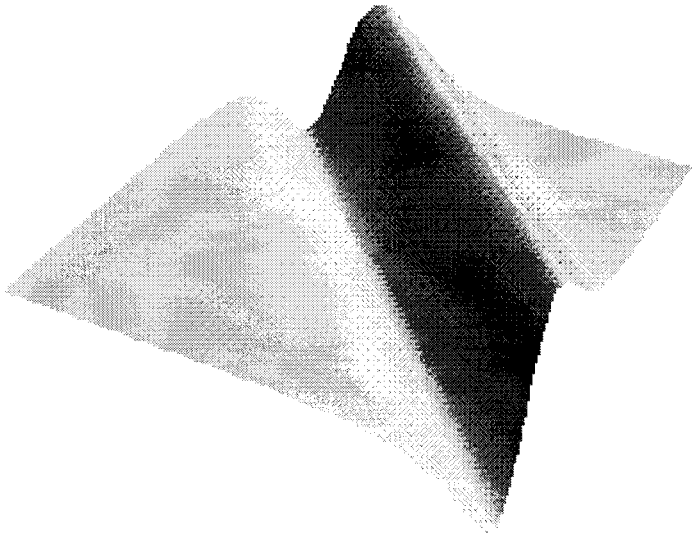

FIG. 2. Odd component of a supersoliton $(h_2(x,t), q=1, x_0=1)$.

$$\boldsymbol{\beta}=\sum_{n=0}^{N-1}\Delta^n\boldsymbol{\gamma}, \tag{37}$$

where $\boldsymbol{\beta}=(\beta_1,\ldots,\beta_N)$ and $\boldsymbol{\gamma}=(\gamma_1,\ldots,\gamma_N)$. It must be observed that the body of f vanishes, so that this class of solutions is not related to any class of the standard KP theory. We will refer to these solutions as *solitino* solutions. The single solitino solution corresponds to $N=1$ and takes the form

$$f=\left[1+\frac{a+(\alpha-\lambda)\beta}{z-q}\right]\cdot f_0,$$

$$w_1=\beta=\omega\ \exp\ r, \quad w_2=a=\lambda(q)\omega\ \exp\ r,$$

where

$$\exp\ r=e(p)e(q)^{-1}=\exp\Bigg[(p-q)x+\sum_{n\geqslant 1}(p^n-q^n)(t_n+\theta\tau_n)-(\lambda(p)-\lambda(q))\theta$$

$$-\sum_{n\geqslant 1}(\lambda(p)p^{n-1}-\lambda(q)q^{n-1})\tau_n\Bigg]. \tag{38}$$

If we take $p_i=-q_i$, $\forall i=1,\ldots,N$, then $z^2\cdot\mathscr{W}\subset\mathscr{W}$ and we obtain a solution of (8). It adopts a convenient way by setting, as we did before, $t_n=0, \forall n\neq 3$ and $\tau_n=0, \forall n\geqslant 1$. Thus the matrix (36) reduces to

$$\Delta_{ij}=\theta\omega_i\ \exp[-2q_i(x+q_i^2t)]$$

and

$$\gamma_i=\omega_i\ \exp[2q_i(x+q_i^2t)],$$

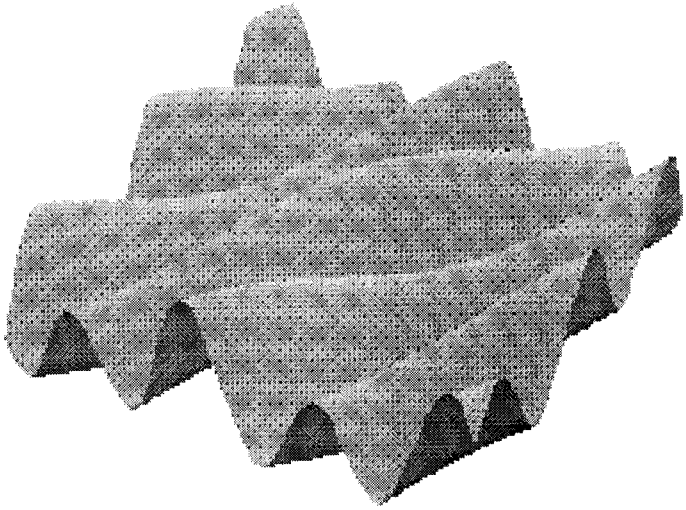

FIG. 3. An even component of a bisolitino solution.

and we find the following multisolitino solution of the SKdV equation (8):

$$v_0 = 4\theta \sum_i q_i^2 \omega_i \exp[-2q_i(x+q_i^2 t)] + 4\sum_{i,j} q_i \omega_i \omega_j \exp[-2q_i(x+q_i^2 t) - 2q_j(x+q_j^2 t)], \tag{39}$$

$$v_1 = 4\sum_i q_i \omega_i \exp[-2q_i(x+q_i^2 t)]. \tag{40}$$

In particular the single solitino solution takes the form

$$v_0 = 4q^2 \theta\omega \exp[-2q(x+q^2 t)], \quad v_1 = 4q\omega \exp[-2q(x+q^2 t)].$$

It is not a localized solution as a function of x. In fact, for imaginary q it is a plane wave.

The multisolitino solution (39) represents a superposition of solitinos which is of a nonlinear character, as it is shown by the presence of quadratic terms in the expression for v_0. See Fig. 3 for a representation of a component of the even part of a bisolitino solution.

C. Rational solutions

A solution K of the SKP hierarchy (2) is said to be rational if the coefficients w_n of its expansion (3) are rational functions of the even coordinates $(x,\mathbf{t})$. Solutions of this kind can be derived by means of asymptotic super-modules similar to those used for solitons and solitinos by imposing instead of the conditions (27) constraints of the type

$$\left(\alpha \frac{\partial}{\partial \alpha} \frac{\partial^{n_i}}{\partial z^{n_i}} + c_i \frac{\partial^{m_i}}{\partial z^{m_i}}\right) \phi(p_i, \alpha) = 0.$$

For example, let us take $\mathscr{W}$ to be the set of superfunctions ϕ analytic on U with the possible exception of a simple pole at a given point $q \neq 0$, and such that

$$\alpha \frac{\partial}{\partial \alpha} \frac{\partial \phi}{\partial z}(0,\alpha) + \phi(0,\alpha) = 0. \tag{41}$$

It is straightforward to get

$$f=\left[1+\frac{a+(\alpha-\lambda)\beta}{z-q}\right]\cdot f_0, \tag{42}$$

with

$$a=q, \quad \beta=-\frac{q(\theta+\tau_1)}{1+q(x+t_1+1)}.$$

As $z^2\cdot\mathscr{W}\subset\mathscr{W}$ this construction leads to a solution of (8) which turns out to be given by

$$v_0=0, \quad v_1=-\frac{2q^2(\theta+\tau_1)}{[1+q(x+t_1+1)]^2}.$$

Another simple example is obtained by replacing (41) by

$$\frac{\partial\phi}{\partial z}(0,\alpha)=0, \tag{43}$$

then the superfunctions a and β in (42) take the form

$$a=q\left(1-\frac{1}{s}+\frac{r\tau_2}{s^3}\right), \quad \beta=\frac{q^2\tau_2}{s^2},$$

where for the MRKP hierarchy

$$s=q(x+t_1+\tau_1\theta)+1, \quad r=q^2(\theta-\tau_1),$$

and for the JKP hierarchy

$$s=q(x+t_1)+1, \quad r=q^2\theta.$$

The condition $z^2\cdot\mathscr{W}\subset\mathscr{W}$ keeps on being satisfied and the corresponding solution of (8) is

$$v_0=-\frac{2q^2}{s^2}+\frac{6q^2r\tau_2}{s^4}, \quad v_1=\frac{4q^3\tau_2}{s^3}.$$

We notice that this solution is a supersymmetric dressing of the elementary rational solution

$$v=\frac{-2q^2}{(qx+1)^2}$$

of the KdV equation.

IV. SUPERGROUP THEORETICAL DESCRIPTION

It is well known the use of $\bar{\partial}$-equations to obtain wave functions for the KP hierarchy.[21,22] This theory was extended to the supersymmetric situation in Ref. 23.

We shall consider solutions of the $\bar{\partial}$-equation,

$$\frac{\partial}{\partial\bar{z}}f(z,\alpha;x,\theta;\mathbf{t},\boldsymbol{\tau})=\int d^2z'\,d\alpha'\,a(z',\alpha';z,\alpha)f(z',\alpha';x,\theta;\mathbf{t},\boldsymbol{\tau}), \tag{44}$$

with $a(z',\alpha';z,\alpha)$ a given distribution of odd parity. We shall denote by $\mathscr{F}$ the space of solutions of Eq. (44) having an asymptotic expansion, $z\to\infty$, of the form

$$F=\left(\sum_{n=-\infty}^{N} u_n z^n+(\alpha-\lambda)\sum_{n=-\infty}^{M} v_n z^n\right) f_0,$$

with coefficients u_n, v_n in $\mathscr{S}$.

By using the properties (9) of the vacuum super-wave function f_0 and the isospectrality of the $\bar{\partial}$-equation (44) (the kernel a of the equation (44) does not depend on x,t), it is immediate that $\mathscr{F}$ is a left module for the algebra of superdifferential operators $\mathscr{E}$. Then, if a unique even solution f of Eq. (44) with the asymptotic expansion Eq. (18) exists, then by Thm. 2, it will be a super-wave equation for a SKP hierarchy.

It was shown in Ref. 23 that solutions of the $\bar{\partial}$-equation are related with the τ-function of the SKP hierarchy generated from the action of the element

$$g=\exp\frac{1}{\pi}\int d^2z'\,d\alpha'\,d^2z\,d\alpha B(z',\alpha')a(z',\alpha';z,\alpha)C(z,\alpha) \tag{45}$$

of the supergroup $GL(\infty|\infty)$ on the vacuum. The quantum fields B, C form a superghost system with commutation and anticommutation relations given by

$$[B(z,\alpha),B(z',\alpha')]=\{C(z,\alpha),C(z',\alpha')\}=0;\quad [B(z,\alpha),C(z',\alpha')]=(\alpha-\alpha')\hat{\delta}_\gamma(z-z'),$$

and $\hat{\delta}_\gamma(z)$ denotes the delta function with support on the circle γ acting on test functions as

$$\int d^2z\,\hat{\delta}_\gamma(z)\phi(z)=\oint_\gamma z\phi(z).$$

One of the advantages of the τ-function formalism for integrable systems is that it allows us to classify the solutions in terms of orbits of symmetry groups. For the SKP hierarchies considered in this paper a τ-function description is already available which exhibits their invariance under the supergroup $GL(\infty|\infty)$.[23] We can thus conclude form the above discussion that the τ-function of the SKP hierarchy generated from the action of (45) on the vacuum is associated with the super-wave function which satisfies the corresponding $\bar{\partial}$ equation.

As for the solutions analyzed in this paper, it is easy to derive the $\bar{\partial}$-equation verified by their associated super-wave functions. For example, the solutions that arise from the constraints (27) and (41) give rise to the kernels

$$a(z',\alpha';z,\alpha)=\pi\sum_{i=1}^{N}(\alpha'-\alpha)(c_i+\alpha'\omega_i)\delta(z-q_i)\delta(z'-p_i) \tag{46}$$

and

$$a(z',\alpha';z,\alpha)=\frac{\delta(z-q)}{2\pi i}\left[\pi(\alpha'-\alpha)\hat{\delta}_{\gamma_1}(z')+\left(\frac{\alpha'-\alpha}{z'}-\frac{\alpha}{(z')^2}\right)\hat{\delta}_{\gamma_2}(z')\right], \tag{47}$$

respectively. Here $\delta(z-q)$ is the usual delta function on the plane and $\hat{\delta}_{\gamma_i}(z)$, $i=1,2$, denotes the delta functions with support on the circles γ_i ($|z|=r_i$), with $r_1>|q|>r_2$. Consequently, we have provided two additional different characterizations for our solutions of the SKP hierarchies. First, from Eq. (45) every solution is associated with an element of $GL(\infty|\infty)$. Second, Eq. (44) shows that the kernel a supplies the spectral description of the solutions.

ACKNOWLEDGMENTS

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Lax–Nijenhuis operators for integrable systems

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The relationship between Lax and bi-Hamiltonian formulations of dynamical systems on finite- or infinite-dimensional phase spaces is investigated. The Lax–Nijenhuis equation is introduced and it is shown that every operator that satisfies that equation satisfies the Lenard recursion relations, while the converse holds for an operator with a simple spectrum. Explicit higher-order Hamiltonian structures for the Toda system, a second Hamiltonian structure of the Euler equation for a rigid body in n-dimensional space, and the quadratic Adler–Gelfand–Dickey structure for the KdV hierarchy are derived using the Lax–Nijenhuis equation. © *1996 American Institute of Physics.* [S0022-2488(96)03411-1]

I. INTRODUCTION

We present an explanation of a long-standing problem: What is the relationship between the Lax formulation of an integrable system and the existence of a bi-Hamiltonian structure?

When considering differential equations in Lax form[1] on a finite- or infinite-dimensional phase-space manifold, according to the problem at hand, one introduces either a matrix of a given size, or a differential operator of a given degree, or, more generally, a pseudo-differential operator whose coefficients are functions of the phase-space coordinates. In other words, the ''Lax operator'' is an A-valued map on phase space, where A is an associative algebra that has to be determined in each problem.

We study the case where the phase-space manifold admits a pair of compatible Poisson structures, i.e., has a bi-Hamiltonian structure.[2–4] (See also Refs. 5–7, and Ref. 8 for a complete exposition and further references.) The term ''Poisson structure'' is most frequently used for finite-dimensional manifolds such as the phase space of dynamical systems defined by evolution ordinary differential equations, while the term ''Hamiltonian structure'' is commonly used in the case of infinite-dimensional manifolds, e.g., manifolds of functions, such as the phase spaces of systems described by evolution partial differential equations. When two Poisson structures satisfying a compatibility condition are present, the term ''bi-Hamiltonian structure'' will be applied. We shall mainly consider the finite-dimensional case, but the extension to the infinite-dimensional situation is straightforward, in the setting of the formal calculus of variations in the sense of Gelfand, Dickey, and Dorfman. (See Refs. 9, 10, and 8.)

As the defining property of a matrix-valued Lax operator, L, in the presence of a bi-Hamiltonian structure (P,Q) we take the so-called Lenard recursion relations,

$$Q\left(d\ \mathrm{tr}\,\frac{L^k}{k}\right)=P\left(d\ \mathrm{tr}\,\frac{L^{k+1}}{k+1}\right). \tag{1.1}$$

When L has distinct eigenvalues, λ_i, these relations imply that

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$$Q(d\lambda_i)=\lambda_i P(d\lambda_i),$$

and in all cases they imply the pairwise involutivity of the eigenvalues of L with respect to both Poisson brackets. Moreover, the traces of powers of L, and hence the eigenvalues of L, are conserved along the flow of each evolution equation in Lax form, $\dot{L}=[L,B]$.

The recursion relations for differential equations in Lax form first appeared in the context of evolution partial differential equations, and they are actually due to Lax.[1] [It is surprising that it has become customary to call them the Lenard recursion relations, probably because, in his paper of 1976, Lax[11] refers to Lenard's contribution to the derivation of the infinite family of higher-order Korteweg–de Vries (KdV) equations as reported in the 1974 article by Gardner, Greene, Kruskal, and Miura.[12] Actually, Gardner *et al.* derived this ''infinite family of equations that leave the eigenvalues of the Schrődinger equation invariant in time'' and they also give ''an alternate derivation of this family due to Lenard,'' and both derivations reveal the recursion operator explicitly but do not relate it to any Hamiltonian property. In that same paper, Lax ascribes the involutivity property of the conserved quantities to Gardner (Ref. 13), where it is not explicit at all! Actually the factorization of the recursion operator as the composition of a Poisson and a symplectic operator is in Lax,[11] Magri,[2] Gelfand and Dorfman,[3] and Fokas and Fuchssteiner.[14]]

In this paper, we show that, under suitable conditions on its spectrum, a Lax operator on a bi-Hamiltonian manifold satisfies a universal equation which we call the Lax–Nijenhuis equation because the vanishing of the Nijenhuis torsion of the recursion operator of a bi-Hamiltonian structure appears as a particular case of this property. Conversely, if L satisfies the Lax–Nijenhuis equation, then L is a Lax operator. We then study the converse problem of determining compatible Hamiltonian structures from Lax–Nijenhuis equations. We treat the Toda system (see Refs. 15–20), the rigid body, the KdV hierarchy (see Refs. 21, 22, and 16), and, more generally, Lax equations that are Hamiltonian with respect to a Poisson bracket defined by an R-matrix (see Ref. 23).

In Sec. II we recall the definition of Hamiltonian and bi-Hamiltonian structures and we prove that functions that satisfy recursion relations (1.1), where P and Q are compatible Poisson structures, are pairwise in involution with respect to either Hamiltonian structure. Nijenhuis operators appear in the theory of bi-Hamiltonian structures (P,Q) when one considers the (1,1)-tensor $N=QP^{-1}$, where the first Poisson structure is assumed to be invertible, i.e., symplectic. (See Refs. 24–27). We analyze the properties of Nijenhuis operators and we observe that the vanishing of the Nijenhuis torsion[28] of a (1,1)-tensor implies the fundamental equation (2.5) that is the prototype of the Lax–Nijenhuis equation that we introduce in (3.6).

Section III contains the main results concerning the relationship between Lax and bi-Hamiltonian formulations of dynamical systems. It is natural to require that the traces of powers of the Lax operator satisfy the Lenard recursion relations (Definition 3.1). It then follows that, under the assumption of the simplicity of its spectrum, such a Lax operator satisfies the Lax–Nijenhuis equation (3.6). Conversely, we show in Proposition 3.5 that, if an operator satisfies the Lax–Nijenhuis equation, it satisfies the Lenard recursion relations, and therefore the traces of its powers are in involution. In addition, we prove that this property remains valid for negative and fractional powers, when they are defined.

The hereditary properties of Nijenhuis operators and of Lax operators compatible with a bi-Hamiltonian structure are derived in Sec. IV. We show that the Lax formulation exists for all vector fields,

$$X_k=Q\alpha_k=P\alpha_{k+1},$$

where α_k is a sequence of differential one-forms satisfying the Lenard recursion relations, provided that X_0 admits a Lax formulation. When all α_ks are closed, the X_ks constitute a bi-Hamiltonian hierarchy, i.e., a sequence of commuting bi-Hamiltonian vector fields, and we state a further commutation property in Proposition 4.3.

The fifth and last section is devoted to examples. For the nonperiodic Toda system, we explicitly determine a sequence of skewsymmetric higher-order bivectors satisfying Lax–Nijenhuis equations. The first three elements of this sequence coincide with the known linear, quadratic, and cubic Poisson structures. We treat the case of the Euler equations for the n-dimensional rigid body rotating about a fixed point, and some generalizations of it. We then study the Lax–Nijenhuis equation for the KdV equation, and, more generally, for the first equation in the nth KdV hierarchy, where the Lax operator takes values in a manifold of nth-order differential operators in the graded, associative algebra of formal pseudodifferential operators, and we obtain the second Adler–Gelfand–Dickey Hamiltonian structure from the first one. Finally, this construction is further generalized to determine the quadratic bracket associated with the linear Poisson bracket defined by an R-matrix, i.e., a solution of the modified classical Yang–Baxter equation.

For background and many results on integrable systems, we refer to Refs. 29 and 30. See Ref. 31 for a discussion closely connected with ours, but undertaken from a different point of view.

II. LENARD RECURSION RELATIONS ON A BI-HAMILTONIAN MANIFOLD

In this section, we recall some well-known results on Lenard recursion relations which we shall need for the study of Lax operators in Sec. III. First we introduce the concept of a bi-Hamiltonian manifold.

A Poisson manifold (also called a Hamiltonian manifold) is a manifold equipped with a Poisson bracket. We recall that a Poisson bracket can be defined in terms of a field of bivectors (a bivector for short) called the Poisson bivector. If P is a bivector on a manifold M, we identify P with the linear bundle map,

$$P: T^*M \to TM,$$

defined by $\langle \beta, P\alpha \rangle = P(\alpha, \beta)$, for $\alpha, \beta \in T^*M$. We set $X_f = Pdf$, for any function $f \in C^\infty(M)$, and we call X_f the Hamiltonian vector field with Hamiltonian f. We also define the Poisson bracket,

$$\{f,g\}_P = X_f \cdot g,$$

for f and $g \in C^\infty(M)$. Recall that a bivector P on M is a Poisson bivector if and only if one of the following equivalent conditions is satisfied:

(1) $[P,P]=0$, where $[\ ,\ ]$ is the Schouten bracket,
(2) the Poisson bracket $\{\ ,\ \}_P$ satisfies the Jacobi identity,
(3) $[X_f, X_g] = X_{\{f,g\}_P}$, for $f, g \in C^\infty(M)$.

These conditions are equivalent because, by the definition of the Schouten and Poisson brackets,

$$\begin{aligned} -\tfrac{1}{2}[P,P](df,dg,dh) &= \{f,\{g,h\}_P\}_P + \{g,\{h,f\}_P\}_P + \{h,\{f,g\}_P\}_P \\ &= ([Pdf, Pdg] - Pd(P(df,dg))).h \\ &= ([X_f, X_g] - X_{\{f,g\}_P}).h, \end{aligned}$$

for $f, g, h \in C^\infty(M)$.

Definition 2.1: A bi-Hamiltonian manifold (M,P,Q) is a manifold M equipped with Poisson structures, P and Q, which are compatible, i.e., such that any linear combination of P and Q is a Poisson structure. A (locally) bi-Hamiltonian vector field on (M,P,Q) is a vector field leaving P and Q invariant.

Thus, on a bi-Hamiltonian manifold there exists a pencil of Poisson structures, $P_\lambda = Q - \lambda P$, for $\lambda \in \mathbb{R} \cup \{\infty\}$. A sufficient condition for a vector field X to be (locally) bi-Hamiltonian is that

there exist closed differential one-forms α and β such that $X=P\beta=Q\alpha$. In particular, if there exist functions f and g such that $X=P(dg)=Q(df)$, then X is bi-Hamiltonian.

Lemma 2.2: Let P and Q be Poisson structures on M. Then P and Q are compatible if and only if one of the following equivalent conditions is satisfied:

(i) $[P, Q]=0$,
(ii) $\circlearrowleft(\{f,\{g,h\}_P\}_Q+\{f,\{g,h\}_Q\}_P)=0$, *where* $\circlearrowleft$ *denotes the sum over the circular permutations of* f,g,h,
(iii) $[X_f, Y_g]+[Y_f, X_g]=X_{\{f,g\}_Q}+Y_{\{f,g\}_P}$,

for $f,g\in C^\infty(M)$, *where* $X_f=Pdf$ *and* $Y_f=Qdf$.

Proof: In fact, each of these conditions is the polarization of the corresponding condition for a single Poisson structure, and each is obtained by bilinearity from the corresponding conditions for P,Q and $P+Q$. ■

For a Hamiltonian system on a symplectic manifold—the phase space—to be completely integrable in the sense of Liouville and Arnold,[32] there must exist a number of independent conserved quantities, equal to half the dimension of the symplectic manifold, which are pairwise in involution. Here we consider the case where the phase space is a bi-Hamiltonian manifold, and we show that when a sequence of functions defined on it satisfies the Lenard recursion relations, these functions are pairwise in involution. We shall denote the positive integers by $\mathbb{N}^*$.

Proposition 2.3: Let P and Q be Poisson structures on a manifold, M, and let $(f_k), k\in\mathbb{N}^*$, be a sequence of complex-valued functions on M that satisfy the Lenard recursion relation,

$$Q(df_k)=P(df_{k+1}), \tag{2.1}$$

for $k\in\mathbb{N}^*$. Then the functions, f_k, are pairwise in involution with respect to both Poisson brackets.

Proof: Let m be a non-negative integer, and let (C_m) be the property that, for all $k\geqslant 1$, $P(df_k,df_{k+m})=0$ and $Q(df_k,df_{k+m})=0$. Clearly (C_0) holds. Now for any $k\geqslant 1, m\geqslant 0$,

$$P(df_k,df_{k+m+1})=-\langle df_k,P(df_{k+m+1})\rangle=-\langle df_k,Q(df_{k+m})\rangle,$$

and

$$Q(df_k,df_{k+m+1})=\langle df_{k+m+1},Q(df_k)\rangle=\langle df_{k+m+1},P(df_{k+1})\rangle.$$

Thus it is clear that (C_{m+1}) holds if (C_m) holds. Therefore (C_m) is proved for all non-negative integers, m. Thus $P(df_k,df_l)=Q(df_k,df_l)=0$ for any $k,l\in\mathbb{N}^*$. ■

We remark that this proof uses only (2.1) and the skewsymmetry of P and Q. However, the assumption that P and Q are compatible Poisson structures is essential in order to guarantee the existence of functions, f_k, fulfilling the Lenard recursion relations (2.1). The question of the existence of such functions in the case of an arbitrary bi-Hamiltonian structure is a difficult problem which is beyond the scope of the present paper. Here, we shall demonstrate their existence in a special case, that of a bi-Hamiltonian manifold, (M,P,Q), where P is an *invertible* Poisson structure, i.e., a symplectic structure. The field of (1,1)-tensors,

$$N=QP^{-1}, \tag{2.2}$$

is called the *recursion operator* or the *Nijenhuis operator* of the bi-Hamiltonian structure. The first name is justified by the fact that N maps symmetries of a bi-Hamiltonian system into symmetries of the same system (see Sec. IV), while the second name is justified by the well-known result proved in Lemma 2.5 below. Nijenhuis operators provide the basic examples of the Lax–Nijenhuis operators to be defined in Sec. III B.

We recall that the Nijenhuis torsion of a field of (1,1)-tensors N on a manifold M is the vector-valued two-form $T(N)$ on M defined by

$$T(N)(X,\ Y)=[NX,\ NY]-N([NX,\ Y]+[X,\ NY])+N^2[X,\ Y], \tag{2.3}$$

for all vector fields X,Y on M.

Definition 2.4: A field of (1,1)*-tensors with vanishing Nijenhuis torsion is called a Nijenhuis tensor or Nijenhuis operator.*

Lemma 2.5: If (P,Q) *is a bi-Hamiltonian structure on* M*, and* $Q=NP$*, where* N *is a* (1,1)*-tensor on* M*, then the Nijenhuis torsion,* $T(N)$*, of* N *vanishes on the image of* P*. In particular, if* (P,Q) *is a bi-Hamiltonian structure, with* P *invertible, then the recursion operator,* $N=QP^{-1}$*, is a Nijenhuis operator.*

Proof: Assume that $Q=NP$. It is enough to show that $T(N)$ vanishes on any pair of vectors (Pdf,Pdg) where $f,g\in C^\infty(M)$. In fact, using the notations of Lemma 2.2,

$$\begin{aligned}T(N)(Pdf,Pdg)&=[NPdf,\ NPdg]-N([NPdf,\ Pdg]+[Pdf,\ NPdg])+N^2[Pdf,\ Pdg]\\&=[Y_f,\ Y_g]-N([Y_f,\ X_g]+[X_f,\ Y_g])+N^2[X_f,\ X_g].\end{aligned}$$

Using the results of Lemma 2.2, we obtain

$$T(N)(Pdf,Pdg)=Y_{\{f,g\}_Q}-N(X_{\{f,g\}_Q}+Y_{\{f,g\}_P})+N^2X_{\{f,g\}_P},$$

which vanishes since $NX_h=Y_h$, for $h\in C^\infty(M)$. ■

The condition that $T(N)=0$ is equivalent to the condition that

$$\mathscr{L}_{NX}N-N\mathscr{L}_XN=0, \tag{2.4}$$

for all vector fields X on M, where $\mathscr{L}_X$ denotes the Lie derivative with respect to X. In fact,

$$T(N)(X,Y)=\mathscr{L}_{NX}(NY)-N\mathscr{L}_{NX}Y-N(\mathscr{L}_X(NY)-N(\mathscr{L}_XY))=(\mathscr{L}_{NX}N)Y-N(\mathscr{L}_XN)Y.$$

Therefore the following proposition holds.

Proposition 2.6: Let N *be a Nijenhuis tensor on a manifold* M*. Then*

$$\mathscr{L}_{NX}N-\mathscr{L}_X\left(\frac{N^2}{2}\right)=\left[N,\ \frac{1}{2}\,\mathscr{L}_XN\right], \tag{2.5}$$

for all vector fields, X*, on* M*.*

Proof: Relation (2.5) follows from the preceding expression of $T(N)$ and the assumption that $T(N)=0$. ■

For the Nijenhuis operator, $N=QP^{-1}$, of a bi-Hamiltonian structure, (P,Q), where P is invertible, Eq. (2.5) becomes

$$\mathscr{L}_{Q\alpha}\,N-\mathscr{L}_{P\alpha}\left(\frac{N^2}{2}\right)=[N,\ \hat{N}(\alpha)] \tag{2.6}$$

for all differential forms α on M, where $\hat{N}(\alpha)=\frac{1}{2}\mathscr{L}P_\alpha N$. This property is the prototype of that of Lax operators on bi-Hamiltonian manifolds.

III. LAX OPERATORS

We first describe the development of the notion of Lax operator from the simplest case to that of Lax operators on Hamiltonian and bi-Hamiltonian phase spaces. We then motivate our definition of Lax–Nijenhuis operators.

A. Lax operators on Hamiltonian and bi-Hamiltonian phase spaces

A dynamical system, $dx/dt=X(x)$, on a manifold M is said to admit a Lax formulation if there exist square matrices L and B, by no means unique, whose coefficients depend on x, such that the given dynamical system is equivalent to

$$\frac{dL}{dt}=[L,\ B], \tag{3.1}$$

where $[L,\ B]=LB-BL$ is the usual commutator. Usually, L is called the Lax operator or the Lax matrix. In fact, both L and B are maps from the manifold M (the space of dependent variables) to the associative algebra of square matrices of a given size. The existence of a Lax formulation for a given dynamical system is important because it implies the existence of a sequence of conserved quantities,

$$J_k=\frac{1}{k}\ \mathrm{tr}\ L^k, \tag{3.2}$$

for $k\in\mathbb{N}^*$, where tr denotes the trace of a matrix. (These conserved quantities need not be functionally independent.) In fact,

$$\frac{dJ_k}{dt}=\mathrm{tr}\ L^{k-1}\ \frac{dL}{dt}=\mathrm{tr}\ L^{k-1}[L,\ B]=\mathrm{tr}(L^kB-L^{k-1}BL)=0.$$

If, moreover, the Lax mapping L is defined on a phase space with a Hamiltonian structure, i.e., on a Poisson manifold, then it is natural to require that the traces of powers of L, which are conserved quantities, be pairwise in involution. In this case, this requirement becomes part of the definition of a Lax operator.

Let us now consider the case where the phase space is a bi-Hamiltonian manifold (M,P,Q). We have seen in Sec. II that, on a bi-Hamiltonian manifold, recursion relations (2.1) for functions f_k imply the pairwise involutivity of these functions. It is natural to require that a Lax operator L defined on a bi-Hamiltonian phase space (M,P,Q) be such that quantities J_k defined by (3.2), proportional to the traces of powers of L, satisfy the so-called Lenard recursion relations

$$Q(dJ_k)=P(dJ_{k+1}), \tag{3.3}$$

for $k\in\mathbb{N}^*$. So, we are led to introduce the following definition of Lax operators on a bi-Hamiltonian phase space (M,P,Q).

Recall that a trace on an associative algebra A over the field of real or complex numbers is a linear form, tr, on A, such that

$$\mathrm{tr}\ L_1L_2=\mathrm{tr}\ L_2L_1, \tag{3.4}$$

for all L_1 and L_2 in A.

Definition 3.1: Let (M,P,Q) be a bi-Hamiltonian manifold. A Lax operator compatible with (P,Q) is an A-valued function L on M, where A is an associative algebra with unit and trace, such that the functions, $J_k=(1/k)\mathrm{tr}\ L^k$, $k\in\mathbb{N}^*$, satisfy the Lenard recursion relations (3.3).

Under this definition, by Proposition 2.3, the traces of the powers of a Lax mapping compatible with (P,Q) are pairwise in involution with respect to both P and Q.

B. Lax–Nijenhuis operators

To understand what relates L to P and Q, we shall consider the simplest case where L is a matrix, but we shall first review some facts about the geometry of associative algebras.

Let A be an associative algebra with a trace. We assume that the symmetric bilinear form on A, $(L_1,L_2)=\operatorname{tr} L_1L_2$, defines an isomorphism of A with its dual A^* and, by means of this isomorphism, we identify A^* with A. We equip A with the Lie algebra structure defined by the associative product,

$$[L_1,\ L_2]=L_1L_2-L_2L_1.$$

Since $\operatorname{tr} L_1L_2L_3=\operatorname{tr} L_3L_1L_2$, the symmetric bilinear form $(\ ,\ )$ is invariant, i.e.,

$$(L_1,[L_2,\ L_3])=([L_1,\ L_2],L_3),$$

Thus the coadjoint action of the Lie algebra A on A^* is identified with the adjoint action of A on itself, and the tangent space at L in A to the coadjoint orbit of L is $\{[L,B]|B\in A\}$. (See also VIII.4 of Ref. 33 for the role of coadjoint orbits in the theory of Lax operators.)

Proposition 3.2: Let A be the algebra of square $n\times n$ matrices, where n is a positive integer. Let L be an A-valued Lax operator compatible with the bi-Hamiltonian structure (P,Q). We assume that L is semi-simple. Then, at each point where the eigenvalues of L are distinct, and for each differential one-form α on M, there exists a matrix $\widetilde{L}(\alpha)$ such that

$$\mathscr{L}_{Q\alpha}L-L\mathscr{L}_{P\alpha}L=[L,\ \widetilde{L}(\alpha)]. \tag{3.5}$$

Proof: Let α be any differential one-form on M. Then, by the definition of a Lax operator, L, compatible with (P,Q), and the skewsymmetry of P and Q, for all one-forms α and for all $k\in\mathbb{N}^*$,

$$\frac{1}{k}\operatorname{tr}\mathscr{L}_{Q\alpha}L^k=\frac{1}{k+1}\operatorname{tr}\mathscr{L}_{P\alpha}L^{k+1},$$

and therefore we obtain

$$\operatorname{tr} L^{k-1}(\mathscr{L}_{Q\alpha}L-L\mathscr{L}_{P\alpha}L)=0.$$

This condition expresses the fact that for all k, the vector field with value $\mathscr{L}_{Q\alpha}L-L\mathscr{L}_{P\alpha}L$ at L leaves $\operatorname{tr} L^k$ invariant, which implies that it leaves all eigenvalues of L invariant. This condition is clearly satisfied if $\mathscr{L}_{Q\alpha}L-L\mathscr{L}_{P\alpha}L$ is tangent to the coadjoint orbit of L, and the converse holds if L is semi-simple with distinct eigenvalues. Thus, under the assumptions of the proposition on the spectrum of L, for each α there exists a matrix, $\widetilde{L}(\alpha)$, such that Eq. (3.5) is satisfied. ■

We shall now allow L to be a section of an associative algebra bundle with trace, $\mathscr{A}$, over M. By this we mean a vector bundle over M such that each fiber $\mathscr{A}_x$ of $\mathscr{A}$, for x in M, is an associative algebra with unit and trace, depending smoothly on x. Obviously an A-valued function L on M corresponds to the case where $\mathscr{A}$ is the trivial vector bundle, $\mathscr{A}=M\times A$. However, we formulate our definition in this more general situation in order to include the case of the Nijenhuis operators that was considered in Sec. II. At each point x in M, $\operatorname{End}(T_xM)$ is an associative algebra with trace, to which we can apply the preceding remarks. Equation (3.5) means that for each differential form α on M, and for each x in M, the vertical vector, $(\mathscr{L}_{Q\alpha}L-L(\mathscr{L}_{P\alpha}L))(x)$, is tangent to the coadjoint orbit of $L(x)$ in $\mathscr{A}_x$. It is easy to show that this is equivalent to the fact

that the vertical vector, $(\mathscr{L}_{Q\alpha} L - \mathscr{L}_{P\alpha}(L^2/2))(x)$, is tangent to this orbit. We assume that M has a bi-Hamiltonian structure, (P,Q). Motivated by the discussion in the previous subsections, we define the following.

Definition 3.3: A section L of an associative algebra bundle $\mathscr{A}$ with trace over a bi-Hamiltonian manifold (M,P,Q) is a Lax–Nijenhuis operator if, for all differential forms α on M, $\mathscr{L}_{Q\alpha}L - \mathscr{L}_{P\alpha}(L^2/2)$ is tangent to the coadjoint orbit of $L(x)$ in the fiber $\mathscr{A}_x$ of $\mathscr{A}$, for each x in M.

Identifying a section of $T^*\mathscr{A}$ over L with a section of $T\mathscr{A}$ over L and using the identification of the dual of the vertical space at x, $(V(\mathscr{A}_x))^* = \mathscr{A}_x^*$, with the vertical space $V(\mathscr{A}_x) = \mathscr{A}_x$, we obtain immediately the following.

Proposition 3.4: A section $L: M \to \mathscr{A}$ is a Lax–Nijenhuis operator if there exists a lifting of L into a section $\hat{L}: T^*M \to T^*\mathscr{A}$ such that

$$\mathscr{L}_{Q\alpha} L - \mathscr{L}_{P\alpha}\left(\frac{L^2}{2}\right) = [L,\ \hat{L}(\alpha)], \tag{3.6}$$

for each section α of T^*M.

Equation (3.6) is called the *Lax–Nijenhuis equation.*

Examples. By (2.6), the recursion operator of a bi-Hamiltonian manifold (M,P,Q) with P invertible is a Lax–Nijenhuis operator.

Proposition 3.2 shows that any matrix-valued Lax operator with a simple spectrum compatible with (P,Q) is a Lax–Nijenhuis operator.

C. Properties of Lax–Nijenhuis operators

We shall now prove that the traces of powers of any matrix-valued Lax–Nijenhuis operator on a bi-Hamiltonian manifold, (M,P,Q), satisfy the Lenard recursion relations (3.3), and that the operator is therefore, by Definition 3.1, a Lax operator compatible with (P,Q).

Proposition 3.5: Let L be a matrix-valued Lax–Nijenhuis operator on a bi-Hamiltonian manifold (M,P,Q). Then the functions $J_k = (1/k)\operatorname{tr} L^k$, $k \in \mathbb{N}^*$, satisfy the Lenard recursion relations (3.3), and L is a Lax operator compatible with (P,Q). Moreover, if L is invertible, relation (3.3) holds when k is a negative integer, and, if L admits a fractional power, $L^{1/r}$, relation (3.3) also holds when k is an integral multiple of $1/r$.

Proof: Relation (3.6) implies that, for any $k \in \mathbb{N}^*$,

$$L^{k-1}\mathscr{L}_{Q\alpha} L - L^{k-1}\mathscr{L}_{P\alpha}\left(\frac{L^2}{2}\right) = [L,\ L^{k-1}\hat{L}(\alpha)],$$

for any α. Taking traces of both sides implies that

$$\mathscr{L}_{Q\alpha}\left(\frac{1}{k}\operatorname{tr} L^k\right) = \mathscr{L}_{P\alpha}\left(\frac{1}{k+1}\operatorname{tr} L^{k+1}\right),$$

or, with the notation of (3.2),

$$\langle Q\alpha, dJ_k\rangle = \langle P\alpha, dJ_{k+1}\rangle.$$

Since this relation holds for any differential form α, we obtain relation (3.3) by the skewsymmetry of P and Q. It follows from Definition 3.1 that L is a Lax operator compatible with (P,Q).

We now show that relation (3.3) holds for negative and fractional powers of Lax–Nijenhuis operators, when they are defined. When α is a fixed differential form, we introduce the convenient notations

$$\mathscr{L}_{P\alpha} L = \frac{dL}{dt_1}, \quad \mathscr{L}_{Q\alpha} L = \frac{dL}{dt_2}, \quad \hat{L}(\alpha) = B.$$

Using the following elementary formulas, valid for L, $B \in A$ and $k \in \mathbb{N}^*$,

$$[L^k, B] = \sum_{j=0}^{k-1} [L, L^j B L^{k-1-j}] = \sum_{j=0}^{k-1} L^j [L, B] L^{k-1-j} \tag{3.7}$$

and

$$\frac{dL^k}{dt} = \sum_{j=0}^{k-1} L^j \frac{dL}{dt} L^{k-1-j}, \tag{3.8}$$

we obtain from (3.6), by induction on k,

$$\frac{dL^k}{dt_2} - \frac{1}{2}\left(L \frac{dL^k}{dt_1} + \frac{dL^k}{dt_1} L \right) = [L^k, B], \tag{3.9}$$

for k a positive integer. Let us prove that, if L is invertible, (3.9) is also valid for k a negative integer. In fact, for $k = -1$,

$$\begin{aligned}
&\frac{dL^{-1}}{dt_2} - \frac{1}{2}\left(L \frac{dL^{-1}}{dt_1} + \frac{dL^{-1}}{dt_1} L \right) = -L^{-1} \frac{dL}{dt_2} L^{-1} + \frac{1}{2}\left(\frac{dL}{dt_1} L^{-1} + L^{-1} \frac{dL}{dt_1} \right) \\
&= -\frac{1}{2} L^{-1}\left(L \frac{dL}{dt_1} + \frac{dL}{dt_1} L \right) L^{-1} + \frac{1}{2}\left(\frac{dL}{dt_1} L^{-1} + L^{-1} \frac{dL}{dt_1} \right) - L^{-1}[L, B] L^{-1} \\
&= -BL^{-1} + L^{-1} B = [L^{-1}, B],
\end{aligned}$$

and, more generally, formula (3.9) for $k < -1$ is proved by recursion.

We now assume that L admits a fractional power D, namely $D^r = L$, for some positive integer r. Then using (3.7) and (3.8), we obtain

$$\begin{aligned}
0 &= \frac{dD^r}{dt_2} - \frac{1}{2}\left(D^r \frac{dD^r}{dt_1} + \frac{dD^r}{dt_1} D^r \right) - [D^r, B] \\
&= \sum_{j=1}^{r} \left(D^{r-j} \frac{dD}{dt_2} D^{j-1} - \frac{1}{2}\left(D^r D^{r-j} \frac{dD}{dt_1} D^{j-1} + D^{r-j} \frac{dD}{dt_1} D^{j-1} D^r \right) - D^{r-j}[D,B] D^{j-1} \right),
\end{aligned}$$

thus

$$\sum_{j=1}^{r} D^{r-j}\left(\frac{dD}{dt_2} - \frac{1}{2}\left(L \frac{dD}{dt_1} + \frac{dD}{dt_1} L \right) - [D, B] \right) D^{j-1} = 0. \tag{3.10}$$

Still more generally, if $D^r = L$, and h is a positive integer, we can prove

$$\sum_{j=1}^{r} D^{r-j}\left(\frac{dD^h}{dt_2} - \frac{1}{2}\left(L \frac{dD^h}{dt_1} + \frac{dD^h}{dt_1} L \right) - [D^h, B] \right) D^{j-1} = 0. \tag{3.11}$$

In fact, we first write (3.10), left-multiply by D^{h-1-i}, then right-multiply by D^i, and sum from $i=0$ to $h-1$. In the resulting equality, we use (3.7) and (3.8) to obtain (3.11). Taking traces in (3.11) and using

$$\frac{1}{b}\,\mathrm{tr}\,D^a\,\frac{dD^b}{dt}=\frac{1}{a+b}\,\mathrm{tr}\,\frac{dD^{a+b}}{dt},$$

we obtain

$$\frac{1}{r+h-1}\,\mathrm{tr}\,\frac{dD^{r+h-1}}{dt_2}=\frac{1}{2r+h-1}\,\mathrm{tr}\,\frac{dD^{2r+h-1}}{dt_1}. \tag{3.12}$$

Setting $(r+h-1)/r=k$, we obtain relation (3.3) for any k that is an integral multiple of $1/r$. Combining the previous results, we see that this formula also holds for negative rational numbers, when such powers of L are defined. ■

IV. BI-HAMILTONIAN HIERARCHIES AND LAX FORMULATION

We have emphasized the striking analogies between the properties of a Lax operator compatible with a bi-Hamiltonian structure and those of a Nijenhuis operator. In this section, we shall continue by considering the ''hereditary properties'' of both types of operators.

The simplest hereditary property of a Nijenhuis operator, N, is that it maps symmetries of N into symmetries of N. In fact, if a vector field X is a symmetry of N, i.e., is such that

$$\mathscr{L}_X N=0,$$

then, by relation (2.4), and as a consequence of the vanishing of the torsion of N,

$$\mathscr{L}_{NX} N=0.$$

Thus, if X is a symmetry of N, so are NX and, more generally, N^kX, for $k\in\mathbb{N}$. The property has been ''inherited'' by the iterated vector fields $NX, N^2X,\ldots$.

We now consider a sequence of differential one-forms, α_k, $k\in\mathbb{N}$, on a bi-Hamiltonian manifold, (M,P,Q), that satisfy the recursion relations,

$$Q\alpha_k=P\alpha_{k+1}. \tag{4.1}$$

Let us consider the sequence of vector fields,

$$X_k=Q\alpha_k=P\alpha_{k+1}. \tag{4.2}$$

If P is invertible, then, by Lemma 2.5, $N=QP^{-1}$ is a Nijenhuis operator and it satisfies

$$X_{k+1}=NX_k. \tag{4.3}$$

If we now assume that the vector field X_0 is a symmetry of the Nijenhuis operator N, then so is X_k, for each $k\in\mathbb{N}$, by the hereditary property of N, recalled above.

Let us now examine the corresponding property for Lax–Nijenhuis operators. Let L be a matrix-valued Lax–Nijenhuis operator on a bi-Hamiltonian manifold (M,P,Q), in the sense of Definition 3.3, and let α_k and X_k be forms and vectors as above. We assume that the vector field X_0 is such that there exists a matrix-valued mapping A_0 on M satisfying

$$\frac{dL}{dt_0}=[L,\,A_0],\quad \text{where } \frac{dL}{dt_0}=\mathscr{L}_{X_0}L. \tag{4.4}$$

We shall prove by recursion that, for any vector field X_k in the associated sequence, there exists a matrix-valued mapping A_k on M satisfying

$$\frac{dL}{dt_k}=[L,\ A_k], \quad \text{where } \frac{dL}{dt_k}=\mathscr{L}_{X_k}L. \tag{4.5}$$

In fact, let us assume (4.5) for 0,1,...,$k-1$. Then, from (3.6), we obtain

$$\begin{aligned}\mathscr{L}_{X_k}L=\mathscr{L}_{Q\alpha_k}L&=\mathscr{L}_{P\alpha_k}\frac{L^2}{2}L+[L,\ \hat{L}(\alpha_k)]\\&=\tfrac{1}{2}(L\mathscr{L}_{X_{k-1}}L+(\mathscr{L}_{X_{k-1}}L)L)+[L,\ \hat{L}(\alpha_k)]\\&=[L,\ \tfrac{1}{2}(LA_{k-1}+A_{k-1}L)+\hat{L}(\alpha_k)].\end{aligned}$$

Setting $A_k=\frac{1}{2}(LA_{k-1}+A_{k-1}L)+\hat{L}(\alpha_k)$, we obtain (4.5) for k.

Remark: Setting $\hat{L}(\alpha_k)=C_k$, $k\in\mathbb{N}$, an explicit expression for A_k, $k\in\mathbb{N}^*$, is

$$A_k=\frac{1}{2^k}\sum_{h=0}^{k}\binom{k}{h}L^hA_0L^{k-h}+\sum_{h=0}^{k-1}\sum_{p=0}^{h}\frac{1}{2^h}\binom{h}{p}L^pC_{k-h}L^{h-p}.$$

In fact, this formula is valid for $k=1$ and is proved by recursion.

The following proposition summarizes this discussion.

Proposition 4.1: Let α_k, $k\in\mathbb{N}$, be a sequence of differential one-forms on the bi-Hamiltonian manifold (M,P,Q), with α_k satisfying recursion relations (4.1) and let $X_k=Q\alpha_k=P\alpha_{k+1}=d/dt_k$ be the corresponding sequence of vector fields. If the vector field $X_0=d/dt_0$ admits a Lax formulation,

$$\frac{dL}{dt_0}=[L,\ A_0],$$

where L is a matrix-valued Lax–Nijenhuis operator, then for each $k\in\mathbb{N}$, there exists a matrix-valued mapping A_k on M satisfying (4.5).

In particular, we shall consider the case when there exists a sequence of closed differential one-forms α_k satisfying recursion relations (4.1). When P is invertible, we set $N=QP^{-1}$, and we denote the transpose of N by ${}^tN$. Then (4.1) is written

$$\alpha_{k+1}={}^tN(\alpha_k) \quad \text{or} \quad \alpha_k=({}^tN)^k\alpha_0,$$

and (4.3) is written

$$X_k=N^k(X_0).$$

Proposition 4.2: Let (M,P,Q) be a bi-Hamiltonian manifold with P invertible. Assume that the differential one-forms α_0 and α_1 are closed. Then all α_k's are closed and the vector fields X_k, $k\in\mathbb{N}$, are (locally) bi-Hamiltonian vector fields which commute in pairs.

Proof: Using the fact that N has vanishing Nijenhuis torsion (Lemma 2.5), we find that

$$d\alpha_k(X,Y)=d\alpha_{k-1}(NX,Y)+d\alpha_{k-1}(X,NY)-d\alpha_{k-2}(NX,NY),$$

for $k\geqslant 2$ and for all vector fields X,Y on M. Thus all the α_k's are closed.

Therefore each vector field X_k is (locally) bi-Hamiltonian.

$$\mathscr{L}_{X_k}P=0, \quad \mathscr{L}_{X_k}Q=0,$$

and hence each X_k is a symmetry of N,

$$\mathscr{L}_{X_k}N=0.$$

(This fact also follows from $\mathscr{L}_{X_0}N = 0$ and the hereditary property of N.)

Thus

$$\begin{aligned}[X_k, X_l]=\mathscr{L}_{X_k}(N^lX_0)&=(\mathscr{L}_{X_k}N^l)X_0+N^l\mathscr{L}_{X_k}X_0\\&=-N^l\mathscr{L}_{X_0}(N^kX_0)\\&=-N^l(\mathscr{L}_{X_0}N^k)(X_0)-N^{l+k}\mathscr{L}_{X_0}X_0=0.\end{aligned}$$ ■

Remark: If X is any (locally) bi-Hamiltonian vector field, then $\mathscr{L}_XN=0$. It follows that if Y is a symmetry of X, so is NY. This justifies the term ''recursion operator'' for the Nijenhuis operator N of a bi-Hamiltonian structure (P,Q), with P invertible.

Remark: Let k and l be non-negative integers. For any Nijenhuis operator N and vector field X, it follows from (2.4) by recursion that

$$\mathscr{L}_{NX}(N^l)=N\mathscr{L}_X(N^l)$$

and that

$$\mathscr{L}_{N^kX}(N^l)=N^k\mathscr{L}_X(N^l).$$

For $k=l$, we recover the well-known fact that any positive power of a Nijenhuis operator is a Nijenhuis operator, and that negative and fractional powers of a Nijenhuis operator, when they are defined, are also Nijenhuis operators.

A sequence of commuting bi-Hamiltonian vector fields is called a *bi-Hamiltonian hierarchy*. When X_k, $k\in\mathbb{N}$, is a bi-Hamiltonian hierarchy, we obtain further properties for the sequence of Lax equations (4.5). In fact, writing that $\mathscr{L}_{X_j}\mathscr{L}_{X_k}L - \mathscr{L}_{X_k}\mathscr{L}_{X_j}L = 0$ for all $j, k\in\mathbb{N}$, we obtain

$$\begin{aligned}0&=\mathscr{L}_{X_j}[L, A_k]-\mathscr{L}_{X_k}[L, A_j]\\&=\left[\frac{\partial L}{\partial t_j}, A_k\right]+\left[L, \frac{\partial A_k}{\partial t_j}\right]-\left[\frac{\partial L}{\partial t_k}, A_j\right]-\left[L, \frac{\partial A_j}{\partial t_k}\right]\\&=[[L, A_j], A_k]-[[L, A_k], A_j]+\left[L, \frac{\partial A_k}{\partial t_j}-\frac{\partial A_j}{\partial t_k}\right]\\&=\left[L, [A_j, A_k]+\frac{\partial A_k}{\partial t_j}-\frac{\partial A_j}{\partial t_k}\right],\end{aligned}$$

by the Jacobi identity. Thus the operator, which can be called the curvature of the connection defined by A_k,

$$[A_j, A_k]+\frac{\partial A_k}{\partial t_j}-\frac{\partial A_j}{\partial t_k}$$

commutes with L. Summarizing, we obtain the following.

Proposition 4.3: When X_k is a bi-Hamiltonian hierarchy with Lax formulation (4.5), the curvature of the connection with components A_k commutes with the Lax operator L.

V. EXAMPLES

In this section, we give four examples showing how the Lax–Nijenhuis equation can be used to compute higher-order Hamiltonian structures associated with a Hamiltonian system admitting a Lax formulation. We write the Lax–Nijenhuis equation (3.6) in the form

$$\mathscr{L}_{Q\alpha} L = \tfrac{1}{2}(L\mathscr{L}_{P\alpha} L + (\mathscr{L}_{P\alpha} L)L) + [L, \hat{L}(\alpha)], \tag{5.1}$$

and we use the information on L and the arbitrariness of α to split this equation into two parts: the first determines the unknown map $\hat{L}$, up to some still arbitrary constants, the second part determines $\mathscr{L}_{Q\alpha} L$ and then Q. The condition of skewsymmetry on Q then determines the constants. The discussion is quite similar to a problem with constraints coming from the restrictions imposed on L, where the role of the Lagrange multipliers is played by the mapping $\hat{L}$.

A. The Toda system

We shall consider the Toda system and its well-known Lax formulation. Let $M = \mathbb{R}^{2n+1}$ with coordinates $x^I = (a_j, b_l)$, $j = 1,\ldots,n$, $l = 1,\ldots,n+1$, $I = 1,\ldots,2n+1$. We consider the Poisson bivector P_0 defined by

$$\begin{aligned} \{a_j, b_j\} &= -a_j, \quad j = 1,2,\ldots,n \\ \{a_j, b_{j+1}\} &= a_j, \quad j = 1,2,\ldots,n, \end{aligned} \tag{5.2}$$

all other Poisson brackets being equal to 0. Thus the Poisson bivector P_0 has matrix

$$(P_0^{IJ}) = \begin{pmatrix} & & & & & a_1 & -a_1 & & & \\ & & & & & & a_2 & -a_2 & & 0 \\ & & & 0 & & & & \ddots & \ddots & \\ & & & & & & 0 & & \ddots & \ddots \\ & & & & & & & & & a_n & -a_n \\ -a_1 & & & & & & & & & & \\ a_1 & -a_2 & & 0 & & & & & & & \\ & a_2 & \ddots & & & & & & & & \\ & & \ddots & \ddots & & & & 0 & & & \\ & 0 & & \ddots & -a_n & & & & & & \\ & & & & a_n & & & & & & \end{pmatrix}.$$

When $H = \Sigma_{j=1}^{n} a_j^2 + 1/2\Sigma_{l=1}^{n+1} b_l^2$, the Hamiltonian vector field $X = P_0 dH$ is the Toda vector field. In fact, the evolution equation $dx/dt = X(x)$ is the system

$$\frac{da_j}{dt} = \{a_j, H\}, \quad j = 1,2,\ldots,n,$$

$$\frac{db_l}{dt} = \{b_l, H\}, \quad l = 1,2,\ldots,n+1,$$

and, setting $a_0 = a_{n+1} = 0$, this system becomes

$$\frac{da_j}{dt}=a_j(b_{j+1}-b_j), \quad j=1,2,\ldots,n,$$
$$\frac{db_l}{dt}=2(a_l^2-a_{l-1}^2), \quad l=1,2,\ldots,n+1, \tag{5.3}$$

which are the equations of the Toda system in Flaschka coordinates.[15] A Lax formulation for the Toda system is

$$\frac{dL}{dt}=[L, A],$$

where

$$L=\begin{pmatrix} b_1 & a_1 & & & & & \\ a_1 & b_2 & a_2 & & & 0 & \\ & a_2 & b_3 & a_3 & & & \\ & & a_3 & \ddots & \ddots & & \\ & & & \ddots & \ddots & \ddots & \\ & 0 & & & \ddots & b_n & a_n \\ & & & & & a_n & b_{n+1} \end{pmatrix}, \quad A=\begin{pmatrix} 0 & a_1 & & & & & \\ a_1 & 0 & a_2 & & & 0 & \\ & a_2 & 0 & a_3 & & & \\ & & a_3 & \ddots & \ddots & & \\ & & & \ddots & \ddots & \ddots & \\ & 0 & & & \ddots & 0 & a_n \\ & & & & & a_n & 0 \end{pmatrix}. \tag{5.4}$$

Now let P and Q be Poisson structures such that (5.1) is satisfied for L symmetric and tridiagonal, as above. We assume that P is known, and we consider Q to be an unknown, higher-order, Poisson structure. We shall assume that $\hat{L}(\alpha)$ depends linearly on α, and we shall denote the matrix $\hat{L}(dx^I)$ of order $n+1$ by C^I. Then (5.1) becomes

$$L\left(P^{IJ}\frac{\partial L}{\partial x^J}+2C^I\right)+\left(P^{IJ}\frac{\partial L}{\partial x^J}-2C^I\right)L=2Q^{IJ}\frac{\partial L}{\partial x^J}, \tag{5.5}$$

where the summation over $J=1,2,\ldots,2n+1$ is understood.

We shall assume that C^I is a skewsymmetric tridiagonal matrix, for each $I=1,\ldots,2n+1$,

$$C^I=\begin{pmatrix} 0 & c^{I1} & & & & & \\ -c^{I1} & 0 & c^{I2} & & & 0 & \\ & -c^{I2} & 0 & c^{I3} & & & \\ & & -c^{I3} & \ddots & \ddots & & \\ & & & \ddots & \ddots & \ddots & \\ & 0 & & & \ddots & 0 & c^{In} \\ & & & & & -c^{In} & 0 \end{pmatrix}, \tag{5.6}$$

where $c_1^I,\ldots,c_n^I$ are to be determined. This choice is the simplest possible and it guarantees that $[L, C^I]$ is a symmetric penta-diagonal matrix. Any other choice of C^I would yield a matrix $[L, C^I]$ with more entries, and so with more constraints to be imposed.

For each $I=1,\ldots,2n+1$, $P^{IJ}(\partial L/\partial x^J)$ is the symmetric tridiagonal matrix

$$\begin{pmatrix} P^{I,n+1} & P^{I1} & & & 0 \\ P^{I1} & P^{I,n+2} & P^{I2} & & \\ & P^{I2} & \ddots & \ddots & \\ & & \ddots & P^{I,2n} & P^{In} \\ 0 & & & P^{In} & P^{I,2n+1} \end{pmatrix},$$

and therefore $(P^{IJ}(\partial L/\partial x^J)-2C^I)L$ is the transpose of $L(P^{IJ}(\partial L/\partial x^J)+2C^I)$. Thus condition (5.5) implies that, for fixed I, matrix C^I is such that the symmetric part of $L(P^{IJ}(\partial L/\partial x^J)+2C^I)$ is tridiagonal. Writing this condition explicitly, one obtains

$$\sum_{k=1}^{n-1}(a_k(P^{J,k+1}+2c^{J,k+1})+a_{k+1}(P^{Jk}-2c^{Jk}))=0.$$

Solving this system for c^{Jk} in terms of P^{Jk} yields the existence of multipliers λ_k^J, $k=1,2,\ldots,n$, such that

$$2c^{Jk}=P^{Jk}+2\lambda_k^J a_k\,.$$

We assume that P^{Jk} is divisible by a_k. This assumption is satisfied for $P=P_0$ defined by (5.2). Setting $\lambda_1^J=\lambda^J$, we obtain

$$2c^{Jk}=P^{Jk}+2a_k\left(\lambda^J-\sum_{j=2}^{k}\frac{P^{Jj}}{a_j}\right).$$

(By convention, here and below the last sum vanishes if $k<2$.)

From relations (5.5), we then obtain the coefficients of the higher-order Poisson structure Q,

$$Q^{Jk}=\tfrac{1}{2}a_k(P^{J,n+k}+P^{J,n+k+1})+\tfrac{1}{2}b_k(P^{Jk}+2c^{Jk})+\tfrac{1}{2}b_{k+1}(P^{Jk}-2c^{Jk}),$$

$$Q^{J,n+l}=a_l(P^{Jl}-2c^{Jl})+a_{l-1}(P^{J,l-1}+2c^{J,l-1})+b_lP^{J,n+l}.$$

We now replace the c^{Jk}s by their values in terms of the parameters λ^J, and we impose the conditions that the diagonal terms of Q vanish. These $2n+1$ conditions imply

$$2(b_{k+1}-b_k)\left(\lambda^k-\sum_{j=2}^{k-1}\frac{P^{kj}}{a_j}\right)=P^{k,n+k}+P^{k,n+k+1},$$

$$a_1^2\lambda^{n+1}=0,$$

$$(a_l^2-a_{l-1}^2)\left(\lambda^{n+l}-\sum_{j=2}^{l-1}\frac{P^{n+l,j}}{a_j}\right)=a_{l-1}P^{n+l,l-1}+a_lP^{n+l,l},$$

for $l=2,\ldots,n+1$.

Thus, we have obtained

$$Q^{Jk}=\frac{1}{2}\,a_k(P^{J,n+k}+P^{J,n+k+1})+b_kP^{Jk}+a_k(b_k-b_{k+1})\left(\lambda^J-\sum_{j=2}^{k-1}\frac{P^{Jj}}{a_j}\right),$$

$$Q^{J,n+l}=2(a_{l-1}P^{J,l-1}+a_lP^{Jl})+b_lP^{J,n+l}+2(a_{l-1}^2-a_l^2)\left(\lambda^J-\sum_{j=2}^{l-1}\frac{P^{Jj}}{a_j}\right),$$

where the λ^Js are given above in terms of a_k, b_l, and P^{IJ}.

Let us assume that all a_ks are nonvanishing and let us introduce the matrix M of order $2n+1$, depending on $a_1,\ldots,a_n,b_1,\ldots,b_{n+1}$, such that M applied to the column with entries $A_1,\ldots,A_n,B_1,\ldots,B_{n+1}$, is the column with entries

$$\overline{A_k}=\frac{1}{2}\,a_k(B_k+B_{k+1})+b_kA_k+a_k(b_{k+1}-b_k)\sum_{j=2}^{k}\frac{A_j}{a_j},$$

$$\overline{B_1}=b_1B_1,\quad \overline{B_2}=b_2B_2+2(a_1A_1+a_2A_2), \tag{5.7}$$

$$\overline{B_l}=b_lB_l+2(a_{l-1}A_{l-1}+a_lA_l)+2(a_l^2-a_{l-1}^2)\sum_{j=2}^{l-1}\frac{A_j}{a_j},$$

for $l=3,\ldots,n+1$.

We see that

$$Q=MP+X\otimes\lambda,$$

where X is the Toda vector field with components

$$a_1(b_2-b_1),a_2(b_3-b_2),\ldots,a_n(b_{n+1}-b_n),2a_1^2,2(a_2^2-a_1^2),\ldots,-2a_n^2,$$

and λ is the vector with components $\lambda^1,\ldots,\lambda^n,\lambda^{n+1},\ldots,\lambda^{2n+1}$. We observe that, although Q is skewsymmetric, this expression does not constitute a decomposition of Q into a sum of skewsymmetric two-tensors.

Thus the Lax–Nijenhuis equation yields an explicit determination of the bivector Q in terms of P. For $P=P_0$, we see that the corresponding vector $\lambda=\lambda_{(0)}$ is the row-matrix with entries

$$\lambda_{(0)}^J=-\tfrac{1}{2}\delta_{n+2}^J. \tag{5.8}$$

It is easy to check that

$$P_1=MP_0+X\otimes\lambda_{(0)}$$

coincides with the second Poisson structure of the Toda system.[17,19,20] For example, if $n=3$, the matrix MP_0 is equal to

$$\begin{pmatrix} b_1 & 0 & 0 & \frac{a_1}{2} & \frac{a_1}{2} & 0 & 0 \\ 0 & b_3 & 0 & 0 & \frac{a_2}{2} & \frac{a_2}{2} & 0 \\ 0 & U & b_4 & 0 & 0 & \frac{a_3}{2} & \frac{a_3}{2} \\ 0 & 0 & 0 & b_1 & 0 & 0 & 0 \\ 2a_1 & 2a_2 & 0 & 0 & b_2 & 0 & 0 \\ 0 & 2\frac{a_3^2}{a_2} & 2a_3 & 0 & 0 & b_3 & 0 \\ 0 & -2\frac{a_3^2}{a_2} & 0 & 0 & 0 & 0 & b_4 \end{pmatrix} \begin{pmatrix} & & & a_1 & -a_1 & 0 & 0 \\ & 0 & & 0 & a_2 & -a_2 & 0 \\ & & & 0 & 0 & a_3 & -a_3 \\ -a_1 & 0 & 0 & & & & \\ a_1 & -a_2 & 0 & & & & \\ 0 & a_2 & -a_3 & & & 0 & \\ 0 & 0 & a_3 & & & & \end{pmatrix},$$

where $U=(a_3/a_2)(b_4-b_3)$, and

$$X\otimes\lambda_{(0)}=\begin{pmatrix} a_1(b_2-b_1) \\ a_2(b_3-b_2) \\ a_3(b_4-b_3) \\ 2a_1^2 \\ 2(a_2^2-a_1^2) \\ 2(a_3^2-a_2^2) \\ -2a_3^2 \end{pmatrix} \otimes {}^t(0 \quad 0 \quad 0 \quad 0 \quad -\tfrac{1}{2} \quad 0 \quad 0),$$

so that

$$P_1=MP_0+X\otimes\lambda_{(0)}=\begin{pmatrix} 0 & -\frac{1}{2}a_1a_2 & 0 & a_1b_1 & -a_1b_2 & 0 & 0 \\ \frac{1}{2}a_1a_2 & 0 & -\frac{1}{2}a_2a_3 & 0 & a_2b_2 & -a_2b_3 & 0 \\ 0 & \frac{1}{2}a_2a_3 & 0 & 0 & 0 & a_3b_3 & -a_3b_4 \\ -a_1b_1 & 0 & 0 & 0 & -2a_1^2 & 0 & 0 \\ a_1b_2 & -a_2b_2 & 0 & 2a_1^2 & 0 & -2a_2^2 & 0 \\ 0 & a_2b_3 & -a_3b_3 & 0 & 2a_2^2 & 0 & -2a_3^2 \\ 0 & 0 & a_3b_4 & 0 & 0 & 2a_3^2 & 0 \end{pmatrix}.$$

Repeating the process, we have to compute the bivector

$$P_2=MP_1+X\otimes\lambda_{(1)},$$

where $\lambda_{(1)}$ is the vector corresponding to P_1. We can show that

$$\lambda_{(1)}=M\lambda_{(0)}.$$

For example, if $n=3$,

$$\lambda_{(1)}=(-\tfrac{1}{4}a_1,-\tfrac{1}{4}a_2,0,0,-\tfrac{1}{2}b_2,0,0)$$

and P_2 is the skewsymmetric matrix

$$P_2 = MP_1 + X \otimes \lambda_{(1)}$$

$$= \begin{pmatrix} 0 & -a_1a_2b_2 & 0 & a_1b_1^2+a_1^3 & -a_1b_2^2-a_1^3 & -a_1a_2^2 & 0 \\ & 0 & -a_2a_3b_3 & a_1^2a_2 & a_2b_2^2+a_2^3 & -a_2b_3^2-a_2^3 & -a_2a_3^2 \\ & & 0 & 0 & a_2^2a_3 & a_3b_3+a_3^2 & -a_3b_4^2-a_3^2 \\ & & & 0 & -2a_1^2(b_1+b_2) & 0 & 0 \\ & & & & 0 & -2a_2^2(b_2+b_3) & 0 \\ & & & & & 0 & -2a_3^2(b_3+b_4) \\ & & & & & & 0 \end{pmatrix}.$$

In this case, P_2 coincides with the opposite of the third Poisson structure of the Toda system described in Refs. 17 and 20.

Thus if M is the matrix of order $2n+1$ defined by (5.7), the bivectors P_i obtained from the Lax–Nijenhuis equation satisfy

$$P_{i+1} = MP_i + X \otimes \lambda_{(i)},$$

where X is the Toda vector field and $\lambda_{(i)}$ is the vector corresponding to P_i.

In particular, it follows that each coefficient P_i^{Jk} of the bivector P_i is divisible by a_k, so the iteration can be carried out.

Let us show that in fact the skewsymmetry of P_i and P_{i+1} implies that

$$\lambda_{(i+1)} = M\lambda_{(i)}.$$

Thus we consider

$$P_i = MP_{i-1} + X \otimes \lambda_{(i-1)},$$

$$P_{i+1} = MP_i + X \otimes \lambda_{(i)}.$$

Since P_{i+1} is assumed to be skewsymmetric, $\lambda_{(i)}$ must satisfy

$$P_i{}^tM - MP_i = X \otimes \lambda_{(i)} + \lambda_{(i)} \otimes X.$$

Moreover, from the skewsymmetry of P_i, we obtain

$$P_i = MP_{i-1} + X \otimes \lambda_{(i-1)} = P_{i-1}{}^tM - \lambda_{(i-1)} \otimes X,$$

where

$$P_i{}^tM - MP_i = X \otimes M\lambda_{(i-1)} + M\lambda_{(i-1)} \otimes X.$$

We thus obtain $\lambda_{(i)} = M\lambda_{(i-1)}$. The following proposition summarizes this discussion.

Proposition 5.1: Let M be the matrix of order $2n+1$ defined by (5.7). The bivectors obtained from the Lax–Nijenhuis equation satisfy

$$P_{i+1} = MP_i + X \otimes M^i\lambda_{(0)},$$

where $\lambda_{(0)}$ is the vector given by (5.8).

B. The *n*-dimensional rigid body

The Euler equations for the n-dimensional rigid body rotating about a fixed point can be written

$$\dot{M} = [M,\ \Omega],$$

where M is the angular momentum, a time-dependent element of the Lie algebra so(n), and

$$M = J\Omega + \Omega J.$$

Here J is a diagonal matrix with positive entries $J_1, J_2, \ldots, J_n$ defined in terms of the principal moments of inertia, and Ω is the angular velocity. These equations admit a Lax formulation, with a spectral parameter,

$$\dot{L} = [L,\ B],$$

where $L = M/\lambda + J^2$ and $B = \Omega + \lambda J$.

Moreover, it is well known (see, e.g., Refs. 10 and 34) that these equations can be written in Hamiltonian form, with respect to the linear Poisson structure of so(n) induced by the identification of the Lie algebra so(n) with its dual by means of the trace of the product of matrices. Making use of this identification, this Poisson structure P is defined by P_M:so(n)$\to$so(n), for each M in so(n), where

$$P_M = ad_M.$$

If $K(M) = \frac{1}{2}\,\mathrm{tr}(M\Omega)$, then the gradient of K [the differential of K identified with a matrix in so(n)] is the constant matrix Ω, and therefore the Euler equations can be written as the Hamiltonian equation

$$\dot{M} = P(dK).$$

Let us use the Lax–Nijenhuis equation in order to find a possible form of a second Hamiltonian structure that will make this equation a bi-Hamiltonian system. Setting $\dot{L} = dL/dt_1$, it follows from the definitions and from the Euler equation that

$$\frac{d(L^2)}{dt_1} = \frac{1}{\lambda}\,(L[M,\ \Omega] + [M,\ \Omega]L),$$

and therefore, by a simple computation,

$$\frac{1}{2}\,\frac{d(L^2)}{dt_1} = \frac{1}{2\lambda}\,[L,\ M\Omega + \Omega M] + \frac{1}{\lambda}\,(M\Omega L - L\Omega M).$$

By the definition of L, $M\Omega L - L\Omega M = M\Omega J^2 - J^2\Omega M$. This suggests that we should set

$$\frac{dM}{dt_2} = M\Omega J^2 - J^2\Omega M.$$

We observe that if M and Ω are skewsymmetric, so is dM/dt_2. In fact, Q defined by

$$Q_M(V) = MVJ^2 - J^2VM,$$

for $M, V \in$ so(n), is the second, compatible Poisson structure on so(n) that was recently found by Morosi and Pizzocchero.[34] This second Poisson structure Q is actually a deformation of the first, linear one, P, under the linear map $M \to JMJ$. The Euler equation can be written

$$\dot{M} = Q(dH),$$

where $H(M)=-\frac{1}{2}\,\mathrm{tr}(J^{-1}MJ^{-1}\Omega)$, since the gradient of H is $-J^{-1}\Omega J^{-1}$.

We now show how to extend this procedure to the determination of Poisson structures compatible with the linear Poisson structures on the sum of several copies of a simple Lie algebra, considered in Refs. 30 and 35. Let us consider, for instance, the Hamiltonian system

$$\frac{dM_0}{dt_1}=[M_0,\ V_1],$$

$$\frac{dM_1}{dt_1}=[M_0,\ V_0]+[M_1,\ V_1],$$

where V_0 and V_1 are the components of the gradient of a Hamiltonian function K. We introduce the Lax matrix depending on the spectral parameter λ,

$$L=\frac{M_0}{\lambda^2}+\frac{M_1}{\lambda}+A.$$

Computing the derivative of the square of this matrix, we find that

$$\frac{1}{2}\,\frac{d(L^2)}{dt_1}=\left[L,\ \frac{(M_0V_1+V_1M_0)}{2\lambda^2}+\frac{(M_0V_0+V_0M_0)+(M_1V_1+V_1M_1)}{2\lambda}\right]$$

$$+\frac{1}{\lambda^2}\,(M_0V_0M_1-M_1V_0M_0+M_0V_1A-AV_1M_0)$$

$$+\frac{1}{\lambda}\,(M_0V_0A-AV_0M_0+M_1V_1A-AV_1M_1).$$

Therefore the Lax–Nijenhuis equation suggests that we should set

$$\frac{dM_0}{dt_2}=(M_0V_0M_1-M_1V_0M_0)+(M_0V_1A-AV_1M_0),$$

$$\frac{dM_1}{dt_2}=(M_0V_0A-AV_0M_0)+(M_1V_1A-AV_1M_1).$$

A computation shows that this is actually a Poisson structure on the direct sum of two copies of so(n). It is clearly compatible with the first, because it can be obtained by deforming A into $A+\lambda I$.

C. The KdV equation

We now enter the field of nonlinear partial differential equations by considering the Korteweg–de Vries (KdV) equation

$$\frac{du}{dt}=u_{xxx}-6uu_x.$$

We use the notations of the formal calculus of variations.[9,10,8] As is well known, the KdV equation is Hamiltonian since it can be written in the form

$$\frac{\partial u}{\partial t}=\partial\,\frac{\delta H}{\delta u},$$

where

$$H(u)=-\int\left(\frac{1}{2}\,u_x^2+u^3\right)dx,$$

and $\partial=d/dx$ is the Gardner Hamiltonian structure.[13] It admits a Lax representation, $du/dt=[L,\,B]$, with

$$L=\partial^2-u,\quad B=4\partial^3-3(u\partial+\partial u).$$

We now want to use the Lax–Nijenhuis equation (5.1), where $P=\partial$, to find the second Hamiltonian structure of the KdV equation. Since L is a second-order differential operator, we assume that $\hat{L}(\alpha)$ is a first-order differential operator,

$$\hat{L}(\alpha)=\lambda+\mu\partial,$$

where λ and μ depend linearly on the one-form α. A simple computation yields

$$\tfrac{1}{2}\mathscr{L}_{P\alpha}(L^2)=-\alpha_x\partial^2-\alpha_{xx}\partial+(u\alpha_x-\tfrac{1}{2}\alpha_{xxx}),$$

$$[L,\,\hat{L}(\alpha)]=2\mu_x\partial^2+(2\lambda_x+\mu_{xx})\partial+(\lambda_{xx}+\mu u_x).$$

By inserting these formulas into the Lax–Nijenhuis equation and by equating the coefficients of ∂^2, ∂, and ∂^0, we get

$$(2\mu-\alpha)_x=0,$$

$$(2\lambda+\mu_x-\alpha_x)_x=0,$$

$$-\mathscr{L}_{Q\alpha}(u)=u\alpha_x-\tfrac{1}{2}\alpha_{xxx}+\lambda_{xx}+\mu u_x\,.$$

The first two equations yield the solution $\mu=\frac{1}{2}\alpha$, $\lambda=\frac{1}{4}\alpha_x$, while the third one yields the second Hamiltonian structure of the KdV equation,

$$Q_u(\alpha)=\tfrac{1}{4}\alpha_{xxx}-u\alpha_x-\tfrac{1}{2}u_x\alpha.$$

The recursion operator is the nonlocal operator, $R_u=\frac{1}{4}\partial^2-u-\frac{1}{2}u_x\partial^{-1}$.

D. The second Adler–Gelfand–Dickey bracket

We now generalize the previous example to the first equation of the nth KdV hierarchy. The unknowns are functions $u_0,u_1,\ldots,u_{n-1}$ on the circle, whose time evolution is being studied. It admits a Lax formulation,

$$\frac{dL}{dt}=[L,B],$$

where

$$L=\partial^n+u_{n-1}\partial^{n-1}+\cdots+u_0\,,$$

and B is a suitable differential operator of order $n+1$. Here L takes values in a manifold $\mathscr{L}_n$ of invertible elements in the algebra A_n of formal pseudodifferential operators of order $\leqslant n$ on the circle.[36] This equation is Hamiltonian with respect to the Poisson structure P on $\mathscr{L}_n$ which, in the operator formalism, is defined by

$$P_L(\alpha)=[\alpha,L]_+\,, \tag{5.9}$$

where α is the pseudodifferential operator,

$$\alpha=\partial^{-1}\alpha_0+\partial^{-2}\alpha_1+\cdots+\partial^{-n}\alpha_{n-1}\,,$$

which is considered as a one-form on $\mathscr{S}_n$. The value of α on any tangent vector $U=U_{n-1}\partial^{n-1}+\cdots+U_1\partial+U_0$ is, by definition,

$$\langle\alpha,U\rangle=\int \operatorname{res}_{\partial^{-1}}(\alpha\circ U)=\int(\alpha_0U_0+\cdots+\alpha_{n-1}U_{n-1})dx.$$

In Eq. (5.9) the symbol $[L,\alpha]_+$ means that we consider the differential part of the pseudodifferential operator obtained by computing the commutator of the operators L and α by the usual (formal) rules of the algebra of pseudodifferential operators. See, e.g., Refs. 36 and 37.

The Lax–Nijenhuis equation (5.1) then takes the form

$$\mathscr{S}_{Q\alpha}(L)=\tfrac{1}{2}(L[\alpha,L]_+-[\alpha,L]_+L)+[L,\hat{L}(\alpha)].$$

Since L is a monic differential operator of order n and

$$\mathscr{S}_{Q\alpha}(L)=\mathscr{S}_{Q\alpha}(u_0)+\mathscr{S}_{Q\alpha}(u_1)\partial+\cdots+\mathscr{S}_{Q\alpha}(u_{n-1})\partial^{n-1},$$

we can solve this equation by looking for operators

$$\hat{L}(\alpha)=\lambda_0+\lambda_1\partial+\cdots+\lambda_{n-1}\partial^{n-1}.$$

(The reasons for this choice and that made in the case of the Toda system are similar.) Then we observe that the Lax–Nijenhuis equation can also be written in the form

$$\mathscr{S}_{Q\alpha}(L)=[\alpha,L]_+L+[L,M(\alpha)] \tag{5.10}$$

if we set

$$M(\alpha)=\hat{L}(\alpha)+\tfrac{1}{2}[\alpha,L]_+\,.$$

To split Eq. (5.10) in two parts, one determining $M(\alpha)$ and the other determining $\mathscr{S}_{Q\alpha}(L)$, we observe that the constraints on L imply that

$$(\mathscr{S}_{Q\alpha}(L)L^{-1})_+=0.$$

Then we get

$$(\mathscr{S}_{Q\alpha}(L)\cdot L^{-1})_+=([\alpha,\,L]_++[L,\,M(\alpha)L^{-1}])_+=0,$$

$$(\mathscr{S}_{Q\alpha}(L)\cdot L^{-1})_-=([\alpha,L]_++[L,M(\alpha)L^{-1}])_-$$

or

$$[L,(M(\alpha)-\alpha L)L^{-1}]_+=0, \tag{5.11}$$

$$\mathscr{S}_{Q\alpha}(L)=[L,M(\alpha)L^{-1}]_-\cdot L. \tag{5.12}$$

Now $[L,(\alpha L)_-L^{-1}]_+=0$, since

$$(L(\alpha L)_- L^{-1} - (\alpha L)_-)_+ = (L(\alpha L)_- L^{-1})_+ = 0.$$

In fact, we know that for any strictly pseudodifferential operator X, such that $X_+ = 0$,

$$(LXL^{-1})_+ = 0.$$

The constraint equation (5.11) can therefore be written in the form

$$[L, (M(\alpha) - (\alpha L)_+) L^{-1}]_+ = 0,$$

and the simplest solution of (5.11) is thus

$$M(\alpha) = (\alpha L)_+ .$$

If we now insert this solution into Eq. (5.12), we get

$$\mathscr{S}_{Q\alpha}(L) = [L, (\alpha L)_+ L^{-1}]_- \cdot L,$$

or

$$\begin{aligned} Q_L(\alpha) = (L(\alpha L)_+ L^{-1})_- L &= L(\alpha L)_+ L^{-1} L - (L(\alpha L)_+ L^{-1})_+ L \\ &= L(\alpha L)_+ - (L\alpha L L^{-1} - L(\alpha L)_- L^{-1})_+ L \\ &= L(\alpha L)_+ - (L\alpha)_+ L. \end{aligned}$$

This is the second Adler–Gelfand–Dickey bracket.[21,16,10,37]

E. The *R*-matrix bracket

It is well known that the Poisson structure (5.9) on $\mathscr{S}_n$ is a particular case of the Poisson structure P defined by

$$P_L(\alpha) = R([L, \alpha]) - [L, R\alpha] \tag{5.13}$$

associated with any skewsymmetric R-matrix satisfying the modified classical Yang–Baxter equation,

$$[RX, RY] - R([RX, Y] + [X, RY]) = -[X, Y].$$

Indeed to obtain (5.9) from (5.13) it is enough to choose as an R-matrix on the algebra of formal pseudodifferential operators half the difference,

$$R = \tfrac{1}{2}(\pi_+ - \pi_-),$$

between the projections π_+ and π_- onto the positive and negative parts into which the algebra of formal pseudodifferential operators naturally splits. In fact

$$R([L, \alpha]) - [L, R\alpha] = \tfrac{1}{2}[L, \alpha]_+ - \tfrac{1}{2}[L, \alpha]_- + \tfrac{1}{2}[L, \alpha] = [L, \alpha]_+ .$$

Therefore, it is natural to try to generalize the previous example by solving the Lax–Nijenhuis equation corresponding to

$$\mathscr{S}_{P\alpha}(L) = R([L, \alpha]) - [L, R(\alpha)].$$

To this end we remark that

$$\mathscr{L}_{P\alpha}(L^2)=LR([L,\alpha])+R([L,\alpha])L-[L,LR(\alpha)+R(\alpha)L]$$

so that the Lax–Nijenhuis condition takes the form

$$\mathscr{L}_{Q\alpha}(L)=\tfrac{1}{2}(LR([L,\alpha])+R([L,\alpha])L)+[L,\hat{L}(\alpha)-\tfrac{1}{2}(LR(\alpha)+R(\alpha)L)].$$

In this case we have no obvious supplementary conditions on L to be used to determine $\hat{L}(\alpha)$. However, to do this we can use the skewsymmetry of Q (as in the Toda example). The idea is to split the linear operator

$$M_L(\alpha)=LR([L,\alpha])+R([L,\alpha])L$$

into its symmetric and skewsymmetric parts. Since

$${}^tM_L(\alpha)=[L,R(\alpha L+L\alpha)],$$

we can write

$$\mathscr{L}_{Q\alpha}(L)=\tfrac{1}{2}(M_L(\alpha)-{}^tM_L(\alpha))+[L,\hat{L}(\alpha)+\tfrac{1}{2}(R(\alpha L+L\alpha))-LR(\alpha)-R(\alpha)L].$$

Now we can choose

$$\hat{L}(\alpha)=\tfrac{1}{2}(LR(\alpha)+R(\alpha)L)-\tfrac{1}{2}R(\alpha L+L\alpha)$$

so as to annihilate the commutator and to get $\mathscr{L}_{Q\alpha}(L)=\tfrac{1}{2}(M_L(\alpha)-{}^tM_L(\alpha))$, a manifestly skewsymmetric mapping. The explicit result that we finally get is

$$\mathscr{L}_{Q\alpha}(L)=\tfrac{1}{2}(LR([L,\alpha])+R([L,\alpha])L-[L,R(\alpha L+L\alpha)]),$$

and thus

$$Q_L(\alpha)=R(L\alpha)L-LR(\alpha L).$$

This is the well known form[23] of the second (quadratic) Poisson bivector associated with the R-bracket (5.13).

VI. CONCLUSION

These examples may help to explain the role of the Lax–Nijenhuis equation and its limits. This equation does not define the second (''quadratic'') Poisson bracket, Q, associated with a Lax operator, but it provides a systematic way of deriving this bracket. The previous examples show that, in many cases, the form of L and the form of the first, given Poisson tensor suggest natural choices for the form of $\hat{L}(\alpha)$ which make Q uniquely defined. This is the value of the method. Its limits are that it does not provide a proof of the fact that we indeed obtain a second Poisson tensor compatible with the given one.

In Ref. 38, there appears a Lax formulation for the evolution of the recursion operator of the KdV hierarchy, whose geometric interpretation along the lines of the present exposition remains to be clarified.

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A geometrical method towards first integrals for dynamical systems

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We develop a method, based on Darboux's and Liouville's works, to find first integrals and/or invariant manifolds for a physically relevant class of dynamical systems, without making any assumption on these elements' forms. We apply it to three dynamical systems: Lotka–Volterra, Lorenz and Rikitake. © *1996 American Institute of Physics.* [S0022-2488(96)03511-6]

I. HISTORICAL OVERVIEW

In Refs. 1 and 2, Roger Liouville and A. Tresse developed a method for deciding whether two differential equations of the form

$$\frac{d^2y}{dx^2}+a_1(x,y)\left(\frac{dy}{dx}\right)^3+3\,a_2(x,y)\left(\frac{dy}{dx}\right)^2+3\,a_3(x,y)\frac{dy}{dx}+a_4(x,y)=0, \tag{1}$$

where the a_i are arbitrary functions of the real or complex variables x and y, are geometrically equivalent, i.e., can be transformed into each other by the most general dependent and independent variable change

$$x'=\varphi(x,y), \quad y'=\psi(x,y). \tag{2}$$

This method was based on the construction of a ''relative invariant'' function called ν_5 of the a_i and of their derivatives, such that in any transformation (2) it becomes $\nu_5'=J(x,y)^{-5}\nu_5$ where $J(x,y)$ is the Jacobian of the transformation. In the general case, two equations such that their ν_5 are non-zero and proportional to each other are indeed equivalent. If $\nu_5=0$ for both, however, one cannot conclude at first, and other invariants, involving higher derivatives of the a_i, must be calculated in order to decide. As an application, Liouville proposed the effective reduction of Equation (1) into its simplest canonical form, which in most cases leads to an explicit integration.

Here we will adopt another point of view. We have derived from these theories a method for finding out first integrals for a wide and physically important class of dynamical systems without having to make any ansatz on their functional form. In the rest of this section, we shall recall some mathematical results of Darboux,[3] Liouville and Tresse. Then we explain our method in Section II, and apply it in Section III to three well-known dynamical systems. Finally, Section IV discusses our results summarised in Table I.

A. Essentials of Liouville theory

Consider a differential equation like (1). Liouville[1] defined the following functions — which are seen as functions of (x,y), forgetting the supposed relation between those variables:

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TABLE I. Results obtained by our method.

DS	ν_5	Denominator	Parameters	Information obtained
Lotka (a,b,c)	(y,z):(17)	$y-abz$	$(0,2,c)$	DE: $(y;x)$
			$(1/(2\,b),b,1)$	DE: $(bx-z;y)$
			$(1,b,2/b)$	DE: $(x-cy;z)$
			$(1/4,2,-5)$	DE: $(16\,y^2-2\,xz-8\,yz+z^2;2\,x)$
			$(-1/5,1/2,4)$	DE: $(100\,y^2-25\,xy+40\,yz+4\,z^2;x)$
			$(1,2,-2)$	DE: $(y^2-xz-yz;2\,x+z)$
			$(-1/2,1/2,1)$	DE: $(-2\,xy+2\,yz+z^2;x+y)$
			$(1,1,1)$	none
			$(-1/2,0,1)$	none
			$(0,2/3,1)$	DE: $(3\,z-2\,x;y)$
	other		cyclic permutation of the above results	
Lorenz (b,σ,ϱ)	(x,y):(22)	$x-y$	$(-1-\sigma,\sigma,\varrho)$	none
			$(2/3,1/3,\varrho)$	none
			$(-16/5,-1/5,-7/5)$	none
	(x,z):(24)	$bz-x^2$	$(2\,\sigma,\sigma,\varrho)$	FI: $(x^2-2\,\sigma z)\,e^{2\,\sigma\,t}$
			$(-1-\sigma,\sigma,\varrho)$	none
	(z,y):(26)	$bz(\varrho-z)-y^2$	$(1,\sigma,0)$	FI: $(z^2+y^2)\,e^{2\,t}$
			$(-1-\sigma,\sigma,\varrho)$	none
Rikitake (α,β,μ)	(x,y):(28)	$\mu(y^2-x^2)$ $+2\,\beta xy$	$(\alpha,0,\mu)$	FI: $(y^2-x^2)\,e^{2\,\mu t}$
			$(\alpha,\beta,0)$	none
	other	...		nothing more

$$L_2=\frac{\partial}{\partial x}\left(\frac{\partial a_1}{\partial x}-3\,a_1a_3\right)+\frac{\partial}{\partial y}\left(\frac{\partial a_3}{\partial y}-2\,\frac{\partial a_2}{\partial x}+a_1a_4\right)$$
$$-3\,a_2\left(\frac{\partial a_3}{\partial y}-2\,\frac{\partial a_2}{\partial x}+a_1a_4\right)+a_1\left(\frac{\partial a_4}{\partial y}+3\,a_2a_4\right), \tag{3}$$

$$L_1=\frac{\partial}{\partial y}\left(\frac{\partial a_4}{\partial y}+3\,a_2a_4\right)-\frac{\partial}{\partial x}\left(2\,\frac{\partial a_3}{\partial y}-\frac{\partial a_2}{\partial x}+a_1a_4\right)$$
$$-3\,a_3\left(2\,\frac{\partial a_3}{\partial y}-\frac{\partial a_2}{\partial x}+a_1a_4\right)-a_4\left(\frac{\partial a_1}{\partial x}-3\,a_1a_3\right), \tag{4}$$

$$\nu_5=L_2\left(L_1\frac{\partial L_2}{\partial x}-L_2\frac{\partial L_1}{\partial x}\right)+L_1\left(L_2\frac{\partial L_1}{\partial y}-L_1\frac{\partial L_2}{\partial y}\right)-a_1L_1^3+3\,a_2L_1^2L_2-3\,a_3L_1L_2^2+a_4L_2^3. \tag{5}$$

The equation $\nu_5=0$ means that

$$L_1dx+L_2dy=0 \tag{6}$$

defines a particular solution of Equation (1). We shall call (6) a *subequation* of Equation (1), i.e., (1) is a differential consequence of (6). Notice that in the case $L_2\equiv 0$ the solution is *not* $L_1\equiv 0$ — which would mean an unexpected lowering of this equation's differential order — but $dx=0$, an absurdity as x is seen as the independent variable. Similarly if $L_1\equiv 0$, the solution is $dy=0$, a solution possibly present in Equation (1) but not very interesting.

Now suppose neither L_1 nor L_2 vanish identically and define $\alpha=-L_2/L_1$. Then

$$\nu_5=L_1^3\left(\alpha\frac{\partial\alpha}{\partial y}+\frac{\partial\alpha}{\partial x}+a_1\alpha^3+3\,a_2\alpha^2+3\,a_3\alpha+a_4\right) \tag{7}$$

and Equation (6) can be rewritten $dy/dx=\alpha(x,y)$. Conversely suppose there is a first-order subequation to Equation (1), namely $dy/dx=A(x,y)$. Then A is a solution to the first-order non-linear PDE

$$A\frac{\partial A}{\partial y}+\frac{\partial A}{\partial x}+a_1A^3+3\,a_2A^2+3\,a_3A+a_4=0 \tag{8}$$

we shall discuss later. Liouville theory is a finite effort tool for finding particular solutions to Equation (8).

B. Darboux polynomials and first integrals for polynomial dynamical systems

Consider an autonomous polynomial dynamical system

$$\dot{x}_i=V_i(x),\quad i=1,\ldots,n. \tag{9}$$

We say that a polynomial $f(x_1,\ldots,x_n)$ is a *Darboux polynomial*[3] of (9) if there exists a polynomial ''eigenvalue'' p such that

$$\frac{df}{dt}\equiv\sum_{i=1}^{n}V_i\frac{\partial f}{\partial x_i}=pf.$$

In other words, there is an algebraic variety, defined by $f(x_1,\ldots,x_n)=0$, which is invariant by the flow of V. In this respect, this notion is a neighbour of the notion of subequation we have seen.

Darboux polynomials are tools for finding out,[4,5] but also proving the non-existence (cf. Ref. 6 for an example) of first integrals to polynomial dynamical systems. We shall not enter into the details. Let us just notice that a polynomial first integral is simply a Darboux polynomial with eigenvalue 0, and that a Darboux polynomial f with constant eigenvalue α gives rise to the time-dependent first integral $f\,e^{-\alpha t}$. More rational and algebraic first integrals can be built with the ''basic blocks'' of Darboux polynomials,[4,5] and, conversely, a theorem of Bruns[7] says there cannot be an algebraic first integral of (9) unless there is a rational one, which in turn implies the existence of Darboux polynomials.

In brief, the problems of existence of first integrals and Darboux polynomials for a polynomial dynamical system are very tightly linked. Notice also that all these objects, like ordinary eigenvectors and -values of linear endomorphisms, naturally live in $\mathbf{C}$.

II. PRINCIPLE OF THE METHOD

We shall draw our interest to autonomous three-dimensional polynomial dynamical systems which are of *first degree* in one of their three variables, e.g., z. Their general form is thus

$$\dot{x}=V_x^0(x,y)+zV_x^1(x,y),\quad \dot{y}=V_y^0(x,y)+zV_y^1(x,y),$$

$$\dot{z}=V_z^0(x,y)+zV_z^1(x,y), \tag{10}$$

which we may abbreviate as $\dot{X}=V(X)$. Dynamical systems of this kind are frequently met in physics: well-known examples are the Lorenz model, or the various three-wave interaction prob-

lems (Rabinovich, etc.). Very often they are indeed of first degree in *all* their variables. We can use this feature for harvesting more information — an example is given in the paragraph about the Lorenz model.

We assume to have found out and studied all solutions with $x=$ cst. Assuming x nonconstant, we shall transform the system (10) into a non-autonomous second-order differential equation linking y and x which will turn out to be of type (1).

Now we settle in a region of space where $\dot{x} \neq 0$ and take x as the independent variable, parametrising the integral curves of (10). The relation

$$(V_x^0(x,y)+zV_x^1(x,y))\frac{dy}{dx}=V_y^0(x,y)+zV_y^1(x,y) \tag{11}$$

is satisfied along all integral curves. Hence, writing $p=dy/dx$,

$$z(V_x^1 p-V_y^1)=V_y^0-pV_x^0. \tag{12}$$

These equations define the mappings $\phi:(x,y,z)\mapsto(x,y,p)$ and $\phi^*:(x,y,p)\mapsto(x,y,z)$, which are homographic and hence:

(1) They are one-to-one wherever they are defined and their determinant $C(x,y)=V_x^0V_y^1-V_y^0V_x^1$ is non-zero; as it involves only the variables x and y the surface $\Sigma=\{C(x,y)=0\}$ can be seen either as a submanifold in the (x,y,z) space or in the (x,y,p) space.

(2) The surfaces $S_1=\{V_x^0(x,y)+zV_x^1(x,y)=0\}$ in the (x,y,z) space and $S_2=\{V_x^1(x,y)p-V_y^1(x,y)=0\}$ in the (x,y,p) space are singular. Any point on $S_1\backslash\Sigma$ is sent to $p=\infty$: this happens when $\dot{x}=0$, and the tangent to the integral curve is orthogonal to the x-axis, i.e., ''vertical'' in (x,y) representation $(dy/dx=\infty)$. Similarly any point on $S_2\backslash\Sigma$ is sent to $z=\infty$.

(3) On Σ, ϕ and ϕ^* are ''constant along fibres,'' i.e., two points of Σ having different z (or p) are sent to the same image, having the same (x,y) as the original point, hence lying on Σ. Thus it is always possible to get it as the image of a point on $\Sigma\backslash S_1$ and calculating it that way shows that $\phi(\Sigma)=\Sigma\cap S_2$; and similarly $\phi^*(\Sigma)=\Sigma\cap S_1$.

Since we are concerned with a differential problem, we have to study what the vector field $V(X)$ becomes under the action of the tangent map $T_X\phi$. And, indeed, points X on Σ differing only in the z coordinate have the same image by ϕ, but different $V(X)$ such that the corresponding $T_X\phi(V(X))$ also generally differ. As all these vectors are attached to the common image of the points X, this can cause a loss of information, leading, as we shall see, to important practical difficulties.

Similarly, we find that

$$(V_x^0(x,y)+zV_x^1(x,y))\frac{dz}{dx}=V_z^0(x,y)+zV_z^1(x,y).$$

We calculate dz/dx by differentiating (12) with respect to x, putting the result into the previous formula, and then replacing z itself with its value in function of p given by Equation (12). This leads to a differential equation in p which, in Cauchy form, reads

$$\frac{dp}{dx}=\frac{N(x,y,p)}{C(x,y)^2}, \tag{13}$$

where N is polynomial in (x,y,p) and of degree three in p. Interpreting p as dy/dx, we see Equation (13) as a differential equation of Liouville type like (1). There are two essential facts in

these computations. One is that the denominator of (13) is exactly the square of the determinant $C(x,y)$ of ϕ, so Equation (13) will not set any further problem as long as its construction is valid. The other one is that Equations (10) are of degree one in z: it ensures not only the good behaviour of the $z \leftrightarrow p$ correspondence but also the Liouville form of the differential equation (13).

We intend to apply Liouville theory to Equation (13) in order to obtain subequations for it. Now, we must take care of their possible relationships with the forbidden surfaces. If a subequation defines a curve in the (x,y,p) space which is not contained in Σ or S_2, there is no problem: it will be pulled back into the (x,y,z) space by the ϕ^* map, which coincides then with the reciprocal of ϕ.

But in the computation of Equation (13), we have used the $z=\phi^*(x,y,p)$ map, and then suppressed the denominator $V_x^1 p - V_y^1$. Thus, the singular manifold at S_2 has disappeared in (13). But consider a curve plotted on S_2 (i.e., $V_x^1 p - V_y^1 \equiv 0$) which is, moreover, a *jet* (i.e., $p \equiv dy/dx$). Then, identically

$$\frac{dy}{dx} = A(x,y) = \frac{V_y^1(x,y)}{V_x^1(x,y)}.$$

We can check that this A is always a solution to Equation (8), whatever the vector field V may be. Hence *any jet plotted on S_2 is a subequation of Equation (13).* However, this jet cannot yield an invariant manifold in the (x,y,z) space unless it is made of images by ϕ of points in this space. Now, it is easy to show that the only points on S_2 that can be written as $\phi(x,y,z)$ are those on $\Sigma \cap S_2$; therefore, as we have seen, they are images of points also lying on Σ.

Yet we know that the pullback of the vector field V is not necessarily well-behaved on Σ. Thus, the system (10) and the differential equation (13) can behave quite differently on Σ.

If we find as Equation (6) the equation of a jet on S_2, we have to check independently whether Σ is an invariant manifold for V or not. In dynamical systems containing parameters, this can be rephrased as: *find at what condition on the system's parameters the equation denominator $C(x,y)$ is a Darboux polynomial for the system (10).*

III. RESULTS FOR SEVERAL DYNAMICAL SYSTEMS

We have applied the method exposed in Section II to three different dynamical systems of type (10) depending on real parameters: Lotka–Volterra, Lorenz, Rikitake. We shall discuss the results obtained in the rest of this section.

A. The (a,b,c) Lotka–Volterra system

This remarkably symmetric system

$$\dot{x} = x(cy+z), \quad \dot{y} = y(az+x), \quad \dot{z} = z(bx+y), \tag{14}$$

appeared first as a model for three-species competition, yet has been found later in plasma physics. A considerable amount of research has been done on it, using many techniques.[6,8–10] Here we shall follow the process exposed in Section II.

Since Equations (14) are invariant by simultaneous circular permutations of (x,y,z) and (a,b,c), it is equivalent to perform the method with any couple of variables. Once this is done, more results can be obtained by the above symmetry. There is also a symmetry in taking $x=x'/b, y=z'/c, z=y'/a$ and $a=1/c', b=1/b', c=1/a'$, which will appear in the distribution of the $\nu_5=0$ cases.

So, we take z as the independent variable and eliminate x, and find

$$L_1 = \frac{(b-1)(1+abc)Q_{abc}^1(y,z)}{z(y-abz)^4} \tag{15}$$

and

$$L_2=\frac{(b-1)(1+abc)Q^2_{abc}(y,z)}{z(y-abz)^4} \tag{16}$$

and

$$\nu_5=\frac{(b-1)^3(1+abc)^3P_{abc}(y,z)}{z^2y^2(y-abz)^{10}}, \tag{17}$$

where $P_{abc},Q^1_{abc},Q^2_{abc}$ are polynomials whose coefficients depend on (a,b,c) and which we do not write down for the sake of brevity. The cases $1+abc=0$ and $b=1$ are known: the first one is the full integrability of the system, with, in particular, the first integral $abx+y-az$; in the second one we have the Darboux polynomial $y-az$ whose eigenvalue is x. We remark this Darboux polynomial is exactly the denominator. Notice also that in those two cases, L_1 and L_2 vanish together with ν_5 so that Equation (6) is an identity and cannot be used for finding out Darboux polynomials.

Now the cases where all coefficients of P_{abc} are zero are listed below in Table I. We notice the presence of the symmetry $a=1/c',b=1/b',c=1/a'$ in this list; one case $(a=1,b=1,c=1)$ is self-symmetric. We shall handle in some detail one of these ''exotic'' cases, viz. $(a=1/4,b=2,c=-5)$. The subequation (6) reads

$$y(-3z^2+16zy-32y^2)+4z\frac{dy}{dz}(z^2-7zy+16y^2)=0. \tag{18}$$

Reverting to the original variables (x,y,z) changes this equation in

$$y(z-2y)(16y^2-2xz-8yz+z^2)=0. \tag{19}$$

The expression $z-2y$ is proportional to the equation denominator; its presence here is an artefact due, as we have seen, to a former suppression of denominator. It should not be taken in account since it corresponds to $b=1$. On the other hand, the other two factors are Darboux polynomials, since their derivatives with respect to the system (14) are $\dot{y}=y(z/4+x)$ and

$$\frac{d}{dt}(16y^2-2xz-8yz+z^2)=2x(16y^2-2xz-8yz+z^2).$$

This illustrates the validity of the method in the general case. The results for all cases are summarised in Table I. We get no information for the self-symmetric case since it is a specialisation of $b=1$, so our method cannot be applied.

B. The Lorenz model

Another well-known and intensively studied[11–15] dynamical system, the Lorenz model

$$\dot{x}=\sigma(y-x),\quad \dot{y}=\varrho x-y-xz,\quad \dot{z}=xy-bz, \tag{20}$$

originally thought of as a simple model for atmospheric turbulence, was the first example of a low-dimensional chaotic deterministic dynamical system.[11] All known first integrals have been obtained or reobtained by Kuś,[13] using the non-decisive procedure of Carleman embedding. Here we shall recover some of them *methodically* by the means of Liouville theory.

Since there is no symmetry among variables here, we can proceed three times to the calculation of the $L_{1,2}$ and ν_5 functions, eliminating each time one of the three variables. Indeed, the

Liouville equation like (13) contains no more information than the dynamical system like (10) does, but it has more singularities; yet, as we have seen, these singularities often contain useful matter about the dynamical system's invariant manifold structure.

Eliminating z and choosing x as the independent variable yields $C(x,y)=\sigma x(y-x)$. Neither $x=0$ nor $y-x=0$ can be interesting invariant manifolds, since both imply $\dot{x}=0$, so $x=$ cst and $y=$ cst. This, in turn, also implies that z is constant, and the manifold reduces to a fixed point.

The functions L_2 and ν_5 are (cf. Ref. 16)

$$L_2=\frac{1+b+\sigma}{\sigma(y-x)^3} \tag{21}$$

and

$$\nu_5=\frac{(1+b+\sigma)P_{b\sigma\varrho}(x,y)}{\sigma^5x^2(y-x)^{10}}. \tag{22}$$

In the obvious case $1+b+\sigma=0$, we also have $L_2=0$. Thus, as explained in Section I, our choice of variables was a bad one. Looking for other cases, we only get three points in the (b,σ,ϱ) space, viz. $(b=0,\sigma=-1)$, $(b=2/3,\sigma=1/3)$ and $(b=-16/5,\sigma=-1/5,\varrho=-7/5)$. They are specialisations either of known cases[13] or of the $1+b+\sigma=0$ case. In those cases, we get subequations that do not give rise to Darboux polynomials, i.e., equations that represent jets plotted on the surface S_2.

Now, if we eliminate y and choose x as the independent variable, we get as equation denominator $C(x,z)=bz-x^2$. Its derivative with respect to the system (20) is

$$\begin{aligned}\frac{d}{dt}(bz-x^2)&=(b-2\,\sigma)xy-(b^2z-2\,\sigma x^2)\\&=-2\,\sigma(bz-x^2)+(b-2\,\sigma)(xy-bz).\end{aligned} \tag{23}$$

The remainder is of degree one in x. Thus C is a Darboux polynomial iff $b=2\,\sigma$; then the eigenvalue is $-2\,\sigma$, so $I=(x^2-2\,\sigma z)\,\mathrm{e}^{2\,\sigma t}$ is a first integral.[12]

We have calculated ν_5 and found

$$\nu_5=\frac{(b-2\,\sigma)(1+b+\sigma)P_{b\sigma\varrho}}{\sigma^5(bz-x^2)^{10}}, \tag{24}$$

$P_{b\sigma\varrho}$ being such that its coefficients never simultaneously vanish. In the case $b=2\,\sigma$, Equation (6) yields $x-\sigma dz/dx=0$. This is the equation of a jet on S_2, and since we are in the good case, we find Σ as the invariant surface.

When $1+b+\sigma=0$, Equation (6) still yields $x-\sigma dz/dx=0$. But in this case, Σ is not invariant and we do not have a Darboux polynomial.

Finally, we have taken z as the independent variable and eliminated x. We find $C(y,z)=b\varrho z-bz^2-y^2$ and

$$\begin{aligned}\frac{dC}{dt}&=xy((b-2)\varrho+2\,(1-b)z)+2\,y^2+2\,b^2z^2-b^2\varrho z\\&=-2\,(b\varrho z-bz^2-y^2)+R(x,y,z),\end{aligned} \tag{25}$$

the remainder R being of first degree in y; hence C is a Darboux polynomial iff $b=1$ and $\varrho=0$. Then, $dC/dt=-2\,C$ and we get that way the first integral $I=(z^2+y^2)\,\mathrm{e}^{2t}$.[12]

As for ν_5, it is equal to

$$\nu_5=\frac{(1+b+\sigma)yP_{b\sigma\varrho}(y,z)}{(b\varrho z-bz^2-y^2)^{10}}, \tag{26}$$

where $P_{b\sigma\varrho}(y,z)\equiv 0$ iff $b=1$ and $\varrho=0$. Let us handle first the latter case. In that case, $L_1=-\sigma zy/(z^2+y^2)^2$ and $L_2=-\sigma y^2/(z^2+y^2)^2$, so Equation (6) simplifies as $zdz+ydy=0$. This is the equation of a jet on S_2, and we get Σ as invariant manifold.

Now, in the case $1+b+\sigma=0$, there is another simplification in Equation (6), namely $yL_1\equiv(z-\varrho)L_2$ and hence $(z-\varrho)dz+ydy=0$. But this is the jet on S_2, so we get no information in this case.

C. The Rikitake dynamo

This dynamical system[8]

$$\dot{x}=-\mu x+y(z+\beta),\quad \dot{y}=-\mu y+x(z-\beta),\quad \dot{z}=\alpha-xy, \tag{27}$$

models the variation of the earth's magnetic field with time.

Let us take x as the privileged variable and eliminate z. The denominator in Equation (13) is $C(x,y)=\mu(y^2-x^2)+2\,\beta xy$, and

$$\nu_5=\frac{\beta^2\mu^2P_{\alpha\beta\mu}(x,y)}{(\mu(y^2-x^2)+2\,\beta xy)^{10}}, \tag{28}$$

where the coefficients of $P_{\alpha\beta\mu}$ cannot vanish together unless $\beta=0$ or $\mu=0$.

The derivative of $C(x,y)$ with respect to the system (27) is

$$\frac{dC}{dt}=(y^2-x^2)(2\,\beta^2-2\,\mu^2)-2\,\beta xy+2\,\beta z(x+y). \tag{29}$$

Assume C is a Darboux polynomial of eigenvalue $P(x,y,z)=A(x,y)+zB(x,y)$. Then the identification of the z terms in Equation (29) gives $BC=2\,\beta(x+y)$. Since C is of second degree, this is impossible unless $\beta=0$.

When $\beta=0$, Equation (29) reads $dC/dt=-2\,\mu C$, so C is a Darboux polynomial of this system, which gives the first integral $(y^2-x^2)\,\mathrm{e}^{2\mu t}$. On the other hand,

$$L_1=\frac{4\,x^2y}{\mu^2(x^2-y^2)^2},\quad L_2=\frac{-4\,xy^2}{\mu^2(x^2-y^2)^2},$$

hence Equation (6) becomes $-xdx+ydy=0$. This is a jet on S_2, but we are in the ''good'' case, and we recover the Darboux polynomial y^2-x^2.

If now $\mu=0$, then

$$L_1=\frac{-\alpha(3\,x^4+2\,x^2y^2+3\,y^4)}{4\,\beta^2x^3y^4},\quad L_2=\frac{\alpha(3\,x^4+2\,x^2y^2+3\,y^4)}{4\,\beta^2x^4y^3},$$

so the subequation is once more $-xdx+ydy=0$, the jet on S_2. Hence we do not obtain any Darboux polynomial unless $\beta=0$.

We have also performed the computations with the other two couples of variables. They have not given more information than the previous ones.

IV. CONCLUSION

We have obtained, *by a methodic procedure*, numerous cases of Darboux polynomials for the Lotka–Volterra system. This ''Darboux polynomial searcher'' can be seen as an input to algorithms which need Darboux polynomials, such as the Prelle–Singer procedure. Up to now, that procedure began with a systematic search, which obliged to set an *a priori* limit on the polynomial's degree in all its variables.[4] Some new results[5] allow the refinement of the search by restricting the choice of the possible highest-degree homogeneous components of the tentative Darboux polynomials, while speeding it up when the system's coefficients are rational numbers. Yet they are valid for dynamical systems of dimension 2, and until now have no counterpart in dimension 3.

Our method has also reobtained some known first integrals for the Lorenz and Rikitake systems, though all cases have not been found, and despite the ''divergence enigma'' we now explain.

In both Lorenz and Rikitake systems, the divergence is a constant, respectively $-1-b-\sigma$ and $-2\,\mu$. In both cases, its vanishing triggers the vanishing of ν_5, but also the reduction of Equation (6) to a singularity from which no information can be extracted. However, the Rikitake dynamo possesses when $\mu=0$ a time-dependent first integral $I=x^2-y^2+4\,\beta z-4\,\alpha\beta t$; this kind of first integral cannot be detected by our method, since it does not arise from a Darboux polynomial, but from a polynomial $f(x,y,z)$ such that $df/dt=$ cst. Such a first integral may exist only for dynamical systems having a constant term, so there is no chance to find any for the Lorenz model. But there may be a first integral of some special kind — indeed, numerical experiments exhibit a regular behaviour when $1+b+\sigma=0$.

Table I summarises the results obtained by our method. Abbreviations are: DS for ''dynamical system,'' FI for ''first integral,'' and DE for ''Darboux element,'' i.e., a couple of polynomials (f,p) such that $df/dt=pf$.

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The Kadomtsev–Petviashvili equation as a source of integrable model equations

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A new integrable and nonlinear partial differential equation (PDE) in 2+1 dimensions is obtained, by an asymptotically exact reduction method based on Fourier expansion and spatiotemporal rescaling, from the Kadomtsev–Petviashvili equation. The integrability property is explicitly demonstrated, by exhibiting the corresponding Lax pair, that is obtained by applying the reduction technique to the Lax pair of the Kadomtsev–Petviashvili equation. This model equation is likely to be of applicative relevance, because it may be considered a consistent approximation of a large class of nonlinear evolution PDEs. © *1996 American Institute of Physics.* [S0022-2488(96)03109-X]

I. INTRODUCTION

In the last years, various authors have studied the wave modulation induced by weak nonlinear effects, for a large class of nonlinear evolution equations in 1+1 and 2+1 dimensions, with a dispersive linear part. The most interesting result is that only a very limited number of model equations are necessary. These model equations are usually of applicative relevance (in plasma physics, nonlinear optics, hydrodynamics), because they are obtained by means of a reduction method from a large class of nonlinear evolution equations, under opportune approximations.[1–6]

It is clear from this method that the property of integrability is inherited through this limit technique and then our model equations are integrable, being sufficient that only an integrable equation is present in the large class from which they have been obtained. This method can be also applied to the weakly nonlinear ordinary differential equations.[7]

The first step of the reduction method (in 2+1 dimensions) is to use a moving frame of reference via the transformation

$$\xi=\epsilon^{p_1}(x-V_1t),\quad \eta=\epsilon^{p_2}(y-V_2t),\quad \tau=\epsilon^{q}t, \tag{1.1}$$

where $p_1,p_2>0$, $q>0$, and $V_1=V_1(K_1,K_2)$, $V_2=V_2(K_1,K_2)$ are the components of the group velocity $\mathbf{V}(\mathbf{K})\equiv(V_1(K_1,K_2),V_2(K_1,K_2))$ of the linearized equation, i.e. of the equation obtained after neglecting all the nonlinear terms and ϵ is the expansion parameter, supposed to be sufficiently small. The linear evolution is most appropriately described in terms of Fourier modes, which have a constant amplitude and a well-defined group velocity (the speed with which a wave packet peaked at that Fourier mode would move in ordinary space). To identify the nonlinear effects, we consider a specific Fourier mode and the frame of reference (1.1), which moves with the corresponding group velocity. We study the modulation, in terms of the variables defined above, of the amplitude of the Fourier mode, due to nonlinear effects. The modulation (that would remain constant in the absence of nonlinear effects) is best described in terms of the rescaled variables ξ,η,τ, that account for the need to look on larger space and time scales, to obtain a not negligible contribution from the nonlinear term.

In a precedent paper, this method has been applied to the Boussinesq equation and a new integrable nonlinear evolution PDE in 1+1 dimensions has been derived.[8] This line of research is now applied in 2+1 dimensions and the variable change (1.1) can be used, in case with a different

rescaling in the spatial variables ($p_1 \neq p_2$): if $p_1 > p_2$, the spatial scale for X is greater than the scale for Y, and *vice versa* if $p_1 < p_2$. In particular, we consider the Kadomtsev–Petviashvili (KP) equation[9] (integrable by means of the spectral transform[10]):

$$U_{xt}(x,y,t) + U_{xxxx}(x,y;t) + sU_{yy}(x,y,t) - 3(U^2(x,y,t))_{xx} = 0, \tag{1.2}$$

where $U = U(x,y,t)$ is real, $s = \pm 1$, and the subscripts denote differentiation. In the second section, we demonstrate that the modulation is governed by a model equation of nonlinear Schrodinger type, if $p_1 = p_2$:

$$i\Psi_\tau(\xi,\eta,\tau) + L_1\Psi(\xi,\eta,\tau) + \Psi(\xi,\eta,\tau)\Phi(\xi,\eta,\tau) = 0, \tag{1.3a}$$

$$L_2\Phi(\xi,\eta,\tau) = 2L_1(|\Psi(\xi,\eta,\tau)|^2), \tag{1.3b}$$

with $\Psi = \Psi(\xi,\eta,\tau)$ complex, $\Phi = \Phi(\xi,\eta,\tau)$ real, and the linear differential operators L_1 and L_2 given by

$$L_1 = \frac{1}{4}(1 - s\lambda^2)\frac{\partial^2}{\partial\xi^2} + s\lambda\frac{\partial}{\partial\xi}\frac{\partial}{\partial\eta} - s\frac{\partial^2}{\partial\eta^2}, \tag{1.3c}$$

$$L_2 = -\frac{1}{4}(1 + s\lambda^2)\frac{\partial^2}{\partial\xi^2} + s\lambda\frac{\partial}{\partial\xi}\frac{\partial}{\partial\eta} - s\frac{\partial^2}{\partial\eta^2}, \tag{1.3d}$$

with $\lambda = K_2/\sqrt{3}K_1^2$. The equation (1.3) belongs to a class first studied by Shulman.[11] If $p_1 \neq p_2$, a new model equation can be derived,

$$i\Psi_\tau(\xi,\eta,\tau) + \Psi_{\xi\xi}(\xi,\eta,\tau) + \Psi(\xi,\eta,\tau)\Phi(\xi,\eta,\tau) = 0, \tag{1.4a}$$

$$\Phi_\tau(\xi,\eta,\tau) + \Phi_\eta(\xi,\eta,\tau) + (|\Psi(\xi,\eta,\tau)|^2)_\xi = 0, \tag{1.4b}$$

with $\Psi = \Psi(\xi,\eta,\tau)$ complex and $\Phi = \Phi(\xi,\eta,\tau)$ real. Taking into account the above-mentioned reasons, it is expected that the equation (1.4) is of applicative relevance. If we take $\xi = \eta$, we recover the integrable equation in $1+1$ dimensions obtained in a precedent paper.[8]

In the third section, the Lax pair relative to Eqs. (1.4) is deduced from the Lax pair of the KP equation. Note that if we eliminate $\Phi_\eta(\xi,\eta,\tau)$ in the last equation (1.4b) by means of a trivial change of variables, at the same time a term $\Psi_\eta(\xi,\eta,\tau)$ appears in the first equation (1.4a).

Finally, in the last section the most important results are recapitulated and some possible extensions and generalizations indicated.

II. MODEL NONLINEAR PDEs OBTAINED FROM THE KADOMTSEV–PETVIASHVILI EQUATION

The linear dispersive part of the Kadomtsev–Petviashvili equation (1.2) is simply described in terms of Fourier modes, with a group velocity $\mathbf{V}(\mathbf{K}) = (V_1(K_1,K_2), V_2(K_1,K_2))$,

$$V_1(K_1,K_2) = -3K_1^2 - s\frac{K_2^2}{K_1^2}, V_2(K_1,K_2) = \frac{2sK_2}{K_1}. \tag{2.1}$$

We introduce a formal asymptotic Fourier expansion,

$$U(x,y,t) = \sum_{n=-\infty}^{n=+\infty} \epsilon^{\gamma_n}\psi_n(\xi,\eta,\tau;\epsilon)\exp\{in(K_1x + K_2y - \omega t)\}, \tag{2.2}$$

with $\gamma_n=|n|$, $\gamma_0=1+r$ a real number to be determined later on, and $\psi_{-n}(\xi,\eta,\tau;\epsilon)=\psi_n^*(\xi,\eta,\tau;\epsilon)$, because $U(x,y,t)$ is real. It is assumed that the limit of $\psi_n(\xi,\eta,\tau,\epsilon)$'s, for $\epsilon\to 0$, exists and is finite.

The final goal is to obtain the evolution equation for the modulation amplitude $\psi_1(\xi,\eta,\tau,\epsilon\to 0)=\Psi(\xi,\eta,\tau)$ and to understand how it is modified by choosing different wave numbers. In particular, an interesting result shall be derived, if the special condition $3K_1^4-K_2^2=0$ is verified.

The standard procedure is to consider the different equations obtained from the coefficients of the Fourier modes. To simplify the treatment, it is more convenient to separate the contributions from the linear and nonlinear parts: $\epsilon^{\gamma_n}[D_n\psi_n]=\epsilon^2 F_n$, where D_n is a linear differential operator acting on $\psi_n(\xi,\eta,\tau)$ and F_n is the contribution of the nonlinear part. The operator D_n is

$$D_n=|(-in\omega+\epsilon^q\partial_\tau-V_1(K_1,K_2)\epsilon^{p_1}\partial_\xi-V_2(K_1,K_2)\epsilon^{p_2}\partial_\eta)\times(\epsilon^{p_1}\partial_\xi+inK_1)+(inK_1+\epsilon^{p_1}\partial_\xi)^4+s(inK_2+\epsilon^{p_2}\partial_\eta)^2. \tag{2.3}$$

It is easily seen that the first F_n has the following explicit form:

$$F_0=6(|\Psi(\xi,\eta,\tau|^2)_{\xi\xi}\epsilon^{2p_1}+o(\epsilon^{2p_1+2},\epsilon^{2p_1+2r}), \tag{2.4a}$$

$$F_2=-12K_1^2\Psi^2(\xi,\eta,\tau)+o(\epsilon^{p_1}), \tag{2.4b}$$

$$F_1=-6K_1^2\Phi(\xi,\eta,\tau)\Psi(\xi,\eta,\tau)\epsilon^r-6K_1^2\psi_2(\xi,\eta,\tau)\Psi^*(\xi,\eta,\tau)\epsilon+O(\epsilon^{p_1+r},\epsilon^{p_1+1}), \tag{2.4c}$$

where $\Phi(\xi,\eta,\tau)=\psi_0(\xi,\eta,\tau)$. After taking $q=2$, $p_1=p_2=1$, $r=1$ for the proper balance of terms, we obtain for $n=0$,

$$V_1(K_1,K_2)\Phi_{\xi\xi}(\xi,\eta,\tau)+V_2(K_1,K_2)\Phi_{\xi\eta}(\xi,\eta,\tau)-s\Phi_{\eta\eta}(\xi,\eta,\tau)+6(|\Psi(\xi,\eta,\tau)|^2)_{\xi\xi}=0, \tag{2.5a}$$

and for $n=1$,

$$iK_1\Psi_\tau(\xi,\eta,\tau)-(6K_1+V_1(K_1,K_2))\Psi_{\xi\xi}(\xi,\eta,\tau)-V_2(K_1,K_2)\Psi_{\xi\eta}(\xi,\eta,\tau)+s\Psi_{\eta\eta}(\xi,\eta,\tau)+6(K_1^2\Phi(\xi,\eta,\tau)\Psi(\xi,\eta,\tau)-|\Psi(\xi,\eta,\tau)|^2\Psi(\xi,\eta,\tau))=0. \tag{2.5b}$$

After a trivial rescaling we arrive at the model equation (1.3). Note that for $K_2=\lambda=0$, we reproduce the Davey–Stewartson equation,[12] whose integrability is well known.[13] However, even if $\lambda\neq 0$, by means of a trivial transformation in the spatial variables, the λ can be eliminated, reducing thereby (1.3) to the Davey–Stewartson equation.

If $p_2>p_1$, a different result is obtained for $n=0$,

$$\Phi(\xi,\eta,\tau)=\frac{6K_1^2}{3K_1^4-K_2^2}\,|\Psi(\xi,\eta,\tau)|^2, \tag{2.6a}$$

with $\gamma_0=1+r=2$, and for $n=1$,

$$i\Psi_\tau(\xi,\eta,\tau)+A(K_1,K_2)\Psi_{\xi\xi}(\xi,\eta,\tau)+6K_1(\Phi(\xi,\eta,\tau)\times\Psi(\xi,\eta,\tau)+\psi_2(\xi,\eta,\tau)\Psi^*(\xi,\eta,\tau))=0, \tag{2.6b}$$

with $2p_1=q=2$. The standard unidimensional nonlinear Schrödinger equation is obtained,

$$i\Psi_\tau(\xi,\eta,\tau)+A(K_1,K_2)\Psi_{\xi\xi}(\xi,\eta,\tau)+B(K_1,K_2)|\Psi(\xi,\eta,\tau)|^2\Psi(\xi,\eta,\tau)=0, \tag{2.7a}$$

with

$$A(K_1,K_2)=-\frac{(3K_1^4+K_2^2)}{K_1^3}, \quad B(K_1,K_2)=\frac{6(3K_1^4+K_2^2)}{(3K_1^5-K_2^2K_1)}. \tag{2.7b}$$

If the relation $3K_1^4=K_2^2$ is verified, then $B(K_1,K_2)$ diverges and another derivation is necessary. For $n=0$ a new equation arises:

$$\Phi_\tau(\xi,\eta,\tau)+2K_1\sqrt{3}\Phi_\eta(\xi,\eta,\tau)-6(|\Psi(\xi,\eta,\tau)|^2)_\xi=0, \tag{2.8a}$$

with $p_2=q$, $r=1+p_1-p_2$.

Taking $n=1$, a new model nonlinear PDE is obtained:

$$i\Psi_\tau(\xi,\eta,\tau)-6K_1\Psi_{\xi\xi}(\xi,\eta,\tau)+6K_1\Psi(\xi,\eta,\tau)\Phi(\xi,\eta,\tau)=0, \tag{2.8b}$$

with $r+1=2p_1$, i.e., $p_1=\frac{2}{3}$, $p_2=\frac{4}{3}$, $r=\frac{1}{3}$, $q=\frac{4}{3}$.

After a trivial rescaling, we arrive at the nonlinear model equation (1.4). It is expected that it is integrable, taking into account that it has been obtained from an equation integrable by the spectral transform.

III. THE LAX PAIR FOR THE MODEL NONLINEAR PDE

The reduction method can be applied to the Lax pair of the Kadomtsev–Petviashvili equation, in order to demonstrate the integrability of (1.3) and (1.4) by the spectral transform. The Lax operators are

$$L=\frac{i}{\sqrt{3}}\frac{\partial}{\partial y}+\frac{\partial^2}{\partial x^2}-U(x,y,t), \quad L\varphi(x,y,t)=0, \tag{3.1}$$

$$A=4\frac{\partial^3}{\partial y^3}-6U(x,y,t)\frac{\partial}{\partial x}-3U_x(x,y,t)+i\sqrt{3}W(x,y,t), \tag{3.2}$$

with $W_x(x,y,t)=U_y(x,y,t)$ and

$$\varphi_t(x,y,t)+A\varphi(x,y,t)=0. \tag{3.3}$$

We introduce an asymptotic Fourier expansion,

$$\varphi(x,y,t)=\sum_{n=-\infty}^{n=+\infty}\epsilon^{\tilde{\gamma}_n}\varphi_n(\xi,\eta,\tau;\epsilon)\exp\left[i\frac{n}{2}z+i(\lambda_1x+\lambda_2y+\lambda_3t)\right], \tag{3.4}$$

where n is odd, $z=K_1x+K_2y-\omega t$, $\tilde{\gamma}_{n+2}=1+\tilde{\gamma}_n$ for $n>0$, $\tilde{\gamma}_{n-2}=\tilde{\gamma}_n+1$ for $n<0$, $\varphi_n(\xi,\eta,\tau,\epsilon)$'s are functions that parametrically depend on ϵ and remain finite if $\epsilon\to0$, and $\lambda_1,\lambda_2,\lambda_3$ are real constants to be determined later on. Inserting now the expression for $\sigma(x,y,t)$ in (3.1), the coefficients of the Fourier modes generate a series of relations; each relation must be valid for a given order of approximation in ϵ. In particular, for the fundamental harmonics $\varphi_\pm(x,y,t)=\varphi_{\pm1}(x,y,t)$, considering terms $O(\epsilon^0)$ in (3.1) and (3.3), the constants $\lambda_1,\lambda_2,\lambda_3$ can be fixed:

$$\lambda_1 = -\frac{K_1}{2}, \quad \lambda_2 = -\frac{\sqrt{3}}{2} K_1^2, \quad \lambda_3 = -2K_1^3. \tag{3.5}$$

The new spectral problem is obtained by means of the successive order ϵ for the equation (3.1), after choosing $\tilde{\gamma}_{-1} = \tilde{\gamma}_1 + \frac{1}{3}$ for the proper balance of terms,

$$i\varphi_{+,\eta}(\xi,\eta,\tau) - \varphi_{+,\xi\xi}(\xi,\eta,\tau) - \Phi(\xi,\eta,\tau)\varphi_+(\xi,\eta,\tau) + \Psi(\xi,\eta,\tau)\varphi_-(\xi,\eta,\tau) = 0, \tag{3.6a}$$

$$i\varphi_{-,\xi}(\xi,\eta,\tau) - \tfrac{1}{2}\Psi^*(\xi,\eta,\tau)\varphi_+(\xi,\eta,\tau) = 0. \tag{3.6b}$$

If the other equation (3.3) is considered, the spectral problem can be again obtained. The temporal evolution can be revealed, taking into account the next order of approximation of (3.3), but in doing so new quantities, the corrections $\tilde{\varphi}_\pm(\xi,\eta,\tau)$ of order ϵ to the fundamental harmonics $\varphi_\pm(\xi,\eta,\tau)$, appear. These unknown quantities can be eliminated in (3.3) taking advantage of the relation obtained from (3.1), considering terms of order ϵ^2. This elimination is possible only because Eqs. (3.1) and (3.3) are identical at the first order. The Lax pair of (1.4) is then

$$L = iD_1 \frac{\partial}{\partial\eta} + iD_2 \frac{\partial}{\partial\xi} + D_3 \frac{\partial^2}{\partial\xi^2} - \tilde{\Psi}(\xi,\eta,\tau), \quad L\hat{\varphi}(\xi,\eta,\tau) = 0, \tag{3.7a}$$

with

$$D_1 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad D_2 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad D_3 = \begin{pmatrix} -1 & 0 \\ 0 & 0 \end{pmatrix}, \tag{3.7b}$$

$$\tilde{\Psi}(\xi,\eta,\tau) = \begin{pmatrix} \Phi(\xi,\eta,\tau) & -\Psi(\xi,\eta,\tau) \\ \frac{1}{2}\Psi^*(\xi,\eta,\tau) & 0 \end{pmatrix}, \quad |\hat{\varphi}(\xi,\eta,\tau) = \begin{pmatrix} \varphi_+ \\ \varphi_- \end{pmatrix}, \tag{3.7c}$$

and

$$A = -iD_1\Phi(\xi,\eta,\tau) - iD_1 \frac{\partial^2}{\partial\xi^2} - \hat{\Psi}(\xi,\eta,\tau) \frac{\partial}{\partial\xi} + \hat{\Psi}_\xi(\xi,\eta,\tau), \tag{3.7d}$$

with

$$\hat{\varphi}_\tau(\xi,\eta,\tau) + A\hat{\varphi}(\xi,\eta,\tau) = 0, \tag{3.7e}$$

$$\hat{\Psi}(\xi,\eta,\tau) = \begin{pmatrix} 0 & 0 \\ \frac{1}{2}\Psi^*(\xi,\eta,\tau) & 0 \end{pmatrix}. \tag{3.7f}$$

A similar calculation permits us to obtain the well-known Lax pair of the Davey–Stewartson equation (1.3).

IV. CONCLUSION

The results obtained in this paper identify a research line devoted to discovery nonlinear evolution PDEs, which are integrable and of applicative relevance. In particular, a new integrable nonlinear evolution PDE has been derived from the Kadomtsev–Petviashvili equation, by means of a reduction method based on Fourier decomposition and space–time rescalings [see (1.4)]. Moreover, the integrability property is explicitly demonstrated, because the Lax pair has been deduced, by applying the reduction method to the Lax pair of the original equation. Possible extensions and generalizations are now indicated: (i) study of the characteristics of the solutions of

(1.3); (ii) research of universal and integrable nonlinear PDEs in 2+1 and 3+1 dimensions obtained by the reduction method; (iii) approximate solution of a physically relevant nonlinear equation through the study of the correspondent integrable model equation.

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Wronskian solutions of the constrained Kadomtsev–Petviashvili hierarchy

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The integrable Kadomtsev–Petviashvili (KP) hierarchy is compatible with generalized k-constraints of the type $(L^k)_- = \Sigma_i\, q_i \partial_x^{-1} r_i$. A large class of solutions—among them solitons—can be represented by Wronskian determinants of functions satisfying a set of linear equations. In this paper we shall obtain additional conditions for these functions imposed by the constraints. © *1996 American Institute of Physics.* [S0022-2488(96)04111-4]

I. THE CONSTRAINED KP HIERARCHY

The dynamics of the KP hierarchy is defined by the Lax equations

$$L_{t_n} = [L, (L^n)_-], \tag{I.1}$$

with the micro-differential operator $L = \partial_x + u_2 \partial_x^{-1} + u_3 \partial_x^{-2} + \ldots$. The dressing operator $W = 1 + w_1 \partial_x^{-1} + w_2 \partial_x^{-2} + \ldots$, related to the Lax operator by $L = W \partial_x W^{-1}$, satisfies Sato's equations

$$W_{t_n} = -(W \partial_x^n W^{-1})_- W. \tag{I.2}$$

The essence of Sato's theory[1–5] is the fact that solutions of Sato's equations can be expressed by a single function τ, which has to satisfy a hierarchy of *bilinear* equations. It is well-known[6–11] that the KP dynamics (I.1) is compatible with generalized k-constraints of the form

$$(L^k)_- = \sum_{i=1}^{M} q_i \partial_x^{-1} r_i \tag{I.3}$$

with suitable functions q_i and r_i. We note that such Lax operators are characterized by the existence of an M-th order differential operator

$$A = \partial_x^M + a_{M-1} \partial_x^{M-1} + \cdots + a_0$$

such that AL^k is a differential operator. The factor A needs to annihilate the functions q_i, i.e., $A(q_1) = \cdots = A(q_N) = 0$. Since an operator may be reconstructed from its kernel, A is uniquely determined if the Wronskian determinant $\mathscr{W}(q_1, \ldots, q_N)$ does not vanish. Similarly, there exists

$$B = \partial_x^M + b_{M-1} \partial_x^{M-1} + \cdots + b_0$$

such that $L^k B$ is a differential operator. The functions r_i span the kernel of the adjoint B^*. The constraint (1.3) reduces the KP dynamics to the hierarchy

$$(L^k)_{t_n} = [L^k, (L^n)_-], \quad (q_i)_{t_n} = (L^n)_+ (q_i), \quad (r_i)_{t_n} = -(L^{*n}) + (r_i)$$

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of 1+1-dimensional integrable equations. For $M=1$ the first three constraints yield the the AKNS hierarchy ($k=1$), the Yajima–Oikawa hierarchy ($k=2$) and a coupled Boussinesq type ($k=3$) hierarchy.[6–11]

II. WRONSKIAN SOLUTIONS

In the following we consider linearly independent functions $f_1,\ldots,f_N$ satisfying the infinite set of linear equations

$$\frac{\partial f_i}{\partial t_n}=f_i^{(n)}\equiv\frac{\partial^n f_i}{\partial x^n}. \tag{II.1}$$

Their Wronskian determinant

$$\mathscr{W}(f_1,\ldots,f_N)=\begin{vmatrix} f_1^{(0)} & \cdots & f_1^{(N-1)} \\ \vdots & \ddots & \vdots \\ f_N^{(0)} & \cdots & f_N^{(N-1)} \end{vmatrix}$$

is a τ-function of the KP hierarchy.[4] This implies that the N-th order differential operator $W=\partial_x^N+w_1\partial_x^{N-1}+\cdots+w_N$ given by

$$W=\frac{1}{\mathscr{W}(f_1,\ldots,f_N)}\begin{vmatrix} f_1^{(0)} & f_1^{(1)} & \cdots & f_1^{(N)} \\ \vdots & \vdots & \ddots & \vdots \\ f_N^{(0)} & f_N^{(1)} & \cdots & f_N^{(N)} \\ 1 & \partial_x & \cdots & \partial_x^N \end{vmatrix} \tag{II.2}$$

provides a dressing operator satisfying (1.2). [The finite micro-differential operator $W\partial_x^{-N}=1+w_1\partial_x^{-1}+\cdots+w_N\partial_x^{-N}$ also satisfies (I.2) and is the dressing operator of Sato's theory.] In this formal determinant an expansion with respect to the last row is understood, in which all subdeterminants are collected on the left of the differential symbols. With this representation it is clear that the action of W on an arbitrary function g is given by

$$W(g)=\frac{\mathscr{W}(f_1,\ldots,f_N,g)}{\mathscr{W}(f_1,\ldots,f_N)}. \tag{II.3}$$

In particular, $W(f_1)=\cdots=W(f_N)=0$, so that formula (II.2) provides the reconstruction of a normalized ordinary differential operator from its kernel.

We shall study the effect of the k-constraint on the entries of the Wronskian τ-function. We will make use of the following technical lemma:

Lemma: The micro-differential inverse of the dressing operator (II.2) *is given by*

$$W^{-1}=\sum_{i=1}^{N} f_i\partial_x^{-1}g_i$$

with

$$g_i=(-1)^{N-i}\,\frac{\mathscr{W}(f_1,\ldots,f_{i-1},f_{i+1},\ldots,f_N)}{\mathscr{W}(f_1,\ldots,f_N)}. \tag{II.4}$$

Proof: The functions g_i are the solutions of the linear system

$$\begin{pmatrix} f_1^{(0)} & \cdots & \cdots & f_N^{(0)} \\ \vdots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ f_1^{(N-1)} & \cdots & \cdots & f_N^{(N-1)} \end{pmatrix} \begin{pmatrix} g_1 \\ \vdots \\ \vdots \\ g_N \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}.$$

From these equations and using the algebraic rule

$$f\partial_x^{-1} = \partial_x^{-1} f + \partial_x^{-2} f^{(1)} + \partial_x^{-3} f^{(2)} + \ldots,$$

for the symbol ∂_x^{-1} one finds

$$\left(W \sum_{i=1}^{N} f_i \partial_x^{-1} g_i \right)_+ = \left(W \sum_{k=0}^{\infty} \partial_x^{-k-1} \sum_{i=1}^{N} f_i^{(k)} g_i \right)_+ = \left(W \partial_x^{-N} \left(1 + \sum_{k=N}^{\infty} \partial_x^{N-k-1} \sum_{i=1}^{N} f_i^{(k)} g_i \right) \right)_+ = 1.$$

On the other hand,

$$\left(W \sum_{i=1}^{N} f_i \partial_x^{-1} g_i \right)_- = \sum_{i=1}^{N} (W(f_i)) \partial_x^{-1} g_i = 0,$$

whence $W\Sigma_i f_i \partial_x^{-1} g_i = 1$. Q.E.D.

The following theorem provides a simple criterion for the Wronskian entries $f_1, \ldots, f_N$ leading to k-constrained KP flows:

Theorem: *The KP solution $L = W\partial_x W^{-1}$ generated by the Wronskian τ-function $\mathscr{W}(f_1, \ldots, f_N) \neq 0$ satisfies the k-constraint (I.3) with some suitable functions $q_1, \ldots, q_M$ and $r_1, \ldots, r_M$ if and only if*

$$\mathscr{W}(f_1, \ldots, f_N, f_{i_1}^{(k)}, \ldots, f_{i_{M+1}}^{(k)}) = 0 \tag{II.5}$$

for all $(M+1)$-tupel of indices $1 \leqslant i_1 < \cdots < i_{M+1} \leqslant N$, which is equivalent to

$$\mathscr{W}\left(\frac{\mathscr{W}(f_1, \ldots, f_N, f_{i_1}^{(k)})}{\mathscr{W}(f_1, \ldots, f_N)}, \ldots, \frac{\mathscr{W}(f_1, \ldots, f_N, f_{i_{M+1}}^{(k)})}{\mathscr{W}(f_1, \ldots, f_N)} \right) = 0 \tag{II.6}$$

for all such indices.

Proof: The equivalence between (II.5) and (II.6) is provided by the Wronskian identity

$$\mathscr{W}\left(\frac{\mathscr{W}(f_1, \ldots, f_N, h_1)}{\mathscr{W}(f_1, \ldots, f_N)}, \ldots, \frac{\mathscr{W}(f_1, \ldots, f_N, h_{M+1})}{\mathscr{W}(f_1, \ldots, f_N)} \right) = \frac{\mathscr{W}(f_1, \ldots, f_N, h_1, \ldots, h_{M+1})}{\mathscr{W}(f_1, \ldots, f_N)}, \tag{II.7}$$

which holds for arbitrary functions $f_1, \ldots, f_N$ and $h_1, \ldots, h_{M+1}$. It is proven in the appendix.

Using the previous lemma one finds

$$(L^k)_- = (W\partial_x^k W^{-1})_- = \sum_{i=1}^{N} (W(f_i^{(k)})) \partial_x^{-1} g_i \tag{II.8}$$

with g_i defined by (II.4). Hence, the constraint (I.3) with $M = N$ is always satisfied for KP solutions generated by $N \times N$-Wronskians. It is claimed that the conditions (II.5)/(II.6) reduce the sum from N to M terms.

First, we show that (II.6) follows from (I.3). As already remarked in Section I, for L satisfying (I.3) there exists an M-th order differential operator A such that AL^k is a differential operator. Application to $W(f_i)=0$ yields

$$0=AL^k(W(f_i))=AW\partial_x^k(f_i)=A(W(f_i^{(k)})).$$

Formula (II.3) leads to

$$W(f_i^{(k)})=\frac{\mathscr{W}(f_1,\ldots,f_N,f_i^{(k)})}{\mathscr{W}(f_1,\ldots,f_N)}\in kernel\ \ (A).$$

Since the kernel of A has dimension M, at most M of these functions can be linearly independent, whence (II.6) obtains. Conversely, if (II.6) holds, then at most M of the functions $W(f_i^{(k)})$ are linearly independent. Consequently, they can be expressed by M functions $q_1,\ldots,q_M$:

$$\frac{\mathscr{W}(f_1,\ldots,f_N,f_i^{(k)})}{\mathscr{W}(f_1,\ldots,f_N)}=\sum_{i=1}^{M} c_{ij}q_j,\quad i=1,\ldots,N,$$

with some constants c_{ij} and (II.8) reduces to

$$(L^k)=\sum_{i=1}^{N}\left(\sum_{j=1}^{M} c_{ij}q_j\right)\partial_x^{-1}g_i=\sum_{j=1}^{M} q_j\partial_x^{-1}\left(\sum_{i=1}^{N} c_{ij}g_i\right). \tag{II.9}$$

$Q.E.D.$

III. EXAMPLE

We consider 2×2-Wronskians $\tau=\mathscr{W}(f_1,f_2)$ with

$$f_1=\exp(c_1+\lambda_1 x+\lambda_1^2 y+\lambda_1^3 t)+\exp(d+\mu x+\mu^2 y+\mu^3 t),$$

$$f_2=\exp(c_2+\lambda_2 x+\lambda_2^2 y+\lambda_2^3 t)+\exp(c_3+\lambda_3 x+\lambda_3^2 y+\lambda_3^3 t)$$

with arbitrary constants c_i,λ_i,d,μ. These functions satisfy the linear equations (II.1) with $t_1=x,t_2=y$ and $t_3=t$, whence $u(x,y,t)=\ln(\tau)_{xx}$ satisfies the KP equation

$$4u_{tx}=(u_{xxx}+12uu_x)_x+3u_{yy}. \tag{III.1}$$

Using the theorem in the last section we will derive conditions on the parameters such that the k-constraint (I.3) with $M=1$ is satisfied. The criterion (II.5) yields a single equation

$$0=\mathscr{W}(f_1,f_2,f_1^{(k)},f_2^{(k)})=(\mu^k-\lambda_1^k)(\lambda_2^k-\lambda_3^k)V(\lambda_1,\lambda_2,\lambda_3,\mu)e^{c_1+c_2+c_3+d}e^{(\lambda_1+\lambda_2+\lambda_3+\mu)x}e^{(\lambda_1^2+\lambda_2^2+\lambda_3^2+\mu^2)y}e^{(\lambda_1^3+\lambda_2^3+\lambda_3^3+\mu^3)t}$$

with the Vandermonde determinant

$$V(\lambda_1,\lambda_2,\lambda_3,\mu)=\begin{vmatrix}1&\lambda_1&\lambda_1^2&\lambda_1^3\\1&\lambda_2&\lambda_2^2&\lambda_2^3\\1&\lambda_3&\lambda_3^2&\lambda_3^3\\1&\mu&\mu^2&\mu^3\end{vmatrix}.$$

It may be satisfied by the choice $\mu=\lambda_2$. Putting $d=c_2$, the τ-function yields

$$\tau=(\lambda_2-\lambda_1)e^{\eta_1+\eta_2}+(\lambda_3-\lambda_2)e^{\eta_2+\eta_3}+(\lambda_3-\lambda_1)e^{\eta_1+\eta_3},$$

where

$$\eta_i=c_i+\lambda_i x+\lambda_i^2 y+\lambda_i^3 t, \quad i=1,2,3.$$

The constraint $(L^k)_-=q\partial_x^{-1}r$ is satisfied with

$$q:=(\lambda_3^k-\lambda_2^k)\frac{\mathscr{W}(f_1,f_2,f_1^{(k)})}{\mathscr{W}(f_1,f_2)}=(\lambda_1^k-\lambda_2^k)\frac{\mathscr{W}(f_1,f_2,f_2^{(k)})}{\mathscr{W}(f_1,f_2)}$$
$$=\frac{(\lambda_1-\lambda_2)(\lambda_2-\lambda_3)(\lambda_3-\lambda_1)(\lambda_1^k-\lambda_2^k)(\lambda_3^k-\lambda_2^k)}{(\lambda_2-\lambda_1)e^{-\eta_3}+(\lambda_3-\lambda_1)e^{-\eta_2}+(\lambda_3-\lambda_2)e^{-\eta_1}},$$

and, according to (II.9)/(II.4),

$$r:=\left(\frac{f_2}{(\lambda_2^k-\lambda_3^k)}+\frac{f_1}{(\lambda_1^k-\lambda_2^k)}\right)\frac{1}{\mathscr{W}(f_1,f_2)}$$
$$=\frac{e^{-\eta_1-\eta_2-\eta_3}}{(\lambda_1^k-\lambda_2^k)(\lambda_3^k-\lambda_2^k)}\frac{(\lambda_3^k-\lambda_2^k)e^{\eta_1}+(\lambda_3^k-\lambda_1^k)e^{\eta_2}+(\lambda_2^k-\lambda_1^k)e^{\eta_3}}{(\lambda_3-\lambda_2)e^{-\eta_1}+(\lambda_3-\lambda_1)e^{-\eta_2}+(\lambda_2-\lambda_1)e^{-\eta_3}}.$$

These functions are regular for $\lambda_1<\lambda_2<\lambda_3$ and, for fixed y and t, bounded in x, if $\lambda_1<0$, $\lambda_2=0$, $\lambda_3>0$. The KP solution $u=\ln(\tau)_{xx}$ consists of three solitary waves located in (x,y,t)-space along the planes $\eta_1\approx\eta_2$, $\eta_2\approx\eta_3$ and $\eta_1\approx\eta_3$, respectively. In particular, choosing $\lambda_1=$, $\lambda_2=0$, $\lambda_3=-\lambda$, $c_1=c$, $c_2=0$, $c_3=-c$ one finds

$$q=\frac{(-1)^k\lambda^{2(k+1)}}{1+e^{-\lambda^2 y}\cosh(c+\lambda x+\lambda^3 t)}$$

and

$$r=\begin{cases}-\dfrac{1}{\lambda^{k+1}}\dfrac{e^{-\lambda^2 y}+\cosh(c+\lambda x+\lambda^3 t)}{e^{\lambda^2 y}+\cosh(c+\lambda x+\lambda^3 t)} & \text{for odd } k,\\ -\dfrac{1}{\lambda^{k+1}}\dfrac{\sinh(c+\lambda x+\lambda^3 t)}{e^{\lambda^2 y}+\cosh(c+\lambda x+\lambda^3 t)} & \text{for even } k.\end{cases}$$

For $k=1$ one has $L=\partial_x+q\partial_x^{-1}r$, whence q,r satisfy the first flows of the AKNS hierarchy

$$q_y=q_{xx}+2q^2r, \quad r_y=-r_{xx}-2qr^2$$

and

$$q_t=q_{xxx}+6qrq_x, \quad r_t=r_{xxx}+6qrr_x,$$

respectively. A solution of the KP equation (III.1) is given by $u=qr$. Plots of u and q in the (x,y)-plane at time $t=0$ are given in Figures 1 and 2 for $\lambda_1=-1$, $\lambda_2=0$, $\lambda_3=1$, $c_1=c_2=c_3=0$.

IV. CONCLUDING REMARKS

We have found necessary and sufficient conditions reducing a Wronskian solution of the general KP hierarchy to solutions of the k-constrained hierarchy. We have relied on properties of differential operators resulting from *finite* dressing operators. Of course, the same goal could have

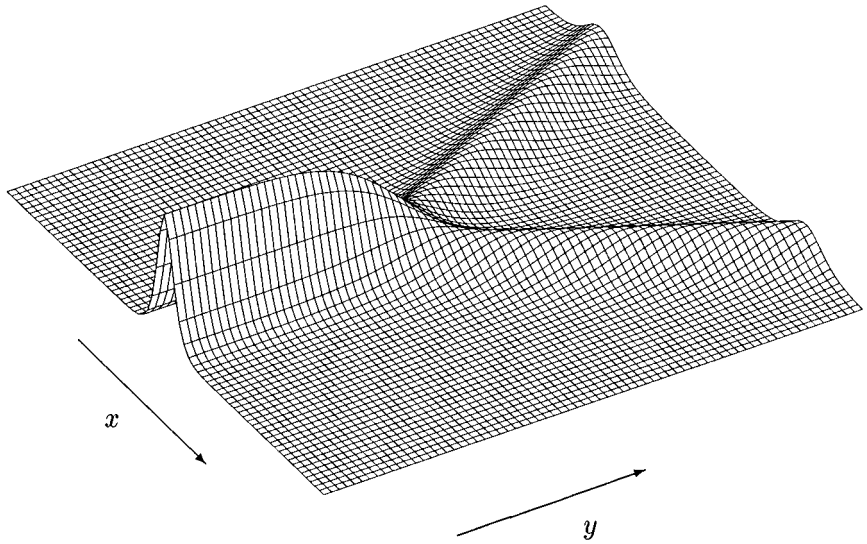

FIG. 1. $u(x,y,t)$ for $t = 0$.

been achieved by formulating additional equations for general τ-functions which then might be specialized to τ-functions of Wronskian type. The constraints for general τ-functions, however, are technically more involved. For special cases some results exist: the simplest additional condition on the τ-function in the cases $k=1$ and 2, respectively, is a trilinear form[12,13] and a quattrolinear form,[13,14] respectively. For Wronskian τ-functions these general conditions reduce to the results of the theorem in Sec. II.

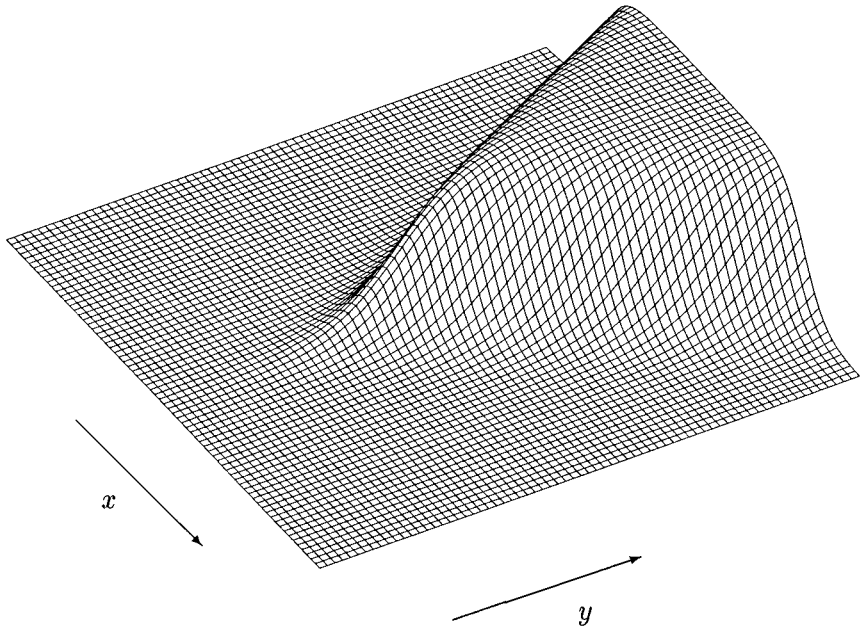

FIG. 2. $q(x,y,t)$ for $t = 0$.

APPENDIX: PROOF OF THE WRONSKIAN IDENTITY (II.7)

With some given family of functions $f_{n+1}^{[n]}, f_{n+2}^{[n]}, \ldots$, one considers ''iterated Darboux transformations'' defined by the recursion

$$f_i^{[k+1]} := \frac{\mathscr{W}(f_{k+1}^{[k]}, f_i^{[k]})}{f_{k+1}^{[k]}}, \quad i,k = n, n+1, \ldots .$$

Crum's classical result[15] is that after K such recursive steps the resulting functions have the Wronskian representation

$$f_i^{[n+K]} = \frac{\mathscr{W}(f_{n+1}^{[n]}, \ldots, f_{n+k}^{[n]}, f_i^{[n]})}{\mathscr{W}(f_{n+1}^{[n]}, \ldots, f_{n+K}^{[n]})}. \tag{A.1}$$

Comparing the results for $(n,K) = (0, N+m)$ and $(n,K) = (N,m)$ one finds for $i = N+m+1$:

$$f_{N+m+1}^{[N+m]} = \frac{\mathscr{W}(f_1^{[0]}, \ldots, f_{N+m+1}^{[0]})}{\mathscr{W}(f_1^{[0]}, \ldots, f_{N+m}^{[0]})} = \frac{\mathscr{W}(f_{N+1}^{[N]}, \ldots, f_{N+m+1}^{[N]})}{\mathscr{W}(f_{N+1}^{[N]}, \ldots, f_{N+m}^{[N]})}. \tag{A.2}$$

Denoting $f_i^{[0]} = f_i$ for $i = 1, \ldots, N$ and $f_{N+i}^{[0]} = h_i$ for $i = 1, \ldots, m+1$ one has

$$f_{N+i}^{[N]} = \frac{\mathscr{W}(f_1, \ldots, f_N, h_i)}{\mathscr{W}(f_1, \ldots, f_N)}, \quad i = 1, \ldots, m+1$$

from (A.1) with $n=0$, $K=N$ and (A.2) yields

$$f_{N+m+1}^{[N+m]} = \frac{\mathscr{W}(f_1, \ldots, f_N, h_1, \ldots, h_{m+1})}{\mathscr{W}(f_1, \ldots, f_N, h_1, \ldots, h_m)} = \frac{\mathscr{W}\left(\frac{\mathscr{W}(f_1, \ldots, f_N, h_1)}{\mathscr{W}(f_1, \ldots, f_N)}, \ldots, \frac{\mathscr{W}(f_1, \ldots, f_N, h_{m+1})}{\mathscr{W}(f_1, \ldots, f_N)}\right)}{\mathscr{W}\left(\frac{\mathscr{W}(f_1, \ldots, f_N, h_1)}{\mathscr{W}(f_1, \ldots, f_N)}, \ldots, \frac{\mathscr{W}(f_1, \ldots, f_N, h_m)}{\mathscr{W}(f_1, \ldots, f_N)}\right)}.$$

Multiplication of these identities with $m = 0, \ldots, M$ yields (II.7). Q.E.D.

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Higher-order Melnikov theory for adiabatic systems

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In this paper, we study adiabatic Hamiltonian systems including those subject to small-amplitude forcing and damping. It is known that simple zeroes of the adiabatic Poincare–Arnold–Melnikov function imply the existence of primary intersection points of the stable and unstable manifolds of hyperbolic orbits. Here, we present an Nth-order Melnikov function whose simple zeroes correspond to Nth-order transverse intersection points and hence to N-pulse homoclinic orbits. Using this function, it can be shown that N-pulse homoclinic orbits arise in a plethora of adiabatic models, including systems with slowly varying potentials. The theory is illustrated on a damped Hamiltonian system with a slowly varying cubic potential. In addition, the Nth-order adiabatic Melnikov function is useful for showing the existence of multi-pulse resonant periodic orbits in the special class of slow, time-periodic systems. © *1996 American Institute of Physics.*
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I. INTRODUCTION

Adiabatic invariance theory in mechanics has a long and rich history; see, e.g., Ref. 1. Adiabatic invariance theory was developed for slowly varying $[\mathcal{O}(\varepsilon)]$ Hamiltonian systems, and it applies to all orbits in regions where the ratio of the small parameter ε to the instantaneous orbit frequency is small. The terms in the series for the adiabatic invariant become disordered and the expansion ceases to be valid, however, near slowly-varying separatrices where the instantaneous orbital frequency approaches zero.

The dynamics of special and general orbits in these separatrix-swept regions has been the object of much recent study, for applications and development of the theory (see, e.g., Refs. 1–10 and also the references in Ref. 11). In time-periodic adiabatic systems, the existence of many resonant hyperbolic periodic orbits in these regions has been established via topological shooting,[7,8] and via matched asymptotic expansions,[4,12] among others. Moreover, for general adiabatic systems with general, not necessarily periodic, hyperbolic orbits in these regions, adiabatic separatrix crossing theory gives the change in a general orbit's adiabatic invariant and the canonically conjugate phase variable after it crosses an instantaneous separatrix. See Refs. 1, 5, and 6 for the full development and references to earlier works; see also Ref. 13.

For time periodic systems, chaos has been discovered in these regions.[3] The existence of the periodic orbits and bounded nonperiodic orbits in a Smale–Birkhoff horseshoe, as well as a kneading theory, have been established in two examples via topological shooting.[7,8] Moreover, the presence of Smale–Birkhoff homoclinic chaos can also be shown using the adiabatic Melnikov function.[2,4,14,15] Further studies of the chaotic structure in these separatrix-swept regions—including lobe area, homoclinic tangle geometry, island size, and the genericity of these results—are presented in Refs. 9, 16, and 17. The main tools used in these later works include an adiabatic separatrix crossing map[16] and an action theoretic derivation of the adiabatic Melnikov function.[9,17] See also Ref. 18.

Many of the physical problems modeled by slowly varying systems are not purely Hamiltonian, however, and are instead subject to small amplitude forcing and damping. For example, the slowly varying system arising in the model of resonant sloshing[7,12] is only Hamiltonian when viscosity is neglected. The presence of viscosity results in small amplitude dissipation in the governing equations.[12] Dissipation also plays an important role in capture-into-resonance, particle

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dynamics in modulated waves, transport in charged particle beams, and other physical systems.

While one expects many of the homoclinic and periodic orbits to survive when forcing and damping are added, there exists a general need to detect precisely which ones do, and where they lie in phase space and for what range of forcing and damping they exist. The Hamiltonian methods used in Refs. 9, 16, and 17 are not applicable when dissipation is included. In contrast, the adiabatic Melnikov function still applies, and hence the existence of persistent homoclinic orbits can still be demonstrated. Also, numerical evidence is presented in Ref. 12 showing that the resonant periodic orbits in the sloshing model can be continued into the nonzero dissipation regime, and it is thought that the topological shooting method can be extended, as well, as indicated in Ref. 7.

Many questions, however, remain open. How can one detect multiple pulse homoclinic orbits? For what parameter values do they occur? Near which parameter values do homoclinic tangencies occur? For special time-periodic systems, what is the geometry of the single-pulse and multi-pulse periodic orbits near these homoclinic orbits?, just to name a few.

In this paper, we develop a method to answer some of these questions. In particular, we establish a higher-order adiabatic Melnikov theory for slowly modulated Hamiltonian systems, which may also be subject to forcing and damping:

$$\dot{q}=\frac{\partial H}{\partial p}(q,p,z)+\varepsilon\mu f_1(q,p,z),\quad \dot{p}=-\frac{\partial H}{\partial q}(q,p,z)+\varepsilon\mu f_2(q,p,z),\quad \dot{z}=\varepsilon, \tag{1.1}$$

where $0<\varepsilon\ll 1$, $\mu>0$, the Hamiltonian H is four times continuously differentiable with a slowly varying parameter z, and f_1, f_2 are $\mathcal{C}^3$. When $\varepsilon=0$, (1.1) is a one-parameter family of ''frozen'' or unperturbed systems. Under the assumption that for each z in a finite interval this system possesses an orbit that is homoclinic (or heteroclinic) to a saddle fixed point(s), we construct a function of ε and z that we call the Nth-order adiabatic Melnikov function. Our main result shows that simple zeroes of this function imply the existence of transverse Nth-order homoclinic intersections of stable and unstable manifolds of (1.1) corresponding to N-pulse homoclinic orbits for the full system (1.1), provided ε is sufficiently small. First-order intersection points are points at which the finite segments of the local manifolds between the fixed point and the intersection point have only the intersection point in common, and these first-order intersections correspond to one-pulse homoclinic orbits. Secondary intersection points are points at which a segment of one manifold between two adjacent (as measured by arclength) first intersection points intersects the other local manifold, and they correspond to two-pulse homoclinic orbits, and so forth for all finite N.

Of course, in the special case of H being periodic in z, the existence of one principal intersection point automatically implies the existence of infinitely many of them, as Poincare showed. However, this new higher-order function is needed to establish the existence of higher-order intersection points for general H.

Also, in the special case of H being periodic in z, the existence and local uniqueness of periodic orbits of all periods automatically follows from the Smale–Birkhoff Homoclinic Theorem (see, e.g., Ref. 19). The precise geometric location of these periodic orbits can be determined using the Lambda Lemma (for scalar z) or by geometric singular perturbation theory (in the case of scalar z, and also for vector valued z) in conjunction with the Nth-order Melnikov function (see Ref. 10 for applications). These periodic orbits make one or more fast excursions away from a hyperbolic periodic solution. In this way, the Nth-order adiabatic Melnikov function enables one to generalize the results of Refs. 7, 8, and 12 for special conservative cases of slowly varying sinusoidal and cubic potentials to the entire class of systems (1.1), even to those with dissipation. During their fast excursions, the multi-pulse resonant periodic orbits stay close to the multi-pulse homoclinic orbits studied here. Thus, precise asymptotic information about the location of many N-pulse periodic orbits can also be gained with the Nth-order adiabatic Melnikov function.

In the global bifurcations at which segments of stable and unstable manifolds are tangent to each other, pairs of stable and unstable periodic orbits are created. Tangencies of these manifolds occur when the Nth-order adiabatic Melnikov function has higher-order zeroes. Hence, the Nth-order adiabatic Melnikov function can also be used to detect homoclinic tangencies and the associated creation of resonant periodic orbits.

The theory developed here is illustrated on an example of a Hamiltonian system, including dissipation, with a cubic potential whose slow variation in z is periodic. We identify and classify all the higher-order intersection points—and their corresponding multi-pulse homoclinic orbits—obtained by the intersection of a segment of the unstable manifold and a segment of the stable manifold. We find several different types of multi-pulse homoclinic orbits, including those that make their fast excursions in rapid succession and those that spend a longer amount of time in between excursions.

In the special case when $\mu=0$ in (1.1) and when H is periodic in z, the general theoretical method developed here is similar to the adiabatic separatrix-crossing map used in Ref. 16. In their vertex–intervertex map, the energy and time variables for an orbit are updated using the slow rate of change of the action and the period, respectively, evaluated at the appropriate vertices. By comparison, in our work, the energy change is measured by the adiabatic Melnikov function, and the period is essential for measuring the time between vertices, and hence for calculating the slow time at which to evaluate the Melnikov function. The methods yield the same result since the adiabatic Melnikov function is equal to the rate of pulsation of the critical (instantaneous separatrix) action, as shown in Refs. 9 and 17. Thus, the set of zeroes of M_A corresponds to the set Λ_e in Ref. 16, and the exact location of higher-order intersection points may be determined either by applying the separatrix-crossing map as demonstrated in Sec. 3.5 of Ref. 16 or by computing the appropriate higher-order adiabatic Melnikov function.

Finally, we remark that our work was inspired in part by the recently developed[20] higher-order Melnikov theory for planar Hamiltonian systems subject to general, small-amplitude, time-periodic perturbations:

$$\dot{x}=\frac{\partial H}{\partial y}(x,y)+\delta g_1(x,y,t), \quad \dot{y}=-\frac{\partial H}{\partial y}(x,y)+\delta g_2(x,y,t),$$

where $0<\delta\ll 1$. Our proof strategy borrows heavily from Ref. 20. For these systems, the secondary Melnikov function[20] depends on the $\mathcal{O}(1)$ phase t_0, and the existence of secondary intersection points is established by the zeroes of the function. In contrast, our second-order and Nth-order ($N>2$) adiabatic Melnikov functions which depend on slowly varying $\mathcal{O}(\varepsilon)$ phases. Also, we work directly on (1.1), whereas the Whisker map is used in Ref. 20.

The theory of multi-pulse homoclinic orbits has also been developed recently in a number of other contexts. For n degree of freedom Hamiltonian systems subject to small amplitude perturbations, dubbed as system I in Ref. 19, the work in Refs. 21 and 22 has shown the existence of different types of multi-pulse orbits. For the same types of systems, Ref. 23 develops a higher-order Melnikov theory. In each of these works, the central variable is a rapidly—($\mathcal{O}(1)$)—varying phase. The energy function of Ref. 21, the Melnikov functions used in Ref. 22, and the higher-order Melnikov function of Ref. 23 are functions of the appropriate $\mathcal{O}(1)$ variable, in contrast to our higher-order Melnikov function which is a function of a slowly varying parameter. In addition, the techniques of proof are fundamentally different.

Finally, homoclinic explosions (and implosions) in which infinitely many multi-pulse homoclinic orbits are created (disappear) have recently been discovered[24] in a slowly varying Hamiltonian system. This system is related to the Ginzburg–Landau equation and may be written in the form of (1.1) by replacing the third component of the vector field by a particular function of the form $\varepsilon F(q,p,z)$ and then analyzing the bifurcations that occur along the persistent slow manifold.

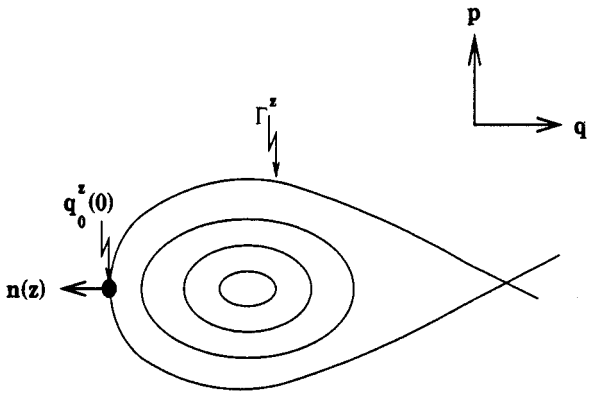

FIG. 1. The geometry of the unperturbed system.

The paper is organized as follows. We state the two structural assumptions on (1.1) in Sec. II. In Sec. III, we present a heuristic derivation of the Nth-order Melnikov function for the (1.1) with $\mu=0$. This heuristic derivation is extended to (1.1) with $\mu\neq 0$ in Sec. VIII. We state the main theorem for (1.1) with $\mu=0$ and its corollary for (1.1) with $\mu\neq 0$ in Sec. IV. We present an example in Sec. V. Section VI contains local estimates that are necessary for the proof of the Theorem. Finally, the theorem and corollary are proven in Secs. VII and VIII, respectively.

II. STRUCTURAL ASSUMPTION

We begin by making the following assumption on (1.1) when $\varepsilon=0$:

Assumption 1: For each fixed z in a finite interval, the instantaneous or frozen system

$$\dot{q}=\frac{\partial H}{\partial p}(q,p,z), \quad \dot{p}=-\frac{\partial H}{\partial q}(q,p,z), \quad \dot{z}=0, \tag{2.1}$$

has a saddle fixed point at $(q_e(z),p_e(z))$ *that satisfies the condition* $H(q_e(z),p_e(z),z)=0$. *For each z, this saddle is connected to itself by a homoclinic orbit* Γ^z. *The graph of* Γ^z *varies smoothly with z, and* Γ^z *is parametrized by the solution* $\mathbf{q}_0^z(t)\equiv(q_0^z(t),p_0^z(t),z)$. *Finally, the interior of the region bounded by* $(q_e(z),p_e(z))\cup\Gamma^z$ *is filled with a continuous family of periodic orbits,* $\mathbf{q}_\alpha^z$, *for* $\alpha\in(-1,0)$, *each with energy* $h_z^\alpha<0$ *and period* $P_z^\alpha=P(h_z^\alpha)$. *Moreover,* P_z^α *is differentiable in* $h^\alpha(z)$, *and* $dP_z^\alpha/dh_z^\alpha<0$.

For definiteness and without loss of generality, we take Γ^z to be as shown in Fig. 1. Let $\mathbf{n}(z)$ denote the unit normal vector to Γ^z at the point $\mathbf{q}_0^z(0)$ in the $q-p$ plane. In $q-p-z$ space, the union of the saddle equilibria over z forms a one-dimensional normally hyperbolic manifold γ_0 that must be either compact (e.g., H is periodic in z) or with boundary and that has two-dimensional stable and unstable manifolds $W^s(\gamma_0)$ and $W^u(\gamma_0)$, respectively. We remark that when $\epsilon=0$, one branch of each of these manifolds coincide in a homoclinic manifold, which is simply the union of the homoclinic orbits Γ^z over all z. The results of Sec. IV are readily generalized to the case in which (2.1) possesses heteroclinic orbits, and hence they are applicable to all of the examples cited in the Introduction.

III. HEURISTIC DERIVATION OF THE *N*TH-ORDER MELNIKOV FUNCTION

Consider the system (1.1) with $\mu=0$:

$$\dot{q}=\frac{\partial H}{\partial p}(q,p,z), \quad \dot{p}=-\frac{\partial H}{\partial q}(q,p,z), \quad \dot{z}=\varepsilon. \tag{3.1}$$

Fenichel theory,[25] states that for ε sufficiently small, γ_0 persists as a slow manifold γ_ε along with its two-dimensional local stable and unstable manifolds, $W^s_{\rm loc}(\gamma_\varepsilon)$ and $W^u_{\rm loc}(\gamma_\varepsilon)$, respectively. The global counterparts of these perturbed manifolds no longer coincide in general, and instead they can transversely intersect one another. We now present a heuristic derivation of the *N*th-order Melnikov function used to detect the *N*th-order transverse intersections of $W^s(\gamma_\varepsilon)$ and $W^u(\gamma_\varepsilon)$ in which the *N*-pulse orbits homoclinic to γ_ε lie for $N=2,3,\ldots$. This derivation will be extended to the $\mu\neq 0$ case in Sec. VIII.

Let $\mathbf{q}^u(t;z_0,\varepsilon)=(x^u(t),y^u(t),z)$ be a solution on the unstable manifold $W^u(\gamma_\varepsilon)$ that crosses the normal $\mathbf{n}(z)$ for the first time with $z=z_0=\varepsilon t_0$, and hits the negative x axis near γ_ε at $t=t_1^*$ with energy $H_1<0$. See Fig. 2 for a sketch. This solution exists when ε is sufficiently small. Using the chain rule, we compute

$$H_1\equiv\int_{-\infty}^{t_1^*}\frac{dH}{dt}(\mathbf{q}^u(t;z_0,\varepsilon))dt=\varepsilon\int_{-\infty}^{t_1^*}\frac{\partial H}{\partial z}(\mathbf{q}^u(t;z_0,\varepsilon))dt. \tag{3.2}$$

At a time $z_0-\Delta z$, for some fixed Δz, $\mathbf{q}^u(t;z_0,\varepsilon)$ is exponentially close to γ_ε; i.e., $|\mathbf{q}^u(t;z_0,\varepsilon)|=\mathcal{O}(e^{-c/\varepsilon})$, for some $c>0$. So for all $z<z_0-\Delta z$, we know that $|\partial H/\partial z(\mathbf{q}^u(t;z_0,\varepsilon))| = \mathcal{O}(e^{-c_1/\varepsilon})$, with $c_1>0$. For $z\in[z_0-\Delta z,\, z_0]$, we Taylor expand $\partial H/\partial z(\mathbf{q}^u(t;z_0,\varepsilon))$ about $\mathbf{q}=\mathbf{q}_0^{z_0}(t)$ and make an error of $\mathcal{O}(\varepsilon)$. This expansion holds for all $z\in[z_0-\Delta z,\, z_0+\Delta z]$. Hence, (3.2) becomes

$$H_1=\varepsilon\int_{-\infty}^{t_1^*}\left[\frac{\partial H}{\partial z}(\mathbf{q}_0^{z_0}(t))+\mathcal{O}(\varepsilon)\right]dt.$$

We introduce the following definitions to keep the length of formulas under control. Let $h_1(z_0)\equiv\int_{-\infty}^{\infty}(\partial H/\partial z)(\mathbf{q}_0^{z_0}(t))dt$, and let $R_s(z_0,t_1^*)\equiv-\varepsilon\int_{t_1^*}^{\infty}\partial H/\partial z(\mathbf{q}_0^{z_0}(t))dt+\mathcal{O}(\varepsilon^2)$. In terms of these new symbols, the above formula for H_1 becomes

$$H_1=\varepsilon h_1(z_0)+R_s(z_0,t_1^*). \tag{3.3}$$

We remark that $h_1(z_0)$ is precisely the (one-pulse) adiabatic Melnikov function $M_A(z_0)$.[2,4,14,15]

We will classify systems of the form (1.1) that satisfy our assumption as systems of type I or of type II. Systems of type I satisfy the extra condition

$$\frac{\partial H}{\partial z}=\alpha(z)L(q,p,z), \quad \text{where} \quad \int_{-\infty}^{\infty}(\mathbf{q}_0{}^z(t))dt>0 \quad \text{for all } z.$$

Thus, for systems of type I the adiabatic Melnikov function is written as $M_A(z)=\alpha(z)\int_{-\infty}^{\infty}(\mathbf{q}_0{}^z(t);\, u)dt$, where for μ sufficiently small, this last integral is positive and $\hat{L}(\mathbf{q}_0{}^z(t);0)\equiv L(\mathbf{q}_0{}^z(t))$. We call systems of type II those that do not satisfy it.

We have chosen the form given in (3.3) to express H_1, since we will show in Sec. VII A that the remainders are of higher order. In fact, for type I systems $R_s(z_0,t_1^*)=\mathcal{O}(\varepsilon^2)$ as $\varepsilon\to 0$ for systems of type II, $R_s(z_0,t_1^*)=\mathcal{O}(\varepsilon^2\ln(1/\varepsilon))$ as $\varepsilon\to 0$. This completes the first part of the heuristic derivation.

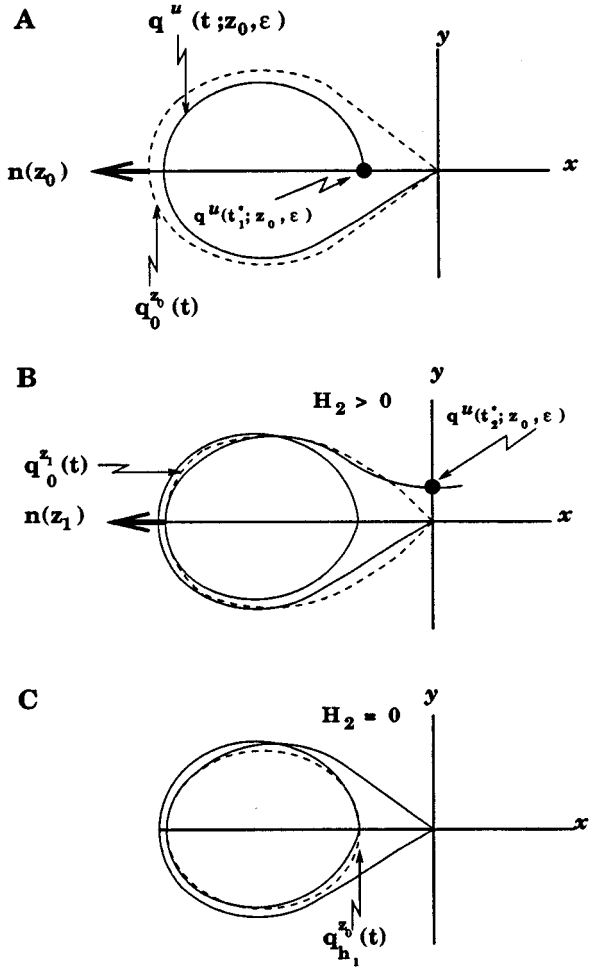

FIG. 2. Projections onto the $x-y$ plane of the perturbed solution $\mathbf{q}^u(t;z_0,\varepsilon)$ on the unstable manifold $W^u(\gamma_\varepsilon)$. (a) The projection is up to time $t=t_1^*$. The dotted curve represents the unperturbed homoclinic orbit $\mathbf{q}_0^{z_0}$ at $z=z_0$. (b) When $H_2>0$, $\mathbf{q}^u(t_2^*;z_0,\varepsilon)$ is on the positive y axis. The dotted curve corresponds to the unperturbed homoclinic $\mathbf{q}_0^{z_1}$. (c) When $H_2=0$, we have that t_2^* is infinite. The dotted curve represents the unperturbed periodic orbit $\mathbf{q}_{h_1}^{z_0}$ at $z=z_0$, with energy εh_1.

Now, since we assumed $H_1<0$, we know that $\mathbf{q}^u(t;z_0,\varepsilon)$ is not a primary homoclinic solution. As we follow this solution beyond t_1^*, it will make a second fast excursion away from γ_ε, crossing $\mathbf{n}(z)$ now at some $z=z_1=\varepsilon t_1$, and then it will come back to the neighborhood of γ_ε, again for ε sufficiently small. Moreover, in this neighborhood this solution either hits the x axis or the y axis at $t=t_2^*$ with energy H_2, or it is forward asymptotic to γ_ε (when $H_2=0$ and t_2^* is infinite). An exact computation yields

$$H_2=H_1+\int_{t_1^*}^{t_2^*}\frac{dH}{dt}\,(\mathbf{q}^u(t;z_0,\varepsilon))dt.$$

In order to arrive at a suitable approximation of H_2, we proceed as we did with the first excursion and write the second fast excursion as an expansion about the instantaneous separatrix at $z=z_1$:

$$H_2=H_1+\varepsilon\int_{-\infty}^{\infty}\frac{\partial H}{\partial z}(\mathbf{q}_0^{z_1}(t))dt-\varepsilon\int_{-\infty}^{t_1^*}\frac{\partial H}{\partial z}(\mathbf{q}_0^{z_1}(t))dt-\varepsilon\int_{t_2^*}^{\infty}\frac{\partial H}{\partial z}(\mathbf{q}_0^{z_1}(t))dt+\mathcal{O}(\varepsilon^2).$$

Therefore, using the remainder notation introduced above, we rewrite this formula as

$$H_2=\varepsilon(h_1(z_0)+h_1(z_1))+R_s(z_0,t_1^*)+R_s(z_1,t_2^*)+R_u(z_1,t_1^*), \tag{3.4}$$

where $R_u(z_1,t_1^*)\equiv-\varepsilon\int_{-\infty}^{t_1^*}(\partial H/\partial z)(\mathbf{q}_0^{z_1}(t))dt+\mathcal{O}(\varepsilon^2)$.

Finally, we use an asymptotic relation between z_0 and z_1. Since z_1-z_0 is the amount of slow time between consecutive crossings of $\mathbf{q}^u(t;z_0,\varepsilon)$ with $\mathbf{n}(z)$, we expect that the period $P(H_1)$ of the unperturbed periodic orbit of the frozen system (2.1) with $z=z_0$, with energy $H_1=h^{\alpha}_{z_0}$, where α is determined by H_1, provides a good approximation of the amount of time the solution $\mathbf{q}^u(t;z_0,\varepsilon)$ spends in the oscillatory regime. In fact, using (3.3), the leading order asymptotic behavior as $\varepsilon\to0$ will be shown in Sec. VII B to be

$$z_1\sim z_0+\varepsilon P(\varepsilon h_1(z_0)). \tag{3.5}$$

Therefore, the above results motivate us to study the function

$$h_2(z_0,\varepsilon)\equiv h_1(z_0)+h_1(z_0+\varepsilon P(h_1(z_0))), \tag{3.6}$$

whose zeroes will be shown to correspond to secondary homoclinic orbits. For N-pulse homoclinic orbits, the value of the function H after N excursions is given exactly as

$$\begin{aligned}H_N&=H_{N-1}+\int_{t_{N-1}^*}^{t_N^*}\frac{dH}{dt}(\mathbf{q}_0^u(t;z_0,\varepsilon))dt\\&=H_{N-1}+\varepsilon h_1(z_{N-1})+R_s(z_{N-1},t_N^*)+R_u(z_{N-1},t_{N-1}^*).\end{aligned} \tag{3.7}$$

Hence, we need the inductively defined function

$$h_N(z_0,\varepsilon)\equiv h_{N-1}(z_0,\varepsilon)+h_1\left(z_0+\varepsilon\sum_{j=1}^{N-1}P(\varepsilon h_j)\right), \tag{3.8}$$

where $h_1\equiv h_1(z_0)$ and $h_j\equiv h_j(z_0,\varepsilon)$ for $j=2,\ldots,N-1$.

This completes the heuristic derivation. As remarked above, $h_1(z_0)=M_A(z_0)$. We will also use $M_{1,A}(z_0)$ to denote $M_A(z_0)$. Therefore, the functions $h_1,\ldots,h_N$ lead us to define the second order and Nth-order for $N\geqslant2$ adiabatic Melnikov functions inductively as

$$\begin{aligned}M_{2,A}(z_0,\varepsilon)&=M_{1,A}(z_0)+M_{1,A}(z_0+\varepsilon P(\varepsilon h_1)),\\M_{N,A}(z_0,\varepsilon)&=M_{N-1,A}(z_0,\varepsilon)+M_{1,A}\left(z_0+\varepsilon\sum_{j=1}^{N-1}P(\varepsilon h_j)\right).\end{aligned} \tag{3.9}$$

The theorem for $\mu=0$ and the corollary for $\mu\neq0$ formulated in the next section show that $\varepsilon M_{N,A}(z_0,\varepsilon)$ is a good approximation to H_N for $N=2,\ldots$, and that simple zeroes of $M_{N,A}(z_0,\varepsilon)$ imply simple zeroes of H_N, and hence transverse Nth-order intersections for systems (1.1).

Remark 1: There is an alternative derivation of H_N which we briefly present for the $N=2$ case. Let $\mathbf{q}^u(t;z_0,\varepsilon)$ be as above, and $\mathbf{q}^s(t;z_1,\varepsilon)$ be a solution on the stable manifold $W^s(\gamma_\varepsilon)$ that in backward time crosses the normal $\mathbf{n}(z_1)$ for the first time at $z=z_1$, and hits the negative x axis in the neighborhood of γ_ε at $t = t_1^*$. The difference in the value of H for these two orbits at the time $t = t_1^*$, when both of them are on the x axis (see Fig. 3), is also a measure of the distance between $W^u(\gamma_\varepsilon)$ and $W^s(\gamma_\varepsilon)$. This difference is given by

$$\Delta H = \int_{-\infty}^{t_1^*} \frac{dH}{dt}\,(\mathbf{q}^u(t;z_0,\varepsilon))dt - \int_{\infty}^{t_1^*} \frac{dH}{dt}\,(\mathbf{q}^s(t;z_1,\varepsilon))dt.$$

After approximating $\mathbf{q}^u(t;z_0,\varepsilon)$ with $\mathbf{q}_0^{z_0}$ the solution on the instantaneous separatrix, and $\mathbf{q}^s(t;z_1,\varepsilon)$ with $\mathbf{q}_0^{z_1}$, we obtain

$$\begin{aligned}\Delta H &= \int_{-\infty}^{\infty} \frac{dH}{dt}\,(\mathbf{q}_0^{z_0}(t))dt + \int_{-\infty}^{\infty} \frac{dH}{dt}\,(\mathbf{q}_0^{z_1}(t))dt + R_s(z_0,t_1^*) + R_u(z_1,t_1^*)\\ &= \varepsilon(h_1(z_0)+h_1(z_1)) + R_s(z_0,t_1^*) + R_u(z_1,t_1^*). \qquad (3.10)\end{aligned}$$

So ΔH is H_2 up to a remainder term and so H_2 can be interpreted as the signed distance between $W^u(\gamma_\varepsilon)$ and $W^s(\gamma_\varepsilon)$ in the neighborhood of γ_ε. For general $N\geqslant 2$, H_N can similarly be interpreted as the signed distance between these two manifolds. When N is even, this distance is measured along the x axis in the neighborhood of γ_ε, while for odd N, the distance is measured along some normal $\mathbf{n}(z)$.

Remark 2: In some cases, the symmetries of the Hamiltonian allow us to improve the error in (3.10), and therefore in (3.4). If $H(q,p,z)$ is invariant under the change of coordinates $p\to -p$, then the remainder terms $R_s(z_0,t_1^*)$ and $R_u(z_1,t_1^*)$ cancel each other out, and (3.10) becomes $\Delta H=\varepsilon(h_1(z_0)+h_1(z_1))+\mathcal{O}(\varepsilon^2)$.

IV. STATEMENT OF THE MAIN RESULT

Theorem 1: *Let (3.1) satisfy Assumption 1. Let $M_{N,A}(z,\varepsilon)$ denote the Nth-order adiabatic Melnikov function for (3.1), where N is a fixed positive integer. If (z_0,ε_0) is such that*

(1) $M_{N,A}(z_0,\varepsilon_0)=0$,
(2) $M_{1,A}(z_0)<-\kappa<0$ *and* $M_{j,A}(z_0,\varepsilon_0)<-\kappa<0$ *for* $j=2,\ldots,N-1$, *and*
(3) $dM_{N,A}/dz(z_0,\varepsilon_0)>\nu>0$,

then there exists a constant $\hat{\varepsilon}=\hat{\varepsilon}(\kappa,\nu,\alpha,\beta)$ where $0<\beta<\alpha<\frac{1}{2}$, such that for every $\varepsilon<\hat{\varepsilon}$ in an $\mathcal{O}(\varepsilon_0^{1+\alpha})$ size neighborhood of ε_0, and for some $z\in[z_0-\Delta z,z_0+\Delta z]$ with $\Delta z=\mathcal{O}(\varepsilon_0^{\beta})$, $W_\varepsilon^u(\gamma_\varepsilon)$ and $W_\varepsilon^s(\gamma_\varepsilon)$ intersect transversely in an N-pulse homoclinic orbit. Furthermore, the remainder terms in calculating M_N are $\mathcal{O}(\varepsilon^2)$ for type I systems and of $\mathcal{O}(\varepsilon^2\ln(1/\varepsilon))$ for type II systems.

When the expansion of $h_1(z_0+\varepsilon\Sigma_{j=1}^{N-1}P(\varepsilon j_j))$ in ε about z_0 is considered in expression (3.9), the first and second terms of this asymptotic expansion are significant for systems of type I, while for type II systems, the second term in this expansion is of the same order as the remainder.

Remark 3: If the system (2.1) possesses multiple homoclinic orbits, the theory can be applied to each one separately, and further homoclinic orbits might be possible in which near-separatrix excursions occur near different homoclinic loops. Also, the theory can be immediately extended to the case of one or more heteroclinic orbits, with the relevant integrals being evaluated along the appropriate heteroclinic, as opposed to homoclinic, orbits. Finally, the second condition of the theorem can be relaxed by just requiring that $M_{1,A}(z_0)$ and $M_{j,A}(z_0,\varepsilon_0)$ for $j=2,\ldots,N-1$ are bounded away from zero. In systems where the topography is correct, such as a slowly varying Duffing equation, this extension enables the detection of a wider class of homoclinic solutions. In

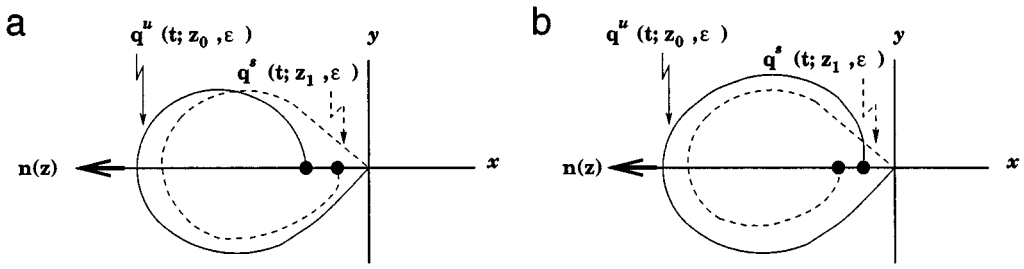

FIG. 3. Illustration of Remark 1 showing projections onto the $x-y$ plane of the solutions $\mathbf{q}^u(t;z_0,\varepsilon)$ on $W^u(\gamma_\varepsilon)$ (solid curve) and $\mathbf{q}^s(t;z_1,\varepsilon)$ on $W^s(\gamma_\varepsilon)$ (dashed curve). At time $t=t_1^*$ both solutions are on the x axis. Depending on the sign of $H(\mathbf{q}^u(t_1^*;z_0,\varepsilon),z_1^*)-H(\mathbf{q}^s(t_1^*;z_0,\varepsilon),z_1^*)$ we have (a) $H_2<0$ and (b) $H_2>0$.

some geometries, such as the slowly varying cubic, however, this extension is not relevant, since orbits with $M_{j,A}>0$ for some j never return to the neighborhood of γ_ε. In fact, in the example below, they escape from the slowly varying potential well.

Corollary 1: For the full damped and forced system (1.1) with $\mu\neq 0$ satisfying Assumption 1, with $M_{N,A}(z,\varepsilon)$ denoting its corresponding adiabatic Melnikov function, and for values (z_0,ε_0) that satisfy conditions (1), (2), and (3) of Theorem 1, the results of Theorem 1 hold.

Theorem 1 is proven in Secs. VI and VII, and the Corollary is proven in Sec. VIII.

V. AN EXAMPLE

In this section, we will deal with the case in which the Hamiltonian is periodic in z:

$$\dot{q}=p,\quad \dot{p}=q^2-F(z)-\varepsilon\mu p,\quad \dot{z}=\varepsilon, \tag{5.1}$$

where $F(z)\equiv 1+c+\cos(z)$, $c>0$, and $\mu>0$ is the dissipation parameter.[7,12] Its Hamiltonian has a slowly varying cubic potential: $H(p,q;z)=p^2/2-q^3/3+qF(z)-\frac{2}{3}F(z)^{3/2}$. System (5.1) is of type I and clearly satisfies our assumption: the $\varepsilon=0$ or frozen system has a saddle at $(q=-F(z)^{1/2}, p=0)$ for each $z\in[0,2\pi)$ so that γ_0 is compact and boundaryless. Each saddle is connected to itself by a homoclinic orbit Γ^z. Γ^z is parametrized by t as follows:

$$(F^{1/2}(z)(1-3\,\mathrm{sech}^2(F^{1/4}(z)t/\sqrt{2})),3\sqrt{2}F^{3/4}(z)\mathrm{sech}^2(F^{1/4}(z)t/\sqrt{2})\tanh(F^{1/4}(z)t/\sqrt{2})).$$

This expression for the instantaneous separatrix facilitates a direct computation of the adiabatic Melnikov function:

$$M_{1,A}(z_0;\mu)=\int_{-\infty}^{\infty}\frac{\partial H}{\partial z}(\mathbf{q}_0^{z_0}(t))dt=6\sqrt{2}F^{1/4}(z_0)\left(\sin(z_0)-\frac{4}{5}\mu F(z_0)\right).$$

Figure 4(a) shows plots of $M_{1,A}(z_0;\mu)$ as a function of z_0, for some values of μ. Each of its simple zeroes implies (via the implicit function theorem) a transverse intersection of $W^u(\gamma_\varepsilon)$ and $W^s(\gamma_\varepsilon)$. In the rest of the figures and the subsequent discussion, we set $\mu=0$ to simplify the numerical computations. We comment on the $\mu>0$ case in the remarks, as well as on the more general case in which the Hamiltonian is not periodic in z.

The zeroes of $M_{1,A}(z_0;0)\equiv M_{1,A}(z_0)$ of the form $\hat{z}_0=2k\pi$, where k is any integer (for which $M'_{1,A}(\hat{z}_0)>0$), correspond to a homoclinic orbit of (5.1) with a fast excursion near a maximum instantaneous separatrix. Each zero of the form $\hat{z}_0=(2k+1)\pi$ [for which $M'_{1,A}(\hat{z}_0)<0$] corresponds to a homoclinic orbit with a fast excursion near a minimum instantaneous separatrix.

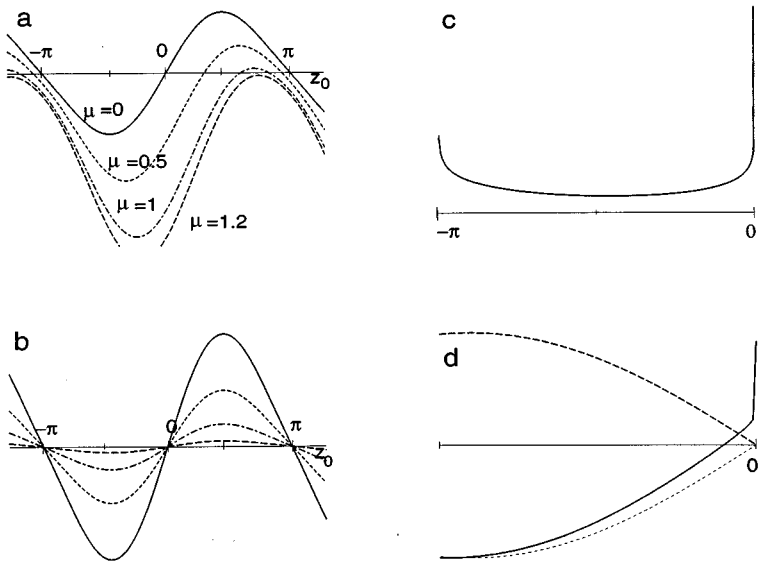

FIG. 4. Analysis of the example in Sec. V. (a) Plots of $M_{1,A}(z_0;\mu)$ for different values of μ. (b) Plots of $\varepsilon M_{1,A}(z_0;0)=\varepsilon M_{1,A}(z_0)$ for different values of ε: $\varepsilon=1$ (solid curve), $\varepsilon=0.5$ (long dashed curve), $\varepsilon=0.2$ (short and long dashed curve), and $\varepsilon=0.05$ (short dashed curve). (c) Behavior of $P(\varepsilon h_1(z_0))=P(\varepsilon M_{1,A}(z_0;0))$. (d) Intersection of $M_{1,A}(z_0+\varepsilon P(\varepsilon h_1(z_0)))$ (solid curve) with $-M_{1,A}(z_0)$ (long dashed curve). $M_{1,A}(z_0)$ (dotted curve) is also shown for $z_0\in(-\pi/2,0]$.

Figure 5 displays the intersection of $W^u(\gamma_\varepsilon)$ and $W^s(\gamma_\varepsilon)$ with the Poincaré section at $z=0$, $\Pi_{z=0}$, for some values of ε as ε decreases. In what follows, we denote $W^u(\gamma_\varepsilon)\cap\Pi_{z=0}$ by W^u, and $W^s(\gamma_\varepsilon)\cap\Pi_{z=0}$ by W^s. We label the primary intersection points of W^u and W^s by P_1; P_{1m}^{π}, $P_{1m}^{-\pi}$, where P_1 belongs to the homoclinic orbit with an excursion close to the maximum instantaneous separatrix at $z=0$. The orbits through P_{1m}^{π} and $P_{1m}^{-\pi}$ are the principal homoclinic orbits with excursions at the minimum instantaneous separatrices at $z=\pi$ and $z=-\pi$, respectively.

We proceed to find the intersection points that belong to the N-pulse homoclinic orbits described in Theorem 1. Beginning with $N=2$, the secondary adiabatic Melnikov function is:

$$M_{2,A}(z_0,\varepsilon)=M_{1,A}(z_0)+M_{1,A}(z_0+\varepsilon P(\varepsilon h_1(z_0))). \tag{5.2}$$

We look for zeroes of (5.2) that satisfy conditions 2 and 3 of Theorem 1. From Fig. 4(a), we see that z_0 must belong to the interval $(-\pi/2,0)$. To find these zeroes, we look first at the expression $\varepsilon P(\varepsilon h_1(z_0))$ in the argument of the second term of (5.2). Figure 4(b) shows plots of $\varepsilon h_1(z_0)=\varepsilon M_{1,A}(z_0)$ as ε decreases, and Fig. 4(c) displays the behavior of $P(\varepsilon h_1(z_0))$, where for each z_0, $P(\varepsilon h_1(z_0))$ denotes the period of the periodic orbit of the frozen system (system (5.1) with $\varepsilon=0$) with $z=z_0$, with energy $\varepsilon h_1(z_0)$. Thus, $P(\varepsilon h_1(z_0))$ can be obtained via complete elliptic integrals of the first kind. For ε small, $P(\varepsilon h_1(z_0))=\mathcal{O}(\ln(1/\varepsilon h_1(z_0)))$; hence the graph in Fig. 4(c) diverges at $z_0=0$. However, as $\varepsilon\to 0$, $\varepsilon P(\varepsilon h_1(z_0))\to 0$, at least for $h_1(z_0)$ not exponentially small. Thus, for ε small, the graph of $M_{1,A}(z_0+\varepsilon P(\varepsilon h_1(z_0)))$ is the graph of $M_{1,A}(z_0)$ slightly translated (nonuniformly) to the left. Finally, as Fig. 4(d) shows, the zero $z_{0,2}$ of $M_{2,A}(z_0,\varepsilon)$ is obtained by the intersection of the graph of $M_{1,A}(z_0+\varepsilon P(\varepsilon h_1(z_0)))$ and that of $-M_{1,A}(z_0,\varepsilon)$.

We now use our estimate of $\varepsilon P(\varepsilon h_1(z_0))$ to obtain an estimate on the size of $z_{0,2}$. We expand $M_{1,A}(z_0+\varepsilon P(\varepsilon h_1(z_0)))$ about z_0: $M_{1,A}(z_0+\varepsilon P(\varepsilon h_1(z_0)))=M_{1,A}(z_0)+M'_{1,A}(z_0)\mathcal{O}(\varepsilon\ln 1/\varepsilon)+\mathcal{O}(\varepsilon^2\ln^2 1/\varepsilon)$. Equation (5.2) becomes

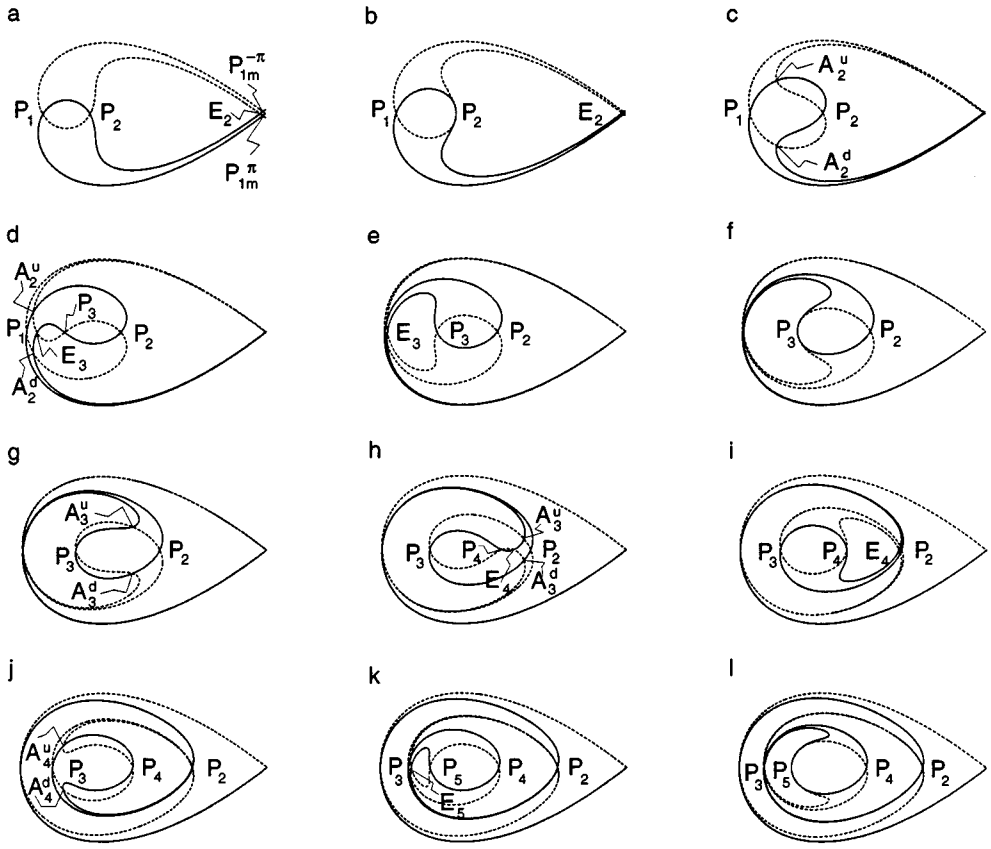

FIG. 5. Poincaré sections at $z=0$ of the intersections of W^u (solid) and W^s (dashed) for system (5.1) with $\mu=0$ for decreasing values of ε. Intersection points are labelled as P_i, E_i, and $A_i^{u,d}$. The P_i intersection points correspond to the i-pulse homoclinic orbits whose existence is established via Theorem 1. These pictures were obtained by numerical simulations based on the algorithm also used in Ref. 17. We used a symplectic integration method, and the code was developed by Steven P. Weibel. The values of ε in each of the panels are (a) $\varepsilon=1$, (b) $\varepsilon=0.9$, (c) $\varepsilon=0.8$, (d) $\varepsilon=0.68$, (e) $\varepsilon=0.6$, (f) $\varepsilon=0.54$, (g) $\varepsilon=0.5$, (h) $\varepsilon=0.45$, (i) $\varepsilon=0.4$, (j) $\varepsilon=0.35$, (k) $\varepsilon=0.325$, and (l) $\varepsilon=0.3$.

$$M_{2,A}(z_0,\varepsilon)=2M_{1,A}(z_0)+M'_{1,A}(z_0)\mathcal{O}\left(\varepsilon\ \ln\frac{1}{\varepsilon}\right)+\mathcal{O}\left(\varepsilon^2\ \ln^2\frac{1}{\varepsilon}\right),$$

where we are interested in the case $M'_{1,A}(z_0)>0$. Note that $M'_{1,A}(z_0)=\mathcal{O}(1)$. Then, $M_{2,A}(z_0,\varepsilon)=0$ implies

$$0=2M_{1,A}(z_{0,2})+M'_{1,A}(z_{0,2})\mathcal{O}\left(\varepsilon\ \ln\frac{1}{\varepsilon}\right)+\mathcal{O}\left(\varepsilon^2\ \ln^2\frac{1}{\varepsilon}\right).$$

The first two terms on the right cancel each other out when $M_{1,A}(z_{0,2})$ is itself $\mathcal{O}(\varepsilon \ln 1/\varepsilon)$, which in turn makes $z_{0,2}$ of $\mathcal{O}(\varepsilon \ln 1/\varepsilon)$. In fact, $z_{0,2}$ is $\mathcal{O}(\varepsilon \ln 1/\varepsilon)$ to the left of the zero $z=0$ of $M_{1,A}$. From Theorem 1, we conclude that $W^u(\gamma_\varepsilon)$ and $W^s(\gamma_\varepsilon)$ intersect in a two-pulse homoclinic orbit that makes two excursions near the maximum separatrix. The first excursion reaches its minimum in q at $z=z_{0,2}=\mathcal{O}(\varepsilon \ln 1/\varepsilon)$ to the left of $z=0$. It is not difficult to see that the second fast excursion reaches its minimum in q at $z=z_{1,2}=\mathcal{O}(\varepsilon \ln 1/\varepsilon)$ to the right of $z=0$, since we can

always write $M_{2,A}(z_1,\varepsilon)=M_{1,A}(z_1-\varepsilon P(\varepsilon h_1(z_1)))+M_{1,A}(z_1,\varepsilon)$, where z_1 corresponds to the second time the solution $\mathbf{q}^u(t;z_0,\varepsilon)$ reaches a normal $\mathbf{n}(z)$. In Fig. 5, this two-pulse homoclinic orbit corresponds to the intersection point labelled as P_2.

Remark 4: When the Hamiltonian is odd about its zero, as in this example with $\mu=0$ in (5.1), the points $z_{0,2}$ and $z_{1,2}$ are equidistant from $z=0$, a zero of $M_{1,A}$. Using (3.4), and expanding z_0 and z_1 about $z=0$, we get $M_{2,A} = 2h_1(0) + h_1'(0)z_0 + h_1'(0)z_1 + h_1''(0)z_0^2 + h_1''(0)z_1^2 + \mathcal{O}(z_0^3;z_1^3)$. Since $h_1(0) = h_1''(0) = 0$, then $M_{2,A}=0$ implies $z_0=-z_1$, at least up to $\mathcal{O}(\varepsilon^2)$ terms. See Remark 2. However, when the Hamiltonian is not odd about its zero as in the case of $\mu>0$ in (5.1), $h''(0)\neq 0$, and then the equality $z_0=-z_1$ holds up to $\mathcal{O}(\varepsilon^2 \ln^2 1/\varepsilon)$ terms.

We proceed now to consider the tertiary Melnikov function:

$$M_{3,A}(z_0,\varepsilon)=M_{2,A}(z_0,\varepsilon)+M_{1,A}(z_0+\varepsilon P(\varepsilon h_1(z_0))+\varepsilon P(\varepsilon h_2(z_0))). \tag{5.3}$$

Again, asymptotically as $\varepsilon\to 0$, $\varepsilon P(\varepsilon h_1(z_0))+\varepsilon P(\varepsilon h_2(z_0))=\mathcal{O}(\varepsilon \ln 1/\varepsilon)$, so (5.3) can be written as follows:

$$M_{3,A}(z_0,\varepsilon)=3M_{1,A}(z_0,\varepsilon)+2M_{1,A}'(z_0)\mathcal{O}\left(\varepsilon \ln\frac{1}{\varepsilon}\right)+\mathcal{O}\left(\varepsilon^2 \ln^2\frac{1}{\varepsilon}\right),$$

which yields that the zero $z_{0,3}$ of this function is $\mathcal{O}(\varepsilon \ln 1/\varepsilon)$ to the left of $z_{0,2}$, for ε sufficiently small. The intersection point corresponding to this three-pulse homoclinic orbit is labelled as P_3 in Fig. 5.

Proceeding in the same manner, for any finite N, and for ε sufficiently small, we find that

$$M_{N,A}(z_0,\varepsilon)=NM_{1,A}(z_0,\varepsilon)+(N-1)M_{1,A}'(z_0)\mathcal{O}\left(\varepsilon \ln\frac{1}{\varepsilon}\right)+\mathcal{O}\left(\varepsilon^2 \ln^2\frac{1}{\varepsilon}\right).$$

Hence, our N-pulse homoclinic orbits make N excursions close to the maximum instantaneous separatrix, and its successive minima in q are $\mathcal{O}(\varepsilon \ln 1/\varepsilon)$ apart. These orbits correspond to the intersection points labeled as P_2, P_3, P_4, P_5,... in Fig. 5.

In what follows we discuss the intersection points labeled E_i and A_i in Fig. 5. Consider first Figs. 5(a) and 5(b). Let $S[P_1,\ P_{1m}^{-\pi}]$ be the segment of W^s between the two primary intersection points (pips) P_1 and $P_{1m}^{-\pi}$. After one period, all points in this segment of W^s will be mapped to the neighborhood of γ_ε, and will remain there forever after. Similarly, let $U[P_{1m}^{\pi},\ P_1]$ be the segment of W^u between the pips P_{1m}^{π} and P_1. All previous images of this segment under the Poincaré map stay in the neighborhood of γ_ε.

Now, consider the point $E_2\in S[P_1,\ P_{1m}^{-\pi}]$. All of its forward images under the Poincaré map will stay in the neighborhood of γ_ε, getting closer and closer to it. Also, since $E_2\in U[P_{1m}^{\pi},\ P_1]$, all of its preimages were in the neighborhood of γ_ε. Here E_2 is on the q axis, inside a box $\mathcal{B}$ in the neighborhood of γ_ε. See Sec. VI for the definition of $\mathcal{B}$. In Sec. VI, we write a normal form [see Eq. (6.1)] for Eqs. (5.1) in $\mathcal{B}$. Using this normal form, we conclude that the orbit through E_2 should leave the box $\mathcal{B}$, and therefore it should make another excursion away from γ_ε to finally asymptote to γ_ε. We do a similar analysis for the backward orbit through E_2. Thus, E_2 corresponds to a two-pulse homoclinic orbit. As $\varepsilon\to 0$, the distance between E_2 and $P_{1m}^{-\pi}$ gets exponentially small, as measured on $U[P_1,\ P_{1m}^{-\pi}]$.

The same reasoning applies to P_2: its image after one period is in the neighborhood of γ_ε, and remains there ever after. All of its preimages are in the neighborhood of γ_ε. Note also, as measured in arclength along $U[P_1,\ P_{1m}^{-\pi}]$, that P_1 is closer to P_2 than E_2, so P_2 must correspond to the two-pulse homoclinic whose existence is guaranteed by the zero of $M_{2,A}(z_0,\varepsilon)$. The main difference between P_2 and E_2 is the time their orbits spend in between their fast excursions away from γ_ε. As $\varepsilon\to 0$, the orbit through P_2 takes an $\mathcal{O}(\varepsilon \ln 1/\varepsilon)$ amount of z-time during this excursion, while the one through E_2 spends an $\mathcal{O}(1)$ amount of z-time, since it gets exponentially close

to γ_ε the second time it reaches the q axis. See Figs. 5(b) and 5(c). Also, since it is exponentially close to $P_{1m}^{-\pi}$ along $U[P_1, P_{1m}^{-\pi}]$, and exponentially close to P_{1m}^{π} along $S[P_{1m}^{\pi}, P_1]$, we expect this two-pulse homoclinic orbit to make its fast excursions exponentially close to the primary homoclinic orbits at the minimum separatrices occuring at $z=-\pi$ and $z=\pi$. See Fig. 6.

Each of the points labelled by A_2^d and A_2^u (the letter A is chosen to refer to asymmetric) corresponds also to a two-pulse homoclinic orbit. These orbits are born when, as ε decreases, the angle formed by the segment of W^u and that of W^s at their intersection at P_2 changes sign, that is, when W^u and W^s are tangent at P_2. See Fig. 5(b). Once born, as $\varepsilon\to 0$, these points get exponentially close to P_1 [see the cases 5(d) and 5(e)]. Thus, their corresponding homoclinic orbits make one excursion at a maximum separatrix and one at a minimum one. A_2^d first makes an excursion exponentially close to the one-pulse homoclinic orbit with a fast excursion at $z=-\pi$, and another one exponentially close to the one-pulse homoclinic that makes a fast excursion at $z=0$. A_2^u makes first an excursion exponentially close to the maximum principal homoclinic orbit (at $z=0$) and then one exponentially close to the minimum one (at $z=\pi$). See Fig. 6.

Remark 5: In principle, the tangency in which A_2^u and A_2^d are born can be detected by computing higher derivatives of $H_2(z_0,\varepsilon)$. When $H_2(z_0^*,\varepsilon^*)=0$, there are three different ways for W^u and W^s to intersect at P_2, as is shown in Fig. 7. Using the interpretation of $H_2(z_0,\varepsilon)$ as a signed distance between W^u and W^s (see Remark 1 in Sec. III), one can distinguish among these three possibilities by looking at the sign of $\partial H_2/\partial z_0$. Thus, the tangency at which A_2^u and A_2^d are born occurs at the value of ε that satisfies

$$H_2(z_0^*,\varepsilon^*)=0, \quad \frac{\partial H_2}{\partial z_0}(z_0^*,\varepsilon^*)=0, \quad \text{and} \quad \frac{\partial^2 H_2}{\partial \varepsilon\, \partial z_0}(z_0^*,\varepsilon^*)<0.$$

However, we cannot compute this ε^*, since our results for approximating H_2 with εh_2 are valid asymptotically as $\varepsilon\to 0$, and for ε sufficiently small it is always the case that $\partial h_2/\partial z_0>0$. For example, from Fig. 5(b), we can see that the value for (5.1) is $\varepsilon^*\approx 0.9$.

We now continue with the description of Fig. 5. As ε decreases, one notices that more and more intersection points appear. In Fig. 5(d), two tertiary intersection points have been born: P_3 and E_3. P_3 corresponds to the three-pulse homoclinic orbit obtained from the zero of $M_{3,A}(z_0,\varepsilon)$. The intersection point E_3 gets exponentially close to P_1 as $\varepsilon\to 0$, which means that its corresponding homoclinic orbit spends $\mathcal{O}(1)$ amount of z-time in between its fast excursions; these excursions occur at $z=-\pi$, $z=0$, and $z=\pi$, each of which is exponentially close to the corresponding one-pulse homoclinic. In Fig. 5(g), A_3^u and A_3^d have appeared. They were born in the tangency of the segments of W^u and W^s at P_3. See case 5(f). We point out that this is the same type of tangency that gave birth to A_2^u and A_2^d. As $\varepsilon\to 0$, A_3^u and A_3^d get exponentially close to P_2, and the corresponding three-pulse homoclinic orbits look like those shown in Fig. 6.

As ε continues to decrease, we see that P_4 and E_4 appear, followed by A_4^u and A_4^d. Then P_5 and E_5 are born, and so on. Figure 8 summarizes the location of some of these intersection points with respect to the q axis.

All the intersection points labeled as P_i correspond to the i-pulse homoclinic orbits that are detected by the zeroes of $M_{i,A}(z_0,\varepsilon)$, as explained at the beginning of this section. As $\varepsilon\to 0$, the homoclinic orbits corresponding to E_i intersection points make fast excursions that are exponentially close to the minimum instantaneous separatrix $z=-\pi$, then to the homoclinic orbit corresponding to P_{i-2}, and finally to the minimum instantaneous separatrix at $z=\pi$. The ones corresponding to the $A_i^{u,d}$ intersection points make an excursion exponentially close to the homoclinic orbit of P_{i-1}, and to one of the minimum instantaneous separatrices (see Fig. 6). All the $A_i^{u,d}$ intersection points are born when W^u and W^s are tangent at P_i. As mentioned in Remark 5, these tangencies can be detected, in principle, via the higher derivatives of H_i.

Although the existence of all the P_i, E_i, and $A_i^{u,d}$ intersection points in the z periodic Hamiltonian case follows automatically from the existence of primary intersection points, a de-

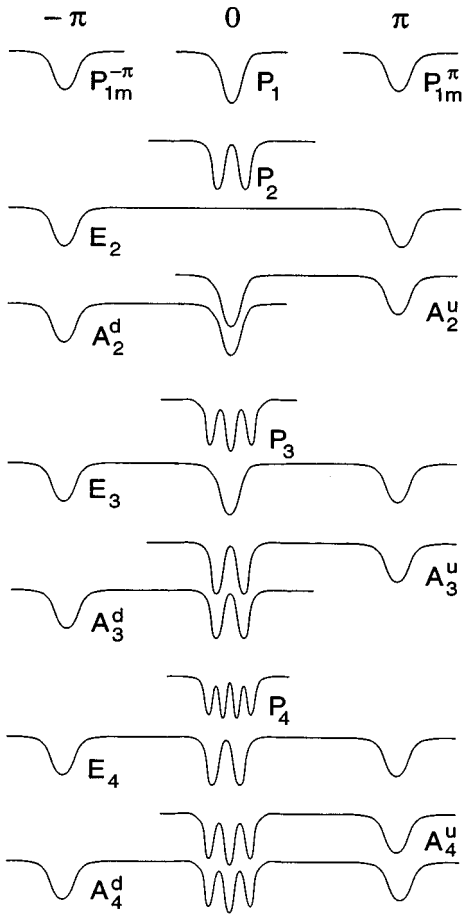

FIG. 6. Diagram of the behavior of the multi-pulse homoclinic orbits corresponding to the different intersection points described in Fig. 5 for ε sufficiently small. Slow time z increases from left to right. The top three curves represent the principal homoclinic orbits, whose existence is established by the zeroes of the one-pulse adiabatic Melnikov function. The curves labelled as P_i for $i \geq 2$ represent homoclinic orbits with i fast excursions close to the maximum instantaneous separatrix. The curves labelled as E_i for $i \geq 2$ correspond to homoclinic orbits that make a fast excursion exponentially close to the principal homoclinic orbit with a fast excursion at $z = -\pi$, then make $i-2$ fast excursions exponentially close to the fast excursions of the homoclinic orbit corresponding to P_{i-2}, and finally they make another fast excursion exponentially close to the fast excursion of the principal homoclinic orbit that makes its fast excursion close to the minimum instantaneous separatrix at $z = \pi$.

tailed characterization of the corresponding homoclinic orbits is given by the above results. As we have shown, Theorem 1 can be used to obtain asymptotics of the homoclinic orbits corresponding to the P_i. Moreover, the existence and local uniqueness of the orbits corresponding to the E_i and $A_i^{u,d}$ intersection points is rigorously shown using the techniques developed in Refs. 10 and 22. This method has the advantage that, in addition to providing a more detailed description of the location in phase space of these multi-pulse homoclinic orbits, it also can be used in the dissipative case, in the nonperiodic Hamiltonian case, and in other higher-dimensional[22] and non-Hamiltonian systems.[26,27] We now briefly describe the use of this method in the case of the two-pulse homoclinic orbit corresponding to E_2 for our example. The main idea is to construct it as the transverse intersection of two invariant manifolds. One of these manifolds, $\mathcal{M}_\varepsilon$, is chosen so that all initial conditions on it leave the neighborhood of γ_ε exponentially close to $W^u(\gamma_\varepsilon)$ in an open interval of z values containing $z = \pi$. Since $\mathcal{M}_\varepsilon$ is exponentially close to $W^u(\gamma_\varepsilon)$ on exit and since

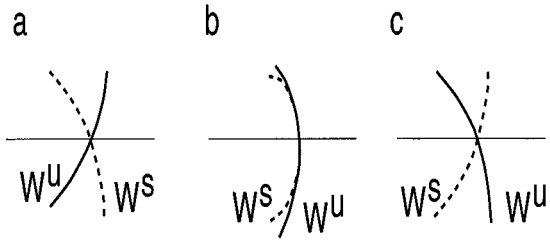

FIG. 7. Intersections of W^u and W^s at P_2. Case (a) corresponds to $\partial H_2/\partial z_0<0$, case (b) to $\partial H_2/\partial z_0=0$, and case (c) to $\partial H_2/\partial z_0>0$.

$W^u(\gamma_\varepsilon)$ and $W^s(\gamma_\varepsilon)$ intersect transversely in the principal homoclinic orbit close to the minimum instantaneous separatrix with a fast excursion at $z=\pi$, then $\mathscr{M}_\varepsilon$ and $W^s(\gamma_\varepsilon)$ will intersect transversely, yielding the orbit corresponding to E_2 for positive z. A similar construction gives the orbit segment for negative z. Note, however that the extra symmetry in the Hamiltonian yields the same result (and also the symmetry of the homoclinic orbit through E_2).

Remark 6: Once it has been established that a system of the form (3.1), whose Hamiltonian is periodic in z, possesses (for ε sufficiently small) an N-pulse homoclinic orbit that corresponds to the P_N intersection point, we can show that there is a periodic orbit close to it. The method of proof is that of Ref. 10, where we construct the periodic orbit as the transverse intersection of two invariant manifolds, say $\mathscr{M}_\varepsilon$ and $\mathscr{N}_\varepsilon$. $\mathscr{M}_\varepsilon$ is obtained by flowing an appropriate set of ''initial conditions'' forward in time, and the other invariant manifold, $\mathscr{N}_\varepsilon$, by flowing a set of ''final conditions'' backward in time. These sets of initial and final conditions are chosen so that when $\mathscr{M}_\varepsilon$ and $\mathscr{N}_\varepsilon$ leave the neighborhood $\mathscr{B}$ of γ_ε, they do so exponentially close to $W^u(\gamma_\varepsilon)$ and $W^s(\gamma_\varepsilon)$, respectively. [This result requires the use of a technical tool, ELESE,[28] that allows the tracking of invariant manifolds while orbits on them spend $\mathscr{O}(1/\varepsilon)$ amounts of time near a slow manifold.] Furthermore, $\mathscr{M}_\varepsilon$ and $\mathscr{N}_\varepsilon$ are $\mathscr{C}^1$-exponentially close to $W^u(\gamma_\varepsilon)$ and $W^s(\gamma_\varepsilon)$ in the regions where $W^u(\gamma_\varepsilon)$ and $W^s(\gamma_\varepsilon)$ intersect transversely in an N-pulse homoclinic orbit. Thus, automatically, our invariant manifolds also intersect transversely, and their intersection is exponentially close to the N-pulse homoclinic orbit during its fast excursions away from γ_ε. Finally, if the sets of initial and final conditions are chosen properly, the resulting orbit is periodic.

Remark 7: The identification of the intersection points of W^u and W^s that we have carried out for the system (5.1) with $\mu=0$ suggests that the periodic orbits obtained in Remark 6 may be related to (and may even be the same as) the periodic orbits that were found via topological shooting in Ref. 7, and via matched asymptotic expansions in Ref. 12. The asymptotics of the periodic orbits obtained in Remark 6 satisfy the properties of the spikes of the periodic orbits in Ref. 7. In Ref. 7 the periodic orbits were labelled as (i,j), for $i=0,1,2,3...$, and $j=0,1$; i denotes the number of fast excursions the orbit makes in the neighborhood of the maximum instantaneous

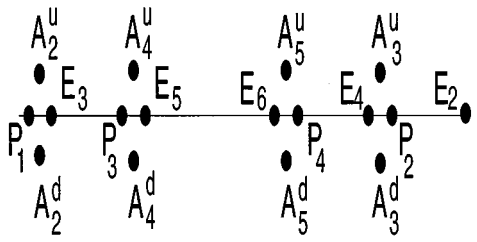

FIG. 8. A schematic representation of the location of the intersection points (up to $i=6$) of W^u and W^s of system (5.1) with $\mu=0$ with respect to the q axis.

separatrix, and j corresponds to either zero or one excursions close to the instantaneous minimum separatrix. Borrowing the same (i,j) labelling, our $(i,0)$ periodic orbits are close to the i-pulse homoclinic orbits whose existence we show via the zero of $M_{i,A}(z_0,\varepsilon)$ and correspond to the intersection point P_i, and the $(i,1)$ periodic orbits are close to the i-pulse homoclinic orbits associated to the A^u_{i-1} intersection point. We point out that, for ε sufficiently small, the homoclinic orbits corresponding to the P_i intersection points which make i fast excursions, occur only close to the maximum instantaneous separatrix, not to the minimum one. This suggests that the periodic orbits found by the method of Remark 6 may not have more than one excursion near the minimum instantaneous separatrix, as is the case for those found in Ref. 7 and 12.

VI. LOCAL ESTIMATES

In this section, we present a local analysis of (3.1) near γ_ε when $0<\varepsilon\ll 1$ and near γ_0 when $\varepsilon=0$. In particular, we study the Fenichel normal forms for both systems. The first one gives the local behavior of Eqs. (3.1) in a neighborhood $\hat{\mathscr{B}}$ of γ_ε. The second one is for Eqs. (3.1) with $\varepsilon=0$ and $z=z_0$ fixed; i.e., for the unperturbed case. Then, using these normal forms, we compute in Lemma 1 the time that $\mathbf{q}^{z_0}_{h_1}$, the unperturbed periodic solution with $z=z_0$ and energy εh_1, spends inside $\hat{\mathscr{B}}$. In Lemma 2, we perform a similar computation for the perturbed trajectory $\mathbf{q}^u(t;z_0,\varepsilon)$ on $W^u(\gamma_\varepsilon)$ that has energy H_1 at time $t=t_1^*$. To homogenize notation, we call this solution $\mathbf{q}^u_{H_1}$.

We begin by deriving the Fenichel normal form for Eqs. (3.1) in a neighborhood $\hat{\mathscr{B}}$ of γ_ε. The instantaneous eigenvalues for the linearization about the saddle $(q_e(z),p_e(z))$ are $\pm S(z)$, where $S(z)\equiv[H^2_{qp}-H_{pp}H_{qq}]^{1/2}(q_e(z),p_e(z),z)$. Hence, using the instantaneous eigenvectors as new coordinate axes, we define the variables

$$\xi\equiv-\left(\frac{1}{2}+\frac{H_{qp}}{2S(z)}\right)x-\frac{H_{pp}}{2S(z)}\,y,$$

$$\eta\equiv-\left(\frac{1}{2}-\frac{H_{qp}}{2S(z)}\right)x+\frac{H_{pp}}{2S(z)}\,y,$$

where all partial derivatives are evaluated at $(q_e(z),p_e(z),z)$. The inverse coordinate change is then given by:

$$x\equiv-\xi-\eta,$$

$$y\equiv-\left(\frac{S(z)-H_{qp}}{H_{pp}}\right)\xi+\left(\frac{S(z)+H_{qp}}{H_{pp}}\right)\eta.$$

In terms of these new coordinates, Eqs. (3.1) can be written as

$$\dot{\xi}=S(z)\xi+\tilde{g}_1(\xi,\eta,z;\varepsilon),\quad \dot{\eta}=-S(z)\eta+\tilde{g}_2(\xi,\eta,z;\varepsilon),\quad \dot{z}=\varepsilon,$$

in the neighborhood of γ_ε, where $\tilde{g}_i$, $i=1,2$, are C^r functions representing terms that are nonlinear in ξ and η, as well as linear terms in ξ and η that are $\mathscr{O}(\varepsilon)$. This form of the equations is almost good enough. We need only one more coordinate change to bring the system into its most useful form.

Fenichel theory[25] (see also Ref. 29) asserts the existence of C^r smooth functions $\varphi^s(\eta,z;\varepsilon)$ and $\varphi^u(\xi,z;\varepsilon)$, for any $r>0$, defined for ξ and η in $\hat{\mathscr{B}}$ such that the sets

$$\{\xi=\varphi^s(\eta,z;\varepsilon)\}\quad\text{and}\quad\{\eta=\varphi^u(\xi,z;\varepsilon)\}$$

are the invariant manifolds $W^s_{\rm loc}(\gamma_\varepsilon)$ and $W^u_{\rm loc}(\gamma_\varepsilon)$, respectively. Moreover, these functions satisfy the properties $\varphi^s(0,z;\varepsilon)=0$, $(\partial\varphi^s/\partial\eta)(0,z;\varepsilon)=0$, $\varphi^u(0,z;\varepsilon)=0$, and $(\partial\varphi^u/\partial\xi)(0,z;\varepsilon)=0$. Hence, defining final variables as

$$a\equiv\xi-\varphi^s(\eta,z;\varepsilon) \quad \text{and} \quad b\equiv\eta-\varphi^u(\xi,z;\varepsilon),$$

the local manifolds are straightened out and given by the sets $\{a=0\}$ and $\{b=0\}$. Therefore, since these sets are invariant, Eqs. (3.1) can be written in the neighborhood of γ_ε as

$$\begin{aligned}\dot a&=S(z)a+g_1(a,b,z;\varepsilon)a,\\ \dot b&=-S(z)b+g_2(a,b,z;\varepsilon)b,\\ \dot z&=\varepsilon.\end{aligned}\tag{6.1}$$

This completes the derivation for the perturbed normal form in $\hat{\mathscr{B}}$. For $\Delta>0$ small, let $\mathscr{B}=\{(a,b,z):|a|\leqslant\Delta,|b|\leqslant\Delta\}$ be a neighborhood of γ_ε for which the normal form (6.1) is valid. From this point on, we replace $\hat{\mathscr{B}}$ with $\mathscr{B}$.

For the system (3.1), with $\varepsilon=0$ and $z=z_0$ we follow the same procedure as above to obtain nice local coordinates. First, we perform a linear coordinate change in the neighborhood of the saddle fixed point, which turns its eigenvectors into the coordinate axes. To avoid confusion with the $\varepsilon>0$ case, these coordinates will have the superscript "o". Thus (2.1) becomes

$$\begin{aligned}\dot\xi^o&=S(z_0)\xi^o+g_1^o(\eta^o,\xi^o;z_0),\\ \dot\eta^o&=S(z_0)\eta^o+g_2^o(\eta^o,\xi^o;z_0).\end{aligned}\tag{6.2}$$

Then we make another change of coordinates that will make the stable and unstable manifolds of the saddle fixed point become the new coordinate axes:

$$\begin{aligned}\dot a^o&=S(z_0)a^o+G_1(a^o,b^o;z_0)a^o,\\ \dot b^o&=-S(z_0)b^o+G_2(a^o,b^o;z_0)b^o.\end{aligned}\tag{6.3}$$

This Fenichel normal form holds inside a neighborhood of the form $\mathscr{B}^o=\{(a^o,b^o,z_0):|a^o|\leqslant\Delta_1,|b^o|\leqslant\Delta_1\}$, where we take Δ_1 such that $\mathscr{B}\subset\mathscr{B}^o$.

In the two following lemmas, we estimate the time for both the perturbed $\mathbf{q}^u_{H_1}$ and unperturbed $\mathbf{q}^{z_0}_{h_1}$ trajectories inside $\mathscr{B}$, where both (6.1) and (6.3) are valid. These results will be used in Sec. VII for the proof of Theorem 1. The reader may skip their proofs on an initial reading.

For clarity of notation, the times for the unperturbed system will also have a superscript "o". We split the time the unperturbed periodic orbit $\mathbf{q}^{z_0}_{h_1}$ spends in $\mathscr{B}$ in two intervals: first, from the entrance to the box at $t^o_{\rm in}$, to the x axis at t^{o*}_1, and second, from the x axis to the exit of $\mathscr{B}$ at $t^o_{\rm out}$. Let $(a^o_{\rm in},b^o_{\rm in})$ be the (a^o,b^o) coordinates at entry at $t^o_{\rm in}$ and (a^{o*},b^{o*}) the coordinates upon reaching the x axis at t^{o*}_1. Given the way the a^o and b^o coordinate axes were set up the trajectory has positive a^o and b^o coordinates throughout the flight inside $\mathscr{B}$ (see Fig. 9). By choice of construction, $b^o_{\rm in}=\Delta+\mathscr{O}(\varepsilon)$ and $a^o_{\rm out}=\Delta+\mathscr{O}(\varepsilon)$. We now introduce similar notation for the perturbed trajectory $\mathbf{q}^u_{H_1}$. Let $t_{\rm in}$ and $t_{\rm out}$ be the entry and exit times of $\mathbf{q}^u_{H_1}$ to and from the box $\mathscr{B}$, so that $b(t_{\rm in})=\Delta$ and $a(t_{\rm out})=\Delta$. Here t^*_1 is the time at which this trajectory reaches the x axis, with local coordinates (a^*,b^*). The time of flight of $\mathbf{q}^u_{H_1}$ in $\mathscr{B}$ will be also divided in two intervals, the first one being $t^*_1-t_{\rm in}$ and the second one $t_{\rm out}-t^*_1$.

Lemma 1: The amount of (fast) time $t^o_{\rm out}-t^o_{\rm in}$ the periodic orbit $\mathbf{q}^{z_0}_{h_1}$ spends in the box $\mathscr{B}$ is

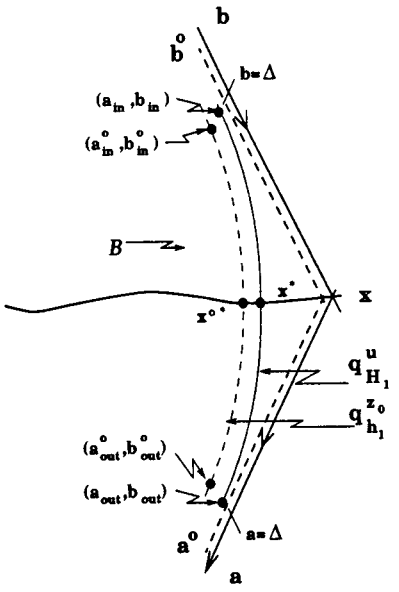

FIG. 9. Schematic representation of the perturbed $\mathbf{q}^{u}_{H_1}$ and unperturbed $\mathbf{q}^{z_0}_{h_1}$ trajectories inside the box $\mathscr{B}$.

$$\frac{-1}{S(z_0)}\left[\ln\left(\frac{1}{2V(z_0)}\sqrt{\frac{|\varepsilon h_1|}{a_3(z_0)}}\right)+\ln\left(\frac{1}{2U(z_0)}\sqrt{\frac{|\varepsilon h_1|}{a_3(z_0)}}\right)\right]+\frac{2}{S(z_0)}\ln\Delta+\mathscr{O}(\Delta,\varepsilon^{1/3}),$$

where

$$V(z_0)\equiv\frac{S(z_0)}{S(z_0)-H_{qp}(q_e(z_0),p_e(z_0))}\quad\text{and}\quad U(z_0)\equiv\frac{S(z_0)}{S(z_0)+H_{qp}(q_e(z_0),p_e(z_0))}.$$

Proof: We will use the second equation of (6.3) to estimate the first part of the flight $t_1^{o*}-t_{\text{in}}^{o}$ since we have control of the b^o coordinate on entry. The first equation in (6.3) will be used for the second interval $t_{\text{out}}^{o}-t_1^{o*}$.

The time $t_1^{o*}-t_{\text{in}}^{o}$ for the orbit $\mathbf{q}^{z_0}_{h_1}$ to travel from $(a^o_{\text{in}},b^o_{\text{in}})$ to (a^{o*},b^{o*}) is

$$\int_{t_{\text{in}}^{o}}^{t_1^{o*}}dt=\int_{b_{\text{in}}^{o}}^{b^{o*}}\frac{db^o}{-S(z_0)b^o+G_2(a^o,b^o;z_0)b^o}. \tag{6.4}$$

The singular part of the integrand is $-1/S(z_0)b^o$, so we add it and subtract it in the integrand above, to obtain

$$t_1^{o*}-t_{\text{in}}^{o}=\int_{b_{\text{in}}^{o}}^{b^{o*}}\frac{db^o}{-S(z_0)b^o}+\int_{b_{\text{in}}^{o}}^{b^{o*}}\frac{\overline{G_2}db^o}{-S(z_0)b^o(1-\overline{G_2})}, \tag{6.5}$$

where $\overline{G_2}\equiv G_2(a^o,b^o;z_0)/S(z_0)=k_1(z_0)a^o+k_2(z_0)b^o+k_3(z_0)a^{o2}+k_4(z_0)a^ob^o+k_5(z_0)b^{o2}+\mathscr{O}(a^{o3},a^{o2},\underline{b^o},a^ob^{o2},b^{o3})$. By directly computing the first integral in (6.5), and by using the expansion of G_2 together with the binomial expansion of $1/(1-G_2)$ in the second integral, (6.5) implies to leading order:

$$t_1^{o*}-t_{\rm in}^o=\frac{-1}{S(z_0)}\ln b^{o*}+\frac{1}{S(z_0)}\ln b_{\rm in}^o+\frac{-1}{S(z_0)}I^o, \tag{6.6}$$

where $I^o\equiv k_1(z_0)\,I_1^o+k_2(z_0)\,I_2^o+(k_1^2(z_0)+k_3(z_0))\,I_3^o+(2k_1(z_0)\,k_2(z_0)+k_4(z_0))\,I_4^o+(k_2^2(z_0)+k_5(z_0))I_5^o$. Here $I_1^o\equiv\int_{b_{\rm in}^o}^{b^{o*}}(a^o/b^o)db^o$, $I_2^o\equiv\int_{b_{\rm in}^o}^{b^{o*}}db^o$, $I_3^o\equiv\int_{b_{\rm in}^o}^{b^{o*}}a^{o2}/b^o db^o$, $I_4^o\equiv\int_{b_{\rm in}^o}^{b^{o*}}a^o db^o$ and $I_5^o\equiv\int_{b_{\rm in}^o}^{b^{o*}}b^o db^o$. In (6.6), higher-order terms involving integrands of $\mathcal{O}(3)$ have been neglected.

Now we relate b^{o*} to $x^{o*}\equiv x(t_1^{o*})$, the x-coordinate of $\mathbf{q}_{h_1}^{z_0}$ when it reaches the x axis. From the changes of coordinates that led us to (6.2), and since $y(t_1^{o*})=0$, we have $\xi^{o*}=-x^{o*}/2U(z_0)$, $\eta^{o*}=-x^{o*}/2V(z_0)$. The latter expressions give, to leading order, $a^{o*}=-x^{o*}/2U(z_0)$ and $b^{o*}=-x^{o*}/2V(z_0)$. Next, we relate x^{o*} to the ''energy'' εh_1 that the orbit has at time t_1^{o*}, using an expansion of the frozen Hamiltonian and recalling that $y(t_1^{o*})=0$, we obtain $H_1=-a_3(z_0)(x^{o*})^2+\mathcal{O}(3)$, where $a_3(z_0)>0$. Thus, $x^{o*}=-\sqrt{|\varepsilon h_1|/a_3(z_0)}(1+\mathcal{O}(\sqrt{\varepsilon}))$, which yields

$$\begin{aligned} a^{o*}&=\frac{1}{2U(z_0)}\sqrt{\frac{|\varepsilon h_1|}{a_3(z_0)}}\,(1+\mathcal{O}(\sqrt{\varepsilon})),\\ b^{o*}&=\frac{1}{2V(z_0)}\sqrt{\frac{|\varepsilon h_1|}{a_3(z_0)}}\,(1+\mathcal{O}(\sqrt{\varepsilon})). \end{aligned} \tag{6.7}$$

Replacing b^{o*} in the first logarithmic term of (6.6) with (6.7), and $b_{\rm in}^o$ with $\Delta+\mathcal{O}(\varepsilon)$ in the second logarithmic term, (6.6) becomes

$$t_1^{o*}-t_{\rm in}^o=\frac{-1}{S(z_0)}\ln\left(\frac{1}{2V(z_0)}\sqrt{\frac{|\varepsilon h_1|}{a_3(z_0)}}\right)+\frac{1}{S(z_0)}\ln\Delta-\frac{1}{S(z_0)}I^o+\mathcal{O}(\sqrt{\varepsilon}). \tag{6.8}$$

Thus, we have almost obtained the desired result for the first part of the trajectory. It remains to be shown that I^o is $\mathcal{O}(\Delta,\varepsilon^{1/3})$. We now estimate I_i^o for $i=1,2,...,5$.

I_2^o and I_5^o can be directly integrated: $I_2^o=b^{o*}-b_{\rm in}^o$, $I_5=\frac{1}{2}(b^{o*2}-b_{\rm in}^{o2})$. Next, since a^o is at most $\mathcal{O}(a^{o*})$ and b^o is at least $\mathcal{O}(b^{o*})$, I_3^o and I_4^o can be immediately estimated: $I_3^o=\mathcal{O}(a^{o*}|b^{o*}-b_{\rm in}^o|)$, and $I_4^o=\mathcal{O}(a^{o*}|b^{o*}-b_{\rm in}^o|)$. And, since $b_{\rm in}^o=\Delta+\mathcal{O}(\varepsilon)$, $b^{o*}=\mathcal{O}(\sqrt{\varepsilon})$, and $a^{o*}=\mathcal{O}(\sqrt{\varepsilon})$, we obtain

$$I_2^o=\mathcal{O}(\Delta,\sqrt{\varepsilon}),\quad I_3^o=\mathcal{O}(\sqrt{\varepsilon}),\quad I_4^o=\mathcal{O}(\sqrt{\varepsilon}),\quad \text{and } I_5^o=\mathcal{O}(\Delta^2,\sqrt{\varepsilon}). \tag{6.9}$$

To estimate I_1^o, we divide the interval of integration in two parts. The first part, from $b_{\rm in}^o$ to some $b_{\rm int}^o$ (an intermediate value of b^o to be specified later), and the second part from $b_{\rm int}^o$ to b^{o*}. Thus

$$I_1^o=\int_{b_{\rm in}^o}^{b_{\rm int}^o}\frac{a^o}{b^o}\,db^o+\int_{b_{\rm int}^o}^{b^{o*}}\frac{a^o}{b^o}\,db^o.$$

In the first integral, we take $a^o=\mathcal{O}(\sqrt{\varepsilon})$, and in the second one we use that a^o/b^o is at most a^{o*}/b^{o*}, which is $\mathcal{O}(1)$. Thus

$$I_1^o=\mathcal{O}(\sqrt{\varepsilon}|\ln b_{\rm int}^o-\ln b_{\rm in}^o|)+\mathcal{O}(|b^{o*}-b_{\rm int}^o|).$$

So, choosing $b_{\rm int}^o=\mathcal{O}(\varepsilon^\alpha)$ for $0<\alpha<\frac{1}{2}$ the last term of the above expression is $O(\varepsilon^\alpha)$. Without loss of generality, we let $\alpha=\frac{1}{3}$. Hence

$$I_1^o = \mathcal{O}(\sqrt{\varepsilon}\ \ln\ \varepsilon^{-1}, \varepsilon^{1/3}).$$

Combined with (6.9) this last estimate allows us to write

$$t_1^{o*} - t_{\text{in}}^o = \frac{-1}{S(z_0)} \ln\left(\frac{1}{2V(z_0)} \sqrt{\frac{|\varepsilon h_1|}{a_3(z_0)}} \right) + \frac{1}{S(z_0)} \ln\ \Delta + \mathcal{O}(\Delta, \varepsilon^{1/3}). \tag{6.10}$$

Thus, the desired difference is obtained for the first part of the flight inside $\mathcal{B}$. To estimate the time it takes for the second part of the flight inside, we start with the first equation of (6.3) and get

$$\int_{t_1^{o*}}^{t_{\text{out}}^o} dt = \int_{a^{o*}}^{a_{\text{out}}^o} \frac{da^o}{S(z_0)a^o + G_1(a^o, b^o; z_0)a^o}.$$

Then, we perform similar computations as above to obtain

$$t_{\text{out}}^o - t_1^{o*} = \frac{-1}{S(z_0)} \ln\left(\frac{1}{2U(z_0)} \sqrt{\frac{|\varepsilon h_1|}{a_3(z_0)}} \right) + \frac{1}{S(z_0)} \ln\ \Delta + \mathcal{O}(\Delta, \varepsilon^{1/3}). \tag{6.11}$$

Hence after adding (6.10) and (6.11), we arrive at the result claimed in Lemma 1.

Lemma 2: The (fast) time it takes for the solution $\mathbf{q}_{H_1}^u$ *on the unstable manifold to travel inside* $\mathcal{B}$ *is given by*

$$\frac{-1}{S(z_0)} \left[\ln\left(\frac{1}{2V(z_0)} \sqrt{\frac{|H_1|}{a_3(z_0)}} \right) + \ln\left(\frac{1}{2U(z_0)} \sqrt{\frac{|H_1|}{a_3(z_0)}} \right) \right] + \frac{2}{S(z_0)} \ln\ \Delta + \mathcal{O}(\Delta, |H_1|^{1/3}). \tag{6.12}$$

Remark 8: It will be seen in Sec. VII that $|H_1| = \mathcal{O}(\varepsilon)$, thus $\mathcal{O}(\Delta)$ is the dominant error. Also, we do not explicitly write out higher-order terms that are bounded by $\mathcal{O}(\sqrt{\varepsilon}\ \ln|H_1|^{-1})$.

Proof: Although the estimates are slightly more involved than for the unperturbed case, the calculation proceeds in the same fashion. Assume ε is small enough so that $\mathbf{q}_{H_1}^u(t_1^*)$ is in $\mathcal{B}$. Using Fenichel theory, we can explicitly state what the relationships between the nonlinear terms in the perturbed and unperturbed normal forms (6.1) and (6.3) are. We know that γ_ε and γ_0 are $\mathcal{C}^r$ $\mathcal{O}(\varepsilon)$ close. Also, $W_{\text{loc}}^s(\gamma_\varepsilon)$ and $W_{\text{loc}}^s(\gamma_0)$ are $\mathcal{C}^r$ $\mathcal{O}(\varepsilon)$ close, and so are $W_{\text{loc}}^u(\gamma_\varepsilon)$ and $W_{\text{loc}}^u(\gamma_0)$. Furthermore, the functions whose graphs are the perturbed stable and unstable manifolds are r times differentiable in z. See Ref. 25, or the exposition in Ref. 29. Taking these facts into consideration, one can see that for $i = 1,2$,

$$g_i(a,b,z;\varepsilon) = G_i(a,b;z_0) + \frac{\partial g_i}{\partial z}(a,b,z_0;0)(z - z_0) + \mathcal{O}(\varepsilon, (z-z_0)^2). \tag{6.13}$$

We now start by expanding $S(z)$ about z_0 and using (6.13) in the second equation of (6.1):

$$\dot{b} = -S(z_0)b + [G_2(a,b;z_0) + \mu(a,b;z_0)(z - z_0) + \mathcal{O}(\varepsilon, (z-z_0)^2)]b, \tag{6.14}$$

where $\mu(a,b;z_0) \equiv -S_z(z_0)/2S(z_0) + (\partial g_2/\partial z)(a,b,z_0;0)$. Then, we recall that $b^* \equiv b(t_1^*)$, so

$$\int_{t_{\text{in}}}^{t_1^*} dt = \int_{\Delta}^{b^*} \frac{db}{-S(z_0)b + [G_2 + \mu(z - z_0) + \mathcal{O}(\varepsilon, (z-z_0)^2)]b},$$

where G_2 and μ denote $G_2(a,b;z_0)$ and $\mu(a,b;z_0)$, respectively. We now add and subtract the singular part in the integrand to obtain

$$t_1^* - t_{\rm in} = \int_\Delta^{b^*} \frac{-db}{S(z_0)b} + \int_\Delta^{b^*} \frac{F db}{-S(z_0)b(1-F)}, \tag{6.15}$$

where $F \equiv \overline{G_2} + \overline{\mu}(z-z_0) + \mathcal{O}(\varepsilon,(z-z_0)^2)$, $\overline{G_2} \equiv G_2/S(z_0)$, and $\overline{\mu} \equiv \mu/S(z_0)$. Direct evaluation of the first integral gives

$$\int_\Delta^{b^*} \frac{-db}{S(z_0)b} = \frac{-1}{S(z_0)} \ln b^* + \frac{1}{S(z_0)} \ln \Delta.$$

To write b^* in terms of the energy of $\mathbf{q}^u_{H_1}$, we first write it in terms of its x coordinate x^* and then write this x^* in terms of H_1. Going back to the coordinate transformations described before Lemma 1, and recalling that $y^u(t_1^*) = 0$, we have

$$\xi^* = \frac{-1}{2U(z)} x^* \quad \text{and} \quad \eta^* = \frac{-1}{2V(z)} x^*.$$

In addition, using the properties of φ^s and φ^u, we know that

$$a^* \equiv a(t_1^*) = \xi^* + \mathcal{O}(\eta^{*2}) \quad \text{and} \quad b^* \equiv b(t_1^*) = \eta^* + \mathcal{O}(\xi^{*2}).$$

Hence, to leading order

$$x^* = -2V(z)b^* \quad \text{or} \quad x^* = -2U(z)a^*. \tag{6.16}$$

We then use the Taylor expansions of $V(z)$ and $U(z)$ around z_0,

$$\begin{aligned} V(z) &= V(z_0) + \varepsilon V'(z_0)(t_1^* - t_0) + \mathcal{O}(\varepsilon^2) \\ &= V(z_0) + \varepsilon V'(z_0)(t_1^* - t_{\rm in}) + \varepsilon V'(z_0)(t_{\rm in} - t_0) + \mathcal{O}(\varepsilon^2) = V(z_0)[1 + \mathcal{O}(\varepsilon(t_1^* - t_{\rm in}))], \end{aligned}$$

$$U(z) = U(z_0)[1 + \mathcal{O}(\varepsilon(t_1^* - t_{\rm in}))],$$

and substitute this in (6.16) to get

$$a^* = \frac{-x^*}{2U(z_0)} (1 + \mathcal{O}(\varepsilon(t_1^* - t_{\rm in}))) \quad \text{and} \quad b^* = \frac{-x^*}{2V(z_0)} (1 + \mathcal{O}(\varepsilon(t_1^* - t_{\rm in}))). \tag{6.17}$$

Now we proceed to estimate x^* in terms of the energy H_1 of the orbit we are studying when $x^u(t_1^*) = x^*$. By definition, we have $H_1 = H(x^*, 0, z_0 + \varepsilon r_1^*)$, where $t_1^* = z_0/\varepsilon + r_1^*$. In a neighborhood of γ_ε,

$$H_1 = -a_3(z)x^{*2} + a_4(z)x^{*3} + \mathcal{O}(4). \tag{6.18}$$

Solving (6.18) for x^* yields

$$x^* = -|H_1|^{1/2} \left[\frac{1}{\sqrt{a_3(z_0)}} - \frac{1}{2} \frac{a_3'(z_0)}{a_3^{3/2}(z_0)} \varepsilon r_1^* + \mathcal{O}(\varepsilon^2) \right] \left(1 + \frac{1}{2} \frac{a_4(z)}{a_3(z)} x^* + \mathcal{O}((x^*)^2) \right).$$

Hence,

$$x^* = \frac{-|H_1|^{1/2}}{\sqrt{a_3(z_0)}} [1 + \mathcal{O}(\varepsilon(t_1^* - t_{\rm in}), |H_1|^{1/2})]. \tag{6.19}$$

Using (6.17) and (6.19) in the integral for the singular part, we get

$$\int_{\Delta}^{b^*} \frac{-db}{S(z_0)b} = \frac{-1}{S(z_0)} \ln\left(\frac{1}{2V(z_0)} \sqrt{\frac{|H_1|}{a_3(z_0)}} \right) + \frac{1}{S(z_0)} \ln \Delta + \mathcal{O}(\varepsilon(t_1^* - t_{\text{in}}), \sqrt{|H_1|}). \quad (6.20)$$

Next, we estimate the second integral in (6.15). First, we decompose it:

$$\int_{\Delta}^{b^*} \frac{F db}{-S(z_0)b(1-F)} = \frac{-1}{S(z_0)} (I_g + I_\mu).$$

Here,

$$\begin{aligned} I_g \equiv & k_1(z_0)I_1 + k_2(z_0)I_2 + (k_1^2(z_0) + k_3(z_0))I_3 \\ & + (2k_1(z_0)k_2(z_0) + k_4(z_0))I_4 + (k_2^2(z_0) + k_3(z_0))I_5, \end{aligned}$$

where

$$I_1 \equiv \int_{\Delta}^{b^*} \frac{a}{b}\, db, \quad I_2 \equiv \int_{\Delta}^{b^*} db, \quad I_3 \equiv \int_{\Delta}^{b^*} \frac{a^2}{b}\, db, \quad I_4 \equiv \int_{\Delta}^{b^*} a\, db, \quad I_5 \equiv \int_{\Delta}^{b^*} b\, db,$$

and

$$\begin{aligned} I_\mu \equiv \int_{\Delta}^{b^*} \frac{1}{b} [& \overline{\mu}(z - z_0) + 2(k_1(z_0)a + k_2(z_0)b)\overline{\mu}(z - z_0) \\ & + \mathcal{O}((z - z_0)^2, a^2(z - z_0), ab(z - z_0), b^2(z - z_0), a(z - z_0)^2, b(z - z_0)^2, \varepsilon)] db. \end{aligned}$$

We note here that the integrands of I_i have the same form as those of I_i^o for $i = 1,...,5$.

We can directly integrate I_2 and I_5:

$$I_2 = b^* - \Delta, \quad I_5 = \tfrac{1}{2}(b^{*2} - \Delta^2).$$

Since a is at most $\mathcal{O}(a^*)$ and b is at least $\mathcal{O}(b^*)$, we get $I_3 = \mathcal{O}(a^*|b^* - \Delta|)$ and $I_4 = \mathcal{O}(a^*|b^* - \Delta|)$. Now, using (6.19) in (6.17), we obtain

$$\begin{aligned} a^* &= \mathcal{O}(\sqrt{|H_1|}, \sqrt{|H_1|}\varepsilon(t_1^* - t_{\text{in}})), \\ b^* &= \mathcal{O}(\sqrt{|H_1|}, \sqrt{|H_1|}\varepsilon(t_1^* - t_{\text{in}})), \end{aligned} \quad (6.21)$$

which yields

$$I_2 = \mathcal{O}(\Delta), \quad I_3 = \mathcal{O}(\sqrt{|H_1|}), \quad I_4 = \mathcal{O}(\sqrt{|H_1|}), \quad \text{and } I_5 = \mathcal{O}(\Delta^2).$$

To estimate I_1, we break the interval of integration in two:

$$I_1 = \int_{\Delta}^{b_{\text{int}}} \frac{a}{b}\, db + \int_{b_{\text{int}}}^{b^*} \frac{a}{b}\, db$$

where $b_{\text{int}} = \mathcal{O}(|H_1|^{1/3})$. This is similar to what we did for estimating I_1 in the unperturbed case and yields $I_1 = \mathcal{O}(\sqrt{|H_1|}\, \ln|H_1|^{-1}, |H_1|^{1/3})$ and hence

$$I_g = \mathcal{O}(\Delta, |H_1|^{1/3}).$$

Next, we estimate I_μ:

$$I_\mu \sim M\varepsilon(t_1^*-t_{\text{in}})|\ln b^*-\ln\Delta|+2M\varepsilon(t_1^*-t_{\text{in}})(k_2(z_0)|b^*-\Delta|+k_1(z_0)|H_1|^{1/3}), \quad (6.22)$$

where $M=\max\mu$, and since $b^*=\mathcal{O}(\sqrt{|H_1|})$,

$$I_\mu=\mathcal{O}(\varepsilon\ \ln|H_1|^{-1}(t_1^*-t_{\text{in}})).$$

Putting the estimates for I_g and I_μ together we arrive at the estimate for the first part of the flight inside $\mathcal{B}$.

$$t_1^*-t_{\text{in}}=\frac{-1}{S(z_0)}\ln\left(\frac{1}{2V(z_0)}\sqrt{\frac{|H_1|}{a_3(z_0)}}\right)+\frac{1}{S(z_0)}\ln\Delta+\mathcal{O}(\Delta,|H_1|^{1/3}). \quad (6.23)$$

Similarly, using the second equation of (6.3) and the fact that $a_{\text{out}}=a_{\text{out}}^o+\mathcal{O}(\varepsilon)$, the second part of the flight in $\mathcal{B}$ is

$$t_{\text{out}}-t_1^*=\frac{-1}{S(z_0)}\ln\left(\frac{1}{2U(z_0)}\sqrt{\frac{|H_1|}{a_3(z_0)}}\right)+\frac{1}{S(z_0)}\ln\Delta+\mathcal{O}(\Delta,|H_1|^{1/3}). \quad (6.24)$$

Finally adding (6.23) and (6.24), Lemma 2 is proved.

Remark 9: The technicality of splitting the trajectory at some intermediate b value was also used in adiabatic separatrix crossing theories (see Ref. 5, for example). It reflects the singular perturbation nature of the problem, with the trajectory from b_{in} to b_{int} being part of the inner solution extended into the overlap domain, and the trajectory from b_{int} to b^* being part of the outer solution similarly extended.

VII. PROOF OF THEOREM 1

We will divide the proof of Theorem 1 in five steps. The first step consists of showing $R_u(z_0,t_1^*)=\mathcal{O}(\varepsilon^2)$ as $\varepsilon\to 0$ for type I systems, and $R_u(z_0,t_1^*)=\mathcal{O}(\varepsilon^2\ln(1/\varepsilon))$ as $\varepsilon\to 0$ for type II systems. Thus, the value H_1 of the function H that the solution $\mathbf{q}^u(t;z_0,\varepsilon)$ has upon reaching the x axis at $t=t_1^*$ is $\varepsilon h_1(z_0)$ to leading order. We remark that this same proof shows that the remainders (3.7) involved in the N-pulse homoclinic orbits are also $\mathcal{O}(\varepsilon^2)$ for type I systems, while for type II systems they are $\mathcal{O}(\varepsilon^2\ln 1/\varepsilon)$. In step 2, we show that $z_1-z_0\sim\varepsilon P(\varepsilon h_1(z_0))$ as $\varepsilon\to 0$. Next, in step 3, we show that H_2 is given to leading order by $\varepsilon h_2(z_0,\varepsilon)=\varepsilon M_{2,A}(z_0,\varepsilon)$. Then, we show in step 4 that simple zeroes of h_2 [i.e., of the secondary Melnikov function $M_{2,A}(z_0,\varepsilon)$] correspond to simple zeroes of H_2. Thus step 4 shows how to obtain the existence of double pulse homoclinic orbits. Finally, we extend the double pulse result to a criterion for the existence of N-pulse homoclinic orbits involving the Nth-order Melnikov function $M_{N,A}(z_0,\varepsilon)$ in step 5. All the estimates in steps 3 through 5 have been carried out for type II systems, since their remainder terms are larger than those for type I systems. The estimates for type I systems are identical, with the estimates of the remainders improved as in Step 1.

A. Step 1

In this subsection we show that for systems of type I, $R_s(z_0,t_1^*)=\mathcal{O}(\varepsilon^2,\varepsilon|H_1|^{3/2}\ \ln|H_1|)$ and for type II systems, $R_s(z_0,t_1^*)=\mathcal{O}(|H_1|\varepsilon\ \ln 1/\varepsilon,\varepsilon^2)$ where we also obtain $H_1=\theta(\varepsilon)$ so the remainders are as claimed above. We start by recalling

$$-\varepsilon\int_{t_1^*}^{\infty}\frac{\partial H}{\partial z}(\mathbf{q}_0^{z_0}(t))dt=-\int_{t_1^*}^{\infty}\frac{dH}{dt}(\mathbf{q}_0^{z_0}(t))dt=H(\mathbf{q}_0^{z_0}(t_1^*),z_1^*),$$

where $z_1^*=\varepsilon t_1^*$. We expand this last expression in the z variable about z_0:

$$H(x_0^{z_0}(t_1^*),y_0^{z_0}(t_1^*),z_1^*)=\frac{\partial H}{\partial z}\,(x_0^{z_0}(t_1^*),y_0^{z_0}(t_1^*),z_0)(z_0-z_1^*)+\mathcal{O}((z_0-z_1^*)^2). \tag{7.1}$$

Here we have used $H(x_0^{z_0},y_0^{z_0},z_0)=0$, since we are evaluating H on an instantaneous separatrix. We first estimate $\mathbf{q}_0^{z_0}(t_1^*)\equiv(x_0^{z_0}(t_1^*),y_0^{z_0}(t_1^*),z_0)$, and then evaluate the partial derivative of H using $\partial H/\partial z=\mathcal{O}(x^2,xy,y^2)$ in the neighborhood of γ_ε. Moreover, $z_0-z_1^*=\mathcal{O}(\varepsilon\,\ln|H_1|)$ by (6.23) in Lemma 2. Putting these estimates together yields the desired result.

The linear approximation of the x coordinate of the instantaneous separatrix $\mathbf{q}_0^{z_0}$ is $x_0^{z_0}(t)\sim Ce^{-S(z_0)(t-t_{\rm in})}$, for large t. Hence, for $t=t_1^*$,

$$x_0^{z_0}(t_1^*)\sim Ce^{-S(z_0)(t_1^*-t_{\rm in})}.$$

Replacing $t_1^*-t_{\rm in}$ by the right-hand side of (6.23), we obtain

$$x_0^{z_0}(t_1^*)\sim C\left(\frac{1}{2V(z_0)\Delta}\,\sqrt{\frac{|H_1|}{a_3(z_0)}}\right)\exp(\mathcal{O}(\Delta,|H_1|^{1/3},\varepsilon(\ln|H_1|^{-1})^2,\sqrt{|H_1|}\,\ln|H_1|^{-1})),$$

which upon expansion yields

$$x_0^{z_0}(t_1^*)\sim C(1+\mathcal{O}(\Delta))\left(\frac{1}{2V(z_0)\Delta}\,\sqrt{\frac{|H_1|}{a_3(z_0)}}\right)+\mathcal{O}(|H_1|^{5/6}).$$

Similarly, we obtain $y_0^{z_0}(t_1^*)=\mathcal{O}(\sqrt{|H_1|})$. Putting these estimates of $x_0^{z_0}(t_1^*)$ and $y_0^{z_0}(t_1^*)$ into the expansion for $\partial H/\partial z$ yields $\partial H/\partial z(x_0^{z_0}(t_1^*),y_0^{z_0}(t_1^*),z_0)=\mathcal{O}(|H_1|)$ for type II systems. Thus, (7.1) becomes

$$H(\mathbf{q}_0^{z_0}(t_1^*),z_1^*)=\mathcal{O}(\varepsilon|H_1|\ln|H_1|).$$

For type I systems we can improve the estimate of the remainder. Since the z_0 we are interested in are $\mathcal{O}(\varepsilon\,\ln|H_1|)$ to the zero of $M_A(z)$, by (3.4) we have that $\alpha(z_0)=\mathcal{O}(\varepsilon\,\ln|H_1|)$, which together with the Taylor expansion of H in (x,y) about $(x,y)=(0,0)$ yields $(\partial H/\partial z)(x_0^{z_0}(t_1^*),\,y_0^{z_0}(t_1^*),z_0)=\mathcal{O}(|H_1|\varepsilon\,\ln|H_1|)$. Therefore (7.1) becomes of $\mathcal{O}(\varepsilon^2,\varepsilon^2|H_1|\ln^2|H_1|)$ and we have the desired result.

In conclusion, we now have

$$H_1=\varepsilon h_1+\mathcal{O}(\varepsilon^2),$$

$$H_1=\varepsilon h_1+\mathcal{O}\left(\varepsilon^2\,\ln\frac{1}{\varepsilon}\right) \tag{7.2}$$

for type I and type II systems, respectively.

B. Step 2

In this second step, we compare the (slow) time, z_1-z_0, that $\mathbf{q}_{H_1}^{\mu}$ spends in the oscillating regime with the period (in slow time), $\varepsilon P(\varepsilon h_1)$, of $\mathbf{q}_{h_1}^{z_0}$. The difference will be shown to be $\mathcal{O}(\varepsilon^{4/3})$. The proof holds for both type I and type II systems.

To accomplish this, we recall Lemmas 1 and 2 in which the time each of these trajectories spends inside $\mathcal{B}$ is computed. The difference in these slow times is calculated as $\mathcal{O}(\varepsilon^{4/3})$ in Corollary 2. Then, we show that the difference in the slow times of flight of these two trajectories outside of $\mathcal{B}$ is $\mathcal{O}(\varepsilon^{3/2})$. Hence, the total difference is $\mathcal{O}(\varepsilon^{4/3})$.

Corollary 2: Inside the box $\mathscr{B}$, the (fast) times of passage of $\mathbf{q}_{h_1}^{z_0}$ and $\mathbf{q}_{H_1}^{u}$ differ by $\mathscr{O}(|\varepsilon h_1|^{1/3})$, so that the slow times differ by $\mathscr{O}(\varepsilon^{4/3})$.

Proof: We rewrite (6.23), the first part of the time of flight of $\mathbf{q}_{H_1}^{u}$ inside $\mathscr{B}$, using (7.2):

$$t_1^* - t_{\text{in}} = -\frac{1}{S(z_0)} \ln\left(\frac{1}{2V(z_0)} \sqrt{\frac{|\varepsilon h_1|}{a_3(z_0)}} \right) + \frac{1}{S(z_0)} \ln \Delta - \frac{1}{S(z_0)} (I_g + I_\mu) + \mathscr{O}(\sqrt{\varepsilon}), \quad (7.3)$$

where, recall, $I_g = k_2(z_0) I_2 + (k_2^2(z_0) + k_5(z_0)) I_5 + \mathscr{O}(|\varepsilon h_1|^{1/3})$, $I_2 = b^* - \Delta$, $I_5 = \frac{1}{2}(b^{*2} - \Delta^2)$, and $I_\mu = \mathscr{O}(\varepsilon(\ln|\varepsilon h_1|^{-1})^2)$.

We compare this expression with (6.8), which corresponds to the time that the unperturbed periodic orbit $\mathbf{q}_{h_1}^{z_0}$ takes in its first part of the flight inside $\mathscr{B}$:

$$t_1^{o*} - t_{\text{in}}^{o} = -\frac{1}{S(z_0)} \ln\left(\frac{1}{2V(z_0)} \sqrt{\frac{|\varepsilon h_1|}{a_3(z_0)}} \right) + \frac{1}{S(z_0)} \ln \Delta - \frac{1}{S(z_0)} I^o + \mathscr{O}(\sqrt{\varepsilon})$$

where $I^o = k_2(z_0) I_2^o + (k_2^2(z_0) + k_5(z_0)) I_5^o + \mathscr{O}(\varepsilon^{1/3})$, $I_2^o = (b^{o*} - b_{\text{in}}^o)$ and $I_5^o = \frac{1}{2}(b^{o*2} - b_{\text{in}}^{o2})$. Thus, substituting $b_{\text{in}}^o = \Delta + \mathscr{O}(\sqrt{\varepsilon})$ and $b^{o*} = b^*(1 + \mathscr{O}(\sqrt{\varepsilon}))$ in I_2^o and I_5^o, we get

$$I_2 = I_2^o + \mathscr{O}(\sqrt{\varepsilon}) \quad \text{and} \quad I_5 = I_5^o + \mathscr{O}(\sqrt{\varepsilon}).$$

Hence, we can now compare the two time intervals:

$$t_1^* - t_{\text{in}} = t_1^{o*} - t_{\text{in}}^o + \mathscr{O}(\varepsilon^{1/3}).$$

A similar result is obtained when we compare the second half of the flights inside $\mathscr{B}$. This completes the proof of the corollary.

We now complete Step 2. By choice of construction, we know that the trajectories we are tracking satisfy $b_{\text{in}}^o = b_{\text{in}} + \mathscr{O}(\varepsilon) = \Delta + \mathscr{O}(\varepsilon)$ on entry to $\mathscr{B}$, and $a_{\text{out}}^o = a_{\text{out}} + \mathscr{O}(\varepsilon) = \Delta + \mathscr{O}(\varepsilon)$ upon exiting. On the other hand, given that a^{o*} is $\mathscr{O}(\sqrt{\varepsilon})$ and that the periodic orbit $\mathbf{q}_{h_1}^{z_0}$ takes an $\mathscr{O}(\ln|\varepsilon h_1|^{-1})$ amount of time in its first part of the flight in $\mathscr{B}$, we must have $a_{\text{in}}^o \ll \sqrt{\varepsilon}$ by (6.3). Similarly, for the perturbed trajectory $\mathbf{q}_{H_1}^{u}$: a^* is $\mathscr{O}(\sqrt{\varepsilon})$ and the first part of the flight in $\mathscr{B}$ takes an $\mathscr{O}(\ln|H_1|^{-1})$ amount of time. Hence, we must also have $a_{\text{in}} \ll \sqrt{\varepsilon}$ by (3.1). Now, since γ_0 and γ_ε are $\mathscr{C}^r\mathscr{O}(\varepsilon)$ close, and so are their local stable manifolds (given respectively by the sets $\{a^o = 0\}$ and $\{a = 0\}$) and the unstable ones (given by the sets $\{b^o = 0\}$ and $\{b = 0\}$), it follows that a_{in}^o and a_{in} are at least $\mathscr{O}(\sqrt{\varepsilon})$ close. Thus, $a_{\text{in}}^o = a_{\text{in}} + \mathscr{O}(\sqrt{\varepsilon})$. A similar argument shows that $b_{\text{out}}^o = b_{\text{out}} + \mathscr{O}(\sqrt{\varepsilon})$.

To compute the time difference outside $\mathscr{B}$, we start by using the result from the previous discussion for $\mathbf{q}_{H_1}^{u}$ and $\mathbf{q}_{h_1}^{z_0}$ at the exit of $\mathscr{B}$. Upon exiting $\mathscr{B}$, the orbits are $\mathscr{O}(\varepsilon^{1/2})$ close. Gronwall-type estimates guarantee that they will remain $\mathscr{O}(\varepsilon^{1/2})$ close when $\mathbf{q}_{h_1}^{z_0}$ reaches a maximum of the norm of its q coordinate at time t_1^o, since it spends an $\mathscr{O}(1)$ amount of time outside $\mathscr{B}$. This means that at this moment, $\mathbf{q}_{H_1}^{u}$ will be $\mathscr{O}(\varepsilon^{1/2})$ close to the q axis. Now, it will take $\mathbf{q}_{H_1}^{u}$ an $\mathscr{O}(\varepsilon^{1/2})$ amount of time to reach the normal $\mathbf{n}(z)$ at $t_1 = z_1/\varepsilon$, since the vector field is $\mathscr{O}(1)$ there. Thus in this part of the flight outside $\mathscr{B}$, the difference in the respective times of flight is $\mathscr{O}(\varepsilon^{1/2})$. Hence, $t_1 - t_1^* = t_1^o - t_1^{o*} + \mathscr{O}(\varepsilon^{1/2})$. For the other part of the flight outside $\mathscr{B}$, the difference is also $\mathscr{O}(\varepsilon^{1/2})$. Combining this time difference for the times spent outside $\mathscr{B}$ with the estimate in Corollary 2 for the difference while in $\mathscr{B}$, we have shown that

$$\varepsilon P(\varepsilon h_1(z_0)) = z_1 - z_0 + \mathscr{O}(|\varepsilon h_1|^{4/3}). \quad (7.4)$$

C. Step 3

We now proceed to compute the estimate of H_2. Recall that we are carrying out the estimates in this and all further steps explicitly for type II systems. Those for type I systems are identical with the improved estimate of the remainder as given in Step 1. So far, for the orbit $\mathbf{q}^u(t;z_0,\varepsilon)$, we have

$$H_2 = H_1 + \int_{t_1^*}^{t_2^*} \frac{dH}{dt}\,dt = \varepsilon h_1(z_0) + \varepsilon h_1(z_1) + \mathcal{O}\left(|\varepsilon h_1|\varepsilon \ln\frac{1}{\varepsilon}, |\varepsilon h_2|\varepsilon \ln\frac{1}{\varepsilon}, \varepsilon^2 \right),$$

where the result of Step 1 has been used in all of the remainder terms in (3.4). The leading error terms are $\mathcal{O}(\varepsilon^2 \ln 1/\varepsilon)$, since h_1 and h_2 are $\mathcal{O}(1)$.

We now substitute the relationship (7.4) between z_1 and z_0 computed in Step 2 for $\varepsilon h_1(z_1)$ in the above equation:

$$H_2 = \varepsilon[M_A(z_0) + M_A((z_0 + \varepsilon P(\varepsilon h_1(z_0)) + \mathcal{O}(\varepsilon^{4/3}))] + \mathcal{O}\left(\varepsilon^2 \ln\frac{1}{\varepsilon}\right).$$

Finally, we recall that $h_2(z_0,\varepsilon) \equiv M_A(z_0) + M_A(z_0 + \varepsilon P(\varepsilon h_1(z_0)))$, so that for $z_0 \in \{z : M_A(z) \leqslant \kappa < 0\}$, we take the Taylor expansion of H_2 and conclude

$$H_2(z_0,\varepsilon) = \varepsilon h_2(z_0,\varepsilon) + \mathcal{O}\left(\varepsilon^2 \ln\frac{1}{\varepsilon}\right). \tag{7.5}$$

D. Step 4

We now show that the existence of a simple zero of h_2 at $(z = z_0,\ \varepsilon = \varepsilon_0)$ guarantees that H_2 has a simple zero for some (z,ε) near (z_0,ε_0). Our method follows closely the strategy used in Ref. 20, since the implicit function theorem cannot be used because $N = 2,3,...$, pulse homoclinic orbits do not exist when $\varepsilon = 0$.

Let $0 < \beta < \alpha < \frac{1}{2}$, $\Delta z = K\varepsilon_0^\beta$, where $K > 0$, and $\Delta\varepsilon = J\varepsilon_0^{1+\alpha}$, where $J \in \mathbb{R}$. We will prove that $H_2(z_0 - \Delta z, \varepsilon_0 + \Delta\varepsilon)$ and $H_2(z_0 + \Delta z, \varepsilon_0 + \Delta\varepsilon)$ are of different signs.

We begin by considering the Taylor expansion of H_2 about (z_0,ε_0):

$$\begin{aligned} H_2(z_0 + \Delta z, \varepsilon_0 + \Delta\varepsilon) = {} & H_2(z_0,\varepsilon_0) + \frac{\partial H_2}{\partial z}(z_0,\varepsilon_0) K\varepsilon_0^\beta + \frac{1}{2}\frac{\partial^2 H_2}{\partial z^2}(z_0,\varepsilon_0) K^2 \varepsilon_0^{2\beta} \\ & + \frac{\partial^2 H_2}{\partial z\,\partial\varepsilon}(z_0,\varepsilon_0) KJ\varepsilon_0^{1+\alpha+\beta} + \frac{\partial H_2}{\partial\varepsilon}(z_0,\varepsilon_0) J\varepsilon_0^{1+\alpha} \\ & + \mathcal{O}(\varepsilon_0^{3\beta}, \varepsilon_0^{2(1+\alpha)}, \varepsilon^{1+\alpha+2\beta}). \end{aligned}$$

Then we use the asymptotic formula (7.5) derived in Step 3 to replace H_2 with h_2:

$$\begin{aligned} H_2(z_0 + \Delta z, \varepsilon_0 + \Delta\varepsilon) = {} & K\frac{\partial h_2}{\partial z}(z_0,\varepsilon_0)\varepsilon_0^{1+\beta} + K^2\frac{1}{2}\frac{\partial^2 h_2}{\partial z^2}\varepsilon_0^{1+2\beta} + KJ\frac{\partial^2(\varepsilon h_2)}{\partial z\,\partial\varepsilon}(z_0,\varepsilon_0)\varepsilon_0^{1+\alpha+\beta} \\ & + J\frac{\partial(\varepsilon h_2)}{\partial\varepsilon}(z_0,\varepsilon_0)\varepsilon_0^{1+\alpha} + \mathcal{O}\left(\varepsilon_0^2 \ln\frac{1}{\varepsilon_0}, \varepsilon_0^{3\beta+1}\right), \end{aligned} \tag{7.6}$$

where we have used the fact that $h_2(z_0,\varepsilon_0) = 0$. Next, we make the following estimates. First, $P(\varepsilon h_1(z_0)) = \mathcal{O}(\ln|\varepsilon h_1|^{1/2}) = \mathcal{O}(\ln 1/\varepsilon)$; and, second, $\partial(\varepsilon h_2)/\partial\varepsilon = \varepsilon\,\partial h_2/\partial\varepsilon + h_2$, where

$$\frac{\partial h_2}{\partial \varepsilon} = M_A'(z_0)\left[\varepsilon\,\frac{dP}{d\varepsilon} + P(\varepsilon h_1(z_0))\right] = M_A'(z_0)\left[\mathcal{O}(1) + \mathcal{O}\left(\ln\frac{1}{\varepsilon}\right)\right] = \mathcal{O}\left(\ln\frac{1}{\varepsilon}\right),$$

and we have used the fact that $dP/d\varepsilon$ also has an asymptotic expansion as $\varepsilon \to 0$, namely $dP/d\varepsilon = \mathcal{O}(1/\varepsilon)$.

Finally, note that $K(\partial h_2/\partial z)(z_0,\varepsilon_0)\varepsilon_0^{1+\beta}$ is the dominant term, since the two terms with partial derivatives in ε in (7.6) are $\mathcal{O}(\varepsilon_0^{2+\alpha+\beta}\ln(1/\varepsilon_0))$ and $\mathcal{O}(\varepsilon_0^{2+\alpha}\ln(1/\varepsilon_0))$, respectively. Thus, we write

$$H_2(z_0+\Delta z,\varepsilon_0+\Delta\varepsilon) = K\,\frac{\partial h_2}{\partial z}\,(z_0,\varepsilon_0)\varepsilon_0^{1+\beta} + \mathcal{O}\left(\varepsilon_0^{1+2\beta}, \varepsilon_0^2\,\ln\frac{1}{\varepsilon_0}\right), \tag{7.7}$$

and similarly

$$H_2(z_0-\Delta z,\varepsilon_0+\Delta\varepsilon) = -K\,\frac{\partial h_2}{\partial z}\,(z_0,\varepsilon_0)\varepsilon_0^{1+\beta} + \mathcal{O}\left(\varepsilon_0^{1+2\beta}, \varepsilon_0^2\,\ln\frac{1}{\varepsilon_0}\right). \tag{7.8}$$

Since by hypothesis $(\partial h_2/\partial z)(z_0,\varepsilon_0) \neq 0$, we see from the two expressions above that H_2 has a simple zero when $z_0 \in [z_0-\Delta z, z_0+\Delta z]$, for every ε in an interval of size $\mathcal{O}(\varepsilon_0^{1+\alpha})$ about ε_0.

E. Step 5

In this final step, we prove inductively that

$$H_N(z_0,\varepsilon) = \varepsilon h_N + \mathcal{O}\left(\varepsilon^2\,\ln\frac{1}{\varepsilon}\right) \tag{7.9}$$

by making use of the results in Steps 1–3 at each step of the induction process. The proof that simple zeroes of h_N imply simple zeroes of H_N is identical to the one presented for $N=2$ in Step 4, and we omit it.

Assume $H_j(z_0,\varepsilon) = \varepsilon h_j + \mathcal{O}(\varepsilon^2 \ln 1/\varepsilon)$ holds for $j=1,\ldots,N-1$. From (3.7) we have

$$H_N = H_{N-1} + \varepsilon h_1(z_{N-1}) + \mathcal{O}\left(\varepsilon^2|h_{N-1}|\ln\frac{1}{\varepsilon}, \varepsilon^2|h_N|\ln\frac{1}{\varepsilon}, \varepsilon^2\right),$$

where the last term was obtained by combining the remainder terms in (3.7) and using the result from Step 1.

We consider the second term

$$\varepsilon h_1(z_{N-1}) = \varepsilon h_1(z_{N-2} + \varepsilon P(\varepsilon h_{N-1})) + \mathcal{O}(\varepsilon^{7/3}),$$

where we have used the result from Step 2; i.e.,

$$z_{N-1} = z_{N-2} + \varepsilon P(\varepsilon h_{N-1}) + \mathcal{O}(|\varepsilon h_{N-1}|^{4/3}).$$

Proceeding inductively, we see that

$$\varepsilon h_1(z_{N-1}) = \varepsilon h_1\left(z_0 + \varepsilon\sum_{j=1}^{N-1} P(\varepsilon h_j)\right) + \mathcal{O}(\varepsilon^{7/3}).$$

Finally, using the above expression and our induction hypothesis $H_{N-1} = \varepsilon h_{N-1}(z_0,\varepsilon) + \mathcal{O}(\varepsilon^2 \ln 1/\varepsilon)$ in the expression for H_N, we obtain

$$H_N = \varepsilon h_{N-1} + \varepsilon h_1\left(z_0 + \varepsilon \sum_{j=1}^{N-1} P(\varepsilon h_j)\right) + \mathcal{O}\left(\varepsilon^2 \ln \frac{1}{\varepsilon}\right).$$

Recalling the definition for h_N, we finally obtain

$$H_N(z_0,\varepsilon) = \varepsilon h_N + \mathcal{O}\left(\varepsilon^2 \ln \frac{1}{\varepsilon}\right),$$

which completes the proof of the Theorem.

VIII. EXTENSION TO (1.1) WITH $\mu>0$

Up until now, we have dealt with slowly varying Hamiltonian systems without any damping or forcing. The above proof of Theorem 1 can now readily be extended to systems of the form (1.1) with $\mu \neq 0$ and satisfying Assumption 1, to show that Corollary 1 holds.

We will begin by showing that an Nth-order adiabatic Melnikov function can be derived in a manner that totally parallels the heuristic derivation for the slowly varying Hamiltonian case in Sec. III. The main difference is that we no longer can talk about the ''energy'' of the system. However, we will exploit the fact that for every z fixed, the level curves of the function H provide us with a system of reference curves that help us set up nice coordinates along $\mathbf{n}(z)$.

We specifically derive $M_{2,A}(z_0,\varepsilon,\mu)$, since the generalization to $M_{N,A}(z_0,\varepsilon,\mu)$ is evident. Again, let $\mathbf{q}^u(t;z_0,\varepsilon,\mu)$ be a solution on $W^u(\gamma_\varepsilon)$ that crosses the normal $\mathbf{n}(z)$ at a time $z=z_0=\varepsilon t_0$ and reaches the negative x axis in the neighborhood of γ_ε at a time t_1^*. At that point, it will cross some level curve of H, with value $H_1 = H(\mathbf{q}^u(t_1^*;z_0,\varepsilon,\mu),\varepsilon t_1^*)$, that can be computed as

$$\begin{aligned} H_1 &= \int_{-\infty}^{t_1^*} \frac{dH}{dt}(\mathbf{q}^u(t;z_0,\varepsilon,\mu))dt \\ &= \varepsilon \int_{-\infty}^{t_1^*} \frac{\partial H}{\partial z}(\mathbf{q}^u(t;z_0,\varepsilon,\mu))dt + \varepsilon\mu \int_{-\infty}^{t_1^*} (f_2(\mathbf{q}^u(t;z_0,\varepsilon,\mu))\dot{q}^u(t;z_0,\varepsilon,\mu) \\ &\quad - f_1(\mathbf{q}^u(t;z_0,\varepsilon,\mu))\dot{p}^u(t;z_0,\varepsilon,\mu))dt, \end{aligned}$$

which reduces to (3.2) when $\mu=0$.

As we did in Sec. III, we then approximate $\mathbf{q}^u(t;z_0,\varepsilon,\mu)$ with the unperturbed separatrix at $z=z_0$, so (3.3) now becomes

$$H_1 = \varepsilon M_A(z_0,\mu) + R_s(z_0,\mu,t_1^*)$$

where

$$\begin{aligned} M_A(z_0,\mu) \equiv & \int_{-\infty}^{t_1^*} \frac{\partial H}{\partial z}(\mathbf{q}^u(t;z_0,\varepsilon,\mu))dt + \mu \int_{-\infty}^{t_1^*} (f_2(\mathbf{q}^u(t;z_0,\varepsilon,\mu))\dot{q}^u(t;z_0,\varepsilon,\mu) \\ & - f_1(\mathbf{q}^u(t;z_0,\varepsilon,\mu))\dot{p}^u(t;z_0,\varepsilon,\mu))dt, \end{aligned}$$

and the remainder term is

$$R_s(z_0,\mu,t_1^*) = -\varepsilon \int_{t_1^*}^{\infty} \frac{dH}{dt}(\mathbf{q}_0^{z_0}(t))dt + \mathcal{O}(\varepsilon^2) = H(\mathbf{q}_0^{z_0}(t_1^*)) + \mathcal{O}(\varepsilon^2).$$

From here, just as in the undamped case,

$$H_2 = \int_{-\infty}^{t_2^*} \frac{dH}{dt}(\mathbf{q}^u(t;z_0,\varepsilon,\mu))dt$$
$$= \varepsilon M_A(z_0,\mu) + \varepsilon M_A(z_1,\mu)$$
$$+ R_s(z_0,\mu,t_1^*) + R_s(z_1,\mu,t_2^*) + R_u(z_1,\mu,t_1^*), \tag{8.1}$$

where z_1 is the second (slow) time of crossing the normal $\mathbf{n}(z)$.

Now, the very same arguments we used in the $\mu=0$ case to estimate the time spent in the rotating regime [and, in fact, the same proof presented in Step 2 with the obvious changes in the expressions of the Fenichel normal forms (6.1) and (6.3)] yield

$$z_1 \sim z_0 + \varepsilon P(\varepsilon M_A(z_0,\mu)).$$

Combining these last two expressions, we arrive at the secondary adiabatic Melnikov function

$$M_{2,A}(z_0,\varepsilon,\mu) \equiv M_A(z_0,\mu) + M_A(z_0+\varepsilon P(\varepsilon M_A(z_0,\mu)),\mu).$$

Finally, we point out that the proof that all the remainders in (8.1) are of higher order, namely, $\mathcal{O}(\varepsilon^2)$ for type I systems, and for type II systems they are $\mathcal{O}(\varepsilon^2 \ln 1/\varepsilon)$, is identical to that for the $\mu=0$ case. The proofs of all the five steps are identical as well.

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Probing quantum gravity through exactly soluble midi-superspaces I

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It is well-known that the Einstein-Rosen solutions to the 3+1- dimensional vacuum Einstein's equations are in one to one correspondence with solutions of 2+1-dimensional general relativity coupled to axi-symmetric, zero rest mass scalar fields. We first re-examine the quantization of this midi-superspace paying special attention to the asymptotically flat boundary conditions and to certain functional analytic subtleties associated with regularization. We then use the resulting quantum theory to analyze several conceptual and technical issues of quantum gravity. © *1996 American Institute of Physics.* [S0022-2488(96)02312-2]

I. INTRODUCTION

Many of the central problems of quantum gravity can be traced back to two main difficulties: (i) the absence of a background space-time metric and (ii) the presence of an infinite number of degrees of freedom.

Let us begin with the first set of issues. The absence of a background geometry implies that the theory has to be diffeomorphism invariant and this feature makes it difficult to construct observables and formulate precisely questions of direct physical interest. It also gives rise to the celebrated ''problem of time'': if there is no background metric, what are we to make of the notion of ''time evolution''? Indeed, if the diffeomorphisms are to be regarded as gauge, at first sight, dynamics also appears as a part of gauge. Can one disentangle dynamics from gauge unambiguously? These questions are of course not new. (For a detailed discussion, see, e.g. Ref. 1.) To gain insight into these issues, a number of mini-superspace models have been discussed in the literature (see, e.g., Ref. 2). In Bianchi models, for example, one restricts attention only to spatially homogeneous solutions of Einstein's equations and, in the quantum theory, addresses the issue of time via ''de-parametrization.'' Perhaps a more striking model is presented by 2+1-dimensional vacuum general relativity which, like the 3+1 theory, is fully diffeomorphism invariant. Quantization of this model[3,4] has shed light on the notion of observables, role of discrete symmetries, etc. These models have also given us considerable insights into the technical problems that arise due to the underlying diffeomorphism invariance. For example, since we have no Poincaré group to help us, the problem of finding the correct inner-product on the space of quantum states requires a new strategy. The 2+1 model has provided a method which, moreover, is free of ambiguities that arise, e.g., in the de-parametrization procedure.

However, these models do not come to grips with the second main difficulty mentioned above: the presence of an infinite number of degrees of freedom. To face this difficulty, we need to consider genuine field theories which do not require a background space-time metric. An obvious strategy would be to again consider symmetry reductions which, however, are mild enough to leave behind *local* degrees of freedom. To locate convenient choices, let us briefly return to the 2+1-dimensional vacuum general relativity. This theory can be obtained by a symmetry reduction of 3+1-dimensional general relativity with respect to a single space-like Killing field which is hyper-surface orthogonal and whose norm is *constant*. Therefore, as a next step, it is natural to drop the severe condition on the norm. The symmetry reduced system now has an infinite number of degrees of freedom. In fact it is now equivalent to 2+1-dimensional general relativity coupled to a zero rest mass scalar field (which is given by the logarithm of the norm of

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the Killing field).[5,6] Unfortunately, this midi-superspace is a bit too complicated in that the issue of global existence of such solutions is still largely unexplored in the classical theory. However, if we require that there be another hyper-surface orthogonal Killing field in the 3+1 theory which commutes with the first one, the situation simplifies dramatically. For now one can in effect ''decouple'' gravity and the scalar field. More precisely, the equation satisfied by the scalar field on the curved 2+1-dimensional space-time is equivalent to the wave equation on a fictitious *flat* 2+1-dimensional space-time. Therefore, one can first solve the second equation without any reference to the physical metric and then use the solution to obtain the physical metric by simple integration. Classically, one now has complete control on the issue of global existence.

Such space-times were considered by Einstein and Rosen in the thirties for the case when the first Killing field is a translation in the ''z-direction'' and the second is a ''x-y rotation.'' Thus, they represent cylindrical gravitational waves (with only one polarization because of the hyper-surface orthogonality requirement.) Their quantization was considered in a remarkable paper by Kuchař[7] already in 1971. The problem was considered again from a 2+1-dimensional perspective by Allen[8] in 1987 (without, however, realizing that this is precisely a symmetry reduced version of Ref. 7.) In the present paper, we shall return to this midi-superspace. Our purpose is two-fold: (i) to supplement the analyses by Kuchař and Allen with a careful treatment of boundary conditions in the classical theory and of certain functional analytic issues in the quantum theory and (ii) to use the resulting quantum theory to analyze several conceptual and technical problems of quantum gravity. Since the model itself is simple enough to be exactly soluble, it provides a concrete arena to examine these vexing issues and to see how they can be resolved in practice.

Specifically, following Refs. 7 and 8, we will use a canonical approach. Since in this approach one *begins* with a 2+1 decomposition of space-time, *a priori* it is not clear if quantized *space-time* geometries can emerge in the final theory. Indeed, one often hears the criticism that, since it is tied to space-like surfaces, the canonical approach may be inadequate to handle ''space-time issues'' such as ''fluctuations of the light cone.'' Here, we have a complete quantum theory. It is therefore natural to ask: are there operators on the final Hilbert space corresponding to space-time geometries? If so, is there adequate structure to analyze how the light cones fluctuate? More generally, can we tie the canonically quantized theory to the quantum description that emerges from covariant approaches? Can we compute S-matrices? In the classical theory, there is a positive energy theorem.[6,9] Does it continue to hold in the quantum theory? Is the true ground state ''peaked around'' Minkowski space-time? Or, does the ground state contain wild quantum fluctuations with Planck energy density as suggested by Wheeler?[10] If so, the true ground state would not have much resemblance to Minkowski space, except perhaps on a suitable coarse-graining. Another question which plays an important role in semi-classical considerations is: Are there ''coherent states'' which are peaked at classical solutions?

There is a non-perturbative approach to full quantum gravity which is based on connections and triads (see, e.g., Ref. 4). A basic assumption in that approach is that the ''Wilson-loop operators,'' which correspond to traces of holonomies of a connection around space-like loops, should be well-defined. *A priori* it is not clear if this assumption is a reasonable one since in the definition of these operators, one appears to smear a quantum field along a *one*-dimensional object (rather than three or four). It is natural to ask for the status of this assumption in a completely solved model. Are these Wilson loop operators well-defined on the explicitly known quantum Hilbert space?

Of course, the fact that such questions are answered in one way in a specific solution to this model does not imply that they would not be answered in another way in another solution and, more importantly, in full 3+1-dimensional quantum gravity. Nonetheless, the ability to answer them in detail in an explicit solution can contribute substantially to our overall intuition for quantum gravity. Our analysis is primarily motivated by such considerations. We will find that most of these questions can be answered in detail but that the analysis involves several rather subtle points.

The plan of the paper is as follows. In section II, we consider the classical Hamiltonian formulation and isolate the true degrees of freedom by a gauge fixing procedure. Because we are in an asymptotically flat situation, by treating the boundary conditions carefully, we can distinguish gauge from dynamics. In particular, the true degrees of freedom are naturally subject to non-trivial dynamics (without the need of any ''deparametrization.'') In section III, we calculate the classical Wilson loop functions and express them in terms of the true degrees of freedom. Quantization is taken up in section IV. As in Refs. 7 and 8 the Hilbert space of states is a Fock space for scalar fields in $2+1$ dimensions. Subtleties arise, however, because the geometrical observables, such as the space-time metric and the Wilson loops, are expressed as integrals of quadratic functionals of these elementary excitations. Thus, in a rough terminology, geometric excitations arise as non-local ''collective modes'' of the primary mathematical entity, the quantum scalar field. Finally, questions raised earlier in this section are analyzed within this solution. Section V summarizes the main results and points out directions for further work.

II. HAMILTONIAN FORMULATION

A. The midi-superspace

Let us begin with a precise specification of our midi-superspace. For definiteness, we will work in the $2+1$-dimensional formulation. Thus, we will consider asymptotically flat, axi-symmetric solutions of $2+1$-dimensional general relativity coupled to zero rest mass scalar-fields (where the rotational Killing field is hyper-surface orthogonal). The underlying manifold M will be topologically R^3 and the space-time metric will have signature $-,+,+$. For simplicity, we will assume that all fields under consideration are C^∞.

Denote by σ^a the rotational Killing field. Hyper-surface orthogonality of σ^a implies that the space-time metric g_{ab} has the form

$$g_{ab}=h_{ab}+R^2\nabla_a\sigma\nabla_b\sigma, \tag{1}$$

where R is the norm of the Killing field and σ is the ''angular coordinate''; $\nabla_a\sigma=R^{-2}g_{ab}\sigma^b$. The field h_{ab} so defined is a metric of signature $-$, $+$ on the two-manifolds orthogonal to σ^a. Let us introduce a space-like foliation of this two-manifold by lines $t=\text{const}$ and a dynamical vector field $t^a=Nn^a+N^r\hat{r}^a$, where n^a is the unit, time-like normal to the foliation and $\hat{r}^a$ the unit (outgoing) vector field within each slice. The pair N,N^r constitutes the lapse and the shift. If we now introduce a radial coordinate r on any one leaf such that $r=0$ at the axis (i.e., where $R=0$) and r tends to infinity at spatial infinity, the two-metric h_{ab} can be written as

$$h_{ab}=(-N^2+(N^r)^2)\nabla_a t\nabla_b t+2N^r\nabla_{(a}t\nabla_{b)}r+e^\gamma\nabla_a r\nabla_b r, \tag{2}$$

where N,N^r and γ are functions of r and t. It is because of axi-symmetry that the three-metric g_{ab} has only four independent components and they are functions only of two variables.

Thus, our midi-superspace consists of five functions (N,N^r,γ,R,ψ) on the space-time manifold M where ψ is the zero rest mass scalar field (which is also Lie-dragged by the rotational Killing field). The five fields are subject to the following field equations:

$$G_{ab}=T_{ab} \quad \text{and} \quad g^{ab}\nabla_a\nabla_b\psi=0\,, \tag{3}$$

where G_{ab} is the Einstein tensor of g_{ab} which is determined by the fields (N,N^r,γ,R) via (2) and T_{ab} is the stress-energy tensor of the scalar field ψ:

$$T_{ab}=\nabla_a\psi\nabla_b\psi-\frac{1}{2}(g^{cd}\nabla_c\psi\nabla_d\psi)g_{ab}\,. \tag{4}$$

(Here, we have used a normalization that arises naturally in the reduction from the 3+1 theory to the 2+1. From the 2+1 perspective, it is natural to regard $\phi := \psi/\sqrt{8\pi G}$ as the physical Klein-Gordon field, where G is Newton's constant.)

Asymptotic flatness and regularity at the axis imply certain boundary conditions on our dynamical fields. We first note that g_{ab} reduces to a Minkowskian metric when $N=1$, $N^r=0$, $\gamma=0$, $R=r$ and $\psi=0$. The general asymptotic flatness conditions can be written as

$$N=1+N_1(r,t), \quad N^r=N^r_o(t)+N^r_1(r,t),$$
$$\gamma(r,t)=\gamma_\infty(t)+\gamma_1(r,t), \quad R(r,t)=r(1+R_1(r,t)), \tag{5}$$

where, on any $t=$const surface, $N_1, N^r_1, \gamma_1, R_1$ and the scalar fields ψ are of asymptotic order $O(1/r)$. (We will say that a function $f(r)$ is of asymptotic order $1/r$ if $rf(r), r^2f'(r)$ and $r^3f''(r)$ admits limits as r tends to infinity, where a prime denotes a derivative with respect to r.) While the conditions imposed on N, N^r, R and ψ are the obvious ones, the condition on the field γ seems surprising at first. For, even at infinity, γ is not required to approach its Minkowskian value, 0. The reason is that the asymptotic value of γ contains the information about mass: If $\gamma_\infty=0$, the spatial metric has a deficit angle at infinity which measures the ADM mass.[6,9] Thus, there is a striking contrast with asymptotic flatness in 3+1 dimensions; the space-time metrics in our midi-superspace do *not* approach a fixed Minkowskian metric at infinity. Note finally that these boundary conditions are somewhat simpler than those used in Ref. 9 where general 2+1-dimensional space-times were considered. Here, we can exploit the fact that we are now working in a highly restrictive context of cylindrical waves.

Finally, regularity at the axis is ensured by requiring that N^r, γ and R vanish there for all t. (Recall also that by assumption, N, N^r, γ, R^2 and ψ are C^∞ everywhere and, in particular, at $r=0$.)

B. Phase space

Let us begin with the three-dimensional action with appropriate boundary terms:

$$S(g,\psi) := \frac{1}{16\pi G}\int_{M'} d^3x\sqrt{g}[\mathscr{R} - g^{ab}\nabla_a\psi\nabla_b\psi] + \frac{1}{8\pi G}\oint_{\partial M'} d^2x[K\sqrt{h} - K_o\sqrt{h_o}], \tag{6}$$

where M' is an open set in M; $\partial M'$, its boundary in M; $\mathscr{R}$, the scalar curvature of g; K and h, the trace of the extrinsic curvature of, and the determinant of the intrinsic metric on $\partial M'$ induced by g_{ab}; and K_o and h_o are the corresponding fields induced by the Minkowski metric $\mathring{g}_{ab}$ (obtained by setting $N=1$, $N^r=0$, $\gamma=0$, $R=r$ and $\psi=0$).

To pass to the Hamiltonian formulation, one performs a 2+1-decomposition. Let us substitute in (6) the form of the metric given by Eqs. (1) and (2). Then, the action reduces to the standard form:

$$S = \frac{1}{8G}\int dt(dr(p_\gamma\dot{\gamma} + p_R\dot{R} + p_\psi\dot{\psi}) - H[N,N^r]) \tag{7}$$

The Hamiltonian H is given by

$$H[N,N^r] = \frac{1}{8G}\int dr(NC + N^rC_r) + \frac{1}{4G}(1-e^{-\gamma_\infty/2}), \tag{8}$$

where C and C_r are functions of the canonical variables,

$$C = e^{-\gamma/2}(2R'' - \gamma'R' - p_\gamma p_R) + \frac{1}{2}Re^{-\gamma/2}\left(\frac{p_\psi{}^2}{R^2} + \psi'^2\right),$$

$$C_r = e^{-\gamma}(-2p'_\gamma + \gamma' p_\gamma + R' p_R) + e^{-\gamma} p_\psi \psi', \tag{9}$$

and γ_∞ is the value of γ at $r=\infty$. (Here primes denote derivatives with respect to r.)

As expected, the lapse and shift functions N, N^r appear as Lagrange multipliers; they are not dynamical variables. Thus, the phase-space Γ consists of three canonically conjugate pairs, $(\gamma, p_\gamma; R, p_R; \psi, p_\psi)$, on a two-manifold Σ which is topologically R^2. The boundary conditions on the configuration variables (γ, R, ψ) have already been discussed. The conditions on the momenta can be deduced from their definitions in terms of these fields and their time derivatives. At infinity, p_γ and p_R fall off as $O(1/r^2)$ while p_ψ falls off as $O(1/r)$. (Note that these conditions imply that action $\int dr p_\gamma \delta\gamma, \int dr p_R \delta R$ and $\int dr p_\psi \delta\psi$ of the momenta on the tangent vectors $\delta\gamma, \delta R, \delta\psi$ to our configuration space are all finite, so that we have a well-defined (weakly non-degenerate) symplectic structure.) There are two first class constraints, $C=0$ and $C_r=0$, obtained by varying the action with respect to the Lagrange multipliers N and N^r. The Hamiltonian is given by H. (It is because of the underlying axi-symmetry that we have only one diffeomorphism constraint, C_r.)

Let us begin by analyzing the canonical transformations generated by constraints. For this, we have to first smear the constraints and obtain well-defined functions on the phase space, say, $C[N_g] := \int dr N_g C$ and $C[N^r_g] = \int dr N^r_g C_r$. Using the boundary conditions on the phase space variables, it is straightforward to verify that these functions are well-defined *and* differentiable on the phase space if N_g vanishes on the axis and is of asymptotic order $O(1/r)$ and N^r_g admits a limit at infinity. (From now on, the subscript g on smearing fields will indicate that they satisfy these boundary conditions.) Since the constraints are of first class, and since we are in the asymptotically flat context, the canonical transformations generated by these constraints can be regarded as ''gauge'' in an appropriate sense. As one might expect, $C[N_g]$ generates ''bubble time evolutions'' via lapses which go to zero at infinity while $C[N^r_g]$ generates spatial diffeomorphisms which are bounded at infinity. The situation with the Hamiltonian constraint is the same as the one we normally encounter in the 3+1-dimensional theory. For the diffeomorphism constraint, on the other hand, the situation is quite different since the diffeomorphisms generated by $N^r_g \hat{r}^a$ are not necessarily asymptotically identity. This is, however, the standard situation in 2+1 dimensions (see e.g., Refs. 6 and 9): In 2+1 dimensions, there are no asymptotic Killing fields corresponding to spatial translations and the ADM two-momentum vanishes.

To obtain genuine time translations, we have to allow lapses which tend to 1 at infinity and on the axis. When this is done, the constraint function $C[N]$ continues to exist everywhere on the phase space. However, due to the presence of the first two terms involving derivatives of γ and R in the expression of C, the function $C[N]$ fails to be differentiable. To make it differentiable, one has to add a surface term. As one might expect, this is precisely the surface term in the expression (8) of the Hamiltonian. Thus, the function which generates the canonical transformation corresponding to (asymptotically unit) time translation is precisely the Hamiltonian $H[N]$ (obtained by setting $N^r=0$ in Eq. (8)). On physical states, i.e., when the constraints are satisfied, the numerical value of the Hamiltonian is given by the surface term in (8):

$$E = \frac{1}{4G}(1 - e^{-(1/2)\gamma_\infty}), \tag{10}$$

As usual, in the space-time picture, the evolution generated by the Hamiltonian on the phase space corresponds to motions along the vector field t^a.

Let us summarize the discussion of this sub-section. Because we are in the asymptotically flat context, there is a clean separation between gauge and dynamics. As usual, when it comes to physical interpretation, the ''gauge transformations'' of general relativity have a somewhat different status from that in Yang-Mills theory. It is not that the diffeomorphisms generated by $C[N_g]$ and $C[N^r_g]$ are ''unphysical.'' Rather, they are ''redundant'' when it comes to extracting

the physical content of the theory. As we will see below, we can gauge fix these constraints and extract the true degrees of freedom. The Hamiltonian generates ''time evolution'' among these gauge fixed points. Knowing this evolution, we can reconstruct the entire solution; motions generated by constraints are not needed and are in this sense ''redundant.''

C. Gauge fixing

Since the canonical transformations generated by $C[N_g]$ and $C[N_g^r]$ are to be regarded as gauge, as in Yang-Mills theory, to gauge fix the system we need to extract one point from each orbit of the corresponding Hamiltonian vector fields. This is achieved by imposing gauge fixing conditions which, together with the constraints, constitute a second class system. As in Ref. 7, we will choose these conditions to make the space-time geometry transparent. Let us demand

$$R(r)=r \quad \text{and} \quad p_\gamma(r)=0. \tag{11}$$

The first condition is motivated by the fact that, in any solution to the field equations (satisfying our boundary conditions), the gradient $\nabla_a R$ of the norm of the Killing field $\partial/\partial\sigma$ is space-like everywhere on M.[11] Since furthermore $R\sim r$ at the axis and at infinity, it is natural to use R itself as the radial coordinate. After this condition is imposed, R will no longer be a dynamical variable. The second gauge fixing condition will remove γ from our list of dynamical variables. Thus, if these conditions are admissible, the true degrees of freedom will all reside in the field ψ, in accordance with our general expectation that in $2+1$ dimensions, all the local degrees of freedom are carried by matter fields.

To see if our gauge fixing conditions are admissible, let us compute their Poisson brackets with the constraints. We have

$$\{R(r)-r,\, C_r[N_g^r]\}=N_g^r e^{-\gamma}R',$$

$$\{p_\gamma,\, C[N_g]\}=\left[\frac{N_g}{2}\left(-p_\gamma p_R+\frac{p_\psi^2}{2R}+\frac{R}{2}\psi'^2\right)-N_g' R'\right]e^{-\gamma/2}, \tag{12}$$

where, as before, N_g^r and N_g are pure gauge lapses and shifts. If $N_g^r \neq 0$ and $N_g \neq 0$, the right sides of (12) do not vanish at any point on the intersection of the surfaces defined by constraints and gauge fixing conditions (11). Hence, as needed, the gauge fixed surface intersects the gauge orbits transversely.

The question now is whether we can choose lapse and shift such that the dynamical evolution generated by the Hamiltonian $H[N,N^r]$ preserves the gauge conditions. More precisely, since the Hamiltonian $H[N,N^r]$ weakly commutes with the constraints $C[N_g],C[N_g^r]$, we know that the dynamical evolution it generates maps entire gauge orbits to entire gauge orbits. The question is if we can select N,N^r such that the image under evolution of any gauge fixed point on the constraint surface is another gauge fixed point. General considerations from symplectic geometry imply that if such a pair exists, it is unique. We will now establish the existence. Let us begin with the Poisson brackets between the gauge conditions and the Hamiltonian:

$$\{R(r)-r,\, H[N,N^r]\}\approx N^r e^{-\gamma},$$

$$\{p_\gamma(r),\, H[N,N^r]\}\approx\left[\frac{N}{4r}(p_\psi^2+r^2\psi'^2)-N'\right]e^{-\gamma/2},$$

where $\approx$ stands for equality modulo constraints and gauge conditions. We seek N and N^r which satisfy our boundary conditions (namely, $N=1+O(1/r)$ and $N^r=N_o^r+O(1/r)$ at infinity) and for which the right hand sides of (13) vanish (modulo constraints and gauge conditions). The only solutions are

$$N(r)=\exp-\frac{1}{4}\int_r^\infty dr_1 r_1\left(\frac{(p_\psi)^2}{r_1^2}+(\psi')^2\right) \quad \text{and} \quad N^r(r)=0. \tag{14}$$

Finally, let us extract the true degrees of freedom of the theory. In order to accomplish this, we need to eliminate redundant variables by solving the set of second class constraints (9) and use gauge conditions (11). By setting $R=r$ and $p_\gamma=0$ in (9), we can trivially solve for γ and p_R in terms of ψ and p_ψ (using the Hamiltonian and the diffeomorphism constraints respectively). The result is

$$\gamma(R)=\frac{1}{2}\int_0^R dR_1 R_1\left(\frac{{p_\psi}^2}{R_1^2}+{\psi'}^2\right), \tag{15}$$

$$p_R=-p_\psi\psi'. \tag{16}$$

Substituting (15) in (14), we can also express the lapse N in terms of γ. Thus, as expected, the true degrees of freedom reside just in the matter variables. Indeed, the space-time metric is now completely determined by ψ and p_ψ:

$$g_{ab}=e^{\gamma(R,t)}(-e^{-\gamma_\infty}\nabla_a t\nabla_b t+\nabla_a R\nabla_b R)+R^2\nabla_a\sigma\nabla_b\sigma, \tag{17}$$

where, from now on, γ will only serve as an abbreviation for the right side of (15).

D. Reduced phase space

It is obvious from the above discussion that the reduced phase space $\overline{\Gamma}$ can be coordinatized by the pair $(\psi(R),p_\psi(R))$. The (non-degenerate) symplectic structure on the reduced phase space Γ is the pull-back of the symplectic structure on Γ. Thus,

$$\{\psi(R_1),p_\psi(R_2)\}=\delta(R_1,R_2) \tag{18}$$

on $\overline{\Gamma}$. Next, let us write the reduced action by substituting (11), (15) and (16) in (6),

$$S[\psi,p_\psi]=\frac{1}{8G}\int dt\left[\int dR(p_\psi\dot{\psi})-2(1-e^{-(1/2)\gamma_\infty})\right], \tag{19}$$

where, as before, $\gamma_\infty=\gamma(r=\infty)$. By varying the action (19) with respect to ψ and p_ψ we then obtain equations of motion:

$$\dot{\psi}=e^{-(1/2)\gamma_\infty}\frac{p_\psi}{R} \quad \text{and} \quad \dot{p}_\psi=e^{-(1/2)\gamma_\infty}(R\psi')'. \tag{20}$$

Due to the presence of $\exp(-\gamma_\infty/2)$ factors, these equations are highly non-linear. However, using (20) it is straightforward to check that $\gamma_\infty(t)$ is a *constant of motion*. Hence, given any *one* solution, we can define a new time coordinate T on M via a constant rescaling: $T:=(\exp-\frac{1}{2}\gamma_\infty)t$. Then, the field ψ satisfies the following *linear* second-order equation of motion:

$$-\frac{\partial^2\psi}{\partial T^2}+\frac{\partial^2\psi}{\partial R^2}+\frac{1}{R}\frac{\partial\psi}{\partial R}=0. \tag{21}$$

This is *exactly* the Klein-Gordon equation for a scalar field propagating on a Minkowskian background g^o_{ab}, given by

$$g^o_{ab} = -\nabla_a T \nabla_b T + \nabla_a R \nabla_b R + R^2 \nabla_a \sigma \nabla_b \sigma. \tag{22}$$

Thus, a remarkable simplification has occurred. We can just solve for a free scalar field ψ in Minkowski space (M, g^o_{ab}), *define* a function γ through (15), and construct a curved metric g_{ab} through (17). Then the pair (g_{ab}, ψ) satisfies the non-linear Einstein–Klein–Gordon equations.

This decoupling is not surprising from the space-time perspective. Indeed, it has been exploited repeatedly in the literature. However, it is illuminating to see how the decoupling comes about from a phase space perspective especially since the dynamics of the true degrees of freedom is driven only by the boundary term Hamiltonian which, furthermore, seems quite complicated at first sight. Note also that, while from a space-time perspective the passage between t and T involves only a constant rescaling, since the constant varies from solution to solution, from a phase space perspective it is a rather complicated ''q-number'' transformation. Thus, in quantum theory, if one variable in the pair (t, T) is taken as a ''time-parameter,'' the other will be a genuine operator. It is therefore instructive to contrast the two notions of time. By construction, t can be identified with the affine parameter along the Hamiltonian vector field defined by (8) on the phase space. Given any dynamical trajectory, we obtain a space-time metric g_{ab} and t can then be thought of as a time coordinate on M with the property that $\partial/\partial t$ generates a *unit* time translation at infinity. The parameter T, on the other hand, does not have a direct and simple physical interpretation in our phase space framework. Its most direct interpretation comes from the fiducial Minkowskian metric g^o_{ab} on M. Even at infinity, the norm of the vector field $\partial/\partial T$ varies from one physical metric g_{ab} to another. For the decoupling procedure, on the other hand, it is natural to fix, once and for all, the Minkowskian metric g^o_{ab} on M and regard g_{ab} simply as a ''derived'' quantity. Then T does have a natural interpretation of time. Finally, note that this somewhat peculiar situation arose because, in $2+1$ dimensions, the physical metrics g_{ab} do not approach a fixed Minkowskian metric even at infinity (or alternatively, because in $3+1$ dimensions, cylindrical waves fail to be asymptotically flat in the conventional sense.)

We will conclude this section with a remark. To begin with, one can ignore the broad physical problem of interest and focus just on a free scalar field satisfying the wave equation on the Minkowskian background (M, g^o_{ab}). The phase space for this system is the same as our reduced phase space and the Hamiltonian is given by γ_∞. However, γ_∞ does *not* have a direct physical interpretation in terms of the original coupled system; the physical energy of our system is given by (10).

III. HOLONOMY

As explained in the introduction, there is a non-perturbative approach[4] to quantum general relativity in $3+1$ dimensions which is based on the assumption that traces of holonomies of a certain connection are well-defined operators in the quantum theory. We would like to investigate the status of this assumption in the context of our midi-superspace. Therefore, in this section, we will make a short detour to compute the holonomy in question in the classical theory. Readers who are not familiar with this approach to quantum gravity may skip this section without loss of continuity.

In the first-order (Palatini) formalism for $2+1$ general relativity the fundamental variables are triads e^I_a and connection one-forms which take values in the Lie-algebra of $SU(1,1)$.[4,12] Let us denote the $SO(2,1)$ connection by ${}^3A^I_a$ and its pull-back to the two-dimensional slice Σ by A^I_a, where $I, J, \cdots = 0,1,2$ are internal indices with respect to a basis τ_I in the Lie algebra of $SU(1,1)$. The internal indices are raised and lowered with a Minkowski metric η_{IJ} with signature $(-,+,+)$.

A. $SO(2,1)$ connection

To obtain the internal connection for the space-time metric (17), we need to fix the internal (i.e., $SU(1,1)$) gauge. This is accomplished by fixing the triads e^I_a. Our choice will be

$$e^I_a \tau_I = \sqrt{2} e^{(1/2)\,(\gamma(R,t)-\gamma_\infty)} (\nabla_a t)\,\tau_0 + \sqrt{2} e^{(1/2)\,\gamma(R,t)} (\nabla_a R)\,\tau_1 + \sqrt{2} R (\nabla_a \sigma)\,\tau_2 . \tag{23}$$

It is straightforward to check that the space-time metric (17) is recovered via $g_{ab} = \eta_{IJ} e^I_a e^J_b$ with the convention $\eta_{IJ} = 2Tr(\tau_I \tau_J)$.

The triad determines the (Christoffel symbols and the) internal connection ${}^3A^I_a$ uniquely. Its pull-back to the spatial slice Σ turns out to be

$$A_a = A^I_a \tau_I = \frac{\dot{\gamma}}{2} e^{(1/2)\,\gamma_\infty} (\nabla_a R)\,\tau_2 + e^{-(1/2)\,\gamma} (\nabla_a \sigma)\,\tau_0 . \tag{24}$$

Note, however, that since R, σ fail to be smooth at $R=0$ our connection also fails to be smooth there. However, our boundary conditions do ensure that all physical fields are smooth at the origin. Thus, this singularity is merely a reflection of a bad choice of gauge (which has in effect introduced a ''source'' at the origin). We can remedy this situation by a gauge transformation. The general form of gauge transformations is

$$A'_a = g A_a g^{-1} - (\partial_a g) g^{-1} \quad \text{with} \quad g = e^{\tau_I \Lambda^I(R,\sigma)} . \tag{25}$$

By choosing the transformation parameters to be $\Lambda^0 = e^{-(1/2)\,\gamma(0)} \sigma$ and $\Lambda^1 = \Lambda^2 = 0$, we obtain a smooth connection as desired:

$$A'_a = A'^I_a \tau_I = \frac{\dot{\gamma}}{2} e^{(1/2)\,\gamma_\infty} \nabla_a R [\cos\,\sigma \tau_2 - \sin\,\sigma \tau_1] + [e^{-(1/2)\,\gamma} - 1] \nabla_a \sigma \tau_0 . \tag{26}$$

B. Holonomy computation

The holonomy of A'^I_a along a loop η is given by a path ordered exponential of the integral of A'^I_a along η:

$$U_\eta[A] := \mathscr{P} \exp\left(\oint_\eta A_a dS^a \right) . \tag{27}$$

For quantum considerations, it turns out that the most interesting loops are the integral curves of the rotational Killing vector σ^a. Note that, along these curves, only the second term in the expression (26) of the connection contributes. Since the internal vector in this term is constant, this part of the connection is effectively Abelian. Recall that in the case of an Abelian connection the path ordered exponential reduces to an ordinary exponential. Hence, if η is chosen to be the integral curve of the Killing field with radius r_o, the holonomy can be easily evaluated. We have

$$U_\eta[A'] = \cos[\pi(1 - e^{-(1/2)\,\gamma(r_o)})] - 2\tau_0\, \sin[\pi(1 - e^{-(1/2)\gamma(r_o)})], \tag{28}$$

where we have used the fundamental representation of $SU(1,1)$. For our purposes, it will suffice to consider these particular loops.

Of special interest to the quantization program under consideration are the functions $T^0_\eta[A]$ of connections defined by the trace of the holonomy. Taking the trace of (28) yields

$$T^0_\eta[A'] = 2 \cos[\pi(1 - e^{-(1/2)\,\gamma(r_o)})] . \tag{29}$$

Note, incidentally, that if η is chosen to be the loop at infinity, $T^0_\eta[A]$ reduces to a simple function of the total energy of the coupled system. For the reduced system, $\gamma(r_o)$ represents precisely the energy of ψ in a box of radius r_o (where ψ is regarded as a scalar field propagating on the

Minkowskian background.) The question of whether the T^0_η can be promoted to a well-defined operator will therefore reduce to the question of whether the operator corresponding to the energy of a scalar field in a box can be satisfactorily regulated.

IV. QUANTUM THEORY

A. Quantization

The reduced phase space of section II D serves as the natural point of departure for quantization. Since the constraints have been solved, the algebra $\mathscr{A}$ of observables is easy to construct. The obvious complete set of classical observables is given by the smeared fields and momenta, $\psi(f) := \int dr f(r)\psi(r)$ and $p_\psi(g) := \int dr g(r) p_\psi(r)$, where f,g belong to the Schwartz space $\mathscr{S}$ of smooth test functions with rapid decay at infinity. Thus, the quantum algebra $\mathscr{A}$ is generated by operators $\hat{\psi}(f)$ and $\hat{p}_\psi(g)$, subject to the canonical commutation relations:

$$[\hat{\psi}(f),\hat{\psi}(g)]=0, \quad [\hat{p}_\psi(f),\hat{p}_\psi(g)]=0, \quad [\hat{\psi}(f),\hat{p}_\psi(g)]=i\int dr f g \hat{I}. \tag{30}$$

Our task is to find a representation of $\mathscr{A}$ which, furthermore, carries a well-defined Hamiltonian operator $\hat{H}$, the quantum analog of $(1/4G)(1-\exp(-\gamma_\infty/2))$.

For technical simplicity, we will regard $\hat{\psi}$ and $\hat{p}_\psi$ as operator-valued distributions in two (space) dimensions and incorporate rotational symmetry by restricting the states to be axisymmetric at the very end. Our experience from low dimensional, interacting scalar quantum field theories now suggests that we use as our Hilbert space $\mathscr{H}=L^2(\mathscr{S}',d\mu)$ where $\mathscr{S}'$ is the space of all tempered distributions on R^2, and μ a suitable measure thereon. (For details, see, e.g., Ref. 13). Since γ_∞ is the Hamiltonian of the free scalar field in Minkowski space, to make the quantum Hamiltonian operator well-defined, it is natural to use for μ the standard Gaussian measure for a free, massless scalar field with covariance $\frac{1}{2}\triangle^{-1/2}$, where $\triangle$ is the Laplacian on R^2 with respect to the flat metric

$$q^o_{ab}=\nabla_a R \nabla_b R + r^2 \nabla_a \theta \nabla_b \theta.$$

Thus, μ is defined by

$$\int_{\mathscr{S}'} d\mu e^{i\int d^2x f(\vec{x})\tilde{\psi}(\vec{x})} = e^{-(1/2)\int d^2x f(\vec{x})\triangle^{-1/2} f(\vec{x})}, \tag{31}$$

where $\tilde{\psi} \in \mathscr{S}'$. (Heuristically, ''$d\mu=[\exp-\frac{1}{2}\int d^2x(\psi\triangle^{1/2}\psi)]\mathscr{D}\psi$.'') The action of the basic operators is then given by

$$\hat{\psi}(f)\cdot\Psi(\psi)=\left(\int d^2x f\psi\right)\Psi(\psi) \quad \text{and} \quad \hat{p}_\psi(g)\cdot\Psi(\psi)=-i\int d^2x\left[g\frac{\delta}{\delta\psi}+\frac{1}{2}\psi\triangle^{1/2}g\right]\Psi(\psi) \tag{32}$$

where Ψ belongs to the dense sub-space of cylindrical functions in $\mathscr{H}$. The operators $\hat{\psi}(f)$ and $\hat{p}_\psi(f)$ admit self-adjoint extensions to $\mathscr{H}$. We will see below that the Hamiltonian is also represented by a self-adjoint operator and that, like its classical counterpart, it is positive.

This choice of representation is also suggested by the mathematical equivalence between our physical system and a free massless scalar field on Minkowski space defined by g^o_{ab} (see Eq. (21)). Thus, although our viewpoint is somewhat different, our final choice of representation is the same as that of Refs. 7 and 8.

In a more familiar terminology, our representation can be obtained by introducing an operator-valued distribution $\hat{\psi}(\vec{x},T)$ in the fictitious Minkowskian background (M,g^o_{ab}):

$$\hat{\psi}(\vec{x},T)=\frac{1}{2\pi}\int\frac{d^2k}{\sqrt{2\omega_k}}[\hat{A}(\vec{k})e^{i(\vec{k}\cdot\vec{x}-\omega_k T)}+\hat{A}^\dagger(\vec{k})e^{-i(\vec{k}\cdot\vec{x}-\omega_k T)}], \tag{33}$$

where $\omega_k=\sqrt{\vec{k}\cdot\vec{k}}$, and $\hat{A}(\vec{k})$ and $\hat{A}^\dagger(\vec{k})$ are the standard creation and annihilation operators. The Hilbert space $\mathscr{H}$ can be generated by repeated actions of creation operators on the vacuum. There is a well-defined self-adjoint operator $\hat{L}_\sigma$ on $\mathscr{H}$ which represents the total angular momentum along the Killing field $\partial/\partial\sigma$. The physical Hilbert space $\mathscr{H}_P$ is the eigenspace of $\hat{L}_\sigma$ with zero eigenvalue. Since zero is a discrete eigenvalue, $\mathscr{H}_P$ is a sub-space of $\mathscr{H}$.

The physical Hilbert space can also be obtained more directly by using, instead of (33), an operator valued distribution in which the zero angular momentum constraint has already been incorporated, namely,

$$\hat{\psi}(R,T)=\int_0^\infty dk[f_k^+(R,T)\hat{A}(k)+f_k^-(R,T)\hat{A}^\dagger(k)]. \tag{34}$$

Here $f_k^+(R,T)=[f_k^-(R,T)]^*=(1/\sqrt{2})J_0(kR)e^{-i\omega_k T}$, where, from now on, $J_n(kR)$ will denote the n-th order Bessel function of the first kind. Note that $f_k^+(R)$ are solutions of the equation of motion (21) and provide an orthonormal basis for the one-particle Hilbert space with respect to the Klein-Gordon inner-product. (Our normalization is such that the creation and annihilation operators satisfy the commutation relations $[\hat{A}(k),\hat{A}^\dagger(k')]=\delta(k,k')$.) The physical Hilbert space $\mathscr{H}_P$ can be generated by repeatedly acting on the vacuum by the creation operators $\hat{A}^\dagger(k)$. In what follows, we will use both the two-dimensional as well as the one-dimensional descriptions given by (33) and (34).

We will conclude this sub-section with three remarks.

(1) Since the physical Hilbert space has a Fock structure, it is tempting to refer to the quanta created by $\hat{A}^\dagger(k)$ as (scalar) ''particles'' and we will often do so. Note, however, that from the point of view of the coupled Einstein-Klein-Gordon system we began with, this description is gauge dependent. The system has one local degree of freedom and we chose to put it in the scalar field. Another gauge choice could put it in the gravitational field and the interpretation of quantum states would then be different. However, the interpretation *is* unambiguous at null infinity, i.e., for asymptotic states, because one does not need to fix gauge there (see below).

(2) We now have the full Hilbert space of states. So, it is natural to examine if one can generate a picture of space-*time*, as opposed to just spatial, quantum geometry in spite of our use of the canonical approach. As one might expect from our gauge-fixing procedure, the answer is in the affirmative. In the fixed chart (T,R,σ) on M, the metric operator can be (heuristically) written as

$$\text{``}\hat{g}_{ab}=:e^{\hat{\gamma}(R,T)}:(-\nabla_a T\nabla_b T+\nabla_a R\nabla_b R)+R^2\nabla_a\sigma\nabla_b\sigma,\text{''} \tag{35}$$

where, as usual, the double-dots indicate normal ordering. (The reason behind the qualification ''heuristic'' and the quotes will become clear in section IV C.)

We can now ask if there are well-defined semi-classical states peaked at classical solutions. The answer is again in the affirmative. Consider, in the Fock space, a coherent state $|\Psi_c\rangle$ which is peaked at a classical solution $c(R,T)$ of (21). In the configuration representation, these are Gaussians for which the uncertainty in the field operator and its momentum are ''shared equally,'' the product of the two uncertainties being minimum *for all times T*. On these states, the expectation value of the metric operator (35) *is well-defined* and is given just by

$$\langle\Psi_c|\hat{g}_{ab}|\Psi_c\rangle=e^{\gamma[c,p_c]}(-\nabla_a T\nabla_b T+\nabla_a R\nabla_b R)+R^2\nabla_a\sigma\nabla_b\sigma, \tag{36}$$

where $\gamma[c,p_c]$ is the right side of (16), evaluated on the initial data of the classical solution c. Thus, every coherent states in our physical Hilbert space $\mathscr{H}_o$ remains peaked at a classical scalar field c *and* a metric g_{ab}, satisfying the coupled Einstein-Klein-Gordon equation. While the result is technically rather simple, conceptually it is somewhat surprising. For the coupled system satisfies highly non-linear equations and the wave packets do not disperse in spite of these non-linearities.

(3) It is well-known that there exist an infinite number of unitarily inequivalent representations of the algebra $\mathscr{A}$. Our additional requirements are that the Hamiltonian operator be well-defined and that the physical states be invariant under the rotational symmetry corresponding to $\partial/\partial\sigma$. Unfortunately, these requirements by themselves are not strong enough to select a representation uniquely. To single out the Fock representation in Minkowskian quantum field theories, one needs additional conditions that refer to the action of the Poincaré group. In our case, the Minkowski space-time (M,g^o_{ab}) is only a fictitious background and its Poincaré group has no physical significance in the full, coupled system.

Nonetheless, it *is* possible to single out our representation by two methods. The first involves the imposition of reality conditions as indicated in Ref. 4: The measure μ on $\mathscr{S}'$ is singled out by the condition that the operators $\hat{\psi}(f)$ and $\hat{p}_\psi(g)$ of (32) be self-adjoint. The second method invokes the S-matrix theory. It turns out that the Einstein-Rosen waves are all asymptotically flat at null infinity in $2+1$ dimensions.[14] Furthermore, the classical S-matrix is well-defined: the data on past null infinity determines the solution uniquely which in turn determines the data on future null infinity. Hence, it is natural to use the asymptotic quantization scheme[15] to quantize the coupled system *at* past and future null infinity. It turns out that our Fock representation is naturally isomorphic to the simplest representation obtained by asymptotic quantization (either at past *or* future null infinity). Details will appear elsewhere.

B. Hamiltonian and time

Recall that, after reduction, the classical Hamiltonian is given by $H=(1/4G)[1-\exp-(\frac{1}{2}\gamma_\infty)]$. Since γ_∞ is the Hamiltonian of a free scalar field in Minkowski space, the normal-ordered operator $:\hat{\gamma}_\infty:$ admits the standard self-adjoint extension which, for simplicity, we will denote also by $:\hat{\gamma}_\infty:$. Then, the standard spectral theorems ensure that

$$\hat{H} := \frac{1}{4G}(1-e^{-(1/2):\hat{\gamma}_\infty:}) \equiv \frac{1}{4G}(1-e^{-\int k dk \hat{A}^\dagger(k)\hat{A}(k)}) \tag{37}$$

is a well-defined, self-adjoint operator. Since $:\hat{\gamma}_\infty:$ is a non-negative, unbounded operator and since $f(\lambda)=(1-e^{-\lambda/2})$ takes values in $[0,1]$ for $\lambda \in [0,\infty]$, it follows that the spectrum of H is given by $[0, 1/4G]$. If we consider states in $\mathscr{H}_P$ with higher and higher frequency, the expectation value of $\hat{\gamma}_\infty$, i.e., the energy in the field from the mathematical, Minkowskian perspective, increases unboundedly. However, the expectation value of the *physical* Hamiltonian $\hat{H}$ remains bounded and tends to the limit $1/4G$. Thus, the situation is completely analogous to that in the classical theory.[6]

Let us now examine the ground state. Since $|0\rangle$ is the unique ground state of $:\hat{\gamma}_\infty:$ on $\mathscr{H}_P$, it follows immediately that it is also the unique ground state of $\hat{H}$. Since $|0\rangle$ is, in particular, a coherent state, it is peaked at a classical solution to the coupled system. As one might expect, the solution is: $\psi=0$ and $g_{ab}=g^o_{ab}$ Thus, the quantum ground state is peaked on Minkowski space-time. The ground state geometry is thus quite tame; there is no evidence of wild fluctuations at the Planck scale.

What is the situation with general coherent states? Given a coherent state $|\Psi_c\rangle := \exp[\int dk c(k)\hat{A}^\dagger(k)]\cdot|0\rangle$, peaked at a classical solution c, we have

$$\left[\exp-\frac{1}{2}:\hat{\gamma}_\infty:\right]\cdot\Psi_c=\left[\exp\int dke^k c(k)\hat{A}^\dagger(k)\right]\cdot|0\rangle=:\Psi_{c'}, \tag{38}$$

where $c'(k)=e^k c(k)$. Thus, the image is again a coherent state but its peak is shifted. Therefore, the expectation value of the Hamiltonian in a coherent state Ψ_c is given by

$$\frac{\langle\Psi_c,\hat{H}\cdot\Psi_c\rangle}{\langle\Psi_c,\Psi_c\rangle}=\frac{1}{4G}\left[1-\exp\frac{1}{\hbar}\int dk(e^{-\hbar k}-1)|c(k)|^2\right], \tag{39}$$

where, to bring out the quantum effects, we have restored the factors of $\hbar$. (Recall also that, from the perspective of the 2+1-dimensional theory, the scalar field has to be rescaled by factors involving $\sqrt{G}$. The net effect is to replace $\hbar$ in (39) by $\hbar G$ which has the physical dimension of length.) In contrast, the classical energy (10) of the solution to the Einstein-Klein-Gordon equation determined by c is $E(c)=(1/4G)\,[1-\exp-\int dkk|c(k)|^2]$. If we expand out $\exp-\hbar k$ in (39), the leading term yields the classical answer. In general, the classical energy is a good approximation to the expectation value of the quantum Hamiltonian if $c(k)$ is concentrated on low frequencies. Quantum corrections (of order $(G\hbar)$ and higher) become more and more significant if the support of $c(k)$ is shifted to higher and higher frequencies.

Next, let us consider the issue of time. Recall that, in the classical theory, the Hamiltonian evolution is tied to time t, the affine parameter along the Hamiltonian vector field in the phase space. Each dynamical trajectory gives rise to a space-time and t can then be interpreted as a time coordinate in *that* space-time, $\partial/\partial t$ being an unit asymptotic time translation. From the decoupling viewpoint, on the other hand, it is the variable T that arises naturally; it represents time in the fixed Minkowskian background. What is the situation in the quantum theory? Now, our measure μ on $\mathscr{S}'$ which dictates the Hilbert structure is rooted in the flat two-geometry induced by g^o_{ab} or, alternatively, in the positive and negative frequency decomposition with respect to the Minkowskian time T. Indeed, since the field equation (20) in terms of t is non-linear, positive frequency decomposition with respect to t is not meaningful *a priori*. Thus, while t and T are on equal footing in the classical theory, our choice of representation breaks this symmetry in the quantum theory.

We can mimic the situation in the classical theory and introduce a dynamical parameter λ, analogous to the classical t, associated with the Hamiltonian:

$$i\hbar\frac{\partial\Psi}{\partial\lambda}=\hat{H}\cdot\Psi. \tag{40}$$

However, unlike in the classical theory, now a solution to the dynamical equation does *not* define a hyperbolic space-time and hence we can not interpret λ as a time parameter in the familiar sense, i.e., in space-time terms. However, a key simplification occurs if we restrict ourselves to coherent states Ψ_c. Since each of these states is peaked at a classical space-time, we can ask if, given any one of these states, we can interpret λ as a time parameter in the corresponding classical space-time. The answer is in the affirmative. In fact λ can be identified with the time coordinate t of that space-time! Thus, as one might have hoped, the familiar notion of time re-emerges in the semi-classical regime. In the full quantum theory, however, the dynamical parameter defined by the Hamiltonian does not have a simple space-time interpretation.

We will conclude this discussion with a remark. There is an obvious alternative form for the Hamiltonian: We can further normal-order $\hat{H}$ and define a new Hamiltonian $\hat{H}'=:\hat{H}:$. One can verify that $\hat{H}'$ is densely defined and admits a self-adjoint extension. It also annihilates $|0\rangle$. Furthermore, the expectation values of $\hat{H}'$ on a coherent state $|\Psi_c\rangle$ equals the classical energy of c. It thus appears to be an attractive alternative. However, its spectrum is the *entire real line*! This comes about because the overall normal ordering ensures that, while acting on n-particle states,

only the first $n+1$ terms in the expansion of the exponential in $\hat{H}'$ have non-vanishing contributions. Thus, for example, on one-particle states, $\hat{H}'$ has the same action as $\frac{1}{8}:\hat{\gamma}_\infty:$, which is unbounded above. Similarly, on two particle states, it is unbounded below. Given that the classically allowed energy values lie in the interval $[0, 1/4G]$, we can not take $\hat{H}'$ as the physically admissible quantum analog of the classical Hamiltonian.

C. Metric operator

Since we are dealing with a system with an infinite number of degrees of freedom, operators corresponding to physical observables have to be regulated. For the Hamiltonian, this was achieved via normal ordering. In this section, we will focus on the metric operator.

A formal expression for the metric operator was already given in (35), where regularization again consisted of normal ordering. Consider the sub-space of $\mathscr{H}_{\mathscr{P}}$ which is spanned by finite linear combinations of coherent states. It is easy to show that the sub-space is dense and that the matrix elements of the metric operator $\hat{g}_{ab}$ are well-defined on it. Thus, the formal expression (35) does lead to a well-defined *quadratic form*; in a field theory terminology, $\hat{g}_{ab}$ exists in the LSZ sense. However, this does *not* imply that $\hat{g}_{ab}$ is well-defined *as an operator* on this sub-space. Note that this is *not* a peculiarity of quantum field theory; one encounters such situations already in non-relativistic quantum mechanics. Consider, for example, a one-dimensional harmonic oscillator. The operator $\exp(\alpha a^\dagger a^\dagger)$ has finite matrix elements on the basis $|n\rangle$ for all complex numbers α. However, if $|\alpha|>1$, the norm $\|e^{\alpha a^\dagger a^\dagger}|n\rangle\|$ diverges for any $|n\rangle$, whence the operator fails to be defined on the sub-space spanned by these basis vectors.

It turns out that the situation with the metric operator is quite analogous (which is the reason behind the quotes in (35)). To see this, let us begin with the first non-trivial term in the expansion of $\hat{g}_{RR}$ or $\hat{g}_{TT}$. Setting for simplicity $T=0$ in (34), we have

$$:\hat{\gamma}(R):=\frac{1}{2}\int dk_1\int dk_2[2F_+(R,k_1,k_2)(\hat{A}^\dagger(k_1)\hat{A}(k_2)) + F_-(R,k_1,k_2)(\hat{A}(k_1)\hat{A}(k_2)+\hat{A}^\dagger(k_1)\hat{A}^\dagger(k_2))], \tag{41}$$

where

$$F_\pm(R,k_1,k_2)=\pm k_1k_2\int_0^R rdr(J_0(k_1r)J_0(k_2r)\pm J_1(k_1r)J_1(k_2r)). \tag{42}$$

For any fixed R, one can regard the coefficient $F_-(R,k_1,k_2)$ of $\hat{A}^\dagger(k_1)\hat{A}^\dagger(k_2)$ as a ''potential two-particle state'' in the Fock space. However, a direct calculation shows that its norm is ultraviolet divergent. This immediately implies that the norm $\|:\hat{\gamma}(R):|0\rangle\|$ also diverges, whence the operator fails to be well-defined on the vacuum state. Further calculations show that the same result holds for any coherent state.

What is the origin of this divergence? Recall that $:\hat{\gamma}(R,T):$, obtained by promoting (15) to an operator, has the same functional form as the restriction of the Hamiltonian of a scalar field to a box of size R. That is,

$$:\hat{\gamma}(R):=\frac{1}{2}\int_0^\infty dr\,\theta(R-r):\left(\frac{\hat{p}_\psi{}^2}{r}+r(\hat{\psi}')^2\right):, \tag{43}$$

where $\theta(R-r)$ denotes the Heaviside step-function, which equals 1 if $r<R$ and 0 otherwise. Normal ordering softens the singularity that arises from the fact that fields are being multiplied at

the same point. However, this turns out to be insufficient because of two simultaneous pathologies: the operator contains products of derivatives of the field $\hat{\psi}(R,T)$ and these are integrated on a region with *sharp* boundary.

Now, a natural strategy to obtain a well-defined metric operator in such circumstance is to soften the sharp boundary of the box. This can be achieved by replacing the Heaviside function $\theta(R-r)$ in (43) with a smooth function $f_R(r)$ which equals 1 for $r\leqslant R-\epsilon$, then it smoothly decreases to zero and equals zero for $r\geqslant R+\epsilon$, where ϵ is a small parameter. An example of such a regulator is

$$f_R(r)=\begin{cases}1, & \text{if } r\leqslant R-\epsilon,\\ \exp\left(-\dfrac{4\epsilon^2}{[r-(R+\epsilon)]^2}+1\right), & \text{if } R-\epsilon\leqslant r\leqslant R+\epsilon,\\ 0, & \text{if } r\geqslant R+\epsilon.\end{cases}$$

Now, in Minkowskian field theories, while one can begin with such a regulator, after suitable renormalization, one has to take the regulator away to ensure Poincaré invariance. In the present case, however, we need only respect the rotational symmetry and hence there is no *a priori* need to take the limit $\epsilon\to 0$. Indeed, the Planck length is now a natural candidate for ϵ.

Let us therefore fix a regulator f_R and consider the smeared version of (41):

$$:\hat{\gamma}(f_R,T):=\frac{1}{2}\int dk_1\int dk_2[2F_+(f_R,k_1,k_2)(\hat{A}^\dagger(k_1)\hat{A}(k_2)e^{i(k_1-k_2)T})+F_-(f_R,k_1,k_2)$$
$$\times(\hat{A}(k_1)\hat{A}(k_2)e^{-i(k_1+k_2)T}+\hat{A}^\dagger(k_1)\hat{A}^\dagger(k_2)e^{i(k_1+k_2)T})], \tag{44}$$

where

$$F_\pm(f_R,k_1,k_2)=\pm k_1k_2\int_0^\infty dr f_R(r)r(J_0(k_1r)J_0(k_2r)\pm J_1(k_1r)J_1(k_2r)). \tag{45}$$

The rest of this section is devoted to showing that this operator is well-defined so long as the smearing function f_R belongs to the Schwartz space $\mathscr{S}$.

The proof is technically simpler if we adopt the two-dimensional version of the Fock space introduced before (see (33)). For, we can then mimic the proofs of analogous statements from Ref. 16. Now, we can take as our smearing fields, elements $f_R(\vec{x})$ of the Schwartz space on R^2. (Thus, the results will in fact be slightly more general than what is need; $f_R(r)$ above is a special case of $f_R(\vec{x})$.)

Let us then write the smeared version of the operator (43) expressed in terms of the creation and annihilation operators given by (33). We have

$$:\hat{\gamma}(f_R,T):=\frac{1}{8\pi}\int d^2k_1\int d^2k_2[2G_+(f_R,\vec{k}_1,\vec{k}_2)\hat{A}^\dagger(\vec{k}_1)\hat{A}(\vec{k}_2)e^{i(\omega_{k_1}-\omega_{k_2})T}-G_-(f_R,\vec{k}_1,\vec{k}_2)$$
$$\times(\hat{A}(\vec{k}_1)\hat{A}(\vec{k}_2)e^{-i(\omega_{k_1}+\omega_{k_2})T}+\hat{A}^\dagger(\vec{k}_1)\hat{A}^\dagger(\vec{k}_2)e^{i(\omega_{k_1}+\omega_{k_2})T})], \tag{46}$$

where

$$G_\pm(f_R,\vec{k}_1,\vec{k}_2)=\pm\left(\frac{\omega_{k_1}\omega_{k_2}+\vec{k}_1\cdot\vec{k}_2}{\sqrt{\omega_{k_1}\omega_{k_2}}}\right)f(\vec{k}_1\mp\vec{k}_2), \tag{47}$$

and $f(\vec{k}_1 \pm \vec{k}_2)$ is the Fourier transform of the smearing function,

$$f(\vec{k}_1 \pm \vec{k}_2) = \frac{1}{2\pi} \int d^2x f_R(\vec{x}) e^{i(\vec{k}_1 \pm \vec{k}_2)\cdot \vec{x}}. \tag{48}$$

Let us begin by showing that the action of the operator (46) is well-defined on the vacuum state. Since $\hat{A}(\vec{k})$ annihilates the vacuum state, we have

$$\| :\hat{\gamma}(f_R): |0\rangle \|^2 = \int d^2k_1 \int d^2k_2 |G_-(f_R, \vec{k}_1, \vec{k}_2)|^2. \tag{49}$$

It follows immediately from (47) that this integral has no infra-red divergences. Therefore, from now on, let us concentrate only on the ultra-violet behavior of the integrand. The factor in the round brackets is ultra-violet divergent. The multiplicative factor f provides a damping, but only for large $|\vec{k_1} + \vec{k_2}|$. However, using simple algebra one can bound $G_-(f_R, \vec{k}_1, \vec{k}_2)$ of Eq (47) by

$$|G_-(f_R, \vec{k}_1, \vec{k}_2)| \leqslant \frac{|\vec{k}_1 + \vec{k}_2|^2 |f(\vec{k}_1 + \vec{k}_2)}{\sqrt{\omega_{k_1} \omega_{k_2}}}. \tag{50}$$

Now, because the smearing function $f_R(\vec{x})$ belongs to the Schwartz space, its Fourier transform $f(\vec{k}_1 + \vec{k}_2)$ falls faster than any polynomial in $|\vec{k_1} + \vec{k_2}|$. This in turn implies that $G_-(f_R, \vec{k}_1, \vec{k}_2)$ is square integrable. Note that the smearing function plays a crucial role in this argument. Had we replaced $f_R(\vec{x})$ by the Heaviside function θ the corresponding Fourier transformed function $f(\vec{k}_1 + \vec{k}_2)$ would behave as $1/|\vec{k}_1 + \vec{k}_2|$ which would not be sufficient to ensure square-integrability of $G_-(f_R, \vec{k}_1, \vec{k}_2)$ (see (50)). Finally, as a side remark, note that the procedure followed above to prove that $G_-(f_R, \vec{k}_1, \vec{k}_2)$ is square integrable does not go through for G_+ because of the minus sign in the argument of the function $f(\vec{k}_1 - \vec{k}_2)$ (see (47)).

Next, one can show that the action of this operator is in fact well-defined on a generic n-particle state on the Fock space,

$$|\Psi_n\rangle = \int d^2k_1 \cdots d^2k_n g^{(n)}(\vec{k}_1, \cdots, \vec{k}_n) \hat{A}^\dagger(\vec{k}_1) \cdots \hat{A}^\dagger(\vec{k}_n) |0\rangle, \tag{51}$$

where $g^{(n)}(\vec{k}_1, \cdots, \vec{k}_n) = \langle \vec{k}_1, \cdots, \vec{k}_n | \Psi_n \rangle$, and $\int d^2k |g^{(n)}(\cdots, \vec{k}, \cdots)|^2 < \infty$. Now the terms involving annihilation operators will also contribute. The final result is that $\| :\hat{\gamma}(f_R): |\Psi_n\rangle \|$ is finite provided that $|\Psi_n\rangle$ is a state such that $\int d^2k |\vec{k}|^2 |g^{(n)}(\cdots, \vec{k}, \cdots)|^2 < \infty$. (This restriction comes from the ''particle number preserving term'' in (46).) Since finite linear combinations of these states form a dense subset of the Hilbert space, we have now established that the operator $:\hat{\gamma}(f_R):$ is densely defined on $\mathscr{H}_{\mathscr{F}}$.

By inspection, it is also symmetric on this space. We will now show that it admits a self-adjoint extension to $\mathscr{H}_P$. For this, by a theorem due to Von-Neumann,[17] it is sufficient to exhibit on $\mathscr{H}_P$ an anti-linear operator $\hat{C}$ with $\hat{C}^2 = 1$ which leaves the domain of $:\hat{\gamma}(f_R):$ invariant and commutes with it. We can take $\hat{C}$ to be the complex-conjugation operator on $\mathscr{H}_P = L^2(\mathscr{S}', d\mu)$. It is straightforward to show that $\hat{C}$ commutes with $\hat{\psi}(\vec{x}, T)$ whence $\hat{C}\hat{A}(\vec{k}) = \hat{A}(-\vec{k})\hat{C}$ and $\hat{C}\hat{A}^\dagger(\vec{k}) = \hat{A}^\dagger(-\vec{k})\hat{C}$. Finally, since $G_\pm(f_R, \vec{k}_1, \vec{k}_2)$ is real and equals $G_\pm(f_R, -\vec{k}_1, -\vec{k}_2)$, it follows that $\hat{C}$ satisfies the conditions of Von-Neumann's theorem. Again, for notational simplicity, we will denote the self-adjoint extension also by $:\hat{\gamma}(f_R):$.

We can now return to the metric. Since $:\hat{\gamma}(f_R):$ is a self-adjoint operator on $\mathscr{H}_P$, it follows that $\exp:\hat{\gamma}(f_R):$ is also self-adjoint. Thus, we can now give meaning to the formal expression (35) and define a regulated operator for the full space-*time* metric:

$$\hat{g}_{ab}(f) = e^{:\hat{\gamma}:(f_R,T)}(-\nabla_a T\nabla_b T + \nabla_a R\nabla_b R) + R^2\nabla_a\sigma\nabla_b\sigma, \tag{52}$$

within canonical quantization. In the classical theory, the existence theorems ensure that a space-time metric can be recovered from the canonical framework. There is, however, no such general result in the quantum theory. Our success can be traced back to the use of a well-suited gauge fixing procedure. (Whether a different choice of gauge will give equivalent results is far from being clear.)

At first, it is somewhat confusing that while we do not need a smearing function to obtain a well-defined quadratic form, we need one to obtain a well-defined operator. Note, however, that the situation is rather similar even in the classical theory! The metric component $\exp\gamma(R)$ is a well-defined functional on (a dense sub-space of) the reduced phase space. However, precisely because of the sharpness of the boundary, this functional *fails* to give rise to a well-defined Hamiltonian vector field. To obtain a Hamiltonian vector field, one again needs to soften the boundaries using a smearing function. The fact that the unsmeared functional is well-defined is analogous to the fact that, in the quantum theory, the quadratic form is well-defined without smearing. The smeared quantum operator is the analog of the smeared classical observable with a well-defined Hamiltonian vector field. From this perspective, in fact it would have been surprising if a self-adjoint metric operator had existed without smearing; it would then have defined a one-parameter group of motions on the Hilbert space which would have no classical counterpart.

D. Quantum geometry

We will now briefly investigate three consequences of the results obtained in the last three sub-sections. The discussion will be rather general and we will only indicate the directions along which more detailed work could be done.

The first concerns the issue of vacuum fluctuations of geometry. To compute these, we need a well-defined operator; quadratic forms do not suffice. Let us therefore consider the regulated metric operator (52). Since it is completely determined by $:\hat{\gamma}(f_R,T):$, let us focus on this latter operator. The vacuum expectation value of this operator is zero. However, because of the vacuum fluctuations, there is a non-zero probability of finding other values as well. A qualitative measure of these probabilities is given by the uncertainty

$$[\delta:\hat{\gamma}(f_R,T):]^2 := \langle 0|(:\hat{\gamma}(f_R,T):)^2|0\rangle - \langle 0|:\hat{\gamma}(f_R,T):|0\rangle^2 = \int dk_1 dk_2 |F_-(f_R,k_1,k_2)|^2. \tag{53}$$

The right side is a measure of the fluctuation of the metric coefficients around the mean. An immediate consequence of the above result is the existence of the fluctuations of the light cone. To see this, consider a vector k^a in the tangent space of a point (T,R,σ) which is null with respect to g^o_{ab}. Now, due to the vacuum fluctuations of the metric operator, the value of the norm of k^a is uncertain and, since the fluctuation can have either sign, there is in general a non-zero probability for k^a to be space-like or time-like. The exception occurs if the vector k^a is radial, i.e., orthogonal to $\partial/\partial\sigma$. Then, because of the specific form (52) of the metric operator, k^a continues to be null. (Similar considerations obviously apply to time-like and space-like vectors.) This simple example illustrates that, contrary to an oft-expressed view, the canonical framework *is* capable of addressing space-*time* issues such as the fluctuations of the causal structure.

The second feature we wish to discuss concerns the commutator of the metric operators at the same value of T. Again, in this calculation, quadratic forms do not suffice and we must use the regulated operator (52). A straightforward calculation yields

$$[:\hat{\gamma}(f_R):,:\hat{\gamma}(g_{R'}):]=\frac{i}{2}\int d^2x(f(\vec{x})\nabla^a g(\vec{x})-g(\vec{x})\nabla^a f(\vec{x}))\times:(\hat{p}_\psi(\vec{x})\nabla_a\hat{\psi}(\vec{x})+\nabla_a\hat{\psi}(\vec{x})\hat{p}_\psi(\vec{x})):. \tag{54}$$

Thus, the commutator does *not* vanish; the non-vanishing contribution comes from the smeared boundary at the smaller of R and R'. At first the result seems surprising since $\hat{\gamma}(f_R)$ and $\hat{\gamma}(g_{R'})$ dictate the ''value'' of the metric operator at points R and R' which can be widely separated (and have the same value of T). However, the result does not contradict any physical principle. For, although the basic field operators $\hat{\psi}$ and $\hat{p}_\psi$ associated with such points do commute, the metric operator is a *non-local* functional of these.

Indeed, the result has a classical analog. As we pointed out at the end of the last sub-section, the unsmeared metric g_{ab} does not define a Hamiltonian vector field on the reduced phase space. Hence, to evaluate Poisson brackets, we are forced to use the smeared metric. Then, it is easy to verify that the Poisson brackets between the functionals $\gamma(f_R)$ and $\gamma(g_{R'})$ fail to vanish even when R and R' are widely separated. In fact these Poisson brackets just mirror the commutators given above.

The last point we wish to discuss concerns the holonomies computed in section III. We found that the expression of the holonomy involves the exponential of the integral of the connection along a loop on Σ. Now, as we indicated in the Introduction, there is a canonical quantization program which is based on the assumption that the quantum analogs of these holonomies are well-defined operators. The present model provides a good testing ground for the validity of this assumption.

To see that the issue is non-trivial, let us first recall the situation in the well-understood Maxwell theory, say in $2+1$ dimensions. There, the connection is generally promoted to an operator-valued distribution and the holonomies (of real connections) fail to be well-defined in the standard Fock representation. For in a $2+1$-dimensional theory, the operator-valued connection has to be smeared with two-dimensional test fields while loops have only one-dimensional support. In the present case, we are also using a Fock representation. A natural question therefore arises: Is the situation then analogous to the Maxwell theory? If so, the basic assumption mentioned above would fail to hold in our solution.

Now, because of axi-symmetry, smearing along a path in the radial direction in effect corresponds to a two-dimensional smearing. Hence, the acid test is provided by loops $R=\text{const}$ where one can not take advantage of axi-symmetry. Can the classical expression (29) of the trace of the holonomy along such a loop, η, be promoted to a well-defined, regulated operator? Following the procedure we used in section IV C, we find that the answer is in the affirmative. The quantum operator is given by

$$\hat{T}^0_\eta=2\cos[\pi(1-e^{-(1/2):\hat{\gamma}(f_R):})]. \tag{55}$$

The standard spectral theorems ensure that the operator on the right is well-defined, self-adjoint and has spectrum bounded between -1 and $+1$. Thus, the situation is very different from that in the Maxwell case. Indeed, in the present case, it is the scalar field that is subject to Fock quantization. The connection, like the metric, is a *non-local* functional of the elementary scalar field; its expression involves two-dimensional integrals of the basic fields. It is because of this that the trace of the holonomy can be promoted to a well-defined operator on $\mathscr{H}_P$. As in the case of the metric, if we were interested only in quadratic forms, there would be no need to use any smearing fields; they are needed only if one wishes to obtain genuine operators.

V. DISCUSSION

The mathematical structure of the classical Einstein-Rosen waves has been well-known for a long time. In light of those results, it is not at all surprising that the true degrees of freedom can

be coded in a scalar field satisfying the wave equation with respect to a fictitious Minkowski space and quantization of this field in itself is trivial. Thus, the underlying structure of our final theory is the expected one. The main purpose of the analysis was, rather, to apply the standard canonical quantization method, which is applicable in the more general context, to arrive at this final picture systematically. That is, since the model is technically sufficiently simple to be exactly soluble, we used it to better understand the standard quantization techniques and to probe conceptual and technical issues of quantum general relativity.

Indeed, the analysis shed light on a number of these. At the classical level, we saw that one can effectively exploit asymptotic flatness to disentangle gauge from dynamics. Gauge conditions can be imposed to handle constraints and to extract the true degrees of freedom. In the final picture, we are still left with a non-trivial Hamiltonian. Consequently, the issue of deparametrization never enters our analysis. Similarly, we did not find it necessary to introduce ''clock degrees of freedom''[18] at infinity to extract dynamics. In the quantum theory, we saw that there exist semi-classical states which are peaked at classical solutions of the coupled Einstein-scalar field system. The positive energy theorem goes over to the quantum theory and the quantum Hamiltonian has the same upper bound as the classical one. The solution also confirms the general expectation about the issue of time in quantum theory in the asymptotically flat context. The parameter t arises as the affine parameter along the Hamiltonian vector field on the classical phase space and has the space-time interpretation of time in the three-metric defined by any dynamical trajectory in the phase space. (This is also the situation in full general relativity.) In the quantum theory, an analogous parameter enters the Schrödinger equation (40). However, since general quantum states do not correspond to classical space-times, this parameter does not have the standard interpretation of time. This interpretation emerges only in the semi-classical regime: in any coherent state, the parameter can be identified with the classical t. Finally, we saw that the regulated metric and holonomy operators can be constructed by a careful smearing procedure which smoothens the sharp boundaries that enter the definition of their classical analogs. The associated functional analysis subtleties are non-trivial even from the mathematical perspective of a free field in Minkowski space.

In the technical discussion, we made a liberal use of the fictitious Minkowskian background g^o_{ab} and the associated time parameter T. However, this was done primarily for pedagogical reasons, i.e., to bring out the relation between the final quantum theory and the expected one. We could have arrived at our Hilbert space of states directly from the reduced phase space either by making use of the ''reality condition'' strategy[4] or by making an appeal to null infinity and the S-matrix theory, without having to explicitly introduce g^o_{ab}.

How do these results compare with those available in the literature? Our analysis is closely related to that of Refs. 7 and 8. In the classical theory, the main difference lies in our systematic handling of the asymptotically flat boundary conditions. In particular, in our treatment, the true Hamiltonian arose directly from the boundary term in the action. This point could not have been realized in the early analyses because the relation between $3+1$- and $2+1$-dimensional theories was not well-known and, more importantly, because a clear understanding of asymptotic flatness in $2+1$ dimensions has emerged only recently. (Indeed, given what was known in the early seventies, the treatment of Ref. 7 seems to be surprisingly ahead of its time!) In the quantum theory, the difference lies in the treatment of certain functional analytical subtleties. That it is necessary to regularize the metric operator was realized in Ref. 8. However, the suggestion there that the softening of the sharp boundaries can be brought about by a simple ultra-violet cut off in the momentum space is incorrect; one needs suitable smearing fields *in space-time*. Thus, our regularization differs from that in Ref. 8. Finally, our isolation of true degrees of freedom was carried out in $2+1$ dimensions. When translated to a $3+1$-dimensional perspective, our result is equivalent to the definition of true observables given in Ref. 19.

Since the model has been solved exactly within the standard canonical framework, it opens

doors for further analysis in a number of directions. We will conclude by mentioning a few of these.

First, we can now explore quantum field theory on a *quantum* geometry. Part of the motivation here is similar to that of quantum field theory in curved space-times; one wishes to investigate the effects of a non-trivial background geometry on quantum fields. Furthermore, this analysis can also shed light on the nature of quantum geometry itself. For instance, we may choose as our background a coherent state. The geometry influences the dynamical evolution of the quantum field because the metric appears in the expression of the Hamiltonian of the test field. Now, in the quantum theory, we have two alternatives. First, we can consider just the quadratic form that is determined by the (normal-ordered, unsmeared) metric (35) and substitute its value in a coherent state in the expression of the Hamiltonian. Since this value is just the classical metric, this would lead us just to the standard quantum field theory in curved space-times. To probe the effects of the *quantum* nature of geometry, we would have to look beyond just the expectation values. This can not be handled by a quadratic form alone; we need a genuine operator. Thus, the second, and much more interesting, possibility is to use the smeared metric operator in the expression of the Hamiltonian of the test field. Then, one would see the effects of the quantum geometry on the evolution of the matter, even in the case when the geometry is assumed to be in the vacuum state (initially). This analysis would be interesting because much of the standard apparatus of quantum field theory in curved space-times uses the fixed causal structure of the classcial geometry which is now absent. Using the canonical framework, one would be able to do quantum theory of test fields even when the causal structure is subject to quantum fluctuations of its own.

Recall that, in the regularization of the metric operator, we needed a smearing function f_R. There is, however, no ''canonical'' choice; while we know what the qualitative behavior of f_R should be, there is considerable freedom in its detailed form. Thus, we do not have a ''canonical'' regularized metric operator. All choices provide the required ultra-violet cut-offs but the precise damping depends on the specific form of f_R. The differences will show up, for example, in the evolution of test fields. It would be interesting to investigate these differences and see if one can restrict the choice of the smearing functions through thought experiments. If one can not, there would a genuine quantization ambiguity. The situation would be similar to that in non-relativistic quantum mechanics where, in general, the factor ordering ambiguities can not be resolved purely on theoretical grounds.

We saw that the regularized operators corresponding to the traces of holonomies of connections are well-defined on the quantum Hilbert space. Now, in the approach to quantum gravity based on these holonomies,[4] a striking picture of quantum geometry has emerged in which geometrical operators such as areas and volumes have a *discrete* spectrum. It is therefore natural to ask if the same is true in the present case. The question is now manageable, thanks to the regularized metric operators. Since the basic operator $:\hat{\gamma}:$ is the regularized version of the restriction of the Hamiltonian in a box, it is quite likely that its spectrum is discrete. If so, the lengths in the radial directions and areas will be quantized. This would be a striking result coming from a Fock-like representation.

Another direction for further investigation is provided by the Gowdy models. Since these are spatially compact and have initial curvature singularities, new issues arise. These will be discussed in the sequel to this paper. While both these problems deal only with the ''one polarization'' case—the two Killing fields are hyper-surface orthogonal in the $3+1$-dimensional picture—one can also investigate the two polarization case.[11] In the case when the translational Killing field is time-like, this case was analyzed in detail by Korotkin and Nicolai[20] recently. Their quantization is mathematically complete but somewhat unconventional in the sense that the relation between their Hamiltonian description and the standard Poisson-brackets of classical general relativity is unclear. It would be interesting to compare the results obtained here with the reduction of their model to the one polarization case. More recently, an infinite number of conserved quantities have been constructed in the classical theory with two polarizations.[21] Using these, one may be able to

extract the true degrees of freedom in this more general case and quantize the model along the lines of this paper.

Finally, the present model itself offers an attractive setting to explore the idea of ''fuzzing'' of space-time points using techniques involving null infinity.[22] As mentioned in section IV A, the $2+1$-dimensional space-times considered here are asymptotically flat at null infinity.[14] Furthermore, since the form of the metric is sufficiently simple, it should be possible to integrate the null geodesics and express the ''light cone cuts of null infinity'' explicitly in terms of the initial data for the scalar field at null infinity. These cuts label space-time points. The asymptotic quantization of the scalar field,[15] which is equivalent to the quantization presented here, would then lead to fuzzy points. So far, in this approach, detailed calculations have been carried out only in the linearized approximation.[22] The underlying simplicity of cylindrical waves provides an interesting arena where these results can be extended beyond the linear context.

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Loop variables and holonomies for a class of conical space–times

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We compute the loop variables for a class of space–times with topological defects. In particular we compute these quantities for multiple moving cosmic strings and two plane topological defects crossed by a cosmic string, showing that these quantities are elements of the homogeneous Lorentz group. We also compute the loop variables for a multi-chiral cone and we show that in the context of Einstein theory the loop variables are elements of the inhomogeneous Lorentz group, but in the context of Einstein-Cartan theory they are elements of the homogeneous Lorentz group. © *1996 American Institute of Physics.* [S0022-2488(96)00411-2]

I. INTRODUCTION

In the loop space formalism for gauge theories[1] the fields depend on paths rather than on space–time points, and a gauge field is described by associating with each path in space–time an element of the corresponding gauge group. The fundamental quantity that arises from this path-dependent approach, the non-integrable phase factor[2] (or loop variable) represents the electromagnetic field or a general gauge field more adequately than the field strength or the integral of the vector potential.[2] In the electromagnetic case, for example, as observed by Wu and Yang,[2] in a situation where global aspects are taken into consideration the field strength underdescribes the theory and the integral of the vector potential for every loop overdescribes it. The exact description is given by the factor $\exp((ie/\hbar c)\oint_c A_\mu dx^\mu)$.

The extension of the loop formalism to the theory of gravity was first considered by Mandelstam[3] who established several equations involving the loop variables, and also by Voronov and Makeenko.[4] Recently, Bollini *et al.*[5] computed the loop variables for the gravitational field corresponding to the Kerr metric.

The loop variables in the theory of gravity are matrices representing parallel transport along contours in a space–time with a given affine connection. They are connected with the holonomy transformations which contain important topological information. These mathematical objects contain information, for example, about how vectors change when parallel transported around a closed curve. The computation of these quantities is definitely interesting, although perhaps its main significance is for a fairly narrow area of physics.

Suppose that we have a vector v^α at a point P in a space–time and a closed curve C which begins and ends at P. Then, one can produce a vector $\overline{v^\alpha}$ at P which, in general, will be different from v^α, by parallel transporting v^α around C. In this case, we associate with the point P and the curve C a linear map U^α_β such that for any vector v^α at P, the vector $\overline{v^\alpha}$ at P results from parallel transporting v^α around C and is given by $\overline{v^\alpha}=U^\alpha_\beta v^\beta$. The linear map U^α_β is called holonomy transformation associated with the point P and the curve C. If we choose a tetrad frame and a

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parameter $\lambda \in [0,1]$ for the curve C such that $C(0)=C(1)=P$, then in parallel transporting a vector v^{α} from $C(\lambda)$ to $C(\lambda+d\lambda)$, the vector components change by $\delta v^{\alpha}=M^{\alpha}_{\beta}[x(\lambda)]v^{\beta}$, where M^{α}_{β} is a linear map which depends on the tetrad, the affine connection of the space–time and the value of λ. Then, it follows that the holonomy transformation U^{α}_{β} is given by the ordered matrix product of the N linear maps,

$$U^{\alpha}_{\beta}=\lim_{N\to\infty}\prod_{i=1}^{N}\left\{\delta_{\alpha\beta}+\frac{1}{N}M^{\alpha}_{\beta}[x(\lambda)]_{\lambda=i/N}\right\}. \tag{1.1}$$

One often writes the expression in Eq. (1.1) as

$$U(C)=P\ \exp\left(\int_{C}M\right), \tag{1.2}$$

where P means ordered product along a curve C. Equation (1.2) should be understood as an abbreviation of the right hand side of Eq. (1.1). Note that if M^{α}_{β} is independent of λ, then it follows from Eq. (1.1) that U^{α}_{β} is given by $U^{\alpha}_{\beta}=(\exp M)^{\alpha}_{\beta}$.

In this paper we shall use the notation

$$U_{BA}(C)=P\ \exp\left(\int_{A}^{B}\Gamma_{\mu}(x(\lambda))\frac{dx^{\mu}}{d\lambda}d\lambda\right), \tag{1.3}$$

where Γ_{μ} is the tetradic connection and A,B are the initial and final points, respectively, of the path. Then, associated with every path C from a point A to point B, we have a loop variable given by Eq. (1.3) which is a function of the path C as a geometrical object.

The purpose of this paper is to compute loop variables and holonomy transformations for some conical space–times and show how these quantities depend on the parameters defining the topological defects. In particular, we compute the loop variables in a space–time with a topological defect corresponding to the multiple parallel chiral strings in the context of Einstein[6] and Einstein-Cartan theories,[7] and the multiple moving crossed cosmic strings.[8] Finally, we consider the topological defects corresponding to two domain walls crossed by a cosmic string[9] and two plane topological defects crossed by a cosmic string[9] also.

II. LOOP VARIABLES IN THE SPACE-TIME OF MULTIPLE MOVING CROSSED COSMIC STRINGS

Recently, Letelier and Gal'tsov[8] found an exact solution of the Einstein equations describing an arbitrary number of non-parallel straight infinitely long cosmic strings moving with different constant velocities. The metric corresponding to this configuration of strings is given by

$$ds^2=-e^{-4V}(dx+F_1dt+G_1dz)^2-e^{-4V}(dy+F_2dt+G_2dz)-dz^2+dt^2, \tag{2.1}$$

where $V=2\Sigma_{i=1}^{N}\mu_i\ln r_i$, with $r_i=|\zeta-\alpha_i|$ and $\zeta=x+iy$, $\alpha_j=v_{xj}t+m_{xj}z+x_{0j}+i(v_{yj}t+m_{yj}z+y_{0j})$. The functions $F_1(G_1)$ and $F_2(G_2)$ are the real and imaginary parts of two analytic functions on the variable ζ; also these functions depend on t and z through the combinations α_i. The explicit form of these functions will not play a major role in our analysis, and they can be found in Ref. 8.

Our interest in computing loop variables for this space–time is to show how we can construct the parallel transport operators using the tetrad formalism, a subject which is definitely interesting. To do this let us introduce a set of four vectors $e^{\mu}_{(a)}$ ($a=1,2,3,4$ is a tetradic index) which are orthonormal at each point with respect to the metric with Minkowski signature, that is,

$g_{\mu\nu}e^{\mu}_{(a)}e^{\nu}_{(b)}=\eta_{ab}=\mathrm{diag}(-1,-1,-1,+1)$. We assume that the $e^{\mu}_{(a)}$'s are matrix invertible, that is, that there exists an inverse frame $e^{(a)}_{\mu}$ given by $e^{(a)}_{\mu}e^{\nu}_{(a)}=\delta^{\nu}_{\mu}$ and $e^{(a)}_{\mu}e^{\mu}_{(b)}=\delta^{a}_{b}$.

Now define the 1-forms θ^a as

$$\theta^1=e^{-2V}(dx+F_1dt+G_1dz),$$

$$\theta^2=e^{-2V}(dy+F_2dt+G_2dz), \tag{2.2}$$

$$\theta^3=dz, \quad \theta^4=dt.$$

Then, in the coordinate system $(x^1=x,\ x^2=y,\ x^3=z,\ x^4=t)$, the tetrad frame defined by $\theta^a=e^{(a)}_{\mu}dx^{\mu}$ is given by

$$e^{(1)}_1=e^{-2V}, \quad e^{(1)}_3=e^{-2V}G_1, \quad e^{(1)}_4=e^{-2V}F_1, \quad e^{(2)}_2=e^{-2V},$$
$$e^{(2)}_3=e^{-2V}G_2, \quad e^{(2)}_4=e^{-2V}F_2, \quad e^{(3)}_3=1, \quad e^{(4)}_4=1. \tag{2.3}$$

Using Cartan's structure equations $d\theta^a+\omega^a_b\wedge\theta^b=0$, for arbitrary functions V, F_1, G_1, F_2 and G_2 we get the following expressions for the tetradic connection:

$$\Gamma^1_{\mu3}dx^{\mu}=-e^{-2V}\chi_1dx-\tfrac{1}{2}e^{-2V}(\chi_2+2F_1\chi_1)dt-e^{-2V}G_1\chi_1dz=-\Gamma^3_{\mu1}dx^{\mu},$$

$$\Gamma^2_{\mu1}dx^{\mu}=-2\frac{\partial V}{\partial y}dx-2\frac{\partial V}{\partial x}dy+\frac{1}{2}\left(\xi_1+4F_2\frac{\partial V}{\partial x}-4F_1\frac{\partial V}{\partial y}\right)dt+\left(2G_2\frac{\partial V}{\partial x}-2G_1\frac{\partial V}{\partial y}+\xi_2\right)dz$$
$$=-\Gamma^1_{\mu2}dx^{\mu},$$

$$\Gamma^2_{\mu3}dx^{\mu}=e^{-2V}\chi_1dy+e^{-2V}G_2\chi_1)dz=-\Gamma^3_{\mu2}dx^{\mu}, \tag{2.4}$$

$$\Gamma^3_{\mu4}dx^{\mu}=\frac{1}{2}e^{-4V}\eta_1(dy+F_2dt+G_2dz)+\frac{1}{2}e^{-4V}\chi_2(dx+F_1dt+G_1dz)=\Gamma^4_{\mu3}dx^{\mu},$$

$$\Gamma^4_{\mu1}dx^{\mu}=e^{-2V}\chi_4dx+e^{-2V}F_1\chi_3dt+\frac{1}{2}e^{-2V}(\chi_2+2G_2\chi_3)dz=\Gamma^1_{\mu4}dx^{\mu},$$

$$\Gamma^4_{\mu2}dx^{\mu}=e^{-2V}F_2\eta_2dt+e^{-2V}\eta_2dy+\frac{1}{2}e^{-2V}(2G_2\eta_2+\eta_1)dz=\Gamma^2_{\mu4}dx^{\mu},$$

where

$$
\begin{aligned}
\eta_1 &= -\frac{\partial G_2}{\partial t}+\frac{\partial G_2}{\partial x}F_1+\frac{\partial G_2}{\partial y}F_2-\frac{\partial F_2}{\partial x}G_1-\frac{\partial F_2}{\partial y}G_2+\frac{\partial F_2}{\partial z},\\
\eta_2 &= 2\frac{\partial V}{\partial t}-2\frac{\partial V}{\partial x}F_1-2\frac{\partial V}{\partial y}F_2+\frac{\partial F_2}{\partial y},\\
\chi_1 &= 2\frac{\partial V}{\partial x}G_1+2\frac{\partial V}{\partial y}G_2-2\frac{\partial V}{\partial z}-\frac{\partial G_1}{\partial x},\\
\chi_2 &= -\frac{\partial G_1}{\partial t}+\frac{\partial G_1}{\partial x}F_1+\frac{\partial G_1}{\partial y}F_2-\frac{\partial F_1}{\partial x}G_1-\frac{\partial F_1}{\partial y}G_2+\frac{\partial F_1}{\partial z},\\
\chi_3 &= 2\frac{\partial V}{\partial t}-2\frac{\partial V}{\partial x}F_1-2\frac{\partial V}{\partial y}F_2+\frac{\partial F_1}{\partial x},\\
\xi_1 &= \frac{\partial F_1}{\partial y}+\frac{\partial F_2}{\partial x},\quad \xi_2=\frac{\partial G_1}{\partial y}-\frac{\partial F_2}{\partial x}.
\end{aligned}
\tag{2.5}
$$

In obtaining Eq. (2.5), we have used the property of analycity of the function $F(x+iy)=F_1+iF_2$ and similarly of $G=G_1+iG_2$.

Using the tetradic connections given by Eq. (2.4) we can compute the loop variables. In our case we are interested in computing the loop variables for segments in the t, x, y and z directions. For a translation in time $\Gamma_\mu dx^\mu=\Gamma_t dt$ with Γ_t being

$$
\Gamma_t=\begin{pmatrix} 0 & B & C & A\\ B & 0 & -F & -D\\ C & F & 0 & E\\ A & D & -E & 0 \end{pmatrix}=-iFJ_{12}-iDJ_{13}-iEJ_{23}-iBJ_{41}-iCJ_{42}-iAJ_{43}, \tag{2.6}
$$

where the boost parameters A, B, C are given by

$$
A=\tfrac{1}{2}e^{-4V}(\eta_1F_2+\chi_2F_1),\quad B=e^{-2V}\chi_3F_1,\quad C=e^{-2V}\eta_2F_2, \tag{2.7}
$$

and the rotation parameters D, E, F are

$$
\begin{aligned}
D &= -\frac{1}{2}e^{-2V}(\chi_2+2F_1\chi_1),\quad E=e^{-2V}\chi_1F_2,\\
F &= -\frac{1}{2}\left(\xi_1+4F_2\frac{\partial V}{\partial x}-4F_1\frac{\partial V}{\partial y}\right).
\end{aligned}
\tag{2.8}
$$

In Eq. (2.6), J_{23}, J_{13} and J_{12} are, respectively, generators of rotations about the x, y and z axis in the three-dimensional space, and J_{41}, J_{42} and J_{43} are, respectively, the generators of boosts in the Ox, Oy and Oz directions.

Then, for a segment in the time direction, the loop variable is a combination of boosts in all directions and rotations around the three axis in space.

Using Eq. (2.6) we get, for a time translation between t_1 and t_2, the following expression for the loop variable:

$$
U_{t_2t_1}(C)=\exp\left[\int_{t_1}^{t_2}(-iFJ_{12}-iDJ_{13}-iEJ_{23}-iBJ_{41}-iCJ_{42}-iAJ_{43})dt\right]. \tag{2.9}
$$

Now, let us consider a segment in the z-direction. In this case we have $\Gamma_{\mu 3}dx^{\mu}=\Gamma_z dz$, where

$$\Gamma_z=\begin{pmatrix} 0 & B' & C' & A' \\ B' & 0 & -F' & -D' \\ C' & F' & 0 & E' \\ A' & D' & -E' & 0 \end{pmatrix}=-iF'J_{12}-iD'J_{13}-iE'J_{23}-iB'J_{41}-iC'J_{42}-iA'J_{43}, \tag{2.10}$$

where

$$A'=\tfrac{1}{2}e^{-4V}(\eta_1 G_2+\chi_2 G_1),\quad B'=\tfrac{1}{2}e^{-2V}(\chi_2+2\chi_3 G_1),$$
$$C'=\tfrac{1}{2}e^{-2V}(2\chi_3 G_2+\eta_1),\quad D'=-e^{-2V}\chi_1 G_1, \tag{2.11}$$
$$E'=e^{-2V}\chi_1 G_2,\quad F'=-2\left(G_2\frac{\partial V}{\partial x}-G_1\frac{\partial V}{\partial y}\right).$$

As in the previous case, the loop variable along the z-direction is a combination of boosts and rotations. For a segment that goes from z_1 to z_2, the loop variable is given by

$$U_{z_2 z_1}(C)=\exp\left[\int_{z_1}^{z_2}(-iF'J_{12}-iD'J_{13}-iE'J_{23}-iB'J_{41}-iC'J_{42}-iA'J_{43})dz\right]. \tag{2.12}$$

Similarly, if we consider segments in the x- and y-directions, at fixed t and z, we get that

$$U_{x_2 x_1}(C)=\exp\left[\int_{x_1}^{x_2}\left(-2i\frac{\partial V}{\partial y}J_{12}-i\overline{D}J_{13}-i\overline{A}J_{43}-i\overline{B}J_{41}\right)dx\right] \tag{2.13}$$

and

$$U_{y_2 y_1}(C)=\exp\left[\int_{y_1}^{y_2}\left(-2i\frac{\partial V}{\partial x}J_{12}-i\overline{E}J_{23}-i\overline{A'}J_{43}-i\overline{C}J_{42}\right)dy\right], \tag{2.14}$$

where

$$\overline{A}=\tfrac{1}{2}e^{-4V}\chi_2,\quad \overline{B}=e^{-2V}\chi_3,\quad \overline{C}=e^{-2V}\eta_2,$$
$$\overline{A'}=\tfrac{1}{2}e^{-4V}\eta_1,\quad \overline{D}=e^{-2V}\chi_1,\quad \overline{E}=\tfrac{1}{2}e^{-4V}\chi_1. \tag{2.15}$$

Using previous results, we can write a general expression for $U(C)$. In the general case, $U(C)$ reads as

$$U(C)=P\ \exp\left(-\frac{i}{2}\int_C \Gamma_{\mu}^{ab}J_{ab}dx^{\mu}\right), \tag{2.16}$$

where J_{ab} are the generators of the Lorentz group $SO(3,1)$ and Γ_{μ}^{ab} are the appropriate tetradic connections. In general, J_{ab} generate the representation of the Lorentz group which acts on the transported quantity (a vector or a spinor). In the spinor case, instead of the group $SO(3,1)$, we have a covering group of this one. Therefore, when we have fermions, the loop variables are elements of the covering group of the Lorentz group.

III. LOOP VARIABLES IN A MULTIPLE CHIRAL CONICAL SPACE–TIME

In a recent paper Gal'tsov and Letelier[6] showed that the chiral conical space–time arises naturally from the spinning particle solution of (2+1)-dimensional gravity by an appropriate boost. This chiral conical space–time provides the gravitational counterpart for the infinitely thin straight chiral strings in the same way that an ordinary conical space–time is associated with the usual string.[10] The metric associated to the chiral conical space–time[6] (spinning string with cosmic dislocation) is given by

$$ds^2=-\overline{r^{8\mu}}(dr^2+r^2d\varphi^2)-(dz+4J^zd\varphi)^2+(dt+4J^td\varphi)^2, \tag{3.1}$$

where J^t represents the string angular momentum, $2J^z/\pi$ is the analogous of the Burgers-vector of dislocation and μ is the linear mass density of the string. The angle φ takes the values $0\leqslant\varphi\leqslant 2\pi$, and the other variables: $-\infty<t<\infty$, $0<r<\infty$, and $-\infty<z<\infty$. If we consider a Cartesian system of coordinates $x=r\cos\varphi$, $y=r\sin\varphi$, we can write Eq. (3.1) as

$$ds^2=-e^{-4V}(dx^2+dy^2)-\left(dz+4J^z\,\frac{xdy-ydx}{r^2}\right)^2+\left(dt-4J^t\,\frac{xdy-ydx}{r^2}\right)^2, \tag{3.2}$$

with $V=2\mu\ln r$.

The generalization of the chiral cone to a multiple chiral cone can[6] be obtained by introducing the parameters μ_i, J_i^t, J_i^z, $i=1,2,\ldots,N$, defining each chiral string located at the points $\vec{r}=\vec{r}_i$ of the plane $z=0$. The resulting metric has the form of Eq. (3.2) with the following interchanges:

$$\begin{aligned}
&J^t\,\frac{xdy-ydx}{r^2}\to\sum_{i=1}^{N}J_i^t\,\frac{(x-x_i)dy-(y-y_i)dx}{|\vec{r}-\vec{r}_i|^2},\\
&J^z\,\frac{xdy-ydx}{r^2}\to\sum_{i=1}^{N}J_i^z\,\frac{(x-x_i)dy-(y-y_i)dx}{|\vec{r}-\vec{r}_i|^2},\\
&V=2\mu\,\ln r\to V=\sum_{i=1}^{N}\mu_i\,\ln[r^2-2rr_i\cos(\varphi-\varphi_i)+r_i^2].
\end{aligned} \tag{3.3}$$

As a consequence of Eq. (3.3), the space–time generated by N multiple chiral cosmic string can be written as[6]

$$ds^2=-e^{-4V}(dx^2+dy^2)-\left[dz-\sum_{i=1}^{N}B_i(W_i^1dy-W_i^2dx)\right]^2+\left[dt-\sum_{i=1}^{N}A_i(W_i^1dy-W_i^2dx)\right]^2, \tag{3.4}$$

where

$$A_i=4J_i^t,\quad B_i=4J_i^z,\quad W_i^1=\frac{x-x_i}{|\vec{r}-\vec{r}_i|^2},\quad W_i^2=\frac{y-y_i}{|\vec{r}-\vec{r}_i|^2}. \tag{3.5}$$

In the previous case, static one, the loop variable was calculated directly from the metric. For the present case, stationary one, it is possible to do the same, but with a slight redefinition of the loop variables. This can be done because this solution of the Einstein equation can be patched together from flat coordinates patches but connected by some additional matching condition in order to take into account the time helical structure and the shift in the z-direction. First of all let us recover a previous result concerning the holonomy in the static case,[11] specifically in the space of a multiple cosmic string.[12] In this case one calculates the holonomy transformation correspond-

ing to circles in the xy-plane directly from the metric. Then, when we parallel transport a vector around multiple cosmic strings at rest at $\vec{r}=\vec{r}_i$ along a circle, this vector acquires a phase given by[11] $U(C)=\exp[-8\pi i(\Sigma_{j=1}^{N}\mu_j)J_{12}]$, where J_{12} is the generator of rotations in the xy-plane, around the z-axis. Therefore, when we go around the multiple cosmic string from the point $(\vec{x},t)$ to $(\vec{x}',t')$, the column vectors $(\vec{x},t)$ and $(\vec{x}',t')$ are related by

$$\begin{pmatrix} x' \\ y' \\ z' \\ t' \end{pmatrix} = \begin{pmatrix} \cos(8\pi\tilde{\mu}) & \sin(8\pi\tilde{\mu}) & 0 & 0 \\ -\sin(8\pi\tilde{\mu}) & \cos(8\pi\tilde{\mu}) & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \\ t \end{pmatrix}, \tag{3.6}$$

where we have set

$$\tilde{\mu}=\sum_{j=1}^{N}\mu_j . \tag{3.7}$$

Since the space-time outside the multiple cosmic string is locally flat, we can describe the analytic solution purely in terms of space–time patches with Minkowski metric, but connected by some matching conditions which are given by Eq. (3.6), that relates points $(\vec{x},t)$ and $(\vec{x}',t')$ along the edges.

As in the multiple cosmic string case, the space-time of the multiple chiral cosmic string is locally flat, and consequently we can describe it in terms of space–time patches with Minkowski metric, but connected by some conditions which are the same as in the static multiple string case, except those concerning the t and z coordinates. These conditions are expressed by relating points $(\vec{x},t)$ and $(\vec{x}',t')$ as follows:

$$x'=\cos(8\pi\tilde{\mu})x+\sin(8\pi\tilde{\mu})y, \quad y'=-\sin(8\pi\tilde{\mu})x+\cos(8\pi\tilde{\mu})y, \tag{3.8}$$

$$z'=z+8\pi\left(\frac{r}{|\vec{r}-\vec{r}_i|^2}\right)^2 J_i^z, \quad t'=t+8\pi\left(\frac{r}{|\vec{r}-\vec{r}_i|^2}\right)^2 J_i^t,$$

where we are considering as paths circles in the xy-plane.

The transformations given by Eq. (3.8) can be cast in the form of a homogeneous matrix multiplication as follows: let M_A^B be a five dimensional matrix, with A and B running from 1 to 5. We take M_ν^μ equal to the rotation matrix given by,[11] $U(C)=\exp(-8\pi i\tilde{\mu}J_{12})$, $M_5^4=8\pi(r/|\vec{r}-\vec{r}_i|^2)^2 J_i^t$ and $M_5^5=8\pi(r/|\vec{r}-\vec{r}_i|^2)^2 J_i^z$, so that

$$\begin{pmatrix} x' \\ y' \\ z' \\ t' \\ 1 \end{pmatrix} = \begin{pmatrix} \cos(8\pi\tilde{\mu}) & \sin(8\pi\tilde{\mu}) & 0 & 0 & 0 \\ -\sin(8\pi\tilde{\mu}) & \cos(8\pi\tilde{\mu}) & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 8\pi\left(\frac{r}{|\vec{r}-\vec{r}_i|^2}\right)^2 J_i^z \\ 0 & 0 & 0 & 1 & 8\pi\left(\frac{r}{|\vec{r}-\vec{r}_i|^2}\right)^2 J_i^z \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \\ t \\ 1 \end{pmatrix}$$

$$= \exp\left[-8\pi\left(\frac{r}{|\vec{r}-\vec{r}_k|^2}\right)^2 J_k^z M_3\right] \exp\left[-8\pi\left(\frac{r}{|\vec{r}-\vec{r}_k|^2}\right)^2 J_k^t M_4\right] \exp(-8\pi\tilde{\mu} J_{12}) \begin{pmatrix} x \\ y \\ z \\ t \\ 1 \end{pmatrix}, \tag{3.9}$$

where M_3 and M_4 are the following matrices:

$$M_3 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & i \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad M_4 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & i \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}. \tag{3.10}$$

Equation (3.9) is the exact expression for the holonomy for circles in the space-time. By defining $y^A=(y^\mu,1)$ we can cast the conditions (3.8) as $y'^A = M^A_B y^B$ which tells us that the points $(\vec{x},t)$ and $(\vec{x}',t')$ along the edges are related by the phase given by Eq. (3.9) that depends on the parameters μ_j, J_j^t and J_j^z.

The existence of locally flat coordinates in this space-time permits us to consider Eq. (3.9) as a ''parallel transport'' matrix. Then we can say that when we carry a vector along a circle in this space-time it acquires a phase that depends on μ_j, J_j^t and J_j^z which prevents it from being equal to the unit matrix. This effect is exclusively due to the non-trivial topology of the space-time under consideration. This is a gravitational analogue[11,13] of the Aharanov-Bohm effect,[14] but in this case, purely at the classical level.

We can also compute the holonomy transformations for circles in the multiple chiral conical space-time in the context of the Einstein-Cartan theory. In this case the connection 1-forms appropriately chosen give us[7]

$$\Gamma^1_{\mu 2} dx^\mu = 2(\partial_x V dy - \partial_y V dx) = -\Gamma^2_{\mu 1} dx^\mu, \tag{3.11}$$

which can be written in cylindrical coordinates $(x^1=r,\ x^2=\varphi,\ x^3=z,\ x^4=t)$ as

$$\Gamma^1_{\mu 2} dx^\mu = -\frac{2}{r}\frac{\partial V}{\partial \varphi} dr - \left(1 - 2r\frac{\partial V}{\partial r}\right) d\varphi = -\Gamma^2_{\mu 1} dx^\mu. \tag{3.12}$$

Now, consider the same previous circle, at constant time. In this case $U_{2\pi,0}(C)$ is given by

$$U_{2\pi,0}(C) = \exp\left(\int_0^{2\pi} \Gamma_\varphi d\varphi\right) = \exp\left[-8\pi i\left(\sum_{j=1}^{N} \mu_j\right) J_{12}\right], \tag{3.13}$$

where

$$\Gamma_{\varphi}=i\left[1-4\sum_{j=1}^{N}\mu_j\frac{R(R-r_i\cos(\varphi-\varphi_i))}{(R^2-2Rr_i\cos(\varphi-\varphi_i)+r_i^2)}\right]J_{12}, \tag{3.14}$$

R being the radius of the circle. Into Eq. (3.12) we have dropped out the factor $\exp(-2\pi i J_{12})$ which is equal to the 4×4 identity matrix. Note that in this case the holonomy transformation has a simple expression and it belongs to the homogeneous Lorentz group. In this context it does not carry information concerning angular momentum and torsion and coincides with a previous result[11] concerning the multiple cosmic string solution.[12] Then, the concept of holonomy can be used to detect different connections that come out from Einstein and Einstein-Cartan theories. The holonomy for a single chiral string has been studied recently in Ref. 15.

From Eq. (3.13), we conclude that the phase factor acquired by a vector when parallel transported in the space-time corresponding to a multiple chiral cosmic string is affected by chiral strings inside the curves along which the vector is parallel transported. Then, from the global point of view the space-time surrounding n strings ($n\leqslant N$) can be seen to correspond to a chiral cone with deficiency angle $\Sigma_{j=1}^{n}\mu_j$. The chiral strings with $n\geqslant N$ do not contribute to the phase.

It is interesting to call attention to the fact that in the context of Einstein theory, the resulting holonomy transformation is an element of the inhomogeneous Lorentz group. The appearance of the group ISO(3,1) as a holonomy group is fascinating and can suggest important parallel with the better understood $(2+1)$ dimensional case, in which gravity is equivalent to an $ISO(2,1)$ Chern-Simons gauge theory,[16] in which case the triad $e_{(a)}^{\mu}$ is a gauge field. As far as we know there is no corresponding result in $(3+1)$ dimensional gravity, in general. Our result, evidently, is valid for the special case under consideration.

IV. LOOP VARIABLES IN OTHER CONICAL SPACE–TIMES

The purpose of this section is to complete a previous work[17] in which we computed the loop variables for some curves in space–times with a topological defect. We considered a single domain wall crossed by multiple cosmic strings. Other simple examples of conical space–times include two domain walls crossed by a cosmic string of linear mass density μ and two planes topological defects plus a cosmic string. A variety of conical space–time of different topologies can be found in Ref. 9.

Now let us consider two domain walls parallels to the xy-plane that intersect the z-axis at $\pm h$ and crossed by a single cosmic string. The metric corresponding to the space-time generated by this configuration is

$$ds^2=e^{-4\pi\sigma|h^2-z^2|}[-e^{4\pi\sigma t}\rho^{-4\mu}(d\rho^2+\rho^2d\varphi^2)-4z^2dz^2+dt^2], \tag{4.1}$$

where σ is the matter density of the wall and μ is the linear mass density of the cosmic string.

Proceeding in the same way of the previous cases let us define the appropriate 1-forms θ^a that give the usual flat space–time limit $\sigma=0$, $\mu=0$ as

$$\begin{aligned}\theta^1&=e^{-2\pi\sigma|h^2-z^2|+2\pi\sigma t}(\rho^{-2\mu}\cos\varphi d\rho-\rho^{-2\mu+1}\sin\varphi d\varphi),\\ \theta^2&=e^{-2\pi\sigma|h^2-z^2|+2\pi\sigma t}(\rho^{-2\mu}\sin\varphi d\rho+\rho^{-2\mu+1}\cos\varphi d\varphi),\\ \theta^3&=2ze^{-2\pi\sigma|h^2-z^2|}dz,\quad \theta^4=e^{-2\pi\sigma|h^2-z^2|}dt.\end{aligned} \tag{4.2}$$

In a coordinate system $(x^1=\rho,\ x^2=\varphi,\ x^3=z,\ x^4=t)$, the tetrad vectors are given by

$$e_1^{(1)}=\rho^{-2\mu}e^{-2\pi\sigma|h^2-z^2|+2\pi\sigma t}\cos\varphi,\quad e_2^{(1)}=-\rho^{-2\mu+1}e^{-2\pi\sigma|h^2-z^2|+2\pi\sigma t}\sin\varphi,$$

$$e_1^{(2)}=\rho^{-2\mu}e^{-2\pi\sigma|h^2-z^2|+2\pi\sigma t}\sin\varphi,\quad e_2^{(2)}=\rho^{-2\mu+1}e^{-2\pi\sigma|h^2-z^2|+2\pi\sigma t}\cos\varphi, \tag{4.3}$$

$$e_3^{(3)}=2ze^{-2\pi\sigma|h^2-z^2|},\quad e_4^{(4)}=e^{-2\pi\sigma|h^2-z^2|}.$$

Using these results we can compute the tetradic connections which are

$$\Gamma^1_{\mu 2}dx^\mu=(1-4\mu)d\varphi=-\Gamma^2_{\mu 1}dx^\mu,$$

$$\Gamma^1_{\mu 3}dx^\mu=2\pi\sigma\,\frac{|h^2-z^2|}{h^2-z^2}\,e^{2\pi\sigma t}\rho^{-4\mu}d\varphi=-\Gamma^3_{\mu 1}dx^\mu,$$

$$\Gamma^2_{\mu 3}dx^\mu=2\pi\sigma\,\frac{|h^2-z^2|}{h^2-z^2}\,e^{2\pi\sigma t}\rho^{-4\mu+1}d\varphi=-\Gamma^3_{\mu 2}dx^\mu,$$

$$\Gamma^4_{\mu 1}dx^\mu=2\pi\sigma e^{2\pi\sigma t}\rho^{-4\mu}d\varphi=\Gamma^1_{\mu 4}dx^\mu, \tag{4.4}$$

$$\Gamma^4_{\mu 2}dx^\mu=2\pi\sigma e^{2\pi\sigma t}\rho^{-4\mu+1}d\varphi=\Gamma^2_{\mu 4}dx^\mu,$$

$$\Gamma^4_{\mu 3}dx^\mu=2\pi\sigma\,\frac{|h^2-z^2|}{h^2-z^2}\,dt=\Gamma^3_{\mu 4}dx^\mu.$$

Let us consider the path C as a circle centered on the z axis with radius R lying on a plane parallel to the xy-plane at a fixed time. In this case we have that $\Gamma_\mu dx^\mu=\Gamma_\varphi d\varphi$ where

$$\Gamma_\mu=i(1-4\mu)J_{12}-2\pi i\sigma e^{2\pi\sigma t}\rho^{-4\mu+1}\left(J_{24}+\frac{|h^2-z^2|}{h^2-z^2}\,J_{23}\right). \tag{4.5}$$

From Eq. (4.5) we get

$$U_{2\pi,0}(C)=\exp\left[-8\pi i\mu J_{12}-4\pi^2 i\sigma e^{2\pi\sigma t}\rho^{-4\mu+1}\left(J_{24}+\frac{|h^2-z^2|}{h^2-z^2}\,J_{23}\right)\right]. \tag{4.6}$$

Equation (4.6) is the exact expression for the holonomy transformation for a circle with center at the cosmic string and that is parallel to the domain walls.

The holonomy transformation associated to the circle C that corresponds to the domain walls only ($\mu=0$) and to the cosmic string only ($\sigma=0$) are given, respectively, by

$$U_{2\pi,0}(C)=\exp\left[-4\pi^2 i\sigma e^{2\pi\sigma t}\rho\left(J_{24}-\frac{|h^2-z^2|}{h^2-z^2}\,J_{23}\right)\right] \tag{4.7}$$

and

$$U_{2\pi,0}(C)=\exp(-8\pi i\mu J_{12}). \tag{4.8}$$

From these results we see that the holonomy transformations detect the topological defects in all cases. In particular, for the domain walls plus a cosmic string, the value of $U_{2\pi,0}(C)$ depends on the radius of the circle. Note that $U_{2\pi,0}(C)$ distinguishes the regions $z<-h$, $-h<z<h$ and $z>h$ in the cases of two domain walls crossed by a cosmic string and two domain walls only.

In the case of two planes topological defects crossed by a cosmic string with an equation of state $p=-\gamma\sigma(\gamma<1)$, the metric is given by

$$ds^2=-\rho^{-8\mu}e^H(d\rho^2+\rho^2d\varphi^2)+e^F(-4z^2dz^2+dt^2), \tag{4.9}$$

where

$$\begin{aligned} e^H&=(t-|h^2-z^2|)^{1/2(1-\gamma)},\\ e^F&=\frac{1}{8\pi\sigma(1-\gamma)}\,\frac{1}{t-|h^2-z^2|}\left[\frac{t-|h^2-z^2|}{t+|h^2-z^2|}\right]^{1/4(\gamma-1)}. \end{aligned} \tag{4.10}$$

The holonomy transformation for the same circle C described above is given by

$$U_{2\pi,0}(C)=\exp\left[-8\pi i\mu J_{12}-\frac{\pi i e^{(H-F)/2}}{4(1-\gamma)(t-|h^2-z^2|)}\,\rho^{-4\mu+1}\left(J_{24}-\frac{|h^2-z^2|}{h^2-z^2}\,J_{23}\right)\right]. \tag{4.11}$$

To get Eq. (4.11), we have used the following relations between the tetradic connections:

$$\begin{aligned} &\Gamma^1_{\mu2}dx^\mu=(1-4\mu)dy=-\Gamma^2_{\mu1}dx^\mu,\\ &\Gamma^1_{\mu3}dx^\mu=\frac{e^{-F/2}}{2z}\,\frac{\partial}{\partial z}\,(e^{H/2})\rho^{-4\mu}d\rho=-\Gamma^3_{\mu1}dx^\mu,\\ &\Gamma^2_{\mu3}dx^\mu=\frac{e^{-F/2}}{2z}\,\frac{\partial}{\partial z}\,(e^{H/2})\rho^{-4\mu+1}d\varphi=-\Gamma^3_{\mu2}dx^\mu,\\ &\Gamma^4_{\mu1}dx^\mu=e^{-F/2}\,\frac{\partial}{\partial t}\,(e^{H/2})\rho^{-4\mu}d\rho=\Gamma^1_{\mu4}dx^\mu,\\ &\Gamma^4_{\mu2}dx^\mu=e^{-F/2}\,\frac{\partial}{\partial t}\,(e^{H/2})\rho^{-4\mu+1}d\varphi=\Gamma^2_{\mu4}dx^\mu,\\ &\Gamma^4_{\mu3}dx^\mu=\frac{e^{-F/2}}{2z}\,\frac{\partial}{\partial z}\,(e^{F/2})dt+2ze^{-F/2}\,\frac{\partial}{\partial t}\,(e^{F/2})dz=\Gamma^3_{\mu4}dx^\mu. \end{aligned} \tag{4.12}$$

As in the previous case corresponding to two domain walls plus a string, the presence of the topological defect is coded in the holonomy transformation, which distinguishes the different regions $z<-h$, $-h<z<h$ and $z>h$. Also in this case, the holonomy transformation is an element of the Lorentz group.

V. CONCLUDING REMARKS

We have shown by explicit computation from the metric corresponding to a multiple parallel chiral cosmic string that the loop variables are combinations of rotations around the three axis and boosts with appropriate parameters that depend on the characteristics of each chiral string defined by μ_i, J^t_i and J^z_i. The holonomy transformation, in this space–time, are elements of the inhomogeneous Lorentz group. It assumes a simple form in the context of the Einstein-Cartan theory which recover an expression for the case of multiple cosmic strings. The loop variables associated with the multiple moving crossed cosmic strings are also combinations of rotations and boosts in the directions of the three spatial axis. They are elements of the homogeneous Lorentz group.

In the two domain walls and two planes topological defects plus the cosmic string, the holonomy transformation distinguishes the presence of strings and membranes and depends on whether the loop encircles the strings and in which side of the planes topological defects are located. Again, they are elements of $SO(3,1)$.

Our approach provides a unified way to obtain the phase factor acquired by a vector or a spinor when parallel transported in these gravitational fields, showing up the dependence of the phase factors with the parameters associated with the defects.

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Asymptotic behavior of a class of inhomogeneous scalar field cosmologies

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The asymptotic behavior of a class of inhomogeneous scalar field cosmologies with a Liouville type of potential is studied. We define a set of new variables for which the phase space of the system of Einstein equations is bounded. This allows us to perform a complete analysis of the evolution of these cosmologies. We also discuss the extension of the cosmic no-hair theorem. © *1996 American Institute of Physics.* [S0022-2488(96)03311-7]

I. INTRODUCTION

Since the proposal by Misner[1] of the ''chaotic cosmology program,'' the idea that the Universe emerged from a highly irregular state and that the inhomogeneities and the anisotropies were washed away giving place to a highly symmetric universe, has been one of the most attractive ideas in cosmology. In spite of the theorem proved by Collins and Hawking[2] which states that only a subclass of measure zero of the space of homogeneous solutions approach isotropy and the alternative approaches that postulated, according to the second law of thermodynamics,[3] that the universe began in a highly regular state, Misner's idea has come back due to the success of the inflationary scenarios.

The cosmic ''no-hair'' theorems of Wald[4] for homogeneous models and of Jensen and Stein-Schabes[5] for inhomogeneous space–times pointed out how the introduction of a cosmological constant, which can be considered as induced by a scalar field (inflaton), allows the models to isotropize approaching the de Sitter solution. This situation, however, may dramatically change if one takes into account the dynamical behavior of the scalar field. Heusler,[6] for example, extending the theorem of Collins and Hawking to the case of convex and positive potentials of the scalar field possessing a local minimum, has shown that only the homogeneous Bianchi models which admit a FRW solution as a particular case approach isotropy. Kitada and Maeda[7] and Ibáñez *et al.*[8] have shown that when one assumes a Liouville type of potential for the scalar field (exponential potential), the Wald theorem for homogeneous solutions still applies if the exponential potential is quite flat.

Although Jensen and Stein-Schabes[5] extended the Wald theorem to inhomogeneous solutions, little is known about the effect of the dynamics of the scalar field on the asymptotic behavior of the models. The first attempts to incorporate the effect of the dynamical evolution of the scalar field was made by Goldwirth and Piran[9] using numerical studies of inhomogeneous models and, later on, by Calzetta and Sakellariadou[10] by studying the evolution of a family of inhomogeneous Cauchy data. The first inhomogeneous scalar field exact solutions with exponential potential of the Einstein field equations were obtained by Feinstein and Ibáñez[11] and it was shown there that the scalar field does not guarantee by itself that the model inflates or isotropizes. Although there are some exact inhomogeneous solutions obtained up to now, we are lacking a result similar to Heusler's. In particular, for the exponential potential, it would be interesting to study the conditions on the scalar field leading to inflation and isotropization.

The asymptotic behavior of homogeneous but anisotropic solutions for a perfect fluid has been widely studied. By using the kinematical quantities of the fluid as variables, the field equations can be written as an autonomous system of ordinary differential equations.[12] One of the most distinctive features is that the equilibrium points of these systems are self-similar solutions. This analysis

has recently been extended to the case when the matter source is a scalar field with exponential potential.[13] Since the scalar field is homogeneous, one can globally associate with it a perfect fluid, and then, by using the kinematical variables of the fluid, the Einstein field equations decouple and the phase space of the system becomes bounded.

The main difficulty in analyzing the asymptotic behavior of inhomogeneous solutions is related to the fact that the field equations involve partial derivatives. The study of such systems was initiated in Ref. 14, where a particular family of self-similar solutions with perfect fluid, for which the Einstein equations reduced to an autonomous system, was studied. Since the source of the metric was a perfect fluid, the kinematical quantities could be used again to analyze the asymptotic behavior of the system, as in the homogeneous case.

In dealing with an inhomogeneous scalar field one can not apply the analysis developed in Ref. 14 due to the fact that one can not globally interpret the scalar field as a perfect fluid. Therefore in order to investigate whether the inhomogeneous scalar field cosmologies undergo an inflationary epoch leading to the homogenization and the isotropization of the space–time, one does have to look for a different way to tackle this problem.

In this paper we initiate the study of the asymptotic behavior of the scalar field cosmologies by considering, as a first step, a two-parameter family of G_2 self-similar solutions. The fact that the scalar field is not equivalent to a perfect fluid prevents the use of the kinematical quantities to describe the evolution of the solutions. Despite the lack of a preferred timelike congruence in the space–time, we manage to find a set of new variables in terms of which the phase space of the system becomes bounded. This allows us to perform a complete analysis of the asymptotic behavior of these space–times. In addition, the way to introduce the set of new variables is a promising method for dealing with more general solutions.

The plan of the paper is as follows: in Sec. II we present the metric and introduce the new variables. Section III is devoted to the analysis of the phase space and in Sec. IV we discuss the results.

II. THE METRIC AND THE COMPACTIFIED PHASE SPACE

We will consider solutions with one-dimensional inhomogeneity. These metrics are described by the generalized Einstein–Rosen space–times which admit an Abelian group of isometries G_2. If the two Killing vectors are hypersurface orthogonal, the line element can be written as

$$ds^2 = e^F(-dt^2+dz^2)+G(e^h dx^2+e^{-h}dy^2), \tag{1}$$

where the metric functions depend on t and z and the Killing vectors are ∂_x and ∂_y.

The matter source for the metric is that of a minimally coupled scalar field with potential, for which the stress-energy tensor is given by

$$T_{ab} = \overline{\phi}_{,a}\overline{\phi}_{,b} - g_{ab}\left(\tfrac{1}{2}\,\overline{\phi}_{,c}\overline{\phi}^{,c} + V(\overline{\phi})\right) \tag{2}$$

(Latin indices run from 0–3), with the Liouville type of the potential

$$V(\overline{\phi}) = \Lambda e^{k\overline{\phi}}, \quad \Lambda \geqslant 0. \tag{3}$$

It is well known[15] that as long as the gradient of the scalar field remains timelike, (2) can be rewritten as a perfect fluid stress-energy tensor.

To simplify the equations we will concentrate in this paper on the class of solutions for which the element of transitivity surface G is homogeneous,

$$G = G(t), \tag{4}$$

which is suitable for a description of cosmological models.

It was shown in Ref. 16 that if one assumes separability of the metric and separability, in the additive sense, of the scalar field one obtains, from the field equations, that the dependence of these functions on the variable z is linear;

$$h(t,z)=p(t)+az, \quad F(t,z)=f(t)+cz, \quad \overline{\phi}(t,z)=\phi(t)+bz, \tag{5}$$

where a, b, and c are arbitrary constants which drive the inhomogeneity. This linear behavior for the inhomogeneity has been recently considered, in a different context, by Vilenkin.[17] The general solution for this class of metrics and the study of a few particular examples were given in Ref. 11.

Before going to the field equations, it is worth mentioning that the metric (1)–(5) admits a homothetic vector field given by

$$\mathbf{H}=\frac{2}{c}\frac{\partial}{\partial \mathbf{z}}+\left(1-\frac{a}{c}\right)x\frac{\partial}{\partial \mathbf{x}}+\left(1+\frac{a}{c}\right)y\frac{\partial}{\partial \mathbf{y}}. \tag{6}$$

It was conjectured in Ref. 14 that the self-similar solutions could be the attractors of the G_2 cosmologies and in this sense the metric (1)–(5) would play an important role in the study of the asymptotic behavior of the inhomogeneous solutions. The metric (1)–(5) is similar to the metric studied by Hewitt *et al.*[14] [it is obtained interchanging t by z in (5)]. Both metrics, however, differ in the character of the orbits of the similarity group and in the type of the source. In our case the orbits of (6) are spacelike given by $t=$constant and the scalar field is inhomogeneous and, therefore, it is not equivalent, in general, to a perfect fluid.

The Einstein equations and the Klein–Gordon equation for the scalar field with the ansatz (5) are given by

$$\frac{\ddot{G}}{G}-2V(\overline{\phi})e^{F}=0, \tag{7}$$

$$\ddot{p}+\frac{\dot{G}}{G}\dot{p}=0, \tag{8}$$

$$a\dot{p}-c\frac{\dot{G}}{G}+2b\dot{\phi}=0, \tag{9}$$

$$\frac{\ddot{G}}{G}-\frac{1}{2}\left(\frac{\dot{G}}{G}\right)^2-\dot{f}\frac{\dot{G}}{G}+\frac{1}{2}\dot{p}^2+\dot{\phi}^2+\frac{1}{2}a^2+b^2=0, \tag{10}$$

$$\ddot{f}-\frac{1}{2}\left(\frac{\dot{G}}{G}\right)^2+\frac{1}{2}\dot{p}^2+\dot{\phi}^2-\frac{1}{2}a^2-b^2=0, \tag{11}$$

$$\ddot{\phi}+\frac{\dot{G}}{G}\dot{\phi}+kV(\overline{\phi})e^{F}=0. \tag{12}$$

For a massless scalar field, $V=0$, the former system of equations turns out to be easily integrable, giving the following solution;

$$\begin{aligned} &p(t)=A\ \ln t, \quad \phi(t)=B\ \ln t, \quad G(t)=t,\\ &f(t)=(\tfrac{1}{2}A^2+B^2-\tfrac{1}{2})\ln t+\tfrac{1}{2}(\tfrac{1}{2}a^2+b^2)t^2, \end{aligned} \tag{13}$$

where A and B are constants subject to the condition

$$aA - c + 2bB = 0. \tag{14}$$

When $V \neq 0$, from (7) or (12), and due to the exponential form of the potential,

$$c = -kb. \tag{15}$$

In this case if the constant $b=0$, then, from (9), either $\dot{p}=0$ and the metric is Bianchi type VI_0, or $a=0$ and the metric is Bianchi type I. Let us note that whatever value V takes, when $a=b=0$ the metric is Bianchi type I.

In order to look for a suitable set of new variables to compactify the phase space, we write the generalized Friedman equation which is obtained from (7) and (10):

$$-\frac{1}{2}\left(\frac{\dot{G}}{G}\right)^2 - \dot{f}\,\frac{\dot{G}}{G} + \frac{1}{2}\,\dot{p}^2 + \dot{\phi}^2 + \frac{1}{2}\,a^2 + b^2 + 2V(\phi)e^f = 0. \tag{16}$$

This equation suggests the introduction of the following set of variables

$$\begin{aligned} \beta &= \frac{\dot{p}}{\dot{G}/G + \dot{f}}, \quad \Psi = \sqrt{2}\,\frac{\dot{\phi}}{\dot{G}/G + \dot{f}}, \\ \Phi &= \frac{\dot{f}}{\dot{G}/G + \dot{f}}, \quad \Gamma = \frac{2\sqrt{Ve^f}}{\dot{G}/G + \dot{f}}. \end{aligned} \tag{17}$$

In terms of these new variables, (16) is written as

$$1 - \beta^2 - \Psi^2 - \Phi^2 - \Gamma^2 = \frac{(a^2 + 2b^2)}{(\dot{G}/G + \dot{f})^2} \geqslant 0. \tag{18}$$

Therefore the space of solutions described by the variables (17) is bounded to the inside of the four-sphere (18). Let us note that, from (16), $\dot{G}/G + \dot{f}$ has to be different from zero, unless Λ be negative.

In dealing with perfect fluid models new variables were defined as the kinematical quantities of the fluid divided by an appropriate power of the rate of expansion θ. This assures good behavior of these variables near the initial singularity. Let us note that our new variables (17) are divided by the quantity $\dot{G}/G + \dot{f}$, which is not related to the expansion of any timelike congruence. Nevertheless, from the general behavior near the initial singularity found by Belinskii *et al.*[18] and from the work of Isenberg and Moncrief[19] we can assume that the metric (1)–(5), near the initial singularity behaves, for each value of the coordinate z, like a Kasner model. Therefore, when $t \to 0$

$$G \sim t, \quad f \sim p \sim \phi \sim \ln t, \tag{19}$$

and the variables (17) remain bounded when t tends to zero.

From (18) we see that the points on the surface of the four-sphere represent either homogeneous Bianchi type I solutions (when constants a and b are zero) or the initial singularity of the models.

By using (17), (9) is written as

$$a\beta + b\sqrt{2}\Psi - c(1 - \Phi) = 0. \tag{20}$$

Except for the trivial case when $a=b=0$, this equation gives a constraint for the constants a and b. Alternatively, if a and b are fixed, one can look at this equation as giving a plane, the

intersection of which with the sphere (18) describes the phase space. In the study of the equilibrium points in the next section, a and b will be arbitrary, chosen constrained by (20).

Using the variables (17), (7) becomes

$$\frac{\ddot{G}}{G}=\frac{1}{2}\left(\frac{\Gamma}{1-\Phi}\right)^2\left(\frac{\dot{G}}{G}\right)^2. \tag{21}$$

This equation decouples from the rest of the field equations if we introduce a new time coordinate

$$\frac{d\tau}{dt}=\frac{\dot{G}}{G}+\dot{f}=\frac{1}{1-\Phi}\frac{\dot{G}}{G}. \tag{22}$$

Near the initial singularity

$$\frac{d\tau}{dt}\sim\frac{1}{t}\Rightarrow\tau\rightarrow-\infty, \tag{23}$$

thus τ varies from $-\infty$ to $+\infty$. In terms of this new time the field equations are written as

$$\beta'=-\beta(1-\beta^2-\Psi^2-\Phi^2), \tag{24}$$

$$\Psi'=-\Psi(1-\beta^2-\Psi^2-\Phi^2)-\frac{k}{2\sqrt{2}}\Gamma^2, \tag{25}$$

$$\Phi'=(1-\Phi)(1-\beta^2-\Psi^2-\Phi^2)-\tfrac{1}{2}\Gamma^2, \tag{26}$$

$$\Gamma'=-\Gamma\left(-\beta^2-\Psi^2-\Phi^2+\frac{1}{2}\Phi-\frac{k}{2\sqrt{2}}\Psi\right), \tag{27}$$

where $'$ means derivative with respect to the new time τ. Differentiating (20) with respect to τ one can easily see that the constraint equation (20) holds for all values of τ, as long as the initial conditions verify the equation (20). Therefore (24)–(27) along with the constraint equation (20) describe the evolution of the metric (1)–(5).

III. THE EQUILIBRIUM POINTS AND THE INVARIANT SETS

In this section we shall study the qualitative behavior of the trajectories of the system (24)–(27). Let us first note that the system admits the discrete symmetry $\Gamma\rightarrow-\Gamma$, and, therefore, without loss of generality the study of the equilibrium points will be restricted to $\Gamma\geqslant 0$.

A. Equilibrium points

The equilibrium points of an autonomous system play an important role in describing the qualitative behavior of its solutions. The local stability of the equilibrium points are given by the eigenvalues of the linearized differential equations. The equilibrium points of the system (24)–(27) can be found explicitly and we now give them and their character:

$$\text{(I)}\quad\left\{\beta=0\quad\Psi=-\frac{k\sqrt{2}}{2+k^2}\quad\Phi=\frac{k^2}{2+k^2}\quad\Gamma=\frac{2\sqrt{2}}{2+k^2}\right\}.$$

This point is outside the sphere when $k^2<2$ and it is on the surface of the sphere when $k^2=2$. The constraint equation (20) is trivially satisfied for all values of the constants a and b. The corresponding metric and the scalar field when $k^2>2$ are

$$ds^2 = Ce^{k^2At/2-kbz}(-dt^2+dz^2)+e^{At}(e^{az}dx^2+e^{-az}dy^2),$$
$$\phi = -\frac{k}{2}At+bz, \tag{28}$$

where

$$C=\frac{A^2}{\Lambda}, \quad A=\sqrt{\frac{2(a^2+2b^2)}{k^2-2}}. \tag{29}$$

This metric was obtained in Ref. 11 and is of Bianchi type VI. The eigenvalues of the linearized system are

$$\frac{-2}{k^2+2}, \quad \frac{-2}{k^2+2}, \quad \frac{-1+\sqrt{5-2k^2}}{k^2+2}, \quad \frac{-1-\sqrt{5-2k^2}}{k^2+2}. \tag{30}$$

When $k^2<\frac{5}{2}$, the equilibrium point is a stable node and when $k^2>5/2$ it is a stable focus.

$$\text{(II)} \quad \left\{\beta=0 \quad \Psi=-\frac{k}{2\sqrt{2}} \quad \Phi=\frac{1}{2} \quad \Gamma=\frac{\sqrt{6-k^2}}{2\sqrt{2}}\right\}.$$

This equilibrium point is on the surface of the sphere. It disappears when $k^2>6$ and coincides with the former equilibrium point when $k^2=2$. Substituting the former values of the variables of the equilibrium point into (17) one easily gets that the solution corresponds to a homogeneous Bianchi type I solution ($a=b=0$). The line element and the scalar field are

$$ds^2=Ct^m(-dt^2+dz^2)+t^m(dy^2+dz^2), \quad m=\frac{4}{k^2-2}, \quad \phi=-\frac{2k}{k^2-2}\ln t, \tag{31}$$

where

$$C=\frac{2(6-k^2)}{\Lambda(k^2-2)^2}, \tag{32}$$

and the metric represents the FRW universe with massless minimally coupled scalar field as a source. The eigenvalues of the linearized system are

$$-\tfrac{1}{8}(6-k^2), \quad -\tfrac{1}{4}(2-k^2), \quad -\tfrac{1}{8}(6-k^2), \quad -\tfrac{1}{8}(6-k^2). \tag{33}$$

When $k^2<2$ this equilibrium point is a stable node, but when $2<k^2<6$ it is a saddle point.

It is important to note that the constraint equation (20) is satisfied not only because a and b vanish but because $\beta=0$ and $\sqrt{2}\Psi+k(1-\Phi)=0$. If we look into the evolution in time of a particular solution with a and b different from zero, and with $k^2<2$, β, Ψ, and Φ will take values such that the constraint equation will be always satisfied and as $t\to\infty$ the solution will approach this equilibrium point becoming, therefore, homogeneous and isotropic.

$$\text{(III)} \quad \{\beta^2+\Psi^2+\Phi^2=1, \quad \Gamma=0\}.$$

This ring of equilibrium points belongs to the surface of the sphere and represents, therefore, Bianchi type I solutions with a minimally coupled massless scalar field. By choosing a particular point on the surface, i.e., $\beta=a_1$, $\Psi=a_2$, and $\Phi=a_3$ with $a_1^2+a_2^2+a_3^2=1$, the eigenvalues of the linearized system are

$$\frac{1}{2}\left(2-a_3+\frac{k}{\sqrt{2}}\,a_2\right),\quad 2(1-a_3),\quad 0,\quad 0. \tag{34}$$

Hence, any of these points are unstable, except when $\Phi=1$ ($a_3=1$), which corresponds to the Minkowski space–time.

B. Invariant sets

Besides the equilibrium points, the existence of invariant sets help to describe the qualitative behavior of the solutions of an autonomous system. In our case, there are three invariant sets, two of them describing massless and exponential potential scalar field solutions, respectively, while the third gives the Bianchi type I solutions.

The points with $\Gamma=0$ (massless scalar field space–times) compose an invariant set of the dynamical system (24)–(27) whose solutions are given by (13) and (14). The dynamics of the points of this subspace can be easily studied: when $\Gamma=0$, the dynamical system reduces to

$$\begin{aligned}\beta' &= -\beta(1-\beta^2-\Psi^2-\Phi^2),\\ \Psi' &= -\Psi(1-\beta^2-\Psi^2-\Phi^2),\\ \Phi' &= (1-\Phi)(1-\beta^2-\Psi^2-\Phi^2),\end{aligned} \tag{35}$$

with straight lines as solutions:

$$\Phi=\frac{\Phi_0-1}{\beta_0}\,\beta+1,\quad \Psi=\frac{\Psi_0}{\beta_0}\,\beta. \tag{36}$$

These lines start on the surface of the sphere $\beta^2+\Psi^2+\Phi^2=1$ and intersect at the point $\beta=\Psi=0$, $\Phi=1$. Thus the solutions evolve from the Kasner initial singularity to the Minkowski space–time.

The second invariant set is given by the points with $\Gamma>0$ (and by symmetry $\Gamma<0$), with equilibrium points being the points I and II described above.

Finally, the third invariant set is given by the points on the surface of the sphere ($\beta^2+\Psi^2+\Phi^2+\Gamma^2=1$). In this case the dynamical system is reduced to

$$\begin{aligned}\beta' &= -\beta(1-\beta^2-\Psi^2-\Phi^2),\\ \Psi' &= -\left(\Psi+\frac{k}{2\sqrt{2}}\right)(1-\beta^2-\Psi^2-\Phi^2),\\ \Phi' &= (\tfrac{1}{2}-\Phi)(1-\beta^2-\Psi^2-\Phi^2).\end{aligned} \tag{37}$$

The solutions of this system are again straight lines:

$$\Phi=\left(\Phi_0-\frac{1}{2}\right)\frac{\beta}{\beta_0}+1,\quad \Psi=\left(\Psi_0+\frac{k}{2\sqrt{2}}\right)\frac{\beta}{\beta_0}-\frac{k}{2\sqrt{2}}, \tag{38}$$

and the equilibrium points of the system (37) are the points II and III.

The behavior of the system (24)–(27) can be visualized in Fig. 1 where the phase space for $\beta=0$ and $\Gamma\geqslant 0$ is depicted for different values of the constant k. The positions of the equilibrium point I as a function of k are represented by the dashed line. All the solutions start on the circle $\Phi^2+\Psi^2=1$, $\Gamma=0$. When $\Gamma=0$ (massless scalar field), for all the cases, the solutions tend to the

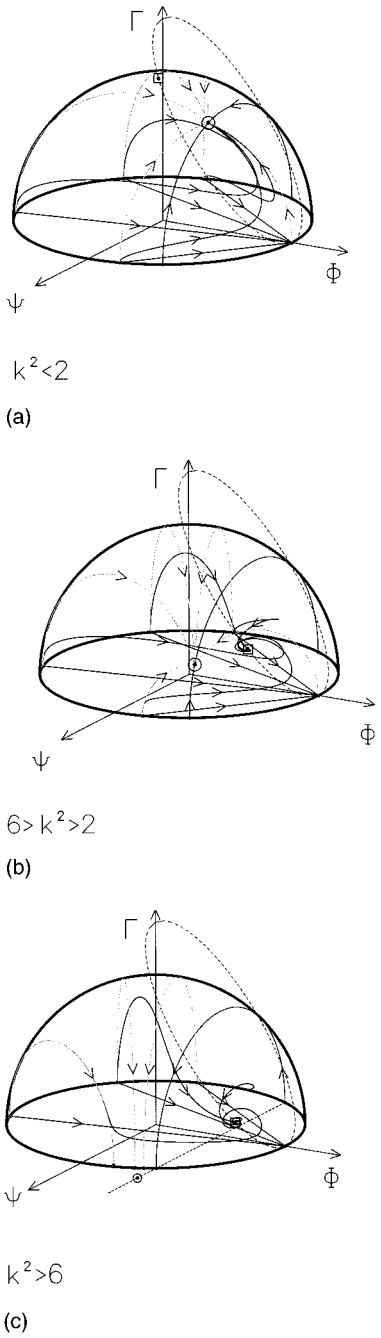

FIG. 1. Phase space when $\beta=0$ and $\Gamma\geqslant 0$, and for different values of the constant k. The equilibrium point I is represented by a square and the equilibrium point II by a circle. The dashed line describes the position of the point I for different values of k. Faded lines represent the trajectories of the solutions lying on the surface of the sphere which is an invariant set. The plane $\Gamma=0$ is an invariant set describing the massless scalar field solutions.

point $\Phi=1$, $\Psi=0$. When $k^2<2$, the point I is outside the sphere and the solutions tend to the equilibrium point II. When $2<k^2<6$, point I is inside the sphere and the solutions evolve either to the point I (those that go inside the sphere) or to the point II (those that lie on the boundary of the sphere). When $k^2>6$, the only attracting point is point I (inside the sphere). The trajectories on the

surface start and finish on the circle $\Phi^2+\Psi^2=1$, $\Gamma=0$, in such a way that their projections on the plane $\Gamma=0$ are a straight line directed to the point $\Psi=-(k/2\sqrt{2})$ $\Phi=\frac{1}{2}$ which is outside the surface.

The behavior described above remains the same when β is different from zero.

IV. CONCLUSIONS

We have studied in this paper the asymptotic behavior of a particular class of inhomogeneous solutions with a minimally coupled scalar field with an exponential potential. The metric belongs to the class of G_2 cosmologies.

We have succeeded in defining a set of new variables for which the entire phase space is bounded by a four-sphere. From the analysis of the dynamical system obtained for this metric, we deduce the following:

(i) As in the homogeneous case,[13] the dynamical behavior of the metric depends on the parameter k which is related to the mass of the scalar field. The parameters a and b which drive the inhomogeneity do not play a significant role in this behavior.

(ii) When $k^2<2$, the only equilibrium point is that given by the FRW universe. The trajectories evolve from the surface of the four-sphere, representing the Kasner regime near the initial singularity, towards the isotropic equilibrium point II. When $k^2>2$, there are two equilibrium points: one is the homogeneous Bianchi type VI (point I) and the second is the FRW solution which is a saddle point and, therefore, unstable against small changes of the initial conditions. This means that the cosmic no-hair theorem holds in this case provided $k^2<2$.

The behavior described above is almost identical to that of homogeneous models,[13] indicating that the introduction of the inhomogeneity through the constants a and b does not affect remarkably the dynamical system. It is likely that the presence of a more ''strong'' inhomogeneity, assuming another dependence on the spatial coordinate, may change the behavior of the solutions and the conditions to isotropize. We consider, therefore, that it is important to extend this analysis to a more general class of inhomogeneous scalar field solutions.

As to the inflation of the models, for inhomogeneous solutions there is no natural way to see whether the models inflate. The hypersurfaces $\phi=$constant do not define a globally timelike observer and, therefore, one should use a weaker way to specify the inflationary behavior. It has been suggested,[20] for example, to look at the fulfillment of the strong energy condition, the breaking of which is a necessary condition for a model to inflate. The energy density and the pressure of the scalar field are given by

$$\rho=-\tfrac{1}{2}\,\overline{\phi}_{,a}\overline{\phi}^{,a}+V,\quad p=-\tfrac{1}{2}\overline{\phi}_{,a}\overline{\phi}^{,a}-V. \tag{39}$$

In terms of the new variables, the breaking of the energy condition is written as

$$3p+\rho=e^{-F}\left(\frac{\dot{G}}{G}+\dot{f}\right)^2\left[\Psi^2-\frac{1}{2}\,\Gamma^2-\frac{2b^2}{(\dot{G}/G+\dot{f})^2}\right]<0. \tag{40}$$

For the equilibrium points I and II the expression $\Psi^2-\frac{1}{2}\Gamma^2$ turns out to be

$$\frac{2(k^2-2)}{(2+k^2)^2}\quad\text{and}\quad\frac{3(k^2-2)}{16}, \tag{41}$$

respectively. That means that if $k^2<2$, both points describe space–times inflating, but if $k^2>2$, the energy condition could be broken only by the solution represented by the point I depending on the value of b. This behavior is similar again to that of the homogeneous models.[8]

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On the distribution of gravitational energy in the de Sitter space

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We calculate the total gravitational energy and the gravitational energy density of the de Sitter space using the definition of localized gravitational energy that naturally arises in the framework of the teleparallel equivalent of general relativity. We find that the gravitational energy can only be defined within the cosmological horizon and is largely concentrated in regions far from the center of spherical symmetry, i.e., in the vicinity of the maximal spacelike radial coordinate $R = \sqrt{3/\Lambda}$. The smaller the cosmological constant, the farther the concentration of energy. This result complies with the phenomenological features of the de Sitter solution, namely, the existence of a radial acceleration directed away from the center of symmetry experienced by a test particle in the de Sitter space. Einstein already contemplated the de Sitter solution as a world with a surface distribution of matter, a picture which is in agreement with the present analysis. © *1996 American Institute of Physics.* [S0022-2488(96)01012-2]

I. INTRODUCTION

The difficulty in defining gravitational energy density within the framework of the Hilbert–Einstein Lagrangian formulation has led to the belief that the gravitational energy cannot be localized. It is widely assumed that an expression for the localized energy density of the gravitational field does not exist. However, it is well known that the total energy of a given asymptotically flat space–time can be calculated by means of pseudotensor methods, which make use of coordinate-dependent expressions. A different approach to the construction of an energy expression for the gravitational field is based on the idea of quasilocal energy. The quasilocal definition of energy, momentum, and angular momentum associates these quantities to an arbitrary spacelike two-surface S in an arbitrary space–time manifold. The inexistence of an unequivocal definition of gravitational energy still remains an actual problem, important in its own right. Furthermore, such definition may play a major role in the thermodynamics of self-gravitating systems. This problem has been recently addressed in Ref. 1, where a comprehensive bibliography on quasi-local energy is presented. Although all attempts so far have led to interesting mathematical developments, they did not allow the achievement of a definite solution, either because of conceptual or mathematical difficulties.

Recently the problem of localization of energy in general relativity has been reconsidered in the framework of the teleparallel equivalent of general relativity (TEGR).[2] The Lagrangian formulation of the TEGR is established by means of the tetrad field $e^a{}_\mu$ and the spin affine connection $\omega_{\mu ab}$, which are taken to be completely independent field variables, even at the level of field equations. This formulation has been investigated in the past in the context of Poincaré gauge theories.[3,4] However, as we will explain ahead, this is not an alternative theory of gravity. This is just an *alternative formulation* of general relativity, in which the curvature tensor constructed out of $\omega_{\mu ab}$ vanishes, but the torsion tensor is nonvanishing. The physical content of the theory is dictated by Einstein's equations. As we will show, in this alternative geometrical formulation the gravitational energy density can be naturally defined.

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The expression for the localized energy density of the gravitational field has arisen in the context of the Hamiltonian formulation of the TEGR.[5] It has been demonstrated that under a suitable gauge fixing of $\omega_{\mu ab}$, already at the Lagrangian level, the Hamiltonian formulation of the TEGR is well defined.[5] The resulting constraints are first class constraints. In fact, the Hamiltonian formulation looks very similar to the usual Arnowitt–Deser–Misner (ADM) formulation.[6] However, there are crucial differences. The integral form of the Hamiltonian constraint equation $C=0$ in the TEGR can be written in the form $C=H-E_{\mathrm{ADM}}=0$, when we restrict considerations to asymptotically flat space–times.[2] The quantity $\varepsilon(x)$ which appears in the expression of C and which under intergration yields E_{ADM} is recognized as the gravitational energy density. We have applied the expression of $\varepsilon(x)$ to the calculation of the energy inside a surface of constant radius, both for the Schwarzschild[2] and for the Kerr metric,[7] and the results are remarkably the same as those obtained by means of the quasilocal energy definition proposed by Brown and York.[1] Moreover, the calculational scheme is rather simple, as we will see shortly, and is exempt of some complications inherent to the latter. Therefore, for asymptotically flat space–times, the gravitational energy density has a definite and unambiguous expression within the framework of the TEGR.

We recall that the gravitational energy can also be calculated by means of the surface term that appears in the expression of the gravitational Hamiltonian.[8,9] However, such surface term yields only the *total* gravitational energy, as the integration has to be necessarily carried out over the whole three-dimensional spacelike hypersurface, in which case the lapse function $N(x)$ goes over into its asymptotic value $N\rightarrow 1$ at spatial infinity.

The action integrals for space–times with different topologies require surface terms that are specific to each topology. Thus the corresponding Hamiltonian also acquires a surface term that is determined by the topological boundary conditions.[10] However, the Hamiltonian constraint for a space–time foliated by spacelike hypersurfaces always has the same basic structure, irrespective of boundary conditions [*additional* terms such as the cosmological constant may appear in the Hamiltonian constraint, as we will see ahead in Eq. (10)].

Therefore the question immediately arises as to whether the Hamiltonian constraint equation in the TEGR can always be written as $C=H-E=0$, in which case $\varepsilon(x)$ would be the gravitational energy density for any curved space–time.

One of the simplest deviations from asymptotically flat geometries are space–times with conical defects. We have applied our expression of gravitational energy density to the calculation of the energy per unit length of defects of topological nature, which include disclinations, i.e., cosmic strings, and dislocations.[11] The result is quite encouraging. We arrive at precisely the same well-known expression for the energy per unit length of a cosmic string (not even multiplicative factors have to be adjusted). Moreover, the total energy of a dislocation is zero, a result which is in close analogy with the statements of the theory of elasticity, which asserts that disclinations and dislocations are defects which require high energy and low energy, respectively.

In this paper we consider the de Sitter space, which is topologically of the type $S^3\times R$. We restrict the considerations to the static region within the cosmological horizon (i.e., the region for which $-g_{00}>0$) and calculate both the total energy and the distribution of energy along the radial direction. Again the result is rather remarkable. We will show that the cosmological constant induces a distribution of gravitational energy in such a way that the energy is largely concentrated in the peripheral region, i.e., in the vicinity of the maximal spacelike radial coordinate $R=\sqrt{3/\Lambda}$. As we will show in Sec. III, this picture is in total agreement with the phenomenological features of the de Sitter solution, and is as well in agreement with Einstein's belief, according to which the de Sitter's solution represents a space–time with a surface distribution of matter.[12] This fact strongly supports the validity of our expression for the gravitational energy density and also represents a clear indication that the Hamiltonian constraint equation in the TEGR can be unambiguously interpreted as an energy equation of the type $H-E=0$.

Notation: The space–time indices $\mu,\nu,\ldots$, and local Lorentz indices $a, b,\ldots$, run from 0–3. In

the 3+1 decomposition, Latin indices from the middle of the alphabet indicate space indices according to $\mu=0,i$, $a=(0),(i)$. The tetrad field $e^a{}_\mu$ and the spin connection $\omega_{\mu ab}$ yield the usual definitions of the torsion and curvature tensors: $R^a{}_{b\mu\nu}=\partial_\mu\omega_\nu{}^a{}_b+\omega_\mu{}^a{}_c\omega_\nu{}^c{}_b-\cdots$, $T^a{}_{\mu\nu}=\partial_\mu e^a{}_\nu+\omega_\mu{}^a{}_b e^b{}_\nu-\cdots$. The flat space–time metric is fixed by $\eta_{(0)(0)}=-1$.

II. THE LAGRANGIAN AND HAMILTONIAN FORMULATIONS OF THE TEGR

In the TEGR the tetrad field $e^a{}_\mu$ and the spin connection $\omega_{\mu ab}$ are independent field variables, not related by any of the field equations. The spin connection is enforced to satisfy the condition of zero curvature. The Lagrangian density in empty space–time is given by[2,5]

$$L(e,\omega,\lambda)=-ke(\tfrac{1}{4}T^{abc}T_{abc}+\tfrac{1}{2}T^{abc}T_{bac}-T^aT_a)+e\lambda^{ab\mu\nu}R_{ab\mu\nu}(\omega), \tag{1}$$

where $k=1/16\pi G$, G is the gravitational constant, $e=\det(e^a{}_\mu)$, $\lambda^{ab\mu\nu}$ are Lagrange multipliers, and T_a is the trace of the torsion tensor defined by $T_a=T^b{}_{ba}$.

The equivalence of the TEGR with Einstein's general relativity is guaranteed by the identity

$$eR(e,\omega)=eR(e)+e(\tfrac{1}{4}T^{abc}T_{abc}+\tfrac{1}{2}T^{abc}T_{acb}-T^aT_a)-2\partial_\mu(eT^\mu), \tag{2}$$

which is obtained by just substituting the arbitrary spin connection $\omega_{\mu ab}={}^0\omega_{\mu ab}(e)+K_{\mu ab}$ in the scalar curvature tensor $R(e,\omega)$ on the left-hand side of (2); ${}^0\omega_{\mu ab}(e)$ is the Levi–Civita connection and $K_{\mu ab}=\frac{1}{2}e_a{}^\lambda e_b{}^\nu(T_{\lambda\mu\nu}+T_{\nu\lambda\mu}-T_{\mu\nu\lambda})$ is the contorsion tensor. The vanishing of $R^a{}_{b\mu\nu}(\omega)$, which is one of the field equations derived from (1), implies the equivalence of the scalar curvature $R(e)$, constructed out of $e^a{}_\mu$ only, and the quadratic combination of the torsion tensor. It also ensures that the field equation arising from the variation of L with respect to $e^a{}_\mu$ is strictly equivalent to Einstein's equations in tetrad form. Let $\delta L/\delta e^{a\mu}=0$ denote the field equation satisfied by $e_{a\mu}$. It can be shown by explicit calculations that

$$\frac{\delta L}{\delta e^{a\mu}}=\frac{1}{2}\left\{R_{a\mu}(e)-\frac{1}{2}\,e_{a\mu}R(e)\right\}$$

(we refer the reader to Ref. 5 for additional details).

For *asymptoticaly flat* space–times the total divergence in (2) does *not* contribute to the action integral. Therefore the latter does not require additional surface terms, as it is already invariant under coordinate transformations that preserve the asymptotic structure of the field quantities.[9] It is well known that for compact geometries a surface term has to be included in the action, in order to make the variations of the field variables well defined. This surface term is constructed out of the trace of the extrinsic curvature on the boundary. However, we will no longer worry about surface terms in the Lagrangian or in the Hamiltonian, as we will be interested only in the constraint structure of the theory.

The Hamiltonian formulation of the TEGR can be successfully implemented if we fix the gauge $\omega_{0ab}=0$ from the outset, since in this case the constraints constitute a *first class* set.[5] The condition $\omega_{0ab}=0$ is achieved by breaking the local Lorentz symmetry of (1). We still make use of the residual time-independent gauge symmetry to fix the usual time gauge condition $e_{(k)}{}^0=e_{(0)i}=0$. Because of $\omega_{0ab}=0$, H does not depend on P^{kab}, the momentum canonically conjugated to ω_{kab}. Therefore arbitrary variations of $L=p\dot{q}-H$ with respect to P^{kab} yields $\dot{\omega}_{kab}=0$. Thus in view of $\omega_{0ab}=0$, ω_{kab} drops out from our considerations. The above gauge fixing can be understood as the fixation of a *global* reference frame.

Under the above gauge fixing, the canonical action integral obtained from (1) becomes[5]

$$A_{TL}=\int d^4x\{\Pi^{(j)k}\dot{e}_{(j)k}-H\}, \tag{3}$$

$$H = NC + N^i C_i + \Sigma_{mn}\Pi^{mn}. \tag{4}$$

In expression (4) above we are omitting surface terms. Here N and N^i are the lapse and shift functions and $\Pi^{mn} = e_{(j)}{}^m \Pi^{(j)n}$ and $\Sigma_{mn} = -\Sigma_{nm}$ are Lagrange multipliers. The constraints are defined by

$$C = \partial_j(2keT^j) - ke\Sigma^{kij}T_{kij} - \frac{1}{4ke}\left(\Pi^{ij}\Pi_{ji} - \frac{1}{2}\Pi^2\right), \tag{5}$$

$$C_k = -e_{(j)k}\partial_i \Pi^{(j)i} - \Pi^{(j)i}T_{(j)ik}, \tag{6}$$

with $e = \det(e_{(j)k})$, $T^i = g^{ik}e^{(j)l}T_{(j)lk}$, and $T_{(j)lk} = \partial_l e_{(j)k} - \partial_k e_{(j)l}$. We remark that (3) and (4) are invariant under *global* SO(3) and general coordinate transformations. [In Eqs. (1) and (2), e is the determinant of the *space–time* tetrad field; from Eq. (3) on, e stands for the determinant of the triads restricted to the three-dimensional spacelike hypersurface.]

If we assume the asymptotic behavior $e_{(j)k} \approx \eta_{jk} + \frac{1}{2}h_{jk}(1/r)$ for $r \to \infty$, which is appropriate for an asymptotically flat space–time, then in view of the relation

$$\frac{1}{8\pi G}\int d^3x \partial_j(eT^j) = \frac{1}{16\pi G}\int_S dS_k(\partial_i h_{ik} - \partial_k h_{ii}) \equiv E_{\mathrm{ADM}}, \tag{7}$$

where the surface integral is evaluated for $r \to \infty$, we note that the integral form of the Hamiltonian constraint $C = 0$ may be rewritten as

$$\int d^3x \left\{ ke\Sigma^{kij}T_{kij} + \frac{1}{4ke}\left(\Pi^{ij}\Pi_{ji} - \frac{1}{2}\Pi^2\right)\right\} = E_{\mathrm{ADM}}. \tag{8}$$

The integration is over the whole three-dimensional space. Given that $\partial_j(eT^j)$ is a scalar density, from (7) and (8) we define the gravitational energy density enclosed by a volume V of the space as[2]

$$E_g = \frac{1}{8\pi G}\int_V d^3x \partial_j(eT^j). \tag{9}$$

It must be noted that this expression is also invariant under global SO(3) transformations.

One is immediately led to ask whether the Hamiltonian constraint for topologically different space–times can also be written as Eq. (8). In the next section we will consider the de Sitter space. Before addressing the latter, let us recall here some applications of E_g. We have calculated the gravitational energy inside a surface of constant radius r_0 both for the Schwarzschild[2] and for the Kerr solution,[7] using Boyer and Lindquist coordinates.[13,14] These quantities have also been calculated by means of Brown and York's procedure, in Refs. 1 and 15, respectively. The expressions found by using (9) are in total agreement with those obtained via the method of Ref. 1. Moreover, E_g can be calculated for any volume in the three-dimensional spacelike hypersurface, at least through numerical integration, whereas the evaluation of the energy in Ref. 15 can only be carried out in the limit of slow rotation of the black hole (the application of Brown and York's procedure to the Kerr solution with arbitrary parameters meets some technical difficulties, as discussed in Ref. 15).

Definition (9) has also been applied to a class of conical space–time defects, in which disclinations (cosmic strings) and dislocations are considered altogether. For the space–time of a single cosmic string, i.e., for a pure disclination, we obtain precisely the well-known value of energy per unit length of the string.[11] Furthermore, the *total* gravitational energy for a pure dislocation vanishes. This is a very interesting result, because we know from the theory of elasticity that

disclinations are defects that require a large amount of energy to be formed, whereas dislocations require low energy (see sections 6.3.2 and 6.5 of Ref. 16 for a discussion as to why the energy demanded for the formation of a disclination in a crystal is very high). Therefore the above calculations of energy are in close agreement with the statements of the theory of elasticity [in this respect we recall that attempts were made a long time ago which envisaged the space–time as a continuum with microstructure (see Ref. 4, section 1.2)].

III. GRAVITATIONAL ENERGY IN THE dE SITTER SPACE

We will consider now the theory defined by the Lagrangian density (1) supplemented by a term containing the cosmological constant Λ. Thus we add to (1) the quantity $2^4e\Lambda$, where ${}^4e = Ne$ is the determinant of the *space–time* tetrad field $e_{a\mu}$. This additional term will contribute to the action integral (3) only as an extra term of the Hamiltonian constraint. The new Hamiltonian constraint reads

$$C=\partial_j(2keT^j)-ke\Sigma^{kij}T_{kij}-\frac{1}{4ke}\left(\Pi^{ij}\Pi_{ji}-\frac{1}{2}\,\Pi^2\right)-2e\Lambda. \tag{10}$$

The most general spherically symmetric solution of the field equations with a positive cosmological constant is the Schwarzschild–de Sitter solution (throughout this section we will make $G=1$):

$$ds^2=-\left(1-\frac{2m}{r}-\frac{r^2}{R^2}\right)dt^2+\left(1-\frac{2m}{r}-\frac{r^2}{R^2}\right)^{-1}dr^2+r^2\ d\theta^2+r^2\ \sin^2\ \theta d\phi^2. \tag{11}$$

This metric represents the gravitational field of a particle of mass m located at the origin of a globally hyperbolic space–time. The vacuum solution, obtained by setting $m=0$ in (11), is the de Sitter solution. Here R is the maximal spacelike radial coordinate for the (vacuum) de Sitter space and is given by $R=\sqrt{3/\Lambda}$.

Strictly speaking, de Sitter space–time corresponds to a four-dimensional surface in a flat five-dimensional space with metric $(-,+,+,+,+)$ described by

$$-z_0^2+z_1^2+z_2^2+z_3^2+z_3^2+z_4^2=\frac{3}{\Lambda},\quad \Lambda>0.$$

The coordinates (t,r,θ,ϕ) in (11) cover only half of the space defined by the relation above. However we will be interested just in (11), as it suffices for our purposes. Moreover, we will restrict the considerations to the physical region between the Schwarzschild (black hole) and the cosmological horizons.

Expression (9) allows us to calculate the gravitational energy for any volume in space. We wish to obtain the energy contained within a surface of constant radius r_0. For this purpose we will calculate $eT^1=eT^r$ for a space–time whose spacelike section is described by the line element

$$dl^2=\alpha^2dr^2+r^2d\theta^2+r^2\ \sin^2\ \theta d\phi^2, \tag{12}$$

where α is a function of the coordinate r. The triads that correspond to (12) are given by

$$e_{(k)i}=\begin{pmatrix} \alpha\ \sin\ \theta\ \cos\ \phi & r\ \cos\ \theta\ \cos\ \phi & -r\ \sin\ \theta\ \sin\ \phi \\ \alpha\ \sin\ \theta\ \sin\ \phi & r\ \cos\ \theta\ \sin\ \phi & r\ \sin\ \theta\ \cos\ \phi \\ \alpha\ \cos\ \theta & -r\ \sin\ \theta & 0 \end{pmatrix}. \tag{13}$$

Here (k) is the line index and i is the column index.

The determinant e of (13) reads $e=\alpha r^2 \sin\theta$. After a lengthy but otherwise straightforward calculation of

$$eT^1 = eg^{1j}g^{im}e^{(k)}{}_m T_{(k)ij},$$

we arrive at

$$eT^1 = 2r \sin\theta\left(1-\frac{1}{\alpha}\right). \tag{14}$$

Therefore for the Schwarzschild–de Sitter solution we have

$$eT^1 = 2r \sin\theta\left(1-\sqrt{1-\frac{2m}{r}-\frac{r^2}{R^2}}\right). \tag{15}$$

The energy contained within a surface of constant radius r_0 is thus given by

$$E_g = \frac{1}{8\pi}\int_S d\theta d\phi eT^1 = r_0\left(1-\sqrt{1-\frac{2m}{r_0}-\frac{r_0^2}{R^2}}\right), \tag{16}$$

where S is a surface of constant radius r_0.

Let us evaluate expression (16) for the range of values of r_0 such that

$$\frac{2m}{r_0} \ll 1, \quad \frac{r_0^2}{R^2} \ll 1,$$

in which case we assume the cosmological constant to be very small. Expanding (16) and neglecting all powers of both $2m/r_0$ and r_0^2/R^2 we arrive at

$$E_g = r_0 + m \equiv E_{dS} + m. \tag{17}$$

Here E_{dS} is the value of energy we would obtain in the absence of the mass m, and therefore it represents the background (vacuum) energy. Upon subtraction of this term we obtain the standard ADM value of energy for a particle of mass m. Of course in (17) we expect r_0 to be much larger than m.

The total gravitational energy contained within the cosmological horizon can be easily calculated, but for this purpose one has to find the roots of the equation $1-2m/r-r^2/R^2=0$. The result is not illuminating. If $R \gg m$, we find that $E_g^{\text{total}} = r_{\max}$, where $r_{\max}$ is slightly smaller than R and is a solution of the equation above. In what follows we will rather consider the vacuum de Sitter solution only, since in this case the analysis of the energy density is most easily carried out, and the main features are not altered by the introduction of a mass m at $r=0$.

Before proceeding we mention that the present analysis is different from that carried out by Abbott and Deser.[17] These authors provide an expression for the energy of the gravitational field *about* the de Sitter background, i.e., they calculate the energy of a field configuration that deviates from the de Sitter metric and which vanish at infinity. In contrast, by means of expression (9) we can compute the energy of the whole gravitational field configuration, including the background.

The total gravitational energy E_{dS} contained in the physical region of the vacuum de Sitter space is obtained from (16) by making $m=0$ and $r_0=R$:

$$E_{dS} = R = \sqrt{\frac{3}{\Lambda}}. \tag{18}$$

The total volume of the compact spacelike section equals $2\pi^2R^3$. Therefore the average energy density is given by

$$\frac{E_{dS}}{2\pi^2R^3}=\frac{\Lambda}{6\pi^2}. \tag{19}$$

Let us obtain now the distribution of gravitational energy in the de Sitter space. In view of the spherical symmetry we will be interested in calculating the density of energy per unit radial distance $\varepsilon(r)$, which is obtained by integrating $(1/8\pi)\partial_r(eT^1{}_1)$ in θ and ϕ. Thus $\varepsilon(r)$ yields the gravitational energy contained between the spherical shells of radii r and $r+dr$. Considering $m=0$ in (15) we obtain upon integration in the angular variables and differentiation in r:

$$\varepsilon(r)=1+\frac{2\beta^2-1}{\sqrt{1-\beta^2}}. \tag{20}$$

where we have set $\beta^2=r^2/R^2$. The function $\varepsilon(r)$ has the following properties. In the range $0\leqslant\beta\leqslant1$, $\varepsilon(r)$ vanishes only for $r=0$. Moreover for $\beta=1$ it diverges: $\varepsilon(\beta=1)\to\infty$. It is straightforward to check that this is a monotonically increasing function, largely concentrated in the vicinity of $\beta=1$: $\varepsilon(\beta=0.1)=0.015$; $\varepsilon(\beta=0.5)=0.423$; $\varepsilon(\beta=0.9)=2,422$. The total energy contained inside the surfaces of radii $0.1R$, $0.5R$, and $0.9R$ are given by $E_g=5.01\times10^{-4}R$, $E_g=0,067R$, and $E_g=0.51R$, respectively.

Therefore almost half of the gravitational energy is located between $\beta=0.9$ and $\beta=1$. This result is in total agreement with the phenomenological features of the de Sitter solution, and can be verified in the following way. The g_{00} component of (11) can be written as

$$g_{00}=1+2\phi,$$

where ϕ is given by

$$\phi=-\frac{m}{r}-\frac{1}{6}\Lambda r^2.$$

Here ϕ is the potential in classical mechanics which would induce motion of a test particle approximately along the geodesics of (11). Therefore even in the absence of a mass m a test particle would be subject to a radial acceleration

$$a=\tfrac{1}{3}\Lambda r,$$

directed away from $r=0$.

The acceleration increases with the distance r, indicating that the gravitational field is more intense at points far from the origin. Therefore when $m=0$ the gravitational field given by (11) acts on physical bodies as if there were a radially symmetric distribution of matter about the origin, beyond the cosmological horizon, just as m represents the mass of a black hole, concentrated inside the black hole horizon.

This is precisely the picture we obtain from (20). By applying (9) to the de Sitter solution we find that the cosmological constant induces a spherically symmetric distribution of gravitational energy, concentrated in regions distant from the origin, due to the gravitational field that acts on a test particle placed in the vacuum de Sitter space. Such a field can be thought of as due to some matter distribution.

One may think of (11) as representing the gravitational field of a spherical cavity inside some spherically symmetric distribution of matter (this idea is discussed, for instance, in Ref. 18). In this respect we recall that Einstein already conjectured that the de Sitter solution would correspond to

a world with a surface distribution of matter.[12] Such conjecture has found a natural explanation within the present geometrical framework, and shows that (9) yields a consistent expression for the gravitational energy in the de Sitter space.

We will briefly discuss how our procedure applies to the anti-de Sitter solution. The latter is obtained by making the replacement $r^2/R^2 \to -r^2/R^2$ in (11). The anti-de Sitter space is a noncompact manifold with constant negative curvature. The energy contained within a surface of constant radius r_0 can be easily calculated and reads

$$E_g = r_0\left(1 - \sqrt{1+\frac{r_0^2}{R^2}}\right), \tag{21}$$

where we have ignored the mass term m. Here r_0 ranges from 0 to ∞. Therefore as $r_0 \to \infty$, we find that $E_g \to -\infty$. This is an expected result, since the anti-de Sitter space is noncompact. The density of energy per unit radial distance $\varepsilon(r)$ in this case is given by

$$\varepsilon(r) = 1 - \frac{1+\dfrac{2r^2}{R^2}}{\sqrt{1+\dfrac{r^2}{R^2}}}. \tag{22}$$

We find that $\varepsilon(r)=0$ only for $r=0$. This point is also the only global maximum for $\varepsilon(r)$; for $r \to \infty$ we clearly see that $\varepsilon(r) \to -\infty$. Thus $\varepsilon(r)$ is a nonpositive monotonically decreasing function.

IV. DISCUSSION

The definition of gravitational energy is a long-standing problem in the theory of general relativity. Numerous attempts have been made in the past for a solution. This problem still attracts considerable attention in the literature, and remains an important issue to be settled. Essentially all of these previous attempts are in one or another way unsatisfactory. In particular it is widely claimed that the gravitational energy cannot be localized. We do not share this opinion. The mathematical structure of the TEGR shows that not only do we have a consistent and unambiguous definition of gravitational energy for asymptotically flat space–times, naturally built in the Hamiltonian formulation, but also that the gravitational energy is localized. The gravitational energy in the framework of the TEGR is given by expression (9). This expression has been successfully applied to a number of space–times, as we mentioned in Sec. II, whose gravitational energy is already known. A justification for the extension of this definition to more general space–times is not straightforward. In the case of asymptotically flat space–times, the Hamiltonian constraint equation can be written as $C = H - E_{\mathrm{ADM}} = 0$. We assume that this form of the constraint is a general feature of the theory, namely, that we can write the Hamiltonian constraint as $C = H - E$ for an arbitrary space–time, since the constraint structure in general relativity is fixed and does not depend on any particular topology.

In the above we considered the de Sitter solution and concluded that the cosmological constant induces a distribution of gravitational energy largely concentrated in the vicinity of the maximal spacelike radial distance R. This result is in total agreement with the fact that a test particle in the de Sitter space is subject to a radial acceleration directed away from the center of symmetry. Therefore the outcome of our analysis complies with the phenomenological behavior of a test particle in the de Sitter space. To our knowledge this is the first time that such analysis has been provided.

By inspecting Eq. (18) we see that if we make $\Lambda \to 0$ the total energy E_g diverges. The vanishing of Λ in (11) amounts to a change from a compact to a noncompact topology. Therefore such a change is not smooth, as it requires an infinite amount of energy. This fact seems to indicate that, at the classical level, topology changing processes are forbidden.

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Gravitational energy of rotating black holes

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In the teleparallel equivalent of general relativity the energy density of asymptotically flat gravitational fields can be naturally defined as a scalar density restricted to a three-dimensional spacelike hypersurface Σ. Integration over the whole Σ yields the standard ADM energy. Here we obtain the formal expression of the localized energy for a Kerr black hole. The expression of the energy inside a surface of constant radius can be explicitly calculated in the limit of small a, the specific angular momentum. Such expression turns out to be exactly the same as the one obtained by means of the method proposed recently by Brown and York [Phys. Rev. D **47**, 1407 (1993)]. We also calculate the energy contained within the outer horizon of the black hole, for *any* value of a. The result is practically indistinguishable from $E=2M_{ir}$, where M_{ir} is the irreducible mass of the black hole. © *1996 American Institute of Physics.* [S0022-2488(96)02912-X]

I. INTRODUCTION

Although it is widely believed that Einstein's equations describe the dynamics of the gravitational field, it has not been possible so far to arrive at a definite expression for the gravitational energy in the context of Einstein's general relativity. Attempts based on the Hilbert–Einstein action integral fail to yield an expression for the gravitational energy *density*.[1,2] The *total* gravitational energy is normally obtained from surface terms in the action or in the Hamiltonian,[3,4] or from pseudotensor methods which make use of coordinate dependent expressions.

Recently an expression for quasilocal energy has been proposed by Brown and York.[5] Such expression is derived directly from the action functional A_{cl}. The latter is identified as Hamilton's principal function and, in similarity with the classical Hamilton–Jacobi equation, which expresses the energy of a classical solution as minus the time rate of the change of the action, the quasilocal gravitational energy is identified as minus the proper time rate of change of the Hilbert-Einstein action (with surface terms included). Expressions for the quasilocal energy have been obtained for the Schwarzschild solution[5] and for the Kerr solution.[6]

Einstein's equations can also be obtained from the teleparallel equivalent of general relativity (TEGR). The Lagrangian formulation of the TEGR is established by means of the tetrad field $e^{a}{}_{\mu}$ and the spin affine connection $\omega_{\mu ab}$, which are taken to be completely independent field variables, even at the level of field equations. This formulation has been investigated in the past in the context of Poincaré gauge theories.[7,8] However, as we will explain ahead, this is not an alternative theory of gravity. This is just an *alternative formulation* of general relativity, in which the curvature tensor constructed out of $\omega_{\mu ab}$ vanishes, but the torsion tensor is nonvanishing. The physical content of the theory is dictated by Einsten's equations. In this alternative geometrical formulation the gravitational energy density can be naturally defined.

The expression for the gravitational energy density arises in the framework of the Hamiltonian formulation of the TEGR.[9] It has been demonstrated that under a suitable gauge fixing of $\omega_{\mu ab}$, already at the Lagrangian level, the Hamiltonian formulation of the TEGR is well defined. The resulting constraints are first class constraints.[9] The Hamiltonian formulation turns out to be very much similar to the usual ADM formulation.[3] However, there are crucial differences. The integral form of the Hamiltonian constraint equation $C=0$ in the TEGR can be written in the form

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$C=H-E_{\mathrm{ADM}}=0$, when we restrict considerations to asymptotically flat space–times.[10] The quantity $\varepsilon(x)$, which appears in the expression of C and which under integration yields E_{ADM}, is recognized as the gravitational energy density.

We have calculated the energy inside a sphere of radius r_0 in a Schwarzschild space–time by means of $\varepsilon(x)$.[10] The expression turns out to be exactly the same as the one obtained by means of the procedure of Ref. 5 [expression (6.14) of Ref. 5]. In this paper we consider the Kerr black hole. We obtain the formal expression for the energy contained in any space volume in terms of nontrivial integrals. In the limit of slow rotation (small specific angular momentum) the energy contained within a surface of constant radius r_0 can be calculated. Again the result obtained here is exactly the same as that obtained by Martinez[6] who adopted Brown and York's procedure. The advantage of our procedure rests on the fact that the localized energy associated with a Kerr space–time can be calculated in the general case, without recourse to particular limits, at least by means of numerical integration, whereas in Brown and York's procedure one has to calculate the subtraction term ε^0 and for this purpose it is necessary to embed an arbitrary two-dimensional boundary surface of the Kerr space Σ in the appropriate reference space (E^3, say), which is not always possible.[6]

We have also calculated the energy contained within the outer horizon of the black hole. Such a quantity has been obtained by Martinez[6] in the limit of small a, and reads $E=2M_{ir}$ [plus corrections of order $O(a^4/M_{ir}^4)$], where M_{ir} is the irreducible mass of the black hole. The concept of irreducible mass was introduced by Christodoulou.[11] He showed that the mass of a rotating black hole cannot be decreased to values below M_{ir} by means of Penrose's process of extraction of energy. One would thus consider $E=2M_{ir}$ to be the energy that cannot escape from the black hole. Here we obtain the expression of the energy contained within the horizon for *any* value of a. The result is striking. The numerical values of this expression are practically coincident with $2M_{ir}$ in the whole range $0\leqslant a\leqslant m$, although the expression is algebraically different from $2M_{ir}$.

In Sec. II we present the mathematical preliminaries of the TEGR, its Hamiltonian formulation, and the expression of the energy for an arbitrary asymptotically flat space–time. The establishment of a reference space–time, whose gravitational energy is zero, is performed in Sec. III. In Sec. IV we carry out the construction of triads for a three-dimensional spacelike hypersurface of the Kerr type, obtain the general expression of the energy contained in a volume V of space, and provide the exact expression of the latter in the limit of slow rotation. Comments and conclusions are presented in Sec. V.

Notation: space–time indices $\mu,\nu,\ldots$, and local Lorentz indices $a,b,\ldots$, run from 0–3. In the 3+1 decomposition Latin indices from the middle of the alphabet indicate space indices according to $\mu=0,i$, $a=(0),(i)$. The tetrad field $e^a{}_\mu$ and the spin connection $\omega_{\mu ab}$ yield the usual definitions of the torsion and curvature tensors: $R^a{}_{b\mu\nu}=\partial_\mu\omega_\nu{}^a{}_b+\omega_\mu{}^a{}_c\ \ \omega_\nu{}^c{}_b-\ldots$, $T^a{}_{\mu\nu}=\partial_\mu e^a{}_\nu+\omega_\mu{}^a{}_b e^b{}_\nu-\cdots$. The flat space–time metric is fixed by $\eta_{(0)(0)}=-1$.

II. THE TEGR IN HAMILTONIAN FORM

In the TEGR the tetrad field $e^a{}_\mu$ and the spin connection $\omega_{\mu ab}$ are completely independent field variables. The latter is enforced to satisfy the condition of zero curvature. The Lagrangian density in empty space–time is given by

$$L(e,\omega,\lambda)=-ke(\tfrac{1}{4}T^{abc}T_{abc}+\tfrac{1}{2}T^{abc}T_{bac}-T^aT_a)+e\lambda^{ab\mu\nu}R_{ab\mu\nu}(\omega), \tag{1}$$

where $k=1/16\pi G$, G is the gravitational constant, $e=\det(e^a{}_\mu)$, $\lambda^{ab\mu\nu}$ are Lagrange multipliers, and T_a is the trace of the torsion tensor defined by $T_a=T^b{}_{ba}$.

The equivalence of the TEGR with Einstein's general relativity is based on the identity

$$eR(e,\omega)=eR(e)+e(\tfrac{1}{4}T^{abc}T_{abc}+T^{abc}T_{bac}-T^aT_a)-2\partial_\mu(eT^\mu), \tag{2}$$

which is obtained by just substituting the arbitrary spin connection $\omega_{\mu ab}={}^{o}\omega_{\mu ab}(e)+K_{\mu ab}$ in the scalar curvature tensor $R(e,\omega)$ on the left-hand side; ${}^{o}\omega_{\mu ab}(e)$ is the Levi-Civita connection and $K_{\mu ab}=\frac{1}{2}e_a{}^{\lambda}e_b{}^{\nu}(T_{\lambda\mu\nu}+T_{\nu\lambda\mu}-T_{\mu\nu\lambda})$ is the contorsion tensor. The vanishing of $R^{a}{}_{b\mu\nu}(\omega)$, which is one of the field equations derived from (1), implies the equivalence of the scalar curvature $R(e)$, constructed out of $e^{a}{}_{\mu}$ only, and the quadratic combination of the torsion tensor. It also ensures that the field equation arising from the variation of L with respect to $e^{a}{}_{\mu}$ is strictly equivalent to Einstein's equations in tetrad form. Let $\delta L/\delta e^{a\mu}=0$ denote the field equations satisfied by $e^{a\mu}$. It can be shown by explicit calculations that

$$\frac{\delta L}{\delta e^{a\mu}}=\frac{1}{2}\left\{R_{a\mu}(e)-\frac{1}{2}\,e_{a\mu}R(e)\right\} \tag{3}$$

(we refer the reader to Ref. 9 for additional details).

It is important to notice that for asymptotically flat space–times the total divergence in (2) does *not* contribute to the action integral. This term is a scalar density that falls off as $1/r^3$ when $r\to\infty$. In this limit we should consider variations in $g_{\mu\nu}$ or in $e_{a\mu}$ that preserve the asymptotic structure of the flat space–time metric; the allowed coordinate transformations must be of the Poincaré type. The variation of $\partial_{\mu}(eT^{\mu})$ at infinity under such variations of $e_{a\mu}$ vanishes. Moreover all surface integrals arising from partial integration in the variation of the action integral vanish as well. Therefore the action does not require additional surface terms, as it is invariant under transformations that preserve the asymptotic structure of the field quantities. This property fixes the action integral, together with the requirement that the variation of the latter must yield Einstein's equations (the Hilbert–Einstein Lagrangian requires the addition of a surface term for the variation of the action to be well defined; a clear discussion of this point is given in Ref. 12). In what follows we will be interested in asymptotically flat space–times.

The Hamiltonian formulation of the TEGR can be successfully implemented if we fix the gauge $\omega_{0ab}=0$ from the outset, since in this case the constraints (to be shown below) constitute a *first class* set.[9] The condition $\omega_{0ab}=0$ is achieved by breaking the local Lorentz symmetry of (1). We still make use of the residual time-independent gauge symmetry to fix the usual time gauge condition $e_{(k)}{}^{0}=e_{(0)i}=0$. Because of $\omega_{0ab}=0$, H does not depend on P^{kab}, the momentum canonically conjugated to ω_{kab}. Therefore arbitrary variations of $L=p\dot{q}-H$ with respect to P^{kab} yields $\dot{\omega}_{kab}=0$. Thus in view of $\omega_{0ab}=0$, ω_{kab} drops out from our considerations. The above gauge fixing can be understood as the fixation of a *global* reference frame.

Under the above gauge fixing the canonical action integral obtained from (1) becomes[9]

$$A_{TL}=\int d^4x\{\Pi^{(j)k}\dot{e}_{(j)k}-H\}, \tag{4}$$

$$H=NC+N^{i}C_i+\Sigma_{mn}\Pi^{mn}+\frac{1}{8\pi G}\,\partial_k(NeT^{k})+\partial_k(\Pi^{jk}N_j). \tag{5}$$

Here N and N^{i} are the lapse and shift functions, and $\Sigma_{mn}=-\Sigma_{nm}$ are Lagrange multipliers.

The constraints are defined by

$$C=\partial_j(2keT^{j})-ke\Sigma^{kij}T_{kij}-\frac{1}{4ke}\left(\Pi^{ij}\Pi_{ji}-\frac{1}{2}\,\Pi^{2}\right), \tag{6}$$

$$C_k=-e_{(j)k}\,\partial_i\Pi^{(j)i}-\Pi^{(j)i}T_{(j)ik}, \tag{7}$$

with $e=\det(e_{(j)k})$ and $T^{i}=g^{ik}e^{(j)l}T_{(j)lk}$, where $T_{(j)lk}=\partial_l e_{(j)k}-\partial_k e_{(j)l}$. We remark that (4) and (5) are invariant under global SO(3) and general coordinate transformations.

We assume the asymptotic behavior $e_{(j)k}\approx\eta_{jk}+\frac{1}{2}h_{jk}(1/r)$ for $r\to\infty$. In view of the relation

$$\frac{1}{8\pi G}\int d^3x\ \partial_j(eT^j)=\frac{1}{16\pi G}\int_S dS_k(\partial_i h_{ik}-\partial_k h_{ii})=E_{\mathrm{ADM}}, \tag{8}$$

where the surface integral is evaluated for $r\to\infty$, the integral form of the Hamiltonian constraint $C=0$ may be rewritten as

$$\int d^3x\left\{ke\Sigma^{kij}T_{kij}+\frac{1}{4ke}\left(\Pi^{ij}\Pi_{ji}-\frac{1}{2}\Pi^2\right)\right\}=E_{\mathrm{ADM}}. \tag{9}$$

The integration is over the whole three-dimensional space. Given that $\partial_j(eT^j)$ is a scalar density, from (7) and (8) we define the gravitational energy density enclosed by a volume V of the space as

$$E_g=\frac{1}{8\pi G}\int_V d^3x\ \partial_j(eT^j). \tag{10}$$

It must be noted that E_g depends only on the triads $e_{(k)i}$ restricted to a three-dimensional spacelike hypersurface; the inverse quantities $e^{(k)i}$ can be written in terms of $e_{(k)i}$. From the identity (3) we observe that the dynamics of the triads does not depend on $\omega_{\mu ab}$. Therefore E_g given above does not depend on the fixation of any gauge for $\omega_{\mu ab}$.

III. THE REFERENCE SPACE–TIME

One of the motivations for considering the TEGR was the possibility of establishing a kind of background structure, a space–time on which the gravitational field would be defined, just like the other ordinary fields are defined on Minkowski space–time. This property would follow from the vanishing of $R_{ab\mu\nu}(\omega)$, but eventually is not achieved. Rather than obtaining such a background structure, we arrive at a *reference space–time*, which can be understood as follows. Consider a space with coordinates q^a such that $ds^2=\eta_{ab}\,dq^a\,dq^b$. We can make a coordinate transformation $dq^a=e^a{}_\mu(x)dx^\mu$ and rewrite the infinitesimal element as $ds^2=\eta_{ab}e^a{}_\mu(x)e^b{}_\nu(x)dx^\mu\,dx^\nu=g_{\mu\nu}\,dx^\mu\,dx^\nu$. This transformation can be *holonomic* or *anholonomic*.

Since we are concerned with the Hamiltonian formulation, we will restrict the considerations to spatial coordinates only. In this case the transformation is given by $dq^{(i)}=e^{(i)}{}_j\,dx^j$. As a simple example, consider

$$x^j=(r,\theta,\phi),\quad q^{(i)}=(r\sin\theta\sin\phi, r\sin\theta\cos\phi, r\cos\theta).$$

The infinitesimals $dq^{(i)}$ and dx^j are related by

$$e^{(i)}{}_j(x)=\frac{\partial q^{(i)}}{\partial x^j}=\begin{pmatrix}\sin\theta\cos\phi & r\cos\theta\cos\phi & -r\sin\theta\sin\phi\\ \sin\theta\sin\phi & r\cos\theta\sin\phi & r\sin\theta\cos\phi\\ \cos\theta & -r\sin\theta & 0\end{pmatrix},$$

where (i) is the line index and j the column index. Since the relation $dq^{(i)}=e^{(i)}{}_j\,dx^j$ can be integrated over the whole three-dimensional space, the transformation $q^{(i)}\to x^i$ does correspond to a single-valued global transformation and therefore it is called holonomic. Both sets of coordinates, $\{q^{(i)}\}$ and $\{x^j\}$, describe the three-dimensional Euclidean space.

However, in the general case this relation cannot be globally integrated, since $e^{(i)}{}_j$ may not be written as the gradient of a function, i.e., in general $e^{(i)}{}_j$ is not of the type $\partial q^{(i)}/\partial x^j$. If the quantities $e^{(i)}{}_j$ are such that $\partial_j e^{(i)}{}_k-\partial_k e^{(i)}{}_j\neq 0$, then the transformation is called anholonomic.

For the triads above the torsion tensor $T_{(i)jk}=\partial_j e_{(i)k}-\partial_k e_{(i)j}$ vanishes identically. A crucial result is that $T_{(i)jk}$ vanishes if and only if $\{e^{(i)}{}_j\}$ are gradient vectors.[13] The Levi-Civita connection

${}^{o}\omega_{m(i)(j)} = -\frac{1}{2}e^{(k)}{}_{m}(\Omega_{(i)(j)(k)} - \Omega_{(j)(i)(k)} - \Omega_{(k)(i)(j)})$, $\Omega_{(i)(j)(k)}=e_{(i)m}(e_{(j)}{}^{n}\,\partial_n e_{(k)}{}^{m} - e_{(k)}{}^{n}\,\partial_n e_{(j)}{}^{m})$, constructed out of triads which are gradient vectors, vanishes identically, and so does the curvature tensor $R_{(i)(j)mn}({}^{o}\omega)$. Thus the triads $e^{(i)}{}_{j}=\partial_j q^{(i)}$ are necessarily equivalent to the triads of the flat Euclidean space (the metric $g_{ij}=\partial_i q^{(m)}\,\partial_j q^{(n)}\,\eta_{(m)(n)}$ can be interpreted as a coordinate transformation of the constant flat metric).

In the framework of the Hamiltonian formulation of the TEGR the gravitational field corresponds to a configuration for which $T_{(i)jk}\neq 0$. Therefore *every* gravitational field is *anholonomically* related to the three-dimensional Euclidean space, which is to be taken as the reference space. Since the torsion tensor vanishes for the latter, as we have seen, the total gravitational energy of the reference space is zero (the gravitational energy density vanishes as well).

IV. ENERGY OF THE KERR GEOMETRY

The Kerr solution[14] describes the field of a rotating black hole. In terms of Boyer and Lindquist coordinates[15] (t,r,θ,ϕ) it is described by the metric

$$ds^2=-\frac{\Delta}{\rho^2}\,[dt-a\,\sin^2\,\theta\,d\phi]^2+\frac{\sin^2\,\theta}{\rho^2}\,[(r^2+a^2)d\phi-a\,dt]^2+\frac{\rho^2}{\Delta}\,dr^2+\rho^2\,d\theta^2,$$

$$\Delta\equiv r^2-2mr+a^2, \tag{11}$$

$$\rho^2\equiv r^2+a^2\,\cos^2\,\theta;$$

a is the specific angular momentum defined by $a=J/m$. The components of the metric restricted to the three-dimensional spacelike hypersurface are given by $g_{11}=\rho^2/\Delta$, $g_{22}=\rho^2$, and $g_{33}=(\Sigma^2/\rho^2)\sin^2\,\theta$, where Σ is defined by

$$\Sigma^2=(r^2+a^2)^2-\Delta a^2\,\sin^2\,\theta.$$

We define the triads $e_{(k)i}$ as

$$e_{(k)i}=\begin{pmatrix} \frac{\rho}{\sqrt{\Delta}}\sin\,\theta\,\cos\,\phi & \rho\,\cos\,\theta\,\cos\,\phi & -\frac{\Sigma}{\rho}\sin\,\theta\,\sin\,\phi \\ \frac{\rho}{\sqrt{\Delta}}\sin\,\theta\,\sin\,\phi & \rho\,\cos\,\theta\,\sin\,\phi & \frac{\Sigma}{\rho}\sin\,\theta\,\cos\,\phi \\ \frac{\rho}{\sqrt{\Delta}}\cos\,\theta & -\rho\,\sin\,\theta & 0 \end{pmatrix}, \tag{12}$$

(k) is the line index and i is the column index. The one form $e^{(k)}$ is defined by

$$e^{(k)}=e^{(k)}{}_{r}\,dr+e^{(k)}{}_{\theta}\,d\theta+e^{(k)}{}_{\phi}\,d\phi;$$

from what follows

$$e^{(k)}e_{(k)}=\frac{\rho^2}{\Delta}\,dr^2+\rho^2\,d\theta^2+\frac{\Sigma^2}{\rho^2}\,\sin^2\,\theta\,d\phi^2.$$

We also obtain $e=\det(e_{(k)i})=(\rho\Sigma/\sqrt{\Delta})\sin\,\theta$. Therefore the triads given by (12) describe the components of the Kerr solution restricted to the three-dimensional spacelike hypersurface.

One readily notices that there is another set of triads that yields the Kerr solution, namely, the set which is diagonal and whose entries are given by the square roots of g_{ii}. This set is not

appropriate for our purposes, and the reason can be understood even in the simple clase of flat space–time. In the limit when both a and m go to zero, (12) describes flat space: the curvature tensor *and* the torsion tensor vanish in this case, as we have seen in Sec. III. However, for the diagonal set of triads (again requiring $a\to 0$ and $m\to 0$),

$$e^{(r)}=dr, \quad e^{(\theta)}=r d\theta, \quad e^{(\phi)}=r\ \sin\ \theta\ d\phi,$$

some components of the torsion tensor do not vanish, $T_{(2)12}=1$, $T_{(3)13}=\sin\theta$, and E_g calculated out of the diagonal set above diverges when integrated over the whole space. Therefore the use of (12) is mandatory in the present context, as it is the only possible choice [modulo global SO(3) rotations].

The components of the torsion tensor can be calculated in a straightforward way from (12). Only $T_{(3)13}$ and $T_{(3)23}$ are vanishing. The others are given by

$$T_{(1)12}=\cos\ \theta\ \cos\ \phi\left(\frac{r}{\rho}+\frac{a^2}{\rho\sqrt{\Delta}}\sin^2\ \theta-\frac{\rho}{\sqrt{\Delta}}\right),$$

$$T_{(1)13}=\sin\ \theta\ \sin\ \phi\left\{-\frac{1}{\rho\Sigma}\left[2r(r^2+a^2)-a^2\ \sin^2\ \theta(r-m)\right]+\frac{r\Sigma}{\rho^3}+\frac{\rho}{\sqrt{\Delta}}\right\},$$

$$T_{(1)23}=\cos\ \theta\ \sin\ \phi\left\{\rho-\frac{\Sigma}{\rho}+a^2\ \sin^2\ \theta\left(\frac{\Delta}{\rho\Sigma}-\frac{\Sigma}{\rho^3}\right)\right\},$$

$$T_{(2)12}=\cos\ \theta\ \sin\ \phi\left(\frac{r}{\rho}+\frac{a^2}{\rho\sqrt{\Delta}}\sin^2\ \theta-\frac{\rho}{\sqrt{\Delta}}\right),$$

$$T_{(2)13}=-\sin\ \theta\ \cos\ \phi\left\{-\frac{1}{\rho\Sigma}\left[2r(r^2+a^2)-a^2\ \sin^2\ \theta(r-m)\right]+\frac{r\Sigma}{\rho^3}+\frac{\rho}{\sqrt{\Delta}}\right\},$$

$$T_{(2)23}=-\cos\ \theta\ \cos\ \phi\left\{\rho-\frac{\Sigma}{\rho}+a^2\ \sin^2\ \theta\left(\frac{\Delta}{\rho\Sigma}-\frac{\Sigma}{\rho^3}\right)\right\},$$

$$T_{(3)12}=\sin\ \theta\left[-\frac{r}{\rho}+\frac{\rho}{\sqrt{\Delta}}+\frac{a^2}{\rho\sqrt{\Delta}}\cos^2\ \theta\right].$$

In order to evaluate (9) we need to obtain T^i. After a long calculation we arrive at

$$T^1=\frac{\sqrt{\Delta}}{\rho^2}+\frac{\sqrt{\Delta}}{\Sigma}-\frac{\Delta}{\rho^2\Sigma^2}\left[2r(r^2+a^2)-a^2\ \sin^2\ \theta(r-m)\right],$$

$$T^2=\sin\ \theta\ \cos\ \theta\frac{a^2}{\rho^4}+\frac{1}{\rho\Sigma}\frac{\cos\ \theta}{\sin\ \theta}\left[\rho-\frac{\Sigma}{\rho}+a^2\ \sin^2\ \theta\left(\frac{\Delta}{\rho\Sigma}-\frac{\Sigma}{\rho^3}\right)\right],$$

$$T^3=0.$$

The gravitational energy density inside a volume V of a three-dimensional spacelike hypersurface of the Kerr solution can now be easily calculated (in what follows we will make $G=1$). It is given by

$$E_g=\frac{1}{8\pi}\int_V dr\ d\theta\ d\phi\Bigg\{\frac{\partial}{\partial r}\left[\sin\theta\left[\rho+\frac{\Sigma}{\rho}-\frac{\sqrt{\Delta}}{\rho\Sigma}\left(2r(r^2+a^2)-a^2\sin^2\theta(r-m)\right)\right]\right]$$
$$+\frac{\partial}{\partial\theta}\left[\frac{\Sigma a^2}{\sqrt{\Delta}\rho^3}\sin^2\theta\cos\theta+\frac{\cos\theta}{\sqrt{\Delta}}\left(\rho-\frac{\Sigma}{\rho}+a^2\sin^2\theta\left(\frac{\Delta}{\rho\Sigma}-\frac{\Sigma}{\rho^3}\right)\right)\right]\Bigg\}. \tag{13}$$

Next we specialize E_g to the case when the volume V is contained within a surface with constant radius $r=r_o$ assuming $r_o\geqslant r_+$, where $r_+=m+\sqrt{m^2-a^2}$ is the outer horizon of the black hole. The integrations in ϕ and r are trivial. Also, because we integrate θ between 0 and π, the second line of the expression above vanishes. We then obtain

$$E_g=\frac{1}{4}\int_0^\pi d\theta\sin\theta\left\{\rho+\frac{\Sigma}{\rho}-\frac{\sqrt{\Delta}}{\rho\Sigma}\left(2r(r^2+a^2)-a^2\sin^2\theta(r-m)\right)\right\}_{r=r_o}. \tag{14}$$

We have not managed to evaluate exactly the integral above. However, in the limit of slow rotation, namely, when $a/r_o\ll 1$, all integrals have a simple structure and we can obtain the approximate expression of E_g. It reads

$$E_g=r_o\left(1-\sqrt{1-\frac{2m}{r_o}+\frac{a^2}{r_o^2}}\right)+\frac{a^2}{6r_o}\left[2+\frac{2m}{r_o}+\left(1+\frac{2m}{r_o}\right)\sqrt{1-\frac{2m}{r_o}+\frac{a^2}{r_o^2}}\right]. \tag{15}$$

This is exactly the expression found by Martinez[6] for the energy inside the surface of constant radius r_o in a spacelike hypersurface of a Kerr black hole, in the limit of small specific angular momentum. As in Ref. 6, we have not expanded the square root which appears in (15) in powers in a^2/r_o^2.

We remark that the expansion of $\rho+\Sigma/\rho$ in the integrand of (14) yields $-\varepsilon_0$, whereas the remaining term corresponds exactly to ε, expressions (3.17) and (3.1), respectively, of Ref. 6. It does not seem to be possible, however, to split $\partial_i(eT^i)$ into two terms such that their integrals arise in the form $\varepsilon-\varepsilon_0$.

As a very interesting application of (14), let us calculate the energy contained within the outer horizon, i.e., we will calculate (14) when the surface of constant radius is defined by $r_o=r_+$. This surface is characterized by $\Delta=0$. The integral can be calculated exactly for *any* value of a. The latter is parametrized in terms of the black hole mass m according to

$$a=km,\quad 0\leqslant k\leqslant 1.$$

After a number of integrations we arrive at

$$E_g=m\left[\frac{\sqrt{2p}}{4}+\frac{6p-k^2}{4k}\ln\left(\frac{\sqrt{2p}+k}{p}\right)\right], \tag{16}$$

where p is defined by

$$p=1+\sqrt{1-k^2}.$$

This is the amount of energy expected not to escape from the black hole by any process in which the black hole interacts with external particles. It is then important to compare (16) with $E=2M_{ir}$.

We recall that a rotating black hole can have its mass decreased by means of Penrose's process of extraction of energy.[16] The idea is the following. We consider a particle that is emitted towards the black hole and penetrates into the ergosphere. Suppose we arrange the particle to break up into two fragments, in such a way that one of the fragments has total negative energy.

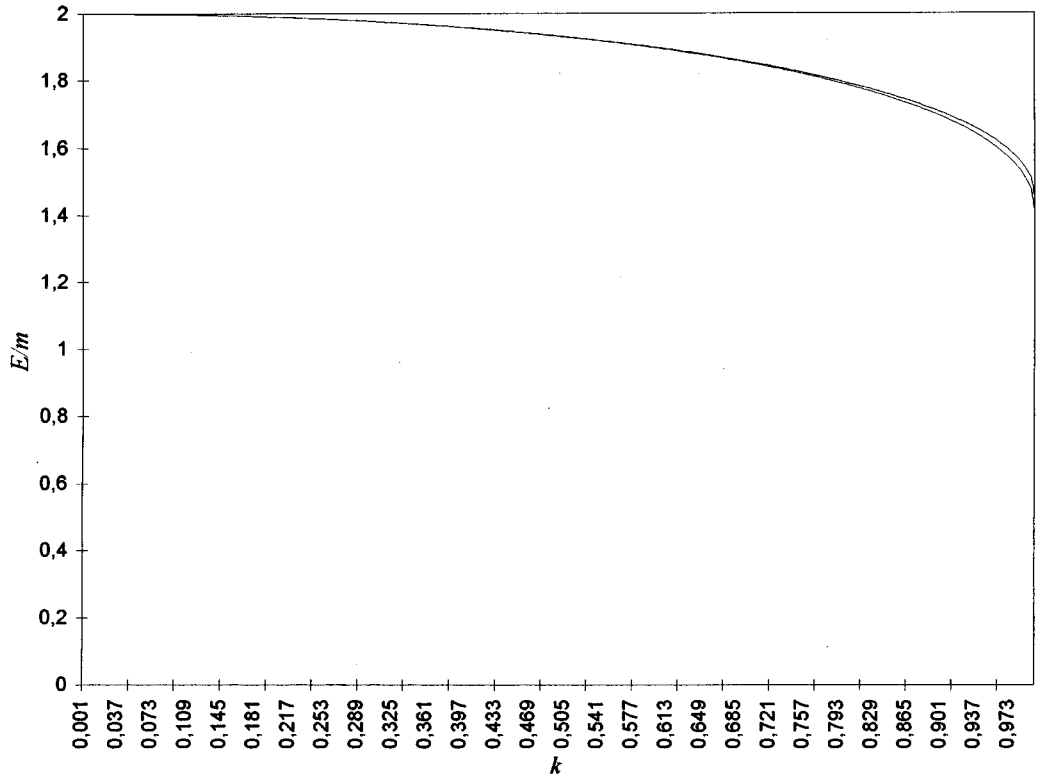

FIG. 1. E/m against k. The upper curve represents the energy expression (16), the lower one (17).

This is possible in principle, since the energy need not be positive in the ergosphere. By conservation of energy, the fragment with positive energy has an energy greater than that of the incident particle. Thus energy will be extracted from the black hole if the positive energy particle escapes to infinity, while the black hole absorbs the negative energy one. As a consequence, the mass of the black hole is decreased. We expect, however, that not the whole energy of the black hole can be extracted in this manner. The existence of the horizon certainly prevents one from exhausting the total energy. Christodoulou[11] has given an argument to determine how much energy can be extracted from the black hole by Penrose's process. He concluded that at the end of this process (when the ergosphere disappears and the black hole becomes static) the final (irreducible) mass of the black hole is given by

$$M_{ir}=\tfrac{1}{2}\sqrt{r_+^2+a^2}.$$

Martinez[6] has calculated the energy inside the horizon of the Kerr black hole in the limit of small a. He arrived at $E=2M_{ir}[1+O(a^4/M_{ir}^4)]$. A similar result (in the same approximation) has been obtained by Zaslavskii[17] in the analysis of a generic axially symmetric space–time. The question immediately arises as to whether this relationship holds for *any* value of a. This is, in fact, the conjecture made in Ref. 6.

Since expressions (14) and (16) are valid for *any* value of a in the appropriate range, it is worth comparing (16) with $2M_{ir}$. In our parametrization we have

$$E=2M_{ir}=m\sqrt{2p}. \tag{17}$$

The expression above certainly looks different from (16). However, in the range $0 \leqslant a \leqslant m$ expressions (16) and (17) as functions of k are strikingly indistinguishable, as we can see in Fig. 1. In the latter we have plotted E/m against k. The upper curve represents (16), the lower one (17). We see that for small values of the parameter k the two curves are essentially coincident. A tiny deviation occurs for values of k near 1. Inspite of this deviation, this is a remarkable result in favor of (14).

Unfortunately we have not been able to explain such small deviation between (16) and (17) for values of k near 1, although we expect such explanation to be of fundamental importance. It might be related to some physical property of the Kerr black hole which we do not understand yet.

V. COMMENTS

The gravitational energy E_g defined by (14) can be evaluated for an arbitrary value of a by means of numerical integration. This is the major advantage of our procedure as compared to that of Brown and York.[5] By means of the latter one cannot construct expressions like (13) and (14), which may be useful in the study of astrophysical problems, since in a general situation Brown and York's procedure requires the embedding of an arbitrary two-dimensional boundary surface of the Kerr space in the reference space E^3, a construction which is not possible in general[6] (the evaluation of ε_0 in Ref. 6 is only possible in the limit $a/r_0 \ll 1$). Therefore the present approach is more general than that of Ref. 6. Finally we remark that we expect expression (10) to be useful in the study of the thermodynamics of self-gravitating systems, where the gravitational energy plays the role of the thermodynamical internal energy that is conjugate to the inverse temperature. We hope to come to this issue in the future.

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Subalgebras with converging star products in deformation quantization: An algebraic construction for $\mathbb{C}P^n$

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Based on a closed formula for a star product of Wick type on $\mathbb{C}P^n$, which has been discovered in an earlier article of the authors, we explicitly construct a subalgebra of the formal star algebra (with coefficients contained in the uniformly dense subspace of representative functions with respect to the canonical action of the unitary group) that consists of *converging* power series in the formal parameter, thereby giving an elementary algebraic proof of a convergence result already obtained by Cahen, Gutt, and Rawnsley. In this subalgebra the formal parameter can be substituted by a real number α: the resulting associative algebras are infinite dimensional, except for the case $\alpha=1/K$, K a positive integer, where they turn out to be isomorphic to the finite-dimensional algebra of linear operators in the Kth energy eigenspace of an isotropic harmonic oscillator with $n+1$ degrees of freedom. Other examples like the $2n$ torus and the Poincaré disk are discussed. © *1996 American Institute of Physics.* [S0022-2488(96)04112-6]

I. INTRODUCTION

The concept of deformation quantization as defined by Bayen *et al.* in 1978 (cf. Ref. 1) consists in a formal local deformation of the commutative algebra (a so-called star product) of all smooth complex-valued functions on a symplectic manifold, such that the first-order commutator equals the Poisson bracket and pointwise complex conjugation remains an antilinear involution. The existence of star products on every symplectic manifold was proved by DeWilde and Lecomte in 1983 (cf. Ref. 2) and independently by Fedosov in 1985.[3,4] A third existence proof was given by Omori, Maeda, and Yoshioka.[5]

One of the problems with these star products is the fact that the formal series involved is shown to never converge on the space of *all* complex-valued smooth functions (see, e.g., Ref. 6), i.e. for every complex number there are two functions whose star product diverges when the formal parameter is substituted for that number.

This paper is a continuation of our work[7] in which we gave a closed formula for a star product of the Wick type on complex projective space by a version of quantum phase space reduction. Star products on complex projective space have already been constructed by Omori, Maeda, and Yoshioka[8] and by Moreno[9] in a less explicit way. $\mathbb{C}P^n$ can also be regarded as a coadjoint orbit of the unitary group $U(n+1)$ (see the work of Arnal, Ludwig, and Masmoudi for the existence of covariant star products on more general coadjoint orbits in Ref. 10 and references therein).

The aim of the present paper is twofold: first, we use our formula to explicitly compute the star product for a uniformly dense subalgebra of representative functions for the $U(n+1)$ action on complex projective space. Second, we would like to use the example $\mathbb{C}P^n$ in order to illustrate the following *algebraic* procedure to deal with the above convergence problem.

(i) Find a complex subalgebra $\mathscr{A}$ of the $*$ algebra of all formal power series in ν with smooth

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coefficients, such that (1) all elements of $\mathscr{U}$ are power series with infinite radius of convergence in ν, and (2) their coefficients may be chosen in a ''sufficiently large'' (e.g., uniformly dense) subspace of the space of all smooth complex-valued functions.

(ii) Verify whether the subspace $\mathscr{I}_\alpha$ of $\mathscr{U}$ defined by

$$\mathscr{I}_\alpha := \{\Phi(\nu) \in \mathscr{U} | \Phi(\alpha) = 0\}, \tag{1}$$

is a star ideal of $\mathscr{U}$.

(iii) Identify the quotient $\mathscr{U}/\mathscr{I}_\alpha$ with the associative algebra of quantum observables related to the ''$\hbar$ value'' α and try to find a representation of this quotient in some Hilbert space.

From the physical point of view it is often required that the subalgebra $\mathscr{U}$ contains certain ''important observables,'' which are in some cases related to the presence of additional symmetries of the classical phase space. For a general symplectic manifold the viability of the above procedure (in particular the existence of a sufficiently large subalgebra $\mathscr{U}$) is—to our best knowledge—an open problem in the theory of deformation quantization.

Nevertheless, in several examples having a large symmetry group (e.g., the Moyal product on the 2-torus or the Wick product on $\mathbb{C}^{n+1}$) the above program may be carried out. For such manifolds the space of representative functions of the symmetry group plays a prominent role for the construction of $\mathscr{U}$: in a remarkable article of Cahen, Gutt, and Rawnsley[11] the convergence of a star product for these functions has been proved for all compact Hermitian spaces (in particular, for $\mathbb{C}P^n$) by analytic methods of complex differential geometry. They start from the finite-dimensional operator algebras of geometric quantization in tensor powers of a very ample regular prequantum line bundle over a compact Kähler manifold and use coherent states (see Refs. 12 and 13) to first construct star products for the Berezin–Rawnsley symbols (Refs. 12 and 13) for each tensor power separately. In a second step an asymptotic expansion of these star products in the inverse tensor power is shown to define a local star product on the manifold where the formal parameter appears as a sort of interpolation of the inverse tensor powers.

The approach of this paper is in some sense reverse to the program of Cahen, Gutt, and Rawnsley (cf. Refs. 14, 11, 15, and 16) and only makes use of elementary algebraic methods: We start from the explicit star product on $\mathbb{C}P^n$ (see Ref. 7) and define $\mathscr{U}$ as a certain proper subspace of the space of all polynomials in the formal parameter with coefficients in the uniformly dense subspace of representative functions for the unitary group $U(n+1)$. Since all occurring star products can explicitly be computed the analysis of the ideals $\mathscr{I}_\alpha$ and the quotient algebras $\mathscr{U}/\mathscr{I}_\alpha$ becomes relatively simple. The main result is that for inverse integer values of the formal parameter ν the quotient algebras turn out to be finite-dimensional full complex matrix algebras, whereas all noninteger quotients are of infinite dimension and define converging star products on the space of representative functions for these values, as has been stated in Ref. 11.

From the physical point of view one can regard the finite-dimensional quantum algebras as the set of all quantum observables restricted to the eigenspace of integral energy of a harmonic oscillator of $n+1$ degrees of freedom (where the ground state energy is zero for the Wick quantization rule).

The advantage of the above algebraic program of prescribing a real value to the formal parameter of deformation quantization is that one may hope to transfer it to physical situations with an infinite number of degrees of freedom, i.e. field theories, where the powerful analytical methods in the theory of finite-dimensional manifolds are no longer well defined.

The paper is organized as follows: after briefly reviewing the concepts and formulas of our last paper,[7] in Sec. II we compute the star product of two Berezin–Rawnsley symbols in Sec. III and discuss the unitary symmetry action on the star product. Section IV is then devoted to defining the algebra $\mathscr{U}$, to compute the ideals $\mathscr{I}_\alpha$ and the quotient algebras $\mathscr{U}/\mathscr{I}_\alpha$. In Sec. V we briefly consider other phase spaces already dealt with in the literature for which the above program works: the complex vector space $\mathbb{C}^{n+1}$ with the Wick product, the $2n$-torus T^{2n} with the Moyal

product, and the Poincaré disk. For this last example we can recover the formula of the star product for the corresponding Berezin–Rawnsley symbols given by Cahen, Gutt, and Rawnsley in Ref. 15.

Notation: Throughout this paper we use the Einstein summation convention, i.e. summation over repeated indices is automatic. Moreover, the symbol $F(z)$ for a complex-valued function F of a complex vector z does *not* necessarily imply that F is holomorphic.

II. REVIEW OF STAR PRODUCTS ON COMPLEX PROJECTIVE SPACE

In this section we shall give a short review of earlier work[7] in which we derived an explicit formula for a star product of the Wick type on the complex projective space $\mathbb{C}P^n$.

Let $\pi:\mathbb{C}^{n+1}\backslash\{0\}\to\mathbb{C}P^n$ be the canonical projection of a complex vector z onto the complex ray through it. Let $x:=\overline{z^l}z^i$. The usual Wick product on $\mathbb{C}^{n+1}\backslash\{0\}$ of two complex-valued functions $F,G\in C^\infty(\mathbb{C}^{n+1}\backslash\{0\})$ is given as the following formal power series in the parameter λ:

$$F*G=\sum_{r=0}^{\infty}\frac{\lambda^r}{r!}\frac{\partial^r F}{\partial z^{i_1}\cdots\partial z^{i_r}}\frac{\partial^r G}{\partial\overline{z^{i_1}}\cdots\partial\overline{z^{i_r}}}. \tag{2}$$

We have called a function $F\in C^\infty(\mathbb{C}^{n+1}\backslash\{0\})$ *homogeneous* iff it is invariant under the natural action of the group $\mathbb{C}\backslash\{0\}$. These functions are precisely given by pullbacks of functions $f\in C^\infty(\mathbb{C}P^n)$, $F=f\circ\pi=\pi^*f$. We have called a function $R\in C^\infty(\mathbb{C}^{n+1}\backslash\{0\})$ *radial* iff it is a function of x, i.e. iff there is a smooth function $\rho:\mathbb{R}^+\to\mathbb{C}$ such that $R=\rho\circ x$. We have defined a formal differential operator $S:C^\infty(\mathbb{C}^{n+1}\backslash\{0\})[[\lambda]]\to C^\infty(\mathbb{C}^{n+1}\backslash\{0\})[[\lambda]]$ depending only on x and $\partial_x:=(1/2x)(z^i\partial_{z^i}+\overline{z^i}\partial_{\overline{z^i}})$ whose standard symbol $\hat{S}(x,\alpha):=(Se_\alpha)(x)e^{-\alpha x}$ (e_α denoting the exponential function $x\mapsto e^{\alpha x}$ for $\alpha\in\mathbb{R}$) is given by [setting the series D in Ref. 7, Eq. (9) equal to 1]:

$$\hat{S}(x,\alpha)=\exp\left(\frac{x}{\lambda}(\log(1+\lambda\alpha)-\lambda\alpha)\right). \tag{3}$$

S and its inverse S^{-1} act trivially on homogeneous functions, i.e. $SF=F=S^{-1}F$, but do in general transform radial functions into radial ones, in particular (for a non-negative integer r) [Ref. 7, Eq. (14)]

$$Sx=x,\quad Sx^r=x^r\prod_{k=0}^{r}\left(1-k\frac{\lambda}{x}\right),\quad Sx^{-r}=x^{-r}\prod_{k=0}^{r}\left(1+k\frac{\lambda}{x}\right)^{-1}. \tag{4}$$

We have used S as an equivalence transformation for a modified Wick product of two functions $F,G\in C^\infty(\mathbb{C}^{n+1}\backslash\{0\})$:

$$F\tilde{*}G:=S(S^{-1}F*S^{-1}G). \tag{5}$$

For two radial functions R_1, R_2 and a homogeneous function F on $\mathbb{C}^{n+1}\backslash\{0\}$ this new star product is just pointwise multiplication [Ref. 7, Eq. (12)]:

$$R_1\tilde{*}R_2=R_1R_2=R_2\tilde{*}R_1,\quad R_1\tilde{*}F=R_1F=F\tilde{*}R_1, \tag{6}$$

whereas for two smooth homogeneous functions F,G we obtain

$$(F\tilde{*}G)(z)=\sum_{r=0}^{\infty}\frac{1}{r!}\left(\frac{\lambda}{x}\right)^r\prod_{k=1}^{r}\left(1+k\frac{\lambda}{x}\right)^{-1}x^r\frac{\partial^r F}{\partial z^{i_1}\cdots\partial z^{i_r}}(z)\frac{\partial^r G}{\partial\overline{z^{i_1}}\cdots\partial\overline{z^{i_r}}}(z). \tag{7}$$

The main result of Ref. 7 was the fact that this formula can directly be projected to $\mathbb{C}P^n$ by phase space reduction via the $U(1)$-momentum map $J:\mathbb{C}^{n+1}\backslash\{0\}\to\mathbb{R}:z\mapsto -x/2$ of the canonical $U(1)$ action on $\mathbb{C}^{n+1}\backslash\{0\}$: for a negative real number μ and a $U(1)$ invariant function F in $C^\infty(\mathbb{C}^{n+1}\backslash\{0\})$ we write F_μ for the unique function in $C^\infty(\mathbb{C}P^n)$ obtained by first restricting F to the odd sphere $J^{-1}(\mu)$ and then projecting it to $\mathbb{C}P^n$ (Ref. 17, Sec. 4.3). Then the formula,

$$F_\mu *^\mu G_\mu := (F\tilde{*}G)_\mu, \tag{8}$$

was shown to define a star product on $\mathbb{C}P^n$. The explicit form of $*^\mu$ is obtained by replacing λ/x by $\lambda/(-2\mu)$ in (7) and noting that the bidifferential operator $\tilde{M}_r(f,g)(\pi(z)) := x^r[\partial^r \pi^* f(z)/\partial z^{i_1}\cdots\partial z^{i_r}][\partial^r \pi^* g(z)/\partial \overline{z^{i_1}}\cdots\partial \overline{z^{i_r}}]$ is well defined on $f,g\in C^\infty(\mathbb{C}P^n)$. For simplicity we shall work with the redefined formal parameter $\nu:=\lambda/(-2\mu)$ in what follows.

Lemma 1: The standard symbol of S^{-1} is described by the formula

$$\widehat{S^{-1}}(x,\alpha) = e^{(x/\lambda)(e^{\alpha\lambda}-1-\alpha\lambda)} = e^{*\alpha x}e^{-\alpha x}, \tag{9}$$

where the last term involves the star exponential[1] of the function x with respect to the usual Wick product (2).

Proof: Since $Se_\beta = e_{(1/\lambda)\log(1+\beta\lambda)}$ we obviously get $e_\beta = S^{-1}e_{(1/\lambda)\log(1+\beta\lambda)}$, which proves the first equation after the substitution $\alpha:=(1/\lambda)\log(1+\beta\lambda)$. Second, note that

$$e^{*\alpha x} = S^{-1}Se^{*\alpha S^{-1}x} = S^{-1}e^{\tilde{*}\alpha x} \overset{(6)}{=} S^{-1}e^{\alpha x} = \widehat{S^{-1}}(x,\alpha)e^{\alpha x},$$

which proves the second equality. □

Remark: Note that the function $H:=1/2x$ equals the usual Hamiltonian function of an isotropic harmonic oscillator in $n+1$ degrees of freedom. The above star exponential of x for $\alpha=-it/2\hbar$ and $\lambda=2\hbar$ then corresponds to the quantum mechanical time development operator for this system.

III. A STAR PRODUCT FOR REPRESENTATIVE FUNCTIONS ON COMPLEX PROJECTIVE SPACE

Let $p:\mathbb{C}^{n+1}\to\mathbb{C}:z\mapsto P(z)$ be a polynomial function (in the $2n+2$ variables $z^0,\ldots,z^n,\overline{z^0},\ldots,\overline{z^n}$). We shall call *$p$ homogeneous of degree (k,k)* for a non-negative integer k iff $p(\lambda z)=(\lambda\lambda)^k p(z)$ for all $\lambda\in\mathbb{C}\backslash\{0\}$. We denote by $\mathscr{E}_k$ the following subspace of $C^\infty(\mathbb{C}P^n)$:

$$\mathscr{E}_k := \left\{ \phi \;\middle|\; \text{there is a homogeneous polynomial } p_k \text{ of degree } (k,k) \text{ s.t. } (\pi^*\phi)(z) = \frac{1}{x^k}\, p_k(z) \right\}. \tag{10}$$

Lemma 2:

(i) For each integer $k\geqslant:\mathscr{E}_k\subset\mathscr{E}_{k+1}$.

(ii) $\mathscr{E}:=\cup_{k=0}^\infty \mathscr{E}_k$ is a filtered subalgebra of $C^\infty(\mathbb{C}P^n)$ with respect to the pointwise multiplication. It is closed under complex conjugation.

(iii) $\mathscr{E}$ separates points and is therefore a dense subalgebra of $C^\infty(\mathbb{C}P^n)$ with respect to the uniform topology.

Proof: (i) Clearly $p_k/x^k = xp_k/x^{k+1}\in\pi^*\mathscr{E}_{k+1}$. (ii) This is obvious. (iii) Consider the complex rays $\pi(z_{(1)})\neq\pi(z_{(2)})$ for $z_{(1)},z_{(2)}\in\mathbb{C}^{n+1}\backslash 0$. This is true iff $z_{(1)},z_{(2)}$ are linearly independent iff there is a $y\in\mathbb{C}^{n+1}$, such that $\langle y,z_{(1)}\rangle=1$ and $\langle y,z_{(2)}\rangle=0$, where $\langle y,z\rangle$ denotes the standard ses-

quilinear form $\langle y,z\rangle=\overline{y^k}z^k$. Then $\phi\in\mathscr{E}_1$ defined by $\phi(\pi(z)):=|\langle y,z\rangle|^2/x$ separates $\pi(z_{(1)})$ and $\pi(z_{(2)})$. The density of $\mathscr{E}$ follows from the Stone–Weierstrass Theorem. □

Consider the standard action of the unitary group $U(n+1)$ on $\mathbb{C}^{n+1}\backslash\{0\}$: $(g,z)\mapsto gz=:\Phi_g(z)$ and its induced action on $\mathbb{C}P^n$: $(g,\pi(z))\mapsto\pi(gz)=:\Psi_g(\pi(z))$. A smooth complex-valued function f on $\mathbb{C}P^n$ is called *representative* with respect to the $U(n+1)$ action iff

$$\mathbb{C}\text{-span}\{f\circ\Psi_g|g\in U(n+1)\}\ \text{ is finite dimensional.} \tag{11}$$

We now get a characterization of $\mathscr{E}$ that should be fairly standard (see Ref. 11, Sec. 3, Lemma 1).

Lemma 3: The algebra $\mathscr{E}$ is equal to the set of all representative functions on $\mathbb{C}P^n$.

Proof: Since x and the finite-dimensional space of all homogeneous polynomials of degree (k,k) are invariant under $U(n+1)$, it follows that $\mathscr{E}$ consists of representative functions. In order to prove the reversed inclusion we can use a more general argument: $\mathbb{C}P^n$ is a homogeneous space G/H for the compact Lie group $G=U(n+1)$ with compact isotropy subgroup $H=U(1)\times U(n)$. Now the space of all representative functions f on G/H [defined as in (11) with $U(n+1)$ replaced by any compact Lie group G] is clearly in one-to-one correspondence with the space of its pullback to G under the natural projection $G\to G/H$: this in turn is given by the space of all H right invariant representative functions on G with respect to left multiplication. Both this space and the pullback of $\mathscr{E}$ to G are G modules and are therefore closed in the space of all representative functions on G with respect to the uniform topology on G [see, e.g., Ref. 18, p. 126, Prop. (1.4) (iii)]. Since the pullback obviously is a continuous closed linear map with respect to the uniform topologies and $\mathscr{E}$ is dense in the space of all representative functions on G/H; thanks to the previous Lemma it follows that $\mathscr{E}$ is equal to that space. □

Yet another equivalent description of $\mathscr{E}$ is obtained in terms of the *Berezin–Rawnsley symbols* known from geometric quantization (Refs. 12–14): for a fixed non-negative integer k take the vector space $\mathscr{H}^{(k)}$ of complex-valued holomorphic polynomials ψ on $\mathbb{C}^{n+1}$, which are homogeneous of degree k, i.e. $\psi(\lambda z)=\lambda^k\psi(z)$ for all complex numbers λ. The dimension of this space is clearly $N:=\binom{n+k}{k}$ and we shall henceforth identify $\mathscr{H}^{(k)}$ with $\mathbb{C}^N$ by means of the base $(z^{i_1}\cdots z^{i_k})$. Consider the space $B(\mathscr{H}^{(k)})$ of complex linear endomorphisms of $\mathscr{H}^{(k)}$. Any $A\in B(\mathscr{H}^{(k)})$ can be viewed as a complex $N\times N$ matrix $A_{i_1\cdots i_k,j_1\cdots j_k}$, where each of the indices $i_1,\ldots,i_k,j_1,\ldots,j_k$ ranges over 0,1,...,n and the matrix elements are symmetric with respect to all permutations among the $i_1,\ldots,i_k$ and among the $j_1,\ldots,j_k$. To each $A\in B(\mathscr{H}^{(k)})$ one can associate the polynomial function,

$$\widetilde{\sigma}(A):\mathbb{C}^{n+1}\to\mathbb{C}:z\mapsto\overline{z^{i_1}}\cdots\overline{z^{i_k}}z^{j_1}\cdots z^{j_k}A_{i_1\cdots i_k,j_1\cdots j_k}. \tag{12}$$

Clearly, $\widetilde{\sigma}(A)$ is homogeneous of degree (k,k), and by counting dimensions it can be seen that every homogeneous polynomial function of degree (k,k) is of that form. The *Berezin–Rawnsley symbol $\sigma(A)$ associated to A* is then defined by

$$\sigma(A):\mathbb{C}P^n\to\mathbb{C}:\pi(z)\mapsto\frac{\widetilde{\sigma}(A)(z)}{x^k}. \tag{13}$$

Then the following corollary is clear.

Corollary 1: For each nonnegative integer k the space $\mathscr{E}_k$ is spanned by all the Berezin–Rawnsley symbols $\sigma(A)$ associated to $A\in B(\mathscr{H}^{(k)})$.

Both on $\mathbb{C}^{n+1}\backslash\{0\}$ and $\mathbb{C}P^n$ there are momentum maps (see Ref. 17 for general definitions) for the $U(n+1)$ action, which can be expressed in terms of Berezin–Rawnsley symbols contained in $\mathscr{E}_1$.

Lemma 4: Let $\mathfrak{u}(n+1)$ denote the space of complex anti-Hermitean $(n+1)\times(n+1)$ matrices, i.e. the Lie algebra of the unitary group $U(n+1)$. Then the following occurs.

(i) The following map:

$$\widetilde{P}:\mathbb{C}^{n+1}\backslash\{0\}\to\mathfrak{u}(n+1)^*:z\mapsto(A\mapsto\widetilde{\sigma}(A)) \tag{14}$$

is a momentum map for the $U(n+1)$ action on $\mathbb{C}^{n+1}\backslash\{0\}$.

(ii) The following map:

$$P:=\widetilde{P}_\mu:\mathbb{C}P^n\to\mathfrak{u}(n+1)^*:\pi(z)\mapsto(A\mapsto-2\mu\sigma(A)(\pi(z))=\widetilde{\sigma}(A)_\mu(\pi(z))) \tag{15}$$

is a momentum map for the $U(n+1)$ action on $\mathbb{C}P^n$.

Recall that the index μ refers to the $U(1)$-phase space reduction of $\mathbb{C}^{n+1}\backslash\{0\}$ by the $U(1)$ momentum map $J(z)=-x/2$.

Proof: (i) The Hamiltonian vector field of $P(A)$ is given by $X_{\widetilde{\sigma}(A)}(z) = (2/i)(A_{ij}z^j\partial_{z^i} + A_{ij}\overline{z^j}\partial_{\overline{z^i}})$, since $A_{ij}=-A_{ji}$, which obviously equals the infinitesimal generator $A_{\mathbb{C}^{n+1}\backslash\{0\}}$ of the $U(n+1)$ action. The Ad^* equivariance of this map is obvious.

(ii) Recall the projection $\pi_\mu:J^{-1}(\mu)\to\mathbb{C}P^n$ to the reduced phase space (compare Ref. 17, Sec. 4.3). Since $\Phi_g\circ\pi_\mu=\pi_\mu\circ\Psi_g$ it is clear that $T\pi_\mu A_{\mathbb{C}^{n+1}\backslash\{0\}} = A_{\mathbb{C}P^n}\pi_\mu$, where $A_{\mathbb{C}P^n}$ is the infinitesimal generator of the $U(n+1)$ action on $\mathbb{C}P^n$. Using the identity $A_{\mathbb{C}P^n}\pi_\mu(z) = X_{\widetilde{\sigma}(A)_\mu}\pi(z)$ we get by phase-space reduction

$$T_z\pi_\mu X_{\widetilde{\sigma}(A)_\mu}(z)=T_z\pi_\mu A_{\mathbb{C}^{n+1}\backslash\{0\}}(z)=X_{\widetilde{\sigma}(A)_\mu}(\pi(z)).$$

The Ad^* equivariance of this map follows at once from the Ad^* equivariance of $\widetilde{P}$. □

We shall now compute star products for elements of $\mathscr{E}$: Set $\nu:=\lambda/(-2\mu)$, $\nu^{(0)}:=1$, $\nu^{(1)}:=1$ and

$$\nu^{(k)}:=(1-\nu)\cdots(1-(k-1)\nu). \tag{16}$$

Theorem 1: *For $f\in\mathscr{E}_k$, $g\in\mathscr{E}_l$ we get*

$$(\pi^*f)\widetilde{*}(\pi^*g)(z)=\sum_{r=0}^{\min(k,l)}\frac{\lambda^r}{r!}\frac{S(x^{k+l-r})}{(Sx^k)(Sx^l)}\frac{1}{x^{k+l-r}}\frac{\partial^r(x^k\pi^*f)}{\partial z^{i_1}\cdots\partial z^{i_r}}(z)\frac{\partial^r(x^l\pi^*g)}{\partial\overline{z^{i_1}}\cdots\partial\overline{z^{i_r}}}(z) \tag{17}$$

and

$$f*^\mu g=\sum_{r=0}^{\min(k,l)}\frac{\nu^r}{r!}\frac{\nu^{(k+l-r)}}{\nu^{(k)}\nu^{(l)}}M_r^{(k,l)}(f,g), \tag{18}$$

with the following bidifferential operator on $C^\infty(\mathbb{C}P^n)$:

$$\pi^*M_r^{(k,l)}(f,g):=\frac{1}{x^{k+l-r}}\frac{\partial^r(x^k\pi^*f)}{\partial z^{i_1}\cdots\partial z^{i_r}}\frac{\partial^r(x^l\pi^*g)}{\partial\overline{z^{i_1}}\cdots\partial\overline{z^{i_r}}}. \tag{19}$$

Proof: The usual Wick product (2) of the two *polynomials* $\widetilde{f}_k:=x^k\pi^*f$, $\widetilde{g}_l:=x^l\pi^*g$ is given by

$$\widetilde{f}_k*\widetilde{g}_l=\sum_{r=0}^{\min(k,l)}\frac{\lambda^r}{r!}\frac{\partial^r\widetilde{f}_k}{\partial z^{i_1}\cdots\partial z^{i_r}}\frac{\partial^r\widetilde{g}_l}{\partial\overline{z^{i_1}}\cdots\partial\overline{z^{i_r}}}. \tag{20}$$

Using definition (5) and the formulas (6) and (4), we find

$$(Sx^k)(Sx^l)(\pi^*f)\widetilde{*}(\pi^*g)=(S(x^k\pi^*f))\widetilde{*}(S(x^l\pi^*g))=S((x^k\pi^*f)*(x^l\pi^*g))$$
$$=S\left(\sum_{r=0}^{\min(k,l)}\frac{\lambda^r}{r!}\frac{\partial^r\widetilde{f}_k}{\partial z^{i_1}\cdots\partial z^{i_r}}\frac{\partial^r\widetilde{g}_l}{\partial\overline{z^{i_1}}\cdots\partial\overline{z^{i_r}}}\right)$$

$$= \sum_{r=0}^{\min(k,l)} \frac{\lambda^r}{r!} S\left(x^{k+l-r} \frac{1}{x^{k+l-r}} \frac{\partial^r \widetilde{f}_k}{\partial z^{i_1} \cdots \partial z^{i_r}} \frac{\partial^r \widetilde{g}_l}{\partial \overline{z^{i_1}} \cdots \partial \overline{z^{i_r}}} \right)$$

$$= \sum_{r=0}^{\min(k,l)} \frac{\lambda^r}{r!} S(x^{k+l-r}) \frac{1}{x^{k+l-r}} \frac{\partial^r \widetilde{f}_k}{\partial z^{i_1} \cdots \partial z^{i_r}} \frac{\partial^r \widetilde{g}_l}{\partial \overline{z^{i_1}} \cdots \partial \overline{z^{i_r}}},$$

which proves the first equation. The second equation immediately follows by the reduction formula (8). □

Remark: Thanks to the straightforward recursion formulas $M_r^{(k+1,l)} = M_r^{(k,l)} + r(l-(r-1))M_{r-1}^{(k,l)}$ and $M_r^{(k,l+1)} = M_r^{(k,l)} + r(k-(r-1))M_{r-1}^{(k,l)}$ it can easily be checked that the right-hand side of (17) is well defined, i.e., if, e.g., f is regarded as an element of $\mathscr{E}_{k+a}$ for a positive integer a.

Corollary 2: For $A,B \in B(\mathscr{H}^{(1)})$ we have

$$\sigma(A)^k *^\mu \sigma(B)^l = \sum_{r=0}^{\min(k,l)} \frac{\nu^r}{r!} \frac{k!l!}{(k-r)!(l-r)!} \frac{\nu^{(k+l-r)}}{\nu^{(k)}\nu^{(l)}} \sigma(AB)^r \sigma(A)^{k-r} \sigma(B)^{l-r}. \tag{21}$$

Proof: This is easily seen by setting $f=\sigma(A)^k$ and $g=\sigma(B)^l$ and using Theorem 1. □

We shall now show that the momentum map P for the $U(n+1)$ action on $\mathbb{C}P^n$ is even a quantum momentum map. More precisely we see the following.

Lemma 5: P is a quantum momentum mapping on $\mathbb{C}P^n$ for the $U(n+1)$ action, i.e. for every smooth function $\phi:\mathbb{C}P^n \to \mathbb{C}$ the following equation holds:

$$P(A) *^\mu \phi - \phi *^\mu P(A) = \frac{i\lambda}{2} \{P(A), \phi\}_\mu, \tag{22}$$

i.e. the star product $*^\mu$ is strongly $U(n+1)$ invariant.

Proof: First we prove the equation $\pi^*\sigma(A) \widetilde{*} f - f \widetilde{*} \pi^*\sigma(A) = (i\lambda/2)\{\pi^*\sigma(A), f\}$ for $f=\pi^*\phi$. Then Eq. (22) follows Eq. (8). We have the strong invariance of the Wick product,

$$\widetilde{\sigma}(A) * f - f * \widetilde{\sigma}(A) = \frac{i\lambda}{2} \{\widetilde{\sigma}(A), f\}.$$

With the equivalence transformation S we find

$$S^{-1}(S\widetilde{\sigma}(A) \widetilde{*} Sf - Sf \widetilde{*} S\widetilde{\sigma}(A)) = \frac{i\lambda}{2} \{\widetilde{\sigma}(A), f\},$$

and with $\pi^*\sigma(A) = x\widetilde{\sigma}(A)$ and $Sf=f$ this leads to

$$Sx(\pi^*\sigma(A) \widetilde{*} f - f \widetilde{*} \pi^*\sigma(A)) = \frac{i\lambda}{2} S(\{x\pi^*\sigma(A), f\}).$$

The Poisson bracket $\{x\pi^*\sigma(A), f\} = x\{\pi^*\sigma(A), f\}$ is again homogeneous. Hence the right-hand side of the last equation is simply $x\{\pi^*\sigma(A), f\}$. With $Sx=x$ the proof is complete. □

Remark: The case $k=l=1$ in Corollary, Eq. (2) shows that the functions $\sigma(A)$ and $\sigma(B)$ commute with respect to $*^\mu$ iff the operators A and B commute. Let $A_1,\ldots,A_n$ be a linearly independent set of commuting traceless Hermitian matrices. It follows in particular that the functions $\sigma(A_1),\ldots,\sigma(A_n)$ are functionally independent and in involution, i.e., the Poisson bracket of $\sigma(A_i)$ with $\sigma(A_j)$ vanishes for all i,j. In other words they form a *completely integrable system* in the sense of Liouville on $\mathbb{C}P^n$. Note that this system is nontrivial in the sense that there is no global chart of action-angle variables, i.e. $\mathbb{C}P^n$ is not symplectomorphic to some $T^r \times \mathbb{R}^{2n-r}$ for a

non-negative integer $r \leqslant n$. The above Corollary now implies that these functions also commute with respect to the star product and can be viewed as a *quantum integrable system* on $\mathbb{C}P^n$.

IV. CONSTRUCTION OF THE SUBALGEBRA $\mathscr{U}$, THE IDEALS $\mathscr{I}_\alpha$, AND THE QUOTIENTS $\mathscr{U}/\mathscr{I}_\alpha$

If we take two functions $\phi_k \in \mathscr{E}_k$ and $\psi_l \in \mathscr{E}_l$ and multiply them with the ν polynomial $\nu^{(k)}$ and $\nu^{(l)}$, respectively, then formula (18) shows that their $*^\mu$ product contains only polynomials in the parameter ν. Moreover, that particular combination is restored, i.e. the functions $M_t^{(k,l)}(\phi_k, \psi_l) \in \mathscr{E}_{k+l-t}$ appear only in combination with $\nu^{(k+l-t)}$.This motivates the definition of the following subspaces of $C^\infty(\mathbb{C}P^n)[[\nu]]$:

$$\mathscr{U}_0 := \mathscr{E}_0 \quad \text{and} \quad \mathscr{U}_k := \nu^{(k)}\mathscr{E}_k + \nu\nu^{(k-1)}\mathscr{E}_{k-1} + \cdots + \nu^{k-1}\nu^{(1)}\mathscr{E}_1 + \nu^k\mathscr{E}_0, \quad \forall k \in \mathbb{N}, \tag{23}$$

where each $\mathscr{U}_k$ is a (not necessarily direct) sum of subspaces of $C^\infty(\mathbb{C}P^n)[[\nu]]$. We denote by $\mathscr{E}[\nu]$ the *polynomials* in ν with coefficients in $\mathscr{E}$. The following theorem describes the structure of $\mathscr{U}$.

Theorem 2:

(i) For each integer k: $\mathscr{U}_k \subset \mathscr{U}_{k+1}$. Define $\mathscr{U} := \cup_k^\infty \mathscr{U}_k$. Then $\mathscr{U}$ is a proper $\mathbb{C}[\nu]$ submodule of $\mathscr{E}[\nu]$.

(ii) $\mathscr{U}$ is a filtered subalgebra of $C^\infty(\mathbb{C}P^n)[[\nu]]$ with respect to $*^\mu$, i.e.

$$\mathscr{U}_k *^\mu \mathscr{U}_l \subset \mathscr{U}_{k+l}.$$

Proof: (i) Let $\Phi \in \mathscr{U}_k$. Φ is of the form $\Phi = \Sigma_{r=0}^k \nu^r \nu^{(k-r)} \phi_{k-r}$ with $\phi_{k-r} \in \mathscr{E}_{k-r}$. The filtration of $\mathscr{E}$ implies $\phi_{k-r} \in \mathscr{E}_{k-r+1}$ so $\nu^r \nu^{(k-r+1)} \phi_{k-r} \in \mathscr{U}_{k+1}$. The element $\nu^{r+1}\nu^{(k-r)}\phi_{k-r}$ is also contained in $\mathscr{U}_{k+1}$. By Eq. (16) we get $\nu^{(k-r+1)} = (1-(k-r)\nu)\nu^{(k-r)}$. Hence

$$\nu^r \nu^{(k-r)} \phi_{k-r} = \nu^r \nu^{(k-r+1)} \phi_{k-r} + (k-r)\nu^{r+1}\nu^{(k-r)}\phi_{k-r} \in \mathscr{U}_{k+1},$$

which proves the inclusion $\mathscr{U}_k \subset \mathscr{U}_{k+1}$. It is clear from the definition (23) that $\nu\mathscr{U}_k \subset \mathscr{U}_{k+1} \subset \mathscr{E}[\nu]$ whence $\mathscr{U}$ is $\mathbb{C}[\nu]$ submodule of $\mathscr{E}[\nu]$. Note that for fixed $y \in \mathbb{C}^{n+1}\backslash\{0\}$ the function $\pi(z) \mapsto |\langle y, z\rangle|^4/x^2 \in \mathscr{E}_2$ is not contained in $\mathscr{U}$. (*ii*) By Theorem 1 the star product for arbitrary $\Phi_k = \Sigma_{r=0}^k \nu^{k-r}\nu^{(r)}\phi_r \in \mathscr{U}_k$ and $\Psi_l = \Sigma_{s=0}^l \nu^{l-s}\nu^{(s)}\psi_s \in \mathscr{U}_l$ with $\phi_r \in \mathscr{E}_r$ and $\psi_s \in \mathscr{E}_s$ is given by

$$\Phi_k *^\mu \Psi_l = \sum_{r=0}^{k} \sum_{s=0}^{l} \sum_{t=0}^{\min(r,s)} \frac{1}{t!}\, \nu^{k-r+l-s+t}\nu^{(r+s-t)} M_t^{(r,s)}(\phi_r, \psi_s),$$

hence each summand is an element of $\mathscr{U}_{k+l}$. This proves the second part. □

We should now like to substitute the formal parameter ν for a fixed nonzero real number α. In the subalgebra $\mathscr{U}$ this is well defined because $\mathscr{U}$ only contains polynomials in ν. The kernel of the substitution homomorphism,

$$\mathscr{I}_\alpha := \{\Phi(\nu) \in \mathscr{U} \,|\, \Phi(\alpha) = 0\}, \tag{24}$$

will turn out to be a $*^\mu$ ideal.

Lemma 6: $\mathscr{I}_\alpha$ is a $*^\mu$ ideal and the general form of an element $\Phi \in \mathscr{I}_\alpha \cap \mathscr{U}_k$ is the following: (i) for $\alpha \in \{1, 1/2, 1/3, \ldots\}$,

$$\Phi(\nu) = (\nu - \alpha) u_{k-1}(\nu), \quad \textit{with} \quad u_{k-1}(\nu) \in \mathscr{U}_{k-1}; \tag{25}$$

(ii) for $\alpha = 1/K$ with $K \in \mathbb{N}\backslash\{0\}$ for $k \leqslant K$,

$$\Phi(\nu) = \left(\nu - \frac{1}{K}\right) u_{k-1}(\nu), \tag{26}$$

and for $k>K$,

$$\Phi(\nu)=\nu^{(k)}\phi_k+\cdots+\nu^{k-K-1}\nu^{(k-K+1)}\phi_{k-K+1}+\left(\nu-\frac{1}{K}\right)u_{k-1}(\nu), \tag{27}$$

with some $u_{k-1}(\nu)\in\mathscr{U}_{k-1}$ *and* $\phi_r\in\mathscr{E}_r$.

Proof: It is clear that $\mathscr{T}_\alpha$ is a $*^\mu$ ideal if Eq. (25), resp. (26), and (27) are valid because of the form of $\nu^{(k)}$ in Eq. (16) and Eq. (18) for the $*^\mu$ product. So we only have to prove Eq. (25) and Eqs. (26) and (27).

Case (i). $\alpha\notin\{1,1/2,1/3,...\}$ We prove (25) by induction on k. With $\mathscr{U}_1=\nu\mathscr{E}_0+\mathscr{E}_1$ we get $\Phi(\nu)=c+\nu\sigma(A)$ for some $c\in\mathbb{C}$ and $\sigma(A)\in\mathscr{E}_1$. $\Phi(\alpha)=0$ implies $A=-(c/\alpha)\mathbf{1}$, where $\mathbf{1}$ is the unit matrix. So we have $\Phi(\nu)=c(1-\nu/\alpha)$. This proves the case $k=1$.

Consider now the induction step $k-1\to k$. Since $\mathscr{U}_k=\nu^{(k)}\mathscr{E}_k+\nu\mathscr{U}_{k-1}$ we write for $\Phi\in\mathscr{U}_k$

$$\Phi(\nu)=\nu^{(k)}\phi_k+\nu u_{k-1}(\nu),\quad \text{with}\quad \phi_k\in\mathscr{E}_k\quad\text{and}\quad u_{k-1}(\nu)\in\mathscr{U}_{k-1}.$$

Then $\Phi(\alpha)=0$ implies $\phi_k=-[\alpha/\alpha^{(k)}]u_{k-1}(\alpha)\in\mathscr{E}_{k-1}$ because $\alpha^{(k)}\neq 0$. Writing $\nu^{(k)}=(1-(k-1)\nu)\nu^{(k-1)}$ we get

$$\Phi(\nu)=\nu^{(k-1)}\phi_k+\nu(-(k-1)\nu^{(k-1)}\phi_k+u_{k-1}(\nu))=:\nu^{(k-1)}\phi_k+\nu u'_{k-1}(\nu),$$

with $u'_{k-1}(\nu)\in\mathscr{U}_{k-1}$. In $\Phi(\nu)=(\nu-\alpha)u'_{k-1}(\nu)+\nu^{(k-1)}\phi_k+\alpha u'_{k-1}(\nu)$ the first term vanishes at $\nu=\alpha$, so we have

$$\nu^{(k-1)}\phi_k+\alpha u'_{k-1}(\nu)\big|_{\nu=\alpha}=0.$$

But $\nu^{(k-1)}\phi_k+\alpha u'_{k-1}(\nu)$ is an element in $\mathscr{U}_{k-1}$ so we can apply the induction and conclude

$$\Phi(\nu)=(\nu-\alpha)u'_{k-1}(\nu)+(\nu-\alpha)u''_{k_2}(\nu),$$

with some $u''_{k-2}(\nu)\in\mathscr{U}_{k-2}$. This proves the first part.

Case (ii). Let $\alpha=1/K$ with $K\in\mathbb{N}\setminus\{0\}$ and $\Phi(\nu)\in\mathscr{U}_k$. We have to consider the two cases $k\leqslant K$ and $k>K$ separately:

(a) For $k\leqslant K$ we have $(1/K)^{(k)}\neq 0$, and we can apply the same arguments as in the first part; hence $\Phi(\nu)=(\nu-1/K)u_{k-1}(\nu)$ with $u_{k-1}(\nu)\in\mathscr{U}_{k-1}$.

(b) For $k>K$ we have for $r\geqslant 1$ $\nu^{(K+r)}\big|_{\nu=1/K}=0$ according to the definition (16) of $\nu^{(k)}$. Hence, in every $\Phi(\nu)\in\mathscr{U}_k$,

$$\Phi(\nu)=\nu^{(k)}\phi_k+\cdots+\nu^{k-K-1}\nu^{(K+1)}\phi_{K+1}+\nu^{k-K}u_K(\nu),$$

the first terms are automatically elements of $\mathscr{T}_{1/K}$ and $\Phi(1/K)=0$ implies $u_K(1/K)=0$. But this is an element of $\mathscr{U}_K$ and we can apply case (a). Hence $u_K(\nu)=(\nu-1/K)u'_{K-1}(\nu)$, which proves the second part. □

The quotient algebras $\mathscr{U}/\mathscr{T}_\alpha$ can now easily be described.

Theorem 3: *The quotient algebra* $\mathscr{A}_\alpha:=\mathscr{U}/\mathscr{T}_\alpha$ *is isomorphic to one of the following algebras.*

(*i*) *For* α *not equal to one of the rational numbers 1,1/2,1/3,..., the algebra* $\mathscr{A}_\alpha$ *is isomorphic to the vector space of representative functions* $\mathscr{E}$ *equipped with the multiplication* $*_\alpha$ *defined by* ($f\in\mathscr{E}_k$, $g\in\mathscr{E}_l$; $k,l\in\mathbb{N}$):

$$f*_\alpha g:=\sum_{r=0}^{\min(k,l)}\frac{\alpha^r}{r!}\frac{\alpha^{(k+l-r)}}{\alpha^{(k)}\alpha^{(l)}}M_r^{(k,l)}(f,g), \tag{28}$$

where the real number $\alpha^{(k)}$ *is defined by the formula (16) and* $M_r^{(k,l)}(f,g)$ *is given in (19).*

(ii) *Let* α *be equal to* $1/K$ *with* K *a positive integer. Then* $\mathscr{A}_\alpha$ *is isomorphic to the finite-dimensional complex algebra of linear endomorphisms of* $\mathbb{C}^N$ *with* $N:=\binom{n+K}{K}$. *The isomorphism is given by the map*

$$A\mapsto \frac{\nu^{(K)}}{(1/K)^{(K)}}\,\sigma(A) \mod \mathscr{T}_{1/K}, \tag{29}$$

where $\sigma(A)$ *is the Berezin-Rawnsley symbol of the complex* $N\times N$*-matrix* A *[see (13)]. The matrix product* $(AB)_{i_1\cdots i_K,j_1\cdots j_K}$ *is given by* $A_{i_1\cdots i_K,a_1\cdots a_K}B_{a_1\cdots a_K,j_1\cdots j_K}$.

Proof: (i) According to the preceding Lemma the ideal $\mathscr{T}_\alpha$ is equal to $(\nu-\alpha)\mathscr{U}$, which amounts to simply substituting $\nu=\alpha$ in (18) which is obviously well defined.

(ii) According to the second part of the preceding Lemma we get $\mathscr{U}_k/\mathscr{T}_{1/K}=\mathscr{U}_K/\mathscr{T}_{1/K}$ for $k\geqslant K$. For $\mathscr{U}_K$ we may substitute ν for $1/K$ since $(1/K)^{(k)}\neq 0$ for $k\leqslant K$. Hence $\dim \mathscr{A}_{1/K}=\dim \mathscr{E}_K=\binom{n+K}{K}^2$. Moreover,

$$\begin{aligned}
&\frac{\nu^{(K)}}{(1/K)^{(K)}}\,\sigma(A)*^{\mu}\frac{\nu^{(K)}}{(1/K)^{(K)}}\,\sigma(B) \mod \mathscr{T}_{1/K}\\
&\quad=\sum_{r=0}^{K}\frac{\nu^r}{r!}\,\frac{\nu^{(2K-r)}}{(1/K)^{(K)}(1/K)^{(K)}}\,M_r^{(K,K)}(\sigma(A),\sigma(B)) \mod \mathscr{T}_{1/K}\\
&\quad=\frac{(1/K)^K}{K!}\,\frac{\nu^{(K)}}{(1/K)^{(K)}(1/K)^{(K)}}\,M_K^{(K,K)}(\sigma(A),\sigma(B)) \mod \mathscr{T}_{1/K}\\
&\quad=\frac{\nu^{(K)}}{(1/K)^{(K)}}\,\sigma(AB) \mod \mathscr{T}_{1/K},
\end{aligned}$$

since a simple calculation shows that

$$\pi^*(M_K^{(K,K)}(\sigma(A),\sigma(B)))(z)=K!K!\,\frac{\widetilde{\sigma}(AB)(z)}{x^K}.$$

This proves the Theorem. □

Remarks: Note that for each $A\in\mathfrak{u}(n+1)$ the Berezin–Rawnsley symbol $\sigma(A)$ is contained in $\mathscr{E}_K$ and thus uniquely corresponds to a linear operator in $B(\mathscr{H}^{(K)})$, which is mapped via the linear map (29) to $\mathscr{A}_{1/K}$. By Lemma 5 it follows that this defines a *representation* of $\mathfrak{u}(n+1)$ in $\mathbb{C}^N$, which is *irreducible*: in fact, by Lemma 5 we know that the momentum map $P(A)$ star commutes with some function iff it Poisson commutes with that function, which is only possible iff that function is constant since the unitary group acts transitively on $\mathbb{C}P^n$. Since the Poisson bracket with $P(A)$ obviously preserves each $\mathscr{E}_k$, it follows that this reasoning carries over to the quotient by $\mathscr{T}_{1/K}$.

From the physical point of view the second part of the preceding Theorem can be viewed as follows: The classical phase space reduction of $\mathbb{C}^{n+1}\backslash\{0\}$ to $\mathbb{C}P^n$ was motivated by the $U(1)$ action on $\mathbb{C}^{n+1}\backslash\{0\}$, which is just the flow of the classical isotropic $(n+1)$-dimensional harmonic oscillator with Hamiltonian $H=1/2x$ (the frequency and mass are normalized to 1). Passing from $\mathbb{C}^{n+1}\backslash\{0\}$ to $\mathbb{C}P^n$ for a fixed value $\mu\in\mathbb{R}^-$ of the momentum mapping $J=-1/2x$ means classically that the harmonic oscillator is considered at a fixed energy $E=-\mu$. This is also true in the quantum mechanical case, but now the energy is quantized. Only for the discrete values $1/K$, K a positive integer, of the formal parameter $\nu=\lambda/(-2\mu)$ one obtains *finite-dimensional* algebras of observables $\mathscr{U}/\mathscr{T}_{1/K}$ as one would physically expect for the *compact phase space* $\mathbb{C}P^n$ because the

phase volume is finite and each state ''occupies a phase cell of volume not smaller than $\hbar^n$,'' which results in a finite-dimensional Hilbert space for the quantum mechanical states. With $\lambda=2\hbar$ the quantized energy is given by

$$E_K=\hbar K$$

[where the usual ground state energy $1/2\hbar(n+1)$ is absent because of the Wick ordering]. Note that in this interpretation the formal parameter $\lambda=2\hbar$ is *not* quantized but the energy $E=-\mu$ is. The dimensions of the operator algebras for a fixed $K\in\mathbb{N}$ correspond to the well-known degeneracy of the Kth energy eigenvalue of the isotropic harmonic oszillator [see, e.g., Ref. 19, Eq. (XII.64)].

V. OTHER EXAMPLES

In this section we briefly sketch how the program mentioned in the Introduction applies to the deformation quantization of other phase spaces that have been dealt with in the literature.

(1) Consider complex $n+1$ space $\mathbb{C}^{n+1}$ as a symplectic manifold in the usual manner, i.e. with symplectic form $\omega=i/2\Sigma_{i=0}^{n}dz^i\wedge d\overline{z^i}$. The Wick product (2) then defines a star product on this space. It is natural to consider the action of $\mathbb{C}^{n+1}$ on itself by translations. Suppose that the smooth complex-valued function F on $\mathbb{C}^{n+1}$ is representative with respect to this group action, i.e. there is a finite number L of linearly independent smooth complex-valued functions $F_1,\ldots,F_L$ on $\mathbb{C}^{n+1}$ such that $F(z+v)=\Sigma_{a=1}^{L}\beta_a(v)F_a(z)$ with smooth complex-valued coefficients β_a. The same equation holds for each F_a thus giving rise to a coefficient matrix $\beta_{ab}(v)$. Since $\mathbb{C}^{n+1}$ is Abelian, $\beta_{ab}(v)$ commutes with each $\beta_{ab}(w)$ whence all these matrices can simultaneously be transformed to the Jordan normal form. It can easily be seen that the generalized eigenvectors of $\beta_{ab}(v)$ are of the form $p(z)e^{b_iz^i+c_i\overline{z^i}}$, where p is a complex-valued polynomial function of $(z,\overline{z})$ and b_i,c_j are complex numbers. Conversely, it is easy to see that each linear combination of the functions of this form is indeed representative. Since this space of functions is a subalgebra of the algebra of all smooth complex-valued functions on $\mathbb{C}^{n+1}$ (with respect to pointwise multiplication), which clearly is closed under complex conjugation, contains a unit element, and separates points it is dense in $C^\infty(\mathbb{C}^{n+1})$ with respect to the uniform topology on compacta thanks to the Stone–Weierstrass Theorem. Note that the space of polynomials is a dense proper $\mathbb{C}^{n+1}$ submodule of representative functions that would be impossible for compact Lie groups (compare the proof of Lemma 3).

Writing $e_{(a,b)}$ for the exponential function $z\mapsto e^{a_iz^i+b_i\overline{z^i}}$ parameterized by two complex vectors $a,b\in\mathbb{C}^{n+1}$, we easily obtain the following formula:

$$e_{(\alpha+\rho,b+\sigma)}*e_{(a'+\rho',b'+\sigma')}=e^{\lambda(a_i+\rho_i)(b_i'+\sigma_i')}e_{(a+\rho,b+\sigma)}e_{(a'+\rho',b'+\sigma')}, \tag{30}$$

where a, a', b, b', ρ, ρ', σ, $\sigma'\in\mathbb{C}^{n+1}$. After differentiating this formula a finite number of times with respect to the components of ρ, ρ', σ, σ' at $\rho=\rho'=\sigma=\sigma'=0$ (which generates polynomial prefactors), we see that the Wick product of two representative functions is again representative and entirely analytic in the formal parameter λ. Therefore the algebra $\mathscr{U}$ can be chosen to be the subalgebra of $C^\infty(\mathbb{C}^{n+1})[[\lambda]]$ which consists of polynomials in λ with coefficients in the space of representative functions. Substituting λ for a real number α then is straightforward.

(2) Consider now the $2n$-torus $T^{2n}:=S^1\times\cdots\times S^1$ ($2n$ factors). Let $(\varphi^1,\ldots,\varphi^{2n})=:\varphi$, $0\leqslant\varphi^i<1$, denote the standard angle coordinates on T^{2n} and take any nondegenerate complex $2n\times 2n$ matrix (Λ_{ij}). The Moyal product may then be defined by for two smooth, complex-valued functions f,g on T^{2n} as follows:

$$f*g:=\sum_{r=0}^{\infty}\frac{(\lambda/2\pi\mathbf{i})^r}{r!}\Lambda^{i_1j_1}\cdots\Lambda^{i_rj_r}\frac{\partial^r f}{\partial\varphi^{i_1}\cdots\varphi^{i_r}}\frac{\partial^r g}{\partial\varphi^{j_1}\cdots\varphi^{j_r}}. \tag{31}$$

It is known that this formula defines an associative deformation for the pointwise multiplication in $C^\infty(T^{2n})$ (see, e.g., Ref. 1). The space of representative functions for the torus action on itself is spanned by the Fourier modes $T_k(\varphi) := e^{2\pi \mathbf{i} k_i \varphi^i}$, $k \in \mathbb{Z}^{2n}$: indeed, it is clear that the complex span of the Fourier modes consists of representative functions. Since it is a subalgebra of $C^\infty(T^{2n})$ that is closed under complex conjugation and contains a unit element, and separates points, it is a dense T^{2n} submodule of the space of all representative functions (by the Stone–Weierstrass Theorem) that has to be equal to that space since T^{2n} is compact [compare again the proof of Lemma (3)]. The Moyal product of two Fourier modes is then simply computed by

$$T_k * T_{k'} = e^{2\pi \mathbf{i} \lambda \Lambda^{ij} k_i k'_j} T_k T_{k'}, \tag{32}$$

which again is an entire function in the formal parameter λ, whence the choice of $\mathscr{U}$ and the substitution of the formal parameter is completely analogous to the previous example.

Suppose now that the matrix (Λ^{ij}) is integral and the greatest common divisor of the matrix elements is equal to 1. Choosing $\lambda = 1/K$, K a positive integer, it is easily seen from the above formula (32) that the subspace $\mathscr{T}_{1/K}$ spanned by all elements of the form $T_k - T_{k+Kk'}$ with $k, k' \in \mathbb{Z}^{2n}$ is a $*$ ideal in the $*$ algebra of representative functions. It can be shown (see Ref. 20) that the quotient algebra is a simple complex algebra of dimension K^{2n}, which is related to the geometric quantization on the $2n$ torus in the theta bundle and its tensor powers.

(3) Let $\mathbb{D} := \{v \in \mathbb{C} \,|\, |v|^2 < 1\}$ be the Poincaré disk in the complex plane. As we have indicated in the last section of Ref. 7, we can use the projective representation of $\mathbb{D}$: in $\mathbb{C}^2 \setminus \{0\}$. Consider the open subset defined by the inequality $0 < y := |z^0|^2 - |z^1|^2$ (the function y was defined with an erroneous sign in Ref. 7). The image of this open set under the projection π is an open set of $\mathbb{C}P^1$ that is holomorphically diffeomorphic to $\mathbb{D}$ via $\pi(z) \mapsto v := z^1/z^0$. In their article,[15] Cahen, Gutt, and Rawnsley have considered the following functions $f_{p,q}(v)$ $(p, q \in \mathbb{N})$ on $\mathbb{D}$:

$$f_{p,q}(v) := v^p \left(\frac{\overline{v}}{1 - |v|^2} \right)^q. \tag{33}$$

Their pullback to $\mathbb{C}^2 \setminus \{0\}$ is simply given by $(\pi^* f_{p,q})(z) = (z^1/z^0)^p (z^0 \overline{z^1})^q / y^q$. In Ref. 7 we have defined a star product on $\mathbb{D}$ by essentially replacing x by y and the operators M_r by

$$\check{M}_r(G, H) := y^r g^{i_1 j_1} \cdots g^{i_r j_r} \frac{\partial^r G}{\partial z^{i_1} \cdots \partial z^{i_r}} \frac{\partial^r G}{\partial \overline{z^{j_1}} \cdots \partial \overline{z^{j_r}}}, \tag{34}$$

with $g^{ij} := \mathrm{diag}(1, -1)$. Observing that Eqs. (17) and (18) remain valid for arbitrary smooth complex-valued functions when the upper bound of the sum is ∞ and that these formulas pass to the noncompact case with the above replacements and adapting the sign and ordering conventions of Ref. 15, we obtain the following star product:

$$\begin{aligned}
(f_{p,q} * f_{r,s})(\pi(z)) = \sum_{m=0}^{\infty} & \frac{(-\nu)^m}{m!} \frac{(-\nu)^{(q+s-m)}}{(-\nu)^{(q)} (-\nu)^{(s)}} y^{m-q-s} g^{i_1 j_1} \cdots g^{i_m j_m} \frac{\partial^r (y^q \pi^* f_{p,q})}{\partial \overline{z^{i_1}} \cdots \partial \overline{z^{i_m}}}(z) \\
& \times \frac{\partial^r (y^s \pi^* f_{r,s})}{\partial z^{j_1} \cdots \partial z^{j_m}}(z) \\
= \sum_{m=0}^{\infty} & \frac{(-\nu)^m}{m!} \frac{(-\nu)^{(q+s-m)}}{(-\nu)^{(q)} (-\nu)^{(s)}} y^{m-q-s} (-1)^m \\
& \times \frac{\partial^m ((z^1/z^0)^p (z^0 \overline{z^1})^q)}{\partial (\overline{z^1})^m}(z) \frac{\partial^m ((z^1/z^0)^r (z^0 \overline{z^1})^s)}{\partial (z^1)^m}(z)
\end{aligned}$$

$$= \sum_{m=0}^{\min(q,r)} \frac{\nu^m}{m!} \frac{(-\nu)^{(q+s-m)}}{(-\nu)^{(q)}(-\nu)^{(s)}} \frac{q!}{(q-m)!} \frac{r!}{(r-m)!} f_{p+r-m,q+s-m}(\pi(z)),$$

which reproduces the result of Ref. 15. In Ref. 16 star products were computed on more general bounded symmetric domains.

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$(T^*\mathcal{B})_q$, q-analog of model space and the Clebsch–Gordan coefficients generating matrices

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We study relations between the deformed cotangent bundle $(T^*\mathcal{B})_q$ for the Borel subgroup $\mathcal{B}$ of a given simple Lie group G, the quantum Lie algebra $\mathcal{J}_q$ associated with the corresponding quantum group G_q and the matrices generating Clebsch–Gordan coefficients for $\mathcal{J}_q$. We reveal the connection of these objects to quantum analog of the model space $\mathcal{M}$ and q-tensor operators. © *1996 American Institute of Physics.* [S0022-2488(96)00612-3]

I. INTRODUCTION

Among different representations of a given compact Lie group G the model space $\mathcal{M}$ plays a distinguished role. By definition,[1] the model space is a direct sum of all irreducible representations $\mathcal{H}_j$ with multiplicity one

$$\mathcal{M}=\sum_j \oplus \mathcal{H}_j \tag{1.1}$$

realized in some universal way. A most popular form of $\mathcal{M}$ is a space of holomorphic functions on the Borel subgroup $\mathcal{B}$ of complexified form of the group G. In this construction the Borel subgroup is considered as an affine space.

A study of model spaces provides a natural language for investigation of physical models. For example, the popular model of two-dimensional quantum gravity, introduced by Polyakov,[2] may be interpreted in terms of the model space of Virasoro algebra.[3] A finite-dimensional quantum group with deformation parameter, depending on the central charge, naturally appears in this context.

In the present paper, which was written with an intent to find new applications of model space in modern mathematical physics, we discuss a q-analog of the model space related to q-deformed Lie group G_q. For this purpose we introduce and examine several ''coordinatizations'' of the quantum space $(T^*\mathcal{B})_q$. As a by-product we obtain some generating matrices for the set of Clebsch–Gordan coefficients (CGC). To our knowledge this result is new even for the nondeformed case.

Throughout the paper we systematically and intentionally make use of the R-matrix formalism, which we believe is the most convenient and powerful tool to get explicit results in the domain of quantum groups.

To avoid the known difficulties with compact forms of quantum groups we adopt here a convention to work with complexified objects (groups, algebras) and their finite-dimensional

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representations on a formal algebraic level. We also do not discuss subtleties arising in the case of q being a root of unity.

Most of formulas given in this paper in R-matrix form have universal validity. However, the concrete results are illustrated on the simplest example $G_q=\mathrm{SL}_q(2)$. The generalization to other groups needs more technical details such as an explicit structure of R-matrices and related objects.

Mentioned above, ''coordinatizations'' of $(T^*\mathscr{B})_q$ arise from two possible decompositions of the matrix L (in usual notations $L=L_+L_-^{-1}$, it comprises all generators of the corresponding quantum Lie algebra):

$$L=UDU^{-1} \quad \text{and} \quad L=ABA^{-1},$$

where D is a diagonal unimodular matrix, U is a deformation of unitary matrix, and A and B are unimodular upper and lower triangular matrices. As we shall clarify below, the matrices A and B admit a natural interpretation as the coordinates in the base and in the fiber of $(T^*\mathscr{B})_q$, whereas entries of the matrix U will be shown to provide basic shifts on the model space $\mathscr{M}$ and generate q-analogs of Clebsch–Gordan coefficients for the quantum group G_q. The explicit connection between U and (A,B) will be demonstrated on the example of $\mathrm{SL}_q(2)$.

It should be mentioned that an object like the matrix U appeared first in Refs. 4 and 5 (later it was used also in Ref. 6), where it was interpreted as a ''chiral'' component of the quantum grouplike element g. In the present paper we give another interpretation and application of the matrix U in the context of a model space.

Let us briefly describe the contents of the present paper. In Sec. II the definition of the cotangent bundle for a quantum group is reminded. Next we introduce an object of especial interest for us—the algebra $\mathscr{U}$ generated by the entries of the matrix U which diagonalizes the coordinate in a fiber of $(T^*G)_q$. We derive explicit relations for this algebra in the case of $G=\mathrm{SL}(2)$.

In Sec. III we consider a nondeformed limit ($q=1$) of the algebra $\mathscr{U}$ and construct an explicit representation. For the case of $G=\mathrm{SL}(2)$ we show that the matrix U_0 generates Clebsch–Gordan coefficients (CGC) for the corresponding nondeformed Lie algebra. The Borel subgroup $\mathscr{B}$ and the space $T^*\mathscr{B}$ naturally appear here. Finally, we discuss a connection of our results with the Wigner–Eckart theorem.

In Sec. IV we construct representations of the algebra $\mathscr{U}$ (for $q\neq 1$) for the case of SL(2) in two different ways. The first one uses the language of q-oscillators. The second is based on explicit realization of $(T^*\mathscr{B})_q$ and hence involves a notion of quantum model space. Here we show that the matrix U is a ''generating matrix'' for CGC for deformed Lie algebra. We also give some comments on the generalized version of the Wigner–Eckart theorem.

II. $(T^*G)_q$ AND RELATED OBJECTS

There exist three symplectic manifolds (from the physical point of view they are phase spaces) naturally related to a given Lie group G and its Lie algebra $\mathscr{J}$:

(1) T^*G—the cotangent bundle for the group G;
(2) $T^*\mathscr{B}$—the cotangent bundle for the Borel subgroup $\mathscr{B}$;
(3) $\mathscr{O}$—an orbit of the coadjoint action of G on $\mathscr{J}^*$.

For instance, in the case of $G=\mathrm{SL}(2)$ (which will be our main example) these spaces are six-, four-, and two-dimensional, correspondingly.

The method of geometric quantization[7] provides a representation theory for (1), (2), (3). Turning from classical to quantum groups, one can try to construct a representation theory for the deformed analogs of these manifolds. In the present paper we shall deal with deformations of the spaces (1) and (2).

A. Description of $(T^*G)_q$

Let G_q be a deformation of the Lie group G and $\mathscr{J}_q$ be a deformation of the corresponding Lie algebra $\mathscr{J}$. The deformed cotangent bundle $(T^*G)_q$ is a noncommutative manifold, i.e., according to the ideology developed by A. Connes,[8] its coordinates are (noncommuting) generators of some associative algebra. A point on this manifold is parametrized by the pair (g,L), where $g \in G_q$ is a coordinate in the base of the bundle, and L is a coordinate in a fiber.

The structure of $(T^*G)_q$ is defined via commutation relations between the coordinates in the base and in a fiber. An appropriate R-matrix form of these relations was proposed in Ref. 5:

$$\overset{1\,2}{R}_{\pm} \overset{2\,1}{g g} = \overset{2\,1}{g g} \overset{1}{R}_{\pm}, \tag{2.1}$$

$$\overset{1\,2}{R}_{-} \overset{2}{g} \overset{1}{L} = \overset{2}{L} \overset{1}{R}_{+} \overset{1}{g}, \tag{2.2}$$

$$\overset{1}{L} \overset{-1}{R}_{-} \overset{2}{L} \overset{2}{R}_{-} = \overset{-1}{R}_{+} \overset{2}{L} \overset{1}{R}_{+} \overset{1}{L}. \tag{2.3}$$

Here and below we use the formalism developed in Ref. 9, i.e., objects like g and L are considered as matrices (say, $L \in \mathscr{J}_q \otimes V$, where V stands for auxiliary space). We use the standard notations for tensor products: $\overset{1}{L} = L \otimes I \in \mathscr{J}_q \otimes V \otimes V$, etc.

Let us take the parameter q, which appears in the theory of quantum groups, in the following form:

$$q = e^{\gamma \hbar}, \tag{2.4}$$

where $\hbar$ is the Planck constant (the parameter of quantization) and γ is the deformation parameter. In physical applications it is most natural to suppose that γ is either pure real (q belongs to the real axis) or pure imaginary (q belongs to the unit circle at the complex plane).

The second form of q is typical for the WZW theory.[4,6,10] For $|q|=1$ we suppose also that q is not a root of unity. It should be mentioned that for both variants of choice of γ in (2.4) the definition of q-number

$$[x] \equiv \frac{q^x - q^{-x}}{q - q^{-1}} \tag{2.5}$$

is invariant with respect to complex conjugation of q, i.e., $\overline{[x]} = [\overline{x}]$. This property becomes important if one discusses involutions of deformed Lie algebras.

Definition 1: The algebra $\mathscr{L}$ is an associative algebra generated by entries of the matrix L which obeys relation (2.3).

An important fact—the connection of algebra $\mathscr{L}$ with the corresponding quantum Lie algebra $\mathscr{J}_q$ was established in Ref. 11 in the following form:

Proposition 1: Let matrices L_+ and L_- obey the following exchange relations:

$$\overset{1\,2}{R}_{\pm} \overset{1\,2}{L_+ L_+} = \overset{2\,1}{L_+ L_+} \overset{1}{R}_{\pm}, \quad \overset{1\,2}{R}_{\pm} \overset{1\,2}{L_- L_-} = \overset{2\,1}{L_- L_-} \overset{1}{R}_{\pm}, \quad \overset{1\,2}{R}_{+} \overset{1\,2}{L_+ L_-} = \overset{2\,1}{L_- L_+} \overset{1}{R}_{+}. \tag{2.6}$$

Then the matrix $L = L_+ L_-^{-1}$ satisfies the relation (2.3).

This statement implies that the algebra $\mathscr{L}$ is isomorphic (up to some technical details which we do not discuss here) to corresponding quantum Lie algebra $U_q(\mathscr{J})$ [which is defined by (2.6), see, e.g., Ref. 9].

Consider now the relations (2.1)–(2.3) for g and L being 2×2 matrices,

$$g=\begin{pmatrix} g_1 & g_2 \\ g_3 & g_4 \end{pmatrix}, \quad L=\begin{pmatrix} A & B \\ C & D \end{pmatrix} \tag{2.7}$$

and the R-matrices taken in the form

$$R_+=q^{-1/2}\begin{pmatrix} q & 0 & 0 & 0 \\ 0 & 1 & \omega & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & q \end{pmatrix}, \quad \omega\equiv q-q^{-1}; \quad R_-=PR_+^{-1}P \tag{2.8}$$

(P denotes the permutation operator: $Pg^{1}P=g^{2}$, etc.). In this case (2.1)–(2.3) define the cotangent bundle for the quantum group $G_q=\mathrm{GL}_q(2)$; each of R-matrix equations (2.1) and (2.3) is equivalent to six independent relations:

$$\begin{gathered} qg_1g_2=g_2g_1, \quad qg_1g_3=g_3g_1, \quad qg_2g_4=g_4g_2, \quad qg_3g_4=g_4g_3, \\ g_2g_3=g_3g_2, \quad g_1g_4-q^{-1}g_4g_1=-\omega g_2g_3; \end{gathered} \tag{2.9}$$

and

$$\begin{gathered} [A,B]=-q^{-1}\omega BD, \quad [A,C]=q^{-1}\omega DC, \quad [A,D]=0, \\ CD=q^2DC, \quad BD=q^{-2}DB, \quad [B,C]=q^{-1}\omega D(D-A). \end{gathered} \tag{2.10}$$

The equation (2.2) gives the following relations:

$$\begin{gathered} g_1A=qAg_1+\omega Bg_3, \quad g_1B=Bg_1, \\ g_2A=qAg_2+\omega Bg_4, \quad g_2B=Bg_2, \\ g_3A=q^{-1}Ag_3+\omega g_1C, \quad g_3B=Bg_3+\omega g_1D, \\ g_4A=q^{-1}Ag_4+\omega g_2C, \quad g_4B=Bg_4+\omega g_2D, \\ g_1C=Cg_1+q^{-1}\omega Dg_3, \quad g_1D=q^{-1}Dg_1, \\ g_2C=Cg_2+q^{-1}\omega Dg_4, \quad g_2D=q^{-1}Dg_2, \\ g_3C=Cg_3, \quad g_3D=qDg_3, \\ g_4C=Cg_4, \quad g_4D=qDg_4. \end{gathered} \tag{2.11}$$

Next, let us recall the well-known statement (see, e.g., Ref. 9):

Proposition 2: The algebra generated by the entries of the matrix g obeying (2.9) possesses the central element (''deformed determinant'')

$$\det_q g=g_1g_4-q^{-1}g_2g_3. \tag{2.12}$$

Similarly, for the algebra $\mathscr{L}$ in the case of $\mathrm{GL}_q(2)$ one can check the following.

Proposition 3: The algebra with generators A,B,C,D obeying (2.10) possesses two central elements:

$$K_1 = qA + q^{-1}D, \quad K_2 = q^{-1}AD - qBC. \tag{2.13}$$

Finally, using the commutation relations (2.11), one can check the following.

Proposition 4: The operators $\det_q g$ *and* K_2 *commute with all entries of the matrices* g *and* L.

This implies that, fixing values of $\det_q g$ and K_2, one gets a certain subalgebra of the algebra defined by (2.9)–(2.11).

Definition 2: Relations (2.9)–(2.11) for $\det_q g = 1$ *and* $K_2 = \text{const}$ *define the cotangent bundle for the quantum group* $G_q = \mathrm{SL}_q(2)$.

Let us underline that the above definitions and statements can be easily generalized, say to the case of $\mathrm{SL}_q(N)$.

In our case the algebra $\mathscr{L}$ is isomorphic to the quantum Lie algebra $\mathscr{J}_q = U_q(\mathrm{sl}(2))$ (introduced first in Ref. 12) which is defined by the relations

$$[l_+, l_-] = \frac{q^{2l_3} - q^{-2l_3}}{q - q^{-1}} \equiv [2l_3], \quad q^{l_3} l_\pm = q^{\pm 1} l_\pm q^{l_3}, \tag{2.14}$$

and the matrices $L_\pm$ can be chosen as follows:

$$L_+ = \begin{pmatrix} q^{l_3} & \omega q^{1/2} l_- \\ 0 & q^{-l_3} \end{pmatrix}, \quad L_- = \begin{pmatrix} q^{-l_3} & 0 \\ -\omega q^{-1/2} l_+ & q^{l_3} \end{pmatrix}. \tag{2.15}$$

Note that the matrix L in the Proposition 1 is defined only up to a scaling factor. Thus, for L_+ and L_- given in (2.15), we may choose L as follows:

$$L = q^2 L_+ L_-^{-1} = \begin{pmatrix} qC - q^{-2l_3} & q^{5/2} \omega l_- q^{-l_3} \\ q^{-1/2} \omega l_+ q^{-l_3} & q^2 q^{-2l_3} \end{pmatrix}. \tag{2.16}$$

Here C stands for the Casimir operator of $\mathrm{U}_q(\mathrm{sl}(2))$:

$$C = \omega^2 l_- l_+ + q^{2l_3+1} + q^{-(2l_3+1)} = q^{2\hat{j}+1} + q^{-(2\hat{j}+1)}, \tag{2.17}$$

where $\hat{j}$ is the operator of spin.

According to Proposition 1, the matrix (2.16) satisfies (2.3). Therefore, it provides a (fundamental) representation of the algebra $\mathscr{L}$ for $\mathrm{U}_q(\mathrm{sl}(2))$. In this representation the central elements (2.13) are given by

$$K_1 = q^2 C, \quad K_2 = q^3, \tag{2.18}$$

Note that the scaling factor q^2 introduced in (2.16) has changed the values of K_1 and K_2. The choice of such a normalization in (2.16) will be explained later.

B. Connection with quantum 6*j*-symbols

Let us remember the theorem which describes an important property of the algebra $\mathscr{L}$ for $U_q(\mathrm{sl}(2))$ (this statement first appeared in Ref. 5).

Theorem 1: *Let* $D \equiv D(p)$ *be the unimodular diagonal matrix*

$$D = \begin{pmatrix} q^{p/\hbar} & \\ & q^{-p/\hbar} \end{pmatrix}, \tag{2.19}$$

and let 2×2 *matrix* U *satisfy the following exchange relations:*

$$\overset{1\ 2}{D}\overset{2\ 1}{U}=\overset{2\ 1}{U}\overset{1\ 2}{D}\sigma, \quad \overset{2\ 1}{D}\overset{1\ 2}{U}=\overset{1\ 2}{U}\overset{2\ 1}{D}\sigma, \quad \sigma=\mathrm{diag}(q^{-1},q,q,q^{-1}), \tag{2.20}$$

$$R_+\overset{1\ 2}{U}\overset{2\ 1}{U}=\overset{2\ 1}{U}\overset{1\ 2}{U}\mathscr{R}_+(p), \quad R_-\overset{1\ 2}{U}\overset{2\ 1}{U}=\overset{2\ 1}{U}\overset{1\ 2}{U}\mathscr{R}_-(p), \tag{2.21}$$

where $R_\pm$ are the standard R-matrices (2.8) and

$$\mathscr{R}_+(p)=P\mathscr{R}_-^{-1}(p)P=q^{-1/2}\begin{pmatrix} q & & & \\ & \dfrac{\sqrt{[p/\hbar+1][p/\hbar-1]}}{[p/\hbar]} & \dfrac{q^{p/\hbar}}{[p/\hbar]} & \\ & -\dfrac{q^{-p/\hbar}}{[p/\hbar]} & \dfrac{\sqrt{[p/\hbar+1][p/\hbar-1]}}{[p/\hbar]} & \\ & & & q \end{pmatrix}, \tag{2.22}$$

(here $[x]$ denotes a ''q-number'' (2.5)). Then matrix L constructed by means of the similarity transformation

$$L=UDU^{-1}, \tag{2.23}$$

satisfies the relation (2.3) and therefore its entries generate an algebra $\mathscr{L}$ isomorphic to $\mathrm{U}_q(\mathrm{sl}(2))$.

The proof is given in Appendix A. It makes use of the identity

$$\mathscr{R}_-(p)=\overset{1}{(D)}^{-1}\mathscr{R}_+(p)\sigma\overset{1}{D}. \tag{2.24}$$

Remark: A consequence of (2.20) is the commutativity of L and D

$$\overset{1\ 2}{L}\overset{2\ 1}{D}=\overset{2\ 1}{D}\overset{1\ 2}{L}, \tag{2.25}$$

which implies that p commutes with all elements of $\mathscr{L}$. Later we shall interpret p as the operator of spin.

Remark: Properly generalizing objects which enter Theorem 1, one can extend this theorem to the case of any quantum semisimple Lie algebra.[13] In particular, the matrix D for $\mathrm{U}_q(\mathrm{sl}(N))$ is found to be: $D(\mathbf{p}) = \mathrm{const}\cdot q^{\mathbf{H}\otimes\mathbf{p}}$, where $\mathbf{p}$ consists of the operators corresponding to components of the weight vector (i.e., on each irreducible representation they are multiples of unity) and $\mathbf{H}$ consists of the generators H_i of the Cartan subalgebra. An explicit form of $\mathscr{R}(p)$ for $\mathrm{U}_q(\mathrm{sl}(N))$ was obtained in Ref. 14.

Remark: The matrix $\mathscr{R}(p)$ obeys the deformed Yang–Baxter equation,[5,14–16] which can be written, for example, as follows:

$$\overset{1\ 23}{Q}\mathscr{R}_+(p)\overset{1}{(Q)}^{-1}\mathscr{R}_+(p)\overset{3\ 12}{Q}\mathscr{R}_+(p)\overset{3}{(Q)}^{-1}=\mathscr{R}_+(p)\overset{2\ 13}{Q}\mathscr{R}_+(p)\overset{2}{(Q)}^{-1}\mathscr{R}_+(p), \tag{2.26}$$

where for $\mathscr{J}_q=\mathrm{U}_q(\mathrm{sl}(2))$ the matrix $Q = \begin{pmatrix} e^{i\xi} & \\ & e^{-i\xi} \end{pmatrix}$ contains an extra variable ξ, conjugated with p:

$$[p,\ \xi]=-i\hbar, \quad q^{p/\hbar}e^{i\xi}=qe^{i\xi}q^{p/\hbar}. \tag{2.27}$$

This variable ξ belongs to the algebra $\mathscr{U}$ but does not enter matrix L. An explicit expression for ξ will be given below. The general form of Q for $\mathrm{U}_q(\mathrm{sl}(N))$ can be easily found:[13] $Q = e^{i\mathbf{H}\otimes\boldsymbol{\xi}}$, where components ξ_i are operators conjugated to p_i: $[p_j, \xi_k] = -i\hbar\,\delta_{jk}$.

The matrix $\mathscr{R}(p)$ was discussed in physical literature in different contexts. In particular, it plays significant role in studies of quantum Liouville[15,16] and WZW[4–6] models; its relation to the Calogero–Moser model was recently discussed in Ref. 17. But for us the more important fact is a connection of $\mathscr{R}(p)$ with the quantum $6j$-symbols: the entries of (2.22) calculated on irreducible representations coincide (up to some normalization) with the values of some $6j$-symbols for $\mathrm{U}_q(\mathrm{sl}(2))$ (exact formulas are given in Ref. 20, generalizations are discussed in Ref. 13). This connection allows us to assume that objects like the matrix U should be interpreted in terms of Clebsch–Gordan coefficients (CGC). Below we demonstrate that U is indeed a ''generating matrix'' for CGC and clarify its relation to $(T^*\mathscr{B})_q$.

C. Algebra $\mathscr{U}$

Definition 3: The algebra $\mathscr{U}$ is an associative algebra generated by entries of matrix

$$U=\begin{pmatrix} U_1 & U_2 \\ U_3 & U_4 \end{pmatrix}$$

and the operator p such that relations (2.19)–(2.22) hold.

Remark: For simplicity we restricted our consideration to the case of $\mathscr{U}$ associated with $U_q(\mathrm{sl}(2))$. Let us stress that the case of $\mathscr{U}$ associated with $\mathrm{U}_q(\mathrm{sl}(N))$ can be studied similarly but it will involve more technical details. On the other hand, it might be rather cumbrous to obtain exact formulas for $\mathscr{U}$ associated with $\mathrm{U}_q(\mathscr{F})$ in the case of $\mathscr{F}$ being generic semisimple Lie algebra.

Let us give an explicit form of the defining relations (2.21):

$$U_1U_3=q^{-1}U_3U_1, \quad U_2U_4=q^{-1}U_4U_2, \tag{2.28}$$

$$U_1U_2=U_2U_1\sqrt{\frac{[p/\hbar-1]}{[p/\hbar+1]}}, \quad U_3U_4=U_4U_3\sqrt{\frac{[p/\hbar-1]}{[p/\hbar+1]}}, \tag{2.29}$$

$$U_1U_4=U_4U_1\,\frac{\sqrt{[p/\hbar+1][p/\hbar-1]}}{[p/\hbar]}-U_3U_2\,\frac{q^{p/\hbar}}{[p/\hbar]}, \tag{2.30}$$

$$U_3U_2=U_2U_3\,\frac{\sqrt{[p/\hbar+1][p/\hbar-1]}}{[p/\hbar]}-U_1U_4\,\frac{q^{-p/\hbar}}{[p/\hbar]}. \tag{2.31}$$

The rest of the relations contained in (2.21) are not independent and can be deduced from (2.28)–(2.31).

Additionally, from (2.20) one gets

$$\begin{aligned} &q^{p/\hbar}U_1=q^{-1}U_1q^{p/\hbar}, \quad q^{p/\hbar}U_2=qU_2q^{p/\hbar}, \\ &q^{p/\hbar}U_3=q^{-1}U_3q^{p/\hbar}, \quad q^{p/\hbar}U_4=qU_4p^{p/\hbar}. \end{aligned} \tag{2.32}$$

Thus, relations (2.28)–(2.32) describe the algebra $\mathscr{U}$. Using them, one may verify the following statement:

Proposition 5: A central element of $\mathscr{U}$ is given by the ''deformed'' determinant of the matrix U:

$$\text{Det } U \equiv U_1 U_4 \sqrt{\frac{[p/\hbar+1]}{[p/\hbar]}} - U_2 U_3 \sqrt{\frac{[p/\hbar-1]}{[p/\hbar]}} = q U_4 U_1 \sqrt{\frac{[p/\hbar-1]}{[p/\hbar]}} - q U_3 U_2 \sqrt{\frac{[p/\hbar+1]}{[p/\hbar]}}. \tag{2.33}$$

For a fixed value of Det U, the algebra $\mathscr{U}$ contains only four independent generators. In classical limit ($\hbar=0$) they become the coordinates on four-dimensional phase space.

For further discussion it is convenient to introduce new variables instead of U_i:

$$\hat{U}_i = U_i \sqrt{[p/\hbar]}. \tag{2.34}$$

The coordinates $\{p, \hat{U}_i\}$ form a new set of generators of the algebra $\mathscr{U}$. The commutation relations (2.28)–(2.32) rewritten in terms of the new generators acquire a simpler form:

$$\hat{U}_1 \hat{U}_3 = q^{-1} \hat{U}_3 \hat{U}_1, \quad \hat{U}_2 \hat{U}_4 = q^{-1} \hat{U}_4 \hat{U}_2, \quad \hat{U}_1 \hat{U}_2 = \hat{U}_2 \hat{U}_1, \quad \hat{U}_3 \hat{U}_4 = \hat{U}_4 \hat{U}_3 \tag{2.35}$$

$$\hat{U}_1 \hat{U}_4 = \hat{U}_4 \hat{U}_1 \frac{[p/\hbar+1]}{[p/\hbar]} - \hat{U}_3 \hat{U}_2 \frac{q^{p/\hbar}}{[p/\hbar]}, \tag{2.36}$$

$$\hat{U}_3 \hat{U}_2 = \hat{U}_2 \hat{U}_3 \frac{[p/\hbar+1]}{[p/\hbar]} - \hat{U}_1 \hat{U}_4 \frac{q^{-p/\hbar}}{[p/\hbar]}, \tag{2.37}$$

$$\begin{aligned} &q^{p/\hbar} \hat{U}_1 = q^{-1} \hat{U}_1 q^{p/\hbar}, \quad q^{p/\hbar} \hat{U}_2 = q \hat{U}_2 q^{p/\hbar}, \\ &q^{p/\hbar} \hat{U}_3 = q^{-1} \hat{U}_3 q^{p/\hbar}, \quad q^{p/\hbar} \hat{U}_4 = q \hat{U}_4 q^{p/\hbar}. \end{aligned} \tag{2.38}$$

The central element (2.33) in new variables looks as follows:

$$\text{Det } U \equiv (\hat{U}_1 \hat{U}_4 - \hat{U}_2 \hat{U}_3) \frac{1}{[p/\hbar]} = (\hat{U}_4 \hat{U}_1 - \hat{U}_3 \hat{U}_2) \frac{q}{[p/\hbar]}. \tag{2.39}$$

The explicit form of the matrix inverse to $\hat{U}$, which we shall need later, is

$$\hat{U}^{-1} = \frac{1}{\text{Det } U} \begin{pmatrix} \hat{U}_4 & -q\hat{U}_2 \\ -\hat{U}_3 & q\hat{U}_1 \end{pmatrix} \frac{1}{[p/\hbar]}. \tag{2.40}$$

Finally, from (2.34) we conclude that the expression (2.23) for the matrix L looks similar in terms of new matrix $\hat{U}$:

$$L = UDU^{-1} = \hat{U} D \hat{U}^{-1}. \tag{2.41}$$

III. NONDEFORMED CASE

A. Representation of algebra $\mathscr{U}_0$

First, we consider the limit $\gamma \to 0$, $\hbar \neq 0$ (note that q-numbers turn into ordinary numbers), i.e., here we deal with a well understood situation—the representation theory of SL(2). An investigation of this simple nondeformed case will make further results more transparent.

Let us denote the corresponding limit algebra as $\mathscr{U}_0$. The defining R-matrix relations (2.21) now degenerate to

$$\overset{1}{U_0}\overset{2}{U_0} = \overset{2}{U_0}\overset{1}{U_0} \mathscr{R}^{0}_{\pm}(p), \tag{3.1}$$

where

$$\mathscr{R}^0_+(p)=\mathscr{R}^0_-(p)=\begin{pmatrix} 1 & & & \\ & \dfrac{\sqrt{(p/\hbar+1)(p/\hbar-1)}}{(p/\hbar)} & \dfrac{\hbar}{p} & \\ & -\dfrac{\hbar}{p} & \dfrac{\sqrt{(p/\hbar+1)(p/\hbar-1)}}{(p/\hbar)} & \\ & & & 1 \end{pmatrix}. \tag{3.2}$$

The analogs of relations (2.35)–(2.38) for $\mathscr{U}_0$ are (from now on we omit the index 0 for the generators of $\mathscr{U}_0$)

$$p\hat{U}_1=\hat{U}_1(p-\hbar),\quad p\hat{U}_2=\hat{U}_2(p+\hbar),\quad p\hat{U}_3=\hat{U}_3(p-\hbar),\quad p\hat{U}_4=\hat{U}_4(p+\hbar), \tag{3.3}$$

$$[\hat{U}_1,\hat{U}_2]=[\hat{U}_1,\hat{U}_3]=[\hat{U}_2,\hat{U}_4]=[\hat{U}_3,\hat{U}_4]=0, \tag{3.4}$$

$$[\hat{U}_1,\hat{U}_4]=\mathrm{Det}\ U_0,\quad [\hat{U}_3,\hat{U}_2]=-\mathrm{Det}\ U_0, \tag{3.5}$$

where Det U_0 stands for a limit version of (2.39):

$$\mathrm{Det}\ U_0=(\hat{U}_1\hat{U}_4-\hat{U}_2\hat{U}_3)\,\frac{\hbar}{p}=(\hat{U}_4\hat{U}_1-\hat{U}_3\hat{U}_2)\,\frac{\hbar}{p}. \tag{3.6}$$

Proposition 6: A possible solution for (3.3)–(3.6) is

$$\hat{U}_1=\partial_1,\quad \hat{U}_2=z_2,\quad \hat{U}_3=-\partial_2,\quad \hat{U}_4=z_1; \tag{3.7}$$

$$p=\hbar(z_1\partial_1+z_2\partial_2+1), \tag{3.8}$$

where we denote $\partial_i\equiv\partial/\partial z_i$.

Remark: The representation given by (3.7) and (3.8) is not unique. In particular, the rescaling $\hat{U}_i\to c_i\hat{U}_i$ (where c_i are numerical constants such that $c_1c_4=c_2c_3$) is allowable.

Proposition 6 together with the connection formula (2.34) allows us to write out the explicit form of the matrix U_0:

$$U_0=\begin{pmatrix} \partial_1 & z_2 \\ -\partial_2 & z_1 \end{pmatrix}\sqrt{\frac{\hbar}{p}}. \tag{3.9}$$

Note that this matrix is ''unimodular,'' i.e., Det $U_0=(\partial_1z_1+z_2\partial_2)\hbar/p=1$.

To describe the obtained representation of the algebra $\mathscr{U}_0$ completely one has to define a space where operators (3.7)–(3.9) act. It is natural to think that this space is $D(z_1,z_2)$—a space of holomorphic functions of two complex variables.

Let us recall that $D(z_1,z_2)$ is a space spanned on the vectors

$$|j,m\rangle=\frac{z_1^{j+m}z_2^{j-m}}{\sqrt{(j+m)!(j-m)!}},\quad j=0,\ \tfrac{1}{2},\ 1,\ \tfrac{3}{2},\ldots,\quad m=-j,\ldots,j, \tag{3.10}$$

and equipped with the scalar product

$$\langle f,g\rangle=\frac{1}{(2\pi i)^2}\int \overline{f(z_1,z_2)}g(z_1,z_2)e^{-z_1\overline{z}_1-z_2\overline{z}_2}dz_1d\overline{z_1}dz_2d\overline{z_2}. \tag{3.11}$$

The system (3.10) is orthonormal with respect to the scalar product (3.11), that is $\langle j,m|j',m'\rangle = \delta_{jj'}\delta_{mm'}$. For the given scalar product a rule of conjugation of operators looks as follows:

$$(z_i)^* = \partial_i, \quad (\partial_i)^* = z_i. \tag{3.12}$$

The question concerning unitarity of the matrix U_0 is discussed in Appendix B.

B. Connection with $T^*\mathscr{B}$

The generators of sl(2) can be realized on $D(z_1,z_2)$ as differential operators:

$$l_+ = z_1\partial_2, \quad l_- = z_2\partial_1, \quad l_3 = \tfrac{1}{2}(z_1\partial_1 - z_2\partial_2). \tag{3.13}$$

Using these expressions we can compare the representation of the algebra $\mathscr{L}$ (or, more precisely, its limit version $\mathscr{L}_0$) given by Theorem 1 with the representation given by Proposition 1.

Indeed, in the limit $\gamma\to 0$ the initial formula (2.23) acquires the form

$$L = I + \gamma L_0 + O(\gamma^2), \quad L_0 = U_0 \begin{pmatrix} p & \\ & -p \end{pmatrix} U_0^{-1}. \tag{3.14}$$

Substituting here the explicit expressions for p, U_0, (3.8) and (3.9) and using the representation (3.13) for generators of sl(2), one derives the following limit form of the L-operator:

$$L_0 = \hbar \begin{pmatrix} 2 + z_1\partial_1 - z_2\partial_2 & 2z_2\partial_1 \\ 2z_1\partial_2 & 2 - z_1\partial_1 + z_2\partial_2 \end{pmatrix} = 2\hbar \begin{pmatrix} 1 + l_3 & l_- \\ l_+ & 1 - l_3 \end{pmatrix}. \tag{3.15}$$

Notice that (3.15) exactly coincides with (2.16) taken in the limit $\gamma\to 0$. This explains why we had to introduce the factor q^2 in (2.16).

The next observation concerning the limit of the L-operator reads as follows.

Proposition 7: The matrix L_0 in the representation (3.15) admits the decomposition

$$L_0 = A_0 B_0 A_0^{-1}, \tag{3.16}$$

where

$$A_0 = \begin{pmatrix} z_1^{-1/2} & -z_1^{-1/2} z_2 \\ 0 & z_1^{1/2} \end{pmatrix}, \quad B_0 = \hbar \begin{pmatrix} p/\hbar + 1/2 & 0 \\ 2\partial_2 & -(p/\hbar - 1/2) \end{pmatrix} \tag{3.17}$$

and p is defined as in (3.8).

This statement can be verified directly.

Let us comment on the meaning of this proposition. First, note that A_0 is a realization of a grouplike element of the Borel subgroup of SL(2). Moreover, this explicit form of A_0 is straightly connected with the construction of the model space $\mathscr{M}$ developed by Gelfand *et al.*[1] Indeed, the space $D(z_1,z_2)$ being a realization of the model space for SL(2) [compare (1.1) and (3.10)] is spanned on monomials with arguments which are combinations of the entries of A_0. On the other hand, B_0 is of opposite (with respect to A_0) triangularity and its entries are operators acting on a given realization of the model space. Therefore, B_0 can be regarded as an element of the space dual to the corresponding Borel subalgebra.

Thus, A_0 and B_0 are coordinates in the base and in a fiber of the cotangent bundle $T^*\mathscr{B}$. At this stage the appearance of $T^*\mathscr{B}$ ''inside'' the algebra $\mathscr{L}$ looks somewhat mysterious, but we shall clarify it later.

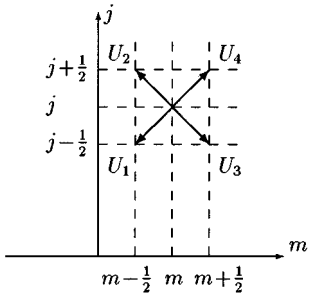

FIG. 1. Action of the operators U_i on the model space.

C. Clebsch–Gordan coefficients

Let us consider an action of the generators of the algebra $\mathscr{U}_0$ defined in (3.8) and (3.9) on the space $D(z_1,z_2)$ (which is a realization of the model space). The action of these operators on the basic vectors (3.10) is given by

$$p|j,m\rangle=(2j+1)\hbar|j,m\rangle, \tag{3.18}$$

$$U_1|j,m\rangle=\left(\frac{j+m}{2j+1}\right)^{1/2}|j-\frac{1}{2},m-\frac{1}{2}\rangle,\quad U_2|j,m\rangle=\left(\frac{j-m+1}{2j+1}\right)^{1/2}|j+\frac{1}{2},m-\frac{1}{2}\rangle,$$
$$U_3|j,m\rangle=-\left(\frac{j-m}{2j+1}\right)^{1/2}|j-\frac{1}{2},m+\frac{1}{2}\rangle,\quad U_4|j,m\rangle=\left(\frac{j+m+1}{2j+1}\right)^{1/2}|j+\frac{1}{2},m+\frac{1}{2}\rangle. \tag{3.19}$$

Formula (3.18) allows us to identify the operator p as $p=2\hat{j}+1$, where $\hat{j}$ is the operator of spin. Hence, invariant subspaces of p on the model space are those with fixed value of spin j.

Formulas (3.19) show that U_i are generators of the basic shifts on the model space (as illustrated on Fig. 1). This observation is very important. As we shall see later, the same picture holds for $q\neq 1$.

Now comparing the matrix elements $\langle j'',m''|U_i|j,m\rangle$ following from (3.19) with values of the Clebsch–Gordon coefficients (CGC) for decomposition of the tensor product of irreducible representations $V_j\otimes V_{1/2}$ for sl(2) which are given by the Van-der-Waerden formula

$$\begin{Bmatrix} j & \frac{1}{2} & j'' \\ m & m' & m'' \end{Bmatrix}=\delta_{m'',m+m'}\sqrt{\frac{(j+\frac{1}{2}-j'')!(j+j''-\frac{1}{2})!(j''+\frac{1}{2}-j)!}{(j+j''+\frac{3}{2})!}}$$
$$\times\sum_{r\geqslant 0}\frac{(-1)^r\sqrt{(j+m)!(j-m)!(j''+m'')!(j''-m'')!(2j''+1)}}{r!(j+\frac{1}{2}-j''-r)!(j-m-r)!(\frac{1}{2}+m'-r)!(j''-\frac{1}{2}+m+r)!(j''-j-m'+r)!}, \tag{3.20}$$

we establish the following correspondence:

$$\langle j'',m''|U_1|j,m\rangle=\delta_{j'',j-1/2}\begin{Bmatrix} j & \frac{1}{2} & j'' \\ m & -\frac{1}{2} & m'' \end{Bmatrix},\quad \langle j'',m''|U_2|j,m\rangle=\delta_{j'',j+1/2}\begin{Bmatrix} j & \frac{1}{2} & j'' \\ m & -\frac{1}{2} & m'' \end{Bmatrix},$$
$$\langle j'',m''|U_3|j,m\rangle=\delta_{j'',j-1/2}\begin{Bmatrix} j & \frac{1}{2} & j'' \\ m & \frac{1}{2} & m'' \end{Bmatrix},\quad \langle j'',m''|U_4|j,m\rangle=\delta_{j'',j+1/2}\begin{Bmatrix} j & \frac{1}{2} & j'' \\ m & \frac{1}{2} & m'' \end{Bmatrix}. \tag{3.21}$$

Thus, we proved the following statement:

Proposition 8: The generators U_i of the algebra $\mathscr{U}_0$ are operators of the basic shifts on the model space for sl(2) *and they generate the Clebsch–Gordan coefficients corresponding to decomposition of the product $V_j\otimes V_{1/2}$ of the irreps of* sl*(2).*

This statement allows us to call the matrix U_0 a ''generating matrix'' (by analogy with the notion of a generating function) for CGC.

Remark: Usually, introducing a generating object (well-known examples are the generating functions for different sets of polynomials, e.g., for the Legendre polynomials), one makes properties of the objects under consideration more evident. We think that the notion of generating matrix will be useful for calculations involving CGC of classical and quantum algebras.

D. Wigner–Eckart theorem

One should underline a connection of the results obtained above (Proposition 8) and the well-known mathematical construction—Wigner–Eckart theorem,[18] which has important applications in quantum mechanics.

Let us remember that the Wigner–Eckart theorem gives CGC for classical Lie algebra $\mathscr{J}$ as matrix elements of some set of operators. These operators are called *tensor operators*. They map the corresponding model space $\mathscr{M}$ onto itself and have special transformation properties under adjoint action of the algebra. In the case of $\mathscr{J}=$sl(2) the Wigner–Eckart theorem reads as follows.

Theorem 2: *Let l_+, l_- and l_3 be the generators of* sl(2) *and let T^j_m, $m=-j,\ldots,j$, be a system of operators acting on $\mathscr{M}$ and obeying the commutation relations*

$$[l_3,T^j_m]=mT^j_m,\quad [l_\pm,\,T^j_m]=\sqrt{(j\mp m)(j\pm m+1)}\,T^j_{m\pm1}, \tag{3.22}$$

where $j(j+1)$ is an eigenvalue of the Casimir operator for sl(2). *Then the matrix elements of T^j_m on $\mathscr{M}$ are proportional to Clebsch–Gordan coefficients:*

$$\langle j''m''|T^j_m|j'm'\rangle=C^j_{j''j'}\begin{Bmatrix} j' & j & j'' \\ m' & m & m'' \end{Bmatrix},$$

where the coefficients $C^j_{j''j'}$ do not depend on m, m', m''.

Proposition 8 says that any tensor operators of spin $j=1/2$ (that is, $\{T^{1/2}_{1/2},T^{1/2}_{-1/2}\}$, $T^{1/2}_m: V_j\mapsto V_j\otimes V_{1/2}=V_{j+1/2}\oplus V_{j-1/2}$) may be constructed via the operators U_i (in fact, it is evident from Fig. 1). Indeed, comparing the commutation relations obtained directly from (3.9) and (3.13)

$$\begin{gathered}[l_+,U_1]=U_3,\quad [l_+,U_2]=U_4,\quad [l_+,U_3]=0,\quad [l_+,U_4]=0,\\ [l_-,U_1]=0,\quad [l_-,U_2]=0,\quad [l_-,U_3]=U_1,\quad [l_-,U_4]=U_2,\\ [l_3,U_1]=-\tfrac{1}{2}U_1,\quad [l_3,U_2]=-\tfrac{1}{2}U_2,\quad [l_3,U_3]=\tfrac{1}{2}U_3,\quad [l_3,U_4]=\tfrac{1}{2}U_4\end{gathered} \tag{3.23}$$

with Theorem 2, we get the following.

Proposition 9: The generators U_i of the algebra $\mathscr{U}_0$ form a basis for tensor operators of spin 1/2, that is components $T^{1/2}_{1/2}$ and $T^{1/2}_{-1/2}$ of any tensor operator of spin 1/2 can be realized as linear combinations of U_i:

$$T^{1/2}_{-1/2}=\mu(p)U_1+\nu(p)U_2, \quad T^{1/2}_{1/2}=\mu(p)U_3+\nu(p)U_4, \tag{3.24}$$

where $\mu(p)$ and $\nu(p)$ are functions only of $p=2\hat{j}+1$.

IV. DEFORMED CASE

Now we want to extend the results obtained in the previous section to the case of $q\neq 1$. In particular, we are going to examine the representations of the algebra $\mathscr{U}$ (see Definition 3 above) and to show that the corresponding matrix U generates Clebsch–Gordan coefficients for the deformed Lie algebra. For these purposes we shall exploit a natural connection of $\mathscr{U}$ with $(T^*\mathscr{B})_q$.

A. The q-oscillators approach

There exist different ways to obtain desirable representations of the algebra $\mathscr{U}$. First we describe a more direct but less instructive method, which is similar to that used in the nondeformed case.

By analogy with the nondeformed case studied above, one can assume that the entries of the matrix U might be realized as operators (deformations of those obtained in Proposition 6) acting on the space of two complex variables. Indeed, using the definition (2.33) of the central element of $\mathscr{U}$ and taking into account the identity for q-numbers

$$[a]q^b+[b]q^{-a}=[a+b], \tag{4.1}$$

we can rewrite (2.35)–(2.37) in the following way:

$$\hat{U}_1\hat{U}_3=q^{-1}\hat{U}_3\hat{U}_1, \quad \hat{U}_2\hat{U}_4=q^{-1}\hat{U}_4\hat{U}_2, \quad \hat{U}_1\hat{U}_2=\hat{U}_2\hat{U}_1, \quad \hat{U}_3\hat{U}_4=\hat{U}_4\hat{U}_3, \tag{4.2}$$

$$\hat{U}_1\hat{U}_4-q^{-1}\hat{U}_4\hat{U}_1=q^{-1}\ \mathrm{Det}\ U\ q^{p/\hbar}, \quad \hat{U}_3\hat{U}_2-q\hat{U}_2\hat{U}_3=-\mathrm{Det}\ U\ q^{-p/\hbar}. \tag{4.3}$$

The relations (4.3) are well known in the theory of q-oscillators (q-bosons).[19] Recall that q-analogs of creation, annihilation, and number operators form a deformed Heisenberg algebra defined by the commutation relations

$$aa^+-qa^+a=N^{-1}, \quad Na=q^{-1}aN, \quad Na^+=qa^+N, \tag{4.4}$$

and they can be realized in terms of multiplication and difference operators:

$$a^+=z, \quad a=z^{-1}[z\partial_z], \quad N=q^{z\partial_z}. \tag{4.5}$$

Using two pairs of generators of the deformed Heisenberg algebra, one can construct the generators of $\mathrm{U}_q(\mathrm{sl}(2))$: $l_+=a_1^+a_2$, $l_-=a_2^+a_1$, and $q^{l_3}=N_1^{1/2}N_2^{-1/2}$. Applying here the representation (4.5) one gets

$$l_+=z_1z_2^{-1}[z_2\partial_2], \quad l_-=z_2z_1^{-1}[z_1\partial_1], \quad q^{l_3}=q^{1/2(z_1\partial_1-z_2\partial_2)}. \tag{4.6}$$

The Casimir operator (2.17) of $\mathrm{U}_q(\mathrm{sl}(2))$ in this realization is given by

$$C=qN_1N_2+q^{-1}N_1^{-1}N_2^{-1}. \tag{4.7}$$

Now, comparing, (4.2) and (4.3) with (4.4), it is easy to conclude that the pairs $(\hat{U}_1, \hat{U}_4)$ and $(\hat{U}_2, \hat{U}_3)$ are similar to two pairs of q-boson operators.

Taking into account the Weyl-like form of relations (4.2) and having already found explicit expressions (3.7) and (3.8) for the generators of algebra $\mathscr{U}_0$, one gets an answer for D and $\hat{U}$ in terms of q-oscillators. More precisely, a straightforward calculation allows us to verify the following statement:

Proposition 10: Equations (4.2) and (4.3) have the family of solutions:

$$q^{p/\hbar} = qN_1N_2, \quad \hat{U} = \begin{pmatrix} \alpha_0 a_1 N_1^{\alpha} N_2^{-\beta} & \beta_0 a_2^+ N_1^{\beta} N_2^{-\alpha} \\ -\gamma_0 a_2 N_1^{-(1+\beta)} N_2^{\alpha} & \delta_0 a_1^+ N_1^{-\alpha} N_2^{1+\beta} \end{pmatrix}, \tag{4.8}$$

where $\alpha_0\delta_0 = q\beta_0\gamma_0$.

Let us note that this form of $\hat{U}$ is consistent with the condition (2.32).

Taking into account the connection formula (2.34) and applying to the generators a_i, a_i^+, and N_i the representation (4.5), one obtains from (4.8) a family of representations of the algebra $\mathscr{U}$. To select some of them, we have to impose an additional condition.

As mentioned above [see (3.14) and (3.15)], in the nondeformed case substitution of the generating matrix U_0 in the formula (2.23) gives the matrix L_0 which exactly coincides with the limit version of the matrix (2.16). It is natural to suppose that the generating matrix U corresponding to deformed algebra produces in the same way the matrix (2.16) itself. Bearing in mind the property (2.41), we obtain the following.

Proposition 11: The condition $\hat{U}D\hat{U}^{-1} = L$, *where* L *is the matrix (2.16),* D *is given by*

$$D = \begin{pmatrix} p^{p/\hbar} & \\ & q^{-p/\hbar} \end{pmatrix} = \begin{pmatrix} qN_1N_2 & \\ & q^{-1}N_1^{-1}N_2^{-1} \end{pmatrix}, \tag{4.9}$$

and $\hat{U}$ is given by (4.8), imposes the following restrictions:

$$\alpha + \beta + \tfrac{1}{2} = 0, \quad \alpha_0 = q\gamma_0, \quad \beta_0 = \delta_0. \tag{4.10}$$

Substitution of (4.10) into (4.8) completes description of $\hat{U}$ in terms of q-oscillators.

B. Connection with $(T^*\mathscr{B})_q$

Now we are going to develop another approach to constructing representations of $\mathscr{U}$. It is more universal since it is based on the connection (which takes place for arbitrary quantum Lie algebra) of the algebra $\mathscr{L}$ (see Definition 1) with $(T^*\mathscr{B})_q$ and on the interpretation of the deformed Borel subgroup $\mathscr{B}_q$ as a quantum model space.

To clarify the announced connection we start with the following theorem (this is a version of the theorem given in Ref. 10 for L-operators with nonultralocal relations).

Theorem 3: *Let the matrices* A and B *obey the relations of type (2.1),*

$$R_{\pm}^{12} A^2 A^1 = A^2 A^1 R_{\pm}^{21}, \quad R_{\pm}^{12} B^2 B^1 = B^2 B^1 R_{\pm}^{21}, \tag{4.11}$$

and the additional exchange relation

$$A^1 B^2 = B^2 A^1 R_+^{21}, \quad A^2 B^1 R_-^{21} = B^1 A^2. \tag{4.12}$$

Then the L*-operator constructed by means of similarity transformation*

$$L = ABA^{-1} \tag{4.13}$$

satisfies the relation (2.3).

Remark: Since (4.11) defines a quantum group structure, A^{-1} in (4.13) should be understood as an antipode of A.

Proof of Theorem 3 is straightforward:

$$\begin{aligned} \overset{1}{L}\overset{-1}{R}\overset{2}{L}\overset{}{R}_- &= \overset{1\,1}{A}\overset{1}{B}(A)^{-1}\overset{-1}{R}\overset{2\,2}{A}\overset{2}{B}(A)^{-1}R_- = \overset{1\,1\,2}{ABA}\overset{-1}{R}\overset{1}{(A)}^{-1}\overset{2}{B}\overset{2}{(A)}^{-1}R_- \\ &= \overset{1\,2\,1\,2}{AABB}\overset{-1}{R}\overset{1}{(A)}^{-1}\overset{2}{(A)}^{-1}R_- = \overset{-1}{R}\overset{2\,1\,2\,1}{AABB}R_-\overset{2}{(A)}^{-1}\overset{1}{(A)}^{-1} \\ &= \overset{-1}{R}\overset{2\,2\,1}{ABA}R_+\overset{2}{(A)}^{-1}\overset{1\,1}{B}(A)^{-1} = \overset{-1}{R}\overset{2\,2\,2}{AB}(A)^{-1}R_+\overset{1\,1\,1}{AB}(A)^{-1} = \overset{-1}{R}\overset{2}{L}\overset{}{R}_+\overset{1}{L}. \end{aligned}$$

Thus, for a given quantum group G_q, the algebra $\mathscr{S}$ is embedded into the algebra generated by entries of A and B obeying (4.11) and (4.12). To argue that (4.11) and (4.12) describe a q-analog of $T^*\mathscr{B}$, let us notice that the nonsymmetric (with respect to R-matrices) form of the relations (4.12) imposes some restriction on the structure of the matrices A and B. Say, if R_+ is an upper triangular matrix, then A and B must be upper and lower triangular, respectively. Therefore, one may think of A and B as coordinates in the deformed Borel subgroup $\mathscr{B}_q$ and in the dual quantum space, respectively. In other words, the matrices A and B are coordinate and momentum on the deformed phase space $(T^*\mathscr{B})_q$, respectively. Thus (4.11) and (4.12) may be regarded as a definition of $(T^*\mathscr{B})_q$ (for additional comments see Ref. 10).

We should underline here that, although the matrices A and B look similar on the quantum level, they transform into different objects when $q\to 1$. Indeed, in the limit $q\to 1$ one has $L\to I+\gamma\hbar L_0$ and the corresponding limit forms of A and B are

$$A\to A_0, \quad B\to I+\gamma\hbar B_0, \tag{4.14}$$

where A_0 is a grouplike element, whereas B_0 is rather an element of algebra [see (3.17) as an example of A_0 and B_0 for sl(2)].

Comparing the statements of Theorems 1 and 3 and taking into account the equality (2.41), we get the formula

$$L=ABA^{-1}=\hat{U}D\hat{U}^{-1}, \tag{4.15}$$

which points out a possibility to construct the matrix $\hat{U}$ obeying (2.35)–(2.38) via the generators of $(T^*\mathscr{B})_q$. This connection is very important; below we consider it for $\mathrm{SL}_q(2)$ in all details.

Now let us turn to the example of $\mathrm{SL}_q(2)$. For $R_\pm$ defined as in (2.8) one can choose

$$A=\begin{pmatrix} a & c \\ 0 & a^{-1} \end{pmatrix}, \quad B=\begin{pmatrix} b & 0 \\ d & b^{-1} \end{pmatrix}. \tag{4.16}$$

Explicit relations for the generators of $(T^*\mathscr{B})_q$ following from (4.11) and (4.12) are

$$ac=q^{-1}ca, \quad bc=q^{1/2}cb, \quad ab=q^{1/2}ba; \tag{4.17}$$

$$bd=q^{-1}db, \quad ad=q^{1/2}da, \quad cd=q^{-1/2}dc+q^{-1/2}\omega b^{-1}a. \tag{4.18}$$

Performing the following decomposition,

$$d=d_0+d_1=d_0+q^{1/2}c^{-1}b^{-1}a, \tag{4.19}$$

we transform (4.18) to homogeneous form:

$$bd_0 = q^{-1}d_0 b, \quad ad_0 = q^{1/2}d_0 a, \quad cd_0 = q^{-1/2}d_0 c. \tag{4.20}$$

Thus, (4.17) and (4.20) describe four variables obeying Weyl-like commutation relations. Using the jargon of conformal field theory, we shall call these formulas ''free field representation'' and the generators a, b, c, and d_0 ''free field'' variables.

Remark: The last of equations (4.18) is nothing but a commutation relation entering the definition of deformed Heisenberg algebra. Indeed, comparing (4.17) and (4.18) with (4.4), one can establish the following correspondence (ρ stands for arbitrary numerical constant):

$$c \sim N^{\rho} a^{+}, \quad d \sim -\omega N^{-1/2-\rho} a, \quad b^{-1}a \sim q^{\rho} N^{-3/2}.$$

Thus, the transformation (4.19) can be interpreted as ''bosonization'' of q-oscillators.

Now, substituting (4.16) in (4.13), we get

$$\begin{aligned} L &= q^{1/2} \begin{pmatrix} a & c \\ 0 & a^{-1} \end{pmatrix} \begin{pmatrix} b & 0 \\ d & b^{-1} \end{pmatrix} \begin{pmatrix} a^{-1} & -qc \\ 0 & a \end{pmatrix} \\ &= \begin{pmatrix} q(b+b^{-1}) + a^{-1}cd_0 & -q^2 ac(b + qa^{-1}cd_0) \\ (ac)^{-1}(b^{-1} + q^{-1}a^{-1}cd_0) & -q^2 a^{-1}cd_0 \end{pmatrix}. \end{aligned} \tag{4.21}$$

This matrix provides a ''free field'' realization of the algebra $\mathscr{L}$ for $U_q(\mathrm{sl}(2))$. Note that the additional scaling factor $q^{1/2}$ was introduced in (4.21) to ensure a coincidence of the Casimir operators calculated by formulas (2.13) for the matrix (4.21):

$$K_1 = q^2(b + b^{-1}), \quad K_2 = q^3 \tag{4.22}$$

with those for the matrix (2.16). In fact, we redefined the matrix B in (4.16) as

$$\widetilde{B} = q^{1/2} B. \tag{4.23}$$

Comparing the Casimir operator K_1 given by (4.22) with one given by (2.18), we identify the operator b with the power of the operator of spin $\hat{j}$:

$$b = q^{2\hat{j}+1}. \tag{4.24}$$

It follows from (4.22) that matrix L contains only three independent variables [it is easy to see from the explicit form (4.21) that these are b, ac, and $a^{-1}cd_0$]. Moreover, direct calculation using (4.17) and (4.20) shows that all elements of the matrix L commute with operator b. That agrees with the property (2.25).

Now exploiting the connection described by formula (4.15), one can obtain an exact expression for $\hat{U}$.

Theorem 4: *The algebra $\mathscr{U} \equiv \{\hat{U}, p\}$ with defining relations (2.35)–(2.38) has the following realization in terms of generators a, b, c,* and d_0:

$$b = q^{p/\hbar}, \quad \hat{U} = \begin{pmatrix} \dfrac{1}{\omega}\, a(b + a^{-1}cd_0)e^{-i\xi/2} & ce^{i\xi/2} \\ \dfrac{1}{\omega}\, c^{-1}(b^{-1} + q^{-1}a^{-1}cd_0)e^{-i\xi/2} & a^{-1}e^{i\xi/2} \end{pmatrix}, \tag{4.25}$$

where $\omega \equiv q - q^{-1}$, d_0 is defined in (4.19), and

$$e^{i\xi}=a^{-1}b^{\gamma}c^{-1}d_0^{-1} \tag{4.26}$$

with γ being an arbitrary constant.

This theorem gives a ''free field'' representation of the algebra $\mathscr{U}$. Let us remark that the remaining freedom in (4.26) corresponds only to canonical transformations (since ξ and p are conjugate variables).

The formulated theorem will be proved in several steps. First, we introduce a lower-triangular matrix which diagonalizes the matrix $\widetilde{B}$:

$$V=\begin{pmatrix} v_1 & 0 \\ v_3 & v_2 \end{pmatrix}, \quad \widetilde{B}=V\widetilde{B}_0V^{-1}, \quad \widetilde{B}_0=\begin{pmatrix} q^{1/2}b & 0 \\ 0 & q^{1/2}b^{-1} \end{pmatrix}\equiv q^{1/2}B_0. \tag{4.27}$$

Proposition 12: A possible solution for the matrix V is

$$v_1=v_1(b), \quad v_2=v_2(b), \quad v_3=dv_1(b)f(b), \tag{4.28}$$

where $v_1(b)$ and $v_2(b)$ are arbitrary functions of b and $f(b)=(b-qb^{-1})^{-1}$.

Thus, matrix L given by (4.21) admits a decomposition of the form

$$L=\hat{U}_0\widetilde{B}_0\hat{U}_0^{-1}, \quad \hat{U}_0=AV. \tag{4.29}$$

However, this diagonalization is not unique. Using an arbitrary power of the diagonal matrix Q, which depends on the variable conjugate to b,

$$Q=\begin{pmatrix} e^{i\xi} & \\ & e^{-i\xi} \end{pmatrix}, \quad be^{i\xi}=qe^{i\xi}b, \tag{4.30}$$

we obtain a family of diagonalizing matrices:

$$L=\hat{U}_\delta\,\widetilde{B}_\delta\,\hat{U}_\delta^{-1}, \quad \hat{U}_\delta=AVQ^\delta, \quad \widetilde{B}_\delta=Q^{-\delta}\widetilde{B}_0Q^\delta=q^\delta\widetilde{B}_0=q^{\delta+1/2}B_0. \tag{4.31}$$

An explicit form of the diagonalizing matrix is

$$\hat{U}_\delta=AVQ^\delta=\begin{pmatrix} (av_1+cdv_1f\ )e^{i\delta\xi} & cv_2e^{-i\delta\xi} \\ a^{-1}dv_1fe^{i\delta\xi} & a^{-1}v_2e^{-i\delta\xi} \end{pmatrix}. \tag{4.32}$$

Here we should describe a new object $e^{i\xi}$ which appeared in the matrix $\hat{U}$. We assume that the following Weyl-like relations hold:

$$ae^{i\xi}=q^\alpha e^{i\xi}a, \quad be^{i\xi}=qe^{i\xi}b, \quad ce^{i\xi}=q^\beta e^{i\xi}c, \quad d_0e^{i\xi}=q^\gamma e^{i\xi}d_0. \tag{4.33}$$

Proposition 13: The set of equations (4.33) is equivalent to

$$e^{i\xi}=a^{\beta+(\gamma-1)/2}b^\gamma c^{(\gamma-1)/2-\alpha}d_0^{-1}. \tag{4.34}$$

Now we have to remember that the matrix U (and $\hat{U}$ as well) described in Theorem 1 has to satisfy the relation (2.20) or, equivalently, the relation

$$\overset{1}{B}_0\overset{2}{\hat{U}}_\delta=\overset{2}{\hat{U}}_\delta\overset{1}{B}_0\sigma, \tag{4.35}$$

where σ and B_0 were introduced in (2.20) and (4.27), respectively. A straightforward calculation using (4.17) and (4.18) leads to the following.

Proposition 14: The matrix $\hat{U}_\delta$ given by (4.32) satisfies the relation (4.35) only for $\delta=-1/2$.

It is worth mentioning that such a choice of δ exactly compensates the renormalization of the matrix B in (4.23), i.e., $\widetilde{B}_{-1/2}=B_0$.

Bearing in mind the formula (4.19), one can rewrite (4.32) for $\delta=-1/2$ as follows,

$$\hat{U}\equiv\hat{U}_{-1/2}=\begin{pmatrix} a(b+a^{-1}cd_0)we^{-i\xi/2} & cve^{i\xi/2} \\ c^{-1}(b^{-1}+q^{-1}a^{-1}cd_0)we^{-i\xi/2} & a^{-1}ve^{i\xi/2} \end{pmatrix}, \tag{4.36}$$

where $w\equiv f(b)v_1(b)$ and $v\equiv v_2(b)$.

Finally, a direct check shows (see Appendix C) that the matrix (4.36) obeys Eqs. (2.35)–(2.38) if the functions w and v are constant [we chose them as follows: $v(b)=1$, $w(b)=1/\omega$] and the coefficients in (4.33) and (4.34) satisfy the conditions $\beta=-\alpha$ and $\gamma=\alpha-\beta-1=2\alpha-1$. Thus, Theorem 4 is proven.

Let us end the discussion of relation of $(T^*\mathscr{B})_q$ to algebras $\mathscr{L}$ and $\mathscr{U}$ with one more statement:

Theorem 5: *The algebra generated by coordinates on $(T^*\mathscr{B})_q$ is isomorphic to the algebra generated by entries of the matrix L and Q.*

Proof: Indeed, formulas (4.21) and (4.26) provide explicit expressions for entries of L and Q via the generators a, b, c, and d_0 [up to unessential canonical transformation in (4.26)]. Conversely, suppose matrix L and the element $e^{i\xi}$ are given. Then, as it follows from (4.21), one can construct from entries of L the combinations b, ac, and $a^{-1}cd_0$. Together with (4.26) this allows us to recover the ''coordinates'' a, b, c, and d_0.

Although we considered this theorem only for the case of $\mathrm{SL}_q(2)$, there is, evidence that it holds for the generic case. For example, in the case of $G_q=\mathrm{SL}_q(N)$ a point on the quantum bundle $(T^*\mathscr{B})_q$ is parametrized by $N\times N$ matrices A and B. As above, the matrix $L=ABA^{-1}$ satisfies (2.3) and therefore its entries generate the corresponding algebra $\mathscr{L}$. However, the dimension of $(T^*\mathscr{B})_q$ exceeds the dimension of $\mathscr{L}$: $\dim(T^*\mathscr{B})_q-\dim\mathscr{L}=(N^2+N-2)-(N^2-1)=N-1$. It is very probable that the remaining $(N-1)$ generators are exactly those that enter the diagonal unimodular $N\times N$ matrix Q.

C. Explicit representation

Now we face the problem of constructing an explicit representation for the generators a, b, c, and d_0. A Weyl-like form of the commutation relations (4.17) and (4.20) points out the possibility of getting a realization for these generators in terms of two pairs of canonical variables. This also means [due to the interpretation of (4.19) as ''bosonization'' of q-oscillators] that the generators a, b, c, and d admit a realization via q-oscillators. Evidently, such a representation is not unique.

It is natural to realize a, b, c, and d_0 as operators acting on the q-analog of the space $D(z_1,z_2)$. We shall denote this space as $D_q(z_1,z_2)$. The space $D_q(z_1,z_2)$ is spanned on the basic vectors of form (remember that $[x]$ stands for q-numbers)

$$|j,m\rangle=\frac{z_1^{j+m}z_2^{j-m}}{\sqrt{[j+m]![j-m]!}},\ j=0,\ \tfrac{1}{2},\ 1,\ \tfrac{3}{2},\ldots,\quad m=-j,..,j. \tag{4.37}$$

One can define on $D_q(z_1,z_2)$ such a scalar product that the system (4.37) is orthonormal, that is $\langle j,m|j',m'\rangle=\delta_{jj'}\delta_{mm'}$.

Remark: This scalar product is a deformation of (3.11). Its explicit form makes use of the q-exponent and the Jackson integral. See Ref. 19 for details.

In all formulas concerning the space $D_q(z_1,z_2)$ we suppose that q is chosen as described in Sec. II (i.e., it belongs either to the real axis or to the unit circle at the complex plane). In this case an analog of the rule of conjugation (3.12) is

$$(z_i)^* = z_i^{-1}[z_i\partial_i], \quad (z_i\partial_i)^* = z_i\partial_i\,. \tag{4.38}$$

The formulas (4.24) and (4.25) imply that the generator b is a power of the operator of spin. Hence, on the space $D_q(z_1,z_2)$ it is given by

$$b = q^{z_1\partial_1 + z_2\partial_2 + 1} = qN_1N_2\,. \tag{4.39}$$

Next, let us remember that we already know the limit versions of the generators a, b, c, and d [see Proposition 7; one should take into account the rescaling (4.23)]. Their appropriate deformations for generic q are described by

Proposition 15: The set of operators (with arbitrary constants λ_i, ν_i*)*

$$\begin{gathered} a = q^{\lambda_0} z_1^{-1/2}\, N_1^{\lambda_1}, \quad c = q^{\nu_0}\, z_1^{-1/2} z_2\, N_1^{\lambda_1 - 2} N_2^{\nu_2}, \\ b = qN_1N_2, \quad d = -q^{\lambda_0 - \nu_0 + \nu_2}\, z_2^{-1}(N_2 - N_2^{-1}) N_1 N_2^{-\nu_2} \end{gathered} \tag{4.40}$$

satisfies (4.17) and (4.18) and gives in the limit $\gamma \to 0$ *the generators found in (3.17).*

Although due to Theorem 4 this proposition gives a family of representations for $\mathscr{U}$, we again should impose an additional condition using the matrix (2.16) as a standard (justification for this trick was given above).

Proposition 16: Matrix L given by (4.21) coincides with the matrix (2.16) taken in the representation (4.6) provided that

$$b = qN_1N_2, \quad ac = q^{-1/2} z_1^{-1} z_2 N_1^{-1/2} N_2^{-1/2}, \quad a^{-1} c d_0 = -N_1^{-1} N_2\,. \tag{4.41}$$

Comparing the statements of Propositions 15 and 16, we derive

$$\begin{gathered} a = q^{\lambda_0} z_1^{-1/2} N_1^{3/4}, \quad b = qN_1N_2, \quad c = q^{\nu_0} z_1^{-1/2} z_2 N_1^{-5/4} N_2^{-1/2}, \\ d_0 = -q^{\lambda_0 - \nu_0 - 1/2} z_2^{-1} N_1 N_2^{3/2}, \quad q^{\lambda_0 + \nu_0} = q^{-1/8}. \end{gathered} \tag{4.42}$$

Substituting (4.42) into (4.26) [and remember that (4.26) is defined only up to a coefficient], we get

$$e^{i\xi} = q^{2\epsilon} z_1 N_1^{\gamma - 1/2} N_2^{\gamma - 1}, \tag{4.43}$$

where γ and ϵ are arbitrary. Finally, substituting (4.42) and (4.43) into (4.36), we obtain (one should remember that U and $\hat{U}$ are defined only up to arbitrary scaling factor)

$$\hat{U} = \begin{pmatrix} \dfrac{1}{\omega}\, \alpha_0 z_1^{-1} N_1^{1-\gamma/2} N_2^{3/2-\gamma/2} (N_1 - N_1^{-1}) & \beta_0 z_2 N_1^{\gamma/2 - 3/2} N_2^{\gamma/2 - 1} \\ -\dfrac{1}{\omega}\, q^{-1} \alpha_0 z_2^{-1} N_1^{1/2-\gamma/2} N_2^{1-\gamma/2} (N_2 - N_2^{-1}) & \beta_0 z_1 N_1^{\gamma/2 - 1} N_2^{\gamma/2 - 1/2} \end{pmatrix}. \tag{4.44}$$

It is easy to check that the family of matrices (4.44) exactly coincides with what was obtained in q-oscillator approach (see Propositions 10 and 11).

D. Quantum Clebsch–Gordan coefficients

Using the connection formula (2.34) we get from (4.44) a family of matrices U which provide possible representations of the algebra $\mathscr{U}$. It is natural to study an action of the entries of these matrices on the space $D_q(z_1,z_2)$ described above. On the basic vectors (4.37) these operators act as follows:

$$
\begin{aligned}
U_1|j,m\rangle &= C_1 q^{(1/2)(j-m+1)} \sqrt{\frac{[j+m]}{[2j+1]}}\,|j-\tfrac{1}{2},m-\tfrac{1}{2}\rangle,\\
U_2|j,m\rangle &= C_2 q^{-(1/2)(j+m)} \sqrt{\frac{[j-m+1]}{[2j+1}}|j+\tfrac{1}{2},m-\tfrac{1}{2}\rangle,\\
U_3|j,m\rangle &= -C_3 q^{-(1/2)(j+m+1)} \sqrt{\frac{[j-m]}{[2j+1]}}\,|j-\tfrac{1}{2},m+\tfrac{1}{2}\rangle,\\
U_4|j,m\rangle &= C_4 q^{(1/2)(j-m)} \sqrt{\frac{[j+m+1]}{[2j+1]}}\,|j+\tfrac{1}{2},m+\tfrac{1}{2}\rangle,
\end{aligned}
\tag{4.45}
$$

where the coefficients C_i do not depend on m.

Note that, similar to the classical case, the operators U_i correspond to the basic shifts on the model space. Comparing the matrix elements $\langle j',m'|U_i|j,m\rangle$ following from (4.45) to values of CGC for $\mathrm{U}_q(\mathrm{sl}(2))$ given by q-analog of the Van-der-Waerden formula,[20,21] which for the decomposition of $V_j\otimes V_{1/2}$ looks like following,

$$
\begin{aligned}
&\begin{Bmatrix} j & \frac{1}{2} & j'' \\ m & m' & m'' \end{Bmatrix}_q \\
&= \delta_{m'',m+m'} \left(\frac{[j+\frac{1}{2}-j'']![j+j''-\frac{1}{2}]![j''+\frac{1}{2}-j]!}{[j+j''+\frac{3}{2}]!} \right)^{1/2} q^{(1/2)(j+1/2-j'')(j+j''+3/2)+jm'-(1/2)m} \\
&\times \sum_{r\geqslant 0} \frac{(-1)^r q^{-r(j+j''+3/2)}([j+m]![j-m]![j''+m'']![j''-m'']![2j''+1])^{1/2}}{[r]![j+\frac{1}{2}-j''-r]![j-m-r]![\frac{1}{2}+m'-r]![j''-\frac{1}{2}+m+r]![j''-j-m'+r]!},
\end{aligned}
\tag{4.46}
$$

we establish the following correspondence:

$$
\begin{aligned}
\langle j'',m''|U_1|j,m\rangle &= \delta_{j'',j-1/2}\ \alpha_0\ q^{(1-\gamma/2)j-1/2} \begin{Bmatrix} j & \frac{1}{2} & j'' \\ m & -\frac{1}{2} & m'' \end{Bmatrix}_q,\\
\langle j'',m''|U_2|j,m\rangle &= \delta_{j'',j+1/2}\ \beta_0\ q^{(\gamma/2-1)j} \begin{Bmatrix} j & \frac{1}{2} & j'' \\ m & -\frac{1}{2} & m'' \end{Bmatrix}_q,\\
\langle j'',m''|U_3|j,m\rangle &= \delta_{j'',j-1/2}\ \alpha_0\ q^{(1-\gamma/2)j-1/2} \begin{Bmatrix} j & \frac{1}{2} & j'' \\ m & \frac{1}{2} & m'' \end{Bmatrix}_q,\\
\langle j'',m''|U_4|j,m\rangle &= \delta_{j'',j+1/2}\ \beta_0\ q^{(\gamma/2-1)j} \begin{Bmatrix} j & \frac{1}{2} & j'' \\ m & \frac{1}{2} & m'' \end{Bmatrix}_q.
\end{aligned}
$$

Thus we derive an analog of Proposition 8:

Proposition 17: The generators U_i of the algebra $\mathscr{U}$ are operators of the basic shifts on the model space for $\mathrm{U}_q(\mathrm{sl}(2))$ *and they generate the q-Clebsch–Gordan coefficients corresponding to decomposition of the product $V_j\otimes V_{1/2}$ of irreps of* $\mathrm{U}_q(\mathrm{sl}(2))$.

Remark: Putting $\alpha_0=q^{1/2}$, $\beta_0=1$, and $\gamma=2$ in (4.44), we get the following generating matrix:

$$U=\begin{pmatrix} z_1^{-1}[z_1\partial_1]q^{(1/2)(z_2\partial_2+1)} & z_2q^{-(1/2)z_1\partial_1} \\ -z_2^{-1}[z_2\partial_2]q^{-(1/2)(z_1\partial_1+1)} & z_1q^{(1/2)z_2\partial_2} \end{pmatrix}\frac{1}{\sqrt{[p/\hbar]}},\quad \text{Det } U=q^{1/2}, \tag{4.47}$$

which may be called ''exact'' as it satisfies (4.45) with $C_i=1$. The question about unitarity of the matrix (4.47) is discussed in Appendix B.

E. Generalized Wigner–Eckart theorem

As we demonstrated in the previous section, entries of the matrix U_0 are tensor operators of spin 1/2 for $\mathscr{J}=\mathrm{sl}(2)$, hence they provide a realization of the Wigner–Eckart theorem. Let us now consider the matrix U from this point of view.

The theory of tensor operators for quantum algebras was discussed by many authors (see, e.g., Ref. 22). In particular, the generalized Wigner–Eckart theorem [in the case of $\mathscr{J}_q=U_q(\mathrm{sl}(2))$] reads as follows.

Theorem 6: *Let l_+, l_-, and l_3 be the generators of $U_q(\mathrm{sl}(2))$ and let T^j_m, $m=-j,..,j$, be a system of operators acting on the deformed model space $\mathscr{M}$ and obeying the commutation relations*

$$[l_3,\ T^j_m]=mT^j_m,\quad l_\pm T^j_m q^{l_3}-q^{l_3\mp 1}T^j_m l_\pm=\sqrt{[j\mp m][j\pm m+1]}\,T^j_{m\pm 1}. \tag{4.48}$$

Then the matrix elements of T^j_m on $\mathscr{M}$ are proportional to q-Clebsch–Gordan coefficients:

$$\langle j''m''|T^j_m|j'm'\rangle=C^j_{j''j'}\begin{Bmatrix} j' & j & j'' \\ m' & m & m'' \end{Bmatrix}_q,$$

where the coefficients $C^j_{j''j'}$ do not depend on m, m', and m''.

Proposition 17 implies that U_i may be regarded as q-tensor operators. Indeed, using (4.44) and (4.6), one can check that U_i satisfy (4.48) [one obtains for U_i deformations of relations (3.23)]. Similarly to the classical case we have the following.

Proposition 18: The generators U_i of the algebra $\mathscr{U}$ form a basis for q-tensor operators of spin 1/2, that is components $T^{1/2}_{1/2}$ and $T^{1/2}_{-1/2}$ of any q-tensor operator of spin 1/2 can be realized as linear combinations of U_i:

$$T^{1/2}_{-1/2}=\mu(p)U_1+\nu(p)U_2,\quad T^{1/2}_{1/2}=\mu(p)U_3+\nu(p)U_4, \tag{4.49}$$

where $\mu(p)$ and $\nu(p)$ are functions only of p.

Remark: Unlike the classical case, solution (4.44) gives a family of matrices U. However, the corresponding matrix elements $\langle j''m''|U_i|j'm'\rangle$ differ only by factors which do not depend on m' and m''. Thus, any representative of the obtained family of matrices U may be used in Proposition 18.

Let us end the description of the algebra $\mathscr{U}$ from the point of view of theory of q-tensor operators with the following statement:

Proposition 19: The matrices U and L defined in Theorem 1 obey the relation

$$R_-\overset{1\,2}{U}L=L\overset{2}{R}_+\overset{1}{U}. \tag{4.50}$$

The proof is straightforward:

$$R_{-}^{1\,2}UL = R_{-}^{1\,2}UU^{2}D(U)^{-1} = U^{2}U^{1}\mathscr{R}_{-}D^{2}(U)^{-1} = U^{2}U^{1}D^{2}\sigma\mathscr{R}_{+}^{2}(U)^{-1}$$

$$= U^{2}D^{2}U^{1}\mathscr{R}_{+}^{2}(U)^{-1} = U^{2}D^{2}(U)^{-1}R_{+}^{1}U^{2}L^{1} = LR_{+}U;$$

it makes use of the relations (2.20) and (2.21) and the property (2.24).

A remarkable fact is that (4.50) may be used for definition of q-tensor operators instead of (4.48). Indeed, in the limit $\gamma\to 0$ it turns into

$$[U_0^{1}, L_0^{2}] = \Lambda U_0^{1}, \quad \Lambda = \begin{pmatrix} 1/2 & & & \\ & -1/2 & 1 & \\ & 1 & -1/2 & \\ & & & 1/2 \end{pmatrix}. \tag{4.51}$$

Using the explicit form of L_0 given in (3.14), one can easily check that this matrix relation is equivalent to (3.23). More on R-matrix description of q-tensor operators is given in Ref. 23.

V. CONCLUSION

In this paper we have constructed the q-analog of the phase space $T^*\mathscr{B}$ and clarified its role in description of the model representation of the corresponding quantum group G_q. We unraveled a connection between the algebras generated by entries of matrix (A,B), (U,D), and (L,Q). The general formulas were concretized by the example of $G=\mathrm{SL}(2)$.

An extension of the described scheme to the case of arbitrary group G will definitely improve understanding of the role played by the matrix $\mathscr{R}(p)$ which so far has been discussed in the literature much less than standard matrix R.

The results of this paper can be generalized in several directions even for the case of SL(2). The first is a consideration of the matrix U with an auxiliary space corresponding to the higher spin representation. It must lead to an exact form of the generating matrix for all CGC. The work in this direction is in progress now. The second point to be discussed is the case of q being a root of unity. The structure of $\mathscr{R}(p)$ allows us to hope that reduction on so-called ''good'' representations will be quite natural in our formalism. However, this case is to be examined more carefully.

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APPENDIX A: PROOF OF THEOREM 1

Using (2.20) and (2.21) together with the identity (2.24) and taking into account that matrices D^{1}, D^{2}, and σ mutually commute, we check

$$
\begin{aligned}
\overset{1}{L}\overset{-1}{R}_{-}\overset{2}{L}R_{-} &= \overset{1\,1}{U}\overset{1}{D}(U)^{-1}\overset{-1}{R}_{-}\overset{2\,2}{U}\overset{2}{D}(U)^{-1}R_{-} \\
&= \overset{1\,1\,2}{U}D\overset{-1}{U}\mathscr{R}_{-}(p)(\overset{1}{U})^{-1}\overset{2\,2}{D}(U)^{-1}R_{-} \\
&= \overset{1\,2\,1}{U}U D\sigma\mathscr{R}_{-}^{-1}(p)\overset{2}{D}\sigma(\overset{1}{U})^{-1}(\overset{2}{U})^{-1}R_{-} \\
&= R_{+}^{-1}\overset{2\,1}{U}U\mathscr{R}_{+}(p)\overset{1}{D}\sigma\mathscr{R}_{-}^{-1}(p)\overset{2}{D}\sigma\mathscr{R}_{-}(p)(\overset{2}{U})^{-1}(\overset{1}{U})^{-1} \\
&= R_{+}^{-1}\overset{2\,1\,2}{U}UD\sigma\overset{1}{D}\mathscr{R}_{-}(p)(\overset{2}{U})^{-1}(\overset{1}{U})^{-1} \\
&= R_{+}^{-1}\overset{2\,2\,1}{U}DU\mathscr{R}_{+}(p)\sigma\overset{1}{D}(\overset{2}{U})^{-1}(\overset{1}{U})^{-1} \\
&= R_{+}^{-1}\overset{2\,2\,1}{U}DU\mathscr{R}_{+}(p)(\overset{2}{U})^{-1}\overset{1}{D}(\overset{1}{U})^{-1} \\
&= R_{+}^{-1}\overset{2\,2}{U}\overset{2}{D}(U)^{-1}R_{+}\overset{1\,1}{U}\overset{1}{D}(U)^{-1} = \overset{-1}{R}_{+}\overset{2}{L}R_{+}\overset{1}{L}.
\end{aligned}
$$

APPENDIX B: ON CONJUGATION OF U_0 AND U

First we consider the matrix U_0. Using the rules of conjugation (3.12) (and taking into account that $p^*=p$), one can check that the matrix conjugated to U_0 does not coincide with U_0^{-1}; that is, the matrix U_0 itself is not unitary. However, it turns out that the transposed matrix [one should remember that in general $(U^T)^{-1}\neq(U^{-1})^T$ for matrices with noncommuting entries]

$$
U_0^T=\begin{pmatrix} \partial_1 & -\partial_2 \\ z_2 & z_1 \end{pmatrix}\sqrt{\frac{\hbar}{p}}
$$

satisfies the unitarity condition:

$$
(U_0^T)^*=\sqrt{\frac{\hbar}{p}}\begin{pmatrix} z_1 & \partial_2 \\ -z_2 & \partial_1 \end{pmatrix}=(U_0^T)^{-1}.
$$

In the deformed case (recall that q can be either real or $|q|=1$) the matrix U includes the operator N which conjugates in different ways for the different choices of q. Let us consider the matrix U given by (4.47). The conjugated matrix can be constructed according to the rules (4.38). Using the formula (4.1), one can check that the unitarity condition $(U^T)^*U^T=U^T(U^T)^*=I$ (i.e., the same as in the nondeformed case) for the transposed matrix holds only for real q. For $|q|=1$, see Ref. 13.

APPENDIX C: PROOF OF THEOREM 4

Here we complete the proof of Theorem 4, i.e., we have to prove that matrix (4.36) satisfies (2.35)–(2.37) if the following conditions,

$$
\alpha+\beta=0, \quad \gamma+\beta-\alpha+1=0, \quad v(b)=1, \quad w(b)=1/\omega, \tag{C1}
$$

are fulfilled.

First, using relations (4.17), (4.20), and (4.33) and conditions (C1), we check

$$\hat{U}_1\hat{U}_2 = a(b+a^{-1}cd_0)e^{-i\xi}ce^{i\xi} = q^{-1/2+\beta/2}ca(b+qa^{-1}cd_0)e^{i\xi}e^{-i\xi}$$
$$= q^{\alpha/2+\beta/2}ce^{i\xi}a(b+q^{(\gamma+\beta-\alpha+1)/2}a^{-1}cd_0)e^{-i\xi} = \hat{U}_2\hat{U}_1,$$

$$\hat{U}_1\hat{U}_3 = a(b+a^{-1}cd_0)e^{-i\xi}c^{-1}(b^{-1}+q^{-1}a^{-1}cd_0)e^{-i\xi}$$
$$= q^{1/2-\beta/2}c^{-1}a(b+q^{-1}a^{-1}cd_0)e^{-i\xi}(b^{-1}+q^{-1}a^{-1}cd_0)e^{-i\xi}$$
$$= q^{-\beta/2}c^{-1}a(b^{-1}+q^{-1}a^{-1}cd_0)(b+q^{-1}a^{-1}cd_0)e^{-i\xi}e^{-i\xi}$$
$$= q^{-1/2-\beta/2}c^{-1}(b^{-1}+q^{-1}a^{-1}cd_0)a(b+q^{-1}a^{-1}cd_0)e^{-i\xi}e^{-i\xi}$$
$$= q^{-1-\alpha/2-\beta/2}c^{-1}(b^{-1}+q^{-1}a^{-1}cd_0)ae^{-i\xi}(b+a^{-1}cd_0)e^{-i\xi}$$
$$= q^{-1}\hat{U}_3\hat{U}_1.$$

The rest of relations (2.35) can be proved similarly.

Next, note that relation (2.36) can be rewritten as follows:

$$\hat{U}_1\hat{U}_4(b-b^{-1}) - \hat{U}_4\hat{U}_1(qb-q^{-1}b^{-1}) = -\omega\hat{U}_3\hat{U}_2b. \tag{C2}$$

To prove this quality we transform its lhs and rhs as follows

$$\hat{U}_1\hat{U}_4(b-b^{-1}) - \hat{U}_4\hat{U}_1(qb-q^{-1}b^{-1})$$
$$= a(b+a^{-1}cd_0)e^{-i\xi}a^{-1}e^{i\xi}(b-b^{-1}) - a^{-1}e^{i\xi}a(b+a^{-1}cd_0)e^{-i\xi}(qb-q^{-1}b^{-1})$$
$$= q^{-\alpha/2}(q^{1/2}b+q^{-1/2}a^{-1}cd_0)(b-b^{-1}) - q^{-\alpha/2}(q^{-1/2}b+q^{1/2}a^{-1}cd_0)(qb-q^{-1}b^{-1})$$
$$= -q^{-\alpha/2}\omega(q^{1/2}a^{-1}cd_0b+q^{-1/2});$$

$$\hat{U}_3\hat{U}_2b = c^{-1}(b^{-1}+q^{-1}a^{-1}cd_0)e^{-i\xi}ce^{i\xi}b$$
$$= q^{\beta/2}(q^{-1/2}b^{-1}+q^{1/2}a^{-1}cd_0)b = q^{\beta/2}(q^{-1/2}+q^{1/2}a^{-1}cd_0b).$$

Thus, the equality (C2) is fulfilled if conditions (C1) are valid. The relation (2.37) can be proved in the same way.

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Relations between the Casimir operators of sl(1|2) and osp(2|2) superalgebras

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The superalgebras sl(1|2) and osp(2|2) are isomorphic. Their Casimir operators have been published in the form of a quadratic (K_2) and a cubic (K_3) operator for sl(1|2) and a quadratic (I_2) and a quartic (I_4) operator for osp(2|2). In this note we derive the algebraic relations between both sets of Casimir operators. © *1996 American Institute of Physics.* [S0022-2488(96)02511-X]

I. INTRODUCTION

The special linear superalgebra sl(1|2) and the orthosymplectic superalgebra osp(2|2) are isomorphic.[1] The independent Casimir operators of both superalgebras have been published in the literature in the following form:

(i) a quadratic (K_2) and a cubic (K_3) operator for sl(1|2),[2] and
(ii) a quadratic (I_2) and a quartic (I_4) operator for osp(2|2).[3]

Because of the isomorphy between both superalgebras, there must exist algebraic relations between both sets (I_2, I_4) and (K_2, K_3). The aim of this letter is to exhibit these relations.

In 1977, Scheunert, Nahm, and Rittenberg[4] introduced the concept of grade star representation for superalgebras. Also, they defined two types of representations:

(i) the *typical representations*, such that the even and the odd parts of the representation space have the same dimension, and
(ii) the *atypical representations*, such that the even and the odd parts of the representation space do not have the same dimension.

Only typical representations can be characterized by the eigenvalues of the Casimir operators, since these vanish for the atypical representations.

II. CASIMIR OPERATORS OF sl(1|2) SUPERALGEBRA

Considering the bosonic subalgebra gl(1)⊕sl(2), Scheunert, Nahm, and Rittenberg[2] showed that the irreducible representations of sl(1|2) are characterized by two numbers (b,q), $b \in \mathbb{R}$, $2q \in \mathbb{N}$, and by the parity λ that takes the value 0 or 1. These representations are typical if $|b| \neq q$ and atypical if $|b| = q$. Then, using a *positive definite* scalar product in the representation space, Scheunert *et al.* derived the star and the grade star representations of sl(1|2). They found two classes $\mathscr{S}^{\pm}$ of star representations for $\pm b > q$, and one class of grade star representations for $q = \frac{1}{2}$ and $|b| < \frac{1}{2}$. They concluded that considering grade star representations of sl(1|2) is almost useless.

In a recent article,[5] these results have been extended by consideration of the embedding of osp(1|2) in sl(1|2), and making use of a *nonpositive definite* scalar product which generalizes that defined by Minnaert and Mozrzymas for osp(1|2).[6] For typical representations, there are three classes of grade star representations

$$\mathscr{G}^{\pm}, \quad \text{for} \quad \pm b > q \quad \text{and} \quad \mathscr{G}^{0}, \quad \text{for} \quad |b| < q.$$

The classes $\mathscr{G}^{\pm}$ are equivalent to $\mathscr{S}^{\pm}$ for star representations while $\mathscr{G}^{0}$ generalizes the grade star representation class defined in Ref. 2 for positive definite scalar product.

The two independent Casimir operators K_2 and K_3 of the sl(1|2) superalgebra are built in the following way.[7] Let X_μ be the generators of sl(1|2). One defines metric forms

$$g_{\mu\nu}=\mathrm{Tr}(\gamma X_\mu X_\nu), \quad g_{\mu\nu\rho}=\mathrm{Tr}(\gamma X_\mu X_\nu X_\rho), \tag{1}$$

where γ is a diagonal matrix with eigenvalues $+1$ (resp. -1) in the even (resp. odd) subspace. Then, the Casimir operators are simply defined by

$$K_2=g_{\mu\nu}X^\mu X^\nu, \quad K_3=g_{\mu\nu\rho}X^\mu X^\nu X^\rho, \tag{2}$$

where $X^\mu=g^{\mu\nu}X_\nu$.

Explicitly, with the notations of Ref. 2, the sl(1|2) generators $\{\mathbf{Q}, B, V_\alpha, W_\alpha\}$ $(\alpha=\pm\frac{1}{2})$ satisfy the (anti)commutation relations

$$\begin{aligned}
&[Q_i,Q_j]=i\varepsilon_{ijk}Q_k, \quad [B,V_\alpha]=\tfrac{1}{2}V_\alpha, \quad [B,W_\alpha]=-\tfrac{1}{2}W_\alpha,\\
&[\mathbf{Q},B]=0, \quad [\mathbf{Q},V_\alpha]=\tfrac{1}{2}V_\beta(\boldsymbol{\tau})^\beta{}_\alpha, \quad [\mathbf{Q},W_\alpha]=\tfrac{1}{2}W_\beta(\boldsymbol{\tau})^\beta{}_\alpha,\\
&\{V_\alpha,V_\beta\}=\{W_\alpha,W_\beta\}=0, \quad \{V_\alpha,W_\beta\}=(C\boldsymbol{\tau})_{\alpha\beta}\cdot\mathbf{Q}+C_{\alpha\beta}B,
\end{aligned} \tag{3}$$

where $\boldsymbol{\tau}$ are the usual Pauli matrices and $C=i\tau_2$ is the charge conjugation matrix. Then, the expressions of the Casimir operators K_2 and K_3 of sl(1|2) are

$$K_2=\mathbf{Q}^2-B^2+\tfrac{1}{2}(VCW+WCV), \tag{4}$$

$$K_3=BK_2+\tfrac{1}{4}B(VCW+WCV)+\tfrac{1}{6}(V\mathbf{Q}\cdot\boldsymbol{\tau}\mathbf{C}\mathbf{W}-W\mathbf{Q}\cdot\boldsymbol{\tau}CV)+\tfrac{1}{12}(V\boldsymbol{\tau}CW-W\boldsymbol{\tau}CV)\cdot\mathbf{Q}. \tag{5}$$

Note that, as pointed out by V. Rittenberg,[8] there is a misprint in the original article: the coefficient of the second term in K_3 is indeed $\frac{1}{4}$ instead of $\frac{1}{2}$. This misprint was reproduced in Refs. 1 and 5.

In the grade star (b,q)-representation of sl(1|2), the eigenvalues k_2 and k_3 of the Casimir operators K_2 and K_3 take the values

$$k_2=q^2-b^2 \quad \text{and} \quad k_3=b(q^2-b^2). \tag{6}$$

III. CASIMIR OPERATORS OF osp(2|2) SUPERALGEBRA

The osp(2|2) superalgebra can be described in a compact form by a super-antisymmetric tensor $T=\{T_{ab}\}$ $(a,b=1,2,\pm\frac{1}{2})$, i.e.,

$$T_{ba}=-(-1)^{ab}T_{ab},$$

with the short notations $(-1)^{ab}=(-1)^{\nu(a)\nu(b)}$ and $(-1)^{a+b}=(-1)^{\nu(a)+\nu(b)}$, where the Grassman degree $\nu(a)=0$ for $a=1,2$ and $\nu(a)=1$ for $a=\pm\frac{1}{2}$. The supercommutator of two tensor components is defined as

$$[T_{ab},T_{cd}]_s=T_{ab}T_{cd}-(-1)^{(a+b)(c+d)}T_{cd}T_{ab}.$$

Then, the T tensor components verify the following supercommutation relation that characterizes the osp(2|2) super algebra

$$[T_{ab},T_{cd}]_s=\frac{1}{i}\{g_{bc}T_{ad}-(-1)^{cd}g_{bd}T_{ac}-(-1)^{ab}g_{ac}T_{bd}+(-1)^{ab+cd}g_{ad}T_{bc}\},$$

where the metric tensor g_{ab} is defined as $g_{ab}=(\delta_{ij},-C_{\alpha\beta})$. The contravariant tensor g^{ab}, such that $g_{ab}g^{bc}=g^{cb}g_{ba}=\delta_a^c$, writes $g^{ab}=(\delta_{ij},C_{\alpha\beta})=g_{ba}=(-1)^{ab}g^{ba}$. Because the T tensor is super-antisymmetric, its trace vanishes: $\mathrm{Tr}(T)\equiv g^{ab}T_{ab}=0$. The contracted products are tensors ($n\in N^*$)

$$(T^2)_{ab}=T_{ac}g^{cd}T_{db},\quad (T^n)_{ab}=T_{ac}g^{cd}(T^{n-1})_{db},$$

and their traces are invariant, $[\mathrm{Tr}(T^n),\ T_{ab}]_s=0$.

The osp(2|2) superalgebra possesses two independent Casimir operators. Because of the identity $\mathrm{Tr}(T^3)=i\ \mathrm{Tr}(T^2)$, these Casimir operators can be chosen as

$$I_2=-\tfrac{1}{2}(T^2)\quad\text{and}\quad I_4=\tfrac{1}{2}(T^4). \tag{7}$$

Note that an equivalent description of this superalgebra is given in Ref. 3.

Up to an equivalence, the finite-dimensional irreducible representations of the osp(2|2) superalgebra can be characterized by two integer or half-integer non-negative numbers (p,q) and by a parity λ taking the value 0 or 1. For such representations, the eigenvalues i_2 and i_4 of the Casimir operators I_2 and I_4 are

$$i_2=p^2-4q^2, \tag{8}$$

$$i_4=(p^2-4q^2)(p^2+4q^2+1). \tag{9}$$

IV. RELATIONS BETWEEN CASIMIR OPERATORS

The isomorphism of the two superalgebras sl(1|2) and osp(2|2) can be expressed by the following relations between the eight generators of sl(1|2), cf. Eq. (3), and the components of the tensor T_{ab}:

$$B=\frac{1}{2}T_{12},\quad \mathbf{Q}=\frac{i}{4}(\boldsymbol{\tau}C)^{\alpha\beta}T_{\alpha\beta}, \tag{10}$$

$$V_\alpha=\frac{1}{2i}(T_{1\alpha}+iT_{2\alpha}),\quad W_\alpha=\frac{1}{2i}(T_{1\alpha}-iT_{2\alpha}). \tag{11}$$

Then, it is easy to see that the parameters p and b satisfy the relation $p=2b$ and that both quadratic operators I_2 and K_2 are proportional:

$$I_2=-4K_2, \tag{12}$$

An algebraic relation between the other Casimir operators I_4 and K_3 can be derived by elimination of the parameters $p(p=2b)$ and q between the expressions (6) and (9) of the eigenvalues k_3 and i_4 in a (p,q)-representation. The result is a relation that involves also the eigenvalue k_2 of the quadratic operator

$$k_2i_4+32k_3^2+16k_2^3+4k_2^2=0. \tag{13}$$

General theorems in the theory of algebra representations imply that such relations between eigenvalues can be extended to relations between Casimir operators themselves. Therefore, the Casimir operators must satisfy the following algebraic relation:

$$K_2 I_4 + 32K_3^2 + 16K_2^3 + 4K_2^2 = 0, \tag{14}$$

which is of sixth degree in the generators. Indeed, this relation can be verified directly on the operators, using the definitions (4), (5), and (7) of Casimir operators and the relations (10) and (11) between both sets of generators.

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Wavelet frames and admissibility in higher dimensions

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This paper is concerned with the relations between discrete and continuous wavelet transforms on k-dimensional Euclidean space. We start with the construction of continuous wavelet transforms with the help of square-integrable representations of certain semidirect products, thereby generalizing results of Bernier and Taylor. We then turn to frames of $L^2(\mathbb{R}^k)$ and to the question, when the functions occurring in a given frame are admissible for a given continuous wavelet transform. For certain frames we give a characterization which generalizes a result of Daubechies to higher dimensions. © *1996 American Institute of Physics.*
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I. INTRODUCTION

The usual approach to the construction of multivariate wavelets uses the notions of multiresolution analysis and frames. In this context, a wavelet is a function f in $L^2(\mathbb{R}^k)$, such that certain translates and dilates of f constitute a frame of the space $L^2(\mathbb{R}^k)$ (possibly along with translates and dilates of other functions). A different approach, introduced to wavelet theory by Grossmann, Morlet and Paul,[1] uses the theory of square-integrable representations of nonunimodular groups, as it was developed independently by Duflo and Moore[2] and Carey.[3] Murenzi[4] as well as Bernier and Taylor[5] followed this approach to construct higher-dimensional analogues of the one-dimensional continuous wavelet transform. They considered the semidirect product of $\mathbb{R}^k$ with certain matrix groups (which served as dilations) and constructed natural representations of these groups on $L^2(\mathbb{R}^k)$, which under suitable conditions turned out to be square-integrable. The general theory then supplies a continuous wavelet transform on $L^2(\mathbb{R}^k)$. Now, in the group-theoretical setting, a wavelet is understood to be an admissible element in the sense that the positive-definite function associated to it is square-integrable.

Hence, depending on whether one generalizes the discrete or the continuous wavelet transform to higher dimensions, one arrives at different concepts, and the relations between these concepts are not clear. In the one-dimensional case, it has been shown by Daubechies,[6] that both notions are equivalent. In the higher-dimensional case, while there has been work done concerning discretization of the continuous wavelet transforms associated to square-integrable representations[5,7,8] to our knowledge there has been no attempt to reverse the process, i.e. consider the question of admissibility of the functions constituting a frame. This is mainly due to the greater practical use of frames for implementation, whereas the continuous wavelet transform rather serves as a vehicle for the construction of frames. Moreover, in higher dimensions the number of groups in question increases (and, at the same time, the number of different notions of admissibility), making it hard to decide which is the natural choice. However, such notions as multiresolution analysis should have some interpretation in terms of group representations, and the question of admissibility of the functions spanning the multiresolution analysis suggests itself as a means of judging the relationship between a given continuous and discrete wavelet transform.

In section II we establish some notation and preliminary results. In particular we introduce the class of semidirect products and their quasiregular representations on $L^2(\mathbb{R}^k)$, which we are going to use for the construction of continuous wavelet transforms.

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In sections III and IV we decide which of these quasiregular representations actually yield continuous wavelet transforms, section III being devoted to irreducibility and section IV to square-integrability.

Section V gives an admissibility criterion for the continuous wavelet transform which is analogous to the well-known integral criterion for univariate wavelets.

Section VI gives two short examples.

In section VII we turn to frames and to the question of admissibility of the functions constituting a given frame. For certain frames we give a characterization which generalizes a result from Ref. 6 to higher dimensions.

II. PRELIMINARIES AND NOTATION

As a natural generalization of the one-dimensional affine group and the wavelet-transform associated to it, D. Bernier and K. Taylor suggest the following construction:[5] Given the k-dimensional vector group $\mathbb{R}^k$ and a closed subgroup H of $\mathrm{GL}(k,\mathbb{R})$, let G denote the semidirect product $\mathbb{R}^k \rtimes H$. Then G acts on $\mathbb{R}^k$ by translations (corresponding to the elements of the vector group) and dilations (corresponding to elements of H), which gives rise to a natural unitary representation π of G on $\mathrm{L}^2(\mathbb{R}^k)$, defined as follows: For a given pair $(x,h) \in G$ and $f \in \mathrm{L}^2(\mathbb{R}^k)$, let $\pi(x,h)f$ be the function defined almost everywhere by

$$\pi(x,h)f(y) = |\det(h)|^{-1/2} f(h^{-1}(y-x)).$$

We study this setup with a view to constructing continuous wavelet transforms, which means that we are interested in the case where π is square-integrable or at least has square-integrable subrepresentations. For the group $H := \mathbb{R}^+ \cdot \mathbf{SO}(k)$, Murenzi showed that indeed we obtain a square-integrable representation. The authors of Ref. 5 considered a whole family of groups H which yield square-integrable representations. However their results do not cover Murenzi's group (at least not for $k>2$), which suggested that there was room for generalizations.

Hence, in the first half of our paper, we examine the situation sketched above with focus on the following questions:

(i) When does π have square-integrable subrepresentations?
(ii) Which are the admissible functions? Is there an admissibility criterion similar to that of the one-dimensional affine case?

It will be seen that, if the action of H on the dual space $\widehat{\mathbb{R}^k}$ satisfies a certain regularity condition, these questions can be answered in a quite satisfactory way. On the other hand, if the regularity condition fails, things seem to become all the more difficult.

Let us now fix some notation and collect the basic facts used in this paper. λ denotes the standard Lebesgue measure on $\mathbb{R}^k$ (or $\widehat{\mathbb{R}^k}$). We will denote the left Haar measure on a locally compact group G by μ_G and its modular function by Δ_G. In our case of the semidirect product $G = \mathbb{R}^k \rtimes H$, we have Haar measure

$$d\mu_G(x,h) = |\det(h)|^{-1} d\lambda(x) d\mu_H(h),$$

and the modular function on G is given by

$$\Delta_G(x,h) = \Delta_H(h) |\det(h)|^{-1}.$$

We use $\widehat{\ }$ to denote both Plancherel and Fourier transform, the exact meaning being clear from the context. $\check{\ }$ denotes the inverse Plancherel transform. By a representation we mean a strongly continuous unitary group representation.

It is useful to calculate the action of π on the Plancherel transform side. Proposition 1 from Ref. 5 provides the following formula, for all $(x,h) \in G$ and all $f \in L^2(\mathbb{R}^k)$:

$$(\pi(x,h)f)^\wedge(\gamma) = |\det(h)|^{1/2} e^{2\pi i \gamma x} \hat{f}(\gamma h), \text{ for almost all } \gamma \in \widehat{\mathbb{R}^k}. \tag{1}$$

III. IRREDUCIBLE SUBREPRESENTATIONS OF THE QUASIREGULAR REPRESENTATION

This section is devoted to finding all irreducible subrepresentations of π, which can be done quite systematically: We give a characterization of the invariant subspaces which is transparent enough to identify the irreducible subspaces.

As was already observed in Ref. 5, the key to invariant subspaces lies in the dual action of H on $\widehat{\mathbb{R}^k}$. If one identifies $\widehat{\mathbb{R}^k}$ as row vectors and defines the duality between $\mathbb{R}^k$ and $\widehat{\mathbb{R}^k}$ by $\langle x,\xi\rangle = e^{2\pi i \xi x}$, then the dual action of H is just matrix multiplication on the right. It will be seen that a very promising class of subspaces is contained in the following definition:

Definition 1: Let $U \subset \widehat{\mathbb{R}^k}$ be measurable. We let $\mathscr{H}_U$ be the closed subspace of $L^2(\mathbb{R}^k)$ consisting of all $f \in L^2(\mathbb{R}^k)$, whose Plancherel transforms $\hat{f}$ satisfy $\hat{f}(\xi) = 0$ for almost all ξ outside of U.

The space $\mathscr{H}_U$ is sometimes called the *generalized Hardy space belonging to U*. The following theorem shows that generalized Hardy spaces are suitable candidates for invariant subspaces:

Theorem 2: *Let $U \subset \widehat{\mathbb{R}^k}$ be invariant under the action of H. Then the Hardy space $\mathscr{H}_U$ is G-invariant. On the other hand: For every G-invariant subspace $\mathscr{H}$ there is an H-invariant subset U of $\widehat{\mathbb{R}^k}$ such that $\mathscr{H} = \mathscr{H}_U$.*

Proof: We start by observing that every G-invariant subspace $\mathscr{H}$ is in particular translation-invariant, and by general Fourier theory[9] this entails $\mathscr{H} = \mathscr{H}_U$ for some measurable $U \subset \widehat{\mathbb{R}^k}$. However, since changing U by any set of measure zero does not affect $\mathscr{H}_U$, U cannot be expected to be H-invariant.

The first step towards finding an equivalent invariant set is the observation that, since $\mathscr{H}_U$ is translation-invariant, $\mathscr{H}_U$ is G-invariant if it is H-invariant. By Eq. (1) from above we know that for every $f \in L^2(\mathbb{R}^k)$ and almost every $\gamma \in \widehat{\mathbb{R}^k}$,

$$(\pi(0,h)f)^\wedge(\gamma) = |\det(h)|^{1/2} \hat{f}(\gamma h).$$

As an immediate consequence: If U is H-invariant, then so is $\mathscr{H}_U$ (with respect to a different action of course), which settles the first part of our theorem.

Now suppose that $\mathscr{H}_U$ is H-invariant. We then claim that U is *invariant up to sets of measure zero*, i.e. for all $h \in H$ we have $\lambda(U \triangle Uh) = 0$, where $\triangle$ denotes the symmetric difference.

For the proof, assume the contrary. Then there exist a set $A \subset U$ having positive finite measure and $h \in H$ such that $Ah^{-1} \cap U = \emptyset$. Let $f \in L^2(\mathbb{R}^k)$ be the function having Plancherel transform χ_A. Then, by Eq. (1),

$$(\pi(0,h)f)^\wedge(\xi) = |\det(h)|^{1/2} \chi_A(\xi h) = |\det(h)|^{1/2} \chi_{Ah^{-1}}(\xi),$$

hence, since Ah^{-1} does not have measure zero, $\pi(0,h)f \notin \mathscr{H}_U$.

Since Lebesgue measure on $\widehat{\mathbb{R}^k}$ is quasi-invariant under matrix multiplication (and hence under the action of H), H acts on the Boolean algebra of equivalence classes of measurable sets modulo sets of measure zero. The equivalence class of U is then invariant under the action on the Boolean algebra, and hence the following theorem by Mackey provides a set V which is equivalent to U and H-invariant, hence $\mathscr{H} = \mathscr{H}_U = \mathscr{H}_V$ as desired.

The missing part of our proof is provided by the following theorem, which is Theorem 3 of Ref. 10. The finiteness of the measure required in the theorem is no real obstacle (replace λ by an equivalent finite measure μ).

Theorem 3 (Mackey): *Let S be a standard Borel G-space, where G is separable and locally compact. Let μ be a finite quasi-invariant measure defined on the Borel subsets of S. Let E be a Borel set in S such that the corresponding Boolean-algebra element is invariant under G. Then E differs by a null set from a Borel set which is invariant under G.*

From now on let U be an H-invariant subset of $\widehat{\mathbb{R}^k}$, and let π_U be the restriction of π to $\mathscr{H}_U$. We can now easily classify the irreducible subrepresentations:

Corollary 4: Let $U \subset \mathbb{R}^k$ be measurable and H-invariant. Then π_U is irreducible iff the action of H on U is ergodic.

Proof: By Theorem 2, any decomposition of $\mathscr{H}_U$ into nontrivial invariant subspaces corresponds to a decomposition of U into H-invariant subsets of positive measure and vice versa.

We now take a closer look at the dual action. The first thing to note is that, H being σ-compact, every orbit is measurable. We are particularly interested in the case where the H-orbits in $\widehat{\mathbb{R}^k}$ are *countably separated*; i.e. there exists a countable family $(U_n)_{n\in\mathbb{N}}$ of measurable H-invariant sets separating the orbits. This is the above-mentioned regularity condition. One well-known consequence of this condition is that in this case ergodicity is essentially the same as transitivity (compare Ref. 11, 6.36):

Proposition 5: Let G be a locally compact group acting ergodically on the locally compact space X with regular Borel measure μ. If the orbits of G are countably separated, then there is an orbit $\mathscr{O}$ such that $\mu(X\backslash\mathscr{O})=0$.

The following corollary summarizes the results of our search for irreducible subrepresentations:

Corollary 6: Let H be a closed subgroup of $GL(k,\mathbb{R})$, and let G and π be constructed as above. Then π has an irreducible subrepresentation iff H acts ergodically on a subset $U \subset \widehat{\mathbb{R}^k}$ of positive measure.

If the orbits are countably separated, then π has an irreducible subrepresentation iff there exists an H-orbit of positive measure.

IV. SQUARE-INTEGRABILITY OF π_U

Now suppose we are given an H-invariant subset U of positive measure on which H acts ergodically. Our next aim is to determine when π_U is square-integrable. Recall that this means that for some nontrivial $f,g \in \mathscr{H}_U$, the matrix coefficient

$$V_{f,g}: G \ni (x,h) \mapsto \langle f, \pi(x,h)g \rangle,$$

is a square-integrable function on G. By the results of Duflo and Moore,[2] the square-integrability of $V_{f,g}$ for some nontrivial f implies square-integrability of $V_{f,g}$ for every f. g is then called *admissible* and the mapping

$$\mathrm{L}^2(\mathbb{R}^k) \ni f \mapsto V_{f,g} \in \mathrm{L}^2(G)$$

is a multiple of an isometry, the so-called *continuous wavelet-transform associated to the wavelet g*.

For the remainder of the paper, we restrict our attention to the case of countably separated orbits. This simplifies matters in two ways: On the one hand, as was seen above, we can assume U to be an orbit. In addition, according to the following well-known theorem by Glimm,[12] nice measure-theoretic behavior (i.e., countable separatedness) of the action is related to nice topological behavior. The latter will also be useful in our further discussion.

Theorem 7 (Glimm): *Let G be a locally compact second countable group, acting on a locally compact space X. Then the following are equivalent*:

(i) *The G-orbits are countably separated.*
(ii) *For every $x \in X$ the natural mapping $G/G_x \to Gx$, where $G_x < G$ is the stability subgroup of x, is a homeomorphism.*
(iii) *Every G-orbit is locally closed in X; or, equivalently, is locally compact in the relative topology.*

The following simple observation is a first step towards calculating the L^2-norm of $V_{f,g}$:

Lemma 8: For $\gamma \in U$ let $p_\gamma : H \to U$, $h \mapsto \gamma h$. Then, for any two $\gamma, \delta \in U$ and any positive measurable function g on U we have the following equality:

$$\int_H (g \circ p_\gamma)(h) d\mu_H(h) = \int_H (g \circ p_\delta)(h) d\mu_H(h).$$

Proof: Since U is an orbit, there exists $k \in H$ such that $\gamma = \delta k$. Then we have

$$\begin{aligned}\int_H (g \circ p_\gamma)(h) d\mu_H(h) &= \int_H g(\gamma h) d\mu_H(h) = \int_H g(\delta k h) d\mu_H(h) \\ &= \int_H g(\delta h) d\mu_H(h) = \int_H (g \circ p_\delta)(h) d\mu_H(h).\end{aligned}$$

Now we are able to give a formula for the L^2-norm of $V_{f,g}$:

Lemma 9: Let $f, g \in \mathscr{H}_U$. Then, for any $\gamma_0 \in U$,

$$\|V_{f,g}\|_{L^2(G)} = \|f\|_{L^2(\mathbb{R}^k)} \|\hat{g} \circ p_{\gamma_0}\|_{L^2(H)}.$$

Hence, g is admissible iff $\hat{g} \circ p_{\gamma_0} \in L^2(H)$.

Proof: The following calculation is essentially the same as in Ref. 5. We include it for the sake of completeness:

$$\begin{aligned}\|V_{f,g}\|^2_{L^2(G)} &= \int_G \left| \langle f, \pi(x,h) g \rangle \right|^2 d\mu_G(x,h) = \int_G \left| \langle \hat{f}, (\pi(x,h) g)^\wedge \rangle \right|^2 d\mu_G(x,h) \\ &= \int_G \left| \int_{\widehat{\mathbb{R}^k}} \hat{f}(\gamma) \left| \det(h) \right|^{1/2} e^{-2\pi i \gamma x} \overline{\hat{g}(\gamma h)} d\lambda(\gamma) \right|^2 d\mu_G(x,h) \\ &= \int_H \int_{\mathbb{R}^k} \left| \int_{\widehat{\mathbb{R}^k}} \hat{f}(\gamma) e^{-2\pi i \gamma x} \overline{\hat{g}(\gamma h)} d\lambda(\gamma) \right|^2 d\lambda(x) d\mu_H(h) \\ &= \int_H \int_{\mathbb{R}^k} \left| \mathscr{F}(\phi_h)(x) \right|^2 d\lambda(x) d\mu_H(h), \qquad (2)\end{aligned}$$

where $\phi_h(\gamma) = \hat{f}(\gamma) \overline{\hat{g}(\gamma h)}$, which is in $L^1(\widehat{\mathbb{R}^k})$, and $\mathscr{F}$ denotes the Fourier transform on $L^1(\widehat{\mathbb{R}^k})$. After an application of Plancherel's formula, (2) becomes

$$\int_H \int_{\widehat{\mathbb{R}}^k} |\phi_h(\gamma)|^2 d\lambda(\gamma) d\mu_H(h) = \int_H \int_{\widehat{\mathbb{R}}^k} |\hat{f}(\gamma)|^2 |\hat{g}(\gamma h)|^2 d\lambda(\gamma) d\mu_H(h)$$
$$= \int_{\widehat{\mathbb{R}}^k} |\hat{f}(\gamma)|^2 \left(\int_H \left| \hat{g}(\gamma h) \right|^2 d\mu_H(h) \right) d\lambda(\gamma)$$
$$= \int_{\mathbb{R}^k} |f(x)|^2 d\lambda(x) \int_H |\hat{g}(\gamma_0 h)|^2 d\mu_H(h),$$

the last equation being due to Lemma 8. This proves the statement except for one technicality: By referring to $\hat{g} \circ p_{\gamma_0}$ as an element of $L^2(G)$ we have implicitly assumed that changing $\hat{g}$ on a null set results in changing $\hat{g} \circ p_{\gamma_0}$ on a null set. This assumption holds because by Glimm's theorem we can identify U and H/H_γ, and then Ref. 11, Theorem 2.64 yields that preimages of null sets are again null sets.

Theorem 10: *π_U is square-integrable iff the stabilizers associated to the orbit U are compact.*

Proof: By the previous lemma, $g \in \mathscr{H}_U$ is admissible iff $\hat{g} \circ p_\gamma \in L^2(H)$, for some (and hence every) $\gamma \in U$. Now, if the stabilizer H_γ of some $\gamma \in U$ is compact and $\hat{g}$ is the characteristic function of some compact set with positive measure, then so is $\hat{g} \circ p_\gamma$. In particular g is admissible.

On the other hand, suppose $g \in \mathscr{H}_U$ is admissible and let $\gamma \in U$. $|\hat{g}|^2$ can be approximated from below by simple functions, hence there is a measurable subset $A \subset U$ having positive, finite measure and such that $\chi_A \leqslant c|\hat{g}|^2$, for some positive constant c. Since $\hat{g} \circ p_\gamma$ is square-integrable, $\mu_H(p_\gamma^{-1}(A)) < \infty$. Moreover, by Ref. 11, Theorem 2.64, $\mu_H(p_\gamma^{-1}(A)) > 0$. We have $H_\gamma p_\gamma^{-1}(A) = p_\gamma^{-1}(A)$, hence, by the following lemma, H_γ is compact.

The following can be viewed as a generalization of the well-known fact that a group having finite Haar measure is compact,[13] and indeed its proof consists of a slight modification of the proof to that result. We include it for the sake of completeness.

Lemma 11: Let H be a locally compact group, $H_0 < H$ a closed noncompact subgroup. Then, for any measurable subset A of H satisfying either $AH_0 = A$ or $H_0 A = A$, we have $\mu_H(A) \in \{0, \infty\}$.

Proof: Suppose that $AH_0 = A$, and $\mu_H(A) \neq 0$. By regularity of μ there is a compact subset $C \subset A$ having positive measure. Pick any $x_0 \in H_0$ and recursively

$$x_{n+1} \in H_0 \setminus \left(\left(\bigcup_{i=1}^{n} C^{-1} C x_i \right) \cup \left(\bigcup_{i=1}^{n} x_i C^{-1} C \right) \right).$$

x_{n+1} exists since H_0 is not compact. Then, for $m \neq n$, we have $Cx_n \cap Cx_m = \emptyset$ and $Cx_n^{-1} \cap Cx_m^{-1} = \emptyset$. Now suppose $\mu_H(A)$ is finite. Because of $\cup_n Cx_n \subset CH_0 \subset AH_0 \subset A$ we have

$$\infty > \mu_H(A) \geqslant \sum_{n=1}^{\infty} \mu_H(Cx_n) = \mu_H(C) \sum_{n=1}^{\infty} \Delta_H(x_n)^{-1},$$

implying that $\Delta_H(x_n)^{-1} \to 0$, as n tends to ∞. On the other hand, using the same argument for Cx_n^{-1}, we get

$$\infty > \mu_H(C) \sum_{n=1}^{\infty} \Delta_H(x_n),$$

but the latter tends to infinity. Hence $\mu_H(A) = \infty$.

The proof for the case $H_0 A = A$ uses the same idea, the argument being simplified by left invariance of μ_H.

Remark 12: At this point let us roughly sketch the case where H acts ergodically but not transitively on a set U of positive measure. Then, for every $g \in \mathscr{H}_U$, the map

$$U \ni \gamma \mapsto \int_H |\hat{g}(\gamma h)|^2 d\mu_H(h)$$

is measurable and H-invariant, hence, by ergodicity, it is constant almost everywhere. By the same calculation as in the proof of Lemma 9 we see that g is admissible if the constant is finite. We can apply this criterion to show that for the construction of square-integrable representations discrete groups of dilations are useless:

Let $H < \mathrm{GL}(\mathbb{R},k)$ be a discrete subgroup acting ergodically on some invariant subset U of $\widehat{\mathbb{R}^k}$. (For instance, take $\mathrm{SL}(2,\mathbb{Z})$, which acts ergodically on $\widehat{\mathbb{R}^2}$.[14]) We will show that π_U is not square-integrable. Clearly it suffices to show that for every measurable subset $A \subset U$ having finite positive measure the function $(\chi_A)^\vee$ is not admissible. By the admissibility criterion from above, this amounts to showing that the set $\gamma H \cap A$ is infinite for almost every $\gamma \in U$. To see this, choose a sequence $(A_n)_{n\in\mathbb{N}}$ of pairwise disjoint subsets of A satisfying $\lambda(A_n) > 0$. Then, for any fixed n, the set $B_n := \{\gamma \in U : \gamma H \cap A_n \neq \emptyset\}$ is H-invariant and contains A_n, hence, by ergodicity, it is a conull set. Then the intersection B of all B_n is a conull set, and for every $\gamma \in B$ the set $\gamma H \cap A$ is infinite, the A_n being disjoint.

Arguing as in the proof of Theorem 10, we see that also in the case of H acting ergodically but not transitively on U, the stabilizer of almost every $\gamma \in U$ must be compact. But as the example of $\mathrm{SL}(2,\mathbb{Z})$ shows, the compactness is no longer sufficient: It is easily seen that the stabilizer of $\gamma \in \widehat{\mathbb{R}^2}$ is trivial whenever the coordinates of γ have irrational quotient, i.e. the stabilizer is trivial a.e.

Summarizing the results of our search for square-integrable representations, we could say that the task lies in finding a group H ''having just the right size:'' It should be ''big enough'' to yield orbits of positive measure and ''small enough'' to have compact stabilizers.

V. THE ADMISSIBILITY CONDITION FOR π_U

Our next aim is to find a more concrete admissibility criterion than the one given in the last section. In particular, we would like to be able to replace integration on H by integration on U, as has been done previously.[4,5] It will be seen that, due to the compactness of the stabilizers, this is indeed possible in much the same way as in the paper of Bernier and Taylor.[5] Also, the formal dimension operator associated to π_U as in Ref. 2 can easily be calculated.

Theorem 13: *Fix $\gamma \in U$. Define a function Ψ on U by*

$$\Psi(\gamma h) := \Delta_H(h)|\det(h)|^{-1}.$$

Then Ψ is a well-defined continuous function on U and for every $g \in \mathscr{H}_U$:

$$g \text{ is admissible} \Leftrightarrow \int_U |\hat{g}(\xi)|^2 \Psi(\xi) d\lambda(\xi) < \infty.$$

Proof: For a measurable subset $A \subset U$, let $\tilde{\mu}(A) := \mu_H(p_\gamma^{-1}(A))$. This defines a regular Borel measure $\tilde{\mu}$ on U, as is readily seen using the compactness of the stabilizers. Moreover, $\tilde{\mu}$ is strongly quasi-invariant under the action of H. To be more precise, if the translate $\tilde{\mu}_h$ of $\tilde{\mu}$ is defined by $\tilde{\mu}_h(A) := \tilde{\mu}(Ah^{-1})$, the Radon–Nikodym-derivative is given by

$$\frac{d\tilde{\mu}_h}{d\tilde{\mu}}(\gamma) = \Delta_H(h).$$

On the other hand, the measure λ on U is strongly quasi-invariant with Radon–Nikodym-derivative

$$\frac{d\lambda_h}{d\lambda}(\gamma)=|\det(h)|.$$

Note that, the operation being on the right, in both cases the translation of the measure by h consists of multiplication of the argument by h^{-1}. By Theorem 2.59 from Ref. 11, λ arises from a so-called **rho-function** on H, i.e. there is a function ρ_λ on H such that

$$\int_U f(\xi)d\lambda(\xi)=\int_H f(\gamma h^{-1})\rho_\lambda(h)d\mu_H(h),$$

for every positive measurable function f on U. Here we have once again used the fact that U and H/H_γ are homeomorphic. Analogously, let $\rho_{\tilde{\mu}}$ be the ρ-function belonging to $\tilde{\mu}$. By Theorem 2.56 from Ref. 11, we can calculate the ρ-functions from the Radon–Nikodym-derivatives, obtaining the equations:

$$\rho_{\tilde{\mu}}(h)=\rho_{\tilde{\mu}}(1)\Delta_H(h),$$

$$\rho_\lambda(h)=\rho_\lambda(1)|\det(h)|.$$

The Radon–Nikodym-derivative of $\tilde{\mu}$ with respect to λ can then be calculated as the quotient of the ρ-functions:

$$\frac{d\tilde{\mu}}{d\lambda}(\gamma h)=\frac{\rho_{\tilde{\mu}}(h)}{\rho_\lambda(h)}=c_0\Psi(\gamma h),$$

with $c_0=\rho_{\tilde{\mu}}(1)/\rho_\lambda(1)$. In particular: Ψ is well-defined and continuous, since the ρ-functions are continuous. Finally, we have for $g\in\mathscr{H}_U$

$$\begin{aligned}\int_H|(\hat{g}\circ p_\gamma)(h)|^2d\mu_H(h)&\\ =\int_U|\hat{g}(\xi)|^2d\tilde{\mu}(\xi)&\\ =\int_U|\hat{g}(\xi)|^2\frac{d\tilde{\mu}}{d\lambda}(\xi)d\lambda(\xi)=\int_U|\hat{g}(\xi)|^2c_0\Psi(\xi)d\lambda(\xi),&\end{aligned}$$

which, along with Lemma 9, proves the admissibility criterion.

Remark 14: Just as in the cases considered in Ref. 5, Ψ allows a concrete interpretation of the (usually unbounded) formal dimension operator K associated to π_U as in Ref. 2: If T denotes the densely defined operator on $L^2(U)$ obtained by pointwise multiplication with $(c_0\Psi)^{-1}$ (c_0 as defined in the proof), then $K=\mathscr{P}^{-1}T\mathscr{P}$, where $\mathscr{P}$ is the Plancherel transform.

VI. EXAMPLES

In this section we apply our results to two groups which we will need for further discussion.

Example 15 [Bernier/Taylor]: Let $H<\mathrm{GL}(k,\mathbb{R})$ be the group consisting of diagonal matrices. Then H acts freely on the orbit $U=\{(\xi_1,\xi_2,\ldots,\xi_n):\Pi\xi_i\neq 0\}=(1,1,\ldots,1)H$, whose complement

has measure zero. Hence π is a square-integrable representation on $L^2(\mathbb{R}^k)$. H is unimodular, and for any $\xi \in U$, the group element h mapping (1,1,…,1) to ξ has determinant $\xi_1\xi_2\cdots\xi_n$. Hence the admissibility criterion is given by:

$$g \text{ is admissible} \Leftrightarrow \int_U \frac{|\hat{g}(\xi)|^2}{|\xi_1\xi_2\ldots\xi_n|}\,d\lambda(\xi)<\infty.$$

Example 16 [Murenzi]: Let $H:=\mathbb{R}^+\cdot\mathbf{SO}(k)$. Then $\widehat{\mathbb{R}^k}\backslash\{0\}$ and $\{0\}$ are the only two orbits, hence π is irreducible. Moreover, the stabilizer of (1,0,…,0) is isomorphic to $\mathbf{SO}(k\text{-}1)$, hence compact, whence we conclude that π is square-integrable. Again H is unimodular. For a given $\xi \in \widehat{\mathbb{R}^k}\backslash\{0\}$, an element $h \in H$ mapping (1,0,…,0) to ξ is obtained by rotating (1,0,…,0) to $\xi/|\xi|$ and then multiplying by $|\xi|$. Hence, $|\det(h)|=|\xi|^k$, which leads to the following admissibility criterion:

$$g \text{ is admissible} \Leftrightarrow \int_U \frac{|\hat{g}(\xi)|^2}{|\xi|^k}\,d\lambda(\xi)<\infty.$$

VII. WAVELET FRAMES AND ADMISSIBILITY

We now turn to frames and the question, whether for a given square-integrable representation π_U as constructed above, the functions involved are admissible. In this paper we will only consider frames of a certain kind, as they arise from multiresolution analysis. To be more precise, we study frames obtained in the following way:

Definition 17: Let $\psi_1,\ldots,\psi_N \in \mathscr{H}_U$, $a_0>0$ *be such that* $a_0 \in H$ (*identifying* a_0 *with* $a_0\cdot\mathbf{id}$). *We say that* $(\psi_1,\ldots,\psi_N;a_0;\mathbb{Z}^k)$ **determines a frame of** $\mathscr{H}_U$ *if the set*

$$\{\pi_U(a_0^m n, a_0^m)\psi_i : m\in\mathbb{Z}, n\in\mathbb{Z}^k, \quad 1\leqslant i\leqslant N\}$$

constitutes a frame of $\mathscr{H}_U$.

The condition that the dilation a_0 be in H is natural, since we want to interpret the dilation as an element of the group G. The following example shows that this condition alone does not guarantee that the functions constituting the frame are admissible:

Example 18: Let ϕ be a continuous scaling function of a dyadic multiresolution which is not a wavelet, i.e. not admissible with respect to the affine group. In fact, any scaling function with compact support and nonzero integral would do (for instance one of Daubechies's scaling functions), by 1.1.5 of Ref. 15. Let ψ be any wavelet belonging to ϕ. Then taking the tensor products yields a dyadic multiresolution of $L^2(\mathbb{R}^2)$, which means that $(\psi\otimes\phi,\phi\otimes\psi,\psi\otimes\psi;2;\mathbb{Z}^2)$ determines a frame in $L^2(\mathbb{R}^2)$ (see Ref. 15, 2.2.16). Let $H<\mathrm{GL}(2,\mathbb{R})$ be the two-dimensional diagonal group. Then 2 is an element of H, hence it makes sense to consider the question of admissibility w.r.t. the quasiregular representation. In order to apply the admissibility criterion from Example 15, we calculate

$$\begin{aligned}\int_{\widehat{\mathbb{R}^2}} \frac{|(\psi\otimes\phi)\hat{}(\xi)|^2}{|\xi_1\xi_2|}\,d\lambda(\xi_1,\xi_2) &= \int_{\widehat{\mathbb{R}^2}} \frac{|\hat{\psi}(\xi_1)\hat{\phi}(\xi_2)|^2}{|\xi_1\xi_2|}\,d\lambda(\xi_1,\xi_2)\\ &= \int_{\hat{\mathbb{R}}} \frac{|\hat{\psi}(\xi)|^2}{|\xi|}\,d\lambda(\xi)\int_{\hat{\mathbb{R}}} \frac{|\hat{\phi}(\xi)|^2}{|\xi|}\,d\lambda(\xi).\end{aligned}$$

Since ϕ is not admissible, the latter integral diverges, hence $\psi\otimes\phi$, as well as $\phi\otimes\psi$, is not admissible.

From now on let H_0 denote the subgroup of H generated by a_0. Since a_0 is in the center of H, H_0 is a normal subgroup. We normalize the Haar measure μ_{H/H_0} such that Weil's formula holds (see Ref. 11, 2.65), i.e. for all positive measurable f we have

$$\int_H f(x)d\mu_H(x)=\int_{H/H_0}\sum_{n\in\mathbb{Z}} f(xa_0^m)d\mu_{H/H_0}(xH_0).$$

The remainder of this paper will be devoted to proving the next theorem, which links the L^2-norms of certain matrix coefficients with the measure μ_{H/H_0} and thus leads to a compactness condition on H/H_0. It is the analogue of Daubechies's result for univariate wavelets,[6] and the proof is modelled after the proof of that statement.

Theorem 19: *Suppose that* $(\psi_1,\ldots,\psi_N;a_0;\mathbb{Z}^k)$ *determines a frame of* $\mathscr{H}_U$, *with* $a_0\in H$. *Then all* ψ_i *are admissible iff* μ_{H/H_0} *is finite,* i.e. *iff* H/H_0 *is compact.*

To be more precise: If $\phi\in\mathscr{H}_U$ *is normed and admissible, and* $0<A<B<\infty$ *are lower and upper frame bounds (respectively), the following inequalities hold:*

$$A\mu_{H/H_0}(H/H_0)\leqslant\sum_{i=1}^{n}\|V_{\phi,\psi_i}\|^2_{L^2(G)}\leqslant B\mu_{H/H_0}(H/H_0).$$

Remark 20: Since a_0 is in the kernel of Δ_H, the compactness criterion of Theorem 19 implies that H is unimodular.

Remark 21: Applying Theorem 19 to the tensor wavelets of example 18 and Murenzi's group $H:=\mathbb{R}^+\cdot\mathbf{SO}(k)$, we see that since H/H_0 is compact, the tensor wavelets are admissible w.r.t. the quasiregular representation of $\mathbb{R}^k\rtimes H$. (Here H_0 denotes the subgroup generated by 2.) In fact any frame arising from a dyadic multiresolution analysis consists of admissible vectors.

On the other hand, since the quotient of the diagonal group by H_0 is noncompact, we see that every wavelet frame obtained from a dyadic multiresolution contains at least one function which is not admissible w.r.t. the quasiregular representation associated to the diagonal group.

The proof of the theorem uses a family of auxiliary functions t_λ on G. We start by constructing suitable functions on $\mathbb{R}^k$.

Lemma 22: Let $f\in C_c^\infty(\mathbb{R})$, *and let* $f_k:\mathbb{R}^k\to\mathbb{R}$ *be the k-fold tensor product of f. Suppose that f is positive and has* L^1*-norm* 1. *Then, for every* $m\in\mathbb{N}_0$, *there exists a constant* $c_{m,k}$ *such that for every positive real number a and every* $y\in\mathbb{R}^k$, *we have*

$$\left|a^{-k}-\sum_{n\in\mathbb{Z}^k} f_k(y+an)\right|\leqslant a^m c_{m,k}.$$

Proof: We will only need the $c_{0,k}$ later on, but the stronger result has an easier inductive proof. We start with $k=1$. We can treat the cases $a\geqslant 1$ and $a<1$ separately and note that the statement is obvious for $a\geqslant 1$. For a given $0<a<1$ and $y\in\mathbb{R}$ pick $N\in\mathbb{N}$ such that $\mathrm{supp}(f)\subset[y-aN,y+aN]$. In particular, for $l\in\mathbb{N}$, we have $f^{(2l+2)}(y\pm aN)=0$, hence, by Euler–MacLaurin's formula:[16]

$$\sum_{n=-\infty}^{\infty} f(y+an)=\sum_{n=-N}^{N} f(y+an)=a^{-1}\int_{y-aN}^{y+aN} f(t)d\lambda(t)+a^{2l+1}\frac{B_{2l+2}}{(2l+2)!}f^{(2l+2)}(x)$$

$$=a^{-1}+a^{2l+1}\frac{B_{2l+2}}{(2l+2)!}f^{(2l+2)}(x),$$

for some $x\in\mathrm{supp}(f)$, with B_n being the nth Bernoulli number. Hence,

$$\left| a^{-1} - \sum_{n=-\infty}^{\infty} f(y+an) \right| \leq a^{2l+1} \frac{|B_{2l+2}|}{(2l+2)!} \sup_{x \in \mathrm{supp}(f)} |f^{(2l+2)}(x)|,$$

which proves the statement for all odd m. Since $a<1$, the statement for the even m follows immediately.

Now suppose the $c_{m,k}$ are given for $k \geq 1$ and all $m \in \mathbb{N}_0$. Again we can restrict our attention to the case $a<1$. Letting $\tilde{y}=(y_2,\ldots,y_{k+1}) \in \mathbb{R}^k$, we calculate:

$$\begin{aligned}
\left| a^{-k-1} - \sum_{n \in \mathbb{Z}^{k+1}} f_{k+1}(an+y) \right| &= \left| a^{-1}a^{-k} - \left(\sum_{n \in \mathbb{Z}} f(an+y_1) \right) \left(\sum_{l \in \mathbb{Z}^k} f_k(al+\tilde{y}) \right) \right| \\
&\leq \left| a^{-1} - \sum_{n \in \mathbb{Z}} f(an+y_1) \right| a^{-k} \\
&\quad + \left| a^{-k} - \sum_{l \in \mathbb{Z}^k} f_k(al+\tilde{y}) \right| \left| \sum_{n \in \mathbb{Z}} f(an+y_1) \right|.
\end{aligned}$$

Applying the induction hypothesis, we see that the first term is less or equal to $a^m c_{m+k,1}$ and the second term is less or equal to $a^{m+1} c_{m+1,k}(a^{-1}+c_{0,1})$. Hence, since $a<1$, the sum can be estimated by $a^m(c_{m+1,k}+c_{0,1}+c_{m+k,1})$.

From now on fix f and f_k as in Lemma 22. Let $C \subset H$ be a measurable fundamental domain for the subgroup H_0, i.e. $CH_0=H$ and $C \cap a_0^m C = \emptyset$, for all $0 \neq m \in \mathbb{Z}$.[17] Define, for $\lambda>0$, a function t_λ on G by

$$t_\lambda(x,h) := \chi_C(h) f_k(\lambda \Delta_G(x,h)^{1/k} x).$$

The next two lemmas collect the properties of t_λ needed for the proof.

Lemma 23: t_λ is a positive measurable function with

$$\int_G t_\lambda(x,h)\, d\mu_G(x,h) = \lambda^{-k} \mu_H(C).$$

Proof: Straightforward computation, observing that $\mu_H(C) = \mu_H(C^{-1})$ by Weil's formula, both C and C^{-1} being fundamental domains.

Lemma 24: For every $(x,h) \in G$, we have

$$\left| \lambda^{-k} \Delta_G(x,h)^{-1} - \sum_{m \in \mathbb{Z}} \sum_{n \in \mathbb{Z}^k} t_\lambda((a_0^m n, a_0^m) \cdot (x,h)) \right| \leq c_{0,k}.$$

Proof: The proof consists of rather straightforward calculations:

$$\begin{aligned}
\sum_{m \in \mathbb{Z}} \sum_{n \in \mathbb{Z}^k} t_\lambda((a_0^m n, a_0^m) \cdot (x,h)) &= \sum_{m \in \mathbb{Z}} \sum_{n \in \mathbb{Z}^k} t_\lambda((a_0^m(n+x), a_0^m h)) \\
&= \sum_{m \in \mathbb{Z}} \sum_{n \in \mathbb{Z}^k} \chi_C(a_0^m h) f_k(\lambda \Delta_G(a_0^m(n+x), a_0^m h)^{1/k} a_0^m(n+x)) \\
&= \sum_{m \in \mathbb{Z}} \sum_{n \in \mathbb{Z}^k} \chi_C(a_0^m h) f_k(\lambda \Delta_H(a_0^m h)^{1/k} |\det(a_0^m h)|^{-1/k} a_0^m(n+x))
\end{aligned}$$

$$= \sum_{m\in\mathbb{Z}} \sum_{n\in\mathbb{Z}^k} \chi_C(a_0^m h) f_k(\lambda \Delta_H(h)^{1/k} |\det(h)|^{-1/k}(n+x))$$
$$= \left(\sum_{m\in\mathbb{Z}} \chi_C(a_0^m h) \right) \left(\sum_{n\in\mathbb{Z}^k} f_k(\lambda \Delta_H(h)^{1/k} |\det(h)|^{-1/k}(n+x)) \right)$$
$$= \left(\sum_{m\in\mathbb{Z}} \chi_C(a_0^m h) \right) \left(\sum_{n\in\mathbb{Z}^k} f_k(\lambda \Delta_G(x,h)^{1/k}(n+x)) \right).$$

By choice of C, the first factor equals one, and using Lemma 22, we can estimate the second factor by

$$\left| \sum_{n\in\mathbb{Z}^k} f_k(\lambda \Delta_G(x,h)^{1/k}(n+x)) - \lambda^{-k} \Delta_G(x,h)^{-1} \right| \leq c_{0,k}.$$

Proof of Theorem 19: We only prove the inequalities, starting with the second one. Let A,B be the frame bounds and let ϕ be a normed admissible vector. By Weil's formula, we have $\mu_H(C) = \mu_{H/H_0}(H/H_0)$, hence, by Lemma 23,

$$\lambda^{-k} B \mu_{H/H_0}(H/H_0) = \int_G B t_\lambda(x,h) d\mu_G(x,h) = \int_G t_\lambda(x,h) B \| \pi_U(x,h)\phi \|^2 d\mu_G(x,h).$$

Since B is an upper bound of the frame, we can estimate the last integral by

$$\int_G t_\lambda(x,h) B \| \pi_U(x,h)\phi \|^2 d\mu_G(x,h) \geq \int_G t_\lambda(x,h) \sum_{i,m,n} |\langle \pi_U(x,h)\phi, \pi_U(a_0^m n, a_0^m)\psi_i \rangle|^2 d\mu_G(x,h)$$
$$= \sum_{i,m,n} \int_G t_\lambda(x,h) |\langle \pi_U((a_0^m n, a_0^m)^{-1} \cdot (x,h))\phi, \psi_i \rangle|^2 d\mu_G(x,h)$$
$$= \sum_{i,m,n} \int_G t_\lambda((a_0^m n, a_0^m)\cdot(x,h)) |\langle \pi_U(x,h)\phi, \psi_i \rangle|^2 d\mu_G(x,h)$$
$$= \sum_i \int_G \sum_{m,n} t_\lambda((a_0^m n, a_0^m)\cdot(x,h)) \times |\langle \pi_U(x,h)\phi, \psi_i \rangle|^2 d\mu_G(x,h).$$

Note that all functions involved are positive, hence Fubini's Theorem is applicable. Now we can apply Lemma 24:

$$\sum_i \int_G \sum_{m,n} t_\lambda((a_0^m n, a_0^m)\cdot(x,h)) |\langle \pi_U(x,h)\phi, \psi_i \rangle|^2 d\mu_G(x,h)$$
$$\geq \sum_i \int_G (\lambda^{-k} \Delta_G(x,h)^{-1} - c_{0,k}) |\langle \pi_U(x,h)\phi, \psi_i \rangle|^2 d\mu_G(x,h)$$

$$= \sum_i \left(-c_{0,k} \left\| V_{\psi_i,\phi} \right\|^2_{\mathrm{L}^2(G)} + \lambda^{-k} \int_G \Delta_G(x,h)^{-1} |\langle \pi_U(x,h)\phi, \psi_i \rangle|^2 d\mu_G(x,h) \right)$$

$$= \sum_i \left(-c_{0,k} \left\| V_{\psi_i,\phi} \right\|^2_{\mathrm{L}^2(G)} + \lambda^{-k} \int_G |\langle \pi_U((x,h)^{-1})\phi, \psi_i \rangle|^2 d\mu_G(x,h) \right)$$

$$= \sum_i \left(-c_{0,k} \| V_{\psi_i,\phi} \|^2_{\mathrm{L}^2(G)} + \lambda^{-k} \| V_{\phi,\psi_i} \|^2_{\mathrm{L}^2(G)} \right).$$

We have thus derived the inequality

$$B\mu_{H/H_0}(H/H_0) \geqslant \sum_i \| V_{\phi,\psi_i} \|^2_{\mathrm{L}^2(G)} - \lambda^k c_{0,k} \sum_i \| V_{\psi_i,\phi} \|^2_{\mathrm{L}^2(G)}.$$

Since ϕ is admissible, $\Sigma_i \| V_{\psi_i,\phi} \|^2_{\mathrm{L}^2(G)}$ is finite. Hence, letting λ tend to zero, we obtain the desired inequality.

The first inequality is obtained in quite the same fashion: Using the lower inequality of the frame property, we arrive at

$$A\mu_{H/H_0}(H/H_0) \leqslant \sum_i \| V_{\phi,\psi_i} \|^2_{\mathrm{L}^2(G)} + \lambda^k c_{0,k} \sum_i \| V_{\psi_i,\phi} \|^2_{\mathrm{L}^2(G)},$$

and letting λ tend to zero gives the desired result.

VIII. CONCLUDING REMARKS

The usual procedure to construct discrete wavelet transforms from square-integrable representations[5,7,8] consists of finding a certain discrete subset of the underlying group and certain admissible functions $\psi_1, \ldots, \psi_n$. The discrete wavelet transform of an element f is then obtained by sampling the continuous wavelet transforms V_{f,ψ_i} on the discrete subset. The difficulty lies in choosing the sampling set and the admissible functions such that, by letting the subset of the group act on the admissible functions, we obtain a frame. Theorem 19 considers this situation in reverse perspective: Here a sampling set

$$\{(a_0^m n, a_0^m) : m \in \mathbb{Z}, n \in \mathbb{Z}^k, 1 \leqslant i \leqslant N\}$$

and a set of functions $\psi_1, \ldots, \psi_n$ yielding a frame (under the action of the sampling set) are given, and the question of admissibility is decided by looking at the relationship between the sampling set and the whole group. It would be desirable to find ways to incorporate both approaches into one result relating sampling sets, frames and admissibility.

A more concrete generalization of Theorem 19 would consist of considering other lattices than $\mathbb{Z}^k$ and (finite sets of) nonscalar dilations a_0. While taking a different lattice causes no serious problems, the use of a nonscalar dilation has graver consequences: In the first place, the choice of the auxiliary functions t_λ requires more care. Moreover, since a_0 need not be central any more, $H/\langle a_0 \rangle$ might not even carry an invariant measure, hence we cannot expect to obtain a compactness (or at least finite measure) condition on $H/\langle a_0 \rangle$.

While this paper is concerned only with wavelet transforms arising from representations which are square-integrable in the strict sense, there are generalizations which yield similar transforms for a wider class of representations.[18,19] The notion used here is that of square-integrability on homogeneous spaces. It may be expected that this approach allows the construction of wavelet transforms under somewhat weaker requirements than the compactness condition of Theorem 10.

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An algebra arising from 2-state chiral Potts model and Sklyanin algebra

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We construct a $\mathbb{C}$-algebra $\mathscr{C}$ associated with an R-matrix of the 2-state chiral Potts model. This algebra will be shown to coincide with the Sklyanin algebra at an 8-torsion point and, in the self-dual case, with $U_q(sl_2)$ at the fourth root of unity.
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I. INTRODUCTION

In this paper we will construct an algebra associated with an R-matrix of the 2-state chiral Potts model by so-called RLL formalism (Theorem 1), and reveal that our algebra $\mathscr{C}$ coincides with the Sklyanin algebra $\mathscr{A}_\eta$ (Ref. 1) when η is an 8-torsion point on an elliptic curve. Moreover, we will show that the quantum group $U_q(sl_2)$ when $q^4=1$ is derived from our algebra in the self-dual case.

Our R-matrix here is defined according to the discussion of Gaudin.[2] It is described by the quadratic formula of the Boltzmann weights of the 2-state chiral Potts model so that it is different from those in Refs. 3 or 4.

Let us recall the definition of the Sklyanin algebra $\mathscr{A}_\eta$: Let σ_α ($\alpha=0,...,3$) be the Pauli matrices. In Ref. 1, Sklyanin defined the well-known Sklyanin algebra $\mathscr{A}_\eta$ as a $\mathbb{C}$-algebra generated by $\{S_0,S_1,S_2,S_3\}$ with the fundamental relation

$$R(u-v)L_1(u)L_2(v)=L_2(v)L_1(u)R(u-v) \quad (u,v\in\mathbb{C}). \tag{1}$$

Here $R(u)$ is Baxter's elliptic R-matrix which has the form

$$R(u)=\sigma_0\otimes\sigma_0+\sum_{\alpha=1}^{3} w_\alpha(u)\sigma_\alpha\otimes\sigma_\alpha \tag{2}$$

and the L-operator $L(u)$ is defined by

$$L(u)=\sigma_0 S_0+\sum_{\alpha=1}^{3} w_\alpha(u)\sigma_\alpha S_\alpha\in \mathrm{End}(\mathbb{C}^2)\otimes\mathscr{A}_\eta, \tag{3}$$

where the coefficients $w_\alpha(u)$ are expressed by the elliptic theta functions (cf. Ref. 5). Then it is seen that (1) is equivalent to the following commutation relations:

$$[S_0,S_\alpha]_-=\sqrt{-1}J_{\beta\gamma}[S_\beta,S_\gamma]_+, \quad [S_\alpha,S_\beta]_-=\sqrt{-1}[S_0,S_\gamma]_+. \tag{4}$$

Here (α,β,γ) are cyclic permutations of (1,2,3), and $J_{\alpha\beta}$ are the structure constants described by

$$\begin{aligned} J_{12}&=k'^2\,\frac{\mathrm{sn}^2}{\mathrm{cn}^2\mathrm{dn}^2}(\eta,k),\\ J_{23}&=k^2\,\frac{\mathrm{sn}^2\mathrm{cn}^2}{\mathrm{dn}^2}(\eta,k), \quad J_{31}=-\frac{\mathrm{sn}^2\mathrm{dn}^2}{\mathrm{cn}^2}(\eta,k). \end{aligned} \tag{5}$$

Letting $\eta=K/2$ (i.e., η is an 8-torsion point), we will show that $\mathscr{A}_{K/2}$ coincides with our quantum algebra $\mathscr{C}$. Furthermore, we will show that our algebra $\mathscr{C}$ in the self-dual case gives $U_q(sl_2)$ at the fourth root of unity.

This paper is organized as follows: In Sec. II we summarize the results of Au-Yang and Perk,[6] and introduce an R-matrix by combining two Boltzmann weights of the N-state chiral Potts model (cf. Ref. 2). In Sec. III we construct a quantum algebra $\mathscr{C}$ which comes from the 2-state chiral Potts model (Theorem 1), and give the proof by using the addition theorems for the theta functions. Further, the link between the Sklyanin algebra and our algebra $\mathscr{C}$ will be clarified. In Sec. IV we give another proof of Theorem 1 by using the star-triangle relation that holds among the Boltzmann weights. Moreover, our quantum algebra $\mathscr{C}$ in the self-dual case will be shown to coincide with $U_q(sl_2)$ when $q=\sqrt{-1}$. Finally, in Sec. V we mention the significance of extending our result to the N-state, i.e., the higher-genus case.

II. *N*-STATE CHIRAL POTTS MODEL

In Ref. 6, Au-Yang and Perk introduced the Boltzmann weights $W_{pq}(n)$ and $\overline{W}_{pq}(n)$ of the N-state chiral Potts model through

$$\begin{aligned}\frac{W_{pq}(n)}{W_{pq}(0)}&=\prod_{j=1}^{n}\left(\frac{d_pb_q-a_pc_q\omega^j}{b_pd_q-c_pa_q\omega^j}\right),\\ \frac{\overline{W}_{pq}(n)}{\overline{W}_{pq}(0)}&=\prod_{j=1}^{n}\left(\frac{\omega a_pd_q-d_pa_q\omega^j}{c_pb_q-b_pc_q\omega^j}\right),\end{aligned}\tag{6}$$

where $\omega:=e^{2\pi\sqrt{-1}/N}$. The parameters (a_p,b_p,c_p,d_p) and (a_q,b_q,c_q,d_q) denote points on an algebraic curve

$$a^N+k'b^N=kd^N,\quad k'a^N+b^N=kc^N,\quad (k^2+k'^2=1),\tag{7}$$

which has the genus $g=N^2(N-2)+1$. Then these Boltzmann weights satisfy the periodic condition

$$W_{pq}(n+N)=W_{pq}(n),\quad \overline{W}_{pq}(n+N)=\overline{W}_{pq}(n)$$

and the star–triangle relation (STR)

$$\sum_{l=1}^{N}\overline{W}_{qr}(j-l)W_{pr}(i-l)\overline{W}_{pq}(l-k)=R_{pqr}W_{pq}(i-j)\overline{W}_{pr}(j-k)W_{qr}(i-k).\tag{8}$$

Here the states i, j, and k belong to $\mathbb{Z}_N$, and R_{pqr} is a constant that is independent of these states. Furthermore, the constant R_{pqr} has the following form (Matveev and Smirnov[7]):

$$\begin{aligned}R^N_{pqr}&=\frac{f^N_{pq}f^N_{qr}}{f^N_{pr}},\\ f_{pq}&:=\left[\prod_{m=1}^{N}\left(\sum_{k=1}^{N}\omega^{mk}\overline{W}_{pq}(k)\right)\Big/\prod_{m=1}^{N}W_{pq}(m)\right]^{1/N}.\end{aligned}\tag{9}$$

Next we introduce an R-matrix associated with the N-state chiral Potts model: Following the discussion of Gaudin in the self-dual case,[2] we put a matrix $R(p,q)\in\mathrm{End}(V^{\otimes 2})$ $(V:=\mathbb{C}^N)$ by

$$R(p,q):=\sum_{i,j,k,l\in\mathbb{Z}_N} R_{ij}^{kl}(p,q)E_{ik}\otimes E_{jl},$$
$$R_{ij}^{kl}(p,q):=\overline{W}_{pq}(j-k)W_{pq}(i+j)\delta_{i+j,k+l}. \tag{10}$$

It is easily proved that $R(p,q)$ satisfies the Yang–Baxter equation (YBE)

$$R_{12}(p,q)R_{13}(p,r)R_{23}(q,r)=R_{23}(q,r)R_{13}(p,r)R_{12}(p,q) \quad \text{on} \quad V^{\otimes 3}. \tag{11}$$

Now we rewrite (10) in a more convenient form. Introducing X and $Y\in\mathrm{End}(V)$ through

$$X:=\begin{pmatrix} 1 & & & \\ & \omega & & \\ & & \ddots & \\ & & & \omega^{N-1} \end{pmatrix}, \quad Y:=\begin{pmatrix} 0 & 1 & & \\ & \ddots & \ddots & \\ & & 0 & 1 \\ 1 & & & 0 \end{pmatrix},$$

we see that

$$R(p,q)=\frac{1}{N}\sum_{\alpha,\alpha',\beta,\beta'\in\mathbb{Z}_N}\{\omega^{(\alpha+\beta)(\alpha'-\beta')}\hat{W}_{pq}(\beta)\overline{W}_{pq}(\beta')(X^{-\alpha-2\beta}Y^{-\alpha'}\otimes X^{\alpha}Y^{\alpha'})\}, \tag{12}$$

where $\hat{W}_{pq}$ is the Fourier transform

$$\hat{W}_{pq}(m)=\frac{1}{N}\sum_{k\in\mathbb{Z}_N}\omega^{mk}W_{pq}(k).$$

III. QUANTUM ALGEBRA ARISING FROM 2-STATE CHIRAL POTTS MODEL

In analogy with the construction of the Sklyanin algebra,[1] let us define the L-operator $L(p,q)$ for our R-matrix (12) by

$$L(p,q):=\frac{1}{N}\sum_{\alpha,\alpha',\beta,\beta'\in\mathbb{Z}_N}\{\omega^{(\alpha+\beta)(\alpha'-\beta')}\hat{W}_{pq}(\beta)\overline{W}_{pq}(\beta')X^{-\alpha-2\beta}Y^{-\alpha'}S_{\alpha\alpha'}\}, \tag{13}$$

where $\{S_{\alpha\alpha'}\}_{0\leqslant\alpha,\alpha'\leqslant N-1}$ are temporarily unknown quantities. Then we impose on the L-operator (13) a relation

$$R(p,q)L_1(p,r)L_2(q,r)=L_2(q,r)L_1(p,r)R(p,q) \quad \text{for all } p,q, \text{ and } r, \tag{14}$$

where $L_1=L\otimes I$ and $L_2=I\otimes L$.

We will consider only the 2-state case in the following. In this case the genus of the curve (7) is equal to 1, namely, the curve is elliptic. The parameters (a_p,b_p,c_p,d_p) can be expressed by Jacobi's theta functions[6]

$$(a_p,b_p,c_p,d_p)=(-H(p),H_1(p),\Theta_1(p),\Theta(p)). \tag{15}$$

We obtain the following theorem.

Theorem 1: *In the case of $N=2$, (14) is equivalent to the following commutation relations for the variables $\{S_{00},S_{01},S_{10},S_{11}\}$:*

$$
\begin{aligned}
&[S_{00},S_{01}]_-=[S_{10},S_{11}]_+, && [S_{00},S_{01}]_+=[S_{10},S_{11}]_-,\\
&[S_{00},S_{10}]_-=-[S_{01},S_{11}]_+, && [S_{00},S_{10}]_+=-[S_{01},S_{11}]_-,\\
&[S_{00},S_{11}]_-=\frac{1-k'}{1+k'}[S_{01},S_{10}]_+, && [S_{00},S_{11}]_+=-[S_{01},S_{10}]_-.
\end{aligned}
\tag{16}
$$

Proof: Here we will derive the third formula in (16) below. In the 2-state case (12) and (13) have the following forms:

$$
R(p,q)=\begin{pmatrix}
\overline{W}_{pq}(0)W_{pq}(0) & & & \overline{W}_{pq}(1)W_{pq}(0)\\
& \overline{W}_{pq}(1)W_{pq}(1) & \overline{W}_{pq}(0)W_{pq}(1) & \\
& \overline{W}_{pq}(0)W_{pq}(1) & \overline{W}_{pq}(1)W_{pq}(1) & \\
\overline{W}_{pq}(1)W_{pq}(0) & & & \overline{W}_{pq}(0)W_{pq}(0)
\end{pmatrix}, \tag{17}
$$

$$
L(p,q)=\frac{1}{2}\begin{pmatrix}
\overline{W}_{\underline{pq}}(0)W_{pq}(0)(S_{00}+S_{10}) & \overline{W}_{\underline{pq}}(0)W_{pq}(1)(S_{01}-S_{11})\\
+W_{pq}(1)W_{pq}(1)(S_{00}-S_{10}) & +W_{pq}(1)W_{pq}(0)(S_{01}+S_{11})\\
\overline{W}_{\underline{pq}}(0)W_{pq}(1)(S_{01}+S_{11}) & \overline{W}_{\underline{pq}}(0)W_{pq}(0)(S_{00}-S_{10})\\
+W_{pq}(1)W_{pq}(0)(S_{01}-S_{11}) & +W_{pq}(1)W_{pq}(1)(S_{00}+S_{10})
\end{pmatrix}. \tag{18}
$$

Here the Boltzmann weights are expressed by

$$
\frac{W_{pq}(1)}{W_{pq}(0)}=\frac{d_pb_q+a_pc_q}{b_pd_q+c_pa_q},\quad \frac{\overline{W}_{pq}(1)}{\overline{W}_{pq}(0)}=\frac{-a_pd_q+d_pa_q}{c_pb_q+b_pc_q}, \tag{19}
$$

where

$$
a^2+k'b^2=kd^2,\quad k'a^2+b^2=kc^2,\quad (k^2+k'^2=1). \tag{20}
$$

Substituting (17) and (18) in (14), we see that there exists the following relation between $[S_{00},S_{11}]_-$ and $[S_{01},S_{10}]_+$:

$$
A_{pqr}[S_{00},S_{11}]_-+B_{pqr}[S_{01},S_{10}]_+=0, \tag{21}
$$

where

$$
\begin{aligned}
A_{pqr}:=&(-\overline{W}_{pq}(0)W_{pq}(1)+\overline{W}_{pq}(1)W_{pq}(0))\\
&\times(\overline{W}_{pr}(0)W_{pr}(0)+\overline{W}_{pr}(1)W_{pr}(1))(-\overline{W}_{qr}(0)W_{qr}(1)+\overline{W}_{qr}(1)W_{qr}(0))\\
&+(\overline{W}_{pq}(0)W_{pq}(0)+\overline{W}_{pq}(1)W_{pq}(1))\\
&\times(-\overline{W}_{pr}(0)W_{pr}(1)+\overline{W}_{pr}(1)W_{pr}(0))(\overline{W}_{qr}(0)W_{qr}(0)+\overline{W}_{qr}(1)W_{qr}(1)),\\
B_{pqr}:=&(\overline{W}_{pq}(0)W_{pq}(1)+\overline{W}_{pq}(1)W_{pq}(0))\\
&\times(\overline{W}_{pr}(0)W_{pr}(0)-\overline{W}_{pr}(1)W_{pr}(1))(\overline{W}_{qr}(0)W_{qr}(1)+\overline{W}_{qr}(1)W_{qr}(0))\\
&-(\overline{W}_{pq}(0)W_{pq}(0)-\overline{W}_{pq}(1)W_{pq}(1))\\
&\times(\overline{W}_{pr}(0)W_{pr}(1)+\overline{W}_{pr}(1)W_{pr}(0))(\overline{W}_{qr}(0)W_{qr}(0)-\overline{W}_{qr}(1)W_{qr}(1)).
\end{aligned}
\tag{22}
$$

Using the parametrizations (15) and the identity

$$
\Theta(u)H(v)+H(u)\Theta(v)=\frac{2H\left(\frac{u+v}{2}\right)\Theta\left(\frac{u+v}{2}\right)H_1\left(\frac{u-v}{2}\right)\Theta_1\left(\frac{u-v}{2}\right)}{H_1(0)\Theta_1(0)}
$$

in Ref. 8, we obtain the following lemma.

Lemma 1: We can rewrite (19) in the form

$$\frac{W_{pq}(1)}{W_{pq}(0)}=-\frac{H\left(\frac{p-q}{2}-\frac{K}{2}\right)\Theta\left(\frac{p-q}{2}-\frac{K}{2}\right)}{H_1\left(\frac{p-q}{2}-\frac{K}{2}\right)\Theta_1\left(\frac{p-q}{2}-\frac{K}{2}\right)},$$
$$\frac{\overline{W}_{pq}(1)}{\overline{W}_{pq}(0)}=\frac{H\left(\frac{p-q}{2}\right)\Theta\left(\frac{p-q}{2}\right)}{H_1\left(\frac{p-q}{2}\right)\Theta_1\left(\frac{p-q}{2}\right)}, \tag{23}$$

where K is the complete elliptic integral of the first kind.

Substituting (23) in (22) and using the identity

$$H(u)\Theta(u)H_1(v)\Theta_1(v)-H(v)\Theta(v)H_1(u)\Theta_1(u)=H(u-v)\Theta(u+v)H_1(0)\Theta_1(0)$$

in Ref. 8, we have

$$\frac{B_{pqr}}{A_{pqr}}=\left\{\frac{H\left(\frac{K}{2}\right)}{\Theta\left(\frac{K}{2}\right)}\right\}^4\frac{S(u,v)}{T(u,v)}. \tag{24}$$

Here

$$\begin{aligned}S(u,v):=&\Theta\left(u-\frac{K}{2}\right)\Theta_1\left(u+v-\frac{K}{2}\right)\Theta\left(v-\frac{K}{2}\right)\Theta_1\left(\frac{K}{2}\right)\\&-\Theta_1\left(u-\frac{K}{2}\right)\Theta\left(u+v-\frac{K}{2}\right)\Theta_1\left(v-\frac{K}{2}\right)\Theta\left(\frac{K}{2}\right),\\T(u,v):=&H\left(u-\frac{K}{2}\right)H_1\left(u+v-\frac{K}{2}\right)H\left(v-\frac{K}{2}\right)H_1\left(\frac{K}{2}\right)\\&+H_1\left(u-\frac{K}{2}\right)H\left(u+v-\frac{K}{2}\right)H_1\left(v-\frac{K}{2}\right)H\left(\frac{K}{2}\right),\end{aligned}$$

and $u:=p-q$, $v:=q-r$. In (24), making use of the addition theorem for the theta functions

$$\begin{aligned}&\vartheta_{00}(x)\vartheta_{00}(y)\vartheta_{01}(u)\vartheta_{01}(v)-\vartheta_{01}(x)\vartheta_{01}(y)\vartheta_{00}(u)\vartheta_{00}(v)\\&\quad+\vartheta_{10}(x)\vartheta_{10}(y)\vartheta_{11}(u)\vartheta_{11}(v)-\vartheta_{11}(x)\vartheta_{11}(y)\vartheta_{10}(u)\vartheta_{10}(v)\\&=-2\,\vartheta_{11}\left(\frac{x+y+u+v}{2}\right)\vartheta_{11}\left(\frac{x+y-u-v}{2}\right)\vartheta_{10}\left(\frac{x-y+u-v}{2}\right)\vartheta_{10}\left(\frac{x-y-u+v}{2}\right)\end{aligned}$$

in Ref. 9 and the identities

$$\frac{H(u)}{\Theta(u)}=k^{1/2}\,\mathrm{sn}(u),\quad \mathrm{sn}\left(\frac{K}{2}\right)=(1+k')^{-1/2},$$

we conclude that (21) is equivalent to

$$[S_{00},S_{11}]_- = \frac{1-k'}{1+k'}\,[S_{01},S_{10}]_+ .$$

Other relations can be proved in a similar way.

Definition 1: The quantum algebra $\mathscr{C}$ is defined to be a $\mathbb{C}$-algebra on the generators $\{S_{00},S_{01},S_{10},S_{11}\}$ subject to the relations (16).

We observe that our quantum algebra $\mathscr{C}$ is a special case of the Sklyanin algebra $\mathscr{A}_\eta(4)$. Actually, substituting $\eta=K/2$ in the structure constants $J_{\alpha\beta}$ that are given by (5), we have

$$(J_{12},J_{23},J_{31}) = \left(1, \frac{1-k'}{1+k'}, -1\right).$$

Therefore, we obtain the following proposition.

Proposition 1: The quantum algebra $\mathscr{C}$ coincides with the Sklyanin algebra $\mathscr{A}_\eta$ when η is an 8-torsion point ($\eta=K/2$) by replacing $(S_{00},\sqrt{-1}S_{11},S_{01},S_{10})$ by (S_0,S_1,S_2,S_3).

Remark 1: We observe the meaning of the 8-torsion point from the viewpoint of the R-matrix. Making use of Lemma 1, we obtain the following relation between our R-matrix (17) and that of the 8-vertex model:

$$\frac{2}{H\left(\frac{K}{2}\right)\Theta\left(\frac{K}{2}\right)H_1(0)\Theta_1(0)}\,R_{2-\text{state chiral Potts}} = P^{-1}R_{8\text{-vertex at the 8-torsion point}}P,$$

$$P := \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & -1 \end{pmatrix}.$$

Further it is also known that the 8-vertex model at the 8-torsion point corresponds to the double Ising model.[8]

IV. ANOTHER DERIVATION OF THE QUANTUM ALGEBRA

We will prove Theorem 1 in another way, which is to use the star–triangle relation (8). Let us recall the relations (21) and (22) as mentioned in Sec. III. We can read (22) as

$$\begin{aligned} A_{pqr} &= \sum_{i,j=0}^{1}\left\{(-1)^{i+j}W_{pq}(j)\overline{W_{pr}}(i+j-1)W_{qr}(i)\sum_{k=0}^{1}\overline{W_{pq}}(i+k)W_{pr}(k)\overline{W_{qr}}(j-k)\right\} \\ &\quad + \sum_{i,j=0}^{1}\left\{W_{pq}(j+1)\overline{W_{pr}}(i+j)W_{qr}(i+1)\sum_{k=0}^{1}(-1)^{k}\overline{W_{pq}}(i+k)W_{pr}(k)\overline{W_{qr}}(j-k)\right\}, \\ B_{pqr} &= \sum_{i,j=0}^{1}\left\{(-1)^{i+j-1}W_{pq}(j)\overline{W_{pr}}(i+j-1)W_{qr}(i)\sum_{k=0}^{1}\overline{W_{pq}}(i+k)W_{pr}(k)\overline{W_{qr}}(j-k)\right\} \\ &\quad + \sum_{i,j=0}^{1}\left\{W_{pq}(j+1)\overline{W_{pr}}(i+j)W_{qr}(i+1)\sum_{k=0}^{1}(-1)^{k}\overline{W_{pq}}(i+k)W_{pr}(k)\overline{W_{qr}}(j-k)\right\}. \end{aligned} \tag{25}$$

Deforming (25) by using the STR in this case

$$\begin{aligned}
&\overline{W}_{pq}(0)W_{pr}(0)\overline{W}_{qr}(0)+\overline{W}_{pq}(1)W_{pr}(1)\overline{W}_{qr}(1)=R_{pqr}W_{pq}(0)\overline{W}_{pr}(0)W_{qr}(0),\\
&\overline{W}_{pq}(1)W_{pr}(0)\overline{W}_{qr}(0)+\overline{W}_{pq}(0)W_{pr}(1)\overline{W}_{qr}(1)=R_{pqr}W_{pq}(0)\overline{W}_{pr}(1)W_{qr}(1),\\
&\overline{W}_{pq}(0)W_{pr}(0)\overline{W}_{qr}(1)+\overline{W}_{pq}(1)W_{pr}(1)\overline{W}_{qr}(0)=R_{pqr}W_{pq}(1)\overline{W}_{pr}(1)W_{qr}(0),\\
&\overline{W}_{pq}(1)W_{pr}(0)\overline{W}_{qr}(1)+\overline{W}_{pq}(0)W_{pr}(1)\overline{W}_{qr}(0)=R_{pqr}W_{pq}(1)\overline{W}_{pr}(0)W_{qr}(1),
\end{aligned}$$

we have

$$\begin{aligned}
A_{pqr}=&\frac{1}{R_{pqr}}\{R_{pqr}^2(W_{pq}(0)^2-W_{pq}(1)^2)(\overline{W}_{pr}(1)\overline{W}_{pr}(0))(W_{qr}(0)^2-W_{qr}(1)^2)\\
&+4(\overline{W}_{pq}(1)\overline{W}_{pq}(0))(W_{pr}(0)^2-W_{pr}(1)^2)(\overline{W}_{qr}(1)\overline{W}_{qr}(0))\},\\
B_{pqr}=&\frac{-1}{R_{pqr}}\{R_{pqr}^2(W_{pq}(0)^2-W_{pq}(1)^2)(\overline{W}_{pr}(1)\overline{W}_{pr}(0))(W_{qr}(0)^2-W_{qr}(1)^2)\\
&-4(\overline{W}_{pq}(1)\overline{W}_{pq}(0))(W_{pr}(0)^2-W_{pr}(1)^2)(\overline{W}_{qr}(1)\overline{W}_{qr}(0))\}.
\end{aligned}\tag{26}$$

Here the constant R_{pqr} (9) has the form

$$R_{pqr}^2=\frac{(\overline{W}_{pq}(0)^2-\overline{W}_{pq}(1)^2)(W_{pr}(1)W_{pr}(0))(\overline{W}_{qr}(0)^2-\overline{W}_{qr}(1)^2)}{(W_{pq}(1)W_{pq}(0))(\overline{W}_{pr}(0)^2-\overline{W}_{pr}(1)^2)(W_{qr}(1)W_{qr}(0))}.\tag{27}$$

Substituting (27) and (19) in (26), we can express A_{pqr} and B_{pqr} as polynomials of the parameters (a,b,c,d). Actually, letting

$$\begin{aligned}
U_{pq}:=&\{(c_pb_q+b_pc_q)^2-(-a_pd_q+d_pa_q)^2\}\{(b_pd_q+c_pa_q)^2-(d_pb_q+a_pc_q)^2\},\\
V_{pq}:=&(c_pb_q+b_pc_q)(-a_pd_q+d_pa_q)(b_pd_q+c_pa_q)(d_pb_q+a_pc_q),
\end{aligned}\tag{28}$$

we obtain

$$\frac{B_{pqr}}{A_{pqr}}=-\frac{U_{pq}V_{pr}U_{qr}-4V_{pq}U_{pr}V_{qr}}{U_{pq}V_{pr}U_{qr}+4V_{pq}U_{pr}V_{qr}}.$$

Moreover, using relations (20) in (28), we have

$$V_{pq}=\frac{k'}{4}U_{pq}.$$

Therefore, we conclude that relation (21) is equivalent to

$$[S_{00},S_{11}]_-=\frac{1-k'}{1+k'}[S_{01},S_{10}]_+.$$

The proofs of other relations are likewise.

Finally, we observe that our quantum algebra $\mathscr{C}$ in the self-dual case coincides with the quantum group $U_q(sl_2)$ at the fourth root of unity. The self-dual case means that the Boltzmann weights satisfy the relation $\hat{W}_{pq}(n)=W_{pq}(n)$, which is realized by the limit

$$k' \to 1, \quad c = d \to 1.$$

In this case the third formula of the defining relations (16) is modified to

$$[S_{00}, S_{11}]_- = 0. \tag{29}$$

Next let

$$E_\pm := \frac{1}{\sqrt{2}} (S_{01} \pm S_{10}), \quad S_\pm := \frac{1}{\sqrt{2}} (S_{00} \pm S_{11}).$$

From (29) it is assured that S_+ and S_- are commutative. In order to make clear the link between $U_q(sl_2)$ and our algebra $\mathscr{C}$, we need to impose a further assumption that $(S_+ S_-)^2 = 1$ in the following. Let $q := \sqrt{-1}$, and z_1, z_2 be normalizing factors that satisfy the relation $z_1 z_2 = q - q^{-1} = 2\sqrt{-1}$. Then we define e, f, and t by

$$z_1 e := E_+, \quad z_2 f := E_-, \quad t := S_+^2.$$

We obtain from (16) and (29) that $\{e, f, t^{\pm 1}\}$ satisfy the fundamental relations of $U_q(sl_2)$

$$tt^{-1} = 1 = t^{-1}t, \quad tet^{-1} = q^2 e, \quad tft^{-1} = q^{-2} f, \quad [e,f]_- = \frac{t - t^{-1}}{q - q^{-1}}.$$

V. DISCUSSION

We proved our main theorem in two ways: One is to make use of the addition theorems for the theta functions since the Boltzmann weights are associated with the elliptic curve, the other is to use the STR. The latter is applicable to the N-state, i.e., the higher-genus case. In this paper we observe the 2-state case and clarify the natural link between the Sklyanin algebra and our result (Proposition 1, Remark 1). It is important to generalize our algebra $\mathscr{C}$ to the N-state case by the latter method because there is a possibility that a quantum algebra attached to algebraic curves of genus >1 is constructed. For the first step to achieve this program, we are now studying the 3-state case (genus 10).

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Cohomology and connections on fiber bundles and applications to field theories

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Given any connection on a fiber bundle $B(M,F,G)$, we discuss the question which closed differential forms on the fiber F can be extended to closed forms on the whole bundle B in a canonical way such that the horizontal parts of the extended forms are given in terms of the gauge fields. Such questions arise for many models in theoretical physics such as the skyrmion bundle and related theories with non-Abelian groups G. We introduce the notion of a G-transgressive form as a sufficient condition for the form to be extendable to any bundle which comes along with a given left action $L:G\times F\to F$. Using Lie algebra cohomology we prove that if the structure group G of the bundle is semisimple, then every closed n-form, $n\leqslant 2$, on the fiber which is invariant under L is G-transgressive and thus defines a unique de Rham cohomology class on any bundle which comes along with L. © *1996 American Institute of Physics.* [S0022-2488(96)02011-7]

I. MOTIVATION

In theoretical physics the following general problem quite often occurs: suppose a field theory is defined for some manifold F, i.e., we have matter fields described by differentiable maps $f:M\to F$ from space-time M to the manifold F. (Examples are wide-spread, let us only mention case of Dirac spinors, where $F=\mathbb{C}^4$, or the Skyrme model and related theories, where $F=\mathrm{SU}_n$, cf. Skyrme,[1] Witten,[2] and Zahed and Brown.[3]) For computations one has integrals like the action integral, where the Lagrangian is combined with the volume form of space-time, but also integrals over closed differential forms ϕ on F (i.e., $d\phi=0$), which are integrated over space-time by means of the pullbacks $f^\star$.

Next suppose, we also have a symmetry group G and we gauge our field theory with respect to this Lie group. From the mathematicians point of view, one has to construct a fiber bundle B with base manifold M, (global) projection $\pi:B\to M$, (standard) fiber F and structure group G, that acts on F via an effective left action $L:G\times F\to F$, cf. Steenrod[4] or Kobayashi and Numizu.[5] For a cover $\mathfrak{U}=\{U_\alpha\}_{\alpha\in A}$ of the base manifold M, we have a bundle atlas $\{(U_\alpha,\psi_\alpha)\}_{\alpha\in A}$ with local trivializations $\psi_\alpha:\pi^{-1}(U_\alpha)\to U_\alpha\times F$, local projections $\pi_\alpha=\mathrm{pr}_F\circ\psi_\alpha$ onto F and local injections $i_{\alpha,x}=(\pi_{\alpha,x})^{-1}$ of F onto the fiber over $x\in M$, where $\pi_{\alpha,x}:=\pi_\alpha|_{\pi^{-1}(x)}:\pi^{-1}(x)\to F$. For every $f\in F$ and $g\in G$ define $L^f:G\to F$ and $L_g:F\to F$ by $L^f(g)=L_g(f)=L(g,f)$. Then on every overlap region $U_{\alpha\beta}=U_\alpha\cap U_\beta$ the change of bundle charts is given by transition functions $g_{\alpha\beta}:U_{\alpha\beta}=U_\alpha\cap U_\beta\to G$, such that $\pi_{\alpha,x}\circ(\pi_{\beta,x})^{-1}=\pi_{\alpha,x}\circ i_{\beta,x}=L_{g_{\alpha\beta}(x)}$ for all $x\in U_{\alpha\beta}$.

The bundle $B(M,F,G)$ is associated to a principal bundle $P(M,G)$, where the structure group acts on itself by left multiplication. We will use the same symbols π, ψ_α, π_α, etc., for the bundles P and B. On the principle bundle we also have a free right action $R:P\times G\to P$ and a connection Γ defined by a connection 1-form ω^Γ and its exterior covariant derivative, the curvature 2-form Ω^Γ. Let e denote the neutral element of G and $\sigma_{\alpha,e}:U_\alpha\to\pi^{-1}(U_\alpha)=P|_{U_\alpha}$ denote the local sections given by $\sigma_{\alpha,e}(x):=\psi_\alpha^{-1}(x,e)$. (Recall that a section σ obeys $\pi\circ\sigma=\mathrm{id}_M$.) Then the gauge potentials A^α and the gauge fields F^α of the field theory are the local forms on the sets U_α defined by $\mathrm{A}^\alpha=\sigma_{\alpha,e}^\star\omega^\Gamma$, resp., $\mathrm{F}^\alpha=\sigma_{\alpha,e}^\star\Omega^\Gamma$.

Now the problem is as follows: since the matter fields now appear as global sections $f:M\to B$, it is necessary to ''generalize'' the given closed differential forms $\phi\in\mathscr{A}(F)$ to the bundle case (such that the pullbacks $f^\star\phi$ are well-defined): one needs a closed form $\psi\in\mathscr{A}(B)$

such that ψ reproduces ϕ when restricted to the fibers: $\phi = i^{\star}_{\alpha,x}\psi$ for all $\alpha \in A$ and all $x \in U_\alpha$.

Recall that the de Rham cohomology of a manifold denotes the vector space of the closed forms modulo the exact forms on the manifold, i.e., it denotes the kernel of the exterior derivative $d: \mathscr{A}(M) \to \mathscr{A}(M), \mathscr{A}_{p-1}(M) \to \mathscr{A}_p(M)$ modulo its image. Since d is a differential operator ($d \circ d = 0$), all exact forms are closed and thus the vector space of the closed modulo the exact p-forms is well-defined. This quotient space is called the p-th de Rham cohomology group $H^p(M)$ and the (total) cohomology of M means the direct sum $H^*(M) := \oplus_{p=0}^{\infty} H^p(M)$.

We may reformulate the problem in terms of the de Rham cohomology: Given a cohomology class $[\phi] \in H^*(F)$ we ask whether $[\phi]$ generates a cohomology class in $[\psi] \in H^*(B)$, such that $[\phi] = [i^{\star}_{\alpha,x}][\psi]$. Moreover, we also need a representative ψ for this generated cohomology class.

The problem of computing the cohomology of a fiber bundle from $H^*(M)$ and $H^*(F)$ is a delicate mathematical problem. For a trivial bundle, i.e., a direct product $M \times F$, we have the Künneth formula

$$H^*(M \times F) \cong H^*(M) \otimes H^*(F).$$

This formula is based on the fact that we have two global projections pr_M and pr_F. Using their pullbacks we may extend any form on M and F to the bundle. Since d commutes with pullbacks, this also holds for the cohomology classes. For a nontrivial bundle we only have one global projection π, which indeed allows us to lift any form on M and any cohomology class in $H^*(M)$ onto the bundle. (Nevertheless, the induced homomorphism $[\pi^*]: H^*(M) \to H^*(B)$ needs not be injective nor surjective.) Yet there is no such mean for forms on F and thus the situation becomes much more complicated as in the trivial case and leads to the theory of spectral sequences, cf. Bott and Tu.[6] Spectral sequences compute $H^*(B)$ from $H^*(M)$ and $H^*(F)$. They also answer the question which closed forms on the fiber can be extended to closed forms on the bundle and thus generate a unique cohomology class in $H^*(B)$ in the manner above. We call these forms 0-transgressive. Not all closed forms on F are 0-transgressive. In general it will depend on the structure of the bundle whether a given form is 0-transgressive: obviously for trivial bundles all closed forms on F are 0-transgressive.

If a form $\phi \in \mathscr{A}(F)$ is 0-transgressive, spectral sequences also provide a formula for ψ (Ref. 6, Prop. 9.5). Nevertheless this ''Collating formula'' involves a partition of unity subordinate to the given cover $\mathfrak{U}$ of M. For any such partition the formula gives a different form ψ within the generated cohomology class. (Note that, a priori, ψ is not unique but defined only up to an exact form on B, whose restriction to the fibers is zero.)

From the physicists point of view, this situation is quite unsatisfactory since a partition of unity does not bear any physical meaning and there is no reason why one partition — and the corresponding form ψ — should be better than another. In fact one would like to obtain a representative ψ for the generated cohomology class that can be associated with the physics in question, that is the gauge potentials and the gauge fields of the field theory.

This takes us back to connections on fiber bundles. Recall that a connection on a fiber bundle defines global horizontal and vertical projections of vector fields such that the $C^\infty(B)$-module $\mathscr{D}^1(B)$ of the vector fields on B splits: $\mathscr{D}^1(B) = h\mathscr{D}^1(B) \oplus v\mathscr{D}^1(B)$. Once a connection on a principal bundle is defined via ω^Γ, resp., the gauge potentials A^α, it also defines connections on all associated fiber bundles, cf. Section III.

In addition, Γ defines lifts of vector fields on the base onto horizontal fields on the bundle and projections of forms on the bundle. These lifts and projections now can be used to extend forms on the fiber to the bundle. In fact, for every differential form $\phi \in \mathscr{A}(F)$ that is invariant under the given left action L (i.e., $L_g^{\star}\phi = \phi$ for all $g \in G$), there exists exactly one vertical form on the bundle, say $\phi v \in \mathscr{A}(B)$, such that $\phi v|_{\pi^{-1}(x)} = \phi$. From the physicists point of view, this seems to be a satisfactory generalization, but unfortunately we are not done with that, since the diagram in Figure 1 does *not* commute.

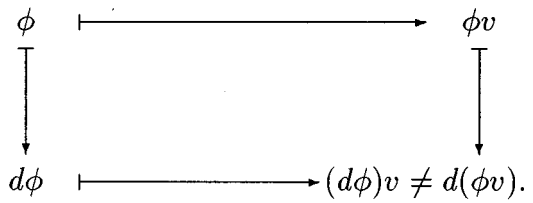

FIG. 1. Exterior derivative and vertical projection do not commute.

Thus although we start with a closed form ϕ, the generated vertical form ϕv needs not be closed. In general, we are not able to find a vertical representative for this cohomology class generated by a 0-transgressive form, but we need to admit horizontal terms. Thus the question will be whether we can find such a representative where these horizontal terms are ''naturally'' given by the connection Γ, in fact, by the gauge fields. In that case, we call the resulting form adapted to Γ. Those forms are candidates for the desired generalizations of closed forms in field theories.

II. BASIC DEFINITIONS

Let M denote any manifold and V,W finite dimensional vector spaces. Every vector field $\mathscr{X} \in \mathscr{D}^1(M)$ differentiably associates with every $x \in M$ an element $\mathscr{X}_x$ in the tangent space $T_x(M)$. Now $\mathscr{D}_p(M,V)$, resp., $\mathscr{A}_p(M,V)$, denote the $C^\infty(M)$-modules of p-linear, resp., alternating p-linear, maps $\phi_p : \mathscr{D}^1(M) \times \cdots \times \mathscr{D}^1(M) \to C^\infty(M,V)$. They associate with every $x \in M$ an element $\phi_x = (\phi_p)_x$ in $\mathrm{Hom}(\otimes^p T_x(M), V)$, resp., in $\mathrm{Alt}_p(T_x(M),V)$, where $\mathrm{Alt}_p(W,V)$ means the vector space of all alternating p-linear maps from W^p to V. The alternations $A_p : \mathscr{D}_p(M,V) \to \mathscr{D}_p(M,V)$ are the canonical projections of $\mathscr{D}_p(M,V)$ onto $\mathscr{A}_p(M,V)$. The exterior product (or wedge product) of forms will be denoted by $\wedge$: for $\phi_p \in \mathscr{A}_p(M)$ and $\phi_r \in \mathscr{A}_r(M)$ we have $\phi_p \wedge \phi_r := A_{p+r}(\phi_p \otimes \phi_r) \in \mathscr{A}_{p+r}(M)$.

Also if a bilinear mapping $\varphi : V \times V \to V$ is given, $\wedge$ extends to an exterior product $\wedge_\varphi$ of V-valued differential forms. For $\phi = \hat{\phi} \otimes v \in \mathscr{A}(M) \otimes V \cong \mathscr{A}(M,V)$ and $\psi = \hat{\psi} \otimes w \in \mathscr{A}(M) \otimes V$, the exterior product is given by

$$\phi \wedge_\varphi \psi := (\hat{\phi} \wedge \hat{\psi}) \otimes \varphi(v,w). \tag{1}$$

Everything in the sequel will also work for infinite dimensional vector spaces V, if we consider $\mathscr{A}(M) \otimes V$ instead of $\mathscr{A}(M,V)$. Yet for our purposes, we will restrict ourselves to finite dimensional V and identify $\mathscr{A}(M) \otimes V$ and $\mathscr{A}(M,V)$.

As mentioned above, we are heading for differential forms whose horizontal parts are given in terms of the gauge fields. Let us denote the $C^\infty(B)$-module of horizontal forms on B by $\mathscr{A}(B)h$ and the vertical counterpart by $\mathscr{A}(B)v$. (Note that only $\mathscr{A}_1(B)$ splits into $\mathscr{A}_1(B)h \oplus \mathscr{A}_1(B)v$, whereas $\mathscr{A}_0(B)h = \mathscr{A}_0(B)v = \mathscr{A}_0(B) = C^\infty(B)$ and for $p \geqslant 2$ $\mathscr{A}_p(B)$ contains also ''mixed'' forms, i.e., exterior products of horizontal and vertical forms.) Normally one would try to split a form into a sum $\phi = \Sigma_{i \in I} \phi_i$, where the ϕ_i are given by $\phi_i = \phi_i^1 \wedge \phi_i^2$ with $\phi_i^1 \in \mathscr{A}(B)h$ and $\phi_i^2 \in \mathscr{A}(B)v$.

Yet in our case such a splitting is impossible, since the gauge fields and the gauge potentials are Lie algebra valued differential forms: $\mathrm{A}^\alpha \in \mathscr{A}_1(U_\alpha, \mathfrak{g})$ and $\mathrm{F}^\alpha \in \mathscr{A}_2(U_\alpha, \mathfrak{g})$, where $\mathfrak{g}$ denotes the Lie algebra of the structure group G. In contrast, $\phi \in \mathscr{A}(F)$ — and thus also $\psi \in \mathscr{A}(B)$ — will be real or complex valued. Thus we need a generalization of the wedge product that combines $\mathfrak{g}$-valued forms with $(\mathfrak{g} \otimes \cdots \otimes \mathfrak{g})^*$-valued forms in order to produce real or complex valued forms. This is the task of the following definition.

Definition II.1: For $\chi_r^s \in \mathscr{A}_r(M, \mathrm{Hom}(\otimes^s \mathfrak{g}, V))$ *and* $\phi_p \in \mathscr{A}_p(M, \mathfrak{g})$, $p,r,s-1 \in \mathbb{N}_0$, *let* $d_{r+sp} \in \mathscr{D}_{r+sp}(M,V)$ *with*

$$d_{r+sp}(\mathscr{X}^1,\ldots,\mathscr{X}^{r+sp})(x):=[\chi_x(\mathscr{X}^1_x,\ldots,\mathscr{X}^r_x)]\circ[\phi_x(\mathscr{X}^{r+1}_x,\ldots,\mathscr{X}^{r+p}_x)$$

$$\otimes\cdots\otimes\phi_x(\mathscr{X}^{r+(s-1)p+1}_x,\ldots,\mathscr{X}^{r+sp}_x)]$$

for all $x\in M$ and define $\chi^s_r\bullet\phi_p:=A_{r+sp}(d_{r+sp})\in\mathscr{A}_{r+sp}(M,V)$ and $\chi^0_r\bullet\phi_p:=\chi^0_r$.

Roughly speaking, the bullet operator means the following: for any $x\in M$ and $\mathscr{X}^i\in\mathscr{D}^1(M)$, $\chi_x(\mathscr{X}^1_x,\ldots,\mathscr{X}^r_x)$ defines an element in $\mathrm{Hom}(\otimes^s\mathfrak{g},V)$. Thus we need s vectors in $\mathfrak{g}$ as input for this map. But again for any $x\in M$ and $\mathscr{Y}^i\in\mathscr{D}^1(M)$, $\phi_x(\mathscr{Y}^1_x,\ldots,\mathscr{Y}^p_x)$ defines such a vector in $\mathfrak{g}$. Altogether the combination of χ and s factors ϕ defines an element $d^{sq}_{r+sp}\in\mathscr{D}_{r+sp}(M,V)$. Using the alternation A_{r+sp}, we finally obtain a form in $\mathscr{A}_{r+sp}(M,V)$.

Note that this construction works with any finite dimensional vector space W instead of $\mathfrak{g}$, and even with differential forms $\phi^q_p\in\mathscr{A}_p(M,\mathrm{Hom}(\otimes^qX,W))$, where X is another finite dimensional vector space. In the latter case the construction produces a differential form $\chi^s_r\bullet\phi^q_p\in\mathscr{A}_{r+sp}(M,\mathrm{Hom}(\otimes^{sq}X,V))$. Yet we only need $\bullet$ in the way defined above, especially for $V=\mathbb{R},\mathbb{C}$ and $\chi^s_r\in\mathscr{A}_r(M,\mathrm{Sym}_s(\mathfrak{g},V))$, where $\mathrm{Sym}_s(\mathfrak{g},V)$ denotes the vector space of symmetric s-linear maps from $\mathfrak{g}^s$ to V, i.e., the image of the canonical symmetrization $\mathrm{Sym}:\mathrm{Hom}(\otimes^s\mathfrak{g},V)\to\mathrm{Hom}(\otimes^s\mathfrak{g},V)$.

For vectors $E_j\in\mathfrak{g}$, $j=1,\ldots,s$, let $E_1\otimes\cdots\otimes E_s$: $\mathrm{Hom}(\otimes^s\mathfrak{g},V)\to V$ denote the canonical (evaluation) morphism. For any form $\chi^s_r\in\mathscr{A}_r(M,\mathrm{Hom}(\otimes^s\mathfrak{g},V))$ define $\chi^{E_1,\ldots,E_s}_r\in\mathscr{A}_r(M,V)$ to be the push-out of χ^s_r under this morphism: $\chi^{E_1,\ldots,E_s}_r:=(E_1\otimes\cdots\otimes E_s)_\star\chi^s_r$ i.e., for all $x\in M$ and $\mathscr{X}^i\in\mathscr{D}^1(M)$, $i=1,\ldots,r$,

$$(\chi^{E_1,\ldots,E_s}_r)_x(\mathscr{X}^1_x,\ldots,\mathscr{X}^r_x):=(E_1\otimes\cdots\otimes E_s)\circ(\chi^s_r)_x(\mathscr{X}^1_x,\ldots,\mathscr{X}^r_x)$$

$$=[(\chi^s_r)_x(\mathscr{X}^1_x,\ldots,\mathscr{X}^r_x)](E_1\otimes\cdots\otimes E_s). \tag{2}$$

With this convention we obtain the following lemma:

Lemma II.2: Let $p,r,s-1\in\mathbb{N}_0$. If $\phi_p=\Sigma^m_{i=1}\phi^i\otimes E_i$ with $\phi^i\in\mathscr{A}_p(M)$ and $E_i\in\mathfrak{g}$, then

$$\chi^s_r\bullet\phi_p=\sum_{i_1,\ldots,i_s=1}^{m}\chi^{E_{i_1},\ldots,E_{i_s}}_r\wedge\phi^{i_1}\wedge\cdots\wedge\phi^{i_s}.$$

Proof: Take $x\in M$ and $\mathscr{X}^i\in\mathscr{D}^1(M)$. Then for d_{r+sp} in Definition II we obtain

$$\begin{aligned}
&(d_{r+sp})_x(\mathscr{X}^1_x,\ldots,\mathscr{X}^{r+sp}_x):\\
&\quad=[\chi_x(\mathscr{X}^1_x,\ldots,\mathscr{X}^r_x)](\phi_x(\mathscr{X}^{r+1}_x,\ldots,\mathscr{X}^{r+p}_x)\\
&\qquad\otimes\cdots\otimes\phi_x(\mathscr{X}^{r+(s-1)p+1}_x,\ldots,\mathscr{X}^{r+sp}_x))\\
&\quad=\sum_{i_1,\ldots,i_s=1}^{m}[\chi_x(\mathscr{X}^1_x,\ldots,\mathscr{X}^r_x)]\Big((E_{i_1}\otimes\cdots\otimes E_{i_s})\\
&\qquad\cdot\prod_{j=1}^{s}\phi^{i_j}_x(\mathscr{X}^{r+(j-1)p+1}_x,\ldots,\mathscr{X}^{r+jp}_x)\Big)\\
&\quad=\sum_{i_1,\ldots,i_s=1}^{m}[(\chi^{E_{i_1},\ldots,E_{i_s}}_r)_x(\mathscr{X}^1_x,\ldots,\mathscr{X}^r_x)]\\
&\qquad\cdot\prod_{j=1}^{s}\phi^{i_j}_x(\mathscr{X}^{r+(j-1)p+1}_x,\ldots,\mathscr{X}^{r+jp}_x).
\end{aligned}$$

Thus if S_{r+sp} denotes the group of permutations of $r+sp$ elements and $(-1)^\rho$ means the signum of $\rho \in S_{r+sp}$, we get

$$
\begin{aligned}
(\chi_r^s \bullet \phi_p)_x(\mathscr{X}_x^1, \ldots, \mathscr{X}_x^{r+sp}) &:= [A_{r+sp}(d_{r+sp})]_x(\mathscr{X}_x^1, \ldots, \mathscr{X}_x^{r+sp}) \\
&= \sum_{\rho \in S_{r+sp}} \frac{(-1)^\rho}{(r+sp)!} \sum_{i_1, \ldots, i_s=1}^{m} [(\chi_r^{E_{i_1}, \ldots, E_{i_s}})_x(\mathscr{X}_x^{\rho(1)}, \ldots, \mathscr{X}_x^{\rho(r)})] \\
&\quad \cdot \prod_{j=1}^{s} \phi_x^{i_j}(\mathscr{X}_x^{\rho(r+(j-1)p+1)}, \ldots, \mathscr{X}_x^{\rho(r+jp)}) \\
&= \sum_{i_1, \ldots, i_s=1}^{m} [A_{r+sp}(\chi_r^{E_{i_1}, \ldots, E_{i_s}} \otimes \phi^{i_1} \otimes \cdots \otimes \phi^{i_s})]_x(\mathscr{X}_x^1, \ldots, \mathscr{X}_x^{r+sp}) \\
&= \left(\sum_{i_1, \ldots, i_s=1}^{m} \chi_r^{E_{i_1}, \ldots, E_{i_s}} \wedge \phi^{i_1} \wedge \cdots \wedge \phi^{i_s} \right)_x (\mathscr{X}_x^1, \ldots, \mathscr{X}_x^{r+sp}),
\end{aligned}
$$

where the last identity follows immediately from the definition of the exterior product $\wedge$. □

Lemma II.2 proves that if p is even, then only the symmetric part of χ_r^s counts: $\chi_r^s \bullet \phi_p = (\mathrm{Sym}_\star \chi_r^s) \bullet \phi_p$. Thus we may concentrate on $\chi_r^s \in \mathscr{A}_r(M, \mathrm{Sym}_s(\mathfrak{g}, V))$, in order to construct forms $\chi_r^s \bullet \mathrm{F}$ with the 2-forms F^α.

Let $\mathrm{Ad}^\star : G \times \mathrm{Hom}(\otimes^s \mathfrak{g}, V) \to \mathrm{Hom}(\otimes^s \mathfrak{g}, V)$ denote the right representation induced by the adjoint action: for $K \in \mathrm{Hom}(\otimes^s \mathfrak{g}, V)$, $g \in G$ and $E_i \in \mathfrak{g}$, it is defined by

$$
(\mathrm{Ad}(g)^\star K)(E_1, \ldots, E_s) := K(\mathrm{Ad}(g)E_1, \ldots, \mathrm{Ad}(g)E_s).
$$

A differential form $\chi_n^s \in \mathscr{A}_n(F, \mathrm{Hom}(\otimes^s \mathfrak{g}, V))$ is called (G-)equivariant if $L_g^\star \chi_n^s = (\mathrm{Ad}(g^{-1})^\star)_\star \chi_n^s$. (For $s=0$ this obviously means that χ_n^0 is invariant under L.) On the other hand a differential form $\phi \in \mathscr{A}(F, \mathfrak{g})$ is called (G-)equivariant if $L_g^\star \phi = \mathrm{Ad}(g)_\star \phi$, e.g., $\omega^\Gamma \in \mathscr{A}_1(P, \mathfrak{g})$ and $\Omega^\Gamma \in \mathscr{A}_2(P, \mathfrak{g})$ are equivariant, since $R_g^\star \omega^\Gamma = \mathrm{Ad}(g^{-1})_\star \omega^\Gamma$, resp., $R_g^\star \Omega^\Gamma = \mathrm{Ad}(g^{-1})_\star \Omega^\Gamma$. We denote the sets of these equivariant differential forms by $\mathscr{A}(F, \mathrm{Hom}(\otimes^s \mathfrak{g}, V))_{\mathrm{equiv}}$, resp., $\mathscr{A}(F, \mathfrak{g})_{\mathrm{equiv}}$. They are modules of the exterior algebra $\mathscr{A}(P)_{\mathrm{inv}}$ of invariant differential forms.

Lemma II.3: If $\chi_n^s \in \mathscr{A}_n(F, \mathrm{Hom}(\otimes^s \mathfrak{g}, V))_{\mathrm{equiv}}$ and $\phi_p \in \mathscr{A}_p(F, \mathfrak{g})_{\mathrm{equiv}}$, then $\chi_n^s \bullet \phi_p$ is invariant.

For our purposes we also need further operators on differential forms that transform V-valued forms into $\mathrm{Alt}_i(\mathfrak{g}, V)$-valued forms. Recall that for any Lie group action $L : G \times F \to F$, every $X \in \mathfrak{g}$ canonically induces a vector field $\mathscr{L}_X \in \mathscr{D}^1(F)$ by $(\mathscr{L}_X)_f := (dL^f)_e(X)$, where $(dL^f)_e : T_e(G) \to T_f(F)$ denotes the differential of the map L^f. The operator $-\mathscr{L} : \mathfrak{g} \to \mathscr{D}^1(F)$ is a Lie algebra homomorphism, in fact we have

$$
[\mathscr{L}_X, \mathscr{L}_Y] = \mathscr{L}_{[Y,X]} = -\mathscr{L}_{[X,Y]} \text{ for all } X, Y \in \mathfrak{g}, \tag{3}
$$

$$
(L_g)_\star \mathscr{L}_X = \mathscr{L}_{\mathrm{Ad}(g)X} \text{ for all } g \in G, X \in \mathfrak{g}. \tag{4}
$$

Analogously for the right action R on a principal bundle, $\mathscr{R} : \mathfrak{g} \to \mathscr{D}^1(P)$ is a Lie algebra homomorphism, and the $\mathscr{R}_X$ are the so-called fundamental vector fields on P. Now we may define:

Definition II.4: Let L be a Lie group action of G on F and $\omega_n \in \mathscr{A}_n(F, V)$. We define differential forms $L_\bullet^i \omega_n \in \mathscr{A}_{n-i}(F, \mathrm{Alt}_i(\mathfrak{g}, V))$, $i = 0, \ldots, n$, for all $\mathscr{X}^j \in \mathscr{D}^1(F)$, $E_k \in \mathfrak{g}$ and $f \in F$ by

$$[(L^i_\bullet \omega_n)(\mathscr{X}^1,\ldots,\mathscr{X}^{n-i})(f)](E_1,\ldots,E_i) := \frac{n!}{(n-i)!}\,\omega_n(\mathscr{L}^1,\ldots,\mathscr{L}^i,\mathscr{X}^1,\ldots,\mathscr{X}^{n-i})(f) \in V,$$

where $\mathscr{L}^i := \mathscr{L}_{E_i}$. *For* $i>n$ *we put* $L^i_\bullet \omega_n = 0$. *In the case* $i=1$ *we also define for* $\chi^s_n \in \mathscr{A}_n(F,\mathrm{Hom}(\otimes^s \mathfrak{g},V))$

$$L^\vee_\bullet \chi^s_n := \mathrm{Sym}_\star(L_\bullet \chi^s_n) \in \mathscr{A}_{n-1}(F,\mathrm{Sym}_{s+1}(\mathfrak{g},V)).$$

(Obviously $\mathrm{Sym}_\star(L^i_\bullet \chi^s_n)=0$ for $i>1$.) Now if $\imath_{\mathscr{X}}:\mathscr{A}_n(M,V)\to\mathscr{A}_{n-1}(M,V)$ denotes the interior product with respect to $\mathscr{X}\in\mathscr{D}^1(M)$, which is given by

$$(\imath_{\mathscr{X}}\omega_n)(\mathscr{Y}^1,\ldots,\mathscr{Y}^{n-1}) := n\,\omega_n(\mathscr{X},\mathscr{Y}^1,\ldots,\mathscr{Y}^{n-1}),$$

then we have the following relation with regard to our convention (2):

$$(L^i_\bullet \omega_n)^{E_1,\ldots,E_i}_{n-i} = (\imath_{\mathscr{L}^i}\circ\cdots\circ\imath_{\mathscr{L}^1})\,\omega_n .$$

The following lemma is quite immediate by (4):

Lemma II.5: For all $i\leqslant n$, *the operator* $L^i_\bullet:\mathscr{A}_n(F,V)\to\mathscr{A}_{n-i}(F,\mathrm{Alt}_i(\mathfrak{g},V))$ *is* $C^\infty(F)$*-linear. For* $\omega_n\in\mathscr{A}_n(F,V)$ *and* $\chi^s_n\in\mathscr{A}_n(F,\mathrm{Hom}(\otimes^s\mathfrak{g},V))_{\mathrm{equiv}}$ *we have*

$$L^0_\bullet\omega_n=\omega_n,\quad (L^n_\bullet\omega_n)(f)=n!\,[(L^f)^\star\omega_n]_e \text{ for all } f\in F, \tag{5}$$

$$L^\star_g(L^i_\bullet\omega_n)=(\mathrm{Ad}(g^{-1})^\star)_\star[L^i_\bullet(L^\star_g\omega_n)],\quad \text{thus} \tag{6}$$

$$L^\star_g(L^i_\bullet\chi^s_n)=(\mathrm{Ad}(g^{-1})^\star)_\star(L^i_\bullet\chi^s_n) \text{ and } \quad L^\star_g(L^\vee_\bullet\chi^s_n)=(\mathrm{Ad}(g^{-1})^\star)_\star(L^\vee_\bullet\chi^s_n). \tag{7}$$

Equation (7) yields that $L^i_\bullet\omega_n$ and $L^\vee_\bullet\omega_n$ are G-equivariant if ω_n is invariant under L.

III. EXTENDING FORMS TO THE BUNDLE

If P is a principal bundle with free right Lie group action R, and L is a left effective Lie group action of G on a manifold F, then the associated fiber bundle with fiber F that comes along with L is the quotient manifold $B(M,F,G)=P\times_G F$ of the direct product $P\times F$ under the free right action $\widetilde{R}:(P\times F)\times G\to P\times F$, which is defined by

$$\widetilde{R}_g(p,f) := (R_g(p),L_{g^{-1}}(f)) \text{ for all } p\in P, f\in F.$$

In fact, $P\times F$ is a principal bundle over B with projection $\widetilde{\pi}$ and fiber G. Every connection Γ on a principal bundle, given by a connection 1-form ω^Γ, canonically induces a connection $\widetilde{\Gamma}$ on $(P\times F)(B,G)$ by $\widetilde{\omega}^{\widetilde{\Gamma}}=\mathrm{pr}_P^\star\omega^\Gamma$. In turn, $\widetilde{\Gamma}$ defines horizontal lifts of vector fields $\widetilde{\mathbb{L}}:\mathscr{D}^1(B)\to\widetilde{h}\mathscr{D}^1(P\times F)_{\mathrm{inv}}$. $\widetilde{\mathbb{L}}$ is a $C^\infty(B)$-module isomorphism with inverse morphism $d\widetilde{\pi}$. If h^{nat} and v^{nat} denote the natural projections of vector fields on the direct product $P\times F$, then we also have projections h, v on $\mathscr{D}^1(B)$

$$h=d\widetilde{\pi}h^{\mathrm{nat}}\widetilde{\mathbb{L}},\quad v=d\widetilde{\pi}v^{\mathrm{nat}}\widetilde{\mathbb{L}},$$

so

$$\mathscr{D}^1(B)=h\mathscr{D}^1(B)\oplus v\mathscr{D}^1(B).$$

This is the induced connection on the associated bundle B, as mentioned above. Let $\mathscr{X}^i \in \mathscr{D}^1(B)$, then for any $\omega_n \in \mathscr{A}_n(B,V)$, $n>0$, the horizontal and vertical projections $\omega_n h \in \mathscr{A}_n(B,V)h$, resp., $\omega_n v \in \mathscr{A}_n(B,V)v$, are given by

$$\omega_n h(\mathscr{X}^1, \ldots, \mathscr{X}^n) := \omega_n(h\mathscr{X}^1, \ldots, h\mathscr{X}^n),$$

$$\omega_n v(\mathscr{X}^1, \ldots, \mathscr{X}^n) := \omega_n(v\mathscr{X}^1, \ldots, v\mathscr{X}^n).$$

Obviously these projections commute with $\bullet$, i.e.,

$$(\chi_n^s \bullet \phi_p)h = \chi_n^s h \bullet \phi_p h, \quad (\chi_n^s \bullet \phi_p)v = \chi_n^s v \bullet \phi_p v.$$

Recall that, by definition, ω^Γ is a vertical form. The exterior covariant derivative of forms on P is defined by $d^\Gamma\phi := (d\phi)h$. Thus $\Omega^\Gamma = d^\Gamma\omega^\Gamma = (d\omega^\Gamma)h$ is a horizontal form.

If ϕ is a differential form on F, then $\mathrm{pr}_F^\star\phi$ is a form on $P\times F$, and if $\mathscr{Y}^i$ are vector fields on B, then $(\mathrm{pr}_F^\star\phi)(\ldots, \widetilde{\mathbb{L}}\mathscr{Y}^i, \ldots)$ is a function on $P\times F$. Now if ϕ is invariant under L, one can prove that this function is invariant under $\widetilde{R}$ and thus defines a map on B. But this defines a form on B. In fact, we have the following proposition:[7]

Proposition III.1: $\phi \in \mathscr{A}(F,V)$ defines a vertical V-valued form ϕv on $B(M,F,G)$ iff ϕ is invariant under all $L_g^\star$ For such a ϕ and all $\mathscr{Y}^i \in \mathscr{D}^1(B)$ then there exists $f \in C^\infty(B,V)$ with

$$(\mathrm{pr}_F^\star\phi)(\ldots, \widetilde{\mathbb{L}}\mathscr{Y}^i, \ldots) = f \circ \widetilde{\pi}.$$

If h^α and v^α denote the local projections of fields and forms induced by Γ, then this generated form ϕv locally is given by

$$\phi v\big|_{\pi^{-1}(U_\alpha)} = (\pi_\alpha^\star\phi)v^\alpha. \tag{8}$$

Proposition III.1 is a special case of the following theorem:

Theorem III.2: *If $\chi_n^s \in \mathscr{A}_n(F, \mathrm{Hom}(\otimes^s\mathfrak{g}, V))_{\mathrm{equiv}}$ and $\phi \in \mathscr{A}_p(P,\mathfrak{g})_{\mathrm{equiv}}$, $p \in \mathbb{N}_0$, then $(\mathrm{pr}_F^\star\chi_n^s)\bullet(\mathrm{pr}_P^\star\phi) \in \mathscr{A}_{n+sp}(P\times F, V)$ defines a V-valued form on B: for all vector fields $\mathscr{Y}^i \in \mathscr{D}^1(B)$ then there exists $f \in C^\infty(B,V)$ such that*

$$[(\mathrm{pr}_F^\star\chi_n^s)\bullet(\mathrm{pr}_P^\star\phi)](\ldots, \widetilde{\mathbb{L}}\mathscr{Y}^i, \ldots)$$
$$= [(\mathrm{pr}_F^\star\chi_n^s)\bullet(\mathrm{pr}_P^\star\phi h)](\ldots, \widetilde{\mathbb{L}}\mathscr{Y}^i, \ldots) = f \circ \widetilde{\pi}.$$

$(\mathrm{pr}_F^\star\chi)$ defines the vertical and $(\mathrm{pr}_P^\star\phi)$ defines the horizontal part of the form.

The proof of Theorem III.2 relies on Lemma II.3: under the assumed conditions one shows that $(\mathrm{pr}_F^\star\chi_n^s)$ and $(\mathrm{pr}_P^\star\phi)$ are equivariant with respect to $\widetilde{R}$, and thus $(\mathrm{pr}_F^\star\chi_n^s)\bullet(\mathrm{pr}_P^\star\phi)$ is invariant by Lemma II.3.

Natural candidates for $\phi \in \mathscr{A}_p(P,\mathfrak{g})_{\mathrm{equiv}}$ are ω^Γ and Ω^Γ. Nevertheless, since ω^Γ is vertical, Theorem III.2 yields that the generated form on B is zero. For Ω^Γ, the generated form is locally given by

$$[(\pi_\alpha^\star\chi_n^s)v^\alpha]\bullet(\pi^\star\mathrm{F}^\alpha) \in \mathscr{A}_{n+2s}(\pi^{-1}(U_\alpha), V).$$

For that reason, we will denote this generated form by $(\chi_n^s v)\bullet\mathrm{F}$ or simply $\chi v\bullet\mathrm{F}$.

Finally we need to compute the exterior derivative of these generated differential forms. We thus cite the following theorem from Ref. 8:

Theorem III.3: *Let* Γ *be a connection on a principal fiber bundle* $P(M,G)$ *and let* $B(M,F,G)$ *be an associated bundle,* V *any vector space,* $\chi_n^s \in \mathscr{A}_n(F)\otimes \mathrm{Hom}(\otimes^s \mathfrak{g},V)$ *be* G*-equivariant and* $\phi_n \in \mathscr{A}_n(F)\otimes V$ *be invariant under* G*. Then*

$$\begin{aligned} d(\chi_n^s v\bullet \mathrm{F}) &= [(d\chi_n^s)v]_{n+1}^s \bullet \mathrm{F} + [(L_\bullet \chi_n^s)v]_{n-1}^{s+1}\bullet \mathrm{F}, \\ &= [(d\chi_n^s)v]_{n+1}^s \bullet \mathrm{F} + [(L_\bullet^\vee \chi_n^s)v]_{n-1}^{s+1}\bullet \mathrm{F}, \end{aligned}$$

$$d(\phi_n v) = (d\phi_n)v + [(L_\bullet \phi_n)v]_{n-1}^1 \bullet \mathrm{F}.$$

Note that the second identity follows from the already mentioned fact that, in combination with F, only the symmetric part of $(L_\bullet \chi_n^s)v$ counts, cf. Lemma II.2. The last identity is a simple corollary to the first one, since for $s=0$, G-equivariance means invariance, $\mathrm{Hom}(\otimes^0 \mathfrak{g},V)=V$, and $\chi_r^0\bullet \mathrm{F}=\chi_r^0$ by definition.

Theorem III.3 proves that the diagram in Section I does not commute in general. Only for 0-forms ϕ, i.e., functions $\phi \in C^\infty(F,V)$, we know that $L_\bullet \phi = 0$.

IV. Γ-ADAPTED AND *G*-TRANSGRESSIVE DIFFERENTIAL FORMS

Now we are prepared for the notion of Γ-adapted differential forms on a bundle:

Definition IV.1: Let Γ *be a connection on* $P(M,G)$ *and* $B=P\times_G F$*. A differential form* $\phi^A \in \mathscr{A}(B,V)$ *is called* Γ-adapted if $\chi^i \in \mathscr{A}_{n(i)}(F,\mathrm{Hom}(\otimes^{s(i)}\mathfrak{g},V))_{\mathrm{equiv}}$ *are given such that*

$$\phi^A = \sum_i \chi^i v\bullet \mathrm{F}.$$

It is this splitting into a sum of $\chi^i v\bullet \mathrm{F}$ that we have in mind when we say that a form can be presented in such a way that all horizontal terms are given by the gauge fields F^α.

We will be concerned with the question whether we can find such a Γ-adapted representative for a cohomology class in $H^*(B)$ that is generated by a 0-transgressive invariant form $\phi \in \mathscr{A}(F)$. For the physical applications in mind, this concentration on invariant forms is no real restriction. Recall from the general theory of fiber bundles that, for every bundle over a paracompact manifold M with a connected structure group G, this Lie group G is reducible to its maximal compact connected subgroup K, i.e., G may be *a priori* chosen to be compact. For example, if we are dealing with electromagnetic interactions, we have $G=\mathrm{U}_1$; if we are dealing with electroweak interactions within the Glashow, Salam and Weinberg theory, then $G=\mathrm{SU}_2\times \mathrm{U}_1$; and for strong interactions covered by quantum chromodynamics (QCD), $G=\mathrm{SU}_3$. In general, for Yang-Mills theories we have $G=\mathrm{U}_n\times \mathrm{U}_n$ or a subgroup $H<G$.

For any compact Lie group we have the normalized Haar measure μ, and we can project any form $\phi \in \mathscr{A}(F,V)$ onto an invariant form ϕ_{inv} defined by

$$\phi_{\mathrm{inv}} := \int_G L_g^\star \phi \, d\mu(g). \tag{9}$$

(Analogous projections onto equivariant forms also exist.) On the other hand, if G is connected, then all maps L_g are homotopic to the identity map $L_e=\mathrm{id}_F$, which yields that $[L_g^\star]=\mathrm{id}_{H^*(F)}$. Thus, if we denote the cohomology of the invariant closed forms on F modulo the invariant exact forms by $H^*_{\mathrm{inv}}(F)$, we have the following proposition:

Proposition IV.2: If G *is a compact connected Lie group acting on* F*, then* $H^*(F)\cong H^*_{\mathrm{inv}}(F)$*, and the isomorphims are induced by the above projection onto invariant forms, resp., the injection* $i:\mathscr{A}(F)_{\mathrm{inv}}\to \mathscr{A}(F)$.

$\mathscr{A}(F,V)_{\mathrm{inv}}$ contains an important subset, whose elements we will call G-transgressive forms. Let $[r]:=\max_{z\in\mathbb{Z}}\{z\leqslant r\}$ for all $r\in\mathbb{R}$. Then their definition is as follows:

Definition IV.3: Let $L:G\times F\to F$ be a left Lie group action. An invariant closed differential form $\phi_n\in\mathscr{A}_n(F,V)_{\mathrm{inv}}$ will be called G-transgressive if equivariant differential forms $\chi^i\in\mathscr{A}_{n-2i}(F,\mathrm{Sym}_i(\mathfrak{g},V))_{\mathrm{equiv}}$ exist for $0\leqslant i\leqslant[n/2]$ with

$$\chi^0=\phi_n,\ -L^{\vee}_{\bullet}\chi^i=d\chi^{i+1}\ \text{for all}\ \ 0\leqslant i\leqslant[n/2]-1\ \text{and}\ \ L^{\vee}_{\bullet}\chi^{[n/2]}=0. \tag{10}$$

Denote the set of all G-transgressive forms on F by $\mathscr{A}(F,V)_{G-\mathrm{trans}}$.

Note IV.4: The reader who is familiar with equivariant cohomology will recognize that G-transgressive forms define equivariant cohomology classes for the given G-manifold F, cf. Atiyah and Bott[9] or Mathai and Quillen[10] and Section VIII.

Recall the definition of the exterior product of vector valued differential forms from (1). For $K_r\in\mathrm{Sym}_r(\mathfrak{g},\mathbb{R})$ and $K_s\in\mathrm{Sym}_s(\mathfrak{g},\mathbb{R})$ we have the symmetric product $K_r\vee K_s:=\mathrm{Sym}(K_r\otimes K_s)$. For any bilinear $\varphi:V\times V\to V$ this extends to a bilinear mapping on the (infinite dimensional) vector space $\mathrm{Sym}(\mathfrak{g},V):=\oplus_{s=0}^{\infty}\mathrm{Sym}_s(\mathfrak{g},V)$ analogously to (1), which we also denote by $\vee$. This in turn defines the exterior product $\wedge_{\vee}$. With respect to $\wedge_{\vee}$, the set $\mathscr{A}(F)\otimes\mathrm{Sym}(\mathfrak{g},V)$ is an exterior algebra with subalgebra $\mathscr{A}(F)_{\mathrm{equiv}}\otimes\mathrm{Sym}(\mathfrak{g},V)$.

Lemma IV.5: d and $L^{\vee}_{\bullet}$ are skew-derivations of degree 1, *resp.* -1, *of the algebras $\mathscr{A}(P)\otimes\mathrm{Sym}(\mathfrak{g},V)$ and $\mathscr{A}(P)_{\mathrm{equiv}}\otimes\mathrm{Sym}(\mathfrak{g},V)$. For all $\alpha_n\in\mathscr{A}_n(P)\otimes\mathrm{Sym}(\mathfrak{g},V)$ and $\omega\in\mathscr{A}(P)\otimes\mathrm{Sym}(\mathfrak{g},V)$,*

$$d(\alpha_n\wedge_{\vee}\omega)=(d\alpha_n)\wedge_{\vee}\omega+(-1)^n\alpha_n\wedge_{\vee}(d\omega),$$

$$L^{\vee}_{\bullet}(\alpha_n\wedge_{\vee}\omega)=(L^{\vee}_{\bullet}\alpha_n)\wedge_{\vee}\omega+(-1)^n\alpha_n\wedge_{\vee}(L^{\vee}_{\bullet}\omega).$$

Lemma IV.5 is the main ingredient in the proof of the following proposition:

*Proposition IV.6: $\mathscr{A}(F,V)_{G-\mathrm{trans}}$ is a $\mathbb{R}$-subalgebra of $\mathscr{A}(F,V)$, whenever a bilinear map $\varphi:V\times V\to V$ and thus a wedge product $\wedge_{\varphi}$ is defined. If ϕ_m and ψ_n are G-transgressive and $\chi^i\in\mathscr{A}_{m-2i}(F,\mathrm{Sym}_i(\mathfrak{g},V))_{\mathrm{equiv}}$, resp. $\xi^i\in\mathscr{A}_{n-2j}(F,\mathrm{Sym}_j(\mathfrak{g},V))_{\mathrm{equiv}}$, are the differential forms given by (*10) *for ϕ_m, resp. ψ_n, then*

$$\zeta^k:=\sum_{i+j=k}\chi^i\wedge_{\vee}\xi^j\in\mathscr{A}_{m+n-2k}(F,\mathrm{Sym}_k(\mathfrak{g},V))_{\mathrm{equiv}}$$

for $0\leqslant k\leqslant[m/2]+[n/2]$ (and $\zeta^{[(m+n)/2]}:=0$ if m and n are odd) are the corresponding forms for $\phi_m\wedge_{\vee}\psi_n$.

Proof: Obviously $\mathscr{A}(F,V)_{G-\mathrm{trans}}$ is a $\mathbb{R}$-subspace of $\mathscr{A}(F,V)$. Hence we only have to check if the ζ^k, for $0\leqslant k\leqslant[(m+n)/2]$, obey the identities (10) for $\phi_m\wedge_{\vee}\psi_n=\phi_m\wedge_{\varphi}\psi_n\in\mathscr{A}_{m+n}(F,V)_{\mathrm{inv}}$. Obviously $\phi_m\wedge_{\vee}\psi_n$ is closed and $\zeta^0=\chi^0\wedge_{\vee}\xi^0=\phi_m\wedge_{\vee}\psi_n$. By definition of $\wedge_{\vee}$, the differential forms ζ^k are elements of $\mathscr{A}_{m+n-2k}(F,\mathrm{Sym}_k(\mathfrak{g},V))$ and

$$L_g^{\star}\zeta^k=\sum_{i+j=k}L_g^{\star}\chi^i\wedge_{\vee}L_g^{\star}\xi^j=\sum_{i+j=k}(\mathrm{Ad}(g^{-1})^{\star})_{\star}\chi^i\wedge_{\vee}(\mathrm{Ad}(g^{-1})^{\star})_{\star}\xi^j=(\mathrm{Ad}(g^{-1})^{\star})_{\star}\zeta^k,$$

whence all ζ^k are G-equivariant. Next for $0\leqslant k\leqslant[m/2]+[n/2]-1$, we obtain from Lemma IV.5, using $d\chi^0=d\xi^0=0$,

$$
\begin{aligned}
d\zeta^{k+1} &= \sum_{i+j=k+1} d(\chi^i \wedge_\vee \xi^j) \\
&= \sum_{i+j=k+1} [d\chi^i \wedge_\vee \xi^j + (-1)^{m-2i} \chi^i \wedge_\vee d\xi^j] \\
&= d\chi^0 \wedge_\vee \xi^{k+1} + \sum_{i+j=k} [d\chi^{i+1} \wedge_\vee \xi^j + (-1)^m \chi^i \wedge_\vee d\xi^{j+1}] \\
&\quad + (-1)^m \chi^{k+1} \wedge_\vee d\xi^0 \\
&= -\sum_{i+j=k} [L_\bullet^\vee \chi^i \wedge_\vee \xi^j + (-1)^m \chi^i \wedge_\vee L_\bullet^\vee \xi^j] \\
&= -\sum_{i+j=k} L_\bullet^\vee (\chi^i \wedge_\vee \xi^j) = -L_\bullet^\vee \zeta^k.
\end{aligned}
$$

Analogously, since $L_\bullet^\vee \chi^{[m/2]} = L_\bullet^\vee \xi^{[n/2]} = 0$,

$$
\begin{aligned}
L_\bullet^\vee \zeta^{[m/2]+[n/2]} &= \sum_{i+j=[m/2]+[n/2]} L_\bullet^\vee (\chi^i \wedge_\vee \xi^j) \\
&= L_\bullet^\vee \chi^{[m/2]} \wedge_\vee \xi^{[n/2]} + (-1)^m \chi^{[m/2]} \wedge_\vee L_\bullet^\vee \xi^{[n/2]} = 0.
\end{aligned}
$$

But $[m/2]+[n/2]=[(m+n)/2]$, except if m and n are both odd, where $[m/2]+[n/2]=[(m+n)/2]-1$. In that case, we have just shown that $-L_\bullet^\vee \zeta^{[(m+n)/2]-1}=0$, whence we may choose $\zeta^{[(m+n)/2]} := 0$. This completes the proof that $\phi_m \wedge_\vee \psi_n$ is G-transgressive. □

Now we are ready for the following theorem:

Theorem IV.7: *Let Γ be a connection on a principal bundle $P(M,G)$ and $B=P\times_G F$ an associated bundle with left Lie group action $L: G\times F \to F$. Let V denote any vector space. If the form $\phi_n \in \mathscr{A}_n(F,V)_{\text{inv}}$ is G-transgressive and the equivariant forms $\chi^i_{n-2i} \in \mathscr{A}_{n-2i}(F, \text{Sym}_i(\mathfrak{g},V))_{\text{equiv}}$ are given by (*10), then

$$
\phi_n^A := \sum_{i=0}^{[n/2]} (\chi^i_{n-2i} v) \bullet \mathrm{F} \in \mathscr{A}_n(B,V)
$$

is closed and Γ-adapted. Its restriction to the fibers is ϕ_n, i.e., for any $\alpha \in A$ and all $x \in U_\alpha$, we have $i^\star_{\alpha,x} \phi_n^A = \phi_n$.

Proof: ϕ_n^A is obviously adapted to Γ. Furthermore Theorem III.3 yields

$$
\begin{aligned}
d\phi_n^A &= \sum_{i=0}^{[n/2]} (d\chi^i_{n-2i}) v \bullet \mathrm{F} + (L_\bullet^\vee \chi^i_{n-2i}) v \bullet \mathrm{F} \\
&= (d\phi_n) v + \sum_{i=0}^{[n/2]-1} (d\chi^{i+1}_{n-2i-2} + L_\bullet^\vee \chi^i_{n-2i}) v \bullet \mathrm{F} + (L_\bullet^\vee \chi^{[n/2]}_{n-2[n/2]}) v \bullet \mathrm{F} = 0,
\end{aligned}
$$

since ϕ_n is G-transgressive. Finally, since $i^\star_{\alpha,x} \pi^\star \mathrm{F}^\alpha = 0$ for all $x \in U_\alpha$, we obtain $i^\star_{\alpha,x} \phi_n^A = i^\star_{\alpha,x}(\chi^0 v) = i^\star_{\alpha,x}(\phi_n v)$. But naturally $i^\star_{\alpha,x}(\phi_n v) = \phi_n$. □

Note that the property of being G-transgressive only depends on L and F. Thus G-transgressive forms define de Rham cohomology classes on all fiber bundles where L is the

action of the structure group G on the fiber F. In particular, this condition is independent of the base M and of the question whether the bundle is trivial or not. Indeed we have the following:

Corollary IV.8: Let $L:G\times F\to F$ be a left Lie group action. If a form $\phi_n \in \mathscr{A}_n(F)$ is G-transgressive, it is 0-transgressive for any bundle $B(M,F,G)$ that comes along with L. Thus ϕ_n defines a unique cohomology class $[\phi_n^A] \in H^n(B)$ with $[i_{\alpha,x}^\star][\phi_n^A]=[\phi_n] \in H^n(F)$, independently of the paracompact base M and the transition functions $g_{\alpha\beta}$.

Proof: By the existence theorem for connections, every principal bundle $P(M,G)$ over a paracompact manifold M admits a connection Γ (Ref. 5, p. 67). Thus ϕ_n^A is well-defined and Theorem IV applies. □

Corollary IV.9: If Γ and Γ' are two connections on $P(M,G)$ and $\phi\in\mathscr{A}(F)$ is G-transgressive, then there exists $\psi \in \mathscr{A}(B)$ such that the forms ϕ^A and $\phi^{A'}$ obey:

$$\phi^A-\phi^{A'}=d\psi \quad \text{with} \quad d(i_{\alpha,x}^\star\psi)=0.$$

Let us derive the analogue to Theorem IV.7 for 1-dimensional Abelian Lie groups G like the electromagnetic structure group $G_{\text{em}}\cong \mathrm{U}_1\cong \mathbb{S}^1$. According to the following lemma, we may reformulate the notion of G-transgressive forms in that case:

Lemma IV.10: If G is Abelian with $\mathfrak{g}=E\mathbb{R}$, then $\phi_n\in\mathscr{A}(F,V)_{\text{inv}}$ is G-transgressive iff $\chi^i \in \mathscr{A}_{n-2i}(F,V)_{\text{inv}}$ exist for $0\leqslant i\leqslant[n/2]$ such that with $\nu^i:=\imath_{\mathscr{Z}_E}\chi^i$ the following equations hold:

$$\chi^0=\phi_n,\ -\nu^i=d\chi^{i+1} \text{ for all } \ 0\leqslant i\leqslant[n/2]-1 \text{ and} \nu^{[n/2]}=0. \tag{11}$$

Also since $\mathfrak{g}\cong\mathbb{R}$, we can replace $\bullet$ by the exterior product and as a corollary to Theorem IV.7 and Lemma II.2 we obtain the following.

Theorem IV.11: *Let Γ be a connection on a principal bundle $P(M,G)$, where G is Abelian with $\mathfrak{g}=E\mathbb{R}$, and let $B=P\times_G F$ be any associated bundle with left Lie group action $L:G\times F\to F$. If $\phi_n \in \mathscr{A}_n(F,V)_{\text{inv}}$ is G-transgressive and $\chi^i_{n-2i} \in \mathscr{A}_{n-2i}(F,V)_{\text{inv}}$ are given by (11), then with $\widetilde{\mathrm{F}}:=1/E\ \pi^\star\mathrm{F} \in \mathscr{A}_2(B)$,*

$$\phi_n^A=\sum_{i=0}^{[n/2]}(\chi^i_{n-2i}v)\underbrace{\widetilde{\mathrm{F}}\wedge\cdots\wedge\widetilde{\mathrm{F}}}_{i}$$

$$=\sum_{i=0}^{[n/2]}\underbrace{\widetilde{\mathrm{F}}\text{-}\wedge\cdots\wedge\widetilde{\mathrm{F}}}_{i}\wedge(\chi^i_{n-2i}v)\in\mathscr{A}_n(B,V)$$

is closed and Γ-adapted. Its restriction to the fibers is ϕ_n, i.e., for any $x \in U_\alpha$, $i_{\alpha,x}^\star\phi_n^A=\phi_n$.

Finally, in order to evaluate Theorem IV.11, we note that for any form $\phi\in\mathscr{A}(F,V)$, the vertical projections (8) are given by

$$\phi v|_{\pi^{-1}(U_\alpha)}=(\pi_\alpha^\star\phi)v^\alpha=\pi_\alpha^\star\phi+\widetilde{\mathrm{A}}^\alpha\wedge\pi_\alpha^\star(\imath_{\mathscr{Z}_E}\phi) \tag{12}$$

with $\widetilde{\mathrm{A}}^\alpha:=1/E\ \pi^\star\mathrm{A}^\alpha$.[7] Hence, since $(\imath_{\mathscr{Z}_E})^2=0$, we have $(\imath_{\mathscr{Z}_E}\phi)v|_{\pi^{-1}(U_\alpha)}=\pi_\alpha^\star(\imath_{\mathscr{Z}_E}\phi)$.

V. SKYRMION BUNDLE AND RELATED YANG–MILLS THEORIES

These results are quite important for the skyrmion bundle in theoretical nuclear physics which treats interactions of mesons and baryons — described within the (ungauged) Skyrme model[1,3] —

with electromagnetic fields.[11–13] In order to show this, we need some basic results from current algebra. Denote the left and right invariant 1-forms on a Lie group $H \leqslant \mathrm{Gl}_n(\mathbb{C})$ by $\Theta^L \in \mathscr{A}_1^L(H,\mathfrak{h})$, resp., $\Theta^R \in \mathscr{A}_1^R(H,\mathfrak{h})$, i.e.,

$$\Theta_h^L(h\cdot X)=\Theta_h^R(X\cdot h)=X \quad \text{for all} \quad h\in H, X\in\mathfrak{h},$$

where $h\cdot X$ and $X\cdot h$ are elements of $T_h(H)$. In the literature, these forms are also called invariant ''currents'' and we find the notations $h^{-1}dh$ and L for Θ^L, resp., dhh^{-1} and R for Θ^R. If $\wedge$ denotes the exterior product of matrix-valued forms with respect to matrix multiplication, then for all $k\in\mathbb{N}$,

$$(\Theta^L)^k := \underbrace{\Theta^L\wedge\cdots\wedge\Theta^L}_{k} \in \mathscr{A}_k^L(H,\mathbb{C}^{n\times n})$$

and

$$(\Theta^R)^k := \underbrace{\Theta^R\wedge\cdots\wedge\Theta^R}_{k} \in \mathscr{A}_k^R(H,\mathbb{C}^{n\times n})$$

are well-defined left, resp., right, invariant k-forms on H, and so are

$$\lambda_k^M := \mathrm{Tr}[M\cdot(\Theta^L)^k]\in\mathscr{A}_k^L(H,\mathbb{C})$$

and

$$\rho_k^M := \mathrm{Tr}[M\cdot(\Theta^R)^k]\in\mathscr{A}_k^R(H,\mathbb{C}),$$

for any matrix $M\in\mathbb{C}^{n\times n}$. Especially for $M=\mathbb{1}$, we obtain the bi-invariant

$$\omega_k := \lambda_k^{\mathbb{1}}=\rho_k^{\mathbb{1}}\in\mathscr{A}_k(H,\mathbb{C})_{\mathrm{inv}},$$

and one easily checks that $\omega_{2k}=0$. Now the Maurer–Cartan identities yield the following.

Lemma V.1: $d(\Theta^L)^{2k-1}=-(\Theta^L)^{2k}$ *and* $d(\Theta^R)^{2k-1}=(\Theta^R)^{2k}$. *As a consequence for any matrix* $M\in\mathbb{C}^{n\times n}$, *we have* $d\lambda_{2k-1}^M=-\lambda_{2k}^M$, $d\rho_{2k-1}^M=\rho_{2k}^M$ *hence* $d\omega_{2k-1}=0$ *and* $d\lambda_{2k}^M=d\rho_{2k}^M=0$.

In addition, recall that the cohomology of SU_n and U_n is generated as an algebra by ω_3, ω_5, $\ldots$, ω_{2n-1} for SU_n, resp., by ω_1, ω_3, $\ldots$, ω_{2n-1} for U_n, cf. Greub, Halperin, and Vanstone.[14]

In the ungauged Skyrme model, the meson fields occur as maps $U:M\to\mathrm{SU}_n$, where M denotes space–time and n denotes the number of flavors in QCD. The configuration $U\equiv\mathbb{1}$ represents the vacuum. Baryons appear as topological soliton solutions, as ''skyrmions,'' of these fields. The number of baryons represented by a given mesonic field configuration is computed by an integration of $U^\star\omega_3$ over the space manifold (which is compactified at infinity, where the fields are required to tend to the vacuum value $\mathbb{1}$). For $n\geqslant 3$, the action integral splits into two parts, the nonamomalous action and the Wess–Zumino term. The latter is an integral over the differential form ω_5.[2]

In order to treat interactions with electromagnetic fields (especially those of magnetic monopoles,[11,12]) one constructs a fiber bundle $B(M,\mathrm{SU}_n,G_{\mathrm{em}})$, cf. Section I. If e denotes the electric unit charge, then the left action of $G_{\mathrm{em}}=1/e\cdot\mathbb{S}^1$ on SU_n is given by the inner automorphisms

$$L(g,U):=e^{-iegQ}Ue^{+iegQ} \tag{13}$$

for $g\in G_{\mathrm{em}}$ and $U\in\mathrm{SU}_n$. Q is the $n\times n$-matrix containing the quark charges in units of e: for $n=2,3$,

$$Q=\begin{pmatrix} \frac{2}{3} & 0 \\ 0 & -\frac{1}{3} \end{pmatrix}, \text{ resp., } Q=\begin{pmatrix} \frac{2}{3} & 0 & 0 \\ 0 & -\frac{1}{3} & 0 \\ 0 & 0 & -\frac{1}{3} \end{pmatrix}.$$

We put $\phi^\alpha:=\pi_\alpha^\star\phi$ for any $\phi\in\mathscr{A}(F,V)$. Under a change of bundle charts we then have

$$U^\alpha(x)=L(g_{\alpha\beta},U^\beta)(x)=e^{-ieg_{\alpha\beta}(x)Q}U^\beta(x)e^{+ieg_{\alpha\beta}(x)Q},$$

and for the canonical vector field $\mathscr{S}_E\in\mathscr{D}^1(\mathrm{SU}_n)$ induced by $E=1/e\in\mathfrak{g}$, we obtain

$$\mathscr{S}_E(U)=-i[Q,U] \text{ for all } U\in\mathrm{SU}_n. \tag{14}$$

Now (12) yields

$$(dU^\alpha)v=dU^\alpha-ie\mathrm{A}^\alpha[Q,U^\alpha].$$

For the invariant forms ρ_k^Q, λ_k^Q and ω_{2k+1}, we obtain the following lemma:[13]

*Lemma V.2: For the action given in (*13),

$$\imath_{\mathscr{S}_E}\omega_{2k+1}=-(2k+1)i(\rho_{2k}^Q-\lambda_{2k}^Q),$$

$$\imath_{\mathscr{S}_E}(\rho_{2k}^Q-\lambda_{2k}^Q)=0,$$

$$\begin{aligned}\imath_{\mathscr{S}_E}(\rho_{2k+1}^Q+\lambda_{2k+1}^Q)=&-2i\sum_{j=1}^{k}\mathrm{Tr}[QU(\Theta^L)^{2j-1}Q(\Theta^L)^{2k-2j+1}U^{-1}]\\&-i\sum_{j=0}^{k}\mathrm{Tr}[Q(\Theta^R)^{2j}Q(\Theta^R)^{2k-2j}-Q(\Theta^L)^{2j}Q(\Theta^L)^{2k-2j}].\end{aligned}$$

In order to define a baryon number and an anomalous action for the skyrmion bundle, we have to extend the forms ω_3 and ω_5 to the bundle. Several approaches ''by trial and error'' have been made to ''generalize'' ω_3 and ω_5, cf. Callan and Witten,[11] Kaymakcalan *et al.*,[15] or Pak and Rossi.[16] In terms of the language we are using, we would like to obtain differential forms ω_3^{A} and ω_5^{A} that are adapted to the Maxwell connection given by the electromagnetic fields. Thus we will examine whether ω_3 and ω_5 are G_{em}-transgressive.

This is indeed the case. According to Lemma IV.10 we have to find $\chi_{n-2i}^i\in\mathscr{A}_n(\mathrm{SU}_n,\mathbb{C})$ and $\nu_{n-2i-1}^i=\imath_{\mathscr{S}_E}\chi_{n-2i}^i$ that obey (11) for $\phi=\omega_3$, resp., $\phi=\omega_5$. From Lemma V.2 we conclude that for $\phi=\omega_{2k+1}$, we have $\nu_{2k}^0=-(2k+1)i(\rho_{2k}^Q-\lambda_{2k}^Q)$. Now Lemma V.1 yields that

$\rho^Q_{2k}-\lambda^Q_{2k}=d(\rho^Q_{2k-1}+\lambda^Q_{2k-1})$, so $\chi^1_{2n-1}=(2k+1)i(\rho^Q_{2k-1}+\lambda^Q_{2k-1})$. For ω_3 we are already done, since χ^1_1 is global and vertical due to Lemma V.2: $\nu^1_0=0$. For χ^1_3, again Lemma V.2 yields $\nu^2_2=-10i^2\mathrm{Tr}[Q^2((\Theta^R)^2-(\Theta^L)^2)+QdU^{-1}\wedge QdU]$. One easily verifies that

$$\chi^2_1=10i^2(\rho_1^{Q^2}+\lambda_1^{Q^2})+5i^2\mathrm{Tr}(QdUQU^{-1}-QUQdU^{-1})+ri^2d\mathrm{Tr}(QU^{-1}QU),r\in\mathbb{R},$$

is an admissible choice and that $\nu^2_0=0$, thus χ^2_1 is global and vertical. For physical reasons (parity invariance[15]), we put $r=0$. We thus obtain from Theorem IV.11:[13] the following.

Theorem V.3: *ω_3 and ω_5 are G_{em}-transgressive and generate de Rham cohomology groups isomorphic to $\mathbb{R}$ for any skyrmion bundle. Representatives for the generated cohomology groups, that are adapted to the Maxwell connection, are*

$$\begin{aligned}\omega^{\mathrm{A}}_3&=\omega_3 v+ie\mathrm{F}\wedge\chi^1_1 v\\&=[\omega^\alpha_3-3ie\mathrm{A}^\alpha\wedge(\rho^Q_2-\lambda^Q_2)]+3ie\mathrm{F}\wedge(\rho^Q_1+\lambda^Q_1),\end{aligned}$$

$$\begin{aligned}\omega^{\mathrm{A}}_5&=\omega_5 v+ie\mathrm{F}\wedge\chi^1_3 v+(ie)^2\mathrm{F}\wedge\mathrm{F}\wedge\chi^2_1 v\\&=[\omega^\alpha_5-5ie\mathrm{A}^\alpha\wedge(\rho^Q_4-\lambda^Q_4)]+5ie\mathrm{F}\wedge\{(\rho^Q_3+\lambda^Q_3)^\alpha\\&\quad-2ie\mathrm{A}^\alpha\wedge\mathrm{Tr}[Q^2((\Theta^R)^2-(\Theta^L)^2)+QdU^{-1}\wedge QdU]^\alpha\}+5(ie)^2\mathrm{F}\wedge\mathrm{F}\wedge[2(\rho_1^{Q^2}+\lambda_1^{Q^2})^\alpha\\&\quad+\mathrm{Tr}(QdUQU^{-1}-QUQdU^{-1})^\alpha].\end{aligned}$$

In fact, one can prove that all differential forms ω_{2k-1} are G_{em}-transgressive.[17]

In comparison to the literature cited, our formalism has led to quite compact notations for ω^{A}_3 and ω^{A}_5. This advantage becomes even more obvious when generalizations to other gauge groups, especially non-Abelian gauge groups, are considered, e.g., instead of $G\cong\mathbb{S}^1$ and $F=\mathrm{SU}_n$ take a Yang–Mills theory where $G=\mathrm{U}^L_n\times\mathrm{U}^R_n$ and $F=\mathrm{U}_n$ with $L_{(g_L,g_R)}(U)=g_LUg_R^{-1}$. As a generalization of (14) we have for all $(X_L,X_R)\in\mathrm{u}^L_n\oplus\mathrm{u}^R_n$

$$\mathscr{L}_{(X_L,X_R)}(U)=X_LU-UX_R\quad\text{for all}\quad U\in\mathrm{SU}_n.\tag{15}$$

Now the gauge fields take their values in $\mathrm{u}^L_n\oplus\mathrm{u}^R_n$, i.e., $\mathrm{A}^\alpha=(\mathrm{A}^\alpha_L,\mathrm{A}^\alpha_R)\in\mathscr{A}(U_\alpha,\mathrm{u}^L_n\oplus\mathrm{u}^R_n)$ define the connection Γ on $P(M,G)$. In this case, omitting the superscripts α, we obtain $dUv=dU+\mathrm{A}_LU-U\mathrm{A}_R$, hence

$$\Theta^Lv=\Theta^L+U^{-1}\mathrm{A}_LU-\mathrm{A}_R,$$

$$\Theta^Rv=\Theta^R+\mathrm{A}_L-U\mathrm{A}_RU^{-1},$$

$$\omega_1v=\omega_1+\mathrm{Tr}(\mathrm{A}_L-\mathrm{A}_R).$$

Moreover, we have $L_\bullet\omega_1=\mathrm{Tr}(\pi_L-\pi_R)$ with the projections $\pi^{L/R}:\mathfrak{g}=\mathrm{u}^L_n\oplus\mathrm{u}^R_n\to\mathrm{u}^{L/R}_n$. Thus for any LIE subgroup $H<G$, the closed invariant form ω_1 is H-transgressive iff $\mathrm{Tr}(X_L-X_R)=0$ for all $(X_L,X_R)\in\mathfrak{h}$, e.g., we could choose a subgroup of the diagonal $D_n=\mathrm{U}^L_n\times\mathrm{U}^L_n$ in G such that $g_L=g_R$ for all $(g_L,g_R)\in D_n$. (Note that this is the case for the skyrmion bundle.) Or we could choose $H=\mathrm{SU}^L_n\times\mathrm{SU}^R_n$, resp., a subgroup of H. In Section VII we will prove that in the latter case, ω_1 is necessarily H-transgressive because $\mathrm{SU}^L_n\times\mathrm{SU}^R_n$ is semisimple for $n>2$, cf. Theorem VII.4.

For ω_3 we obtain $L_\bullet\omega_3=3\mathrm{Tr}[(\Theta^R)^2\pi^L-(\Theta^L)^2\pi^R]$, thus

$$\chi^1_1:=-3\mathrm{Tr}(\Theta^R\pi^L+\Theta^L\pi^R)\in\mathscr{A}_1(\mathrm{U}_n,\mathrm{Hom}(\mathfrak{g},\mathbb{C}))$$

obeys $d\chi_1^1 = -L_\bullet \omega_3$ due to Lemma V.1. Omitting the symmetrization $\vee$, we compute $L_\bullet^\vee \chi_1^1 = 3\mathrm{Tr}(\pi^R\pi^R - \pi^L\pi^L)$, i.e.,

$$(L_\bullet^\vee \chi_1^1)((X_L,X_R),(Y_L,Y_R)) = 3\mathrm{Tr}(X_R Y_R - X_L Y_L) \neq 0.$$

Thus ω_3 is not G-transgressive. In fact, take any $\tilde{\chi}_1^1 \in \mathscr{A}_1(U_n, \mathrm{Hom}(\mathfrak{g},\mathbb{C}))_{\mathrm{equiv}}$ with $d\tilde{\chi}_1^1 = -L_\bullet \omega_3$. Then $\xi_1^1 := \tilde{\chi}_1^1 - \chi_1^1 \in \mathscr{A}_1(U_n, \mathrm{Hom}(\mathfrak{g},\mathbb{C}))_{\mathrm{equiv}}$ with $d\xi_1^1 = 0$. Since $H^1(\mathrm{SU}_n) = 0$, we find $\xi_0^1 \in C^\infty(U_n, \mathrm{Hom}(\mathfrak{g},\mathbb{C}))$ with $d\xi_0^1 = \xi_1^1$. In fact, we may choose ξ_0^1 equivariant, because SU_n is compact, analogously to (9). But then for all $X, Y \in \mathfrak{g}$,

$$\begin{aligned} L_\bullet^\vee \xi_1^1(X,Y) &= (\imath_{\mathscr{L}_X} d\xi_0^1)(Y) + (\imath_{\mathscr{L}_Y} d\xi_0^1)(X) \\ &= \mathscr{L}_X(\xi_0^1)(Y) + \mathscr{L}_Y(\xi_0^1)(X) \\ &= \xi_0^1([Y,X]) + \xi_0^1([X,Y]) = 0. \end{aligned}$$

Thus $(L_\bullet^\vee \tilde{\chi}_1^1) = (L_\bullet^\vee \chi_1^1) \neq 0$. Since ω_3 is not G-transgressive, the generated Γ-adapted form

$$\omega_3^{\mathrm{A}} = \omega_3 v + \chi_1^1 v \bullet \mathrm{F} \in \mathscr{A}_3(B(M, \mathrm{U}_n, G), \mathbb{C})$$

is not closed in general: $d\omega_3^{\mathrm{A}} = (L_\bullet^\vee \chi_1^1) v \bullet \mathrm{F} = (L_\bullet^\vee \chi_1^1) \bullet \mathrm{F}$. Yet if we again restrict L to a subgroup $H < G$ with generators $X^\sigma = (X_L^\sigma, X_R^\sigma)$, $\sigma \in I$, such that $\mathrm{Tr}(X_L^\sigma X_L^\tau) = \mathrm{Tr}(X_R^\sigma X_R^\tau)$ for all $\sigma, \tau \in I$, then $L_\bullet^\vee \chi_1^1 = 0$ and ω_3 is H-transgressive. Note that this condition holds for any subgroup of the diagonal D_n and thus for the skyrmion bundle.

Finally, some cumbersome calculations show that the voluminous expressions for the Wess-Zumino term in Ref. 15, (4.18), resp., Ref. 2, (24), are equal to the integral over the Γ-adapted differential form

$$\omega_5^{\mathrm{A}} = \omega_5 v + \chi_3^1 v \bullet \mathrm{F} + \chi_1^2 v \bullet \mathrm{F} \in \mathscr{A}_5(B(M, \mathrm{U}_n, G), \mathbb{C}),$$

where the forms $\chi_{5-2l}^l \in \mathscr{A}_{5-2l}(\mathrm{U}_n, \mathrm{Sym}_l(\mathfrak{g},\mathbb{C}))_{\mathrm{equiv}}$ are given by

$$\chi_3^1 := -5\mathrm{Tr}[(\Theta^R)^3 \pi^L + (\Theta^L)^3 \pi^R],$$

$$\chi_1^2 := 10\mathrm{Tr}[(\Theta^R)\pi^L\pi^L + (\Theta^L)\pi^R\pi^R] + 5\mathrm{Tr}(dU\pi^R U^{-1}\pi^L - d(U^{-1})\pi^L U \pi^R).$$

Analogously to the skyrmion case, one may add a term

$$r[d\mathrm{Tr}(\pi^L U \pi^R U^{-1}) v] \bullet \mathrm{F} = r d\mathrm{Tr}(F_L U F_R U^{-1}), r \in \mathbb{C},$$

or exclude it by parity invariance.[15] Also in this case, the differential form ω_5 is not G-transgressive: we obtain $L_\bullet^\vee \chi_1^2 = 10\mathrm{Tr}(\pi^L\pi^L\pi^L - \pi^R\pi^R\pi^R)$, thus again ω_5 is H-transgressive for any subgroup $H \leqslant D$. More generally, ω_5 is H-transgressive if and only if the generators of H obey $\mathrm{Tr}(X_L^\sigma X_L^\tau X_L^\upsilon) = \mathrm{Tr}(X_R^\sigma X_R^\tau X_R^\upsilon)$ for all $\sigma, \tau, \upsilon \in I$, specifically, only if $\mathrm{Tr}[(X_L^\sigma)^3] = \mathrm{Tr}[(X_R^\sigma)^3]$ for all $\sigma \in I$, which is the usual condition for cancellation of anomalies on the quark level.[2]

Nevertheless note that $d\omega_5^{\mathrm{A}} = (L_\bullet^\vee \chi_1^2) \bullet \mathrm{F}$ consists of a 6-form on the base. Thus as long as we stick to space–time M — or even a five-dimensional extension — this form vanishes and ω_5^{A} is in fact closed. The same holds for ω_3^{A}: although it might not be closed on space–time M, ω_3^{A} is closed, of course, when restricted to three-dimensional space.

VI. LIE ALGEBRA COHOMOLOGY

Back to the general case, we want to derive which closed invariant n-forms ϕ_n on the fiber F are G-transgressive in the cases where $n=0$, 1 or 2. To this purpose we need some basic results on Lie algebra cohomology.

Suppose $\mathfrak{g}$ is a $\mathbb{K}$-Lie algebra (for $\mathbb{K}=\mathbb{R},\mathbb{C}$) and $l:\mathfrak{g}\to\mathrm{gl}(V)$ is a (left) representation of $\mathfrak{g}$ on a (possibly infinte dimensional) $\mathbb{K}$-vector space V. Then $\mathrm{Alt}(\mathfrak{g},V)=\oplus_{p=0}^{\infty}\mathrm{Alt}_p(\mathfrak{g},V)$ becomes a differential complex C_l with the following differential operator $\mathbf{d}^l=(\mathbf{d}_p^l: C_l^p\to C_l^{p+1})_{p\in\mathbb{N}_0}$: for $c\in C_l^p:=\mathrm{Alt}_p(\mathfrak{g},V)$ and $X_i\in\mathfrak{g}$,

$$\mathbf{d}_p^l c(X_1,\ldots,X_{p+1}):=\sum_{i=1}^{p+1}(-1)^{i+1}l(X_i)(c(\ldots,\widehat{X_i},\ldots))+\sum_{i=1}^{p}\sum_{j=i+1}^{p+1}(-1)^i c(\ldots,\widehat{X_i},\ldots,X_{j-1},[X_i,X_j],X_{j+1},\ldots)$$

(where $\widehat{\ }$ indicates that the term is omitted).

Our definition of $\mathbf{d}^l$ differs slightly from the definitions in Ref. 14, resp., in Hilgert and Neeb,[18] where analogously to the definition of the exertior derivative d, the second term reads

$$+\sum_{i=1}^{p}\sum_{j=i+1}^{p+1}(-1)^{i+j}c([X_i,X_j],X_1,\ldots,\widehat{X_i},\ldots,\widehat{X_j},\ldots).$$

Obviously both definitions coincide on C_l. Nevertheless with our definition not only $\mathrm{Alt}(\mathfrak{g},V)$ becomes a differential complex, but also $\mathrm{Hom}(\mathscr{T}(\mathfrak{g}),V)$ becomes a complex C_l with subcomplex C_l. [$\mathscr{T}(\mathfrak{g})$ denotes the tensor algebra of $\mathfrak{g}$.] Indeed we can prove — analogously to the proof for $d^2=0$ — that $\mathbf{d}_{p+1}^l\circ\mathbf{d}_p^l=0$ on C_l for any representation $l:\mathfrak{g}\to\mathrm{gl}(V)$ of $\mathfrak{g}$. Now the cohomology of this complex, $H_l^p(\mathfrak{g},V):=H_{\mathbf{d}}^p(C_l)$ is called the pth (Chevalley) cohomology space of $\mathfrak{g}$ with values in V with regard to l. We put $H_l^p(\mathfrak{g}):=H_l^p(\mathfrak{g},\mathbb{K})$. Analogously, $\overline{H_l^p}(\mathfrak{g},V):=\overline{H_{\mathbf{d}}^p}(C_l)$ and $\overline{H_l^p}(\mathfrak{g}):=\overline{H_l^p}(\mathfrak{g},\mathbb{K})$.

Lemma VI.1: Let $o:\mathfrak{g}\to\mathrm{gl}(V)$ denote the trivial representation of $\mathfrak{g}$. Then

(1) $H_o^0(\mathfrak{g},V)=\overline{H_o^0}(\mathfrak{g},V)=V$.
(2) $H_o^1(\mathfrak{g},V)=\overline{H_o^1}(\mathfrak{g},V)=\{c\in\mathrm{Hom}(\mathfrak{g},V)\,|\,c([\mathfrak{g},\mathfrak{g}])=\{0\}\leqslant V\}=[\mathfrak{g},\mathfrak{g}]^{\perp}$, *thus $\mathbf{d}_1^o$ is injective and $H_o^1(\mathfrak{g},V)=\{0\}$ for all Lie algebras $\mathfrak{g}$ with $\mathfrak{g}=[\mathfrak{g},\mathfrak{g}]$*, e.g., *semisimple Lie algebras.*
(3) *If $\mathfrak{a}$ is Abelian, then $H_o^p(\mathfrak{a},V)=\mathrm{Alt}_p(\mathfrak{a},V)$ and $H_o^p(\mathfrak{a},V)=\mathrm{Hom}(\otimes^p\mathfrak{a},V)$.*

Moreover, if V is finite dimensional, then Whitehead's lemmas yield that $H_l^1(\mathfrak{g},V)=H_l^2(\mathfrak{g},V)=0$ for any representation $l:\mathfrak{g}\to\mathrm{gl}(V)$ of a semisimple Lie algebra $\mathfrak{g}$.

Recall that a double complex $C^{*,*}:=\oplus_{p,q\in\mathbb{N}_0}C^{p,q}$ is a doubly graded differential complex with two commuting differential operators, a horizontal operator $\delta:C^{p,q}\to C^{p+1,q}$ and a vertical operator $d:C^{p,q}\to C^{p,q+1}$. Every double complex is associated with a singly graded complex C^* by summing along the antidiagonal lines, i.e., C^n is given by $C^n=\oplus_{p+q=n}C^{p,q}$. The (total) cohomology of such a double complex is then defined to be the cohomology of the associated singly graded complex with regard to the differential operator $D=\delta+(-1)^p d$ on $C^{p,q}$. Note that indeed $D:C^n\to C^{n+1}$. The alternating sign guaranties that $D\circ D=0$.[6]

Given a Lie group action $L:G\times F\to F$, we want to combine the invariant cohomology on F with the Lie algebra cohomology of $\mathfrak{g}$. To this purpose, we form the double complex

$$C^{*,*}:=\mathscr{A}(F)\otimes\mathrm{Hom}(\mathscr{T}(\mathfrak{g}),V)=\oplus_{p,q\in\mathbb{N}_0}\mathscr{A}_q(F,\mathrm{Hom}(\otimes^p\mathfrak{g},V)).$$

$(-1)^p d_{(q)}: C^{p,q} \to C^{p,q+1}$ is the vertical operator, and for the horizontal operator we have $\delta := -\mathbf{d}^l_{(q)}: C^{p,q} \to C^{p+1,q}$. For the representation $l: \mathfrak{g} \to \mathrm{gl}(\mathscr{A}(F,V))$ several choices are possible. e. g., one can take the trivial representation o. Then $\mathbf{d}^o$ and d obviously commute.

Instead we choose l defined by $l(X) := -L_{\mathscr{L}_X}$, where $L_{\mathscr{X}}: \mathscr{A}(F,V) \to \mathscr{A}(F,V)$ denotes the Lie derivative of forms with respect to a vector field $\mathscr{X} \in \mathscr{D}^1(F)$. Recall that $L_{\mathscr{X}}$ is given by $L_{\mathscr{X}} = d \circ \imath_{\mathscr{X}} + \imath_{\mathscr{X}} \circ d$. Since Lie differentiation and exterior differentiation commute, δ and d commute on the double complex and define an operator D.

With regard to these operators we obtain (Ref. 8, Lemma 3.4) the following.

Lemma VI.2: For all $\omega_n \in \mathscr{A}_n(F,V)$ and all $i \leqslant n+1$,

$$L^i_\bullet d\omega_n - (-1)^i dL^i_\bullet \omega_n = \delta_{i-1} L^{i-1}_\bullet \omega_n .$$

$A^{*,*} := \mathscr{A}(F) \otimes \mathrm{Alt}(\mathfrak{g},V)$ is a subcomplex of $C^{*,*}$ and $A^{*,*}_{\mathrm{inv}} := \mathscr{A}(F)_{\mathrm{inv}} \otimes \mathrm{Alt}(\mathfrak{g},V)$ and $A^{*,*}_{\mathrm{equiv}} := \mathscr{A}(F)_{\mathrm{equiv}} \otimes \mathrm{Alt}(\mathfrak{g},V)$ are subcomplexes of $A^{*,*}$, on which the horizontal operators are given by $\delta = -\mathbf{d}^o$, resp., $\delta = +\mathbf{d}^o$.

Recall that a chain map $f: A \to B$ between two differential complexes A and B is a homomorphism that commutes with the differential operators of A and B: $f \circ D_A = D_B \circ f$, e.g., all pullbacks $f^\star: \mathscr{A}(M,V) \to \mathscr{A}(N,V)$ are chain maps.

Definition VI.3: For any Lie group action $L: G \times F \to F$, the homomorphism $\mathbf{L}: \mathscr{A}(F,V) \to \mathscr{A}(F) \otimes \mathrm{Alt}(\mathfrak{g},V)$ *is defined by* $\mathbf{L}\omega_n := \Sigma_{i=0}^n L^i_\bullet \omega_n$ *for all* $\omega_n \in \mathscr{A}_n(F,V)$.

The homomorphism $L^*_\bullet: \mathscr{A}(F,V) \to \mathrm{Alt}(\mathfrak{g},V)$ *is given by* $L^*_\bullet \omega := \Sigma_{n=0}^\infty L^n_\bullet \omega_n$ *for all* $\omega = \Sigma_{n=0}^\infty \omega_n$ *with* $\omega_n \in \mathscr{A}_n(F,V)$.

Let $p_0: \mathscr{A}(F) \otimes \mathrm{Alt}(\mathfrak{g},V) \to \mathscr{A}(P,V)$ denote the canonical projection. Since $p_0 \circ D = d \circ p_0$, p_0 is a chain map. Obviously $p_0 \circ \mathbf{L} = \mathrm{id}_{\mathscr{A}(F,V)}$, thus if $\mathbf{L}$ is a chain map, we obtain $[p_0] \circ [\mathbf{L}] = \mathrm{id}_{H^*(P,V)}$ and $[\mathbf{L}]$ is injective. Indeed we find the following.

Proposition VI.4:

(1) $\mathbf{L}$ *is a chain map and induces an injective homomorphism*

$$[\mathbf{L}]: H^*(F,V) \to H^*_D(\mathscr{A}(F) \otimes \mathrm{Alt}(\mathfrak{g},V)).$$

(2) $L^*_\bullet$ *is a chain map and thus induces a homomorphism*

$$[L^*_\bullet]: H^*(F,V) \to H^*_l(\mathfrak{g},V).$$

Proof:

(1) By Lemma VI.2 we have

$$\begin{aligned} D(\mathbf{L}\omega) &= \sum_{i=0}^n D(L^i_\bullet \omega_n) = \sum_{i=0}^n [\delta_i L^i_\bullet \omega_n + (-1)^i dL^i_\bullet \omega_n] \\ &= \sum_{i=0}^n [L^{i+1}_\bullet d\omega_n + (-1)^i dL^{i+1}_\bullet \omega_n + (-1)^i dL^i_\bullet \omega_n] \\ &= \sum_{i=0}^n (L^{i+1}_\bullet d\omega_n) + (-1)^n dL^{n+1}_\bullet \omega_n + d\omega_n \\ &= \mathbf{L}(d\omega_n) \end{aligned}$$

since $L^{n+1}_\bullet \omega_n = 0$.

(2) follows from Lemma VI.2 if we put $i = n+1$. □

Finally we find the following result with regard to our purposes:

Theorem VI.5: *If the Lie algebra* $\mathfrak{g}$ *is semisimple and the form* $\omega \in \mathscr{A}_2(F,V)_{\text{inv}}$ *is closed, then there exists a unique* $\chi \in \mathscr{A}_0(F,\text{Alt}_1(\mathfrak{g},V))_{\text{equiv}}$, *such that*

$$d\chi = -L_\bullet \omega \quad \text{and} \quad \delta\chi = L^2_\bullet \omega.$$

Proof: By Lemma VI.2, $\delta L^2_\bullet \omega = 0$ holds. Since $H^2_o(\mathfrak{g},V) = 0$ by Whitehead's second lemma, we find $\chi \in \mathscr{A}_0(F,\text{Alt}_1(\mathfrak{g},V))_{\text{equiv}}$ with $\delta\chi = L^2_\bullet \omega$. Lemma VI.1 yields that δ_1 is injective, so χ is unique. On the other hand we know from $D\mathbf{L}\omega = \mathbf{L}d\omega = 0$ that $-\delta L_\bullet \omega = dL^2_\bullet \omega = d\,\delta\chi = \delta d\chi$. Thus $d\chi + L_\bullet \omega \in \ker\delta_1$. But δ_1 is injective. □

VII. *G*-TRANSGRESSIVE *N*-FORMS FOR $N \leqslant 2$

Now we are prepared to compute which closed invariant n-forms ϕ_n, $n \leqslant 2$, on the fiber are G-transgressive.

$d\phi_0 = 0$ means that $\phi_0 \in C^\infty(F)$ is locally constant. Obviously $L^\vee_\bullet \phi_0 = 0$. So every closed G-invariant $\phi_0 \in C^\infty(F)$ is G-transgressive. Since ϕ_0 is invariant, it is global and vertical. Thus $(\phi_0^A)^\alpha = \pi_\alpha^\star \phi_0$ and $[i^\star_{\alpha,x}][\phi_0^A] = [\phi_0]$. This proves the following.

Lemma VII.1: Every closed G-invariant $\phi_0 \in C^\infty(F)$ *is G-transgressive and thus for any* $\alpha \in A$ *and* $x \in U_\alpha$, $[i^\star_{\alpha,x}]: H^0(B(M,F,G)) \to H^0_{\text{inv}}(F)$ *is surjective.*

[Note that this also implies $H^0_{\text{inv}}(F) \leqslant H^0(F)$, if we put $B := \{x\} \times F$, but this is nothing new.]

For $n = 1$ and $\phi_1 \in \mathscr{A}(F)_{\text{inv}}$, Lemma VI.2 yields that $d\phi_1 = 0$ implies $\mathbf{d}_1^0 L_\bullet \phi_1 = 0$, i.e., for all $f \in F$, $[L_\bullet \phi_1(f)] \in [\mathfrak{g},\mathfrak{g}]^\perp$ by Lemma VI.1. Thus for a semisimple Lie algebra $\mathfrak{g}$, $L_\bullet \phi_1 = 0$. As a consequence for any bundle $B(M,F,G)$ that comes along with L, $\{\pi_\alpha^\star \phi_1\}_{\alpha \in A}$ defines a global vertical form on B. We have proved the following.

Lemma VII.2: If L *is a Lie group action of a semisimple Lie group* G *on* F, *then every closed invariant* 1*-form* $\phi_1 \in \mathscr{A}_1(F)_{\text{inv}}$ *is G-transgressive and defines a unique cohomology class* $[\phi_1 v] = [\{\pi_\alpha^\star \phi_1\}_{\alpha \in A}] \in H^1(B)$ *for any bundle* $B(M,F,G)$ *that comes along with* L. *Thus for any* $x \in U_\alpha$, $[i^\star_{\alpha,x}]: H^1(B(M,F,G)) \to H^1_{\text{inv}}(F)$ *is surjective.*

To show that the condition ''G semisimple'' is necessary, take $G = \mathbb{S}^1 \cong \mathbb{R}/\mathbb{Z}$ acting on itself by left multiplication, thus $\mathfrak{g} = \mathbb{R}$. For every Lie group, the (left) canonical 1-form $\Theta^L \in \mathscr{A}_1(G,\mathfrak{g})$, defined by $\Theta^L_g(\mathscr{X}_g) := d\lambda_{g^{-1}}(\mathscr{X}_g)$, is (left) invariant by definition. Since $\mathbb{S}^1$ is Abelian, $d\Theta^L = 0$ in this case. Θ^L is the volume form on $\mathbb{S}^1$ and generates $H^1_{\text{inv}}(\mathbb{S}^1) \cong H^1(\mathbb{S}^1) \cong \mathbb{R}$, cf. Proposition IV.2. Yet $(L_\bullet \Theta^L)(X) = \Theta^L(\mathscr{L}_X) = X$ for all $X \in \mathbb{R}$. Thus $L_\bullet \Theta^L = \text{id}_{\mathbb{R}}$ and Θ^L is *not* $\mathbb{S}^1$-transgressive.

In fact, take the principal bundles $P_m(\mathbb{S}^2,\mathbb{S}^1)$, $m \in \mathbb{Z}$, that classify all fiber bundles over $\mathbb{S}^2$ with structure group $\mathbb{S}^1$ according to the Classification theorem (Ref. 4, p. 99). For $m = 0$ we have the trivial bundle $\mathbb{S}^2 \times \mathbb{S}^1$ and for $m = 1$ we obtain the Hopf fibering of the 3-sphere, $\pi: \mathbb{S}^3 \to \mathbb{S}^2$. For the de Rham cohomology $H^*(P_m)$ one obtains from the spectral sequence for P_m with $m \neq 0$:

$$H^0(P_m) \cong \mathbb{R}, \quad H^1(P_m) = 0, \quad H^2(P_m) = 0, \quad H^3(P_m) \cong \mathbb{R}.$$

So no $[i^\star_{\alpha,x}]: H^1(P_m) \to H^1_{\text{inv}}(G)$ is surjective. Moreover, we always have $\Theta^L v = \omega^\Gamma$, even for $m = 0$. Since $d\omega^\Gamma = d^\Gamma \omega^\Gamma = \Omega^\Gamma$, our canonical construction does not produce closed forms on P_m, in general.

Finally we consider the case $n = 2$ for semisimple Lie groups. Using Theorem VI.5 we obtain that every closed invariant 2-form on F is G-transgressive. Thus we have the following.

Corollary VII.3: If L *is a Lie group action of a semisimple Lie group* G *on* F, *then every closed invariant* 2*-form* $\phi_2 \in \mathscr{A}_2(F)_{\text{inv}}$ *is G-transgressive and defines a unique cohomology class* $[\phi_2^A] \in H^2(B)$ *for any bundle* $B(M,F,G)$ *that comes along with* L. *If* $\chi_0^1 \in C^\infty(F)_{\text{equiv}} \otimes \text{Hom}(\mathfrak{g},\mathbb{R})$ *is the unique map with* $d\chi_0^1 = -L_\bullet \phi_2$ *and* $\delta\chi_0^1 = L^2_\bullet \phi_2$ *according to* Theorem VI.5, *then* ϕ_2^A *is given by*

$$\phi_2^A = \phi_2 v + (\chi_0^1 v)\bullet \mathrm{F} \in \mathscr{A}_2(B).$$

Thus for any $x \in U_\alpha$, $[i_{\alpha,x}^\star]: H^2(B(M,F,G)) \to H^2_{\mathrm{inv}}(F)$ *is surjective.*

In view of Proposition IV.2 we thus have proved the following.

Theorem VII.4: *If* L *is a Lie group action of a semisimple Lie group* G *on* F*, then every closed invariant* $\phi_n \in \mathscr{A}_n(F)_{\mathrm{inv}}$, $n \leqslant 2$*, is* G*-transgressive and defines a unique cohomology class* $[\phi_n^A] \in H^n(B)$ *for any bundle* $B(M,F,G)$ *that comes along with* L*. For any* $x \in U_\alpha$, $[i_{\alpha,x}^\star]: H^n(B(M,F,G)) \to H^n_{\mathrm{inv}}(F)$ *is surjective.*

If in addition, G *is compact and connected, then* $H^n_{\mathrm{inv}}(F) \cong H^n(F)$*. Thus for every bundle* $B(M,F,G)$, $H^n(B)$ *contains a subgroup isomorphic to* $H^n(F)$ *for* $n \leqslant 2$.

Theorem VII.4 applies to QCD, where $G \cong \mathrm{SU}_3$ and to Yang–Mills theories with $G < \mathrm{SU}_n \times \mathrm{SU}_n$.

This theorem is sharp in the sense that it does not hold for $n = 3$, e.g., take $G = \mathbb{S}^3 \cong \mathrm{SU}_2$ acting on itself by left multiplication. Then the volume form on $\mathbb{S}^3$ is closed and invariant and generates $H^3(\mathbb{S}^3) \cong \mathbb{R}$. If this form were G-transgressive, then for all principal bundles $P(M,\mathbb{S}^3)$, the cohomology group $H^3(P)$ would contain a subgroup isomorphic to $\mathbb{R}$, independently of M and the transition functions $g_{\alpha\beta}$. Yet we know that $\mathbb{S}^7$ is a principal bundle over $\mathbb{S}^4$ with fiber $\mathbb{S}^3$, and $H^3(\mathbb{S}^7) = 0$. Thus the volume form on $\mathbb{S}^3$ cannot be G-transgressive.

VIII. FINAL REMARKS

According to Corollary IV.8, every G-transgressive form is 0-transgressive for all bundles with fiber and left action L. The reverse is also true for compact connected Lie groups. This can be proved, e.g., in terms of universal bundles, the Weil algebra and the equivariant cohomology of the G-manifold F.[9,10] In fact, G-transgressive forms are exactly those forms on F that generate equivariant cohomology classes (but not every equivariant cohomology class is generated by a form on F). Now there is a natural isomorphism between this equivariant cohomology and the de Rham cohomology of the universal bundle for the given left action L, which yields that equivariant cohomology classes define de Rham cohomology classes on all bundles that come with L.

We have not used these notions here for several reasons: First of all, we did not want to restrict ourselves *a priori* to compact connected Lie groups, where equivariant cohomology is usually settled. Second, we were not interested in the whole cohomology of the bundles (resp., the whole equivariant cohomology), but only in those cohomology classes that have their origin in forms on F. And last, for the applications in theoretical physics, we were interested in explicit formulas for the generated differential forms and not in a more abstract notion like the Weil algebra.

For non-compact Lie groups the reverse of Corollary IV.8 is false, e.g., take $G = \mathbb{R}$ and define $L: \mathbb{R} \times \mathbb{R}^k \to \mathbb{R}^k$ by $L(r,\vec{v}) = \vec{v} + r\vec{z}$ with $\vec{z} \in \mathbb{R}^k$. Then all forms ϕ_n with constant coefficients are closed and invariant. Because every bundle with structure group $\mathbb{R}$ (even more general, with $G \cong \mathbb{R}^m$) is trivial, every ϕ_n defines a closed form $\mathrm{pr}_{\mathbb{R}^k}^\star \phi_n$ on the bundle. But ϕ_n is not G-transgressive, in general, e.g., for $\phi_1 \in \mathscr{A}_1(\mathbb{R}^k)$ defined by $\phi_1(\vec{v})(\vec{x}) := \langle \vec{v}, \vec{z} \rangle$ for all $\vec{x} \in \mathbb{R}^k$ and $\vec{v} \in T_{\vec{x}}(\mathbb{R}^k)$, where $L_\bullet \phi_1(\vec{x}) = \mathrm{id}_{\mathbb{R}} \neq 0$. Thus ϕ_1 is not G-transgressive.

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An Itzykson–Zuber-like integral and diffusion for complex ordinary and supermatrices

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We compute an analogue of the Itzykson–Zuber integral for the case of arbitrary complex matrices. The calculation is done for both ordinary and supermatrices by transferring the Itzykson–Zuber diffusion equation method to the space of arbitrary complex matrices. The integral is of interest for applications in quantum chromodynamics and the theory of two-dimensional quantum gravity. © *1996 American Institute of Physics.* [S0022-2488(96)03412-3]

I. INTRODUCTION

In 1980, Itzykson and Zuber[1] presented their result on a certain integral over the unitary group which had great impact in several areas of mathematical physics. Let U be a matrix parameterizing the unitary group $U(N)$ with the invariant Haar measure $d\mu(U)$. Moreover, consider two diagonal matrices x and y with entries x_n and y_n, respectively, where $n=1,\ldots,N$. The Itzykson–Zuber integral can then be written in the form

$$\int d\mu(U)\exp(i\ \mathrm{tr}\ U^{-1}xUy)=\frac{\det[\exp(ix_ny_m)]_{n,m=1,\ldots,N}}{\Delta_N(x)\Delta_N(y)}, \tag{1.1}$$

where the function

$$\Delta_N(x)=\prod_{n<m}(x_n-x_m) \tag{1.2}$$

is the Vandermonde determinant of order N. Although it was later realized that this formula is a special case of a more general result due to Harish–Chandra,[2] it prompted many investigations in various fields. In 1983, Mehta and Pandey[3,4] used this formula to work out, in the framework of random matrix theory, the spectral correlations of a generic quantum chaotic system which undergoes a transition from conserved to broken time-reversal invariance. There are also numerous applications in field theory, particularly in the theory of two-dimensional quantum gravity; a review can be found in Ref. 5.

Recently, Shatashvili[6] showed that the integral (1.1) itself and all correlations in the Itzykson–Zuber model can be evaluated using the Gelfand–Tzetlin coordinates for an explicit calculation. Remarkably, Itzykson and Zuber had not derived their result by an explicit calculation but related the integral (1.1) to a diffusion process. They showed that it can be viewed as the kernel of a diffusion equation in the curved space of the eigenvalues of Hermitian matrices. Since the space of Hermitian matrices is Cartesian and, therefore, easy to treat, the result (1.1) can be found by comparison with the curved space without actually calculating it explicitly. The crucial point is the separability of the Laplacian operator in the curved space of the eigenvalues. This diffusion equation technique turned out to be a very powerful tool.

Some years ago, it was realized by one of the present authors[7] that the Itzykson–Zuber diffusion can be directly transferred to supermathematics. After the pioneering mathematical

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achievements of Berezin,[8] supermathematics was brought into the theory of matrix models by Efetov[9] and Verbaarschot, Weidenmüller, and Zirnbauer.[10] In Ref. 7 it was shown that there is, completely analogously to the case of ordinary matrices, a diffusion equation in the space of the eigenvalues of Hermitian supermatrices whose kernel is the supersymmetric generalization of the Itzykson–Zuber integral (1.1). Thus the integral can be worked out generalizing the methods of Ref. 1. Again, the crucial point is the separability of the Laplacian in the curved space of the eigenvalues.[7] The result has been used to evaluate, in the framework of random matrix theory, the effect of symmetry breaking on the spectral correlations of a chaotic time-reversal non-invariant system.[11] Recently, it was shown that the supersymmetric generalization of the Itzykson–Zuber diffusion has not only a mathematical, but also a physical meaning: In random matrix theory, it describes the transition from arbitrary to chaotic fluctuations.[12] These results could be used to work out the crossover from Poisson regularity to chaos in a time-reversal non-invariant system.

Let u be a supermatrix, parameterizing the unitary supergroup $U(k_1/k_2)$, with invariant Haar–Berezin measure $d\mu(u)$, and let s and r be diagonal matrices, both having the form $s=\mathrm{diag}(s_1, is_2)$ with $s_j=\mathrm{diag}(s_{1j},\ldots,s_{k_j j})$, $j=1,2$. Then, in its most general form, the supersymmetric Itzykson–Zuber integral[7] can be written as[13,14]

$$\int d\mu(u)\exp(i\ \mathrm{trg}\ usu^{-1}r)=\frac{\det[\exp(is_{p1}r_{p'1})]_{p,p'=1,\ldots,k_1}\ \det[\exp(is_{q2}r_{q'2})]_{q,q'=1,\ldots,k_2}}{B_{k_1k_2}(s)B_{k_1k_2}(r)}, \tag{1.3}$$

where the symbol trg stands for the supertrace, often also denoted by str. The supersymmetric generalization of the Vandermonde determinant is given by

$$B_{k_1k_2}(s)=\frac{\Delta_{k_1}(s_1)\Delta_{k_2}(is_2)}{\Pi_{p,q}(s_{p1}-is_{q2})}. \tag{1.4}$$

It is worth mentioning that $B_{k_1k_2}(s)$ reduces to a determinant[7] via Cauchy's lemma in the case $k_1=k_2$ such that $B_{k_1k_1}(s) = \det[1/(s_{p1} - is_{q2})]_{p,q=1,\ldots,k_1}$. Furthermore, by setting $k_1=N$ and $k_2=0$, one easily sees that formula (1.3) includes formula (1.1) as desired. However, for k_1 and k_2 both non-zero, there is an important caveat: In superanalysis, a change of variables can induce a certain class of singularities. Here, this implies that, if further integration over, say, the s-variables in Eq. (1.3) is required, we have to deal with new types of boundary contributions which have no analogue in ordinary analysis. The general theory of this effect, which is sometimes overlooked in the literature, was given by Rothstein.[15] In Refs. 7 and 16 it was shown how to treat these contributions in the case of the supersymmetric Itzykson–Zuber integral. Regarding integrations over the supersymmetric Itzykson–Zuber integral, yet another comment is in order: In applications in statistical mechanics,[3,4,7,11,12] the integrand, containing formulae (1.1) or (1.3), possesses some invariances under permutations. This allows one to replace the numerator of the right hand sides of these equations by $\exp(i\ \mathrm{tr}\ xy)$ or $\exp(i\ \mathrm{trg}\ sr)$, respectively, which makes the calculations more transparent. We emphasize this trivial point since it has stirred some confusion lately.

It is the purpose of this work to transfer all the results which have been reviewed so far from Hermitian to arbitrary complex matrices. We will do this for the case of ordinary and supermatrices. We will derive closed formulae for the analogues of the ordinary and the supersymmetric Itzykson–Zuber integral in the space of complex matrices. To the best of our knowledge, those have not been worked out yet. Our results are of considerable interest in the theory of matrix models. Several models in two-dimensional quantum gravity involve complex instead of Hermitian matrices.[17,18] Recently, the so-called chiral Gaussian ensembles,[19] also based on complex matrices, have been introduced and proved to be very useful in studying certain aspects of quantum chromodynamics (QCD).[20–23] In particular, the integral we compute will be crucial for a further analysis of the spectral correlations of the Dirac operator of QCD in the framework of

random-matrix models at finite temperatures, in the presence of mass terms, or at finite chemical potential. Via the Banks–Casher formula,[24] such analysis is also important for the study of questions related to the chiral phase transition of QCD.

To derive our results, we transfer the diffusion equation technique to complex ordinary and supermatrices. Again, the crucial point turns out to be the separability in the curved space of, in this case, radial coordinates. We have no doubt that the explicit formula could also be evaluated using other techniques. Especially, Gelfand–Tzetlin coordinates could be used as in Ref. 6 for ordinary Hermitian matrices. Recently, Gelfand–Tzetlin coordinates were derived for Hermitian supermatrices[14] such that this method could also be used for complex supermatrices. Moreover, regarding the case of ordinary matrices, we do not exclude the possibility that our results might be derivable directly from Harish–Chandra's formula.[2] To the best of our knowledge, Harish–Chandra's result has not been transferred to superanalysis yet. Nevertheless, here we will focus on the diffusion equation technique. So far, this technique was, for Hermitian matrices, viewed as a purely mathematical tool. However, as mentioned before, the diffusion in superspace describes the transition from arbitrary to chaotic fluctuations in random matrix theory[12] and, therefore, also has a direct physical meaning. We strongly believe that similar features are likely to exist in the case of the diffusion in the space of complex matrices which we will discuss in the present work.

The paper is organized as follows. In Sec. II, we state our results and derive them by constructing an eigenvalue equation. In Sec. III, we discuss the diffusion and questions related to it. We summarize and discuss our results in Sec. IV. Three appendices are provided for the derivation of intermediate results used in the text. In a fourth appendix, we discuss some boundary contributions which occur in the case of Hermitian supermatrices.

II. DERIVATION OF THE INTEGRAL BY CONSTRUCTING AN EIGENVALUE EQUATION

In Sec. II A, we state the integral for both cases, for ordinary and supermatrices. The derivation is performed for ordinary and supermatrices in Secs. II B and II C, respectively.

A. Statement of the integral

Let X be an arbitrary, square, complex ordinary matrix of dimension N. It is well known[25] that it can be written in the so-called pseudo-diagonal form

$$X = UxV \quad \text{with} \quad x = \mathrm{diag}(x_1,\ldots,x_N), \tag{2.1}$$

where the N variables x_n are real and non-negative. Note that these are not eigenvalues, they will be referred to as radial coordinates. While the matrix U explores the full parameter space of the unitary group $U(N)$, the matrix V is, in order to remove a double counting of phases, restricted to a subspace defined as the quotient of the unitary group and the Cartan subgroup, hence we have $U \in U(N)$ and $V \in U(N)/U^N(1)$.

We now multiply X by a diagonal matrix y of the same form as x and consider the expression i Re tr $UxVy$. The integral we wish to compute is the angular average over both unitary matrices of the exponential of this trace,

$$\Phi(x,y) = \int d\mu(U) \int d\mu(V) \exp(i \ \mathrm{Re\ tr}\ UxVy), \tag{2.2}$$

with $d\mu(U)$ and $d\mu(V)$ being the corresponding invariant Haar measures. We show that this integral is given by

$$\Phi(x,y) = \frac{(2\pi)^{N^2}}{N!} \frac{\det[J_0(x_n y_m)]_{n,m=1,\ldots,N}}{\Delta_N(x^2)\Delta_N(y^2)}, \tag{2.3}$$

where $J_0(z)$ is the ordinary Bessel function of zeroth order. The Vandermonde determinant was defined in Eq. (1.2).

Remarkably and fully analogously to the case of Hermitian matrices, this result can straightforwardly be generalized to supermatrices. An arbitrary complex supermatrix σ of dimension k_1+k_2 can be written as

$$\sigma = us\overline{v} \quad \text{with} \quad s = \mathrm{diag}(s_1, is_2) \tag{2.4}$$

and $s_j = \mathrm{diag}(s_{1j},...,s_{k_j j})$ for $j=1,2$. Again, while the matrix u explores the full parameter space of the unitary supergroup, the matrix $\overline{v}$ has to be restricted to a subspace in order to remove phases, we thus have $u \in U(k_1/k_2)$ and $\overline{v} \in U(k_1/k_2)/U^{k_1+k_2}(1)$.

Analogously to the case of ordinary matrices, we multiply the matrix σ by a diagonal matrix r of the same form as s and consider the expression $i\,\mathrm{Re\,trg}\,us\overline{v}r$. The generalization of the integral in the ordinary case is given by replacing the trace by the supertrace and the invariant measures by the corresponding ones in superspace, $d\mu(u)$ and $d\mu(\overline{v})$, respectively. We show that the double average

$$\varphi(s,r) = \int d\mu(u) \int d\mu(\overline{v}) \exp(i\ \mathrm{Re\ trg}\ us\overline{v}r) \tag{2.5}$$

is given by

$$\varphi(s,r) = \frac{(2\pi)^{(k_1-k_2)^2}}{2^{2k_1k_2}k_1!k_2!} \frac{\det[J_0(s_{p1}r_{p'1})]_{p,p'=1,\ldots,k_1} \det[J_0(s_{q2}r_{q'2})]_{q,q'=1,\ldots,k_2}}{B_{k_1k_2}(s^2)B_{k_1k_2}(r^2)} \tag{2.6}$$

where the generalized Vandermonde determinant was defined in Eq. (1.4).

Obviously, formula (2.6) includes formula (2.3) as can be seen by putting $k_1=N$ and $k_2=0$. Hence, in principle, it is sufficient to perform the derivation solely in superspace. However, we decided not to do so. We prove both results separately, first, in order to give those readers with little interest in supermathematics the opportunity to understand the ordinary case without being burdened by undesired information and, second, in order to help those readers with little experience in supermathematics to approach this area starting from more familiar grounds.

Note that our discussion is related to the harmonic analysis in the corresponding matrix spaces. The functions $\Phi(x,y)$ and $\varphi(s,r)$ can be viewed as the lowest order Bessel functions in these spaces.

B. Derivation for ordinary matrices

Besides X, we introduce a second arbitrary complex matrix Y of dimension N whose pseudodiagonalization reads $Y=U'yV'$ with y defined in Sec. II A. We have $U' \in U(N)$ and $V' \in U(N)/U^N(1)$. We observe that the ''plane wave''

$$W(X,Y) = \exp(i\ \mathrm{Re\ tr}\ XY^\dagger) \tag{2.7}$$

in this matrix space obeys the ''wave equation''

$$\Delta W(X,Y) = -(\mathrm{tr}YY^\dagger)W(X,Y). \tag{2.8}$$

where the Laplacian is defined as

$$\Delta = \sum_{n,m} \left(\frac{\partial^2}{\partial(\mathrm{Re}\ X_{nm})^2} + \frac{\partial^2}{\partial(\mathrm{Im}\ X_{nm})^2} \right). \tag{2.9}$$

Due to the invariance of the Haar measures we can express the function (2.2) as the angular average of the matrix plane wave,

$$\Phi(x,y)=\int d\mu(U')\int d\mu(\overline{V'})W(X,Y). \tag{2.10}$$

The crucial observation is now, just as in the case of Hermitian matrices, that $\Phi(x,y)$ satisfies the wave equation (2.8). This can be seen by averaging both sides of (2.8) over the matrices U' and V' using $\mathrm{tr}\, YY^{\dagger}=\mathrm{tr}\, y^2$. Consequently, since $\Phi(x,y)$ depends only on the radial coordinates, we can replace the Laplacian Δ by its radial part Δ_x. To construct it we have to transform the Cartesian volume element

$$d[X]=\prod_{n,m} d\ \mathrm{Re}\ X_{nm} d\ \mathrm{Im}\ X_{nm} \tag{2.11}$$

to radial and angular coordinates,

$$d[X]=J(x)d[x]d\mu(U)d\mu(\overline{V}),$$

$$d[x]=\prod_{n=1}^{N} dx_n, \quad J(x)=\Delta_N^2(x^2)\prod_{n=1}^{N} x_n, \tag{2.12}$$

where the Jacobian $J(x)$ was worked out in Ref. 25. It is then easily shown that the radial part of the Laplace operator reads

$$\Delta_x=\sum_{n=1}^{N} \frac{1}{J(x)}\frac{\partial}{\partial x_n} J(x)\ \frac{\partial}{\partial x_n}, \tag{2.13}$$

and we thus arrive at the eigenvalue equation

$$\Delta_x\Phi(x,y)=-(\mathrm{tr}\, y^2)\Phi(x,y) \tag{2.14}$$

in the curved space of the radial coordinates.

The key to the solution of the above equation is the separability of the radial Laplacian. For an arbitrary function $\Lambda(x)$ we have the identity

$$\Delta_x \frac{\Lambda(x)}{\Delta_N(x^2)}=\frac{1}{\Delta_N(x^2)}\ \Delta_x'\Lambda(x). \tag{2.15}$$

where the reduced part of the radial Laplacian is

$$\Delta_x'=\sum_{n=1}^{N}\left(\frac{\partial^2}{\partial x_n^2}+\frac{1}{x_n}\frac{\partial}{\partial x_n}\right). \tag{2.16}$$

The proof of this fact is given in Appendix A. Hence, the ansatz

$$\Phi(x,y)=\frac{\Psi(x,y)}{\Delta_N(x^2)\Delta_N(y^2)} \tag{2.17}$$

in which, for symmetry reasons, x and y are treated on the same footing, reduces the radial equation (2.14) to the much simpler form

$$\Delta_x' \Psi(x,y) = -(\mathrm{tr}\, y^2)\Psi(x,y). \tag{2.18}$$

This equation is again separable by a product ansatz for $\Psi(x,y)$ which yields N Bessel differential equations of zeroth order for each of the N functions. Hence, each of them can be written as a linear combination of the Bessel and Weber functions J_0 and N_0, respectively. Note that the indices of the eigenvalues y_n^2 of these N Bessel differential equations can be permuted arbitrarily implying that the most general solution is a linear combination of all these permuted products. However, the integral representation (2.2) imposes certain boundary conditions on the solution of the differential equation (2.18). Since the integral has a finite value for all x and y we have to exclude the Weber function from the solution. Additionally, we have to take into account that the integral is invariant under permutations of the indices. Since $\Delta_N(x^2)$, the Vandermonde determinant, is really a determinant, the function $\Psi(x,y)$ has to have the same properties under permutations of the indices. Incorporating these boundary conditions we find

$$\Psi(x,y) = \frac{(2\pi)^{N^2}}{N!} \det[J_0(x_n y_m)]_{n,m=1,\ldots,N}, \tag{2.19}$$

which yields immediately the result (2.3). Of course, the normalization constant is arbitrary. We will show later why our choice is useful.

C. Derivation for supermatrices

All steps are completely analogous to the ordinary case. In order to make the notation more transparent, we write the supermatrix σ in the boson-fermion block form[7,10]

$$\sigma = \begin{bmatrix} \sigma^{11} & \sigma^{12} \\ \sigma^{21} & i\sigma^{22} \end{bmatrix}, \tag{2.20}$$

where σ^{jl} is a $k_j \times k_l$ complex matrix whose entries are commuting if $j=l$ and anticommuting if $j \neq l$. The factor i in front of σ^{22} is, as usual, introduced to ensure convergence.[9,10] Again, besides σ, we introduce a second arbitrary complex supermatrix ρ of the same form whose pseudo-diagonalization reads $\rho = u' r \overline{v'}$ with r defined in Sec. II A and with $u' \in U(k_1/k_2)$ and $\overline{v'} \in U(k_1/k_2)/U^{k_1+k_2}(1)$. There is also a ''plane wave''

$$w(\sigma,\rho) = \exp(i\ \mathrm{Re\ trg}\ \sigma\rho^\dagger) \tag{2.21}$$

in this matrix space. Note that the expression $\mathrm{Re\,trg}\,\sigma\rho^\dagger$ has, for explicit calculations, to be interpreted as half the sum of $\mathrm{trg}\,\sigma\rho^\dagger$ and its complex conjugate since we will not introduce the real and the imaginary part of Grassmann variables. The plane wave satisfies the ''wave equation''

$$\Delta w(\sigma,\rho) = -(\mathrm{trg}\ \rho\rho^\dagger) w(\sigma,\rho), \tag{2.22}$$

where the Laplacian is defined as

$$\Delta = \sum_{j=1}^{2} \sum_{p,q} \left(\frac{\partial^2}{\partial(\mathrm{Re}\ \sigma_{pq}^{jj})^2} + \frac{\partial^2}{\partial(\mathrm{Im}\ \sigma_{pq}^{jj})^2} \right) + 4 \sum_{j \neq l} \sum_{p,q} \frac{\partial^2}{\partial \sigma_{pq}^{jl} \sigma_{pq}^{jl*}}. \tag{2.23}$$

The invariance of the Haar measures allows us to express the function (2.5) as the angular average of the matrix plane wave,

$$\varphi(s,r) = \int d\mu(u') \int d\mu(\overline{v'}) w(\sigma,\rho). \tag{2.24}$$

As in the ordinary case, we integrate both sides of the wave equation over the matrices u' and $\overline{v'}$ using $\mathrm{trg}\,\rho\rho^{\dagger}=\mathrm{trg}\,r^2$ and observe that $\varphi(s,r)$ satisfies the wave equation (2.22). Again, since $\varphi(s,r)$ depends only on the radial coordinates, we can replace the Laplacian Δ by its radial part Δ_s. The transformation of the Cartesian volume element

$$d[\sigma]=\prod_{j=1}^{2}\prod_{p,q} d(\mathrm{Re}\ \sigma_{pq}^{jj})d(\mathrm{Im}\ \sigma_{pq}^{jj})\prod_{j\neq l}\prod_{p,q} d\sigma_{pq}^{jl*}\ \ d\sigma_{pq}^{jl} \tag{2.25}$$

to radial and angular coordinates reads

$$\begin{aligned} d[\sigma]&=J(s)d[s]d\mu(u)d\mu(\overline{v}),\\ d[s]&=\prod_{j=1}^{2}\prod_{p=1}^{k_j} ds_{pj}, \quad J(s)=B_{k_1k_2}^{2}(s^2)\prod_{j=1}^{2}\prod_{p=1}^{k_j} s_{pj}, \end{aligned} \tag{2.26}$$

where the Jacobian or Berezinian $J(s)$ is computed in Appendix B. The radial part of the Laplace operator takes the form

$$\Delta_s=\sum_{j=1}^{2}\sum_{p=1}^{k_j}\ \frac{1}{J(s)}\frac{\partial}{\partial s_{pj}}J(s)\ \frac{\partial}{\partial s_{pj}}, \tag{2.27}$$

details are given in Appendix B. Hence, we have to solve the equation

$$\Delta_s\varphi(s,r)=-(\mathrm{trg}\ r^2)\varphi(s,r) \tag{2.28}$$

in the curved space of the radial coordinates.

In the case of ordinary matrices, the key for the solution was the separability of the radial Laplacian. It is essential that this feature is also present in the case of supermatrices. This closely parallels the situation for Hermitian matrices.[7] For an arbitrary function $\lambda(s)$ we find

$$\Delta_s\ \frac{\lambda(s)}{B_{k_1k_2}(s^2)}=\frac{1}{B_{k_1k_2}(s^2)}\ \Delta_s'\lambda(s), \tag{2.29}$$

where the reduced part of the Laplacian reads

$$\Delta_s'=\sum_{j=1}^{2}\sum_{p=1}^{k_j}\left(\frac{\partial^2}{\partial s_{pj}^2}+\frac{1}{s_{pj}}\frac{\partial}{\partial s_{pj}}\right). \tag{2.30}$$

The derivation is given in Appendix C. Thus the ansatz

$$\varphi(s,r)=\frac{\psi(s,r)}{B_{k_1k_2}(s^2)B_{k_1k_2}(r^2)} \tag{2.31}$$

yields the reduced equation

$$\Delta_s'\psi(s,r)=-(\mathrm{trg}\ r^2)\psi(s,r) \tag{2.32}$$

which, again, is separable by a product ansatz for $\psi(s,r)$. We obtain k_1+k_2 Bessel differential equations of zeroth order. The boundary conditions imposed by the integral representation (2.5) are very similar to the ones in the ordinary case. First, we have to construct the solution using the Bessel function J_0 and to reject the Weber function N_0. Second, we have to take into account the

invariance under permutations. Here, however, we see from the Jacobian that this invariance exists only within the boson-boson or fermion-fermion block, respectively. Since these boundary conditions imply that the solution is given by

$$\psi(s,r)=\frac{(2\pi)^{(k_1-k_2)^2}}{2^{2k_1k_2}k_1!k_2!}\det[J_0(s_{p1}r_{p'1})]_{p,p'=1,\ldots,k_1}\det[J_0(s_{q2}r_{q'2})]_{q,q'=1,\ldots,k_2}, \tag{2.33}$$

we arrive at the final result (2.6). Again, the normalization constant is arbitrary, we will comment on our choice later.

III. DIFFUSION EQUATION AND FOURIER TRANSFORM

We now discuss a diffusion equation which is closely related to the plane waves and the eigenvalue equations we constructed in the previous section. Our goal is to show that the concept of diffusion equations which is so useful in the case of Hermitian matrices can be transferred straightforwardly to arbitrary complex matrices. However, since these considerations are more of conceptual interest and do not require so many explicit calculations, we study only the case of supermatrices. The case of ordinary matrices is always recovered by setting $k_1=N$ and $k_2=0$. In Sec. III A, we introduce the concepts in Cartesian space. We go over to the curved space of the radial coordinates in Sec. III B. In Sec. III C, we discuss some questions related to boundary terms.

A. Cartesian space

We introduce a time coordinate t and consider the diffusion equation

$$\frac{1}{2}\Delta F(\sigma,t)=\frac{\partial}{\partial t}F(\sigma,t) \tag{3.1}$$

for a given initial condition $F_0(\sigma)$ such that

$$\lim_{t\to 0}F(\sigma,t)=F_0(\sigma). \tag{3.2}$$

The kernel of this diffusion satisfies the equations

$$\frac{1}{2}\Delta G(\sigma,t)=\frac{\partial}{\partial t}G(\sigma,t)\quad\text{and}\quad\lim_{t\to 0}G(\sigma,t)=\delta(\sigma), \tag{3.3}$$

where the δ-function is given by

$$\delta(\sigma)=\prod_{j=1}^{2}\prod_{p,q}\delta(\mathrm{Re}\ \sigma_{pq}^{jj})\delta(\mathrm{Im}\ \sigma_{pq}^{jj})\prod_{j\neq l}\prod_{p,q}\delta(\sigma_{pq}^{jl*})\delta(\sigma_{pq}^{jl}). \tag{3.4}$$

The δ-function of an anticommuting variable β is defined by $\delta(\beta)=\sqrt{2\pi}\beta$.[7,10] Similar to the discussion in Refs. 1 and 16, the kernel is the Gaussian

$$G(\sigma,t)=\frac{2^{2k_1k_2}}{(2\pi t)^{(k_1-k_2)^2}}\exp\left(-\frac{1}{2t}\,\mathrm{trg}\ \sigma\sigma^{\dagger}\right). \tag{3.5}$$

and the solution of the diffusion process can be written as the convolution

$$F(\sigma,t)=\int G(\sigma-\sigma',t)F_0(\sigma')d[\sigma']. \tag{3.6}$$

Moreover, this solution is also expressible as

$$F(\sigma,t)=\exp\left(\frac{t}{2}\,\Delta\right)F_0(\sigma) \tag{3.7}$$

which has to be viewed as a formal power series.

We will now show how the diffusion can be related to the plane waves of the previous section and to the theory of Fourier transforms. To this end, we remark that the δ-function (3.4) can be expanded in the plane waves (2.21),

$$\delta(\sigma)=\frac{2^{4k_1k_2}}{(2\pi)^{2(k_1-k_2)^2}}\int w(\sigma,\rho)d[\rho], \tag{3.8}$$

which allows us to introduce the Fourier transform $\widetilde{P}(\rho)$ of a function $P(\sigma)$ and its inverse by

$$\widetilde{P}(\rho)=\frac{2^{2k_1k_2}}{(2\pi)^{(k_1-k_2)^2}}\int P(\sigma)w^*(\sigma,\rho)d[\sigma] \quad \text{and} \quad P(\sigma)=\frac{2^{2k_1k_2}}{(2\pi)^{(k_1-k_2)^2}}\int \widetilde{P}(\rho)w(\sigma,\rho)d[\rho]. \tag{3.9}$$

The Fourier transform can be used to derive the explicit form (3.5) of the diffusion kernel defined in Eq. (3.3), this works as follows. The diffusion kernel can, according to Eq. (3.7), be expressed in the form

$$G(\sigma,t)=\exp\left(\frac{t}{2}\,\Delta\right)\delta(\sigma) \tag{3.10}$$

in which we insert the expansion (3.8),

$$G(\sigma,t)=\frac{2^{4k_1k_2}}{(2\pi)^{2(k_1-k_2)^2}}\int \exp\left(\frac{t}{2}\,\Delta\right)w(\sigma,\rho)d[\rho]. \tag{3.11}$$

We write the exponential as a power series and, by virtue of the eigenvalue equation (2.22), perform all derivatives. The resummation of the series gives the diffusion kernel as the Fourier transform of a Gaussian

$$G(\sigma,t)=\frac{2^{4k_1k_2}}{(2\pi)^{2(k_1-k_2)^2}}\int \exp\left(-\frac{t}{2}\,\mathrm{trg}\;\rho\rho^{\dagger}\right)w(\sigma,\rho)d[\rho], \tag{3.12}$$

which is in agreement with Eq. (3.5).

B. Curved space of the radial coordinates

We now assume that the initial condition depends only on the radial coordinates, i.e., $F_0(\sigma)=F_0(s)$. Thus it is useful to use the coordinates (2.4) in the integral representation (3.6) of the solution of the diffusion equation (3.1). This has some important consequences. The invariance of the Haar measures implies that this solution is also a function of the radial coordinates only, hence we have $F(\sigma,t)=F(s,t)$. Consequently, the diffusion takes place in the curved space of the radial coordinates alone,

$$\tfrac{1}{2}\,\Delta_s F(s,t)=\frac{\partial}{\partial t}F(s,t) \quad \text{and} \quad \lim_{t\to 0}F(s,t)=F_0(s), \tag{3.13}$$

where Δ_s is the radial part of the Laplacian defined in Eq. (2.27). Moreover, we may conclude from the integral representation (3.6) that the kernel of the diffusion (3.13) is given by

$$\Gamma(s,s',t)=\int d\mu(u)\int d\mu(\overline{v})G(us\overline{v}-s',t). \tag{3.14}$$

There are two ways of evaluating this double average. First, since the kernel $G(\sigma,t)$ is Gaussian, a direct comparison of Eq. (3.5) with Eq. (2.5) shows that

$$\Gamma(s,s',t)=\frac{2^{2k_1k_2}}{(2\pi t)^{(k_1-k_2)^2}}\exp\left(-\frac{1}{2t}\,\mathrm{trg}(s^2+s'^2)\right)\varphi(-is/t,s'), \tag{3.15}$$

which means that this double average can be expressed in terms of the one we have calculated in the previous section. Hence, with the help of the result (2.6) and after a reordering of factors, we can write the diffusion kernel in the curved space in the form

$$\Gamma(s,s',t)=\frac{1}{k_1!k_2!}\,\frac{\det[\,\gamma(s_{p1},s'_{p'1},t)]_{p,p'=1,\ldots,k_1}\,\det[\,\gamma(s_{q2},s'_{q'2},t)]_{q,q'=1,\ldots,k_2}}{B_{k_1k_2}(s^2)B_{k_1k_2}(s'^2)}, \tag{3.16}$$

in which the entries of the determinants are given by the function

$$\gamma(s_{pj},s'_{qj},t)=\frac{1}{t}\exp\left(-\frac{s_{pj}^2+s_{qj}'^2}{2t}\right)I_0\left(\frac{s_{pj}s'_{qj}}{t}\right) \tag{3.17}$$

for all values of $j=1,2$ and $p,q=1,\ldots,k_j$. The function $I_0(z)$ is the modified Bessel function of zeroth order.

Alternatively, if the result (2.6) was unknown, formula (3.16) could be derived by a procedure similar to the one in Sec. II C. The separability of the radial part Δ_s leads to a reduced diffusion equation involving the reduced operator Δ_s' defined in (2.30). This equation can be solved by a product ansatz leading to the diffusion equation

$$\frac{1}{2}\left(\frac{\partial^2}{\partial s_{pj}^2}+\frac{1}{s_{pj}}\,\frac{\partial}{\partial s_{pj}}\right)\gamma(s_{pj},s'_{qj},t)=\frac{\partial}{\partial t}\,\gamma(s_{pj},s'_{qj},t), \tag{3.18}$$

where the differential operator is just the radial part of the Laplacian in a two-dimensional space. In order to construct the solution, we express it as the formal series

$$\gamma(s_{pj},s'_{qj},t)=\exp\left(\frac{t}{2}\left(\frac{\partial^2}{\partial s_{pj}^2}+\frac{1}{s_{pj}}\,\frac{\partial}{\partial s_{pj}}\right)\right)\,\frac{\delta(s_{pj}-s'_{qj})}{\sqrt{s_{pj}s'_{qj}}} \tag{3.19}$$

acting on the proper radial δ-function in this two-dimensional space. Inserting Hankel's expansion [Ref. 26, 14·4.(1)] of this δ-function,

$$\frac{\delta(s_{pj}-s'_{qj})}{\sqrt{s_{pj}s'_{qj}}}=\int_0^\infty J_0(s_{pj}z)J_0(s'_{qj}z)z\;dz, \tag{3.20}$$

we can perform all derivatives and resum the series. We arrive at

$$\gamma(s_{pj},s'_{qj},t)=\int_0^\infty \exp\left(-\frac{t}{2}\,z^2\right)J_0(s_{pj}z)J_0(s'_{qj}z)z\;dz, \tag{3.21}$$

which is precisely Weber's representation [Ref. 26, 13·31.(1)] of the function (3.17). It is easy to see in a direct calculation that this function is indeed the kernel of the diffusion equation (3.18). According to an elementary result [Ref. 26, 13·3.(1)] of the theory of Bessel functions, $\gamma(s_{pj},s'_{qj},t)$ is properly normalized,

$$\int_0^\infty \gamma(s_{pj},s'_{qj},t)s_{pj}\,ds_{pj}=1, \tag{3.22}$$

where we have used the radial part $s_{pj}\,ds_{pj}$ of the measure in the two-dimensional space. Furthermore, since $I_0(z)$ behaves like $\exp(z)/\sqrt{2\pi z}$ for large values of the argument, the function $\gamma(s_{pj},r_{qj},t)$ approaches the δ-function

$$\lim_{t\to 0}\ \gamma(s_{pj},s'_{qj},t)=\frac{\delta(s_{pj}-s'_{qj})}{\sqrt{s_{pj}s'_{qj}}} \tag{3.23}$$

for vanishing time t.

The limit relation (3.23) implies that the kernel (3.16) satisfies the correct limit relation in the curved space of all radial coordinates, we write this in the form

$$\begin{aligned}\lim_{t\to 0}\Gamma(s,s',t)&=\int d\mu(u)\int d\mu(\overline{v})\delta(us\overline{v}-s')\\ &=\frac{1}{k_1!k_2!}\,\frac{\det[\,\delta(s_{p1}-s'_{p'1})]_{p,p'=1,\ldots,k_1}\,\det[\,\delta(s_{q2}-s'_{q'2})]_{q,q'=1,\ldots,k_2}}{\sqrt{J(s)J(s')}}\end{aligned} \tag{3.24}$$

where the Berezinian $J(s)$ is defined in Eq. (2.26). Using this result, it is easily checked that the constant $1/k_1!k_2!$ ensures the correct normalization. This, in turn, motivates our choice of the normalization constants in Eqs. (2.19) and (2.33).

C. Questions related to boundary contributions

The function $\Gamma(s,s',t)$ given in Eq. (3.16) is, as we have shown, the kernel of the diffusion equation (3.13) in the curved space of the radial coordinates. Thus the solution of the integral (3.14) as it stands is indeed given by formula (3.16). However, there is a very subtle point about kernels of this type which has an important impact on applications. Although we will present some applications of our results to physical problems in a forthcoming publication, we already give a short, more intuitive, discussion of this subtlety here. We do so to acquaint the reader who is not yet familiar with supersymmetry with this point which is sometimes overlooked in the literature.

In Cartesian space, the normalization of the Gaussian diffusion kernel (3.5) implies that the equation

$$\int\ G(\sigma-\sigma',t)d[\sigma']=1 \tag{3.25}$$

holds for all values of t and for all matrices σ. Thus after performing the angular integration, one would naively assume that the radial integral

$$\eta(s,t)=\int\Gamma(s,s',t)J(s')d[s'] \tag{3.26}$$

also yields unity for all values of t and for all diagonal matrices s. In the ordinary case, i.e., for $k_1=N$ and $k_2=0$, it can be checked by a straightforward, direct calculation that we indeed have

$\eta(s,t)=1$. However, in the case of supermatrices this is, for non-trivial reasons, no longer true. The singularities of the Berezinian $J(s)$ compensate the vanishing of some angular Grassmann integrals such that a finite, non-zero result remains. This effect leads to certain contributions to the integral which are often called Efetov–Wegner–Parisi–Sourlas terms in the more physics-oriented literature. There are various methods to construct those contributions in the applications of supersymmetry.[7,9–11,27] From a strictly mathematical point of view, these terms arise as boundary contributions due to the fact that the integrals are ill-defined for non-compact supermanifolds. A full-fledged theory can be found in Ref. 15. It is instructive to think of these boundary contributions as being necessary to restore the translational invariance of the integrals in Cartesian space, as obvious in Eq. (3.25), which is broken in Eq. (3.26) if $\eta(s,t)$ differs from unity.[28] To illustrate this, we calculate the function $\eta(s,t)$ for the simplest non-trivial case, namely $k_1=k_2=1$. We have

$$\eta(s,t)=(s_{11}^2+s_{12}^2)\int_0^\infty\int_0^\infty ds'_{11}ds'_{12}\,\frac{s'_{11}s'_{12}}{s'^2_{11}+s'^2_{12}}\,\gamma(s_{11},s'_{11},t)\,\gamma(s_{12},s'_{12},t). \tag{3.27}$$

By expressing the denominator of the Berezinian as the integral

$$\frac{1}{s'^2_{11}+s'^2_{12}}=\int_0^\infty \exp(-(s'^2_{11}+s'^2_{12})z)dz, \tag{3.28}$$

we can evaluate the double integral (3.27) by standard methods [Ref. 26, 13·3 (1)]. We arrive at

$$\eta(s,t)=1-\exp\left(-\frac{s_{11}^2+s_{12}^2}{2t}\right) \tag{3.29}$$

which equals unity only in the limit $t\to 0$. Note that the exponential is, apart from a numerical factor, nothing else but the Cartesian kernel at $\sigma'=0$ which is just $G(\sigma,t)=G(s,t)$. This is, of course, no accidental coincidence.

The case $k_1=k_2$, where k_1 is arbitrary, is physically the most interesting one. Due to the determinant structure of the function $B_{k_1k_1}(s'^2)$, the evaluation of the function $\eta(s,t)$ reduces to the double integral (3.27) already computed, and we arrive at

$$\eta(s,t)=\frac{1}{B_{k_1k_1}(s^2)}\det\left[\frac{1}{s_{p1}^2+s_{q2}^2}\,1\left(-\exp\left(-\frac{s_{p1}^2+s_{q2}^2}{2t}\right)\right)\right]_{p,q=1,\ldots,k_1}. \tag{3.30}$$

As evident from the definition (3.26), this function is a solution of diffusion equation (3.13), we have

$$\frac{1}{2}\,\Delta_s\eta(s,t)=\frac{\partial}{\partial t}\,\eta(s,t). \tag{3.31}$$

However, it is not a kernel of the diffusion process in the usual sense since it obeys different limit relations,

$$\lim_{t\to 0}\eta(s,t)\big|_{s\neq 0}=1 \quad\text{and}\quad \lim_{t\to\infty}\eta(s,t)=0, \tag{3.32}$$

which reflect the existence of the new boundary contributions. The function $\eta(s,t)$ can be viewed as the envelope solution corresponding to the kernel $\Gamma(s,s',t)$. The function $B_{k_1k_1}(s^2)\Gamma(s,s',t)$ possesses a product structure in the kernels $\gamma(s_{p1},s'_{q2},t)$. Due to the integration, this property has

vanished in $B_{k_1 k_1}(s^2)\,\eta(s,t)$, which factorizes only in functions of the combinations $s_{p1}^2+s_{q2}^2$. Along the lines given in Refs. 7, 10, and 28, one can show that the diffusion kernel in the curved space of the radial coordinates has to be replaced by

$$\Gamma(s,s',t)\to(1-\eta(s,t))\,\frac{\delta(s')}{J(s')}+\Gamma(s,s',t) \tag{3.33}$$

if further integration over the primed variables s' is required. This replacement cures the problem of the boundary contributions for $k_1=k_2$ in the physically most interesting cases. Hence, for a well-behaved initial condition $F_0(s)$, the solution $F(s,t)$ of the diffusion equation in the curved space of the radial coordinates reads

$$F(s,t)=(1-\eta(s,t))F_0(0)+\int \Gamma(s,s',t)F_0(s')J(s')d[s']. \tag{3.34}$$

We emphasize that this result is really a solution of the diffusion process (3.13), including its initial condition. Note that there are very peculiar cases in which further boundary contributions can arise. Those, however, have to be constructed using the full theory which is given in Ref. 15.

In Appendix D, we reconsider the boundary contributions to the supersymmetric Itzykson–Zuber integral for Hermitian supermatrices as derived in Ref. 7.

IV. SUMMARY AND DISCUSSION

We have calculated an analogue of the Itzykson–Zuber integral in the space of arbitrary complex matrices. We arrived at explicit formulae for the case of ordinary and supermatrices, where the latter includes the former. We performed our calculation by transferring the diffusion equation technique of Itzykson and Zuber for Hermitian matrices, which works in ordinary[1] and in superspace,[7,13] to complex matrices. For the actual derivation, we used an eigenvalue equation for the plane waves in these matrix spaces which is closely related to this diffusion. Similar to the Hermitian case, the integral in question turns out to be the kernel of the diffusion in the curved spaces of the radial coordinates. The explicit results can be computed due to a separability of the Laplacian in these radial spaces. We discussed certain types of boundary contributions to the full solution of the diffusion equation which can arise in superspace.

We have no doubts that our explicit results can also be derived by other methods. In particular, the use of Gelfand–Tzetlin coordinates for the unitary group in ordinary[6] and superspace[14] ought to be mentioned here since it allows a recursive evaluation of correlation functions in the corresponding matrix models. Most importantly, as far as the case of ordinary matrices is concerned, it does not seem unlikely that the explicit formula for the integral we presented here can be derived directly from the Harish–Chandra integral. At first sight, one would not think so since the Harish–Chandra integral is an average over one unitary matrix whereas our result is a double average over two unitary matrices. This can be seen from the fact that our explicit formula contains Bessel functions where the Itzykson–Zuber integrals contain exponentials, i.e., plane waves. The Bessel function of zeroth order is just the angular average over a plane wave in a two-dimensional space. This might indicate that the angular average over two unitary matrices is essential and cannot be replaced by an average over one unitary matrix. Nevertheless, we do not exclude the possibility that a clever reordering of the trace in the matrix plane waves which combines these two unitary matrices can be done in such a way that the essential part of the calculation reduces to an application of the Harish–Chandra formula. These considerations, however, do not apply to the case of supermatrices, for which, to the best of our knowledge, Harish–Chandra's result has not been transferred yet.

For the reasons discussed above, we do not want to present our explicit formulae for the integrals as our most important findings. Rather, we consider the Itzykson–Zuber-like diffusion

which we constructed here as our most interesting result. We strongly believe that this diffusion is more than a mathematical tool to calculate integrals. In the case of Hermitian supermatrices, it was shown[12] that the Itzykson–Zuber diffusion models the transition from arbitrary to chaotic fluctuations of all orders in a very general way. We are convinced that the diffusion in the space of complex matrices also has a physical meaning of similar significance.

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APPENDIX A: SEPARABILITY IN ORDINARY SPACE

We use a more convenient form of Δ_x.

$$\Delta_x = \sum_{n=1}^{N} \left(\frac{\partial^2}{\partial x_n^2} + \frac{\partial \ln J(x)}{\partial x_n} \frac{\partial}{\partial x_n} \right). \tag{A1}$$

The derivatives in Eq. (2.15) are evaluated in a straightforward manner, and we arrive at the intermediate result

$$\Delta_x \frac{\Lambda(x)}{\Delta_N(x^2)} = \frac{1}{\Delta_N(x^2)} \sum_{n=1}^{N} \left(\frac{\partial^2}{\partial x_n^2} + \frac{1}{x_n} \frac{\partial}{\partial x_n} - 4D_n \right) \Lambda(x), \tag{A2}$$

where $D_n = S_n + x_n^2(S_n^2 - T_n)$ with

$$S_n = \sum_{\substack{m=1 \\ m \neq n}}^{N} \frac{1}{x_n^2 - x_m^2} \quad \text{and} \quad T_n = \sum_{\substack{m=1 \\ m \neq n}}^{N} \frac{1}{(x_n^2 - x_m^2)^2}. \tag{A3}$$

We now show that $\Sigma_{n=1}^{N} D_n = 0$. The fact that

$$\sum_{n=1}^{N} S_n = \sum_{m \neq n} \frac{1}{x_n^2 - x_m^2} = 0 \tag{A4}$$

is easily seen by renaming summation indices. The remaining term is

$$R = \sum_{n=1}^{N} x_n^2 (S_n^2 - T_n) = \sum_{\Omega(n,m,m')} \frac{x_n^2}{(x_n^2 - x_m^2)(x_n^2 - x_{m'}^2)}, \tag{A5}$$

where the symbol $\Omega(n,m,m')$ denotes summation over three indices n,m,m' which are pairwise different. We now rename $n \leftrightarrow m$ and $n \leftrightarrow m'$ to obtain

$$2R = \sum_{\Omega(n,m,m')} \left[\frac{x_m^2}{(x_m^2 - x_n^2)(x_m^2 - x_{m'}^2)} + \frac{x_{m'}^2}{(x_{m'}^2 - x_m^2)(x_{m'}^2 - x_n^2)} \right] = -R, \tag{A6}$$

from which $R = 0$ follows immediately. This completes the proof.

APPENDIX B: DERIVATION OF THE BEREZINIAN AND THE RADIAL PART OF THE LAPLACIAN

We wish to compute the Berezinian of the transformation $\sigma = us\overline{v}$, defined in Eq. (2.4). We first construct

$$d\sigma = u(u^\dagger\, du\, s + ds + s\, d\overline{v\, v^\dagger})\overline{v}. \tag{B1}$$

Writing $u^\dagger\, du = du'$ and $d\overline{v\, v^\dagger} = d\overline{v'}$, and noting that $s^\dagger = s$, we obtain the invariant length element

$$\mathrm{trg}\; d\sigma\; d\sigma^\dagger = \mathrm{trg}(du'\, s + ds + s\, d\overline{v'})(s\, du'^\dagger + ds + d\overline{v'^\dagger}\, s) \tag{B2}$$

from which the Berezinian can be read off. Since du' and $d\overline{v'}$ are also in the algebra we are entitled to drop the primes. This gives

$$\mathrm{trg}\; d\sigma\; d\sigma^\dagger = \mathrm{trg}\; ds^2 + \mathrm{trg}\; s\; ds(du + du^\dagger + d\overline{v} + d\overline{v^\dagger}) + \mathrm{trg}(du\, s + s\, d\overline{v})(s\, du^\dagger + d\overline{v^\dagger}\, s). \tag{B3}$$

where we have made use of the fact that s and ds are diagonal. Since du and $d\overline{v}$ are anti-Hermitian, the second term in the above expression yields zero. The vanishing of this term also shows that the Laplace operator separates into two sums over radial and angular coordinates, respectively, a fact which has been used in Sec. II C. The first term in Eq. (B3) contributes a factor of 1 to the Berezinian so that we are left with the third term only. Using boson-fermion block notation, we write

$$du = \begin{bmatrix} du^{C_1} & du^A \\ -du^{A^\dagger} & du^{C_2} \end{bmatrix}. \tag{B4}$$

A note about the number of degrees of freedom: du^{C_j} is an anti-Hermitian matrix with k_j^2 commuting degrees of freedom whereas du^A and $du^{A^\dagger}$ each have $k_1 k_2$ anticommuting degrees of freedom. Similar notation is used for $d\overline{v}$, the main difference being that the diagonal elements of $d\overline{v}^{C_j}$ are zero. It is convenient to separate the diagonal elements of du^{C_j} and to define

$$du\, s + s\, d\overline{v} = \eta + \omega = \begin{bmatrix} \eta^{11} & 0 \\ 0 & \eta^{22} \end{bmatrix} + \begin{bmatrix} \omega^{11} & \omega^{12} \\ \omega^{21} & \omega^{22} \end{bmatrix}. \tag{B5}$$

where $\eta^{11} = \mathrm{diag}(du_{11}^{C_1}\, s_{11}, \ldots, du_{k_1 k_1}^{C_1}\, s_{k_1 1})$, $\eta^{22} = \mathrm{diag}(du_{11}^{C_2}\, is_{12}, \ldots, du_{k_2 k_2}^{C_2}\, is_{k_2 2})$, the diagonal elements of ω^{11} and ω^{22} are zero, and

$$\begin{aligned} \omega_{pp'}^{11} &= du_{pp'}^{C_1}\, s_{p'1} + s_{p1}\, d\overline{v}_{pp'}^{C_1}, \quad (p \neq p'), \\ \omega_{qq'}^{22} &= du_{qq'}^{C_2}\, is_{q'2} + is_{q2}\, d\overline{v}_{qq'}^{C_2}, \quad (q \neq q'), \\ \omega_{pq}^{12} &= du_{pq}^{A}\, is_{q2} + s_{p1}\, d\overline{v}_{pq}^{A}, \\ \omega_{qp}^{21} &= -du_{qp}^{A^\dagger}\, s_{p1} - is_{q2}\, d\overline{v}_{qp}^{A^\dagger}. \end{aligned} \tag{B6}$$

We now consider

$$\begin{aligned} \mathrm{trg}(\eta + \omega)(\eta^\dagger + \omega^\dagger) = \mathrm{trg}(\eta\eta^\dagger + \omega\omega^\dagger) = \mathrm{trg}\; \eta\eta^\dagger + \mathrm{tr}\; \omega^{11}\omega^{11\dagger} - \mathrm{tr}\; \omega^{22}\omega^{22\dagger} \\ - \mathrm{tr}(\omega^{12}\omega^{12\dagger} + \omega^{21}\omega^{21\dagger}). \end{aligned} \tag{B7}$$

where in the first equality we have employed the fact that η is diagonal and that the diagonal elements of ω are zero by definition. Each independent variable appears in one and only one of the four terms in the above expression so that their contribution to the Berezinian is multiplicative. The contribution from the first term can be read off immediately, we obtain

$$\mathrm{trg}\ \eta\eta^{\dagger}\rightarrow\prod_{j=1}^{2}\prod_{p=1}^{k_j} s_{pj}\,. \tag{B8}$$

We now write $\mathrm{tr}\ \omega^{11}\omega^{11\dagger}=\Sigma_{p<p'}(|\omega^{11}_{pp'}|^2+|\omega^{11}_{p'p}|^2)$. Each term in the sum contains only independent variables which do not appear in any other term so that the contribution of these terms to the Berezinian is multiplicative again. Using Eq. (B6) and the anti-Hermiticity of du^{C_1} and $d\overline{v^{C_1}}$ we obtain for the contribution to the Berezinian

$$\mathrm{tr}\ \omega^{11}\omega^{11\dagger}\rightarrow\prod_{p<p'}^{k_1}(s^2_{p1}-s^2_{p'1})^2=\Delta^2_{k_1}(s^2_1). \tag{B9}$$

In complete analogy,

$$-\mathrm{tr}\ \omega^{22}\omega^{22\dagger}\rightarrow\prod_{q<q'}^{k_2}(s^2_{q2}-s^2_{q'2})^2=\Delta^2_{k_2}(s^2_s). \tag{B10}$$

Similar arguments are made for the remaining term in Eq. (B7). Since ω^{12} and ω^{21} couple commuting and anticommuting variables, their contribution to the Berezinian appears in the denominator. Specifically, we obtain

$$-\mathrm{tr}(\omega^{12}\omega^{12\dagger}+\omega^{21}\omega^{21\dagger})\rightarrow\left(\prod_{p=1}^{k_1}\prod_{q=1}^{k_2}(s^2_{p1}+s^2_{q2})\right)^{-2}. \tag{B11}$$

Collecting terms, we finally obtain the Berezinian (2.26).

Since Eq. (B3) implies that the metric tensor in the subspace of the radial coordinates is just the unit matrix, the radial part of the Laplacian has the form (2.27).

APPENDIX C: SEPARABILITY IN SUPERSPACE

Again, we write Δ_s in a more convenient form,

$$\Delta_s=\sum_{j=1}^{2}\sum_{p=1}^{k_j}\left(\frac{\partial^2}{\partial s^2_{pj}}+\frac{\partial\ \ln J(s)}{\partial s_{pj}}\frac{\partial}{\partial s_{pj}}\right). \tag{C1}$$

We now evaluate the derivatives in Eq. (2.29) in analogy to the case of ordinary matrices. The calculation is somewhat more involved but still reasonably straightforward so that we only mention the intermediate result

$$\Delta_s\frac{\lambda(s)}{B_{k_1k_2}(s^2)}=\frac{1}{B_{k_1k_2}(s^2)}\sum_{j=1}^{2}\sum_{p=1}^{k_j}\left(\frac{\partial^2}{\partial s^2_{pj}}+\frac{1}{s_{pj}}\frac{\partial}{\partial s_{pj}}-4D_{pj}\right)\lambda(s), \tag{C2}$$

where $D_{pj}=s_{pj}+s^2_{pj}(S^2_{pj}-T_{pj})$. Here, $S_{pj}=\widetilde{S}_{pj}-\overline{S_{pj}}$ and $T_{pj}=\widetilde{T}_{pj}-\overline{T_{pj}}$ with

$$\widetilde{S}_{pj}=\sum_{\substack{q=1\\q\neq p}}^{k_j}\frac{1}{s^2_{pj}-s^2_{qj}},\quad \overline{S_{pj}}=\sum_{q=1}^{k_{\chi(j)}}\frac{1}{s^2_{pj}+s^2_{q\chi(j)}}, \tag{C3}$$

$$\widetilde{T}_{pj}=\sum_{\substack{q=1\\q\neq p}}^{k_j}\frac{1}{(s_{pj}^2-s_{qj}^2)^2},\quad \overline{T_{pj}}=\sum_{q=1}^{k_{\chi(j)}}\frac{1}{(s_{pj}^2+s_{q\chi(j)}^2)^2}. \tag{C4}$$

In the above, we have introduced the convention

$$\chi(j)=\begin{cases}1 & \text{if } j=2\\ 2 & \text{if } j=1\end{cases}. \tag{C5}$$

We now show that $\Sigma_{j=1}^{2}\Sigma_{p=1}^{k_j}D_{pj}=0$. According to the definition, we have

$$D_{pj}=\widetilde{S}_{pj}+s_{pj}^2(\widetilde{S}_{pj}^2-\widetilde{T}_{pj})-\overline{S_{pj}}+s_{pj}^2(\overline{S_{pj}^2}-2\widetilde{S}_{pj}\overline{S_{pj}}+\overline{T_{pj}}). \tag{C6}$$

For each j, the sum over p of the first two terms is zero in analogy to the case of ordinary matrices which was discussed in Appendix A. We are thus left with the remaining two terms which we denote by $-D'_{pj}$. Summing over p and j, some algebra leads to

$$\sum_{j=1}^{2}\sum_{p=1}^{k_j}D'_{pj}=\sum_{p=1}^{k_1}\sum_{q=1}^{k_2}\frac{1}{s_{p1}^2+s_{q2}^2}\left(\sum_{\substack{p'=1\\p'\neq p}}^{k_1}\frac{s_{q2}^2(s_{p1}^2+s_{p'1}^2)+2s_{p1}^2s_{p'1}^2}{(s_{p1}^2-s_{p'1}^2)(s_{p'1}^2+s_{q2}^2)}\right.$$
$$\left.+\sum_{\substack{q'=1\\q'\neq q}}^{k_2}\frac{s_{p1}^2(s_{q2}^2+s_{q'2}^2)+2s_{q2}^2s_{q'2}^2}{(s_{q2}^2-s_{q'2}^2)(s_{p1}^2+s_{q'2}^2)}\right). \tag{C7}$$

Renaming $p\leftrightarrow p'$ and $q\leftrightarrow q'$ in the first and second term, respectively, shows that each of the two sums yields zero individually. This completes the proof.

APPENDIX D: ON BOUNDARY CONTRIBUTIONS IN THE CASE OF HERMITIAN SUPERMATRICES

The purpose of this Appendix is to clarify the role of some boundary contributions to the supersymmetric Itzykson–Zuber integral which arise in the case of Hermitian supermatrices. This discussion is not directly related to the main content of the present paper.

After we had computed the result (3.30) for the function $\eta(s,t)$, P.-B. Gossiaux pointed out to us that the structure of these contributions in the case of Hermitian supermatrices ought to be very similar. Indeed, this is true. A careful reexamination of the considerations following Eq. (B33) in Appendix B of Ref. 7 leads to additional terms very similar to the ones in Eq. (3.30). To clarify this, we calculate the function

$$\eta(s,t)=\frac{1}{B_k(s)}\det[\,\widetilde{\eta}(s_{p1},is_{q2},t)\,]_{p,q=1,\ldots,k} \tag{D1}$$

in the case of Hermitian supermatrices for $k_1=k_2=k$. Here, the entries of the determinant are given by

$$\widetilde{\eta}(s_{p1},is_{q2},t)=\frac{1}{2\pi t}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\frac{dr_1\,dr_2}{r_1-ir_2}\exp\left(-\frac{1}{2t}\left((s_{p1}-r_1)^2+(s_{p2}-r_2)^2\right)\right). \tag{D2}$$

We introduce polar coordinates $r_1+ir_2=\kappa\exp(i\vartheta)$ and $s_{p1}+is_{q2}=\mu\exp(i\psi)$ and find

$$\tilde{\eta}(s_{p1}, is_{q2}, t) = \frac{1}{2\pi t} \int_0^\infty d\kappa \, \exp\left(-\frac{1}{2t} (\kappa^2 + \mu^2) \right) \int_0^{2\pi} d\vartheta \, \exp(i\vartheta) \exp\left(\frac{\kappa\mu}{t} \cos(\vartheta - \psi) \right). \tag{D3}$$

The angular integration yields the modified Bessel function $I_1(\kappa\mu/t)$ [Ref. 26, 3·71.(9) and 6·22.(4)]. The radial integration can then be performed using standard methods [Ref. 26, 13·3.(2)]. Collecting everything, we arrive at

$$\eta(s,t) = \frac{1}{B_k(s)} \det\left[\frac{1}{s_{p1} - is_{q2}} \left(1 - \exp\left(-\frac{s_{p1}^2 + s_{q2}^2}{2t} \right) \right) \right]_{p,q=1,\ldots,k}. \tag{D4}$$

As in the case of complex matrices, this function satisfies the diffusion equation

$$\frac{1}{2} \Delta_s \eta(s,t) = \frac{\partial}{\partial t} \eta(s,t), \tag{D5}$$

where the radial part Δ_s of the Laplacian is defined in Eq. (B19) of Ref. 7. The main results of Ref. 7 do not change due to these additional contributions.

NOTE ADDED IN PROOF

After submission of the manuscript, we learned that our results Eq. (2.3) and Eq. (2.6) were also obtained independently by Jackson, Şener, and Verbaarschot [A. D. Jackson, M. K. Şener, and J. J. M. Verbaarschot (preprint hep-th/9605183)] who also generalized Eq. (2.3) to rectangular ordinary matrices.

Furthermore, we were informed by G. Olshanski that the integral for complex rectangular ordinary matrices had already appeared in a short note in Russian by F. A. Berezin and F. I. Karpelevich [F. A. Berezin and F. I. Karpelevich, Doklady Akad. Nauk SSSR **118**, 9–12 (1958)]. We thank G. Olshanski for sending us this paper and V. Kagalovsky for help with the translation. Our main result Eq. (2.6), however, has not been derived before to the best of our knowledge.

In the meantime, we have also generalized our result Eq. (2.6) to rectangular supermatrices. Let σ be a complex supermatrix whose boson-boson and fermion-fermion blocks have dimension $k_1 \times k_1'$ and $k_2 \times k_2'$, respectively. Such a matrix can only be pseudodiagonalized as $\sigma = usv^{-1}$ if the condition $(k_1' - k_1)(k_2' - k_2) \geqslant 0$ is satisfied. For definiteness, let us assume that $k_1' \geqslant k_1$ and $k_2' \geqslant k_2$ and define $d = k_1' - k_1 - (k_2' - k_2)$, $d_1 = d$, $d_2 = -d$. The Berezinian analogous to (2.26) is then given by

$$J(s) = B_{k_1 k_2}^2(s^2) \prod_{j=1}^{2} \prod_{p=1}^{k_j} s_{pj}^{1+2d_j}. \tag{I}$$

The reduced part of the Laplacian analogous to (2.30) becomes

$$\Delta_s' = \sum_{j=1}^{2} \sum_{p=1}^{k_j} \left(\frac{\partial^2}{\partial s_{pj}^2} + \frac{1 + 2d_j}{s_{pj}} \frac{\partial}{\partial s_{pj}} \right). \tag{II}$$

The integral analogous to (2.6) yields

$$\varphi(s,r) = \frac{(2\pi)^{(k_1 - k_2)(k_1' - k_2')}}{2^{k_1 k_2' + k_1' k_2} k_1! k_2!} \frac{\det[J_{d_1}(s_{p1} r_{p'1})]_{p,p'=1,\ldots,k_1} \det[J_{d_2}(s_{q2} r_{q'2})]_{q,q'=1,\ldots,k_2}}{B_{k_1 k_2}(s^2) B_{k_1 k_2}(r^2) \prod_{j=1}^{2} \prod_{p=1}^{k_j} (s_{pj} r_{pj})^{d_j}}. \tag{III}$$

It should be emphasized that the appearance of additional singularities in the Berezinian (I) gives rise to further contributions to the Efetov–Wegner term $\eta(s,t)$.

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Classification of invariant wave equations

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In this paper we characterize the possible symmetry groups of wave equations and certain evolutionary generalizations, in a single time variable and one or more spatial variables. Furthermore, we describe a complete classification of two-dimensional wave equations $u_{tt}=F[u]$ and potential evolutionary equations $u_{xt}=F[u]$ having a point or contact symmetry group. The results rely on Lie's classification of planar transformation groups and their relative differential invariants. © *1996 American Institute of Physics.* [S0022-2488(96)03211-2]

I. INTRODUCTION

One of the most basic constructions of modern physics is the formulation of field equations (or variational principles) admitting a known symmetry group. It has been known since the days of Sophus Lie that this can be readily done, in the regular case, by assembling suitable combinations of differential invariants of the transformation group. Although Lie's general theorem would appear to completely resolve the issue of classifying differential equations admitting prescribed symmetry groups, a more subtle question has recently been of importance, and cannot be quite so immediately answered. The problem is to classify invariant differential equations of a specified form admitting a prescribed symmetry group. For example, the classification of geometric diffusion equations admitting symmetry groups of visual significance is a problem of importance in computer vision and image processing. In Refs. 1 and 2, a complete classification for subgroups of the projective group was determined. More generally, one can ask for a complete list of invariant evolution equations admitting a prescribed symmetry group, and the latter problem was completely solved in Ref. 3, using the theory of relative invariants. It was found that any transformation group in the field and spatial variables (but fixing the time variable) always admits an infinite collection of invariant evolution equations; see Theorem 4.11 below and also the work of Sokolov.[4] The reason why this problem is not an immediate consequence of the classification of differential invariants for the transformation group in question is that it may not be so evident which combinations of differential invariants, *if any*, can be used to produce the equation having the specified form. In the case of evolution equations, the fact that the time variable introduces an additional coordinate into the picture implies that one needs to compute a new basis of fundamental differential invariants, even when the purely spatial derivative invariants are known.

In this paper, we shall consider the classification of wave equations in both one and several space variables, and a single time variable admitting a prescribed finite-dimensional symmetry group. This problem is of interest in computer vision and other applications, first since one might desire to use hyperbolic, rather than parabolic, processing on an image. A second reason arises in image enhancement, in which one uses a hyperbolic regularization to effect a backwards (and hence ill-posed) parabolic equation (cf. Ref. 5). (See also Ref. 6 for equations of Euler–Poisson–Darboux type.) Since the image smoothing was done in a group-invariant manner, one might reasonably ask for similarly invariant hyperbolic enhancers. Surprisingly, the above-mentioned

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result for evolution equations is no longer valid—*not* every spatial transformation group admits an invariant hyperbolic wave equation. We determine a complete set of conditions that a transformation group admit an invariant evolutionary or wave equation. Further, using the differential invariants for the groups, completely characterize all possible invariant equations admitted by a symmetry group of the prescribed type. In the planar case (one independent spatial variable and one dependent variable), we then use Lie's complete classification of groups of point and contact transformations in the plane to find a complete list of invariant wave equations.

We shall assume that the reader is familiar with the basic theory of symmetry groups of differential equations, as presented in Refs. 7 and 8. We shall make extensive use of the theory of differential invariants, as presented in the latter book, as well as in Refs. 9 and 10. Since we are relying on Lie's classification of finite-dimensional transformation groups acting on a two-dimensional complex manifold cf. (Refs. 8 and 11); we shall assume that the variables are, in general, complex valued. In the case of point transformation groups, the extension of these results to real differential equations is not difficult. Unfortunately, there is, as far as we know, no complete classification of real groups of contact transformations acting in two dimensions. The present paper can be viewed as a start towards the classification of differential invariants for surfaces under transformation groups in three-dimensional space, where the group acts completely trivially on the time coordinate. In Ref. 12 Lie describes a partial classification of three-dimensional transformation groups, and claims that he has completed it but these results never appeared in print. An important task awaiting completion is the complete classification of the differential invariants of Lie's three-dimensional transformation groups.

II. JET SPACES AND PROLONGATIONS

Before proceeding to a detailed discussion of our results, we need to first review the theory of differential invariants and, more generally, relative differential invariants. Since all our considerations are local, we will not lose any generality by working in Euclidean space. We will consider the total space $E \simeq X \times U$, where, in the cases considered in this paper, $U \simeq \mathbb{R}$ has coordinate u, the scalar-dependent variable, whereas $X \simeq \mathbb{R}^p$, has coordinates $x = (x^1, \dots, x^p)$, representing the spatial independent variables. The nth jet space $\mathrm{J}^n E$ thus has coordinates $(x, u^{(n)})$, where $u^{(n)}$ stands for all partial derivatives

$$u_K = \frac{\partial^k u}{(\partial x^1)^{k_1} \cdots (\partial x^p)^{k_p}}, \quad \text{where} \quad \begin{matrix} K = (k_1, \dots, k_p), \\ k = \#K = k_1 + \cdots + k_p \leqslant n. \end{matrix} \tag{2.1}$$

We will use the basic multi-indices e_i, $i = 0, \dots, p$, which has a single 1 in the ith position and zeros elsewhere. Thus $u_i = u_{e_i} = \partial u / \partial x^i$. Moreover, we write $L \subseteq K$ if all entries of L are less than or equal to those of K, so $0 \leqslant l_j \leqslant k_j$, $j = 0, \dots, p$. Similarly, we write $L \subset K$ if $L \subseteq K$, but $L \neq K$. Note that the difference $K - L$ is a well-defined multi-index if and only if $L \subseteq K$. Finally, we write $\binom{K}{L}$ for the standard multinomial coefficient, which is nonzero provided $L \subseteq K$. A function $F(x, u^{(n)})$ depending on independent and dependent variables and their derivatives is known as a *differential function*, and $n = \operatorname{ord} F$ is its order, which means that F really does depend on nth-order derivatives of u.

We shall consider both point transformation groups, which are local transformation groups $G = G^{(0)}$ acting on the space $E = X \times U$, and contact transformation groups, which, by Bäcklund's Theorem,[13,8] are at most first order, and thus realized as a local transformation group $G^{(1)}$ on the first jet space $\mathrm{J}^1 E$ preserving the contact ideal generated by the contact form $\theta = du - \sum_{i=1}^p u_i dx^i$. In both cases, the group induces a corresponding transformation group $G^{(n)}$ on the nth jet space $\mathrm{J}^n E$, called the nth prolongation of G, which can be uniquely characterized as the nth-order contact transformation group projecting back to the original group action.

We let $\mathfrak{g}$ denote the Lie algebra of G. Consider an infinitesimal generator of the group action

$$\mathbf{v}^{(0)}=\sum_{i=1}^{p}\ \xi^i\ \frac{\partial}{\partial x^i}+\varphi\ \frac{\partial}{\partial u},\tag{2.2}$$

corresponding to the Lie algebra element $\mathbf{v}\in\mathfrak{g}$. In the case of point transformations, the coefficients ξ^i and φ of $\mathbf{v}^{(0)}$ depend on x and u. The group is fiber preserving (or projectable[7]) if $\xi^i=\xi^i(x)$ only depend on the independent variables. Finally, the group consists of *affine bundle maps* if it consists of transformations $(x,u)\mapsto(\Phi(x),A(x)u+B(x))$ which are fiber preserving and affine in the dependent variable u at each point; the infinitesimal generators have $\varphi=\alpha(x)u+\beta(x)$. For instance, most linear partial differential equations have affine bundle symmetry groups. The infinitesimal generators of a contact transformation group have the same form (2.2), but the coefficients ξ^i and φ are allowed to depend on the first-order derivatives of u provided they satisfy the *contact conditions*

$$\frac{\partial\varphi}{\partial u_k}=\sum_{i=1}^{p}\ u_i\ \frac{\partial\xi^i}{\partial u_k},\quad k=1,\ldots,p.\tag{2.3}$$

In all cases, the *characteristic* of the vector field (2.2) is defined to be the first-order differential function

$$Q(x,u^{(1)})=\varphi-\sum_{i=1}^{p}\ \xi^i u_i\,.\tag{2.4}$$

The vector field can be recovered from its characteristic by solving (2.4) for φ and using

$$\xi^i(x,u^{(1)})=-\frac{\partial Q(x,u^{(1)})}{\partial u_i},\tag{2.5}$$

which is a consequence of the contact conditions (2.3), to construct the coefficients ξ^i. The corresponding infinitesimal generator

$$\mathbf{v}^{(n)}=\sum_{i=1}^{p}\ \xi^i\ \frac{\partial}{\partial x^i}+\sum_{\#K\leqslant n}\ \varphi^K\ \frac{\partial}{\partial u_K}\tag{2.6}$$

of $G^{(n)}$ defines the nth prolongation of $\mathbf{v}$, whose coefficients are given by the standard prolongation formula

$$\varphi^K=D_KQ+\sum_{i=1}^{p}\ \xi^i u_{Ki}\,.\tag{2.7}$$

Here D_K is the total derivative corresponding to the multi-index K, and we use the notation $u_{Ki}=u_{K+e_i}=D_iu_K$.

For later reference, we require some elementary formulas for higher-order total derivatives of certain types of differential functions. Both results are easy to prove by induction using Leibniz' rule.

Lemma 2.1: Suppose $\varphi(x,u)$ is a zeroth-order differential function. Then its first and second-order total derivatives have the form

$$D_i\varphi=\frac{\partial\varphi}{\partial u}\ u_i+\frac{\partial\varphi}{\partial x^i},$$

$$D_iD_j\varphi=\frac{\partial\varphi}{\partial u}\,u_{ij}+\frac{\partial^2\varphi}{\partial u^2}\,u_iu_j+\frac{\partial^2\varphi}{\partial u\,\partial x^i}\,u_j+\frac{\partial^2\varphi}{\partial u\,\partial x^j}\,u_i+\frac{\partial^2\varphi}{\partial x^i\partial x^j}. \tag{2.8}$$

Furthermore, for any multi-index K with $k=\#K\geqslant 3$,

$$D_K\varphi=\varphi_u u_K+\sum_{i=1}^{p} k_i(D_i\varphi_u)u_{K-e_i}+F(x,u^{(k-2)}), \tag{2.9}$$

where F is a differential function depending on at most $(k-2)$*nd-order derivatives of u*

Lemma 2.2: Suppose $Q(x,u^{(1)})$ *is a first-order differential function. Then its first- and second-order total derivatives have the form*

$$\begin{aligned} D_iQ&=\sum_{l=1}^{p}\frac{\partial Q}{\partial u_l}\,u_{il}+\frac{\partial Q}{\partial u}\,u_i+\frac{\partial Q}{\partial x^i},\\ D_iD_jQ&=\sum_{l=1}^{p}\frac{\partial Q}{\partial u_l}\,u_{ijl}+\sum_{l,m=1}^{p}\frac{\partial^2 Q}{\partial u_l\partial u_m}\,u_{il}u_{jm}+\frac{\partial Q}{\partial u}\,u_{ij}\\ &\quad+\sum_{l=1}^{p}\left(\frac{\partial^2 Q}{\partial u_l\partial u}\,(u_ju_{il}+u_iu_{jl})+\frac{\partial^2 Q}{\partial u_l\partial x^i}\,u_{jl}+\frac{\partial^2 Q}{\partial u_l\partial x^j}\,u_{il}\right)+R(x,u^{(1)}), \end{aligned} \tag{2.10}$$

where R is a first-order differential function. Furthermore, for any multi-index K with $k=\#K\geqslant 3$,

$$D_KQ=\sum_{l=1}^{p}\frac{\partial Q}{\partial u_l}\,u_{Kl}+Q_uu_K+\sum_{i,l=1}^{p}k_iD_i\left(\frac{\partial Q}{\partial u_l}\right)u_{K-e_i+e_l}+R(x,u^{(k-1)}), \tag{2.11}$$

where R is a differential function depending on at most $(k-1)$*st-order derivatives of u*.

Note that in both sets of formulas, the multi-indices of orders 1 and 2 do not fit into the general higher-order pattern.

III. RELATIVE DIFFERENTIAL INVARIANTS

Throughout this section, we let G be a transformation group (either point or contact) acting via prolongation on the jet spaces J^nE over a bundle $E=X\times U$. Recall that an (absolute) differential invariant is an invariant differential function for a prolonged group action. A differential operator is said to be G-invariant if it maps differential invariants to higher-order differential invariants, and thus, by iteration, produces hierarchies of differential invariants of arbitrarily large order. A general theorem guarantees the existence of sufficiently many such differential operators so as to completely generate all the higher-order independent differential invariants of the group by successively differentiating lower-order differential invariants. Thus, a complete description of all the differential invariants is provided by a collection of low-order ''fundamental'' differential invariants along with the requisite invariant differential operators.

Theorem 3.1: *Suppose that G is a group of point or contact transformations. Then there exist* $p=\dim X$ *invariant differential operators* $\mathscr{D}_1,\ldots,\mathscr{D}_p$, *and a system of fundamental differential invariants* $J_1,\ldots,J_m$, *such that, locally, every differential invariant can be written as a function of the iterated derivatives* $\mathscr{D}_{j_1}\ldots\mathscr{D}_{j_\kappa}J_\nu$.

A relative differential invariant is, roughly speaking, a differential function which is invariant, up to a factor, under the prolonged group action. The theory of relative differential invariants is a particular case of the general theory of relative invariants of transformation group actions, in which the group acts by prolongation on a suitable jet space (cf. Ref. 8). See Ref. 14 for a detailed development and recent results describing general classification of relative invariants.

Definition 3.2: A differential multiplier of order n is a linear map $\mathbf{v}\mapsto H_{\mathbf{v}}(x,u^{(n)})$ that maps each Lie algebra element $\mathbf{v}\in\mathfrak{g}$ to a differential function $H_{\mathbf{v}}(x,u^{(n)})$, and satisfies the *cocycle condition*

$$\mathbf{v}^{(n)}(H_{\mathbf{w}}(x,u^{(n)}))-\mathbf{w}^{(n)}(H_{\mathbf{v}}(x,u^{(n)}))=H_{[\mathbf{v},\mathbf{w}]}(x,u^{(n)}). \tag{3.1}$$

The cocycle condition (3.1) implies that the associated infinitesimal generators of the differential multiplier representation

$$\mathscr{D}_{\mathbf{v}}=\mathbf{v}^{(n)}-H_{\mathbf{v}}(x,u^{(n)}) \tag{3.2}$$

form a Lie algebra of first-order differential operators on J^nE having the same commutation relations as the Lie algebra $\mathfrak{g}$. In this paper, we only need consider scalar multipliers, although extensions to matrix-valued multipliers are straightforward.[14,8]

Definition 3.3: A differential function $R(x,u^{(n)})$ is called a *relative differential invariant* for the differential multiplier $H_{\mathbf{v}}$ if it satisfies

$$\mathscr{D}_{\mathbf{v}}(R)=\mathbf{v}^{(n)}(R)-H_{\mathbf{v}}\cdot R=0, \quad \text{for all} \quad \mathbf{v}\in\mathfrak{g}. \tag{3.3}$$

Thus ordinary (or absolute) differential invariants are relative differential invariants for the trivial differential multiplier $H_{\mathbf{v}}\equiv 0$. Note that if R is a relative differential invariant for the multiplier $H_{\mathbf{v}}$ and S is a relative differential invariant for the multiplier $K_{\mathbf{v}}$, then the product $R\cdot S$ is a relative differential invariant for the sum $H_{\mathbf{v}}+K_{\mathbf{v}}$. If R_0 is one particular relative differential invariant of weight $H_{\mathbf{v}}$, then every other such relative differential invariant has the form $R=IR_0$, where I is an arbitrary absolute differential invariant.

Relative differential invariants can be used to construct invariant differential equations. The following result is standard; see Ref. 14 for a proof and Ref. 15 for additional applications.

Theorem 3.4: *A regular partial differential equation $\Delta(x,u^{(n)})=0$ admits G as a symmetry group if and only if Δ is a relative differential invariant for some differential multiplier of G.*

Proposition 3.5: Suppose $R(x,u^{(n)})$ is a relative differential invariant of weight $H_{\mathbf{v}}$. Then the partial differential equation $R(x,u^{(n)})=S(x,u^{(n)})$ admits G as a symmetry group if and only if $S(x,u^{(n)})$ is also a relative differential invariant of weight $H_{\mathbf{v}}$.

The existence of relative differential invariants of sufficiently high order is a consequence of general results in Refs. 8 and 10; see also Ref. 14 for generalizations. Recall that a group is said to act *effectively freely* on the manifold M if the quotient group G/G_0 of G by its global isotropy subgroup $G_0=\{g\in G\,|\,g\cdot x=x \text{ for all } x\in M\}$ acts freely.

Theorem 3.6: *Let $H_{\mathbf{v}}(x,u^{(n)})$ be an nth-order differential multiplier. If $G^{(n)}$ acts effectively freely on (an open subset of) J^nE, then there exists a nontrivial relative invariant of weight $H_{\mathbf{v}}$.*

The next theorem is originally due to Ovsiannikov;[10] see also Ref. 8.

Theorem 3.7: *If G is a local transformation group on E, then, for n sufficiently large, G acts effectively freely on the open subset of J^nE where its orbits have maximal dimension.*

Combining Theorems 3.6 and 3.7, we conclude that any transformation group admits a nontrivial relative differential invariant, provided we allow it to have a sufficiently high order.

Theorem 3.8: *Any differential multiplier $H_{\mathbf{v}}(x,u^{(n)})$ of a transformation group G admits a nonzero relative invariant $R_0(x,u^{(m)})\not\equiv 0$. Moreover, every other relative invariant of weight $H_{\mathbf{v}}$ has the form $R=I\cdot R_0$, where I is an arbitrary absolute differential invariant of G.*

Example 3.9: The total divergence multiplier $D_{\mathbf{v}}$ is defined as the total divergence of the independent variable coefficients of the infinitesimal generator (2.2), so that

$$D_{\mathbf{v}}=\operatorname{Div}\boldsymbol{\xi}=\sum_{i=1}^{p} D_i\xi^i. \tag{3.4}$$

The total divergence multiplier arises in the study of invariant variational problems. The standard infinitesimal invariance criterion[7] that G be a strict variational symmetry group (i.e., without divergence terms) of a variational problem $\int L(x,u^{(n)})dx$ is

$$\mathbf{v}^{(n)}(L)+L\ \mathrm{Div}\ \boldsymbol{\xi}=0. \tag{3.5}$$

However, (3.5) is just the condition that the Lagrangian $L(x,u^{(n)})$ is a relative differential invariant for the negative total divergence multiplier $\widetilde{D}_{\mathbf{v}}=-\mathrm{Div}\ \boldsymbol{\xi}$. For example, if $X=\mathbb{R}^2$, then the usual surface area integral,

$$\mathscr{S}[u]=\int \sqrt{1+u_x^2+u_y^2}\,dx\wedge dy, \tag{3.6}$$

clearly admits the Euclidean group $G=\mathrm{E}(3)$, consisting of translations and rotations in the three-dimensional space coordinatized by (x,y,u), as a symmetry group. This means that $S=\sqrt{1+u_x^2+u_y^2}$ is a relative differential invariant for $D_{\mathbf{v}}=-D_x\xi-D_y\eta$, corresponding to the infinitesimal generator $\mathbf{v}^{(0)}=\xi\partial_x+\eta\partial_y+\varphi\partial_u$.

Example 3.10: A second important differential multiplier is the *characteristic multiplier*

$$K_{\mathbf{v}}=Q_u, \tag{3.7}$$

where $Q(x,u^{(1)})$ is the characteristic of the vector field (2.2) given in (2.4). The importance of this differential multiplier lies in its connection with the Euler–Lagrange equations for invariant variational problems. See Refs. 8 and 3 for the proof of the following result.

Theorem 3.11: *Let G be a transformation group. Suppose that $\int L(x,u^{(n)})dx$ is a G-invariant variational problem, so that L is a relative differential invariant for the total divergence multiplier. Then its Euler–Lagrange expression* $\mathrm{E}(L)$ *is a relative differential invariant of weight* $-Q_u-\mathrm{Div}\ \boldsymbol{\xi}$.

If one chooses the G-invariant volume element $\int L\,dx$ as the invariant variational problem, then the Euler–Lagrange equation forms the G-invariant minimal hypersurface equation in E. For example, if $G=\mathrm{E}(3)$ is the Euclidean group in $\mathbb{R}^3$, then the Euler–Lagrange equation for the surface area integral (3.6) is the standard (Euclidean-invariant) three-dimensional minimal surface equation

$$0=\mathrm{E}(S)=-D_x(S_{u_x})-D_y(S_{u_y})=\frac{-(1+u_y^2)u_{xx}+2u_xu_yu_{xy}-(1+u_x^2)u_{yy}}{(1+u_x^2+u_y^2)^{3/2}}.$$

The right-hand side of this equation is a relative invariant of weight $-Q_u-D_x\xi-D_y\eta$.

Using the multiplicative property of relative invariants, we readily establish the following useful result.

Corollary 3.12: Every relative invariant for the characteristic multiplier $K_{\mathbf{v}}=Q_u$ has the form

$$F=\frac{L}{\mathrm{E}(L)}\,I, \tag{3.8}$$

where I is an arbitrary differential invariant of G, and $\int L(x,u^{(n)})dx$ is a G-invariant variational problem having nontrivial Euler–Lagrange expression $\mathrm{E}(L)\not\equiv 0$.

IV. INVARIANCE CONDITIONS

Our primary purpose is determining symmetry groups of evolutionary-type equations, and so we shall extend the preceding considerations to include an additional independent variable, the ''time'' t. Now, the total space is $\hat{E}\simeq\mathbb{R}\times E\simeq Z\times U$, where $U\simeq\mathbb{R}$ has coordinate u, whereas

$Z \simeq \mathbb{R}\times\mathbb{R}^p$ has coordinates $t=x^0$, representing time, and $x=(x^1,\dots,x^p)$, representing the spatial independent variables. The nth jet space $\mathrm{J}^n\hat{E}$ thus has coordinates[16] $(x,u^{[n]})$, where $u^{[n]}$ stands for all partial derivatives

$$u_K=\frac{\partial^k u}{(\partial t)^{k_0}(\partial x^1)^{k_1}\cdots(\partial x^p)^{k_p}}, \quad \text{where} \quad \begin{matrix} K=(k_0,k_1,\dots,k_p), \\ k=\#K=k_0+k_1+\cdots+k_p\leqslant n. \end{matrix} \tag{4.1}$$

In this framework, an nth-order *evolution equation* is a partial differential equation of the form

$$u_t=F[u], \tag{4.2}$$

where $F:\mathrm{J}^nE\to\mathbb{R}$ is a smooth differential function, depending on spatial derivatives of u up to order n. More generally, we consider higher-order *evolutionary-type equations*

$$u_K=F[u], \tag{4.3}$$

where $K=L+e_0$ is a multi-index that contains at least one time derivative in it, so $k_0\geqslant 1$, and F is again a spatial differential function. Particular cases include the *wave equation*

$$u_{tt}=F[u], \tag{4.4}$$

where $K=2e_0=(2,0,\dots,0)$, and the *potential evolution equation*

$$\frac{\partial^2 u}{\partial t\,\partial x^i}=u_{it}=F[u], \tag{4.5}$$

where $K=e_0+e_i$. Note that differentiating the evolution equation (4.2) with respect to x^i, or replacing u by its ith potential function $u\mapsto u_i$, will convert (4.2) into an equation of the form (4.5). In each of these examples, one could, of course, go further and allow F to also depend on some lower-order temporal derivatives of u; for example, one might allow the right-hand side of the wave equation (4.4) to depend on u_t. However, for most of our results, we will restrict attention to purely spatial right-hand sides; extensions will be briefly discussed in Sec. VI.

We are interested in classifying the *spatial* symmetry groups of such evolutionary-type equations. The restriction to spatial implies that the time variable t is not affected by the group transformations, and so we consider a connected Lie group G of either point or contact transformations, which acts on the space $E=X\times U$ of spatial coordinates, and hence determines the corresponding spatially prolonged actions $G^{(n)}$ on the jet space J^nE. In addition, one can include the time t as an additional variable not affected by the group transformations, and thus induce a temporal prolongation $G^{[n]}$ acting on the extended jet space $\mathrm{J}^n\hat{E}$. In the point transformation case, this is found by prolonging the extended action $(t,x,u)\mapsto(t,g\cdot(x,u))$ on $\hat{E}\simeq\mathbb{R}\times E$; in the case of contact transformations, we extend the action to $\mathrm{J}^1\hat{E}\simeq\mathbb{R}^2\times\mathrm{J}^1E$, so that the t variable is not affected, while the action on the time derivative coordinate u_t is determined by the chain rule:

$$\overline{u_t}=\left(\frac{\partial\Phi}{\partial u}-\sum_{i=1}^{p}\overline{u_i}\,\frac{\partial\Xi^i}{\partial u}\right)u_t, \quad \text{where} \quad \begin{matrix} \overline{t}=t, & \overline{x^i}=\Xi^i(x,u^{(1)}), \\ \overline{u}=\Phi(x,u^{(1)}), & \overline{u_i}=\Psi_i(x,u^{(1)}). \end{matrix} \tag{4.6}$$

In this manner, a contact transformation on J^1E extends in a natural way to a contact transformation on $\mathrm{J}^1\hat{E}$.

Given a Lie algebra element $\mathbf{v}\in\mathfrak{g}$, the corresponding infinitesimal generator $\mathbf{v}^{(0)}$ is a spatial vector field, as in (2.2), whose extended action on $\hat{E}=\mathbb{R}\times E$ has the same form, $\mathbf{v}^{[0]}=\mathbf{v}^{(0)}$, since the time variable is not changed. Let $\mathbf{v}^{[n]}$ denote the nth prolongation of $\mathbf{v}$ to $\mathrm{J}^n\hat{E}$. Note that, according

to the prolongation formula, the coefficients of temporal and mixed derivatives in $\mathbf{v}^{[n]}$ are *not* necessarily trivial even though t is unaffected by the group transformations; for instance, using (2.5), the coefficient of ∂_{u_t} is

$$\varphi^t = D_t Q + \sum_{i=1}^{p} \xi^i u_{it} = Q_u u_t . \tag{4.7}$$

Thus $\mathbf{v}^{[1]}(u_t) = Q_u u_t$, and we discover that u_t is a relative differential invariant for the characteristic multiplier Q_u. Proposition 3.5 thus implies that the evolution equation (4.2) admits G as a symmetry group if and only if the right-hand side $F[u]$ is also a relative differential invariant of weight Q_u. Combining this observation with the characterization of such relative differential invariants in Corollary 3.12 produces the main result of Ref. 3.

Theorem 4.1: *An evolution equation $u_t = F[u]$ admits the connected spatial transformation group G as a symmetry group if and only if F is a relative invariant of weight Q_u, and hence of the form (3.8).*

In particular, every spatial transformation group admits an invariant evolution equation! The most effective method for analyzing the symmetry groups of differential equations is by use of infinitesimal generators. Our starting point is the standard infinitesimal invariance criterion for differential equations.

Theorem 4.2: *An evolutionary-type equation $u_K = F$ admits a connected transformation group G as a symmetry group if and only if*

$$\mathbf{v}^{[n]}(u_K - F) = 0 \quad \text{whenever} \quad u_K = F. \tag{4.8}$$

We proceed to analyze this criterion for spatial transformation groups. The prolongation formula (2.6), coupled with (2.7) and (2.4), implies that we can replace (4.8) by

$$D_K Q + \sum_{i=1}^{p} \xi^i u_{Ki} = \mathbf{v}^{(n)}(F) \quad \text{whenever} \quad u_K = F. \tag{4.9}$$

Recall that $k = \#K$ is the order of K, which contains at least one t derivative. Note first that the left-hand side of (4.9) does not contain any terms involving derivatives of order $k+1$ since the terms $\xi^i u_{Ki}$ cancel the corresponding terms obtained by differentiating the characteristic. [This still holds for contact transformations due to the contact conditions (2.5).]

We begin by assuming that K has order $k = \#K \geqslant 3$, postponing the analysis of the second-order cases, namely the wave equation (4.4) and potential evolution equations (4.5), until later. However, unless specifically stated otherwise, the intervening theorems also apply to second-order equations, albeit with slightly different proofs. For $\#K \geqslant 3$, according (2.11), the only terms on the left-hand side of (4.9) which involve derivatives of order k are

$$Q_u u_K - \sum_{i=1}^{p} \sum_{j=0}^{p} k_j (D_j \xi^i) u_{K - e_j + e_i}, \tag{4.10}$$

where we have used (2.5) to identify the derivatives of the characteristic with respect to the derivative variables u_i. On solutions to (4.3) we can replace u_K by F, and hence the terms involving u_K in (4.10) only depend on spatial derivatives of u. On the other hand, because the coefficients φ and ξ^i do not depend on t, all other terms on the left-hand side of (4.9) will involve at least one temporal derivative of u, which cannot be replaced by a spatial derivative. Therefore, the infinitesimal invariance condition (4.9) splits into three components. The first part contains only spatial derivatives of u, and is obtained by equating the terms involving u_K in (4.10) to the right-hand side of (4.9), leading to our first key result.

Theorem 4.3: *If the evolutionary-type equation $u_K = F[u]$ admits a spatial symmetry group G, then the right-hand side satisfies*

$$\mathbf{v}^{(n)}(F) = \left(Q_u - \sum_{i=1}^{p} k_i D_i \xi^i \right) F, \quad \text{for all} \quad \mathbf{v} \in \mathfrak{g}. \tag{4.11}$$

Thus, Eq. (4.11) says that the right-hand side F of an invariant differential equation of evolutionary type forms a relative differential invariant for the differential multiplier

$$H^K_{\mathbf{v}}(x, u^{(2)}) = Q_u - \sum_{i=1}^{p} k_i D_i \xi^i. \tag{4.12}$$

In particular, the order of t differentiation on the left-hand side of the equation does not affect the type of relative invariant that the right-hand side assumes.

Corollary 4.4: If a purely temporal evolutionary-type equation,

$$\frac{\partial^n u}{\partial t^n} = F[u], \tag{4.13}$$

admits G as a symmetry group, then F is relative invariant of weight Q_u, and hence of the form (3.8).

Thus if (4.13) admits G, then so does the evolution equation (4.2) with the same right-hand side. The converse, though, is *not* true since there are additional invariance conditions that (4.13) must satisfy that are not required for the invariance of the simple evolution equation (4.2). The additional terms on the left-hand side of the infinitesimal condition (4.9) will end up providing fairly severe restrictions on the types of transformation groups which have, say, invariant wave equations.

Corollary 4.5: If an equation of the form (4.13) admits a symmetry group G, then the corresponding evolution equation $u_t = F$ is also G-invariant. The converse holds provided G fulfills the symmetry conditions in Theorem 4.11 below.

The second set of invariance conditions arise from the other kth-order terms in (4.10), which are equated to 0. We find

$$D_j \xi^i = 0, \quad \text{whenever} \quad k_j > 0, \quad j = 0, \dots, p, \quad j \neq i. \tag{4.14}$$

In particular, $k_0 \geqslant 1$ by assumption, and hence (4.14) implies $D_t \xi^i = 0$, $i = 1, \dots, p$. This automatically requires that $\xi^i = \xi^i(x)$ depends only on the spatial variables, and hence the symmetry group is fiber preserving.

Proposition 4.6: If G is a symmetry group of an evolutionary-type equation (4.3) with left-hand side of order $\#K \geqslant 3$, then G is necessarily a fiber-preserving transformation group.

$$Q(x, u^{(1)}) = \varphi(x, u) - \sum_{i=1}^{p} \xi^i(x) u_i. \tag{4.15}$$

Given a multi-index $K = (k_0, k_1, \dots, k_p)$, let us divide the spatial variables into two sets: the *principal spatial variables*, which are those appearing in the derivative u_K, and the *parametric spatial variables*, which are all the rest. Thus x^j, $1 \leqslant j \leqslant p$, is principal if $k_j > 0$, and parametric if $k_j = 0$. In particular, for the purely temporal evolutionary-type equation (4.13), all spatial variables are parametric. For notational convenience, let us number the spatial variables so that the first s, namely $x^1, \dots, x^s$, are principal, while the remainder $x^{s+1}, \dots, x^p$ are parametric.

Proposition 4.7: Suppose G is a symmetry group of an evolutionary-type equation $u_K = F[u]$ in which $\#K \geqslant 3$. Let $\mathbf{v} \in \mathfrak{g}$ determine an infinitesimal generator (2.2). Then the coefficients $\xi^{s+1},\dots,\xi^p$ corresponding to the parametric spatial variables $x^{s+1},\dots,x^p$ depend only on parametric variables:

$$\xi^i = \xi^i(x^{s+1},\dots,x^p), \quad i = s+1,\dots,p, \tag{4.16}$$

while the coefficients corresponding to the principal spatial variables $x^1,\dots,x^s$ have the form

$$\xi^i = \xi^i(x^i,x^{s+1},\dots,x^p), \quad i = 1,\dots,s. \tag{4.17}$$

Proposition 4.7 allows us to properly justify the statement in Theorem 4.3. In fact, if G is an arbitrary spatial transformation group, then the function (4.12) is, in fact, not an infinitesimal multiplier. However, the additional conditions contained in Proposition 4.7 are precisely those needed to make (4.12) satisfy the infinitesimal multiplier conditions (3.1). Indeed, we can readily produce a basic relative invariant that is associated with (4.12).

Proposition 4.8: Let us split the independent variables into parametric and principal variables in accordance with the multi-index K. Suppose G is a spatial transformation group satisfying the conditions in Proposition 4.7. Suppose that

$$\omega = \sum_{i=1}^{p} A_i(x,u^{(n)})\,dx^i \tag{4.18}$$

is a G-invariant one-form. Then, for each principal variable x^i, the coefficient A_i satisfies[17]

$$\mathbf{v}^{(n)}(A_i) + (D_i\xi^i)A_i = 0, \tag{4.19}$$

and hence defines a relative invariant of weight $-D_i\xi^i$.

Proof: The infinitesimal invariance conditions for a horizontal one-form (4.18) on J^n (up to contact forms—see Ref. 8) are

$$0 = \mathbf{v}^{(n)}(\omega) = \sum_{i=1}^{p} \{\mathbf{v}^{(n)}(A_i)\,dx^i + A_i \mathrm{D}\xi^i\}, \tag{4.20}$$

where

$$\mathrm{D}\xi^i = \sum_{j=1}^{p} D_j\xi^i\,dx^j \tag{4.21}$$

is the total (or horizontal) differential of ξ^i. On the other hand, according to the conditions (4.14), for any principal variable x^i, only the term when $j = i$ contributes to the coefficient of dx^i. Therefore, the coefficient of dx^i in (4.20) is precisely the left-hand side of (4.19). Q.E.D.

Theorem 4.9: *If the evolutionary-type equation $u_K = F[u]$ admits a spatial symmetry group G, then its right-hand side is necessarily of the form*

$$F = \frac{A^K L}{\mathrm{E}(L)}\, I. \tag{4.22}$$

Here I is an arbitrary absolute differential invariant, $\int L(x,u^{(n)})\,dx$ is a G-invariant variational problem with Euler–Lagrange expression $\mathrm{E}(L) \not\equiv 0$, and $\omega = A_1\,dx^1 + \cdots + A_p\,dx^p$ is a G-invariant one-form, such that the product

$$A^K=\prod_{i=1}^{s}(A_i)^{k_i}\not\equiv 0.$$

It is worth reemphasizing at this point that not every spatial transformation group admits an invariant evolutionary-type equation of a prescribed form. For equations in more than two spatial variables, Proposition 4.7 provides some restrictions on the types of symmetry groups allowed. Further restrictions are obtained by analyzing the lower-order terms in the infinitesimal invariance conditions (4.9).

We have already analyzed the terms depending on kth-order derivatives. All remaining terms in (4.8) must vanish since they involve lower-order temporal derivatives of u. We number the spatial variables so that $x^1,\dots,x^s$ are the principal variables, and $x^{s+1},\dots,x^p$ are the parametric variables. We now use Leibniz' rule and (2.9) to find that the terms involving derivatives of order $k-1$ are

$$\sum_{i=0}^{p} k_i(D_i\varphi_u)u_{K-e_i}-\sum_{j=1}^{p}\binom{k_j}{2}(D_j^2\xi^j)u_{K-e_j}=0. \tag{4.23}$$

In particular, setting $i=0$ in the first summation shows that $D_t\varphi_u=0$, and hence

$$\varphi(x,u)=\eta(x)u+\sigma(x). \tag{4.24}$$

This implies that the group consists of affine bundle maps.

Proposition 4.10: A connected symmetry group of an evolutionary-type equation which is not an evolution equation or a potential evolution equation consists of affine bundle maps.

(The case of a wave equation will be demonstrated later.) The additional terms in (4.23) imply that

$$\frac{\partial\eta}{\partial x^i}=\frac{k_i-1}{2}\frac{\partial^2\xi^i}{(\partial x^i)^2},\quad k_i\neq 0. \tag{4.25}$$

In the ordinary case, the group is fiber preserving, and so hence, in terms of the principal variables,

$$\eta(x)=\sum_{i=1}^{s}\frac{k_i-1}{2}\frac{\partial\xi^i}{\partial x^i}+\zeta(x^{s+1},\dots,x^p). \tag{4.26}$$

Furthermore, if $k_i\geqslant 2$, then the $(k-2)$nd-order derivative u_{K-2e_i} in (4.9) has coefficient

$$\binom{k_i}{2}D_i^2\eta=\binom{k_i}{3}D_i^3\xi^i,\quad \text{or}\quad D_i^2\eta=\frac{k_i-2}{3}D_i^3\xi^i,\quad k_i\geqslant 2. \tag{4.27}$$

However, differentiating (4.25) and subtracting, we find

$$D_i^3\xi^i=0,\quad \text{whenever}\quad k_i\geqslant 2. \tag{4.28}$$

Therefore

$$\xi^i=\alpha^i(x^i)^2+\beta^i x^i+\gamma^i,\quad k_i\geqslant 2, \tag{4.29}$$

where α^i, β^i, and γ^i are functions of the parametric variables $x^{s+1},\dots,x^p$ only. This implies all the lower-order derivative terms are also zero; indeed the only term left unaccounted for is $D_K\sigma=0$; but this is automatic since σ only depends on spatial coordinates and K contains at least

one time derivative. We have completed our analysis of the infinitesimal symmetry conditions (4.8) for $\#K \geqslant 3$, and therefore characterized the possible symmetry groups for higher-order evolutionary-type equations.

The analysis in the second-order cases proceeds similarly. The wave equation case (4.4) is completely analogous, using (2.8) and (2.10) instead of the higher-order counterparts, and left to the reader. On the other hand, if the equation is a potential evolution equation, (4.5) (with $i=1$ for consistency in notation), then the conditions arising from second-order derivatives in (4.9) require

$$\frac{\partial^2 Q}{\partial u_l \partial u_m} = \frac{\partial^2 Q}{\partial u_l \partial x^1} = 0 \quad \text{whenever} \quad l, m \neq 1,$$

whereas

$$\frac{\partial^2 Q}{\partial u \partial u_j} = \frac{\partial^2 Q}{\partial u^2} = \frac{\partial^2 Q}{\partial u \partial x^1} = 0 \qquad \text{for} \quad \text{all} \quad j = 1, \dots, p.$$

These imply that the characteristic must have the special form

$$Q(x, u^{(1)}) = \theta(x, u_1) + \zeta(x^2, \dots, x^p) u - \sum_{i=2}^{p} \xi^i(x^2, \dots, x^p) u_i . \tag{4.30}$$

Therefore, potential evolution equations can admit contact symmetry groups, but only of a very special type, with infinitesimal generators of the form

$$-\frac{\partial \theta}{\partial u_1} \frac{\partial}{\partial x^1} + \sum_{i=2}^{p} \xi^i(x^2, \dots, x^p) \frac{\partial}{\partial x^i} + \left[\zeta(x^2, \dots, x^p) u + \theta(x, u_1) + u_1 \frac{\partial \theta}{\partial u_1} \right] \frac{\partial}{\partial u}. \tag{4.31}$$

We have thus completed our analysis of the infinitesimal symmetry conditions (4.8), and have thus proved the following general result governing the possible symmetry groups of evolutionary-type equations.

Theorem 4.11: *Let G be a connected spatial transformation group, and suppose that $u_K = F[u]$, $k_0 > 0$, is an evolutionary-type equation admitting G as a symmetry group. Assume that $x^1, \dots, x^s$ are the principal variables, and $x^{s+1}, \dots, x^p$ are the parametric variables.*

(i) *If the equation is an evolution equation, $u_t = F$, then there are no conditions on G.*

(ii) *If the equation is a potential evolution equation, $u_{xt} = F$, where $x = x^1$, then G can be a contact transformation group whose generators have the form (4.31).*

(iii) *In all other cases, the group is necessarily a group of affine bundle maps, whose infinitesimal generators have coefficients of the form (4.16), (4.17), (4.24), and (4.26). Moreover, if the left-hand side contains a principal derivative having order 2 or more, i.e., $k_i \geqslant 2$, then the corresponding coefficient has the form (4.29).*

In all cases, a group G of the prescribed form does admit a nontrivial invariant evolutionary-type equation $u_K = F_0$ with $F_0 \not\equiv 0$ a relative invariant of weight (4.12) as given in (4.22). Moreover, the most general G-invariant equation of this form is $u_K = I F_0$, where I is an arbitrary absolute differential invariant of G.

Proof: The only part left to demonstrate is the existence of a suitably invariant evolution equation. This follows from the general existence result for relative invariants given in Theorem 3.8. Q.E.D.

Remark: The equation $u_K = 0$ is invariant under any transformation group that meets the invariance conditions in Theorem 4.11.

Remark: If the right-hand side of an evolutionary-type equation is nontrivial, $F \not\equiv 0$, then u_K/F is an (absolute) differential invariant of the group G acting on $\mathrm{J}^n\hat{E}$.

A useful observation is that in every case, the symmetry group admits an invariant foliation, namely that provided by the vertical fibration $\{x=c\}$ of either E or, in the contact case, J^1E, and hence, by definition, must form an imprimitive group of transformations on E. Indeed, Proposition 4.7 implies that the group is ''multiply imprimitive'' since any collection of independent variables that includes all the parametric variables also defines an invariant foliation.

Proposition 4.12: Any connected symmetry group of an evolutionary-type equation $u_K=F[u]$ which is not *an evolution equation is necessarily an imprimitive transformation group.*

This result is of great value in simplifying the classification procedure, since it allows us to immediately eliminate many geometrically important transformation groups (which tend to act primitively) from consideration.

An alternative mechanism for generating invariant evolutionary-type equations whose left-hand sides have higher-order spatial derivatives is by differentiating lower-order equations of evolutionary type. The preceding remark shows how this may be used to provide alternative absolute temporal differential invariants.

Theorem 4.13: *If the evolutionary-type equation $u_K=F[u]$ admits a spatial symmetry group G, then any spatial derivative $u_{K+L}=D_LF$, where $l_0=0$, also admits G as a symmetry group provided G satisfies the restrictions for the differentiated evolutionary-type equation prescribed in Theorem 4.11.*

Proof: This is a direct consequence of the standard commutation formula

$$\mathbf{v}^{(n+1)}\cdot D_i = D_i\cdot \mathbf{v}^{(n)} - \sum_{j=1}^{p} (D_i\xi^j) D_j, \tag{4.32}$$

between prolonged vector fields and total derivatives (cf. Ref. 7). Suppose $L=e_i$, so that x^i is now a principal variable for $K+L=K+e_i$, whether or not it was one for K. Assume first that G satisfies the conditions of Proposition 4.7, with K replaced by $K+L=K+e_i$. Thus, if F satisfies (4.11), then (4.8) implies

$$\begin{aligned}\mathbf{v}^{(n+1)}D_iF = D_i\mathbf{v}^{(n)}(F) - (D_i\xi^i)D_iF &= D_i\left[\left(Q_u - \sum_{j=1}^{p} k_j D_j\xi^j\right)F\right] - (D_i\xi^i)D_iF \\ &= \left(Q_u - \sum_{j=1}^{p} l_j D_j\xi^j\right)D_iF + [D_i\phi - k_iD_i^2\xi^i]F. \end{aligned}\tag{4.33}$$

Now (4.25), which, according to our hypothesis, must hold with k_i replaced by $l_i=k_i+1$, implies that the coefficient of F in the final term in (4.33) vanishes, and so D_iF is a relative invariant of the correct weight for the multi-index L [cf. (4.12)]. Q.E.D.

An interesting question is how to connect this approach with that in Theorem 4.9.

V. CLASSIFICATION IN ONE SPACE DIMENSION

The previous sections dealt with the general theory of invariant equations of evolutionary type in multidimensional space. We now restrict our attention to evolutionary-type equations in one space dimension, so that $p=1$ and there is a single spatial variable, x. The advantage here is that the spatial transformation groups act on a two-dimensional space $E\simeq\mathbb{R}^2$, or, in the complex case $E\simeq\mathbb{C}^2$, and hence we can use Lie's classification of transformation groups acting on two-dimensional manifolds—see the Tables below, which are based on Ref. 11, as simplified in Ref. 8. Our goal now is to classify *all* the invariant equations in a single spatial variable for each of the finite-dimensional transformation groups in the plane. (We leave aside the classification of equations admitting infinite-dimensional pseudo-groups, since, by a linearization theorem of Bluman

and Kumei,[18,8] most of these differential equations can be linearized.) For simplicity, we restrict to the complex case here, although extensions to the five additional real forms[19,8] are readily done utilizing the same methods.

Thus we consider an evolutionary-type equation

$$u_{mn}=\frac{\partial^{m+n}u}{\partial x^m \partial t^n}=F[u], \tag{5.1}$$

where $n\geqslant 1$, and F depends on x, u, and the spatial derivatives $u_k=D_x^k u$ of u. The symmetry generators are vector fields of the form

$$\mathbf{v}^{(0)}=\xi(x,u,u_x)\partial_x+\sigma(x,u,u_x)\partial_u, \tag{5.2}$$

where the dependence on the derivative $u_x=u_1$ allows us to also admit contact transformation groups. Let $N=\max\{m+n,\operatorname{ord} F\}$ denote the order of the partial differential equation (5.1). Let us begin by restating our basic Theorem 4.11 in the scalar spatial case.

Theorem 5.1: *Let G be a connected spatial transformation group acting on $E=X\times U\simeq\mathbb{R}^2$ which is a symmetry group of an evolutionary-type equation (5.1).*

(i) *$m=0$, $n=1$: If the equation is an evolution equation, $u_t=F$, then there are no conditions on G.*

(ii) *$m=0$, $n\geqslant 2$: If the equation is purely evolutionary, i.e., of the form $\partial^n u/\partial t^n=F$, then the infinitesimal generators of G have the form*

$$\mathbf{v}^{(0)}=\xi(x)\partial_x+[\eta(x)u+f(x)]\partial_u, \tag{5.3}$$

where ξ,η,f are functions of x.

(iii) *$m=1$, $n=1$: If the equation is a potential evolution equation, $u_{xt}=F$, then G can be a contact transformation group whose infinitesimal generators have the form*

$$\mathbf{v}^{(0)}=\xi(x,u_x)\partial_x+[ku+\theta(x,u_x)]\partial_u, \tag{5.4}$$

where k is a constant.

(iv) *$m=1$, $n\geqslant 2$: If the equation is the potential form of a higher-order purely evolution equation, $u_{xn}=F$ with $n\geqslant 2$, then the infinitesimal generators of G have the form*

$$\mathbf{v}^{(0)}=\xi(x)\partial_x+[ku+f(x)]\partial_u, \tag{5.5}$$

where k is a constant and ξ and f are functions of x.

(v) *$m\geqslant 2$: In all other cases, the infinitesimal generators have the form*

$$\mathbf{v}^{(0)}=[a_2x^2+a_1x+a_0]\partial_x+[(m-1)a_2u+b_0]\partial_u, \tag{5.6}$$

where a_0, a_1, a_2, and b_0 are constants (and thus the symmetry group is at most four-dimensional).

We also generalize Theorem 4.9 to the scalar case. Now the G-invariant one-form can be taken to be the same as the G-invariant Lagrangian $\omega=L\,dx$.

Theorem 5.2. *In one spatial variable, if an evolutionary-type equation (5.1) admits a spatial transformation group G, then its right-hand side satisfies*

$$\mathbf{v}^{(N)}(F)=(Q_u-mD_x\xi)F, \tag{5.7}$$

and hence is a relative differential invariant of the form

$$F=\frac{L^{m+1}}{E(L)}\,I. \tag{5.8}$$

TABLE I. Lie algebras of point transformations in $\mathbb{C}^2$.

	Generators	Dim	Structure
1.1	$\partial_x, x\partial_x - u\partial_u, x^2\partial_x - 2xu\partial_u$	3	$\mathfrak{sl}(2)$
1.2	$\partial_x, x\partial_x - u\partial_u, x^2\partial_x - (2xu+1)\partial_u$	3	$\mathfrak{sl}(2)$
1.3	$\partial_x, x\partial_x, u\partial_u, x^2\partial_x - xu\partial_u$	4	$\mathfrak{gl}(2)$
1.4	$\partial_x, x\partial_x, x^2\partial_x, \partial_u, u\partial_u, u^2\partial_u$	6	$\mathfrak{sl}(2)\oplus\mathfrak{sl}(2)$
1.5	$\partial_x, \eta_1(x)\partial_u, \ldots, \eta_k(x)\partial_u$	$k+1$	$\mathbb{C}\ltimes\mathbb{C}^k$
1.6	$\partial_x, u\partial_u, \eta_1(x)\partial_u, \ldots, \eta_k(x)\partial_u$	$k+2$	$\mathbb{C}^2\ltimes\mathbb{C}^k$
1.7	$\partial_x, \partial_u, x\partial_x + \alpha u\partial_u, x\partial_u, \ldots, x^{k-1}\partial_u$	$k+2$	$\mathfrak{a}(1)\ltimes\mathbb{C}^k$
1.8	$\partial_x, \partial_u, x\partial_u, \ldots, x^{k-1}\partial_u, x\partial_x + (ku+x^k)\partial_u$	$k+2$	$\mathbb{C}\ltimes(\mathbb{C}\ltimes\mathbb{C}^k)$
1.9	$\partial_x, \partial_u, x\partial_x, u\partial_u, x\partial_u, x^2\partial_u, \ldots, x^{k-1}\partial_u$	$k+3$	$(\mathfrak{a}(1)\oplus\mathbb{C})\ltimes\mathbb{C}^k$
1.10	$\partial_x, \partial_u, 2x\partial_x + (k-1)u\partial_u, x^2\partial_x + (k-1)xu\partial_u, x\partial_u, x^2\partial_u, \ldots, x^{k-1}\partial_u$	$k+3$	$\mathfrak{sl}(2)\ltimes\mathbb{C}^k$
1.11	$\partial_x, \partial_u, x\partial_x, u\partial_u, x^2\partial_x + (k-1)xu\partial_u, x\partial_u, x^2\partial_u, \ldots, x^{k-1}\partial_u$	$k+4$	$\mathfrak{gl}(2)\ltimes\mathbb{C}^k$
2.1	$\partial_x, \partial_u, x\partial_x - u\partial_u, u\partial_x, x\partial_u$	5	$\mathfrak{sa}(2)$
2.2	$\partial_x, \partial_u, x\partial_x, u\partial_x, x\partial_u, u\partial_u$	6	$\mathfrak{a}(2)$
2.3	$\partial_x, \partial_u, x\partial_x, u\partial_x, x\partial_u, u\partial_u, x^2\partial_x + xu\partial_u, xu\partial_x + u^2\partial_u$	8	$\mathfrak{sl}(3)$
3.1	$\zeta_1(x)\partial_u, \ldots, \zeta_k(x)\partial_u$	k	$\mathbb{C}^k$
3.2	$\zeta_1(x)\partial_u, \ldots, \zeta_k(x)\partial_u, u\partial_u$	$k+1$	$\mathbb{C}\ltimes\mathbb{C}^k$
3.3	$\partial_x, x\partial_x, x^2\partial_x$	3	$\mathfrak{sl}(2)$

In Cases 1.5 and 1.6, the functions $\eta_1(x),\ldots,\eta_k(x)$ satisfy a kth-order constant coefficient homogeneous linear ordinary differential equation $\mathscr{D}[u]=0$. In Cases 3.1 and 3.2, the functions $\zeta_1(x),\ldots,\zeta_k(x)$ are arbitrary. In Cases 1.5–1.11 we require $k\geqslant 1$.

Note: We use $\mathfrak{a}(n)$ to denote the Lie algebra of the affine group of $\mathbb{C}^n$, and $\mathfrak{sa}(n)$ for the Lie algebra of the special affine group consisting of volume-preserving affine transformations.

Here I is an arbitrary differential invariant of G, and $\omega = L(x,u^{(n)})dx$ is a G-invariant one-form having nontrivial Euler–Lagrange expression $\mathrm{E}(L)\not\equiv 0$.

Lie's local classification of nonsingular transformation groups[20] that act on a two-dimensional complex manifold appears in Tables I and II. Table I provides a complete list of canonical forms for the infinitesimal generators of all possible finite-dimensional transformation groups in the plane. In this case, two transformation groups are equivalent if they can be mapped to each other by a point transformation. Cases 1.1–1.11 list the transitive imprimitive groups; Cases 2.1–2.3 list the primitive transformation groups; and Cases 3.1–3.3 list the intransitive cases. As for contact transformation groups, there are three additional cases not equivalent to point transformation groups, given in Table II. Any other finite-dimensional contact transformation group is equivalent, now via a contact transformation, to one of these three or one of the previously listed point

TABLE II. Lie algebras of contact transformations in $\mathbb{C}^2$.

	Generators
4.1	$\partial_x, x\partial_x, \partial_u, x\partial_u, x^2\partial_u, 2u_x\partial_x + u_x^2\partial_u$
4.2	$\partial_x, x\partial_x, u\partial_u, \partial_u, x\partial_u, x^2\partial_u, 2u_x\partial_x + u_x^2\partial_u$
4.3	$\partial_x, x\partial_x, \partial_u, x\partial_u, x^2\partial_u, u\partial_u, (2-x)x\partial_x, 2u_x\partial_x + u_x^2\partial_u, xu_x^2\partial_u - 2(u-xu_x)\partial_x,$ $2x(2u-xu_x)\partial_x + (2u-xu_x)(2u+xu_x)\partial_u$

It is convenient to separate some special cases of the families of algebras given in Tables I and II. Thus 1.7a, 1.7b and 1.7c denote family 1.7 with $\alpha\neq k$, $\alpha=0$, and $\alpha=k$, respectively. Any starred designation 1.5$*$–1.11$*$ means the respective family of algebras with the parameter k set to 1. Analogously, 1.11$**$ is 1.11 with $k=2$.

In the following tables we give the fundamental differential invariants and invariant derivatives of the algebras of Tables I and II. First the action on the jet space of variables (x,u) is considered, denoted as ''2-D.'' The last two columns refer to the action on the jet space of (t,x,u). When no invariant derivative with a component in D_t is given in the third column, D_t is meant to be the second invariant derivative.

TABLE III. Differential invariants.

	2-D invariant derivative	2-D fundamental invariant(s)	Invariant derivatives	Fundamental invariants
1.1	$u^{-1}D_x$	$\frac{u_{xx}}{u^3}-\frac{3}{2}\frac{u_x^2}{u^4}$	$u^{-1}D_x$	$\frac{u_t}{u}, \frac{u_{xx}}{u^3}-\frac{3}{2}\frac{u_x^2}{u^4}$
1.2	$\frac{D_x}{\sqrt{u_x-u^2}}$	$\frac{u_{xx}-6uu_x+4u^3}{(u_x-u^2)^{3/2}}$	$u_t^{-1}D_x$	$\frac{u_t}{\sqrt{u_x-u^2}}$
1.3	$uQ_2^{-1/2}D_x$	$Q_2^{-3/2}S_3$	$u^{-1}u_tD_x$	$u^{-1}u_t, Q_2^{-3/2}S_3$
1.4	$\frac{u_xD_x}{\sqrt{Q_3}}$	$\frac{U_5}{Q_3^3}$	$\frac{u_t}{u_x}D_x$	$\frac{u_{tt}}{u_t}-\frac{u_{xt}}{u_x}, \frac{u_t^2Q_3}{u_x^4}$
1.5	D_x	$\mathscr{D}[u]$	D_x	$u_t, \mathscr{D}[u]$
1.6	D_x	$D_x\log(\mathscr{D}[u])$	D_x	$\frac{u_{xt}}{u_t}, \frac{u_{tt}}{u_t}, \frac{\mathscr{D}[u]}{u_t}$
1.7a	$u_k^{1/(\alpha-k)}D_x$	$u_k^{1/(\alpha-k)-1}u_{k+1}$	$u_t^{1/\alpha}D_x$	$\frac{u_{xt}}{u_t^{1-1/\alpha}}, \frac{u_{tt}}{u_t}, \frac{u_k}{u_t^{1-k/\alpha}}$
1.7b	$u_k^{-1/k}D_x$	$u_k^{-1/k-1}u_{k+1}$	$u_{xt}^{-1}D_x$	$u_t\frac{u_{xxt}}{u_{xt}^2}, \frac{u_k}{u_{xt}^k}$
1.7c	$\frac{D_x}{u_{k+1}}$	$u_k, \frac{u_{k+2}}{u_{k+1}^2}$	$u_t^{1/k}D_x$	$\frac{u_{xt}}{u_t^{1-1/k}}, \frac{u_{tt}}{u_t}, u_k$
1.8	$e^{u_k/k!}D_x$	$e^{u_k/k!}u_{k+1}$	$u_t^{1/k}D_x$	$\frac{u_{xt}}{u_t^{1-1/k}}, \frac{u_{tt}}{u_t}, \frac{u_t}{e^{u_k(k-1)!}}$
1.9	$\frac{u_kD_x}{u_{k+1}}$	$\frac{u_ku_{k+2}}{u_{k+1}^2}$	$\frac{u_t}{u_{xt}}D_x$	$\frac{u_{tt}}{u_t}, \frac{u_tu_{xxt}}{u_{xt}^2}, \frac{u_t^{k-1}u_k}{u_{xt}^k}$
1.10	$u_k^{-2/(k+1)}D_x$	$u_k^{-2-4/(k+1)}Q_{k+2}$	$u_t^{2/(k-1)}D_x$	$u_t^{-1}u_{tt}, u_t^{k+1}u_k^{k-1}$
1.10*	$u_x^{-1}D_x$	$u_x^{-4}Q_3$	$u_x^{-1}D_x$	$u_t, u_t^{-1}u_{tt}, u_x^{-4}Q_3$
1.11	$\frac{u_k}{\sqrt{Q_{k+2}}}D_x$	$Q_{k+2}^{-3/2}S_{k+3}$	$\frac{u_t^2}{Y_3}D_x$	$\frac{u_{tt}}{u_t}, \frac{\tilde{Z}_{k3}}{Y_3^2}, \frac{u_t^{2k-1}u_k}{Y_3^k}$
1.11*	$\frac{u_x}{\sqrt{Q_3}}D_x$	$Q_3^{-3/2}S_4$	$\frac{u_t}{u_x}D_x$	$\frac{u_{xt}}{u_t}, \frac{u_{tt}}{u_t}, \frac{u_t^2Q_3}{u_x^4}$
1.11**	$\frac{u_{xx}}{\sqrt{Q_4}}D_x$	$Q_4^{-3/2}S_5$	$\sqrt{\frac{u_t}{u_{xx}}}D_x$	$\frac{u_{tt}}{u_t}, \frac{W_3}{\sqrt{u_tu_{xx}^3}}, \frac{u_{xxt}}{u_{xx}}$

transformation groups. [Some of the point transformation canonical forms are equivalent under a contact transformation—one example is the two transitive actions of SL(2) given in 1.1 and 1.2.]

We proceed to classify the possible evolutionary-type equations that admit a finite-dimensional symmetry groups. We leave aside evolution equations, since any transformation group admits an invariant evolution equation. Thus, according to Proposition 4.12 we can immediately restrict our attention to the imprimitive groups. The first step of the classification is to check if the representative Lie algebra of a class fulfills the invariance conditions. If this is so, then, according to Theorem 5.2, knowledge of the fundamental absolute invariants, a relative invariant $R=L/E(L)$, and a nontrivial Lagrangian L of the group allows us to generate all invariant equations (5.1). In Tables III and IV we give all the fundamental absolute invariants and invariant derivatives of the algebras acting over E (two-dimensional action) and $\hat{E}$. The Lagrangian L is the reciprocal of the coefficient of D_x in the invariant two-dimensional derivative. In Table V we give the simplest invariant evolution equations, its right-hand side serving as the needed relative invariant R [not necessarily equal to $L/E(L)$], together with the corresponding invariant wave and potential evolution equations.

TABLE IV. Differential invariants.

	2-D invariant derivative	2-D fundamental invariants	Invariant derivatives	Fundamental invariants
2.1	$u_{xx}^{-1/3} D_x$	$\frac{R_4}{u_{xx}^{8/3}}$	$\left\{ \frac{D_x}{u_{xx}^{1/3}}, \ \frac{u_{xt}}{u_{tt}} D_x - D_t \right.$	$\frac{u_{xx}}{u_t^3}, \ \frac{U_2}{u_t^4}, \ \frac{V_3}{u_x^5}$
2.2	$\frac{u_{xx}}{\sqrt{R_4}} D_x$	$\frac{S_5}{R_4^{3/2}}$	$\left\{ \frac{\sqrt{U_2} D_x}{u_{xx}}, \right.$ $\left. \frac{u_{xt}}{u_{tt}} D_x - D_t \right.$	$\frac{U_2}{u_t u_{xx}}, \ \frac{V_3}{u_t^{1/2} u_{xx}^{3/2}}, \ \frac{X_3}{u_{xx}^2}$
2.3	$\frac{u_{xx}}{S_5^{1/3}} D_x$	$\frac{V_7}{S_5^{8/3}}$	$\left\{ \sqrt{\frac{u_t}{u_x}} D_x, \right.$ $\left. \left(\frac{u_{xt}}{2u_{xx}} + \frac{u_t u_{xxx}}{6u_{xx}^2} \right) D_x - D_t \right.$	$\frac{L_3}{u_t u_{xx}^3}, \ \frac{M_3}{u_t^{3/2} u_{xx}^{9/2}}, \ \frac{N_3}{u_t^2 u_{xx}^6}$
3.1	D_x	$x, \mathscr{D}[u]$	D_x	$x, u_t, \mathscr{D}[u]$
3.2a	D_x	$x, D_x \log(\mathscr{D}[u])$	D_x	$x, \frac{\mathscr{D}[u]}{u_t}$
3.2b	D_x	$x, D_x \log(\mathscr{D}[u])$	D_x	$x, \frac{u_{xt}}{u_t}, \frac{u_{tt}}{u_t}, \frac{\mathscr{D}[u]}{u_t}$
3.3	D_x	$x, \frac{Q_3}{u_x^2}$	D_x	$x, \frac{u_t}{u_x}, \frac{Q_3}{u_x^2}$
4.1	$\frac{D_x}{u_{xxx}^{1/3}}$	$\frac{\widetilde{R}_5}{u_{xxx}^{8/3}}$	$\left\{ \frac{D_x}{u_{xt}}, \right.$ $\left. \frac{u_{tt}}{u_{xt}} D_x - D_t \right.$	$u_t, \ \frac{u_{xxx}}{u_{xt}^3}, \ \frac{A_3}{u_{xt}^3}, \ \frac{B_3}{u_{xt}^3}, \ \frac{C_3}{u_{xt}^3}$
4.2	$\frac{u_{xxx}}{\sqrt{\widetilde{R}_5}} D_x$	$\widetilde{R}_5^{-3/2} \widetilde{S}_6$	$\left\{ \frac{u_t}{u_{xt}} D_x, \right.$ $\left. \frac{u_{tt}}{u_{xt}} D_x - D_t \right.$	$\frac{u_t^2 u_{xxx}}{u_{xt}^3}, \ \frac{u_t A_3}{u_{xt}^3}, \ \frac{B_3}{u_{xt}^3}, \ \frac{C_3}{u_t u_{xt}^3}$
4.3	$\frac{u_{xxx}}{T_7^{-5.2}} Z_9 \mathscr{D}_x$	$T_7^{-5/2} Z_9$	$\left\{ \left(\frac{u_t}{u_{xxx}} \right)^{-1/3} D_x, \right.$ $\left. \frac{\widetilde{Z}_{33} D_x}{2u_t^3 u_{xxx}} - D_t \right.$	$\frac{D_3}{u_t^{8/3} u_{xxx}^{4/3}}, \ \frac{E_3}{u_t^4 u_{xxx}^2}, \ \frac{F_4}{u_t^2 u_{xxx}^2}$

Regardless of the existence of invariant equations for the representative algebra, the possibility remains that a change of variables could yield a point or contact-equivalent algebra satisfying the invariance conditions, and hence admitting invariant equations in the new coordinates. Alternatively, we can think that the representative algebra admits an invariant equation which is not of the prescribed form (4.2), but that can be converted into one by an appropriate equivalence transformation, which leaves its invariance untouched.

The second step is to find the required changes of variables, and the corresponding additional invariant equations. We begin with the case of point transformations, which, by Theorem 5.1, covers all but the potential evolution equations. Consider a change of variables

$$\overline{x} = \chi(x,u), \quad \overline{u} = \psi(x,u). \tag{5.9}$$

TABLE IV. (*Continued.*)

In the previous tables, given functions $\eta_1(x),\dots,\eta_k(x)$, we let $\mathscr{D}$ be a kth-order linear ordinary differential operator whose kernel is spanned by $\eta_1(x),\dots,\eta_k(x)$, and let $W(x)$ denote their Wronskian determinant. Furthermore,

$Q_{k+2}=(k+1)u_k u_{k+2}-(k+2)u_{k+1}^2$,
$R_4=3u_2u_4-5u_3^2$,
$\widetilde{R}_5=3u_3u_5-5u_4^2$,
$S_{k+3}=(k+1)^2u_k^2u_{k+3}-3(k+1)(k+3)u_k u_{k+1}u_{k+2}+2(k+2)(k+3)u_{k+1}^3$,
$\widetilde{S}_6=9u_3^2u_6-45u_3u_4u_5+40u_4^3$,
$U_5=u_1^2[Q_3D_x^2Q_3-\frac{5}{4}(D_xQ_3)^2]+u_1u_2Q_3D_xQ_3-(2u_1u_3-u_2^2)Q_3^2$,
$V_7=u_2^2[S_5D_x^2S_5-\frac{7}{6}(D_xS_5)^2]+u_2u_3S_5D_xS_5-\frac{1}{2}(9u_2u_4-7u_3^2)S_5^2$,
$Z_9=u_3^2[T_7D_x^2T_7-\frac{9}{8}(D_xT_7)^2]+u_3u_4T_7D_xT_7-\frac{4}{5}(7u_3u_5-5u_4^2)T_7^2$,
$T_7=10u_3^3u_7-70u_3^2u_4u_6-49u_3^2u_5^2+280u_3u_4^2u_5-175u_4^4$,
$U_2=u_{xx}u_{tt}-u_{xt}^2$,
$V_3=u_tu_{xxx}-3u_{xt}u_{xx}$,
$W_3=u_tu_{xxx}+3u_{xt}u_{xx}$,
$X_3=u_{xx}u_{xxt}-u_{xt}u_{xxx}$,
$Y_3=u_tu_{xtt}-u_{xt}u_{tt}$,
$\widetilde{Z}_{k3}=(k-1)u_t^3u_{xxt}-(k-2)u_t^2u_{xt}^2$,
$L_3=12u_tu_{xx}^2u_{xxt}-9u_{xx}^2u_{xt}^2-6u_tu_{xx}u_{xt}u_{xxx}-u_t^2u_{xxx}^2$,
$M_3=54u_tu_{xx}^4u_{xtt}-18u_t^2u_{xx}^2u_{xxx}u_{xxt}-54u_tu_{xx}^3u_{xt}u_{xxt}+27u_{xx}^3u_{xt}^3-54u_{xx}^4u_{xt}u_{tt}+27u_tu_{xx}^2u_{xt}^2u_{xxx}+9u_t^2u_{xx}u_{xt}u_{xxx}^2+u_t^3u_{xxx}^3$,
$N_3=288u_tu_{xx}^6u_{ttt}-144u_t^2u_{xx}^4u_{xxx}u_{xtt}-432u_tu_{xx}^5u_{xt}u_{xtt}+24u_t^3u_{xx}^2u_{xxx}^2u_{xxt}+144u_t^2u_{xx}^3u_{xt}u_{xxx}u_{xxt}+216u_tu_{xx}^4u_{xt}^2u_{xxt}$
$-81u_{xx}^4u_{xt}^4+432u_{xx}^5u_{xt}^2u_{tt}-432u_{xx}^6u_{tt}^2-108u_tu_{xx}^3u_{xt}^3u_{xxx}+144u_tu_{xx}^4u_{xt}u_{tt}u_{xxx}-54u_t^2u_{xx}^2u_{xt}^2u_{xxx}^2$
$-12u_t^3u_{xx}u_{xt}u_{xxx}^3-u_t^4u_{xxx}^4$,
$A_3=u_{xt}u_{xxt}-u_{tt}u_{xxx}$,
$B_3=u_{xt}^2u_{xtt}-2u_{xt}u_{tt}u_{xxt}+u_{tt}^2u_{xxx}$,
$C_3=u_{xt}^3u_{ttt}-3u_{xt}^2u_{tt}u_{xtt}+3u_{xt}u_{tt}^2u_{xxt}-u_{tt}^3u_{xxx}$,
$D_3=4u_t^2u_{xxx}u_{xtt}-4u_t^2u_{xxt}^2+4u_tu_{xt}^2u_{xxt}-4u_tu_{xt}u_{tt}u_{xxx}-u_{xt}^4$,
$E_3=4u_t^3u_{xxx}^2u_{ttt}-12u_t^3u_{xxx}u_{xxt}u_{xtt}+6u_t^2u_{xt}^2u_{xxx}u_{xtt}+8u_t^3u_{xxt}^3-12u_t^2u_{xt}^2u_{xxt}^2+12u_t^2u_{xt}u_{tt}u_{xxx}u_{xxt}+6u_tu_{xt}^4u_{xxt}$
$-6u_t^2u_{tt}^2u_{xxx}^2-6u_tu_{xt}^3u_{tt}u_{xxx}-u_{xt}^6$,
$F_4=2u_t^2u_{xxx}u_{xxxt}-2u_t^2u_{xxt}u_{xxxx}+u_tu_{xt}^2u_{xxxx}-4u_tu_{xt}u_{xxx}u_{xxt}+u_tu_{tt}u_{xxx}^2+2u_{xt}^3u_{xxx}$.

If the transformed group admits an invariant equation, it must be generated by vector fields of the form

$$\overline{\mathbf{v}}=\overline{\xi(x)}\partial_{\bar{x}}+[k(\overline{xu}+f(\overline{x})]\partial_{\bar{u}}=\overline{\xi(\chi)}\partial_{\bar{x}}+[k(\chi)\psi+f(\chi)]\partial_{\bar{u}},$$

with the appropriate form of k depending on the type of the invariant equation considered. This means that

$$\begin{aligned}\mathbf{v}(\chi)&=\overline{\xi(\chi)},\\ \mathbf{v}(\psi)&=\xi\psi_x+\varphi\psi_u=k(\chi)\psi+f(\chi),\end{aligned}\tag{5.10}$$

and thus the level sets of the function χ form an invariant foliation. In terms of the intermediate variables

$$(\widetilde{x},\widetilde{u})=\begin{cases}(\chi,u), & \text{if } \chi_x\neq 0,\\ (\chi,x), & \text{if } \chi_x=0,\end{cases}$$

TABLE V. Evolution, u_{xt} and u_{tt}-invariant equations

	$u_t=F$	$u_{tt}=F$	$u_{xt}=F$
1.1	u	u	$\cdots$
1.2	$\sqrt{u_x-u^2}$	$\sqrt{u_x-u^2}$	$\cdots$
1.3	u	u	$\cdots$
1.4	$\dfrac{u_x^2}{\sqrt{Q_3}}$	$\cdots$	$\cdots$
1.5	1	1	1
1.6	$\mathscr{D}[u]$	$\mathscr{D}[u]$	$\mathscr{D}[u]$
1.7ab	$u_k^{\alpha/(\alpha-k)}$	$u_k^{\alpha/(\alpha-k)}$	$u_k^{(\alpha-1)/(\alpha-k)}$
1.7c	u_{k+1}^{-k}	u_{k+1}^{-k}	u_{k+1}^{-k+1}
1.8	$e^{u_k/(k-1)!}$	$e^{u_k/(k-1)!}$	$e^{(k-1)u_k/k!}$
1.9	$\dfrac{u_k^{k+1}}{u_{k+1}^k}$	$\dfrac{u_k^{k+1}}{u_{k+1}^k}$	$\dfrac{u_k^k}{u_{k+1}^{k-1}}$
1.10	$u_k^{-(k-1)/(k+1)}$	$\cdots$	$\cdots$
1.10*	1	1	u_x
1.11	$\dfrac{u_k^{k+1}}{Q_{k+2}^{k/2}}$	$\cdots$	$\cdots$
1.11*	$\dfrac{u_x^2}{Q_3^{1/2}}$	$\dfrac{u_x^2}{Q_3^{1/2}}$	u_x
2.1	$u_{xx}^{1/3}$	$\cdots$	$\cdots$
2.2	$\dfrac{R_4}{u_{xx}^{7/3}}$	$\cdots$	$\cdots$
2.3	$\dfrac{u_{xx}^3}{S_5^{2/3}}$	$\cdots$	$\cdots$
3.1	1	1	1
3.2	$\mathscr{D}[u]$	$\mathscr{D}[u]$	$\mathscr{D}[u]$
3.3	u_x	u_x	u_x
4.1	1	1	$u_{xxx}^{-1/3}$
4.2	$\dfrac{u_{xxx}^4}{\widetilde{R}_5^{3/2}}$	$\dfrac{u_{xxx}^4}{\widetilde{R}_5^{3/2}}$	$\dfrac{u_{xxx}^3}{\widetilde{R}_5}$
4.3	$\dfrac{u_{xxx}^4}{T_7^{3/4}}$	$\cdots$	$\cdots$

we have

$$\widetilde{\mathbf{v}}=\widetilde{\xi}(\widetilde{x})\,\partial_{\widetilde{x}}+\widetilde{\varphi}(\widetilde{x},\overline{u})\,\partial_{\overline{u}}.$$

Differentiating (5.10) with respect to $\overline{u}$ we obtain

$$\widetilde{\xi}\psi_{\widetilde{x}\,\overline{u}}+\widetilde{\varphi}_{\overline{u}}\psi_{\widetilde{u}}+\widetilde{\varphi}\psi_{\widetilde{u}\,\overline{u}}=k\psi_{\overline{u}},$$

that is to say,

$$\widetilde{\mathbf{v}}(\psi_{\overline{u}})-(k-\widetilde{\varphi}_{\overline{u}})\psi_{\overline{u}}=0.$$

Therefore the function $\phi_{\overline{u}}$ *must be a relative invariant* of weight $k-\widetilde{\varphi}_{\overline{u}}$. Explicitly in the original variables we have

TABLE VI. Invariant foliations.

Algebra	Invariant foliation
1.1,1.2,1.3,1.5,1.6,1.7,1.8,1.9,1.10,1.11,3.1,3.2	$x=\lambda$
1.4,1.9*,1.10*,1.11*,3.2*,3.3	$x=\lambda,\ u=\mu$
1.5*,1.6*,1.7bc*	$ax+bu=\lambda$
3.1*	$u-f(x)=\lambda$
4.1,4.2	$x=\lambda,\ u_x=\mu$

$$(\widetilde{\varphi}_{\overline{u}},\psi_{\overline{u}})=\begin{cases}\left(\varphi_u-\dfrac{\chi_u}{\chi_x}\,\varphi_x,\psi_u-\dfrac{\chi_u}{\chi_x}\,\psi_x\right), & \text{if } \chi_x\neq 0,\\ (\varphi_x,\psi_x), & \text{if } \chi_x=0.\end{cases}$$

Contact transformations can be treated analogously. Consider a contact transformation

$$\overline{x}=\chi(x,u,u_x),\quad \overline{u}=\psi(x,u,u_x),\quad \chi D_x\psi=\psi D_x\chi.$$

The transformed group is now generated by vector fields of the form

$$\overline{\mathbf{v}}=\overline{\xi}(\overline{x},\overline{u_x})\partial_{\overline{x}}+[k(\overline{x},\overline{u_x})\overline{u}+f(\overline{x},\overline{u_x})]\partial_{\overline{u_x}}=\overline{\xi}(\chi,\overline{u_x})\partial_{\overline{x}}+\left[k\left(\chi,\frac{D_x\psi}{D_x\chi}\right)\psi+f\left(\chi,\frac{D_x\psi}{D_x\chi}\right)\right]\partial_{\overline{u}}.$$

Beginning with an invariant foliation by lines $\chi(x,u,u_x)=\lambda$, and $\eta(x,u,u_x)=\mu$ of the space J^1E, we conclude that the function

$$\Psi=\Psi(x,u,u_x)=-\frac{(\chi_u\eta_{u_x}-\chi_{u_x}\eta_u)\psi_x-(\chi_u\eta_x-\chi_x\eta_u)\psi_{u_x}}{\chi_x\eta_{u_x}-\chi_{u_x}\eta_x}+\psi_u$$

must be a relative invariant:

$$\mathbf{v}(\Psi)-\left(k+\frac{(\chi_u\eta_{u_x}-\chi_{u_x}\eta_u)\varphi_x-(\chi_u\eta_x-\chi_x\eta_u)\varphi_{u_x}}{\chi_x\eta_{u_x}-\chi_{u_x}\eta_x}-\varphi_u\right)\Psi=0.$$

In Table VI we give the invariant foliations of the actions of the considered groups, needed for determining changes of variables discussed above. Given an invariant foliation $\chi(x,u)$ there exists always a class of ''affine transformations''

$$\overline{x}=\chi,\quad \overline{u}=c(\chi)u+d(\chi)$$

that respects the form and symmetries of a family of invariant equations. We have found that there exists only one class of algebras having two inequivalent representatives with invariant equations, related by a *non*-affine transformation. It is class 1.1, and the additional representative is studied in Table VII.

TABLE VII. Additional algebra with invariant equations.

	Change	Algebra	Invariant derivative	2-D fundamental invariant	Fundamental invariants	$u_t=F$	$u_{xt}=F$
1.1	$\psi=u^{-1}$	$\partial_x, x\partial_x-\partial_u,$ $x^2\partial_x-2x\partial_u$	$\dfrac{D_x}{e^u}$	$\dfrac{2u_{xx}-u_x^2}{e^{2u}}$	$u_t,\ \dfrac{2u_{xx}-u_x^2}{e^{2u}}$	$\dfrac{2u_{xx}-u_x^2}{e^{2u}}$	$\dfrac{2u_{xx}-u_x^2}{e^{u}}$

VI. GENERALIZATIONS

So far we have restricted our attention to evolutionary-type equations in which the right-hand side is purely a function of the spatial variables and spatial derivatives of the dependent variable. In this section, we relax this condition by permitting the right-hand side to also depend on time derivatives of u. Here the computations become more complicated because there is not an immediate separation in the infinitesimal symmetry criteria into purely spatial and temporal parts.

According to Theorem 3.4, a general scalar differential equation

$$R(x,u^{(n)})=0 \tag{6.1}$$

is invariant under a group of transformations if and only if R forms a relative differential invariant of the group, and so satisfies (3.3) for some differential multiplier $H_{\mathbf{v}}$. However, if we solve the differential equation (6.1) for one of the derivatives,

$$u_K=F[u], \quad F:\mathrm{J}^n\hat{E}\to\mathbb{R}, \tag{6.2}$$

then the two components u_K and F may or may not form individual relative differential invariants. (If they do, then Proposition 3.5 implies that they must have the same weight.) As we have seen, this splitting of the equation into relative invariants does occur if (6.2) is of evolutionary type, meaning that K has at least one time derivative, and F depends on purely spatial derivatives. However, in more general situations, F is an ''inhomogeneous relative differential invariant,'' and the existence is more problematic (cf. Ref. 14). This has an advantage and a disadvantage. The disadvantage of studying equations with an isolated variable is then the inhomogeneity of the associated relative invariant. The advantage is that the weights are precisely determined, allowing a more systematic approach. The following result, which is analogous to Theorem 4.3 for an evolutionary-type equation, characterizes the right-hand side of the general equation (6.2) as an inhomogeneous relative differential invariant.

Proposition 6.1: If the general equation $u_K=F[u]$ admits a spatial symmetry group G, then the right-hand side satisfies

$$\mathbf{v}^{[n]}(F)=\left(Q_u-\sum_{i=1}^{p}k_iD_i\xi^i\right)F+\left[D_KQ-\left(Q_u-\sum_{i=1}^{p}k_iD_i\xi^i\right)u_K\right], \tag{6.3}$$

for all infinitesimal generators $\mathbf{v}\in\mathfrak{g}$.

Our first result characterizes those equations that impose an affine symmetry condition on its symmetry group.

Proposition 6.2: Consider a differential equation

$$u_K=F(t,x,u,u_t,u_1,\ldots,u_p,\ldots,u_L,\ldots), \tag{6.4}$$

with the right-hand side depending on variables u_L with temporal derivatives of lower order than the one on the left-hand side. That is to say, if $K=(k_0,k_1,\ldots,k_p)$ and $L=(l_0,l_1,\ldots,l_p)$, then $l_0<k_0$ for all variables u_L in F. If K is not a purely temporal multi-index, $K\neq k_0e_0$, then any connected spatial symmetry group of equation (6.4) is composed of affine bundle maps.

Proof: Apply Theorem 4.2, and expand the infinitesimal symmetry condition (4.8) to obtain

$$D_KQ+\sum_{i=1}^{p}\xi^iu_{Ki}=\mathbf{v}^{[n]}(F), \tag{6.5}$$

in analogy to (4.9). Consider terms on the left-hand side of maximal and submaximal orders k and $k-1$, but with maximal temporal order k_0. The right-hand side of (6.5) does not contain temporal

derivatives of order k_0, and then equating to zero the corresponding coefficients we obtain conditions (4.14) and $D_j Q_u = 0$, where j runs over principal spatial variables. Q.E.D.

In the case of an equation (6.4), the right-hand side of (6.5) contains terms depending on temporal derivatives [compare with (4.9)]. This means that now the expression on the left can contain them also, and that the term on u_K will not be the only one different from zero, i.e., $G \neq 0$ and instead of Theorem 4.3, Proposition 6.1 must be used.

Theorem 6.3: *Let G be a connected spatial symmetry group of an equation of type*

$$\frac{\partial^{m+n} u}{\partial x^m \partial t^n} = F(x, u^{(N)}, u_t) = F(x, u, u_x, u_t, u_{xx}, u_{xt}, \ldots, u_{kl}, \ldots), \quad l < n. \tag{6.6}$$

i.e., with right-hand sides that can depend on temporal derivatives of order $l < n$.

(i) *If the equation is purely evolutionary, i.e., of the form $\partial^n u / \partial t^n = F$, then there are no restrictions on G.*

(ii) *If the equation is the potential form $\partial^{n+1} u / \partial x \partial t^n$ of a purely evolutionary equation, then G can be a contact transformation group whose infinitesimal generators have the form*

$$\mathbf{v}^{(0)} = \xi(x, u_x)\partial_x + (ku + f(x, u_x))\partial_u, \tag{6.7}$$

where k is a constant.

(iii) *All the remaining equations, with $m \geqslant 2$, have the same type of symmetry groups as the corresponding evolutionary-type equations (5.1).*

We can also generalize Theorem 4.9 and Theorem 5.2 to this case. (The existence of suitable inhomogeneous relative invariants is, however, not immediate.)

Theorem 6.4: *In one spatial variable, if an equation (6.4) admits a spatial transformation group G, then its right-hand side satisfies*

$$\mathbf{v}^{(N)}(F) - (Q_u - m D_x \xi) F = H, \tag{6.8}$$

where the form of H follows from (6.3). Thus F is an inhomogeneous relative differential invariant of the form

$$F = \frac{L^{m+1}}{\mathrm{E}(L)} I + F_0, \tag{6.9}$$

where I is an absolute differential invariant of G depending on temporal derivatives of u of order less than n, $\omega = L(x, u^{(n)})dx$ is a G-invariant one-form having nontrivial Euler–Lagrange expression $\mathrm{E}(L) \not\equiv 0$, and F_0 is a particular inhomogeneous differential invariant of the same weight as F.

As our final examples, let us apply the previous ideas to general wave equations of type (6.4) and to potential evolution equations with an additional dependence on u_t on the right-hand side.

Example 6.5: In this example we discuss invariant wave equations of type (6.4):

$$u_{tt} = F(x, u, u_t, u_x, u_{xt}, \ldots, u_{m-1}, u_{m-1,t}), \tag{6.10}$$

i.e., those whose right-hand sides are allowed to depend on spatial derivatives of u and on first-order time derivatives. According to Theorem 6.3, the symmetry group G can be any group of transformations—imprimitive, primitive, and contact. Moreover F must be an inhomogeneous relative invariant (6.9) satisfying

$$\mathbf{v}^{(N)}(F) - Q_u F = u_t D_t Q_u - u_{xt} D_t \xi. \tag{6.11}$$

TABLE VIII. Invariant equations of the form $u_{xt}=F[x,u_t]$.

	R	F_0
1.1	u^2	$\frac{u_x u_t}{u}$
1.2	u^2-u_x	$2uu_t$
1.3	$\sqrt{\frac{u_t}{u}Q_2}$	$\frac{u_x u_t}{u}$
1.4	u_x	$\frac{u_t U_4}{u_x Q_3}$
1.5	1	0
1.6	u_t	0
1.7	$u_t^{(\alpha-1)/\alpha}$	0
1.7b	$u_k^{1/k}$	0
1.8	$u_t^{(k-1)/k}$	0
1.9	$(u_t^{k-1}u_k)^{1/k}$	0
1.10	$u_t^{(k-3)/(k-1)}$	$-\frac{k-1}{k+1}\frac{u_{k+1}u_t}{u_k}$
1.10*	u_x	0
1.11	$u_t^{(k-1)/k}u_k^{1/k}$	$-\frac{k-1}{k+1}\frac{u_{k+1}u_t}{u_k}$
2.1	$u_{xx}^{2/3}$	0
2.2	$\sqrt{u_t u_{xx}}$	0
2.3	$\sqrt{u_t u_{xx}}$	$\frac{u_x S_5^{1/3}}{3^{2/3}u_{xx}}+\frac{u_x V_6}{u_{xx}S_5}$
3.1	u_t	0
3.2	u_t	0
3.3	u_t	$\frac{u_t u_{xx}}{u_x}$
4.1	$u_{xxx}^{1/3}$	0
4.2	$(u_t^2 u_{xxx})^{1/3}$	0
4.3	$(u_t^2 u_{xxx})^{1/3}$	$\frac{u_x T_7^{1/4}}{u_{xxx}}+\frac{u_x Z_8}{2u_{xxx}T_7}$

In Table VIII we give the simplest homogeneous part of F, corresponding to some relative invariant $R=L^2I/\mathrm{E}(L)$, and the simplest inhomogeneous part F_0.

Example 6.6: In this example we discuss invariant potential evolution equations

$$u_{xt}=F(x,u,u_t,u_x,u_{xx},\ldots,u_m) \tag{6.12}$$

whose right-hand sides are allowed to depend on spatial derivatives of u and the time derivative u_t. Note that potential evolution equations do not belong to the class (6.4), and can be invariant, in principle, under any kind of transformation group. We find that the right-hand side F must be an inhomogeneous relative invariant (6.9) satisfying

$$\mathbf{v}^{(N)}(F)-(Q_u-D_x\xi)F=u_t D_x Q_u\,. \tag{6.13}$$

TABLE IX. Invariant equations of the form $u_{tt}=F[x,u_t,u_{xt},\ldots]$.

	R	F_0
1.1	u	0
1.2	u_t	0
1.3	u	0
1.4	u_t	$\dfrac{u_t u_{xt}}{u_x}$
1.5	1	0
1.6	u_t	0
1.7	u_t	0
1.8	u_t	0
1.9	u_t	0
1.10	u_t	0
1.10*	1	0
1.11	u_t	0
2.1	u_t	$\dfrac{u_{xt}^2}{u_{xx}}$
2.2	u_t	$\dfrac{u_{xt}^2}{u_{xx}}$
2.3	u_t	$\dfrac{G_4}{3u_{xx}^2}$
3.1	1	0
3.2	u_t	0
3.2	1	0
4.1	1	$\dfrac{u_{xt}u_{xxt}}{u_{xxx}}$
4.2	u_t	$\dfrac{u_{xt}u_{xxt}}{u_{xxx}}$
4.3	u_t	$\dfrac{-F_4}{u_t u_{xxx}^2}$

We have used the notations

$$U_4=-6u_2^3+6u_1u_2u_3-u_1^2u_4,$$
$$G_4=3u_tu_{xx}^2-12u_{xx}u_{xt}^2-8u_tu_{xt}u_{xxx}+18u_tu_{xx}u_{xxt}-u_t^2u_{xxxx},$$
$$V_6=120u_3^4-185u_2u_3^2u_4+30u_2^2u_4^2+45u_2^2u_3u_5-6u_2^3u_6,$$
$$Z_8=-1400u_4^5+2870u_3u_4^3u_5-1085u_3^2u_4u_5^2-770u_3^2u_4^2u_6+252u_3^3u_5u_6+140u_3^3u_4u_7-15u_3^4u_8.$$

In Table IX we give the simplest homogeneous part R and the simplest inhomogeneous part F_0 of the right-hand side F.

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Superintegrability and associated polynomial solutions: Euclidean space and the sphere in two dimensions

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In this work we examine the basis functions for those classical and quantum mechanical systems in two dimensions which admit separation of variables in at least two coordinate systems. We do this for the corresponding systems defined in Euclidean space and on the two-dimensional sphere. We present all of these cases from a unified point of view. In particular, all of the special functions that arise via variable separation have their essential features expressed in terms of their zeros. The principal new results are the details of the polynomial bases for each of the nonsubgroup bases, not just the subgroup Cartesian and polar coordinate cases, and the details of the structure of the quadratic algebras. We also study the polynomial eigenfunctions in elliptic coordinates of the n-dimensional isotropic quantum oscillator. © *1996 American Institute of Physics.* [S0022-2488(96)03212-4]

I. INTRODUCTION

It has long been known that there are potentials for which a given Hamiltonian system in classical mechanics admits a solution via separation of variables in more than one coordinate system.[1] The methodical search for such potentials was initiated by Smorodinsky and Winternitz *et al.* in two and three dimensions,[2–4] and there has been a considerable amount of work for various examples.[5–9] A subset of such systems is called *maximal* in dimension N if there exist $2N-1$ functionally independent integrals of motion. In some papers, such systems are called *superintegrable*.[10,11] In this work we examine the basis functions for those classical and quantum mechanical systems in two dimensions which admit separation of variables in at least two coordinate systems. We do this for the corresponding systems defined in Euclidean space and on the two-dimensional sphere. In a subsequent work we shall study systems defined in two-dimensional hyperbolic spaces and in complex two-dimensional spaces.

For each of the superintegrable systems we observe that, for the discrete spectrum of the quantum mechanical Hamiltonian, one can consider this operator as acting on a space of polynomials.[12] Each eigenvalue is multiply degenerate. However, each separable coordinate system gives rise to an orthonormal basis of polynomial eigenfunctions in this space and breaks the degeneracy. These bases are characterized as simultaneous eigenfunctions of second-order symmetry operators for the Hamiltonian.[13] We show that under commutation these symmetry operators close to form a quadratic algebra.[14] The superintegral systems are of two types: the ''normal type'' in which the original Hamiltonian is diagonalized, and the ''conformal type'' in which the Hamiltonian is modified by multiplying the eigenvalue equation by a function and considering the energy as fixed. The modified equation is then interpreted as the eigenvalue equation for a Hamiltonian on a conformal Euclidean space with a ''charge'' as the eigenvalue. We present all of these cases from a unified point of view. In particular, all of the special functions that arise via variable separation have their essential features expressed in terms of their zeros. The principal new results

are the details of the polynomial bases for each of the nonsubgroup bases, not just the subgroup Cartesian and polar coordinate cases, and the details of the structure of the quadratic algebras. (For those coordinate systems which correspond to subgroup type coordinates, the finite solutions have already been found. The contribution of this article is to indicate how the remaining finite solutions can be obtained. This invariably involves the use of a Niven-type ansatz for the finite solutions; every quantity of interest can be computed in terms of the zeros of the corresponding polynomial solutions.) For the sake of completeness we list all the finite solutions that are possible. We analyze each of the potentials systematically.

In Secs. II and III we consider the superintegrable systems in Euclidean two-space and on the two-dimensional sphere, respectively. In Sec. IV we examine the polynomial eigenfunctions in elliptic coordinates of the n-dimensional isotropic quantum oscillator.

II. TWO-DIMENSIONAL EUCLIDEAN SPACE

As is well known[1,13] there are exactly four coordinate systems on the Euclidean plane in which the free particle Schrödinger equation separates: Cartesian, polar, parabolic, and elliptic. We describe these coordinate systems. Let x and y be the **Cartesian coordinates. Polar coordinates** are defined by

$$\begin{aligned} x&=r\ \cos\ \theta, \quad r>0,\\ y&=r\ \sin\ \theta, \quad 0\leqslant\theta<2\pi. \end{aligned} \tag{1}$$

Parabolic coordinates. We can define two mutually perpendicular parabolic systems:

$$x=\tfrac{1}{2}(\xi^2-\eta^2), \quad y=\xi\eta, \quad \xi\in\mathbf{R}, \eta>0, \tag{2}$$

and

$$x=\overline{\xi}\,\overline{\eta}, \quad y=\tfrac{1}{2}(\overline{\xi^2}-\overline{\eta^2}), \quad \overline{\xi}\in\mathbf{R}, \overline{\eta}>0. \tag{3}$$

The connection $(\xi,\eta)\mapsto(\overline{\xi},\overline{\eta})$ is a rotation of angle $\pi/4$ in the (ξ,η) space. The transformation $(x,y)\mapsto(\xi,\eta)$ actually is the two-dimensional realization of the Levi-Civita transformation[15] which has the form

$$x=\xi^2-\eta^2, \quad y=2\xi\eta, \quad \xi\in\mathbf{R}, \eta>0. \tag{4}$$

Elliptic coordinates in algebraic form are defined by $(e_1<u_1<e_2<u_2)$

$$x^2=\frac{(u_1-e_1)(u_2-e_1)}{e_2-e_1}, \quad y^2=\frac{(u_1-e_2)(u_2-e_2)}{e_1-e_2}. \tag{5}$$

Replacing $x\mapsto x+\sqrt{e_2-e_1}$ yields a coordinate system which is called *elliptic II coordinates*:[16]

$$x=\sqrt{\frac{(u_1-e_1)(u_2-e_1)}{e_2-e_1}}+\sqrt{e_2-e_1}, \quad y=\sqrt{\frac{(u_1-e_2)(u_2-e_2)}{e_1-e_2}}. \tag{6}$$

It is interesting that the two elliptic coordinates are connected by the Levi-Civita transformation. Indeed, if we use parabolic coordinates (ξ,η) in Eq. (4) as Cartesian coordinates in Eq. (5), we have

$$x=\sqrt{\frac{(\overline{u_1}-\overline{e_1})(\overline{u_2}-\overline{e_1})}{\overline{e_2}-\overline{e_1}}}+\sqrt{\overline{e_2}-\overline{e_1}}, \quad y=\sqrt{\frac{(\overline{u_1}-\overline{e_2})(\overline{u_2}-\overline{e_2})}{\overline{e_1}-\overline{e_2}}}, \tag{7}$$

TABLE I. The two-dimensional superintegrable potentials.

Potential $V(x,y)$	Coordinate system
$V_1=\frac{1}{2}\omega^2(x^2+y^2)+\frac{1}{2}\left(\frac{k_1^2-\frac{1}{4}}{x^2}+\frac{k_2^2-\frac{1}{4}}{y^2}\right)$	Cartesian polar elliptic
$V_2=\frac{1}{2}\omega^2(4x^2+y^2)+k_1x+\frac{1}{2}\frac{k_2^2-\frac{1}{4}}{y^2}$	Cartesian parabolic
$V_3=-\frac{\alpha}{\sqrt{x^2+y^2}}+\frac{1}{4}\frac{1}{\sqrt{x^2+y^2}}$ $\times\left(\frac{k_1^2-\frac{1}{4}}{\sqrt{x^2+y^2}+x}+\frac{k_2^2-\frac{1}{4}}{\sqrt{x^2+y^2}-x}\right)$	Polar elliptic II parabolic
$V_4=-\frac{\alpha}{\sqrt{x^2+y^2}}+\frac{1}{4}\frac{1}{\sqrt{x^2+y^2}}$ $\times(\beta_1\sqrt{\sqrt{x^2+y^2}+x}+\beta_2\sqrt{\sqrt{x^2+y^2}-x})$	Mutually parabolic

where

$$\overline{u_i}=u_i^2-u_1(e_1+e_2),\quad \overline{e_1}=-\tfrac{1}{4}(e_1+e_2)^2,\quad \overline{e_2}=-e_1e_2. \tag{8}$$

As shown in Refs. 2–4 there are four classes of potentials for which multiple separation occurs in Euclidean space (see Table I).

We treat the cases in order. In each case the Schrödinger equation is ($\hbar=m=1$)

$$-\tfrac{1}{2}\Delta\Psi+V_i(x,y)\Psi=E\Psi,\quad i=1,\ldots,4. \tag{9}$$

(i) The potential in the first case is

$$V_1(x,y)=\frac{1}{2}\,\omega^2(x^2+y^2)+\frac{1}{2}\left(\frac{k_1^2-\frac{1}{4}}{x^2}+\frac{k_2^2-\frac{1}{4}}{y^2}\right). \tag{10}$$

The corresponding Schrödinger equation is ($k_1,k_2>0$)

$$\left[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right]\Psi+\left[2E-\omega^2(x^2+y^2)-\frac{k_1^2-\frac{1}{4}}{x^2}-\frac{k_2^2-\frac{1}{4}}{y^2}\right]\Psi=0.$$

See Refs. 2, 3, and 16–18 for an earlier treatment. This equation separates in three different separable coordinate systems: Cartesian, polar, and elliptical coordinates.

If we rewrite the Schrödinger equation by putting

$$\Psi=e^{-\omega(x^2+y^2)/2}x^{1/2\pm k_1}y^{1/2\pm k_2}\Phi(x,y), \tag{11}$$

then the equation for $\Phi(x,y)$ is $Q\Phi=-2E\Phi$ or

$$\left[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\left(\frac{1\pm 2k_1}{x}-2\omega x\right)\frac{\partial}{\partial x}+\left(\frac{1\pm 2k_2}{y^2}-2\omega y\right)\frac{\partial}{\partial y}-2\omega(2\pm k_1\pm k_2)\right]\Phi=-2E\Phi. \tag{12}$$

Clearly the operator Q maps polynomials (in x^2,y^2) into polynomials, without increasing the order. Since the original Hamiltonian is self-adjoint with respect to the measure $dx\ dy$ in the plane, the operator Q acting on polynomials in x^2 and y^2 is self-adjoint with respect to the measure

$$d\rho(x,y)=e^{-\omega(x^2+y^2)}x^{1\pm 2k_1}y^{1\pm 2k_2}\ dx\ dy$$

in the quadrant $x>0$, $y>0$. We assume that the positive sign at the k_i has to be taken if $k_i>\frac{1}{2}$ and both the positive and the negative sign must be taken if $0<k_i<\frac{1}{2}$, so that the polynomials have finite norm.[16]

To find the eigenfunctions in the case of Cartesian coordinates we look for separable solutions $\Phi(x,y)=X(x)Y(y)$. Then the separation equation in x becomes

$$\left[\frac{\partial^2}{\partial x^2}+\left(-2\omega+\frac{1\pm 2k_1}{x^2}\right)x\frac{\partial}{\partial x}-(1\pm 2k_1)\omega\right]X=2\lambda_1 X. \tag{13}$$

If we look for solutions of the form

$$X(x)=\prod_{m=1}^{q}(x^2-\theta_m),$$

the θ_m must satisfy

$$\omega\theta_\ell=1\pm k_1+2\sum_{j\neq\ell}\frac{\theta_\ell}{\theta_\ell-\theta_j}$$

and

$$\lambda_1=-\omega(2q\pm k_1+\tfrac{1}{2}),$$

where q is a non-negative integer. The solutions are $X(x)=L_q^{k_1}(\omega x^2)$ where $L_n^{\alpha}(z)$ is a Laguerre polynomial.

Thus the corresponding set of orthonormal eigenfunctions which are normalized in quadrant $x>0$, $y>0$ by

$$\int_0^\infty dx\int_0^\infty dy\,\Psi^*_{n_1'n_2'}(x,y)\Psi_{n_1n_2}(x,y)=\frac{1}{4}\,\delta_{n_1'n_1}\delta_{n_2'n_2} \tag{14}$$

is

$$\Psi(x,y)\equiv\Psi^{(k_1,k_2)}_{n_1,n_2}(x,y)=\sqrt{\frac{\omega n_1!n_2!}{\Gamma(n_1\pm k_1+1)\Gamma(n_2\pm k_2+1)}}\,(\sqrt{\omega}x)^{1/2\pm k_1}(\sqrt{\omega}y)^{1/2\pm k_2}$$
$$\times e^{-(\omega/2)(x^2+y^2)}L_{n_1}^{\pm k_1}(\omega x^2)L_{n_2}^{\pm k_2}(\omega y^2), \tag{15}$$

where $E_n=\omega(2n\pm k_1\pm k_2+2)$ and $n=n_1+n_2$ is the principal quantum number.

The corresponding classical operator is

$$L_1 = p_x^2 - \left(\omega^2 x^2 + \frac{k_1^2 - \frac{1}{4}}{x^2} \right).$$

These eigenfunctions satisfy

$$\hat{L}_1 \Psi = \left(\frac{\partial^2}{\partial x^2} - \omega^2 x^2 - \frac{k_1^2 - \frac{1}{4}}{x^2} \right) \Psi = 2\lambda_1 \Psi. \tag{16}$$

In polar coordinates the Schrödinger equation is

$$\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2} \right) \Psi + \left[2E - \omega^2 r^2 \Psi - \frac{1}{r^2} \left(\frac{k_1^2 - \frac{1}{4}}{\cos^2 \theta} + \frac{k_2^2 - \frac{1}{4}}{\sin^2 \theta} \right) \right] \Psi = 0.$$

If we write $\Psi = R(r)T(\theta)$, then the separation equation for $T(\theta)$ is

$$\frac{d^2}{d\theta^2} T(\theta) - \left(\frac{k_1^2 - \frac{1}{4}}{\cos^2 \theta} + \frac{k_2^2 - \frac{1}{4}}{\sin^2 \theta} \right) T(\theta) = \lambda T(\theta).$$

If we now put

$$T(\theta) = (\cos \theta)^{1/2 \pm k_1} (\sin \theta)^{1/2 \pm k_2} P(z),$$

where $z = \cos 2\theta$, this separation equation becomes

$$\left\{ (1 - z^2) \frac{\partial^2}{\partial z^2} - [(2 \pm k_1 \pm k_2)z + (\pm k_1 \mp k_2)] \frac{\partial}{\partial z} - \frac{1}{4} [\lambda + (1 \pm k_1 \pm k_2)^2] \right\} P(z) = 0.$$

If we try solutions of the form $P(z) = \Pi_{m=1}^{q} (z - \theta_m)$, we find that the zeros of the polynomial $P(z)$ satisfy

$$2 \sum_{m \neq l} \frac{1}{\theta_l - \theta_m} = \frac{1 \pm k_2}{(1 - \theta_l)} - \frac{1 \pm k_1}{(1 + \theta_l)}, \tag{17}$$

where $\lambda = -(2q \pm k_1 \pm k_2 + 1)^2$. These are just the equations satisfied by the zeros of the Jacobi polynomials. In fact the solutions of this eigenvalue equation have the form

$$T(\theta) = (\cos \theta)^{1/2 \pm k_1} (\sin \theta)^{1/2 \pm k_2} P_q^{(\pm k_1, \pm k_2)} (\cos 2\theta).$$

The classical constant of the motion is

$$L_2 = (x p_y - y p_x)^2 - \left[\frac{k_1^2 - \frac{1}{4}}{x^2} + \frac{k_2^2 - \frac{1}{4}}{y^2} \right] (x^2 + y^2)$$

and the corresponding eigenvalue equation satisfied by the eigenfunctions Ψ is

$$\hat{L}_2 \Psi = \left[\left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right)^2 + \left(\frac{\frac{1}{4} - k_1^2}{x^2} + \frac{\frac{1}{4} - k_2^2}{y^2} \right) (x^2 + y^2) \right] \Psi = \lambda \Psi. \tag{18}$$

The orthonormal [as in Eq. (14)] eigenfunctions in these coordinates are

$$\Psi(r,\theta)\equiv\Psi_{n_r,q}^{(\pm k_1,\pm k_2)}(r,\theta)=\Phi_q^{(\pm k_1,\pm k_2)}(\theta)\sqrt{\frac{2\omega n!}{\Gamma(n+2q\pm k_1\pm k_2+1)}}$$
$$\times e^{-\omega r^2/2}(\sqrt{\omega}r)^{(2q\pm k_1\pm k_2+1)}L_n^{2q\pm k_1\pm k_2+1}(\omega r^2), \tag{19}$$

where

$$\Phi_q^{(\pm k_1,\pm k_2)}(\theta)=\sqrt{\frac{(2q\pm k_1\pm k_2+1)q!\Gamma(q\pm k_1\pm k_2+1)}{2\Gamma(q\pm k_2+1)\Gamma(q\pm k_1+1)}}$$
$$\times(\cos\theta)^{1/2\pm k_1}(\sin\theta)^{1/2\pm k_2}P_q^{(\pm k_1,\pm k_2)}(\cos 2\theta) \tag{20}$$

and $E=\omega(2n\pm k_1\pm k_2+2)$, with $n=n_r+q$. Using (11) we can easily split off the polynomial portion of (20) from the multiplier.

In elliptical coordinates we adopt a similar approach. Using the identity

$$\frac{x^2}{\theta-e_1}+\frac{y^2}{\theta-e_2}-1=-\frac{(u_1-\theta)(u_2-\theta)}{(\theta-e_1)(\theta-e_2)}, \tag{21}$$

we look for solutions (11) of the form[19]

$$\Phi(x,y)=\prod_{m=1}^{q}\left(\frac{x^2}{\theta_m-e_1}+\frac{y^2}{\theta_m-e_2}-1\right).$$

The θ_m must satisfy

$$\frac{1\pm k_1}{\theta_m-e_1}+\frac{1\pm k_2}{\theta_m-e_2}+\sum_{j\neq m}\frac{2}{(\theta_m-\theta_j)}-\omega=0, \tag{22}$$

where $E=\omega(2q\pm k_1\pm k_2+2)$. If we write the Schrödinger equation for this potential in elliptical coordinates we obtain

$$\frac{4(u_1-e_1)(u_1-e_2)}{u_1-u_2}\left[\frac{\partial^2\Psi}{\partial u_1^2}+\frac{1}{2}\left(\frac{1}{u_1-e_1}+\frac{1}{u_1-e_2}\right)\frac{\partial\Psi}{\partial u_1}\right]$$
$$+\frac{4(u_2-e_1)(u_2-e_2)}{u_2-u_1}\left[\frac{\partial^2\Psi}{\partial u_2^2}+\frac{1}{2}\left(\frac{1}{u_2-e_1}+\frac{1}{u_2-e_2}\right)\frac{\partial\Psi}{\partial u_2}\right]$$
$$+\left[2E-\omega^2(u_1+u_2-e_1-e_2)+\frac{(\frac{1}{4}-k_1^2)(e_2-e_1)}{(u_1-e_1)(u_2-e_1)}+\frac{(\frac{1}{4}-k_2^2)(e_1-e_2)}{(u_1-e_2)(u_2-e_2)}\right]\Psi=0.$$

This equation admits separable solutions $\Psi=U_1(u_1)U_2(u_2)$ and separation equations

$$\left\{4(u_i-e_1)(u_i-e_2)\left[\frac{\partial^2}{\partial u_i^2}+\frac{1}{2}\left(\frac{1}{u_i-e_1}+\frac{1}{u_i-e_2}\right)\frac{\partial}{\partial u_i}\right]-\omega^2[u_i^2-(e_1+e_2)u_i]\right.$$
$$\left.+\frac{(k_1^2-\frac{1}{4})(e_1-e_2)}{(u_1-e_1)}+\frac{(k_2^2-\frac{1}{4})(e_2-e_1)}{(u_1-e_2)}+2Eu_i+\lambda\right\}U_i(u_i)=0,\quad i=1,2.$$

The additional operator describing this coordinate system is

$$\hat{L}_3\Psi=\frac{4u_2(u_1-e_1)(u_1-e_2)}{u_1-u_2}\left[\frac{\partial^2\Psi}{\partial u_1^2}+\frac{1}{2}\left(\frac{1}{u_1-e_1}+\frac{1}{u_1-e_2}\right)\frac{\partial\Psi}{\partial u_1}\right]$$
$$+\frac{4u_1(u_2-e_1)(u_2-e_2)}{u_2-u_1}\left[\frac{\partial^2\Psi}{\partial u_2^2}+\frac{1}{2}\left(\frac{1}{u_2-e_1}+\frac{1}{u_2-e_2}\right)\frac{\partial\Psi}{\partial u_2}\right]$$
$$+\left[-u_1u_2\omega^2+\frac{(k_1^2-\frac{1}{4})(e_1-e_2)}{(u_1-e_1)(u_2-e_1)}+\frac{(k_2^2-\frac{1}{4})(e_1-e_2)}{(u_1-e_2)(u_2-e_2)}\right]\Psi$$
$$=\left[\left(x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x}\right)^2+e_2\frac{\partial^2}{\partial x^2}+e_1\frac{\partial^2}{\partial y^2}-\omega^2(e_2x^2+e_1y^2+e_1e_2)\right.$$
$$\left.+\frac{\frac{1}{4}-k_1^2}{x^2}(x^2+y^2+e_2)+\frac{\frac{1}{4}-k_2^2}{y^2}(x^2+y^2+e_1)\right]\Psi=\lambda\Psi, \tag{23}$$

where

$$\lambda=-(1\pm k_1\pm k_2)^2-2e_2\omega(1\pm k_1)-2e_1\omega(1\pm k_2)-\omega^2e_1e_2-4\sum_{m=1}^{q}\left[e_2\frac{1\pm k_1}{\theta_m-e_1}+e_1\frac{1\pm k_2}{\theta_m-e_2}\right].$$

The corresponding classical operator is

$$L_3=(xp_y-yp_x)^2+e_2p_x^2+e_1p_y^2-\omega^2(e_2x^2+e_1y^2+e_1e_2)$$
$$+\frac{(\frac{1}{4}-k_1^2)}{x^2}(x^2+y^2+e_2)+\frac{(\frac{1}{4}-k_2^2)}{y^2}(x^2+y^2+e_1). \tag{24}$$

If we now use the redefined operators

$$M_1=L_1,\quad M_2=L_2-\tfrac{1}{2}+k_1^2+k_2^2,\quad M_3=L_3-\tfrac{1}{2}+k_1^2+k_2^2,$$

and

$$H=p_x^2+p_y^2-\omega^2(x^2+y^2)+\frac{\frac{1}{4}-k_1^2}{x^2}+\frac{\frac{1}{4}-k_2^2}{y^2},$$

we observe the following relations:

$$M_{12}=\{M_1,M_2\}=4(xp_y-yp_x)(p_xp_y-\omega^2xy)+\frac{\frac{1}{4}-k_2^2}{y^2}xp_x-\frac{\frac{1}{4}-k_1^2}{x^2}yp_y, \tag{25}$$

$$\{M_{12},M_1\}=8(M_1^2-M_1H)-16\omega^2M_2, \tag{26}$$

$$\{M_{12},M_2\}=8M_2(H-2M_1)-4(1-4k_2^2)M_2+4(1-4k_1^2)(H-M_1), \tag{27}$$

$$M_{12}^2=16M_1M_2(H-M_1)+16\omega^2L_2^2-4(1-4k_2^2)M_1^2-4(1-4k_2^2)(H-M_1)^2$$
$$+4\omega^2(1-4k_1^2)(1-4k_2^2).$$

We have not included M_3 in these calculations as it is linearly dependent on H, M_1 and M_2 via the relation $M_3=M_2+(e_2-e_1)M_1+e_1H$. The constants of the motion M_1, M_2 and H generate a quadratic algebra.

(ii) The potential is now

$$V_2(x,y)=\frac{1}{2}\,\omega^2(4x^2+y^2)+\frac{k_2^2-\frac{1}{4}}{2y^2}. \tag{28}$$

For $k_1=0$ this potential is also known as a Holt potential.[20] The Schrödinger equation for $k_1=0$ has the form

$$\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\Psi-\left[\omega^2(4x^2+y^2)+\frac{k_2^2-\frac{1}{4}}{y^2}\right]\Psi=-2E\Psi.$$

There are two coordinate systems of relevance here: Cartesian coordinates x,y and parabolic coordinates ξ,η. If we express solutions of the Schrödinger equations in the form

$$\Psi=e^{-\omega x^2-\omega y^2/2}y^{1/2\pm k_2}\Phi(x,y), \tag{29}$$

then the function $\Phi(x,y)$ satisfies the equation $R\Phi=-2E\Phi$ or

$$\left[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{(1\pm 2k_2)}{y}\,\frac{\partial}{\partial y}-2\omega\left(2x\,\frac{\partial}{\partial x}+y\,\frac{\partial}{\partial y}\right)-2\omega(2\pm k_2)\right]\Phi(x,y)=-2E\Phi. \tag{30}$$

It follows that the operator R maps polynomials (in x,y^2) into polynomials, without increasing the order. Since the original Hamiltonian is self-adjoint with respect to the measure $dx\,dy$ in the plane, the operator R, acting on polynomials in x,y^2 is self-adjoint with respect to the measure

$$d\rho(x,y)=e^{-\omega(x^2+y^2)}y^{1\pm 2k_2}\,dx\,dy$$

in the upper half-plane $y>0$. We assume that the positive sign at the k_2 has to be taken if $k_2>\frac{1}{2}$ and both the positive and the negative sign must be taken if $0<k_2<\frac{1}{2}$, so that the polynomials have finite norm.[16]

Equation (30) admits a separable solution of the form $\Phi=X(x)Y(y)$ where the function $X(x)$ satisfies the separation equation

$$\left[\frac{\partial^2}{\partial x^2}-4\omega x\,\frac{\partial}{\partial x}-2\omega-\lambda\right]X=0.$$

If we try solutions of the form $X=\Pi_{m=1}^{q}(x-\theta_m)$, the relations among the θ_m are

$$4\omega\theta_\ell=\sum_{m\neq\ell}\frac{1}{\theta_\ell-\theta_m} \tag{31}$$

and the eigenvalues are $\lambda=-2(2q+1)\omega$ with solutions $X=H_q(\sqrt{2\omega}x)$. The solutions for the function $Y(y)$ correspond exactly to those given for the potential V_1 viz

$$Y(y)=L_n^{\pm k_2}(y^2).$$

The orthonormal eigenfunctions are

$$\Psi(x,y)=\sqrt{2}\,\omega^{(1/2)(1\pm k_2)}\sqrt{\frac{n!}{\Gamma(n\pm k_2+1)}}\,y^{1/2\pm k_2}e^{-1/2\omega y^2}L_n^{\pm k_2}(\omega y^2)$$
$$\times\left(\frac{2\omega}{\pi}\right)^{1/4}\frac{1}{\sqrt{2^q q!}}\,e^{-\omega x^2}H_q(\sqrt{2\omega}x). \tag{32}$$

The energy E takes the values $E=\omega[2(q+n+1)\pm k_2]$.

In the case of *parabolic coordinates* we note that

$$\frac{y^2}{\lambda^2}+2x-\lambda^2=\frac{(\xi^2-\lambda^2)(\eta^2+\lambda^2)}{\lambda^2}.$$

If we try a solution of (30) in the form

$$\Phi(x,y)=\prod_{\ell=1}^{q}\left(\frac{y^2}{\lambda_\ell^2}+2x-\lambda_\ell^2\right), \tag{33}$$

it follows that the λ_ℓ must satisfy

$$\frac{1}{\lambda_\ell^2}+\sum_{m\neq\ell}\frac{4}{\lambda_\ell^2-\lambda_m^2}-2\omega\lambda_\ell^2=0$$

and $E=\omega(2q+2\pm k_2)$. The Schrödinger equation written in terms of parabolic coordinates is

$$\frac{1}{\xi^2+\eta^2}\left(\frac{\partial^2\Psi}{\partial\xi^2}+\frac{\partial^2\Psi}{\partial\eta^2}\right)+\left[2E-\omega^2(\xi^4-\xi^2\eta^2+\eta^4)+\frac{\frac{1}{4}-k_2^2}{\xi^2\eta^2}\right]\Psi=0. \tag{34}$$

If we look for separable solutions of the form $\Psi=X_1(\xi)X_2(\eta)$, the separation equations are

$$\left[\frac{\partial^2}{\partial\mu^2}+\left(-\omega^2\mu^6+\frac{\frac{1}{4}-k_2^2}{\mu^2}+2E\mu^2+\lambda\right)\right]X_j=0,$$

where $\mu=\xi$ if $j=1$ and $\mu=\eta$ if $j=2$. The operator whose eigenvalue is λ is

$$\hat{L}_2\Psi=\frac{1}{\xi^2+\eta^2}\left[\xi^2\frac{\partial^2\Psi}{\partial\eta^2}-\eta^2\frac{\partial^2\Psi}{\partial\xi^2}\right]+\left[\omega^2\xi^2\eta^2+\frac{\frac{1}{4}-k_2^2}{\xi^2\eta^2}\right](\xi^2-\eta^2)\Psi$$
$$=2x\frac{\partial^2\Psi}{\partial y^2}-2y\frac{\partial^2\Psi}{\partial x\partial y}-\frac{\partial\Psi}{\partial x}+\left[2\omega^2xy^2+\frac{\frac{1}{4}-k_2^2}{y^2}x\right]\Psi. \tag{35}$$

The eigenvalues are

$$\lambda=2(k_2+1)\prod_{j=1}^{q}\lambda_j^2\left(\sum_{m=1}^{q}\lambda_m^{-2}\right).$$

If we define the classical operators associated with this separable system as

$$H=p_x^2+p_y^2-\omega^2(4x^2+y^2)+\frac{\frac{1}{4}-k_2^2}{y^2},$$

$$L_1=p_x^2-4\omega^2x^2,\quad L_2=2p_y(xp_y-yp_x)+2\omega^2xy^2+\frac{\frac{1}{4}-k_2^2}{y^2}\,x,$$

then the defining relations of the quadratic algebra are

$$L_{12}=\{L_1,L_2\}=4\left[p_xp_y^2+\omega^2y^2p_x+2\,\frac{\frac{1}{4}-k_2^2}{y^2}\,p_x-4\omega^2xyp_y\right],$$

$$L_{12}^2=16(H-L_1)^2L_1+16\omega^2L_2^2+16\omega^2(1-4k_2^2),\quad \{L_1,L_{12}\}=-16\omega^2L_2, \tag{36}$$

$$\{L_2,L_{12}\}=16L_1(H-L_1)-8(H-L_1)^2-8\omega^2(1-4k_2^2).$$

(iii) The potential is now

$$V_3=\frac{-\alpha}{\sqrt{x^2+y^2}}+\frac{1}{4\sqrt{x^2+y^2}}\left[\frac{k_1^2-\frac{1}{4}}{\sqrt{x^2+y^2}+x}+\frac{k_2^2-\frac{1}{4}}{\sqrt{x^2+y^2}-x}\right]. \tag{37}$$

The Schrödinger equation separates variables in polar coordinates, parabolic coordinates, and modified elliptic coordinates. If we look for solutions of the Schrödinger equation of the form

$$\Psi=e^{-(1/2)\sqrt{-2E}(\xi^2+\eta^2)}\xi^{1/2\pm k_1}\eta^{1/2\pm k_2}\Phi(\xi,\eta), \tag{38}$$

where ξ and η are *parabolic coordinates*, we find that the equation for $\Phi(\xi,\eta)$ is $S\Phi=-4\alpha\Phi$ or

$$\left[\frac{\partial^2\Phi}{\partial\xi^2}+\frac{\partial^2\Phi}{\partial\eta^2}+\frac{(1\pm2k_1)}{\xi}\,\frac{\partial\Phi}{\partial\xi}+\frac{(1\pm2k_2)}{\eta}\,\frac{\partial\Phi}{\partial\eta}\right.$$
$$\left.+2\sqrt{-2E}\left(\xi\,\frac{\partial\Phi}{\partial\xi}+\eta\,\frac{\partial\Phi}{\partial\eta}\right)-2\sqrt{-2E}(2\pm k_1\pm k_2)\right]\Phi=-4\alpha\Phi. \tag{39}$$

For fixed E we can consider this as an eigenvalue equation for S with eigenvalue -4α. Moreover, S maps polynomials (in ξ^2, η^2, or, what is the same thing, in $r=\sqrt{x^2+y^2}$, x) into polynomials, without increasing the order. Since the original Hamiltonian is self-adjoint with respect to the measure $dx\,dy$ in the plane, the operator S, acting on polynomials in ξ^2 and η^2, is self-adjoint with respect to the measure

$$d\rho(x,y)=e^{-\sqrt{-2E}(\xi^2+\eta^2)}\xi^{1\pm2k_1}\eta^{1\pm2k_2}(\xi^2+\eta^2)d\xi\,d\eta.$$

We assume that the positive sign at the k_i has to be taken if $k_i>\frac{1}{2}$ and both the positive and the negative sign must be taken if $0<k_i<\frac{1}{2}$, so that the polynomials have finite norm.[16] For polynomial eigenfunctions we must have the quantisation condition

$$2\alpha=\sqrt{-2E}[2(q+1)\pm k_1\pm k_2] \tag{40}$$

for integer q.

In *polar coordinates* with potential V_3 the Schrödinger equation has the form

$$\left[\frac{\partial^2}{\partial r^2}+\frac{1}{r}\,\frac{\partial}{\partial r}+\frac{1}{r^2}\,\frac{\partial^2}{\partial\theta^2}\right]\Psi+\left[2E+\frac{2\alpha}{r}+\frac{1}{2r^2}\left(\frac{\frac{1}{4}-k_1^2}{1+\cos\,\theta}+\frac{\frac{1}{4}-k_2^2}{1-\cos\,\theta}\right)\right]\Psi=0.$$

If we write solutions Ψ in the form

$$\Psi = R(r)S(\theta),$$

the θ separation equation is

$$\frac{d^2}{d\theta^2}S(\theta) + \frac{1}{16}\left[\frac{1-4k_1^2}{\cos^2(\theta/2)} + \frac{1-4k_2^2}{\sin^2(\theta/2)}\right]S(\theta) = -\lambda^2 S(\theta), \tag{41}$$

which has solutions

$$S(\theta) = \left(\sin\frac{\theta}{2}\right)^{1/2\pm k_2}\left(\cos\frac{\theta}{2}\right)^{1/2\pm k_1} P_m^{(\pm k_1, \pm k_2)}(\cos\,\theta),$$

where $\lambda = m + \frac{1}{2}(1 \pm k_1 \pm k_2)$. The separation equation for $R(r)$ is

$$\left[\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} - \frac{\lambda^2}{r^2} + \frac{2\alpha}{r} + 2E\right]R(r) = 0, \tag{42}$$

which has the solution

$$R_{n\lambda}(r) = e^{-\sqrt{-2E}r}(2\sqrt{-2E}r)^{\lambda} L_n^{\lambda}(2\sqrt{-2E}r),$$

where

$$E = \frac{-2\alpha^2}{[2(m+n+1) \pm k_1 \pm k_2]^2}.$$

The orthonormal basis of eigenfunctions is

$$\Psi = \sqrt{\frac{\alpha n!}{\Gamma(2n+2\lambda+1)(2n+2\lambda+1)}}\, R_{n\lambda}(r)\Phi_n^{(\pm k_2, \pm k_1)}\left(\frac{\theta}{2}\right). \tag{43}$$

The operator whose eigenvalue is μ^2 is, in Cartesian coordinates,

$$L_1\Psi = \left[\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)^2 - \frac{1}{2}\sqrt{x^2+y^2}\left(\frac{k_1^2-\frac{1}{4}}{\sqrt{x^2+y^2}+x} + \frac{k_2^2-\frac{1}{4}}{\sqrt{x^2+y^2}-x}\right)\right]\Psi. \tag{44}$$

In *parabolic coordinates* Schrödinger's equation has the form

$$H\Psi = \frac{1}{\xi^2+\eta^2}\left[\frac{\partial^2\Psi}{\partial\xi^2} + \frac{\partial^2\Psi}{\partial\eta^2}\right] + \left[4\alpha + \left(\frac{\frac{1}{4}-k_1^2}{\xi^2} + \frac{\frac{1}{4}-k_2^2}{\eta^2}\right)\right]\Psi = -2E\Psi.$$

The separation equations are

$$\frac{\partial^2}{\partial\mu^2}X_j + \left(\frac{\frac{1}{4}-k_j^2}{\mu^2} + 2E\mu^2 + \lambda_j\right)X_j = 0 \tag{45}$$

with $\lambda_1+\lambda_2=4\alpha$. The orthonormal bound state eigenfunctions of Schrödinger's equation in these coordinates are

$$\begin{aligned}\Psi &= X_1(\xi)X_2(\eta)\\ &= \sqrt{\frac{\alpha}{[2(n_1+n_2)\pm k_1\pm k_2+2]^3}}\ \sqrt{\frac{n_1!n_2!}{\Gamma(n_1\pm k_1+1)\Gamma(n_2\pm k_2+1)}}\ e^{-(1/2)\sqrt{-2E}(\xi^2+\eta^2)}\\ &\quad\times(\sqrt{-2E}\,\xi)^{1/2\pm k_1}(\sqrt{-2E}\,\eta)^{1/2\pm k_2}L_{n_1}^{\pm k_1}(\sqrt{-2E}\,\xi^2)L_{n_2}^{\pm k_2}(\sqrt{-2E}\,\eta^2),\end{aligned}\tag{46}$$

where $\lambda_j=2\sqrt{-2E}(2n_j\pm k_j+1)$, $j=1,2$, and

$$E=-\frac{2\alpha^2}{[2(n_1+n_2)\pm k_1\pm k_2+2]^2}.$$

If we choose $\lambda_1=2\alpha+\lambda$ and $\lambda_2=2\alpha-\lambda$, then the symmetry operator with eigenvalue λ is

$$\begin{aligned}L_2\Psi &= 2x\frac{\partial^2\Psi}{\partial y^2}-2y\frac{\partial^2\Psi}{\partial x\partial y}-\frac{\partial\Psi}{\partial x}+\left[-\left(k_1^2-\frac{1}{4}\right)\frac{\sqrt{x^2+y^2}-x}{\sqrt{x^2+y^2}(\sqrt{x^2+y^2}+x)}\right.\\ &\quad\left.+\left(k_2^2-\frac{1}{4}\right)\frac{\sqrt{x^2+y^2}+x}{\sqrt{x^2+y^2}(\sqrt{x^2+y^2}-x)}+\frac{4\alpha}{\sqrt{x^2+y^2}}\right]\Psi\\ &= \frac{1}{\xi^2+\eta^2}\left[\xi^2\frac{\partial^2\Psi}{\partial\eta^2}-\eta^2\frac{\partial^2\Psi}{\partial\xi^2}\right]+\left[\left(\frac{1}{4}-k_1^2\right)\frac{\eta^2}{\xi^2(\xi^2+\eta^2)}\right.\\ &\quad\left.+\left(k_2^2-\frac{1}{4}\right)\frac{\xi^2}{\eta^2(\xi^2+\eta^2)}+2\alpha\frac{\xi^2-\eta^2}{\xi^2+\eta^2}\right]\Psi.\end{aligned}$$

For the case of *elliptical coordinates* we proceed as follows. The normal elliptical coordinates will not separate variables. However, if we compare (12) and (39) we are motivated to choose coordinates such that

$$\xi^2=\frac{(u_1-e_1)(u_2-e_1)}{e_1-e_2},\quad \eta^2=\frac{(u_1-e_2)(u_2-e_2)}{e_2-e_1}.\tag{47}$$

If we then try a solution of (39) in the form

$$\Phi(\xi,\eta)=\prod_{m=1}^{q}\left[\frac{\xi^2}{\theta_m-e_1}+\frac{\eta^2}{\theta_m-e_2}-1\right],\tag{48}$$

we see that the θ_m must satisfy

$$\frac{1\pm k_1}{\theta_m-e_1}+\frac{1\pm k_2}{\theta_m-e_2}+\sum_{j\neq m}\frac{2}{\theta_m-\theta_j}-\sqrt{-2E}=0,$$

and the quantization condition (40). In this choice of coordinates the Schrödinger equation has the form

$$\frac{4(u_1-e_1)(u_1-e_2)}{u_1-u_2}\left[\frac{\partial^2\Phi}{\partial u_1^2}+\frac{1}{2}\left(\frac{1}{u_1-e_1}+\frac{1}{u_1-e_2}\right)\frac{\partial\Phi}{\partial u_1}\right]$$

$$+\frac{4(u_2-e_1)(u_2-e_2)}{u_2-u_1}\left[\frac{\partial^2\Phi}{\partial u_2^2}+\frac{1}{2}\left(\frac{1}{u_2-e_1}+\frac{1}{u_2-e_2}\right)\frac{\partial\Phi}{\partial u_2}\right]$$

$$+\left[2E(u_1+u_2-e_1-e_2)+\frac{(\frac{1}{4}-k_1^2)(e_2-e_1)}{(u_1-e_1)(u_2-e_1)}+\frac{(\frac{1}{4}-k_2^2)(e_1-e_2)}{(u_1-e_2)(u_2-e_2)}+4\alpha\right]\Phi=0.$$

This equation admits separable solutions $\Phi=U_1(u_1)U_2(u_2)$ and separation equations

$$\left\{4(u_i-e_1)(u_i-e_2)\left(\frac{\partial^2}{\partial u_i^2}+\frac{1}{2}\left[\frac{1}{u_i-e_1}+\frac{1}{u_i-e_2}\right]\frac{\partial}{\partial u_i}\right)+2E[u_i^2-(e_1+e_2)u_i]\right.$$

$$\left.+\frac{(k_1^2-\frac{1}{4})(e_1-e_2)}{u_1-e_1}+\frac{(k_2^2-\frac{1}{4})(e_2-e_1)}{u_1-e_2}+4\alpha u_i+\lambda\right\}U_i(u_i)=0,\quad i=1,2. \tag{49}$$

The additional operator describing this coordinate system is

$$\hat{L}_3\Phi=\frac{4}{(u_1-u_2)(u_1+u_2-e_1-e_2)}\left\{u_2(u_1-e_1)(u_1-e_2)\left(\frac{\partial^2\Phi}{\partial u_1^2}+\frac{1}{2}\left[\frac{1}{u_1-e_1}+\frac{1}{u_1-e_2}\right]\frac{\partial\Phi}{\partial u_1}\right)\right.$$

$$\left.-u_1(u_2-e_1)(u_2-e_2)\left(\frac{\partial^2\Phi}{\partial u_2^2}+\frac{1}{2}\left[\frac{1}{u_2-e_1}+\frac{1}{u_2-e_2}\right]\frac{\partial\Phi}{\partial u_2}\right)\right\}$$

$$+\frac{k_1^2-\frac{1}{4}}{(u_1-e_1)(u_2-e_1)}\left\{u_1+u_2-e_1-e_2-\frac{[(u_1-e_2)(u_2-e_2)+e_1e_2]}{(u_1+u_2-e_1-e_2)}\right\}\Phi$$

$$+\frac{k_2^2-\frac{1}{4}}{(u_1-e_2)(u_2-e_2)}\left\{u_1+u_2-e_1-e_2-\frac{[(u_1-e_1)(u_2-e_1)+e_1e_2]}{(u_1+u_2-e_1-e_2)}\right\}\Phi$$

$$+\frac{4\alpha u_1u_2}{u_1+u_2-e_1-e_2}\Phi. \tag{50}$$

In Cartesian coordinates the solutions have the form

$$\Psi=e^{-\sqrt{-2E}(x^2+y^2)}(\sqrt{x^2+y^2}+x)^{(1/4)(1\pm2k_1)}(\sqrt{x^2+y^2}-x)^{(1/4)(1\pm2k_2)}$$

$$\times\prod_{m=1}^{q}\left(\frac{\sqrt{x^2+y^2}+x}{\theta_m-e_1}+\frac{\sqrt{x^2+y^2}-x}{\theta_m-e_2}-1\right). \tag{51}$$

Acting on the functions Ψ the operator L_3 has the form

$$L_3\Psi=\left[\left(\xi\frac{\partial}{\partial\eta}-\eta\frac{\partial}{\partial\xi}\right)^2+e_2\frac{\partial^2}{\partial\xi^2}+e_1\frac{\partial^2}{\partial\eta^2}-(e_2\xi^2+e_1\eta^2+e_1e_2)H\right.$$
$$\left.+\left(\frac{1}{4}-k_1^2\right)\frac{(\xi^2+\eta^2+e_2)}{\xi^2}+\left(\frac{1}{4}-k_2^2\right)\frac{(\xi^2+\eta^2+e_2)}{\eta^2}\right]\Psi$$
$$=\left[-4\left(x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x}\right)^2-(e_1-e_2)\left(2x\frac{\partial^2}{\partial y^2}-2y\frac{\partial^2}{\partial x\partial y}-\frac{\partial}{\partial x}\right)-e_1e_2H\right.$$
$$-\frac{2\alpha}{\sqrt{x^2+y^2}}[e_1(\sqrt{x^2+y^2}-x)+e_2(\sqrt{x^2+y^2}+x)]-\left(\frac{1}{4}-k_1^2\right)$$
$$\times\frac{(e_1-e_2)(\sqrt{x^2+y^2}-x)}{2\sqrt{x^2+y^2}(\sqrt{x^2+y^2}+x)}-\left(\frac{1}{4}-k_2^2\right)\frac{(e_1-e_2)(\sqrt{x^2+y^2}+x)}{2\sqrt{x^2+y^2}(\sqrt{x^2+y^2}-x)}$$
$$\left.+\left(\frac{1}{4}-k_1^2\right)\frac{\sqrt{x^2+y^2}-x}{\sqrt{x^2+y^2}+x}+\left(\frac{1}{4}-k_2^2\right)\frac{\sqrt{x^2+y^2}+x}{\sqrt{x^2+y^2}-x}+\frac{1}{2}-k_1^2-k_2^2\right]\Psi, \tag{52}$$

where in Cartesian coordinates

$$H\Psi=\frac{\partial^2\Psi}{\partial x^2}+\frac{\partial^2\Psi}{\partial y^2}+\left[\frac{-\alpha}{\sqrt{x^2+y^2}}+\frac{1}{4\sqrt{x^2+y^2}}\left[\frac{k_1^2-\frac{1}{4}}{\sqrt{x^2+y^2}+x}+\frac{k_2^2-\frac{1}{4}}{\sqrt{x^2+y^2}-x}\right]\right]\Psi.$$

The eigenvalues of the operator L_3 are

$$\lambda=-(1\pm k_1\pm k_2)^2-2\sqrt{-2E}[e_2(1\pm k_1)-2e_1(1\pm k_2)]$$
$$+2Ee_1e_2-4\sum_{m=1}^{q}\left[e_2\frac{k_1+1}{\theta_m-e_1}+e_1\frac{k_2+1}{\theta_m-e_2}\right]. \tag{53}$$

The corresponding quadratic algebra can be generated by the classical constants

$$L_1=(\xi p_\eta-\eta p_\xi)^2+(\xi^2+\eta^2)\left[\frac{\frac{1}{4}-k_1^2}{\xi^2}+\frac{\frac{1}{4}-k_2^2}{\eta^2}\right],$$

$$L_2=\frac{1}{\xi^2+\eta^2}\left[\xi^2p_\eta^2-\eta^2p_\xi^2-\frac{\eta^2}{\xi^2}\left(\frac{1}{4}-k_1^2\right)-\frac{\xi^2}{\eta^2}\left(\frac{1}{4}-k_2^2\right)+2\alpha(\xi^2-\eta^2)\right],$$

$$L_3=(\xi p_\eta-\eta p_\xi)^2+e_2p_\xi^2+e_1p_\eta^2-(e_2\xi^2+e_1\eta^2)H$$
$$+\left(\frac{1}{4}-k_1^2\right)\frac{(\xi^2+\eta^2+e_2)}{\xi^2}+\left(\frac{1}{4}-k_2^2\right)\frac{(\xi^2+\eta^2+e_2)}{\eta^2},$$

$$H=\frac{1}{\xi^2+\eta^2}\left[p_\xi^2+p_\eta^2+4\alpha+\left(\frac{\frac{1}{4}-k_1^2}{\xi^2}+\frac{\frac{1}{4}-k_2^2}{\eta^2}\right)\right].$$

Here, L_1, L_2, and L_3 are functionally dependent via the relation

$$L_3^2=L_1^2+2(e_1-e_2)L_1L_2+(e_1-e_2)^2L_2^2-2[(k_1+k_2)+2(e_1+e_2)\alpha]L_1$$
$$-[4\alpha^2(e_1^2-e_2^2)+2(e_1-e_2)(k_1+k_2)]L_2-(k_1+k_2+2\alpha(e_1+e_2))^2. \tag{54}$$

The only additional quantity that we need is

$$L_{12}=\{L_1,L_2\}=\frac{1}{\xi^2+\eta^2}\left[4(\xi p_\eta-\eta p_\xi)^2(\xi p_\xi-\eta p_\eta)-16\xi\eta(\xi p_\eta-\eta p_\xi)\right.$$
$$+\left[\left(4\frac{\xi^3}{\eta^2}+8\xi\right)\left(\frac{1}{4}-k_2^2\right)+4\frac{\eta^2}{\xi}\left(\frac{1}{4}-k_1^2\right)\right]p_\xi$$
$$\left.-\left[\left(4\frac{\eta^3}{\xi^2}+8\eta\right)\left(\frac{1}{4}-k_1^2\right)+4\frac{\xi^2}{\eta}\left(\frac{1}{4}-k_2^2\right)\right]p_\eta\right].$$

The nontrivial independent commutation relations are

$$\{L_{12},L_1\}=-16L_1L_2+32\alpha(k_1^2-k_2^2),\quad \{L_{12},L_2\}=-16HL_1+8L_2^2. \tag{55}$$

We should also observe the relations

$$\{L_1,L_3\}=(e_1-e_2)\{L_1,L_2\},\quad \{L_1,L_2\}=\{L_3,L_2\},$$
$$\{L_{12},L_3\}=16(e_1-e_2)HL_1-8(e_1-e_2)L_2^2-16L_1L_2$$
$$-16(e_1-e_2)H-32\alpha(\alpha(e_1-e_2)+(k_1^2-k_2^2)). \tag{56}$$

(iv) The fourth potential is

$$V_4=\frac{-\alpha}{\sqrt{x^2+y^2}}+\frac{B_1}{4}\frac{\sqrt{\sqrt{x^2+y^2}+x}}{\sqrt{x^2+y^2}}+\frac{B_2}{4}\frac{\sqrt{\sqrt{x^2+y^2}-x}}{\sqrt{x^2+y^2}}. \tag{57}$$

The corresponding Schrödinger equation separates in two versions of parabolic coordinates.

In *regular parabolic coordinates* (2) the Schrödinger equation has the form

$$\frac{1}{\xi^2+\eta^2}\left[\frac{\partial^2\Psi}{\partial\xi^2}+\frac{\partial^2\Psi}{\partial\eta^2}+(4\alpha-B_1\xi-B_2\eta)\Psi\right]=-2E\Psi. \tag{58}$$

If we write the solutions Ψ in the form $X(\xi)Y(\eta)$, the separation equations are

$$\frac{\partial^2X}{\partial\xi^2}+(2\alpha-\lambda-B_1\xi+2E\xi^2)X=0,\quad \frac{\partial^2Y}{\partial\eta^2}+(2\alpha+\lambda-B_2\eta+2E\eta^2)Y=0.$$

The solutions of these equations are

$$X(\xi)=e^{(1/2\sqrt{-2E})[-2E\xi^2+B_1\xi]}H_n\left(\sqrt{-2E}\left(\xi-\frac{B_1}{4E}\right)\right) \tag{59}$$

and

$$Y(\eta)=e^{(1/2\sqrt{-2E})[-2E\eta^2+B_2\eta]}H_m\left(\sqrt{-2E}\left(\eta-\frac{B_2}{4E}\right)\right), \tag{60}$$

where

$$2\alpha-\lambda-\frac{B_1^2}{8E}=-(n+1)\sqrt{-2E},\quad 2\alpha+\lambda-\frac{B_2^2}{8E}=-(m+1)\sqrt{-2E}.$$

From this we see that the energy eigenstates are solutions of

$$4\alpha-\frac{1}{8E}(B_1^2+B_2^2)=-(m+n+2)\sqrt{-2E}. \tag{61}$$

Moreover, it follows from (59) and (60) that

$$\Psi(\xi,\eta)=e^{(1/2\sqrt{-2E})[-2E(\xi^2+\eta^2)+B_1\xi+B_2\eta]}\Phi(\xi,\eta),$$

where Φ is a polynomial in ξ and η. If (58) is written as a differential equation for Φ, it can be interpreted as an eigenvalue equation, with eigenvalue -4α, for an E-dependent operator acting on a space of polynomials. The operator whose eigenvalue is λ is

$$\begin{aligned}L_1\Psi&=\frac{1}{\xi^2+\eta^2}\left\{\eta^2\frac{\partial^2\Psi}{\partial\xi^2}-\xi^2\frac{\partial^2\Psi}{\partial\eta^2}+[-B_1\xi\eta^2+B_2\eta\xi^2+2(\eta^2-\xi^2)\alpha]\Psi\right\}\\&=-2x\frac{\partial^2\Psi}{\partial y^2}+2y\frac{\partial^2\Psi}{\partial x\partial y}+\frac{\partial\Psi}{\partial x}+\left[\frac{B_1}{2}\sqrt{\sqrt{x^2+y^2}+x}\left(1-\frac{x}{\sqrt{x^2+y^2}}\right)\right.\\&\quad\left.+\frac{B_2}{2}\sqrt{\sqrt{x^2+y^2}-x}\left(1+\frac{x}{\sqrt{x^2+y^2}}\right)-\frac{2x\alpha}{\sqrt{x^2+y^2}}\right]\Psi.\end{aligned} \tag{62}$$

The second coordinate system is a *variant of parabolic coordinates* (3) in terms of which the Schrödinger equation has the form

$$\frac{1}{\mu^2+\nu^2}\left\{\frac{\partial^2\Psi}{\partial\mu^2}+\frac{\partial^2\Psi}{\partial\nu^2}+\left[4\alpha-\frac{B_1}{\sqrt{2}}(\mu+\nu)-\frac{B_2}{\sqrt{2}}(\mu-\nu)\right]\Psi\right\}=-2E\Psi.$$

The separation equations for $\Psi=X(\mu)Y(\nu)$ are

$$\frac{\partial^2X}{\partial\mu^2}+\left(2\alpha-\lambda-\frac{1}{\sqrt{2}}(B_1+B_2)\mu+2E\mu^2\right)X=0,$$

$$\frac{\partial^2Y}{\partial\nu^2}+\left(2\alpha+\lambda-\frac{1}{\sqrt{2}}(B_1-B_2)\nu+2E\nu^2\right)Y=0.$$

The operator whose eigenvalue is λ is

$$\begin{aligned}L_2\Psi&=\frac{1}{\mu^2+\nu^2}\left[\nu^2\frac{\partial^2\Psi}{\partial\mu^2}-\mu^2\frac{\partial^2\Psi}{\partial\nu^2}-\frac{\mu\nu^2}{\sqrt{2}}(B_1+B_2)\Psi+\frac{\nu\mu^2}{\sqrt{2}}(B_1-B_2)\Psi+2(\nu^2-\mu^2)\alpha\Psi\right]\\&=-2y\frac{\partial^2\Psi}{\partial x^2}+2x\frac{\partial^2\Psi}{\partial x\partial y}+\frac{\partial\Psi}{\partial y}+\left[-\frac{1}{2\sqrt{2}}(B_1+B_2)\sqrt{\sqrt{x^2+y^2}+x}\left(1-\frac{x}{\sqrt{x^2+y^2}}\right)\right.\\&\quad\left.+\frac{1}{2\sqrt{2}}(B_1-B_2)\sqrt{\sqrt{x^2+y^2}-x}\left(1+\frac{x}{\sqrt{x^2+y^2}}\right)-\frac{2x\alpha}{\sqrt{x^2+y^2}}\right]\Psi.\end{aligned} \tag{63}$$

The space of polynomials in ξ,η coincides with the space of polynomials in ν,μ. The classical operators associated with this separable system are, using the ξ,η coordinates,

$$L_1=\frac{1}{\xi^2+\eta^2}\,[\,\eta^2 p_\xi^2-\xi^2 p_\eta^2-B_1\xi\eta^2+B_2\eta\xi^2+2(\eta^2-\xi^2)\alpha],$$

$$L_2=\frac{1}{\xi^2+\eta^2}\left[(\xi p_\xi-\eta p_\eta)(\xi p_\eta-\eta p_\xi)-4\xi\eta\alpha+\frac{1}{2}(\xi^2-\eta^2)(\eta B_1-\xi B_2)\right],$$

$$H=\frac{1}{\xi^2+\eta^2}\,[p_\xi^2+p_\eta^2+(4\alpha-B_1\xi-B_2\eta)],$$

together with

$$L_{12}=\{L_1,L_2\}=\frac{1}{\xi^2+\eta^2}\,[2(\xi p_\eta-\eta p_\xi)(p_\xi^2+p_\eta^2)+8\alpha(\xi p_\eta-\eta p_\xi)$$
$$+((\eta^2-\xi^2)p_\eta+2\xi\eta p_\xi)B_1+((\eta^2-\xi^2)p_\xi+2\xi\eta p_\eta)B_2].$$

The defining relations of the quadratic algebra are

$$L_{12}^2=4L_1^2H+4L_2^2H-16\alpha^2H+(B_2^2-B_1^2)L_1-2B_1B_2L_2-2\alpha^2(B_1^2+B_2^2),$$
$$\{L_{12},L_1\}=-4L_1^2H+B_1B_2,\quad \{L_{12},L_2\}=4L_1H-\tfrac{1}{2}(B_1^2-B_2^2). \tag{64}$$

There are, of course, quantum analogs for all the quadratic algebras that occur for each potential. These operator algebras can be obtained via the replacement of the Poisson bracket by the commutator bracket. [Indeed the relations (64) for the classical version of the algebras remain unchanged under this replacement.] One can ask the question what are the consequences of such an algebra on the eigenfunction spaces of the operators L_1 and L_2? Let the eigenspace corresponding to a fixed bound state energy E be of dimension N. This eigenspace can be spanned by eigenfunctions of both L_1 and L_2. Let the corresponding eigenvectors be ϕ_m and ψ_m, respectively, satisfying

$$L_1\phi_m=\lambda_m\phi_m,\quad L_2\psi_n=\rho_n\psi_n,$$

where $\lambda_n=2\alpha-B_1^2/8E-(2n+1)\sqrt{-2E}$ and $\rho_m=2\alpha-(B_1+B_2)^2/16E-(2m+1)\sqrt{-2E}$. Using the quantum version of the defining relations of the quadratic algebra, what can we deduce? If we use the second of the relations (64) acting on ψ_n and write $L_1\psi_n=\Sigma_{\tau=1}^N C_{n\tau}\psi_\tau$ we deduce that

$$[(\rho_n-\rho_\tau)^2+8E]C_{n\tau}=-[\tfrac{1}{2}(B_1^2-B_2^2)+16\alpha E]\,\delta_{n\tau}.$$

This relation implies that $C_{nn}=-[\frac{1}{2}(B_1^2-B_2^2)+16\alpha E]/8E$ and $C_{pq}\neq 0$ if $|p-q|\leqslant 1$ and zero otherwise. Here we have used the relation $(\rho_n-\rho_\tau)^2+8E=0$ for $|n-\tau|=1$. If we apply the second relation to the function ψ_n we obtain the relation

$$\sum_{\tau=1}^{N} C_{n\tau}C_{\tau\sigma}(2\rho_\tau-\rho_n-\rho_\sigma)=(8E\rho_n+B_1B_2+16\alpha E)\,\delta_{n\sigma}.$$

If we assume that the basis functions ψ_n are orthonormal and observe that the operator L_1 is self-adjoint, then we can assume $C_{n+1,n}=C_{n,n+1}^*$. The only nontrivial consequence of this relation is when $n=\sigma$. The result is

$$4\sqrt{-2E}(|C_{n,n+1}|^2-|C_{n-1,n}|^2)=8E\rho_n+B_1B_2+16\alpha E.$$

If we act on the functions ϕ_m, we generate similar relations. In fact, if we write $L_2\phi_m=\Sigma_{\tau=1}^N D_{m\tau}\phi_\tau$, the corresponding results are

$$D_{nn}=-(B_1B_2+16\alpha E)/8E$$

and $D_{pq}\neq 0$ if $|p-q|\leqslant 1$ and is zero otherwise. Furthermore,

$$4\sqrt{-2E}(|D_{n,n+1}|^2-|D_{n-1,n}|^2)=-8\lambda_\sigma E-\tfrac{1}{2}(B_1^2-B_2^2)-16\alpha E.$$

From these relations we can, in principle, calculate the matrices C_{pq} and D_{pq}. Once these are known, relations are also implied for the matrices relating the two bases. If we denote $\langle\phi_m,\psi_q\rangle=A_{mq}$, then these matrices must satisfy

$$C_{tr}=\sum_{m=1}^N \lambda_m A_{mr}^* A_{mt}, \quad D_{tr}=\sum_{m=1}^N \rho_m A_{mr} A_{mt}^*.$$

Thus, from the consequences of the quadratic algebra we can, in principle, calculate the overlap functions A_{rs}. The only ambiguity is in the choice of the phases of the wavefunctions.

III. THE TWO-DIMENSIONAL SPHERE

In the case of the two-dimensional sphere there are two potentials that are separable in more than one coordinate system, and these each separate in two systems. To work with the two-dimensional sphere it is convenient to use projective coordinates: s_i, $i=1,2,3$, $s_1^2+s_2^2+s_3^2=1$.

(i) The first superintegrable potential on the sphere is

$$V_1=\frac{1}{2}\left(\frac{k_1^2-\frac{1}{4}}{s_1^2}+\frac{k_2^2-\frac{1}{4}}{s_2^2}+\frac{k_3^2-\frac{1}{4}}{s_3^2}\right). \tag{65}$$

In terms of *spherical coordinates*

$$s_1=\sin\,\theta\,\cos\,\varphi, \quad s_2=\sin\,\theta\,\sin\,\varphi, \quad s_3=\cos\,\theta, \tag{66}$$

the corresponding Schrödinger equation has the form

$$\left[\left(s_1\frac{\partial}{\partial s_2}-s_2\frac{\partial}{\partial s_1}\right)^2+\left(s_1\frac{\partial}{\partial s_3}-s_3\frac{\partial}{\partial s_1}\right)^2+\left(s_3\frac{\partial}{\partial s_2}-s_2\frac{\partial}{\partial s_3}\right)^2\right]\Psi$$
$$-\left[\frac{k_1^2-\frac{1}{4}}{s_1^2}+\frac{k_2^2-\frac{1}{4}}{s_2^2}+\frac{k_3^2-\frac{1}{4}}{s_3^2}\right]\Psi=-2E\Psi, \tag{67}$$

or, in terms of θ and φ,

$$\frac{1}{\sin\,\theta}\frac{\partial}{\partial\theta}\left(\sin\,\theta\,\frac{\partial\Psi}{\partial\theta}\right)+\frac{1}{\sin^2\,\theta}\frac{\partial^2\Psi}{\partial\varphi^2}+\frac{1}{\sin^2\,\theta}\left(\frac{\frac{1}{4}-k_1^2}{\cos^2\,\varphi}+\frac{\frac{1}{4}-k_2^2}{\sin^2\,\varphi}\right)\Psi+\frac{\frac{1}{4}-k_3^2}{\cos^2\,\theta}\,\Psi=-2E\Psi.$$

This equation admits separable solutions of the form $\Psi=T(\theta)\Phi(\varphi)$ such that

$$\frac{\partial^2\Phi}{\partial\varphi^2}+\left(\frac{\frac{1}{4}-k_1^2}{\cos^2\varphi}+\frac{\frac{1}{4}-k_2^2}{\sin^2\varphi}\right)\Phi=-\lambda\Phi,$$

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial T}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\lambda T+\frac{\frac{1}{4}-k_3^2}{\cos^2\theta}T=-2ET.$$

These equations have the solutions

$$\Phi=(\sin\varphi)^{k_2+1/2}(\cos\varphi)^{k_1+1/2}P_n^{(k_2,k_1)}(\cos 2\varphi),$$

where $\lambda=(2n+1+k_1+k_2)^2$ and n is an integer, and

$$T(\theta)=(\cos\theta)^{k_3+1/2}(\sin\theta)^{2n+k_1+k_2+1}P_m^{(2n+k_1+k_2+1,k_3)}(\cos 2\theta),$$

where $E=\frac{1}{2}[2(m+n+1)+(k_1+k_2+k_3)]^2-\frac{1}{8}$. The orthonormal basis eigenfunctions are

$$\Psi=(\sin\theta)^{-1}\Phi_n^{(k_2,k_1)}(\varphi)\Phi^{(2n+k_1+k_2,k_3)}(\theta). \tag{68}$$

The operator which characterizes this solution and separation is

$$L_1\Psi=\left[\left(s_1\frac{\partial}{\partial s_2}-s_2\frac{\partial}{\partial s_1}\right)^2+\left(\frac{1}{4}-k_1^2\right)\frac{s_1^2+s_2^2}{s_1^2}+\left(\frac{1}{4}-k_2^2\right)\frac{s_1^2+s_2^2}{s_2^2}\right]\Psi=\lambda\Psi. \tag{69}$$

Note that after the multiplier $(\sin\varphi)^{k_2+1/2}(\cos\varphi)^{k_1+1/2}(\cos\theta)^{k_3+1/2}(\sin\theta)^{k_1+k_2+1}=\Pi_{\ell=1}^3 s_\ell^{k_\ell+1/2}$ is split off, the eigenfunctions are polynomials in the variables s_2^2 and s_2^3. See Refs. 21–24 for a complete discussion of the polynomial setting for this eigenvalue equation.

For the second coordinate system we choose *Lamé coordinates* given by

$$s_i^2=\frac{(u_1-e_i)(u_2-e_i)}{(e_i-e_j)(e_i-e_k)},\quad i,j,k=1,2,3,\quad \text{and } i,j,k \text{ pairwise distinct.}$$

The Schrödinger equation written in terms of these coordinates is

$$\begin{aligned}&\frac{4}{(u_1-u_2)}\left[(u_1-e_1)(u_1-e_2)(u_1-e_3)\left[\frac{\partial^2\Psi}{\partial u_1^2}+\frac{1}{2}\left(\frac{1}{u_1-e_1}+\frac{1}{u_1-e_2}+\frac{1}{u_1-e_3}\right)\frac{\partial\Psi}{\partial u_1}\right]\right.\\&\quad\left.-(u_2-e_1)(u_2-e_2)(u_2-e_3)\left[\frac{\partial^2\Psi}{\partial u_2^2}-\frac{1}{2}\left(\frac{1}{u_2-e_1}+\frac{1}{u_2-e_2}+\frac{1}{u_2-e_3}\right)\frac{\partial\Psi}{\partial u_2}\right]\right]\\&\quad+\left[\left(k_1^2-\frac{1}{4}\right)\frac{(e_1-e_2)(e_1-e_3)}{(u_1-e_1)(u_2-e_1)}+\left(k_2^2-\frac{1}{4}\right)\frac{(e_2-e_1)(e_2-e_3)}{(u_1-e_2)(u_2-e_2)}\right.\\&\quad\left.+\left(k_3^2-\frac{1}{4}\right)\frac{(e_3-e_2)(e_3-e_1)}{(u_1-e_3)(u_2-e_3)}\right]\Psi=2E\Psi.\end{aligned} \tag{70}$$

The separation equations are

$$(\rho-e_1)(\rho-e_2)(\rho-e_3)\left[\frac{\partial^2}{\partial\rho^2}+\frac{1}{2}\left(\frac{1}{\rho-e_1}+\frac{1}{\rho-e_2}+\frac{1}{\rho-e_3}\right)\frac{\partial\Psi}{\partial\rho}\right]-\left[\left(k_1^2-\frac{1}{4}\right)\frac{(e_1-e_2)(e_1-e_3)}{\rho-e_1}\right.$$
$$\left.+\left(k_2^2-\frac{1}{4}\right)\frac{(e_2-e_1)(e_2-e_3)}{\rho-e_2}+\left(k_3^2-\frac{1}{4}\right)\frac{(e_3-e_2)(e_3-e_1)}{\rho-e_3}+2E\rho+\mu\right]\Psi=0, \tag{71}$$

where $\rho=u_1, u_2$. The operator whose eigenvalue is μ is

$$L_2\Psi=\frac{-4}{(u_1-u_2)}\left[u_2\left[(u_1-e_1)(u_1-e_2)(u_1-e_3)\left[\frac{\partial^2\Psi}{\partial u_1^2}+\frac{1}{2}\left(\frac{1}{u_1-e_1}+\frac{1}{u_1-e_2}+\frac{1}{u_1-e_3}\right)\frac{\partial\Psi}{\partial u_1}\right]\right]\right.$$
$$-u_1\left[(u_2-e_1)(u_2-e_2)(u_2-e_3)\left[\frac{\partial^2\Psi}{\partial u_2^2}-\frac{1}{2}\left(\frac{1}{u_2-e_1}+\frac{1}{u_2-e_2}+\frac{1}{u_2-e_3}\right)\frac{\partial\Psi}{\partial u_2}\right]\right]$$
$$+\left[\left(k_1^2-\frac{1}{4}\right)\frac{(e_1-e_2)(e_1-e_3)}{(u_1-e_1)(u_2-e_1)}(u_1+u_2-e_1)+\left(k_2^2-\frac{1}{4}\right)\frac{(e_2-e_1)(e_2-e_3)}{(u_1-e_2)(u_2-e_2)}\right.$$
$$\left.\left.\times(u_1+u_2-e_2)+\left(k_3^2-\frac{1}{4}\right)\frac{(e_3-e_2)(e_3-e_1)}{(u_1-e_3)(u_2-e_3)}(u_1+u_2-e_3)\right]\Psi. \right. \tag{72}$$

Expressed in terms of coordinates on the sphere this has the form

$$L_2=e_3\left(s_1\frac{\partial}{\partial s_2}-s_2\frac{\partial}{\partial s_1}\right)^2+e_2\left(s_1\frac{\partial}{\partial s_3}-s_3\frac{\partial}{\partial s_1}\right)^2+e_1\left(s_3\frac{\partial}{\partial s_2}-s_2\frac{\partial}{\partial s_3}\right)^2+\left(\frac{1}{4}-k_1^2\right)\left[\frac{e_2s_2^2+e_3s_3^2}{s_1^2}\right.$$
$$\left.+e_1-e_2-e_3\right]+\left(\frac{1}{4}-k_2^2\right)\left[\frac{e_1s_1^2+e_3s_3^2}{s_2^2}+e_2-e_1-e_3\right]+\left(\frac{1}{4}-k_3^2\right)\left[\frac{e_2s_2^2+e_1s_1^2}{s_3^2}+e_3-e_2-e_1\right]. \tag{73}$$

The eigenfunctions Ψ can readily be calculated from the Schrödinger equation (67). In order to find the bound state solutions we try a solution of the form

$$\Psi=\left(\prod_{\ell=1}^{3}s_\ell^{k_\ell+1/2}\right)\prod_{j=1}^{q}\left(\frac{s_1^2}{\theta_j-e_1}+\frac{s_2^2}{\theta_j-e_2}+\frac{s_3^2}{\theta_j-e_3}\right) \tag{74}$$

(Ref. 19) and observe that

$$\frac{s_1^2}{\theta_j-e_1}+\frac{s_2^2}{\theta_j-e_2}+\frac{s_3^2}{\theta_j-e_3}=\frac{\Pi_{\ell=1}^2(u_\ell-\theta_j)}{\Pi_{m=1}^3(\theta_j-e_m)}.$$

For solutions, the zeros θ_p must satisfy the equations

$$\frac{k_1+1}{\theta_m-e_1}+\frac{k_2+1}{\theta_m-e_2}+\frac{k_3+1}{\theta_m-e_3}+\sum_{j\neq m}\frac{2}{\theta_m-\theta_j}=0, \tag{75}$$

and the eigenvalues E and μ in this case are

$$E=\tfrac{1}{2}(2q+2+k_1+k_2+k_3)^2-\tfrac{1}{8},$$

$$\mu=-2[k_1(e_2+e_3)+k_2(e_1+e_3)+k_3(e_2+e_1)+e_3k_1k_2+e_2k_1k_3+e_1k_2k_3]$$
$$-\frac{3}{2}(e_1+e_2+e_3)-4e_2e_3(k_1+1)\sum_{m=1}^{q}\frac{1}{(\theta_m-e_1)}-4e_1e_3(k_2+1)$$
$$\times\sum_{m=1}^{q}\frac{1}{(\theta_m-e_2)}-4e_2e_1(k_3+1)\sum_{m=1}^{q}\frac{1}{(\theta_m-e_3)}.$$

If we take the constants of the motion to be

$$H=M_{12}^2+M_{13}^2+M_{23}^2+\frac{k_1^2-\frac{1}{4}}{s_1^2}(s_2^2+s_3^2)+\frac{k_2^2-\frac{1}{4}}{s_2^2}(s_1^2+s_3^2)+\frac{k_3^2-\frac{1}{4}}{s_3^2}(s_2^2+s_1^2),$$

$$L_1=M_{12}^2+\left(k_1^2-\frac{1}{4}\right)\frac{s_2^2}{s_1^2}+\left(k_2^2-\frac{1}{4}\right)\frac{s_1^2}{s_2^2},$$

$$L_2=e_3M_{12}^2+e_2M_{13}^2+e_1M_{32}^2+\frac{k_1^2-\frac{1}{4}}{s_1^2}(e_3s_2^2+e_2s_3^2)+\frac{k_2^2-\frac{1}{4}}{s_2^2}(e_3s_1^2+e_1s_3^2)+\frac{k_3^2-\frac{1}{4}}{s_3^2}(e_1s_2^2+e_2s_1^2),$$

the corresponding defining relations are

$$L_{12}=\{L_1,L_2\}=4(e_1-e_2)\left[M_{12}M_{13}M_{32}-\left(k_1^2-\frac{1}{4}\right)\frac{s_3s_2}{s_1^2}M_{23}\right.$$
$$\left.-(k_2^2-\tfrac{1}{4})\frac{s_3s_1}{s_2^2}M_{31}-\left(k_3^2-\frac{1}{4}\right)\frac{s_1s_2}{s_3^2}M_{12}\right],$$

$$\begin{aligned}L_{12}^2=&-16L_1(e_2H+(e_3-e_2)L_1-L_2)(e_1H+(e_3-e_1)L_1-L_2)\\&-16\left(k_3^2-\frac{1}{4}\right)(e_1-e_2)^2L_1^2\\&-16\left(k_1^2-\frac{1}{4}\right)(e_2H+(e_3-e_2)L_1-L_2)^2\\&-16\left(k_2^2-\frac{1}{4}\right)(e_1H+(e_3-e_1)L_1-L_2)^2-\frac{4}{3}\prod_{\ell=1}^{3}\left(k_\ell^2-\frac{1}{4}\right)(e_1-e_2)^2,\end{aligned}\tag{76}$$

$$\{L_{12},L_1\}=-(8L_1+16)\left(k_2^2-\frac{1}{4}\right)(e_1H+(e_3-e_1)L_1-L_2)$$
$$-(8L_1+16)\left(k_1^2-\frac{1}{4}\right)(e_2H+(e_3-e_2)L_1-L_2),$$

$$\{L_{12},L_2\}=-8(e_2H+(e_3-e_2)L_1-L_2)(e_1H+(e_3-e_1)L_1-L_2)-8(e_2-e_3)L_1(e_1H+(e_3-e_1)L_1-L_2)-8(e_1-e_3)L_1(e_2H+(e_3-e_2)L_1-L_2)+16\left(\left(k_1^2-\frac{1}{4}\right)(e_3-e_2)+\left(k_2^2-\frac{1}{4}\right)(e_3-e_1)\right)L_2-16\left(\left(k_1^2-\frac{1}{4}\right)(e_3-e_2)^2+\left(k_2^2-\frac{1}{4}\right)\times(e_3-e_1)^2+\left(k_3^2-\frac{1}{4}\right)(e_1-e_2)^2\right)L_1+16e_1(e_1-e_3)\left(k_2^2-\frac{1}{4}\right)+16e_2(e_2-e_3)H.$$

(ii) The second potential on the sphere is

$$V_2=\frac{-\alpha s_3}{2\sqrt{s_1^2+s_2^2}}+\frac{1}{4\sqrt{s_1^2+s_2^2}}\left[\frac{k_1^2-\frac{1}{4}}{\sqrt{s_1^2+s_2^2}+s_1}+\frac{k_2^2-\frac{1}{4}}{\sqrt{s_1^2+s_2^2}-s_1}\right]. \tag{77}$$

In *polar coordinates* the Schrödinger equation has the form

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Psi}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2\Psi}{\partial\varphi^2}+\frac{\alpha\cos\theta}{\sin\theta}\Psi+\frac{1}{2\sin^2\theta}\left(\frac{\frac{1}{4}-k_1^2}{1+\cos\varphi}+\frac{\frac{1}{4}-k_2^2}{1-\cos\varphi}\right)\Psi=-2E\Psi.$$

This equation can be solved by a separation of variables via the substitution $\Psi=T(\theta)\Phi(\varphi)$, and the separation equations are

$$\frac{\partial^2\Phi}{\partial\varphi^2}+\frac{1}{2}\left(\frac{\frac{1}{4}-k_1^2}{1+\cos\varphi}+\frac{\frac{1}{4}-k_2^2}{1-\cos\varphi}\right)\Phi=-\lambda^2\Phi,$$

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial T}{\partial\theta}\right)+\frac{\alpha\cos\theta}{\sin\theta}T-\frac{\lambda^2}{\sin^2\theta}T=-2ET.$$

The solutions of the first equation are $\Phi_m^{(k_1,k_2)}(\varphi/2)$ [see (20)], where $\lambda^2=\frac{1}{4}(2m+k_1+k_2+1)^2$. The solution of the θ separation equation is given by

$$S_{nm}(\theta)=\frac{1}{\Gamma(2m+2+k_1+k_2)}\sqrt{\left(1+\frac{\alpha^2}{(n+m+1+\frac{1}{2}(k_1+k_2))^4}\right)\frac{\Gamma(n+2(m+1)+k_1+k_2)\Gamma(i\sigma+m+1+\frac{1}{2}(k_1+k_2))}{m!\Gamma(i\sigma+m+\frac{1}{2}(k_1+k_2))}}\times(2\sin\theta)^{m+1+(1/2)(k_1+k_2)}e^{i\theta(i\sigma-n)}{}_2F_1(-n,i\sigma+m+1+\tfrac{1}{2}(k_1+k_2);2m+2+k_1+k_2;1-e^{2i\theta}), \tag{78}$$

where $\sigma=\alpha/(n+m+1+\frac{1}{2}(k_1+k_2))$, and the orthonormal eigenfunctions are

$$\Psi=S_{nm}(\theta)\Phi_m^{(k_1,k_2)}\left(\frac{\varphi}{2}\right).$$

The operator which characterizes the separable solutions in this coordinate system is

$$L_1\Psi=\left[\left(s_1\frac{\partial}{\partial s_2}-s_2\frac{\partial}{\partial s_1}\right)^2+\left(\frac{1}{4}-k_1^2\right)\frac{\sqrt{s_1^2+s_2^2}}{2(\sqrt{s_1^2+s_2^2}+s_1)}+\left(\frac{1}{4}-k_2^2\right)\frac{\sqrt{s_1^2+s_2^2}}{2(\sqrt{s_1^2+s_2^2}-s_1)}\right]\Psi$$
$$=-\lambda^2\Psi.$$

For the second coordinate system we must choose a *variant of the standard elliptical coordinates*. A suitable choice is

$$s_1=\cos f\, x_1+\sin f\, x_3,\quad s_2=x_2,\quad s_3=-\sin f\, x_1+\cos f\, x_3,$$

where

$$x_i^2=\frac{(y_1-e_i)(y_2-e_i)}{(e_i-e_j)(e_i-e_k)},\quad i,j,k=1,2,3\quad\text{and } i,j,k\text{ pairwise distinct},\quad \sin f=\sqrt{\frac{e_2-e_1}{e_3-e_1}}.$$

To see how this works it is convenient to define the new variables E_+, E_-, Z_1, and Z_2 according to

$$e_1=e_2+\frac{1}{4}(E_++E_-)^2,\quad e_3=e_2+\frac{1}{4}(E_+-E_-)^2,$$

$$y_j=e_2+\frac{1}{4}(E_+^2+E_-^2)+\frac{1}{4}E_+E_-\left(Z_j+\frac{1}{Z_j}\right).$$

In terms of these variables Schrödinger's equation has the form

$$-\frac{4Z_1Z_2}{(Z_1-Z_2)(Z_1Z_2-1)}\left[(Z_1+\Omega_+)(Z_1+\Omega_-)Z_1\left[\frac{\partial^2\Psi}{\partial Z_1^2}+\frac{1}{2}\left(\frac{1}{Z_1+\Omega_+}+\frac{1}{Z_1+\Omega_-}+\frac{1}{Z_1}\right)\frac{\partial\Psi}{\partial Z_1}\right]\right.$$
$$\left.-(Z_2+\Omega_+)(Z_2+\Omega_-)Z_2\left[\frac{\partial^2\Psi}{\partial Z_2^2}+\frac{1}{2}\left(\frac{1}{Z_2+\Omega_+}+\frac{1}{Z_2+\Omega_-}+\frac{1}{Z_2}\right)\frac{\partial\Psi}{\partial Z_2}\right]\right]$$
$$+\left[\frac{2i\alpha(Z_1Z_2+1)}{(Z_1Z_2-1)}+\left(k_1^2-\frac{1}{4}\right)\frac{(1-\Omega_-^2)Z_1Z_2}{(Z_1Z_2-1)(Z_2+\Omega_+)(Z_1+\Omega_+)}\right.$$
$$\left.+\left(k_2^2-\frac{1}{4}\right)\frac{(1-\Omega_+^2)Z_1Z_2}{(Z_1Z_2-1)(Z_2+\Omega_-)(Z_1+\Omega_-)}\right]\Psi=-2E\Psi,\tag{79}$$

where $\Omega_+=E_+/E_-$ and $\Omega_-=E_-/E_+$, so $\Omega_+\Omega_-=1$. The separation equations are

$$4(Z_j+\Omega_+)(Z_j+\Omega_-)Z_j\left[\frac{\partial^2\Psi}{\partial Z_j^2}+\frac{1}{2}\left(\frac{1}{Z_j+\Omega_+}+\frac{1}{Z_j+\Omega_-}+\frac{1}{Z_j}\right)\frac{\partial\Psi}{\partial Z_j}\right]$$
$$+\left[2(-i\alpha+E)Z_j+2(i\alpha+E)\frac{1}{Z_j}+\frac{(k_1^2-\frac{1}{4})(\Omega_-^2-1)}{Z_j+\Omega_-}+\frac{(k_2^2-\frac{1}{4})(\Omega_+^2-1)}{Z_j+\Omega_+}+\mu\right]\Psi=0.$$

In terms of the variables Z_j the operator which describes the separation is

$$L_2\Psi=\frac{4}{(Z_1-Z_2)(Z_1Z_2-1)}\Bigg[-(Z_2+1)Z_1(Z_1+\Omega_+)(Z_1+\Omega_-)$$
$$\times\left[\frac{\partial^2\Psi}{\partial Z_1^2}+\frac{1}{2}\left(\frac{1}{Z_1+\Omega_+}+\frac{1}{Z_1+\Omega_-}+\frac{1}{Z_1}\right)\frac{\partial\Psi}{\partial Z_1}\right]$$
$$+(Z_1+1)Z_2(Z_2+\Omega_+)(Z_2+\Omega_-)\left[\frac{\partial^2\Psi}{\partial Z_2^2}+\frac{1}{2}\left(\frac{1}{Z_2+\Omega_+}+\frac{1}{Z_2+\Omega_-}+\frac{1}{Z_2}\right)\frac{\partial\Psi}{\partial Z_2}\right]\Bigg]$$
$$+\left[\frac{(1-\Omega_-^2)(Z_1Z_2(Z_1+Z_2)+\Omega_-(Z_1Z_2-1))}{(Z_1Z_2-1)(Z_1+\Omega_-)(Z_2+\Omega_-)}\left(k_1^2-\frac{1}{4}\right)\right.$$
$$\left.+\frac{(1-\Omega_+^2)(Z_1Z_2(Z_1+Z_2)+\Omega_+(Z_1Z_2-1))}{(Z_1Z_2-1)(Z_1+\Omega_+)(Z_2+\Omega_+)}\left(k_2^2-\frac{1}{4}\right)+\frac{4i\alpha(Z_1+Z_2)}{Z_1Z_2-1}\right]\Psi. \tag{80}$$

Indeed if we consider the elliptical coordinates

$$U_3^2=Z_1Z_2,\quad U_1^2=\frac{(Z_1+\Omega_-)(Z_2+\Omega_-)}{\Omega_-^2-1},\quad U_2^2=\frac{(Z_1+\Omega_+)(Z_2+\Omega_+)}{\Omega_+^2-1}, \tag{81}$$

then putting $k_3=\sqrt{\frac{1}{4}+2(E-i\alpha)}$ and $\widetilde{E}=i\alpha+E$ and multiplying the Schrödinger equation by $(1/Z_1Z_2-1)$ we see that the resulting equation has the form

$$H\Psi=\frac{\partial^2\Psi}{\partial U_1^2}+\frac{\partial^2\Psi}{\partial U_2^2}+\frac{\partial^2\Psi}{\partial U_3^2}-\left(U_1\frac{\partial}{\partial U_1}+U_2\frac{\partial}{\partial U_2}+U_3\frac{\partial}{\partial U_3}\right)^2\Psi$$
$$-\left(U_1\frac{\partial\Psi}{\partial U_1}+U_2\frac{\partial\Psi}{\partial U_2}+U_3\frac{\partial\Psi}{\partial U_3}\right)+\left[\frac{\frac{1}{4}-k_1^2}{U_1^2}+\frac{\frac{1}{4}-k_2^2}{U_2^2}+\frac{\frac{1}{4}-k_3^2}{U_3^2}\right]\Psi+2\widetilde{E}\Psi=0. \tag{82}$$

We recognize this as Eq. (67) that we obtained in the case of the potential V_1. Thus the solutions are of the form

$$\Psi=\left(\prod_{\ell=1}^{3}U_\ell^{k_\ell+1/2}\right)\prod_{j=1}^{q}\left(\frac{U_1^2}{\theta_j-e_1}+\frac{U_2^2}{\theta_j-e_2}+\frac{U_3^2}{\theta_j-e_3}\right). \tag{83}$$

The zeros θ_p satisfy the equations

$$\frac{k_1+1}{\theta_m+\Omega_-}+\frac{k_2+1}{\theta_m+\Omega_+}+\frac{\sqrt{\frac{1}{4}+2(E-i\alpha)}+1}{\theta_m}+\sum_{j\neq m}\frac{2}{\theta_m-\theta_j}=0, \tag{84}$$

and the eigenvalues E and μ are determined by

$$E=\frac{1}{2}\left(2q+2+k_1+k_2+\sqrt{\frac{1}{4}+2(E-i\alpha)}\right)^2-\frac{1}{8},$$

$$\begin{aligned}\mu=&2\left[\Omega_-\left(k_2+\sqrt{\frac{1}{4}+2(E-i\alpha)}\right)+\Omega_+\left(k_1+\sqrt{\frac{1}{4}+2(E-i\alpha)}\right)\right]\\&+2[\Omega_+k_1+\Omega_-k_2]\sqrt{\frac{1}{4}+2(E-i\alpha)}+\frac{3}{2}(\Omega_++\Omega_-)+\sqrt{\frac{1}{4}+2(E-i\alpha)}\\&\times\left[4\Omega_+(k_1+1)\sum_{m=1}^{q}\frac{1}{(\theta_m+\Omega_-)}+4\Omega_-(k_2+1)\sum_{m=1}^{q}\frac{1}{(\theta_m+\Omega_+)}\right]\\&-4\Omega_+\Omega_-\left(\sqrt{\frac{1}{4}+2(E-i\alpha)}+1\right)\sum_{m=1}^{q}\frac{1}{\theta_m}.\end{aligned}\tag{85}$$

The classical constants of the motion associated with this potential are

$$\begin{aligned}H=&-\frac{4Z_1Z_2}{(Z_1-Z_2)(Z_1Z_2-1)}[(Z_1+\Omega_+)(Z_1+\Omega_-)Z_1P_{Z_1}^2-(Z_2+\Omega_+)(Z_2+\Omega_-)Z_2P_{Z_2}^2]\\&+\left[\frac{2i\alpha(Z_1Z_2+1)}{(Z_1Z_2-1)}+\left(k_1^2-\frac{1}{4}\right)\frac{(1-\Omega_-^2)Z_1Z_2}{(Z_1Z_2-1)(Z_2+\Omega_+)(Z_1+\Omega_+)}\right.\\&\left.+\left(k_2^2-\frac{1}{4}\right)\frac{(1-\Omega_+^2)Z_1Z_2}{(Z_1Z_2-1)(Z_2+\Omega_-)(Z_1+\Omega_-)}\right],\end{aligned}$$

$$\begin{aligned}L_2=&\frac{4}{(Z_1-Z_2)(Z_1Z_2-1)}[-(Z_2+1)Z_1(Z_1+\Omega_+)(Z_1+\Omega_-)P_{Z_1}^2\\&+(Z_1+1)Z_2(Z_2+\Omega_+)(Z_2+\Omega_-)P_{Z_2}^2]\\&+\frac{(1-\Omega_-^2)(Z_1Z_2(Z_1+Z_2)+\Omega_-(Z_1Z_2-1))}{(Z_1Z_2-1)(Z_1+\Omega_-)(Z_2+\Omega_-)}\left(k_1^2-\frac{1}{4}\right)\\&+\frac{(1-\Omega_+^2)(Z_1Z_2(Z_1+Z_2)+\Omega_+(Z_1Z_2-1))}{(Z_1Z_2-1)(Z_1+\Omega_+)(Z_2+\Omega_+)}\left(k_2^2-\frac{1}{4}\right)+\frac{4i\alpha(Z_1+Z_2)}{Z_1Z_2-1}\\=&(\Omega_++\Omega_-)(M_{12}^2-M_{13}^2-M_{23}^2)-2i(\Omega_--\Omega_+)M_{12}M_{13}+\left[\frac{\Omega_+(s_3-is_1)+\Omega_-(s_3+is_1)}{\sqrt{s_1^2+s_2^2}}\right]\alpha\\&+\frac{k_1^2-\frac{1}{4}}{2(\sqrt{s_1^2+s_2^2}+s_1)}\left[\frac{\Omega_+(s_3-is_1)+\Omega_-(s_3+is_1)}{\sqrt{s_1^2+s_2^2}(\sqrt{s_1^2+s_2^2}-s_3)}+\Omega_-(\sqrt{s_1^2+s_2^2}+is_3)\right]\\&+\frac{k_2^2-\frac{1}{4}}{2(\sqrt{s_1^2+s_2^2}-s_1)}\left[\frac{\Omega_+(s_3-is_1)+\Omega_-(s_3+is_1)}{\sqrt{s_1^2+s_2^2}(\sqrt{s_1^2+s_2^2}-s_3)}+\Omega_+(\sqrt{s_1^2+s_2^2}+is_3)\right],\end{aligned}$$

$$L_1=-\frac{(Z_1+\Omega_+)(Z_1+\Omega_-)(Z_2+\Omega_+)(Z_2+\Omega_-)}{(Z_1-Z_2)^2}(Z_1P_{Z_1}-Z_2P_{Z_2})^2$$
$$+\frac{1}{4}\left(k_2^2-\frac{1}{4}\right)\frac{(\Omega_+^2-1)(Z_1Z_2-1)}{(Z_1+\Omega_+)(Z_2+\Omega_+)}+\frac{1}{4}\left(k_1^2-\frac{1}{4}\right)\frac{(\Omega_-^2-1)(Z_1Z_2-1)}{(Z_1+\Omega_-)(Z_2+\Omega_-)}$$
$$=M_{12}^2-\frac{1}{2}\left[\frac{\sqrt{s_1^2+s_2^2}}{\sqrt{s_1^2+s_2^2}+s_1}\left(k_1^2-\frac{1}{4}\right)+\frac{\sqrt{s_1^2+s_2^2}}{\sqrt{s_1^2+s_2^2}-s_1}\left(k_2^2-\frac{1}{4}\right)\right].$$

The corresponding defining relations for the quadratic algebra are

$$L_{12}^2=-64L_1^2-4(\Omega_++\Omega_-)^2H^2L_1+64HL_2^2+16(\Omega_++\Omega_-)L_3L_2^2-4L_1L_2^2-8(\Omega_++\Omega_-)L_1L_2H$$
$$+(\Omega_+-\Omega_-)-4(\Omega_-(4k_1^2-1)-\Omega_+(4k_2^2-1))L_1^2-4(\Omega_-(1-k_2^2-3k_1^2)$$
$$-\Omega_+(1-k_1^2-3k_2^2))HL_1+4(k_1^2-k_2^2)L_1L_2-4i\alpha(k_1^2-k_2^2)L_2+8i\alpha(\Omega_-(k_2^2-k_1^2-2i\alpha)$$
$$+\Omega_+(k_1^2-k_2^2+2i\alpha))L_1-(k_1^2-k_2^2)(\Omega_-(k_2^2-k_1^2+4i\alpha)+\Omega_+(k_1^2-k_2^2+4i\alpha))H$$
$$+2i\alpha(\Omega_+-\Omega_-)((k_1^2-k_2^2)^2+2i\alpha(2(k_1^2+k_2^2)-1)),$$

$$\{L_{12},L_1\}=8(\Omega_++\Omega_-)L_1^2-4L_1L_2-4(\Omega_++\Omega_-)L_1H+2(k_1^2-k_2^2)L_1$$
$$-2i\alpha(k_1^2-k_2^2)(\Omega_+-\Omega_-), \tag{86}$$

$$\{L_{12},L_2\}=-2(\Omega_++\Omega_-)^2H^2-96L_1^2-2L_2^2+16L_2L_1-4(\Omega_++\Omega_-)L_2H-2L_1H(\Omega_+-\Omega_-)$$
$$\times[\Omega_+(k_1^2+3k_2^2-1)-\Omega_-(k_2^2+3k_1^2-1)]H-4(\Omega_+(1-4k_2^2)-\Omega_+(1-4k_2^2))L_1$$
$$+4i\alpha((k_1^2-k_2^2)(\Omega_+-\Omega_-)+2i\alpha(\Omega_+-\Omega_-)).$$

IV. THE *n*-DIMENSIONAL ISOTROPIC OSCILLATOR

It is well known that the quantum isotropic harmonic oscillator can be solved by the method of separation of variables in a number of coordinate systems, including Cartesian coordinates and elliptical coordinates (see, e.g., Refs. 25 and 26). We present a new derivation of the eigenfunctions associated with *elliptic coordinates*. We will adopt the convention of defining this equation by

$$H\Psi=[-\tfrac{1}{2}\Delta+\tfrac{1}{2}\omega^2(x_1^2+\cdots+x_n^2)]\Psi=E\Psi, \tag{87}$$

where $\Delta=\partial_{x_1}^2+\cdots+\partial_{x_n}^2$. Elliptical coordinates in Euclidean n space are defined by

$$x_j^2=\frac{\Pi_{\ell=1}^n(u_\ell-e_j)}{\Pi_{k\neq j}(e_k-e_j)} \tag{88}$$

for $e_1<u_1<e_2<\cdots<e_n<u_n$. To obtain polynomial solutions of this equation in these coordinates we note the identity

$$\sum_{k=1}^n\frac{x_k^2}{\theta-e_k}-1=-\frac{\Pi_{h=1}^n(\theta-u_h)}{\Pi_{\ell=1}^n(\theta-e_\ell)}.$$

If we rewrite Eq. (87) in terms of Φ where $\Psi=\exp[-1/2\omega^2r^2]\Phi$ and r is the radial coordinate, we obtain the eigenvalue equation

$$\left[\Delta-2\omega\left(\sum_{m=1}^{n} x_m\,\partial_{x_m}\right)-n\omega\right]\Phi=-2E\Phi. \tag{89}$$

Note that the operator on the left-hand side maps polynomials in the variables x_j to polynomials, without increasing the order. For this equation we look for solutions of the form

$$\Phi=\prod_{\ell=1}^{q} x_\ell^{\alpha_\ell}\zeta(x_1,\ldots,x_n),$$

where $\alpha_\ell=0$ or 1. The equation for ζ is then

$$\left[\Delta+\sum_{m=1}^{n}\left(\frac{2\alpha_m}{x_m}\,\partial_{x_m}-2\omega x_m\partial_{x_m}\right)\right]\zeta=\left(-2E+n\omega+2\omega\sum_{\ell=1}^{n}\alpha_\ell\right)\zeta.$$

We now look for solutions of the form

$$\zeta=\prod_{m=1}^{q}\left[\sum_{k=1}^{n}\frac{x_k^2}{\theta_m-e_k}-1\right]. \tag{90}$$

Substituting this ansatz into the equation for ζ we obtain the requirements

$$\sum_{k=1}^{n}\frac{1+2\alpha_k}{\theta_\ell-e_k}+\sum_{j\neq\ell}\frac{4}{\theta_\ell-\theta_j}=-2\omega,\quad E=\omega\left(2m+\frac{n}{2}+\sum_{p=1}^{n}\alpha_p\right). \tag{91}$$

The operators which describe the separation constants are

$$\Lambda_j=\sum_{k\neq\ell}S_{j-1}^{k\ell}M_{kl}^2+\sum_{\ell\neq j}S_j^{\ell}Q_{\ell\ell},\quad j=1,\ldots,n-1,$$

where $M_{k\ell}=x_k\partial_{x_\ell}-x_\ell\partial_{x_k}$, and

$$Q_{ik}=\partial_{x_i}\partial_{x_k}-\omega^2x_ix_k,\quad S_j^{kl}=\frac{1}{j!}\sum_{i_1,\ldots,i_j}e_{i_1}\cdots e_{i_j},$$

where $i_m\neq i_{m'}$, $i_m\neq k,l$ for $m\neq m'$ and $m,m'=1\cdots j$, and

$$S_j^k=S_j^k[e_1,\ldots,e_n]=\frac{1}{j!}\sum_{i_1,\ldots,i_j}e_{i_1}\cdots e_{i_j},\quad i_1,\ldots,i_j \text{ pairwise distinct},$$

where $i_m\neq i_{m'}$, $i_m\neq k$ for $m\neq m'$ and $m,m'=1\cdots j$. In coordinate form these operators are

$$\Lambda_j=\sum_{k=1}^{n}\frac{S_j^k[u_1,\ldots,u_n]}{\Pi_{\ell\neq k}(u_\ell-u_k)}\left(4\sqrt{\Pi_{\ell=1}^{n}(u_k-e_\ell)}\,\partial_{u_k}\sqrt{\Pi_{\ell=1}^{n}(u_k-e_\ell)}\,\partial_{u_k}-\omega^2\Pi_{\ell=1}^{n}(u_k-e_\ell)\right). \tag{92}$$

They have the eigenvalues

$$\sum_{\ell}S_j^{\ell}\left[\omega(2\alpha_\ell+1)-\sum_{m=1}^{q}\frac{2(\alpha_\ell+1)}{\theta_m-e_\ell}\right]. \tag{93}$$

These operators form a closed algebra under the commutation relations

$$[M_{kl},\ M_{ij}]=M_{lj}\delta_{ki}+M_{ki}\delta_{lj}-M_{kj}\delta_{li}-M_{li}\delta_{kj},$$

$$[Q_{ik},\ Q_{jl}]=\omega^2[M_{ij}\delta_{lk}+M_{il}\delta_{jk}+M_{kj}\delta_{li}+M_{kl}\delta_{ji}],$$

$$[Q_{ik},\ M_{jl}]=Q_{ij}\delta_{kl}+Q_{kj}\delta_{il}+Q_{il}\delta_{kj}+Q_{kl}\delta_{ij}.$$

The eigenfunctions can be normalized by using their representation in terms of Cartesian coordinates. For the assumed form of the eigenfunctions given above the norm N is readily calculated to be

$$N^2=\sum_{p=0}^{n}\sum_{s_{i_1}s_{i_2},\ldots,s_{i_p}}\sum_{i_1,\ldots,i_p\neq}(-1)^q\omega^{-(n/2+\Sigma_{h=1}^{n}\alpha_h)}$$
$$\times\frac{\Pi_{j=1}^{p}[(-\omega)^{-A_{i_j}}\Gamma(\alpha_{i_j}+s_{i_j}+\tfrac{1}{2})]\Pi_{k=p+1}^{n}\Gamma(\alpha_{i_k}+\tfrac{1}{2})}{\Pi_{r=1}^{p}\Pi_{\not r}^{s_{i_r}}(\theta_{i_r\not r}-e_{i_r})},\tag{94}$$

where $0\leqslant s_{i_j}\leqslant 2q$, $0\leqslant\Sigma_{j=1}^{p}s_{i_j}\leqslant 2q$, $0\leqslant p\leqslant n$. Each of the s_{i_j} are integers, $\theta_{i_r\not r}\in\{\theta_1,\ldots,\theta_m\}$ and $\theta_{i_r\not r}\neq\theta_{j_w\not w}$ if $i_r\neq j_w$, and if i_r is fixed then at most two $\theta_{i_r\not r}$ can be equal. From these results we have the satisfactory situation that both the eigenvalues and the normalizations can be computed in terms of the zeros $\theta_1,\ldots,\theta_m$.

As an example of the simplest normalized eigenfunction we give the following:

$$\Psi=\sqrt{\frac{\omega}{\pi}}\left[\frac{3}{4\omega^2}\left(\frac{1}{(\theta-e_1)^2}+\frac{1}{(\theta-e_2)^2}\right)+\frac{1}{2\omega^2(\theta-e_1)(\theta-e_2)}+1\right]^{-1/2}$$
$$\times e^{-(x^2+y^2)/2}\left[\frac{x^2}{\theta-e_1}+\frac{y^2}{\theta-e_2}-1\right].$$

For this eigenfunction the varable θ is a solution of

$$\frac{1}{(\theta-e_1)}+\frac{1}{(\theta-e_2)}=0,$$

i.e., $\theta=(e_1+e_2)/2$. If we substitute this into the above equations we obtain

$$\Psi=\sqrt{\frac{\omega}{\pi}}\left[\left(\frac{2}{\omega(e_1-e_2)}\right)^2+1\right]^{-1/2}e^{-\omega(x^2+y^2)/2}\left[\frac{2(x^2-y^2)}{(e_2-e_1)}-1\right].$$

The orthonormalized eigenfunctions calculated in this way form a complete set.

In this paper we have established that once the zeros of a given set of special eigenfunctions, which are essentially polynomials, are known, then all the other properties such as normalization and eigenvalues can be determined from them in terms of algebraic expressions.

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Multiplicity, invariants, and tensor product decompositions of compact groups

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Decomposing tensor products of irreducible representations of compact groups almost always involves multiplicity, wherein some irreducible representations occur more than once in the direct sum decomposition. We show that the multiplicity can always be specified by polynomial group invariants. The setting is a Bargmann–Segal–Fock space in $n\times N$ complex variables, where n is the number of labels needed to specify the tensor product and N is the dimension of the fundamental representation of the compact group. Both the tensor product and direct sum bases are realized as polynomials in this space, and it is shown how Clebsch–Gordan and Racah coefficients can be computed by suitably differentiating these polynomials. The example of SU(N) is discussed in detail, and it is shown that the multiplicity can be computed as the solution of certain diophantine equations arising from powers of group invariants, namely minors of determinants. © *1996 American Institute of Physics.* [S0022-2488(96)02711-9]

I. INTRODUCTION

Clebsch–Gordan and Racah coefficients for SU(2) are well known, and closed form expressions for them are available, as well as programs for explicitly evaluating any desired coefficients. For other compact groups much less is known about these coefficients. Some procedures and partial results for SU(3) have been published,[1–3] but beyond this almost nothing is known. In this paper we will present techniques for calculating Clebsch–Gordan and Racah coefficients for arbitrary tensor products of the compact groups, using Bargmann space techniques developed in earlier papers.[4]

The general problem can be stated as follows. Given a compact G, whose irreducible representations are all assumed known, choose a basis $|\lambda,\xi\rangle$ in the irreducible representation space V^{λ}. Form the p-fold tensor product $\lambda_1\otimes\lambda_2\otimes\cdots\otimes\lambda_p$ and calculate the number of times the irreducible representation λ occurs in the tensor product. There are a number of ways for computing this multiplicity, but most of them are rather long and tedious. We will show a relatively simple way for computing this multiplicity, as solutions of diophantine equations arising from group invariants. In any event we assume the multiplicity is known. Next choose a (possibly new) basis in V^{λ}, say $|\lambda,\zeta\rangle$; then the Clebsch–Gordan coefficients are the overlap between the tensor product basis and the direct sum basis in the tensor product decomposition, namely $\langle\lambda_1\xi_1\cdots\lambda_p\xi_p|\lambda\zeta\eta\rangle$. Similarly, the Racah coefficients are the overlap between direct sum bases with different multiplicity labels: $\langle\lambda\zeta\eta'|\lambda\zeta\eta\rangle$. Here η and η' are multiplicity labels, that is, labels that distinguish the equivalent representations. For SU(2) the Clebsch–Gordan and Racah coefficients are reasonably well known for $p=3,4,5$, when η refers to a stepwise coupling set of labels, generated by intermediate angular momenta, in which case the Racah coefficients are called $6J$, $9J$, $12J$, etc. symbols.

If $\lambda_1=\lambda_2=\cdots=\lambda_p$, a new symmetry occurs, a permutation symmetry that can be used to help label the multiplicity. Moreover, it is often desirable to have coefficients that have definite per-

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mutation symmetry; we will show that such permutation symmetry arises naturally using the techniques presented in this paper.

Our procedure for computing Clebsch–Gordan and Racah coefficients is as follows: we realize all irreducible representations of G on Bargmann space; in particular, the states $|\lambda,\xi\rangle$ are realized as polynomials $f_{|\lambda,\xi\rangle}(Z)$ of a multicomponent complex variable Z. The tensor product states can then also be realized as polynomials $|\lambda_1,\xi_1,\ldots,\lambda_p,\xi_p\rangle \rightarrow f_{|\lambda_1,\xi_1,\ldots,\lambda_p,\xi_p\rangle}(Z)$. The problem is how to realize the state $|\lambda,\zeta,\eta\rangle$ as a polynomial. If this were known, using the differentiation inner product [see Eq. (2.1)] in Bargmann space, the Clebsch–Gordan coefficients would be

$$\langle \lambda_1,\xi_1,\ldots,\lambda_p,\xi_p|\lambda,\zeta,\eta\rangle = f^*_{|\lambda\zeta\eta'\rangle}(D) f_{|\lambda\zeta\eta\rangle}(Z)|_{Z=0}$$

and the Racah coefficients

$$\langle \lambda,\zeta,\eta'|\lambda,\zeta,\eta\rangle = f^*_{|\lambda\eta'\rangle}(D) f_{|\lambda\zeta\eta\rangle}(Z)|_{Z=0}.$$

The Racah coefficients are actually basis independent, so that the basis element ζ can be conveniently chosen as the highest weight. Though the Clebsch–Gordan coefficients are not basis independent, it often suffices to compute these coefficients for the highest weight and then get the other coefficients using raising and lowering operators from the Lie algebra of G. However, the techniques discussed in the next sections allow one to calculate Clebsch–Gordan coefficients directly in any basis of interest.

Our strategy for realizing $|\lambda,\zeta,\eta\rangle$ as a polynomial is as follows: instead of computing the number of times λ occurs in the tensor product $\lambda_1\otimes\cdots\otimes\lambda_p$ we look at what is equivalent, namely the number of times the identity representation occurs in the augmented tensor product $\lambda_1\otimes\cdots\otimes\lambda_p\otimes\lambda^{\surd}$, where $\lambda^{\surd}$ is the contragradient representation of λ. For completeness we show in Sec. II that these multiplicities are the same; that is,

$$\#(\lambda\subset\lambda_1\otimes\cdots\otimes\lambda_p)=\#(1\subset\lambda_1\otimes\cdots\otimes\lambda_p\otimes\lambda^{\surd}),$$

where # means ''number of times.'' Shifting the problem to a study of the multiplicity of the identity representation means that the full power of invariant theory can be brought to bear on computing $f_{|\lambda\zeta\eta\rangle}(Z)$.

Assume that a set of functionally independent invariants $I_\eta(Z,W)$ in the augmented tensor product space is known [i.e., $I_\eta(Zg,Wg)=I_\eta(Z,W)$ for all $g\in G$]. Then as will be shown in Sec. II, the polynomial $f^*_{|\lambda^{\surd}\zeta^{\surd}\rangle}(D_w)I_\eta(Z,W)_{W=0}$ transforms under G as the polynomial $f_{|\lambda\zeta\eta\rangle}(Z)$ and, if properly normalized, can be used to calculate the Clebsch–Gordan and Racah coefficients of G.

The goal of this paper is to prove these theorems (Sec. II) and then apply them to $G=\mathrm{SU}(N)$ (Sec. III), where use is made of the fact that all $\mathrm{SU}(N)$ invariants are minors of determinants. The invariants $I_\eta(Z,W)$ are then products of minors of determinants with certain transformation properties.

Finally in Sec. IV we give a number of examples to demonstrate the power and generality of our methods. These examples show that although we cannot calculate closed form expressions for Clebsch–Gordan and Racah coefficients, we have reduced the computation of these coefficients to solving linear diophantine equations and differentiating certain polynomials. With the availability of symbolic manipulation computer programs, this is almost equivalent to having closed form expressions.

II. GENERAL THEORY

Let $\mathbb{C}^{n\times N}$ denote the vector space of all $n\times N$ complex matrices. If $Z=(Z_{ij})$ is an element of $\mathbb{C}^{n\times N}$, let Z^* denote its complex conjugate and write $Z_{ij}=X_{ij}+\sqrt{-1}Y_{ij}$; $1\leqslant i\leqslant n$, $1\leqslant j\leqslant N$. If dX_{ij} (resp. dY_{ij}) denotes Lebesque measure on $\mathbb{R}$, we let dZ denote the Lebesque product measure on $\mathbb{R}^{nN}$. Define a Gaussian measure $d\mu$ on $\mathbb{C}^{n\times N}$ by

$$d\mu(Z)=\pi^{-nN}\exp[-\mathrm{tr}(ZZ^{\dagger})]dZ,$$

where tr denotes the trace of a matrix and $Z^{\dagger}$ is the transpose of Z^*.

A function $f:\mathbb{C}^{n\times N}\to\mathbb{C}$ is *holomorphic square integrable* if it is holomorphic on the entire domain $\mathbb{C}^{n\times N}$, and if

$$\int_{\mathbb{C}^{n\times N}}|f(Z)|^2 d\mu(Z)<\infty.$$

Clearly the holomorphic square-integrable functions form a Hilbert space, the *Bargmann–Segal–Fock space*, with respect to the inner product

$$\langle f_1|f_2\rangle=\int_{\mathbb{C}^{n\times N}}f_1^*(Z)f_2(Z)d\mu(Z).$$

Let $\mathscr{F}\equiv\mathscr{F}(\mathbb{C}^{n\times N})$ denote this Hilbert space. From Ref. 4 this inner product also can be defined by the following formula:

$$\langle f_1|f_2\rangle=f_1^*(D)f_2(Z)|_{Z=0}, \tag{2.1}$$

where $f(D)$ is the differential operator obtained by formally replacing Z_{ij} by the partial derivative $\partial/\partial Z_{ij}$ $(1\leqslant i\leqslant n,\ 1\leqslant j\leqslant N)$. It follows that the representation R of $U(N)$ of $\mathscr{F}$ defined by $[R(g)f](Z)=f(Zg)$, $g\in U(N)$, is unitary.

Let G be a closed subgroup of $\mathrm{SU}(N)$ [the important cases are the classical groups $G=\mathrm{SU}(N)$, $\mathrm{SO}(N)$, or $\mathrm{Sp}(N)$, N even for the latter]. Then by the Borel–Weil theorem an irreducible representation R^{λ} of G of signature λ can be realized on a space of polynomial functions V^{λ} that can be embedded in $\mathscr{F}$ where G acts by right translation on V^{λ}. Since G is a closed subgroup of $\mathrm{SU}(N)$, the contragradient (or in this case complex conjugate) of the representation R^{λ} can also be realized on a subspace of polynomial functions V^{λ^*} of $\mathscr{F}$ [for example, if $G=\mathrm{SU}(3)$, $\lambda=(4,1,0)$ then $\lambda^*=(4,3,0)$].

A polynomial function $f\in\mathscr{F}$ is said to be G-invariant if $R(g)f=f$ for all $g\in G$. The following theorem relates the multiplicity of an irreducible representation R^{λ} in the p-fold tensor product $V^{\lambda_1}\otimes\cdots\otimes V^{\lambda_p}\subset\mathscr{F}$ with the G-invariant polynomial functions in $\mathscr{F}$.

Theorem 2.1: *Let G be a closed subgroup of* $\mathrm{SU}(N)$ *and let $(R^{\lambda},V^{\lambda})$ denote an irreducible representation of G with signature λ. Then the multiplicity of the irreducible representation R^{λ} in the tensor product $V^{\lambda_1}\otimes\cdots\otimes V^{\lambda_p}\subset\mathscr{F}$ is equal to the dimension of the G-invariant subspace in $V^{\lambda_1}\otimes\cdots\otimes V^{\lambda_p}\otimes V^{\lambda^*}\subset\mathscr{F}$.*

Proof: To prove the theorem we use the following well-known fact which we prove for the sake of completeness.

Lemma 2.2: Let G be a compact group and let ρ_i, $i=1,2$, be irreducible unitary representations of G on the Hilbert spaces H_i, $i=1,2$, respectively. Then the identity representation of G occurs in $\rho_1\otimes\rho_2^*|G$ (with multiplicity exactly 1) if and only if ρ_1 is equivalent to ρ_2.

Proof of the lemma: If ρ is a representation of G, let χ_{ρ} denote the character of ρ. Let I denote the identity representation of G. For all $g\in G$ it is well known that $\chi_I(g)=1$ and $\chi_{\rho_1\otimes\rho_2^*}(g,g)$

$= \chi_{\rho_1}(g)\chi_{\rho_2^*}(g)$. If $[\rho\otimes\rho^*|_G : I]$ denotes the multiplicity of the identity representation in $\rho_1 \otimes \rho_2^*|_G$, then the Schur orthogonality relations for compact groups imply that

$$[\rho_1\otimes\rho_2^*|_G : I] = \int_G \chi_{\rho_1\otimes\rho_2^*}(g,g)\chi_I^*(g)dg,$$

where dg denotes the normalized Haar measure of G. However, as remarked above, we have

$$\int_G \chi_{\rho_1\otimes\rho_2^*}(g,g)\chi_I^*(g)dg = \int_G \chi_{\rho_1}(g)\chi_{\rho_2^*}(g)dg,$$

which, again by the Schur orthogonality relations, is equal to

$$\delta_{\rho_1,\rho_2} = \begin{cases} 1 & \text{if } \rho_1 \approx \rho_2, \\ 0 & \text{if } \rho_1 \not\approx \rho_2. \end{cases}$$

This achieves the proof of the lemma.

From the lemma it follows immediately by iteration that the multiplicity of R^λ in $V^{\lambda_1} \otimes \cdots \otimes V^{\lambda_p}$ is equal to the multiplicity of the identity representation I in $V^{\lambda_1} \otimes \cdots \otimes V^{\lambda_p} \otimes V^{\lambda^*}$. Since $V^{\lambda_1} \otimes \cdots \otimes V^{\lambda_p} \otimes V^{\lambda^*}$ consists of polynomial functions in $\mathscr{F}$ and G acts on $V^{\lambda_1} \otimes \cdots \otimes V^{\lambda_p} \otimes V^{\lambda^*}$ by right translation, it follows that the identity representation occurs in $V^{\lambda_1} \otimes \cdots \otimes V^{\lambda_p} \otimes V^{\lambda^*}$ if and only if there exist polynomial functions $f \in V^{\lambda_1} \otimes \cdots \otimes V^{\lambda_p} \otimes V^{\lambda^*}$ such that $R^\lambda(g)f = R(g)f = f$ for all $g \in G$, i.e., f is G-invariant. Each of these polynomial functions f spans a one-dimensional subspace of $V^{\lambda_1} \otimes \cdots \otimes V^{\lambda_p} \otimes V^{\lambda^*}$. This implies immediately that the dimension of the G-invariant subspace of $V^{\lambda_1} \otimes \cdots \otimes V^{\lambda_p} \otimes V^{\lambda^*}$ is equal to the multiplicity of R^λ in $V^{\lambda_1} \otimes \cdots \otimes V^{\lambda_p}$.

The next theorem will give us a very simple way to compute Clebsch–Gordan coefficients for the tensor product $V^{\lambda_1} \otimes \cdots \otimes V^{\lambda_p}$. The proof of the theorem relies heavily on the properties of the ''differentiation'' inner product (2.1) of $\mathscr{F}$. Thus we start by establishing some properties of this inner product. For $f \in \mathscr{F}$, the polynomial differential operator with constant coefficients $f(D)$ also acts on $\mathscr{F}$ in the obvious fashion. If $y \in \mathrm{GL}(N,\mathbb{C})$, then it can be shown (cf. Ref. 5a) that

$$R(y)f(D)R(y^{-1}) = (R(y^\vee)f)(D), \tag{2.2}$$

where $y^\vee = (y^{-1})^t$; in particular, if $y \in U(N)$, then $y^\vee = y^*$, the complex-conjugate of y. For $f \in \mathscr{F}$ we define the linear functional $\Phi(f)$ on $\mathscr{F}$ by

$$[\Phi f](h) = \langle f|h\rangle = f^*(D)h(Z)|_{Z=0}, \quad h \in \mathscr{F}.$$

Then Φ is a *conjugate-linear isomorphism* (or anti-isomorphism) of $\mathscr{F}$ onto its dual $\mathscr{F}^*$. If R is a representation of a closed subgroup G of $\mathrm{SU}(N)$ which is defined by right translation on a subspace V of $\mathscr{F}$, then we can define the contragradient $R^\vee$ (or in this case the complex-conjugate R^*) by the equation

$$[R^\vee(g)\Phi(f)](h) := [\Phi(f)](R(g^{-1})h) = \langle f|R(g^{-1})h\rangle = \langle R(g)f|h\rangle = [\Phi(R(g)f)](h)$$

for all $g \in G$ and $h, f \in \mathscr{F}$.

It follows that

$$[R^{\vee}(g_1g_2)\Phi(f)](h)=[\Phi(R(g_1g_2)f)](h)=[\Phi(R(g_1)(R(g_2)f))](h)$$
$$=[R^{\vee}(g_1)\Phi(R(g_2)f)](h)$$
$$=[R^{\vee}(g_1)R^{\vee}(g_2)\Phi f](h),$$

for all $g_1,g_2\in G$ and $f,h\in\mathscr{F}$. Thus Φ is a *conjugate-linear isomorphism* (or *anti-isomorphism*) *intertwining operator*. In particular if $(R^{\lambda},V^{\lambda})$ is an irreducible representation of G, then $(R^{\lambda^{\vee}},\Phi(V^{\lambda}))$ is also an irreducible unitary representation of G. Since G is a subgroup of SU(N) the G-module $(R^{\lambda^{\vee}},\Phi(V^{\lambda}))$ can be unitarily mapped onto $(R^{\lambda^*},V^{\lambda^*})$, a G-submodule of $\mathscr{F}$. [In the Appendix this map is carried out explicitly for the case $G=\mathrm{SU}(N)$.] Thus $V^{\lambda_i}(V^{\lambda^*})$ can be realized as a subspace of holomorphic square-integrable functions on $\mathbb{C}^{r_i\times N}(\mathbb{C}^{s\times N})$ which *transform covariantly with respect* to $B_i(B_s)$, $1\leqslant i\leqslant p$, i.e., $f(b_iZ_i)=\lambda_i(b_i)f(Z_i)$, $Z_i\in\mathbb{C}^{r_i\times N}$, and which may satisfy some additional properties [for example, when $G=\mathrm{SO}(N)$ or $\mathrm{Sp}(N)$, $V^{\lambda_i}(V^{\lambda^*})$ must also be G-harmonic polynomials (see Refs. 5a and 5b)]. For $Z_i\in\mathbb{C}^{r_i\times N}$, $1\leqslant i\leqslant p$, write

$$Z=(Z_1,\ldots,Z_p)\equiv\begin{bmatrix}Z_1\\ \vdots\\ Z_p\end{bmatrix},$$

and for $W\in\mathbb{C}^{s\times N}$ write $(Z,W)\equiv\begin{bmatrix}Z\\ W\end{bmatrix}$. Let $d\mu(Z)$, $d\mu(W)$, and $d\mu(Z,W)$ denote the Gaussian measures on $\mathbb{C}^{r\times N}(r=\Sigma_{i=1}^{p}r_i)$, $\mathbb{C}^{s\times N}$, and $\mathbb{C}^{(r+s)\times N}$, respectively. Let $\mathscr{I}\equiv\mathscr{I}(V^{\lambda_1}\otimes\cdots\otimes V^{\lambda_p}\otimes V^{\lambda^*})$ denote the space of G-invariants in $V^{\lambda_1}\otimes\cdots\otimes V^{\lambda_p}\otimes V^{\lambda^*}$ as in Theorem 2.1. Then we have the following:

Theorem 2.3: *Let $\{f^{\lambda_i}_{\xi_i}\}_{\xi_i}$ be a basis of state vectors in V^{λ_i}, $1\leqslant i\leqslant p$. Let $\{f^{\lambda}_{\zeta}\}_{\zeta}$ be a basis of state vectors in V^{λ} and let $\{f^{\lambda^*}_{\xi^*}\}$ be its anti-isomorphic image in V^{λ^*}. Let $\{\mathscr{I}_{\eta}\}_{\eta}$ be a basis of state vectors in $\mathscr{I}$. Let*

$$\tilde{f}^{\lambda,\eta}_{\zeta}(Z)=f^{*\lambda^*}_{\zeta^*}(D)\mathscr{I}_{\eta}(Z,W)|_{W=0}\equiv\int_{\mathbb{C}^{s\times N}}f^{\lambda^*}_{\zeta^*}(W)I_{\eta}(Z,W)d\mu(W).\tag{2.3}$$

Then $\{\tilde{f}^{\lambda,\eta}_{\zeta}\}_{\zeta}$ is an isomorphic image of $\{f^{\lambda}_{\zeta}\}_{\zeta}$ in $V^{\lambda_1}\otimes\cdots\otimes V^{\lambda_p}$ indexed by the multiplicity label η and we have the following relation of Clebsch–Gordan coefficients,

$$\langle f^{\lambda_1}_{\xi_1}f^{\lambda_2}_{\xi_2}\cdots f^{\lambda_p}_{\xi_p}f^{\lambda^*}_{\zeta^*}|\mathscr{I}_{\eta}\rangle=\langle f^{\lambda_1}_{\xi_1}\cdots f^{\lambda_p}_{\xi_p}|\tilde{f}^{\lambda,\eta}_{\zeta}\rangle.\tag{2.4}$$

Proof: Let A: $\phi(V^{\lambda})\to V^{\lambda^*}$ denote the linear isomorphism intertwining $\phi(V^{\lambda})$ and V^{λ^*}. Then $f^{\lambda^*}_{\zeta^*}=A\Phi(f^{\lambda}_{\zeta})$. Using the inner product (2.1) or its equivalent integral inner product, we have

$$\tilde{f}^{\lambda,\eta}_{\zeta}(Z)=f^{*\lambda^*}_{\zeta^*}(D)I_{\eta}(Z,W)|_{W=0}=\int_{\mathbb{C}^{s\times N}}\overline{f^{\lambda^*}_{\zeta^*}(W)}\mathscr{I}_{\eta}(Z,W)d\mu(W).$$

Note that in Eq. (2.3) $\tilde{f}^{\lambda,\eta}_{\zeta}(Z)$ is the inner product $\langle f^{\lambda^*}_{\zeta^*},I_{\eta}\rangle$, where I_{η} is considered as a function of the variable W. Clearly $\tilde{f}^{\lambda,\eta}_{\zeta}(Z)$ is a polynomial function in Z and if $b=(b_1,\ldots,b_p)\in B_1\times\cdots\times B_p$, then

$$\tilde{f}^{\lambda,\eta}_{\zeta}(Z)=f^{\lambda,\eta}_{\zeta}(b_1Z_1,\ldots,b_pZ_p)=\int_{\mathbb{C}^{s\times N}}\overline{f^{\lambda^*}_{\zeta^*}(W)}\mathscr{I}_{\eta}(b_1Z_1,\ldots,b_pZ_p,W)d\mu(W).$$

Since I_η is an element of $V^{\lambda_1}\otimes\cdots\otimes V^{\lambda_p}\otimes V^{\lambda^*}$, it follows immediately that

$$\mathscr{T}_\eta(b_1Z_1,\ldots,b_pZ_p,W)=\lambda_1(b_1),\ldots,\lambda_p(b_p)\mathscr{T}_\eta(Z_1,\ldots,Z_p,W).$$

Hence

$$\tilde{f}^{\lambda,\eta}_{\zeta}(bZ)=\lambda_1(b_1),\ldots,\lambda_p(b_p)\tilde{f}^{\lambda,\eta}_{\zeta}(Z).$$

Moreover, if $\mathscr{T}_\eta(Z,W)$ is required to satisfy any additional property in order for it to belong to $V^{\lambda_1}\otimes\cdots\otimes V^{\lambda_p}\otimes V^{\lambda^*}$, then it follows that $\tilde{f}^{\lambda,\eta}_{\zeta}$ must satisfy a similar property in order for it to belong to $V^{\lambda_1}\otimes\cdots\otimes V^{\lambda_p}$ [for example, if $\mathscr{T}_\eta(Z,W)$ must be a G-harmonic polynomial, then by interchanging differentiation and integration, that is, differentiating under the integral sign, one can easily show that $\tilde{f}^{\lambda,\eta}_{\zeta}(Z)$ is G-harmonic polynomial in the variable Z]. In conclusion, $\tilde{f}^{\lambda,\eta}_{\zeta}$ belong to $V^{\lambda_1}\otimes\cdots\otimes V^{\lambda_p}$. Then

$$\begin{aligned}R(g)\tilde{f}^{\lambda}_{\zeta}&=R(g)f^{*\lambda^*}_{\zeta^*}(D)\mathscr{T}_\eta\\&=\underbrace{(R(g)f^{*\lambda^*}_{\zeta^*}(D)R(g^{-1}))}(R(g)\mathscr{T}_\eta)\\&=(R(g^*)f^{*\lambda^*}_{\zeta^*})(D)\mathscr{T}_\eta\end{aligned}$$

by Eq. (2.2) and the fact that $\mathscr{T}_\eta$ is G-invariant. Now $R(g^*)f^{*\lambda^*}_{\zeta^*}=(R(g)f^{\lambda^*}_{\zeta^*})^*$, and

$$R(g)f^{\lambda^*}_{\zeta^*}=R(g)A\Phi(f^{\lambda}_{\zeta})=A\Phi(R(g)f^{\mu}_{\xi}).$$

However, $R(g)f^{\lambda}_{\zeta}=\Sigma_{\xi'}D^{\mu}_{\xi'\xi}(g)f^{\mu}_{\xi'}$, where $D^{\mu}_{\zeta'\zeta}$ are the D-functions of R^λ. So

$$R(g)f^{\lambda^*}_{\zeta^*}=\sum_{\zeta'}D^{*\lambda}_{\zeta'\zeta}(g)A\phi(f^{\lambda}_{\zeta'}),$$

where in the last equality we use the fact that Φ is a conjugate-linear isomorphism. It follows that

$$(R(g)f^{\lambda^*}_{\zeta^*})^*=\sum_{\zeta'}D^{\lambda}_{\zeta'\zeta}(g)f^{\lambda^*}_{\zeta^*},$$

and

$$R(g)\tilde{f}^{\lambda}_{\zeta}=\sum_{\zeta'}D^{\lambda}_{\zeta'\zeta}(g)(f^{\lambda^*}_{\zeta^*},(D)\mathscr{T}_\eta)=\sum_{\zeta'}D^{\lambda}_{\zeta'\zeta}(g)\tilde{f}^{\lambda}_{\zeta'}.$$

This last equality shows that $\{\tilde{f}^{\lambda}_{\zeta}\}$ transforms under R in the same manner as $\{f^{\lambda}_{\zeta}\}$.

Now

$$\begin{aligned}\langle f^{\lambda_1}_{\xi_1}\cdots f^{\lambda_p}_{\xi_p}f^{\lambda^*}_{\zeta^*}|\mathscr{T}_\eta\rangle&=f^{*\lambda_1}_{\xi_1}(D)\cdots f^{*\lambda_p^*}_{\xi_p}(D)f^{*\lambda^*}_{\zeta^*}(D)\mathscr{T}_\eta(Z,W)|_{(Z,W)=(0,0)}\\&=f^{*\lambda_1}_{\xi_1}(D)\cdots f^{*\lambda_p}_{\xi_p}(D)\tilde{f}^{\lambda,\eta}_{\zeta}(Z)|_{Z=0}=\langle f^{\lambda_1}_{\xi_1}\cdots f^{\lambda_p}_{\xi_p}|\tilde{f}^{\lambda,\eta}_{\zeta}\rangle\end{aligned}$$

which is Eq. (2.4).

Remark 2.4: (i) In Eq. (2.3) the invariant polynomial $\mathscr{I}_\eta(Z,W)$ can be viewed as a kernel function and the index η can be used as the multiplicity label of the representation λ in the tensor product $\lambda_1\otimes\cdots\otimes\lambda_p$.

(ii) We could also use the integration inner product to give another proof of Theorem 2.3. Indeed, for $g\in G$ we have from Eq. (2.3)

$$R(g)\tilde{f}^{\lambda,\eta}_{\zeta}(Z)=\tilde{f}^{\lambda,\eta}_{\zeta}(Zg)=\int_{\mathbb{C}^{s\times N}} f^{\lambda *}_{\zeta *}(W)\mathscr{I}_\eta(Zg,W)d\mu(W).$$

However, $\mathscr{I}_\eta(Zg,W)=\mathscr{I}_\eta(Zgg^{-1},Wg^{-1})=\mathscr{I}_\eta(Z,Wg^{-1})$ since $\mathscr{I}_\eta$ is G-invariant. In making the change of variable $W'=Wg^{-1}$ and using the fact that the measure $d\mu(W)$ is G-invariant, we obtain

$$R(g)\tilde{f}^{\lambda,\eta}_{\zeta}(Z)=\int_{\mathbb{C}^{s\times N}}\overline{f^{\lambda *}_{\zeta *}(W'g)}\mathscr{I}_\eta(Z,W')d\mu(W').$$

Now

$$\begin{aligned} f^{\lambda *}_{\zeta *}(Wg)=[R(g)A\Phi(f^{\lambda}_{\zeta})](W)=[A\Phi R(g)f^{\lambda}_{\zeta}](W)&=\left[A\Phi\sum_{\zeta'}D^{\lambda}_{\zeta'\zeta}(g)f^{\lambda}_{\zeta'}\right](W)\\ &=\sum_{\zeta'}\overline{D^{\lambda}_{\zeta'\zeta}(g)}[A\Phi f^{\lambda}_{\zeta'}(W)]\\ &=\sum_{\zeta'}\overline{D^{\lambda}_{\zeta'\zeta}(g)}f^{\lambda *}_{\zeta *'}(W).\end{aligned}$$

Therefore,

$$\begin{aligned} R(g)\tilde{f}^{\lambda,\eta}_{\zeta}(Z)&=\int_{\mathbb{C}^{s\times N}}\overline{\left(\sum_{\zeta'}\overline{D^{\lambda}_{\zeta'\zeta}(g)}f^{\lambda *}_{\zeta *'}\right)}(W')\mathscr{I}_\eta(Z,W')d\mu(W')\\ &=\sum_{\zeta'}D^{\lambda}_{\zeta'\zeta}(g)\int_{\mathbb{C}^{s\times N}}f^{\lambda *}_{\zeta *'}(W')\mathscr{I}_\eta(Z,W')d\mu(W')\\ &=\sum_{\zeta'}D^{\lambda}_{\zeta'\zeta}(g)\tilde{f}^{\lambda,\eta}_{\zeta'}(Z).\end{aligned}$$

Also,

$$\langle f^{\lambda_1}_{\xi_1}\cdots f^{\lambda_p}_{\xi_p}f^{\lambda *}_{\zeta *}|\mathscr{I}_\eta\rangle=\int_{\mathbb{C}^{(r+s)\times N}}\overline{f^{\lambda_1}_{\xi_1}(Z_1)\cdots f^{\lambda_p}_{\xi_p}(Z_p)f^{\lambda *}_{\zeta *}(W)}f(Z,W)d\mu(Z,\mu),$$

which by Fubini's theorem is equal to

$$\begin{aligned}&\int_{\mathbb{C}^{r\times N}}d\mu(Z)\overline{f^{\lambda_1}_{\xi_1}(Z_1)\cdots f^{\lambda_p}_{\xi_p}(Z_p)}\left(\int_{\mathbb{C}^{s\times N}}d\mu(W)\overline{f^{\lambda *}_{\zeta *}}(W)\mathscr{I}_\eta(Z,W)\right)\\ &=\int_{\mathbb{C}^{r\times N}}\overline{f^{\lambda_1}_{\xi_1}(Z_1)\cdots f^{\lambda_p}_{\xi_p}(Z_p)}\tilde{f}^{\lambda,\eta}_{\zeta}(Z)d\mu(Z)\\ &=\langle f^{\lambda_1}_{\xi_1}\cdots f^{\lambda_p}_{\xi_p}|\tilde{f}^{\lambda,\eta}_{\zeta}\rangle.\end{aligned}$$

III. APPLICATION TO SU(*N*)

We have shown that the problem of finding the multiplicity of an irreducible unitary representation R^{λ} in the tensor product $V^{\lambda_1}\otimes\cdots\otimes V^{\lambda_p}$ of p irreducible unitary representations of a closed subgroup of SU(N) is equivalent to that of finding the dimension of the G-invariant subspace in $V^{\lambda_1}\otimes\cdots\otimes V^{\lambda_p}\otimes V^{\lambda^*}$ (Theorem 2.1). Also, the Clebsch–Gordan coefficients of R^{λ} in $R^{\lambda_1}\otimes\cdots\otimes R^{\lambda_p}$ are essentially inner products of state vectors $f^{\lambda_1}_{\zeta_1}\cdots f^{\lambda_p}_{\zeta_p}f^{\lambda^*}_{\xi^*}$ with basis vectors of G-invariants in $V^{\lambda_1}\otimes\cdots\otimes V^{\lambda_p}\otimes V^{\lambda^*}$ (Theorem 2.3). It is therefore crucial to find explicit bases for the space $\mathscr{T}\equiv\mathscr{T}^{\lambda_1,\ldots,\lambda_p,\lambda^*}$ of G-invariant polynomial functions in $V^{\lambda_1}\otimes\cdots\otimes V^{\lambda_p}\otimes V^{\lambda^*}$. This also will give a resolution of the multiplicity problem, i.e., the problem of labelling different isomorphic copies of an irreducible representation R^{λ} which occurs in $R^{\lambda_1}\otimes\cdots\otimes R^{\lambda_p}$. However, the theory of polynomial invariants of the classical groups is well known (see Ref. 6, for example), and for many other reductive groups this problem has been thoroughly investigated (see Ref. 7, for example). We start in this paper with the simplest but nevertheless very important case when $G=\mathrm{SU}(N)$. For this the ''first main theorem'' of invariants of $\mathrm{SL}(N,\mathbb{C})$ [and hence of SU(N)] can be stated as (see Ref. 7, Ch. II):

Theorem 3.1: *Let* $\mathbb{P}(\mathbb{C}^{k\times N})$, $k\geqslant N$, *be the subspace of* $\mathscr{T}(\mathbb{C}^{n\times N})$, $n\geqslant k$, *of all polynomial functions on* $\mathbb{C}^{k\times N}$. *Then the algebra of all* $\mathrm{SL}(N,\mathbb{C})$*-invariant polynomials in* $\mathbb{P}(\mathbb{C}^{k\times N})$ *is generated by the polynomials*

$$\Delta^{i_1\ldots i_N}_{1,2\ldots N}(Z),\quad Z\in\mathbb{C}^{k\times N},$$

where $(i_1,\ldots,i_N)$ *is an N-shuffle, i.e., a strictly increasing sequence of integers in the segment* $[1,k]$, *and* $\Delta^{i_1\ldots i_N}_{12\ldots N}(Z)$ *is the determinant of the* $N\times N$ *matrix formed by the rows* $i_1,\ldots,i_N$ *and the columns* 1,...,N of Z.

Next we consider tensor products of p irreducible SU(N)-modules V^{λ_i} with $V^{(\lambda^*)}$. Each signature λ_i and λ^* can be labelled by a highest weight of the form $(m^i_1,\ldots,m^i_{N-1},0)$ where the integers $m^i_1,\ldots,m^i_{N-1}$ satisfy the dominant condition $m^i_1\geqslant m^i_2\geqslant\cdots\geqslant m^i_{N-1}\geqslant 0$. We discard those m^i_j which are equal to zero and form the k-tuple of positive integers $(m^1_1,\ldots,m^1_{r_1},m^2_1,\ldots,m_{r_2},\ldots,m^p_1,\ldots,m^p_{r_p},M_1,\ldots,M_s)$, where

$$\underbrace{(M_1,\ldots,M_s,0,\ldots,0)}_{N}$$

is the highest weight of λ^* and $m^i_1\geqslant m^i_2\geqslant m^i_r>0$ for $i=1,\ldots,p$. Let B_i denote the subgroup of $\mathrm{GL}(r_i,\mathbb{C})$ consisting of all lower triangular matrices, $i=1,\ldots,p$, and let B_s denote the lower triangular subgroup of $\mathrm{GL}(s,\mathbb{C})$. Then the group $B_1\times B_2\times\ldots\times B_p\times B_s$ can be identified with the group of all $k\times k$ lower triangular block matrices β of the form

$$\begin{array}{l} r_1\\ r_2\\ \vdots\\ r_p\\ s \end{array}\begin{pmatrix} \boxed{b_1} & & & & \\ & \boxed{b_2} & & \bigcirc & \\ & & \ddots & & \\ & \bigcirc & & \boxed{b_p} & \\ & & & & \boxed{b_s} \end{pmatrix} b_1\in B_i, b_s\in B_s.$$

Then we have the following:

Theorem 3.2: *Let* $\mathbb{P}(\mathbb{C}^{k\times N})$, $k\geqslant N$, *be the subspace of* $\mathscr{T}(\mathbb{C}^{n\times N})$, $n\geqslant k$, *of all polynomial functions on* $\mathbb{C}^{k\times N}$. *Then the tensor product* $V^{\lambda_1}\otimes\cdots\otimes V^{\lambda_p}\otimes V^{\lambda^*}$ *of irreducible unitary SU(N)-modules can be realized as the subspace of* $\mathbb{P}(\mathbb{C}^{k\times N})$ *of all polynomial functions* f *which satisfy the covariant condition*

$$f(\beta Z)=\left(\prod_{i=1,\ldots,p}\lambda_i(b_i)\right)\lambda^*(b_s)f(Z), \tag{3.2}$$

where $Z\in\mathbb{C}^{k\times N}$, β *is given by Eq. (3.1), and* $\lambda_i(b_i)=(b_i)_{11}^{m_1^i}\cdots(b_i)_{r_ir_i}^{m_{ri}^i}$, $\lambda^*(b_s)=(b_s)_{11}^{M_1}\cdots(b_s)_{ss}^{M_s}$. *The SU(N)-invariant polynomials in* $V^{\lambda_1}\otimes\ldots\otimes V^{\lambda_p}\otimes V^{\lambda^*}$ *are linear combinations of polynomials of the form*

$$(\Delta_{12\ldots N}^{12\ldots N}(Z))^{\ell_{1\ldots N}}\cdots(\Delta_{1\ldots N}^{i_1\ldots i_N}(Z))^{\ell_{i_1\ldots i_N}}\cdots(\Delta_{1,\ldots,N}^{k-N+1,\ldots,k}(Z))^{\ell_{k-N+1,\ldots,k}}, \tag{3.3}$$

with

$$\begin{aligned}
&\ell_{12\ldots N}+\cdots+\ell_{1i_2\ldots i_N}+\cdots\ell_{1,\ldots,k}=m_1^1,\\
&\ell_{12\ldots N}+\cdots+\ell_{12\ldots i_N}+\cdots\ell_{2,\ldots,k}=m_2^1,\\
&\qquad\vdots\\
&\ell_{1\ldots k}+\cdots+\ell_{i_1\ldots i_{N-1,k}}+\cdots+\ell_{k-N+1,\ldots,k}=M_s,
\end{aligned} \tag{3.4}$$

where in Eq. (3.3) a minor $\Delta_{1\ldots N}^{i_1\ldots i_N}(Z)$ *appears if and only if it satisfies*

$$\Delta_{1\ldots N}^{i_1\ldots i_N}(\beta Z)=\beta_{i_1i_1}\cdots\beta_{i_Ni_N}\Delta_{1\ldots N}^{i_1\ldots i_N}(Z), \tag{3.5}$$

and where in Eq. (3.4) the $l_{i_1\ldots i_N}$ *are non-negative integers and the shuffles* $(i_1\ldots i_N)$ *are lexicographically ordered. Moreover, the number of linearly independent solutions of Eq. (3.3) which satisfy the constraints (3.5) and the system of linear diophantine equations (3.4) is the multiplicity of* λ *in the Clebsch–Gordan series of* $\lambda_1\otimes\ldots\otimes\lambda_p$.

Proof: The fact that the tensor product $V^{\lambda_1}\otimes\cdots\otimes V^{\lambda_p}\otimes V^{\lambda^*}$ of irreducible SU(N)-modules can be realized as the subspace of all polynomial functions in $\mathcal{P}(\mathbb{C}^{k\times N})$ which satisfy the covariant condition (3.2) is a consequence of the Borel–Weil theorem and a detailed proof can be found in Ref. 4a. It remains to show that the SU(N)-invariant polynomials in $V^{\lambda_1}\otimes\cdots\otimes V^{\lambda_p}\otimes V^{\lambda^*}$ are spanned by polynomials of the form (3.3) which satisfy the constraints (3.4) and (3.5). From Theorem 3.1 it follows that the polynomials of the form (3.3) will span the subspace of SU(N)-invariants in $V^{\lambda_1}\otimes\cdots\otimes V^{\lambda_p}\otimes V^{\lambda^*}$ if and only if they also satisfy the covariant condition (3.2). Thus it remains to show that a polynomial of the form (3.3) satisfies the covariant condition (3.2) if and only if it satisfies the constraints (3.4) and (3.5). Since in a polynomial of the form (3.3), where only the minors $\Delta_{1\ldots N}^{i_1\ldots i_N}$ which satisfy (3.5) occur, the constraints (3.4) imply the condition (3.2), it is clear that the condition is sufficient. To show that the condition is necessary we first observe that it is easy to verify that

$$\Delta_{1\ldots N}^{i_1\ldots i_N}(yZ)=\sum_{j_1<\cdots<j_N}\Delta_{j_1\ldots j_N}^{i_1\ldots i_N}(y)\Delta_{1\ldots N}^{j_1\ldots j_N}(Z) \tag{3.6}$$

for all $y\in\mathbb{C}^{k\times k}$ and $Z\in\mathbb{C}^{k\times N}$, and where in Eq. (3.6) the summation ranges over all N-shuffles $(j_1,\ldots,j_N)$. Next, let f be an element of the form (3.3) and consider a typical factor $(\Delta_{1\ldots N}^{i_1\ldots i_N})^{l_1\ldots l_N}$ of f. The condition that f must satisfy Eq. (3.2) together with the equality (3.6) with $y=\beta$, a matrix of form (3.1), force $\Delta_{j_1\ldots j_N}^{i_1\ldots i_N}(\beta)=0$ if the shuffle $(j_1,\ldots,j_N)$ is different from $(i_1,\ldots,i_N)$. Thus Eq. (3.6) becomes

$$\Delta^{i_1\cdots i_N}_{1\cdots N}(\beta Z)=\Delta^{i_1\cdots i_N}_{i_1\cdots i_N}(\beta)\Delta^{i_1\cdots i_N}_{1\cdots N}(Z). \tag{3.7}$$

However, in Eq. (3.7) β is an invertible lower triangular matrix, therefore,

$$\Delta^{i_1\cdots i_N}_{i_1\cdots i_N}(\beta)=\beta_{i_1 i_1}\cdots\beta_{i_N i_N}.$$

It follows immediately that in order that f satisfies Eq. (3.2), it is necessary that the minors $\Delta^{i_1\cdots i_N}_{1\cdots N}$ appearing in f must satisfy Eq. (3.5) and the exponents $l_{i_1\cdots i_N}$ must satisfy the constraints (3.4).

Remark 3.3: For any concrete example it is very easy to determine which minors $\Delta^{i_1\cdots i_N}_{1\cdots N}(Z)$ satisfy condition (3.5). This reduces the problem of finding the subspace of SU(N)-invariant polynomials in $V^{\lambda_1}\otimes\cdots\otimes V^{\lambda_p}\otimes V^{\lambda *}$ to that of solving the system of linear diophantine equations (3.4), which is a well-studied problem in integer programming (e.g., the Branch bound method). In general, the polynomials given by Eq. (3.3) which satisfy the constraints (3.4) are not necessarily linearly independent, as we shall see in an example in the next section. However, the problem of finding a basis for a spanning set of polynomial functions is also well studied in computer programming.

IV. EXAMPLES

To illustrate our procedures we consider below several examples.

Example 1: This is the same example given in Refs. 4b and 4c. It will serve to prove the power and the simplicity of our present method versus the more elaborate one in the former. Consider the tensor product $V^{(2,0,0)}\otimes V^{(2,0,0)}\otimes V^{(1,0,0)}$ of SU(3) which has the following Clebsch–Gordan series,

$$(2,0)\otimes(2,0)\otimes(1,0)=(5,0)+2(4,1)+(3,2)+(2,0)+(1,1), \tag{4.1}$$

where in Eq. (4.1) only two integers are needed to label an irreducible representation of SU(3). The representation with signature (4,1) occurs with multiplicity two and its contragradient representation has signature (4,3). So in accordance with Theorem 3.2 we consider the polynomial space $\mathscr{P}(\mathbb{C}^{5\times 3})$. The minors $\Delta^{i_1 i_2 i_3}_{123}(Z)$ which satisfy the condition (3.5) for $z\in\mathbb{C}^{5\times 3}$ and

$$\beta=\begin{bmatrix}\beta_{11} & & & & \\ & \beta_{22} & & & \\ & & \beta_{33} & & \\ & & & \beta_{44} & 0 \\ & & & \beta_{54} & \beta_{55}\end{bmatrix}$$

are

$$\Delta^{123}_{123},\quad \Delta^{124}_{123},\quad \Delta^{134}_{123},\quad \Delta^{145}_{123},\quad \Delta^{234}_{123},\quad \Delta^{245}_{123},\quad \text{and}\quad \Delta^{345}_{123}.$$

So the diophantine linear equation (3.4) for this case is

$$\ell_{123}+\ell_{124}+\ell_{134}+\ell_{145}=2,$$

$$\ell_{123}+\ell_{124}+\ell_{234}+\ell_{245}=2,$$

$$\ell_{123}+\ell_{134}+\ell_{234}+\ell_{345}=1,$$

$$\ell_{124}+\ell_{134}+\ell_{145}+\ell_{234}+\ell_{245}+\ell_{345}=4,$$

$$\ell_{145}+\ell_{245}+\ell_{345}=3,$$

which, using a Maple V program, gives the solutions

$$\ell_{123}=\ell_{134}=\ell_{234}=0,\quad \ell_{124}=\ell_{145}=\ell_{245}=\ell_{345}=1,$$

$$\ell_{123}=\ell_{124}=\ell_{134}=\ell_{345}=0,\quad \ell_{145}=2,\quad \ell_{234}=\ell_{245}=1,$$

and

$$\ell_{123}=\ell_{124}=\ell_{234}=\ell_{345}=0,\quad \ell_{134}=\ell_{145}=1,\quad \ell_{245}=2.$$

It follows that the polynomials

$$\Delta^{124}_{123}(Z)\Delta^{145}_{123}(Z)\Delta^{245}_{123}(Z)\Delta^{345}_{123}(Z),\quad (\Delta^{145}_{123}(Z))^2\Delta^{234}_{123}(Z)\Delta^{245}_{123}(Z),\quad \text{and}\quad \Delta^{134}_{123}(Z)\Delta^{145}_{123}(Z)(\Delta^{245}_{123}(Z))^2,$$

which are easily verified to be linearly dependent [in fact, $\Delta^{124}_{123}(Z)\Delta^{145}_{123}(Z)\Delta^{245}_{123}(Z)\times\Delta^{345}_{123}(Z)+(\Delta^{145}_{123}(Z))^2\Delta^{234}_{123}(Z)\Delta^{245}_{123}(Z)=\Delta^{134}_{123}(Z)\Delta^{145}_{123}(Z)(\Delta^{245}_{123}(Z))^2$], span the two-dimensional subspace of all SU(3)-invariants in the tensor product

$$V^{(2,0,0)}\otimes V^{(2,0,0)}\otimes V^{(1,0,0)}\otimes V^{(4,3,0)}.$$

In Eq. (4.1) the other irreducible representation which occurs with multiplicity two is (3,2). Its contragradient representation has signature (3,1). So proceeding as above, we obtain the polynomials

$$f_1(Z)=(\Delta^{124}_{123}(Z))^2\Delta^{345}_{123}(Z),\quad f_2(Z)=\Delta^{124}_{123}(Z)\Delta^{134}_{123}(Z)\Delta^{245}_{123}(Z),$$

and

$$f_3(Z)=\Delta^{124}_{123}(Z)\Delta^{145}_{123}(Z)\Delta^{234}_{123}(Z)$$

which span the subspace of all SU(3)-invariants in the tensor product.

$$V^{(2,0,0)}\otimes V^{(2,0,0)}\otimes V^{(1,0,0)}\otimes V^{(3,1,0)}.$$

Using a Maple V program, we easily verify the f_1, f_2, and f_3 span a two-dimensional vector space with $f_1+f_3-f_2=0$.

Example 2: Threefold tensor products of SU(2) and S_3 permutation symmetry.

We consider in this example the threefold SU(2) tensor product $j\otimes j\otimes j$, which, since all the irreducible representations are the same, generates an S_3 permutation symmetry. The decomposition into irreducible representations is

$$j\otimes j\otimes j=3j\oplus(3j-1)\oplus(3j-2)\oplus\cdots,$$

$$\text{Symmetry type}=S\quad M\quad S,M\ldots,$$

$$\text{Multiplicity}=1\quad 2\quad 3\ldots.$$

The Clebsch–Gordan coefficients are not particularly difficult to compute for $J=3j-1,3j-2$; here we simply wish to show how the polynomial invariants carry a representation of S_3. According to the general formalism set up in Secs. II and III, we have the augmented Bargmann–Segal–Fock space $\mathcal{P}(\mathbb{C}^{4\times 2})$ of all polynomial functions f which satisfy the covariant condition

$$f(dZ)=d_1^{2j}d_2^{2j}d_3^{2j}d_4^{2J}f(Z),\quad \text{for all}\quad d=\begin{bmatrix} d_1 & & & \\ & d_2 & & \\ & & d_3 & \\ & & & d_4 \end{bmatrix}\quad \text{and}\quad Z\in\mathbb{C}^{4\times 2},\tag{4.2}$$

with invariants of the form $(\Delta_{12}^{12}(Z))^{\ell_{12}}(\Delta_{12}^{13}(Z))^{\ell_{13}}\cdots(\Delta_{12}^{34}(Z))^{\ell_{34}}$. The non-negative integers ℓ_{ij} must be chosen to satisfy Eq. (4.2). That means the equations

$$\begin{aligned} &\ell_{12}+\ell_{13}+\ell_{14}=2j,\quad \ell_{12}+\ell_{23}+\ell_{24}=2j,\\ &\ell_{13}+\ell_{23}+\ell_{34}=2j,\quad \ell_{14}+\ell_{24}+\ell_{34}=2J \end{aligned}\tag{4.3}$$

must be satisfied. For $J=3j-1$ the solutions are

$$\begin{aligned} f_1(Z)&=(\Delta_{12}^{14}(Z))^{2j}(\Delta_{12}^{24}(Z))^{2j-1}(\Delta_{12}^{34}(Z))^{2j-1}(\Delta_{12}^{23}(Z)),\\ f_2(Z)&=(\Delta_{12}^{14}(Z))^{2j-1}(\Delta_{12}^{24}(Z))^{2j}(\Delta_{12}^{34}(Z))^{2j-1}(\Delta_{12}^{13}(Z)),\\ f_3(Z)&=(\Delta_{12}^{14}(Z))^{2j-1}(\Delta_{12}^{24}(Z))^{2j-1}(\Delta_{12}^{34}(Z))^{2j}(\Delta_{12}^{12}(Z)). \end{aligned}\tag{4.4}$$

However, the multiplicity for $J=3j-1$ is 2, not 3, so we see that the f_i must be linearly dependent. To extract the permutation symmetry, we note that

$$(L_\sigma f\ )(Z)=f(\sigma^{-1}Z),\quad \sigma\in S_3,\tag{4.5}$$

defines the action of the permutation group S_3 on the subspace of invariants. Applied to f_i gives

$$\begin{aligned} &L_{(12)(3)}f_1=f_2,\quad L_{(12)(3)}f_2=f_1,\quad L_{(12)(3)}f_3=-f_2,\\ &L_{(123)}f_1=-f_2,\quad L_{(132)}f_2=-f_3,\quad L_{(132)}f_3=f_1, \end{aligned}\tag{4.6}$$

which means the f_i carry a mixed and antisymmetric representation of S_3. From this it follows that the antisymmetric linear combination, f_A, must give the linear dependence:

$$f_A:=f_1-f_2+f_3=0.\tag{4.7}$$

The mixed representation can be chosen such that the S_2 subgroup carries a symmetric and antisymmetric representation. Then

$$f_\pm=f_1\pm f_2=(\Delta_{12}^{14})^{2j-1}(\Delta_{12}^{24})^{2j-1}(\Delta_{12}^{34})^{2j-1}[\Delta_{12}^{14}\Delta_{12}^{23}\pm\Delta_{12}^{24}\Delta_{12}^{13}]\tag{4.8}$$

gives the two mixed representation states needed to calculate the Clebsch–Gordan coefficients

$$\langle j,m_1;j,m_2;j,m_3|J=3j-1,M;\pm\rangle.$$

Similarly for $J=3j-2$, with threefold degeneracy, the solutions to Eq. (4.3) are

$$\begin{aligned} f_1&:=(\Delta_{12}^{14})^{2j-2}(\Delta_{12}^{24})^{2j-1}(\Delta_{12}^{34})^{2j-1}\Delta_{12}^{12}\Delta_{12}^{13},\\ f_2&:=(\Delta_{12}^{14})^{2j-1}(\Delta_{12}^{24})^{2j-1}(\Delta_{12}^{34})^{2j-1}\Delta_{12}^{12}\Delta_{12}^{23},\\ f_3&:=(\Delta_{12}^{14})^{2j-1}(\Delta_{12}^{24})^{2j-1}(\Delta_{12}^{34})^{2j-2}\Delta_{12}^{13}\Delta_{12}^{23}, \end{aligned}\tag{4.9}$$

and since the multiplicity for $J=3j-2$ is 3, these f_i must all be linearly independent. To get the permutation type, we again use Eq. (4.5) to get

$$\begin{gathered} L_{(12)(3)}f_1=-f_2, \quad L_{(12)(3)}f_2=-f_1, \quad L_{(12)(3)}f_3=-f_3, \\ L_{(132)}f_1=-f_2, \quad L_{(132)}f_2=-f_3, \quad L_{(132)}f_3=f_1, \end{gathered} \tag{4.10}$$

from which it follows that the symmetry types are S (symmetric) and M (mixed) with

$$f_S=f_1-f_2+f_3, \quad f_{M,\pm}=f_1\mp f_2. \tag{4.11}$$

We conclude this example with a computation of the polynomial invariants where the Clebsch–Gordan coefficients are not so easy to compute by conventional means, namely the lowest weights in the tensor product decomposition. Consider first the case where j is an integer; the lowest weight is $J=0$ with multiplicity 1. Using Eq. (4.3) with $J=0$ gives

$$f_A=(\Delta_{12}^{12})^{2j}(\Delta_{12}^{13})^{2j}(\Delta_{12}^{23})^{2j} \tag{4.12}$$

and is always antisymmetric as can be checked by computing $L_{(12)(3)}f_A=-f_A$. The coefficients are given directly by

$$\begin{aligned} &\frac{\|f_A\|^{-1}}{\sqrt{(j+m_1)!(j-m_1)!(j+m_2)!(j-m_2)!(j+m_3)!(j-m_3)!}} \\ &\quad\times\frac{\partial^{j+m_1}}{\partial z_{11}^{j+m_1}}\frac{\partial^{j-m}}{\partial z_{12}^{j-m_1}}\frac{\partial^{j+m_2}}{\partial z_{21}^{j+m_2}}\frac{\partial^{j-m_2}}{\partial z_{22}^{j-m_2}}\frac{\partial^{j+m_3}}{\partial z_{31}^{j+m_3}}\frac{\partial^{j-m_3}}{\partial z_{32}^{j-m_3}}f_A(Z)|_{Z=0} \\ &\quad=\langle j,m_1;j_1m_2;j,m_3|J=0\rangle. \end{aligned} \tag{4.13}$$

For j a half-odd integer the lowest weight is $J=\frac{1}{2}$ with multiplicity 2. Using Eq. (4.3) gives three polynomials, namely,

$$\begin{aligned} f_1&:=(\Delta_{12}^{12})^{j-1/2}(\Delta_{12}^{13})^{j-1/2}(\Delta_{12}^{23})^{j+1/2}\Delta_{12}^{14}, \\ f_2&:=(\Delta_{12}^{12})^{j-1/2}(\Delta_{12}^{13})^{j+1/2}(\Delta_{12}^{23})^{j-1/2}\Delta_{12}^{24}, \\ f_3&:=(\Delta_{12}^{12})^{j+1/2}(\Delta_{12}^{13})^{j-1/2}(\Delta_{12}^{23})^{j-1/2}\Delta_{12}^{34}, \end{aligned} \tag{4.14}$$

with permutation structure

$$\begin{gathered} L_{(12)(3)}f_1=(-1)^{j-1/2}f_2, \quad L_{(12)(3)}f_2=(-1)^{j-1/2}f_1, \quad L_{(12)(3)}f_3=(-1)^{j+1/2}f_3, \\ L_{(132)}f_1=(-1)^{2j}f_2, \quad L_{(132)}f_2=(-1)^{2j}f_1, \quad L_{(132)}f_3=f_1, \end{gathered} \tag{4.15}$$

which gives a mixed representation and symmetric or antisymmetric depending on whether $(-1)^{j+1/2}$ is one or minus one. However, for any half-odd integer j, the linear dependence is given by

$$f=f_1-f_2+f_3=0 \tag{4.16}$$

and $L_{(12)(3)}(f_1\pm f_2)=\pm(-1)^{j-1/2}(f_1\pm f_2)$ gives the two mixed representation polynomials.

V. CONCLUSION

Calculating Clebsch–Gordan and Racah coefficients for tensor products of irreducible representations of compact groups almost always involves multiplicity. We have shown how the multiplicity problem can be restated in terms of group invariants, polynomials in $n\times N$ complex variables that are invariant under the right action of the group. Our setting is the Bargmann–Segal–Fock space $\mathscr{F}(\mathbb{C}^{n\times N})$, defined in Sec. II, where n refers to the number of labels needed to specify the tensor product and N is the dimension of the fundamental representation of the group.

We have shown in previous papers that all of the irreducible representations of the compact groups can be realized as polynomials in an appropriate Bargmann–Segal–Fock space; these we write as $f_{|\lambda\zeta\eta\rangle}(Z)$, where λ is the irreducible representation label and ξ is a basis label in the irreducible representation space. A p-fold tensor product state is then a product of these polynomials, written as $f_{|\lambda_1\xi_1\ldots\lambda_p\xi_p\rangle}(Z)\in\mathscr{F}(\mathbb{C}^{n\times N})$, where the irreducible representation labels $\lambda_1,\ldots,\lambda_p$ provide a total of n (nonzero) labels.

What is needed to compute Clebsch–Gordan and Racah coefficients are polynomial realizations of the direct sum basis elements, written $f_{|\lambda\zeta\eta\rangle}(Z)\in\mathscr{F}(\mathbb{C}^{n\times N})$. Here ζ is a (possibly new) set of basis labels in the λ irreducible representation space and η are multiplicity labels. The polynomials $f_{|\lambda\zeta\eta\rangle}(Z)$ are obtained by augmenting the tensor product $\lambda_1\otimes\cdots\otimes\lambda_p$ to $\lambda_1\otimes\cdots\otimes\lambda_p\otimes\lambda^{\vee}$, where $\lambda^{\vee}$ is the representation contragradient to λ, and looking for a set of functionally independent polynomial group invariants $\mathscr{I}_\eta(Z,W)$ in the augmented Bargmann–Segal–Fock space. As shown in Sec. II the number of such functionally independent polynomial invariants is just the multiplicity—the number of times the augmented tensor product contains the identity representation. In Sec. II we then showed that the polynomial $f_{|\lambda\zeta\eta\rangle}(Z)$ is, up to a normalization constant, the polynomial $f^{*}_{|\lambda^{\vee}\zeta^{\vee}\rangle}(D_w)\mathscr{I}_\eta(Z,W)|_{W=0}$.

There are many different ways of choosing a set of functionally independent group invariants to label the multiplicity. As shown through the example of SU(N) in Sec. III, these sets arise as products of fundamental group invariants satisfying certain transformation properties [see Eq. (3.2)]. As such they can be orthogonalized and used to label the multiplicity. However, it is desirable to have a more systematic procedure in which the invariants are manipulated to become eigenvectors of operators. The natural choice here are operators from the centralizer of the outer product group $G\times\cdots\times G$ with respect to G itself. That is, the operators are chosen from that set of operators in the universal enveloping algebra of the Lie algebra of $G\times\cdots\times G$ that commute with G. These operators can be specified more precisely by passing to the duals of $G\times\cdots\times G$ and G on $\mathscr{F}(\mathbb{C}^{n\times N})$. We plan to address the issue of operators from the centralizer being used to diagonalize invariant polynomials in a future paper. In any event, it is clear that the conventional Racah coefficients for SU(2), called $6J,9J,\ldots$ symbols, are all defined via centralizer elements; in this case these operators correspond to various choices of intermediate angular momentum operators.

The use of polynomial invariants allows for great flexibility in computing Clebsch–Gordan and Racah coefficients. It is possible to use any basis for both the tensor product and direct sum states. The price paid is that no attempt is made to find closed form expressions for the coefficients. Rather the goal is to specify procedures to a computer to obtain coefficients of physical interest. This is to be contrasted with other methods, such as that of Vilenkin and Klimyk (Ref. 2) or Prakash and Sharatchandra (Ref. 3), where basis choices are made at the outset [for SU(N) the Gelfand–Zetlin basis] and a specific choice for multiplicity is made (Vilenkin and Klimyk use the Biedenharn–Louck tensor operators). The goal is to find closed form expressions; the complexity of these coefficients, even for SU(3), suggests that while it would be nice to have such expressions, for physical applications much less is needed.

For example, often the irreducible representations generating the tensor product are the same; such is the case for various quark models, where p refers to the number of bound state quarks and the tensor product is the p-fold product of the fundamental representation of SU(6), with $N=6$

coming from the product of $SU(2)_{spin}$ and $SU(3)_{flavor}$. When $p=3$ one gets the standard picture of a baryon-one object (such as a proton) as a bound state of three quarks. However, there has been interest in five quark bound states, where one quark is a heavy anticharm quark, bound to four lighter quarks; then $p=4$.

In this situation it is desirable to label (direct sum) states by their permutation symmetry (in order to respect Pauli statistics). For $p=4$ the relevant group is S_4, the permutation group on four letters. However, this is equivalent to demanding that the invariant polynomials $\mathcal{I}_\eta(Z,W)$ transform as irreducible representations under S_4. In Sec. IV we have worked out several examples of invariant polynomials with definite permutation symmetry for the simpler SU(2) group to show how the multiplicity arising from threefold tensor products can be labeled by irreducible representations of S_3.

There remains the problem of using the known fundamental invariant polynomials of subgroups of SU(N) to calculate the invariants $\mathcal{I}_\eta(Z,W)$ for tensor products of subgroups such as SO(N) and Sp(N). This we intend to take up in a subsequent publication. Here again it should be possible to use computers to obtain invariant polynomials, and by differentiating these polynomials in the right way, compute Clebsch–Gordan and Racah coefficients for arbitrary tensor products of any compact group.

APPENDIX: HOLOMORPHIC REPRESENTATIONS OF GL(N,$\mathbb{C}$)

In this Appendix we will review some facts on holomorphic representations of GL(N,$\mathbb{C}$) and show explicitly how raising and lowering operators of an irreducible GL(N,$\mathbb{C}$)-module are mapped onto lowering and raising operators, respectively, of the corresponding contragradient module. Also we shall see how the highest weight vector is mapped onto the lowest weight vector in this correspondence. This theory allows us to realize explicitly the contragradient SU(N)-module V^{λ^*}, and have the tensor product $V^{\lambda_1}\otimes\cdots\otimes V^{\lambda_p}\otimes V^{\lambda^*}$, as a subspace of the Bargmann–Segal–Fock space $\mathcal{F}(\mathbb{C}^{n\times N})$ discussed in Secs. II–IV.

For $g\in\mathrm{GL}(N,\mathbb{C})$ we set

$$\Delta_\ell(g)=\begin{vmatrix} g_{11} & \cdots & g_{1\ell} \\ \vdots & & \\ g_{\ell 1} & \cdots & g_{\ell\ell} \end{vmatrix},$$

the ℓth minor of g, $1\leqslant\ell\leqslant N$. Then g is called *regular* if $\Delta_\ell(g)\neq 0$ for all ℓ. Let D_N, U_N^-, and U_N^+ denote the diagonal, lower triangular unipotent, and upper triangular unipotent subgroups of GL(N,$\mathbb{C}$), respectively. Then every regular element $g\in G$ can be uniquely represented in the form $g=duv$, where $d\in D_N$, $u\in U_N^-$, and $v\in U_N^+$ (see, e.g., Ref. 8, Chap. VI). Let T be a representation of GL(N,$\mathbb{C}$) in a finite-dimensional complex vector space V. Then a nonzero vector $f\in V$ is called a *weight vector* of *weight* α of the representation T with respect to D_N if $T(d)f=\alpha(d)f$, for all $d\in D_N$, where α is holomorphic character of D_N. A nonzero vector $f_{\max}\in V$ is called a *highest weight vector* with *highest weight* α of the representation T if, in addition to being a weight vector, $f_{\max}$ also satisfies

$$T(v)f_{\max}=f_{\max},\quad \text{for all } v\in U_N^+.$$

Similarly, a nonzero vector $f_{\min}\in V$ is called a *lowest weight vector* of *lowest weight* β if

$$T(d)f_{\min}=\beta(d)f_{\min},\quad \text{and}\quad T(u)f_{\min}=f_{\min}\quad \text{for all } d\in D_N, u\in U_N^-.$$

Now let V^λ denote an irreducible holomorphic representation of GL(N,$\mathbb{C}$) with signature λ. Then V^λ can be explicitly realized on a space of holomorphic functions on $\mathbb{C}^{N\times N}$. The signature $\lambda\equiv\lambda_{(m)}$ is a holomorphic character of D_N defined by

$$\lambda(d)=d_1^{m_1}\cdots d_N^{m_N},\quad d=(d_1,\ldots,d_N)\in D_N,$$

where the m_is are integers which satisfy the dominant condition $m_1\geqslant m_2\geqslant\cdots\geqslant m_N$. Then the space V^λ consists of all holomorphic functions f on $\mathbb{C}^{N\times N}$ which satisfy the covariant condition

$$f(duZ)=\lambda(d)f(Z),\quad \text{for all}\quad d\in D_N, u\in U_N^-,$$

and $Z\in\mathbb{C}^{N\times N}$. The representation R^λ is defined on V^λ by the formula

$$[R^\lambda(g)f](Z)=f(Zg),\quad \text{for all}\quad g\in \mathrm{GL}(N,\mathbb{C}).$$

Then it can be shown (see, e.g., Ref. 3, Chap. VI) that V^λ admits a ''unique'' (i.e., up to a nonzero scalar multiple) highest weight vector $f_{\max}$ of weight $\lambda_{(m)}=(m_1,\ldots,m_N)$, and a ''unique'' lowest weight vector $f_{\min}$ of weight $(m_N,m_{N-1},\ldots,m_1)$. In fact, $f_{\max}$ can be defined as

$$f_{\max}(Z)=\Delta_1^{m_1-m_2}(Z)\Delta_2^{m_2-m_3}(Z)\cdots\Delta_N^{m_N}(Z),$$

and it is straightforward to verify that $f_{\max}(dZ)=d_1^{m_1}\cdots d_N^{m_N}f_{\max}(Z)$, and $f_{\max}(Zv)=f_{\max}$, for all $d\in D_N$ and $v\in U_N^+$. Let

$$s=\begin{bmatrix} & & 1\\ & \iddots & \\ 1 & & \end{bmatrix}$$

be the $N\times N$ matrix with 1's on the reverse diagonal and 0 elsewhere, and define $f_{\min}=R^\lambda(s)f_{\max}$. Then

$$Z_s=\begin{bmatrix} Z_{1N} & Z_{1,N-1} & \ldots Z_{12} & Z_{11}\\ \vdots & \vdots & \vdots & \vdots\\ Z_{NN} & Z_{N,N-1} & \ldots Z_{N2} & Z_{N1}\end{bmatrix},$$

$$\Delta_\ell(Zs)=\begin{vmatrix} Z_{1N} & \ldots & Z_{1,N-i+1}\\ \vdots & & \vdots\\ Z_{\ell,N} & & Z_{\ell,N-i+1}\end{vmatrix}=(-1)\mathrm{sgn}(\sigma)\begin{vmatrix} Z_{1,N-i+1} & \ldots & Z_{1N}\\ \vdots & & \\ Z_{\ell,N-i+1} & \ldots & Z_{\ell,N}\end{vmatrix},$$

where $\mathrm{sgn}(\sigma)$ is the sign of the permutation

$$\sigma=\begin{pmatrix} N-\ell+1 & N-\ell+2 & \ldots & N\\ N & N-1 & & N-\ell+1\end{pmatrix},$$

and

$$f_{\min}(Z)=(\Delta_1(Zs))^{m_1-m_2}\cdots(\Delta_N(Zs))^{m_N}.$$

It follows that

$$[R^\lambda(d)f_{\min}](Z)=[R^\lambda(d)(R^\lambda(s)f_{\max})](Z)=f_{\max}(Zds)=f_{\max}(Zs(sds))=d_1^{m_N}\cdots d_N^{m_1}f_{\max}(Zs)$$
$$=d_1^{m_N}\cdots d_N^{m_1}f_{\min}(Z)$$

since $s=s^{-1}$ and $sds=(d_N,\ldots,d_1)$. Also,

$$[R^{\lambda}(u)f_{\min}(Z)=[R^{\lambda}(u)(R^{\lambda}(s)f_{\max})](Z)=f_{\max}(Zus)=f_{\max}(Zs(sus)),\quad u\in U^{-}.$$

However, it is easy to verify that $sus\in U^{+}$ so that

$$f_{\max}(Zs(sus))=f_{\max}(Zs)=f_{\min}(Z).$$

The differential representation of R^{λ} is given by the infinitesimal generators

$$R^{\lambda}_{ij}=\sum_{s=1,\ldots,N} Z_{is}\frac{\partial}{\partial Z_{js}},\quad 1\leqslant i,j\leqslant N.$$

The differential operators R^{λ}_{ij} with $i<j$ (resp. $i>j$) are called *raising* (resp. lowering) operators. It follows immediately that, in terms of raising and lowering operators, a highest vector $f_{\max}$ (resp. lowest weight vector $f_{\min}$) is characterized by the condition

$$R^{\lambda}_{ij}f_{\max}=0,\quad \forall i<j(\text{resp. } R^{\lambda}_{ij}f_{\min}=0,\forall i>j).$$

Let $(R^{\lambda})^{\vee}$ denote the contragradient representation of R^{λ} on $(V^{\lambda})^{*}$, the dual of V. Then $(R^{\lambda})^{\vee}$ is defined by the equation

$$[(R^{\lambda})^{\vee}(g)f^{*}](h)=f^{*}(R^{\lambda}(g^{-1})h),\quad \text{for all } g\in \mathrm{GL}(N,\mathbb{C}),f^{*}\in(V^{\lambda})^{*},\quad \text{and } h\in V^{\lambda}.$$

Let Φ: $V^{\lambda}\to(V^{\lambda})^{*}$ denote the conjugate-linear isomorphism introduced in Sec. II. Then it is easy to show, using Eq. (2.2), that Φ intertwines R^{λ} and $(R^{\lambda})^{\vee}$. We have the following:

Theorem A1: *Let* $(R^{\lambda},V^{\lambda})$ *be an irreducible holomorphic representation of* $\mathrm{GL}(N,\mathbb{C})$ *and let* $((R^{\lambda})^{\vee},(V^{\lambda})^{*})$ *be the contragradient* $\mathrm{GL}(N,\mathbb{C})$*-module. Under the map* Φ: $V^{\lambda}\to(V^{\lambda})^{*}$ *defined above, the raising operators of* R^{λ} *are mapped onto the lowering operators of* $(R^{\lambda})^{\vee}$ *and vice versa. Moreover, the highest weight vector of* R^{λ} *is mapped onto the lowest weight vector of* $(R^{\lambda})^{\vee}$*, and vice versa.*

Proof: Let $\mathscr{B}=\{f_i\}$ be a basis for V^{λ} and let $\mathscr{B}^{*}=\{f_i^{*}\}$ be its dual basis defined by

$$f_i^{*}(f_j)=\delta_{ij},\quad \forall i_{ij}.$$

Then $(R^{\lambda})^{\vee}(g)f_i^{*}=\Sigma_k(D^{\lambda})^{\vee}_{ki}(g)f_k^{*}$, where $(D_{\lambda})^{\vee}_{ki}(g)$ are the matrix coefficients of $(R^{\lambda})^{\vee}(g)$ relative to $\mathscr{B}^{*}$. Therefore,

$$[(R^{\lambda})^{\vee}(g)f_i^{*}](f_j)=\sum_k (D^{\lambda})^{\vee}_{ki}(g)f_k^{*}(f_j)=(D^{\lambda})^{\vee}_{ji}(g).$$

On the other hand, by definition

$$[(R^{\lambda})^{Nr}(g)(fi^{*})](f_i):=f_i^{*}((R^{\lambda})(g^{-1})f_j)=f_i^{*}\left(\sum_k D^{\lambda}_{kj}(g^{-1})f_k\right)=\sum_k D^{\lambda}_{kj}(g^{-1})f_i^{*}(f_k)$$

$$=D^{\lambda}_{ij}(g^{-1}).$$

Thus we have the following equations:

$$(D^{\lambda})^{\vee}_{ij}(g)=D^{\lambda}_{ji}(g^{-1})\quad \forall i,j,\quad \text{or } [(R^{\lambda})^{\vee}(g)]_{\mathscr{B}^{*}}=[R^{\lambda}(g^{-1})]^{t}_{\mathscr{B}}. \tag{A1}$$

From the matrix form of Eq. (A1) it follows that the infinitesimal operators of R^{λ} and $(R^{\lambda})^{\vee}$ are in a one-to-one correspondence:

$$(R^{\lambda})^{\surd}_{ij} \leftrightarrow -R^{\lambda}_{ji}, \quad 1 \leqslant i,j \leqslant N. \tag{A2}$$

From Eq. (A2) it follows that raising operators of R^{λ} correspond to lowering operators of $(R^{\lambda})^{\surd}$, and vice versa.

If $f_{\max}$ is a highest weight vector of R^{λ}, then by definition

$$\begin{aligned} R^{\lambda}_{ii} f_{\max} &= m_i f_{\max} \quad \forall i = 1,\ldots,N, \\ R^{\lambda}_{ij} f_{\max} &= 0 \quad \forall \leqslant i < j \leqslant N. \end{aligned} \tag{A3}$$

Using the fact that Φ: $V^{\lambda} \rightarrow (V^{\lambda})^*$ is a conjugate-linear intertwining operator and Eq. (A2) we see that

$$\begin{aligned} (R^{\lambda})^{\surd}_{ii} \Phi(f_{\max}) &= \Phi(-R^{\lambda}_{ii} f_{\max}) = -m_i \Phi(f_{\max}) \quad \forall i = 1,\ldots,N, \\ (R^{\lambda})^{\surd}_{ij} \Phi(f_{\max}) &= \Phi(-R^{\lambda}_{ij} f_{\max}) = \Phi(0) \quad \text{for all } 1 \leqslant i < j \leqslant N. \end{aligned} \tag{A4}$$

Equation (A4) shows that $\Phi(f_{\max})$ is the lowest weight vector of $(R^{\lambda})^{\surd}$ [where $\lambda^{\surd} = -(m_N,\ldots,-m_1)$] with weight $(-m_1,\ldots,-m_N)$. Similarly, one can show that $\Phi(f_{\min})$ is the highest weight vector of $(R^{\lambda})^{\surd}$ with weight $(-m_N,\ldots,-m_1)$. □

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On the essential spectrum of transport operators on L_1-spaces

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In a recent article by the first author [J. Math. Phys. **35**, 6199–6212 (1994)] the essential spectrum of transport operator was analyzed in L_p-spaces for $p \in (1,+\infty)$. The purpose of the present work is to extend this analysis to the case of L_1-spaces. After establishing preliminary results we define the notion of the weak spectrum which we characterize by means of Fredholm operators. We show, in particular, that in L_1-spaces the weak spectrum is nothing else but the essential spectrum. Using the same techniques as in the above-mentioned work, we prove the stability of the essential spectrum of a one-dimensional transport operator with general boundary conditions where an abstract boundary operator relates the incoming and the outgoing fluxes. Sufficient conditions are given in terms of boundary and collision operators, assuring the stability of the essential spectrum. We show also that our results remain valid for neutron transport operators in arbitrary dimension.
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I. INTRODUCTION

In this article we are concerned with the essential spectrum of the following integrodifferential operator

$$A_H\psi(x,\xi) = -\xi\,\frac{\partial\psi}{\partial x}(x,\xi)\sigma(\xi)\psi(x,\xi) + \int_{-1}^{1}\kappa(\xi,\xi')\psi(x,\xi')d\xi' = T_H\psi + K\psi \tag{1.1}$$

with general boundary conditions where $x \in [-a,\ a]$ for a parameter $0<a<\infty$ and $\xi\in[-1,\ 1]$. This operator describes the transport of particles (neutrons, photons, molecules of gas, etc.) in a plane parallel domain with a width of $2a$ mean free paths. The function $\psi(x,\xi)$ represents the number (or probability) density of gas particles having the position x and the direction cosine of propagation ξ. The function $\sigma(.)$ and $\kappa(.,.)$ are called, respectively, the collision frequency and the scattering kernel. The boundary conditions are modeled by

$$\psi_{|\Gamma_-} = H(\psi_{|\Gamma_+}), \tag{1.2}$$

where Γ_- (resp. Γ_+) is the incoming (resp. outgoing) part of the phase space boundary, $\psi_{|\Gamma_-}$ (resp. $\psi_{|\Gamma_+}$) is the restriction of ψ to Γ_- (resp. Γ_+), and H is a linear bounded operator from a suitable function space on Γ_- to a similar one on Γ_+. The known classical boundary conditions (vacuum boundary, specular reflections, periodic, diffuse reflections, generalized and mixed type boundary conditions[1–5]) are special examples of our general framework. Our general assumptions are

$$\begin{cases} \sigma(.) \in L^{\infty}(-1,1), \\ H \text{ is a bounded boundary operator}, \\ K \in \mathscr{L}(L_1[(-a,a)\times(-1,1)]), \end{cases}$$

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where K is the partially integral operator with kernel $\kappa(\xi,\xi')$.

In Ref. 6, the essential spectrum of the operator (1.1) supplemented with the boundary conditions (1.2) was investigated on L_p-spaces for $p\in(1,+\infty)$. In particular, it has been proved that if K is regular (see Definition 4.1), then $\sigma_{\text{ess}}(T_H+K)=\sigma_{\text{ess}}(T_H)$ regardless of the boundary operator H [$\sigma_{\text{ess}}(.)$ denotes the essential spectrum]. Further, sufficient conditions on the boundary operator H under which $\sigma_{\text{ess}}(T_H)=\sigma_{\text{ess}}(T_0)$ were given where T_0 is the well-known streaming operator in neutron transport theory ($H=0$) whose spectrum was analyzed in detail in Ref. 6.

Note that even though the spectral theory of transport operators is a classical theme in transport theory, generally, the analysis focuses on the point spectrum of these operators (see, for instance, any of Refs. 7–13). In fact, the knowledge of the (peripheral) point spectrum permits us to obtain a simple description of the time asymptotic behavior ($t\to\infty$) of the solution of the associated Cauchy problem (cf. Ref. 7, 12, 14, or 15).

The purpose of the present work is to investigate the essential spectrum of a one-dimensional transport operator with general boundary conditions and to extend the results obtained in Ref. 6 to L_1-spaces. The idea may be summarized as follows:

Let (Ω,Σ,μ) be an arbitrary positive measure space. After some abstract preliminary results, we define the notion of the weak spectrum [which we denote by $\sigma_w(.)$] on $L_1(\Omega,d\mu)$ and we prove that if B and C are closed densely defined linear operators on $L_1(\Omega,d\mu)$ and if for some $\lambda\in\rho(B)\cap\rho(C)$, the operator $(\lambda-B)^{-1}-(\lambda-C)^{-1}$ is a weakly compact, then $\sigma_w(B)=\sigma_w(C)$. Second, we show the equality (in the sense of the inclusion) of the sets $\sigma_{\text{ess}}(.)$ and $\sigma_w(.)$ on $L_1(\Omega,d\mu)$. Finally, using these remarks, the same strategy as in Ref. 6 leads to the desired results on $L_1[(-a,a)\times(-1,1),dxd\xi]$.

The plan of this article is as follows. In Sec. II, some preliminary abstract results concerning Fredholm operators needed in the sequel are given. Section III is devoted to the analysis of the weak spectrum on L_1-spaces. The main results of this section are Theorems 3.1 and 3.2. In Sec. IV we take advantage of the results of the previous sections to prove the stability of the essential spectrum of a one-dimensional transport operator with general boundary conditions. Sufficient conditions in terms of H and K assuring the stability of the essential spectrum are given. We close this section by discussing the essential spectrum of a transport operator with vacuum boundary conditions in arbitrary dimension.

II. PRELIMINARY RESULTS

Let Z be a Banach space. A closed densely defined linear operator A with domain $D(A)$ is said to be Fredholm if $R(A)$ is closed and both $\alpha(A)=\dim[N(A)]$ and $\beta(A)=\operatorname{codim}[R(A)]$ are finite where $R(A)$ and $N(A)$ are, respectively, the range and the null space of A. The set of Fredholm operators on Z is denoted by $\Phi(Z)$ while the number $i(A)=\alpha(A)-\beta(A)$ is called the index of A. We denote by Φ_A the set

$$\Phi_A:=\{\lambda\in\mathbf{C}\ \text{such that}\ \lambda-A\ \text{is a Fredholm operator on}\ Z\}.$$

We define the essential spectrum of A by

$$\sigma_{\text{ess}}(A)=\bigcap_{C\in\mathscr{K}(Z)}\sigma(A+C),$$

where $\mathscr{K}(Z)$ stands for the ideal of all compact operators on Z.

Similarly, we define the weak spectrum of A by

$$\sigma_w(A)=\bigcap_{F\in\mathscr{F}(Z)}\sigma(A+F),$$

where $\mathscr{F}(Z)$ denotes the set of all weakly compact operators on Z.

Let $\mathscr{P}(Z)$ denote the set

$$\mathscr{P}(Z)=\{F\in\mathscr{L}(Z) \text{ such that there exists } r\in\mathbf{N}^* \text{ satisfying } F^r\in\mathscr{K}(Z)\}.$$

We first prove the following auxiliary lemma:

Lemma 2.1: Let F be an arbitrary element of $\mathscr{P}(Z)$ and set $A=I-F$. Then

(i) *dim*$[N(A)]<\infty$,

(ii) $R(A)$ *is closed,*

(iii) *codim*$[R(A)]<\infty$. ◇

Proof: (i) Since $F\in\mathscr{P}(Z)$, there exists $r\in N^*$ such that $F^r\in.\mathscr{K}(Z)$. Let $x\in N(A)$, then $F^rx=x$, i.e., $x\in N(I-F^r)$ and therefore $N(A)\subset N(I-F^r)$. On the other hand, the identity I restricted to the kernel of $(I-F^r)$ is equal to F^r and consequently compact. Hence $N(I-F^r)$ is finite dimensional and therefore dim$[N(A)]<\infty$.

(ii) Since A commutes with I, Newton's binomial formula gives

$$F^r=(I-A)^r=I+\sum_{k=1}^{r}(-1)^kC_r^kA^k. \tag{2.1}$$

Let E be a closed complement for $N(A)$, so that $Z=N(A)\oplus E$. Thus, we obtain two linear continuous maps $A_{|E}:E\to Z$ and $F_{|E}:E\to Z$, the restrictions of A and F to E. It is clear that the kernel of $A_{|E}$ is $\{0\}$. In order to conclude, it suffices to show that $A_{|E}(E)=A(E)=A(Z)$ is closed. For this it suffices to show that the map $(A_{|E})^{-1}:A(E)\to E$ is continuous. By linearity, it even suffices to prove that $(A_{|E})^{-1}$ is continuous at 0. Suppose that this is not the case. Then we can find a sequence $\{x_n\}$ in E such that $Ax_n\to 0$, but $\{x_n\}$ does not converge to 0. Selecting a suitable subsequence we can assume without loss of generality that $\|x_n\|\geqslant\eta>0$ for all n. Then $1/\|x_n\|\leqslant 1/\eta$ for all n and consequently $A(x_n/\|x_n\|)$ also converges to 0. Furthermore, $x_n/\|x_n\|$ has norm 1, and hence some subsequence of $F^r(x_n/\|x_n\|)$ converges. It follows from (2.1) that $x_n/\|x_n\|$ has a converging subsequence to an element z in E verifying $\|z\|=1$ and $F^r(z)=z$. On the other hand, $F^r=F-FA-F^2A-\cdots-F^{r-1}A$ and so we get $F^r(z)=F(z)$. Hence, we infer that $F(z)-z=0$, which implies that $z\in N(A)$. This contradicts the fact that $E\cap N(A)=\{0\}$ (because $\|z\|=1$) and completes the proof of (ii).

(iii) If $A(Z)$ does not have finite codimension, we can find a sequence of closed subspaces

$$A(Z)=M_0\subset M_1\subset M_2\subset\cdots\subset M_n\subset\cdots$$

such that each M_n is closed and of codimension 1 in M_{n+1} just by adding one-dimensional spaces to $A(Z)$ inductively. By Riesz's lemma (Ref. 16, Lemma 3, p. 578) we can find in each M_n an element x_n such that $\|x_n\|=1$ and $\|x_n-y\|\geqslant 1-\varepsilon$ for all y in M_{n-1} with $0<\varepsilon<1$. Then, by using (2.1) together with the fact that $Z\supset R(A)\supset R(A^2)\supset\cdots\supset R(A^n)\supset\cdots$, for all $k<n$ we get

$$\begin{aligned}\|F^rx_n-F^rx_k\|&=\left\|x_n-\sum_{i=1}^{r}(-1)^iC_r^iA^ix_n-x_k+\sum_{i=1}^{r}(-1)^iC_r^iA^ix_k\right\|\\&=\left\|x_n-x_k-\sum_{i=1}^{r}(-1)^iC_r^iA^i(x_n-x_k)\right\|\geqslant 1-\epsilon\end{aligned}$$

because $x_k+\Sigma_{i=1}^{r}(-1)^iC_r^iA^i(x_n-x_k)\in M_{n-1}$. This proves that the sequence $(F^rx_n)_n$ cannot have a convergent subsequence, and contradicts the compactness of F^r. Q.E.D.

Theorem 2.1: *Assume that the hypothesis of Lemma 2.1 holds. Then $A=I-F$ is a Fredholm operator and $i(A)=0$.* ◇

Proof: The first part of the theorem follows from Lemma 2.1. In order to complete the proof it suffices to show that dim$[N(A)]=$dim$[R(A)^{\perp}]$. To do this, note first that the operator dual A' of A is given by $A'=I'-F'$. The use of Schauder's theorem and Lemma 2.1 (i) gives

$\dim[N(A')]<\infty$. Accordingly, by using the relation $R(A)^{\perp}=N(A')$, we need only to prove $\dim[N(A)]=\dim[N(A')]$. Now the rest of the proof may be sketched in a similar way to that in Ref. 17, pp. 94–100. It suffices to replace $\|Fz_n-Fz_m\|$ by $\|F^r z_n-F^r z_m\|$ and to use the relation $F^r=F-FA-F^2A-\cdots-F^{r-}A$. The details are therefore omitted.

Q.E.D.

Remark 2.1: Note that for $r=1$, Theorem 2.1 is nothing but the classical Riesz's theorem for compact operators (see, for instance, Ref. 17, Theorem 3.2, p. 94). ◇

We close this section with the following result which we need in the sequel.

Theorem 2.2: *Let A be a closed densely defined operator on Z. Suppose that there exist $A_1, A_2 \in \mathscr{L}(Z)$, $F_1, F_2 \in \mathscr{F}(Z)$ such that $A_1A=I-F_1$ on $D(A)$ and $AA_2=I-F_2$ on Z. Then $A \in \Phi(Z)$.* ◇

Proof: In view of the fact that $N(A)\subset N(A_1A)$, we have $\alpha(A)\leqslant\alpha(I-F_1)$. On the other hand, $R(A)\supset R(AA_2)=R(I-F_2)$ and therefore $R(A)^{\perp}\subset R(I-F_2)^{\perp}$. Accordingly, we have $\beta(A)\leqslant\alpha(I'-F_2')$. Now Theorem 2.1 together with Schauder's theorem gives $\alpha(A)<\infty$ and $\beta(A)<\infty$. In order to complete the proof it suffices to show that $R(A)$ is closed. This last assertion follows from Ref. 17, Lemma 2.2, p. 111. Q.E.D.

Theorem 2.2 generalizes Theorem 1.2, p. 163, in Ref. 17.

III. THE IDENTITY OF $\sigma_w(.)$ AND $\sigma_{ess}(.)$ ON L_1-SPACES

In this section we are concerned with the study of the essential spectrum on L_1-spaces. In particular, we prove the equality (in the sense of the inclusion) of the sets $\sigma_w(A)$ and $\sigma_{ess}(A)$, where A is a closed densely defined linear operator. The analysis is essentially based on the results obtained in the previous section.

Let (Ω,Σ,μ) be an arbitrary positive measure space. Throughout this section X_1 denotes the space $L_1(\Omega,d\mu)$.

Theorem 3.1: *Let A be a closed densely defined linear operator on X_1. Then we have*

$$\sigma_w(A)=\sigma_{ess}(A).$$

. ◇

Proof: From $\mathscr{K}(X_1)\subset\mathscr{F}(X_1)$ we infer that $\sigma_w(A)\subset\sigma_{ess}(A)$. In order to conclude, it suffices to show that $\sigma_{ess}(A)\subset\sigma_w(A)$. To this end, suppose that $\lambda\notin\sigma_w(A)$. Then there exists $F\in\mathscr{F}(X_1)$ such that $\lambda\in\rho(A+F)$. This implies that $\lambda\in\Phi_{(A+F)}$ and $i(\lambda-A-F)=0$. Since $F\in\mathscr{F}(X_1)$ we have $(\lambda-A-F)^{-1}F\in\mathscr{F}(X_1)$. Hence by Ref. 16, Corollary 13, p. 510, we get $[(\lambda-A-F)^{-1}F]^2\in\mathscr{K}(X_1)$. Now by representing $\lambda-A$ as $\lambda-A=(\lambda-A-F)[I+(\lambda-A-F)^{-1}F]$ and by using Ref. 17, Theorem 1.3, p. 163, together with Theorem 2.1, we obtain $\lambda\in\Phi_A$ and $i(\lambda-A)=0$. Now Ref. 18, Theorem 4.5, p. 15, gives the wanted inclusion and achieves the proof. Q.E.D.

By Theorem 3.1 and Ref. 6, Lemma 4.1, we have the following:

Corollary 3.1: Let A be a closed densely defined linear operator on X_1. Then

(i) $\sigma C(A)\subset\sigma_w(A)$,
(ii) $\sigma R(A)\subset\sigma_w(A)$,

where $\sigma C(A)$ [resp. $\sigma R(A)$] denotes the continuous spectrum (resp. the residual spectrum) of A. ◇

The following result provides a characterization of the weak spectrum on L_1-spaces.

Corollary 3.2: Let A be a closed densely defined linear operator on X_1. Then

$$\lambda\notin\sigma_w(A) \text{ if and only if } \lambda\in\Phi_A \text{ and } i(\lambda-A)=0.$$

◇

Proof: This corollary immediately follows from Theorem 3.1 and Ref. 18, Theorem 4.5, p. 15. Q.E.D.

We end this section with the following result which provides a practical criterion for the stability of the weak spectrum on L_1-spaces.

Theorem 3.2: *Let A, B be closed densely defined operators on X_1. If for some $\lambda \in \rho(A) \cap \rho(B)$ the operator $(\lambda - A)^{-1} - (\lambda - B)^{-1}$ is weakly compact on X_1, then*

$$\sigma_w(A) = \sigma_w(B).$$

◇

Proof: Without loss of generality, suppose $\lambda = 0$. Thus $A^{-1} = B^{-1} + F$ where F is a weakly compact operator on X_1. Let $\mu \in \Phi_{A^{-1}}$. Then by Ref. 17, Theorem 2.1, p. 110, there exist $A_1, A_2 \in \mathscr{L}(X_1)$ and $K_1, K_2 \in \mathscr{K}(X_1)$ such that $(\mu - A^{-1})A_1 = I - K_1$ and $A_2(\mu - A^{-1}) = I - K_2$. This implies

$$(\mu - B^{-1})A_1 = I - K_1 + FA_1 = I - F_1,$$

$$A_2(\mu - B^{-1}) = I - K_2 + A_2F = I - F_2,$$

where $F_1 = K_1 - FA_1$ and $F_2 = K_2 - A_2F$ are weakly compact. It follows from Theorem 2.2 that $\mu \in \Phi_{B^{-1}}$, i.e., $\Phi_{A^{-1}} \subset \Phi_{B^{-1}}$. Similarly, by writing $B^{-1} = A^{-1} - F$, we obtain $\Phi_{B^{-1}} \subset \Phi_{A^{-1}}$ and consequently $\Phi_{A^{-1}} = \Phi_{B^{-1}}$. On the other hand, the weak compactness of F_1 and F_2, Ref. 16, Corollary 13, p. 510, and Theorem 2.1 give $i(\mu - A^{-1}) = i(\mu - B^{-1})$ for all $\mu \in \Phi_{A^{-1}}$. Hence, by using Ref. 18, Lemma 4.6, p. 16, we obtain $\Phi_A = \Phi_B$ and $i(\tau - A) = i(\tau - B)$ for all $\tau \in \Phi_A$. The result is now a consequence of Corollary 3.2. Q.E.D.

IV. APPLICATION TO TRANSPORT EQUATIONS

The aim of this section is the analysis of the essential spectrum of one-dimensional transport operators with abstract boundary conditions on L_1-spaces. Our analysis uses the results of Secs. II and III and follows closely Ref. 6.

Let

$$X = L_1[(-a,a) \times (-1,1); dx d\xi], \quad a > 0,$$

and

$$X^o := L_1[\{-a\} \times (-1,0); |\xi| d\xi] \times L_1[\{a\} \times (0,1); |\xi| d\xi] := X_1^o \times X_2^o$$

equipped with the norm

$$\|\psi^o; X^o\| = \|\psi_1^o; X_1^o\| + \|\psi_2^o; X_2^o\| = \int_{-1}^{0} |\psi(-a,\xi)||\xi| d\xi + \int_{0}^{1} |\psi(a,\xi)||\xi| d\xi,$$

and

$$X^i := L_1[\{-a\} \times (0,1); |\xi| d\xi] \times L_1[\{a\} \times (-1,0); |\xi| d\xi] := X_1^i \times X_2^i$$

equipped with the norm

$$\|\psi^i; X^i\| = \|\psi_1^i; X_1^i\| + \|\psi_2^i; X_2^i\| = \int_{0}^{1} |\psi(-a,\xi)||\xi| d\xi + \int_{-1}^{0} |\psi(a,\xi)||\xi| d\xi.$$

We define the partial Sobolev space W by

$$W=\left\{\psi\in X \text{ such that } \xi\frac{\partial\psi}{\partial x}\in X\right\}.$$

It is well known that any function $\psi\in W$ has traces on $\{-a\}$ and $\{a\}$ in X^o and X^i (see, for instance, Ref. 19 or 20). They are denoted, respectively, by ψ^o and ψ^i, and represent the outgoing and the incoming fluxes (''o'' for outgoing and ''i'' for incoming).

Let H be the following boundary operator:

$$\begin{cases} H:X^o\to X^i, \\ u\to Hu, \\ Hu:=\begin{pmatrix} H_{11} & H_{12}\\ H_{21} & H_{22}\end{pmatrix}\begin{pmatrix} u_1\\ u_2\end{pmatrix}, \end{cases}$$

where $H_{11}\in\mathscr{L}(X_1^o,X_1^i)$, $H_{12}\in\mathscr{L}(X_2^o,X_1^i)$, $H_{21}\in\mathscr{L}(X_1^o,X_2^i)$, and $H_{22}\in\mathscr{L}(X_2^o,X_2^i)$.

We define the streaming operator T_H by

$$\begin{cases} T_H:D(T_H)\subset X\to X, \\ \psi\to T_H\psi(x,\xi)=-\xi\dfrac{\partial\psi}{\partial x}-\sigma(\xi)\psi(x,\xi), \\ D(T_H)=\{\psi\in W \text{ such that } H\psi^o=\psi^i\}. \end{cases}$$

Let

$$\lambda_0:=\begin{cases} -\lambda^*, & \text{if } \|H\|\leqslant 1, \\ -\lambda^*+\dfrac{1}{2a}\operatorname{Log}(\|H\|), & \text{if } \|H\|>1, \end{cases}$$

where

$$\lambda^*=-\lim_{|\xi|\to 0}\inf\sigma(\xi).$$

For $\operatorname{Re}\lambda>\lambda_0$, $\lambda\in\rho(T_H)$ and the resolvent of T_H are given by

$$(\lambda-T_H)^{-1}=\sum_{n\geqslant 0}B_\lambda H(M_\lambda H)^n G_\lambda+C_\lambda,$$

where B_λ, C_λ, G_λ, and M_λ are linear bounded operators. For the details, see Ref. 21. Note that C_λ is nothing but $(\lambda-T_0)^{-1}$, so we have

$$(\lambda-T_H)^{-1}-(\lambda-T_0)^{-1}=Q_\lambda,$$

where $Q_\lambda=\Sigma_{n\geqslant 0}B_\lambda H(M_\lambda H)^n G_\lambda$.

Theorem 4.1: *Let H be a bounded boundary operator. If H is weakly compact, then*

$$\sigma_{\text{ess}}(T_H)=\sigma_{\text{ess}}(T_0).$$

◇

Proof: The weak compactness of H implies that of Q_λ on X. In view of Theorem 3.2, we have $\sigma_w(T_H)=\sigma_w(T_0)$. Now, the result follows from Theorem 3.1. Q.E.D.

Remark 4.1: It should be noted that Theorem 4.1 shows not only that the result of Ref. 6, Theorem 4.1, remains valid for $p=1$ but also the hypothesis on the boundary operator H may be weakened. ◇

Remark 4.2: Let $\widetilde{H}$ be the boundary operator defined by

$$\begin{cases} \widetilde{H}: X^0 \to X^i, \\ u \to \widetilde{H}u, \\ \widetilde{H}u = \begin{pmatrix} H_{11} & 0 \\ H_{21} & 0 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}, \end{cases}$$

where

$$\begin{cases} H_{11}: X_1^0 \to X_1^i, \\ u(-a,\xi) \to u(-a,\xi), \end{cases}$$

and H_{21} is an arbitrary operator of $\mathscr{L}(X_1^o, X_2^i)$. In spite of the fact that $\widetilde{H}$ is not compact, it has shown in Ref. 6, Proposition 4.1, that $\sigma_{\text{ess}}(T_{\widetilde{H}}) = \sigma_{\text{ess}}(T_0)$. Since H_{11} and H_{22} are not weakly compact, the operator $\widetilde{H}$ is not weakly compact either. So, by a similar reasoning to that in the proof of Ref. 6, Proposition 4.1, we get $\sigma_{\text{ess}}(T_{\widetilde{H}}) = \sigma_{\text{ess}}(T_0)$. This shows that the result of Theorem 4.1 is not optimal. ◇

Next we consider the transport operator $A_H := T_H + K$, where K is a bounded partially integral operator on X defined by

$$\begin{cases} K: X \to X, \\ \psi \to \displaystyle\int_{-1}^{1} \kappa(\xi,\xi')\psi(x,\xi')d\xi'. \end{cases}$$

The scattering kernel $\kappa: (-1,1)\times(-1,1) \to \mathbf{R}$ is assumed to be measurable.

Definition 4.1: A bounded operator K, defined as above, is said to be regular if its restriction to $L_1([-1,1],d\xi)$ is compact. ◇

Remark 4.3: Note that the fact that K is regular does not imply the compactness of K on X. To see this, suppose that $\kappa(\xi,\xi') = f(\xi)g(\xi')$ where $f \in L_1([-1,1],d\xi)$, $g \in L^{\infty}([-1,1],d\xi)$. Thus K is regular because it is of rank one on $L_1([-1,1],d\xi)$ but it is not compact on X because its spectrum $\sigma(K) = \overline{\{f(\xi), -1 \leqslant \xi \leqslant 1\}}$ is not necessary discrete. ◇

Let $\lambda \in \rho(T_H)$ be such that $r_\sigma[(\lambda - T_H)^{-1}K] < 1$ [$r_\sigma(.)$ denotes the spectral radius]. Then $\lambda \in \rho(A_H)$ and

$$(\lambda - A_H)^{-1} - (\lambda - T_H)^{-1} = \sum_{n \geqslant 1} [(\lambda - T_H)^{-1}K]^n (\lambda - T_H)^{-1}. \tag{4.1}$$

By using Eq. (4.1), Theorems 3.1 and 3.2, and Ref. 21, Theorem 2.1, we have the following.

Theorem 4.2: *Let H be a bounded boundary operator. Assume that the collision operator K is regular on X. Then*

$$\sigma_{\text{ess}}(A_H) = \sigma_{\text{ess}}(T_H). \quad \diamond$$

Theorems 4.1 and 4.2 and Ref. 6, Theorem 3.1, imply the following:

Corollary 4.1: Let H be a bounded boudary operator. If K is regular on X and H is weakly compact, then

$$\sigma_{\text{ess}}(A_H)=\{\lambda\in\mathbf{C}\ \ such\ \ that\ \ \text{Re}\ \lambda\leqslant-\lambda^*\}.$$ ◇

Remark 4.4: Theorems 4.2 and 4.3 and Corollary 4.1 generalize the results of Ref. 6 to the case $p=1$ and give positive answers to the problems indicated therein. ◇

We close this section by discussing briefly the essential spectrum of the multidimensional neutron transport equation. To this purpose, consider the neutron transport operator

$$A_0\psi(x,v)=-v\ \frac{\partial\psi}{\partial x}\ (x,v)-\sigma(v)\psi(x,v)+\int_V\kappa(v,v')\psi(x,v')dv'=T_0\psi+K\psi,$$

where T_0 is the streaming operator and K denotes the integral part of A_0 (the collision operator), $(x,v)\in D\times V$, where the configuration space D is an open and bounded subset of R^N, $N\geqslant 1$. The velocity space V is an arbitrary open subset of R^N. The unbounded operator A_0 (i.e., $H=0$) is studied in the Banach space $L_1(D\times V)$. Its domain is

$$D(A_0)=D(T_0)=\left\{\psi\in L_1(D\times V)\text{such that}\ v\ \frac{\partial\psi}{\partial x}\in L_1(D\times V),\quad \psi_{|\Gamma_-}=0\right\},$$

where $\Gamma_-=\{(x,v)\in\partial D\times V$ such that v is ingoing at $x\in\partial D\}$.

It is well known that

$$\sigma(T_0)=\{\lambda\in\mathbf{C}\ \ such\ \ that\ \ \text{Re}\ \lambda\leqslant-\lambda^*\}$$

(see, for instance, Ref. 22, Corollary 12.11, p. 272). More precisely we have

$$\sigma_{\text{ess}}(T_0)=\sigma C(T_0)=\{\lambda\in\mathbf{C}\ \ such\ \ that\ \ \text{Re}\ \lambda\leqslant-\lambda^*\}$$

(see Ref. 6, p. 6211).

The existence of the eigenvalues of T_0+K in the half-plane $\{\lambda\in\mathbf{C}/\text{Re}\ \lambda>-\lambda^*\}$ is related to the compactness of some iterate of $(\lambda-T_0)^{-1}K$ (see Ref. 22, Chap. 12). Unfortunately, this does not prevent the appearance of holes, included in the resolvent set of A_0, in the region $\{\lambda\in\mathbf{C}$ such that $\text{Re}\ \lambda\leqslant-\lambda^*\}$. However, if K is compact on $L_1(V)$, then $(\lambda-T_0)^{-1}K$ is weakly compact on $L_1(D\times V)$ (see Ref. 15, Lemma 2.1) and consequently we have the following result.

Theorem 4.3: *Suppose that K is compact on $L_1(V,dv)$. Then*

$$\sigma_{\text{ess}}(A_0)=\{\lambda\in\mathbf{C}\ \ such\ \ that\ \ \text{Re}\ \lambda\leqslant-\lambda^*\}.$$

◇

Proof: Let λ be such that $\text{Re}\ \lambda>s(A_0)$ (the spectral bound of A_0). Then we may write

$$(\lambda-A_0)^{-1}-(\lambda-T_0)^{-1}=\sum_{n\geqslant 1}\ [(\lambda-T_0)^{-1}K]^n(\lambda-T_0)^{-1}.$$

The hypothesis on K together with Ref. 15, Lemma 2.1, implies the weak compactness of

$$\sum_{n\geqslant 1}\ [(\lambda-T_0)^{-1}K]^n(\lambda-T_0)^{-1}.$$

Now the result follows from Theorems 3.1 and 3.2. Q.E.D.

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Braided geometry of the conformal algebra

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We show that the action of the special conformal transformations of the usual (undeformed) conformal group is the $q\to 1$ scaling limit of the braided adjoint action or R-commutator of q-Minkowski space on itself. We also describe the q-deformed conformal algebra in R-matrix form and its quasi-$*$ structure. © *1996 American Institute of Physics.* [S0022-2488(96)03611-0]

I. INTRODUCTION

It is a standard geometrical fact that the action of the momentum generators of the Poincaré algebra in physics is determined by the additive group structure of space–time, by differentiation as an infinitesimal addition. In this note we provide a novel geometrical picture of the special conformal transformations c_i similarly in terms of the structure of space–time itself. Namely, we show that they act as the $q\to 1$ limit of the braided adjoint action by which any braided group acts upon itself. In the case of q-deformed space–time,[1] this is the R-commutator

$$c_i\cdot(x_{i_1}\cdots x_{i_n})=\frac{x_{i_1}\cdots x_{i_n}x_i-x_{a_1}x_{j_1}\cdots x_{j_n}\mathbf{R}^{j_1}{}_{i_1}{}^{a_1}{}_{a_2}\mathbf{R}^{j_2}{}_{i_2}{}^{a_2}{}_{a_3}\cdots\mathbf{R}^{j_n}{}_{i_n}{}^{a_n}{}_{i}}{q-q^{-1}},$$

where the x_i are the noncommuting space–time-coordinates with braid statistics controlled by the appropriate Yang–Baxter matrix $\mathbf{R}^{i}{}_{j}{}^{k}{}_{l}$. We take the limit $q\to 1$. The formula also works for $q\neq 1$ and extends the q-Poincaré action in Ref. 2 to an action of the q-deformed conformal algebra.

We believe that this result is interesting as an application of q-deformation techniques to classical geometry: the picture which it provides is rather simpler than the usual picture of the c_i in terms of conjugation under conformal inversion of space-time translation, but is only possible when $q\neq 1$. One may work with the c_i in our $q\neq 1$ setting and afterwards set $q=1$. The result adds weight to the idea that q-deformed geometry is conceptually simpler and more regular than classical geometry, with certain notions unified in ways that are singular when $q=1$.

In a previous paper[3] we showed that the braided adjoint action with respect to the *multiplicative* braided group structure[4] of q-Minkowski space (as Hermitian 2×2 matrices being multiplied) corresponds in a $q\to 1$ scaling limit to the internal symmetry Lie algebra $su(2)\times u(1)$. Our result now is for the *additive* braided group structure due to Meyer.[5] It appears that both adjoint actions have important scaling limits as $q\to 1$.

We note that while a lot of effort has been expended in q-deforming geometrical structures, in particular in the author's ''braided groups approach'' [1,4,6] (which included specific proposals[7] in a general and systematic R-matrix form), this program has been stuck in recent years due to the following ''dilaton problem:'' when one tries to q-deform the q-Poincaré group one finds quite generally[2] that, for the types of deformations of interest, one must include a scale generator as well. The purely Poincaré sector in this family does not close as a Hopf algebra. A related problem is that even after this extension, it does not seem possible to obtain a Hopf $*$-algebra (i.e., to define

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complex conjugation of the generators) in any conventional sense. Moreover, the extended q-Poincaré Hopf algebra is not in general quasitriangular, i.e., not a strict quantum group in the sense of Drinfeld.[8]

Here we solve these three problems as follows. First, we propose to embrace the dilaton generator and q-deform the entire conformal algebra. This algebra is isomorphic to the standard Drinfeld–Jimbo deformation $U_q(so(4,2))$ or a cocycle twisting of it, but obtained now as an example of a new R-matrix construction. We use the categorical double-bosonization theory developed recently in Ref. 9. From a physical point of view, this focus on the conformal algebra limits our theories at first to massless ones. This is not, however, an unreasonable starting point, especially if we are interested in fundamental theories where observed particles are essentially massless compared to the Planck mass scale. Second, we show that the natural $*$-structure on the q-conformal algebra for real q makes it into a *quasi-*$*$ Hopf algebra in the sense recently introduced in Ref. 10 for the Poincaré case. There is also a quasitriangular structure. This work provides a first step towards the development of a q-twistor theory based on the properties of q-Minkowski space and the q-conformal algebra.

For quantum groups and braided groups, we adopt the conventions and notation in Refs. 11 and 12. Briefly, a quantum group H has a coproduct $\Delta: H\to H\otimes H$ which is a homomorphism to the usual tensor product. By contrast, a braided group B has a map $\underline{\Delta}: B\to B\underline{\otimes}B$ which is a homomorphism to a braided or noncommuting tensor product. This concept and many examples have been introduced by the author.[4] In physical terms, the elements of B enjoy braid statistics. When discussing quasitriangular structures, we will require formal power series in a deformation parameter in the usual way. All other constructions are algebraic.

Although we emphasize the construction in Proposition 2.1 below as a q-conformal algebra, we can also choose R from other standard families such as su_n. Then the construction takes us up one in the family, i.e., it allows the construction of quantum groups by induction.[9] Or we can choose nonstandard R and obtain altogether new quantum groups. Also, it has been pointed out to us that there are some superficial similarities between some of the relations in Proposition 2.1 and some of the relations independently proposed for a Hopf algebra construction in Ref. 13. The two constructions are, however, not at all the same.

II. q-CONFORMAL ALGEBRA

In this preliminary section we define a quasitriangular Hopf algebra which we call the conformal algebra associated to regular R-matrix data. When R is the so_n R-matrix, one obtains $U_q(so_{n+2})$. The construction is a specific example of a left-module version of a recent abstract construction in Ref. 9. This is explained further in the Appendix; here we describe only the resulting algebra. In fact, the construction of the dilaton-extended q-Poincaré algebra in R-matrix form has already been obtained (by the author) in Refs. 2 and 10. We use exactly the results and conventions developed for this, extending it now by the special conformal transformations.

Thus, let $\mathbf{R},\mathbf{R}'\in M_n\otimes M_n$ be invertible matrices obeying the conditions in Ref. 2 for the construction of a linear (momentum) braided group $V(\mathbf{R}',\mathbf{R})$ and its associated extended q-Poincaré algebra, which we denote $P(\mathbf{R}',\mathbf{R})$. The momentum sector has generators p^i and relations and braid statistics[2]

$$\mathbf{p}_1\mathbf{p}_2=\mathbf{R}'\mathbf{p}_2\mathbf{p}_1,\quad \mathbf{p}_1'\mathbf{p}_2=\mathbf{R}\mathbf{p}_2\mathbf{p}_1', \tag{1}$$

while $\mathbf{p}'$ denotes the generators of the second copy. We use a standard compact notation where suffices denote tensor contraction positions. The braided coproduct $\Delta\mathbf{p}=\mathbf{p}\otimes 1+1\otimes\mathbf{p}\equiv\mathbf{p}+\mathbf{p}'$ is called a *braided coaddition*. The braided antipode is $\underline{S}\mathbf{p}=-\mathbf{p}$. The rotation sector has matrix generators $l^{\pm i}{}_j$ and the usual relations[14]

$$\mathbf{l}_1^{\pm}\mathbf{l}_2^{\pm}\mathbf{R}=\mathbf{R}\mathbf{l}_2^{\pm}\mathbf{l}_1^{\pm},\quad \mathbf{l}_1^{+}\mathbf{l}_2^{-}\mathbf{R}=\mathbf{R}\mathbf{l}_2^{-}\mathbf{l}_1^{+}. \tag{2}$$

We also require other relations beyond these quadratic ones, such that the $\mathbf{l}^{\pm}$ with matrix coproduct $\Delta\mathbf{l}^{\pm}=\mathbf{l}^{\pm}\otimes\mathbf{l}^{\pm}$ define a quasitriangular Hopf algebra under which (1) and (5) remain covariant. For the so_n R-matrix the $\mathbf{l}^{\pm}$ generate $U_q(so_n)$ in the FRT form.[14] Our construction is not limited to this case, however. The dilatation sector is an additional generator ς with coproduct $\Delta\varsigma=\varsigma\otimes\varsigma$. The q-Poincaré algebra is generated by these subalgebras, with the cross relations[2]

$$\mathbf{l}_1^+\mathbf{p}_2=\lambda^{-1}\mathbf{R}_{21}^{-1}\mathbf{p}_2\mathbf{l}_1^+,\quad \mathbf{l}_1^-\mathbf{p}_2=\lambda\mathbf{R}\mathbf{p}_2\mathbf{l}_1^-,\quad \varsigma\mathbf{p}=\lambda^{-1}\mathbf{p}\varsigma,\quad [\mathbf{l}^{\pm},\,\varsigma]=0, \tag{3}$$

where λ is the *quantum group normalization constant*[2] appearing in the fundamental representation $\rho(\mathbf{l}^+)=\lambda\mathbf{R}$, $\rho(\mathbf{l}^-)=\lambda^{-1}\mathbf{R}_{21}^{-1}$ of the rotation sector. The braided coproduct and antipode of the $\mathbf{p}$ generators do not appear directly in the extended q-Poincaré algebra (which is an ordinary Hopf algebra), but in the bosonized form

$$\Delta\mathbf{p}=\mathbf{p}\otimes 1+\varsigma\mathbf{l}^-\otimes\mathbf{p},\quad S\mathbf{p}=-(S\mathbf{l}^-)\varsigma^{-1}\mathbf{p}. \tag{4}$$

To this construction, we add now the special conformal transformations as the linear braided group $V\check{}(\mathbf{R}',\mathbf{R})^{\mathrm{op}}$ with generators c_i and relations and braid statistics

$$\mathbf{c}_2\mathbf{c}_1=\mathbf{c}_1\mathbf{c}_2\mathbf{R}',\quad \mathbf{c}_2'\mathbf{c}_1=\mathbf{c}_1\mathbf{c}_2'\mathbf{R}. \tag{5}$$

There is a linear braided coproduct $\underline{\Delta}\mathbf{c}=\mathbf{c}+\mathbf{c}'$.

Proposition 2.1: The extended q-Poincaré algebra (1)–(4) has a further extension by generators c_i obeying

$$\mathbf{c}_2\mathbf{c}_1=\mathbf{c}_1\mathbf{c}_2\mathbf{R}',\quad \mathbf{l}_1^+\mathbf{c}_2=\lambda\mathbf{c}_2\mathbf{l}_1^+\mathbf{R}_{21},\quad \mathbf{l}_1^-\mathbf{c}_2=\lambda^{-1}\mathbf{c}_2\mathbf{l}_1^-\mathbf{R}^{-1},$$

$$\varsigma\mathbf{c}=\lambda\mathbf{c}\varsigma,\quad [\mathbf{p},\,\mathbf{c}]=\frac{\mathbf{l}^+\varsigma^{-1}-\mathbf{l}^-\varsigma}{q-q^{-1}},\quad \Delta\mathbf{c}=\mathbf{c}\otimes\mathbf{l}^+\varsigma^{-1}+\mathbf{l}\otimes\mathbf{c},\quad S\mathbf{c}=-\mathbf{c}\varsigma S\mathbf{l}^+,$$

where it is assumed that $\mathbf{R}$ *depends on a parameter q such that* $\mathbf{R}_{21}\mathbf{R}=\mathrm{id}+O(q-q^{-1})$. *We call this the q-conformal algebra* $C(\mathbf{R}',\mathbf{R})$ *associated to our R-matrix data.*

Proof: An abstract derivation is in the Appendix, but a direct proof is also possible. Indeed, it is clear that $\mathbf{c}$, $\mathbf{l}^{\pm}$, and ς generate a ''conjugate'' Hopf algebra to the extended q-Poincaré one: their relations are analogous under a symmetry. Hence it suffices to verify that the coproduct is compatible with the cross relations. Thus,

$$\begin{aligned}[\Delta p^i,\,\Delta c_j]&=[p^i,\,c_a]\otimes l^{+a}{}_j\varsigma^{-1}+\varsigma l^{-i}{}_a\otimes[p^a,\,c_j]+\varsigma l^{-i}{}_a c_b\otimes p^a l^{+b}{}_j\varsigma^{-1}-c_b\varsigma l^{-i}{}_a\otimes l^{+b}{}_j\varsigma^{-1}p^a\\
&=[p^i,\,c_a]\otimes l^{+a}{}_j\varsigma^{-1}+\varsigma l^{-i}{}_a\otimes[p^a,\,c_j]+\varsigma c_d l^{-i}{}_c\mathbf{R}^{-1c}{}_a{}^d{}_b\otimes p^a l^{+b}{}_j\varsigma^{-1}\\
&\quad -c_b\varsigma l^{-i}{}_a\otimes l^{+b}{}_j\varsigma^{-1}p^a\\
&=\frac{l^{+i}{}_a\varsigma^{-1}\otimes l^{+a}{}_j\varsigma^{-1}-l^{-i}{}_a\varsigma\otimes l^{-a}{}_j\varsigma}{q-q^{-1}}\\
&=\Delta\,\frac{l^{+i}{}_j\varsigma^{-1}-l^{-i}{}_j\varsigma}{q-q^{-1}}=\Delta[p^i,\,c_j]\end{aligned}$$

as required. We used the stated $\mathbf{c},\mathbf{l}^-$ and $\mathbf{p},\mathbf{l}^+$ relations for the second and third equalities, as well as the $[\mathbf{p},\mathbf{c}]$ relations for the latter.

Note that the $q-q^{-1}$ factor ensures that our algebra has a reasonable limit as $q\to 1$ but is not needed for the Hopf algebra structure itself (any factor will do for this). □

In a setting where $q=e^{t/2}$, there is typically a quasitriangular structure $\mathscr{R}_L$ for the Lorentz/rotation sector as a formal power series in t. In this setting, we have the following.

Proposition 2.2: The q-conformal Hopf algebra above is quasitriangular, with

$$\mathscr{R}=\mathscr{R}_L\lambda^{-\xi\otimes\xi}\exp(\mathbf{c}|\mathbf{p})^{-1}, \tag{6}$$

where $\mathscr{R}_L$ *is the q-Lorentz quantum group quasitriangular structure,* $\varsigma=\lambda^{\xi}$ *and* $\exp(\mathbf{c}|\mathbf{p})\in V^{\vee}\otimes V$ *is the* braided exponential *or canonical element associated with the braided group duality pairing between V and* $V^{\vee}$ *as linear braided groups.*

Proof: This follows from the general construction[9] underlying the above proposition; see the Appendix. To verify it directly, one may use the bicharacter property of the braided exponentials under the braided coproduct,[15] with the corresponding properties with respect to the bosonized coproduct. □

The braided exponential $\exp(\mathbf{c}|\mathbf{p})$ here is a $\mathbf{p}$-eigenfunction or plane wave in the copy of q-space–time generated by the c_i (and likewise a plane wave in the copy generated by p^i).

III. QUASI $*$-STRUCTURE ON THE CONFORMAL GENERATORS

So far, we have considered the complexified picture. We now consider $*$-structures on our algebras. The specification of the $*$-structure in the momentum sector determines which linear combinations are 'real' in the sense of being invariant under $*$. This determines which representations are unitary (such elements should be Hermitian) and also determines, when there is a quantum metric, whether it is of Euclidean, Minkowski, or another type according to the form of its restriction to such elements. The $*$-structures for the extended q-Poincaré group have already been-analyzed in Ref. 10, and we extend this now to the q-conformal case. We recall from Ref. 10 that one needs the notion of a quasi-$*$ Hopf algebra $\mathscr{H}$. This is a Hopf algebra over $\mathbb{C}$ which is a $*$-algebra, and an invertible element $\mathscr{S}\in\mathscr{H}\otimes\mathscr{H}$ such that

$$(*\otimes*)\circ\Delta\circ*=\mathscr{S}^{-1}(\tau\circ\Delta\ )\mathscr{S},\ \ (\Delta\otimes\mathrm{id})\mathscr{S}=\mathscr{S}_{13}\mathscr{S}_{23},\ \ (\mathrm{id}\otimes\Delta)\mathscr{S}=\mathscr{S}_{13}\mathscr{S}_{12},\ \ \mathscr{S}^{*\otimes*}=\mathscr{S}_{21}, \tag{7}$$

where τ denotes transposition. One can show that $\mathscr{S}$ obeys the quantum Yang–Baxter equations or QYBE (but we do not denote it here by $\mathscr{R}$, to avoid confusion with the quasitriangular structure also present). To have such a structure in our R-matrix setting we suppose that the R-matrix in the preceding section is of one of the two real types in Ref. 16. We also suppose a quantum metric η compatible with $\mathbf{R}$ (see Ref. 1) and of corresponding reality type:

$$\overline{\mathbf{R}^{i\ k}_{\ j\ l}}=\begin{cases}\mathbf{R}^{l\ j}_{\ k\ i} & \text{Real Type I,}\\ \mathbf{R}^{j\ \bar{i}}_{\ l\ \bar{k}} & \text{Real Type II,}\end{cases}\qquad \overline{\eta_{ij}}=\begin{cases}\eta^{ji} & \text{Real Type I,}\\ \eta_{\bar{j}\,\bar{i}} & \text{Real Type II,}\end{cases} \tag{8}$$

where η^{ij} is the transposed inverse of η_{ij} and $\bar{i}$ is an involution on the indices assumed in the type II case. We assume $\lambda^*=\lambda$ as well. These reality conditions hold for the standard choices of $\mathbf{R}$, when their parameter q is real.

The extended q-Poincaré algebra has the quasi-$*$-structure[10]

$$p^{i*}=\begin{cases}\eta_{i\bar{a}}p^a & \text{Real Type I,}\\ p^{\bar{i}} & \text{Real Type II,}\end{cases}\qquad l^{\pm i}{}_j{}^*=\begin{cases}\eta_{ib}l^{\mp b}{}_a\eta^{ja} & \text{Real Type I,}\\ l^{\mp\bar{i}}{}_{\bar{j}} & \text{Real Type II,}\end{cases}$$

$$\varsigma^*=\varsigma^{-1},\quad \mathscr{S}=\mathscr{R}_L\lambda^{-\xi\otimes\xi}, \tag{9}$$

where $\mathscr{R}_L\lambda^{-\xi\otimes\xi}$ is the dilaton-extended q-Lorentz quasitriangular structure and $\varsigma=\lambda^{\xi}$. Note that the real type II case used in Ref. 10 was chosen such that on the Lorentz generators in function-algebra form it appears as $t^i{}_j{}^*=t^{\bar{i}}{}_{\bar{j}}$, which corresponds to $l^{\pm i}{}_j{}^*=S^2l^{\mp\bar{i}}{}_{\bar{j}}$. We can equivalently put the S^2 automorphism on the function algebra side as $t^i{}_j{}^*=S^2t^{\bar{i}}{}_{\bar{j}}$, as we prefer now.

Proposition 3.1: The quasi-∗ structure (9) extends to one on the q-conformal algebra in Proposition 2.1, with

$$c_i{}^* = \begin{cases} c_a \eta^{ia}, & \text{Real Type I,} \\ c_{\bar{i}}, & \text{Real Type II.} \end{cases}$$

Moreover,

$$(*\otimes *)\circ\Delta\circ * = \exp(\mathbf{c}|\mathbf{p})^{-1}(\Delta\ )\exp(\mathbf{c}|\mathbf{p})$$

holds for the coproduct on any element of the q-conformal algebra.

Proof: The proof of compatibility of this ∗ with the $\mathbf{c},\mathbf{l}^{\pm}$ relations is similar to that for $\mathbf{p},\mathbf{l}^{\pm}$. Explicitly, in the type I case,

$$\begin{aligned}(\lambda c_b l^{+i}{}_a \mathbf{R}^b{}_k{}^a{}_j)^* &= \lambda \mathbf{R}^j{}_a{}^k{}_b \eta^{bd}\eta_{ic} l^{-c}{}_e \eta^{ae} c_d = \lambda \mathbf{R}^j{}_a{}^k{}_b \eta^{bd}\eta_{ic}\eta^{ae}\lambda^{-1} c_g l^{-c}{}_f \mathbf{R}^{-1 f}{}_e{}^g{}_d \\ &= c_a \eta^{ka}\eta_{ic} l^{-c}{}_d \eta^{jd} = (l^{+i}{}_j c_k)^*,\end{aligned}$$

using invariance of R under conjugation by $\eta\otimes\eta$. In addition, we have

$$[p^i,\ c_j]^* = [c_j{}^*,\ p^{i*}] = [c_a \eta^{ja}, p^b \eta_{ib}] = -\eta^{ja}\eta_{ib}\left(\frac{l^{+b}{}_a \mathfrak{s}^{-1} - l^{-b}{}_a \mathfrak{s}}{q-q^{-1}}\right) = \left(\frac{l^{+i}{}_j \mathfrak{s}^{-1} - l^{-i}{}_j \mathfrak{s}}{q-q^{-1}}\right)^*,$$

as required. Hence we have a ∗-algebra in this case. In the type II case, the calculation is

$$(\lambda c_b l^{+i}{}_a \mathbf{R}^b{}_k{}^a{}_j)^* = \lambda l^{-\bar{i}}{}_{\bar{a}} c_{\bar{b}} \mathbf{R}^{\bar{a}}{}_j{}^{\bar{b}}{}_{\bar{k}} = c_{\bar{k}} l^{-\bar{i}}{}_{\bar{j}} = (l^{+i}{}_j c_k)^*,$$

$$[p^i,\ c_j]^* = [c_{\bar{j}},\ p^{\bar{i}}] = -\left(\frac{l^{+\bar{i}}{}_{\bar{j}} \mathfrak{s}^{-1} - l^{-\bar{i}}{}_{\bar{j}} \mathfrak{s}}{q-q^{-1}}\right) = \left(\frac{l^{+i}{}_j \mathfrak{s}^{-1} - l^{-i}{}_j \mathfrak{s}}{q-q^{-1}}\right)^*.$$

In either case, the sub-Hopf algebra generated by $\mathfrak{s},\mathbf{c},\mathbf{l}^{\pm}$ forms a quasi-∗ Hopf algebra with the same cocycle $\mathcal{J} = \mathcal{R}_L \lambda^{-\xi\otimes\xi}$, by analogous arguments to the proof for the extended q-Poincaré algebra in Ref. 10. Combining (7) with Proposition 2.2 gives the form of $(*\otimes *)\circ\Delta\circ *$ stated. □

Although the q-conformal algebra with the above ∗-operation is not a Hopf ∗-algebra in the usual sense, we see that Δ fails to be a ∗-algebra map only up to conjugation by the plane wave $\exp(\mathbf{c}|\mathbf{p})$. More precisely, to every quasi-∗ Hopf algebra the conjugate coproduct $\Delta = (*\otimes *)\circ\Delta\circ *$ also provides a quasi-∗ Hopf algebra structure, in general different from Δ. In our case, this comes out as

$$\overline{\Delta\mathbf{c}} = \mathbf{c}\otimes\mathbf{l}^{-}\mathfrak{s} + 1\otimes\mathbf{c} \tag{10}$$

for either the real type I or type II ∗-structures above (similarly for $\overline{\Delta\mathbf{p}}$ in Ref. 10); Proposition 3.1 tells us that this Δ and the coproduct Δ in Proposition 2.1 are conjugate by $\exp(\mathbf{c}|\mathbf{p})$.

IV. SPINORIAL FORMULATION

An important class of examples of our data $\mathbf{R}',\mathbf{R}$ is provided by a ''spinorial'' construction starting from a smaller Yang–Baxter matrix $R\in M_s\otimes M_s$, where $n=s^2$. We require this to be q-Hecke in the sense $(PR-q)(PR+q^{-1})=0$, where P is the permutation matrix. The extended q-Poincaré algebra in this setting has been given in Ref. 10, while the momentum sector or q-space–time itself is from Refs. 4, 5, and 17 and reviewed in Ref. 1 or 11, Ch. 10. We include now the q-conformal algebra in this spinorial approach. In fact, the construction has two versions which are strictly ''gauge equivalent'' in a certain algebraic sense. These are the ''Euclidean'' and ''Minkowski'' gauges of the same construction, introduced in Ref. 17 and 4 and 5, respectively.

The Euclidean gauge construction is[17]

$$\mathbf{R}'^{i}{}_{j}{}^{k}{}_{l}=R^{-1}{}^{l_0}{}_{k_0}{}^{j_0}{}_{i_0}R^{i_1}{}_{j_1}{}^{k_1}{}_{l_1},\quad \mathbf{R}^{i}{}_{j}{}^{k}{}_{l}=R^{j_0}{}_{i_0}{}^{l_0}{}_{k_0}R^{i_1}{}_{j_1}{}^{k_1}{}_{l_1} \tag{11}$$

and is equivalent for R the standard su_2 R-matrix to taking for $\mathbf{R}$ the standard so_4 R-matrix. Of course, the construction is more general and can be used just as well to define nonstandard space–times by taking other nonstandard R. We write $i=i_0i_1$, $j=j_0j_1$, etc., as multi-indices.

We also write $p^i = p^{i_1}{}_{i_0}$. Then the relations (1) in the momentum sector (which will also be the relations of q-space–time) become[17]

$$R_{21}\mathbf{p}_1\mathbf{p}_2=\mathbf{p}_2\mathbf{p}_1R. \tag{12}$$

More nontrivially, we replace the vectorial q-Lorentz algebra generated by $l^{\pm i}{}_j$ by a spinorial version generated by two sets of generators $l^{\pm i_0}{}_{j_0}$ and $m^{\pm i_1}{}_{j_1}$ obeying relations like (2) with respect to R. For R the su_2 R-matrix, the momentum and space–time sectors are isomorphic to the quantum matrices $M_q(2)$, and the Lorentz/rotation sector is $U_q(su_2)\otimes U_q(su_2)$. The natural $*$-structure in this gauge is the unitary type one which corresponds to $SU_q(2)$ as a q-deformed three-sphere in $M_q(2)$. The dilation sector is generated by ς as before, commuting with $\mathbf{l}^{\pm},\mathbf{m}^{\pm}$. The cross-relations between these various sectors and the coproducts are obtained in Ref. 10. In the present (slightly different) conventions they come out as

$$\mathbf{p}_1\mathbf{l}_2^{+}=\lambda^{-1/2}R^{-1}\mathbf{l}_2^{+}\mathbf{p}_1,\quad \mathbf{p}_1\mathbf{l}_2^{-}=\lambda^{1/2}R_{21}\mathbf{l}_2^{+}\mathbf{p}_1,\quad \mathbf{p}_1\mathbf{m}_2^{+}=\lambda^{1/2}R\mathbf{m}_2^{+}\mathbf{p}_1,\quad \mathbf{p}_1\mathbf{m}_2^{-}=\lambda^{-1/2}R_{21}^{-1}\mathbf{m}_2^{-}\mathbf{p}_1,$$

$$\varsigma\mathbf{p}=\lambda^{-1}\mathbf{p}\varsigma,\quad \Delta\mathbf{p}=\mathbf{p}\otimes 1+\varsigma S^{-1}(S\mathbf{m}^{-}(\ )\mathbf{l}^{-})\otimes\mathbf{p},\quad \epsilon(\mathbf{p})=0, \tag{13}$$

where the space is for the matrix indices of $\mathbf{p}$ to be inserted.

To this spinorial extended q-Poincaré algebra, we add the special conformal transformations $c_i = c^{i_0}{}_{i_1}$. Note that the assignment is transposed relative to the assignment for p^i.

Proposition 4.1: In the Euclidean gauge, the spinorial extended q-Poincaré algebra in Ref. 10 *has a further extension by a matrix of generators* $\mathbf{c}$ *obeying*

$$R\mathbf{c}_1\mathbf{c}_2=\mathbf{c}_2\mathbf{c}_1R_{21},\quad \mathbf{l}_1^{+}\mathbf{c}_2=\lambda^{-1/2}\mathbf{c}_2\mathbf{l}_1^{+}R^{-1},\quad \mathbf{l}_1^{-}\mathbf{c}_2=\lambda^{1/2}\mathbf{c}_2\mathbf{l}_1^{-}R_{21},$$

$$\mathbf{m}_1^{+}\mathbf{c}_2=\lambda^{1/2}\mathbf{c}_2\mathbf{m}_1^{+}R,\quad \mathbf{m}_1^{-}\mathbf{c}_2=\lambda^{-1/2}\mathbf{c}_2\mathbf{m}_1^{-}R_{21}^{-1},\quad \varsigma\mathbf{c}=\lambda\mathbf{c}\varsigma,$$

$$[p^{i_1}{}_{i_0},\, c^{j_0}{}_{j_1}]=\frac{\varsigma^{-1}(S^{-1}l^{+j_0}{}_{i_0})m^{+i_1}{}_{j_1}-\varsigma(S^{-1}l^{-j_0}{}_{i_0})m^{-i_1}{}_{j_1}}{q-q^{-1}},$$

$$\Delta\mathbf{c}=\mathbf{c}\otimes\varsigma^{-1}(S^{-1}\mathbf{l}^{+})(\ )\mathbf{m}^{+}+1\otimes\mathbf{c},\quad \epsilon(\mathbf{c})=0,$$

and forming a quasitriangular Hopf algebra. This is the spinorial q-conformal algebra in the Euclidean gauge.

Proof: The $\mathbf{c}$, $\mathbf{l}^{\pm}$, $\mathbf{m}^{\pm}$, ς relations are obtained along the same lines as in Ref. 10 via double-bosonization. They are consistent with Proposition 2.1 using (11) and the ansatz $l^{\pm i}{}_j = (S^{-1}l^{\pm j_0}{}_{i_0})m^{\pm i_1}{}_{j_1}$. The $\mathbf{c}$, $\mathbf{p}$ relations and the coproduct follow at once from this form of $l^{\pm i}{}_j$. We note that if we use the (slightly different) identification $\eta_{ia}p^a = p^{i_0}{}_{i_1}$ used in Ref. 10, and the expression $\eta_{ij} = \epsilon^{i_0j_0}\epsilon_{i_1j_1}$ in terms of the spinor metric associated to R, then the $[p^i,c_j]$ relations come out as

$$[p^{i_0}{}_{i_1},c^{j_0}{}_{j_1}]=\frac{\varsigma^{-1}l^{+i_0}{}_{a_0}\epsilon^{a_0j_0}\epsilon_{a_1i_1}m^{+a_1}{}_{j_1}-\varsigma l^{-i_0}{}_{a_0}\epsilon^{a_0j_0}\epsilon_{a_1i_1}m^{-a_1}{}_{j_1}}{q-q^{-1}}. \tag{14}$$

The spinor metric also converts the $*$-structure in Sec. III into a matrix form. □

The Minkowski gauge for the same construction is[4,5]

$$\mathbf{R}'^{i}{}_{j}{}^{k}{}_{l}=R^{-1}{}^{d}{}_{k_0}{}^{j_0}{}_{a}R^{k_1}{}_{b}{}^{a}{}_{i_0}R^{i_1}{}_{c}{}^{b}{}_{l_1}\widetilde{R}^{c}{}_{j_1}{}^{l_0}{}_{d},\quad \mathbf{R}^{i}{}_{j}{}^{k}{}_{l}=R^{j_0}{}_{a}{}^{d}{}_{k_0}R^{k_1}{}_{b}{}^{a}{}_{i_0}R^{i_1}{}_{c}{}^{b}{}_{l_1}\widetilde{R}^{c}{}_{j_1}{}^{l_0}{}_{d}. \tag{15}$$

The momentum or space–time sector in this case has the braided matrix relations[4]

$$R_{21}\mathbf{p}_1R\mathbf{p}_2=\mathbf{p}_2R_{21}\mathbf{p}_1R, \tag{16}$$

where $\eta_{ia}p^a = p^{i_0}{}_{i_1}$, and yields the braided matrices $BM_q(2)$ for the standard su_2 R-matrix. The natural space–time $*$-structure in this case is a Hermitian one, justifying the name for this gauge. [The unit sphere here is actually isomorphic to $U_q(su_2)$ as a $*$-algebra when $q\neq 1$.] The Lorentz sector in this standard case is $U_q(su_2)\blacktriangleright\!\!\blacktriangleleft U_q(su_2)$ (with a more complicated coproduct than in the Euclidean gauge).

The Euclidean gauge for q-space–time was introduced in Ref. 17 precisely as gauge equivalent to the Minkowski gauge (which was found first). At the Lorentz algebra level the gauges are related by twisting by a quantum cocycle (see Ref. 2, Sec. 4, in a dual form). This was extended to the level of the extended q-Poincaré algebra in Ref. 10, using the same cocycle viewed in the bigger algebra. The cocycle is $\chi=\mathscr{R}_{23}^{-1}$ where $\mathscr{R}$ is the quasitriangular structure of $U_q(su_2)$ in the standard example.

Proposition 4.2: The same quantum cocycle χ viewed in the spinorial form of the q-conformal algebra twists its structure from the Euclidean to the Minkowski gauge.

Proof: This is true for the sub-Hopf algebra generated by $\mathbf{c},\mathbf{l}^{\pm},\varsigma$ by analogous arguments to those for the extended q-Poincaré algebra. Since the coproduct is entirely defined by its restriction to either of these two sub-Hopf algebras, we conclude the same twisting result for the entire q-conformal algebra. □

In view of this, we will not give the structure in detail in the Minkowski gauge: the structure of the spinorial form of the extended q-Poincaré algebra is given in Ref. 10. To this, we add the special conformal transformations in the form $R_{21}\mathbf{c}_1R\mathbf{c}_2=\mathbf{c}_2R_{21}\mathbf{c}_1R$, where $c_i = c^{i_1}{}_{i_0}$ and $\overline{R^{i}{}_{j}{}^{k}{}_{l}}=R^{l}{}_{k}{}^{j}{}_{i}$. The cross relations with $\mathbf{l}^{\pm}$ are similar to those between $\mathbf{p}$ and $\mathbf{l}^{\pm}$ in Ref. 10.

V. CONFORMAL TRANSFORMATIONS OF SPACE–TIME

So far, we have called our quasitriangular Hopf algebra $C(\mathbf{R}',\mathbf{R})$ the q-conformal one because of its structural form, which is analogous to that of the conformal Lie algebra. We are now ready to justify the terminology in geometrical terms, i.e., by its action on q-space–time. For the latter, we take the linear braided group $V^{\check{}}(\mathbf{R}',\mathbf{R})$ with generators x_i and relations and braid statistics

$$\mathbf{x}_1\mathbf{x}_2=\mathbf{x}_2\mathbf{x}_1\mathbf{R}',\quad \mathbf{x}_1'\mathbf{x}_2=\mathbf{x}_2\mathbf{x}_1'\mathbf{R}. \tag{17}$$

There is a linear coproduct $\underline{\Delta}\mathbf{x}=\mathbf{x}+\mathbf{x}'$ and a $*$-structure

$$x_i^*=\begin{cases} x_a\eta^{ia}, & \text{Real Type I,}\\ x_{\bar{i}}, & \text{Real Type II,}\end{cases}$$

which we take of the same form as for $\mathbf{c}$ in Sec. III.

From the theory of braided groups, it is known[2] that the extended q-Poincaré algebra acts covariantly on q-space–time by q-rotations (via the fundamental representation defined by $\mathbf{R}$) and braided-differentiation for the momentum sector[2,10]

$$\mathbf{l}_1^{+}\triangleright\mathbf{x}_2=\mathbf{x}_2\lambda\mathbf{R}_{21},\quad \mathbf{l}_1^{-}\triangleright\mathbf{x}_2=\mathbf{x}_2\lambda^{-1}\mathbf{R}^{-1},\quad p^i\triangleright x_j=-\delta^i{}_j,\quad \varsigma\triangleright x_i=\lambda x_i. \tag{18}$$

To this, we add the following.

Proposition 5.1: The q-conformal algebra in Proposition 2.1 acts covariantly on q-space–time by (18) and

$$\mathbf{c}_2 \triangleright \mathbf{x}_1 = \frac{\mathbf{x}_1\mathbf{x}_2 - \mathbf{x}_2\mathbf{x}_1\mathbf{R}}{q-q^{-1}}.$$

Proof: This follows from general theory in Ref. 9; the required action of $\mathbf{c}$ is derived in the Appendix. The direct proof that the $\mathbf{c}$, $\mathbf{l}^{\pm}$, ς relations are represented is similar to that for $\mathbf{p}$, $\mathbf{l}^{\pm}$, ς. For the $\mathbf{p}$, $\mathbf{c}$ relations we can check it easily at lowest order, as $(q-q^{-1})[p^i,c_j]\triangleright x_k = p^i\triangleright(x_k x_j - x_b x_a \mathbf{R}^a{}_k{}^b{}_j) + c_j \triangleright \delta^i{}_k = -\delta^i{}_k x_j - x_a \mathbf{R}^{-1}{}^i{}_j{}^a{}_k + \delta^i{}_b x_a \mathbf{R}^a{}_k{}^b{}_j + x_c \mathbf{R}^{-1}{}^i{}_a{}^c{}_b \mathbf{R}^a{}_k{}^b{}_j = (\varsigma^{-1} l^{+i}{}_j - \varsigma l^{-i}{}_j)\triangleright x_k$, where the outer two terms cancelled. We used the action of p^i on products $x_j x_k$ via the braided-Leibniz rule with R_{21}^{-1}.[10] One can proceed similarly for the higher order case, using the action of c_i on products obtained below. □

Note that both the action of p^i and c_i extend to products via a braided-Leibniz rule because they originate as braided module algebra structures (this is equivalent to the statement that the actions form a module-algebra structure with respect to the Hopf algebra coproducts.) In the case of p^i, the action on a general monomial comes out in terms of the braided-integer matrices with respect to $\mathbf{R}_{21}^{-1}$ (see Ref. 10). For the c_i we have:

Lemma 5.2: The action of c_i on a general product is

$$\mathbf{c}_n \triangleright \mathbf{x}_1\mathbf{x}_2\cdots\mathbf{x}_{n-1} = \mathbf{x}_1\mathbf{x}_2\cdots\mathbf{x}_n\left(\frac{1-(P\mathbf{R})_{12}(P\mathbf{R})_{23}\cdots(P\mathbf{R})_{n-1n}}{q-q^{-1}}\right),$$

where P is the permutation matrix.

Proof: We first compute the braided-Leibniz rule for c_i. As explained in the Appendix, its natural form is as a right-handed (braided) derivation $c_i\triangleright = \delta_i$ acting from the right. Then

$$(ab)\,\delta_i = a(b\,\delta_i) + a\Psi(b\otimes\delta_i),$$

where the braiding is the braiding for the covector braided group $V^{\vee}(\mathbf{R}',\mathbf{R})$, i.e., defined by $\mathbf{R}$. Hence

$$(\mathbf{x}_1\cdots\mathbf{x}_{n-1})\,\delta_n = \mathbf{x}_1\cdots\mathbf{x}_n\left(\frac{1-(P\mathbf{R})_{n-1n}}{q-q^{-1}}\right) + (\mathbf{x}_1\cdots\mathbf{x}_{n-2})\,\delta_{n-1}\mathbf{x}_n(P\mathbf{R})_{n-1n}.$$

The result then follows by induction. □

Another way to describe the action is in terms of the algebra structure of the corresponding semidirect product of space–time crossed by the q-conformal group. The cross relations between the extended q-Poincaré algebra and space–time is[10]

$$\mathbf{l}_1^+\mathbf{x}_2 = \mathbf{x}_2\lambda\mathbf{R}_{21}\mathbf{l}_1^+, \quad \mathbf{l}_1^-\mathbf{x}_2 = \mathbf{x}_2\lambda^{-1}\mathbf{R}^{-1}\mathbf{l}_1^-, \quad \mathbf{x}_2\mathbf{R}^{-1}\mathbf{p}_1 - \mathbf{p}_1\mathbf{x}_2 = \mathrm{id}, \quad \varsigma\mathbf{x} = \lambda\mathbf{x}\varsigma. \tag{19}$$

The $\mathbf{x},\mathbf{p}$ relations are the ''braided Heisenberg algebra'' in the present conventions. To this we now add the following.

Proposition 5.3: The q-conformal group acting as above and $\mathbf{x}$ acting by left multiplication on q-space–time form a representation of the algebra $V^{\vee}(\mathbf{R}',\mathbf{R})\bowtie C(\mathbf{R}',\mathbf{R})$ with the additional $\mathbf{c},\mathbf{x}$ cross relations

$$\left[\mathbf{c}_1 + \frac{\mathbf{x}_1\mathbf{l}_1^+\varsigma^{-1}}{q-q^{-1}}, \mathbf{x}_2\right] = 0.$$

Proof: We make a left-handed semidirect product using the coproduct in Proposition 2.1, the action of c_i above, and the already-known cross-relations (19). Thus

$$c_i x_j = (c_{i(1)} \triangleright x_j) c_{i(2)} = (c_a \triangleright x_j) \mathbf{l}^{+a}{}_i \mathbf{s}^{-1} + x_j c_i = \frac{x_j x_a - x_d x_c R^{c}{}_{j}{}^{d}{}_{a}}{q - q^{-1}} \, l^{+a}{}_i \mathbf{s}^{-1} + x_j c_i$$

$$= \frac{x_j x_a l^{+a}{}_i \mathbf{s}^{-1} - x_a l^{+a}{}_i \mathbf{s}^{-1} x_j}{q - q^{-1}} + x_j c_i ,$$

as stated. Because the action in Proposition 5.1 is covariant (q-space–time forms a module algebra under it), we know from the general theory of Hopf algebra cross products that these relations define an associative algebra structure on the tensor product vector space, and that the action on q-space–time extends to it with x_i acting by left-multiplication. □

We can also use the spinorial form of the q-conformal algebra. The action of the spinorial form of the extended q-Poincaré algebra is given in Ref. 10. To this, we add the following.

Proposition 5.4: The spinorial form of the q-conformal algebra in the Euclidean gauge acts as in Ref. 10 and

$$\mathbf{c}_2 \triangleright \mathbf{x}_1 = -\mathbf{x}_1 \mathbf{x}_2 P R.$$

Proof: We use the form of $\mathbf{R}$ in (11) in Proposition 5.1 and $R = R_{21}^{-1} + (q - q^{-1})P$ from the q-Hecke assumption in Sec. IV. Thus

$$(q - q^{-1}) c_j \triangleright x_i = x_i x_j - x_b x_a \mathbf{R}^{a}{}_{i}{}^{b}{}_{j} = x^{i_0}{}_{i_1} x^{j_0}{}_{j_1} - x^{b_0}{}_{b_1} x^{a_0}{}_{a_1} R^{-1 i_0}{}_{a_0}{}^{j_0}{}_{b_0} R^{a_1}{}_{i_1}{}^{b_1}{}_{j_1}$$

$$- (q - q)^{-1} x^{b_0}{}_{b_1} x^{a_0}{}_{a_1} \delta^{i_0}_{b_0} \delta^{j_0}_{a_0} R^{a_1}{}_{i_1}{}^{b_1}{}_{j_1}.$$

The first two terms then give zero due to the form of $\mathbf{R}'$ in (11) and the relations for the x_i. □

We are now in position to compute this action for our standard q-space–time.[1] The classical formula $c_j \triangleright x_i = \frac{1}{2} \eta_{ij} \mathbf{x} \cdot \mathbf{x} - x_i x_j$ would be

$$\begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \triangleright \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} -a^2 & -ba & -ac & -bc \\ -ab & -b^2 & -ad & -bd \\ -ca & -da & -c^2 & -dc \\ -cb & -db & -cd & -d^2 \end{pmatrix}, \tag{20}$$

where

$$c = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}, \quad \mathbf{x} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \text{ and } \quad \eta = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

is the metric on complexified space–time in these spinor coordinates (different linear combinations are considered real space–time coordinates in the Minkowski and Euclidean cases).

Example 5.5: For the standard q-space–time in the Euclidean gauge, we have

$$\begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \triangleright \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} -a^2 & -q^2 ab & -ca & -bc \\ -ba & -b^2 & -da & -db \\ -ac & -ad - (q - q^{-1}) bc & -c^2 & -qdc \\ -bc & -bd & -dc & -d^2 \end{pmatrix}.$$

This is a q-deformation of the usual action of the special conformal transformations on space–time.

Proof: This is computed easily from Proposition 5.4 with

$$R=\begin{pmatrix} q & 0 & 0 & 0 \\ 0 & 1 & q-q^{-1} & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & q \end{pmatrix},$$

which is the standard su_2 R-matrix in the q-Hecke normalization. The relations between the noncommutative spinor space–time coordinates in this case are given explicitly in Ref. 17. The quantum group normalization of the corresponding $\mathbf{R}$ is $\lambda=q^{-1}$. □

This justifies our proposal for $C(\mathbf{R}',\mathbf{R})$ as q-conformal group. Note that the metric does not play any direct role in our definition of the q-conformal group and its action on spacetime, i.e., our approach is a novel one even when $q=1$. It is remarkable therefore that it coincides for our standard example with the action (20) defined through a metric. The connection is quite general, however.

Lemma 5.6: If η is a quantum metric such that $\mathbf{x}\cdot\mathbf{x}=x_a x_b \eta^{ba}$ is central, then it is preserved by the q-conformal group up to scaling, in the sense

$$c_i\triangleright(\mathbf{x}\cdot\mathbf{x})^m=\left(\frac{1-\lambda^{-2m}}{q-q^{-1}}\right)x_i(\mathbf{x}\cdot\mathbf{x})^m,\quad \text{i.e.,}\quad c_i\triangleright f(\mathbf{x}\cdot\mathbf{x})=\left(\frac{1-\lambda^{-2}}{q-q^{-1}}\right)x_i\mathbf{x}\cdot\mathbf{x}(\partial_{\lambda^{-2}}f\,)(\mathbf{x}\cdot\mathbf{x}).$$

Proof: We compute $(q-q^{-1})c_i\triangleright(x_q x_b\eta^{ba})=x_a x_b x_i\eta^{ba}-x_c x_d x_e\mathbf{R}^{d}{}_{a}{}^{c}{}_{f}\mathbf{R}^{e}{}_{b}{}^{f}{}_{i}\eta^{ba}$ $=x_a x_b x_i\eta^{ba}-x_c x_d x_e\mathbf{R}^{d}{}_{a}{}^{c}{}_{f}\eta^{eb}\lambda^{-2}\mathbf{R}^{-1a}{}_{b}{}^{f}{}_{i}=\mathbf{x}\cdot\mathbf{x}x_i-\lambda^{-2}x_i\mathbf{x}\cdot\mathbf{x}$, using the covariance properties of the quantum metric. Under a further condition on the quantum metric (true in the main examples, see Ref. 1) one knows that $\mathbf{x}\cdot\mathbf{x}$ is also central. This gives the result for $m=1$. From the covariance properties of the quantum metric, we likewise compute the braiding $\mathbf{x}'\cdot\mathbf{x}'x_i=x'_a x'_b x_i\eta^{ba}$ $=x'_a x_d x'_c R^{c}{}_{b}{}^{d}{}_{i}\eta^{ba}=x'_a x_d x'_c\lambda^{-2}R^{-1a}{}_{b}{}^{d}{}_{i}\eta^{cb}=x_f x'_e x'_c R^{e}{}_{a}{}^{f}{}_{d}\lambda^{-2}R^{-1a}{}_{b}{}^{d}{}_{i}\eta^{cb}=\lambda^{-2}x_i\mathbf{x}'\cdot\mathbf{x}'$, i.e., $\Psi(\mathbf{x}\cdot\mathbf{x}\otimes x_i)=\lambda^{-2}\mathbf{x}_i\otimes\mathbf{x}\cdot\mathbf{x}$. The q-Leibniz rule for the action of c_i then implies $c_i\triangleright(\mathbf{x}\cdot\mathbf{x})^m=(\mathbf{x}\cdot\mathbf{x})^{m-1}x_i((1-\lambda^{-2})/(q-q^{-1}))\mathbf{x}\cdot\mathbf{x}+(c_i\triangleright(\mathbf{x}\cdot\mathbf{x})^{m-1})\mathbf{x}\cdot\mathbf{x}\lambda^{-2}$, which provides the general result by induction. We alternatively write this in terms of a λ^{-2}-deformed derivative defined in a usual way. □

Thus, our q-conformal group and its action do not *a priori* involve a metric, but when there is one, it is preserved in some sense. Instead, the structures and formulas which we normally associate with preservation up to scale of a metric are obtained from the braided adjoint action. For example, we see that the standard q-Gaussian g_η in the setting of Lemma 5.6, which is a λ^{-2}-exponential of $\mathbf{x}\cdot\mathbf{x}$, is preserved in the sense

$$c_i\triangleright g_\eta=-q^{-1}\left(\frac{1-\lambda^{-2}}{1-q^{-4}}\right)x_i(\mathbf{x}\cdot\mathbf{x})g_\eta,$$

in addition to its usual properties under the extended q-Poincaré algebra.

Finally, when a quasi-$*$ Hopf algebra acts covariantly on a $*$-algebra, its conjugate quasi-$*$ Hopf algebra acts with a conjugate action.[10] In the case of the extended q-Poincaré algebra it was shown that the action of $\mathbf{1}^{\pm},\varsigma$ on q-space–time is self-conjugate, while the conjugate action of the $\mathbf{p}$ generators is by braided-differentiation with $\mathbf{R}_{21}^{-1}$ replaced by $\mathbf{R}$.

Proposition 5.7: The conjugate action of the q-conformal algebra on q-space–time is

$$\mathbf{c}_2\overline{\triangleright}\mathbf{x}_1=\frac{\mathbf{x}_1\mathbf{x}_2-\mathbf{x}_2\mathbf{x}_1\mathbf{R}_{21}^{-1}}{q-q^{-1}}.$$

Moreover, $c_i \underline{\triangleright} \underline{S}(\ ) = \underline{S}(c_i \overline{\underline{\triangleright}}(\ ))$*, where* $\underline{S}$ *is the braided antipode or parity operator on q-space–time.*

Proof: The abstract treatment for the conjugate action of the special conformal generators is in the Appendix, from which one may compute the explicit form stated. In our R-matrix setting, a direct proof is as follows, using the $*$-structures in Sec. III for either the real type I or type II cases. In the type I case,

$$c_i \overline{\underline{\triangleright}} x_j = (Sc_a \eta^{ia} \underline{\triangleright} x_b \eta^{jb})^* = -(\eta^{ia} c_d \underline{\varsigma} Sl^{+d}{}_a \underline{\triangleright} x_b \eta^{jb})^* = -(\eta^{ia} c_d \underline{\triangleright} x_e R^{-1e}{}_b{}^d{}_a \eta^{jb})^*$$
$$= \left(\left(\frac{-x_e x_d + x_f x_g R^{g}{}_e{}^f{}_d}{q - q^{-1}} \right) \eta^{ia} R^{-1e}{}_b{}^d{}_a \eta^{jb} \right)^* = \frac{x_j x_i - x_a x_b R^{-1a}{}_i{}^b{}_j}{q - q^{-1}}$$

using the usual covariance properties of the quantum metric. In the type II case,

$$c_i \overline{\underline{\triangleright}} x_j = (Sc_i \underline{\triangleright} x_j)^* = -(c_a \underline{\varsigma} Sl^{+a}{}_i \underline{\triangleright} x_j)^* = -(c_a \underline{\triangleright} x_b R^{-1b}{}_j{}^a{}_i)^*$$
$$= \left(\left(\frac{-x_b x_a + x_d x_c R^{c}{}_b{}^d{}_a}{q - q^{-1}} \right) R^{-1b}{}_j{}^a{}_i \right)^*$$

which likewise computes to the stated formula.

For the result that the action and conjugate action are intertwined by $\underline{S}$, we have on the generators $\underline{S}(\mathbf{c}_2 \overline{\underline{\triangleright}} \mathbf{x}_1) = (q - q^{-1})^{-1} \underline{S}(\mathbf{x}_1 \mathbf{x}_2 - \mathbf{x}_2 \mathbf{x}_1 \mathbf{R}_{21}^{-1}) = (q - q^{-1})^{-1}((-\mathbf{x}_2)(-\mathbf{x}_1)\mathbf{R} - (-\mathbf{x}_1)(\mathbf{x}_2))$ $= \mathbf{c}_2 \underline{\triangleright} (-\mathbf{x}_1)$ using the braided-antimultiplicativity of the braided antipode $\underline{S}(\mathbf{x}) = -\mathbf{x}$. □

The same applies to the action on products of q-space–time generators: we use $\mathbf{R}_{21}^{-1}$ in place of $\mathbf{R}$ in Lemma 5.2. Thus the q-conformal group exhibits the same novel phenomenon demonstrated for the extended q-Poincaré algebra in Ref. 10 whereby $*$-conjugation is implemented in braided geometry by reversal of braid crossings. The equivalence of the action and conjugate action via the braided-parity operator also applies to all orders of products of q-space–time generators. This is the sense within braided geometry in which the operators c_i are ''anti-Hermitian.'' This also holds for the momentum p^i generators as the main result in Ref. 10.

The present work suggests the possibility of a systematic theory of massless spinning particles based on invariance under the q-conformal group. This will be attempted elsewhere. Classically, it requires the construction of fields with conformal weights defined as sections of certain vector bundles over compactified spacetime. In the q-deformed case one needs therefore nontrivial quantum homogeneous spaces and their associated bundles, for example along the lines in Ref. 18.

APPENDIX: ABSTRACT RESULTS

Most of the formulas for the q-conformal group in the text above have been given at the level of R-matrices and matrix relations. In principle, one also has to check a large number of nonquadratic relations, in particular associated with the $\mathbf{l}^{\pm}$ generators (they are not independent). These are needed to form a (quasitriangular) Hopf algebra in the Lorentz sector. Fortunately, such details are ensured by the abstract braided group and quantum group constructions underlying the R-matrix formulas. This is given for the extended q-Poincaré algebra in Ref. 10 and we extend this now for the q-conformal case. The basis for the latter is a recent construction[9] which associates to a braided group B in the category of H-modules (H is a quasitriangular Hopf algebra), a new quasitriangular Hopf algebra built from B, H, B^*, called the *double-bosonization* of B. Here we state without proof the relevant left-module version of the double-bosonization formulas (different right-module conventions are used in Ref. 9, for the purposes there). Then we study $*$-structures in this abstract setting, which is the new result of this Appendix.

Familiarity with abstract quantum group[11] and braided group[12] techniques is assumed. In particular, $\Delta h = h_{(1)} \otimes h_{(2)}$ denotes the coproduct of $h \in H$ and $\underline{\Delta} b = \underline{b_{(1)}} \otimes \underline{b_{(2)}}$ the braided coproduct of $b \in B$. Also, $\mathscr{R} = \mathscr{R}^{(1)} \otimes \mathscr{R}^{(2)}$ denotes the quasitriangular structure of $\overline{H}$, and $v = \mathscr{R}^{(1)} S \mathscr{R}^{(2)}$.

Let B be a braided group with invertible braided antipode in the braided category of left H-modules, dual to another braided group C. So $B = C^\star$. (In the infinite-dimensional case, we suppose a duality pairing ev: $B \otimes C \to k$ of braided groups.) The *double-bosonization* of B is the Hopf algebra $U(B)$ containing B, C^{op}, H as subalgebras and the cross relations, coproduct and antipode (cf. Ref. 9)

$$\begin{gathered} hb = (h_{(1)} \triangleright b) h_{(2)}, \quad hc = (h_{(2)} \triangleright c) h_{(1)}, \\ \underline{b_{(1)}} \mathscr{R}^{(2)} \underline{c_{(1)}} \mathrm{ev}(\mathscr{R}^{(1)} \triangleright \underline{b_{(2)}}, \underline{c_{(2)}}) = \mathrm{ev}(\underline{b_{(1)}}, \mathscr{R}^{(2)} \triangleright \underline{c_{(1)}}) \underline{c_{(2)}} \mathscr{R}^{(1)} \underline{b_{(2)}}, \\ \Delta b = \underline{b_{(1)}} \mathscr{R}^{(2)} \otimes \mathscr{R}^{(1)} \triangleright \underline{b_{(2)}}, \quad \Delta c = \mathscr{R}^{(2)} \triangleright \underline{c_{(1)}} \otimes \underline{c_{(2)}} \mathscr{R}^{(1)}, \\ Sb = (u \mathscr{R}^{(1)} \triangleright \underline{S} b) S \mathscr{R}^{(2)}, \quad Sc = \mathscr{R}^{-(1)} \underline{S}^{-1} (v^{-1} \mathscr{R}^{-(2)} \triangleright c), \end{gathered} \tag{21}$$

where $\triangleright$ denotes the action of H whereby B, C live in the braided category of H-modules. The pairing is assumed covariant, so $\mathrm{ev}(h \triangleright b, c) = \mathrm{ev}(b, (Sh) \triangleright c)$. The unit and counit are the trivial tensor product ones and H has its usual coproduct and antipode (it is a sub-Hopf algebra). Similar proofs to those in Ref. 9 show that this defines a Hopf algebra. The bosonization $B \bowtie H$ appears as a sub-Hopf algebra and a certain ''conjugate bosonization'' generated by C^{op}, H also appears as a sub-Hopf algebra.

When the pairing is nondegenerate, we have as a formal power series a canonical element $\exp = e_\alpha \otimes f^\alpha$ for the pairing, where $\{e_\alpha\}$ is a basis of C and $\{f^\alpha\}$ is a dual basis. Its inverse in the algebra $C^{\mathrm{op}} \otimes B$ is $\exp^{-1} = (\underline{S} e_\alpha \otimes f^\alpha)$ from the pairing axioms. In this case the double-bosonization is quasitriangular with

$$\mathscr{R}_{U(B)} = \mathscr{R}\, \exp^{-1}, \tag{22}$$

where we view $\mathscr{R}$ and exp in $U(B) \otimes U(B)$.

This describes the left-handed version of the formulas in Ref. 9. It underlies the formulas in Sec. II: we take H generated by $\mathbf{l}^{\pm}$, $\mathfrak{s}$ and B generated by $\mathbf{p}$. We take C generated by $\mathbf{c}$ which are dual to the $\mathbf{p}$ in the usual way except scaled so that $\mathrm{ev}(p^i, c_j) = (q - q^{-1})^{-1} \delta^i{}_j$. We then use the same methods as in Refs. 2 and 10 for the calculation of the extended q-Poincaré algebra as $B \bowtie H$. Similarly for the conjugate bosonization generated by H, C^{op}. The remaining cross relations are $[p^i, c_j] = \mathrm{ev}(p^i, c_a) \langle t^a{}_j g, \mathscr{R}^{(2)} \rangle \mathscr{R}^{(1)} - \mathscr{R}^{(2)} \langle S t^i{}_a g^{-1}, \mathscr{R}^{(1)} \rangle \mathrm{ev}(p^a, c_j)$ from (21) and the linear form of the braided coproducts on B, C. It is convenient to compute the action of $\mathscr{R}$ here on C as evaluation against the coaction of the matrix quantum group dual to H, with generators $\mathbf{t}, g$. We derive the formula in Proposition 2.1 in this way. The same method gives the spinorial formulas in Sec. IV.

Also given in Ref. 9 is a fundamental representation of $U(B)$. In our conventions it appears on C, making it into a left $U(B)$-module algebra as follows: first, B acts on C by the braided left coregular representation studied in Ref. 10, Sec. 2. Together with the given action $\triangleright$ of H on C, we have (Ref. 10, Cor. 2.2) a covariant action of $B \bowtie H$ on C (it defines the action of the extended q-Poincaré algebra on space–time). Second, C acts on itself by the right braided-adjoint action. This is given by the diagrams in Ref. 3 reflected in a mirror followed by reversal of braid crossings. We view this as a left action of C^{op} on itself (cf. Ref. 19). These actions fit together to give an action of $U(B)$ covariantly on C (i.e., respecting its product). Explicitly,

$$b \triangleright x = \mathrm{ev}(\underline{S}^{-1} b, \underline{x_{(1)^{\mathrm{op}}}}) \underline{x_{(2)^{\mathrm{op}}}}, \quad c \triangleright x = (\mathscr{R}^{(2)} \triangleright \underline{S} \underline{c_{(1)}}) (\mathscr{R}^{(1)} \triangleright x) \underline{c_{(2)}} \tag{23}$$

when acting on $x\in C$. Here $x_{\underline{(1)}^{\rm op}}\otimes x_{\underline{(2)}^{\rm op}}=\mathscr{R}^{-(1)}\triangleright x_{\underline{(2)}}\otimes\mathscr{R}^{-(2)}\triangleright x_{\underline{(1)}}$ is the opposite braided coproduct of C. This action underlies the formulas in Sec. V. The action of $p^i\in B$ is by braided differentiation as studied in Ref. 10. The action of $c_i\in C$ is computed as

$$c_i\triangleright x_j=(\mathscr{R}^{(2)}\triangleright \underline{S}c_i)x_a\langle\mathscr{R}^{(1)},t^a{}_jg\rangle+x_jc_i=x_jc_i-(\varsigma^{-1}Sl^{-a}{}_j\triangleright c_i)x_a=\frac{x_jx_i-x_ax_bR^b{}_j{}^a{}_i}{q-q^{-1}},$$

where $x_i\in C$ are the usual (not scaled) generators dual to p^i [so $c_i=(q-q^{-1})x_i$], and $\underline{S}x_i=-x_i$. This derives the action used in Sec. V.

Next we move on to new abstract considerations beyond.[9] We suppose that B,C are $*$-braided groups in the usual sense,[16] H is a real-quasitriangular Hopf $*$-algebra, and its action on B is unitary in the Hopf algebraic sense. Thus

$$(h\triangleright b)^*=(Sh)^*\triangleright b^*,\quad (h\triangleright c)^\star=(S(h^*))\triangleright c^\star. \tag{24}$$

As explained in Ref. 10, the second formula is dictated by the first one and braided group duality. We use $\bigstar$ to define the $*$-structure on $C^{\rm op}$ as the same antilinear map.

Proposition A.1: In this setting, the double bosonization $U(B)$ is a quasi-$*$ Hopf algebra with cocycle $\mathscr{R}$ viewed in $U(B)\otimes U(B)$. Moreover,

$$(*\otimes *)\circ\Delta\circ *=\exp^{-1}(\Delta\ )\exp$$

in $U(B)$.

Proof: It is proven in Ref. 10 that, in this setting, $B\bowtie H$ becomes a quasi-$*$ Hopf algebra with cocycle $\mathscr{R}$. By a similar calculation, we find that the conjugate bosonization generated by $C^{\rm op}$, H is also a quasi-$*$ Hopf algebra with the same cocycle $\mathscr{R}$. We verify that these $*$-structures are compatible with the cross-relations in (21). Applying $*$ to both sides:

$$\begin{aligned}(b_{\underline{(1)}}\mathscr{R}^{(2)}c_{\underline{(1)}})^*\overline{{\rm ev}(\mathscr{R}^{(1)}\triangleright b_{\underline{(2)}},c_{\underline{(2)}})}&=c_{\underline{(1)}}{}^*\mathscr{R}^{(2)*}b_{\underline{(1)}}{}^*{\rm ev}((\mathscr{R}^{(1)}\triangleright b_{\underline{(2)}})^*,c_{\underline{(2)}}{}^*)\\&=c^*{}_{\underline{(2)}}\mathscr{R}^{(1)}b^*{}_{\underline{(2)}}{\rm ev}(S^{-1}\mathscr{R}^{(2)}\triangleright b^*{}_{\underline{(1)}},c^*{}_{\underline{(1)}})\\&=c^*{}_{\underline{(2)}}\mathscr{R}^{(1)}b^*{}_{\underline{(2)}}{\rm ev}(b^*{}_{\underline{(1)}},\mathscr{R}^{(2)}\triangleright c^*{}_{\underline{(1)}})\\&={\rm ev}(\mathscr{R}^{(1)}\triangleright b^*{}_{\underline{(2)}},c^*{}_{\underline{(2)}})b^*{}_{\underline{(1)}}\mathscr{R}^{(2)}c^*{}_{\underline{(1)}}\\&={\rm ev}(b^*{}_{\underline{(2)}},S\mathscr{R}^{(1)}\triangleright c^*{}_{\underline{(2)}})b^*{}_{\underline{(1)}}\mathscr{R}^{(2)}c^*{}_{\underline{(1)}}\\&={\rm ev}(b_{\underline{(1)}}{}^*,(\mathscr{R}^{(2)}\triangleright c_{\underline{(1)}})^*)b_{\underline{(2)}}{}^*\mathscr{R}^{(1)*}c_{\underline{(2)}}{}^*\\&=\overline{{\rm ev}(b_{\underline{(1)}},\mathscr{R}^{(2)}\triangleright c_{\underline{(1)}})}(c_{\underline{(2)}}\mathscr{R}^{(1)}b_{\underline{(2)}})^*\end{aligned}$$

using $\overline{{\rm ev}(b\otimes c)}={\rm ev}(b^*,c^*)$, reality of $\mathscr{R}$ in the sense $\mathscr{R}^{*\otimes *}=\mathscr{R}_{21}$, our assumption (24), invariance of ev, and the cross-relations in (21) applied to b^*, c^*. This checks consistency of the relations under $*$ and implies that we have a $*$-algebra structure on $U(B)$. Since its two sub-Hopf algebras mentioned above are quasi-$*$ Hopf algebras with cocycle $\mathscr{R}$, it becomes a quasi-$*$ Hopf algebra as well, with the same cocycle.

Since $U(B)$ is also (in the nondegenerately paired case) quasitriangular via (22), we deduce that $(*\otimes *)\circ\Delta\circ *=\mathscr{R}^{-1}(\tau\circ\Delta\ )\mathscr{R}=\mathscr{R}^{-1}\mathscr{R}_{U(B)}(\Delta\ )\mathscr{R}_{U(B)}^{-1}\mathscr{R}=\exp^{-1}(\Delta\ )\exp$, as stated. □

We see from this proposition that the plane wave exp controls the extent that the double bosonization fails to be a Hopf $*$-algebra in the usual sense. This, in turn, expresses the sense in which the tensor product of unitaries fails to be unitary: they are unitary only up to a cocycle isomorphism expressed by the action of exp.

From the theory of quasi-$*$ Hopf algebras in Ref. 10, Lemma 4.7, it is known that if a quasi-$*$ Hopf algebra $\mathscr{H}$ acts covariantly on a $*$-algebra C by $\triangleright$, then the conjugate quasi-$*$ Hopf algebra [with coproduct $\overline{\Delta}=(*\otimes *)\circ\Delta\circ *$] acts covariantly on C by a conjugate action $\overline{\triangleright}$ defined by

$$h\overline{\triangleright}x=(S(h^*)\triangleright x^*)^* \tag{25}$$

for all $h\in\mathscr{H}$ and $x\in C$.

Theorem A.2: *The conjugate of the action of $U(B)$ as a quasi-$*$ Hopf algebra acting on C is $h\overline{\triangleright}x=h\triangleright x$ and $b\overline{\triangleright}x=\mathrm{ev}(b,x_{\underline{(1)}})x_{\underline{(2)}}$ as in* Ref. 10, *and*

$$c\overline{\triangleright}x=(\mathscr{R}^{-(1)}\triangleright\underline{S}^{-1}c_{\underline{(1)}^{\mathrm{op}}})(\mathscr{R}^{-(2)}\triangleright x)c_{\underline{(2)}^{\mathrm{op}}}.$$

Moreover, $(\ )\triangleright\underline{S}x=\underline{S}((\ )\overline{\triangleright}x)$, i.e., the action and conjugate action of $U(B)$ are intertwined by the braided antipode of C.

Proof: The conjugate actions of $h\in H$ and $b\in B$ are covered in the conjunction of Ref. 10, Cor. 2.4 and Prop. 4.8. To this we add now the conjugate of the action of $c\in C$. We compute

$$\begin{aligned}
c\overline{\triangleright}x&=(S(c^*)\triangleright x^*)^*=(\mathscr{R}^{-(1)}\triangleright((v^{-1}\mathscr{R}^{-(2)}\triangleright\underline{S}^{-1}c^*)\triangleright x^*))^*\\
&=S(\mathscr{R}^{-(1)}*)\triangleright((v^{-1}\mathscr{R}^{-(2)}\triangleright\underline{S}^{-1}c^*)\triangleright x^*)^*\\
&=S(\mathscr{R}^{-(1)}*)\triangleright((\mathscr{R}^{(2)}\triangleright\underline{S}(v^{-1}\mathscr{R}^{-(2)}\triangleright\underline{S}^{-1}c^*)_{\underline{(1)}})(\mathscr{R}^{(1)}\triangleright x^*)(v^{-1}\mathscr{R}^{-(2)}\triangleright\underline{S}^{-1}c^*)_{\underline{(2)}})^*\\
&=S(\mathscr{R}^{-(1)}*)\triangleright((v^{-1}\mathscr{R}^{-(2)}\triangleright\underline{S}^{-1}c^*)^*_{\underline{(1)}}(S(\mathscr{R}^{(1)}*)\triangleright x)\\
&\qquad\times(S(\mathscr{R}^{(2)}*)\triangleright\underline{S}(v^{-1}\mathscr{R}^{-(2)}\triangleright\underline{S}^{-1}c^*)^*_{\underline{(2)}}))\\
&=\mathscr{R}^{-(2)}\triangleright((u^{-1}\mathscr{R}^{-(1)}\triangleright\underline{S}^{-1}c)_{\underline{(1)}}(\mathscr{R}^{(2)}\triangleright x)(\mathscr{R}^{(1)}\triangleright\underline{S}(u^{-1}\mathscr{R}^{-(1)}\triangleright\underline{S}^{-1}c)_{\underline{(2)}}))\\
&=\mathscr{R}_2{}^{-(2)}\mathscr{R}_1{}^{-(2)}\triangleright((u^{-1}\mathscr{R}_1{}^{(2)}\mathscr{R}_2{}^{(1)}\mathscr{R}_1{}^{-(1)}\mathscr{R}^{-(1)}\triangleright\underline{S}^{-1}c_{\underline{(2)}})(\mathscr{R}^{(2)}\triangleright x)\\
&\qquad\times(\mathscr{R}^{(1)}u^{-1}\mathscr{R}_1{}^{(1)}\mathscr{R}_2{}^{(2)}\mathscr{R}_2{}^{-(1)}\mathscr{R}^{-(2)}\triangleright c_{\underline{(1)}})),
\end{aligned}$$

where we use the antipode of $U(B)$ from (21) and repeatedly use (24). For the fifth equality we use the axiom $c_{\underline{(1)}}{}^*\otimes c_{\underline{(2)}}{}^*=c^*{}_{\underline{(2)}}\otimes c^*{}_{\underline{(1)}}$ for $*$-braided groups. We then use the reality property of $\mathscr{R}$, which also implies that $v^{-1}{}^*=\overline{v}^{-1}$. Here $Sv^{-1}=u^{-1}=\mathscr{R}^{(2)}S^2\mathscr{R}^{(1)}$. For the last equality we use covariance of $\underline{\Delta}$ under the action of H [along with standard facts about quasitriangular Hopf algebras to compute Δu^{-1} and $(\Delta\otimes\mathrm{id})\mathscr{R}^{-1}$], and the braided anticomultiplicativity $\underline{\Delta}S^{-1}c=\mathscr{R}^{-(1)}\triangleright\underline{S}^{-1}c_{\underline{(2)}}\otimes\mathscr{R}^{-(2)}\triangleright\underline{S}^{-1}c_{\underline{(1)}}$ from Ref. 12. Numerical suffices on $\mathscr{R}$, $\mathscr{R}^{-1}$ are used to distinguish the various copies. The remaining steps are a tedious but straightforward computation: we use the QYBE for $\mathscr{R}$ to cancel some of the $\mathscr{R}$ factors. Then we compute the action of $\mathscr{R}_1{}^{-(2)}\mathscr{R}_2{}^{-(2)}$ on products using covariance, converting coproducts on $\mathscr{R}^{-1}$ into more copies of $\mathscr{R}^{-1}$. Using $u(\ )u^{-1}=S^2$ and $\mathscr{R}^{-(2)}u^{-1}\mathscr{R}^{-(1)}=1$, we can then cancel most of the $\mathscr{R}$, $\mathscr{R}^{-1}$ factors to obtain the result stated. Here $c_{\underline{(1)}^{\mathrm{op}}}\otimes c_{\underline{(2)}^{\mathrm{op}}}$ denotes the braided opposite coproduct of C as usual.

Next, we show that the action and conjugate action are intertwined by the braided antipode $\underline{S}$ of the copy of C in which we are acting. For the action of $h\in H$ this is covariance of the braided antipode. For $b\in B$ this is Ref. 10, Cor. 2.4. To this we now add

$$\underline{S}(c\overline{\triangleright x}) = (.\mathscr{R}^{(2)}\triangleright \underline{S}c_{\underline{(2)}^{\mathrm{op}}})(.\mathscr{R}^{(1)}\triangleright \underline{S}((.\mathscr{R}^{-(1)}\triangleright \underline{S}^{-1}c_{\underline{(1)}^{\mathrm{op}}})(.\mathscr{R}^{-(2)}\triangleright x)))$$
$$= (.\mathscr{R}_1{}^{(2)}.\mathscr{R}_2{}^{(2)}\triangleright \underline{S}c_{\underline{(2)}^{\mathrm{op}}})(.\mathscr{R}_1{}^{(1)}\triangleright \underline{S}x)(.\mathscr{R}_2{}^{(1)}\triangleright c_{\underline{(1)}^{\mathrm{op}}})$$
$$= (.\mathscr{R}^{(2)}\triangleright \underline{S}c_{\underline{(1)}})(.\mathscr{R}^{(1)}\triangleright \underline{S}x)c_{\underline{(2)}} = c\triangleright \underline{S}x$$

using braided-antimultiplicativity of $\underline{S}$ twice. This part of the proof can also be done diagrammatically. □

This therefore extends the abstract unitarity and quasi-$*$ considerations for bosonizations and the extended q-Poincaré algebra in Ref. 10 to double-bosonizations and the q-conformal algebra. It is used in Secs. III and V.

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The algebra of q-pseudodifferential symbols and the q-$\mathbf{W}_{\mathrm{KP}}^{(n)}$ algebra

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In this paper we continue with the program to explore the topography of the space of W-type algebras. In the present case, the starting point is the work of Khesin, Lyubashenko, and Roger on the algebra of q-deformed pseudodifferential symbols and their associated integrable hierarchies. The analysis goes on by studying the associated Hamiltonian structures for which compact expressions are found. The fundamental Poisson brackets yield q-deformations of $\mathbf{W}_{\mathrm{KP}}$ and related $\mathbf{W}$-type algebras which, in specific cases, coincide with the ones constructed by Frenkel and Reshetikhin. The construction underlies a continuous correspondence between the Hamiltonian structures of the Toda lattice and the KP hierarchies. © *1996 American Institute of Physics.* [S0022-2488(96)04011-X]

I. INTRODUCTION

The literature concerning the so-called **W** algebras increases as the belief that the *w* stands for ''wild.'' In fact they are wild objects in that they still resist all efforts to achieve a clear and unified understanding of their physical meaning or at least of their geometrical origin. On the other hand, the fascination about them stems from the way they underlie so many *a priori* disconnected physical and mathematical constructions: two-dimensional conformal field theory,[1] soliton systems,[2] vertex-operator and Kac–Moody algebras,[3] classical and quantum fluids,[4,5] 2-D quantum gravity,[6] generalized particle systems,[7] and many others.

On the way to taming the **W** algebras different proposals have been pursued. On one hand, in the last years some effort has been posed in setting up a classification program. It has been realized that a natural arena to handle this program is the phase space of integrable soliton systems, where very many of the known **W** algebras arise either as Poisson bracket algebras, or as symmetries of the evolution equations. On the other hand, searching for an interpretation of **W** algebras in physical terms, some simplifications have been produced, yielding somewhat simpler objects which still preserve many of the distinguishing features of **W** algebras. Among them, the presence of the Virasoro subalgebra plays a central role. Thus for example the ''dispersionless'' or ''classical'' limit, in which the operator ∂ is smoothly replaced by a commuting symbol ξ (Ref. 8), has shed some light about the geometry of classical **W**-morphisms in relation to ''area preserving diffeomorphisms'' [9] and Hamiltonian mechanics[10] (see also Ref. 11 for other interesting proposals).

Another interesting simplification should occur if we replaced the derivative ∂ by the q-derivative ∂_q. The q-derivative is in fact a difference operator, i.e., let F denote the ring of complex-valued polynomials in z and z^{-1} ($\mathbf{C}[z, z^{-1}]$) and $q \in \mathbf{C}$:

$$\partial_q f(z) \equiv \frac{f(qz)-f(z)}{z(q-1)},$$

where ∂ is recovered in the $\lim_{q\to 1}\partial_q = \partial$. Using ∂_q instead of ∂ provides a sort of short distance cutoff. For this reason it has been widely investigated in connection with the problem of regulating quantum field theories.[12] In the last years, a few works have been concerned with the issue of the

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q-deformed Virasoro and **W** algebras; in Refs. 13 and 14 we have listed the references we are aware of, where structures deserving such a name have been constructed. The generic approach in them exploits heavily the use of the q-affine algebras, q-vertex operators, and a q-deformed version of the Miura transformation. The connection of these algebras with integrable systems remained unclear, until the recent work of E. Frenkel.[15] In this paper it is claimed that the q-deformed W algebras constructed in Ref. 14 provide bi-Hamiltonian structures for a particular set of differential—q-difference integrable systems, which naturally deserve the name of q-deformed KdV hierarchies.

Our original motivation was to pursue the line of research developed in Ref. 16. In this work the central object of study was the Lie algebra of so-called q-pseudodifferential symbols ∂_q, its extensions and contractions, as well as the associated Lax systems. Actually, the q-deformed n-KdV integrable hierarchies defined there turn out to be the same as those in Ref. 15, albeit in a different basis. With respect to this work, ours is somewhat complementary in that we asked ourselves: first, what are the most general hierarchies that one could write in terms of Lax operators involving q-pseudodifferential symbols and, second, what are their Hamiltonian structures.[2] To perform the analysis, the unified framework described in Ref. 17 proved to be instrumental. As an output, a large class of q-deformations of classical W algebras are found, including those of $\mathbf{W}_{\mathrm{KP}}$, GD_n, or the centrally extended $W_{1+\infty}$. In specific cases we find agreement with the results of Ref. 15. We also comment on some obstruction found when trying to define a q-deformation of W_n.

This paper is organized as follows: for completeness, Secs. II and III are devoted to the introductory material. In the former, some basic notions about the algebra of q-pseudodifferential operators are included; the latter gives an overview of the r-matrix approach to integrable systems. In both sections we have followed closely the clear expositions of Refs. 16 and 17, respectively.

Section IV is a straightforward application of the machinery of Sec. III. The analysis is performed in a twisted basis T, which we refer to as the ''Toda lattice'' basis. In particular, three tri-Hamiltonian hierarchies of nonlinear differential-difference equations are found. The Poisson brackets are explicitly computed and agree in special cases with those found in Ref. 15. One of the advantages of the present formalism is the possibility of carrying out a transparent treatment of reductions. Some of them are investigated at the end of this section.

Section V is a reelaboration of the previous findings in the basis ∂_q introduced in Sec. I, and named q-KP basis after its direct relationship with the standard KP basis. The nonlinear infinite-dimensional algebra which we obtain and compute is connected with the $\mathbf{W}_{\mathrm{KP}}^{(n)}$ algebra[18] in the limit $q\to 1$; thereafter, we name it the q-$\mathbf{W}_{\mathrm{KP}}^{(n)}$ algebra. Reductions are treated at the end. Of utmost importance are the reductions of q-KP to q-KdV. We comment about the possibility of obtaining several q-deformations of the Virasoro algebra within the present formalism.

Finally, in Sec. VI we bring the logarithm of the q-differential symbol $\log \partial_q$ into the game. We do this by formally continuing the order n of the Lax operator to real values and taking afterwards a suitable limit $n\to 0$. The resulting algebra can be considered as a q-deformation of the centerful $W_{1+\infty}$ algebra.

II. THE ALGEBRA OF q-PSEUDODIFFERENTIAL OPERATORS

It will be useful to define the ''shift'' $\tau f(z)=f(qz)$, $\tau^{\beta} f(z)=f(q^{\beta}z)$, $\beta\in\mathbf{C}$. So, ∂_q is a q-derivative in the following sense:

$$\partial_q(fg)=\partial_q(f\,)g+\tau(f\,)\partial_q(g), \tag{2.1}$$

which can be proven by explicit computation. The actions of τ and ∂_q are not commutative but rather q-commutative, i.e., $\partial_q(\tau(f\,))=q\,\tau(\partial_q f\,)$

Definition 2.2: An algebra ΨDO_q of q-pseudodifferential operators is a vector space of formal series

$$\Psi DO_q=\left\{ A(x,\partial_q)=\sum_{-\infty}^{n} u_i(z)\partial_q^i \,\middle|\, u_i\in F \right\} \tag{2.3}$$

with respect to ∂_q. The multiplication law in ψDO_q is defined by the following rule: F is a subalgebra of ψDO_q and there are commutation relations ($u\in F$):

$$\begin{aligned} \partial_q u&=(\partial_q u)+\tau(u)\partial_q,\\ \partial_q^{-1}u&=\sum_{k\geqslant 0}(-1)^k q^{-k(k+1)/2}(\tau^{-k-1}(\partial_q^k u))\partial_q^{-k-1}. \end{aligned} \tag{2.4}$$

Each term of the product of two Laurent series in ∂_q is found by applying these rules a finite number of times. The formula (2.4) is built so that $\partial_q^{-1}\partial_q u=\partial_q\partial_q^{-1}u=u$. For $q=1$ these formulas recover the ''classical'' definition of multiplication law in the algebra of pseudodifferential operators ψDO.

The commutation rule for ∂_q^n (with any integer n) and $u(z)$ join these formulas in one

$$\partial_q^n u=\sum_{k\geqslant 0}\begin{bmatrix} n\\ k\end{bmatrix}_q(\tau^{n-k}(\partial_q^k u))\partial_q^{n-k}, \tag{2.5}$$

where we use the following notation for q-numbers and q-binomials.

$$(n)_q=\frac{q^n-1}{q-1},$$

$$\begin{bmatrix} m\\ k\end{bmatrix}_q=\frac{(m)_q(m-1)_q\cdots(m-k+1)_q}{(1)_q(2)_q\cdots(k)_q}.$$

The q-analog of the Leibnitz rule of multiplication of two q-pseudodifferential operators $A(x,\partial_q)$ and $B(x,\partial_q)$ can be written as the following operation on their symbols,

$$A(x,\partial_q)B(x,\partial_q)=\sum_{k\geqslant 0}\frac{1}{(k)_q!}\left(\frac{d^k}{d\partial_q^k}A\right)*(\partial_q^k B), \tag{2.6}$$

where for any complex value of α

$$\frac{d^k}{d\partial_q^k}(f\partial_q^\alpha)=(\alpha)_q(\alpha-1)_q\cdots(\alpha-k+1)_q f\partial_q^{\alpha-k}$$

and the $*$ multiplication of symbols obeys the following commutation rule for the generators:

$$f*\partial_q=f\partial_q,\quad \partial_q*f=\tau(f\ )\partial_q,\quad \partial_q^{-1}*f=\tau^{-1}(f\ )\partial_q^{-1}. \tag{2.7}$$

This follows by a straightforward verification of the formula (2.6) for the product $\partial_q^n u(z)$, which gives the same answer as (2.5).

Define the Lie algebra $\mathcal{G}_q$ as the set ΨDO_q of all q-pseudodifferential symbols equipped with the commutator bracket $[A,\ B]=AB-BA$.

With this setup in mind, it is straightforward to construct a q-deformed analog of the KP hierarchy. The phase space for this dynamical system is the set $\{L_q=\partial_q+u_1(z)+u_2(z)\partial_q^{-1}+u_3(z)\partial_q^{-2}+\cdots\}$, and the equations of motion adopt the familiar Lax form

$$\frac{dL_q}{dt_m}=[L_q,(L_q^m)_+]=[(L_q^m)_-,L_q]. \tag{2.8}$$

Notice that unlike in the differential case, the potential $u_1(z)$ has a nontrivial evolution. This is due to the fact that now the highest degree of the commutator of two q-pseudodifferential operators is the sum of their respective highest degrees, this being a consequence of the nonconmutativity of the multiplication of symbols as shown in (2.7).

III. *R*-MATRIX APPROACH TO INTEGRABLE SYSTEMS

We recall here the rudiments of r-matrix and refer the interested reader to the literature.[19] In this section we shall follow closely the clear introduction given in Ref. 17. A classical r-matrix on a Lie algebra g is a linear map $\mathscr{R}$: $g\to g$ such that the modified bracket

$$[a,\ b]_{\mathscr{R}}=[\mathscr{R}(a),\ b]+[a,\ \mathscr{R}(b)]$$

is a Lie bracket, thus providing a second Lie algebra structure on g. As was shown in Ref. 19, a sufficient condition for a linear map $\mathscr{R}$ to be an r-matrix is given by the so-called *modified Yang–Baxter* equation [m-YB(α) for short].

$$[\mathscr{R}(a),\ \mathscr{R}(b)]-\mathscr{R}([a,\ b]_{\mathscr{R}})=-\alpha[a,\ b], \tag{3.1}$$

where α is any real number. Now let us assume that in g there is an ad-invariant (under the natural Lie bracket [,] in g) inner product $\langle,\rangle$: $g\times g\to\mathbf{C}$ under which g can be identified with its dual g^*. Immediately we know of a natural Poisson structure that lives on $\mathbf{C}^\infty(g^*)$, namely the Lie–Poisson bracket arising from the modified Lie bracket $[,]_{\mathscr{R}}$:

$$\{f_1,f_2\}_1(L)\equiv\langle L,[\mathscr{R}df_1,\ df_2]+[df_1,\ \mathscr{R}df_2]\rangle, \tag{3.2}$$

evaluated at a point $L\in g=g^*$. This Poisson bracket, termed *linear* after its dependence on L, is the first of a series of other ''potential'' Poisson brackets:

$$\{f_1,f_2\}_2\equiv\langle L,[\mathscr{R}(Ldf_1+df_1L),\ df_2]+[df_1,\ \mathscr{R}(Ldf_2+df_2L)]\rangle, \tag{3.3}$$

$$\{f_1,f_2\}_3\equiv\langle L,[\mathscr{R}(Ldf_1L),\ df_2]+[df_1,\ \mathscr{R}(Ldf_2L)]\rangle. \tag{3.4}$$

Using ad-invariance of the inner product, and the definition of the adjoint r-matrix as $\langle\mathscr{R}(a),b\rangle=\langle a,\mathscr{R}^*(b)\rangle$, we may encode the above ''potential'' Poisson brackets in terms of the associated Poisson map J, defined by

$$\{f_1,f_2\}_s(L)=\langle J_L^{(s)}(df_1),df_2\rangle,\quad s=1,2,3, \tag{3.5}$$

as follows

$$\begin{aligned}
J_L^{(1)}(df\ )&=[L,\ \mathscr{R}(df\ )]+\mathscr{R}^*([L,\ df]),\\
J_L^{(2)}(df\ )&=[L,\ \mathscr{R}(Ldf+dfL)]+L\mathscr{R}^*([L,\ df])+\mathscr{R}^*([L,\ df])L,\\
J_L^{(3)}(df\ )&=[L,\ \mathscr{R}(LdfL)]+L\mathscr{R}^*([L,\ df])L.
\end{aligned} \tag{3.6}$$

Now the crucial question: for what $\mathscr{R}$ will the above maps define Hamiltonian maps? The findings of Refs. 17 and 20 specify the following.

(a) $J_L^{(1)}$ is Hamiltonian for any r-matrix $\mathscr{R}$ on g.

(b) $J_L^{(2)}$ is Hamiltonian if $\mathscr{R}$ and its skew-symmetric combination $\frac{1}{2}(\mathscr{R}-\mathscr{R}^*)$ *both* satisfy the m-YB(α) equation (3.1).
(c) $J_L^{(3)}$ is Hamiltonian if $\mathscr{R}$ is an r-matrix which satisfies m-YB(α) equation.

The three maps are related with one another by simple deformations

$$J_{L+\epsilon 1}^{(2)}=J_L^{(2)}+2\epsilon J_L^{(1)},$$

$$J_{L+\epsilon 1}^{(3)}=J_L^{(3)}+\epsilon J_L^{(2)}+\epsilon^2 J_L^{(1)},$$

where 1 is the generator of the center in g. This, by the way, shows the compatibility of the three ''would be'' Poisson structures.

The construction of integrable systems that are Hamiltonian with respect to the above brackets refers to the existence of a (possibly maximal) set of conserved functions in involution. Here, an important piece in the game is played by the set of Casimir (invariant) functions, i.e., those functions $C\in\mathbf{C}^\infty(g^*)$ satisfying $ad_L^*(C(L))=0$ or, equivalently,

$$ad_L(dC(L))=[L,\ dC(L)]=0.$$

If one has a chance to characterize the Casimir functions (in short, the centralizer of $L\in g$), then a short look at the form of $J^{(s)}$ in (3.6) reveals the following.

(i) The associated Hamiltonian flows adopt the Lax form

$$\frac{dL}{dt}=J_L^{(1)}(dC)=[L,\ \mathscr{R}(dC)],$$

$$\frac{dL}{dt}=J_L^{(2)}(dC)=[L,\ \mathscr{R}(2LdC)],$$

$$\frac{dL}{dt}=J_L^{(3)}(dC)=[L,\ \mathscr{R}(L^2dC)].$$

(ii) The Casimir functions are in involution. For example, when $s=1$

$$\{C_1,C_2\}_1=\langle[L,\ \mathscr{R}(dC_1)],dC_2\rangle=-\langle[L,\ dC_2],\mathscr{R}(dC_1)\rangle=0.$$

A particular (partial) solution is given by the traces of powers of L:

$$C_p(L)\equiv\frac{1}{k}\,\mathrm{Tr}(L^p),\quad dC_p(L)=L^{(k-1)},\quad p=1,2,\ldots\ .$$

For this particular set of functions, the Lax equations are tri-Hamiltonian

$$\frac{dL}{dt_p}\equiv[L,\ \mathscr{R}(L^p)]=J_L^{(1)}(dC_{p+1})=J_L^{(2)}(dC_p)=J_L^{(3)}(dC_{p-1}).$$

In some cases (n-KdV), p may be a fraction of the order of L.

The classification of solutions to (3.1) has been achieved partially. A class of them fall into the following characterization: if $g=g_+\oplus g_-$ is a decomposition into Lie subalgebras, denoting by P_+ (P_-) the projection of g_+ (resp. g_-) along g_- (resp. g_+), then $\mathscr{R}=\frac{1}{2}(P_+-P_-)$ satisfies the modified Yang–Baxter equation (3.1) with $\alpha=\frac{1}{4}$ since $[a,\ b]_{\mathscr{R}}$ is easily calculated to be $[a_+,\ b_+]-[a_-,\ b_-]$ in obvious notation.

We may give the particular form of (3.6) whenever adapted to the present situation (hereafter we shall obviate the dependence of $J_L^{(s)}$ on L, and write simply $J^{(s)}$):

$$
\begin{aligned}
J^{(1)}(df) &= [L,\ P_+ df] - P_-^*[L,\ df] = -[L,\ P_- df] + P_+^*[L,\ df], \\
J^{(2)}(df) &= [L,\ P_+(L df + df\, L)] - L(P_-^*[L,\ df]) - (P_-^*[L,\ df])L \\
&= -[L,\ P_-(L df + df\, L)] + L(P_+^*[L,\ df]) + (P_+^*[L,\ df])L, \\
J^{(3)}(df) &= [L,\ P_+(L df\, L)] - L(P_-^*[L,\ df])L = -[L,\ P_-(L df\, L)] + L(P_+^*[L,\ df])L.
\end{aligned}
\tag{3.7}
$$

Moreover, if g_+ and g_- are isotropic, then clearly $\mathscr{R}$ is skew-adjoint with respect to the inner product $\langle \mathscr{R}(a), b\rangle = \langle a, \mathscr{R}^*(b)\rangle$, i.e., $\mathscr{R}^* = -\mathscr{R}$. In this case $P_\pm^* = P_\mp$ and the three structures in (3.6) reduce to the following form ($X \equiv df$):

$$
\begin{aligned}
J_L^{(1)}(z) &= [L,\ X_+]_- - [L,\ X_-]_+, \\
J_L^{(2)}(z) &= L(XL)_+ - (LX)_+ L = -L(XL)_- + (LX)_- L, \\
J_L^{(3)}(z) &= [L,\ (LXL)_+]_- - L[L, X]_+ L.
\end{aligned}
\tag{3.8}
$$

IV. THE "TODA LATTICE" BASIS

Let us return to the q-deformation of the KP hierarchy that we showed in the introduction (2.8). Define, for $q \neq 1$,

$$
\begin{aligned}
T &= z(q-1)\partial_q + 1, \\
T^{-1} &= \frac{1}{z(q-1)\partial_q + 1} = \sum_{i=1}^{\infty} -\frac{(-q)^i}{(q-1)^i} z^{-i} \partial_q^{-i}.
\end{aligned}
\tag{4.1}
$$

Any element of ΨDO_q of the form (2.3) admits a similar expression in this "twisted" basis

$$
A = \sum_{-\infty}^{n} a_i(z)\partial_q^i = \sum_{-\infty}^{n} t_i(z) T^i. \tag{4.2}
$$

Hence we will be describing the same algebra $\mathscr{G}_q$ in this basis. The relevant composition law is the following, which can be proven by elementary manipulations: For any $f \in F$,

$$
Tf = \tau(f)T, \tag{4.3}
$$

in particular $Tz = qzT$. We will use the notation (Tf) to mean that T acts only on f, i.e., $(Tf) \equiv TfT^{-1} = \tau(f)$.

The algebraic approach to integrability relies heavily on the existence of an ad-invariant symmetric bilinear form. As a step in this direction, a linear functional $\int : f \in \mathbf{C}$ is defined satisfying $\int \tau(f) = \int f$ for all $f \in F$. In agreement with this requirement, we further specify that $\int z^n = \delta_{n,0}$. A particular realization of this definition is given by the usual Riemann integration over S^1 of the Fourier basis functions $z^n = e^{in\theta}$, where the action of τ is seen as a shift of $(-i \log q)$ in θ. Also $\delta(z) = \Sigma_{k \in \mathbf{Z}} z^k$.

Now, let $A = \Sigma_i a_i T^i \in \Psi DO_q$. We define the residue $\mathrm{res}_T : \Psi DO_q \to f$ by

$$
\mathrm{res}_T\left(\sum_i a_i T^i \right) = a_0
$$

and the trace Tr: $\Psi DO_q \to \mathbf{C}$ by

$$\mathrm{Tr}\ A = \int \mathrm{res}_T\ A$$

Lemma 4.4: The bilinear form $\langle , \rangle : \mathscr{G}_q \times \mathscr{G}_q \mathbf{C}$, *given by*

$$\langle A, B \rangle = \mathrm{Tr}\ AB = \int \mathrm{res}_T\ AB, \tag{4.5}$$

defines an ad-invariant bilinear symmetric inner product in $\mathscr{G}_q$

Proof: By direct computation and use of the defining ''shift'' invariance of $\int$ we find

$$\mathrm{Tr}\ AB = \int \mathrm{res}_T\ a_i T^i b_j T^j = \int a_i \tau^i(b_{-i}) = \int b_{-i} \tau^{-i}(a_i)$$

$$= \int \mathrm{res}_T\ b_j \tau^j(a_i) T^{j+1} = \int \mathrm{res}_T\ b_j T^j a_i T^i = \mathrm{Tr}\ BA.$$

■

We would like to stress that this bilinear product is the same (up to factors of q) as the one defined in Ref. 16, as we shall show in Sec. V. The previous lemma is fully equivalent to theorem 3.3 in that reference. With respect to this inner product, the adjoint of τ is $\tau^* = \tau^{-1}$, i.e., $(T^* f) = (T^{-1} f)$.

Let us investigate the possible splittings of the form $\mathscr{G}_q = \mathscr{G}_1 \oplus \mathscr{G}_2$, where $\mathscr{G}_1$ and $\mathscr{G}_2$ are Lie subalgebras. In view of the generic (graded) commutation relations

$$[t_i T^i,\ t_j T^j] = (t_i \tau^i(t_j) - t_j \tau^j(t_i)) T^{i+j},$$

we find only three possibilities as follows:

(1) $(\sigma = -1)$: $\mathscr{G}_q = \mathscr{G}_{\geqslant 0} \oplus \mathscr{G}_{\leqslant -1}$

$$\mathscr{G}_{\geqslant 0} \equiv \left\{ \sum_{i \geqslant 0} t_i(z) T^i \right\}; \quad \mathscr{G}_{\leqslant -1} \equiv \left\{ \sum_{i \leqslant -1} t_i(z) T^i \right\};$$

(2) $(\sigma = +1)$: $\mathscr{G}_q = \mathscr{G}_{\geqslant 1} \oplus \mathscr{G}_{\leqslant 0}$:

$$\mathscr{G}_{\geqslant 1} \equiv \left\{ \sum_{j \geqslant 1} t_j(z) T^j \right\}; \quad \mathscr{G}_{\leqslant 0} \equiv \left\{ \sum_{j \leqslant 0} t_j(z) T^j \right\};$$

(3) $(\sigma = 0)$: $\mathscr{G}_q = \mathscr{G}_{0+} \oplus \mathscr{G}_{0-}$

$$\mathscr{G}_{0+} \equiv \left\{ \sum_{k \geqslant 0} t_k(z) T^k,\ t_0 \in z\mathbf{C}[z] \right\};$$

$$\mathscr{G}_{0-} \equiv \left\{ \sum_{k \geqslant 0} t_k(z) T^k,\ t_0 \in z^{-1}\mathbf{C}[z^{-1}] \right\}.$$

Remark 4.6: As mentioned in Ref. 16, the interest of the last case comes from the fact that, relative to the inner product defined in (4.5), it is the only one where $\mathscr{G}_{0\pm}$ are isotropic. Hence $(\mathscr{G}, \mathscr{G}_{0+}, \mathscr{G}_{0-})$ is a Manin triple and $(\mathscr{G}, \mathscr{G}_{0-})$ a Lie double.

A. The fundamental Poisson brackets

In order to define the phase space where our dynamics will take place, let

$$L=\sum_{i=m}^{n} t_i(z)T^i, \tag{4.7}$$

where $n, m\in\mathbf{Z}$ and $n>m$. We regard any of these difference operators as ''points'' on a manifold $\mathscr{M}_T^{(n,m)}$. The dynamics is governed by differential—q-difference equations derived from the usual Lax system

$$\frac{dL}{dt_p}=[L,\ (L^p)_+]=[(L^p)_-,\ L], \tag{4.8}$$

which is manifestly consistent for L of the form given in (4.7). Here $\pm$ refers to any one of the $\sigma=0,\ \pm1$ splittings defined above.

In the case of $\sigma=-1$ with $(n,m)=(1,-\infty)$, this system is none other than the simplest version of the Toda lattice hierarchy involving one set of time parameters.[21,22] Indeed, in these works the Toda lattice hierarchy is formulated in terms of a Lax operator of the form

$$L=e^{\partial}+\sum_{n=0}^{\infty} u_{n+1}e^{-n\partial},$$

which involves the difference operator e^{∂} acting as $e^{n\partial}u_i(x)=u_i(x+n)e^{n\partial}$. The isomorphism between both formulations is made patent after identifying $u_i(x)$ with $t_i(z=q^x\zeta)$ where $\zeta\in\mathbf{C}$ is any fixed complex number.

Remark that only for $m=0$ and the splitting $\sigma=-1$, or $n=0$ and $\sigma=+1$, equations (4.8) are empty since in this case the commutator vanishes identically. The nontrivial flows may come then from fractional powers of L.[15,16] For example, let $n=N$ and $m=0$. Then

$$\frac{dL}{dt_p}=[L,\ (L^{p/N})_+]=[(L^{p/N})_-,\ L]$$

are nontrivial differential difference equations as long as p is not a multiple of N. An analogous way to characterize these flows is to consider an operator of the form $L\in\mathscr{M}_T^{1,-\infty}$ of the form $L=t_0T+t_1+t_2T^{-1}+...$, constrained to satisfy $L_-^N=0$.

On $\mathscr{M}_T^{(n,m)}$ the (linear) functionals of interest have the form $f_X(L)=\mathrm{Tr}\,LX$ with

$$X=\sum_{j=m}^{n} T^{-j}x_j(z).$$

Clearly f_X adopts the form of a Euclidean scalar product $f_X=\int\Sigma_{i=m}^{n}t_ix_i$. Defining the gradient $d:F\to\mathscr{G}_q$ by

$$\langle df,\delta L\rangle\equiv\frac{d}{d\epsilon}\,f_X(L+\epsilon\delta L)\bigg|_{\epsilon=0},$$

it turns out that $df_X(L)=X$.

We are interested in the fundamental Poisson brackets among the fields $t_i(z)$. Since the Poisson maps $J^{(s)}(df_X)$ are linear in $df_X=X$, we may expand

$$J^{(s)}(X)=\sum_{i=m}^{n}\sum_{j=m}^{n}(J_{ji}^{(s)}x_i)(z)T^j, \tag{4.9}$$

where $J_{ij}^{(s)}$ is some function of q-difference operators T. Plugging this back in (3.5) we obtain

$$\{f_X,f_Y\}=\int (J_{ij}x_j)y_i=\int x_i(J_{ji}^{*}y_j)=-\int x_i(J_{ij}y_j),$$

where the last equation follows from the antisymmetry $\{f_X,f_Y\}=-\{f_Y,f_X\}$, which implies that $J_{ji}^{*}=-J_{ij}$. Finally, comparing this expression with

$$\{f_X,f_Y\}_r=\int x_i(z)\int\{u_i(z),u_j(w)\}_s y_j(w)$$

shows that

$$\{u_i(z),u_j(w)\}_s=-(J_{ij}^{(s)}(z)\,\delta(z/w)), \tag{4.10}$$

where $\delta(z/w)=\Sigma_{j\in\mathbf{Z}}(z/w)^j$, and the operators J_{ij} act at z.

It is time to analyze in detail the potential Poisson structures on $\mathscr{M}_T^{(n,m)}$. We will do this by taking into consideration, case by case, the three possible splittings of $\mathscr{G}_q$: $\sigma=0,\pm1$. Notice that for all cases, the linear and cubic brackets in (3.2) and (3.4) define Poisson brackets, since $\mathscr{R}=\frac{1}{2}(P_+-P_-)$, with $P_\pm$ in each case the relevant projection operators, yields automatically an r-matrix obeying the m-YB($\frac{1}{4}$) equation (3.1). Therefore, further analysis is only required for the quadratic bracket.

1. ($\sigma=-1$): $\mathscr{G}_q=\mathscr{G}_{\geqslant 0}\oplus\mathscr{G}_{\leqslant -1}$

This splitting is, among the three, the most analogous to the one of the standard KP hierarchy. Notice, however, the important difference: now the subalgebra $\mathscr{G}_{\geqslant 0}$ is *not isotropic*, and in consequence the r-matrix is not anti-self-adjoint. Thus, whether the ''antisymmetric'' combination $\frac{1}{2}(\mathscr{R}-\mathscr{R}^*)$ satisfies the m-YB($\frac{1}{4}$) equation as well must be checked independently. In more concrete terms, let

$$\mathscr{R}=\tfrac{1}{2}(P_{\geqslant 0}-P_{\leqslant -1}).$$

In view of the definition of the inner product (4.5), $\mathscr{R}^*=\frac{1}{2}(P_{\leqslant 0}-P_{\geqslant 1})$, and therefore

$$\tfrac{1}{2}(\mathscr{R}-\mathscr{R}^*)=\tfrac{1}{2}(P_{\geqslant 1}-P_{\leqslant -1}). \tag{4.11}$$

It follows from an easy calculation that this linear map satisfies (3.1) with $\alpha=\frac{1}{4}$ as well. Hence all three brackets in (3.2) and (3.4) are Poisson brackets. Using the general formula (3.7) we may particularize to the present case and get ($X\equiv df$)

$$J^{(1)}(X)=[L,\,X_{\geqslant 0}]_{\leqslant 0}-[L,\,X_{\leqslant -1}]_{\geqslant 1}, \tag{4.12}$$

$$\begin{aligned}J^{(2)}(X)&=2L(XL)_{\geqslant 0}-2(LX)_{\geqslant 0}L+L\ \mathrm{res}_T([L,\,X])+\mathrm{res}_T([L,\,X])L\\&=-2L(XL)_{\leqslant -1}+2(LX)_{\leqslant -1}L+L\ \mathrm{res}_T([L,\,X])+\mathrm{res}_T([L,\,X])L,\end{aligned} \tag{4.13}$$

$$J^{(3)}(X)=[L,\,(LXL)_{\geqslant 0}]-L[L,\,X]_{\geqslant 1}L. \tag{4.14}$$

A word about consistency is needed. Concerning the *first structure* (4.12), in order that $J^{(1)}(X)$ describes a deformation of L we must demand that $n\geqslant 0$ and $1\geqslant m$ (in fact, for the particular case of $\mathscr{M}_T^{(n>0,0)}$ expression (4.12) appeared in Ref. 15). This may be seen from (4.12) written in the following form:

$$J^{(1)}(X)=[L_{\leqslant 0},\, X_{\geqslant 0}]_{\leqslant 0}-[L_{\geqslant 2},\, X_{\leqslant -1}]_{\geqslant 1}.$$

The first term on the right-hand side bounds the lowest order of $J^{(1)}(X)$ to be higher or equal to the lowest order of L. The second one bounds the highest order of the map to be strictly lower than the highest order of L. The constraints in n and m come from the projectors outside the commutators.

It is remarkable that for the *second structure* $J^{(2)}$ there is not such a restriction and $J(X)$ parametrizes a deformation of L for any (n,m).

The case of the cubic or *third structure* is more extreme. From (4.14) is evident that $\mathscr{M}_T^{(n,m)}$ is not an invariant subspace under the action of $J^{(3)}$, unless $(n,m)=(\infty,0)$, $(0,-\infty)$, or $(\infty,-\infty)$. For this reason we do not consider this algebra to be of much interest and we will not write down its explicit form. Hereafter we shall restrict our attention to the two other structures.

In terms of the fundamental Poisson brackets we obtain for $J^{(1)}$ the following difference operators $J_{ij}^{(1)}$:

$$J_{ij}^{(1)}=t_{i+j}T^i-T^{-j}t_{i+j}, \tag{4.15}$$

if either $i,j\geqslant 1$ with $n\geqslant i+j$ or, up to a sign, when $0\geqslant i,j$ with $i+j\geqslant m$. In all other cases $J_{ij}^{(1)}=0$. For the sake of comparison with similar results in the literature,[13–15] we may write down the Poisson brackets explicitly:

$$\{t_i(z),t_j(w)\}_1=-t_{i+j}(z)\,\delta\left(\frac{q^i z}{w}\right)+t_{i+j}(w)\,\delta\left(\frac{z}{q^j w}\right). \tag{4.16}$$

with the same set of restrictions upon the indices i,j. This expression exhibits the splitting of the linear Poisson bracket algebra in two graded subalgebras spanned by either positive or nonpositive values of i,j.

For $J_{ij}^{(2)}$ an analogous computation yields

$$J_{ij}^{(2)}=2\sum_{k=\max(m,i+j-n)}^{\min(n,i)}(t_kT^{k-j}t_{i+j-k}-t_{i+j-k}T^{i-k}t_k)+t_i(1+T^i)(1-T^{-j})t_j$$

or, again

$$\{t_i(z),t_j(w)\}_{(2)}=2\sum_{k=\max(m,i+j-n)}^{\min(n,i)}\left(t_{i+j-k}(z)t_k(w)\,\delta\left(\frac{q^{i-k}z}{w}\right)-t_k(z)t_{i+j-k}(w)\,\delta\left(\frac{z}{q^{j-k}w}\right)\right)$$
$$-t_i(z)t_j(w)\sum_{l\in\mathbf{Z}}\left(\frac{z}{w}\right)^l(1+q^i)(1-q^{-j})$$

2. ($\sigma=+1$): $\mathscr{G}_q=\mathscr{G}_{\geqslant 1}\oplus\mathscr{G}_{\leqslant 0}$

This situation is symmetric with respect to the one above. Notice that at the level of the algebra, this splitting transforms into the previous one upon the substitution $T\to T^{-1}$. Therefore, the formulas obtained from (4.12)–(4.14) can be adapted to the present case by a simple replacement $q\to q^{-1}$ and $m\leftrightarrow n$.

3. ($\sigma=0$): $\mathscr{G}_q=\mathscr{G}_{\mathbf{0}^+}\oplus\mathscr{G}_{\mathbf{0}^-}$

This is the standard case of a Lie bialgebra. The three maps in (3.8) automatically define Poisson brackets. The fundamental ones are a slight modification of the ones above, and involve an additional operator $\mathbf{p}_{\pm}$, which projects any element $f\in F$ into its Taylor and Laurent parts, respectively, i.e., $\mathbf{p}_+ z^m=z^m$ iff $m\geqslant 1$ and zero otherwise, and vice versa. Here $\mathbf{p}_+$ and $\mathbf{p}_-$ are mutually adjoint with respect to the inner product defined with $\int$ and commute with T.

As before, the linear structure is a direct sum of two subalgebras, spanned by the fields $t_0^+\equiv\mathbf{p}_+ t_0$ and $\{t_i,\ i=1,\ldots,n\}$ on one side, and $t_0^-\equiv\mathbf{p}_- t_0$ and $\{t_i,\ i=-1,-2,\ldots,m\}$ on the other. Therefore, as long as $i,j\geqslant 1$ but $n\geqslant i+j$,

$$J_{ij}^{(1)}=-(t_{i+j}T^i-T^{-j}t_{i+j}). \tag{4.17}$$

The same expression with opposite sign holds if $-1\geqslant i,j$ with $i+j\geqslant m$. Finally,

$$J_{0j}^{(1)}=\Theta(j-1)\mathbf{p}_+(T^{-j}-1)t_j-\Theta(-j-1)\mathbf{p}_-(T^{-j}-1)t_j \tag{4.18}$$

and $J_{i0}^{(1)}=-J_{0i}^{(1)*}$. In all other cases $J_{ij}=0$. In formula (4.18) Θ stands for the usual step function $\Theta(x)=1$ iff $x\geqslant 0$ and 0 otherwise. The quadratic brackets are computed along the same lines:

$$J_{ij}^{(2)}=2\sum_{k=\max(m,i+j-n)}^{\min(n,i)}(t_kT^{k-j}t_{i+j-k}-t_{i+j-k}T^{i-k}t_k)+2t_i(1-T^{i-j})\mathbf{p}_-t_j\,.$$

B. Some reductions

Let us focus on the $\sigma=-1$ splitting (the case $\sigma=+1$ follows a symmetric pattern). Remark that as far as the Lax equations are concerned, the field t_n is not dynamical. Let $\widetilde{\mathscr{M}}_T^{(n,m)}$ represent the submanifold of $\mathscr{M}_T^{(n,m)}$ defined by the constraint $t_n=1$ (or any constant). From $J^{(1)}$ in (4.12) we observe that, as long as $n\geqslant 1$, the highest positive order of $J^{(1)}$ is $n-1$ and therefore the Hamiltonian map is automatically tangent to the constraint submanifold. When $m=0$ this is also the case for a similar constraint on the lowest field $t_0=$constant; indeed (4.12) shows that in this case the contribution of $J^{(1)}(X)$ to order zero is $[L_0,\ X_0]=0$. In a few words, both constraints are first class, and the Poisson brackets are defined by simple restriction of (4.16).

For $J^{(2)}$, things are more involved. Notice in fact from the expression (4.13) that the highest order of $J^{(2)}(X)$ is n, i.e., the same as that of L. Therefore, in order to define Poisson brackets on $\widetilde{\mathscr{M}}_T^{(n,m)}$ we would follow the standard prescription for second class constraints due to Dirac. However, instead of plugging here the formula of the Dirac brackets, we will pause briefly to describe how they appear in our context. Given the projection map, such as $\mathscr{M}_T^{(n,m)}\to\widetilde{\mathscr{M}}_T^{(n,m)}$ that sets $t_n\to 1$, at each point L, the induced projection of vectors on the tangent subspace is unique. This is not so for one-forms. To see this notice that if we want to compute Poisson brackets of functions f,g on $\widetilde{\mathscr{M}}_T^{(n,m)}$ via (4.13), we first need to extend them to $\mathscr{M}_T^{(n,m)}$. This extension, being nonunique, renders the component $x_n=\delta f/\delta t_n$ in the gradient

$$df(L)=\sum_{k=m}^{n}T^{-k}x_k$$

undefined. Therefore some additional structure is required in order to specify the cotangent subspace. Since we have $J^{(2)}$ at hand, a map from one-forms to vectors, we may fix this ambiguity by demanding that the associated Hamiltonian vector fields be tangent to $\widetilde{\mathscr{M}}_T^{(n,m)}$. In other words, we fix x_n by the requirement that $J_2(df(L))$ should have no term of order n. This form of computing the algebra is fully equivalent to the Dirac bracket prescription as we show next.[23] The demand that $J(z)$ should stay tangent to the constraint manifold implies for $df(L)$ that

$$\sum_{j=m}^{n} J_{nj}x_j = 0$$

and this may be solved for $x_n = -\Sigma_{j=m}^{n-1} J_{nn}^{-1} J_{nj} x_j$. Plugging this back into (4.9) we have

$$J(z) = \sum_{i,j=m}^{n-1} (\tilde{J}_{ij} x_j) T^i,$$

where

$$\tilde{J}_{ij} = J_{ij} - J_{in} J_{nn}^{-1} J_{nj}, \quad i,j = 1,\ldots,n-1, \tag{4.19}$$

are the corresponding Dirac brackets on the constraint surface. For the explicitly reduced brackets we find a nonlocal expression as follows:

$$\tilde{J}_{ij}^{(2)} = 2 \sum_{k=\max(m,i+j-n)}^{\min(n,i)} (t_k T^{k-j} t_{i+j-k} - t_{i+j-k} T^{i-k} t_k) + 2 t_i \frac{(1-T^{i-n})(1-T^{-j})}{(1-T^{-n})} t_j. \tag{4.20}$$

Indeed, the interest in the reduction $t_n = 1$ stemmed from the fact that the Lax flows (4.8) stabilize this constraint. Likewise, if $m = 0$ the Lax equation for t_0 is trivial, hence we may want to set it also to a constant. However, in contrast to the previous case, the contribution of $J^{(2)}(X)$ to order zero is $2L_0(XL)_0 - 2(LX)_0 L_0 + 2L_0[L, X]_0 = 0$; in other words, for all j, $J_{0j}^{(2)}$ vanishes and therefore this constraint is first class and does not lead to any modification of the algebra. If we put $m = 0$, (4.20) is equivalent to formula (3.6) in Ref. 15.

V. THE q-KP BASIS

We recall that our main purpose is to construct a q-deformation of the algebra $\mathbf{W}_{\mathrm{KP}}$. For this reason it will be interesting to reformulate the findings of the previous section in terms of the basis ∂_q, i.e.,

$$\partial_q = \frac{1}{z(q-1)} (T-1). \tag{5.1}$$

Written in this basis, the limit $q \to 1$ should yield directly $\mathbf{W}_{\mathrm{KP}}^{(n)}$ in Ref. 18. We recall here the relevant formulas for the change of basis:

$$\begin{aligned} T &= z(q-1)\partial_q + 1, \\ T^{-1} &= \frac{1}{z(q-1)\partial_q + 1} \equiv -\sum_{i=1}^{\infty} \frac{(-q)^i}{(q-1)^i} z^{-i} \partial_q^{-i} \end{aligned} \tag{5.2}$$

These imply in particular that the phase space $\mathscr{M}_T^{(n,m)}$ will be coordinatized now by q-pseudodifferential operators L of the form

$$L = \sum_{j=-\infty}^{n} u_j(z) \partial_q^j, \tag{5.3}$$

$(m+n)$ being still the number of degrees of freedom. Yet the manifold of all q-pseudodifferential operators of the form (5.3), which we will denote by $\mathscr{M}_{\partial_q}^{(n)}$, is much bigger than $\mathscr{M}_T^{(n,m)}$. Rather, we have that the set of all these spaces $\{\mathscr{M}_T^{(n,m)}, m = 1,2,3,\ldots\}$ is dense in $\mathscr{M}_{\partial_q}^{(n)}$.

Notice that (5.2) involves a specific choice of the expansion point, namely around $\partial_q=\infty$. Other choices may lead to different W-algebras. In the q-KP basis we may grade $\mathscr{G}_q$ by the scaling dimension: if z has degree -1, ∂_q will have $+1$ and we may make L homogeneous of a certain degree, n, by further assignment of degree j to u_j. This gives us a chance to look for a q-deformation of the Virasoro algebra in the subalgebra spanned by the counterpart of the energy momentum tensor (the field u_2 in the context of the classical $\mathbf{W}_{\mathrm{KP}}$ algebra), which will be a particular x-dependent combination of various fields in the Toda basis (where the grading was a different one).

In order to study the Hamiltonian structures we have to redefine the residue and trace functionals in the new basis. The point is the following; let

$$L(T)_{\geqslant 0}=\sum_{i=0}^{n} t_i T^i=\sum_{i=0}^{n} u_i \partial_q^i=L(\partial_q)_{\geqslant 0},$$

where in each case the projection is performed with respect to the relevant basis. Making use of (5.1) we may write t_0 in terms of u_i:

$$t_0(u_i)=(-1)^m \frac{u_m}{z^m(q-1)^m}+(-1)^{m-1} \frac{u_{m-1}}{z^{m-1}(q-1)^{m-1}}+\cdots-\frac{u_1}{z(q-1)}+u_0. \tag{5.4}$$

If $L(T)\equiv t_i T^i$, $t_0=\mathrm{res}_T\, L(T)$. How can we manage to extract $t_0(u_i)$ out of $L(\partial_q)$ as given by the right-hand side of (5.4)? Notice that we may take advantage of the fact that the projections (in the respective basis) $(\ )_{\geqslant 0}$ and $(\ )_{\leqslant -1}$ commute with the change of basis $T\leftrightarrow\partial_q$, hence

$$(L(T))_0=(L(T)T^{-1})_{-1}=(L(T)_{\geqslant 0}T^{-1})_{-1}=\frac{z(q-1)}{q}\,(L(\partial_q)_{\geqslant 0}T^{-1}(\partial_q))_{-1}.$$

In the last expression $T^{-1}(\partial_q)$ stands for the second relation in (5.2). Thus

$$t_0(u_i)=\frac{z(q-1)}{q}\,\mathrm{res}_{\partial_q}(L(\partial_q)T^{-1}),$$

where we have introduced the symbol $\mathrm{res}_{\partial_q}\, a_i\partial_q^i \equiv a_{-1}$. Concerning the ad-invariant symmetric bilinear product, we find the same expression that was considered in Ref. 16 (modulo a constant factor)

$$\langle A,B\rangle=\langle B,A\rangle=\int \mathrm{res}_T\, AB=\frac{q-1}{q}\int z\,\mathrm{res}_{\partial_q}\, ABT^{-1}. \tag{5.5}$$

In this basis the natural integral functional is $\int_{-1}\equiv\int z$ which, in spite of not being scale invariant $\int_{-1}\tau(f\,)=q^{-1}\int_{-1} f$ satisfies the desirable property that $\int_{-1}(\partial_q f\,)=0$. With respect to the above inner product, the adjoints of τ and ∂_q are easy to compute, yielding

$$\tau^*=\frac{1}{q}\,\tau^{-1};\quad \partial_q^*=-\partial_q^*\tau^{-1}. \tag{5.6}$$

For later use we shall introduce the following compact notation:

$$\Omega(A)\equiv\frac{z(q-1)}{q}\,\mathrm{res}_{\partial_q}(A).$$

Next, we must characterize the three possible splittings of $\mathscr{G}_q(\sigma=0,\pm 1)$ in the ∂_q basis:

The untwisted basis is naturally adapted to the case $\sigma=-1$,

$$\mathscr{G}_{\geqslant 0}(T)=\mathscr{G}_{\geqslant 0}(\partial_q),\quad \mathscr{G}_{\leqslant -1}(T)=\mathscr{G}_{\leqslant -1}(\partial_q).$$

Here $\sigma=+1$ looks a little bit more contrived:

$$\mathscr{G}_{\leqslant 1}(T)=\widetilde{\mathscr{G}}_{\geqslant 0}(\partial_q)\equiv\left\{L=\sum_{j=0}^{m} u_j\partial_q^j \middle| \operatorname{res}_{\partial_q}(LT^{-1})=0\right\},$$

$$\mathscr{G}_{\leqslant 0}(T)=\mathscr{G}_{\leqslant 0}(\partial_q)=\left\{L=\sum_{j=-\infty}^{0} u_j\partial_q^j\right\}.$$

Last, the characterization of $\sigma=0$ in the untwisted basis makes this splitting very unnatural:

$$\mathscr{G}_{0^+}(\partial_q)\equiv\left\{L=\sum_{j=0}^{m} u_j\partial_q^j \middle| z\ \operatorname{res}_{\partial_q}(LT^{-1})\in z\mathbf{C}[z]\right\},$$

$$\mathscr{G}_{0^-}(\partial_q)\equiv\left\{L=\sum_{j=-\infty}^{0} u_j\partial_q^j \middle| u_0\in z^{-1}\mathbf{C}[z^{-1}]\right\}.$$

We want to consider again the Poisson maps (3.7). Now in order to compute the analog of (4.12)–(4.14) we have to say what the relevant projection operators are. From the form of the scalar product (5.5) it is clear that

$$\begin{aligned} &P_{\geqslant 0}L=L_{\geqslant 0},\quad P^*_{\geqslant 0}L=(LT^{-1})_{\leqslant -1}T,\\ &P_{\leqslant -1}L=L_{\leqslant -1},\quad P^*_{\leqslant -1}L=(LT^{-1})_{\geqslant 0}T. \end{aligned} \tag{5.7}$$

We may simplify these expressions, remembering that the projections $(\ )_{\geqslant 0}$ and $(\ )_{\leqslant -1}$ commute with the change of basis $T\leftrightarrow\partial_q$. So for $L=t_iT^i=u_j\partial_q^j$,

$$\begin{aligned} P^*_{\geqslant 0}L&=(L(\partial_q)T^{-1}(\partial_q))_{\leqslant -1}T=(L(T)T^{-1})_{\leqslant -1}T=(L(T))_{\leqslant 0}\\ &=(L(T))_{\leqslant -1}+t_0=(L(\partial_q))_{\leqslant -1}+\Omega(L), \end{aligned}$$

where we made use of (5.2). Similarly

$$\begin{aligned} P^*_{\leqslant -1}L&=(L(\partial_q)T^{-1})_{\geqslant 0}T=(L(T)T^{-1})_{\geqslant 0}T=L(T)_{\geqslant 1}T^{-1}T\\ &=L(T)_{\geqslant 0}-t_0=L(\partial_q)_{\geqslant 0}-\Omega(L). \end{aligned}$$

With these results the antisymmetric part of the r-matrix is

$$\tfrac{1}{2}(\mathscr{R}-\mathscr{R}^*)=\tfrac{1}{2}(P_{\geqslant 0}-P_{\leqslant -1}-\Omega)=\mathscr{R}-\tfrac{1}{2}\Omega. \tag{5.8}$$

It is not evident that this expression also satisfies the m-YB($\frac{1}{4}$) equation. However, an explicit computation shows that the only nonvanishing contribution to (3.1) has the form $\Omega([a_{\geqslant 0},\ b_{\geqslant 0}])$, which vanishes. An easy way to convince oneself of this fact is that when written in the T basis this is $\operatorname{res}_T[a(T)_{\geqslant 0},\ b(T)_{\leqslant 0}]=0$.

With all this information, it is now an easy exercise to find the explicit expressions for (3.7) as adapted to the present case. Let again $X\equiv df$:

$$J^{(1)}(X)=[L,\ X_{\geqslant 0}]_{\leqslant -1}-[L,\ X_{\leqslant -1}]_{\geqslant 0}+\Omega([L,\ X]), \tag{5.9}$$

$$J^{(2)}(X)=2L(XL)_{\geqslant 0}-2(LX)_{\geqslant 0}L+L\Omega([L,\,X])+\Omega([L,\,X])L$$
$$=-2L(XL)_{\leqslant -1}+2(LX)_{\leqslant -1}L+L\Omega([L,X])+\Omega([L,X])L, \tag{5.10}$$

$$J^{(3)}(X)=[L,\,(LXL)_{\geqslant 0}]-L[L,\,X]_{\geqslant 0}L+L\Omega([L,\,X])L. \tag{5.11}$$

Notice that as compared with the analogous expressions for the $\mathbf{W}_{\mathrm{KP}}$ algebra,[18] the ones above present additional terms which vanish in the limit $q\to 1$. However, these terms are not active whenever f is a Casimir function, and hence, in particular for the Lax–Hamiltonian flows.

In order to compute the algebra of fundamental Poisson brackets we have to describe the manifold and the class of functionals for which $J^{(i)}$, $i=1,2,3$, describe tangent maps. We will work on $\mathscr{M}_{\partial_q}^{(n)}$ whose points are parametrized as

$$L^{(n)}=\sum_{i=0}^{\infty} u_i\partial^{n-i}\quad (n\in\mathbf{Z}). \tag{5.12}$$

Accordingly, in order to define linear functionals of the form $f_X=\int_{-1}u_ix_i$ as $f_X=\int_{-1}\mathrm{res}_{\partial_q}LXT^{-1}$, our gradient one-forms will be q-pseudodifferential operators of the form

$$X\equiv df_X=\sum_{j=0}^{\infty}\partial_q^{j-n-1}Tx_j\,.$$

After a straightforward computation, we list the full set of fundamental brackets for $J^{(1)}$ as follows: first we have that for all j: $J_{00}^{(1)}=J_{0j}^{(1)}=J_{j0}^{(1)}=0$. If $i,j\geqslant n+1$,

$$J_{ij}^{(1)}=\sum_{k=0}^{i+j-n-1}\begin{bmatrix} i-n-1\\ k\end{bmatrix}_q q^{k(k+1)/2}\left(q^{n-i-1}(q-1)u_{i+j-n-k}(-\partial_q)^kx+\frac{1}{q}\,u_{i+j-n-k-1}(-\partial_q)^k\right)$$
$$\times T^{n-i}-\sum_{k=0}^{i+j-n}\begin{bmatrix} j-n\\ k\end{bmatrix}_q\frac{(q-1)}{q}\,T^{j-n-k}\partial_q^ku_{i+j-n-k}x$$
$$-\sum_{k=0}^{i+j-n-1}\begin{bmatrix} j-n-1\\ k\end{bmatrix}_q\frac{1}{q}\,T^{j-n-k-1}\partial_q^ku_{i+j-n-k-1}. \tag{5.13}$$

If, however, $1\leqslant i,j\leqslant n-1$, the same expression (5.13) is valid with the opposite sign.

Finally, when $j=n$,

$$J_{in}^{(1)}=\left\{\sum_{k=0}^{i-n-1}\left(\begin{bmatrix} i-n-1\\ k\end{bmatrix}_q q^{k(k+1)/2+n-i-1}(q-1)u_{i-k}(-\partial_q)^kxT^{n-i}\right)-\frac{1}{q}\,(q-1)xu_i\right\}$$
$$\times\Theta(i-(n+1))+\left\{-\sum_{k=0}^{i-1}\begin{bmatrix} i-n-1\\ k\end{bmatrix}_q q^{k(k+1)/2}\left(q^{n-i-1}(q-1)u_{i-k}(-\partial_q)^kx\right.\right.$$
$$\left.\left.+\frac{1}{q}\,u_{i-k-1}(-\partial_q)^k\right)+\frac{(q-1)}{q}\,xu_i+\sum_{k=0}^{i-1}\begin{bmatrix} -1\\ k\end{bmatrix}_q\frac{1}{q}\,T^{-k-1}\partial_q^ku_{i-k-1}\right\}$$
$$\times\Theta(n-i)+\frac{x(q-1)}{q}\left(u_n-\sum_{k=0}^{n}\begin{bmatrix} -1\\ k\end{bmatrix}_q T^{-k}\partial_q^ku_{n-k}\right)\delta_{i,n}\,. \tag{5.14}$$

The rest of the brackets can be computed making use of the identity $J_{ij}=-J_{ji}^{*}$ and (5.6).

Concerning reductions, as long as $n\geqslant 1$, the highest order of $J^{(1)}(X)$ is $n-1$ and thereafter its action is tangent to the submanifold defined by $u_0=$constant. Again this reduction is therefore first class. Two other consistent reductions of L are of the form $L=L_{\geqslant 0}$ with $J^{(1)}(X)=-[L_{\geqslant 0},\, X_{\leqslant -1}]_{\geqslant 0}+\Omega([L_{\geqslant 0},\, X_{\leqslant -1}])$ or $L=L_{\leqslant 0}$, in which case $J^{(1)}(X)=[L_{\leqslant 0},\, X_{\geqslant -1}]_{\leqslant -1}+\Omega([L_{\leqslant 0},\, X_{\geqslant -1}])$. The relevant explicit form of the Poisson brackets can be obtained in each case from (5.9) after suitably setting to zero the corresponding fields u_i and its duals x_i.

Written in this basis, the formula (5.13) exhibits a nested sequence of subalgebras $N=1,2,...$, spanned by $\{u_{n+N+k},\, k=0,1,2,...\}$. In the continuum limit $q\to 1$ these contract to the nested set truncations of the centerless $W_{1+\infty}$ algebra known as $W_{-N+\infty}$.[18]

For $J^{(2)}$ we have in turn

$$
\begin{aligned}
J^{(2)}_{ij}=&\,2\sum_{k=0}^{i-1}\sum_{l=0}^{k}\begin{bmatrix} l-k-1 \\ l \end{bmatrix}_q q^{(l-1)(k+1)}u_{j+k-l}\partial_q^l T^{-k}u_{i-k-1}\\
&-2\sum_{k=0}^{i-1}\sum_{l=0}^{j+k}\sum_{m=0}^{i-k-1}\begin{bmatrix} j-n-1 \\ l \end{bmatrix}_q\begin{bmatrix} n-m \\ i-k-m-1 \end{bmatrix}_q\\
&\times q^{(l-1)(l-j+n+1)+(i+l-k-m-2)(i-k-n-1)}u_m\partial_q^{i+l-k-m-1}T^{j+k-i-l+1}u_{j+k-l}\\
&+2\sum_{k=0}^{i}\sum_{l=0}^{k}\begin{bmatrix} l-k-1 \\ l \end{bmatrix}_q q^{(l-1)(k+1)}(q-1)xu_{j+k-l}\partial_q^l T^{-k}u_{i-k}\\
&-2\sum_{k=0}^{i}\sum_{l=0}^{j+k}\sum_{m=0}^{i-k}\begin{bmatrix} j-n-1 \\ l \end{bmatrix}_q\begin{bmatrix} n-m \\ i-k-m \end{bmatrix}_q q^{(l-1)(l-j+n+1)+(i+l-k-m-1)(i-k-n)}\\
&\times(q-1)xu_m\partial_q^{i+l-k-m}T^{j+k-i-l}u_{j+k-l}-(1-q^{-1})xu_iu_j\\
&+\sum_{k=0}^{i}\sum_{l=0}^{j}\begin{bmatrix} j-n-1 \\ l \end{bmatrix}_q\begin{bmatrix} n-k \\ i-k \end{bmatrix}_q q^{(l-1)(l-j+n+1)+(i+l-k-1)(i-n)}(q-1)xu_k\partial_q^{i+l-k}T^{j-i-l}u_{j-l}\\
&+\sum_{k=0}^{i-1}\sum_{l=0}^{j}\begin{bmatrix} j-n-1 \\ l \end{bmatrix}_q\begin{bmatrix} n-k \\ i-k-1 \end{bmatrix}_q q^{(l-1)(l-j+n+1)+(i+l-k-1)(i-n-1)}(q^{n-i+1}-1)\\
&\times u_k\partial_q^{i+l-k-1}T^{j-i-l+1}u_{j-l}+\sum_{k=0}^{i}\begin{bmatrix} n-k \\ i-k \end{bmatrix}_q q^{(i-k)(i-n)}(1-q^{-1})u_k\partial_q^{i-k}T^{n-i}xu_j\\
&-\sum_{k=0}^{j}\begin{bmatrix} j-n-1 \\ k \end{bmatrix}_q q^{(k-1)(k-j+n+1)}(q-1)xu_i\partial_q^k T^{j-k-n}u_{j-k}. \qquad (5.15)
\end{aligned}
$$

This expression reduces in the limit $q\to 1$ to the one of the W_{KP} algebra. Contrary to $J^{(1)}$,$J^{(2)}(X)$ does not stabilize the field u_0; i.e., from (5.10) we see that the highest order of $J^{(2)}(X)$ is the same as that of L. Therefore the constraint $u_0=1$ is second class. The same discussion that was developed in the T basis holds here *mutatis mutandi*. We will refrain from giving the explicit form of the reduced Poisson brackets, whose computation follows again the standard Dirac's recipe.

A. Reductions. Where is $q-W_n$?

Let us consider here the very important reductions of q-KP to q-KdV. The expressions in (5.9) and (5.10) are perfectly consistent when applied to purely q-differential operators $L=u_0\partial_q^n+u_1\partial_q^{n-1}+\cdots+u_n$. The related algebras are simply obtained by restricting the subindices of the fields appearing in (5.13)–(5.15) to take values in the range $i,j\in[0,\, n]$, and neglecting

all other fields. In a strict sense, these algebras should be considered as deformations of GD_n, the second Gelfand–Dickey bracket over the phase space of Lax operators of the form $L=\partial^n+u_1\partial^{n-1}+\cdots+u_n$. Hence we will name them $q-GD_n$ algebras.

An important point arises here: as compared with GD_n, $q-GD_n$ contain an additional generator u_0. In the limit $q\to 1$ this field decouples because $\lim_{q\to 1} J_{0j}=0$, $\forall j$ and we may set $u_0=1$. One could argue that in order to construct a true q-deformation of GD_n which involves exactly n generators we should first reduce $u_0=0$ via Dirac brackets. However, the projection involved in the reduction *is not a continuous* step and nothing guarantees that the resulting algebra will still recover the desired limit when $q\to 1$.

Let us give an example of this phenomenon by considering the simplest Lax operator $L=u_0\partial_q+u_1$. The Poisson brackets for u_0 and u_1 generate $q-GD_1$, whose brackets are given by

$$\begin{aligned} J_{00}^{(2)}&=\frac{q-1}{2q}\,u_0(T-T^{-1})zu_0,\\ J_{01}^{(2)}&=\frac{1}{2q}\,u_0(T-T^{-1})u_0,\\ J_{10}^{(2)}&=\frac{1}{2q}\,u_0(qT-q^{-1}T^{-1})u_0,\\ J_{11}^{(2)}&=\frac{1}{2zq(q-1)}\,u_0(T-T^{-1})u_0, \end{aligned} \tag{5.16}$$

which in the limit $q\to 1$ reproduce the free boson algebra GD_1 after u_0 is set to 1, i.e., $J_{11}^{(2)}\to\partial$, and $J_{0i}^{(2)}\to 0$. However, if we insisted in reducing $u_0=1$ before taking the limit, the Dirac formula gives us a vanishing answer for $\widetilde{J}_{11}^{(2)}$:

$$\begin{aligned} \widetilde{J}_{11}^{(2)}&=J_{11}^{(2)}-J_{10}^{(2)}(J_{00}^{(2)})^{-1}J_{01}^{(2)}\\ &=u_0\,\frac{1}{2q(q-1)}\left(\frac{1}{z}\,(T-T^{-1})-(qT-q^{-1}T^{-1})\,\frac{1}{z}\right)u_0=0. \end{aligned} \tag{5.17}$$

One cannot cure this result by multiplying the starting brackets by global factors of $(q-1)$, because the Dirac bracket is homogeneous under such rescalings. This vanishing result is also independent of any q-dependent redefinition of the field u_0.

We expect that a similar discussion applies to the classical W_n algebras although we do not have a general proof. These algebras arise as Hamiltonian reductions of GD_n where the generator u_1 is set to 0. The first generator, u_2, closes a linear subalgebra which is none other than the ubiquitous Virasoro algebra. It is in this sense that W_n algebras are sometimes defined as (nonlinear) extensions of the Virasoro algebra. A continuous q-deformation of W_n in $n-1$ fields $u_2,\ldots,u_n$ would present the same problems that we have exposed above in the case of GD_n. The naive procedure, of starting from $q-GD_n$ and reducing $u_0=1$ and $u_1=0$, may spoil the continuous correspondence with W_n in the limit $q\to 1$. We feel this is an important point that deserves further attention.

VI. ANALYTIC CONTINUATION

Notice that the expression for the algebra $q-\mathbf{W}_{\mathrm{KP}}^{(n)}$ as given in (5.15) admits analytic continuation to complex values of $n=\alpha\in\mathbf{C}$. This happens in contrast to the first structure, given in (5.13) and (5.14), where n appears explicitly in the limits of summatories. The best way to understand this is by implementing the analytic continuation right from the beginning. Actually the whole

formalism is susceptible of such a continuation along the lines advocated in Refs. 18 and 24. Hence $q-\mathbf{W}_{\mathrm{KP}}^{(\alpha)}$ describes a *two-parameter* family of nonlinear $\mathbf{W}_\infty$-type algebras.

There is an important technical question concerning the triviality of such deformation parameters, i.e., whether the algebras for different pairs (q,α) and (q',α') are isomorphic or not. At least in the continuum case $q=1$ we know positively that α represents a nontrivial deformation parameter.[25]

The second issue we intend to address in this concern is the possibility of connecting the linear and quadratic structures by a suitable contraction of the parameter α. In Ref. 18 the limit $\alpha\to 0$ was shown to yield an extension of the linear algebra $\mathbf{W}_{1+\infty}$ by means of the Khesin–Kravchenko cocycle.[26] This fact was also understood in Refs. 24 and 27 from a Poisson–Lie group theoretical point of view.

In more concrete terms, let us introduce a second parameter β and define $L^{(\alpha,\beta)}\in \mathscr{M}_{\partial_q}^{(\alpha)}$ such that

$$L^{(\alpha,\beta)}=\beta\partial_q^\alpha+\sum_{j=0}^{\infty} u_j(z)\partial_q^{\alpha-1}\equiv\beta\partial_q^\alpha+L^{(\alpha)}. \tag{6.1}$$

Correspondingly, the one-forms X will look as

$$X=\sum_{j=0}^{\infty}\partial_q^{j-\alpha-1}Tx_j\,.$$

We will be interested in the following ''scaling'' limit in which α tends to 0 and β to ∞ in such a way that $\alpha\beta=c$, a finite constant. It will be convenient to normalize $J^{(2)}$ in the following form:

$$J^{(2)}_{L^{(\alpha,\beta)}}(z)=\frac{1}{\beta}\{L^{(\alpha,\beta)}(XL^{(\alpha,\beta)})_{\geqslant 0}-(L^{(\alpha,\beta)}X)_{\geqslant 0}L^{(\alpha,\beta)}$$
$$+\tfrac{1}{2}\,L^{(\alpha,\beta)}\Omega([L^{(\alpha,\beta)},\,X])+\tfrac{1}{2}\,\Omega([L^{(\alpha,\beta)},\,X])L^{(\alpha,\beta)}\}.$$

Plugging (6.1) in this expression we may first gather all the terms quadratic in $\beta\partial_q^\alpha$:

$$\beta(\partial_q^\alpha(X\partial_q^\alpha)_{\geqslant 0}-(\partial_q^\alpha X)_{\geqslant 0}\partial_q^\alpha+\tfrac{1}{2}\partial_q^\alpha(\Omega[\partial_q^\alpha,\,X])+\tfrac{1}{2}\Omega([\partial_q^\alpha,\,X])\partial_q^\alpha).$$

Expanding $\partial_q^\alpha=1+\alpha\log\partial_q+O(\alpha^2)$ the surviving terms in the desired limit yield

$$c[\log\partial_q,\,X_{\geqslant 0}]-c[\log\partial_q,\,X]_{\geqslant 0}+c\Omega([\log\partial_q,\,X])=c[\log\partial_q,\,X_{\geqslant 0}]_{\leqslant -1}+c\Omega([\log\partial_q,\,X]).$$

In the linear terms the β dependence cancels out and we obtain

$$[L^{(0)},\,X_{\geqslant 0}]-[L^{(0)},\,X]_{\geqslant 0}+\Omega([L^{(\alpha)},\,X])=[L^{(0)},\,X_{\geqslant 0}]_{\leqslant -1}+\Omega([L^{(0)},tX]).$$

In summary, the limiting Hamiltonian structure yields

$$J_{1+\infty;q}(X)=[c\,\log\partial_q+L^{(0)},\,X_{\geqslant 0}]_{\leqslant -1}+\Omega([c\,\log\partial_q+L^{(0)},\,X]). \tag{6.2}$$

Consistency of $J(X)$ as a tangent map demands that L be of the form

$$L=\log\partial_q+u_0+\sum_{i=1}^{\infty}u_i\partial^{-i}.$$

The expression $\log\partial_q$ has to be understood as an outer automorphism of the Lie algebra of q-pseudodifferential symbols. Its action can be defined and computed as a limit:

$$[\log \partial_q,\ f\partial_q^p]=\lim_{\alpha\to 0}\frac{1}{\alpha}\,(\partial_q^{\alpha} f\partial_q^p\partial_q^{-\alpha}-f\partial_q^p)$$

$$=\log q f'\partial_q^p-\sum_{k\geqslant 1}\frac{\log q}{(q-1)}\begin{bmatrix}-1\\ k\end{bmatrix}_q q^k\tau^{-k}(\partial_q^k f\ )\partial_q^{p-k}.$$

The notation in (6.2) intends to make explicit that this algebra is a q-deformation of the centrally extended $W_{1+\infty}$ algebra. We will not write down explicitly the Poisson brackets here. They agree with the ones given in (5.13) and (5.14) with $n=0$ except for the central terms, which are the only ones that require corrections proportional to $\log q$.

VII. CONCLUSIONS AND OUTLOOK

The picture of an atlas of **W** algebras is slowly emerging. In this landscape, W_∞ algebras provide natural landmarks and, among them, the algebra $\mathbf{W}_{\mathrm{KP}}$ is a cornerstone. In Ref. 28 this algebra was shown to be related with a large amount of the known classical W-type algebras by continuous deformation or truncation. The main result of the present paper is that many of the points in that atlas admit yet another deformation, parametrized by q. Of particular importance are $q-\mathbf{W}_{\mathrm{KP}}^{(\alpha)}$, $q-GD_n$, and $q-W_{1+\infty}$.

It has been amusing to observe how many structures that worked fine for the algebra of pseudodifferential operators are robust enough to resist their implementation in the algebra of q-deformed pseudodifferential operators, as well. It certainly points out that perhaps other well-known results could be exported. To be more precise, we think about issues like the dressing transformation, the embedding of the Lie algebra of differential operators into W_n (Ref. 29), or the Kupershmidt–Wilson–Yu theorem.[30] In fact, concerning this last important theorem, a straightforward implementation of the proof given in Ref. 31 for a quadratic structure of the form (3.3) works fine in the case of an isotropic splitting. This requirement is only fulfilled in the present work for the splitting $\sigma=0$ and hence there is a q-deformed version of the Kupershmidt–Wilson–Yu theorem in this case. For $\sigma=\pm 1$ we have not been able to establish a similar result. In this respect we should mention that a proposal for a q-deformed Miura transformation has appeared in Ref. 14. Its connection to some peculiar way to factorize the Lax operator has been addressed in Ref. 15.

We should emphasize the existence of three consistent splittings ($\sigma=0,\pm 1$) for the algebra ΨDO_q. They all yield integrable Hamiltonian systems and thereafter **W**-type algebras. In Refs. 32 and 33 the m-KdV hierarchy was investigated in the scalar Lax formalism. It was recognized that this system is related to a nonstandard splitting of the algebra of ordinary ΨDO. Indeed $L=L_{\geqslant k}+L_{<k}$ yields consistent subalgebras for $k=0$, 1, and 2. It would be interesting to find out whether a possible q-deformation of these nonstandard splittings could be related to the cases $\sigma=0$ and $\sigma=+1$ in this paper.

The connection of the KP hierarchy with the Toda lattice hierarchy is a subject of recent interest which has received the attention of different groups.[22,34,35] We believe that our approach is substantially different from these and closer, at least in spirit, to the lattice deformation of Ref. 36. We expect that the powerful techniques that have been used in this paper can be implemented also in the context of the Calogero–Sutherland model, especially in the formulation that makes use of the exchange operators.[37]

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A calculus for SU(3) leading to an algebraic formula for the Clebsch–Gordan coefficients

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We develop a simple computational tool for SU(3) analogous to Bargmann's calculus for SU(2). Crucial new inputs are (i) explicit representation of the Gelfand–Zetlin basis in terms of polynomials in four variables and positive or negative integral powers of a fifth variable, (ii) an auxiliary Gaussian measure with respect to which the Gelfand–Zetlin states are orthogonal but not normalized, (iii) simple generating functions for generating all basis states and also all invariants. As an illustration of our techniques, an algebraic formula for the Clebsch–Gordan coefficients is obtained for the first time. This involves only Gaussian integrations. Thus SU(3) is made as accessible for computations as SU(2) is. © *1996 American Institute of Physics.* [S0022-2488(96)04309-5]

I. INTRODUCTION

Compact Lie groups have been extensively studied from different viewpoints.[1–12] In spite of this, there are gaps in our understanding which are keenly felt in specific applications. This has mostly to do with the absence of a viable scheme of general computations. For example, there is no algebraic formula for the Clebsch–Gordan coefficients of even the SU(3) group, despite extensive work by a generation of mathematical physicists. This is in contrast to the SU(2) group, where it seems that everything can be computed in more than one way. Somehow, every technique that works for SU(2) does not appear to have a simple generalization for other groups.

In this paper we develop techniques which provide a simple computation tool for SU(3). Our aim is to highlight the flexibility available for computations of various objects of interest in representation theory. In particular we obtain a closed formula for the Clebsch–Gordan coefficients of SU(3). With a couple of new inputs it might be possible to use our techniques for other groups also. We have borrowed ideas heavily from many earlier workers. We have made some conceptual and technical advances which together have enabled us to provide a simple tool.

We now give a summary of the earlier works, with specific reference to SU(3). An excellent summary of the situation up to 1971 is contained in the Appendix of the review by Smorodonskii and Shelepin.[13] Our summary is by no means complete and accurate.

In the SU(2)[13,14] case there are broadly three computational tools: (a) an infinitesimal approach; (b) a polynomial basis and generating invariants; and (c) use of the relationship with the symmetric group. Within each approach there have been many different ways[13,14] of deriving formulas for the Clebsch–Gordan coefficients. Almost every one of these variations has been tried for SU(3), but each has led to obstacles.

A major obstacle encountered in any approach is the outer multiplicity problem. In the decomposition into irreducible representations (IRs) of a Kronecker product of two IRs of SU(n), $n>3$, a given IR may appear more than once. These repeating IRs cannot be distinguished by the matrix-elements of the generators. We need to understand how the repeating IRs may be distinguished, labeled in a convenient and canonical way, and handled. Extensive efforts have been put into this problem. At least in the SU(3) case, the problem has been essentially resolved by many authors using diverse techniques and often without the knowledge of previous works. New Ca-

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simirs (''Chiral Casimirs'') which distinguish between repeating IRs have been constructed.[15–17] Biedenharn and his collaborators have obtained a ''canonical resolution'' of the multiplicity problem.[18,19] An explicit formula for multiplicity has been obtained by Coleman[20] by analyzing the Littlewood–Richardson rule; by Jasselette[21,22] and Resnikoff[23] by applying the theory of invariants; and by O'Reilly[24] by a detailed and careful analysis of the Kronecker product. Anishetty *et al.*[25] recently reinterpreted these results to give the most explicit formula, analogous to the triangle rule for the addition of angular momenta in SU(2). The advantage of this formula is that the IRs in the Kronecker product are labeled by *free* integers which are subject only to additive constraints by the two IRs one started with. This therefore provides a ''natural labeling'' of the repeating IRs. Gadiyar and Sharatchandra[26] have recently solved the multiplicity problem for SU(n) for any n. This is done by obtaining an explicit algebraic solution of the Littlewood–Richardson rule in terms of free integers.

In the infinitesimal approach to SU(2), the Clebsch–Gordan coefficients are computed as follows. A recursion relation is obtained by considering the action of the Lie algebra on the direct product space. This does not work as it does for SU(3) and other groups. The Lie algebra does not provide a large enough number of recursion relations to be able to compute all Clebsch–Gordan coefficients. The reason is the multiplicity problem. Biedenharn and collaborators[27,28] have emphasized the need to define a basic set of irreducible tensor operators. The set they construct provides a ''canonical resolution'' of the multiplicity problem. For a review see Refs. 19, 29, and 30. Their ''pattern calculus'' provides a framework for computing the Clebsch–Gordan coefficients. There has been extensive formal work in this direction. It has led to significant concepts such as a global algebraic formulation of SU(3) tensor operator structure[27] and the denominator functions[28] which have wider ramifications.[31–35] In addition, this approach has been very useful for practical algorithms[36–38] and symbolic manipulation programs.[39] However the approach has not (yet!) led to an algebraic formula for the Clebsch–Gordan coefficients of SU(3).

The starting point of the second approach is the construction of a convenient *model space,* i.e., a concrete realization of (say, on a function space) the basis of every irreducible unitary representation of the group. In the case of SU(2), the simplest realization of the basis is as polynomials in two complex variables. This was known to Weyl[8] and was used by van der Waerden,[40] Cartan,[41] and Kramers.[42,43] It is related to the spinor representation of SO(3). Schwinger's[44] boson calculus is also related to this. This approach reached the peak in the work of Bargmann[54,42] where all computations in SU(2) are reduced to evaluation of Gaussian integrals. The computation of Clebsch–Gordan coefficients amounts to the construction of invariant polynomials. We will refer to this package of tools as the Bargmann calculus. We give a constructive analysis of this calculus in Sec. II. Though there are other model spaces for SU(2), e.g., the spherical harmonics, none provide as simple a computational tool.

There has been extensive work to generalize this second approach to other groups. Many model spaces have been constructed. Realization using polynomials[15,45,2,21,23,46,47] boson calculus[33,48,34] harmonic functions, i.e., functions on coset spaces.[55,49,50] Gelfand and collaborators[45] have obtained a differential equation which yields the measure with respect to which the Gelfand–Zetlin basis states are orthonormal. Jasselette,[21,22] Resnikoff,[23] and Karasev[46] have constructed invariant polynomials from which the Clebsch–Gordan coefficients may be obtained in principle. Resnikoff[23] made progress in using a Gaussian measure to extract the Clebsch–Gordan coefficients.

In spite of all this work, the situation is not comparable to the SU(2) case. Some of the coefficients[23,22,46] in the formula for the Clebsch–Gordan coefficients cannot be explicitly computed. The stumbling blocks in this approach which make it so much harder to handle SU(3) are the following. The realization of the basis functions in terms of polynomials is much more complicated. In fact all earlier realizations[15,47] are analogous to the harmonic polynomials (i.e., those which are annihilated by the Laplacian operators) obtained from the defining representation of SO(3) rather than to the monomials obtained from the spinor representation. Explicit construc-

tion of such basis vectors[15,48] and working with them is not easy. Moreover the measure with respect to which the basis is orthonormal is not known in a closed form.[45] Even were it known explicitly, the hope of computing with it appears remote. Invariant polynomials in the space of three IRs can be easily built.[21,23,46] However the invariant polynomial consistent with the three given IRs is not unique in general. The coefficients have to be fixed by demanding that they be expandable in terms of the constrained polynomials representing the basis vectors. Even this does not fix the invariant polynomial completely. This is a consequence of the multiplicity problem and requires a choice of basis to be made in the space of repeating IRs. After all this, there is no easy way of extracting the Clebsch–Gordan coeffients.[15,21–23,46]

In this paper we show how these stumbling blocks may all be overcome. We develop a calculus which is almost as simple as Bargmann's calculus. All computations are effectively reduced to Gaussian integrations.

The first simplification we have achieved is in the explicit realization[51] of the Gelfand–Zetlin basis vectors, free of constraints. We realized this in Sec. III. Our realization uses polynomials in four complex variables and positive or negative integral powers of a fifth variable. It is related to the functions on the cone $\vec{w}\cdot\vec{z}=0$ where $\vec{z}$ and $\vec{w}$ each are triplets of complex variables.[2,47] We choose a specific parametrization of the cone (i.e., eliminating w_3) and explicitly construct a Gelfand–Zetlin basis for the functions on the space. With our parametrization, we are using all polynomials and not just a subset as in earlier works.

Our realization is not as simple as the monomial basis for SU(2). However, in Sec. IV we use a generating function which generates all the (unnormalized) basis functions of every IR. This generating function is as simple as the ''principal vectors'' of Bargmann's calculus.[52,53]

At this stage of our formulation the normalizations of our basis vectors are not known. The normalization is to be determined by requiring that the representation matrix for each IR be unitary. It is always a headache to compute the normalization.[15,48] The great advantage of Bargmann's calculus is the Gaussian measure which permits explicit and easy computations. It is fortuitous that in the SU(2) case the measure with respect to which the Gelfand–Zetlin states are orthonormal is so simple. In order to retain this computability, we construct an auxiliary Gaussian measure with respect to which the Gelfand–Zetlin basis vectors are orthogonal but are not automatically normalized (Sec. V). In fact we use this measure to compute the normalization itself by requiring that the representation matrix in each IR be unitary (Sec. VI). This way we are killing two birds with one stone: To start with, the normalization and the measure are both unknown. A simple auxiliary measure is constructed and used to compute the normalization itself. The basis we use also leads to a simplification in the form of invariants in the direct product space of three IRs (Sec. VIII). This is a consequence of using the cone $\vec{w}\cdot\vec{z}=0$. The invariant polynomial corresponding to a choice of a repeating IR is now uniquely known and there are no unknown coefficients to be fixed separately (Sec. VIII). Therefore the Clebsch–Gordan coefficients (Sec. VII) can be obtained by simply expanding this polynomial in the basis vectors of each IR. We are assured that such an expansion exists because our basis spans all polynomials in contrast to the constrained polynomials of the earlier works.

In the SU(2) case, the Clebsch–Gordan coefficients are simply obtained by reading off the coefficients of the right monomial in the invariant polynomial. But our basis is more complicated. In order to obtain the coefficients in the expansion, we again use our auxiliary measure. We introduce a generating function for the invariant polynomials themselves (Sec. IX). This way all Clebsch–Gordan coefficients are being computed in one shot. Moreover, it is easier to do these computations than with each invariant polynomial individually. The Gaussian measure is used to find the inner product of the generating function for the basis vectors of the three IRs with the generating function for the invariant polynomials (Sec. X). There are terms in the exponent which are *apparently* cubic in this integration—a consequence of the ''multiplicity problem.'' Remarkably however, because of the specific measure we have chosen, the integrals can all be explicitly computed.

II. AN ANALYSIS OF BARGMANN'S TECHNIQUE FOR SU(2)

Bargmann[54] used an axiomatic approach in his analysis. This presumes many results known from other methods. In this section we give a constructive analysis of Bargmann's techniques for SU(2). This will set the stage for our techniques for SU(3), making it clear as to where new ideas are required. SU(2) is the group of simple unitary 2×2 matrices. Its action on $\mathscr{C}_2$, the two-dimensional complex Euclidean space, is given by

$$\begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \to \mathscr{U} \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \tag{1}$$

where $\mathscr{U} \in \mathrm{SU}(2)$. The doublet of complex numbers (z_1, z_2) transforms as the irreducible representation (IR) $\underline{2}$ of SU(2). In particular, z_1 represents the spin ''up'' state and z_2, the spin ''down'' state. States of an arbitrarily high spin can be obtained from a large enough collection of spin 1/2 particles. In particular, states of spin J can be obtained from a system of $2J$ number of identical spin 1/2 particles, i.e., from $2J$ copies of $\mathscr{C}_2$. (The $2J$ boxes in the row of the Young table represent spin J). This corresponds to a realization of the IRs in the space of polynomials in z_1 and z_2: the monomial

$$z_1^m z_2^n \tag{2}$$

describes, up to a normalization, the basis states

$$|JM\rangle, \quad 2J = m+n, \quad 2M = m-n. \tag{3}$$

We notice that as m and n range independently over all non-negative integers, every basis state $|JM\rangle$ of every IR is realized uniquely. This means the following.

Consider the space $\mathscr{F}_2$ whose elements are, roughly speaking, polynomials in z_1 and z_2. In this space, every IR is realized, and moreover each IR is realized once only. Thus it is a model space (see Sec. I for the definition). In addition, the standard basis states [Eq. (3)] are simply realized as monomials. Thus this space is very convenient for calculations. There are further surprises to follow. The action of the group on any state is obtained in this model by transforming z_1 and z_2 in Eq. (2) as given by Eq. (1). To express this action on an arbitrary state, it is very convenient to work with the generating function,

$$\mathscr{Z}(a,b) = \exp(az_1 + bz_2). \tag{4}$$

Simply by extracting the coefficient of $a^m b^n$, an unnormalized basis state [Eq. (3)] can be extracted. This way, we are handling all states of all IRs in one shot. Moreover, the action of the group on the generating function is very simple:

$$\mathscr{U}: \mathscr{Z}(a,b) \to \mathscr{Z}((a,b)\mathscr{U}). \tag{5}$$

The normalizations of the basis states (within an IR) are obtained by demanding the unitarity of the representation matrices on the space. It is sufficient to use group elements close to the identity for this purpose. An SU(2) matrix close to identity may be represented as follows:

$$\mathscr{U} \simeq 1 + i(\epsilon_3 \sigma_3 + \epsilon_+ \sigma_+ + \epsilon_- \sigma_-), \tag{6}$$

where

$$\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}; \quad \sigma_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}; \quad \sigma_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \tag{7}$$

(note that we are not using conventional normalization for the generators).

For unitarity, $\mathscr{U}^{\dagger}\mathscr{U}=1$, we require

$$\epsilon_{+}^{*}=\epsilon_{-}, \quad \epsilon_{3}^{*}=\epsilon_{3} \tag{8}$$

{det $\mathscr{U}=1$ is satisfied because the matrices [Eq. (7)] are traceless}. Using Eq. (6) in Eq. (5), we get the following representation for the generators on our model space,

$$\pi^{0}=a\,\frac{\partial}{\partial a}-b\,\frac{\partial}{\partial b}; \quad \pi^{-}=a\,\frac{\partial}{\partial b}; \quad \pi^{+}=b\,\frac{\partial}{\partial a}, \tag{9}$$

where the generators correspond to σ_3, σ_+, and σ_-, respectively. The notation we are using is motivated by the isospin triplet of pions. The requirement of unitarity of the representation matrix translates into the following condition on the generators:

$$(\pi^{0})^{*}=\pi^{0}, \quad (\pi^{+})^{*}=\pi^{-}, \tag{10}$$

where the asterisk stands for the adjoint. We write formally,

$$\mathscr{Z}(a,b)=\sum_{m,n} a^{m}b^{n}|m,n), \tag{11}$$

where

$$|m,n)=\frac{z_1^{m}z_2^{n}}{m!n!} \tag{12}$$

represent unnormalized basis states. The normalized basis

$$|J,M\rangle\equiv|m,n\rangle=N^{-1/2}(m,n)|mn), \quad 2J=m+n \quad 2M=m-n \tag{13}$$

are to be obtained by requiring,

$$\langle m'n'|T^{*}|mn\rangle=\langle mn|T|m'n'\rangle^{*} \tag{14}$$

for every generator T. Let

$$T|mn)=\sum_{m'n'} T(mn;m'n')|m'n'). \tag{15}$$

This action can be easily computed using the generating function [Eq. (4)] and the representation [Eq. (9)] of the generators. In terms of normalized states this means,

$$N^{1/2}(m,n)T|mn\rangle=\sum_{m'n'} T(mn;m'n')N^{1/2}(m',n')|m'n'\rangle. \tag{16}$$

Using orthonormality,

$$\langle m'n'|mn\rangle=\delta_{m'm}\delta_{n'n}, \tag{17}$$

we get

$$\langle m'n'|T|mn\rangle=T(mn;m'n')\,\frac{N^{1/2}(m',n')}{N^{1/2}(m,n)}. \tag{18}$$

Define $T^*(mn;m'n')$ for the generator T^*, analogously to Eq. (15). Condition (14) gives

$$\left|\frac{N(m,n)}{N(m'n')}\right| = \frac{T(mn;m'n')}{T^*(m'n';mn)}. \tag{19}$$

This way, the relative normalizations of basis states within an IR may be computed. For the present case,

$$\begin{aligned}
\pi^0 \sum a^m b^n|mn) &= \sum (m-n) a^m b^n|mn), \\
\pi^- \sum a^m b^n|mn) &= \sum a^{m+1} b^{n-1} n|mn), \\
\pi^+ \sum a^m b^n|mn) &= \sum a^{m-1} b^{n+1} m|mn).
\end{aligned} \tag{20}$$

Comparing like powers of a and b, we get,

$$\begin{aligned}
\pi^0(mn;mn) &= m-n, \\
\pi^-(mn;m-1,n+1) &= (n+1), \\
\pi^+(mn;m+1,n-1) &= (m+1).
\end{aligned} \tag{21}$$

Other matrix elements are zero. π^0 in Eq. (19) does not lead to any constraints on the normalizations. This is because it is diagonal in the chosen basis. However, using Eq. (19) for $\pi^{\pm}$, we get,

$$\left|\frac{N(m,n)}{N(m-1,n+1)}\right| = \frac{n+1}{m}. \tag{22}$$

We choose the solution,

$$N(m,n) = \frac{1}{m!n!}. \tag{23}$$

The solution is determined only up to (i) any function of the sum $m+n=2J$ and (ii) an arbitrary phase factor: (i) means that the relative normalization of states in different IRs is not fixed by our criterion. This is to be expected because unitarity of the representation matrix constrains relative normalizations of the basis states only within each IR. For any phase, unitarity is assured, and corresponds to a choice of the phases of the basis states.

Our orthonormalized basis states are represented by

$$|mn\rangle = \frac{z_1^m z_2^m}{\sqrt{m!}\sqrt{n!}}. \tag{24}$$

It would be easy to guess the measure with respect to which this basis is orthonormal. Define the inner product:

$$(f,g) = \int \frac{d^2z_1}{\pi}\frac{d^2z_2}{\pi} \exp(-\overline{z_1}z_1 - \overline{z_2}z_2)\overline{f(z_1,z_2)}g(z_1,z_2) \tag{25}$$

for functions in $\mathscr{F}_2$. The states [Eq. (24)] are orthonormal with respect to this measure. Note that the measure is invariant under the action of the group Eq. (1). We are led to a simple, Gaussian measure. As a consequence, it is easy to obtain a general formula for the Clebsch–Gordan coefficients. We now review this method.

Consider the direct product of two IRs, J_1 and J_2. This representation of the group is reducible in general. Consider its decomposition into various irreducible components:

$$|(J_1J_2)J_3M_3\rangle=\sum_{M_1,M_2} C^{J_1J_2J_3}_{M_1M_2M_3}|J_1M_1\rangle|J_2M_2\rangle. \tag{26}$$

The coefficients in the expansion are the Clebsch–Gordan coefficients. It is more convenient and symmetric to write this as follows. Given two IRs, J_1 and J_2, it is possible to form a nontrivial combination invariant under the group, only if $J_1=J_2$ and in this case,

$$\sum\ (-1)^{(J-M)}|J,M\rangle|J,-M\rangle=\text{invariant}. \tag{27}$$

As a consequence Eq. (26) may be reinterpreted as follows. Given three IRs, J_1, J_2 and J_3, try and form a (nontrivial) invariant combination

$$\sum_{M_1,M_2,M_3}\begin{pmatrix} J_1 & J_2 & J_3 \\ M_1 & M_2 & M_3\end{pmatrix}|J_1M_1\rangle|J_2M_2\rangle|J_3M_3\rangle. \tag{28}$$

The coefficients are the $3-j$ symbols.

Now represent the three IRs by homogeneous polynomials of degrees $2J_1,2J_2,2J_3$ in variables (z_1^1,z_2^1), (z_1^2,z_2^2), and (z_1^3,z_2^3), respectively. Then Eq. (28) corresponds to forming an invariant combination out of such polynomials. It is easy to do this. Invariant theory implies that any invariant polynomial in the six variables is a polynomial in the three independent invariants,

$$(z_1^1z_2^2-z_2^1z_1^2),\quad (z_1^2z_2^3-z_2^2z_1^3),\quad (z_1^3z_2^1-z_2^3z_1^1). \tag{29}$$

In order to satisfy our homogeneity requirements, we need non-negative integers N_1, N_2 and N_3 in

$$(z_1^1z_2^2-z_2^1z_1^2)^{N_3}(z_1^2z_2^3-z_2^2z_1^3)^{N_1}(z_1^3z_2^1-z_2^3z_1^1)^{N_2} \tag{30}$$

such that

$$2J_1=N_2+N_3,\quad 2J_2=N_3+N_1,\quad 2J_3=N_1+N_2. \tag{31}$$

For given J_1, J_2 and J_3, the only solution is

$$\begin{aligned} N_1&=J_2+J_3-J_1,\\ N_2&=J_3+J_1-J_2,\\ N_3&=J_1+J_2-J_3 \end{aligned} \tag{32}$$

if the right-hand sides are all non-negative. Thus if J_1, J_2, and J_3 satisfy the triangle condition, there is a unique invariant. Otherwise there is no nontrivial invariant. Thus the $3-j$ symbols are obtained (up to an overall normalization depending only on the total spins J_1, J_2, and J_3) by simply extracting in Eq. (30) the coefficients of the monomials [Eq. (24)] in the three sets of variables.

To obtain a formula for the $3-j$ symbols, we have to apply the binomial theorem, and extract the relevant powers of the monomials. We get (up to a normalization),

$$\sum_{p_a,q_a} \prod_{a=1}^{3} \frac{(-1)^{q_a}}{p_a! q_a!} \tag{33}$$

where the sum is over all nonnegative integers p_a, q_a satisfying the following matrix equation:

$$\begin{pmatrix} N_1 & N_2 & N_3 \\ m^1 & m^2 & m^3 \\ n^1 & n^2 & n^3 \end{pmatrix} = \begin{pmatrix} q_1+p_1 & q_2+p_2 & q_3+p_3 \\ q_2+p_3 & q_3+p_1 & q_1+p_2 \\ q_3+p_2 & q_1+p_3 & q_2+p_1 \end{pmatrix}. \tag{34}$$

III. A MODEL SPACE FOR SU(3)

Our first task is to construct a convenient model space for SU(3) (model space has been defined in Sec. I). It is not possible to get a model space as simple as the one for SU(2). But, we have constructed[47] a model space which is simple enough for obtaining general formulas. We provide an *ab initio* review of this construction in this section.

In the case of SU(2) all IRs could be constructed from the defining representation $\underline{2}$. This is no longer true for other semisimple groups. Consider a triplet (z_1, z_1, z_3) of complex numbers transforming as the defining representation $\underline{3}$ of SU(3). By considering polynomials in these complex variables we can only build totally symmetric tensors of SU(3). Such IRs are represented by Young's table with just our row. A general Young's table has two rows, some columns having two boxes and the rest having one box. In order to build a general IR, observe that an IR with one column of two rows corresponds to the $\underline{3^*}$ of SU(3). Therefore a general IR can be built using a direct product of $\underline{3^*}$s and $\underline{3}$s. Further, the tensors corresponding to the Young's table are symmetric in indices along each row. This means that it suffices to consider direct products which are totally symmetric in the $\underline{3^*}$s and in the $\underline{3}$s. Therefore, we may build a general IR in the space of polynomials in two triplets of complex numbers (z_1, z_2, z_3) and (w_1, w_2, w_3) transforming as $\underline{3}$ and $\underline{3}^*$ of SU(3), respectively. (All this is a heuristic explanation of a result proven in Refs. 1 and 2).

IRs of SU(3) are conveniently labeled by two arbitrary non-negative integers (M,N) which stand for the number of columns with one box and two boxes, respectively. Such an IR can be realized using polynomials of degree M in the z's and N in the w's, i.e., polynomials built from the monomials,

$$z_1^{m_1} z_2^{m_2} z_3^{m_3} w_1^{n_1} w_2^{n_2} w_3^{n_3} \tag{35}$$

with

$$m_1+m_2+m_3=M, \quad n_1+n_2+n_3=N. \tag{36}$$

However, this space contains some other IRs (M',N') with $M'<M$ and $N'<N$. The reason is that it is possible to form an SU(3) invariant $\vec{w}\cdot\vec{z}$. This is again a major difference from the SU(2) case. A simple way to remove the unwanted IRs is to impose the constraint,

$$\vec{w}\cdot\vec{z}=0, \tag{37}$$

where

$$\vec{w}\cdot\vec{z}=w_1z_1+w_2z_2+w_3z_3 \tag{38}$$

(i.e., we are constraining our variables to a cone in C_6). The IR(M,N) is now uniquely realized in the subspace with constraints [Eq. (36)].

We are forced to contend with the constraint [Eq. (37)] in order to get a model space. We obtain an explicit and simple enough basis by simply eliminating w_3 (say), in favor of the other five variables

$$w_3 = -\frac{1}{z_3}(w_1 z_1 + w_2 z_2). \tag{39}$$

Thus our space is spanned by the monomials (allowing for negative powers of z_3),

$$z_1^{m_1} z_2^{m_2} w_z^{n_1} w_2^{n_2} (w_1 z_1 + w_2 z_2)^{n_3} z_3^{m_3 - n_3}. \tag{40}$$

In order to get an explicit realization of the Gelfand–Zetlin basis in this space, we proceed as follows. Note that (z_1, z_2) transforms as a $\underline{2}$ and (w_1, w_2) as a $\underline{2}^*$ (which is equivalent to $\underline{2}$) under the isospin SU(2) subgroup of SU(3). The combination $(w_1 z_1 + w_2 z_2)$ in Eq. (3.6) is an SU(2) singlet built of these two doublets. This suggests that it is useful to use the coupled basis for the isospin group. This is done as follows. The monomials $z_1^{m_1} z_2^{m_2}$ and $w_1^{n_1} w_2^{n_2}$ with

$$m_1 + m_2 = 2I', \quad n_1 + n_2 = 2I'' \tag{41}$$

span the IRs of (iso)spin I' and I'', respectively. Therefore the direct product of these two spaces is a direct sum of spaces with isospin $I' + I'', I' + I'' - 1, \ldots, |I' - I''|$, each isospin appearing just once. This decomposition can be performed explicitly by the following trick: Introduce an (external) doublet (p,q) transforming as a $\underline{2}^*$ of SU(2). Then the following combination is invariant under SU(2):

$$(p z_1 + q z_2)^R (p w_2 - q w_1)^S (w_1 z_1 + w_2 z_2)^T. \tag{42}$$

Now,

$$\frac{p^P q^Q}{\sqrt{P!}\sqrt{Q!}} \sim \left| I = \frac{P+Q}{2}, \quad I_3 = \frac{-P+Q}{2} \right\rangle \tag{43}$$

under SU(2) transformations. On using Eq. (1) this means that the coefficient of the monomial $p^P q^Q$ corresponds to the state,

$$|(I'I'')I\, I_3\rangle \tag{44}$$

of the coupled basis, where

$$\begin{aligned} R + S = P + Q = 2I, \quad S + T = n_1 + n_2 = 2I'', \\ T + R = m_1 + m_2 = 2I', \quad P - Q = 2I_3. \end{aligned} \tag{45}$$

This way, we are able to explicitly construct basis vectors of the coupled basis. By allowing for all non-negative integer values of P, Q, R, S, and T subject to the constraints of Eq. (45) we are simply making a change of basis from the basis [Eq. (41)]. We make this change of basis in the space spanned by (Eq. 40) (further constrained by Eq. (41). We get an equivalent basis (as coefficients of $p^P q^Q$) in,

$$(p z_1 + q z_2)^R (p w_2 - q w_1)^S (w_1 z_1 + w_2 z_2)^{T + n_3} z_3^{m_3 - n_3}. \tag{46}$$

In terms of the new parameters we have

$$R+T+m_3=M, \quad S+T+n_3=N. \tag{47}$$

We now notice that distinct values of m_3, n_3, and T such that $T+n_3$ and $T+m_3$ have the same values correspond to the same basis vector on the cone $\vec{w}\cdot\vec{z}=0$. This is the way that the repeating IRs in C_6 spanned by $(\vec{w},\vec{z})$ get identified on the five-(complex) dimensional cone $\vec{w}\cdot\vec{z}=0$. Redefine

$$T+m_3=U, \quad T+n_3=V, \tag{48}$$

where U and V are non-negative integers. In terms of these variables, Eq. (47) is

$$R+U=M, \quad S+V=N. \tag{49}$$

Also, from Eq. (44)

$$P+Q=R+S. \tag{50}$$

We started with freely ranging non-negative integers m_i and n_i, subject only to the constraints of Eq. (36). This translates to free non-negative integers P, Q, R, S, U, and V subject to the constraints of Eqs. (49) and (50).

We have finally arrived at the following explicit and convenient realization of the (unnormalized) Gelfand–Zetlin basis of an arbitrary IR of SU(3): Extract the coefficients of various monomials $p^P q^Q$ in

$$(pz_1+qz_2)^R(pw_2-qw_1)^S z_3^U w_3^V, \tag{51}$$

where w_3 is given by Eq. (39). We will denote the space spanned by these basis vectors by $\mathscr{S}(M,N)$.

In the quark model, the basis within each IR is labeled by the quantum numbers I (total isospin), I_3 (the third component of isospin), and Y (the hypercharge) (or equivalently strangeness). These are related to our labels $(PQRSUV)$ as follows:

$$2I=P+Q=R+S, \quad 2I_3=P-Q,$$

$$Y=\tfrac{1}{3}(M-N)+V-U\equiv\tfrac{2}{3}(N-M)-(S-R). \tag{52}$$

Our labels are better because allowed quantum numbers within each IR (M,N) can be read off easily: R takes all values from 0 to M. S takes all values from 0 to N. For a given R and S, Q takes all values from 0 to $R+S$.

IV. THE GENERATING FUNCTION

Our representation [Eq. (51)] of the basis vectors of the IRs of SU(3) is not as simple as the monomial basis of Bargmann for SU(3). We need to use specific polynomials. In spite of this it has enough features of the Bargmann's basis as to be useful for general calculations. We demonstrate this in the following sections.

The first important feature of our basis is the following. By allowing for all possible non-negative integral values for our labels $(PQRSUV)$ subject to the constraint [Eq. (50)], the basis for every IR is realized and moreover realized once only. Further there are homogeneity restrictions on the $\vec{z}$ and $\vec{w}$ variables. Even though we are forced to use polynomials instead of the

monomials for the basis, the polynomials needed can be obtained as the coefficients of a monomial $p^P q^Q$. As a consequence of all this a simple generating function can be used to easily and uniquely generate all unnormalized basis states.

$$\mathbf{g}(p,q,r,s,u,v)=\exp(r(pz_1+qz_2)+s(pw_2-qw_1)+uz_3+vw_3). \tag{53}$$

The coefficient of the *monomial*,

$$p^P q^Q r^R s^S u^U v^V, \tag{54}$$

generates the *unnormalized* Gelfand–Zetlin basis denoted by $|P,Q,R,S,U,V)$. Thus,

$$\mathbf{g}=\sum_{P,Q,R,S,U,V} p^P q^Q r^R s^S u^U v^V |PQRSUV). \tag{55}$$

Note that the constraint [Eq. (50)], $P+Q=R+S$, is automatically satisfied in the Taylor expansion of Eq. (53). We refer to the variables p, q, r, s, u, and v as the sources and collectively denote them by j. Similarly, we refer to the labels P,Q,R,S,U, and V as the quantum numbers and collectively denote them by E. By using the generating function [Eq. (53)] we have come even closer to the Bargmann's techniques for SU(2).

In order to calculate the normalizations of our unnormalized basis vectors, we have to first obtain (as in Sec. II) the representation of the generators as differential operators on $\mathscr{G}$. An infinitesimal SU(3) matrix may be parametrized as follows:

$$\begin{aligned}\mathscr{U}\sim 1+i(&\epsilon(\pi^0)\pi^0+\epsilon(\eta)\eta+\epsilon(\pi^+)\pi^+ +\epsilon(\pi^-)\pi^- \\ &+\epsilon(K^+)K^+ +\epsilon(K^-)K^- +\epsilon(K^0)K^0 +\epsilon(\overline{K^0})\overline{K^0}),\end{aligned} \tag{56}$$

where the (unnormalized) generators are

$$\pi^0=\begin{pmatrix}1&0&0\\0&-1&0\\0&0&0\end{pmatrix};\quad \eta=\begin{pmatrix}1&0&0\\0&1&0\\0&0&-2\end{pmatrix};\quad \pi^-=\begin{pmatrix}0&1&0\\0&0&0\\0&0&0\end{pmatrix},$$

$$\pi^+=\begin{pmatrix}0&0&0\\1&0&0\\0&0&0\end{pmatrix};\quad K^-=\begin{pmatrix}0&0&1\\0&0&0\\0&0&0\end{pmatrix};\quad K^+=\begin{pmatrix}0&0&0\\0&0&0\\1&0&0\end{pmatrix}, \tag{57}$$

$$K^0=\begin{pmatrix}0&0&0\\0&0&1\\0&0&0\end{pmatrix};\quad \overline{K^0}=\begin{pmatrix}0&0&0\\0&0&0\\0&1&0\end{pmatrix}.$$

For unitarity, we have

$$\begin{gathered}\epsilon(\pi^0)^*=\epsilon(\pi^0);\quad \epsilon(\eta)^*=\epsilon(\eta);\\ \epsilon(\pi^+)^*=\epsilon(\pi^-);\quad \epsilon(K^+)^*=\epsilon(K^-);\quad \epsilon(K^0)^*=\epsilon(\overline{K^0}).\end{gathered} \tag{58}$$

Under an SU(3) transformation,

$$\begin{pmatrix} z_1 \\ z_2 \\ z_3 \end{pmatrix} \to \mathscr{U} \begin{pmatrix} z_1 \\ z_2 \\ z_3 \end{pmatrix},$$

$$(w_1 \quad w_2 \quad w_3) \to (w_1 \quad w_2 \quad w_3)\mathscr{U}^+, \tag{59}$$

where $\mathscr{U} \in \mathrm{SU}(3)$. This transformation is true even when w_3 is eliminated in favor of the other variables since the constraint [Eq. (37)] is itself invariant under SU(3). In order to obtain the transformation of **g**, it is convenient to write the exponent in Eq. (53) as follows:

$$(r_p \quad r_q \quad u) \cdot \begin{pmatrix} z_1 \\ z_2 \\ z_3 \end{pmatrix} + (w_1 \quad w_2 \quad w_3) \cdot \begin{pmatrix} s_q \\ s_p \\ v \end{pmatrix}, \tag{60}$$

where

$$r_p = rp, \quad r_q = rq, \quad s_p = sp, \quad s_q = -sq. \tag{61}$$

It is convenient to regard r_p, r_q, s_p, and s_q as independent variables and not related by Eq. (61). Only at the end of the calculations we may set the values [Eq. (61)] and generate the required basis vectors. We will refer to this operation as ''*going on shell*.'' Thus we define the *generalized generating function*:

$$\mathscr{G}(r_p, r_q, u, s_q, s_p, v) = \exp\left((r_p \quad r_q \quad u) \begin{pmatrix} z_1 \\ z_2 \\ z_3 \end{pmatrix} + (w_1 \quad w_2 \quad w_3) \cdot \begin{pmatrix} s_q \\ s_p \\ v \end{pmatrix} \right). \tag{62}$$

Its transformation is

$$\mathscr{G}(r_p, r_q, u, s_q, s_p, v) \to \mathscr{G}\left((r_p \quad r_q \quad u)\mathscr{U}, \mathscr{U}^\dagger \begin{pmatrix} s_q \\ s_p \\ v \end{pmatrix} \right). \tag{63}$$

Substitute Eq. (56) and collect the coefficients of $\epsilon(\pi^+)$, etc., after using Eq. (58).

We get the following representation of the generators:

$$\hat{\pi}^0 = r_p \frac{\partial}{\partial r_p} - r_q \frac{\partial}{\partial r_q} - s_q \frac{\partial}{\partial s_q} + s_p \frac{\partial}{\partial s_p},$$

$$\hat{\pi}^- = r_p \frac{\partial}{\partial r_q} - s_p \frac{\partial}{\partial s_q}, \quad \hat{\pi}^+ = r_q \frac{\partial}{\partial r_p} - s_q \frac{\partial}{\partial s_p},$$

$$\hat{K}^- = r_p \frac{\partial}{\partial u} - v \frac{\partial}{\partial s_q}, \quad \hat{K}^+ = u \frac{\partial}{\partial r_p} - s_q \frac{\partial}{\partial v}, \tag{64}$$

$$\hat{K}^0 = r_q \frac{\partial}{\partial u} - v \frac{\partial}{\partial s_p}, \quad \overline{\hat{K}^0} = u \frac{\partial}{\partial r_q} - s_p \frac{\partial}{\partial v},$$

$$\hat{\eta} = r_p \frac{\partial}{\partial r_p} + r_q \frac{\partial}{\partial r_q} - 2u \frac{\partial}{\partial u} - s_p \frac{\partial}{\partial s_p} - s_q \frac{\partial}{\partial s_q} + 2v \frac{\partial}{\partial v}.$$

For $\hat{\pi}^0$, $\hat{\pi}^\pm$, and $\hat{\eta}$ we may use Eq. (61) and get the following expressions:

$$\hat{\pi}^0 = p\,\frac{\partial}{\partial p} - q\,\frac{\partial}{\partial q}, \quad \hat{\pi}^- = p\,\frac{\partial}{\partial q},$$
$$\hat{\pi}^+ = q\,\frac{\partial}{\partial p}, \quad \hat{\eta} = r\,\frac{\partial}{\partial r} - s\,\frac{\partial}{\partial s} - 2u\,\frac{\partial}{\partial u} + 2v\,\frac{\partial}{\partial v}. \tag{65}$$

However, in order to represent the other generators as differential operators, we need to regard r_p, r_q, s_p and s_q as independent variables. As a result we face the following problem. It is not easy to calculate the matrix elements,

$$(P'Q'R'S'U'V'|T|PQRSUV) \tag{66}$$

of these generators, which are needed to evaluate the normalizations (see Sec. II). Consider for example the action of $\hat{K}^-$ on $\mathbf{g}$:

$$\hat{K}^-\mathbf{g} = (rpz_3 - vw_1)\mathbf{g}. \tag{67}$$

We need to reexpress the effect of z_3 or w_1 multiplying a basis state [Eq. (51)] as a linear combination of such states. But this is not easy.

This is another stumbling block compared to the situation in SU(2). We devise the technique to overcome this problem in Sec. V.

V. AN AUXILIARY GAUSSIAN MEASURE

An important reason for the efficiency of Bargmann's techniques for SU(2) is the Gaussian measure, using calculations which can be performed explicitly and easily. It is obtained as the measure with respect to which the Gelfand–Zetlin vectors form an orthonormal set and the representation matrices are unitary. We have discussed this in Sec. II.

We have a model space using five complex variables $(z_1, z_2, z_3, w_1, w_2)$. The measure in this space with respect to which properly normalized basis vectors form an orthonormal set exists, in principle. Gelfand *et al.*[45] have obtained this measure as the solution of a differential equation in a related context. Unfortunately, this measure does not have the simplicity of the Gaussian measure for SU(2). It appears that using it as a calculational tool to obtain general formulas is quite remote. This is yet another stumbling block in extending the Bargmann techniques to SU(3).

We evade this problem in the following way. We construct an auxiliary measure which is amenable to computations by relaxing the condition that it gives correct *normalizations* of the Gelfand–Zetlin states. We only require that the basis states do form an *orthogonal* set with respect to the measure. This is in fact sufficient for calculations of formulas. The correct normalization of the basis states (which gives a unitary representation) is itself computed using the same measure.

Our condition on the measure may be expressed in terms of the generating function as follows. Define the inner product,

$$(\mathbf{g}', \mathbf{g}) = \int d\mu\, \exp\overline{(r'(p'z_1 + q'z_2) + s'(p'w_2 - q'w_1) + u'z_3 + v'w_3)}$$
$$\times \exp(r(pz_1 + qz_2) + s(pw_2 - qw_1) + (uz_3 + vw_3) \tag{68}$$

between generating functions for different sets of arguments. (The over line in the first exponential means complex conjugation of the expression under it.) The integration is over the variables $(z_1, z_2, z_3, w_1, w_2)$, w_3 being expressed in terms of these other variables. We want this inner product to be of the following type:

$$(\mathbf{g}', \mathbf{g}) = F(\overline{p'}p, \overline{q'}q, \overline{r'}r, \overline{s'}s, \overline{u'}u, \overline{v'}v), \tag{69}$$

where the function F has a Taylor expansion in its arguments about the origin with every coefficient positive definite. Such a form implies that the inner product is zero whenever the powers of the variables (p,q,r,s,u,v) do not match the powers of the corresponding variables (p',q',r',s',u',v'), i.e., Gelfand–Zetlin basis vectors are mutually orthogonal. Moreover the square of the norm given by the corresponding coefficient in the Taylor expansion is positive definite.

Our measure is closely related to Bargmann's. We have two doublets (z_1,z_2) and (w_1,w_2) of SU(2) and the coupled basis built using them. We know that coupled basis is obtained by a unitary transformation of the direct product basis. This means that Bargmann's measure for these two doublets ensures orthogonality of our SU(3) basis vectors in so far as the (z_1,z_2,w_1,w_2) variables are concerned. To be explicit we consider,

$$
\begin{aligned}
F=\int \frac{d^2z_1}{\pi}\frac{d^2z_2}{\pi}\frac{d^2w_1}{\pi}\frac{d^2w^2}{\pi}\exp(-\overline{z_1}z_1-\overline{z_2}z_2-\overline{w_1}w_1-\overline{w_2}w_2)\\
\times\exp\left(\overline{r'(p'z_1+q'z_2)+s'(p'w_2-q'w_1)-\frac{v'}{z_3}(z_1w_1+z_2w_2)+u'z_3}\right)\\
\times\exp\left(r(pz_1+qz_2)+s(pw_2-qw_1)-\frac{v}{z^3}(z_1w_1+z_2w_2)+uz_3\right). \qquad (70)
\end{aligned}
$$

This can be evaluated easily. Write the exponent as

$$
\begin{aligned}
&-(\overline{z_1}\ w_1)\begin{pmatrix}1 & \overline{\left(\frac{v'}{z_3}\right)}\\ \frac{v}{z_3} & 1\end{pmatrix}\begin{pmatrix}z_1\\ \overline{w_1}\end{pmatrix}-(\overline{z_2}\quad w_2)\begin{pmatrix}1 & \overline{\left(\frac{v'}{z_3}\right)}\\ \frac{v}{z_3} & 1\end{pmatrix}\begin{pmatrix}z_2\\ \overline{w_2}\end{pmatrix}+(rp-\overline{(s'q')})\begin{pmatrix}z_1\\ \overline{w_1}\end{pmatrix}\\
&+(\overline{z_1}\ w_1)\begin{pmatrix}\overline{r'p'}\\ -sq\end{pmatrix}+(rq\quad(\overline{s'p'}))\begin{pmatrix}z_2\\ \overline{w_2}\end{pmatrix}+(\overline{z_2}\quad w_2)\begin{pmatrix}\overline{(r'q')}\\ sp\end{pmatrix}+\overline{(u'z_3)}+uz_3. \qquad (71)
\end{aligned}
$$

Use the formula,

$$
\prod_{i=1}^{n}\int\frac{d^2z_i}{\pi}\exp(-\overline{z}^TXz+A^Tz+\overline{z}^T\overline{B})=(\det X)^{-1}\exp(A^TX^{-1}\overline{B}) \qquad (72)
$$

which is valid whenever the Hermitian part of X is positive definite. Here z is the column vector of the complex variables $(z_1,z_2,\ldots,z_n)$. We get,

$$
\begin{aligned}
F=\left(1-\frac{\overline{v'}v}{|z_3|^2}\right)^{-2}\exp\left[\left((1-\overline{v'}v/|z_3|^2)^{-1}\left((rp,-\overline{s'q'})\begin{pmatrix}1 & -\overline{v'}/\overline{z_3}\\ -v/z_3 & 1\end{pmatrix}\begin{pmatrix}\overline{r'p'}\\ -sq\end{pmatrix}\right.\right.\\
\left.\left.+(rq',\overline{s'p'})\begin{pmatrix}1 & -\overline{v'}/\overline{z_3}\\ -v/x_3 & 1\end{pmatrix}\begin{pmatrix}\overline{r'q'}\\ sp\end{pmatrix}\right)+\overline{u'z_3}+uz_3\right]. \qquad (73)
\end{aligned}
$$

Thus,

$$F=\left(1-\frac{\overline{v'}v}{|z_3|^2}\right)^{-2}\exp\left(\frac{(\overline{r'}r+\overline{s'}s)(\overline{p'}p+\overline{q'}q)}{(1-\overline{v'}v/|z_3|^2)}+\overline{u'z_3}+uz_3\right). \tag{74}$$

Note that this has the features [Eq. (69)] we required for the inner product, so far as the variables p, q, r, s, and v are concerned. This was to be expected, because the coupled basis constructed out of two doublets $(z_1 \quad z_2)$ and $(w_1 \quad w_2)$ is an orthogonal set with respect to Bargmann's measure.

We have to now propose a workable measure for integration over the z_3 variable. Note that $|z_3|^2$ appears in the denominators in Eq. (74). This suggests that it is best to set

$$z_3=\epsilon^{i\theta} \tag{75}$$

so that $|z_3|^2=1$. This means that our realization of the basis vectors is in terms of four complex variables z_1, z_2, w_1, w_2, and a phase variable $e^{i\theta}$. Setting the constraint [Eq: (75)] is no problem, because we have used only the variable z_3 and not $\overline{z_3}$ in our basis vectors. (See the Appendix for a more detailed discussion.) Our requirement on the measure for the θ variable is that (i) it is simple and (ii) we get a function of only the combination $\overline{u'}u$. From Eq. (74) we see that it is sufficient to average over θ. Thus the measure we use is

$$(\mathbf{g}',\mathbf{g})=\int_{-\pi}^{+\pi}\frac{d0}{2\pi}\int\frac{d^2z_1}{\pi}\frac{d^2z_2}{\pi}\frac{d^2w_1}{\pi}\frac{d^2w_2}{\pi}\,\overline{\mathbf{g}'}\mathbf{g}. \tag{76}$$

The inner product between two generating functions is

$$(\mathbf{g}',\mathbf{g})=(1-\overline{v'}v)^{-2}\left(\sum_{n=0}^{\infty}\frac{(\overline{u'}u)^n}{(n!)^2}\right)\exp[(1-\overline{v'}v)^{-1}(\overline{p'}p+\overline{q'}q)(\overline{r'}r+\overline{s'}s)]. \tag{77}$$

Notice that the coefficients of the Taylor expansion are all positive definite. This is a satisfactory inner product which we may use do to computations explicitly.

For our calculations, we need the inner product between any two generalized generating functions [Eq. (62)]. In place of Eq. (74), we get

$$\begin{aligned}(\mathscr{G}',\mathscr{G})=\int\frac{d\theta}{2\pi}(1-\overline{v'}v)^{-2}\exp\Bigg[&(1-\overline{v'}v)^{-1}(r_p \quad \overline{s'_q})\begin{pmatrix}1 & -\overline{v'}e^{i\theta}\\ -ve^{-i\theta} & 1\end{pmatrix}\begin{pmatrix}\overline{r'_p}\\ s_q\end{pmatrix}\\ &+\left((r_q \quad \overline{s'_p})\begin{pmatrix}1 & -\overline{v'}e^{+i\theta}\\ -ve^{-i\theta} & 1\end{pmatrix}\begin{pmatrix}\overline{r'_q}\\ s_p\end{pmatrix}+\overline{u'}e^{-i\theta}+ue^{i\theta}.\right.\end{aligned} \tag{78}$$

Therefore,

$$\begin{aligned}(\mathscr{G}',\mathscr{G})=&(1-\overline{v'}v)^{-2}\exp[(1-\overline{v'}v)^{-1}(\overline{r'_p}r_p+\overline{r'_q}r_q+\overline{s'_p}s_p+\overline{s'_q}s_q)]\\ &\times\left[\sum_{n=0}^{\infty}\frac{1}{(n!)^2}\left(\overline{u'}-v\,\frac{(\overline{r'_ps'_q}+\overline{r'_qs'_p})}{(1-\overline{v'}v)}\right)^n\left(u-\overline{v'}\,\frac{(r_ps_q+r_qs_p)}{(1-\overline{v'}v)}\right)^n\right].\end{aligned} \tag{79}$$

VI. CALCULATION OF THE NORMALIZATIONS

We now compute the normalization of our representation [Eq. (51)] of the (unnormalized) basis vectors. As discussed in Sec. II, this is obtained from the requirement that the representation matrix be unitary in each IR. Our technique differs from the one discussed in Sec. II in one crucial respect.

Let $|E)$ denote any unnormalized basis vector defined by the expansion [Eq. (55)]. E stands for the set of quantum numbers used in the basis. For any generator T let

$$T|E) = \sum_{E'} T(E,E')|E'). \tag{80}$$

We want to compute $N(E)$ defined by

$$|E) = N^{1/2}(E)|E\rangle, \tag{81}$$

where $|E\rangle$ denotes any Gelfand–Zetlin normalized basis vector:

$$\langle E'|E\rangle = \delta_{E'E}. \tag{82}$$

The representation matrix is unitary when the basis vectors $|E\rangle$ are used. $N(E)$ is obtained by the requirement,

$$\langle E'|T|E\rangle = \langle E|T^*|E'\rangle^* \tag{83}$$

for every generator T and for any normalized basis vectors $|E\rangle$ and $|E'\rangle$. We have from Eq. (80) and Eq. (81),

$$N^{1/2}(E)T|E\rangle = \sum_{E'} T(E,E')N^{1/2}(E')|E'\rangle \tag{84}$$

so that,

$$\langle E'|T|E\rangle = T(E,E')\,\frac{N^{1/2}(E')}{N^{1/2}(E)}. \tag{85}$$

Therefore, Eq. (83) gives

$$\left|\frac{N(E)}{N(E')}\right| = \frac{T(E,E')}{(T(E',E))^*}. \tag{86}$$

This means we need to evaluate $T(E,E')$, defined in Eq. (80). For this we use our ''auxiliary'' inner product given by Eq. (76). We denote this inner product between two vectors $|1)$ and $|2)$ by

$$(2\|1) \tag{87}$$

to distinguish it from the ''true'' inner product given by Eq. (82). The Gelfand–Zetlin normalized basis vectors $|E\rangle$ do form an orthogonal set but have a different norm with respect to the auxiliary inner product. Therefore,

$$(E'\|E) = \delta_{E'E}M(E), \tag{88}$$

where $M(E)$ is different from $N(E)$ in general. Using Eq. (88) in Eq. (80) we get

$$(E'\|(T|E)) = T(E,E')M(E'). \tag{89}$$

Therefore Eq. (86) gives

$$\left|\frac{N(E)}{N(E')}\right| = \frac{(E'\|T|E)}{(E\|T^*|E')^*}\,\frac{M(E)}{M(E')}. \tag{90}$$

Thus we can fix the normalization using an ''auxiliary'' inner product which allows explicit computation, even though it is not the ''true'' inner product.

$M(P,Q,R,S,U,V)$ can be read off as the coefficient of the monomial:

$$(\overline{p'}p)^P(\overline{q'}q)^Q(\overline{r'}r)^R(\overline{s'}s)^S(\overline{u'}u)^U(\overline{v'}v)^V$$

in Eq. (77).

We have

$$(\mathbf{g}',\mathbf{g})=\left(\sum_{2I=0}^{\infty}\frac{(\overline{p'}p+\overline{q'}q)^{2I}(\overline{r'}r+\overline{s'}s)^{2I}}{(2I)!(1-\overline{v'}v)^{2I+2}}\right)\left(\sum_{V=0}^{\infty}\frac{(\overline{u'}u)^U}{(U!)^2}\right). \tag{91}$$

Using

$$(x+y)^n=\sum_{m=0}^{n}{}^nC_m x^m y^{n-m} \tag{92}$$

and

$$\frac{1}{(1-x)^{m+1}}=\sum_{n=0}^{\infty}{}^{(n+m)}C_n x^n \tag{93}$$

we get

$$M(P,Q,R,S,U,V)=\frac{(V+2I+1)!}{P!Q!R!S!(U!)^2V!(2I+1)}. \tag{94}$$

We have used $2I=P+Q=R+S$.

We now apply the formula of Eq. (90) for each of our generators [Eq. (64)]. The generators $\hat{\pi}^0$ and $\hat{\eta}$ are diagonal in the chosen basis and therefore do not lead to any constraints on the relative normalizations of the basis vectors. Consider $\hat{\pi}^-$ as given by Eq. (65). We get

$$(\mathbf{g}',\hat{\pi}^-\mathbf{g})=p\,\frac{\partial}{\partial q}\,(\mathbf{g}',\mathbf{g})=p\overline{q'}\,\frac{(\overline{r'}r+\overline{s'}s)}{(1-\overline{v'}v)}\,(\mathbf{g}',\mathbf{g}) \tag{95}$$

on using Eq. (77). Extracting like powers of the monomials from both sides of Eq. (92), we get

$$(P,Q+1,R,S,U,V)\|\hat{\pi}^-|P+1,Q,R,S,U,V)=M_3(P,Q,R,S,U,V) \tag{96}$$

as the only nonzero auxiliary matrix element of $\hat{\pi}^-$. This is expected because $\hat{\pi}^-$ only lowers the I_3 value by 1 [see (Eq. (52)]. $M_3(P,Q,R,S,U,V)$ is listed in Table I. Similarly we get

$$(P+1,Q,R,S,U,V\|\hat{\pi}^+|P,Q+1,R,S,U,V)=M_3(P,Q,R,S,U,V). \tag{97}$$

Thus, in the present case,

$$(P,Q+1,R,S,U,V\|\hat{\pi}^-|P+1,Q,R,S,U,V)=(P+1,Q,R,S,U,V\|\hat{\pi}^+|P,Q+1,R,S,U,V) \tag{98}$$

since $M_3(P,Q,R,S,U,V)$ is real. Therefore the auxiliary normalization, also gives the Gelfand–Zetlin normalizations, is in this case:

$$\left|\frac{N(P+1,Q,R,S,U,V)}{N(P,Q+1,R,S,U,V)}\right|=\frac{M(P+1,Q,R,S,U,V)}{M(P,Q+1,R,S,U,V)}. \tag{99}$$

TABLE I. Normalization constants.

$M(P,Q,R,S,U,V)$	$\frac{\exp[(1-\overline{v}'v)^{-1}(\overline{p}'p+\overline{q}'q)(\overline{r}'r+\overline{s}'s)]}{(1-\overline{v}'v)^2}\sum_n \frac{(\overline{u}'u)^n}{(n!)^2}$	$\frac{(2I+1+V)!}{P!Q!R!S!U!V!}\frac{1}{U!(2I+1)}$
$M_1(P,Q,R,S,U,V)$	$\frac{\exp[(1-\overline{v}'v)^{-1}(\overline{p}'p+\overline{q}'q)(\overline{r}'r+\overline{s}'s)]}{(1-\overline{v}'v)^3}\sum_n \frac{(\overline{u}'u)^n}{(n!)^2}$	$\frac{(2I+2+V)!}{P!Q!R!S!U!V!}\frac{1}{U!(2I+1)(2I+2)}$
$M_2(P,Q,R,S,U,V)$	$\frac{\exp[(1-\overline{v}'v)^{-1}(\overline{p}'p+\overline{q}'q)(\overline{r}'r+\overline{s}'s)]}{(1-\overline{v}'v)^4}\sum_n \frac{(\overline{u}'u)^n}{(n!)^2}$	$\frac{(2I+3+V)!}{P!Q!R!S!U!V!}\frac{1}{U!(2I+1)(2I+2)(2I+3)}$
$M_3(P,Q,R,S,U,V)$	$\frac{\exp[(1-\overline{v}'v)^{-1}(\overline{p}'p+\overline{q}'q)(\overline{r}'r+\overline{s}'s)]}{(1-\overline{v}'v)^3}\times(\overline{r}'r+\overline{s}'s)\sum_n \frac{(\overline{u}'u)^n}{(n!)^2}$	Not needed
$M_4(P,Q,R,S,U,V)$	$\frac{\exp[(1-\overline{v}'v)^{-1}(\overline{p}'p+\overline{q}'q)(\overline{r}'r+\overline{s}'s)]}{(1-\overline{v}'v)^4}\times(\overline{p}'p+\overline{q}'q)(\overline{r}'r+\overline{s}'s)\sum_n \frac{(\overline{u}'u)^n}{(n!)^2}$	$\frac{(2I+2+V)!}{P!Q!R!S!U!V!}\frac{2I}{U!(2I+1)(2I+2)}$
$M_5(P,Q,R,S,U,V)$	$\frac{\exp[(1-\overline{v}'v)^{-1}(\overline{p}'p+\overline{q}'q)(\overline{r}'r+\overline{s}'s)]}{(1-\overline{v}'v)^2}\sum_n \frac{(\overline{u}'u)^n}{(n+1)!n!}$	$\frac{(2I+1+V)!}{P!Q!R!S!U!V!}\frac{1}{(U+1)!(2I+1)}$
$M_6(P,Q,R,S,U,V)$	$\frac{\exp[(1-\overline{v}'v)^{-1}(\overline{p}'p+\overline{q}'q)(\overline{r}'r+\overline{s}'s)]}{(1-\overline{v}'v)^3}\sum_n \frac{(\overline{u}'u)^n}{(n+1)!n!}$	$\frac{(2I+2+V)!}{P!Q!R!S!U!V!}\frac{1}{(U+1)!(2I+1)(2I+2)}$

The reason for this matching is that for the SU(2) subgroup we are using just the Bargmann measure. Using Table I we get,

$$\left|\frac{N(P+1,Q,R,S,U,V)}{N(P,Q+1,R,S,U,V)}\right|=\frac{Q+1}{P+1}, \tag{100}$$

exactly as in the SU(2) case (Sec. II). Thus the relative normalizations of basis vectors within an isospin multiplet are determined and are the same as in the SU(2) case:

$$N(P,Q,R,S,U,V)\sim\frac{1}{P!Q!}. \tag{101}$$

The dependence on the total isospin $P+Q=R+S$ as also on quantum numbers, R, S, U, and V are not determined at this stage.

We now compute the relative normalizations implied by $\hat{K}^{\pm}$. To calculate, $(\mathbf{g}',\hat{K}^{-}\mathbf{g})$ we use the generalized partition function:

$$(\mathbf{g}',\hat{K}^{-}\mathbf{g})=\left(r_p\frac{\partial}{\partial u}-v\frac{\partial}{\partial s_q}\right)(\mathscr{G}',\mathscr{G})\Big|, \tag{102}$$

where the vertical line at the end of this equation means that after applying a differential operator on $(\mathscr{G}',\mathscr{G})$, we need to set the values [Eq. (61)] for the sources. For instance,

$$(r_p s_q+r_q s_p)\big|=0;\quad (\overline{r_p}'\overline{s_q}'+\overline{r_q}'\overline{s_p}')\big|=0. \tag{103}$$

We get

$$(\mathbf{g}',\hat{K}^-\mathbf{g}) = \frac{1}{(1-\overline{v'}v)^2}\exp[(1-\overline{v'}v)^{-1}(\overline{p'}p+\overline{q'}q)(\overline{r'}r+\overline{s'}s)] \times\left[rp\sum_{n=0}^{\infty}\frac{\overline{u'}^{n+1}u^n}{(n+1)!n!}+\frac{v\overline{s'q'}}{(1-\overline{v'}v)}\sum_{n=0}^{\infty}\frac{\overline{u'}^n u^n}{(n!)^2}+\frac{v\overline{v'}rp}{(1-\overline{v'}v)}\sum_{n=0}^{\infty}\frac{\overline{u'}^{n+1}u^n}{(n+1)!n!}\right]. \tag{104}$$

Matching coefficients of like powers we get (Table I)

$$(P,Q,R,S,U+1,V\|\hat{K}^-|P+1,Q,R+1,S,U,V) = M_5(P,Q,R,S,U,V)+M_6(P,Q,R,S,U,V-1), \tag{105}$$

$$(P,Q+1,R,S+1,U,V\|\hat{K}^-|P,Q,R,S,U,V+1)=M_4(P,Q,R,S,U,V). \tag{106}$$

These nonzero matrix elements are as expected for $I=\frac{1}{2}$, $I_3=-\frac{1}{2}$, $Y=+1$ quantum numbers for $\hat{K}^-$. Similarly,

$$(P+1,Q,R+1,S,U,V)\|\hat{K}^+|P,Q,R,S,U+1,V)=M_4(P,Q,R,S,U,V), \tag{107}$$

$$(P,Q,R,S,U,V+1\|\hat{K}^+|P,Q+1,R,S+1,U,V) = M_6(P,Q,R,S,U-1,V)+2M_4(P,Q,R,S,U,V)+M_4(P,Q,R,S,U,V). \tag{108}$$

Using Eq. (91) we get the following constraints on relative normalizations from Eqs. (103)–(106):

$$\left|\frac{N(P+1,Q,R+1,S,U,V)}{N(P,Q,R,S,U+1,V)}\right|=(V+2I+2)\frac{(U+1)}{(P+1)(R+1)}\frac{(2I+1)}{(2I+2)}, \tag{109}$$

$$\left|\frac{N(P,Q+1,R,S+1,U,V)}{N(P,Q,R,S,U,V+1)}\right|=(U+2I+2)\frac{(V+1)}{(Q+1)(S+1)}\frac{(2I+1)}{(2I+2)}. \tag{110}$$

A solution for Eqs. (107) and (108) is

$$N(P,Q,R,S,U,V)=\frac{(U+2I+1)!(V+2I+1)!}{P!Q!R!S!U!V!(2I+1)}. \tag{111}$$

We now consider the nonuniqueness in this solution. The quantum numbers, Q, S, V, $P+U$, and $R+U$ do not change between the numerator and the denominator of Eq. (109). Therefore dependence of $N(P,Q,R,S,U,V)$ on these quantum numbers are not fixed by Eq. (109). However, Eq. (110) serves to fix the dependence on Q,S,V. Therefore the only ambiguity is in dependence of the combinations $P+U$ and $R+U$. We may hope that this ambiguity is removed by the constraints coming from the remaining generators $\hat{K}^0$ and $\hat{\bar{K}}^0$. The nonzero matrix elements of these generators in the unnormalized basis are:

$$(P,Q,R,S,U+1,V\|\hat{K}^0|P,Q+1,R+1,S,U,V) = M_5(P,Q,R,S,U,V)+M_6(P,Q,R,S,U,V-1), \tag{112}$$

$$(P+1,Q,R,S+1,U,V\|\hat{K}^0|P,Q,R,S,U,V+1)=-M_1(P,Q,R,S,U,V), \tag{113}$$

$$(P,Q+1,R+1,S,U,V\|\hat{K}^0|P,Q,R,S,U+1,V)=M_1(P,Q,R,S,U,V), \tag{114}$$

$$(P,Q,R,S,U,V+1)\|\hat{K}^0|P+1,Q,R,S+1,U,V)$$
$$=-M_6(P,Q,R,S,U-1,V)-2M_1(P,Q,R,S,U,V)-M_4(P,Q,R,S,U,V). \tag{115}$$

This gives the constraints,

$$\left|\frac{N(P,Q+1,R+1,S,U,V)}{N(P,Q,R,S,U+1,V)}\right|=(V+2I+2)\,\frac{(U+1)}{(Q+1)(R+1)}\,\frac{(2I+1)}{(2I+2)}, \tag{116}$$

$$\left|\frac{N(P+1,Q,R,S+1,U,V)}{N(P,Q,R,S,U,V+1)}\right|=(U+2I+2)\,\frac{(V+1)}{(P+1)(S+1)}\,\frac{(2I+1)}{(2I+2)}. \tag{117}$$

As expected, these constraints fix the dependence on $P+U$ and $R+U$. Thus the normalization factor of our unnormalized basis states is uniquely fixed by Eq. (111). It is worth noting that the matrix elements Eqs. (106), (108), and (114) are all equal and differ only in sign from Eq. (113). Similarly, Eqs. (105) and (112) are equal, whereas Eq. (108) only differs in sign from Eq. (115). As a consequence, there is a certain symmetry in the constraints [Eqs. (109), (110), (116), and (117) of the normalizations. (See Table I.) These relations between matrix elements with respect to auxiliary inner product between unnormalized basis states is a consequence of our choices of the inner product and basis states. They do not seem to have any group theoretic reason. Anyway we are only interested in matrix elements between normalized states.

VII. THE 3-G SYMBOLS

In this section, we mostly review well-known material[1,2,15,48,23] in order to fix our notations and for logical continuity. In addition we emphasize the relation between the multiplicity in the Clebsch–Gordan series and the distinct invariants that can be constructed out of three IRs. Consider a compact group G. We denote the basis of states of unitary irreducible representations by

$$\left|\begin{matrix}\lambda\\ \alpha\end{matrix}\right\rangle, \tag{118}$$

where λ labels the IRs and α labels the basis for the IRs. For SU(3), for instance, we may use the ordered pair (M,N) for λ and (I,I_3,Y) for α. Consider the direct product of two IRs, λ and λ'. This can be completely reduced to the IRs of the group. In general, the same IR λ'' may appear more than once in the decomposition. Therefore we need extra labels for the IRs of the decomposition. We denote these additional labels collectively by k. (We discuss this in detail[25,26] for SU(3) in Sec. VIII). Thus we may write

$$\left|\begin{matrix}\lambda''\\ \alpha''\end{matrix}\right\rangle^k=\sum_{\alpha,\alpha'}\left|\begin{matrix}\lambda\\ \alpha\end{matrix}\right\rangle\left|\begin{matrix}\lambda'\\ \alpha'\end{matrix}\right\rangle\left\langle\begin{matrix}\lambda\lambda'\\ \alpha\alpha'\end{matrix}\right|\left.\begin{matrix}\lambda''\\ \alpha''\end{matrix}\right\rangle^k, \tag{119}$$

where $|{}^{\lambda''}_{\alpha''}\rangle^k$ are the basis vectors of the repeating IR λ'' and where the repetitions are labeled by k. The coefficients in this expansion,

$$\left\langle\begin{matrix}\lambda\lambda'\\ \alpha\alpha'\end{matrix}\right|\left.\begin{matrix}\lambda''\\ \alpha''\end{matrix}\right\rangle^k, \tag{120}$$

are the Wigner–Clebsch–Gordan coefficients of G. Equation (119) provides a unitary transformation from the basis of the IRs of the decomposition to the direct product basis. Inverse transformation may be written as

$$\left|\begin{matrix}\lambda\\ \alpha\end{matrix}\right\rangle\left|\begin{matrix}\lambda'\\ \alpha'\end{matrix}\right\rangle=\sum_{\alpha'',k}\left|\begin{matrix}\lambda''\\ \alpha''\end{matrix}\right\rangle^{k\,k}\left\langle\begin{matrix}\lambda''\\ \alpha''\end{matrix}\middle|\begin{matrix}\lambda\lambda'\\ \alpha\alpha'\end{matrix}\right\rangle. \tag{121}$$

We get

$$\sum_{\lambda'',k,\alpha''}\left\langle\begin{matrix}\lambda\lambda'\\ \alpha\alpha'\end{matrix}\middle|\begin{matrix}\lambda''\\ \alpha''\end{matrix}\right\rangle^{k\,k}\left\langle\begin{matrix}\lambda''\\ \alpha''\end{matrix}\middle|\begin{matrix}\lambda\lambda'\\ \beta\beta'\end{matrix}\right\rangle=\delta_{\alpha\beta}\delta_{\alpha'\beta'}, \tag{122}$$

$$\sum_{\alpha,\alpha'}{}^{k}\left\langle\begin{matrix}\lambda''\\ \alpha''\end{matrix}\middle|\begin{matrix}\lambda\lambda'\\ \alpha\alpha'\end{matrix}\right\rangle\left\langle\begin{matrix}\lambda\lambda'\\ \alpha\alpha'\end{matrix}\middle|\begin{matrix}\lambda'''\\ \alpha'''\end{matrix}\right\rangle^{k'}=\delta_{kk'}\delta_{\lambda''\lambda'''}\delta_{\alpha''\alpha'''}. \tag{123}$$

Let $D(g)^{\lambda}$ denote the unitary representation matrix of an element $g\in G$ in the IR λ. Thus under the group action,

$$g:\left|\begin{matrix}\lambda\\ \alpha\end{matrix}\right\rangle\rightarrow\sum_{\beta}D^{\lambda}_{\alpha\beta}(g)\left|\begin{matrix}\lambda\\ \beta\end{matrix}\right\rangle. \tag{124}$$

The matrices $\overline{D^{\lambda}}(g)$ whose elements are complex conjugates of $D^{\lambda}(g)$,

$$(\overline{D(g)})_{\alpha\beta}=(D^{\lambda}(g))^{*}_{\alpha\beta}, \tag{125}$$

also provide an irreducible representation of the group called the representation $\overline{\lambda}$ conjugate to λ. For SU(3), the IR (N,M) is the conjugate of (M,N). Define basis states

$$\left|\begin{matrix}\lambda\\ \alpha\end{matrix}\right\rangle_{c} \tag{126}$$

transforming like

$$g:\left|\begin{matrix}\lambda\\ \alpha\end{matrix}\right\rangle_{c}\rightarrow\sum_{\beta}(D(g)^{\lambda}_{\alpha\beta})^{*}\left|\begin{matrix}\lambda\\ \beta\end{matrix}\right\rangle_{c}. \tag{127}$$

This means

$$\begin{aligned}g:\sum_{\alpha}\left|\begin{matrix}\lambda\\ \alpha\end{matrix}\right\rangle\left|\begin{matrix}\lambda\\ \alpha\end{matrix}\right\rangle_{c}&\rightarrow\sum_{\alpha}\left(\sum_{\beta}(D(g))^{\lambda}_{\alpha\beta}\left|\begin{matrix}\lambda\\ \beta\end{matrix}\right\rangle\right)\left(\sum_{\gamma}(D(g)^{\lambda}_{\alpha\gamma})^{*}\left|\begin{matrix}\lambda\\ \gamma\end{matrix}\right\rangle_{c}\right)\\ &=\sum_{\beta,\gamma}(D^{\lambda\dagger}(g)D(g)^{\lambda})_{\gamma\beta}\left|\begin{matrix}\lambda\\ \beta\end{matrix}\right\rangle\left|\begin{matrix}\lambda\\ \gamma\end{matrix}\right\rangle_{c}=\sum_{\alpha}\left|\begin{matrix}\lambda\\ \alpha\end{matrix}\right\rangle\left|\begin{matrix}\lambda\\ \alpha\end{matrix}\right\rangle_{c}\end{aligned} \tag{128}$$

since $D(g)$ is unitary. Therefore

$$\frac{1}{\sqrt{d_{\lambda}}}\sum_{\alpha}\left|\begin{matrix}\lambda\\ \alpha\end{matrix}\right\rangle\left|\begin{matrix}\lambda\\ \alpha\end{matrix}\right\rangle_{c} \tag{129}$$

(where d_λ is the dimension of the IR λ) (i) is invariant under the group; (ii) is the unique invariant vector in the direct product space of λ and $\bar{\lambda}$ (since there is one, and only one singlet in the decomposition of the direct product of λ and $\bar{\lambda}$.); (iii) it has unit norm. Now $|^{\lambda''}_{\alpha''}\rangle^k$ in Eq. (119) transforms like the IR λ'' for every k. Therefore,

$$\frac{1}{\sqrt{d_\lambda}} \sum_{\alpha''} \left|\begin{matrix}\lambda'' \\ \alpha''\end{matrix}\right\rangle^k \left|\begin{matrix}\lambda'' \\ \alpha''\end{matrix}\right\rangle_c \tag{130}$$

is an invariant with unit norm for every k. Use this in Eq. (119). We get, in the direct product of three IRs, λ, λ' and λ'',

$$\frac{1}{\sqrt{d''_\lambda}} \sum_{\alpha,\alpha',\alpha''} \left\langle\begin{matrix}\lambda\lambda' \\ \alpha\alpha'\end{matrix}\middle|\begin{matrix}\lambda'' \\ \alpha''\end{matrix}\right\rangle^k \left|\begin{matrix}\lambda \\ \alpha\end{matrix}\right\rangle \left|\begin{matrix}\lambda' \\ \alpha'\end{matrix}\right\rangle \left|\begin{matrix}\lambda'' \\ \alpha''\end{matrix}\right\rangle_c \tag{131}$$

(i) is, for each k, an invariant of unit norm, (ii) are linearly independent vectors in the direct product space for various k's. (This is because $|^{\lambda''}_{\alpha''}\rangle^k$ in Eq. (119) are linearly independent for various k.) (iii) are the only invariant vectors in the direct product space of λ, λ' and λ''. This is because Eq. (129) are the only invariant vectors formed from $|^{\lambda''}_{\alpha''}\rangle^k$. We will rewrite Eq. (131) in the following way. Define the 3–G *symbols*,

$$\left[\begin{matrix}\lambda\lambda'\lambda'' \\ \alpha\alpha'\alpha''\end{matrix}\right]_k = \frac{1}{\sqrt{d_{\lambda''}}} \left\langle\begin{matrix}\lambda\lambda' \\ \alpha\alpha'\end{matrix}\middle|\begin{matrix}\lambda'' \\ \alpha''\end{matrix}\right\rangle^k_c . \tag{132}$$

Noting that

$$\left(\left|\begin{matrix}\lambda \\ \alpha\end{matrix}\right\rangle_c\right)_c = \left|\begin{matrix}\lambda \\ \alpha\end{matrix}\right\rangle, \tag{133}$$

we see that,

$$\sum_{\alpha,\alpha',\alpha''} \left[\begin{matrix}\lambda\lambda'\lambda'' \\ \alpha\alpha'\alpha''\end{matrix}\right]_k \left|\begin{matrix}\lambda \\ \alpha\end{matrix}\right\rangle \left|\begin{matrix}\lambda' \\ \alpha'\end{matrix}\right\rangle \left|\begin{matrix}\lambda'' \\ \alpha''\end{matrix}\right\rangle \tag{134}$$

give all linearly independent invariant vectors in the direct product space of three IRs λ, λ', and λ''. This gives the generalization of the definition [Eq. (28)] of $3j$ symbols. Thus the number of linearly independent invariant vectors and hence the 3–G symbols, are given by the outer multiplicity of λ'' in the direct product of λ and λ'. For SU(2) there is just one.

We now consider the normalization of the 3–G symbols. The basis vectors of all three IRs in Eq. (119) are orthonormal. Therefore we get

$$\sum_{\alpha\alpha'} \left\langle\begin{matrix}\lambda\lambda' \\ \alpha\alpha'\end{matrix}\middle|\begin{matrix}\lambda'' \\ \alpha''\end{matrix}\right\rangle^k \left\langle\begin{matrix}\lambda\lambda' \\ \alpha\alpha'\end{matrix}\middle|\begin{matrix}\lambda''' \\ \alpha'''\end{matrix}\right\rangle^{k'} = \delta_{kk'}\delta_{\lambda''\lambda'''}\delta_{\alpha''\alpha'''} . \tag{135}$$

For 3–G symbols, this gives [see Eq. (132)]

$$\sum_{\alpha\alpha'} \left[\begin{matrix}\lambda\lambda'\lambda'' \\ \alpha\alpha'\alpha''\end{matrix}\right]_k \left[\begin{matrix}\lambda\lambda'\lambda''' \\ \alpha\alpha'\alpha'''\end{matrix}\right]^*_{k'} = \frac{1}{d_{\lambda''}} \delta_{kk'}\delta_{\lambda''\lambda'''}\delta_{\alpha''\alpha'''} . \tag{136}$$

VIII. INVARIANTS IN THE SPACE $S(M^1N^1)\otimes S(M^2N^2)\otimes S(M^3N^3)$

The next step in obtaining a formula for the Clebsch–Gordan coefficients is to construct the invariants [Eq. (134)] using our realization of the basis vectors. This corresponds to Eq. (30) in the case of SU(2). However, the computation for SU(3) is more complicated for the following reasons.

(1) The variables (z_1,z_2,θ,w_1,w_2) that we use do not transform linearly under SU(3) in contrast to the variables (z_1,z_2) of the SU(2) case (see the Appendix).
(2) We can form more than one invariant in contrast to the SU(2) case.

To analyze the situation we first ignore the constraint $\vec{w}\cdot\vec{z}=0$. Consider three vector spaces, $\mathscr{P}(M^1,N^1)$, $\mathscr{P}(M^2N^2)$, and $\mathscr{P}(M^3N^3)$ built of polynomials in variables $(\vec{z}^1,\vec{w}^1)$, $(\vec{z}^2,\vec{w}^2)$, and $(\vec{z}^3,\vec{w}^3)$, respectively. $\mathscr{P}(M^a,N^a)$, $a=1$, 2, or 3 is the space of polynomials homogeneous of degree M in (z_1,z_2,z_3) and of degree N in (w_1,w_2,w_3), respectively. Invariant theory can be applied[15,21,23] to this situation. The result is that any invariant can be constructed out of the basic invariants,

$$\vec{z}^1\cdot\vec{w}^1,\quad \vec{z}^1\cdot\vec{w}^2,\quad \vec{z}^1\cdot\vec{w}^3,$$

$$\vec{z}^2\cdot\vec{w}^1,\quad \vec{z}^2\cdot\vec{w}^2,\quad \vec{z}^2\cdot\vec{w}^3,$$

$$\vec{z}^3\cdot\vec{w}^1,\quad \vec{z}^3\cdot\vec{w}^2,\quad \vec{z}^3\cdot\vec{w}^3, \tag{137}$$

$$\vec{z}^1\cdot\vec{z}^2\times\vec{z}^3,\quad \vec{w}^1\cdot\vec{w}^2\times\vec{w}^3. \tag{138}$$

Further, these invariants are not all independent, because

$$(\vec{z}^1\cdot\vec{z}^2\times\vec{z}^3)(\vec{w}_1\cdot\vec{w}^2\times\vec{w}^3)$$
$$=\begin{vmatrix} z_1^1 & z_2^1 & z_3^1\\ z_1^2 & z_2^2 & z_3^2\\ z_1^3 & z_2^3 & z_3^3\end{vmatrix}\times\begin{vmatrix} w_1^1 & w_1^2 & w_1^3\\ w_2^1 & w_2^2 & w_2^3\\ w_3^1 & w_3^2 & w_3^3\end{vmatrix}=\begin{vmatrix} \vec{z}^1\cdot\vec{w}^1 & \vec{z}^1\cdot\vec{w}^2 & \vec{z}^1\cdot\vec{w}^3\\ \vec{z}^2\cdot\vec{w}^1 & \vec{z}^2\cdot\vec{w}^2 & \vec{z}^2\cdot\vec{w}^3\\ \vec{z}^3\cdot\vec{w}^1 & \vec{z}^3\cdot\vec{w}^2 & \vec{z}^3\cdot\vec{w}^3\end{vmatrix}. \tag{139}$$

Thus we may remove either $\vec{z}^1\cdot\vec{z}^2\times\vec{z}^3$ or $\vec{w}^1\cdot\vec{w}^2\times\vec{w}^3$ from the list of basic invariants Eq. (137) and (138). Any invariant is a function of the remaining ten invariants. To decide which of the two invariants [Eq. (139)] is to be kept, note that we are interested in polynomials in the three sets of six variables. Therefore, we permit only positive integral powers of *either* $\vec{z}^1\cdot\vec{z}^2\times\vec{z}^3$ or $\vec{w}^1\cdot\vec{w}^2\times\vec{w}^3$ in addition to those of Eq. (137). This gives all independent invariant polynomials. We will not be repeating polynomials which are identical on using Eq. (139). This is because if we were to replace $\vec{z}^1\cdot\vec{z}^2\times\vec{z}^2$ in a polynomial by $\vec{w}^1\cdot\vec{w}^2\times\vec{w}^3$ using Eq. (139), the latter would be appearing in the denominator. Therefore it would not coincide with any linear combination of the other polynomials we have considered.

Thus a general invariant polynomial is a linear combination of the following invariants:

$$\mathscr{P}(N(1,1),N(1,2),N(1,3),N(2,1),N(2,2),N(2,3),N(3,1),N(3,2),N(3,3),L)$$
$$=(z^1\cdot w^1)^{N(1,1)}(z^1\cdot w^2)^{N(1,2)}(z^1\cdot z^3)^{N(1,3)}(z^2\cdot z^1)^{N(2,1)}(z^2\cdot w^2)^{N(2,2)}(z^2\cdot w^3)^{N(2,3)}$$
$$\times(\vec{z}^3\cdot\vec{w}^1)^{N(3,1)}(\vec{z}^3\cdot\vec{w}^2)^{N(3,2)}(\vec{z}^3\cdot\vec{w}^3)^{N(3,3)}((\vec{z}^1\cdot\vec{z}^2\times\vec{z}^3)^L \text{ or } (\vec{w}^1\cdot\vec{w}^2\times\vec{w}^3)^{-L}). \tag{140}$$

We have adopted the following notation. If L is a positive (likewise negative) integer, the invariant has the term $(z^1 \cdot z^2 \times z^3)^L$ [likewise $(w^1 \cdot w^2 \times w^3)^{-L}$]. This way, both possibilities are labeled by a single integer L taking both positive and negative values. The other labels, $N(a,b), a,b=1, 2,$ or 3 freely range over all non-negative integers.

The invariants in the space $\mathscr{F}(M^1,N^1)\otimes\mathscr{F}(M^2,N^2)\otimes\mathscr{F}(M^3,N^3)$ have to be built from a linear combination of those invariants [Eq. (140)] for which

$$\begin{aligned} &\sum_{b=1}^{3} N(a,b)+L\,\epsilon(L)=M^a, \\ &\sum_{b=1}^{3} N(b,a)+|L|\,\epsilon(-L)=N^a, \quad a=1,2,3. \end{aligned} \tag{141}$$

Here,

$$\begin{aligned} &\epsilon(L)=1, \quad L\geqslant 0, \\ &\epsilon(L)=-1, \quad L<0. \end{aligned} \tag{142}$$

For three given IRs, this gives six equations for ten unknowns $N(a,b)$ and L. Therefore, there are many independent invariants, in general.

In order to obtain the 3-SU(3) symbols (Sec. VII) we have to expand these invariants in terms of a realization of the SU(3) basis vectors as polynomials in $\vec{z}^a$ and $\vec{w}^a$. The analogous procedure for SU(2), discussed in Sec. II, is very simple because we have a simple monomial basis. All that is needed there is to collect coefficients in the Taylor's expansion. However in the SU(3) case the basis is more complicated. In the realization using six complex variables used in earlier works,[15,21–23] the basis spans only a subspace of the space of all polynomials. As a result, one is not even assured that a general invariant satisfying Eq. (139) can be expanded in the basis vectors. That it be so expandable imposes restrictions on the coefficients of the linear combinations of the basic invariants [Eq. (140)]. In fact each of the three IRs imposes one restriction on the linear combination. This effectively reduces the number of independent linear combinations that may be chosen. Any freedom that is left corresponds to the repeating IRs in the decomposition. We may hope that requiring the invariant polynomial to be an eigenstate of the chiral Casimir[15,23,17] uniquely determines the invariant polynomial corresponding to each of the repeating IRs in the decomposition.

In this way the 3-SU(3) symbols can be extracted—in principle. However, extracting an explicit formula for the symbols this way has not been possible. The closest has been a formula with some undetermined coefficients.[23] We are able to overcome all these hurdles here for the following reasons. (i) our basis is simpler, (ii) the relevant invariants are completely determined, (iii) we use our auxiliary measure to calculate the expansion coefficients, and (iv) we use a generating function for the basis states and also for the invariants. This way calculations for all IRs are being done in one shot. Moreover, all calculations effectively reduce to Gaussian integrations.

We now describe why the relevant invariants are completely determined in our basis.

We are using the five-(complex)-dimensional subspace $\vec{w}\cdot\vec{z}=0$ in our basis. This constraint is invariant under SU(3). Therefore, invariants in the larger six-dimensional space are also invariants when restricted to our subspace. However all invariants with nonzero $N(1,1)$, $N(2,2)$, and $N(3,3)$ vanish identically because in our basis

$$\vec{w}^a\cdot\vec{z}^a=0, \quad a=1,2,3. \tag{143}$$

Thus the basic invariants are only

$$I(N(1,2),N(2,3),N(3,1),N(2,1),N(3,2),N(1,3),L)$$

$$= (\vec{z}^1 \cdot \vec{w}^2)^{N(1,2)} (\vec{z}^2 \cdot \vec{w}^3)^{N(2,3)} (\vec{z}^3 \cdot \vec{w}^1)^{N(3,1)} (\vec{z}^2 \cdot \vec{w}^1)^{N(2,1)} (\vec{z}^3 \cdot \vec{w}^2)^{N(3,2)} (\vec{z}^1 \cdot \vec{w}^3)^{N(1,3)}$$
$$\times [(\vec{z}^1 \cdot \vec{z}^2 \times \vec{z}^3)^L \quad \text{or} \quad (\vec{w}^1 \cdot \vec{w}^2 \times \vec{w}^3)^{-|L|}]. \tag{144}$$

We now simply have

$$N(1,2)+N(1,3)+L\epsilon(L)=M^1, \quad N(2,3)+N(2,1)+L\epsilon(L)=M^2,$$
$$N(3,1)+N(3,2)+L\epsilon(L)=M^3, \quad N(2,1)+N(3,1)+|L|\epsilon(-L)=N^1, \tag{45}$$
$$N(3,2)+N(1,2)+|L|\epsilon(-L)=N^2, \quad N(1,3)+N(2,3)+|L|\epsilon(-L)=N^3.$$

Thus we are led to the same equations for multiplicity as obtained in Ref. 25 from other considerations.

Note that Eq. (142) implies

$$3L=\sum_{a=1}^{3} (M^a-N^a). \tag{146}$$

Thus L is completely determined by the three IRs chosen and is not an independent parameter. It counts the number of invariants formed using $\det(\mathscr{U})=1$ condition. It may be called the ''chirality number'' of the invariant.

As a result, when we consider three given IRs λ^1, λ^2, and λ^3, we have just six non-negative integers $N(a,b)$, $a \neq b$, constrained by five linearly independent equations [Eq. (145)]. Therefore, there can be more than one solution for the set $N(a,b)$. This corresponds to the multiplicity problem in the decomposition of the Kronecker product.

It is possible, in principle, that there are more invariants in our subspace which do not have an invariant extension into the larger space of $\vec{z}^a$ and $\vec{w}^a$ variables. We now argue that there are no further invariants constructed out of our basis vectors from three IRs. In Sec. III, we obtained our basis vectors from basis vectors in the space of $\vec{z}$ and $\vec{w}$ variables by retaining those which are distinct in our subspace. Now a basis for *all invariants* in the larger space are catalogued by Eq. (140). Therefore, by simply imposing the constraints [Eq. (142)] and retaining nontrivial and distinct invariants, we get all invariants for our case.

In earlier approaches one was not assured that an arbitrary linear combination of the basic invariants [Eq. (140)] could be expanded in the basis vectors of the three IRs. We do not have such a problem now. This is because our basis vectors form all polynomials in four variables z_1, z_2, w_1, and w_2 and all (positive or negative integral) powers of z_3. Thus, even the basic invariants. [Eq. (140)] with constraints [Eq. (142)] can be expanded in our basis. This means the following. We may simply regard each of basic invariants [Eq. (140)] as the (unnormalized) linearly independent invariant vectors in the direct product space of three IRs. For a given basic invariant [Eq. (140)], the three IRs of which it is composed are given by Eq. (144)].

Thus the $3-\mathrm{SU}(3)$ symbols are naturally labeled by the set of integers,

(1) $N(1,2)$, $N(2,3)$, $N(3,1)$, $N(2,1)$, $N(3,2)$, $N(1,3)$, L.
(2) $P^a, Q^a, R^a, S^a, U^a, V^a$, $a=1,2,3$.

In place of (2) we may use the quark-model labels,

(3) $M^a, N^a, I^a, I_3^a, Y^a$, $a=1,2,3$.

These labels are related by the constraints. These constraints may be displayed as follows:

$$\left[\begin{array}{cccccccc} & N(1,2) & & N(1,3) & & N(2,3) & & N(2,1) \\ N^2 & & M^1 & & N^3 & & M^2 & \\ & & U^1,R^1 & & V^3,S^3 & & U^2,R^2 & \\ & & P^1 & & P^3 & & P^2 & \end{array}\right.$$

$$\left.\begin{array}{cccccc} & N(3,1) & & N(3,2) & & \\ N^1 & & M^3 & & N^2 & \\ & V^1,S^1 & & U^3,R^3 & & V^2,S^2 \\ & Q^1 & & Q^3 & & Q^2 \end{array}\right]_L . \tag{147}$$

This is the analog of the $3-j$ symbol of SU(2) prescribed as an array of nine integers, [Eq. (34)]. As in that case, this array is highly redundant. This notation is nevertheless useful, because the allowed values can be easily read off. For convenience, we will adopt the following notation for the $3-$SU(3) symbols:

$$\left[\begin{array}{ccccccc} N(1,2) & N(2,3) & N(3,1) & L & N(1,3) & N(3,2) & N(2,1) \\ & M^1N^1 & & M^2N^2 & & M^3N^3 & \\ & I'I_3'Y' & & I^2I_3^2Y^2 & & I^3I_3^3Y^3 & \end{array}\right]. \tag{148}$$

IX. A GENERATING FUNCTION FOR THE INVARIANTS

Though our basis has simplified many aspects, it is still not simple enough to allow the expansion coefficients to be read off from the invariants [Eq. (145)]. In order to compute these coefficients we will use our auxiliary inner product. We will also use generating functions [Eq. (53)] for the basis states and also a generating function for the invariants. This simplifies the computations drastically. Moreover we are doing computations for all IRs in one shot.

Define the generating function for the invariants,

$$\begin{aligned} &\mathscr{I}_{\pm}(j_{12},j_{23},j_{31},j_{21},j_{32},j_{13},j_{\pm}) \\ &= \exp(j_{12}\vec{z}^1\cdot\vec{w}^2 + j_{23}\vec{z}^2\cdot\vec{w}^3 + j_{31}\vec{z}^3\cdot\vec{w}^1 + j_{21}\vec{z}^2\cdot\vec{w}^1 + j_{32}\vec{z}^3\cdot\vec{w}^2 + j_{13}\vec{z}^1\cdot\vec{w}^3 \\ &\quad + (j_+\vec{z}^1\cdot\vec{z}^2\times\vec{z}^3 \ \text{ or } \ j_-\vec{w}^1\cdot\vec{w}^2\times\vec{w}^3). \end{aligned} \tag{149}$$

By a Taylor expansion in the sources j we generate all basic invariants [Eq. (145)]. Note that we use *either* j_+ *or* j_- because we do not need both $z^1\cdot z^2\times z^3$ and $w^1\cdot w^2\times w^3$ together.

The exponent in Eq. (149) is linear in each of the variables separately. This is an important feature which allows explicit computations.

We may write

$$\begin{aligned} \mathscr{I}_{\pm} = &\sum_{N(1,2)\ldots,|L|} j_{12}^{N(1,2)} j_{23}^{N(2,3)} j_{31}^{N(3,1)} j_{21}^{N(2,1)} j_{32}^{N(3,2)} j_{13}^{N(1,3)} (j_{\pm})^{|L|} \\ &\times |N(1,2),N(2,3),N(3,1),N(2,1),N(3,2),N(1,3),\pm|L|). \end{aligned} \tag{150}$$

The kets on the right-hand side of Eq. (150) are the unnormalized invariant vectors [Eq. (134)] in the direct product of three IRs. For the corresponding normalized invariant vectors, we have

$$
\begin{aligned}
&|N(1,2),N(2,3),N(3,1),N(2,1),N(3,2),N(1,3),\pm|L|\rangle \\
&\quad\equiv n^{-1/2}(N(1,2),N(2,3),N(3,1),N(2,1),N(3,2),N(1,3),\pm|L|) \\
&\qquad\times|N(1,2)\ldots,\pm|L|) \qquad (151)\\
&\quad=\sum_{\{P^a,Q^a,R^a,S^a,U^a,V^a\}}\begin{bmatrix} N(1,2) & N(2,3) & N(3,1) & L & N(1,3) & N(3,2) & N(2,1)\\ & M^1N^1 & & M^2N^2 & & M^3N^3 & \\ & I^1I_3^1Y^1 & & I^2I_3^2Y^2 & & I^3I_3^3Y^3 & \end{bmatrix} \\
&\qquad\times|P^1,Q^1,R^1,S^1,U^1,V^1\rangle|P^2,Q^2,R^2,S^2,U^2,V^2\rangle|P^3,Q^3,R^3,S^3,U^3,V^3\rangle,
\end{aligned}
$$

where n is the normalization factor. We have used our labeling [Eq. (55)] for the basis vectors. The variables on the right-hand side of Eq. (151) are related by Eqs. (49), (50), and (52) for each $a=1,2,3$.

Consider the auxiliary inner product of $\mathscr{T}_\pm$ with $\mathbf{g}^1\mathbf{g}^2\mathbf{g}^3$ which is the product of the partition functions for basis vectors of the three IRs. Using Eq. (55) and noting from Eqs. (81) and (88)

$$
\begin{aligned}
&(P,Q,R,S,U,V\|P',Q',R',S',U',V'\rangle \\
&\quad=N^{-1/2}(P,Q,R,S,U,V)M(P,Q,R,S,U,V)\delta_{PP'}\delta_{QQ'}\delta_{RR'}\delta_{SS'}\delta_{UU'}\delta_{VV'}, \qquad (152)
\end{aligned}
$$

we get

$$
\begin{aligned}
&\int_\pm\equiv(\mathbf{g}^1\mathbf{g}^2\mathbf{g}^3,\mathscr{T}_\pm) \\
&\quad=\sum\prod_{a=1}^{3}(\overline{p^a}^{P^a}\overline{q^a}^{Q^a}\overline{r^a}^{R^a}\overline{s^a}^{S^a}\overline{u^a}^{U^a}\overline{v^a}^{V^a}N^{-1/2}(P^a,Q^a,R^a,S^a,U^a,V^a) \\
&\qquad\times M(P^a,Q^a,R^a,S^a,U^a,V^a))j_{12}^{N(1,2)}j_{23}^{N(2,3)}j_{31}^{N(3,1)}j_{21}^{N(2,1)}j_{32}^{N(3,2)}j_{13}^{N(1,3)} \\
&\qquad\times(j_\pm)^{|L|}n^{+1/2}(N(1,2),N(2,3),N(3,1),N(2,1),N(3,2),N(1,3),\pm L) \\
&\qquad\times\begin{bmatrix} N(1,2) & N(2,3) & N(3,1) & L & N(1,3) & N(3,2) & N(2,1)\\ & M^1N^1 & & M^2N^2 & & M^3N^3 & \\ & I^1I_3^1Y^1 & & I^2I_3^2Y^2 & & I^3I_3^3Y^3 & \end{bmatrix}. \qquad (153)
\end{aligned}
$$

Thus the $3-\mathrm{SU}(3)$ symbols can be computed by calculating $(\mathbf{g}_1\mathbf{g}_2\mathbf{g}_3,\ \mathscr{T}_\pm)$ with respect to the auxiliary inner product. The normalization n in Eq. (153) has to be evaluated separately, using Eq. (136).

X. EVALUATION OF $\int_+$

We now evaluated $\int_+$. We have,

$$
\int_\pm=\int d\mu^1\int d\mu^2\int d\mu^3\ \ \mathbf{g}^1\mathbf{g}^2\mathbf{g}^3.\mathscr{T}_\pm. \qquad (154)
$$

Here,

$$\int d\mu^a = \int_0^{2\pi} \frac{d\theta^a}{2\pi} \int \frac{d^2z_1^a}{\pi} \int \frac{d^2z_2^a}{\pi} \int \frac{d^2w_1^a}{\pi} \int \frac{d^2w_2^a}{\pi} \exp(-\overline{z_1^a} z_1^a - \overline{z_2^a} z_2^a - \overline{w_1^a} w_1^a - \overline{w_2^a} w_2^a), \tag{155}$$

$$\overline{\mathbf{g}^a} = \exp(\overline{r_p^a z_1^a + r_q^a z_2^a + s_q^a w_1^a + s_p^a w_2^a + u^a e^{i\theta^a} - v^a e^{-i\theta^a}(z_1^a w_1^a + z_2^a w_2^a)}), \quad a = 1,2,3. \tag{156}$$

In Eq. (156), it is sufficient to use the ''mass shell'' values [Eq. (61)] for the sources. Further, in $\mathscr{I}_{\pm}$ [see Eq. (149)], we have

$$\vec{z}^1 \cdot \vec{w}^2 = z_1^1 w_1^2 + z_2^1 w_2^2 - \exp(i\theta^1 - i\theta^2)(z_1^2 w_1^2 + z_2^2 w_2^2), \text{ etc.} \tag{157}$$

Also,

$$\vec{z}^1 \cdot \vec{z}^2 \times \vec{z}^3 = e^{i\theta^1}(z_1^2 z_2^3 - z_1^3 z_2^2) + (\text{cyclic}). \tag{158}$$

Note that all exponents in $\int_+$ are bilinear in $z_{1,2}^a$ and $w_{1,2}^a$ variables. Therefore these integrations can be explicitly done. The only term that could have caused problems is $\vec{z}^1 \cdot \vec{z}^2 \times z^3$ [Eq. (158)], which is related to the multiplicity problem and is apparently cubic. However, since $z_3^a = e^{i\theta^a}$, $a = 1,2,3$, this term is also bilinear. On the other hand, $\vec{w}^1 \cdot \vec{w}^2 \times \vec{w}^3$ appearing in $\int_-$ is not bilinear after elimination of w_3^a. We will handle this problem in Sec. XII.

The form of $\int_+$ suggests the following operations. First, dependence on θ^a, $a = 1,2,3$, can be completely transferred to the sources. Make a change of variables,

$$\begin{aligned} z_1^a &\to e^{i\theta^a} z_1^a; \quad & z_2^a &\to e^{i\theta^a} z_2^a, \\ \overline{z_1^a} &\to e^{-i\theta^a} \overline{z_1^a}; \quad & \overline{z_2^a} &\to e^{-i\theta^a} \overline{z_2^a}, \\ w_1^a &\to e^{-i\theta^a} w_1^a; \quad & w_2^a &\to e^{-i\theta^a} w_2^a, \\ \overline{w_1^a} &\to e^{-i\theta^a} \overline{w_1^a}; \quad & \overline{w_2^a} &\to e^{-i\theta^a} \overline{w_2^a} \end{aligned} \tag{159}$$

and the measure [Eq. (155)], remains unchanged. On the other hand,

$$\begin{aligned} \mathbf{g}^a \to \exp(&\overline{(r_p^a e^{i\theta^a}) z_1^a + (r_q^a e^{i\theta^a}) z_2^a + (s_q^a e^{-i\theta^a}) w_1^a + (s_p^a e^{-i\theta^a}) w_2^a} \\ &+ \overline{(u^a c^{i\theta^a}) - (v^a e^{-i\theta^a})(z_1^a w_1^a + z_2^a w_2^a)}). \end{aligned} \tag{160}$$

Also,

$$j_{12} \vec{z}^1 \cdot \vec{w}^2 \to j_{12} e^{i\theta^1 - i\theta^2}(z_1^1 w_1^2 + z_2^1 w_2^2 - z_1^2 w_1^2 - z_2^2 w_2^2) \tag{161}$$

with similar changes for $j_{23} \vec{z}^2 \cdot \vec{w}^3$, $j_{21} \vec{z}^2 \cdot \vec{w}^1$, etc. Lastly,

$$j_+ \vec{z}^1 \cdot \vec{z}^2 \times \vec{z}^3 \to j_+ e^{i\theta^1 + i\theta^2 + i\theta^3}((z_1^2 z_2^3 - z_1^3 z_2^2) + (\text{cyclic})). \tag{162}$$

This change of variables makes integration over θ^a, $a = 1,2,3$ very easy. Indeed, these integrations only implement one additive conservation law for each of the three IRs, since

$$\int_0^{2\pi} \frac{d\theta}{2\pi} e^{in\theta} = \delta_{n,0}. \tag{163}$$

The three kinds of charges for various sources as can be read off from Eq. (160)–(162) are displayed in Table II. In effect, each of (z_1^a, z_2^a, z_3^a) is given Q^a charge $+1$ and each of (w_1^a, w_2^a, w_3^a) has $Q^a = -1$.

TABLE II. $\overline{p^a}$, $\overline{q^a}$, $a=1,2,3$ do not carry any of these charges.

$Q^1=+1$	$\overline{s^1}$	$\overline{v^1}$	j_{12}	j_{13}	j_+
$Q^1=-1$	$\overline{r^1}$	$\overline{u^1}$	j_{21}	j_{31}	
$Q^2=+1$	$\overline{s^2}$	$\overline{v^2}$	j_{23}	j_{21}	j_+
$Q^2=-1$	$\overline{r^2}$	$\overline{u^2}$	j_{32}	j_{12}	
$Q^3=+1$	$\overline{s^3}$	$\overline{v^3}$	j_{31}	j_{32}	j_+
$Q^3=-1$	$\overline{r^3}$	$\overline{u^3}$	j_{13}	j_{23}	

The sources have the corresponding compensating charges. As a consequence, it is not necessary to explicitly do θ^a integrations. We may simply ignore the dependencies on θ^a. After integration over z^a and w^a variables, we only keep polynomial in sources each term of which is neutral with respect to Q^1, Q^2 and Q^3 charges.

From Table II and our definitions of quantum numbers, powers of the sources in the polynomials have to satisfy

$$\sum_{b\neq a} N(a,b)+L-\sum_{b\neq a} N(b,a)=R^a+U^a-S^a-V^a, \quad a=1,2,3. \tag{164}$$

From Eqs. (49) and (145), we notice that both sides of Eq. (164), are M^a-N^a. (see Table II.) Thus the θ integration is only implementing equality of M^a-N^a as calculated using the invariants [Eq. (145)] and the states [Eq. (49)]. However, we know that M and N evaluated in these two ways should each be separately equal. This stronger equality should be a consequence of integration over the z and w variables.

We now consider the integrations over the z and w variables. It is convenient to employ the following matrix notation:

$$Z_1=\begin{pmatrix} z_1^1 \\ z_1^2 \\ z_1^3 \end{pmatrix}, \quad \overline{Z_1}=\begin{pmatrix} \overline{z_1^1} \\ \overline{z_1^2} \\ \overline{z_1^3} \end{pmatrix}, \quad \overline{R_p}=\begin{pmatrix} \overline{r_p^1} \\ \overline{r_p^2} \\ \overline{r_p^3} \end{pmatrix} \tag{165}$$

with similar notations for $Z_2,\overline{Z_2},W_1,\overline{W_1},W_2,\overline{W_2},\overline{R_q},\overline{S_p},\overline{S_q}$. Further, define,

$$\overline{V}=\begin{pmatrix} \overline{v^1} & 0 & 0 \\ 0 & \overline{v^2} & 0 \\ 0 & 0 & \overline{v^3} \end{pmatrix}, \tag{166}$$

$$J=\begin{pmatrix} +j_{31}+j_{21} & -j_{12} & -j_{13} \\ -j_{21} & +j_{12}+j_{32} & -j_{23} \\ -j_{31} & -j_{32} & +j_{23}+j_{13} \end{pmatrix}, \tag{167}$$

$$A=\begin{pmatrix} 0 & 1 & -1 \\ -1 & 0 & 1 \\ 1 & -1 & 0 \end{pmatrix}. \tag{168}$$

In terms of these objects the integral we need is

$$\int \frac{d^2Z_1 d^2Z_2}{\pi^3\pi^3}\frac{d^2W_1 d^2W_2}{\pi^3\pi^3}\exp\Big(-\overline{Z}_1^T Z_1-\overline{Z}_2^T Z_2-\overline{W}_1^T W_1-\overline{W}_2^T W_2+\overline{Z}_1^T\overline{R_p}+\overline{Z}_2^T\overline{R_q}$$

$$+\overline{W}_1^T\overline{S_q}+\overline{W}_2^T\overline{S_p}-\overline{Z}_1^T\overline{VW_1}-\overline{Z}_2^T\overline{VW_2}-Z_1^T JW_1-Z_2^T JW_2+j_+Z_1^T AZ_2+\sum_{a=1}^{3}\overline{u^a}\Big), \tag{169}$$

where

$$\int \frac{d^2Z_1}{\pi^3}=\int\frac{d^2z_1^1}{\pi}\int\frac{d^2z_1^2}{\pi}\int\frac{d^2z_1^3}{\pi}, \tag{170}$$

etc. We now use Eq. (72) in the following order. Integrate over W_1 and W_2. We get,

$$\int \frac{d^2Z_1 d^2Z_2}{\pi^3\pi^3}\exp\Big(-\overline{Z}_1^T Z_1-\overline{Z}_2^T Z_2+\overline{Z}_1^T\overline{R_p}+\overline{Z}_2^T\overline{R_q}+Z_1^T J\overline{VZ_1}+Z_2^T J\overline{VZ_2}$$

$$-Z_1^T J\overline{S_q}-Z_2^T J\overline{S_p}+j_+Z_1^T AZ_2+\sum_{a=1}^{3}\overline{u^a}\Big). \tag{171}$$

Now integrating over Z_2, we get

$$\int \frac{d^2Z_1}{\pi^3}\det(1-\overline{VJ}^T)^{-1}\exp\Big(-\overline{Z}_1^T(1-\overline{VJ}^T)Z_1+\overline{Z}_1^T\overline{R_p}-\overline{S}_q^T J^T Z_1$$

$$-\overline{S}_p^T J^T(1-\overline{VJ}^T)^{-1}\overline{R_q}+j_+Z_1^T A(1-\overline{VJ}^T)^{-1}\overline{R_q}+\sum_{a=1}^{a}\overline{u^a}\Big). \tag{172}$$

Final integration over Z_1 gives

$$\det(1-\overline{VJ}^T)^{-2}\exp\Big(-\overline{S}_q^T J^T(1-\overline{VJ}^T)^{-1}\overline{R_p}-\overline{S}_p^T J^T(1-\overline{VJ}^T)^{-1}\overline{R_q}$$

$$+j_+\overline{R}_q^T(1-\overline{VJ}^T)^{T^{-1}}A^T(1-\overline{VJ}^T)^{-1}\overline{R_p}+\sum_{a=1}^{a}\overline{u^a}\Big). \tag{173}$$

We rewrite this as

$$\exp\Big(-\overline{R}_p^T BJ\overline{S_q}-\overline{R}_q^T BJ\overline{S_p}+j_+\overline{R}_p^T BAB^T\overline{R_q}+2\mathrm{tr}(\ln B)+\sum_{a=1}^{a}\overline{u^a}\Big), \tag{174}$$

where

$$B=(1-J\overline{V})^{-1}=\sum_{n=0}^{\infty}\frac{(J\overline{V})^n}{n!}. \tag{175}$$

XI. ALGEBRAIC FORMULA FOR 3-SU(3) COEFFICIENTS WHEN $L\geqslant 0$

To get 3-SU(3) symbols for a given set of three IRs, we have to expand Eq. (174) in powers of the various sources. On mass shell we have

$$-\overline{R_p^T}BJ\overline{S_q}-\overline{R_q^T}BJ\overline{S_p}=(\overline{r^1}(BJ)_{12}\overline{s^2}-\overline{r^2}(BJ)_{21}\overline{s^1})(\overline{p^1q^2}-\overline{q^1p^2})+\text{cyclic}. \tag{176}$$

Notice that we always have combinations such as $(\overline{p^1q^2}-\overline{q^1p^2})$ which are invariant under the (isospin) SU(2) transformations of the sources. This is to be expected because our measure is manifestly invariant under this subgroup. Note also that the diagonal terms of the matrix (BJ) do not appear on the right-hand side (this is because of the negative sign in $\overline{s_q^a}=-\overline{s^aq^a}$, $a=1,2,3$, etc.) This is again required by SU(2) invariance. With such diagonal terms we would get terms like $\overline{p^aq^a}$ which are not SU(2) invariant. We also have

$$\overline{R_p^T}BAB^T\overline{R_q}=\overline{r^1r^2}(\overline{p^1q^2}-\overline{q^1p^2})(BAB^T)_{12}+\text{cyclic}. \tag{177}$$

Again we get SU(2) invariant combinations. The reason now is the antisymmetry of the matrix A and hence of BAB^T.

Explicitly inverting the 3×3 matrix $(1-J\overline{V})$, we obtain quite simple expressions for the relevant matrix elements:

$$\begin{aligned}(BJ)_{12}&=\|B\|(-j_{12}+j_{12}(j_{23}+j_{13})\overline{v^3}+j_{13}\overline{v^3}j_{32}),\\ (BJ)_{21}&=\|B\|(-j_{21}+j_{21}(j_{23}+j_{13})\overline{v^3}+j_{23}\overline{v^3}j_{31})\end{aligned} \tag{178}$$

and corresponding cyclic expressions. Here,

$$\|B^{-1}\|=\det(1-J\overline{V})=1-((j_{31}+j_{21})\overline{v^1}+\text{cyclic})+((j_{31}j_{12}+j_{31}j_{32}+j_{21}j_{32})\overline{v^1}\overline{v^2}+\text{cyclic}). \tag{179}$$

Also notice that,

$$A_{ij}=\epsilon_{ijk}c_k, \tag{180}$$

where

$$\overline{c}=(c_k)=(1,1,1). \tag{181}$$

Therefore,

$$(BAB^T)_{il}=B_{ij}\epsilon_{jkm}c_mB_{lk}=\|B\|\epsilon_{iln}c_m(B^{-1})_{mn}. \tag{182}$$

Now,

$$c_m(B^{-1})_{mn}=\sum_{m=1}^{3}(1-J\overline{V})_{mn}=1 \quad \text{for each } n. \tag{183}$$

Thus,

$$(BAB^T)_{12}=(BAB^T)_{23}=(BAB^T)_{31}=\|B\|. \tag{184}$$

Now we have an explicit expression for $\int_+$:

$$\begin{aligned}\int_+ \sim\|B\|^2\ \exp[\|B\|\{&(\overline{u^1}+j_+\overline{r^1}\overline{r^2}-\overline{r^1}j_{12}\overline{s^2}+\overline{r^2}j_{21}\overline{s^1}+\overline{r^1}j_{12}\overline{s^2}(j_{23}+j_{13})\overline{v^3}\\ &-\overline{r^2}j_{21}\overline{s^1}(j_{23}+j_{13})\overline{v^3}+\overline{r^1}j_{13}\overline{v^3}j_{32}\overline{s^2}-\overline{r^2}j_{23}\overline{v^3}j_{31}\overline{s^1})(\overline{p^1q^2}-\overline{p^2q^1})+(\text{cyclic})\}],\end{aligned} \tag{185}$$

where $\sim$ means that we are supposed to keep only terms consistent with the conservation laws [Eq. (164)].

This form implies another conservation law. Note that j_{21} and j_{31} always appear with the $\overline{s^1}$ or $\overline{v^1}$. Therefore,

$$N(2,1)+N(3,1)=S^1+V^1, \tag{186}$$

which we expect because both sides equal N^1. We have similar equations for N^2 and N^3 also. Taken with Eq. (164), which are a consequence of θ^a, $a=1,2,3$ integrations, we get separate conservations of M^a and N^a $a=1,2,3$ as computed from the states and from the invariants.

We now change the right-hand side of Eq. (185) to a form which automatically gives the conservation law:

$$N(1,2)+N(1,3)+L=R^1+U^1 \tag{187}$$

and corresponding cyclic expressions. For this we remove $\exp(\Sigma_{a=1}^3 \overline{u^a})$ and insert $\overline{u^1},\overline{u^2},\overline{u^3}$ factors suitably in the other terms of the exponent and in $\|B\|$:

$$\begin{aligned}\int_+ \rightarrow \|\widetilde{B}\|^2 \exp[\|\widetilde{B}\|\{&((j_+\overline{r^1r^2u^3}-\overline{r^1}j_{12}\overline{s^2}+\overline{r^2}j_{21}\overline{s^1}+\overline{r^1}j_{12}\overline{s^2})(\overline{u^2}j_{23}\overline{v^3}+\overline{u^1}j_{13}\overline{v^3})\\ &-\overline{r^2}j_{21}\overline{s^1}(\overline{u^2}j_{23}\overline{v^3}+\overline{u^1}j_{13}\overline{v^3})+\overline{r^1}j_{13}\overline{v^3}\overline{u^3}j_{32}\overline{s^2}\\ &-\overline{r^2}j_{23}\overline{v^3}\overline{u^3}j_{31}\overline{s^1})(\overline{p^1q^2}-\overline{p^2q^1})\ +(\text{cyclic})\},\end{aligned} \tag{188}$$

where

$$\begin{aligned}\|\widetilde{B}\|=1-(&\overline{u^3}j_{31}\overline{v^1}+\overline{u^2}j_{21}\overline{v^1}+(\text{cyclic}))+(\overline{u^3}j_{31}\overline{v^1}\overline{u^1}j_{12}\overline{v^2}\\ &+\overline{u^3}j_{31}\overline{v^1}\overline{u^3}j_{32}\overline{v^2}+\overline{u^2}j_{21}\overline{v^1}\overline{u^3}j_{32}\overline{v^2}+(\text{cyclic})).\end{aligned} \tag{189}$$

Now j_{12} and j_{13} always appears with $\overline{r^1}$ or $\overline{u^1}$ except in the terms $\overline{r^1r^2u^3}+(\text{cyclic})$. The effect of these last terms is to provide monomials where the powers R^a+U^a, $a=1,2,3$ are equal. The net effect is to imply Eq. (187) and corresponding cyclic expressions where L is given by the sum of the powers of $\overline{r^1r^2u^3}$, $\overline{r^2r^3u^1}$ and $\overline{r^3r^1u^2}$. Thus the right-hand side of Eq. (188) automatically takes care of conservations laws, Eqs. (186) and (187) and corresponding cyclic expressions. It also gives $\int_+$ exactly except for the additional factor

$$\frac{1}{U^1!U^2!U^3!} \tag{190}$$

(coming from $\exp(\overline{u^1}+\overline{u^2}+\overline{u^3})$) to be associated with $(\overline{u^a})^{U^a}$, $a=1,2,3$.

We have to now expand the right-hand side of Eq. (188) in powers of the various monomials in the exponent and determinant. This is exactly analogous to the SU(2) case [Eq. (33)]. As in that case, we have to collect all the terms contributing to the monomial. For this we have first to adopt a notation for the powers of the monomials. This is presented in Table III.

We have deliberately adopted this notation for the powers because, the arguments in the symbols uniquely characterize the term being considered. Thus for example $l(123)$ is associated with $(j_+)(\overline{p^1r^1})(\overline{q^2r^2})(\overline{u^3})$. We have such variables associated with every permutation of (123) arising from the term $j_+\overline{r^1r^2u^3}(\overline{p^1q^2}-\overline{p^2q^1})+\text{cyclic}$ in the exponent in Eq. (188). In Table IV, we catalogue all allowed arguments in our variables of Table III. The advantage of our notation is

TABLE III. Definition of the variables $l(\cdots)$, ... , $g(\cdots)$.

Monomial	$j_+\overline{p^1q^2r^1r^2u^3}$	$\overline{p^2q^1r^1r^2u^3}$	$\overline{p^1q^2r^1}j_{12}\overline{s^2}$	$\overline{p^2q^1r^1}j_{12}\overline{s^2}$
Order used in label	$\overline{p^1q^2u^3}$	$\overline{p^2q^1u^3}$	$\overline{p^1q^2r^1s^2}$	$\overline{p^2q^1r^1s^2}$
Power	$l(123)$	$l(213)$	$k(1212)$	$k(2112)$

$\overline{p^1q^2r^2}j_{21}\overline{s^1}$	$\overline{p^1q^2r^1}j_{12}\overline{s^2u^2}j_{23}\overline{v^3}$	$\overline{p^1q^2r^1}j_{12}\overline{s^2u^1}j_{13}\overline{v^3}$	$\overline{p^1q^2r^1}j_{13}\overline{v^3u^3}j_{32}\overline{s^2}$
$\overline{p^1q^2r^2s^1}$	$\overline{p^1q^2r^1s^2u^2v^3}$	$\overline{p^1q^2r^1s^2u^1v^3}$	$\overline{p^1q^2r^1s^2u^3v^3}$
$k(1221)$	$m(121223)$	$m(121213)$	$n(12123)$

$\overline{u^3}j_{31}\overline{v^1}$	$\overline{u^2}j_{21}\overline{v^1}$	$\overline{u^3}j_{31}\overline{v^1u^1}j_{12}\overline{v^2}$	$\overline{u^2}j_{21}\overline{v^1u^1}j_{32}\overline{v^2}$	$\overline{u^3}j_{31}\overline{v^1u^3}j_{32}\overline{v^2}$
$\overline{u^3v^1}$	$\overline{u^2v^1}$	$\overline{u^3v^1u^1v^2}$	$\overline{u^3v^2u^2v^1}$	$\overline{u^3u^3v^2v^1}$
$e(31)$	$e(21)$	$f(3112)$	$f(3221)$	$g(321)$

that we can easily trace the terms that involve a given source j_{12}, $\overline{p^1}$, etc. Thus for example, we can write the conservation laws in a compact form as below. By collecting the powers of each source, we get

$$P^\alpha=\sum\ (l(\alpha--)+k(\alpha---)+m(\alpha------)+n(\alpha------));$$

$$Q^\alpha=\sum\ (l(-\alpha-)+k(-\alpha--)+m(-\alpha----)+n(-\alpha----));$$

$$R^\alpha=\sum\ (l(\alpha--)+l(-\alpha-)+k(--\alpha-)+m(--\alpha---)+n(--\alpha---));$$

$$S^\alpha=\sum\ (k(---\alpha)+m(---\alpha--)+n(---\alpha--));$$

TABLE IV. Permitted arguments of $l(\cdots)$, ... , $g(\cdots)$.

$\alpha,\beta,\gamma\cdots=1$, 2, or 3	
$l(\alpha\beta\gamma)$	$(\alpha\beta\gamma)$ is a permutation of (123)
$k(\alpha\beta\gamma\delta)$	$(\alpha\beta)$ is same or transpose of $(\gamma\delta)$
$m(\alpha\beta\gamma\delta\epsilon\phi)$	$(\gamma\delta\phi)$ is a permutation of (123); $(\alpha\beta)$ is same or transpose of $(\gamma\delta)$; ϕ is either γ or δ.
$n(\alpha\beta\gamma\delta\epsilon)$	$(\gamma\delta\epsilon)$ is a permutation of (123); $(\alpha\beta)$ is same or transpose of $(\gamma\delta)$.
$e(\alpha\beta)$: $\alpha\neq\beta$.	
$f(\alpha\beta\gamma\delta)$	$\beta=\gamma$ and $(\alpha\beta\delta)$ is a permutation of (123):
$g(\alpha\beta\gamma)$	$(\alpha\beta\gamma)$ only even permutation of (123)

$$U^\alpha=\sum\ (l(--\alpha)+m(----\alpha-)+n(-----\alpha-))+e(\alpha-)$$
$$+f(\alpha---)+f(--\alpha-)+2g(\alpha\beta\gamma));$$

$$V^\alpha=\sum\ (m(------\alpha)+n(-------\alpha))+e(-\alpha)+f(-\alpha--)$$
$$+f(---\alpha)+g(-\alpha-)+g(--\alpha));$$

$$L=\sum\ l(---);$$

$$N(\alpha,\beta)=\sum\ (k(--\alpha\beta)+m(--\alpha\beta--))+m(----\alpha\beta)+n(--\alpha\beta--)$$
$$+n(---\alpha\beta)+e(\alpha\beta)+f(\alpha\beta--)+f(--\alpha\beta)+g(\alpha\beta-)+g(\alpha-\beta));$$
(191)

Here we have used the following notation: Σ stands for summation over all allowed arguments in the blank spaces.

Note that Eqs. (190) and (191) express the non-negative integers, $P^\alpha,\ldots,V^\alpha$, $N(\alpha,\beta)$, and L, α, β=1,2, or 3 in terms of yet other non-negative integers of Table III. It is easy to see that the constraint $P^\alpha+Q^\alpha=R^\alpha+S^\alpha$ for the labels of each IR α=1,2, or 3 is satisfied. Also the constraints [Eqs. (186) and (187)] are satisfied as is seen from the positions of the labels and Table III.

We may read off various conservation laws in the 3-SU(3) symbols from Eq. (191):

$$\sum_{\alpha=1}^{3} P^\alpha=\sum_{\alpha=1}^{3} Q^\alpha.$$ (192)

This is valid because we are summing over all positions of α in the labels. This is simply a statement of the conservation of I_3.

Similarly,

$$\sum_{\alpha=1}^{3} U^\alpha=\sum_{\alpha=1}^{3} V^\alpha+L.$$ (193)

This implies conservation of hypercharge as seen by rewriting it as

$$\sum_{\alpha=1}^{3}\left(\frac{1}{3}(M^\alpha-N^\alpha)+V^\alpha-U^\alpha\right)=0.$$ (194)

When we expand the exponent in powers of each monomial, we collect a factor

$$\|\widetilde{B}\|^{1+h}$$ (195)

in Eq. (188). Here

$$-1+h=\sum\ (l()+k()+m()+n()).$$ (196)

Alternately, note that the number of $\|\tilde{B}\|$ factors is the sum of the number of s^α variables ($\alpha=1,2,3$) and the power of j_+, i.e.,

$$-1+h=L+S^1+S^2+S^3. \tag{197}$$

We may now apply the formula

$$\left(1-\sum_{k=1}^{K} x_k\right)^{-1-h}=\sum_{n_1,n_2=0}^{\infty} \frac{(h+\Sigma n_k)!}{h!\Pi_k(n_k!)}\prod_{k=1}^{K} x_k^{n_k} \tag{198}$$

to calculate coefficients of various monomials in Eq. (195) where $\|\tilde{B}\|$ is as in Eq. (188). This gives the coefficient of the monomials in the expansion of the RHS of Eq. (188) to be

$$\frac{1+\Sigma(l()+k()+m()+n()+e()+f()+g())!}{(1+\Sigma(l()+k()+m()+n()))!\Pi(l()!(k()!(m()!(n()!(e()!(f()!(g()!}$$
$$\times\exp[i\pi\Sigma_s(k()+n())+\Sigma_A m()+\Sigma(f()+g())]. \tag{199}$$

Here Σ and Π are over all possible arguments of the variables indicated. Σ_S (respectively Σ_A) correspond to summations over only those arguments ($\alpha\beta\gamma\delta\cdots$) such that $\alpha\beta$ is same as (respectively transposes of) $\gamma\delta$.

In order to get the coefficient of the monomial in $\int_+$, we have to multiply Eq. (199) by the factor Eq. (190). We may now extract the 3-SU(3) symbol from Eq. (153), by supplying factors of $N^{1/2}$ and M^{-1} as required. We get the 3-SU(3) symbol for $L\geqslant 0$,

$$\begin{bmatrix} N(1,2) & N(2,3) & N(3,1) & L & N(1,3) & N(3,2) & N(2,1) \\ & M^1N^1 & & M^2N^2 & & M^3N^3 & \\ & I^1I_3^1Y^1 & & I^2I_3^2Y^2 & & I^3I_3^3Y^3 & \end{bmatrix}$$
$$=n^{-1/2}(N(1,2),N(2,3),N(3,1),N(2,1),N(3,2),N(1,3),L)$$
$$\times\left[\prod_{\alpha=1}^{3}\frac{P^\alpha!Q^\alpha!R^\alpha!S^\alpha!U^\alpha!V^\alpha!(U^\alpha+2I^\alpha+1)!(2I^\alpha+1)}{(V^\alpha+2I^\alpha+1)!}\right]^{1/2}$$
$$\times\sum_{e,f,g,k,l,m,n}\frac{(1+\Sigma(e()+f()+g()+k()+l()+m()+n()))!}{(1+\Sigma(k()+l()+m()+n()))!\Pi(l()!\ldots n())!}$$
$$\times\exp[i\pi\Sigma_S(k()+n())+\Sigma_A m()+\Sigma(f()+g())]. \tag{200}$$

This is the exact analog of Eq. (33) of SU(2). The Clebsch–Gordan coefficients are presented as a sum over non-negative integers which satisfy conditions Eq. (191). (See Tables III and IV.)

XII. DISCUSSION

In our calculations for SU(3) we have ignored the questions involving the choice of phases until now. We will now make a careful analysis. With our definition [Eq. (55)] of the unnormalized basis vectors, note that the $\mathfrak{Z}^*$ is represented by $(-w_1,w_2,w_3)$ up to a normalization constant. Our computations of the relative normalization, Eqs. (109) and (110) fix only the magnitude of the normalizations. The phases may be chosen arbitrarily as discussed in Sec. II for the SU(2) case. Under a change of phases,

$$|E\rangle\rightarrow\exp(i\theta_E)|E\rangle, \tag{201}$$

the representation matrix changes as

$$(D(g))_{EE'} \to e^{i\theta_E}(D(g))_{EE'}e^{-i\theta_{E'}} \tag{202}$$

and remains unitary.

However one may want to make a choice of phases to rid the formulas of phases and relative signs if possible. For instance, we may choose the phase to have $\underline{3}^*$ be represented by $1/\sqrt{2}(w_1, w_2, w_3)$.

Fortunately our basis vectors [Eqs. (53)–(55)] have real coefficients even though they are represented by polynomials in complex variables. Similarly, our invariants [Eq. (140)] have real coefficients. Thus we are assured that the 3-SU(3) symbols are real as is checked in Eq. (200).

We now address the ambiguity in the phase of the Clebsch–Gordan coefficients. In the definition of Eq. (119), various coupled basis vectors $|\lambda''\alpha''>^k$, are required to transform as an IR(λ''). This fixes phases of all 3-SU(3) symbols except for an overall phase for each λ'' and k.

In previous sections we calculated 3-SU(3) symbols only for the $L \geqslant 0$ case. With our choice of regarding w_3 as a dependent variable, the relevant integrations could be explicitly computed in this case. We now show the 3-SU(3) symbols can be obtained for $L<0$ also.

In constructing the basis vectors, we could have as well chosen to eliminate z_3 instead of w_3. We could have done all computations with this basis. In this case, the integrations for 3-SU(3) symbols can be done explicitly for $L<0$ instead of $L>0$.

This is related to the invariance of the 3-SU(3) symbols under conjugation of the IRs involved. (It is possible that the invariance is only up to an additional phase factor as may happen if the phases of the basis states are not chosen carefully.) In our formalism this invariance may be seen as follows. Consider an expansion of an invariant [Eq. (140)] with $L \geqslant 0$ as a linear combination of the basis vectors of Eqs. (53)–(55). Now consider an interchange $\vec{z} \leftrightarrow \vec{w}$ in this expansion. The effect on the invariant is to change it to another invariant with

$$N(\alpha, \beta) \to N(\beta, \alpha), L \to -L. \tag{203}$$

This means

$$M^a \leftrightarrow N^a, \quad a = 1,2,3. \tag{204}$$

The effect of $\vec{z} \leftrightarrow \vec{w}$ on the generating functions [Eq. (53)] is equivalent to the following changes:

$$p^a \to -q^a, \quad q^a \to p^a, \quad r^a \to s^a, \quad s^a \to -r^a, \quad u^a \to v^a, \quad v^a \to u^a. \tag{205}$$

Thus the effect on the unnormalized basis states [Eq. (55)] is

$$|PQRSUV) \to (-1)^{Q+R}|QPSRVU). \tag{206}$$

In the usual notation,

$$M^a \leftrightarrow N^a, \quad I^a \to I^a, \quad I_3^a \to -I_3^a, \quad Y^a \to -Y^a \tag{207}$$

and in addition an additional phase factor $(-1)^{Q+R}$ is picked up.

In Eq. (188), note that the isospin dependence is always contained in the SU(2) invariant combination of sources, $(\overline{p^1 q^2} - \overline{p^2 q^1})$, etc. As a consequence, it is possible to extract isoscalar factors also.[3] However, we will not pursue this here. Equation (188) can be used, in principle, to extract Regge symmetries[62] of SU(3) Clebsch–Gordan coefficients. We do not attempt this here.

XIII. SUMMARY OF RESULTS

For easy accessibility we summarize our results in a self-contained way here.

(i) Labels for the basic vectors. Normalized basis vectors are denoted by $|M,N;P,Q,R,S,U,V\rangle$. All labels are non-negative integers. All IRs are uniquely labeled by (M,N). For a given IR (M,N), labels (P,Q,R,S,U,V) take all non-negative integral values subject to the constraints:

$$R+U=M, \quad S+V=N, \quad P+Q=R+S.$$

The allowed values can be read off easily: R takes all values from 0 to M, and S from 0 to N. For a given R and S, Q takes all values from 0 to $R+S$.

(ii) Explicit realization of the basis states. Consider the coefficient of the monomial

$$p^P q^Q r^R s^S u^U v^V$$

in

$$\exp(r(pz_1+qz_2)+s(pw_2-qw_1)+uz_3+vw_3).$$

Divide it by the normalization,

$$\left[\frac{(U+2I+1)!(V+2I+1)!}{P!Q!R!S!U!V!(2I+1)}\right]^{1/2}.$$

This then provides an explicit realization of the normalized basis state $|PQRSUV\rangle$.

(iii) Generating function for the invariants. All Clebsch–Gordan coefficients can be extracted from the following generating function of the invariants:

$$\mathcal{J}_{\pm}(j_{12},j_{23},j_{31},j_{21},j_{32},j_{13},j_{\pm}) = \exp(j_{12}\vec{z}^1\cdot\vec{w}^2+j_{23}\vec{z}^2\cdot\vec{w}^3+j_{31}\vec{z}^3\cdot\vec{w}^1+j_{21}\vec{z}^2\cdot\vec{w}^1+j_{32}\vec{z}^3\cdot\vec{w}^2 + j_{13}\vec{z}^1\cdot\vec{w}^3+(j_+\vec{z}^1\cdot\vec{z}^2\times\vec{z}^3 \text{ or } j_-\vec{w}^1\cdot\vec{w}^2\times\vec{w}^3)).$$

(iv) Multiplicity labels for the Clebsch–Gordan series. For three given IRs, $(M',N'),(M'',N''),(M''',N''')$, construct all solutions of

$$N(1,2)+N(1,3)+L\epsilon(L)=M^1, \quad N(2,3)+N(2,1)+L\epsilon(L)=M^2,$$

$$N(3,1)+N(3,2)+L\epsilon(L)=M^3, \quad N(2,1)+N(3,1)+|L|\epsilon(-L)=N^1,$$

$$N(3,2)+N(1,2)+|L|\epsilon(-L)=N^2, \quad N(1,3)+N(2,3)+|L|\epsilon(-L)=N^3,$$

$$3L=\sum_{a=1}^{3}(M^a-N^a),$$

where $N(a,b)$, $a\neq b$ are non-negative integers. They provide unambiguous labels for the Clebsch–Gordan series as follows.

For given two IRs (M,N) and (M',N'), construct all (M'',N'') for which $N(a,b)$, $a\neq b$ have non-negative integer solutions. Then the reversed pair (N'',M'') gives all IRs in the Clebsch–Gordan series. Multiplicity of solutions for one (M'',N'') provides the multiplicity of repeating IRs. Therefore $N(a,b)$ unambiguously provide the multiplicity labels.

(v) 3−SU(3) symbol. The $3-G$ symbols are related to the Clebsch–Gordan coefficients as in Eq. (132), and have more explicit symmetry than the latter. The 3−SU(3) symbol is represented by,

$$\begin{bmatrix} N(1,2) & N(1,3) & N(2,3) & N(2,1) & N(3,1) & N(3,2) & \\ N^2 & M^1 & N^3 & M^2 & N^1 & M^3 & N^2 \\ & U^1,R^1 & V^3,S^3 & U^2,R^2 & V^1,S^1 & U^3,R^3 & V^2,S^2 \\ & P^1 & P^3 & P^2 & Q^1 & Q^3 & Q^2 \end{bmatrix}_L .$$

Here the top row specifies the multiplicity labels: the second and third rows specify the usual complete set of labels for the basis states of the three IRs.

(vi) Generating function for the 3−SU(3) symbol for $L>0$. Extract coefficient of the monomial

$$j_{12}^{N(1,2)} j_{21}^{N(2,1)} j_{13}^{N(1,3)} j_{31}^{N(3,1)} j_{23}^{N(2,3)} j_{32}^{N(3,2)} j_{+}^{L} \prod_{\alpha=1}^{3} \overline{p}^{\alpha P^\alpha} \overline{q}^{\alpha Q^\alpha} \overline{r}^{\alpha R^\alpha} \overline{s}^{\alpha S^\alpha} \overline{u}^{\alpha U^\alpha} \overline{v}^{\alpha V^\alpha}$$

in

$$\int_{+} \to \|\tilde{B}\|^2 \exp[\|\tilde{B}\|((j_{+}\overline{r}^{1}\overline{r}^{2}\overline{u}^{3} - \overline{r}^{1} j_{12} \overline{s}^{2} + \overline{r}^{2} j_{21} \overline{s}^{1} + \overline{r}^{1} j_{12} \overline{s}^{2}(\overline{u}^{2} j_{23} \overline{v}^{3} + \overline{u}^{1} j_{13} \overline{v}^{3})$$
$$- \overline{r}^{2} j_{21} \overline{s}^{1}(\overline{u}^{2} j_{23} \overline{v}^{3} + \overline{u}^{1} j_{13} \overline{v}^{3}) + \overline{r}^{1} j_{13} \overline{v}^{3} \overline{u}^{3} j_{32} \overline{s}^{2} - \overline{r}^{2} j_{23} \overline{v}^{3} \overline{u}^{3} j_{31} \overline{s}^{1})$$
$$\times (\overline{p}^{1}\overline{q}^{2} - \overline{p}^{2}\overline{q}^{1}) + (\text{cyclic})]$$

Multiply by the factor

$$\prod_{\alpha=1}^{3} \left[\frac{P^\alpha! Q^\alpha! R^\alpha! R^\alpha! S^\alpha! U^\alpha! V^\alpha! (U^\alpha + 2I^\alpha + 1)! (2I^\alpha + 1)}{(V^\alpha + 2I^\alpha + 1)!} \right]^{1/2} .$$

This gives the 3−SU(3) symbol up to an overall normalization depending only on IRs involved.

(vii) Formula for 3−SU(3) symbol for $L>0$. We have obtained an explicit analog of the Bargmann's formula for the $3-j$ symbol of SU(2), [Eq. (33)]. This formula for 3−SU(3) symbols (for $L>0$) is presented in Eq. (187). The notation used for the summation variables is defined in Tables III and IV as explained in detail in Sec. XI.

(viii) Generating function and formula for 3−SU(3) symbol for $L<0$ case. These can be obtained from those for $L>0$ by making the changes indicated in Eqs. (203)–(207).

APPENDIX: GROUP ACTION ON THE VARIABLES

In Sec. V, we set $|z_3|=1$ in constructing the auxiliary measure. Thus the IRs are realized in the space of polynomials in z_1, z_2, w_1, w_2 and $e^{i\theta}$. We clarify here the manner in which the group acts on these variables.

The action of the group on $\vec{z}$ and $\vec{w}$ is given by,

$$\mathscr{U}: z_i \to \mathscr{U}_{ij} z_i \equiv z_i' , \quad w_i = \mathscr{U}_{ij}^{*} w_j \equiv w_i' . \tag{A1}$$

We have imposed the constraint, $\vec{w}\cdot\vec{z}=0$ and regarded (z_1,z_2,z_3,w_1,w_2) as independent variables. The action of the group on these variables is,

$$\mathscr{U}: (z_1,z_2,z_3,w_1,w_2) \to (z_1',z_2',z_3',w_1',w_2'), \tag{A2}$$

where the primed variables are defined in Eq. (A1).

Now let us take $|z_3|=1$ i.e., $z_3=e^{i\theta}$. However, under the action [Eq. (A)], $z_3\neq 0$ in general:

$$z_3' = |z_3'| \exp(i\theta') . \tag{A3}$$

Now define,

$$z_1''=\frac{z_1'}{|z_3'|},\quad z_2''=\frac{z_2'}{|z_3'|},\quad w_1''=\frac{w_1'}{|z_3'|},\quad w_2''=\frac{w_2'}{|z_3'|}. \tag{A4}$$

Then action of the group is defined by,

$$\mathscr{U}:(z_1,z_2,w_1,w_2,\theta)\rightarrow(z_1'',z_2'',w_1'',w_2'',\theta'). \tag{A5}$$

This action is nonlinear as seen from Eqs. (A1) and (A4). In spite of this it serves our purpose as a calculating tool. This realization is intimately related to the optimal boson calculus for SU(3).[51]

Also the action is ambiguous whenever $z_3'=0$, because θ' is then undefined. However, this does not pose a problem for us, because we use a generic situation in our calculations. $z_3'=0$ is a set of measure zero in our space of variables, (z_1,z_2,z_3,w_1,w_2).

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Orbit–orbit branching rules between classical simple Lie algebras and maximal reductive subalgebras

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Complete orbit–orbit branching rules are found for the classical algebra–maximal reductive subalgebra pairs $A_{m+n+1}\supset A_m\oplus A_n\oplus u(1)$, $B_{m+1}\supset B_m\oplus u(1)$, $C_{m+1}\supset A_m\oplus u(1)$, $D_{m+1}\supset D_m\oplus u(1)$, and $D_{m+1}\supset A_m\oplus u(1)$. © *1996 American Institute of Physics.* [S0022-2488(96)02812-5]

I. INTRODUCTION

In a recent paper,[1] to be referred to as **I**, we found orbit–orbit branching rules for the classical algebra–subalgebra pairs $C_{m+n}\supset C_m\oplus C_n$, $B_{m+n}\supset D_m\oplus B_n$, $D_{m+n}\supset D_m\oplus D_n$. Our motivation here is similar, and we refer to **I** for an account of it.

We now consider the algebra–subalgebra pairs $A_{m+n+1}\supset A_m\oplus A_n\oplus u(1)$, $B_{m+1}\supset B_m\oplus u(1)$, $C_{m+1}\supset A_m\oplus u(1)$, $D_{m+1}\supset D_m\oplus u(1)$, $D_{m+1}\supset A_m\oplus u(1)$, in which the subalgebra contains the factor $u(1)$; this completes the cases in which the algebra is classical and the subalgebra is maximal and equal rank [we regard $u(1)$ as contributing 1 to the subalgebra rank]. As for the cases considered in **I**, explicit representation–representation branching rules for the present algebra–subalgebra pairs are not known for general values of m,n. Weyl sectors of algebra and subalgebra line up, i.e., each subalgebra sector contains only complete algebra sectors.

In recent publications[2,3] it is shown that for the cases under consideration (equal rank algebra–subalgebra pairs, with Weyl sectors lining up) the integrity basis (elementary Weyl orbits), in terms of which the subalgebra Weyl orbits (or, simply, orbits) contained in all algebra orbits may be expressed as stretched products (all orbit labels additive, i.e., each algebra and subalgebra label of the product orbit is equal to the sum of the corresponding labels of the factor orbits) consists entirely of the subalgebra orbits contained in the fundamental orbits of the algebra. We label an orbit by the components of its highest weight in a fundamental weights basis; a fundamental orbit is one which has a fundamental weight as its highest weight (one label is unity, the rest zero).

We use orthonormal vectors e_i for the most part as our basis in weight space rather than the more commonly used fundamental weights—it is easier then to recognize to which algebra orbit a subalgebra orbit belongs.

The $u(1)$ label, u, is centered so that its sum over all states of an algebra orbit vanishes, and its scale is such that the spacing between adjacent values in the same algebra orbit is unity. Unlike other orbit labels u can take negative and fractional values.

For each algebra–subalgebra pair we define a $u(1)$ fundamental weight ω_u. It is orthogonal to the other subalgebra fundamental weights (and roots) and points in the $u(1)$ direction. The presence of $u\omega_u$ in the weight of a state indicates that its $u(1)$ label is u.

The branching rules given in **I** for $B_{m+n}\supset D_m\oplus B_n$ and $D_{m+n}\supset D_m\oplus D_n$ are inapplicable for $m=1$, when D_m becomes $u(1)$; that is why $B_{m+1}\supset B_m\oplus u(1)$ and $D_{m+1}\supset D_m\oplus u(1)$ are treated here.

II. THE ALGEBRA–SUBALGEBRA PAIR $A_{m+n+1}\supset A_m\oplus A_n\oplus u(1)$

As basis vectors in weight space we use the $l+1$ ($l=m+n+1$) orthonormal vectors e_i, $i=1,\ldots,l+1$. The Weyl group is generated by the interchanges $e_i\leftrightarrow e_j$.

The simple roots of A_l are $\alpha_i=e_i-e_{i+1}$, $i=1,\ldots,l$. The fundamental weights ω_i are expressed in terms of the simple roots by the reciprocal of the Cartan matrix

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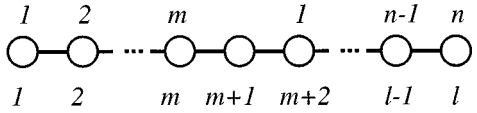

FIG. 1. The Dynkin–Coxeter diagram for $A_{m+n+1}\supset A_m\oplus A_n\oplus u(1)$. The numbers below the diagram label the simple roots of $A_l=A_{m+n+1}$. The first m above label those of A_m and the last n above label those of A_n. The direction unlabeled above corresponds to that of $u(1)$, orthogonal to the other $l-1=m+n$ simple roots of A_l.

$$\omega_i=\sum_{h=1}^{l}(C^{-1})_{ih}\alpha_h,\quad (i=1,\ldots,l); \tag{1}$$

in terms of the orthonormal basis we find

$$\omega_i=(l+1)^{-1}\left[(l-i+1)\sum_{h=1}^{i}e_h-i\sum_{h=i+1}^{l+1}e_h\right]. \tag{2}$$

α_i and ω_i are all orthogonal to $\Sigma_{h=1}^{l+1}e_h$ and hence lie in an $l=m+n+1$ dimensional weight space.

For any weight of the fundamental orbit $[i]$ according to Eq. (2) the number of e_h with coefficient $(l-i+1)/(l+1)$ is i and the number with coefficient $-i/(l+1)$ is $l-i+1$.

The simple roots of A_l, A_m, and A_n are shown in Fig. 1. In terms of the simple roots of A_l the simple roots α'_j of A_m and α''_k of A_n are $\alpha'_j=\alpha_j$, $j=1,\ldots,m$ and $\alpha''_k=\alpha_{m+k+1}$, $k=1,\ldots,n$. The fundamental weights ω'_j of A_m and ω''_k of A_n are

$$\begin{aligned}\omega'_j&=(m+1)^{-1}\left[(m-j+1)\sum_{h=1}^{j}e_h-j\sum_{h=j+1}^{m+1}e_h\right],\quad j=1,\ldots,m,\\ \omega''_k&=(n+1)^{-1}\left[(n-k+1)\sum_{h=m+2}^{m+k+1}e_h-k\sum_{h=m+k+2}^{l+1}e_h\right],\quad k=1,\ldots,n.\end{aligned} \tag{3}$$

The fundamental $u(1)$ weight is

$$\omega_u=(m+1)^{-1}\sum_{h=1}^{m+1}e_h-(n+1)^{-1}\sum_{h=m+2}^{l+1}e_h. \tag{4}$$

The algebra weight $[\lambda_1,\lambda_2,\ldots,\lambda_l]$ becomes, in the subalgebra basis, $[\lambda_1,\lambda_2,\ldots,\lambda_m;\lambda_{m+2},\lambda_{m+3},\ldots,\lambda_l;u]$, where

$$u=(l+1)^{-1}\left[(n+1)\sum_{i=1}^{m+1}i\lambda_i+(m+1)\sum_{j=1}^{n}(n-j+1)\lambda_{m+j+1}\right]. \tag{5}$$

The elementary $A_m\oplus A_n\oplus u(1)$ orbits are those contained in the fundamental A_l orbits $[i]$. A representative one, $[j;k]$, in $[i]$ has as the weight of its highest state $\omega'_j+\omega''_k+u\omega_u$, where

$$k=i-j, \tag{6}$$

$$u=(l+1)^{-1}[j(n+1)-k(m+1)]. \tag{7}$$

Thus

$$[i] \supset \sum_{j=\max(0,i-n-1)}^{\min(m+1,i)} [j;i-j]. \tag{8}$$

When $j=0$ or $m+1$ the point orbit of A_m is understood; similarly for the A_n orbit when $k=0$ or $n+1$. It may be checked that the weights $\omega'_j + \omega''_k + u\omega_u$ have i e's with coefficient $(l-i+1)/(l+1)$ and $l-i+1$ with coefficient $-i/(l+1)$ and therefore belong to the A_l orbit $[i]$; moreover the weights of $[j;k]$ exhaust those of $[i]$.

It remains to find the compatibility rules between pairs of elementary orbits. Consider the stretched product $[j;k]\cdot[j';k']$; it implies the orbit $[j,j';k,k']$ of $A_m \oplus A_n \oplus u(1)$ where the A_m orbit $[j,j']$ is that with labels $\lambda'_h = \delta_{hj} + \delta_{hj'}$ and similarly for the orbit $[k,k']$ of A_n. The pair $[j;k],[j';k']$ is compatible if and only if their stretched product belongs to the orbit $[i,i']$ of A_l, where $i=j+k$ and $i'=j'+k'$. We may suppose $i'>i$ (two elementary orbits in the same A_l orbit are known to be incompatible). We may also suppose $j'>j$ (otherwise interchange the roles of A_m and A_n). Now a weight of the A_l orbit $[i,i']$ has i e's with coefficient $(2l-i-i'+2)/(l+1)$, $i'-i$ with coefficient $(l-i-i'+1)/(l+1)$ and $l-i'+1$ with coefficient $-(i+i')/(l+1)$.

The A_m orbit $[j,j']$ has weight $\omega'_j + \omega'_{j'} + [(j+j')(l-m) - (k+k')(m+1)][(l+1)(m+1)]^{-1}\Sigma_{h=1}^{m+1} e_h$; we have included the part of the $u(1)$ weight component for which $h \leqslant m+1$. There are j e's with coefficient $(2l-i-i'+2)/(l+1)$, $j'-j$ with coefficient $(l-i-i'+1)/(l+1)$ and $m+1-j'$ with coefficient $-(i+i')/(l+1)$. Comparing this with the number of e's in the A_l orbit with each coefficient we conclude that in the A_n part of the weight there are k e's with coefficient $(2l-i-i'+2)/(l+1)$, $k'-k$ with coefficient $(l-i-i'+1)/(l+1)$ and $n-k'+1$ with coefficient $-(i+i')/(l+1)$. This is possible only if $k' \geqslant k$. So $[j;k]$ and $[j';k']$ are compatible if and only if $j' \geqslant j$ and $k' \geqslant k$ (recall $i'>i$). The compatibility condition is shown diagrammatically in Fig. 2. Two elementary orbits are incompatible if one lies above and to the right of the other.

So the orbit–orbit branching rules are complete. To get the $A_m \oplus A_n \oplus u(1)$ orbit content of the A_l orbit $[\lambda_1,\lambda_2,...,\lambda_l]$, choose a series of boxes $[j_i;k_i]$, one from each diagonal row $i=j_i+k_i$ for which $\lambda_i \neq 0$, such that each is compatible with the last preceding i (and therefore with all preceding i). Each such series contributes one subalgebra orbit $[\lambda'_1,\ldots,\lambda'_m;\lambda''_1,\ldots,\lambda''_n]$ with $\lambda'_h = \Sigma_i \lambda_i \delta_{hj_i}$, $\lambda''_h = \Sigma_i \lambda_i \delta_{hk_i}$ (the stretched product of the chosen mutually compatible orbits); the $u(1)$ labels are also additive. The same strategy can be used to get the subalgebra orbit content of an arbitrary algebra orbit for the algebra–subalgebra pairs considered in the next four sections; we will not repeat it for them.

III. THE ALGEBRA–SUBALGEBRA PAIR $B_{m+1} \supset B_m \oplus u(1)$

In this and the next three sections (III–VI), to save space, we state our results without detailed proofs; the proofs are very similar to those given in Sec. II for $A_{m+n+1} \supset A_m \oplus A_n \oplus u(1)$. The roots of B_l $(l=m+1)$ are $\pm e_i$, $i=1,\ldots,l$ and $\pm e_i \pm' e_j$, $i=1,\ldots,l-1$ and $j=i+1,\ldots,l$ where e_i, $i=1,\ldots,l$ are orthonormal vectors; the prime above is to indicate that the $\pm$ signs are independent. The Weyl group is generated by sign reversals $e_i \to -e_i$ and interchanges $e_i \leftrightarrow e_j$.

The simple roots of B_l are $\alpha_i = e_i - e_{i+1}$, $i=1,\ldots,l-1$ and $\alpha_l = e_l$. The fundamental weights are given by

$$\omega_i = \sum_{h=1}^{i} e_h, \quad i=1,\ldots,l-1, \quad \omega_l = \frac{1}{2}\sum_{h=1}^{l} e_h. \tag{9}$$

In any weight of the fundamental orbit $[i]$, $i=1,\ldots,l-1$, the number of e_h with coefficient ± 1 is i, the number with coefficient 0 is $l-i$; in the fundamental orbit $[l]$, all l e_h have coefficient $\pm\frac{1}{2}$.

The simple roots of B_l and B_m are shown in Fig. 3. The simple roots of B_m are $\alpha'_i = \alpha_{i+1}$.

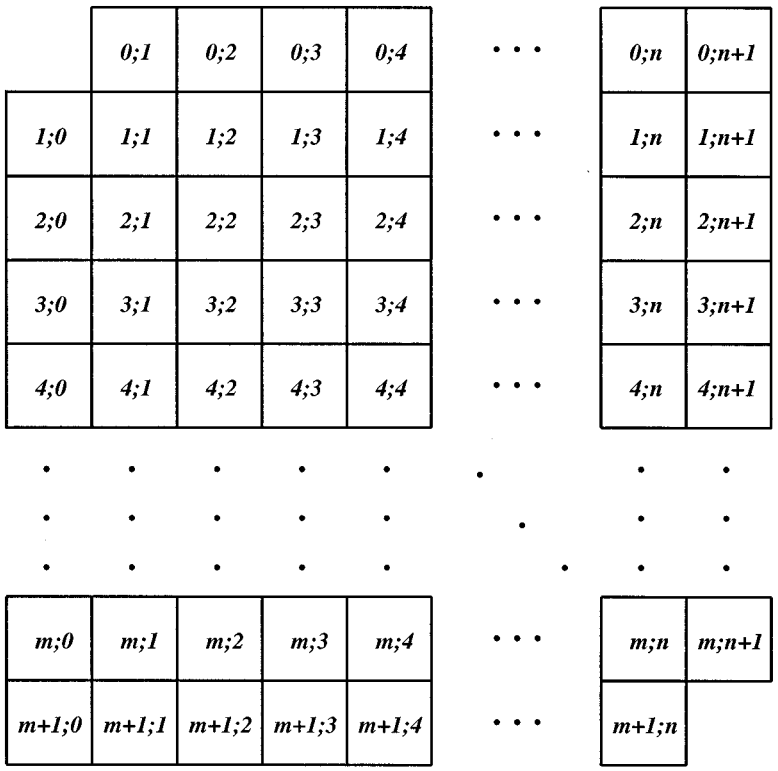

FIG. 2. The elementary $A_{m+n+1}\supset A_m\oplus A_n\oplus u(1)$ W orbits. The elementary orbit $[j;k]$ belongs to the $(j+k)$th fundamental orbit of A_{m+n+1}. Two elementary orbits are compatible only if one lies below and/or to the right of the other.

The fundamental weights of B_m are

$$\omega_i'=\sum_{h=2}^{i+1} e_h\,,\quad i=1,\ldots,m-1,$$

$$\omega_m'=\frac{1}{2}\sum_{h=2}^{l} e_h\,. \tag{10}$$

The fundamental $u(1)$ weight is

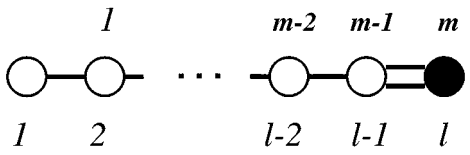

FIG. 3. The Dynkin–Coxeter diagram for $B_{m+1}\supset B_m\oplus u(1)$. The numbers below the diagram label the simple roots of $B_l=B_{m+1}$. Those above label those of B_m. The direction unlabeled above corresponds to that of $u(1)$, orthogonal to the simple roots and fundamental weights of B_m.

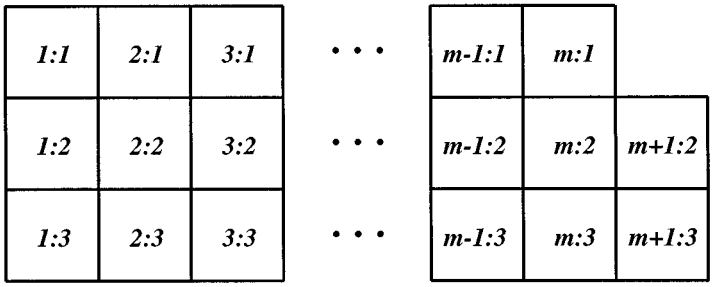

FIG. 4. The elementary subalgebra orbits for $B_{m+1}\supset B_m\oplus u(1)$. Those in the ith column belong to the ith fundamental orbit of $B_l=B_{m+1}$. One in the first row is compatible with all those to its right, in any row. One in the second or third row is compatible with one to its right only if they are in the same row.

$$\omega_u=e_1. \tag{11}$$

The algebra weight $[\lambda_1,\lambda_2,...,\lambda_l]$ becomes, in the subalgebra basis, $[\lambda_2,\lambda_3,...,\lambda_l;u]$ with

$$u=\sum_{h=1}^{l-1}\lambda_h+\frac{1}{2}\lambda_l. \tag{12}$$

The elementary $B_m\oplus u(1)$ orbits are those contained in the fundamental B_l orbits $[i]$. The first m orbits contain 3 elementary orbits each and the lth contains 2

$$\begin{gathered}[i]\supset[i{:}1]\oplus[i{:}2]\oplus[i{:}3],\quad i=1,\ldots,m,\\ [l]\supset[l{:}2]\oplus[l{:}3],\end{gathered} \tag{13}$$

where

$$\begin{gathered}[i{:}1]=[i;0],\quad i=1,\ldots,m-1,\quad [m{:}1]=[2m;0],\\ [i{:}2]=[i-1;1],\quad i=1,\ldots,m,\\ [i{:}3]=[i-1;-1],\quad i=1,\ldots,m,\\ [l{:}2]=[m;\tfrac{1}{2}],\quad [l{:}3]=[m;-\tfrac{1}{2}],\end{gathered} \tag{14}$$

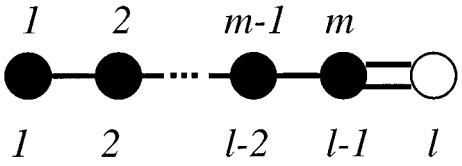

FIG. 5. The Dynkin–Coxeter diagram for $C_{m+1}\supset A_m\oplus u(1)$. The numbers below the diagram label the simple roots of $C_l=C_{m+1}$. Those above label those of A_m. The direction unlabeled above corresponds to that of $u(1)$, orthogonal to the simple roots and fundamental weights of A_m.

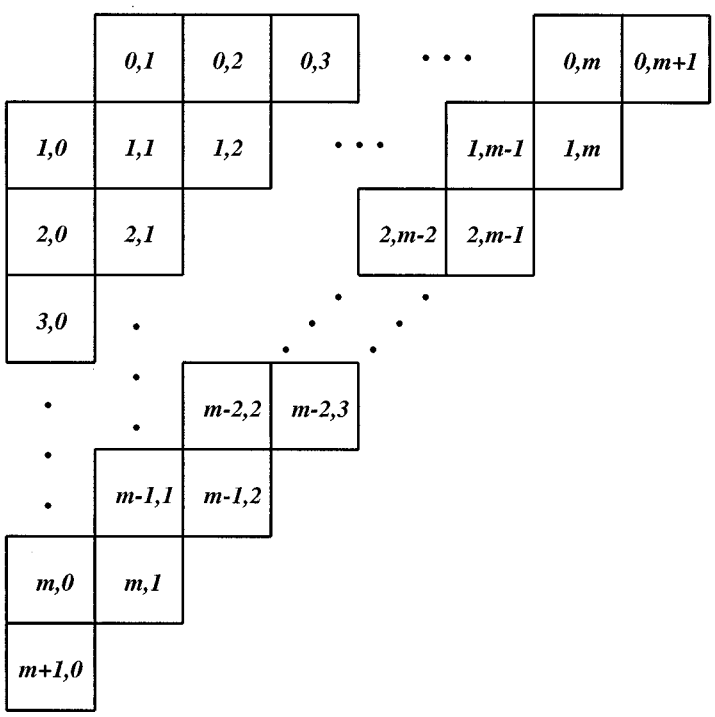

FIG. 6. The elementary $C_{m+1}\supset A_m\oplus u(1)$ orbits $[j,k]$. The orbit $[j,k]$ belongs to the ith$=(j+k)$th fundamental orbit of $C_l=C_{m+1}$. Two elementary orbits are incompatible if and only if one lies to the right and above the other.

The numbers i, $i-1$, m mean the corresponding B_m fundamental orbits; $2m$ means the B_m orbit whose mth label is 2, the others 0; $i-1$ means the point orbit when $i=1$. The symbol on the right of the semicolon is the $u(1)$ label of the orbit.

Two elementary orbits $[j{:}k]$ and $[j';k']$, with $j'>j$, are compatible if $k=1$, or if k and k' are equal; if $k\neq 1$ and $k'\neq k$ they are incompatible; see Fig. 4.

IV. THE ALGEBRA–SUBALGEBRA PAIR $C_{m+1}\supset A_m\oplus u(1)$

The roots of C_l $(l=m+1)$ are $\pm e_i$, $1\leqslant i\leqslant l$ and $\pm e_i\pm' e_j$, $1\leqslant i<j\leqslant l$, where e_i, e_j are orthonormal weight space vectors. Weyl reflections are generated by sign reversals $e_i\rightarrow -e_i$ and

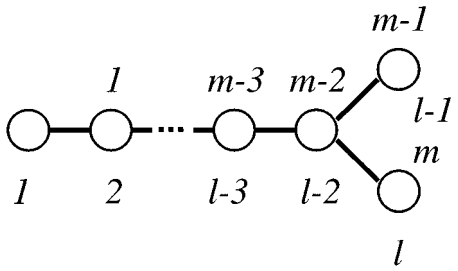

FIG. 7. The Dynkin–Coxeter diagram for $D_{m+1}\supset D_m\oplus u(1)$. The numbers below the diagram label the simple roots of D_l $(l=m+1)$. Those above label those of D_m. The direction unlabeled above corresponds to that of $u(1)$, orthogonal to the simple roots and fundamental weights of D_m.

interchanges $e_i \leftrightarrow e_j$. The simple roots are $\alpha_i = e_i - e_{i+1}$, $i = 1,\ldots,l-1$ and $\alpha_l = 2e_l$ (for simplicity we have multiplied them and the fundamental weights below by $\sqrt{2}$). In terms of the orthonormal basis the fundamental weights are

$$\omega_i = \sum_{h=1}^{i} e_h, \quad i = 1,\ldots,l. \tag{15}$$

Any weight of the fundamental orbit $[i]$, with highest weight ω_i, has i e's with coefficient ± 1, $l-i$ with coefficient 0.

The simple roots of C_l and A_m are shown in Fig. 5. Those of A_m are $\alpha'_i = \alpha_i$, $i = 1,\ldots,m$. The fundamental weights ω'_j of A_m are

$$\omega'_j = l^{-1}\left[(l-j)\sum_{h=1}^{j} e_h - j\sum_{h=j+1}^{l} e_h\right]. \tag{16}$$

The fundamental $u(1)$ weight is

$$\omega_u = 2l^{-1}\sum_{h=1}^{l} e_h. \tag{17}$$

The algebra weight $[\lambda_1,\ldots,\lambda_l]$ becomes, in the subalgebra basis, $[\lambda_1,\ldots,\lambda_{l-1};u]$ with

$$u = \frac{1}{2}\sum_{i=1}^{l} i\lambda_i. \tag{18}$$

The elementary $A_m \oplus u(1)$ orbits are the ones contained in the fundamental C_l orbits $[i]$. A representative one, $[j;k]$, in $[i]$ has as the weight of its highest state $\omega_j + \omega_{l-k} + u\omega_u$, where

$$k = i - j, \tag{19}$$

$$u = \tfrac{1}{2}(j-k). \tag{20}$$

Thus

$$[i] \supset \sum_{j=0}^{i} [j, i-j], \quad i = 1,\ldots,l. \tag{21}$$

The elementary orbit $[j,k]$, where $k = i-j$, has A_m orbit labels

$$\lambda_h = \delta_{hj} + \delta_{h,l-k}, \tag{22}$$

where δ_{hj} or $\delta_{h,l-k}$ is taken as zero when j or k, respectively, is 0 or l. The u label of the orbit $[j,k]$, suppressed in Eq. (21), is given by Eq. (20). When $i = l$, j and $l-k$ are equal and nonzero A_m orbit labels are all 2.

It can be shown that two elementary orbits $[j,k]$ and $[j',k']$ (we may suppose $i' = j' + k' > i = j + k$) are compatible if and only if $j' \geqslant j$ and $k' \geqslant k$ (only one of the $\geqslant$ signs can be $=$). The elementary orbits and their compatibility rules are shown graphically in Fig. 6.

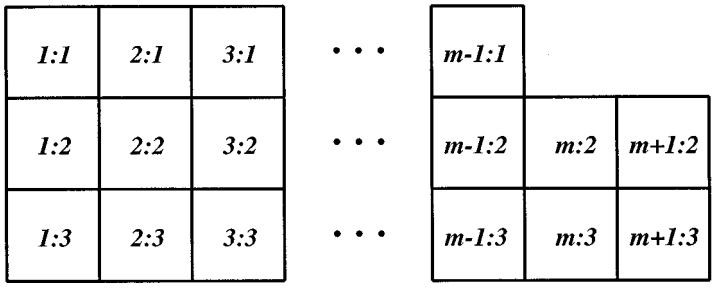

FIG. 8. The elementary subalgebra orbits for $B_{m+1}\supset B_m\oplus u(1)$. Those in the ith column belong to the ith fundamental B_l orbit, $l=m+1$. One in the first row is compatible with all those to its right, in any row. Each in rows 2 and 3 is compatible with those to its right in the same row, and both in the mth column are compatible with both in the $(m+1)$th column.

V. THE ALGEBRA–SUBALGEBRA PAIR $D_{m+1}\supset D_m\oplus u(1)$

The roots of D_l $(l=m+1)$ are $\pm e_i\pm' e_j$, $1\leqslant i<j\leqslant l$ where e_i, e_j are orthonormal weight space vectors. The Weyl group is generated by two sign reversals at a time $e_i\rightarrow -e_i$, $e_j\rightarrow -e_j$ and interchanges $e_i\leftrightarrow e_j$.

The simple roots are $\alpha_i=e_i-e_{i+1}$, $i=1,\ldots,l-1$, $\alpha_l=e_{l-1}+e_l$. The fundamental weights are

$$\omega_i=\sum_{h=1}^{i} e_h, \quad i=1,\ldots,l-2,$$

$$\omega_{l-1}=\frac{1}{2}\left[\sum_{h=1}^{l-1} e_h-e_l\right], \quad \omega_l=\frac{1}{2}\left[\sum_{h=1}^{l-1} e_h+e_l\right]. \tag{23}$$

Thus a weight of the orbit $[i]$, $i\leqslant l-2$, has i e_h with coefficient ± 1, the rest with coefficient 0; one of $[l-1]$ has an odd number with coefficient $-\frac{1}{2}$, the rest with coefficient $\frac{1}{2}$; one of $[l]$ has an even number with coefficient $-\frac{1}{2}$, the rest with coefficient $\frac{1}{2}$.

The simple roots of D_l and D_m are shown in Fig. 7. The simple roots of D_m are $\alpha_i'=\alpha_{i+1}$, $i=1,\ldots,m$. The fundamental weights of D_m are

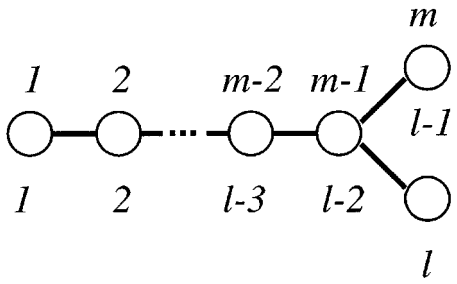

FIG. 9. The Dynkin–Coxeter diagram for $D_{m+1}\supset A_m\oplus u(1)$. The numbers below the nodes label the simple roots of D_l $(l=m+1)$. Those above label those of A_m. The direction unlabeled above corresponds to that of $u(1)$, orthogonal to the roots and fundamental weights of A_m.

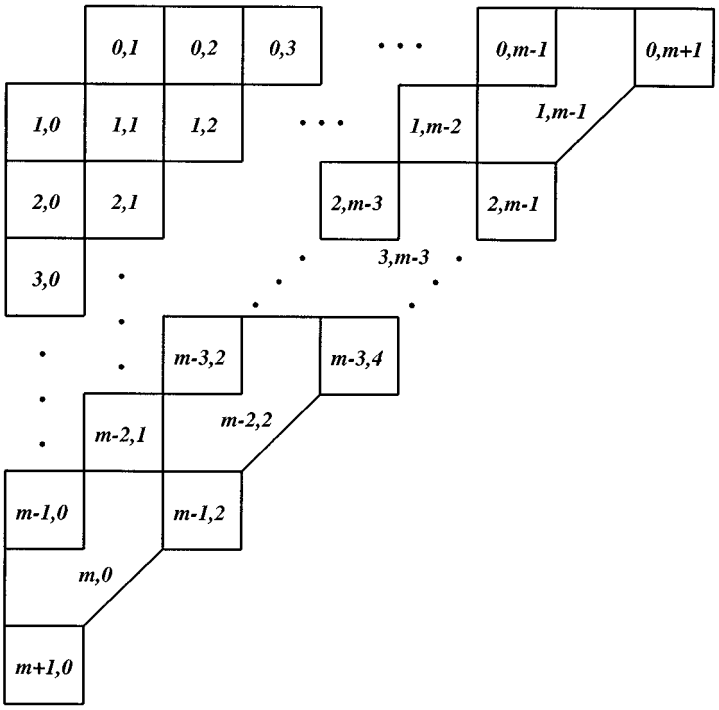

FIG. 10. The elementary $D_{m+1}\supset A_m\oplus u(1)$ orbits for $l=m+1$ even. Two orbits are compatible only if one is to the right of and/or below the other, or, in case one of them is in the diagonal row $l-1$, if either of its squares is to right of and/or below the other or to the left of and/or above the other.

$$\omega_i'=\sum_{h=2}^{i+1} e_h\,,\quad i=1,\ldots,m-2,$$
$$\omega_{m-1}'=\frac{1}{2}\left[\sum_{h=2}^{l-1} e_h-e_l\right],\quad \omega_m'=\frac{1}{2}\sum_{h=2}^{l} e_h\,. \tag{24}$$

The fundamental $u(1)$ weight is

$$\omega_u=e_1\,. \tag{25}$$

A D_l weight $[\lambda_1,\ldots,\lambda_l]$, in a $D_m\oplus u(1)$ basis, becomes $[\lambda_2,\lambda_3,\ldots,\lambda_l;u]$ with

$$u=\sum_{i=1}^{l-2}\lambda_i+\frac{1}{2}(\lambda_{l-1}+\lambda_l). \tag{26}$$

The elementary $D_m\oplus u(1)$ orbits are those contained in the fundamental D_l orbits $[i]$. The first $l-2$ orbits contain 3 elementary orbits each; the $(l-1)$th and lth each contains 2

$$[i]\supset[i{:}1]\oplus[i{:}2]\oplus[i{:}3],\quad i=1,\ldots,l-2,$$
$$[l-1]\supset[l-1{:}2]\oplus[l-1{:}3],\quad [l]\supset[l{:}2]\oplus[l{:}3], \tag{27}$$

where

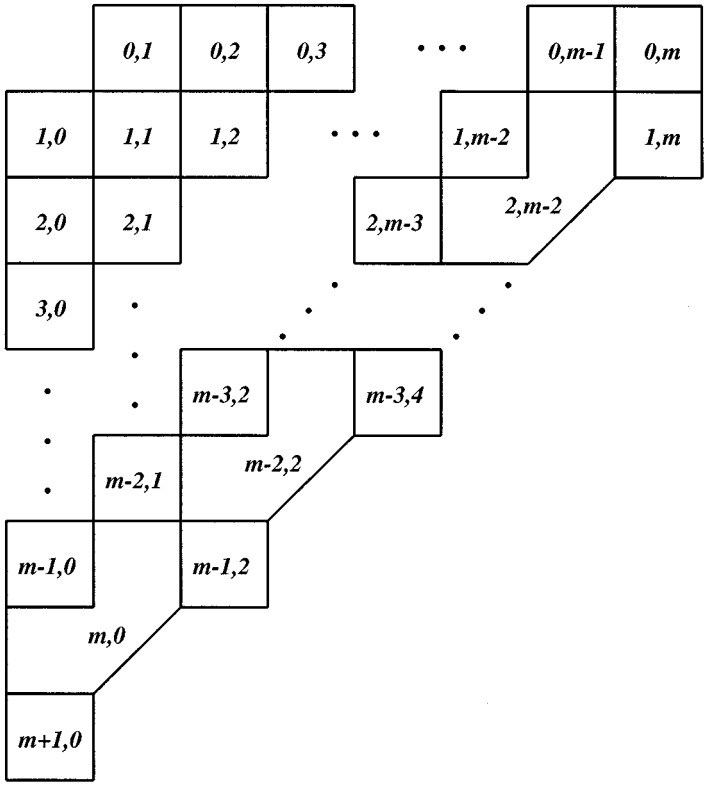

FIG. 11. The elementary $D_{m+1}\supset A_m\oplus u(1)$ orbits for $l=m+1$ odd. The compatibility condition for two orbits is the same as that in the caption of Fig. 10.

$$
\begin{gathered}
[i{:}1]=[i;0],\quad i=1,\ldots,l-3,\\
[l-2{:}1]=[m-1,m;0]\ \text{(the last two } D_m \text{ labels are 1, the rest 0)}\\
[i{:}2]=[i-1;1],\quad i=1,\ldots,l-2,\\
[i{:}3]=[i-1;-1],\quad i=1,\ldots,l-2,\\
[l-1{:}2]=[m-1;\tfrac{1}{2}],\quad [l-1{:}3]=[m;-\tfrac{1}{2}],\\
[l{:}2]=[m;\tfrac{1}{2}],\quad [l{:}3]=[m-1;-\tfrac{1}{2}].
\end{gathered}
\tag{28}
$$

The numbers $i,i-1,m,m-1$ mean the corresponding D_m fundamental orbits, i.e., the corresponding D_m orbit label is 1. The number to the right of the semicolon is the $u(1)$ label.

Two elementary orbits $[j{:}k]$ and $[j'{:}k']$, with $j'>j$, are compatible if $k=1$ or if k and k' are equal or if $j=m$ and $j'=m+1$; otherwise they are incompatible; see Fig. 8.

VI. THE ALGEBRA–SUBALGEBRA PAIR $D_{m+1}\supset A_m\oplus u(1)$

The roots and fundamental weights of D_l $(l=m+1)$ are of course the same as those given in the first paragraph of Sec. V.

The simple roots of D_l and A_m are shown in Fig. 9. The simple roots of A_m are $\alpha_i' = \alpha_i$, $i=l,\ldots,m$. The fundamental weights of A_m are

$$\omega_i' = (m+1)^{-1}\left[(m-i+1)\sum_{h=1}^{i} e_h - i\sum_{h=i+1}^{m+1} e_h\right]. \tag{29}$$

The fundamental $u(1)$ weight ω_u is

$$\omega_u = \frac{2}{l}\sum_{h=1}^{l} e_h . \tag{30}$$

The D_l weight $[\lambda_1,\ldots,\lambda_l]$ becomes, in the $A_m \oplus u(1)$ basis, $[\lambda_1,\ldots,\lambda_{l-1};u]$, with

$$u = \frac{1}{2}\sum_{i=1}^{l-2} i\lambda_i + \frac{l-2}{4}\lambda_{l-1} + \frac{l}{4}\lambda_l . \tag{31}$$

The elementary $A_m \oplus u(1)$ orbits are those contained in the fundamental D_l orbits $[i]$. We find

$$[i] \supset \sum_{j=0}^{i} [j,i-j], \quad i=1,\ldots l-2, \tag{32}$$

$$[i] \supset \sum_{j=0}^{[(1/2)\,i]} [i-2j,2j], \quad i=l-1,l. \tag{33}$$

In Eq. (32) the elementary orbit $[j,k]$, with $k=i-j$, is that with labels

$$\lambda_h = \delta_{hj} + \delta_{h,l-k}, \tag{34}$$

i.e., the nonzero (unit) labels are the jth and $(l-k)$th; if j (or k) is 0 or l the corresponding Kronecker δ in Eq. (34) is 0. The u label of the orbit $[j,k]$, suppressed in Eq. (32), is

$$u = \tfrac{1}{2}(j-k). \tag{35}$$

In Eq. (33) $[\frac{1}{2}i]$ means the integer part of $\frac{1}{2}i$, i.e., $\frac{1}{2}i$ or $\frac{1}{2}(i-1)$ according to whether i is even or odd. The elementary orbit $[i-2j,2j]$ is that with labels

$$\lambda_h = \delta_{h,i-2j}, \tag{36}$$

i.e., there is one nonzero (unit) label, the $(i-2j)$th; if $i-2j$ is 0 or l the Kronecker δ in Eq. (36) is 0 and we have the point or zero orbit of A_m. The u-label of $[i-2j,2j]$ is

$$u = \tfrac{1}{2}i - j - \tfrac{1}{4}l. \tag{37}$$

The elementary orbits and their compatibility rules are shown graphically in Figs. 10 and 11, for l even and odd, respectively.

For the $(l-1)$th fundamental orbit we associate with the elementary orbit $[m-2j,2j]$ also the labels $[m-2j-1,2j+1]$ (except when $m-2j=0$), so it is represented by two boxes in Figs. 10 and 11. Two elementary orbits $[j,k],[j',k']$ are incompatible if $j'>j$ and $k'<k$ or if $j'<j$ and $k'>k$. In case $j+k=m$ or $j'+k'=m$ these inequalities must hold for both versions of $[j,k]$ or $[j',k']$; see the caption of Fig. 10.

VII. CONCLUSIONS

This work concludes the computation of branching rules for Weyl orbits of classical Lie algebras and their maximal reductive regular subalgebras. Work on a similar problem for Kac–Moody algebras is in progress.

ACKNOWLEDGMENTS

The work was supported in part by the National Science and Engineering Research Council of Canada and by the Fonds FCAR du Québec.

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Comments on a recent paper by S. Adler on projective group representations in quaternionic Hilbert spaces

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A version of Schur's lemma is proven that elucidates some issues raised by that paper. © *1996 American Institute of Physics.* [S0022-2488(96)03712-7]

I. PRELIMINARIES: PROJECTIVE REPRESENTATIONS OF INDIVIDUAL SYMMETRIES

In a paper[1] recently published in this journal, Adler mentions divergences between his approach and that taken by the present author[2] in connection with a then new proof[3,4] for Wigner's theorem (also see notes No. 5–7 for Bargmann's review[5] on the several proofs that appeared at the time). It seems worth pointing out that these divergences are not due, as Adler states, to a ''failure'' that ''can lead to erroneous conclusions,'' but rather to subtle shifts in the assumptions.

Let us first recall that in Refs. 2 and 3 a *symmetry* of an irreducible quaternionic quantum system is defined as an isomorphism μ of the canonically relatively orthocomplemented lattice $\mathscr{P}(\mathscr{H}_{\mathbf{H}})$ of all projectors of a Hilbert space $\mathscr{H}_{\mathbf{H}}$ on the field $\mathbf{H}$ of the real quaternions. To make things as unambiguous as is compatible with conciseness, we only mention here that the scalar product in $\mathscr{H}_{\mathbf{H}}$ is a positive definite sesquilinear form, linear in its first factor: $(q\phi,\psi)=q(\phi,\psi)$ and $(\phi,\psi)=(\psi,\phi)^*$, $\forall q\in\mathbf{H}$; $\phi,\psi\in\mathscr{H}_{\mathbf{H}}$; and that μ is an isomorphism of $\mathscr{P}(\mathscr{H}_{\mathbf{H}})$ exactly when it is a bijective map, such that

$$P\subset Q\Rightarrow\mu P\subset\mu Q;\quad (\mu P)^{\perp}=\mu(P^{\perp}),\quad \forall P,Q\in\mathscr{P}(\mathscr{H}_{\mathbf{H}}). \tag{1.1}$$

The interpretation of this formulation has its roots in the work of Birkhoff and von Neumann:[6] the elements of $\mathscr{P}$ are to be interpreted as the ''propositions'' (or ''questions'' or ''yes–no'' experiments) on the physical system considered. Hence (1.1) is the pragmatic requirement that *if Q is true whenever P is true, i.e. if P implies Q, then μP implies μQ; and the negation $(\mu P)^{\perp}$ of μP is the image through μ of the negation $P^{\perp}$ of P*.

As a consequence[3] of the first fundamental theorem of projective geometry,[7] every such μ is implemented by a bijective semilinear map of $\mathscr{H}_{\mathbf{H}}$ into itself:

$$\mu(P)=S^{-1}PS,\quad \forall P\in\mathscr{P}(\mathscr{H}_{\mathbf{H}}), \tag{1.2}$$

with

$$S(\phi+\psi)=S\phi+S\psi\quad\text{and}\quad S(q\phi)=q_S^{-1}qq_SS\phi,\forall q\in\mathbf{H};\quad \phi,\psi\in\mathscr{H}_{\mathbf{H}}. \tag{1.3}$$

Clearly, then, one can assume without loss of generality that there exists a bijective, *linear* map of $\mathscr{H}_{\mathbf{H}}$ onto itself, namely $S_0\equiv q_sS$, which implements the same symmetry:

$$S_0^{-1}PS_0=\mu(P)=S^{-1}PS,\quad \forall P\in\mathscr{P}(\mathscr{H}_{\mathbf{H}}). \tag{1.4}$$

Proposition 1 (A Quaternionic Schur's lemma): The bijective semilinear map S of $\mathscr{H}_{\mathbf{H}}$ which implements a symmetry μ of $\mathscr{P}(\mathscr{H}_{\mathbf{H}})$ is unique up to a multiplicative constant ω; i.e., if $S_k(k=1,2)$ are two bijective semilinear maps such that

$$S_1^{-1}PS_1=S_2^{-1}PS_2,\forall P\in\mathscr{P}(\mathscr{H}_{\mathbf{H}}); \tag{1.5}$$

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then

$$S_1 = \omega S_2, \quad \text{for some non-zero} \quad \omega \in \mathbf{H}. \tag{1.6}$$

As the proof of this result bears directly on the main issue of this paper, it is given with some details here.

Proof: Let $S \equiv S_1 S_2^{-1}$ and let $S_0 \equiv q_s S$ be the corresponding bijective, *linear* map [cf. (1.4)]. We have then

$$PS_0 = S_0 P, \quad \forall P \in \mathscr{P}(\mathscr{H}_{\mathbf{H}}). \tag{1.7}$$

For every $\psi \in \mathscr{H}_{\mathbf{H}}$ with $\|\psi\| = 1$, let P_ψ denote the projector

$$P_\psi : \phi \in \mathscr{H}_H \to (\phi, \psi)\psi \in \mathscr{H}_{\mathbf{H}}. \tag{1.8}$$

From (1.7) we have in particular for all ϕ and ψ on the unit sphere of $\mathscr{H}_{\mathbf{H}}$:

$$P_\psi S_0 \phi = S_0 P_\psi \phi, \tag{1.9}$$

which reads as (recall that S_0 is linear)

$$(S_0\phi, \psi)\psi = (\phi, \psi) S_0 \psi, \tag{1.10}$$

and thus in particular, for $\phi = \psi$:

$$S_0\phi = \omega_0(\phi)\phi, \quad \forall \phi \in \mathscr{H}_{\mathbf{H}} \quad \text{with} \quad \|\phi\| = 1. \tag{1.11}$$

The essence of Proposition 1 is to assert that any explicit dependence of ω on ϕ would not be compatible with the definition (1.1) of a symmetry. Indeed, we first notice that, whenever $(\phi, \psi) \neq 0$, (1.9) reads as

$$S_0\psi = \omega_0(\psi)\psi, \quad \text{with} \quad \omega_0(\psi) = (\phi, \psi)^{-1}\omega_0(\phi)(\phi, \psi). \tag{1.12}$$

Upon using the above argument again for $\chi = (\|\phi + \psi\|)^{-1}(\phi + \psi)$ whenever ϕ and ψ are linearly independent and not orthogonal, we have

$$\omega_0(\chi)\phi + \omega_0(\chi)\psi = (\|\phi + \psi\|) S_0 \chi = \omega_0(\phi)\phi + \omega_0(\psi)\psi, \tag{1.13}$$

i.e., upon using linear independence of ϕ and ψ,

$$\omega_0(\phi) = \omega_0(\psi). \tag{1.14}$$

For ϕ, ψ as above, and $q \in \mathbf{H}$ with $\|q\| = 1$, the previous argument, now with $\phi' = q\phi$, used instead of ϕ, gives

$$\omega_0(q\phi) = \omega_0(\psi), \tag{1.15}$$

i.e., together with (1.12) and (1.14),

$$q\omega_0(\phi)q^* = \omega_0(\phi), \quad \forall q \in \mathbf{H} \quad \text{with} \quad \|q\| = 1. \tag{1.16}$$

This implies that $\omega_0(\phi)$ is *real*.

Finally, when $(\phi, \psi) = 0$ let $\zeta = (1/\sqrt{2})(\phi + \psi)$ to get similarly

$$\omega_0(\phi) = \omega_0(\zeta) \quad \text{and} \quad \omega_0(\zeta) = \omega_0(\psi), \tag{1.17}$$

so that (1.14) holds again in this case. Hence, there is an ω_0 real, and *independent* of ϕ, such that

$$S_0\phi=\omega_0\phi, \quad \forall\,\phi\in\mathscr{H}_{\mathbf{H}} \quad \text{with } \|\phi\|=1. \tag{1.18}$$

Since ω_0 is real, we have

$$S_0\phi=\omega_0\phi, \quad \forall\,\phi\in\mathscr{H}_{\mathbf{H}}, \text{ i.e., } S_0=\omega_0 I. \tag{1.19}$$

Returning now to the first line of the proof, we see that (1.19) proves the proposition, namely

$$S_1=\omega S_2, \quad \text{with } \omega=q_S^{-1}\omega_0. \tag{1.20}$$

Remark: Without loss of generality, we can assume[2–4] that the transformations S implementing any symmetry μ are not only semilinear but counitary, i.e.,

$$(S\phi,S\psi)=q_S(\phi,\psi)q_S^{-1}, \quad \forall\,\phi,\psi\in\mathscr{H}_{\mathbf{H}}. \tag{1.21}$$

We can therefore require, without loss of generality, that the quaternion ω in the conclusion (1.6) is of norm 1.

II. THE ISSUE: PROJECTIVE REPRESENTATIONS OF SYMMETRY GROUPS

Having predicated our analysis (as Adler apparently did his) on the idea that the natural language in which to express the primary concepts of the theory of symmetries is *projective geometry*, we defined[2] a *projective representation* μ of a group G as a *group homomorphism*,

$$\mu: g\in G\mapsto\mu(g)\in \mathrm{Aut}\{\mathscr{P}(\mathscr{H}_{\mathbf{H}})\}, \tag{2.1}$$

where Aut $\{\mathscr{P}(\mathscr{H}_{\mathbf{H}})\}$ is the group of all bijective maps of $\mathscr{P}(\mathscr{H}_{\mathbf{H}})$ onto itself, satisfying (1.1). Since the theory of group representations on vector spaces is still (and certainly was in the 1930s) better developed than the corresponding theory for projective spaces, the interest of Wigner's theorem is to help reduce the study of the latter to that of the former. Specifically, we defined a *lifting* of a projective representation μ as a map

$$S: g\in G\mapsto S(g)\in \mathrm{Aut}\{\mathscr{H}_H)\}, \quad \text{with } S(g)^{-1}PS(g)=\mu P, \quad \forall\,P\in\mathscr{P}(\mathscr{H}_{\mathbf{H}})), \tag{2.2}$$

where Aut $\{\mathscr{H}_{\mathbf{H}})\}$ denotes the group of all bijective semilinear maps of $\mathscr{H}_{\mathbf{H}}$ onto itself. Note that, while the map S implements μ, this is not sufficient to ensure that the map S is itself a group homomorphism. Nevertheless, since for any pair g_1, g_2 of elements of G, $S(g_1)S(g_2)$ and $S(g_1g_2)$ implement the same symmetry, we have

$$[S(g_1)S(g_2)]^{-1}P[S(g_1)S(g_2)]=[S(g_1g_2)]^{-1}P[S(g_1g_2)], \quad \forall\,P\in\mathscr{P}(\mathscr{H}_{\mathbf{H}}). \tag{2.3}$$

Proposition 1 thus implies that there exists a nonzero quaternion $\omega(g_1,g_2)$ (which one can actually take to be of norm 1; see the remark at the end of Sec. I), such that

$$S(g_1)S(g_2)=\omega(g_1,g_2)S(g_1g_2). \tag{2.4}$$

Adler collapses these two definitions [projective representation, i.e. (2.1); and lifting i.e. (2.2)] into one, namely that

$$[S(g_1)S(g_2)]\phi=\omega(\phi;g_1,g_2))[S(g_1g_2)]\phi, \tag{2.5}$$

holds ''for one particular complete set of states.''

III. DISCUSSION

Adler emphasizes that one should allow for an actual dependence of ω on ϕ in (2.5); also see his book;[8] especially its Sec. 4.6 (his Ref. 4) that he cites to support his version, formula (2), of the above (2.5). Adler points out correctly that this requires restricting (2.5) to hold only on a particular set of vectors rather than on the whole unit sphere of $\mathscr{H}_{\mathbf{H}}$; indeed the latter would imply that one of the transformations $S(g_1)$, $S(g_2)$, or $S(g_1g_2)$ would not be semilinear, thus violating Wigner's theorem.

This is to say that the definitions (2.1–2.2) and (2.5) (with an explicit dependence on ϕ) are not compatible unconditionally; specifically, condition (2.5) holds only if condition (2.3) is violated in such a way that one cannot go past (1.11) in the proof of Proposition 1 (see Sec. I); hence, the weakening of condition (2.3) must be such as to exclude, in that proof, the consideration of pairs ψ, ϕ of (unit) vectors in $\mathscr{H}_{\mathbf{H}}$ that are not orthogonal. This then requires (i) that in (2.3) $\mathscr{P}(\mathscr{H}_{\mathbf{H}})$ be replaced by the atomic maximal Boolean orthocomplemented sublattice $\mathscr{P}_0$ of $\mathscr{P}(\mathscr{H}_{\mathbf{H}})$ corresponding to a complete orthonormal basis $\{\psi_n\}$ in $\mathscr{H}_{\mathbf{H}}$; and (ii) that the modified condition (2.3) holds only on pure states on $\mathscr{P}_0$; i.e., that ψ and ϕ run over the members of $\{\psi_n\}$.

For consistency reasons, one may then wish to pursue Adler's more general definition, involving only ''one particular complete set of states,'' into the actual premises of the theory, namely the axiomatic (i.e., physical) definition of a symmetry. One would then have to take into account the fact that the first fundamental theorem of projective geometry does not hold in such a weakened environment, invalidating thereby the usual arguments (Refs. 3–5, i.e., Adler's Refs. Nos. 1–3) that are intimately linked to the derivation and axiomatic implications of Wigner's representation of individual symmetries by semilinear transformations of the underlying Hilbert space.

Thus, we thought that what ultimately amounts to a subtle shift in assumptions—rather than to some erroneous deductions from accepted basic premises—deserved to be pinpointed, as it clarifies the genuine scope of the new horizons opened by Adler's generalization.

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Response to the Comment by G. Emch on projective group representations in quaternionic Hilbert space

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We discuss the differing definitions of complex and quaternionic projective group representations employed by us and by Emch. The definition of Emch (termed here a strong projective representation) is too restrictive to accommodate quaternionic Hilbert space embeddings of complex projective representations. Our definition (termed here a weak projective representation) encompasses such embeddings, and leads to a detailed theory of quaternionic, as well as complex, projective group representations. © *1996 American Institute of Physics.* [S0022-2488(96)03812-1]

I. PRELIMINARIES NOT INVOLVING GROUP STRUCTURE

Before turning to a discussion of what is an appropriate definition of a quaternionic projective group representation, we first address several issues that do not involve the notion of a *group* of symmetries. We follow throughout the Dirac notation used in our recent book,[1] in which linear operators in Hilbert space act on ket states from the left and on bra states from the right, as in $\mathcal{O}|f\rangle$ and $\langle f|\mathcal{O}$, while quaternionic scalars in Hilbert space act on ket states from the right and on bra states from the left, as in $|f\rangle\omega$ and $\omega\langle f|$.

We begin by recalling the statement (see Sec. 2.3 of Ref. 1) of the quaternionic extension of Wigner's theorem, which gives the Hilbert space representation of an individual symmetry in quantum mechanics. Physical states in quaternionic quantum mechanics are in one-to-one correspondence with unit rays of the form $|\mathbf{f}\rangle=\{|f\rangle\omega\}$, with $|f\rangle$ a unit normalized Hilbert space vector and ω a quaternionic phase of unit magnitude. A symmetry operation $\mathcal{S}$ is a mapping of the unit rays $|\mathbf{f}\rangle$ onto images $|\mathbf{f}'\rangle$, which preserves all transition probabilities,

$$\mathcal{S}|\mathbf{f}\rangle=|\mathbf{f}'\rangle, \quad |\langle\mathbf{f}'|\mathbf{g}'\rangle|=|\langle\mathbf{f}|\mathbf{g}\rangle|. \tag{1}$$

Wigner's theorem, as extended to quaternionic Hilbert space, asserts that by an appropriate $\mathcal{S}$-dependent choice of ray representatives for the states, the mapping $\mathcal{S}$ can always be represented (in Hilbert spaces of dimension greater than 2) by a unitary transformation $U_{\mathcal{S}}$ on the state vectors, so that

$$|f'\rangle=U_{\mathcal{S}}|f\rangle. \tag{2}$$

Conversely, any unitary transformation of the form of Eq. (2) clearly implies the preservation of transition probabilities, as in Eq. (1). When only one symmetry transformation is involved, the issue of projective representations does not enter, since Wigner's theorem asserts that this transformation can be given a unitary representation on appropriate ray representative states in Hilbert space. The issue of projective representations arises only when we are dealing with two (or more) symmetry transformations, in which case the ray representative choices which reduce the first symmetry transformation to unitary form may not be compatible with the ray representative choices which reduce a second symmetry transformation to unitary form. Thus we disagree with Emch's statement, in the semifinal paragraph of his Comment, that Wigner's theorem (which he notes is a form of the first fundamental theorem of projective geometry) may be dependent on the definition adopted for quaternionic projective group representations.

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In the first section of his Comment, Emch proves a Proposition stating that if an operator $\mathcal{O}$ commutes with all of the projectors $|f\rangle\langle f|$ of a quaternionic Hilbert space of dimension 2 or greater, then $\mathcal{O}$ must be a real multiple of the unit operator 1 in Hilbert space. When $\mathcal{O}$ is further restricted to be a unitary operator (as obtained from a symmetry transformation via the Wigner theorem), the real multiple is further restricted to be ± 1. Since we will refer to this result in the next section, let us give an alternative proof, based on the spectral representation of a general unitary operator U in quaternionic Hilbert space,

$$U=\sum_{\ell} |u_{\ell}\rangle e^{i\theta_{\ell}}\langle u_{\ell}|, \quad 0\leqslant\theta_{\ell}\leqslant\pi, \tag{3}$$

in which the sum over ℓ spans a complete set of orthonormal eigenstates of U. Let us focus on a two state subspace spanned by $|u_1\rangle$ and $|u_2\rangle$, and construct the projector $P=|\Phi\rangle\langle\Phi|$, with

$$|\Phi\rangle=|u_1\rangle+|u_2\rangle\omega, \quad \overline{\omega}=-\omega, \quad \omega=\omega_\alpha+j\omega_\beta, \quad \omega_\alpha\omega_\beta\neq 0, \tag{4}$$

where $\omega_{\alpha,\beta}$ are symplectic components lying in the complex subalgebra of the quaternions spanned by 1 and i. Then the projector P is given by

$$P=|u_1\rangle\langle u_1|+|u_2\rangle\langle u_2|+|u_2\rangle\omega\langle u_1|-|u_1\rangle\omega\langle u_2|, \tag{5a}$$

and the part of U lying in the $|u_{1,2}\rangle$ subspace is

$$U_{1,2}=|u_1\rangle e^{i\theta_1}\langle u_1|+|u_2\rangle e^{i\theta_2}\langle u_2|. \tag{5b}$$

The commutator of U and P is then given by

$$[U,P]=[U_{1,2},P]=|u_2\rangle(e^{i\theta_2}\omega-\omega e^{i\theta_1})\langle u_1|-|u_1\rangle(e^{i\theta_1}\omega-\omega e^{i\theta_2})\langle u_2|, \tag{6}$$

which vanishes only if $e^{i\theta_1}=e^{i\theta_2}$ (from equating to zero the coefficient of ω_α) and $e^{i\theta_1}=e^{-i\theta_2}$ (from equating to zero the coefficient of ω_β). Since $0\leqslant\theta_{1,2}\leqslant\pi$, this requires either $\theta_1=\theta_2=0$ or $\theta_1=\theta_2=\pi$. Repeating the argument for each dimension 2 subspace in turn, we learn that $U=\pm 1$. Note that in a complex Hilbert space, the analogous argument shows only that $e^{i\theta_1}=e^{i\theta_2}$, from which we conclude (again by repeating the argument for each dimension 2 subspace in turn) that $U=e^{i\theta}$, which commutes with all projectors because any complex number is a c-number in complex Hilbert space.

Clearly, the argument just given involves only elementary properties of the projectors in Hilbert space, and makes no reference to the notion of a group of symmetries. The same is true of the proposition given in Sec. I of Emch's Comment. Since Schur's lemma ordinarily describes the restrictions on an operator that commutes with the representation matrices of an irreducible group representation, and since the projectors in Hilbert space do not form a group (they are not invertible and the product of two different projectors is not a projector), it is a misnomer to describe Emch's Proposition, or the corollary given here, as a ''quaternionic Schur's lemma.'' In addition to disagreeing with Emch's terminology, we also disagree with his statement, in the second paragraph of Sec. III of his Comment, that the analysis leading to his Proposition is dependent on the definition adopted for quaternionic projective group representations; in fact, the notion of a group of symmetries does not enter into either his analysis, or the corollary for unitary matrices proved here.

II. HOW SHOULD ONE DEFINE QUATERNIONIC PROJECTIVE GROUP REPRESENTATIONS?

Let us now address the central question of how one should generalize to quaternionic Hilbert space the notion of a projective group representation. We begin by reviewing how projective

group representations arise in complex Hilbert space. Let $\mathscr{G}$ be a symmetry group composed of abstract elements a with group multiplication ab. By Wigner's theorem, each group element is represented, after an a-dependent choice of ray representatives, by a unitary operator U_a acting on the states of Hilbert space. In the simplest case, in which the U_a are said to form a vector representation, the U's obey a multiplication law isomorphic to that of the corresponding abstract group elements,

$$U_a U_b = U_{ab}\,. \tag{7}$$

However, when the complex rephasings of the states used in Wigner's theorem are taken into account, there exists the more general possibility that for any state $|f\rangle$, the states $U_a U_b|f\rangle$ and $U_{ab}|f\rangle$ are not equal, but rather differ from one another by a change of ray representative, i.e.,

$$U_a U_b|f\rangle = U_{ab}|f\rangle e^{i\phi(a,b;f)}. \tag{8}$$

Corresponding to Eq. (8), there are two possible definitions of a projective representation in complex Hilbert space

Definition (1): In a *weak* projective representation, the multiplication law of the U's obeys Eq. (8) on one complete set of states $\{|f\rangle\}$. This suffices, by superposition, to determine the multiplication law of the U's on all states.

Definiton (2): In a *strong* projective representation, the multiplication law of the U's obeys Eq. (8) on all states in Hilbert space. In this case, we can easily prove that the phases $\phi(a,b;f)$ are independent of the state label f. To see this, let us define $V_{ab} = U_{ab}^{-1} U_a U_b$; then Eq. (8) implies that

$$V_{ab}|f\rangle = |f\rangle e^{i\phi(a,b;f)}, \tag{9}$$

which immediately implies that V_{ab} commutes with the projector $|f\rangle\langle f|$, for all states $|f\rangle$ in Hilbert space. But invoking the complex Hilbert space specialization of the result of the preceding section, we learn that V_{ab} must be a c-number, $V_{ab} = e^{i\phi(a,b)}$. This is the customary definition of a projective representation in complex Hilbert space, and is well known to have nontrivial realizations.

Let us now turn to the question of how to define projective representations in quaternionic Hilbert space. Emch choses as his generalization the strong definition given above, which by the reasoning following Eq. (9), and the quaternionic result of Sec. I, implies that $V_{ab} = (-1)^{n_{a,b}}$, with $n_{a,b}$ an integer that can depend in general on a and b. In other words, *the only strong quaternionic projective representations are real projective representations*.

The problem with adopting the strong definition, however, is that it excludes from consideration as a quaternionic projective representation the embedding into quaternionic Hilbert space of a nontrivial complex projective representation realized on a complex Hilbert space. Thus potentially interesting structure is lost. To avoid this problem, Ref. 1 adopts as the quaternionic generalization of the notion of a projective representation the weak definition given above, which in quaternionic Hilbert space states that

$$U_a U_b|f\rangle = U_{ab}|f\rangle \omega_{a,b}\,, \quad |\omega_{a,b}| = 1 \tag{10}$$

for one particular complete set of states $\{|f\rangle\}$. As discussed in Ref. 1, Eq. (10) can also be rewritten in the operator form

$$U_a U_b = U_{ab}\Omega(a,b), \tag{11a}$$

with

$$\Omega(a,b)=\sum_f |f\rangle\omega(a,b;f)\langle f|. \tag{11b}$$

Since the operator Ω depends on the particular complete set of states on which the projective phases are given, a more complete notation (not employed in Ref. 1) would in fact be $\Omega(a,b;\{|f\rangle\})$. Using the result of an analysis[2] of the associativity condition for weak quaternionic projective representations, Tao and Millard[3] have recently given a beautiful complete structural classification theorem for weak quaternionic projective representations. The complex specialization of their Corollary 2, incidentally, states that in a complex Hilbert space, the weak definition of a projective representation implies the strong one.

Can the weak definition of a quaternionic projective representation be weakened even further, by using a *different* complete set of states $\{|f\rangle\}$ to specify the projective phases for each pair of group elements a and b?[4] In this case, the operator Ω takes the form $\Omega(a,b;\{|f\rangle\}_{a,b})$. However, since any unitary operator is diagonalizable on some complete set of states, this further weakening allows an arbitrary specification of Ω for each a,b, and any relationship of the unitary representation to the underlying group structure is lost.

III. DISCUSSION

We conclude that the difference between our analysis and that of Emch is traceable to what I have here termed the difference between a *strong* and a *weak* definition of projective representation. The strong definition is the customary one in complex Hilbert space, but it excludes potentially interesting structure when applied to quaternionic Hilbert space. Since the weak definition leads to a detailed theory[1–3] of projective group representations in quaternionic Hilbert space, and since it implies[3] the strong definition in complex Hilbert space, the weak definition is in fact the more appropriate one in both complex and quaternionic Hilbert spaces.

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[1] S. L. Adler, *Quaternionic Quantum Mechanics and Quantum Fields* (Oxford University Press, London, 1995).
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[4] T. Tao (private communication).

Erratum: Gauge invariant perturbations of black holes. I. Schwarzschild space–time [J. Math. Phys. 37, 836–857 (1996)]

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An error appeared in the final printed version of this paper. The operators A and A' which occur throughout the paper should be replaced with $\mathfrak{p}$ and $\mathfrak{p}'$, respectively, to adhere to proper convention.

Erratum: Remarks on the quantization of gauge theories [J. Math. Phys. 37, 1713–1723 (1996)]

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(1) Superscripts on q: throughout the paper, the first superscript on q is its space–time index while the second one, wherever it occurs, is its exponent.
For example, on p. 1714, Eq. (1.1) should read $\phi \equiv (q^1)^2 + (q^2)^2 + p_1^2 + p_2^2 - R^2 = 0$ and the exponent in Eq. (3.5) is $-[(q^1)^2 + (q^2)^2]/2$.
Other places where such double-superscripts should be resolved are:
p. 1717, Eq. (3.4) and
p. 1718, Eq. (3.11).
(2) In the second line on p. 1715, (θ', ϑ') should read (θ', φ').
(3) (Weil's) ''integrability'' (condition) should read (Weil's) ''integrality'' (condition) in the following:
p. 1716, last but two lines,
p. 1718, 7th line after Eq. (3.11),
p. 1719, Sec. IV, 5th line and
p. 1721, line preceding Eq. (A15).
(4) In the Appendix, subscripts on ∇:
Eq. (A7) should read $\hat{f} = -i\hbar\nabla_{X_f} + f$ and
Eq. (A8) should read $\nabla_{X_{m^s}} = 0$.

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